Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 01:14 AM EDT

PDB ID	:	2M9U
BMRB ID	:	19299
Title	:	Solution NMR structure of the C-terminal domain (CTD) of Moloney murine leukemia virus integrase, Northeast Structural Genomics Target OR41A
Authors	:	Aiyer, S.; Rossi, P.; Schneider, W.M.; Chander, A.; Roth, M.J.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2013-06-19

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:

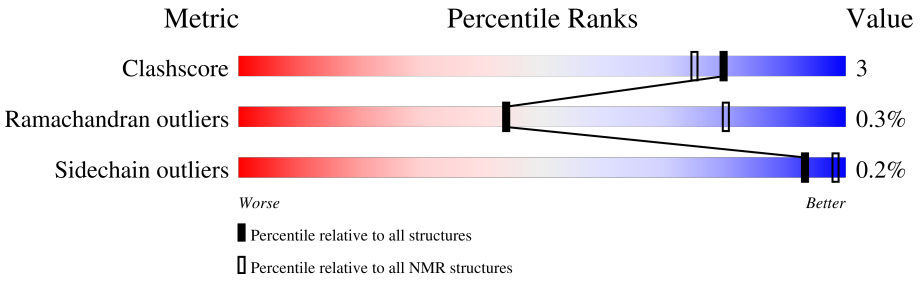
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 82%.

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	89	47% • 52%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:9-A:18, A:27-A:59 (43)	0.56	1

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1442 atoms, of which 725 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Integrase p46.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1442	451	725	147	118	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P03355
A	2	HIS	-	expression tag	UNP P03355
A	3	HIS	-	expression tag	UNP P03355
A	4	HIS	-	expression tag	UNP P03355
A	5	HIS	-	expression tag	UNP P03355
A	6	HIS	-	expression tag	UNP P03355
A	7	SER	-	expression tag	UNP P03355
A	8	HIS	-	expression tag	UNP P03355
A	9	MET	-	expression tag	UNP P03355

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: Integrase p46

Chain A: 47% • 52%

H1 H2 H3 H4 H5 H6 S7 H8 R17 R18 H19 Q20 T21 K22 N23 L24 E25 P26 D60 P61 G62 G63 G64 P65 S66 S67 R68 L69 T70 W71 R72 V73 Q74 R75 S76 Q77 N78 P79 L80 K81 I82 R83 L84 T85 R86 E87 A88 P89

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 (medoid)

• Molecule 1: Integrase p46

Chain A: 45% • 52%

H1 H2 H3 H4 H5 H6 S7 H8 D12 H19 Q20 T21 K22 N23 L24 E25 P26 V34 P39 D60 P61 G62 G63 G64 P65 S66 S67 R68 L69 T70 W71 R72 V73 Q74 R75 S76 Q77 N78 P79 L80 K81 I82 R83 L84 T85 R86 E87 A88 P89

4.2.2 Score per residue for model 2

• Molecule 1: Integrase p46

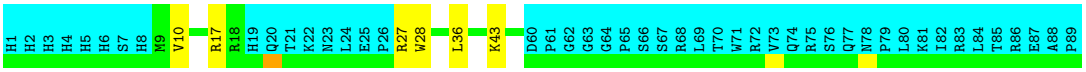
Chain A: 46% • 52%

H1 H2 H3 H4 H5 H6 S7 H8 D12 H19 Q20 T21 K22 N23 L24 E25 P26 V34 D60 P61 G62 G63 G64 P65 S66 S67 R68 L69 T70 W71 R72 V73 Q74 R75 S76 Q77 N78 P79 L80 K81 I82 R83 L84 T85 R86 E87 A88 P89

4.2.3 Score per residue for model 3

- Molecule 1: Integrase p46

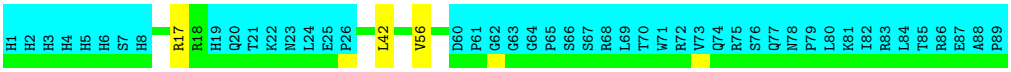
Chain A: 42% 7% 52%



4.2.4 Score per residue for model 4

- Molecule 1: Integrase p46

Chain A: 45% • 52%



4.2.5 Score per residue for model 5

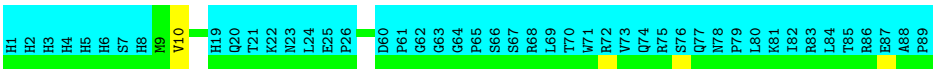
- Molecule 1: Integrase p46

Chain A: 45% • 52%

4.2.6 Score per residue for model 6

- Molecule 1: Integrase p46

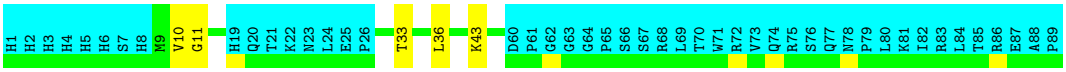
Chain A: 47% • 52%



4.2.7 Score per residue for model 7

- Molecule 1: Integrase p46

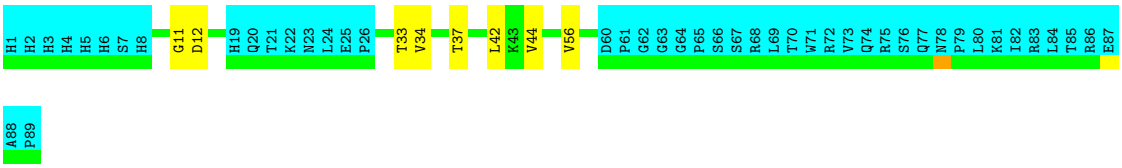
Chain A: 43% 6% 52%



4.2.8 Score per residue for model 8

- Molecule 1: Integrase p46

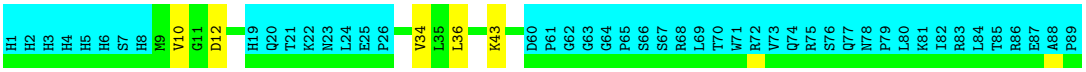
Chain A: 39% 9% 52%



4.2.9 Score per residue for model 9

- Molecule 1: Integrase p46

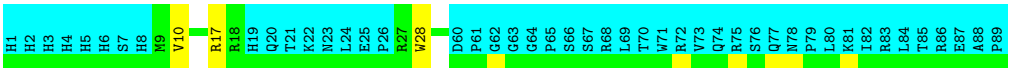
Chain A: 43% 6% 52%



4.2.10 Score per residue for model 10

- Molecule 1: Integrase p46

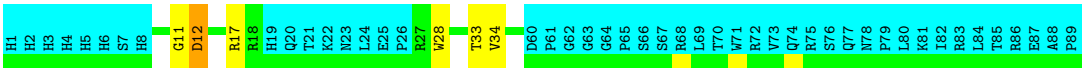
Chain A: 45% • 52%



4.2.11 Score per residue for model 11

- Molecule 1: Integrase p46

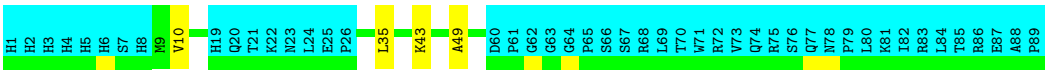
Chain A: 42% 6% • 52%



4.2.12 Score per residue for model 12

- Molecule 1: Integrase p46

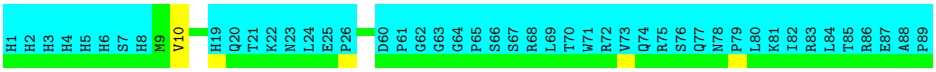
Chain A: 44% • 52%



4.2.13 Score per residue for model 13

- Molecule 1: Integrase p46

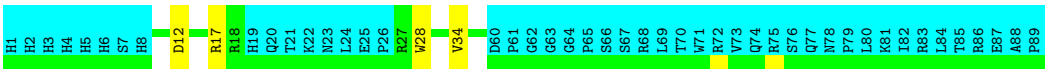
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Integrase p46

Chain A:



4.2.15 Score per residue for model 15

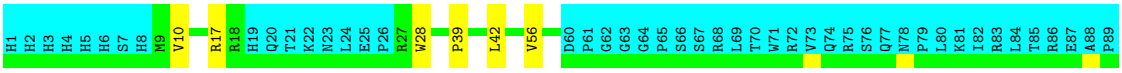
- Molecule 1: Integrase p46

Chain A:

4.2.16 Score per residue for model 16

- Molecule 1: Integrase p46

Chain A:



4.2.17 Score per residue for model 17

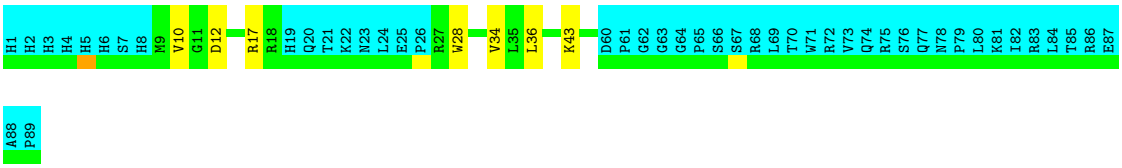
- Molecule 1: Integrase p46

Chain A:

4.2.18 Score per residue for model 18

- Molecule 1: Integrase p46

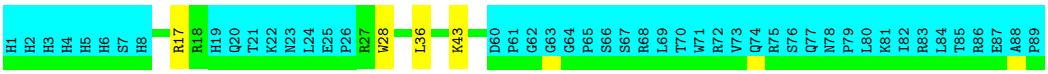
Chain A: 40% 8% 52%



4.2.19 Score per residue for model 19

- Molecule 1: Integrase p46

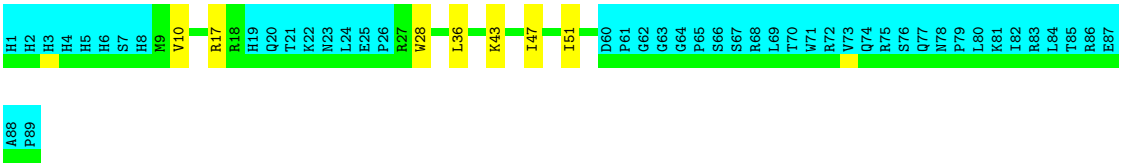
Chain A: 44% • 52%



4.2.20 Score per residue for model 20

- Molecule 1: Integrase p46

Chain A: 40% 8% 52%



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	**Classification**	**Version**
AutoStructure	structure solution	2.2.1
CYANA	geometry optimization	2.1
CYANA	structure solution	2.1
CNS	geometry optimization	2.0.6
CNS	refinement	2.0.6

