



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 AM UTC

PDB ID : 2LL8 / pdb_00002ll8
BMRB ID : 18032
Title : Solution NMR structure of the specialized holo-acyl carrier protein RPA2022 from *Rhodopseudomonas palustris* refined with NH RDCs, Northeast Structural Genomics Consortium Target RpR324
Authors : Ramelot, T.A.; Ni, S.; Rossi, P.; Yang, Y.; Wang, H.; Ciccocanti, C.; Maglaqui, M.; Janjua, H.; Nair, R.; Roset, B.; Acton, T.B.; Xiao, R.; Everett, J.K.; Prestegard, J.H.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-10-31

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
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

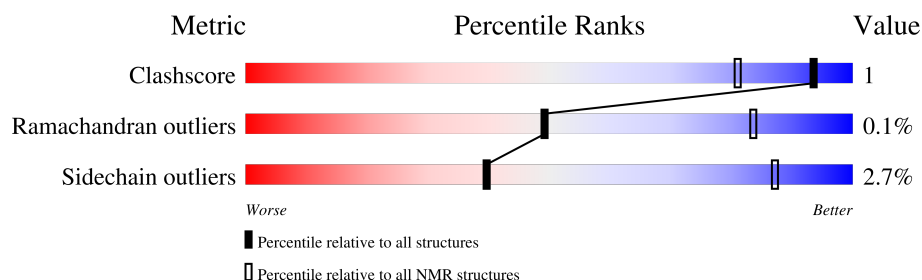
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 96%.

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	101	

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:4-A:90 (87)	0.58	18

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1622 atoms, of which 804 are hydrogens and 0 are deuteriums.

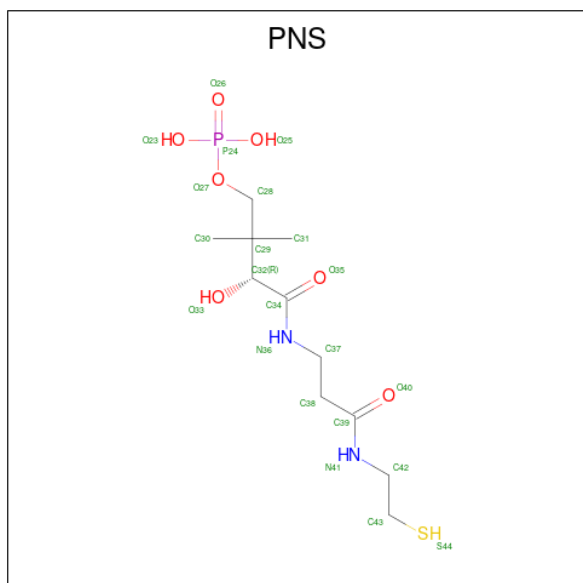
- Molecule 1 is a protein called Specialized acyl carrier protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1580	505	783	135	155	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LEU	-	expression tag	UNP Q6N882
A	95	GLU	-	expression tag	UNP Q6N882
A	96	HIS	-	expression tag	UNP Q6N882
A	97	HIS	-	expression tag	UNP Q6N882
A	98	HIS	-	expression tag	UNP Q6N882
A	99	HIS	-	expression tag	UNP Q6N882
A	100	HIS	-	expression tag	UNP Q6N882
A	101	HIS	-	expression tag	UNP Q6N882

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



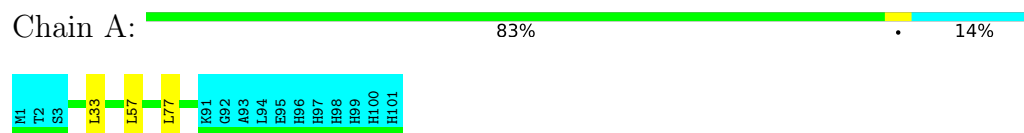
Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
2	A	1	42	11	21	2	6	1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Specialized acyl carrier protein

