



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 06:53 PM UTC

PDB ID : 2LLY / pdb_00002lly
BMRB ID : 18093
Title : NMR structures of the transmembrane domains of the nAChR $\alpha 4$ subunit
Authors : Bondarenko, V.; Mowrey, D.; Tillman, T.; Cui, T.; Liu, L.T.; Xu, Y.; Tang, P.
Deposited on : 2011-11-18

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

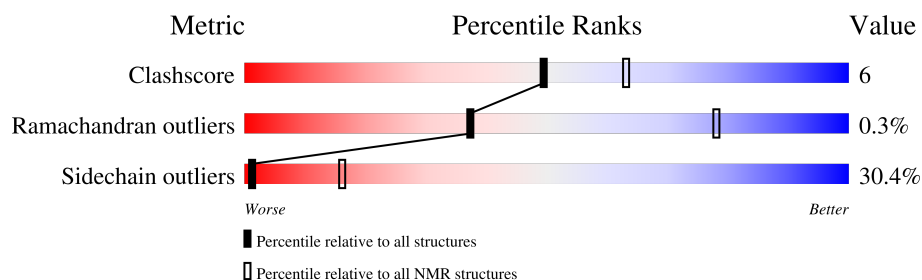
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	137	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:61, A:69-A:94, A:108-A:129 (102)	1.13	11

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 6, 8, 10, 16, 17, 18, 20
2	2, 3, 4, 7, 9, 13
3	5, 11, 15, 19
Single-model clusters	12; 14

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2132 atoms, of which 1095 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neuronal acetylcholine receptor subunit alpha-4.

Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2132	699	1095	151	180	7	

There are 15 discrepancies between the modelled and reference sequences:

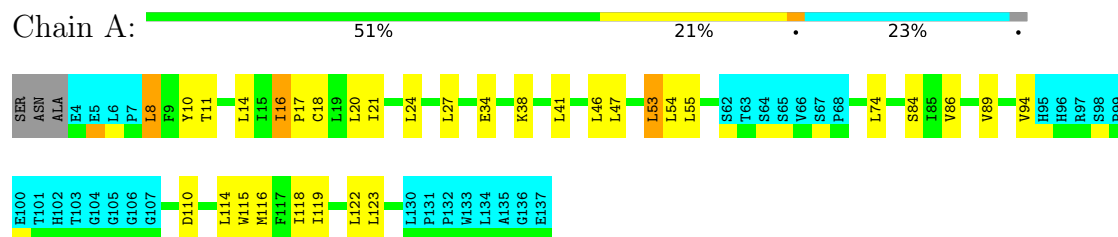
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P43681
A	2	ASN	-	expression tag	UNP P43681
A	3	ALA	-	expression tag	UNP P43681
A	4	GLU	ARG	engineered mutation	UNP P43681
A	5	GLU	ARG	engineered mutation	UNP P43681
A	65	SER	LEU	engineered mutation	UNP P43681
A	67	SER	ILE	engineered mutation	UNP P43681
A	69	SER	LEU	engineered mutation	UNP P43681
A	100	GLU	ARG	engineered mutation	UNP P43681
A	104	GLY	-	linker	UNP P43681
A	105	GLY	-	linker	UNP P43681
A	106	GLY	-	linker	UNP P43681
A	107	GLY	-	linker	UNP P43681
A	108	GLY	-	linker	UNP P43681
A	137	GLU	MET	engineered mutation	UNP P43681

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

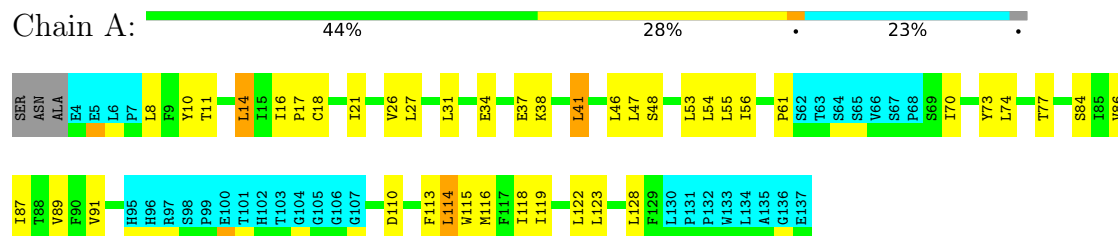


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

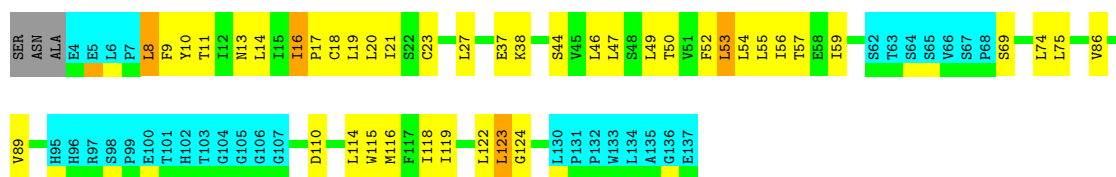
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



4.2.2 Score per residue for model 2

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

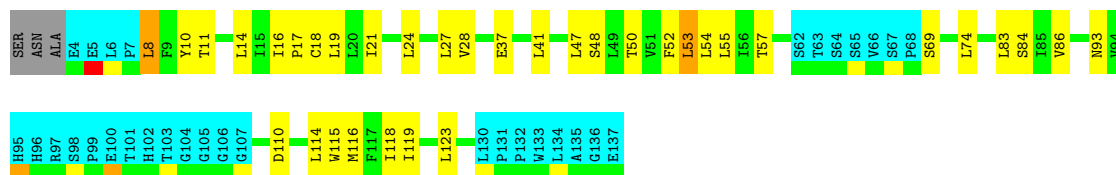




4.2.3 Score per residue for model 3

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

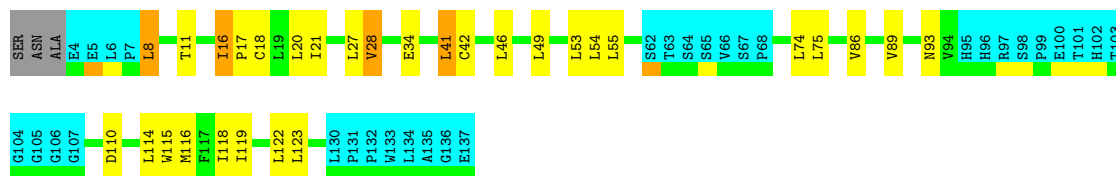
Chain A: 49% 24% 23%



4.2.4 Score per residue for model 4

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

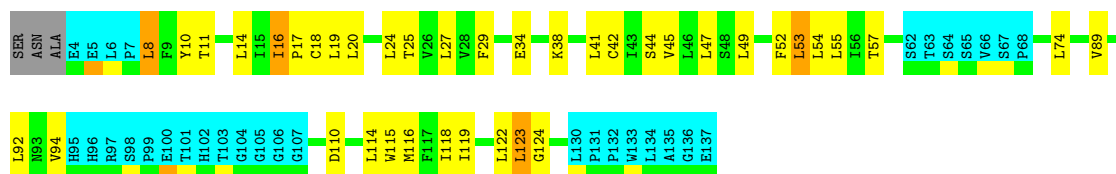
Chain A: 53% 19% 23%



4.2.5 Score per residue for model 5

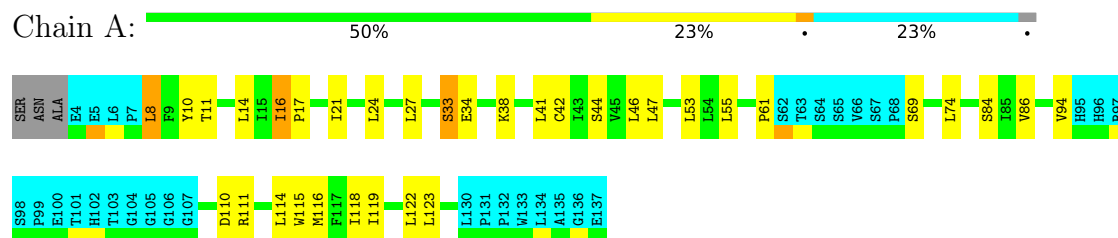
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

Chain A: 46% 26% 23%



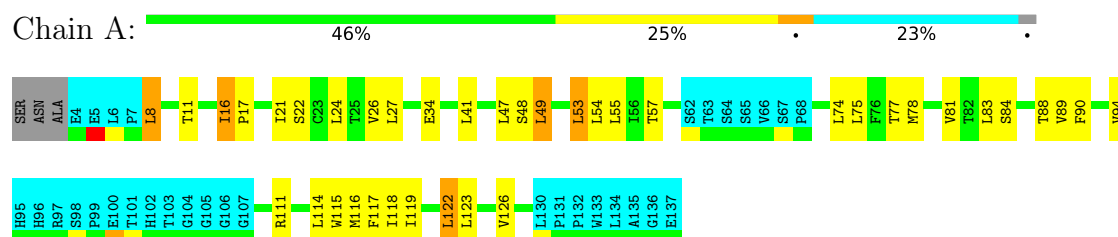
4.2.6 Score per residue for model 6

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



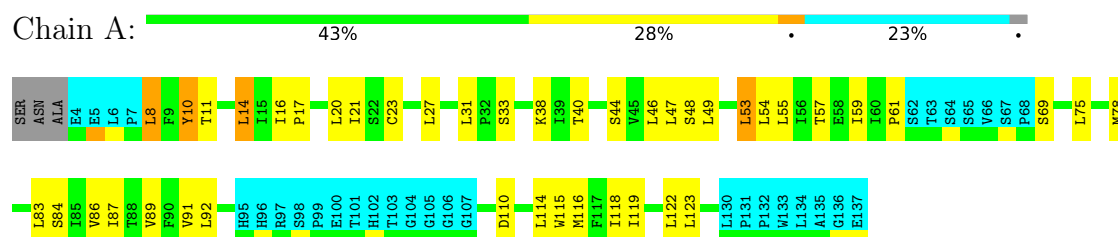
4.2.7 Score per residue for model 7

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



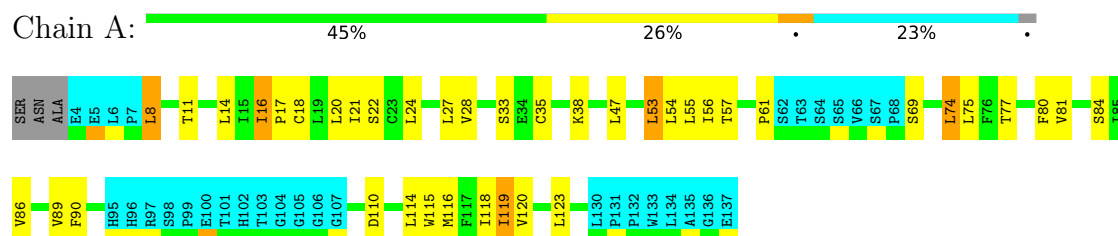
4.2.8 Score per residue for model 8

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



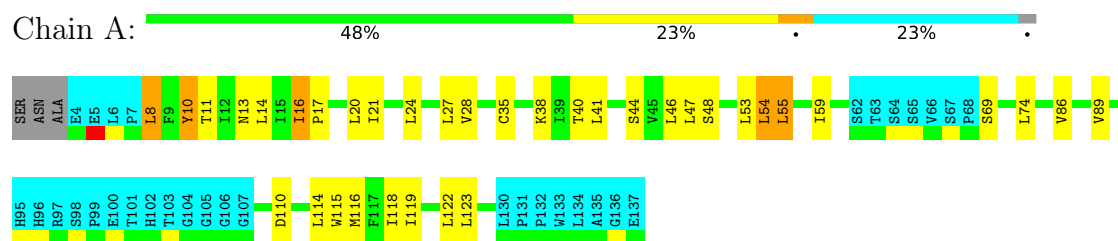
4.2.9 Score per residue for model 9

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



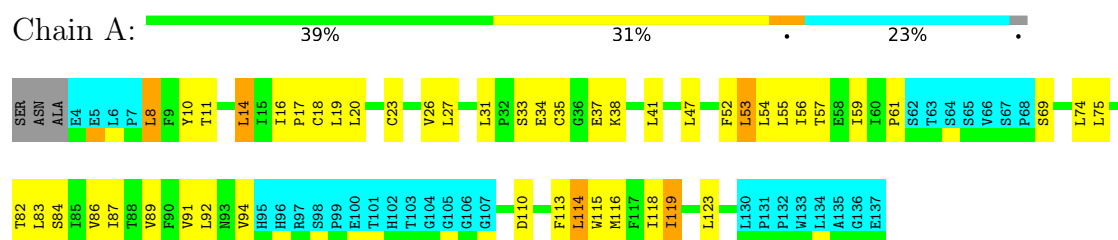
4.2.10 Score per residue for model 10

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



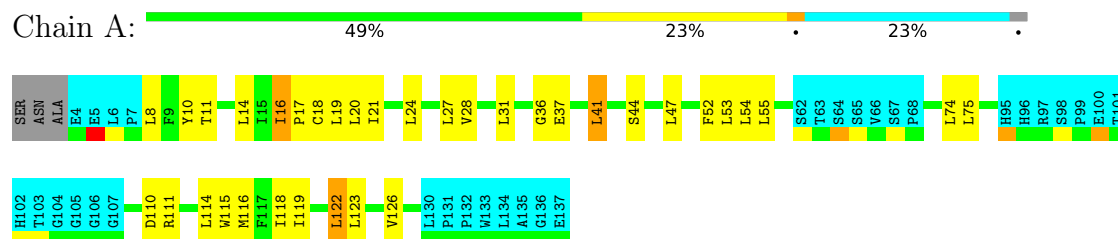
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



