Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 02:49 PM EDT

PDB ID	:	6U19
Title	:	Solution Structure of the RAZUL domain from 26S proteasome subunit hRpn10/S5a complexed with the AZUL domain from E3 ligase E6AP/UBE3A
Authors	:	Chen, X.; Walters, K.J.
Deposited on	:	2019-08-15

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:

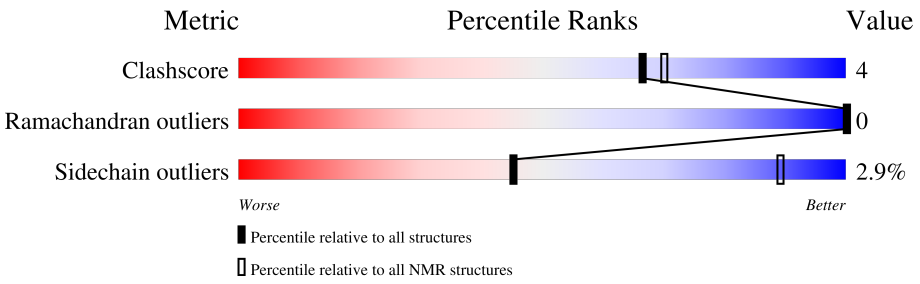
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 91%.

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	73	45% · 53%
2	B	64	84% 6% 9%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 4 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:327-A:360, B:25-B:82 (92)	0.55	4

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2072 atoms, of which 1015 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	73	1078	332	523	91	129	3	0

- Molecule 2 is a protein called Ubiquitin-protein ligase E3A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	64	993	312	492	90	92	7	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	B	1	1	1

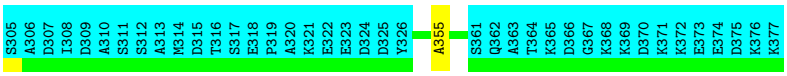
4 Residue-property plots (i)

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: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 45% • 53%



• Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 84% 6% 9%

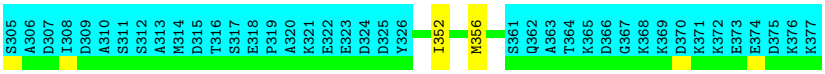
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 44% • 53%



• Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 81% 9% 9%

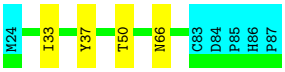
4.2.2 Score per residue for model 2

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 40% 7% 53%

- Molecule 2: Ubiquitin-protein ligase E3A

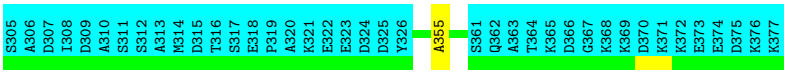
Chain B: 84% 6% 9%



4.2.3 Score per residue for model 3

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 45% • 53%



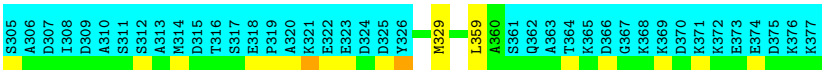
- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 77% 14% 9%

4.2.4 Score per residue for model 4 (medoid)

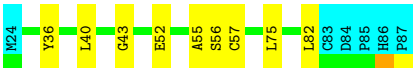
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 44% • 53%



- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 77% 14% 9%



4.2.5 Score per residue for model 5

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 45% • 53%

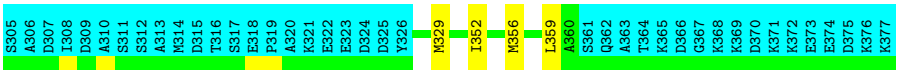
- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 81% 9% 9%

4.2.6 Score per residue for model 6

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 41% 5% 53%



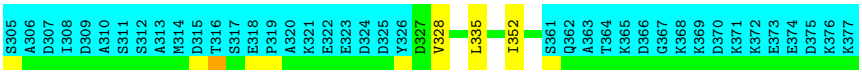
- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 81% 9% 9%

4.2.7 Score per residue for model 7

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 42% • 53%



- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 77% 12% • 9%

4.2.8 Score per residue for model 8

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 45% • 53%

S305 A306 D307 I308 D309 A310 S311 S312 A313 M314 D315 T316 S317 E318 P319 A320 K321 E322 E323 D324 D325 Y326 A355 S361 Q362 A363 T364 K365 D366 G367 K368 K369 D370 K371 K372 E373 E374 D375 K376 K377

- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 78% 12% 9%

M24 Y37 T41 E42 G43 N51 A55 N66 I70 L82 C83 D84 P85 H86 P87

4.2.9 Score per residue for model 9

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 44% • 53%

S305 A306 D307 I308 D309 A310 S311 S312 A313 M314 D315 T316 S317 E318 P319 A320 K321 E322 E323 D324 D325 Y326 M329 L359 A360 S361 Q362 A363 T364 K365 D366 G367 K368 K369 D370 K371 K372 E373 E374 D375 K376 K377

- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 84% 6% 9%

M24 G43 A55 E74 I78 C83 D84 P85 H86 P87

4.2.10 Score per residue for model 10

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 38% 8% 53%

S305 A306 D307 I308 D309 A310 S311 S312 A313 M314 D315 T316 S317 E318 P319 A320 K321 E322 E323 D324 D325 Y326 M329 Q330 D331 I352 A355 L359 A360 S361 Q362 A363 T364 K365 D366 G367 K368 K369 D370 K371 K372 E373 E374 D375 K376 K377

- Molecule 2: Ubiquitin-protein ligase E3A

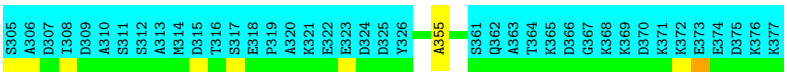
Chain B: 83% 8% 9%

M24 Y36 E42 A55 I70 L82 C83 D84 P85 H86 P87

4.2.11 Score per residue for model 11

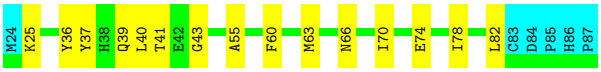
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 45% • 53%



- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 67% 23% 9%



4.2.12 Score per residue for model 12

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 41% 5% 53%

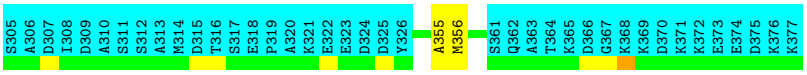
- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 80% 11% 9%

4.2.13 Score per residue for model 13

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 44% • 53%



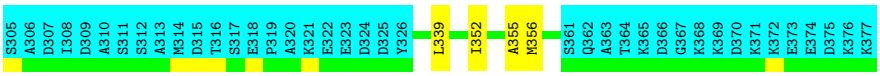
- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 77% 14% 9%

4.2.14 Score per residue for model 14

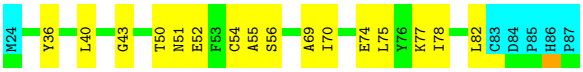
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 41% 5% 53%



- Molecule 2: Ubiquitin-protein ligase E3A

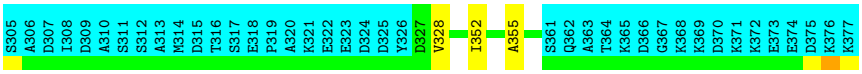
Chain B: 66% 25% 9%



4.2.15 Score per residue for model 15

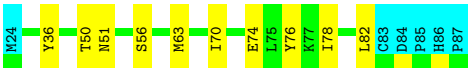
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A: 42% • 53%



- Molecule 2: Ubiquitin-protein ligase E3A

Chain B: 75% 16% 9%



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	

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	1618
Number of shifts mapped to atoms	1618
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	256	244	244	2±1
2	B	454	451	449	5±2
All	All	10665	10425	10395	85

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:40:LEU:O	2:B:55:ALA:HB2	0.76	1.81	3	6
2:B:40:LEU:HD11	2:B:60:PHE:CZ	0.70	2.22	5	1
1:A:329:MET:SD	1:A:359:LEU:HD21	0.67	2.30	4	5
2:B:36:TYR:CD2	2:B:82:LEU:HD21	0.67	2.24	11	4
2:B:40:LEU:HD11	2:B:75:LEU:CD1	0.61	2.25	14	3
2:B:74:GLU:O	2:B:78:ILE:HG22	0.60	1.97	15	5
2:B:43:GLY:CA	2:B:55:ALA:HB3	0.57	2.28	14	10
2:B:50:THR:O	2:B:50:THR:HG23	0.56	2.00	15	3
2:B:37:TYR:O	2:B:41:THR:HG23	0.56	2.01	13	1
2:B:40:LEU:HD11	2:B:60:PHE:CE1	0.56	2.35	11	3
2:B:50:THR:O	2:B:50:THR:HG22	0.56	2.01	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:82:LEU:HD12	2:B:82:LEU:N	0.55	2.17	15	2
2:B:43:GLY:HA3	2:B:55:ALA:HB3	0.54	1.77	7	6
1:A:328:VAL:HG21	2:B:76:TYR:OH	0.53	2.03	15	2
1:A:355:ALA:CB	2:B:70:ILE:HD12	0.53	2.34	11	9
2:B:36:TYR:CE2	2:B:82:LEU:HD21	0.52	2.40	4	2
2:B:43:GLY:HA2	2:B:55:ALA:HB3	0.52	1.82	13	3
2:B:82:LEU:HD12	2:B:82:LEU:H	0.48	1.68	15	2
1:A:352:ILE:HD12	1:A:352:ILE:N	0.48	2.23	2	7
2:B:42:GLU:O	2:B:55:ALA:HB3	0.47	2.09	10	1
2:B:37:TYR:CZ	2:B:41:THR:HG21	0.47	2.45	11	2
1:A:339:LEU:HD22	2:B:69:ALA:HB1	0.44	1.88	14	1
2:B:37:TYR:CE1	2:B:68:ALA:HB3	0.44	2.47	1	1
1:A:338:VAL:HG11	2:B:33:ILE:HG21	0.42	1.91	12	2
1:A:342:LEU:HD22	2:B:37:TYR:CD2	0.41	2.50	2	1
2:B:42:GLU:C	2:B:55:ALA:HB3	0.41	2.36	1	1
1:A:328:VAL:CG1	1:A:335:LEU:HD21	0.40	2.46	7	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	34/73 (47%)	34±1 (99±2%)	0±1 (1±2%)	0±0 (0±0%)	100	100
2	B	58/64 (91%)	56±1 (97±2%)	2±1 (3±2%)	0±0 (0±0%)	100	100
All	All	1380/2055 (67%)	1348 (98%)	32 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	29/62 (47%)	29±0 (99±2%)	0±0 (1±2%)	74 96
2	B	46/52 (88%)	44±1 (96±3%)	2±1 (4±3%)	34 82
All	All	1125/1710 (66%)	1092 (97%)	33 (3%)	45 89

All 14 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)
2	B	66	ASN	5
1	A	356	MET	4
2	B	56	SER	4
2	B	63	MET	4
2	B	57	CYS	3
2	B	52	GLU	3
2	B	39	GLN	2
2	B	65	ASN	2
2	B	59	THR	1
2	B	25	LYS	1
2	B	82	LEU	1
1	A	331	ASP	1
2	B	31	HIS	1
2	B	54	CYS	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 91% for the well-defined parts and 92% 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	1618
Number of shifts mapped to atoms	1618
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
$^{13}C_{\alpha}$	137	-0.17 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	132	0.44 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	136	-0.15 ± 0.05	None needed (< 0.5 ppm)
^{15}N	130	-0.72 ± 0.41	None needed (imprecise)

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 91%, i.e. 1116 atoms were assigned a chemical shift out of a possible 1224. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	456/456 (100%)	184/184 (100%)	184/184 (100%)	88/88 (100%)
Sidechain	632/695 (91%)	433/451 (96%)	187/215 (87%)	12/29 (41%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	28/73 (38%)	28/35 (80%)	0/34 (0%)	0/4 (0%)
Overall	1116/1224 (91%)	645/670 (96%)	371/433 (86%)	100/121 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1616 atoms were assigned a chemical shift out of a possible 1762. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	673/676 (100%)	270/272 (99%)	273/274 (100%)	130/130 (100%)
Sidechain	910/996 (91%)	621/639 (97%)	276/319 (87%)	13/38 (34%)
Aromatic	33/90 (37%)	33/43 (77%)	0/41 (0%)	0/6 (0%)
Overall	1616/1762 (92%)	924/954 (97%)	549/634 (87%)	143/174 (82%)

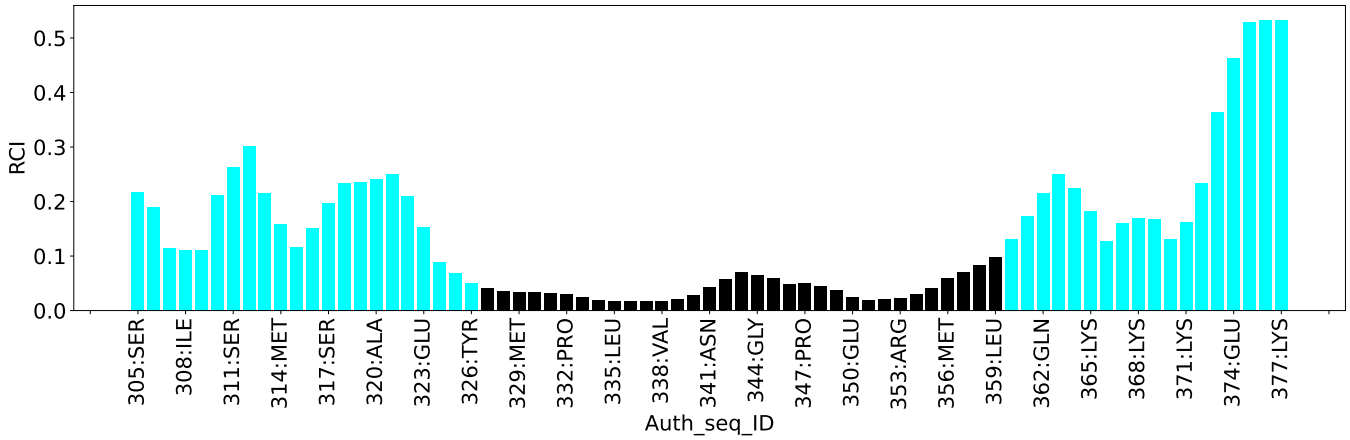
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