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	900
Number of shifts mapped to atoms	900
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	336	352	350	2±1
All	All	6720	7040	7000	37

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ASP:HB3	1:A:34:VAL:HB	0.55	1.77	8	8
1:A:11:GLY:HA2	1:A:33:THR:HB	0.55	1.78	15	4
1:A:17:ARG:HA	1:A:28:TRP:HA	0.52	1.82	14	9
1:A:36:LEU:HB3	1:A:43:LYS:HB3	0.51	1.81	19	6
1:A:42:LEU:HD12	1:A:56:VAL:HG11	0.51	1.83	8	4
1:A:10:VAL:HA	1:A:35:LEU:HA	0.43	1.89	12	1
1:A:11:GLY:HA2	1:A:33:THR:HG23	0.42	1.91	7	1
1:A:43:LYS:HG3	1:A:49:ALA:O	0.42	2.14	12	1
1:A:37:THR:HG22	1:A:42:LEU:HD22	0.41	1.93	8	1
1:A:34:VAL:HG22	1:A:44:VAL:HG22	0.40	1.94	8	1
1:A:47:ILE:HG21	1:A:51:ILE:HG12	0.40	1.92	20	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	43/89 (48%)	40±1 (92±3%)	3±1 (7±2%)	0±0 (0±1%)	44 80
All	All	860/1780 (48%)	794 (92%)	63 (7%)	3 (0%)	44 80

All 2 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	39	PRO	2
1	A	12	ASP	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	33/75 (44%)	33±0 (100±1%)	0±0 (0±1%)	93 98
All	All	660/1500 (44%)	659 (100%)	1 (0%)	93 98

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	10	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 71% 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	900
Number of shifts mapped to atoms	900
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	79	-0.06 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	73	-0.17 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	79	0.20 ± 0.05	None needed (< 0.5 ppm)
^{15}N	70	0.25 ± 0.49	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 497 atoms were assigned a chemical shift out of a possible 605. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	198/214 (93%)	80/87 (92%)	81/86 (94%)	37/41 (90%)
Sidechain	255/330 (77%)	176/220 (80%)	79/98 (81%)	0/12 (0%)

Continued on next page...

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	44/61 (72%)	22/30 (73%)	19/24 (79%)	3/7 (43%)
Overall	497/605 (82%)	278/337 (82%)	179/208 (86%)	40/60 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 900 atoms were assigned a chemical shift out of a possible 1263. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	379/437 (87%)	151/177 (85%)	158/178 (89%)	70/82 (85%)
Sidechain	465/689 (67%)	313/450 (70%)	152/205 (74%)	0/34 (0%)
Aromatic	56/137 (41%)	28/68 (41%)	24/45 (53%)	4/24 (17%)
Overall	900/1263 (71%)	492/695 (71%)	334/428 (78%)	74/140 (53%)

7.1.4 Statistically unusual chemical shifts (i)

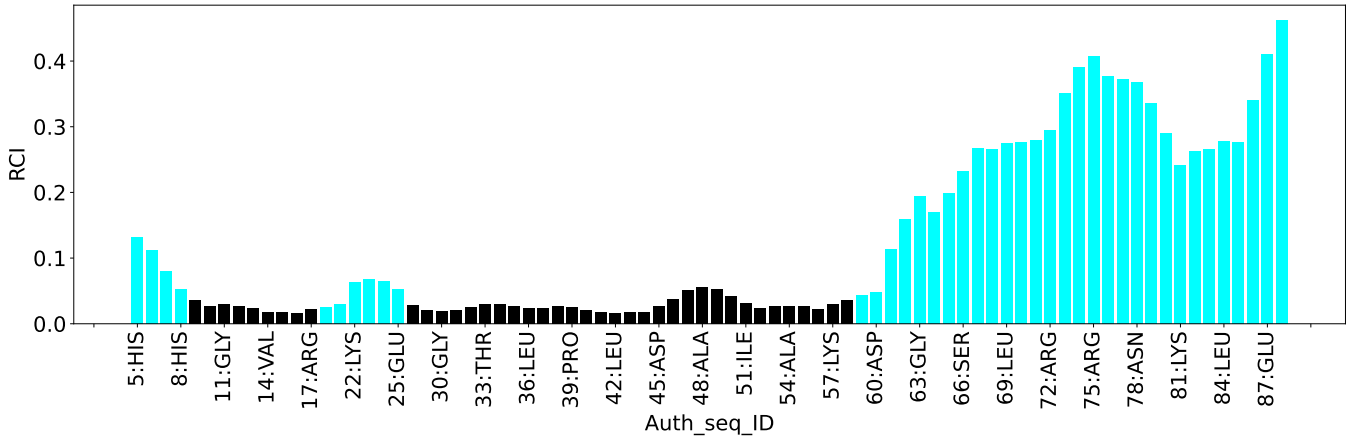
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	43	LYS	HB2	0.27	0.58 – 2.97	-6.3

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:


RCI
0.0
0.1
0.2
0.3
0.4
5:HIS
8:HIS
11:GLY
14:VAL
17:ARG
22:LYS
25:GLU
30:GLY
33:THR
36:LEU
39:PRO
42:LEU
45:ASP
48:ALA
51:ILE
54:ALA
57:LYS
60:ASP
63:GLY
66:SER
69:LEU
72:ARG
75:ARG
78:ASN
81:LYS
84:LEU
87:GLU
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	474
Intra-residue (|i-j|=0)	118
Sequential (|i-j|=1)	115
Medium range (|i-j|>1 and |i-j|<5)	40
Long range (|i-j|≥5)	157
Inter-chain	0
Hydrogen bond restraints	44
Disulfide bond restraints	0
Total dihedral-angle restraints	147
Number of unmapped restraints	0
Number of restraints per residue	7.0
Number of long range restraints per residue[1]	2.2

[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)	1.4	0.19
0.2-0.5 (Medium)	1.1	0.5
>0.5 (Large)	2.8	1.94

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)	17.9	8.8
10.0-20.0 (Medium)	None	None
>20.0 (Large)	0.2	149.5

9 Distance violation analysis (i)

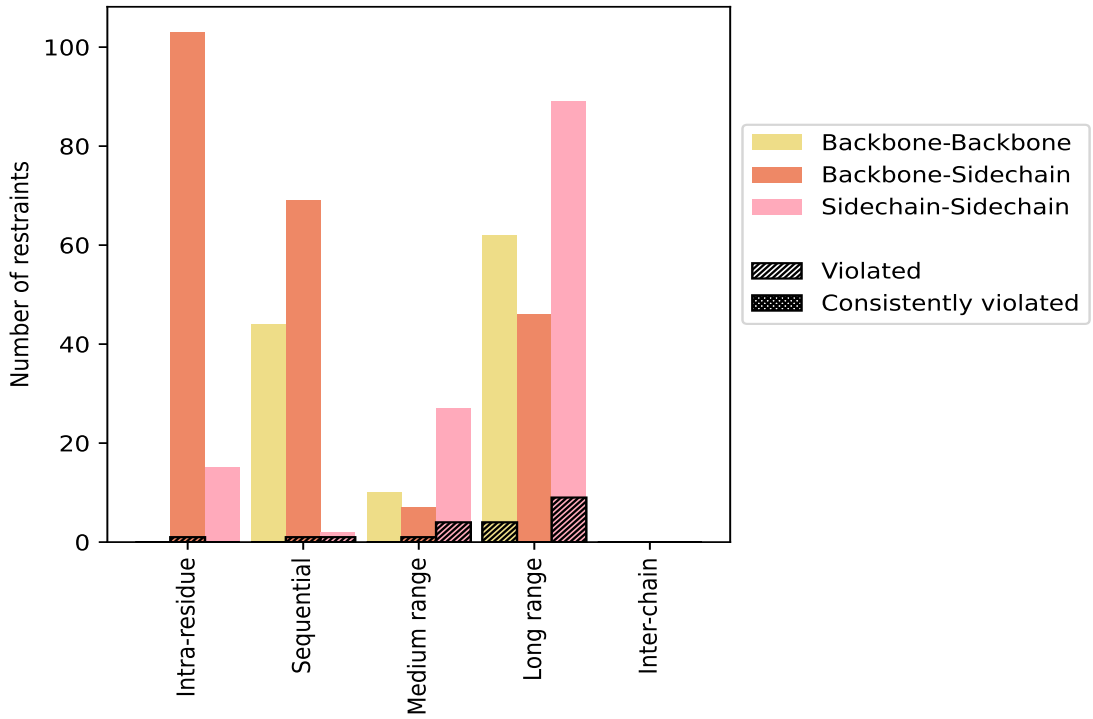
9.1 Summary of distance violations (i)