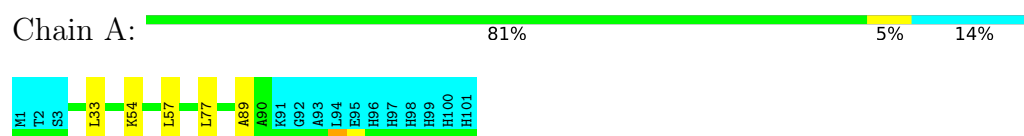


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

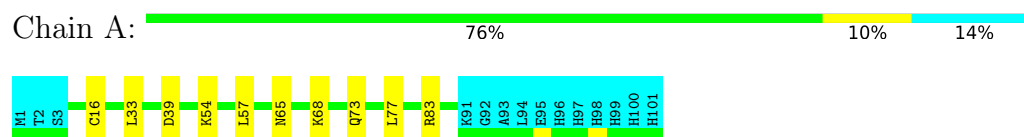
4.2.1 Score per residue for model 1

- Molecule 1: Specialized acyl carrier protein



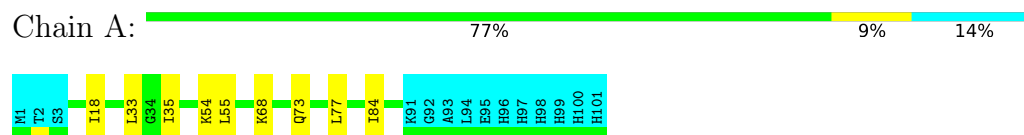
4.2.2 Score per residue for model 2

- Molecule 1: Specialized acyl carrier protein



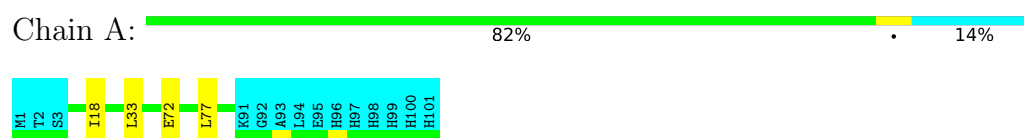
4.2.3 Score per residue for model 3

- Molecule 1: Specialized acyl carrier protein



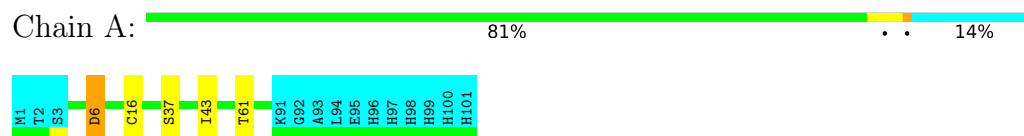
4.2.4 Score per residue for model 4

- Molecule 1: Specialized acyl carrier protein



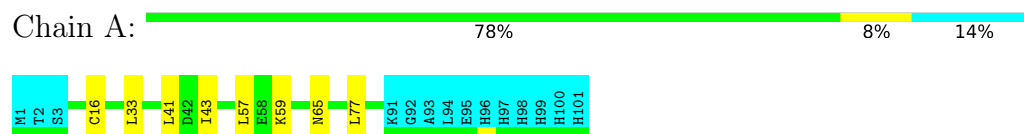
4.2.5 Score per residue for model 5

- Molecule 1: Specialized acyl carrier protein



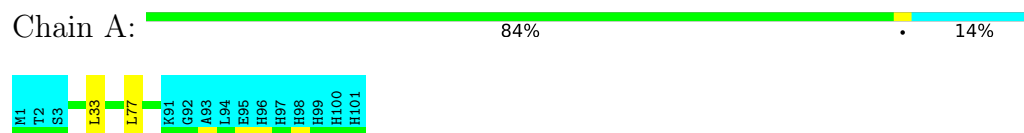
4.2.6 Score per residue for model 6

- Molecule 1: Specialized acyl carrier protein



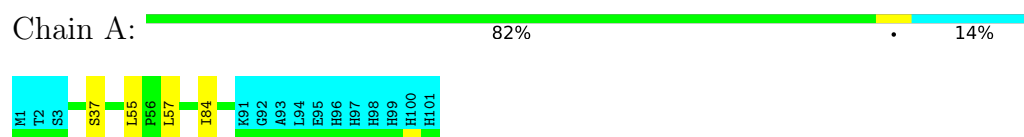
4.2.7 Score per residue for model 7

- Molecule 1: Specialized acyl carrier protein



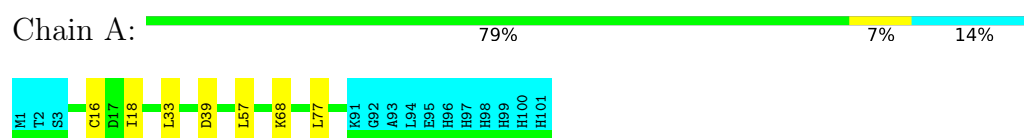
4.2.8 Score per residue for model 8

- Molecule 1: Specialized acyl carrier protein



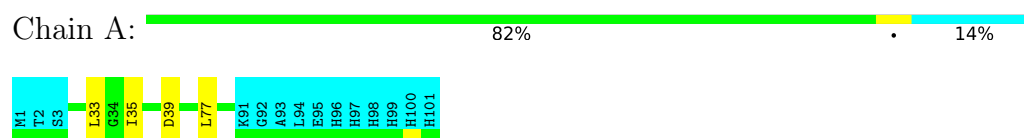
4.2.9 Score per residue for model 9

- Molecule 1: Specialized acyl carrier protein



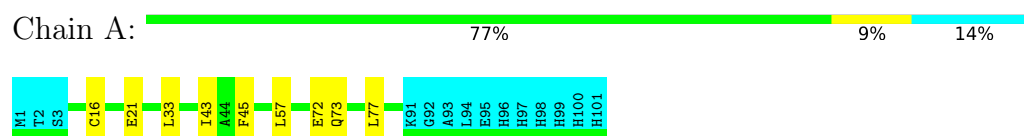
4.2.10 Score per residue for model 10

- Molecule 1: Specialized acyl carrier protein



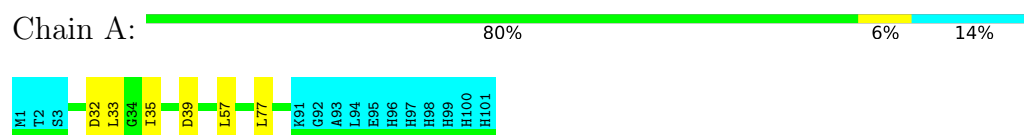
4.2.11 Score per residue for model 11

- Molecule 1: Specialized acyl carrier protein



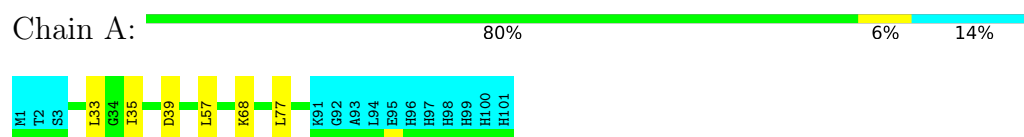
4.2.12 Score per residue for model 12

- Molecule 1: Specialized acyl carrier protein



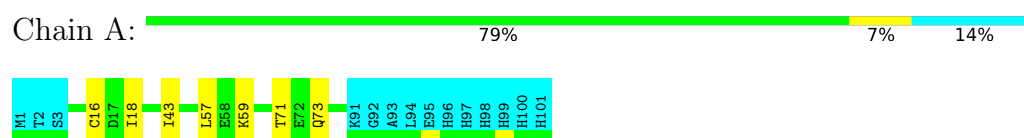
4.2.13 Score per residue for model 13

- Molecule 1: Specialized acyl carrier protein



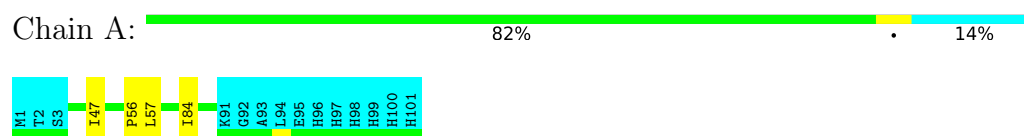
4.2.14 Score per residue for model 14

- Molecule 1: Specialized acyl carrier protein



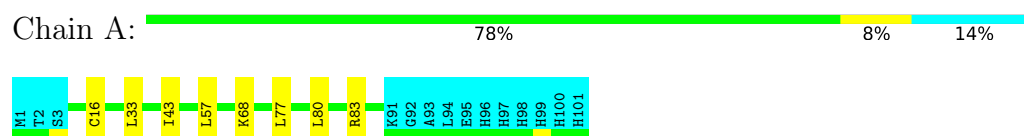
4.2.15 Score per residue for model 15

- Molecule 1: Specialized acyl carrier protein



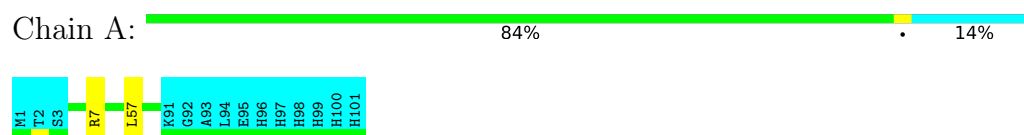
4.2.16 Score per residue for model 16

- Molecule 1: Specialized acyl carrier protein



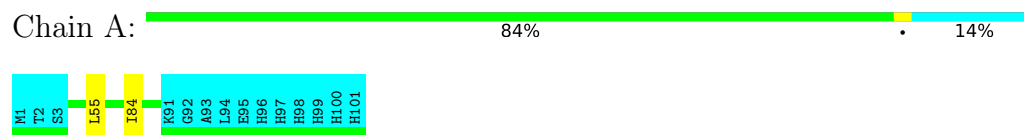
4.2.17 Score per residue for model 17

- Molecule 1: Specialized acyl carrier protein



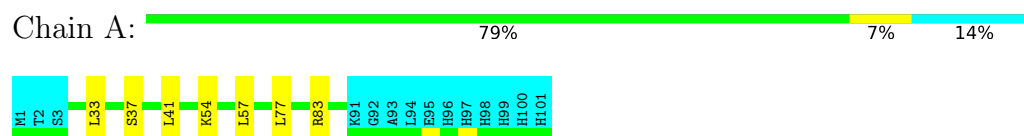
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Specialized acyl carrier protein



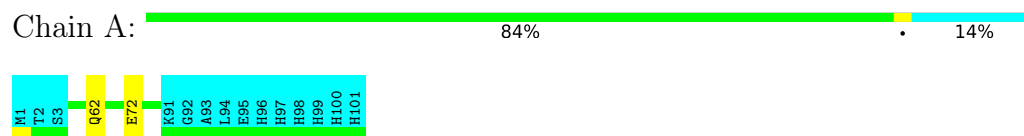
4.2.19 Score per residue for model 19

- Molecule 1: Specialized acyl carrier protein



4.2.20 Score per residue for model 20

- Molecule 1: Specialized acyl carrier protein



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.25
CNS	refinement	1.3
PSVS	refinement	1.4
PdbStat	structure solution	5.4
CYANA	structure solution	2.1
FMCGUI	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	1260
Number of shifts mapped to atoms	1260
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	96%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.24±0.02	0±0/692 (0.0± 0.1%)	1.10±0.01	0±0/943 (0.0± 0.0%)
All	All	1.24	4/13840 (0.0%)	1.10	0/18860 (0.0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	18	ILE	CA-CB	7.14	1.59	1.54	9	3
1	A	56	PRO	CA-CB	6.00	1.57	1.53	15	1

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	680	674	674	2±1
2	A	21	21	21	0±0
All	All	14020	13900	13900	36

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD11	1:A:77:LEU:HD11	0.60	1.71	7	13
1:A:37:SER:HB2	1:A:61:THR:HG21	0.48	1.85	5	1
1:A:16:CYS:SG	1:A:43:ILE:HD11	0.48	2.48	16	5
1:A:55:LEU:HD21	1:A:84:ILE:HG12	0.46	1.88	8	3
1:A:35:ILE:HG23	1:A:39:ASP:HB2	0.46	1.88	10	3
1:A:80:LEU:HA	1:A:83:ARG:NH1	0.45	2.26	16	1
1:A:16:CYS:SG	1:A:39:ASP:HB3	0.44	2.52	9	2
1:A:47:ILE:HG21	1:A:84:ILE:HD13	0.43	1.90	15	1
1:A:41:LEU:HD23	1:A:57:LEU:HD12	0.43	1.90	6	1
1:A:18:ILE:HG13	1:A:35:ILE:HD11	0.43	1.90	3	1
2:A:102:PNS:H32	2:A:102:PNS:O26	0.42	2.15	14	1
1:A:68:LYS:HE2	1:A:68:LYS:HA	0.41	1.93	3	1
1:A:37:SER:O	1:A:41:LEU:HG	0.41	2.15	19	1
2:A:102:PNS:O25	2:A:102:PNS:H302	0.40	2.15	19	1
2:A:102:PNS:O25	2:A:102:PNS:H301	0.40	2.16	5	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	87/101 (86%)	84±1 (97±2%)	3±1 (3±2%)	0±0 (0±0%)	49	83
All	All	1740/2020 (86%)	1681 (97%)	58 (3%)	1 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	32	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	73/85 (86%)	71±2 (97±2%)	2±2 (3±2%)	40 87
All	All	1460/1700 (86%)	1421 (97%)	39 (3%)	40 87

All 14 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	57	LEU	12
1	A	54	LYS	4
1	A	68	LYS	4
1	A	73	GLN	4
1	A	72	GLU	3
1	A	65	ASN	2
1	A	83	ARG	2
1	A	59	LYS	2
1	A	6	ASP	1
1	A	37	SER	1
1	A	21	GLU	1
1	A	45	PHE	1
1	A	71	THR	1
1	A	62	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PNS	A	102	1	14,20,21	1.25±0.11	1±0 (7±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PNS	A	102	1	18,26,29	0.62±0.14	0±0 (0±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PNS	A	102	1	-	0±0,24,26,27	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	102	PNS	C28-C29	4.41	1.59	1.52	13	20
2	A	102	PNS	C38-C39	2.13	1.55	1.51	2	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	102	PNS	C38-C39-N41	2.25	120.44	116.34	2	1
2	A	102	PNS	C37-C38-C39	2.00	115.73	112.39	16	1

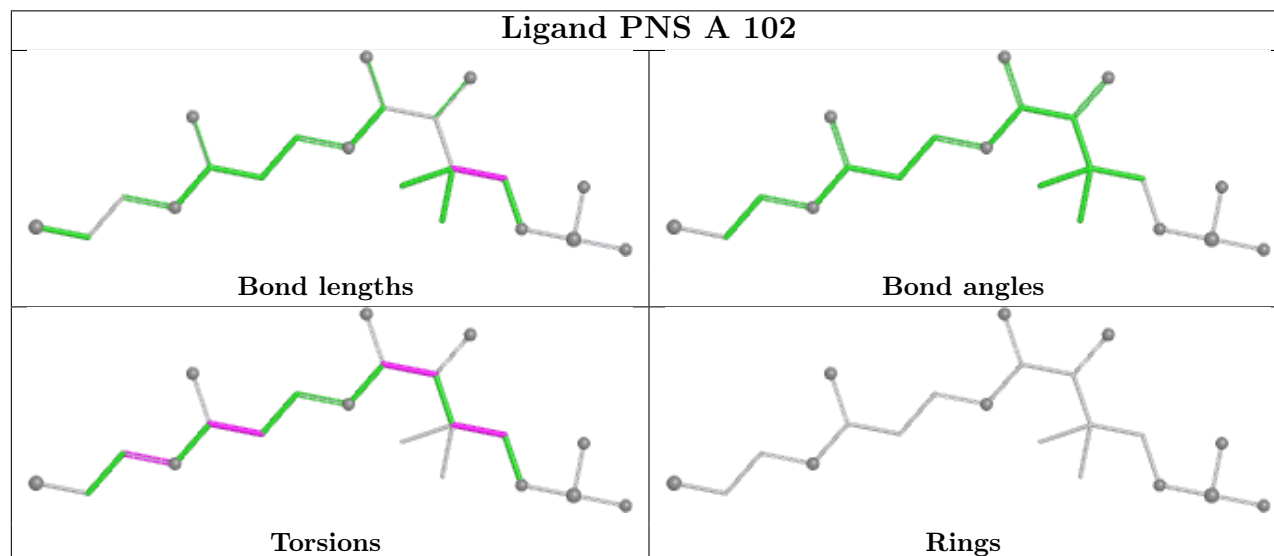
There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	102	PNS	C32-C34-N36-C37	2

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 96% for the well-defined parts and 90% 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	1260
Number of shifts mapped to atoms	1260
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	96	-0.62 ± 0.09	Should be checked
$^{13}\text{C}_\beta$	92	0.25 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	89	-0.41 ± 0.12	None needed (< 0.5 ppm)
^{15}N	91	0.23 ± 0.48	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 96%, i.e. 1134 atoms were assigned a chemical shift out of a possible 1179. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	427/432 (99%)	174/174 (100%)	169/174 (97%)	84/84 (100%)
Sidechain	631/668 (94%)	428/436 (98%)	194/214 (91%)	9/18 (50%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	76/79 (96%)	37/39 (95%)	36/37 (97%)	3/3 (100%)
Overall	1134/1179 (96%)	639/649 (98%)	399/425 (94%)	96/105 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1228 atoms were assigned a chemical shift out of a possible 1372. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	466/503 (93%)	190/203 (94%)	185/202 (92%)	91/98 (93%)
Sidechain	686/742 (92%)	465/485 (96%)	212/238 (89%)	9/19 (47%)
Aromatic	76/127 (60%)	37/63 (59%)	36/49 (73%)	3/15 (20%)
Overall	1228/1372 (90%)	692/751 (92%)	433/489 (89%)	103/132 (78%)