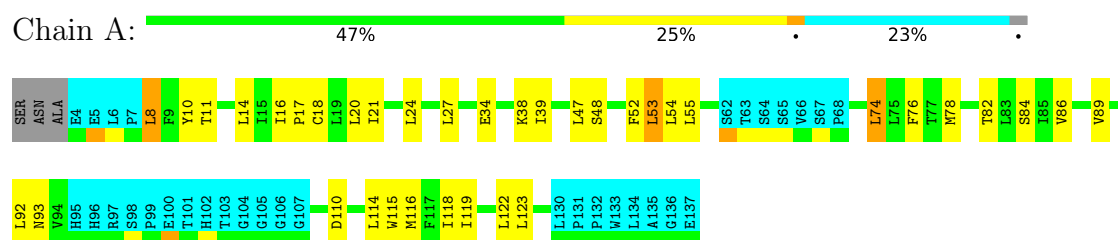
4.2.12 Score per residue for model 12

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



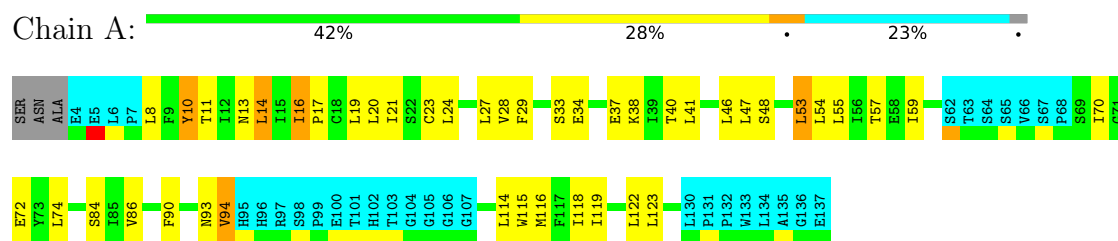
4.2.13 Score per residue for model 13

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



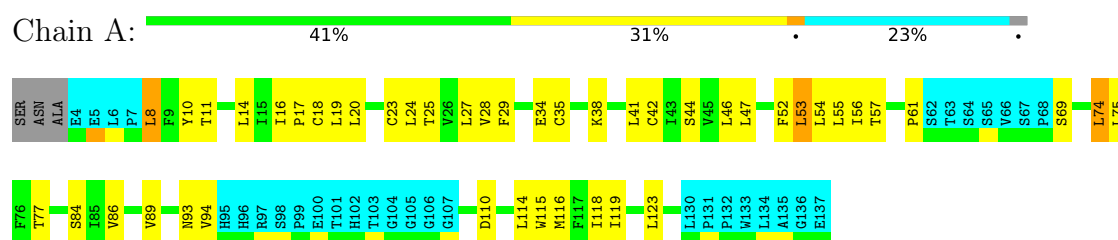
4.2.14 Score per residue for model 14

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



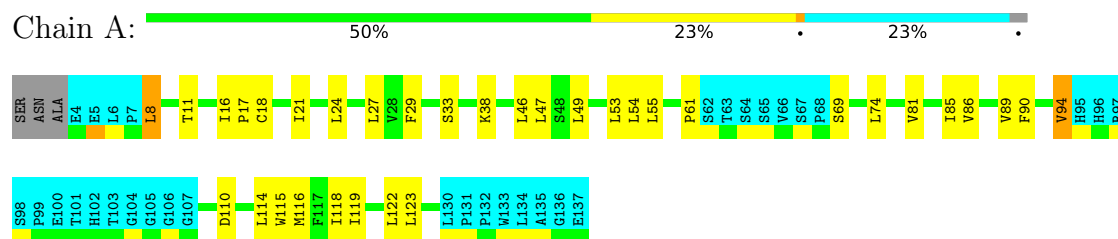
4.2.15 Score per residue for model 15

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



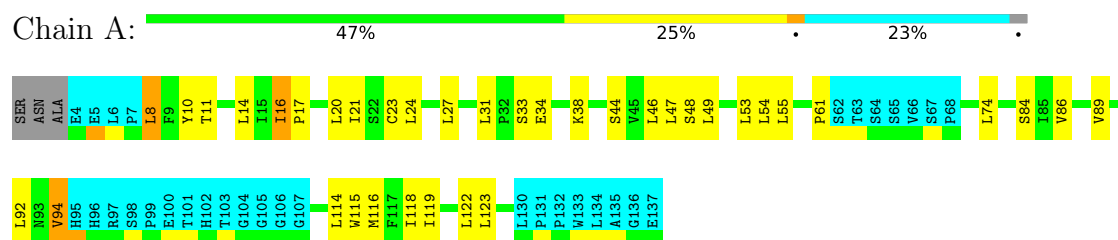
4.2.16 Score per residue for model 16

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



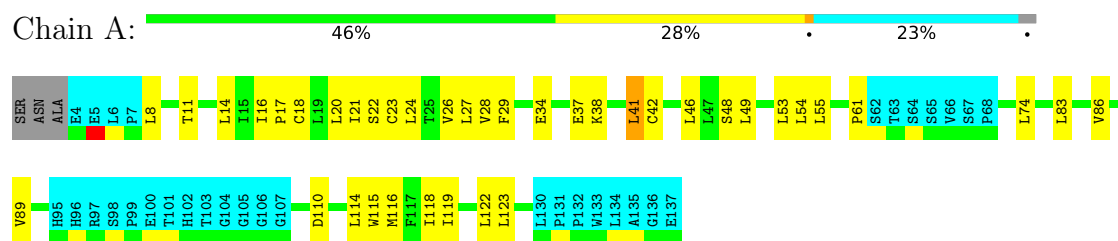
4.2.17 Score per residue for model 17

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



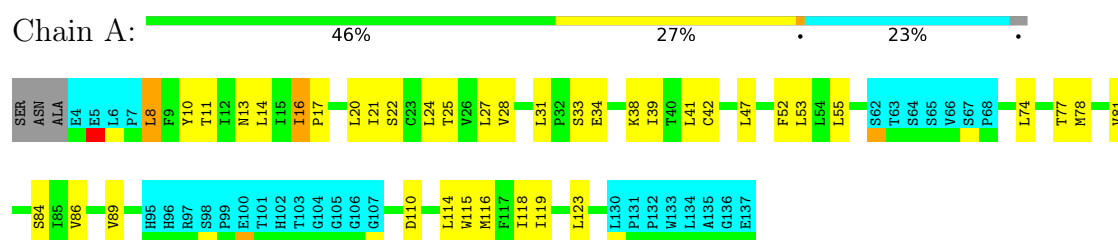
4.2.18 Score per residue for model 18

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



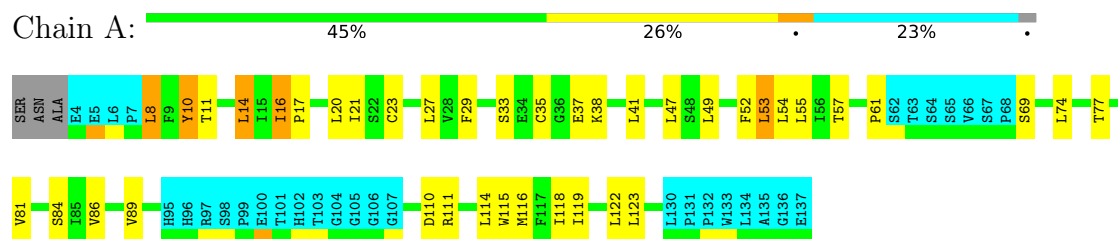
4.2.19 Score per residue for model 19

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



4.2.20 Score per residue for model 20

- Molecule 1: Neuronal acetylcholine receptor subunit alpha-4



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	3.0
CYANA	refinement	3.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1569
Number of shifts mapped to atoms	1554
Number of unparsed shifts	0
Number of shifts with mapping errors	15
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	804	884	884	10±3
All	All	16080	17680	17680	192

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:VAL:HG11	1:A:41:LEU:HD13	0.71	1.62	12	1
1:A:28:VAL:HG21	1:A:41:LEU:HD22	0.71	1.63	10	5
1:A:10:TYR:CZ	1:A:14:LEU:HD11	0.66	2.25	12	5
1:A:10:TYR:CE2	1:A:14:LEU:HD11	0.65	2.26	3	7
1:A:14:LEU:HD21	1:A:70:ILE:HD11	0.61	1.71	1	1
1:A:14:LEU:HD22	1:A:52:PHE:CE1	0.61	2.30	2	7
1:A:53:LEU:O	1:A:57:THR:HG23	0.60	1.97	2	10
1:A:14:LEU:HD11	1:A:52:PHE:CE1	0.58	2.32	11	1
1:A:10:TYR:OH	1:A:59:ILE:HD13	0.58	1.98	8	3
1:A:73:TYR:CE1	1:A:128:LEU:HD21	0.57	2.33	1	1
1:A:26:VAL:HG11	1:A:114:LEU:CB	0.57	2.30	1	2
1:A:56:ILE:HD13	1:A:59:ILE:HD11	0.56	1.77	2	2
1:A:28:VAL:CG2	1:A:41:LEU:HD22	0.56	2.31	14	3
1:A:10:TYR:CE1	1:A:14:LEU:HD23	0.56	2.36	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:VAL:HG21	1:A:41:LEU:HD13	0.55	1.77	4	1
1:A:80:PHE:CZ	1:A:120:VAL:HG11	0.55	2.36	9	1
1:A:77:THR:O	1:A:81:VAL:HG22	0.54	2.03	9	4
1:A:10:TYR:O	1:A:14:LEU:HD12	0.54	2.03	20	2
1:A:8:LEU:O	1:A:8:LEU:HD13	0.54	2.03	17	20
1:A:87:ILE:O	1:A:91:VAL:HG12	0.53	2.04	8	3
1:A:115:TRP:CE3	1:A:118:ILE:HD11	0.52	2.40	9	20
1:A:49:LEU:HD22	1:A:78:MET:HE2	0.51	1.82	7	1
1:A:53:LEU:HD13	1:A:74:LEU:HD22	0.51	1.82	9	1
1:A:28:VAL:HG11	1:A:41:LEU:CD1	0.51	2.36	12	1
1:A:10:TYR:CE1	1:A:14:LEU:HD11	0.50	2.41	12	1
1:A:14:LEU:HD22	1:A:52:PHE:CD1	0.50	2.41	19	1
1:A:55:LEU:O	1:A:59:ILE:HG23	0.49	2.08	10	1
1:A:10:TYR:OH	1:A:56:ILE:HD12	0.49	2.08	1	1
1:A:25:THR:CG2	1:A:45:VAL:HG11	0.49	2.38	5	1
1:A:16:ILE:N	1:A:17:PRO:HD2	0.48	2.23	6	20
1:A:26:VAL:HG11	1:A:114:LEU:HB2	0.48	1.84	11	2
1:A:81:VAL:O	1:A:85:ILE:HD12	0.47	2.09	16	1
1:A:28:VAL:HG21	1:A:41:LEU:HB2	0.47	1.86	14	1
1:A:14:LEU:HD11	1:A:52:PHE:CZ	0.47	2.45	11	1
1:A:92:LEU:O	1:A:92:LEU:HD23	0.46	2.10	17	4
1:A:52:PHE:CZ	1:A:74:LEU:HD11	0.46	2.45	15	1
1:A:24:LEU:O	1:A:28:VAL:HG23	0.46	2.11	9	1
1:A:22:SER:O	1:A:26:VAL:HG23	0.46	2.10	7	2
1:A:53:LEU:CD1	1:A:54:LEU:HD22	0.45	2.41	10	1
1:A:14:LEU:HD21	1:A:52:PHE:CE1	0.45	2.47	20	1
1:A:122:LEU:O	1:A:126:VAL:HG23	0.44	2.12	7	2
1:A:25:THR:HA	1:A:41:LEU:HD21	0.44	1.88	15	1
1:A:8:LEU:HD13	1:A:8:LEU:C	0.44	2.38	12	3
1:A:73:TYR:CD1	1:A:128:LEU:HD21	0.44	2.47	1	1
1:A:92:LEU:C	1:A:92:LEU:HD13	0.44	2.38	13	1
1:A:123:LEU:HD13	1:A:124:GLY:N	0.43	2.29	2	2
1:A:26:VAL:HG13	1:A:113:PHE:CE1	0.42	2.48	1	2
1:A:41:LEU:O	1:A:41:LEU:HD13	0.42	2.13	1	1
1:A:28:VAL:CB	1:A:41:LEU:HD22	0.42	2.45	19	2
1:A:53:LEU:HB2	1:A:74:LEU:HD22	0.42	1.92	13	1
1:A:25:THR:HA	1:A:41:LEU:HD11	0.42	1.92	5	1
1:A:14:LEU:HD23	1:A:70:ILE:HD12	0.42	1.92	14	1
1:A:56:ILE:HG23	1:A:61:PRO:HG3	0.42	1.91	11	3
1:A:16:ILE:HG22	1:A:17:PRO:N	0.41	2.30	17	15
1:A:53:LEU:O	1:A:53:LEU:HD12	0.41	2.14	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:TRP:O	1:A:119:ILE:HD12	0.41	2.15	9	2
1:A:26:VAL:HG22	1:A:117:PHE:CD2	0.41	2.51	7	1
1:A:26:VAL:HG11	1:A:114:LEU:HB3	0.41	1.93	1	1
1:A:16:ILE:CB	1:A:17:PRO:CD	0.40	3.00	11	6
1:A:53:LEU:HD11	1:A:54:LEU:HD22	0.40	1.93	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/137 (74%)	99±1 (97±1%)	3±2 (3±2%)	0±1 (0±1%)	37	78
All	All	2040/2740 (74%)	1972 (97%)	61 (3%)	7 (0%)	37	78

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	33	SER	3
1	A	94	VAL	3
1	A	36	GLY	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/125 (78%)	68±3 (70±3%)	30±3 (30±3%)	1	16
All	All	1940/2500 (78%)	1350 (70%)	590 (30%)	1	16

