STUDI IDENTIFIKASI *HEMAGGLUTININ* VIRUS INFLUENZA A PENYEBAB PANDEMIK BERKAITAN DENGAN SPESIFITASNYA TERHADAP RESEPTOR *SIALIC ACID* SECARA *IN SILICO*

RAMDHAN

0305030522

UNIVERSITAS INDONESIA

FAKULTAS MATEMATIKA DAN ILMU PENGETAHUAN ALAM

DEPARTEMEN KIMIA

DEPOK

2009

STUDI IDENTIFIKASI *HEMAGGLUTININ* VIRUS INFLUENZA A PENYEBAB PANDEMIK BERKAITAN DENGAN SPESIFITASNYA TERHADAP RESEPTOR *SIALIC ACID* SECARA *IN SILICO*

Skripsi ini diajukan sebagai salah satu syarat

untuk memperoleh gelar Sarjana Sains

Oleh :

RAMDHAN

0305030522

DEPOK

2009

SKRIPSI : STUDI IDENTIFIKASI *HEMAGGLUTININ* VIRUS INFLUENZA A PENYEBAB PANDEMIK BERKAITAN DENGAN SPESIFITASNYA TERHADAP RESEPTOR *SIALIC ACID* SECARA *IN SILICO*

NAMA : RAMDHAN

NPM : 0305030522

SKRIPSI INI TELAH DIPERIKSA DAN DISETUJUI

DEPOK, JULI 2009

Prof. Dr. Usman Sumo Friend Tambunan

PEMBIMBING

Tanggal Lulus Ujian Sidang Sarjana :	**Juli 2009**
Penguji I	**: .....**
Penguji II	**: .....**
Penguji III	**: .....**

KATA PENGANTAR

Bismillahirrahmanirrahim

Puji syukur penulis panjatakan atas kehadirat Allah SWT yang telah melimpahkan taufiq, hidayah dan rahmat-Nya sehingga penulis dapat menyelesaikan tugas akhir ini.

Tugas akhir ini berisi tentang Studi Identifikasi Hemagglutinin Virus Influenza A Penyebab Pandemik Berkaitan dengan Spesifitasnya Terhadap Reseptor Sialic Acid Secara *In Silico*. Tugas akhir ini diajukan sebagai salah satu syarat untuk memperoleh gelar Sarjana Sains Program Studi Kimia Fakultas Matematika dan Ilmu Pengetahuan Alam Universitas Indonesia.

Penulis tidak lupa ingin mengucapkan rasa terima kasih kepada semua pihak yang telah bersedia dan turut serta memberikan andil. Terima kasih atas sumbangan tenaga dan pemikirannya dengan penuh kerelaan dan keikhlasan serta bentuan kepada penulis berupa spiritual, moril, materiil sebelum, selama dan sesudah penyusunan skripsi ini, yaitu kepada:

1. Ibu dan Ayahku, untuk cinta dan kasih sayangnya dan juga semua nasihat yang selalu senantiasa kalian berikan kepadaku. Harapan kalian merupakan motivasi besar dan semangat dalam kehidupanku.
2. Prof. Dr Usman Sumo Friend Tambunan sebagai Penasihat Akademik dan dosen pembimbing penelitian atas pengarahan, bimbingan, kesabaran serta dorongan moril selama proses penyusunan skripsi ini.

3. Dr. Ridla Bakri sebagai ketua Departemen Kimia Fakultas Matematika dan Ilmu Pengetahuan Alam Universitas Indonesia.
4. Tresye Utari M.Si sebagai koordinator penelitian dan Prof. Dr. Sumi Hudiyono sebagai Ketua KBI Biokimia yang telah memberikan kesempatan dan bantuan dalam penelitian.
5. Seluruh staf pengajar Program Studi Kimia FMIPA UI yang telah memberikan bimbingn dan motivasi selama mengikuti perkuliahan.
6. Rekan-rekan satu kelompok penelitian Bioinformatika : Danang, Ronggo dan Samira. Terima kasih atas kerjasama, kebersamaan dalam suka dan duka, serta semangat untuk saling memberikan motivasi. Terima kasih kepada Fitri Amelia M.Si yang telah memberikan dasar-dasar Bioinformatika dengan baik.
7. Yayu R, alumni Farmasi UI, untuk kasih sayang, semangat, motivasi dan kebersamaanya dalam suka maupun duka serta yang selama ini dengan sabar selalu menemaniku.
8. Sahabatku Agung, Faruk, Syarif, Yusni, untuk kebersamaanya dan rasa percaya yang diberikan, terima kasih atas persahabatan selama 4 tahun ini dan semoga terus berlanjut selamanya.
9. Sahabar-sahabat Kimia UI angkatan 2005 atas persahabatn selama 4 tahun ini yang telah memberikan banyak kenangan yang begitu indah.
10. Semua pihak yang tidak bisa penulis sebutkan satu per satu, atas segala bantuan dan dukungannya dalam proses penyusunan skripsi ini hingga selesai.

Semoga Allah SWT memberikan balasan dan selalu diberikan berkah, rahmat dan hidayah-Nya. Amiin.

Penulis menyadari bahwa skripsi ini masih jauh dari kesempurnaan dan terdapat banyak kekurangan, namun demikian penulis berharap semoga skripsi ini dapat memberikan manfaat dalam dunia Biokimia khususnya Studi Bioinformatika.

Penulis

2009

ABSTRAK

Salah satu faktor yang berperan dalam infeksi virus influenza A adalah adanya kecocokan antara *Hemagglutinin* (HA) dari virus dengan reseptor permukaan sel dari host. Permukaan sel host mengandung gugus terminal *sialyl-galactosyl* [Sia(α2-3)Gal] atau [Sia(α2-6)Gal]. Virus Influenza A yang berasal dari unggas cenderung berikatan dengan Sia(α2-3)Gal sedangkan yang berasal dari isolat manusia cenderung berikatan dengan Sia(α2-6)Gal. Hasil Alignment subtipe H1N1 menunjukan bahwa diperlukan mutasi asam amino pada posisi 190 dan 225 menjadi Asam Aspartat pada Hemagglutinin untuk mengenali reseptor Sia(α2-6)Gal sedangkan pada subtipe H2N2 dan H3N2 memerlukan mutasi asam amino pada posisi 226 dan 228 menjadi Leusin dan Serin. Berdasarkan analisis mutasi terhadap HA subtipe H1N1, H2N2, dan H3N2 yang telah menjadi pandemik, dapat diperkirakan bahwa *Hemagglutinnin* subtipe H5N1 memerlukan mutasi pada posisi 190 dan 225 menjadi Asam Aspartat pada HA untuk mengenali reseptor Sia(α2-6)Gal. Kemungkinan lain adalah memerlukan mutasi asam amino pada posisi 226 dan 228 menjadi Leusin dan Serin. Metode simulasi *molecular docking* mampu membentuk kompleks antara *Hemagglutinin* dengan Reseptor Sia(α2-6)Gal dan Sia(α2-3)Gal. Berdasarkan hasil kompleks yang terbentuk, metode simulasi *molecular docking* berhasil mengidentifikasi spesifitas *Hemagglutinin* terhadap Sia(α2-3)Gal atau Sia(α2-6)Gal

Kata kunci : *Hemagglutinin*, Influenza A, Sia(α2-6)Gal, Sia(α2-3)Gal.

xv + 165 hlm;gbr;tab;lamp

DAFTAR ISI

DAFTAR GAMBAR

DAFTAR TABEL

DAFTAR LAMPIRAN

BAB I

PENDAHULUAN

1.1 Latar Belakang

Pada abad 20 telah terjadi tiga pandemik Influenza A di seluruh dunia. Periode tahun 1918-1919 terjadi pandemik pertama yang disebabkan oleh virus Influenza A subtipe H1N1. Pandemik ini mengakibatkan lima puluh juta orang meninggal dunia. Pandemik kedua terjadi pada tahun 1957-1958 yang diakibatkan oleh virus Influenza A subtipe H2N2 dan diperkirakan mengakibatkan satu juta korban jiwa. Pandemik ketiga terjadi pada tahun 1967-1968 yang diakibatkan oleh virus Influenza A subtipe H3N2 dengan jumlah kematian diperkirakan satu juta korban jiwa (Kamps, Hoffman, & Preiser, 2006).

Pada tahun 1997, virus Influenza A subtipe H5N1 pertama kali terdeteksi di Hongkong. Virus ini menyerang dan menewaskan 6 orang dari 18 orang yang terinfeksi . Virus influenza A subtipe H5N1 telah menyebar di kawasan benua Asia mulai dari Jepang di utara hingga Indonesia di selatan. Hingga saat ini penelitian membuktikan bahwa infeksi virus Influenza H5N1 ke manusia akibat kontak langsung dari unggas dan belum mampu menyebar antar manusia (Horimoto T, Kawaoka Y. 2001). Hingga 2 Juni 2009, tercatat 433 orang terinfeksi virus Influenza A subtipe H5N1 dan 262 diantaranya meninggal dunia

(www.who.int/entity/csr/disease/avian_influenza/cases_table_2009_06_02/en /index.html, diakses pada hari Rabu 3 Juni 2009 pukul 09.18 WIB).

Sekitar bulan April 2009, virus Influenza A subtipe H1N1 kembali merebak di Meksiko dan mulai menyebar ke seluruh dunia. Pada 26 Juni 2009 tercatat 59.814 orang telah terinfeksi dan 263 orang diantaranya telah meninggal dunia. Penyebaran yang sangat cepat membuat lembaga WHO menetapkan status virus Influenza A subtipe H1N1 sebagai pandemik global. Ini adalah pandemik Influenza pertama di abad ke-21 (www.who.int/csr/don/2009_06_26/en/index.html, diakses pada hari Senin 29 Juni 2009 pukul 10.30 WIB).

Strain Virus Influenza untuk menjadi pandemik harus memenuhi tiga syarat utama. Virus mempunyai kemampuan untuk menginfeksi, menyebabkan kematian, dan mampu bertransmisi antar manusia secara mudah. Kemampuan Hemagglutinin Virus Influenza untuk mengenali SA(α2,6)Gal akan mendukung kemampuan Virus untuk menginfeksi, dan menyebar antar manusia sehingga akan memenuhi dua syarat yang dibutuhkan strain Influenza untuk menjadi pandemik (Kamps, Hoffman, & Preiser, 2006).

Salah satu faktor yang berperan dalam infeksi virus Influenza adalah adanya kecocokan antara *Hemagglutinin* (HA) dari virus dengan reseptor pada permukaan sel dari *host*. Permukaan sel *host* mengandung gugus terminal *sialyl-galactosyl* [Sia(α2-3)Gal] atau [Sia(α2-6)Gal]. Virus Influenza A yang berasal dari unggas cenderung berikatan dengan Sia(α2-3)Gal

sedangkan yang berasal dari isolat manusia cenderung berikatan dengan Sia(α2-6)Gal. Sia(α2-3)Gal merupakan reseptor sel permukaan pada Unggas sedangkan Sia(α2-6)Gal merupakan reseptor sel permukaan pada manusia (Matrosovich, 2004).

Mutasi dapat terjadi pada protein *Hemagglutinin* dan memungkinkan *Hemagglutinin* mampu mengenali reseptor Sia(α2-6)Gal. Potensi virus inilah yang dikhawatirkan sehingga virus dapat membuat varian-varian baru dari strain *Hemagglutinin* yang mampu menular antar manusia (Russel CJ and Webster RG. 2005;Stevens J. *et. al*. 2006).

1.2 Kedudukan Terhadap Penelitian Sebelumnya

Studi secara *in silico* terhadap mutasi *Hemagglutinin* dan *Neuraminidase* virus Influenza A (H5N1) telah dilakukan oleh kelompok Studi Bioinformatika dari Departemen Kimia Universitas Indonesia. Hasil studi telah menunjukan bahwa sekuen *Hemagglutinin* dari *Strain* Virus H5N1 isolat Indonesia belum mengalami mutasi secara signifikan dan belum terbentuk strain yang mampu menular dari manusia ke manusia. Hasil analisis filogenetik menunjukan bahwa sekuen *Hemagglutinin* dan *Neuraminidase* untuk virus Influenza A(H5N1) lebih dekat kekerabatannya dengan virus Influenza A(H1N1) dibandingkan dengan subtipe H2N2 dan H3N2 (Tambunan *et al*., 2008;Ridlo N.,2008;Hikmawan O.,2007).

Studi mengenai mekanisme pengikatan *Hemagglutinin* subtipe H5N1 dengan Sia(α2-3)Gal dan Sia(α2-6)Gal berdasarkan metode *Molecular*

Docking, Molecular Mechanic, dan *Molecular Dynamic* telah dilakukan. Hasil studi ini menunjukan bahwa hemagglutinin dari H5N1 berinteraksi dengan Sia(α2-3)Gal membentuk 11 ikatan Hidrogen sedangkan dengan Sia(α2-6)Gal hanya membentuk 3 ikatan Hidrogen. Hasil penelitian ini mendukung spesifitas *Hemagglutinin* subtipe H5N1 terhadap Sia(α2-3)Gal (Minyong Li& Binghe Wang.2006).

1.3 Perumusan Masalah

Pemahaman lebih jelas berkaitan dengan spesifitas *Hemagglutinin* terhadap Sia(α2-3)Gal dan Sia(α2-6)Gal sangat diperlukan untuk mengantisipasi kemungkinan pandemik Influenza. Oleh karena itu, penelitian secara *in silico* lebih lanjut perlu dilakukan terhadap *Hemagglutinin* dari subtipe yang telah menjadi pandemik. Berdasarkan sekuen *Hemagglutinin* yang berasal dari subtipe H1N1, H2N2, dan H3N2 akan dibandingkan perbedaan penyusun *Receptor Binding Domain* pada *Hemagglutinin* antara *host* manusia dan *host* unggas. Analisis mutasi dari subtipe *Hemagglutinin* yang telah menjadi pandemik dapat digunakan untuk memprediksikan kemungkinan mutasi pada subtipe H5N1 yang mampu mengenali Sia(α2-6)Gal. Pada penelitian ini juga akan menguji keberhasilan metode simulasi *Molecular Docking* untuk mengidentifikasi spesifitas *Hemagglutinin* terhadap Sia(α2-3)Gal atau Sia(α2-6)Gal

1.4 Tujuan Penelitian

Penelitian ini diharapkan dapat mengidentifikasi beberapa asam amino yang sangat mempengaruhi spesifitas *Hemagglutinin* subtipe H1N1, H2N2, dan H3N2 yang telah menyebabkan pandemik terhadap Sia(α2-3)Gal atau Sia(α2-6)Gal. Hasil identifikasi mutasi asam amino pada subtipe yang telah menyebabkan pandemik akan menjadi modal penting untuk memprediksi mutasi yang diperlukan untuk mengubah *Receptor Binding Domain Hemagglutinin* subtipe H5N1dari hanya mengenali Sia(α2-3)Gal menjadi mampu mengenali Sia(α2-6)Gal. Penelitian ini juga diharapkan dapat mengetahui keberhasilan metode simulasi *Molecular Docking* untuk mengidentifikasi spesifitas *Hemagglutinin* terhadap Sia(α2-3)Gal atau Sia(α2-6)Gal.

BAB II

TINJAUAN PUSTAKA

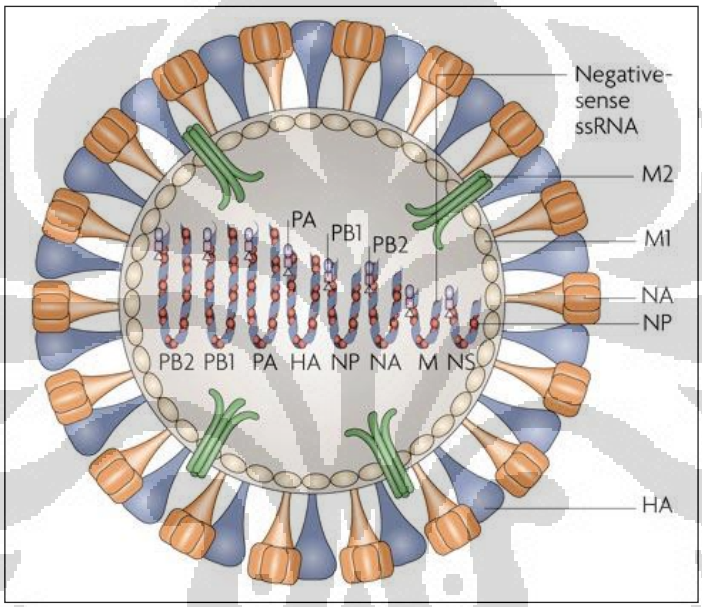
2.1 Definisi Virus Influenza

Virus Influenza merupakan virus yang termasuk dalam famili *Orthomyxoviridae* yang mempunyai selubung (*envelope*) dengan genom RNA berupa rangkaian tunggal berpolaritas negatif (*negative sense)* sebanyak 7-8 segmen. Pada manusia virus ini dapat menyebabkan demam, pusing, batuk dan dalam beberapa kasus serius, menyebabkan pneumonia pada anak-anak dan orang tua hingga menyebabkan kematian (Kamps, Hoffman, & Preiser, 2006).

2.2 Klasifikasi Virus Influenza

Perbedaan sifat antigen internal dari *nucleocapsid protein* (NP) dan *matriks* protein (MP) menjadi dasar dari pembagian Virus Influenza menjadi tipe A, tipe B, dan Tipe C. Virus Influenza A dan B terdiri dari delapan segmen RNA sedangkan virus Influenza C hanya terdiri dari tujuh segmen. Virus influenza A dapat menginfeksi unggas maupun mamalia (termasuk manusia) dan bersifat patogen terhadap hospesnya, sedangkan virus influenza B dan C dapat diisolasi dari mamalia (termasuk manusia) dan umumnya kurang patogen dibandingkan dengan virus influenza tipe A (Kamps, Hoffman, & Preiser, 2006)

Antigen Eksternal permukaan glikoprotein yang tersusun dari *Hemagglutinin* (HA) dan *Neuraminidase* (NA) menjadi dasar pengelompokkan lebih lanjut Influenza A menjadi beberapa subtipe. Virus Influenza A mempunyai 16 jenis Hemagglutinin dan 9 Neuraminidase. (Kamps, Hoffman, & Preiser, 2006)



Gambar 1. Struktur Influenza

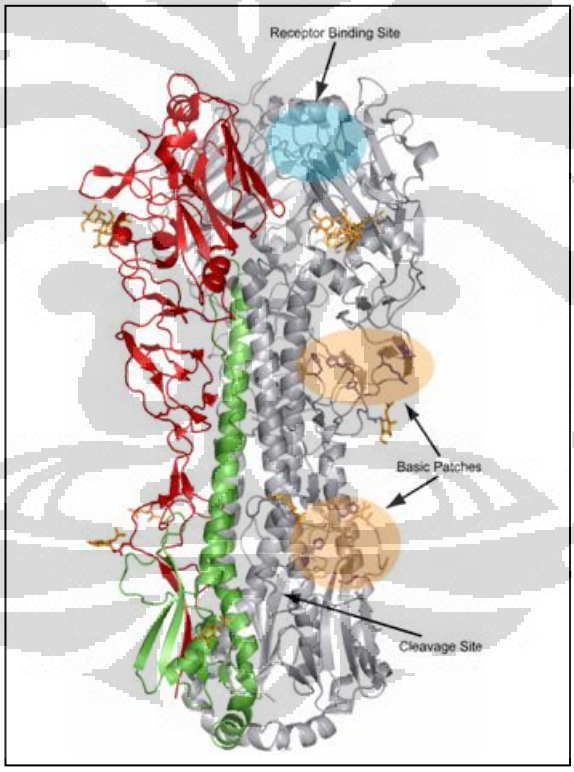
(Horimoto, T., et. al, 2005)

2.3 *Hemagglutinin* (HA)

Hemagglutinin merupakan *Homotrimer* glikoprotein yang memiliki dua atau tiga *glycosylation site* dengan berat molekul sekitar 76.000. *Hemaglutinin* ini mengelilingi membran lipid pada sisi luarnya dan setidaknya memiliki 5 daerah antigenik (*epitope*) yaitu A, B(membawa *receptor binding*

site), C, D, dan E. *Antigenic sites* berada dipuncak dari molekul HA sedangkan bagian bawahnya mengikat *lipid layer*. Bagian tengah HA memiliki *stalk region* dan *fusiogenic domain* yang dibutuhkan untuk *membran fusion* ketika virus menginfeksi sel baru (Kamps, Hoffman, & Preiser, 2006).

Hemagglutinin berfungsi sebagai reseptor dalam pengikatan virus terhadap sel host. *Hemagglutinin* akan berikatan dengan *sialic acid* (N-acetyl-neuraminic acid) dan menstimulasi penetrasi materi genetik virus dengan *membrane fusion.* (Kamps, Hoffman, & Preiser, 2006).



Gambar 2. Struktur *Hemagglutinin*

(Stevens J. *et. al*. 2006)

2.4 *Neuraminidase* (NA)

Neuraminidase merupakan glikoprotein seperti *Hemagglutinin* yang berada di permukaan virus membentuk struktur *tetramer* dengan rata-rata berat molekul 220.000 (Kamps, Hoffman, & Preiser, 2008). *Neuraminidase* berfungsi sebagai suatu enzim yang dapat menghidrolisis ikatan antara galaktosa dan *sialic acid* pada rantai ujung oligosakarid-glikoprotein. Fungsi lain dari *Neuraminidase* adalah untuk melepaskan partikel virus yang sudah selesai replikasi dalam sel *host* dan mencegah virus yang sudah terbentuk menempel kembali pada reseptor *sialic acid* melalui tonjolan Hemagglutinin. Oleh karena itu, efisiensi replikasi Avian Influenza sangat bergantung pada kerjasama protein *Hemagglutinin* dan *Neuraminidase* dari virus (Kamps, Hoffman, & Preiser, 2006; Suzuki *et al*. 2000).

Oseltamivir merupakan inhibitor yang mampu menghambat kerja Neuraminidase. Adanya inhibitor Oseltamivir akan menghambat pelepasan partikel virus yang selesai bereplikasi sehingga aktivitas infeksi virus akan berkurang (Kamps, Hoffman, & Preiser, 2006).

2.5 Protein Matriks (M)

Gen Matriks dari virus Influenza A menyandi dua macam protein yaitu protein Matriks 1 (M1) dan protein Matriks 2 (M2). Protein Matriks mempunyai peran dalam penyusunan *virion* virus Influenza. Bersama dengan

protein *Hemagglutinin* dan *Neuraminidase*, protein Matriks 2 menyusun struktur amplop virus dan berperan sebagai saluran ion. Protein Matriks 2 tidak hanya sebagai komponen struktural virus, tetapi juga berperan dalam proses awal infeksi dalam pemisahan protein M1 dari ribonucleoprotein (RNP) untuk masuk ke dalam sitoplasma sel *host*. Pemisahan ini dipicu pemindahan ion hidrogen melewati membran virus oleh protein Matriks 2 (Kamps, Hoffman, & Preiser, 2006).

2.6 *Polymerase basic* 1 (PB 1), *Polymerase basic* 2 (PB 2), dan *Polymerase acidic* (PA)

Ketiga jenis polimerase PB1, PB2 dan PA berperan dalam proses replikasi dan transkripsi. Gen *Polymerase Basic* (PB) menyandi *transkriptase* yang berperan diantaranya dalam *capbinding* dan *elongation*. Ketiganya memiliki aktivitas endonuklease dan terikat dengan ribonuleoprotein (Asmara, W. 2007; Kamps, Hoffman, & Preiser, 2006)

2.7 *Nonstructural protein* (NS)

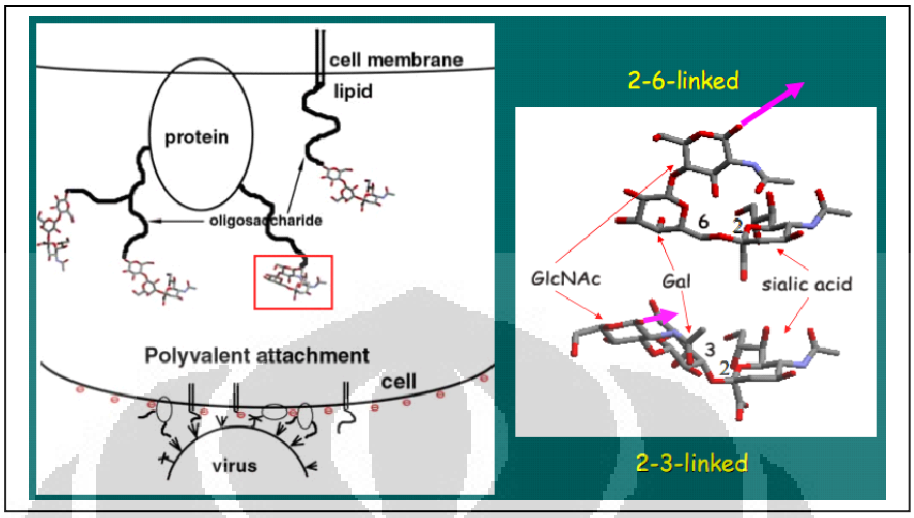
Gen Nonstructural menyandi 2 macam protein yaitu Nonstructural 1 (NS1) dan Nonstructural 2 (NS2). NS1 memiliki berat molekul sekitar 26.000 dan membentuk *dimer* yang dapat menginhibisi transfer mRNA sel *host* dari nukleus, sehingga memberikan kemudahan bagi viral RNA untuk bisa dibawa ke ribosom dan ditranslasikan. Selain itu NS1 juga dapat berperan dalam

resistensi terhadap respon interferon pada sistem imun sel host (Kamps,Hoffman&Preiser 2006)

NS2 merupakan molekul kecil dengan berat molekul 11.000. Protein ini kemungkinan terikat dengan M1 protein dan diyakini memiliki fungsi untuk memfasilitasi transport ribonuleoprotein yang baru terbentuk dari nukleus ke sitoplasma sehingga dapat mempercepat replikasi dari virus (Kamps, Hoffman, & Preiser, 2006).

2.8 Reseptor Sel Permukaan pada Saluran Pernapasan

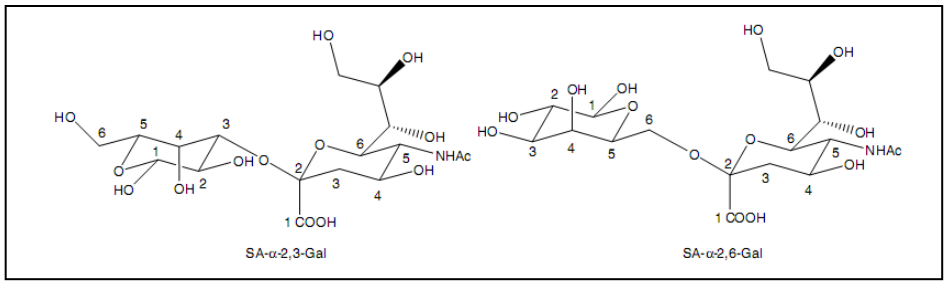
Salah satu faktor virus Influenza dapat menginfeksi manusia disebabkan karena adanya kecocokan antara *Hemagglutinin* virus dengan reseptor *sialic acid* pada permukaan sel dari *host*. Permukaan sel *host* mengandung gugus terminal *sialyl-galactosyl* Sia(α2-3)Gal atau Sia(α2-6)Gal. Virus Influenza A yang berasal dari unggas cenderung berikatan dengan Sia(α2-3)Gal sedangkan yang berasal dari isolat manusia cenderung berikatan dengan Sia(α2-6)Gal. Sia(α2-3)Gal merupakan reseptor sel permukaan pada Unggas sedangkan Sia(α2-6)Gal merupakan reseptor sel permukaan pada manusia (Matrosovich, 2004).



Gambar 3. Reseptor sel permukaan

(Matrosovich, 2004)

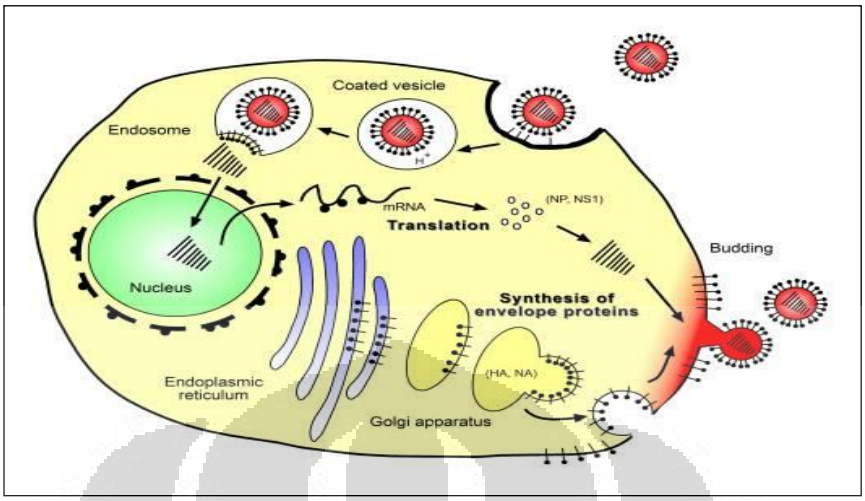
Penelitian akhir-akhir ini telah mengungkapkan bahwa pada manusia juga sedikit mempunyai reseptor sel permukaan Sia(α2-3)Gal pada saluran pernapasan bagian bawah. Penemuan ini menjelaskan kemampuan Hemagglutinin yang mampu bereplikasi pada manusia meskipun Hemagglutinin tersebut mempunyai spesifitas terhadap Sia(α2-3)Gal. Penemuan yang lain mengungkapkan bahwa tidak semua unggas hanya memiliki reseptor sel permukaan Sia(α2-3)Gal tetapi juga mempunyai Sia(α2-6)Gal seperti pada ayam dan burung puyuh. Berbeda dengan ayam dan burung puyuh, bebek hanya memiliki reseptor sel permukaan Sia(α2-3)Gal (Matrosovich, 2004).



Gambar 4. Struktur Sia(α2-3)Gal dan Sia(α2-6)Gal (Minyong Li & Binghe Wang, 2006).

2.9 Infeksi Virus Influenza A

Tahap pertama proses infeksi virus adalah proses pengikatan *Hemagglutinin* dengan *sialic acid* dari sel permukaan host. Langkah selanjutnya, virus akan masuk melalui proses fusi antara amplop virus dengan membran *endosomal* sel *host*. Langkah ini dilakukan dengan proses *endositosis* melalui mediasi penurunan pH pada phagosom. Penurunan pH akan dihentikan oleh kerja protein M2 setelah komponen virus telah masuk ke dalam sel *host*. Selanjutnya akan terjadi serangkaian penataan ulang protein matrix-1 (M1) dan kompleks glikoprotein *homotrimerik Hemagglutinin* sehingga menghasilkan sebuah *domain* yang sangat lipofilik dan fusogenik dari setiap monomer *Hemagglutinin* yang masuk ke dalam membran *endolisomal*. Proses ini akan memerlukan bantuan protease sel *host* untuk mengaktivasi prekursor *Hemagglutinin* (HA0) menjadi fragmen 1 (HA1) dan fragmen 2 (HA2) yang akan memungkinkan virus melepaskan ribonukleoproteinnya (RNP) (Asmara, W. 2007; Kamps, Hoffman, & Preiser, 2006).



Gambar 5. Siklus Replikasi Virus Influenza A

(Cox & Kawaoka, 1997)

Langkah berikutnya adalah transport RNP ke nukleus, dimana kompleks polimerase terikat pada viral RNA. Pada tahap ini terjadi pemutusan viral RNA oleh aktivitas endonuklease dan secara simultan terjadilah proses *elongation*. Pembentukan dari viral RNA akan dibatasi oleh NP yang akan membentuk mRNA. Viral RNA (vRNA) dikopi dari (-) sense menjadi (+) cRNA dan mRNA. cRNA akan tetap berada inti yang berfungsi sebagai template pada produksi (-) sense vRNA baru, sedangkan mRNA akan berpindah ke sitoplasma untuk memproduksi protein (Kamps, Hoffman, & Preiser, 2006).

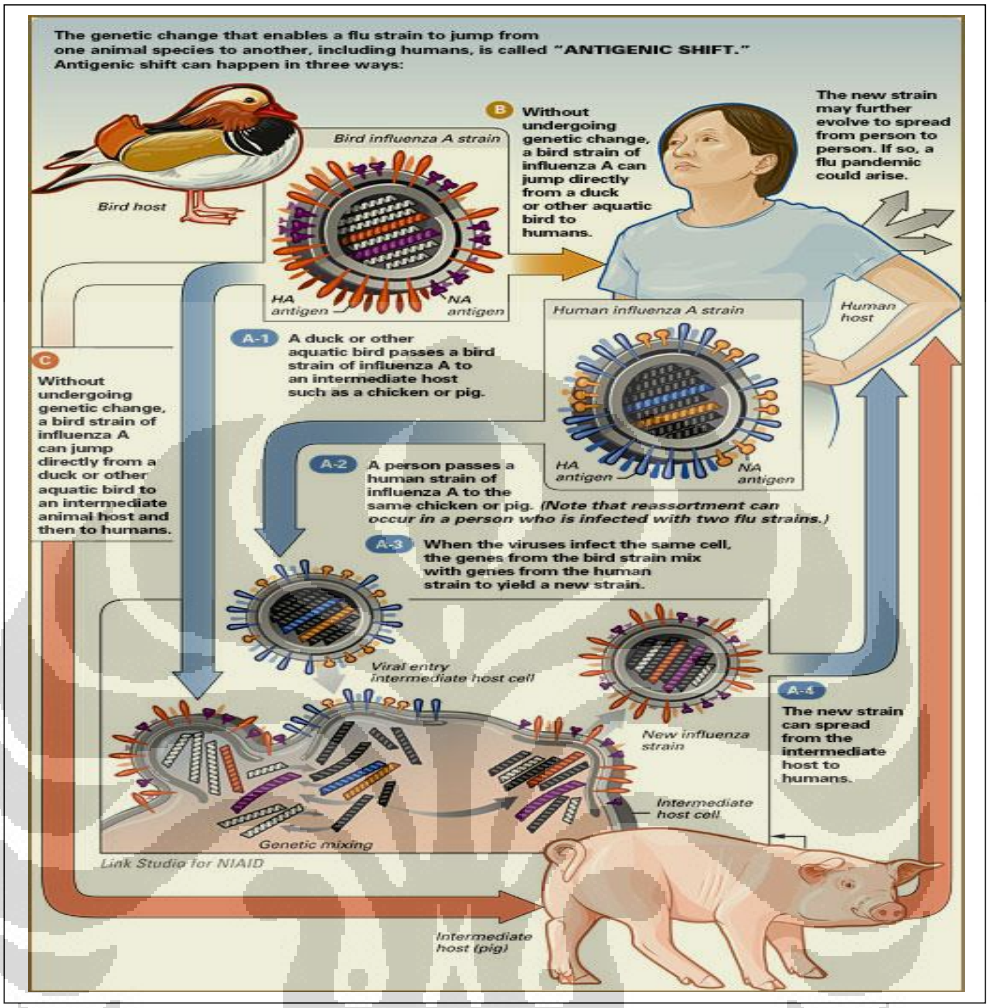
Langkah berikutnya viral protein yang baru terbentuk kembali lagi ke inti sel untuk membentuk vRNA lagi dan membentuk RNP atau viral protein yang baru terbentuk dikeluarkan menuju badan golgi dimana terjadi proses

glikosilasi. Protein yang dibentuk ini kemudian dibawa ke membran sel dimana mereka akan terikat dengan *lipid bilayer (Kamps, Hoffman, & Preiser, 2006).*

Tahap terakhir adalah vRNA dan inti viral meninggalkan inti sel menuju membran dan melakukan pemisahan dengan sel host melalui aktivitas NA, proses ini dikenal dengan sebutan *budding* (Kamps, Hoffman, & Preiser, 2006).

2.10 Antigenik Shift

Antigenik shift merupakan mutasi yang terjadi akibat *gene reassortment* (pertukaran atau pencampuran gen) yang terjadi pada dua atau lebih virus influenza tipe A sehingga terjadi penyusunan kembali suatu galur virus baru yang bermanifestasi sebagai genom virus Influenza yang baru. Antigenik shift terjadi oleh adanya perubahan struktur antigenik yang bersifat dominan pada genom virus Influenza. Sebagai contoh virus dengan Hemagglutinin subtipe H1 digantikan dengan subtipe H5 menghasilkan genom baru dari virus ini. Hal ini dapat terjadi ketika suatu sel *host* terinfeksi oleh 2 tipe virus Influenza yang berbeda secara bersamaan sehingga segmen gen dari kedua virus tersebut saling bertukar selama proses replikasi (Guan, Yi. 2007; Tumpey *et al*. 2002).



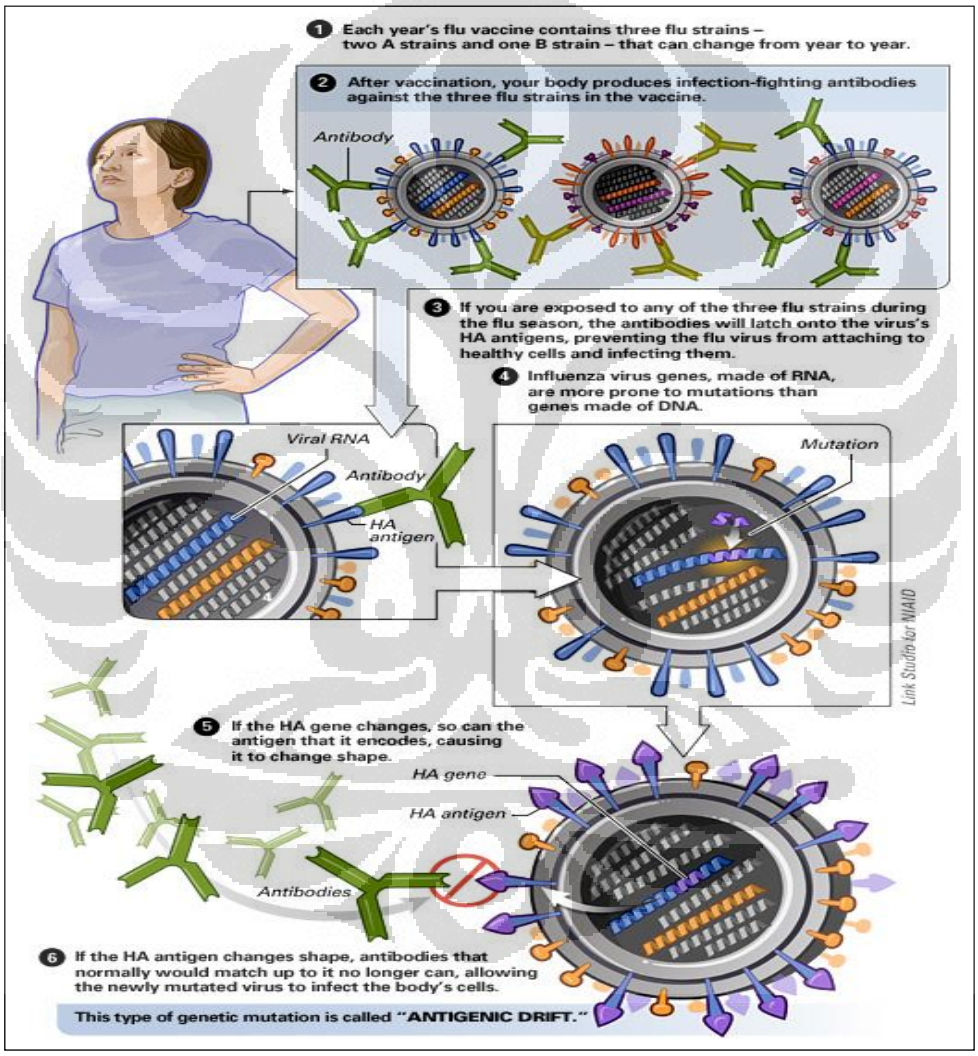
Gambar 6. Antigenik shift

(National Institute of Allergy and Infectious Disease)

2.11 Antigenik drift

Antigenik drift terjadi jika terdapat perubahan susunan asam amino ketika virus Influenza melakukan encoding terhadap genom virus setiap kali virus bereplikasi sehingga menghasilkan strain yang baru. Antigenik drift dapat terjadi oleh adanya perubahan struktur antigenik yang bersifat minor

pada genom dari virus Influenza. Antigenik drift berlangsung lambat, tetapi progresif dan cenderung menimbulkan penyakit yang terbatas pada suatu kawasan. Mutasi pada materi genetik dapat menimbulkan perubahan polipeptida virus, yaitu sekitar 2-3 kali substitusi asam amino per tahun (Asmara, W. 2007; Soepadi PZ. 2005).



Gambar 7. Antigenik drift

(National Institute of Allergy and Infectious Disease)

2.12 Struktur Protein

Protein tersusun oleh kombinasi asam amino melalui ikatan peptida membentuk struktur primer, sekunder, tersier, dan kuartener. Protein dapat merupakan satu rantai polipeptida maupun beberapa rantai polipeptida yang satu dengan lainnya membentuk ikatan atau interaksi tertentu. Perbedaan komposisi dan urutan asam amino penyusunnya mengakibatkan perbedaan sifat protein satu dengan lainnya (Baxevanis dan Oullete, 2001).

Struktur primer protein merupakan polipeptida yang menunjukan urutan asam amino penyusun serta ikatan disulfida (jika ada). Struktur sekunder menggambarkan struktur primer dan ikatan hidrogen antar residu asam amino yang berdekatan membentuk struktru α *heliks*, β *strands* dan *loop* Struktur tersier protein adalah nama lain dari struktur tiga dimensi suatu protein. Struktur ini terbentuk dari interaksi berbagai struktur sekunder yang berbeda dan membentuk folding dengan konformasi paling stabil sedangkan struktur kuartener merupakan interaksi antar struktur tersier (Baxevanis dan Oullete, 2001).

Struktur protein dapat diidentifikasi dari urutan asam aminonya, namun sifat biologis dari protein tidak muncul dari urutan asam amino yang linear. Melalui penentuan struktur tiga dimensi protein yang pertama kali pada tahun 1958, didapatkan suatu konsep dalam Biologi Molekular dan Bioinformatika, yaitu fungsi protein terkait erat dengan struktur tiga dimensi protein tersebut. Dua protein yang memiliki struktur tiga dimensi yang sama maka fungsi

kedua protein tersebut dapat dikatakan sama (Claverie & Notredame, 2003).

2.13 Definisi dan Ruang Lingkup Bioinformatika

Bioinformatika merupakan bidang ilmu yang menggunakan pendekatan komputasional untuk menyelesaikan persoalan biologis. Bioinformatika meliputi pengelolaan informasi biologis yang diperoleh dari berbagai penelitian yang menghasilkan data dalam jumlah banyak dan kompleks seperti pemetaan genom manusia. Bioinformatika mampu memberikan prediksi maupun simulasi dengan mempertimbangkan hubungan serta pola data biologis (Baxevanis dan Oullete, 2001).

Bioinformatika juga dapat diartikan sebagai teknologi pengumpulan, penyimpanan, analisis, interpretasi, penyebaran dan aplikasi dari data-data biologi molekul. Perangkat utama Bioinformatika adalah software yang didukung oleh kesediaan internet dan server *world wide web*. Bioinformatika menjadi penting karena perkembangan teknologi informasi dan peningkatan ilmu komputer, khususnya pada bidang biologi molekuler, membuka sudut pandang baru dalam menyelesaikan persoalan biologi molekuler (Baxevanis dan Oullete, 2001).

2.14 Database

Kumpulan data yang diatur sedemikian rupa untuk memudahkan penggunanya. Pada database bioinformatika, data yang diatur merupakan data sekuen DNA atau protein yang didapat melalui percobaan laboratorium

yang biasanya disimpan dalam file komputer. Setiap file dari suatu sekuen berisi informasi mengenai asal organisme, nama sekuen, dan juga nomor akses yang digunakan untuk mengidentifikasi sekuen tersebut. (Mount, 2004)

GenBank merupakan suatu institusi yang menyimpan dan mengelola database urutan DNA suatu gen dan ekspresi asam aminonya. Urutan DNA diperoleh dari berbagai penelitian yang dengan sukarela memberikan hasil penelitiannya untuk masyarakat umum. GenBank didirikan oleh *National Center for Biotechnology Information* (NCBI) bersama dengan DNA *Data Bank of Japan* (DDBJ) dan *European Bioinformatics Institute* (EBI). Diantara format-format database yang ada, GenBank Flatfile Format (GBFF) dan FASTA merupakan format yang umum digunakan pada Bioinformatika. (Baxevanis dan Oullete, 2001).

2.15 GenBank Flatfile Format (GBFF)

Format GBFF memiliki tiga bagian terpisah yaitu *header*, *feature*, dan sekuen . Bagian *header* berisi tentang informasi identitas organisme asal sekuen nukleotida atau asam amino seperti nama gen, waktu publikasi, nomor akses, produk ekspresi, dan nama peneliti yang memetakan sekuen nukleotida tersebut. Bagian feature memuat nama genus, spesies, jaringan, kromosom, galur, dan organisme asal sekuen beserta daerah gen, urutan asam amino yang disandi, dan nomor identitas produk proteinnya. Bagian terakhir GBFF merupakan bagian yang berisi susunan lengkap sekuen nukleotida atau protein dari organisme yang bersangkutan (Baxevanis dan

Oullete, 2001).

2.16 Format FASTA

Format FASTA terdiri atas definition line dan sekuen asam amino atau nukleotida. Format ini merupakan format input (*query sequence)* untuk berbagai program analisis bioinformatika. Format FASTA tergolong kurang informatif dibandingkan format lainnya, namun format ini lebih praktis jika digunakan dalam analisis sekuen (Baxevanis dan Oullete, 2001).

2.17 Format PDB

Format file yang berbasiskan teks yang memetakan koordinat dari suatu molekul sehingga dapat menggambarkan struktur tiga dimensi dari suatu molekul. Mayoritas informasi yang disimpan dalam format PDB adalah struktur tiga dimensi dari protein. Selain memetakan koordinat dari suatu molekul, format PDB juga dapat memuat informasi tentang peneliti yang telah memetakan struktur molekul tersebut (Baxevanis dan Oullete, 2001).

2.18 *Sequence Alignment*

Metoda penjajaran dua atau lebih sekuen nukleotida atau asam amino menggunakan algoritma tertentu dengan bantuan komputer, sehingga didapatkan area yang memiliki urutan relatif identik satu sama lain. Metoda ini berfungsi mencari homologi antar sekuen nukleotida atau asam amino. Konsertivitas menunjukan adanya hubungan evolusi antara dua atau lebih

sekuen nukleotida yang mengalami perubahan akibat substitusi, insersi, dan delesi (Baxevanis dan Oullete, 2001).

Sequence Alignment dibagi menjadi dua jenis berdasarkan jumlah sekuen yang digunakan sebagai input. *Pairwise sequence alignment* melibatkan dua sekuen, sedangkan *multiple sequence alignment* melibatkan lebih dari dua sekuen. *Multiple sequence alignment* memberikan hasil yang lebih akurat dan representatif dibandingkan *pairwise sequence alignment* karena peningkatan jumlah input sekuen meningkatkan kepercayaan dan akurasi output. Peningkatan jumlah sekuen yang dimasukkan berarti meningkatkan kompleksitas proses sequence alignment (Baxevanis dan Oullete, 2001).

2.19 *Database Similarity Searching*

Sequence alignment digunakan untuk membandingkan pasangan sekuen yang spesifik. Jika suatu sekuens yang belum diketahui pembandingnya maka digunakan *Database Similarity Searching.* Metode ini akan mencari kecocokan sekuens input terhadap *database* dan hasilnya berupa suatu daftar beserta berbagai nilai dan statistik (Baxevanis dan Oullete, 2001).

Program *Basic Local Alignment Search Tool* (BLAST) dikembangkan sesuai dengan tipe sekuen *query* dan *subject*, protein atau nukleotida. Jika tipe sekuen berbeda, sekuen nukleotida akan terlebih dahulu ditranslasikan oleh program. BLASTp digunakan untuk *query* protein terhadap *subject*

protein. BLASTn digunakan untuk *query* nukleotida (ditranslasikan) terhadap *subject* protein. TBLASTn digunakan untuk *query* protein terhadap *subject* nukleotida (ditranslasikan). TBLASTx digunakan untuk *query* dan *subject* berupa nukleotida, tetapi keduanya ditranslasikan terlebih dahulu kemudian dibandingkan sebagai protein.

2.20 Prediksi *Conserved Region*

Metoda ini untuk mendapatkan daerah sekuen yang memiliki similaritas antar nukleotida atau asam amino yang rapat. *Hasil conserved region* dapat diinterpretasikan bahwa sekuen tersebut berperan vital dalam aktivitas biologis karena tetap dipertahankan selama proses evolusi berlangsung. Jika *conserved region* tersebut menyandi suatu protein, kemungkinan besar ia menyandi pusat aktif enzim yang umumnya tidak berubah selama protein tersebut mempunyai fungsi yang sama. Tidak tertutup kemungkinan bahwa *conserved region* itu terbentuk dari sekuen nukleotida non fungsional yang belum berubah sehingga menyandikan area yang tidak memiliki fungsi penting pada protein (Baxevanis dan Oullete, 2001).

2.21 *Molecular Docking*

Metode untuk mencari posisi optimal molekul *ligand* terhadap sisi aktif pengikatan dari struktur target (*receptor*). *Molecular Docking* dapat memprediksikan afinitas pengikatan kompleks yang terbentuk antara *receptor*

dengan ligand menggunakan berbagai skor sperti ΔG° binding, *Konstanta Inhibition*, ikatan hidrogen dan kontak hidrofobik. *Molecular Docking* sangat berguna dalam proses *Drug Design*, seperti untuk memprediksi afinitas pengikatan dari inhibitor yang didesain terhadap enzim tertentu yang ingin dihambat aktivitasnya (Yeturu & Nagasuma, 2008)

BAB III

METODE PENELITIAN

Penelitian dilakukan menggunakan metode *in silico* yang memanfaatkan perangkat komputer dan data-data yang tersedia di database. Data-data digunakan untuk dianalisis dan diinterpretasikan dengan berbagai software yang didukung oleh ketersedian jaringan internet. Secara garis besar, penelitian ini dilakukan dengan pencarian sekuen, *multiple alignment,* pencarian struktur tiga dimensi, *superimpose*, dan *molecular docking*.

3.1 Pencarian dan Pemilihan Sekuen

Sekuen Hemagglutinin dari subtipe H1N1, H2N2, H3N2, H5N1 di*download* dari *Influenza Virus Resource database* yang disediakan oleh N*ational Center for Biotechnology Information* (NCBI) dan dapat diakses melalui *http://ncbi.nlm.nih.gov/genomes/FLU/Database.html*. Sekuen yang didownload adalah sekuen isolat asal bebek dan manusia dengan format FASTA. Pemilihan sekuen didasarkan pada tahun ketika terjadi pandemik dan untuk H5N1 pada tahun awal kemunculan serta strain yang sering digunakan untuk sampel penelitian.

3.2 Multiple Alignment

Sekuen dari tiap subtipe dialignment menggunakan program Clustal W2 antara isolat dari bebek dan manusia. Program Clustal W2 disediakan

secara online dengan mengakses *www.ebi.ac.uk/Tools/clustalw2/index.html*. Hasil *alignment* diinterpretasikan untuk mengetahui posisi asam amino yang berbeda pada *Region Receptor Binding Domain* antara isolat asal bebek dan manusia untuk tiap subtipe. Proses *editing alignment* digunakan *software* Bioedit.

3.3 Pencarian Struktur tiga dimensi.

Pencarian dilakukan dengan melakukan *Basic Local Alignment Search Tools* (BLAST) antara sekuen *Hemagglutinin* asal isolat bebek dan manusia tiap subtipe terhadap database struktur tiga dimensi yang dapat diakses melalui *www.rcsb.org/pdb/static.do?p=search/index.html*. Struktur tiga dimensi yang dipilih adalah yang mempunyai kesamaan 100 % terhadap *Receptor Binding Domain* sekuen *Hemagglutinin* yang telah dipilih sebelumnya. Kemudian didownload juga struktur tiga dimensi dari Sia(α2-3)Gal dan Sia(α2-6)Gal yang mewakili reseptor sel permukaan dari host bebek dan manusia.

3.4 Superimpose Struktur Tiga Dimensi

Struktur tiga dimensi dari *Receptor Binding Domain* asal isolat bebek dan manusia untuk tiap subtipe dilakukan superimpose menggunakan *software* Pymol. Berdasarkan hasil super impose akan dilihat keterkaitan struktur tiga dimensi *Receptor Binding Domain Hemagglutinin* asal isolat

bebek dan manusia dalam satu subtipe menggunakan nilai *Root Mean Square Deviation* (RMSD). Analisis juga dilakukan terhadap kedekatan struktur *Receptor Binding Domain* antara subtipe H5 dengan subtipe H3 dan H1.

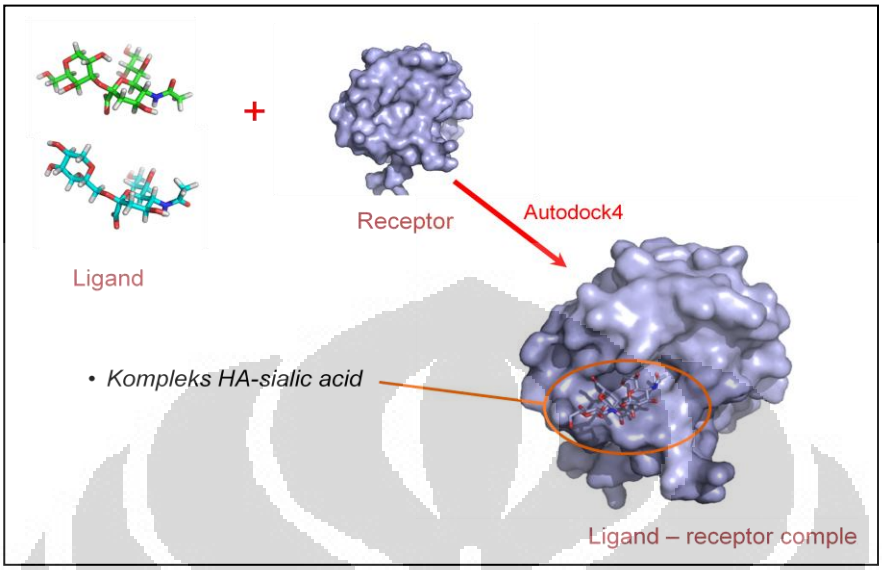
3.5 Molecular Docking

Setiap struktur tiga dimensi *Hemagglutin* dilakukan *Molecular Docking* terhadap reseptor Sia(α2-3)Gal dan Sia(α2-6)Gal. Sebelum dilakukan *Molecular Docking*, terlebih dahulu dilakukan preparasi awal terhadap struktur *Macromolecule* (*Hemagglutinin)* dan struktur *Ligand* (Sia α2-3 Gal dan Siaα2-6Gal). Preparasi yang dilakukan adalah Penghapusan molekul air, penambahan atom Hidrogen, penghitungan *Charges* dan proses minimasi (metode Conjugate Gradient) menggunakan *software* VegaZZ.

Program *Molecular Docking* yang digunakan adalah Autodock4 dengan bantuan program Autogrid4, dan Auto Dock Tools. Program Auto Dock Tools digunakan untuk pembuatan parameter-parameter yang diperlukan oleh program Autodock4 dan Autogrid4.

Autodock4 akan mengevaluasi kompleks yang terjadi antara *Hemagglutinin* dengan Sia(α2-3)Gal dan Sia(α2-6)Gal dengan nilai ΔG°*binding* dan *Konstanta Inhibition*. Selanjutnya hasil *molecular docking* divisualisasikan menggunakan *Software* Pymol untuk melihat interaksi dan kompleks yang terbentuk antara *Hemagglutinin* dengan Sia(α2-3)Gal dan

Sia(α2-6)Gal.



Gambar 8. Skema perancangan simulasi *Molecular Docking*

BAB IV

HASIL DAN PEMBAHASAN

4.1 Pencarian Sekuen Hemagglutinin

Sekuen protein *Hemagglutinin* Virus Influenza A yang digunakan sebagai bahan penelitian adalah sekuen yang berasal dari subtipe H1N1, H2N2, H3N2, dan H5N1. Pemilihan subtipe H1N1, H2N2, dan H3N2 dikarenakan subtipe ini telah menyebabkan pandemik global. Kemampuan menyebabkan pandemik menunjukan bahwa subtipe H1N1, H2N2, dan H3N2 asal isolat manusia memiliki kemampuan mengenali Sia(α2-6)Gal sehingga mampu menyebar antar manusia secara mudah. Berdasarkan hal ini, sekuen protein *Hemagglutinin* subtipe H1N1, H2N2, dan H3N2 asal isolat manusia yang berasal dari tahun terjadinya pandemik dapat dijadikan sampel protein *Hemagglutinin* yang mengenali reseptor Sia(α2-6)Gal.

Hemagglutinin yang berasal dari isolat unggas mampu mengenali Sia(α2-3)Gal yang merupakan reseptor sel permukaan paling dominan pada unggas. Pada *host* unggas juga terdapat reseptor sel permukaan Sia(α2-6)Gal, seperti pada ayam dan burung puyuh. Berbeda dengan ayam dan burung puyuh, bebek hanya memiliki reseptor sel permukaan Sia(α2-3)Gal. Berdasarkan hal ini, sekuen protein *Hemagglutinin* yang berasal dari isolat bebek dapat dijadikan sampel protein *Hemagglutinin* yang mengenali Sia(α2-6)Gal.

Subtipe H5N1 merupakan virus Influenza yang dikhawatirkan dapat menjadi pandemik. Subtipe H5N1 telah mampu menginfeksi manusia dan memiliki patogenesitas yang tinggi, namun belum mampu menyebar antar manusia. Sampel yang digunakan untuk mewakili subtipe H5N1 berasal dari tahun 1997 yang merupakan awal kemunculan subtipe ini dan sekuen yang telah sering digunakan oleh beberapa penelitian.

Pada tahun 2009, virus Influenza subtipe H1N1 kembali merebak dan lembaga WHO telah menetapkan phase 6 untuk virus ini. Phase 6 menunjukan bahwa telah terjadi pandemik global. Oleh karena itu, analisis Hemagglutinin pada strain virus ini perlu dilakukan untuk melihat keterkaitan terhadap subtipe H1N1 yang telah menyebabkan pandemik pada tahun 1918-1919.

Pencarian sekuen protein *Hemagglutinin* dilakukan pada server database *GenBank* yang diakses melalui *Influenza Virus Resource* pada website *National Center for Biotechnology Information* (*http://ncbi.nlm.nih.gov/genomes/FLU/Database.html*). Format yang terdapat pada database tersebut berbentuk *GenBank Flatfile Format* (GBFF). Format ini terdiri atas *Header*, *Feature*, serta sekuen nukleotida dan protein. *Software* Bioinformatika memerlukan input file dengan format FASTA. Format FASTA hanya berisi *definition line* dan sekuen asam amino menggunakan kode satu huruf. Oleh karena itu, format file terlebih dahulu dirubah menjadi format FASTA sebelum di*download*.

Tabel 1. Hasil pencarian sekuen *Hemagglutinin*

Subtipe H1	
A/duck/Alberta/35/76(H1N1)	A/Brevig_Mission/1/18(H1N1)
A/mallard/Alberta/35/1976(H1N1)	A/New_York/1/18(H1N1)
A/duck/Bavaria/1/1977 (H1N1)	A/South Carolina/1/1918(H1N1)
A/duck/Miyagi/66/1977(H1N1)	A/Puerto Rico/8/34(H1N1)
A/swine/Iowa/15/1930(H1N1)	A/Mexico/4108/2009(H1N1)
A/swine/1931(H1N1)	A/Mexico/4108/2009(H1N1)
A/swine/Ohio/23/1935(H1N1)	A/Mexico/3955/2009(H1N1)
A/swine/Jamesburg/1942(H1N1)	A/Mexico/4635/2009(H1N1)
Subtipe H2	
A/mallard/MT/Y61 (H2N2)	A/Guiyang/1/1957(H2N2)
A/duck/Hong Kong/273/78 (H2N2)	A/Japan/305/1957(H2N2)
A/duck/Hong Kong/319/1978(H2N2)	A/Japan/305/1957(H2N2)
A/mallard/New York/6750/1978(H2N2)	A/Kayano/57(H2N2)
Subtipe H3	
A/duck/Hong Kong/7/1975(H3N2)	A/Aichi/2/1968(H3N2)
A/duck/Alberta/78/1976(H3N2)	A/Aichi/2/1968(H3N2)
A/pintail duck/ALB/86/1976(H3N2)	A/Hong Kong/1/1968(H3N2)
A/duck/Ukraine/1963(H3N8)	A/Memphis/1/68(H3N2)
Subtipe H5	
A/duck/Minnesota/1525/81(H5N1)	A/Hong Kong/156/97(H5N1)
A/Duck/Hong Kong/p46/97 (H5N1)	A/Thailand/2(SP-33)/2004(H5N1)
A/duck/Guangxi/07/1999(H5N1)	A/Viet Nam/1194/2004(H5N1)
A/duck/Zhejiang/11/2000(H5N1)	A/Viet Nam/1203/2004(H5N1)

Hasil pencarian sekuen didapatkan total 40 sekuen *Hemagglutinin* yang di*download* sebagai sampel. Sekuen sampel dalam format FASTA dapat dilihat di Lampiran 3.

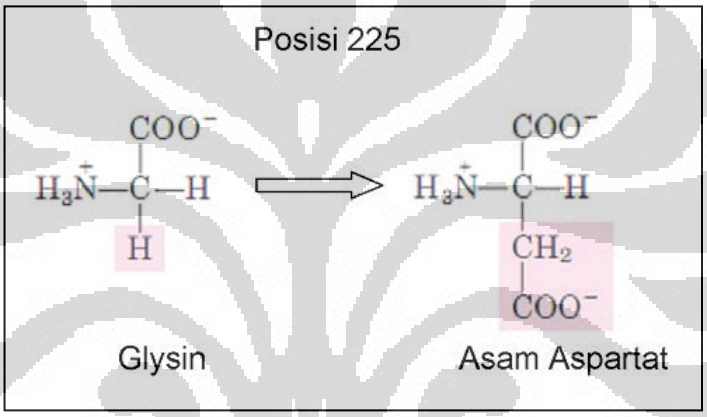
4.2 Multiple Sequence Alignment

Proses multiple sequence alignment dilakukan menggunakan program ClustalW2 yang diakses secara online melalui website *http://www.ebi.ac.uk/Tools/clustalw2/index.html.* Program ini akan menyejajarkan susunan asam amino sehingga dapat dianalisis mutasi-mutasi yang terjadi pada sekuen hemagglutinin asal isolat bebek dan manusia untuk setiap subtipe. Penomoran posisi asam amino pada tiap strain mengikuti penomoran berdasarkan struktur tiga dimensi dari subtipe H3N2 untuk menghindari kerancuan penomoran yang berbeda dari tiap subtipe. Analisis yang dilakukan terhadap mutasi hanya akan dibatasi pada asam amino yang berperan dalam *Receptor Binding Domain* (RBD). Posisi *Receptor Binding Domain* berada pada 130 loop (residu 134-138), 190 helix (residu 190-198), dan 220 loop (residu 221-228). Perhatian khusus diberikan untuk posisi 190, 225, 226, dan 228 karena posisi ini berinteraksi langsung terhadap pengikatan reseptor *sialic acid.*

Tabel 2. Hasil analisis *sequence alignment*

Posisi AA	H1		H2		H3		H5	
	Bebek	Manusia	Bebek	Manusia	Bebek	Manusia	Bebek	Manusia
190	E	D	E	E	E	E	E	E
225	G	D	G	G	G	G	G	G
226	Q	Q	Q	L	Q	L	Q	Q
228	G	G	G	S	G	S	G	G

Hasil dari Alignment antara isolat asal bebek dan manusia untuk subtipe H1N1 menunjukan bahwa terjadi mutasi pada posisi 225 dan 190. Pada posisi 225 dari *Hemagglutinin* asal isolat bebek memiliki asam amino Glysin (G) sedangkan pada *Hemagglutinin* asal isolat manusia memiliki asam amino Asam Aspartat (D). Mutasi terjadi dari asam amino yang memiliki karakteristik *Hidrofobik* menjadi asam amino yang *Hidrofilik* dan bermuatan negatif.

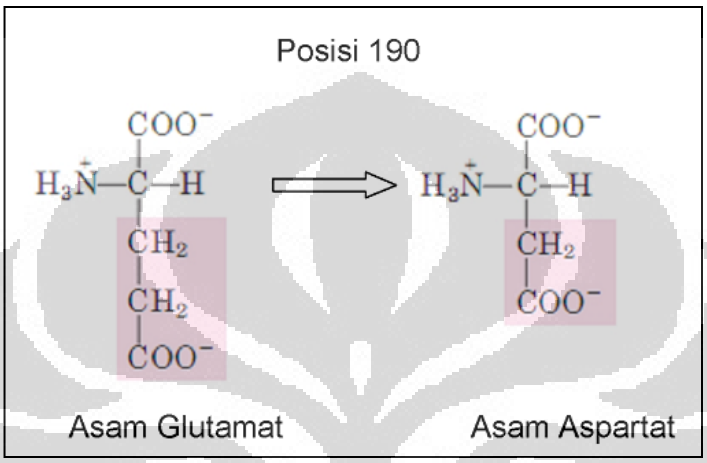


Gambar 9. Mutasi RBD dari isolat bebek ke manusia pada subtipe H1N1

Pada posisi 190 terjadi mutasi dari asam amino Asam Glutamat (E) pada isolat bebek menjadi Asam Aspartat (D) pada isolat manusia. Kedua asam amino ini memiliki karakteristik hampir sama dan hanya sedikit berbeda ukuran. Asam Glutamat asal isolat bebek memiliki 1 atom C lebih banyak dibandingkan Asam Aspartat pada isolat manusia.

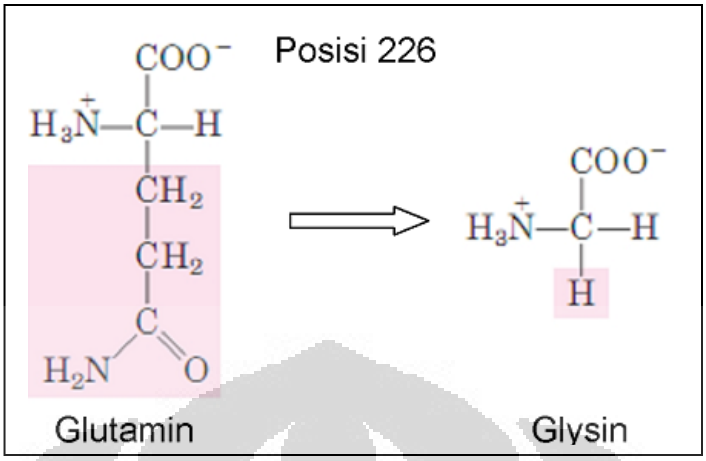
Hemagglutinin subtipe H1N1 isolat tahun 2009 memiliki susunan asam amino *Receptor Binding Domain* yang sama dengan subtipe H1N1 isolat manusia tahun 1918. Hal ini menunjukan bahwa sekuen *Hemagglutinin* isolat

manusia tahun 2009 telah mampu mengenali reseptor Sia(α2-6)Gal. Hal ini juga dibuktikan dengan keadaan saat ini yang telah menjadi pandemik global, meskipun tidak memakan korban jiwa sebanyak ketika pandemik tahun 1918 terjadi.

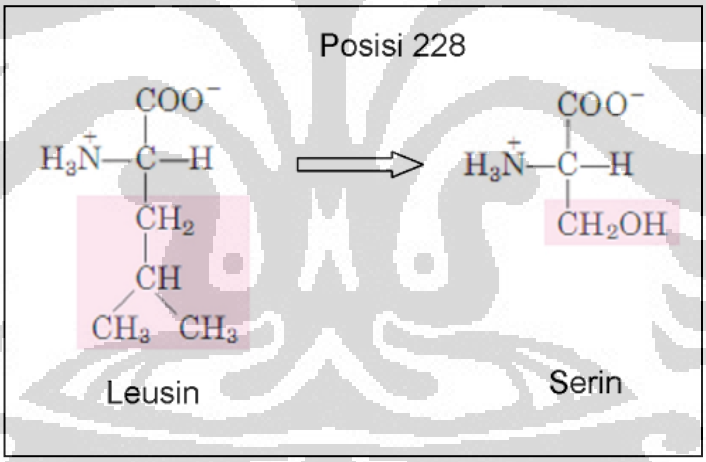


Gambar 10. Mutasi RBD dari isolat bebek ke manusia pada subtipe H1N1

Hasil *multiple alignment* untuk subtipe H2N2 dan H3N2 menunjukan terdapat mutasi pada posisi 226 dan 228 antara isolat bebek dan manusia. Isolat bebek memiliki asam amino Glutamin (Q) pada posisi 226 dan Glysin (G) pada posisi 228. Isolat asal manusia memiliki asam amino Leusin (L) pada posisi 226 dan Serin (S) pada posisi 228. Pada posisi 226, asam amino Glutamin asal isolat bebek memiliki karakteristik *hidrofilik*, sedangkan Leusin asal isolat manusia memilki karakteristik *hidrofobik*. Pada posisi 228, asam amino Glysin asal isolat bebek memiliki karakteristik *hidrofobik*, sedangkan asam amino Serin asal isolat manusia bersifat *Hidrofilik*.