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)	118	24.9	1	0.8	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	103	21.7	1	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	15	3.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	115	24.3	2	1.7	0.4	0	0.0	0.0
Backbone-Backbone	44	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	69	14.6	1	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	2	0.4	1	50.0	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	40	8.4	5	12.5	1.1	0	0.0	0.0
Backbone-Backbone	6	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	1.5	1	14.3	0.2	0	0.0	0.0
Sidechain-Sidechain	27	5.7	4	14.8	0.8	0	0.0	0.0
Long range (|i-j|≥5)	157	33.1	9	5.7	1.9	0	0.0	0.0
Backbone-Backbone	22	4.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	46	9.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	89	18.8	9	10.1	1.9	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	44	9.3	4	9.1	0.8	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	474	100.0	21	4.4	4.4	0	0.0	0.0
Backbone-Backbone	116	24.5	4	3.4	0.8	0	0.0	0.0
Backbone-Sidechain	225	47.5	3	1.3	0.6	0	0.0	0.0
Sidechain-Sidechain	133	28.1	14	10.5	3.0	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	1	1	1	5	0	8	0.61	1.86	0.6	0.34
2	1	0	1	3	0	5	0.84	1.78	0.56	0.63
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	1	1	1	4	0	7	0.69	1.74	0.62	0.44
5	1	0	2	4	0	7	0.6	1.69	0.52	0.46
6	1	0	1	5	0	7	0.81	1.32	0.38	0.76
7	1	0	1	7	0	9	0.67	1.94	0.57	0.64
8	1	0	1	4	0	6	0.79	1.65	0.41	0.64
9	1	0	2	5	0	8	0.58	1.35	0.41	0.54
10	0	0	0	4	0	4	0.12	0.16	0.02	0.12
11	1	0	1	5	0	7	0.69	1.69	0.64	0.37

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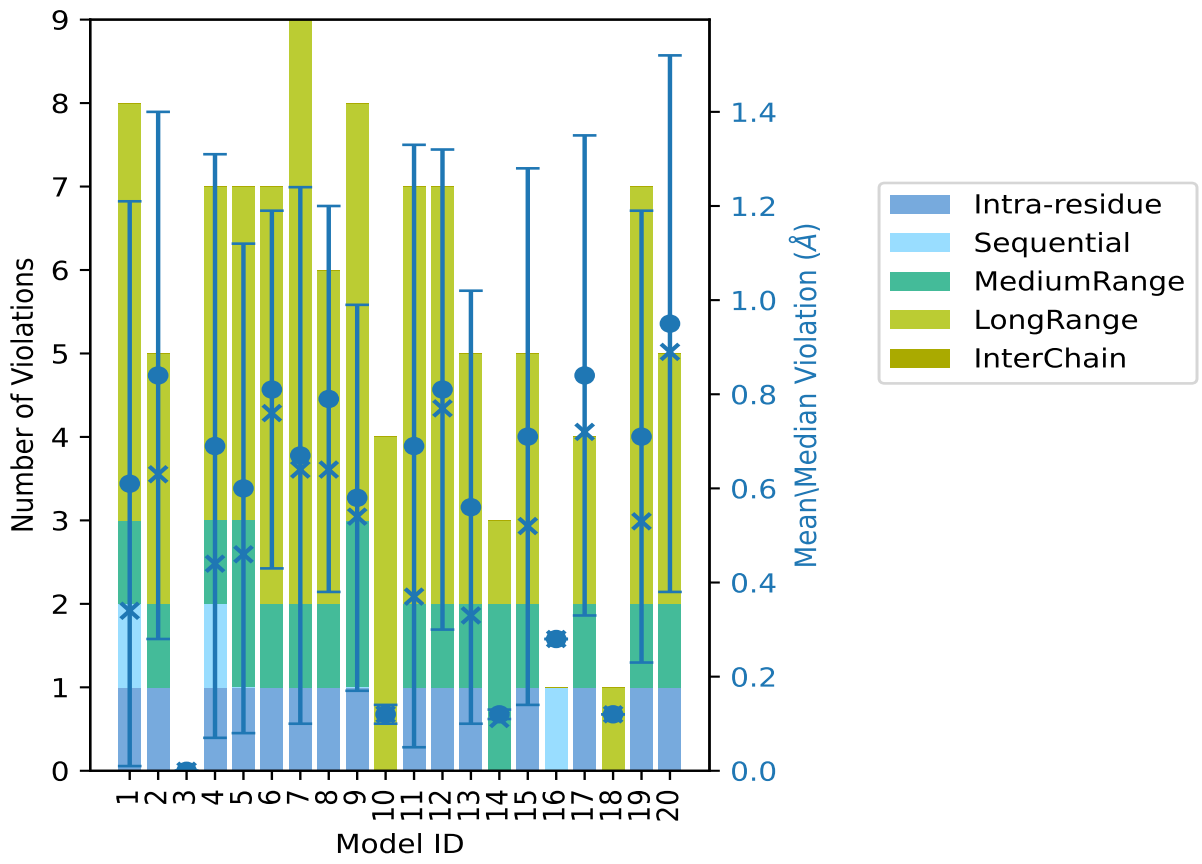
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	0	1	5	0	7	0.81	1.71	0.51	0.77
13	1	0	1	3	0	5	0.56	1.45	0.46	0.33
14	0	0	2	1	0	3	0.12	0.13	0.01	0.11
15	1	0	1	3	0	5	0.71	1.75	0.57	0.52
16	0	1	0	0	0	1	0.28	0.28	0.0	0.28
17	1	0	1	2	0	4	0.84	1.66	0.51	0.72
18	0	0	0	1	0	1	0.12	0.12	0.0	0.12
19	1	0	1	5	0	7	0.71	1.48	0.48	0.53
20	1	0	1	3	0	5	0.95	1.7	0.57	0.89

[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

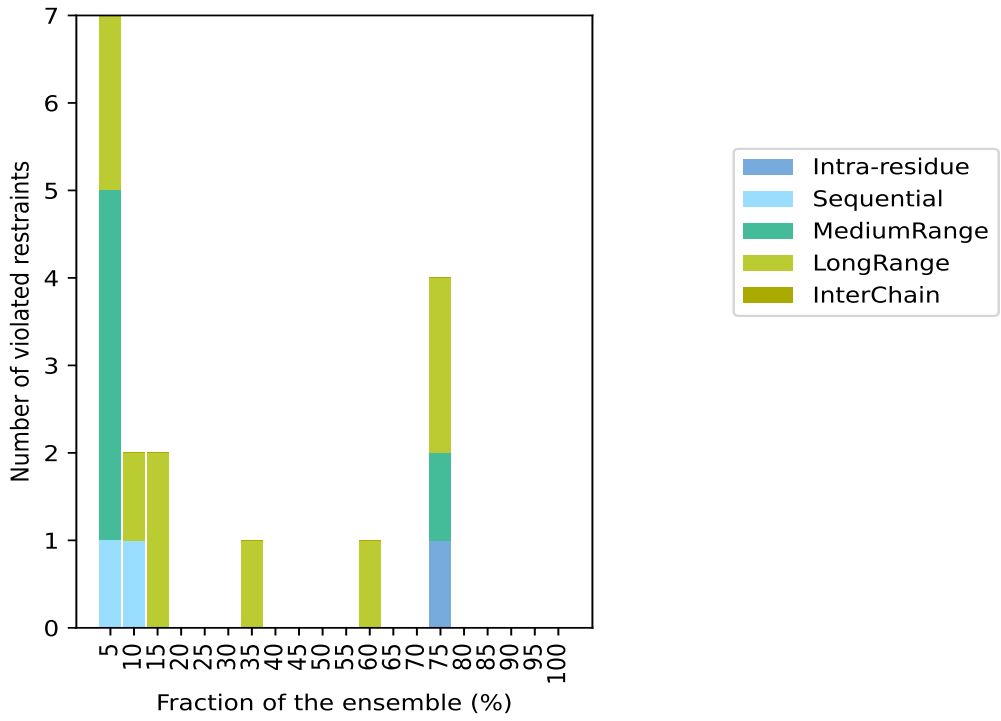
9.3 Distance violation statistics for the ensemble (i)

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, 413(IR:117, SQ:113, MR:35, LR:148, 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]	%
0	1	4	2	0	7	1	5.0
0	1	0	1	0	2	2	10.0
0	0	0	2	0	2	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	1	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
1	0	1	2	0	4	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	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

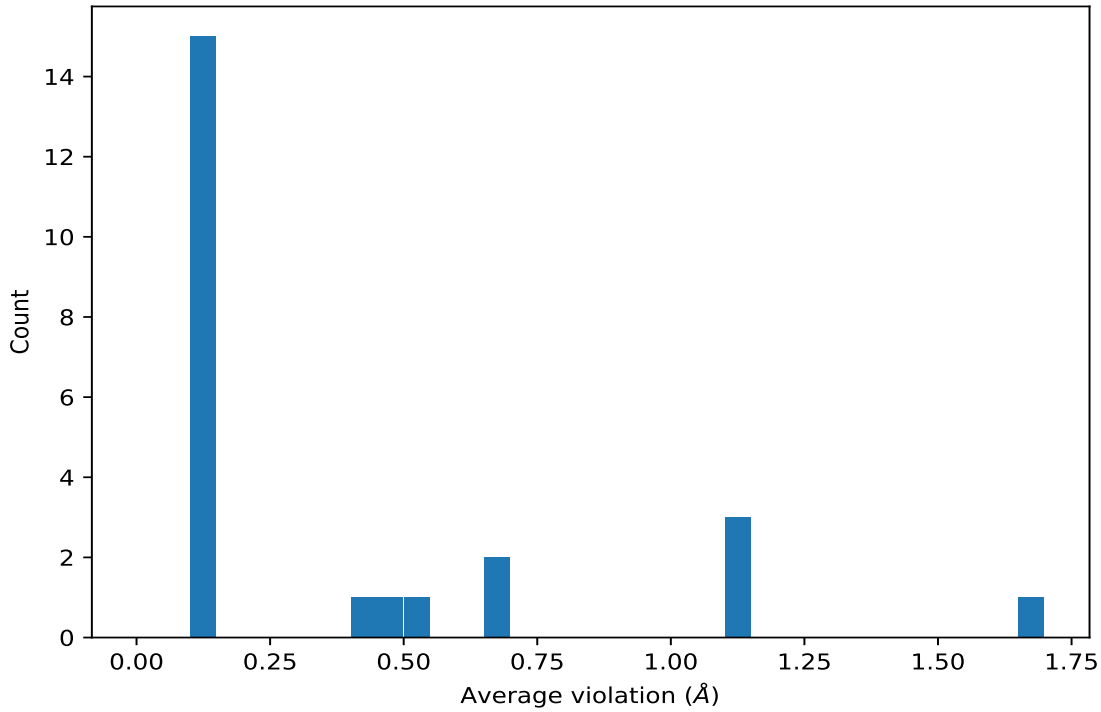
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	15	1.65	0.18	1.69
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	15	1.11	0.35	1.16
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	15	1.11	0.35	1.16
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	15	1.11	0.35	1.16
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	15	0.67	0.1	0.64
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	15	0.67	0.1	0.64
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	15	0.4	0.13	0.37
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	12	0.51	0.31	0.43
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	7	0.48	0.2	0.49
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	7	0.12	0.01	0.12
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB2	3	0.13	0.03	0.11
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB3	3	0.13	0.03	0.11
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG21	3	0.12	0.01	0.12
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG22	3	0.12	0.01	0.12
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG23	3	0.12	0.01	0.12
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG21	3	0.12	0.01	0.12