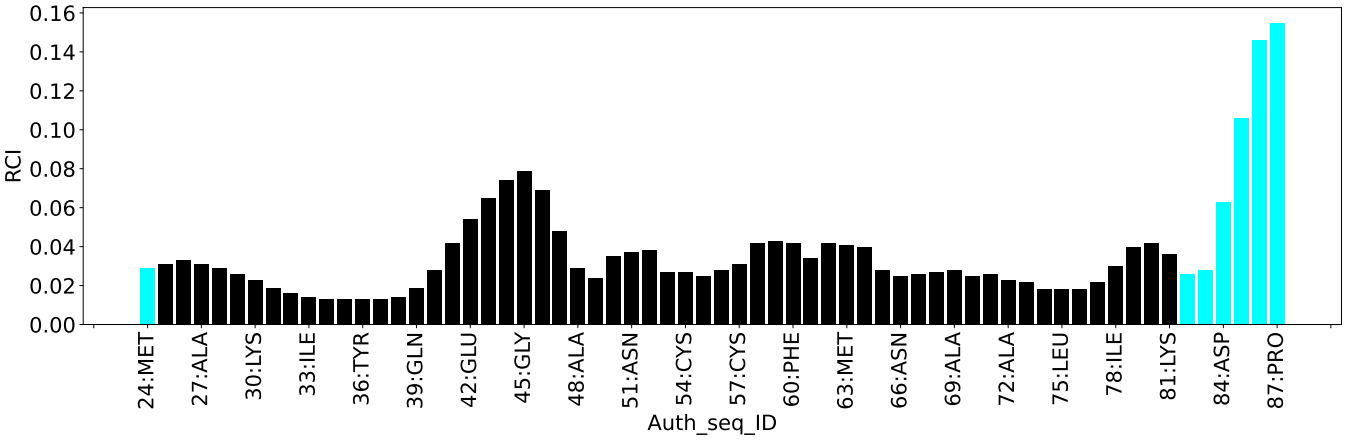
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:


RCI
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
24:MET
27:ALA
30:LYS
33:ILE
36:TYR
39:GLN
42:GLU
45:GLY
48:ALA
51:ASN
54:CYS
57:CYS
60:PHE
63:MET
66:ASN
69:ALA
72:ALA
75:LEU
78:ILE
81:LYS
84:ASP
87:PRO
Auth_seq_ID

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	2097
Intra-residue (|i-j|=0)	799
Sequential (|i-j|=1)	449
Medium range (|i-j|>1 and |i-j|<5)	375
Long range (|i-j|≥5)	171
Inter-chain	219
Hydrogen bond restraints	74
Disulfide bond restraints	10
Total dihedral-angle restraints	176
Number of unmapped restraints	0
Number of restraints per residue	16.6
Number of long range restraints per residue[1]	1.3

[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)	22.9	0.2
0.2-0.5 (Medium)	9.3	0.5
>0.5 (Large)	0.5	2.23

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)	7.1	9.2
10.0-20.0 (Medium)	1.0	20.0
>20.0 (Large)	0.3	30.0

9 Distance violation analysis (i)

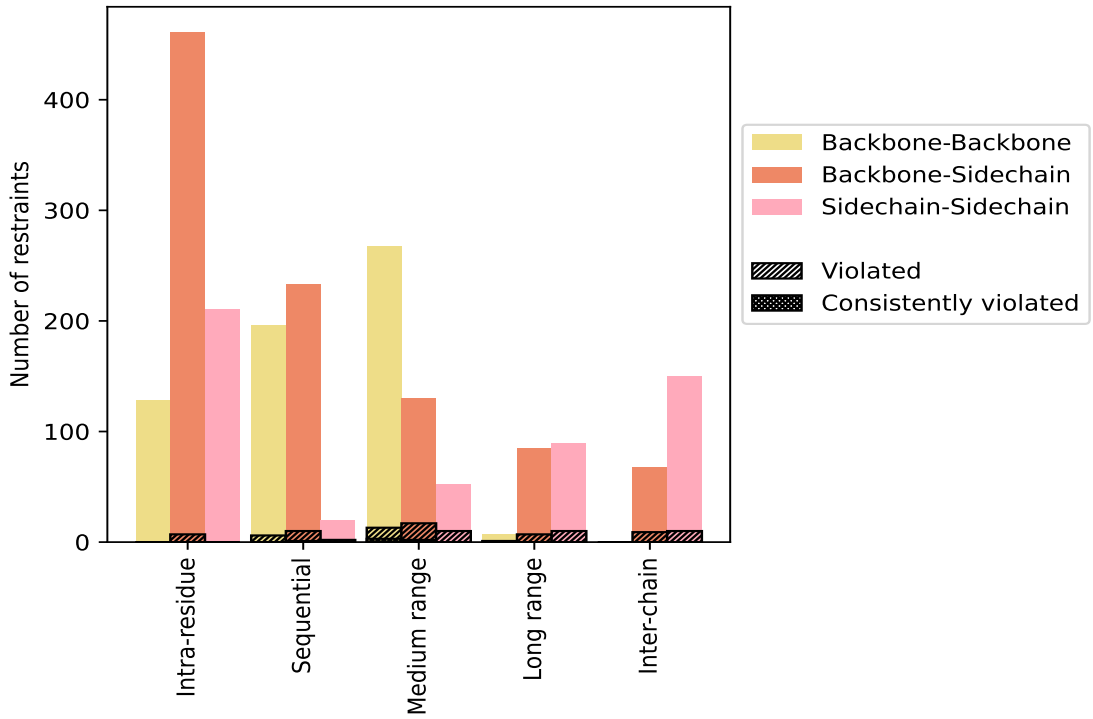
9.1 Summary of distance violations (i)

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)	799	38.1	7	0.9	0.3	0	0.0	0.0
Backbone-Backbone	128	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	461	22.0	7	1.5	0.3	0	0.0	0.0
Sidechain-Sidechain	210	10.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	449	21.4	18	4.0	0.9	1	0.2	0.0
Backbone-Backbone	196	9.3	6	3.1	0.3	0	0.0	0.0
Backbone-Sidechain	233	11.1	10	4.3	0.5	1	0.4	0.0
Sidechain-Sidechain	20	1.0	2	10.0	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	375	17.9	40	10.7	1.9	5	1.3	0.2
Backbone-Backbone	193	9.2	13	6.7	0.6	3	1.6	0.1
Backbone-Sidechain	130	6.2	17	13.1	0.8	2	1.5	0.1
Sidechain-Sidechain	52	2.5	10	19.2	0.5	0	0.0	0.0
Long range (|i-j|≥5)	171	8.2	17	9.9	0.8	0	0.0	0.0
Backbone-Backbone	7	0.3	1	14.3	0.0	0	0.0	0.0
Backbone-Sidechain	85	4.1	7	8.2	0.3	0	0.0	0.0
Sidechain-Sidechain	79	3.8	9	11.4	0.4	0	0.0	0.0
Inter-chain	219	10.4	19	8.7	0.9	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	68	3.2	9	13.2	0.4	0	0.0	0.0
Sidechain-Sidechain	150	7.2	10	6.7	0.5	0	0.0	0.0
Hydrogen bond	74	3.5	0	0.0	0.0	0	0.0	0.0
Disulfide bond	10	0.5	1	10.0	0.0	0	0.0	0.0
Total	2097	100.0	102	4.9	4.9	6	0.3	0.3
Backbone-Backbone	599	28.6	20	3.3	1.0	3	0.5	0.1
Backbone-Sidechain	977	46.6	50	5.1	2.4	3	0.3	0.1
Sidechain-Sidechain	521	24.8	32	6.1	1.5	0	0.0	0.0

[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	6	14	5	6	31	0.19	0.5	0.09	0.16
2	0	9	21	4	4	38	0.17	0.43	0.08	0.14
3	1	6	15	9	4	35	0.18	0.43	0.07	0.15
4	2	9	17	6	1	35	0.21	0.44	0.1	0.17
5	0	6	16	6	4	32	0.18	0.45	0.08	0.15
6	0	4	15	3	5	27	0.18	0.36	0.07	0.16
7	2	7	17	6	4	36	0.29	2.23	0.37	0.18
8	0	4	15	3	3	25	0.17	0.34	0.06	0.14
9	0	3	18	6	5	32	0.16	0.32	0.06	0.14
10	0	9	19	6	4	38	0.21	0.56	0.1	0.18
11	1	3	18	9	6	37	0.21	1.57	0.23	0.15

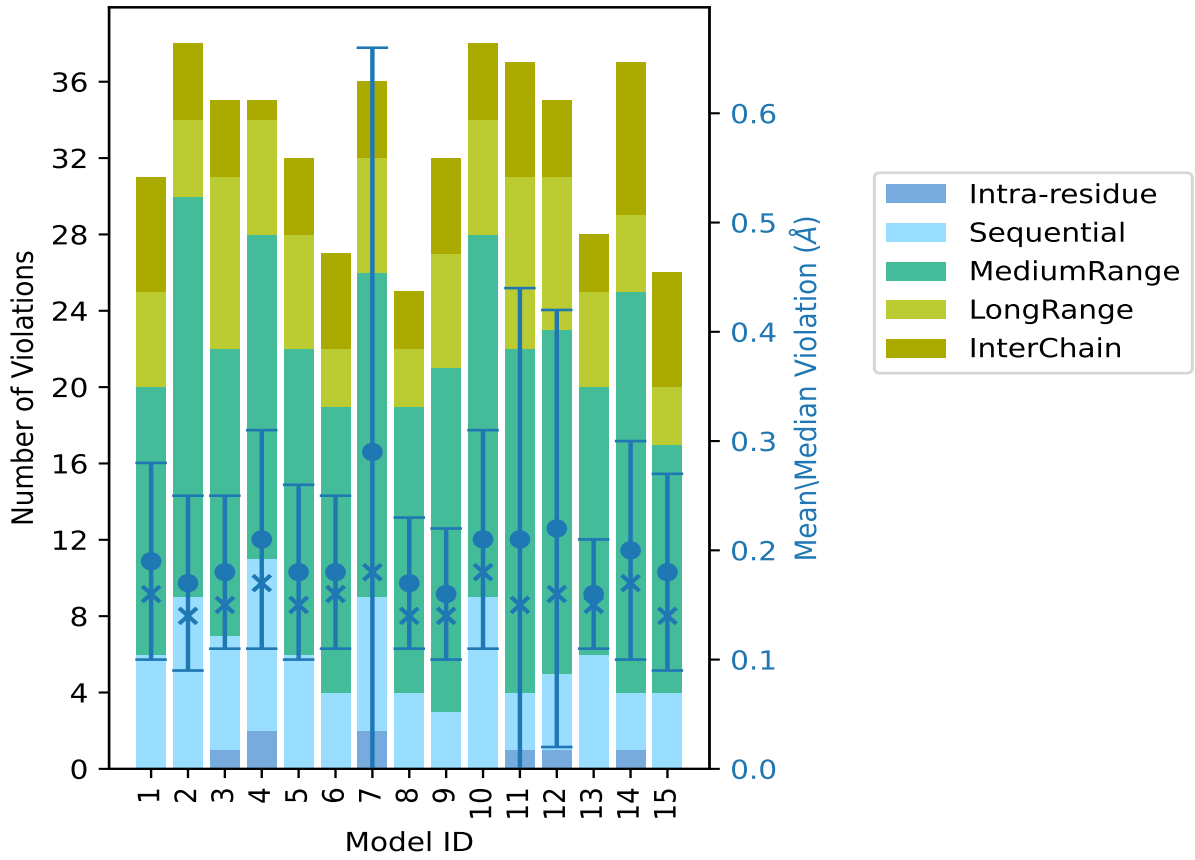
Continued on next page...

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	1	4	18	8	4	35	0.22	1.31	0.2	0.16
13	0	6	14	5	3	28	0.16	0.29	0.05	0.15
14	1	3	21	4	8	37	0.2	0.59	0.1	0.17
15	0	4	13	3	6	26	0.18	0.52	0.09	0.14

[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)

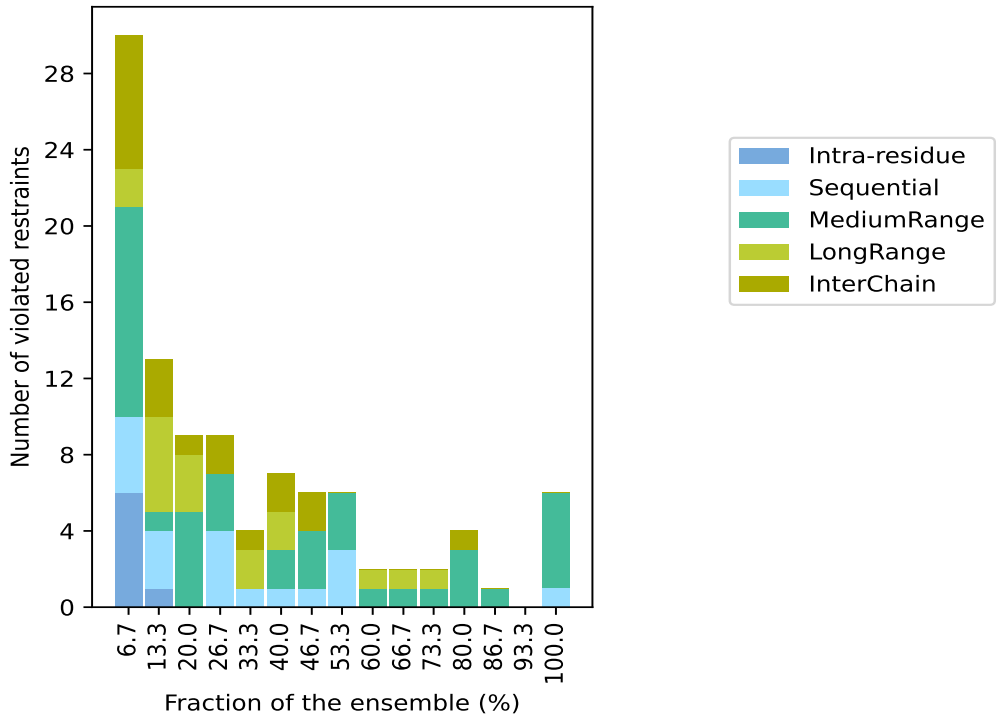
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints

for a given fraction of the ensemble. In total, 1912(IR:792, SQ:431, MR:335, LR:154, IC:200) 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]	%
6	4	11	2	7	30	1	6.7
1	3	1	5	3	13	2	13.3
0	0	5	3	1	9	3	20.0
0	4	3	0	2	9	4	26.7
0	1	0	2	1	4	5	33.3
0	1	2	2	2	7	6	40.0
0	1	3	0	2	6	7	46.7
0	3	3	0	0	6	8	53.3
0	0	1	1	0	2	9	60.0
0	0	1	1	0	2	10	66.7
0	0	1	1	0	2	11	73.3
0	0	3	0	1	4	12	80.0
0	0	1	0	0	1	13	86.7
0	0	0	0	0	0	14	93.3
0	1	5	0	0	6	15	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