7.1.4 Statistically unusual chemical shifts ⓘ

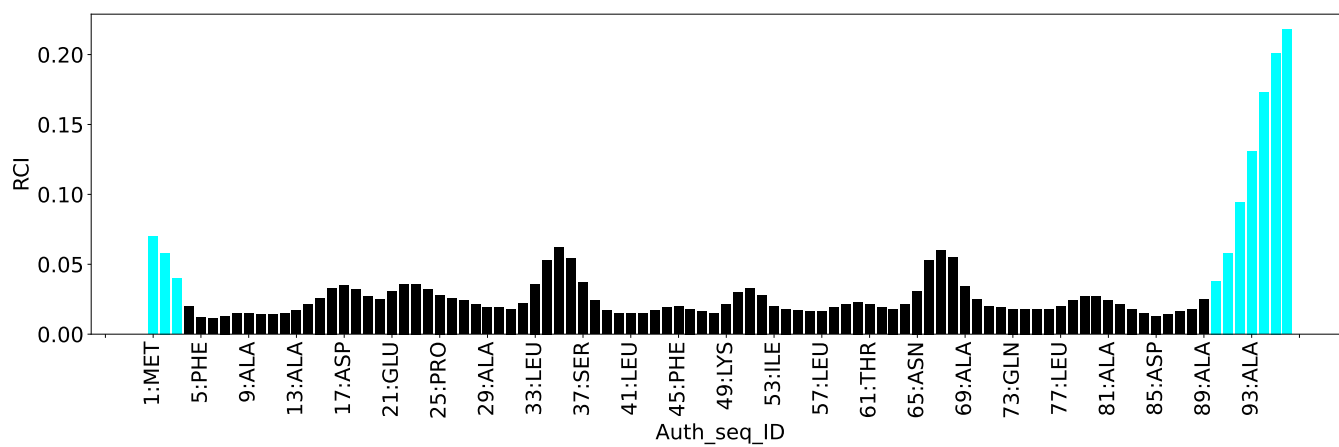
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	15	THR	HG1	5.36	0.08 – 2.19	20.0
1	A	25	PRO	HG2	0.27	0.41 – 3.45	-5.5

7.1.5 Random Coil Index (RCI) plots ⓘ

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	2025
Intra-residue ($ i-j =0$)	501
Sequential ($ i-j =1$)	466
Medium range ($ i-j >1$ and $ i-j <5$)	515
Long range ($ i-j \geq 5$)	443
Inter-chain	6
Hydrogen bond restraints	94
Disulfide bond restraints	0
Total dihedral-angle restraints	144
Number of unmapped restraints	0
Number of restraints per residue	21.3
Number of long range restraints per residue ¹	4.4

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)	5.1	0.2
0.2-0.5 (Medium)	1.4	0.42
>0.5 (Large)	None	None

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)	1.4	5.34
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

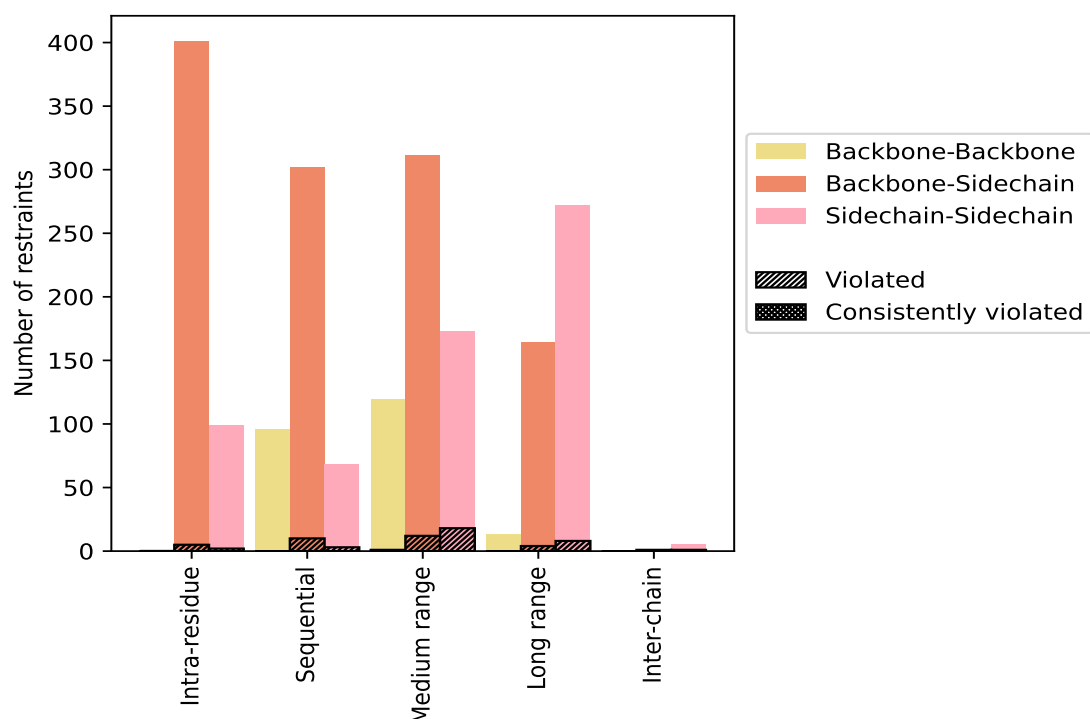
9.1 Summary of distance violations ⓘ

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)	501	24.7	7	1.4	0.3	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	401	19.8	5	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	99	4.9	2	2.0	0.1	0	0.0	0.0
Sequential (i-j =1)	466	23.0	13	2.8	0.6	0	0.0	0.0
Backbone-Backbone	96	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	302	14.9	10	3.3	0.5	0	0.0	0.0
Sidechain-Sidechain	68	3.4	3	4.4	0.1	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	515	25.4	24	4.7	1.2	0	0.0	0.0
Backbone-Backbone	119	5.9	1	0.8	0.0	0	0.0	0.0
Backbone-Sidechain	223	11.0	5	2.2	0.2	0	0.0	0.0
Sidechain-Sidechain	173	8.5	18	10.4	0.9	0	0.0	0.0
Long range (i-j ≥5)	443	21.9	12	2.7	0.6	0	0.0	0.0
Backbone-Backbone	13	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	158	7.8	4	2.5	0.2	0	0.0	0.0
Sidechain-Sidechain	272	13.4	8	2.9	0.4	0	0.0	0.0
Inter-chain	6	0.3	2	33.3	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.0	1	100.0	0.0	0	0.0	0.0
Sidechain-Sidechain	5	0.2	1	20.0	0.0	0	0.0	0.0
Hydrogen bond	94	4.6	7	7.4	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2025	100.0	65	3.2	3.2	0	0.0	0.0
Backbone-Backbone	229	11.3	1	0.4	0.0	0	0.0	0.0
Backbone-Sidechain	1179	58.2	32	2.7	1.6	0	0.0	0.0
Sidechain-Sidechain	617	30.5	32	5.2	1.6	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	2	4	0	1	0	7	0.19	0.33	0.09	0.15
2	2	2	1	2	0	7	0.14	0.23	0.04	0.12
3	1	0	3	1	0	5	0.19	0.37	0.1	0.15
4	2	1	2	2	0	7	0.21	0.42	0.1	0.18
5	1	0	1	3	0	5	0.16	0.25	0.06	0.13
6	1	0	1	1	0	3	0.13	0.19	0.04	0.11
7	1	2	4	3	0	10	0.16	0.36	0.08	0.12
8	1	2	5	1	0	9	0.14	0.19	0.04	0.12
9	2	1	3	1	0	7	0.19	0.33	0.07	0.17
10	1	1	1	2	1	6	0.22	0.34	0.09	0.22

Continued on next page...

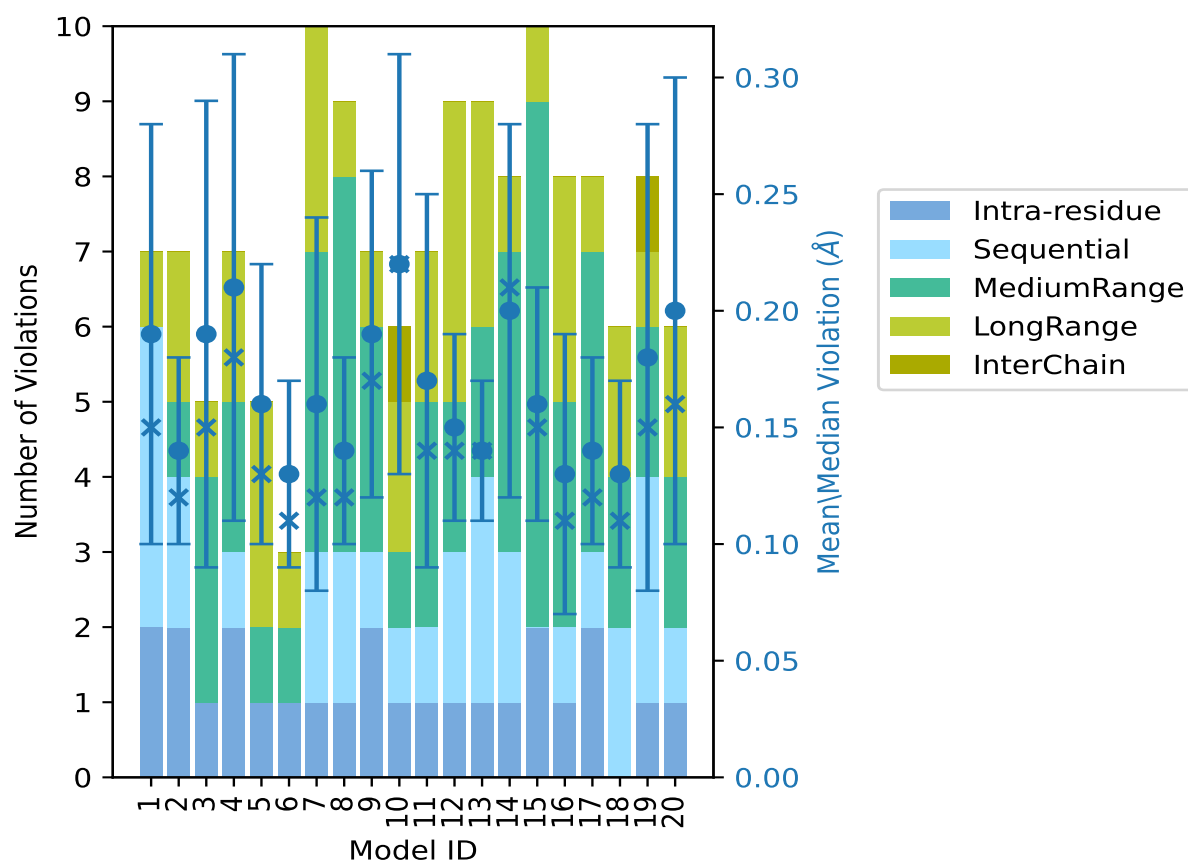
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	1	3	2	0	7	0.17	0.35	0.08	0.14
12	1	2	2	4	0	9	0.15	0.23	0.04	0.14
13	1	3	2	3	0	9	0.14	0.2	0.03	0.14
14	1	2	4	1	0	8	0.2	0.31	0.08	0.21
15	2	0	7	1	0	10	0.16	0.3	0.05	0.15
16	1	1	3	3	0	8	0.13	0.29	0.06	0.11
17	2	1	4	1	0	8	0.14	0.22	0.04	0.12
18	0	2	2	2	0	6	0.13	0.21	0.04	0.11
19	1	3	2	1	1	8	0.18	0.41	0.1	0.15
20	1	1	2	2	0	6	0.2	0.41	0.1	0.16

