



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 08:08 PM UTC

PDB ID : 2M5T / pdb_00002m5t
BMRB ID : 19079
Title : Solution structure of the 2A proteinase from a common cold agent, human rhinovirus RV-C02, strain W12
Authors : Lee, W.; Frederick, R.; Tonelli, M.; Troupis, A.T.; Reinin, N.; Suchy, F.P.; Moyer, K.; Watters, K.; Aceti, D.; Palmenberg, A.C.; Markley, J.L.
Deposited on : 2013-03-07

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

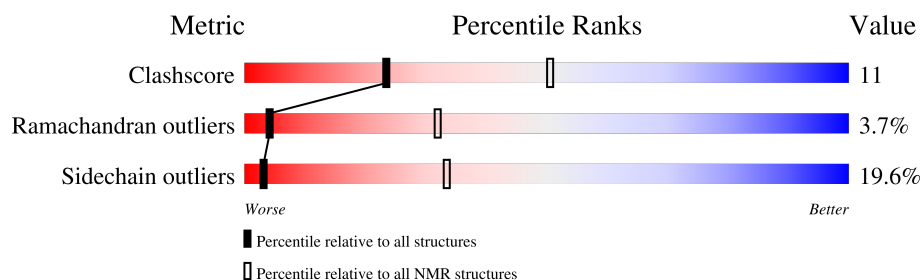
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	142	56% 37% • 6%

2 Ensemble composition and analysis

This entry contains 15 models. Model 8 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:6-A:138 (133)	1.13	8

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2119 atoms, of which 1027 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called human rhinovirus 2A proteinase.

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2118	685	1027	183	216	7	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	CYS	engineered mutation	UNP I2CMJ2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

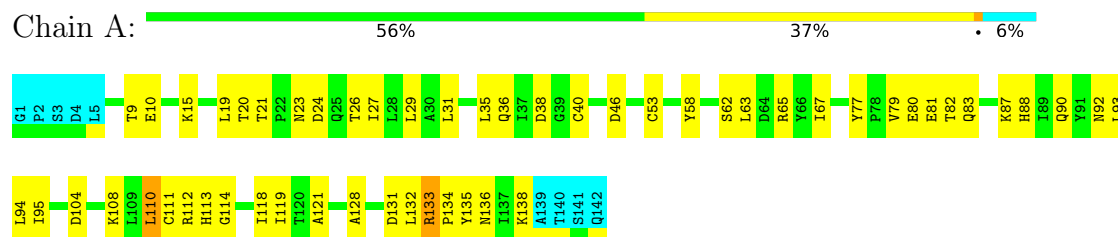
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: human rhinovirus 2A proteinase

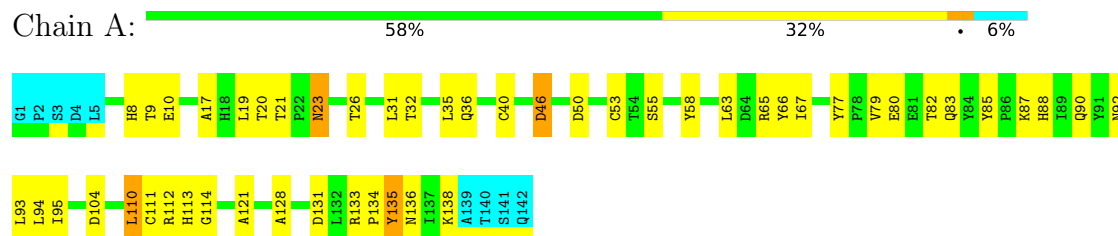


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

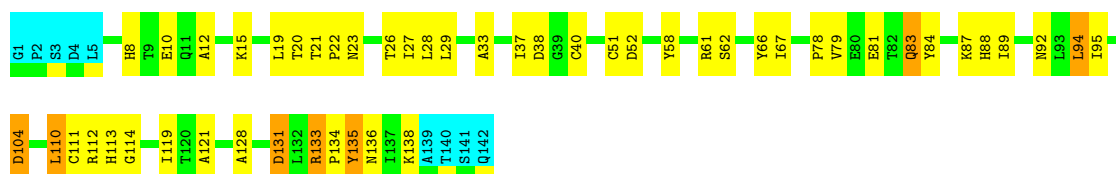
- Molecule 1: human rhinovirus 2A proteinase



4.2.2 Score per residue for model 2

- Molecule 1: human rhinovirus 2A proteinase

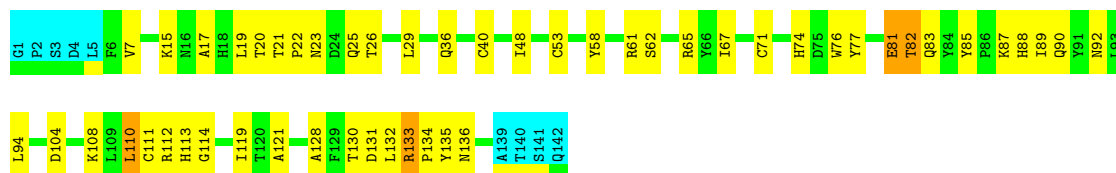




4.2.3 Score per residue for model 3

- Molecule 1: human rhinovirus 2A proteinase

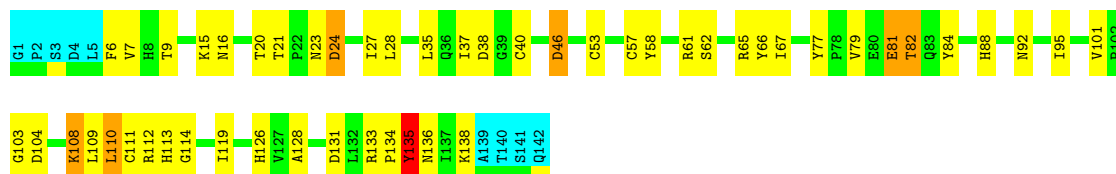
Chain A: 58% 33% 6%



4.2.4 Score per residue for model 4

- Molecule 1: human rhinovirus 2A proteinase

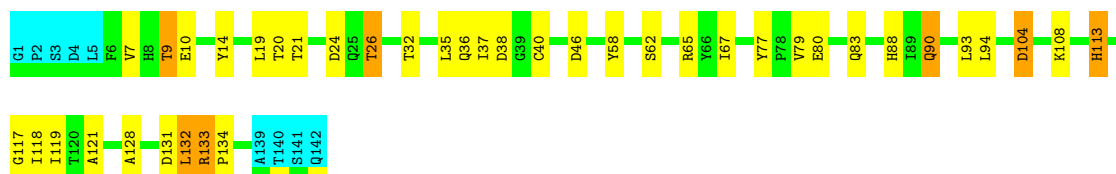
Chain A: 58% 31% 6%



4.2.5 Score per residue for model 5

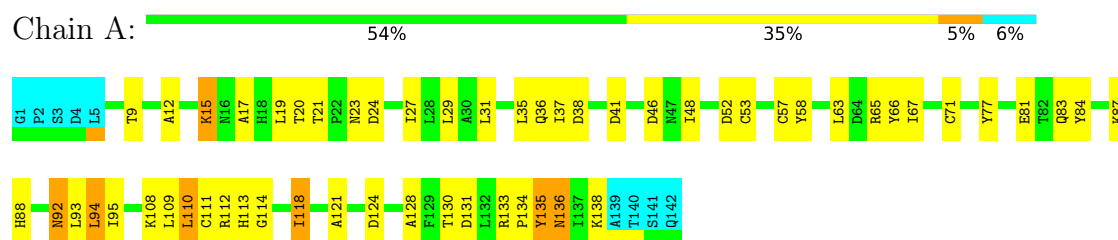
- Molecule 1: human rhinovirus 2A proteinase

Chain A: 65% 23% 5% 6%



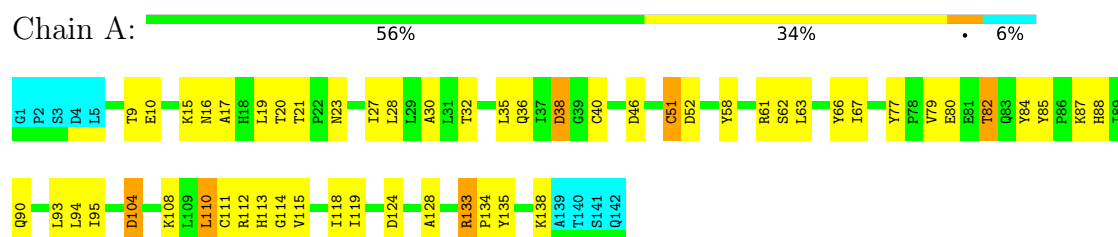
4.2.6 Score per residue for model 6

- Molecule 1: human rhinovirus 2A proteinase



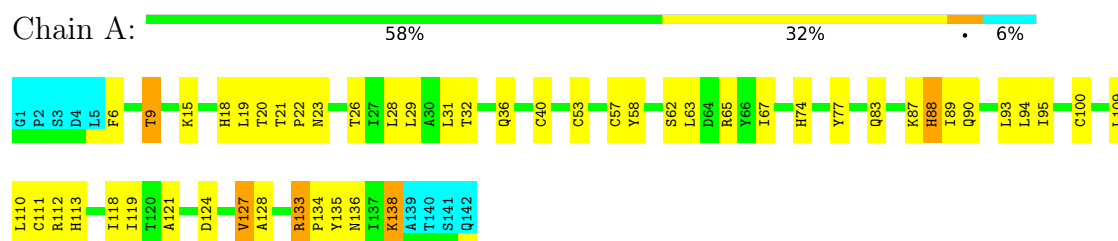
4.2.7 Score per residue for model 7

- Molecule 1: human rhinovirus 2A proteinase



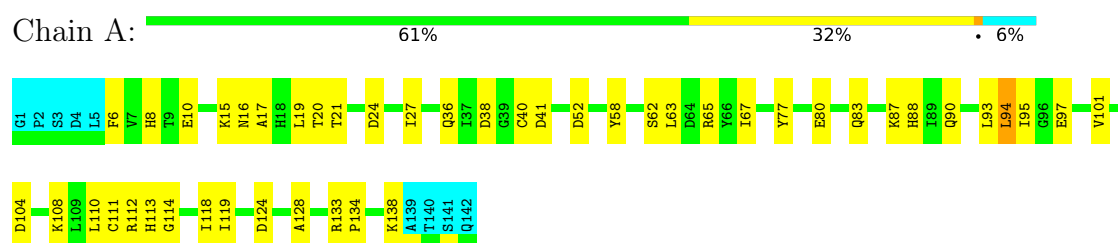
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: human rhinovirus 2A proteinase



