MODELLER 9.22, 2019/06/19, r11413

PROTEIN STRUCTURE MODELLING BY SATISFACTION OF SPATIAL RESTRAINTS

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Kind, OS, HostName, Kernel, Processor: 4, Linux watson.cgl.ucsf.edu 3.10.0-1160.6.1.el7.x86\_64 x86\_64

Date and time of compilation : 2019/06/19 14:00:54

MODELLER executable type : x86\_64-intel8

Job starting time (YY/MM/DD HH:MM:SS): 2021/03/27 11:25:20

openf\_\_\_224\_> Open $(LIB)/restyp.lib

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/resgrp.lib

rdresgr\_266\_> Number of residue groups: 2

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/sstruc.lib

Dynamically allocated memory at amaxlibraries [B,KiB,MiB]: 191566 187.076 0.183

Dynamically allocated memory at amaxlibraries [B,KiB,MiB]: 192094 187.592 0.183

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/resdih.lib

Dynamically allocated memory at amaxlibraries [B,KiB,MiB]: 240694 235.053 0.230

rdrdih\_\_263\_> Number of dihedral angle types : 9

Maximal number of dihedral angle optima: 3

Dihedral angle names : Alph Phi Psi Omeg chi1 chi2 chi3 chi4 chi5

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/radii.lib

Dynamically allocated memory at amaxlibraries [B,KiB,MiB]: 253994 248.041 0.242

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/radii14.lib

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/af\_mnchdef.lib

rdwilmo\_274\_> Mainchain residue conformation classes: APBLE

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/mnch.lib

rdclass\_257\_> Number of classes: 5

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/mnch1.lib

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/mnch2.lib

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/mnch3.lib

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/xs4.mat

rdrrwgh\_268\_> Number of residue types: 21

openf\_\_\_224\_> Open alignment.ali

Dynamically allocated memory at amaxalignment [B,KiB,MiB]: 269801 263.478 0.257

Dynamically allocated memory at amaxalignment [B,KiB,MiB]: 284893 278.216 0.272

Dynamically allocated memory at amaxalignment [B,KiB,MiB]: 300293 293.255 0.286

Dynamically allocated memory at amaxalignment [B,KiB,MiB]: 331093 323.333 0.316

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 331873 324.095 0.316

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 332657 324.860 0.317

Read the alignment from file : alignment.ali

Total number of alignment positions: 200

# Code #\_Res #\_Segm PDB\_code Name

-------------------------------------------------------------------------------

1 Template- 196 1 Template-4o

2 USP\_recep 197 1 USP\_recepto

check\_a\_343\_> >> BEGINNING OF COMMAND

openf\_\_\_224\_> Open ./Template-4ozr.pdb\_0\_0.pdb

readlinef\_\_W> File: ./Template-4ozr.pdb\_0\_0.pdb, Line: 472

Modeller will only read the first 80 characters of this line.

readlinef\_\_W> File: ./Template-4ozr.pdb\_0\_0.pdb, Line: 473

Modeller will only read the first 80 characters of this line.

readlinef\_\_W> File: ./Template-4ozr.pdb\_0\_0.pdb, Line: 477

Modeller will only read the first 80 characters of this line.

readlinef\_\_W> File: ./Template-4ozr.pdb\_0\_0.pdb, Line: 495

Modeller will only read the first 80 characters of this line.

readlinef\_\_W> File: ./Template-4ozr.pdb\_0\_0.pdb, Line: 515

Modeller will only read the first 80 characters of this line.

readlinef\_\_W> File: ./Template-4ozr.pdb\_0\_0.pdb, Line: 550

No more warnings will be printed for truncated lines in this file.

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 393182 383.967 0.375

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 393182 383.967 0.375

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 393353 384.134 0.375

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 394203 384.964 0.376

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 395461 386.192 0.377

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 397365 388.052 0.379

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 397365 388.052 0.379

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 397455 388.140 0.379

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 400311 390.929 0.382

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 400311 390.929 0.382

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 400446 391.061 0.382

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 404730 395.244 0.386

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 404730 395.244 0.386

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 404928 395.438 0.386

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 411354 401.713 0.392

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 411354 401.713 0.392

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 411651 402.003 0.393

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 421273 411.399 0.402

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 421273 411.399 0.402

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 421723 411.839 0.402

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 436173 425.950 0.416

Dynamically allocated memory at amaxsequence [B,KiB,MiB]: 436173 425.950 0.416

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 436848 426.609 0.417

Dynamically allocated memory at amaxcoordinates [B,KiB,MiB]: 458506 447.760 0.437

Dynamically allocated memory at amaxstructure [B,KiB,MiB]: 458245 447.505 0.437

check\_ali\_\_\_> Checking the sequence-structure alignment.

Implied intrachain target CA(i)-CA(i+1) distances longer than 8.0 angstroms:

ALN\_POS TMPL RID1 RID2 NAM1 NAM2 DIST

----------------------------------------------

END OF TABLE

check\_a\_344\_> << END OF COMMAND

openf\_\_\_224\_> Open ${LIB}/top\_allh.lib

read\_to\_681\_> topology.submodel read from topology file: 1

openf\_\_\_224\_> Open ${LIB}/par.lib

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 669725 654.028 0.639

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 671325 655.591 0.640

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 675305 659.478 0.644

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 677305 661.431 0.646

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 680305 664.360 0.649

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 684805 668.755 0.653

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 690377 674.196 0.658

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 693177 676.931 0.661

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 697377 681.032 0.665

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 703677 687.185 0.671

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 706449 689.892 0.674

Dynamically allocated memory at amaxparameters [B,KiB,MiB]: 707849 691.259 0.675

read\_pa\_232\_> parameters BONDS ANGLS DIHEDS IMPROPS MODE

227 561 661 112 0

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 738621 721.310 0.704

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 1056239 1031.483 1.007

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 1097503 1071.780 1.047

getf\_\_\_\_\_\_\_W> RTF restraint not found in the atoms list:

residue type, indices: 7 1

atom names : N -C CA H

atom indices : 1 0 3 2

mkilst\_\_\_\_\_\_> segment topology constructed from sequence and RTF:

segments residues atoms bonds angles dihedrals impropers:

1 197 3222 3252 0 0 952

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 1305179 1274.589 1.245

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 1442899 1409.081 1.376

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 1443055 1409.233 1.376

patch\_\_\_\_\_\_\_> segment topology patched using RTF: 1 ; HIS ; NTER

segments residues atoms bonds angles dihedrals impropers:

1 197 3224 3254 5879 8582 952

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 1443127 1409.304 1.376

patch\_\_\_\_\_\_\_> segment topology patched using RTF: 197 ; VAL ; CTER

segments residues atoms bonds angles dihedrals impropers:

1 197 3225 3255 5881 8585 953

genseg\_\_\_\_\_\_> segment topology constructed from sequence and RTF:

segments residues atoms bonds angles dihedrals impropers:

1 197 3225 3255 5881 8585 953

transfe\_506\_> MODEL is an average of all templates.

transfe\_511\_> Number of templates for coordinate transfer: 1

After transferring coordinates of the equivalent template atoms,

there are defined, undefined atoms in MODEL: 1196 2029

The following 1 residues contain 6-membered rings with poor geometries

after transfer from templates. Rebuilding rings from internal coordinates:

<Residue 22 (type PHE)>

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

make\_re\_417\_> Restraint type to be calculated: stereo

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1550176 1513.844 1.478

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1558368 1521.844 1.486

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1574752 1537.844 1.502

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1607520 1569.844 1.533

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1640288 1601.844 1.564

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1705824 1665.844 1.627

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1738592 1697.844 1.658

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1771360 1729.844 1.689

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1836896 1793.844 1.752

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 1967968 1921.844 1.877

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 2033504 1985.844 1.939

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 2099040 2049.844 2.002

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 2230112 2177.844 2.127

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 2492256 2433.844 2.377

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 2623328 2561.844 2.502

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 2754400 2689.844 2.627

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 3016544 2945.844 2.877

generat\_607W> Cannot find params in params file:

CHARMM atoms : NY CA CPT H

IUPAC atoms : NE1 CD1 CE2 HE1

Atom indices : 3184 3182 3186 3185

Residues : TRP TRP TRP TRP

addprm\_\_440W> Adding params (mean,force,period): 1.0035 60.0000 0

For atoms: NY CA CPT H

r\_stere\_606\_> Stereochemical restraints were constructed from RTF & PRMF.

Added bond,angle,dihedral,improper restraints : 3255 5881 7138 948

Total number of restraints before, now : 0 17222

make\_re\_422\_> Number of previous, current restraints : 0 17222

make\_re\_423\_> Number of previous, current selected restraints: 0 17222

make\_re\_417\_> Restraint type to be calculated: phi-psi\_binormal

Dynamically allocated memory at amaxstructure [B,KiB,MiB]: 3186502 3111.818 3.039

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/mnch1.bin

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/mnch1.mdt

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 5 10 GLN

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 5 193 ASP

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 5 194 MET

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 5 195 LEU

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 6 10 GLN

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 6 193 ASP

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 6 194 MET

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 6 195 LEU

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 7 10 GLN

errdih\_\_638\_> Missing atoms in a dihedral, residue index, residue type: 7 194 MET

getdata\_643\_> Protein accepted: Template-4ozr.pdb\_0\_0

getdata\_289\_> Proteins (all/accepted): 1 1

make\_re\_422\_> Number of previous, current restraints : 17222 17417

make\_re\_423\_> Number of previous, current selected restraints: 17222 17417

make\_re\_417\_> Restraint type to be calculated: omega\_dihedral

Dynamically allocated memory at amaxstructure [B,KiB,MiB]: 3186518 3111.834 3.039

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/omega.bin

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/omega.mdt

getdata\_643\_> Protein accepted: Template-4ozr.pdb\_0\_0

getdata\_289\_> Proteins (all/accepted): 1 1

omgdel\_\_425\_> Unselected all O C +N +CA dihedrals: 201

(This is to avoid clashes between STEREO

and OMEGA\_DIHEDRAL restraints)

make\_re\_422\_> Number of previous, current restraints : 17417 17613

make\_re\_423\_> Number of previous, current selected restraints: 17417 17412

make\_re\_417\_> Restraint type to be calculated: chi1\_dihedral

Dynamically allocated memory at amaxstructure [B,KiB,MiB]: 3186518 3111.834 3.039

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi1234.bin

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi1.mdt

getdata\_643\_> Protein accepted: Template-4ozr.pdb\_0\_0

getdata\_289\_> Proteins (all/accepted): 1 1

make\_re\_422\_> Number of previous, current restraints : 17613 17792

make\_re\_423\_> Number of previous, current selected restraints: 17412 17591

make\_re\_417\_> Restraint type to be calculated: chi2\_dihedral

Dynamically allocated memory at amaxstructure [B,KiB,MiB]: 3186518 3111.834 3.039

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi1234.bin

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi2.mdt

getdata\_643\_> Protein accepted: Template-4ozr.pdb\_0\_0

getdata\_289\_> Proteins (all/accepted): 1 1

make\_re\_422\_> Number of previous, current restraints : 17792 17934

make\_re\_423\_> Number of previous, current selected restraints: 17591 17733

make\_re\_417\_> Restraint type to be calculated: chi3\_dihedral

Dynamically allocated memory at amaxstructure [B,KiB,MiB]: 3186518 3111.834 3.039

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi1234.bin

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi3.mdt

getdata\_643\_> Protein accepted: Template-4ozr.pdb\_0\_0

getdata\_289\_> Proteins (all/accepted): 1 1

make\_re\_422\_> Number of previous, current restraints : 17934 17990

make\_re\_423\_> Number of previous, current selected restraints: 17733 17789

make\_re\_417\_> Restraint type to be calculated: chi4\_dihedral

Dynamically allocated memory at amaxstructure [B,KiB,MiB]: 3186518 3111.834 3.039

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi1234.bin

openf\_\_\_224\_> Open ${MODINSTALL9v22}/modlib/chi4.mdt

mdtrsr\_\_446W> A potential that relies on one protein is used, yet you have at

least one known structure available. MDT, not library, potential is used.

getdata\_643\_> Protein accepted: Template-4ozr.pdb\_0\_0

getdata\_289\_> Proteins (all/accepted): 1 1

make\_re\_422\_> Number of previous, current restraints : 17990 18012

make\_re\_423\_> Number of previous, current selected restraints: 17789 17811

make\_re\_417\_> Restraint type to be calculated: DISTANCE

Dynamically allocated memory at amaxhash\_contac [B,KiB,MiB]: 4115282 4018.830 3.925

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 4639570 4530.830 4.425

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 4901714 4786.830 4.675

make\_re\_422\_> Number of previous, current restraints : 18012 21349

make\_re\_423\_> Number of previous, current selected restraints: 17811 21148

make\_re\_417\_> Restraint type to be calculated: DISTANCE

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 5163858 5042.830 4.925

make\_re\_422\_> Number of previous, current restraints : 21349 24753

make\_re\_423\_> Number of previous, current selected restraints: 21148 24552

make\_re\_417\_> Restraint type to be calculated: DISTANCE

make\_re\_422\_> Number of previous, current restraints : 24753 26443

make\_re\_423\_> Number of previous, current selected restraints: 24552 26242

make\_re\_417\_> Restraint type to be calculated: DISTANCE

make\_re\_422\_> Number of previous, current restraints : 26443 26845

make\_re\_423\_> Number of previous, current selected restraints: 26242 26644

0 atoms in HETATM/BLK residues constrained

to protein atoms within 2.30 angstroms

and protein CA atoms within 10.00 angstroms

make\_re\_417\_> Restraint type to be calculated: DISTANCE

make\_re\_422\_> Number of previous, current restraints : 26845 26845

make\_re\_423\_> Number of previous, current selected restraints: 26644 26644

make\_re\_417\_> Restraint type to be calculated: DISTANCE

make\_re\_422\_> Number of previous, current restraints : 26845 26845

make\_re\_423\_> Number of previous, current selected restraints: 26644 26644

make\_re\_417\_> Restraint type to be calculated: DISTANCE

make\_re\_422\_> Number of previous, current restraints : 26845 26845

make\_re\_423\_> Number of previous, current selected restraints: 26644 26644

make\_re\_417\_> Restraint type to be calculated: DISTANCE

make\_re\_422\_> Number of previous, current restraints : 26845 26845

make\_re\_423\_> Number of previous, current selected restraints: 26644 26644

0 atoms in residues without defined topology

constrained to be rigid bodies

make\_re\_417\_> Restraint type to be calculated: DISTANCE

make\_re\_422\_> Number of previous, current restraints : 26845 26845

make\_re\_423\_> Number of previous, current selected restraints: 26644 26644

rmdupl\_\_427\_> 1292 redundant cosine dihedral restraints were unselected.

condens\_443\_> Restraints marked for deletion were removed.

Total number of restraints before, now: 26845 25352

openf\_\_\_224\_> Open USP\_receptor\_Luc.rsr

openf\_\_\_224\_> Open USP\_receptor\_Luc.rsr

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 5322831 5198.077 5.076

rdcsr2\_\_307\_> Number of restraints read : 25352

Number of excluded pairs read: 0

Number of pseudo atoms read : 0

rdcsrs\_\_304\_> Restraints in memory, selected restraints: 25352 25352

Explicitly excluded atom pairs in memory : 0

Pseudo atoms in memory : 0

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 5322855 5198.101 5.076

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 5692835 5559.409 5.429

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 5770235 5634.995 5.503

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 5925035 5786.167 5.651

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_485\_> OD1/2 will be swapped: 124.8202 2 2

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 124.8202

iupac\_m\_487\_> NH1/2 swapped: 175.3792 6 6

iupac\_m\_486\_> OE1/2 will be swapped: -123.6535 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -123.6535

iupac\_m\_487\_> NH1/2 swapped: -180.0000 55 55

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 124.6920 57 57

iupac\_m\_487\_> NH1/2 swapped: -178.9010 70 70

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 104.9632 77 77

iupac\_m\_486\_> OE1/2 will be swapped: -143.4353 105 105

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -143.4353

iupac\_m\_485\_> OD1/2 will be swapped: 126.0876 117 117

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 126.0876

iupac\_m\_487\_> NH1/2 swapped: -176.1397 118 118

iupac\_m\_486\_> OE1/2 will be swapped: 120.7613 125 125

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 120.7613

iupac\_m\_486\_> OE1/2 will be swapped: 111.0201 128 128

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 111.0201

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 113.5882 133 133

iupac\_m\_487\_> NH1/2 swapped: 179.6690 139 139

iupac\_m\_487\_> NH1/2 swapped: -178.6254 145 145

iupac\_m\_485\_> OD1/2 will be swapped: 138.2817 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 138.2817

