

Project2_FirstDraft

May 31, 2022

Introduction (20 points) - 5 points for specific, measurable, and clear scientific question - 5 points for background on the protein/gene/species of interest and where the data is sourced from - 5 points for clear, specific, and measurable scientific hypothesis that is in the form of an if-then statement - 5 points for description of what analyses were done and how the data was downloaded for the project

Scientific question: WISP-1 is a protein from the CCN protein family which is known to act as an oncogene in most type of cancers to promote cancer cell proliferation, progression, metastasis, and invasion. What might be the structural basis of WISP-1-induced tumor growth?

Background WNT1 inducible signaling pathway protein 1 (WISP1), a member 4 protein from the CCN family (CCN4), is a secreted matricellular protein found in the extracellular matrix (ECM) and affects different cell responses like other ECM proteins. It plays a part in cellular functions such as differentiation, proliferation, migration, and survival. and was demonstrated to its overexpression has oncogenic properties in most cancers. An in vitro study found that recombinant WISP-1 treatment increased cell proliferation in a breast cancer context (1). Since WISP-1 interacts with other proteins in the ECM to signal downstream pathways, inhibiting the interactions might limit cellular pathway signaling for cellular responses like cell proliferation and halt its oncogenic functions, making it a potential target of cancer therapeutic. Another study regarding downstream target of WISP-1 found that disrupting WISP-1 reduces the activating phosphorylation of Akt (pAkt-Ser473), indicating that WISP-1 might be regulating Akt activity, specifically phosphorylation, in glioma stem cells (GSC). It was also found that WISP-1 trigger its downstream signaling and enhances Akt phosphorylation by binding to integrin $\alpha 6 \beta 1$ for its autocrine function (2). The PI3K/Akt/mTOR pathway is often over-activated in cancer different signaling pathway, among which is the induction carcinogenesis and progression by inhibiting tumor suppressor that suppressors cancer cell growth and proliferation (3). The interface of WISP-1 and integrin $\alpha 6 \beta 1$ does warrant study in order to determine competent inhibitors for the interaction. Since no experimental structure of WISP-1 exists, homology modeling might be able to construct a useful model for further analysis in molecular interaction and docking between WISP-1 and integrin $\alpha 6 \beta 1$.

Sources: 1. <https://www.nature.com/articles/srep08686> 2. <https://www.nature.com/articles/s41467-020-16827-z> 3. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC839409>

Where the data is sourced from (input)

Scientific hypothesis If WISP-1 can bind a series of protein partners which includes different integrin subunits to modulate specific cell functions such as tumor cell proliferation, then there are

structural domains on WISP-1 that engage in specific interactions with its downstream interacting protein integrin $\alpha 6 \beta 1$ to promote tumorigenesis potentially via activation of the AKT pathway.

Description of analysis (input)

How the data was downloaded

- Search CCN family member 4 in NCBI within the protein category, select CCN family member 4 isoform 1 precursor [Homo sapiens]. The page should be https://www.ncbi.nlm.nih.gov/protein/NP_003873.1
- select “Send to” on the upper right corner, choose FASTA format, and click create file. Upload the “sequence.fasta” file downloaded to the same directory as the Jupyter notebook.

Loading in Packages (15 points) - 10 points for definition of each of the packages loaded - 5 points for correctly loading all of the packages needed and stating anything that needs to be done to load the packages (downloading the packages)

Packages loaded Biopython: - <https://github.com/biopython/biopython> - Biopython is a package for computational molecular biology with Python tools, for example, it contains code for dealing with BLAST programs and output.

Numpy - <https://numpy.org/doc/stable/> - NumPy is the fundamental package for scientific computing in Python

Modeller - <https://salilab.org/modeller/> - Modeller is a package used for homology modeling of protein 3D structure - Installation & activation: need to go to home page → registration → sign the agreement to obtain a license key from the website and input the license in the correct document file following the error message upon initial attempt of activation

Ngl viewer - <http://nglviewer.org/nglview/release/v0.5.1/> - NGL Viewer is a collection of tools for web-based molecular graphics such as displaying protein structures

Prody - <http://prody.csb.pitt.edu/index.html> - Prody is a package for protein structural dynamics analysis and contains functions like flexible PDB parsers

```
[12]: !pip install -U ProDy
```

```
Requirement already satisfied: ProDy in
/Users/yingyinli/opt/anaconda3/lib/python3.9/site-packages (2.2.0)
Requirement already satisfied: biopython<=1.76 in
/Users/yingyinli/opt/anaconda3/lib/python3.9/site-packages (from ProDy) (1.76)
Requirement already satisfied: pyparsing in
/Users/yingyinli/opt/anaconda3/lib/python3.9/site-packages (from ProDy) (3.0.4)
Requirement already satisfied: numpy>=1.10 in
/Users/yingyinli/opt/anaconda3/lib/python3.9/site-packages (from ProDy) (1.20.3)
Requirement already satisfied: scipy in
/Users/yingyinli/opt/anaconda3/lib/python3.9/site-packages (from ProDy) (1.7.1)
```

```
[6]: conda install modeller
```

```
Collecting package metadata (current_repodata.json): done
Solving environment: \
The environment is inconsistent, please check the package plan carefully
The following packages are causing the inconsistency:
```

```
- bjornfjohansson/noarch::cai==1.0.3=py_0
done
```

```
## Package Plan ##
```

```
environment location: /Users/yingyinli/opt/anaconda3
```

```
added / updated specs:
```

```
- modeller
```

```
The following packages will be downloaded:
```

package	build		
biopython-1.79	py39h89e85a6_1	2.6 MB	conda-forge
Total:		2.6 MB	

```
The following NEW packages will be INSTALLED:
```

```
biopython          conda-forge/osx-64::biopython-1.79-py39h89e85a6_1
```

```
Downloading and Extracting Packages
```

```
biopython-1.79      | 2.6 MB      | ##### | 100%
```

```
Preparing transaction: done
```

```
Verifying transaction: done
```

```
Executing transaction: done
```

```
Note: you may need to restart the kernel to use updated packages.
```

```
[13]: from prody import *
```

```
[3]: from Bio import SeqIO
import numpy as np
from Bio.Blast import NCBIWWW
from Bio.Blast import NCBIXML

from modeller import *
from Bio.PDB import *
```

```
import nglview as ngv

env = environ()
```

environ___W> The class 'environ' is deprecated; use 'Environ' instead

Performing Bioinformatics Analysis (20 points) - 5 points for a description each of the bioinformatics method that includes data types read in and how the method works. - 5 points for code working correctly - 5 points for adequate commenting in the code and code checks - 5 points for a function written that performs some part of the bioinformatics analyses

0.0.1 1. Blast

```
[4]: #!/update_blastdb.pl --decompress pdbaa #to download the pdbaa database locally
'psiblast -db pdbaa -query "protein.faa" -inclusion_ethresh 1e-3 -evaluate 1e-3
↪-num_iterations 0

#could not for the life of me get anything to run after couple hours of failed
↪attempts
#leaving this line here to mourn for my sanity
#did another BLAST method using the protein sequence
```

/bin/bash: psiblast: command not found

```
[4]: WISP1_protein = SeqIO.read('sequence.fasta', 'fasta')
#code check
#print(WISP1_gene)
#print(len(WISP1_gene))
```

```
[5]: #extract the string for using blastpdb function to cross check if potential
↪blast template has an existing pdb structure on file
WISP1_protein_seq = WISP1_protein.seq
#code check
#str(WISP1_protein_seq)
```

Blast code source: http://prody.csb.pitt.edu/tutorials/structure_analysis/blastpdb.html

```
[17]: #blast search
blast_record = blastPDB(str(WISP1_protein_seq))
```

@> Blast searching NCBI PDB database for "MRWFL..."
 @> Blast search completed in 63.2s.

```
[18]: #save this record on disk, as NCBI may not respond to repeated searches for the
↪same sequence
import pickle
pickle.dump(blast_record, open('WISP1_blast_record.pkl', 'wb'))
blast_record = pickle.load(open('WISP1_blast_record.pkl', 'rb'))
```

```
[21]: #template selection
best = blast_record.getBest()
best['pdb_id']
```

```
[21]: '5nb8'
```

```
[27]: best['percent_identity']
```

```
[27]: 53.521126760563384
```

```
[30]: best['evalue']
```

```
[30]: 2.45677e-19
```

Template selected being '5nb8' with a 53.52% sequence identity and an e-value of 2.45677e-19.

0.0.2 2. Target-Template Alignment

Code Source: <https://salilab.org/modeller/tutorial/basic.html>

```
[61]: #alignment
      #PAP easier to visualize
      #PIR is what modeller works with
      from modeller import *

      env = Environ()
      aln = Alignment(env)
      mdl = Model(env, file='5nb8', model_segment=('FIRST:A','LAST:A'))
      aln.append_model(mdl, align_codes='5nb8', atom_files='5nb8.pdb')
      aln.append(file='WISP1.ali', align_codes='WISP1')
      aln.align2d(max_gap_length=50)
      aln.write(file='WISP1-5nb8.ali', alignment_format='PIR')
      aln.write(file='WISP1-5nb8.pap', alignment_format='PAP')
```

```
mkapsa_637W> No residue topology library is in memory.
              Better radii would be used if topology.read() is called first.
iup2crm_280W> No topology library in memory or assigning a BLK residue.
              Default CHARMM atom type assigned: N --> N
              This message is written only for the first such atom.
```

Pairwise dynamic programming alignment (ALIGN2D):

Residue-residue metric	:	\$(LIB)/as1.sim.mat
Diagonal	:	100
Overhang	:	0
Maximal gap length	:	50
Local alignment	:	F
MATRIX_OFFSET (local aln):		0.0000

```

FIX_OFFSETS      :      0.0    -1.0    -2.0    -3.0    -4.0
N_SUBOPT         :              0
SUBOPT_OFFSET    :      0.0000
Alignment block   :              1
Gap introduction penalty :    -100.0000
Gap extension penalty  :       0.0000
Gap diagonal penalty  :       0.0000
Structure gap penalties :    3.500    3.500    3.500    0.200    4.000    6.500
2.000    0.000
Break-break bonus   :   10000.0000
Length of alignment :           367
Score               :   48435.6133

```

[62]: *#Observe the alignment of the template 5nb8 and the target WISP1.*
!cat WISP1-5nb8.pap

```

 _aln.pos      10      20      30      40      50      60
5nb8      M-----E-----
WISP1      MRWFLPWTLAAVTA AA STVLATALSPAPTTMDFTPAPLEDTSSRPQFCKWPCECPPSPPRCPLGVSL
_consrvd   *                               *

 _aln.p      70      80      90      100     110     120     130
5nb8      -----GDNC-----VFDGVIYRNGEKF
WISP1      ITDGCECCKMCAQQLGDNCTEAAICDPHRGLYCDYSGDRPRYAIGVCAQVVGVGCVLDGVRYNNGQSF
_consrvd           ****                      * * * * *

 _aln.pos     140     150     160     170     180     190     200
5nb8      EPNCQYHCTCRDGQIGCVPRCQ-----L-----DVLLPG-----P-----D-----
WISP1      QPNCKYNCTCIDGAVGCTPLCLRV RPPRLWC P HRRVSIPGHCCEQWVCEDDAKRPRKTAPRDTGAFD
_consrvd   *** * * * * * * * * * * * * * * *

 _aln.pos     210     220     230     240     250     260     270
5nb8      -----C-----PAPKK
WISP1      AVGEVEAWHRNCIAYTSPWSPCSTSCGLGVSTRISNVNAQCWPEQESRLCNLRPCDVDIHTLIKAGKK
_consrvd           *                               * * *

 _aln.pos     280     290     300     310     320     330     340
5nb8      -VAV--P-----G-----ECC-----EKWTCG-----
WISP1      CLAVYQPEASMNFTLAGCISTRSYQPKYCGVCMDNRCCIPYKSKTIDVSFQCPDGLGFSRQVLWINAC
_consrvd   ** *           *           **           *

 _aln.pos     350     360
5nb8      -----
WISP1      FCNLSCRNPNDIFADLESYPDFSEIAN
_consrvd

```

```
[82]: #import 5nb8 structure & put in the same directory as notebook

import Bio
from Bio.PDB import PDBList
pdbl=PDBList()
pdbl.retrieve_pdb_file('5nb8',file_format='pdb',pdir='/Users/yingyinli//BIMM143/
↳5_28 2C')
```

Downloading PDB structure '5nb8'...

```
[82]: '/Users/yingyinli//BIMM143/5_28 2C/pdb5nb8.ent'
```

```
[83]: #rename downloaded pdb to run the next function takes takes in argument in_
↳specific naming format
!mv pdb5nb8.ent 5nb8.pdb
```

```
[86]: #model construction based on modeller

from modeller import *
from modeller.automodel import *
from modeller import soap_protein_od

env = Environ()
a = AutoModel(env, alnfile='WISP1-5nb8.ali',
               knowns='5nb8', sequence='WISP1',
               assess_methods=(assess.DOPE,
                               soap_protein_od.Scorer(),
                               assess.GA341))

a.starting_model = 1
a.ending_model = 5
a.make()
```

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

read_to_681_> topology.submodel read from topology file: 3

patch_s_522_> Number of disulfides patched in MODEL: 5

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.

0 atoms in HETATM/BLK residues constrained
to protein atoms within 2.30 angstroms
and protein CA atoms within 10.00 angstroms

```

0 atoms in residues without defined topology
constrained to be rigid bodies
condens_443_> Restraints marked for deletion were removed.
                Total number of restraints before, now:      16583      13904
iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle
the H atom.
iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle
the H atom.
iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle
the H atom.
iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle
the H atom.
iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle
the H atom.
>> Model assessment by DOPE potential
iatmcls_286W> MODEL atom not classified:  ASN:OXT  ASN

```

```

>> ENERGY; Differences between the model's features and restraints:
Number of all residues in MODEL                :      367
Number of all, selected real atoms              :      2804      2804
Number of all, selected pseudo atoms           :           0           0
Number of all static, selected restraints      :     13904     13904
COVALENT_CYS                                  :           F
NONBONDED_SEL_ATOMS                          :           1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):    350313
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                               :     -19561.4375

```

```

<< end of ENERGY.
DOPE score                                : -19561.437500
>> Model assessment by SOAP-Protein-OD score
preppdf_455W> None of the non-bonded terms selected.
pair2___701W> Insufficient system memory to allocate storage for cell-based
                (NlogN) nonbond list algorithm; falling back to N*N method.

```


Warning 1 of 10; further warnings will be suppressed.

```
>> ENERGY; Differences between the model's features and restraints:
Number of all residues in MODEL           :      367
Number of all, selected real atoms        :    2804    2804
Number of all, selected pseudo atoms     :         0         0
Number of all static, selected restraints :    13904    13904
COVALENT_CYS                             :         F
NONBONDED_SEL_ATOMS                      :         1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):         0
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                            :    0.000
DYNAMIC_PAIRS,_SPHERE,_COULOMB,_LENNARD,_MODELLER :         T         F         F
F         F
SPHERE_STDV                              :    0.050
RADII_FACTOR                             :    0.820
Current energy                            :              0.0000
```

<< end of ENERGY.

SOAP-Protein-OD score : 0.000000

>> Model assessment by GA341 potential

```
Surface library           :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/surf5.de
Pair library              :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/pair9.de
Chain identifier          : _
% sequence identity       :    62.856998
Sequence length           :         367
Compactness               :    0.012427
Native energy (pair)      :    74.187079
Native energy (surface)   :    41.164093
Native energy (combined)  :    8.783159
Z score (pair)            :   -3.828903
Z score (surface)         :   -1.095584
Z score (combined)        :   -3.287000
GA341 score               :    0.973716
```

```
>> ENERGY; Differences between the model's features and restraints:
Number of all residues in MODEL                :      367
Number of all, selected real atoms              :      2804      2804
Number of all, selected pseudo atoms           :           0           0
Number of all static, selected restraints      :     13904     13904
COVALENT_CYS                                  :           F
NONBONDED_SEL_ATOMS                          :           1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):      4418
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                              :           2115.5510
```

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	2881	0	0	0.003	0.003
8.0481	1.000					
2	Bond angle potential	3935	0	1	1.786	1.786
236.08	1.000					
3	Stereochemical cosine torsion poten:	1962	0	81	50.259	50.259
768.76	1.000					
4	Stereochemical improper torsion pot:	1155	0	0	0.938	0.938
21.032	1.000					

5 Soft-sphere overlap restraints	:	4418	0	0	0.003	0.003
3.5749 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)	:	765	0	4	1.295	1.295
108.48 1.000						
10 Distance restraints 2 (N-O)	:	973	0	11	1.669	1.669
178.00 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:		366	0	0	3.338	3.338
48.102 1.000						
14 Sidechain Chi_1 dihedral restraints:		315	0	2	84.674	84.674
97.588 1.000						
15 Sidechain Chi_2 dihedral restraints:		209	0	1	76.192	76.192
86.232 1.000						
16 Sidechain Chi_3 dihedral restraints:		98	0	0	80.861	80.861
52.483 1.000						
17 Sidechain Chi_4 dihedral restraints:		34	0	0	105.462	105.462
23.723 1.000						
18 Disulfide distance restraints	:	5	0	0	0.007	0.007
0.39089E-01 1.000						
19 Disulfide angle restraints	:	10	0	0	1.873	1.873
0.77495 1.000						
20 Disulfide dihedral angle restraints:		5	0	0	20.174	20.174
2.0034 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)	:	643	0	0	0.630	0.630
31.940 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:		365	205	54	37.936	134.248
416.39 1.000						
26 Distance restraints 4 (SDCH-SDCH)	:	183	0	2	2.228	2.228
32.307 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				

Heavy relative violation of each residue is written to: WISP1.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: 61820.8125

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.

 Feature 25 : Phi/Psi pair of dihedral restraints
 List of the RVIOL violations larger than : 6.5000

#	ICSR	RESN01/2	ATM1/2	INDATM1/2	FEAT	restr	viol	rviol
RESTR	VIOL	RVIOL						
1	9954	1M 2R C	N	7 9	-142.52	-125.20	17.41	0.65
-63.00	-166.38	31.59						
1		2R 2R N	CA	9 10	142.36	140.60		
-41.10								
2	9955	2R 3W C	N	18 20	-119.80	-124.90	15.85	0.64
-63.00	-178.30	20.20						
2		3W 3W N	CA	20 21	128.39	143.40		
-44.20								
3	9956	3W 4F C	N	32 34	-111.47	-124.20	34.32	1.25
-63.20	163.04	19.70						
3		4F 4F N	CA	34 35	111.43	143.30		
-44.30								
4	9957	4F 5L C	N	43 45	-132.67	-108.50	29.60	1.63
-63.50	171.21	21.05						
4		5L 5L N	CA	45 46	115.41	132.50		
-41.20								
5	9959	6P 7W C	N	58 60	-165.89	-124.90	47.36	1.55
-63.00	-179.19	29.48						
5		7W 7W N	CA	60 61	167.12	143.40		
-44.20								
6	9960	7W 8T C	N	72 74	-117.76	-124.80	10.73	0.64
-63.20	175.03	26.07						
6		8T 8T N	CA	74 75	151.59	143.50		
-42.10								
7	9961	8T 9L C	N	79 81	-99.78	-108.50	18.22	0.87
-63.50	161.82	20.68						
7		9L 9L N	CA	81 82	116.50	132.50		
-41.20								
8	9962	9L 10A C	N	87 89	-161.24	-134.00	32.32	0.78
-62.50	-176.45	35.32						
8		10A 10A N	CA	89 90	164.38	147.00		
-40.90								
9	9963	10A 11A C	N	92 94	81.03	-134.00	153.31	3.60
-62.50	-171.47	29.69						
9		11A 11A N	CA	94 95	-163.14	147.00		
-40.90								
10	9965	12V 13T C	N	104 106	-74.75	-78.10	33.06	1.31
-63.20	159.43	19.71						
10		13T 13T N	CA	106 107	116.91	149.80		

-42.10	11	9966	13T	14A	C	N	111	113	-148.95	-134.00	15.13	0.42
-62.50	-169.47		35.85									
	11		14A	14A	N	CA	113	114	149.32	147.00		
-40.90												
	12	9967	14A	15A	C	N	116	118	-82.34	-68.20	15.81	1.09
-62.50	167.91		28.53									
	12		15A	15A	N	CA	118	119	152.37	145.30		
-40.90												
	13	9968	15A	16A	C	N	121	123	-82.79	-68.20	29.58	1.92
-62.50	149.46		25.54									
	13		16A	16A	N	CA	123	124	171.03	145.30		
-40.90												
	14	9969	16A	17A	C	N	126	128	-58.95	-68.20	22.85	1.53
-62.50	165.35		27.27									
	14		17A	17A	N	CA	128	129	124.41	145.30		
-40.90												
	15	9970	17A	18S	C	N	131	133	-171.02	-136.60	56.54	1.96
-64.10	167.51		19.84									
	15		18S	18S	N	CA	133	134	-163.95	151.20		
-35.00												
	16	9971	18S	19T	C	N	137	139	-60.30	-78.10	17.84	1.11
-63.20	166.87		21.21									
	16		19T	19T	N	CA	139	140	151.05	149.80		
-42.10												
	17	9972	19T	20V	C	N	144	146	-59.84	-62.40	7.11	0.79
-125.40	-179.98		10.14									
	17		20V	20V	N	CA	146	147	-49.04	-42.40		
143.30												
	18	9973	20V	21L	C	N	151	153	-72.30	-70.70	5.17	0.45
-63.50	178.11		24.24									
	18		21L	21L	N	CA	153	154	136.69	141.60		
-41.20												
	19	9974	21L	22A	C	N	159	161	-119.23	-134.00	20.46	0.60
-62.50	-177.23		27.78									
	19		22A	22A	N	CA	161	162	132.85	147.00		
-40.90												
	20	9975	22A	23T	C	N	164	166	-99.76	-78.10	61.33	2.06
-63.20	116.60		17.38									
	20		23T	23T	N	CA	166	167	-152.82	149.80		
-42.10												
	21	9976	23T	24A	C	N	171	173	-63.21	-68.20	5.64	0.39
-62.50	176.43		28.95									
	21		24A	24A	N	CA	173	174	142.67	145.30		
-40.90												
	22	9978	25L	26S	C	N	184	186	-118.70	-136.60	31.99	1.16
-64.10	168.76		10.39									
	22		26S	26S	N	CA	186	187	124.68	151.20		

-35.00	23	9980	27P	28A	C	N	197	199	-121.37	-134.00	43.71	2.12
-62.50	23	157.47	23.73	28A	28A	N	CA	199	200	105.15	147.00	
-40.90	24	9983	30T	31T	C	N	216	218	-98.76	-78.10	60.31	2.03
-63.20	24	116.98	17.36	31T	31T	N	CA	218	219	-153.54	149.80	
-42.10	25	9984	31T	32M	C	N	223	225	-66.03	-73.00	18.75	1.39
-63.40	25	159.11	23.96	32M	32M	N	CA	225	226	160.41	143.00	
-40.50	26	9991	38P	39L	C	N	276	278	-44.82	-70.70	26.25	2.51
-63.50	26	173.81	23.13	39L	39L	N	CA	278	279	146.00	141.60	
-41.20	27	9993	40E	41D	C	N	293	295	-131.30	-96.50	34.82	1.42
-63.30	27	167.63	17.86	41D	41D	N	CA	295	296	113.22	114.20	
-40.00	28	9995	42T	43S	C	N	308	310	-74.82	-72.40	3.22	0.26
-64.10	28	175.05	13.35	43S	43S	N	CA	310	311	150.28	152.40	
-35.00	29	9996	43S	44S	C	N	314	316	-110.91	-136.60	35.68	1.98
-64.10	29	156.21	14.58	44S	44S	N	CA	316	317	175.97	151.20	
-35.00	30	9997	44S	45R	C	N	320	322	-99.22	-125.20	27.88	1.37
-63.00	30	172.06	25.75	45R	45R	N	CA	322	323	150.70	140.60	
-41.10	31	9999	46P	47Q	C	N	338	340	-79.28	-73.00	30.72	2.14
-63.80	31	151.72	21.52	47Q	47Q	N	CA	340	341	110.63	140.70	
-40.30	32	10000	47Q	48F	C	N	347	349	-139.67	-124.20	25.02	0.72
-63.20	32	170.80	28.63	48F	48F	N	CA	349	350	162.97	143.30	
-44.30	33	10002	49C	50K	C	N	364	366	-98.67	-118.00	24.97	0.85
-62.90	33	167.95	20.13	50K	50K	N	CA	366	367	123.29	139.10	
-40.80	34	10003	50K	51W	C	N	373	375	-128.29	-124.90	19.31	1.01
-63.00	34	-179.21	19.94	51W	51W	N	CA	375	376	124.39	143.40	

-44.20											
35	10004	51W	52P	C	N	387	389	-51.58	-58.70	12.28	0.75
-64.50	172.78		13.59								
35		52P	52P	N	CA	389	390	-40.50	-30.50		
147.20											
36	10006	53C	54E	C	N	400	402	-98.51	-117.80	19.49	0.79
-63.60	-176.74		22.69								
36		54E	54E	N	CA	402	403	139.60	136.80		
-40.30											
37	10010	57P	58S	C	N	429	431	-65.23	-72.40	23.45	1.16
-64.10	165.08		11.89								
37		58S	58S	N	CA	431	432	130.07	152.40		
-35.00											
38	10012	59P	60P	C	N	442	444	-62.98	-58.70	4.88	0.69
-64.50	179.97		13.51								
38		60P	60P	N	CA	444	445	-32.83	-30.50		
147.20											
39	10013	60P	61R	C	N	449	451	55.35	-72.10	131.45	10.70
-63.00	-172.94		21.50								
39		61R	61R	N	CA	451	452	174.05	141.90		
-41.10											
40	10015	62C	63P	C	N	466	468	-64.47	-58.70	8.41	0.58
-64.50	171.58		12.80								
40		63P	63P	N	CA	468	469	-24.38	-30.50		
147.20											
41	10016	63P	64L	C	N	473	475	-77.10	-70.70	11.95	0.74
-63.50	167.66		24.08								
41		64L	64L	N	CA	475	476	151.69	141.60		
-41.20											
42	10017	64L	65G	C	N	481	483	140.48	-167.20	52.33	1.02
82.20	175.08		11.26								
42		65G	65G	N	CA	483	484	173.59	174.60		
8.50											
43	10019	66V	67S	C	N	492	494	-163.15	-136.60	33.39	1.03
-64.10	-177.28		20.39								
43		67S	67S	N	CA	494	495	171.45	151.20		
-35.00											
44	10020	67S	68L	C	N	498	500	-105.73	-108.50	17.57	0.98
-63.50	174.14		26.77								
44		68L	68L	N	CA	500	501	149.85	132.50		
-41.20											
45	10022	69I	70T	C	N	514	516	-85.17	-78.10	18.42	0.61
-63.20	152.68		21.04								
45		70T	70T	N	CA	516	517	166.80	149.80		
-42.10											
46	10023	70T	71D	C	N	521	523	-100.83	-96.50	81.41	3.42
-63.30	82.00		8.70								
46		71D	71D	N	CA	523	524	32.91	114.20		

-40.00											
47	10024	71D	72G	C	N	529	531	75.47	78.70	13.48	0.51
82.20	172.45	8.03									
47		72G	72G	N	CA	531	532	-179.18	-166.10		
8.50											
48	10026	73C	74E	C	N	539	541	-125.03	-117.80	7.23	0.26
-63.60	-172.42	22.26									
48		74E	74E	N	CA	541	542	136.93	136.80		
-40.30											
49	10029	76C	77K	C	N	560	562	47.65	-70.20	127.89	10.34
-62.90	170.00	20.18									
49		77K	77K	N	CA	562	563	-169.95	140.40		
-40.80											
50	10030	77K	78M	C	N	569	571	-77.14	-73.00	15.36	0.98
-63.40	162.29	25.32									
50		78M	78M	N	CA	571	572	157.79	143.00		
-40.50											
51	10032	79C	80A	C	N	583	585	-77.78	-68.20	45.26	3.31
-62.50	130.47	22.16									
51		80A	80A	N	CA	585	586	-170.46	145.30		
-40.90											
52	10033	80A	81Q	C	N	588	590	-49.15	-73.00	23.88	1.68
-63.80	-179.63	27.30									
52		81Q	81Q	N	CA	590	591	139.47	140.70		
-40.30											
53	10034	81Q	82Q	C	N	597	599	-63.79	-73.00	11.13	0.87
-63.80	172.74	25.40									
53		82Q	82Q	N	CA	599	600	146.96	140.70		
-40.30											
54	10035	82Q	83L	C	N	606	608	-80.74	-70.70	24.15	1.52
-63.50	156.18	22.71									
54		83L	83L	N	CA	608	609	163.57	141.60		
-41.20											
55	10040	87C	88T	C	N	640	642	-128.78	-124.80	7.40	0.23
-63.20	-179.51	27.47									
55		88T	88T	N	CA	642	643	149.75	143.50		
-42.10											
56	10041	88T	89E	C	N	647	649	-136.77	-117.80	24.11	0.73
-63.60	-176.73	28.55									
56		89E	89E	N	CA	649	650	151.67	136.80		
-40.30											
57	10042	89E	90A	C	N	656	658	-63.60	-68.20	10.99	0.73
-62.50	176.22	28.83									
57		90A	90A	N	CA	658	659	135.32	145.30		
-40.90											
58	10043	90A	91A	C	N	661	663	173.98	-134.00	53.97	2.35
-62.50	-146.99	32.08									
58		91A	91A	N	CA	663	664	132.64	147.00		

-40.90											
59	10045	92I	93C	C	N	674	676	-64.59	-63.00	12.43	1.63
-117.90	173.84		7.50								
59		93C	93C	N	CA	676	677	-53.43	-41.10		
141.10											
60	10046	93C	94D	C	N	680	682	-172.16	-96.50	77.59	3.19
-63.30	-156.96		21.63								
60		94D	94D	N	CA	682	683	131.39	114.20		
-40.00											
61	10049	96H	97R	C	N	705	707	-179.65	-125.20	61.50	1.86
-63.00	-170.22		33.21								
61		97R	97R	N	CA	707	708	169.20	140.60		
-41.10											
62	10050	97R	98G	C	N	716	718	135.74	-167.20	57.37	1.24
82.20	168.82		10.74								
62		98G	98G	N	CA	718	719	168.61	174.60		
8.50											
63	10051	98G	99L	C	N	720	722	-132.19	-108.50	34.94	1.59
-63.50	174.69		28.51								
63		99L	99L	N	CA	722	723	158.18	132.50		
-41.20											
64	10052	99L	100Y	C	N	728	730	-105.70	-98.40	7.80	0.43
-63.50	179.57		26.46								
64		100Y	100Y	N	CA	730	731	131.14	128.40		
-43.40											
65	10054	101C	102D	C	N	746	748	-94.63	-96.50	2.07	0.08
-63.30	158.22		17.86								
65		102D	102D	N	CA	748	749	115.09	114.20		
-40.00											
66	10055	102D	103Y	C	N	754	756	-133.05	-124.30	25.72	1.05
-63.50	171.72		30.69								
66		103Y	103Y	N	CA	756	757	159.59	135.40		
-43.40											
67	10056	103Y	104S	C	N	766	768	-72.91	-72.40	18.24	1.06
-64.10	154.62		11.75								
67		104S	104S	N	CA	768	769	170.63	152.40		
-35.00											
68	10058	105G	106D	C	N	776	778	-66.38	-70.90	9.70	0.70
-63.30	161.15		20.08								
68		106D	106D	N	CA	778	779	158.89	150.30		
-40.00											
69	10059	106D	107R	C	N	784	786	-69.54	-72.10	3.68	0.24
-63.00	179.76		24.72								
69		107R	107R	N	CA	786	787	139.26	141.90		
-41.10											
70	10061	108P	109R	C	N	802	804	-89.93	-72.10	25.60	1.66
-63.00	160.90		23.59								
70		109R	109R	N	CA	804	805	160.27	141.90		

