Full wwPDB NMR Structure Validation Report (i)

Dec 13, 2023 – 10:34 PM EST

PDB ID	:	2JN4
BMRB ID	:	15085
Title	:	Solution NMR Structure of Protein RP4601 from Rhodopseudomonas palustris. Northeast Structural Genomics Consortium Target RpT2; Ontario Center for Structural Proteomics Target RP4601.
Authors	:	Lemak, A.; Srisailam, S.; Yee, A.; Karra, M.D.; Lukin, J.A.; Arrowsmith, C.H.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2006-12-22

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

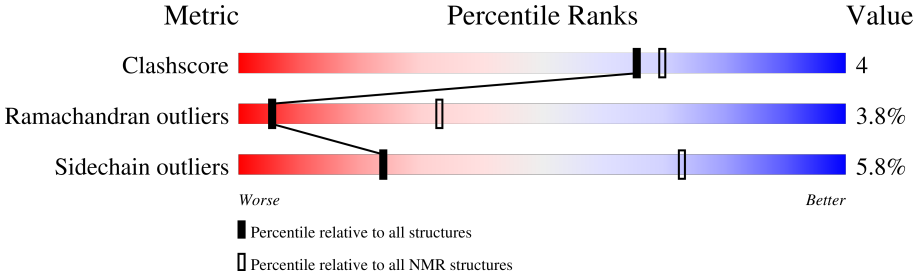
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 87%.

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	87	69% 7% 24%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *all calculated structures submitted*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:66 (66)	0.86	12

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1039 atoms, of which 532 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein fixU, nifT.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	66	1039	325	532	85	93	4	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	cloning artifact	UNP Q6N0Y6
A	-19	GLY	-	cloning artifact	UNP Q6N0Y6
A	-18	SER	-	cloning artifact	UNP Q6N0Y6
A	-17	SER	-	cloning artifact	UNP Q6N0Y6
A	-16	HIS	-	expression tag	UNP Q6N0Y6
A	-15	HIS	-	expression tag	UNP Q6N0Y6
A	-14	HIS	-	expression tag	UNP Q6N0Y6
A	-13	HIS	-	expression tag	UNP Q6N0Y6
A	-12	HIS	-	expression tag	UNP Q6N0Y6
A	-11	HIS	-	expression tag	UNP Q6N0Y6
A	-10	SER	-	cloning artifact	UNP Q6N0Y6
A	-9	SER	-	cloning artifact	UNP Q6N0Y6
A	-8	GLY	-	cloning artifact	UNP Q6N0Y6
A	-7	ARG	-	cloning artifact	UNP Q6N0Y6
A	-6	GLU	-	cloning artifact	UNP Q6N0Y6
A	-5	ASN	-	cloning artifact	UNP Q6N0Y6
A	-4	LEU	-	cloning artifact	UNP Q6N0Y6
A	-3	TYR	-	cloning artifact	UNP Q6N0Y6
A	-2	PHE	-	cloning artifact	UNP Q6N0Y6
A	-1	GLN	-	cloning artifact	UNP Q6N0Y6
A	0	GLY	-	cloning artifact	UNP Q6N0Y6

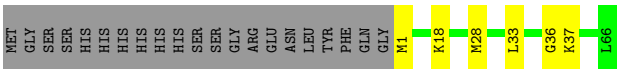
4 Residue-property plots (i)

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: Hypothetical protein fixU, nifT

Chain A: 69% 7% 24%



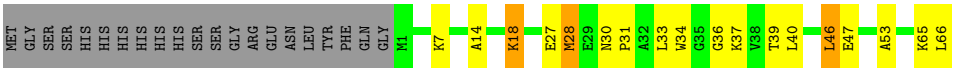
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Hypothetical protein fixU, nifT

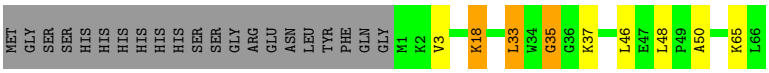
Chain A: 55% 17% • 24%



4.2.2 Score per residue for model 2

• Molecule 1: Hypothetical protein fixU, nifT

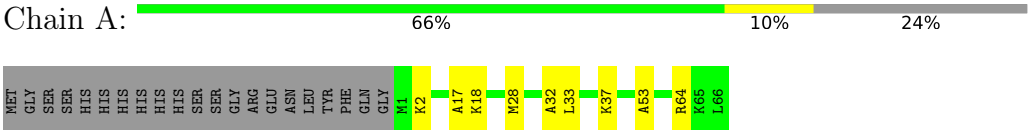
Chain A: 66% 7% • 24%



4.2.3 Score per residue for model 3

• Molecule 1: Hypothetical protein fixU, nifT

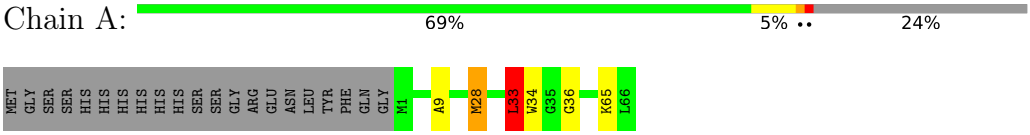
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Hypothetical protein fixU, nifT

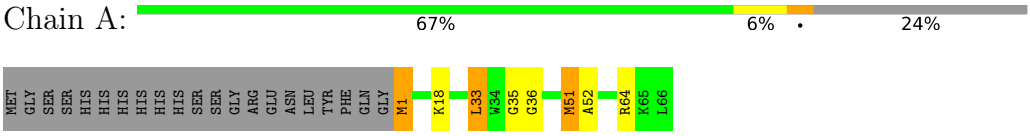
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Hypothetical protein fixU, nifT

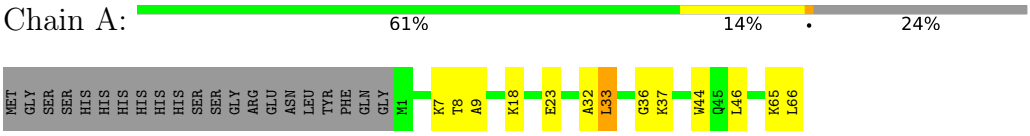
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Hypothetical protein fixU, nifT

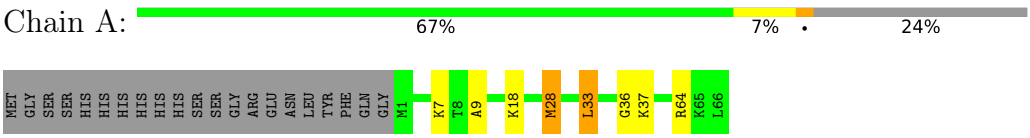
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Hypothetical protein fixU, nifT

Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Hypothetical protein fixU, nifT

Chain A: 63% 13% 24%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 R6 A14 K18 M28 L33 W34 G35 G36 L40 A50 L57 P58 L66

4.2.9 Score per residue for model 9

• Molecule 1: Hypothetical protein fixU, nifT

Chain A: 62% 11% • 24%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 K18 L21 E22 M28 E29 N30 P31 A32 L33 K37 W44 R64 K65 L66

4.2.10 Score per residue for model 10

• Molecule 1: Hypothetical protein fixU, nifT

Chain A: 62% 13% • 24%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 K7 K18 M28 L33 W34 G35 G36 K37 L46 E47 D54 R64 K65 L66

4.2.11 Score per residue for model 11

• Molecule 1: Hypothetical protein fixU, nifT

Chain A: 64% 11% 24%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 K18 K19 D20 L21 M28 E29 N30 L33 G36 W44 E62 L66

4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: Hypothetical protein fixU, nifT

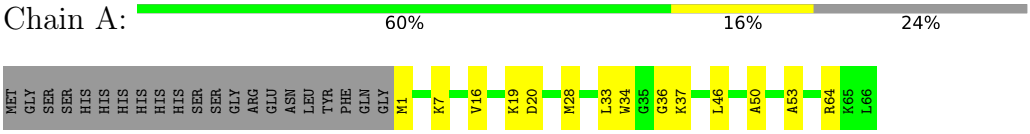
Chain A: 67% 7% • 24%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY M1 A9 K19 M28 E29 L33 W34 G35 G36 K37 L66

4.2.13 Score per residue for model 13

• Molecule 1: Hypothetical protein fixU, nifT

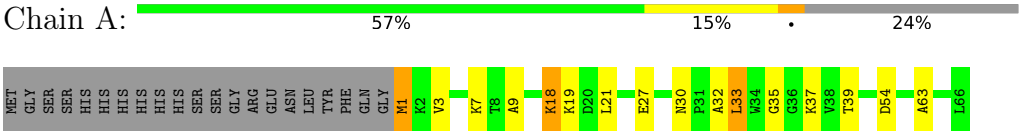
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Hypothetical protein fixU, nifT