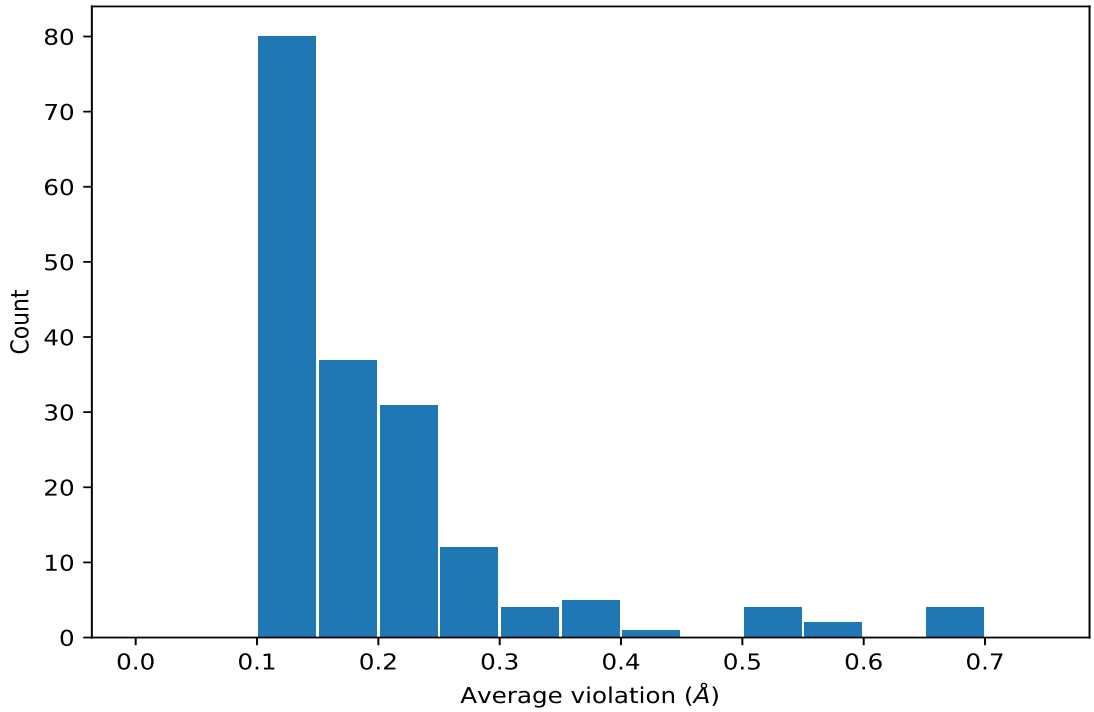
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	15	0.31	0.02	0.31
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	15	0.31	0.02	0.31
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	15	0.31	0.02	0.31
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	15	0.27	0.08	0.26
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	15	0.27	0.08	0.26
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	15	0.21	0.03	0.21
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	15	0.19	0.04	0.18
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	15	0.18	0.06	0.16
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	15	0.18	0.06	0.16
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	15	0.16	0.03	0.16
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	13	0.13	0.01	0.13
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	12	0.21	0.04	0.22
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	12	0.21	0.12	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	12	0.21	0.12	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	12	0.21	0.12	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	12	0.21	0.12	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	12	0.21	0.12	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	12	0.21	0.12	0.17
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	12	0.14	0.03	0.15
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	12	0.14	0.02	0.14
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	11	0.21	0.06	0.24
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	11	0.21	0.06	0.24
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	11	0.15	0.02	0.16
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	10	0.23	0.03	0.23
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	10	0.14	0.03	0.13
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	10	0.14	0.03	0.13
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	10	0.14	0.03	0.13
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	10	0.12	0.01	0.12
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	9	0.15	0.04	0.14
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	9	0.13	0.02	0.13
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	9	0.13	0.02	0.13
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	9	0.13	0.02	0.13
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	8	0.33	0.03	0.34
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	8	0.2	0.03	0.2
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	8	0.17	0.06	0.16
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	8	0.17	0.06	0.16
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	8	0.17	0.06	0.16
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	8	0.16	0.03	0.16
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	8	0.16	0.03	0.16
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	8	0.16	0.03	0.16
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	8	0.12	0.02	0.12
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	8	0.12	0.02	0.12
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	8	0.11	0.0	0.11
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	7	0.25	0.04	0.24
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	7	0.25	0.04	0.24
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	7	0.24	0.04	0.24
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	7	0.24	0.04	0.24
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	7	0.24	0.04	0.24
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	7	0.23	0.08	0.27
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	7	0.23	0.08	0.27
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	7	0.15	0.04	0.13
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	7	0.15	0.04	0.13
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	7	0.15	0.04	0.13
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	7	0.13	0.01	0.12
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	7	0.13	0.01	0.12
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	7	0.12	0.01	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	7	0.12	0.01	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	7	0.12	0.01	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	7	0.12	0.01	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	7	0.12	0.01	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	7	0.12	0.01	0.11
(2,1024)	2:B:63:MET:HG2	2:B:68:ALA:H	6	0.3	0.1	0.34
(2,1024)	2:B:63:MET:HG3	2:B:68:ALA:H	6	0.3	0.1	0.34
(2,389)	1:A:352:ILE:HD11	1:A:353:ARG:H	6	0.19	0.05	0.22
(2,389)	1:A:352:ILE:HD12	1:A:353:ARG:H	6	0.19	0.05	0.22
(2,389)	1:A:352:ILE:HD13	1:A:353:ARG:H	6	0.19	0.05	0.22
(2,819)	2:B:44:CYS:H	2:B:56:SER:H	6	0.17	0.04	0.16
(2,1288)	2:B:78:ILE:HB	2:B:80:ALA:H	6	0.15	0.01	0.15
(2,1057)	2:B:68:ALA:H	2:B:65:ASN:H	6	0.13	0.02	0.13
(2,1900)	1:A:339:LEU:HD11	2:B:73:LEU:HG	6	0.13	0.02	0.12
(2,1900)	1:A:339:LEU:HD12	2:B:73:LEU:HG	6	0.13	0.02	0.12
(2,1900)	1:A:339:LEU:HD13	2:B:73:LEU:HG	6	0.13	0.02	0.12
(2,1900)	1:A:339:LEU:HD21	2:B:73:LEU:HG	6	0.13	0.02	0.12
(2,1900)	1:A:339:LEU:HD22	2:B:73:LEU:HG	6	0.13	0.02	0.12
(2,1900)	1:A:339:LEU:HD23	2:B:73:LEU:HG	6	0.13	0.02	0.12
(2,1809)	1:A:328:VAL:HG11	2:B:26:ARG:HA	6	0.12	0.01	0.12
(2,1809)	1:A:328:VAL:HG12	2:B:26:ARG:HA	6	0.12	0.01	0.12
(2,1809)	1:A:328:VAL:HG13	2:B:26:ARG:HA	6	0.12	0.01	0.12
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG2	5	0.52	0.54	0.31
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG3	5	0.52	0.54	0.31
(2,1973)	1:A:356:MET:HE1	2:B:70:ILE:HA	5	0.27	0.16	0.17
(2,1973)	1:A:356:MET:HE2	2:B:70:ILE:HA	5	0.27	0.16	0.17
(2,1973)	1:A:356:MET:HE3	2:B:70:ILE:HA	5	0.27	0.16	0.17
(2,919)	2:B:36:TYR:HE1	2:B:80:ALA:H	5	0.17	0.03	0.17
(2,919)	2:B:36:TYR:HE2	2:B:80:ALA:H	5	0.17	0.03	0.17
(2,305)	1:A:339:LEU:HB2	1:A:338:VAL:H	5	0.12	0.01	0.12
(2,305)	1:A:339:LEU:HB3	1:A:338:VAL:H	5	0.12	0.01	0.12
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD21	4	0.66	0.91	0.16
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD22	4	0.66	0.91	0.16
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD21	4	0.66	0.91	0.16
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD22	4	0.66	0.91	0.16
(5,8)	1:A:323:GLU:OE1	2:B:25:LYS:NZ	4	0.36	0.2	0.36
(5,8)	1:A:323:GLU:OE2	2:B:25:LYS:NZ	4	0.36	0.2	0.36
(2,966)	2:B:25:LYS:HE2	2:B:26:ARG:H	4	0.28	0.08	0.3
(2,966)	2:B:25:LYS:HE3	2:B:26:ARG:H	4	0.28	0.08	0.3
(2,323)	1:A:321:LYS:HA	1:A:322:GLU:H	4	0.26	0.08	0.28
(2,1357)	2:B:34:GLU:HG2	2:B:31:HIS:HA	4	0.16	0.06	0.14
(2,1357)	2:B:34:GLU:HG3	2:B:31:HIS:HA	4	0.16	0.06	0.14
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD21	4	0.15	0.06	0.12
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD22	4	0.15	0.06	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB2	4	0.14	0.02	0.14
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB3	4	0.14	0.02	0.14
(2,1179)	2:B:55:ALA:H	2:B:56:SER:H	4	0.12	0.01	0.12
(2,1077)	2:B:81:LYS:H	2:B:82:LEU:H	4	0.11	0.0	0.11
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE2	3	0.52	0.56	0.15
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE3	3	0.52	0.56	0.15
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD11	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD12	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD13	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD21	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD22	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD23	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD11	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD12	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD13	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD21	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD22	3	0.2	0.01	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD23	3	0.2	0.01	0.2
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB1	3	0.18	0.1	0.12
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB2	3	0.18	0.1	0.12
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB3	3	0.18	0.1	0.12
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB1	3	0.18	0.1	0.12
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB2	3	0.18	0.1	0.12
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB3	3	0.18	0.1	0.12
(2,841)	2:B:54:CYS:H	2:B:57:CYS:H	3	0.15	0.01	0.15
(2,1330)	2:B:80:ALA:HB1	2:B:78:ILE:HB	3	0.15	0.01	0.15
(2,1330)	2:B:80:ALA:HB2	2:B:78:ILE:HB	3	0.15	0.01	0.15
(2,1330)	2:B:80:ALA:HB3	2:B:78:ILE:HB	3	0.15	0.01	0.15
(4,6)	2:B:49:CYS:CB	3:B:201:ZN:ZN	3	0.14	0.01	0.14
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB2	3	0.13	0.01	0.13
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB3	3	0.13	0.01	0.13
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB2	3	0.13	0.01	0.13
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB3	3	0.13	0.01	0.13
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG12	3	0.13	0.0	0.13
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG13	3	0.13	0.0	0.13
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB2	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB3	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB2	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB3	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB2	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB3	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB2	3	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