All 60 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	11	THR	20
1	A	27	LEU	20
1	A	55	LEU	20
1	A	114	LEU	20
1	A	116	MET	20
1	A	119	ILE	20
1	A	123	LEU	20
1	A	53	LEU	19
1	A	74	LEU	19
1	A	47	LEU	18
1	A	54	LEU	18
1	A	21	ILE	17
1	A	86	VAL	17
1	A	110	ASP	17
1	A	38	LYS	16
1	A	89	VAL	16
1	A	8	LEU	16
1	A	122	LEU	15
1	A	20	LEU	15
1	A	84	SER	13
1	A	24	LEU	13
1	A	18	CYS	12
1	A	34	GLU	12
1	A	16	ILE	12
1	A	46	LEU	11
1	A	14	LEU	10
1	A	69	SER	10
1	A	41	LEU	9
1	A	48	SER	9
1	A	49	LEU	9
1	A	37	GLU	8
1	A	23	CYS	8
1	A	44	SER	8
1	A	75	LEU	8
1	A	19	LEU	7
1	A	94	VAL	7
1	A	33	SER	7
1	A	31	LEU	6
1	A	42	CYS	6
1	A	29	PHE	6
1	A	10	TYR	6
1	A	83	LEU	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	93	ASN	5
1	A	35	CYS	5
1	A	13	ASN	4
1	A	111	ARG	4
1	A	90	PHE	4
1	A	40	THR	3
1	A	78	MET	3
1	A	77	THR	2
1	A	50	THR	2
1	A	28	VAL	2
1	A	22	SER	2
1	A	82	THR	2
1	A	39	ILE	2
1	A	9	PHE	1
1	A	88	THR	1
1	A	76	PHE	1
1	A	72	GLU	1
1	A	25	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1569
Number of shifts mapped to atoms	1554
Number of unparsed shifts	0
Number of shifts with mapping errors	15
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 15 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ASN	HA	4.732	0.007	1
1	A	2	ASN	HB2	2.824	0.015	2
1	A	2	ASN	HB3	2.792	0.000	2
1	A	2	ASN	C	175.227	0.000	1
1	A	2	ASN	CA	53.626	0.029	1
1	A	2	ASN	CB	38.934	0.113	1
1	A	3	ALA	H	8.378	0.003	1
1	A	3	ALA	HA	4.216	0.003	1
1	A	3	ALA	HB1	1.374	0.002	1
1	A	3	ALA	HB2	1.374	0.002	1
1	A	3	ALA	HB3	1.374	0.002	1
1	A	3	ALA	C	177.924	0.000	1
1	A	3	ALA	CA	53.514	0.025	1
1	A	3	ALA	CB	19.029	0.061	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	ALA	N	124.347	0.020	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	133	-0.84 ± 0.09	Should be checked
$^{13}\text{C}_\beta$	114	0.17 ± 0.03	None needed (< 0.5 ppm)
$^{13}\text{C}'$	123	-0.11 ± 0.05	None needed (< 0.5 ppm)
^{15}N	124	0.95 ± 0.18	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1267 atoms were assigned a chemical shift out of a possible 1505. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	487/509 (96%)	196/206 (95%)	195/204 (96%)	96/99 (97%)
Sidechain	724/867 (84%)	493/589 (84%)	230/272 (85%)	1/6 (17%)
Aromatic	56/129 (43%)	28/63 (44%)	27/65 (42%)	1/1 (100%)
Overall	1267/1505 (84%)	717/858 (84%)	452/541 (84%)	98/106 (92%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1554 atoms were assigned a chemical shift out of a possible 1882. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	630/664 (95%)	255/270 (94%)	252/268 (94%)	123/126 (98%)
Sidechain	856/1056 (81%)	578/713 (81%)	277/334 (83%)	1/9 (11%)
Aromatic	68/162 (42%)	34/81 (42%)	32/76 (42%)	2/5 (40%)
Overall	1554/1882 (83%)	867/1064 (81%)	561/678 (83%)	126/140 (90%)

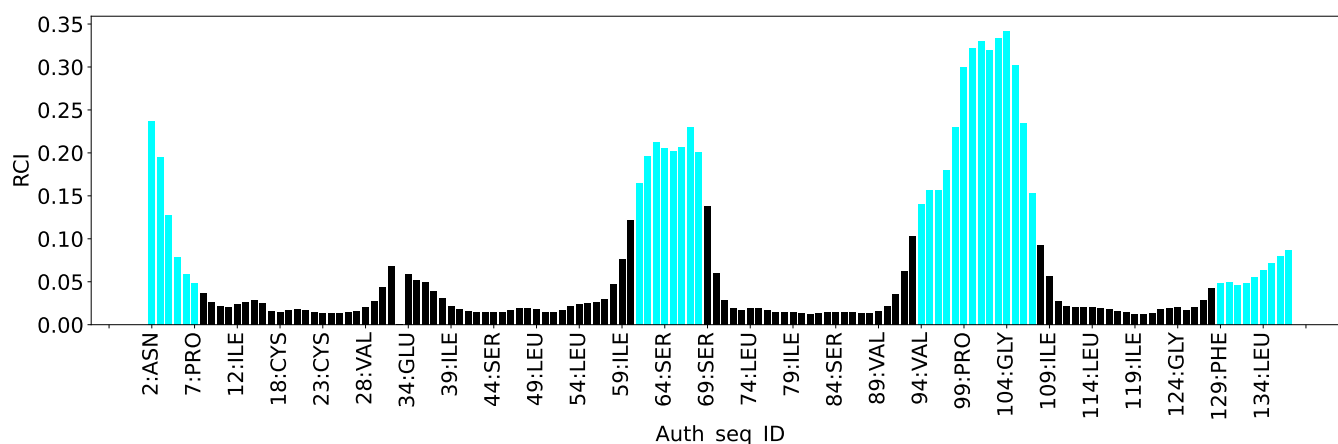
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1334
Intra-residue ($ i-j =0$)	351
Sequential ($ i-j =1$)	411
Medium range ($ i-j >1$ and $ i-j <5$)	322
Long range ($ i-j \geq 5$)	28
Inter-chain	0
Hydrogen bond restraints	222
Disulfide bond restraints	0
Total dihedral-angle restraints	180
Number of unmapped restraints	0
Number of restraints per residue	11.1
Number of long range restraints per residue ¹	0.2

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	9.2	0.2
0.2-0.5 (Medium)	23.1	0.5
>0.5 (Large)	49.4	4.03

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

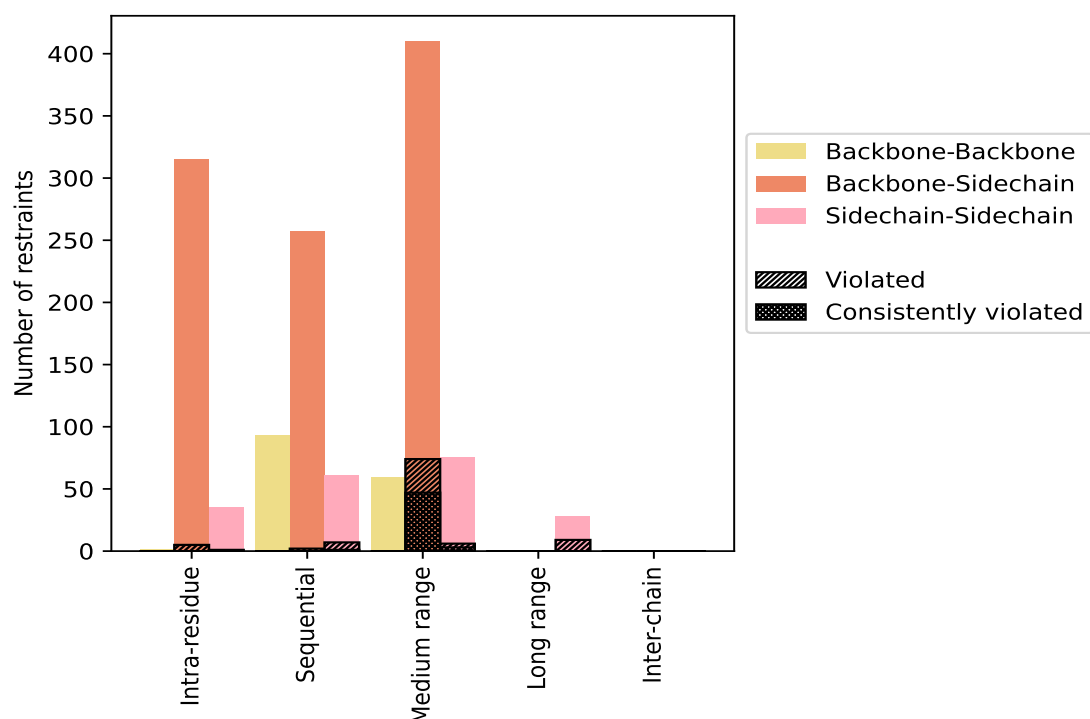
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	351	26.3	6	1.7	0.4	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	315	23.6	5	1.6	0.4	0	0.0	0.0
Sidechain-Sidechain	35	2.6	1	2.9	0.1	0	0.0	0.0
Sequential ($i-j =1$)	411	30.8	9	2.2	0.7	1	0.2	0.1
Backbone-Backbone	93	7.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	257	19.3	2	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	61	4.6	7	11.5	0.5	1	1.6	0.1
Medium range ($i-j >1$ & $i-j <5$)	322	24.1	6	1.9	0.4	3	0.9	0.2
Backbone-Backbone	59	4.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	188	14.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	75	5.6	6	8.0	0.4	3	4.0	0.2
Long range ($i-j \geq 5$)	28	2.1	9	32.1	0.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	28	2.1	9	32.1	0.7	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	222	16.6	74	33.3	5.5	47	21.2	3.5
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1334	100.0	104	7.8	7.8	51	3.8	3.8
Backbone-Backbone	153	11.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	982	73.6	81	8.2	6.1	47	4.8	3.5
Sidechain-Sidechain	199	14.9	23	11.6	1.7	4	2.0	0.3

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	2	4	67	4	0	77	0.64	3.18	0.55	0.55
2	1	1	72	4	0	78	0.68	3.83	0.7	0.54
3	3	1	72	5	0	81	0.69	3.86	0.7	0.51
4	1	4	71	7	0	83	0.72	3.51	0.71	0.58
5	1	1	72	5	0	79	0.68	3.6	0.65	0.58
6	2	4	68	9	0	83	0.79	4.03	0.76	0.61
7	2	2	77	4	0	85	0.63	3.7	0.66	0.52
8	4	5	71	5	0	85	0.67	3.67	0.62	0.57
9	2	5	70	4	0	81	0.67	3.52	0.65	0.56
10	3	4	70	5	0	82	0.67	4.01	0.63	0.56

Continued on next page...

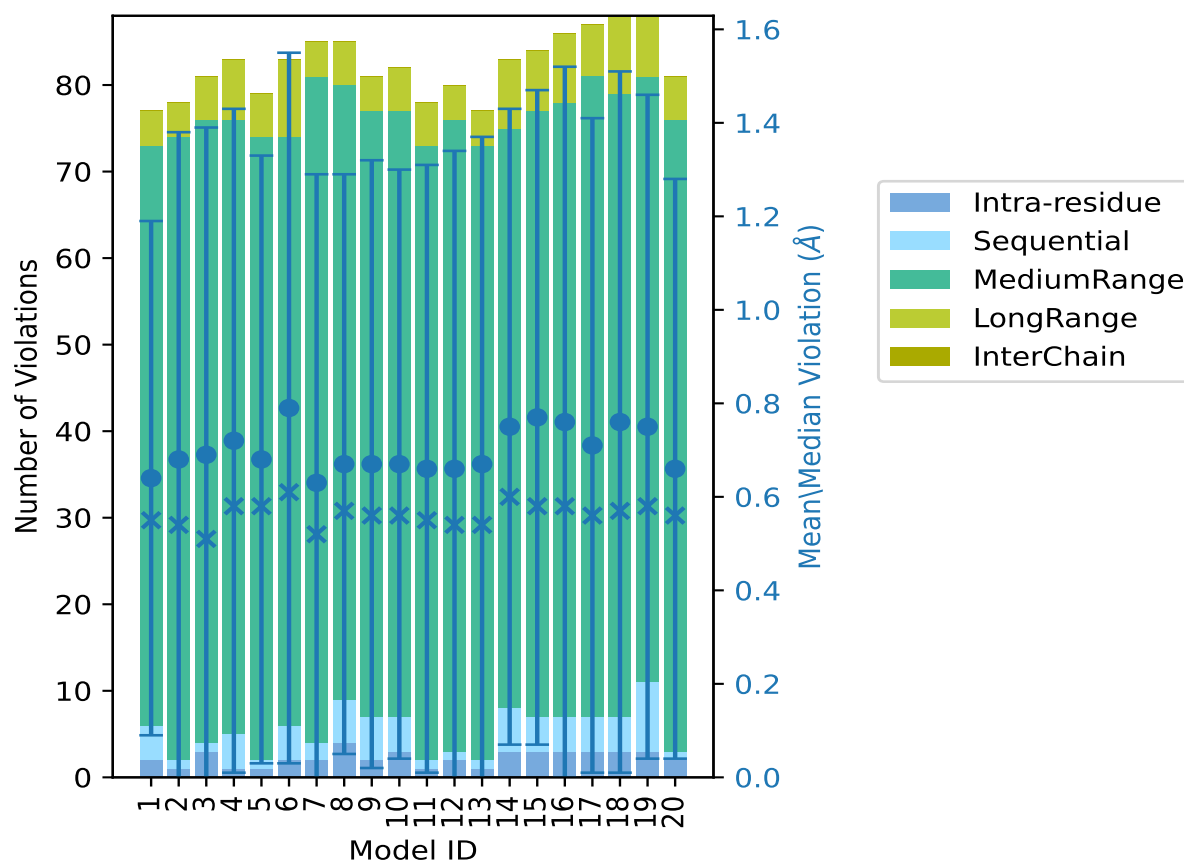
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	1	71	5	0	78	0.66	3.58	0.65	0.55
12	2	1	73	4	0	80	0.66	3.86	0.68	0.54
13	1	1	71	4	0	77	0.67	3.82	0.7	0.54
14	3	5	67	8	0	83	0.75	3.88	0.68	0.6
15	3	4	70	7	0	84	0.77	3.53	0.7	0.58
16	3	4	71	8	0	86	0.76	3.88	0.76	0.58
17	3	4	74	6	0	87	0.71	3.93	0.7	0.56
18	3	4	72	9	0	88	0.76	3.72	0.75	0.57
19	3	8	70	7	0	88	0.75	3.61	0.71	0.58
20	2	1	73	5	0	81	0.66	3.85	0.62	0.56

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

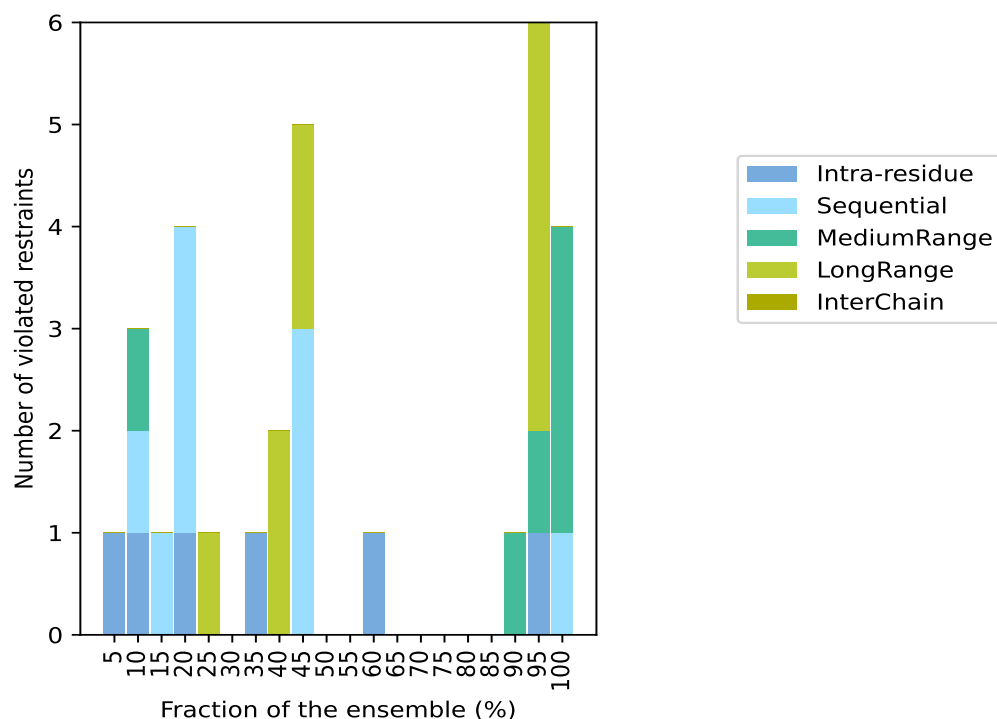
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1082(IR:345, SQ:402, MR:316, LR:19, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	0	0	0	0	1	1	5.0
1	1	1	0	0	3	2	10.0
0	1	0	0	0	1	3	15.0
1	3	0	0	0	4	4	20.0
0	0	0	1	0	1	5	25.0
0	0	0	0	0	0	6	30.0
1	0	0	0	0	1	7	35.0
0	0	0	2	0	2	8	40.0
0	3	0	2	0	5	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
1	0	0	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
1	0	1	4	0	6	19	95.0
0	1	3	0	0	4	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