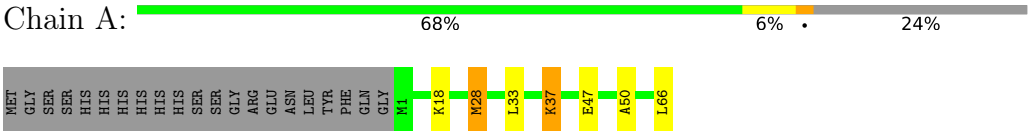
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Hypothetical protein fixU, nifT

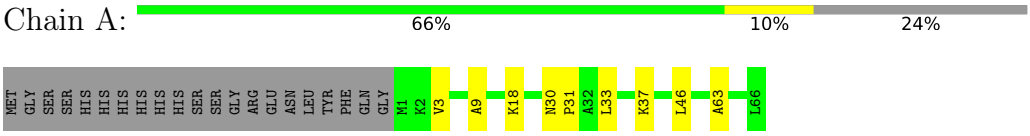
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Hypothetical protein fixU, nifT

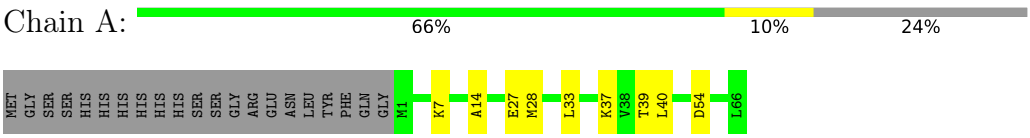
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Hypothetical protein fixU, nifT

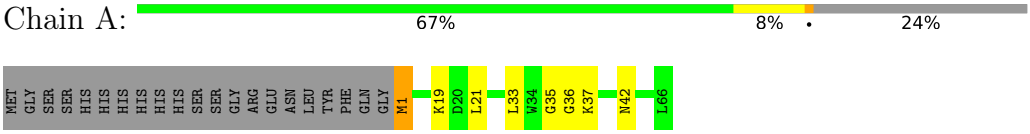
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Hypothetical protein fixU, nifT

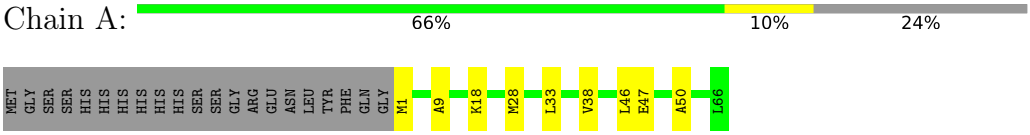
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical protein fixU, nifT

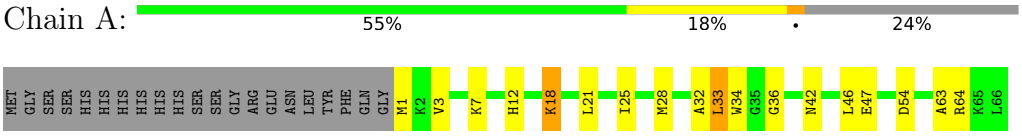
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein fixU, nifT

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 150 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
CYANA	structure solution	2.1
CNS	refinement	1.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	789
Number of shifts mapped to atoms	789
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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	507	532	533	4±2
All	All	10140	10640	10660	86

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:SD	1:A:64:ARG:NH1	0.68	2.67	10	1
1:A:7:LYS:HE2	1:A:54:ASP:HA	0.64	1.69	20	1
1:A:1:MET:SD	1:A:18:LYS:HD3	0.64	2.32	9	1
1:A:1:MET:SD	1:A:1:MET:N	0.61	2.73	5	4
1:A:19:LYS:HG3	1:A:21:LEU:HB2	0.61	1.71	11	1
1:A:1:MET:HG3	1:A:63:ALA:HB3	0.57	1.77	20	1
1:A:1:MET:SD	1:A:64:ARG:HG2	0.57	2.39	13	1
1:A:28:MET:SD	1:A:28:MET:N	0.56	2.79	4	9
1:A:19:LYS:HD3	1:A:19:LYS:O	0.53	2.03	14	3
1:A:32:ALA:HB3	1:A:53:ALA:HB1	0.52	1.82	3	1
1:A:19:LYS:HD2	1:A:21:LEU:HB2	0.51	1.83	14	2
1:A:21:LEU:HD11	1:A:42:ASN:HD22	0.51	1.66	18	1
1:A:34:TRP:HB2	1:A:53:ALA:HA	0.50	1.83	1	2
1:A:46:LEU:HD13	1:A:47:GLU:N	0.49	2.23	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ALA:O	1:A:33:LEU:HB2	0.48	2.07	20	3
1:A:44:TRP:HZ2	1:A:65:LYS:HD2	0.48	1.69	9	1
1:A:27:GLU:HB3	1:A:39:THR:HB	0.47	1.86	14	3
1:A:64:ARG:HH11	1:A:64:ARG:HG3	0.47	1.68	5	1
1:A:14:ALA:HB3	1:A:40:LEU:HD11	0.47	1.86	1	3
1:A:3:VAL:HB	1:A:63:ALA:HB2	0.46	1.86	20	3
1:A:6:ARG:HD3	1:A:58:PRO:HB3	0.46	1.87	8	1
1:A:33:LEU:HB3	1:A:34:TRP:CD1	0.46	2.46	20	1
1:A:8:THR:HG22	1:A:9:ALA:H	0.45	1.71	6	1
1:A:18:LYS:NZ	1:A:18:LYS:HB2	0.45	2.26	1	2
1:A:7:LYS:NZ	1:A:54:ASP:O	0.45	2.49	10	3
1:A:44:TRP:HZ2	1:A:65:LYS:HE2	0.45	1.72	6	1
1:A:28:MET:SD	1:A:28:MET:O	0.45	2.74	15	1
1:A:12:HIS:CD2	1:A:33:LEU:HD23	0.44	2.47	20	1
1:A:66:LEU:HD12	1:A:66:LEU:N	0.44	2.28	1	2
1:A:2:LYS:HD2	1:A:17:ALA:HB2	0.44	1.89	3	1
1:A:3:VAL:HG11	1:A:46:LEU:HD21	0.44	1.89	2	1
1:A:1:MET:SD	1:A:18:LYS:NZ	0.44	2.87	20	1
1:A:33:LEU:HB3	1:A:34:TRP:HD1	0.43	1.73	4	1
1:A:37:LYS:HA	1:A:47:GLU:HA	0.43	1.89	15	1
1:A:7:LYS:HD3	1:A:33:LEU:HG	0.43	1.90	7	1
1:A:57:LEU:HB2	1:A:58:PRO:HD2	0.43	1.89	8	1
1:A:33:LEU:HG	1:A:48:LEU:HD21	0.43	1.90	2	1
1:A:38:VAL:HG12	1:A:46:LEU:O	0.43	2.13	19	1
1:A:64:ARG:HG3	1:A:64:ARG:NH1	0.43	2.28	5	1
1:A:30:ASN:OD1	1:A:31:PRO:HD2	0.42	2.14	16	3
1:A:19:LYS:CG	1:A:21:LEU:HB2	0.42	2.43	11	1
1:A:16:VAL:O	1:A:20:ASP:N	0.42	2.52	13	1
1:A:7:LYS:NZ	1:A:7:LYS:HB3	0.42	2.29	1	1
1:A:21:LEU:HD11	1:A:44:TRP:CE3	0.42	2.50	11	1
1:A:18:LYS:NZ	1:A:18:LYS:HB3	0.42	2.30	2	1
1:A:51:MET:SD	1:A:52:ALA:N	0.42	2.87	5	1
1:A:1:MET:O	1:A:62:GLU:HA	0.42	2.14	11	1
1:A:35:GLY:HA2	1:A:50:ALA:HB2	0.41	1.91	2	1
1:A:37:LYS:HD3	1:A:37:LYS:O	0.41	2.15	9	1
1:A:29:GLU:HB2	1:A:37:LYS:HD3	0.41	1.92	12	1
1:A:21:LEU:HD21	1:A:42:ASN:HD21	0.41	1.76	20	1
1:A:47:GLU:HB3	1:A:64:ARG:HB2	0.41	1.91	20	1
1:A:21:LEU:HD23	1:A:22:GLU:N	0.40	2.31	9	1
1:A:12:HIS:HB2	1:A:25:ILE:HB	0.40	1.92	20	1
1:A:66:LEU:N	1:A:66:LEU:HD12	0.40	2.32	6	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	64/87 (74%)	55±2 (86±3%)	7±2 (11±3%)	2±1 (4±1%)	5 33
All	All	1280/1740 (74%)	1095 (86%)	136 (11%)	49 (4%)	5 33

All 5 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	33	LEU	20
1	A	36	GLY	12
1	A	35	GLY	7
1	A	9	ALA	6
1	A	50	ALA	4

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	53/71 (75%)	50±1 (94±2%)	3±1 (6±2%)	24 73
All	All	1060/1420 (75%)	999 (94%)	61 (6%)	24 73