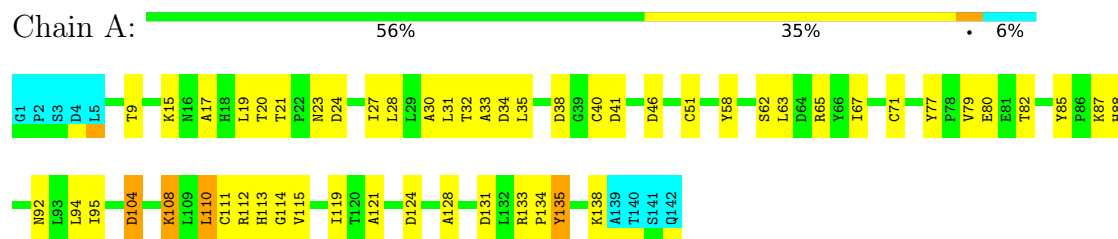
4.2.9 Score per residue for model 9

- Molecule 1: human rhinovirus 2A proteinase



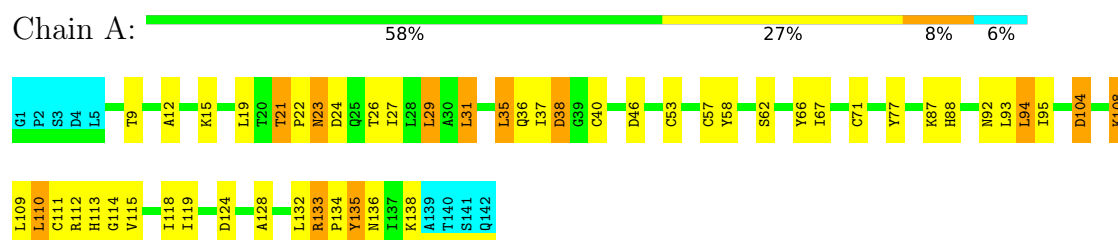
4.2.10 Score per residue for model 10

- Molecule 1: human rhinovirus 2A proteinase



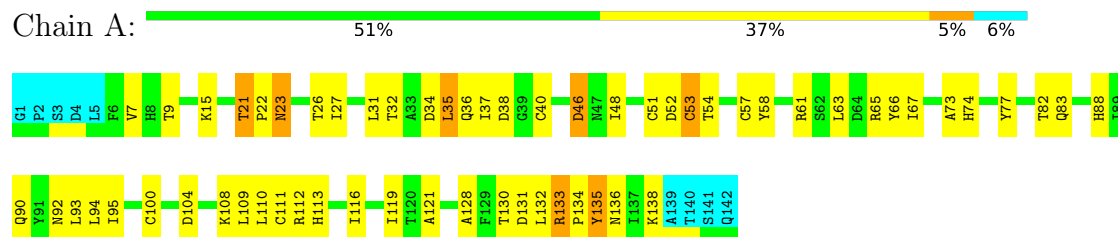
4.2.11 Score per residue for model 11

- Molecule 1: human rhinovirus 2A proteinase



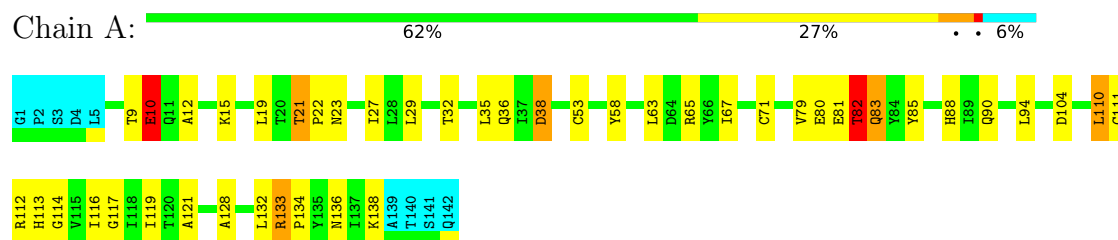
4.2.12 Score per residue for model 12

- Molecule 1: human rhinovirus 2A proteinase



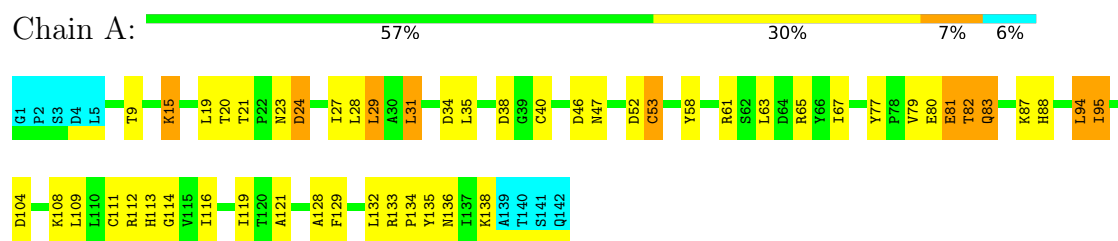
4.2.13 Score per residue for model 13

- Molecule 1: human rhinovirus 2A proteinase



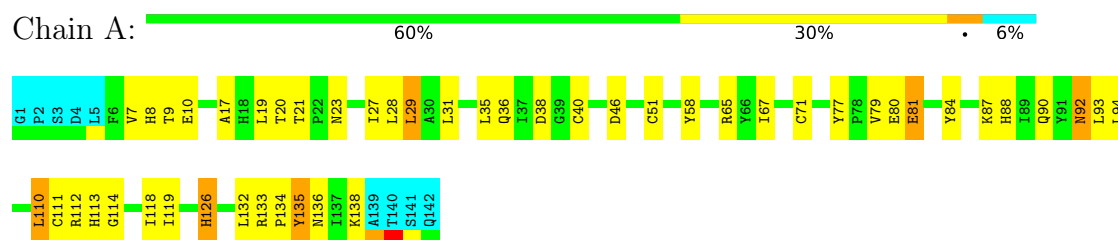
4.2.14 Score per residue for model 14

- Molecule 1: human rhinovirus 2A proteinase



4.2.15 Score per residue for model 15

- Molecule 1: human rhinovirus 2A proteinase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 200 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
CYANA	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	1485
Number of shifts mapped to atoms	1485
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

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

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	1031	972	972	22±4
All	All	15480	14580	14581	332

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ALA:HB3	1:A:128:ALA:HB3	0.99	1.31	10	10
1:A:29:LEU:HD11	1:A:31:LEU:HD22	0.70	1.62	14	3
1:A:52:ASP:O	1:A:116:ILE:HD12	0.68	1.89	14	2
1:A:95:ILE:CD1	1:A:128:ALA:HB2	0.66	2.21	14	9
1:A:26:THR:HG21	1:A:36:GLN:CD	0.66	2.16	12	1
1:A:90:GLN:CB	1:A:93:LEU:HD11	0.64	2.23	7	7
1:A:90:GLN:HB2	1:A:93:LEU:HD11	0.64	1.68	8	4
1:A:104:ASP:O	1:A:119:ILE:HD12	0.63	1.94	3	10
1:A:58:TYR:CD2	1:A:119:ILE:HD11	0.61	2.30	10	4
1:A:121:ALA:HB3	1:A:128:ALA:CB	0.61	2.24	1	6
1:A:17:ALA:HB2	1:A:36:GLN:HG3	0.60	1.73	7	5
1:A:109:LEU:HD23	1:A:129:PHE:CE2	0.59	2.33	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ILE:HG23	1:A:133:ARG:NH2	0.59	2.13	12	1
1:A:9:THR:CG2	1:A:12:ALA:HB3	0.59	2.28	13	1
1:A:90:GLN:HB3	1:A:93:LEU:HD11	0.58	1.76	5	4
1:A:108:LYS:HA	1:A:118:ILE:HG22	0.58	1.76	6	5
1:A:37:ILE:HD11	1:A:135:TYR:CD1	0.58	2.33	11	2
1:A:30:ALA:HB3	1:A:135:TYR:CZ	0.57	2.34	10	1
1:A:35:LEU:HD23	1:A:36:GLN:N	0.57	2.14	13	2
1:A:58:TYR:CE2	1:A:67:ILE:HD11	0.57	2.34	13	2
1:A:27:ILE:HD12	1:A:38:ASP:HA	0.56	1.75	11	11
1:A:21:THR:N	1:A:22:PRO:HD2	0.56	2.15	11	3
1:A:9:THR:O	1:A:10:GLU:C	0.56	2.48	13	1
1:A:111:CYS:O	1:A:112:ARG:C	0.56	2.48	7	14
1:A:29:LEU:HD22	1:A:36:GLN:OE1	0.56	1.99	13	1
1:A:110:LEU:HD23	1:A:114:GLY:HA2	0.56	1.76	15	11
1:A:9:THR:HG22	1:A:46:ASP:O	0.56	2.01	1	7
1:A:35:LEU:HD13	1:A:36:GLN:N	0.56	2.16	5	3
1:A:132:LEU:O	1:A:133:ARG:C	0.56	2.48	12	1
1:A:52:ASP:OD2	1:A:94:LEU:HD11	0.55	2.00	9	1
1:A:26:THR:HG22	1:A:38:ASP:OD1	0.55	2.01	11	1
1:A:58:TYR:CE1	1:A:67:ILE:HD11	0.55	2.36	3	13
1:A:31:LEU:HD23	1:A:85:TYR:OH	0.55	2.02	1	1
1:A:133:ARG:H	1:A:133:ARG:NE	0.55	1.99	12	1
1:A:29:LEU:HD11	1:A:31:LEU:CD2	0.55	2.32	14	3
1:A:9:THR:HG22	1:A:12:ALA:O	0.54	2.02	13	1
1:A:79:VAL:HG11	1:A:90:GLN:CD	0.54	2.28	13	1
1:A:58:TYR:CE2	1:A:119:ILE:HD11	0.54	2.38	10	2
1:A:35:LEU:HD23	1:A:135:TYR:CE1	0.54	2.37	7	1
1:A:48:ILE:HD12	1:A:136:ASN:CG	0.53	2.28	6	1
1:A:7:VAL:HG12	1:A:14:TYR:O	0.53	2.04	5	1
1:A:95:ILE:HD13	1:A:128:ALA:HB2	0.53	1.79	14	1
1:A:113:HIS:CD2	1:A:113:HIS:N	0.53	2.77	5	1
1:A:26:THR:HG21	1:A:36:GLN:NE2	0.53	2.19	8	2
1:A:71:CYS:SG	1:A:94:LEU:HD12	0.53	2.43	15	3
1:A:9:THR:HG21	1:A:136:ASN:OD1	0.52	2.04	8	1
1:A:57:CYS:C	1:A:109:LEU:HD12	0.52	2.30	12	5
1:A:15:LYS:CD	1:A:20:THR:HG21	0.52	2.35	14	2
1:A:31:LEU:HD22	1:A:84:TYR:CE2	0.52	2.40	6	1
1:A:48:ILE:HG12	1:A:132:LEU:HD23	0.52	1.81	3	1
1:A:9:THR:HG22	1:A:46:ASP:HB3	0.51	1.82	12	1
1:A:17:ALA:HB2	1:A:36:GLN:CG	0.51	2.35	9	2
1:A:7:VAL:HG21	1:A:108:LYS:HE2	0.51	1.83	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ALA:HB1	1:A:37:ILE:CG2	0.51	2.36	6	2
1:A:115:VAL:HG12	1:A:132:LEU:HD12	0.51	1.81	11	1
1:A:92:ASN:O	1:A:93:LEU:HD23	0.50	2.06	15	3
1:A:118:ILE:HD12	1:A:119:ILE:O	0.50	2.06	8	2
1:A:129:PHE:C	1:A:129:PHE:CD1	0.50	2.89	14	1
1:A:48:ILE:HD12	1:A:136:ASN:ND2	0.50	2.22	6	1
1:A:23:ASN:HB3	1:A:26:THR:HG23	0.50	1.84	11	1
1:A:29:LEU:CD1	1:A:31:LEU:HD22	0.50	2.37	15	3
1:A:62:SER:O	1:A:63:LEU:HD13	0.50	2.06	10	1
1:A:108:LYS:NZ	1:A:115:VAL:HG11	0.49	2.21	10	1
1:A:9:THR:OG1	1:A:12:ALA:HB3	0.49	2.06	11	1
1:A:100:CYS:HB2	1:A:127:VAL:HG22	0.49	1.83	8	1
1:A:95:ILE:HD11	1:A:128:ALA:HB2	0.49	1.83	12	9
1:A:31:LEU:HD12	1:A:85:TYR:OH	0.49	2.07	10	1
1:A:20:THR:O	1:A:21:THR:C	0.49	2.56	4	12
1:A:76:TRP:CE3	1:A:89:ILE:HG21	0.49	2.43	3	1
1:A:117:GLY:HA2	1:A:132:LEU:HD13	0.49	1.85	5	2
1:A:88:HIS:C	1:A:89:ILE:HD12	0.48	2.34	8	1
1:A:133:ARG:N	1:A:134:PRO:HD2	0.48	2.23	11	15
1:A:52:ASP:OD2	1:A:73:ALA:HB2	0.48	2.09	12	1
1:A:71:CYS:HB2	1:A:94:LEU:HD12	0.47	1.85	3	2
1:A:15:LYS:O	1:A:35:LEU:HD12	0.47	2.09	6	2
1:A:35:LEU:HD13	1:A:35:LEU:C	0.47	2.35	5	1
1:A:35:LEU:C	1:A:35:LEU:HD13	0.47	2.34	14	1
1:A:110:LEU:HD23	1:A:114:GLY:CA	0.46	2.41	15	4
1:A:26:THR:HG21	1:A:36:GLN:OE1	0.46	2.10	12	1
1:A:66:TYR:CE2	1:A:110:LEU:HD12	0.46	2.45	12	7
1:A:133:ARG:CB	1:A:134:PRO:CD	0.46	2.94	8	13
1:A:21:THR:CB	1:A:22:PRO:CD	0.46	2.94	13	2
1:A:48:ILE:HG23	1:A:133:ARG:HH22	0.46	1.70	12	1
1:A:21:THR:N	1:A:22:PRO:CD	0.46	2.79	11	4
1:A:30:ALA:HB3	1:A:135:TYR:OH	0.46	2.11	10	1
1:A:115:VAL:CG1	1:A:132:LEU:HD12	0.45	2.42	11	1
1:A:15:LYS:CE	1:A:20:THR:HG21	0.45	2.41	14	1
1:A:94:LEU:CB	1:A:129:PHE:CE2	0.45	2.99	14	1
1:A:130:THR:O	1:A:130:THR:HG23	0.45	2.11	6	2
1:A:17:ALA:CB	1:A:29:LEU:HD12	0.45	2.42	6	1
1:A:48:ILE:HD12	1:A:136:ASN:HB2	0.45	1.88	3	1
1:A:17:ALA:HB3	1:A:34:ASP:O	0.45	2.12	10	1
1:A:17:ALA:HB2	1:A:36:GLN:HB3	0.44	1.88	6	1
1:A:30:ALA:HB3	1:A:35:LEU:O	0.44	2.13	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ILE:HD11	1:A:135:TYR:CE1	0.44	2.47	12	1
1:A:37:ILE:HD11	1:A:135:TYR:HD1	0.44	1.73	4	1
1:A:94:LEU:HD13	1:A:129:PHE:CZ	0.43	2.48	14	1
1:A:101:VAL:HG22	1:A:104:ASP:HB3	0.43	1.90	4	1
1:A:35:LEU:HD12	1:A:36:GLN:H	0.43	1.74	1	1
1:A:35:LEU:HD23	1:A:135:TYR:CD1	0.43	2.47	7	1
1:A:71:CYS:HB2	1:A:94:LEU:HD23	0.43	1.90	11	1
1:A:51:CYS:O	1:A:116:ILE:HG22	0.43	2.14	12	1
1:A:82:THR:N	1:A:85:TYR:O	0.43	2.51	13	1
1:A:108:LYS:CE	1:A:115:VAL:HG11	0.43	2.44	7	1
1:A:26:THR:HG22	1:A:37:ILE:O	0.43	2.13	5	1
1:A:81:GLU:O	1:A:82:THR:HG23	0.43	2.14	14	3
1:A:58:TYR:HE1	1:A:67:ILE:HD11	0.42	1.74	5	4
1:A:111:CYS:HB3	1:A:116:ILE:HD13	0.42	1.91	12	1
1:A:78:PRO:HA	1:A:89:ILE:HD13	0.42	1.90	2	1
1:A:33:ALA:HB3	1:A:135:TYR:CZ	0.42	2.50	10	1
1:A:35:LEU:HD12	1:A:36:GLN:N	0.42	2.29	1	1
1:A:7:VAL:HG13	1:A:46:ASP:CG	0.42	2.39	15	1
1:A:82:THR:HG21	1:A:84:TYR:CE2	0.42	2.49	7	1
1:A:114:GLY:O	1:A:116:ILE:HG23	0.42	2.14	14	2
1:A:33:ALA:HB3	1:A:135:TYR:OH	0.41	2.15	2	1
1:A:126:HIS:CD2	1:A:126:HIS:C	0.41	2.97	15	1
1:A:63:LEU:HD22	1:A:63:LEU:N	0.41	2.30	10	5
1:A:63:LEU:N	1:A:63:LEU:HD22	0.41	2.31	1	4
1:A:7:VAL:HG21	1:A:108:LYS:NZ	0.41	2.30	4	1
1:A:95:ILE:HD13	1:A:128:ALA:CA	0.41	2.46	4	1
1:A:15:LYS:HE2	1:A:20:THR:HG21	0.40	1.93	8	1
1:A:94:LEU:HD11	1:A:131:ASP:OD2	0.40	2.16	2	1
1:A:81:GLU:C	1:A:82:THR:HG22	0.40	2.42	13	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	133/142 (94%)	102±4 (77±3%)	26±4 (20±3%)	5±2 (4±1%)	4	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1995/2130 (94%)	1528 (77%)	393 (20%)	74 (4%)	4	32