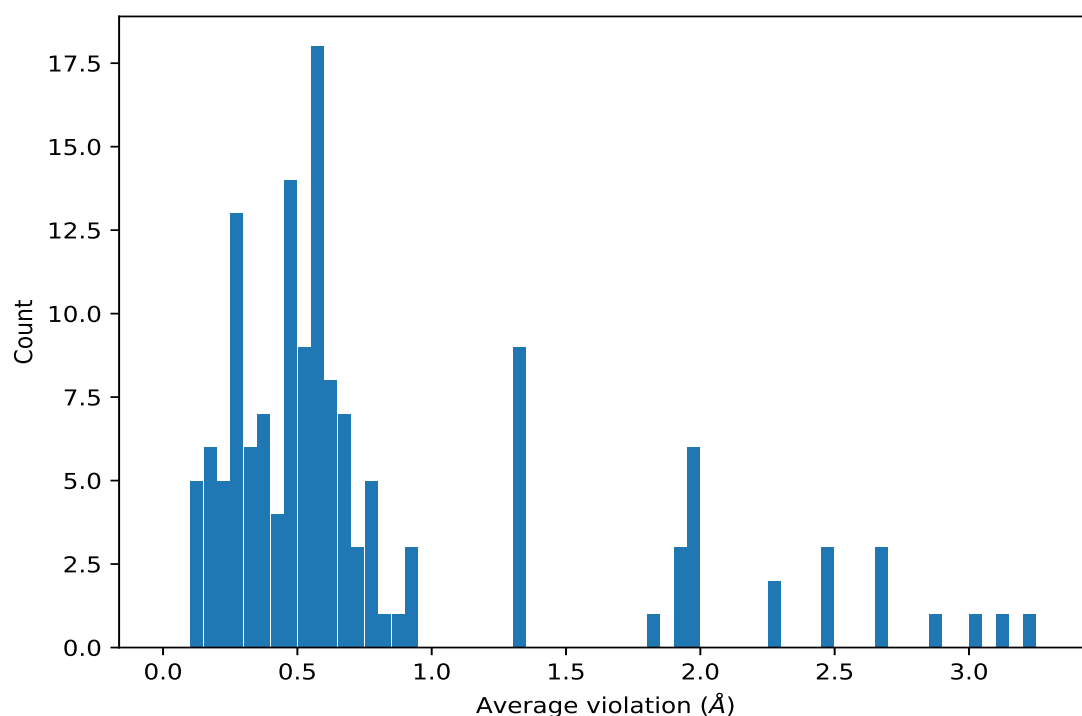
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	20	3.01	0.2	3.0
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	20	2.66	0.08	2.67
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	20	2.66	0.08	2.67
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	20	2.66	0.08	2.67
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	20	0.79	0.17	0.76
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	20	0.79	0.17	0.76
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	20	0.79	0.17	0.76
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	20	0.78	0.01	0.78
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	20	0.76	0.0	0.76
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	20	0.74	0.02	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	20	0.73	0.04	0.74
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	20	0.7	0.05	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	20	0.69	0.02	0.7
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	20	0.68	0.05	0.68
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	20	0.66	0.16	0.72
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	20	0.65	0.03	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	20	0.65	0.0	0.65
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	20	0.65	0.1	0.68
(2,174)	1:44:A:SER:O	1:48:A:SER:N	20	0.64	0.13	0.68
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	20	0.64	0.08	0.64
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	20	0.63	0.1	0.67
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	20	0.63	0.03	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	20	0.62	0.01	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	20	0.62	0.01	0.62
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	20	0.61	0.08	0.64
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	20	0.59	0.03	0.58
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	20	0.58	0.07	0.58
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	20	0.58	0.09	0.58
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	20	0.57	0.15	0.57
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	20	0.57	0.04	0.57
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	20	0.56	0.06	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	20	0.56	0.01	0.56
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	20	0.56	0.04	0.55
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	20	0.55	0.06	0.57
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	20	0.54	0.04	0.54
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	20	0.52	0.06	0.51
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	20	0.52	0.13	0.53
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	20	0.5	0.13	0.5
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	20	0.5	0.1	0.52
(2,192)	1:78:A:MET:O	1:82:A:THR:N	20	0.5	0.12	0.54
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	20	0.48	0.07	0.45
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	20	0.47	0.11	0.46
(2,170)	1:40:A:THR:O	1:44:A:SER:N	20	0.45	0.16	0.47
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	20	0.42	0.0	0.42
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	20	0.39	0.12	0.37
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	20	0.37	0.13	0.36
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	20	0.36	0.12	0.38
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	20	0.35	0.15	0.36
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	20	0.34	0.01	0.34
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	20	0.33	0.15	0.31
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	20	0.31	0.01	0.32
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	20	0.29	0.13	0.25
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	20	0.29	0.13	0.27
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	20	0.19	0.03	0.2
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	20	0.11	0.0	0.11
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	19	3.21	0.72	3.58
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	19	2.88	0.84	2.75
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	19	2.27	0.7	2.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	19	2.27	0.7	2.59
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	19	1.95	0.5	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	19	1.95	0.5	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	19	1.95	0.5	2.07
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	19	0.93	0.26	0.88
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	19	0.93	0.26	0.88
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	19	0.93	0.26	0.88
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	19	0.61	0.03	0.61
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	19	0.58	0.1	0.58
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	19	0.58	0.09	0.58
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	19	0.45	0.2	0.51
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	19	0.39	0.12	0.4
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	19	0.37	0.14	0.32
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	18	1.34	0.32	1.31
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	18	1.34	0.32	1.31
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	18	1.34	0.32	1.31
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	18	1.34	0.32	1.31
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	18	1.34	0.32	1.31
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	18	1.34	0.32	1.31
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	18	0.42	0.16	0.44
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	18	0.41	0.21	0.45
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	18	0.3	0.08	0.34
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	18	0.26	0.18	0.19
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	18	0.18	0.07	0.16
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	17	0.41	0.14	0.36
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	17	0.32	0.16	0.29
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	17	0.3	0.14	0.25
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	16	0.59	0.13	0.61
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	16	0.24	0.12	0.22
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	15	0.29	0.14	0.27
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	15	0.25	0.07	0.26
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	13	0.23	0.09	0.21
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	13	0.23	0.13	0.17
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	12	0.82	0.26	0.79
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	12	0.17	0.07	0.15
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	11	0.26	0.12	0.26
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	10	0.16	0.05	0.15
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	9	3.13	0.08	3.16
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	9	2.48	0.07	2.46
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	9	2.48	0.07	2.46
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	9	2.48	0.07	2.46
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	9	1.99	0.53	1.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	9	1.99	0.53	1.78
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	9	1.99	0.53	1.78
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	9	1.9	0.2	1.83
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	9	1.9	0.2	1.83
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	9	1.9	0.2	1.83
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	9	0.85	0.04	0.85
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	8	0.54	0.13	0.52
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	8	0.54	0.13	0.52
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	8	0.54	0.13	0.52
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	8	0.45	0.24	0.46
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	8	0.45	0.24	0.46
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	8	0.45	0.24	0.46
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	8	0.2	0.11	0.16
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	7	0.37	0.15	0.36
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	7	0.15	0.05	0.13
(2,198)	1:84:A:SER:O	1:88:A:THR:N	6	0.26	0.16	0.24
(1,15)	1:114:A:LEU:HD21	1:30:A:TYR:HD1	5	1.31	0.56	1.14
(1,15)	1:114:A:LEU:HD22	1:30:A:TYR:HD1	5	1.31	0.56	1.14
(1,15)	1:114:A:LEU:HD23	1:30:A:TYR:HD1	5	1.31	0.56	1.14
(1,235)	1:28:A:VAL:HB	1:29:A:PHE:HD1	4	1.81	0.24	1.75
(1,449)	1:29:A:PHE:H	1:29:A:PHE:HD1	4	0.67	0.05	0.66
(1,859)	1:28:A:VAL:HG11	1:29:A:PHE:HE1	4	0.56	0.19	0.5
(1,859)	1:28:A:VAL:HG12	1:29:A:PHE:HE1	4	0.56	0.19	0.5
(1,859)	1:28:A:VAL:HG13	1:29:A:PHE:HE1	4	0.56	0.19	0.5
(1,859)	1:28:A:VAL:HG21	1:29:A:PHE:HE1	4	0.56	0.19	0.5
(1,859)	1:28:A:VAL:HG22	1:29:A:PHE:HE1	4	0.56	0.19	0.5
(1,859)	1:28:A:VAL:HG23	1:29:A:PHE:HE1	4	0.56	0.19	0.5
(1,773)	1:29:A:PHE:HD1	1:30:A:TYR:H	4	0.23	0.08	0.24
(1,858)	1:28:A:VAL:HG11	1:29:A:PHE:HD1	3	0.25	0.12	0.17
(1,858)	1:28:A:VAL:HG12	1:29:A:PHE:HD1	3	0.25	0.12	0.17
(1,858)	1:28:A:VAL:HG13	1:29:A:PHE:HD1	3	0.25	0.12	0.17
(1,858)	1:28:A:VAL:HG21	1:29:A:PHE:HD1	3	0.25	0.12	0.17
(1,858)	1:28:A:VAL:HG22	1:29:A:PHE:HD1	3	0.25	0.12	0.17
(1,858)	1:28:A:VAL:HG23	1:29:A:PHE:HD1	3	0.25	0.12	0.17
(2,162)	1:23:A:CYS:O	1:27:A:LEU:N	3	0.15	0.03	0.16
(1,980)	1:89:A:VAL:HG11	1:90:A:PHE:HE1	2	0.48	0.28	0.48
(1,980)	1:89:A:VAL:HG12	1:90:A:PHE:HE1	2	0.48	0.28	0.48
(1,980)	1:89:A:VAL:HG13	1:90:A:PHE:HE1	2	0.48	0.28	0.48
(1,980)	1:89:A:VAL:HG21	1:90:A:PHE:HE1	2	0.48	0.28	0.48
(1,980)	1:89:A:VAL:HG22	1:90:A:PHE:HE1	2	0.48	0.28	0.48
(1,980)	1:89:A:VAL:HG23	1:90:A:PHE:HE1	2	0.48	0.28	0.48
(1,747)	1:90:A:PHE:H	1:90:A:PHE:HD1	2	0.46	0.02	0.46

Continued on next page...

Continued from previous page...