-41.10	71	10062	109R	110Y	C	N	813	815	-64.38	-98.40	34.07	1.31
-63.50	173.80	27.53										
	71		110Y	110Y	N	CA	815	816	130.40	128.40		
-43.40												
	72	10063	110Y	111A	C	N	825	827	-110.95	-134.00	27.60	0.67
-62.50	179.38	27.46										
	72		111A	111A	N	CA	827	828	131.81	147.00		
-40.90												
	73	10065	112I	113G	C	N	838	840	-67.71	-80.20	53.97	1.54
82.20	-172.21	6.94										
	73		113G	113G	N	CA	840	841	121.60	174.10		
8.50												
	74	10067	114V	115C	C	N	849	851	-58.21	-63.00	13.35	1.39
-117.90	175.79	7.63										
	74		115C	115C	N	CA	851	852	-53.56	-41.10		
141.10												
	75	10068	115C	116A	C	N	855	857	-142.31	-134.00	12.47	0.74
-62.50	-164.39	29.39										
	75		116A	116A	N	CA	857	858	137.70	147.00		
-40.90												
	76	10069	116A	117Q	C	N	860	862	-102.58	-121.10	18.53	0.68
-63.80	-176.48	25.11										
	76		117Q	117Q	N	CA	862	863	139.08	139.70		
-40.30												
	77	10072	119V	120G	C	N	883	885	-94.16	-80.20	38.25	0.93
82.20	-122.69	18.35										
	77		120G	120G	N	CA	885	886	-150.29	174.10		
8.50												
	78	10078	125L	126D	C	N	919	921	46.98	-70.90	127.57	10.67
54.50	158.36	11.05										
	78		126D	126D	N	CA	921	922	-160.92	150.30		
40.90												
	79	10079	126D	127G	C	N	927	929	-67.96	-62.40	6.98	1.02
82.20	156.90	11.83										
	79		127G	127G	N	CA	929	930	-36.98	-41.20		
8.50												
	80	10111	158L	159R	C	N	1163	1165	-145.23	-125.20	30.36	0.95
-63.00	175.89	29.33										
	80		159R	159R	N	CA	1165	1166	163.41	140.60		
-41.10												
	81	10113	160V	161R	C	N	1181	1183	113.99	-125.20	131.96	4.09
-63.00	-143.19	27.50										
	81		161R	161R	N	CA	1183	1184	-166.32	140.60		
-41.10												
	82	10118	165L	166W	C	N	1225	1227	-59.92	-71.30	37.98	2.56
-63.00	146.99	18.56										
	82		166W	166W	N	CA	1227	1228	102.76	139.00		

-44.20											
83	10122	169H	170P	C	N	1262	1264	-70.41	-58.70	25.28	1.48
-64.50	155.40	11.91									
83		170P	170P	N	CA	1264	1265	-8.09	-30.50		
147.20											
84	10123	170P	171R	C	N	1269	1271	-70.21	-72.10	50.32	3.91
-63.00	126.92	17.63									
84		171R	171R	N	CA	1271	1272	-167.82	141.90		
-41.10											
85	10130	177G	178H	C	N	1323	1325	-132.72	-125.60	28.46	0.94
-63.20	166.55	25.35									
85		178H	178H	N	CA	1325	1326	166.36	138.80		
-42.30											
86	10133	180C	181E	C	N	1345	1347	-70.97	-69.30	14.15	1.02
-63.60	163.31	22.18									
86		181E	181E	N	CA	1347	1348	156.56	142.50		
-40.30											
87	10134	181E	182Q	C	N	1354	1356	-61.48	-73.00	18.62	1.07
-63.80	166.39	24.59									
87		182Q	182Q	N	CA	1356	1357	126.07	140.70		
-40.30											
88	10135	182Q	183W	C	N	1363	1365	-151.21	-124.90	50.45	1.78
-63.00	156.57	25.48									
88		183W	183W	N	CA	1365	1366	-173.56	143.40		
-44.20											
89	10138	185C	186E	C	N	1390	1392	-78.24	-69.30	19.40	1.17
-63.60	160.65	22.23									
89		186E	186E	N	CA	1392	1393	159.72	142.50		
-40.30											
90	10140	187D	188D	C	N	1407	1409	-122.47	-96.50	26.00	1.06
-63.30	166.15	17.85									
90		188D	188D	N	CA	1409	1410	115.26	114.20		
-40.00											
91	10141	188D	189A	C	N	1415	1417	-166.61	-134.00	32.93	1.27
-62.50	-154.90	39.16									
91		189A	189A	N	CA	1417	1418	142.39	147.00		
-40.90											
92	10142	189A	190K	C	N	1420	1422	177.09	-118.00	65.89	2.69
-62.90	-153.07	24.07									
92		190K	190K	N	CA	1422	1423	127.77	139.10		
-40.80											
93	10143	190K	191R	C	N	1429	1431	-139.91	-125.20	25.67	1.42
-63.00	178.12	20.30									
93		191R	191R	N	CA	1431	1432	119.56	140.60		
-41.10											
94	10145	192P	193R	C	N	1447	1449	-67.05	-72.10	9.35	0.81
-63.00	169.18	23.13									
94		193R	193R	N	CA	1449	1450	149.77	141.90		

-41.10											
95	10146	193R	194K	C	N	1458	1460	-68.84	-70.20	18.57	1.31
-62.90	162.79	20.82									
95		194K	194K	N	CA	1460	1461	121.88	140.40		
-40.80											
96	10148	195T	196A	C	N	1474	1476	-80.70	-68.20	20.15	1.27
-62.50	159.04	26.99									
96		196A	196A	N	CA	1476	1477	161.11	145.30		
-40.90											
97	10149	196A	197P	C	N	1479	1481	-67.43	-58.70	13.81	0.89
-64.50	167.03	12.62									
97		197P	197P	N	CA	1481	1482	-19.80	-30.50		
147.20											
98	10150	197P	198R	C	N	1486	1488	-107.33	-125.20	17.92	0.69
-63.00	-175.12	28.04									
98		198R	198R	N	CA	1488	1489	139.42	140.60		
-41.10											
99	10152	199D	200T	C	N	1505	1507	-158.25	-124.80	34.82	1.57
-63.20	-169.82	30.48									
99		200T	200T	N	CA	1507	1508	153.18	143.50		
-42.10											
100	10153	200T	201G	C	N	1512	1514	162.75	-167.20	30.07	0.55
82.20	-174.49	12.69									
100		201G	201G	N	CA	1514	1515	175.61	174.60		
8.50											
101	10154	201G	202A	C	N	1516	1518	-164.33	-134.00	43.76	1.35
-62.50	173.57	33.81									
101		202A	202A	N	CA	1518	1519	178.54	147.00		
-40.90											
102	10155	202A	203F	C	N	1521	1523	-91.16	-71.40	29.07	2.56
-63.20	166.05	21.25									
102		203F	203F	N	CA	1523	1524	119.38	140.70		
-44.30											
103	10156	203F	204D	C	N	1532	1534	-120.33	-96.50	43.66	1.84
-63.30	178.57	25.73									
103		204D	204D	N	CA	1534	1535	150.78	114.20		
-40.00											
104	10157	204D	205A	C	N	1540	1542	-123.05	-134.00	13.43	0.74
-62.50	175.13	31.94									
104		205A	205A	N	CA	1542	1543	154.78	147.00		
-40.90											
105	10159	206V	207G	C	N	1552	1554	-123.29	-80.20	43.67	2.67
82.20	-128.29	17.57									
105		207G	207G	N	CA	1554	1555	-178.82	174.10		
8.50											
106	10160	207G	208E	C	N	1556	1558	-68.85	-69.30	1.14	0.10
-63.60	176.23	23.79									
106		208E	208E	N	CA	1558	1559	143.55	142.50		

-40.30											
107	10162	209V	210E	C	N	1572	1574	-127.13	-63.60	96.56	16.20
-63.60	96.56	16.20									
107		210E	210E	N	CA	1574	1575	-113.02	-40.30		
-40.30											
108	10163	210E	211A	C	N	1581	1583	-58.06	-68.20	10.37	0.95
-62.50	171.67	27.92									
108		211A	211A	N	CA	1583	1584	147.49	145.30		
-40.90											
109	10164	211A	212W	C	N	1586	1588	-65.87	-71.30	26.58	1.86
-63.00	157.21	19.48									
109		212W	212W	N	CA	1588	1589	112.98	139.00		
-44.20											
110	10165	212W	213H	C	N	1600	1602	166.71	-125.60	70.65	2.05
-63.20	-154.79	33.76									
110		213H	213H	N	CA	1602	1603	159.00	138.80		
-42.30											
111	10166	213H	214R	C	N	1610	1612	-158.17	-125.20	49.58	1.55
-63.00	170.34	29.31									
111		214R	214R	N	CA	1612	1613	177.63	140.60		
-41.10											
112	10168	215N	216C	C	N	1629	1631	-65.90	-63.00	7.86	1.18
-117.90	178.24	7.66									
112		216C	216C	N	CA	1631	1632	-48.40	-41.10		
141.10											
113	10170	217I	218A	C	N	1643	1645	-78.60	-68.20	46.92	3.42
-62.50	129.05	21.98									
113		218A	218A	N	CA	1645	1646	-168.94	145.30		
-40.90											
114	10171	218A	219Y	C	N	1648	1650	-27.18	-98.40	72.87	3.03
-63.50	176.55	26.25									
114		219Y	219Y	N	CA	1650	1651	143.82	128.40		
-43.40											
115	10172	219Y	220T	C	N	1660	1662	-54.36	-78.10	24.85	1.30
-63.20	175.64	21.95									
115		220T	220T	N	CA	1662	1663	142.48	149.80		
-42.10											
116	10173	220T	221S	C	N	1667	1669	-162.43	-136.60	44.48	1.58
-64.10	169.11	19.35									
116		221S	221S	N	CA	1669	1670	-172.59	151.20		
-35.00											
117	10175	222P	223W	C	N	1680	1682	-109.22	-124.90	17.13	0.59
-63.00	-174.83	26.20									
117		223W	223W	N	CA	1682	1683	136.49	143.40		
-44.20											
118	10176	223W	224S	C	N	1694	1696	-147.48	-136.60	18.77	1.06
-64.10	-169.84	12.06									
118		224S	224S	N	CA	1696	1697	135.90	151.20		

-35.00											
119	10180	227S	228T	C	N	1719	1721	-149.00	-124.80	26.39	1.09
-63.20	-175.03	29.27									
119		228T	228T	N	CA	1721	1722	154.03	143.50		
-42.10											
120	10181	228T	229S	C	N	1726	1728	-139.94	-136.60	3.92	0.21
-64.10	-168.50	19.27									
120		229S	229S	N	CA	1728	1729	149.16	151.20		
-35.00											
121	10183	230C	231G	C	N	1738	1740	-146.86	-167.20	23.33	0.38
82.20	-157.35	15.26									
121		231G	231G	N	CA	1740	1741	163.17	174.60		
8.50											
122	10184	231G	232L	C	N	1742	1744	-114.02	-108.50	8.16	0.46
-63.50	175.14	21.99									
122		232L	232L	N	CA	1744	1745	126.49	132.50		
-41.20											
123	10185	232L	233G	C	N	1750	1752	133.87	-167.20	58.95	1.16
82.20	172.29	10.83									
123		233G	233G	N	CA	1752	1753	172.86	174.60		
8.50											
124	10187	234V	235S	C	N	1761	1763	-164.99	-136.60	28.49	1.07
-64.10	-161.05	21.68									
124		235S	235S	N	CA	1763	1764	153.53	151.20		
-35.00											
125	10188	235S	236T	C	N	1767	1769	-121.47	-124.80	36.02	1.45
-63.20	160.68	17.48									
125		236T	236T	N	CA	1769	1770	107.64	143.50		
-42.10											
126	10189	236T	237R	C	N	1774	1776	-134.58	-125.20	9.41	0.36
-63.00	-168.62	30.77									
126		237R	237R	N	CA	1776	1777	141.41	140.60		
-41.10											
127	10191	238I	239S	C	N	1793	1795	-109.30	-136.60	50.82	1.87
-64.10	150.29	9.26									
127		239S	239S	N	CA	1795	1796	108.33	151.20		
-35.00											
128	10192	239S	240N	C	N	1799	1801	-119.65	-119.90	2.85	0.12
-63.20	-175.87	20.45									
128		240N	240N	N	CA	1801	1802	134.17	137.00		
-41.10											
129	10194	241V	242N	C	N	1814	1816	-71.44	-71.20	6.96	0.44
-63.20	169.35	21.63									
129		242N	242N	N	CA	1816	1817	149.76	142.80		
-41.10											
130	10195	242N	243A	C	N	1822	1824	-63.93	-68.20	30.54	2.31
-62.50	155.96	25.49									
130		243A	243A	N	CA	1824	1825	115.06	145.30		

-40.90											
131	10196	243A	244Q	C	N	1827	1829	-175.80	-121.10	74.39	2.38
-63.80	171.28	30.57									
131		244Q	244Q	N	CA	1829	1830	-169.89	139.70		
-40.30											
132	10197	244Q	245C	C	N	1836	1838	-58.54	-63.00	20.48	2.24
-117.90	168.60	7.34									
132		245C	245C	N	CA	1838	1839	-61.09	-41.10		
141.10											
133	10198	245C	246W	C	N	1842	1844	-167.47	-124.90	43.04	2.05
-63.00	-152.94	32.91									
133		246W	246W	N	CA	1844	1845	137.02	143.40		
-44.20											
134	10200	247P	248E	C	N	1863	1865	-81.88	-69.30	16.42	1.51
-63.60	173.21	22.14									
134		248E	248E	N	CA	1865	1866	131.94	142.50		
-40.30											
135	10201	248E	249Q	C	N	1872	1874	-85.88	-73.00	13.93	0.89
-63.80	175.10	26.92									
135		249Q	249Q	N	CA	1874	1875	146.00	140.70		
-40.30											
136	10202	249Q	250E	C	N	1881	1883	-119.63	-117.80	14.64	0.76
-63.60	171.96	20.42									
136		250E	250E	N	CA	1883	1884	122.28	136.80		
-40.30											
137	10203	250E	251S	C	N	1890	1892	63.13	-72.40	135.62	9.83
-64.10	-149.64	15.19									
137		251S	251S	N	CA	1892	1893	157.47	152.40		
-35.00											
138	10204	251S	252R	C	N	1896	1898	-111.77	-125.20	83.32	3.71
-63.00	110.78	12.61									
138		252R	252R	N	CA	1898	1899	58.37	140.60		
-41.10											
139	10205	252R	253L	C	N	1907	1909	-135.79	-108.50	32.41	1.77
-63.50	172.13	21.13									
139		253L	253L	N	CA	1909	1910	115.02	132.50		
-41.20											
140	10207	254C	255N	C	N	1921	1923	-100.34	-119.90	22.08	1.14
-63.20	175.64	24.07									
140		255N	255N	N	CA	1923	1924	147.24	137.00		
-41.10											
141	10209	256L	257R	C	N	1937	1939	138.70	-125.20	98.95	3.39
-63.00	-138.67	39.69									
141		257R	257R	N	CA	1939	1940	164.21	140.60		
-41.10											
142	10211	258P	259C	C	N	1955	1957	-66.93	-63.00	4.42	0.79
-117.90	-176.99	7.84									
142		259C	259C	N	CA	1957	1958	-43.13	-41.10		

141.10											
143	10212	259C	260D	C	N	1961	1963	-67.92	-70.90	5.36	0.18
-63.30	174.22	21.79									
143		260D	260D	N	CA	1963	1964	145.85	150.30		
-40.00											
144	10214	261V	262D	C	N	1976	1978	-96.42	-70.90	46.96	1.60
-63.30	134.42	18.72									
144		262D	262D	N	CA	1978	1979	-170.28	150.30		
-40.00											
145	10216	263I	264H	C	N	1992	1994	59.75	56.30	5.95	0.48
-63.20	145.73	25.01									
145		264H	264H	N	CA	1994	1995	35.95	40.80		
-42.30											
146	10217	264H	265T	C	N	2002	2004	-107.87	-124.80	16.96	0.92
-63.20	178.99	25.93									
146		265T	265T	N	CA	2004	2005	144.58	143.50		
-42.10											
147	10218	265T	266L	C	N	2009	2011	-105.71	-108.50	17.11	0.95
-63.50	174.59	26.83									
147		266L	266L	N	CA	2011	2012	149.38	132.50		
-41.20											
148	10222	269A	270G	C	N	2039	2041	137.89	78.70	67.56	3.79
-80.20	151.26	8.02									
148		270G	270G	N	CA	2041	2042	-133.53	-166.10		
174.10											
149	10229	276V	277Y	C	N	2087	2089	168.78	-124.30	66.99	5.13
-63.50	-142.73	29.97									
149		277Y	277Y	N	CA	2089	2090	132.36	135.40		
-43.40											
150	10230	277Y	278Q	C	N	2099	2101	-72.74	-73.00	9.47	0.61
-63.80	171.77	24.80									
150		278Q	278Q	N	CA	2101	2102	131.24	140.70		
-40.30											
151	10232	279P	280E	C	N	2115	2117	-99.49	-117.80	25.55	1.36
-63.60	168.94	24.55									
151		280E	280E	N	CA	2117	2118	154.62	136.80		
-40.30											
152	10233	280E	281A	C	N	2124	2126	-62.10	-68.20	10.32	0.65
-62.50	177.88	29.17									
152		281A	281A	N	CA	2126	2127	136.98	145.30		
-40.90											
153	10234	281A	282S	C	N	2129	2131	-126.81	-136.60	23.76	0.96
-64.10	176.10	10.87									
153		282S	282S	N	CA	2131	2132	129.55	151.20		
-35.00											
154	10236	283M	284N	C	N	2143	2145	-76.27	-71.20	9.93	0.77
-63.20	175.85	21.29									
154		284N	284N	N	CA	2145	2146	134.26	142.80		

-41.10	155	10239	286T	287L	C	N	2169	2171	-108.56	-108.50	7.55	0.41
-63.50	-175.66	28.36										
	155		287L	287L	N	CA	2171	2172	140.05	132.50		
-41.20												
	156	10240	287L	288A	C	N	2177	2179	-121.06	-134.00	14.53	0.33
-62.50	-171.93	33.94										
	156		288A	288A	N	CA	2179	2180	140.38	147.00		
-40.90												
	157	10244	291I	292S	C	N	2200	2202	-76.90	-72.40	8.13	0.37
-64.10	166.33	12.86										
	157		292S	292S	N	CA	2202	2203	159.16	152.40		
-35.00												
	158	10245	292S	293T	C	N	2206	2208	-130.19	-124.80	27.91	1.04
-63.20	161.56	25.10										
	158		293T	293T	N	CA	2208	2209	170.88	143.50		
-42.10												
	159	10246	293T	294R	C	N	2213	2215	-109.76	-125.20	18.58	0.55
-63.00	177.63	21.26										
	159		294R	294R	N	CA	2215	2216	130.27	140.60		
-41.10												
	160	10247	294R	295S	C	N	2224	2226	-145.36	-136.60	14.47	0.82
-64.10	-167.34	12.12										
	160		295S	295S	N	CA	2226	2227	139.68	151.20		
-35.00												
	161	10248	295S	296Y	C	N	2230	2232	-121.01	-124.30	13.24	0.57
-63.50	175.66	25.24										
	161		296Y	296Y	N	CA	2232	2233	122.57	135.40		
-43.40												
	162	10249	296Y	297Q	C	N	2242	2244	-146.68	-121.10	32.18	1.00
-63.80	-179.38	30.86										
	162		297Q	297Q	N	CA	2244	2245	159.22	139.70		
-40.30												
	163	10251	298P	299K	C	N	2258	2260	73.10	56.60	128.53	10.46
-62.90	-155.19	24.44										
	163		299K	299K	N	CA	2260	2261	166.07	38.60		
-40.80												
	164	10252	299K	300Y	C	N	2267	2269	-105.47	-98.40	13.58	1.23
-63.50	165.62	24.28										
	164		300Y	300Y	N	CA	2269	2270	116.81	128.40		
-43.40												
	165	10254	301C	302G	C	N	2285	2287	-155.42	-167.20	17.05	0.39
82.20	-163.48	14.68										
	165		302G	302G	N	CA	2287	2288	162.28	174.60		
8.50												
	166	10257	304C	305M	C	N	2302	2304	-73.63	-73.00	41.78	2.81
-63.40	135.11	20.98										
	166		305M	305M	N	CA	2304	2305	-175.22	143.00		

-40.50											
167	10258	305M	306D	C	N	2310	2312	-76.42	-96.50	61.47	2.59
-63.30	97.00	11.24									
167		306D	306D	N	CA	2312	2313	56.11	114.20		
-40.00											
168	10259	306D	307N	C	N	2318	2320	-117.88	-119.90	4.82	0.26
-63.20	-174.25	26.34									
168		307N	307N	N	CA	2320	2321	141.38	137.00		
-41.10											
169	10264	311I	312P	C	N	2357	2359	-59.09	-58.70	2.24	0.22
-64.50	179.99	13.15									
169		312P	312P	N	CA	2359	2360	-32.71	-30.50		
147.20											
170	10266	313Y	314K	C	N	2376	2378	-74.82	-70.20	8.35	0.51
-62.90	172.26	23.04									
170		314K	314K	N	CA	2378	2379	147.35	140.40		
-40.80											
171	10268	315S	316K	C	N	2391	2393	-80.99	-70.20	11.68	0.94
-62.90	177.66	22.14									
171		316K	316K	N	CA	2393	2394	135.93	140.40		
-40.80											
172	10269	316K	317T	C	N	2400	2402	-125.08	-124.80	31.59	1.36
-63.20	165.98	18.00									
172		317T	317T	N	CA	2402	2403	111.91	143.50		
-42.10											
173	10270	317T	318I	C	N	2407	2409	-68.01	-63.40	5.41	1.02
-120.60	-175.61	8.60									
173		318I	318I	N	CA	2409	2410	-46.43	-43.60		
130.30											
174	10271	318I	319D	C	N	2415	2417	160.90	-96.50	119.88	4.98
-63.30	-162.21	32.71									
174		319D	319D	N	CA	2417	2418	176.20	114.20		
-40.00											
175	10272	319D	320V	C	N	2423	2425	-61.42	-62.40	8.47	1.02
-73.50	170.41	14.71									
175		320V	320V	N	CA	2425	2426	-50.81	-42.40		
139.20											
176	10278	325P	326D	C	N	2469	2471	-169.04	-70.90	130.12	5.64
-63.30	135.21	22.86									
176		326D	326D	N	CA	2471	2472	-124.27	150.30		
-40.00											
177	10280	327G	328L	C	N	2481	2483	-61.72	-70.70	20.39	1.28
-63.50	164.51	22.94									
177		328L	328L	N	CA	2483	2484	123.30	141.60		
-41.20											
178	10282	329G	330F	C	N	2493	2495	-139.95	-124.20	18.92	0.49
-63.20	179.19	29.84									
178		330F	330F	N	CA	2495	2496	153.78	143.30		

-44.30	179	10283	330F	331S	C	N	2504	2506	-111.05	-136.60	25.64	0.96
-64.10	-177.83	16.43										
	179		331S	331S	N	CA	2506	2507	148.98	151.20		
-35.00												
	180	10284	331S	332R	C	N	2510	2512	-73.20	-72.10	1.11	0.09
-63.00	177.42	24.66										
	180		332R	332R	N	CA	2512	2513	141.77	141.90		
-41.10												
	181	10285	332R	333Q	C	N	2521	2523	-124.63	-121.10	17.96	0.79
-63.80	173.41	28.72										
	181		333Q	333Q	N	CA	2523	2524	157.31	139.70		
-40.30												
	182	10287	334V	335L	C	N	2537	2539	-109.13	-108.50	2.25	0.11
-63.50	-178.31	23.04										
	182		335L	335L	N	CA	2539	2540	134.67	132.50		
-41.20												
	183	10288	335L	336W	C	N	2545	2547	-142.02	-124.90	22.05	0.70
-63.00	177.11	27.46										
	183		336W	336W	N	CA	2547	2548	157.29	143.40		
-44.20												
	184	10290	337I	338N	C	N	2567	2569	-121.33	-119.90	7.56	0.37
-63.20	-179.70	19.94										
	184		338N	338N	N	CA	2569	2570	129.57	137.00		
-41.10												
	185	10291	338N	339A	C	N	2575	2577	-145.27	-134.00	11.63	0.29
-62.50	-171.61	35.31										
	185		339A	339A	N	CA	2577	2578	149.87	147.00		
-40.90												
	186	10293	340C	341F	C	N	2586	2588	-137.35	-124.20	13.41	0.60
-63.20	-169.93	31.23										
	186		341F	341F	N	CA	2588	2589	140.69	143.30		
-44.30												
	187	10295	342C	343N	C	N	2603	2605	-138.03	-119.90	19.48	0.63
-63.20	-169.85	28.01										
	187		343N	343N	N	CA	2605	2606	144.10	137.00		
-41.10												
	188	10296	343N	344L	C	N	2611	2613	-125.03	-108.50	18.58	0.99
-63.50	176.31	21.85										
	188		344L	344L	N	CA	2613	2614	124.03	132.50		
-41.20												
	189	10297	344L	345S	C	N	2619	2621	-132.88	-136.60	10.32	0.43
-64.10	-170.50	11.71										
	189		345S	345S	N	CA	2621	2622	141.58	151.20		
-35.00												
	190	10299	346C	347R	C	N	2631	2633	-138.62	-125.20	16.11	0.48
-63.00	-174.50	30.23										
	190		347R	347R	N	CA	2633	2634	149.51	140.60		

-41.10											
191	10300	347R	348N	C	N	2642	2644	-111.97	-119.90	14.69	0.47
-63.20	172.76	19.33									
191		348N	348N	N	CA	2644	2645	124.64	137.00		
-41.10											
192	10302	349P	350N	C	N	2657	2659	-116.73	-119.90	21.37	0.89
-63.20	165.84	18.34									
192		350N	350N	N	CA	2659	2660	115.87	137.00		
-41.10											
193	10303	350N	351D	C	N	2665	2667	-134.81	-96.50	38.37	1.56
-63.30	168.21	17.88									
193		351D	351D	N	CA	2667	2668	112.25	114.20		
-40.00											
194	10305	352I	353F	C	N	2681	2683	-113.65	-124.20	24.95	0.87
-63.20	172.54	20.88									
194		353F	353F	N	CA	2683	2684	120.69	143.30		
-44.30											
195	10306	353F	354A	C	N	2692	2694	-169.18	-134.00	36.73	0.89
-62.50	-166.39	37.38									
195		354A	354A	N	CA	2694	2695	157.54	147.00		
-40.90											
196	10307	354A	355D	C	N	2697	2699	-124.81	-96.50	43.61	1.79
-63.30	135.76	14.41									
196		355D	355D	N	CA	2699	2700	81.03	114.20		
-40.00											
197	10308	355D	356L	C	N	2705	2707	-111.58	-108.50	5.86	0.33
-63.50	175.43	22.11									
197		356L	356L	N	CA	2707	2708	127.51	132.50		
-41.20											
198	10309	356L	357E	C	N	2713	2715	-109.27	-117.80	11.51	0.36
-63.60	175.42	21.22									
198		357E	357E	N	CA	2715	2716	129.07	136.80		
-40.30											
199	10310	357E	358S	C	N	2722	2724	-75.74	-72.40	5.48	0.43
-64.10	177.33	13.57									
199		358S	358S	N	CA	2724	2725	148.05	152.40		
-35.00											
200	10311	358S	359Y	C	N	2728	2730	-120.00	-124.30	11.12	0.45
-63.50	177.76	25.60									
200		359Y	359Y	N	CA	2730	2731	125.14	135.40		
-43.40											
201	10313	360P	361D	C	N	2747	2749	-104.13	-96.50	22.81	0.95
-63.30	138.84	15.15									
201		361D	361D	N	CA	2749	2750	92.71	114.20		
-40.00											
202	10314	361D	362F	C	N	2755	2757	-126.98	-124.20	3.14	0.08
-63.20	-177.55	29.54									
202		362F	362F	N	CA	2757	2758	144.76	143.30		

```

-44.30
  203  10315  362F  363S  C   N   2766  2768 -142.15 -136.60    7.28    0.23
-64.10 -173.76   19.07
  203           363S  363S  N   CA   2768  2769  155.90  151.20
-35.00
  204  10316  363S  364E  C   N   2772  2774  -80.97  -69.30   16.65    0.93
-63.60  166.23   23.13
  204           364E  364E  N   CA   2774  2775  154.38  142.50
-40.30
  205  10318  365I  366A  C   N   2789  2791 -126.48 -134.00   10.69    0.63
-62.50  176.50   32.35
  205           366A  366A  N   CA   2791  2792  154.60  147.00
-40.90

```

report_____> Distribution of short non-bonded contacts:

```

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:    0    0    0    0    0   18   31  140  171  197  220  240  267
290  328

```

<< end of ENERGY.

iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls_286W> MODEL atom not classified: ASN:OXT ASN

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

```

Number of all residues in MODEL           :      367
Number of all, selected real atoms         :      2804      2804
Number of all, selected pseudo atoms       :         0         0
Number of all static, selected restraints  :     13904     13904
COVALENT_CYS                             :         F
NONBONDED_SEL_ATOMS                      :         1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):    350489
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      :    -19009.3887

```

<< end of ENERGY.

```
DOPE score           : -19009.388672
```

>> Model assessment by SOAP-Protein-OD score

```
preppdf_455W> None of the non-bonded terms selected.
```

```
pair2___701W> Insufficient system memory to allocate storage for cell-based
               (NlogN) nonbond list algorithm; falling back to N*N method.
```

```
Warning          2 of          10; further warnings will be suppressed.
```

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

```

Number of all residues in MODEL           :      367
Number of all, selected real atoms        :    2804    2804
Number of all, selected pseudo atoms      :         0         0
Number of all static, selected restraints :    13904    13904
COVALENT_CYS                             :         F
NONBONDED_SEL_ATOMS                      :         1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):         0
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                           :    0.000
DYNAMIC_PAIRS,_SPHERE,_COULOMB,_LENNARD,_MODELLER :      T      F      F
F      F
SPHERE_STDV                             :     0.050
RADII_FACTOR                            :     0.820
Current energy                           :              0.0000

```

<< end of ENERGY.

```
SOAP-Protein-OD score           :      0.000000
```

>> Model assessment by GA341 potential

```

Surface library      :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/surf5.de
Pair library        :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/pair9.de
Chain identifier     : -
% sequence identity  : 62.856998
Sequence length      : 367
Compactness          : 0.011921
Native energy (pair) : 92.750579
Native energy (surface) : 58.330122
Native energy (combined) : 11.881281
Z score (pair)       : -4.129315
Z score (surface)    : 0.984446
Z score (combined)   : -2.122395
GA341 score          : 0.678443

```

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

```

Number of all residues in MODEL      : 367
Number of all, selected real atoms   : 2804 2804
Number of all, selected pseudo atoms : 0 0
Number of all static, selected restraints : 13904 13904
COVALENT_CYS                         : F
NONBONDED_SEL_ATOMS                 : 1
Number of non-bonded pairs (excluding 1-2,1-3,1-4): 4697
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                       : 2058.1731

```

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 $-\ln(\text{pdf}) > \text{VIOL_REPORT_CUT2}[i]$.
 RMS_1 ... RMS(feature, minimally_violated_basis_restraint, NUMB).
 RMS_2 ... RMS(feature, best_value, NUMB).
 MOL.PDF ... scaled contribution to $-\ln(\text{Molecular pdf})$.