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 90.0987 156 156

iupac\_m\_486\_> OE1/2 will be swapped: 122.5115 165 165

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 122.5115

iupac\_m\_487\_> NH1/2 swapped: 175.7650 167 167

iupac\_m\_487\_> NH1/2 swapped: -172.6271 185 185

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.141946

Native energy (pair) : -247.880951

Native energy (surface) : -10.223727

Native energy (combined) : -10.645743

Z score (pair) : -7.695558

Z score (surface) : -6.798227

Z score (combined) : -9.931092

GA341 score : 1.000000

openf\_\_\_224\_> Open ${LIB}/atmcls-mf.lib

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5925455 5786.577 5.651

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5925519 5786.640 5.651

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5925577 5786.696 5.651

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5925641 5786.759 5.651

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5925707 5786.823 5.651

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5925771 5786.886 5.651

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5925927 5787.038 5.651

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5926055 5787.163 5.652

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5926349 5787.450 5.652

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5926541 5787.638 5.652

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5927045 5788.130 5.652

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5927301 5788.380 5.653

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5928297 5789.353 5.654

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5928681 5789.728 5.654

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5929257 5790.290 5.655

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5931291 5792.276 5.657

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5932187 5793.151 5.657

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5936639 5797.499 5.662

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5937983 5798.812 5.663

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5947601 5808.204 5.672

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5949585 5810.142 5.674

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5970231 5830.304 5.694

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 5973239 5833.241 5.697

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6019205 5878.130 5.740

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6023685 5882.505 5.745

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6124905 5981.353 5.841

openf\_\_\_224\_> Open ${LIB}/dist-mf.lib

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6125301 5981.739 5.842

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6126097 5982.517 5.842

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6126893 5983.294 5.843

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6128081 5984.454 5.844

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6128481 5984.845 5.845

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6129081 5985.431 5.845

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6129981 5986.310 5.846

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6131329 5987.626 5.847

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6131529 5987.821 5.847

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6133553 5989.798 5.849

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6133853 5990.091 5.850

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6136889 5993.056 5.853

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6137337 5993.493 5.853

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6141889 5997.938 5.857

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6142561 5998.595 5.858

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6149389 6005.263 5.865

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6150397 6006.247 5.865

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6160641 6016.251 5.875

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6161241 6016.837 5.876

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6161641 6017.228 5.876

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6163153 6018.704 5.878

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6178517 6033.708 5.892

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6179417 6034.587 5.893

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6180017 6035.173 5.894

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6182285 6037.388 5.896

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6205333 6059.896 5.918

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6206677 6061.208 5.919

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6207577 6062.087 5.920

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6210981 6065.411 5.923

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6245553 6099.173 5.956

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6247569 6101.142 5.958

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6248917 6102.458 5.959

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6254021 6107.442 5.964

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6305877 6158.083 6.014

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6308901 6161.036 6.017

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6310925 6163.013 6.019

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6318581 6170.489 6.026

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6396365 6246.450 6.100

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6400901 6250.880 6.104

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6403937 6253.845 6.107

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6415421 6265.060 6.118

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6532097 6379.001 6.229

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6538901 6385.646 6.236

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6543453 6390.091 6.240

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6560681 6406.915 6.257

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6735697 6577.829 6.424

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6745909 6587.802 6.433

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6752737 6594.470 6.440

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 6778577 6619.704 6.465

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7041101 6876.075 6.715

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7056413 6891.028 6.730

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7066657 6901.032 6.739

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7105417 6938.884 6.776

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7499201 7323.438 7.152

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7522169 7345.868 7.174

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7537533 7360.872 7.188

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 7595673 7417.649 7.244

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 8186349 7994.481 7.807

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 8220801 8028.126 7.840

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 8243849 8050.634 7.862

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 8331061 8135.802 7.945

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 9217077 9001.052 8.790

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 9268761 9051.524 8.839

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 9303333 9085.286 8.872

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 9434149 9213.036 8.997

Dynamically allocated memory at amaxgroup\_restr [B,KiB,MiB]: 10763173 10510.911 10.265

read\_pa\_232\_> parameters BONDS ANGLS DIHEDS IMPROPS MODE

0 0 0 0 12561

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 11365545 11099.165 10.839

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 11984745 11703.853 11.430

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 13223145 12913.228 12.611

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 15699945 15331.978 14.973

Dynamically allocated memory at amaxrestraints [B,KiB,MiB]: 20653545 20169.477 19.697

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1091916

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -22075.4395

<< end of ENERGY.

DOPE score : -22075.439453

>> Normalized DOPE z score: -0.420

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20449

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 63877.0000

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 3255 32 32 0.193 0.193 55180. 1.000

2 Bond angle potential : 5881 261 330 9.632 9.632 6815.4 1.000

3 Stereochemical cosine torsion poten: 5645 0 48 26.388 26.388 639.84 1.000

4 Stereochemical improper torsion pot: 948 62 75 6.168 6.168 602.80 1.000

5 Soft-sphere overlap restraints : 20449 0 0 0.001 0.001 4.9990 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 1 0.341 0.341 132.55 1.000

10 Distance restraints 2 (N-O) : 3404 0 6 0.413 0.413 176.16 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 4 4.186 4.186 40.507 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 3 73.330 73.330 57.178 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 1 81.246 81.246 56.788 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 81.300 81.300 41.399 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 101.430 101.430 15.567 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.389 0.389 30.417 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 15 24 30.302 43.039 2.8601 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 2 9 1.300 1.300 80.885 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990001

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990001

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 36124.1055

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 3.27 1.00 2.27 88.93 1.00 2.27 88.93

2 100 6R 6R NH1 HH12 95 97 2.56 1.00 1.56 61.24 1.00 1.56 61.24

3 101 6R 6R NH2 HH21 98 99 2.56 1.00 1.56 61.21 1.00 1.56 61.21

4 102 6R 6R NH2 HH22 98 100 3.27 1.00 2.27 88.88 1.00 2.27 88.88

5 903 55R 55R NH1 HH11 894 895 2.57 1.00 1.57 61.61 1.00 1.57 61.61

6 904 55R 55R NH1 HH12 894 896 3.27 1.00 2.27 89.05 1.00 2.27 89.05

7 905 55R 55R NH2 HH21 897 898 3.27 1.00 2.27 89.04 1.00 2.27 89.04

8 906 55R 55R NH2 HH22 897 899 2.57 1.00 1.57 61.68 1.00 1.57 61.68

9 1150 70R 70R NH1 HH11 1137 1138 2.56 1.00 1.56 61.31 1.00 1.56 61.31

10 1151 70R 70R NH1 HH12 1137 1139 3.27 1.00 2.27 88.93 1.00 2.27 88.93

11 1152 70R 70R NH2 HH21 1140 1141 3.27 1.00 2.27 88.86 1.00 2.27 88.86

12 1153 70R 70R NH2 HH22 1140 1142 2.57 1.00 1.57 61.39 1.00 1.57 61.39

13 1928 118R 118R NH1 HH11 1908 1909 3.26 1.00 2.26 88.80 1.00 2.26 88.80

14 1929 118R 118R NH1 HH12 1908 1910 2.56 1.00 1.56 61.10 1.00 1.56 61.10

15 1930 118R 118R NH2 HH21 1911 1912 2.55 1.00 1.55 60.98 1.00 1.55 60.98

16 1931 118R 118R NH2 HH22 1911 1913 3.26 1.00 2.26 88.80 1.00 2.26 88.80

17 2263 139R 139R NH1 HH11 2240 2241 2.57 1.00 1.57 61.49 1.00 1.57 61.49

18 2264 139R 139R NH1 HH12 2240 2242 3.27 1.00 2.27 88.94 1.00 2.27 88.94

19 2265 139R 139R NH2 HH21 2243 2244 2.57 1.00 1.57 61.63 1.00 1.57 61.63

20 2266 139R 139R NH2 HH22 2243 2245 3.27 1.00 2.27 89.00 1.00 2.27 89.00

21 2380 145R 145R NH1 HH11 2356 2357 3.27 1.00 2.27 88.94 1.00 2.27 88.94

22 2381 145R 145R NH1 HH12 2356 2358 2.57 1.00 1.57 61.58 1.00 1.57 61.58

23 2382 145R 145R NH2 HH21 2359 2360 3.27 1.00 2.27 89.07 1.00 2.27 89.07

24 2383 145R 145R NH2 HH22 2359 2361 2.57 1.00 1.57 61.42 1.00 1.57 61.42

25 2739 167R 167R NH1 HH11 2711 2712 3.27 1.00 2.27 88.96 1.00 2.27 88.96

26 2740 167R 167R NH1 HH12 2711 2713 2.56 1.00 1.56 61.35 1.00 1.56 61.35

27 2741 167R 167R NH2 HH21 2714 2715 3.27 1.00 2.27 89.00 1.00 2.27 89.00

28 2742 167R 167R NH2 HH22 2714 2716 2.57 1.00 1.57 61.39 1.00 1.57 61.39

29 3029 185R 185R NH1 HH11 3000 3001 2.57 1.00 1.57 61.64 1.00 1.57 61.64

30 3030 185R 185R NH1 HH12 3000 3002 3.27 1.00 2.27 88.97 1.00 2.27 88.97

31 3031 185R 185R NH2 HH21 3003 3004 3.27 1.00 2.27 89.09 1.00 2.27 89.09

32 3032 185R 185R NH2 HH22 3003 3005 2.58 1.00 1.58 61.83 1.00 1.58 61.83

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15731 2D 3V C N 30 32 -86.27 -125.40 87.40 3.16 -62.40 110.17 12.73

1 3V 3V N CA 32 34 65.15 143.30 -42.40

2 15733 4S 5F C N 57 59 -83.68 -124.20 99.02 3.50 -63.20 99.39 12.49

2 5F 5F N CA 59 61 52.96 143.30 -44.30

3 15797 68N 69N C N 1105 1107 -134.10 -119.90 103.36 5.00 -63.20 103.73 11.48

3 69N 69N N CA 1107 1109 34.62 137.00 -41.10

4 15845 116S 117D C N 1878 1880 -83.30 -96.50 34.40 1.45 -63.30 124.06 14.21

4 117D 117D N CA 1880 1882 82.43 114.20 -40.00

5 15880 151M 152S C N 2440 2442 -57.55 -136.60 80.32 3.56 -64.10 159.73 11.20

5 152S 152S N CA 2442 2444 165.40 151.20 -35.00

6 15881 152S 153L C N 2451 2453 -161.07 -108.50 57.57 2.55 -63.50 -170.19 32.35

6 153L 153L N CA 2453 2455 155.98 132.50 -41.20

7 15883 154V 155F C N 2486 2488 27.09 -63.20 127.30 22.77 -63.20 127.30 22.77

7 155F 155F N CA 2488 2490 45.45 -44.30 -44.30

8 15884 155F 156F C N 2506 2508 -144.19 -124.20 55.54 2.05 -63.20 145.26 25.16

8 156F 156F N CA 2508 2510 -164.88 143.30 -44.30

9 15902 173N 174A C N 2802 2804 88.97 55.40 52.07 2.42 -62.50 156.48 31.38

9 174A 174A N CA 2804 2806 -1.61 38.20 -40.90

10 15904 175E 176M C N 2827 2829 93.73 -125.60 146.74 6.82 -125.60 146.74 6.82

10 176M 176M N CA 2829 2831 98.75 140.50 140.50

11 15905 176M 177C C N 2844 2846 -94.53 -117.90 94.21 3.32 -63.00 96.25 10.13

11 177C 177C N CA 2846 2848 49.84 141.10 -41.10

12 15906 177C 178F C N 2855 2857 -111.04 -63.20 77.49 8.76 -63.20 77.49 8.76

12 178F 178F N CA 2857 2859 16.65 -44.30 -44.30

13 15909 180L 181K C N 2905 2907 -77.90 -118.00 84.75 3.40 -62.90 106.30 13.06

13 181K 181K N CA 2907 2909 64.44 139.10 -40.80

14 15911 182L 183K C N 2946 2948 77.47 -62.90 149.40 21.72 -62.90 149.40 21.72

14 183K 183K N CA 2948 2950 -91.95 -40.80 -40.80

15 15924 195W 196D C N 3195 3197 -32.52 -70.90 39.45 2.63 -63.30 -178.52 20.72

15 196D 196D N CA 3197 3199 141.15 150.30 -40.00

-------------------------------------------------------------------------------------------------

Feature 26 : Distance restraints 4 (SDCH-SDCH)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 25287 138L 156F CG CE1 2212 2520 9.58 3.65 5.93 4.59 3.65 5.93 4.59

2 25294 138L 156F CD2 CE1 2218 2520 10.38 3.82 6.55 5.00 3.82 6.55 5.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 584 1948 1.306

serious non-bonded atom clash: 813 2691 1.330

serious non-bonded atom clash: 816 1715 1.417

serious non-bonded atom clash: 841 923 1.397

serious non-bonded atom clash: 937 1040 1.295

serious non-bonded atom clash: 944 1444 1.470

serious non-bonded atom clash: 1262 1338 1.315

serious non-bonded atom clash: 1327 2849 1.413

serious non-bonded atom clash: 1692 2574 1.481

serious non-bonded atom clash: 1739 2219 1.314

serious non-bonded atom clash: 1747 2201 1.478

serious non-bonded atom clash: 1762 2565 1.460

serious non-bonded atom clash: 1951 2041 1.306

serious non-bonded atom clash: 1977 2022 1.457

serious non-bonded atom clash: 2074 2129 1.319

serious non-bonded atom clash: 2211 2477 1.425

serious non-bonded atom clash: 2299 2519 1.310

serious non-bonded atom clash: 2461 2561 1.368

serious non-bonded atom clash: 2464 2539 1.322

serious non-bonded atom clash: 2467 2509 1.302

serious non-bonded atom clash: 2469 2566 1.295

serious non-bonded atom clash: 2730 2744 1.319

serious non-bonded atom clash: 3009 3020 1.442

serious non-bonded atom clash: 3036 3053 1.364

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 467 224 243 374 441 612 628 730 770 874 990 1084 1128 1146 1236

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990001.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_485\_> OD1/2 will be swapped: 118.0181 2 2

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 118.0181

iupac\_m\_487\_> NH1/2 swapped: 172.4493 6 6

iupac\_m\_486\_> OE1/2 will be swapped: 143.2433 10 10

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 143.2433

iupac\_m\_486\_> OE1/2 will be swapped: -173.7087 21 21

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -173.7087

iupac\_m\_486\_> OE1/2 will be swapped: 97.4191 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 97.4191

iupac\_m\_487\_> NH1/2 swapped: 176.1659 52 52

iupac\_m\_487\_> NH1/2 swapped: -174.9388 55 55

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 91.3096 65 65

iupac\_m\_484W> Dihedral still outside +-90: -91.0427

iupac\_m\_487\_> NH1/2 swapped: 177.9482 70 70

iupac\_m\_485\_> OD1/2 will be swapped: 119.2630 75 75

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 119.2630

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 98.3904 77 77

iupac\_m\_485\_> OD1/2 will be swapped: 112.7289 84 84

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 112.7289

iupac\_m\_485\_> OD1/2 will be swapped: 114.2924 88 88

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 114.2924

iupac\_m\_487\_> NH1/2 swapped: 179.1843 94 94

iupac\_m\_483\_> CD1/2 CE1/2 swapped: -98.7551 97 97

iupac\_m\_486\_> OE1/2 will be swapped: -120.8215 105 105

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -120.8215

iupac\_m\_485\_> OD1/2 will be swapped: 124.4951 117 117

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 124.4951

iupac\_m\_487\_> NH1/2 swapped: 178.9489 118 118

iupac\_m\_486\_> OE1/2 will be swapped: -118.6765 122 122

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -118.6765

iupac\_m\_486\_> OE1/2 will be swapped: -144.2368 123 123

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -144.2368

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 96.3698 133 133

iupac\_m\_487\_> NH1/2 swapped: 174.7716 139 139

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 90.1734 141 141

iupac\_m\_487\_> NH1/2 swapped: 179.6579 145 145

iupac\_m\_485\_> OD1/2 will be swapped: -98.5005 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -98.5005

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 91.6573 178 178

iupac\_m\_487\_> NH1/2 swapped: 175.6206 185 185

iupac\_m\_486\_> OE1/2 will be swapped: 102.5306 193 193

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 102.5306

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.149314

Native energy (pair) : -222.845548

Native energy (surface) : -8.946776

Native energy (combined) : -9.870062

Z score (pair) : -7.095279

Z score (surface) : -6.516498

Z score (combined) : -8.351258

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1092482

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -21691.2227

<< end of ENERGY.

DOPE score : -21691.222656

>> Normalized DOPE z score: -0.282

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20449

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 71068.1953

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 3255 36 36 0.205 0.205 61869. 1.000

2 Bond angle potential : 5881 240 328 9.870 9.870 7170.5 1.000

3 Stereochemical cosine torsion poten: 5645 0 42 26.983 26.983 686.31 1.000

4 Stereochemical improper torsion pot: 948 61 70 6.485 6.485 665.70 1.000

5 Soft-sphere overlap restraints : 20449 0 0 0.001 0.001 4.3794 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 0 0.351 0.351 142.96 1.000

10 Distance restraints 2 (N-O) : 3404 0 3 0.398 0.398 177.70 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 3 4.492 4.492 46.636 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 5 82.784 82.784 86.237 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 3 84.829 84.829 76.540 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 80.999 80.999 39.060 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 81.737 81.737 14.022 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.413 0.413 30.867 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 16 21 30.912 44.654 0.77233 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 3 1.103 1.103 56.965 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990002

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990002

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 39543.5234

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 3.28 1.00 2.28 89.30 1.00 2.28 89.30