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

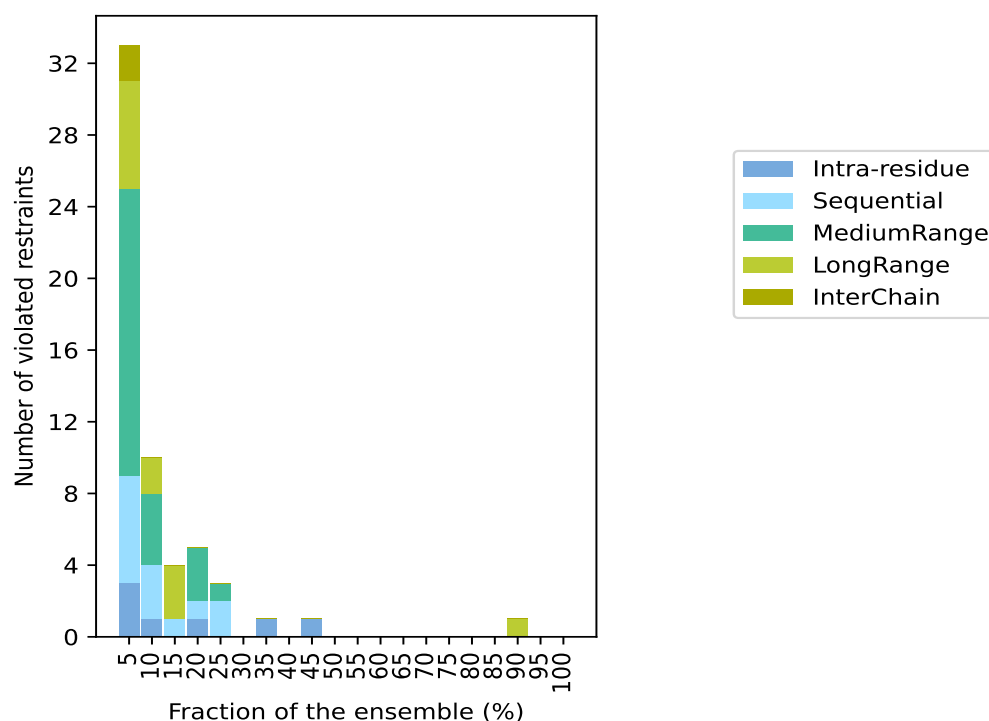
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1873(IR:494, SQ:453, MR:491, LR:431, IC:4) restraints are 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	%
3	6	16	6	2	33	1	5.0
1	3	4	2	0	10	2	10.0
0	1	0	3	0	4	3	15.0
1	1	3	0	0	5	4	20.0
0	2	1	0	0	3	5	25.0
0	0	0	0	0	0	6	30.0
1	0	0	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
1	0	0	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	1	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

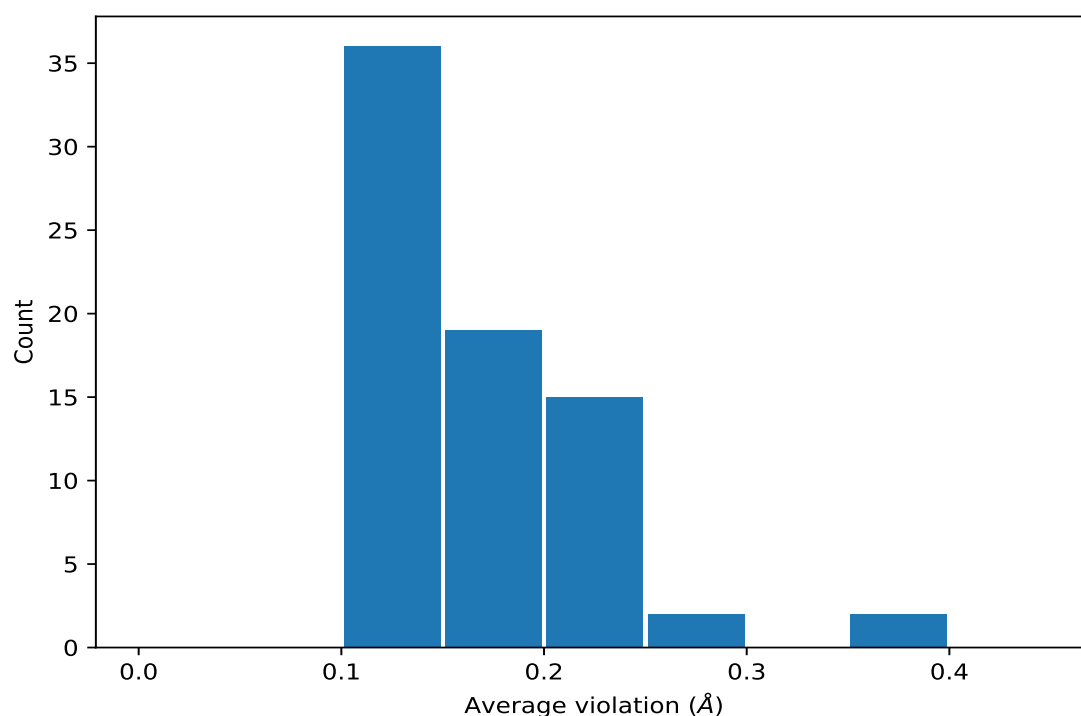
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	18	0.21	0.07	0.19
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	18	0.21	0.07	0.19
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	18	0.21	0.07	0.19
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	18	0.21	0.07	0.19
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	18	0.21	0.07	0.19
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	18	0.21	0.07	0.19
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	9	0.11	0.01	0.11
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	7	0.37	0.04	0.37
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	7	0.37	0.04	0.37
(1,475)	1:33:A:LEU:HD11	1:34:A:GLY:H	5	0.14	0.04	0.13
(1,475)	1:33:A:LEU:HD12	1:34:A:GLY:H	5	0.14	0.04	0.13
(1,475)	1:33:A:LEU:HD13	1:34:A:GLY:H	5	0.14	0.04	0.13
(1,891)	1:51:A:PHE:H	1:53:A:ILE:HG12	5	0.14	0.03	0.13
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD1	5	0.13	0.03	0.13
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD2	5	0.13	0.03	0.13
(1,13)	2:102:A:PNS:H301	2:102:A:PNS:H41	4	0.2	0.03	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,13)	2:102:A:PNS:H302	2:102:A:PNS:H41	4	0.2	0.03	0.2
(1,13)	2:102:A:PNS:H303	2:102:A:PNS:H41	4	0.2	0.03	0.2
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB2	4	0.17	0.08	0.15
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB3	4	0.17	0.08	0.15
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB2	4	0.17	0.08	0.15
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB3	4	0.17	0.08	0.15
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB2	4	0.17	0.08	0.15
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB3	4	0.17	0.08	0.15
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD2	4	0.16	0.04	0.16
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD3	4	0.16	0.04	0.16
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD2	4	0.16	0.04	0.16
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD3	4	0.16	0.04	0.16
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE2	4	0.12	0.02	0.12
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE3	4	0.12	0.02	0.12
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE2	4	0.12	0.02	0.12
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE3	4	0.12	0.02	0.12
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD21	4	0.12	0.01	0.12
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD22	4	0.12	0.01	0.12
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD23	4	0.12	0.01	0.12
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG2	3	0.25	0.07	0.27
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG3	3	0.25	0.07	0.27
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG2	3	0.2	0.07	0.23
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG3	3	0.2	0.07	0.23
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG2	3	0.2	0.07	0.23
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG3	3	0.2	0.07	0.23
(2,63)	1:76:A:VAL:H	1:72:A:GLU:O	3	0.16	0.03	0.15
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD21	3	0.14	0.04	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD22	3	0.14	0.04	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD23	3	0.14	0.04	0.11
(1,1747)	1:55:A:LEU:HD21	1:87:A:LEU:H	3	0.12	0.01	0.12
(1,1747)	1:55:A:LEU:HD22	1:87:A:LEU:H	3	0.12	0.01	0.12
(1,1747)	1:55:A:LEU:HD23	1:87:A:LEU:H	3	0.12	0.01	0.12
(1,1918)	1:94:A:LEU:HA	1:95:A:GLU:HG2	2	0.24	0.12	0.24
(1,1918)	1:94:A:LEU:HA	1:95:A:GLU:HG3	2	0.24	0.12	0.24
(1,154)	1:16:A:CYS:HB2	1:18:A:ILE:HG12	2	0.18	0.05	0.18
(1,154)	1:16:A:CYS:HB2	1:18:A:ILE:HG13	2	0.18	0.05	0.18
(1,154)	1:16:A:CYS:HB3	1:18:A:ILE:HG12	2	0.18	0.05	0.18
(1,154)	1:16:A:CYS:HB3	1:18:A:ILE:HG13	2	0.18	0.05	0.18
(1,981)	1:57:A:LEU:HB2	1:58:A:GLU:HG2	2	0.17	0.03	0.17
(1,981)	1:57:A:LEU:HB2	1:58:A:GLU:HG3	2	0.17	0.03	0.17
(1,981)	1:57:A:LEU:HB3	1:58:A:GLU:HG2	2	0.17	0.03	0.17
(1,981)	1:57:A:LEU:HB3	1:58:A:GLU:HG3	2	0.17	0.03	0.17

Continued on next page...

Continued from previous page...