Gambar 11. Mutasi RBD isolat bebek ke manusia pada subtipe H2N2 & H3N2



Gambar 12.Mutasi RBD isolat bebek ke manusia pada subtipe H2N2 & H3N2

Pada subtipe H5N1 tidak ditemukan adanya mutasi pada daerah *Receptor Binding Domain* antara isolat asal bebek dan manusia. Pada posisi 190 terdapat asam amino Asam Glutamat (E), sedangkan pada posisi 225,

226, dan 228 terdapat asam amino Glysin (G), Glutamin (Q), dan Gysin (G). Hal ini menunjukan bahwa subtipe H5N1 hanya mampu mengenali Sia(α2-3)Gal.

Berdasarkan kajian dari subtipe yang telah menjadi pandemik, kemungkinan subtipe H5N1 mampu mengenali Sia(α2-6)Gal jika terjadi mutasi pada asam amino posisi 190 dan 225 menjadi Asam aspartat. Kemungkinan lainnya jika terjadi mutasi pada posisi 226 dan 228 menjadi asam amino Leusin dan Serin.

4.3 Pencarian Struktur Tiga Dimensi Protein Hemagglutinin

Pencarian struktur tiga dimensi dilakukan melalui server yang diakses melalui *http://www.rcsb.org/pdb/static.do?p=search/index.html*. Pada server ini, pencarian struktur tiga dimensi dapat dilakukan dengan beberapa cara seperti memasukan kode *input* PDB, berdasarkan nama protein atau dengan membandingkan sekuen input terhadap database. Metode yang digunakan dalam penelitian ini adalah membandingkan sekuen *Hemagglutinin* yang telah dianalisis dengan *multiple alignment t*erhadap sekuen pada database yang telah diketahui strukturnya. Proses ini disebut *Basic Local Alignment Search Tool* (BLAST).

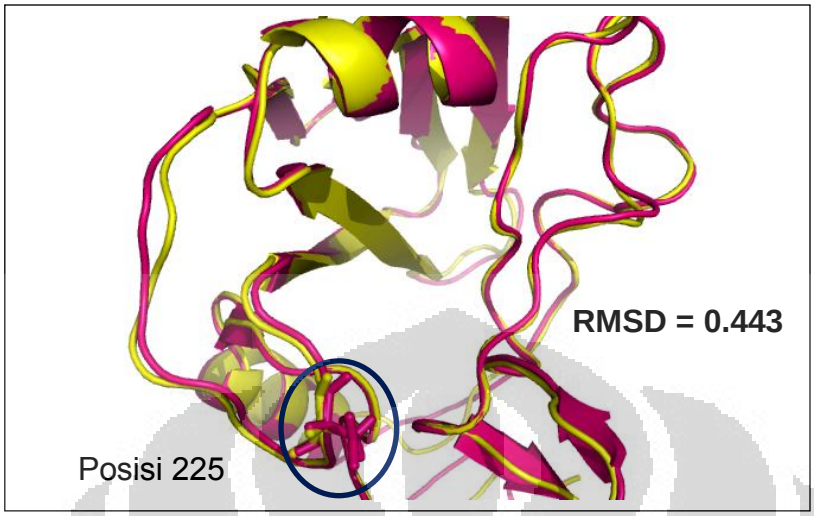
Struktur tiga dimensi yang dicari adalah *Hemagglutinin* asal isolat bebek dan manusia untuk subtipe H1, H3, dan H5. Struktur tiga dimensi yang dicari harus memiliki kesamaan 100% pada *Receptor Binding Domain* terhadap sekuen input.

Struktur yang didapatkan dari proses ini adalah 1RVT asal isolat babi dan 1RD8 asal isolat manusia untuk subtipe H1. 1MQN asal isolat bebek dan 1HGF asal isolat manusia untuk subtipe H3 serta 2FK0 untuk subtipe H5. File struktur tiga dimensi yang didownload berupa format PDB.

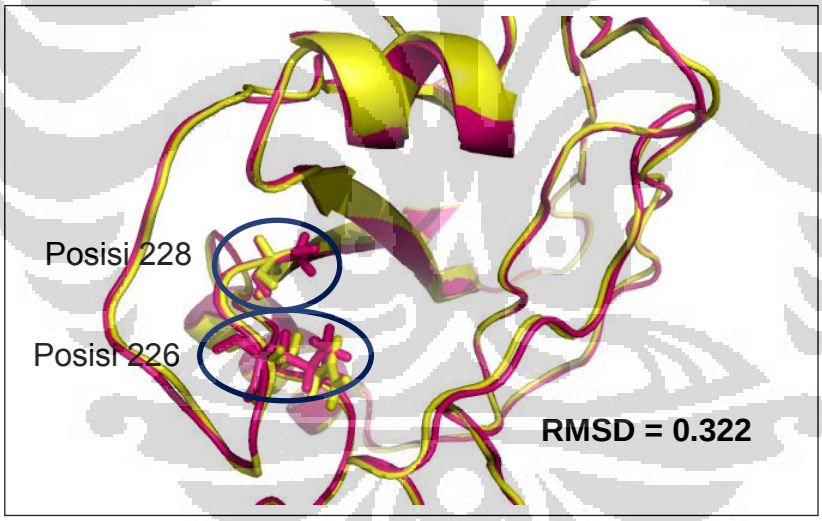
4.4 Superimpose Struktur Tiga Dimensi

Asam amino *backbone* yang terdapat di selain *Receptor Binding Domain* juga dapat mempengaruhi bentuk pelipatan celah dari *Receptor Binding Domain*. Karakteristik keterkaitan pelipatan celah dari *Receptor Binding Domain* asal isolat bebek dan manusia dilakukan untuk mengetahui seberapa besar peran dari asam amino *backbone* tersebut. Metode yang digunakan untuk memeriksa keterkaitan antar struktur adalah *superimpose* dan dilakukan menggunakan *software* Pymol. Pada metode ini, posisi Cα untuk tiap asam amino di bandingkan antara isolat bebek dan manusia dengan menggunakan nilai *Root Mean Square Deviation* (RMSD). Nilai RMSD ini akan berguna untuk menunjukan hubungan antar struktur yang dibandingkan.

Nilai RMSD dari hasil *superimpose* antara isolat bebek dengan isolat manusia pada subtipe H1 sebesar 0.604 Angstroms. Pada subtipe H3 sebesar 0.416 Angstroms dan pada subtipe H5 sebesar 0.573 Angstroms



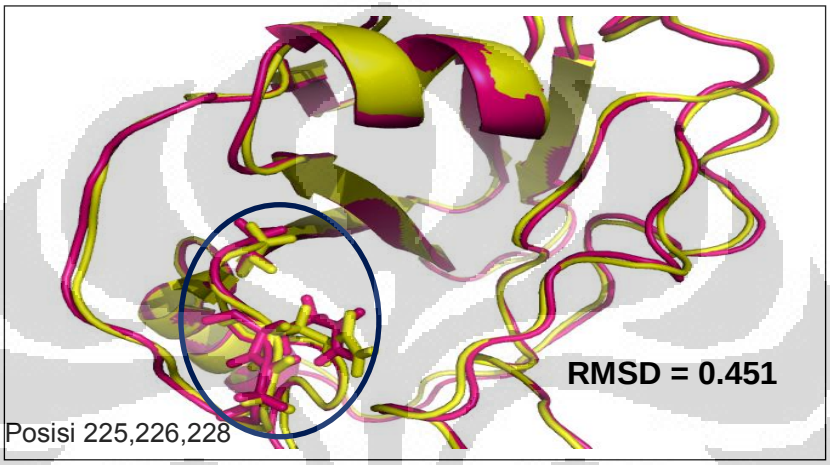
Gambar 13. *Superimpose* subtipe H1 isolat babi (kuning) & manusia (merah)



Gambar14.*Superimpose* subtipe H3 isolat bebek(kuning) & manusia (merah)

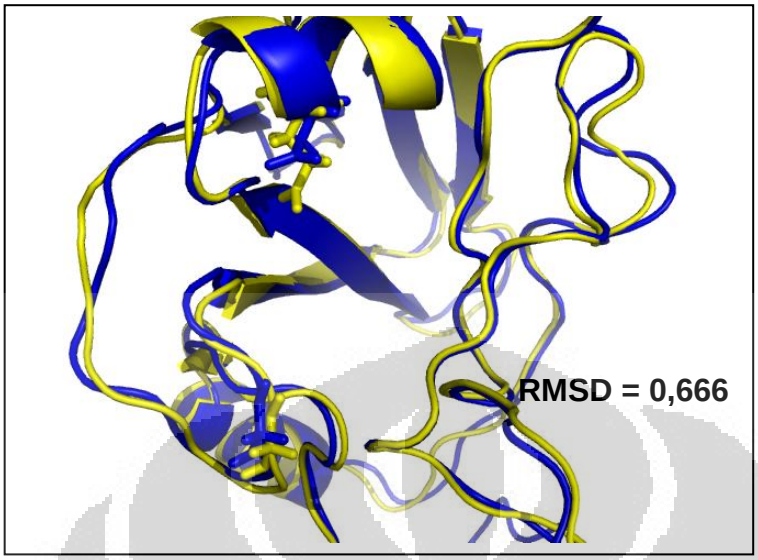
Hasil dari *superimpose* menunjukan bahwa struktur *Receptor Binding Domain* untuk isolat bebek dan manusia dalam satu subtipe memilki bentuk mirip. Hal ini menunjukan bahwa asam amino *backbone* dalam satu subtipe tidak secara signifikan mempengaruhi pola pelipatan celah dari *Receptor*

Binding Domain. Berdasarkan hal tersebut dapat diasumsikan bahwa spesifisitas *Hemagglutinin* dalam satu subtipe hanya dipengaruhi oleh susunan asam amino pada *Receptor Binding Domain* yang berinteraksi secara langsung dengan reseptor sel *sialic acid*.

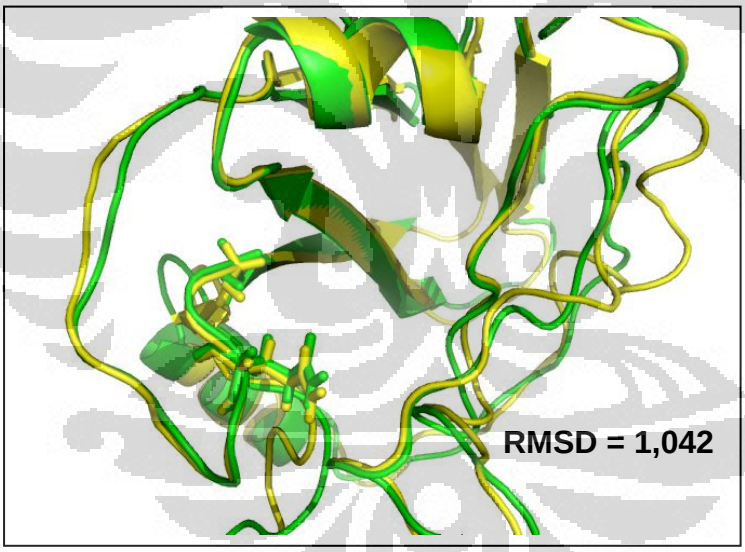


Gambar 15.*Superimpose* subtipe H5 isolat bebek (kuning) & manusia(merah)

Hasil *superimpose* untuk struktur *Receptor Binding Domain* antara subtipe H1 dengan H5 menghasilkan nilai RMSD sebesar 0,666 Angstroms. Pada subtipe antara H5 dan H3 menghasilkan nilai RMSD 1,042 Angstroms. Berdasarkan hasil ini didapatkan kesimpulan bahwa struktur *Receptor Binding Domain* subtipe H5 memiliki keterkaitan struktur lebih dekat dengan subtipe H1 dibandingkan dengan subtipe H3. Hal ini sekaligus mendukung pernyataan, Ridlo 2008, mengenai kedekatan subtipe H5N1 terhadap subtipe H1N1 dibandingkan dengan H3N2 dengan menggunakan analisis *phylogenetic tree*



Gambar 16.*Superimpose* antara subtipe H5(kuning) dengan subtipe H1 (biru)



Gambar 17.*Superimpose* antara subtipe H5(kuning) dengan subtipe H3(hijau)

4.5 Molecular Docking

Struktur tiga dimensi yang telah di*download* kemudian dilakukan simulasi *molecular docking* terhadap ligand Sia(α2-3)Gal dan Sia(α2-6)Gal.

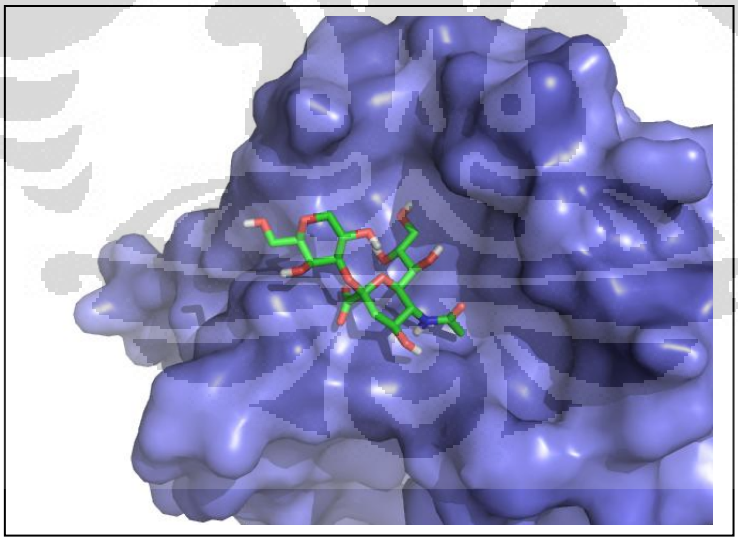
Simulasi *molecular docking* menggunakan software Autodock4 dengan *Lamarckian-Genetic Algorithm* dan hasil docking divisualisasikan menggunakan software Pymol. Kompleks yang terbentuk antara *Hemagglutinin* dengan Sia(α2-3)Gal dan Sia(α2-3)Gal mempunyai nilai perkiraan ΔG°*binding* dan *Konstanta Inhibition* yang dihitung oleh program Autodock.

Tabel 3. Hasil perkiraan ΔG°*binding* dan *Konstanta Inhibition*

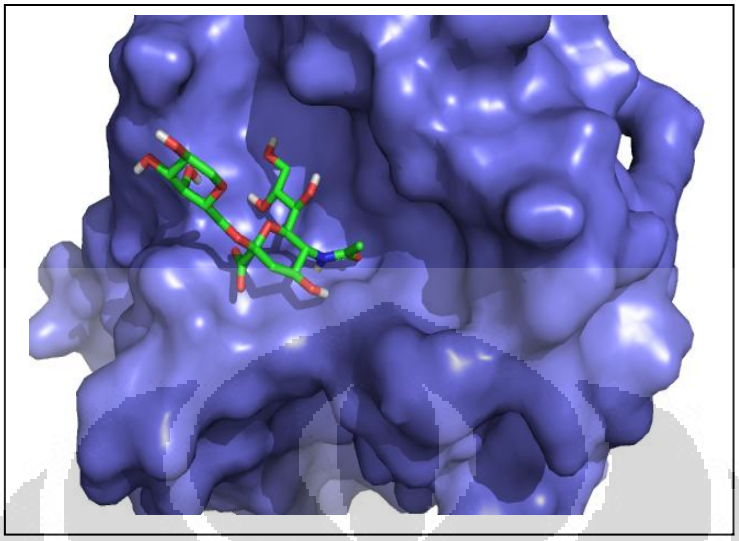
Subtipe H1N1		
1RVT (babi) - Sia(α2-3)Gal	ΔG°*binding*	-1.37 kcal/mol
	Ki	99.71 mM
1RVT (babi) - Sia(α2-6)Gal	ΔG°*binding*	-1.98 kcal/mol
	Ki	35.67 mM
1RD8 (manusia) - Sia(α2-3)Gal	ΔG°*binding*	-1.86 kcal/mol
	Ki	43.12 mM
1RD8 (manusia) - Sia(α2-6)Gal	ΔG°*binding*	-1.99 kcal/mol
	Ki	34.75 mM
Subtipe H3N2		
1MQN (bebek) - Sia(α2-3)Gal	ΔG°*binding*	-1.06 kcal/mol
	Ki	166.46 mM
1MQN (bebek) - Sia(α2-6)Gal	ΔG°*binding*	-1.59 kcal/mol
	Ki	68.55 mM
1HGF (manusia) - Sia(α2-3)Gal	ΔG°*binding*	-0.75 kcal/mol
	Ki	283.94 mM
1HGF (manusia) - Sia(α2-6)Gal	ΔG°*binding*	-0.20 kcal/mol
	Ki	716.54 mM
Subtipe H5N1		
2FK0 (manusia) - Sia(α2-3)Gal	ΔG°*binding*	-1.14 kcal/mol
	Ki	145.55 mM
2FK0 (manusia) - Sia(α2-6)Gal	ΔG°*binding*	-1.50 kcal/mol
	Ki	79.72 mM

Berdasarkan nilai ΔG°*binding* dan *Konstanta Inhibition* tidak terjadi perbedaan signifikan antara kompleks asal isolat bebek dan dengan asal isolat manusia. Hal ini mengakibatkan nilai ΔG°*binding* dan *Konstanta Inhibition* hasil output dari program Autodock tidak dapat dijadikan acuan untuk menentukan spesifitas *Hemagglutinin.*

Penentuan spesifitas harus dilakukan dengan melihat secara manual dan meneliti kompleks yang terbentuk. Apabila residu *sialic acid* dapat memasuki celah Receptor Binding Domain (RBD) maka dapat disimpulkan bahwa *Hemagglutinin* mampu berikatan dengan reseptor *sialic acid* tersebut. Pada *Hemagglutinin* yang tidak memilki kecocokan dengan reseptor *sialic acid* terbentuk kompleks yang menunjukan residu *sialic acid* tidak dapat memasuki celah RBD.

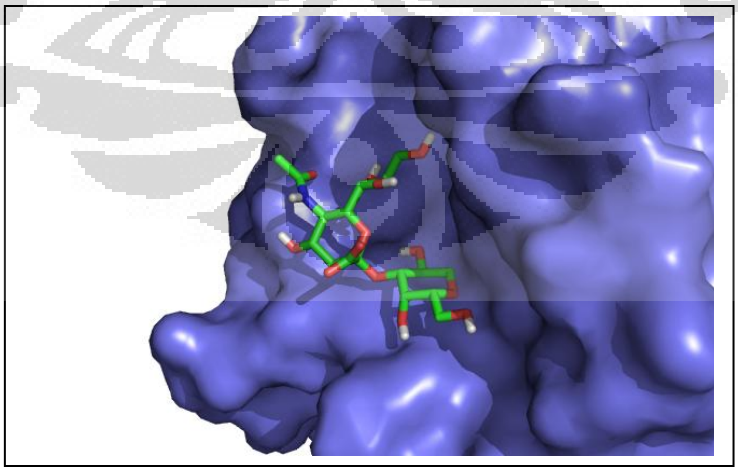


Gambar 18. Kompleks Hemagglutinin 1RVT dengan Sia(α2-3)Gal

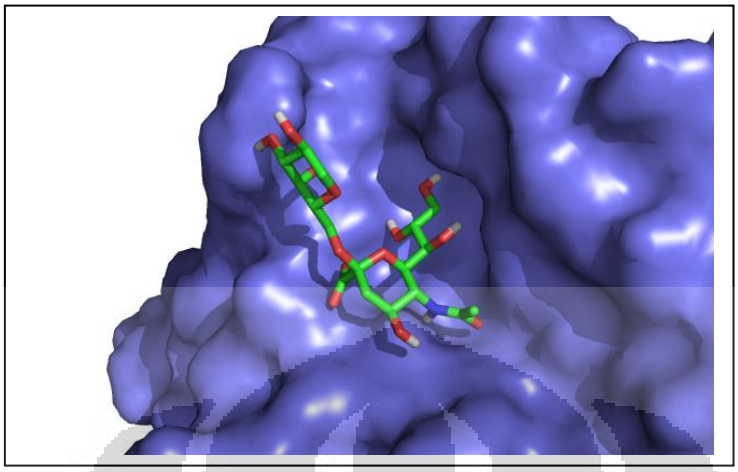


Gambar 19. Kompleks Hemagglutinin 1RVT dengan Sia(α2-6)Gal

Berdasarkan hasil visualisasi kompleks dari *molecular docking* pada subtipe H1 didapatkan bahwa struktur 1RVT (isolat babi) dapat berikatan dengan *ligand* Sia(α2-3)Gal dan Sia(α2-6)Gal. Hal ini terlihat dari hasil kompleks yang divisualisasikan menunjukan bahwa residu *sialic acid* dari Sia(α2-3)Gal dan Sia(α2-6)Gal dapat memasuki celah RBD.



Gambar 20. Kompleks Hemagglutinin 1RD8 dengan Sia(α2-3)Gal

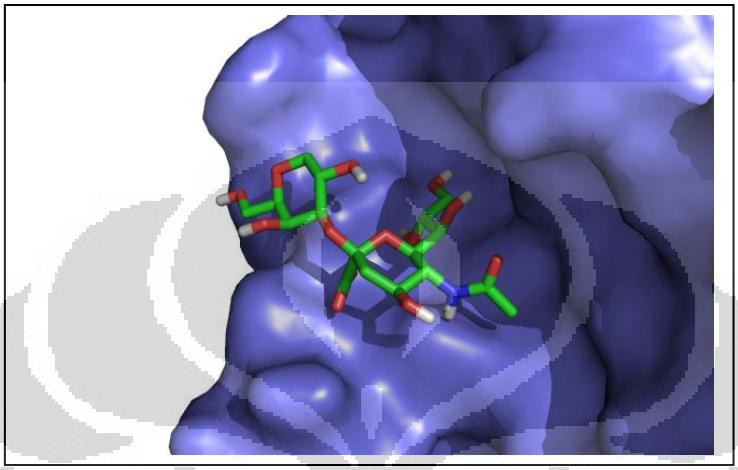


Gambar 21. Kompleks Hemagglutinin 1RD8 dengan Sia(α2-6)Gal

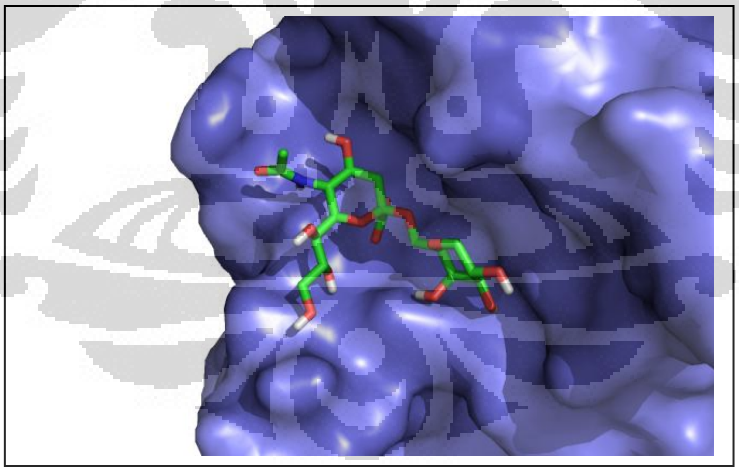
Hal berbeda ditunjukan pada kompleks antara 1RD8 (isolat manusia) dengan Sia(α2-3)Gal dan Sia(α2-6)Gal. Kompleks yang terjadi antara 1RD8 dengan Sia(α2-3)Gal menunjukan bahwa residu *sialic acid* dari Sia(α2-3)Gal tidak dapat memasuki celah dari RBD. Berdasarkan hal ini dapat diperkirakan bahwa Sia(α2-3)Gal tidak mampu berikatan dengan 1RD8. Hal berbeda terjadi pada kompleks antara 1RD8 dengan Sia(α2-6)Gal. Pada kompleks tersebut terlihat bahwa residu *sialic acid* dapat memasuki celah RBD. Berdasarkan hal ini dapat disimpulkan bahwa struktur *Hemagglutinin* 1RD8 memiliki spesifitas terhadap reseptor Sia(α2-6)Gal.

Hasil *molecular docking* untuk subtipe H3 menunjukan bahwa struktur 1MQN (asal isolat bebek) memiliki spesifitas terhadap Sia(α2-3)Gal. Hal tersebut dapat dilihat berdasarkan kompleks yang terbentuk dengan Sia(α2-3)Gal dan Sia(α2-6)Gal. Pada kompleks dengan Sia(α2-3)Gal terlihat bahwa gugus residu *sialic acid* memasuki celah RBD, namun hal ini tidak

terjadi pada kompleks dengan Sia(α2-6)Gal. Residu *sialic acid* dari Sia(α2-6)Gal hanya tepat berada di depan celah RBD tanpa mampu memasukinya.



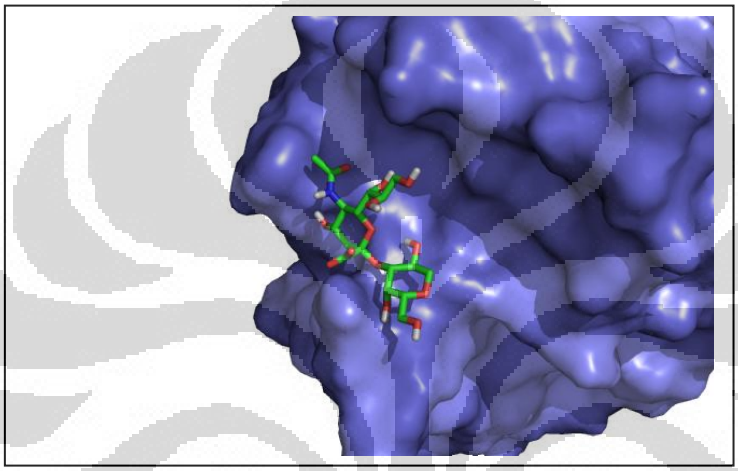
Gambar 22. Kompleks *Hemagglutinin* 1MQN dengan Sia(α2-3)Gal



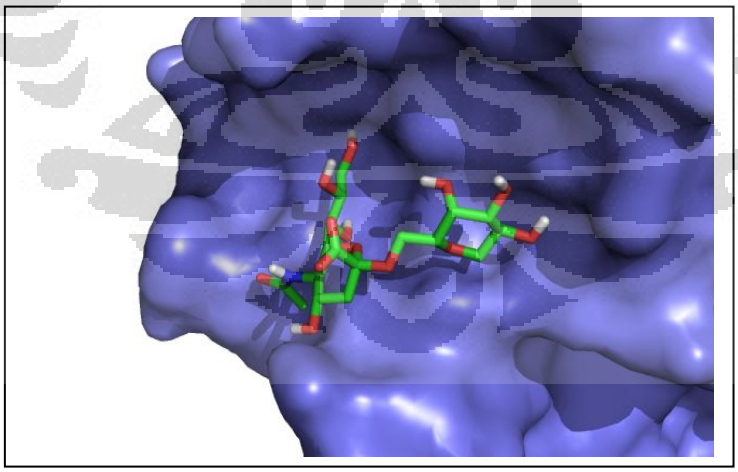
Gambar 23. Kompleks *Hemagglutinin* 1MQN dengan Sia(α2-6)Gal

Pada struktur 1HGF (asal isolat manusia) yang masih termasuk subtipe H3, memilki spesifitas berbeda dengan 1MQN (asal isolat bebek).

1HGF memiliki spesifitas terhadap Sia(α2-6)Gal. Pada kompleks 1HGF dengan Sia(α2-3)Gal dan Sia(α2-6)Gal menunjukan hal berlawanan dengan kompleks 1MQN. Residu *sialic acid* Sia(α2-3)Gal tidak mampu memasuki celah RBD sedangkan residu *sialic acid* Sia(α2-6)Gal mampu memasuki RBD.

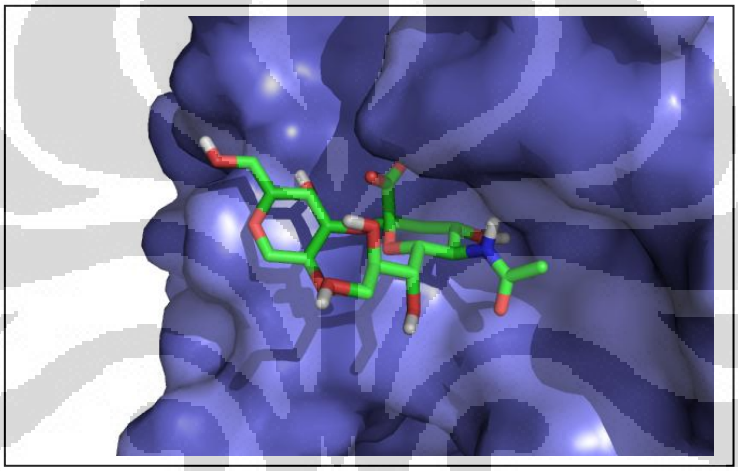


Gambar 24. Kompleks *Hemagglutinin* 1HGF dengan Sia(α2-3)Gal

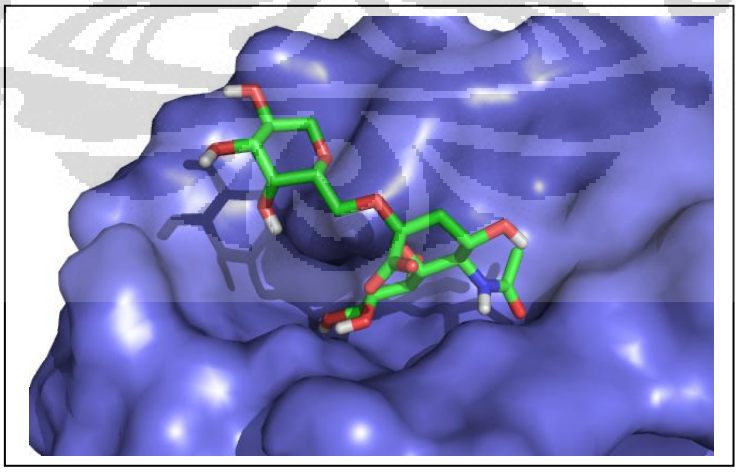


Gambar 25. Kompleks *Hemagglutinin* 1HGF dengan Sia(α2-6)Gal

Pada struktur 2FK0 asal isolat manusia yang juga memiliki susunan asam amino RBD yang sama dengan asal isolat bebek menunjukan spesifitas terhadap Sia(α2-3)Gal. Kompleks yang terbentuk menunjukan residu *sialic acid* dari Sia(α2-3)Gal mampu memasuki celah sempit RBD namun residu *sialic acid* dari Sia(α2-6)Gal terlihat hanya mampu sedikit memasuki celah RBD.



Gambar 26. Kompleks *Hemagglutinin* 2FK0 dengan Sia(α2-3)Gal



Gambar 27. Kompleks *Hemagglutinin* 2FK0 dengan Sia(α2-6)Gal

Hasil *molecular docking* dengan autodock berhasil memprediksikan spesifitas *Hemagglutinin* melalui evaluasi kompleks yang terbentuk meskipun gagal dalam memprediksikan spesifitas melalui nilai ΔG°*binding* dan *Konstanta Inhibition.* Hasil penelitian ini dapat dijadikan salah satu dasar dilakukannya uji spesifitas dari sekuen *Hemagglutinin* yang belum diuji di laboratorium melalui metode komputasional. Penggabungan metode *homology modelling* dan *molecular docking* terhadap suatu sekuen *Hemagglutinin* dapat memprediksikan spesifitas dari suatu *Hemagglutinin* dengan cepat dan murah. Selanjutnya hasil dari penelitian ini diharapkan dapat dijadikan informasi awal dalam perancangan inhibitor yang mampu menghalangi pengikatan *Hemagglutinin* terhadap reseptor sel Sia(α2-6)Gal yang ada pada saluran pernapasan manusia.

BAB V

KESIMPULAN DAN SARAN

5.1 Kesimpulan

Hasil *alignment* subtipe H1N1 menunjukan bahwa diperlukan mutasi asam amino pada posisi 190 dan 225 menjadi Asam Aspartat pada hemagglutinin untuk mengenali reseptor Sia(α2-6)Gal. Pada subtipe H2N2 dan H3N2 memerlukan mutasi yang berbeda dengan subtipe H1N1. Subtipe H2N2 dan H3N2 memerlukan mutasi asam amino pada posisi 226 dan 228 menjadi Leusin dan Serin untuk mengenali reseptor Sia(α2-6)Gal.

Berdasarkan Analisis mutasi terhadap *Hemagglutinin* yang telah menjadi pandemik, dapat diperkirakan bahwa *Hemagglutinnin* subtipe H5N1 memerlukan mutasi pada posisi 190 dan 225 menjadi Asam Aspartat untuk mengenali reseptor Sia(α2-6)Gal. Kemungkinan lain adalah memerlukan mutasi asam amino pada posisi 226 dan 228 menjadi Leusin dan Serin.

Metode simulasi *molecular docking* mampu membentuk kompleks antara *Hemagglutinin* dengan Reseptor Sia(α2-6)Gal dan Sia(α2-3)Gal. Berdasarkan hasil kompleks yang terbentuk, metode simulasi *molecular docking* berhasil mengidentifikasi spesifitas Hemagglutinin terhadap Sia(α2-3)Gal atau Sia(α2-6)Gal

5.2 Saran

Simulasi *molecular docking* dapat dilakukan dengan menggunakan program selain autodock sebagai perbandingan. Perbandingan program *molecular docking* dapat lebih memastikan keberhasilan dari metode simulasi *molecular docking* untuk mengidentifikasi spesifitas *Hemagglutinin* terhadap Sia(α2-3)Gal atau Sia(α2-6)Gal.

Analisis *molecular mechanic* dan *molecular dynamic* perlu dilakukan lebih lanjut terhadap hasil docking yang telah dilakukan. Analisis *molecular mechanic* dan *molecular dynamic* dapat memberikan penjelasan lebih lanjut mengenai interaksi ikatan *Hemagglutinin* dengan reseptor *sialic acid*. Metode ini juga dapat meningkatkan keakuratan simulasi mekanisme pengikatan *Hemagglutinin* dengan reseptor *sialic acid*.

DAFTAR PUSTAKA

Asmara, W. 2007. *Peran Biologi Molekuler Dalam Pengendalian Avian Influenza dan Flu Burung*. Pidato Pengukuhan Jabatan Guru besar pada FKH UGM.

Baxevanis, A. D., Ouelette, B.F.F. 2005. *Bioinformatics A Practical Guide to The Analysis of Genes and Proteins.* 3rd ed. Wiley Interscience

Claverie, M. J., Notredame, C. 2003. Bioinformatics for Dummies. Wiley Publishing.

Cox NJ, Kawaoka Y. Orthomyxoviruses: Influenza. In: Topley & Wilson's Microbiology and Microbial Infections, 9th ed., Collier L, Balows A., Sussman M., eds., Edward Arnold, London Vol.1, 1997: 385-433

Guan, Yi *et al*. 2007. *Avian Influenza Virus (H5N1): a Threat to Human Health*. Clin. Microbiol.**20**: 243-267.

Higgins,D.G. and Sharp,P.M. (1989) *Fast and sensitive multiple sequence alignments on a microcomputer*. CABIOS 5,151-153.

Higgins,D.G. and Sharp,P.M. (1988) *CLUSTAL: a package for performing multiple sequence alignment on a microcomputer*. Gene 73,237-244.

Hikmawan O., 2007. *Studi In Silico Mutasi Virus Influenza A H5N1 strain Indonesia.* Departemen Kimia Universitas Indonesia.

Horimoto, T., et. al., *Influenza: Lessons from past pandemics, warnings from current incidents*, Nature Reviews Microbiology 3, 591-600

Horimoto, T., and Kawaoka, Y. 2001. *Pandemic Threat Posed By Avian Influenza A Viruses.* Clin. Microbiol. Rev. **14**: 129-149

Iwatsuki-Horimoto, K. Kanazawa, R. Sugii, S. Kawaoka, Y. & Horimoto, T.2004. *The index influenza A virus subtype H5N1 isolated from a human in 1997 differs in its receptor-binding properties from a virulent avian influenza virus*," *J. Gen. Virol.*, vol. 85, pp. 1001–1005, 2004.

Kamps, Hoffman, & Preiser S.B., 2006. *Influenza report 2006*. Flying Publisher. Paris, Cagliari, Sevilla.

Larkin,M.A., Blackshields, G., Brown, N.P., Chenna, R., McGettigan, P.A., McWilliam, H., Valentin, F., Wallace, I.M., Wilm, A., Lopez, R., Thompson, J.D., Gibson, T.J., Higgins, D.G. (2007) *Clustal W and Clustal X version 2.0.* Bioinformatics, 23:2947-2948.

Li, Minyong., Binghe Wang. 2006. *Computational Studies of H5N1 Hemagglutinin binding with Sia(α2-3)Gal and Sia(α2-6)Gal*. Sciencedirect 347 : 662-668

Li-Ching, W. Jorng-Tzong, H. Hsien-Da, H., and Wei-Long C. 2008. *Identifying Discriminative Amino Acids Within the Hemagglutinin of Human Influenza A H5N1 Virus Using a Decision Tree*. Information Technology in Biomedicine, vol. 12, no. 6, november 2008

Matrosovich, M.N., Matrosovich, T.Y., Gray, T., Roberts, N.A., and Klenk, H.D. 2004. *Human and Avian Influenza Viruses Target diferent Cell Types in Cultures of Human Airway Epithelium*. PNAS. **101** (13) : 4620-2624.

G. M. Morris, D. S. Goodsell, R. S. Halliday, R. Huey,W. E.Hart, R. K. Belew

and A. J. Olson. *Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function*. Journal of Computational Chemistry,19 (14):1639–1662, 1999. ISSN 1096-987X.

Michel F. Sanner. Python: A Programming Language for Software Integration and Development. J. Mol. Graphics Mod., 1999, Vol 17, February. pp57-61

Mount, D.W., 2004. *Bioinformatics sequences and genome analysis*. Cold Spring Harbor Laboratory Press. New York.

Reid, A.H *et al*. 2002. *Characterization of The 1918 Spanish Influenza Virus Matrix Gene Segment*. J. Virol. **76**: 10717-10723.

Ridlo, N. 2008. *Studi Mekanisme Mutasi Virus Influenza A Membentuk Subtipe H5N1 pada Manusia Secara in silico.* Departemen Kimia Universitas Indonesia.

Stevens J. *et. al*. 2006. *Structure and Receptor Specificity of the Hemagglutinin from an H5N1 Influenza Virus*. Science : 1124513

Supandi PZ. 2005. *Influenza Burung pada Manusia*. Prosiding simposium. Jakarta: Departemen Pulmonologi dan Ilmu Kedokteran Respirasi FKUI.

Tambunan S.F, Hikmawan O., & Theofilus A., 2008. *In Silico Mutation Study of Hemagglutinin and Neuraminidase on Banten Province Strain Influenza A H5N1 Virus*. Trends in Bioinformatic : Science Allert

Thompson,J.D., Gibson,T.J., Plewniak,F., Jeanmougin,F. and Higgins,D.G (1997*) The ClustalX windows interface: flexible strategies for multiple*

sequence alignment aided by quality analysis tools. Nucleic Acids Research, 25:4876-4882.

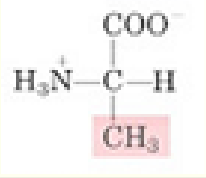
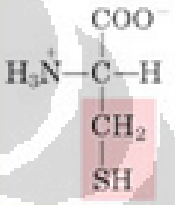
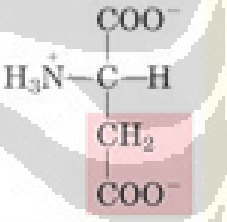
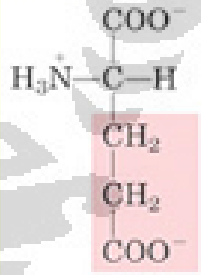
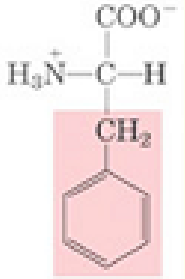
Tumpey, T.M., Suarez, D.L., Perkin, L.E.L. 2002. *characterization of Highly Pathogenic H5N1 Avian Influenza A Virus Isolated From Duck Meat*. J. Virol. **76** (12): 6344-6355.

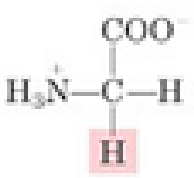
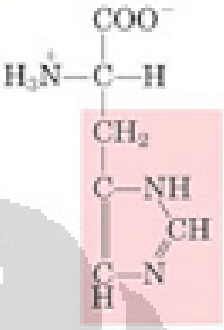
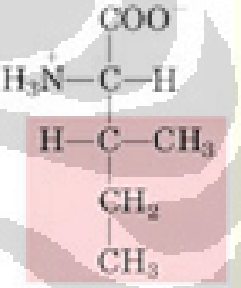
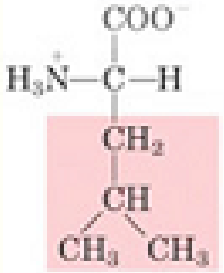
Y. Kalidas, and N. Chandra,.2008. *Structural Bioinformatics: Transforming protein structures into biologicl insight.* Journal of the Indian Institute of Science VOL 88:2

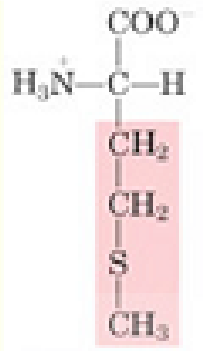
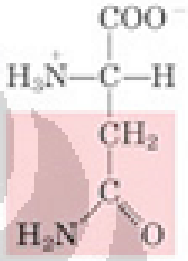
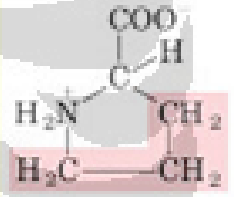
www.who.int/csr/don/2009_06_26/en/index.html, diakses pada hari Senin 29 Juni 2009 pukul 18.00 WIB

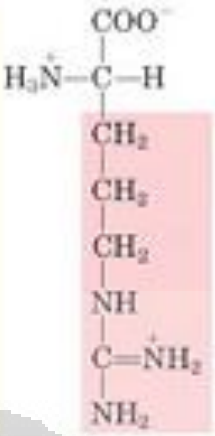
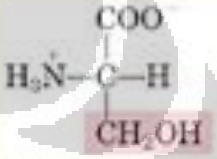
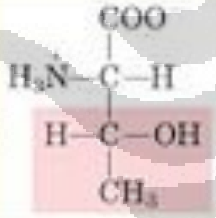
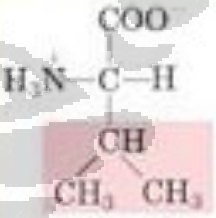
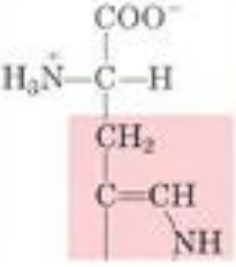
www.who.int/entity/csr/disease/avian_influenza/cases_table_2009_06_02/en/index.html, diakses pada hari Rabu 3 Juni 2009 pukul 09.18 WIB

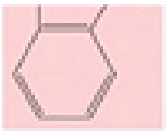
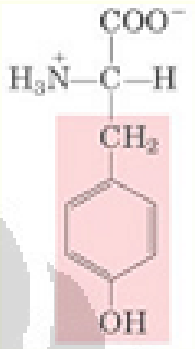
Lampiran 1. Tabel Asam Amino

A	Ala	Alanine	aliphatic hydrophobic neutral	GCT GCC GCA GCG	
B		either aspartic acid or asparagine			
C	Cys	Cysteine	polar hydrophobic neutral	TGT TGC	
D	Asp	Aspartic Acid	polar hydrophilic charged (-)	GAT GAC	
E	Glu	Glutamic Acid	polar hydrophilic charged (-)	GAA GAG	
F	Phe	Phenylalanine	aromatic hydrophobic neutral	TTT TTC	

G	Gly	Glycine		GGT GGC GGA GGG	
H	His	Histidine	aromatic polar hydrophilic charged (+)	CAT CAC	
I	Ile	Isoleucine	aliphatic hydrophobic neutral	ATT ATC ATA	
K	Lys	Lysine		AAA AAG	
L	Leu	Leucine	aliphatic hydrophobic neutral	TTG TTA CTT CTC CTA CTG	

M	Met	Methionine	hydrophobic neutral	ATG	
N	Asn	Asparagine	polar hydrophilic neutral	AAT AAC	
P	Pro	Proline	hydrophobic neutral	CCT CCC CCA CCG	
Q	Gln	Glutamine	polar hydrophilic neutral	CAA CAG	

R	Arg	Arginine	polar hydrophilic charged (+)	CGT CGC CGA CGG AGA AGG	
S	Ser	Serine	polar hydrophilic neutral	TCT TCC TCA TCG AGT AGC	
T	Thr	Threonine	polar hydrophilic neutral	ACT ACC ACA ACG	
V	Val	Valine	aliphatic hydrophobic neutral	GTT GTC GTA GTG	
W	Trp	Tryptophan	aromatic hydrophobic neutral	TGG	

					
X		UNKNOWN			
Y	Tyr	Tyrosine	aromatic polar hydrophobic	TAT TAC	
Z		either glutamic acid or glutamine			
	End	Terminator		TAA TAG	

Lampiran 2. Keterkaitan struktur berdasarkan nilai RMSD

RMSD(Å)	Structure Comparison Comment
>12	Completely Unrelated
7	Dubious relationship
5	May be structurally related
4	Good structural relationship
2	Closely related
1,5	Very Closely Related
0,8	Differences are not obvious
0,4	Essentially indistinguishable

(Baxevanis dan Oullete, 2001).

Lampiran 3. Sekuen Sampel Hemagglutinin dalam format FASTA

>gi|4585161|gb|AAD25304| /Avian/HA/H1N1/Canada/1976/// hemagglutinin precursor [influenza A virus (A/duck/Alberta/35/76(H1N1))]
MEAKLFVLFCTFTVLKADTICVGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCSLNGIAPLQLG
KCNVAGWLLGNPECDLLLTANSWSYIIETSNSENGTCYPGEFIDYEELREQLSSVSSFEKFEIFPKASSW
PNHETTKGVTAACSYSGASSFYRNLLWITKKGTSYPKLSKSYTNNKGKEVLVLWGVHHPPSVSEQQSLYQ
NADAYVSVGSSKYNRRFAPEIAARPKVRGQAGRMNYYWTLLDQGDTITFEATGNLIAPWYAFALNKGSDS
GIITSDAPVHNCDTRCQTPHGALNSSLPFQNVHPITIGECPKYVKSTKLRMATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQNAIDGITSKVNSVIEKMNTQFTAVGKEFNNLERR
IENLNKKVDDGFLDVWTYNAELLVLLENERTLDFHDSNVRNLYEKVKSQLRNNAKEIGNGCFEFYHKCDD
ECMESVKNGTYDYPKYSEESKLNREEIDGVKLESMGVYQILAIYSTVASSLVLLVSLGAISFWMCSNGSL
QCRICI
>gi|221300|gb|BAA01280| /Avian/HA/H1N1/Canada/1976/// haemagglutinin [Influenza A virus (A/mallard/Alberta/35/1976(H1N1))]
MEAKLFVLFCTFTVLKADTICVGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCSLNGIAPLQLG
KCNVAGWLLGNPECDLLLTANSWSYIIETSNSENGTCYPGEFIDYEELREQLSSISSFEKFEIFPKASSW
PNHETTKGVTAACSYSGASSFYRNLLWITKKGTSYPKLSKSYTNNKGKEVLVLWGVHHPPSVSEQQSLYQ
NADAYVSVGSSKYNRRFAPEIAARPEVRGQAGRMNYYWTLLDQGDTITFEATGNLIAPWYAFALNKGSDS
GIITSDAPVHNCDTRCQTPHGALNSSLPFQNVHPITIGECPKYVKSTKLRMATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQNAIDGITSKVNSVIEKMNTQFTAVGKEFNNLERR
IENLNKKVDDGFLDVWTYNAELLVLLENERTLDFHDSNVRNLYEKVKSQLRNNAKEIGNGCFEFYHKCDD
ECMESVKNGTYDYPKYSEESKLNREEIDGVKLESMGVYQILAIYSTVASSLVLLVSWGAISFWMCSNGSL
QCRICI
>gi|4585169|gb|AAD25308| /Avian/HA/H1N1/Germany/1977/// hemagglutinin precursor[Influenza A virus (A/duck/Bavaria/1/1977 (H1N1))]
MEVKLFVLFCTFTALKADTICVGYHANNSTDTVDTVLEKNVTVTHSVNLLENSHNGKLCSLNGIAPLQLG
KCNVAGWILGNPECDLLLTANSWSYIIETSNSENGTCYPGEFIDYEELREQLSSVSSFEKFEIFPKASSW
PNHETTKGVTAACSYSGASSFYRNLLWITKKGTSYPKLSKSYTNNKGKEVLVIWGVHHPPTADEQQSLYQ
NADAYVSVGSSKYNRRFTPEIAARPKVRGQAGRMNYYWTLLDQGDTITFEATGNLIAPWYAFALNKDSGS
GIITSDAPVHNCDTKCQTPRGALNSSLPFQNIHPITIGECPKYVKSTKLRMATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQNAIDGITNKVNSVIEKMNTQFTAVGKEFNNLERR
IENLNKKVDDGFLDVWTYNAELLVLLENERTLDFHDSNVRNLYEKVKSQLRNNAKEIGNGCFEFYHKCDD
ECMESVKNGTYDYPKYSEESKLNREEIDGVKLESMGVYQILAIYSTVASSLVLLVSLGAISFWMCSNGSL
QCRICI
>gi|113531185|gb|BAF03627| /Avian/HA/H1N1/Japan/1977/// haemagglutinin[Influenza A virus (A/duck/Miyagi/66/1977(H1N1))]
MEAKLFVLFCTFTALKADTICIGYHANNSTDTVDTVLEKNVTVTHSVNLLENSHNGKLCSLNGIAPLQLG
KCNVAGWLLGNPECDLLLTASSWSYIIETSNSENGTCYPGEFIDYEELREQLSSVSSFEKFEIFPKASSW
PNHETTKGVTAACSYSGASSFYRNLLWITEKGTSYPKLSKSYTNNKGKEVLVLWGVHHPPTTNEQQSLYQ
NADAYVSVGSSKYNRRFTPEIAARPKVRGQAGRMNYYWTLLDQGDTITFEATGNLIAPWYAFALNKGSDS
GIITSDAPVHNCDTKCQTPHGALNSSLPFQNVHPITIGECPKYVKSTKLRMATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQSAIDGITNKVNSVIEKMNTQFTAVGKEFNNLERR
IENLNKKVDDGFLNVWTYNAELLVLLENERTLDFHDSNVRNLYEKVKSQLRNNAKEIGNGCFEFYHKCDD
ECMESVKNGTYDYPKYSEESKLNREEIDGVKLESMGVYQILAIYSTVASSLVLLVSLGAISFWMCSNGSL
QCRICI

>gi|4325018|gb|AAD17218| /Human/HA/H1N1/USA/1918/// hemagglutinin [influenza A virus (A/Brevig_Mission/1/18(H1N1))]
MEARLLVLLCAFAATNADTICIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCKLKGIAPLQLG
KCNIAGWLLGNPECDLLLTASSWSYIVETSNSENGTCYPGDFIDYEELREQLSSVSSFEKFEIFPKTSSW
PNHETTKGVTAACSYAGASSFYRNLLWLTKKGSSYPKLSKSYVNNKGKEVLVLWGVHHPPTGTDQQSLYQ
NADAYVSVGSSKYNRRFTPEIAARPKVRDQAGRMNYYWTLLEPGDTITFEATGNLIAPWYAFALNRGSGS
GIITSDAPVHDCNTKCQTPHGAINSSLPFQNIHPVTIGECPKYVRSTKLRMATGLRNIPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQNAIDGITNKVNSVIEKMNTQ

>gi|4325020|gb|AAD17219| /Human/HA/H1N1/USA/1918/// hemagglutinin [influenza A virus (A/New_York/1/18(H1N1))]
MEARLLVLLCAFAATNADTICIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCKLKGIAPLQLG
KCNIAGWLLGNPECDLLLTASSWSYIVETSNSENGTCYPGDFIDYEELREQLSSVSSFEKFEIFPKTSSW
PNHETTKGVTAACSYAGASSFYRNLLWLTKKGSSYPKLSKSYVNNKGKEVLVLWGVHHPPTGTDQQSLYQ
NADAYVSVGSSKYNRRFTPEIAARPKVRGQAGRMNYYWTLLEPGDTITFEATGNLIAPWYAFALNRGSGS
GIITSDAPVHDCNTKCQTPHGAINSSLPFQNIHPVTIGECPKYVRSTKLRMATGLRNIPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQNAIDGITNKVNSVIEKMNTQ
>gi|4325039|gb|AAD17229| /Human/HA/H1N1/USA/1918/// hemagglutinin[Influenza A virus (A/South Carolina/1/1918(H1N1))]
MEARLLVLLCAFAATNADTICIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCKLKGIAPLQLG
KCNIAGWLLGNPECDLLLTASSWSYIVETSNSENGTCYPGDFIDYEELREQLSSVSSFEKFEIFPKTSSW
PNHETTKGVTAACSYAGASSFYRNLLWLTKKGSSYPKLSKSYVNNKGKEVLVLWGVHHPPTGTDQQSLYQ
NADAYVSVGSSKYNRRFTPEIAARPKVRDQAGRMNYYWTLLEPGDTITFEATGNLIAPWYAFALNRGSGS
GIITSDAPVHDCNTKCQTPHGAINSSLPFQNIHPVTIGECPKYVRSTKLRMATGLRNIPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQNAIDGITNKVNSVIEKMNTQFTAVGKEFNNLERR
IENLNKKVDDGFLDIWTYNAELLVLLENERTLDFHDSNVRNLYEKVKSQLKNNAKEIGNGCFEFYHKCDD
ACMESVRNGTYDYPKYSEESKLNREEIDGVKLESMGVYQILAIYSTVASSLVLLVSLGAISFWMCSNGSL
QCRICI
>gi|89779321|gb|ABD77675| /Human/HA/H1N1/Puerto Rico/1934/// hemagglutinin [Influenza A virus (A/Puerto Rico/8/34(H1N1))]
MKANLLVLLCALAAADADTICIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCRLKGIAPLQLG
KCNIAGWLLGNPECDPLLPVRSWSYIVETPNSENGICYPGDFIDYEELREQLSSVSSFERFEIFPKESSW
PNHNTNGVTAACSHEGKSSFYRNLLWLTEKEGSYPKLKNSYVNKKGKEVLVLWGIHHPPNSKEQQNLYQN
ENAYVSVVTSNYNRRFTPEIAERPKVRDQAGRMNYYWTLLKPGDTIIFEANGNLIAPMYAFALSRGFGSG
IITSNASMHECNTKCQTPLGAINSSLPYQNIHPVTIGECPKYVRSAKLRMVTGLRNIPSIQSRGLFGAIA
GFIEGGWTGMIDGWYGYHHQNEQGSGYAADQKSTQNAINGITNKVNTVIEKMNIQFTAVGKEFNKLEKRM
ENLNKKVDDGFLDIWTYNAELLVLLENERTLDFHDSNVKNLYEKVKSQLKNNAKEIGNGCFEFYHKCDNE
CMESVRNGTYDYPKYSEESKLNREKVDGVKLESMGIYQILAIYSTVASSLVLLVSLGAISFWMCSNGSLQ
CRICI

>gi|157168440|gb|ABV25634| /Swine/HA/H1N1/USA/1930/// hemagglutinin [Influenza A virus (A/swine/Iowa/15/1930(H1N1))]
MKAILLVLLCAFAATNADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCRLGGIAPLQLG
KCNIAGWLLGNPECDLLLTVSSWSYIVETSNSDNGTCYPGDFIDYEELREQLSSVSSFEKFEIFPKTSSW
PNHETTRGVTAACPYAGASSFYRNLLWLVKKENSYPKLSKSYVNNKGKEVLVLWGVHHPPTSTDQQSLYQ
NADAYVSVGSSKYDRRFTPEIAARPKVRGQAGRMNYYWTLLEPGDTITFEATGNLVAPRYAFALNRGSES
GIITSDAPVHDCDTKCQTPHGAINSSLPFQNIHPVTIGECPKYVKSTKLRMVTGLRNIPSIQSRGLFGAI
AGFIEGGWTGLIDGWYGYHHQNGQGSGYAADQKSTQNAIDGITNKVNSVIEKMNTQFTVVGKEFNNLERR
IKNLNKKVDDGFLDVWTYNAELLVLLENERTLDFHDSNVKNLYEKARSQLRNNAKEIGNGCFEFYHKCDD
ACMESVRNGTYDYPKYSEESKLNREEIDGVKLESMMVYQILAIYSTVASSLVLLVSLGAISFWMCSNGSL
QCRICI
>gi|89941382|gb|ABD79255| /Swine/HA/H1N1//1931/// hemagglutinin [Influenza A virus (A/swine/1931(H1N1))]
MKAILLVLLCAFAATNADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCRLGGIAPLQLG
KCNIAGWLLGNPECDLLLTVSSWSYIVETSNSDNGTCYPGDFIDYEELREQLSSVSSFEKFEIFPKTSSW
PNHETTRGVTAACPYAGASSFYRNLLWLVKKENSYPKLSKSYVNNKGKEVLVLWGVHHPPTSTDQQSLYQ
NADAYVSVGSSKYDRRFTPEIAARPKVRGQAGRMNYYWTLLEPGDTITFEATGNLVAPRYAFALNRGSES
GIITSDAPVHDCDTKCQTPHGAINSSLPFQNIHPVTIGECPKYVKSTKLRMVTGLRNIPSIQSRGLFGAI
AGFIEGGWTGLIDGWYGYHHQNGQGSGYAADQKSTQNAIDGITNKVNSVIEKMNTQFTVVGKEFNNLERR
MKNLNKKVDDGFLDVWTYNAEXLVLLENERTLDFHDSNVKNLYEKARSQLRNNAKEIGNGCFEFYHKCDD
ACMESVRNGTYDYPKYSEESKLNREEIDGVKLESMMVYQILAIYSTVASSLVLLVSLGAISFWMCSNGSL
QCRICI
>gi|158525224|gb|ABW71481| /Swine/HA/H1N1/USA/1935/// hemagglutinin [Influenza A virus (A/swine/Ohio/23/1935(H1N1))]
MKARLLVLLCALAATNADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCRLGGIAPLQLG
KCNIAGWLLGNPECDLLLTVSSWSYIVETSNSDNGTCYPGDFIDYEELREQLSSVSSFERFEIFPKTSSW
PNHETTXGVTAACPYAGANSFYRNLLWLVKKGDSYPKLSKSYVNNKGKEVLVLWGVHHPPTSTXQQSLYQ
NADAYVSVGSSKYNRRFTPEIAARPKVRGQAGRMNYYWTLLEPGDTITFEATGNLVAPRYAFALNKGSGS
GVITSDAPVHDCDTKCQTPHGAINSSLPFQNIHPVTIGECPKYVKSTKLRMATGLRNIPSIQSRGLFGAI

AGFIEGGWTGMIDGWYGYHQQNGQGSGYAADQKSTQNAIDGITNKVNSVIEKMNTQFTAVGKEFNNLERR
IENLNKKVDDGFLDVWTYNAELLVLLENERTLDFHDSNVKNLYEKVRSQLRNNAKEIGNGCFEFYHKCDN
ACMESVRNGTYDYPKYSEESKLNREEIDGVKLESMRVYQILAIYSTVASSLVLSVSLGAISFWMCSNGSL
QCRICI
>gi|158426690|gb|ABW38010| /Swine/HA/H1N1/USA/1942/// hemagglutinin
[Influenza A virus (A/swine/Jamesburg/1942(H1N1))]
MKARLLVLLCAFAATNADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDSHNGKLCRLGGIAPLQLG
KCNIAGWLLGNPECDSLLTVSSWSYIVETSDSDNGTCYPGDFIDYEELREQLSSVSSFEKFEIFPKTSSW
PNHETTRGVTAACPYAGASSFYRNLLWLVKKENSYPKLSKSYVNNKGKEVLVLWGVHHPPTSTDQQSLYQ
NADAYVSVGSSKYYRRFTPEIAARPKVRGQAGRMNYYWTLLEPGDTITFEATGNLVAPRYAFALNRGSGS
GIITSNAPVHDCDTKCQTPHGAINSSLPFQNVHPVTIGECPKYVKSTKLRMVTGLRNIPSIQSRGLFGAI
AGFIEGGWTGMIDGWYGYHHQNGQGSGYAADQKSTQKAIDGITNKVNSVIEKMNTQFTAVGKEFNNLERR
IENLNKKVDDGFLDIWTYNAELLVLLENERTLDFHDSNVKNLYEKVRSQLRNNAKEIGNGCFEFYHKCDD
ACMESVRNGTYDYPKYSEESKLNREEIDGVKLESMMVYQILAIYSTVASSLVLLVSLGAISFWMCSNGSL
QCRICI
>gi|237511804|gb|ACQ99613| /Human/HA/H1N1/Mexico/2009/04/02/
hemagglutinin[Influenza A virus (A/Mexico/4108/2009(H1N1))]
MKAILVVLLYTFATANADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDKHNGKLCKLRGVAPLHLG
KCNIAGWILGNPECESLSTASSWSYIVETSSSDNGTCYPGDFIDYEELREQLSSVSSFERFEIFPKTSSW
PNHDSNKGVTAACPHAGAKSFYKNLIWLVKKGNSYPKLSKSYINDKGKEVLVLWGIHHPSTSADQQSLYQ
NADAYVFVGSSRYSKKFKPEIAIRPKVRDQEGRMNYYWTLVEPGDKITFEATGNLVVPRYAFAMERNAGS
GIIISDTPVHDCNTTCQTPKGAINTSLPFQNIHPITIGKCPKYVKSTKLRLATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMVDGWYGYHHQNEQGSGYAADLKSTQNAIDEITNKVNSVIEKMNTQFTAVGKEFNHLEKR
IENLNKKVDDGFLDIWTYNAELLILLENERTLDYHDSNVKNLYEKVRSQLKNNAKEIGNGCFEFYHKCDN
TCMESVKNGTYDYPKYSEEAKLNREEIDGVKLESTRIYQILAIYSTVASSLVLVVSLGAISFWMCSNGSL
QCRICI
>gi|237659618|gb|ACR09364| /Human/HA/H1N1/Mexico/2009/04/02/
hemagglutinin[Influenza A virus (A/Mexico/4108/2009(H1N1))]
MKAILVVLLYTFATANADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDKHNGKLCKLRGVAPLHLG
KCNIAGWILGNPECESLSTASSWSYIVETSSSDNGTCYPGDFIDYEELREQLSSVSSFERFEIFPKTSSW
PNHDSNKGVTAACPHAGAKSFYKNLIWLVKKGNSYPKLSKSYINDKGKEVLVLWGIHHPSTSADQQSLYQ
NADAYVFVGSSRYSKKFKPEIAIRPKVRDXEGRMNYYWTLVEPGDKITFEATGNLVVPRYAFAMERNAGS
GIIISDTPVHDCNTTCQTPKGAINTSLPFQNIHPITIGKCPKYVKSTKLRLATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMVDGWYGYHHQNEQGSGYAADLKSTQNAIDEITNKVNSVIEKMNTQFTAVGKEFNHLEKR
IENLNKKVDDGFLDIWTYNAELLILLENERTLDYHDSNVKNLYEKVRSQLKNNAKEIGNGCFEFYHKCDN
TCMESVKNGTYDYPKYSEEAKLNREEIDGVKLESTRIYQILAIYSTVASSLVLVVSLGAISFWMCSNGSL
QCRICI
>gi|237659634|gb|ACR09372| /Human/HA/H1N1/Mexico/2009/04/02/
hemagglutinin[Influenza A virus (A/Mexico/3955/2009(H1N1))]
MKAILVVLLYTFATANADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDKHNGKLCKLRGVAPLHLG
KCNIAGWILGNPECESXSTASSWSYIVETSSSDNGTCYPGDFIDYEELREQLSSVSSFERFEIFPKTSSW
PNHDSNKGVTAACPHAGAKSFYKNLIWLVKKGNSYPKLSKSYINDKGKEVLVLWGIHHPSTSADQQSLYQ
NADAYVFVGSSRYSKKFKPEIAIRPKVRGQEGRMNYYWTLVEPGDKITFEATGNLVVPRYAFAMERNAGS
GIIISDTPVHDCNTTCQTPKGAINTSLPFQNIHPITIGKCPKYVKSTKLRLATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMVDGWYGYHHQNEQGSGYAADLKSTQNAIDEITNKVNSVIEKMNTQFTAVGKEFNHLEKR
IENLNKKVDDGFLDIWTYNAELLILLENERTLDYHDSNVKNLYEKVRSQLKNNAKEIGNGCFEFYHKCDN
TCMESVKNGTYDYPKYSEEAKLNREEIDGVKLESTRIYQILAIYSTVASSLVLVVSLGAISFWMCSNGSL
QCRICI
>gi|237659640|gb|ACR09375| /Human/HA/H1N1/Mexico/2009/04/20/
hemagglutinin[Influenza A virus (A/Mexico/4635/2009(H1N1))]
MKAILVVLLYTFATANADTLCIGYHANNSTDTVDTVLEKNVTVTHSVNLLEDKHNGKLCKLRGVAPLHLG
KCNIAGWILGNPECESLSTASSWSYIVETSSSDNGTCYPGDFIDYEELREQLSSVSSFERFEIFPKTSSW
PNHDSNKGVTAACPHAGAKSFYKNLIWLVKKGNSYPKLSKSYINDKGKEVLVLWGIHHPSTSADQQSLYQ
NADAYVFVGSSRYSKKFKPEIAIRPKVRDQEGRMNYYWTLVEPGDKITFEATGNLVVPRYAFAMEKNAGS
GIIISDTPVHDCNTTCQTPKGAINTSLPFQNIHPITIGKCPKYVKSTKLRLATGLRNVPSIQSRGLFGAI
AGFIEGGWTGMVDGWYGYHHQNEQGSGYAADLKSTQNAIDEITNKVNSVIEKMNTQFTAVGKEFNHLEKR
IENLNKKVDDGFLDIWTYNAELLVLLENERTLDYHDSNVKNLYEKVRSQLKNNAKEIGNGCFEFYHKCDN
TCMESVKNGTYDYPKYSEEAKLNREEIDGVKLESTRIYQILAIYSTVASSLVLVVSLGAISFWMCSNGSL
QCRICI

