Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:51 PM EDT

PDB ID	:	2K6S
BMRB ID	:	15880
Title	:	Structure of Rab11-FIP2 C-terminal Coiled-coil Domain
Authors	:	Wei, J.; Liu, Y.; Baleja, J.D.
Deposited on	:	2008-07-18

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 (i) 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 (1)) were used in the production of this report:

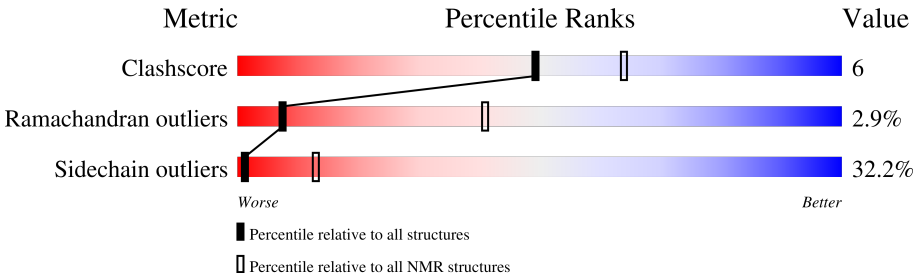
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 32%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	41	59% 37% 5%
1	B	41	61% 34% 5%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 23 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:1-A:41, B:1-B:41 (82)	0.41	23

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	3, 5, 6, 7, 8, 9, 11, 12, 13, 16, 17, 20, 22, 23, 25, 26, 30
2	1, 2, 4, 19, 21, 24
3	27, 28, 29
4	10, 14
Single-model clusters	15; 18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1433 atoms, of which 732 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Rab11fip2 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	41	716	221	366	62	66	1	0
1	B	41	717	221	366	62	67	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q7L804
B	1	GLY	-	expression tag	UNP Q7L804

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

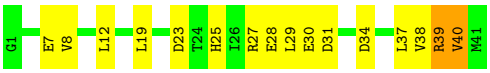
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Rab11fip2 protein

Chain A:

• Molecule 1: Rab11fip2 protein

Chain B:



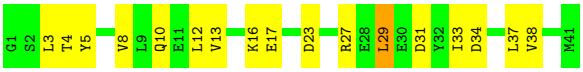
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

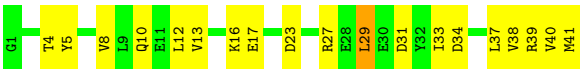
• Molecule 1: Rab11fip2 protein

Chain A:



• Molecule 1: Rab11fip2 protein

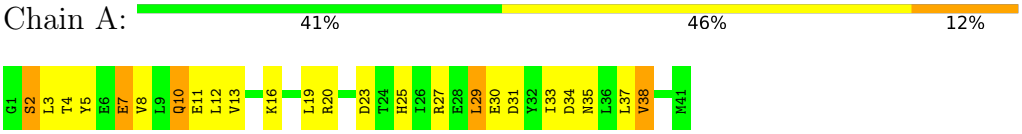
Chain B:



4.2.2 Score per residue for model 2

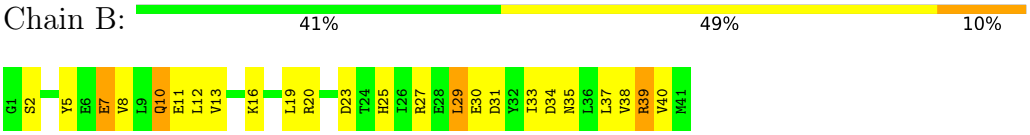
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

Chain B:



4.2.3 Score per residue for model 3

- Molecule 1: Rab11fip2 protein

Chain A:

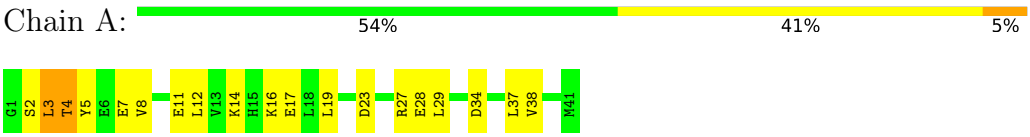
- Molecule 1: Rab11fip2 protein

Chain B:

4.2.4 Score per residue for model 4

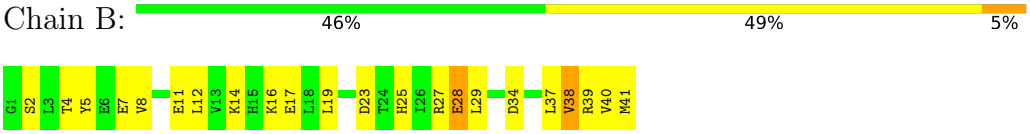
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

Chain B:



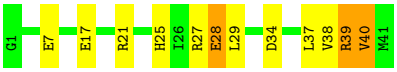
4.2.5 Score per residue for model 5

- Molecule 1: Rab11fip2 protein

Chain A:

- Molecule 1: Rab11fip2 protein

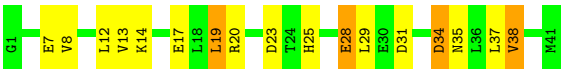
Chain B:



4.2.6 Score per residue for model 6

- Molecule 1: Rab11fip2 protein

Chain A:



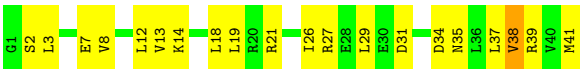
- Molecule 1: Rab11fip2 protein

Chain B:

4.2.7 Score per residue for model 7

- Molecule 1: Rab11fip2 protein

Chain A:



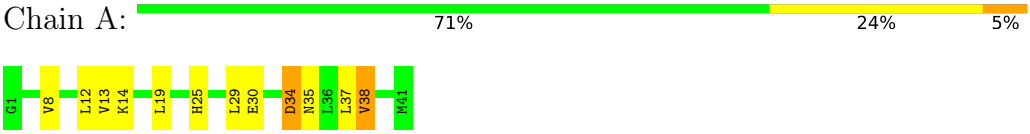
- Molecule 1: Rab11fip2 protein

Chain B:

4.2.8 Score per residue for model 8

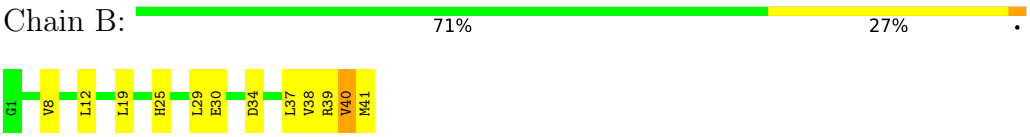
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

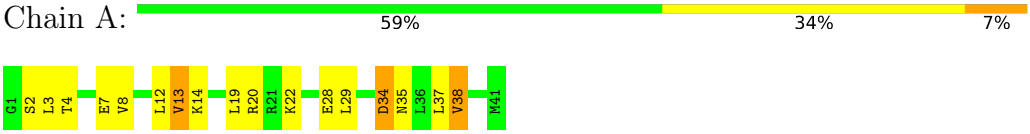
Chain B:



4.2.9 Score per residue for model 9

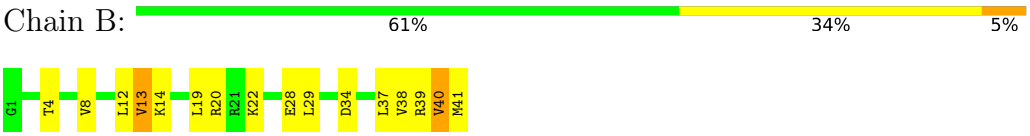
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

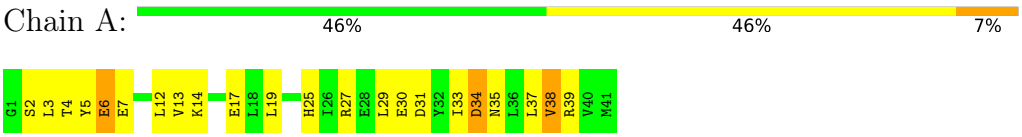
Chain B:



4.2.10 Score per residue for model 10

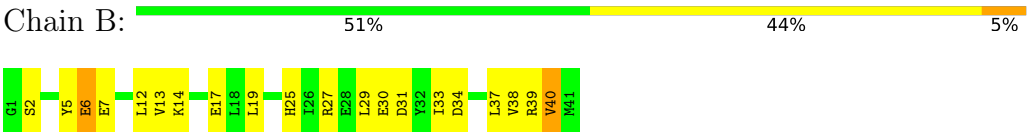
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

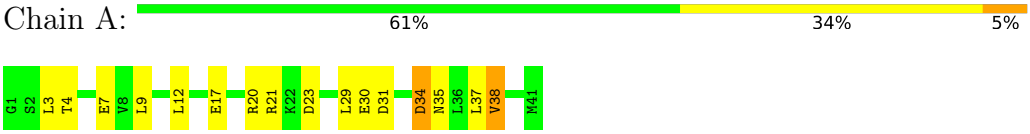
Chain B:



4.2.11 Score per residue for model 11

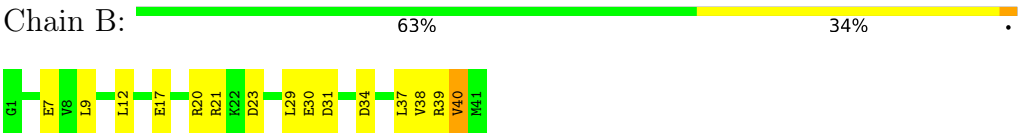
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

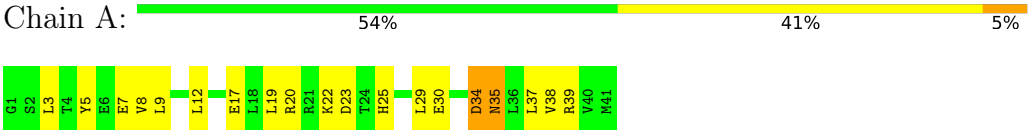
Chain B:



4.2.12 Score per residue for model 12

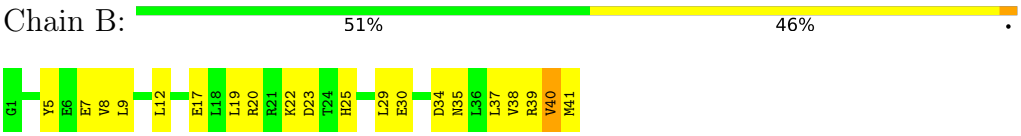
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

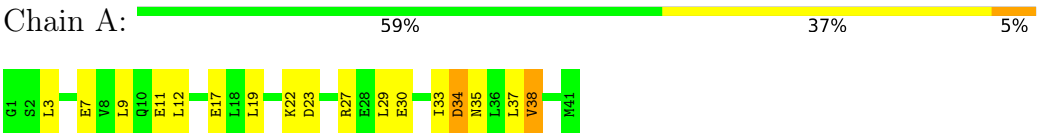
Chain B:



4.2.13 Score per residue for model 13

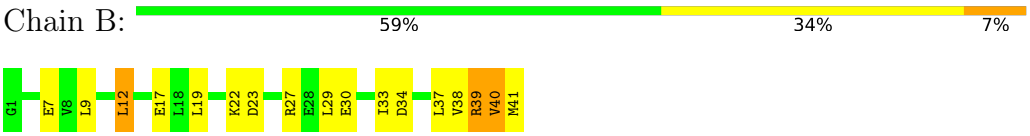
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

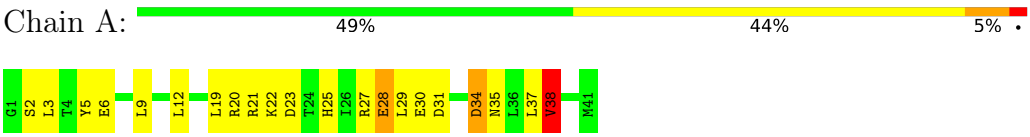
Chain B:



4.2.14 Score per residue for model 14

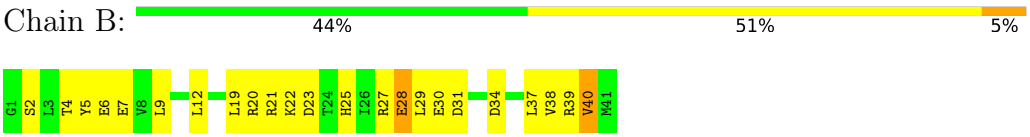
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

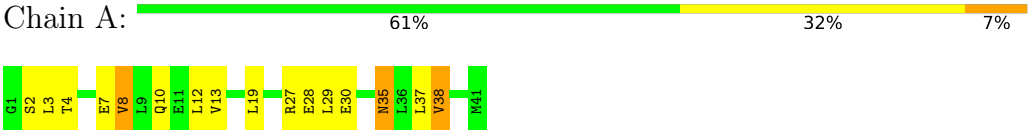
Chain B:



4.2.15 Score per residue for model 15

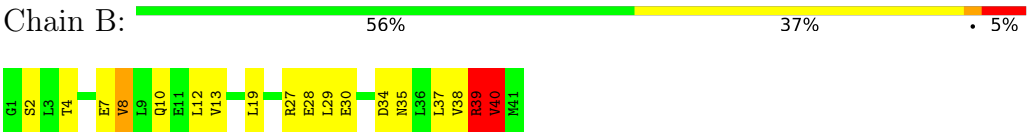
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

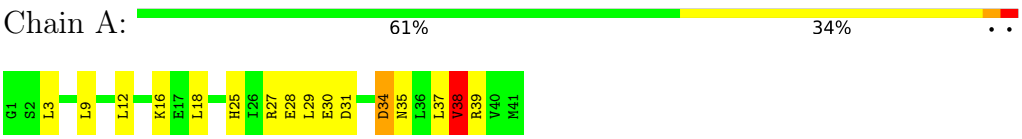
Chain B:



4.2.16 Score per residue for model 16

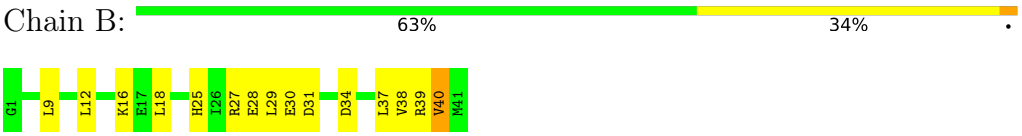
- Molecule 1: Rab11fip2 protein

Chain A:



- Molecule 1: Rab11fip2 protein

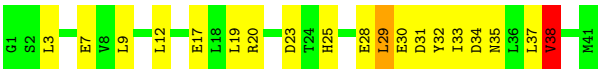
Chain B:



4.2.17 Score per residue for model 17

- Molecule 1: Rab11fip2 protein

Chain A: 54% 41%



- Molecule 1: Rab11fip2 protein

Chain B: 56% 37% 7%

4.2.18 Score per residue for model 18

- Molecule 1: Rab11fip2 protein

Chain A: 44% 44% 12%

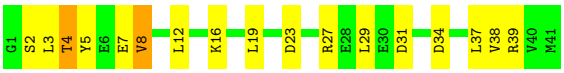
- Molecule 1: Rab11fip2 protein

Chain B: 51% 41% 7%

4.2.19 Score per residue for model 19

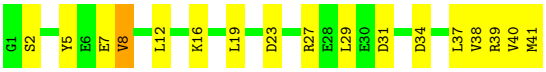
- Molecule 1: Rab11fip2 protein

Chain A: 59% 37% 5%



- Molecule 1: Rab11fip2 protein

Chain B: 59% 39%



4.2.20 Score per residue for model 20

- Molecule 1: Rab11fip2 protein

Chain A: 56% 37% 7%

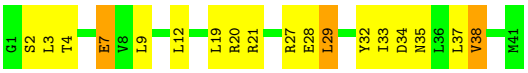
- Molecule 1: Rab11fip2 protein

Chain B: 59% 37% 5%

4.2.21 Score per residue for model 21

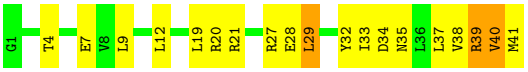
- Molecule 1: Rab11fip2 protein

Chain A: 56% 37% 7%



- Molecule 1: Rab11fip2 protein

Chain B: 54% 39% 7%



4.2.22 Score per residue for model 22

- Molecule 1: Rab11fip2 protein

Chain A: 59% 37%

- Molecule 1: Rab11fip2 protein

Chain B: 51% 44% 5%

4.2.23 Score per residue for model 23 (medoid)

- Molecule 1: Rab11fip2 protein

Chain A: 54% 39% 7%

G1 S2 L3 E7 V8 L12 V13 K14 L19 K22 D23 T24 H25 E28 L29 E30 D31 D34 N35 L36 L37 V38 M41

- Molecule 1: Rab11fip2 protein

Chain B: 59% 37% 5%

G1 V8 L12 V13 K14 L19 K22 D23 T24 H25 E28 L29 E30 D31 D34 L37 V38 R39 V40 M41

4.2.24 Score per residue for model 24

- Molecule 1: Rab11fip2 protein

Chain A: 63% 34% •

G1 S2 L3 T4 Y5 E6 E7 V8 L12 E28 L29 E30 D31 D34 N35 L36 L37 V38 M41

- Molecule 1: Rab11fip2 protein

Chain B: 63% 32% 5%

G1 T4 Y5 E6 E7 V8 L12 E28 L29 E30 D31 D34 L37 V38 R39 V40 M41

4.2.25 Score per residue for model 25

- Molecule 1: Rab11fip2 protein

Chain A: 59% 37% 5%

G1 S2 L3 T4 Y5 E6 E7 L12 E17 L18 L19 K22 H25 E28 L29 E30 D31 D34 N35 L36 L37 V38 R39 V40 M41

- Molecule 1: Rab11fip2 protein

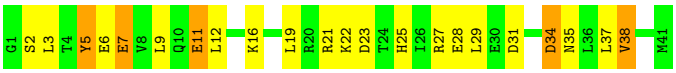
Chain B: 63% 34% •

G1 Y5 E6 E7 L12 E17 L18 L19 K22 H25 E28 L29 E30 D31 D34 L37 V38 R39 V40 M41

4.2.26 Score per residue for model 26

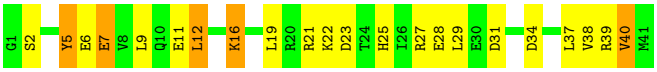
- Molecule 1: Rab11fip2 protein

Chain A: 46% 41% 12%



- Molecule 1: Rab11fip2 protein

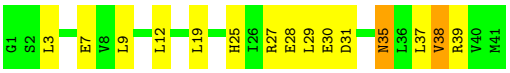
Chain B: 46% 41% 12%



4.2.27 Score per residue for model 27

- Molecule 1: Rab11fip2 protein

Chain A: 63% 32% 5%



- Molecule 1: Rab11fip2 protein

Chain B: 56% 39% 5%

4.2.28 Score per residue for model 28

- Molecule 1: Rab11fip2 protein

Chain A: 59% 37% 5%

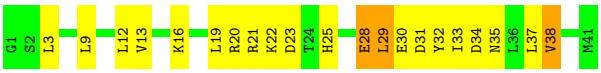
- Molecule 1: Rab11fip2 protein

Chain B: 61% 29% 5% 5%

4.2.29 Score per residue for model 29

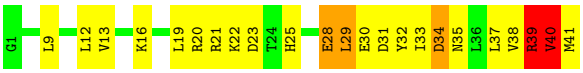
- Molecule 1: Rab11fip2 protein

Chain A: 49% 44% 7%



- Molecule 1: Rab11fip2 protein

Chain B: 44% 44% 7% 5%



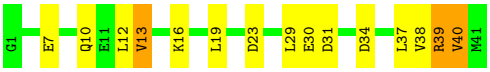
4.2.30 Score per residue for model 30

- Molecule 1: Rab11fip2 protein

Chain A: 59% 34% 5%

- Molecule 1: Rab11fip2 protein

Chain B: 63% 29% 7%



5 Refinement protocol and experimental data overview (i)

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

Of the 30 calculated structures, 30 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	refinement	1.1

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	401
Number of shifts mapped to atoms	401
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	32%

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	350	366	364	5±2
1	B	351	366	364	5±3
All	All	21030	21960	21840	261

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:19:LEU:HD21	1:B:19:LEU:HD21	0.93	1.41	9	4
1:A:8:VAL:HG11	1:B:8:VAL:HG11	0.92	1.42	19	11
1:B:38:VAL:O	1:B:38:VAL:HG12	0.67	1.88	15	4
1:A:35:ASN:HA	1:A:38:VAL:HG12	0.67	1.67	20	26
1:A:10:GLN:O	1:A:13:VAL:HG12	0.65	1.92	2	3
1:B:39:ARG:O	1:B:40:VAL:HG13	0.65	1.92	28	4
1:B:10:GLN:O	1:B:13:VAL:HG12	0.63	1.92	2	3
1:A:35:ASN:HB3	1:A:40:VAL:HG12	0.63	1.70	18	1
1:A:29:LEU:HD23	1:A:33:ILE:HD11	0.62	1.72	2	4
1:A:19:LEU:HD11	1:B:19:LEU:HD11	0.61	1.70	6	1
1:B:29:LEU:HD23	1:B:33:ILE:HD11	0.61	1.72	2	4
1:B:34:ASP:O	1:B:38:VAL:HG23	0.60	1.95	27	4
1:B:5:TYR:O	1:B:8:VAL:HG12	0.58	1.99	19	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:TYR:O	1:A:8:VAL:HG12	0.56	1.99	19	6
1:A:11:GLU:HB3	1:B:12:LEU:HD21	0.56	1.78	26	2
1:A:8:VAL:HG11	1:B:8:VAL:CG1	0.54	2.33	23	4
1:B:34:ASP:C	1:B:38:VAL:HG23	0.52	2.25	27	4
1:B:39:ARG:C	1:B:40:VAL:HG22	0.52	2.25	27	4
1:B:28:GLU:HG3	1:B:29:LEU:N	0.52	2.19	3	3
1:A:2:SER:O	1:A:7:GLU:HB2	0.51	2.06	15	9
1:B:38:VAL:O	1:B:38:VAL:CG1	0.51	2.59	15	1
1:A:28:GLU:HG3	1:A:29:LEU:N	0.51	2.19	3	3
1:A:5:TYR:HB2	1:B:5:TYR:HB2	0.51	1.81	10	3
1:A:13:VAL:CG1	1:A:14:LYS:N	0.50	2.74	9	1
1:B:13:VAL:CG1	1:B:14:LYS:N	0.49	2.75	9	1
1:A:3:LEU:O	1:A:4:THR:HG23	0.49	2.07	10	1
1:B:25:HIS:O	1:B:28:GLU:HG3	0.49	2.08	27	10
1:A:25:HIS:O	1:A:28:GLU:HG3	0.48	2.08	27	9
1:B:2:SER:O	1:B:7:GLU:HB2	0.48	2.08	15	6
1:A:19:LEU:HD21	1:B:19:LEU:CD2	0.48	2.38	4	1
1:A:34:ASP:O	1:A:38:VAL:HB	0.48	2.08	16	19
1:A:35:ASN:HA	1:A:38:VAL:CG1	0.48	2.38	15	2
1:B:2:SER:O	1:B:7:GLU:CB	0.47	2.63	10	1
1:B:13:VAL:HG13	1:B:14:LYS:N	0.47	2.25	23	6
1:A:14:LYS:O	1:A:17:GLU:HG2	0.46	2.11	4	1
1:A:2:SER:O	1:A:4:THR:N	0.46	2.48	4	5
1:A:13:VAL:HG13	1:A:14:LYS:N	0.46	2.25	6	6
1:B:40:VAL:HG12	1:B:40:VAL:O	0.46	2.11	24	6
1:B:14:LYS:O	1:B:17:GLU:HG2	0.46	2.11	4	1
1:B:5:TYR:CE2	1:B:9:LEU:HD11	0.46	2.46	12	1
1:B:35:ASN:HA	1:B:38:VAL:CG2	0.45	2.41	29	1
1:A:2:SER:O	1:A:7:GLU:CB	0.45	2.64	10	1
1:B:35:ASN:O	1:B:38:VAL:HG23	0.45	2.12	21	2
1:B:7:GLU:O	1:B:11:GLU:HG3	0.45	2.11	4	1
1:B:38:VAL:O	1:B:40:VAL:N	0.45	2.50	8	25
1:A:10:GLN:HA	1:A:13:VAL:HG12	0.45	1.88	15	1
1:B:10:GLN:HA	1:B:13:VAL:HG12	0.45	1.88	15	1
1:B:38:VAL:HG12	1:B:39:ARG:H	0.45	1.71	18	1
1:A:19:LEU:CD1	1:B:19:LEU:HD11	0.45	2.41	6	1
1:A:5:TYR:CE2	1:A:9:LEU:HD11	0.45	2.46	12	1
1:A:25:HIS:O	1:A:28:GLU:HG2	0.44	2.12	16	2
1:B:25:HIS:O	1:B:28:GLU:HG2	0.44	2.12	16	2
1:A:8:VAL:HG21	1:B:8:VAL:HG13	0.44	1.88	18	1
1:A:7:GLU:O	1:A:11:GLU:HG3	0.44	2.11	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:VAL:HG13	1:A:39:ARG:N	0.44	2.27	20	4
1:B:38:VAL:HG12	1:B:39:ARG:N	0.44	2.28	18	1
1:B:35:ASN:CA	1:B:38:VAL:HG23	0.43	2.42	29	1
1:A:19:LEU:CD2	1:B:19:LEU:HD21	0.42	2.40	4	2
1:B:33:ILE:HG22	1:B:33:ILE:O	0.42	2.14	13	1
1:B:2:SER:O	1:B:4:THR:N	0.42	2.52	14	2
1:A:33:ILE:HG22	1:A:33:ILE:O	0.42	2.15	13	2
1:A:38:VAL:HG22	1:A:39:ARG:H	0.42	1.74	25	1
1:B:8:VAL:CG1	1:B:9:LEU:N	0.41	2.83	18	1
1:B:28:GLU:OE2	1:B:29:LEU:HD12	0.41	2.16	18	1
1:A:28:GLU:OE2	1:A:29:LEU:HD12	0.41	2.16	18	1
1:B:33:ILE:O	1:B:33:ILE:HG22	0.41	2.15	17	1
1:A:8:VAL:CG1	1:A:9:LEU:N	0.41	2.83	18	1
1:A:8:VAL:HG13	1:B:8:VAL:HG21	0.41	1.91	19	1
1:B:39:ARG:HD2	1:B:39:ARG:O	0.41	2.16	21	1
1:B:12:LEU:HD12	1:B:16:LYS:HD2	0.41	1.93	26	1
1:A:5:TYR:O	1:A:7:GLU:N	0.40	2.54	10	1
1:B:5:TYR:O	1:B:7:GLU:N	0.40	2.54	10	1
1:B:8:VAL:O	1:B:11:GLU:HB2	0.40	2.16	3	1
1:B:39:ARG:O	1:B:40:VAL:HG22	0.40	2.16	27	1
1:A:8:VAL:O	1:A:11:GLU:HB2	0.40	2.16	3	1
1:A:13:VAL:HG13	1:A:14:LYS:H	0.40	1.76	6	1
1:A:35:ASN:CA	1:A:38:VAL:HG12	0.40	2.46	8	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	39/41 (95%)	33±2 (84±4%)	6±2 (15±4%)	0±1 (1±1%)	24	71
1	B	39/41 (95%)	31±2 (79±4%)	6±2 (15±4%)	2±0 (5±1%)	4	25
All	All	2340/2460 (95%)	1912 (82%)	360 (15%)	68 (3%)	7	41