2 100 6R 6R NH1 HH12 95 97 2.58 1.00 1.58 62.13 1.00 1.58 62.13

3 101 6R 6R NH2 HH21 98 99 2.59 1.00 1.59 62.49 1.00 1.59 62.49

4 102 6R 6R NH2 HH22 98 100 3.27 1.00 2.27 89.18 1.00 2.27 89.18

5 852 52R 52R NH1 HH11 843 844 2.55 1.00 1.55 60.82 1.00 1.55 60.82

6 853 52R 52R NH1 HH12 843 845 3.26 1.00 2.26 88.67 1.00 2.26 88.67

7 854 52R 52R NH2 HH21 846 847 2.55 1.00 1.55 60.66 1.00 1.55 60.66

8 855 52R 52R NH2 HH22 846 848 3.26 1.00 2.26 88.76 1.00 2.26 88.76

9 903 55R 55R NH1 HH11 894 895 3.26 1.00 2.26 88.63 1.00 2.26 88.63

10 904 55R 55R NH1 HH12 894 896 2.55 1.00 1.55 60.76 1.00 1.55 60.76

11 905 55R 55R NH2 HH21 897 898 3.26 1.00 2.26 88.78 1.00 2.26 88.78

12 906 55R 55R NH2 HH22 897 899 2.55 1.00 1.55 60.70 1.00 1.55 60.70

13 1150 70R 70R NH1 HH11 1137 1138 3.27 1.00 2.27 88.89 1.00 2.27 88.89

14 1151 70R 70R NH1 HH12 1137 1139 2.56 1.00 1.56 61.29 1.00 1.56 61.29

15 1152 70R 70R NH2 HH21 1140 1141 3.27 1.00 2.27 88.95 1.00 2.27 88.95

16 1153 70R 70R NH2 HH22 1140 1142 2.56 1.00 1.56 61.35 1.00 1.56 61.35

17 1533 94R 94R NH1 HH11 1516 1517 3.27 1.00 2.27 88.95 1.00 2.27 88.95

18 1534 94R 94R NH1 HH12 1516 1518 2.58 1.00 1.58 61.95 1.00 1.58 61.95

19 1535 94R 94R NH2 HH21 1519 1520 3.27 1.00 2.27 89.16 1.00 2.27 89.16

20 1536 94R 94R NH2 HH22 1519 1521 2.58 1.00 1.58 61.95 1.00 1.58 61.95

21 1928 118R 118R NH1 HH11 1908 1909 3.26 1.00 2.26 88.74 1.00 2.26 88.74

22 1929 118R 118R NH1 HH12 1908 1910 2.56 1.00 1.56 61.19 1.00 1.56 61.19

23 1930 118R 118R NH2 HH21 1911 1912 3.27 1.00 2.27 89.03 1.00 2.27 89.03

24 1931 118R 118R NH2 HH22 1911 1913 2.56 1.00 1.56 61.07 1.00 1.56 61.07

25 2263 139R 139R NH1 HH11 2240 2241 3.27 1.00 2.27 88.89 1.00 2.27 88.89

26 2264 139R 139R NH1 HH12 2240 2242 2.56 1.00 1.56 61.28 1.00 1.56 61.28

27 2265 139R 139R NH2 HH21 2243 2244 2.55 1.00 1.55 60.96 1.00 1.55 60.96

28 2266 139R 139R NH2 HH22 2243 2245 3.27 1.00 2.27 88.95 1.00 2.27 88.95

29 2380 145R 145R NH1 HH11 2356 2357 3.27 1.00 2.27 88.90 1.00 2.27 88.90

30 2381 145R 145R NH1 HH12 2356 2358 2.56 1.00 1.56 61.19 1.00 1.56 61.19

31 2382 145R 145R NH2 HH21 2359 2360 2.57 1.00 1.57 61.55 1.00 1.57 61.55

32 2383 145R 145R NH2 HH22 2359 2361 3.27 1.00 2.27 88.88 1.00 2.27 88.88

33 3029 185R 185R NH1 HH11 3000 3001 3.26 1.00 2.26 88.58 1.00 2.26 88.58

34 3030 185R 185R NH1 HH12 3000 3002 2.54 1.00 1.54 60.48 1.00 1.54 60.48

35 3031 185R 185R NH2 HH21 3003 3004 2.53 1.00 1.53 60.04 1.00 1.53 60.04

36 3032 185R 185R NH2 HH22 3003 3005 3.26 1.00 2.26 88.49 1.00 2.26 88.49

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15731 2D 3V C N 30 32 -102.90 -125.40 32.11 0.90 -62.40 167.75 19.22

1 3V 3V N CA 32 34 120.39 143.30 -42.40

2 15733 4S 5F C N 57 59 -79.86 -124.20 86.42 2.77 -63.20 114.64 14.83

2 5F 5F N CA 59 61 69.12 143.30 -44.30

3 15734 5F 6R C N 77 79 -106.07 -63.00 95.95 10.91 -63.00 95.95 10.91

3 6R 6R N CA 79 81 44.64 -41.10 -41.10

4 15785 56R 57Y C N 924 926 -100.04 -98.40 88.79 9.43 -63.50 90.72 12.81

4 57Y 57Y N CA 926 928 39.63 128.40 -43.40

5 15797 68N 69N C N 1105 1107 -131.22 -119.90 80.44 3.90 -63.20 119.68 12.90

5 69N 69N N CA 1107 1109 57.36 137.00 -41.10

6 15845 116S 117D C N 1878 1880 -95.65 -96.50 37.13 1.56 -63.30 121.46 13.37

6 117D 117D N CA 1880 1882 77.08 114.20 -40.00

7 15880 151M 152S C N 2440 2442 47.46 -64.10 173.54 20.61 -64.10 173.54 20.61

7 152S 152S N CA 2442 2444 97.92 -35.00 -35.00

8 15883 154V 155F C N 2486 2488 -82.55 -71.40 13.23 1.11 -63.20 178.94 23.57

8 155F 155F N CA 2488 2490 133.59 140.70 -44.30

9 15884 155F 156F C N 2506 2508 167.89 -124.20 96.10 2.59 -63.20 165.89 29.89

9 156F 156F N CA 2508 2510 -148.70 143.30 -44.30

10 15902 173N 174A C N 2802 2804 86.81 55.40 53.53 2.24 -62.50 153.53 30.72

10 174A 174A N CA 2804 2806 -5.14 38.20 -40.90

11 15904 175E 176M C N 2827 2829 95.26 -125.60 149.26 7.19 -125.60 149.26 7.19

11 176M 176M N CA 2829 2831 86.49 140.50 140.50

12 15905 176M 177C C N 2844 2846 -82.26 -63.00 86.81 9.46 -63.00 86.81 9.46

12 177C 177C N CA 2846 2848 43.55 -41.10 -41.10

13 15909 180L 181K C N 2905 2907 -79.94 -118.00 84.70 3.44 -62.90 105.62 12.88

13 181K 181K N CA 2907 2909 63.43 139.10 -40.80

14 15911 182L 183K C N 2946 2948 63.90 -62.90 131.01 19.77 -62.90 131.01 19.77

14 183K 183K N CA 2948 2950 -73.77 -40.80 -40.80

15 15923 194I 195W C N 3171 3173 -62.67 -71.30 9.38 0.76 58.80 163.67 7.04

15 195W 195W N CA 3173 3175 142.69 139.00 33.00

16 15924 195W 196D C N 3195 3197 -57.18 -70.90 19.50 0.78 -63.30 176.54 22.17

16 196D 196D N CA 3197 3199 136.44 150.30 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 37 3035 1.356

serious non-bonded atom clash: 91 100 1.446

serious non-bonded atom clash: 123 179 1.309

serious non-bonded atom clash: 321 766 1.447

serious non-bonded atom clash: 425 438 1.464

serious non-bonded atom clash: 460 1866 1.425

serious non-bonded atom clash: 516 536 1.495

serious non-bonded atom clash: 645 1844 1.418

serious non-bonded atom clash: 673 1845 1.312

serious non-bonded atom clash: 718 1833 1.310

serious non-bonded atom clash: 820 2691 1.475

serious non-bonded atom clash: 823 2687 1.374

serious non-bonded atom clash: 835 916 1.300

serious non-bonded atom clash: 935 1048 1.299

serious non-bonded atom clash: 1018 1180 1.393

serious non-bonded atom clash: 1171 1241 1.410

serious non-bonded atom clash: 1174 2940 1.465

serious non-bonded atom clash: 1211 1392 1.472

serious non-bonded atom clash: 1390 1448 1.339

serious non-bonded atom clash: 1430 2745 1.335

serious non-bonded atom clash: 1484 2692 1.448

serious non-bonded atom clash: 1593 2459 1.494

serious non-bonded atom clash: 1749 2210 1.343

serious non-bonded atom clash: 1763 2566 1.449

serious non-bonded atom clash: 1766 2642 1.469

serious non-bonded atom clash: 1858 2042 1.484

serious non-bonded atom clash: 2005 2027 1.444

serious non-bonded atom clash: 2298 2517 1.378

serious non-bonded atom clash: 2304 2513 1.333

serious non-bonded atom clash: 2454 2468 1.299

serious non-bonded atom clash: 2479 2489 1.472

serious non-bonded atom clash: 2800 2847 1.496

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 442 207 233 403 485 577 623 713 744 950 955 1021 1168 1216 1351

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990002.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_485\_> OD1/2 will be swapped: -151.8677 2 2

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -151.8677

iupac\_m\_487\_> NH1/2 swapped: 177.7690 6 6

iupac\_m\_486\_> OE1/2 will be swapped: -123.9905 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -123.9905

iupac\_m\_487\_> NH1/2 swapped: -177.8976 52 52

iupac\_m\_487\_> NH1/2 swapped: 177.5983 55 55

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 107.6204 57 57

iupac\_m\_487\_> NH1/2 swapped: 178.7351 70 70

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 113.8207 72 72

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 91.7076 77 77

iupac\_m\_486\_> OE1/2 will be swapped: 178.3592 87 87

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 178.3592

iupac\_m\_485\_> OD1/2 will be swapped: 175.2534 88 88

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 175.2534

iupac\_m\_487\_> NH1/2 swapped: -180.0000 94 94

iupac\_m\_487\_> NH1/2 swapped: 180.0000 118 118

iupac\_m\_485\_> OD1/2 will be swapped: -170.6784 136 136

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -170.6784

iupac\_m\_487\_> NH1/2 swapped: -175.9095 139 139

iupac\_m\_487\_> NH1/2 swapped: 178.2017 145 145

iupac\_m\_485\_> OD1/2 will be swapped: 177.8591 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 177.8591

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 99.2425 156 156

iupac\_m\_486\_> OE1/2 will be swapped: 166.7939 165 165

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 166.7939

iupac\_m\_486\_> OE1/2 will be swapped: 128.3206 175 175

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 128.3206

iupac\_m\_487\_> NH1/2 swapped: -175.6438 185 185

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.182035

Native energy (pair) : -212.418822

Native energy (surface) : -9.799134

Native energy (combined) : -9.844034

Z score (pair) : -6.896365

Z score (surface) : -6.729669

Z score (combined) : -8.853036

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1106669

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -21997.5605

<< end of ENERGY.

DOPE score : -21997.560547

>> Normalized DOPE z score: -0.392

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20576

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 71704.7266

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 3255 36 36 0.205 0.205 62208. 1.000

2 Bond angle potential : 5881 284 359 10.120 10.120 7531.2 1.000

3 Stereochemical cosine torsion poten: 5645 0 55 26.828 26.828 657.34 1.000

4 Stereochemical improper torsion pot: 948 63 81 6.533 6.533 675.25 1.000

5 Soft-sphere overlap restraints : 20576 0 0 0.002 0.002 5.5782 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 4 0.371 0.371 152.50 1.000

10 Distance restraints 2 (N-O) : 3404 0 1 0.405 0.405 169.07 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 5 4.423 4.423 45.215 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 7 77.293 77.293 71.638 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 1 83.285 83.285 67.495 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 1 86.645 86.645 39.115 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 100.637 100.637 17.029 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.443 0.443 35.767 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 16 17 29.359 48.236 -27.203 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 4 1.168 1.168 56.470 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990003

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990003

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 38540.5273

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

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Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 3.27 1.00 2.27 89.08 1.00 2.27 89.08

2 100 6R 6R NH1 HH12 95 97 2.58 1.00 1.58 61.84 1.00 1.58 61.84

3 101 6R 6R NH2 HH21 98 99 2.58 1.00 1.58 62.06 1.00 1.58 62.06

4 102 6R 6R NH2 HH22 98 100 3.27 1.00 2.27 89.00 1.00 2.27 89.00

5 852 52R 52R NH1 HH11 843 844 3.27 1.00 2.27 88.89 1.00 2.27 88.89

6 853 52R 52R NH1 HH12 843 845 2.57 1.00 1.57 61.59 1.00 1.57 61.59

7 854 52R 52R NH2 HH21 846 847 2.57 1.00 1.57 61.46 1.00 1.57 61.46

8 855 52R 52R NH2 HH22 846 848 3.27 1.00 2.27 89.08 1.00 2.27 89.08

9 903 55R 55R NH1 HH11 894 895 3.27 1.00 2.27 88.89 1.00 2.27 88.89

10 904 55R 55R NH1 HH12 894 896 2.56 1.00 1.56 61.17 1.00 1.56 61.17

11 905 55R 55R NH2 HH21 897 898 3.27 1.00 2.27 88.86 1.00 2.27 88.86

12 906 55R 55R NH2 HH22 897 899 2.56 1.00 1.56 61.35 1.00 1.56 61.35

13 1150 70R 70R NH1 HH11 1137 1138 3.27 1.00 2.27 88.97 1.00 2.27 88.97

14 1151 70R 70R NH1 HH12 1137 1139 2.56 1.00 1.56 61.28 1.00 1.56 61.28

15 1152 70R 70R NH2 HH21 1140 1141 3.27 1.00 2.27 88.85 1.00 2.27 88.85

16 1153 70R 70R NH2 HH22 1140 1142 2.58 1.00 1.58 61.79 1.00 1.58 61.79

17 1533 94R 94R NH1 HH11 1516 1517 3.27 1.00 2.27 89.08 1.00 2.27 89.08

18 1534 94R 94R NH1 HH12 1516 1518 2.57 1.00 1.57 61.56 1.00 1.57 61.56

19 1535 94R 94R NH2 HH21 1519 1520 2.57 1.00 1.57 61.72 1.00 1.57 61.72

20 1536 94R 94R NH2 HH22 1519 1521 3.27 1.00 2.27 89.11 1.00 2.27 89.11

21 1928 118R 118R NH1 HH11 1908 1909 3.26 1.00 2.26 88.82 1.00 2.26 88.82

22 1929 118R 118R NH1 HH12 1908 1910 2.56 1.00 1.56 61.23 1.00 1.56 61.23

23 1930 118R 118R NH2 HH21 1911 1912 3.26 1.00 2.26 88.75 1.00 2.26 88.75

24 1931 118R 118R NH2 HH22 1911 1913 2.56 1.00 1.56 61.25 1.00 1.56 61.25

25 2263 139R 139R NH1 HH11 2240 2241 2.58 1.00 1.58 62.13 1.00 1.58 62.13

26 2264 139R 139R NH1 HH12 2240 2242 3.27 1.00 2.27 89.21 1.00 2.27 89.21

27 2265 139R 139R NH2 HH21 2243 2244 3.28 1.00 2.28 89.22 1.00 2.28 89.22

28 2266 139R 139R NH2 HH22 2243 2245 2.59 1.00 1.59 62.23 1.00 1.59 62.23

29 2380 145R 145R NH1 HH11 2356 2357 3.27 1.00 2.27 89.02 1.00 2.27 89.02

30 2381 145R 145R NH1 HH12 2356 2358 2.57 1.00 1.57 61.66 1.00 1.57 61.66

31 2382 145R 145R NH2 HH21 2359 2360 2.57 1.00 1.57 61.61 1.00 1.57 61.61

32 2383 145R 145R NH2 HH22 2359 2361 3.27 1.00 2.27 88.96 1.00 2.27 88.96

33 3029 185R 185R NH1 HH11 3000 3001 3.27 1.00 2.27 88.87 1.00 2.27 88.87

34 3030 185R 185R NH1 HH12 3000 3002 2.57 1.00 1.57 61.50 1.00 1.57 61.50

35 3031 185R 185R NH2 HH21 3003 3004 3.27 1.00 2.27 88.84 1.00 2.27 88.84

36 3032 185R 185R NH2 HH22 3003 3005 2.57 1.00 1.57 61.41 1.00 1.57 61.41

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15733 4S 5F C N 57 59 -82.23 -124.20 81.98 2.63 -63.20 118.72 15.25

1 5F 5F N CA 59 61 72.89 143.30 -44.30

2 15734 5F 6R C N 77 79 -118.70 -63.00 93.36 10.64 -63.00 93.36 10.64

2 6R 6R N CA 79 81 33.82 -41.10 -41.10

3 15797 68N 69N C N 1105 1107 -130.71 -119.90 74.21 3.60 -63.20 124.57 13.40

3 69N 69N N CA 1107 1109 63.58 137.00 -41.10

4 15845 116S 117D C N 1878 1880 -81.99 -96.50 22.48 0.94 -63.30 138.31 16.02

4 117D 117D N CA 1880 1882 97.04 114.20 -40.00

5 15880 151M 152S C N 2440 2442 106.67 -136.60 139.46 7.41 -64.10 -156.93 26.53

5 152S 152S N CA 2442 2444 74.89 151.20 -35.00

6 15882 153L 154V C N 2470 2472 -67.61 -62.40 13.00 1.97 -125.40 172.36 9.66

6 154V 154V N CA 2472 2474 -54.31 -42.40 143.30

7 15883 154V 155F C N 2486 2488 -167.48 -124.20 45.04 2.11 -63.20 -156.17 23.10

7 155F 155F N CA 2488 2490 130.83 143.30 -44.30

8 15884 155F 156F C N 2506 2508 173.97 -124.20 97.73 2.79 -63.20 156.34 28.19

8 156F 156F N CA 2508 2510 -141.02 143.30 -44.30

9 15902 173N 174A C N 2802 2804 90.49 55.40 59.17 2.50 -62.50 156.19 31.12

9 174A 174A N CA 2804 2806 -9.44 38.20 -40.90

10 15904 175E 176M C N 2827 2829 92.30 -125.60 145.72 6.56 -125.60 145.72 6.56

10 176M 176M N CA 2829 2831 108.23 140.50 140.50

11 15905 176M 177C C N 2844 2846 -86.80 -63.00 93.57 10.07 -63.00 93.57 10.07

11 177C 177C N CA 2846 2848 49.40 -41.10 -41.10

12 15909 180L 181K C N 2905 2907 -84.69 -118.00 84.10 3.51 -62.90 104.97 12.60

12 181K 181K N CA 2907 2909 61.88 139.10 -40.80

13 15911 182L 183K C N 2946 2948 112.04 -118.00 139.56 4.65 -62.90 -142.51 27.99

13 183K 183K N CA 2948 2950 -170.02 139.10 -40.80

14 15912 183K 184N C N 2968 2970 -66.11 -119.90 57.17 1.89 -63.20 158.76 19.69

14 184N 184N N CA 2970 2972 117.63 137.00 -41.10

15 15923 194I 195W C N 3171 3173 -62.08 -71.30 13.14 0.77 58.80 154.76 7.35

15 195W 195W N CA 3173 3175 129.63 139.00 33.00

16 15924 195W 196D C N 3195 3197 -88.36 -96.50 19.35 0.80 -63.30 173.58 20.03

16 196D 196D N CA 3197 3199 131.76 114.20 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 65 2976 1.305

serious non-bonded atom clash: 521 536 1.435

serious non-bonded atom clash: 529 583 1.443

serious non-bonded atom clash: 584 1948 1.439

serious non-bonded atom clash: 706 1903 1.480

serious non-bonded atom clash: 805 2801 1.306

serious non-bonded atom clash: 816 1715 1.387

serious non-bonded atom clash: 889 898 1.469

serious non-bonded atom clash: 914 920 1.472

serious non-bonded atom clash: 1021 1180 1.448

serious non-bonded atom clash: 1076 1256 1.481

serious non-bonded atom clash: 1188 1228 1.431

serious non-bonded atom clash: 1262 1337 1.390

serious non-bonded atom clash: 1390 1449 1.476

serious non-bonded atom clash: 1486 2739 1.385

serious non-bonded atom clash: 1533 1603 1.480

serious non-bonded atom clash: 1658 1667 1.305

serious non-bonded atom clash: 1738 2152 1.499

serious non-bonded atom clash: 1739 2216 1.321

serious non-bonded atom clash: 1741 2148 1.445

serious non-bonded atom clash: 1809 2154 1.389

serious non-bonded atom clash: 1858 2039 1.491

serious non-bonded atom clash: 1951 1989 1.466

serious non-bonded atom clash: 2152 2221 1.325

serious non-bonded atom clash: 2229 2523 1.310

serious non-bonded atom clash: 2251 2317 1.324

serious non-bonded atom clash: 2296 2489 1.499

serious non-bonded atom clash: 2450 2511 1.383

serious non-bonded atom clash: 2499 2566 1.473

serious non-bonded atom clash: 2707 2713 1.464

serious non-bonded atom clash: 2851 2899 1.356

serious non-bonded atom clash: 2866 2925 1.303

serious non-bonded atom clash: 2981 3036 1.347

serious non-bonded atom clash: 2996 3009 1.366

serious non-bonded atom clash: 3035 3054 1.312

serious non-bonded atom clash: 3045 3116 1.374

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 468 226 252 346 456 593 656 717 799 942 937 1048 1132 1113 1317