>gi|408553|gb|AAA43345| /Avian/HA/H2N2/USA/1961/// hemagglutinin [Influenza A virus (A/mallard/MT/Y61 (H2N2))]
MAIIYLILLFTAVRGDQICIGYHSNNSTEKVDTILERNVTVTHAQNILEKTHNGKLCKLNGIPPLELGDC
SIAGWLLGNPECDRLLTVPEWSYIMEKENPRNGLCYPGSFNDYEELKHLLSSVTHFEKVKILPKDRWTQH
TTTGGSRACAVSGNPSFFRNMVWLTKKGSNYPIAKGSYNNTSGEQMLIIWGVHHPNDETEQRTLYQNVGT
YVSIGTSTLNKRSIPVIATRPKVNGQGGRMEFSWTILDIWDTINFESTGNLIAPEYGFRISKRGSSGIMK
TEGTLENCETKCQTPLGAINTTLPFHNVHPLTIGECPKYVKSERLVLATGLRNVPQIESRGLFGAIAGFI
EGGWQGMIDGWYGYHHSNDQGSGYAADKESTQKAIDGITNRVNSVIEKMNTQFEAVGKEFSNLEKRLENL
NKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDRVRMQLRDNAKELGNGCFEFYHKCDDECMN
SVKNGTYDYPKYEEESKLNRNEIKGVKLSNMGVYQILAIYATVAGSLSLAIMIAGISLWMCSNGSLQCRI
CI
>gi|408521|gb|AAA43243| /Avian/HA/H2N2/Hong Kong/1978/// hemagglutinin [Influenza A virus (A/duck/Hong Kong/273/78 (H2N2))]
MAIIYLILLLTVVKGDQICIGYHANNSTETVDTILERNVTVTHAKNILEKTHNGKLCKLNGIPPLELGDC
SIAGWLLGNPECDRLLSIPEWSYIMEKENPRNGLCYPGSFNDYEELKLLLSSVTHFEKVKILPRDRWTQH
TTTGGSRACAVSGNPSFFRNMVWLTTKGSNYPVAKGSYNNTNGEQILIIWGVHHPNDETEQRTLYQNVGT
YVSVGTSTLNKRSIPEIATRPKVNGQGGRMEFSWTLLDMWDTINFESTGNLIAPEYGFKISRRGNSGIMK
TEGTLENCETKCQTPLGAINTTLPFHNVHPLTIGECPKYVKSEKLVLATGLRNAHKMESRGLFGAIAGFI
EGGWQGMVDGWYGYHHSNDQGSGYAADKESTQKAVDGITNKVNSVIEKMNTQFEAVGKEFNNLERRLENL
NKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRMQLRDNAKEIGNGCFEFYHKCDDECMN
SVKNGTYDYPKYEEESRLNRNEIKGVKLSNMGVYQILAIYATVAGSLSLAIMMAGISFWMCSNGSLQCRI
CI
>gi|78097440|gb|ABB20229| /Avian/HA/H2N2/Hong Kong/1978/// hemagglutinin [Influenza A virus (A/duck/Hong Kong/319/1978(H2N2))]
MTIIYFILLLTVVKGDQICIGYHANNSTEKVDTILERNVTVTHAKDILEKTHNGKLCKLNGIPPLELGDC
SIAGWLLGNPECDRLLSVPEWSYIMEKENPRNGLCYPGSFNDYEELKHLLSSVTHFEKVKILPRDRWTQH
TTTGGSRACAVSGNPSFFRNMVWLTMKGSNYPVAKGSYNNTNGEQILIIWGIHHPNDETEQRTLYQNVGT
YVSVGTSTLNKRSTPEIATRPKVNGQGGRMEFSWTLLDMWDTINFESTGNLIAPEYGFKISKRGSSGIMK
TEGTLENCETKCQTPLGAINTTLPFHNVHPLTIGECPKYVKSEKLVLATGLRNVPQMESRGLFGAIAGFI
EGGWQGMVDGWYGYHHSNDQGSGYAADKESTQKAVDGITNKVNFVIEKMNTQFEAVGKEFNNLERRLENL
NKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRMQLRDNAKEIGNGCFEFYHKCDDECMN
SVRNGTYNYPKYEEESRLNRNEIKGVKLSSMGVYQILAIYATVAGSLSLAIIIAGISFWMCSNGSLQCRI
CI
>gi|408599|gb|AAA43576| /Avian/HA/H2N2/USA/1978/// hemagglutinin[Influenza A virus (A/mallard/New York/6750/1978(H2N2))]
MTITFLILLFTVVKGDQICIGYHANNSTEKVDTILERNVTVTHAKDILEKTHNGKLCRLSGIPPLELGDC
SIAGWLLGNPECDRLLSVPEWSYIVEKENPANGLCYPGNFNDYEELKHLLTRVTHFEKIKILPRDQWTQH
TTTGGSRACAVSGNPSFFRNMVWLTKKGSNYPVAKGSYNNTSGEQMLVIWGIHHPNDDTEQRTLYQNVGT
YVSVGTSTLNKRSIPEIATRPKVNGQGGRMEFSWTLLETWDVINFESTGNLIAPEYGFKISKRGSSGIMK
TEKTLENCETKCQTPLGAINTTLPFHNIHPLTIGECPKYVKSDRLVLATGLRNVPQIESRGLFGAIAGFI
EGGWQGMIDGWYGYHHSNDQGSGYAADKESTQKAIDGITNKVNSVIEKMNTQFEAVGKEFNNLERRLENL
NKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRMQLRDNAKEIGNGCFEFYHKCDDECMN
SVRNGTYDYPKYEEESKLNRNEIKGVKLSNMGVYQILAIYATVAGSLSLAIMIAGISFWMCSNGSLQCRI
CI
>gi|189230499|gb|ACD85231| /Human/HA/H2N2/China/1957/// hemagglutinin [Influenza A virus (A/Guiyang/1/1957(H2N2))]
IIYLILLFTAVRGDQICIGYHANNSTEKVDTILERNVTVTHAKDILEKTHNGKLCKLNGIPPLELGDCSI
AGWLLGNPECDRLLSVPEWSYIMEKENPRDGLCYPGSFNDYEELKHLLSSVTHFEKVKILPRDRWTQHTT
TGGSRACAVSGNPSFFRNMVWLTEKGSNYPVAKGSYNNTSGEQMLIIWGVHHPNDETEQRTLYQNVGTYV
SVGTSTLNKRSTPEIATRPKVNGLGSRMEFSWILLDMWDTINFESTGNLIAPEYGFKISKRGSSGIMKTE
GTLENCETKCQTPLGAINTTLPFHNVHPLTIGECPKYVKSEKLVLATGLRNVPQIESRGLFGAIAGFIEG
GWQGMVDGWYGYHHSNDQGSGYAADKESTQKAFDGITNKVNSVIEKMNIQFEAVGKEFSNLERRLENLNK
KMEDGFRDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRMQLRDNAKELGNGCFEFYHKCDDECMNSV
KNGTYDYPKYEEESKLNRNEIKGVKLSSMGVYQILAIYATVAGSLSLAIMMAGISFWMCSNGSLQCRICI
>gi|324146|gb|AAA43185| /Human/HA/H2N2/Japan/1957/// hemagglutinin precursor [Influenza A virus (A/Japan/305/1957(H2N2))]
MAIIYLILLFTAVRGDQICIGYHANNSTEKVDTNLERNVTVTHAKDILEKTHNGKLCKLNGIPPLELGDC
SIAGWLLGNPECDRLLSVPEWSYIMEKENPRDGLCYPGSFNDYEELKHLLSSVKHFEKVKILPKDRWTQH
TTTGGSRACAVSGNPSFFRNMVWLTKEGSDYPVAKGSYNNTSGEQMLIIWGVHHPIDETEQRTLYQNVGT

YVSVGTSTLNKRSTPEIATRPKVNGQGGRMEFSWTLLDMWDTINFESTGNLIAPEYGFKISKRGSSGIMK
TEGTLENCETKCQTPLGAINTTLPFHNVHPLTIGECPKYVKSEKLVLATGLRNVPQIESRGLFGAIAGFI
EGGWQGMVDGWYGYHHSNDQGSGYAADKESTQKAFDGITNKVNSVIEKMNTQFEAVGKEFGNLERRLENL
NKRMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRMQLRDNVKELGNGCFEFYHKCDDECMN
SVKNGTYDYPKYEEESKLNRNEIKGVKLSSMGVYQILAIYATVAGSLSLAIMMAGISFWMCSNGSLQCRI
CI
>gi|94481522|gb|ABF21270| /Human/HA/H2N2/Japan/1957///
hemagglutinin[Influenza A virus (A/Japan/305/1957(H2N2))]
MAIIYLILLFTAVRGDQICIGYHANNSTEMVDTILERNVTVTHAKDILEKTHNGKLCKLNGIPPLELGDC
SIAGWLLGNPECDRLLSVPEWSYIMEKENPRDGLCYPGSFNDYEELKHLLSSVKHFEKVKILPKDRWTQH
TTTGGSRACAVSGNPSFFRNMVWLTKKGSDYPVAKGSYNNTSGEQMLIIWGVHHPNDETEQRTLYQNVGT
YVSVGTSTLNKRSTPEIATRLKVNGQGGRMEFSWTLLDMWDTINFESTGNLIAPEYGFKISKRGSSGIMK
TEGTLENCETKCQTPLGAINTTLPFHNVHPLTIGECPKYVKSEKLVLATGLRNVPQIESRGLFGAIAGFI
EGGWQGMVDGWYGYHHSNDQGSGYAADKESTQKAFDGITNKVNSVIEKMNTQFEAVGKEFSNLERRLENL
NKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRMQLRDNVKELGNGCFEFYHKCDDECMN
SVKTGTYDYPKYEEESKLNRNEIKGVKLSSMGVYQILAIYATVAGSLSLAIMMAGISFWMCSNGSLQCRI
CI
>gi|26453383|gb|BAC43764| /Human/HA/H2N2/Japan/1957/// hemagglutinin
[Influenza A virus (A/Kayano/57(H2N2))]
MAIIYLILLFTAVRGDQICIGYHANNSTEKVDTILERNVTVTHAKNILEKTHNGKLCKLNGIPPLELGDC
SIAGWLLGNPECDRLLIVPEWSYIMEKENPRDGLCYPGSFNDYEELKHLLSSVKHFEKVKILPKDRWTQH
TTTGGSRACAVSGNPSFFRNMVWLTKKGSNYPVAKGSYNNTSGEQMLIIWGVHHPIDETEQITLYQNVGT
YVSVGTSTLNKRSTPEIATRPKVNGLGSRMEFSWTLLDMWDTINFESTGNLIAPEYGFKISKRGSSGIMK
TEGTLENCETKCQTPLGAINTTLPFHNVHPLTIGECPKYVKSEKLVLATGLRNVPQIESRGLFGAIAGFI
EGGWQGMVDGWYGYHHSNDQGSGYAADKESTQKAFDGITNKVNSVIEKMNTQFEAVGKEFSNLERRLENL
NKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRMQLRDNVKELGNGCFEFYHKCDDECMN
SVKNGTYDYPKYEEESKLNRNEIKGVKLSSMGVYQILAIYATVAGSLSLAIMMAGISFWMCSNGSLQFRI
CI

>gi|82654665|gb|ABB88256| /Avian/HA/H3N2/Hong Kong/1975///
hemagglutinin[Influenza A virus (A/duck/Hong Kong/7/1975(H3N2))]
MKTIIALSYIFCLAFGQDLPRNDNSTATLCLGHHAVPNGTIVKTITDDQIEVTNATELVQSSSTGKICNN
PHKILDGRDCTLIDALLGDPHCDVFQDETWDLFVERGNAFSSCYPYDVPDYASLRSLVASSGTLEFITEG
FTWTGVTQNGGSSACKRGPASGFFSRLNWLTKSGSTYPVLNVTMPNNDNFDKLYIWGVHHPSTNQEQTNL
YVQASGRVTVSTRRSQQTIIPNIGSRPWVRGQSGRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCVSECITPNGSIPNDKPFQNVNKITYGACPKYVKQNSLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINGKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSYNAELLVALENQHTIDLTDSEMNKLFEKTRRQLRENAEDMGNGCFKIYHKCD
NACIESIRNGTYDHDIYRDEALNNRFQIKGVELKSGYKDWILWISFAISCFLLCVVLLGFIMWACQRGNI
RCNICI
>gi|98991137|gb|ABF60581| /Avian/HA/H3N2/Canada/1976/// hemagglutinin
[Influenza A virus (A/duck/Alberta/78/1976(H3N2))]
MKTIIVLSYFFCLALSQDYSESNNSTATLCLGHHAVPNGTIVKTITDDQIEVTNATELVQSSSTGKICNN
PHRILDGRDCTLIDALLGDPHCDVFQDETWDLYVERSSAFSNCYPYDVPDYDSLRSLVASSGTLEFITEG
FTWTGVTQNGGSNACKRGPASGFFSRLNWLTKSGSTYPVLNVTMPNNDNFDKLYVWGVHHPSTNQEQTNL
YVQASGRVTVSTRRSQQTIIPNIGSRPWVRGQSGRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCISECITPNGSIPNDMPFQNVNKITYGACPKYVKQGTLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINGKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSDNAELLVALENQHTIDLTDSEMNKLFEKTRRQLRENAEVMGNGCFKIYHKCD
NACIESIRNGTYDHDIYRDEALNNRFQIKGVELKSGYKDWILWISFAISCFLLCVVLLGFIMWACQRGNI
RCNICI
>gi|82652543|gb|ABB87377| /Avian/HA/H3N2/Canada/1976/08/13/
hemagglutinin[Influenza A virus (A/pintail duck/ALB/86/1976(H3N2))]
MKTIIVLSYFFCLALSQDYSESNNSTATLCLGHHAVPNGTIVKTITDDQIEVTNATELVQSSSTGKICNN
PHRILDGRDCTLIDALLGDPHCDVFQDETWDLYVERSSAFSNCYPYDVPDYASLRSLVASSGTLEFITEG
FTWTGVTQNGGSNACKRGPASGFFSRLNWLTKSGSTYPVLNVTMPNNDNFDKLYVWGVHHPSTNQEQTNL
YVQASGRVTVSTRRSQQTIIPNIGSRPWVRGQSGRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCISECITPNGSIPNDKPFQNVNKITYGACPKYVKQGTLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINGKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSYNAELLVALENQHTIDLTDSEMNKLFEKTRRQLRENAEDMGNGCFKIYHKCD

NACIESIRNGTYDHDIYRDEALNNRFQIKGVELKSGYKDWILWISFAISCFLLCVVLLGFIMWACQRGNI
RCNICI
>gi|60757|gb|CAA24271| /Avian/HA/H3N8/Ukraine/1963/// unnamed protein
product [Influenza A virus (A/duck/Ukraine/1963(H3N8))]
MKTVIALSYILCLTFGQDLPGNDNSTATLCLGHHAVPNGTIVKTITDDQIEVTNATELVQSSSTGKICNN
PHRILDGRACTLIDALLGDPHCDVFQNETWDLFVERSNAFSNCYPYDIPDYASLRSLVASSGTLEFITEG
FTWTGVTQNGGSSACKRGPANGFFSRLNWLTKSESAYPVLNVTMPNNDNFDKLYIWGVHHPSTNQEQTNL
YVQASGRVTVSTRRSQQTIIPNIGSRPWVRGQPGRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCISECITPNGSIPNDKPFQNVNKITYGACPKYVKQNTLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINRKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSYNAELLVALENQHTIDLADSEMNKLFEKTRRQLRENAEDMGNGCFKIYHKCD
NACIESIRNGTYDHDIYRDEALNNRFQIKGVELKSGYKDWILWISFAISCLLLCVVLLGFIMWACQRGNI
RCNICI

>gi|118420992|gb|BAF37221| /Human/HA/H3N2/Japan/1968/// hemagglutinin
[Influenza A virus (A/Aichi/2/1968(H3N2))]
MKTIIALSYIFCLAIGQDLPGNDNSTATLCLGHHAVPNGTLVKTITDDQIEVTNATELVQSSSTGKICNN
PHRILDGIDCTLIDALLGDPHCDVFQNETWDLFVERSKAFSNCYPYDVPDYASLRSLVASSGTLEFITEG
FTWTGVTQNGGSNACKRGPSSGFFSRLNWLTKSGSTYPVLNVTMPNNDNFDKLYIWGVHHPSTNQEQTSL
YVQASGRVTVSTRRSQQTIIPNIGSRPWVGGLSSRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCISECITPNGSIPNDKPFQNVNKITYGACPKYVKQNTLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINGKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSYNAELLVALENQHTIDLTDSEMNKLFEKTRRQLRENAEDMGNGCFKIYHKCD
NACIESIRNGTYDHDVYRDEALNNRFQIKGVELKSGYKDWILWISFAISCFLLCVVLLGFIMWACQRGNI
RCNICI
>gi|126567435|gb|BAF48361| /Human/HA/H3N2/Japan/1968/// haemagglutinin
[Influenza A virus (A/Aichi/2/1968(H3N2))]
MKTIIALSYIFCLALGQDLPGNDNSTATLCLGHHAVPNGTLVKTITDDQIEVTNATELVQSSSTGKICNN
PHRILDGIDCTLIDALLGDPHCDVFQNETWDLFVERSKAFSNCYPYDVPDYASLRSLVASSGTLEFITEG
FTWTGVTQNGGSNACKRGPGSGFFSRLNWLTKSGSTYPVLNVTMPNNDNFDKLYIWGVHHPSTNQEQTSL
YVQASGRVTVSTRRSQQTIIPNIESRPWVRGLSSRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCISECITPNGSIPNDKPFQNVNKITYGACPKYVKQNTLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINGKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSYNAELLVALENQHTIDLTDSEMNKLFEKTRRQLRENAEDMGNGCFKIYHKCD
NACIESIRNGTYDHDVYRDEALNNRFQIKGVELKSGYKDWILWISFAISCFLLCVVLLGFIMWACQRGNI
RCNICI
>gi|14009692|gb|AAK51718| /Human/HA/H3N2/Hong Kong/1968///
hemagglutinin[Influenza A virus (A/Hong Kong/1/1968(H3N2))]
MKTIIALSYIFCLALGQDLPGNDNSTATLCLGHHAVPNGTLVKTITDDQIEVTNATELVQSSSTGKICNN
PHRILDGIDCTLIDALLGDPHCDVFQNETWDLFVERSKAFSNCYPYDVPDYASLRSLVASSGTLEFITEG
FTWTGVTQNGGSNACKRGPGSGFFSRLNWLTKSGSTYPVLNVTMPNNDNFDKLYIWGVHHPSTNQEQTSL
YVQASGRVTVSTRRSQQTIIPNIGSRPWVRGLSSRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCISECITPNGSIPNDKPFQNVNKITYGACPKYVKQNTLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINGKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSYNAELLVALENQHTIDLTDSEMNKLFEKTRRQLRENAEDMGNGCFKIYHKCD
NACIESIRNGTYDHDVYRDEALNNRFQIKGVELKSGYKDWILWISFAISCFLLCVVLLGFIMWACQRGNI
RCNICI
>gi|80977928|gb|ABB54514| /Human/HA/H3N2/USA/1968/// hemagglutinin
[Influenza A virus (A/Memphis/1/68(H3N2))]
MKTIIALSYIFCLALGQDLPGNDNSTATLCLGHHAVPNGTLVKTITDDQIEVTNATELVQSSSTGKICNN
PHRILDGINCTLIDALLGDPHCDVFQDETWDLFVERSKAFSNCYPYDVPDYASLRSLVASSGTLEFITEG
FTWTGVTQNGGSNACKRGPGSGFFSRLNWLTKSGSTYPVLNVTMPNNDNFDKLYIWGVHHPSTNQEQTSL
YVQASGRVTVSTRRSQQTIIPNIGSRPWVRGLSSRISIYWTIVKPGDVLVINSNGNLIAPRGYFKMRTGK
SSIMRSDAPIDTCISECITPNGSIPNDKPFQNVNKITYGACPKYVKQNTLKLATGMRNVPEKQTRGLFGA
IAGFIENGWEGMIDGWYGFRHQNSEGTGQAADLKSTQAAIDQINGKLNRVIEKTNEKFHQIEKEFSEVEG
RIQDLEKYVEDTKIDLWSYNAELLVALENQHTIDLTDSEMNKLFEKTRRQLRENAEDMGNGCFKIYHKCD
NACIESIRNGTYDHDVYRDEALNNRFQIKGVELKSGYKDWILWISFAISCFLLCVVLLGFIMWACQRGNI
RCNICI

>gi|4240448|gb|AAD13572| /Avian/HA/H5N1/USA/1981/// hemagglutinin H5
[Influenza A virus (A/duck/Minnesota/1525/81(H5N1))]
MERIVIALAIISVVKGDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILEKEHNGKLCSLKGVRPLILKD
CSVAGWLLGNPMCDEFLNVPEWSYIVEKDNPVNGLCYPGDFNDYEELKHLMSSTNHFEKIQIIPRSSWSN
HDASSGVSSACPYNGRSSFFRNVVWLIKKNNAYPTIKRTYNNTNMEDLLILWGIHHPNDAAEQTKLYQNS
NTYVSVGTSTLNQRSIPEIATRPKVNGQSGRMEFFWTILRPNDAISFESNGNFIAPEYAYKIVKKGDSAM
MKSELEYGNCNTKCQTPVGAINSSMPFHNVHPLTIGECPKYVKSDKLVLATGLRNVPQRETRGLFGAIAG
FIEGGWQGMVDGWYGYHHSNRQGSGYAADKESTQKAIDGITNKVNSIIDKMNTQFEAVGKEFNNLERRIE
NLNKKMEDGFIDVWTYNAELLVLMENERTLDFHDSNVRNLYDKVRLQLRDNAKELGNGCFEFYHKCDNEC
MESVRNGTYDYPQYSEESRLNREEIDGVKLESMGTYQILSIYSTVASSLALAIMVAGLSFWMCSNGSLQC
RICI
>gi|6048757|gb|AAF02306| /Avian/HA/H5N1/Hong Kong/1997/// hemagglutinin
[Influenza A virus (A/Duck/Hong Kong/p46/97 (H5N1))]
VKMEKIVLLLATVSLVKSDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILERTHNGKLCDLNGVKPLIL
RDCSVAGWLLGNPMCDEFINVPEWSYIVEKASPANDLCYPGNFNDYEELKHLLSRINHFEKIQIIPKSSW
SNHDASSGVSSACPYLGRSSFFRNVVWLIKKNSAYPTIKRSYNNTNQEDLLVLWGIHHPNDAAEQTKLYQ
NPTTYISVGTSTLNQRLVPEIATRPKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGDS
TIMKSELEYGNCNTKCQTPMGAINSSMPFHNIHPLTIGECPKYVKSNRLVLATGLRNTPQRERRRKKRGL
FGAIAGFIEGGWQGMVDGWYGYHHSNEQGSGYAADKESTQKAIDGVTNKVNSIINKMNTQFEAVGREFNN
LERRIENLNKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRLQLRDNAKELGNGCFEFYH
KCDNECMESVKNGTYDYPQYSEEARLNREEISGVKLESMGTYQILSIYSTVASSLALAIMVAGLSLWMCS
NGSLQCRICI
>gi|47156281|gb|AAT12028| /Avian/HA/H5N1/China/1999///
hemagglutinin[Influenza A virus (A/duck/Guangxi/07/1999(H5N1))]
MEKIVLLLAIVSLVESDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILEKTHNGKLCNLNGVKPLILRD
CSVAGWLLGNPMCDEFINVPEWSYIVEKASPANDLCYPGDLNDYEELKHLLSSTNHFEKIQIIPKNSWSN
HDASSGVSSACPYHGRSSFFRNVVWLTKKNSAYPTIKRSYNNTNPEDLLILWGIHHPNDAAEQTKLYQNP
TTYVSVGTSTLNQRLVPEIATRPKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGDSAI
MKSELEYSNCNTKCQTPIGAINSSMPFHNIHPLTIGECPKYVKSNRLVLATGLRNTPQREKRRKKRGLFG
AIAGFIEGGWQGMVDGWYGYHHSNEQGSGYAADKESTQKAIDGVTNKVNSIIDKMNTQFEAVGREFNNLE
RRIENLNKKMEDGFLDVWTYNAELLVLMENERTLYFHDSNVKDLYDKVRLQLRDNAKELGNGCFEFYHKC
DNECMESVRNGTYDYPQYSEEARLNREEISGVKLESMGTYQILSIYSTVASSLALAIMVAGLSLWMCSNG
SLQCRICI
>gi|47156297|gb|AAT12036| /Avian/HA/H5N1/China/2000///
hemagglutinin[Influenza A virus (A/duck/Zhejiang/11/2000(H5N1))]
MEKIVLLLAIVSLVKSDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILEKTHNGKLCDLNGVKPLILRD
CSVAGWLLGNPMCDEFTNVPEWSYIVEKANPANDLCYPGDFNDYEELKHLLSRINHFEKIQIIPKSSWSN
HDASSGVSSACPYHGRSSFFRNVVWLIKKNSTYPTIKRSYNNTNQEDLLVLWGIHHPNDAAEQTKLYQNP
TTYISVGTSTLNQRLVPEIATRPKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGDSAI
MKSELEYGNCNTKCQTPMGAINSSMPFHNIHPLTIGECPKYVKSNRLVLATGLRNTPQRERRRKKRGLFG
AIAGFIEGGWQGMVDGWYGYHHSNEQGSGYAADKESTQKAIDGVTNKVNSIIDKMNTQFEAVGREFNNLE
RRIESLNKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRLQLRDNAKELGNGCFEFYHKC
DNECMESVKNGTYDYPQYSEEARLNREEISGVKLESMGTYQILSIYSTVASSLALAIMVAGLSLWMCSNG
SLQCRICI
>gi|2865380|gb|AAC40508| /Human/HA/H5N1/Hong Kong/1997/// hemagglutinin
[Influenza A virus (A/Hong Kong/156/97(H5N1))]
MERTVLLLATVSLVKSDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILERTHNGKLCDLNGVKPLILRD
CSVAGWLLGNPMCDEFINVPEWSYIVEKASPANDLCYPGNFNDYEELKHLLSRINHFEKIQIIPKSSWSN
HDASSGVSSACPYLGRSSFFRNVVWLIKKNSAYPTIKRSYNNTNQEDLLVLWGVHHPNDAAEQTKLYQNP
TTYISVGTSTLNQRLVPEIATRPKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGDSTI
MKSELEYGNCNTKCQTPMGAINSSMPFHNIHPLTIGECPKYVKSNRLVLATGLRNTPQRERRRKKRGLFG
AIAGFIEGGWQGMVDGWYGYHHSNEQGSCYSADKESTQKAIDGVTNKVNSIINKMNTQFEAVGREFNNLE
RRIENLNKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRLQLRDNAKELGNGCFEFYHKC
DNECMESVKNGTYDYPQYSEEARLNREEISGVKLESMGTYQILSIYSTVASSLALAIMVAGLSLWMCSNG
SLQCRICI
>gi|45453834|gb|AAS65618| /Human/HA/H5N1/Thailand/2004/// hemagglutinin
[Influenza A virus (A/Thailand/2(SP-33)/2004(H5N1))]
MEKIVLLFAIVSLVKSDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILEKTHNGKLCDLDGVKPLILRD
CSVAGWLLGNPMCDEFINVPEWSYIVEKANPVNDLCYPGDFNDYEELKHLLSRINHFEKIQIIPKSSWSS
HEVSLGVSSACPYQGKSSFFRNVVWLIKKNSTYPTIKRSYNNTNQEDLLVLWGIHHPNDAAEQTKLYQNP

TTYISVGTSTLNQRLVPRIATRSKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGDSTI
MKSELEYGNCNTKCQTPMGAINSSMPFHNIHPLTIGECPKYVKSNRLVLATGLRNSPQRERRRKKRGLFG
AIAGFIEGGWQGMVDGWYGYHHSNEQGSGYAAAKESTQKAIDGVTNKVNSIIDKMNTQFEAVGREFNNLE
RRIENLNKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRLQLKDNAKELGNGCFEFYHKC
DNECMESVRNGTYDYPQYSEEARLKREEISGVKLESIGIYQILSIYSTVASSLALAIMVAGLSLWMCSNG
SLQCRICI
>gi|50296051|gb|AAT73273| /Human/HA/H5N1/Viet Nam/2004/// hemagglutinin
[Influenza A virus (A/Viet Nam/1194/2004(H5N1))]
MEKIVLLFAIVSLVKSDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILEKTHNGKLCDLDGVKPLILRD
CSVAGWLLGNPMCDEFINVPEWSYIVEKANPVNDLCYPGDFNDYEELKHLLSRINHFEKIQIIPKSSWSS
HEASLGVSSACPYQGKSSFFRNVVWLIKKNSTYPTIKRSYNNTNQEDLLVLWGIHHPNDAAEQTKLYQNP
TTYISVGTSTLNQRLVPRIATRSKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGDSTI
MKSELEYGNCNTKCQTPMGAINSSMPFHNIHPLTIGECPKYVKSNRLVLATGLRNSPQRERRRKKRGLFG
AIAGFIEGGWQGMVDGWYGYHHSNEQGSGYAADKESTQKAIDGVTNKVNSIIDKMNTQFEAVGREFNNLE
RRIENLNKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRLQLRDNAKELGNGCFEFYHKC
DNECMESVRNGTYDYPQYSEEARLKREEISGVKLESIGIYQILSIYSTVASSLALAIMVAGLSLWMCSNG
SLQCR
>gi|159144903|gb|ABW90126| /Human/HA/H5N1/Viet Nam/2004/// hemagglutinin
[Influenza A virus (A/Viet Nam/1203/2004(H5N1))]
MEKIVLLFAIVSLVKSDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILEKKHNGKLCDLDGVKPLILRD
CSVAGWLLGNPMCDEFINVPEWSYIVEKANPVNDLCYPGDFNDYEELKHLLSRINHFEKIQIIPKSSWSS
HEASLGVSSACPYQGKSSFFRNVVWLIKKNSTYPTIKGSYNNTNQEDLLVLWGIHHPNDAAEQTKLYQNP
TTYISVGTSTLNQRLVPRIATRSKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGDSTI
MKSELEYGNCNTKCQTPMGAINSSMPFHNIHPLTIGECPKYVKSNRLVLATGLRNSPQRETRGLFGAIAG
FIEGGWQGMVDGWYGYHHSNEQGSGYAADKESTQKAIDGVTNKVNSIIDKMNTQFEAVGREFNNLERRIE
NLNKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRLQLRDNAKELGNGCFEFYHKCDNEC
MESVRNGTYDYPQYSEEARLKREEISGVKLESIGIYQILSIYSTVASSLALAIMVAGLSLWMCSNGSLQC
RICI
>gi|11596242|gb|AAG38534| /Avian/HA/H5N3/Malaysia/1997/// hemagglutinin
[Influenza A virus (A/duck/Malaysia/F119-3/97(H5N3))]
MEKIVLLLAIVSLVKSDQICIGYHANNSTEQVDTIMEKNVTVTHAQDILEKTHNGKLCSLNGVKPLILRD
CSVAGWLLGNPMCDEFLNVPEWSYIVEKDNPVNGLCYPGDFNDYEELKHLLSSTNHFEKIRIIPRSSWSN
HDASSGVSSACPYNGRSSFFRNVVWLIKKNNAYPTIKRSYNNTNQEDLLILWGIHHPNDAAEQTKLYQNP
TTYVSVGTSTLNQRSVPEIATRPKVNGQSGRMEFFWTILKPNDAINFESNGNFIAPEYAYKIVKKGGSAI
MKSGLEYGNCNTKCQTPMGAINSSMPFHNIHPLTIGECPKYVKSGRLVLATGLRNVPQRETRGLFGAIAG
FIEGGWQGMVDGWYGYHHSNEQGSGYAADKESTQKAIDGITNKVNSIIDKMNTQFEAVGKEFNNLERRIE
NLNKKMEDGFLDVWTYNAELLVLMENERTLDFHDSNVKNLYDKVRLQLRDNAKELGNGCFEFYHKCDNEC
MESVKNGTYDYPQYSEEARLNREEISGVKLESMGIYQILSIYSTVASSLALAIMIAGLSFWMCSNGSLQC
RICI

Lampiran 4. Hasil Mutiple Alignment

```
                ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                    5          15         25         35         45         55
gi|4585161    --ADTICVGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCSLNGI APLQLGKCNV
gi|221300|    --ADTICVGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCSLNGI APLQLGKCNV
gi|4585169    --ADTICVGY HANNSTDTVD TVLEKNVTVT HSVNLLENSH NGKLCSLNGI APLQLGKCNV
gi|1135311    --ADTICIGY HANNSTDTVD TVLEKNVTVT HSVNLLENSH NGKLCSLNGI APLQLGKCNV
gi|4325018    --ADTICIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCKLKGI APLQLGKCNI
gi|4325020    --ADTICIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCKLKGI APLQLGKCNI
gi|4325039    --ADTICIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCKLKGI APLQLGKCNI
gi|8977932    --ADTICIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCRLKGI APLQLGKCNI
gi|1571684    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCRLGGI APLQLGKCNI
gi|8994138    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCRLGGI APLQLGKCNI
gi|1585252    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCRLGGI APLQLGKCNI
gi|1584266    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDSH NGKLCRLGGI APLQLGKCNI
gi|2375118    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDKH NGKLCKLRGV APLHLGKCNI
gi|2376596    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDKH NGKLCKLRGV APLHLGKCNI
gi|2376596    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDKH NGKLCKLRGV APLHLGKCNI
gi|2376596    --ADTLCIGY HANNSTDTVD TVLEKNVTVT HSVNLLEDKH NGKLCKLRGV APLHLGKCNI
gi|408553|    --GDQICIGY HSNNSTEKVD TILERNVTVT HAQNILEKTH NGKLCKLNGI PPLELGDCSI
gi|408521|    --GDQICIGY HANNSTETVD TILERNVTVT HAKNILEKTH NGKLCKLNGI PPLELGDCSI
gi|7809744    --GDQICIGY HANNSTEKVD TILERNVTVT HAKDILEKTH NGKLCKLNGI PPLELGDCSI
gi|408599|    --GDQICIGY HANNSTEKVD TILERNVTVT HAKDILEKTH NGKLCRLSGI PPLELGDCSI
gi|1892304    --GDQICIGY HANNSTEKVD TILERNVTVT HAKDILEKTH NGKLCKLNGI PPLELGDCSI
gi|324146|    --GDQICIGY HANNSTEKVD TNLERNVTVT HAKDILEKTH NGKLCKLNGI PPLELGDCSI
gi|9448152    --GDQICIGY HANNSTEMVD TILERNVTVT HAKDILEKTH NGKLCKLNGI PPLELGDCSI
gi|2645338    --GDQICIGY HANNSTEKVD TILERNVTVT HAKNILEKTH NGKLCKLNGI PPLELGDCSI
gi|8265466    NSTATLCLGH HAVPNGTIVK TITDDQIEVT NATELVQSSS TGKICN-NPH KILDGRDCTL
gi|9899113    NSTATLCLGH HAVPNGTIVK TITDDQIEVT NATELVQSSS TGKICN-NPH RILDGRDCTL
gi|8265254    NSTATLCLGH HAVPNGTIVK TITDDQIEVT NATELVQSSS TGKICN-NPH RILDGRDCTL
gi|60757|g    NSTATLCLGH HAVPNGTIVK TITDDQIEVT NATELVQSSS TGKICN-NPH RILDGRACTL
gi|1184209    NSTATLCLGH HAVPNGTLVK TITDDQIEVT NATELVQSSS TGKICN-NPH RILDGIDCTL
gi|1265674    NSTATLCLGH HAVPNGTLVK TITDDQIEVT NATELVQSSS TGKICN-NPH RILDGIDCTL
gi|1400969    NSTATLCLGH HAVPNGTLVK TITDDQIEVT NATELVQSSS TGKICN-NPH RILDGIDCTL
gi|8097792    NSTATLCLGH HAVPNGTLVK TITDDQIEVT NATELVQSSS TGKICN-NPH RILDGINCTL
gi|4240448    --GDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILEKEH NGKLCSLKGV RPLILKDCSV
gi|6048757    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILERTH NGKLCDLNGV KPLILRDCSV
gi|4715628    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILEKTH NGKLCNLNGV KPLILRDCSV
gi|4715629    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILEKTH NGKLCDLNGV KPLILRDCSV
gi|2865380    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILERTH NGKLCDLNGV KPLILRDCSV
gi|4545383    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILEKTH NGKLCDLDGV KPLILRDCSV
gi|5029605    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILEKTH NGKLCDLDGV KPLILRDCSV
gi|1591449    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILEKKH NGKLCDLDGV KPLILRDCSV
gi|1159624    --SDQICIGY HANNSTEQVD TIMEKNVTVT HAQDILEKTH NGKLCSLNGV KPLILRDCSV
Clustal Co      :*:*: *:  .   *. *  : :: ** :: ::::    .**:*       *    *.:

                ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                   65         75         85         95        105        115
gi|4585161    AGWLLGNPEC DLLLTANSWS YIIETSNSEN GTCYPGEFID YEELREQLSS VSSFEKFEIF
gi|221300|    AGWLLGNPEC DLLLTANSWS YIIETSNSEN GTCYPGEFID YEELREQLSS ISSFEKFEIF
gi|4585169    AGWILGNPEC DLLLTANSWS YIIETSNSEN GTCYPGEFID YEELREQLSS VSSFEKFEIF
gi|1135311    AGWLLGNPEC DLLLTASSWS YIIETSNSEN GTCYPGEFID YEELREQLSS VSSFEKFEIF
gi|4325018    AGWLLGNPEC DLLLTASSWS YIVETSNSEN GTCYPGDFID YEELREQLSS VSSFEKFEIF
gi|4325020    AGWLLGNPEC DLLLTASSWS YIVETSNSEN GTCYPGDFID YEELREQLSS VSSFEKFEIF
gi|4325039    AGWLLGNPEC DLLLTASSWS YIVETSNSEN GTCYPGDFID YEELREQLSS VSSFEKFEIF
gi|8977932    AGWLLGNPEC DPLLPVRSWS YIVETPNSEN GICYPGDFID YEELREQLSS VSSFERFEIF
gi|1571684    AGWLLGNPEC DLLLTVSSWS YIVETSNSDN GTCYPGDFID YEELREQLSS VSSFEKFEIF
gi|8994138    AGWLLGNPEC DLLLTVSSWS YIVETSNSDN GTCYPGDFID YEELREQLSS VSSFEKFEIF
gi|1585252    AGWLLGNPEC DLLLTVSSWS YIVETSNSDN GTCYPGDFID YEELREQLSS VSSFERFEIF
gi|1584266    AGWLLGNPEC DSLLTVSSWS YIVETSDSDN GTCYPGDFID YEELREQLSS VSSFEKFEIF
gi|2375118    AGWILGNPEC ESLSTASSWS YIVETSSSDN GTCYPGDFID YEELREQLSS VSSFERFEIF

gi|2376596    AGWILGNPEC ESLSTASSWS YIVETSSSDN GTCYPGDFID YEELREQLSS VSSFERFEIF
gi|2376596    AGWILGNPEC ESXSTASSWS YIVETSSSDN GTCYPGDFID YEELREQLSS VSSFERFEIF
```

```
gi|2376596   AGWILGNPEC ESLSTASSWS YIVETSSSDN GTCYPGDFID YEELREQLSS VSSFERFEIF
gi|408553|   AGWLLGNPEC DRLLTVPEWS YIMEKENPRN GLCYPGSFND YEELKHLLSS VTHFEKVKIL
gi|408521|   AGWLLGNPEC DRLLSIPEWS YIMEKENPRN GLCYPGSFND YEELKLLLSS VTHFEKVKIL
gi|7809744   AGWLLGNPEC DRLLSVPEWS YIMEKENPRN GLCYPGSFND YEELKHLLSS VTHFEKVKIL
gi|408599|   AGWLLGNPEC DRLLSVPEWS YIVEKENPAN GLCYPGNFND YEELKHLLTR VTHFEKIKIL
gi|1892304   AGWLLGNPEC DRLLSVPEWS YIMEKENPRD GLCYPGSFND YEELKHLLSS VTHFEKVKIL
gi|324146|   AGWLLGNPEC DRLLSVPEWS YIMEKENPRD GLCYPGSFND YEELKHLLSS VKHFEKVKIL
gi|9448152   AGWLLGNPEC DRLLSVPEWS YIMEKENPRD GLCYPGSFND YEELKHLLSS VKHFEKVKIL
gi|2645338   AGWLLGNPEC DRLLIVPEWS YIMEKENPRD GLCYPGSFND YEELKHLLSS VKHFEKVKIL
gi|8265466   IDALLGDPHC DVFQD-ETWD LFVERGNAFS -SCYPYDVPD YASLRSLVAS SG---TLEFI
gi|9899113   IDALLGDPHC DVFQD-ETWD LYVERSSAFS -NCYPYDVPD YDSLRSLVAS SG---TLEFI
gi|8265254   IDALLGDPHC DVFQD-ETWD LYVERSSAFS -NCYPYDVPD YASLRSLVAS SG---TLEFI
gi|60757|g   IDALLGDPHC DVFQN-ETWD LFVERSNAFS -NCYPYDIPD YASLRSLVAS SG---TLEFI
gi|1184209   IDALLGDPHC DVFQN-ETWD LFVERSKAFS -NCYPYDVPD YASLRSLVAS SG---TLEFI
gi|1265674   IDALLGDPHC DVFQN-ETWD LFVERSKAFS -NCYPYDVPD YASLRSLVAS SG---TLEFI
gi|1400969   IDALLGDPHC DVFQN-ETWD LFVERSKAFS -NCYPYDVPD YASLRSLVAS SG---TLEFI
gi|8097792   IDALLGDPHC DVFQD-ETWD LFVERSKAFS -NCYPYDVPD YASLRSLVAS SG---TLEFI
gi|4240448   AGWLLGNPMC DEFLNVPEWS YIVEKDNPVN GLCYPGDFND YEELKHLMSS TNHFEKIQII
gi|6048757   AGWLLGNPMC DEFINVPEWS YIVEKASPAN DLCYPGNFND YEELKHLLSR INHFEKIQII
gi|4715628   AGWLLGNPMC DEFINVPEWS YIVEKASPAN DLCYPGDLND YEELKHLLSS TNHFEKIQII
gi|4715629   AGWLLGNPMC DEFTNVPEWS YIVEKANPAN DLCYPGDFND YEELKHLLSR INHFEKIQII
gi|2865380   AGWLLGNPMC DEFINVPEWS YIVEKASPAN DLCYPGNFND YEELKHLLSR INHFEKIQII
gi|4545383   AGWLLGNPMC DEFINVPEWS YIVEKANPVN DLCYPGDFND YEELKHLLSR INHFEKIQII
gi|5029605   AGWLLGNPMC DEFINVPEWS YIVEKANPVN DLCYPGDFND YEELKHLLSR INHFEKIQII
gi|1591449   AGWLLGNPMC DEFINVPEWS YIVEKANPVN DLCYPGDFND YEELKHLLSR INHFEKIQII
gi|1159624   AGWLLGNPMC DEFLNVPEWS YIVEKDNPVN GLCYPGDFND YEELKHLLSS TNHFEKIRII
Clustal Co    . :**:* * :      *.   :*  .. .   *** .. * * .*:  ::        .::

             ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
               125        135        145        155        165        175
gi|4585161   PKASSWPNHE TTKGVTAACS YSGASSFYRN LLWITKKGTS YPKLSKSYTN NKGKEVLVLW
gi|221300|   PKASSWPNHE TTKGVTAACS YSGASSFYRN LLWITKKGTS YPKLSKSYTN NKGKEVLVLW
gi|4585169   PKASSWPNHE TTKGVTAACS YSGASSFYRN LLWITKKGTS YPKLSKSYTN NKGKEVLVIW
gi|1135311   PKASSWPNHE TTKGVTAACS YSGASSFYRN LLWITEKGTS YPKLSKSYTN NKGKEVLVLW
gi|4325018   PKTSSWPNHE TTKGVTAACS YAGASSFYRN LLWLTKKGSS YPKLSKSYVN NKGKEVLVLW
gi|4325020   PKTSSWPNHE TTKGVTAACS YAGASSFYRN LLWLTKKGSS YPKLSKSYVN NKGKEVLVLW
gi|4325039   PKTSSWPNHE TTKGVTAACS YAGASSFYRN LLWLTKKGSS YPKLSKSYVN NKGKEVLVLW
gi|8977932   PKESSWPNHN TN-GVTAACS HEGKSSFYRN LLWLTEKEGS YPKLKNSYVN KKGKEVLVLW
gi|1571684   PKTSSWPNHE TTRGVTAACP YAGASSFYRN LLWLVKKENS YPKLSKSYVN NKGKEVLVLW
gi|8994138   PKTSSWPNHE TTRGVTAACP YAGASSFYRN LLWLVKKENS YPKLSKSYVN NKGKEVLVLW
gi|1585252   PKTSSWPNHE TTXGVTAACP YAGANSFYRN LLWLVKKGDS YPKLSKSYVN NKGKEVLVLW
gi|1584266   PKTSSWPNHE TTRGVTAACP YAGASSFYRN LLWLVKKENS YPKLSKSYVN NKGKEVLVLW
gi|2375118   PKTSSWPNHD SNKGVTAACP HAGAKSFYKN LIWLVKKGNS YPKLSKSYIN DKGKEVLVLW
gi|2376596   PKTSSWPNHD SNKGVTAACP HAGAKSFYKN LIWLVKKGNS YPKLSKSYIN DKGKEVLVLW
gi|2376596   PKTSSWPNHD SNKGVTAACP HAGAKSFYKN LIWLVKKGNS YPKLSKSYIN DKGKEVLVLW
gi|2376596   PKTSSWPNHD SNKGVTAACP HAGAKSFYKN LIWLVKKGNS YPKLSKSYIN DKGKEVLVLW
gi|408553|   PK-DRWTQHT TTGG-SRACA VSGNPSFFRN MVWLTKKGSN YPIAKGSYNN TSGEQMLIIW
gi|408521|   PR-DRWTQHT TTGG-SRACA VSGNPSFFRN MVWLTTKGSN YPVAKGSYNN TNGEQILIIW
gi|7809744   PR-DRWTQHT TTGG-SRACA VSGNPSFFRN MVWLTMKGSN YPVAKGSYNN TNGEQILIIW
gi|408599|   PR-DQWTQHT TTGG-SRACA VSGNPSFFRN MVWLTKKGSN YPVAKGSYNN TSGEQMLVIW
gi|1892304   PR-DRWTQHT TTGG-SRACA VSGNPSFFRN MVWLTEKGSN YPVAKGSYNN TSGEQMLIIW
gi|324146|   PK-DRWTQHT TTGG-SRACA VSGNPSFFRN MVWLTKEGSD YPVAKGSYNN TSGEQMLIIW
gi|9448152   PK-DRWTQHT TTGG-SRACA VSGNPSFFRN MVWLTKKGSD YPVAKGSYNN TSGEQMLIIW
gi|2645338   PK-DRWTQHT TTGG-SRACA VSGNPSFFRN MVWLTKKGSN YPVAKGSYNN TSGEQMLIIW
gi|8265466   TEGFTWTGVT QNGG-SSACK RGPASGFFSR LNWLTKSGST YPVLNVTMPN NDNFDKLYIW
gi|9899113   TEGFTWTGVT QNGG-SNACK RGPASGFFSR LNWLTKSGST YPVLNVTMPN NDNFDKLYVW
gi|8265254   TEGFTWTGVT QNGG-SNACK RGPASGFFSR LNWLTKSGST YPVLNVTMPN NDNFDKLYVW
gi|60757|g   TEGFTWTGVT QNGG-SSACK RGPANGFFSR LNWLTKSESA YPVLNVTMPN NDNFDKLYIW
gi|1184209   TEGFTWTGVT QNGG-SNACK RGPSSGFFSR LNWLTKSGST YPVLNVTMPN NDNFDKLYIW
gi|1265674   TEGFTWTGVT QNGG-SNACK RGPGSGFFSR LNWLTKSGST YPVLNVTMPN NDNFDKLYIW
gi|1400969   TEGFTWTGVT QNGG-SNACK RGPGSGFFSR LNWLTKSGST YPVLNVTMPN NDNFDKLYIW
gi|8097792   TEGFTWTGVT QNGG-SNACK RGPGSGFFSR LNWLTKSGST YPVLNVTMPN NDNFDKLYIW
gi|4240448   PR-SSWSNHD ASSGVSSACP YNGRSSFFRN VVWLIKKNNA YPTIKRTYNN TNMEDLLILW
gi|6048757   PK-SSWSNHD ASSGVSSACP YLGRSSFFRN VVWLIKKNSA YPTIKRSYNN TNQEDLLVLW
gi|4715628   PK-NSWSNHD ASSGVSSACP YHGRSSFFRN VVWLTKKNSA YPTIKRSYNN TNPEDLLILW
gi|4715629   PK-SSWSNHD ASSGVSSACP YHGRSSFFRN VVWLIKKNST YPTIKRSYNN TNQEDLLVLW
gi|2865380   PK-SSWSNHD ASSGVSSACP YLGRSSFFRN VVWLIKKNSA YPTIKRSYNN TNQEDLLVLW
gi|4545383   PK-SSWSSHE VSLGVSSACP YQGKSSFFRN VVWLIKKNST YPTIKRSYNN TNQEDLLVLW
```

```
gi|5029605   PK-SSWSSHE ASLGVSSACP YQGKSSFFRN VVWLIKKNST YPTIKRSYNN TNQEDLLVLW
gi|1591449   PK-SSWSSHE ASLGVSSACP YQGKSSFFRN VVWLIKKNST YPTIKGSYNN TNQEDLLVLW
gi|1159624   PR-SSWSNHD ASSGVSSACP YNGRSSFFRN VVWLIKKNNA YPTIKRSYNN TNQEDLLILW
Clustal Co   ..   *.     . * : **       .*: . : *:  .    **  . :  *  .  : * :*

                ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                   185        195        205        215        225        235
gi|4585161   GVHHPPSVSE QQSLYQNADA YVSVGSSKYN RRFAPEIAAR PKVRGQAGRM NYYWTLLDQG
gi|221300|   GVHHPPSVSE QQSLYQNADA YVSVGSSKYN RRFAPEIAAR PEVRGQAGRM NYYWTLLDQG
gi|4585169   GVHHPPTADE QQSLYQNADA YVSVGSSKYN RRFTPEIAAR PKVRGQAGRM NYYWTLLDQG
gi|1135311   GVHHPPTTNE QQSLYQNADA YVSVGSSKYN RRFTPEIAAR PKVRGQAGRM NYYWTLLDQG
gi|4325018   GVHHPPTGTD QQSLYQNADA YVSVGSSKYN RRFTPEIAAR PKVRDQAGRM NYYWTLLEPG
gi|4325020   GVHHPPTGTD QQSLYQNADA YVSVGSSKYN RRFTPEIAAR PKVRGQAGRM NYYWTLLEPG
gi|4325039   GVHHPPTGTD QQSLYQNADA YVSVGSSKYN RRFTPEIAAR PKVRDQAGRM NYYWTLLEPG
gi|8977932   GIHHPPNSKE QQNLYQNENA YVSVVTSNYN RRFTPEIAER PKVRDQAGRM NYYWTLLKPG
gi|1571684   GVHHPPTSTD QQSLYQNADA YVSVGSSKYD RRFTPEIAAR PKVRGQAGRM NYYWTLLEPG
gi|8994138   GVHHPPTSTD QQSLYQNADA YVSVGSSKYD RRFTPEIAAR PKVRGQAGRM NYYWTLLEPG
gi|1585252   GVHHPPTSTX QQSLYQNADA YVSVGSSKYN RRFTPEIAAR PKVRGQAGRM NYYWTLLEPG
gi|1584266   GVHHPPTSTD QQSLYQNADA YVSVGSSKYY RRFTPEIAAR PKVRGQAGRM NYYWTLLEPG
gi|2375118   GIHHPSTSAD QQSLYQNADA YVFVGSSRYS KKFKPEIAIR PKVRDQEGRM NYYWTLVEPG
gi|2376596   GIHHPSTSAD QQSLYQNADA YVFVGSSRYS KKFKPEIAIR PKVRDXEGRM NYYWTLVEPG
gi|2376596   GIHHPSTSAD QQSLYQNADA YVFVGSSRYS KKFKPEIAIR PKVRGQEGRM NYYWTLVEPG
gi|2376596   GIHHPSTSAD QQSLYQNADA YVFVGSSRYS KKFKPEIAIR PKVRDQEGRM NYYWTLVEPG
gi|408553|   GVHHPNDETE QRTLYQNVGT YVSIGTSTLN KRSIPVIATR PKVNGQGGRM EFSWTILDIW
gi|408521|   GVHHPNDETE QRTLYQNVGT YVSVGTSTLN KRSIPEIATR PKVNGQGGRM EFSWTLLDMW
gi|7809744   GIHHPNDETE QRTLYQNVGT YVSVGTSTLN KRSTPEIATR PKVNGQGGRM EFSWTLLDMW
gi|408599|   GIHHPNDDTE QRTLYQNVGT YVSVGTSTLN KRSIPEIATR PKVNGQGGRM EFSWTLLETW
gi|1892304   GVHHPNDETE QRTLYQNVGT YVSVGTSTLN KRSTPEIATR PKVNGLGSRM EFSWILLDMW
gi|324146|   GVHHPIDETE QRTLYQNVGT YVSVGTSTLN KRSTPEIATR PKVNGQGGRM EFSWTLLDMW
gi|9448152   GVHHPNDETE QRTLYQNVGT YVSVGTSTLN KRSTPEIATR LKVNGQGGRM EFSWTLLDMW
gi|2645338   GVHHPIDETE QITLYQNVGT YVSVGTSTLN KRSTPEIATR PKVNGLGSRM EFSWTLLDMW
gi|8265466   GVHHPSTNQE QTNLYVQASG RVTVSTRRSQ QTIIPNIGSR PWVRGQSGRI SIYWTIVKPG
gi|9899113   GVHHPSTNQE QTNLYVQASG RVTVSTRRSQ QTIIPNIGSR PWVRGQSGRI SIYWTIVKPG
gi|8265254   GVHHPSTNQE QTNLYVQASG RVTVSTRRSQ QTIIPNIGSR PWVRGQSGRI SIYWTIVKPG
gi|60757|g   GVHHPSTNQE QTNLYVQASG RVTVSTRRSQ QTIIPNIGSR PWVRGQPGRI SIYWTIVKPG
gi|1184209   GVHHPSTNQE QTSLYVQASG RVTVSTRRSQ QTIIPNIGSR PWVGGLSSRI SIYWTIVKPG

gi|1265674   GVHHPSTNQE QTSLYVQASG RVTVSTRRSQ QTIIPNIESR PWVRGLSSRI SIYWTIVKPG
gi|1400969   GVHHPSTNQE QTSLYVQASG RVTVSTRRSQ QTIIPNIGSR PWVRGLSSRI SIYWTIVKPG
gi|8097792   GVHHPSTNQE QTSLYVQASG RVTVSTRRSQ QTIIPNIGSR PWVRGLSSRI SIYWTIVKPG
gi|4240448   GIHHPNDAAE QTKLYQNSNT YVSVGTSTLN QRSIPEIATR PKVNGQSGRM EFFWTILRPN
gi|6048757   GIHHPNDAAE QTKLYQNPTT YISVGTSTLN QRLVPEIATR PKVNGQSGRM EFFWTILKPN
gi|4715628   GIHHPNDAAE QTKLYQNPTT YVSVGTSTLN QRLVPEIATR PKVNGQSGRM EFFWTILKPN
gi|4715629   GIHHPNDAAE QTKLYQNPTT YISVGTSTLN QRLVPEIATR PKVNGQSGRM EFFWTILKPN
gi|2865380   GVHHPNDAAE QTKLYQNPTT YISVGTSTLN QRLVPEIATR PKVNGQSGRM EFFWTILKPN
gi|4545383   GIHHPNDAAE QTKLYQNPTT YISVGTSTLN QRLVPRIATR SKVNGQSGRM EFFWTILKPN
gi|5029605   GIHHPNDAAE QTKLYQNPTT YISVGTSTLN QRLVPRIATR SKVNGQSGRM EFFWTILKPN
gi|1591449   GIHHPNDAAE QTKLYQNPTT YISVGTSTLN QRLVPRIATR SKVNGQSGRM EFFWTILKPN
gi|1159624   GIHHPNDAAE QTKLYQNPTT YVSVGTSTLN QRSVPEIATR PKVNGQSGRM EFFWTILKPN
Clustal Co   *:***     * .** :    : : :    :   * *  *   *  .*: .  * ::

                ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                   245        255        265        275        285        295
gi|4585161   DTITFEATGN LIAPWYAFAL NKGSDSGIIT SDAPVHNCDT RCQTPHGALN SSLPFQNVHP
gi|221300|   DTITFEATGN LIAPWYAFAL NKGSDSGIIT SDAPVHNCDT RCQTPHGALN SSLPFQNVHP
gi|4585169   DTITFEATGN LIAPWYAFAL NKDSGSGIIT SDAPVHNCDT KCQTPRGALN SSLPFQNIHP
gi|1135311   DTITFEATGN LIAPWYAFAL NKGSDSGIIT SDAPVHNCDT KCQTPHGALN SSLPFQNVHP
gi|4325018   DTITFEATGN LIAPWYAFAL NRGSGSGIIT SDAPVHDCNT KCQTPHGAIN SSLPFQNIHP
gi|4325020   DTITFEATGN LIAPWYAFAL NRGSGSGIIT SDAPVHDCNT KCQTPHGAIN SSLPFQNIHP
gi|4325039   DTITFEATGN LIAPWYAFAL NRGSGSGIIT SDAPVHDCNT KCQTPHGAIN SSLPFQNIHP
gi|8977932   DTIIFEANGN LIAPMYAFAL SRGFGSGIIT SNASMHECNT KCQTPLGAIN SSLPYQNIHP
gi|1571684   DTITFEATGN LVAPRYAFAL NRGSESGIIT SDAPVHDCDT KCQTPHGAIN SSLPFQNIHP
gi|8994138   DTITFEATGN LVAPRYAFAL NRGSESGIIT SDAPVHDCDT KCQTPHGAIN SSLPFQNIHP
gi|1585252   DTITFEATGN LVAPRYAFAL NKGSGSGVIT SDAPVHDCDT KCQTPHGAIN SSLPFQNIHP
gi|1584266   DTITFEATGN LVAPRYAFAL NRGSGSGIIT SNAPVHDCDT KCQTPHGAIN SSLPFQNVHP
gi|2375118   DKITFEATGN LVVPRYAFAM ERNAGSGIII SDTPVHDCNT TCQTPKGAIN TSLPFQNIHP
gi|2376596   DKITFEATGN LVVPRYAFAM ERNAGSGIII SDTPVHDCNT TCQTPKGAIN TSLPFQNIHP
gi|2376596   DKITFEATGN LVVPRYAFAM ERNAGSGIII SDTPVHDCNT TCQTPKGAIN TSLPFQNIHP
```

```
gi|2376596   DKITFEATGN LVVPRYAFAM EKNAGSGIII SDTPVHDCNT TCQTPKGAIN TSLPFQNIHP
gi|408553|   DTINFESTGN LIAPEYGFRI SKRGSSGIMK TEGTLENCET KCQTPLGAIN TTLPFHNVHP
gi|408521|   DTINFESTGN LIAPEYGFKI SRRGNSGIMK TEGTLENCET KCQTPLGAIN TTLPFHNVHP
gi|7809744   DTINFESTGN LIAPEYGFKI SKRGSSGIMK TEGTLENCET KCQTPLGAIN TTLPFHNVHP
gi|408599|   DVINFESTGN LIAPEYGFKI SKRGSSGIMK TEKTLENCET KCQTPLGAIN TTLPFHNIHP
gi|1892304   DTINFESTGN LIAPEYGFKI SKRGSSGIMK TEGTLENCET KCQTPLGAIN TTLPFHNVHP
gi|324146|   DTINFESTGN LIAPEYGFKI SKRGSSGIMK TEGTLENCET KCQTPLGAIN TTLPFHNVHP
gi|9448152   DTINFESTGN LIAPEYGFKI SKRGSSGIMK TEGTLENCET KCQTPLGAIN TTLPFHNVHP
gi|2645338   DTINFESTGN LIAPEYGFKI SKRGSSGIMK TEGTLENCET KCQTPLGAIN TTLPFHNVHP
gi|8265466   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCVS ECITPNGSIP NDKPFQNVNK
gi|9899113   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCIS ECITPNGSIP NDMPFQNVNK
gi|8265254   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCIS ECITPNGSIP NDKPFQNVNK
gi|60757|g   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCIS ECITPNGSIP NDKPFQNVNK
gi|1184209   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCIS ECITPNGSIP NDKPFQNVNK
gi|1265674   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCIS ECITPNGSIP NDKPFQNVNK
gi|1400969   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCIS ECITPNGSIP NDKPFQNVNK
gi|8097792   DVLVINSNGN LIAPRGYFKM R-TGKSSIMR SDAPIDTCIS ECITPNGSIP NDKPFQNVNK
gi|4240448   DAISFESNGN FIAPEYAYKI VKKGDSAMMK SELEYGNCNT KCQTPVGAIN SSMPFHNVHP
gi|6048757   DAINFESNGN FIAPEYAYKI VKKGDSTIMK SELEYGNCNT KCQTPMGAIN SSMPFHNIHP
gi|4715628   DAINFESNGN FIAPEYAYKI VKKGDSAIMK SELEYSNCNT KCQTPIGAIN SSMPFHNIHP
gi|4715629   DAINFESNGN FIAPEYAYKI VKKGDSAIMK SELEYGNCNT KCQTPMGAIN SSMPFHNIHP
gi|2865380   DAINFESNGN FIAPEYAYKI VKKGDSTIMK SELEYGNCNT KCQTPMGAIN SSMPFHNIHP
gi|4545383   DAINFESNGN FIAPEYAYKI VKKGDSTIMK SELEYGNCNT KCQTPMGAIN SSMPFHNIHP
gi|5029605   DAINFESNGN FIAPEYAYKI VKKGDSTIMK SELEYGNCNT KCQTPMGAIN SSMPFHNIHP
gi|1591449   DAINFESNGN FIAPEYAYKI VKKGDSTIMK SELEYGNCNT KCQTPMGAIN SSMPFHNIHP
gi|1159624   DAINFESNGN FIAPEYAYKI VKKGGSAIMK SGLEYGNCNT KCQTPMGAIN SSMPFHNIHP
Clustal Co   * : :::.** ::.*   : :      * ::  :     * :  * ** *::  .  *::*::

             ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                305        315        325        335        345        355
gi|4585161   ITIGECPKYV KSTKLRMATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|221300|   ITIGECPKYV KSTKLRMATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|4585169   ITIGECPKYV KSTKLRMATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|1135311   ITIGECPKYV KSTKLRMATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|4325018   VTIGECPKYV RSTKLRMATG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|4325020   VTIGECPKYV RSTKLRMATG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|4325039   VTIGECPKYV RSTKLRMATG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|8977932   VTIGECPKYV RSAKLRMVTG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|1571684   VTIGECPKYV KSTKLRMVTG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG LIDGWYGYHH
gi|8994138   VTIGECPKYV KSTKLRMVTG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG LIDGWYGYHH
gi|1585252   VTIGECPKYV KSTKLRMATG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHQ
gi|1584266   VTIGECPKYV KSTKLRMVTG LRNIPSIQ-- --SRGLFGAI AGFIEGGWTG MIDGWYGYHH
gi|2375118   ITIGKCPKYV KSTKLRLATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MVDGWYGYHH
gi|2376596   ITIGKCPKYV KSTKLRLATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MVDGWYGYHH
gi|2376596   ITIGKCPKYV KSTKLRLATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MVDGWYGYHH
gi|2376596   ITIGKCPKYV KSTKLRLATG LRNVPSIQ-- --SRGLFGAI AGFIEGGWTG MVDGWYGYHH
gi|408553|   LTIGECPKYV KSERLVLATG LRNVPQIE-- --SRGLFGAI AGFIEGGWQG MIDGWYGYHH
gi|408521|   LTIGECPKYV KSEKLVLATG LRNAHKME-- --SRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|7809744   LTIGECPKYV KSEKLVLATG LRNVPQME-- --SRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|408599|   LTIGECPKYV KSDRLVLATG LRNVPQIE-- --SRGLFGAI AGFIEGGWQG MIDGWYGYHH
gi|1892304   LTIGECPKYV KSEKLVLATG LRNVPQIE-- --SRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|324146|   LTIGECPKYV KSEKLVLATG LRNVPQIE-- --SRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|9448152   LTIGECPKYV KSEKLVLATG LRNVPQIE-- --SRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|2645338   LTIGECPKYV KSEKLVLATG LRNVPQIE-- --SRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|8265466   ITYGACPKYV KQNSLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|9899113   ITYGACPKYV KQGTLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|8265254   ITYGACPKYV KQGTLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|60757|g   ITYGACPKYV KQNTLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|1184209   ITYGACPKYV KQNTLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|1265674   ITYGACPKYV KQNTLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|1400969   ITYGACPKYV KQNTLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|8097792   ITYGACPKYV KQNTLKLATG MRNVPEKQ-- --TRGLFGAI AGFIENGWEG MIDGWYGFRH
gi|4240448   LTIGECPKYV KSDKLVLATG LRNVPQRE-- --TRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|6048757   LTIGECPKYV KSNRLVLATG LRNTPQRERR RKKRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|4715628   LTIGECPKYV KSNRLVLATG LRNTPQREKR RKKRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|4715629   LTIGECPKYV KSNRLVLATG LRNTPQRERR RKKRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|2865380   LTIGECPKYV KSNRLVLATG LRNTPQRERR RKKRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|4545383   LTIGECPKYV KSNRLVLATG LRNSPQRERR RKKRGLFGAI AGFIEGGWQG MVDGWYGYHH
```

```
gi|5029605   LTIGECPKYV KSNRLVLATG LRNSPQRERR RKKRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|1591449   LTIGECPKYV KSNRLVLATG LRNSPQRE-- --TRGLFGAI AGFIEGGWQG MVDGWYGYHH
gi|1159624   LTIGECPKYV KSGRLVLATG LRNVPQRE-- --TRGLFGAI AGFIEGGWQG MVDGWYGYHH
Clustal Co   :* * ***** :.  * :.** :**  . :     .******* *****.** * ::*****:::

                ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                   365        375        385        395        405        415
gi|4585161   QNEQGSGYAA DQKSTQNAID GITSKVNSVI EKMNTQFTAV GKEFNNLERR IENLNKKVDD
gi|221300|   QNEQGSGYAA DQKSTQNAID GITSKVNSVI EKMNTQFTAV GKEFNNLERR IENLNKKVDD
gi|4585169   QNEQGSGYAA DQKSTQNAID GITNKVNSVI EKMNTQFTAV GKEFNNLERR IENLNKKVDD
gi|1135311   QNEQGSGYAA DQKSTQSAID GITNKVNSVI EKMNTQFTAV GKEFNNLERR IENLNKKVDD
gi|4325018   QNEQGSGYAA DQKSTQNAID GITNKVNSVI EKMNTQ---- ---------- ----------
gi|4325020   QNEQGSGYAA DQKSTQNAID GITNKVNSVI EKMNTQ---- ---------- ----------
gi|4325039   QNEQGSGYAA DQKSTQNAID GITNKVNSVI EKMNTQFTAV GKEFNNLERR IENLNKKVDD
gi|8977932   QNEQGSGYAA DQKSTQNAIN GITNKVNTVI EKMNIQFTAV GKEFNKLEKR MENLNKKVDD
gi|1571684   QNGQGSGYAA DQKSTQNAID GITNKVNSVI EKMNTQFTVV GKEFNNLERR IKNLNKKVDD
gi|8994138   QNGQGSGYAA DQKSTQNAID GITNKVNSVI EKMNTQFTVV GKEFNNLERR MKNLNKKVDD
gi|1585252   QNGQGSGYAA DQKSTQNAID GITNKVNSVI EKMNTQFTAV GKEFNNLERR IENLNKKVDD
gi|1584266   QNGQGSGYAA DQKSTQKAID GITNKVNSVI EKMNTQFTAV GKEFNNLERR IENLNKKVDD
gi|2375118   QNEQGSGYAA DLKSTQNAID EITNKVNSVI EKMNTQFTAV GKEFNHLEKR IENLNKKVDD
gi|2376596   QNEQGSGYAA DLKSTQNAID EITNKVNSVI EKMNTQFTAV GKEFNHLEKR IENLNKKVDD
gi|2376596   QNEQGSGYAA DLKSTQNAID EITNKVNSVI EKMNTQFTAV GKEFNHLEKR IENLNKKVDD
gi|2376596   QNEQGSGYAA DLKSTQNAID EITNKVNSVI EKMNTQFTAV GKEFNHLEKR IENLNKKVDD
gi|408553|   SNDQGSGYAA DKESTQKAID GITNRVNSVI EKMNTQFEAV GKEFSNLEKR LENLNKKMED
gi|408521|   SNDQGSGYAA DKESTQKAVD GITNKVNSVI EKMNTQFEAV GKEFNNLERR LENLNKKMED
gi|7809744   SNDQGSGYAA DKESTQKAVD GITNKVNFVI EKMNTQFEAV GKEFNNLERR LENLNKKMED
gi|408599|   SNDQGSGYAA DKESTQKAID GITNKVNSVI EKMNTQFEAV GKEFNNLERR LENLNKKMED
gi|1892304   SNDQGSGYAA DKESTQKAFD GITNKVNSVI EKMNIQFEAV GKEFSNLERR LENLNKKMED
gi|324146|   SNDQGSGYAA DKESTQKAFD GITNKVNSVI EKMNTQFEAV GKEFGNLERR LENLNKRMED
gi|9448152   SNDQGSGYAA DKESTQKAFD GITNKVNSVI EKMNTQFEAV GKEFSNLERR LENLNKKMED
gi|2645338   SNDQGSGYAA DKESTQKAFD GITNKVNSVI EKMNTQFEAV GKEFSNLERR LENLNKKMED
gi|8265466   QNSEGTGQAA DLKSTQAAID QINGKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|9899113   QNSEGTGQAA DLKSTQAAID QINGKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|8265254   QNSEGTGQAA DLKSTQAAID QINGKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|60757|g   QNSEGTGQAA DLKSTQAAID QINRKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|1184209   QNSEGTGQAA DLKSTQAAID QINGKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|1265674   QNSEGTGQAA DLKSTQAAID QINGKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|1400969   QNSEGTGQAA DLKSTQAAID QINGKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|8097792   QNSEGTGQAA DLKSTQAAID QINGKLNRVI EKTNEKFHQI EKEFSEVEGR IQDLEKYVED
gi|4240448   SNRQGSGYAA DKESTQKAID GITNKVNSII DKMNTQFEAV GKEFNNLERR IENLNKKMED
gi|6048757   SNEQGSGYAA DKESTQKAID GVTNKVNSII NKMNTQFEAV GREFNNLERR IENLNKKMED
gi|4715628   SNEQGSGYAA DKESTQKAID GVTNKVNSII DKMNTQFEAV GREFNNLERR IENLNKKMED
gi|4715629   SNEQGSGYAA DKESTQKAID GVTNKVNSII DKMNTQFEAV GREFNNLERR IESLNKKMED
gi|2865380   SNEQGSCYSA DKESTQKAID GVTNKVNSII NKMNTQFEAV GREFNNLERR IENLNKKMED
gi|4545383   SNEQGSGYAA AKESTQKAID GVTNKVNSII DKMNTQFEAV GREFNNLERR IENLNKKMED
gi|5029605   SNEQGSGYAA DKESTQKAID GVTNKVNSII DKMNTQFEAV GREFNNLERR IENLNKKMED
gi|1591449   SNEQGSGYAA DKESTQKAID GVTNKVNSII DKMNTQFEAV GREFNNLERR IENLNKKMED
gi|1159624   SNEQGSGYAA DKESTQKAID GITNKVNSII DKMNTQFEAV GKEFNNLERR IENLNKKMED
Clustal Co   .* :*:  :*   :*** *.:  :. ::* :* :* * :

                ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                   425        435        445        455        465        475
gi|4585161   GFLDVWTYNA ELLVLLENER TLDFHDSNVR NLYEKVKSQL RNNAKEIGNG CFEFYHKCDD
gi|221300|   GFLDVWTYNA ELLVLLENER TLDFHDSNVR NLYEKVKSQL RNNAKEIGNG CFEFYHKCDD
gi|4585169   GFLDVWTYNA ELLVLLENER TLDFHDSNVR NLYEKVKSQL RNNAKEIGNG CFEFYHKCDD
gi|1135311   GFLNVWTYNA ELLVLLENER TLDFHDSNVR NLYEKVKSQL RNNAKEIGNG CFEFYHKCDD
gi|4325018   ---------- ---------- ---------- ---------- ---------- ----------
gi|4325020   ---------- ---------- ---------- ---------- ---------- ----------
gi|4325039   GFLDIWTYNA ELLVLLENER TLDFHDSNVR NLYEKVKSQL KNNAKEIGNG CFEFYHKCDD
gi|8977932   GFLDIWTYNA ELLVLLENER TLDFHDSNVK NLYEKVKSQL KNNAKEIGNG CFEFYHKCDN
gi|1571684   GFLDVWTYNA ELLVLLENER TLDFHDSNVK NLYEKARSQL RNNAKEIGNG CFEFYHKCDD
gi|8994138   GFLDVWTYNA EXLVLLENER TLDFHDSNVK NLYEKARSQL RNNAKEIGNG CFEFYHKCDD
gi|1585252   GFLDVWTYNA ELLVLLENER TLDFHDSNVK NLYEKVRSQL RNNAKEIGNG CFEFYHKCDN
gi|1584266   GFLDIWTYNA ELLVLLENER TLDFHDSNVK NLYEKVRSQL RNNAKEIGNG CFEFYHKCDD
gi|2375118   GFLDIWTYNA ELLILLENER TLDYHDSNVK NLYEKVRSQL KNNAKEIGNG CFEFYHKCDN
gi|2376596   GFLDIWTYNA ELLILLENER TLDYHDSNVK NLYEKVRSQL KNNAKEIGNG CFEFYHKCDN
gi|2376596   GFLDIWTYNA ELLILLENER TLDYHDSNVK NLYEKVRSQL KNNAKEIGNG CFEFYHKCDN
gi|2376596   GFLDIWTYNA ELLVLLENER TLDYHDSNVK NLYEKVRSQL KNNAKEIGNG CFEFYHKCDN
```

```
gi|408553|   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDRVRMQL RDNAKELGNG CFEFYHKCDD
gi|408521|   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRMQL RDNAKEIGNG CFEFYHKCDD
gi|7809744   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRMQL RDNAKEIGNG CFEFYHKCDD
gi|408599|   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRMQL RDNAKEIGNG CFEFYHKCDD
gi|1892304   GFRDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRMQL RDNAKELGNG CFEFYHKCDD
gi|324146|   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRMQL RDNVKELGNG CFEFYHKCDD
gi|9448152   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRMQL RDNVKELGNG CFEFYHKCDD
gi|2645338   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRMQL RDNVKELGNG CFEFYHKCDD
gi|8265466   TKIDLWSYNA ELLVALENQH TIDLTDSEMN KLFEKTRRQL RENAEDMGNG CFKIYHKCDN
gi|9899113   TKIDLWSDNA ELLVALENQH TIDLTDSEMN KLFEKTRRQL RENAEVMGNG CFKIYHKCDN
gi|8265254   TKIDLWSYNA ELLVALENQH TIDLTDSEMN KLFEKTRRQL RENAEDMGNG CFKIYHKCDN
gi|60757|g   TKIDLWSYNA ELLVALENQH TIDLADSEMN KLFEKTRRQL RENAEDMGNG CFKIYHKCDN
gi|1184209   TKIDLWSYNA ELLVALENQH TIDLTDSEMN KLFEKTRRQL RENAEDMGNG CFKIYHKCDN
gi|1265674   TKIDLWSYNA ELLVALENQH TIDLTDSEMN KLFEKTRRQL RENAEDMGNG CFKIYHKCDN
gi|1400969   TKIDLWSYNA ELLVALENQH TIDLTDSEMN KLFEKTRRQL RENAEDMGNG CFKIYHKCDN
gi|8097792   TKIDLWSYNA ELLVALENQH TIDLTDSEMN KLFEKTRRQL RENAEDMGNG CFKIYHKCDN
gi|4240448   GFIDVWTYNA ELLVLMENER TLDFHDSNVR NLYDKVRLQL RDNAKELGNG CFEFYHKCDN
gi|6048757   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRLQL RDNAKELGNG CFEFYHKCDN
gi|4715628   GFLDVWTYNA ELLVLMENER TLYFHDSNVK DLYDKVRLQL RDNAKELGNG CFEFYHKCDN
gi|4715629   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRLQL RDNAKELGNG CFEFYHKCDN
gi|2865380   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRLQL RDNAKELGNG CFEFYHKCDN
gi|4545383   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRLQL KDNAKELGNG CFEFYHKCDN
gi|5029605   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRLQL RDNAKELGNG CFEFYHKCDN
gi|1591449   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRLQL RDNAKELGNG CFEFYHKCDN
gi|1159624   GFLDVWTYNA ELLVLMENER TLDFHDSNVK NLYDKVRLQL RDNAKELGNG CFEFYHKCDN
Clustal Co

             ....|....| ....|....| ....|....| ....|....| ....|....| ....|....|
                485        495        505        515        525        535
gi|4585161   ECMESVKNGT YDYPKYSEES KLNREEIDGV KLESMGVYQI LAIYSTVASS LVLLVSLGAI
gi|221300|   ECMESVKNGT YDYPKYSEES KLNREEIDGV KLESMGVYQI LAIYSTVASS LVLLVSWGAI
gi|4585169   ECMESVKNGT YDYPKYSEES KLNREEIDGV KLESMGVYQI LAIYSTVASS LVLLVSLGAI
gi|1135311   ECMESVKNGT YDYPKYSEES KLNREEIDGV KLESMGVYQI LAIYSTVASS LVLLVSLGAI
gi|4325018   ---------- ---------- ---------- ---------- ---------- ----------
gi|4325020   ---------- ---------- ---------- ---------- ---------- ----------
gi|4325039   ACMESVRNGT YDYPKYSEES KLNREEIDGV KLESMGVYQI LAIYSTVASS LVLLVSLGAI
gi|8977932   ECMESVRNGT YDYPKYSEES KLNREKVDGV KLESMGIYQI LAIYSTVASS LVLLVSLGAI
gi|1571684   ACMESVRNGT YDYPKYSEES KLNREEIDGV KLESMMVYQI LAIYSTVASS LVLLVSLGAI
gi|8994138   ACMESVRNGT YDYPKYSEES KLNREEIDGV KLESMMVYQI LAIYSTVASS LVLLVSLGAI
gi|1585252   ACMESVRNGT YDYPKYSEES KLNREEIDGV KLESMRVYQI LAIYSTVASS LVLSVSLGAI
gi|1584266   ACMESVRNGT YDYPKYSEES KLNREEIDGV KLESMMVYQI LAIYSTVASS LVLLVSLGAI
gi|2375118   TCMESVKNGT YDYPKYSEEA KLNREEIDGV KLESTRIYQI LAIYSTVASS LVLVVSLGAI
gi|2376596   TCMESVKNGT YDYPKYSEEA KLNREEIDGV KLESTRIYQI LAIYSTVASS LVLVVSLGAI
gi|2376596   TCMESVKNGT YDYPKYSEEA KLNREEIDGV KLESTRIYQI LAIYSTVASS LVLVVSLGAI
gi|2376596   TCMESVKNGT YDYPKYSEEA KLNREEIDGV KLESTRIYQI LAIYSTVASS LVLVVSLGAI
gi|408553|   ECMNSVKNGT YDYPKYEEES KLNRNEIKGV KLSNMGVYQI LAIYATVAGS LSLAIMIAGI
gi|408521|   ECMNSVKNGT YDYPKYEEES RLNRNEIKGV KLSNMGVYQI LAIYATVAGS LSLAIMMAGI
gi|7809744   ECMNSVRNGT YNYPKYEEES RLNRNEIKGV KLSSMGVYQI LAIYATVAGS LSLAIIIAGI
gi|408599|   ECMNSVRNGT YDYPKYEEES KLNRNEIKGV KLSNMGVYQI LAIYATVAGS LSLAIMIAGI
gi|1892304   ECMNSVKNGT YDYPKYEEES KLNRNEIKGV KLSSMGVYQI LAIYATVAGS LSLAIMMAGI
gi|324146|   ECMNSVKNGT YDYPKYEEES KLNRNEIKGV KLSSMGVYQI LAIYATVAGS LSLAIMMAGI
gi|9448152   ECMNSVKTGT YDYPKYEEES KLNRNEIKGV KLSSMGVYQI LAIYATVAGS LSLAIMMAGI
gi|2645338   ECMNSVKNGT YDYPKYEEES KLNRNEIKGV KLSSMGVYQI LAIYATVAGS LSLAIMMAGI
gi|8265466   ACIESIRNGT YDHDIYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C FLLCVVLLGF
gi|9899113   ACIESIRNGT YDHDIYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C FLLCVVLLGF
gi|8265254   ACIESIRNGT YDHDIYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C FLLCVVLLGF
gi|60757|g   ACIESIRNGT YDHDIYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C LLLCVVLLGF
gi|1184209   ACIESIRNGT YDHDVYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C FLLCVVLLGF
gi|1265674   ACIESIRNGT YDHDVYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C FLLCVVLLGF
gi|1400969   ACIESIRNGT YDHDVYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C FLLCVVLLGF
gi|8097792   ACIESIRNGT YDHDVYRDEA LNNRFQIKGV ELKSGYKDWI LWISFAIS-C FLLCVVLLGF
gi|4240448   ECMESVRNGT YDYPQYSEES RLNREEIDGV KLESMGTYQI LSIYSTVASS LALAIMVAGL
gi|6048757   ECMESVKNGT YDYPQYSEEA RLNREEISGV KLESMGTYQI LSIYSTVASS LALAIMVAGL
gi|4715628   ECMESVRNGT YDYPQYSEEA RLNREEISGV KLESMGTYQI LSIYSTVASS LALAIMVAGL
gi|4715629   ECMESVKNGT YDYPQYSEEA RLNREEISGV KLESMGTYQI LSIYSTVASS LALAIMVAGL
gi|2865380   ECMESVKNGT YDYPQYSEEA RLNREEISGV KLESMGTYQI LSIYSTVASS LALAIMVAGL
gi|4545383   ECMESVRNGT YDYPQYSEEA RLKREEISGV KLESIGIYQI LSIYSTVASS LALAIMVAGL
gi|5029605   ECMESVRNGT YDYPQYSEEA RLKREEISGV KLESIGIYQI LSIYSTVASS LALAIMVAGL
```

```
gi|1591449   ECMESVRNGT YDYPQYSEEA RLKREEISGV KLESIGIYQI LSIYSTVASS LALAIMVAGL
gi|1159624   ECMESVKNGT YDYPQYSEEA RLNREEISGV KLESMGIYQI LSIYSTVASS LALAIMIAGL
Clustal Co

             ....|....| ....|.
                545        555
gi|4585161   SFWMCSNGSL QCRICI
gi|221300|   SFWMCSNGSL QCRICI
gi|4585169   SFWMCSNGSL QCRICI
gi|1135311   SFWMCSNGSL QCRICI
gi|4325018   ---------- ------
gi|4325020   ---------- ------
gi|4325039   SFWMCSNGSL QCRICI
gi|8977932   SFWMCSNGSL QCRICI
gi|1571684   SFWMCSNGSL QCRICI
gi|8994138   SFWMCSNGSL QCRICI
gi|1585252   SFWMCSNGSL QCRICI
gi|1584266   SFWMCSNGSL QCRICI
gi|2375118   SFWMCSNGSL QCRICI
gi|2376596   SFWMCSNGSL QCRICI
gi|2376596   SFWMCSNGSL QCRICI
gi|2376596   SFWMCSNGSL QCRICI
gi|408553|   SLWMCSNGSL QCRICI
gi|408521|   SFWMCSNGSL QCRICI
gi|7809744   SFWMCSNGSL QCRICI
gi|408599|   SFWMCSNGSL QCRICI
gi|1892304   SFWMCSNGSL QCRICI
gi|324146|   SFWMCSNGSL QCRICI
gi|9448152   SFWMCSNGSL QCRICI
gi|2645338   SFWMCSNGSL QFRICI
gi|8265466   IMWACQRGNI RCNICI
gi|9899113   IMWACQRGNI RCNICI
gi|8265254   IMWACQRGNI RCNICI
gi|60757|g   IMWACQRGNI RCNICI
gi|1184209   IMWACQRGNI RCNICI
gi|1265674   IMWACQRGNI RCNICI
gi|1400969   IMWACQRGNI RCNICI
gi|8097792   IMWACQRGNI RCNICI
gi|4240448   SFWMCSNGSL QCRICI
gi|6048757   SLWMCSNGSL QCRICI
gi|4715628   SLWMCSNGSL QCRICI
gi|4715629   SLWMCSNGSL QCRICI
gi|2865380   SLWMCSNGSL QCRICI
gi|4545383   SLWMCSNGSL QCRICI
gi|5029605   SLWMCSNGSL QCR---
gi|1591449   SLWMCSNGSL QCRICI
gi|1159624   SFWMCSNGSL QCRICI
Clustal Co
```