All 21 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	23	ASN	12
1	A	53	CYS	9
1	A	135	TYR	8
1	A	10	GLU	7
1	A	24	ASP	6
1	A	124	ASP	6
1	A	46	ASP	4
1	A	51	CYS	4
1	A	83	GLN	3
1	A	81	GLU	3
1	A	84	TYR	2
1	A	136	ASN	1
1	A	26	THR	1
1	A	6	PHE	1
1	A	103	GLY	1
1	A	52	ASP	1
1	A	138	LYS	1
1	A	97	GLU	1
1	A	100	CYS	1
1	A	82	THR	1
1	A	47	ASN	1

6.3.2 Protein sidechains ⓘ

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	112/119 (94%)	90±3 (80±3%)	22±3 (20±3%)	3	33
All	All	1680/1785 (94%)	1351 (80%)	329 (20%)	3	33

All 63 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	88	HIS	15
1	A	113	HIS	15
1	A	19	LEU	13
1	A	40	CYS	13
1	A	77	TYR	13
1	A	138	LYS	13
1	A	65	ARG	12
1	A	87	LYS	11
1	A	110	LEU	11
1	A	83	GLN	10
1	A	94	LEU	10
1	A	15	LYS	9
1	A	79	VAL	8
1	A	80	GLU	8
1	A	82	THR	8
1	A	92	ASN	8
1	A	131	ASP	8
1	A	62	SER	8
1	A	133	ARG	8
1	A	136	ASN	8
1	A	32	THR	7
1	A	104	ASP	7
1	A	135	TYR	7
1	A	28	LEU	7
1	A	29	LEU	6
1	A	61	ARG	6
1	A	8	HIS	4
1	A	81	GLU	4
1	A	35	LEU	4
1	A	108	LYS	4
1	A	38	ASP	4
1	A	31	LEU	4
1	A	23	ASN	3
1	A	26	THR	3
1	A	74	HIS	3
1	A	16	ASN	3
1	A	24	ASP	3
1	A	9	THR	3
1	A	132	LEU	3
1	A	41	ASP	3
1	A	21	THR	3
1	A	52	ASP	2
1	A	85	TYR	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	90	GLN	2
1	A	126	HIS	2
1	A	6	PHE	2
1	A	34	ASP	2
1	A	53	CYS	2
1	A	50	ASP	1
1	A	55	SER	1
1	A	84	TYR	1
1	A	25	GLN	1
1	A	118	ILE	1
1	A	51	CYS	1
1	A	18	HIS	1
1	A	127	VAL	1
1	A	101	VAL	1
1	A	93	LEU	1
1	A	46	ASP	1
1	A	54	THR	1
1	A	130	THR	1
1	A	10	GLU	1
1	A	95	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1485
Number of shifts mapped to atoms	1485
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	-0.18 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	125	-0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	114	0.38 ± 0.10	None needed (< 0.5 ppm)
^{15}N	125	0.43 ± 0.38	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1401 atoms were assigned a chemical shift out of a possible 1728. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	614/658 (93%)	261/269 (97%)	236/266 (89%)	117/123 (95%)
Sidechain	782/915 (85%)	532/596 (89%)	250/292 (86%)	0/27 (0%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	5/155 (3%)	5/76 (7%)	0/72 (0%)	0/7 (0%)
Overall	1401/1728 (81%)	798/941 (85%)	486/630 (77%)	117/157 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1482 atoms were assigned a chemical shift out of a possible 1824. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	656/702 (93%)	278/287 (97%)	253/284 (89%)	125/131 (95%)
Sidechain	821/967 (85%)	559/630 (89%)	262/309 (85%)	0/28 (0%)
Aromatic	5/155 (3%)	5/76 (7%)	0/72 (0%)	0/7 (0%)
Overall	1482/1824 (81%)	842/993 (85%)	515/665 (77%)	125/166 (75%)

7.1.4 Statistically unusual chemical shifts [i](#)

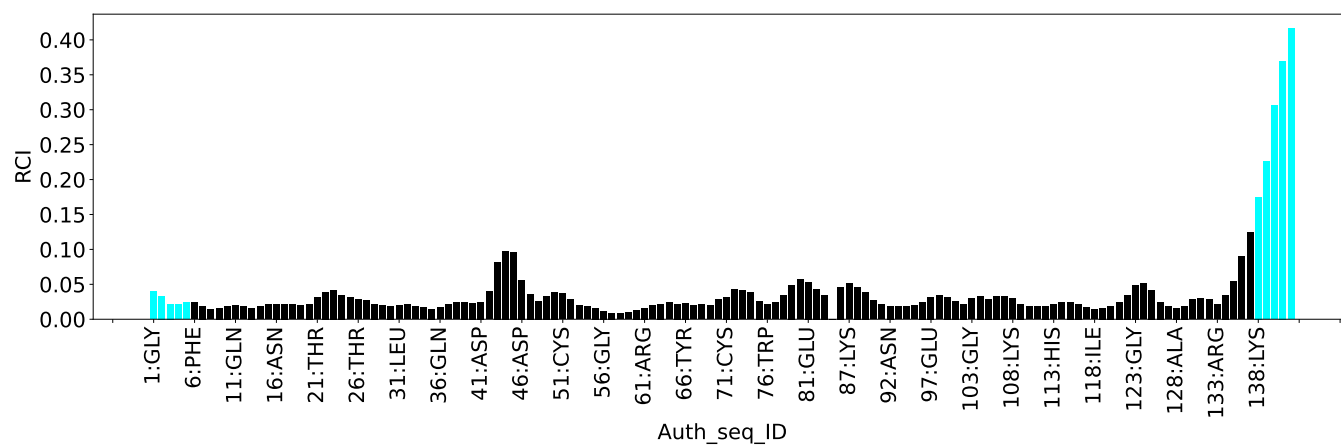
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	20	THR	HG1	4.20	0.08 – 2.19	14.5
1	A	2	PRO	CD	43.70	45.11 – 55.58	-6.3
1	A	109	LEU	HG	-0.34	-0.13 – 3.16	-5.6

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1073
Intra-residue ($ i-j =0$)	198
Sequential ($ i-j =1$)	167
Medium range ($ i-j >1$ and $ i-j <5$)	112
Long range ($ i-j \geq 5$)	487
Inter-chain	0
Hydrogen bond restraints	105
Disulfide bond restraints	0
Total dihedral-angle restraints	142
Number of unmapped restraints	0
Number of restraints per residue	8.5
Number of long range restraints per residue ¹	3.9

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	18.1	0.2
0.2-0.5 (Medium)	6.3	0.5
>0.5 (Large)	3.2	3.84

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)	4.1	3.9
10.0-20.0 (Medium)	0.9	19.8
>20.0 (Large)	0.1	21.98

9 Distance violation analysis ⓘ

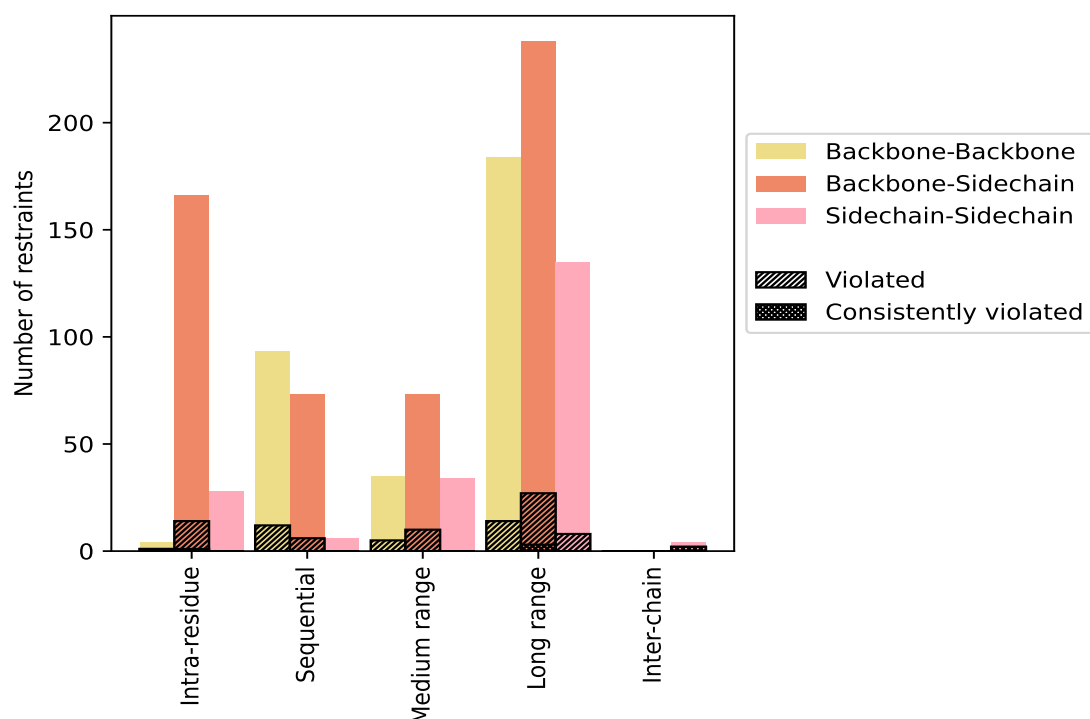
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	198	18.5	15	7.6	1.4	2	1.0	0.2
Backbone-Backbone	4	0.4	1	25.0	0.1	1	25.0	0.1
Backbone-Sidechain	166	15.5	14	8.4	1.3	1	0.6	0.1
Sidechain-Sidechain	28	2.6	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	167	15.6	18	10.8	1.7	0	0.0	0.0
Backbone-Backbone	92	8.6	12	13.0	1.1	0	0.0	0.0
Backbone-Sidechain	69	6.4	6	8.7	0.6	0	0.0	0.0
Sidechain-Sidechain	6	0.6	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	112	10.4	9	8.0	0.8	0	0.0	0.0
Backbone-Backbone	31	2.9	4	12.9	0.4	0	0.0	0.0
Backbone-Sidechain	47	4.4	5	10.6	0.5	0	0.0	0.0
Sidechain-Sidechain	34	3.2	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	487	45.4	38	7.8	3.5	1	0.2	0.1
Backbone-Backbone	162	15.1	13	8.0	1.2	0	0.0	0.0
Backbone-Sidechain	190	17.7	17	8.9	1.6	1	0.5	0.1
Sidechain-Sidechain	135	12.6	8	5.9	0.7	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	105	9.8	17	16.2	1.6	2	1.9	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1073	100.0	99	9.2	9.2	7	0.7	0.7
Backbone-Backbone	316	29.5	32	10.1	3.0	1	0.3	0.1
Backbone-Sidechain	550	51.3	57	10.4	5.3	4	0.7	0.4
Sidechain-Sidechain	207	19.3	10	4.8	0.9	2	1.0	0.2

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	5	5	4	6	2	22	0.26	0.76	0.18	0.18
2	6	5	5	9	2	27	0.27	1.1	0.23	0.16
3	6	5	3	13	2	29	0.25	1.01	0.23	0.16
4	6	3	4	14	2	29	0.27	1.23	0.24	0.16
5	5	6	3	7	2	23	0.24	0.72	0.19	0.14
6	8	5	5	11	2	31	0.27	1.05	0.21	0.16
7	7	6	5	11	2	31	0.36	3.84	0.67	0.16
8	6	5	5	10	2	28	0.26	0.98	0.21	0.18
9	4	6	3	14	2	29	0.19	0.9	0.16	0.13
10	7	5	6	14	2	34	0.25	1.1	0.23	0.16

Continued on next page...