All 12 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	18	LYS	14
1	A	37	LYS	14
1	A	28	MET	11
1	A	46	LEU	5
1	A	65	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	64	ARG	3
1	A	1	MET	3
1	A	33	LEU	2
1	A	7	LYS	2
1	A	30	ASN	2
1	A	51	MET	1
1	A	23	GLU	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 87% for the well-defined parts and 87% 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	789
Number of shifts mapped to atoms	789
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	65	0.10 ± 0.24	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	59	0.05 ± 0.23	None needed (< 0.5 ppm)
$^{13}C'$	56	0.49 ± 0.20	None needed (< 0.5 ppm)
^{15}N	58	0.38 ± 0.47	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 87%, i.e. 789 atoms were assigned a chemical shift out of a possible 905. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	306/326 (94%)	127/132 (96%)	121/132 (92%)	58/62 (94%)
Sidechain	472/538 (88%)	324/355 (91%)	146/168 (87%)	2/15 (13%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	11/41 (27%)	9/20 (45%)	0/17 (0%)	2/4 (50%)
Overall	789/905 (87%)	460/507 (91%)	267/317 (84%)	62/81 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 789 atoms were assigned a chemical shift out of a possible 905. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	306/326 (94%)	127/132 (96%)	121/132 (92%)	58/62 (94%)
Sidechain	472/538 (88%)	324/355 (91%)	146/168 (87%)	2/15 (13%)
Aromatic	11/41 (27%)	9/20 (45%)	0/17 (0%)	2/4 (50%)
Overall	789/905 (87%)	460/507 (91%)	267/317 (84%)	62/81 (77%)

7.1.4 Statistically unusual chemical shifts (i)

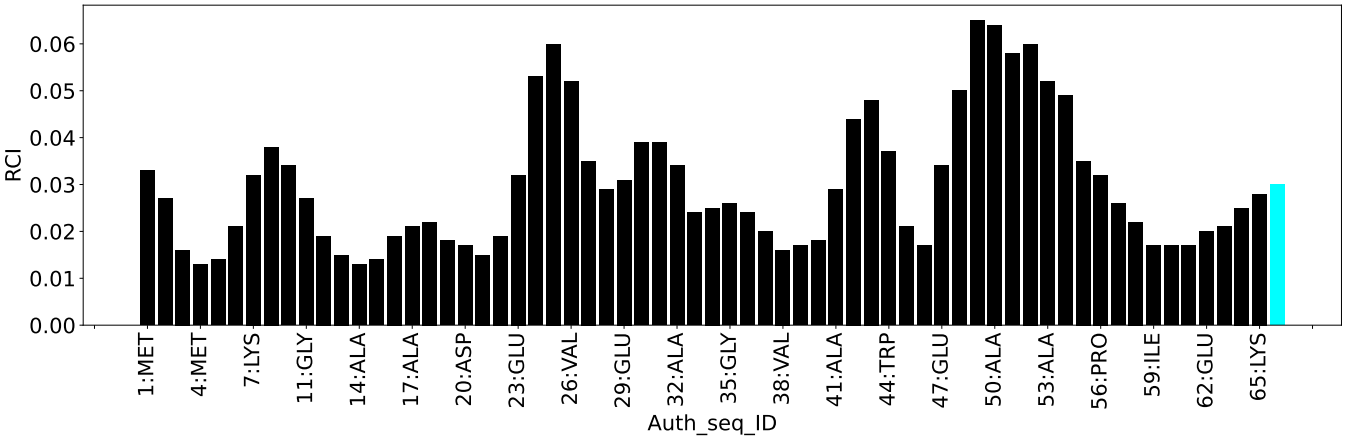
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	65	LYS	HE2	1.58	1.95 – 3.88	-6.9
1	A	65	LYS	HE3	1.58	1.92 – 3.89	-6.7

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
0.00
0.01
0.02
0.03
0.04
0.05
0.06
1:MET
4:MET
7:LYS
11:GLY
14:ALA
17:ALA
20:ASP
23:GLU
26:VAL
29:GLU
32:ALA
35:GLY
38:VAL
41:ALA
44:TRP
47:GLU
50:ALA
53:ALA
56:PRO
59:ILE
62:GLU
65:LYS
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	1312
Intra-residue (|i-j|=0)	262
Sequential (|i-j|=1)	351
Medium range (|i-j|>1 and |i-j|<5)	138
Long range (|i-j|≥5)	561
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	64
Number of unmapped restraints	0
Number of restraints per residue	15.8
Number of long range restraints per residue[1]	6.4

[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)	2.5	0.2
0.2-0.5 (Medium)	0.9	0.47
>0.5 (Large)	5.0	3.44

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)	1.9	4.82
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

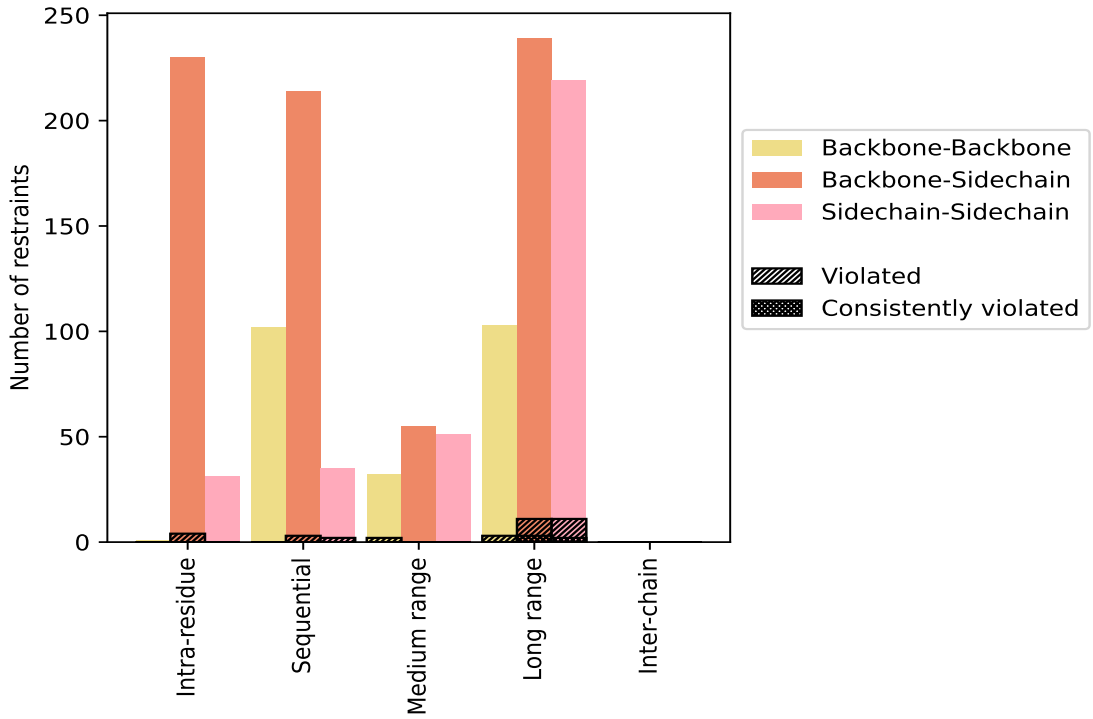
9.1 Summary of distance violations (i)

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)	262	20.0	4	1.5	0.3	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	230	17.5	4	1.7	0.3	0	0.0	0.0
Sidechain-Sidechain	31	2.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	351	26.8	5	1.4	0.4	0	0.0	0.0
Backbone-Backbone	102	7.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	214	16.3	3	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	35	2.7	2	5.7	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	138	10.5	2	1.4	0.2	0	0.0	0.0
Backbone-Backbone	32	2.4	2	6.2	0.2	0	0.0	0.0
Backbone-Sidechain	55	4.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	51	3.9	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	561	42.8	25	4.5	1.9	5	0.9	0.4
Backbone-Backbone	103	7.9	3	2.9	0.2	0	0.0	0.0
Backbone-Sidechain	239	18.2	11	4.6	0.8	3	1.3	0.2
Sidechain-Sidechain	219	16.7	11	5.0	0.8	2	0.9	0.2
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1312	100.0	36	2.7	2.7	5	0.4	0.4
Backbone-Backbone	238	18.1	5	2.1	0.4	0	0.0	0.0
Backbone-Sidechain	738	56.2	18	2.4	1.4	3	0.4	0.2
Sidechain-Sidechain	336	25.6	13	3.9	1.0	2	0.6	0.2

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	1	0	8	0	10	0.81	2.68	0.84	0.4
2	2	1	0	6	0	9	0.97	2.74	0.88	0.6
3	0	0	0	7	0	7	1.26	3.03	0.95	1.03
4	0	3	0	7	0	10	0.99	3.07	0.91	0.88
5	1	2	0	6	0	9	1.01	2.9	0.88	0.89
6	0	2	0	6	0	8	1.12	3.21	0.96	0.9
7	0	1	1	6	0	8	1.19	3.33	1.07	0.82
8	0	2	1	8	0	11	0.75	2.66	0.83	0.15
9	0	3	0	7	0	10	1.02	3.44	1.04	0.62
10	0	1	0	5	0	6	1.3	3.19	0.98	1.09
11	0	1	0	6	0	7	1.14	3.11	0.95	1.24