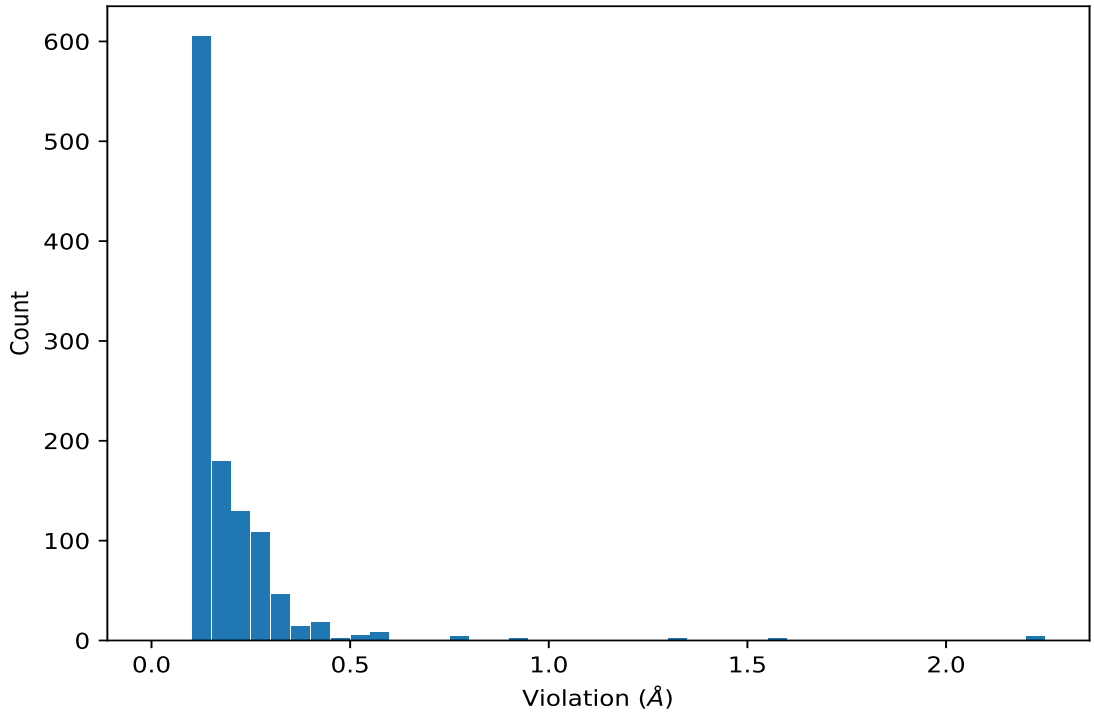
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB3	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB2	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB3	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB2	3	0.12	0.01	0.12
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB3	3	0.12	0.01	0.12
(5,7)	1:A:324:ASP:OD1	2:B:25:LYS:NZ	2	0.56	0.36	0.56
(5,7)	1:A:324:ASP:OD2	2:B:25:LYS:NZ	2	0.56	0.36	0.56
(2,1244)	2:B:32:LEU:HG	2:B:33:ILE:H	2	0.4	0.02	0.4
(2,1035)	2:B:52:GLU:HG2	2:B:52:GLU:H	2	0.39	0.01	0.39
(2,1035)	2:B:52:GLU:HG3	2:B:52:GLU:H	2	0.39	0.01	0.39
(2,1280)	2:B:75:LEU:HG	2:B:76:TYR:H	2	0.36	0.0	0.36
(2,1184)	2:B:60:PHE:HE1	2:B:62:ARG:H	2	0.2	0.04	0.2
(2,1184)	2:B:60:PHE:HE2	2:B:62:ARG:H	2	0.2	0.04	0.2
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD11	2	0.18	0.0	0.18
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD12	2	0.18	0.0	0.18
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD13	2	0.18	0.0	0.18
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD11	2	0.18	0.0	0.18
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD12	2	0.18	0.0	0.18
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD13	2	0.18	0.0	0.18
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB1	2	0.16	0.01	0.16
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB2	2	0.16	0.01	0.16
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB3	2	0.16	0.01	0.16
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB1	2	0.16	0.01	0.16
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB2	2	0.16	0.01	0.16
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB3	2	0.16	0.01	0.16
(4,8)	2:B:83:CYS:CB	3:B:201:ZN:ZN	2	0.16	0.02	0.16
(2,922)	2:B:62:ARG:H	2:B:63:MET:H	2	0.12	0.02	0.12
(2,1994)	1:A:342:LEU:HD11	2:B:69:ALA:H	2	0.12	0.0	0.12
(2,1994)	1:A:342:LEU:HD12	2:B:69:ALA:H	2	0.12	0.0	0.12
(2,1994)	1:A:342:LEU:HD13	2:B:69:ALA:H	2	0.12	0.0	0.12
(2,1994)	1:A:342:LEU:HD21	2:B:69:ALA:H	2	0.12	0.0	0.12
(2,1994)	1:A:342:LEU:HD22	2:B:69:ALA:H	2	0.12	0.0	0.12
(2,1994)	1:A:342:LEU:HD23	2:B:69:ALA:H	2	0.12	0.0	0.12
(4,7)	2:B:54:CYS:CB	3:B:201:ZN:ZN	2	0.12	0.01	0.12
(2,750)	2:B:58:PRO:HD2	2:B:51:ASN:H	2	0.11	0.0	0.11
(2,750)	2:B:58:PRO:HD3	2:B:51:ASN:H	2	0.11	0.0	0.11
(2,1436)	2:B:60:PHE:HE1	2:B:40:LEU:HA	2	0.11	0.0	0.11
(2,1436)	2:B:60:PHE:HE2	2:B:40:LEU:HA	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)
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD21	7	2.23
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD22	7	2.23
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD21	7	2.23
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD22	7	2.23
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG2	11	1.57
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG3	11	1.57
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE2	12	1.31
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE3	12	1.31
(5,7)	1:A:324:ASP:OD1	2:B:25:LYS:NZ	7	0.92
(5,7)	1:A:324:ASP:OD2	2:B:25:LYS:NZ	7	0.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,801)	2:B:53:PHE:HD1	2:B:51:ASN:HD21	7	0.76
(2,801)	2:B:53:PHE:HD1	2:B:51:ASN:HD22	7	0.76
(2,801)	2:B:53:PHE:HD2	2:B:51:ASN:HD21	7	0.76
(2,801)	2:B:53:PHE:HD2	2:B:51:ASN:HD22	7	0.76
(5,8)	1:A:323:GLU:OE1	2:B:25:LYS:NZ	14	0.59
(5,8)	1:A:323:GLU:OE2	2:B:25:LYS:NZ	14	0.59
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	10	0.56
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	10	0.56
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	10	0.56
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	10	0.56
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	10	0.56
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	10	0.56
(5,8)	1:A:323:GLU:OE1	2:B:25:LYS:NZ	15	0.52
(5,8)	1:A:323:GLU:OE2	2:B:25:LYS:NZ	15	0.52
(2,1973)	1:A:356:MET:HE1	2:B:70:ILE:HA	1	0.5
(2,1973)	1:A:356:MET:HE2	2:B:70:ILE:HA	1	0.5
(2,1973)	1:A:356:MET:HE3	2:B:70:ILE:HA	1	0.5
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	5	0.45
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	5	0.45
(2,299)	1:A:323:GLU:HG2	1:A:323:GLU:H	4	0.44
(2,299)	1:A:323:GLU:HG3	1:A:323:GLU:H	4	0.44
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	3	0.43
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	3	0.43
(2,1973)	1:A:356:MET:HE1	2:B:70:ILE:HA	14	0.43
(2,1973)	1:A:356:MET:HE2	2:B:70:ILE:HA	14	0.43
(2,1973)	1:A:356:MET:HE3	2:B:70:ILE:HA	14	0.43
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG2	12	0.43
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG3	12	0.43
(2,1244)	2:B:32:LEU:HG	2:B:33:ILE:H	2	0.43
(2,1790)	1:A:324:ASP:HA	2:B:25:LYS:HE2	14	0.41
(2,1790)	1:A:324:ASP:HA	2:B:25:LYS:HE3	14	0.41
(2,1035)	2:B:52:GLU:HG2	2:B:52:GLU:H	7	0.4
(2,1035)	2:B:52:GLU:HG3	2:B:52:GLU:H	7	0.4
(2,1024)	2:B:63:MET:HG2	2:B:68:ALA:H	1	0.4
(2,1024)	2:B:63:MET:HG3	2:B:68:ALA:H	1	0.4
(2,1024)	2:B:63:MET:HG2	2:B:68:ALA:H	10	0.4
(2,1024)	2:B:63:MET:HG3	2:B:68:ALA:H	10	0.4
(2,1231)	2:B:77:LYS:HE2	2:B:77:LYS:H	12	0.39
(2,1231)	2:B:77:LYS:HE3	2:B:77:LYS:H	12	0.39
(2,1244)	2:B:32:LEU:HG	2:B:33:ILE:H	10	0.38
(2,1035)	2:B:52:GLU:HG2	2:B:52:GLU:H	4	0.38
(2,1035)	2:B:52:GLU:HG3	2:B:52:GLU:H	4	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,966)	2:B:25:LYS:HE2	2:B:26:ARG:H	4	0.37
(2,966)	2:B:25:LYS:HE3	2:B:26:ARG:H	4	0.37
(2,1024)	2:B:63:MET:HG2	2:B:68:ALA:H	4	0.37
(2,1024)	2:B:63:MET:HG3	2:B:68:ALA:H	4	0.37
(2,323)	1:A:321:LYS:HA	1:A:322:GLU:H	7	0.36
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	4	0.36
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	4	0.36
(2,1280)	2:B:75:LEU:HG	2:B:76:TYR:H	2	0.36
(2,1280)	2:B:75:LEU:HG	2:B:76:TYR:H	6	0.36
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	4	0.35
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	5	0.35
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	7	0.35
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	7	0.35
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	7	0.35
(2,438)	1:A:342:LEU:HG	1:A:342:LEU:H	11	0.34
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	7	0.34
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	8	0.34
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	10	0.34
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	12	0.34
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	2	0.34
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	2	0.34
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	2	0.34
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	10	0.34
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	10	0.34
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	10	0.34
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	10	0.34
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	10	0.34
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	2	0.33
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	2	0.33
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	3	0.32
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB1	12	0.32
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB2	12	0.32
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB3	12	0.32
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB1	12	0.32
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB2	12	0.32
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB3	12	0.32
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	4	0.32
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	4	0.32
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	4	0.32
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	5	0.32
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	5	0.32
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	5	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	9	0.32
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	9	0.32
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	9	0.32
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG2	4	0.31
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG3	4	0.31
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	12	0.31
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	12	0.31
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	12	0.31
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	14	0.31
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	14	0.31
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	14	0.31
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	15	0.31
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	15	0.31
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	15	0.31
(2,966)	2:B:25:LYS:HE2	2:B:26:ARG:H	10	0.3
(2,966)	2:B:25:LYS:HE3	2:B:26:ARG:H	10	0.3
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	1	0.3
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	1	0.3
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	1	0.3
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	6	0.3
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	6	0.3
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	6	0.3
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	11	0.3
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	11	0.3
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	11	0.3
(2,1024)	2:B:63:MET:HG2	2:B:68:ALA:H	5	0.3
(2,1024)	2:B:63:MET:HG3	2:B:68:ALA:H	5	0.3
(2,966)	2:B:25:LYS:HE2	2:B:26:ARG:H	9	0.29
(2,966)	2:B:25:LYS:HE3	2:B:26:ARG:H	9	0.29
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	2	0.29
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	9	0.29
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	9	0.29
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	11	0.29
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	11	0.29
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	13	0.29
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	13	0.29
(2,323)	1:A:321:LYS:HA	1:A:322:GLU:H	13	0.29
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	1	0.29
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	1	0.29
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	1	0.29
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	12	0.29
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	12	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	12	0.29
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	12	0.29
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	12	0.29
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	12	0.29
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	12	0.29
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	12	0.29
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	13	0.29
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	13	0.29
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	13	0.29
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	4	0.28
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	4	0.28
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	12	0.28
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	12	0.28
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	10	0.28
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	10	0.28
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	10	0.28
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	6	0.28
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	6	0.28
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	8	0.28
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	8	0.28
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	8	0.28
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	5	0.28
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	5	0.28
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	15	0.28
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	15	0.28
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	3	0.28
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	3	0.28
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	3	0.28
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	6	0.28
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	5	0.27
(2,323)	1:A:321:LYS:HA	1:A:322:GLU:H	3	0.27
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	8	0.27
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	8	0.27
(2,1357)	2:B:34:GLU:HG2	2:B:31:HIS:HA	14	0.27
(2,1357)	2:B:34:GLU:HG3	2:B:31:HIS:HA	14	0.27
(2,1261)	2:B:59:THR:HG21	2:B:59:THR:H	14	0.27
(2,1261)	2:B:59:THR:HG22	2:B:59:THR:H	14	0.27
(2,1261)	2:B:59:THR:HG23	2:B:59:THR:H	14	0.27
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	6	0.27
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	6	0.27
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	7	0.27
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	1	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	1	0.26
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD21	7	0.26
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD22	7	0.26
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	7	0.26
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	7	0.26
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	7	0.26
(2,1793)	1:A:323:GLU:HG2	2:B:25:LYS:HE2	14	0.26
(2,1793)	1:A:323:GLU:HG2	2:B:25:LYS:HE3	14	0.26
(2,1793)	1:A:323:GLU:HG3	2:B:25:LYS:HE2	14	0.26
(2,1793)	1:A:323:GLU:HG3	2:B:25:LYS:HE3	14	0.26
(2,1759)	2:B:78:ILE:HB	2:B:75:LEU:HA	1	0.26
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	11	0.26
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	11	0.26
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	14	0.26
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	14	0.26
(2,1273)	2:B:70:ILE:HD11	2:B:73:LEU:H	3	0.26
(2,1273)	2:B:70:ILE:HD12	2:B:73:LEU:H	3	0.26
(2,1273)	2:B:70:ILE:HD13	2:B:73:LEU:H	3	0.26
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	1	0.26
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	7	0.26
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	14	0.26
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	1	0.26
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	11	0.26
(2,987)	2:B:71:LYS:HE2	2:B:71:LYS:H	3	0.25
(2,987)	2:B:71:LYS:HE3	2:B:71:LYS:H	3	0.25
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	4	0.25
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	10	0.25
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	10	0.25
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	10	0.25
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	3	0.25
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	3	0.25
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	5	0.25
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	5	0.25
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	5	0.25
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	5	0.25
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	5	0.25
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	6	0.25
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	6	0.25
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	7	0.25
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	3	0.24
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	8	0.24
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	14	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	14	0.24
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	14	0.24
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	14	0.24
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	14	0.24
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	9	0.24
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	9	0.24
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	2	0.24
(2,1184)	2:B:60:PHE:HE1	2:B:62:ARG:H	14	0.24
(2,1184)	2:B:60:PHE:HE2	2:B:62:ARG:H	14	0.24
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	15	0.24
(2,919)	2:B:36:TYR:HE1	2:B:80:ALA:H	11	0.23
(2,919)	2:B:36:TYR:HE2	2:B:80:ALA:H	11	0.23
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	6	0.23
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	10	0.23
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	14	0.23
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	7	0.23
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	2	0.23
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	2	0.23
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	14	0.23
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	14	0.23
(2,389)	1:A:352:ILE:HD11	1:A:353:ARG:H	5	0.23
(2,389)	1:A:352:ILE:HD12	1:A:353:ARG:H	5	0.23
(2,389)	1:A:352:ILE:HD13	1:A:353:ARG:H	5	0.23
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	15	0.23
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	15	0.23
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	15	0.23
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	10	0.23
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	10	0.23
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	11	0.23
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	11	0.23
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	13	0.23
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	13	0.23
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	7	0.23
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	7	0.23
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	11	0.23
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	11	0.23
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	9	0.23
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	4	0.23
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	10	0.23
(2,819)	2:B:44:CYS:H	2:B:56:SER:H	10	0.22
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	6	0.22
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	11	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	3	0.22
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	7	0.22
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	7	0.22
(2,389)	1:A:352:ILE:HD11	1:A:353:ARG:H	3	0.22
(2,389)	1:A:352:ILE:HD12	1:A:353:ARG:H	3	0.22
(2,389)	1:A:352:ILE:HD13	1:A:353:ARG:H	3	0.22
(2,389)	1:A:352:ILE:HD11	1:A:353:ARG:H	12	0.22
(2,389)	1:A:352:ILE:HD12	1:A:353:ARG:H	12	0.22
(2,389)	1:A:352:ILE:HD13	1:A:353:ARG:H	12	0.22
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	4	0.22
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	15	0.22
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	15	0.22
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	15	0.22
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	3	0.22
(2,819)	2:B:44:CYS:H	2:B:56:SER:H	7	0.21
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	4	0.21
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	12	0.21
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	8	0.21
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	8	0.21
(2,389)	1:A:352:ILE:HD11	1:A:353:ARG:H	4	0.21
(2,389)	1:A:352:ILE:HD12	1:A:353:ARG:H	4	0.21
(2,389)	1:A:352:ILE:HD13	1:A:353:ARG:H	4	0.21
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	3	0.21
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	3	0.21
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	3	0.21
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	3	0.21
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	3	0.21
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	3	0.21
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD11	14	0.21
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD12	14	0.21
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD13	14	0.21
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD21	14	0.21
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD22	14	0.21
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD23	14	0.21
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD11	14	0.21
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD12	14	0.21
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD13	14	0.21
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD21	14	0.21
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD22	14	0.21
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD23	14	0.21
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	10	0.21
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	7	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	7	0.21
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	7	0.21
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	8	0.21
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	14	0.21
(5,8)	1:A:323:GLU:OE1	2:B:25:LYS:NZ	11	0.2
(5,8)	1:A:323:GLU:OE2	2:B:25:LYS:NZ	11	0.2
(5,7)	1:A:324:ASP:OD1	2:B:25:LYS:NZ	15	0.2
(5,7)	1:A:324:ASP:OD2	2:B:25:LYS:NZ	15	0.2
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	8	0.2
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD21	11	0.2
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD22	11	0.2
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD21	11	0.2
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD22	11	0.2
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	1	0.2
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	15	0.2
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	1	0.2
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	12	0.2
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	2	0.2
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	2	0.2
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	2	0.2
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG12	15	0.2
(2,1653)	2:B:75:LEU:HA	2:B:78:ILE:HG13	15	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD11	10	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD12	10	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD13	10	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD21	10	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD22	10	0.2
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD23	10	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD11	10	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD12	10	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD13	10	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD21	10	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD22	10	0.2
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD23	10	0.2
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	2	0.2