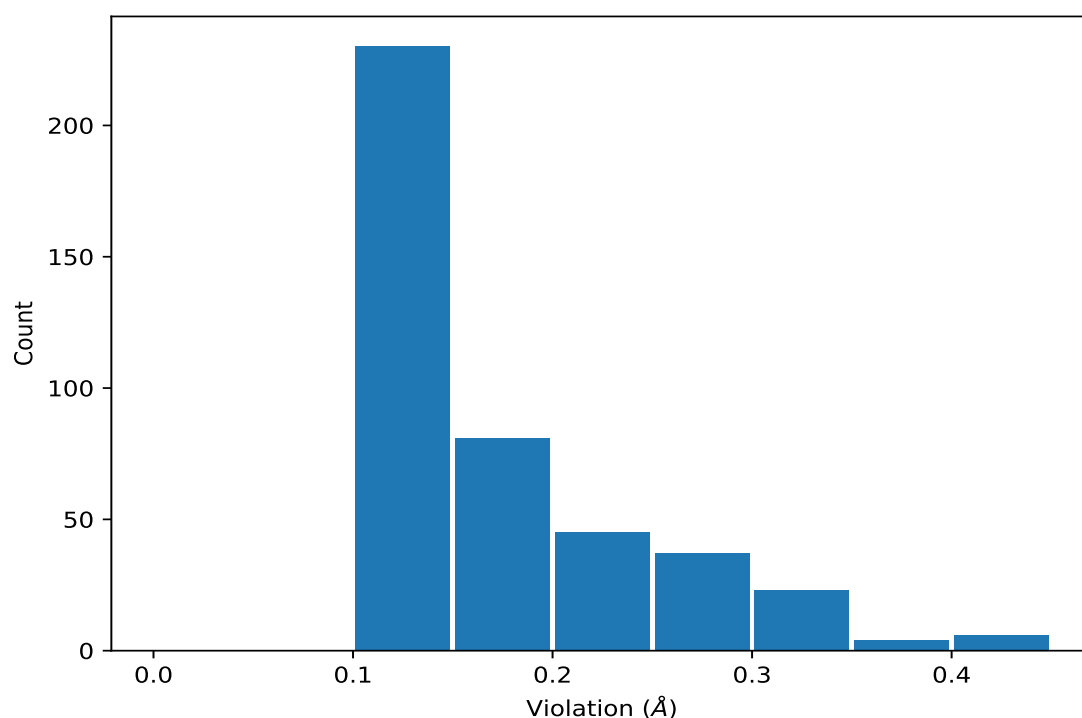
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1262)	1:70:A:THR:HG21	1:72:A:GLU:H	2	0.15	0.0	0.15
(1,1262)	1:70:A:THR:HG22	1:72:A:GLU:H	2	0.15	0.0	0.15
(1,1262)	1:70:A:THR:HG23	1:72:A:GLU:H	2	0.15	0.0	0.15
(2,91)	1:91:A:LYS:H	1:87:A:LEU:O	2	0.15	0.03	0.15
(1,182)	1:18:A:ILE:HB	1:19:A:PRO:HD3	2	0.14	0.02	0.14
(1,1726)	1:86:A:GLU:H	1:86:A:GLU:HB2	2	0.14	0.02	0.14
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD11	2	0.13	0.03	0.13
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD12	2	0.13	0.03	0.13
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD13	2	0.13	0.03	0.13
(1,1212)	1:4:A:THR:HG21	1:7:A:ARG:HB3	2	0.12	0.01	0.12
(1,1212)	1:4:A:THR:HG22	1:7:A:ARG:HB3	2	0.12	0.01	0.12
(1,1212)	1:4:A:THR:HG23	1:7:A:ARG:HB3	2	0.12	0.01	0.12
(1,1298)	1:60:A:TRP:HH2	1:74:A:TYR:HD1	2	0.12	0.02	0.12
(1,1298)	1:60:A:TRP:HH2	1:74:A:TYR:HD2	2	0.12	0.02	0.12
(2,93)	1:92:A:GLY:H	1:88:A:VAL:O	2	0.12	0.01	0.12
(1,825)	1:4:A:THR:HB	1:51:A:PHE:HZ	2	0.12	0.0	0.12