#	RESTRAINT_GROUP	NUM	NUMVI	NUMVP	RMS_1	RMS_2
MOL.PDF	S_i					

1	Bond length potential	2881	0	0	0.003	0.003
7.2587	1.000					
2	Bond angle potential	3935	0	1	1.705	1.705
214.41	1.000					
3	Stereochemical cosine torsion poten:	1962	0	92	51.760	51.760
803.93	1.000					
4	Stereochemical improper torsion pot:	1155	0	0	0.939	0.939
20.541	1.000					
5	Soft-sphere overlap restraints	4697	0	0	0.003	0.003
5.1733	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)	765	0	8	1.447	1.447
113.62	1.000					
10	Distance restraints 2 (N-O)	973	0	12	1.596	1.596
151.96	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:	366	0	0	2.853	2.853
35.120	1.000					
14	Sidechain Chi_1 dihedral restraints:	315	0	0	84.607	84.607
92.544	1.000					
15	Sidechain Chi_2 dihedral restraints:	209	0	1	74.590	74.590
83.937	1.000					
16	Sidechain Chi_3 dihedral restraints:	98	0	0	81.062	81.062
51.484	1.000					
17	Sidechain Chi_4 dihedral restraints:	34	0	0	105.174	105.174
22.703	1.000					
18	Disulfide distance restraints	5	0	0	0.004	0.004
0.13046E-01	1.000					
19	Disulfide angle restraints	10	0	0	2.119	2.119
0.99125	1.000					
20	Disulfide dihedral angle restraints:	5	0	0	24.182	24.182

2.9986	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)	:	643	0	2	0.632	0.632
28.250	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:		365	209	47	36.563	135.382
386.62	1.000					
26 Distance restraints 4 (SDCH-SDCH)	:	183	0	0	2.147	2.147
36.618	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					

Heavy relative violation of each residue is written to: WISP1.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: 62327.9180

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 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	9954	1M 2R C N	7 9	-161.17	-125.20	41.80	1.24	
-63.00	-174.85	31.56						
1		2R 2R N CA	9 10	161.91	140.60			
-41.10								
2	9955	2R 3W C N	18 20	-72.29	-71.30	12.32	0.91	
-63.00	164.79	21.18						
2		3W 3W N CA	20 21	151.28	139.00			
-44.20								
3	9956	3W 4F C N	32 34	-83.34	-71.40	30.97	2.73	
-63.20	157.71	20.58						
3		4F 4F N CA	34 35	112.12	140.70			
-44.30								
4	9957	4F 5L C N	43 45	-129.99	-108.50	43.12	2.06	
-63.50	163.08	26.76						
4		5L 5L N CA	45 46	169.89	132.50			
-41.20								
5	9959	6P 7W C N	58 60	-89.94	-71.30	48.33	4.06	
-63.00	141.20	16.26						
5		7W 7W N CA	60 61	94.41	139.00			
-44.20								
6	9960	7W 8T C N	72 74	-153.61	-124.80	30.55	1.33	
-63.20	-172.52	29.87						

6		8T	8T N	CA	74	75	153.66	143.50		
-42.10										
7	9961	8T	9L C	N	79	81	-118.64	-108.50	12.77	0.71
-63.50	174.86	21.82								
7		9L	9L N	CA	81	82	124.74	132.50		
-41.20										
8	9962	9L	10A C	N	87	89	-140.81	-134.00	8.06	0.19
-62.50	-174.83	34.54								
8		10A	10A N	CA	89	90	151.31	147.00		
-40.90										
9	9963	10A	11A C	N	92	94	-115.71	-134.00	20.78	0.48
-62.50	-174.18	28.36								
9		11A	11A N	CA	94	95	137.14	147.00		
-40.90										
10	9965	12V	13T C	N	104	106	-60.86	-78.10	34.21	1.12
-63.20	162.37	20.98								
10		13T	13T N	CA	106	107	120.25	149.80		
-42.10										
11	9966	13T	14A C	N	111	113	-170.99	-134.00	49.29	1.38
-62.50	176.74	34.64								
11		14A	14A N	CA	113	114	179.58	147.00		
-40.90										
12	9967	14A	15A C	N	116	118	-65.29	-68.20	5.02	0.49
-62.50	169.73	27.95								
12		15A	15A N	CA	118	119	149.39	145.30		
-40.90										
13	9968	15A	16A C	N	121	123	-64.14	-68.20	7.01	0.68
-62.50	168.09	27.63								
13		16A	16A N	CA	123	124	151.02	145.30		
-40.90										
14	9969	16A	17A C	N	126	128	-59.20	-68.20	22.44	1.51
-62.50	165.67	27.31								
14		17A	17A N	CA	128	129	124.74	145.30		
-40.90										
15	9970	17A	18S C	N	131	133	165.98	-136.60	66.12	2.02
-64.10	-168.26	23.22								
15		18S	18S N	CA	133	134	-176.02	151.20		
-35.00										
16	9971	18S	19T C	N	137	139	-81.39	-78.10	56.54	2.53
-63.20	136.67	16.39								
16		19T	19T N	CA	139	140	93.35	149.80		
-42.10										
17	9973	20V	21L C	N	151	153	-63.64	-70.70	21.60	1.40
-63.50	162.39	22.54								
17		21L	21L N	CA	153	154	121.19	141.60		
-41.20										
18	9974	21L	22A C	N	159	161	-169.79	-134.00	37.29	0.90
-62.50	-165.98	37.48								

18		22A	22A	N	CA	161	162	157.44	147.00		
-40.90											
19	9976	23T	24A	C	N	171	173	-135.87	-134.00	8.49	0.43
-62.50	179.50	33.35									
19		24A	24A	N	CA	173	174	155.28	147.00		
-40.90											
20	9977	24A	25L	C	N	176	178	-118.57	-108.50	11.79	0.52
-63.50	-171.92	23.59									
20		25L	25L	N	CA	178	179	138.64	132.50		
-41.20											
21	9978	25L	26S	C	N	184	186	-122.03	-136.60	16.18	0.50
-64.10	-171.72	11.60									
21		26S	26S	N	CA	186	187	144.15	151.20		
-35.00											
22	9982	29P	30T	C	N	209	211	-125.95	-124.80	4.35	0.22
-63.20	-170.70	28.43									
22		30T	30T	N	CA	211	212	139.30	143.50		
-42.10											
23	9983	30T	31T	C	N	216	218	-123.95	-124.80	17.13	0.76
-63.20	168.62	25.63									
23		31T	31T	N	CA	218	219	160.60	143.50		
-42.10											
24	9985	32M	33D	C	N	231	233	-57.13	-70.90	16.20	1.36
-63.30	161.28	19.54									
24		33D	33D	N	CA	233	234	158.84	150.30		
-40.00											
25	9986	33D	34F	C	N	239	241	-70.76	-71.40	50.11	4.02
-63.20	135.11	18.26									
25		34F	34F	N	CA	241	242	90.60	140.70		
-44.30											
26	9988	35T	36P	C	N	257	259	-67.11	-58.70	23.61	1.42
-64.50	155.66	11.75									
26		36P	36P	N	CA	259	260	-8.44	-30.50		
147.20											
27	9993	40E	41D	C	N	293	295	179.87	-96.50	90.36	3.73
-63.30	-152.42	33.03									
27		41D	41D	N	CA	295	296	148.42	114.20		
-40.00											
28	9994	41D	42T	C	N	301	303	-137.33	-124.80	18.34	0.58
-63.20	177.26	27.58									
28		42T	42T	N	CA	303	304	156.89	143.50		
-42.10											
29	9995	42T	43S	C	N	308	310	-85.07	-72.40	17.75	0.84
-64.10	161.53	13.07									
29		43S	43S	N	CA	310	311	164.83	152.40		
-35.00											
30	9996	43S	44S	C	N	314	316	-149.75	-136.60	23.69	0.86
-64.10	176.29	18.94									

30		44S	44S	N	CA	316	317	170.91	151.20		
-35.00											
31	9997	44S	45R	C	N	320	322	-99.90	-125.20	26.80	0.87
-63.00	176.76		21.63								
31		45R	45R	N	CA	322	323	131.77	140.60		
-41.10											
32	9999	46P	47Q	C	N	338	340	-152.50	-121.10	34.88	1.08
-63.80	-172.84		32.10								
32		47Q	47Q	N	CA	340	341	154.89	139.70		
-40.30											
33	10000	47Q	48F	C	N	347	349	-100.73	-124.20	38.35	1.12
-63.20	161.70		20.09								
33		48F	48F	N	CA	349	350	112.98	143.30		
-44.30											
34	10002	49C	50K	C	N	364	366	-147.52	-118.00	29.66	1.17
-62.90	-163.79		22.55								
34		50K	50K	N	CA	366	367	136.23	139.10		
-40.80											
35	10003	50K	51W	C	N	373	375	-152.14	-124.90	33.25	1.06
-63.00	177.35		28.17								
35		51W	51W	N	CA	375	376	162.48	143.40		
-44.20											
36	10004	51W	52P	C	N	387	389	-66.63	-58.70	9.28	0.83
-64.50	172.90		13.01								
36		52P	52P	N	CA	389	390	-25.69	-30.50		
147.20											
37	10006	53C	54E	C	N	400	402	-110.65	-117.80	8.70	0.44
-63.60	-175.95		27.20								
37		54E	54E	N	CA	402	403	141.76	136.80		
-40.30											
38	10010	57P	58S	C	N	429	431	-144.40	-136.60	13.22	0.47
-64.10	-178.19		18.92								
38		58S	58S	N	CA	431	432	161.88	151.20		
-35.00											
39	10013	60P	61R	C	N	449	451	-152.33	-125.20	37.73	1.14
-63.00	176.38		29.82								
39		61R	61R	N	CA	451	452	166.82	140.60		
-41.10											
40	10016	63P	64L	C	N	473	475	-70.76	-70.70	3.12	0.24
-63.50	179.83		24.56								
40		64L	64L	N	CA	475	476	138.48	141.60		
-41.20											
41	10017	64L	65G	C	N	481	483	60.34	78.70	37.16	0.56
82.20	143.97		8.07								
41		65G	65G	N	CA	483	484	-133.79	-166.10		
8.50											
42	10019	66V	67S	C	N	492	494	-69.86	-72.40	14.93	0.97
-64.10	157.99		11.80								

42		67S	67S N	CA	494	495	167.11	152.40		
-35.00										
43	10020	67S	68L C	N	498	500	-64.47	-70.70	11.43	0.71
-63.50	173.22	24.00								
43		68L	68L N	CA	500	501	132.02	141.60		
-41.20										
44	10022	69I	70T C	N	514	516	-85.99	-78.10	8.50	0.56
-63.20	172.76	23.67								
44		70T	70T N	CA	516	517	146.65	149.80		
-42.10										
45	10023	70T	71D C	N	521	523	-89.21	-70.90	45.11	1.53
-63.30	131.07	17.83								
45		71D	71D N	CA	523	524	-168.48	150.30		
-40.00										
46	10024	71D	72G C	N	529	531	102.63	78.70	48.70	0.73
82.20	144.43	8.02								
46		72G	72G N	CA	531	532	151.48	-166.10		
8.50										
47	10026	73C	74E C	N	539	541	-103.36	-117.80	14.52	0.49
-63.60	179.97	22.05								
47		74E	74E N	CA	541	542	135.22	136.80		
-40.30										
48	10029	76C	77K C	N	560	562	-111.67	-118.00	6.41	0.23
-62.90	-174.58	21.91								
48		77K	77K N	CA	562	563	138.09	139.10		
-40.80										
49	10030	77K	78M C	N	569	571	-134.47	-125.60	21.67	0.82
-63.40	174.37	31.64								
49		78M	78M N	CA	571	572	160.27	140.50		
-40.50										
50	10032	79C	80A C	N	583	585	-147.01	-134.00	25.79	1.03
-62.50	172.03	32.70								
50		80A	80A N	CA	585	586	169.26	147.00		
-40.90										
51	10033	80A	81Q C	N	588	590	-71.40	-73.00	17.85	1.20
-63.80	161.39	24.13								
51		81Q	81Q N	CA	590	591	158.48	140.70		
-40.30										
52	10034	81Q	82Q C	N	597	599	-96.33	-73.00	34.15	1.97
-63.80	157.46	24.89								
52		82Q	82Q N	CA	599	600	165.64	140.70		
-40.30										
53	10035	82Q	83L C	N	606	608	-88.17	-70.70	59.90	3.94
-63.50	122.42	18.50								
53		83L	83L N	CA	608	609	-161.11	141.60		
-41.20										
54	10040	87C	88T C	N	640	642	-86.51	-78.10	36.40	1.31
-63.20	134.71	18.83								

54		88T	88T N	CA	642	643	-174.78	149.80		
-42.10										
55	10041	88T	89E C	N	647	649	47.11	-69.30	120.75	7.99
-63.60	-172.99	30.89								
55		89E	89E N	CA	649	650	110.41	142.50		
-40.30										
56	10042	89E	90A C	N	656	658	170.04	-134.00	63.19	1.45
-62.50	-168.63	37.93								
56		90A	90A N	CA	658	659	176.35	147.00		
-40.90										
57	10043	90A	91A C	N	661	663	-109.59	-134.00	28.04	0.65
-62.50	-179.64	27.65								
57		91A	91A N	CA	663	664	133.20	147.00		
-40.90										
58	10046	93C	94D C	N	680	682	-140.92	-96.50	51.40	2.13
-63.30	-164.03	29.21								
58		94D	94D N	CA	682	683	140.06	114.20		
-40.00										
59	10048	95P	96H C	N	695	697	-63.99	-67.60	8.69	0.56
-63.20	174.39	21.75								
59		96H	96H N	CA	697	698	132.09	140.00		
-42.30										
60	10049	96H	97R C	N	705	707	-139.12	-125.20	27.78	0.98
-63.00	172.02	28.42								
60		97R	97R N	CA	707	708	164.64	140.60		
-41.10										
61	10050	97R	98G C	N	716	718	-63.79	-62.40	9.43	1.35
82.20	151.47	11.34								
61		98G	98G N	CA	718	719	-31.87	-41.20		
8.50										
62	10051	98G	99L C	N	720	722	-53.46	-70.70	17.26	1.54
-63.50	178.41	24.21								
62		99L	99L N	CA	722	723	140.67	141.60		
-41.20										
63	10052	99L	100Y C	N	728	730	-126.23	-124.30	12.87	0.60
-63.50	179.77	31.67								
63		100Y	100Y N	CA	730	731	148.13	135.40		
-43.40										
64	10054	101C	102D C	N	746	748	-81.14	-70.90	31.59	1.12
-63.30	140.95	18.52								
64		102D	102D N	CA	748	749	-179.82	150.30		
-40.00										
65	10055	102D	103Y C	N	754	756	-61.50	-98.40	37.07	1.51
-63.50	168.34	26.81								
65		103Y	103Y N	CA	756	757	124.92	128.40		
-43.40										
66	10056	103Y	104S C	N	766	768	-150.61	-136.60	14.62	0.48
-64.10	-169.61	20.00								

66	104S	104S	N	CA	768	769	155.39	151.20		
-35.00										
67	10059	106D	107R	C	N	784	786	-83.46	-72.10	14.23
-63.00	175.63	22.41								1.23
67		107R	107R	N	CA	786	787	133.33	141.90	
-41.10										
68	10061	108P	109R	C	N	802	804	-72.94	-72.10	3.79
-63.00	179.57	23.60								0.31
68		109R	109R	N	CA	804	805	138.20	141.90	
-41.10										
69	10062	109R	110Y	C	N	813	815	-132.79	-124.30	22.39
-63.50	174.80	31.17								0.90
69		110Y	110Y	N	CA	815	816	156.12	135.40	
-43.40										
70	10063	110Y	111A	C	N	825	827	-66.69	-68.20	2.43
-62.50	175.76	29.01								0.15
70		111A	111A	N	CA	827	828	143.39	145.30	
-40.90										
71	10065	112I	113G	C	N	838	840	-96.15	-80.20	36.37
82.20	-119.26	18.61								0.85
71		113G	113G	N	CA	840	841	-153.21	174.10	
8.50										
72	10068	115C	116A	C	N	855	857	-68.88	-68.20	2.89
-62.50	176.73	29.28								0.26
72		116A	116A	N	CA	857	858	142.49	145.30	
-40.90										
73	10072	119V	120G	C	N	883	885	-110.33	-80.20	38.51
82.20	-140.69	17.02								2.79
73		120G	120G	N	CA	885	886	150.11	174.10	
8.50										
74	10074	121V	122G	C	N	894	896	-103.31	-80.20	56.80
82.20	-151.73	16.27								3.36
74		122G	122G	N	CA	896	897	122.22	174.10	
8.50										
75	10111	158L	159R	C	N	1163	1165	-150.74	-125.20	28.86
-63.00	-173.23	31.17								0.87
75		159R	159R	N	CA	1165	1166	154.03	140.60	
-41.10										
76	10113	160V	161R	C	N	1181	1183	178.36	-125.20	79.86
-63.00	170.03	30.38								2.44
76		161R	161R	N	CA	1183	1184	-162.89	140.60	
-41.10										
77	10116	163P	164R	C	N	1206	1208	-162.11	-125.20	78.46
-63.00	147.37	26.18								2.84
77		164R	164R	N	CA	1208	1209	-150.16	140.60	
-41.10										
78	10118	165L	166W	C	N	1225	1227	-107.80	-124.90	29.27
-63.00	155.25	22.38								1.68

78	166W 166W N	CA	1227 1228	167.16	143.40		
-44.20							
79	10121 168P 169H C	N	1252 1254	-53.02	-67.60	16.25	1.41
-63.20	170.82 20.74						
79	169H 169H N	CA	1254 1255	147.18	140.00		
-42.30							
80	10122 169H 170P C	N	1262 1264	-60.00	-58.70	6.82	0.47
-64.50	171.06 12.53						
80	170P 170P N	CA	1264 1265	-23.80	-30.50		
147.20							
81	10123 170P 171R C	N	1269 1271	-102.65	-125.20	95.62	4.07
-63.00	97.23 11.13						
81	171R 171R N	CA	1271 1272	47.67	140.60		
-41.10							
82	10124 171R 172R C	N	1280 1282	-105.01	-125.20	95.82	4.15
-72.10	100.51 8.38						
82	172R 172R N	CA	1282 1283	46.93	140.60		
141.90							
83	10130 177G 178H C	N	1323 1325	-58.76	-67.60	13.05	0.78
-63.20	172.76 21.88						
83	178H 178H N	CA	1325 1326	130.40	140.00		
-42.30							
84	10133 180C 181E C	N	1345 1347	-128.65	-117.80	21.15	0.80
-63.60	177.12 27.28						
84	181E 181E N	CA	1347 1348	154.95	136.80		
-40.30							
85	10134 181E 182Q C	N	1354 1356	-95.10	-73.00	36.19	2.77
-63.80	155.52 21.35						
85	182Q 182Q N	CA	1356 1357	112.04	140.70		
-40.30							
86	10135 182Q 183W C	N	1363 1365	-151.18	-124.90	39.66	1.29
-63.00	167.75 26.89						
86	183W 183W N	CA	1365 1366	173.10	143.40		
-44.20							
87	10136 183W 184V C	N	1377 1379	-61.26	-62.40	3.14	0.35
-125.40	-177.02 10.28						
87	184V 184V N	CA	1379 1380	-45.32	-42.40		
143.30							
88	10138 185C 186E C	N	1390 1392	-84.36	-69.30	17.49	1.02
-63.60	169.60 23.77						
88	186E 186E N	CA	1392 1393	151.38	142.50		
-40.30							
89	10139 186E 187D C	N	1399 1401	-72.52	-70.90	17.54	0.95
-63.30	173.08 20.82						
89	187D 187D N	CA	1401 1402	132.84	150.30		
-40.00							
90	10141 188D 189A C	N	1415 1417	-57.66	-68.20	20.09	1.29
-62.50	169.17 27.96						

90	189A	189A	N	CA	1417	1418	128.20	145.30		
-40.90										
91	10143	190K	191R	C	N	1429	1431	-123.33	-125.20	20.50 1.03
-63.00	169.03	26.99								
91	191R	191R	N	CA	1431	1432	161.01	140.60		
-41.10										
92	10144	191R	192P	C	N	1440	1442	-53.39	-64.50	19.06 1.12
-58.70	162.30	13.84								
92	192P	192P	N	CA	1442	1443	131.71	147.20		
-30.50										
93	10145	192P	193R	C	N	1447	1449	-137.51	-125.20	15.92 0.47
-63.00	-176.04	29.95								
93	193R	193R	N	CA	1449	1450	150.70	140.60		
-41.10										
94	10146	193R	194K	C	N	1458	1460	-149.39	-118.00	112.36 4.95
-62.90	112.67	19.42								
94	194K	194K	N	CA	1460	1461	-113.01	139.10		
-40.80										
95	10147	194K	195T	C	N	1467	1469	-80.73	-78.10	43.04 1.75
-63.20	126.36	17.37								
95	195T	195T	N	CA	1469	1470	-167.24	149.80		
-42.10										
96	10148	195T	196A	C	N	1474	1476	-60.09	-68.20	17.91 1.18
-62.50	170.25	28.02								
96	196A	196A	N	CA	1476	1477	129.34	145.30		
-40.90										
97	10150	197P	198R	C	N	1486	1488	-120.77	-125.20	18.96 0.81
-63.00	173.18	20.22								
97	198R	198R	N	CA	1488	1489	122.16	140.60		
-41.10										
98	10152	199D	200T	C	N	1505	1507	-151.28	-124.80	33.05 1.16
-63.20	177.95	28.47								
98	200T	200T	N	CA	1507	1508	163.28	143.50		
-42.10										
99	10153	200T	201G	C	N	1512	1514	-135.42	-167.20	48.25 1.16
82.20	-167.35	14.89								
99	201G	201G	N	CA	1514	1515	138.28	174.60		
8.50										
100	10154	201G	202A	C	N	1516	1518	-119.58	-134.00	18.63 0.50
-62.50	-174.89	28.15								
100	202A	202A	N	CA	1518	1519	135.20	147.00		
-40.90										
101	10155	202A	203F	C	N	1521	1523	-143.93	-124.20	19.80 0.72
-63.20	-171.18	31.44								
101	203F	203F	N	CA	1523	1524	145.01	143.30		
-44.30										
102	10156	203F	204D	C	N	1532	1534	-112.14	-96.50	15.69 0.64
-63.30	162.85	17.74								

102		204D	204D	N	CA	1534	1535	115.36	114.20		
-40.00											
103	10157	204D	205A	C	N	1540	1542	-128.95	-134.00	12.08	0.53
-62.50	-171.01	28.56									
103		205A	205A	N	CA	1542	1543	136.03	147.00		
-40.90											
104	10162	209V	210E	C	N	1572	1574	-107.71	-117.80	13.21	0.41
-63.60	174.26	21.13									
104		210E	210E	N	CA	1574	1575	128.28	136.80		
-40.30											
105	10163	210E	211A	C	N	1581	1583	-68.09	-68.20	5.01	0.41
-62.50	168.88	27.95									
105		211A	211A	N	CA	1583	1584	150.32	145.30		
-40.90											
106	10164	211A	212W	C	N	1586	1588	-63.37	-71.30	26.12	1.76
-63.00	158.31	19.77									
106		212W	212W	N	CA	1588	1589	114.11	139.00		
-44.20											
107	10165	212W	213H	C	N	1600	1602	-146.61	-125.60	22.78	0.96
-63.20	-168.58	20.40									
107		213H	213H	N	CA	1602	1603	129.99	138.80		
-42.30											
108	10166	213H	214R	C	N	1610	1612	-159.02	-125.20	56.69	1.86
-63.00	163.88	28.44									
108		214R	214R	N	CA	1612	1613	-173.90	140.60		
-41.10											
109	10167	214R	215N	C	N	1621	1623	-60.83	-71.20	10.55	0.81
-63.20	174.19	21.65									
109		215N	215N	N	CA	1623	1624	144.72	142.80		
-41.10											
110	10168	215N	216C	C	N	1629	1631	-62.61	-63.00	2.01	0.22
-117.90	-175.69	7.94									
110		216C	216C	N	CA	1631	1632	-43.07	-41.10		
141.10											
111	10170	217I	218A	C	N	1643	1645	160.94	-134.00	66.55	1.73
-62.50	-151.08	41.30									
111		218A	218A	N	CA	1645	1646	160.99	147.00		
-40.90											
112	10171	218A	219Y	C	N	1648	1650	-118.54	-124.30	23.43	1.02
-63.50	165.51	23.75									
112		219Y	219Y	N	CA	1650	1651	112.69	135.40		
-43.40											
113	10172	219Y	220T	C	N	1660	1662	-157.18	-63.20	107.75	18.56
-63.20	107.75	18.56									
113		220T	220T	N	CA	1662	1663	-94.80	-42.10		
-42.10											
114	10173	220T	221S	C	N	1667	1669	-59.16	-72.40	13.47	0.88
-64.10	175.15	12.40									

114		221S	221S	N	CA	1669	1670	149.92	152.40		
-35.00											
115	10175	222P	223W	C	N	1680	1682	58.49	-71.30	131.69	8.79
-63.00	-158.39	33.29									
115		223W	223W	N	CA	1682	1683	116.69	139.00		
-44.20											
116	10176	223W	224S	C	N	1694	1696	-169.56	-136.60	44.83	1.42
-64.10	178.01	20.51									
116		224S	224S	N	CA	1696	1697	-178.41	151.20		
-35.00											
117	10179	226C	227S	C	N	1713	1715	-166.14	-136.60	31.09	1.01
-64.10	-166.75	21.36									
117		227S	227S	N	CA	1715	1716	160.88	151.20		
-35.00											
118	10180	227S	228T	C	N	1719	1721	-137.03	-124.80	15.17	0.54
-63.20	-178.85	28.07									
118		228T	228T	N	CA	1721	1722	152.47	143.50		
-42.10											
119	10181	228T	229S	C	N	1726	1728	-137.72	-136.60	7.44	0.40
-64.10	-166.59	12.00									
119		229S	229S	N	CA	1728	1729	143.85	151.20		
-35.00											
120	10183	230C	231G	C	N	1738	1740	-139.53	-167.20	47.58	1.27
82.20	-172.00	14.51									
120		231G	231G	N	CA	1740	1741	135.89	174.60		
8.50											
121	10184	231G	232L	C	N	1742	1744	-133.49	-108.50	53.59	2.58
-63.50	155.52	25.92									
121		232L	232L	N	CA	1744	1745	179.91	132.50		
-41.20											
122	10185	232L	233G	C	N	1750	1752	-67.44	-80.20	21.13	0.56
82.20	-149.00	6.62									
122		233G	233G	N	CA	1752	1753	157.26	174.10		
8.50											
123	10187	234V	235S	C	N	1761	1763	-130.16	-136.60	12.17	0.69
-64.10	176.31	17.46									
123		235S	235S	N	CA	1763	1764	161.53	151.20		
-35.00											
124	10188	235S	236T	C	N	1767	1769	-103.03	-124.80	55.32	1.81
-63.20	140.51	15.73									
124		236T	236T	N	CA	1769	1770	92.65	143.50		
-42.10											
125	10189	236T	237R	C	N	1774	1776	176.99	-125.20	67.35	2.00
-63.00	-172.75	33.00									
125		237R	237R	N	CA	1776	1777	175.16	140.60		
-41.10											
126	10191	238I	239S	C	N	1793	1795	-90.68	-72.40	39.37	1.82
-64.10	140.27	11.94									

126		239S	239S	N	CA	1795	1796	-172.73	152.40		
-35.00											
127	10192	239S	240N	C	N	1799	1801	-60.92	-71.20	10.55	0.81
-63.20	173.76	21.60									
127		240N	240N	N	CA	1801	1802	145.16	142.80		
-41.10											
128	10195	242N	243A	C	N	1822	1824	-59.76	-68.20	12.75	0.80
-62.50	176.66	29.09									
128		243A	243A	N	CA	1824	1825	135.74	145.30		
-40.90											
129	10196	243A	244Q	C	N	1827	1829	-157.69	-121.10	44.21	1.37
-63.80	-178.62	31.46									
129		244Q	244Q	N	CA	1829	1830	164.51	139.70		
-40.30											
130	10198	245C	246W	C	N	1842	1844	-65.95	-71.30	6.07	0.50
-63.00	173.96	21.93									
130		246W	246W	N	CA	1844	1845	141.87	139.00		
-44.20											
131	10200	247P	248E	C	N	1863	1865	-125.75	-117.80	8.17	0.35
-63.60	-174.07	22.03									
131		248E	248E	N	CA	1865	1866	134.93	136.80		
-40.30											
132	10201	248E	249Q	C	N	1872	1874	-132.31	-121.10	33.86	1.75
-63.80	163.13	21.17									
132		249Q	249Q	N	CA	1874	1875	107.75	139.70		
-40.30											
133	10203	250E	251S	C	N	1890	1892	-124.91	-136.60	31.13	1.75
-64.10	157.19	15.71									
133		251S	251S	N	CA	1892	1893	-179.96	151.20		
-35.00											
134	10204	251S	252R	C	N	1896	1898	-62.84	-72.10	11.90	1.03
-63.00	169.52	22.89									
134		252R	252R	N	CA	1898	1899	149.38	141.90		
-41.10											
135	10205	252R	253L	C	N	1907	1909	-101.44	-108.50	28.10	1.58
-63.50	163.56	25.03									
135		253L	253L	N	CA	1909	1910	159.70	132.50		
-41.20											
136	10207	254C	255N	C	N	1921	1923	-89.53	-71.20	31.89	2.50
-63.20	159.98	18.67									
136		255N	255N	N	CA	1923	1924	116.70	142.80		
-41.10											
137	10208	255N	256L	C	N	1929	1931	-137.68	-108.50	31.83	1.41
-63.50	-171.25	30.80									
137		256L	256L	N	CA	1931	1932	145.24	132.50		
-41.20											
138	10209	256L	257R	C	N	1937	1939	-74.44	-72.10	4.00	0.35
-63.00	-179.88	23.58									