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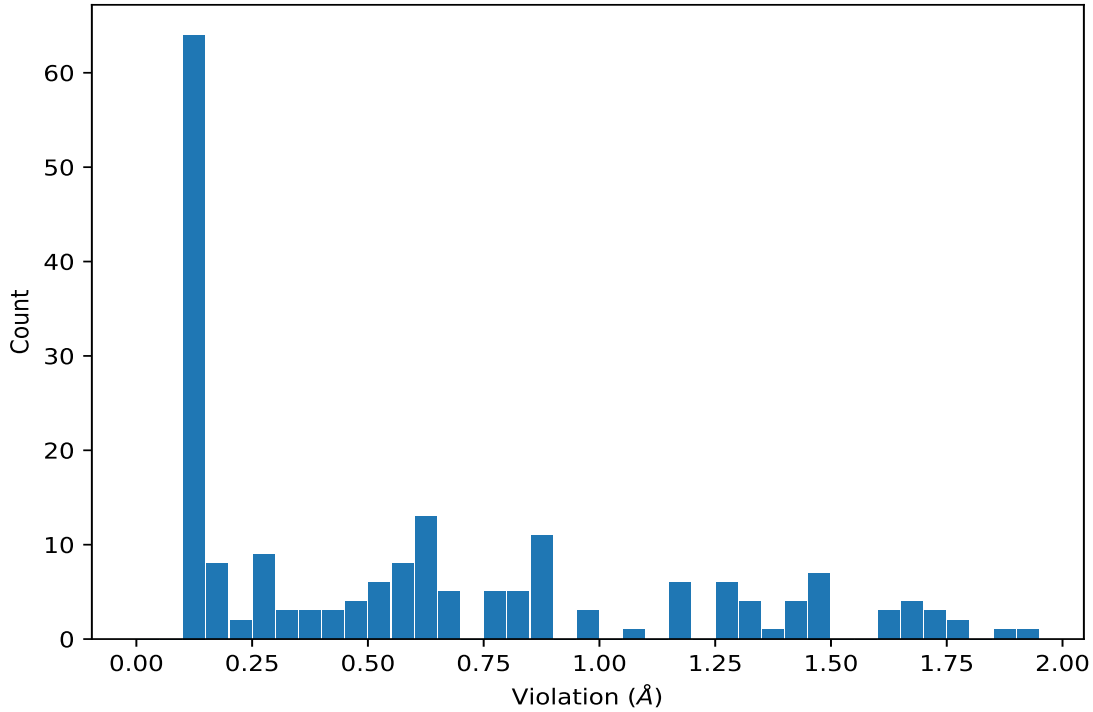
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG22	3	0.12	0.01	0.12
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG23	3	0.12	0.01	0.12
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG21	3	0.12	0.01	0.12
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG22	3	0.12	0.01	0.12
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG23	3	0.12	0.01	0.12
(2,415)	1:A:74:GLN:HB2	1:A:80:LEU:HB2	2	0.14	0.02	0.14
(2,415)	1:A:74:GLN:HB3	1:A:80:LEU:HB2	2	0.14	0.02	0.14
(2,4)	1:A:32:TYR:HD1	1:A:33:THR:H	2	0.12	0.0	0.12

[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)
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	7	1.94
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	1	1.86
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	2	1.78
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	15	1.75
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	4	1.74
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	12	1.71
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	20	1.7
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	5	1.69
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	11	1.69
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	17	1.66
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	8	1.65
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	11	1.6
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	11	1.6
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	11	1.6
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	19	1.48
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	19	1.48
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	19	1.48
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	4	1.45
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	4	1.45
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	4	1.45
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	13	1.45
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	20	1.44
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	20	1.44
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	20	1.44
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	19	1.4
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	9	1.35
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	12	1.34
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	12	1.34
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	12	1.34
(2,12)	1:A:32:TYR:HD1	1:A:44:VAL:HB	6	1.32
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	1	1.29
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	1	1.29
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	1	1.29
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	6	1.28
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	6	1.28
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	6	1.28
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	2	1.16
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	2	1.16
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	2	1.16
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	7	1.16
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	7	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	7	1.16
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	9	1.08
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	5	0.95
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	5	0.95
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	5	0.95
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	20	0.89
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	20	0.89
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	6	0.88
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	7	0.88
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	8	0.87
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	8	0.87
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	8	0.87
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	15	0.86
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	15	0.86
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	15	0.86
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	12	0.85
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	17	0.82
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	17	0.82
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	17	0.82
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	11	0.8
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	11	0.8
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	4	0.79
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	4	0.79
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	12	0.77
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	12	0.77
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	6	0.76
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	8	0.68
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	8	0.68
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	7	0.68
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	6	0.65
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	6	0.65
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	1	0.64
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	1	0.64
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	5	0.64
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	5	0.64
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	7	0.64
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	7	0.64
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	19	0.64
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	19	0.64
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	2	0.63
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	2	0.63
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	17	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	17	0.63
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	6	0.61
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	8	0.59
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	20	0.59
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	9	0.58
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	9	0.58
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	9	0.58
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	13	0.57
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	13	0.57
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	9	0.56
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	19	0.53
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	9	0.52
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	9	0.52
(2,382)	1:A:30:GLY:HA2	1:A:32:TYR:HD2	15	0.52
(2,382)	1:A:30:GLY:HA3	1:A:32:TYR:HD2	15	0.52
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	19	0.5
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	8	0.49
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	12	0.49
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	5	0.46
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	8	0.45
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	4	0.44
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	12	0.4
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	1	0.4
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	11	0.37
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	7	0.36
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	2	0.35
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG21	13	0.33
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG22	13	0.33
(2,15)	1:A:32:TYR:HD1	1:A:44:VAL:HG23	13	0.33
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	1	0.29
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	2	0.29
(2,421)	1:A:79:PRO:HB2	1:A:80:LEU:HG	16	0.28
(2,421)	1:A:79:PRO:HB3	1:A:80:LEU:HG	16	0.28
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	9	0.27
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	15	0.27
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	17	0.27
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	19	0.27
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	5	0.25
(2,87)	1:A:32:TYR:H	1:A:32:TYR:HD2	13	0.22
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	13	0.22
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	4	0.19
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB2	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB3	19	0.18
(2,416)	1:A:74:GLN:HB2	1:A:80:LEU:HG	10	0.16
(2,416)	1:A:74:GLN:HB3	1:A:80:LEU:HG	10	0.16
(2,415)	1:A:74:GLN:HB2	1:A:80:LEU:HB2	15	0.16
(2,415)	1:A:74:GLN:HB3	1:A:80:LEU:HB2	15	0.16
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	6	0.15
(2,7)	1:A:16:VAL:HB	1:A:32:TYR:HE2	11	0.14
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG21	12	0.14
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG22	12	0.14
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG23	12	0.14
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG21	12	0.14
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG22	12	0.14
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG23	12	0.14
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG21	12	0.14
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG22	12	0.14
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG23	12	0.14
(2,253)	1:A:34:VAL:HG11	1:A:37:THR:HG21	9	0.14
(2,253)	1:A:34:VAL:HG11	1:A:37:THR:HG22	9	0.14
(2,253)	1:A:34:VAL:HG11	1:A:37:THR:HG23	9	0.14
(2,253)	1:A:34:VAL:HG12	1:A:37:THR:HG21	9	0.14
(2,253)	1:A:34:VAL:HG12	1:A:37:THR:HG22	9	0.14
(2,253)	1:A:34:VAL:HG12	1:A:37:THR:HG23	9	0.14
(2,253)	1:A:34:VAL:HG13	1:A:37:THR:HG21	9	0.14
(2,253)	1:A:34:VAL:HG13	1:A:37:THR:HG22	9	0.14
(2,253)	1:A:34:VAL:HG13	1:A:37:THR:HG23	9	0.14
(2,11)	1:A:16:VAL:HB	1:A:32:TYR:HD2	1	0.14
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	1	0.14
(2,402)	1:A:65:PRO:HB2	1:A:69:LEU:HB2	14	0.13
(2,402)	1:A:65:PRO:HB2	1:A:69:LEU:HB3	14	0.13
(2,402)	1:A:65:PRO:HB3	1:A:69:LEU:HB2	14	0.13
(2,402)	1:A:65:PRO:HB3	1:A:69:LEU:HB3	14	0.13
(2,298)	1:A:65:PRO:HB3	1:A:69:LEU:HG	5	0.13
(2,4)	1:A:32:TYR:HD1	1:A:33:THR:H	1	0.12
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG21	4	0.12
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG22	4	0.12
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG23	4	0.12
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG21	4	0.12
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG22	4	0.12
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG23	4	0.12
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG21	4	0.12
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG22	4	0.12
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG23	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,307)	1:A:12:ASP:HB2	1:A:34:VAL:HG21	10	0.12
(2,307)	1:A:12:ASP:HB2	1:A:34:VAL:HG22	10	0.12
(2,307)	1:A:12:ASP:HB2	1:A:34:VAL:HG23	10	0.12
(1,9)	1:A:14:VAL:O	1:A:32:TYR:H	11	0.12
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	7	0.12
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	18	0.12
(2,415)	1:A:74:GLN:HB2	1:A:80:LEU:HB2	7	0.11
(2,415)	1:A:74:GLN:HB3	1:A:80:LEU:HB2	7	0.11
(2,4)	1:A:32:TYR:HD1	1:A:33:THR:H	4	0.11
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB2	9	0.11
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB3	9	0.11
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB2	20	0.11
(2,392)	1:A:36:LEU:HB3	1:A:43:LYS:HB3	20	0.11
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG21	10	0.11
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG22	10	0.11
(2,347)	1:A:42:LEU:HD11	1:A:51:ILE:HG23	10	0.11
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG21	10	0.11
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG22	10	0.11
(2,347)	1:A:42:LEU:HD12	1:A:51:ILE:HG23	10	0.11
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG21	10	0.11
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG22	10	0.11
(2,347)	1:A:42:LEU:HD13	1:A:51:ILE:HG23	10	0.11
(2,343)	1:A:72:ARG:HB2	1:A:75:ARG:HG3	14	0.11
(1,31)	1:A:36:LEU:H	1:A:43:LYS:O	5	0.11
(1,25)	1:A:18:ARG:O	1:A:27:ARG:H	7	0.11
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	10	0.11
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	11	0.11
(1,13)	1:A:12:ASP:H	1:A:34:VAL:O	14	0.11