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)
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	4	0.42
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	4	0.42
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	19	0.41
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	19	0.41
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	20	0.41
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	20	0.41
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	3	0.37
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	3	0.37
(1,1918)	1:94:A:LEU:HA	1:95:A:GLU:HG2	7	0.36
(1,1918)	1:94:A:LEU:HA	1:95:A:GLU:HG3	7	0.36
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	11	0.35
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	11	0.35
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	11	0.35
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	11	0.35
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	11	0.35
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	11	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	10	0.34
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	10	0.34
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	9	0.33
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	9	0.33
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG2	1	0.33
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG3	1	0.33
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG2	1	0.31
(1,1730)	1:86:A:GLU:H	1:86:A:GLU:HG3	1	0.31
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	10	0.31
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	10	0.31
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	10	0.31
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	10	0.31
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	10	0.31
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	10	0.31
(1,1249)	1:70:A:THR:HA	1:71:A:THR:HG21	14	0.31
(1,1249)	1:70:A:THR:HA	1:71:A:THR:HG22	14	0.31
(1,1249)	1:70:A:THR:HA	1:71:A:THR:HG23	14	0.31
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	15	0.3
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	15	0.3
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	15	0.3
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	15	0.3
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	15	0.3
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	15	0.3
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	16	0.29
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	16	0.29
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	16	0.29
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	16	0.29
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	16	0.29
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	16	0.29
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB2	14	0.29
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB3	14	0.29
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB2	14	0.29
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB3	14	0.29
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB2	14	0.29
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB3	14	0.29
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG2	10	0.27
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG3	10	0.27
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG2	10	0.27
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG3	10	0.27
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG2	14	0.27
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG3	14	0.27
(1,1229)	1:7:A:ARG:H	1:7:A:ARG:HG2	4	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	5	0.25
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	5	0.25
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	5	0.25
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	5	0.25
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	5	0.25
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	5	0.25
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	14	0.25
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	14	0.25
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	14	0.25
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	14	0.25
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	14	0.25
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	14	0.25
(1,154)	1:16:A:CYS:HB2	1:18:A:ILE:HG12	9	0.24
(1,154)	1:16:A:CYS:HB2	1:18:A:ILE:HG13	9	0.24
(1,154)	1:16:A:CYS:HB3	1:18:A:ILE:HG12	9	0.24
(1,154)	1:16:A:CYS:HB3	1:18:A:ILE:HG13	9	0.24
(1,19)	1:37:A:SER:H	2:102:A:PNS:H301	19	0.24
(1,19)	1:37:A:SER:H	2:102:A:PNS:H302	19	0.24
(1,19)	1:37:A:SER:H	2:102:A:PNS:H303	19	0.24
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG2	12	0.23
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG3	12	0.23
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG2	12	0.23
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG3	12	0.23
(1,13)	2:102:A:PNS:H301	2:102:A:PNS:H41	2	0.23
(1,13)	2:102:A:PNS:H302	2:102:A:PNS:H41	2	0.23
(1,13)	2:102:A:PNS:H303	2:102:A:PNS:H41	2	0.23
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	3	0.22
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	3	0.22
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	3	0.22
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	3	0.22
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	3	0.22
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	3	0.22
(1,13)	2:102:A:PNS:H301	2:102:A:PNS:H41	17	0.22
(1,13)	2:102:A:PNS:H302	2:102:A:PNS:H41	17	0.22
(1,13)	2:102:A:PNS:H303	2:102:A:PNS:H41	17	0.22
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	18	0.21
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	18	0.21
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	18	0.21
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	18	0.21
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	18	0.21
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	18	0.21
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD2	20	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD3	20	0.21
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD2	20	0.21
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD3	20	0.21
(2,63)	1:76:A:VAL:H	1:72:A:GLU:O	20	0.2
(1,981)	1:57:A:LEU:HB2	1:58:A:GLU:HG2	7	0.2
(1,981)	1:57:A:LEU:HB2	1:58:A:GLU:HG3	7	0.2
(1,981)	1:57:A:LEU:HB3	1:58:A:GLU:HG2	7	0.2
(1,981)	1:57:A:LEU:HB3	1:58:A:GLU:HG3	7	0.2
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD21	5	0.2
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD22	5	0.2
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD23	5	0.2
(1,475)	1:33:A:LEU:HD11	1:34:A:GLY:H	4	0.2
(1,475)	1:33:A:LEU:HD12	1:34:A:GLY:H	4	0.2
(1,475)	1:33:A:LEU:HD13	1:34:A:GLY:H	4	0.2
(1,214)	1:20:A:ARG:HD2	1:21:A:GLU:H	13	0.2
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	7	0.19
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	7	0.19
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	7	0.19
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	7	0.19
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	7	0.19
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	7	0.19
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	13	0.19
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	13	0.19
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	13	0.19
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	13	0.19
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	13	0.19
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	13	0.19
(1,644)	1:41:A:LEU:H	1:43:A:ILE:HD11	6	0.19
(1,644)	1:41:A:LEU:H	1:43:A:ILE:HD12	6	0.19
(1,644)	1:41:A:LEU:H	1:43:A:ILE:HD13	6	0.19
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB2	8	0.19
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB3	8	0.19
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB2	8	0.19
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB3	8	0.19
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB2	8	0.19
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB3	8	0.19
(1,13)	2:102:A:PNS:H301	2:102:A:PNS:H41	9	0.19
(1,13)	2:102:A:PNS:H302	2:102:A:PNS:H41	9	0.19
(1,13)	2:102:A:PNS:H303	2:102:A:PNS:H41	9	0.19
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	4	0.18
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	4	0.18
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	4	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	4	0.18
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	4	0.18
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	4	0.18
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	8	0.18
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	8	0.18
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	8	0.18
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	8	0.18
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	8	0.18
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	8	0.18
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	12	0.18
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	12	0.18
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	12	0.18
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	12	0.18
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	12	0.18
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	12	0.18
(1,891)	1:51:A:PHE:H	1:53:A:ILE:HG12	15	0.18
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD1	12	0.18
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD2	12	0.18
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD2	7	0.18
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD3	7	0.18
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD2	7	0.18
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD3	7	0.18
(2,91)	1:91:A:LYS:H	1:87:A:LEU:O	14	0.17
(1,1906)	1:93:A:ALA:H	1:94:A:LEU:HG	8	0.17
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	2	0.17
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	2	0.17
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	2	0.17
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	2	0.17
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	2	0.17
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	2	0.17
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	9	0.17
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	9	0.17
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	9	0.17
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	9	0.17
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	9	0.17
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	9	0.17
(1,1088)	1:59:A:LYS:HG2	1:63:A:GLU:HG2	11	0.17
(1,408)	1:28:A:HIS:H	1:31:A:ASP:H	8	0.17
(1,263)	1:20:A:ARG:HD3	1:23:A:ILE:HD11	13	0.17
(1,263)	1:20:A:ARG:HD3	1:23:A:ILE:HD12	13	0.17
(1,263)	1:20:A:ARG:HD3	1:23:A:ILE:HD13	13	0.17
(1,18)	1:37:A:SER:HB2	2:102:A:PNS:H311	10	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:37:A:SER:HB2	2:102:A:PNS:H312	10	0.17
(1,18)	1:37:A:SER:HB2	2:102:A:PNS:H313	10	0.17
(1,18)	1:37:A:SER:HB3	2:102:A:PNS:H311	10	0.17
(1,18)	1:37:A:SER:HB3	2:102:A:PNS:H312	10	0.17
(1,18)	1:37:A:SER:HB3	2:102:A:PNS:H313	10	0.17
(1,1726)	1:86:A:GLU:H	1:86:A:GLU:HB2	15	0.16
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG2	19	0.16
(1,978)	1:57:A:LEU:HB2	1:58:A:GLU:HG3	19	0.16
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD11	15	0.16
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD12	15	0.16
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD13	15	0.16
(1,182)	1:18:A:ILE:HB	1:19:A:PRO:HD3	17	0.16
(2,63)	1:76:A:VAL:H	1:72:A:GLU:O	4	0.15
(1,1262)	1:70:A:THR:HG21	1:72:A:GLU:H	3	0.15
(1,1262)	1:70:A:THR:HG22	1:72:A:GLU:H	3	0.15
(1,1262)	1:70:A:THR:HG23	1:72:A:GLU:H	3	0.15
(1,1262)	1:70:A:THR:HG21	1:72:A:GLU:H	4	0.15
(1,1262)	1:70:A:THR:HG22	1:72:A:GLU:H	4	0.15
(1,1262)	1:70:A:THR:HG23	1:72:A:GLU:H	4	0.15
(1,1119)	1:61:A:THR:HB	1:65:A:ASN:HB2	15	0.15
(1,1119)	1:61:A:THR:HB	1:65:A:ASN:HB3	15	0.15
(1,891)	1:51:A:PHE:H	1:53:A:ILE:HG12	19	0.15
(1,853)	1:8:A:VAL:HG11	1:51:A:PHE:HE1	13	0.15
(1,853)	1:8:A:VAL:HG11	1:51:A:PHE:HE2	13	0.15
(1,853)	1:8:A:VAL:HG12	1:51:A:PHE:HE1	13	0.15
(1,853)	1:8:A:VAL:HG12	1:51:A:PHE:HE2	13	0.15
(1,853)	1:8:A:VAL:HG13	1:51:A:PHE:HE1	13	0.15
(1,853)	1:8:A:VAL:HG13	1:51:A:PHE:HE2	13	0.15
(1,475)	1:33:A:LEU:HD11	1:34:A:GLY:H	1	0.15
(1,475)	1:33:A:LEU:HD12	1:34:A:GLY:H	1	0.15
(1,475)	1:33:A:LEU:HD13	1:34:A:GLY:H	1	0.15
(1,15)	2:102:A:PNS:H311	2:102:A:PNS:H41	15	0.15
(1,15)	2:102:A:PNS:H312	2:102:A:PNS:H41	15	0.15
(1,15)	2:102:A:PNS:H313	2:102:A:PNS:H41	15	0.15
(1,13)	2:102:A:PNS:H301	2:102:A:PNS:H41	1	0.15
(1,13)	2:102:A:PNS:H302	2:102:A:PNS:H41	1	0.15
(1,13)	2:102:A:PNS:H303	2:102:A:PNS:H41	1	0.15
(1,1647)	1:53:A:ILE:HG12	1:84:A:ILE:HA	11	0.14
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	1	0.14
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	1	0.14
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	1	0.14
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	1	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	1	0.14
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	1	0.14
(1,1298)	1:60:A:TRP:HH2	1:74:A:TYR:HD1	13	0.14
(1,1298)	1:60:A:TRP:HH2	1:74:A:TYR:HD2	13	0.14
(1,981)	1:57:A:LEU:HB2	1:58:A:GLU:HG2	19	0.14
(1,981)	1:57:A:LEU:HB2	1:58:A:GLU:HG3	19	0.14
(1,981)	1:57:A:LEU:HB3	1:58:A:GLU:HG2	19	0.14
(1,981)	1:57:A:LEU:HB3	1:58:A:GLU:HG3	19	0.14
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD1	11	0.14
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD2	11	0.14
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD2	9	0.14
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD3	9	0.14
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD2	9	0.14
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD3	9	0.14
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE2	11	0.14
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE3	11	0.14
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE2	11	0.14
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE3	11	0.14
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE2	12	0.14
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE3	12	0.14
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE2	12	0.14
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE3	12	0.14
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD21	12	0.14
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD22	12	0.14
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD23	12	0.14
(2,93)	1:92:A:GLY:H	1:88:A:VAL:O	17	0.13
(2,63)	1:76:A:VAL:H	1:72:A:GLU:O	9	0.13
(1,1747)	1:55:A:LEU:HD21	1:87:A:LEU:H	5	0.13
(1,1747)	1:55:A:LEU:HD22	1:87:A:LEU:H	5	0.13
(1,1747)	1:55:A:LEU:HD23	1:87:A:LEU:H	5	0.13
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	12	0.13
(1,1701)	1:53:A:ILE:HD11	1:85:A:ASP:H	2	0.13
(1,1701)	1:53:A:ILE:HD12	1:85:A:ASP:H	2	0.13
(1,1701)	1:53:A:ILE:HD13	1:85:A:ASP:H	2	0.13
(1,1212)	1:4:A:THR:HG21	1:7:A:ARG:HB3	7	0.13
(1,1212)	1:4:A:THR:HG22	1:7:A:ARG:HB3	7	0.13
(1,1212)	1:4:A:THR:HG23	1:7:A:ARG:HB3	7	0.13
(1,891)	1:51:A:PHE:H	1:53:A:ILE:HG12	14	0.13
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD1	18	0.13
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD2	18	0.13
(1,475)	1:33:A:LEU:HD11	1:34:A:GLY:H	20	0.13
(1,475)	1:33:A:LEU:HD12	1:34:A:GLY:H	20	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:33:A:LEU:HD13	1:34:A:GLY:H	20	0.13
(1,154)	1:16:A:CYS:HB2	1:18:A:ILE:HG12	17	0.13
(1,154)	1:16:A:CYS:HB2	1:18:A:ILE:HG13	17	0.13
(1,154)	1:16:A:CYS:HB3	1:18:A:ILE:HG12	17	0.13
(1,154)	1:16:A:CYS:HB3	1:18:A:ILE:HG13	17	0.13
(2,91)	1:91:A:LYS:H	1:87:A:LEU:O	8	0.12
(1,1747)	1:55:A:LEU:HD21	1:87:A:LEU:H	20	0.12
(1,1747)	1:55:A:LEU:HD22	1:87:A:LEU:H	20	0.12
(1,1747)	1:55:A:LEU:HD23	1:87:A:LEU:H	20	0.12
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	14	0.12
(1,1496)	1:4:A:THR:HB	1:8:A:VAL:HB	7	0.12
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	20	0.12
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	20	0.12
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	20	0.12
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	20	0.12
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	20	0.12
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	20	0.12
(1,1212)	1:4:A:THR:HG21	1:7:A:ARG:HB3	10	0.12
(1,1212)	1:4:A:THR:HG22	1:7:A:ARG:HB3	10	0.12
(1,1212)	1:4:A:THR:HG23	1:7:A:ARG:HB3	10	0.12
(1,1005)	1:3:A:SER:H	1:6:A:ASP:HB3	13	0.12
(1,997)	1:59:A:LYS:HA	1:59:A:LYS:HG3	11	0.12
(1,891)	1:51:A:PHE:H	1:53:A:ILE:HG12	16	0.12
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD1	13	0.12
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD2	13	0.12
(1,825)	1:4:A:THR:HB	1:51:A:PHE:HZ	16	0.12
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD21	2	0.12
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD22	2	0.12
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD23	2	0.12
(1,230)	1:19:A:PRO:HD3	1:22:A:THR:HG21	15	0.12
(1,230)	1:19:A:PRO:HD3	1:22:A:THR:HG22	15	0.12
(1,230)	1:19:A:PRO:HD3	1:22:A:THR:HG23	15	0.12
(1,223)	1:18:A:ILE:HG21	1:22:A:THR:HB	15	0.12
(1,223)	1:18:A:ILE:HG22	1:22:A:THR:HB	15	0.12
(1,223)	1:18:A:ILE:HG23	1:22:A:THR:HB	15	0.12
(1,150)	1:16:A:CYS:HB3	1:18:A:ILE:HG12	17	0.12
(2,93)	1:92:A:GLY:H	1:88:A:VAL:O	18	0.11
(2,43)	1:49:A:LYS:H	1:45:A:PHE:O	15	0.11
(2,37)	1:46:A:ALA:H	1:42:A:ASP:O	15	0.11
(2,23)	1:23:A:ILE:H	1:20:A:ARG:O	2	0.11
(1,1918)	1:94:A:LEU:HA	1:95:A:GLU:HG2	1	0.11
(1,1918)	1:94:A:LEU:HA	1:95:A:GLU:HG3	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1861)	1:88:A:VAL:HG11	1:91:A:LYS:HE2	8	0.11
(1,1861)	1:88:A:VAL:HG11	1:91:A:LYS:HE3	8	0.11
(1,1861)	1:88:A:VAL:HG12	1:91:A:LYS:HE2	8	0.11
(1,1861)	1:88:A:VAL:HG12	1:91:A:LYS:HE3	8	0.11
(1,1861)	1:88:A:VAL:HG13	1:91:A:LYS:HE2	8	0.11
(1,1861)	1:88:A:VAL:HG13	1:91:A:LYS:HE3	8	0.11
(1,1726)	1:86:A:GLU:H	1:86:A:GLU:HB2	7	0.11
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	2	0.11
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	5	0.11
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	6	0.11
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	16	0.11
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	17	0.11
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG2	16	0.11
(1,1605)	1:74:A:TYR:HD1	1:83:A:ARG:HG3	16	0.11
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG2	16	0.11
(1,1605)	1:74:A:TYR:HD2	1:83:A:ARG:HG3	16	0.11
(1,1298)	1:60:A:TRP:HH2	1:74:A:TYR:HD1	12	0.11
(1,1298)	1:60:A:TRP:HH2	1:74:A:TYR:HD2	12	0.11
(1,1150)	1:63:A:GLU:HB3	1:67:A:GLY:H	17	0.11
(1,1093)	1:62:A:GLN:HG2	1:63:A:GLU:H	2	0.11
(1,1092)	1:62:A:GLN:HG3	1:63:A:GLU:H	10	0.11
(1,1086)	1:59:A:LYS:HG3	1:63:A:GLU:HG3	16	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD21	4	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD22	4	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD23	4	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD21	18	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD22	18	0.11
(1,961)	1:44:A:ALA:H	1:57:A:LEU:HD23	18	0.11
(1,955)	1:40:A:PHE:HE1	1:57:A:LEU:HD21	7	0.11
(1,955)	1:40:A:PHE:HE1	1:57:A:LEU:HD22	7	0.11
(1,955)	1:40:A:PHE:HE1	1:57:A:LEU:HD23	7	0.11
(1,955)	1:40:A:PHE:HE2	1:57:A:LEU:HD21	7	0.11
(1,955)	1:40:A:PHE:HE2	1:57:A:LEU:HD22	7	0.11
(1,955)	1:40:A:PHE:HE2	1:57:A:LEU:HD23	7	0.11
(1,825)	1:4:A:THR:HB	1:51:A:PHE:HZ	7	0.11
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD2	8	0.11
(1,759)	1:45:A:PHE:HE1	1:49:A:LYS:HD3	8	0.11
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD2	8	0.11
(1,759)	1:45:A:PHE:HE2	1:49:A:LYS:HD3	8	0.11
(1,758)	1:45:A:PHE:HD1	1:49:A:LYS:HG2	11	0.11
(1,758)	1:45:A:PHE:HD1	1:49:A:LYS:HG3	11	0.11
(1,758)	1:45:A:PHE:HD2	1:49:A:LYS:HG2	11	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:45:A:PHE:HD2	1:49:A:LYS:HG3	11	0.11
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE2	3	0.11
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE3	3	0.11
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE2	3	0.11
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE3	3	0.11
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE2	5	0.11
(1,757)	1:45:A:PHE:HD1	1:49:A:LYS:HE3	5	0.11
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE2	5	0.11
(1,757)	1:45:A:PHE:HD2	1:49:A:LYS:HE3	5	0.11
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD21	1	0.11
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD22	1	0.11
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD23	1	0.11
(1,475)	1:33:A:LEU:HD11	1:34:A:GLY:H	19	0.11
(1,475)	1:33:A:LEU:HD12	1:34:A:GLY:H	19	0.11
(1,475)	1:33:A:LEU:HD13	1:34:A:GLY:H	19	0.11
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB2	3	0.11
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB3	3	0.11
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB2	3	0.11
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB3	3	0.11
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB2	3	0.11
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB3	3	0.11
(1,265)	1:20:A:ARG:HG2	1:23:A:ILE:HG21	12	0.11
(1,265)	1:20:A:ARG:HG2	1:23:A:ILE:HG22	12	0.11
(1,265)	1:20:A:ARG:HG2	1:23:A:ILE:HG23	12	0.11
(1,265)	1:20:A:ARG:HG3	1:23:A:ILE:HG21	12	0.11
(1,265)	1:20:A:ARG:HG3	1:23:A:ILE:HG22	12	0.11
(1,265)	1:20:A:ARG:HG3	1:23:A:ILE:HG23	12	0.11
(1,182)	1:18:A:ILE:HB	1:19:A:PRO:HD3	16	0.11
(2,53)	1:62:A:GLN:H	1:58:A:GLU:O	16	0.1
(1,1747)	1:55:A:LEU:HD21	1:87:A:LEU:H	6	0.1
(1,1747)	1:55:A:LEU:HD22	1:87:A:LEU:H	6	0.1
(1,1747)	1:55:A:LEU:HD23	1:87:A:LEU:H	6	0.1
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	8	0.1
(1,1725)	1:86:A:GLU:H	1:86:A:GLU:HB3	13	0.1
(1,1361)	1:26:A:GLU:HG2	1:76:A:VAL:HG11	12	0.1
(1,1361)	1:26:A:GLU:HG2	1:76:A:VAL:HG12	12	0.1
(1,1361)	1:26:A:GLU:HG2	1:76:A:VAL:HG13	12	0.1
(1,1361)	1:26:A:GLU:HG3	1:76:A:VAL:HG11	12	0.1
(1,1361)	1:26:A:GLU:HG3	1:76:A:VAL:HG12	12	0.1
(1,1361)	1:26:A:GLU:HG3	1:76:A:VAL:HG13	12	0.1
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE1	17	0.1
(1,1328)	1:30:A:ILE:HG21	1:75:A:PHE:HE2	17	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE1	17	0.1
(1,1328)	1:30:A:ILE:HG22	1:75:A:PHE:HE2	17	0.1
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE1	17	0.1
(1,1328)	1:30:A:ILE:HG23	1:75:A:PHE:HE2	17	0.1
(1,951)	1:40:A:PHE:HB2	1:57:A:LEU:HD21	19	0.1
(1,951)	1:40:A:PHE:HB2	1:57:A:LEU:HD22	19	0.1
(1,951)	1:40:A:PHE:HB2	1:57:A:LEU:HD23	19	0.1
(1,951)	1:40:A:PHE:HB3	1:57:A:LEU:HD21	19	0.1
(1,951)	1:40:A:PHE:HB3	1:57:A:LEU:HD22	19	0.1
(1,951)	1:40:A:PHE:HB3	1:57:A:LEU:HD23	19	0.1
(1,891)	1:51:A:PHE:H	1:53:A:ILE:HG12	7	0.1
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD1	8	0.1
(1,829)	1:50:A:ALA:HA	1:51:A:PHE:HD2	8	0.1
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD21	9	0.1
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD22	9	0.1
(1,595)	1:40:A:PHE:H	1:41:A:LEU:HD23	9	0.1
(1,531)	1:37:A:SER:H	1:38:A:LEU:HD11	18	0.1
(1,531)	1:37:A:SER:H	1:38:A:LEU:HD12	18	0.1
(1,531)	1:37:A:SER:H	1:38:A:LEU:HD13	18	0.1
(1,475)	1:33:A:LEU:HD11	1:34:A:GLY:H	13	0.1
(1,475)	1:33:A:LEU:HD12	1:34:A:GLY:H	13	0.1
(1,475)	1:33:A:LEU:HD13	1:34:A:GLY:H	13	0.1
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB2	18	0.1
(1,331)	1:24:A:THR:HG21	1:26:A:GLU:HB3	18	0.1
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB2	18	0.1
(1,331)	1:24:A:THR:HG22	1:26:A:GLU:HB3	18	0.1
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB2	18	0.1
(1,331)	1:24:A:THR:HG23	1:26:A:GLU:HB3	18	0.1
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD11	19	0.1
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD12	19	0.1
(1,264)	1:20:A:ARG:HD2	1:23:A:ILE:HD13	19	0.1
(1,149)	1:16:A:CYS:HB3	1:18:A:ILE:HG13	14	0.1