138	257R	257R	N	CA	1939	1940	138.66	141.90			
-41.10											
139	10212	259C	260D	C	N	1961	1963	-119.85	-96.50	34.85	1.43
-63.30	140.23	14.94									
139	260D	260D	N	CA	1963	1964	88.33	114.20			
-40.00											
140	10213	260D	261V	C	N	1969	1971	-63.74	-62.40	10.96	1.47
-125.40	174.67	9.82									
140	261V	261V	N	CA	1971	1972	-53.28	-42.40			
143.30											
141	10214	261V	262D	C	N	1976	1978	-118.78	-96.50	37.47	1.57
-63.30	-175.78	26.32									
141	262D	262D	N	CA	1978	1979	144.33	114.20			
-40.00											
142	10216	263I	264H	C	N	1992	1994	-121.70	-125.60	19.48	0.66
-63.20	172.25	18.69									
142	264H	264H	N	CA	1994	1995	119.71	138.80			
-42.30											
143	10217	264H	265T	C	N	2002	2004	-104.89	-124.80	38.67	1.20
-63.20	158.05	17.84									
143	265T	265T	N	CA	2004	2005	110.35	143.50			
-42.10											
144	10218	265T	266L	C	N	2009	2011	-134.00	-108.50	25.53	1.20
-63.50	-171.38	23.28									
144	266L	266L	N	CA	2011	2012	133.75	132.50			
-41.20											
145	10225	272K	273C	C	N	2061	2063	65.23	57.40	16.35	0.56
-117.90	-146.56	9.14									
145	273C	273C	N	CA	2063	2064	21.64	36.00			
141.10											
146	10229	276V	277Y	C	N	2087	2089	-101.04	-98.40	34.26	3.62
-63.50	142.67	20.86									
146	277Y	277Y	N	CA	2089	2090	94.24	128.40			
-43.40											
147	10230	277Y	278Q	C	N	2099	2101	-79.53	-73.00	31.82	1.95
-63.80	148.69	22.70									
147	278Q	278Q	N	CA	2101	2102	171.84	140.70			
-40.30											
148	10232	279P	280E	C	N	2115	2117	-120.31	-117.80	7.08	0.30
-63.60	-174.82	27.90									
148	280E	280E	N	CA	2117	2118	143.42	136.80			
-40.30											
149	10233	280E	281A	C	N	2124	2126	-122.21	-134.00	12.55	0.58
-62.50	178.09	32.38									
149	281A	281A	N	CA	2126	2127	151.32	147.00			
-40.90											
150	10234	281A	282S	C	N	2129	2131	79.14	-136.60	145.87	5.25
-64.10	-150.98	16.49									

150		282S	282S	N	CA	2131	2132	172.78	151.20		
-35.00											
151	10235	282S	283M	C	N	2135	2137	-110.20	-125.60	23.34	0.74
-63.40	170.04	22.21									
151		283M	283M	N	CA	2137	2138	122.96	140.50		
-40.50											
152	10236	283M	284N	C	N	2143	2145	-123.29	-119.90	7.58	0.26
-63.20	-174.85	26.57									
152		284N	284N	N	CA	2145	2146	143.78	137.00		
-41.10											
153	10239	286T	287L	C	N	2169	2171	91.89	-108.50	159.62	7.62
-63.50	-127.95	41.42									
153		287L	287L	N	CA	2171	2172	131.13	132.50		
-41.20											
154	10240	287L	288A	C	N	2177	2179	-123.56	-134.00	10.69	0.28
-62.50	-175.19	33.55									
154		288A	288A	N	CA	2179	2180	144.68	147.00		
-40.90											
155	10241	288A	289G	C	N	2182	2184	-64.29	-62.40	4.62	0.79
82.20	156.10	11.93									
155		289G	289G	N	CA	2184	2185	-45.42	-41.20		
8.50											
156	10244	291I	292S	C	N	2200	2202	-80.85	-72.40	8.80	0.68
-64.10	175.84	13.81									
156		292S	292S	N	CA	2202	2203	149.96	152.40		
-35.00											
157	10245	292S	293T	C	N	2206	2208	-114.06	-124.80	73.11	2.82
-63.20	124.18	13.33									
157		293T	293T	N	CA	2208	2209	71.18	143.50		
-42.10											
158	10246	293T	294R	C	N	2213	2215	-163.69	-125.20	42.76	1.31
-63.00	-171.23	32.21									
158		294R	294R	N	CA	2215	2216	159.22	140.60		
-41.10											
159	10247	294R	295S	C	N	2224	2226	-79.25	-72.40	9.88	0.47
-64.10	166.18	13.00									
159		295S	295S	N	CA	2226	2227	159.52	152.40		
-35.00											
160	10248	295S	296Y	C	N	2230	2232	-118.67	-124.30	14.43	0.58
-63.50	174.47	25.14									
160		296Y	296Y	N	CA	2232	2233	122.11	135.40		
-43.40											
161	10249	296Y	297Q	C	N	2242	2244	-120.51	-121.10	9.05	0.42
-63.80	-179.87	23.92									
161		297Q	297Q	N	CA	2244	2245	130.67	139.70		
-40.30											
162	10251	298P	299K	C	N	2258	2260	-141.65	-118.00	38.31	1.42
-62.90	169.37	26.70									

162		299K	299K	N	CA	2260	2261	169.25	139.10		
-40.80											
163	10252	299K	300Y	C	N	2267	2269	-106.90	-98.40	9.15	0.46
-63.50	173.93	25.52									
163		300Y	300Y	N	CA	2269	2270	125.03	128.40		
-43.40											
164	10254	301C	302G	C	N	2285	2287	-71.24	-80.20	28.78	0.74
82.20	-153.47	6.86									
164		302G	302G	N	CA	2287	2288	146.75	174.10		
8.50											
165	10257	304C	305M	C	N	2302	2304	-73.84	-73.00	38.68	2.60
-63.40	138.22	21.46									
165		305M	305M	N	CA	2304	2305	-178.33	143.00		
-40.50											
166	10258	305M	306D	C	N	2310	2312	-60.75	-70.90	10.49	0.86
-63.30	167.07	20.47									
166		306D	306D	N	CA	2312	2313	152.95	150.30		
-40.00											
167	10259	306D	307N	C	N	2318	2320	-125.03	-119.90	35.03	1.47
-63.20	159.71	23.47									
167		307N	307N	N	CA	2320	2321	171.65	137.00		
-41.10											
168	10260	307N	308R	C	N	2326	2328	-115.83	-125.20	155.09	7.69
-125.20	155.09	7.69									
168		308R	308R	N	CA	2328	2329	-64.60	140.60		
140.60											
169	10265	312P	313Y	C	N	2364	2366	-111.13	-98.40	12.74	0.50
-63.50	178.77	26.11									
169		313Y	313Y	N	CA	2366	2367	128.91	128.40		
-43.40											
170	10266	313Y	314K	C	N	2376	2378	-81.46	-70.20	13.93	0.84
-62.90	171.60	23.34									
170		314K	314K	N	CA	2378	2379	148.61	140.40		
-40.80											
171	10267	314K	315S	C	N	2385	2387	-66.91	-72.40	49.79	2.74
-64.10	137.95	9.83									
171		315S	315S	N	CA	2387	2388	102.92	152.40		
-35.00											
172	10268	315S	316K	C	N	2391	2393	179.92	-118.00	71.51	2.37
-62.90	-173.87	31.01									
172		316K	316K	N	CA	2393	2394	174.59	139.10		
-40.80											
173	10269	316K	317T	C	N	2400	2402	-87.44	-78.10	95.29	4.39
-63.20	100.05	11.40									
173		317T	317T	N	CA	2402	2403	54.97	149.80		
-42.10											
174	10270	317T	318I	C	N	2407	2409	-65.89	-63.40	3.92	0.73
-120.60	-174.80	8.58									

174		318I	318I	N	CA	2409	2410	-46.63	-43.60		
130.30											
175	10271	318I	319D	C	N	2415	2417	57.90	54.50	13.92	0.78
-63.30	138.67	23.68									
175		319D	319D	N	CA	2417	2418	27.40	40.90		
-40.00											
176	10272	319D	320V	C	N	2423	2425	173.95	-125.40	83.07	2.28
-73.50	127.95	8.68									
176		320V	320V	N	CA	2425	2426	-159.94	143.30		
139.20											
177	10278	325P	326D	C	N	2469	2471	-67.58	-96.50	30.23	1.24
-63.30	145.48	17.70									
177		326D	326D	N	CA	2471	2472	105.41	114.20		
-40.00											
178	10279	326D	327G	C	N	2477	2479	-130.68	-167.20	37.22	0.57
82.20	-143.45	16.48									
178		327G	327G	N	CA	2479	2480	167.41	174.60		
8.50											
179	10280	327G	328L	C	N	2481	2483	-102.09	-108.50	19.62	1.11
-63.50	172.14	26.26									
179		328L	328L	N	CA	2483	2484	151.04	132.50		
-41.20											
180	10281	328L	329G	C	N	2489	2491	-73.84	-80.20	16.96	0.41
82.20	-143.64	6.92									
180		329G	329G	N	CA	2491	2492	158.38	174.10		
8.50											
181	10282	329G	330F	C	N	2493	2495	-112.76	-124.20	12.74	0.65
-63.20	173.98	27.47									
181		330F	330F	N	CA	2495	2496	148.92	143.30		
-44.30											
182	10283	330F	331S	C	N	2504	2506	-117.85	-136.60	18.75	0.76
-64.10	-178.53	16.89									
182		331S	331S	N	CA	2506	2507	151.67	151.20		
-35.00											
183	10284	331S	332R	C	N	2510	2512	-121.64	-125.20	5.00	0.27
-63.00	-175.63	28.95									
183		332R	332R	N	CA	2512	2513	144.10	140.60		
-41.10											
184	10285	332R	333Q	C	N	2521	2523	-106.76	-121.10	15.55	0.71
-63.80	179.19	28.64									
184		333Q	333Q	N	CA	2523	2524	145.73	139.70		
-40.30											
185	10287	334V	335L	C	N	2537	2539	-140.09	-108.50	44.08	2.47
-63.50	162.19	19.87									
185		335L	335L	N	CA	2539	2540	101.76	132.50		
-41.20											
186	10288	335L	336W	C	N	2545	2547	-142.44	-124.90	23.83	1.36
-63.00	-171.02	20.75									

186		336W 336W N	CA	2547 2548	127.27	143.40		
-44.20								
187	10290	337I 338N C	N	2567 2569	-123.97	-119.90	22.61	1.11
-63.20	167.29	18.31						
187		338N 338N N	CA	2569 2570	114.76	137.00		
-41.10								
188	10291	338N 339A C	N	2575 2577	-176.08	-134.00	42.18	1.29
-62.50	-156.16	39.42						
188		339A 339A N	CA	2577 2578	149.85	147.00		
-40.90								
189	10293	340C 341F C	N	2586 2588	-126.31	-124.20	8.56	0.45
-63.20	-169.91	22.64						
189		341F 341F N	CA	2588 2589	135.01	143.30		
-44.30								
190	10295	342C 343N C	N	2603 2605	-113.17	-119.90	24.91	0.96
-63.20	162.02	17.99						
190		343N 343N N	CA	2605 2606	113.02	137.00		
-41.10								
191	10296	343N 344L C	N	2611 2613	-129.99	-108.50	23.91	1.27
-63.50	176.24	21.74						
191		344L 344L N	CA	2613 2614	122.01	132.50		
-41.20								
192	10297	344L 345S C	N	2619 2621	-137.28	-136.60	10.42	0.54
-64.10	-169.58	11.83						
192		345S 345S N	CA	2621 2622	140.80	151.20		
-35.00								
193	10299	346C 347R C	N	2631 2633	-132.20	-125.20	9.09	0.49
-63.00	-170.99	21.85						
193		347R 347R N	CA	2633 2634	134.79	140.60		
-41.10								
194	10300	347R 348N C	N	2642 2644	-115.35	-119.90	27.15	1.12
-63.20	160.07	17.68						
194		348N 348N N	CA	2644 2645	110.24	137.00		
-41.10								
195	10302	349P 350N C	N	2657 2659	-123.00	-119.90	15.19	0.75
-63.20	173.84	19.11						
195		350N 350N N	CA	2659 2660	122.13	137.00		
-41.10								
196	10303	350N 351D C	N	2665 2667	-122.72	-96.50	28.31	1.15
-63.30	155.33	16.60						
196		351D 351D N	CA	2667 2668	103.52	114.20		
-40.00								
197	10305	352I 353F C	N	2681 2683	-133.66	-124.20	9.46	0.37
-63.20	-173.85	30.46						
197		353F 353F N	CA	2683 2684	143.40	143.30		
-44.30								
198	10306	353F 354A C	N	2692 2694	-148.63	-134.00	15.75	0.36
-62.50	-172.72	35.30						

198		354A	354A	N	CA	2694	2695	152.81	147.00		
-40.90											
199	10307	354A	355D	C	N	2697	2699	-97.30	-96.50	5.03	0.21
-63.30	153.06	17.11									
199		355D	355D	N	CA	2699	2700	109.24	114.20		
-40.00											
200	10308	355D	356L	C	N	2705	2707	-109.38	-108.50	1.64	0.08
-63.50	-178.99	22.94									
200		356L	356L	N	CA	2707	2708	133.89	132.50		
-41.20											
201	10309	356L	357E	C	N	2713	2715	-118.82	-117.80	3.43	0.15
-63.60	-172.08	28.18									
201		357E	357E	N	CA	2715	2716	140.07	136.80		
-40.30											
202	10310	357E	358S	C	N	2722	2724	-128.67	-136.60	9.60	0.51
-64.10	-179.65	17.63									
202		358S	358S	N	CA	2724	2725	156.60	151.20		
-35.00											
203	10311	358S	359Y	C	N	2728	2730	-119.72	-124.30	7.99	0.32
-63.50	-178.81	26.15									
203		359Y	359Y	N	CA	2730	2731	128.85	135.40		
-43.40											
204	10312	359Y	360P	C	N	2740	2742	-53.28	-58.70	6.53	0.56
-64.50	179.01	13.96									
204		360P	360P	N	CA	2742	2743	-34.15	-30.50		
147.20											
205	10313	360P	361D	C	N	2747	2749	53.04	54.50	2.30	0.13
-63.30	142.72	24.25									
205		361D	361D	N	CA	2749	2750	42.68	40.90		
-40.00											
206	10314	361D	362F	C	N	2755	2757	-109.16	-124.20	17.31	0.46
-63.20	-175.17	22.79									
206		362F	362F	N	CA	2757	2758	134.73	143.30		
-44.30											
207	10315	362F	363S	C	N	2766	2768	-136.27	-136.60	6.97	0.36
-64.10	-178.22	18.31									
207		363S	363S	N	CA	2768	2769	158.16	151.20		
-35.00											
208	10316	363S	364E	C	N	2772	2774	-73.68	-69.30	5.49	0.31
-63.60	174.18	23.78									
208		364E	364E	N	CA	2774	2775	145.81	142.50		
-40.30											
209	10318	365I	366A	C	N	2789	2791	-121.64	-134.00	12.36	0.42
-62.50	-178.39	32.92									
209		366A	366A	N	CA	2791	2792	147.39	147.00		
-40.90											

report_____> Distribution of short non-bonded contacts:

```
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:      0      0      0      0      0     23     36    156    179    237    229    268    272
327   335
```

<< end of ENERGY.

iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls_286W> MODEL atom not classified: ASN:OXT ASN

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

```
Number of all residues in MODEL           :      367
Number of all, selected real atoms         :      2804      2804
Number of all, selected pseudo atoms       :           0           0
Number of all static, selected restraints  :     13904     13904
COVALENT_CYS                             :           F
NONBONDED_SEL_ATOMS                       :           1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):    324540
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                             :     -17263.9219
```

<< end of ENERGY.

DOPE score : -17263.921875

>> Model assessment by SOAP-Protein-OD score

preppdf_455W> None of the non-bonded terms selected.

```
pair2___701W> Insufficient system memory to allocate storage for cell-based
               (NlogN) nonbond list algorithm; falling back to N*N method.
Warning        3 of          10; further warnings will be suppressed.
```

```
>> ENERGY; Differences between the model's features and restraints:
Number of all residues in MODEL           :      367
Number of all, selected real atoms        :      2804      2804
Number of all, selected pseudo atoms      :           0           0
Number of all static, selected restraints :     13904     13904
COVALENT_CYS                             :           F
NONBONDED_SEL_ATOMS                      :           1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):       0
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                            :      0.000
DYNAMIC_PAIRS,_SPHERE,_COULOMB,_LENNARD,_MODELLER :          T          F          F
F          F
SPHERE_STDV                             :      0.050
RADII_FACTOR                             :      0.820
Current energy                           :              0.0000
```

```
<< end of ENERGY.
SOAP-Protein-OD score                    :      0.000000
>> Model assessment by GA341 potential
```

```
Surface library                          :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/surf5.de
Pair library                             :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/pair9.de
Chain identifier                         : _
% sequence identity                     :      62.856998
Sequence length                         :           367
Compactness                             :      0.011363
Native energy (pair)                    :     175.468621
Native energy (surface)                  :      50.866196
Native energy (combined)                 :      13.135105
Z score (pair)                          :     -1.120854
Z score (surface)                       :     -0.510135
Z score (combined)                      :     -1.080186
GA341 score                             :      0.329538
```

```
>> ENERGY; Differences between the model's features and restraints:
Number of all residues in MODEL           :      367
Number of all, selected real atoms         :    2804    2804
Number of all, selected pseudo atoms       :         0         0
Number of all static, selected restraints  :   13904   13904
COVALENT_CYS                             :         F
NONBONDED_SEL_ATOMS                       :         1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):    4720
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                             :    2089.6370
```

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	2881	0	0	0.003	0.003
6.9683	1.000					
2	Bond angle potential	3935	0	1	1.692	1.692
214.67	1.000					
3	Stereochemical cosine torsion poten:	1962	0	80	51.281	51.281
785.63	1.000					

4 Stereochemical improper torsion pot:	1155	0	0	0.935	0.935
21.334 1.000					
5 Soft-sphere overlap restraints :	4720	0	0	0.003	0.003
5.7840 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) :	765	0	8	1.243	1.243
116.63 1.000					
10 Distance restraints 2 (N-O) :	973	2	11	1.519	1.519
164.76 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:	366	0	2	3.165	3.165
43.231 1.000					
14 Sidechain Chi_1 dihedral restraints:	315	0	3	86.654	86.654
106.32 1.000					
15 Sidechain Chi_2 dihedral restraints:	209	0	0	77.151	77.151
80.077 1.000					
16 Sidechain Chi_3 dihedral restraints:	98	0	0	94.302	94.302
53.264 1.000					
17 Sidechain Chi_4 dihedral restraints:	34	0	0	82.369	82.369
19.650 1.000					
18 Disulfide distance restraints :	5	0	0	0.003	0.003
0.99187E-02 1.000					
19 Disulfide angle restraints :	10	0	0	1.264	1.264
0.35293 1.000					
20 Disulfide dihedral angle restraints:	5	0	0	34.888	34.888
4.9679 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) :	643	0	0	0.633	0.633
21.258 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:	365	216	48	37.732	135.937
417.98 1.000					
26 Distance restraints 4 (SDCH-SDCH) :	183	0	4	1.640	1.640
26.748 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				

Heavy relative violation of each residue is written to: WISP1.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: 64216.6016

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 10 : Distance restraints 2 (N-O)
List of the RVIOL violations larger than : 4.5000

#	ICSR	RESN01/2	ATM1/2	INDATM1/2	FEAT	restr	viol	rviol
RESTR	VIOL	RVIOL						
1	12119	40E 148D N	0	286 1102	8.49	5.54	2.95	4.52
5.54	2.95	4.52						
2	12251	130Y 87C N	0	951 641	4.77	2.66	2.11	4.62
2.66	2.11	4.62						

Feature 25 : Phi/Psi pair of dihedral restraints
List of the RVIOL violations larger than : 6.5000

#	ICSR	RESN01/2	ATM1/2	INDATM1/2	FEAT	restr	viol	rviol
RESTR	VIOL	RVIOL						
1	9954	1M 2R C N	7 9	-129.55 -125.20	8.83	0.49		
-63.00	-173.69	21.60						
1		2R 2R N CA	9 10	132.92 140.60				
-41.10								
2	9955	2R 3W C N	18 20	-140.40 -124.90	19.23	0.61		
-63.00	178.65	27.54						
2		3W 3W N CA	20 21	154.79 143.40				
-44.20								
3	9956	3W 4F C N	32 34	-133.88 -124.20	11.21	0.58		
-63.20	-168.44	31.24						
3		4F 4F N CA	34 35	137.65 143.30				
-44.30								
4	9957	4F 5L C N	43 45	-142.28 -108.50	36.99	1.64		
-63.50	-171.53	31.05						
4		5L 5L N CA	45 46	147.58 132.50				
-41.20								
5	9959	6P 7W C N	58 60	-130.37 -124.90	10.11	0.35		
-63.00	177.21	26.68						
5		7W 7W N CA	60 61	151.90 143.40				
-44.20								
6	9960	7W 8T C N	72 74	-119.26 -124.80	5.55	0.29		
-63.20	-176.73	27.23						
6		8T 8T N CA	74 75	143.41 143.50				
-42.10								

7	9961	8T	9L	C	N	79	81	-107.31	-108.50	1.95	0.11
-63.50	-179.36		22.96								
7		9L	9L	N	CA	81	82	134.05	132.50		
-41.20											
8	9962	9L	10A	C	N	87	89	-119.39	-134.00	14.78	0.41
-62.50	-176.64		33.08								
8		10A	10A	N	CA	89	90	144.79	147.00		
-40.90											
9	9963	10A	11A	C	N	92	94	-113.24	-134.00	23.68	0.55
-62.50	-176.35		28.08								
9		11A	11A	N	CA	94	95	135.60	147.00		
-40.90											
10	9965	12V	13T	C	N	104	106	-111.61	-124.80	23.80	0.74
-63.20	172.71		19.36								
10		13T	13T	N	CA	106	107	123.69	143.50		
-42.10											
11	9966	13T	14A	C	N	111	113	-141.74	-134.00	8.07	0.20
-62.50	-172.57		34.96								
11		14A	14A	N	CA	113	114	149.25	147.00		
-40.90											
12	9967	14A	15A	C	N	116	118	-129.41	-134.00	6.36	0.19
-62.50	-171.23		34.51								
12		15A	15A	N	CA	118	119	142.59	147.00		
-40.90											
13	9968	15A	16A	C	N	121	123	-135.76	-134.00	2.18	0.06
-62.50	-174.13		34.38								
13		16A	16A	N	CA	123	124	148.28	147.00		
-40.90											
14	9969	16A	17A	C	N	126	128	-117.19	-134.00	20.97	0.54
-62.50	-176.31		27.98								
14		17A	17A	N	CA	128	129	134.46	147.00		
-40.90											
15	9970	17A	18S	C	N	131	133	46.97	-72.40	123.30	7.81
-64.10	-168.05		21.93								
15		18S	18S	N	CA	133	134	121.54	152.40		
-35.00											
16	9971	18S	19T	C	N	137	139	-121.12	-124.80	4.64	0.16
-63.20	-173.55		27.76								
16		19T	19T	N	CA	139	140	140.67	143.50		
-42.10											
17	9972	19T	20V	C	N	144	146	-62.19	-62.40	5.97	0.74
-125.40	179.81		10.11								
17		20V	20V	N	CA	146	147	-48.36	-42.40		
143.30											
18	9973	20V	21L	C	N	151	153	-140.24	-108.50	32.76	1.48
-63.50	-166.00		31.69								
18		21L	21L	N	CA	153	154	140.62	132.50		
-41.20											

19	9974	21L	22A	C	N	159	161	-63.01	-68.20	5.74	0.40
-62.50	176.25	28.91									
19		22A	22A	N	CA	161	162	142.85	145.30		
-40.90											
20	9976	23T	24A	C	N	171	173	-153.74	-134.00	22.26	0.51
-62.50	-174.21	35.32									
20		24A	24A	N	CA	173	174	157.27	147.00		
-40.90											
21	9977	24A	25L	C	N	176	178	-77.27	-70.70	20.10	1.30
-63.50	158.80	22.86									
21		25L	25L	N	CA	178	179	160.59	141.60		
-41.20											
22	9978	25L	26S	C	N	184	186	-69.45	-72.40	10.16	0.70
-64.10	162.96	12.13									
22		26S	26S	N	CA	186	187	162.13	152.40		
-35.00											
23	9980	27P	28A	C	N	197	199	-120.21	-134.00	13.87	0.52
-62.50	-179.92	32.59									
23		28A	28A	N	CA	199	200	148.53	147.00		
-40.90											
24	9982	29P	30T	C	N	209	211	-91.87	-78.10	22.32	0.76
-63.20	153.24	21.56									
24		30T	30T	N	CA	211	212	167.37	149.80		
-42.10											
25	9984	31T	32M	C	N	223	225	-71.79	-73.00	2.91	0.22
-63.40	174.06	26.65									
25		32M	32M	N	CA	225	226	145.64	143.00		
-40.50											
26	9985	32M	33D	C	N	231	233	-99.25	-96.50	52.79	2.22
-63.30	107.66	11.62									
26		33D	33D	N	CA	233	234	61.48	114.20		
-40.00											
27	9986	33D	34F	C	N	239	241	-138.39	-124.20	20.17	0.54
-63.20	175.04	29.16									
27		34F	34F	N	CA	241	242	157.63	143.30		
-44.30											
28	9987	34F	35T	C	N	250	252	-79.43	-78.10	2.33	0.14
-63.20	170.79	22.98									
28		35T	35T	N	CA	252	253	147.88	149.80		
-42.10											
29	9989	36P	37A	C	N	264	266	-96.43	-68.20	32.89	3.21
-62.50	172.70	26.84									
29		37A	37A	N	CA	266	267	128.43	145.30		
-40.90											
30	9991	38P	39L	C	N	276	278	76.60	-63.50	144.79	26.28
-63.50	144.79	26.28									
30		39L	39L	N	CA	278	279	-4.67	-41.20		
-41.20											

31	9992	39L	40E	C	N	284	286	-61.89	-63.60	17.40	2.23
-69.30	160.05	12.48									
31		40E	40E	N	CA	286	287	-57.62	-40.30		
142.50											
32	9993	40E	41D	C	N	293	295	-103.77	-70.90	50.94	1.89
-63.30	136.90	19.51									
32		41D	41D	N	CA	295	296	-170.78	150.30		
-40.00											
33	9994	41D	42T	C	N	301	303	-76.63	-78.10	2.83	0.17
-63.20	166.22	22.21									
33		42T	42T	N	CA	303	304	152.22	149.80		
-42.10											
34	9995	42T	43S	C	N	308	310	-69.92	-72.40	18.48	1.00
-64.10	169.19	11.92									
34		43S	43S	N	CA	310	311	134.09	152.40		
-35.00											
35	9996	43S	44S	C	N	314	316	-169.71	-136.60	34.40	1.15
-64.10	-164.53	21.78									
35		44S	44S	N	CA	316	317	160.52	151.20		
-35.00											
36	9997	44S	45R	C	N	320	322	50.10	57.30	15.64	0.77
-63.00	146.41	26.52									
36		45R	45R	N	CA	322	323	51.88	38.00		
-41.10											
37	9999	46P	47Q	C	N	338	340	-109.15	-121.10	12.81	0.40
-63.80	-178.86	24.49									
37		47Q	47Q	N	CA	340	341	135.07	139.70		
-40.30											
38	10000	47Q	48F	C	N	347	349	-134.78	-124.20	16.02	0.45
-63.20	175.61	29.04									
38		48F	48F	N	CA	349	350	155.34	143.30		
-44.30											
39	10002	49C	50K	C	N	364	366	-138.18	-118.00	20.25	0.74
-62.90	-166.36	29.65									
39		50K	50K	N	CA	366	367	140.79	139.10		
-40.80											
40	10003	50K	51W	C	N	373	375	-125.62	-124.90	2.38	0.10
-63.00	-178.71	26.86									
40		51W	51W	N	CA	375	376	145.67	143.40		
-44.20											
41	10006	53C	54E	C	N	400	402	-74.05	-69.30	6.07	0.34
-63.60	173.73	23.74									
41		54E	54E	N	CA	402	403	146.29	142.50		
-40.30											
42	10010	57P	58S	C	N	429	431	-138.02	-136.60	9.41	0.45
-64.10	-179.65	18.34									
42		58S	58S	N	CA	431	432	160.49	151.20		
-35.00											

43	10013	60P	61R	C	N	449	451	-119.29	-125.20	11.95	0.66
-63.00	177.10	27.81									
43		61R	61R	N	CA	451	452	150.98	140.60		
-41.10											
44	10015	62C	63P	C	N	466	468	-67.05	-58.70	10.39	0.85
-64.50	171.54	12.94									
44		63P	63P	N	CA	468	469	-24.32	-30.50		
147.20											
45	10016	63P	64L	C	N	473	475	-76.40	-70.70	7.51	0.49
-63.50	172.79	24.75									
45		64L	64L	N	CA	475	476	146.49	141.60		
-41.20											
46	10017	64L	65G	C	N	481	483	152.35	-167.20	41.52	1.03
82.20	171.73	11.57									
46		65G	65G	N	CA	483	484	165.26	174.60		
8.50											
47	10019	66V	67S	C	N	492	494	-134.42	-136.60	7.42	0.41
-64.10	-179.06	18.11									
47		67S	67S	N	CA	494	495	158.29	151.20		
-35.00											
48	10020	67S	68L	C	N	498	500	-97.94	-108.50	16.01	0.73
-63.50	165.30	21.23									
48		68L	68L	N	CA	500	501	120.48	132.50		
-41.20											
49	10022	69I	70T	C	N	514	516	-72.45	-78.10	9.12	0.57
-63.20	161.20	21.28									
49		70T	70T	N	CA	516	517	156.96	149.80		
-42.10											
50	10023	70T	71D	C	N	521	523	-64.47	-70.90	23.68	0.88
-63.30	167.51	20.61									
50		71D	71D	N	CA	523	524	127.51	150.30		
-40.00											
51	10024	71D	72G	C	N	529	531	62.25	78.70	20.16	0.59
82.20	164.17	8.96									
51		72G	72G	N	CA	531	532	-154.45	-166.10		
8.50											
52	10026	73C	74E	C	N	539	541	-85.14	-69.30	42.59	3.73
-63.60	144.88	18.22									
52		74E	74E	N	CA	541	542	102.96	142.50		
-40.30											
53	10029	76C	77K	C	N	560	562	-113.39	-118.00	11.71	0.49
-62.90	176.51	20.73									
53		77K	77K	N	CA	562	563	128.33	139.10		
-40.80											
54	10030	77K	78M	C	N	569	571	-138.67	-125.60	20.67	0.66
-63.40	179.52	32.73									
54		78M	78M	N	CA	571	572	156.52	140.50		
-40.50											

55	10032	79C	80A	C	N	583	585	-68.53	-68.20	3.16	0.27
-62.50	177.04	29.31									
55		80A	80A	N	CA	585	586	142.16	145.30		
-40.90											
56	10033	80A	81Q	C	N	588	590	-126.12	-121.10	25.55	1.12
-63.80	167.01	27.85									
56		81Q	81Q	N	CA	590	591	164.75	139.70		
-40.30											
57	10034	81Q	82Q	C	N	597	599	-83.95	-73.00	51.48	3.59
-63.80	132.24	18.44									
57		82Q	82Q	N	CA	599	600	90.40	140.70		
-40.30											
58	10035	82Q	83L	C	N	606	608	-143.02	-108.50	44.27	1.97
-63.50	177.40	29.55									
58		83L	83L	N	CA	608	609	160.22	132.50		
-41.20											
59	10040	87C	88T	C	N	640	642	3.37	-78.10	121.01	4.30
-63.20	122.15	19.87									
59		88T	88T	N	CA	642	643	60.32	149.80		
-42.10											
60	10041	88T	89E	C	N	647	649	-129.58	-117.80	16.50	0.88
-63.60	178.21	20.94									
60		89E	89E	N	CA	649	650	125.25	136.80		
-40.30											
61	10042	89E	90A	C	N	656	658	-125.37	-134.00	30.69	1.88
-62.50	155.90	28.92									
61		90A	90A	N	CA	658	659	176.45	147.00		
-40.90											
62	10043	90A	91A	C	N	661	663	-130.78	-134.00	12.04	0.73
-62.50	174.43	32.24									
62		91A	91A	N	CA	663	664	158.59	147.00		
-40.90											
63	10045	92I	93C	C	N	674	676	-65.28	-63.00	2.35	0.36
-117.90	-174.00	7.98									
63		93C	93C	N	CA	676	677	-40.49	-41.10		
141.10											
64	10046	93C	94D	C	N	680	682	-64.12	-70.90	23.36	0.86
-63.30	167.94	20.68									
64		94D	94D	N	CA	682	683	127.94	150.30		
-40.00											
65	10048	95P	96H	C	N	695	697	-83.43	-67.60	20.80	1.23
-63.20	165.44	21.98									
65		96H	96H	N	CA	697	698	153.50	140.00		
-42.30											
66	10049	96H	97R	C	N	705	707	-137.12	-125.20	30.51	1.17
-63.00	167.51	27.67									
66		97R	97R	N	CA	707	708	168.68	140.60		
-41.10											