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	9	0.2
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	9	0.2
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	15	0.2
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	15	0.2
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	15	0.2
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	3	0.2
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	5	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	6	0.2
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	9	0.19
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	5	0.19
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	5	0.19
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	5	0.19
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	5	0.19
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	5	0.19
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	5	0.19
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD11	4	0.19
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD12	4	0.19
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD13	4	0.19
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD21	4	0.19
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD22	4	0.19
(2,1518)	2:B:71:LYS:HE2	2:B:75:LEU:HD23	4	0.19
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD11	4	0.19
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD12	4	0.19
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD13	4	0.19
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD21	4	0.19
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD22	4	0.19
(2,1518)	2:B:71:LYS:HE3	2:B:75:LEU:HD23	4	0.19
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	3	0.19
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	10	0.19
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	10	0.19
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	10	0.19
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	10	0.19
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	10	0.19
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	12	0.19
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	12	0.19
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	12	0.19
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	13	0.19
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	2	0.19
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	2	0.19
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	2	0.19
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	2	0.19
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	1	0.18
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	7	0.18
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	7	0.18
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	13	0.18
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	13	0.18
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD11	11	0.18
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD12	11	0.18
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD13	11	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD11	11	0.18
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD12	11	0.18
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD13	11	0.18
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	1	0.18
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	1	0.18
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	1	0.18
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	1	0.18
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	1	0.18
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	1	0.18
(2,1493)	2:B:42:GLU:HG2	2:B:41:THR:HB	10	0.18
(2,1493)	2:B:42:GLU:HG3	2:B:41:THR:HB	10	0.18
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	1	0.18
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	1	0.18
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	1	0.18
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	3	0.18
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	3	0.18
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	3	0.18
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	12	0.18
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	10	0.18
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	8	0.18
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	12	0.18
(2,1026)	2:B:54:CYS:H	2:B:51:ASN:H	12	0.18
(2,1024)	2:B:63:MET:HG2	2:B:68:ALA:H	9	0.18
(2,1024)	2:B:63:MET:HG3	2:B:68:ALA:H	9	0.18
(4,8)	2:B:83:CYS:CB	3:B:201:ZN:ZN	14	0.17
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	13	0.17
(2,919)	2:B:36:TYR:HE1	2:B:80:ALA:H	3	0.17
(2,919)	2:B:36:TYR:HE2	2:B:80:ALA:H	3	0.17
(2,919)	2:B:36:TYR:HE1	2:B:80:ALA:H	6	0.17
(2,919)	2:B:36:TYR:HE2	2:B:80:ALA:H	6	0.17
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	4	0.17
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	13	0.17
(2,861)	2:B:60:PHE:HD1	2:B:62:ARG:H	14	0.17
(2,861)	2:B:60:PHE:HD2	2:B:62:ARG:H	14	0.17
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	5	0.17
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	8	0.17
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	9	0.17
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	11	0.17
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB2	5	0.17
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB3	5	0.17
(2,1973)	1:A:356:MET:HE1	2:B:70:ILE:HA	6	0.17
(2,1973)	1:A:356:MET:HE2	2:B:70:ILE:HA	6	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1973)	1:A:356:MET:HE3	2:B:70:ILE:HA	6	0.17
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD11	8	0.17
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD12	8	0.17
(2,1959)	1:A:352:ILE:HG12	2:B:70:ILE:HD13	8	0.17
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD11	8	0.17
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD12	8	0.17
(2,1959)	1:A:352:ILE:HG13	2:B:70:ILE:HD13	8	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	9	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	9	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	9	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	9	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	9	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	9	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	11	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	11	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	11	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	11	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	11	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	11	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	14	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	14	0.17
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	14	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	14	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	14	0.17
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	14	0.17
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB1	12	0.17
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB2	12	0.17
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB3	12	0.17
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB1	12	0.17
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB2	12	0.17
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB3	12	0.17
(2,1535)	2:B:67:ALA:HB1	2:B:64:ASP:HA	2	0.17
(2,1535)	2:B:67:ALA:HB2	2:B:64:ASP:HA	2	0.17
(2,1535)	2:B:67:ALA:HB3	2:B:64:ASP:HA	2	0.17
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	1	0.17
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	1	0.17
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	1	0.17
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	3	0.17
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	7	0.17
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	10	0.17
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	4	0.17
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	4	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	4	0.17
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	11	0.17
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	11	0.17
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	11	0.17
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	14	0.17
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	14	0.17
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	4	0.17
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	4	0.17
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	10	0.17
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	10	0.16
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	11	0.16
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	14	0.16
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	15	0.16
(2,841)	2:B:54:CYS:H	2:B:57:CYS:H	14	0.16
(2,819)	2:B:44:CYS:H	2:B:56:SER:H	13	0.16
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	9	0.16
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	6	0.16
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	6	0.16
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB2	12	0.16
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB3	12	0.16
(2,1953)	1:A:352:ILE:HD11	2:B:69:ALA:HA	6	0.16
(2,1953)	1:A:352:ILE:HD12	2:B:69:ALA:HA	6	0.16
(2,1953)	1:A:352:ILE:HD13	2:B:69:ALA:HA	6	0.16
(2,1900)	1:A:339:LEU:HD11	2:B:73:LEU:HG	12	0.16
(2,1900)	1:A:339:LEU:HD12	2:B:73:LEU:HG	12	0.16
(2,1900)	1:A:339:LEU:HD13	2:B:73:LEU:HG	12	0.16
(2,1900)	1:A:339:LEU:HD21	2:B:73:LEU:HG	12	0.16
(2,1900)	1:A:339:LEU:HD22	2:B:73:LEU:HG	12	0.16
(2,1900)	1:A:339:LEU:HD23	2:B:73:LEU:HG	12	0.16
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	6	0.16
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	6	0.16
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB1	9	0.16
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB2	9	0.16
(2,1542)	2:B:63:MET:HG2	2:B:68:ALA:HB3	9	0.16
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB1	9	0.16
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB2	9	0.16
(2,1542)	2:B:63:MET:HG3	2:B:68:ALA:HB3	9	0.16
(2,1330)	2:B:80:ALA:HB1	2:B:78:ILE:HB	11	0.16
(2,1330)	2:B:80:ALA:HB2	2:B:78:ILE:HB	11	0.16
(2,1330)	2:B:80:ALA:HB3	2:B:78:ILE:HB	11	0.16
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	8	0.16
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	12	0.16
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	12	0.16
(2,1288)	2:B:78:ILE:HB	2:B:80:ALA:H	2	0.16
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	4	0.16
(2,1195)	2:B:82:LEU:HG	2:B:83:CYS:H	12	0.16
(2,1184)	2:B:60:PHE:HE1	2:B:62:ARG:H	10	0.16
(2,1184)	2:B:60:PHE:HE2	2:B:62:ARG:H	10	0.16
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	5	0.16
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	5	0.16
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	6	0.16
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	1	0.16
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	1	0.16
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	1	0.16
(4,6)	2:B:49:CYS:CB	3:B:201:ZN:ZN	11	0.15
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	11	0.15
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	2	0.15
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	5	0.15
(2,919)	2:B:36:TYR:HE1	2:B:80:ALA:H	9	0.15
(2,919)	2:B:36:TYR:HE2	2:B:80:ALA:H	9	0.15
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	5	0.15
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	10	0.15
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	12	0.15
(2,841)	2:B:54:CYS:H	2:B:57:CYS:H	13	0.15
(2,819)	2:B:44:CYS:H	2:B:56:SER:H	1	0.15
(2,737)	2:B:73:LEU:H	2:B:70:ILE:H	3	0.15
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	14	0.15
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	13	0.15
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	13	0.15
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	14	0.15
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	14	0.15
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	14	0.15
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	14	0.15
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	14	0.15
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	14	0.15
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	6	0.15
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	6	0.15
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	6	0.15
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	6	0.15
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	6	0.15
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	6	0.15
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	8	0.15
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	8	0.15
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	1	0.15
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	7	0.15
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	13	0.15
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	15	0.15
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB2	14	0.15
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB3	14	0.15
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB2	14	0.15
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB3	14	0.15
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG2	13	0.15
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG3	13	0.15
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE2	7	0.15
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE3	7	0.15
(2,1357)	2:B:34:GLU:HG2	2:B:31:HIS:HA	7	0.15
(2,1357)	2:B:34:GLU:HG3	2:B:31:HIS:HA	7	0.15
(2,1330)	2:B:80:ALA:HB1	2:B:78:ILE:HB	9	0.15
(2,1330)	2:B:80:ALA:HB2	2:B:78:ILE:HB	9	0.15
(2,1330)	2:B:80:ALA:HB3	2:B:78:ILE:HB	9	0.15
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	2	0.15
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	2	0.15
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	3	0.15
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	3	0.15
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	5	0.15
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	5	0.15
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	5	0.15
(2,1288)	2:B:78:ILE:HB	2:B:80:ALA:H	9	0.15
(2,1288)	2:B:78:ILE:HB	2:B:80:ALA:H	11	0.15
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	5	0.15
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	11	0.15
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	13	0.15
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	3	0.15
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	3	0.15
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	3	0.15
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	1	0.15
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	12	0.15
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	4	0.15
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	4	0.15
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	4	0.15
(2,1057)	2:B:68:ALA:H	2:B:65:ASN:H	7	0.15
(2,1057)	2:B:68:ALA:H	2:B:65:ASN:H	10	0.15
(2,1024)	2:B:63:MET:HG2	2:B:68:ALA:H	12	0.15
(2,1024)	2:B:63:MET:HG3	2:B:68:ALA:H	12	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,8)	2:B:83:CYS:CB	3:B:201:ZN:ZN	11	0.14
(4,6)	2:B:49:CYS:CB	3:B:201:ZN:ZN	14	0.14
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	15	0.14
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	2	0.14
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	15	0.14
(2,966)	2:B:25:LYS:HE2	2:B:26:ARG:H	1	0.14
(2,966)	2:B:25:LYS:HE3	2:B:26:ARG:H	1	0.14
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	4	0.14
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	8	0.14
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	13	0.14
(2,922)	2:B:62:ARG:H	2:B:63:MET:H	2	0.14
(2,919)	2:B:36:TYR:HE1	2:B:80:ALA:H	5	0.14
(2,919)	2:B:36:TYR:HE2	2:B:80:ALA:H	5	0.14
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	2	0.14
(2,841)	2:B:54:CYS:H	2:B:57:CYS:H	9	0.14
(2,819)	2:B:44:CYS:H	2:B:56:SER:H	2	0.14
(2,795)	2:B:77:LYS:HB2	2:B:76:TYR:H	13	0.14
(2,795)	2:B:77:LYS:HB3	2:B:76:TYR:H	13	0.14
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	2	0.14
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	15	0.14
(2,689)	1:A:328:VAL:HG11	1:A:326:TYR:HD1	2	0.14
(2,689)	1:A:328:VAL:HG11	1:A:326:TYR:HD2	2	0.14
(2,689)	1:A:328:VAL:HG12	1:A:326:TYR:HD1	2	0.14
(2,689)	1:A:328:VAL:HG12	1:A:326:TYR:HD2	2	0.14
(2,689)	1:A:328:VAL:HG13	1:A:326:TYR:HD1	2	0.14
(2,689)	1:A:328:VAL:HG13	1:A:326:TYR:HD2	2	0.14
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	5	0.14
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	5	0.14
(2,305)	1:A:339:LEU:HB2	1:A:338:VAL:H	1	0.14
(2,305)	1:A:339:LEU:HB3	1:A:338:VAL:H	1	0.14
(2,305)	1:A:339:LEU:HB2	1:A:338:VAL:H	2	0.14
(2,305)	1:A:339:LEU:HB3	1:A:338:VAL:H	2	0.14
(2,1973)	1:A:356:MET:HE1	2:B:70:ILE:HA	2	0.14
(2,1973)	1:A:356:MET:HE2	2:B:70:ILE:HA	2	0.14
(2,1973)	1:A:356:MET:HE3	2:B:70:ILE:HA	2	0.14
(2,1900)	1:A:339:LEU:HD11	2:B:73:LEU:HG	10	0.14
(2,1900)	1:A:339:LEU:HD12	2:B:73:LEU:HG	10	0.14
(2,1900)	1:A:339:LEU:HD13	2:B:73:LEU:HG	10	0.14
(2,1900)	1:A:339:LEU:HD21	2:B:73:LEU:HG	10	0.14
(2,1900)	1:A:339:LEU:HD22	2:B:73:LEU:HG	10	0.14
(2,1900)	1:A:339:LEU:HD23	2:B:73:LEU:HG	10	0.14
(2,1809)	1:A:328:VAL:HG11	2:B:26:ARG:HA	9	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1809)	1:A:328:VAL:HG12	2:B:26:ARG:HA	9	0.14
(2,1809)	1:A:328:VAL:HG13	2:B:26:ARG:HA	9	0.14
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	2	0.14
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	2	0.14
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	2	0.14
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	2	0.14
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	2	0.14
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	2	0.14
(2,1711)	2:B:77:LYS:HD2	2:B:78:ILE:HG21	13	0.14
(2,1711)	2:B:77:LYS:HD2	2:B:78:ILE:HG22	13	0.14
(2,1711)	2:B:77:LYS:HD2	2:B:78:ILE:HG23	13	0.14
(2,1711)	2:B:77:LYS:HD3	2:B:78:ILE:HG21	13	0.14
(2,1711)	2:B:77:LYS:HD3	2:B:78:ILE:HG22	13	0.14
(2,1711)	2:B:77:LYS:HD3	2:B:78:ILE:HG23	13	0.14
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	2	0.14
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	2	0.14
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	4	0.14
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	4	0.14
(2,1570)	2:B:68:ALA:HB1	2:B:63:MET:HE1	4	0.14
(2,1570)	2:B:68:ALA:HB1	2:B:63:MET:HE2	4	0.14
(2,1570)	2:B:68:ALA:HB1	2:B:63:MET:HE3	4	0.14
(2,1570)	2:B:68:ALA:HB2	2:B:63:MET:HE1	4	0.14
(2,1570)	2:B:68:ALA:HB2	2:B:63:MET:HE2	4	0.14
(2,1570)	2:B:68:ALA:HB2	2:B:63:MET:HE3	4	0.14
(2,1570)	2:B:68:ALA:HB3	2:B:63:MET:HE1	4	0.14
(2,1570)	2:B:68:ALA:HB3	2:B:63:MET:HE2	4	0.14
(2,1570)	2:B:68:ALA:HB3	2:B:63:MET:HE3	4	0.14
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	14	0.14
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	14	0.14
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	14	0.14
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	10	0.14
(2,1330)	2:B:80:ALA:HB1	2:B:78:ILE:HB	6	0.14
(2,1330)	2:B:80:ALA:HB2	2:B:78:ILE:HB	6	0.14
(2,1330)	2:B:80:ALA:HB3	2:B:78:ILE:HB	6	0.14
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	15	0.14
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	15	0.14
(2,1288)	2:B:78:ILE:HB	2:B:80:ALA:H	6	0.14
(2,1288)	2:B:78:ILE:HB	2:B:80:ALA:H	15	0.14
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	11	0.14
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	2	0.14
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	2	0.14
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	8	0.14
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	8	0.14
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	8	0.14
(2,1057)	2:B:68:ALA:H	2:B:65:ASN:H	15	0.14
(5,8)	1:A:323:GLU:OE1	2:B:25:LYS:NZ	13	0.13
(5,8)	1:A:323:GLU:OE2	2:B:25:LYS:NZ	13	0.13
(4,7)	2:B:54:CYS:CB	3:B:201:ZN:ZN	3	0.13
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	6	0.13
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	4	0.13
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	13	0.13
(2,994)	2:B:39:GLN:HA	2:B:41:THR:H	12	0.13
(2,961)	2:B:25:LYS:HG2	2:B:25:LYS:H	7	0.13
(2,961)	2:B:25:LYS:HG3	2:B:25:LYS:H	7	0.13
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	1	0.13
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	6	0.13
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	11	0.13
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	14	0.13
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB2	7	0.13
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB3	7	0.13
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB2	7	0.13
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB3	7	0.13
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB2	7	0.13
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB3	7	0.13
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB2	7	0.13
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB3	7	0.13
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB2	7	0.13
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB3	7	0.13
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB2	7	0.13
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB3	7	0.13
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	4	0.13
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	4	0.13
(2,389)	1:A:352:ILE:HD11	1:A:353:ARG:H	8	0.13
(2,389)	1:A:352:ILE:HD12	1:A:353:ARG:H	8	0.13
(2,389)	1:A:352:ILE:HD13	1:A:353:ARG:H	8	0.13
(2,323)	1:A:321:LYS:HA	1:A:322:GLU:H	10	0.13
(2,1973)	1:A:356:MET:HE1	2:B:70:ILE:HA	13	0.13
(2,1973)	1:A:356:MET:HE2	2:B:70:ILE:HA	13	0.13
(2,1973)	1:A:356:MET:HE3	2:B:70:ILE:HA	13	0.13
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG12	3	0.13
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG13	3	0.13
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG12	12	0.13
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG13	12	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1919)	1:A:342:LEU:HD11	2:B:37:TYR:HE1	11	0.13
(2,1919)	1:A:342:LEU:HD11	2:B:37:TYR:HE2	11	0.13
(2,1919)	1:A:342:LEU:HD12	2:B:37:TYR:HE1	11	0.13
(2,1919)	1:A:342:LEU:HD12	2:B:37:TYR:HE2	11	0.13
(2,1919)	1:A:342:LEU:HD13	2:B:37:TYR:HE1	11	0.13