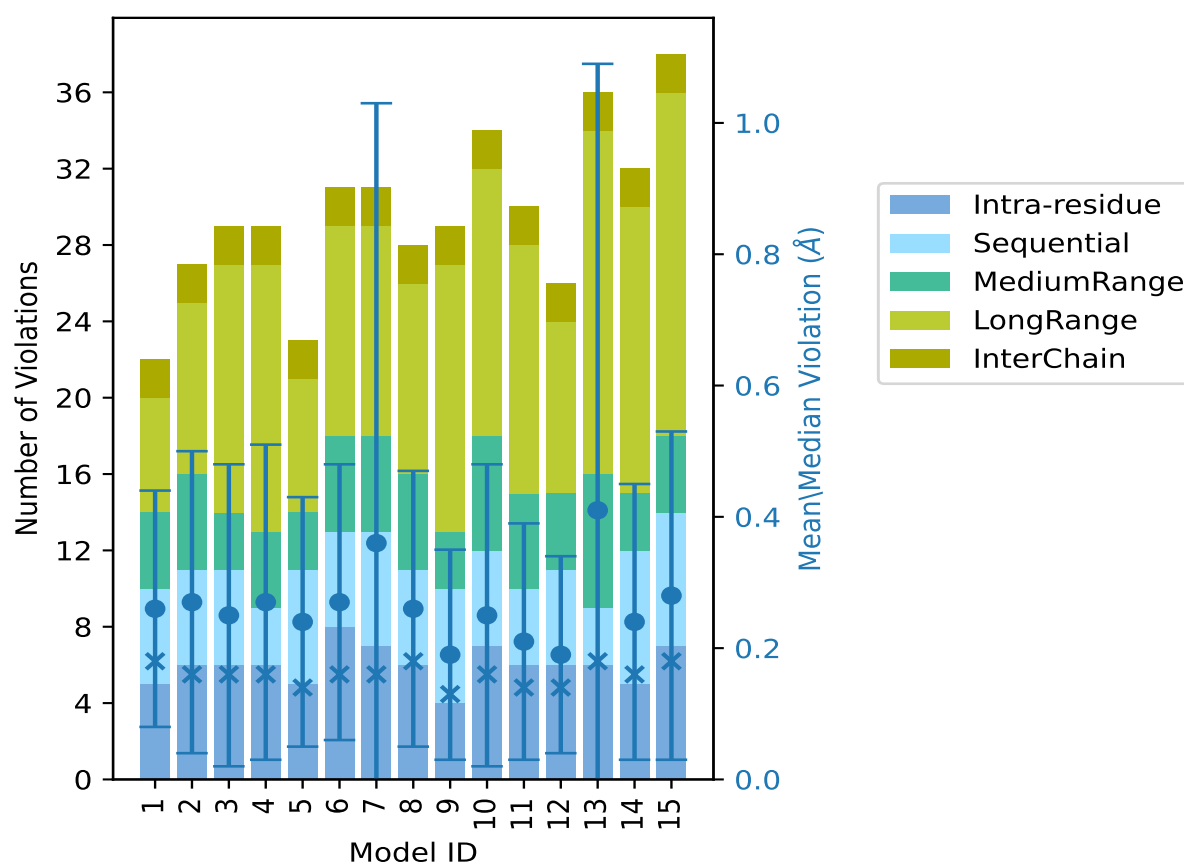
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	6	4	5	13	2	30	0.21	0.9	0.18	0.14
12	6	5	4	9	2	26	0.19	0.77	0.15	0.14
13	6	3	7	18	2	36	0.41	3.77	0.68	0.18
14	5	7	3	15	2	32	0.24	0.92	0.21	0.16
15	7	7	4	18	2	38	0.28	1.14	0.25	0.18

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

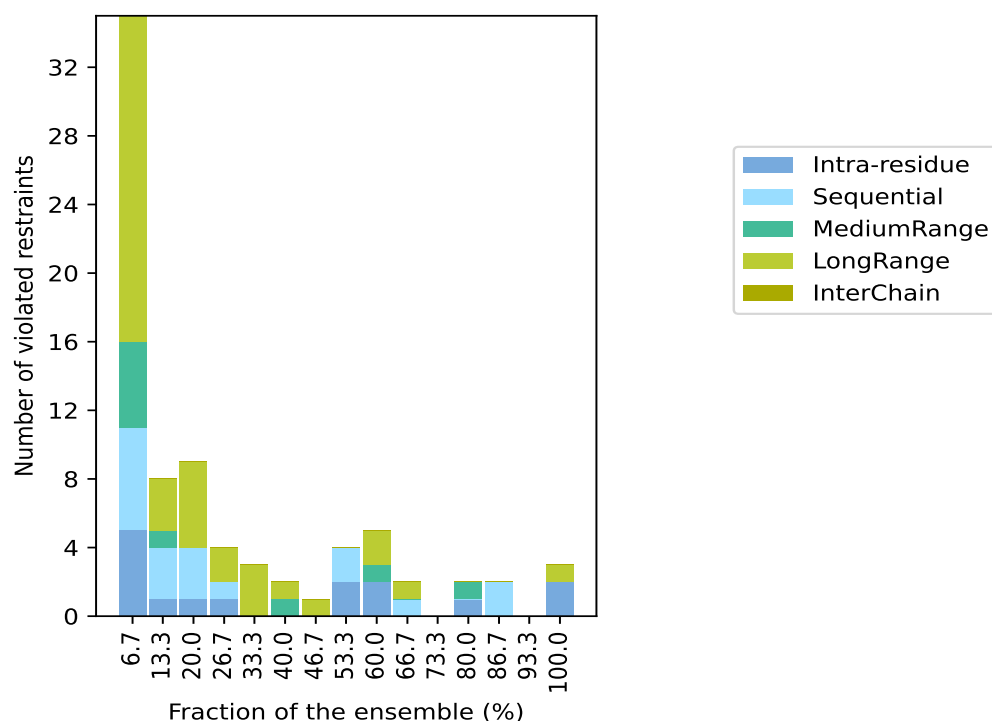
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 884(IR:183, SQ:149, MR:103, LR:449, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	6	5	19	0	35	1	6.7
1	3	1	3	0	8	2	13.3
1	3	0	5	0	9	3	20.0
1	1	0	2	0	4	4	26.7
0	0	0	3	0	3	5	33.3
0	0	1	1	0	2	6	40.0
0	0	0	1	0	1	7	46.7
2	2	0	0	0	4	8	53.3
2	0	1	2	0	5	9	60.0
0	1	0	1	0	2	10	66.7
0	0	0	0	0	0	11	73.3
1	0	1	0	0	2	12	80.0
0	2	0	0	0	2	13	86.7
0	0	0	0	0	0	14	93.3
2	0	0	1	0	3	15	100.0

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

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

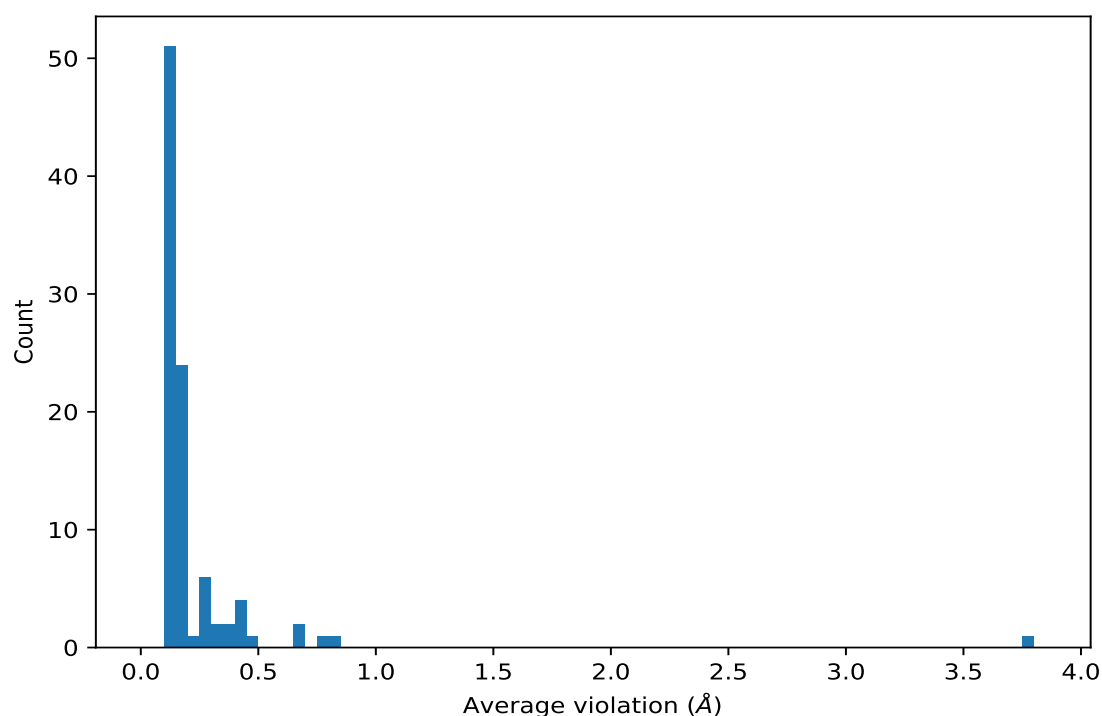
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	15	0.65	0.13	0.71
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	15	0.41	0.07	0.44
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	15	0.4	0.2	0.39
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	15	0.4	0.2	0.39
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	15	0.4	0.2	0.39
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	15	0.35	0.15	0.3
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	15	0.2	0.09	0.18
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	15	0.16	0.0	0.16
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	15	0.13	0.01	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	15	0.13	0.01	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	15	0.13	0.01	0.12
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	14	0.32	0.26	0.2
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	13	0.16	0.01	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	13	0.16	0.01	0.16
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	13	0.11	0.01	0.11
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	12	0.75	0.4	0.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	12	0.27	0.1	0.27
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	12	0.17	0.02	0.16
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	12	0.17	0.02	0.16
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	10	0.13	0.01	0.13
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	10	0.12	0.02	0.11
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	9	0.37	0.09	0.41
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	9	0.17	0.04	0.16
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	9	0.16	0.01	0.16
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	9	0.16	0.01	0.16
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	9	0.12	0.01	0.13
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	9	0.11	0.01	0.11
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	9	0.11	0.01	0.11
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	8	0.49	0.35	0.48
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	8	0.37	0.02	0.38
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	8	0.27	0.01	0.27
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	8	0.16	0.03	0.16
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	8	0.15	0.03	0.15
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	8	0.15	0.03	0.15
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	7	0.25	0.18	0.14
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	7	0.18	0.03	0.19
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	7	0.18	0.03	0.19
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	7	0.18	0.03	0.19
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	7	0.18	0.03	0.19
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	7	0.18	0.03	0.19
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	7	0.18	0.03	0.19
(1,876)	1:124:A:ASP:HA	1:126:A:HIS:H	6	0.17	0.11	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD11	6	0.12	0.02	0.12
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD12	6	0.12	0.02	0.12
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD13	6	0.12	0.02	0.12
(1,605)	1:81:A:GLU:H	1:87:A:LYS:HG2	5	0.69	0.43	0.56
(2,74)	1:7:A:VAL:O	1:14:A:TYR:N	5	0.28	0.15	0.2
(1,637)	1:92:A:ASN:HA	1:131:A:ASP:H	5	0.16	0.04	0.15
(2,55)	1:114:A:GLY:H	1:111:A:CYS:O	5	0.12	0.01	0.12
(1,389)	1:58:A:TYR:H	1:66:A:TYR:HA	5	0.12	0.01	0.11
(3,25)	1:82:A:THR:H	1:86:A:PRO:N	4	0.18	0.11	0.12
(1,883)	1:127:A:VAL:H	1:128:A:ALA:H	4	0.17	0.01	0.16
(1,640)	1:93:A:LEU:H	1:93:A:LEU:HG	4	0.15	0.02	0.14
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG12	4	0.13	0.02	0.12
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG13	4	0.13	0.02	0.12
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG12	4	0.13	0.02	0.12
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG13	4	0.13	0.02	0.12
(1,350)	1:56:A:GLY:H	1:71:A:CYS:H	4	0.13	0.04	0.11

Continued on next page...

Continued from previous page...