10 Dihedral-angle violation analysis (i)

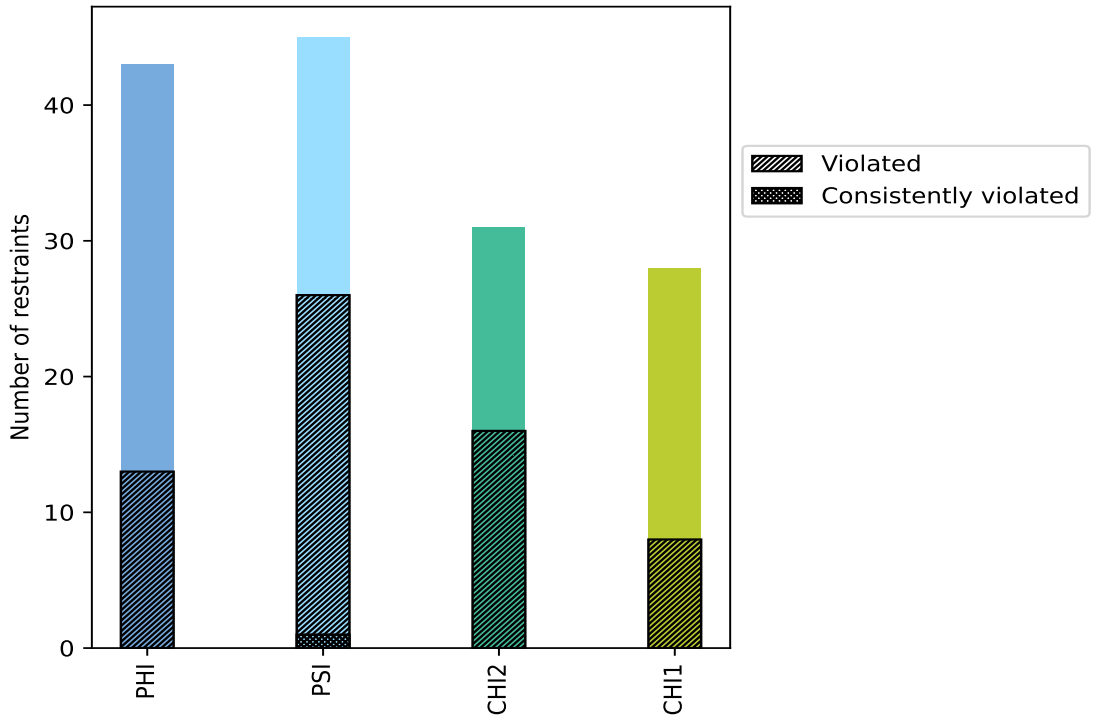
10.1 Summary of dihedral-angle violations (i)

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	43	29.3	13	30.2	8.8	0	0.0	0.0
PSI	45	30.6	26	57.8	17.7	1	2.2	0.7
CHI2	31	21.1	16	51.6	10.9	0	0.0	0.0
CHI1	28	19.0	8	28.6	5.4	0	0.0	0.0
Total	147	100.0	63	42.9	42.9	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)



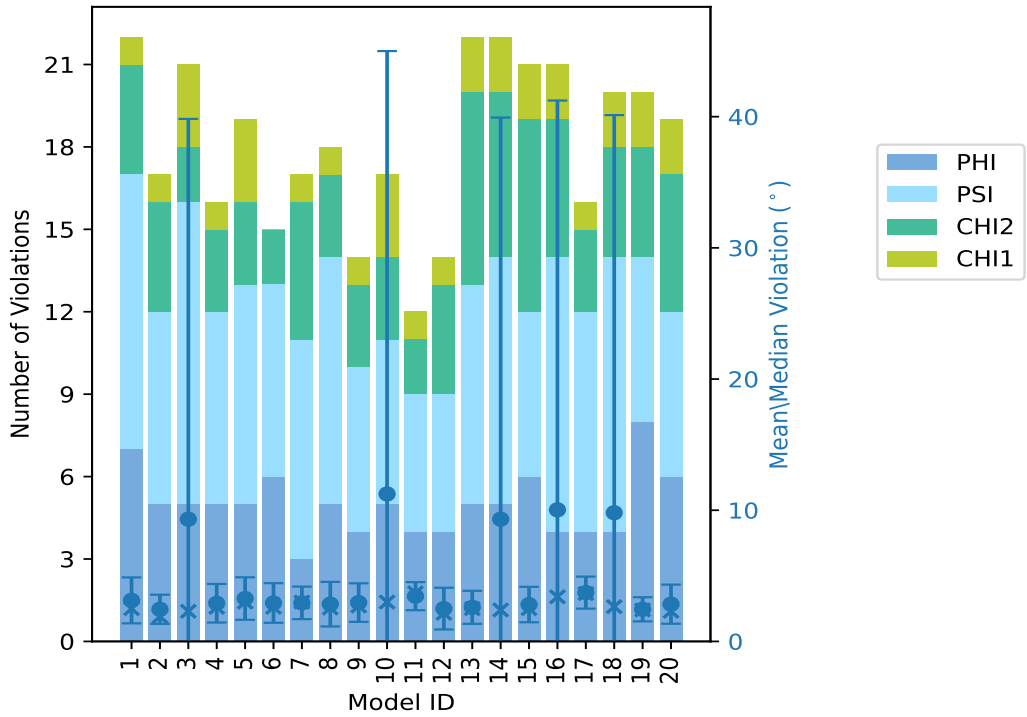
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (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	CHI2	CHI1	Total				
1	7	10	4	1	22	3.13	7.1	1.75	2.5
2	5	7	4	1	17	2.45	4.9	1.11	1.9
3	5	11	2	3	21	9.32	145.7	30.51	2.3
4	5	7	3	1	16	2.91	6.3	1.47	2.6
5	5	8	3	3	19	3.27	7.7	1.62	3.0
6	6	7	2	0	15	2.93	5.7	1.51	2.6
7	3	8	5	1	17	2.94	6.1	1.24	3.0
8	5	9	3	1	18	2.84	8.8	1.7	2.55
9	4	6	3	1	14	2.96	6.5	1.47	2.7
10	5	6	3	3	17	11.24	146.2	33.76	3.0
11	4	5	2	1	12	3.45	5.3	1.07	3.7
12	4	5	4	1	14	2.5	7.4	1.59	2.15
13	5	8	7	2	22	2.6	6.2	1.26	2.5
14	5	9	6	2	22	9.32	149.5	30.61	2.4
15	6	6	7	2	21	2.81	6.5	1.35	2.5
16	4	10	5	2	21	10.03	149.4	31.2	3.4
17	4	8	3	1	16	3.72	6.0	1.22	3.65
18	4	10	4	2	20	9.81	141.8	30.31	2.65
19	8	6	4	2	20	2.45	4.0	0.92	2.4
20	6	6	5	2	19	2.84	6.9	1.49	2.3

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



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

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

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

Number of violated restraints					Fraction of the ensemble	
PHI	PSI	CHI2	CHI1	Total	Count[1]	%
6	2	7	3	18	1	5.0
1	8	2	3	14	2	10.0
0	1	1	0	2	3	15.0
0	3	0	0	3	4	20.0
1	4	1	0	6	5	25.0
0	1	0	0	1	6	30.0
0	1	0	0	1	7	35.0
0	0	0	1	1	8	40.0
0	2	0	0	2	9	45.0
0	0	3	0	3	10	50.0
0	0	0	0	0	11	55.0