(2,1919)	1:A:342:LEU:HD13	2:B:37:TYR:HE2	11	0.13
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	6	0.13
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	6	0.13
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	6	0.13
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	6	0.13
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	6	0.13
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	6	0.13
(2,1809)	1:A:328:VAL:HG11	2:B:26:ARG:HA	14	0.13
(2,1809)	1:A:328:VAL:HG12	2:B:26:ARG:HA	14	0.13
(2,1809)	1:A:328:VAL:HG13	2:B:26:ARG:HA	14	0.13
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	8	0.13
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	8	0.13
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	8	0.13
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	8	0.13
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	8	0.13
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	8	0.13
(2,180)	1:A:361:SER:HA	1:A:363:ALA:H	11	0.13
(2,1706)	2:B:77:LYS:HG2	2:B:74:GLU:HA	15	0.13
(2,1706)	2:B:77:LYS:HG3	2:B:74:GLU:HA	15	0.13
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	3	0.13
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	3	0.13
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	3	0.13
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	6	0.13
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	9	0.13
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB2	5	0.13
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB3	5	0.13
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB2	5	0.13
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB3	5	0.13
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG2	5	0.13
(2,1411)	2:B:54:CYS:HA	2:B:39:GLN:HG3	5	0.13
(2,1344)	2:B:73:LEU:HA	2:B:76:TYR:HD1	2	0.13
(2,1344)	2:B:73:LEU:HA	2:B:76:TYR:HD2	2	0.13
(2,1321)	2:B:71:LYS:HG2	2:B:75:LEU:HD11	9	0.13
(2,1321)	2:B:71:LYS:HG2	2:B:75:LEU:HD12	9	0.13
(2,1321)	2:B:71:LYS:HG2	2:B:75:LEU:HD13	9	0.13
(2,1321)	2:B:71:LYS:HG2	2:B:75:LEU:HD21	9	0.13
(2,1321)	2:B:71:LYS:HG2	2:B:75:LEU:HD22	9	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1321)	2:B:71:LYS:HG2	2:B:75:LEU:HD23	9	0.13
(2,1321)	2:B:71:LYS:HG3	2:B:75:LEU:HD11	9	0.13
(2,1321)	2:B:71:LYS:HG3	2:B:75:LEU:HD12	9	0.13
(2,1321)	2:B:71:LYS:HG3	2:B:75:LEU:HD13	9	0.13
(2,1321)	2:B:71:LYS:HG3	2:B:75:LEU:HD21	9	0.13
(2,1321)	2:B:71:LYS:HG3	2:B:75:LEU:HD22	9	0.13
(2,1321)	2:B:71:LYS:HG3	2:B:75:LEU:HD23	9	0.13
(2,1318)	2:B:75:LEU:HG	2:B:71:LYS:HB2	2	0.13
(2,1318)	2:B:75:LEU:HG	2:B:71:LYS:HB3	2	0.13
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	5	0.13
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	5	0.13
(2,1288)	2:B:78:ILE:HB	2:B:80:ALA:H	14	0.13
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	2	0.13
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	2	0.13
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	2	0.13
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	9	0.13
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	9	0.13
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	9	0.13
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	1	0.13
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	1	0.13
(2,1179)	2:B:55:ALA:H	2:B:56:SER:H	1	0.13
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	7	0.13
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	7	0.13
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	15	0.13
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	15	0.13
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	5	0.13
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	10	0.13
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	10	0.13
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	10	0.13
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	13	0.13
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	13	0.13
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	13	0.13
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	14	0.13
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	14	0.13
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	14	0.13
(4,6)	2:B:49:CYS:CB	3:B:201:ZN:ZN	1	0.12
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	2	0.12
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	5	0.12
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	7	0.12
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	8	0.12
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	9	0.12
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	11	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	15	0.12
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	8	0.12
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	1	0.12
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	2	0.12
(2,819)	2:B:44:CYS:H	2:B:56:SER:H	3	0.12
(2,734)	2:B:78:ILE:HA	2:B:80:ALA:H	6	0.12
(2,728)	2:B:36:TYR:HE1	2:B:32:LEU:H	15	0.12
(2,728)	2:B:36:TYR:HE2	2:B:32:LEU:H	15	0.12
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB2	3	0.12
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB3	3	0.12
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB2	3	0.12
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB3	3	0.12
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB2	3	0.12
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB3	3	0.12
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB2	3	0.12
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB3	3	0.12
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB2	3	0.12
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB3	3	0.12
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB2	3	0.12
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB3	3	0.12
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	2	0.12
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	2	0.12
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	9	0.12
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	9	0.12
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	12	0.12
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	12	0.12
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB2	9	0.12
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB3	9	0.12
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB2	11	0.12
(2,451)	1:A:358:SER:HA	1:A:361:SER:HB3	11	0.12
(2,305)	1:A:339:LEU:HB2	1:A:338:VAL:H	4	0.12
(2,305)	1:A:339:LEU:HB3	1:A:338:VAL:H	4	0.12
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD21	5	0.12
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD22	5	0.12
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD21	9	0.12
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD22	9	0.12
(2,1994)	1:A:342:LEU:HD11	2:B:69:ALA:H	1	0.12
(2,1994)	1:A:342:LEU:HD12	2:B:69:ALA:H	1	0.12
(2,1994)	1:A:342:LEU:HD13	2:B:69:ALA:H	1	0.12
(2,1994)	1:A:342:LEU:HD21	2:B:69:ALA:H	1	0.12
(2,1994)	1:A:342:LEU:HD22	2:B:69:ALA:H	1	0.12
(2,1994)	1:A:342:LEU:HD23	2:B:69:ALA:H	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1994)	1:A:342:LEU:HD11	2:B:69:ALA:H	9	0.12
(2,1994)	1:A:342:LEU:HD12	2:B:69:ALA:H	9	0.12
(2,1994)	1:A:342:LEU:HD13	2:B:69:ALA:H	9	0.12
(2,1994)	1:A:342:LEU:HD21	2:B:69:ALA:H	9	0.12
(2,1994)	1:A:342:LEU:HD22	2:B:69:ALA:H	9	0.12
(2,1994)	1:A:342:LEU:HD23	2:B:69:ALA:H	9	0.12
(2,1974)	1:A:356:MET:HE1	2:B:70:ILE:HD11	1	0.12
(2,1974)	1:A:356:MET:HE1	2:B:70:ILE:HD12	1	0.12
(2,1974)	1:A:356:MET:HE1	2:B:70:ILE:HD13	1	0.12
(2,1974)	1:A:356:MET:HE2	2:B:70:ILE:HD11	1	0.12
(2,1974)	1:A:356:MET:HE2	2:B:70:ILE:HD12	1	0.12
(2,1974)	1:A:356:MET:HE2	2:B:70:ILE:HD13	1	0.12
(2,1974)	1:A:356:MET:HE3	2:B:70:ILE:HD11	1	0.12
(2,1974)	1:A:356:MET:HE3	2:B:70:ILE:HD12	1	0.12
(2,1974)	1:A:356:MET:HE3	2:B:70:ILE:HD13	1	0.12
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG12	5	0.12
(2,1943)	1:A:351:ALA:HA	2:B:70:ILE:HG13	5	0.12
(2,1900)	1:A:339:LEU:HD11	2:B:73:LEU:HG	1	0.12
(2,1900)	1:A:339:LEU:HD12	2:B:73:LEU:HG	1	0.12
(2,1900)	1:A:339:LEU:HD13	2:B:73:LEU:HG	1	0.12
(2,1900)	1:A:339:LEU:HD21	2:B:73:LEU:HG	1	0.12
(2,1900)	1:A:339:LEU:HD22	2:B:73:LEU:HG	1	0.12
(2,1900)	1:A:339:LEU:HD23	2:B:73:LEU:HG	1	0.12
(2,1900)	1:A:339:LEU:HD11	2:B:73:LEU:HG	7	0.12
(2,1900)	1:A:339:LEU:HD12	2:B:73:LEU:HG	7	0.12
(2,1900)	1:A:339:LEU:HD13	2:B:73:LEU:HG	7	0.12
(2,1900)	1:A:339:LEU:HD21	2:B:73:LEU:HG	7	0.12
(2,1900)	1:A:339:LEU:HD22	2:B:73:LEU:HG	7	0.12
(2,1900)	1:A:339:LEU:HD23	2:B:73:LEU:HG	7	0.12
(2,1900)	1:A:339:LEU:HD11	2:B:73:LEU:HG	9	0.12
(2,1900)	1:A:339:LEU:HD12	2:B:73:LEU:HG	9	0.12
(2,1900)	1:A:339:LEU:HD13	2:B:73:LEU:HG	9	0.12
(2,1900)	1:A:339:LEU:HD21	2:B:73:LEU:HG	9	0.12
(2,1900)	1:A:339:LEU:HD22	2:B:73:LEU:HG	9	0.12
(2,1900)	1:A:339:LEU:HD23	2:B:73:LEU:HG	9	0.12
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	3	0.12
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	3	0.12
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	3	0.12
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	3	0.12
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	3	0.12
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	3	0.12
(2,1809)	1:A:328:VAL:HG11	2:B:26:ARG:HA	3	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1809)	1:A:328:VAL:HG12	2:B:26:ARG:HA	3	0.12
(2,1809)	1:A:328:VAL:HG13	2:B:26:ARG:HA	3	0.12
(2,1809)	1:A:328:VAL:HG11	2:B:26:ARG:HA	10	0.12
(2,1809)	1:A:328:VAL:HG12	2:B:26:ARG:HA	10	0.12
(2,1809)	1:A:328:VAL:HG13	2:B:26:ARG:HA	10	0.12
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB1	3	0.12
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB2	3	0.12
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB3	3	0.12
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB1	3	0.12
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB2	3	0.12
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB3	3	0.12
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	12	0.12
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	12	0.12
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	12	0.12
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	13	0.12
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	13	0.12
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	13	0.12
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	4	0.12
(2,1428)	2:B:60:PHE:HD1	2:B:63:MET:HE1	10	0.12
(2,1428)	2:B:60:PHE:HD1	2:B:63:MET:HE2	10	0.12
(2,1428)	2:B:60:PHE:HD1	2:B:63:MET:HE3	10	0.12
(2,1428)	2:B:60:PHE:HD2	2:B:63:MET:HE1	10	0.12
(2,1428)	2:B:60:PHE:HD2	2:B:63:MET:HE2	10	0.12
(2,1428)	2:B:60:PHE:HD2	2:B:63:MET:HE3	10	0.12
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB2	10	0.12
(2,1423)	2:B:60:PHE:HD1	2:B:62:ARG:HB3	10	0.12
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB2	10	0.12
(2,1423)	2:B:60:PHE:HD2	2:B:62:ARG:HB3	10	0.12
(2,1357)	2:B:34:GLU:HG2	2:B:31:HIS:HA	13	0.12
(2,1357)	2:B:34:GLU:HG3	2:B:31:HIS:HA	13	0.12
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	13	0.12
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	13	0.12
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	7	0.12
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	7	0.12
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	7	0.12
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	8	0.12
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	8	0.12
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	8	0.12
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	12	0.12
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	12	0.12
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	12	0.12
(2,1229)	2:B:77:LYS:HD2	2:B:78:ILE:H	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1229)	2:B:77:LYS:HD3	2:B:78:ILE:H	4	0.12
(2,1179)	2:B:55:ALA:H	2:B:56:SER:H	7	0.12
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	2	0.12
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	2	0.12
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	3	0.12
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	3	0.12
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	4	0.12
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	4	0.12
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	3	0.12
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	9	0.12
(2,1103)	2:B:37:TYR:HA	2:B:39:GLN:H	11	0.12
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	5	0.12
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	5	0.12
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	5	0.12
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	7	0.12
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	7	0.12
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	7	0.12
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	9	0.12
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	9	0.12
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	9	0.12
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	6	0.12
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	6	0.12
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	6	0.12
(2,1057)	2:B:68:ALA:H	2:B:65:ASN:H	1	0.12
(2,1057)	2:B:68:ALA:H	2:B:65:ASN:H	3	0.12
(4,7)	2:B:54:CYS:CB	3:B:201:ZN:ZN	9	0.11
(4,5)	2:B:44:CYS:CB	3:B:201:ZN:ZN	12	0.11
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	3	0.11
(4,1)	2:B:44:CYS:SG	3:B:201:ZN:ZN	6	0.11
(2,967)	2:B:46:ASN:H	2:B:47:GLU:H	5	0.11
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	9	0.11
(2,939)	2:B:69:ALA:H	2:B:66:ASN:H	12	0.11
(2,922)	2:B:62:ARG:H	2:B:63:MET:H	15	0.11
(2,885)	2:B:32:LEU:H	2:B:35:ARG:H	3	0.11
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	3	0.11
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	6	0.11
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	7	0.11
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	8	0.11
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	9	0.11
(2,863)	2:B:80:ALA:H	2:B:81:LYS:H	14	0.11
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD21	4	0.11
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD22	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD21	4	0.11
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD22	4	0.11
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD21	14	0.11
(2,802)	2:B:53:PHE:HE1	2:B:51:ASN:HD22	14	0.11
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD21	14	0.11
(2,802)	2:B:53:PHE:HE2	2:B:51:ASN:HD22	14	0.11
(2,750)	2:B:58:PRO:HD2	2:B:51:ASN:H	7	0.11
(2,750)	2:B:58:PRO:HD3	2:B:51:ASN:H	7	0.11
(2,750)	2:B:58:PRO:HD2	2:B:51:ASN:H	10	0.11
(2,750)	2:B:58:PRO:HD3	2:B:51:ASN:H	10	0.11
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB2	12	0.11
(2,695)	1:A:339:LEU:HD11	1:A:347:PRO:HB3	12	0.11
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB2	12	0.11
(2,695)	1:A:339:LEU:HD12	1:A:347:PRO:HB3	12	0.11
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB2	12	0.11
(2,695)	1:A:339:LEU:HD13	1:A:347:PRO:HB3	12	0.11
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB2	12	0.11
(2,695)	1:A:339:LEU:HD21	1:A:347:PRO:HB3	12	0.11
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB2	12	0.11
(2,695)	1:A:339:LEU:HD22	1:A:347:PRO:HB3	12	0.11
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB2	12	0.11
(2,695)	1:A:339:LEU:HD23	1:A:347:PRO:HB3	12	0.11
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE1	11	0.11
(2,687)	1:A:328:VAL:HB	1:A:326:TYR:HE2	11	0.11
(2,389)	1:A:352:ILE:HD11	1:A:353:ARG:H	11	0.11
(2,389)	1:A:352:ILE:HD12	1:A:353:ARG:H	11	0.11
(2,389)	1:A:352:ILE:HD13	1:A:353:ARG:H	11	0.11
(2,305)	1:A:339:LEU:HB2	1:A:338:VAL:H	10	0.11
(2,305)	1:A:339:LEU:HB3	1:A:338:VAL:H	10	0.11
(2,305)	1:A:339:LEU:HB2	1:A:338:VAL:H	12	0.11
(2,305)	1:A:339:LEU:HB3	1:A:338:VAL:H	12	0.11
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD21	6	0.11
(2,1996)	1:A:345:VAL:HA	2:B:65:ASN:HD22	6	0.11
(2,1987)	1:A:326:TYR:HD1	2:B:26:ARG:H	15	0.11
(2,1987)	1:A:326:TYR:HD2	2:B:26:ARG:H	15	0.11
(2,1961)	1:A:352:ILE:HD11	2:B:70:ILE:HB	5	0.11
(2,1961)	1:A:352:ILE:HD12	2:B:70:ILE:HB	5	0.11
(2,1961)	1:A:352:ILE:HD13	2:B:70:ILE:HB	5	0.11
(2,1900)	1:A:339:LEU:HD11	2:B:73:LEU:HG	2	0.11
(2,1900)	1:A:339:LEU:HD12	2:B:73:LEU:HG	2	0.11
(2,1900)	1:A:339:LEU:HD13	2:B:73:LEU:HG	2	0.11
(2,1900)	1:A:339:LEU:HD21	2:B:73:LEU:HG	2	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1900)	1:A:339:LEU:HD22	2:B:73:LEU:HG	2	0.11
(2,1900)	1:A:339:LEU:HD23	2:B:73:LEU:HG	2	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	4	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	4	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	4	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	4	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	4	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	4	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	11	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	11	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	11	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	11	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	11	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	11	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	12	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	12	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	12	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	12	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	12	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	12	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB1	13	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB2	13	0.11
(2,1849)	1:A:334:PHE:HD1	2:B:29:ALA:HB3	13	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB1	13	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB2	13	0.11
(2,1849)	1:A:334:PHE:HD2	2:B:29:ALA:HB3	13	0.11
(2,1809)	1:A:328:VAL:HG11	2:B:26:ARG:HA	8	0.11
(2,1809)	1:A:328:VAL:HG12	2:B:26:ARG:HA	8	0.11
(2,1809)	1:A:328:VAL:HG13	2:B:26:ARG:HA	8	0.11
(2,1809)	1:A:328:VAL:HG11	2:B:26:ARG:HA	11	0.11
(2,1809)	1:A:328:VAL:HG12	2:B:26:ARG:HA	11	0.11
(2,1809)	1:A:328:VAL:HG13	2:B:26:ARG:HA	11	0.11
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB1	15	0.11
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB2	15	0.11
(2,1807)	1:A:326:TYR:HE1	2:B:29:ALA:HB3	15	0.11
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB1	15	0.11
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB2	15	0.11
(2,1807)	1:A:326:TYR:HE2	2:B:29:ALA:HB3	15	0.11
(2,1791)	1:A:324:ASP:HA	2:B:25:LYS:HD2	15	0.11
(2,1791)	1:A:324:ASP:HA	2:B:25:LYS:HD3	15	0.11
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB1	10	0.11
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB2	10	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1635)	2:B:37:TYR:HE1	2:B:72:ALA:HB3	10	0.11
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB1	10	0.11
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB2	10	0.11
(2,1635)	2:B:37:TYR:HE2	2:B:72:ALA:HB3	10	0.11
(2,1544)	2:B:63:MET:HE1	2:B:40:LEU:HD11	10	0.11
(2,1544)	2:B:63:MET:HE1	2:B:40:LEU:HD12	10	0.11
(2,1544)	2:B:63:MET:HE1	2:B:40:LEU:HD13	10	0.11
(2,1544)	2:B:63:MET:HE1	2:B:40:LEU:HD21	10	0.11
(2,1544)	2:B:63:MET:HE1	2:B:40:LEU:HD22	10	0.11
(2,1544)	2:B:63:MET:HE1	2:B:40:LEU:HD23	10	0.11
(2,1544)	2:B:63:MET:HE2	2:B:40:LEU:HD11	10	0.11
(2,1544)	2:B:63:MET:HE2	2:B:40:LEU:HD12	10	0.11
(2,1544)	2:B:63:MET:HE2	2:B:40:LEU:HD13	10	0.11
(2,1544)	2:B:63:MET:HE2	2:B:40:LEU:HD21	10	0.11
(2,1544)	2:B:63:MET:HE2	2:B:40:LEU:HD22	10	0.11
(2,1544)	2:B:63:MET:HE2	2:B:40:LEU:HD23	10	0.11
(2,1544)	2:B:63:MET:HE3	2:B:40:LEU:HD11	10	0.11
(2,1544)	2:B:63:MET:HE3	2:B:40:LEU:HD12	10	0.11
(2,1544)	2:B:63:MET:HE3	2:B:40:LEU:HD13	10	0.11
(2,1544)	2:B:63:MET:HE3	2:B:40:LEU:HD21	10	0.11
(2,1544)	2:B:63:MET:HE3	2:B:40:LEU:HD22	10	0.11
(2,1544)	2:B:63:MET:HE3	2:B:40:LEU:HD23	10	0.11
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD11	2	0.11
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD12	2	0.11
(2,1528)	2:B:67:ALA:HA	2:B:70:ILE:HD13	2	0.11
(2,1436)	2:B:60:PHE:HE1	2:B:40:LEU:HA	5	0.11
(2,1436)	2:B:60:PHE:HE2	2:B:40:LEU:HA	5	0.11
(2,1436)	2:B:60:PHE:HE1	2:B:40:LEU:HA	11	0.11
(2,1436)	2:B:60:PHE:HE2	2:B:40:LEU:HA	11	0.11
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	5	0.11
(2,143)	1:A:349:ASN:H	1:A:351:ALA:H	8	0.11
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE2	9	0.11
(2,1403)	2:B:74:GLU:HA	2:B:77:LYS:HE3	9	0.11
(2,1357)	2:B:34:GLU:HG2	2:B:31:HIS:HA	8	0.11
(2,1357)	2:B:34:GLU:HG3	2:B:31:HIS:HA	8	0.11
(2,1315)	2:B:81:LYS:HG2	2:B:80:ALA:H	14	0.11
(2,1315)	2:B:81:LYS:HG3	2:B:80:ALA:H	14	0.11
(2,1291)	2:B:78:ILE:HG21	2:B:80:ALA:H	4	0.11
(2,1291)	2:B:78:ILE:HG22	2:B:80:ALA:H	4	0.11
(2,1291)	2:B:78:ILE:HG23	2:B:80:ALA:H	4	0.11
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	8	0.11
(2,1282)	2:B:75:LEU:HG	2:B:80:ALA:H	14	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	1	0.11
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	1	0.11
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	1	0.11
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	7	0.11
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	7	0.11
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	7	0.11
(2,1256)	2:B:41:THR:HG21	2:B:68:ALA:H	14	0.11
(2,1256)	2:B:41:THR:HG22	2:B:68:ALA:H	14	0.11
(2,1256)	2:B:41:THR:HG23	2:B:68:ALA:H	14	0.11
(2,1179)	2:B:55:ALA:H	2:B:56:SER:H	4	0.11
(2,1179)	2:B:55:ALA:H	2:B:56:SER:H	10	0.11
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	11	0.11
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	11	0.11
(2,1170)	2:B:26:ARG:HD2	2:B:27:ALA:H	13	0.11
(2,1170)	2:B:26:ARG:HD3	2:B:27:ALA:H	13	0.11
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	2	0.11
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	13	0.11
(2,1116)	2:B:65:ASN:HA	2:B:67:ALA:H	14	0.11
(2,1102)	2:B:37:TYR:H	2:B:40:LEU:H	3	0.11
(2,1077)	2:B:81:LYS:H	2:B:82:LEU:H	2	0.11
(2,1077)	2:B:81:LYS:H	2:B:82:LEU:H	4	0.11
(2,1077)	2:B:81:LYS:H	2:B:82:LEU:H	7	0.11
(2,1077)	2:B:81:LYS:H	2:B:82:LEU:H	8	0.11
(2,1070)	2:B:68:ALA:HB1	2:B:66:ASN:H	12	0.11
(2,1070)	2:B:68:ALA:HB2	2:B:66:ASN:H	12	0.11
(2,1070)	2:B:68:ALA:HB3	2:B:66:ASN:H	12	0.11
(2,1061)	2:B:68:ALA:HB1	2:B:64:ASP:H	11	0.11
(2,1061)	2:B:68:ALA:HB2	2:B:64:ASP:H	11	0.11
(2,1061)	2:B:68:ALA:HB3	2:B:64:ASP:H	11	0.11
(2,1057)	2:B:68:ALA:H	2:B:65:ASN:H	2	0.11