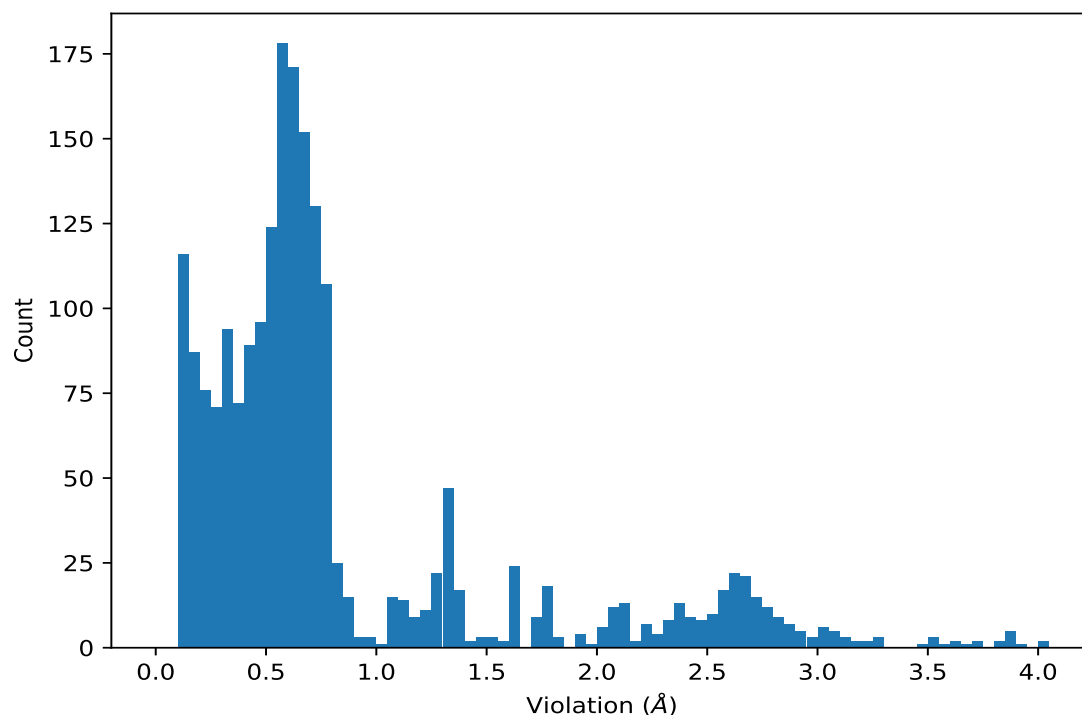
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB1	2	0.11	0.0	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB2	2	0.11	0.0	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB3	2	0.11	0.0	0.11
(2,158)	1:19:A:LEU:O	1:23:A:CYS:N	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	6	4.03
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	10	4.01
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	17	3.93
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	14	3.88
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	16	3.88
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	3	3.86
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	12	3.86
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	20	3.85
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	2	3.83
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	13	3.82
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	18	3.72
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	7	3.7
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	8	3.67
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	19	3.61
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	5	3.6
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	11	3.58
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	15	3.53
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	9	3.52
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	4	3.51
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	6	3.49
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	3	3.29
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	18	3.26
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	17	3.25
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	16	3.22
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	19	3.2
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	1	3.18
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	6	3.16
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	10	3.12
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	14	3.12
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	15	3.11
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	5	3.07
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	17	3.07
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	20	3.06
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	11	3.05
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	14	3.05
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	4	3.02
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	13	3.01
(1,207)	1:80:A:PHE:HD1	1:81:A:VAL:HB	18	3.01
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	16	3.0
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	16	3.0
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	16	3.0
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	8	2.99
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	2	2.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	15	2.98
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	2	2.93
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	2	2.93
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	2	2.93
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	3	2.91
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	3	2.91
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	7	2.89
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	12	2.89
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	13	2.89
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	13	2.89
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	3	2.88
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	9	2.88
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	19	2.86
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	4	2.84
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	16	2.84
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	16	2.84
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	16	2.84
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	7	2.84
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	7	2.84
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	12	2.82
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	12	2.82
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	9	2.81
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	20	2.78
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	20	2.78
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	20	2.78
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	6	2.76
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	6	2.76
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	6	2.76
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	6	2.75
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	6	2.75
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	6	2.75
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	18	2.75
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	18	2.75
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	7	2.75
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	2	2.74
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	2	2.74
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	2	2.74
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	17	2.74
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	17	2.74
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	17	2.74
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	12	2.73
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	12	2.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	12	2.73
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	14	2.71
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	14	2.71
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	14	2.71
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	19	2.7
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	19	2.7
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	19	2.7
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	11	2.68
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	11	2.68
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	11	2.68
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	4	2.68
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	3	2.67
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	3	2.67
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	3	2.67
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	10	2.67
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	10	2.67
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	10	2.67
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	15	2.67
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	15	2.67
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	15	2.67
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	5	2.67
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	5	2.67
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	7	2.65
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	7	2.65
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	7	2.65
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	13	2.65
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	13	2.65
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	13	2.65
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	5	2.64
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	5	2.64
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	5	2.64
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	4	2.63
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	4	2.63
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	4	2.63
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	8	2.63
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	8	2.63
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	8	2.63
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	16	2.63
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	16	2.63
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	16	2.63
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	18	2.62
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	18	2.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	18	2.62
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	9	2.62
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	9	2.62
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	19	2.61
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	9	2.6
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	9	2.6
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	9	2.6
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	13	2.6
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	11	2.59
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	11	2.59
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	15	2.57
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	15	2.57
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	15	2.57
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	8	2.57
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	8	2.57
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	8	2.57
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	18	2.57
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	18	2.57
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	18	2.57
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	16	2.55
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	16	2.55
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	16	2.55
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	17	2.55
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	17	2.55
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	17	2.55
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	6	2.53
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	6	2.53
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	6	2.53
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	19	2.52
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	19	2.52
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	5	2.52
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	4	2.51
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	4	2.51
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	15	2.51
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	15	2.51
(1,279)	1:70:A:ILE:HB	1:73:A:TYR:HD1	1	2.49
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	4	2.46
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	4	2.46
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	4	2.46
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	1	2.45
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	1	2.45
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	1	2.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	12	2.45
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	19	2.43
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	19	2.43
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	19	2.43
(1,86)	1:70:A:ILE:HG21	1:73:A:TYR:HD1	1	2.41
(1,86)	1:70:A:ILE:HG22	1:73:A:TYR:HD1	1	2.41
(1,86)	1:70:A:ILE:HG23	1:73:A:TYR:HD1	1	2.41
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	2	2.4
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	2	2.4
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	2	2.4
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	14	2.39
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	14	2.39
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	14	2.39
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	13	2.37
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	13	2.37
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	13	2.37
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	11	2.37
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	7	2.36
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	7	2.36
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	7	2.36
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG11	18	2.35
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG12	18	2.35
(1,140)	1:80:A:PHE:HD1	1:81:A:VAL:HG13	18	2.35
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	3	2.34
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	3	2.34
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	3	2.34
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	18	2.34
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	18	2.34
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	18	2.34
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	15	2.33
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	20	2.3
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	16	2.28
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	16	2.28
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	16	2.28
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	8	2.28
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	12	2.24
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	12	2.24
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	12	2.24
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	10	2.21
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	5	2.2
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	5	2.2
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	5	2.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	17	2.18
(1,235)	1:28:A:VAL:HB	1:29:A:PHE:HD1	19	2.15
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	9	2.14
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	9	2.14
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	9	2.14
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	18	2.14
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	18	2.14
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	18	2.14
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	16	2.12
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	16	2.12
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	16	2.12
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	6	2.12
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	14	2.11
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	14	2.11
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	14	2.11
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	11	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	11	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	11	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	15	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	15	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	15	2.07
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	15	2.07
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	15	2.07
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	15	2.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	19	2.05
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	19	2.05
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	19	2.05
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	4	2.03
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	4	2.03
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	4	2.03
(1,15)	1:114:A:LEU:HD21	1:30:A:TYR:HD1	18	2.0
(1,15)	1:114:A:LEU:HD22	1:30:A:TYR:HD1	18	2.0
(1,15)	1:114:A:LEU:HD23	1:30:A:TYR:HD1	18	2.0
(1,1)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	14	1.97
(1,15)	1:114:A:LEU:HD21	1:30:A:TYR:HD1	6	1.94
(1,15)	1:114:A:LEU:HD22	1:30:A:TYR:HD1	6	1.94
(1,15)	1:114:A:LEU:HD23	1:30:A:TYR:HD1	6	1.94
(1,235)	1:28:A:VAL:HB	1:29:A:PHE:HD1	10	1.91
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	4	1.83
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	4	1.83
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	4	1.83
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	10	1.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	10	1.78
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	10	1.78
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	19	1.77
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	19	1.77
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	19	1.77
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	14	1.76
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	14	1.76
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	14	1.76
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	14	1.76
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	14	1.76
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	14	1.76
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	17	1.75
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	17	1.75
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	17	1.75
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	17	1.75
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	17	1.75
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	17	1.75
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	6	1.73
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	6	1.73
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	6	1.73
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	20	1.73
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	20	1.73
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	20	1.73
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	17	1.7
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	17	1.7
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	17	1.7
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	8	1.64
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	8	1.64
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	8	1.64
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	8	1.64
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	8	1.64
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	8	1.64
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	20	1.64
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	20	1.64
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	20	1.64
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	20	1.64
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	20	1.64
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	20	1.64
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	1	1.64
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	1	1.64
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	1	1.64
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	6	1.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	6	1.62
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	6	1.62
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	6	1.62
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	6	1.62
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	6	1.62
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG21	1	1.6
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG22	1	1.6
(1,25)	1:80:A:PHE:HD1	1:120:A:VAL:HG23	1	1.6
(1,235)	1:28:A:VAL:HB	1:29:A:PHE:HD1	9	1.59
(1,235)	1:28:A:VAL:HB	1:29:A:PHE:HD1	8	1.57
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	18	1.52
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	18	1.52
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	18	1.52
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	1	1.46
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	1	1.46
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	1	1.46
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	20	1.43
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	20	1.43
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	20	1.39
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	20	1.39
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	20	1.39
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	14	1.39
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	14	1.39
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	14	1.39
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	12	1.36
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	12	1.36
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	12	1.36
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	12	1.36
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	12	1.36
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	12	1.36
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	12	1.36
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	12	1.36
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	12	1.36
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	6	1.35
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	6	1.35
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	13	1.34
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	13	1.34
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	13	1.34
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	13	1.34
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	13	1.34
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	13	1.34
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	17	1.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	17	1.34
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	6	1.33
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	6	1.33
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	6	1.33
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	5	1.31
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	5	1.31
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	5	1.31
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	5	1.31
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	5	1.31
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	5	1.31
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	11	1.31
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	11	1.31
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	11	1.31
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	11	1.31
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	11	1.31
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	11	1.31
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	15	1.31
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	15	1.31
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	15	1.31
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	15	1.31
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	15	1.31
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	15	1.31
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	19	1.31
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	19	1.31
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	19	1.31
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	19	1.31
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	19	1.31
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	19	1.31
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	3	1.3
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	3	1.3
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	3	1.3
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	3	1.3
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	3	1.3
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	3	1.3
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	7	1.3
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	7	1.3
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	7	1.3
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	7	1.3
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	7	1.3
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	7	1.3
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	10	1.29
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	10	1.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	10	1.29
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	10	1.29
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	10	1.29
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	10	1.29
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	10	1.29
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	10	1.29
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	10	1.29
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	17	1.29
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	17	1.29
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	17	1.29
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	8	1.26
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	8	1.26
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	8	1.26
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	16	1.25
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	9	1.25
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	9	1.25
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	9	1.25
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	9	1.25
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	9	1.25
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	9	1.25
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	2	1.23
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	2	1.23
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	2	1.23
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	2	1.23
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	2	1.23
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	2	1.23
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	10	1.23
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	10	1.23
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD11	17	1.22
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD12	17	1.22
(1,19)	1:129:A:PHE:HE1	1:12:A:ILE:HD13	17	1.22
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	8	1.19
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	8	1.19
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	4	1.16
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	4	1.16
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	4	1.16
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	4	1.16
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	4	1.16
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	4	1.16
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	3	1.15
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	15	1.14
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	15	1.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	15	1.14
(1,15)	1:114:A:LEU:HD21	1:30:A:TYR:HD1	3	1.14
(1,15)	1:114:A:LEU:HD22	1:30:A:TYR:HD1	3	1.14
(1,15)	1:114:A:LEU:HD23	1:30:A:TYR:HD1	3	1.14
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	16	1.14
(1,2)	1:10:A:TYR:HE1	1:56:A:ILE:HG13	18	1.13
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	5	1.12
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	5	1.12
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	5	1.12
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	11	1.1
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	11	1.1
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	11	1.1
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	19	1.08
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	19	1.08
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	19	1.08
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG12	14	1.08
(1,21)	1:10:A:TYR:HE1	1:59:A:ILE:HG13	14	1.08
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD11	14	1.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD12	14	1.07
(1,52)	1:10:A:TYR:HD1	1:59:A:ILE:HD13	14	1.07
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	13	1.06
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	13	1.06
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	13	1.06
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	14	1.06
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	14	1.06
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	14	1.06
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	18	1.05
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	15	1.04
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	17	0.98
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	17	0.98
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	17	0.98
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	16	0.94
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	1	0.91
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	17	0.9
(1,859)	1:28:A:VAL:HG11	1:29:A:PHE:HE1	19	0.88
(1,859)	1:28:A:VAL:HG12	1:29:A:PHE:HE1	19	0.88
(1,859)	1:28:A:VAL:HG13	1:29:A:PHE:HE1	19	0.88
(1,859)	1:28:A:VAL:HG21	1:29:A:PHE:HE1	19	0.88
(1,859)	1:28:A:VAL:HG22	1:29:A:PHE:HE1	19	0.88
(1,859)	1:28:A:VAL:HG23	1:29:A:PHE:HE1	19	0.88
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	7	0.88
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	7	0.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	7	0.88
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	6	0.87
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	6	0.87
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	6	0.87
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	15	0.86
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	18	0.86
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	1	0.85
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	3	0.84
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	3	0.84
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	3	0.84
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	18	0.84
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	18	0.84
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	18	0.84
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	6	0.83
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	3	0.83
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	3	0.83
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	3	0.83
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	20	0.83
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	20	0.83
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	20	0.83
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	19	0.82
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	17	0.82
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	4	0.81
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	2	0.81
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	2	0.81
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	2	0.81
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	14	0.81
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	14	0.81
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	14	0.81
(1,15)	1:114:A:LEU:HD21	1:30:A:TYR:HD1	11	0.81
(1,15)	1:114:A:LEU:HD22	1:30:A:TYR:HD1	11	0.81
(1,15)	1:114:A:LEU:HD23	1:30:A:TYR:HD1	11	0.81
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	18	0.79
(1,741)	1:80:A:PHE:HD1	1:81:A:VAL:H	14	0.79
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	10	0.79
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	10	0.79
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	10	0.79
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	13	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	1	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	4	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	6	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	7	0.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	8	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	9	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	10	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	13	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	16	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	17	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	19	0.78
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	20	0.78
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	8	0.78
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	8	0.78
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	8	0.78
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	19	0.78
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	19	0.78
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	19	0.78
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	4	0.77
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	11	0.77
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	8	0.77
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	14	0.77
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	19	0.77
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	5	0.77
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	6	0.77
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	2	0.77
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	3	0.77
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	5	0.77
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	11	0.77
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	12	0.77
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	14	0.77
(2,155)	1:16:A:ILE:O	1:20:A:LEU:N	15	0.77
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	11	0.77
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	11	0.77
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	11	0.77
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	12	0.77
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	12	0.77
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	12	0.77
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	1	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	2	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	3	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	4	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	5	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	6	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	7	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	8	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	9	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	10	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	11	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	12	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	13	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	14	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	15	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	16	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	17	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	18	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	19	0.76
(2,209)	1:113:A:PHE:O	1:117:A:PHE:N	20	0.76
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	6	0.76
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	6	0.76
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	20	0.76
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	8	0.76
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	16	0.76
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	19	0.76
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	3	0.76
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	1	0.76
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	8	0.76
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	14	0.76
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	20	0.76
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	14	0.76
(1,449)	1:29:A:PHE:H	1:29:A:PHE:HD1	19	0.76
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	6	0.76
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	6	0.76
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	6	0.76
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	3	0.75
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	15	0.75
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	11	0.75
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	17	0.75
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	18	0.75
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	5	0.75
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	11	0.75
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	12	0.75
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	13	0.75
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	15	0.75
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	20	0.75
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	7	0.75
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	10	0.75
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	16	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	19	0.75
(1,980)	1:89:A:VAL:HG11	1:90:A:PHE:HE1	14	0.75
(1,980)	1:89:A:VAL:HG12	1:90:A:PHE:HE1	14	0.75
(1,980)	1:89:A:VAL:HG13	1:90:A:PHE:HE1	14	0.75
(1,980)	1:89:A:VAL:HG21	1:90:A:PHE:HE1	14	0.75
(1,980)	1:89:A:VAL:HG22	1:90:A:PHE:HE1	14	0.75
(1,980)	1:89:A:VAL:HG23	1:90:A:PHE:HE1	14	0.75
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	17	0.75
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	17	0.75
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	17	0.75
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	18	0.75
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	18	0.75
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	18	0.75
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	15	0.74
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	18	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	1	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	4	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	7	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	9	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	12	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	13	0.74
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	16	0.74
(2,174)	1:44:A:SER:O	1:48:A:SER:N	4	0.74
(2,174)	1:44:A:SER:O	1:48:A:SER:N	15	0.74
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	6	0.74
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	14	0.74
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	15	0.74
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	13	0.74
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	2	0.74
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	3	0.74
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	9	0.74
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	12	0.74
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	15	0.74
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	17	0.74
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	20	0.74
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	20	0.74
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	20	0.74
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	13	0.74
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	13	0.74
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	13	0.74
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	7	0.73
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	13	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	8	0.73
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	5	0.73
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	16	0.73
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	19	0.73
(2,174)	1:44:A:SER:O	1:48:A:SER:N	7	0.73
(2,174)	1:44:A:SER:O	1:48:A:SER:N	14	0.73
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	10	0.73
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	17	0.73
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	1	0.73
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	6	0.73
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	11	0.73
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	20	0.73
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	7	0.73
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	13	0.73
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	18	0.73
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	8	0.73
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	16	0.73
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	16	0.73
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	16	0.73
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	15	0.73
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	15	0.73
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	15	0.73
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	16	0.72
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	14	0.72
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	12	0.72
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	19	0.72
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	3	0.72
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	19	0.72
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	7	0.72
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	9	0.72
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	17	0.72
(2,174)	1:44:A:SER:O	1:48:A:SER:N	9	0.72
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	14	0.72
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	16	0.72
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	6	0.72
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	4	0.72
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	12	0.72
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	5	0.72