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	39	ARG	29
1	B	40	VAL	25
1	A	38	VAL	6
1	B	38	VAL	3
1	A	6	GLU	2
1	B	6	GLU	2
1	A	3	LEU	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	40/40 (100%)	26±3 (66±7%)	14±3 (34±7%)	1 11
1	B	40/40 (100%)	28±3 (69±6%)	12±3 (31±6%)	1 15
All	All	2400/2400 (100%)	1628 (68%)	772 (32%)	1 13

All 69 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	29	LEU	30
1	A	37	LEU	30
1	B	29	LEU	30
1	B	37	LEU	30
1	A	38	VAL	28
1	A	12	LEU	27
1	B	12	LEU	27
1	A	3	LEU	26
1	A	34	ASP	26
1	B	34	ASP	26
1	A	31	ASP	20
1	B	31	ASP	20
1	A	19	LEU	20
1	B	19	LEU	20
1	A	30	GLU	19
1	B	30	GLU	19
1	A	7	GLU	17
1	B	7	GLU	17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	23	ASP	16
1	A	27	ARG	16
1	B	23	ASP	16
1	B	27	ARG	16
1	A	28	GLU	15
1	B	28	GLU	15
1	B	39	ARG	14
1	B	41	MET	13
1	A	17	GLU	11
1	B	17	GLU	11
1	A	20	ARG	10
1	B	20	ARG	10
1	A	21	ARG	10
1	B	21	ARG	10
1	A	4	THR	9
1	A	16	LYS	9
1	B	16	LYS	9
1	A	22	LYS	9
1	B	22	LYS	9
1	A	9	LEU	9
1	B	9	LEU	9
1	B	4	THR	7
1	A	25	HIS	7
1	B	25	HIS	7
1	A	39	ARG	7
1	A	2	SER	6
1	A	11	GLU	4
1	B	11	GLU	4
1	B	40	VAL	4
1	A	18	LEU	3
1	B	18	LEU	3
1	A	13	VAL	3
1	B	13	VAL	3
1	A	6	GLU	3
1	B	6	GLU	3
1	A	35	ASN	3
1	B	35	ASN	3
1	A	32	TYR	3
1	B	32	TYR	3
1	A	33	ILE	2
1	B	33	ILE	2
1	A	8	VAL	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	8	VAL	2
1	A	5	TYR	2
1	B	5	TYR	2
1	A	10	GLN	1
1	B	10	GLN	1
1	A	26	ILE	1
1	A	41	MET	1
1	B	26	ILE	1
1	B	2	SER	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 monosaccharides 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 (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 32% for the well-defined parts and 32% 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 (i)

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	401
Number of shifts mapped to atoms	401
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	35	-1.20 ± 0.42	Should be checked
$^{13}C_{\beta}$	30	0.34 ± 0.20	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	36	0.37 ± 0.40	None needed (< 0.5 ppm)

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 32%, i.e. 401 atoms were assigned a chemical shift out of a possible 1258. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	146/412 (35%)	75/166 (45%)	35/164 (21%)	36/82 (44%)
Sidechain	244/778 (31%)	213/502 (42%)	30/242 (12%)	1/34 (3%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	11/68 (16%)	11/32 (34%)	0/28 (0%)	0/8 (0%)
Overall	401/1258 (32%)	299/700 (43%)	65/434 (15%)	37/124 (30%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 401 atoms were assigned a chemical shift out of a possible 1258. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	146/412 (35%)	75/166 (45%)	35/164 (21%)	36/82 (44%)
Sidechain	244/778 (31%)	213/502 (42%)	30/242 (12%)	1/34 (3%)
Aromatic	11/68 (16%)	11/32 (34%)	0/28 (0%)	0/8 (0%)
Overall	401/1258 (32%)	299/700 (43%)	65/434 (15%)	37/124 (30%)

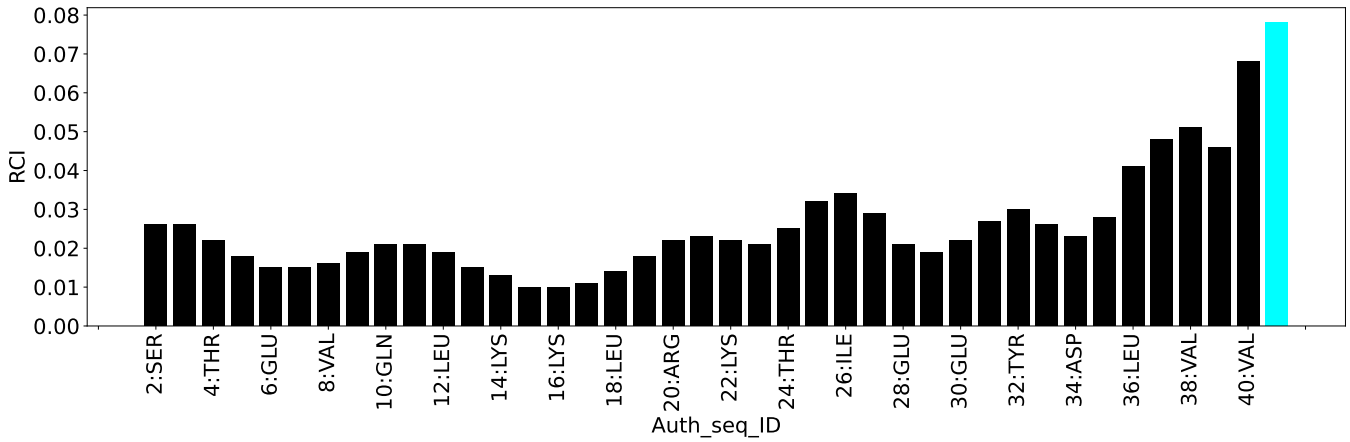
7.1.4 Statistically unusual chemical shifts (i)

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 (i)

8.1 Conformationally restricting restraints (i)

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	1081
Intra-residue (|i-j|=0)	379
Sequential (|i-j|=1)	185
Medium range (|i-j|>1 and |i-j|<5)	445
Long range (|i-j|≥5)	0
Inter-chain	72
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	153
Number of unmapped restraints	0
Number of restraints per residue	15.0
Number of long range restraints per residue[1]	0.0

[1]Long 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 (i)

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 (i)

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)	0.8	0.18
0.2-0.5 (Medium)	1.3	0.48
>0.5 (Large)	6.3	1.17

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	3.2	9.9
10.0-20.0 (Medium)	1.4	20.0
>20.0 (Large)	3.5	24.9

9 Distance violation analysis (i)

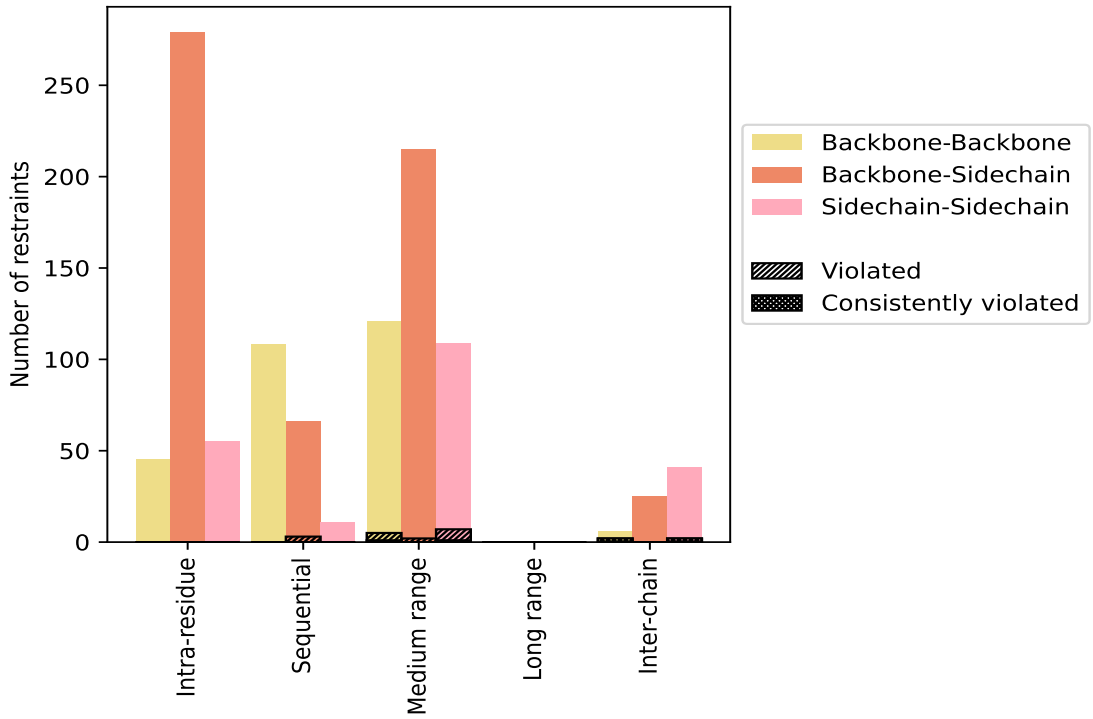
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	379	35.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	45	4.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	279	25.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	55	5.1	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	185	17.1	3	1.6	0.3	0	0.0	0.0
Backbone-Backbone	108	10.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	66	6.1	3	4.5	0.3	0	0.0	0.0
Sidechain-Sidechain	11	1.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	445	41.2	14	3.1	1.3	2	0.4	0.2
Backbone-Backbone	121	11.2	5	4.1	0.5	1	0.8	0.1
Backbone-Sidechain	215	19.9	2	0.9	0.2	0	0.0	0.0
Sidechain-Sidechain	109	10.1	7	6.4	0.6	1	0.9	0.1
Long range (|i-j|≥5)	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
Inter-chain	72	6.7	4	5.6	0.4	4	5.6	0.4
Backbone-Backbone	6	0.6	2	33.3	0.2	2	33.3	0.2
Backbone-Sidechain	25	2.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	41	3.8	2	4.9	0.2	2	4.9	0.2
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1081	100.0	21	1.9	1.9	6	0.6	0.6
Backbone-Backbone	280	25.9	7	2.5	0.6	3	1.1	0.3
Backbone-Sidechain	585	54.1	5	0.9	0.5	0	0.0	0.0
Sidechain-Sidechain	216	20.0	9	4.2	0.8	3	1.4	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	0	1	7	0	4	12	0.58	1.11	0.36	0.52
2	0	1	3	0	4	8	0.7	1.12	0.38	0.7
3	0	0	5	0	4	9	0.89	1.12	0.25	1.04
4	0	0	2	0	4	6	0.9	1.12	0.22	0.9
5	0	0	2	0	4	6	1.07	1.11	0.04	1.08
6	0	0	5	0	4	9	0.83	1.12	0.28	0.96
7	0	0	5	0	4	9	0.84	1.1	0.29	1.01
8	0	0	3	0	4	7	0.9	1.14	0.31	0.94
9	0	0	4	0	4	8	0.8	1.13	0.31	0.81
10	0	0	8	0	4	12	0.66	1.12	0.28	0.59
11	0	0	2	0	4	6	1.04	1.11	0.06	1.05