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

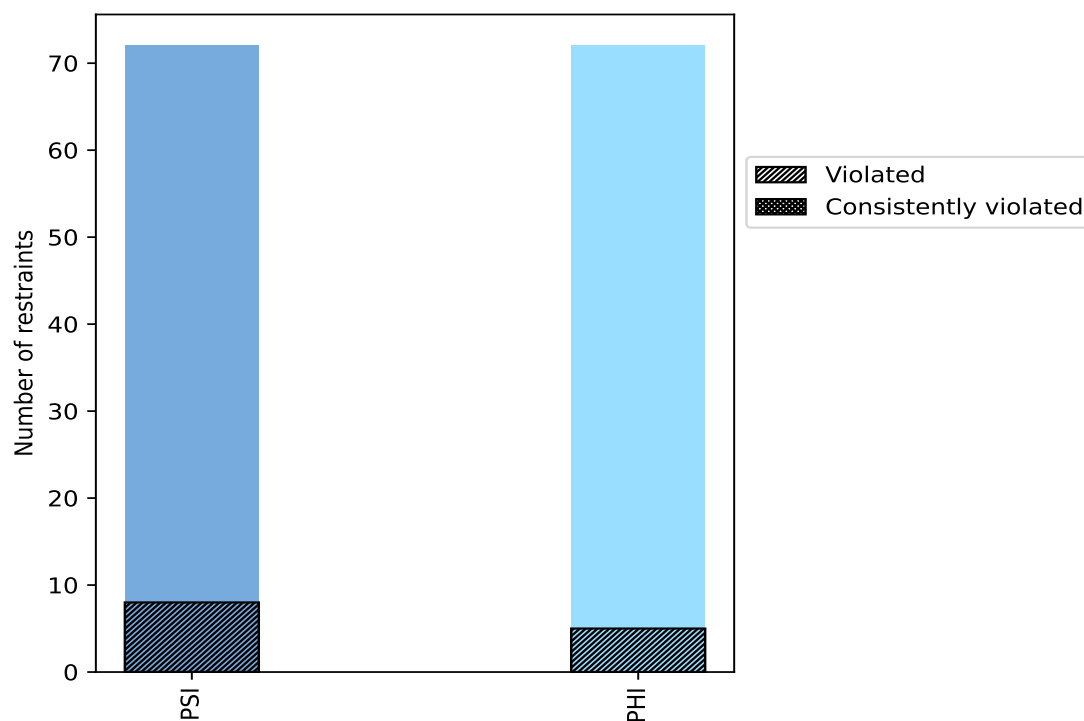
10.1 Summary of dihedral-angle violations [i](#)

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	50.0	8	11.1	5.6	0	0.0	0.0
PHI	72	50.0	5	6.9	3.5	0	0.0	0.0
Total	144	100.0	13	9.0	9.0	0	0.0	0.0

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

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



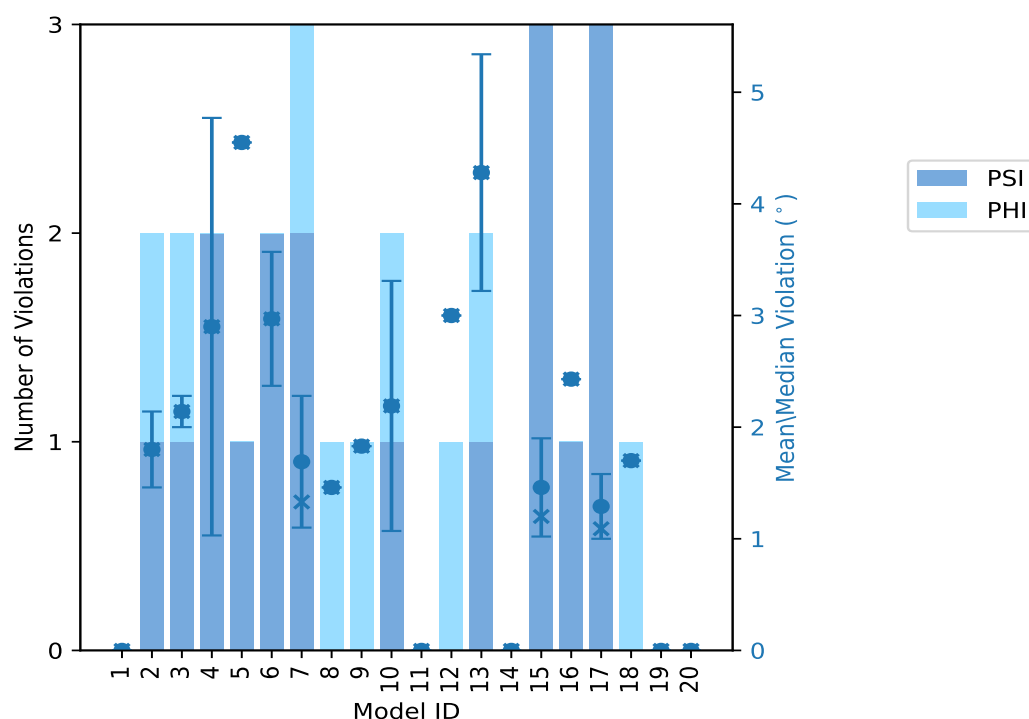
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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	0	0	0	0.0	0.0	0.0	0.0
2	1	1	2	1.8	2.13	0.34	1.8
3	1	1	2	2.14	2.28	0.14	2.14
4	2	0	2	2.9	4.77	1.87	2.9
5	1	0	1	4.55	4.55	0.0	4.55
6	2	0	2	2.97	3.57	0.6	2.97
7	2	1	3	1.69	2.52	0.59	1.33
8	0	1	1	1.46	1.46	0.0	1.46
9	0	1	1	1.83	1.83	0.0	1.83
10	1	1	2	2.19	3.32	1.12	2.19
11	0	0	0	0.0	0.0	0.0	0.0
12	0	1	1	3.0	3.0	0.0	3.0
13	1	1	2	4.28	5.34	1.06	4.28
14	0	0	0	0.0	0.0	0.0	0.0
15	3	0	3	1.46	2.09	0.44	1.2
16	1	0	1	2.43	2.43	0.0	2.43
17	3	0	3	1.29	1.69	0.29	1.09
18	0	1	1	1.7	1.7	0.0	1.7
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