10 Dihedral-angle violation analysis (i)

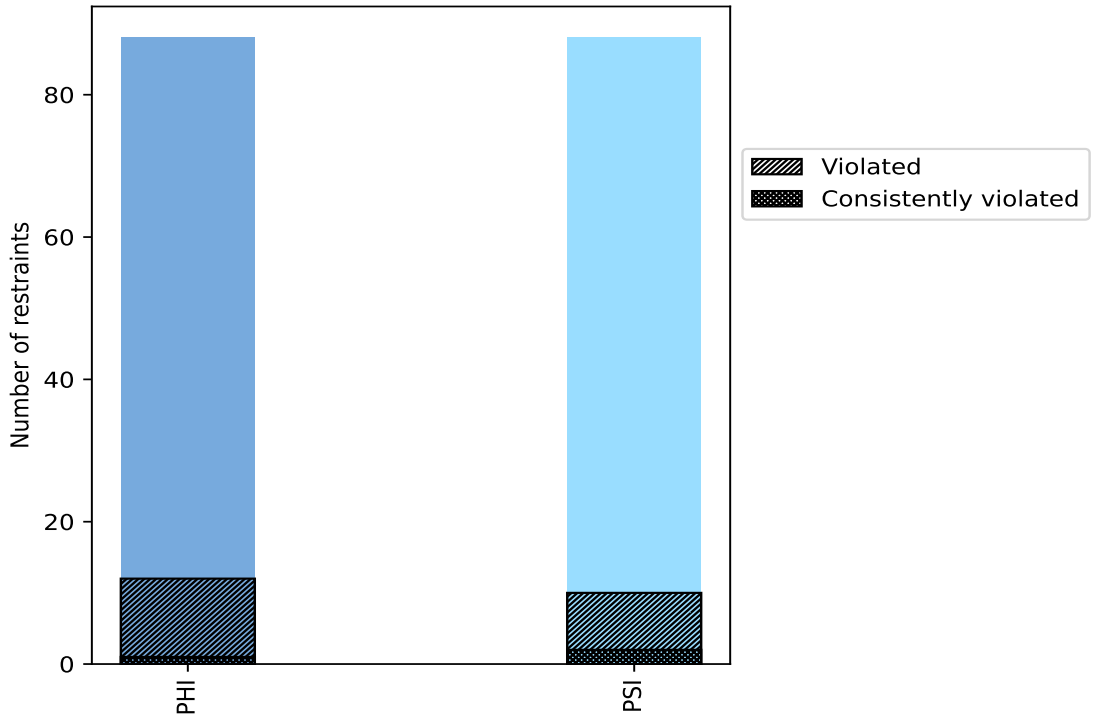
10.1 Summary of dihedral-angle violations (i)

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	88	50.0	12	13.6	6.8	1	1.1	0.6
PSI	88	50.0	10	11.4	5.7	2	2.3	1.1
Total	176	100.0	22	12.5	12.5	3	1.7	1.7

[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)



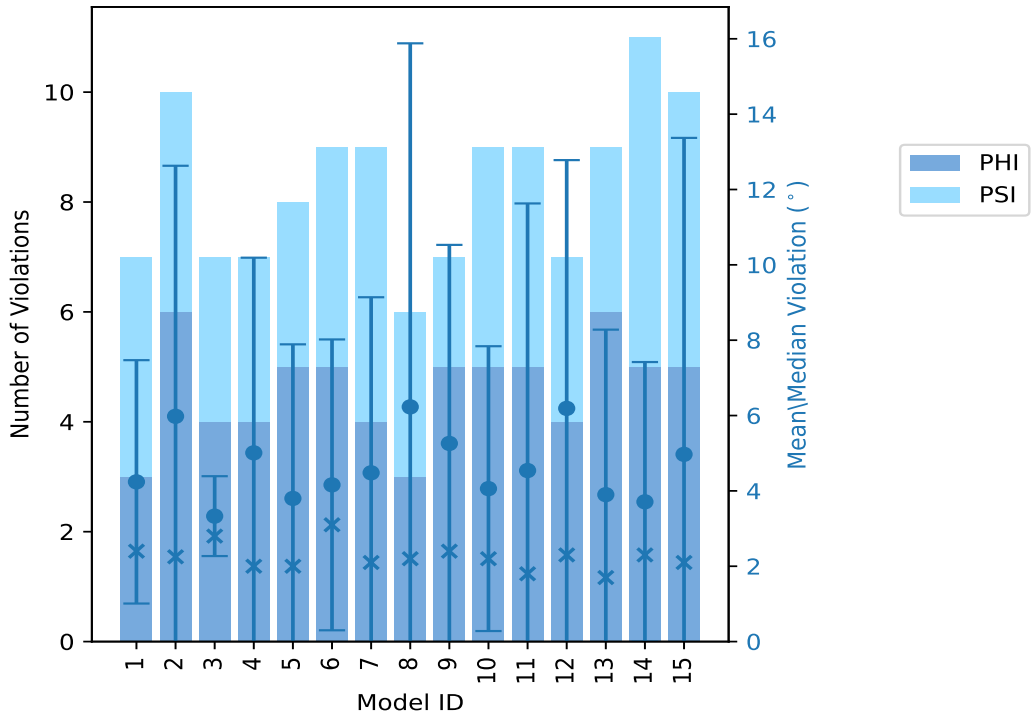
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	3	4	7	4.24	11.0	3.23	2.4
2	6	4	10	5.98	22.7	6.65	2.25
3	4	3	7	3.33	5.3	1.06	2.8
4	4	3	7	5.01	14.5	5.18	2.0
5	5	3	8	3.8	14.1	4.09	2.0
6	5	4	9	4.16	14.4	3.86	3.1
7	4	5	9	4.48	15.4	4.66	2.1
8	3	3	6	6.23	27.8	9.65	2.2
9	5	2	7	5.26	15.8	5.27	2.4
10	5	4	9	4.06	13.2	3.78	2.2
11	5	4	9	4.54	24.3	7.09	1.8
12	4	3	7	6.19	20.0	6.59	2.3
13	6	3	9	3.9	14.3	4.38	1.7
14	5	6	11	3.71	13.4	3.71	2.3
15	5	5	10	4.97	30.0	8.4	2.1