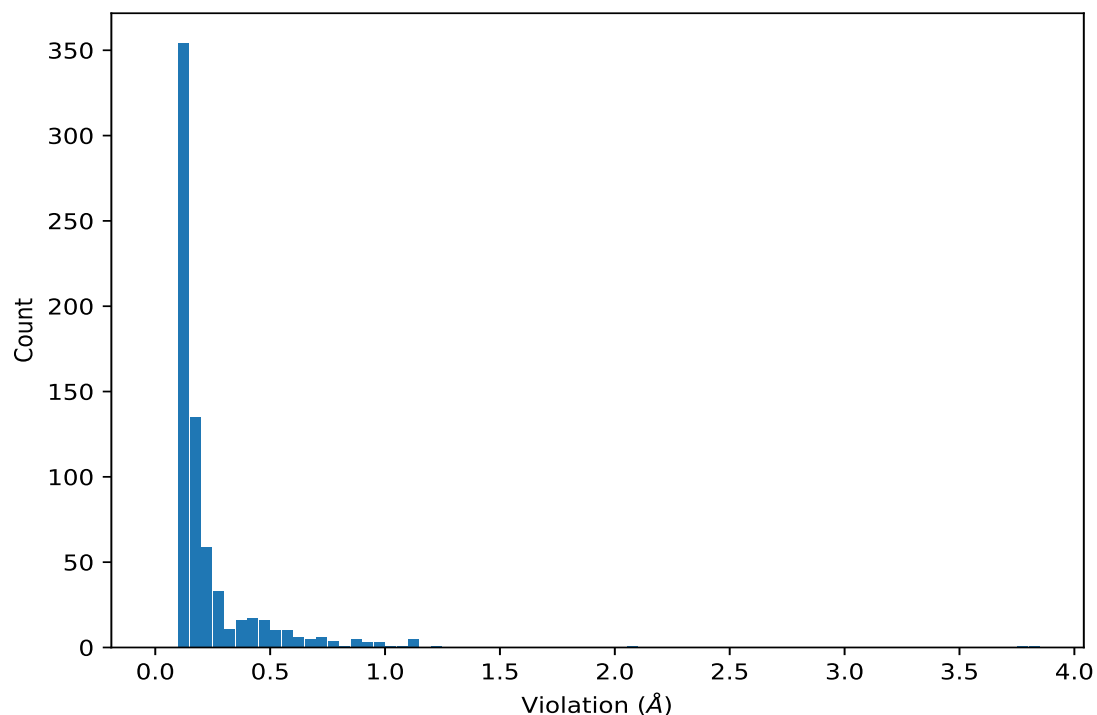
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,600)	1:81:A:GLU:HB3	1:86:A:PRO:HA	3	0.8	0.24	0.76
(1,559)	1:76:A:TRP:HA	1:91:A:TYR:HB3	3	0.26	0.08	0.3
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB2	3	0.17	0.04	0.15
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB3	3	0.17	0.04	0.15
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB2	3	0.17	0.04	0.15
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB3	3	0.17	0.04	0.15
(1,70)	1:13:A:ILE:HD11	1:14:A:TYR:H	3	0.12	0.01	0.13
(1,70)	1:13:A:ILE:HD12	1:14:A:TYR:H	3	0.12	0.01	0.13
(1,70)	1:13:A:ILE:HD13	1:14:A:TYR:H	3	0.12	0.01	0.13
(1,564)	1:76:A:TRP:HA	1:93:A:LEU:HB2	3	0.12	0.0	0.12
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG12	3	0.11	0.01	0.11
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG13	3	0.11	0.01	0.11
(1,751)	1:109:A:LEU:H	1:110:A:LEU:H	3	0.11	0.01	0.11
(1,506)	1:71:A:CYS:H	1:72:A:GLU:HA	3	0.1	0.0	0.1
(2,43)	1:106:A:GLY:H	1:119:A:ILE:O	3	0.1	0.0	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG21	3	0.1	0.0	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG22	3	0.1	0.0	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG23	3	0.1	0.0	0.1
(1,399)	1:58:A:TYR:HD1	1:69:A:VAL:H	2	3.8	0.03	3.8
(1,279)	1:47:A:ASN:H	1:48:A:ILE:H	2	0.29	0.18	0.29
(1,631)	1:91:A:TYR:H	1:92:A:ASN:H	2	0.16	0.05	0.16
(1,166)	1:23:A:ASN:H	1:25:A:GLN:H	2	0.15	0.02	0.15
(1,585)	1:79:A:VAL:HG11	1:87:A:LYS:HE2	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG11	1:87:A:LYS:HE3	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG12	1:87:A:LYS:HE2	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG12	1:87:A:LYS:HE3	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG13	1:87:A:LYS:HE2	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG13	1:87:A:LYS:HE3	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG21	1:87:A:LYS:HE2	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG21	1:87:A:LYS:HE3	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG22	1:87:A:LYS:HE2	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG22	1:87:A:LYS:HE3	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG23	1:87:A:LYS:HE2	2	0.14	0.01	0.14
(1,585)	1:79:A:VAL:HG23	1:87:A:LYS:HE3	2	0.14	0.01	0.14
(1,826)	1:118:A:ILE:HG12	1:130:A:THR:HB	2	0.12	0.02	0.12
(1,826)	1:118:A:ILE:HG13	1:130:A:THR:HB	2	0.12	0.02	0.12
(1,808)	1:117:A:GLY:H	1:118:A:ILE:H	2	0.11	0.01	0.11
(1,159)	1:21:A:THR:H	1:21:A:THR:HB	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:58:A:TYR:HD1	1:69:A:VAL:H	7	3.84
(1,399)	1:58:A:TYR:HD1	1:69:A:VAL:H	13	3.77
(1,47)	1:9:A:THR:H	1:14:A:TYR:HE1	13	2.08
(1,605)	1:81:A:GLU:H	1:87:A:LYS:HG2	4	1.23
(1,605)	1:81:A:GLU:H	1:87:A:LYS:HG2	15	1.14
(1,600)	1:81:A:GLU:HB3	1:86:A:PRO:HA	13	1.11
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	7	1.11
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	2	1.1
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	10	1.1
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	6	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	3	1.01
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	8	0.98
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	15	0.98
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	10	0.96
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	14	0.92
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	11	0.9
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	9	0.9
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	14	0.89
(1,917)	1:137:A:ILE:H	1:137:A:ILE:HG12	15	0.87
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	3	0.86
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	3	0.86
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	3	0.86
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	13	0.84
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	12	0.77
(1,600)	1:81:A:GLU:HB3	1:86:A:PRO:HA	15	0.76
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	1	0.76
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	14	0.75
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	2	0.73
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	5	0.72
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	8	0.72
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	4	0.71
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	10	0.71
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	7	0.71
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	4	0.69
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	4	0.69
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	4	0.69
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	3	0.68
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	6	0.65
(1,19)	1:7:A:VAL:HG11	1:14:A:TYR:HD1	13	0.62
(1,19)	1:7:A:VAL:HG12	1:14:A:TYR:HD1	13	0.62
(1,19)	1:7:A:VAL:HG13	1:14:A:TYR:HD1	13	0.62
(1,19)	1:7:A:VAL:HG21	1:14:A:TYR:HD1	13	0.62
(1,19)	1:7:A:VAL:HG22	1:14:A:TYR:HD1	13	0.62
(1,19)	1:7:A:VAL:HG23	1:14:A:TYR:HD1	13	0.62
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	7	0.59
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	8	0.59
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	8	0.59
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	8	0.59
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	13	0.58
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	2	0.57
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	1	0.56
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	6	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:81:A:GLU:H	1:87:A:LYS:HG2	11	0.56
(2,74)	1:7:A:VAL:O	1:14:A:TYR:N	5	0.55
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	5	0.54
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	3	0.54
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	5	0.54
(1,600)	1:81:A:GLU:HB3	1:86:A:PRO:HA	4	0.53
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	11	0.51
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	5	0.5
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	1	0.5
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	10	0.5
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	10	0.5
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	10	0.5
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	6	0.49
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	2	0.49
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	2	0.49
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	2	0.49
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	6	0.49
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	6	0.49
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	6	0.49
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	14	0.48
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	12	0.47
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	6	0.47
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	15	0.47
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	3	0.46
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	4	0.46
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	6	0.46
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	8	0.46
(1,279)	1:47:A:ASN:H	1:48:A:ILE:H	10	0.46
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	7	0.44
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	13	0.44
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	11	0.43
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	2	0.43
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	1	0.43
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	1	0.43
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	1	0.43
(1,876)	1:124:A:ASP:HA	1:126:A:HIS:H	8	0.42
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	1	0.42
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	7	0.42
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	2	0.41
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	9	0.41
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	8	0.41
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	15	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	1	0.4
(1,605)	1:81:A:GLU:H	1:87:A:LYS:HG2	13	0.4
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	4	0.4
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	2	0.39
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	12	0.39
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	9	0.39
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	9	0.39
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	9	0.39
(2,75)	1:14:A:TYR:O	1:7:A:VAL:N	6	0.38
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	4	0.38
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	8	0.38
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	11	0.38
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	14	0.38
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	15	0.37
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	11	0.37
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	10	0.36
(3,25)	1:82:A:THR:H	1:86:A:PRO:N	13	0.36
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	15	0.36
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	1	0.36
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	3	0.35
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	15	0.35
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	8	0.34
(1,911)	1:134:A:PRO:HD2	1:135:A:TYR:H	6	0.34
(1,559)	1:76:A:TRP:HA	1:91:A:TYR:HB3	2	0.34
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	7	0.34
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	7	0.34
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	7	0.34
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	1	0.32
(2,74)	1:7:A:VAL:O	1:14:A:TYR:N	10	0.32
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	5	0.32
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	13	0.3
(1,559)	1:76:A:TRP:HA	1:91:A:TYR:HB3	7	0.3
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	15	0.3
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	15	0.3
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	15	0.3
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	5	0.29
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	12	0.29
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	13	0.29
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	13	0.29
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	13	0.29
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	4	0.28
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	14	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	2	0.28
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	7	0.28
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	14	0.28
(2,30)	1:82:A:THR:H	1:85:A:TYR:O	13	0.27
(2,3)	1:14:A:TYR:O	1:7:A:VAL:H	9	0.27
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	6	0.27
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	8	0.27
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	10	0.27
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	12	0.27
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	12	0.27
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	12	0.27
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	15	0.26
(1,903)	1:132:A:LEU:HA	1:132:A:LEU:HD11	6	0.26
(1,903)	1:132:A:LEU:HA	1:132:A:LEU:HD12	6	0.26
(1,903)	1:132:A:LEU:HA	1:132:A:LEU:HD13	6	0.26
(1,903)	1:132:A:LEU:HA	1:132:A:LEU:HD21	6	0.26
(1,903)	1:132:A:LEU:HA	1:132:A:LEU:HD22	6	0.26
(1,903)	1:132:A:LEU:HA	1:132:A:LEU:HD23	6	0.26
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	3	0.26
(1,313)	1:50:A:ASP:HA	1:50:A:ASP:HB2	15	0.25
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	3	0.25
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	7	0.24
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	10	0.24
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	9	0.24
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	7	0.23
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	14	0.23
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	15	0.23
(3,17)	1:81:A:GLU:N	1:87:A:LYS:H	13	0.22
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	4	0.22
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	4	0.22
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	4	0.22
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	4	0.22
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	4	0.22
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	4	0.22
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB2	14	0.22
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB3	14	0.22
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB2	14	0.22
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB3	14	0.22
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	4	0.22
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	13	0.21
(3,15)	1:80:A:GLU:O	1:82:A:THR:H	13	0.21
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	11	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	12	0.21
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	14	0.21
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	6	0.21
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	6	0.21
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	6	0.21
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	6	0.21
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	6	0.21
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	6	0.21
(1,655)	1:94:A:LEU:H	1:95:A:ILE:H	15	0.21
(1,637)	1:92:A:ASN:HA	1:131:A:ASP:H	4	0.21
(1,631)	1:91:A:TYR:H	1:92:A:ASN:H	8	0.21
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	1	0.21
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	1	0.21
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	4	0.2
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	12	0.2
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	7	0.2
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	3	0.2
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	4	0.2
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	8	0.2
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	10	0.2
(2,74)	1:7:A:VAL:O	1:14:A:TYR:N	14	0.2
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	15	0.2
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	13	0.2
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	13	0.2
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	13	0.2
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	13	0.2
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	13	0.2
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	13	0.2
(1,582)	1:79:A:VAL:H	1:80:A:GLU:H	9	0.2
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	13	0.2
(1,323)	1:53:A:CYS:H	1:116:A:ILE:HD11	12	0.2
(1,323)	1:53:A:CYS:H	1:116:A:ILE:HD12	12	0.2
(1,323)	1:53:A:CYS:H	1:116:A:ILE:HD13	12	0.2
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	3	0.2
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	3	0.2
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	8	0.2
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	8	0.2
(1,18)	1:7:A:VAL:HB	1:14:A:TYR:H	9	0.2
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	8	0.19
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	10	0.19
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	11	0.19
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	2	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:7:A:VAL:O	1:14:A:TYR:N	9	0.19
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	10	0.19
(1,918)	1:137:A:ILE:HA	1:137:A:ILE:HD11	15	0.19
(1,918)	1:137:A:ILE:HA	1:137:A:ILE:HD12	15	0.19
(1,918)	1:137:A:ILE:HA	1:137:A:ILE:HD13	15	0.19
(1,883)	1:127:A:VAL:H	1:128:A:ALA:H	6	0.19
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	10	0.19
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	10	0.19
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	10	0.19
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	10	0.19
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	10	0.19
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	10	0.19
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	15	0.19
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	15	0.19
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	15	0.19
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	15	0.19
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	15	0.19
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	15	0.19
(1,637)	1:92:A:ASN:HA	1:131:A:ASP:H	15	0.19
(1,350)	1:56:A:GLY:H	1:71:A:CYS:H	14	0.19
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	13	0.19
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	7	0.19
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	7	0.19
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	15	0.19
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	15	0.19
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	1	0.18
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	3	0.18
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	6	0.18
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	9	0.18
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	8	0.18
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	9	0.18
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	1	0.18
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	15	0.18
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	13	0.18
(1,640)	1:93:A:LEU:H	1:93:A:LEU:HG	4	0.18
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	3	0.18
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	14	0.18
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	15	0.18
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	15	0.18
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	1	0.18
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	1	0.18
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	2	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	2	0.18
(5,3)	2:201:A:ZN:ZN	1:53:A:CYS:SG	5	0.17
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	3	0.17
(1,883)	1:127:A:VAL:H	1:128:A:ALA:H	9	0.17
(1,868)	1:123:A:GLY:HA2	1:126:A:HIS:H	10	0.17
(1,868)	1:123:A:GLY:HA3	1:126:A:HIS:H	10	0.17
(1,706)	1:99:A:PRO:HA	1:125:A:GLY:H	8	0.17
(1,681)	1:95:A:ILE:HG12	1:128:A:ALA:H	15	0.17
(1,681)	1:95:A:ILE:HG13	1:128:A:ALA:H	15	0.17
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	14	0.17
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	14	0.17
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	14	0.17
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG12	12	0.17
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG13	12	0.17
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG12	12	0.17
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG13	12	0.17
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	14	0.17
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	14	0.17
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	14	0.17
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	1	0.17
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	1	0.17
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	2	0.17
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	2	0.17
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	2	0.16
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	7	0.16
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	15	0.16
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	11	0.16
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	14	0.16
(1,883)	1:127:A:VAL:H	1:128:A:ALA:H	7	0.16
(1,883)	1:127:A:VAL:H	1:128:A:ALA:H	11	0.16
(1,716)	1:101:A:VAL:HG11	1:105:A:ALA:H	4	0.16
(1,716)	1:101:A:VAL:HG12	1:105:A:ALA:H	4	0.16
(1,716)	1:101:A:VAL:HG13	1:105:A:ALA:H	4	0.16
(1,716)	1:101:A:VAL:HG21	1:105:A:ALA:H	4	0.16
(1,716)	1:101:A:VAL:HG22	1:105:A:ALA:H	4	0.16
(1,716)	1:101:A:VAL:HG23	1:105:A:ALA:H	4	0.16
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	3	0.16
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	3	0.16
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	3	0.16
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	3	0.16
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	3	0.16
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	3	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	2	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	3	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	7	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	8	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	9	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	10	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	13	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	14	0.16
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	15	0.16
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	2	0.16
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	4	0.16