Lampiran 5. Parameter Autogrid

Hemagglutinin 1RVT

```
npts 40 40 40                           # num.grid points in xyz
gridfld 1RVT_EMF.maps.fld               # grid_data_file
spacing 0.375                           # spacing(A)
receptor_types A C HD N NA OA SA        # receptor atom types
ligand_types C HD OA N                  # ligand atom types
receptor 1RVT_EMF.pdbqt                 # macromolecule
gridcenter 76.25 18.935 -22.507         # xyz-coordinates or auto
smooth 0.5                              # store minimum energy w/in
rad(A)
map 1RVT_EMF.C.map                      # atom-specific affinity map
map 1RVT_EMF.HD.map                     # atom-specific affinity map
map 1RVT_EMF.OA.map                     # atom-specific affinity map
map 1RVT_EMF.N.map                      # atom-specific affinity map
elecmap 1RVT_EMF.e.map                  # electrostatic potential map
dsolvmap 1RVT_EMF.d.map                 # desolvation potential map
dielectric -0.1465                      # <0, AD4 distance-dep.diel;>0,
constant
```

Hemagglutinin 1RD8

```
npts 40 40 40                           # num.grid points in xyz
gridfld 1RD8_EMF.maps.fld               # grid_data_file
spacing 0.375                           # spacing(A)
receptor_types A C HD N NA OA SA        # receptor atom types
ligand_types C HD OA N                  # ligand atom types
receptor 1RD8_EMF.pdbqt                 # macromolecule
gridcenter 76.994 19.206 -22.249        # xyz-coordinates or auto
smooth 0.5                              # store minimum energy w/in
rad(A)
map 1RD8_EMF.C.map                      # atom-specific affinity map
map 1RD8_EMF.HD.map                     # atom-specific affinity map
map 1RD8_EMF.OA.map                     # atom-specific affinity map
map 1RD8_EMF.N.map                      # atom-specific affinity map
elecmap 1RD8_EMF.e.map                  # electrostatic potential map
dsolvmap 1RD8_EMF.d.map                 # desolvation potential map
dielectric -0.1465                      # <0, AD4 distance-dep.diel;>0,
constant
```

Hemagglutinin 1MQN

```
npts 40 40 40                           # num.grid points in xyz
gridfld 1MQN_EMF.maps.fld               # grid_data_file
spacing 0.375                           # spacing(A)
receptor_types A C HD N NA OA SA        # receptor atom types
ligand_types C HD OA N                  # ligand atom types
receptor 1MQN_EMF.pdbqt                 # macromolecule
gridcenter 76.25 18.935 -22.507         # xyz-coordinates or auto
```

```
smooth 0.5                              # store minimum energy w/in
rad(A)
map 1MQN_EMF.C.map                      # atom-specific affinity map
map 1MQN_EMF.HD.map                     # atom-specific affinity map
map 1MQN_EMF.OA.map                     # atom-specific affinity map
map 1MQN_EMF.N.map                      # atom-specific affinity map
elecmap 1MQN_EMF.e.map                  # electrostatic potential map
dsolvmap 1MQN_EMF.d.map                 # desolvation potential map
dielectric -0.1465                      # <0, AD4 distance-dep.diel;>0,
constant
```

Hemagglutinin 1HGF

```
npts 40 40 40                           # num.grid points in xyz
gridfld 1HGF_EMF.maps.fld               # grid_data_file
spacing 0.375                           # spacing(A)
receptor_types A C HD N NA OA SA        # receptor atom types
ligand_types C HD OA N                  # ligand atom types
receptor 1HGF_EMF.pdbqt                 # macromolecule
gridcenter 76.994 19.206 -22.249        # xyz-coordinates or auto
smooth 0.5                              # store minimum energy w/in
rad(A)
map 1HGF_EMF.C.map                      # atom-specific affinity map
map 1HGF_EMF.HD.map                     # atom-specific affinity map
map 1HGF_EMF.OA.map                     # atom-specific affinity map
map 1HGF_EMF.N.map                      # atom-specific affinity map
elecmap 1HGF_EMF.e.map                  # electrostatic potential map
dsolvmap 1HGF_EMF.d.map                 # desolvation potential map
dielectric -0.1465                      # <0, AD4 distance-dep.diel;>0,
constant
```

Hemagglutinin 2FK0

```
npts 40 40 40                           # num.grid points in xyz
gridfld 2FK0_EMF.maps.fld               # grid_data_file
spacing 0.375                           # spacing(A)
receptor_types A C HD N NA OA SA        # receptor atom types
ligand_types C HD OA N                  # ligand atom types
receptor 2FK0_EMF.pdbqt                 # macromolecule
gridcenter 76.994 19.206 -22.249        # xyz-coordinates or auto
smooth 0.5                              # store minimum energy w/in
rad(A)
map 2FK0_EMF.C.map                      # atom-specific affinity map
map 2FK0_EMF.HD.map                     # atom-specific affinity map
map 2FK0_EMF.OA.map                     # atom-specific affinity map
map 2FK0_EMF.N.map                      # atom-specific affinity map
elecmap 2FK0_EMF.e.map                  # electrostatic potential map
dsolvmap 2FK0_EMF.d.map                 # desolvation potential map
dielectric -0.1465                      # <0, AD4 distance-dep.diel;>0,
constant
```

Lampiran 6. Parameter Autodock

1RVT-Sia(α2-3)Gal

```
outlev 1                              # diagnostic output level
intelec                               # calculate internal electrostatics
seed pid time                         # seeds for random generator
ligand_types C HD OA N                # atoms types in ligand
fld 1RVT_EMF.maps.fld                 # grid_data_file
map 1RVT_EMF.C.map                    # atom-specific affinity map
map 1RVT_EMF.HD.map                   # atom-specific affinity map
map 1RVT_EMF.OA.map                   # atom-specific affinity map
map 1RVT_EMF.N.map                    # atom-specific affinity map
elecmap 1RVT_EMF.e.map                # electrostatics map
desolvmap 1RVT_EMF.d.map              # desolvation map
move a.pdbqt                          # small molecule
about 76.25 18.935 -22.507            # small molecule center
tran0 random                          # initial coordinates/A or random
quat0 random                          # initial quaternion
ndihe 0                               # number of active torsions
dihe0 random                          # initial dihedrals (relative) or random
tstep 2.0                             # translation step/A
qstep 50.0                            # quaternion step/deg
dstep 50.0                            # torsion step/deg
torsdof 15 0.274000                    # torsional degrees of freedom and coefficient
rmstol 2.0                            # cluster_tolerance/A
extnrg 1000.0                         # external grid energy
e0max 0.0 10000                       # max initial energy; max number of retries
ga_pop_size 150                       # number of individuals in population
ga_num_evals 500000                  # maximum number of energy evaluations
ga_num_generations 27000              # maximum number of generations
ga_elitism 1                          # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                 # rate of gene mutation
ga_crossover_rate 0.8                 # rate of crossover
ga_window_size 10                     #
ga_cauchy_alpha 0.0                   # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                    # Beta parameter Cauchy distribution
set_ga                                # set the above parameters for GA or LGA
sw_max_its 300                        # iterations of Solis & Wets local search
sw_max_succ 4                         # consecutive successes before changing rho
sw_max_fail 4                         # consecutive failures before changing rho
sw_rho 1.0                            # size of local search space to sample
sw_lb_rho 0.01                        # lower bound on rho
ls_search_freq 0.06                   # probability of performing local search on
individual
set_sw1                               # set the above Solis & Wets parameters
compute_unbound_extended              # compute extended ligand energy
ga_run 100                            # do this many hybrid GA-LS runs
analysis                              # perform a ranked cluster analysis
```

1RVT-Sia(α2-6)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 1RVT_EMF.maps.fld                   # grid_data_file
map 1RVT_EMF.C.map                      # atom-specific affinity map
map 1RVT_EMF.HD.map                     # atom-specific affinity map
map 1RVT_EMF.OA.map                     # atom-specific affinity map
map 1RVT_EMF.N.map                      # atom-specific affinity map
elecmap 1RVT_EMF.e.map                  # electrostatics map
desolvmap 1RVT_EMF.d.map                # desolvation map
move h.pdbqt                            # small molecule
about 76.3817 19.6178 -22.5455          # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

1RD8-Sia(α2-6)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 1RD8_EMF.maps.fld                   # grid_data_file
map 1RD8_EMF.C.map                      # atom-specific affinity map
map 1RD8_EMF.HD.map                     # atom-specific affinity map
map 1RD8_EMF.OA.map                     # atom-specific affinity map
map 1RD8_EMF.N.map                      # atom-specific affinity map
elecmap 1RD8_EMF.e.map                  # electrostatics map
desolvmap 1RD8_EMF.d.map                # desolvation map
move h.pdbqt                            # small molecule
about 76.3817 19.6178 -22.5455          # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

1RD8-Sia(α2-3)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 1RD8_EMF.maps.fld                   # grid_data_file
map 1RD8_EMF.C.map                      # atom-specific affinity map
map 1RD8_EMF.HD.map                     # atom-specific affinity map
map 1RD8_EMF.OA.map                     # atom-specific affinity map
map 1RD8_EMF.N.map                      # atom-specific affinity map
elecmap 1RD8_EMF.e.map                  # electrostatics map
desolvmap 1RD8_EMF.d.map                # desolvation map
move a.pdbqt                            # small molecule
about 76.25 18.935 -22.507              # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

1MQN-Sia(α2-3)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 1MQN_EMF.maps.fld                   # grid_data_file
map 1MQN_EMF.C.map                      # atom-specific affinity map
map 1MQN_EMF.HD.map                     # atom-specific affinity map
map 1MQN_EMF.OA.map                     # atom-specific affinity map
map 1MQN_EMF.N.map                      # atom-specific affinity map
elecmap 1MQN_EMF.e.map                  # electrostatics map
desolvmap 1MQN_EMF.d.map                # desolvation map
move a.pdbqt                            # small molecule
about 76.25 18.935 -22.507              # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

1MQN-Sia(α2-6)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 1MQN_EMF.maps.fld                   # grid_data_file
map 1MQN_EMF.C.map                      # atom-specific affinity map
map 1MQN_EMF.HD.map                     # atom-specific affinity map
map 1MQN_EMF.OA.map                     # atom-specific affinity map
map 1MQN_EMF.N.map                      # atom-specific affinity map
elecmap 1MQN_EMF.e.map                  # electrostatics map
desolvmap 1MQN_EMF.d.map                # desolvation map
move h.pdbqt                            # small molecule
about 76.3817 19.6178 -22.5455          # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

1HGF-Sia(α2-3)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 1HGF_EMF.maps.fld                   # grid_data_file
map 1HGF_EMF.C.map                      # atom-specific affinity map
map 1HGF_EMF.HD.map                     # atom-specific affinity map
map 1HGF_EMF.OA.map                     # atom-specific affinity map
map 1HGF_EMF.N.map                      # atom-specific affinity map
elecmap 1HGF_EMF.e.map                  # electrostatics map
desolvmap 1HGF_EMF.d.map                # desolvation map
move a.pdbqt                            # small molecule
about 76.25 18.935 -22.507              # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

1HGF-Sia(α2-6)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 1HGF_EMF.maps.fld                   # grid_data_file
map 1HGF_EMF.C.map                      # atom-specific affinity map
map 1HGF_EMF.HD.map                     # atom-specific affinity map
map 1HGF_EMF.OA.map                     # atom-specific affinity map
map 1HGF_EMF.N.map                      # atom-specific affinity map
elecmap 1HGF_EMF.e.map                  # electrostatics map
desolvmap 1HGF_EMF.d.map                # desolvation map
move h.pdbqt                            # small molecule
about 76.3817 19.6178 -22.5455          # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

2FK0-Sia(α2-3)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 2FK0_EMF.maps.fld                   # grid_data_file
map 2FK0_EMF.C.map                      # atom-specific affinity map
map 2FK0_EMF.HD.map                     # atom-specific affinity map
map 2FK0_EMF.OA.map                     # atom-specific affinity map
map 2FK0_EMF.N.map                      # atom-specific affinity map
elecmap 2FK0_EMF.e.map                  # electrostatics map
desolvmap 2FK0_EMF.d.map                # desolvation map
move a.pdbqt                            # small molecule
about 76.25 18.935 -22.507              # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

2FK0-Sia(α2-6)Gal

```
outlev 1                                # diagnostic output level
intelec                                 # calculate internal electrostatics
seed pid time                           # seeds for random generator
ligand_types C HD OA N                  # atoms types in ligand
fld 2FK0_EMF.maps.fld                   # grid_data_file
map 2FK0_EMF.C.map                      # atom-specific affinity map
map 2FK0_EMF.HD.map                     # atom-specific affinity map
map 2FK0_EMF.OA.map                     # atom-specific affinity map
map 2FK0_EMF.N.map                      # atom-specific affinity map
elecmap 2FK0_EMF.e.map                  # electrostatics map
desolvmap 2FK0_EMF.d.map                # desolvation map
move h.pdbqt                            # small molecule
about 76.3817 19.6178 -22.5455          # small molecule center
tran0 random                            # initial coordinates/A or random
quat0 random                            # initial quaternion
ndihe 0                                 # number of active torsions
dihe0 random                            # initial dihedrals (relative) or random
tstep 2.0                               # translation step/A
qstep 50.0                              # quaternion step/deg
dstep 50.0                              # torsion step/deg
torsdof 15 0.274000                      # torsional degrees of freedom and coefficient
rmstol 2.0                              # cluster_tolerance/A
extnrg 1000.0                           # external grid energy
e0max 0.0 10000                         # max initial energy; max number of retries
ga_pop_size 150                         # number of individuals in population
ga_num_evals 500000                    # maximum number of energy evaluations
ga_num_generations 27000                # maximum number of generations
ga_elitism 1                            # number of top individuals to survive to next
generation
ga_mutation_rate 0.02                   # rate of gene mutation
ga_crossover_rate 0.8                   # rate of crossover
ga_window_size 10                       #
ga_cauchy_alpha 0.0                     # Alpha parameter of Cauchy distribution
ga_cauchy_beta 1.0                      # Beta parameter Cauchy distribution
set_ga                                  # set the above parameters for GA or LGA
sw_max_its 300                          # iterations of Solis & Wets local search
sw_max_succ 4                           # consecutive successes before changing rho
sw_max_fail 4                           # consecutive failures before changing rho
sw_rho 1.0                              # size of local search space to sample
sw_lb_rho 0.01                          # lower bound on rho
ls_search_freq 0.06                     # probability of performing local search on
individual
set_sw1                                 # set the above Solis & Wets parameters
compute_unbound_extended                # compute extended ligand energy
ga_run 100                              # do this many hybrid GA-LS runs
analysis                                # perform a ranked cluster analysis
```

Lampiran 7. Output Hasil Docking

1RVT-Sia(α2-3)Gal

```
                    AutoDock 4.00

                    (c) 1991-2007
          The Scripps Research Institute

             Garrett M. Morris, TSRI
                  Ruth Huey, TSRI
              William E. Hart, Sandia
              William Lindstrom, TSRI
              Alexander Gillet, TSRI
             David S. Goodsell, TSRI
              Arthur J. Olson, TSRI

       Automated Docking of Flexible Ligand
        to Flexible Macromolecular Receptor
```

Number of distinct conformational clusters found = 3, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.69	93	-1.50	68	##
2	-1.37	53	-1.29	31	###############################
3	-0.61	33	-0.61	1	#

Number of multi-member conformational clusters found = 2, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	93	-1.69	0.00	2.55	RANKING
1	2	55	-1.69	0.08	2.55	RANKING
1	3	87	-1.68	0.13	2.55	RANKING
1	4	56	-1.68	0.08	2.55	RANKING
1	5	16	-1.68	0.15	2.54	RANKING
1	6	52	-1.68	0.08	2.55	RANKING
1	7	64	-1.68	0.03	2.55	RANKING
1	8	51	-1.67	0.12	2.55	RANKING
1	9	76	-1.67	0.13	2.54	RANKING
1	10	43	-1.67	0.11	2.56	RANKING
1	11	62	-1.67	0.06	2.55	RANKING
1	12	15	-1.67	0.05	2.55	RANKING
1	13	42	-1.66	0.11	2.57	RANKING
1	14	61	-1.66	0.09	2.56	RANKING
1	15	25	-1.65	0.10	2.56	RANKING
1	16	32	-1.65	0.16	2.56	RANKING
1	17	37	-1.65	0.05	2.55	RANKING
1	18	21	-1.65	0.13	2.54	RANKING
1	19	39	-1.65	0.17	2.54	RANKING
1	20	31	-1.65	0.20	2.54	RANKING
1	21	54	-1.65	0.10	2.57	RANKING
1	22	22	-1.64	0.17	2.54	RANKING
1	23	88	-1.64	0.15	2.54	RANKING
1	24	74	-1.64	0.12	2.57	RANKING
1	25	68	-1.64	0.08	2.55	RANKING
1	26	89	-1.63	0.12	2.57	RANKING
1	27	85	-1.63	0.19	2.55	RANKING
1	28	72	-1.63	0.13	2.54	RANKING
1	29	95	-1.63	0.18	2.54	RANKING
1	30	49	-1.63	0.12	2.56	RANKING
1	31	14	-1.62	0.06	2.55	RANKING
1	32	38	-1.61	0.19	2.54	RANKING
1	33	79	-1.61	0.14	2.53	RANKING
1	34	34	-1.61	0.14	2.56	RANKING
1	35	11	-1.60	0.12	2.55	RANKING
1	36	9	-1.60	0.14	2.55	RANKING
1	37	27	-1.60	0.20	2.53	RANKING
1	38	47	-1.60	0.10	2.56	RANKING
1	39	26	-1.60	0.11	2.57	RANKING
1	40	19	-1.58	0.16	2.56	RANKING
1	41	3	-1.55	0.25	2.52	RANKING
1	42	28	-1.53	0.20	2.54	RANKING
1	43	58	-1.52	0.24	2.53	RANKING
1	44	73	-1.48	0.22	2.51	RANKING
1	45	75	-1.47	0.28	2.51	RANKING
1	46	40	-1.42	0.37	2.51	RANKING
1	47	65	-1.39	0.37	2.50	RANKING
1	48	60	-1.38	0.41	2.50	RANKING
1	49	41	-1.31	0.62	2.49	RANKING
1	50	66	-1.29	0.64	2.49	RANKING
1	51	8	-1.29	0.53	2.48	RANKING
1	52	81	-1.28	0.66	2.49	RANKING
1	53	35	-1.28	0.65	2.50	RANKING
1	54	84	-1.27	0.78	2.48	RANKING
1	55	83	-1.24	0.89	2.47	RANKING
1	56	57	-1.24	0.82	2.48	RANKING
1	57	59	-1.23	0.93	2.47	RANKING
1	58	98	-1.22	0.88	2.47	RANKING
1	59	78	-1.21	1.13	2.46	RANKING
1	60	82	-1.21	0.80	2.48	RANKING
1	61	36	-1.21	1.01	2.46	RANKING
1	62	50	-1.21	1.11	2.47	RANKING
1	63	96	-1.20	1.15	2.47	RANKING
1	64	46	-1.20	0.98	2.46	RANKING
1	65	90	-1.17	1.12	2.46	RANKING
1	66	6	-1.16	1.18	2.46	RANKING
1	67	70	-1.16	0.34	2.61	RANKING
1	68	80	-1.07	1.03	2.43	RANKING
2	1	53	-1.37	0.00	1.43	RANKING

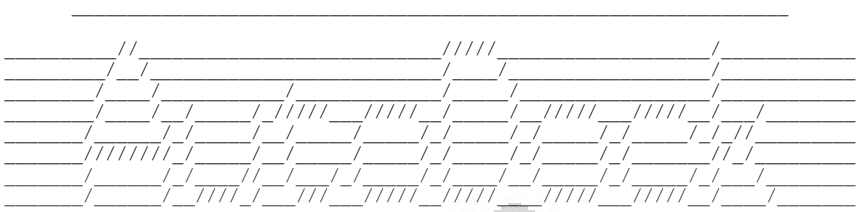
```
   2      2     67       -1.36      0.05      1.42           RANKING
   2      3     23       -1.36      0.05      1.42           RANKING
   2      4     18       -1.35      0.11      1.45           RANKING
   2      5     86       -1.35      0.04      1.43           RANKING
   2      6     94       -1.35      0.11      1.45           RANKING
   2      7    100       -1.35      0.11      1.43           RANKING
   2      8      7       -1.34      0.10      1.42           RANKING
   2      9     20       -1.34      0.09      1.43           RANKING
   2     10      5       -1.34      0.15      1.42           RANKING
   2     11     45       -1.33      0.12      1.40           RANKING
   2     12     24       -1.33      0.11      1.38           RANKING
   2     13      2       -1.32      0.15      1.45           RANKING
   2     14     77       -1.32      0.49      1.53           RANKING
   2     15     63       -1.32      0.31      1.44           RANKING
   2     16     10       -1.31      0.56      1.51           RANKING
   2     17      1       -1.31      0.52      1.51           RANKING
   2     18     97       -1.31      0.57      1.53           RANKING
   2     19     30       -1.30      0.50      1.51           RANKING
   2     20     17       -1.30      0.48      1.49           RANKING
   2     21     91       -1.28      0.62      1.51           RANKING
   2     22     92       -1.28      0.43      1.49           RANKING
   2     23     12       -1.27      0.18      1.38           RANKING
   2     24     71       -1.27      0.57      1.47           RANKING
   2     25      4       -1.24      0.41      1.45           RANKING
   2     26     48       -1.24      0.20      1.38           RANKING
   2     27     13       -1.23      0.71      1.52           RANKING
   2     28     69       -1.21      0.41      1.44           RANKING
   2     29     99       -1.17      0.62      1.52           RANKING
   2     30     29       -1.12      0.38      1.34           RANKING
   2     31     44       -1.05      0.94      1.58           RANKING
   3      1     33       -0.61      0.00      2.83           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.15  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.24           at Temperature, T = 298.15 K
Free energy,        A ~ -2729.90 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -1.43 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       93
USER    Run = 93
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 68
USER
USER    RMSD from reference structure       = 2.549 A
USER
USER    Estimated Free Energy of Binding    =   -1.69 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   57.93 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.80 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.89 kcal/mol
USER        Electrostatic Energy            =   +0.08 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
```

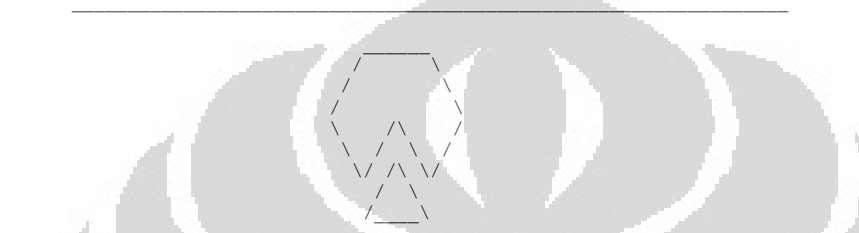
```
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rvta.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      74.417560 17.298233 -22.549715
USER    NEWDPF axisangle0 -0.531901 0.846069 0.035332 -165.086284
USER    NEWDPF quaternion0        -0.527403 0.838914 0.035033 -0.129780
USER
USER                                x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      75.378  16.814 -24.159 -0.01 -0.03    +0.239  2.549
ATOM      2  O1A SIA A3021      76.284  16.420 -24.890 +0.01 +0.07    -0.644  2.549
ATOM      3  O1B SIA A3021      74.645  17.717 -24.560 +0.03 +0.11    -0.644  2.549
ATOM      4  C2  SIA A3021      75.278  16.328 -22.686 -0.08 -0.04    +0.259  2.549
ATOM      5  C3  SIA A3021      76.615  15.767 -22.158 -0.13 -0.01    +0.114  2.549
ATOM      6  C4  SIA A3021      77.668  16.867 -21.965 -0.10 -0.00    +0.149  2.549
ATOM      7  O4  SIA A3021      78.829  16.308 -21.312 -0.09 -0.03    -0.393  2.549
ATOM      8  C5  SIA A3021      77.124  18.043 -21.129 -0.19 -0.00    +0.145  2.549
ATOM      9  N5  SIA A3021      78.108  19.140 -21.161 -0.07 -0.01    -0.352  2.549
ATOM     10  C6  SIA A3021      75.772  18.508 -21.709 -0.13 -0.02    +0.182  2.549
ATOM     11  O6  SIA A3021      74.851  17.375 -21.753 -0.10 +0.07    -0.336  2.549
ATOM     12  C7  SIA A3021      75.108  19.669 -20.936 -0.22 -0.04    +0.180  2.549
ATOM     13  O7  SIA A3021      74.959  19.336 -19.537 -0.24 +0.05    -0.390  2.549
ATOM     14  C8  SIA A3021      73.737  20.044 -21.540 -0.20 -0.04    +0.173  2.549
ATOM     15  O8  SIA A3021      73.884  20.394 -22.934 -0.02 +0.11    -0.391  2.549
ATOM     16  C9  SIA A3021      73.072  21.211 -20.802 -0.31 -0.07    +0.198  2.549
ATOM     17  O9  SIA A3021      71.782  21.496 -21.374 -0.19 +0.14    -0.398  2.549
ATOM     18  C10 SIA A3021      78.544  19.826 -20.075 -0.24 +0.03    +0.214  2.549
ATOM     19  O10 SIA A3021      78.097  19.659 -18.945 -0.60 -0.04    -0.274  2.549
ATOM     20  C11 SIA A3021      79.500  20.950 -20.327 -0.16 +0.02    +0.117  2.549
ATOM     21  H4  SIA A3021      79.481  16.989 -21.193 +0.05 +0.02    +0.210  2.549
ATOM     22  H5  SIA A3021      78.490  19.404 -22.069 +0.03 -0.00    +0.163  2.549
ATOM     23  H7  SIA A3021      74.551  20.050 -19.062 -0.25 -0.01    +0.210  2.549
ATOM     24  H8  SIA A3021      73.041  20.626 -23.306 +0.08 -0.08    +0.210  2.549
ATOM     25  H9  SIA A3021      71.369  22.219 -20.917 -0.10 -0.08    +0.209  2.549
ATOM     26  C1  GAL A3022      70.525  15.414 -22.274 -0.35 -0.03    +0.202  2.549
ATOM     27  C2  GAL A3022      71.981  15.184 -21.832 -0.27 -0.06    +0.173  2.549
ATOM     28  O2  GAL A3022      72.265  15.957 -20.644 -0.04 +0.13    -0.391  2.549
ATOM     29  C3  GAL A3022      72.952  15.597 -22.949 -0.21 -0.04    +0.187  2.549
ATOM     30  O3  GAL A3022      74.315  15.231 -22.569 -0.12 +0.08    -0.336  2.549
ATOM     31  C4  GAL A3022      72.585  14.922 -24.283 -0.14 -0.03    +0.180  2.549
ATOM     32  O4  GAL A3022      72.838  13.501 -24.207 -0.10 +0.07    -0.390  2.549
ATOM     33  C5  GAL A3022      71.104  15.204 -24.615 -0.22 -0.02    +0.176  2.549
ATOM     34  O5  GAL A3022      70.232  14.749 -23.537 -0.22 +0.05    -0.378  2.549
ATOM     35  C6  GAL A3022      70.675  14.527 -25.920 -0.20 -0.02    +0.198  2.549
ATOM     36  O6  GAL A3022      69.309  14.865 -26.233 -0.16 +0.08    -0.398  2.549
ATOM     37  H2  GAL A3022      73.164  15.815 -20.371 -0.37 -0.15    +0.210  2.549
ATOM     38  H4  GAL A3022      72.612  13.085 -25.030 +0.06 -0.02    +0.210  2.549
ATOM     39  H6  GAL A3022      69.043  14.445 -27.042 -0.32 -0.05    +0.209  2.549
TER
ENDMDL
MODEL       53
USER    Run = 53
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 31
USER
USER    RMSD from reference structure       = 1.432 A
USER
USER    Estimated Free Energy of Binding    =   -1.37 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   99.71 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.48 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.15 kcal/mol
USER        Electrostatic Energy            =   -0.33 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rvta.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      76.203137 18.500898 -21.471977
USER    NEWDPF axisangle0 0.600984 0.790487 0.118103 -20.504027
USER    NEWDPF quaternion0        0.106962 0.140689 0.021020 -0.984034
```

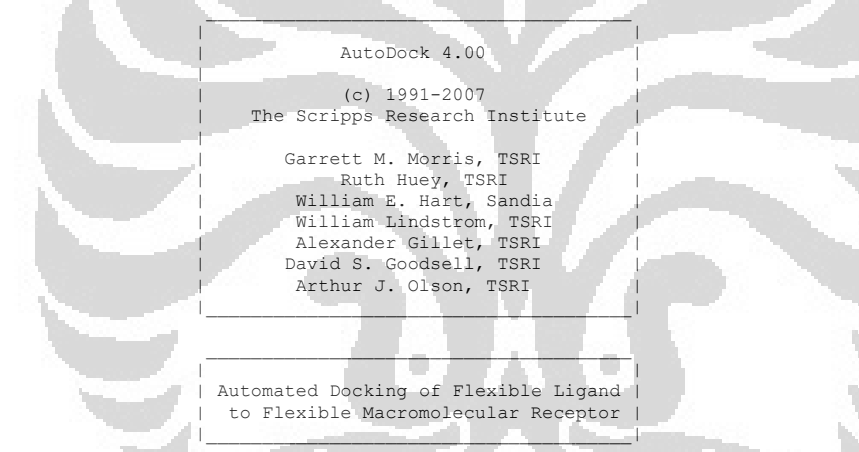
```
USER
USER                                x       y       z    vdW   Elec       q     RMS
ATOM      1  C1  SIA A3021      77.095  17.274 -20.269 -0.18 +0.02    +0.239  1.432
ATOM      2  O1A SIA A3021      77.481  16.220 -19.771 -0.13 -0.08    -0.644  1.432
ATOM      3  O1B SIA A3021      76.831  18.219 -19.524 -0.16 -0.10    -0.644  1.432
ATOM      4  C2  SIA A3021      76.754  17.360 -21.783 -0.10 -0.02    +0.259  1.432
ATOM      5  C3  SIA A3021      76.481  15.975 -22.405 -0.11 -0.01    +0.114  1.432
ATOM      6  C4  SIA A3021      75.162  15.367 -21.908 -0.20 -0.03    +0.149  1.432
ATOM      7  O4  SIA A3021      74.882  14.161 -22.651 -0.10 +0.08    -0.393  1.432
ATOM      8  C5  SIA A3021      73.983  16.350 -22.058 -0.22 -0.04    +0.145  1.432
ATOM      9  N5  SIA A3021      72.806  15.783 -21.377 -0.23 +0.12    -0.352  1.432
ATOM     10  C6  SIA A3021      74.364  17.712 -21.443 -0.21 -0.04    +0.182  1.432
ATOM     11  O6  SIA A3021      75.588  18.201 -22.073 -0.04 +0.05    -0.336  1.432
ATOM     12  C7  SIA A3021      73.270  18.797 -21.558 -0.19 -0.04    +0.180  1.432
ATOM     13  O7  SIA A3021      72.862  18.971 -22.934 -0.07 +0.09    -0.390  1.432
ATOM     14  C8  SIA A3021      73.740  20.145 -20.970 -0.27 -0.04    +0.173  1.432
ATOM     15  O8  SIA A3021      74.132  19.978 -19.589 -0.36 +0.08    -0.391  1.432
ATOM     16  C9  SIA A3021      72.659  21.228 -21.053 -0.31 -0.07    +0.198  1.432
ATOM     17  O9  SIA A3021      73.157  22.474 -20.531 -0.16 +0.18    -0.398  1.432
ATOM     18  C10 SIA A3021      71.560  15.710 -21.909 -0.35 -0.05    +0.214  1.432
ATOM     19  O10 SIA A3021      71.259  16.191 -22.996 -0.21 +0.05    -0.274  1.432
ATOM     20  C11 SIA A3021      70.484  15.155 -21.028 -0.28 -0.02    +0.117  1.432
ATOM     21  H4  SIA A3021      74.065  13.784 -22.343 -0.11 -0.07    +0.210  1.432
ATOM     22  H5  SIA A3021      72.938  15.417 -20.434 -0.41 -0.09    +0.163  1.432
ATOM     23  H7  SIA A3021      72.189  19.637 -23.005 +0.09 -0.06    +0.210  1.432
ATOM     24  H8  SIA A3021      74.421  20.808 -19.227 -0.30 -0.12    +0.210  1.432
ATOM     25  H9  SIA A3021      72.487  23.146 -20.582 -0.26 -0.11    +0.209  1.432
ATOM     26  C1  GAL A3022      78.845  21.566 -23.023 -0.02 +0.01    +0.202  1.432
ATOM     27  C2  GAL A3022      78.315  20.169 -23.391 -0.00 -0.01    +0.173  1.432
ATOM     28  O2  GAL A3022      76.998  20.278 -23.977 +0.01 +0.04    -0.391  1.432
ATOM     29  C3  GAL A3022      78.241  19.278 -22.141 -0.05 -0.00    +0.187  1.432
ATOM     30  O3  GAL A3022      77.881  17.917 -22.534 -0.01 +0.01    -0.336  1.432
ATOM     31  C4  GAL A3022      79.582  19.264 -21.387 -0.08 +0.01    +0.180  1.432
ATOM     32  O4  GAL A3022      80.582  18.568 -22.165 -0.01 -0.01    -0.390  1.432
ATOM     33  C5  GAL A3022      80.023  20.713 -21.088 -0.09 +0.01    +0.176  1.432
ATOM     34  O5  GAL A3022      80.117  21.493 -22.318 -0.00 -0.03    -0.378  1.432
ATOM     35  C6  GAL A3022      81.372  20.759 -20.365 -0.07 +0.01    +0.198  1.432
ATOM     36  O6  GAL A3022      81.721  22.121 -20.045 -0.02 -0.03    -0.398  1.432
ATOM     37  H2  GAL A3022      76.671  19.415 -24.204 +0.02 -0.03    +0.210  1.432
ATOM     38  H4  GAL A3022      81.410  18.559 -21.699 +0.02 +0.00    +0.210  1.432
ATOM     39  H6  GAL A3022      82.557  22.150 -19.596 +0.04 +0.01    +0.209  1.432
TER
ENDMDL
MODEL       33
USER    Run = 33
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 2.827 A
USER
USER    Estimated Free Energy of Binding    =   -0.61 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  357.97 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.72 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.88 kcal/mol
USER        Electrostatic Energy            =   +0.15 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rvta.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      74.528085 16.461649 -22.994829
USER    NEWDPF axisangle0 -0.716954 -0.642421 -0.270689 -125.559250
USER    NEWDPF quaternion0        -0.637554 -0.571276 -0.240711 -0.457414
USER
USER                                x       y       z    vdW   Elec       q     RMS
ATOM      1  C1  SIA A3021      73.380  18.017 -23.097 -0.10 -0.05    +0.239  2.827
ATOM      2  O1A SIA A3021      72.368  18.711 -23.047 +0.01 +0.15    -0.644  2.827
ATOM      3  O1B SIA A3021      74.227  18.267 -23.954 +0.05 +0.13    -0.644  2.827
ATOM      4  C2  SIA A3021      73.504  16.731 -22.233 -0.18 -0.06    +0.259  2.827
ATOM      5  C3  SIA A3021      72.133  16.204 -21.759 -0.33 -0.03    +0.114  2.827
ATOM      6  C4  SIA A3021      71.305  15.625 -22.914 -0.33 -0.03    +0.149  2.827
ATOM      7  O4  SIA A3021      70.117  14.999 -22.383 -0.25 +0.06    -0.393  2.827
ATOM      8  C5  SIA A3021      72.106  14.595 -23.736 -0.22 -0.03    +0.145  2.827
```

```
ATOM      9  N5  SIA A3021      71.328  14.241 -24.937 -0.09 +0.05    -0.352  2.827
ATOM     10  C6  SIA A3021      73.471  15.197 -24.130 -0.10 -0.03    +0.182  2.827
ATOM     11  O6  SIA A3021      74.175  15.625 -22.924 -0.08 +0.07    -0.336  2.827
ATOM     12  C7  SIA A3021      74.383  14.245 -24.936 -0.05 -0.02    +0.180  2.827
ATOM     13  O7  SIA A3021      74.576  12.999 -24.231 -0.06 +0.05    -0.390  2.827
ATOM     14  C8  SIA A3021      75.749  14.895 -25.248 -0.01 -0.02    +0.173  2.827
ATOM     15  O8  SIA A3021      75.561  16.133 -25.969 +0.00 +0.04    -0.391  2.827
ATOM     16  C9  SIA A3021      76.660  13.976 -26.069 -0.01 -0.02    +0.198  2.827
ATOM     17  O9  SIA A3021      77.934  14.607 -26.298 +0.00 +0.03    -0.398  2.827
ATOM     18  C10 SIA A3021      71.100  12.977 -25.372 -0.19 -0.02    +0.214  2.827
ATOM     19  O10 SIA A3021      71.595  11.983 -24.850 -0.14 +0.01    -0.274  2.827
ATOM     20  C11 SIA A3021      70.338  12.832 -26.652 -0.21 -0.01    +0.117  2.827
ATOM     21  H4  SIA A3021      69.604  14.640 -23.098 +0.13 -0.02    +0.210  2.827
ATOM     22  H5  SIA A3021      70.931  15.006 -25.483 +0.07 -0.02    +0.163  2.827
ATOM     23  H7  SIA A3021      75.137  12.414 -24.727 +0.04 -0.02    +0.210  2.827
ATOM     24  H8  SIA A3021      76.401  16.532 -26.161 +0.00 -0.02    +0.210  2.827
ATOM     25  H9  SIA A3021      78.498  14.037 -26.807 +0.00 -0.01    +0.209  2.827
ATOM     26  C1  GAL A3022      78.044  17.114 -20.547 -0.20 +0.03    +0.202  2.827
ATOM     27  C2  GAL A3022      76.607  16.575 -20.428 -0.17 -0.01    +0.173  2.827
ATOM     28  O2  GAL A3022      76.552  15.209 -20.897 -0.17 +0.05    -0.391  2.827
ATOM     29  C3  GAL A3022      75.642  17.435 -21.259 -0.19 -0.03    +0.187  2.827
ATOM     30  O3  GAL A3022      74.268  17.000 -21.014 -0.13 +0.12    -0.336  2.827
ATOM     31  C4  GAL A3022      75.785  18.927 -20.909 -0.23 -0.02    +0.180  2.827
ATOM     32  O4  GAL A3022      75.295  19.174 -19.573 -0.21 +0.05    -0.390  2.827
ATOM     33  C5  GAL A3022      77.263  19.351 -21.045 -0.18 -0.01    +0.176  2.827
ATOM     34  O5  GAL A3022      78.121  18.527 -20.200 -0.64 -0.07    -0.378  2.827
ATOM     35  C6  GAL A3022      77.469  20.823 -20.677 -0.06 -0.00    +0.198  2.827
ATOM     36  O6  GAL A3022      78.846  21.201 -20.878 -0.37 -0.05    -0.398  2.827
ATOM     37  H2  GAL A3022      75.664  14.876 -20.824 +0.02 -0.05    +0.210  2.827
ATOM     38  H4  GAL A3022      75.384  20.095 -19.357 -0.35 -0.06    +0.210  2.827
ATOM     39  H6  GAL A3022      78.974  22.114 -20.649 +0.06 +0.04    +0.209  2.827
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2            # number of dimensions in the field
AVSFLD: nspace=1          # number of physical coordinates
AVSFLD: veclen=7          # vector size
AVSFLD: dim1=39           # atoms
AVSFLD: dim2=3            # conformations
AVSFLD: data=Real       # data type (byte,integer,Real,double)
AVSFLD: field=uniform     # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1rvta.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1rvta.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1rvta.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1rvta.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1rvta.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1rvta.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1rvta.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                 11:45 12" a.m., 06/14/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 44m 47.67s,  CPU= 43m 57.99s,  System= 0.97s
_____________________________________________________________________________
```

1RVT-Sia(α2-6)Gal







Number of distinct conformational clusters found = 2, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.98	92	-1.93	98	##########
2	-1.08	47	-1.08	2	##

Number of multi-member conformational clusters found = 2, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	92	-1.98	0.00	2.01	RANKING
1	2	8	-1.97	0.09	1.99	RANKING
1	3	2	-1.97	0.09	1.97	RANKING
1	4	72	-1.97	0.05	2.01	RANKING
1	5	87	-1.97	0.10	1.99	RANKING
1	6	95	-1.97	0.08	2.01	RANKING
1	7	70	-1.97	0.03	2.02	RANKING
1	8	65	-1.97	0.08	1.97	RANKING
1	9	93	-1.97	0.08	1.97	RANKING
1	10	11	-1.97	0.03	2.01	RANKING
1	11	82	-1.97	0.10	1.99	RANKING
1	12	36	-1.96	0.16	1.94	RANKING
1	13	24	-1.96	0.13	1.96	RANKING
1	14	61	-1.96	0.06	2.00	RANKING
1	15	98	-1.96	0.07	2.01	RANKING
1	16	83	-1.96	0.04	2.01	RANKING
1	17	66	-1.96	0.05	2.00	RANKING
1	18	12	-1.96	0.14	1.95	RANKING
1	19	67	-1.96	0.04	2.03	RANKING
1	20	51	-1.96	0.15	1.95	RANKING
1	21	40	-1.96	0.07	1.98	RANKING
1	22	46	-1.96	0.06	2.03	RANKING
1	23	74	-1.96	0.13	1.97	RANKING
1	24	96	-1.96	0.05	1.99	RANKING
1	25	48	-1.96	0.03	2.00	RANKING
1	26	20	-1.96	0.07	2.00	RANKING
1	27	35	-1.96	0.12	1.96	RANKING
1	28	31	-1.95	0.05	2.02	RANKING
1	29	3	-1.95	0.04	2.00	RANKING
1	30	17	-1.95	0.05	2.02	RANKING
1	31	1	-1.95	0.06	2.01	RANKING
1	32	49	-1.95	0.07	2.01	RANKING
1	33	81	-1.95	0.07	1.98	RANKING
1	34	54	-1.95	0.15	1.97	RANKING
1	35	29	-1.95	0.05	2.01	RANKING
1	36	43	-1.95	0.10	1.99	RANKING
1	37	13	-1.95	0.13	1.97	RANKING
1	38	100	-1.95	0.15	1.97	RANKING
1	39	21	-1.95	0.05	2.00	RANKING
1	40	55	-1.95	0.10	1.99	RANKING
1	41	23	-1.94	0.06	2.02	RANKING
1	42	80	-1.94	0.10	1.98	RANKING
1	43	22	-1.94	0.15	1.98	RANKING
1	44	19	-1.94	0.16	1.93	RANKING
1	45	45	-1.94	0.12	1.97	RANKING
1	46	15	-1.94	0.05	2.02	RANKING
1	47	63	-1.94	0.09	2.00	RANKING
1	48	27	-1.94	0.13	1.94	RANKING
1	49	62	-1.94	0.15	1.93	RANKING
1	50	97	-1.94	0.15	1.95	RANKING
1	51	79	-1.94	0.20	1.93	RANKING
1	52	10	-1.94	0.17	1.95	RANKING
1	53	50	-1.94	0.10	1.97	RANKING
1	54	14	-1.94	0.06	2.01	RANKING
1	55	85	-1.94	0.07	1.99	RANKING
1	56	41	-1.93	0.10	2.04	RANKING
1	57	4	-1.93	0.13	1.96	RANKING
1	58	88	-1.93	0.09	2.04	RANKING
1	59	39	-1.93	0.08	2.04	RANKING
1	60	5	-1.93	0.12	1.96	RANKING
1	61	32	-1.93	0.10	1.97	RANKING
1	62	73	-1.92	0.18	1.94	RANKING
1	63	99	-1.92	0.08	2.00	RANKING
1	64	33	-1.92	0.17	1.99	RANKING
1	65	52	-1.92	0.16	1.98	RANKING
1	66	9	-1.92	0.10	2.01	RANKING
1	67	53	-1.92	0.18	1.98	RANKING
1	68	30	-1.92	0.11	1.98	RANKING
1	69	71	-1.92	0.07	2.00	RANKING
1	70	59	-1.92	0.13	1.94	RANKING
1	71	6	-1.91	0.08	1.98	RANKING
1	72	69	-1.91	0.11	2.00	RANKING
1	73	78	-1.91	0.23	1.92	RANKING
1	74	68	-1.91	0.17	1.99	RANKING

```
   1      75      42       -1.90       0.13       2.06           RANKING
   1      76      16       -1.90       0.11       2.02           RANKING
   1      77      91       -1.89       0.21       1.97           RANKING
   1      78      77       -1.89       0.21       1.99           RANKING
   1      79      60       -1.89       0.13       2.06           RANKING
   1      80      75       -1.89       0.21       1.97           RANKING
   1      81      28       -1.88       0.25       1.95           RANKING
   1      82      56       -1.88       0.23       1.94           RANKING
   1      83      94       -1.88       0.19       2.00           RANKING
   1      84       7       -1.88       0.27       2.00           RANKING
   1      85      64       -1.88       0.21       2.01           RANKING
   1      86      34       -1.87       0.26       1.95           RANKING
   1      87      90       -1.87       0.20       1.99           RANKING
   1      88      25       -1.87       0.16       2.04           RANKING
   1      89      18       -1.87       0.23       2.01           RANKING
   1      90      26       -1.87       0.16       1.98           RANKING
   1      91      58       -1.86       0.22       1.96           RANKING
   1      92      86       -1.86       0.23       2.01           RANKING
   1      93      89       -1.85       0.20       2.00           RANKING
   1      94      57       -1.84       0.35       2.00           RANKING
   1      95      37       -1.84       0.27       1.95           RANKING
   1      96      76       -1.83       0.35       2.02           RANKING
   1      97      84       -1.82       0.17       2.03           RANKING
   1      98      44       -1.77       0.14       2.04           RANKING
   2       1      47       -1.08       0.00       2.75           RANKING
   2       2      38       -1.07       0.12       2.76           RANKING
_____________________________________________________________________

        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________

Information entropy for this clustering = 0.02  (rmstol = 2.00 Angstrom)

_____________________________________________________________________

        STATISTICAL MECHANICAL ANALYSIS
        _______________________________

Partition function, Q =   100.32           at Temperature, T = 298.15 K
Free energy,        A ~ -2730.39 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -1.91 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________

        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       92
USER    Run = 92
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 98
USER
USER    RMSD from reference structure       = 2.013 A
USER
USER    Estimated Free Energy of Binding    =   -1.98 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   35.67 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -6.09 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.73 kcal/mol
USER        Electrostatic Energy            =   -0.36 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rvth.dpf
```

```
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      75.985054 18.454061 -22.421993
USER    NEWDPF axisangle0 0.296829 0.950850 -0.088191 -37.053466
USER    NEWDPF quaternion0        0.094317 0.302130 -0.028022 -0.948176
USER
USER                             x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      77.140  16.666 -20.664 -0.23 -0.00    +0.239  2.013
ATOM      2  O1A SIA A 801      77.519  15.577 -20.239 -0.13 -0.03    -0.644  2.013
ATOM      3  O1B SIA A 801      77.067  17.615 -19.883 -0.35 -0.10    -0.644  2.013
ATOM      4  C2  SIA A 801      76.570  16.800 -22.103 -0.08 -0.03    +0.258  2.013
ATOM      5  C3  SIA A 801      76.093  15.442 -22.664 -0.11 -0.01    +0.114  2.013
ATOM      6  C4  SIA A 801      74.827  14.933 -21.958 -0.24 -0.04    +0.149  2.013
ATOM      7  O4  SIA A 801      74.358  13.742 -22.624 -0.13 +0.10    -0.393  2.013
ATOM      8  C5  SIA A 801      73.720  16.003 -21.945 -0.25 -0.04    +0.145  2.013
ATOM      9  N5  SIA A 801      72.594  15.549 -21.104 -0.24 +0.13    -0.352  2.013
ATOM     10  C6  SIA A 801      74.292  17.325 -21.393 -0.20 -0.05    +0.182  2.013
ATOM     11  O6  SIA A 801      75.438  17.729 -22.203 -0.05 +0.05    -0.336  2.013
ATOM     12  C7  SIA A 801      73.267  18.479 -21.340 -0.18 -0.04    +0.180  2.013
ATOM     13  O7  SIA A 801      72.627  18.655 -22.627 -0.09 +0.09    -0.390  2.013
ATOM     14  C8  SIA A 801      73.914  19.803 -20.875 -0.27 -0.04    +0.173  2.013
ATOM     15  O8  SIA A 801      74.572  19.618 -19.603 -0.29 +0.06    -0.391  2.013
ATOM     16  C9  SIA A 801      72.891  20.937 -20.740 -0.32 -0.06    +0.198  2.013
ATOM     17  O9  SIA A 801      73.543  22.157 -20.339 -0.17 +0.18    -0.398  2.013
ATOM     18  C10 SIA A 801      71.313  15.320 -21.493 -0.33 -0.05    +0.214  2.013
ATOM     19  O10 SIA A 801      70.427  15.183 -20.660 -0.39 +0.02    -0.274  2.013
ATOM     20  C11 SIA A 801      70.986  15.064 -22.937 -0.39 -0.02    +0.117  2.013
ATOM     21  H4  SIA A 801      73.576  13.427 -22.187 -0.37 -0.12    +0.210  2.013
ATOM     22  H5  SIA A 801      72.802  15.389 -20.118 -0.42 -0.10    +0.163  2.013
ATOM     23  H7  SIA A 801      71.997  19.365 -22.595 +0.10 -0.05    +0.210  2.013
ATOM     24  H8  SIA A 801      74.969  20.432 -19.317 -0.35 -0.09    +0.210  2.013
ATOM     25  H9  SIA A 801      72.909  22.860 -20.256 -0.31 -0.12    +0.209  2.013
ATOM     26  C1  GAL A 802      78.786  19.718 -26.176 +0.00 -0.01    +0.202  2.013
ATOM     27  C2  GAL A 802      79.680  20.957 -25.974 +0.01 -0.00    +0.173  2.013
ATOM     28  O2  GAL A 802      80.475  21.203 -27.155 +0.00 +0.01    -0.391  2.013
ATOM     29  C3  GAL A 802      80.609  20.764 -24.760 +0.01 +0.00    +0.180  2.013
ATOM     30  O3  GAL A 802      81.332  21.984 -24.486 +0.01 -0.03    -0.390  2.013
ATOM     31  C4  GAL A 802      79.835  20.316 -23.504 +0.00 +0.00    +0.180  2.013
ATOM     32  O4  GAL A 802      79.021  21.405 -23.014 +0.00 -0.02    -0.390  2.013
ATOM     33  C5  GAL A 802      78.972  19.086 -23.857 +0.00 -0.01    +0.176  2.013
ATOM     34  O5  GAL A 802      78.068  19.424 -24.947 +0.00 +0.03    -0.378  2.013
ATOM     35  C6  GAL A 802      78.158  18.557 -22.676 -0.02 -0.01    +0.206  2.013
ATOM     36  O6  GAL A 802      77.594  17.264 -23.037 -0.00 +0.02    -0.344  2.013
ATOM     37  H2  GAL A 802      81.025  21.967 -27.030 +0.00 +0.00    +0.210  2.013
ATOM     38  H3  GAL A 802      81.905  21.865 -23.737 +0.01 +0.01    +0.210  2.013
ATOM     39  H4  GAL A 802      78.544  21.129 -22.240 +0.04 +0.01    +0.210  2.013
TER
ENDMDL
MODEL       47
USER    Run = 47
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 2
USER
USER    RMSD from reference structure       = 2.753 A
USER
USER    Estimated Free Energy of Binding    =   -1.08 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  160.24 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.20 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.04 kcal/mol
USER        Electrostatic Energy            =   -0.16 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rvth.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      74.711033 19.172527 -22.359769
USER    NEWDPF axisangle0 0.042837 0.170765 -0.984380 -134.262898
USER    NEWDPF quaternion0        0.039470 0.157342 -0.907007 -0.388618
USER
USER                             x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      73.927  19.337 -19.718 -0.32 -0.04    +0.239  2.753
ATOM      2  O1A SIA A 801      73.238  19.673 -18.758 -0.05 +0.04    -0.644  2.753
ATOM      3  O1B SIA A 801      75.052  18.882 -19.510 -0.06 +0.07    -0.644  2.753
```

```
ATOM      4  C2  SIA A 801      73.478  19.663 -21.169 -0.21 -0.06    +0.258  2.753
ATOM      5  C3  SIA A 801      72.446  20.811 -21.209 -0.35 -0.04    +0.114  2.753
ATOM      6  C4  SIA A 801      73.070  22.167 -20.847 -0.29 -0.06    +0.149  2.753
ATOM      7  O4  SIA A 801      72.090  23.209 -21.044 -0.08 +0.15    -0.393  2.753
ATOM      8  C5  SIA A 801      74.324  22.455 -21.692 -0.23 -0.04    +0.145  2.753
ATOM      9  N5  SIA A 801      74.997  23.671 -21.194 -0.19 +0.02    -0.352  2.753
ATOM     10  C6  SIA A 801      75.283  21.249 -21.611 -0.13 -0.05    +0.182  2.753
ATOM     11  O6  SIA A 801      74.584  20.046 -22.055 -0.05 +0.08    -0.336  2.753
ATOM     12  C7  SIA A 801      76.580  21.422 -22.430 -0.08 -0.02    +0.180  2.753
ATOM     13  O7  SIA A 801      76.277  21.788 -23.798 +0.01 +0.05    -0.390  2.753
ATOM     14  C8  SIA A 801      77.458  20.150 -22.394 -0.05 -0.01    +0.173  2.753
ATOM     15  O8  SIA A 801      77.738  19.775 -21.028 -0.10 +0.00    -0.391  2.753
ATOM     16  C9  SIA A 801      78.786  20.337 -23.137 -0.00 -0.00    +0.198  2.753
ATOM     17  O9  SIA A 801      79.554  19.119 -23.107 +0.01 +0.00    -0.398  2.753
ATOM     18  C10 SIA A 801      75.209  24.831 -21.866 -0.33 +0.06    +0.214  2.753
ATOM     19  O10 SIA A 801      75.987  25.669 -21.427 -0.64 -0.19    -0.274  2.753
ATOM     20  C11 SIA A 801      74.376  25.184 -23.065 -0.31 -0.00    +0.117  2.753
ATOM     21  H4  SIA A 801      72.475  24.047 -20.820 -0.14 -0.08    +0.210  2.753
ATOM     22  H5  SIA A 801      75.342  23.635 -20.234 +0.05 -0.02    +0.163  2.753
ATOM     23  H7  SIA A 801      77.075  21.894 -24.302 +0.02 -0.01    +0.210  2.753
ATOM     24  H8  SIA A 801      78.278  18.993 -21.006 +0.06 +0.01    +0.210  2.753
ATOM     25  H9  SIA A 801      80.377  19.234 -23.567 +0.01 -0.00    +0.209  2.753
ATOM     26  C1  GAL A 802      72.202  15.998 -25.036 -0.12 -0.03    +0.202  2.753
ATOM     27  C2  GAL A 802      72.760  14.563 -25.094 -0.10 -0.02    +0.173  2.753
ATOM     28  O2  GAL A 802      71.906  13.722 -25.901 -0.04 +0.04    -0.391  2.753
ATOM     29  C3  GAL A 802      72.879  13.968 -23.678 -0.13 -0.05    +0.180  2.753
ATOM     30  O3  GAL A 802      73.542  12.687 -23.729 -0.12 +0.08    -0.390  2.753
ATOM     31  C4  GAL A 802      73.625  14.912 -22.715 -0.20 -0.05    +0.180  2.753
ATOM     32  O4  GAL A 802      75.026  14.969 -23.069 -0.04 +0.06    -0.390  2.753
ATOM     33  C5  GAL A 802      72.975  16.310 -22.774 -0.21 -0.04    +0.176  2.753
ATOM     34  O5  GAL A 802      73.015  16.806 -24.142 -0.04 +0.07    -0.378  2.753
ATOM     35  C6  GAL A 802      73.643  17.329 -21.851 -0.19 -0.05    +0.206  2.753
ATOM     36  O6  GAL A 802      72.806  18.520 -21.785 -0.12 +0.07    -0.344  2.753
ATOM     37  H2  GAL A 802      72.251  12.838 -25.937 +0.06 -0.02    +0.210  2.753
ATOM     38  H3  GAL A 802      73.616  12.320 -22.856 -0.38 -0.07    +0.210  2.753
ATOM     39  H4  GAL A 802      75.486  15.550 -22.476 +0.06 -0.03    +0.210  2.753
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2            # number of dimensions in the field
AVSFLD: nspace=1          # number of physical coordinates
AVSFLD: veclen=7          # vector size
AVSFLD: dim1=39           # atoms
AVSFLD: dim2=2            # conformations
AVSFLD: data=Real        # data type (byte,integer,Real,double)
AVSFLD: field=uniform     # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1rvth.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1rvth.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1rvth.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1rvth.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1rvth.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1rvth.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1rvth.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                 12:30 14" p.m., 06/14/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 45m 02.06s,  CPU= 44m 23.72s,  System= 1.10s
_____________________________________________________________________________
```