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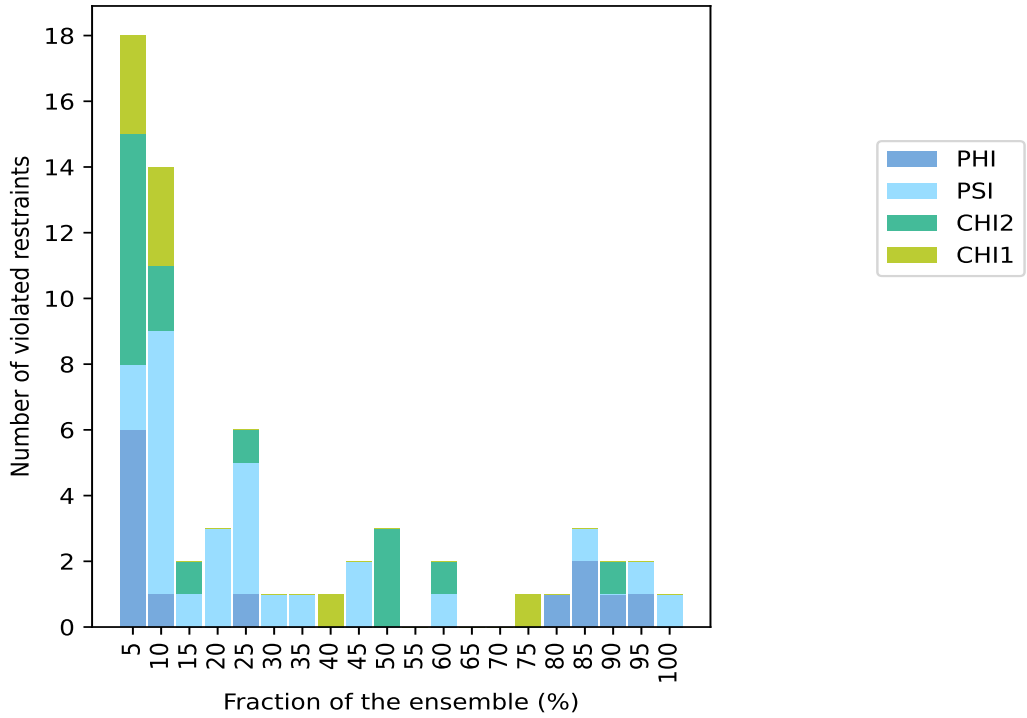
Number of violated restraints					Fraction of the ensemble	
PHI	PSI	CHI2	CHI1	Total	Count[1]	%
0	1	1	0	2	12	60.0
0	0	0	0	0	13	65.0
0	0	0	0	0	14	70.0
0	0	0	1	1	15	75.0
1	0	0	0	1	16	80.0
2	1	0	0	3	17	85.0
1	0	1	0	2	18	90.0
1	1	0	0	2	19	95.0
0	1	0	0	1	20	100.0

[1] Number of models with violations

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

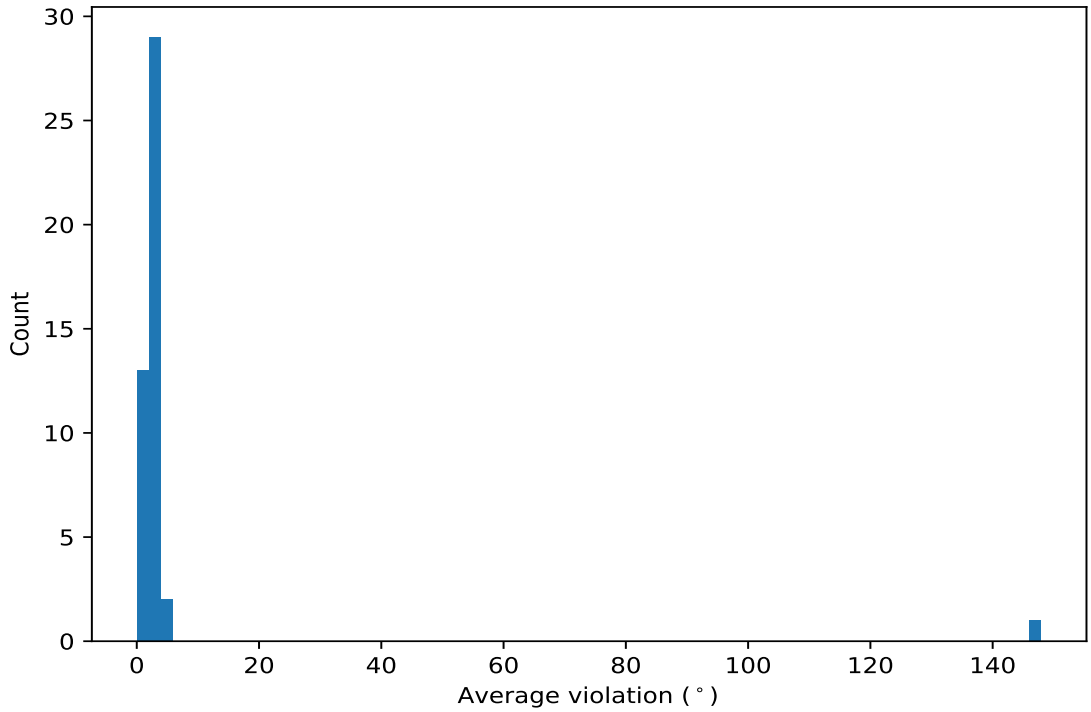


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	20	4.2	1.07	4.05
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	19	5.99	1.26	6.1
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	19	2.89	1.09	2.7
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	18	3.53	1.28	3.35
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	18	3.48	1.3	3.15
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	17	2.88	0.91	2.8
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	17	2.85	0.93	2.6
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	17	2.41	1.04	2.1
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	16	3.58	1.13	3.25
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	15	2.56	0.93	2.3
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	12	2.64	0.78	2.6
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	12	2.57	0.93	2.6
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	10	2.14	0.83	1.85
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	10	2.11	0.54	2.15
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	10	2.07	0.93	1.9
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	9	3.03	1.06	3.1
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	9	1.7	0.4	1.6
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	8	3.02	1.43	2.45
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	7	1.93	0.78	1.6
(1,6)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:C	1:A:10:VAL:N	6	1.5	0.59	1.25

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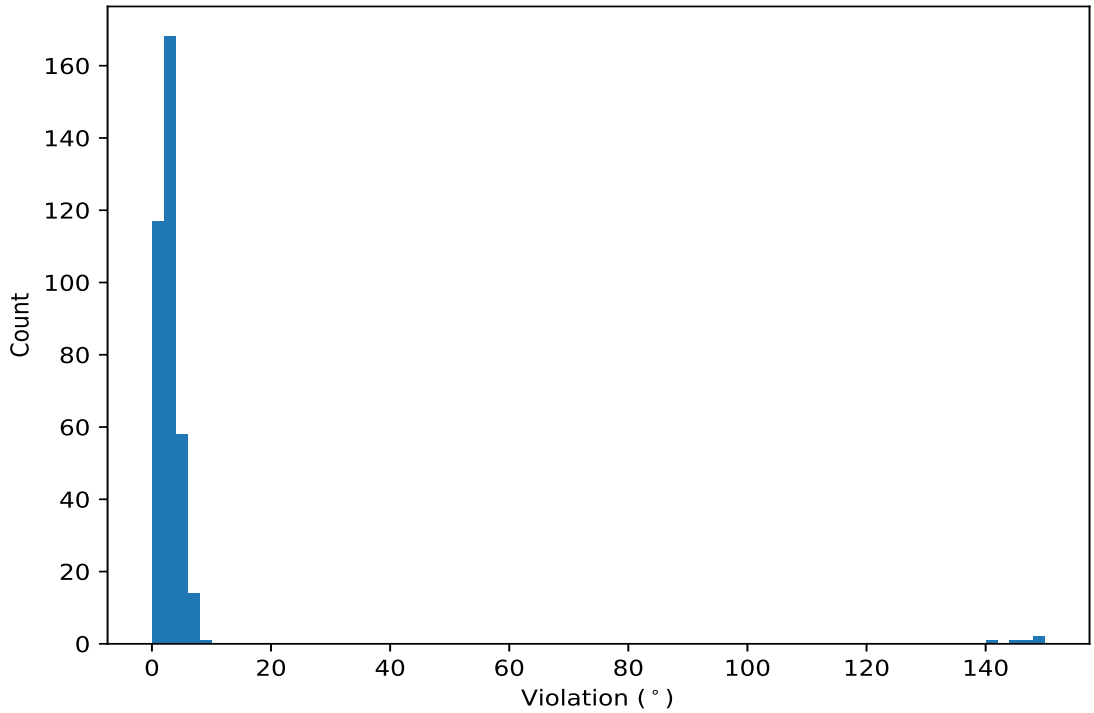
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,99)	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	1:A:32:TYR:CD1	5	146.52	2.84	146.2
(1,78)	1:A:55:HIS:C	1:A:56:VAL:N	1:A:56:VAL:CA	1:A:56:VAL:C	5	3.58	1.03	4.3
(1,46)	1:A:36:LEU:N	1:A:36:LEU:CA	1:A:36:LEU:C	1:A:37:THR:N	5	2.72	1.12	2.4
(1,22)	1:A:17:ARG:N	1:A:17:ARG:CA	1:A:17:ARG:C	1:A:18:ARG:N	5	2.46	0.78	1.9
(1,51)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:THR:N	5	1.88	0.79	1.5
(1,71)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	1:A:51:ILE:N	5	1.8	0.44	1.6
(1,26)	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	1:A:23:ASN:N	4	2.92	0.67	2.75
(1,4)	1:A:8:HIS:N	1:A:8:HIS:CA	1:A:8:HIS:C	1:A:9:MET:N	4	2.17	0.76	1.9
(1,81)	1:A:57:LYS:N	1:A:57:LYS:CA	1:A:57:LYS:C	1:A:58:ALA:N	4	1.48	0.39	1.35
(1,106)	1:A:86:ARG:CA	1:A:86:ARG:CB	1:A:86:ARG:CG	1:A:86:ARG:CD	3	2.63	0.88	3.1
(1,8)	1:A:10:VAL:N	1:A:10:VAL:CA	1:A:10:VAL:C	1:A:11:GLY:N	3	2.13	1.04	1.5
(1,25)	1:A:21:THR:C	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	2	3.85	2.55	3.85
(1,85)	1:A:59:ALA:N	1:A:59:ALA:CA	1:A:59:ALA:C	1:A:60:ASP:N	2	3.65	1.45	3.65
(1,128)	1:A:42:LEU:N	1:A:42:LEU:CA	1:A:42:LEU:CB	1:A:42:LEU:CG	2	2.95	0.05	2.95
(1,110)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	2	2.5	0.6	2.5
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	2	2.2	1.0	2.2
(1,55)	1:A:42:LEU:N	1:A:42:LEU:CA	1:A:42:LEU:C	1:A:43:LYS:N	2	2.1	1.0	2.1
(1,145)	1:A:55:HIS:CA	1:A:55:HIS:CB	1:A:55:HIS:CG	1:A:55:HIS:ND1	2	2.0	0.1	2.0
(1,14)	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	1:A:14:VAL:N	2	1.95	0.05	1.95
(1,88)	1:A:61:PRO:N	1:A:61:PRO:CA	1:A:61:PRO:C	1:A:62:GLY:N	2	1.95	0.55	1.95
(1,48)	1:A:37:THR:N	1:A:37:THR:CA	1:A:37:THR:C	1:A:38:THR:N	2	1.45	0.05	1.45
(1,63)	1:A:46:GLY:N	1:A:46:GLY:CA	1:A:46:GLY:C	1:A:47:ILE:N	2	1.45	0.05	1.45
(1,83)	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	1:A:59:ALA:N	2	1.25	0.15	1.25
(1,105)	1:A:18:ARG:CA	1:A:18:ARG:CB	1:A:18:ARG:CG	1:A:18:ARG:CD	2	1.25	0.15	1.25
(1,114)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:CB	1:A:9:MET:CG	2	1.25	0.15	1.25