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	6	0.16
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	10	0.16
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	10	0.16
(1,166)	1:23:A:ASN:H	1:25:A:GLN:H	11	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	1	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	1	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	3	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	3	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	4	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	4	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	5	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	5	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	6	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	6	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	7	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	7	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	8	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	8	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	9	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	9	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	10	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	10	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	14	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	14	0.16
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	15	0.16
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	15	0.16
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	3	0.16
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	3	0.16
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	4	0.16
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	4	0.16
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	8	0.16
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	12	0.16
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	12	0.16
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	14	0.16
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	14	0.16
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	7	0.15
(2,74)	1:7:A:VAL:O	1:14:A:TYR:N	11	0.15
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	6	0.15
(1,894)	1:130:A:THR:H	1:130:A:THR:HB	12	0.15
(1,876)	1:124:A:ASP:HA	1:126:A:HIS:H	6	0.15
(1,806)	1:116:A:ILE:HA	1:133:A:ARG:H	11	0.15
(1,640)	1:93:A:LEU:H	1:93:A:LEU:HG	10	0.15
(1,637)	1:92:A:ASN:HA	1:131:A:ASP:H	6	0.15
(1,559)	1:76:A:TRP:HA	1:91:A:TYR:HB3	13	0.15
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	1	0.15
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	4	0.15
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	5	0.15
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	6	0.15
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	11	0.15
(1,488)	1:69:A:VAL:H	1:69:A:VAL:HA	12	0.15
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	10	0.15
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	10	0.15
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	10	0.15
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB2	5	0.15
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB3	5	0.15
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB2	5	0.15
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB3	5	0.15
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	1	0.15
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	10	0.15
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	13	0.15
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD11	7	0.15
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD12	7	0.15
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD13	7	0.15
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	2	0.15
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	2	0.15
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	2	0.15
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	2	0.15
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	4	0.15
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	4	0.15
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	9	0.15
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	9	0.15
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	10	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	10	0.15
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	10	0.15
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	10	0.15
(5,2)	2:201:A:ZN:ZN	1:113:A:HIS:NE2	14	0.14
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	14	0.14
(3,25)	1:82:A:THR:H	1:86:A:PRO:N	15	0.14
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	13	0.14
(2,55)	1:114:A:GLY:H	1:111:A:CYS:O	11	0.14
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	8	0.14
(1,826)	1:118:A:ILE:HG12	1:130:A:THR:HB	6	0.14
(1,826)	1:118:A:ILE:HG13	1:130:A:THR:HB	6	0.14
(1,697)	1:97:A:GLU:HA	1:126:A:HIS:H	10	0.14
(1,585)	1:79:A:VAL:HG11	1:87:A:LYS:HE2	15	0.14
(1,585)	1:79:A:VAL:HG11	1:87:A:LYS:HE3	15	0.14
(1,585)	1:79:A:VAL:HG12	1:87:A:LYS:HE2	15	0.14
(1,585)	1:79:A:VAL:HG12	1:87:A:LYS:HE3	15	0.14
(1,585)	1:79:A:VAL:HG13	1:87:A:LYS:HE2	15	0.14
(1,585)	1:79:A:VAL:HG13	1:87:A:LYS:HE3	15	0.14
(1,585)	1:79:A:VAL:HG21	1:87:A:LYS:HE2	15	0.14
(1,585)	1:79:A:VAL:HG21	1:87:A:LYS:HE3	15	0.14
(1,585)	1:79:A:VAL:HG22	1:87:A:LYS:HE2	15	0.14
(1,585)	1:79:A:VAL:HG22	1:87:A:LYS:HE3	15	0.14
(1,585)	1:79:A:VAL:HG23	1:87:A:LYS:HE2	15	0.14
(1,585)	1:79:A:VAL:HG23	1:87:A:LYS:HE3	15	0.14
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB2	12	0.14
(1,382)	1:57:A:CYS:HB2	1:110:A:LEU:HB3	12	0.14
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB2	12	0.14
(1,382)	1:57:A:CYS:HB3	1:110:A:LEU:HB3	12	0.14
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD11	10	0.14
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD12	10	0.14
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD13	10	0.14
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	11	0.14
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	11	0.14
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	5	0.14
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	5	0.14
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	6	0.14
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	6	0.14
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD2	14	0.14
(1,157)	1:20:A:THR:HA	1:22:A:PRO:HD3	14	0.14
(1,51)	1:10:A:GLU:HG2	1:12:A:ALA:H	15	0.14
(1,51)	1:10:A:GLU:HG3	1:12:A:ALA:H	15	0.14
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	4	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	12	0.13
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	13	0.13
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	15	0.13
(2,81)	1:69:A:VAL:O	1:56:A:GLY:N	15	0.13
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	4	0.13
(2,78)	1:13:A:ILE:O	1:38:A:ASP:N	9	0.13
(2,76)	1:9:A:THR:O	1:12:A:ALA:N	5	0.13
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	2	0.13
(2,5)	1:9:A:THR:O	1:12:A:ALA:H	11	0.13
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	15	0.13
(1,648)	1:93:A:LEU:HA	1:129:A:PHE:H	15	0.13
(1,640)	1:93:A:LEU:H	1:93:A:LEU:HG	2	0.13
(1,640)	1:93:A:LEU:H	1:93:A:LEU:HG	11	0.13
(1,605)	1:81:A:GLU:H	1:87:A:LYS:HG2	12	0.13
(1,585)	1:79:A:VAL:HG11	1:87:A:LYS:HE2	4	0.13
(1,585)	1:79:A:VAL:HG11	1:87:A:LYS:HE3	4	0.13
(1,585)	1:79:A:VAL:HG12	1:87:A:LYS:HE2	4	0.13
(1,585)	1:79:A:VAL:HG12	1:87:A:LYS:HE3	4	0.13
(1,585)	1:79:A:VAL:HG13	1:87:A:LYS:HE2	4	0.13
(1,585)	1:79:A:VAL:HG13	1:87:A:LYS:HE3	4	0.13
(1,585)	1:79:A:VAL:HG21	1:87:A:LYS:HE2	4	0.13
(1,585)	1:79:A:VAL:HG21	1:87:A:LYS:HE3	4	0.13
(1,585)	1:79:A:VAL:HG22	1:87:A:LYS:HE2	4	0.13
(1,585)	1:79:A:VAL:HG22	1:87:A:LYS:HE3	4	0.13
(1,585)	1:79:A:VAL:HG23	1:87:A:LYS:HE2	4	0.13
(1,585)	1:79:A:VAL:HG23	1:87:A:LYS:HE3	4	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	9	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	9	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	9	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	12	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	12	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	12	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	13	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	13	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	13	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	15	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	15	0.13
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	15	0.13
(1,389)	1:58:A:TYR:H	1:66:A:TYR:HA	13	0.13
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	4	0.13
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	6	0.13
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	7	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	10	0.13
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	11	0.13
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD11	2	0.13
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD12	2	0.13
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD13	2	0.13
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG12	9	0.13
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG13	9	0.13
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG12	9	0.13
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG13	9	0.13
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	5	0.13
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	5	0.13
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	5	0.13
(1,166)	1:23:A:ASN:H	1:25:A:GLN:H	13	0.13
(1,70)	1:13:A:ILE:HD11	1:14:A:TYR:H	1	0.13
(1,70)	1:13:A:ILE:HD12	1:14:A:TYR:H	1	0.13
(1,70)	1:13:A:ILE:HD13	1:14:A:TYR:H	1	0.13
(1,70)	1:13:A:ILE:HD11	1:14:A:TYR:H	2	0.13
(1,70)	1:13:A:ILE:HD12	1:14:A:TYR:H	2	0.13
(1,70)	1:13:A:ILE:HD13	1:14:A:TYR:H	2	0.13
(3,48)	1:116:A:ILE:N	1:111:A:CYS:H	7	0.12
(3,22)	1:82:A:THR:N	1:84:A:TYR:H	13	0.12
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	8	0.12
(2,55)	1:114:A:GLY:H	1:111:A:CYS:O	7	0.12
(2,55)	1:114:A:GLY:H	1:111:A:CYS:O	12	0.12
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	1	0.12
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	10	0.12
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	14	0.12
(1,871)	1:123:A:GLY:H	1:128:A:ALA:H	10	0.12
(1,808)	1:117:A:GLY:H	1:118:A:ILE:H	14	0.12
(1,807)	1:116:A:ILE:HG21	1:133:A:ARG:HD2	7	0.12
(1,807)	1:116:A:ILE:HG21	1:133:A:ARG:HD3	7	0.12
(1,807)	1:116:A:ILE:HG22	1:133:A:ARG:HD2	7	0.12
(1,807)	1:116:A:ILE:HG22	1:133:A:ARG:HD3	7	0.12
(1,807)	1:116:A:ILE:HG23	1:133:A:ARG:HD2	7	0.12
(1,807)	1:116:A:ILE:HG23	1:133:A:ARG:HD3	7	0.12
(1,789)	1:114:A:GLY:H	1:115:A:VAL:H	5	0.12
(1,751)	1:109:A:LEU:H	1:110:A:LEU:H	12	0.12
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG12	14	0.12
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG13	14	0.12
(1,637)	1:92:A:ASN:HA	1:131:A:ASP:H	3	0.12
(1,637)	1:92:A:ASN:HA	1:131:A:ASP:H	11	0.12
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	9	0.12
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	13	0.12
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	13	0.12
(1,586)	1:79:A:VAL:H	1:88:A:HIS:H	9	0.12
(1,572)	1:78:A:PRO:HA	1:79:A:VAL:HG11	9	0.12
(1,572)	1:78:A:PRO:HA	1:79:A:VAL:HG12	9	0.12
(1,572)	1:78:A:PRO:HA	1:79:A:VAL:HG13	9	0.12
(1,572)	1:78:A:PRO:HA	1:79:A:VAL:HG21	9	0.12
(1,572)	1:78:A:PRO:HA	1:79:A:VAL:HG22	9	0.12
(1,572)	1:78:A:PRO:HA	1:79:A:VAL:HG23	9	0.12
(1,564)	1:76:A:TRP:HA	1:93:A:LEU:HB2	8	0.12
(1,564)	1:76:A:TRP:HA	1:93:A:LEU:HB2	12	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	1	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	1	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	1	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	2	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	2	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	2	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	3	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	3	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	3	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	4	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	4	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	4	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	5	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	5	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	5	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	6	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	6	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	6	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	7	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	7	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	7	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	8	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	8	0.12
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	8	0.12
(1,389)	1:58:A:TYR:H	1:66:A:TYR:HA	15	0.12
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	3	0.12
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	8	0.12
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	3	0.12
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	10	0.12
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG12	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG13	14	0.12
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG12	14	0.12
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG13	14	0.12
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	7	0.12
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	7	0.12
(1,314)	1:50:A:ASP:H	1:51:A:CYS:H	7	0.12
(1,267)	1:41:A:ASP:H	1:41:A:ASP:HB3	6	0.12
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD21	11	0.12
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD22	11	0.12
(1,247)	1:35:A:LEU:H	1:35:A:LEU:HD23	11	0.12
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	6	0.12
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	8	0.12
(1,43)	1:9:A:THR:HA	1:9:A:THR:HG21	13	0.12
(1,43)	1:9:A:THR:HA	1:9:A:THR:HG22	13	0.12
(1,43)	1:9:A:THR:HA	1:9:A:THR:HG23	13	0.12
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	3	0.11
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	7	0.11
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	9	0.11
(3,39)	1:109:A:LEU:N	1:59:A:TYR:H	11	0.11
(3,25)	1:82:A:THR:H	1:86:A:PRO:N	6	0.11
(2,79)	1:38:A:ASP:O	1:13:A:ILE:N	14	0.11
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	1	0.11
(2,57)	1:116:A:ILE:O	1:133:A:ARG:H	11	0.11
(2,55)	1:114:A:GLY:H	1:111:A:CYS:O	9	0.11
(2,55)	1:114:A:GLY:H	1:111:A:CYS:O	10	0.11
(2,47)	1:108:A:LYS:O	1:59:A:TYR:H	4	0.11
(2,43)	1:106:A:GLY:H	1:119:A:ILE:O	13	0.11
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	2	0.11
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	5	0.11
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	7	0.11
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	12	0.11
(1,876)	1:124:A:ASP:HA	1:126:A:HIS:H	7	0.11
(1,876)	1:124:A:ASP:HA	1:126:A:HIS:H	9	0.11
(1,876)	1:124:A:ASP:HA	1:126:A:HIS:H	10	0.11
(1,826)	1:118:A:ILE:HG12	1:130:A:THR:HB	14	0.11
(1,826)	1:118:A:ILE:HG13	1:130:A:THR:HB	14	0.11
(1,751)	1:109:A:LEU:H	1:110:A:LEU:H	5	0.11
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG12	13	0.11
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG13	13	0.11
(1,709)	1:100:A:CYS:HB2	1:127:A:VAL:HB	8	0.11
(1,709)	1:100:A:CYS:HB3	1:127:A:VAL:HB	8	0.11
(1,657)	1:94:A:LEU:HD11	1:109:A:LEU:HG	14	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:94:A:LEU:HD12	1:109:A:LEU:HG	14	0.11
(1,657)	1:94:A:LEU:HD13	1:109:A:LEU:HG	14	0.11
(1,657)	1:94:A:LEU:HD21	1:109:A:LEU:HG	14	0.11
(1,657)	1:94:A:LEU:HD22	1:109:A:LEU:HG	14	0.11
(1,657)	1:94:A:LEU:HD23	1:109:A:LEU:HG	14	0.11
(1,631)	1:91:A:TYR:H	1:92:A:ASN:H	3	0.11
(1,618)	1:88:A:HIS:H	1:79:A:VAL:HG12	9	0.11
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	6	0.11
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	6	0.11
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	11	0.11
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	11	0.11
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	12	0.11
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	12	0.11
(1,565)	1:77:A:TYR:H	1:89:A:ILE:HD11	8	0.11
(1,565)	1:77:A:TYR:H	1:89:A:ILE:HD12	8	0.11
(1,565)	1:77:A:TYR:H	1:89:A:ILE:HD13	8	0.11
(1,564)	1:76:A:TRP:HA	1:93:A:LEU:HB2	3	0.11
(1,506)	1:71:A:CYS:H	1:72:A:GLU:HA	14	0.11
(1,446)	1:60:A:SER:HA	1:67:A:ILE:HD11	10	0.11
(1,446)	1:60:A:SER:HA	1:67:A:ILE:HD12	10	0.11
(1,446)	1:60:A:SER:HA	1:67:A:ILE:HD13	10	0.11
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG21	11	0.11
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG22	11	0.11
(1,392)	1:58:A:TYR:H	1:67:A:ILE:HG23	11	0.11
(1,389)	1:58:A:TYR:H	1:66:A:TYR:HA	3	0.11
(1,389)	1:58:A:TYR:H	1:66:A:TYR:HA	4	0.11
(1,389)	1:58:A:TYR:H	1:66:A:TYR:HA	6	0.11
(1,381)	1:57:A:CYS:HA	1:110:A:LEU:H	13	0.11
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	5	0.11
(1,350)	1:56:A:GLY:H	1:71:A:CYS:H	1	0.11
(1,350)	1:56:A:GLY:H	1:71:A:CYS:H	11	0.11
(1,342)	1:56:A:GLY:H	1:69:A:VAL:HA	15	0.11
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	2	0.11
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	6	0.11
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	7	0.11
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	8	0.11
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	15	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD11	3	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD12	3	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD13	3	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD11	8	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD12	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD13	8	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD11	15	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD12	15	0.11
(1,329)	1:54:A:THR:H	1:116:A:ILE:HD13	15	0.11
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG12	10	0.11
(1,321)	1:52:A:ASP:HB2	1:116:A:ILE:HG13	10	0.11
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG12	10	0.11
(1,321)	1:52:A:ASP:HB3	1:116:A:ILE:HG13	10	0.11
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	5	0.11
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	5	0.11
(1,316)	1:50:A:ASP:HB2	1:51:A:CYS:H	12	0.11
(1,316)	1:50:A:ASP:HB3	1:51:A:CYS:H	12	0.11
(1,312)	1:50:A:ASP:H	1:50:A:ASP:HB3	11	0.11
(1,279)	1:47:A:ASN:H	1:48:A:ILE:H	13	0.11
(1,175)	1:25:A:GLN:H	1:25:A:GLN:HG3	4	0.11
(1,164)	1:22:A:PRO:HB2	1:23:A:ASN:HA	13	0.11
(1,164)	1:22:A:PRO:HB3	1:23:A:ASN:HA	13	0.11
(1,159)	1:21:A:THR:H	1:21:A:THR:HB	12	0.11
(3,25)	1:82:A:THR:H	1:86:A:PRO:N	2	0.1
(2,77)	1:12:A:ALA:O	1:9:A:THR:N	2	0.1
(2,43)	1:106:A:GLY:H	1:119:A:ILE:O	9	0.1
(2,43)	1:106:A:GLY:H	1:119:A:ILE:O	11	0.1
(2,4)	1:14:A:TYR:O	1:7:A:VAL:N	9	0.1
(1,913)	1:136:A:ASN:HA	1:137:A:ILE:HG12	15	0.1
(1,913)	1:136:A:ASN:HA	1:137:A:ILE:HG13	15	0.1
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	3	0.1
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	4	0.1
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	9	0.1
(1,885)	1:127:A:VAL:HA	1:128:A:ALA:HA	11	0.1
(1,876)	1:124:A:ASP:HA	1:126:A:HIS:H	11	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG21	3	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG22	3	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG23	3	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG21	5	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG22	5	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG23	5	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG21	12	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG22	12	0.1
(1,830)	1:119:A:ILE:H	1:119:A:ILE:HG23	12	0.1
(1,808)	1:117:A:GLY:H	1:118:A:ILE:H	12	0.1
(1,751)	1:109:A:LEU:H	1:110:A:LEU:H	14	0.1
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG12	10	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:106:A:GLY:H	1:119:A:ILE:HG13	10	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	1	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	1	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	5	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	5	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	7	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	7	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG2	10	0.1
(1,593)	1:80:A:GLU:HA	1:80:A:GLU:HG3	10	0.1
(1,544)	1:74:A:HIS:H	1:93:A:LEU:HB2	14	0.1
(1,544)	1:74:A:HIS:H	1:93:A:LEU:HB3	14	0.1
(1,530)	1:73:A:ALA:HB1	1:75:A:ASP:H	12	0.1
(1,530)	1:73:A:ALA:HB2	1:75:A:ASP:H	12	0.1
(1,530)	1:73:A:ALA:HB3	1:75:A:ASP:H	12	0.1
(1,506)	1:71:A:CYS:H	1:72:A:GLU:HA	3	0.1
(1,506)	1:71:A:CYS:H	1:72:A:GLU:HA	6	0.1
(1,351)	1:56:A:GLY:HA2	1:109:A:LEU:HG	9	0.1
(1,350)	1:56:A:GLY:H	1:71:A:CYS:H	2	0.1
(1,340)	1:56:A:GLY:H	1:57:A:CYS:H	9	0.1
(1,159)	1:21:A:THR:H	1:21:A:THR:HB	13	0.1
(1,70)	1:13:A:ILE:HD11	1:14:A:TYR:H	5	0.1
(1,70)	1:13:A:ILE:HD12	1:14:A:TYR:H	5	0.1
(1,70)	1:13:A:ILE:HD13	1:14:A:TYR:H	5	0.1