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	5	0.72
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	5	0.72
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	8	0.72
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	8	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	8	0.72
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	9	0.71
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	17	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	5	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	7	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	9	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	11	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	12	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	14	0.71
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	15	0.71
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	18	0.71
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	10	0.71
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	3	0.71
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	6	0.71
(2,174)	1:44:A:SER:O	1:48:A:SER:N	19	0.71
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	4	0.71
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	7	0.71
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	9	0.71
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	5	0.71
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	1	0.71
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	14	0.71
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	15	0.71
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	16	0.71
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	2	0.71
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	5	0.71
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	9	0.71
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	11	0.71
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	2	0.71
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	2	0.71
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	2	0.71
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	4	0.71
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	4	0.71
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	4	0.71
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	7	0.71
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	7	0.71
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	7	0.71
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	15	0.71
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	15	0.71
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	15	0.71
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	6	0.7
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	5	0.7
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	2	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	4	0.7
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	13	0.7
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	1	0.7
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	4	0.7
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	6	0.7
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	2	0.7
(2,174)	1:44:A:SER:O	1:48:A:SER:N	10	0.7
(2,174)	1:44:A:SER:O	1:48:A:SER:N	11	0.7
(2,174)	1:44:A:SER:O	1:48:A:SER:N	18	0.7
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	9	0.7
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	8	0.7
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	12	0.7
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	15	0.7
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	16	0.7
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	17	0.7
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	18	0.7
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	12	0.7
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	20	0.69
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	5	0.69
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	2	0.69
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	5	0.69
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	10	0.69
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	19	0.69
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	15	0.69
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	1	0.69
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	3	0.69
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	16	0.69
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	17	0.69
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	2	0.69
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	14	0.69
(2,174)	1:44:A:SER:O	1:48:A:SER:N	2	0.69
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	3	0.69
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	14	0.69
(2,160)	1:21:A:ILE:O	1:25:A:THR:N	4	0.69
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	9	0.69
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	9	0.69
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	9	0.69
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	9	0.69
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	9	0.69
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	9	0.69
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	16	0.69
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	16	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	16	0.69
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	1	0.69
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	1	0.69
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	1	0.69
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	8	0.68
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	10	0.68
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	1	0.68
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	7	0.68
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	5	0.68
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	17	0.68
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	6	0.68
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	20	0.68
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	19	0.68
(2,174)	1:44:A:SER:O	1:48:A:SER:N	20	0.68
(2,170)	1:40:A:THR:O	1:44:A:SER:N	7	0.68
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	15	0.68
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	17	0.68
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	19	0.68
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	18	0.68
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	10	0.68
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	2	0.68
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	3	0.68
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	5	0.68
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	11	0.68
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	12	0.68
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	14	0.68
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	15	0.68
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	5	0.68
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	9	0.68
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	12	0.68
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	13	0.68
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	15	0.68
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	16	0.67
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	20	0.67
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	18	0.67
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	9	0.67
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	17	0.67
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	18	0.67
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	7	0.67
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	5	0.67
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	8	0.67
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	18	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	16	0.67
(2,174)	1:44:A:SER:O	1:48:A:SER:N	12	0.67
(2,174)	1:44:A:SER:O	1:48:A:SER:N	13	0.67
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	14	0.67
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	5	0.67
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	6	0.67
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	20	0.67
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	11	0.67
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	20	0.67
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	7	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	1	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	2	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	3	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	4	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	6	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	7	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	8	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	10	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	11	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	14	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	19	0.67
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	20	0.67
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	14	0.67
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	4	0.67
(1,449)	1:29:A:PHE:H	1:29:A:PHE:HD1	8	0.67
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	1	0.66
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	9	0.66
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	11	0.66
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	9	0.66
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	6	0.66
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	13	0.66
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	17	0.66
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	15	0.66
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	7	0.66
(2,170)	1:40:A:THR:O	1:44:A:SER:N	10	0.66
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	12	0.66
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	14	0.66
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	19	0.66
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	20	0.66
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	1	0.66
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	3	0.66
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	8	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	10	0.66
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	14	0.66
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	14	0.66
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	14	0.66
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	11	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	1	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	2	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	3	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	4	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	5	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	6	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	7	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	8	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	10	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	12	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	13	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	14	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	15	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	16	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	17	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	18	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	19	0.65
(2,213)	1:117:A:PHE:O	1:121:A:CYS:N	20	0.65
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	10	0.65
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	13	0.65
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	16	0.65
(2,192)	1:78:A:MET:O	1:82:A:THR:N	16	0.65
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	5	0.65
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	8	0.65
(2,174)	1:44:A:SER:O	1:48:A:SER:N	1	0.65
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	8	0.65
(2,170)	1:40:A:THR:O	1:44:A:SER:N	12	0.65
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	18	0.65
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	19	0.65
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	9	0.65
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	18	0.65
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	16	0.65
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	16	0.65
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	17	0.65
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	16	0.65
(1,15)	1:114:A:LEU:HD21	1:30:A:TYR:HD1	5	0.65
(1,15)	1:114:A:LEU:HD22	1:30:A:TYR:HD1	5	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:114:A:LEU:HD23	1:30:A:TYR:HD1	5	0.65
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	5	0.64
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	1	0.64
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	6	0.64
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	14	0.64
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	3	0.64
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	16	0.64
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	5	0.64
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	20	0.64
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	15	0.64
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	3	0.64
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	15	0.64
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	2	0.64
(2,185)	1:55:A:LEU:O	1:59:A:ILE:N	10	0.64
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	2	0.64
(2,174)	1:44:A:SER:O	1:48:A:SER:N	5	0.64
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	16	0.64
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	13	0.64
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	4	0.64
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	19	0.64
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	18	0.64
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	6	0.64
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	7	0.64
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	8	0.64
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	10	0.64
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	20	0.64
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	7	0.64
(1,449)	1:29:A:PHE:H	1:29:A:PHE:HD1	10	0.64
(1,51)	1:70:A:ILE:HD11	1:73:A:TYR:HD1	4	0.64
(1,51)	1:70:A:ILE:HD12	1:73:A:TYR:HD1	4	0.64
(1,51)	1:70:A:ILE:HD13	1:73:A:TYR:HD1	4	0.64
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	20	0.63
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	4	0.63
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	4	0.63
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	6	0.63
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	10	0.63
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	12	0.63
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	15	0.63
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	1	0.63
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	13	0.63
(2,174)	1:44:A:SER:O	1:48:A:SER:N	6	0.63
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	3	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	18	0.63
(2,170)	1:40:A:THR:O	1:44:A:SER:N	6	0.63
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	10	0.63
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	12	0.63
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	8	0.63
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	18	0.63
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	9	0.63
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	13	0.63
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	19	0.63
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	4	0.63
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	14	0.63
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	4	0.63
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	4	0.63
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	4	0.63
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	14	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	2	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	4	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	5	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	6	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	7	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	8	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	10	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	11	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	12	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	13	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	15	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	17	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	18	0.62
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	19	0.62
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	2	0.62
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	1	0.62
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	5	0.62
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	8	0.62
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	11	0.62
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	12	0.62
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	16	0.62
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	19	0.62
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	9	0.62
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	19	0.62
(2,192)	1:78:A:MET:O	1:82:A:THR:N	8	0.62
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	6	0.62
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	7	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	11	0.62
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	1	0.62
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	16	0.62
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	4	0.62
(2,174)	1:44:A:SER:O	1:48:A:SER:N	8	0.62
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	1	0.62
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	10	0.62
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	5	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	1	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	4	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	6	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	7	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	8	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	9	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	10	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	13	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	19	0.62
(2,154)	1:15:A:ILE:O	1:19:A:LEU:N	20	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	1	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	2	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	4	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	5	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	6	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	7	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	8	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	14	0.62
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	15	0.62
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	5	0.62
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	8	0.62
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	9	0.62
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	15	0.62
(1,449)	1:29:A:PHE:H	1:29:A:PHE:HD1	9	0.62
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	15	0.61
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	19	0.61
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	15	0.61
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	13	0.61
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	20	0.61
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	3	0.61
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	9	0.61
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	14	0.61
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	16	0.61
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	20	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	7	0.61
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	15	0.61
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	3	0.61
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	1	0.61
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	8	0.61
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	10	0.61
(2,192)	1:78:A:MET:O	1:82:A:THR:N	6	0.61
(2,192)	1:78:A:MET:O	1:82:A:THR:N	17	0.61
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	11	0.61
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	16	0.61
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	2	0.61
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	17	0.61
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	6	0.61
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	18	0.61
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	9	0.61
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	1	0.61
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	11	0.61
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	19	0.61
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	14	0.61
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	3	0.61
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	10	0.61
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	11	0.61
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	12	0.61
(2,153)	1:14:A:LEU:O	1:18:A:CYS:N	20	0.61
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	12	0.61
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	13	0.61
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	14	0.6
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	5	0.6
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	11	0.6
(2,210)	1:114:A:LEU:O	1:118:A:ILE:N	1	0.6
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	16	0.6
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	19	0.6
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	18	0.6
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	17	0.6
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	14	0.6
(2,192)	1:78:A:MET:O	1:82:A:THR:N	2	0.6
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	14	0.6
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	10	0.6
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	12	0.6
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	20	0.6
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	8	0.6
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	10	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	10	0.6
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	13	0.6
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	17	0.6
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	19	0.6
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	16	0.59
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	6	0.59
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	3	0.59
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	4	0.59
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	6	0.59
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	17	0.59
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	3	0.59
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	14	0.59
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	4	0.59
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	20	0.59
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	9	0.59
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	16	0.59
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	20	0.59
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	15	0.59
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	16	0.59
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	12	0.59
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	18	0.59
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	6	0.59
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	18	0.59
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	7	0.59
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	9	0.59
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	12	0.59
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	13	0.59
(2,181)	1:51:A:VAL:O	1:55:A:LEU:N	10	0.59
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	17	0.59
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	17	0.59
(2,174)	1:44:A:SER:O	1:48:A:SER:N	17	0.59
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	10	0.59
(2,170)	1:40:A:THR:O	1:44:A:SER:N	4	0.59
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	4	0.59
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	18	0.59
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	3	0.59
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	17	0.59
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	3	0.59
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	13	0.59
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	2	0.59
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	11	0.59
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	9	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	16	0.58
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	4	0.58
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	17	0.58
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	18	0.58
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	1	0.58
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	9	0.58
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	3	0.58
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	2	0.58
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	1	0.58
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	4	0.58
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	8	0.58
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	11	0.58
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	3	0.58
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	18	0.58
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	1	0.58
(2,192)	1:78:A:MET:O	1:82:A:THR:N	9	0.58
(2,192)	1:78:A:MET:O	1:82:A:THR:N	19	0.58
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	4	0.58
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	8	0.58
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	5	0.58
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	8	0.58
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	14	0.58
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	15	0.58
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	19	0.58
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	16	0.58
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	6	0.58
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	8	0.58
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	5	0.58
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	15	0.58
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	5	0.58
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	9	0.58
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	11	0.58
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	15	0.58
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	19	0.58
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	18	0.58
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	20	0.58
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	2	0.57
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	8	0.57
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	16	0.57
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	13	0.57
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	2	0.57
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	12	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	20	0.57
(2,202)	1:88:A:THR:O	1:92:A:LEU:N	2	0.57
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	14	0.57
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	13	0.57
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	4	0.57
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	20	0.57
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	16	0.57
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	18	0.57
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	9	0.57
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	14	0.57
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	12	0.57
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	15	0.57
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	13	0.57
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	11	0.57
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	15	0.57
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	8	0.57
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	14	0.57
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	12	0.57
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	13	0.57
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	20	0.57
(2,161)	1:22:A:SER:O	1:26:A:VAL:N	17	0.57
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	11	0.57
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	18	0.57
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	2	0.57
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	3	0.57
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	16	0.57
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	17	0.57
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	10	0.57
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	18	0.56
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	6	0.56
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	5	0.56
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	19	0.56
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	7	0.56
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	5	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	3	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	4	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	5	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	6	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	8	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	10	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	11	0.56
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	13	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	16	0.56
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	12	0.56
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	17	0.56
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	10	0.56
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	19	0.56
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	9	0.56
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	1	0.56
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	2	0.56
(2,192)	1:78:A:MET:O	1:82:A:THR:N	4	0.56
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	16	0.56
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	19	0.56
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	20	0.56
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	8	0.56
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	5	0.56
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	20	0.56
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	15	0.56
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	17	0.56
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	2	0.56
(2,163)	1:24:A:LEU:O	1:28:A:VAL:N	9	0.56
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	20	0.56
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	2	0.56
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	3	0.56
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	16	0.56
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	1	0.55
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	2	0.55
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	10	0.55
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	20	0.55
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	15	0.55
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	7	0.55
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	14	0.55
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	15	0.55
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	17	0.55
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	18	0.55
(2,207)	1:111:A:ARG:O	1:115:A:TRP:N	19	0.55
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	4	0.55
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	10	0.55
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	11	0.55
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	18	0.55
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	14	0.55
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	18	0.55
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	6	0.55
(2,192)	1:78:A:MET:O	1:82:A:THR:N	10	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,192)	1:78:A:MET:O	1:82:A:THR:N	18	0.55
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	18	0.55
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	9	0.55
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	2	0.55
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	18	0.55
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	11	0.55
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	1	0.55
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	6	0.55
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	4	0.55
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	20	0.55
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	5	0.55
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	9	0.55
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	15	0.55
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	19	0.55
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	12	0.54
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	11	0.54
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	14	0.54
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	9	0.54
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	12	0.54
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	19	0.54
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	12	0.54
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	13	0.54
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	20	0.54
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	19	0.54
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	20	0.54
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	5	0.54
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	19	0.54
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	3	0.54
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	10	0.54
(2,170)	1:40:A:THR:O	1:44:A:SER:N	13	0.54
(2,170)	1:40:A:THR:O	1:44:A:SER:N	20	0.54
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	5	0.54
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	7	0.54
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	15	0.54
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	17	0.54
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	6	0.54
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	9	0.54
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	13	0.54
(1,453)	1:73:A:TYR:H	1:73:A:TYR:HD1	6	0.54
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	16	0.54
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	16	0.54
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	16	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	1	0.53
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	8	0.53
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	13	0.53
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	14	0.53
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	6	0.53
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	6	0.53
(2,192)	1:78:A:MET:O	1:82:A:THR:N	7	0.53
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	17	0.53
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	8	0.53
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	15	0.53
(2,182)	1:52:A:PHE:O	1:56:A:ILE:N	10	0.53
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	1	0.53
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	14	0.53
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	2	0.53
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	18	0.53
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	2	0.53
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	15	0.53
(2,170)	1:40:A:THR:O	1:44:A:SER:N	8	0.53
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	7	0.53
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	20	0.53
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	2	0.53
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	2	0.53
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	13	0.53
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	1	0.53
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	13	0.53
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	12	0.53
(1,859)	1:28:A:VAL:HG11	1:29:A:PHE:HE1	9	0.53
(1,859)	1:28:A:VAL:HG12	1:29:A:PHE:HE1	9	0.53
(1,859)	1:28:A:VAL:HG13	1:29:A:PHE:HE1	9	0.53
(1,859)	1:28:A:VAL:HG21	1:29:A:PHE:HE1	9	0.53
(1,859)	1:28:A:VAL:HG22	1:29:A:PHE:HE1	9	0.53
(1,859)	1:28:A:VAL:HG23	1:29:A:PHE:HE1	9	0.53
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	19	0.53
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	19	0.53
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	19	0.53
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	14	0.52
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	17	0.52
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	9	0.52
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	12	0.52
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	19	0.52
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	7	0.52
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	10	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	14	0.52
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	7	0.52
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	7	0.52
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	12	0.52
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	2	0.52
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	19	0.52
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	10	0.52
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	9	0.52
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	2	0.52
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	7	0.52
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	16	0.52
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	19	0.52
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	14	0.52
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	14	0.52
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	14	0.52
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	18	0.51
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	15	0.51
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	2	0.51
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	13	0.51
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	17	0.51
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	19	0.51
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	17	0.51
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	4	0.51
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	7	0.51
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	3	0.51
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	12	0.51
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	6	0.51
(2,170)	1:40:A:THR:O	1:44:A:SER:N	1	0.51
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	2	0.51
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	3	0.51
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	11	0.51
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	8	0.51
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	12	0.51
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	18	0.51
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	20	0.51
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	15	0.51
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	15	0.51
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	15	0.51
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	15	0.51
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	8	0.5
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	2	0.5
(2,214)	1:118:A:ILE:O	1:122:A:LEU:N	8	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	18	0.5
(2,192)	1:78:A:MET:O	1:82:A:THR:N	20	0.5
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	1	0.5
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	11	0.5
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	4	0.5
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	12	0.5
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	6	0.5
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	15	0.5