1RD8-Sia(α2-3)Gal

```
Number of distinct conformational clusters found = 4,  out of 100 runs,
Using an rmsd-tolerance of 2.0 A

        CLUSTERING HISTOGRAM
        ____________________

_____|____________|_____|____________|_____|_____________________________________________
     |            |     |            |     |
Clus | Lowest     | Run | Mean       | Num | Histogram
-ter | Binding    |     | Binding    | in  |
Rank | Energy     |     | Energy     | Clus|    5    10   15   20   25   30   35
_____|____________|_____|____________|_____|____:____|____:____|____:____|____:___
   1 |      -1.86 |  89 |      -1.67 |  52 |##################################################
   2 |      -1.30 |  47 |      -1.29 |   2 |##
   3 |      -1.27 |  63 |      -1.23 |  42 |########################################
   4 |      -0.84 |  87 |      -0.84 |   4 |####
_____|____________|_____|____________|_____|_____________________________________________

Number of multi-member conformational clusters found = 4, out of 100 runs.

        RMSD TABLE
        __________
```

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	89	-1.86	0.00	2.36	RANKING
1	2	19	-1.79	0.18	2.39	RANKING
1	3	95	-1.78	0.49	2.38	RANKING
1	4	65	-1.77	0.41	2.42	RANKING
1	5	44	-1.77	0.14	2.39	RANKING
1	6	72	-1.76	0.16	2.36	RANKING
1	7	24	-1.76	0.22	2.38	RANKING
1	8	38	-1.75	0.22	2.40	RANKING
1	9	67	-1.75	0.54	2.39	RANKING
1	10	31	-1.75	0.45	2.37	RANKING
1	11	80	-1.75	0.48	2.39	RANKING
1	12	16	-1.75	0.49	2.43	RANKING
1	13	18	-1.75	0.49	2.43	RANKING
1	14	40	-1.74	0.46	2.43	RANKING
1	15	30	-1.73	0.45	2.43	RANKING
1	16	29	-1.73	0.33	2.40	RANKING
1	17	70	-1.73	0.35	2.41	RANKING
1	18	27	-1.73	0.49	2.42	RANKING
1	19	11	-1.72	0.30	2.35	RANKING
1	20	94	-1.72	0.32	2.36	RANKING
1	21	22	-1.72	0.26	2.35	RANKING
1	22	57	-1.72	0.56	2.39	RANKING
1	23	85	-1.71	0.34	2.37	RANKING
1	24	83	-1.71	0.46	2.40	RANKING
1	25	79	-1.71	0.54	2.43	RANKING
1	26	9	-1.70	0.56	2.40	RANKING
1	27	1	-1.70	0.33	2.37	RANKING
1	28	3	-1.70	0.43	2.39	RANKING
1	29	77	-1.70	0.34	2.40	RANKING
1	30	60	-1.69	0.31	2.35	RANKING
1	31	58	-1.69	0.40	2.38	RANKING
1	32	34	-1.69	0.64	2.39	RANKING
1	33	86	-1.69	0.35	2.36	RANKING
1	34	12	-1.69	0.35	2.38	RANKING
1	35	61	-1.69	0.36	2.38	RANKING
1	36	41	-1.69	0.30	2.39	RANKING
1	37	13	-1.68	0.33	2.36	RANKING
1	38	48	-1.65	0.58	2.40	RANKING
1	39	43	-1.63	0.63	2.41	RANKING
1	40	37	-1.62	0.61	2.41	RANKING
1	41	84	-1.62	0.45	2.36	RANKING
1	42	97	-1.61	0.64	2.40	RANKING
1	43	78	-1.61	0.62	2.41	RANKING
1	44	71	-1.59	0.46	2.39	RANKING
1	45	56	-1.59	0.64	2.41	RANKING
1	46	53	-1.56	0.75	2.36	RANKING
1	47	39	-1.56	0.49	2.41	RANKING
1	48	54	-1.47	0.69	2.46	RANKING
1	49	8	-1.45	0.48	2.40	RANKING
1	50	99	-1.45	0.52	2.37	RANKING
1	51	35	-1.38	0.70	2.35	RANKING
1	52	14	-1.07	0.91	2.33	RANKING
2	1	47	-1.30	0.00	2.45	RANKING
2	2	96	-1.29	0.11	2.45	RANKING
3	1	63	-1.27	0.00	2.51	RANKING
3	2	20	-1.27	0.14	2.51	RANKING
3	3	74	-1.27	0.06	2.51	RANKING
3	4	36	-1.26	0.21	2.51	RANKING
3	5	28	-1.26	0.07	2.51	RANKING
3	6	66	-1.26	0.10	2.51	RANKING
3	7	98	-1.26	0.09	2.51	RANKING
3	8	90	-1.26	0.06	2.51	RANKING
3	9	69	-1.26	0.10	2.51	RANKING
3	10	23	-1.26	0.07	2.51	RANKING
3	11	2	-1.26	0.04	2.52	RANKING
3	12	76	-1.26	0.06	2.52	RANKING
3	13	82	-1.25	0.25	2.51	RANKING
3	14	68	-1.25	0.11	2.51	RANKING
3	15	17	-1.25	0.23	2.51	RANKING
3	16	52	-1.25	0.11	2.51	RANKING
3	17	100	-1.25	0.13	2.51	RANKING
3	18	75	-1.25	0.07	2.51	RANKING

```
   3     19      6       -1.25      0.14      2.51           RANKING
   3     20     93       -1.24      0.14      2.51           RANKING
   3     21     50       -1.24      0.11      2.51           RANKING
   3     22     10       -1.24      0.18      2.51           RANKING
   3     23     33       -1.24      0.05      2.52           RANKING
   3     24     25       -1.24      0.16      2.52           RANKING
   3     25     81       -1.24      0.17      2.51           RANKING
   3     26     64       -1.24      0.13      2.51           RANKING
   3     27     42       -1.24      0.10      2.50           RANKING
   3     28     59       -1.24      0.25      2.51           RANKING
   3     29     62       -1.24      0.05      2.51           RANKING
   3     30     55       -1.23      0.16      2.51           RANKING
   3     31     21       -1.23      0.18      2.50           RANKING
   3     32     46       -1.23      0.14      2.50           RANKING
   3     33     92       -1.21      0.18      2.50           RANKING
   3     34     45       -1.20      0.16      2.50           RANKING
   3     35     49       -1.20      0.22      2.53           RANKING
   3     36     88       -1.19      0.20      2.50           RANKING
   3     37     32       -1.16      0.26      2.51           RANKING
   3     38     15       -1.16      0.20      2.53           RANKING
   3     39     26       -1.16      0.24      2.50           RANKING
   3     40      4       -1.15      0.21      2.52           RANKING
   3     41     73       -1.14      0.14      2.52           RANKING
   3     42     91       -1.05      0.44      2.52           RANKING
   4      1     87       -0.84      0.00      2.71           RANKING
   4      2      7       -0.84      0.22      2.73           RANKING
   4      3      5       -0.84      0.17      2.70           RANKING
   4      4     51       -0.84      0.31      2.70           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.20  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.24           at Temperature, T = 298.15 K
Free energy,        A ~ -2729.92 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -1.44 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       89
USER    Run = 89
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 52
USER
USER    RMSD from reference structure       = 2.364 A
USER
USER    Estimated Free Energy of Binding    =   -1.86 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   43.12 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.98 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.53 kcal/mol
USER        Electrostatic Energy            =   -0.45 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
```

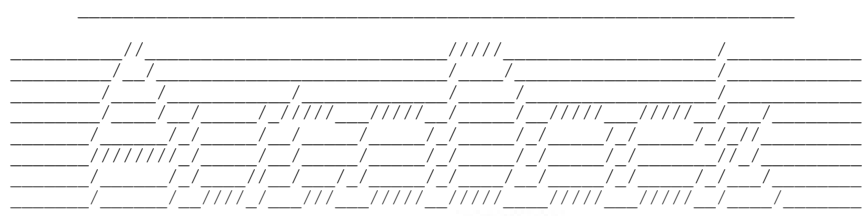
```
USER
USER    DPF = 1rd8a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      74.857621 17.285048 -22.858578
USER    NEWDPF axisangle0 0.524460 -0.823522 0.216223 174.769150
USER    NEWDPF quaternion0        0.523914 -0.822664 0.215998 0.045632
USER
USER                             x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      75.950  16.057 -23.881 -0.04 +0.02    +0.239  2.364
ATOM      2  O1A SIA A3021      76.897  15.341 -24.198 +0.03 -0.07    -0.644  2.364
ATOM      3  O1B SIA A3021      75.339  16.655 -24.767 +0.03 -0.03    -0.644  2.364
ATOM      4  C2  SIA A3021      75.649  16.362 -22.387 -0.13 -0.00    +0.259  2.364
ATOM      5  C3  SIA A3021      76.871  16.116 -21.477 -0.27 +0.00    +0.114  2.364
ATOM      6  C4  SIA A3021      77.979  17.153 -21.705 -0.18 +0.02    +0.149  2.364
ATOM      7  O4  SIA A3021      79.013  16.973 -20.712 -0.25 -0.08    -0.393  2.364
ATOM      8  C5  SIA A3021      77.440  18.596 -21.630 -0.17 +0.01    +0.145  2.364
ATOM      9  N5  SIA A3021      78.505  19.521 -22.058 -0.03 -0.01    -0.352  2.364
ATOM     10  C6  SIA A3021      76.202  18.733 -22.539 -0.07 -0.01    +0.182  2.364
ATOM     11  O6  SIA A3021      75.205  17.739 -22.149 -0.08 +0.02    -0.336  2.364
ATOM     12  C7  SIA A3021      75.549  20.133 -22.527 -0.07 -0.02    +0.180  2.364
ATOM     13  O7  SIA A3021      75.220  20.536 -21.178 -0.10 +0.08    -0.390  2.364
ATOM     14  C8  SIA A3021      74.288  20.181 -23.416 -0.06 -0.04    +0.173  2.364
ATOM     15  O8  SIA A3021      74.615  19.796 -24.770 -0.00 +0.06    -0.391  2.364
ATOM     16  C9  SIA A3021      73.638  21.569 -23.438 -0.10 -0.10    +0.198  2.364
ATOM     17  O9  SIA A3021      72.446  21.553 -24.245 -0.09 +0.35    -0.398  2.364
ATOM     18  C10 SIA A3021      78.870  20.647 -21.396 -0.13 -0.00    +0.214  2.364
ATOM     19  O10 SIA A3021      78.289  21.065 -20.400 -0.58 -0.05    -0.274  2.364
ATOM     20  C11 SIA A3021      79.934  21.487 -22.031 -0.12 -0.03    +0.117  2.364
ATOM     21  H4  SIA A3021      79.699  17.615 -20.852 +0.05 +0.04    +0.210  2.364
ATOM     22  H5  SIA A3021      79.004  19.297 -22.918 +0.03 +0.00    +0.163  2.364
ATOM     23  H7  SIA A3021      74.819  21.397 -21.171 -0.08 -0.08    +0.210  2.364
ATOM     24  H8  SIA A3021      73.839  19.826 -25.318 +0.04 -0.04    +0.210  2.364
ATOM     25  H9  SIA A3021      72.044  22.413 -24.258 -0.20 -0.43    +0.209  2.364
ATOM     26  C1  GAL A3022      70.822  15.836 -22.230 +0.00 +0.03    +0.202  2.364
ATOM     27  C2  GAL A3022      72.198  15.833 -21.539 -0.30 +0.03    +0.173  2.364
ATOM     28  O2  GAL A3022      72.408  17.088 -20.852 -0.25 +0.04    -0.391  2.364
ATOM     29  C3  GAL A3022      73.316  15.628 -22.573 -0.27 +0.03    +0.187  2.364
ATOM     30  O3  GAL A3022      74.596  15.479 -21.883 -0.25 -0.01    -0.336  2.364
ATOM     31  C4  GAL A3022      73.047  14.389 -23.445 -0.25 +0.05    +0.180  2.364
ATOM     32  O4  GAL A3022      73.178  13.187 -22.653 -0.68 -0.25    -0.390  2.364
ATOM     33  C5  GAL A3022      71.640  14.491 -24.069 -0.25 +0.04    +0.176  2.364
ATOM     34  O5  GAL A3022      70.620  14.639 -23.035 -0.25 -0.05    -0.378  2.364
ATOM     35  C6  GAL A3022      71.306  13.264 -24.924 -0.21 +0.04    +0.198  2.364
ATOM     36  O6  GAL A3022      70.013  13.423 -25.542 -0.10 -0.07    -0.398  2.364
ATOM     37  H2  GAL A3022      73.257  17.087 -20.426 -0.31 -0.12    +0.210  2.364
ATOM     38  H4  GAL A3022      73.012  12.422 -23.192 +0.08 +0.14    +0.210  2.364
ATOM     39  H6  GAL A3022      69.806  12.662 -26.073 +0.10 +0.03    +0.209  2.364
TER
ENDMDL
MODEL       47
USER    Run = 47
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 2
USER
USER    RMSD from reference structure      = 2.451 A
USER
USER    Estimated Free Energy of Binding    =   -1.30 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  111.95 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.41 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.27 kcal/mol
USER        Electrostatic Energy            =   -0.14 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rd8a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      74.643578 17.466124 -22.355698
USER    NEWDPF axisangle0 0.259385 0.961534 0.090396 167.469428
USER    NEWDPF quaternion0        0.257835 0.955791 0.089856 0.109132
USER
USER                             x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      73.523  17.240 -23.918 -0.08 +0.00    +0.239  2.451
```

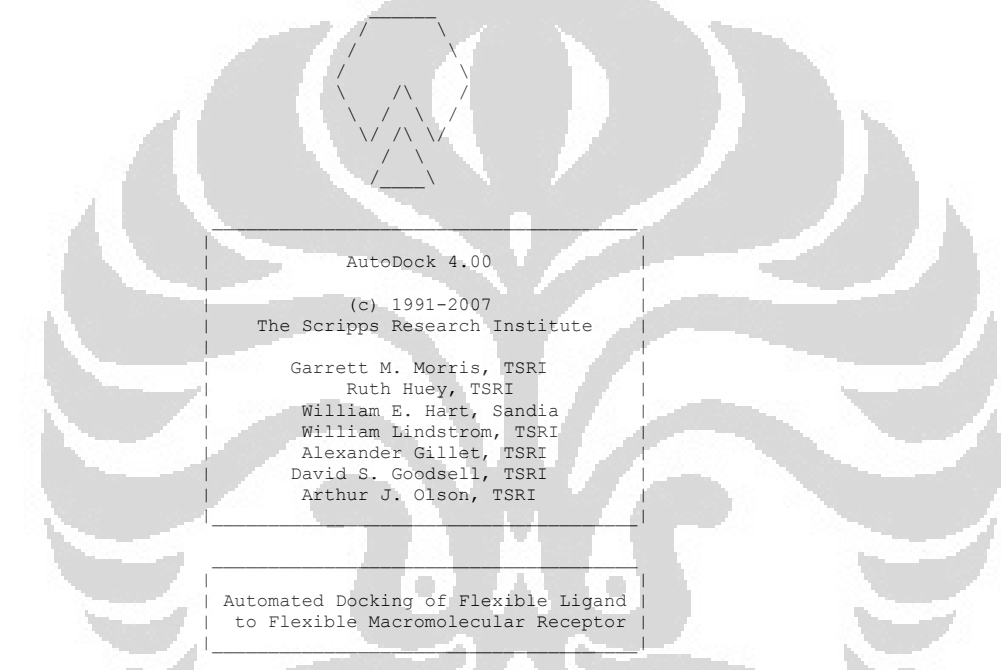
```
ATOM      2  O1A SIA A3021      72.785  16.708 -24.743 +0.03 -0.04    -0.644  2.451
ATOM      3  O1B SIA A3021      74.337  18.079 -24.305 +0.04 +0.02    -0.644  2.451
ATOM      4  C2  SIA A3021      73.571  16.730 -22.450 -0.17 -0.00    +0.259  2.451
ATOM      5  C3  SIA A3021      73.033  15.290 -22.309 -0.34 +0.03    +0.114  2.451
ATOM      6  C4  SIA A3021      73.974  14.256 -22.942 -0.30 +0.05    +0.149  2.451
ATOM      7  O4  SIA A3021      73.505  12.927 -22.628 -0.67 -0.25    -0.393  2.451
ATOM      8  C5  SIA A3021      75.425  14.420 -22.447 -0.22 +0.03    +0.145  2.451
ATOM      9  N5  SIA A3021      76.299  13.540 -23.244 -0.06 -0.09    -0.352  2.451
ATOM     10  C6  SIA A3021      75.858  15.893 -22.592 -0.15 +0.01    +0.182  2.451
ATOM     11  O6  SIA A3021      74.918  16.746 -21.870 -0.10 +0.04    -0.336  2.451
ATOM     12  C7  SIA A3021      77.292  16.192 -22.099 -0.17 +0.01    +0.180  2.451
ATOM     13  O7  SIA A3021      77.466  15.758 -20.731 -0.23 -0.01    -0.390  2.451
ATOM     14  C8  SIA A3021      77.636  17.692 -22.226 -0.10 +0.01    +0.173  2.451
ATOM     15  O8  SIA A3021      77.480  18.127 -23.595 +0.01 -0.01    -0.391  2.451
ATOM     16  C9  SIA A3021      79.063  18.006 -21.764 -0.11 +0.02    +0.198  2.451
ATOM     17  O9  SIA A3021      79.322  19.419 -21.862 -0.04 -0.02    -0.398  2.451
ATOM     18  C10 SIA A3021      77.236  12.704 -22.732 -0.14 +0.07    +0.214  2.451
ATOM     19  O10 SIA A3021      77.518  12.652 -21.540 -0.11 -0.07    -0.274  2.451
ATOM     20  C11 SIA A3021      78.066  11.940 -23.717 -0.09 +0.04    +0.117  2.451
ATOM     21  H4  SIA A3021      74.087  12.287 -23.020 +0.05 +0.13    +0.210  2.451
ATOM     22  H5  SIA A3021      76.190  13.562 -24.258 +0.03 +0.04    +0.163  2.451
ATOM     23  H7  SIA A3021      78.347  15.941 -20.428 -0.05 +0.03    +0.210  2.451
ATOM     24  H8  SIA A3021      77.692  19.050 -23.673 +0.02 -0.00    +0.210  2.451
ATOM     25  H9  SIA A3021      80.207  19.614 -21.576 +0.04 +0.01    +0.209  2.451
ATOM     26  C1  GAL A3022      73.529  20.899 -19.958 -0.08 -0.07    +0.202  2.451
ATOM     27  C2  GAL A3022      73.254  19.388 -20.054 -0.25 -0.02    +0.173  2.451
ATOM     28  O2  GAL A3022      74.329  18.650 -19.429 -0.09 +0.04    -0.391  2.451
ATOM     29  C3  GAL A3022      73.132  18.958 -21.524 -0.24 -0.02    +0.187  2.451
ATOM     30  O3  GAL A3022      72.724  17.556 -21.589 -0.22 +0.03    -0.336  2.451
ATOM     31  C4  GAL A3022      72.113  19.832 -22.276 -0.24 -0.03    +0.180  2.451
ATOM     32  O4  GAL A3022      70.777  19.562 -21.797 -0.12 +0.03    -0.390  2.451
ATOM     33  C5  GAL A3022      72.475  21.321 -22.096 -0.25 -0.06    +0.176  2.451
ATOM     34  O5  GAL A3022      72.532  21.677 -20.682 -0.23 +0.14    -0.378  2.451
ATOM     35  C6  GAL A3022      71.473  22.240 -22.800 -0.23 -0.14    +0.198  2.451
ATOM     36  O6  GAL A3022      71.878  23.618 -22.667 -0.06 +0.40    -0.398  2.451
ATOM     37  H2  GAL A3022      74.159  17.717 -19.488 -0.15 -0.14    +0.210  2.451
ATOM     38  H4  GAL A3022      70.148  20.101 -22.261 +0.12 -0.02    +0.210  2.451
ATOM     39  H6  GAL A3022      71.256  24.188 -23.103 -0.30 -0.32    +0.209  2.451
TER
ENDMDL
MODEL       63
USER    Run = 63
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 42
USER
USER    RMSD from reference structure       = 2.512 A
USER
USER    Estimated Free Energy of Binding    =   -1.27 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  117.08 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.39 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.19 kcal/mol
USER        Electrostatic Energy            =   -0.19 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rd8a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      74.006364 18.584372 -23.124087
USER    NEWDPF axisangle0 -0.533870 0.468387 -0.703986 -126.743165
USER    NEWDPF quaternion0        -0.477243 0.418706 -0.629316 -0.448203
USER
USER                              x       y       z     vdW   Elec       q     RMS
ATOM      1  C1  SIA A3021      75.379  18.233 -21.805 -0.13 -0.02    +0.239  2.512
ATOM      2  O1A SIA A3021      75.976  18.230 -20.731 -0.07 +0.01    -0.644  2.512
ATOM      3  O1B SIA A3021      76.033  18.295 -22.846 +0.04 +0.02    -0.644  2.512
ATOM      4  C2  SIA A3021      73.830  18.356 -21.852 -0.15 -0.03    +0.259  2.512
ATOM      5  C3  SIA A3021      73.245  18.946 -20.551 -0.32 -0.02    +0.114  2.512
ATOM      6  C4  SIA A3021      73.589  20.432 -20.385 -0.35 -0.04    +0.149  2.512
ATOM      7  O4  SIA A3021      72.875  20.963 -19.247 -0.06 +0.11    -0.393  2.512
ATOM      8  C5  SIA A3021      73.231  21.249 -21.643 -0.25 -0.05    +0.145  2.512
ATOM      9  N5  SIA A3021      73.773  22.612 -21.491 -0.10 +0.17    -0.352  2.512
ATOM     10  C6  SIA A3021      73.824  20.564 -22.891 -0.10 -0.05    +0.182  2.512
ATOM     11  O6  SIA A3021      73.343  19.186 -22.959 -0.05 +0.04    -0.336  2.512
```

```
ATOM     12  C7  SIA A3021      73.508  21.275 -24.225 -0.11 -0.10    +0.180  2.512
ATOM     13  O7  SIA A3021      72.083  21.452 -24.388 -0.12 +0.35    -0.390  2.512
ATOM     14  C8  SIA A3021      74.087  20.505 -25.432 -0.07 -0.05    +0.173  2.512
ATOM     15  O8  SIA A3021      75.515  20.342 -25.282 +0.00 +0.06    -0.391  2.512
ATOM     16  C9  SIA A3021      73.805  21.208 -26.764 -0.10 -0.09    +0.198  2.512
ATOM     17  O9  SIA A3021      74.328  20.433 -27.860 -0.01 +0.08    -0.398  2.512
ATOM     18  C10 SIA A3021      73.081  23.755 -21.726 -0.32 -0.10    +0.214  2.512
ATOM     19  O10 SIA A3021      71.941  23.775 -22.177 -0.29 +0.18    -0.274  2.512
ATOM     20  C11 SIA A3021      73.833  25.040 -21.575 -0.45 -0.02    +0.117  2.512
ATOM     21  H4  SIA A3021      73.087  21.883 -19.143 -0.29 -0.16    +0.210  2.512
ATOM     22  H5  SIA A3021      74.742  22.701 -21.186 -0.32 -0.10    +0.163  2.512
ATOM     23  H7  SIA A3021      71.888  21.890 -25.208 -0.00 -0.33    +0.210  2.512
ATOM     24  H8  SIA A3021      75.872  19.868 -26.024 +0.01 -0.02    +0.210  2.512
ATOM     25  H9  SIA A3021      74.153  20.869 -28.686 +0.04 -0.04    +0.209  2.512
ATOM     26  C1  GAL A3022      72.679  15.006 -25.176 -0.09 +0.03    +0.202  2.512
ATOM     27  C2  GAL A3022      72.312  15.872 -23.958 -0.18 +0.02    +0.173  2.512
ATOM     28  O2  GAL A3022      71.547  17.023 -24.383 -0.03 -0.03    -0.391  2.512
ATOM     29  C3  GAL A3022      73.583  16.346 -23.235 -0.16 +0.01    +0.187  2.512
ATOM     30  O3  GAL A3022      73.212  17.038 -22.002 -0.18 +0.02    -0.336  2.512
ATOM     31  C4  GAL A3022      74.511  15.163 -22.909 -0.21 +0.03    +0.180  2.512
ATOM     32  O4  GAL A3022      73.912  14.325 -21.895 -0.68 -0.16    -0.390  2.512
ATOM     33  C5  GAL A3022      74.796  14.358 -24.195 -0.10 +0.04    +0.176  2.512
ATOM     34  O5  GAL A3022      73.553  13.900 -24.809 -0.05 -0.09    -0.378  2.512
ATOM     35  C6  GAL A3022      75.692  13.147 -23.923 -0.13 +0.06    +0.198  2.512
ATOM     36  O6  GAL A3022      75.990  12.458 -25.154 -0.05 -0.13    -0.398  2.512
ATOM     37  H2  GAL A3022      71.321  17.558 -23.631 +0.10 +0.01    +0.210  2.512
ATOM     38  H4  GAL A3022      74.486  13.595 -21.694 +0.08 +0.09    +0.210  2.512
ATOM     39  H6  GAL A3022      76.546  11.707 -24.985 +0.03 +0.09    +0.209  2.512
TER
ENDMDL
MODEL       87
USER    Run = 87
USER    Cluster Rank = 4
USER    Number of conformations in this cluster = 4
USER
USER    RMSD from reference structure       = 2.712 A
USER
USER    Estimated Free Energy of Binding    =   -0.84 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  241.80 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.96 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.66 kcal/mol
USER        Electrostatic Energy            =   -0.30 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rd8a.dpf
USER    NEWDPF move      a.pdbqt
USER    NEWDPF about     76.250000 18.934999 -22.507000
USER    NEWDPF tran0     75.904532 18.798485 -22.571671
USER    NEWDPF axisangle0 -0.586937 0.318069 -0.744538 -106.920992
USER    NEWDPF quaternion0       -0.471573 0.255551 -0.598197 -0.595377
USER
USER                           x       y       z     vdW   Elec       q     RMS
ATOM      1  C1  SIA A3021      76.941  18.948 -20.944 -0.23 +0.02    +0.239  2.712
ATOM      2  O1A SIA A3021      77.217  19.146 -19.763 -0.45 -0.24    -0.644  2.712
ATOM      3  O1B SIA A3021      77.768  19.254 -21.804 +0.01 -0.03    -0.644  2.712
ATOM      4  C2  SIA A3021      75.511  18.507 -21.363 -0.17 -0.02    +0.259  2.712
ATOM      5  C3  SIA A3021      74.455  18.831 -20.286 -0.30 -0.02    +0.114  2.712
ATOM      6  C4  SIA A3021      74.202  20.340 -20.159 -0.31 -0.03    +0.149  2.712
ATOM      7  O4  SIA A3021      73.090  20.564 -19.266 -0.19 +0.08    -0.393  2.712
ATOM      8  C5  SIA A3021      73.903  20.989 -21.526 -0.21 -0.04    +0.145  2.712
ATOM      9  N5  SIA A3021      73.877  22.453 -21.358 -0.04 +0.18    -0.352  2.712
ATOM     10  C6  SIA A3021      74.988  20.577 -22.542 -0.08 -0.04    +0.182  2.712
ATOM     11  O6  SIA A3021      75.053  19.120 -22.614 -0.03 +0.03    -0.336  2.712
ATOM     12  C7  SIA A3021      74.782  21.143 -23.965 -0.04 -0.05    +0.180  2.712
ATOM     13  O7  SIA A3021      73.473  20.798 -24.471 -0.05 +0.16    -0.390  2.712
ATOM     14  C8  SIA A3021      75.873  20.648 -24.938 -0.00 -0.03    +0.173  2.712
ATOM     15  O8  SIA A3021      77.183  21.006 -24.445 +0.01 +0.04    -0.391  2.712
ATOM     16  C9  SIA A3021      75.701  21.218 -26.350 -0.01 -0.04    +0.198  2.712
ATOM     17  O9  SIA A3021      76.715  20.696 -27.229 +0.00 +0.04    -0.398  2.712
ATOM     18  C10 SIA A3021      72.909  23.274 -21.837 -0.29 -0.11    +0.214  2.712
ATOM     19  O10 SIA A3021      71.984  22.888 -22.543 -0.24 +0.22    -0.274  2.712
ATOM     20  C11 SIA A3021      73.100  24.742 -21.614 -0.42 -0.03    +0.117  2.712
ATOM     21  H4  SIA A3021      72.933  21.498 -19.187 -0.19 -0.10    +0.210  2.712
```

```
ATOM     22  H5  SIA A3021      74.645  22.881 -20.842 -0.34 -0.13    +0.163  2.712
ATOM     23  H7  SIA A3021      73.346  21.147 -25.345 +0.05 -0.12    +0.210  2.712
ATOM     24  H8  SIA A3021      77.855  20.702 -25.044 +0.01 -0.01    +0.210  2.712
ATOM     25  H9  SIA A3021      76.609  21.050 -28.104 +0.01 -0.02    +0.209  2.712
ATOM     26  C1  GAL A3022      76.469  15.007 -24.593 -0.03 +0.03    +0.202  2.712
ATOM     27  C2  GAL A3022      75.532  15.669 -23.566 -0.09 +0.02    +0.173  2.712
ATOM     28  O2  GAL A3022      74.543  16.473 -24.247 -0.01 -0.02    -0.391  2.712
ATOM     29  C3  GAL A3022      76.335  16.559 -22.605 -0.12 +0.01    +0.187  2.712
ATOM     30  O3  GAL A3022      75.453  17.056 -21.550 -0.08 +0.05    -0.336  2.712
ATOM     31  C4  GAL A3022      77.509  15.785 -21.978 -0.18 +0.01    +0.180  2.712
ATOM     32  O4  GAL A3022      77.011  14.776 -21.072 -0.19 +0.01    -0.390  2.712
ATOM     33  C5  GAL A3022      78.365  15.151 -23.095 -0.06 +0.02    +0.176  2.712
ATOM     34  O5  GAL A3022      77.556  14.285 -23.946 -0.01 -0.06    -0.378  2.712
ATOM     35  C6  GAL A3022      79.533  14.340 -22.526 -0.07 +0.03    +0.198  2.712
ATOM     36  O6  GAL A3022      80.347  13.819 -23.596 -0.00 -0.05    -0.398  2.712
ATOM     37  H2  GAL A3022      73.965  16.882 -23.613 +0.06 +0.01    +0.210  2.712
ATOM     38  H4  GAL A3022      77.735  14.298 -20.685 -0.41 -0.05    +0.210  2.712
ATOM     39  H6  GAL A3022      81.072  13.315 -23.243 +0.02 +0.03    +0.209  2.712
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2            # number of dimensions in the field
AVSFLD: nspace=1          # number of physical coordinates
AVSFLD: veclen=7          # vector size
AVSFLD: dim1=39           # atoms
AVSFLD: dim2=4            # conformations
AVSFLD: data=Real       # data type (byte,integer,Real,double)
AVSFLD: field=uniform     # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1rd8a.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1rd8a.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1rd8a.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1rd8a.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1rd8a.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1rd8a.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1rd8a.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                 1:14 00" p.m., 06/14/2009



_______________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 43m 45.79s,  CPU= 43m 06.14s,  System= 0.96s
_______________________________________________________________________________
```

1RD8-Sia(α2-6)Gal





Number of distinct conformational clusters found = 4, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.99	4	-1.75	77	##
2	-1.40	2	-1.35	19	###################
3	-1.17	80	-1.15	3	###
4	-1.15	41	-1.15	1	#

Number of multi-member conformational clusters found = 3, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	4	-1.99	0.00	2.14	RANKING
1	2	12	-1.99	0.07	2.09	RANKING
1	3	9	-1.99	0.02	2.15	RANKING
1	4	82	-1.99	0.06	2.13	RANKING
1	5	95	-1.98	0.06	2.13	RANKING
1	6	87	-1.98	0.05	2.15	RANKING
1	7	76	-1.98	0.06	2.13	RANKING
1	8	29	-1.98	0.08	2.09	RANKING
1	9	53	-1.97	0.04	2.13	RANKING
1	10	33	-1.97	0.07	2.20	RANKING
1	11	45	-1.97	0.07	2.11	RANKING
1	12	98	-1.97	0.06	2.18	RANKING
1	13	24	-1.97	0.06	2.12	RANKING
1	14	100	-1.97	0.09	2.09	RANKING
1	15	66	-1.96	0.08	2.12	RANKING
1	16	94	-1.95	0.09	2.18	RANKING
1	17	30	-1.95	0.07	2.11	RANKING
1	18	67	-1.95	0.09	2.11	RANKING
1	19	52	-1.93	0.09	2.11	RANKING
1	20	62	-1.92	0.11	2.09	RANKING
1	21	6	-1.92	0.17	2.08	RANKING
1	22	99	-1.92	0.15	2.02	RANKING
1	23	39	-1.91	0.08	2.11	RANKING
1	24	57	-1.91	0.11	2.21	RANKING
1	25	55	-1.91	0.12	2.04	RANKING
1	26	91	-1.89	0.19	2.12	RANKING
1	27	70	-1.88	0.12	2.09	RANKING
1	28	56	-1.86	0.22	1.99	RANKING
1	29	40	-1.86	0.13	2.08	RANKING
1	30	74	-1.83	0.39	2.15	RANKING
1	31	5	-1.82	0.17	2.08	RANKING
1	32	28	-1.82	0.37	2.15	RANKING
1	33	97	-1.82	0.26	2.19	RANKING
1	34	48	-1.80	0.25	2.04	RANKING
1	35	90	-1.79	0.41	2.11	RANKING
1	36	8	-1.79	0.44	2.10	RANKING
1	37	78	-1.78	0.22	2.10	RANKING
1	38	34	-1.75	0.30	1.99	RANKING
1	39	47	-1.74	0.29	2.20	RANKING
1	40	20	-1.72	0.49	2.02	RANKING
1	41	35	-1.65	1.23	2.14	RANKING
1	42	58	-1.65	1.23	2.14	RANKING
1	43	1	-1.64	1.25	2.14	RANKING
1	44	50	-1.63	1.26	2.14	RANKING
1	45	77	-1.63	1.20	2.15	RANKING
1	46	11	-1.63	1.22	2.17	RANKING
1	47	61	-1.63	1.25	2.16	RANKING
1	48	32	-1.63	1.26	2.16	RANKING
1	49	42	-1.63	1.25	2.12	RANKING
1	50	93	-1.63	1.25	2.12	RANKING
1	51	46	-1.62	1.15	2.15	RANKING
1	52	88	-1.62	1.23	2.14	RANKING
1	53	23	-1.62	1.26	2.14	RANKING
1	54	65	-1.62	1.23	2.19	RANKING
1	55	68	-1.62	1.26	2.10	RANKING
1	56	73	-1.61	1.11	2.18	RANKING
1	57	25	-1.61	1.22	2.17	RANKING
1	58	89	-1.61	1.12	2.19	RANKING
1	59	16	-1.60	1.24	2.16	RANKING
1	60	17	-1.60	1.24	2.17	RANKING
1	61	63	-1.60	1.13	2.19	RANKING
1	62	13	-1.60	1.22	2.14	RANKING
1	63	26	-1.59	1.24	2.19	RANKING
1	64	43	-1.58	0.77	2.07	RANKING
1	65	69	-1.58	1.23	2.13	RANKING
1	66	44	-1.58	1.11	2.19	RANKING
1	67	22	-1.58	1.25	2.20	RANKING
1	68	38	-1.57	1.15	2.23	RANKING
1	69	31	-1.56	1.26	2.16	RANKING
1	70	21	-1.56	1.31	2.17	RANKING
1	71	15	-1.56	1.32	2.20	RANKING

```
   1     72     64       -1.55      1.35      2.21           RANKING
   1     73     49       -1.53      1.38      2.20           RANKING
   1     74     72       -1.52      1.32      2.21           RANKING
   1     75     19       -1.51      1.39      2.23           RANKING
   1     76     85       -1.48      1.48      2.17           RANKING
   1     77     92       -1.45      1.48      2.28           RANKING
   2      1      2       -1.40      0.00      2.72           RANKING
   2      2     75       -1.40      0.03      2.72           RANKING
   2      3     54       -1.38      0.08      2.72           RANKING
   2      4     60       -1.38      0.06      2.71           RANKING
   2      5     27       -1.38      0.44      2.72           RANKING
   2      6     18       -1.37      0.06      2.73           RANKING
   2      7     10       -1.37      0.44      2.74           RANKING
   2      8      7       -1.36      0.12      2.71           RANKING
   2      9     79       -1.36      0.21      2.73           RANKING
   2     10     37       -1.36      0.15      2.73           RANKING
   2     11     86       -1.36      0.18      2.73           RANKING
   2     12     51       -1.34      0.27      2.73           RANKING
   2     13     36       -1.34      0.42      2.73           RANKING
   2     14     81       -1.34      0.28      2.75           RANKING
   2     15      3       -1.34      0.29      2.73           RANKING
   2     16     14       -1.30      0.71      2.78           RANKING
   2     17     83       -1.30      0.74      2.78           RANKING
   2     18     59       -1.30      0.66      2.78           RANKING
   2     19     96       -1.29      0.69      2.78           RANKING
   3      1     80       -1.17      0.00      2.76           RANKING
   3      2     84       -1.14      0.36      2.82           RANKING
   3      3     71       -1.13      0.48      2.83           RANKING
   4      1     41       -1.15      0.00      2.78           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.15  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.28           at Temperature, T = 298.15 K
Free energy,        A ~ -2730.13 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -1.65 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL        4
USER    Run = 4
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 77
USER
USER    RMSD from reference structure       = 2.141 A
USER
USER    Estimated Free Energy of Binding    =   -1.99 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   34.75 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -6.11 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.28 kcal/mol
USER        Electrostatic Energy            =   -0.83 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
```

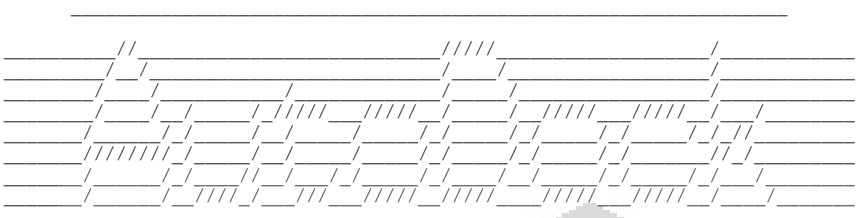
```
USER
USER
USER    DPF = 1rd8h.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      75.539358 20.410131 -22.625543
USER    NEWDPF axisangle0 -0.139699 -0.917934 -0.371324 29.649193
USER    NEWDPF quaternion0        -0.035744 -0.234863 -0.095007 0.966714
USER
USER                              x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      76.804  19.021 -20.602 -0.27 +0.03    +0.239  2.141
ATOM      2  O1A SIA A 801      77.369  18.077 -20.057 -0.40 -0.30    -0.644  2.141
ATOM      3  O1B SIA A 801      76.369  19.937 -19.904 -0.20 -0.06    -0.644  2.141
ATOM      4  C2  SIA A 801      76.460  18.970 -22.117 -0.08 -0.00    +0.258  2.141
ATOM      5  C3  SIA A 801      76.436  17.523 -22.655 -0.10 +0.00    +0.114  2.141
ATOM      6  C4  SIA A 801      75.241  16.722 -22.118 -0.11 -0.01    +0.149  2.141
ATOM      7  O4  SIA A 801      75.200  15.435 -22.770 -0.10 -0.04    -0.393  2.141
ATOM      8  C5  SIA A 801      73.914  17.470 -22.341 -0.18 -0.01    +0.145  2.141
ATOM      9  N5  SIA A 801      72.817  16.761 -21.653 -0.17 +0.01    -0.352  2.141
ATOM     10  C6  SIA A 801      74.039  18.907 -21.795 -0.17 -0.02    +0.182  2.141
ATOM     11  O6  SIA A 801      75.163  19.574 -22.446 -0.03 +0.04    -0.336  2.141
ATOM     12  C7  SIA A 801      72.764  19.759 -21.971 -0.22 -0.03    +0.180  2.141
ATOM     13  O7  SIA A 801      72.317  19.735 -23.348 -0.08 +0.08    -0.390  2.141
ATOM     14  C8  SIA A 801      72.974  21.216 -21.499 -0.27 -0.06    +0.173  2.141
ATOM     15  O8  SIA A 801      73.441  21.236 -20.132 -0.14 +0.17    -0.391  2.141
ATOM     16  C9  SIA A 801      71.692  22.051 -21.593 -0.28 -0.08    +0.198  2.141
ATOM     17  O9  SIA A 801      71.943  23.406 -21.176 -0.24 +0.17    -0.398  2.141
ATOM     18  C10 SIA A 801      71.715  16.201 -22.215 -0.36 +0.02    +0.214  2.141
ATOM     19  O10 SIA A 801      70.768  15.859 -21.518 -0.38 -0.05    -0.274  2.141
ATOM     20  C11 SIA A 801      71.702  15.836 -23.673 -0.24 +0.01    +0.117  2.141
ATOM     21  H4  SIA A 801      74.461  14.939 -22.437 +0.07 +0.04    +0.210  2.141
ATOM     22  H5  SIA A 801      72.895  16.683 -20.638 -0.39 -0.05    +0.163  2.141
ATOM     23  H7  SIA A 801      71.533  20.259 -23.457 +0.10 -0.06    +0.210  2.141
ATOM     24  H8  SIA A 801      73.570  22.131 -19.842 -0.27 -0.18    +0.210  2.141
ATOM     25  H9  SIA A 801      71.148  23.924 -21.235 +0.12 -0.07    +0.209  2.141
ATOM     26  C1  GAL A 802      78.506  22.266 -25.986 +0.01 -0.01    +0.202  2.141
ATOM     27  C2  GAL A 802      79.016  23.697 -25.730 -0.01 +0.01    +0.173  2.141
ATOM     28  O2  GAL A 802      79.904  24.113 -26.791 +0.00 -0.02    -0.391  2.141
ATOM     29  C3  GAL A 802      79.754  23.779 -24.380 -0.08 -0.01    +0.180  2.141
ATOM     30  O3  GAL A 802      80.093  25.149 -24.079 -0.14 -0.21    -0.390  2.141
ATOM     31  C4  GAL A 802      78.923  23.175 -23.230 -0.11 -0.04    +0.180  2.141
ATOM     32  O4  GAL A 802      77.794  24.029 -22.939 -0.11 +0.03    -0.390  2.141
ATOM     33  C5  GAL A 802      78.465  21.757 -23.630 -0.02 -0.02    +0.176  2.141
ATOM     34  O5  GAL A 802      77.695  21.826 -24.863 +0.01 +0.04    -0.378  2.141
ATOM     35  C6  GAL A 802      77.629  21.063 -22.554 -0.06 -0.02    +0.206  2.141
ATOM     36  O6  GAL A 802      77.474  19.660 -22.913 -0.01 +0.01    -0.344  2.141
ATOM     37  H2  GAL A 802      80.218  24.996 -26.634 +0.01 +0.03    +0.210  2.141
ATOM     38  H3  GAL A 802      80.548  25.200 -23.246 -0.44 -0.13    +0.210  2.141
ATOM     39  H4  GAL A 802      77.281  23.657 -22.230 +0.06 -0.05    +0.210  2.141
TER
ENDMDL
MODEL        2
USER    Run = 2
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 19
USER
USER    RMSD from reference structure      = 2.720 A
USER
USER    Estimated Free Energy of Binding    =   -1.40 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   94.16 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.52 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.50 kcal/mol
USER        Electrostatic Energy            =   -0.02 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rd8h.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      74.693338 19.624720 -22.262231
USER    NEWDPF axisangle0 -0.128218 -0.045207 0.990715 135.331422
USER    NEWDPF quaternion0        -0.118600 -0.041815 0.916394 0.380010
USER
USER                              x       y       z    vdW   Elec        q     RMS
```

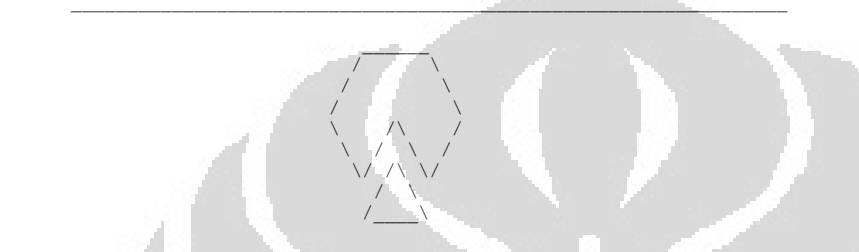
```
ATOM      1  C1  SIA A 801      73.354  20.228 -19.925 -0.31 -0.05    +0.239  2.720
ATOM      2  O1A SIA A 801      72.494  20.736 -19.209 +0.31 +0.11    -0.644  2.720
ATOM      3  O1B SIA A 801      74.367  19.768 -19.400 -0.16 +0.04    -0.644  2.720
ATOM      4  C2  SIA A 801      73.265  20.342 -21.472 -0.19 -0.06    +0.258  2.720
ATOM      5  C3  SIA A 801      72.355  21.509 -21.913 -0.31 -0.04    +0.114  2.720
ATOM      6  C4  SIA A 801      72.981  22.880 -21.613 -0.32 -0.07    +0.149  2.720
ATOM      7  O4  SIA A 801      72.149  23.916 -22.179 -0.20 +0.26    -0.393  2.720
ATOM      8  C5  SIA A 801      74.410  22.983 -22.176 -0.19 -0.06    +0.145  2.720
ATOM      9  N5  SIA A 801      75.042  24.235 -21.714 -0.16 +0.09    -0.352  2.720
ATOM     10  C6  SIA A 801      75.235  21.768 -21.704 -0.06 -0.06    +0.182  2.720
ATOM     11  O6  SIA A 801      74.566  20.540 -22.122 -0.06 +0.07    -0.336  2.720
ATOM     12  C7  SIA A 801      76.691  21.761 -22.216 -0.12 -0.03    +0.180  2.720
ATOM     13  O7  SIA A 801      76.730  21.921 -23.655 +0.01 +0.06    -0.390  2.720
ATOM     14  C8  SIA A 801      77.443  20.477 -21.798 -0.13 -0.01    +0.173  2.720
ATOM     15  O8  SIA A 801      77.383  20.308 -20.365 -0.52 -0.07    -0.391  2.720
ATOM     16  C9  SIA A 801      78.913  20.494 -22.231 -0.07 -0.01    +0.198  2.720
ATOM     17  O9  SIA A 801      79.563  19.266 -21.851 -0.04 -0.02    -0.398  2.720
ATOM     18  C10 SIA A 801      75.484  25.268 -22.477 -0.27 +0.00    +0.214  2.720
ATOM     19  O10 SIA A 801      76.204  26.132 -21.994 -0.54 -0.10    -0.274  2.720
ATOM     20  C11 SIA A 801      74.968  25.462 -23.874 -0.20 -0.03    +0.117  2.720
ATOM     21  H4  SIA A 801      72.535  24.763 -21.993 +0.12 -0.08    +0.210  2.720
ATOM     22  H5  SIA A 801      75.160  24.335 -20.705 -0.10 -0.05    +0.163  2.720
ATOM     23  H7  SIA A 801      77.625  21.917 -23.970 +0.03 -0.02    +0.210  2.720
ATOM     24  H8  SIA A 801      77.845  19.519 -20.107 +0.07 +0.07    +0.210  2.720
ATOM     25  H9  SIA A 801      80.475  19.277 -22.119 +0.03 +0.00    +0.209  2.720
ATOM     26  C1  GAL A 802      72.618  16.173 -24.968 -0.11 +0.02    +0.202  2.720
ATOM     27  C2  GAL A 802      73.068  14.726 -24.690 -0.12 +0.03    +0.173  2.720
ATOM     28  O2  GAL A 802      72.357  13.804 -25.545 -0.04 -0.08    -0.391  2.720
ATOM     29  C3  GAL A 802      72.823  14.354 -23.215 -0.29 +0.06    +0.180  2.720
ATOM     30  O3  GAL A 802      73.386  13.055 -22.928 -0.55 -0.22    -0.390  2.720
ATOM     31  C4  GAL A 802      73.403  15.406 -22.249 -0.29 +0.03    +0.180  2.720
ATOM     32  O4  GAL A 802      74.848  15.353 -22.274 -0.18 -0.03    -0.390  2.720
ATOM     33  C5  GAL A 802      72.887  16.803 -22.656 -0.24 +0.00    +0.176  2.720
ATOM     34  O5  GAL A 802      73.269  17.078 -24.034 -0.04 -0.01    -0.378  2.720
ATOM     35  C6  GAL A 802      73.405  17.926 -21.758 -0.20 -0.02    +0.206  2.720
ATOM     36  O6  GAL A 802      72.665  19.144 -22.058 -0.13 +0.04    -0.344  2.720
ATOM     37  H2  GAL A 802      72.634  12.912 -25.374 +0.06 +0.06    +0.210  2.720
ATOM     38  H3  GAL A 802      73.235  12.826 -22.019 +0.06 +0.20    +0.210  2.720
ATOM     39  H4  GAL A 802      75.206  16.001 -21.678 -0.07 -0.02    +0.210  2.720
TER
ENDMDL
MODEL       80
USER    Run = 80
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 3
USER
USER    RMSD from reference structure       = 2.757 A
USER
USER    Estimated Free Energy of Binding    =   -1.17 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  139.60 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.28 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.82 kcal/mol
USER        Electrostatic Energy            =   -0.47 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rd8h.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      76.210614 19.496068 -22.083795
USER    NEWDPF axisangle0 0.088970 0.090721 -0.991894 -112.235307
USER    NEWDPF quaternion0        0.073861 0.075315 -0.823455 -0.557489
USER
USER                               x       y       z     vdW   Elec       q     RMS
ATOM      1  C1  SIA A 801      74.903  19.565 -19.653 -0.36 -0.01    +0.239  2.757
ATOM      2  O1A SIA A 801      73.963  19.703 -18.875 -0.16 -0.01    -0.644  2.757
ATOM      3  O1B SIA A 801      76.049  19.558 -19.205 -0.08 -0.13    -0.644  2.757
ATOM      4  C2  SIA A 801      74.672  19.601 -21.190 -0.19 -0.04    +0.258  2.757
ATOM      5  C3  SIA A 801      73.344  20.300 -21.557 -0.25 -0.02    +0.114  2.757
ATOM      6  C4  SIA A 801      73.389  21.812 -21.291 -0.25 -0.06    +0.149  2.757
ATOM      7  O4  SIA A 801      72.177  22.418 -21.789 -0.17 +0.19    -0.393  2.757
ATOM      8  C5  SIA A 801      74.617  22.464 -21.953 -0.16 -0.06    +0.145  2.757
ATOM      9  N5  SIA A 801      74.727  23.873 -21.526 -0.13 +0.13    -0.352  2.757
ATOM     10  C6  SIA A 801      75.888  21.689 -21.549 -0.07 -0.05    +0.182  2.757
```

```
ATOM     11  O6  SIA A 801      75.738  20.287 -21.928 -0.06 +0.04    -0.336  2.757
ATOM     12  C7  SIA A 801      77.188  22.252 -22.162 -0.15 -0.04    +0.180  2.757
ATOM     13  O7  SIA A 801      77.062  22.384 -23.599 +0.00 +0.06    -0.390  2.757
ATOM     14  C8  SIA A 801      78.416  21.383 -21.808 -0.15 -0.02    +0.173  2.757
ATOM     15  O8  SIA A 801      78.526  21.234 -20.375 -0.53 -0.05    -0.391  2.757
ATOM     16  C9  SIA A 801      79.725  21.975 -22.343 -0.11 -0.06    +0.198  2.757
ATOM     17  O9  SIA A 801      80.835  21.117 -22.019 -0.03 +0.07    -0.398  2.757
ATOM     18  C10 SIA A 801      74.667  24.981 -22.311 -0.28 -0.03    +0.214  2.757
ATOM     19  O10 SIA A 801      75.013  26.071 -21.873 -0.79 -0.08    -0.274  2.757
ATOM     20  C11 SIA A 801      74.023  24.924 -23.667 -0.15 -0.07    +0.117  2.757
ATOM     21  H4  SIA A 801      72.205  23.353 -21.624 +0.13 -0.11    +0.210  2.757
ATOM     22  H5  SIA A 801      74.863  24.034 -20.528 -0.21 -0.09    +0.163  2.757
ATOM     23  H7  SIA A 801      77.862  22.730 -23.977 +0.04 -0.02    +0.210  2.757
ATOM     24  H8  SIA A 801      79.280  20.700 -20.157 +0.08 +0.03    +0.210  2.757
ATOM     25  H9  SIA A 801      81.646  21.484 -22.351 +0.03 -0.05    +0.209  2.757
ATOM     26  C1  GAL A 802      75.507  15.447 -24.663 -0.03 +0.02    +0.202  2.757
ATOM     27  C2  GAL A 802      76.515  14.305 -24.428 -0.04 +0.03    +0.173  2.757
ATOM     28  O2  GAL A 802      76.174  13.158 -25.238 -0.02 -0.10    -0.391  2.757
ATOM     29  C3  GAL A 802      76.539  13.898 -22.942 -0.14 +0.04    +0.180  2.757
ATOM     30  O3  GAL A 802      77.591  12.937 -22.706 -0.08 -0.10    -0.390  2.757
ATOM     31  C4  GAL A 802      76.715  15.114 -22.012 -0.21 +0.01    +0.180  2.757
ATOM     32  O4  GAL A 802      78.056  15.640 -22.139 -0.07 -0.03    -0.390  2.757
ATOM     33  C5  GAL A 802      75.659  16.180 -22.371 -0.17 +0.00    +0.176  2.757
ATOM     34  O5  GAL A 802      75.804  16.555 -23.770 -0.01 -0.02    -0.378  2.757
ATOM     35  C6  GAL A 802      75.745  17.436 -21.503 -0.09 -0.02    +0.206  2.757
ATOM     36  O6  GAL A 802      74.562  18.251 -21.741 -0.10 +0.04    -0.344  2.757
ATOM     37  H2  GAL A 802      76.796  12.455 -25.094 +0.03 +0.07    +0.210  2.757
ATOM     38  H3  GAL A 802      77.606  12.686 -21.790 +0.05 +0.05    +0.210  2.757
ATOM     39  H4  GAL A 802      78.165  16.390 -21.565 +0.06 +0.02    +0.210  2.757
TER
ENDMDL
MODEL       41
USER    Run = 41
USER    Cluster Rank = 4
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 2.778 A
USER
USER    Estimated Free Energy of Binding    =   -1.15 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  142.73 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.27 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.01 kcal/mol
USER        Electrostatic Energy            =   -0.26 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1rd8h.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      73.480860 18.447003 -23.495842
USER    NEWDPF axisangle0 -0.464361 0.489275 -0.738227 -134.204211
USER    NEWDPF quaternion0        -0.427770 0.450720 -0.680054 -0.389090
USER
USER                             x       y       z     vdW   Elec       q    RMS
ATOM      1  C1  SIA A 801      75.564  18.237 -21.696 -0.14 -0.02    +0.239  2.778
ATOM      2  O1A SIA A 801      76.123  18.245 -20.602 -0.10 -0.02    -0.644  2.778
ATOM      3  O1B SIA A 801      76.253  18.284 -22.715 +0.04 +0.01    -0.644  2.778
ATOM      4  C2  SIA A 801      74.019  18.368 -21.798 -0.15 -0.03    +0.258  2.778
ATOM      5  C3  SIA A 801      73.408  18.988 -20.522 -0.34 -0.02    +0.114  2.778
ATOM      6  C4  SIA A 801      73.760  20.476 -20.372 -0.33 -0.04    +0.149  2.778
ATOM      7  O4  SIA A 801      73.042  21.023 -19.245 -0.04 +0.12    -0.393  2.778
ATOM      8  C5  SIA A 801      73.422  21.267 -21.649 -0.23 -0.05    +0.145  2.778
ATOM      9  N5  SIA A 801      73.939  22.645 -21.537 -0.09 +0.17    -0.352  2.778
ATOM     10  C6  SIA A 801      74.052  20.564 -22.869 -0.09 -0.05    +0.182  2.778
ATOM     11  O6  SIA A 801      73.572  19.186 -22.931 -0.05 +0.04    -0.336  2.778
ATOM     12  C7  SIA A 801      73.772  21.268 -24.214 -0.09 -0.09    +0.180  2.778
ATOM     13  O7  SIA A 801      72.352  21.495 -24.387 -0.10 +0.35    -0.390  2.778
ATOM     14  C8  SIA A 801      74.339  20.471 -25.410 -0.05 -0.05    +0.173  2.778
ATOM     15  O8  SIA A 801      75.750  20.226 -25.223 +0.00 +0.05    -0.391  2.778
ATOM     16  C9  SIA A 801      74.139  21.200 -26.744 -0.08 -0.08    +0.198  2.778
ATOM     17  O9  SIA A 801      74.651  20.407 -27.832 -0.00 +0.07    -0.398  2.778
ATOM     18  C10 SIA A 801      73.224  23.799 -21.547 -0.33 -0.09    +0.214  2.778
ATOM     19  O10 SIA A 801      73.786  24.878 -21.690 -0.37 +0.05    -0.274  2.778
ATOM     20  C11 SIA A 801      71.758  23.794 -21.217 -0.45 -0.05    +0.117  2.778
```

```
ATOM     21  H4  SIA A 801      73.261  21.942 -19.153 -0.30 -0.17    +0.210  2.778
ATOM     22  H5  SIA A 801      74.951  22.742 -21.440 -0.15 -0.08    +0.163  2.778
ATOM     23  H7  SIA A 801      72.179  21.928 -25.215 -0.03 -0.33    +0.210  2.778
ATOM     24  H8  SIA A 801      76.099  19.737 -25.959 +0.01 -0.02    +0.210  2.778
ATOM     25  H9  SIA A 801      74.526  20.859 -28.659 +0.03 -0.04    +0.209  2.778
ATOM     26  C1  GAL A 802      70.591  14.557 -23.732 -0.29 +0.03    +0.202  2.778
ATOM     27  C2  GAL A 802      70.978  13.481 -24.766 -0.25 +0.04    +0.173  2.778
ATOM     28  O2  GAL A 802      70.051  12.375 -24.712 -0.18 -0.08    -0.391  2.778
ATOM     29  C3  GAL A 802      72.408  12.969 -24.507 -0.15 +0.06    +0.180  2.778
ATOM     30  O3  GAL A 802      72.816  12.077 -25.566 -0.08 -0.13    -0.390  2.778
ATOM     31  C4  GAL A 802      73.420  14.123 -24.368 -0.15 +0.04    +0.180  2.778
ATOM     32  O4  GAL A 802      73.620  14.758 -25.651 -0.01 -0.06    -0.390  2.778
ATOM     33  C5  GAL A 802      72.897  15.129 -23.321 -0.24 +0.04    +0.176  2.778
ATOM     34  O5  GAL A 802      71.587  15.616 -23.729 -0.12 -0.05    -0.378  2.778
ATOM     35  C6  GAL A 802      73.830  16.320 -23.105 -0.15 +0.01    +0.206  2.778
ATOM     36  O6  GAL A 802      73.383  17.058 -21.931 -0.17 +0.03    -0.344  2.778
ATOM     37  H2  GAL A 802      70.289  11.712 -25.349 +0.10 +0.04    +0.210  2.778
ATOM     38  H3  GAL A 802      73.698  11.761 -25.407 +0.04 +0.09    +0.210  2.778
ATOM     39  H4  GAL A 802      74.244  15.470 -25.566 +0.03 +0.02    +0.210  2.778
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2           # number of dimensions in the field
AVSFLD: nspace=1         # number of physical coordinates
AVSFLD: veclen=7         # vector size
AVSFLD: dim1=39          # atoms
AVSFLD: dim2=4           # conformations
AVSFLD: data=Real       # data type (byte,integer,Real,double)
AVSFLD: field=uniform    # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1rd8h.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1rd8h.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1rd8h.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1rd8h.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1rd8h.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1rd8h.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1rd8h.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                1:58 40" p.m., 06/14/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 44m 40.08s,  CPU= 44m 37.22s,  System= 0.68s
_____________________________________________________________________________
```

1MQN-Sia(α2-3)Gal





Number of distinct conformational clusters found = 3, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.06	53	-1.00	46	##
2	-0.91	82	-0.89	45	###
3	-0.66	91	-0.65	9	#########

Number of multi-member conformational clusters found = 3, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	53	-1.06	0.00	1.96	RANKING
1	2	79	-1.06	0.07	1.92	RANKING
1	3	46	-1.06	0.03	1.96	RANKING
1	4	56	-1.06	0.09	1.92	RANKING
1	5	78	-1.06	0.03	1.95	RANKING
1	6	10	-1.05	0.04	1.95	RANKING
1	7	93	-1.05	0.09	1.92	RANKING
1	8	13	-1.05	0.07	1.96	RANKING
1	9	1	-1.05	0.05	1.93	RANKING
1	10	67	-1.05	0.18	1.89	RANKING
1	11	20	-1.05	0.07	1.94	RANKING
1	12	5	-1.05	0.03	1.95	RANKING
1	13	76	-1.05	0.10	1.98	RANKING
1	14	90	-1.05	0.07	1.94	RANKING
1	15	88	-1.05	0.07	1.95	RANKING
1	16	23	-1.05	0.08	1.97	RANKING
1	17	94	-1.05	0.12	1.93	RANKING
1	18	14	-1.04	0.06	1.97	RANKING
1	19	61	-1.04	0.07	1.95	RANKING
1	20	6	-1.04	0.05	1.95	RANKING
1	21	40	-1.04	0.07	1.93	RANKING
1	22	11	-1.04	0.14	1.99	RANKING
1	23	86	-1.04	0.12	1.97	RANKING
1	24	63	-1.04	0.08	1.91	RANKING
1	25	72	-1.03	0.15	1.92	RANKING
1	26	73	-1.03	0.20	1.90	RANKING
1	27	68	-1.02	0.16	1.91	RANKING
1	28	21	-1.02	0.19	1.88	RANKING
1	29	22	-1.02	0.18	1.99	RANKING
1	30	48	-1.02	0.24	1.91	RANKING
1	31	15	-1.01	0.14	1.97	RANKING
1	32	44	-0.99	0.43	1.97	RANKING
1	33	43	-0.99	0.39	1.95	RANKING
1	34	18	-0.98	0.41	1.95	RANKING
1	35	9	-0.98	0.46	1.97	RANKING
1	36	98	-0.98	0.28	1.96	RANKING
1	37	60	-0.98	0.42	1.98	RANKING
1	38	81	-0.98	0.28	1.90	RANKING
1	39	27	-0.97	0.42	1.98	RANKING
1	40	74	-0.97	0.44	1.93	RANKING
1	41	65	-0.97	0.34	1.98	RANKING
1	42	97	-0.90	0.16	1.91	RANKING
1	43	85	-0.77	1.09	2.02	RANKING
1	44	7	-0.77	1.08	2.01	RANKING
1	45	64	-0.74	0.98	1.93	RANKING
1	46	39	-0.59	0.94	1.93	RANKING
2	1	82	-0.91	0.00	2.85	RANKING
2	2	3	-0.91	0.09	2.84	RANKING
2	3	24	-0.91	0.10	2.84	RANKING
2	4	55	-0.91	0.04	2.85	RANKING
2	5	51	-0.91	0.07	2.84	RANKING
2	6	62	-0.91	0.04	2.84	RANKING
2	7	17	-0.91	0.07	2.84	RANKING
2	8	33	-0.91	0.08	2.84	RANKING
2	9	34	-0.91	0.05	2.84	RANKING
2	10	84	-0.90	0.05	2.84	RANKING
2	11	16	-0.90	0.07	2.85	RANKING
2	12	36	-0.90	0.10	2.84	RANKING
2	13	28	-0.90	0.07	2.85	RANKING
2	14	12	-0.90	0.14	2.84	RANKING
2	15	95	-0.90	0.04	2.85	RANKING
2	16	71	-0.90	0.16	2.83	RANKING
2	17	19	-0.90	0.04	2.84	RANKING
2	18	75	-0.90	0.17	2.84	RANKING
2	19	4	-0.90	0.15	2.83	RANKING
2	20	80	-0.90	0.09	2.84	RANKING
2	21	57	-0.90	0.11	2.85	RANKING
2	22	42	-0.89	0.12	2.84	RANKING
2	23	41	-0.89	0.12	2.83	RANKING
2	24	99	-0.89	0.09	2.84	RANKING
2	25	59	-0.89	0.26	2.83	RANKING
2	26	31	-0.89	0.19	2.83	RANKING
2	27	38	-0.89	0.20	2.83	RANKING