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990003.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_485\_> OD1/2 will be swapped: -132.2139 2 2

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -132.2139

iupac\_m\_487\_> NH1/2 swapped: 179.7353 6 6

iupac\_m\_486\_> OE1/2 will be swapped: -179.1649 10 10

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -179.1649

iupac\_m\_486\_> OE1/2 will be swapped: -126.3369 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -126.3369

iupac\_m\_487\_> NH1/2 swapped: 178.7420 55 55

iupac\_m\_487\_> NH1/2 swapped: -178.2660 70 70

iupac\_m\_487\_> NH1/2 swapped: 180.0000 74 74

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 91.8416 77 77

iupac\_m\_485\_> OD1/2 will be swapped: 123.9514 84 84

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 123.9514

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 104.1054 92 92

iupac\_m\_483\_> CD1/2 CE1/2 swapped: -139.8378 97 97

iupac\_m\_484W> Dihedral still outside +-90: -90.6811

iupac\_m\_486\_> OE1/2 will be swapped: -163.2122 105 105

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -163.2122

iupac\_m\_487\_> NH1/2 swapped: 179.9515 118 118

iupac\_m\_486\_> OE1/2 will be swapped: -131.7113 123 123

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -131.7113

iupac\_m\_486\_> OE1/2 will be swapped: -175.9773 128 128

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -175.9773

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 91.5528 133 133

iupac\_m\_487\_> NH1/2 swapped: 178.0529 139 139

iupac\_m\_487\_> NH1/2 swapped: -179.1429 145 145

iupac\_m\_486\_> OE1/2 will be swapped: 168.2037 165 165

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 168.2037

iupac\_m\_487\_> NH1/2 swapped: -179.6029 185 185

iupac\_m\_486\_> OE1/2 will be swapped: 179.9515 192 192

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 179.9515

iupac\_m\_485\_> OD1/2 will be swapped: 126.0178 196 196

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 126.0178

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.172805

Native energy (pair) : -230.980288

Native energy (surface) : -6.287314

Native energy (combined) : -9.446010

Z score (pair) : -7.782042

Z score (surface) : -5.379551

Z score (combined) : -8.583765

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1100104

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -21605.1719

<< end of ENERGY.

DOPE score : -21605.171875

>> Normalized DOPE z score: -0.251

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20982

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 64429.0469

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 3255 32 34 0.193 0.193 55145. 1.000

2 Bond angle potential : 5881 269 350 9.832 9.832 7133.2 1.000

3 Stereochemical cosine torsion poten: 5645 4 60 26.320 26.320 673.90 1.000

4 Stereochemical improper torsion pot: 948 67 82 6.934 6.934 850.55 1.000

5 Soft-sphere overlap restraints : 20982 0 2 0.002 0.002 14.047 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 0 0.335 0.335 125.07 1.000

10 Distance restraints 2 (N-O) : 3404 0 3 0.397 0.397 162.97 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 2 4.144 4.144 39.701 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 5 81.555 81.555 73.329 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 4 76.582 76.582 71.976 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 84.165 84.165 35.417 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 104.785 104.785 15.734 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.415 0.415 34.068 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 18 22 31.331 44.839 -7.4795 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 3 1.203 1.203 61.993 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990004

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990004

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 37913.7539

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 2.57 1.00 1.57 61.48 1.00 1.57 61.48

2 100 6R 6R NH1 HH12 95 97 3.27 1.00 2.27 88.98 1.00 2.27 88.98

3 101 6R 6R NH2 HH21 98 99 3.27 1.00 2.27 88.97 1.00 2.27 88.97

4 102 6R 6R NH2 HH22 98 100 2.57 1.00 1.57 61.48 1.00 1.57 61.48

5 903 55R 55R NH1 HH11 894 895 3.27 1.00 2.27 88.91 1.00 2.27 88.91

6 904 55R 55R NH1 HH12 894 896 2.56 1.00 1.56 61.27 1.00 1.56 61.27

7 905 55R 55R NH2 HH21 897 898 3.27 1.00 2.27 88.92 1.00 2.27 88.92

8 906 55R 55R NH2 HH22 897 899 2.56 1.00 1.56 61.21 1.00 1.56 61.21

9 1150 70R 70R NH1 HH11 1137 1138 3.27 1.00 2.27 88.93 1.00 2.27 88.93

10 1151 70R 70R NH1 HH12 1137 1139 2.56 1.00 1.56 61.30 1.00 1.56 61.30

11 1152 70R 70R NH2 HH21 1140 1141 3.27 1.00 2.27 88.93 1.00 2.27 88.93

12 1153 70R 70R NH2 HH22 1140 1142 2.56 1.00 1.56 61.29 1.00 1.56 61.29

13 1221 74R 74R NH1 HH11 1207 1208 3.27 1.00 2.27 88.94 1.00 2.27 88.94

14 1222 74R 74R NH1 HH12 1207 1209 2.56 1.00 1.56 61.33 1.00 1.56 61.33

15 1223 74R 74R NH2 HH21 1210 1211 3.27 1.00 2.27 88.93 1.00 2.27 88.93

16 1224 74R 74R NH2 HH22 1210 1212 2.57 1.00 1.57 61.41 1.00 1.57 61.41

17 1928 118R 118R NH1 HH11 1908 1909 3.27 1.00 2.27 88.99 1.00 2.27 88.99

18 1929 118R 118R NH1 HH12 1908 1910 2.57 1.00 1.57 61.41 1.00 1.57 61.41

19 1930 118R 118R NH2 HH21 1911 1912 2.57 1.00 1.57 61.41 1.00 1.57 61.41

20 1931 118R 118R NH2 HH22 1911 1913 3.27 1.00 2.27 88.97 1.00 2.27 88.97

21 2263 139R 139R NH1 HH11 2240 2241 2.56 1.00 1.56 61.34 1.00 1.56 61.34

22 2264 139R 139R NH1 HH12 2240 2242 3.27 1.00 2.27 88.93 1.00 2.27 88.93

23 2265 139R 139R NH2 HH21 2243 2244 3.27 1.00 2.27 88.93 1.00 2.27 88.93

24 2266 139R 139R NH2 HH22 2243 2245 2.57 1.00 1.57 61.39 1.00 1.57 61.39

25 2380 145R 145R NH1 HH11 2356 2357 2.57 1.00 1.57 61.42 1.00 1.57 61.42

26 2381 145R 145R NH1 HH12 2356 2358 3.27 1.00 2.27 88.91 1.00 2.27 88.91

27 2382 145R 145R NH2 HH21 2359 2360 2.57 1.00 1.57 61.40 1.00 1.57 61.40

28 2383 145R 145R NH2 HH22 2359 2361 3.27 1.00 2.27 88.83 1.00 2.27 88.83

29 3029 185R 185R NH1 HH11 3000 3001 3.27 1.00 2.27 88.96 1.00 2.27 88.96

30 3030 185R 185R NH1 HH12 3000 3002 2.57 1.00 1.57 61.44 1.00 1.57 61.44

31 3031 185R 185R NH2 HH21 3003 3004 2.57 1.00 1.57 61.42 1.00 1.57 61.42

32 3032 185R 185R NH2 HH22 3003 3005 3.27 1.00 2.27 88.96 1.00 2.27 88.96

-------------------------------------------------------------------------------------------------

Feature 2 : Bond angle potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 6110 97Y 97Y CE1 CZ 1570 1574 145.07 120.00 25.07 5.42 120.00 25.07 5.42

2 6113 97Y 97Y CE2 CZ 1572 1574 145.67 120.00 25.67 5.55 120.00 25.67 5.55

-------------------------------------------------------------------------------------------------

Feature 3 : Stereochemical cosine torsion potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 11823 97Y 97Y HD1 CD1 1567 1566 80.96 0.00 80.96 8.19 0.00 80.96 8.19

2 11827 97Y 97Y HD2 CD2 1569 1568 -106.63 180.00 73.37 7.71 180.00 73.37 7.71

3 11837 97Y 97Y CE2 CZ 1572 1574 121.05 180.00 -58.95 6.16 180.00 -58.95 6.16

4 11841 97Y 97Y CE1 CZ 1570 1574 -113.54 180.00 66.46 7.06 180.00 66.46 7.06

-------------------------------------------------------------------------------------------------

Feature 4 : Stereochemical improper torsion potentia

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15260 97Y 97Y CB CG 1562 1565 -158.51 -180.00 21.49 6.55 -180.00 21.49 6.55

2 15263 97Y 97Y CE1 CZ 1570 1574 39.91 0.00 39.91 12.16 0.00 39.91 12.16

3 15264 97Y 97Y CZ CE2 1574 1572 43.29 0.00 43.29 13.18 0.00 43.29 13.18

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15733 4S 5F C N 57 59 -82.91 -63.20 98.26 12.38 -63.20 98.26 12.38

1 5F 5F N CA 59 61 51.96 -44.30 -44.30

2 15734 5F 6R C N 77 79 -91.49 -63.00 95.73 11.31 -63.00 95.73 11.31

2 6R 6R N CA 79 81 50.30 -41.10 -41.10

3 15785 56R 57Y C N 924 926 -100.60 -98.40 76.12 8.08 -63.50 102.65 14.62

3 57Y 57Y N CA 926 928 52.31 128.40 -43.40

4 15797 68N 69N C N 1105 1107 -132.50 -63.20 102.81 11.34 -63.20 102.81 11.34

4 69N 69N N CA 1107 1109 34.85 -41.10 -41.10

5 15845 116S 117D C N 1878 1880 -73.81 -96.50 51.92 2.19 -63.30 108.01 12.73

5 117D 117D N CA 1880 1882 67.50 114.20 -40.00

6 15875 146H 147C C N 2379 2381 -87.09 -117.90 30.95 1.00 -63.00 -179.19 20.53

6 147C 147C N CA 2381 2383 138.10 141.10 -41.10

7 15876 147C 148G C N 2390 2392 93.18 82.20 22.15 0.62 -62.40 158.53 29.35

7 148G 148G N CA 2392 2394 -10.74 8.50 -41.20

8 15881 152S 153L C N 2451 2453 36.13 -63.50 137.78 24.91 -63.50 137.78 24.91

8 153L 153L N CA 2453 2455 53.96 -41.20 -41.20

9 15882 153L 154V C N 2470 2472 -64.12 -62.40 13.98 1.87 -125.40 171.73 9.66

9 154V 154V N CA 2472 2474 -56.27 -42.40 143.30

10 15884 155F 156F C N 2506 2508 -75.34 -124.20 78.40 4.35 -63.20 111.75 16.34

10 156F 156F N CA 2508 2510 -155.39 143.30 -44.30

11 15902 173N 174A C N 2802 2804 88.57 55.40 55.39 2.36 -62.50 155.01 30.98

11 174A 174A N CA 2804 2806 -6.16 38.20 -40.90

12 15904 175E 176M C N 2827 2829 96.17 -125.60 143.84 6.66 -125.60 143.84 6.66

12 176M 176M N CA 2829 2831 100.73 140.50 140.50

13 15905 176M 177C C N 2844 2846 -92.60 -63.00 82.40 8.61 -63.00 82.40 8.61

13 177C 177C N CA 2846 2848 35.81 -41.10 -41.10

14 15909 180L 181K C N 2905 2907 -75.55 -118.00 93.93 3.81 -62.90 96.95 11.95

14 181K 181K N CA 2907 2909 55.32 139.10 -40.80

15 15911 182L 183K C N 2946 2948 54.91 -118.00 173.60 6.30 -62.90 -157.75 33.21

15 183K 183K N CA 2948 2950 123.60 139.10 -40.80

16 15912 183K 184N C N 2968 2970 53.60 55.90 14.03 0.82 -63.20 150.20 24.56

16 184N 184N N CA 2970 2972 53.34 39.50 -41.10

17 15922 193E 194I C N 3152 3154 -26.64 -97.30 74.07 3.51 -120.60 95.89 7.20

17 194I 194I N CA 3154 3156 149.43 127.20 130.30

18 15924 195W 196D C N 3195 3197 -72.18 -70.90 4.63 0.17 -63.30 165.50 20.97

18 196D 196D N CA 3197 3199 154.74 150.30 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 123 179 1.423

serious non-bonded atom clash: 518 536 1.312

serious non-bonded atom clash: 769 1821 1.335

serious non-bonded atom clash: 816 1715 1.308

serious non-bonded atom clash: 820 1776 1.307

serious non-bonded atom clash: 929 935 1.416

serious non-bonded atom clash: 944 1151 1.460

serious non-bonded atom clash: 1076 1256 1.495

serious non-bonded atom clash: 1205 1271 1.433

serious non-bonded atom clash: 1262 1338 1.422

serious non-bonded atom clash: 1478 2624 1.362

serious non-bonded atom clash: 1503 1573 1.279

serious non-bonded atom clash: 1567 1569 1.260

serious non-bonded atom clash: 1596 1642 1.385

serious non-bonded atom clash: 1741 2211 1.289

serious non-bonded atom clash: 1758 2639 1.357

serious non-bonded atom clash: 1764 2566 1.369

serious non-bonded atom clash: 1877 1881 1.491

serious non-bonded atom clash: 2098 2157 1.356

serious non-bonded atom clash: 2110 2171 1.391

serious non-bonded atom clash: 2229 2521 1.305

serious non-bonded atom clash: 2302 2448 1.496

serious non-bonded atom clash: 2303 2473 1.309

serious non-bonded atom clash: 2458 2539 1.488

serious non-bonded atom clash: 2459 2511 1.301

serious non-bonded atom clash: 2475 2575 1.425

serious non-bonded atom clash: 2834 2868 1.302

serious non-bonded atom clash: 2945 2990 1.474

serious non-bonded atom clash: 2981 3035 1.385

serious non-bonded atom clash: 3036 3054 1.425

serious non-bonded atom clash: 3069 3082 1.310

serious non-bonded atom clash: 3096 3117 1.471

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 477 228 259 337 489 672 651 752 786 896 997 1117 1189 1263 1313

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990004.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_487\_> NH1/2 swapped: -179.3073 6 6

iupac\_m\_486\_> OE1/2 will be swapped: -136.8330 10 10

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -136.8330

iupac\_m\_486\_> OE1/2 will be swapped: -175.0265 21 21

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -175.0265

iupac\_m\_486\_> OE1/2 will be swapped: 114.2909 35 35

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 114.2909

iupac\_m\_487\_> NH1/2 swapped: 178.7829 55 55

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 102.9034 57 57

iupac\_m\_485\_> OD1/2 will be swapped: 178.3289 58 58

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 178.3289

iupac\_m\_485\_> OD1/2 will be swapped: 114.2879 75 75

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 114.2879

iupac\_m\_485\_> OD1/2 will be swapped: 177.5098 84 84

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 177.5098

iupac\_m\_485\_> OD1/2 will be swapped: 152.6044 88 88

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 152.6044

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 95.1823 92 92

iupac\_m\_487\_> NH1/2 swapped: 179.3442 94 94

iupac\_m\_486\_> OE1/2 will be swapped: -165.8252 105 105

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -165.8252

iupac\_m\_487\_> NH1/2 swapped: 177.4741 118 118

iupac\_m\_486\_> OE1/2 will be swapped: 176.8006 128 128

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 176.8006

iupac\_m\_485\_> OD1/2 will be swapped: 178.4154 136 136

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 178.4154

iupac\_m\_487\_> NH1/2 swapped: 179.9011 167 167

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 98.9629 178 178

iupac\_m\_487\_> NH1/2 swapped: 179.2958 185 185

iupac\_m\_486\_> OE1/2 will be swapped: 116.0539 193 193

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 116.0539

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.163198

Native energy (pair) : -229.807797

Native energy (surface) : -8.904543

Native energy (combined) : -10.174841

Z score (pair) : -7.993480

Z score (surface) : -6.519361

Z score (combined) : -9.359262

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1095333

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -22083.9141

<< end of ENERGY.