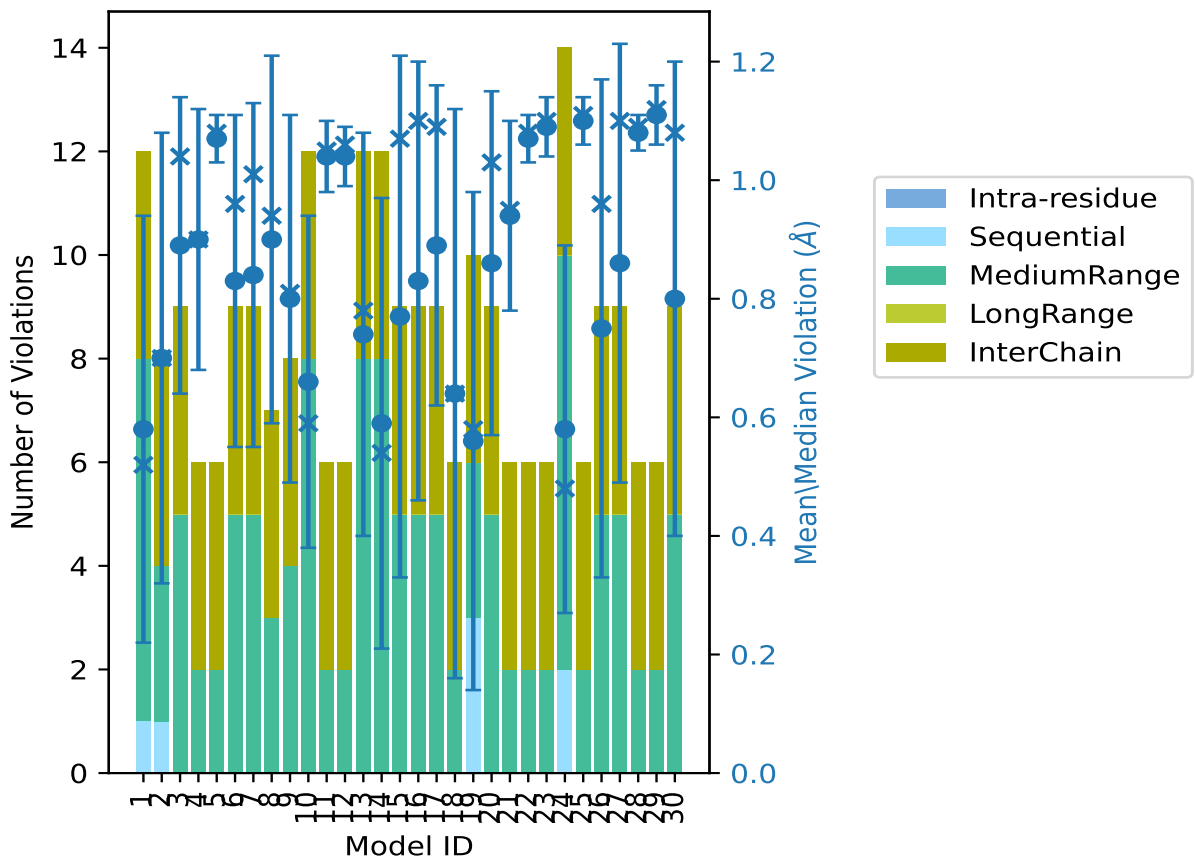
Continued on next page...

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				
12	0	0	2	0	4	6	1.04	1.09	0.05	1.06
13	0	0	8	0	4	12	0.74	1.1	0.34	0.78
14	0	0	8	0	4	12	0.59	1.17	0.38	0.54
15	0	0	5	0	4	9	0.77	1.13	0.44	1.07
16	0	0	5	0	4	9	0.83	1.12	0.37	1.1
17	0	0	5	0	4	9	0.89	1.1	0.27	1.09
18	0	0	2	0	4	6	0.64	1.13	0.48	0.64
19	0	3	3	0	4	10	0.56	1.14	0.42	0.58
20	0	0	5	0	4	9	0.86	1.12	0.29	1.03
21	0	0	2	0	4	6	0.94	1.12	0.16	0.95
22	0	0	2	0	4	6	1.07	1.11	0.04	1.08
23	0	0	2	0	4	6	1.09	1.13	0.05	1.1
24	0	2	8	0	4	14	0.58	1.1	0.31	0.48
25	0	0	2	0	4	6	1.1	1.15	0.04	1.11
26	0	0	5	0	4	9	0.75	1.14	0.42	0.96
27	0	0	5	0	4	9	0.86	1.15	0.37	1.1
28	0	0	2	0	4	6	1.08	1.11	0.03	1.09
29	0	0	2	0	4	6	1.11	1.14	0.05	1.12
30	0	0	5	0	4	9	0.8	1.1	0.4	1.08

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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 (i)

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, 1060(IR:379, SQ:182, MR:431, LR:0, IC:68) 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]	%
0	0	3	0	0	3	1	3.3
0	2	0	0	0	2	2	6.7
0	1	2	0	0	3	3	10.0
0	0	1	0	0	1	4	13.3
0	0	0	0	0	0	5	16.7
0	0	3	0	0	3	6	20.0

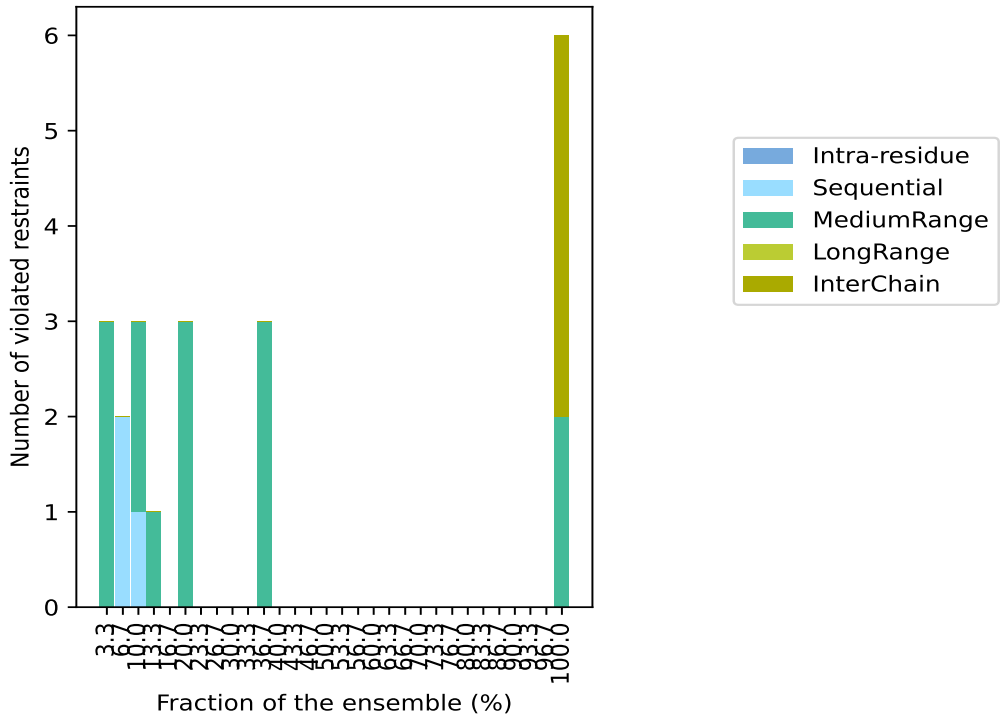
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	0	3	0	0	3	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	2	0	4	6	30	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

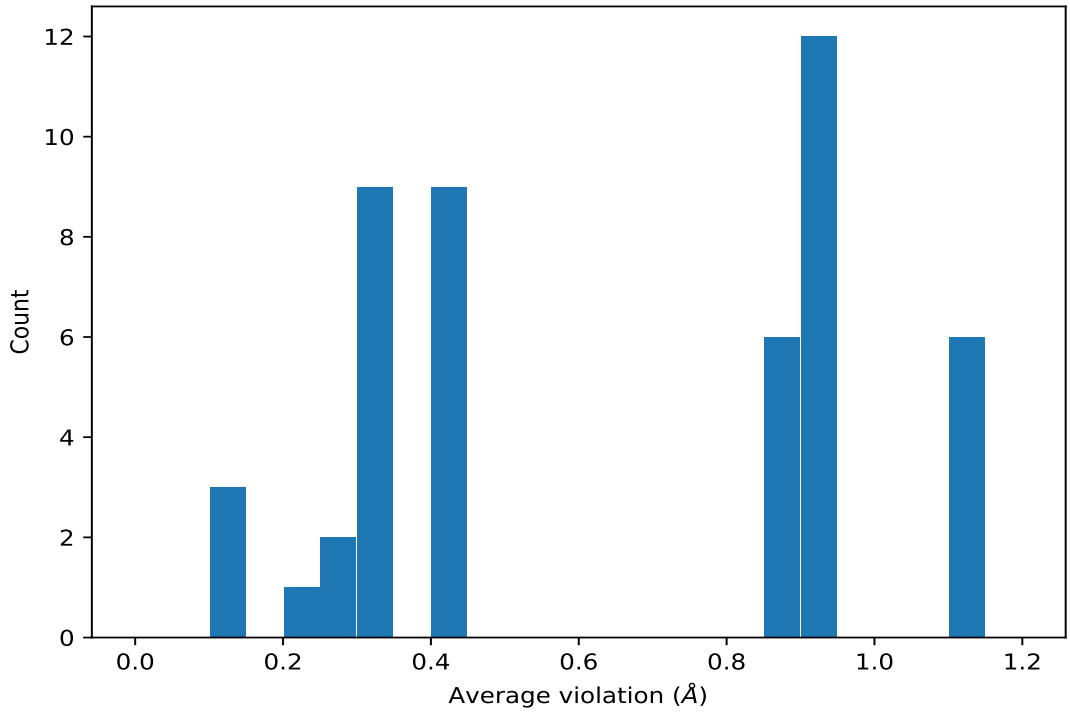
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	30	1.11	0.02	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	30	1.11	0.02	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	30	1.11	0.02	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	30	1.11	0.02	1.12
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	30	1.11	0.02	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	30	1.11	0.02	1.1
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	30	0.92	0.22	1.02
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	30	0.92	0.22	1.02
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	30	0.92	0.22	1.02
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	30	0.92	0.22	1.02
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	30	0.92	0.22	1.02
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	30	0.92	0.22	1.02
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	30	0.92	0.22	1.02
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	30	0.92	0.22	1.02
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	30	0.92	0.22	1.02
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	30	0.92	0.22	1.02

Continued on next page...

Continued from previous page...