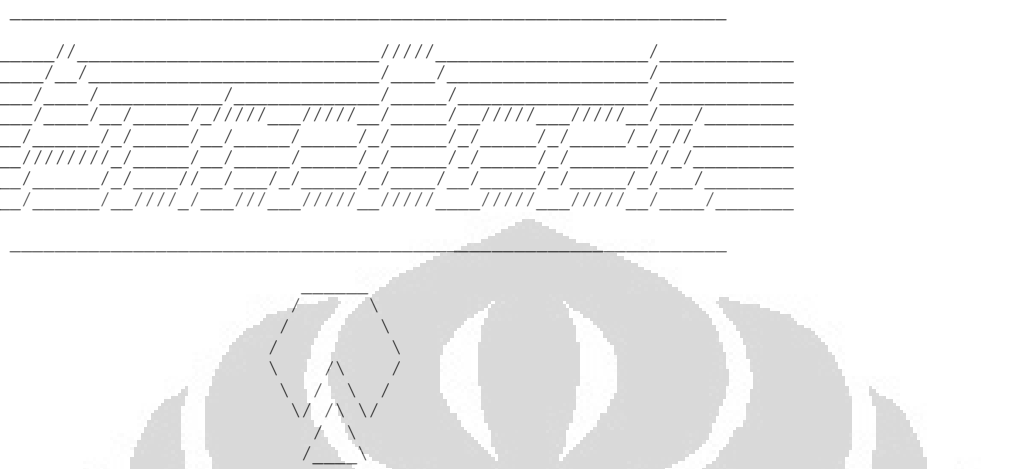
```
   2     28     87       -0.89      0.15      2.85           RANKING
   2     29     35       -0.88      0.15      2.85           RANKING
   2     30     29       -0.88      0.13      2.85           RANKING
   2     31     77       -0.88      0.14      2.84           RANKING
   2     32    100       -0.88      0.23      2.84           RANKING
   2     33     66       -0.88      0.19      2.82           RANKING
   2     34     37       -0.88      0.17      2.83           RANKING
   2     35     54       -0.88      0.12      2.83           RANKING
   2     36     52       -0.88      0.32      2.82           RANKING
   2     37      8       -0.88      0.25      2.82           RANKING
   2     38     58       -0.88      0.15      2.84           RANKING
   2     39     26       -0.87      0.32      2.81           RANKING
   2     40     69       -0.87      0.23      2.81           RANKING
   2     41     96       -0.87      0.32      2.81           RANKING
   2     42     92       -0.87      0.15      2.86           RANKING
   2     43     70       -0.86      0.21      2.84           RANKING
   2     44     45       -0.86      0.31      2.81           RANKING
   2     45     50       -0.85      0.36      2.81           RANKING
   3      1     91       -0.66      0.00      2.75           RANKING
   3      2     25       -0.66      0.02      2.75           RANKING
   3      3     32       -0.65      0.07      2.77           RANKING
   3      4     49       -0.65      0.04      2.76           RANKING
   3      5     47       -0.65      0.05      2.76           RANKING
   3      6     83       -0.64      0.04      2.75           RANKING
   3      7     30       -0.64      0.05      2.74           RANKING
   3      8     89       -0.64      0.08      2.76           RANKING
   3      9      2       -0.63      0.06      2.75           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.20  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.16           at Temperature, T = 298.15 K
Free energy,        A ~ -2729.39 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -0.92 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       53
USER    Run = 53
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 46
USER
USER    RMSD from reference structure       = 1.956 A
USER
USER    Estimated Free Energy of Binding    =   -1.06 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  166.46 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.18 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.86 kcal/mol
USER        Electrostatic Energy            =   -0.32 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
```

```
USER    DPF = 1mqna.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      76.404376 19.624615 -21.256370
USER    NEWDPF axisangle0 -0.693269 -0.656624 -0.297023 35.135204
USER    NEWDPF quaternion0        -0.209250 -0.198189 -0.089651 0.953361
USER
USER                              x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      77.563  18.295 -20.458 -0.24 +0.04    +0.239  1.956
ATOM      2  O1A SIA A3021      78.118  17.218 -20.256 -0.50 -0.21    -0.644  1.956
ATOM      3  O1B SIA A3021      77.295  19.013 -19.495 -0.04 -0.12    -0.644  1.956
ATOM      4  C2  SIA A3021      77.031  18.660 -21.872 -0.07 +0.02    +0.259  1.956
ATOM      5  C3  SIA A3021      76.831  17.419 -22.766 -0.05 +0.01    +0.114  1.956
ATOM      6  C4  SIA A3021      75.656  16.550 -22.296 -0.09 -0.00    +0.149  1.956
ATOM      7  O4  SIA A3021      75.416  15.507 -23.265 -0.01 -0.01    -0.393  1.956
ATOM      8  C5  SIA A3021      74.370  17.378 -22.102 -0.12 -0.01    +0.145  1.956
ATOM      9  N5  SIA A3021      73.353  16.528 -21.459 -0.08 +0.03    -0.352  1.956
ATOM     10  C6  SIA A3021      74.677  18.614 -21.231 -0.18 -0.00    +0.182  1.956
ATOM     11  O6  SIA A3021      75.755  19.383 -21.848 -0.05 -0.00    -0.336  1.956
ATOM     12  C7  SIA A3021      73.468  19.544 -20.988 -0.22 -0.01    +0.180  1.956
ATOM     13  O7  SIA A3021      72.877  19.957 -22.241 -0.06 +0.04    -0.390  1.956
ATOM     14  C8  SIA A3021      73.861  20.783 -20.155 -0.29 -0.03    +0.173  1.956
ATOM     15  O8  SIA A3021      74.437  20.376 -18.894 -0.39 -0.03    -0.391  1.956
ATOM     16  C9  SIA A3021      72.670  21.708 -19.882 -0.34 -0.06    +0.198  1.956
ATOM     17  O9  SIA A3021      73.094  22.866 -19.139 -0.11 +0.22    -0.398  1.956
ATOM     18  C10 SIA A3021      72.065  16.409 -21.870 -0.24 +0.00    +0.214  1.956
ATOM     19  O10 SIA A3021      71.583  17.070 -22.783 -0.15 -0.01    -0.274  1.956
ATOM     20  C11 SIA A3021      71.172  15.541 -21.040 -0.43 +0.01    +0.117  1.956
ATOM     21  H4  SIA A3021      74.688  14.968 -22.974 +0.04 +0.00    +0.210  1.956
ATOM     22  H5  SIA A3021      73.639  15.988 -20.642 -0.41 -0.07    +0.163  1.956
ATOM     23  H7  SIA A3021      72.134  20.528 -22.091 +0.09 -0.03    +0.210  1.956
ATOM     24  H8  SIA A3021      74.679  21.138 -18.381 +0.09 -0.01    +0.210  1.956
ATOM     25  H9  SIA A3021      72.355  23.439 -18.970 -0.20 -0.14    +0.209  1.956
ATOM     26  C1  GAL A3022      78.493  23.272 -22.312 -0.12 -0.01    +0.202  1.956
ATOM     27  C2  GAL A3022      78.073  21.930 -22.937 -0.05 +0.00    +0.173  1.956
ATOM     28  O2  GAL A3022      76.689  21.990 -23.352 -0.01 +0.02    -0.391  1.956
ATOM     29  C3  GAL A3022      78.249  20.789 -21.924 -0.08 +0.02    +0.187  1.956
ATOM     30  O3  GAL A3022      77.990  19.509 -22.581 -0.01 -0.02    -0.336  1.956
ATOM     31  C4  GAL A3022      79.668  20.788 -21.327 -0.11 +0.02    +0.180  1.956
ATOM     32  O4  GAL A3022      80.632  20.414 -22.336 -0.00 -0.02    -0.390  1.956
ATOM     33  C5  GAL A3022      79.986  22.183 -20.748 -0.17 +0.01    +0.176  1.956
ATOM     34  O5  GAL A3022      79.844  23.216 -21.769 -0.08 +0.01    -0.378  1.956
ATOM     35  C6  GAL A3022      81.402  22.249 -20.167 -0.16 +0.02    +0.198  1.956
ATOM     36  O6  GAL A3022      81.640  23.543 -19.578 -0.13 -0.02    -0.398  1.956
ATOM     37  H2  GAL A3022      76.430  21.160 -23.738 +0.02 -0.00    +0.210  1.956
ATOM     38  H4  GAL A3022      81.507  20.413 -21.967 +0.03 +0.01    +0.210  1.956
ATOM     39  H6  GAL A3022      82.518  23.585 -19.218 +0.05 +0.03    +0.209  1.956
TER
ENDMDL
MODEL       82
USER    Run = 82
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 45
USER
USER    RMSD from reference structure       = 2.848 A
USER
USER    Estimated Free Energy of Binding    =   -0.91 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  213.89 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.03 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.84 kcal/mol
USER        Electrostatic Energy            =   -0.19 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1mqna.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      74.044935 17.059465 -22.149537
USER    NEWDPF axisangle0 -0.742479 -0.669519 -0.021633 -126.467248
USER    NEWDPF quaternion0        -0.662923 -0.597781 -0.019315 -0.450354
USER
USER                              x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      72.567  18.298 -22.325 -0.15 -0.00    +0.239  2.848
ATOM      2  O1A SIA A3021      71.457  18.801 -22.173 +0.02 +0.02    -0.644  2.848
```

```
ATOM      3  O1B SIA A3021      73.115  18.395 -23.423 +0.03 -0.00    -0.644  2.848
ATOM      4  C2  SIA A3021      73.185  17.389 -21.226 -0.19 -0.02    +0.259  2.848
ATOM      5  C3  SIA A3021      72.122  16.828 -20.258 -0.21 +0.00    +0.114  2.848
ATOM      6  C4  SIA A3021      71.217  15.788 -20.933 -0.42 +0.02    +0.149  2.848
ATOM      7  O4  SIA A3021      70.363  15.181 -19.939 -0.32 -0.09    -0.393  2.848
ATOM      8  C5  SIA A3021      72.033  14.693 -21.648 -0.26 +0.02    +0.145  2.848
ATOM      9  N5  SIA A3021      71.112  13.857 -22.438 -0.10 -0.02    -0.352  2.848
ATOM     10  C6  SIA A3021      73.091  15.348 -22.559 -0.12 +0.00    +0.182  2.848
ATOM     11  O6  SIA A3021      73.927  16.244 -21.763 -0.10 +0.03    -0.336  2.848
ATOM     12  C7  SIA A3021      73.998  14.349 -23.312 -0.05 +0.01    +0.180  2.848
ATOM     13  O7  SIA A3021      74.636  13.438 -22.389 -0.04 -0.01    -0.390  2.848
ATOM     14  C8  SIA A3021      75.064  15.075 -24.161 -0.01 +0.01    +0.173  2.848
ATOM     15  O8  SIA A3021      74.429  15.974 -25.098 +0.00 -0.02    -0.391  2.848
ATOM     16  C9  SIA A3021      75.958  14.101 -24.936 +0.00 +0.01    +0.198  2.848
ATOM     17  O9  SIA A3021      76.960  14.822 -25.678 +0.00 -0.02    -0.398  2.848
ATOM     18  C10 SIA A3021      71.100  12.500 -22.440 -0.18 +0.00    +0.214  2.848
ATOM     19  O10 SIA A3021      71.921  11.816 -21.839 -0.15 -0.01    -0.274  2.848
ATOM     20  C11 SIA A3021      70.126  11.837 -23.363 -0.22 -0.01    +0.117  2.848
ATOM     21  H4  SIA A3021      69.802  14.537 -20.356 +0.11 +0.05    +0.210  2.848
ATOM     22  H5  SIA A3021      70.432  14.335 -23.029 +0.05 -0.00    +0.163  2.848
ATOM     23  H7  SIA A3021      75.193  12.823 -22.852 +0.03 +0.01    +0.210  2.848
ATOM     24  H8  SIA A3021      75.085  16.421 -25.621 +0.01 +0.01    +0.210  2.848
ATOM     25  H9  SIA A3021      77.514  14.218 -26.158 +0.00 +0.01    +0.209  2.848
ATOM     26  C1  GAL A3022      77.763  19.008 -21.072 -0.18 +0.02    +0.202  2.848
ATOM     27  C2  GAL A3022      76.560  18.312 -20.409 -0.25 +0.02    +0.173  2.848
ATOM     28  O2  GAL A3022      76.728  16.877 -20.465 -0.16 -0.03    -0.391  2.848
ATOM     29  C3  GAL A3022      75.257  18.698 -21.125 -0.19 +0.00    +0.187  2.848
ATOM     30  O3  GAL A3022      74.117  18.150 -20.392 -0.21 +0.02    -0.336  2.848
ATOM     31  C4  GAL A3022      75.116  20.227 -21.238 -0.16 -0.01    +0.180  2.848
ATOM     32  O4  GAL A3022      74.895  20.803 -19.931 -0.13 +0.06    -0.390  2.848
ATOM     33  C5  GAL A3022      76.381  20.816 -21.897 -0.10 +0.00    +0.176  2.848
ATOM     34  O5  GAL A3022      77.578  20.451 -21.147 -0.45 -0.08    -0.378  2.848
ATOM     35  C6  GAL A3022      76.308  22.342 -22.006 -0.10 -0.02    +0.198  2.848
ATOM     36  O6  GAL A3022      77.474  22.851 -22.683 -0.04 +0.02    -0.398  2.848
ATOM     37  H2  GAL A3022      75.985  16.447 -20.056 -0.39 -0.06    +0.210  2.848
ATOM     38  H4  GAL A3022      74.808  21.746 -20.001 -0.29 -0.12    +0.210  2.848
ATOM     39  H6  GAL A3022      77.429  23.797 -22.751 +0.05 -0.02    +0.209  2.848
TER
ENDMDL
MODEL       91
USER    Run = 91
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 9
USER
USER    RMSD from reference structure       = 2.751 A
USER
USER    Estimated Free Energy of Binding    =   -0.66 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  327.60 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.78 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.62 kcal/mol
USER        Electrostatic Energy            =   -0.16 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1mqna.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      75.221124 19.414353 -21.858768
USER    NEWDPF axisangle0 -0.073526 0.242839 -0.967276 -104.433471
USER    NEWDPF quaternion0        -0.058110 0.191924 -0.764471 -0.612676
USER
USER                              x       y       z     vdW   Elec       q    RMS
ATOM      1  C1  SIA A3021      74.777  18.796 -20.079 -0.28 +0.01    +0.239  2.751
ATOM      2  O1A SIA A3021      74.147  18.630 -19.037 -0.02 -0.07    -0.644  2.751
ATOM      3  O1B SIA A3021      76.003  18.882 -20.022 -0.07 -0.07    -0.644  2.751
ATOM      4  C2  SIA A3021      74.038  19.091 -21.415 -0.14 -0.01    +0.259  2.751
ATOM      5  C3  SIA A3021      72.605  19.619 -21.192 -0.25 -0.01    +0.114  2.751
ATOM      6  C4  SIA A3021      72.596  21.038 -20.607 -0.32 -0.03    +0.149  2.751
ATOM      7  O4  SIA A3021      71.241  21.537 -20.584 -0.16 +0.17    -0.393  2.751
ATOM      8  C5  SIA A3021      73.485  22.001 -21.420 -0.21 -0.05    +0.145  2.751
ATOM      9  N5  SIA A3021      73.591  23.277 -20.689 -0.13 +0.19    -0.352  2.751
ATOM     10  C6  SIA A3021      74.879  21.372 -21.623 -0.13 -0.03    +0.182  2.751
ATOM     11  O6  SIA A3021      74.731  20.067 -22.262 -0.03 +0.02    -0.336  2.751
ATOM     12  C7  SIA A3021      75.857  22.233 -22.453 -0.09 -0.02    +0.180  2.751
```

```
ATOM     13  O7  SIA A3021      75.279  22.578 -23.732 -0.00 +0.05    -0.390  2.751
ATOM     14  C8  SIA A3021      77.210  21.518 -22.659 -0.07 +0.00    +0.173  2.751
ATOM     15  O8  SIA A3021      77.800  21.187 -21.382 -0.53 -0.08    -0.391  2.751
ATOM     16  C9  SIA A3021      78.204  22.366 -23.460 -0.03 -0.00    +0.198  2.751
ATOM     17  O9  SIA A3021      79.433  21.643 -23.661 +0.00 -0.01    -0.398  2.751
ATOM     18  C10 SIA A3021      73.420  24.505 -21.239 -0.29 -0.16    +0.214  2.751
ATOM     19  O10 SIA A3021      73.238  24.690 -22.437 -0.17 +0.26    -0.274  2.751
ATOM     20  C11 SIA A3021      73.634  25.681 -20.339 -0.46 -0.06    +0.117  2.751
ATOM     21  H4  SIA A3021      71.235  22.415 -20.222 -0.05 -0.14    +0.210  2.751
ATOM     22  H5  SIA A3021      73.811  23.232 -19.694 -0.30 -0.11    +0.163  2.751
ATOM     23  H7  SIA A3021      75.880  23.108 -24.242 +0.03 -0.02    +0.210  2.751
ATOM     24  H8  SIA A3021      78.633  20.747 -21.509 +0.05 +0.03    +0.210  2.751
ATOM     25  H9  SIA A3021      80.049  22.169 -24.158 +0.01 +0.00    +0.209  2.751
ATOM     26  C1  GAL A3022      76.420  16.204 -24.512 +0.00 +0.01    +0.202  2.751
ATOM     27  C2  GAL A3022      75.160  16.990 -24.104 -0.01 +0.01    +0.173  2.751
ATOM     28  O2  GAL A3022      75.116  18.252 -24.809 +0.00 -0.01    -0.391  2.751
ATOM     29  C3  GAL A3022      75.161  17.255 -22.591 -0.07 -0.00    +0.187  2.751
ATOM     30  O3  GAL A3022      73.891  17.867 -22.203 -0.06 +0.01    -0.336  2.751
ATOM     31  C4  GAL A3022      75.373  15.953 -21.799 -0.02 -0.02    +0.180  2.751
ATOM     32  O4  GAL A3022      74.217  15.096 -21.930 -0.08 +0.03    -0.390  2.751
ATOM     33  C5  GAL A3022      76.648  15.243 -22.302 -0.10 +0.01    +0.176  2.751
ATOM     34  O5  GAL A3022      76.568  14.981 -23.735 +0.00 -0.03    -0.378  2.751
ATOM     35  C6  GAL A3022      76.892  13.922 -21.567 -0.16 +0.03    +0.198  2.751
ATOM     36  O6  GAL A3022      78.123  13.320 -22.016 -0.51 -0.14    -0.398  2.751
ATOM     37  H2  GAL A3022      74.339  18.737 -24.557 +0.03 +0.01    +0.210  2.751
ATOM     38  H4  GAL A3022      74.349  14.293 -21.441 -0.04 -0.01    +0.210  2.751
ATOM     39  H6  GAL A3022      78.274  12.500 -21.561 +0.04 +0.09    +0.209  2.751
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2           # number of dimensions in the field
AVSFLD: nspace=1         # number of physical coordinates
AVSFLD: veclen=7         # vector size
AVSFLD: dim1=39          # atoms
AVSFLD: dim2=3           # conformations
AVSFLD: data=Real       # data type (byte,integer,Real,double)
AVSFLD: field=uniform    # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1mqna.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1mqna.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1mqna.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1mqna.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1mqna.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1mqna.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1mqna.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                2:42 31" p.m., 06/14/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 43m 50.19s,  CPU= 43m 47.69s,  System= 0.60s
_____________________________________________________________________________
```

1MQN-Sia(α2-6)Gal



```
                                AutoDock 4.00

                                (c) 1991-2007
                          The Scripps Research Institute

                             Garrett M. Morris, TSRI
                                  Ruth Huey, TSRI
                              William E. Hart, Sandia
                              William Lindstrom, TSRI
                              Alexander Gillet, TSRI
                             David S. Goodsell, TSRI
                              Arthur J. Olson, TSRI

                       Automated Docking of Flexible Ligand
                         to Flexible Macromolecular Receptor
```

Number of distinct conformational clusters found = 3, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.59	38	-1.54	92	
2	-0.78	62	-0.74	7	#######
3	-0.11	66	-0.11	1	#

Number of multi-member conformational clusters found = 2, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	38	-1.59	0.00	2.95	RANKING
1	2	13	-1.58	0.08	2.95	RANKING
1	3	57	-1.58	0.23	2.94	RANKING
1	4	12	-1.58	0.18	2.94	RANKING
1	5	97	-1.58	0.07	2.95	RANKING
1	6	16	-1.58	0.27	2.95	RANKING
1	7	81	-1.58	0.13	2.95	RANKING
1	8	15	-1.58	0.02	2.95	RANKING
1	9	69	-1.58	0.03	2.95	RANKING
1	10	40	-1.58	0.06	2.95	RANKING
1	11	14	-1.58	0.06	2.96	RANKING
1	12	24	-1.58	0.21	2.94	RANKING
1	13	58	-1.58	0.06	2.95	RANKING
1	14	68	-1.58	0.03	2.95	RANKING
1	15	34	-1.58	0.21	2.94	RANKING
1	16	76	-1.57	0.14	2.94	RANKING
1	17	2	-1.57	0.21	2.94	RANKING
1	18	60	-1.57	0.07	2.96	RANKING
1	19	78	-1.57	0.11	2.94	RANKING
1	20	11	-1.57	0.27	2.95	RANKING
1	21	77	-1.57	0.07	2.95	RANKING
1	22	73	-1.57	0.14	2.95	RANKING
1	23	64	-1.57	0.29	2.95	RANKING
1	24	17	-1.57	0.17	2.94	RANKING
1	25	30	-1.57	0.15	2.95	RANKING
1	26	46	-1.57	0.15	2.94	RANKING
1	27	3	-1.57	0.13	2.94	RANKING
1	28	79	-1.57	0.20	2.95	RANKING
1	29	7	-1.57	0.06	2.95	RANKING
1	30	90	-1.57	0.19	2.95	RANKING
1	31	54	-1.57	0.12	2.95	RANKING
1	32	70	-1.57	0.13	2.95	RANKING
1	33	29	-1.57	0.15	2.94	RANKING
1	34	48	-1.56	0.10	2.94	RANKING
1	35	37	-1.56	0.11	2.96	RANKING
1	36	49	-1.56	0.16	2.95	RANKING
1	37	65	-1.56	0.19	2.96	RANKING
1	38	88	-1.56	0.18	2.95	RANKING
1	39	82	-1.56	0.15	2.95	RANKING
1	40	86	-1.56	0.32	2.94	RANKING
1	41	19	-1.56	0.07	2.95	RANKING
1	42	41	-1.56	0.05	2.95	RANKING
1	43	33	-1.56	0.31	2.94	RANKING
1	44	80	-1.56	0.33	2.95	RANKING
1	45	27	-1.56	0.26	2.94	RANKING
1	46	28	-1.56	0.09	2.94	RANKING
1	47	9	-1.56	0.20	2.94	RANKING
1	48	91	-1.56	0.09	2.94	RANKING
1	49	8	-1.56	0.03	2.96	RANKING
1	50	42	-1.56	0.05	2.95	RANKING
1	51	56	-1.56	0.13	2.95	RANKING
1	52	84	-1.56	0.13	2.94	RANKING
1	53	22	-1.56	0.19	2.95	RANKING
1	54	50	-1.56	0.09	2.95	RANKING
1	55	92	-1.56	0.29	2.95	RANKING
1	56	72	-1.55	0.27	2.94	RANKING
1	57	99	-1.55	0.13	2.94	RANKING
1	58	1	-1.55	0.10	2.94	RANKING
1	59	51	-1.55	0.15	2.96	RANKING
1	60	45	-1.55	0.07	2.95	RANKING
1	61	10	-1.55	0.12	2.95	RANKING
1	62	93	-1.55	0.09	2.94	RANKING
1	63	52	-1.55	0.37	2.95	RANKING
1	64	83	-1.55	0.13	2.94	RANKING
1	65	75	-1.55	0.36	2.95	RANKING
1	66	67	-1.55	0.26	2.95	RANKING
1	67	31	-1.55	0.12	2.94	RANKING
1	68	61	-1.55	0.23	2.95	RANKING
1	69	85	-1.55	0.10	2.94	RANKING
1	70	5	-1.55	0.07	2.95	RANKING

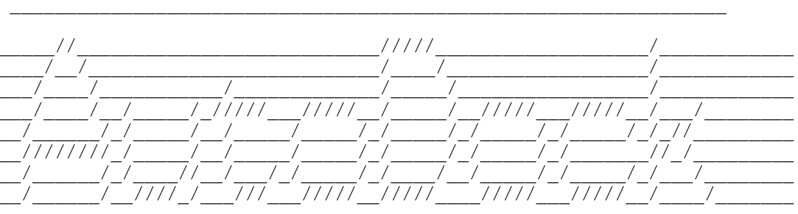
```
   1     71     47       -1.54      0.12      2.95           RANKING
   1     72     35       -1.54      0.15      2.94           RANKING
   1     73     94       -1.54      0.15      2.93           RANKING
   1     74     53       -1.54      0.12      2.93           RANKING
   1     75     98       -1.54      0.13      2.94           RANKING
   1     76     96       -1.54      0.37      2.95           RANKING
   1     77     21       -1.54      0.20      2.97           RANKING
   1     78     89       -1.54      0.39      2.94           RANKING
   1     79     55       -1.54      0.17      2.96           RANKING
   1     80      6       -1.53      0.10      2.94           RANKING
   1     81     87       -1.52      0.18      2.95           RANKING
   1     82     25       -1.52      0.15      2.94           RANKING
   1     83      4       -1.52      0.14      2.94           RANKING
   1     84    100       -1.52      0.14      2.94           RANKING
   1     85     74       -1.49      0.27      2.96           RANKING
   1     86     63       -1.48      0.29      2.94           RANKING
   1     87     36       -1.47      0.23      2.93           RANKING
   1     88     26       -1.45      0.21      2.92           RANKING
   1     89     43       -1.41      0.22      2.94           RANKING
   1     90     95       -1.40      0.35      2.93           RANKING
   1     91     20       -1.33      0.38      2.92           RANKING
   1     92     71       -0.72      0.63      2.91           RANKING
   2      1     62       -0.78      0.00      2.15           RANKING
   2      2     44       -0.78      0.03      2.16           RANKING
   2      3     32       -0.77      0.13      2.21           RANKING
   2      4     23       -0.75      0.17      2.22           RANKING
   2      5     59       -0.73      0.28      2.27           RANKING
   2      6     39       -0.72      0.30      2.26           RANKING
   2      7     18       -0.64      0.56      2.45           RANKING
   3      1     66       -0.11      0.00      3.13           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.07  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.25           at Temperature, T = 298.15 K
Free energy,        A ~ -2729.95 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -1.47 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       38
USER    Run = 38
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 92
USER
USER    RMSD from reference structure       = 2.952 A
USER
USER    Estimated Free Energy of Binding    =   -1.59 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   68.55 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.70 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.74 kcal/mol
USER        Electrostatic Energy            =   +0.04 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
```

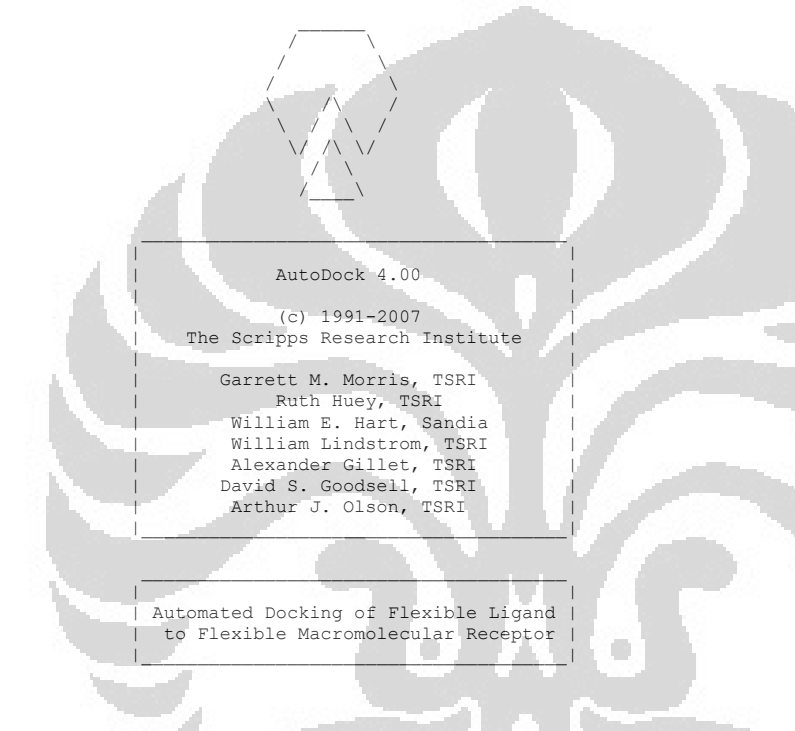
```
USER
USER
USER
USER    DPF = 1mqnh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      74.378049 19.235390 -21.621551
USER    NEWDPF axisangle0 -0.132787 0.098554 0.986233 161.414083
USER    NEWDPF quaternion0        -0.131044 0.097261 0.973289 0.161483
USER
USER                              x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      73.374  20.864 -19.631 -0.27 -0.04    +0.239  2.952
ATOM      2  O1A SIA A 801      72.823  21.846 -19.139 -0.03 +0.20    -0.644  2.952
ATOM      3  O1B SIA A 801      74.027  20.120 -18.899 -0.13 -0.05    -0.644  2.952
ATOM      4  C2  SIA A 801      73.421  20.671 -21.172 -0.17 -0.04    +0.258  2.952
ATOM      5  C3  SIA A 801      73.188  21.998 -21.927 -0.21 -0.04    +0.114  2.952
ATOM      6  C4  SIA A 801      74.371  22.967 -21.777 -0.17 -0.05    +0.149  2.952
ATOM      7  O4  SIA A 801      74.151  24.118 -22.620 -0.08 +0.19    -0.393  2.952
ATOM      8  C5  SIA A 801      75.705  22.291 -22.143 -0.11 -0.02    +0.145  2.952
ATOM      9  N5  SIA A 801      76.829  23.189 -21.813 -0.08 +0.05    -0.352  2.952
ATOM     10  C6  SIA A 801      75.838  20.967 -21.361 -0.12 -0.01    +0.182  2.952
ATOM     11  O6  SIA A 801      74.690  20.115 -21.657 -0.06 +0.02    -0.336  2.952
ATOM     12  C7  SIA A 801      77.142  20.194 -21.655 -0.10 +0.02    +0.180  2.952
ATOM     13  O7  SIA A 801      77.317  20.007 -23.080 -0.00 -0.01    -0.390  2.952
ATOM     14  C8  SIA A 801      77.180  18.832 -20.925 -0.21 +0.02    +0.173  2.952
ATOM     15  O8  SIA A 801      76.982  19.020 -19.507 -0.15 -0.07    -0.391  2.952
ATOM     16  C9  SIA A 801      78.504  18.090 -21.143 -0.18 +0.03    +0.198  2.952
ATOM     17  O9  SIA A 801      78.482  16.815 -20.475 -0.49 -0.12    -0.398  2.952
ATOM     18  C10 SIA A 801      77.740  23.720 -22.669 -0.10 -0.01    +0.214  2.952
ATOM     19  O10 SIA A 801      78.759  24.248 -22.242 -0.13 +0.02    -0.274  2.952
ATOM     20  C11 SIA A 801      77.441  23.822 -24.138 -0.04 -0.01    +0.117  2.952
ATOM     21  H4  SIA A 801      74.882  24.718 -22.527 +0.09 -0.08    +0.210  2.952
ATOM     22  H5  SIA A 801      76.934  23.439 -20.829 -0.12 -0.04    +0.163  2.952
ATOM     23  H7  SIA A 801      78.119  19.531 -23.261 +0.02 +0.01    +0.210  2.952
ATOM     24  H8  SIA A 801      77.006  18.183 -19.058 -0.08 +0.07    +0.210  2.952
ATOM     25  H9  SIA A 801      79.302  16.355 -20.610 +0.03 +0.06    +0.209  2.952
ATOM     26  C1  GAL A 802      71.050  16.602 -23.973 -0.17 +0.01    +0.202  2.952
ATOM     27  C2  GAL A 802      70.752  15.205 -23.395 -0.18 +0.01    +0.173  2.952
ATOM     28  O2  GAL A 802      69.731  14.544 -24.174 -0.07 +0.03    -0.391  2.952
ATOM     29  C3  GAL A 802      70.294  15.310 -21.927 -0.03 +0.01    +0.180  2.952
ATOM     30  O3  GAL A 802      70.165  13.993 -21.350 -0.20 -0.05    -0.390  2.952
ATOM     31  C4  GAL A 802      71.256  16.166 -21.081 -0.39 +0.01    +0.180  2.952
ATOM     32  O4  GAL A 802      72.505  15.463 -20.892 -0.63 -0.03    -0.390  2.952
ATOM     33  C5  GAL A 802      71.477  17.521 -21.785 -0.28 +0.00    +0.176  2.952
ATOM     34  O5  GAL A 802      72.006  17.292 -23.122 -0.08 -0.01    -0.378  2.952
ATOM     35  C6  GAL A 802      72.421  18.453 -21.025 -0.18 -0.01    +0.206  2.952
ATOM     36  O6  GAL A 802      72.355  19.778 -21.627 -0.13 +0.03    -0.344  2.952
ATOM     37  H2  GAL A 802      69.548  13.683 -23.818 -0.29 -0.06    +0.210  2.952
ATOM     38  H3  GAL A 802      69.882  14.057 -20.445 +0.14 +0.06    +0.210  2.952
ATOM     39  H4  GAL A 802      73.098  15.991 -20.370 -0.37 -0.05    +0.210  2.952
TER
ENDMDL
MODEL       62
USER    Run = 62
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 7
USER
USER    RMSD from reference structure      = 2.145 A
USER
USER    Estimated Free Energy of Binding   =   -0.78 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki  =  266.92 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy    =   -4.90 kcal/mol
USER        vdW + Hbond + desolv Energy    =   -4.50 kcal/mol
USER        Electrostatic Energy           =   -0.40 kcal/mol
USER    (2) Final Total Internal Energy    =   +0.00 kcal/mol
USER    (3) Torsional Free Energy          =   +4.12 kcal/mol
USER    (4) Unbound System's Energy        =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1mqnh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      75.878199 19.969041 -21.856107
USER    NEWDPF axisangle0 -0.423761 -0.888631 -0.175387 42.286477
USER    NEWDPF quaternion0        -0.152851 -0.320530 -0.063262 0.932682
USER
```

```
USER                                x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      77.329  18.093 -20.443 -0.23 +0.04    +0.239  2.145
ATOM      2  O1A SIA A 801      77.870  17.014 -20.215 -0.39 -0.20    -0.644  2.145
ATOM      3  O1B SIA A 801      77.155  18.878 -19.511 -0.05 -0.12    -0.644  2.145
ATOM      4  C2  SIA A 801      76.696  18.385 -21.831 -0.08 +0.02    +0.258  2.145
ATOM      5  C3  SIA A 801      76.390  17.086 -22.610 -0.07 +0.00    +0.114  2.145
ATOM      6  C4  SIA A 801      75.233  16.292 -21.986 -0.08 -0.01    +0.149  2.145
ATOM      7  O4  SIA A 801      74.908  15.175 -22.841 -0.03 -0.00    -0.393  2.145
ATOM      8  C5  SIA A 801      73.990  17.177 -21.778 -0.15 -0.01    +0.145  2.145
ATOM      9  N5  SIA A 801      72.968  16.434 -21.014 -0.08 +0.03    -0.352  2.145
ATOM     10  C6  SIA A 801      74.394  18.456 -21.015 -0.21 -0.01    +0.182  2.145
ATOM     11  O6  SIA A 801      75.444  19.148 -21.758 -0.05 -0.00    -0.336  2.145
ATOM     12  C7  SIA A 801      73.223  19.428 -20.754 -0.23 -0.01    +0.180  2.145
ATOM     13  O7  SIA A 801      72.519  19.724 -21.984 -0.09 +0.03    -0.390  2.145
ATOM     14  C8  SIA A 801      73.698  20.733 -20.077 -0.31 -0.03    +0.173  2.145
ATOM     15  O8  SIA A 801      74.420  20.433 -18.863 -0.40 -0.03    -0.391  2.145
ATOM     16  C9  SIA A 801      72.535  21.672 -19.739 -0.33 -0.06    +0.198  2.145
ATOM     17  O9  SIA A 801      73.026  22.887 -19.143 -0.11 +0.22    -0.398  2.145
ATOM     18  C10 SIA A 801      71.718  16.094 -21.422 -0.32 +0.01    +0.214  2.145
ATOM     19  O10 SIA A 801      70.888  15.696 -20.613 -0.50 -0.03    -0.274  2.145
ATOM     20  C11 SIA A 801      71.378  16.040 -22.884 -0.21 +0.01    +0.117  2.145
ATOM     21  H4  SIA A 801      74.193  14.684 -22.455 +0.05 +0.00    +0.210  2.145
ATOM     22  H5  SIA A 801      73.231  16.143 -20.072 -0.36 -0.06    +0.163  2.145
ATOM     23  H7  SIA A 801      71.799  20.322 -21.824 +0.10 -0.03    +0.210  2.145
ATOM     24  H8  SIA A 801      74.711  21.235 -18.447 +0.09 -0.03    +0.210  2.145
ATOM     25  H9  SIA A 801      72.304  23.469 -18.934 -0.19 -0.14    +0.209  2.145
ATOM     26  C1  GAL A 802      78.344  22.227 -25.372 -0.00 +0.00    +0.202  2.145
ATOM     27  C2  GAL A 802      79.066  23.528 -24.971 -0.02 +0.00    +0.173  2.145
ATOM     28  O2  GAL A 802      79.776  24.079 -26.102 -0.00 -0.01    -0.391  2.145
ATOM     29  C3  GAL A 802      80.055  23.269 -23.819 -0.04 +0.00    +0.180  2.145
ATOM     30  O3  GAL A 802      80.612  24.515 -23.349 -0.05 -0.00    -0.390  2.145
ATOM     31  C4  GAL A 802      79.395  22.511 -22.650 -0.06 +0.00    +0.180  2.145
ATOM     32  O4  GAL A 802      78.457  23.377 -21.971 -0.10 +0.02    -0.390  2.145
ATOM     33  C5  GAL A 802      78.697  21.248 -23.197 -0.02 +0.01    +0.176  2.145
ATOM     34  O5  GAL A 802      77.717  21.633 -24.202 +0.00 -0.00    -0.378  2.145
ATOM     35  C6  GAL A 802      78.006  20.420 -22.114 -0.06 +0.02    +0.206  2.145
ATOM     36  O6  GAL A 802      77.613  19.138 -22.685 -0.01 -0.02    -0.344  2.145
ATOM     37  H2  GAL A 802      80.221  24.881 -25.855 +0.01 +0.00    +0.210  2.145
ATOM     38  H3  GAL A 802      81.222  24.355 -22.639 +0.03 +0.00    +0.210  2.145
ATOM     39  H4  GAL A 802      78.050  22.910 -21.250 +0.06 -0.00    +0.210  2.145
TER
ENDMDL
MODEL       66
USER    Run = 66
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 3.126 A
USER
USER    Estimated Free Energy of Binding    =   -0.11 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  835.30 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.22 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.75 kcal/mol
USER        Electrostatic Energy            =   -0.47 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1mqnh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      76.649733 17.001039 -23.251497
USER    NEWDPF axisangle0 -0.311146 -0.859486 0.405552 53.057222
USER    NEWDPF quaternion0        -0.138972 -0.383885 0.181138 0.894711
USER
USER                                x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      77.555  14.882 -21.731 -0.14 +0.05    +0.239  3.126
ATOM      2  O1A SIA A 801      77.669  13.714 -21.368 -0.46 -0.24    -0.644  3.126
ATOM      3  O1B SIA A 801      77.935  15.778 -20.977 -0.11 -0.15    -0.644  3.126
ATOM      4  C2  SIA A 801      76.764  15.237 -23.021 -0.03 +0.02    +0.258  3.126
ATOM      5  C3  SIA A 801      75.795  14.107 -23.433 -0.03 +0.01    +0.114  3.126
ATOM      6  C4  SIA A 801      74.612  13.972 -22.462 -0.10 +0.00    +0.149  3.126
ATOM      7  O4  SIA A 801      73.678  13.002 -22.984 -0.01 -0.02    -0.393  3.126
ATOM      8  C5  SIA A 801      73.905  15.322 -22.244 -0.13 -0.00    +0.145  3.126
ATOM      9  N5  SIA A 801      72.897  15.193 -21.173 -0.07 -0.01    -0.352  3.126
```

```
ATOM     10  C6  SIA A 801      74.950  16.390 -21.860 -0.04 -0.02    +0.182  3.126
ATOM     11  O6  SIA A 801      75.969  16.465 -22.903 -0.02 -0.01    -0.336  3.126
ATOM     12  C7  SIA A 801      74.354  17.794 -21.622 -0.15 -0.01    +0.180  3.126
ATOM     13  O7  SIA A 801      73.542  18.204 -22.748 -0.03 +0.00    -0.390  3.126
ATOM     14  C8  SIA A 801      75.451  18.845 -21.338 -0.16 +0.00    +0.173  3.126
ATOM     15  O8  SIA A 801      76.273  18.422 -20.228 -0.19 -0.04    -0.391  3.126
ATOM     16  C9  SIA A 801      74.868  20.227 -21.020 -0.18 -0.01    +0.198  3.126
ATOM     17  O9  SIA A 801      75.924  21.179 -20.796 -0.19 +0.03    -0.398  3.126
ATOM     18  C10 SIA A 801      71.555  15.372 -21.277 -0.32 +0.03    +0.214  3.126
ATOM     19  O10 SIA A 801      70.862  15.474 -20.272 -0.59 -0.05    -0.274  3.126
ATOM     20  C11 SIA A 801      70.872  15.282 -22.612 -0.24 +0.01    +0.117  3.126
ATOM     21  H4  SIA A 801      72.947  12.919 -22.384 +0.06 +0.01    +0.210  3.126
ATOM     22  H5  SIA A 801      73.249  14.940 -20.249 -0.41 +0.01    +0.163  3.126
ATOM     23  H7  SIA A 801      73.175  19.068 -22.602 +0.07 -0.01    +0.210  3.126
ATOM     24  H8  SIA A 801      76.947  19.068 -20.054 +0.07 +0.03    +0.210  3.126
ATOM     25  H9  SIA A 801      75.562  22.036 -20.599 -0.38 -0.09    +0.209  3.126
ATOM     26  C1  GAL A 802      78.852  17.517 -27.544 +0.00 +0.01    +0.202  3.126
ATOM     27  C2  GAL A 802      80.098  18.423 -27.567 +0.00 +0.01    +0.173  3.126
ATOM     28  O2  GAL A 802      80.665  18.467 -28.895 +0.00 -0.02    -0.391  3.126
ATOM     29  C3  GAL A 802      81.159  17.914 -26.571 +0.00 +0.01    +0.180  3.126
ATOM     30  O3  GAL A 802      82.255  18.850 -26.488 +0.00 -0.02    -0.390  3.126
ATOM     31  C4  GAL A 802      80.566  17.668 -25.170 +0.01 +0.01    +0.180  3.126
ATOM     32  O4  GAL A 802      80.238  18.931 -24.547 +0.01 -0.02    -0.390  3.126
ATOM     33  C5  GAL A 802      79.320  16.767 -25.300 +0.00 +0.01    +0.176  3.126
ATOM     34  O5  GAL A 802      78.352  17.403 -26.183 +0.00 -0.02    -0.378  3.126
ATOM     35  C6  GAL A 802      78.650  16.460 -23.961 -0.00 +0.02    +0.206  3.126
ATOM     36  O6  GAL A 802      77.661  15.409 -24.162 +0.00 -0.03    -0.344  3.126
ATOM     37  H2  GAL A 802      81.433  19.026 -28.909 +0.00 +0.01    +0.210  3.126
ATOM     38  H3  GAL A 802      82.909  18.536 -25.874 +0.00 +0.01    +0.210  3.126
ATOM     39  H4  GAL A 802      79.872  18.780 -23.682 +0.02 +0.01    +0.210  3.126
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2           # number of dimensions in the field
AVSFLD: nspace=1         # number of physical coordinates
AVSFLD: veclen=7         # vector size
AVSFLD: dim1=39          # atoms
AVSFLD: dim2=3           # conformations
AVSFLD: data=Real       # data type (byte,integer,Real,double)
AVSFLD: field=uniform    # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1mqnh.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1mqnh.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1mqnh.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1mqnh.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1mqnh.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1mqnh.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1mqnh.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                  3:28 11" p.m., 06/14/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 45m 40.36s,  CPU= 44m 44.44s,  System= 1.11s
_____________________________________________________________________________
```

1HGF-Sia(α2-3)Gal





Number of distinct conformational clusters found = 5, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-0.75	14	-0.71	93	##
2	-0.33	36	-0.33	1	#
3	-0.12	67	-0.12	1	#
4	-0.10	82	-0.09	3	###
5	-0.04	80	-0.04	2	##

Number of multi-member conformational clusters found = 3, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	14	-0.75	0.00	2.99	RANKING
1	2	70	-0.74	0.04	2.98	RANKING
1	3	40	-0.74	0.03	3.00	RANKING
1	4	90	-0.74	0.02	2.99	RANKING
1	5	85	-0.74	0.04	2.98	RANKING
1	6	49	-0.74	0.03	2.99	RANKING
1	7	92	-0.74	0.04	2.98	RANKING
1	8	79	-0.74	0.05	2.98	RANKING
1	9	38	-0.74	0.04	2.98	RANKING
1	10	48	-0.74	0.05	2.98	RANKING
1	11	55	-0.74	0.03	2.99	RANKING
1	12	62	-0.74	0.03	2.99	RANKING
1	13	2	-0.73	0.06	2.98	RANKING
1	14	78	-0.73	0.06	2.98	RANKING
1	15	12	-0.73	0.05	3.00	RANKING
1	16	32	-0.73	0.08	2.97	RANKING
1	17	5	-0.73	0.11	2.97	RANKING
1	18	15	-0.73	0.05	2.98	RANKING
1	19	91	-0.73	0.10	3.01	RANKING
1	20	42	-0.73	0.09	2.97	RANKING
1	21	71	-0.73	0.05	2.98	RANKING
1	22	26	-0.73	0.05	2.99	RANKING
1	23	19	-0.73	0.04	2.98	RANKING
1	24	24	-0.73	0.05	2.99	RANKING
1	25	93	-0.73	0.06	2.97	RANKING
1	26	86	-0.73	0.15	2.96	RANKING
1	27	99	-0.73	0.11	2.96	RANKING
1	28	73	-0.73	0.07	2.97	RANKING
1	29	72	-0.73	0.05	2.98	RANKING
1	30	22	-0.73	0.05	2.98	RANKING
1	31	64	-0.73	0.06	3.00	RANKING
1	32	3	-0.73	0.07	3.01	RANKING
1	33	54	-0.73	0.05	3.00	RANKING
1	34	50	-0.73	0.09	2.97	RANKING
1	35	33	-0.73	0.16	3.03	RANKING
1	36	100	-0.73	0.05	3.00	RANKING
1	37	4	-0.72	0.09	3.01	RANKING
1	38	97	-0.72	0.05	3.00	RANKING
1	39	44	-0.72	0.15	3.03	RANKING
1	40	11	-0.72	0.09	2.97	RANKING
1	41	31	-0.72	0.10	2.97	RANKING
1	42	63	-0.72	0.03	2.99	RANKING
1	43	74	-0.72	0.13	2.96	RANKING
1	44	60	-0.72	0.05	2.99	RANKING
1	45	69	-0.72	0.12	2.97	RANKING
1	46	25	-0.72	0.06	2.98	RANKING
1	47	75	-0.72	0.09	2.98	RANKING
1	48	77	-0.72	0.15	2.96	RANKING
1	49	18	-0.72	0.08	2.97	RANKING
1	50	45	-0.72	0.06	2.98	RANKING
1	51	17	-0.72	0.10	2.97	RANKING
1	52	35	-0.72	0.08	2.98	RANKING
1	53	51	-0.72	0.10	2.98	RANKING
1	54	68	-0.71	0.09	2.98	RANKING
1	55	84	-0.71	0.07	2.98	RANKING
1	56	37	-0.71	0.06	3.01	RANKING
1	57	7	-0.71	0.10	2.97	RANKING
1	58	27	-0.71	0.10	2.97	RANKING
1	59	47	-0.71	0.05	2.99	RANKING
1	60	6	-0.71	0.14	2.96	RANKING
1	61	61	-0.71	0.11	2.96	RANKING
1	62	87	-0.71	0.12	3.02	RANKING
1	63	30	-0.71	0.14	3.02	RANKING
1	64	95	-0.71	0.14	3.03	RANKING
1	65	13	-0.71	0.15	2.97	RANKING
1	66	88	-0.71	0.15	2.97	RANKING
1	67	1	-0.71	0.08	2.98	RANKING
1	68	81	-0.71	0.08	2.98	RANKING
1	69	16	-0.71	0.12	2.98	RANKING
1	70	9	-0.71	0.15	2.97	RANKING
1	71	65	-0.71	0.09	2.98	RANKING
1	72	23	-0.70	0.18	2.96	RANKING
1	73	59	-0.70	0.11	2.98	RANKING

```
   1      74      52        -0.70       0.07       2.98           RANKING
   1      75      56        -0.70       0.11       2.97           RANKING
   1      76      83        -0.70       0.07       3.00           RANKING
   1      77      39        -0.70       0.06       2.99           RANKING
   1      78      29        -0.70       0.10       2.97           RANKING
   1      79      21        -0.69       0.09       2.98           RANKING
   1      80      43        -0.69       0.18       2.96           RANKING
   1      81      76        -0.69       0.10       3.00           RANKING
   1      82      58        -0.69       0.14       2.97           RANKING
   1      83      10        -0.69       0.09       2.99           RANKING
   1      84      34        -0.69       0.11       2.99           RANKING
   1      85      96        -0.69       0.19       3.05           RANKING
   1      86      41        -0.69       0.19       2.97           RANKING
   1      87      28        -0.68       0.20       2.98           RANKING
   1      88      66        -0.67       0.20       2.98           RANKING
   1      89       8        -0.66       0.10       3.00           RANKING
   1      90      57        -0.66       0.12       3.01           RANKING
   1      91      53        -0.66       0.14       3.00           RANKING
   1      92      94        -0.65       0.25       3.00           RANKING
   1      93      98        -0.60       0.26       3.00           RANKING
   2       1      36        -0.33       0.00       2.93           RANKING
   3       1      67        -0.12       0.00       2.33           RANKING
   4       1      82        -0.10       0.00       2.87           RANKING
   4       2      89        -0.08       0.16       2.86           RANKING
   4       3      20        -0.08       0.57       2.94           RANKING
   5       1      80        -0.04       0.00       2.76           RANKING
   5       2      46        -0.04       0.05       2.77           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.07  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.11           at Temperature, T = 298.15 K
Free energy,        A ~ -2729.15 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -0.67 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       14
USER    Run = 14
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 93
USER
USER    RMSD from reference structure       = 2.990 A
USER
USER    Estimated Free Energy of Binding    =   -0.75 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  283.94 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.86 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.45 kcal/mol
USER        Electrostatic Energy            =   -0.41 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
```

```
USER    DPF = 1hgfa.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      77.740962 19.015653 -22.901579
USER    NEWDPF axisangle0 0.748754 -0.493151 0.442911 157.876992
USER    NEWDPF quaternion0        0.734844 -0.483989 0.434682 0.191863
USER
USER                              x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      79.668  18.837 -22.931 -0.07 +0.08    +0.239  2.990
ATOM      2  O1A SIA A3021      80.849  19.010 -22.641 -0.45 +0.34    -0.644  2.990
ATOM      3  O1B SIA A3021      79.373  18.620 -24.106 +0.00 -0.14    -0.644  2.990
ATOM      4  C2  SIA A3021      78.549  19.079 -21.880 -0.18 +0.07    +0.259  2.990
ATOM      5  C3  SIA A3021      79.017  19.979 -20.717 -0.28 +0.03    +0.114  2.990
ATOM      6  C4  SIA A3021      79.233  21.432 -21.161 -0.21 +0.02    +0.149  2.990
ATOM      7  O4  SIA A3021      79.500  22.251 -20.002 -0.18 -0.02    -0.393  2.990
ATOM      8  C5  SIA A3021      78.008  21.991 -21.914 -0.16 +0.01    +0.145  2.990
ATOM      9  N5  SIA A3021      78.363  23.303 -22.484 -0.08 +0.00    -0.352  2.990
ATOM     10  C6  SIA A3021      77.593  21.008 -23.028 -0.06 +0.02    +0.182  2.990
ATOM     11  O6  SIA A3021      77.342  19.693 -22.442 -0.06 -0.05    -0.336  2.990
ATOM     12  C7  SIA A3021      76.353  21.443 -23.839 -0.03 +0.01    +0.180  2.990
ATOM     13  O7  SIA A3021      75.232  21.703 -22.965 -0.03 +0.01    -0.390  2.990
ATOM     14  C8  SIA A3021      75.966  20.389 -24.898 -0.01 +0.01    +0.173  2.990
ATOM     15  O8  SIA A3021      77.079  20.139 -25.786 +0.00 -0.04    -0.391  2.990
ATOM     16  C9  SIA A3021      74.752  20.813 -25.731 -0.02 +0.01    +0.198  2.990
ATOM     17  O9  SIA A3021      74.405  19.782 -26.674 +0.00 -0.03    -0.398  2.990
ATOM     18  C10 SIA A3021      77.607  24.425 -22.384 -0.19 -0.01    +0.214  2.990
ATOM     19  O10 SIA A3021      76.492  24.446 -21.873 -0.13 +0.02    -0.274  2.990
ATOM     20  C11 SIA A3021      78.114  25.644 -23.090 -0.10 -0.00    +0.117  2.990
ATOM     21  H4  SIA A3021      79.634  23.151 -20.276 -0.27 -0.04    +0.210  2.990
ATOM     22  H5  SIA A3021      79.244  23.372 -22.993 +0.03 +0.01    +0.163  2.990
ATOM     23  H7  SIA A3021      74.470  21.972 -23.464 +0.06 -0.02    +0.210  2.990
ATOM     24  H8  SIA A3021      76.840  19.490 -26.437 +0.00 +0.02    +0.210  2.990
ATOM     25  H9  SIA A3021      73.652  20.046 -27.191 +0.04 +0.02    +0.209  2.990
ATOM     26  C1  GAL A3022      75.695  15.210 -22.575 -0.12 +0.02    +0.202  2.990
ATOM     27  C2  GAL A3022      76.229  16.343 -21.680 -0.14 +0.03    +0.173  2.990
ATOM     28  O2  GAL A3022      75.285  17.439 -21.656 -0.16 -0.04    -0.391  2.990
ATOM     29  C3  GAL A3022      77.580  16.849 -22.206 -0.22 +0.05    +0.187  2.990
ATOM     30  O3  GAL A3022      78.139  17.816 -21.263 -0.49 -0.11    -0.336  2.990
ATOM     31  C4  GAL A3022      78.570  15.687 -22.407 -0.17 +0.06    +0.180  2.990
ATOM     32  O4  GAL A3022      78.958  15.139 -21.128 -0.57 -0.22    -0.390  2.990
ATOM     33  C5  GAL A3022      77.925  14.607 -23.300 -0.08 +0.04    +0.176  2.990
ATOM     34  O5  GAL A3022      76.669  14.136 -22.725 -0.05 -0.07    -0.378  2.990
ATOM     35  C6  GAL A3022      78.856  13.409 -23.508 -0.05 +0.05    +0.198  2.990
ATOM     36  O6  GAL A3022      78.248  12.451 -24.398 +0.01 -0.08    -0.398  2.990
ATOM     37  H2  GAL A3022      75.615  18.139 -21.104 -0.10 +0.02    +0.210  2.990
ATOM     38  H4  GAL A3022      79.569  14.422 -21.252 +0.02 +0.16    +0.210  2.990
ATOM     39  H6  GAL A3022      78.826  11.708 -24.526 +0.01 +0.04    +0.209  2.990
TER
ENDMDL
MODEL       36
USER    Run = 36
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 2.925 A
USER
USER    Estimated Free Energy of Binding    =   -0.33 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  576.51 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.44 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.30 kcal/mol
USER        Electrostatic Energy            =   -0.14 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfa.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      76.290592 20.912758 -23.268706
USER    NEWDPF axisangle0 -0.152354 0.978827 -0.136698 -165.911698
USER    NEWDPF quaternion0        -0.151204 0.971439 -0.135666 -0.122634
USER
USER                              x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      76.586  19.531 -24.592 -0.00 +0.03    +0.239  2.925
ATOM      2  O1A SIA A3021      76.900  18.450 -25.083 +0.02 -0.08    -0.644  2.925
```

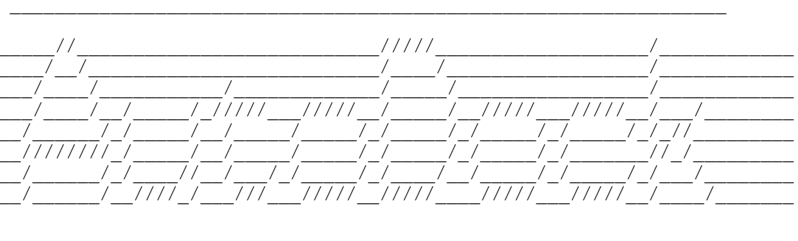
```
ATOM      3  O1B SIA A3021      76.782  20.556 -25.244 +0.02 -0.05    -0.644  2.925
ATOM      4  C2  SIA A3021      76.135  19.628 -23.107 -0.06 +0.03    +0.259  2.925
ATOM      5  C3  SIA A3021      76.594  18.414 -22.271 -0.16 +0.02    +0.114  2.925
ATOM      6  C4  SIA A3021      78.113  18.405 -22.050 -0.20 +0.04    +0.149  2.925
ATOM      7  O4  SIA A3021      78.454  17.350 -21.125 -0.45 -0.18    -0.393  2.925
ATOM      8  C5  SIA A3021      78.622  19.753 -21.503 -0.22 +0.04    +0.145  2.925
ATOM      9  N5  SIA A3021      80.096  19.740 -21.512 -0.11 -0.13    -0.352  2.925
ATOM     10  C6  SIA A3021      78.083  20.904 -22.378 -0.10 +0.02    +0.182  2.925
ATOM     11  O6  SIA A3021      76.624  20.830 -22.425 -0.06 -0.03    -0.336  2.925
ATOM     12  C7  SIA A3021      78.502  22.316 -21.911 -0.15 +0.01    +0.180  2.925
ATOM     13  O7  SIA A3021      78.135  22.530 -20.530 -0.05 +0.00    -0.390  2.925
ATOM     14  C8  SIA A3021      77.883  23.416 -22.801 -0.13 -0.00    +0.173  2.925
ATOM     15  O8  SIA A3021      78.262  23.215 -24.181 -0.01 -0.02    -0.391  2.925
ATOM     16  C9  SIA A3021      78.307  24.824 -22.369 -0.16 -0.01    +0.198  2.925
ATOM     17  O9  SIA A3021      77.674  25.815 -23.200 -0.08 +0.01    -0.398  2.925
ATOM     18  C10 SIA A3021      80.884  20.117 -20.474 -0.13 +0.08    +0.214  2.925
ATOM     19  O10 SIA A3021      80.447  20.594 -19.432 -0.27 -0.09    -0.274  2.925
ATOM     20  C11 SIA A3021      82.362  20.091 -20.706 -0.13 +0.04    +0.117  2.925
ATOM     21  H4  SIA A3021      79.394  17.343 -20.988 +0.05 +0.14    +0.210  2.925
ATOM     22  H5  SIA A3021      80.558  19.425 -22.364 +0.02 +0.07    +0.163  2.925
ATOM     23  H7  SIA A3021      78.393  23.398 -20.243 -0.21 -0.07    +0.210  2.925
ATOM     24  H8  SIA A3021      77.882  23.892 -24.728 +0.03 +0.01    +0.210  2.925
ATOM     25  H9  SIA A3021      77.936  26.688 -22.933 +0.06 -0.00    +0.209  2.925
ATOM     26  C1  GAL A3022      72.297  22.587 -23.436 -0.18 -0.07    +0.202  2.925
ATOM     27  C2  GAL A3022      73.083  21.481 -22.710 -0.25 -0.03    +0.173  2.925
ATOM     28  O2  GAL A3022      73.834  22.049 -21.612 -0.14 +0.12    -0.391  2.925
ATOM     29  C3  GAL A3022      74.050  20.786 -23.680 -0.09 -0.00    +0.187  2.925
ATOM     30  O3  GAL A3022      74.675  19.646 -23.012 -0.05 -0.02    -0.336  2.925
ATOM     31  C4  GAL A3022      73.320  20.309 -24.948 -0.09 +0.01    +0.180  2.925
ATOM     32  O4  GAL A3022      72.423  19.224 -24.626 -0.07 -0.03    -0.390  2.925
ATOM     33  C5  GAL A3022      72.555  21.492 -25.580 -0.18 -0.00    +0.176  2.925
ATOM     34  O5  GAL A3022      71.622  22.080 -24.623 -0.14 +0.04    -0.378  2.925
ATOM     35  C6  GAL A3022      71.781  21.066 -26.831 -0.25 +0.01    +0.198  2.925
ATOM     36  O6  GAL A3022      71.134  22.206 -27.430 -0.26 +0.03    -0.398  2.925
ATOM     37  H2  GAL A3022      74.320  21.366 -21.164 +0.03 -0.03    +0.210  2.925
ATOM     38  H4  GAL A3022      71.972  18.930 -25.409 +0.06 +0.02    +0.210  2.925
ATOM     39  H6  GAL A3022      70.654  21.942 -28.206 -0.19 -0.02    +0.209  2.925
TER
ENDMDL
MODEL       67
USER    Run = 67
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 2.328 A
USER
USER    Estimated Free Energy of Binding    =   -0.12 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  821.64 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.23 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.15 kcal/mol
USER        Electrostatic Energy            =   -0.08 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfa.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      77.664889 19.572835 -22.424198
USER    NEWDPF axisangle0 -0.846365 -0.517650 -0.125319 -156.962660
USER    NEWDPF quaternion0        -0.829319 -0.507225 -0.122796 -0.199687
USER
USER                               x       y       z     vdW   Elec       q    RMS
ATOM      1  C1  SIA A3021      77.024  21.049 -23.501 -0.03 +0.02    +0.239  2.328
ATOM      2  O1A SIA A3021      76.273  21.911 -23.948 +0.04 -0.02    -0.644  2.328
ATOM      3  O1B SIA A3021      77.815  20.497 -24.266 +0.03 -0.07    -0.644  2.328
ATOM      4  C2  SIA A3021      76.850  20.520 -22.049 -0.11 +0.04    +0.259  2.328
ATOM      5  C3  SIA A3021      75.441  20.798 -21.485 -0.23 +0.01    +0.114  2.328
ATOM      6  C4  SIA A3021      74.365  19.946 -22.170 -0.23 +0.01    +0.149  2.328
ATOM      7  O4  SIA A3021      73.106  20.125 -21.485 -0.19 +0.02    -0.393  2.328
ATOM      8  C5  SIA A3021      74.737  18.449 -22.179 -0.22 +0.01    +0.145  2.328
ATOM      9  N5  SIA A3021      73.770  17.727 -23.025 -0.07 -0.03    -0.352  2.328
ATOM     10  C6  SIA A3021      76.170  18.275 -22.721 -0.12 +0.02    +0.182  2.328
ATOM     11  O6  SIA A3021      77.090  19.079 -21.919 -0.10 -0.05    -0.336  2.328
ATOM     12  C7  SIA A3021      76.672  16.815 -22.751 -0.14 +0.03    +0.180  2.328
```

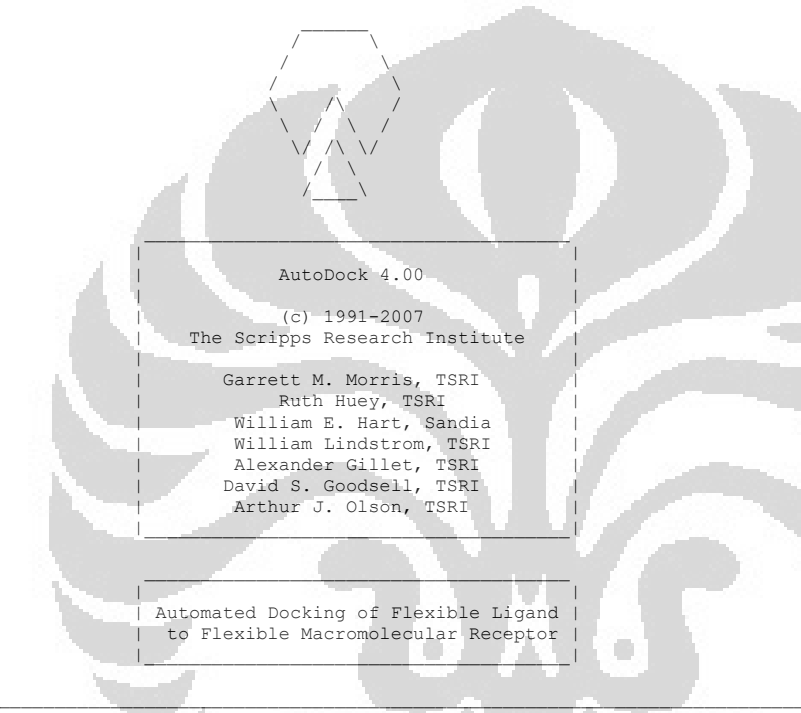
```
ATOM     13  O7  SIA A3021      76.560  16.205 -21.446 -0.15 -0.08    -0.390  2.328
ATOM     14  C8  SIA A3021      78.129  16.724 -23.254 -0.11 +0.04    +0.173  2.328
ATOM     15  O8  SIA A3021      78.243  17.317 -24.567 -0.00 -0.07    -0.391  2.328
ATOM     16  C9  SIA A3021      78.639  15.280 -23.316 -0.10 +0.05    +0.198  2.328
ATOM     17  O9  SIA A3021      80.012  15.250 -23.750 -0.18 -0.14    -0.398  2.328
ATOM     18  C10 SIA A3021      73.135  16.580 -22.676 -0.19 +0.02    +0.214  2.328
ATOM     19  O10 SIA A3021      73.365  15.969 -21.638 -0.17 +0.01    -0.274  2.328
ATOM     20  C11 SIA A3021      72.236  15.968 -23.705 -0.18 +0.01    +0.117  2.328
ATOM     21  H4  SIA A3021      72.439  19.597 -21.909 +0.10 +0.00    +0.210  2.328
ATOM     22  H5  SIA A3021      73.563  18.120 -23.943 +0.04 +0.02    +0.163  2.328
ATOM     23  H7  SIA A3021      76.868  15.307 -21.465 +0.03 +0.05    +0.210  2.328
ATOM     24  H8  SIA A3021      79.140  17.261 -24.877 +0.02 +0.04    +0.210  2.328
ATOM     25  H9  SIA A3021      80.327  14.355 -23.787 +0.03 +0.07    +0.209  2.328
ATOM     26  C1  GAL A3022      81.448  20.413 -20.486 -0.16 +0.07    +0.202  2.328
ATOM     27  C2  GAL A3022      79.937  20.500 -20.210 -0.30 +0.05    +0.173  2.328
ATOM     28  O2  GAL A3022      79.432  19.203 -19.815 -0.32 -0.21    -0.391  2.328
ATOM     29  C3  GAL A3022      79.189  20.973 -21.466 -0.16 +0.03    +0.187  2.328
ATOM     30  O3  GAL A3022      77.781  21.192 -21.141 -0.14 -0.06    -0.336  2.328
ATOM     31  C4  GAL A3022      79.802  22.271 -22.022 -0.12 +0.02    +0.180  2.328
ATOM     32  O4  GAL A3022      79.547  23.369 -21.118 -0.09 +0.05    -0.390  2.328
ATOM     33  C5  GAL A3022      81.317  22.075 -22.242 -0.07 +0.02    +0.176  2.328
ATOM     34  O5  GAL A3022      81.975  21.669 -21.004 -0.03 -0.07    -0.378  2.328
ATOM     35  C6  GAL A3022      81.986  23.349 -22.766 -0.07 +0.02    +0.198  2.328
ATOM     36  O6  GAL A3022      83.385  23.110 -23.021 -0.01 -0.05    -0.398  2.328
ATOM     37  H2  GAL A3022      78.498  19.257 -19.645 -0.29 +0.03    +0.210  2.328
ATOM     38  H4  GAL A3022      79.926  24.169 -21.461 -0.16 -0.03    +0.210  2.328
ATOM     39  H6  GAL A3022      83.800  23.900 -23.346 +0.02 +0.02    +0.209  2.328
TER
ENDMDL
MODEL       82
USER    Run = 82
USER    Cluster Rank = 4
USER    Number of conformations in this cluster = 3
USER
USER    RMSD from reference structure       = 2.874 A
USER
USER    Estimated Free Energy of Binding    =   -0.10 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  848.92 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.21 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.77 kcal/mol
USER        Electrostatic Energy            =   -0.44 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfa.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      77.888293 20.973635 -22.270337
USER    NEWDPF axisangle0 -0.269778 0.715958 -0.643913 174.530114
USER    NEWDPF quaternion0        -0.269471 0.715142 -0.643180 0.047716
USER
USER                              x       y       z     vdW   Elec       q     RMS
ATOM      1  C1  SIA A3021      78.391  19.264 -21.515 -0.15 +0.06    +0.239  2.874
ATOM      2  O1A SIA A3021      78.889  18.438 -20.753 -0.46 -0.33    -0.644  2.874
ATOM      3  O1B SIA A3021      78.356  19.012 -22.719 +0.00 -0.14    -0.644  2.874
ATOM      4  C2  SIA A3021      77.993  20.677 -21.004 -0.15 +0.06    +0.259  2.874
ATOM      5  C3  SIA A3021      78.715  21.055 -19.694 -0.40 +0.03    +0.114  2.874
ATOM      6  C4  SIA A3021      80.214  21.302 -19.909 -0.30 +0.03    +0.149  2.874
ATOM      7  O4  SIA A3021      80.793  21.815 -18.689 -0.22 -0.08    -0.393  2.874
ATOM      8  C5  SIA A3021      80.474  22.296 -21.059 -0.18 +0.01    +0.145  2.874
ATOM      9  N5  SIA A3021      81.920  22.324 -21.341 -0.03 -0.05    -0.352  2.874
ATOM     10  C6  SIA A3021      79.684  21.857 -22.309 -0.09 +0.02    +0.182  2.874
ATOM     11  O6  SIA A3021      78.267  21.746 -21.971 -0.07 -0.03    -0.336  2.874
ATOM     12  C7  SIA A3021      79.839  22.794 -23.528 -0.06 +0.01    +0.180  2.874
ATOM     13  O7  SIA A3021      79.496  24.154 -23.178 -0.08 -0.01    -0.390  2.874
ATOM     14  C8  SIA A3021      78.981  22.322 -24.722 -0.01 +0.01    +0.173  2.874
ATOM     15  O8  SIA A3021      79.333  20.969 -25.087 +0.00 -0.05    -0.391  2.874
ATOM     16  C9  SIA A3021      79.140  23.225 -25.950 -0.01 +0.01    +0.198  2.874
ATOM     17  O9  SIA A3021      78.291  22.770 -27.020 +0.00 -0.03    -0.398  2.874
ATOM     18  C10 SIA A3021      82.662  23.450 -21.486 -0.10 +0.03    +0.214  2.874
ATOM     19  O10 SIA A3021      82.186  24.580 -21.479 -0.08 -0.02    -0.274  2.874
ATOM     20  C11 SIA A3021      84.106  23.265 -21.834 -0.04 +0.01    +0.117  2.874
ATOM     21  H4  SIA A3021      81.722  21.968 -18.822 +0.08 +0.05    +0.210  2.874
ATOM     22  H5  SIA A3021      82.399  21.429 -21.436 +0.04 +0.03    +0.163  2.874
```

```
ATOM     23  H7  SIA A3021      79.592  24.730 -23.927 +0.03 +0.01    +0.210  2.874
ATOM     24  H8  SIA A3021      78.805  20.679 -25.822 +0.01 +0.02    +0.210  2.874
ATOM     25  H9  SIA A3021      78.389  23.330 -27.782 +0.00 +0.02    +0.209  2.874
ATOM     26  C1  GAL A3022      73.642  21.282 -23.077 -0.16 -0.02    +0.202  2.874
ATOM     27  C2  GAL A3022      74.658  21.604 -21.967 -0.17 -0.01    +0.173  2.874
ATOM     28  O2  GAL A3022      75.330  22.850 -22.259 -0.04 +0.04    -0.391  2.874
ATOM     29  C3  GAL A3022      75.700  20.481 -21.853 -0.18 +0.02    +0.187  2.874
ATOM     30  O3  GAL A3022      76.563  20.731 -20.700 -0.26 -0.12    -0.336  2.874
ATOM     31  C4  GAL A3022      75.024  19.106 -21.707 -0.22 +0.02    +0.180  2.874
ATOM     32  O4  GAL A3022      74.370  19.008 -20.423 -0.22 -0.08    -0.390  2.874
ATOM     33  C5  GAL A3022      74.017  18.900 -22.859 -0.16 +0.01    +0.176  2.874
ATOM     34  O5  GAL A3022      73.029  19.974 -22.886 -0.12 -0.00    -0.378  2.874
ATOM     35  C6  GAL A3022      73.289  17.557 -22.745 -0.18 +0.02    +0.198  2.874
ATOM     36  O6  GAL A3022      72.407  17.371 -23.870 -0.08 -0.05    -0.398  2.874
ATOM     37  H2  GAL A3022      75.958  23.049 -21.573 +0.14 -0.01    +0.210  2.874
ATOM     38  H4  GAL A3022      73.952  18.159 -20.333 +0.09 +0.04    +0.210  2.874
ATOM     39  H6  GAL A3022      71.955  16.538 -23.800 +0.07 +0.03    +0.209  2.874
TER
ENDMDL
MODEL       80
USER    Run = 80
USER    Cluster Rank = 5
USER    Number of conformations in this cluster = 2
USER
USER    RMSD from reference structure       = 2.763 A
USER
USER    Estimated Free Energy of Binding    =   -0.04 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  932.22 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.16 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.99 kcal/mol
USER        Electrostatic Energy            =   -0.16 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfa.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      77.423501 17.713872 -23.032683
USER    NEWDPF axisangle0 0.703776 0.710201 -0.017745 160.229491
USER    NEWDPF quaternion0        0.693327 0.699657 -0.017482 0.171676
USER
USER                            x       y       z     vdW   Elec       q     RMS
ATOM      1  C1  SIA A3021      76.088  18.456 -24.222 -0.02 +0.03    +0.239  2.763
ATOM      2  O1A SIA A3021      74.990  18.746 -24.688 +0.03 -0.06    -0.644  2.763
ATOM      3  O1B SIA A3021      77.014  18.210 -24.996 +0.03 -0.09    -0.644  2.763
ATOM      4  C2  SIA A3021      76.264  18.209 -22.697 -0.10 +0.03    +0.259  2.763
ATOM      5  C3  SIA A3021      74.929  17.885 -21.995 -0.25 +0.01    +0.114  2.763
ATOM      6  C4  SIA A3021      74.387  16.504 -22.390 -0.20 +0.01    +0.149  2.763
ATOM      7  O4  SIA A3021      73.237  16.191 -21.575 -0.17 +0.01    -0.393  2.763
ATOM      8  C5  SIA A3021      75.451  15.400 -22.223 -0.09 +0.00    +0.145  2.763
ATOM      9  N5  SIA A3021      74.933  14.152 -22.811 -0.04 -0.02    -0.352  2.763
ATOM     10  C6  SIA A3021      76.757  15.830 -22.923 -0.12 +0.03    +0.182  2.763
ATOM     11  O6  SIA A3021      77.192  17.117 -22.385 -0.13 -0.07    -0.336  2.763
ATOM     12  C7  SIA A3021      77.915  14.815 -22.801 -0.14 +0.05    +0.180  2.763
ATOM     13  O7  SIA A3021      78.177  14.499 -21.415 -0.48 -0.19    -0.390  2.763
ATOM     14  C8  SIA A3021      79.201  15.334 -23.479 -0.08 +0.05    +0.173  2.763
ATOM     15  O8  SIA A3021      78.948  15.635 -24.869 -0.01 -0.08    -0.391  2.763
ATOM     16  C9  SIA A3021      80.356  14.331 -23.390 -0.01 +0.08    +0.198  2.763
ATOM     17  O9  SIA A3021      81.543  14.876 -23.998 -0.46 -0.17    -0.398  2.763
ATOM     18  C10 SIA A3021      74.966  12.936 -22.209 -0.11 +0.02    +0.214  2.763
ATOM     19  O10 SIA A3021      75.514  12.730 -21.132 -0.18 -0.04    -0.274  2.763
ATOM     20  C11 SIA A3021      74.444  11.778 -23.002 -0.06 +0.02    +0.117  2.763
ATOM     21  H4  SIA A3021      72.901  15.336 -21.819 -0.02 -0.00    +0.210  2.763
ATOM     22  H5  SIA A3021      74.518  14.206 -23.741 +0.03 +0.02    +0.163  2.763
ATOM     23  H7  SIA A3021      78.889  13.874 -21.341 +0.06 +0.16    +0.210  2.763
ATOM     24  H8  SIA A3021      79.740  15.955 -25.286 +0.02 +0.04    +0.210  2.763
ATOM     25  H9  SIA A3021      82.258  14.254 -23.943 +0.01 +0.07    +0.209  2.763
ATOM     26  C1  GAL A3022      80.375  20.628 -21.778 -0.12 +0.05    +0.202  2.763
ATOM     27  C2  GAL A3022      79.033  20.033 -21.315 -0.22 +0.05    +0.173  2.763
ATOM     28  O2  GAL A3022      79.255  18.762 -20.663 -0.54 -0.21    -0.391  2.763
ATOM     29  C3  GAL A3022      78.094  19.832 -22.514 -0.11 +0.03    +0.187  2.763
ATOM     30  O3  GAL A3022      76.778  19.409 -22.037 -0.09 -0.05    -0.336  2.763
ATOM     31  C4  GAL A3022      77.958  21.124 -23.338 -0.04 +0.02    +0.180  2.763
ATOM     32  O4  GAL A3022      77.233  22.121 -22.583 -0.04 -0.02    -0.390  2.763
```

```
ATOM     33  C5  GAL A3022      79.360  21.638 -23.730 -0.03 +0.02    +0.176  2.763
ATOM     34  O5  GAL A3022      80.187  21.851 -22.547 -0.02 -0.05    -0.378  2.763
ATOM     35  C6  GAL A3022      79.285  22.943 -24.527 -0.02 +0.01    +0.198  2.763
ATOM     36  O6  GAL A3022      80.606  23.358 -24.932 -0.01 -0.03    -0.398  2.763
ATOM     37  H2  GAL A3022      78.427  18.394 -20.378 -0.37 +0.08    +0.210  2.763
ATOM     38  H4  GAL A3022      77.149  22.918 -23.092 +0.05 +0.00    +0.210  2.763
ATOM     39  H6  GAL A3022      80.559  24.168 -25.426 +0.01 +0.02    +0.209  2.763
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2           # number of dimensions in the field
AVSFLD: nspace=1         # number of physical coordinates
AVSFLD: veclen=7         # vector size
AVSFLD: dim1=39          # atoms
AVSFLD: dim2=5           # conformations
AVSFLD: data=Real       # data type (byte,integer,Real,double)
AVSFLD: field=uniform    # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1hgfa.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1hgfa.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1hgfa.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1hgfa.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1hgfa.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1hgfa.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1hgfa.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                  4:13 04" p.m., 06/14/2009




_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 44m 52.66s,  CPU= 43m 41.61s,  System= 1.28s
_____________________________________________________________________________
```

1HGF-Sia(α2-6)Gal





Number of distinct conformational clusters found = 9, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-0.71	4	-0.59	18	##################
2	-0.20	16	-0.09	52	##
3	+0.01	27	+0.02	9	#########
4	+0.02	82	+0.02	14	##############
5	+0.02	62	+0.02	1	#
6	+0.15	77	+0.15	1	#
7	+0.15	33	+0.16	3	###
8	+0.19	32	+0.19	1	#
9	+0.23	6	+0.23	1	#

Number of multi-member conformational clusters found = 5, out of 100 runs.