[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 (°)
(1,99)	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	1:A:32:TYR:CD1	14	149.5
(1,99)	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	1:A:32:TYR:CD1	16	149.4
(1,99)	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	1:A:32:TYR:CD1	10	146.2
(1,99)	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	1:A:32:TYR:CD1	3	145.7
(1,99)	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	1:A:32:TYR:CD1	18	141.8
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	8	8.8
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	5	7.7
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	12	7.4
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	1	7.1
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	20	6.9
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	9	6.5
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	15	6.5
(1,25)	1:A:21:THR:C	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	1	6.4
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	18	6.3
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	4	6.3
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	13	6.2
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	18	6.1
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	10	6.1
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	7	6.1
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	17	6.0
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	16	5.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	14	5.7
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	16	5.7
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	6	5.7
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	4	5.6
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	1	5.6
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	5	5.5
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	15	5.5
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	16	5.4
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	17	5.4
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	8	5.4
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	15	5.4
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	1	5.3
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	3	5.3
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	6	5.3
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	11	5.3
(1,85)	1:A:59:ALA:N	1:A:59:ALA:CA	1:A:59:ALA:C	1:A:60:ASP:N	20	5.1
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	5	5.0
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1	5.0
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	17	4.9
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	2	4.9
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	17	4.9
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	18	4.8
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	20	4.8
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	6	4.6
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	14	4.6
(1,78)	1:A:55:HIS:C	1:A:56:VAL:N	1:A:56:VAL:CA	1:A:56:VAL:C	14	4.6
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	17	4.6
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	16	4.6
(1,46)	1:A:36:LEU:N	1:A:36:LEU:CA	1:A:36:LEU:C	1:A:37:THR:N	11	4.6
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	5	4.6
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	9	4.5
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	4	4.5
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	5	4.4
(1,78)	1:A:55:HIS:C	1:A:56:VAL:N	1:A:56:VAL:CA	1:A:56:VAL:C	3	4.3
(1,78)	1:A:55:HIS:C	1:A:56:VAL:N	1:A:56:VAL:CA	1:A:56:VAL:C	6	4.3
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	17	4.3
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	7	4.3
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	20	4.3
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	11	4.3
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	11	4.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	2	4.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	10	4.2
(1,24)	1:A:21:THR:N	1:A:21:THR:CA	1:A:21:THR:C	1:A:22:LYS:N	1	4.2
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	14	4.2
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	3	4.2
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	5	4.1
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	12	4.1
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	16	4.1
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	6	4.1
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	18	4.1
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	9	4.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	13	4.1
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	20	4.0
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	7	4.0
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	19	4.0
(1,26)	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	1:A:23:ASN:N	17	4.0
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	9	4.0
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	1	3.9
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	9	3.9
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	13	3.9
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	11	3.9
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	14	3.9
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	17	3.8
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	13	3.8
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	11	3.8
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	6	3.8
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	2	3.8
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	10	3.8
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	13	3.8
(1,69)	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1:A:50:TRP:N	3	3.7
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	1	3.7
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	4	3.7
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	16	3.7
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	7	3.7
(1,109)	1:A:83:ARG:CA	1:A:83:ARG:CB	1:A:83:ARG:CG	1:A:83:ARG:CD	19	3.7
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	5	3.7
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	10	3.7
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	7	3.6
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	11	3.6
(1,8)	1:A:10:VAL:N	1:A:10:VAL:CA	1:A:10:VAL:C	1:A:11:GLY:N	16	3.6
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	13	3.6
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	19	3.6
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	7	3.6
(1,22)	1:A:17:ARG:N	1:A:17:ARG:CA	1:A:17:ARG:C	1:A:18:ARG:N	5	3.6
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	10	3.5
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	17	3.5
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	19	3.5
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	2	3.5
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	4	3.4
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	7	3.4
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	4	3.4
(1,51)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:THR:N	1	3.4
(1,4)	1:A:8:HIS:N	1:A:8:HIS:CA	1:A:8:HIS:C	1:A:9:MET:N	15	3.4
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	16	3.4
(1,106)	1:A:86:ARG:CA	1:A:86:ARG:CB	1:A:86:ARG:CG	1:A:86:ARG:CD	16	3.4
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	16	3.4
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	19	3.4
(1,46)	1:A:36:LEU:N	1:A:36:LEU:CA	1:A:36:LEU:C	1:A:37:THR:N	18	3.3
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	17	3.3
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	9	3.3
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	10	3.3
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	13	3.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	17	3.3
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	19	3.3
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	2	3.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	14	3.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	15	3.2
(1,22)	1:A:17:ARG:N	1:A:17:ARG:CA	1:A:17:ARG:C	1:A:18:ARG:N	7	3.2
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	8	3.2
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	20	3.2
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	2	3.2
(1,55)	1:A:42:LEU:N	1:A:42:LEU:CA	1:A:42:LEU:C	1:A:43:LYS:N	17	3.1
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	3	3.1
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	5	3.1
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	10	3.1
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	13	3.1
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	18	3.1
(1,110)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	18	3.1
(1,106)	1:A:86:ARG:CA	1:A:86:ARG:CB	1:A:86:ARG:CG	1:A:86:ARG:CD	8	3.1
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	11	3.0
(1,97)	1:A:29:LYS:CA	1:A:29:LYS:CB	1:A:29:LYS:CG	1:A:29:LYS:CD	15	3.0
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	4	3.0
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	8	3.0
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	15	3.0
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	7	3.0
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	14	3.0
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	10	3.0
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	5	3.0
(1,128)	1:A:42:LEU:N	1:A:42:LEU:CA	1:A:42:LEU:CB	1:A:42:LEU:CG	3	3.0
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	16	3.0
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	15	2.9
(1,72)	1:A:50:TRP:C	1:A:51:ILE:N	1:A:51:ILE:CA	1:A:51:ILE:C	19	2.9
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	20	2.9
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	1	2.9
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	3	2.9
(1,26)	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	1:A:23:ASN:N	19	2.9
(1,128)	1:A:42:LEU:N	1:A:42:LEU:CA	1:A:42:LEU:CB	1:A:42:LEU:CG	5	2.9
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	12	2.9
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	12	2.8
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	2	2.8
(1,6)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:C	1:A:10:VAL:N	18	2.8
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	1	2.8
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	9	2.8
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	13	2.8
(1,101)	1:A:43:LYS:CA	1:A:43:LYS:CB	1:A:43:LYS:CG	1:A:43:LYS:CD	12	2.8
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	7	2.8
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	20	2.7
(1,78)	1:A:55:HIS:C	1:A:56:VAL:N	1:A:56:VAL:CA	1:A:56:VAL:C	19	2.7
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	8	2.7
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	8	2.7
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	18	2.7
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	8	2.7
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	7	2.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	4	2.7
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	11	2.7
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	13	2.6
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	9	2.6
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	6	2.6
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	6	2.6
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	14	2.6
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	8	2.6
(1,26)	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	1:A:23:ASN:N	13	2.6
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	3	2.6
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	15	2.6