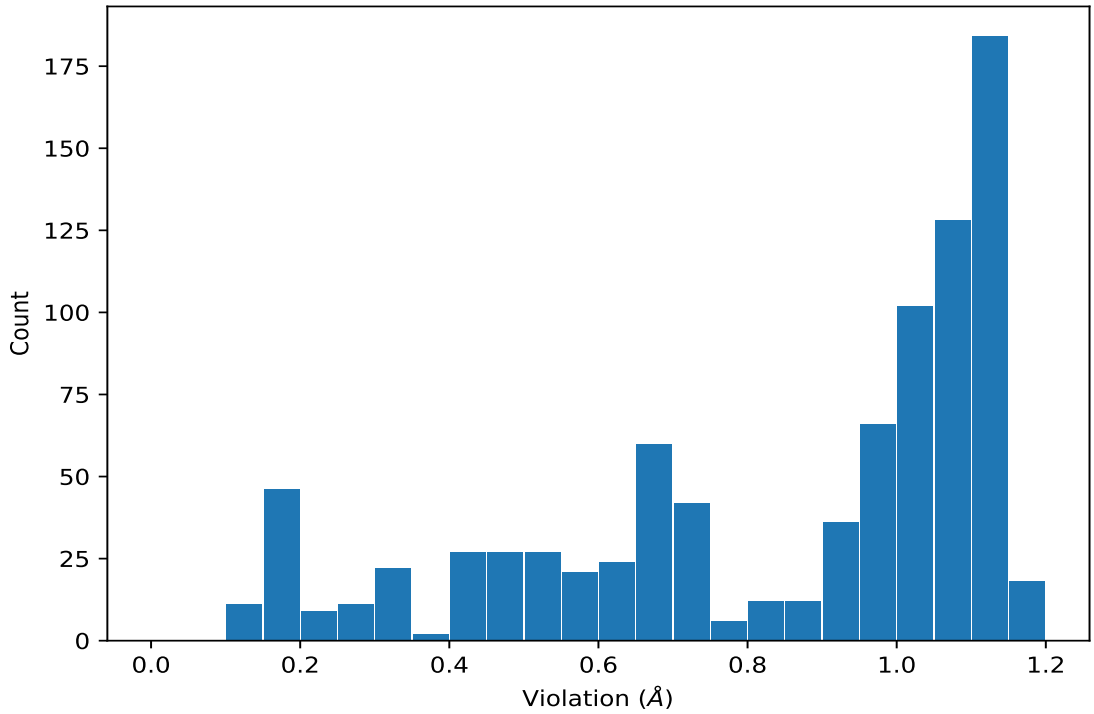
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	30	0.92	0.22	1.02
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	30	0.92	0.22	1.02
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	30	0.86	0.2	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	30	0.86	0.2	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	30	0.86	0.2	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	30	0.86	0.2	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	30	0.86	0.2	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	30	0.86	0.2	0.94
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	11	0.42	0.12	0.46
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	11	0.42	0.12	0.46
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	11	0.42	0.12	0.46
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	11	0.42	0.12	0.46
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	11	0.42	0.12	0.46
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	11	0.42	0.12	0.46
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	11	0.42	0.12	0.46
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	11	0.42	0.12	0.46
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	11	0.42	0.12	0.46
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD21	6	0.3	0.1	0.32
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD22	6	0.3	0.1	0.32
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD23	6	0.3	0.1	0.32
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	6	0.3	0.1	0.32
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	6	0.3	0.1	0.32
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	6	0.3	0.1	0.32
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	6	0.3	0.1	0.32
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	6	0.3	0.1	0.32
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	6	0.3	0.1	0.32
(1,21)	1:A:4:THR:HA	1:A:6:GLU:H	4	0.22	0.11	0.22
(1,379)	1:B:4:THR:HA	1:B:6:GLU:H	3	0.25	0.1	0.29
(1,740)	1:B:4:THR:HA	1:B:6:GLU:H	3	0.25	0.1	0.29
(1,18)	1:A:4:THR:HB	1:A:5:TYR:H	3	0.13	0.0	0.13
(1,378)	1:B:4:THR:HB	1:B:5:TYR:H	2	0.11	0.0	0.11
(1,739)	1:B:4:THR:HB	1:B:5:TYR:H	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard 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)
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	14	1.17
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	14	1.17
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	14	1.17
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	14	1.17
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	27	1.15
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	27	1.15
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	27	1.15
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	27	1.15
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	27	1.15
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	27	1.15
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	25	1.15
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	25	1.15
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	27	1.15
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	27	1.15
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	27	1.15
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	27	1.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	27	1.15
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	27	1.15
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	29	1.14
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	29	1.14
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	29	1.14
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	29	1.14
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	29	1.14
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	29	1.14
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	8	1.14
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	8	1.14
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	26	1.14
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	26	1.14
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	19	1.14
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	19	1.14
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	29	1.14
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	29	1.14
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	29	1.14
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	29	1.14
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	29	1.14
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	29	1.14
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	8	1.14
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	8	1.14
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	26	1.14
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	26	1.14
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	18	1.13
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	18	1.13
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	23	1.13
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	23	1.13
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	25	1.13
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	25	1.13
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	9	1.13
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	9	1.13
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	15	1.13
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	15	1.13
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	29	1.13
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	29	1.13
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	18	1.13
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	18	1.13
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	23	1.13
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	23	1.13
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	25	1.13
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	25	1.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	3	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	3	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	4	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	4	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	6	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	6	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	9	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	9	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	10	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	10	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	15	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	15	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	16	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	16	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	19	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	19	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	20	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	20	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	29	1.12
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	29	1.12
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	2	1.12
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	2	1.12
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	4	1.12
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	4	1.12
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	18	1.12
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	18	1.12
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	21	1.12
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	21	1.12
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	23	1.12
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	23	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	3	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	3	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	4	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	4	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	6	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	6	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	9	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	9	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	10	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	10	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	15	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	15	1.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	16	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	16	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	19	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	19	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	20	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	20	1.12
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	29	1.12
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	29	1.12
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	11	1.11
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	11	1.11
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	22	1.11
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	22	1.11
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	27	1.11
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	27	1.11
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	1	1.11
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	1	1.11
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	5	1.11
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	5	1.11
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	20	1.11
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	20	1.11
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	26	1.11
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	26	1.11
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	28	1.11
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	28	1.11
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	11	1.11
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	11	1.11
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	22	1.11
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	22	1.11
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	27	1.11
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	27	1.11
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	16	1.1
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	16	1.1
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	16	1.1
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	16	1.1
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	16	1.1
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	16	1.1
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	17	1.1
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	17	1.1
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	17	1.1
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	17	1.1
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	17	1.1
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	17	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	1	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	1	1.1
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	2	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	2	1.1
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	5	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	5	1.1
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	7	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	7	1.1
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	13	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	13	1.1
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	21	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	21	1.1
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	24	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	24	1.1
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	30	1.1
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	30	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	3	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	3	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	8	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	8	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	13	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	13	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	16	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	16	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	22	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	22	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	24	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	24	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	27	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	27	1.1
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	30	1.1
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	30	1.1
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	16	1.1
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	16	1.1
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	16	1.1
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	16	1.1
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	16	1.1
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	16	1.1
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	17	1.1
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	17	1.1
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	17	1.1
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	17	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	17	1.1
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	17	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	1	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	1	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	2	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	2	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	5	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	5	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	7	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	7	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	13	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	13	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	21	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	21	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	24	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	24	1.1
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	30	1.1
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	30	1.1
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	25	1.09
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	25	1.09
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	25	1.09
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	25	1.09
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	25	1.09
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	25	1.09
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	28	1.09
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	28	1.09
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	28	1.09
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	28	1.09
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	28	1.09
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	28	1.09
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	12	1.09
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	12	1.09
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	17	1.09
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	17	1.09
(1,714)	1:B:2:SER:HA	1:A:5:TYR:H	28	1.09
(1,714)	1:B:2:SER:HA	1:B:5:TYR:H	28	1.09
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	27	1.09
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	27	1.09
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	27	1.09
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	27	1.09
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	27	1.09
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	27	1.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	7	1.09
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	7	1.09
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	10	1.09
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	10	1.09
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	11	1.09
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	11	1.09
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	17	1.09
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	17	1.09
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	25	1.09
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	25	1.09
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	25	1.09
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	25	1.09
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	25	1.09
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	25	1.09
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	28	1.09
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	28	1.09
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	28	1.09
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	28	1.09
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	28	1.09
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	28	1.09
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	12	1.09
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	12	1.09
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	17	1.09
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	17	1.09
(1,1074)	1:B:2:SER:HA	1:A:5:TYR:H	28	1.09
(1,1074)	1:B:2:SER:HA	1:B:5:TYR:H	28	1.09
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	23	1.08
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	23	1.08
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	23	1.08
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	23	1.08
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	23	1.08
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	23	1.08
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	30	1.08
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	30	1.08
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	30	1.08
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	30	1.08
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	30	1.08
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	30	1.08
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	6	1.08
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	6	1.08
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	12	1.08
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	12	1.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	23	1.08
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	23	1.08
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	23	1.08
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	23	1.08
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	23	1.08
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	23	1.08
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	30	1.08
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	30	1.08
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	30	1.08
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	30	1.08
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	30	1.08
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	30	1.08
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	15	1.07
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	15	1.07
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	15	1.07
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	15	1.07
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	15	1.07
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	15	1.07
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	22	1.07
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	22	1.07
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	22	1.07
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	22	1.07
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	22	1.07
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	22	1.07
(1,353)	1:A:2:SER:HA	1:A:5:TYR:H	14	1.07
(1,353)	1:A:2:SER:HA	1:B:5:TYR:H	14	1.07
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	15	1.07
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	15	1.07
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	15	1.07
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	15	1.07
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	15	1.07
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	15	1.07
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	22	1.07
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	22	1.07
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	22	1.07
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	22	1.07
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	22	1.07
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	22	1.07
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	5	1.06
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	5	1.06
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	5	1.06
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	5	1.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	5	1.06
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	5	1.06
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	5	1.06
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	5	1.06
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	5	1.06
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	5	1.06
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	5	1.06
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	5	1.06
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	13	1.05
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	13	1.05
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	13	1.05
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	13	1.05
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	13	1.05
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	13	1.05
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	13	1.05
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	13	1.05
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	13	1.05
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	13	1.05
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	13	1.05
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	13	1.05
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	3	1.04
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	3	1.04
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	3	1.04
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	3	1.04
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	3	1.04
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	3	1.04
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	3	1.04
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	3	1.04
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	3	1.04
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	3	1.04
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	3	1.04
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	3	1.04
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	12	1.03
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	12	1.03
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	12	1.03
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	12	1.03
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	12	1.03
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	12	1.03
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	20	1.03
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	20	1.03
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	20	1.03
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	20	1.03

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	20	1.03
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	20	1.03
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	16	1.03
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	16	1.03
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	16	1.03
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	16	1.03
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	16	1.03
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	16	1.03
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	25	1.03
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	25	1.03
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	25	1.03
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	25	1.03
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	25	1.03
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	25	1.03
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	12	1.03
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	12	1.03
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	12	1.03
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	12	1.03
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	12	1.03
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	12	1.03
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	20	1.03
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	20	1.03
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	20	1.03
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	20	1.03
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	20	1.03
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	20	1.03
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	13	1.02
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	13	1.02
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	13	1.02
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	13	1.02
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	13	1.02
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	13	1.02
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	30	1.02
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	30	1.02
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	30	1.02
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	30	1.02
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	30	1.02
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	30	1.02
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	7	1.01
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	7	1.01
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	7	1.01
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	7	1.01

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	7	1.01
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	7	1.01
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	11	1.01
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	11	1.01
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	11	1.01
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	11	1.01
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	11	1.01
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	11	1.01
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	17	1.01
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	17	1.01
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	17	1.01
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	17	1.01
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	17	1.01
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	17	1.01
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	28	1.01
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	28	1.01
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	28	1.01
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	28	1.01
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	28	1.01
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	28	1.01
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	7	1.01
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	7	1.01
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	7	1.01
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	7	1.01
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	7	1.01
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	7	1.01
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	11	1.01
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	11	1.01
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	11	1.01
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	11	1.01
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	11	1.01
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	11	1.01
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	23	1.0
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	23	1.0
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	23	1.0
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	23	1.0
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	23	1.0
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	23	1.0
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	5	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	5	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	5	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	5	0.99