RMSD TABLE

_____

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	4	-0.71	0.00	2.58	RANKING
1	2	70	-0.68	0.07	2.58	RANKING
1	3	69	-0.68	0.09	2.57	RANKING
1	4	5	-0.66	0.09	2.57	RANKING
1	5	7	-0.66	0.09	2.58	RANKING
1	6	54	-0.66	0.12	2.57	RANKING
1	7	38	-0.65	0.10	2.58	RANKING
1	8	36	-0.65	0.10	2.57	RANKING
1	9	60	-0.64	0.27	2.59	RANKING
1	10	2	-0.63	0.05	2.58	RANKING
1	11	22	-0.62	0.12	2.57	RANKING
1	12	79	-0.60	0.18	2.56	RANKING
1	13	18	-0.60	0.24	2.58	RANKING
1	14	48	-0.59	0.14	2.57	RANKING
1	15	15	-0.55	0.19	2.57	RANKING
1	16	99	-0.51	0.29	2.60	RANKING
1	17	87	-0.39	0.44	2.58	RANKING
1	18	9	-0.22	0.51	2.55	RANKING
2	1	16	-0.20	0.00	3.35	RANKING
2	2	74	-0.19	0.04	3.36	RANKING
2	3	55	-0.19	0.06	3.38	RANKING
2	4	63	-0.19	0.06	3.35	RANKING
2	5	83	-0.19	0.07	3.32	RANKING
2	6	72	-0.19	0.05	3.35	RANKING
2	7	96	-0.19	0.09	3.33	RANKING
2	8	39	-0.16	0.11	3.35	RANKING
2	9	19	-0.14	0.15	3.31	RANKING
2	10	49	-0.14	0.31	3.42	RANKING
2	11	84	-0.13	0.28	3.32	RANKING
2	12	66	-0.13	0.35	3.31	RANKING
2	13	86	-0.12	0.24	3.40	RANKING
2	14	61	-0.10	1.53	2.89	RANKING
2	15	78	-0.10	1.50	2.88	RANKING
2	16	3	-0.10	1.51	2.88	RANKING
2	17	13	-0.10	1.52	2.89	RANKING
2	18	64	-0.10	1.51	2.89	RANKING
2	19	31	-0.10	1.51	2.89	RANKING
2	20	68	-0.09	1.50	2.90	RANKING
2	21	41	-0.09	1.52	2.88	RANKING
2	22	75	-0.09	1.49	2.89	RANKING
2	23	45	-0.09	1.51	2.88	RANKING
2	24	85	-0.09	1.54	2.90	RANKING
2	25	35	-0.09	1.50	2.88	RANKING
2	26	98	-0.09	1.52	2.88	RANKING
2	27	11	-0.09	1.52	2.88	RANKING
2	28	58	-0.09	1.56	2.89	RANKING
2	29	52	-0.09	1.56	2.90	RANKING
2	30	14	-0.08	1.51	2.87	RANKING
2	31	8	-0.08	1.53	2.87	RANKING
2	32	100	-0.08	1.51	2.87	RANKING
2	33	43	-0.08	1.52	2.88	RANKING
2	34	34	-0.08	1.49	2.88	RANKING
2	35	10	-0.08	1.51	2.89	RANKING
2	36	20	-0.07	1.50	2.87	RANKING
2	37	21	-0.07	1.53	2.87	RANKING
2	38	50	-0.07	1.58	2.89	RANKING
2	39	97	-0.07	1.57	2.89	RANKING
2	40	29	-0.06	1.49	2.89	RANKING
2	41	81	-0.06	1.63	2.89	RANKING
2	42	71	-0.06	1.48	2.88	RANKING
2	43	28	-0.05	1.44	2.88	RANKING
2	44	65	-0.05	1.62	2.85	RANKING
2	45	90	-0.04	1.52	2.92	RANKING
2	46	25	-0.04	1.70	2.88	RANKING
2	47	51	-0.04	1.64	2.88	RANKING
2	48	57	-0.04	1.63	2.85	RANKING
2	49	93	-0.03	1.74	2.85	RANKING
2	50	56	-0.03	1.41	2.88	RANKING
2	51	53	-0.02	1.54	2.82	RANKING
2	52	91	+0.01	1.45	2.80	RANKING
3	1	27	+0.01	0.00	3.02	RANKING

```
   3      2     67       +0.01      0.13      3.02           RANKING
   3      3     73       +0.02      0.18      3.05           RANKING
   3      4     24       +0.02      0.11      3.04           RANKING
   3      5     46       +0.02      0.20      3.07           RANKING
   3      6     88       +0.02      0.14      3.00           RANKING
   3      7     37       +0.03      0.18      3.05           RANKING
   3      8     92       +0.03      0.15      3.08           RANKING
   3      9      1       +0.04      0.14      3.06           RANKING
   4      1     82       +0.02      0.00      2.62           RANKING
   4      2     30       +0.02      0.05      2.63           RANKING
   4      3     95       +0.02      0.04      2.63           RANKING
   4      4     94       +0.02      0.02      2.62           RANKING
   4      5     80       +0.02      0.07      2.59           RANKING
   4      6     59       +0.02      0.05      2.65           RANKING
   4      7     47       +0.02      0.10      2.56           RANKING
   4      8     40       +0.02      0.07      2.60           RANKING
   4      9     76       +0.02      0.07      2.60           RANKING
   4     10     44       +0.02      0.11      2.59           RANKING
   4     11     12       +0.03      0.10      2.58           RANKING
   4     12     17       +0.03      0.07      2.64           RANKING
   4     13     26       +0.03      0.10      2.61           RANKING
   4     14     89       +0.03      0.09      2.65           RANKING
   5      1     62       +0.02      0.00      2.92           RANKING
   6      1     77       +0.15      0.00      3.72           RANKING
   7      1     33       +0.15      0.00      3.08           RANKING
   7      2     42       +0.15      0.06      3.08           RANKING
   7      3     23       +0.17      0.11      3.06           RANKING
   8      1     32       +0.19      0.00      3.62           RANKING
   9      1      6       +0.23      0.00      3.00           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.31  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.02           at Temperature, T = 298.15 K
Free energy,        A ~ -2728.62 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -0.14 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL        4
USER    Run = 4
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 18
USER
USER    RMSD from reference structure       = 2.576 A
USER
USER    Estimated Free Energy of Binding    =   -0.71 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  301.99 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.83 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.58 kcal/mol
USER        Electrostatic Energy            =   -0.25 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
```

```
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      74.475390 18.255895 -22.673825
USER    NEWDPF axisangle0 -0.618040 0.780920 -0.090505 -168.790428
USER    NEWDPF quaternion0        -0.615085 0.777186 -0.090072 -0.097666
USER
USER                              x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      76.386  17.983 -24.648 -0.01 +0.03    +0.239  2.576
ATOM      2  O1A SIA A 801      77.473  17.692 -25.142 +0.02 -0.09    -0.644  2.576
ATOM      3  O1B SIA A 801      75.620  18.707 -25.283 +0.02 -0.07    -0.644  2.576
ATOM      4  C2  SIA A 801      76.063  17.617 -23.172 -0.07 +0.03    +0.258  2.576
ATOM      5  C3  SIA A 801      77.344  17.359 -22.349 -0.21 +0.02    +0.114  2.576
ATOM      6  C4  SIA A 801      78.146  18.646 -22.101 -0.20 +0.03    +0.149  2.576
ATOM      7  O4  SIA A 801      79.244  18.358 -21.209 -0.48 -0.21    -0.393  2.576
ATOM      8  C5  SIA A 801      77.260  19.757 -21.507 +0.01 +0.03    +0.145  2.576
ATOM      9  N5  SIA A 801      78.013  21.025 -21.454 -0.09 -0.06    -0.352  2.576
ATOM     10  C6  SIA A 801      75.999  19.927 -22.379 -0.13 +0.02    +0.182  2.576
ATOM     11  O6  SIA A 801      75.297  18.649 -22.465 -0.09 -0.04    -0.336  2.576
ATOM     12  C7  SIA A 801      75.027  21.015 -21.873 -0.20 +0.00    +0.180  2.576
ATOM     13  O7  SIA A 801      74.702  20.803 -20.478 -0.24 -0.02    -0.390  2.576
ATOM     14  C8  SIA A 801      73.738  21.076 -22.723 -0.19 -0.01    +0.173  2.576
ATOM     15  O8  SIA A 801      74.067  21.265 -24.116 -0.02 +0.01    -0.391  2.576
ATOM     16  C9  SIA A 801      72.801  22.206 -22.281 -0.29 -0.07    +0.198  2.576
ATOM     17  O9  SIA A 801      71.601  22.204 -23.076 -0.20 +0.14    -0.398  2.576
ATOM     18  C10 SIA A 801      78.339  21.747 -20.351 -0.18 +0.03    +0.214  2.576
ATOM     19  O10 SIA A 801      78.751  22.895 -20.460 -0.10 +0.03    -0.274  2.576
ATOM     20  C11 SIA A 801      78.362  21.102 -18.994 -0.35 +0.03    +0.117  2.576
ATOM     21  H4  SIA A 801      79.739  19.153 -21.057 +0.04 +0.10    +0.210  2.576
ATOM     22  H5  SIA A 801      78.325  21.403 -22.349 +0.05 +0.02    +0.163  2.576
ATOM     23  H7  SIA A 801      74.104  21.472 -20.166 -0.31 -0.07    +0.210  2.576
ATOM     24  H8  SIA A 801      73.274  21.303 -24.639 +0.07 -0.01    +0.210  2.576
ATOM     25  H9  SIA A 801      71.020  22.904 -22.802 +0.11 -0.17    +0.209  2.576
ATOM     26  C1  GAL A 802      72.157  14.159 -21.500 -0.29 +0.03    +0.202  2.576
ATOM     27  C2  GAL A 802      70.867  13.855 -22.288 -0.31 +0.03    +0.173  2.576
ATOM     28  O2  GAL A 802      70.297  12.600 -21.855 -0.19 -0.07    -0.391  2.576
ATOM     29  C3  GAL A 802      71.155  13.796 -23.800 -0.15 +0.02    +0.180  2.576
ATOM     30  O3  GAL A 802      69.921  13.663 -24.538 -0.09 +0.01    -0.390  2.576
ATOM     31  C4  GAL A 802      71.933  15.033 -24.290 -0.11 +0.02    +0.180  2.576
ATOM     32  O4  GAL A 802      71.078  16.198 -24.253 -0.09 -0.06    -0.390  2.576
ATOM     33  C5  GAL A 802      73.182  15.227 -23.404 -0.12 +0.02    +0.176  2.576
ATOM     34  O5  GAL A 802      72.772  15.372 -22.014 -0.18 -0.01    -0.378  2.576
ATOM     35  C6  GAL A 802      74.029  16.434 -23.805 -0.07 +0.02    +0.206  2.576
ATOM     36  O6  GAL A 802      75.297  16.375 -23.090 -0.06 -0.04    -0.344  2.576
ATOM     37  H2  GAL A 802      69.502  12.414 -22.341 +0.01 +0.02    +0.210  2.576
ATOM     38  H3  GAL A 802      70.098  13.627 -25.471 +0.06 +0.01    +0.210  2.576
ATOM     39  H4  GAL A 802      71.557  16.961 -24.555 +0.07 +0.03    +0.210  2.576
TER
ENDMDL
MODEL       16
USER    Run = 16
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 52
USER
USER    RMSD from reference structure       = 3.352 A
USER
USER    Estimated Free Energy of Binding    =   -0.20 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  716.54 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.31 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.13 kcal/mol
USER        Electrostatic Energy            =   -0.19 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      78.324142 17.115778 -22.290488
USER    NEWDPF axisangle0 0.712155 0.685363 0.152028 160.734968
USER    NEWDPF quaternion0        0.702114 0.675701 0.149885 0.167328
USER
USER                              x       y       z    vdW   Elec        q     RMS
```

```
ATOM      1  C1  SIA A 801      76.943  18.139 -24.451 -0.01 +0.03    +0.239  3.352
ATOM      2  O1A SIA A 801      75.977  18.558 -25.084 +0.03 -0.07    -0.644  3.352
ATOM      3  O1B SIA A 801      77.963  17.825 -25.063 +0.02 -0.10    -0.644  3.352
ATOM      4  C2  SIA A 801      76.818  17.818 -22.935 -0.09 +0.04    +0.258  3.352
ATOM      5  C3  SIA A 801      75.348  17.602 -22.511 -0.19 +0.01    +0.114  3.352
ATOM      6  C4  SIA A 801      74.765  16.298 -23.075 -0.13 +0.01    +0.149  3.352
ATOM      7  O4  SIA A 801      73.447  16.090 -22.524 -0.12 -0.02    -0.393  3.352
ATOM      8  C5  SIA A 801      75.668  15.092 -22.757 -0.13 +0.01    +0.145  3.352
ATOM      9  N5  SIA A 801      75.175  13.895 -23.466 -0.01 -0.04    -0.352  3.352
ATOM     10  C6  SIA A 801      77.114  15.407 -23.193 -0.09 +0.04    +0.182  3.352
ATOM     11  O6  SIA A 801      77.565  16.624 -22.524 -0.12 -0.08    -0.336  3.352
ATOM     12  C7  SIA A 801      78.116  14.266 -22.915 -0.11 +0.05    +0.180  3.352
ATOM     13  O7  SIA A 801      78.042  13.844 -21.531 -0.33 -0.18    -0.390  3.352
ATOM     14  C8  SIA A 801      79.563  14.668 -23.278 -0.08 +0.06    +0.173  3.352
ATOM     15  O8  SIA A 801      79.629  15.110 -24.651 -0.03 -0.09    -0.391  3.352
ATOM     16  C9  SIA A 801      80.556  13.517 -23.083 -0.10 +0.07    +0.198  3.352
ATOM     17  O9  SIA A 801      81.893  13.946 -23.399 -0.48 -0.15    -0.398  3.352
ATOM     18  C10 SIA A 801      74.727  12.736 -22.918 -0.06 +0.03    +0.214  3.352
ATOM     19  O10 SIA A 801      74.577  11.739 -23.612 -0.01 -0.04    -0.274  3.352
ATOM     20  C11 SIA A 801      74.251  12.697 -21.494 -0.09 +0.01    +0.117  3.352
ATOM     21  H4  SIA A 801      73.087  15.284 -22.873 +0.06 +0.02    +0.210  3.352
ATOM     22  H5  SIA A 801      75.169  13.944 -24.486 +0.02 +0.02    +0.163  3.352
ATOM     23  H7  SIA A 801      78.658  13.142 -21.360 +0.06 +0.13    +0.210  3.352
ATOM     24  H8  SIA A 801      80.519  15.357 -24.875 +0.02 +0.05    +0.210  3.352
ATOM     25  H9  SIA A 801      82.509  13.232 -23.278 +0.02 +0.07    +0.209  3.352
ATOM     26  C1  GAL A 802      79.476  20.370 -18.881 -0.28 +0.06    +0.202  3.352
ATOM     27  C2  GAL A 802      80.840  21.070 -19.039 -0.32 +0.04    +0.173  3.352
ATOM     28  O2  GAL A 802      81.042  22.025 -17.975 -0.18 -0.09    -0.391  3.352
ATOM     29  C3  GAL A 802      80.928  21.788 -20.400 -0.19 +0.03    +0.180  3.352
ATOM     30  O3  GAL A 802      82.259  22.310 -20.603 -0.05 -0.06    -0.390  3.352
ATOM     31  C4  GAL A 802      80.540  20.862 -21.569 -0.13 +0.04    +0.180  3.352
ATOM     32  O4  GAL A 802      81.561  19.857 -21.761 -0.28 -0.15    -0.390  3.352
ATOM     33  C5  GAL A 802      79.170  20.217 -21.268 -0.22 +0.05    +0.176  3.352
ATOM     34  O5  GAL A 802      79.244  19.486 -20.012 -0.46 -0.16    -0.378  3.352
ATOM     35  C6  GAL A 802      78.688  19.274 -22.370 -0.14 +0.05    +0.206  3.352
ATOM     36  O6  GAL A 802      77.295  18.931 -22.117 -0.10 -0.05    -0.344  3.352
ATOM     37  H2  GAL A 802      81.883  22.456 -18.072 +0.09 +0.05    +0.210  3.352
ATOM     38  H3  GAL A 802      82.314  22.752 -21.442 +0.05 +0.03    +0.210  3.352
ATOM     39  H4  GAL A 802      81.322  19.286 -22.482 +0.03 +0.10    +0.210  3.352
TER
ENDMDL
MODEL       27
USER    Run = 27
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 9
USER
USER    RMSD from reference structure       = 3.021 A
USER
USER    Estimated Free Energy of Binding    =   +0.01 kcal/mol  [=(1)+(2)+(3)-(4)]
USER
USER    (1) Final Intermolecular Energy     =   -4.11 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.82 kcal/mol
USER        Electrostatic Energy            =   -0.29 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      77.620773 19.056959 -22.543090
USER    NEWDPF axisangle0 0.903244 -0.151336 0.401557 -61.921135
USER    NEWDPF quaternion0        0.464672 -0.077855 0.206580 -0.857522
USER
USER                               x       y       z     vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      78.260  16.387 -22.255 -0.19 +0.07    +0.239  3.021
ATOM      2  O1A SIA A 801      78.768  15.305 -22.540 -0.05 -0.21    -0.644  3.021
ATOM      3  O1B SIA A 801      77.379  16.421 -21.397 -0.09 -0.20    -0.644  3.021
ATOM      4  C2  SIA A 801      78.575  17.656 -23.095 -0.10 +0.07    +0.258  3.021
ATOM      5  C3  SIA A 801      79.114  17.299 -24.498 -0.05 +0.02    +0.114  3.021
ATOM      6  C4  SIA A 801      78.033  16.684 -25.398 -0.01 +0.02    +0.149  3.021
ATOM      7  O4  SIA A 801      78.564  16.512 -26.729 +0.00 -0.06    -0.393  3.021
ATOM      8  C5  SIA A 801      76.769  17.564 -25.444 -0.00 +0.02    +0.145  3.021
ATOM      9  N5  SIA A 801      75.692  16.857 -26.165 +0.00 -0.04    -0.352  3.021
ATOM     10  C6  SIA A 801      76.319  17.886 -24.004 -0.03 +0.02    +0.182  3.021
ATOM     11  O6  SIA A 801      77.415  18.534 -23.290 -0.03 -0.06    -0.336  3.021
```

```
ATOM     12  C7  SIA A 801      75.058  18.773 -23.924 -0.05 +0.02    +0.180  3.021
ATOM     13  O7  SIA A 801      75.220  19.968 -24.726 +0.00 -0.03    -0.390  3.021
ATOM     14  C8  SIA A 801      74.708  19.147 -22.466 -0.17 +0.01    +0.173  3.021
ATOM     15  O8  SIA A 801      74.569  17.955 -21.664 -0.17 -0.04    -0.391  3.021
ATOM     16  C9  SIA A 801      73.412  19.960 -22.367 -0.23 +0.00    +0.198  3.021
ATOM     17  O9  SIA A 801      73.144  20.315 -20.998 -0.14 +0.04    -0.398  3.021
ATOM     18  C10 SIA A 801      75.076  17.242 -27.312 -0.00 +0.03    +0.214  3.021
ATOM     19  O10 SIA A 801      74.040  16.697 -27.673 -0.00 -0.04    -0.274  3.021
ATOM     20  C11 SIA A 801      75.735  18.220 -28.243 -0.00 +0.01    +0.117  3.021
ATOM     21  H4  SIA A 801      77.895  16.131 -27.286 +0.00 +0.03    +0.210  3.021
ATOM     22  H5  SIA A 801      75.374  15.979 -25.754 +0.01 +0.02    +0.163  3.021
ATOM     23  H7  SIA A 801      74.444  20.514 -24.678 +0.04 +0.01    +0.210  3.021
ATOM     24  H8  SIA A 801      74.354  18.184 -20.768 +0.09 +0.03    +0.210  3.021
ATOM     25  H9  SIA A 801      72.341  20.819 -20.937 -0.21 -0.05    +0.209  3.021
ATOM     26  C1  GAL A 802      81.149  22.145 -21.295 -0.12 +0.03    +0.202  3.021
ATOM     27  C2  GAL A 802      81.157  22.614 -19.827 -0.20 +0.02    +0.173  3.021
ATOM     28  O2  GAL A 802      82.268  23.506 -19.589 -0.14 -0.07    -0.391  3.021
ATOM     29  C3  GAL A 802      81.249  21.410 -18.871 -0.30 +0.04    +0.180  3.021
ATOM     30  O3  GAL A 802      81.102  21.846 -17.503 -0.25 -0.08    -0.390  3.021
ATOM     31  C4  GAL A 802      80.198  20.330 -19.197 -0.29 +0.06    +0.180  3.021
ATOM     32  O4  GAL A 802      78.878  20.810 -18.852 -0.32 -0.10    -0.390  3.021
ATOM     33  C5  GAL A 802      80.291  19.973 -20.695 -0.21 +0.07    +0.176  3.021
ATOM     34  O5  GAL A 802      80.086  21.173 -21.494 -0.05 -0.07    -0.378  3.021
ATOM     35  C6  GAL A 802      79.285  18.905 -21.127 -0.17 +0.09    +0.206  3.021
ATOM     36  O6  GAL A 802      79.626  18.457 -22.471 -0.34 -0.15    -0.344  3.021
ATOM     37  H2  GAL A 802      82.272  23.796 -18.685 +0.08 +0.07    +0.210  3.021
ATOM     38  H3  GAL A 802      81.159  21.104 -16.913 +0.08 +0.03    +0.210  3.021
ATOM     39  H4  GAL A 802      78.230  20.144 -19.053 -0.18 +0.07    +0.210  3.021
TER
ENDMDL
MODEL       82
USER    Run = 82
USER    Cluster Rank = 4
USER    Number of conformations in this cluster = 14
USER
USER    RMSD from reference structure       = 2.618 A
USER
USER    Estimated Free Energy of Binding    =   +0.02 kcal/mol  [=(1)+(2)+(3)-(4)]
USER
USER    (1) Final Intermolecular Energy     =   -4.10 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.63 kcal/mol
USER        Electrostatic Energy            =   -0.47 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      76.123109 17.683912 -23.606476
USER    NEWDPF axisangle0 0.192071 0.974069 -0.119574 -41.661845
USER    NEWDPF quaternion0        0.068303 0.346390 -0.042522 -0.934634
USER
USER                              x       y       z     vdW   Elec       q     RMS
ATOM      1  C1  SIA A 801      77.439  15.983 -21.875 -0.23 +0.07    +0.239  2.618
ATOM      2  O1A SIA A 801      77.855  14.916 -21.431 -0.23 -0.26    -0.644  2.618
ATOM      3  O1B SIA A 801      77.443  16.973 -21.142 -0.12 -0.20    -0.644  2.618
ATOM      4  C2  SIA A 801      76.733  16.045 -23.258 -0.07 +0.04    +0.258  2.618
ATOM      5  C3  SIA A 801      76.202  14.663 -23.697 -0.05 +0.02    +0.114  2.618
ATOM      6  C4  SIA A 801      75.010  14.201 -22.846 -0.10 +0.01    +0.149  2.618
ATOM      7  O4  SIA A 801      74.477  12.979 -23.400 -0.01 -0.05    -0.393  2.618
ATOM      8  C5  SIA A 801      73.910  15.277 -22.784 -0.15 +0.01    +0.145  2.618
ATOM      9  N5  SIA A 801      72.870  14.875 -21.817 -0.13 -0.00    -0.352  2.618
ATOM     10  C6  SIA A 801      74.535  16.622 -22.361 -0.19 +0.01    +0.182  2.618
ATOM     11  O6  SIA A 801      75.599  16.975 -23.298 -0.04 -0.04    -0.336  2.618
ATOM     12  C7  SIA A 801      73.522  17.784 -22.271 -0.18 +0.02    +0.180  2.618
ATOM     13  O7  SIA A 801      72.761  17.897 -23.498 -0.09 -0.04    -0.390  2.618
ATOM     14  C8  SIA A 801      74.213  19.126 -21.942 -0.25 +0.01    +0.173  2.618
ATOM     15  O8  SIA A 801      74.990  19.004 -20.730 -0.06 -0.08    -0.391  2.618
ATOM     16  C9  SIA A 801      73.210  20.273 -21.770 -0.27 -0.01    +0.198  2.618
ATOM     17  O9  SIA A 801      73.899  21.508 -21.498 -0.15 +0.08    -0.398  2.618
ATOM     18  C10 SIA A 801      71.557  14.634 -22.068 -0.32 +0.03    +0.214  2.618
ATOM     19  O10 SIA A 801      70.755  14.548 -21.147 -0.38 -0.07    -0.274  2.618
ATOM     20  C11 SIA A 801      71.092  14.305 -23.458 -0.22 +0.01    +0.117  2.618
ATOM     21  H4  SIA A 801      73.740  12.693 -22.874 +0.05 +0.02    +0.210  2.618
ATOM     22  H5  SIA A 801      73.172  14.767 -20.848 -0.41 -0.06    +0.163  2.618
```

```
ATOM     23  H7  SIA A 801      72.138  18.611 -23.443 +0.08 +0.02    +0.210  2.618
ATOM     24  H8  SIA A 801      75.414  19.829 -20.527 +0.09 +0.08    +0.210  2.618
ATOM     25  H9  SIA A 801      73.277  22.218 -21.392 -0.17 -0.10    +0.209  2.618
ATOM     26  C1  GAL A 802      78.552  18.729 -27.675 +0.00 +0.02    +0.202  2.618
ATOM     27  C2  GAL A 802      79.463  19.971 -27.625 +0.00 +0.02    +0.173  2.618
ATOM     28  O2  GAL A 802      80.141  20.149 -28.888 +0.00 -0.04    -0.391  2.618
ATOM     29  C3  GAL A 802      80.505  19.836 -26.497 +0.00 +0.02    +0.180  2.618
ATOM     30  O3  GAL A 802      81.252  21.064 -26.359 +0.00 -0.04    -0.390  2.618
ATOM     31  C4  GAL A 802      79.854  19.460 -25.151 -0.01 +0.03    +0.180  2.618
ATOM     32  O4  GAL A 802      79.093  20.579 -24.643 +0.00 -0.05    -0.390  2.618
ATOM     33  C5  GAL A 802      78.959  18.219 -25.353 -0.01 +0.03    +0.176  2.618
ATOM     34  O5  GAL A 802      77.955  18.506 -26.368 +0.00 -0.05    -0.378  2.618
ATOM     35  C6  GAL A 802      78.262  17.759 -24.073 -0.04 +0.04    +0.206  2.618
ATOM     36  O6  GAL A 802      77.664  16.452 -24.309 -0.01 -0.06    -0.344  2.618
ATOM     37  H2  GAL A 802      80.702  20.915 -28.858 +0.00 +0.02    +0.210  2.618
ATOM     38  H3  GAL A 802      81.894  20.981 -25.664 +0.01 +0.03    +0.210  2.618
ATOM     39  H4  GAL A 802      78.692  20.347 -23.813 +0.03 +0.03    +0.210  2.618
TER
ENDMDL
MODEL       62
USER    Run = 62
USER    Cluster Rank = 5
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 2.916 A
USER
USER    Estimated Free Energy of Binding    =   +0.02 kcal/mol  [=(1)+(2)+(3)-(4)]
USER
USER    (1) Final Intermolecular Energy     =   -4.09 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.64 kcal/mol
USER        Electrostatic Energy            =   -0.45 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      78.168104 21.492553 -22.512716
USER    NEWDPF axisangle0 -0.152913 0.738629 -0.656540 172.442170
USER    NEWDPF quaternion0        -0.152581 0.737023 -0.655113 0.065907
USER
USER                               x       y       z    vdW   Elec       q     RMS
ATOM      1  C1  SIA A 801      78.911  18.999 -21.589 -0.20 +0.08    +0.239  2.916
ATOM      2  O1A SIA A 801      79.231  18.143 -20.768 -0.26 -0.43    -0.644  2.916
ATOM      3  O1B SIA A 801      79.104  18.778 -22.784 -0.07 -0.19    -0.644  2.916
ATOM      4  C2  SIA A 801      78.460  20.412 -21.125 -0.18 +0.06    +0.258  2.916
ATOM      5  C3  SIA A 801      78.939  20.728 -19.691 -0.40 +0.03    +0.114  2.916
ATOM      6  C4  SIA A 801      80.459  20.931 -19.617 -0.32 +0.04    +0.149  2.916
ATOM      7  O4  SIA A 801      80.816  21.363 -18.286 -0.25 -0.09    -0.393  2.916
ATOM      8  C5  SIA A 801      80.942  21.962 -20.655 -0.18 +0.02    +0.145  2.916
ATOM      9  N5  SIA A 801      82.418  21.995 -20.679 -0.03 -0.06    -0.352  2.916
ATOM     10  C6  SIA A 801      80.399  21.579 -22.047 -0.09 +0.03    +0.182  2.916
ATOM     11  O6  SIA A 801      78.942  21.496 -21.989 -0.06 -0.04    -0.336  2.916
ATOM     12  C7  SIA A 801      80.815  22.550 -23.172 -0.05 +0.02    +0.180  2.916
ATOM     13  O7  SIA A 801      80.491  23.916 -22.816 -0.08 -0.02    -0.390  2.916
ATOM     14  C8  SIA A 801      80.165  22.177 -24.524 -0.01 +0.02    +0.173  2.916
ATOM     15  O8  SIA A 801      80.470  20.808 -24.865 +0.00 -0.05    -0.391  2.916
ATOM     16  C9  SIA A 801      80.633  23.085 -25.667 -0.01 +0.02    +0.198  2.916
ATOM     17  O9  SIA A 801      79.978  22.724 -26.897 +0.00 -0.03    -0.398  2.916
ATOM     18  C10 SIA A 801      83.225  23.047 -20.385 -0.10 +0.03    +0.214  2.916
ATOM     19  O10 SIA A 801      84.414  23.018 -20.677 -0.02 -0.04    -0.274  2.916
ATOM     20  C11 SIA A 801      82.719  24.190 -19.553 -0.12 +0.02    +0.117  2.916
ATOM     21  H4  SIA A 801      81.757  21.489 -18.241 +0.09 +0.05    +0.210  2.916
ATOM     22  H5  SIA A 801      82.885  21.128 -20.947 +0.04 +0.04    +0.163  2.916
ATOM     23  H7  SIA A 801      80.747  24.513 -23.509 +0.03 +0.01    +0.210  2.916
ATOM     24  H8  SIA A 801      80.071  20.579 -25.695 +0.01 +0.03    +0.210  2.916
ATOM     25  H9  SIA A 801      80.268  23.288 -27.605 +0.00 +0.02    +0.209  2.916
ATOM     26  C1  GAL A 802      73.490  22.600 -21.856 -0.22 -0.08    +0.202  2.916
ATOM     27  C2  GAL A 802      72.532  22.221 -23.002 -0.28 -0.05    +0.173  2.916
ATOM     28  O2  GAL A 802      71.175  22.584 -22.665 -0.16 +0.23    -0.391  2.916
ATOM     29  C3  GAL A 802      72.604  20.710 -23.294 -0.22 -0.01    +0.180  2.916
ATOM     30  O3  GAL A 802      71.821  20.391 -24.464 -0.09 -0.01    -0.390  2.916
ATOM     31  C4  GAL A 802      74.055  20.225 -23.480 -0.11 +0.00    +0.180  2.916
ATOM     32  O4  GAL A 802      74.588  20.735 -24.723 -0.00 -0.01    -0.390  2.916
ATOM     33  C5  GAL A 802      74.900  20.689 -22.275 -0.17 +0.00    +0.176  2.916
```

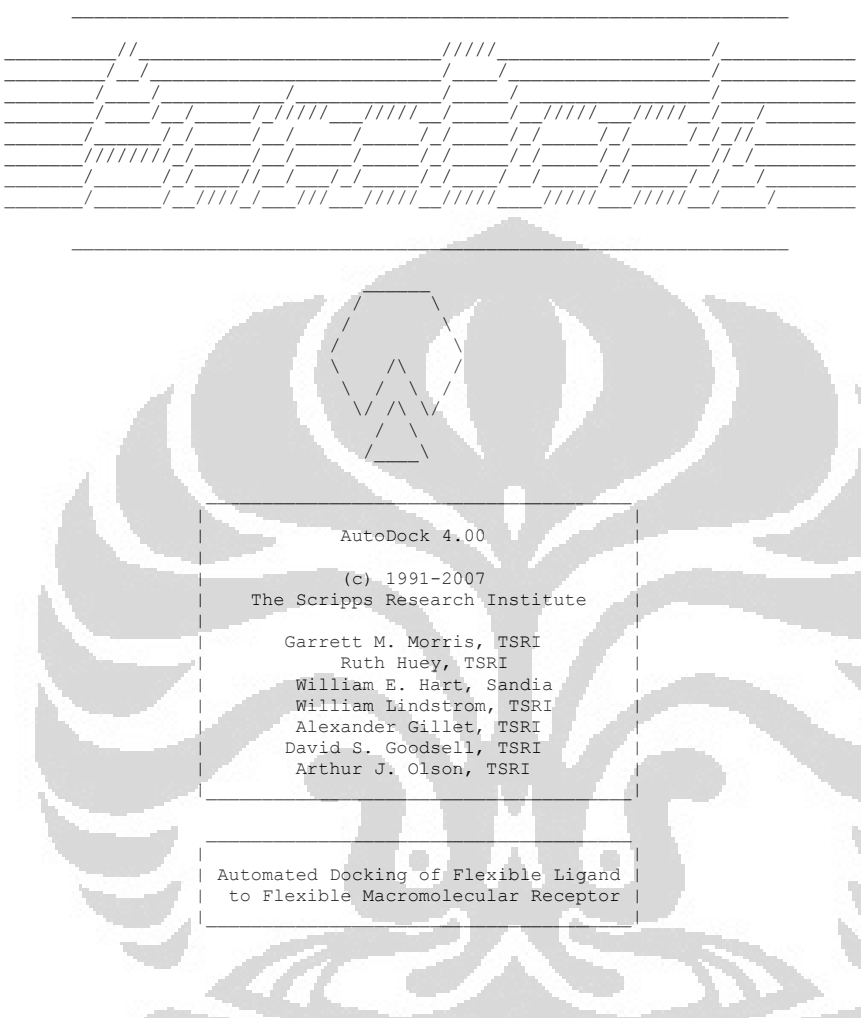
```
ATOM     34  O5  GAL A 802      74.834  22.140 -22.167 -0.08 +0.04    -0.378  2.916
ATOM     35  C6  GAL A 802      76.365  20.259 -22.360 -0.12 +0.02    +0.206  2.916
ATOM     36  O6  GAL A 802      77.002  20.513 -21.075 -0.15 -0.09    -0.344  2.916
ATOM     37  H2  GAL A 802      70.585  22.351 -23.372 +0.16 -0.08    +0.210  2.916
ATOM     38  H3  GAL A 802      71.865  19.459 -24.644 +0.08 +0.02    +0.210  2.916
ATOM     39  H4  GAL A 802      75.483  20.436 -24.838 +0.03 +0.01    +0.210  2.916
TER
ENDMDL
MODEL       77
USER    Run = 77
USER    Cluster Rank = 6
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 3.720 A
USER
USER    Estimated Free Energy of Binding    =   +0.15 kcal/mol  [=(1)+(2)+(3)-(4)]
USER
USER    (1) Final Intermolecular Energy     =   -3.97 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.42 kcal/mol
USER        Electrostatic Energy            =   -0.55 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      77.328908 17.320347 -23.304963
USER    NEWDPF axisangle0 0.082418 0.327063 0.941402 -121.582852
USER    NEWDPF quaternion0        0.071939 0.285477 0.821702 -0.487990
USER
USER                               x       y       z     vdW   Elec       q     RMS
ATOM      1  C1  SIA A 801      79.349  18.698 -22.022 -0.06 +0.10    +0.239  3.720
ATOM      2  O1A SIA A 801      80.351  19.400 -21.913 -0.40 -0.29    -0.644  3.720
ATOM      3  O1B SIA A 801      78.968  18.050 -21.047 -0.41 -0.35    -0.644  3.720
ATOM      4  C2  SIA A 801      78.689  18.468 -23.410 -0.07 +0.06    +0.258  3.720
ATOM      5  C3  SIA A 801      79.667  18.760 -24.569 -0.04 +0.02    +0.114  3.720
ATOM      6  C4  SIA A 801      80.786  17.711 -24.665 -0.05 +0.04    +0.149  3.720
ATOM      7  O4  SIA A 801      81.572  17.963 -25.849 -0.00 -0.07    -0.393  3.720
ATOM      8  C5  SIA A 801      80.216  16.281 -24.703 -0.05 +0.04    +0.145  3.720
ATOM      9  N5  SIA A 801      81.315  15.301 -24.610 -0.03 -0.11    -0.352  3.720
ATOM     10  C6  SIA A 801      79.236  16.090 -23.527 -0.03 +0.05    +0.182  3.720
ATOM     11  O6  SIA A 801      78.187  17.103 -23.604 -0.04 -0.07    -0.336  3.720
ATOM     12  C7  SIA A 801      78.593  14.688 -23.467 -0.08 +0.05    +0.180  3.720
ATOM     13  O7  SIA A 801      77.994  14.344 -24.739 +0.01 -0.07    -0.390  3.720
ATOM     14  C8  SIA A 801      77.549  14.580 -22.333 -0.19 +0.05    +0.173  3.720
ATOM     15  O8  SIA A 801      78.144  14.946 -21.069 -0.50 -0.20    -0.391  3.720
ATOM     16  C9  SIA A 801      76.962  13.169 -22.211 -0.13 +0.05    +0.198  3.720
ATOM     17  O9  SIA A 801      75.971  13.125 -21.168 -0.12 -0.05    -0.398  3.720
ATOM     18  C10 SIA A 801      81.669  14.367 -25.531 -0.01 +0.04    +0.214  3.720
ATOM     19  O10 SIA A 801      82.438  13.462 -25.233 -0.01 -0.06    -0.274  3.720
ATOM     20  C11 SIA A 801      81.263  14.519 -26.969 +0.00 +0.02    +0.117  3.720
ATOM     21  H4  SIA A 801      82.264  17.315 -25.908 +0.01 +0.04    +0.210  3.720
ATOM     22  H5  SIA A 801      81.874  15.328 -23.756 +0.01 +0.09    +0.163  3.720
ATOM     23  H7  SIA A 801      77.598  13.481 -24.703 +0.02 +0.04    +0.210  3.720
ATOM     24  H8  SIA A 801      77.502  14.880 -20.372 +0.05 +0.11    +0.210  3.720
ATOM     25  H9  SIA A 801      75.608  12.250 -21.092 +0.05 +0.04    +0.209  3.720
ATOM     26  C1  GAL A 802      73.665  20.080 -24.885 -0.07 +0.01    +0.202  3.720
ATOM     27  C2  GAL A 802      72.493  20.285 -23.905 -0.18 +0.00    +0.173  3.720
ATOM     28  O2  GAL A 802      71.489  21.142 -24.493 -0.13 +0.01    -0.391  3.720
ATOM     29  C3  GAL A 802      72.991  20.905 -22.585 -0.26 -0.02    +0.180  3.720
ATOM     30  O3  GAL A 802      71.917  20.952 -21.621 -0.20 +0.06    -0.390  3.720
ATOM     31  C4  GAL A 802      74.192  20.135 -22.002 -0.24 +0.00    +0.180  3.720
ATOM     32  O4  GAL A 802      73.759  18.845 -21.514 -0.17 -0.03    -0.390  3.720
ATOM     33  C5  GAL A 802      75.274  19.987 -23.092 -0.09 +0.01    +0.176  3.720
ATOM     34  O5  GAL A 802      74.710  19.299 -24.244 -0.01 -0.03    -0.378  3.720
ATOM     35  C6  GAL A 802      76.516  19.234 -22.616 -0.10 +0.03    +0.206  3.720
ATOM     36  O6  GAL A 802      77.563  19.378 -23.619 -0.01 -0.05    -0.344  3.720
ATOM     37  H2  GAL A 802      70.767  21.268 -23.888 +0.17 -0.02    +0.210  3.720
ATOM     38  H3  GAL A 802      72.224  21.334 -20.807 -0.16 -0.10    +0.210  3.720
ATOM     39  H4  GAL A 802      74.500  18.370 -21.154 +0.09 +0.03    +0.210  3.720
TER
ENDMDL
MODEL       33
USER    Run = 33
USER    Cluster Rank = 7
```

```
USER    Number of conformations in this cluster = 3
USER
USER    RMSD from reference structure       = 3.081 A
USER
USER    Estimated Free Energy of Binding    =   +0.15 kcal/mol  [=(1)+(2)+(3)-(4)]
USER
USER    (1) Final Intermolecular Energy     =   -3.96 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.98 kcal/mol
USER        Electrostatic Energy            =   +0.01 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      75.798124 20.364476 -23.447491
USER    NEWDPF axisangle0 0.179887 -0.234114 -0.955422 -92.315146
USER    NEWDPF quaternion0        0.129743 -0.168854 -0.689096 -0.692677
USER
USER                               x       y       z    vdW   Elec       q     RMS
ATOM      1  C1  SIA A 801      73.581  20.551 -21.813 -0.24 -0.02    +0.239  3.081
ATOM      2  O1A SIA A 801      72.392  20.516 -21.506 -0.05 +0.07    -0.644  3.081
ATOM      3  O1B SIA A 801      74.376  21.096 -21.047 -0.05 +0.06    -0.644  3.081
ATOM      4  C2  SIA A 801      74.049  20.102 -23.225 -0.10 +0.01    +0.258  3.081
ATOM      5  C3  SIA A 801      72.893  20.123 -24.249 -0.16 +0.00    +0.114  3.081
ATOM      6  C4  SIA A 801      72.448  21.552 -24.594 -0.20 -0.01    +0.149  3.081
ATOM      7  O4  SIA A 801      71.472  21.502 -25.656 -0.19 -0.00    -0.393  3.081
ATOM      8  C5  SIA A 801      73.642  22.430 -25.013 -0.11 -0.01    +0.145  3.081
ATOM      9  N5  SIA A 801      73.206  23.833 -25.159 -0.08 +0.10    -0.352  3.081
ATOM     10  C6  SIA A 801      74.751  22.328 -23.946 -0.07 -0.01    +0.182  3.081
ATOM     11  O6  SIA A 801      75.129  20.927 -23.777 -0.02 -0.01    -0.336  3.081
ATOM     12  C7  SIA A 801      76.008  23.165 -24.266 -0.04 -0.01    +0.180  3.081
ATOM     13  O7  SIA A 801      76.499  22.866 -25.595 +0.01 -0.01    -0.390  3.081
ATOM     14  C8  SIA A 801      77.124  22.951 -23.219 -0.07 +0.00    +0.173  3.081
ATOM     15  O8  SIA A 801      76.625  23.228 -21.892 +0.09 +0.01    -0.391  3.081
ATOM     16  C9  SIA A 801      78.347  23.838 -23.480 -0.09 +0.00    +0.198  3.081
ATOM     17  O9  SIA A 801      79.373  23.580 -22.502 -0.09 -0.00    -0.398  3.081
ATOM     18  C10 SIA A 801      73.231  24.593 -26.284 -0.20 -0.04    +0.214  3.081
ATOM     19  O10 SIA A 801      73.072  25.805 -26.217 -0.24 +0.08    -0.274  3.081
ATOM     20  C11 SIA A 801      73.285  23.950 -27.640 -0.21 -0.01    +0.117  3.081
ATOM     21  H4  SIA A 801      71.196  22.386 -25.869 +0.10 +0.00    +0.210  3.081
ATOM     22  H5  SIA A 801      72.846  24.283 -24.317 +0.06 -0.11    +0.163  3.081
ATOM     23  H7  SIA A 801      77.273  23.381 -25.792 +0.02 +0.01    +0.210  3.081
ATOM     24  H8  SIA A 801      77.311  23.096 -21.249 +0.08 -0.01    +0.210  3.081
ATOM     25  H9  SIA A 801      80.131  24.130 -22.664 +0.04 +0.00    +0.209  3.081
ATOM     26  C1  GAL A 802      77.309  15.838 -24.323 -0.02 +0.03    +0.202  3.081
ATOM     27  C2  GAL A 802      78.355  15.267 -23.345 -0.09 +0.04    +0.173  3.081
ATOM     28  O2  GAL A 802      78.695  13.910 -23.708 -0.02 -0.10    -0.391  3.081
ATOM     29  C3  GAL A 802      77.821  15.295 -21.900 -0.27 +0.06    +0.180  3.081
ATOM     30  O3  GAL A 802      78.859  14.902 -20.977 -0.59 -0.26    -0.390  3.081
ATOM     31  C4  GAL A 802      77.268  16.681 -21.515 -0.17 +0.05    +0.180  3.081
ATOM     32  O4  GAL A 802      78.354  17.626 -21.388 -0.47 -0.15    -0.390  3.081
ATOM     33  C5  GAL A 802      76.253  17.135 -22.586 -0.15 +0.03    +0.176  3.081
ATOM     34  O5  GAL A 802      76.904  17.165 -23.888 -0.01 -0.06    -0.378  3.081
ATOM     35  C6  GAL A 802      75.641  18.506 -22.299 -0.15 +0.02    +0.206  3.081
ATOM     36  O6  GAL A 802      74.524  18.719 -23.210 -0.05 -0.03    -0.344  3.081
ATOM     37  H2  GAL A 802      79.340  13.559 -23.105 +0.04 +0.07    +0.210  3.081
ATOM     38  H3  GAL A 802      78.530  14.920 -20.086 +0.08 +0.17    +0.210  3.081
ATOM     39  H4  GAL A 802      78.014  18.481 -21.150 -0.28 +0.04    +0.210  3.081
TER
ENDMDL
MODEL       32
USER    Run = 32
USER    Cluster Rank = 8
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 3.621 A
USER
USER    Estimated Free Energy of Binding    =   +0.19 kcal/mol  [=(1)+(2)+(3)-(4)]
USER
USER    (1) Final Intermolecular Energy     =   -3.92 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.60 kcal/mol
USER        Electrostatic Energy            =   -0.32 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
```

```
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      79.174718 17.735007 -23.195821
USER    NEWDPF axisangle0 -0.457512 -0.876217 0.151416 -84.292542
USER    NEWDPF quaternion0        -0.307002 -0.587964 0.101604 -0.741434
USER
USER                                 x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      76.616  17.442 -22.201 -0.16 +0.04    +0.239  3.621
ATOM      2  O1A SIA A 801      75.714  16.973 -21.510 -0.06 -0.07    -0.644  3.621
ATOM      3  O1B SIA A 801      76.320  18.145 -23.167 +0.03 -0.09    -0.644  3.621
ATOM      4  C2  SIA A 801      78.090  16.996 -21.989 -0.21 +0.08    +0.258  3.621
ATOM      5  C3  SIA A 801      78.183  15.642 -21.253 -0.22 +0.05    +0.114  3.621
ATOM      6  C4  SIA A 801      77.707  14.471 -22.126 -0.22 +0.05    +0.149  3.621
ATOM      7  O4  SIA A 801      77.956  13.230 -21.432 -0.18 -0.18    -0.393  3.621
ATOM      8  C5  SIA A 801      78.415  14.464 -23.494 -0.08 +0.04    +0.145  3.621
ATOM      9  N5  SIA A 801      77.805  13.443 -24.368 +0.01 -0.07    -0.352  3.621
ATOM     10  C6  SIA A 801      78.290  15.858 -24.142 -0.04 +0.04    +0.182  3.621
ATOM     11  O6  SIA A 801      78.848  16.861 -23.238 -0.07 -0.09    -0.336  3.621
ATOM     12  C7  SIA A 801      78.973  15.972 -25.522 -0.01 +0.03    +0.180  3.621
ATOM     13  O7  SIA A 801      80.348  15.523 -25.452 -0.01 -0.08    -0.390  3.621
ATOM     14  C8  SIA A 801      78.904  17.411 -26.081 +0.00 +0.03    +0.173  3.621
ATOM     15  O8  SIA A 801      77.534  17.865 -26.127 +0.01 -0.05    -0.391  3.621
ATOM     16  C9  SIA A 801      79.507  17.521 -27.486 +0.00 +0.03    +0.198  3.621
ATOM     17  O9  SIA A 801      79.453  18.882 -27.952 +0.00 -0.05    -0.398  3.621
ATOM     18  C10 SIA A 801      78.406  12.350 -24.906 +0.00 +0.04    +0.214  3.621
ATOM     19  O10 SIA A 801      77.861  11.720 -25.803 +0.00 -0.04    -0.274  3.621
ATOM     20  C11 SIA A 801      79.665  11.795 -24.302 -0.01 +0.02    +0.117  3.621
ATOM     21  H4  SIA A 801      77.662  12.506 -21.972 +0.06 +0.06    +0.210  3.621
ATOM     22  H5  SIA A 801      76.819  13.573 -24.595 +0.02 +0.03    +0.163  3.621
ATOM     23  H7  SIA A 801      80.768  15.593 -26.301 +0.01 +0.04    +0.210  3.621
ATOM     24  H8  SIA A 801      77.492  18.749 -26.471 +0.00 +0.02    +0.210  3.621
ATOM     25  H9  SIA A 801      79.826  18.950 -28.823 +0.00 +0.02    +0.209  3.621
ATOM     26  C1  GAL A 802      82.208  20.204 -20.324 -0.11 +0.07    +0.202  3.621
ATOM     27  C2  GAL A 802      82.269  21.728 -20.547 -0.11 +0.03    +0.173  3.621
ATOM     28  O2  GAL A 802      83.188  22.336 -19.613 -0.04 -0.07    -0.391  3.621
ATOM     29  C3  GAL A 802      80.873  22.359 -20.381 -0.20 +0.02    +0.180  3.621
ATOM     30  O3  GAL A 802      80.912  23.757 -20.740 -0.13 +0.01    -0.390  3.621
ATOM     31  C4  GAL A 802      79.805  21.627 -21.218 -0.17 +0.03    +0.180  3.621
ATOM     32  O4  GAL A 802      80.020  21.886 -22.624 -0.02 -0.05    -0.390  3.621
ATOM     33  C5  GAL A 802      79.870  20.117 -20.910 -0.24 +0.06    +0.176  3.621
ATOM     34  O5  GAL A 802      81.207  19.620 -21.202 -0.38 -0.18    -0.378  3.621
ATOM     35  C6  GAL A 802      78.847  19.293 -21.692 -0.20 +0.06    +0.206  3.621
ATOM     36  O6  GAL A 802      78.813  17.944 -21.144 -0.57 -0.17    -0.344  3.621
ATOM     37  H2  GAL A 802      83.227  23.276 -19.751 +0.06 +0.04    +0.210  3.621
ATOM     38  H3  GAL A 802      80.052  24.146 -20.638 -0.41 -0.08    +0.210  3.621
ATOM     39  H4  GAL A 802      79.362  21.436 -23.140 +0.04 +0.03    +0.210  3.621
TER
ENDMDL
MODEL        6
USER    Run = 6
USER    Cluster Rank = 9
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 2.995 A
USER
USER    Estimated Free Energy of Binding    =   +0.23 kcal/mol  [=(1)+(2)+(3)-(4)]
USER
USER    (1) Final Intermolecular Energy     =   -3.88 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.52 kcal/mol
USER        Electrostatic Energy            =   -0.36 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 1hgfh.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      75.528386 19.932552 -23.753985
USER    NEWDPF axisangle0 0.103816 -0.921488 -0.374276 42.950804
USER    NEWDPF quaternion0        0.038007 -0.337358 -0.137023 0.930575
USER
```

```
USER                                x       y       z     vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      77.334  19.020 -21.875 -0.08 +0.04    +0.239  2.995
ATOM      2  O1A SIA A 801      78.121  18.241 -21.343 -0.29 -0.16    -0.644  2.995
ATOM      3  O1B SIA A 801      76.912  19.975 -21.223 +0.08 -0.16    -0.644  2.995
ATOM      4  C2  SIA A 801      76.724  18.702 -23.269 -0.05 +0.04    +0.258  2.995
ATOM      5  C3  SIA A 801      76.806  17.197 -23.605 -0.07 +0.02    +0.114  2.995
ATOM      6  C4  SIA A 801      75.860  16.354 -22.737 -0.15 +0.02    +0.149  2.995
ATOM      7  O4  SIA A 801      75.882  14.987 -23.200 -0.03 -0.05    -0.393  2.995
ATOM      8  C5  SIA A 801      74.421  16.902 -22.775 -0.17 +0.01    +0.145  2.995
ATOM      9  N5  SIA A 801      73.585  16.184 -21.793 -0.10 +0.01    -0.352  2.995
ATOM     10  C6  SIA A 801      74.440  18.410 -22.451 -0.18 +0.02    +0.182  2.995
ATOM     11  O6  SIA A 801      75.316  19.096 -23.397 -0.03 -0.03    -0.336  2.995
ATOM     12  C7  SIA A 801      73.046  19.073 -22.467 -0.20 +0.01    +0.180  2.995
ATOM     13  O7  SIA A 801      72.358  18.790 -23.709 -0.09 -0.03    -0.390  2.995
ATOM     14  C8  SIA A 801      73.131  20.599 -22.235 -0.27 -0.01    +0.173  2.995
ATOM     15  O8  SIA A 801      73.838  20.879 -21.007 -0.14 +0.06    -0.391  2.995
ATOM     16  C9  SIA A 801      71.748  21.257 -22.168 -0.32 -0.04    +0.198  2.995
ATOM     17  O9  SIA A 801      71.876  22.679 -21.985 -0.25 +0.25    -0.398  2.995
ATOM     18  C10 SIA A 801      72.489  15.422 -22.042 -0.25 +0.01    +0.214  2.995
ATOM     19  O10 SIA A 801      71.747  15.083 -21.128 -0.37 -0.04    -0.274  2.995
ATOM     20  C11 SIA A 801      72.255  14.842 -23.408 -0.17 +0.01    +0.117  2.995
ATOM     21  H4  SIA A 801      75.297  14.466 -22.663 +0.03 +0.01    +0.210  2.995
ATOM     22  H5  SIA A 801      73.862  16.270 -20.814 -0.28 -0.04    +0.163  2.995
ATOM     23  H7  SIA A 801      71.500  19.198 -23.719 +0.11 +0.02    +0.210  2.995
ATOM     24  H8  SIA A 801      73.890  21.816 -20.864 -0.24 -0.08    +0.210  2.995
ATOM     25  H9  SIA A 801      71.019  23.087 -21.944 -0.04 -0.23    +0.209  2.995
ATOM     26  C1  GAL A 802      77.518  21.587 -27.858 +0.00 +0.02    +0.202  2.995
ATOM     27  C2  GAL A 802      77.857  23.090 -27.894 +0.00 +0.01    +0.173  2.995
ATOM     28  O2  GAL A 802      78.463  23.440 -29.158 +0.00 -0.03    -0.391  2.995
ATOM     29  C3  GAL A 802      78.815  23.459 -26.745 -0.00 +0.01    +0.180  2.995
ATOM     30  O3  GAL A 802      79.006  24.889 -26.694 -0.00 -0.02    -0.390  2.995
ATOM     31  C4  GAL A 802      78.310  22.945 -25.383 -0.01 +0.01    +0.180  2.995
ATOM     32  O4  GAL A 802      77.144  23.697 -24.975 +0.00 -0.01    -0.390  2.995
ATOM     33  C5  GAL A 802      77.992  21.439 -25.499 +0.00 +0.01    +0.176  2.995
ATOM     34  O5  GAL A 802      77.002  21.232 -26.546 +0.00 -0.03    -0.378  2.995
ATOM     35  C6  GAL A 802      77.479  20.825 -24.196 -0.01 +0.02    +0.206  2.995
ATOM     36  O6  GAL A 802      77.461  19.375 -24.336 +0.00 -0.05    -0.344  2.995
ATOM     37  H2  GAL A 802      78.671  24.366 -29.181 +0.00 +0.02    +0.210  2.995
ATOM     38  H3  GAL A 802      79.597  25.117 -25.986 +0.01 +0.01    +0.210  2.995
ATOM     39  H4  GAL A 802      76.832  23.380 -24.135 +0.04 -0.00    +0.210  2.995
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2            # number of dimensions in the field
AVSFLD: nspace=1          # number of physical coordinates
AVSFLD: veclen=7          # vector size
AVSFLD: dim1=39           # atoms
AVSFLD: dim2=9            # conformations
AVSFLD: data=Real        # data type (byte,integer,Real,double)
AVSFLD: field=uniform     # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 1hgfh.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 1hgfh.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 1hgfh.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 1hgfh.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 1hgfh.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 1hgfh.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 1hgfh.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                11:24 39" p.m., 06/14/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 44m 02.82s,  CPU= 43m 55.97s,  System= 0.70s
_____________________________________________________________________________
```

2FK0-Sia(α2-3)Gal



Number of distinct conformational clusters found = 5, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.14	68	-1.04	80	
2	-1.11	77	-1.10	8	########
3	-0.88	12	-0.86	10	##########
4	-0.78	37	-0.78	1	#
5	-0.54	10	-0.54	1	#