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

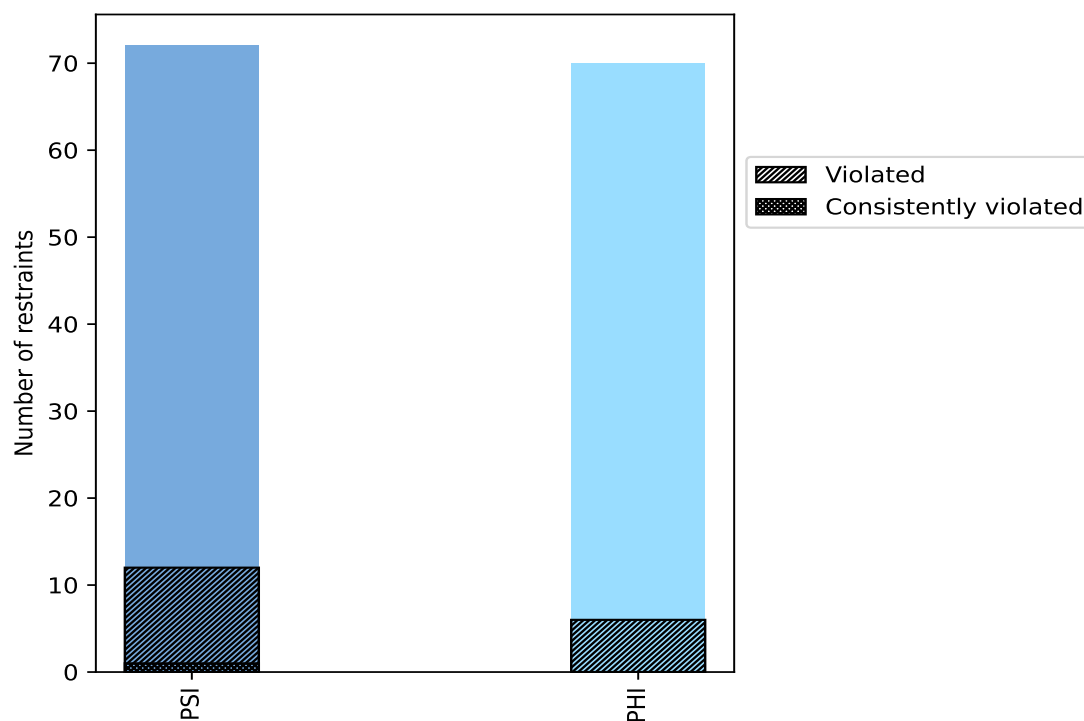
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	72	50.7	12	16.7	8.5	1	1.4	0.7
PHI	70	49.3	6	8.6	4.2	0	0.0	0.0
Total	142	100.0	18	12.7	12.7	1	0.7	0.7

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](#)



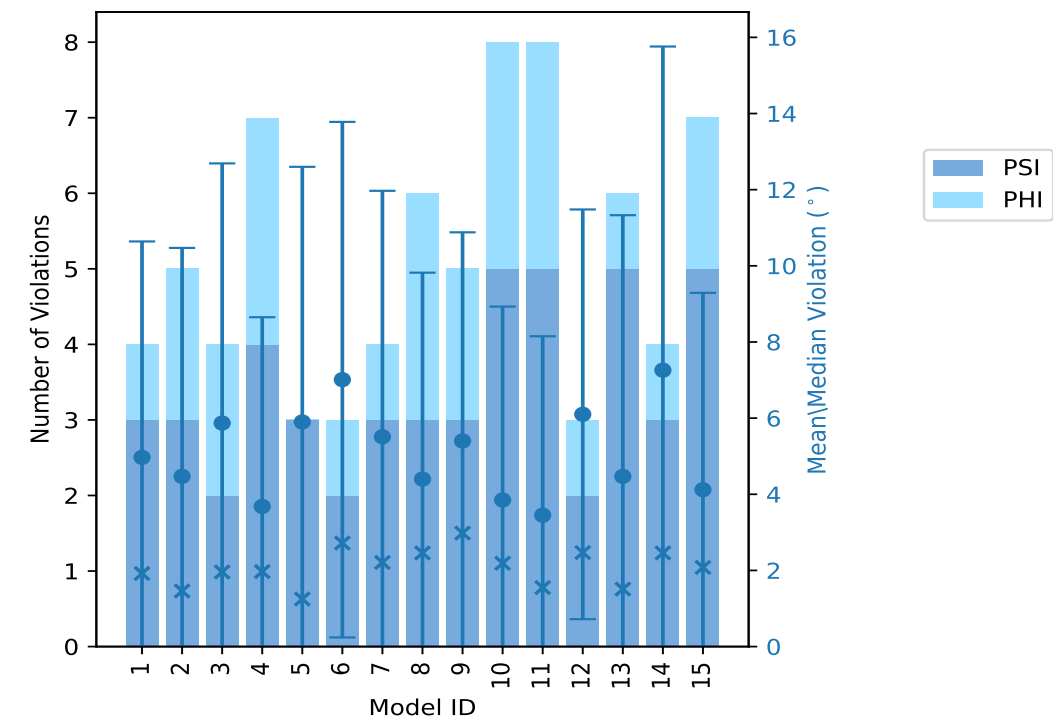
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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 (°)
	PSI	PHI	Total				
1	3	1	4	4.97	14.78	5.67	1.92
2	3	2	5	4.47	16.47	6.0	1.46
3	2	2	4	5.87	17.68	6.82	1.96
4	4	3	7	3.68	15.8	4.97	1.97
5	3	0	3	5.9	15.38	6.7	1.25
6	2	1	3	7.01	16.57	6.77	2.72
7	3	1	4	5.51	16.59	6.46	2.21
8	3	3	6	4.4	16.41	5.42	2.46
9	3	2	5	5.4	16.22	5.48	2.98
10	5	3	8	3.85	17.25	5.08	2.19
11	5	3	8	3.45	15.78	4.7	1.55
12	2	1	3	6.1	13.7	5.38	2.47
13	5	1	6	4.47	19.8	6.86	1.51
14	3	1	4	7.26	21.98	8.5	2.46
15	5	2	7	4.12	16.69	5.17	2.08