DOPE score : -22083.914062

>> Normalized DOPE z score: -0.423

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20412

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 49139.3906

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

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1 Bond length potential : 3255 24 24 0.168 0.168 41494. 1.000

2 Bond angle potential : 5881 258 318 8.835 8.835 5741.9 1.000

3 Stereochemical cosine torsion poten: 5645 0 53 26.751 26.751 649.75 1.000

4 Stereochemical improper torsion pot: 948 64 77 6.414 6.414 652.93 1.000

5 Soft-sphere overlap restraints : 20412 0 0 0.002 0.002 7.6559 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 1 0.332 0.332 125.96 1.000

10 Distance restraints 2 (N-O) : 3404 0 5 0.405 0.405 174.64 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 4 4.304 4.304 42.821 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 5 78.946 78.946 63.250 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 1 86.745 86.745 62.787 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 94.894 94.894 41.369 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 102.209 102.209 14.110 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.388 0.388 29.477 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 15 17 29.618 43.270 -8.3847 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 2 1.079 1.079 46.793 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990005

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990005

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 35597.3672

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 3.27 1.00 2.27 89.13 1.00 2.27 89.13

2 100 6R 6R NH1 HH12 95 97 2.57 1.00 1.57 61.58 1.00 1.57 61.58

3 101 6R 6R NH2 HH21 98 99 2.58 1.00 1.58 61.79 1.00 1.58 61.79

4 102 6R 6R NH2 HH22 98 100 3.27 1.00 2.27 89.13 1.00 2.27 89.13

5 903 55R 55R NH1 HH11 894 895 2.57 1.00 1.57 61.53 1.00 1.57 61.53

6 904 55R 55R NH1 HH12 894 896 3.27 1.00 2.27 88.92 1.00 2.27 88.92

7 905 55R 55R NH2 HH21 897 898 3.27 1.00 2.27 88.95 1.00 2.27 88.95

8 906 55R 55R NH2 HH22 897 899 2.57 1.00 1.57 61.43 1.00 1.57 61.43

9 1533 94R 94R NH1 HH11 1516 1517 3.27 1.00 2.27 89.02 1.00 2.27 89.02

10 1534 94R 94R NH1 HH12 1516 1518 2.57 1.00 1.57 61.72 1.00 1.57 61.72

11 1535 94R 94R NH2 HH21 1519 1520 3.27 1.00 2.27 89.01 1.00 2.27 89.01

12 1536 94R 94R NH2 HH22 1519 1521 2.57 1.00 1.57 61.72 1.00 1.57 61.72

13 1928 118R 118R NH1 HH11 1908 1909 3.27 1.00 2.27 88.97 1.00 2.27 88.97

14 1929 118R 118R NH1 HH12 1908 1910 2.57 1.00 1.57 61.47 1.00 1.57 61.47

15 1930 118R 118R NH2 HH21 1911 1912 3.27 1.00 2.27 88.93 1.00 2.27 88.93

16 1931 118R 118R NH2 HH22 1911 1913 2.57 1.00 1.57 61.48 1.00 1.57 61.48

17 2739 167R 167R NH1 HH11 2711 2712 3.27 1.00 2.27 88.99 1.00 2.27 88.99

18 2740 167R 167R NH1 HH12 2711 2713 2.57 1.00 1.57 61.52 1.00 1.57 61.52

19 2741 167R 167R NH2 HH21 2714 2715 3.27 1.00 2.27 89.00 1.00 2.27 89.00

20 2742 167R 167R NH2 HH22 2714 2716 2.57 1.00 1.57 61.66 1.00 1.57 61.66

21 3029 185R 185R NH1 HH11 3000 3001 3.27 1.00 2.27 88.94 1.00 2.27 88.94

22 3030 185R 185R NH1 HH12 3000 3002 2.57 1.00 1.57 61.72 1.00 1.57 61.72

23 3031 185R 185R NH2 HH21 3003 3004 3.27 1.00 2.27 89.05 1.00 2.27 89.05

24 3032 185R 185R NH2 HH22 3003 3005 2.57 1.00 1.57 61.54 1.00 1.57 61.54

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Feature 2 : Bond angle potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 4569 44C 44C N CA 710 712 122.75 107.00 15.75 4.53 107.00 15.75 4.53

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Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15733 4S 5F C N 57 59 -82.54 -124.20 84.35 2.75 -63.20 115.89 14.84

1 5F 5F N CA 59 61 69.96 143.30 -44.30

2 15734 5F 6R C N 77 79 -109.01 -63.00 90.34 10.22 -63.00 90.34 10.22

2 6R 6R N CA 79 81 36.64 -41.10 -41.10

3 15796 67A 68N C N 1091 1093 -75.18 -119.90 51.44 1.55 -63.20 153.14 18.51

3 68N 68N N CA 1093 1095 111.57 137.00 -41.10

4 15797 68N 69N C N 1105 1107 60.51 55.90 11.21 0.54 -63.20 142.33 23.40

4 69N 69N N CA 1107 1109 29.29 39.50 -41.10

5 15845 116S 117D C N 1878 1880 -70.39 -96.50 43.66 1.83 -63.30 119.41 14.32

5 117D 117D N CA 1880 1882 79.21 114.20 -40.00

6 15875 146H 147C C N 2379 2381 -84.45 -117.90 33.47 1.16 -63.00 177.90 23.24

6 147C 147C N CA 2381 2383 142.30 141.10 -41.10

7 15876 147C 148G C N 2390 2392 94.96 82.20 28.76 0.83 -62.40 159.17 29.28

7 148G 148G N CA 2392 2394 -17.27 8.50 -41.20

8 15881 152S 153L C N 2451 2453 -8.99 -70.70 67.89 5.09 -63.50 163.84 26.12

8 153L 153L N CA 2453 2455 113.31 141.60 -41.20

9 15883 154V 155F C N 2486 2488 22.33 -63.20 127.40 22.65 -63.20 127.40 22.65

9 155F 155F N CA 2488 2490 50.12 -44.30 -44.30

10 15884 155F 156F C N 2506 2508 -125.47 -124.20 68.91 3.22 -63.20 120.79 20.68

10 156F 156F N CA 2508 2510 -147.80 143.30 -44.30

11 15902 173N 174A C N 2802 2804 88.06 55.40 54.24 2.33 -62.50 154.75 30.95

11 174A 174A N CA 2804 2806 -5.11 38.20 -40.90

12 15904 175E 176M C N 2827 2829 90.54 -125.60 149.46 6.90 -125.60 149.46 6.90

12 176M 176M N CA 2829 2831 99.99 140.50 140.50

13 15905 176M 177C C N 2844 2846 -91.63 -63.00 90.60 9.56 -63.00 90.60 9.56

13 177C 177C N CA 2846 2848 44.86 -41.10 -41.10

14 15909 180L 181K C N 2905 2907 -76.08 -118.00 78.97 3.07 -62.90 113.74 14.10

14 181K 181K N CA 2907 2909 72.17 139.10 -40.80

15 15911 182L 183K C N 2946 2948 82.19 -62.90 158.45 22.42 -62.90 158.45 22.42

15 183K 183K N CA 2948 2950 -104.49 -40.80 -40.80

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 90 150 1.370

serious non-bonded atom clash: 184 1089 1.484

serious non-bonded atom clash: 197 215 1.308

serious non-bonded atom clash: 331 399 1.491

serious non-bonded atom clash: 470 1846 1.455

serious non-bonded atom clash: 520 537 1.295

serious non-bonded atom clash: 752 1827 1.435

serious non-bonded atom clash: 803 2690 1.307

serious non-bonded atom clash: 818 1781 1.339

serious non-bonded atom clash: 875 1430 1.350

serious non-bonded atom clash: 937 1039 1.313

serious non-bonded atom clash: 981 1056 1.427

serious non-bonded atom clash: 1161 1251 1.415

serious non-bonded atom clash: 1264 1339 1.393

serious non-bonded atom clash: 1390 1443 1.474

serious non-bonded atom clash: 1486 2670 1.415

serious non-bonded atom clash: 1640 2571 1.396

serious non-bonded atom clash: 1660 1713 1.486

serious non-bonded atom clash: 1695 2483 1.320

serious non-bonded atom clash: 1763 2621 1.355

serious non-bonded atom clash: 1979 2016 1.491

serious non-bonded atom clash: 2175 2221 1.360

serious non-bonded atom clash: 2219 2491 1.481

serious non-bonded atom clash: 2295 2456 1.380

serious non-bonded atom clash: 2445 2546 1.464

serious non-bonded atom clash: 2485 2575 1.436

serious non-bonded atom clash: 2489 2566 1.398

serious non-bonded atom clash: 2497 2585 1.368

serious non-bonded atom clash: 2835 2866 1.424

serious non-bonded atom clash: 3094 3121 1.310

serious non-bonded atom clash: 3162 3174 1.302

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 481 248 260 361 476 637 636 724 733 835 969 1111 1179 1191 1220

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990005.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_486\_> OE1/2 will be swapped: 133.6730 10 10

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 133.6730

iupac\_m\_486\_> OE1/2 will be swapped: 176.9763 21 21

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 176.9763

iupac\_m\_486\_> OE1/2 will be swapped: 169.3451 35 35

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 169.3451

iupac\_m\_486\_> OE1/2 will be swapped: -167.2963 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -167.2963

iupac\_m\_487\_> NH1/2 swapped: 179.2603 52 52

iupac\_m\_487\_> NH1/2 swapped: -178.9391 55 55

iupac\_m\_487\_> NH1/2 swapped: 179.5946 56 56

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 106.6347 57 57

iupac\_m\_487\_> NH1/2 swapped: -179.9344 70 70

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 92.3530 77 77

iupac\_m\_487\_> NH1/2 swapped: -179.4039 94 94

iupac\_m\_485\_> OD1/2 will be swapped: 115.5856 102 102

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 115.5856

iupac\_m\_487\_> NH1/2 swapped: -175.9493 118 118

iupac\_m\_486\_> OE1/2 will be swapped: 97.0250 128 128

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 97.0250

iupac\_m\_487\_> NH1/2 swapped: 174.9628 139 139

iupac\_m\_485\_> OD1/2 will be swapped: 123.2866 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 123.2866

iupac\_m\_483\_> CD1/2 CE1/2 swapped: -94.0743 155 155

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 117.2391 156 156

iupac\_m\_486\_> OE1/2 will be swapped: -177.7591 165 165

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -177.7591

iupac\_m\_487\_> NH1/2 swapped: -179.2369 167 167

iupac\_m\_486\_> OE1/2 will be swapped: 99.2531 175 175

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 99.2531

iupac\_m\_487\_> NH1/2 swapped: 179.1544 185 185

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 116.9414 190 190

iupac\_m\_486\_> OE1/2 will be swapped: 177.7950 192 192

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 177.7950

iupac\_m\_486\_> OE1/2 will be swapped: 173.5251 193 193

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 173.5251

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.213366

Native energy (pair) : -235.486346

Native energy (surface) : -8.449234

Native energy (combined) : -9.827321

Z score (pair) : -7.823203

Z score (surface) : -6.548431

Z score (combined) : -9.058443

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1102578

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -21809.4609

<< end of ENERGY.

DOPE score : -21809.460938

>> Normalized DOPE z score: -0.324

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20389

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 71511.0938

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

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1 Bond length potential : 3255 36 36 0.205 0.205 62070. 1.000

2 Bond angle potential : 5881 282 345 10.071 10.071 7435.1 1.000

3 Stereochemical cosine torsion poten: 5645 0 56 27.481 27.481 674.69 1.000

4 Stereochemical improper torsion pot: 948 70 80 6.506 6.506 670.40 1.000

5 Soft-sphere overlap restraints : 20389 0 0 0.002 0.002 5.8589 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 1 0.352 0.352 130.94 1.000

10 Distance restraints 2 (N-O) : 3404 0 8 0.438 0.438 195.88 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 5 4.687 4.687 50.781 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 3 77.458 77.458 62.368 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 0 83.195 83.195 51.801 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 92.232 92.232 39.179 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 96.289 96.289 15.185 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.368 0.368 26.372 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 15 22 31.153 44.020 16.742 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 9 1.119 1.119 66.164 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990006

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990006

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 38532.2109

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 852 52R 52R NH1 HH11 843 844 2.57 1.00 1.57 61.51 1.00 1.57 61.51

2 853 52R 52R NH1 HH12 843 845 3.27 1.00 2.27 89.05 1.00 2.27 89.05

3 854 52R 52R NH2 HH21 846 847 3.27 1.00 2.27 89.00 1.00 2.27 89.00

4 855 52R 52R NH2 HH22 846 848 2.57 1.00 1.57 61.49 1.00 1.57 61.49

5 903 55R 55R NH1 HH11 894 895 3.27 1.00 2.27 88.92 1.00 2.27 88.92

6 904 55R 55R NH1 HH12 894 896 2.56 1.00 1.56 61.25 1.00 1.56 61.25

7 905 55R 55R NH2 HH21 897 898 2.56 1.00 1.56 61.20 1.00 1.56 61.20

8 906 55R 55R NH2 HH22 897 899 3.26 1.00 2.26 88.78 1.00 2.26 88.78

9 927 56R 56R NH1 HH11 918 919 2.57 1.00 1.57 61.74 1.00 1.57 61.74

10 928 56R 56R NH1 HH12 918 920 3.27 1.00 2.27 89.18 1.00 2.27 89.18

11 929 56R 56R NH2 HH21 921 922 3.27 1.00 2.27 89.03 1.00 2.27 89.03

12 930 56R 56R NH2 HH22 921 923 2.58 1.00 1.58 61.89 1.00 1.58 61.89

13 1150 70R 70R NH1 HH11 1137 1138 2.57 1.00 1.57 61.68 1.00 1.57 61.68

14 1151 70R 70R NH1 HH12 1137 1139 3.27 1.00 2.27 89.00 1.00 2.27 89.00

15 1152 70R 70R NH2 HH21 1140 1141 3.27 1.00 2.27 88.99 1.00 2.27 88.99

16 1153 70R 70R NH2 HH22 1140 1142 2.57 1.00 1.57 61.58 1.00 1.57 61.58

17 1533 94R 94R NH1 HH11 1516 1517 2.56 1.00 1.56 61.05 1.00 1.56 61.05

18 1534 94R 94R NH1 HH12 1516 1518 3.27 1.00 2.27 88.89 1.00 2.27 88.89

19 1535 94R 94R NH2 HH21 1519 1520 3.27 1.00 2.27 88.88 1.00 2.27 88.88

20 1536 94R 94R NH2 HH22 1519 1521 2.56 1.00 1.56 61.15 1.00 1.56 61.15

21 1928 118R 118R NH1 HH11 1908 1909 2.57 1.00 1.57 61.45 1.00 1.57 61.45

22 1929 118R 118R NH1 HH12 1908 1910 3.27 1.00 2.27 88.97 1.00 2.27 88.97

23 1930 118R 118R NH2 HH21 1911 1912 2.57 1.00 1.57 61.75 1.00 1.57 61.75

24 1931 118R 118R NH2 HH22 1911 1913 3.26 1.00 2.26 88.73 1.00 2.26 88.73

25 2263 139R 139R NH1 HH11 2240 2241 3.27 1.00 2.27 88.87 1.00 2.27 88.87

26 2264 139R 139R NH1 HH12 2240 2242 2.56 1.00 1.56 61.32 1.00 1.56 61.32

27 2265 139R 139R NH2 HH21 2243 2244 2.56 1.00 1.56 61.23 1.00 1.56 61.23

28 2266 139R 139R NH2 HH22 2243 2245 3.26 1.00 2.26 88.77 1.00 2.26 88.77

29 2739 167R 167R NH1 HH11 2711 2712 3.27 1.00 2.27 89.07 1.00 2.27 89.07

30 2740 167R 167R NH1 HH12 2711 2713 2.57 1.00 1.57 61.69 1.00 1.57 61.69

31 2741 167R 167R NH2 HH21 2714 2715 3.27 1.00 2.27 88.99 1.00 2.27 88.99

32 2742 167R 167R NH2 HH22 2714 2716 2.57 1.00 1.57 61.69 1.00 1.57 61.69

33 3029 185R 185R NH1 HH11 3000 3001 3.27 1.00 2.27 88.85 1.00 2.27 88.85

34 3030 185R 185R NH1 HH12 3000 3002 2.56 1.00 1.56 61.15 1.00 1.56 61.15

35 3031 185R 185R NH2 HH21 3003 3004 2.56 1.00 1.56 61.04 1.00 1.56 61.04

36 3032 185R 185R NH2 HH22 3003 3005 3.27 1.00 2.27 88.93 1.00 2.27 88.93

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15733 4S 5F C N 57 59 -72.51 -124.20 80.53 2.28 -63.20 126.20 16.90

1 5F 5F N CA 59 61 81.55 143.30 -44.30

2 15845 116S 117D C N 1878 1880 -81.27 -96.50 55.67 2.35 -63.30 102.24 11.64

2 117D 117D N CA 1880 1882 60.65 114.20 -40.00

3 15875 146H 147C C N 2379 2381 -84.25 -117.90 34.04 1.25 -63.00 174.00 22.75

3 147C 147C N CA 2381 2383 146.21 141.10 -41.10

4 15876 147C 148G C N 2390 2392 100.20 82.20 38.54 1.09 -62.40 163.35 29.76

4 148G 148G N CA 2392 2394 -25.58 8.50 -41.20

5 15881 152S 153L C N 2451 2453 27.99 -70.70 119.88 8.24 -63.50 146.76 25.87

5 153L 153L N CA 2453 2455 73.54 141.60 -41.20

6 15883 154V 155F C N 2486 2488 40.77 -71.40 133.05 7.48 -63.20 153.89 27.38

6 155F 155F N CA 2488 2490 69.16 140.70 -44.30

7 15884 155F 156F C N 2506 2508 -177.25 -124.20 73.91 1.97 -63.20 166.23 29.63

7 156F 156F N CA 2508 2510 -165.24 143.30 -44.30

8 15902 173N 174A C N 2802 2804 90.74 55.40 57.81 2.52 -62.50 156.83 31.29

8 174A 174A N CA 2804 2806 -7.55 38.20 -40.90

9 15904 175E 176M C N 2827 2829 92.58 -125.60 151.42 7.26 -125.60 151.42 7.26

9 176M 176M N CA 2829 2831 87.45 140.50 140.50

10 15905 176M 177C C N 2844 2846 -85.38 -63.00 81.00 8.65 -63.00 81.00 8.65

10 177C 177C N CA 2846 2848 36.75 -41.10 -41.10

11 15909 180L 181K C N 2905 2907 -75.92 -118.00 93.62 3.80 -62.90 97.15 11.96

11 181K 181K N CA 2907 2909 55.48 139.10 -40.80

12 15911 182L 183K C N 2946 2948 61.21 -62.90 124.87 21.00 -62.90 124.87 21.00

12 183K 183K N CA 2948 2950 -27.10 -40.80 -40.80

13 15913 184N 185R C N 2982 2984 -75.89 -125.20 58.41 3.07 -63.00 147.56 20.81

13 185R 185R N CA 2984 2986 171.90 140.60 -41.10

14 15914 185R 186K C N 3006 3008 83.40 -62.90 149.81 25.67 -62.90 149.81 25.67

14 186K 186K N CA 3008 3010 -8.59 -40.80 -40.80

15 15924 195W 196D C N 3195 3197 -53.86 -70.90 25.71 0.98 -63.30 171.30 21.73

15 196D 196D N CA 3197 3199 131.04 150.30 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 161 211 1.458

serious non-bonded atom clash: 320 767 1.471

serious non-bonded atom clash: 718 1825 1.339

serious non-bonded atom clash: 873 1428 1.352

serious non-bonded atom clash: 941 1448 1.422

serious non-bonded atom clash: 1018 1180 1.359

serious non-bonded atom clash: 1199 1274 1.429

serious non-bonded atom clash: 1303 2883 1.389

serious non-bonded atom clash: 1482 2741 1.307

serious non-bonded atom clash: 1658 1668 1.329

serious non-bonded atom clash: 1739 2152 1.361

serious non-bonded atom clash: 1748 2210 1.377

serious non-bonded atom clash: 1803 2098 1.467

serious non-bonded atom clash: 1809 2154 1.311

serious non-bonded atom clash: 1951 2041 1.444

serious non-bonded atom clash: 1979 2017 1.380

serious non-bonded atom clash: 2074 2127 1.482

serious non-bonded atom clash: 2211 2493 1.370

serious non-bonded atom clash: 2221 2493 1.411

serious non-bonded atom clash: 2293 2473 1.486

serious non-bonded atom clash: 2293 2477 1.480

serious non-bonded atom clash: 2303 2473 1.437

serious non-bonded atom clash: 2376 2404 1.318

serious non-bonded atom clash: 2459 2511 1.291

serious non-bonded atom clash: 2475 2575 1.446

serious non-bonded atom clash: 2485 2575 1.380

serious non-bonded atom clash: 2501 2594 1.309

serious non-bonded atom clash: 2834 2868 1.312

serious non-bonded atom clash: 3033 3096 1.374

serious non-bonded atom clash: 3036 3053 1.304

serious non-bonded atom clash: 3106 3117 1.406

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 457 216 231 347 501 607 678 708 758 895 956 1121 1078 1167 1309