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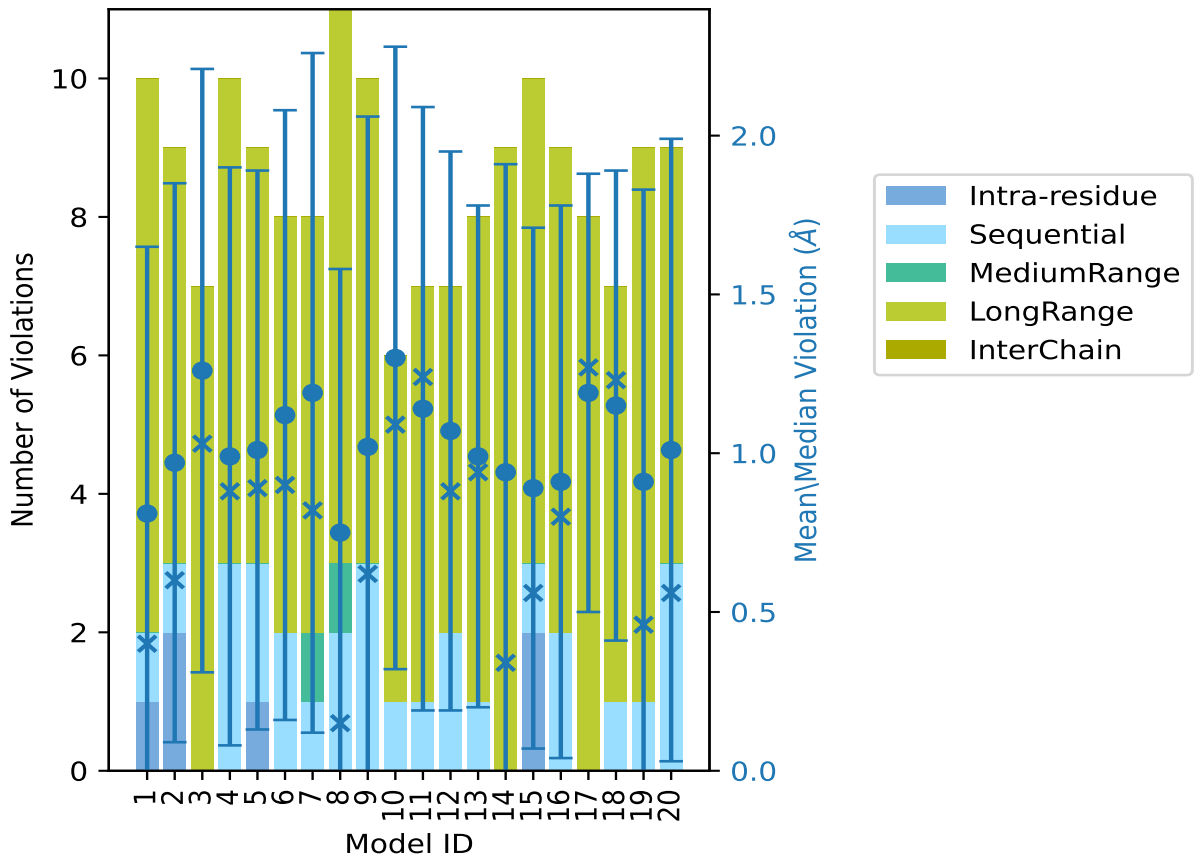
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	0	5	0	7	1.07	2.7	0.88	0.88
13	0	1	0	7	0	8	0.99	2.65	0.79	0.94
14	0	0	0	9	0	9	0.94	3.0	0.97	0.34
15	2	1	0	7	0	10	0.89	2.81	0.82	0.56
16	0	2	0	7	0	9	0.91	2.92	0.87	0.8
17	0	0	0	8	0	8	1.19	2.56	0.69	1.27
18	0	1	0	6	0	7	1.15	2.51	0.74	1.23
19	0	1	0	8	0	9	0.91	3.06	0.92	0.46
20	0	3	0	6	0	9	1.01	3.19	0.98	0.56

[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

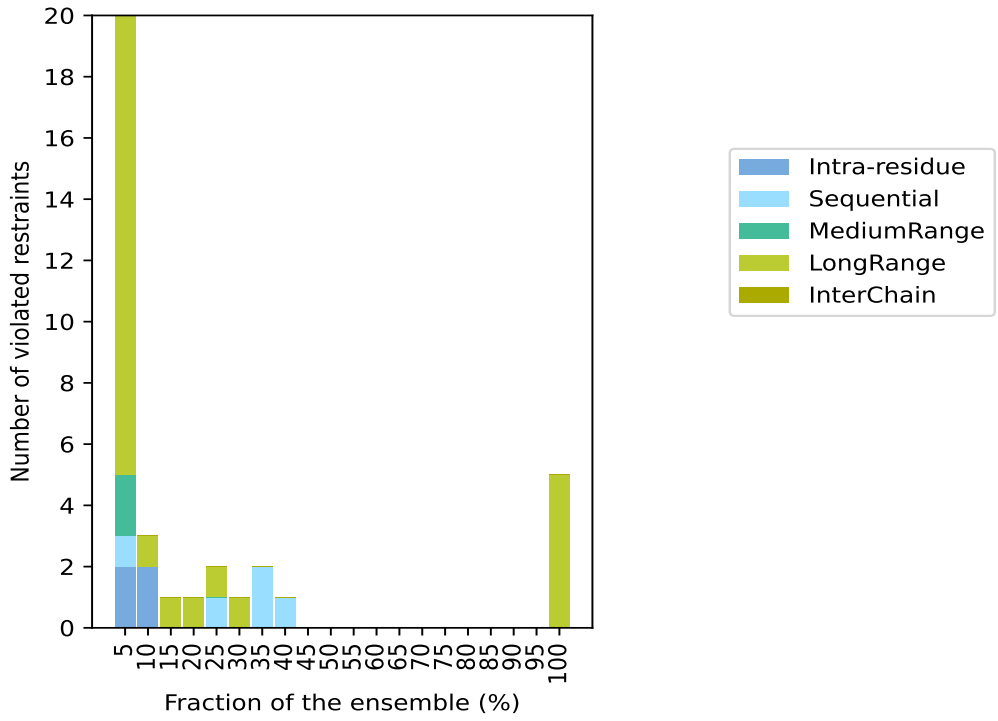
9.3 Distance violation statistics for the ensemble (i)

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, 1276(IR:258, SQ:346, MR:136, LR:536, 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]	%
2	1	2	15	0	20	1	5.0
2	0	0	1	0	3	2	10.0
0	0	0	1	0	1	3	15.0
0	0	0	1	0	1	4	20.0
0	1	0	1	0	2	5	25.0
0	0	0	1	0	1	6	30.0
0	2	0	0	0	2	7	35.0
0	1	0	0	0	1	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	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	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	5	0	5	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

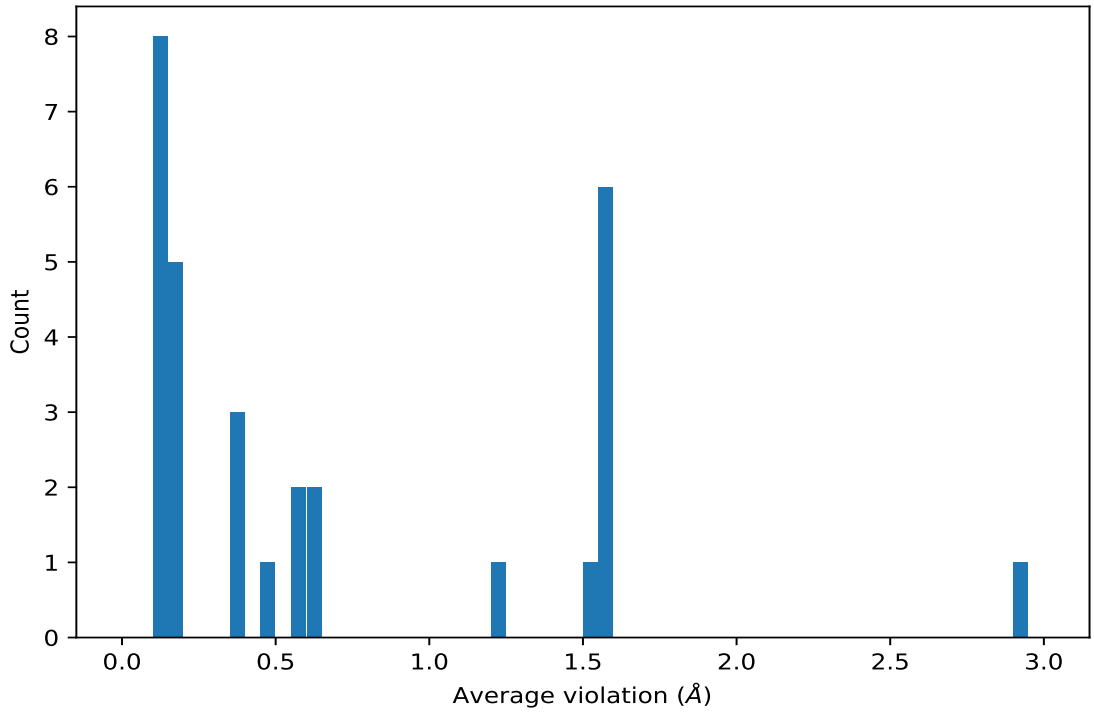
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	20	2.94	0.26	2.96
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	20	1.55	0.31	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	20	1.55	0.31	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	20	1.55	0.31	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	20	1.55	0.31	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	20	1.55	0.31	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	20	1.55	0.31	1.62
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	20	1.52	0.22	1.46
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	20	1.23	0.25	1.23
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	20	0.59	0.16	0.62
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	20	0.59	0.16	0.62
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	8	0.15	0.01	0.14
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	8	0.15	0.01	0.14
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	8	0.15	0.01	0.14
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	7	0.63	0.28	0.56
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	7	0.63	0.28	0.56