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	9	0.5
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	6	0.5
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	6	0.5
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	6	0.5
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	2	0.49
(2,215)	1:119:A:ILE:O	1:123:A:LEU:N	15	0.49
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	6	0.49
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	19	0.49
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	16	0.49
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	8	0.49
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	9	0.49
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	3	0.49
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	13	0.49
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	11	0.49
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	10	0.49
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	1	0.49
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	1	0.49
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	10	0.49
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	5	0.49
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	12	0.49
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	12	0.49
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	10	0.49
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	7	0.48
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	18	0.48
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	6	0.48
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	4	0.48
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	20	0.48
(2,198)	1:84:A:SER:O	1:88:A:THR:N	7	0.48
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	5	0.48
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	2	0.48
(2,196)	1:82:A:THR:O	1:86:A:VAL:N	11	0.48
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	8	0.48
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	17	0.48
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	8	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	10	0.48
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	3	0.48
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	3	0.48
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	15	0.48
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	6	0.48
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	7	0.48
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	2	0.48
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	3	0.48
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	1	0.48
(1,747)	1:90:A:PHE:H	1:90:A:PHE:HD1	14	0.48
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	10	0.47
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	9	0.47
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	10	0.47
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	5	0.47
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	4	0.47
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	16	0.47
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	7	0.47
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	11	0.47
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	12	0.47
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	18	0.47
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	19	0.47
(2,170)	1:40:A:THR:O	1:44:A:SER:N	3	0.47
(2,170)	1:40:A:THR:O	1:44:A:SER:N	17	0.47
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	17	0.47
(2,164)	1:25:A:THR:O	1:29:A:PHE:N	4	0.47
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	18	0.47
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	18	0.47
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	18	0.47
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	18	0.47
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	3	0.46
(2,192)	1:78:A:MET:O	1:82:A:THR:N	1	0.46
(2,192)	1:78:A:MET:O	1:82:A:THR:N	15	0.46
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	9	0.46
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	2	0.46
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	8	0.46
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	11	0.46
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	20	0.46
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	5	0.46
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	3	0.46
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	11	0.46
(1,859)	1:28:A:VAL:HG11	1:29:A:PHE:HE1	8	0.46
(1,859)	1:28:A:VAL:HG12	1:29:A:PHE:HE1	8	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:28:A:VAL:HG13	1:29:A:PHE:HE1	8	0.46
(1,859)	1:28:A:VAL:HG21	1:29:A:PHE:HE1	8	0.46
(1,859)	1:28:A:VAL:HG22	1:29:A:PHE:HE1	8	0.46
(1,859)	1:28:A:VAL:HG23	1:29:A:PHE:HE1	8	0.46
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	3	0.46
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	17	0.45
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	7	0.45
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	1	0.45
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	3	0.45
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	4	0.45
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	8	0.45
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	11	0.45
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	17	0.45
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	5	0.45
(2,192)	1:78:A:MET:O	1:82:A:THR:N	3	0.45
(2,174)	1:44:A:SER:O	1:48:A:SER:N	16	0.45
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	4	0.45
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	14	0.45
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	11	0.45
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	14	0.45
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	10	0.45
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	16	0.45
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	16	0.45
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	16	0.45
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	15	0.44
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	17	0.44
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	3	0.44
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	11	0.44
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	3	0.44
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	16	0.44
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	7	0.44
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	12	0.44
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	14	0.44
(2,192)	1:78:A:MET:O	1:82:A:THR:N	14	0.44
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	10	0.44
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	1	0.44
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	10	0.44
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	7	0.44
(2,170)	1:40:A:THR:O	1:44:A:SER:N	9	0.44
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	5	0.44
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	18	0.44
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	4	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:18:A:CYS:O	1:22:A:SER:N	17	0.44
(1,747)	1:90:A:PHE:H	1:90:A:PHE:HD1	7	0.44
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	3	0.43
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	8	0.43
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	10	0.43
(2,192)	1:78:A:MET:O	1:82:A:THR:N	11	0.43
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	6	0.43
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	10	0.43
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	6	0.43
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	17	0.43
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	20	0.43
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	16	0.43
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	12	0.43
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	3	0.43
(1,651)	1:129:A:PHE:H	1:129:A:PHE:HE1	6	0.43
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	11	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	1	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	2	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	3	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	4	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	5	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	6	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	7	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	8	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	9	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	10	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	11	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	12	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	13	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	14	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	15	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	16	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	17	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	18	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	19	0.42
(2,211)	1:115:A:TRP:O	1:119:A:ILE:N	20	0.42
(2,206)	1:110:A:ASP:O	1:114:A:LEU:N	7	0.42
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	9	0.42
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	11	0.42
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	15	0.42
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	2	0.42
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	8	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	19	0.42
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	2	0.42
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	18	0.42
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	7	0.42
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	13	0.42
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	16	0.42
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	17	0.42
(1,858)	1:28:A:VAL:HG11	1:29:A:PHE:HD1	19	0.42
(1,858)	1:28:A:VAL:HG12	1:29:A:PHE:HD1	19	0.42
(1,858)	1:28:A:VAL:HG13	1:29:A:PHE:HD1	19	0.42
(1,858)	1:28:A:VAL:HG21	1:29:A:PHE:HD1	19	0.42
(1,858)	1:28:A:VAL:HG22	1:29:A:PHE:HD1	19	0.42
(1,858)	1:28:A:VAL:HG23	1:29:A:PHE:HD1	19	0.42
(1,71)	1:85:A:ILE:HB	1:85:A:ILE:HD11	19	0.42
(1,71)	1:85:A:ILE:HB	1:85:A:ILE:HD12	19	0.42
(1,71)	1:85:A:ILE:HB	1:85:A:ILE:HD13	19	0.42
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	17	0.41
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	15	0.41
(2,193)	1:79:A:ILE:O	1:83:A:LEU:N	20	0.41
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	3	0.41
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	7	0.41
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	11	0.41
(2,170)	1:40:A:THR:O	1:44:A:SER:N	19	0.41
(2,159)	1:20:A:LEU:O	1:24:A:LEU:N	16	0.41
(2,198)	1:84:A:SER:O	1:88:A:THR:N	5	0.4
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	6	0.4
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	18	0.4
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	16	0.4
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	17	0.4
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	18	0.39
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	12	0.39
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	15	0.39
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	20	0.39
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	5	0.39
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	6	0.39
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	12	0.39
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	16	0.39
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	16	0.39
(2,152)	1:12:A:ILE:O	1:16:A:ILE:N	17	0.39
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	20	0.38
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	9	0.38
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	11	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	1	0.38
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	19	0.38
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	2	0.38
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	13	0.38
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	18	0.38
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	17	0.38
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	13	0.38
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	2	0.38
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	3	0.38
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	16	0.38
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	20	0.38
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	20	0.38
(2,169)	1:39:A:ILE:O	1:43:A:ILE:N	1	0.38
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	9	0.37
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	1	0.37
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	7	0.37
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	8	0.37
(2,198)	1:84:A:SER:O	1:88:A:THR:N	12	0.37
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	7	0.37
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	4	0.37
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	12	0.37
(2,183)	1:53:A:LEU:O	1:57:A:THR:N	14	0.37
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	15	0.37
(2,170)	1:40:A:THR:O	1:44:A:SER:N	2	0.37
(2,170)	1:40:A:THR:O	1:44:A:SER:N	15	0.37
(1,859)	1:28:A:VAL:HG11	1:29:A:PHE:HE1	10	0.37
(1,859)	1:28:A:VAL:HG12	1:29:A:PHE:HE1	10	0.37
(1,859)	1:28:A:VAL:HG13	1:29:A:PHE:HE1	10	0.37
(1,859)	1:28:A:VAL:HG21	1:29:A:PHE:HE1	10	0.37
(1,859)	1:28:A:VAL:HG22	1:29:A:PHE:HE1	10	0.37
(1,859)	1:28:A:VAL:HG23	1:29:A:PHE:HE1	10	0.37
(1,117)	1:6:A:LEU:HD21	1:10:A:TYR:HE1	10	0.37
(1,117)	1:6:A:LEU:HD22	1:10:A:TYR:HE1	10	0.37
(1,117)	1:6:A:LEU:HD23	1:10:A:TYR:HE1	10	0.37
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	16	0.36
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	8	0.36
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	9	0.36
(2,200)	1:86:A:VAL:O	1:90:A:PHE:N	10	0.36
(2,192)	1:78:A:MET:O	1:82:A:THR:N	5	0.36
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	3	0.36
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	4	0.36
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	14	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	18	0.36
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	19	0.35
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	17	0.35
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	19	0.35
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	12	0.35
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	10	0.35
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	12	0.35
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	1	0.35
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	6	0.35
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	14	0.35
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	16	0.35
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	18	0.35
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	20	0.35
(2,170)	1:40:A:THR:O	1:44:A:SER:N	18	0.35
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	13	0.35
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	16	0.35
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	7	0.35
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	1	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	2	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	3	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	4	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	5	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	6	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	7	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	8	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	10	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	12	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	13	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	14	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	15	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	16	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	17	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	18	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	19	0.34
(2,212)	1:116:A:MET:O	1:120:A:VAL:N	20	0.34
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	1	0.34
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	8	0.34
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	13	0.34
(2,192)	1:78:A:MET:O	1:82:A:THR:N	13	0.34
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	17	0.34
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	14	0.34
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	20	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	1	0.34
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	18	0.34
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	4	0.33
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	8	0.33
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	11	0.33
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	20	0.33
(2,170)	1:40:A:THR:O	1:44:A:SER:N	14	0.33
(2,217)	1:121:A:CYS:O	1:125:A:THR:N	13	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	2	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	3	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	4	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	5	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	10	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	14	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	16	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	17	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	19	0.32
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	20	0.32
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	2	0.32
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	5	0.32
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	3	0.32
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	15	0.32
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	4	0.32
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	4	0.32
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	6	0.32
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	10	0.32
(1,773)	1:29:A:PHE:HD1	1:30:A:TYR:H	8	0.32
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	17	0.32
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	13	0.31
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	6	0.31
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	8	0.31
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	9	0.31
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	12	0.31
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	13	0.31
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	15	0.31
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	11	0.31
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	1	0.31
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	1	0.31
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	6	0.31
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	7	0.31
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	20	0.31
(2,188)	1:74:A:LEU:O	1:78:A:MET:N	15	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	9	0.31
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	11	0.31
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	4	0.31
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	11	0.31
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	11	0.31
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	7	0.31
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	8	0.31
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	20	0.31
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	5	0.31
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	15	0.31
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	4	0.3
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	1	0.3
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	4	0.3
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	2	0.3
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	7	0.3
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	18	0.3
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	20	0.3
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	3	0.3
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	14	0.3
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	2	0.3
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	9	0.3
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	19	0.3
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	7	0.3
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	19	0.3
(1,14)	1:120:A:VAL:HG11	1:80:A:PHE:HD1	4	0.3
(1,14)	1:120:A:VAL:HG12	1:80:A:PHE:HD1	4	0.3
(1,14)	1:120:A:VAL:HG13	1:80:A:PHE:HD1	4	0.3
(2,208)	1:112:A:ILE:O	1:116:A:MET:N	11	0.29
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	5	0.29
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	11	0.29
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	20	0.29
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	3	0.29
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	15	0.29
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	9	0.29
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	13	0.29
(1,773)	1:29:A:PHE:HD1	1:30:A:TYR:H	19	0.29
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	1	0.29
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	1	0.29
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	1	0.29
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	7	0.28
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	20	0.28
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	5	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	1	0.28
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	4	0.28
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	3	0.28
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	4	0.28
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	8	0.28
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	20	0.28
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	9	0.28
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	12	0.28
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	5	0.28
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	13	0.28
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	17	0.28
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	10	0.28
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	1	0.28
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	16	0.28
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	14	0.27
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	3	0.27
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	13	0.27
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	20	0.27
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	9	0.27
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	8	0.27
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	9	0.27
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	13	0.27
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	15	0.27
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	19	0.27
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	17	0.27
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	3	0.27
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	5	0.27
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	10	0.26
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	13	0.26
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	11	0.26
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	13	0.26
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	6	0.26
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	1	0.26
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	9	0.26
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	10	0.26
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	19	0.26
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	20	0.26
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	4	0.26
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	14	0.26
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	5	0.25
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	19	0.25
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	7	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	12	0.25
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	19	0.25
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	4	0.25
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	12	0.25
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	11	0.25
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	3	0.25
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	7	0.25
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	11	0.25
(1,116)	1:6:A:LEU:HD11	1:10:A:TYR:HD1	18	0.25
(1,116)	1:6:A:LEU:HD12	1:10:A:TYR:HD1	18	0.25
(1,116)	1:6:A:LEU:HD13	1:10:A:TYR:HD1	18	0.25
(1,116)	1:6:A:LEU:HD21	1:10:A:TYR:HD1	18	0.25
(1,116)	1:6:A:LEU:HD22	1:10:A:TYR:HD1	18	0.25
(1,116)	1:6:A:LEU:HD23	1:10:A:TYR:HD1	18	0.25
(2,221)	1:125:A:THR:O	1:129:A:PHE:N	7	0.24
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	3	0.24
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	5	0.24
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	12	0.24
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	18	0.24
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	8	0.24
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	15	0.24
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	18	0.24
(2,186)	1:72:A:GLU:O	1:76:A:PHE:N	14	0.24
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	19	0.24
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	3	0.24
(2,170)	1:40:A:THR:O	1:44:A:SER:N	11	0.24
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	4	0.24
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	2	0.24
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	4	0.23
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	17	0.23
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	10	0.23
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	2	0.23
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	13	0.23
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	14	0.23
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	10	0.23
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	5	0.23
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	6	0.23
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	10	0.23
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	1	0.23
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	12	0.22
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	6	0.22
(2,199)	1:85:A:ILE:O	1:89:A:VAL:N	7	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	14	0.22
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	3	0.22
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	5	0.22
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	8	0.22
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	7	0.22
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	9	0.22
(2,172)	1:42:A:CYS:O	1:46:A:LEU:N	13	0.22
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	2	0.22
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	6	0.22
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	4	0.22
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	14	0.22
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	2	0.21
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	12	0.21
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	15	0.21
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	4	0.21
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	16	0.21
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	5	0.21
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	11	0.21
(2,204)	1:90:A:PHE:O	1:94:A:VAL:N	18	0.21
(2,195)	1:81:A:VAL:O	1:85:A:ILE:N	11	0.21
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	16	0.21
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	16	0.21
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	8	0.21
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	8	0.21
(2,166)	1:36:A:GLY:O	1:40:A:THR:N	5	0.21
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	9	0.21
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	1	0.21
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	4	0.21
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	8	0.21
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	20	0.21
(2,149)	1:9:A:PHE:O	1:13:A:ASN:N	1	0.21
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	13	0.2
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	15	0.2
(2,180)	1:50:A:THR:O	1:54:A:LEU:N	2	0.2
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	4	0.2
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	16	0.2
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	4	0.2
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	9	0.2
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	13	0.2
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	16	0.2
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	18	0.2
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	19	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:89:A:VAL:HG11	1:90:A:PHE:HE1	7	0.2
(1,980)	1:89:A:VAL:HG12	1:90:A:PHE:HE1	7	0.2
(1,980)	1:89:A:VAL:HG13	1:90:A:PHE:HE1	7	0.2
(1,980)	1:89:A:VAL:HG21	1:90:A:PHE:HE1	7	0.2
(1,980)	1:89:A:VAL:HG22	1:90:A:PHE:HE1	7	0.2
(1,980)	1:89:A:VAL:HG23	1:90:A:PHE:HE1	7	0.2
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	6	0.19
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	3	0.19
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	13	0.19
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	14	0.19
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	10	0.19
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	17	0.19
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	9	0.19
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	18	0.19
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	2	0.19
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	10	0.19
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	17	0.19
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	2	0.19
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	17	0.19
(1,773)	1:29:A:PHE:HD1	1:30:A:TYR:H	9	0.19
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	11	0.18
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	4	0.18
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	19	0.18
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	15	0.18
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	6	0.18
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	2	0.18
(2,162)	1:23:A:CYS:O	1:27:A:LEU:N	12	0.18
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	7	0.18
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	14	0.18
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	15	0.18
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	16	0.17
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	17	0.17
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	20	0.17
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	7	0.17
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	17	0.17
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	6	0.17
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	14	0.17
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	7	0.17
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	9	0.17
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	8	0.17
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	2	0.17
(2,167)	1:37:A:GLU:O	1:41:A:LEU:N	12	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	18	0.17
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	5	0.17
(1,858)	1:28:A:VAL:HG11	1:29:A:PHE:HD1	8	0.17
(1,858)	1:28:A:VAL:HG12	1:29:A:PHE:HD1	8	0.17
(1,858)	1:28:A:VAL:HG13	1:29:A:PHE:HD1	8	0.17
(1,858)	1:28:A:VAL:HG21	1:29:A:PHE:HD1	8	0.17
(1,858)	1:28:A:VAL:HG22	1:29:A:PHE:HD1	8	0.17
(1,858)	1:28:A:VAL:HG23	1:29:A:PHE:HD1	8	0.17
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	4	0.16
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	10	0.16
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	12	0.16
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	7	0.16
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	12	0.16
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	8	0.16
(2,179)	1:49:A:LEU:O	1:53:A:LEU:N	7	0.16
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	17	0.16
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	3	0.16
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	11	0.16
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	15	0.16
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	16	0.16
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	19	0.16
(2,170)	1:40:A:THR:O	1:44:A:SER:N	16	0.16
(2,168)	1:38:A:LYS:O	1:42:A:CYS:N	18	0.16
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	8	0.16
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	17	0.16
(2,162)	1:23:A:CYS:O	1:27:A:LEU:N	9	0.16
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	3	0.16
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	9	0.15
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	16	0.15
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	17	0.15
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	13	0.15
(2,194)	1:80:A:PHE:O	1:84:A:SER:N	4	0.15
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	3	0.15
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	5	0.15
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	12	0.15
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	3	0.15
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	12	0.15
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	3	0.15
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	20	0.15
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	5	0.15
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	7	0.15
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	9	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:54:A:LEU:O	1:58:A:GLU:N	19	0.15
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	11	0.15
(2,165)	1:26:A:VAL:O	1:30:A:TYR:N	11	0.15
(1,858)	1:28:A:VAL:HG11	1:29:A:PHE:HD1	9	0.15
(1,858)	1:28:A:VAL:HG12	1:29:A:PHE:HD1	9	0.15
(1,858)	1:28:A:VAL:HG13	1:29:A:PHE:HD1	9	0.15
(1,858)	1:28:A:VAL:HG21	1:29:A:PHE:HD1	9	0.15
(1,858)	1:28:A:VAL:HG22	1:29:A:PHE:HD1	9	0.15
(1,858)	1:28:A:VAL:HG23	1:29:A:PHE:HD1	9	0.15
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	5	0.14
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	5	0.14
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	12	0.14
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	1	0.14
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	2	0.14
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	7	0.14
(2,218)	1:122:A:LEU:O	1:126:A:VAL:N	13	0.14
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	11	0.14
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	14	0.14
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	10	0.14
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	5	0.14
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	17	0.14
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	3	0.14
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	7	0.14
(2,174)	1:44:A:SER:O	1:48:A:SER:N	3	0.14
(2,173)	1:43:A:ILE:O	1:47:A:LEU:N	15	0.14
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	19	0.14
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	11	0.14
(2,222)	1:126:A:VAL:O	1:130:A:LEU:N	2	0.13
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	8	0.13
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	19	0.13
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	8	0.13
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	18	0.13
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	20	0.13
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	1	0.13
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	2	0.13
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	12	0.13
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	14	0.13
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	18	0.13
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	2	0.13
(1,773)	1:29:A:PHE:HD1	1:30:A:TYR:H	10	0.13
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	19	0.13
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	19	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	19	0.13
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	2	0.12
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	18	0.12
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	17	0.12
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	7	0.12
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	15	0.12
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	19	0.12
(2,201)	1:87:A:ILE:O	1:91:A:VAL:N	13	0.12
(2,198)	1:84:A:SER:O	1:88:A:THR:N	13	0.12
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	12	0.12
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	13	0.12
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	18	0.12
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	1	0.12
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	16	0.12
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	1	0.12
(2,171)	1:41:A:LEU:O	1:45:A:VAL:N	13	0.12
(2,156)	1:17:A:PRO:O	1:21:A:ILE:N	12	0.12
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	10	0.12
(1,274)	1:129:A:PHE:H	1:129:A:PHE:HD1	8	0.12
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG11	6	0.12
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG12	6	0.12
(1,26)	1:80:A:PHE:HE1	1:120:A:VAL:HG13	6	0.12
(2,220)	1:124:A:GLY:O	1:128:A:LEU:N	10	0.11
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	20	0.11
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	6	0.11
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	9	0.11
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	18	0.11
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	19	0.11
(2,198)	1:84:A:SER:O	1:88:A:THR:N	11	0.11
(2,198)	1:84:A:SER:O	1:88:A:THR:N	20	0.11
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	6	0.11
(2,192)	1:78:A:MET:O	1:82:A:THR:N	12	0.11
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	16	0.11
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	18	0.11
(2,187)	1:73:A:TYR:O	1:77:A:THR:N	11	0.11
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	16	0.11
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	13	0.11
(2,170)	1:40:A:THR:O	1:44:A:SER:N	5	0.11
(2,162)	1:23:A:CYS:O	1:27:A:LEU:N	7	0.11
(2,158)	1:19:A:LEU:O	1:23:A:CYS:N	7	0.11
(2,158)	1:19:A:LEU:O	1:23:A:CYS:N	18	0.11
(2,151)	1:11:A:THR:O	1:15:A:ILE:N	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	6	0.11
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	20	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	1	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	2	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	3	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	4	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	5	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	6	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	7	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	8	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	9	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	10	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	11	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	12	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	13	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	14	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	15	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	16	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	17	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	18	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	19	0.11
(1,428)	1:6:A:LEU:HB2	1:7:A:PRO:HD3	20	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB1	16	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB2	16	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB3	16	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB1	17	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB2	17	0.11
(1,155)	1:132:A:PRO:HB3	1:135:A:ALA:HB3	17	0.11
(2,219)	1:123:A:LEU:O	1:127:A:GLY:N	9	0.1
(2,216)	1:120:A:VAL:O	1:124:A:GLY:N	13	0.1
(2,205)	1:109:A:ILE:O	1:113:A:PHE:N	17	0.1
(2,203)	1:89:A:VAL:O	1:93:A:ASN:N	17	0.1
(2,197)	1:83:A:LEU:O	1:87:A:ILE:N	4	0.1
(2,191)	1:77:A:THR:O	1:81:A:VAL:N	1	0.1
(2,190)	1:76:A:PHE:O	1:80:A:PHE:N	7	0.1
(2,189)	1:75:A:LEU:O	1:79:A:ILE:N	1	0.1
(2,178)	1:48:A:SER:O	1:52:A:PHE:N	20	0.1
(2,177)	1:47:A:LEU:O	1:51:A:VAL:N	12	0.1
(2,176)	1:46:A:LEU:O	1:50:A:THR:N	7	0.1
(2,175)	1:45:A:VAL:O	1:49:A:LEU:N	9	0.1
(2,150)	1:10:A:TYR:O	1:14:A:LEU:N	8	0.1