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990006.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_485\_> OD1/2 will be swapped: -174.5594 36 36

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -174.5594

iupac\_m\_486\_> OE1/2 will be swapped: -179.4443 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -179.4443

iupac\_m\_487\_> NH1/2 swapped: 179.1282 52 52

iupac\_m\_486\_> OE1/2 will be swapped: 124.1204 87 87

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 124.1204

iupac\_m\_485\_> OD1/2 will be swapped: 117.6102 88 88

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 117.6102

iupac\_m\_487\_> NH1/2 swapped: -176.7416 94 94

iupac\_m\_486\_> OE1/2 will be swapped: -101.7166 105 105

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -101.7166

iupac\_m\_487\_> NH1/2 swapped: -178.6726 118 118

iupac\_m\_486\_> OE1/2 will be swapped: 121.0760 122 122

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 121.0760

iupac\_m\_486\_> OE1/2 will be swapped: -108.9578 123 123

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -108.9578

iupac\_m\_486\_> OE1/2 will be swapped: 179.8310 125 125

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 179.8310

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 101.2029 133 133

iupac\_m\_485\_> OD1/2 will be swapped: 178.2582 136 136

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 178.2582

iupac\_m\_487\_> NH1/2 swapped: -176.3640 145 145

iupac\_m\_485\_> OD1/2 will be swapped: 115.2444 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 115.2444

iupac\_m\_483\_> CD1/2 CE1/2 swapped: -94.9682 155 155

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 90.8063 178 178

iupac\_m\_486\_> OE1/2 will be swapped: -179.6620 192 192

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -179.6620

iupac\_m\_485\_> OD1/2 will be swapped: 174.6283 196 196

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 174.6283

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.136576

Native energy (pair) : -231.270460

Native energy (surface) : -9.712568

Native energy (combined) : -10.213902

Z score (pair) : -7.597687

Z score (surface) : -6.605371

Z score (combined) : -9.106425

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1114098

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -22030.8105

<< end of ENERGY.

DOPE score : -22030.810547

>> Normalized DOPE z score: -0.404

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 21045

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 33994.9414

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 3255 16 16 0.137 0.137 27589. 1.000

2 Bond angle potential : 5881 241 300 7.917 7.917 4617.7 1.000

3 Stereochemical cosine torsion poten: 5645 0 50 26.164 26.164 622.57 1.000

4 Stereochemical improper torsion pot: 948 62 76 6.206 6.206 611.17 1.000

5 Soft-sphere overlap restraints : 21045 0 0 0.001 0.001 3.0644 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 0 0.312 0.312 106.78 1.000

10 Distance restraints 2 (N-O) : 3404 0 3 0.377 0.377 149.23 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 5 4.097 4.097 38.800 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 3 80.171 80.171 56.506 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 0 86.813 86.813 63.209 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 89.809 89.809 37.806 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 104.228 104.228 15.468 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.457 0.457 34.916 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 17 20 28.721 46.425 -4.9705 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 0 1.266 1.266 53.833 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990007

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990007

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 33106.8125

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

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Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 852 52R 52R NH1 HH11 843 844 3.27 1.00 2.27 89.09 1.00 2.27 89.09

2 853 52R 52R NH1 HH12 843 845 2.57 1.00 1.57 61.68 1.00 1.57 61.68

3 854 52R 52R NH2 HH21 846 847 3.27 1.00 2.27 89.07 1.00 2.27 89.07

4 855 52R 52R NH2 HH22 846 848 2.57 1.00 1.57 61.69 1.00 1.57 61.69

5 1533 94R 94R NH1 HH11 1516 1517 3.27 1.00 2.27 88.97 1.00 2.27 88.97

6 1534 94R 94R NH1 HH12 1516 1518 2.57 1.00 1.57 61.48 1.00 1.57 61.48

7 1535 94R 94R NH2 HH21 1519 1520 3.27 1.00 2.27 88.98 1.00 2.27 88.98

8 1536 94R 94R NH2 HH22 1519 1521 2.57 1.00 1.57 61.42 1.00 1.57 61.42

9 1928 118R 118R NH1 HH11 1908 1909 3.27 1.00 2.27 88.96 1.00 2.27 88.96

10 1929 118R 118R NH1 HH12 1908 1910 2.57 1.00 1.57 61.56 1.00 1.57 61.56

11 1930 118R 118R NH2 HH21 1911 1912 3.27 1.00 2.27 88.98 1.00 2.27 88.98

12 1931 118R 118R NH2 HH22 1911 1913 2.57 1.00 1.57 61.57 1.00 1.57 61.57

13 2380 145R 145R NH1 HH11 2356 2357 2.56 1.00 1.56 61.02 1.00 1.56 61.02

14 2381 145R 145R NH1 HH12 2356 2358 3.26 1.00 2.26 88.75 1.00 2.26 88.75

15 2382 145R 145R NH2 HH21 2359 2360 2.55 1.00 1.55 60.97 1.00 1.55 60.97

16 2383 145R 145R NH2 HH22 2359 2361 3.26 1.00 2.26 88.78 1.00 2.26 88.78

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Feature 2 : Bond angle potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 7699 152S 152S N CA 2442 2444 126.72 107.00 19.72 5.67 107.00 19.72 5.67

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Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15731 2D 3V C N 30 32 -93.43 -125.40 65.66 2.29 -62.40 132.04 15.16

1 3V 3V N CA 32 34 85.95 143.30 -42.40

2 15733 4S 5F C N 57 59 -78.47 -124.20 79.83 2.41 -63.20 123.13 16.09

2 5F 5F N CA 59 61 77.88 143.30 -44.30

3 15734 5F 6R C N 77 79 -98.10 -63.00 91.17 10.49 -63.00 91.17 10.49

3 6R 6R N CA 79 81 43.04 -41.10 -41.10

4 15796 67A 68N C N 1091 1093 -76.02 -119.90 47.11 1.54 -63.20 161.45 19.51

4 68N 68N N CA 1093 1095 119.85 137.00 -41.10

5 15797 68N 69N C N 1105 1107 59.10 55.90 5.09 0.27 -63.20 144.32 23.73

5 69N 69N N CA 1107 1109 35.54 39.50 -41.10

6 15845 116S 117D C N 1878 1880 -81.80 -96.50 24.32 1.02 -63.30 136.08 15.76

6 117D 117D N CA 1880 1882 94.82 114.20 -40.00

7 15881 152S 153L C N 2451 2453 -67.48 -70.70 64.86 5.04 -63.50 112.49 15.85

7 153L 153L N CA 2453 2455 -153.62 141.60 -41.20

8 15883 154V 155F C N 2486 2488 73.18 -63.20 137.18 22.94 -63.20 137.18 22.94

8 155F 155F N CA 2488 2490 -29.41 -44.30 -44.30

9 15884 155F 156F C N 2506 2508 -70.41 -124.20 57.96 2.85 -63.20 150.98 21.45

9 156F 156F N CA 2508 2510 164.90 143.30 -44.30

10 15902 173N 174A C N 2802 2804 88.82 55.40 56.21 2.38 -62.50 155.07 30.97

10 174A 174A N CA 2804 2806 -7.00 38.20 -40.90

11 15904 175E 176M C N 2827 2829 94.02 -125.60 148.20 7.01 -125.60 148.20 7.01

11 176M 176M N CA 2829 2831 93.00 140.50 140.50

12 15905 176M 177C C N 2844 2846 -94.63 -63.00 82.27 8.56 -63.00 82.27 8.56

12 177C 177C N CA 2846 2848 34.85 -41.10 -41.10

13 15909 180L 181K C N 2905 2907 -80.31 -118.00 78.16 3.12 -62.90 112.78 13.79

13 181K 181K N CA 2907 2909 70.63 139.10 -40.80

14 15911 182L 183K C N 2946 2948 115.53 -118.00 146.70 4.87 -62.90 -152.58 27.86

14 183K 183K N CA 2948 2950 -146.57 139.10 -40.80

15 15912 183K 184N C N 2968 2970 -116.09 -119.90 19.24 0.78 -63.20 167.80 18.59

15 184N 184N N CA 2970 2972 118.14 137.00 -41.10

16 15923 194I 195W C N 3171 3173 -59.74 -71.30 11.56 0.83 58.80 159.16 6.89

16 195W 195W N CA 3173 3175 139.21 139.00 33.00

17 15924 195W 196D C N 3195 3197 -69.15 -70.90 10.07 0.58 -63.30 159.90 20.09

17 196D 196D N CA 3197 3199 160.21 150.30 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 43 2953 1.309

serious non-bonded atom clash: 121 135 1.462

serious non-bonded atom clash: 487 505 1.301

serious non-bonded atom clash: 518 536 1.312

serious non-bonded atom clash: 727 788 1.396

serious non-bonded atom clash: 751 2682 1.305

serious non-bonded atom clash: 820 1711 1.414

serious non-bonded atom clash: 883 1553 1.307

serious non-bonded atom clash: 887 895 1.317

serious non-bonded atom clash: 1142 2893 1.324

serious non-bonded atom clash: 1262 1338 1.348

serious non-bonded atom clash: 1304 1323 1.482

serious non-bonded atom clash: 1484 2687 1.317

serious non-bonded atom clash: 1538 2614 1.337

serious non-bonded atom clash: 1690 1743 1.382

serious non-bonded atom clash: 1695 2481 1.346

serious non-bonded atom clash: 1739 2152 1.376

serious non-bonded atom clash: 1744 2216 1.371

serious non-bonded atom clash: 1766 2568 1.353

serious non-bonded atom clash: 1810 2154 1.306

serious non-bonded atom clash: 2150 2176 1.418

serious non-bonded atom clash: 2152 2217 1.426

serious non-bonded atom clash: 2273 2483 1.307

serious non-bonded atom clash: 2278 2483 1.495

serious non-bonded atom clash: 2296 2459 1.305

serious non-bonded atom clash: 2299 2517 1.435

serious non-bonded atom clash: 2376 2465 1.441

serious non-bonded atom clash: 2458 2473 1.445

serious non-bonded atom clash: 2835 2866 1.305

serious non-bonded atom clash: 2925 2951 1.372

serious non-bonded atom clash: 3041 3091 1.490

serious non-bonded atom clash: 3161 3174 1.340

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 504 237 244 331 494 672 671 766 782 891 941 1135 1164 1236 1327

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990007.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_487\_> NH1/2 swapped: 179.2169 6 6

iupac\_m\_486\_> OE1/2 will be swapped: -170.0822 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -170.0822

iupac\_m\_487\_> NH1/2 swapped: 177.7681 52 52

iupac\_m\_487\_> NH1/2 swapped: -176.1970 55 55

iupac\_m\_485\_> OD1/2 will be swapped: 177.8199 58 58

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 177.8199

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 95.6772 77 77

iupac\_m\_486\_> OE1/2 will be swapped: 120.4085 87 87

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 120.4085

iupac\_m\_485\_> OD1/2 will be swapped: 121.5043 88 88

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 121.5043

iupac\_m\_487\_> NH1/2 swapped: 179.4841 94 94

iupac\_m\_486\_> OE1/2 will be swapped: -130.3584 105 105

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -130.3584

iupac\_m\_485\_> OD1/2 will be swapped: 124.1835 117 117

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 124.1835

iupac\_m\_487\_> NH1/2 swapped: -176.9500 118 118

iupac\_m\_486\_> OE1/2 will be swapped: -122.2205 123 123

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -122.2205

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 105.0221 133 133

iupac\_m\_485\_> OD1/2 will be swapped: -176.7973 136 136

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -176.7973

iupac\_m\_487\_> NH1/2 swapped: 179.7309 139 139

iupac\_m\_485\_> OD1/2 will be swapped: 165.1245 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 165.1245

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 102.6821 178 178

iupac\_m\_487\_> NH1/2 swapped: 175.2330 185 185

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.206865

Native energy (pair) : -233.016540

Native energy (surface) : -11.481187

Native energy (combined) : -10.619193

Z score (pair) : -7.546846

Z score (surface) : -6.993210

Z score (combined) : -9.168443

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1104821

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -21913.7148

<< end of ENERGY.

DOPE score : -21913.714844

>> Normalized DOPE z score: -0.362

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20720

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 56479.4570

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 3255 28 28 0.181 0.181 48377. 1.000

2 Bond angle potential : 5881 257 325 9.228 9.228 6261.2 1.000

3 Stereochemical cosine torsion poten: 5645 0 47 26.225 26.225 631.02 1.000

4 Stereochemical improper torsion pot: 948 63 76 6.250 6.250 618.46 1.000

5 Soft-sphere overlap restraints : 20720 0 0 0.001 0.001 4.2874 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 0 0.306 0.306 105.96 1.000

10 Distance restraints 2 (N-O) : 3404 0 5 0.395 0.395 170.54 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 4 4.657 4.657 50.135 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 5 78.486 78.486 57.368 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 2 82.330 82.330 56.347 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 92.833 92.833 39.163 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 91.704 91.704 14.320 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.385 0.385 27.538 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 17 22 30.975 45.632 9.3100 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 2 1.283 1.283 57.089 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990008

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990008

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 35398.0000

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 2.57 1.00 1.57 61.49 1.00 1.57 61.49

2 100 6R 6R NH1 HH12 95 97 3.27 1.00 2.27 89.11 1.00 2.27 89.11

3 101 6R 6R NH2 HH21 98 99 3.27 1.00 2.27 89.02 1.00 2.27 89.02

4 102 6R 6R NH2 HH22 98 100 2.57 1.00 1.57 61.59 1.00 1.57 61.59

5 852 52R 52R NH1 HH11 843 844 3.27 1.00 2.27 88.95 1.00 2.27 88.95

6 853 52R 52R NH1 HH12 843 845 2.56 1.00 1.56 61.32 1.00 1.56 61.32

7 854 52R 52R NH2 HH21 846 847 3.27 1.00 2.27 88.93 1.00 2.27 88.93

8 855 52R 52R NH2 HH22 846 848 2.57 1.00 1.57 61.37 1.00 1.57 61.37

9 903 55R 55R NH1 HH11 894 895 2.57 1.00 1.57 61.69 1.00 1.57 61.69

10 904 55R 55R NH1 HH12 894 896 3.27 1.00 2.27 89.04 1.00 2.27 89.04

11 905 55R 55R NH2 HH21 897 898 3.27 1.00 2.27 89.05 1.00 2.27 89.05

12 906 55R 55R NH2 HH22 897 899 2.57 1.00 1.57 61.52 1.00 1.57 61.52

13 1533 94R 94R NH1 HH11 1516 1517 3.27 1.00 2.27 88.97 1.00 2.27 88.97

14 1534 94R 94R NH1 HH12 1516 1518 2.57 1.00 1.57 61.37 1.00 1.57 61.37

15 1535 94R 94R NH2 HH21 1519 1520 2.57 1.00 1.57 61.49 1.00 1.57 61.49

16 1536 94R 94R NH2 HH22 1519 1521 3.27 1.00 2.27 88.98 1.00 2.27 88.98

17 1928 118R 118R NH1 HH11 1908 1909 3.27 1.00 2.27 89.01 1.00 2.27 89.01

18 1929 118R 118R NH1 HH12 1908 1910 2.58 1.00 1.58 61.76 1.00 1.58 61.76

19 1930 118R 118R NH2 HH21 1911 1912 2.57 1.00 1.57 61.73 1.00 1.57 61.73

20 1931 118R 118R NH2 HH22 1911 1913 3.27 1.00 2.27 89.06 1.00 2.27 89.06

21 2263 139R 139R NH1 HH11 2240 2241 3.27 1.00 2.27 89.07 1.00 2.27 89.07

22 2264 139R 139R NH1 HH12 2240 2242 2.57 1.00 1.57 61.69 1.00 1.57 61.69

23 2265 139R 139R NH2 HH21 2243 2244 2.57 1.00 1.57 61.71 1.00 1.57 61.71

24 2266 139R 139R NH2 HH22 2243 2245 3.27 1.00 2.27 89.06 1.00 2.27 89.06

25 3029 185R 185R NH1 HH11 3000 3001 3.27 1.00 2.27 88.92 1.00 2.27 88.92

26 3030 185R 185R NH1 HH12 3000 3002 2.57 1.00 1.57 61.38 1.00 1.57 61.38

27 3031 185R 185R NH2 HH21 3003 3004 3.27 1.00 2.27 88.94 1.00 2.27 88.94

28 3032 185R 185R NH2 HH22 3003 3005 2.57 1.00 1.57 61.37 1.00 1.57 61.37

-------------------------------------------------------------------------------------------------