67	10050	97R	98G	C	N	716	718	-58.64	-62.40	16.32	2.28
82.20	155.36	12.03									
67		98G	98G	N	CA	718	719	-57.08	-41.20		
8.50											
68	10051	98G	99L	C	N	720	722	-164.52	-108.50	56.43	2.77
-63.50	-164.87	23.94									
68		99L	99L	N	CA	722	723	125.74	132.50		
-41.20											
69	10054	101C	102D	C	N	746	748	59.06	54.50	18.21	1.01
-63.30	137.75	23.52									
69		102D	102D	N	CA	748	749	23.26	40.90		
-40.00											
70	10055	102D	103Y	C	N	754	756	-74.36	-98.40	25.23	1.31
-63.50	164.48	25.55									
70		103Y	103Y	N	CA	756	757	120.72	128.40		
-43.40											
71	10056	103Y	104S	C	N	766	768	-110.67	-136.60	53.75	2.06
-64.10	146.70	9.04									
71		104S	104S	N	CA	768	769	104.11	151.20		
-35.00											
72	10057	104S	105G	C	N	772	774	-103.77	-80.20	29.35	2.14
82.20	-131.48	17.73									
72		105G	105G	N	CA	774	775	156.61	174.10		
8.50											
73	10058	105G	106D	C	N	776	778	-85.03	-70.90	62.70	2.44
-63.30	110.77	15.06									
73		106D	106D	N	CA	778	779	-148.62	150.30		
-40.00											
74	10059	106D	107R	C	N	784	786	-53.40	-72.10	25.40	2.21
-63.00	160.09	21.00									
74		107R	107R	N	CA	786	787	159.10	141.90		
-41.10											
75	10061	108P	109R	C	N	802	804	-121.64	-125.20	4.95	0.15
-63.00	-172.34	22.06									
75		109R	109R	N	CA	804	805	137.16	140.60		
-41.10											
76	10062	109R	110Y	C	N	813	815	-104.36	-98.40	36.94	3.86
-63.50	141.38	20.52									
76		110Y	110Y	N	CA	815	816	91.95	128.40		
-43.40											
77	10063	110Y	111A	C	N	825	827	164.74	-134.00	116.96	4.56
-62.50	151.25	30.76									
77		111A	111A	N	CA	827	828	-113.37	147.00		
-40.90											
78	10064	111A	112I	C	N	830	832	32.69	-97.30	130.80	5.80
-120.60	154.30	10.12									
78		112I	112I	N	CA	832	833	112.68	127.20		
130.30											

79	10065	112I	113G	C	N	838	840	158.82	-167.20	73.48	2.99
82.20	126.73	9.40									
79		113G	113G	N	CA	840	841	109.45	174.60		
8.50											
80	10068	115C	116A	C	N	855	857	-73.55	-68.20	13.70	0.92
-62.50	161.57	27.03									
80		116A	116A	N	CA	857	858	157.91	145.30		
-40.90											
81	10069	116A	117Q	C	N	860	862	-70.24	-73.00	10.90	0.77
-63.80	168.57	25.13									
81		117Q	117Q	N	CA	862	863	151.25	140.70		
-40.30											
82	10072	119V	120G	C	N	883	885	-128.82	-167.20	51.75	1.09
82.20	-161.36	15.38									
82		120G	120G	N	CA	885	886	139.88	174.60		
8.50											
83	10074	121V	122G	C	N	894	896	80.56	78.70	8.65	0.17
82.20	176.96	8.51									
83		122G	122G	N	CA	896	897	-174.55	-166.10		
8.50											
84	10077	124V	125L	C	N	911	913	173.78	-108.50	-167.73	10.93
-108.50	-167.73	10.93									
84		125L	125L	N	CA	913	914	-43.36	132.50		
132.50											
85	10111	158L	159R	C	N	1163	1165	-128.60	-125.20	39.11	1.81
-63.00	154.01	25.28									
85		159R	159R	N	CA	1165	1166	179.56	140.60		
-41.10											
86	10113	160V	161R	C	N	1181	1183	-173.09	-125.20	66.87	2.03
-63.00	171.60	30.25									
86		161R	161R	N	CA	1183	1184	-172.73	140.60		
-41.10											
87	10116	163P	164R	C	N	1206	1208	-178.61	-125.20	57.60	1.81
-63.00	-165.23	33.87									
87		164R	164R	N	CA	1208	1209	162.15	140.60		
-41.10											
88	10118	165L	166W	C	N	1225	1227	-124.21	-124.90	40.62	1.99
-63.00	145.31	22.29									
88		166W	166W	N	CA	1227	1228	-175.99	143.40		
-44.20											
89	10121	168P	169H	C	N	1252	1254	-167.60	-125.60	57.28	1.41
-63.20	174.61	28.41									
89		169H	169H	N	CA	1254	1255	177.74	138.80		
-42.30											
90	10122	169H	170P	C	N	1262	1264	-66.30	-58.70	18.78	1.10
-64.50	160.53	12.07									
90		170P	170P	N	CA	1264	1265	-13.33	-30.50		
147.20											

91	10123	170P	171R	C	N	1269	1271	-67.83	-72.10	34.77	2.77
-63.00	142.58	19.59									
91		171R	171R	N	CA	1271	1272	176.41	141.90		
-41.10											
92	10130	177G	178H	C	N	1323	1325	-90.70	-67.60	27.88	1.68
-63.20	164.40	22.33									
92		178H	178H	N	CA	1325	1326	155.61	140.00		
-42.30											
93	10132	179C	180C	C	N	1339	1341	-63.87	-63.00	3.70	0.52
-117.90	-177.61	7.85									
93		180C	180C	N	CA	1341	1342	-44.69	-41.10		
141.10											
94	10133	180C	181E	C	N	1345	1347	-103.05	-117.80	14.77	0.52
-63.60	-179.21	22.17									
94		181E	181E	N	CA	1347	1348	136.13	136.80		
-40.30											
95	10134	181E	182Q	C	N	1354	1356	-97.24	-121.10	25.09	0.81
-63.80	175.47	24.17									
95		182Q	182Q	N	CA	1356	1357	131.95	139.70		
-40.30											
96	10135	182Q	183W	C	N	1363	1365	-130.74	-124.90	13.14	0.49
-63.00	174.33	26.35									
96		183W	183W	N	CA	1365	1366	155.17	143.40		
-44.20											
97	10138	185C	186E	C	N	1390	1392	-91.18	-117.80	46.43	1.67
-63.60	141.77	17.53									
97		186E	186E	N	CA	1392	1393	98.76	136.80		
-40.30											
98	10139	186E	187D	C	N	1399	1401	-126.06	-70.90	93.96	3.30
-63.30	112.72	17.89									
98		187D	187D	N	CA	1401	1402	-133.63	150.30		
-40.00											
99	10140	187D	188D	C	N	1407	1409	-56.29	-70.90	21.02	0.83
-63.30	175.32	22.07									
99		188D	188D	N	CA	1409	1410	135.18	150.30		
-40.00											
100	10141	188D	189A	C	N	1415	1417	-78.47	-68.20	18.50	1.18
-62.50	159.22	26.91									
100		189A	189A	N	CA	1417	1418	160.68	145.30		
-40.90											
101	10142	189A	190K	C	N	1420	1422	-64.32	-70.20	6.99	0.43
-62.90	177.43	22.96									
101		190K	190K	N	CA	1422	1423	136.63	140.40		
-40.80											
102	10143	190K	191R	C	N	1429	1431	-116.43	-125.20	14.04	0.78
-63.00	175.67	27.42									
102		191R	191R	N	CA	1431	1432	151.56	140.60		
-41.10											

103	10144	191R	192P	C	N	1440	1442	-50.24	-64.50	25.85	1.51
-58.70	156.36	13.61									
103		192P	192P	N	CA	1442	1443	125.63	147.20		
-30.50											
104	10145	192P	193R	C	N	1447	1449	-130.56	-125.20	43.67	2.22
-63.00	153.97	17.53									
104		193R	193R	N	CA	1449	1450	97.26	140.60		
-41.10											
105	10146	193R	194K	C	N	1458	1460	168.06	-118.00	80.81	2.68
-62.90	-164.02	32.92									
105		194K	194K	N	CA	1460	1461	171.70	139.10		
-40.80											
106	10147	194K	195T	C	N	1467	1469	-93.50	-124.80	94.99	3.22
-63.20	100.59	11.18									
106		195T	195T	N	CA	1469	1470	53.82	143.50		
-42.10											
107	10148	195T	196A	C	N	1474	1476	-158.18	-134.00	24.53	0.67
-62.50	-166.68	36.79									
107		196A	196A	N	CA	1476	1477	151.12	147.00		
-40.90											
108	10150	197P	198R	C	N	1486	1488	-137.26	-125.20	93.60	4.76
-63.00	115.82	13.35									
108		198R	198R	N	CA	1488	1489	47.78	140.60		
-41.10											
109	10152	199D	200T	C	N	1505	1507	-155.55	-124.80	52.23	1.62
-63.20	161.25	26.46									
109		200T	200T	N	CA	1507	1508	-174.28	143.50		
-42.10											
110	10153	200T	201G	C	N	1512	1514	-123.98	-80.20	67.13	4.62
82.20	-168.13	14.97									
110		201G	201G	N	CA	1514	1515	123.20	174.10		
8.50											
111	10154	201G	202A	C	N	1516	1518	-79.65	-68.20	11.95	0.89
-62.50	171.22	28.93									
111		202A	202A	N	CA	1518	1519	148.75	145.30		
-40.90											
112	10155	202A	203F	C	N	1521	1523	-142.24	-124.20	24.62	0.65
-63.20	174.56	29.31									
112		203F	203F	N	CA	1523	1524	160.06	143.30		
-44.30											
113	10156	203F	204D	C	N	1532	1534	-86.96	-96.50	34.27	1.44
-63.30	123.57	13.98									
113		204D	204D	N	CA	1534	1535	81.29	114.20		
-40.00											
114	10159	206V	207G	C	N	1552	1554	-64.84	-80.20	25.26	0.67
82.20	-153.10	6.51									
114		207G	207G	N	CA	1554	1555	154.05	174.10		
8.50											

115	10160	207G	208E	C	N	1556	1558	-77.03	-69.30	13.83	0.80
-63.60	166.28	22.92									
115		208E	208E	N	CA	1558	1559	153.96	142.50		
-40.30											
116	10162	209V	210E	C	N	1572	1574	-58.18	-69.30	22.87	1.36
-63.60	162.90	22.02									
116		210E	210E	N	CA	1574	1575	122.51	142.50		
-40.30											
117	10163	210E	211A	C	N	1581	1583	67.20	-68.20	136.22	12.03
-62.50	-154.95	31.13									
117		211A	211A	N	CA	1583	1584	160.28	145.30		
-40.90											
118	10164	211A	212W	C	N	1586	1588	-68.66	-71.30	4.23	0.25
-63.00	179.98	22.17									
118		212W	212W	N	CA	1588	1589	135.69	139.00		
-44.20											
119	10165	212W	213H	C	N	1600	1602	-65.49	-67.60	3.75	0.23
-63.20	179.22	22.27									
119		213H	213H	N	CA	1602	1603	136.90	140.00		
-42.30											
120	10166	213H	214R	C	N	1610	1612	-119.47	-125.20	5.87	0.20
-63.00	-171.72	29.34									
120		214R	214R	N	CA	1612	1613	139.29	140.60		
-41.10											
121	10167	214R	215N	C	N	1621	1623	-106.37	-119.90	15.45	0.47
-63.20	176.01	19.93									
121		215N	215N	N	CA	1623	1624	129.53	137.00		
-41.10											
122	10169	216C	217I	C	N	1635	1637	-60.70	-63.40	3.53	0.55
-120.60	-173.92	8.47									
122		217I	217I	N	CA	1637	1638	-45.87	-43.60		
130.30											
123	10170	217I	218A	C	N	1643	1645	-72.45	-68.20	5.55	0.35
-62.50	170.52	28.44									
123		218A	218A	N	CA	1645	1646	148.87	145.30		
-40.90											
124	10172	219Y	220T	C	N	1660	1662	-148.45	-124.80	27.44	1.04
-63.20	-178.28	28.81									
124		220T	220T	N	CA	1662	1663	157.42	143.50		
-42.10											
125	10173	220T	221S	C	N	1667	1669	-86.63	-72.40	29.91	1.38
-64.10	148.02	12.21									
125		221S	221S	N	CA	1669	1670	178.71	152.40		
-35.00											
126	10175	222P	223W	C	N	1680	1682	-161.83	-124.90	91.54	3.50
-63.00	132.76	22.93									
126		223W	223W	N	CA	1682	1683	-132.84	143.40		
-44.20											

127	10176	223W	224S	C	N	1694	1696	-52.92	-72.40	19.53	1.44
-64.10	171.43	11.80									
127		224S	224S	N	CA	1696	1697	153.93	152.40		
-35.00											
128	10180	227S	228T	C	N	1719	1721	-43.55	-78.10	47.85	1.78
-63.20	160.01	21.83									
128		228T	228T	N	CA	1721	1722	116.69	149.80		
-42.10											
129	10184	231G	232L	C	N	1742	1744	-117.35	-108.50	26.86	1.34
-63.50	169.71	26.89									
129		232L	232L	N	CA	1744	1745	157.86	132.50		
-41.20											
130	10185	232L	233G	C	N	1750	1752	-149.27	-167.20	29.64	0.77
82.20	-168.11	14.56									
130		233G	233G	N	CA	1752	1753	151.00	174.60		
8.50											
131	10187	234V	235S	C	N	1761	1763	-145.30	-136.60	14.64	0.83
-64.10	-167.60	12.11									
131		235S	235S	N	CA	1763	1764	139.42	151.20		
-35.00											
132	10188	235S	236T	C	N	1767	1769	-123.38	-124.80	1.75	0.11
-63.20	-176.47	27.53									
132		236T	236T	N	CA	1769	1770	144.51	143.50		
-42.10											
133	10189	236T	237R	C	N	1774	1776	-140.45	-125.20	16.29	0.52
-63.00	-170.85	30.85									
133		237R	237R	N	CA	1776	1777	146.34	140.60		
-41.10											
134	10191	238I	239S	C	N	1793	1795	-122.03	-136.60	15.95	0.50
-64.10	-171.19	11.63									
134		239S	239S	N	CA	1795	1796	144.70	151.20		
-35.00											
135	10192	239S	240N	C	N	1799	1801	-134.71	-119.90	20.67	0.60
-63.20	-177.88	26.82									
135		240N	240N	N	CA	1801	1802	151.41	137.00		
-41.10											
136	10194	241V	242N	C	N	1814	1816	-132.18	-119.90	22.22	0.70
-63.20	177.35	26.08									
136		242N	242N	N	CA	1816	1817	155.51	137.00		
-41.10											
137	10195	242N	243A	C	N	1822	1824	-96.23	-68.20	34.15	3.36
-62.50	170.07	26.43									
137		243A	243A	N	CA	1824	1825	125.79	145.30		
-40.90											
138	10196	243A	244Q	C	N	1827	1829	-151.00	-121.10	42.42	1.38
-63.80	173.42	29.97									
138		244Q	244Q	N	CA	1829	1830	169.79	139.70		
-40.30											

139	10197	244Q	245C	C	N	1836	1838	-60.51	-63.00	10.10	1.09
-117.90	177.54	7.68									
139		245C	245C	N	CA	1838	1839	-50.89	-41.10		
141.10											
140	10198	245C	246W	C	N	1842	1844	-132.11	-124.90	13.01	0.74
-63.00	-170.20	20.92									
140		246W	246W	N	CA	1844	1845	132.57	143.40		
-44.20											
141	10200	247P	248E	C	N	1863	1865	-128.81	-117.80	11.86	0.35
-63.60	-169.99	29.02									
141		248E	248E	N	CA	1865	1866	141.23	136.80		
-40.30											
142	10201	248E	249Q	C	N	1872	1874	-129.21	-121.10	12.29	0.41
-63.80	-177.14	30.35									
142		249Q	249Q	N	CA	1874	1875	148.93	139.70		
-40.30											
143	10202	249Q	250E	C	N	1881	1883	-118.43	-117.80	4.58	0.22
-63.60	-173.40	27.98									
143		250E	250E	N	CA	1883	1884	141.34	136.80		
-40.30											
144	10203	250E	251S	C	N	1890	1892	-131.01	-136.60	6.53	0.20
-64.10	-170.61	18.44									
144		251S	251S	N	CA	1892	1893	147.82	151.20		
-35.00											
145	10204	251S	252R	C	N	1896	1898	-84.94	-72.10	14.87	0.99
-63.00	170.92	24.59									
145		252R	252R	N	CA	1898	1899	149.40	141.90		
-41.10											
146	10205	252R	253L	C	N	1907	1909	-99.41	-108.50	20.38	0.99
-63.50	159.56	20.39									
146		253L	253L	N	CA	1909	1910	114.27	132.50		
-41.20											
147	10207	254C	255N	C	N	1921	1923	-86.39	-71.20	43.12	3.18
-63.20	145.40	17.00									
147		255N	255N	N	CA	1923	1924	102.44	142.80		
-41.10											
148	10208	255N	256L	C	N	1929	1931	-110.73	-108.50	11.10	0.62
-63.50	169.54	21.34									
148		256L	256L	N	CA	1931	1932	121.63	132.50		
-41.20											
149	10209	256L	257R	C	N	1937	1939	-116.30	-125.20	22.85	0.88
-63.00	169.27	19.88									
149		257R	257R	N	CA	1939	1940	119.56	140.60		
-41.10											
150	10212	259C	260D	C	N	1961	1963	-95.15	-70.90	54.89	1.84
-63.30	124.60	17.43									
150		260D	260D	N	CA	1963	1964	-160.46	150.30		
-40.00											

151	10216	263I	264H	C	N	1992	1994	-70.74	-67.60	10.42	0.71
-63.20	167.94	21.47									
151		264H	264H	N	CA	1994	1995	149.93	140.00		
-42.30											
152	10218	265T	266L	C	N	2009	2011	-79.69	-70.70	44.32	3.71
-63.50	140.34	18.62									
152		266L	266L	N	CA	2011	2012	98.20	141.60		
-41.20											
153	10219	266L	267I	C	N	2017	2019	-67.28	-63.40	4.23	0.69
-120.60	-179.72	8.35									
153		267I	267I	N	CA	2019	2020	-41.91	-43.60		
130.30											
154	10229	276V	277Y	C	N	2087	2089	-113.48	-124.30	17.77	1.38
-63.50	174.42	30.21									
154		277Y	277Y	N	CA	2089	2090	149.50	135.40		
-43.40											
155	10230	277Y	278Q	C	N	2099	2101	45.01	-73.00	127.58	8.12
-63.80	171.47	30.50									
155		278Q	278Q	N	CA	2101	2102	92.22	140.70		
-40.30											
156	10232	279P	280E	C	N	2115	2117	-57.54	-69.30	28.83	1.78
-63.60	156.59	21.21									
156		280E	280E	N	CA	2117	2118	116.17	142.50		
-40.30											
157	10233	280E	281A	C	N	2124	2126	-90.34	-68.20	29.41	1.87
-62.50	156.93	27.17									
157		281A	281A	N	CA	2126	2127	164.66	145.30		
-40.90											
158	10234	281A	282S	C	N	2129	2131	-70.01	-72.40	15.77	1.01
-64.10	157.12	11.74									
158		282S	282S	N	CA	2131	2132	167.99	152.40		
-35.00											
159	10235	282S	283M	C	N	2135	2137	-74.86	-73.00	59.28	4.04
-63.40	124.77	17.77									
159		283M	283M	N	CA	2137	2138	83.75	143.00		
-40.50											
160	10236	283M	284N	C	N	2143	2145	-163.32	-119.90	50.48	1.51
-63.20	-174.50	28.72									
160		284N	284N	N	CA	2145	2146	162.75	137.00		
-41.10											
161	10237	284N	285F	C	N	2151	2153	-93.81	-71.40	45.02	4.00
-63.20	149.13	18.75									
161		285F	285F	N	CA	2153	2154	101.65	140.70		
-44.30											
162	10238	285F	286T	C	N	2162	2164	-154.84	-124.80	50.26	1.56
-63.20	162.43	26.58									
162		286T	286T	N	CA	2164	2165	-176.21	143.50		
-42.10											

163	10239	286T	287L	C	N	2169	2171	-69.56	-70.70	4.37	0.38
-63.50	173.09	24.38									
163		287L	287L	N	CA	2171	2172	145.82	141.60		
-41.20											
164	10240	287L	288A	C	N	2177	2179	-66.85	-68.20	8.83	0.66
-62.50	177.53	28.88									
164		288A	288A	N	CA	2179	2180	136.58	145.30		
-40.90											
165	10244	291I	292S	C	N	2200	2202	-151.58	-136.60	17.13	0.52
-64.10	-172.81	19.85									
165		292S	292S	N	CA	2202	2203	159.51	151.20		
-35.00											
166	10245	292S	293T	C	N	2206	2208	-130.06	-124.80	13.05	0.42
-63.20	175.68	26.93									
166		293T	293T	N	CA	2208	2209	155.44	143.50		
-42.10											
167	10246	293T	294R	C	N	2213	2215	-115.93	-125.20	13.22	0.40
-63.00	-179.78	21.32									
167		294R	294R	N	CA	2215	2216	131.17	140.60		
-41.10											
168	10247	294R	295S	C	N	2224	2226	-86.41	-72.40	18.06	0.90
-64.10	162.73	13.25									
168		295S	295S	N	CA	2226	2227	163.80	152.40		
-35.00											
169	10248	295S	296Y	C	N	2230	2232	-116.39	-124.30	19.94	0.80
-63.50	168.99	24.37									
169		296Y	296Y	N	CA	2232	2233	117.10	135.40		
-43.40											
170	10249	296Y	297Q	C	N	2242	2244	-148.80	-121.10	30.05	1.38
-63.80	-171.43	24.36									
170		297Q	297Q	N	CA	2244	2245	128.03	139.70		
-40.30											
171	10251	298P	299K	C	N	2258	2260	154.62	-118.00	88.96	3.11
-62.90	-143.22	36.40									
171		299K	299K	N	CA	2260	2261	155.82	139.10		
-40.80											
172	10252	299K	300Y	C	N	2267	2269	-105.86	-98.40	23.95	2.40
-63.50	154.95	22.58									
172		300Y	300Y	N	CA	2269	2270	105.64	128.40		
-43.40											
173	10254	301C	302G	C	N	2285	2287	-170.04	-167.20	26.71	1.07
82.20	176.30	13.11									
173		302G	302G	N	CA	2287	2288	148.04	174.60		
8.50											
174	10257	304C	305M	C	N	2302	2304	-102.67	-125.60	22.99	0.95
-63.40	-178.45	30.24									
174		305M	305M	N	CA	2304	2305	142.25	140.50		
-40.50											

175	10258	305M	306D	C	N	2310	2312	-67.85	-70.90	28.31	1.25
-63.30	162.22	19.75									
175		306D	306D	N	CA	2312	2313	122.15	150.30		
-40.00											
176	10259	306D	307N	C	N	2318	2320	-135.86	-119.90	24.42	0.73
-63.20	178.85	26.47									
176		307N	307N	N	CA	2320	2321	155.48	137.00		
-41.10											
177	10265	312P	313Y	C	N	2364	2366	-133.01	-124.30	52.40	2.42
-63.50	146.99	26.69									
177		313Y	313Y	N	CA	2366	2367	-172.93	135.40		
-43.40											
178	10267	314K	315S	C	N	2385	2387	-93.62	-72.40	25.59	1.33
-64.10	161.03	13.64									
178		315S	315S	N	CA	2387	2388	166.70	152.40		
-35.00											
179	10268	315S	316K	C	N	2391	2393	-82.88	-70.20	15.98	0.96
-62.90	170.26	23.25									
179		316K	316K	N	CA	2393	2394	150.11	140.40		
-40.80											
180	10269	316K	317T	C	N	2400	2402	-119.94	-124.80	6.20	0.38
-63.20	179.75	26.82									
180		317T	317T	N	CA	2402	2403	147.34	143.50		
-42.10											
181	10270	317T	318I	C	N	2407	2409	-64.76	-63.40	4.24	0.74
-120.60	-173.53	8.62									
181		318I	318I	N	CA	2409	2410	-47.61	-43.60		
130.30											
182	10271	318I	319D	C	N	2415	2417	-91.02	-70.90	46.44	1.56
-63.30	130.82	17.92									
182		319D	319D	N	CA	2417	2418	-167.85	150.30		
-40.00											
183	10272	319D	320V	C	N	2423	2425	-60.73	-62.40	7.50	0.87
-73.50	171.56	14.82									
183		320V	320V	N	CA	2425	2426	-49.71	-42.40		
139.20											
184	10277	324C	325P	C	N	2462	2464	-49.15	-58.70	31.32	1.94
-64.50	153.25	12.26									
184		325P	325P	N	CA	2464	2465	-60.32	-30.50		
147.20											
185	10278	325P	326D	C	N	2469	2471	178.23	-96.50	96.54	4.00
-63.30	-160.49	32.08									
185		326D	326D	N	CA	2471	2472	159.48	114.20		
-40.00											
186	10279	326D	327G	C	N	2477	2479	-149.62	-167.20	22.54	0.44
82.20	-161.17	14.96									
186		327G	327G	N	CA	2479	2480	160.49	174.60		
8.50											

187	10280	327G	328L	C	N	2481	2483	-106.87	-108.50	1.68	0.08
-63.50	179.41	22.81									
187		328L	328L	N	CA	2483	2484	132.89	132.50		
-41.20											
188	10281	328L	329G	C	N	2489	2491	-155.02	-167.20	48.44	1.71
82.20	171.13	13.16									
188		329G	329G	N	CA	2491	2492	127.71	174.60		
8.50											
189	10282	329G	330F	C	N	2493	2495	-146.70	-124.20	23.61	0.72
-63.20	-174.88	31.06									
189		330F	330F	N	CA	2495	2496	150.48	143.30		
-44.30											
190	10283	330F	331S	C	N	2504	2506	-126.82	-136.60	18.07	0.66
-64.10	-177.85	11.23									
190		331S	331S	N	CA	2506	2507	136.01	151.20		
-35.00											
191	10284	331S	332R	C	N	2510	2512	-128.69	-125.20	4.45	0.13
-63.00	-172.58	29.84									
191		332R	332R	N	CA	2512	2513	143.37	140.60		
-41.10											
192	10285	332R	333Q	C	N	2521	2523	-106.82	-121.10	21.25	0.71
-63.80	169.80	22.94									
192		333Q	333Q	N	CA	2523	2524	123.95	139.70		
-40.30											
193	10287	334V	335L	C	N	2537	2539	-115.60	-108.50	12.57	0.72
-63.50	171.44	21.45									
193		335L	335L	N	CA	2539	2540	122.13	132.50		
-41.20											
194	10288	335L	336W	C	N	2545	2547	-130.07	-124.90	6.78	0.38
-63.00	-170.92	28.13									
194		336W	336W	N	CA	2547	2548	139.02	143.40		
-44.20											
195	10290	337I	338N	C	N	2567	2569	-123.13	-119.90	8.92	0.47
-63.20	-179.95	19.85									
195		338N	338N	N	CA	2569	2570	128.69	137.00		
-41.10											
196	10291	338N	339A	C	N	2575	2577	-170.16	-134.00	37.87	0.91
-62.50	-166.44	37.42									
196		339A	339A	N	CA	2577	2578	158.25	147.00		
-40.90											
197	10293	340C	341F	C	N	2586	2588	-115.35	-124.20	19.39	0.66
-63.20	178.15	21.55									
197		341F	341F	N	CA	2588	2589	126.05	143.30		
-44.30											
198	10295	342C	343N	C	N	2603	2605	-123.08	-119.90	10.31	0.53
-63.20	178.63	19.69									
198		343N	343N	N	CA	2605	2606	127.20	137.00		
-41.10											

199	10296	343N	344L	C	N	2611	2613	-117.92	-108.50	14.19	0.80
-63.50	171.93	21.45									
199		344L	344L	N	CA	2613	2614	121.89	132.50		
-41.20											
200	10297	344L	345S	C	N	2619	2621	-140.03	-136.60	5.24	0.29
-64.10	-166.70	19.40									
200		345S	345S	N	CA	2621	2622	147.24	151.20		
-35.00											
201	10300	347R	348N	C	N	2642	2644	42.51	55.90	29.52	1.41
-63.20	150.35	24.28									
201		348N	348N	N	CA	2644	2645	65.81	39.50		
-41.10											
202	10302	349P	350N	C	N	2657	2659	-101.21	-119.90	27.14	0.80
-63.20	162.92	18.53									
202		350N	350N	N	CA	2659	2660	117.32	137.00		
-41.10											
203	10303	350N	351D	C	N	2665	2667	-126.84	-96.50	30.89	1.27
-63.30	172.17	18.45									
203		351D	351D	N	CA	2667	2668	120.02	114.20		
-40.00											
204	10305	352I	353F	C	N	2681	2683	-137.04	-124.20	14.10	0.39
-63.20	-177.80	30.10									
204		353F	353F	N	CA	2683	2684	149.13	143.30		
-44.30											
205	10306	353F	354A	C	N	2692	2694	-141.56	-134.00	9.43	0.24
-62.50	-175.70	34.44									
205		354A	354A	N	CA	2694	2695	152.62	147.00		
-40.90											
206	10307	354A	355D	C	N	2697	2699	-95.07	-96.50	19.31	0.81
-63.30	138.63	15.46									
206		355D	355D	N	CA	2699	2700	94.95	114.20		
-40.00											
207	10308	355D	356L	C	N	2705	2707	-111.44	-108.50	3.15	0.14
-63.50	-178.70	22.91									
207		356L	356L	N	CA	2707	2708	133.65	132.50		
-41.20											
208	10309	356L	357E	C	N	2713	2715	-110.96	-117.80	10.06	0.33
-63.60	176.22	21.26									
208		357E	357E	N	CA	2715	2716	129.43	136.80		
-40.30											
209	10310	357E	358S	C	N	2722	2724	-139.07	-136.60	5.29	0.21
-64.10	-175.01	18.74									
209		358S	358S	N	CA	2724	2725	155.87	151.20		
-35.00											
210	10311	358S	359Y	C	N	2728	2730	-118.87	-124.30	8.56	0.36
-63.50	-179.13	26.13									
210		359Y	359Y	N	CA	2730	2731	128.78	135.40		
-43.40											

211	10312	359Y	360P	C	N	2740	2742	-53.51	-58.70	6.80	0.52
-64.50	178.24	13.89									
211		360P	360P	N	CA	2742	2743	-34.90	-30.50		
147.20											
212	10313	360P	361D	C	N	2747	2749	-80.08	-70.90	19.57	0.65
-63.30	153.35	19.98									
212		361D	361D	N	CA	2749	2750	167.58	150.30		
-40.00											
213	10314	361D	362F	C	N	2755	2757	-111.67	-124.20	18.57	1.03
-63.20	165.93	26.27									
213		362F	362F	N	CA	2757	2758	157.01	143.30		
-44.30											
214	10315	362F	363S	C	N	2766	2768	-66.27	-72.40	6.16	0.42
-64.10	173.15	12.67									
214		363S	363S	N	CA	2768	2769	151.86	152.40		
-35.00											
215	10316	363S	364E	C	N	2772	2774	-74.13	-69.30	7.02	0.39
-63.60	172.42	23.57									
215		364E	364E	N	CA	2774	2775	147.60	142.50		
-40.30											
216	10318	365I	366A	C	N	2789	2791	-104.06	-134.00	30.33	0.83
-62.50	-178.18	31.99									
216		366A	366A	N	CA	2791	2792	142.10	147.00		
-40.90											

report_____> Distribution of short non-bonded contacts:

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:	0	0	0	0	0	25	42	190	183	231	254	243	280
	299	342											

<< end of ENERGY.