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

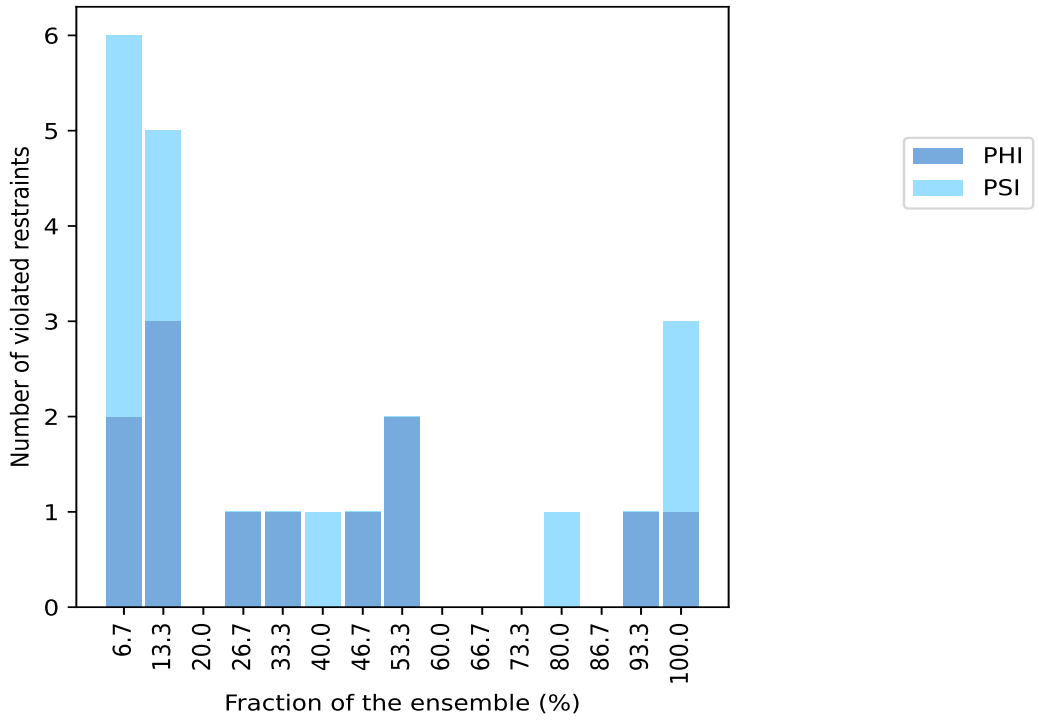
10.3 Dihedral-angle violation statistics for the ensemble (i)

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	4	6	1	6.7
3	2	5	2	13.3
0	0	0	3	20.0
1	0	1	4	26.7
1	0	1	5	33.3
0	1	1	6	40.0
1	0	1	7	46.7
2	0	2	8	53.3
0	0	0	9	60.0
0	0	0	10	66.7
0	0	0	11	73.3
0	1	1	12	80.0
0	0	0	13	86.7
1	0	1	14	93.3
1	2	3	15	100.0

[1] Number of models with violations

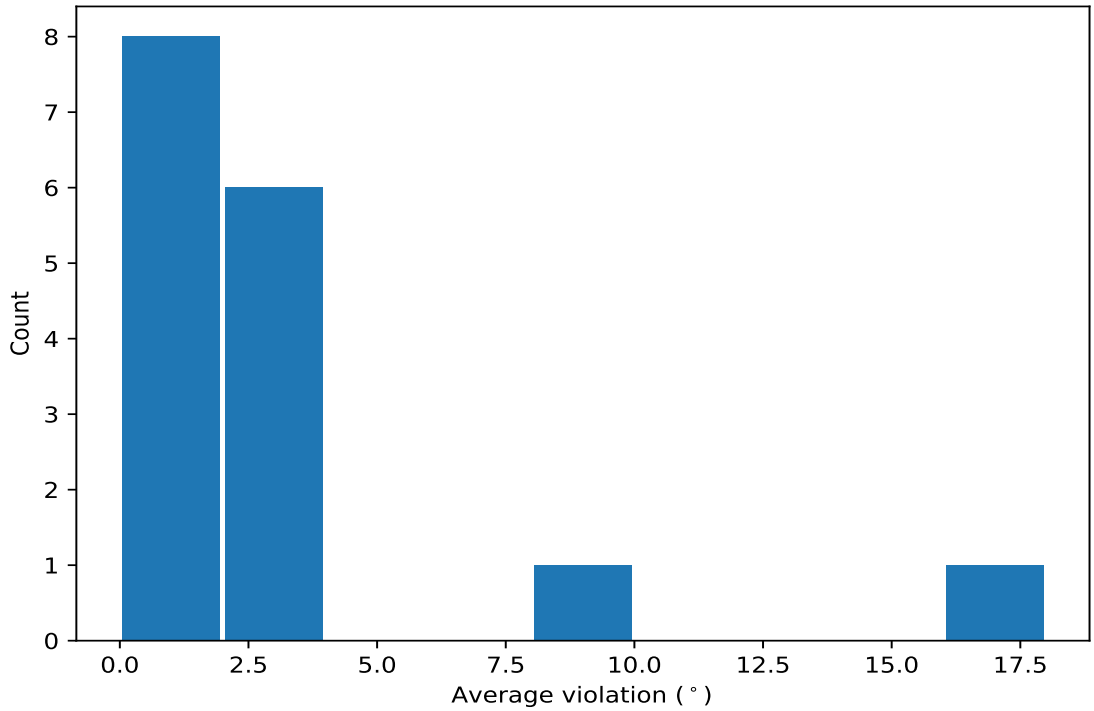
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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.

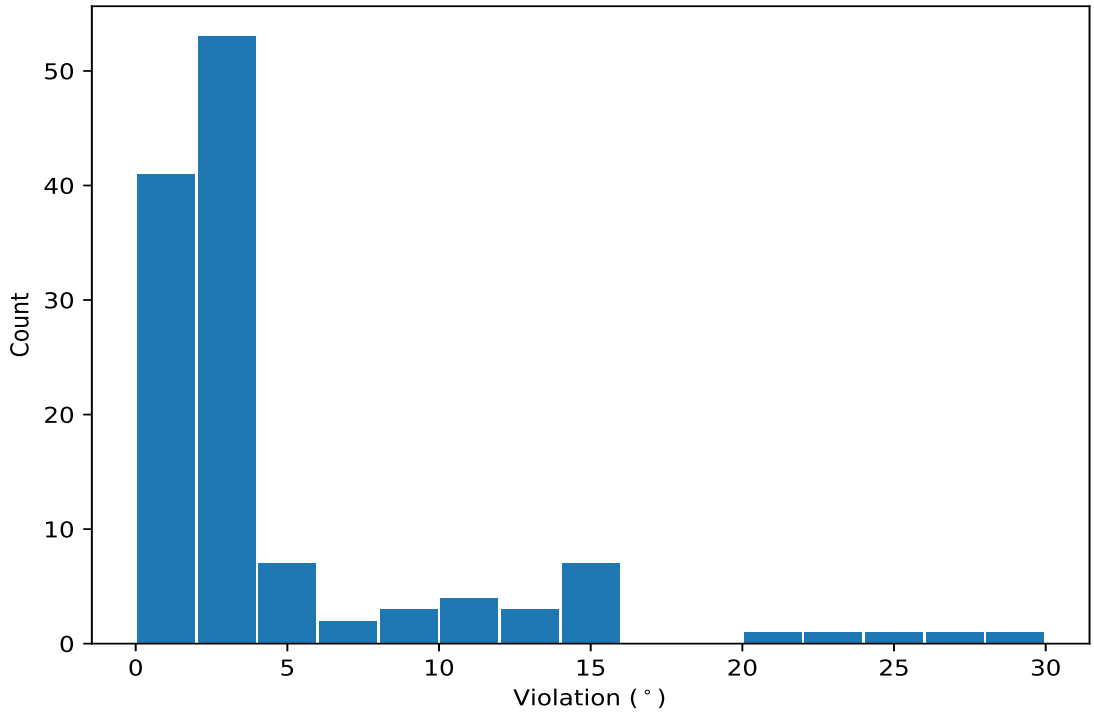
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	15	16.55	6.46	14.4
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	15	2.11	0.28	2.1
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	15	1.99	0.31	2.0
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	14	8.98	4.16	8.7
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	12	2.27	0.41	2.3
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	8	2.53	0.33	2.45
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	8	1.52	0.29	1.4
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	7	2.06	0.82	2.0
(1,139)	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	2:B:45:GLY:N	6	1.48	0.36	1.4
(1,6)	1:A:329:MET:C	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	5	3.14	0.99	3.8
(1,84)	2:B:43:GLY:C	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	4	1.45	0.21	1.35
(1,23)	1:A:347:PRO:C	1:A:348:ASN:N	1:A:348:ASN:CA	1:A:348:ASN:C	2	2.5	0.3	2.5
(1,173)	2:B:81:LYS:N	2:B:81:LYS:CA	2:B:81:LYS:C	2:B:82:LEU:N	2	1.95	0.55	1.95
(1,117)	2:B:79:ASN:C	2:B:80:ALA:N	2:B:80:ALA:CA	2:B:80:ALA:C	2	1.7	0.4	1.7
(1,38)	1:A:329:MET:N	1:A:329:MET:CA	1:A:329:MET:C	1:A:330:GLN:N	2	1.45	0.35	1.45
(1,16)	1:A:340:GLU:C	1:A:341:ASN:N	1:A:341:ASN:CA	1:A:341:ASN:C	2	1.2	0.1	1.2

[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 (°)
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	15	30.0
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	8	27.8
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	11	24.3
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	2	22.7
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	12	20.0
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	9	15.8
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	7	15.4
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	4	14.5
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	6	14.4
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	13	14.3
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	5	14.1
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	2	14.0
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	14	13.4
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	10	13.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	12	12.1
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	4	11.7
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	1	11.0
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	9	10.8
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	7	10.2
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	13	9.2
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	14	9.2
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	10	8.2
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	1	7.1
(1,56)	1:A:348:ASN:N	1:A:348:ASN:CA	1:A:348:ASN:C	1:A:349:ASN:N	2	6.1
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	6	5.7
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	5	5.5
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	11	5.4
(1,20)	1:A:344:GLY:C	1:A:345:VAL:N	1:A:345:VAL:CA	1:A:345:VAL:C	3	5.3
(1,24)	1:A:348:ASN:C	1:A:349:ASN:N	1:A:349:ASN:CA	1:A:349:ASN:C	2	5.2
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	15	4.6
(1,21)	1:A:345:VAL:C	1:A:346:ASP:N	1:A:346:ASP:CA	1:A:346:ASP:C	3	4.1
(1,6)	1:A:329:MET:C	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	3	3.9
(1,6)	1:A:329:MET:C	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	6	3.8
(1,6)	1:A:329:MET:C	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	7	3.8
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	6	3.7
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	10	3.2
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	6	3.1
(1,6)	1:A:329:MET:C	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	15	2.9
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	1	2.9
(1,23)	1:A:347:PRO:C	1:A:348:ASN:N	1:A:348:ASN:CA	1:A:348:ASN:C	12	2.8
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	3	2.8
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	3	2.6
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	13	2.6
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	9	2.6
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	3	2.5
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	14	2.5
(1,173)	2:B:81:LYS:N	2:B:81:LYS:CA	2:B:81:LYS:C	2:B:82:LEU:N	14	2.5
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	8	2.5
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	10	2.5
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	1	2.4
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	4	2.4
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	7	2.4
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	1	2.4
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	9	2.4
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	15	2.4
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	6	2.3
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	14	2.3
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	2	2.3
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	12	2.3
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	12	2.3
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	14	2.3
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	8	2.2
(1,23)	1:A:347:PRO:C	1:A:348:ASN:N	1:A:348:ASN:CA	1:A:348:ASN:C	2	2.2
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	5	2.2
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	8	2.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,139)	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	2:B:45:GLY:N	10	2.2
(1,137)	2:B:40:LEU:N	2:B:40:LEU:CA	2:B:40:LEU:C	2:B:41:THR:N	1	2.2
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	2	2.1
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	12	2.1
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	15	2.1
(1,2)	1:A:324:ASP:C	1:A:325:ASP:N	1:A:325:ASP:CA	1:A:325:ASP:C	5	2.1
(1,175)	2:B:84:ASP:N	2:B:84:ASP:CA	2:B:84:ASP:C	2:B:85:PRO:N	7	2.1
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	3	2.1
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	10	2.1
(1,117)	2:B:79:ASN:C	2:B:80:ALA:N	2:B:80:ALA:CA	2:B:80:ALA:C	10	2.1
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	15	2.1
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	4	2.0
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	9	2.0
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	11	2.0
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	4	2.0
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	11	2.0
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	2	2.0
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	6	2.0
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	14	2.0
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	9	1.9
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	10	1.9
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	5	1.9
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	13	1.9
(1,84)	2:B:43:GLY:C	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	11	1.8
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	5	1.8
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	7	1.8
(1,38)	1:A:329:MET:N	1:A:329:MET:CA	1:A:329:MET:C	1:A:330:GLN:N	14	1.8
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	7	1.8
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	14	1.8
(1,39)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:ASP:N	15	1.7
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	1	1.7
(1,146)	2:B:53:PHE:N	2:B:53:PHE:CA	2:B:53:PHE:C	2:B:54:CYS:N	13	1.7
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	12	1.7
(1,1)	1:A:323:GLU:C	1:A:324:ASP:N	1:A:324:ASP:CA	1:A:324:ASP:C	14	1.7
(1,64)	1:A:356:MET:N	1:A:356:MET:CA	1:A:356:MET:C	1:A:357:GLY:N	2	1.6
(1,139)	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	2:B:45:GLY:N	2	1.6
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	5	1.5
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	11	1.5
(1,139)	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	2:B:45:GLY:N	7	1.5
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	13	1.5
(1,84)	2:B:43:GLY:C	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	8	1.4
(1,173)	2:B:81:LYS:N	2:B:81:LYS:CA	2:B:81:LYS:C	2:B:82:LEU:N	15	1.4
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	4	1.4
(1,140)	2:B:45:GLY:N	2:B:45:GLY:CA	2:B:45:GLY:C	2:B:46:ASN:N	11	1.4
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	11	1.4
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	6	1.3
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	7	1.3
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	8	1.3
(1,94)	2:B:55:ALA:C	2:B:56:SER:N	2:B:56:SER:CA	2:B:56:SER:C	13	1.3
(1,84)	2:B:43:GLY:C	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	13	1.3
(1,84)	2:B:43:GLY:C	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	15	1.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:A:329:MET:C	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	13	1.3
(1,16)	1:A:340:GLU:C	1:A:341:ASN:N	1:A:341:ASN:CA	1:A:341:ASN:C	9	1.3
(1,139)	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	2:B:45:GLY:N	14	1.3
(1,117)	2:B:79:ASN:C	2:B:80:ALA:N	2:B:80:ALA:CA	2:B:80:ALA:C	5	1.3
(1,139)	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	2:B:45:GLY:N	15	1.2
(1,38)	1:A:329:MET:N	1:A:329:MET:CA	1:A:329:MET:C	1:A:330:GLN:N	11	1.1
(1,16)	1:A:340:GLU:C	1:A:341:ASN:N	1:A:341:ASN:CA	1:A:341:ASN:C	4	1.1
(1,139)	2:B:44:CYS:N	2:B:44:CYS:CA	2:B:44:CYS:C	2:B:45:GLY:N	6	1.1
(1,115)	2:B:77:LYS:C	2:B:78:ILE:N	2:B:78:ILE:CA	2:B:78:ILE:C	10	1.1