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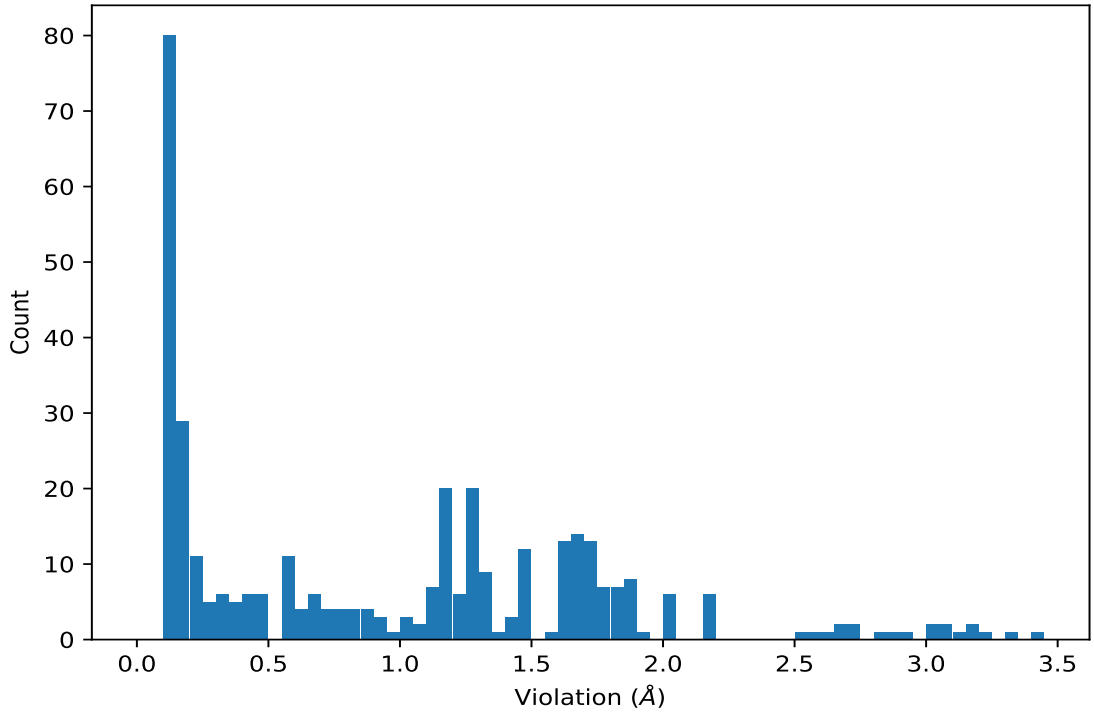
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	7	0.11	0.01	0.11
(1,959)	1:1:A:MET:H	1:63:A:ALA:H	6	0.47	0.35	0.39
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB1	5	0.36	0.13	0.34
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB2	5	0.36	0.13	0.34
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB3	5	0.36	0.13	0.34
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG21	5	0.16	0.04	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG22	5	0.16	0.04	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG23	5	0.16	0.04	0.18
(1,87)	1:23:A:GLU:HB2	1:40:A:LEU:HG	4	0.17	0.01	0.16
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB2	3	0.12	0.02	0.11
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB3	3	0.12	0.02	0.11
(1,731)	1:2:A:LYS:H	1:2:A:LYS:HB3	2	0.18	0.02	0.18
(1,765)	1:65:A:LYS:H	1:65:A:LYS:HB2	2	0.15	0.01	0.15
(1,176)	1:27:A:GLU:HB3	1:39:A:THR:HB	2	0.11	0.01	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	9	3.44
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	7	3.33
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	6	3.21
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	10	3.19
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	20	3.19
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	11	3.11
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	4	3.07
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	19	3.06
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	3	3.03
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	14	3.0
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	16	2.92
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	5	2.9
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	15	2.81
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	2	2.74
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	12	2.7
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	1	2.68
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	8	2.66
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	13	2.65
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	17	2.56
(1,786)	1:15:A:TYR:HD2	1:22:A:GLU:H	18	2.51
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	7	2.16
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	7	2.16
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	7	2.16
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	7	2.16
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	7	2.16
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	7	2.16
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	9	2.02
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	9	2.02
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	9	2.02
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	9	2.02
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	9	2.02
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	9	2.02
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	6	1.92
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	20	1.9
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	20	1.9
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	20	1.9
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	20	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	20	1.9
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	20	1.9
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	3	1.89
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	14	1.87
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	7	1.83
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	1	1.81
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	1	1.81
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	1	1.81
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	1	1.81
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	1	1.81
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	1	1.81
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	2	1.78
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	2	1.78
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	2	1.78
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	2	1.78
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	2	1.78
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	2	1.78
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	4	1.75
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	10	1.72
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	8	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	8	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	8	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	8	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	8	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	8	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	18	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	18	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	18	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	18	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	18	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	18	1.71
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	12	1.7
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	12	1.7
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	12	1.7
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	12	1.7
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	12	1.7
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	12	1.7
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	9	1.69
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	14	1.66
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	14	1.66
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	14	1.66
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	14	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	14	1.66
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	14	1.66
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	20	1.66
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	5	1.63
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	5	1.63
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	5	1.63
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	5	1.63
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	5	1.63
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	5	1.63
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	3	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	3	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	3	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	3	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	3	1.62
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	3	1.62
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	2	1.6
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	5	1.59
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	17	1.49
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	17	1.48
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	17	1.48
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	17	1.48
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	17	1.48
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	17	1.48
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	17	1.48
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	12	1.48
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	19	1.48
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	13	1.47
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	15	1.46
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	11	1.46
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	15	1.45
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	16	1.45
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	4	1.44
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	17	1.39
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	1	1.33
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	8	1.33
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	2	1.32
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	4	1.31
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	4	1.31
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	4	1.31
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	4	1.31
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	4	1.31
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	4	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	15	1.27
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	15	1.27
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	15	1.27
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	15	1.27
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	15	1.27
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	15	1.27
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	13	1.27
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	19	1.26
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	19	1.26
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	19	1.26
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	19	1.26
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	19	1.26
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	19	1.26
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	11	1.25
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	11	1.25
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	11	1.25
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	11	1.25
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	11	1.25
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	11	1.25
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	18	1.25
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	6	1.24
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	11	1.24
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	19	1.23
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	5	1.23
(1,420)	1:15:A:TYR:HD2	1:22:A:GLU:HA	18	1.23
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	16	1.22
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	10	1.2
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	10	1.2
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	10	1.2
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	10	1.2
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	10	1.2
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	10	1.2
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	8	1.2
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	13	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	13	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	13	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	13	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	13	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	13	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	16	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	16	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	16	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	16	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	16	1.17
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	16	1.17