>> Model assessment by DOPE potential

iatmcls_286W> MODEL atom not classified: ASN:OXT ASN

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

Number of all residues in MODEL	:	367	
Number of all, selected real atoms	:	2804	2804
Number of all, selected pseudo atoms	:	0	0
Number of all static, selected restraints	:	13904	13904
COVALENT_CYS	:	F	

```

NONBONDED_SEL_ATOMS           :          1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):    331609
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                 :   -18903.2168

```

<< end of ENERGY.

```
DOPE score                     : -18903.216797
```

>> Model assessment by SOAP-Protein-OD score

```
preppdf_455W> None of the non-bonded terms selected.
```

```
pair2___701W> Insufficient system memory to allocate storage for cell-based
(NlogN) nonbond list algorithm; falling back to N*N method.
```

```
Warning          4 of          10; further warnings will be suppressed.
```

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

```

Number of all residues in MODEL           :          367
Number of all, selected real atoms         :    2804    2804
Number of all, selected pseudo atoms       :          0          0
Number of all static, selected restraints  :   13904   13904
COVALENT_CYS                             :          F
NONBONDED_SEL_ATOMS                       :          1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):          0
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                             :    0.000
DYNAMIC_PAIRS,_SPHERE,_COULOMB,_LENNARD,_MODELLER :          T          F          F
F          F
SPHERE_STDV                               :    0.050
RADII_FACTOR                              :    0.820
Current energy                            :          0.0000

```

<< end of ENERGY.

SOAP-Protein-OD score : 0.000000

>> Model assessment by GA341 potential

Surface library :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/surf5.de
Pair library :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/pair9.de
Chain identifier : -
% sequence identity : 62.856998
Sequence length : 367
Compactness : 0.011643
Native energy (pair) : 99.628431
Native energy (surface) : 50.079533
Native energy (combined) : 10.995486
Z score (pair) : -3.520322
Z score (surface) : -0.720860
Z score (combined) : -2.664887
GA341 score : 0.857862

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

Number of all residues in MODEL	:	367		
Number of all, selected real atoms	:	2804	2804	
Number of all, selected pseudo atoms	:	0	0	
Number of all static, selected restraints	:	13904	13904	
COVALENT_CYS	:	F		
NONBONDED_SEL_ATOMS	:	1		
Number of non-bonded pairs (excluding 1-2,1-3,1-4):	:	4507		
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	:	1996.5691		

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	:	2881	0	0	0.003	0.003
6.6816	1.000						
2	Bond angle potential	:	3935	0	3	1.640	1.640
200.08	1.000						
3	Stereochemical cosine torsion poten:		1962	0	88	51.526	51.526
788.63	1.000						
4	Stereochemical improper torsion pot:		1155	0	1	0.953	0.953
21.110	1.000						
5	Soft-sphere overlap restraints	:	4507	0	0	0.003	0.003
5.5781	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)	:	765	1	6	1.395	1.395
132.41	1.000						
10	Distance restraints 2 (N-O)	:	973	0	21	1.720	1.720
192.56	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:		366	0	1	2.707	2.707
31.630	1.000						
14	Sidechain Chi_1 dihedral restraints:		315	0	2	87.603	87.603
92.354	1.000						
15	Sidechain Chi_2 dihedral restraints:		209	0	1	71.017	71.017
67.644	1.000						
16	Sidechain Chi_3 dihedral restraints:		98	0	0	90.528	90.528
53.214	1.000						

17 Sidechain Chi_4 dihedral restraints:	34	0	0	99.471	99.471
21.859 1.000					
18 Disulfide distance restraints :	5	0	0	0.008	0.008
0.51672E-01 1.000					
19 Disulfide angle restraints :	10	0	0	1.767	1.767
0.68951 1.000					
20 Disulfide dihedral angle restraints:	5	0	0	29.188	29.188
4.0229 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) :	643	0	0	0.585	0.585
16.124 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:	365	196	42	33.960	129.879
352.14 1.000					
26 Distance restraints 4 (SDCH-SDCH) :	183	0	0	1.529	1.529
9.7950 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					


```
# Heavy relative violation of each residue is written to: WISP1.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:    60087.8203
```

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 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	9954	1M 2R C N	7 9	-140.34	-125.20	17.98	0.95	
-63.00	-171.43	21.58						
1		2R 2R N CA	9 10	130.89	140.60			
-41.10								
2	9955	2R 3W C N	18 20	-146.45	-124.90	24.38	0.81	
-63.00	-178.65	28.29						
2		3W 3W N CA	20 21	154.79	143.40			
-44.20								
3	9956	3W 4F C N	32 34	-104.48	-124.20	28.31	0.77	
-63.20	172.31	21.33						
3		4F 4F N CA	34 35	122.99	143.30			
-44.30								
4	9957	4F 5L C N	43 45	-117.30	-108.50	15.91	0.91	
-63.50	169.23	21.10						
4		5L 5L N CA	45 46	119.25	132.50			

-41.20	5	9959	6P	7W	C	N	58	60	-146.12	-124.90	24.53	0.80
-63.00	5	-179.61	28.15									
-44.20	5		7W	7W	N	CA	60	61	155.70	143.40		
-63.20	6	9960	7W	8T	C	N	72	74	-126.11	-124.80	8.05	0.31
-42.10	6	177.95	26.98									
-63.50	6		8T	8T	N	CA	74	75	151.44	143.50		
-41.20	7	9961	8T	9L	C	N	79	81	-102.40	-108.50	8.49	0.38
-63.50	7	172.24	22.00									
-41.20	7		9L	9L	N	CA	81	82	126.59	132.50		
-62.50	8	9962	9L	10A	C	N	87	89	-121.80	-134.00	17.10	0.51
-40.90	8	-174.36	28.18									
-62.50	8		10A	10A	N	CA	89	90	135.02	147.00		
-40.90	9	9963	10A	11A	C	N	92	94	-77.14	-68.20	9.52	0.90
-62.50	9	177.66	29.86									
-40.90	9		11A	11A	N	CA	94	95	142.05	145.30		
-63.20	10	9965	12V	13T	C	N	104	106	-105.66	-124.80	71.58	2.53
-42.10	10	124.11	13.59									
-62.50	10		13T	13T	N	CA	106	107	74.52	143.50		
-40.90	11	9966	13T	14A	C	N	111	113	-164.78	-134.00	31.36	0.83
-62.50	11	-164.92	37.41									
-40.90	11		14A	14A	N	CA	113	114	152.98	147.00		
-62.50	12	9967	14A	15A	C	N	116	118	-77.63	-68.20	11.42	0.75
-40.90	12	168.03	28.30									
-62.50	12		15A	15A	N	CA	118	119	151.75	145.30		
-40.90	13	9968	15A	16A	C	N	121	123	-115.84	-134.00	18.33	0.52
-62.50	13	-177.40	32.76									
-40.90	13		16A	16A	N	CA	123	124	144.47	147.00		
-62.50	14	9969	16A	17A	C	N	126	128	-94.93	-68.20	35.54	3.51
-40.90	14	165.98	25.81									
-62.50	14		17A	17A	N	CA	128	129	121.88	145.30		
-64.10	15	9970	17A	18S	C	N	131	133	-174.21	-136.60	44.45	1.35
-35.00	15	-173.83	21.44									
-63.20	15		18S	18S	N	CA	133	134	174.89	151.20		
-40.90	16	9971	18S	19T	C	N	137	139	-120.87	-124.80	17.77	0.88
-63.20	16	167.32	25.27									
-40.90	16		19T	19T	N	CA	139	140	160.83	143.50		

-42.10											
17	9974	21L	22A	C	N	159	161	-130.28	-134.00	3.72	0.12
-62.50	-174.94	33.96									
17		22A	22A	N	CA	161	162	146.90	147.00		
-40.90											
18	9976	23T	24A	C	N	171	173	-154.88	-134.00	23.15	0.53
-62.50	-173.41	35.51									
18		24A	24A	N	CA	173	174	156.98	147.00		
-40.90											
19	9978	25L	26S	C	N	184	186	-163.32	-136.60	27.85	1.31
-64.10	-155.91	13.30									
19		26S	26S	N	CA	186	187	143.35	151.20		
-35.00											
20	9980	27P	28A	C	N	197	199	-70.71	-68.20	5.61	0.53
-62.50	179.01	29.75									
20		28A	28A	N	CA	199	200	140.28	145.30		
-40.90											
21	9983	30T	31T	C	N	216	218	-118.93	-124.80	12.49	0.70
-63.20	172.62	25.83									
21		31T	31T	N	CA	218	219	154.52	143.50		
-42.10											
22	9984	31T	32M	C	N	223	225	-85.30	-73.00	18.85	1.48
-63.40	170.63	23.85									
22		32M	32M	N	CA	225	226	128.72	143.00		
-40.50											
23	9985	32M	33D	C	N	231	233	-112.12	-96.50	24.91	1.02
-63.30	143.37	15.45									
23		33D	33D	N	CA	233	234	94.80	114.20		
-40.00											
24	9989	36P	37A	C	N	264	266	-160.04	-134.00	27.11	0.66
-62.50	-168.71	36.55									
24		37A	37A	N	CA	266	267	154.55	147.00		
-40.90											
25	9992	39L	40E	C	N	284	286	-124.11	-117.80	40.71	2.14
-69.30	71.50	6.56									
25		40E	40E	N	CA	286	287	96.58	136.80		
142.50											
26	9993	40E	41D	C	N	293	295	-70.24	-70.90	20.52	0.98
-63.30	169.93	20.56									
26		41D	41D	N	CA	295	296	129.79	150.30		
-40.00											
27	9994	41D	42T	C	N	301	303	-109.56	-124.80	43.39	1.45
-63.20	152.21	16.90									
27		42T	42T	N	CA	303	304	102.87	143.50		
-42.10											
28	9997	44S	45R	C	N	320	322	-66.80	-72.10	11.56	0.78
-63.00	172.76	23.09									
28		45R	45R	N	CA	322	323	131.62	141.90		

-41.10											
29	9999	46P	47Q	C	N	338	340	-155.05	-121.10	34.09	1.35
-63.80	-160.89	25.70									
29		47Q	47Q	N	CA	340	341	136.67	139.70		
-40.30											
30	10000	47Q	48F	C	N	347	349	-122.38	-124.20	3.89	0.13
-63.20	-174.47	29.69									
30		48F	48F	N	CA	349	350	139.87	143.30		
-44.30											
31	10002	49C	50K	C	N	364	366	-76.21	-70.20	6.06	0.42
-62.90	178.48	23.93									
31		50K	50K	N	CA	366	367	141.22	140.40		
-40.80											
32	10003	50K	51W	C	N	373	375	-91.81	-71.30	22.65	1.38
-63.00	169.66	23.07									
32		51W	51W	N	CA	375	376	148.61	139.00		
-44.20											
33	10004	51W	52P	C	N	387	389	-66.06	-58.70	9.60	0.74
-64.50	171.54	12.88									
33		52P	52P	N	CA	389	390	-24.33	-30.50		
147.20											
34	10006	53C	54E	C	N	400	402	-96.78	-117.80	21.53	0.69
-63.60	175.62	21.76									
34		54E	54E	N	CA	402	403	132.15	136.80		
-40.30											
35	10010	57P	58S	C	N	429	431	-127.12	-136.60	9.48	0.38
-64.10	-175.33	17.81									
35		58S	58S	N	CA	431	432	151.42	151.20		
-35.00											
36	10013	60P	61R	C	N	449	451	-140.22	-125.20	21.47	0.66
-63.00	-179.67	29.63									
36		61R	61R	N	CA	451	452	155.94	140.60		
-41.10											
37	10016	63P	64L	C	N	473	475	-65.37	-70.70	9.70	0.60
-63.50	174.71	24.15									
37		64L	64L	N	CA	475	476	133.50	141.60		
-41.20											
38	10017	64L	65G	C	N	481	483	84.81	78.70	29.86	0.61
82.20	156.19	7.71									
38		65G	65G	N	CA	483	484	164.68	-166.10		
8.50											
39	10018	65G	66V	C	N	485	487	-63.96	-62.40	1.78	0.30
-125.40	-176.01	10.30									
39		66V	66V	N	CA	487	488	-43.27	-42.40		
143.30											
40	10019	66V	67S	C	N	492	494	-144.65	-136.60	26.89	1.17
-64.10	168.63	18.01									
40		67S	67S	N	CA	494	495	176.85	151.20		

-35.00											
41	10020	67S	68L	C	N	498	500	-65.75	-70.70	5.57	0.56
-63.50	174.64	24.38									
41		68L	68L	N	CA	500	501	144.17	141.60		
-41.20											
42	10022	69I	70T	C	N	514	516	-119.73	-124.80	8.13	0.48
-63.20	177.30	26.49									
42		70T	70T	N	CA	516	517	149.86	143.50		
-42.10											
43	10023	70T	71D	C	N	521	523	-86.00	-96.50	62.25	2.62
-63.30	95.58	10.63									
43		71D	71D	N	CA	523	524	52.85	114.20		
-40.00											
44	10024	71D	72G	C	N	529	531	66.31	78.70	12.64	0.57
82.20	172.83	9.18									
44		72G	72G	N	CA	531	532	-163.59	-166.10		
8.50											
45	10026	73C	74E	C	N	539	541	-108.46	-117.80	20.23	0.79
-63.60	165.36	19.94									
45		74E	74E	N	CA	541	542	118.86	136.80		
-40.30											
46	10029	76C	77K	C	N	560	562	-136.08	-118.00	24.74	1.24
-62.90	178.69	20.57									
46		77K	77K	N	CA	562	563	122.22	139.10		
-40.80											
47	10030	77K	78M	C	N	569	571	-145.44	-125.60	22.92	0.68
-63.40	-173.45	34.29									
47		78M	78M	N	CA	571	572	151.96	140.50		
-40.50											
48	10031	78M	79C	C	N	577	579	-63.74	-63.00	1.08	0.19
-117.90	-174.89	7.96									
48		79C	79C	N	CA	579	580	-41.89	-41.10		
141.10											
49	10032	79C	80A	C	N	583	585	-71.44	-68.20	11.92	0.85
-62.50	162.58	27.09									
49		80A	80A	N	CA	585	586	156.77	145.30		
-40.90											
50	10033	80A	81Q	C	N	588	590	-71.12	-73.00	8.62	0.60
-63.80	170.74	25.49									
50		81Q	81Q	N	CA	590	591	149.12	140.70		
-40.30											
51	10034	81Q	82Q	C	N	597	599	-105.84	-121.10	38.87	2.02
-63.80	150.25	24.34									
51		82Q	82Q	N	CA	599	600	175.45	139.70		
-40.30											
52	10035	82Q	83L	C	N	606	608	-67.27	-70.70	23.71	1.93
-63.50	153.78	21.57									
52		83L	83L	N	CA	608	609	165.06	141.60		

-41.20											
53	10041	88T	89E	C	N	647	649	-156.61	-117.80	46.45	1.37
-63.60	-177.18	29.50									
53		89E	89E	N	CA	649	650	162.31	136.80		
-40.30											
54	10042	89E	90A	C	N	656	658	-160.11	-134.00	26.98	0.67
-62.50	-168.04	36.66									
54		90A	90A	N	CA	658	659	153.81	147.00		
-40.90											
55	10043	90A	91A	C	N	661	663	-83.54	-68.20	21.22	1.34
-62.50	160.52	27.39									
55		91A	91A	N	CA	663	664	159.96	145.30		
-40.90											
56	10045	92I	93C	C	N	674	676	-68.17	-63.00	5.20	0.89
-117.90	-175.94	7.87									
56		93C	93C	N	CA	676	677	-41.68	-41.10		
141.10											
57	10046	93C	94D	C	N	680	682	-53.67	-70.90	31.61	1.08
-63.30	164.08	20.85									
57		94D	94D	N	CA	682	683	123.80	150.30		
-40.00											
58	10048	95P	96H	C	N	695	697	-134.54	-125.60	64.92	2.63
-63.20	136.86	14.57									
58		96H	96H	N	CA	697	698	74.50	138.80		
-42.30											
59	10049	96H	97R	C	N	705	707	61.01	-72.10	140.71	11.66
-63.00	-179.31	21.17									
59		97R	97R	N	CA	707	708	-172.51	141.90		
-41.10											
60	10050	97R	98G	C	N	716	718	-64.93	-80.20	44.92	1.11
82.20	-168.00	6.66									
60		98G	98G	N	CA	718	719	131.85	174.10		
8.50											
61	10051	98G	99L	C	N	720	722	-105.35	-63.50	73.85	9.11
-63.50	73.85	9.11									
61		99L	99L	N	CA	722	723	19.64	-41.20		
-41.20											
62	10052	99L	100Y	C	N	728	730	58.05	-98.40	156.88	6.31
-63.50	-158.92	37.44									
62		100Y	100Y	N	CA	730	731	116.78	128.40		
-43.40											
63	10054	101C	102D	C	N	746	748	-78.92	-96.50	20.38	0.85
-63.30	144.73	16.97									
63		102D	102D	N	CA	748	749	103.89	114.20		
-40.00											
64	10056	103Y	104S	C	N	766	768	26.22	-72.40	116.05	9.34
-64.10	143.44	10.63									
64		104S	104S	N	CA	768	769	-146.43	152.40		

-35.00											
65	10057	104S	105G	C	N	772	774	126.07	78.70	55.97	1.77
82.20	161.63	9.96									
65		105G	105G	N	CA	774	775	164.07	-166.10		
8.50											
66	10058	105G	106D	C	N	776	778	69.17	54.50	37.94	1.88
-63.30	140.20	23.76									
66		106D	106D	N	CA	778	779	5.90	40.90		
-40.00											
67	10059	106D	107R	C	N	784	786	157.83	-125.20	85.94	4.37
-63.00	-160.14	23.51									
67		107R	107R	N	CA	786	787	102.35	140.60		
-41.10											
68	10061	108P	109R	C	N	802	804	-73.17	-72.10	46.88	3.63
-63.00	136.51	17.78									
68		109R	109R	N	CA	804	805	95.03	141.90		
-41.10											
69	10062	109R	110Y	C	N	813	815	-123.46	-124.30	4.90	0.23
-63.50	-175.99	26.45									
69		110Y	110Y	N	CA	815	816	130.57	135.40		
-43.40											
70	10063	110Y	111A	C	N	825	827	-108.02	-134.00	35.45	1.02
-62.50	169.99	26.03									
70		111A	111A	N	CA	827	828	122.88	147.00		
-40.90											
71	10068	115C	116A	C	N	855	857	-115.48	-134.00	18.53	0.59
-62.50	-179.35	32.42									
71		116A	116A	N	CA	857	858	146.39	147.00		
-40.90											
72	10069	116A	117Q	C	N	860	862	-73.80	-73.00	7.45	0.47
-63.80	171.89	25.80									
72		117Q	117Q	N	CA	862	863	148.10	140.70		
-40.30											
73	10072	119V	120G	C	N	883	885	66.99	78.70	15.39	0.40
82.20	165.33	8.79									
73		120G	120G	N	CA	885	886	-156.13	-166.10		
8.50											
74	10074	121V	122G	C	N	894	896	95.52	78.70	39.91	0.60
82.20	149.80	7.94									
74		122G	122G	N	CA	896	897	157.71	-166.10		
8.50											
75	10111	158L	159R	C	N	1163	1165	-140.00	-125.20	35.73	1.35
-63.00	164.87	27.49									
75		159R	159R	N	CA	1165	1166	173.11	140.60		
-41.10											
76	10113	160V	161R	C	N	1181	1183	166.08	-125.20	79.66	2.37
-63.00	-169.76	33.92									
76		161R	161R	N	CA	1183	1184	-179.12	140.60		

-41.10	77	10116	163P	164R	C	N	1206	1208	-177.28	-125.20	54.26	1.81
-63.00	-160.88	34.42										
	77		164R	164R	N	CA	1208	1209	155.84	140.60		
-41.10	78	10118	165L	166W	C	N	1225	1227	-136.82	-124.90	25.45	0.93
-63.00	167.10	25.86										
	78		166W	166W	N	CA	1227	1228	165.89	143.40		
-44.20	79	10120	167C	168P	C	N	1245	1247	-55.62	-58.70	3.08	0.40
-64.50	177.84	12.81										
	79		168P	168P	N	CA	1247	1248	-30.42	-30.50		
147.20	80	10121	168P	169H	C	N	1252	1254	-66.13	-67.60	4.38	0.29
-63.20	178.20	22.10										
	80		169H	169H	N	CA	1254	1255	135.87	140.00		
-42.30	81	10122	169H	170P	C	N	1262	1264	-73.29	-58.70	28.40	1.67
-64.50	153.58	11.93										
	81		170P	170P	N	CA	1264	1265	-6.13	-30.50		
147.20	82	10130	177G	178H	C	N	1323	1325	-78.58	-67.60	14.90	0.88
-63.20	168.34	22.03										
	82		178H	178H	N	CA	1325	1326	150.07	140.00		
-42.30	83	10133	180C	181E	C	N	1345	1347	-148.71	-117.80	34.97	1.02
-63.60	-172.95	29.68										
	83		181E	181E	N	CA	1347	1348	153.14	136.80		
-40.30	84	10134	181E	182Q	C	N	1354	1356	-94.86	-73.00	41.73	3.15
-63.80	148.74	20.37										
	84		182Q	182Q	N	CA	1356	1357	105.16	140.70		
-40.30	85	10135	182Q	183W	C	N	1363	1365	-152.07	-124.90	43.05	1.42
-63.00	165.10	26.61										
	85		183W	183W	N	CA	1365	1366	176.79	143.40		
-44.20	86	10138	185C	186E	C	N	1390	1392	-68.57	-69.30	1.08	0.10
-63.60	176.47	23.80										
	86		186E	186E	N	CA	1392	1393	143.30	142.50		
-40.30	87	10141	188D	189A	C	N	1415	1417	171.82	-134.00	54.31	1.66
-62.50	-149.90	41.03										
	87		189A	189A	N	CA	1417	1418	150.73	147.00		
-40.90	88	10143	190K	191R	C	N	1429	1431	-76.93	-72.10	6.42	0.42
-63.00	173.32	24.36										
	88		191R	191R	N	CA	1431	1432	146.14	141.90		

-41.10											
89	10144	191R	192P	C	N	1440	1442	-75.24	-64.50	10.80	1.06
-58.70	179.56	13.54									
89		192P	192P	N	CA	1442	1443	148.30	147.20		
-30.50											
90	10145	192P	193R	C	N	1447	1449	-127.67	-125.20	2.58	0.12
-63.00	-169.63	30.18									
90		193R	193R	N	CA	1449	1450	139.85	140.60		
-41.10											
91	10146	193R	194K	C	N	1458	1460	-158.20	-118.00	53.52	1.85
-62.90	173.32	28.16									
91		194K	194K	N	CA	1460	1461	174.43	139.10		
-40.80											
92	10148	195T	196A	C	N	1474	1476	-105.75	-134.00	32.27	0.74
-62.50	177.63	27.33									
92		196A	196A	N	CA	1476	1477	131.39	147.00		
-40.90											
93	10150	197P	198R	C	N	1486	1488	173.71	-125.20	65.16	2.08
-63.00	-161.45	34.80									
93		198R	198R	N	CA	1488	1489	163.27	140.60		
-41.10											
94	10152	199D	200T	C	N	1505	1507	-153.77	-124.80	42.93	1.36
-63.20	169.03	27.42									
94		200T	200T	N	CA	1507	1508	175.18	143.50		
-42.10											
95	10153	200T	201G	C	N	1512	1514	170.71	-167.20	30.43	1.13
82.20	170.02	12.16									
95		201G	201G	N	CA	1514	1515	153.68	174.60		
8.50											
96	10154	201G	202A	C	N	1516	1518	-151.49	-134.00	19.47	0.44
-62.50	-173.79	35.27									
96		202A	202A	N	CA	1518	1519	155.54	147.00		
-40.90											
97	10155	202A	203F	C	N	1521	1523	-132.80	-124.20	16.27	0.51
-63.20	173.19	28.58									
97		203F	203F	N	CA	1523	1524	157.11	143.30		
-44.30											
98	10156	203F	204D	C	N	1532	1534	-74.06	-70.90	9.22	0.32
-63.30	161.41	20.59									
98		204D	204D	N	CA	1534	1535	158.96	150.30		
-40.00											
99	10157	204D	205A	C	N	1540	1542	-72.35	-68.20	9.18	0.60
-62.50	165.90	27.68									
99		205A	205A	N	CA	1542	1543	153.49	145.30		
-40.90											
100	10160	207G	208E	C	N	1556	1558	-79.74	-69.30	14.87	0.83
-63.60	167.40	23.22									
100		208E	208E	N	CA	1558	1559	153.08	142.50		

-40.30											
101	10163	210E	211A	C	N	1581	1583	73.17	-68.20	141.62	12.28
-62.50	-146.07	32.49									
101		211A	211A	N	CA	1583	1584	153.70	145.30		
-40.90											
102	10165	212W	213H	C	N	1600	1602	-109.79	-125.60	16.59	0.68
-63.20	-179.97	25.55									
102		213H	213H	N	CA	1602	1603	143.80	138.80		
-42.30											
103	10166	213H	214R	C	N	1610	1612	-74.09	-72.10	2.88	0.19
-63.00	175.27	24.43									
103		214R	214R	N	CA	1612	1613	143.98	141.90		
-41.10											
104	10167	214R	215N	C	N	1621	1623	-99.96	-119.90	27.85	0.81
-63.20	162.86	18.57									
104		215N	215N	N	CA	1623	1624	117.56	137.00		
-41.10											
105	10170	217I	218A	C	N	1643	1645	-178.92	-134.00	59.72	1.67
-62.50	176.57	34.95									
105		218A	218A	N	CA	1645	1646	-173.64	147.00		
-40.90											
106	10171	218A	219Y	C	N	1648	1650	-47.63	-98.40	57.61	3.30
-63.50	161.75	24.87									
106		219Y	219Y	N	CA	1650	1651	155.63	128.40		
-43.40											
107	10172	219Y	220T	C	N	1660	1662	-65.41	-63.20	68.18	8.89
-63.20	68.18	8.89									
107		220T	220T	N	CA	1662	1663	-110.24	-42.10		
-42.10											
108	10173	220T	221S	C	N	1667	1669	-98.27	-72.40	44.02	3.40
-64.10	155.58	9.78									
108		221S	221S	N	CA	1669	1670	116.78	152.40		
-35.00											
109	10175	222P	223W	C	N	1680	1682	-93.55	-71.30	33.60	1.98
-63.00	154.68	21.33									
109		223W	223W	N	CA	1682	1683	164.17	139.00		
-44.20											
110	10176	223W	224S	C	N	1694	1696	-64.01	-72.40	9.59	0.77
-64.10	167.94	12.16									
110		224S	224S	N	CA	1696	1697	157.06	152.40		
-35.00											
111	10179	226C	227S	C	N	1713	1715	-172.42	-136.60	58.61	2.03
-64.10	167.23	19.91									
111		227S	227S	N	CA	1715	1716	-162.41	151.20		
-35.00											
112	10180	227S	228T	C	N	1719	1721	-58.71	-78.10	26.20	0.99
-63.20	174.33	22.65									
112		228T	228T	N	CA	1721	1722	132.17	149.80		

-42.10											
113	10181	228T	229S	C	N	1726	1728	-120.74	-136.60	17.10	0.84
-64.10	176.72	16.77									
113		229S	229S	N	CA	1728	1729	157.60	151.20		
-35.00											
114	10183	230C	231G	C	N	1738	1740	-65.10	-80.20	44.24	1.10
82.20	-167.45	6.66									
114		231G	231G	N	CA	1740	1741	132.51	174.10		
8.50											
115	10184	231G	232L	C	N	1742	1744	-84.69	-70.70	17.70	1.19
-63.50	167.70	24.55									
115		232L	232L	N	CA	1744	1745	152.44	141.60		
-41.20											
116	10185	232L	233G	C	N	1750	1752	-72.98	-80.20	17.49	0.41
82.20	-144.40	6.88									
116		233G	233G	N	CA	1752	1753	158.17	174.10		
8.50											
117	10187	234V	235S	C	N	1761	1763	-112.69	-136.60	25.41	0.82
-64.10	-175.89	11.42									
117		235S	235S	N	CA	1763	1764	142.58	151.20		
-35.00											
118	10188	235S	236T	C	N	1767	1769	-83.75	-78.10	10.27	0.34
-63.20	160.85	21.99									
118		236T	236T	N	CA	1769	1770	158.37	149.80		
-42.10											
119	10189	236T	237R	C	N	1774	1776	-115.39	-125.20	20.05	1.11
-63.00	169.14	26.47									
119		237R	237R	N	CA	1776	1777	158.08	140.60		
-41.10											
120	10191	238I	239S	C	N	1793	1795	-152.97	-136.60	23.63	0.77
-64.10	-179.80	19.45									
120		239S	239S	N	CA	1795	1796	168.23	151.20		
-35.00											
121	10192	239S	240N	C	N	1799	1801	-117.31	-119.90	19.68	0.95
-63.20	171.17	24.48									
121		240N	240N	N	CA	1801	1802	156.51	137.00		
-41.10											
122	10194	241V	242N	C	N	1814	1816	-138.80	-119.90	19.88	0.67
-63.20	-168.67	28.20									
122		242N	242N	N	CA	1816	1817	143.14	137.00		
-41.10											
123	10195	242N	243A	C	N	1822	1824	-116.65	-134.00	21.38	0.54
-62.50	-176.43	27.97									
123		243A	243A	N	CA	1824	1825	134.50	147.00		
-40.90											
124	10196	243A	244Q	C	N	1827	1829	-148.26	-121.10	34.85	1.09
-63.80	179.30	30.73									
124		244Q	244Q	N	CA	1829	1830	161.53	139.70		