Number of multi-member conformational clusters found = 3, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	68	-1.14	0.00	2.54	RANKING
1	2	29	-1.14	0.02	2.54	RANKING
1	3	95	-1.13	0.05	2.54	RANKING
1	4	66	-1.13	0.06	2.53	RANKING
1	5	99	-1.12	0.06	2.53	RANKING
1	6	74	-1.12	0.08	2.52	RANKING
1	7	60	-1.12	0.06	2.53	RANKING
1	8	91	-1.12	0.30	2.59	RANKING
1	9	64	-1.11	0.17	2.58	RANKING
1	10	72	-1.11	0.06	2.55	RANKING
1	11	9	-1.11	0.26	2.58	RANKING
1	12	25	-1.11	0.16	2.57	RANKING
1	13	84	-1.11	0.04	2.53	RANKING
1	14	24	-1.11	0.05	2.54	RANKING
1	15	70	-1.11	0.15	2.57	RANKING
1	16	69	-1.11	0.09	2.55	RANKING
1	17	14	-1.11	0.26	2.59	RANKING
1	18	45	-1.11	0.06	2.55	RANKING
1	19	93	-1.11	0.29	2.59	RANKING
1	20	65	-1.11	0.26	2.59	RANKING
1	21	20	-1.10	0.28	2.59	RANKING
1	22	31	-1.10	0.24	2.59	RANKING
1	23	61	-1.10	0.08	2.54	RANKING
1	24	87	-1.10	0.08	2.55	RANKING
1	25	51	-1.10	0.09	2.57	RANKING
1	26	43	-1.10	0.36	2.59	RANKING
1	27	23	-1.10	0.11	2.56	RANKING
1	28	30	-1.10	0.20	2.59	RANKING
1	29	21	-1.09	0.15	2.57	RANKING
1	30	63	-1.09	0.31	2.59	RANKING
1	31	52	-1.09	0.24	2.58	RANKING
1	32	86	-1.09	0.17	2.57	RANKING
1	33	42	-1.09	0.12	2.55	RANKING
1	34	19	-1.09	0.20	2.58	RANKING
1	35	82	-1.08	0.11	2.56	RANKING
1	36	57	-1.08	0.26	2.59	RANKING
1	37	22	-1.08	0.36	2.60	RANKING
1	38	59	-1.07	0.26	2.59	RANKING
1	39	76	-1.07	0.20	2.57	RANKING
1	40	75	-1.07	0.16	2.52	RANKING
1	41	55	-1.07	0.30	2.58	RANKING
1	42	34	-1.07	0.31	2.59	RANKING
1	43	96	-1.06	0.21	2.58	RANKING
1	44	62	-1.04	0.19	2.58	RANKING
1	45	53	-1.03	0.19	2.54	RANKING
1	46	80	-1.03	0.33	2.58	RANKING
1	47	40	-1.03	0.27	2.55	RANKING
1	48	1	-1.01	0.68	2.51	RANKING
1	49	5	-1.01	0.72	2.50	RANKING
1	50	48	-1.01	0.75	2.50	RANKING
1	51	41	-1.01	0.76	2.49	RANKING
1	52	36	-1.01	0.74	2.50	RANKING
1	53	27	-1.01	0.72	2.50	RANKING
1	54	44	-1.01	0.74	2.50	RANKING
1	55	35	-1.01	0.75	2.49	RANKING
1	56	78	-1.00	0.73	2.50	RANKING
1	57	94	-1.00	0.77	2.49	RANKING
1	58	56	-1.00	0.60	2.53	RANKING
1	59	32	-1.00	0.76	2.51	RANKING
1	60	89	-1.00	0.76	2.49	RANKING
1	61	100	-1.00	0.60	2.53	RANKING
1	62	13	-1.00	0.83	2.48	RANKING
1	63	85	-1.00	0.59	2.53	RANKING
1	64	17	-1.00	0.66	2.52	RANKING
1	65	38	-1.00	0.73	2.50	RANKING
1	66	88	-1.00	0.82	2.48	RANKING
1	67	39	-0.99	0.55	2.54	RANKING
1	68	67	-0.99	0.78	2.49	RANKING
1	69	11	-0.95	1.11	2.44	RANKING

```
   1     70     50       -0.94      1.07      2.43           RANKING
   1     71      3       -0.94      1.09      2.44           RANKING
   1     72     49       -0.94      1.11      2.42           RANKING
   1     73      8       -0.93      1.15      2.42           RANKING
   1     74      2       -0.93      1.19      2.45           RANKING
   1     75     54       -0.92      1.25      2.43           RANKING
   1     76     58       -0.91      1.27      2.42           RANKING
   1     77      7       -0.91      1.18      2.42           RANKING
   1     78     47       -0.88      1.20      2.46           RANKING
   1     79     28       -0.88      1.28      2.45           RANKING
   1     80     81       -0.87      1.32      2.47           RANKING
   2      1     77       -1.11      0.00      3.40           RANKING
   2      2     97       -1.11      0.07      3.39           RANKING
   2      3     73       -1.10      0.11      3.39           RANKING
   2      4     26       -1.10      0.18      3.37           RANKING
   2      5      6       -1.10      0.13      3.37           RANKING
   2      6     33       -1.10      0.23      3.36           RANKING
   2      7     46       -1.09      0.07      3.37           RANKING
   2      8     90       -1.06      0.21      3.34           RANKING
   3      1     12       -0.88      0.00      3.43           RANKING
   3      2     98       -0.88      0.12      3.39           RANKING
   3      3      4       -0.88      0.22      3.36           RANKING
   3      4     92       -0.87      0.15      3.37           RANKING
   3      5     79       -0.87      0.05      3.42           RANKING
   3      6     18       -0.87      0.21      3.36           RANKING
   3      7     16       -0.87      0.19      3.36           RANKING
   3      8     71       -0.85      0.31      3.33           RANKING
   3      9     83       -0.85      0.38      3.29           RANKING
   3     10     15       -0.80      0.46      3.28           RANKING
   4      1     37       -0.78      0.00      3.75           RANKING
   5      1     10       -0.54      0.00      3.05           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.15  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.17           at Temperature, T = 298.15 K
Free energy,        A ~ -2729.50 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -1.02 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       68
USER    Run = 68
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 80
USER
USER    RMSD from reference structure       = 2.537 A
USER
USER    Estimated Free Energy of Binding    =   -1.14 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  145.55 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.26 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.12 kcal/mol
USER        Electrostatic Energy            =   -1.14 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
```

```
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 2fk0a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      75.658502 17.095738 -23.117322
USER    NEWDPF axisangle0 0.818076 0.517290 0.251321 118.751608
USER    NEWDPF quaternion0        0.703977 0.445142 0.216269 0.509405
USER
USER                               x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      74.838  18.838 -22.919 -0.09 +0.18    +0.239  2.537
ATOM      2  O1A SIA A3021      74.017  19.701 -22.618 +0.02 -0.68    -0.644  2.537
ATOM      3  O1B SIA A3021      75.496  18.980 -23.949 -0.13 -0.76    -0.644  2.537
ATOM      4  C2  SIA A3021      74.910  17.501 -22.129 -0.16 +0.04    +0.259  2.537
ATOM      5  C3  SIA A3021      73.611  17.205 -21.350 -0.19 +0.00    +0.114  2.537
ATOM      6  C4  SIA A3021      72.443  16.859 -22.282 -0.30 +0.02    +0.149  2.537
ATOM      7  O4  SIA A3021      71.313  16.428 -21.493 -0.23 -0.05    -0.393  2.537
ATOM      8  C5  SIA A3021      72.819  15.751 -23.288 -0.26 +0.02    +0.145  2.537
ATOM      9  N5  SIA A3021      71.731  15.618 -24.273 -0.07 -0.05    -0.352  2.537
ATOM     10  C6  SIA A3021      74.145  16.116 -23.986 -0.14 +0.04    +0.182  2.537
ATOM     11  O6  SIA A3021      75.178  16.335 -22.977 -0.08 -0.04    -0.336  2.537
ATOM     12  C7  SIA A3021      74.646  15.065 -25.001 -0.06 +0.03    +0.180  2.537
ATOM     13  O7  SIA A3021      74.755  13.763 -24.382 -0.02 -0.02    -0.390  2.537
ATOM     14  C8  SIA A3021      76.001  15.471 -25.621 -0.02 +0.03    +0.173  2.537
ATOM     15  O8  SIA A3021      75.892  16.764 -26.256 -0.03 -0.12    -0.391  2.537
ATOM     16  C9  SIA A3021      76.504  14.453 -26.649 -0.00 +0.02    +0.198  2.537
ATOM     17  O9  SIA A3021      77.786  14.854 -27.167 +0.00 -0.05    -0.398  2.537
ATOM     18  C10 SIA A3021      71.171  14.445 -24.660 -0.23 +0.02    +0.214  2.537
ATOM     19  O10 SIA A3021      71.573  13.348 -24.288 -0.19 +0.00    -0.274  2.537
ATOM     20  C11 SIA A3021      70.120  14.519 -25.723 -0.32 +0.01    +0.117  2.537
ATOM     21  H4  SIA A3021      70.589  16.213 -22.070 +0.14 +0.02    +0.210  2.537
ATOM     22  H5  SIA A3021      71.373  16.474 -24.697 +0.09 +0.04    +0.163  2.537
ATOM     23  H7  SIA A3021      75.062  13.117 -25.006 +0.03 +0.01    +0.210  2.537
ATOM     24  H8  SIA A3021      76.726  17.014 -26.638 +0.01 +0.06    +0.210  2.537
ATOM     25  H9  SIA A3021      78.098  14.222 -27.804 +0.00 +0.02    +0.209  2.537
ATOM     26  C1  GAL A3022      79.703  16.947 -21.570 -0.14 +0.03    +0.202  2.537
ATOM     27  C2  GAL A3022      78.257  16.673 -21.120 -0.24 +0.02    +0.173  2.537
ATOM     28  O2  GAL A3022      77.834  15.370 -21.583 -0.14 -0.01    -0.391  2.537
ATOM     29  C3  GAL A3022      77.310  17.743 -21.683 -0.19 +0.03    +0.187  2.537
ATOM     30  O3  GAL A3022      75.972  17.552 -21.123 -0.10 -0.00    -0.336  2.537
ATOM     31  C4  GAL A3022      77.813  19.160 -21.355 -0.22 +0.04    +0.180  2.537
ATOM     32  O4  GAL A3022      77.702  19.411 -19.936 -0.46 -0.13    -0.390  2.537
ATOM     33  C5  GAL A3022      79.272  19.314 -21.833 -0.15 +0.03    +0.176  2.537
ATOM     34  O5  GAL A3022      80.128  18.298 -21.229 -0.08 -0.01    -0.378  2.537
ATOM     35  C6  GAL A3022      79.836  20.699 -21.502 -0.12 +0.04    +0.198  2.537
ATOM     36  O6  GAL A3022      81.175  20.830 -22.020 -0.04 -0.04    -0.398  2.537
ATOM     37  H2  GAL A3022      76.941  15.201 -21.305 -0.10 -0.03    +0.210  2.537
ATOM     38  H4  GAL A3022      78.013  20.285 -19.734 +0.02 +0.06    +0.210  2.537
ATOM     39  H6  GAL A3022      81.525  21.689 -21.815 +0.04 +0.03    +0.209  2.537
TER
ENDMDL
MODEL       77
USER    Run = 77
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 8
USER
USER    RMSD from reference structure       = 3.399 A
USER
USER    Estimated Free Energy of Binding    =   -1.11 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  153.04 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.23 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.77 kcal/mol
USER        Electrostatic Energy            =   -0.46 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 2fk0a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      77.814347 22.728895 -22.829360
USER    NEWDPF axisangle0 -0.927478 -0.371477 0.042305 -142.716226
USER    NEWDPF quaternion0        -0.878818 -0.351987 0.040085 -0.319652
```

```
USER
USER                                x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      77.101  24.401 -23.494 -0.07 +0.06    +0.239  3.399
ATOM      2  O1A SIA A3021      76.438  25.433 -23.550 +0.05 -0.15    -0.644  3.399
ATOM      3  O1B SIA A3021      77.327  23.786 -24.537 +0.05 -0.18    -0.644  3.399
ATOM      4  C2  SIA A3021      77.480  23.774 -22.124 -0.15 +0.05    +0.259  3.399
ATOM      5  C3  SIA A3021      76.568  24.262 -20.979 -0.30 +0.02    +0.114  3.399
ATOM      6  C4  SIA A3021      75.142  23.707 -21.099 -0.37 -0.01    +0.149  3.399
ATOM      7  O4  SIA A3021      74.392  24.057 -19.915 -0.47 +0.02    -0.393  3.399
ATOM      8  C5  SIA A3021      75.134  22.175 -21.277 -0.21 -0.01    +0.145  3.399
ATOM      9  N5  SIA A3021      73.761  21.742 -21.590 -0.20 +0.04    -0.352  3.399
ATOM     10  C6  SIA A3021      76.101  21.782 -22.413 -0.18 +0.07    +0.182  3.399
ATOM     11  O6  SIA A3021      77.432  22.308 -22.118 -0.21 -0.09    -0.336  3.399
ATOM     12  C7  SIA A3021      76.205  20.262 -22.670 -0.14 +0.11    +0.180  3.399
ATOM     13  O7  SIA A3021      76.555  19.559 -21.457 -0.14 -0.10    -0.390  3.399
ATOM     14  C8  SIA A3021      77.227  19.941 -23.782 -0.06 +0.10    +0.173  3.399
ATOM     15  O8  SIA A3021      76.871  20.629 -25.002 -0.41 -0.37    -0.391  3.399
ATOM     16  C9  SIA A3021      77.327  18.440 -24.070 -0.04 +0.08    +0.198  3.399
ATOM     17  O9  SIA A3021      78.320  18.188 -25.082 +0.01 -0.10    -0.398  3.399
ATOM     18  C10 SIA A3021      73.114  20.711 -20.990 -0.36 -0.01    +0.214  3.399
ATOM     19  O10 SIA A3021      73.642  19.967 -20.172 -0.29 +0.01    -0.274  3.399
ATOM     20  C11 SIA A3021      71.743  20.391 -21.497 -0.41 -0.02    +0.117  3.399
ATOM     21  H4  SIA A3021      73.509  23.714 -19.989 -0.27 -0.10    +0.210  3.399
ATOM     22  H5  SIA A3021      73.258  22.258 -22.312 -0.18 -0.12    +0.163  3.399
ATOM     23  H7  SIA A3021      76.618  18.624 -21.615 +0.08 +0.05    +0.210  3.399
ATOM     24  H8  SIA A3021      77.500  20.432 -25.686 +0.02 +0.11    +0.210  3.399
ATOM     25  H9  SIA A3021      78.382  17.257 -25.260 +0.01 +0.04    +0.209  3.399
ATOM     26  C1  GAL A3022      82.146  22.622 -22.828 -0.02 +0.03    +0.202  3.399
ATOM     27  C2  GAL A3022      80.975  22.971 -21.893 -0.11 +0.03    +0.173  3.399
ATOM     28  O2  GAL A3022      80.429  21.765 -21.313 -0.13 -0.07    -0.391  3.399
ATOM     29  C3  GAL A3022      79.870  23.704 -22.670 -0.10 +0.04    +0.187  3.399
ATOM     30  O3  GAL A3022      78.839  24.158 -21.739 -0.14 -0.06    -0.336  3.399
ATOM     31  C4  GAL A3022      80.438  24.907 -23.444 -0.07 +0.07    +0.180  3.399
ATOM     32  O4  GAL A3022      80.859  25.938 -22.522 -0.02 -0.23    -0.390  3.399
ATOM     33  C5  GAL A3022      81.614  24.444 -24.330 -0.02 +0.04    +0.176  3.399
ATOM     34  O5  GAL A3022      82.648  23.797 -23.529 +0.00 -0.07    -0.378  3.399
ATOM     35  C6  GAL A3022      82.240  25.610 -25.101 -0.02 +0.05    +0.198  3.399
ATOM     36  O6  GAL A3022      83.289  25.132 -25.966 +0.00 -0.06    -0.398  3.399
ATOM     37  H2  GAL A3022      79.705  21.981 -20.736 +0.08 +0.08    +0.210  3.399
ATOM     38  H4  GAL A3022      81.209  26.680 -22.999 +0.03 +0.16    +0.210  3.399
ATOM     39  H6  GAL A3022      83.677  25.855 -26.444 +0.00 +0.03    +0.209  3.399
TER
ENDMDL
MODEL       12
USER    Run = 12
USER    Cluster Rank = 3
USER    Number of conformations in this cluster = 10
USER
USER    RMSD from reference structure       = 3.433 A
USER
USER    Estimated Free Energy of Binding    =   -0.88 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  225.46 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.00 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.34 kcal/mol
USER        Electrostatic Energy            =   -0.65 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 2fk0a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      76.323401 21.824917 -23.589652
USER    NEWDPF axisangle0 0.598188 -0.668201 0.442356 -158.196949
USER    NEWDPF quaternion0        0.587393 -0.656142 0.434373 -0.189122
USER
USER                                x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A3021      77.531  20.331 -23.825 -0.04 +0.12    +0.239  3.433
ATOM      2  O1A SIA A3021      78.566  19.669 -23.817 +0.04 -0.18    -0.644  3.433
ATOM      3  O1B SIA A3021      76.721  20.151 -24.734 -0.43 -0.66    -0.644  3.433
ATOM      4  C2  SIA A3021      77.332  21.505 -22.827 -0.08 +0.10    +0.259  3.433
ATOM      5  C3  SIA A3021      78.667  22.021 -22.248 -0.07 +0.03    +0.114  3.433
ATOM      6  C4  SIA A3021      79.509  22.754 -23.301 -0.05 +0.03    +0.149  3.433
ATOM      7  O4  SIA A3021      80.655  23.356 -22.661 -0.03 -0.08    -0.393  3.433
ATOM      8  C5  SIA A3021      78.697  23.843 -24.030 -0.03 +0.04    +0.145  3.433
```

```
ATOM      9  N5  SIA A3021      79.498  24.357 -25.155 +0.01 -0.09    -0.352  3.433
ATOM     10  C6  SIA A3021      77.368  23.245 -24.537 -0.04 +0.06    +0.182  3.433
ATOM     11  O6  SIA A3021      76.642  22.659 -23.413 -0.07 -0.12    -0.336  3.433
ATOM     12  C7  SIA A3021      76.447  24.251 -25.263 -0.06 +0.04    +0.180  3.433
ATOM     13  O7  SIA A3021      76.186  25.402 -24.430 -0.02 -0.06    -0.390  3.433
ATOM     14  C8  SIA A3021      75.117  23.596 -25.695 -0.06 +0.05    +0.173  3.433
ATOM     15  O8  SIA A3021      75.374  22.454 -26.543 -0.15 -0.34    -0.391  3.433
ATOM     16  C9  SIA A3021      74.199  24.571 -26.439 -0.19 -0.02    +0.198  3.433
ATOM     17  O9  SIA A3021      72.957  23.927 -26.783 -0.37 +0.06    -0.398  3.433
ATOM     18  C10 SIA A3021      79.692  25.670 -25.437 -0.02 +0.08    +0.214  3.433
ATOM     19  O10 SIA A3021      79.145  26.580 -24.825 -0.06 -0.18    -0.274  3.433
ATOM     20  C11 SIA A3021      80.489  25.985 -26.664 -0.01 +0.03    +0.117  3.433
ATOM     21  H4  SIA A3021      81.177  23.810 -23.313 +0.03 +0.05    +0.210  3.433
ATOM     22  H5  SIA A3021      79.940  23.673 -25.769 +0.01 +0.03    +0.163  3.433
ATOM     23  H7  SIA A3021      75.620  26.020 -24.877 +0.07 +0.02    +0.210  3.433
ATOM     24  H8  SIA A3021      74.555  22.051 -26.808 +0.04 +0.28    +0.210  3.433
ATOM     25  H9  SIA A3021      72.388  24.532 -27.245 +0.10 -0.03    +0.209  3.433
ATOM     26  C1  GAL A3022      72.759  20.781 -21.357 -0.41 -0.01    +0.202  3.433
ATOM     27  C2  GAL A3022      74.170  21.351 -21.128 -0.33 -0.01    +0.173  3.433
ATOM     28  O2  GAL A3022      74.189  22.763 -21.437 -0.20 +0.14    -0.391  3.433
ATOM     29  C3  GAL A3022      75.192  20.624 -22.015 -0.21 +0.09    +0.187  3.433
ATOM     30  O3  GAL A3022      76.541  21.074 -21.674 -0.22 -0.08    -0.336  3.433
ATOM     31  C4  GAL A3022      75.094  19.098 -21.840 -0.24 +0.07    +0.180  3.433
ATOM     32  O4  GAL A3022      75.550  18.718 -20.523 -0.22 -0.05    -0.390  3.433
ATOM     33  C5  GAL A3022      73.638  18.643 -22.075 -0.30 +0.07    +0.176  3.433
ATOM     34  O5  GAL A3022      72.723  19.337 -21.174 -0.19 -0.05    -0.378  3.433
ATOM     35  C6  GAL A3022      73.475  17.132 -21.882 -0.29 +0.02    +0.198  3.433
ATOM     36  O6  GAL A3022      72.120  16.735 -22.173 -0.20 -0.06    -0.398  3.433
ATOM     37  H2  GAL A3022      75.061  23.115 -21.296 +0.10 -0.03    +0.210  3.433
ATOM     38  H4  GAL A3022      75.489  17.776 -20.416 -0.26 -0.01    +0.210  3.433
ATOM     39  H6  GAL A3022      72.019  15.798 -22.053 +0.11 +0.02    +0.209  3.433
TER
ENDMDL
MODEL     37
USER    Run = 37
USER    Cluster Rank = 4
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 3.752 A
USER
USER    Estimated Free Energy of Binding    =   -0.78 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  269.57 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.89 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.36 kcal/mol
USER        Electrostatic Energy            =   -1.53 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 2fk0a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      77.983797 22.291034 -23.584940
USER    NEWDPF axisangle0 0.045984 0.970309 -0.237457 124.184686
USER    NEWDPF quaternion0        0.040636 0.857465 -0.209842 0.468048
USER
USER                                 x       y       z     vdW   Elec       q    RMS
ATOM      1  C1  SIA A3021      76.522  21.023 -23.635 +0.07 +0.21    +0.239  3.752
ATOM      2  O1A SIA A3021      75.902  19.970 -23.515 -0.25 -0.82    -0.644  3.752
ATOM      3  O1B SIA A3021      76.248  21.768 -24.576 -0.17 -0.74    -0.644  3.752
ATOM      4  C2  SIA A3021      77.758  21.323 -22.741 -0.07 +0.09    +0.259  3.752
ATOM      5  C3  SIA A3021      78.362  20.045 -22.122 -0.13 +0.03    +0.114  3.752
ATOM      6  C4  SIA A3021      79.048  19.162 -23.174 -0.04 +0.03    +0.149  3.752
ATOM      7  O4  SIA A3021      79.736  18.078 -22.512 -0.04 -0.05    -0.393  3.752
ATOM      8  C5  SIA A3021      80.051  19.961 -24.030 -0.01 +0.02    +0.145  3.752
ATOM      9  N5  SIA A3021      80.511  19.107 -25.139 +0.01 -0.05    -0.352  3.752
ATOM     10  C6  SIA A3021      79.369  21.235 -24.570 +0.00 +0.04    +0.182  3.752
ATOM     11  O6  SIA A3021      78.840  22.011 -23.452 -0.02 -0.09    -0.336  3.752
ATOM     12  C7  SIA A3021      80.285  22.140 -25.423 +0.01 +0.03    +0.180  3.752
ATOM     13  O7  SIA A3021      81.484  22.491 -24.695 +0.01 -0.06    -0.390  3.752
ATOM     14  C8  SIA A3021      79.552  23.419 -25.885 +0.01 +0.04    +0.173  3.752
ATOM     15  O8  SIA A3021      78.363  23.072 -26.629 +0.01 -0.09    -0.391  3.752
ATOM     16  C9  SIA A3021      80.437  24.319 -26.754 +0.00 +0.04    +0.198  3.752
ATOM     17  O9  SIA A3021      79.725  25.515 -27.124 +0.01 -0.08    -0.398  3.752
ATOM     18  C10 SIA A3021      81.807  18.938 -25.505 +0.00 +0.02    +0.214  3.752
```

```
ATOM     19  O10 SIA A3021      82.738  19.552 -24.997 +0.00 -0.03    -0.274  3.752
ATOM     20  C11 SIA A3021      82.061  18.076 -26.702 +0.00 +0.01    +0.117  3.752
ATOM     21  H4  SIA A3021      80.161  17.531 -23.163 +0.03 +0.02    +0.210  3.752
ATOM     22  H5  SIA A3021      79.802  18.605 -25.672 +0.01 +0.03    +0.163  3.752
ATOM     23  H7  SIA A3021      82.047  23.047 -25.220 +0.01 +0.03    +0.210  3.752
ATOM     24  H8  SIA A3021      77.912  23.859 -26.913 +0.02 +0.05    +0.210  3.752
ATOM     25  H9  SIA A3021      80.273  26.073 -27.663 +0.00 +0.04    +0.209  3.752
ATOM     26  C1  GAL A3022      76.974  25.954 -21.501 -0.30 +0.10    +0.202  3.752
ATOM     27  C2  GAL A3022      77.610  24.579 -21.230 -0.20 +0.04    +0.173  3.752
ATOM     28  O2  GAL A3022      78.996  24.586 -21.642 -0.06 -0.07    -0.391  3.752
ATOM     29  C3  GAL A3022      76.859  23.480 -21.996 -0.18 +0.03    +0.187  3.752
ATOM     30  O3  GAL A3022      77.382  22.171 -21.609 -0.10 -0.10    -0.336  3.752
ATOM     31  C4  GAL A3022      75.347  23.540 -21.715 -0.27 -0.02    +0.180  3.752
ATOM     32  O4  GAL A3022      75.079  23.156 -20.348 -0.17 +0.07    -0.390  3.752
ATOM     33  C5  GAL A3022      74.823  24.963 -22.003 -0.30 -0.02    +0.176  3.752
ATOM     34  O5  GAL A3022      75.546  25.954 -21.213 -0.63 -0.17    -0.378  3.752
ATOM     35  C6  GAL A3022      73.325  25.088 -21.709 -0.24 -0.08    +0.198  3.752
ATOM     36  O6  GAL A3022      72.858  26.409 -22.051 -0.34 -0.02    -0.398  3.752
ATOM     37  H2  GAL A3022      79.389  23.737 -21.474 -0.06 +0.03    +0.210  3.752
ATOM     38  H4  GAL A3022      74.146  23.193 -20.175 -0.13 -0.08    +0.210  3.752
ATOM     39  H6  GAL A3022      71.929  26.487 -21.869 +0.14 +0.01    +0.209  3.752
TER
ENDMDL
MODEL       10
USER    Run = 10
USER    Cluster Rank = 5
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 3.048 A
USER
USER    Estimated Free Energy of Binding    =   -0.54 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  401.89 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -4.66 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -3.56 kcal/mol
USER        Electrostatic Energy            =   -1.10 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 2fk0a.dpf
USER    NEWDPF move       a.pdbqt
USER    NEWDPF about      76.250000 18.934999 -22.507000
USER    NEWDPF tran0      79.038617 19.950638 -22.870694
USER    NEWDPF axisangle0 0.663647 0.739583 -0.112203 156.059733
USER    NEWDPF quaternion0        0.649217 0.723501 -0.109764 0.207402
USER
USER                            x       y       z     vdW   Elec       q    RMS
ATOM      1  C1  SIA A3021      77.439  20.438 -23.846 -0.05 +0.13    +0.239  3.048
ATOM      2  O1A SIA A3021      76.250  20.560 -24.129 -0.38 -0.95    -0.644  3.048
ATOM      3  O1B SIA A3021      78.247  20.248 -24.756 +0.02 -0.24    -0.644  3.048
ATOM      4  C2  SIA A3021      77.897  20.328 -22.365 -0.08 +0.08    +0.259  3.048
ATOM      5  C3  SIA A3021      76.751  19.900 -21.424 -0.22 +0.03    +0.114  3.048
ATOM      6  C4  SIA A3021      76.335  18.439 -21.646 -0.23 +0.03    +0.149  3.048
ATOM      7  O4  SIA A3021      75.387  18.052 -20.628 -0.15 -0.02    -0.393  3.048
ATOM      8  C5  SIA A3021      77.546  17.485 -21.610 -0.21 +0.02    +0.145  3.048
ATOM      9  N5  SIA A3021      77.104  16.144 -22.031 -0.09 -0.01    -0.352  3.048
ATOM     10  C6  SIA A3021      78.650  18.014 -22.548 -0.08 +0.03    +0.182  3.048
ATOM     11  O6  SIA A3021      78.997  19.380 -22.163 -0.08 -0.06    -0.336  3.048
ATOM     12  C7  SIA A3021      79.934  17.156 -22.576 -0.08 +0.02    +0.180  3.048
ATOM     13  O7  SIA A3021      80.462  16.976 -21.243 -0.04 -0.05    -0.390  3.048
ATOM     14  C8  SIA A3021      81.012  17.773 -23.494 -0.02 +0.02    +0.173  3.048
ATOM     15  O8  SIA A3021      80.493  17.938 -24.833 +0.01 -0.05    -0.391  3.048
ATOM     16  C9  SIA A3021      82.285  16.924 -23.556 -0.01 +0.02    +0.198  3.048
ATOM     17  O9  SIA A3021      83.273  17.559 -24.388 +0.00 -0.03    -0.398  3.048
ATOM     18  C10 SIA A3021      77.394  14.989 -21.382 -0.15 -0.01    +0.214  3.048
ATOM     19  O10 SIA A3021      78.136  14.929 -20.408 -0.31 -0.01    -0.274  3.048
ATOM     20  C11 SIA A3021      76.903  13.722 -22.010 -0.19 -0.00    +0.117  3.048
ATOM     21  H4  SIA A3021      75.129  17.148 -20.765 -0.35 -0.08    +0.210  3.048
ATOM     22  H5  SIA A3021      76.536  16.080 -22.876 +0.04 +0.01    +0.163  3.048
ATOM     23  H7  SIA A3021      81.251  16.448 -21.261 +0.03 +0.03    +0.210  3.048
ATOM     24  H8  SIA A3021      81.157  18.318 -25.398 +0.00 +0.02    +0.210  3.048
ATOM     25  H9  SIA A3021      84.063  17.033 -24.426 +0.00 +0.01    +0.209  3.048
ATOM     26  C1  GAL A3022      81.754  23.280 -22.304 -0.06 +0.04    +0.202  3.048
ATOM     27  C2  GAL A3022      80.596  22.566 -21.584 -0.13 +0.03    +0.173  3.048
ATOM     28  O2  GAL A3022      81.087  21.381 -20.915 -0.09 -0.04    -0.391  3.048
```

```
ATOM     29  C3  GAL A3022      79.505  22.166 -22.589 -0.07 +0.04    +0.187  3.048
ATOM     30  O3  GAL A3022      78.353  21.626 -21.868 -0.42 -0.13    -0.336  3.048
ATOM     31  C4  GAL A3022      79.067  23.368 -23.443 -0.05 +0.05    +0.180  3.048
ATOM     32  O4  GAL A3022      78.355  24.325 -22.627 -0.08 -0.11    -0.390  3.048
ATOM     33  C5  GAL A3022      80.306  24.014 -24.100 -0.02 +0.05    +0.176  3.048
ATOM     34  O5  GAL A3022      81.283  24.412 -23.092 -0.03 -0.10    -0.378  3.048
ATOM     35  C6  GAL A3022      79.931  25.240 -24.939 -0.03 +0.07    +0.198  3.048
ATOM     36  O6  GAL A3022      81.100  25.777 -25.589 -0.01 -0.12    -0.398  3.048
ATOM     37  H2  GAL A3022      80.372  20.940 -20.470 -0.03 +0.02    +0.210  3.048
ATOM     38  H4  GAL A3022      78.085  25.067 -23.155 +0.06 +0.08    +0.210  3.048
ATOM     39  H6  GAL A3022      80.868  26.537 -26.109 +0.01 +0.07    +0.209  3.048
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2            # number of dimensions in the field
AVSFLD: nspace=1          # number of physical coordinates
AVSFLD: veclen=7          # vector size
AVSFLD: dim1=39           # atoms
AVSFLD: dim2=5            # conformations
AVSFLD: data=Real        # data type (byte,integer,Real,double)
AVSFLD: field=uniform     # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 2fk0a.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 2fk0a.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 2fk0a.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 2fk0a.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 2fk0a.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 2fk0a.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 2fk0a.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                1:37 40" a.m., 06/15/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 44m 06.47s,  CPU= 43m 59.91s,  System= 0.67s
_____________________________________________________________________________
```

2FK0-Sia(α2-6)Gal

Number of distinct conformational clusters found = 2, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.50	17	-1.39	49	##
2	-1.42	61	-1.36	51	##

Number of multi-member conformational clusters found = 2, out of 100 runs.

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern

1	1	17	-1.50	0.00	3.48	RANKING
1	2	11	-1.48	0.13	3.43	RANKING
1	3	38	-1.48	0.15	3.43	RANKING
1	4	82	-1.48	0.12	3.50	RANKING
1	5	66	-1.47	0.04	3.47	RANKING
1	6	1	-1.47	0.17	3.51	RANKING
1	7	100	-1.46	0.09	3.45	RANKING
1	8	42	-1.46	0.12	3.43	RANKING
1	9	48	-1.46	0.09	3.45	RANKING
1	10	31	-1.45	0.27	3.36	RANKING
1	11	43	-1.44	0.08	3.50	RANKING
1	12	98	-1.44	0.18	3.40	RANKING
1	13	12	-1.44	0.18	3.39	RANKING
1	14	36	-1.44	0.11	3.45	RANKING
1	15	62	-1.44	0.18	3.40	RANKING
1	16	52	-1.44	0.25	3.37	RANKING
1	17	39	-1.43	0.23	3.37	RANKING
1	18	60	-1.42	1.61	3.21	RANKING
1	19	13	-1.42	1.61	3.22	RANKING
1	20	19	-1.41	1.57	3.21	RANKING
1	21	22	-1.41	0.33	3.33	RANKING
1	22	73	-1.41	0.33	3.32	RANKING
1	23	69	-1.41	0.27	3.36	RANKING
1	24	15	-1.41	1.58	2.95	RANKING
1	25	79	-1.41	0.34	3.33	RANKING
1	26	29	-1.40	0.21	3.41	RANKING
1	27	87	-1.40	0.26	3.35	RANKING
1	28	47	-1.40	0.30	3.34	RANKING
1	29	77	-1.40	0.35	3.33	RANKING
1	30	71	-1.40	0.34	3.32	RANKING
1	31	57	-1.40	0.17	3.42	RANKING
1	32	8	-1.39	0.45	3.60	RANKING
1	33	88	-1.39	0.39	3.30	RANKING
1	34	55	-1.39	0.52	3.62	RANKING
1	35	4	-1.38	1.58	3.33	RANKING
1	36	14	-1.38	0.34	3.31	RANKING
1	37	58	-1.36	1.61	2.81	RANKING
1	38	27	-1.35	1.55	2.82	RANKING
1	39	92	-1.35	0.45	3.27	RANKING
1	40	78	-1.34	1.55	3.02	RANKING
1	41	26	-1.33	1.58	3.19	RANKING
1	42	89	-1.32	1.59	3.00	RANKING
1	43	34	-1.32	0.47	3.23	RANKING
1	44	74	-1.31	0.53	3.20	RANKING
1	45	18	-1.30	0.56	3.20	RANKING
1	46	93	-1.26	0.62	3.16	RANKING
1	47	10	-1.15	1.42	2.44	RANKING
1	48	81	-1.14	1.82	2.11	RANKING
1	49	91	-1.13	1.60	2.24	RANKING
2	1	61	-1.42	0.00	2.91	RANKING
2	2	6	-1.42	0.03	2.91	RANKING
2	3	7	-1.41	0.04	2.90	RANKING
2	4	40	-1.41	0.06	2.90	RANKING
2	5	65	-1.41	0.07	2.90	RANKING
2	6	80	-1.41	0.12	2.91	RANKING
2	7	2	-1.41	0.04	2.92	RANKING
2	8	35	-1.41	0.06	2.90	RANKING
2	9	33	-1.41	0.08	2.92	RANKING
2	10	68	-1.40	0.06	2.92	RANKING
2	11	41	-1.40	0.11	2.92	RANKING
2	12	99	-1.40	0.09	2.92	RANKING
2	13	97	-1.40	0.07	2.90	RANKING
2	14	3	-1.40	0.05	2.90	RANKING
2	15	16	-1.40	0.06	2.90	RANKING
2	16	30	-1.40	0.10	2.92	RANKING
2	17	56	-1.40	0.15	2.91	RANKING
2	18	51	-1.39	0.05	2.92	RANKING
2	19	84	-1.39	0.12	2.92	RANKING
2	20	44	-1.39	0.15	2.93	RANKING
2	21	21	-1.39	0.18	2.92	RANKING
2	22	53	-1.39	0.11	2.91	RANKING
2	23	37	-1.39	0.15	2.92	RANKING
2	24	90	-1.39	0.13	2.92	RANKING
2	25	25	-1.39	0.10	2.92	RANKING
2	26	45	-1.38	0.16	2.92	RANKING
2	27	54	-1.38	0.08	2.89	RANKING
2	28	76	-1.38	0.09	2.90	RANKING

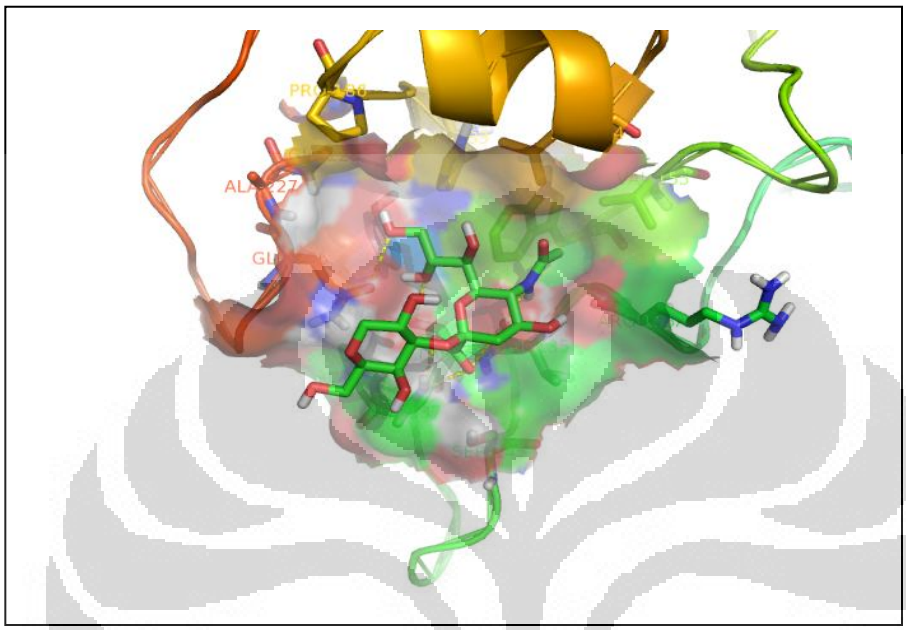
```
   2     29     94       -1.37      0.19      2.92           RANKING
   2     30     95       -1.37      0.14      2.95           RANKING
   2     31     86       -1.36      0.10      2.94           RANKING
   2     32     63       -1.35      0.27      2.94           RANKING
   2     33     83       -1.35      0.14      2.95           RANKING
   2     34     59       -1.35      0.21      2.93           RANKING
   2     35     70       -1.35      0.22      2.95           RANKING
   2     36     96       -1.34      0.22      2.93           RANKING
   2     37     67       -1.34      0.45      3.02           RANKING
   2     38     72       -1.33      0.26      2.93           RANKING
   2     39     75       -1.33      0.29      2.96           RANKING
   2     40     24       -1.32      0.33      2.97           RANKING
   2     41     64       -1.32      0.18      2.96           RANKING
   2     42     46       -1.32      0.15      2.92           RANKING
   2     43      5       -1.32      0.40      2.95           RANKING
   2     44     23       -1.29      0.18      2.90           RANKING
   2     45     28       -1.29      0.38      3.00           RANKING
   2     46     32       -1.28      0.70      3.10           RANKING
   2     47     49       -1.27      0.67      3.06           RANKING
   2     48     50       -1.26      1.01      3.21           RANKING
   2     49     85       -1.26      0.45      2.99           RANKING
   2     50      9       -1.25      1.07      3.25           RANKING
   2     51     20       -1.24      1.10      3.26           RANKING
_____________________________________________________________________


        INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING
        ________________________________________________


Information entropy for this clustering = 0.15  (rmstol = 2.00 Angstrom)

_____________________________________________________________________


        STATISTICAL MECHANICAL ANALYSIS
        _______________________________


Partition function, Q =   100.23           at Temperature, T = 298.15 K
Free energy,        A ~ -2729.85 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -1.37 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       17
USER    Run = 17
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 49
USER
USER    RMSD from reference structure       = 3.476 A
USER
USER    Estimated Free Energy of Binding    =   -1.50 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   79.72 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.61 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.89 kcal/mol
USER        Electrostatic Energy            =   -0.72 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 2fk0h.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      75.669351 19.581819 -24.230921
```

```
USER    NEWDPF axisangle0 -0.282357 -0.955870 -0.081156 69.471017
USER    NEWDPF quaternion0        -0.160884 -0.544644 -0.046242 0.821791
USER
USER                                x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      77.698  17.778 -23.725 -0.02 +0.06    +0.239  3.476
ATOM      2  O1A SIA A 801      78.326  16.726 -23.807 +0.04 -0.10    -0.644  3.476
ATOM      3  O1B SIA A 801      77.959  18.556 -22.808 +0.04 -0.16    -0.644  3.476
ATOM      4  C2  SIA A 801      76.464  18.037 -24.634 -0.05 +0.13    +0.258  3.476
ATOM      5  C3  SIA A 801      75.877  16.724 -25.197 -0.06 +0.04    +0.114  3.476
ATOM      6  C4  SIA A 801      75.195  15.879 -24.111 -0.09 +0.03    +0.149  3.476
ATOM      7  O4  SIA A 801      74.547  14.746 -24.728 -0.01 -0.05    -0.393  3.476
ATOM      8  C5  SIA A 801      74.169  16.705 -23.314 -0.19 +0.04    +0.145  3.476
ATOM      9  N5  SIA A 801      73.671  15.917 -22.170 -0.14 +0.00    -0.352  3.476
ATOM     10  C6  SIA A 801      74.835  18.003 -22.813 -0.18 +0.08    +0.182  3.476
ATOM     11  O6  SIA A 801      75.371  18.741 -23.953 -0.17 -0.35    -0.336  3.476
ATOM     12  C7  SIA A 801      73.894  18.919 -22.002 -0.29 +0.08    +0.180  3.476
ATOM     13  O7  SIA A 801      72.674  19.181 -22.738 -0.29 -0.24    -0.390  3.476
ATOM     14  C8  SIA A 801      74.581  20.247 -21.609 -0.29 +0.06    +0.173  3.476
ATOM     15  O8  SIA A 801      75.809  19.983 -20.896 -0.13 -0.03    -0.391  3.476
ATOM     16  C9  SIA A 801      73.684  21.131 -20.735 -0.26 -0.04    +0.198  3.476
ATOM     17  O9  SIA A 801      74.350  22.369 -20.423 -0.17 +0.16    -0.398  3.476
ATOM     18  C10 SIA A 801      72.394  15.518 -21.934 -0.41 +0.01    +0.214  3.476
ATOM     19  O10 SIA A 801      72.072  15.083 -20.836 -0.78 -0.06    -0.274  3.476
ATOM     20  C11 SIA A 801      71.397  15.445 -23.055 -0.25 +0.01    +0.117  3.476
ATOM     21  H4  SIA A 801      74.126  14.223 -24.057 +0.06 +0.01    +0.210  3.476
ATOM     22  H5  SIA A 801      74.366  15.640 -21.475 -0.38 -0.06    +0.163  3.476
ATOM     23  H7  SIA A 801      72.095  19.745 -22.239 +0.10 +0.04    +0.210  3.476
ATOM     24  H8  SIA A 801      76.230  20.799 -20.655 -0.37 -0.03    +0.210  3.476
ATOM     25  H9  SIA A 801      73.794  22.918 -19.881 -0.32 -0.15    +0.209  3.476
ATOM     26  C1  GAL A 802      76.048  21.945 -28.451 -0.07 +0.07    +0.202  3.476
ATOM     27  C2  GAL A 802      76.818  23.280 -28.419 -0.02 +0.03    +0.173  3.476
ATOM     28  O2  GAL A 802      76.875  23.861 -29.741 +0.00 -0.05    -0.391  3.476
ATOM     29  C3  GAL A 802      78.249  23.069 -27.888 +0.00 +0.03    +0.180  3.476
ATOM     30  O3  GAL A 802      78.911  24.341 -27.718 +0.01 -0.07    -0.390  3.476
ATOM     31  C4  GAL A 802      78.264  22.284 -26.561 -0.00 +0.05    +0.180  3.476
ATOM     32  O4  GAL A 802      77.731  23.106 -25.498 +0.00 -0.12    -0.390  3.476
ATOM     33  C5  GAL A 802      77.442  20.988 -26.733 -0.05 +0.08    +0.176  3.476
ATOM     34  O5  GAL A 802      76.085  21.325 -27.137 -0.08 -0.26    -0.378  3.476
ATOM     35  C6  GAL A 802      77.391  20.130 -25.468 -0.05 +0.12    +0.206  3.476
ATOM     36  O6  GAL A 802      76.827  18.831 -25.807 -0.08 -0.20    -0.344  3.476
ATOM     37  H2  GAL A 802      77.350  24.683 -29.720 +0.01 +0.02    +0.210  3.476
ATOM     38  H3  GAL A 802      79.793  24.211 -27.390 +0.00 +0.04    +0.210  3.476
ATOM     39  H4  GAL A 802      77.740  22.622 -24.680 +0.03 +0.07    +0.210  3.476
TER
ENDMDL
MODEL       61
USER    Run = 61
USER    Cluster Rank = 2
USER    Number of conformations in this cluster = 51
USER
USER    RMSD from reference structure       = 2.910 A
USER
USER    Estimated Free Energy of Binding    =   -1.42 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   91.01 mM (millimolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.54 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -4.99 kcal/mol
USER        Electrostatic Energy            =   -0.55 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.00 kcal/mol
USER    (3) Torsional Free Energy           =   +4.12 kcal/mol
USER    (4) Unbound System's Energy         =   +0.00 kcal/mol
USER
USER
USER
USER    DPF = 2fk0h.dpf
USER    NEWDPF move       h.pdbqt
USER    NEWDPF about      76.381699 19.617800 -22.545500
USER    NEWDPF tran0      75.658987 19.334089 -23.128046
USER    NEWDPF axisangle0 0.099324 0.280660 -0.954654 -126.141504
USER    NEWDPF quaternion0        0.088554 0.250227 -0.851138 -0.452890
USER
USER                                x       y       z    vdW   Elec        q     RMS
ATOM      1  C1  SIA A 801      74.795  18.796 -20.562 -0.32 +0.02    +0.239  2.910
ATOM      2  O1A SIA A 801      74.039  18.808 -19.594 -0.06 -0.03    -0.644  2.910
ATOM      3  O1B SIA A 801      75.971  18.476 -20.392 -0.04 -0.11    -0.644  2.910
ATOM      4  C2  SIA A 801      74.336  19.365 -21.933 -0.23 +0.12    +0.258  2.910
ATOM      5  C3  SIA A 801      73.139  20.330 -21.786 -0.36 +0.04    +0.114  2.910
ATOM      6  C4  SIA A 801      73.537  21.649 -21.107 -0.31 -0.04    +0.149  2.910
```

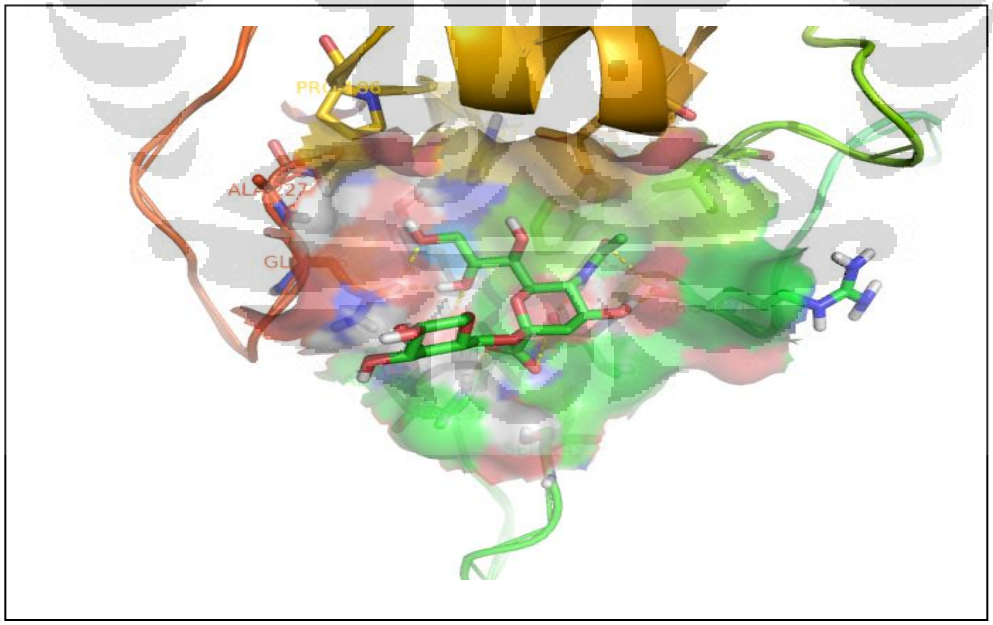
```
ATOM      7  O4  SIA A 801      72.412  22.554 -21.133 -0.18 +0.26    -0.393  2.910
ATOM      8  C5  SIA A 801      74.752  22.296 -21.797 -0.29 -0.01    +0.145  2.910
ATOM      9  N5  SIA A 801      75.215  23.457 -21.012 -0.19 +0.03    -0.352  2.910
ATOM     10  C6  SIA A 801      75.884  21.255 -21.920 -0.19 +0.05    +0.182  2.910
ATOM     11  O6  SIA A 801      75.390  20.091 -22.651 -0.17 -0.29    -0.336  2.910
ATOM     12  C7  SIA A 801      77.158  21.791 -22.607 -0.12 +0.06    +0.180  2.910
ATOM     13  O7  SIA A 801      76.836  22.402 -23.880 -0.06 -0.18    -0.390  2.910
ATOM     14  C8  SIA A 801      78.221  20.685 -22.794 -0.08 +0.05    +0.173  2.910
ATOM     15  O8  SIA A 801      78.523  20.063 -21.526 -0.44 -0.11    -0.391  2.910
ATOM     16  C9  SIA A 801      79.522  21.223 -23.401 -0.02 +0.04    +0.198  2.910
ATOM     17  O9  SIA A 801      80.468  20.154 -23.589 +0.00 -0.06    -0.398  2.910
ATOM     18  C10 SIA A 801      75.261  24.755 -21.407 -0.34 +0.02    +0.214  2.910
ATOM     19  O10 SIA A 801      75.889  25.581 -20.755 -0.78 -0.15    -0.274  2.910
ATOM     20  C11 SIA A 801      74.413  25.238 -22.549 -0.20 -0.04    +0.117  2.910
ATOM     21  H4  SIA A 801      72.658  23.370 -20.713 -0.12 -0.13    +0.210  2.910
ATOM     22  H5  SIA A 801      75.538  23.262 -20.064 +0.04 -0.02    +0.163  2.910
ATOM     23  H7  SIA A 801      77.619  22.732 -24.303 +0.04 +0.07    +0.210  2.910
ATOM     24  H8  SIA A 801      79.176  19.384 -21.641 +0.05 +0.04    +0.210  2.910
ATOM     25  H9  SIA A 801      81.275  20.487 -23.965 +0.01 +0.03    +0.209  2.910
ATOM     26  C1  GAL A 802      73.738  16.496 -26.562 -0.11 +0.07    +0.202  2.910
ATOM     27  C2  GAL A 802      74.514  15.206 -26.894 -0.04 +0.03    +0.173  2.910
ATOM     28  O2  GAL A 802      73.821  14.448 -27.910 -0.01 -0.06    -0.391  2.910
ATOM     29  C3  GAL A 802      74.689  14.337 -25.633 -0.03 +0.02    +0.180  2.910
ATOM     30  O3  GAL A 802      75.544  13.210 -25.919 -0.00 -0.03    -0.390  2.910
ATOM     31  C4  GAL A 802      75.256  15.144 -24.449 -0.05 +0.02    +0.180  2.910
ATOM     32  O4  GAL A 802      76.639  15.482 -24.701 -0.00 -0.06    -0.390  2.910
ATOM     33  C5  GAL A 802      74.398  16.411 -24.245 -0.12 +0.05    +0.176  2.910
ATOM     34  O5  GAL A 802      74.395  17.196 -25.471 -0.05 -0.21    -0.378  2.910
ATOM     35  C6  GAL A 802      74.877  17.288 -23.088 -0.15 +0.06    +0.206  2.910
ATOM     36  O6  GAL A 802      73.865  18.300 -22.817 -0.14 -0.19    -0.344  2.910
ATOM     37  H2  GAL A 802      74.299  13.653 -28.114 +0.01 +0.02    +0.210  2.910
ATOM     38  H3  GAL A 802      75.652  12.674 -25.142 +0.02 +0.01    +0.210  2.910
ATOM     39  H4  GAL A 802      76.989  15.979 -23.971 +0.03 +0.03    +0.210  2.910
TER
ENDMDL


AVSFLD: # AVS field file
AVSFLD: #
AVSFLD: # Created by AutoDock
AVSFLD: #
AVSFLD: ndim=2           # number of dimensions in the field
AVSFLD: nspace=1         # number of physical coordinates
AVSFLD: veclen=7         # vector size
AVSFLD: dim1=39          # atoms
AVSFLD: dim2=2           # conformations
AVSFLD: data=Real       # data type (byte,integer,Real,double)
AVSFLD: field=uniform    # field coordinate layout
AVSFLD: label= x y z vdW Elec q RMS
AVSFLD: variable 1 file = 2fk0h.dlg.pdb filetype = ascii offset = 5 stride = 12
AVSFLD: variable 2 file = 2fk0h.dlg.pdb filetype = ascii offset = 6 stride = 12
AVSFLD: variable 3 file = 2fk0h.dlg.pdb filetype = ascii offset = 7 stride = 12
AVSFLD: variable 4 file = 2fk0h.dlg.pdb filetype = ascii offset = 8 stride = 12
AVSFLD: variable 5 file = 2fk0h.dlg.pdb filetype = ascii offset = 9 stride = 12
AVSFLD: variable 6 file = 2fk0h.dlg.pdb filetype = ascii offset = 10 stride = 12
AVSFLD: variable 7 file = 2fk0h.dlg.pdb filetype = ascii offset = 11 stride = 12
AVSFLD: # end of file

>>> Closing the docking parameter file (DPF)...

This docking finished at:                2:22 12" a.m., 06/15/2009



_____________________________________________________________________________

autodock4: Successful Completion on "ubuntu"

Real= 44m 31.82s,  CPU= 44m 25.06s,  System= 0.57s
_____________________________________________________________________________
```

Lampiran 8. Hasil Visualisasi Docking

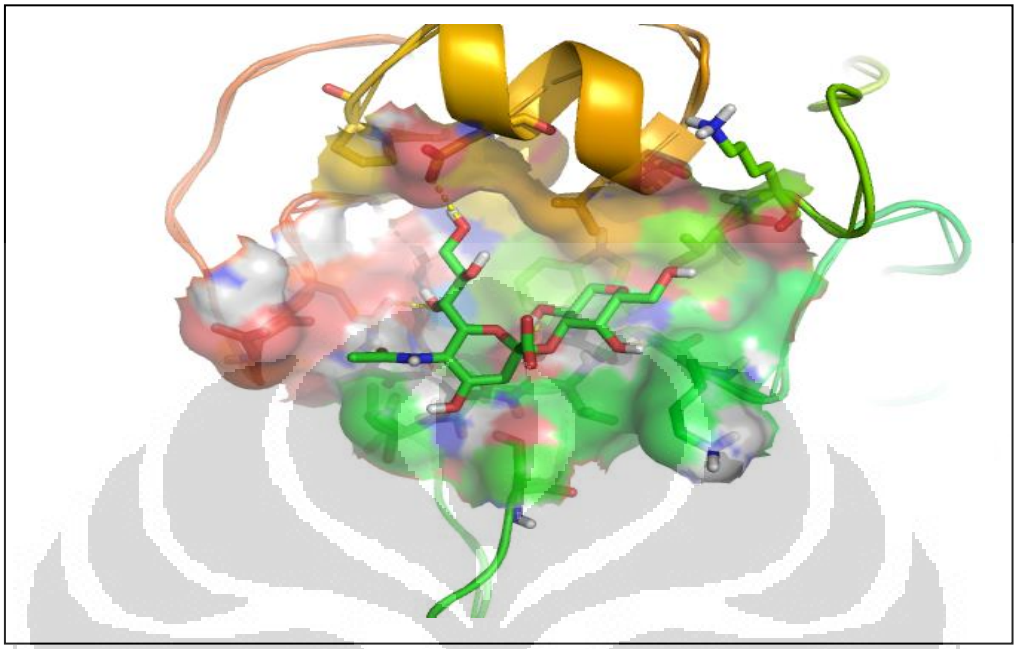
Subtipe H1 1RVT(isolat babi) dengan Sia(α2-3)Gal



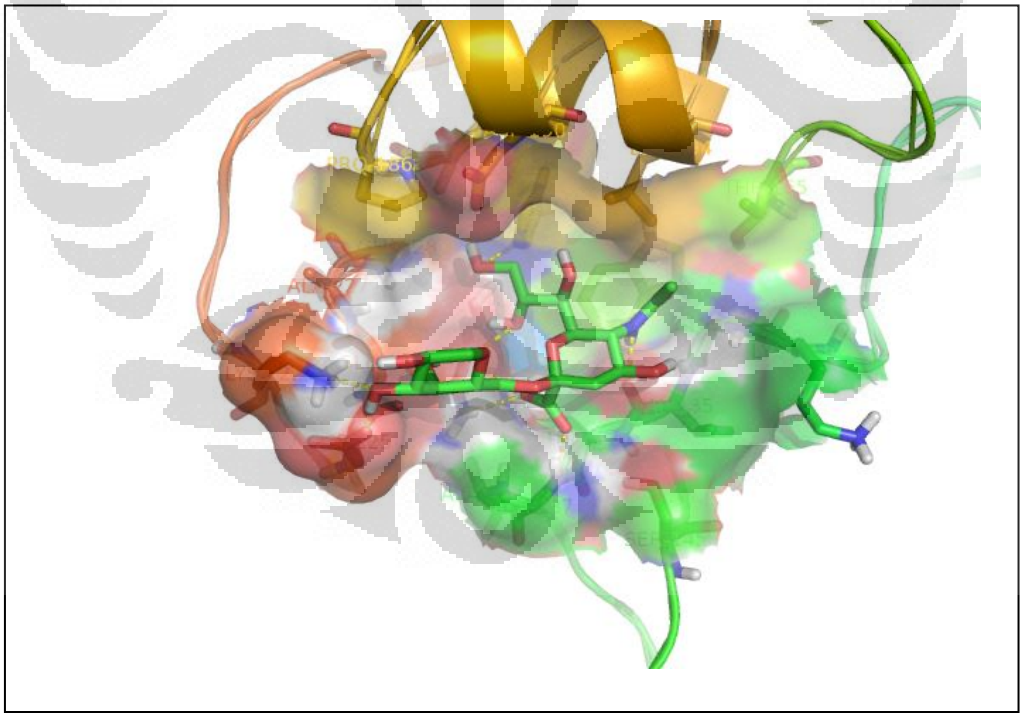
Subtipe H1 1RVT (isolat babi) dengan Sia(α2-6)Gal



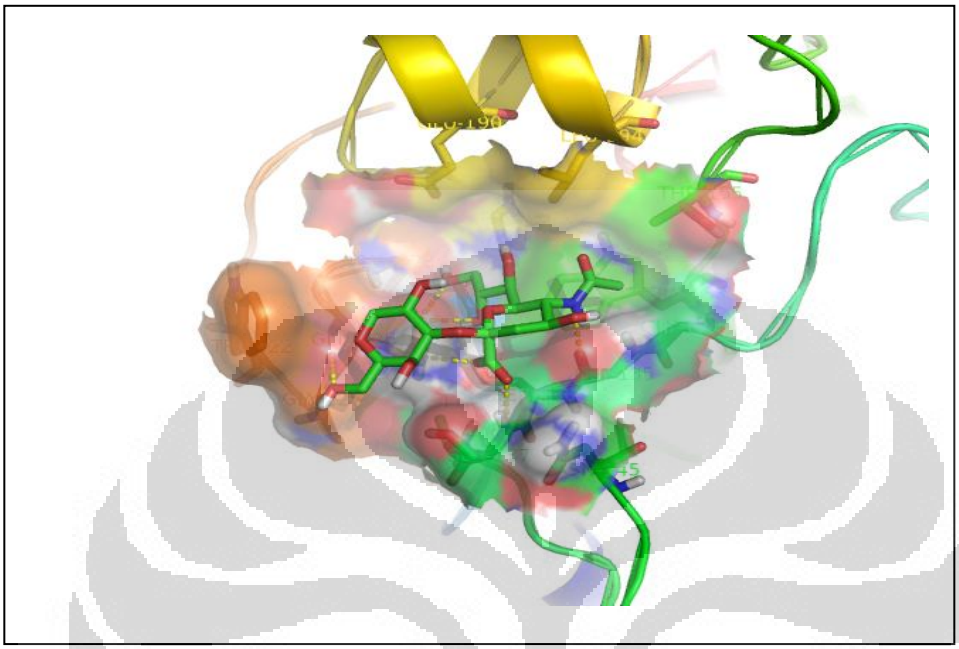
Subtipe H1 1RD8 (isolat manusia) dengan Sia(α2-3)Gal



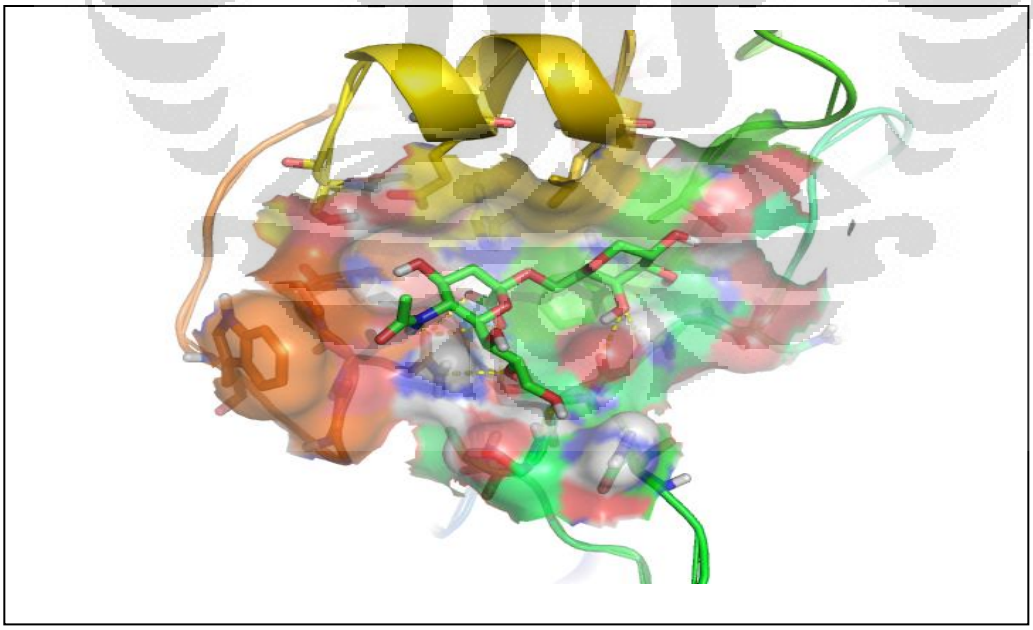
Subtipe H1 1RD8 (isolat manusia) dengan Sia(α2-6)Gal



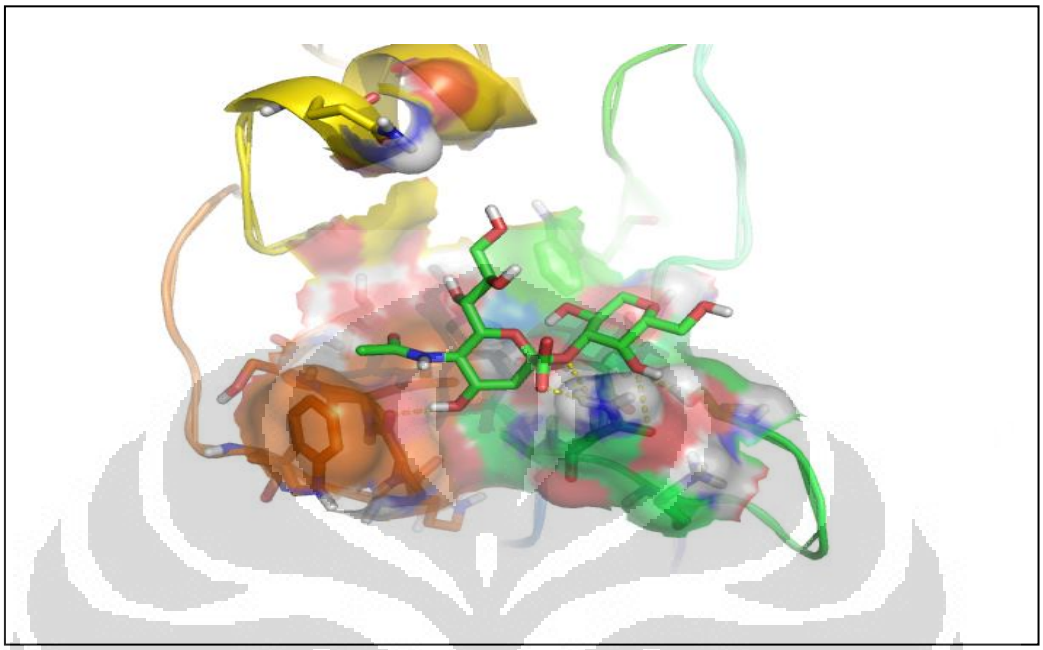
Subtipe H3 1MQN (isolat bebek) dengan Sia(α2-3)Gal



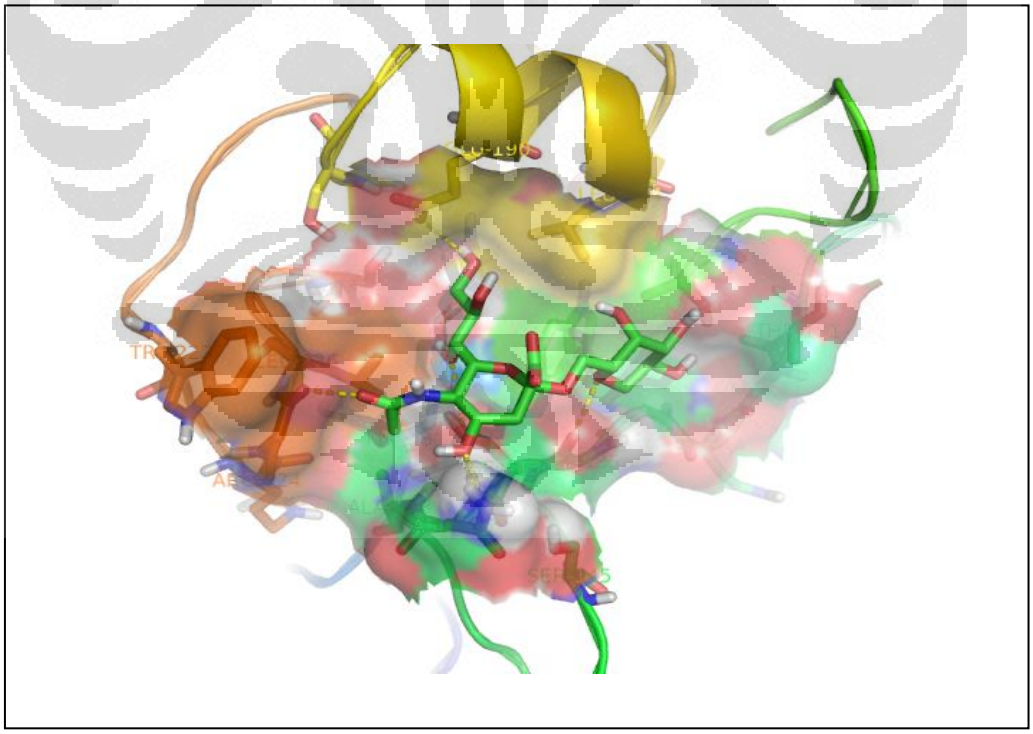
Subtipe H3 1MQN (isolat bebek) dengan Sia(α2-6)Gal



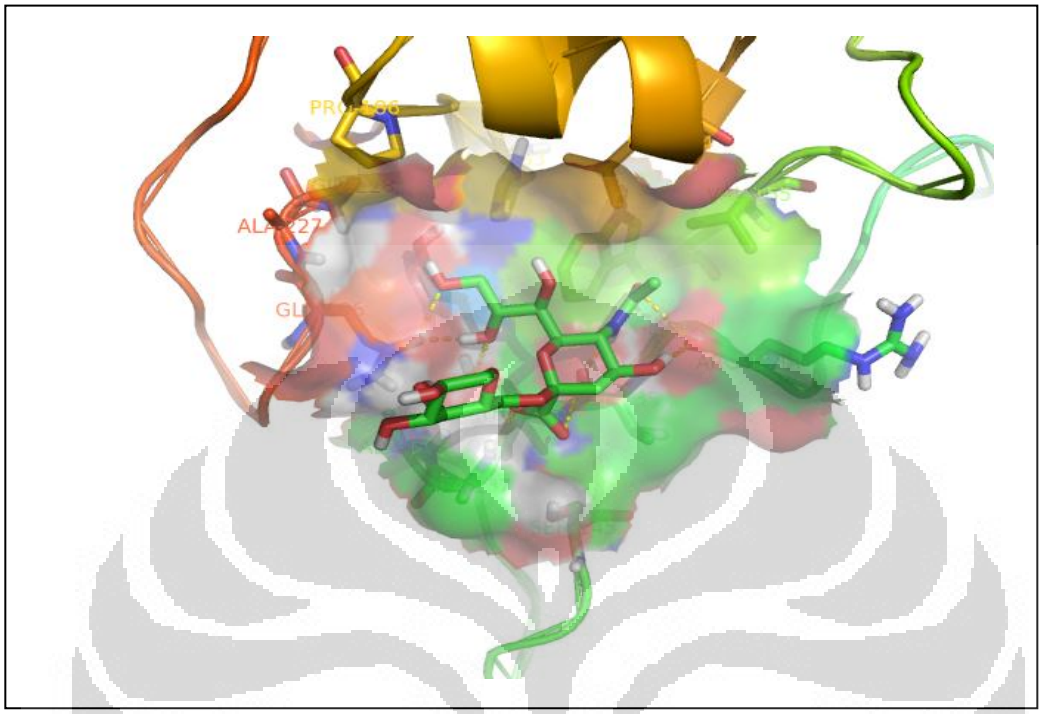
Subtipe H3 1HGF (isolat manusia) dengan Sia(α2-3)Gal



Subtipe H3 1HGF (isolat manusia) dengan Sia(α2-6)Gal



Subtipe H5 2FK0 (isolat manusia) dengan Sia(α2-3)Gal



Subtipe H5 2FK0 (isolat manusia) dengan Sia(α2-6)Gal