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	9	1.17
(1,959)	1:1:A:MET:H	1:63:A:ALA:H	17	1.15
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD11	6	1.1
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD12	6	1.1
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD13	6	1.1
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD21	6	1.1
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD22	6	1.1
(1,1041)	1:15:A:TYR:HD2	1:21:A:LEU:HD23	6	1.1
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	4	1.07
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	4	1.07
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	1	1.04
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	3	1.03
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	14	1.0
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	10	0.98
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	3	0.92
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	3	0.92
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	7	0.9
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	5	0.89
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	5	0.89
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	12	0.88
(1,776)	1:4:A:MET:H	1:15:A:TYR:HD1	20	0.87
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	9	0.81
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	9	0.81
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	16	0.8
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	16	0.8
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	17	0.77
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	17	0.77
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	7	0.75
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	7	0.75
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	13	0.72
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	13	0.72
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	6	0.71
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	6	0.71
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	4	0.68
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	4	0.68
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	11	0.67
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	11	0.67
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	18	0.65
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	8	0.64
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	8	0.64
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	10	0.61
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	10	0.61
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	2	0.6
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	2	0.6
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB1	17	0.59
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB2	17	0.59
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB3	17	0.59
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	20	0.56
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	20	0.56
(1,959)	1:1:A:MET:H	1:63:A:ALA:H	15	0.56
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	15	0.55
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	15	0.55
(1,959)	1:1:A:MET:H	1:63:A:ALA:H	18	0.55
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	1	0.47
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	1	0.47
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	20	0.47
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	20	0.47
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	19	0.46
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	19	0.46
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	5	0.43
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	5	0.43
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	9	0.43
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	9	0.43
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	6	0.43
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	6	0.43
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	12	0.36
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	12	0.36
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB1	7	0.36
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB2	7	0.36
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB3	7	0.36
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	14	0.34
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	14	0.34
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB1	1	0.34
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB2	1	0.34
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB3	1	0.34
(1,913)	1:24:A:LEU:H	1:24:A:LEU:HG	15	0.33
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB2	19	0.3
(1,1042)	1:15:A:TYR:HD2	1:22:A:GLU:HB3	19	0.3
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB1	13	0.28
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB2	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB3	13	0.28
(1,959)	1:1:A:MET:H	1:63:A:ALA:H	14	0.23
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB2	12	0.22
(1,962)	1:1:A:MET:H	1:2:A:LYS:HB3	12	0.22
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB1	6	0.22
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB2	6	0.22
(1,958)	1:1:A:MET:H	1:63:A:ALA:HB3	6	0.22
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG21	9	0.22
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG22	9	0.22
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG23	9	0.22
(1,959)	1:1:A:MET:H	1:63:A:ALA:H	3	0.21
(1,731)	1:2:A:LYS:H	1:2:A:LYS:HB3	2	0.2
(1,87)	1:23:A:GLU:HB2	1:40:A:LEU:HG	13	0.19
(1,1199)	1:37:A:LYS:HE2	1:66:A:LEU:HD11	2	0.18
(1,1199)	1:37:A:LYS:HE2	1:66:A:LEU:HD12	2	0.18
(1,1199)	1:37:A:LYS:HE2	1:66:A:LEU:HD13	2	0.18
(1,1199)	1:37:A:LYS:HE2	1:66:A:LEU:HD21	2	0.18
(1,1199)	1:37:A:LYS:HE2	1:66:A:LEU:HD22	2	0.18
(1,1199)	1:37:A:LYS:HE2	1:66:A:LEU:HD23	2	0.18
(1,1199)	1:37:A:LYS:HE3	1:66:A:LEU:HD11	2	0.18
(1,1199)	1:37:A:LYS:HE3	1:66:A:LEU:HD12	2	0.18
(1,1199)	1:37:A:LYS:HE3	1:66:A:LEU:HD13	2	0.18
(1,1199)	1:37:A:LYS:HE3	1:66:A:LEU:HD21	2	0.18
(1,1199)	1:37:A:LYS:HE3	1:66:A:LEU:HD22	2	0.18
(1,1199)	1:37:A:LYS:HE3	1:66:A:LEU:HD23	2	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG21	4	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG22	4	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG23	4	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG21	20	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG22	20	0.18
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG23	20	0.18
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	15	0.18
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	15	0.18
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	15	0.18
(1,87)	1:23:A:GLU:HB2	1:40:A:LEU:HG	19	0.17
(1,1004)	1:6:A:ARG:HA	1:7:A:LYS:HG2	13	0.16
(1,1004)	1:6:A:ARG:HA	1:7:A:LYS:HG3	13	0.16
(1,765)	1:65:A:LYS:H	1:65:A:LYS:HB2	2	0.16
(1,731)	1:2:A:LYS:H	1:2:A:LYS:HB3	5	0.16
(1,87)	1:23:A:GLU:HB2	1:40:A:LEU:HG	9	0.16
(1,87)	1:23:A:GLU:HB2	1:40:A:LEU:HG	16	0.16
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB3	16	0.15
(1,1147)	1:29:A:GLU:HB3	1:37:A:LYS:HD2	8	0.15
(1,1147)	1:29:A:GLU:HB3	1:37:A:LYS:HD3	8	0.15
(1,1094)	1:21:A:LEU:HD11	1:44:A:TRP:HD1	5	0.15
(1,1094)	1:21:A:LEU:HD12	1:44:A:TRP:HD1	5	0.15
(1,1094)	1:21:A:LEU:HD13	1:44:A:TRP:HD1	5	0.15
(1,1094)	1:21:A:LEU:HD21	1:44:A:TRP:HD1	5	0.15
(1,1094)	1:21:A:LEU:HD22	1:44:A:TRP:HD1	5	0.15
(1,1094)	1:21:A:LEU:HD23	1:44:A:TRP:HD1	5	0.15
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	16	0.15
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	16	0.15
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	16	0.15
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	18	0.15
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	18	0.15
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	18	0.15
(1,1102)	1:24:A:LEU:H	1:24:A:LEU:HD11	15	0.14
(1,1102)	1:24:A:LEU:H	1:24:A:LEU:HD12	15	0.14
(1,1102)	1:24:A:LEU:H	1:24:A:LEU:HD13	15	0.14
(1,1102)	1:24:A:LEU:H	1:24:A:LEU:HD21	15	0.14
(1,1102)	1:24:A:LEU:H	1:24:A:LEU:HD22	15	0.14
(1,1102)	1:24:A:LEU:H	1:24:A:LEU:HD23	15	0.14
(1,765)	1:65:A:LYS:H	1:65:A:LYS:HB2	1	0.14
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	2	0.14
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	2	0.14
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	2	0.14
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	6	0.14
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	6	0.14
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	6	0.14
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	8	0.14
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	8	0.14
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	8	0.14
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	20	0.14
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	20	0.14
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	20	0.14
(1,836)	1:12:A:HIS:HD2	1:34:A:TRP:HE1	20	0.13
(1,769)	1:1:A:MET:HG3	1:63:A:ALA:H	9	0.13
(1,318)	1:32:A:ALA:HB1	1:33:A:LEU:HB2	12	0.13
(1,318)	1:32:A:ALA:HB2	1:33:A:LEU:HB2	12	0.13
(1,318)	1:32:A:ALA:HB3	1:33:A:LEU:HB2	12	0.13
(1,261)	1:49:A:PRO:HD3	1:61:A:VAL:HG11	4	0.13
(1,261)	1:49:A:PRO:HD3	1:61:A:VAL:HG12	4	0.13
(1,261)	1:49:A:PRO:HD3	1:61:A:VAL:HG13	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	16	0.13
(1,959)	1:1:A:MET:H	1:63:A:ALA:H	11	0.12
(1,837)	1:34:A:TRP:HE1	1:53:A:ALA:HA	1	0.12
(1,736)	1:2:A:LYS:H	1:63:A:ALA:HB1	4	0.12
(1,736)	1:2:A:LYS:H	1:63:A:ALA:HB2	4	0.12
(1,736)	1:2:A:LYS:H	1:63:A:ALA:HB3	4	0.12
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG21	11	0.12
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG22	11	0.12
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG23	11	0.12
(1,514)	1:47:A:GLU:HB2	1:64:A:ARG:H	17	0.12
(1,421)	1:36:A:GLY:HA2	1:48:A:LEU:HA	14	0.12
(1,176)	1:27:A:GLU:HB3	1:39:A:THR:HB	14	0.12
(1,164)	1:37:A:LYS:HA	1:47:A:GLU:HA	15	0.12
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	5	0.12
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	8	0.12
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB2	3	0.11
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB3	3	0.11
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB2	19	0.11
(1,1184)	1:37:A:LYS:H	1:48:A:LEU:HB3	19	0.11
(1,932)	1:29:A:GLU:H	1:38:A:VAL:HB	8	0.11
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG21	7	0.11
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG22	7	0.11
(1,735)	1:2:A:LYS:H	1:3:A:VAL:HG23	7	0.11
(1,536)	1:8:A:THR:H	1:12:A:HIS:HA	7	0.11
(1,455)	1:8:A:THR:H	1:11:A:GLY:H	8	0.11
(1,446)	1:36:A:GLY:H	1:48:A:LEU:HD21	14	0.11
(1,446)	1:36:A:GLY:H	1:48:A:LEU:HD22	14	0.11
(1,446)	1:36:A:GLY:H	1:48:A:LEU:HD23	14	0.11
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	1	0.11
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	4	0.11
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	9	0.11
(1,96)	1:21:A:LEU:HD11	1:40:A:LEU:HG	19	0.11
(1,96)	1:21:A:LEU:HD12	1:40:A:LEU:HG	19	0.11
(1,96)	1:21:A:LEU:HD13	1:40:A:LEU:HG	19	0.11
(1,213)	1:37:A:LYS:HB2	1:47:A:GLU:HG3	8	0.1
(1,176)	1:27:A:GLU:HB3	1:39:A:THR:HB	1	0.1
(1,151)	1:30:A:ASN:HB3	1:31:A:PRO:HG2	10	0.1