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	
PSI	PHI	Total	Count ¹	%
4	4	8	1	5.0
1	0	1	2	10.0
2	0	2	3	15.0
0	0	0	4	20.0
0	1	1	5	25.0
1	0	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

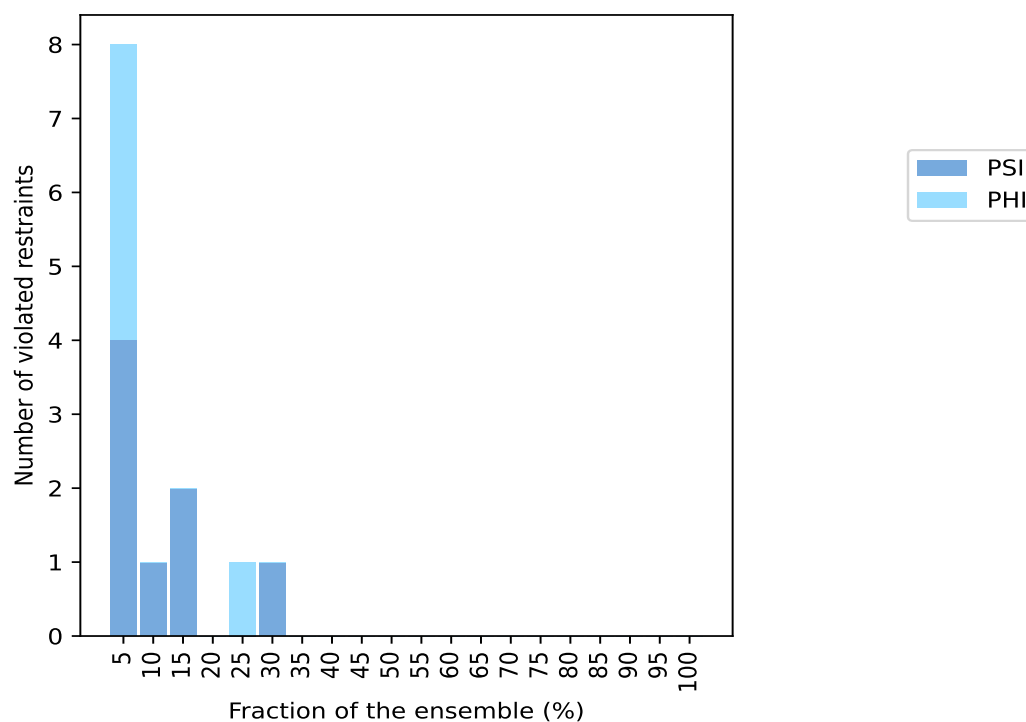
Continued on next page...

Continued from previous page...

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

¹ Number of models with violations

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

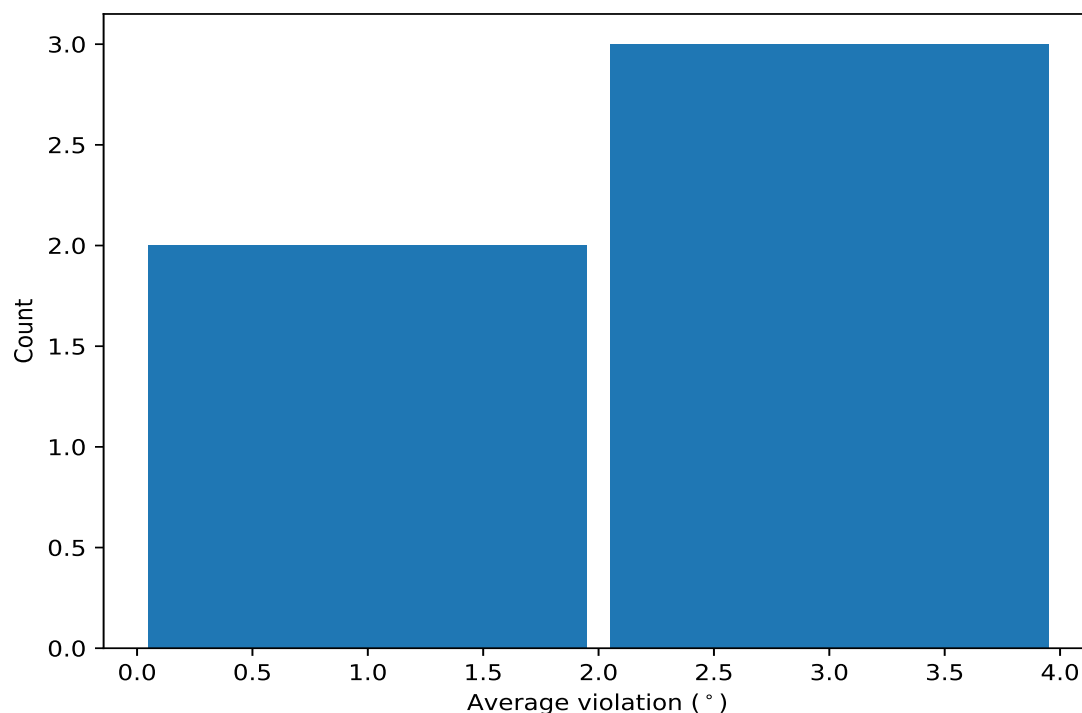


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

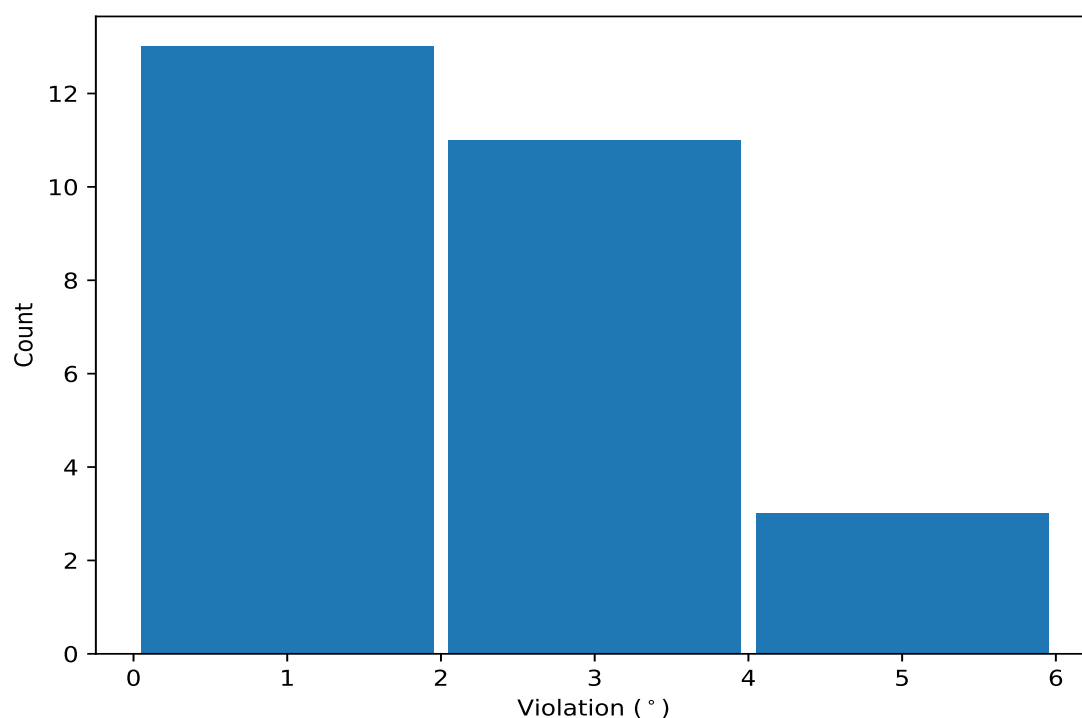
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,54)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:LEU:N	6	2.74	0.95	2.4
(1,79)	1:53:A:ILE:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	5	2.14	0.65	2.28
(1,144)	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	1:93:A:ALA:N	3	3.18	1.48	3.57
(1,40)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:SER:N	3	1.15	0.13	1.1
(1,36)	1:23:A:ILE:N	1:23:A:ILE:CA	1:23:A:ILE:C	1:24:A:THR:N	2	1.27	0.19	1.27

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 (°)
(1,102)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	13	5.34
(1,144)	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	1:93:A:ALA:N	4	4.77
(1,54)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:LEU:N	5	4.55
(1,144)	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	1:93:A:ALA:N	6	3.57
(1,54)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:LEU:N	10	3.32
(1,143)	1:91:A:LYS:C	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	13	3.23
(1,79)	1:53:A:ILE:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	12	3.0
(1,79)	1:53:A:ILE:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	7	2.52
(1,54)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:LEU:N	16	2.43
(1,54)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:LEU:N	6	2.37
(1,79)	1:53:A:ILE:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	3	2.28
(1,51)	1:38:A:LEU:C	1:39:A:ASP:N	1:39:A:ASP:CA	1:39:A:ASP:C	2	2.13
(1,54)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:LEU:N	15	2.09
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:CYS:N	3	2.01
(1,79)	1:53:A:ILE:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	9	1.83
(1,25)	1:15:A:THR:C	1:16:A:CYS:N	1:16:A:CYS:CA	1:16:A:CYS:C	18	1.7
(1,54)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:LEU:N	17	1.69
(1,77)	1:52:A:GLY:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	8	1.46
(1,36)	1:23:A:ILE:N	1:23:A:ILE:CA	1:23:A:ILE:C	1:24:A:THR:N	2	1.46
(1,40)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:SER:N	7	1.33
(1,144)	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	1:93:A:ALA:N	7	1.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,62)	1:44:A:ALA:N	1:44:A:ALA:CA	1:44:A:ALA:C	1:45:A:PHE:N	15	1.2
(1,40)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:SER:N	15	1.1
(1,50)	1:38:A:LEU:N	1:38:A:LEU:CA	1:38:A:LEU:C	1:39:A:ASP:N	17	1.09
(1,36)	1:23:A:ILE:N	1:23:A:ILE:CA	1:23:A:ILE:C	1:24:A:THR:N	17	1.08
(1,79)	1:53:A:ILE:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	10	1.07
(1,40)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:SER:N	4	1.03