Feature 2 : Bond angle potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 4569 44C 44C N CA 710 712 123.03 107.00 16.03 4.61 107.00 16.03 4.61

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15731 2D 3V C N 30 32 -126.75 -125.40 31.39 1.59 -62.40 167.21 18.45

1 3V 3V N CA 32 34 111.94 143.30 -42.40

2 15733 4S 5F C N 57 59 -84.35 -124.20 87.81 2.98 -63.20 111.39 14.11

2 5F 5F N CA 59 61 65.06 143.30 -44.30

3 15785 56R 57Y C N 924 926 -102.27 -98.40 86.49 9.17 -63.50 93.79 13.21

3 57Y 57Y N CA 926 928 42.00 128.40 -43.40

4 15845 116S 117D C N 1878 1880 -75.99 -96.50 34.64 1.45 -63.30 126.91 14.94

4 117D 117D N CA 1880 1882 86.28 114.20 -40.00

5 15880 151M 152S C N 2440 2442 -172.02 -136.60 100.48 4.23 -64.10 134.20 17.29

5 152S 152S N CA 2442 2444 -114.78 151.20 -35.00

6 15881 152S 153L C N 2451 2453 65.64 -63.50 151.76 21.33 -63.50 151.76 21.33

6 153L 153L N CA 2453 2455 -120.92 -41.20 -41.20

7 15883 154V 155F C N 2486 2488 -43.18 -71.40 50.42 3.14 -63.20 144.61 21.43

7 155F 155F N CA 2488 2490 98.92 140.70 -44.30

8 15884 155F 156F C N 2506 2508 -133.98 -124.20 81.48 3.59 -63.20 115.69 20.31

8 156F 156F N CA 2508 2510 -135.81 143.30 -44.30

9 15902 173N 174A C N 2802 2804 86.90 55.40 55.50 2.25 -62.50 153.09 30.57

9 174A 174A N CA 2804 2806 -7.50 38.20 -40.90

10 15904 175E 176M C N 2827 2829 95.36 -125.60 144.51 6.68 -125.60 144.51 6.68

10 176M 176M N CA 2829 2831 101.12 140.50 140.50

11 15905 176M 177C C N 2844 2846 -94.23 -63.00 83.69 8.72 -63.00 83.69 8.72

11 177C 177C N CA 2846 2848 36.55 -41.10 -41.10

12 15909 180L 181K C N 2905 2907 -72.22 -118.00 85.19 3.30 -62.90 108.46 13.60

12 181K 181K N CA 2907 2909 67.26 139.10 -40.80

13 15911 182L 183K C N 2946 2948 74.63 -62.90 137.64 22.79 -62.90 137.64 22.79

13 183K 183K N CA 2948 2950 -35.30 -40.80 -40.80

14 15916 187L 188P C N 3047 3049 -67.79 -64.50 9.11 0.54 -58.70 174.05 15.13

14 188P 188P N CA 3049 3050 155.69 147.20 -30.50

15 15917 188P 189K C N 3061 3063 72.67 -62.90 135.83 22.60 -62.90 135.83 22.60

15 189K 189K N CA 3063 3065 -32.39 -40.80 -40.80

16 15923 194I 195W C N 3171 3173 -102.79 -124.90 24.72 1.34 58.80 -157.85 10.06

16 195W 195W N CA 3173 3175 154.46 143.40 33.00

17 15924 195W 196D C N 3195 3197 -88.03 -96.50 11.48 0.47 -63.30 163.83 18.85

17 196D 196D N CA 3197 3199 121.96 114.20 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 430 438 1.380

serious non-bonded atom clash: 524 537 1.466

serious non-bonded atom clash: 813 1715 1.407

serious non-bonded atom clash: 819 2687 1.492

serious non-bonded atom clash: 941 1018 1.306

serious non-bonded atom clash: 1076 1256 1.357

serious non-bonded atom clash: 1480 2623 1.424

serious non-bonded atom clash: 1695 2477 1.490

serious non-bonded atom clash: 1739 2152 1.295

serious non-bonded atom clash: 1762 2499 1.308

serious non-bonded atom clash: 1802 2099 1.311

serious non-bonded atom clash: 1809 2154 1.391

serious non-bonded atom clash: 1855 2039 1.468

serious non-bonded atom clash: 1951 1989 1.309

serious non-bonded atom clash: 1979 2012 1.487

serious non-bonded atom clash: 2230 2521 1.316

serious non-bonded atom clash: 2304 2459 1.371

serious non-bonded atom clash: 2348 2369 1.304

serious non-bonded atom clash: 2352 2467 1.406

serious non-bonded atom clash: 2450 2454 1.311

serious non-bonded atom clash: 2493 2563 1.298

serious non-bonded atom clash: 2744 2778 1.414

serious non-bonded atom clash: 2835 2868 1.310

serious non-bonded atom clash: 2945 2993 1.307

serious non-bonded atom clash: 3036 3053 1.456

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 492 244 228 358 504 622 695 726 778 860 926 1159 1169 1276 1282

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990008.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_485\_> OD1/2 will be swapped: 175.9668 2 2

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 175.9668

iupac\_m\_487\_> NH1/2 swapped: 179.7093 6 6

iupac\_m\_486\_> OE1/2 will be swapped: -179.1846 10 10

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -179.1846

iupac\_m\_486\_> OE1/2 will be swapped: 118.5168 21 21

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 118.5168

iupac\_m\_486\_> OE1/2 will be swapped: 113.5519 35 35

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 113.5519

iupac\_m\_486\_> OE1/2 will be swapped: -123.2462 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -123.2462

iupac\_m\_487\_> NH1/2 swapped: 179.6625 52 52

iupac\_m\_487\_> NH1/2 swapped: 179.5771 55 55

iupac\_m\_487\_> NH1/2 swapped: 177.7357 56 56

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 112.0275 57 57

iupac\_m\_487\_> NH1/2 swapped: 179.2372 70 70

iupac\_m\_485\_> OD1/2 will be swapped: 119.2104 75 75

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 119.2104

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 102.4264 77 77

iupac\_m\_486\_> OE1/2 will be swapped: 179.3645 87 87

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 179.3645

iupac\_m\_485\_> OD1/2 will be swapped: 178.7321 88 88

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 178.7321

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 98.0424 92 92

iupac\_m\_487\_> NH1/2 swapped: -179.4026 94 94

iupac\_m\_487\_> NH1/2 swapped: 179.6823 118 118

iupac\_m\_486\_> OE1/2 will be swapped: 179.0911 122 122

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 179.0911

iupac\_m\_486\_> OE1/2 will be swapped: 126.5501 125 125

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 126.5501

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 90.8585 133 133

iupac\_m\_485\_> OD1/2 will be swapped: -118.3449 136 136

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -118.3449

iupac\_m\_487\_> NH1/2 swapped: 179.3245 139 139

iupac\_m\_487\_> NH1/2 swapped: 179.8629 145 145

iupac\_m\_485\_> OD1/2 will be swapped: -179.8357 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -179.8357

iupac\_m\_486\_> OE1/2 will be swapped: -122.8490 175 175

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -122.8490

iupac\_m\_487\_> NH1/2 swapped: 178.3304 185 185

iupac\_m\_486\_> OE1/2 will be swapped: -117.5139 193 193

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -117.5139

iupac\_m\_485\_> OD1/2 will be swapped: -171.6809 196 196

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -171.6809

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.150506

Native energy (pair) : -231.916953

Native energy (surface) : -10.261117

Native energy (combined) : -10.374681

Z score (pair) : -7.921496

Z score (surface) : -6.785622

Z score (combined) : -9.357684

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1100074

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -21906.2949

<< end of ENERGY.

DOPE score : -21906.294922

>> Normalized DOPE z score: -0.359

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20735

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 78566.2188

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 3255 40 40 0.216 0.216 68995. 1.000

2 Bond angle potential : 5881 258 323 10.262 10.262 7740.1 1.000

3 Stereochemical cosine torsion poten: 5645 0 56 26.016 26.016 610.93 1.000

4 Stereochemical improper torsion pot: 948 63 70 6.066 6.066 583.67 1.000

5 Soft-sphere overlap restraints : 20735 0 0 0.002 0.002 9.9993 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 0 0.344 0.344 124.86 1.000

10 Distance restraints 2 (N-O) : 3404 0 4 0.421 0.421 182.70 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 0 4 4.383 4.383 44.401 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 4 78.573 78.573 64.229 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 2 81.459 81.459 51.299 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 99.388 99.388 38.839 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 93.881 93.881 14.177 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.397 0.397 34.024 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 17 22 30.693 43.478 21.326 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 1 1.010 1.010 50.363 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990009

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990009

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 38220.8047

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 3.27 1.00 2.27 89.00 1.00 2.27 89.00

2 100 6R 6R NH1 HH12 95 97 2.57 1.00 1.57 61.59 1.00 1.57 61.59

3 101 6R 6R NH2 HH21 98 99 3.27 1.00 2.27 88.96 1.00 2.27 88.96

4 102 6R 6R NH2 HH22 98 100 2.57 1.00 1.57 61.58 1.00 1.57 61.58

5 852 52R 52R NH1 HH11 843 844 3.27 1.00 2.27 89.03 1.00 2.27 89.03

6 853 52R 52R NH1 HH12 843 845 2.57 1.00 1.57 61.56 1.00 1.57 61.56

7 854 52R 52R NH2 HH21 846 847 3.27 1.00 2.27 89.05 1.00 2.27 89.05

8 855 52R 52R NH2 HH22 846 848 2.57 1.00 1.57 61.57 1.00 1.57 61.57

9 903 55R 55R NH1 HH11 894 895 2.57 1.00 1.57 61.38 1.00 1.57 61.38

10 904 55R 55R NH1 HH12 894 896 3.27 1.00 2.27 88.89 1.00 2.27 88.89

11 905 55R 55R NH2 HH21 897 898 3.27 1.00 2.27 88.92 1.00 2.27 88.92

12 906 55R 55R NH2 HH22 897 899 2.56 1.00 1.56 61.21 1.00 1.56 61.21

13 927 56R 56R NH1 HH11 918 919 3.27 1.00 2.27 89.01 1.00 2.27 89.01

14 928 56R 56R NH1 HH12 918 920 2.57 1.00 1.57 61.48 1.00 1.57 61.48

15 929 56R 56R NH2 HH21 921 922 2.57 1.00 1.57 61.60 1.00 1.57 61.60

16 930 56R 56R NH2 HH22 921 923 3.27 1.00 2.27 89.00 1.00 2.27 89.00

17 1150 70R 70R NH1 HH11 1137 1138 2.57 1.00 1.57 61.52 1.00 1.57 61.52

18 1151 70R 70R NH1 HH12 1137 1139 3.27 1.00 2.27 88.98 1.00 2.27 88.98

19 1152 70R 70R NH2 HH21 1140 1141 2.57 1.00 1.57 61.55 1.00 1.57 61.55

20 1153 70R 70R NH2 HH22 1140 1142 3.27 1.00 2.27 88.97 1.00 2.27 88.97

21 1533 94R 94R NH1 HH11 1516 1517 3.27 1.00 2.27 88.98 1.00 2.27 88.98

22 1534 94R 94R NH1 HH12 1516 1518 2.57 1.00 1.57 61.49 1.00 1.57 61.49

23 1535 94R 94R NH2 HH21 1519 1520 2.57 1.00 1.57 61.56 1.00 1.57 61.56

24 1536 94R 94R NH2 HH22 1519 1521 3.27 1.00 2.27 88.97 1.00 2.27 88.97

25 1928 118R 118R NH1 HH11 1908 1909 3.27 1.00 2.27 89.01 1.00 2.27 89.01

26 1929 118R 118R NH1 HH12 1908 1910 2.57 1.00 1.57 61.59 1.00 1.57 61.59

27 1930 118R 118R NH2 HH21 1911 1912 2.57 1.00 1.57 61.50 1.00 1.57 61.50

28 1931 118R 118R NH2 HH22 1911 1913 3.27 1.00 2.27 89.09 1.00 2.27 89.09

29 2263 139R 139R NH1 HH11 2240 2241 3.27 1.00 2.27 88.87 1.00 2.27 88.87

30 2264 139R 139R NH1 HH12 2240 2242 2.56 1.00 1.56 61.03 1.00 1.56 61.03

31 2265 139R 139R NH2 HH21 2243 2244 2.56 1.00 1.56 61.05 1.00 1.56 61.05

32 2266 139R 139R NH2 HH22 2243 2245 3.27 1.00 2.27 88.85 1.00 2.27 88.85

33 2380 145R 145R NH1 HH11 2356 2357 3.27 1.00 2.27 89.00 1.00 2.27 89.00

34 2381 145R 145R NH1 HH12 2356 2358 2.57 1.00 1.57 61.47 1.00 1.57 61.47

35 2382 145R 145R NH2 HH21 2359 2360 3.27 1.00 2.27 89.00 1.00 2.27 89.00

36 2383 145R 145R NH2 HH22 2359 2361 2.57 1.00 1.57 61.55 1.00 1.57 61.55

37 3029 185R 185R NH1 HH11 3000 3001 3.27 1.00 2.27 88.90 1.00 2.27 88.90

38 3030 185R 185R NH1 HH12 3000 3002 2.56 1.00 1.56 61.15 1.00 1.56 61.15

39 3031 185R 185R NH2 HH21 3003 3004 2.56 1.00 1.56 61.27 1.00 1.56 61.27

40 3032 185R 185R NH2 HH22 3003 3005 3.27 1.00 2.27 88.88 1.00 2.27 88.88

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Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15731 2D 3V C N 30 32 -99.28 -125.40 83.08 3.38 -62.40 113.02 12.63

1 3V 3V N CA 32 34 64.43 143.30 -42.40

2 15733 4S 5F C N 57 59 -84.85 -124.20 77.03 2.47 -63.20 123.30 15.72

2 5F 5F N CA 59 61 77.09 143.30 -44.30

3 15797 68N 69N C N 1105 1107 -133.26 -119.90 86.06 4.20 -63.20 116.50 12.61

3 69N 69N N CA 1107 1109 51.98 137.00 -41.10

4 15845 116S 117D C N 1878 1880 -82.48 -96.50 18.24 0.76 -63.30 143.82 16.68

4 117D 117D N CA 1880 1882 102.54 114.20 -40.00

5 15881 152S 153L C N 2451 2453 30.80 -70.70 120.68 8.43 -63.50 150.68 26.58

5 153L 153L N CA 2453 2455 76.32 141.60 -41.20

6 15882 153L 154V C N 2470 2472 -48.00 -62.40 39.29 4.35 -125.40 158.00 9.06

6 154V 154V N CA 2472 2474 -78.96 -42.40 143.30

7 15883 154V 155F C N 2486 2488 -97.02 -63.20 76.79 8.83 -63.20 76.79 8.83

7 155F 155F N CA 2488 2490 24.64 -44.30 -44.30

8 15884 155F 156F C N 2506 2508 -84.97 -63.20 91.73 14.20 -63.20 91.73 14.20

8 156F 156F N CA 2508 2510 -133.41 -44.30 -44.30

9 15902 173N 174A C N 2802 2804 88.81 55.40 54.56 2.39 -62.50 155.52 31.11

9 174A 174A N CA 2804 2806 -4.94 38.20 -40.90

10 15904 175E 176M C N 2827 2829 87.68 -125.60 152.17 7.00 -125.60 152.17 7.00

10 176M 176M N CA 2829 2831 100.15 140.50 140.50

11 15905 176M 177C C N 2844 2846 -90.36 -63.00 89.64 9.49 -63.00 89.64 9.49

11 177C 177C N CA 2846 2848 44.26 -41.10 -41.10

12 15909 180L 181K C N 2905 2907 -71.09 -118.00 75.84 2.81 -62.90 120.60 15.23

12 181K 181K N CA 2907 2909 79.52 139.10 -40.80

13 15911 182L 183K C N 2946 2948 57.54 -62.90 124.33 18.79 -62.90 124.33 18.79

13 183K 183K N CA 2948 2950 -71.66 -40.80 -40.80

14 15913 184N 185R C N 2982 2984 -59.96 -125.20 73.20 3.73 -63.00 145.15 19.41

14 185R 185R N CA 2984 2986 173.78 140.60 -41.10

15 15914 185R 186K C N 3006 3008 81.32 -62.90 144.48 23.28 -62.90 144.48 23.28

15 186K 186K N CA 3008 3010 -49.50 -40.80 -40.80

16 15923 194I 195W C N 3171 3173 -53.46 -71.30 20.41 1.22 58.80 147.77 6.65

16 195W 195W N CA 3173 3175 129.09 139.00 33.00

17 15924 195W 196D C N 3195 3197 -78.08 -70.90 7.19 0.53 -63.30 169.90 21.89

17 196D 196D N CA 3197 3199 150.75 150.30 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 10 21 1.481

serious non-bonded atom clash: 70 135 1.499

serious non-bonded atom clash: 121 136 1.410

serious non-bonded atom clash: 125 2922 1.462

serious non-bonded atom clash: 184 1089 1.377

serious non-bonded atom clash: 319 765 1.432

serious non-bonded atom clash: 372 1729 1.400

serious non-bonded atom clash: 426 1864 1.329

serious non-bonded atom clash: 452 2086 1.461

serious non-bonded atom clash: 766 1778 1.345

serious non-bonded atom clash: 813 1715 1.310

serious non-bonded atom clash: 823 2686 1.398

serious non-bonded atom clash: 857 1039 1.307

serious non-bonded atom clash: 937 1029 1.303

serious non-bonded atom clash: 987 1060 1.491

serious non-bonded atom clash: 1169 2944 1.390

serious non-bonded atom clash: 1171 1241 1.319

serious non-bonded atom clash: 1174 2944 1.499

serious non-bonded atom clash: 1262 1339 1.366

serious non-bonded atom clash: 1426 1480 1.470

serious non-bonded atom clash: 1595 1636 1.310

serious non-bonded atom clash: 1637 2571 1.312

serious non-bonded atom clash: 1741 2152 1.471

serious non-bonded atom clash: 1748 2216 1.479

serious non-bonded atom clash: 1805 2640 1.371

serious non-bonded atom clash: 1951 1989 1.479

serious non-bonded atom clash: 1952 2042 1.310

serious non-bonded atom clash: 2215 2494 1.294

serious non-bonded atom clash: 2217 2489 1.333

serious non-bonded atom clash: 2296 2484 1.426

serious non-bonded atom clash: 2302 2473 1.419

serious non-bonded atom clash: 2369 2400 1.303

serious non-bonded atom clash: 2458 2514 1.418

serious non-bonded atom clash: 2459 2539 1.308

serious non-bonded atom clash: 2465 2519 1.456

serious non-bonded atom clash: 2493 2566 1.459

serious non-bonded atom clash: 2505 2639 1.493

serious non-bonded atom clash: 2728 2749 1.310

serious non-bonded atom clash: 2776 2786 1.308

serious non-bonded atom clash: 2956 2971 1.355

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 495 230 253 381 446 637 639 746 780 893 984 1169 1115 1205 1320

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990009.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

openf\_\_\_224\_> Open USP\_receptor\_Luc.ini

Dynamically allocated memory at amaxmodel [B,KiB,MiB]: 20360797 19883.590 19.418

read\_mo\_297\_> Segments, residues, atoms: 1 197 3225

read\_mo\_298\_> Segment: 1 1 197 3225

randomi\_498\_> Atoms,selected atoms,random\_seed,amplitude: 3225 3225 1 4.0000

randomi\_496\_> Amplitude is > 0; randomization is done.