10 Dihedral-angle violation analysis (i)

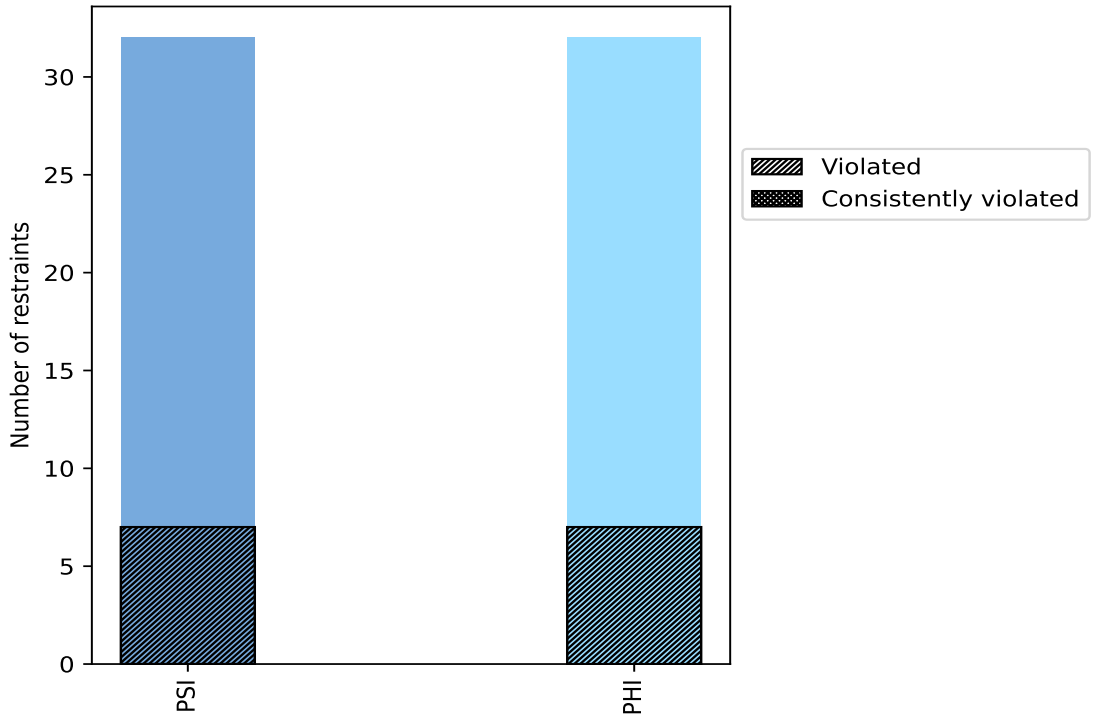
10.1 Summary of dihedral-angle violations (i)

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	32	50.0	7	21.9	10.9	0	0.0	0.0
PHI	32	50.0	7	21.9	10.9	0	0.0	0.0
Total	64	100.0	14	21.9	21.9	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)



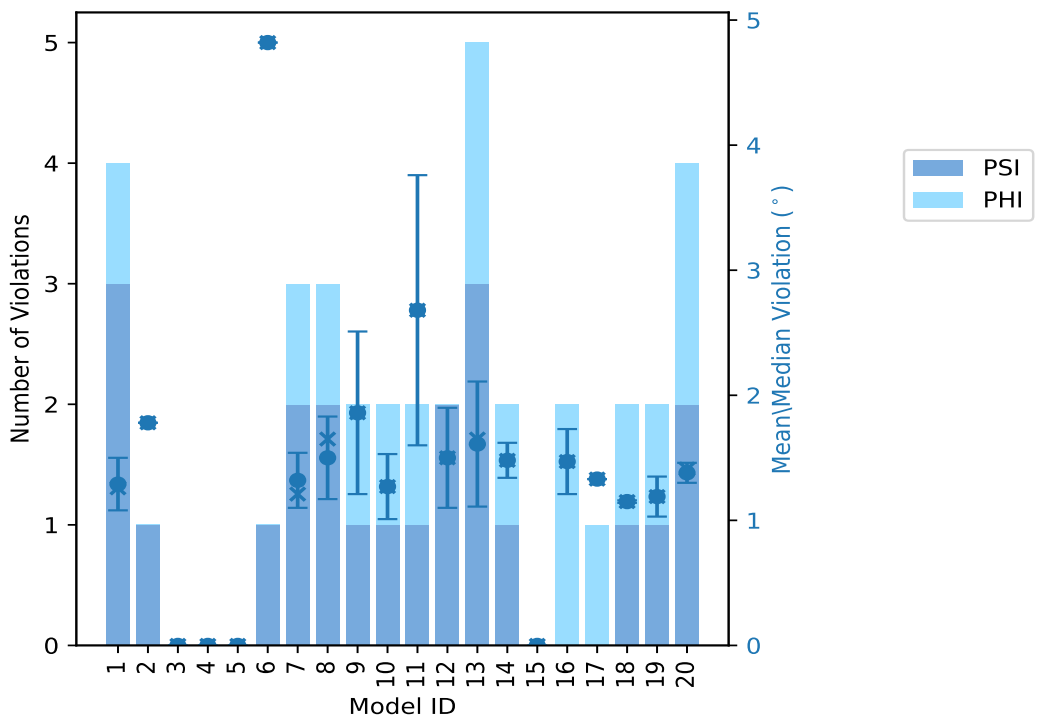
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (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 (°)
	PSI	PHI	Total				
1	3	1	4	1.29	1.62	0.21	1.26
2	1	0	1	1.78	1.78	0.0	1.78
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	1	0	1	4.82	4.82	0.0	4.82
7	2	1	3	1.32	1.63	0.22	1.21
8	2	1	3	1.5	1.81	0.33	1.65
9	1	1	2	1.86	2.51	0.65	1.86
10	1	1	2	1.27	1.52	0.26	1.27
11	1	1	2	2.68	3.77	1.08	2.68
12	2	0	2	1.5	1.91	0.4	1.5
13	3	2	5	1.61	2.46	0.5	1.65
14	1	1	2	1.48	1.62	0.14	1.48
15	0	0	0	0.0	0.0	0.0	0.0
16	0	2	2	1.47	1.73	0.26	1.47
17	0	1	1	1.33	1.33	0.0	1.33
18	1	1	2	1.15	1.16	0.01	1.15
19	1	1	2	1.19	1.35	0.16	1.19
20	2	2	4	1.38	1.47	0.08	1.41

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

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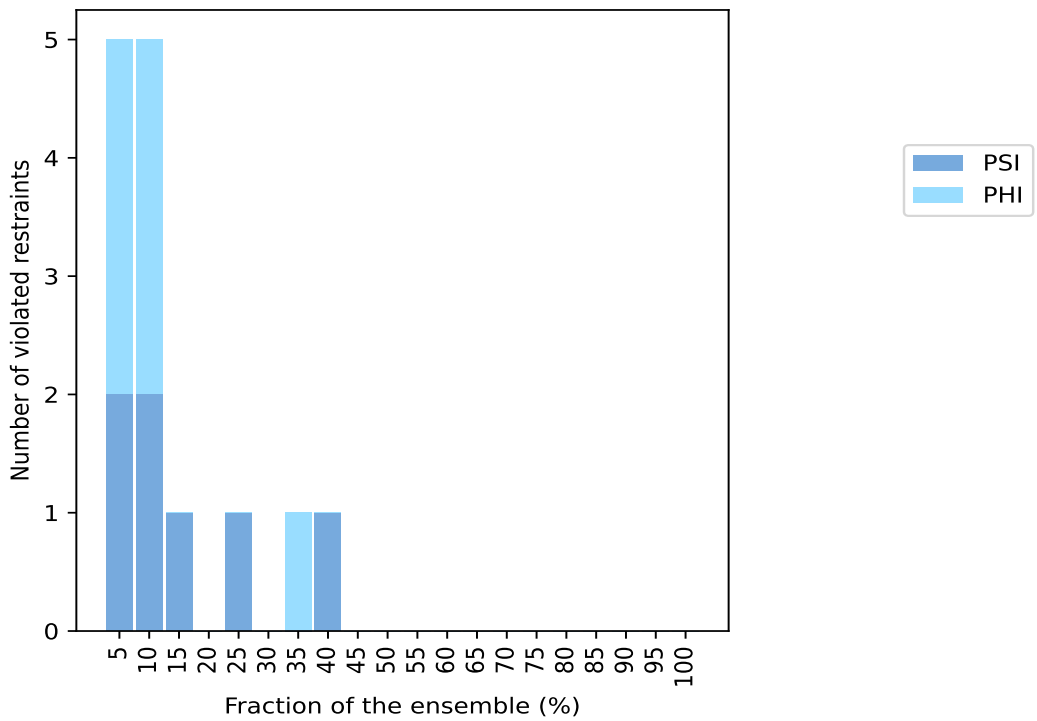
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