-40.30											
125	10198	245C	246W	C	N	1842	1844	89.29	-124.90	150.34	5.69
-63.00	-155.97	24.95									
125		246W	246W	N	CA	1844	1845	-179.97	143.40		
-44.20											
126	10200	247P	248E	C	N	1863	1865	-76.86	-69.30	14.22	0.83
-63.60	165.68	22.83									
126		248E	248E	N	CA	1865	1866	154.55	142.50		
-40.30											
127	10201	248E	249Q	C	N	1872	1874	-67.60	-73.00	7.53	0.44
-63.80	175.80	25.65									
127		249Q	249Q	N	CA	1874	1875	135.45	140.70		
-40.30											
128	10202	249Q	250E	C	N	1881	1883	-146.34	-117.80	47.99	1.69
-63.60	166.35	26.75									
128		250E	250E	N	CA	1883	1884	175.38	136.80		
-40.30											
129	10203	250E	251S	C	N	1890	1892	-72.58	-72.40	21.17	1.24
-64.10	151.67	11.51									
129		251S	251S	N	CA	1892	1893	173.57	152.40		
-35.00											
130	10204	251S	252R	C	N	1896	1898	-75.89	-72.10	60.95	4.77
-63.00	122.84	15.76									
130		252R	252R	N	CA	1898	1899	81.06	141.90		
-41.10											
131	10207	254C	255N	C	N	1921	1923	-113.81	-119.90	12.79	0.68
-63.20	178.00	25.14									
131		255N	255N	N	CA	1923	1924	148.25	137.00		
-41.10											
132	10209	256L	257R	C	N	1937	1939	-121.81	-125.20	26.90	1.37
-63.00	162.62	26.01									
132		257R	257R	N	CA	1939	1940	167.28	140.60		
-41.10											
133	10211	258P	259C	C	N	1955	1957	-61.76	-63.00	6.96	0.77
-117.90	179.93	7.77									
133		259C	259C	N	CA	1957	1958	-47.95	-41.10		
141.10											
134	10212	259C	260D	C	N	1961	1963	-97.23	-96.50	13.38	0.56
-63.30	170.96	19.29									
134		260D	260D	N	CA	1963	1964	127.56	114.20		
-40.00											
135	10214	261V	262D	C	N	1976	1978	-91.76	-70.90	59.77	2.09
-63.30	117.21	16.30									
135		262D	262D	N	CA	1978	1979	-153.69	150.30		
-40.00											
136	10216	263I	264H	C	N	1992	1994	-129.10	-125.60	4.44	0.11
-63.20	-171.91	27.83									
136		264H	264H	N	CA	1994	1995	141.53	138.80		

-42.30											
137	10218	265T	266L	C	N	2009	2011	-134.55	-108.50	27.82	1.24
-63.50	-169.70	30.82									
137		266L	266L	N	CA	2011	2012	142.26	132.50		
-41.20											
138	10229	276V	277Y	C	N	2087	2089	-134.60	-124.30	17.82	1.37
-63.50	178.98	25.30									
138		277Y	277Y	N	CA	2089	2090	120.85	135.40		
-43.40											
139	10230	277Y	278Q	C	N	2099	2101	-140.38	-121.10	21.50	0.67
-63.80	-173.11	31.50									
139		278Q	278Q	N	CA	2101	2102	149.22	139.70		
-40.30											
140	10232	279P	280E	C	N	2115	2117	-161.81	-117.80	44.14	1.54
-63.60	-155.35	32.73									
140		280E	280E	N	CA	2117	2118	140.15	136.80		
-40.30											
141	10233	280E	281A	C	N	2124	2126	-74.04	-68.20	8.22	0.81
-62.50	179.95	30.07									
141		281A	281A	N	CA	2126	2127	139.52	145.30		
-40.90											
142	10234	281A	282S	C	N	2129	2131	-163.35	-136.60	29.66	0.92
-64.10	-170.87	20.86									
142		282S	282S	N	CA	2131	2132	164.00	151.20		
-35.00											
143	10235	282S	283M	C	N	2135	2137	-75.40	-73.00	7.13	0.45
-63.40	170.21	26.36									
143		283M	283M	N	CA	2137	2138	149.71	143.00		
-40.50											
144	10236	283M	284N	C	N	2143	2145	-88.11	-71.20	35.76	2.73
-63.20	154.41	18.04									
144		284N	284N	N	CA	2145	2146	111.29	142.80		
-41.10											
145	10237	284N	285F	C	N	2151	2153	-144.02	-124.20	27.37	0.73
-63.20	173.49	29.25									
145		285F	285F	N	CA	2153	2154	162.18	143.30		
-44.30											
146	10239	286T	287L	C	N	2169	2171	-75.73	-70.70	7.22	0.46
-63.50	172.46	24.67									
146		287L	287L	N	CA	2171	2172	146.77	141.60		
-41.20											
147	10240	287L	288A	C	N	2177	2179	-129.64	-134.00	4.67	0.11
-62.50	-173.69	34.13									
147		288A	288A	N	CA	2179	2180	145.31	147.00		
-40.90											
148	10244	291I	292S	C	N	2200	2202	-156.46	-136.60	27.54	0.88
-64.10	-179.81	19.71									
148		292S	292S	N	CA	2202	2203	170.27	151.20		

-35.00											
149	10245	292S	293T	C	N	2206	2208	-75.99	-78.10	3.23	0.20
-63.20	166.15	22.15									
149		293T	293T	N	CA	2208	2209	152.24	149.80		
-42.10											
150	10246	293T	294R	C	N	2213	2215	-127.13	-125.20	2.87	0.09
-63.00	-172.51	29.75									
150		294R	294R	N	CA	2215	2216	142.72	140.60		
-41.10											
151	10247	294R	295S	C	N	2224	2226	-88.45	-72.40	31.75	1.46
-64.10	147.23	12.28									
151		295S	295S	N	CA	2226	2227	179.80	152.40		
-35.00											
152	10248	295S	296Y	C	N	2230	2232	-96.83	-98.40	2.17	0.18
-63.50	173.53	25.90									
152		296Y	296Y	N	CA	2232	2233	126.90	128.40		
-43.40											
153	10249	296Y	297Q	C	N	2242	2244	-129.64	-121.10	21.05	0.83
-63.80	173.73	29.02									
153		297Q	297Q	N	CA	2244	2245	158.93	139.70		
-40.30											
154	10250	297Q	298P	C	N	2251	2253	-66.87	-58.70	10.26	0.83
-64.50	171.50	12.92									
154		298P	298P	N	CA	2253	2254	-24.29	-30.50		
147.20											
155	10251	298P	299K	C	N	2258	2260	-116.15	-118.00	21.98	1.09
-62.90	166.92	24.85									
155		299K	299K	N	CA	2260	2261	161.00	139.10		
-40.80											
156	10252	299K	300Y	C	N	2267	2269	-105.61	-98.40	27.85	2.84
-63.50	150.90	21.96									
156		300Y	300Y	N	CA	2269	2270	101.50	128.40		
-43.40											
157	10257	304C	305M	C	N	2302	2304	-122.22	-125.60	28.34	1.28
-63.40	163.79	20.76									
157		305M	305M	N	CA	2304	2305	112.37	140.50		
-40.50											
158	10259	306D	307N	C	N	2318	2320	-107.24	-119.90	19.78	1.07
-63.20	172.42	24.06									
158		307N	307N	N	CA	2320	2321	152.21	137.00		
-41.10											
159	10264	311I	312P	C	N	2357	2359	-72.22	-58.70	23.88	1.45
-64.50	158.19	12.22									
159		312P	312P	N	CA	2359	2360	-10.81	-30.50		
147.20											
160	10266	313Y	314K	C	N	2376	2378	-100.38	-118.00	39.90	2.07
-62.90	149.08	21.57									
160		314K	314K	N	CA	2378	2379	174.91	139.10		

-40.80											
161	10268	315S	316K	C	N	2391	2393	-163.38	-62.90	102.27	15.82
-62.90	102.27		15.82								
161		316K	316K	N	CA	2393	2394	-21.76	-40.80		
-40.80											
162	10270	317T	318I	C	N	2407	2409	-68.31	-63.40	7.82	1.19
-120.60	175.78		8.13								
162		318I	318I	N	CA	2409	2410	-37.52	-43.60		
130.30											
163	10271	318I	319D	C	N	2415	2417	-49.81	-70.90	21.25	1.69
-63.30	167.60		19.90								
163		319D	319D	N	CA	2417	2418	152.95	150.30		
-40.00											
164	10278	325P	326D	C	N	2469	2471	-172.21	-96.50	78.02	3.17
-63.30	173.73		18.93								
164		326D	326D	N	CA	2471	2472	95.36	114.20		
-40.00											
165	10279	326D	327G	C	N	2477	2479	-134.39	-167.20	42.58	0.85
82.20	-160.31		15.36								
165		327G	327G	N	CA	2479	2480	147.46	174.60		
8.50											
166	10280	327G	328L	C	N	2481	2483	-106.19	-108.50	6.48	0.37
-63.50	-175.24		23.57								
166		328L	328L	N	CA	2483	2484	138.56	132.50		
-41.20											
167	10281	328L	329G	C	N	2489	2491	-168.48	-167.20	10.06	0.41
82.20	-169.41		13.96								
167		329G	329G	N	CA	2491	2492	164.62	174.60		
8.50											
168	10282	329G	330F	C	N	2493	2495	-130.93	-124.20	25.30	1.01
-63.20	162.77		26.99								
168		330F	330F	N	CA	2495	2496	167.69	143.30		
-44.30											
169	10283	330F	331S	C	N	2504	2506	-60.82	-72.40	12.58	0.73
-64.10	177.56		12.67								
169		331S	331S	N	CA	2506	2507	147.47	152.40		
-35.00											
170	10284	331S	332R	C	N	2510	2512	-101.34	-125.20	29.41	0.87
-63.00	168.91		20.51								
170		332R	332R	N	CA	2512	2513	123.40	140.60		
-41.10											
171	10285	332R	333Q	C	N	2521	2523	-135.39	-121.10	14.46	0.59
-63.80	-168.33		25.10								
171		333Q	333Q	N	CA	2523	2524	137.50	139.70		
-40.30											
172	10287	334V	335L	C	N	2537	2539	-120.25	-108.50	22.06	1.26
-63.50	165.09		20.48								
172		335L	335L	N	CA	2539	2540	113.83	132.50		

-41.20											
173	10288	335L	336W	C	N	2545	2547	-136.76	-124.90	15.09	0.85
-63.00	-167.08	21.23									
173		336W	336W	N	CA	2547	2548	134.06	143.40		
-44.20											
174	10290	337I	338N	C	N	2567	2569	-131.83	-119.90	23.51	1.26
-63.20	172.12	18.70									
174		338N	338N	N	CA	2569	2570	116.74	137.00		
-41.10											
175	10291	338N	339A	C	N	2575	2577	-159.81	-134.00	25.92	0.77
-62.50	-164.34	37.26									
175		339A	339A	N	CA	2577	2578	149.36	147.00		
-40.90											
176	10293	340C	341F	C	N	2586	2588	-120.27	-124.20	14.88	0.59
-63.20	-177.59	21.89									
176		341F	341F	N	CA	2588	2589	128.96	143.30		
-44.30											
177	10295	342C	343N	C	N	2603	2605	-114.32	-119.90	9.65	0.30
-63.20	177.74	19.85									
177		343N	343N	N	CA	2605	2606	129.13	137.00		
-41.10											
178	10296	343N	344L	C	N	2611	2613	-107.04	-108.50	7.19	0.37
-63.50	172.26	21.83									
178		344L	344L	N	CA	2613	2614	125.46	132.50		
-41.20											
179	10297	344L	345S	C	N	2619	2621	-131.60	-136.60	12.63	0.52
-64.10	-172.81	11.57									
179		345S	345S	N	CA	2621	2622	139.60	151.20		
-35.00											
180	10299	346C	347R	C	N	2631	2633	-123.19	-125.20	5.15	0.20
-63.00	-173.09	21.90									
180		347R	347R	N	CA	2633	2634	135.86	140.60		
-41.10											
181	10300	347R	348N	C	N	2642	2644	-106.62	-119.90	25.34	0.82
-63.20	162.43	18.26									
181		348N	348N	N	CA	2644	2645	115.42	137.00		
-41.10											
182	10302	349P	350N	C	N	2657	2659	-104.48	-119.90	19.45	0.57
-63.20	171.30	19.43									
182		350N	350N	N	CA	2659	2660	125.15	137.00		
-41.10											
183	10303	350N	351D	C	N	2665	2667	-109.18	-96.50	62.19	2.60
-63.30	103.99	11.04									
183		351D	351D	N	CA	2667	2668	53.32	114.20		
-40.00											
184	10305	352I	353F	C	N	2681	2683	-120.17	-124.20	10.42	0.38
-63.20	-173.11	22.50									
184		353F	353F	N	CA	2683	2684	133.69	143.30		

-44.30											
185	10306	353F	354A	C	N	2692	2694	-139.38	-134.00	5.38	0.18
-62.50	-171.51	35.01									
185		354A	354A	N	CA	2694	2695	147.00	147.00		
-40.90											
186	10307	354A	355D	C	N	2697	2699	-104.52	-96.50	12.37	0.51
-63.30	150.53	16.53									
186		355D	355D	N	CA	2699	2700	104.78	114.20		
-40.00											
187	10308	355D	356L	C	N	2705	2707	-101.71	-108.50	15.56	0.76
-63.50	164.21	20.94									
187		356L	356L	N	CA	2707	2708	118.51	132.50		
-41.20											
188	10309	356L	357E	C	N	2713	2715	-132.94	-117.80	15.34	0.50
-63.60	-167.47	22.67									
188		357E	357E	N	CA	2715	2716	139.31	136.80		
-40.30											
189	10310	357E	358S	C	N	2722	2724	-132.95	-136.60	4.92	0.16
-64.10	-169.99	18.63									
189		358S	358S	N	CA	2724	2725	147.90	151.20		
-35.00											
190	10311	358S	359Y	C	N	2728	2730	-118.06	-124.30	10.80	0.43
-63.50	178.52	25.79									
190		359Y	359Y	N	CA	2730	2731	126.58	135.40		
-43.40											
191	10312	359Y	360P	C	N	2740	2742	-53.26	-58.70	7.44	0.54
-64.50	177.58	13.85									
191		360P	360P	N	CA	2742	2743	-35.58	-30.50		
147.20											
192	10313	360P	361D	C	N	2747	2749	-98.45	-96.50	11.01	0.46
-63.30	168.74	18.97									
192		361D	361D	N	CA	2749	2750	125.04	114.20		
-40.00											
193	10314	361D	362F	C	N	2755	2757	-110.18	-124.20	17.77	0.46
-63.20	-177.17	22.46									
193		362F	362F	N	CA	2757	2758	132.39	143.30		
-44.30											
194	10315	362F	363S	C	N	2766	2768	-138.23	-136.60	8.65	0.40
-64.10	-178.83	18.41									
194		363S	363S	N	CA	2768	2769	159.69	151.20		
-35.00											
195	10316	363S	364E	C	N	2772	2774	-77.03	-69.30	13.77	0.79
-63.60	166.34	22.92									
195		364E	364E	N	CA	2774	2775	153.90	142.50		
-40.30											
196	10318	365I	366A	C	N	2789	2791	-71.81	-68.20	9.16	0.62
-62.50	165.64	27.61									
196		366A	366A	N	CA	2791	2792	153.72	145.30		

-40.90

report_____> Distribution of short non-bonded contacts:

```
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:      0      0      0      0      1     21     51    166    161    193    215    258    264
295    322
```

<< end of ENERGY.

iupac_m_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls_286W> MODEL atom not classified: ASN:OXT ASN

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

```
Number of all residues in MODEL           :      367
Number of all, selected real atoms         :      2804      2804
Number of all, selected pseudo atoms       :           0           0
Number of all static, selected restraints  :     13904     13904
COVALENT_CYS                             :           F
NONBONDED_SEL_ATOMS                       :           1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):    321041
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                             :     -19025.3555
```

<< end of ENERGY.

DOPE score : -19025.355469

>> Model assessment by SOAP-Protein-OD score

```

preppdf_455W> None of the non-bonded terms selected.
pair2___701W> Insufficient system memory to allocate storage for cell-based
               (NlogN) nonbond list algorithm; falling back to N*N method.
               Warning      5 of      10; further warnings will be suppressed.

```

```

>> ENERGY; Differences between the model's features and restraints:
Number of all residues in MODEL           :      367
Number of all, selected real atoms        :      2804      2804
Number of all, selected pseudo atoms      :           0           0
Number of all static, selected restraints :      13904      13904
COVALENT_CYS                             :           F
NONBONDED_SEL_ATOMS                      :           1
Number of non-bonded pairs (excluding 1-2,1-3,1-4):      0
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                            :      0.000
DYNAMIC_PAIRS,_SPHERE,_COULOMB,_LENNARD,_MODELLER :           T           F           F
F           F
SPHERE_STDV                             :      0.050
RADII_FACTOR                             :      0.820
Current energy                           :           0.0000

```

```

<< end of ENERGY.
SOAP-Protein-OD score                    :      0.000000
>> Model assessment by GA341 potential

```

```

Surface library          :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/surf5.de
Pair library             :
/Users/yingyinli/opt/anaconda3/lib/modeller-10.1/modlib/pair9.de
Chain identifier         : -
% sequence identity      :      62.856998
Sequence length         :           367
Compactness              :      0.013353
Native energy (pair)    :      78.545624
Native energy (surface) :      48.121285
Native energy (combined) :      10.186766
Z score (pair)          :      -3.183653
Z score (surface)       :      -0.856761
Z score (combined)      :      -2.831354

```

GA341 score : 0.900786

```
>> ENERGY; Differences between the model's features and restraints:
Number of all residues in MODEL : 367
Number of all, selected real atoms : 2804 2804
Number of all, selected pseudo atoms : 0 0
Number of all static, selected restraints : 13904 13904
COVALENT_CYS : F
NONBONDED_SEL_ATOMS : 1
Number of non-bonded pairs (excluding 1-2,1-3,1-4): 4280
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 : 1910.7992
```

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	2881	0	0	0.003	0.003
5.6976	1.000					
2	Bond angle potential	3935	0	1	1.657	1.657
207.49	1.000					
3	Stereochemical cosine torsion poten:	1962	0	76	50.892	50.892

778.76	1.000					
4 Stereochemical improper torsion pot:	1155	0	0	0.879	0.879	
18.661	1.000					
5 Soft-sphere overlap restraints :	4280	0	0	0.003	0.003	
3.2089	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) :	765	0	7	1.210	1.210	
92.864	1.000					
10 Distance restraints 2 (N-O) :	973	0	14	1.659	1.659	
170.22	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:	366	0	1	2.941	2.941	
37.329	1.000					
14 Sidechain Chi_1 dihedral restraints:	315	0	1	82.890	82.890	
77.825	1.000					
15 Sidechain Chi_2 dihedral restraints:	209	0	0	69.614	69.614	
72.752	1.000					
16 Sidechain Chi_3 dihedral restraints:	98	0	0	92.088	92.088	
56.170	1.000					
17 Sidechain Chi_4 dihedral restraints:	34	0	0	115.214	115.214	
20.919	1.000					
18 Disulfide distance restraints :	5	0	0	0.007	0.007	
0.38949E-01	1.000					
19 Disulfide angle restraints :	10	0	0	1.934	1.934	
0.82595	1.000					
20 Disulfide dihedral angle restraints:	5	0	0	37.626	37.626	
5.7777	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) :	643	0	0	0.606	0.606	
17.365	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:	365	200	38	32.046	131.145	
321.50	1.000					
26 Distance restraints 4 (SDCH-SDCH) :	183	0	2	1.406	1.406	
23.393	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					

Heavy relative violation of each residue is written to: WISP1.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: 60767.0391

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 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	9955	2R 3W C	N	18 20	-63.37	-71.30	12.56	0.75
-63.00	173.46	21.66						
1		3W 3W N	CA	20 21	129.26	139.00		
-44.20								
2	9956	3W 4F C	N	32 34	-123.32	-124.20	15.20	0.69
-63.20	-177.39	21.77						
2		4F 4F N	CA	34 35	128.13	143.30		
-44.30								
3	9957	4F 5L C	N	43 45	-86.94	-70.70	20.54	1.38
-63.50	166.29	24.50						
3		5L 5L N	CA	45 46	154.17	141.60		
-41.20								
4	9959	6P 7W C	N	58 60	-113.55	-124.90	12.14	0.43
-63.00	-176.19	26.33						
4		7W 7W N	CA	60 61	139.08	143.40		
-44.20								
5	9960	7W 8T C	N	72 74	-91.66	-78.10	27.42	0.90
-63.20	147.06	20.76						
5		8T 8T N	CA	74 75	173.62	149.80		
-42.10								
6	9961	8T 9L C	N	79 81	-98.73	-108.50	9.81	0.46
-63.50	176.43	22.72						
6		9L 9L N	CA	81 82	131.67	132.50		
-41.20								
7	9962	9L 10A C	N	87 89	-135.73	-134.00	6.43	0.32
-62.50	-178.65	33.64						
7		10A 10A N	CA	89 90	153.19	147.00		
-40.90								
8	9963	10A 11A C	N	92 94	-104.32	-134.00	33.94	0.78
-62.50	176.46	27.19						
8		11A 11A N	CA	94 95	130.54	147.00		
-40.90								
9	9965	12V 13T C	N	104 106	-125.06	-124.80	10.35	0.45
-63.20	-174.15	20.42						
9		13T 13T N	CA	106 107	133.15	143.50		
-42.10								

10	9966	13T	14A	C	N	111	113	-153.36	-134.00	21.15	0.48
-62.50	-172.86	35.52									
10		14A	14A	N	CA	113	114	155.50	147.00		
-40.90											
11	9967	14A	15A	C	N	116	118	-133.15	-134.00	1.68	0.07
-62.50	-172.61	34.49									
11		15A	15A	N	CA	118	119	145.54	147.00		
-40.90											
12	9968	15A	16A	C	N	121	123	-140.67	-134.00	11.36	0.41
-62.50	-179.30	33.80									
12		16A	16A	N	CA	123	124	156.19	147.00		
-40.90											
13	9969	16A	17A	C	N	126	128	-89.46	-68.20	34.16	3.34
-62.50	161.73	25.32									
13		17A	17A	N	CA	128	129	118.57	145.30		
-40.90											
14	9970	17A	18S	C	N	131	133	-169.78	-136.60	34.58	1.14
-64.10	-164.86	21.76									
14		18S	18S	N	CA	133	134	160.95	151.20		
-35.00											
15	9971	18S	19T	C	N	137	139	-103.03	-124.80	69.23	2.37
-63.20	126.32	13.97									
15		19T	19T	N	CA	139	140	77.78	143.50		
-42.10											
16	9974	21L	22A	C	N	159	161	-110.28	-134.00	24.18	0.64
-62.50	-176.87	32.54									
16		22A	22A	N	CA	161	162	142.31	147.00		
-40.90											
17	9975	22A	23T	C	N	164	166	-69.59	-78.10	19.41	0.64
-63.20	174.58	21.97									
17		23T	23T	N	CA	166	167	132.36	149.80		
-42.10											
18	9976	23T	24A	C	N	171	173	-73.77	-68.20	6.40	0.43
-62.50	171.01	28.59									
18		24A	24A	N	CA	173	174	148.46	145.30		
-40.90											
19	9978	25L	26S	C	N	184	186	-133.83	-136.60	7.61	0.32
-64.10	-167.80	11.88									
19		26S	26S	N	CA	186	187	144.11	151.20		
-35.00											
20	9979	26S	27P	C	N	190	192	-74.00	-58.70	31.69	1.85
-64.50	150.25	11.72									
20		27P	27P	N	CA	192	193	-2.75	-30.50		
147.20											
21	9983	30T	31T	C	N	216	218	-94.31	-78.10	30.16	0.99
-63.20	146.02	20.80									
21		31T	31T	N	CA	218	219	175.23	149.80		
-42.10											

22	9984	31T	32M	C	N	223	225	-93.08	-73.00	27.02	2.15
-63.40	168.06	22.94									
22		32M	32M	N	CA	225	226	124.92	143.00		
-40.50											
23	9985	32M	33D	C	N	231	233	-83.40	-70.90	18.78	0.72
-63.30	156.98	20.64									
23		33D	33D	N	CA	233	234	164.31	150.30		
-40.00											
24	9987	34F	35T	C	N	250	252	-131.76	-124.80	7.30	0.43
-63.20	-170.57	28.82									
24		35T	35T	N	CA	252	253	141.32	143.50		
-42.10											
25	9989	36P	37A	C	N	264	266	-131.75	-134.00	2.25	0.07
-62.50	-174.43	34.12									
25		37A	37A	N	CA	266	267	146.94	147.00		
-40.90											
26	9991	38P	39L	C	N	276	278	-78.50	-70.70	17.08	1.07
-63.50	162.69	23.48									
26		39L	39L	N	CA	278	279	156.80	141.60		
-41.20											
27	9992	39L	40E	C	N	284	286	-59.35	-63.60	5.86	0.70
-69.30	173.44	13.58									
27		40E	40E	N	CA	286	287	-44.34	-40.30		
142.50											
28	9994	41D	42T	C	N	301	303	-79.58	-78.10	65.51	2.85
-63.20	127.46	15.32									
28		42T	42T	N	CA	303	304	84.31	149.80		
-42.10											
29	9997	44S	45R	C	N	320	322	-95.89	-72.10	25.51	2.13
-63.00	176.87	21.86									
29		45R	45R	N	CA	322	323	132.69	141.90		
-41.10											
30	9999	46P	47Q	C	N	338	340	-112.82	-121.10	8.99	0.41
-63.80	-176.81	29.55									
30		47Q	47Q	N	CA	340	341	143.19	139.70		
-40.30											
31	10000	47Q	48F	C	N	347	349	-117.16	-124.20	13.10	0.41
-63.20	-175.37	22.34									
31		48F	48F	N	CA	349	350	132.26	143.30		
-44.30											
32	10001	48F	49C	C	N	358	360	-65.75	-63.00	6.90	1.05
-117.90	179.23	7.70									
32		49C	49C	N	CA	360	361	-47.42	-41.10		
141.10											
33	10002	49C	50K	C	N	364	366	-79.74	-70.20	9.58	0.72
-62.90	-179.59	24.38									
33		50K	50K	N	CA	366	367	139.57	140.40		
-40.80											

34	10003	50K	51W	C	N	373	375	-111.51	-124.90	15.94	0.51
-63.00	-174.59	20.87									
34		51W	51W	N	CA	375	376	134.75	143.40		
-44.20											
35	10006	53C	54E	C	N	400	402	-60.40	-69.30	10.05	0.60
-63.60	178.17	23.93									
35		54E	54E	N	CA	402	403	137.84	142.50		
-40.30											
36	10010	57P	58S	C	N	429	431	-76.02	-72.40	4.91	0.24
-64.10	169.69	13.04									
36		58S	58S	N	CA	431	432	155.72	152.40		
-35.00											
37	10013	60P	61R	C	N	449	451	-149.62	-125.20	24.61	0.91
-63.00	-164.54	32.30									
37		61R	61R	N	CA	451	452	143.68	140.60		
-41.10											
38	10016	63P	64L	C	N	473	475	-101.48	-108.50	10.80	0.61
-63.50	-177.90	27.60									
38		64L	64L	N	CA	475	476	140.70	132.50		
-41.20											
39	10017	64L	65G	C	N	481	483	85.30	78.70	19.32	0.31
82.20	167.27	8.28									
39		65G	65G	N	CA	483	484	175.74	-166.10		
8.50											
40	10019	66V	67S	C	N	492	494	-114.79	-136.60	35.83	1.25
-64.10	165.71	10.21									
40		67S	67S	N	CA	494	495	122.76	151.20		
-35.00											
41	10020	67S	68L	C	N	498	500	-123.95	-108.50	15.65	0.78
-63.50	-178.44	22.57									
41		68L	68L	N	CA	500	501	130.00	132.50		
-41.20											
42	10022	69I	70T	C	N	514	516	-122.59	-124.80	8.03	0.41
-63.20	176.95	26.62									
42		70T	70T	N	CA	516	517	151.22	143.50		
-42.10											
43	10023	70T	71D	C	N	521	523	-72.91	-70.90	2.02	0.16
-63.30	170.13	21.59									
43		71D	71D	N	CA	523	524	150.14	150.30		
-40.00											
44	10024	71D	72G	C	N	529	531	-171.39	-167.20	13.20	0.45
82.20	-152.09	14.81									
44		72G	72G	N	CA	531	532	-172.88	174.60		
8.50											
45	10026	73C	74E	C	N	539	541	-119.08	-117.80	10.86	0.52
-63.60	-179.17	27.25									
45		74E	74E	N	CA	541	542	147.58	136.80		
-40.30											

46	10028	75C	76C C	N	554	556	-64.88	-63.00	3.17	0.52
-117.90	-176.92		7.87							
46		76C	76C N	CA	556	557	-43.66	-41.10		
141.10										
47	10030	77K	78M C	N	569	571	-82.11	-73.00	13.05	1.03
-63.40	175.15		24.75							
47		78M	78M N	CA	571	572	133.65	143.00		
-40.50										
48	10032	79C	80A C	N	583	585	-61.30	-68.20	7.00	0.55
-62.50	175.00		28.62							
48		80A	80A N	CA	585	586	144.11	145.30		
-40.90										
49	10033	80A	81Q C	N	588	590	-85.98	-73.00	13.26	0.99
-63.80	179.68		25.30							
49		81Q	81Q N	CA	590	591	138.00	140.70		
-40.30										
50	10034	81Q	82Q C	N	597	599	-132.20	-121.10	12.33	0.58
-63.80	-172.45		24.61							
50		82Q	82Q N	CA	599	600	134.33	139.70		
-40.30										
51	10040	87C	88T C	N	640	642	-135.83	-124.80	24.75	0.79
-63.20	168.68		26.37							
51		88T	88T N	CA	642	643	165.66	143.50		
-42.10										
52	10041	88T	89E C	N	647	649	-166.43	-117.80	53.42	1.57
-63.60	-169.14		31.07							
52		89E	89E N	CA	649	650	158.91	136.80		
-40.30										
53	10042	89E	90A C	N	656	658	166.76	-134.00	67.00	1.54
-62.50	-167.86		38.19							
53		90A	90A N	CA	658	659	178.29	147.00		
-40.90										
54	10043	90A	91A C	N	661	663	-69.66	-68.20	6.99	0.51
-62.50	167.12		27.74							
54		91A	91A N	CA	663	664	152.14	145.30		
-40.90										
55	10046	93C	94D C	N	680	682	-119.42	-96.50	24.98	1.03
-63.30	173.47		18.78							
55		94D	94D N	CA	682	683	124.15	114.20		
-40.00										
56	10048	95P	96H C	N	695	697	-108.66	-125.60	46.77	1.43
-63.20	144.82		15.83							
56		96H	96H N	CA	697	698	95.20	138.80		
-42.30										
57	10049	96H	97R C	N	705	707	-165.55	-125.20	51.33	1.52
-63.00	178.88		30.92							
57		97R	97R N	CA	707	708	172.34	140.60		
-41.10										