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	5	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	5	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	20	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	20	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	20	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	20	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	20	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	20	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	29	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	29	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	29	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	29	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	29	0.99
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	29	0.99
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	15	0.98
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	15	0.98
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	15	0.98
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	15	0.98
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	15	0.98
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	15	0.98
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	22	0.98
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	22	0.98
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	22	0.98
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	22	0.98
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	22	0.98
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	22	0.98
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	6	0.96
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	6	0.96
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	6	0.96
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	6	0.96
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	6	0.96
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	6	0.96
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	26	0.96
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	26	0.96
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	26	0.96
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	26	0.96
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	26	0.96
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	26	0.96
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	6	0.96
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	6	0.96
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	6	0.96
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	6	0.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	6	0.96
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	6	0.96
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	26	0.96
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	26	0.96
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	26	0.96
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	26	0.96
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	26	0.96
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	26	0.96
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	3	0.95
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	3	0.95
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	3	0.95
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	3	0.95
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	3	0.95
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	3	0.95
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	7	0.95
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	7	0.95
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	7	0.95
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	7	0.95
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	7	0.95
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	7	0.95
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	8	0.94
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	8	0.94
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	8	0.94
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	8	0.94
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	8	0.94
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	8	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	11	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	11	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	11	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	11	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	11	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	11	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	12	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	12	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	12	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	12	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	12	0.94
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	12	0.94
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	8	0.94
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	8	0.94
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	8	0.94
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	8	0.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	8	0.94
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	8	0.94
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	9	0.91
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	9	0.91
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	9	0.91
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	9	0.91
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	9	0.91
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	9	0.91
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	26	0.91
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	26	0.91
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	26	0.91
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	26	0.91
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	26	0.91
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	26	0.91
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	6	0.88
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	6	0.88
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	6	0.88
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	6	0.88
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	6	0.88
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	6	0.88
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	8	0.86
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	8	0.86
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	8	0.86
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	8	0.86
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	8	0.86
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	8	0.86
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	21	0.8
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	21	0.8
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	21	0.8
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	21	0.8
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	21	0.8
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	21	0.8
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	21	0.8
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	21	0.8
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	21	0.8
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	21	0.8
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	21	0.8
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	21	0.8
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	21	0.75
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	21	0.75
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	21	0.75
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	21	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	21	0.75
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	21	0.75
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	14	0.74
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	14	0.74
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	14	0.74
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	14	0.74
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	14	0.74
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	14	0.74
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	14	0.74
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	14	0.74
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	14	0.74
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	14	0.74
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	14	0.74
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	14	0.74
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	14	0.73
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	14	0.73
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	14	0.73
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	14	0.73
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	14	0.73
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	14	0.73
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	9	0.71
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	9	0.71
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	9	0.71
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	9	0.71
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	9	0.71
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	9	0.71
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	9	0.71
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	9	0.71
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	9	0.71
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	9	0.71
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	9	0.71
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	9	0.71
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	2	0.7
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	2	0.7
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	2	0.7
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	2	0.7
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	2	0.7
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	2	0.7
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	2	0.7
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	2	0.7
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	2	0.7
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	2	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	2	0.7
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	2	0.7
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	4	0.69
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	4	0.69
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	4	0.69
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	4	0.69
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	4	0.69
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	4	0.69
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	4	0.69
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	4	0.69
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	4	0.69
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	4	0.69
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	4	0.69
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	4	0.69
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	1	0.68
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	1	0.68
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	1	0.68
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	1	0.68
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	1	0.68
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	1	0.68
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	10	0.68
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	10	0.68
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	10	0.68
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	10	0.68
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	10	0.68
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	10	0.68
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	1	0.68
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	1	0.68
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	1	0.68
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	1	0.68
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	1	0.68
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	1	0.68
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	10	0.68
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	10	0.68
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	10	0.68
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	10	0.68
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	10	0.68
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	10	0.68
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	10	0.66
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	10	0.66
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	10	0.66
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	10	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	10	0.66
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	10	0.66
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	24	0.65
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	24	0.65
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	24	0.65
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	24	0.65
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	24	0.65
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	24	0.65
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	4	0.65
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	4	0.65
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	4	0.65
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	4	0.65
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	4	0.65
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	4	0.65
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	24	0.65
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	24	0.65
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	24	0.65
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	24	0.65
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	24	0.65
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	24	0.65
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	1	0.62
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	1	0.62
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	1	0.62
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	1	0.62
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	1	0.62
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	1	0.62
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	19	0.61
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	19	0.61
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	19	0.61
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	19	0.61
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	19	0.61
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	19	0.61
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	19	0.61
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	19	0.61
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	19	0.61
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	19	0.61
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	19	0.61
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	19	0.61
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	2	0.6
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	2	0.6
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	2	0.6
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	2	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	2	0.6
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	2	0.6
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	24	0.59
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	24	0.59
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	24	0.59
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	24	0.59
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	24	0.59
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	24	0.59
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	3	0.55
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	3	0.55
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	3	0.55
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	3	0.55
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	3	0.55
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	3	0.55
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	19	0.55
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	19	0.55
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	19	0.55
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	19	0.55
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	19	0.55
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	19	0.55
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	3	0.55
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	3	0.55
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	3	0.55
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	13	0.53
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	13	0.53
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	13	0.53
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	13	0.53
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	13	0.53
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	13	0.53
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	13	0.53
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	13	0.53
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	13	0.53
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	10	0.52
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	10	0.52
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	10	0.52
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	10	0.52
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	10	0.52
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	10	0.52
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	10	0.52
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	10	0.52
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	10	0.52
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	17	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	17	0.51
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	17	0.51
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	17	0.51
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	17	0.51
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	17	0.51
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	17	0.51
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	17	0.51
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	17	0.51
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	24	0.48
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	24	0.48
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	24	0.48
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	24	0.48
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	24	0.48
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	24	0.48
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	24	0.48
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	24	0.48
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	24	0.48
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	20	0.46
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	20	0.46
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	20	0.46
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	20	0.46
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	20	0.46
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	20	0.46
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	20	0.46
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	20	0.46
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	20	0.46
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	6	0.45
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	6	0.45
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	6	0.45
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	6	0.45
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	6	0.45
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	6	0.45
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	6	0.45
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	6	0.45
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	6	0.45
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	7	0.44
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	7	0.44
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	7	0.44
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	7	0.44
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	7	0.44
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	7	0.44
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	7	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	7	0.44
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	7	0.44
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD21	1	0.42
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD22	1	0.42
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD23	1	0.42
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	1	0.41
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	1	0.41
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	1	0.41
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	24	0.41
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	24	0.41
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	24	0.41
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	1	0.41
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	1	0.41
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	1	0.41
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	24	0.41
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	24	0.41
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	24	0.41
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD21	24	0.41
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD22	24	0.41
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD23	24	0.41
(1,740)	1:B:4:THR:HA	1:B:6:GLU:H	10	0.35
(1,379)	1:B:4:THR:HA	1:B:6:GLU:H	10	0.35
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	27	0.34
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	27	0.34
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	27	0.34
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	27	0.34
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	27	0.34
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	27	0.34
(1,21)	1:A:4:THR:HA	1:A:6:GLU:H	14	0.34
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD21	27	0.34
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD22	27	0.34
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD23	27	0.34
(1,738)	1:B:4:THR:HB	1:B:6:GLU:H	9	0.33
(1,377)	1:B:4:THR:HB	1:B:6:GLU:H	9	0.33
(1,21)	1:A:4:THR:HA	1:A:6:GLU:H	10	0.33
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	16	0.31
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	16	0.31
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	16	0.31
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	16	0.31
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	16	0.31
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	16	0.31
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	16	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	16	0.31
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	16	0.31
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	13	0.29
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	13	0.29
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	13	0.29
(1,740)	1:B:4:THR:HA	1:B:6:GLU:H	14	0.29
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	13	0.29
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	13	0.29
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	13	0.29
(1,379)	1:B:4:THR:HA	1:B:6:GLU:H	14	0.29
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD21	13	0.29
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD22	13	0.29
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD23	13	0.29
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	30	0.24
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	30	0.24
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	30	0.24
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	30	0.24
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	30	0.24
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	30	0.24
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	30	0.24
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	30	0.24
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	30	0.24
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	14	0.18
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	14	0.18
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	14	0.18
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	14	0.18
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	14	0.18
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	14	0.18
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD21	14	0.18
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD22	14	0.18
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD23	14	0.18
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	26	0.17
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	26	0.17
(1,864)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	26	0.17
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG21	18	0.17
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG22	18	0.17
(1,715)	1:B:4:THR:HB	1:A:8:VAL:HG23	18	0.17
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG21	18	0.17
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG22	18	0.17
(1,715)	1:B:4:THR:HB	1:B:8:VAL:HG23	18	0.17
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD21	26	0.17
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD22	26	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:B:15:HIS:HB3	1:B:12:LEU:HD23	26	0.17
(1,383)	1:B:4:THR:H	1:B:8:VAL:H	8	0.17
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD21	26	0.17
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD22	26	0.17
(1,143)	1:A:15:HIS:HB3	1:A:12:LEU:HD23	26	0.17
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG21	18	0.17
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG22	18	0.17
(1,1075)	1:B:4:THR:HB	1:A:8:VAL:HG23	18	0.17
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG21	18	0.17
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG22	18	0.17
(1,1075)	1:B:4:THR:HB	1:B:8:VAL:HG23	18	0.17
(1,946)	1:B:24:THR:HG21	1:B:28:GLU:HG3	15	0.15
(1,946)	1:B:24:THR:HG22	1:B:28:GLU:HG3	15	0.15
(1,946)	1:B:24:THR:HG23	1:B:28:GLU:HG3	15	0.15
(1,586)	1:B:24:THR:HG21	1:B:28:GLU:HG3	15	0.15
(1,586)	1:B:24:THR:HG22	1:B:28:GLU:HG3	15	0.15
(1,586)	1:B:24:THR:HG23	1:B:28:GLU:HG3	15	0.15
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG21	18	0.15
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG22	18	0.15
(1,354)	1:A:4:THR:HB	1:A:8:VAL:HG23	18	0.15
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG21	18	0.15
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG22	18	0.15
(1,354)	1:A:4:THR:HB	1:B:8:VAL:HG23	18	0.15
(1,225)	1:A:24:THR:HG21	1:A:28:GLU:HG3	15	0.15
(1,225)	1:A:24:THR:HG22	1:A:28:GLU:HG3	15	0.15
(1,225)	1:A:24:THR:HG23	1:A:28:GLU:HG3	15	0.15
(1,18)	1:A:4:THR:HB	1:A:5:TYR:H	1	0.13
(1,18)	1:A:4:THR:HB	1:A:5:TYR:H	2	0.13
(1,740)	1:B:4:THR:HA	1:B:6:GLU:H	1	0.12
(1,379)	1:B:4:THR:HA	1:B:6:GLU:H	1	0.12
(1,18)	1:A:4:THR:HB	1:A:5:TYR:H	19	0.12
(1,739)	1:B:4:THR:HB	1:B:5:TYR:H	19	0.11
(1,739)	1:B:4:THR:HB	1:B:5:TYR:H	24	0.11
(1,378)	1:B:4:THR:HB	1:B:5:TYR:H	19	0.11
(1,378)	1:B:4:THR:HB	1:B:5:TYR:H	24	0.11
(1,21)	1:A:4:THR:HA	1:A:6:GLU:H	2	0.11
(1,21)	1:A:4:THR:HA	1:A:6:GLU:H	19	0.11

10 Dihedral-angle violation analysis (i)

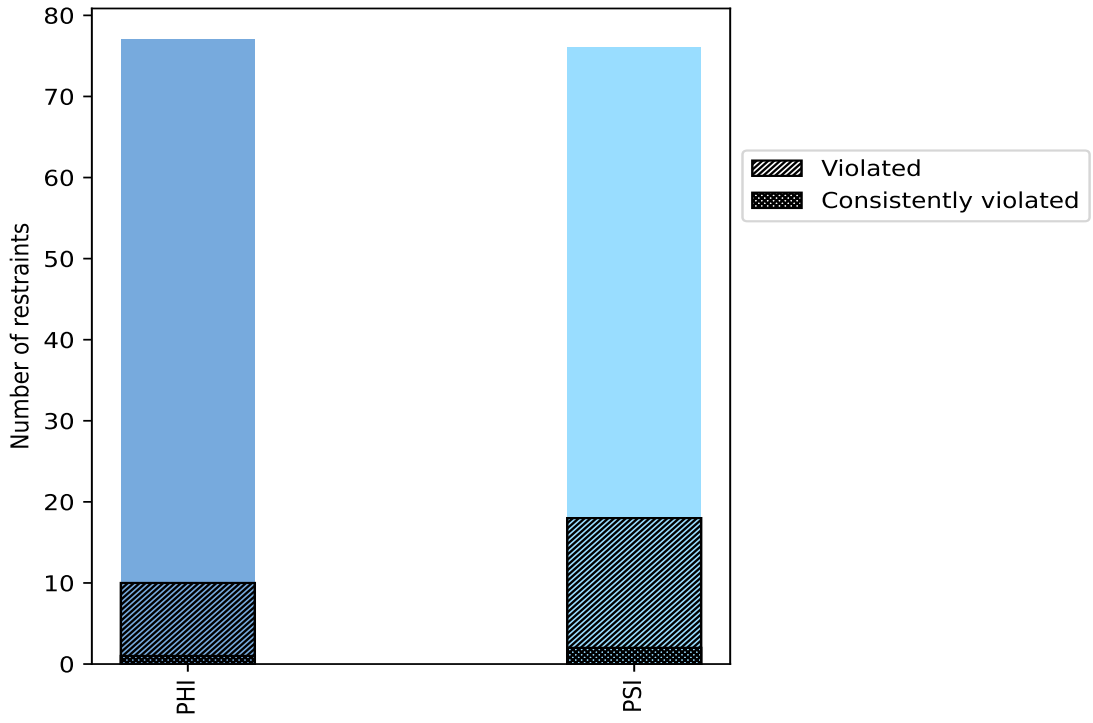
10.1 Summary of dihedral-angle violations (i)

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]
PHI	77	50.3	10	13.0	6.5	1	1.3	0.7
PSI	76	49.7	18	23.7	11.8	2	2.6	1.3
Total	153	100.0	28	18.3	18.3	3	2.0	2.0