10 Dihedral-angle violation analysis [i](#)

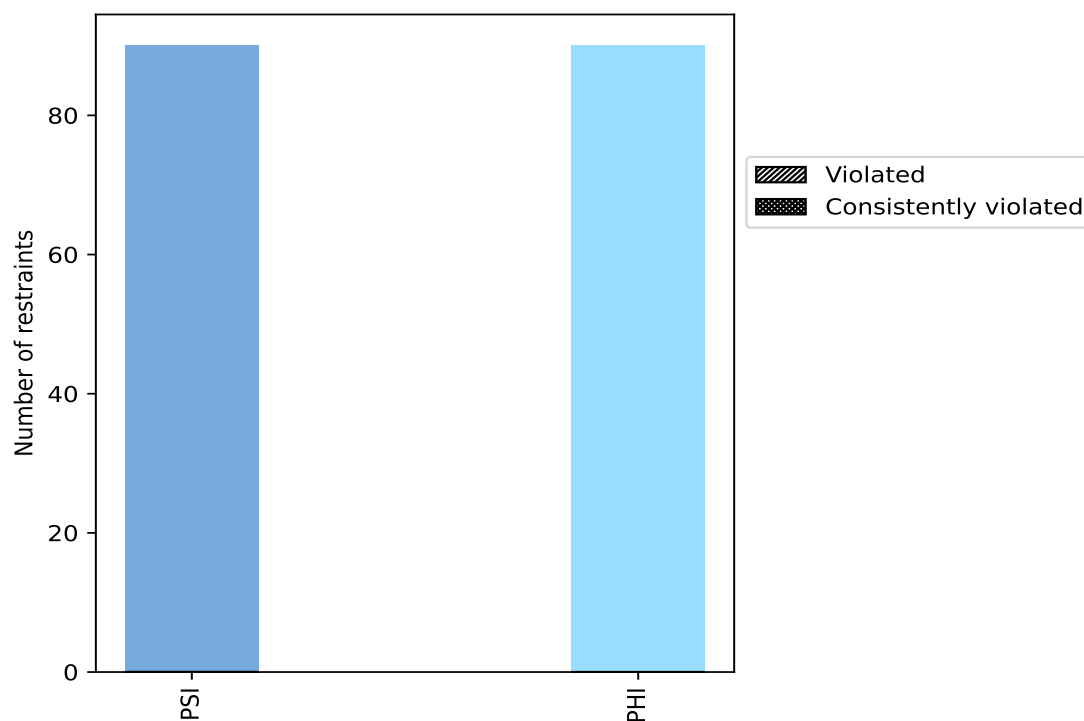
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	90	50.0	0	0.0	0.0	0	0.0	0.0
PHI	90	50.0	0	0.0	0.0	0	0.0	0.0
Total	180	100.0	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

No violations found

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

No violations found

10.5 All violated dihedral-angle restraints [i](#)

No violations found