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	15	2.6
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	18	2.6
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	9	2.5
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	10	2.5
(1,88)	1:A:61:PRO:N	1:A:61:PRO:CA	1:A:61:PRO:C	1:A:62:GLY:N	3	2.5
(1,71)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	1:A:51:ILE:N	5	2.5
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	12	2.5
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	19	2.5
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	4	2.5
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	11	2.5
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	15	2.5
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	18	2.5
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	8	2.5
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	14	2.4
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	17	2.4
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	14	2.4
(1,46)	1:A:36:LEU:N	1:A:36:LEU:CA	1:A:36:LEU:C	1:A:37:THR:N	13	2.4
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	14	2.4
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	13	2.4
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	3	2.3
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	19	2.3
(1,7)	1:A:9:MET:C	1:A:10:VAL:N	1:A:10:VAL:CA	1:A:10:VAL:C	20	2.3
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	4	2.3
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	16	2.3
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	17	2.3
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	16	2.3
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	20	2.3
(1,134)	1:A:36:LEU:N	1:A:36:LEU:CA	1:A:36:LEU:CB	1:A:36:LEU:CG	20	2.3
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	17	2.3
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	14	2.3
(1,85)	1:A:59:ALA:N	1:A:59:ALA:CA	1:A:59:ALA:C	1:A:60:ASP:N	10	2.2
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	1	2.2
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	12	2.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1	2.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	6	2.2
(1,4)	1:A:8:HIS:N	1:A:8:HIS:CA	1:A:8:HIS:C	1:A:9:MET:N	16	2.2
(1,26)	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	1:A:23:ASN:N	3	2.2
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	8	2.2
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	5	2.1
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	8	2.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	19	2.1
(1,81)	1:A:57:LYS:N	1:A:57:LYS:CA	1:A:57:LYS:C	1:A:58:ALA:N	7	2.1
(1,71)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	1:A:51:ILE:N	2	2.1
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	6	2.1
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	15	2.1
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	8	2.1
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	19	2.1
(1,145)	1:A:55:HIS:CA	1:A:55:HIS:CB	1:A:55:HIS:CG	1:A:55:HIS:ND1	15	2.1
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	12	2.1
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	14	2.1
(1,10)	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1:A:12:ASP:N	18	2.1
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	7	2.0
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	18	2.0
(1,78)	1:A:55:HIS:C	1:A:56:VAL:N	1:A:56:VAL:CA	1:A:56:VAL:C	15	2.0
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	15	2.0
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	8	2.0
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	18	2.0
(1,14)	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	1:A:14:VAL:N	16	2.0
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	3	2.0
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	20	2.0
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	15	2.0
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	10	1.9
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	5	1.9
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	14	1.9
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	20	1.9
(1,70)	1:A:49:ALA:C	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	14	1.9
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	3	1.9
(1,51)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:THR:N	5	1.9
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	1	1.9
(1,22)	1:A:17:ARG:N	1:A:17:ARG:CA	1:A:17:ARG:C	1:A:18:ARG:N	1	1.9
(1,145)	1:A:55:HIS:CA	1:A:55:HIS:CB	1:A:55:HIS:CG	1:A:55:HIS:ND1	19	1.9
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	2	1.9
(1,14)	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	1:A:14:VAL:N	5	1.9
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	12	1.9
(1,110)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1	1.9
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	20	1.8
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	18	1.8
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	11	1.8
(1,46)	1:A:36:LEU:N	1:A:36:LEU:CA	1:A:36:LEU:C	1:A:37:THR:N	8	1.8
(1,22)	1:A:17:ARG:N	1:A:17:ARG:CA	1:A:17:ARG:C	1:A:18:ARG:N	4	1.8
(1,22)	1:A:17:ARG:N	1:A:17:ARG:CA	1:A:17:ARG:C	1:A:18:ARG:N	10	1.8
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	13	1.8
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	15	1.8
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	3	1.8
(1,108)	1:A:57:LYS:CA	1:A:57:LYS:CB	1:A:57:LYS:CG	1:A:57:LYS:CD	1	1.8
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	7	1.7
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	11	1.7
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	2	1.7
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	6	1.7
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	20	1.7
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	19	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	15	1.7
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	8	1.7
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	15	1.6
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	15	1.6
(1,90)	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	1:A:12:ASP:OD1	2	1.6
(1,9)	1:A:10:VAL:C	1:A:11:GLY:N	1:A:11:GLY:CA	1:A:11:GLY:C	1	1.6
(1,71)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	1:A:51:ILE:N	14	1.6
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	2	1.6
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	10	1.6
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	13	1.6
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	14	1.6
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	9	1.6
(1,4)	1:A:8:HIS:N	1:A:8:HIS:CA	1:A:8:HIS:C	1:A:9:MET:N	3	1.6
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	12	1.6
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	18	1.6
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	9	1.6
(1,142)	1:A:52:HIS:N	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	13	1.6
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	5	1.6
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	2	1.6
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	4	1.6
(1,92)	1:A:60:ASP:N	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	4	1.5
(1,81)	1:A:57:LYS:N	1:A:57:LYS:CA	1:A:57:LYS:C	1:A:58:ALA:N	4	1.5
(1,8)	1:A:10:VAL:N	1:A:10:VAL:CA	1:A:10:VAL:C	1:A:11:GLY:N	9	1.5
(1,71)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	1:A:51:ILE:N	3	1.5
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	5	1.5
(1,63)	1:A:46:GLY:N	1:A:46:GLY:CA	1:A:46:GLY:C	1:A:47:ILE:N	2	1.5
(1,57)	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	1:A:44:VAL:N	20	1.5
(1,51)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:THR:N	15	1.5
(1,48)	1:A:37:THR:N	1:A:37:THR:CA	1:A:37:THR:C	1:A:38:THR:N	2	1.5
(1,46)	1:A:36:LEU:N	1:A:36:LEU:CA	1:A:36:LEU:C	1:A:37:THR:N	3	1.5
(1,4)	1:A:8:HIS:N	1:A:8:HIS:CA	1:A:8:HIS:C	1:A:9:MET:N	13	1.5
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	4	1.5
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	20	1.5
(1,103)	1:A:17:ARG:CA	1:A:17:ARG:CB	1:A:17:ARG:CG	1:A:17:ARG:CD	20	1.5
(1,88)	1:A:61:PRO:N	1:A:61:PRO:CA	1:A:61:PRO:C	1:A:62:GLY:N	10	1.4
(1,83)	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	1:A:59:ALA:N	6	1.4
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	7	1.4
(1,63)	1:A:46:GLY:N	1:A:46:GLY:CA	1:A:46:GLY:C	1:A:47:ILE:N	14	1.4
(1,6)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:C	1:A:10:VAL:N	16	1.4
(1,58)	1:A:43:LYS:C	1:A:44:VAL:N	1:A:44:VAL:CA	1:A:44:VAL:C	13	1.4
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	17	1.4
(1,53)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	1	1.4
(1,48)	1:A:37:THR:N	1:A:37:THR:CA	1:A:37:THR:C	1:A:38:THR:N	14	1.4
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	8	1.4
(1,114)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:CB	1:A:9:MET:CG	16	1.4
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	10	1.4
(1,106)	1:A:86:ARG:CA	1:A:86:ARG:CB	1:A:86:ARG:CG	1:A:86:ARG:CD	2	1.4
(1,105)	1:A:18:ARG:CA	1:A:18:ARG:CB	1:A:18:ARG:CG	1:A:18:ARG:CD	19	1.4
(1,98)	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:CB	1:A:32:TYR:CG	12	1.3
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	3	1.3
(1,89)	1:A:12:ASP:N	1:A:12:ASP:CA	1:A:12:ASP:CB	1:A:12:ASP:CG	10	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:A:10:VAL:N	1:A:10:VAL:CA	1:A:10:VAL:C	1:A:11:GLY:N	1	1.3
(1,79)	1:A:56:VAL:N	1:A:56:VAL:CA	1:A:56:VAL:C	1:A:57:LYS:N	3	1.3
(1,71)	1:A:50:TRP:N	1:A:50:TRP:CA	1:A:50:TRP:C	1:A:51:ILE:N	9	1.3
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	1	1.3
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	6	1.3
(1,67)	1:A:48:ALA:N	1:A:48:ALA:CA	1:A:48:ALA:C	1:A:49:ALA:N	19	1.3
(1,6)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:C	1:A:10:VAL:N	13	1.3
(1,51)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:THR:N	14	1.3
(1,51)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:THR:N	18	1.3
(1,25)	1:A:21:THR:C	1:A:22:LYS:N	1:A:22:LYS:CA	1:A:22:LYS:C	19	1.3
(1,86)	1:A:59:ALA:C	1:A:60:ASP:N	1:A:60:ASP:CA	1:A:60:ASP:C	16	1.2
(1,81)	1:A:57:LYS:N	1:A:57:LYS:CA	1:A:57:LYS:C	1:A:58:ALA:N	16	1.2
(1,6)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:C	1:A:10:VAL:N	8	1.2
(1,6)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:C	1:A:10:VAL:N	19	1.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	5	1.2
(1,56)	1:A:42:LEU:C	1:A:43:LYS:N	1:A:43:LYS:CA	1:A:43:LYS:C	12	1.2
(1,20)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:ARG:N	9	1.2
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	20	1.2
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	4	1.2
(1,143)	1:A:52:HIS:CA	1:A:52:HIS:CB	1:A:52:HIS:CG	1:A:52:HIS:ND1	6	1.2
(1,135)	1:A:36:LEU:CA	1:A:36:LEU:CB	1:A:36:LEU:CG	1:A:36:LEU:CD1	13	1.2
(1,117)	1:A:15:TRP:CA	1:A:15:TRP:CB	1:A:15:TRP:CG	1:A:15:TRP:CD1	7	1.2
(1,115)	1:A:9:MET:CA	1:A:9:MET:CB	1:A:9:MET:CG	1:A:9:MET:SD	16	1.2
(1,111)	1:A:50:TRP:CA	1:A:50:TRP:CB	1:A:50:TRP:CG	1:A:50:TRP:CD1	7	1.2
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	2	1.1
(1,93)	1:A:60:ASP:CA	1:A:60:ASP:CB	1:A:60:ASP:CG	1:A:60:ASP:OD1	13	1.1
(1,83)	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	1:A:59:ALA:N	3	1.1
(1,81)	1:A:57:LYS:N	1:A:57:LYS:CA	1:A:57:LYS:C	1:A:58:ALA:N	18	1.1
(1,68)	1:A:48:ALA:C	1:A:49:ALA:N	1:A:49:ALA:CA	1:A:49:ALA:C	19	1.1
(1,6)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:C	1:A:10:VAL:N	6	1.1
(1,55)	1:A:42:LEU:N	1:A:42:LEU:CA	1:A:42:LEU:C	1:A:43:LYS:N	18	1.1
(1,47)	1:A:36:LEU:C	1:A:37:THR:N	1:A:37:THR:CA	1:A:37:THR:C	12	1.1
(1,40)	1:A:33:THR:N	1:A:33:THR:CA	1:A:33:THR:C	1:A:34:VAL:N	12	1.1
(1,13)	1:A:12:ASP:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	1	1.1
(1,114)	1:A:9:MET:N	1:A:9:MET:CA	1:A:9:MET:CB	1:A:9:MET:CG	14	1.1
(1,105)	1:A:18:ARG:CA	1:A:18:ARG:CB	1:A:18:ARG:CG	1:A:18:ARG:CD	13	1.1