[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)



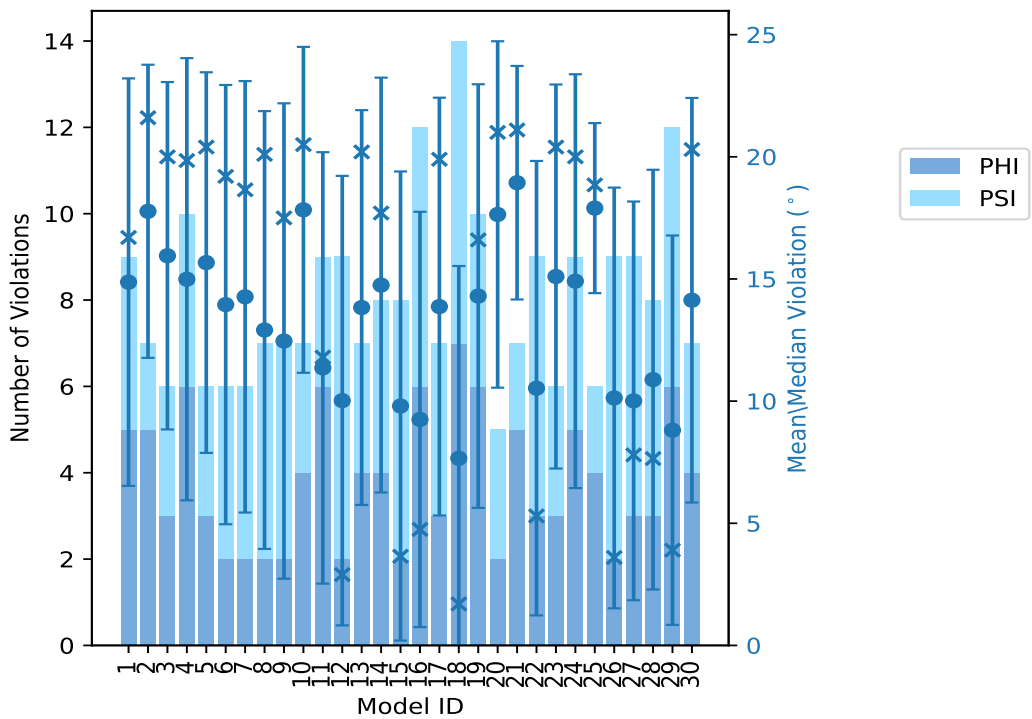
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	5	4	9	14.87	24.3	8.34	16.7
2	5	2	7	17.77	24.1	6.0	21.6
3	3	3	6	15.95	21.1	7.11	20.0
4	6	4	10	14.99	24.6	9.05	19.85
5	3	3	6	15.67	21.7	7.79	20.4
6	2	4	6	13.95	21.3	8.99	19.2
7	2	4	6	14.27	22.6	8.83	18.65
8	2	5	7	12.91	22.1	8.96	20.1
9	2	5	7	12.46	22.9	9.73	17.5
10	4	3	7	17.83	22.7	6.67	20.5
11	6	3	9	11.36	21.0	8.83	11.8
12	2	7	9	10.02	21.6	9.2	2.9
13	4	3	7	13.83	20.8	8.08	20.2
14	4	4	8	14.75	24.3	8.49	17.7
15	2	6	8	9.8	23.4	9.6	3.65
16	6	6	12	9.25	21.7	8.5	4.75
17	3	4	7	13.87	22.0	8.55	19.9
18	7	7	14	7.66	20.5	7.87	1.7
19	6	4	10	14.3	24.8	8.67	16.6
20	2	3	5	17.64	22.0	7.09	21.0
21	5	2	7	18.94	24.9	4.78	21.1
22	3	6	9	10.53	21.1	9.3	5.3
23	3	3	6	15.1	20.8	7.86	20.4
24	5	4	9	14.91	23.6	8.47	20.0
25	4	2	6	17.9	21.1	3.48	18.85
26	2	7	9	10.13	21.6	8.61	3.6
27	3	6	9	10.01	21.4	8.16	7.8
28	3	5	8	10.88	21.9	8.59	7.65
29	6	6	12	8.81	21.2	7.97	3.9
30	4	3	7	14.13	21.1	8.28	20.3

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

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

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
2	1	3	1	3.3
0	4	4	2	6.7
3	4	7	3	10.0
0	4	4	4	13.3
0	1	1	5	16.7
0	0	0	6	20.0
0	1	1	7	23.3
0	0	0	8	26.7
1	0	1	9	30.0
0	0	0	10	33.3
0	0	0	11	36.7

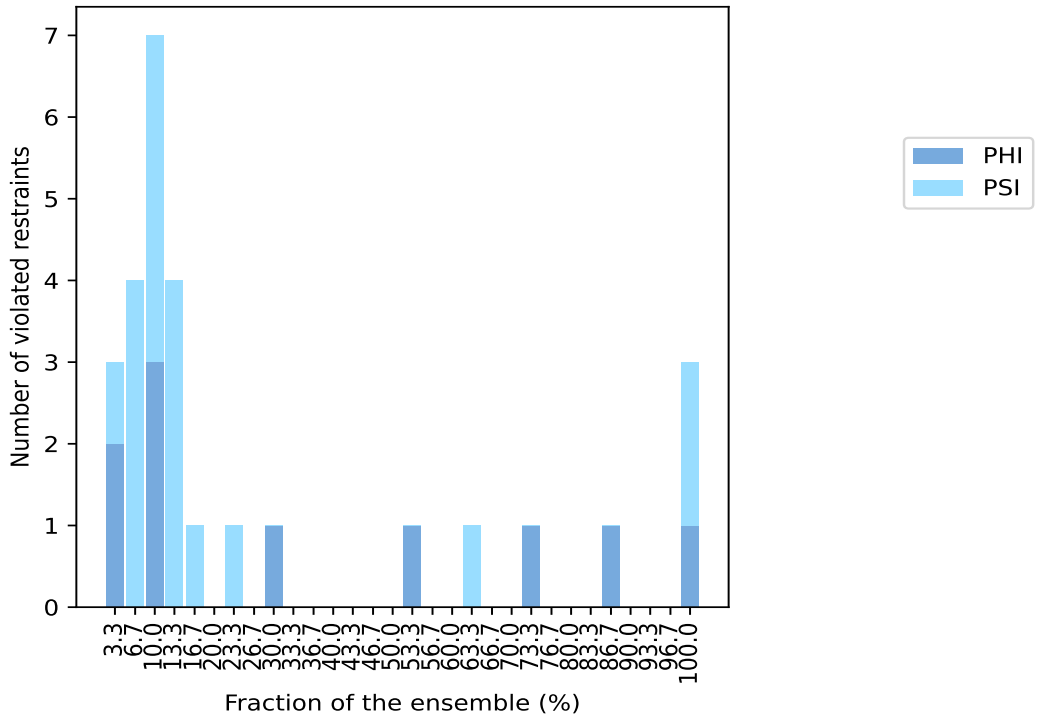
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	40.0
0	0	0	13	43.3
0	0	0	14	46.7
0	0	0	15	50.0
1	0	1	16	53.3
0	0	0	17	56.7
0	0	0	18	60.0
0	1	1	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
1	0	1	22	73.3
0	0	0	23	76.7
0	0	0	24	80.0
0	0	0	25	83.3
1	0	1	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
1	2	3	30	100.0

[1] Number of models with violations

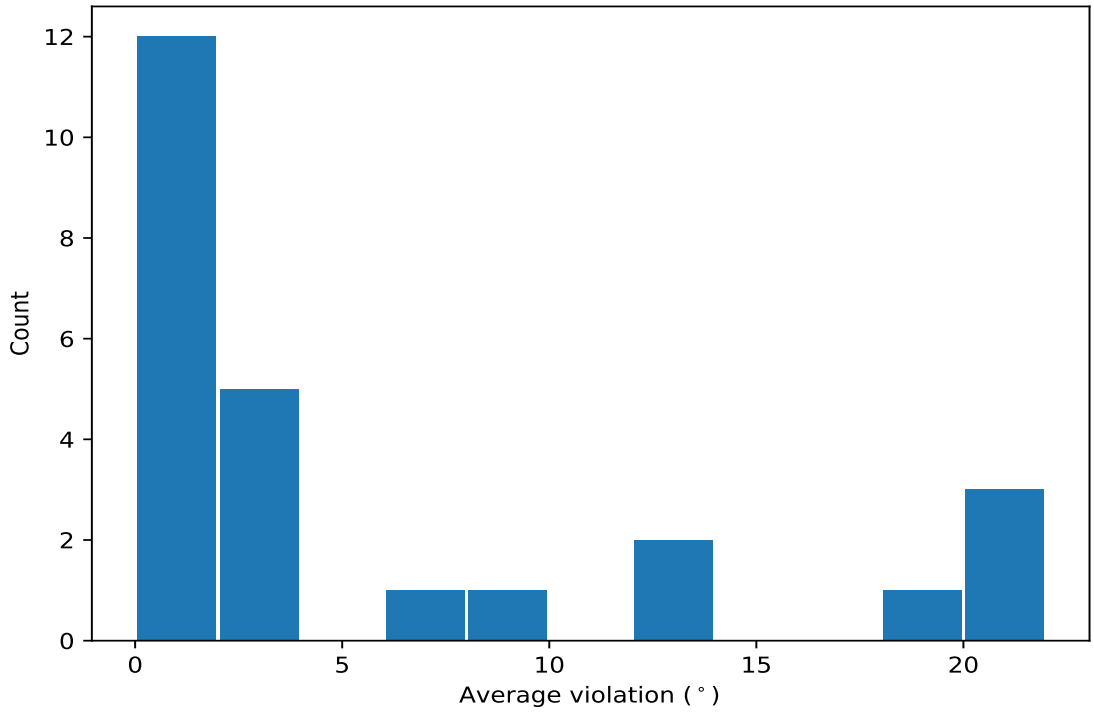
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	30	21.27	1.12	21.3
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	30	21.15	0.57	21.1
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	30	19.88	4.08	20.2
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	26	21.47	0.75	21.3
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	22	12.45	4.33	12.2
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	19	1.88	0.51	1.9
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	16	9.06	4.09	9.55
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	9	13.73	6.49	16.7
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	7	1.39	0.27	1.3
(1,51)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	1:A:18:LEU:N	5	1.56	0.36	1.5
(1,152)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:VAL:N	4	3.95	0.26	3.9
(1,128)	1:B:17:GLU:N	1:B:17:GLU:CA	1:B:17:GLU:C	1:B:18:LEU:N	4	1.65	0.3	1.6
(1,54)	1:A:20:ARG:N	1:A:20:ARG:CA	1:A:20:ARG:C	1:A:21:ARG:N	4	1.35	0.27	1.25
(1,131)	1:B:20:ARG:N	1:B:20:ARG:CA	1:B:20:ARG:C	1:B:21:ARG:N	4	1.3	0.23	1.2
(1,36)	1:A:37:LEU:C	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	3	6.2	5.0	3.6
(1,58)	1:A:24:THR:N	1:A:24:THR:CA	1:A:24:THR:C	1:A:25:HIS:N	3	3.07	0.39	2.9
(1,135)	1:B:24:THR:N	1:B:24:THR:CA	1:B:24:THR:C	1:B:25:HIS:N	3	3.0	0.36	2.8
(1,98)	1:B:22:LYS:C	1:B:23:ASP:N	1:B:23:ASP:CA	1:B:23:ASP:C	3	2.43	0.62	2.6
(1,21)	1:A:22:LYS:C	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	3	2.4	0.59	2.6
(1,46)	1:A:12:LEU:N	1:A:12:LEU:CA	1:A:12:LEU:C	1:A:13:VAL:N	3	1.9	0.45	2.0
(1,123)	1:B:12:LEU:N	1:B:12:LEU:CA	1:B:12:LEU:C	1:B:13:VAL:N	3	1.83	0.46	2.0

Continued on next page...

Continued from previous page...