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 18782

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 19959

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 20754

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 21632

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22229

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 22595

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 23219

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24053

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 24998

pick\_re\_612\_> Number of MODEL atoms, selected restraints; 3225 25352

iupac\_m\_485\_> OD1/2 will be swapped: 163.8641 2 2

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 163.8641

iupac\_m\_487\_> NH1/2 swapped: 178.9944 6 6

iupac\_m\_486\_> OE1/2 will be swapped: 179.8082 21 21

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 179.8082

iupac\_m\_486\_> OE1/2 will be swapped: -117.9738 47 47

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -117.9738

iupac\_m\_487\_> NH1/2 swapped: -177.6437 52 52

iupac\_m\_485\_> OD1/2 will be swapped: -176.4254 58 58

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -176.4254

iupac\_m\_485\_> OD1/2 will be swapped: -112.9130 62 62

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -112.9130

iupac\_m\_487\_> NH1/2 swapped: 176.5496 74 74

iupac\_m\_485\_> OD1/2 will be swapped: 120.9324 75 75

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 120.9324

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 97.4683 77 77

iupac\_m\_485\_> OD1/2 will be swapped: -175.6575 84 84

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -175.6575

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 109.5182 92 92

iupac\_m\_487\_> NH1/2 swapped: 179.6063 94 94

iupac\_m\_486\_> OE1/2 will be swapped: -176.6585 105 105

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -176.6585

iupac\_m\_487\_> NH1/2 swapped: 176.3384 118 118

iupac\_m\_486\_> OE1/2 will be swapped: 174.6876 125 125

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 174.6876

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 96.4582 134 134

iupac\_m\_485\_> OD1/2 will be swapped: 119.7675 136 136

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 119.7675

iupac\_m\_487\_> NH1/2 swapped: -178.7466 145 145

iupac\_m\_485\_> OD1/2 will be swapped: 166.4994 149 149

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 166.4994

iupac\_m\_487\_> NH1/2 swapped: -177.0613 167 167

iupac\_m\_483\_> CD1/2 CE1/2 swapped: 105.7273 178 178

iupac\_m\_487\_> NH1/2 swapped: 179.5454 185 185

iupac\_m\_486\_> OE1/2 will be swapped: -116.4695 193 193

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: -116.4695

>> Model assessment by GA341 potential

Surface library : /usr/lib/modeller9.22/modlib/surf5.de

Pair library : /usr/lib/modeller9.22/modlib/pair9.de

Chain identifier : \_

% sequence identity : 26.531000

Sequence length : 197

Compactness : 0.134481

Native energy (pair) : -223.804166

Native energy (surface) : -5.804411

Native energy (combined) : -8.822233

Z score (pair) : -7.700765

Z score (surface) : -5.405682

Z score (combined) : -8.410973

GA341 score : 1.000000

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: VAL:OXT VAL

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 1097143

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -21677.5273

<< end of ENERGY.

DOPE score : -21677.527344

>> Normalized DOPE z score: -0.277

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 197

Number of all, selected real atoms : 3225 3225

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 25352 25352

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 20990

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 64733.1289

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

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1 Bond length potential : 3255 32 32 0.193 0.193 55243. 1.000

2 Bond angle potential : 5881 305 399 9.958 9.958 7329.8 1.000

3 Stereochemical cosine torsion poten: 5645 0 55 26.957 26.957 669.58 1.000

4 Stereochemical improper torsion pot: 948 80 92 7.049 7.049 786.99 1.000

5 Soft-sphere overlap restraints : 20990 0 0 0.002 0.002 6.5769 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 3337 0 1 0.319 0.319 133.60 1.000

10 Distance restraints 2 (N-O) : 3404 0 11 0.413 0.413 210.46 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 196 1 7 5.095 5.095 59.997 1.000

14 Sidechain Chi\_1 dihedral restraints: 179 0 2 77.336 77.336 51.774 1.000

15 Sidechain Chi\_2 dihedral restraints: 142 0 2 92.130 92.130 71.022 1.000

16 Sidechain Chi\_3 dihedral restraints: 56 0 0 95.644 95.644 38.267 1.000

17 Sidechain Chi\_4 dihedral restraints: 22 0 0 99.207 99.207 18.891 1.000

18 Disulfide distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

19 Disulfide angle restraints : 0 0 0 0.000 0.000 0.0000 1.000

20 Disulfide dihedral angle restraints: 0 0 0 0.000 0.000 0.0000 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 1690 0 0 0.383 0.383 27.257 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 195 23 28 31.519 51.175 22.419 1.000

26 Distance restraints 4 (SDCH-SDCH) : 402 0 4 1.112 1.112 63.958 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

openf\_\_\_224\_> Open USP\_receptor\_Luc.V99990010

# Heavy relative violation of each residue is written to: USP\_receptor\_Luc.V99990010

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 40001.6328

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

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Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 99 6R 6R NH1 HH11 95 96 3.27 1.00 2.27 89.09 1.00 2.27 89.09

2 100 6R 6R NH1 HH12 95 97 2.58 1.00 1.58 61.77 1.00 1.58 61.77

3 101 6R 6R NH2 HH21 98 99 3.27 1.00 2.27 89.15 1.00 2.27 89.15

4 102 6R 6R NH2 HH22 98 100 2.58 1.00 1.58 61.85 1.00 1.58 61.85

5 852 52R 52R NH1 HH11 843 844 3.27 1.00 2.27 88.97 1.00 2.27 88.97

6 853 52R 52R NH1 HH12 843 845 2.57 1.00 1.57 61.46 1.00 1.57 61.46

7 854 52R 52R NH2 HH21 846 847 3.27 1.00 2.27 89.01 1.00 2.27 89.01

8 855 52R 52R NH2 HH22 846 848 2.57 1.00 1.57 61.39 1.00 1.57 61.39

9 1221 74R 74R NH1 HH11 1207 1208 3.27 1.00 2.27 88.99 1.00 2.27 88.99

10 1222 74R 74R NH1 HH12 1207 1209 2.57 1.00 1.57 61.60 1.00 1.57 61.60

11 1223 74R 74R NH2 HH21 1210 1211 3.27 1.00 2.27 88.96 1.00 2.27 88.96

12 1224 74R 74R NH2 HH22 1210 1212 2.57 1.00 1.57 61.59 1.00 1.57 61.59

13 1533 94R 94R NH1 HH11 1516 1517 3.27 1.00 2.27 89.11 1.00 2.27 89.11

14 1534 94R 94R NH1 HH12 1516 1518 2.57 1.00 1.57 61.72 1.00 1.57 61.72

15 1535 94R 94R NH2 HH21 1519 1520 3.27 1.00 2.27 89.15 1.00 2.27 89.15

16 1536 94R 94R NH2 HH22 1519 1521 2.58 1.00 1.58 61.78 1.00 1.58 61.78

17 1928 118R 118R NH1 HH11 1908 1909 3.27 1.00 2.27 89.02 1.00 2.27 89.02

18 1929 118R 118R NH1 HH12 1908 1910 2.57 1.00 1.57 61.53 1.00 1.57 61.53

19 1930 118R 118R NH2 HH21 1911 1912 2.57 1.00 1.57 61.68 1.00 1.57 61.68

20 1931 118R 118R NH2 HH22 1911 1913 3.27 1.00 2.27 89.02 1.00 2.27 89.02

21 2380 145R 145R NH1 HH11 2356 2357 2.56 1.00 1.56 61.22 1.00 1.56 61.22

22 2381 145R 145R NH1 HH12 2356 2358 3.27 1.00 2.27 88.96 1.00 2.27 88.96

23 2382 145R 145R NH2 HH21 2359 2360 2.57 1.00 1.57 61.40 1.00 1.57 61.40

24 2383 145R 145R NH2 HH22 2359 2361 3.27 1.00 2.27 88.91 1.00 2.27 88.91

25 2739 167R 167R NH1 HH11 2711 2712 3.27 1.00 2.27 88.83 1.00 2.27 88.83

26 2740 167R 167R NH1 HH12 2711 2713 2.56 1.00 1.56 61.15 1.00 1.56 61.15

27 2741 167R 167R NH2 HH21 2714 2715 3.27 1.00 2.27 88.88 1.00 2.27 88.88

28 2742 167R 167R NH2 HH22 2714 2716 2.56 1.00 1.56 61.21 1.00 1.56 61.21

29 3029 185R 185R NH1 HH11 3000 3001 3.27 1.00 2.27 88.85 1.00 2.27 88.85

30 3030 185R 185R NH1 HH12 3000 3002 2.56 1.00 1.56 61.18 1.00 1.56 61.18

31 3031 185R 185R NH2 HH21 3003 3004 3.27 1.00 2.27 88.87 1.00 2.27 88.87

32 3032 185R 185R NH2 HH22 3003 3005 2.56 1.00 1.56 61.27 1.00 1.56 61.27

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 15731 2D 3V C N 30 32 -111.15 -125.40 42.86 1.72 -62.40 153.24 17.16

1 3V 3V N CA 32 34 102.88 143.30 -42.40

2 15733 4S 5F C N 57 59 -85.78 -124.20 79.40 2.62 -63.20 120.26 15.25

2 5F 5F N CA 59 61 73.82 143.30 -44.30

3 15734 5F 6R C N 77 79 -106.69 -63.00 78.69 8.92 -63.00 78.69 8.92

3 6R 6R N CA 79 81 24.35 -41.10 -41.10

4 15755 26L 27P C N 431 433 -48.65 -58.70 30.96 1.89 -64.50 153.84 12.33

4 27P 27P N CA 433 434 -59.78 -30.50 147.20

5 15756 27P 28A C N 445 447 -75.39 -62.50 24.03 3.61 55.40 143.40 17.05

5 28A 28A N CA 447 449 -20.61 -40.90 38.20

6 15785 56R 57Y C N 924 926 -98.05 -63.50 86.71 12.25 -63.50 86.71 12.25

6 57Y 57Y N CA 926 928 36.13 -43.40 -43.40

7 15796 67A 68N C N 1091 1093 -65.24 -119.90 56.71 1.97 -63.20 163.01 20.27

7 68N 68N N CA 1093 1095 121.90 137.00 -41.10

8 15797 68N 69N C N 1105 1107 72.36 55.90 35.61 1.70 -63.20 144.14 23.45

8 69N 69N N CA 1107 1109 7.92 39.50 -41.10

9 15845 116S 117D C N 1878 1880 -74.25 -96.50 38.59 1.62 -63.30 123.16 14.57

9 117D 117D N CA 1880 1882 82.68 114.20 -40.00

10 15875 146H 147C C N 2379 2381 -87.71 -117.90 30.73 1.15 -63.00 173.83 22.99

10 147C 147C N CA 2381 2383 146.84 141.10 -41.10

11 15876 147C 148G C N 2390 2392 92.24 82.20 28.67 0.91 -62.40 156.32 28.74

11 148G 148G N CA 2392 2394 -18.35 8.50 -41.20

12 15880 151M 152S C N 2440 2442 -63.68 -136.60 79.39 3.96 -64.10 142.40 10.29

12 152S 152S N CA 2442 2444 -177.40 151.20 -35.00

13 15881 152S 153L C N 2451 2453 -121.33 -108.50 22.89 1.30 -63.50 165.20 20.47

13 153L 153L N CA 2453 2455 113.55 132.50 -41.20

14 15883 154V 155F C N 2486 2488 36.63 -63.20 126.60 22.83 -63.20 126.60 22.83

14 155F 155F N CA 2488 2490 33.56 -44.30 -44.30

15 15884 155F 156F C N 2506 2508 -89.71 -124.20 47.47 2.60 -63.20 142.27 21.54

15 156F 156F N CA 2508 2510 175.92 143.30 -44.30

16 15902 173N 174A C N 2802 2804 89.43 55.40 55.37 2.43 -62.50 156.01 31.19

16 174A 174A N CA 2804 2806 -5.47 38.20 -40.90

17 15904 175E 176M C N 2827 2829 94.55 -125.60 147.52 6.97 -125.60 147.52 6.97

17 176M 176M N CA 2829 2831 93.55 140.50 140.50

18 15905 176M 177C C N 2844 2846 -85.38 -63.00 79.95 8.53 -63.00 79.95 8.53

18 177C 177C N CA 2846 2848 35.66 -41.10 -41.10

19 15909 180L 181K C N 2905 2907 -77.59 -118.00 91.43 3.73 -62.90 98.99 12.13

19 181K 181K N CA 2907 2909 57.09 139.10 -40.80

20 15911 182L 183K C N 2946 2948 76.41 -62.90 149.29 21.54 -62.90 149.29 21.54

20 183K 183K N CA 2948 2950 -94.46 -40.80 -40.80

21 15912 183K 184N C N 2968 2970 -73.23 -119.90 71.85 2.15 -63.20 123.88 14.96

21 184N 184N N CA 2970 2972 82.37 137.00 -41.10

22 15922 193E 194I C N 3152 3154 42.70 -97.30 140.09 5.79 -120.60 163.32 11.40

22 194I 194I N CA 3154 3156 132.21 127.20 130.30

23 15924 195W 196D C N 3195 3197 -74.82 -70.90 18.26 0.72 -63.30 152.31 19.51

23 196D 196D N CA 3197 3199 168.13 150.30 -40.00

report\_\_\_\_\_\_> Distribution of short non-bonded contacts:

serious non-bonded atom clash: 44 60 1.330

serious non-bonded atom clash: 331 404 1.452

serious non-bonded atom clash: 474 596 1.478

serious non-bonded atom clash: 523 537 1.310

serious non-bonded atom clash: 746 2690 1.434

serious non-bonded atom clash: 748 2688 1.287

serious non-bonded atom clash: 811 822 1.469

serious non-bonded atom clash: 814 1715 1.422

serious non-bonded atom clash: 854 864 1.373

serious non-bonded atom clash: 1018 1187 1.304

serious non-bonded atom clash: 1040 1424 1.481

serious non-bonded atom clash: 1262 1339 1.428

serious non-bonded atom clash: 1303 1329 1.441

serious non-bonded atom clash: 1596 1642 1.480

serious non-bonded atom clash: 1603 2570 1.331

serious non-bonded atom clash: 1739 2217 1.349

serious non-bonded atom clash: 1760 2505 1.304

serious non-bonded atom clash: 1810 2636 1.412

serious non-bonded atom clash: 2210 2491 1.410

serious non-bonded atom clash: 2229 2521 1.485

serious non-bonded atom clash: 2273 2479 1.288

serious non-bonded atom clash: 2293 2477 1.399

serious non-bonded atom clash: 2304 2447 1.388

serious non-bonded atom clash: 2352 2361 1.463

serious non-bonded atom clash: 2433 2557 1.303

serious non-bonded atom clash: 2463 2563 1.288

serious non-bonded atom clash: 2501 2582 1.393

serious non-bonded atom clash: 2834 2866 1.291

serious non-bonded atom clash: 2975 3035 1.312

serious non-bonded atom clash: 2975 3054 1.306

DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40

DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50

FREQUENCY: 510 229 265 329 480 634 620 770 782 925 1012 1071 1132 1226 1293

<< end of ENERGY.

openf\_\_\_224\_> Open USP\_receptor\_Luc.B99990010.pdb

wrpdb\_\_\_568\_> Residues, atoms, selected atoms: 197 3225 3225

>> Summary of successfully produced models:

Filename molpdf GA341 score Normalized DOPE score

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USP\_receptor\_Luc.B99990001.pdb 63877.00000 1.00000 -0.41966

USP\_receptor\_Luc.B99990002.pdb 71068.19531 1.00000 -0.28153

USP\_receptor\_Luc.B99990003.pdb 71704.72656 1.00000 -0.39166

USP\_receptor\_Luc.B99990004.pdb 64429.04688 1.00000 -0.25060

USP\_receptor\_Luc.B99990005.pdb 49139.39062 1.00000 -0.42271

USP\_receptor\_Luc.B99990006.pdb 71511.09375 1.00000 -0.32404

USP\_receptor\_Luc.B99990007.pdb 33994.94141 1.00000 -0.40362

USP\_receptor\_Luc.B99990008.pdb 56479.45703 1.00000 -0.36152

USP\_receptor\_Luc.B99990009.pdb 78566.21875 1.00000 -0.35885

USP\_receptor\_Luc.B99990010.pdb 64733.12891 1.00000 -0.27661