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

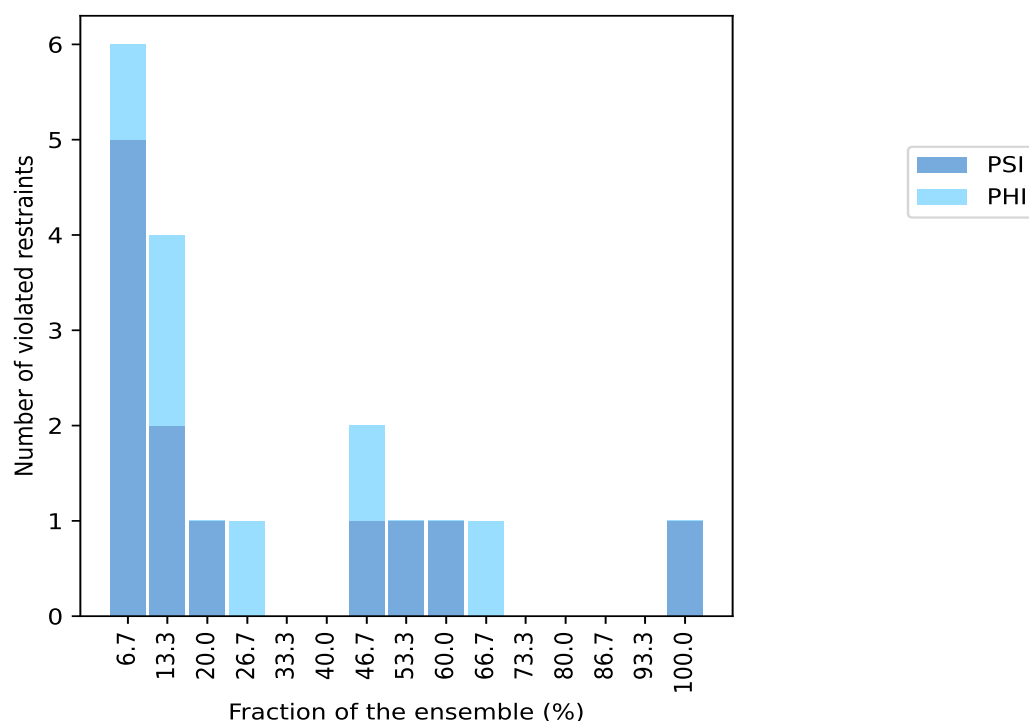
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

¹ Number of models with violations

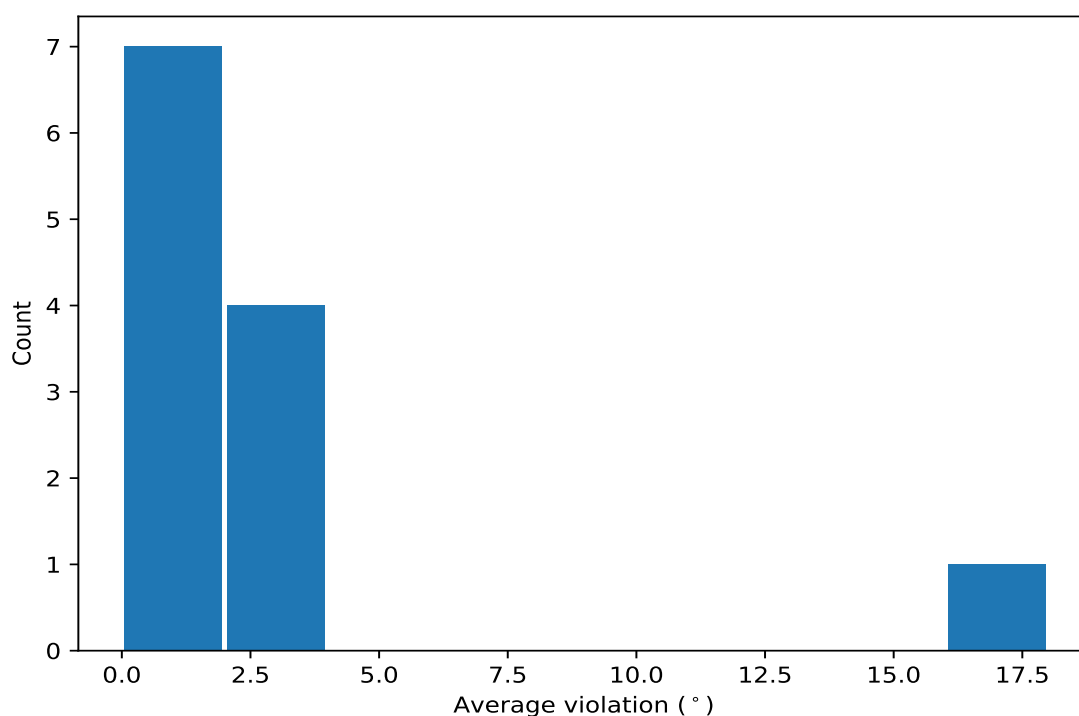
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

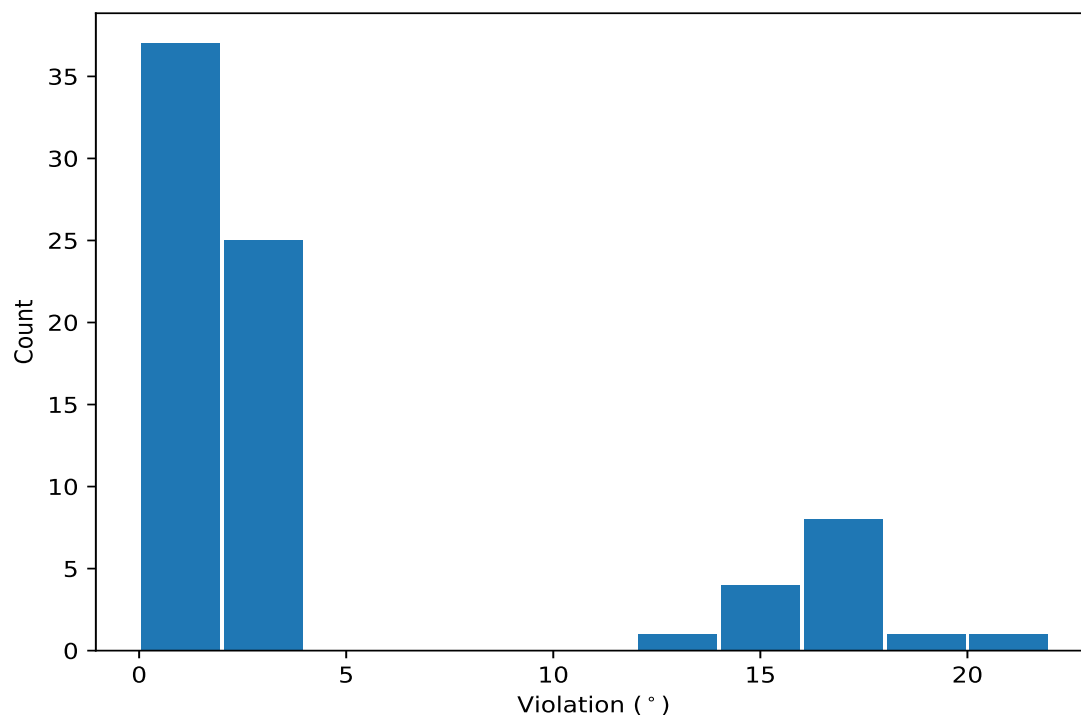
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	15	16.74	1.92	16.47
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	10	2.19	0.36	2.33
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	9	2.09	0.18	2.12
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	8	1.2	0.12	1.17
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	7	1.84	0.58	1.82
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	7	1.7	0.28	1.75
(1,130)	1:121:A:ALA:C	1:122:A:GLY:N	1:122:A:GLY:CA	1:122:A:GLY:C	4	2.96	0.2	2.94
(1,49)	1:44:A:GLY:N	1:44:A:GLY:CA	1:44:A:GLY:C	1:45:A:PRO:N	3	2.8	0.41	2.68
(1,8)	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	1:12:A:ALA:N	2	1.38	0.29	1.38
(1,142)	1:130:A:THR:C	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	2	1.21	0.01	1.21
(1,10)	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	1:13:A:ILE:N	2	1.2	0.08	1.2
(1,132)	1:125:A:GLY:C	1:126:A:HIS:N	1:126:A:HIS:CA	1:126:A:HIS:C	2	1.1	0.03	1.1

¹ Number of violated models, ²Standard 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 (°)
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	14	21.98
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	13	19.8
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	3	17.68
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	10	17.25
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	15	16.69
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	7	16.59
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	6	16.57
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	2	16.47
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	8	16.41
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	9	16.22
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	4	15.8
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	11	15.78
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	5	15.38
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	1	14.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,53)	1:56:A:GLY:N	1:56:A:GLY:CA	1:56:A:GLY:C	1:57:A:CYS:N	12	13.7
(1,1)	1:6:A:PHE:C	1:7:A:VAL:N	1:7:A:VAL:CA	1:7:A:VAL:C	9	3.9
(1,49)	1:44:A:GLY:N	1:44:A:GLY:CA	1:44:A:GLY:C	1:45:A:PRO:N	15	3.35
(1,130)	1:121:A:ALA:C	1:122:A:GLY:N	1:122:A:GLY:CA	1:122:A:GLY:C	7	3.25
(1,130)	1:121:A:ALA:C	1:122:A:GLY:N	1:122:A:GLY:CA	1:122:A:GLY:C	9	2.98
(1,130)	1:121:A:ALA:C	1:122:A:GLY:N	1:122:A:GLY:CA	1:122:A:GLY:C	8	2.91
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	6	2.72
(1,130)	1:121:A:ALA:C	1:122:A:GLY:N	1:122:A:GLY:CA	1:122:A:GLY:C	11	2.7
(1,49)	1:44:A:GLY:N	1:44:A:GLY:CA	1:44:A:GLY:C	1:45:A:PRO:N	9	2.68
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	11	2.59
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	14	2.53
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	8	2.47
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	12	2.47
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	10	2.46
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	8	2.44
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	10	2.41
(1,49)	1:44:A:GLY:N	1:44:A:GLY:CA	1:44:A:GLY:C	1:45:A:PRO:N	14	2.38
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	4	2.25
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	15	2.24
(1,133)	1:126:A:HIS:N	1:126:A:HIS:CA	1:126:A:HIS:C	1:127:A:VAL:N	10	2.22
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	14	2.17
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	10	2.16
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	12	2.12
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	4	2.1
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	15	2.08
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	1	2.04
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	3	1.99
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	15	1.97
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	4	1.97
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	3	1.92
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	3	1.9
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	11	1.82
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	1	1.79
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:GLU:N	2	1.79
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	6	1.75
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	10	1.75
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	13	1.75
(1,8)	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	1:12:A:ALA:N	13	1.68
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	10	1.49
(1,7)	1:10:A:GLU:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	2	1.46
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	2	1.39
(1,137)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:PHE:N	15	1.37
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	4	1.37
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	13	1.34
(1,10)	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	1:13:A:ILE:N	11	1.28
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	1	1.26
(1,109)	1:96:A:GLY:N	1:96:A:GLY:CA	1:96:A:GLY:C	1:97:A:GLU:N	5	1.25
(1,58)	1:58:A:TYR:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	2	1.24
(1,142)	1:130:A:THR:C	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	11	1.22
(1,142)	1:130:A:THR:C	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	4	1.2
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	9	1.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	7	1.17
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	15	1.17
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	11	1.15
(1,132)	1:125:A:GLY:C	1:126:A:HIS:N	1:126:A:HIS:CA	1:126:A:HIS:C	8	1.13
(1,10)	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	1:13:A:ILE:N	13	1.13
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	13	1.11
(1,8)	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	1:12:A:ALA:N	11	1.09
(1,76)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:GLU:N	5	1.07
(1,132)	1:125:A:GLY:C	1:126:A:HIS:N	1:126:A:HIS:CA	1:126:A:HIS:C	10	1.06
(1,113)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:LYS:N	4	1.06
(1,105)	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1:95:A:ILE:N	7	1.04
(1,97)	1:90:A:GLN:N	1:90:A:GLN:CA	1:90:A:GLN:C	1:91:A:TYR:N	8	1.04