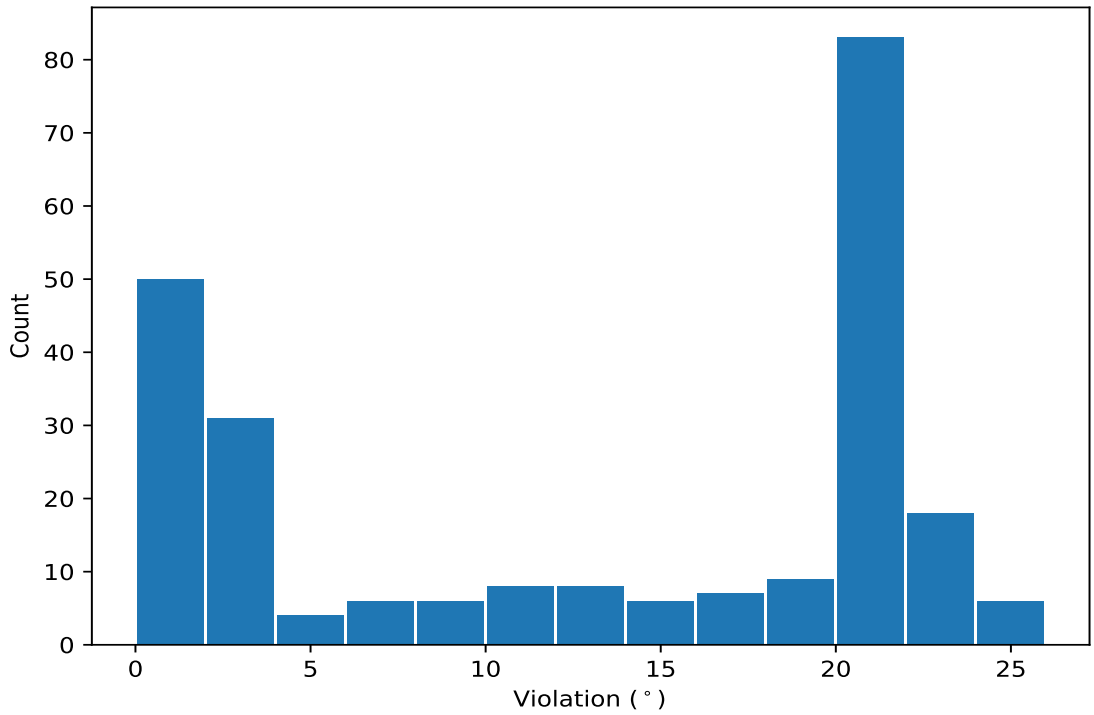
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,57)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:THR:N	2	1.7	0.2	1.7
(1,134)	1:B:23:ASP:N	1:B:23:ASP:CA	1:B:23:ASP:C	1:B:24:THR:N	2	1.7	0.2	1.7
(1,127)	1:B:16:LYS:N	1:B:16:LYS:CA	1:B:16:LYS:C	1:B:17:GLU:N	2	1.4	0.1	1.4
(1,50)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:GLU:N	2	1.35	0.15	1.35

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	21	24.9
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	19	24.8
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	4	24.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	14	24.3
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1	24.3
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	2	24.1
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	24	23.6
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	15	23.4
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	19	23.4
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	9	22.9
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	10	22.7
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	2	22.7
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	4	22.6
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	15	22.6
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	7	22.6
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	1	22.2
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	24	22.2
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	1	22.1
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	4	22.1
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	8	22.1
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	17	22.0
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	1	22.0
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	4	22.0
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	20	22.0
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	9	21.9
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	28	21.9
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	21	21.9
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	2	21.8
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	16	21.7
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	19	21.7
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	5	21.7
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	2	21.6
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	12	21.6
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	24	21.6
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	28	21.6
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	4	21.6
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	17	21.6
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	26	21.6
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	14	21.5
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	19	21.5
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	20	21.5
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	7	21.4
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	21	21.4
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	27	21.4
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	7	21.4
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	5	21.4
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	12	21.4
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	12	21.3
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	6	21.3
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	10	21.3
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	6	21.2
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	29	21.2
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	6	21.2
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	28	21.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	16	21.2
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	5	21.1
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	30	21.1
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	21	21.1
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	22	21.1
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	24	21.1
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	30	21.1
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	3	21.1
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	22	21.1
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	25	21.1
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	20	21.0
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	22	21.0
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	11	21.0
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	16	21.0
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	14	21.0
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	30	21.0
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	25	20.9
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	11	20.8
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	13	20.8
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	3	20.8
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	13	20.8
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	23	20.8
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	9	20.8
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	23	20.8
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	13	20.7
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	10	20.6
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	23	20.6
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	29	20.6
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	11	20.6
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	10	20.5
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	29	20.5
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	18	20.5
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	3	20.4
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	27	20.4
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	10	20.4
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	14	20.4
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	27	20.4
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	18	20.3
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	15	20.3
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	30	20.3
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	8	20.2
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	8	20.2
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	11	20.2
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	13	20.2
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	20	20.2
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	22	20.2
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	23	20.2
(1,113)	1:B:37:LEU:C	1:B:38:VAL:N	1:B:38:VAL:CA	1:B:38:VAL:C	17	20.2
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	19	20.1
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	8	20.1
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	24	20.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,149)	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1:B:5:TYR:N	26	20.0
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	16	20.0
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	17	19.9
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	5	19.7
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	26	19.6
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	21	19.6
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	3	19.6
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	18	19.3
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	25	19.3
(1,72)	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1:A:5:TYR:N	25	18.4
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	4	18.1
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	9	17.5
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	26	17.5
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	10	17.4
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	6	17.2
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	25	16.9
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1	16.7
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	12	16.3
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	7	15.9
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	14	15.0
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	18	15.0
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	29	14.7
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	24	14.2
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	2	14.0
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	2	13.6
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	14	13.4
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	21	13.3
(1,36)	1:A:37:LEU:C	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	18	13.2
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	4	13.1
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	19	13.1
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1	12.2
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	3	12.2
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	11	11.8
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	29	11.5
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	1	11.3
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	27	11.2
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	30	11.1
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	25	10.8
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	21	10.4
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	19	10.1
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	17	9.9
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	28	9.1
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	24	9.0
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	13	8.8
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	5	8.5
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	18	8.4
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	27	7.8
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	16	7.8
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	2	6.6
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	16	6.4
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	28	6.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	23	6.0
(1,2)	1:A:3:LEU:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	22	5.3
(1,152)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:VAL:N	15	4.3
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	29	4.1
(1,152)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:VAL:N	27	4.1
(1,152)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:VAL:N	28	3.7
(1,152)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:VAL:N	29	3.7
(1,58)	1:A:24:THR:N	1:A:24:THR:CA	1:A:24:THR:C	1:A:25:HIS:N	26	3.6
(1,36)	1:A:37:LEU:C	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	19	3.6
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	13	3.5
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	20	3.5
(1,135)	1:B:24:THR:N	1:B:24:THR:CA	1:B:24:THR:C	1:B:25:HIS:N	26	3.5
(1,98)	1:B:22:LYS:C	1:B:23:ASP:N	1:B:23:ASP:CA	1:B:23:ASP:C	16	3.1
(1,37)	1:A:38:VAL:C	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	15	3.0
(1,21)	1:A:22:LYS:C	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	16	3.0
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	11	2.9
(1,79)	1:B:3:LEU:C	1:B:4:THR:N	1:B:4:THR:CA	1:B:4:THR:C	30	2.9
(1,58)	1:A:24:THR:N	1:A:24:THR:CA	1:A:24:THR:C	1:A:25:HIS:N	12	2.9
(1,135)	1:B:24:THR:N	1:B:24:THR:CA	1:B:24:THR:C	1:B:25:HIS:N	12	2.8
(1,58)	1:A:24:THR:N	1:A:24:THR:CA	1:A:24:THR:C	1:A:25:HIS:N	8	2.7
(1,135)	1:B:24:THR:N	1:B:24:THR:CA	1:B:24:THR:C	1:B:25:HIS:N	8	2.7
(1,98)	1:B:22:LYS:C	1:B:23:ASP:N	1:B:23:ASP:CA	1:B:23:ASP:C	29	2.6
(1,21)	1:A:22:LYS:C	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	29	2.6
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	8	2.4
(1,46)	1:A:12:LEU:N	1:A:12:LEU:CA	1:A:12:LEU:C	1:A:13:VAL:N	19	2.4
(1,123)	1:B:12:LEU:N	1:B:12:LEU:CA	1:B:12:LEU:C	1:B:13:VAL:N	19	2.3
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	17	2.2
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	23	2.2
(1,51)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	1:A:18:LEU:N	7	2.2
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	26	2.1
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	27	2.1
(1,128)	1:B:17:GLU:N	1:B:17:GLU:CA	1:B:17:GLU:C	1:B:18:LEU:N	7	2.1
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	13	2.0
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	22	2.0
(1,46)	1:A:12:LEU:N	1:A:12:LEU:CA	1:A:12:LEU:C	1:A:13:VAL:N	4	2.0
(1,123)	1:B:12:LEU:N	1:B:12:LEU:CA	1:B:12:LEU:C	1:B:13:VAL:N	4	2.0
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	10	1.9
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	16	1.9
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	28	1.9
(1,57)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:THR:N	16	1.9
(1,134)	1:B:23:ASP:N	1:B:23:ASP:CA	1:B:23:ASP:C	1:B:24:THR:N	16	1.9
(1,114)	1:B:38:VAL:C	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	18	1.9
(1,54)	1:A:20:ARG:N	1:A:20:ARG:CA	1:A:20:ARG:C	1:A:21:ARG:N	15	1.8
(1,36)	1:A:37:LEU:C	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	4	1.8
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	6	1.7
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	11	1.7
(1,131)	1:B:20:ARG:N	1:B:20:ARG:CA	1:B:20:ARG:C	1:B:21:ARG:N	15	1.7
(1,128)	1:B:17:GLU:N	1:B:17:GLU:CA	1:B:17:GLU:C	1:B:18:LEU:N	26	1.7
(1,98)	1:B:22:LYS:C	1:B:23:ASP:N	1:B:23:ASP:CA	1:B:23:ASP:C	11	1.6
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	3	1.6
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	5	1.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	9	1.6
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	27	1.6
(1,51)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	1:A:18:LEU:N	26	1.6
(1,21)	1:A:22:LYS:C	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	11	1.6
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	18	1.5
(1,57)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:THR:N	29	1.5
(1,51)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	1:A:18:LEU:N	22	1.5
(1,50)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:GLU:N	1	1.5
(1,134)	1:B:23:ASP:N	1:B:23:ASP:CA	1:B:23:ASP:C	1:B:24:THR:N	29	1.5
(1,128)	1:B:17:GLU:N	1:B:17:GLU:CA	1:B:17:GLU:C	1:B:18:LEU:N	22	1.5
(1,127)	1:B:16:LYS:N	1:B:16:LYS:CA	1:B:16:LYS:C	1:B:17:GLU:N	1	1.5
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	28	1.4
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	30	1.4
(1,51)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	1:A:18:LEU:N	12	1.4
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	15	1.3
(1,54)	1:A:20:ARG:N	1:A:20:ARG:CA	1:A:20:ARG:C	1:A:21:ARG:N	9	1.3
(1,46)	1:A:12:LEU:N	1:A:12:LEU:CA	1:A:12:LEU:C	1:A:13:VAL:N	18	1.3
(1,153)	1:B:40:VAL:N	1:B:40:VAL:CA	1:B:40:VAL:C	1:B:41:MET:N	17	1.3
(1,128)	1:B:17:GLU:N	1:B:17:GLU:CA	1:B:17:GLU:C	1:B:18:LEU:N	12	1.3
(1,127)	1:B:16:LYS:N	1:B:16:LYS:CA	1:B:16:LYS:C	1:B:17:GLU:N	24	1.3
(1,82)	1:B:6:GLU:C	1:B:7:GLU:N	1:B:7:GLU:CA	1:B:7:GLU:C	18	1.2
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	12	1.2
(1,74)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ARG:N	14	1.2
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	29	1.2
(1,54)	1:A:20:ARG:N	1:A:20:ARG:CA	1:A:20:ARG:C	1:A:21:ARG:N	18	1.2
(1,50)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:GLU:N	24	1.2
(1,5)	1:A:6:GLU:C	1:A:7:GLU:N	1:A:7:GLU:CA	1:A:7:GLU:C	18	1.2
(1,131)	1:B:20:ARG:N	1:B:20:ARG:CA	1:B:20:ARG:C	1:B:21:ARG:N	9	1.2
(1,131)	1:B:20:ARG:N	1:B:20:ARG:CA	1:B:20:ARG:C	1:B:21:ARG:N	14	1.2
(1,123)	1:B:12:LEU:N	1:B:12:LEU:CA	1:B:12:LEU:C	1:B:13:VAL:N	18	1.2
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	16	1.1
(1,73)	1:A:37:LEU:N	1:A:37:LEU:CA	1:A:37:LEU:C	1:A:38:VAL:N	22	1.1
(1,54)	1:A:20:ARG:N	1:A:20:ARG:CA	1:A:20:ARG:C	1:A:21:ARG:N	27	1.1
(1,51)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	1:A:18:LEU:N	6	1.1
(1,131)	1:B:20:ARG:N	1:B:20:ARG:CA	1:B:20:ARG:C	1:B:21:ARG:N	18	1.1