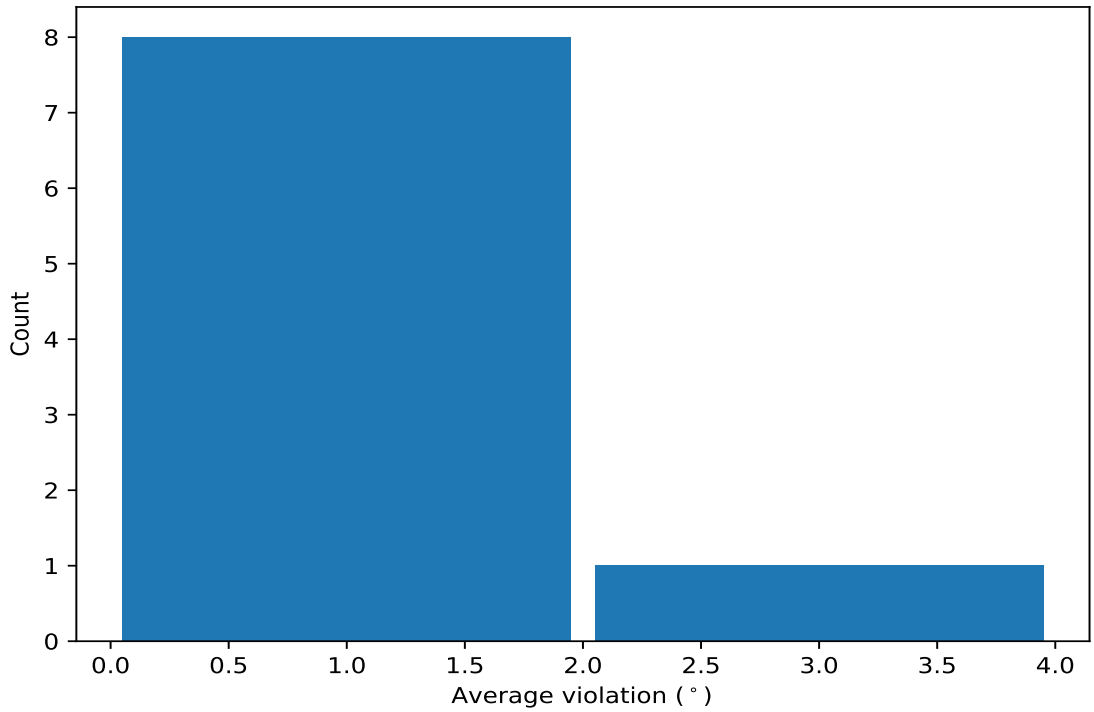


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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.

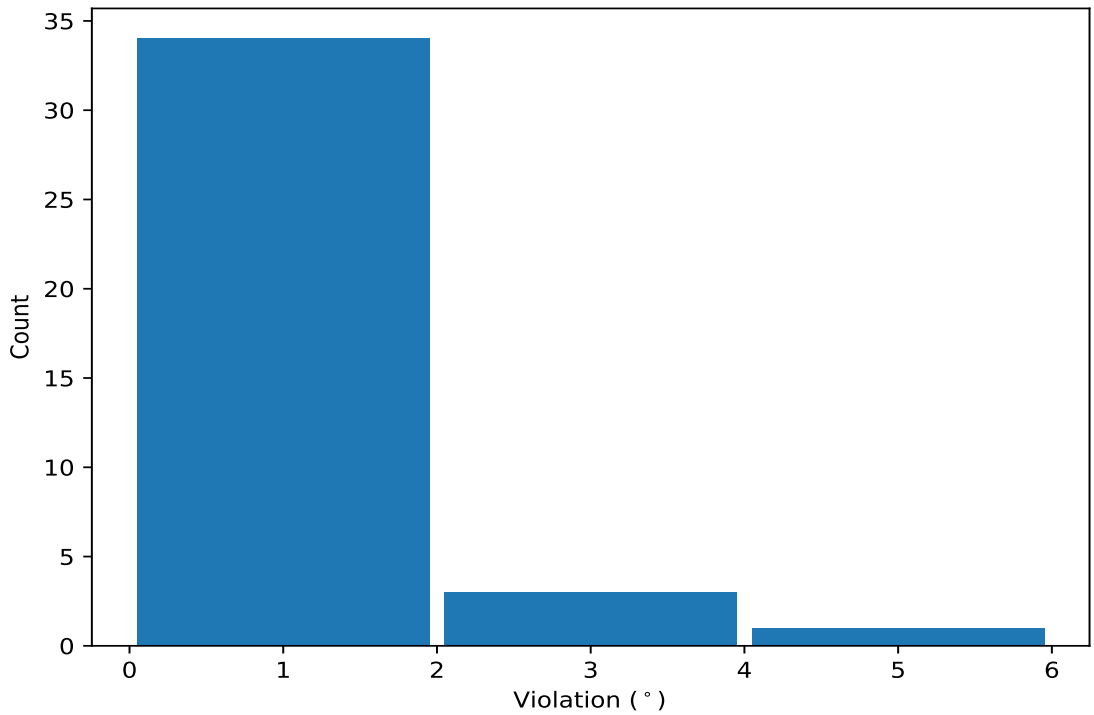
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	8	1.68	0.51	1.61
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	7	1.87	0.79	1.62
(1,18)	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	1:16:A:VAL:N	5	1.57	0.32	1.65
(1,60)	1:63:A:ALA:N	1:63:A:ALA:CA	1:63:A:ALA:C	1:64:A:ARG:N	3	1.27	0.36	1.03
(1,26)	1:22:A:GLU:N	1:22:A:GLU:CA	1:22:A:GLU:C	1:23:A:GLU:N	2	2.98	1.84	2.98
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	2	1.49	0.14	1.49
(1,53)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	2	1.36	0.01	1.36
(1,23)	1:20:A:ASP:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	2	1.17	0.04	1.17
(1,1)	1:1:A:MET:C	1:2:A:LYS:N	1:2:A:LYS:CA	1:2:A:LYS:C	2	1.12	0.09	1.12

[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 (°)
(1,26)	1:22:A:GLU:N	1:22:A:GLU:CA	1:22:A:GLU:C	1:23:A:GLU:N	6	4.82
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	11	3.77
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	9	2.51
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	13	2.46
(1,18)	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	1:16:A:VAL:N	12	1.91
(1,18)	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	1:16:A:VAL:N	8	1.81
(1,60)	1:63:A:ALA:N	1:63:A:ALA:CA	1:63:A:ALA:C	1:64:A:ARG:N	2	1.78
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	16	1.73
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	13	1.7
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	8	1.65
(1,18)	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	1:16:A:VAL:N	13	1.65
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	7	1.63
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	1	1.62
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	14	1.62
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	11	1.6
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	10	1.52
(1,18)	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	1:16:A:VAL:N	20	1.47
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	20	1.44
(1,53)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	20	1.38
(1,53)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	19	1.35
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	14	1.35

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,9)	1:5:A:ILE:C	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	17	1.33
(1,62)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:LYS:N	1	1.3
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	20	1.25
(1,8)	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	1:6:A:ARG:N	1	1.22
(1,1)	1:1:A:MET:C	1:2:A:LYS:N	1:2:A:LYS:CA	1:2:A:LYS:C	13	1.22
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	7	1.21
(1,31)	1:36:A:GLY:C	1:37:A:LYS:N	1:37:A:LYS:CA	1:37:A:LYS:C	9	1.21
(1,23)	1:20:A:ASP:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	16	1.21
(1,35)	1:38:A:VAL:C	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	18	1.16
(1,26)	1:22:A:GLU:N	1:22:A:GLU:CA	1:22:A:GLU:C	1:23:A:GLU:N	18	1.14
(1,23)	1:20:A:ASP:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	7	1.13
(1,58)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:GLU:N	12	1.1
(1,29)	1:27:A:GLU:C	1:28:A:MET:N	1:28:A:MET:CA	1:28:A:MET:C	8	1.05
(1,60)	1:63:A:ALA:N	1:63:A:ALA:CA	1:63:A:ALA:C	1:64:A:ARG:N	19	1.03
(1,1)	1:1:A:MET:C	1:2:A:LYS:N	1:2:A:LYS:CA	1:2:A:LYS:C	1	1.03
(1,60)	1:63:A:ALA:N	1:63:A:ALA:CA	1:63:A:ALA:C	1:64:A:ARG:N	13	1.01
(1,18)	1:15:A:TYR:N	1:15:A:TYR:CA	1:15:A:TYR:C	1:16:A:VAL:N	10	1.01