58	10050	97R	98G	C	N	716	718	-136.36	-167.20	41.25	0.86
82.20	-161.90	15.22									
58		98G	98G	N	CA	718	719	147.21	174.60		
8.50											
59	10051	98G	99L	C	N	720	722	-70.92	-70.70	4.83	0.36
-63.50	172.53	24.39									
59		99L	99L	N	CA	722	723	146.43	141.60		
-41.20											
60	10052	99L	100Y	C	N	728	730	-76.09	-98.40	23.19	1.15
-63.50	165.97	25.70									
60		100Y	100Y	N	CA	730	731	122.09	128.40		
-43.40											
61	10055	102D	103Y	C	N	754	756	-136.49	-124.30	12.20	0.93
-63.50	-167.15	27.37									
61		103Y	103Y	N	CA	756	757	135.11	135.40		
-43.40											
62	10056	103Y	104S	C	N	766	768	-145.41	-136.60	9.00	0.31
-64.10	-169.81	19.59									
62		104S	104S	N	CA	768	769	153.07	151.20		
-35.00											
63	10057	104S	105G	C	N	772	774	-173.81	-167.20	18.29	0.75
82.20	-178.27	13.31									
63		105G	105G	N	CA	774	775	157.54	174.60		
8.50											
64	10058	105G	106D	C	N	776	778	-81.57	-70.90	15.98	0.61
-63.30	158.87	20.75									
64		106D	106D	N	CA	778	779	162.19	150.30		
-40.00											
65	10059	106D	107R	C	N	784	786	-75.22	-72.10	14.96	1.08
-63.00	162.83	22.83									
65		107R	107R	N	CA	786	787	156.53	141.90		
-41.10											
66	10061	108P	109R	C	N	802	804	-72.74	-72.10	6.91	0.52
-63.00	170.40	23.68									
66		109R	109R	N	CA	804	805	148.78	141.90		
-41.10											
67	10062	109R	110Y	C	N	813	815	-72.33	-98.40	26.08	1.02
-63.50	171.08	26.70									
67		110Y	110Y	N	CA	815	816	127.45	128.40		
-43.40											
68	10063	110Y	111A	C	N	825	827	-131.22	-134.00	6.83	0.42
-62.50	179.54	33.10									
68		111A	111A	N	CA	827	828	153.23	147.00		
-40.90											
69	10065	112I	113G	C	N	838	840	67.19	78.70	20.90	0.34
82.20	157.87	8.41									
69		113G	113G	N	CA	840	841	-148.65	-166.10		
8.50											

70	10068	115C	116A	C	N	855	857	-73.93	-68.20	19.51	1.37
-62.50	155.57	26.07									
70		116A	116A	N	CA	857	858	163.95	145.30		
-40.90											
71	10069	116A	117Q	C	N	860	862	-60.53	-73.00	16.33	0.96
-63.80	170.49	25.24									
71		117Q	117Q	N	CA	862	863	130.15	140.70		
-40.30											
72	10074	121V	122G	C	N	894	896	-168.64	-167.20	11.71	0.44
82.20	-151.44	14.94									
72		122G	122G	N	CA	896	897	-173.78	174.60		
8.50											
73	10111	158L	159R	C	N	1163	1165	168.93	-125.20	66.30	2.47
-63.00	-146.56	37.19									
73		159R	159R	N	CA	1165	1166	148.15	140.60		
-41.10											
74	10113	160V	161R	C	N	1181	1183	-178.18	-125.20	78.42	2.44
-63.00	166.68	29.74									
74		161R	161R	N	CA	1183	1184	-161.58	140.60		
-41.10											
75	10116	163P	164R	C	N	1206	1208	178.02	-125.20	80.48	2.46
-63.00	169.89	30.37									
75		164R	164R	N	CA	1208	1209	-162.37	140.60		
-41.10											
76	10118	165L	166W	C	N	1225	1227	-143.17	-124.90	29.22	0.97
-63.00	169.72	26.62									
76		166W	166W	N	CA	1227	1228	166.20	143.40		
-44.20											
77	10119	166W	167C	C	N	1239	1241	-127.21	-63.00	64.55	11.06
-117.90	171.38	6.60									
77		167C	167C	N	CA	1241	1242	-47.77	-41.10		
141.10											
78	10121	168P	169H	C	N	1252	1254	105.28	56.30	124.89	15.59
-63.20	-126.26	26.49									
78		169H	169H	N	CA	1254	1255	155.68	40.80		
-42.30											
79	10122	169H	170P	C	N	1262	1264	-71.42	-58.70	25.53	1.50
-64.50	155.72	11.99									
79		170P	170P	N	CA	1264	1265	-8.36	-30.50		
147.20											
80	10123	170P	171R	C	N	1269	1271	-63.83	-72.10	47.02	3.79
-63.00	130.72	17.71									
80		171R	171R	N	CA	1271	1272	-171.82	141.90		
-41.10											
81	10130	177G	178H	C	N	1323	1325	55.31	56.30	10.60	1.02
-63.20	138.95	23.86									
81		178H	178H	N	CA	1325	1326	30.25	40.80		
-42.30											

82	10133	180C	181E	C	N	1345	1347	-135.82	-117.80	18.23	0.74
-63.60	-171.24	22.12									
82		181E	181E	N	CA	1347	1348	134.09	136.80		
-40.30											
83	10134	181E	182Q	C	N	1354	1356	-122.22	-121.10	34.72	1.67
-63.80	156.61	20.51									
83		182Q	182Q	N	CA	1356	1357	105.00	139.70		
-40.30											
84	10135	182Q	183W	C	N	1363	1365	-151.73	-124.90	42.25	1.39
-63.00	165.56	26.65									
84		183W	183W	N	CA	1365	1366	176.03	143.40		
-44.20											
85	10139	186E	187D	C	N	1399	1401	-91.13	-70.90	33.13	1.19
-63.30	146.14	19.81									
85		187D	187D	N	CA	1401	1402	176.54	150.30		
-40.00											
86	10140	187D	188D	C	N	1407	1409	-114.54	-96.50	32.70	1.37
-63.30	-174.26	26.23									
86		188D	188D	N	CA	1409	1410	141.47	114.20		
-40.00											
87	10141	188D	189A	C	N	1415	1417	-87.43	-68.20	42.42	4.02
-62.50	150.46	23.56									
87		189A	189A	N	CA	1417	1418	107.49	145.30		
-40.90											
88	10142	189A	190K	C	N	1420	1422	45.94	56.60	14.40	0.97
-62.90	140.64	24.27									
88		190K	190K	N	CA	1422	1423	48.27	38.60		
-40.80											
89	10143	190K	191R	C	N	1429	1431	-114.84	-125.20	44.56	1.90
-63.00	147.75	17.16									
89		191R	191R	N	CA	1431	1432	97.26	140.60		
-41.10											
90	10145	192P	193R	C	N	1447	1449	71.62	57.30	33.54	1.63
-63.00	143.18	25.80									
90		193R	193R	N	CA	1449	1450	7.67	38.00		
-41.10											
91	10146	193R	194K	C	N	1458	1460	-172.05	-118.00	54.06	2.03
-62.90	-150.09	33.75									
91		194K	194K	N	CA	1460	1461	139.90	139.10		
-40.80											
92	10148	195T	196A	C	N	1474	1476	-58.35	-68.20	28.42	2.61
-62.50	147.20	23.92									
92		196A	196A	N	CA	1476	1477	171.97	145.30		
-40.90											
93	10150	197P	198R	C	N	1486	1488	-41.64	-72.10	30.46	2.33
-63.00	177.88	22.66									
93		198R	198R	N	CA	1488	1489	142.31	141.90		
-41.10											

94	10152	199D	200T	C	N	1505	1507	-58.23	-78.10	21.51	1.06
-63.20	176.42	22.30									
94		200T	200T	N	CA	1507	1508	141.55	149.80		
-42.10											
95	10153	200T	201G	C	N	1512	1514	-93.80	-80.20	20.97	0.60
82.20	-109.36	19.20									
95		201G	201G	N	CA	1514	1515	-169.94	174.10		
8.50											
96	10154	201G	202A	C	N	1516	1518	-147.27	-134.00	24.74	0.95
-62.50	173.37	32.94									
96		202A	202A	N	CA	1518	1519	167.88	147.00		
-40.90											
97	10155	202A	203F	C	N	1521	1523	-66.64	-71.40	5.59	0.47
-63.20	172.11	24.13									
97		203F	203F	N	CA	1523	1524	143.63	140.70		
-44.30											
98	10156	203F	204D	C	N	1532	1534	-70.69	-70.90	4.84	0.23
-63.30	174.69	22.02									
98		204D	204D	N	CA	1534	1535	145.46	150.30		
-40.00											
99	10157	204D	205A	C	N	1540	1542	-115.11	-134.00	18.92	0.67
-62.50	178.98	32.13									
99		205A	205A	N	CA	1542	1543	148.03	147.00		
-40.90											
100	10159	206V	207G	C	N	1552	1554	89.36	78.70	15.08	0.34
82.20	174.89	8.85									
100		207G	207G	N	CA	1554	1555	-176.76	-166.10		
8.50											
101	10160	207G	208E	C	N	1556	1558	-75.54	-69.30	12.41	0.73
-63.60	166.90	22.91									
101		208E	208E	N	CA	1558	1559	153.22	142.50		
-40.30											
102	10162	209V	210E	C	N	1572	1574	-139.89	-117.80	32.09	1.05
-63.60	176.91	27.86									
102		210E	210E	N	CA	1574	1575	160.08	136.80		
-40.30											
103	10163	210E	211A	C	N	1581	1583	-65.64	-68.20	9.81	0.70
-62.50	176.76	28.81									
103		211A	211A	N	CA	1583	1584	135.83	145.30		
-40.90											
104	10164	211A	212W	C	N	1586	1588	-152.87	-124.90	39.66	1.27
-63.00	169.99	27.29									
104		212W	212W	N	CA	1588	1589	171.51	143.40		
-44.20											
105	10165	212W	213H	C	N	1600	1602	-64.98	-67.60	4.44	0.27
-63.20	178.72	22.23									
105		213H	213H	N	CA	1602	1603	136.41	140.00		
-42.30											

106	10166	213H	214R	C	N	1610	1612	-118.91	-125.20	18.36	0.99
-63.00	170.48	26.89									
106		214R	214R	N	CA	1612	1613	157.85	140.60		
-41.10											
107	10167	214R	215N	C	N	1621	1623	-64.57	-71.20	15.36	0.83
-63.20	170.05	21.19									
107		215N	215N	N	CA	1623	1624	128.94	142.80		
-41.10											
108	10170	217I	218A	C	N	1643	1645	-113.71	-134.00	22.34	1.10
-62.50	170.62	30.69									
108		218A	218A	N	CA	1645	1646	156.35	147.00		
-40.90											
109	10172	219Y	220T	C	N	1660	1662	-110.22	-124.80	27.70	0.86
-63.20	168.73	18.92									
109		220T	220T	N	CA	1662	1663	119.94	143.50		
-42.10											
110	10173	220T	221S	C	N	1667	1669	-154.99	-136.60	21.27	0.65
-64.10	-173.29	20.07									
110		221S	221S	N	CA	1669	1670	161.90	151.20		
-35.00											
111	10175	222P	223W	C	N	1680	1682	-64.95	-71.30	6.92	0.56
-63.00	174.07	21.88									
111		223W	223W	N	CA	1682	1683	141.75	139.00		
-44.20											
112	10176	223W	224S	C	N	1694	1696	-135.64	-136.60	30.12	1.55
-64.10	160.52	16.76									
112		224S	224S	N	CA	1696	1697	-178.70	151.20		
-35.00											
113	10179	226C	227S	C	N	1713	1715	-137.15	-136.60	9.21	0.46
-64.10	-179.92	18.25									
113		227S	227S	N	CA	1715	1716	160.39	151.20		
-35.00											
114	10180	227S	228T	C	N	1719	1721	-90.17	-78.10	20.06	0.68
-63.20	154.45	21.61									
114		228T	228T	N	CA	1721	1722	165.82	149.80		
-42.10											
115	10183	230C	231G	C	N	1738	1740	-119.20	-80.20	49.78	3.61
82.20	-151.94	16.15									
115		231G	231G	N	CA	1740	1741	143.16	174.10		
8.50											
116	10184	231G	232L	C	N	1742	1744	-72.65	-70.70	7.45	0.50
-63.50	170.25	24.17									
116		232L	232L	N	CA	1744	1745	148.79	141.60		
-41.20											
117	10185	232L	233G	C	N	1750	1752	-164.70	-167.20	36.62	1.40
82.20	171.97	13.00									
117		233G	233G	N	CA	1752	1753	138.06	174.60		
8.50											

118	10187	234V	235S	C	N	1761	1763	-127.32	-136.60	11.72	0.36
-64.10	-170.13	11.70									
118		235S	235S	N	CA	1763	1764	144.03	151.20		
-35.00											
119	10188	235S	236T	C	N	1767	1769	-123.20	-124.80	5.00	0.17
-63.20	-171.08	28.21									
119		236T	236T	N	CA	1769	1770	138.76	143.50		
-42.10											
120	10189	236T	237R	C	N	1774	1776	-111.26	-125.20	30.34	1.11
-63.00	162.10	19.15									
120		237R	237R	N	CA	1776	1777	113.65	140.60		
-41.10											
121	10191	238I	239S	C	N	1793	1795	-137.80	-136.60	1.51	0.05
-64.10	-172.06	18.86									
121		239S	239S	N	CA	1795	1796	152.11	151.20		
-35.00											
122	10192	239S	240N	C	N	1799	1801	-127.28	-119.90	17.87	0.63
-63.20	177.59	25.84									
122		240N	240N	N	CA	1801	1802	153.28	137.00		
-41.10											
123	10194	241V	242N	C	N	1814	1816	-171.53	-119.90	82.84	2.51
-63.20	159.54	25.63									
123		242N	242N	N	CA	1816	1817	-158.22	137.00		
-41.10											
124	10195	242N	243A	C	N	1822	1824	-63.04	-68.20	9.23	0.89
-62.50	166.14	27.25									
124		243A	243A	N	CA	1824	1825	152.96	145.30		
-40.90											
125	10196	243A	244Q	C	N	1827	1829	-60.95	-73.00	17.77	1.03
-63.80	167.96	24.85									
125		244Q	244Q	N	CA	1829	1830	127.64	140.70		
-40.30											
126	10198	245C	246W	C	N	1842	1844	-94.99	-71.30	40.67	3.50
-63.00	153.51	17.57									
126		246W	246W	N	CA	1844	1845	105.95	139.00		
-44.20											
127	10200	247P	248E	C	N	1863	1865	-77.44	-69.30	8.18	0.59
-63.60	176.93	24.36									
127		248E	248E	N	CA	1865	1866	143.31	142.50		
-40.30											
128	10201	248E	249Q	C	N	1872	1874	-124.21	-121.10	15.93	0.70
-63.80	175.13	28.95									
128		249Q	249Q	N	CA	1874	1875	155.32	139.70		
-40.30											
129	10202	249Q	250E	C	N	1881	1883	-67.65	-69.30	2.50	0.14
-63.60	179.12	24.10									
129		250E	250E	N	CA	1883	1884	140.62	142.50		
-40.30											

130	10203	250E	251S	C	N	1890	1892	-115.61	-136.60	45.66	1.78
-64.10	154.49		9.52								
130		251S	251S	N	CA	1892	1893	110.65	151.20		
-35.00											
131	10204	251S	252R	C	N	1896	1898	-132.51	-63.00	102.50	11.97
-63.00	102.50		11.97								
131		252R	252R	N	CA	1898	1899	34.23	-41.10		
-41.10											
132	10205	252R	253L	C	N	1907	1909	-142.35	-108.50	40.63	1.79
-63.50	-178.18		30.12								
132		253L	253L	N	CA	1909	1910	154.97	132.50		
-41.20											
133	10207	254C	255N	C	N	1921	1923	-151.89	-119.90	36.83	1.11
-63.20	-173.86		28.24								
133		255N	255N	N	CA	1923	1924	155.25	137.00		
-41.10											
134	10208	255N	256L	C	N	1929	1931	-124.72	-108.50	28.32	1.32
-63.50	174.18		27.97								
134		256L	256L	N	CA	1931	1932	155.73	132.50		
-41.20											
135	10209	256L	257R	C	N	1937	1939	-67.77	-72.10	9.13	0.61
-63.00	175.03		23.33								
135		257R	257R	N	CA	1939	1940	133.86	141.90		
-41.10											
136	10212	259C	260D	C	N	1961	1963	-66.17	-70.90	15.34	0.55
-63.30	175.72		21.52								
136		260D	260D	N	CA	1963	1964	135.70	150.30		
-40.00											
137	10214	261V	262D	C	N	1976	1978	-67.46	-70.90	3.64	0.23
-63.30	170.94		21.35								
137		262D	262D	N	CA	1978	1979	149.12	150.30		
-40.00											
138	10216	263I	264H	C	N	1992	1994	-174.23	-125.60	75.49	1.91
-63.20	164.34		27.36								
138		264H	264H	N	CA	1994	1995	-163.46	138.80		
-42.30											
139	10217	264H	265T	C	N	2002	2004	-63.95	-78.10	34.13	1.12
-63.20	160.84		20.58								
139		265T	265T	N	CA	2004	2005	118.74	149.80		
-42.10											
140	10218	265T	266L	C	N	2009	2011	-98.30	-108.50	45.37	2.33
-63.50	134.09		16.96								
140		266L	266L	N	CA	2011	2012	88.29	132.50		
-41.20											
141	10225	272K	273C	C	N	2061	2063	-61.86	-63.00	9.06	1.03
-117.90	177.87		7.68								
141		273C	273C	N	CA	2063	2064	-50.09	-41.10		
141.10											

142	10229	276V	277Y	C	N	2087	2089	-58.58	-98.40	42.30	2.03
-63.50	173.99	27.35									
142		277Y	277Y	N	CA	2089	2090	142.68	128.40		
-43.40											
143	10230	277Y	278Q	C	N	2099	2101	-55.82	-73.00	36.72	2.13
-63.80	148.76	22.29									
143		278Q	278Q	N	CA	2101	2102	108.24	140.70		
-40.30											
144	10232	279P	280E	C	N	2115	2117	-99.88	-117.80	23.36	0.72
-63.60	166.14	20.38									
144		280E	280E	N	CA	2117	2118	121.82	136.80		
-40.30											
145	10233	280E	281A	C	N	2124	2126	-126.00	-134.00	10.43	0.28
-62.50	-170.26	34.49									
145		281A	281A	N	CA	2126	2127	140.31	147.00		
-40.90											
146	10234	281A	282S	C	N	2129	2131	63.36	-72.40	139.64	10.76
-64.10	-170.72	14.73									
146		282S	282S	N	CA	2131	2132	-174.93	152.40		
-35.00											
147	10235	282S	283M	C	N	2135	2137	-69.21	-73.00	26.19	1.84
-63.40	150.70	22.95									
147		283M	283M	N	CA	2137	2138	168.91	143.00		
-40.50											
148	10236	283M	284N	C	N	2143	2145	-58.86	-71.20	15.18	0.86
-63.20	175.12	22.13									
148		284N	284N	N	CA	2145	2146	133.97	142.80		
-41.10											
149	10237	284N	285F	C	N	2151	2153	-127.63	-124.20	24.01	1.04
-63.20	161.99	26.69									
149		285F	285F	N	CA	2153	2154	167.07	143.30		
-44.30											
150	10239	286T	287L	C	N	2169	2171	-107.95	-108.50	12.58	0.69
-63.50	179.32	27.63									
150		287L	287L	N	CA	2171	2172	145.07	132.50		
-41.20											
151	10240	287L	288A	C	N	2177	2179	-134.93	-134.00	17.38	0.97
-62.50	170.86	31.88									
151		288A	288A	N	CA	2179	2180	164.35	147.00		
-40.90											
152	10244	291I	292S	C	N	2200	2202	80.82	-136.60	145.97	5.03
-64.10	-156.72	16.58									
152		292S	292S	N	CA	2202	2203	-177.55	151.20		
-35.00											
153	10245	292S	293T	C	N	2206	2208	-75.48	-78.10	5.02	0.30
-63.20	164.27	21.88									
153		293T	293T	N	CA	2208	2209	154.09	149.80		
-42.10											

154	10246	293T	294R	C	N	2213	2215	-88.63	-72.10	21.16	1.38
-63.00	165.77	24.16									
154		294R	294R	N	CA	2215	2216	155.12	141.90		
-41.10											
155	10247	294R	295S	C	N	2224	2226	-130.53	-136.60	9.70	0.55
-64.10	179.01	17.67									
155		295S	295S	N	CA	2226	2227	158.77	151.20		
-35.00											
156	10248	295S	296Y	C	N	2230	2232	-124.37	-124.30	4.40	0.23
-63.50	-173.02	32.74									
156		296Y	296Y	N	CA	2232	2233	139.80	135.40		
-43.40											
157	10249	296Y	297Q	C	N	2242	2244	-109.26	-121.10	18.53	0.63
-63.80	171.86	23.14									
157		297Q	297Q	N	CA	2244	2245	125.44	139.70		
-40.30											
158	10251	298P	299K	C	N	2258	2260	51.59	56.60	5.07	0.55
-62.90	139.78	24.30									
158		299K	299K	N	CA	2260	2261	39.38	38.60		
-40.80											
159	10252	299K	300Y	C	N	2267	2269	-133.42	-124.30	15.11	0.62
-63.50	-176.97	32.52									
159		300Y	300Y	N	CA	2269	2270	147.45	135.40		
-43.40											
160	10257	304C	305M	C	N	2302	2304	-71.60	-73.00	17.23	1.19
-63.40	159.53	24.46									
160		305M	305M	N	CA	2304	2305	160.17	143.00		
-40.50											
161	10258	305M	306D	C	N	2310	2312	-60.57	-70.90	34.08	1.23
-63.30	157.85	19.65									
161		306D	306D	N	CA	2312	2313	117.83	150.30		
-40.00											
162	10259	306D	307N	C	N	2318	2320	-140.92	-119.90	24.81	0.74
-63.20	-174.22	27.62									
162		307N	307N	N	CA	2320	2321	150.16	137.00		
-41.10											
163	10265	312P	313Y	C	N	2364	2366	-124.78	-124.30	31.40	1.64
-63.50	161.85	28.74									
163		313Y	313Y	N	CA	2366	2367	166.79	135.40		
-43.40											
164	10268	315S	316K	C	N	2391	2393	-153.36	-118.00	42.67	1.43
-62.90	-179.50	28.83									
164		316K	316K	N	CA	2393	2394	163.00	139.10		
-40.80											
165	10269	316K	317T	C	N	2400	2402	-80.18	-78.10	2.10	0.12
-63.20	168.64	22.75									
165		317T	317T	N	CA	2402	2403	150.12	149.80		
-42.10											

166	10271	318I	319D	C	N	2415	2417	-92.45	-96.50	57.01	2.40
-63.30	101.61	11.11									
166		319D	319D	N	CA	2417	2418	57.34	114.20		
-40.00											
167	10272	319D	320V	C	N	2423	2425	169.48	-125.40	79.15	2.08
-73.50	126.90	8.58									
167		320V	320V	N	CA	2425	2426	-171.71	143.30		
139.20											
168	10278	325P	326D	C	N	2469	2471	-114.38	-70.90	44.58	3.00
-63.30	167.85	24.02									
168		326D	326D	N	CA	2471	2472	160.11	150.30		
-40.00											
169	10279	326D	327G	C	N	2477	2479	-74.52	-80.20	7.85	0.26
82.20	-135.90	6.93									
169		327G	327G	N	CA	2479	2480	168.69	174.10		
8.50											
170	10280	327G	328L	C	N	2481	2483	-85.43	-108.50	29.23	1.30
-63.50	157.29	20.68									
170		328L	328L	N	CA	2483	2484	114.56	132.50		
-41.20											
171	10281	328L	329G	C	N	2489	2491	-73.61	-80.20	44.85	1.44
82.20	-162.58	7.17									
171		329G	329G	N	CA	2491	2492	129.74	174.10		
8.50											
172	10282	329G	330F	C	N	2493	2495	-146.36	-124.20	29.41	0.77
-63.20	174.18	29.48									
172		330F	330F	N	CA	2495	2496	162.65	143.30		
-44.30											
173	10283	330F	331S	C	N	2504	2506	-108.72	-136.60	40.30	1.32
-64.10	163.31	10.11									
173		331S	331S	N	CA	2506	2507	122.10	151.20		
-35.00											
174	10284	331S	332R	C	N	2510	2512	-106.28	-125.20	38.16	1.35
-63.00	154.73	18.40									
174		332R	332R	N	CA	2512	2513	107.46	140.60		
-41.10											
175	10285	332R	333Q	C	N	2521	2523	-135.14	-121.10	17.25	0.53
-63.80	-175.65	30.86									
175		333Q	333Q	N	CA	2523	2524	149.72	139.70		
-40.30											
176	10287	334V	335L	C	N	2537	2539	-61.63	-70.70	13.67	0.86
-63.50	172.59	24.07									
176		335L	335L	N	CA	2539	2540	131.37	141.60		
-41.20											
177	10288	335L	336W	C	N	2545	2547	-117.42	-124.90	12.90	0.44
-63.00	-174.74	20.68									
177		336W	336W	N	CA	2547	2548	132.89	143.40		
-44.20											

178	10290	337I	338N	C	N	2567	2569	-79.01	-71.20	11.64	0.62
-63.20	168.21	21.91									
178		338N	338N	N	CA	2569	2570	151.43	142.80		
-41.10											
179	10291	338N	339A	C	N	2575	2577	-94.00	-68.20	29.41	2.86
-62.50	174.94	27.30									
179		339A	339A	N	CA	2577	2578	131.18	145.30		
-40.90											
180	10293	340C	341F	C	N	2586	2588	-105.17	-124.20	21.83	0.58
-63.20	-178.18	22.60									
180		341F	341F	N	CA	2588	2589	132.61	143.30		
-44.30											
181	10295	342C	343N	C	N	2603	2605	-113.67	-119.90	11.35	0.36
-63.20	176.00	19.67									
181		343N	343N	N	CA	2605	2606	127.51	137.00		
-41.10											
182	10296	343N	344L	C	N	2611	2613	-108.18	-108.50	20.17	1.09
-63.50	159.91	20.12									
182		344L	344L	N	CA	2613	2614	112.34	132.50		
-41.20											
183	10297	344L	345S	C	N	2619	2621	-143.01	-136.60	11.66	0.66
-64.10	-166.70	12.10									
183		345S	345S	N	CA	2621	2622	141.46	151.20		
-35.00											
184	10299	346C	347R	C	N	2631	2633	-102.33	-125.20	41.24	1.40
-63.00	152.53	18.29									
184		347R	347R	N	CA	2633	2634	106.27	140.60		
-41.10											
185	10300	347R	348N	C	N	2642	2644	-130.19	-119.90	22.67	1.21
-63.20	171.52	18.67									
185		348N	348N	N	CA	2644	2645	116.80	137.00		
-41.10											
186	10301	348N	349P	C	N	2650	2652	-55.48	-58.70	14.13	0.93
-64.50	168.78	13.08									
186		349P	349P	N	CA	2652	2653	-44.26	-30.50		
147.20											
187	10302	349P	350N	C	N	2657	2659	-173.05	-119.90	56.93	1.86
-63.20	-164.67	30.44									
187		350N	350N	N	CA	2659	2660	157.39	137.00		
-41.10											
188	10303	350N	351D	C	N	2665	2667	-76.96	-70.90	10.47	0.37
-63.30	161.75	20.81									
188		351D	351D	N	CA	2667	2668	158.83	150.30		
-40.00											
189	10305	352I	353F	C	N	2681	2683	-129.82	-124.20	12.79	0.70
-63.20	-171.70	22.24									
189		353F	353F	N	CA	2683	2684	131.82	143.30		
-44.30											

190	10306	353F	354A	C	N	2692	2694	-147.48	-134.00	16.11	0.86
-62.50	-161.77	29.74									
190		354A	354A	N	CA	2694	2695	138.19	147.00		
-40.90											
191	10307	354A	355D	C	N	2697	2699	-131.99	-96.50	52.45	2.15
-63.30	134.45	14.29									
191		355D	355D	N	CA	2699	2700	75.59	114.20		
-40.00											
192	10308	355D	356L	C	N	2705	2707	-116.32	-108.50	13.11	0.61
-63.50	-176.46	28.74									
192		356L	356L	N	CA	2707	2708	143.03	132.50		
-41.20											
193	10309	356L	357E	C	N	2713	2715	-113.65	-117.80	14.86	0.66
-63.60	170.35	20.40									
193		357E	357E	N	CA	2715	2716	122.53	136.80		
-40.30											
194	10310	357E	358S	C	N	2722	2724	-138.69	-136.60	10.20	0.55
-64.10	-168.64	11.90									
194		358S	358S	N	CA	2724	2725	141.22	151.20		
-35.00											
195	10311	358S	359Y	C	N	2728	2730	-122.61	-124.30	16.69	0.81
-63.50	172.64	24.71									
195		359Y	359Y	N	CA	2730	2731	118.80	135.40		
-43.40											
196	10313	360P	361D	C	N	2747	2749	-131.29	-96.50	44.99	1.84
-63.30	142.89	15.16									
196		361D	361D	N	CA	2749	2750	85.68	114.20		
-40.00											
197	10314	361D	362F	C	N	2755	2757	-136.66	-124.20	18.55	0.51
-63.20	174.84	29.04									
197		362F	362F	N	CA	2757	2758	157.04	143.30		
-44.30											
198	10315	362F	363S	C	N	2766	2768	-113.34	-136.60	25.52	0.79
-64.10	-177.53	11.30									
198		363S	363S	N	CA	2768	2769	140.69	151.20		
-35.00											
199	10316	363S	364E	C	N	2772	2774	-76.33	-69.30	12.14	0.69
-63.60	167.78	23.08									
199		364E	364E	N	CA	2774	2775	152.40	142.50		
-40.30											
200	10318	365I	366A	C	N	2789	2791	-143.47	-134.00	23.35	1.03
-62.50	171.13	32.37									
200		366A	366A	N	CA	2791	2792	168.34	147.00		
-40.90											

report_____> Distribution of short non-bonded contacts:

```
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:      0      0      0      0      0     16     41    139    145    183    217    249    235
295    288
```

```
<< end of ENERGY.
```

```
>> Summary of successfully produced models:
```

Filename	molpdf	DOPE score	GA341 score	SOAP-Protein-OD score
----------	--------	------------	-------------	-----------------------

WISP1.B99990001.pdb	2115.55103	-19561.43750	0.97372	
0.00000				
WISP1.B99990002.pdb	2058.17310	-19009.38867	0.67844	
0.00000				
WISP1.B99990003.pdb	2089.63696	-17263.92188	0.32954	
0.00000				
WISP1.B99990004.pdb	1996.56909	-18903.21680	0.85786	
0.00000				
WISP1.B99990005.pdb	1910.79919	-19025.35547	0.90079	
0.00000				

```
[87]: #select model with the lowest DOPE score
#explanation for DOPE score: https://salilab.org/modeller/10.0/manual/node261.html; https://salilab.org/modeller/tutorial/basic.html
#model selected will be WISP1.B99990001.pdb
```

```
[ ]:
```

Plotting The Results (15 points) - 5 points for description of data analysis method - 5 points for the code working for data analysis method - 5 points for adequate commenting in the code for the data analysis method

0.0.3 Visualizing the structure

model - WISP1.B99990001.pdb

```
[88]: mdl_v = ngv.show_structure_file('WISP1.B99990001.pdb')
mdl_v.display()
```

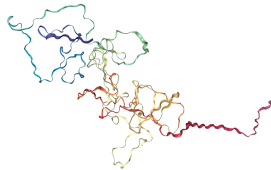
```
NGLWidget()
```



```
[91]: mdl_v.render_image();
```

```
[90]: mdl_v._display_image()
```

```
[90]:
```



```
[92]: #model evaluation?
```

Analyzing the Results (15 points) - 15 points for correctly analyzing the data

Code Formatting Requirements (15 points) - 5 points for comments identifying global variables and local variables with in depth explanations of each - 5 points for use of a built-in Bioconductor or Biopython function (or some other tool that was discussed in class like NumPy or SciPy), and description of what the function reads in and what it returns. - 5 points for hard-coding/redundant code being absent.

```
[ ]:
```

```
[ ]:
```