Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KZV
BMRB ID	:	17020
Title	:	Solution NMR structure of CV_0373(175-257) protein from Chromobacterium violaceum, Northeast Structural Genomics Consortium Target CvR118A
Authors	:	Yang, Y.; Ramelot, T.A.; Wang, D.; Ciccosanti, C.; Mao, L.; Janjua, H.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-06-25

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

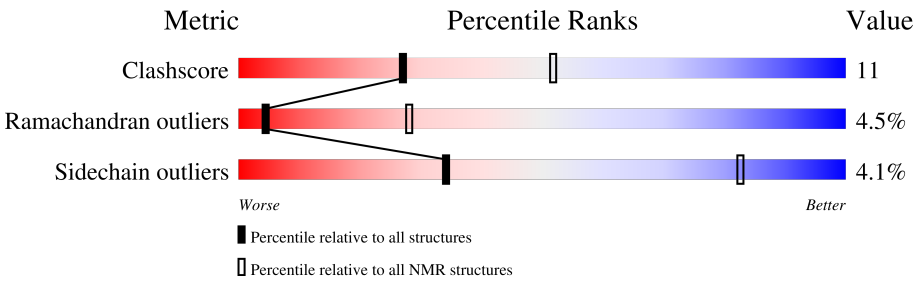
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	92	63% 16% • 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:7-A:81 (75)	1.24	3

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 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1459 atoms, of which 712 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	92	1459	463	712	146	135	3	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q7P141
A	85	LEU	-	expression tag	UNP Q7P141
A	86	GLU	-	expression tag	UNP Q7P141
A	87	HIS	-	expression tag	UNP Q7P141
A	88	HIS	-	expression tag	UNP Q7P141
A	89	HIS	-	expression tag	UNP Q7P141
A	90	HIS	-	expression tag	UNP Q7P141
A	91	HIS	-	expression tag	UNP Q7P141
A	92	HIS	-	expression tag	UNP Q7P141

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: Uncharacterized protein

Chain A: 63% 16% • 18%

M1 P2 H3 K4 E5 K6 H7 A21 R22 D23 S24 G25 W26 Y35 L36 N39 D40 R46 G49 R52 D61 F62 R69 L80 R81 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

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: Uncharacterized protein

Chain A: 57% 21% • 18%

M1 P2 H3 K4 E5 K6 H7 P8 L9 R22 D23 S24 G25 W26 Y35 L36 N39 D40 W48 Q55 M56 F62 Q66 E67 S68 R69 N70 H75 S76 E77 T78 R79 L80 R81 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

4.2.2 Score per residue for model 2

• Molecule 1: Uncharacterized protein

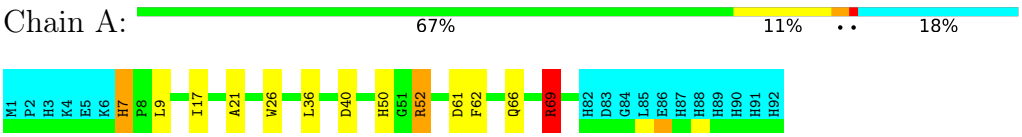
Chain A: 67% 12% • 18%

M1 P2 H3 K4 E5 K6 R22 D23 S24 Y35 L36 N39 D40 R46 M56 F62 L63 T64 R69 R81 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Uncharacterized protein

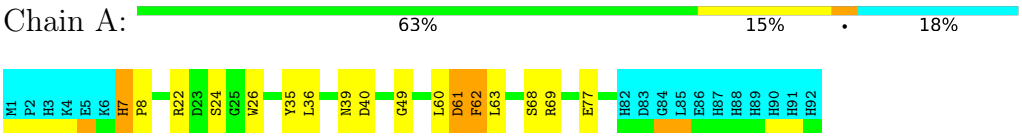
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

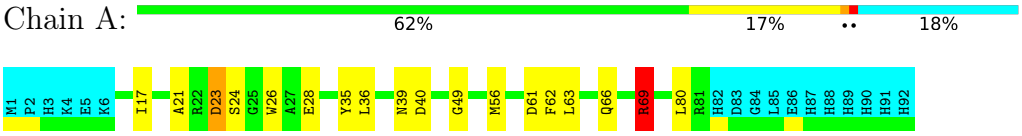
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein

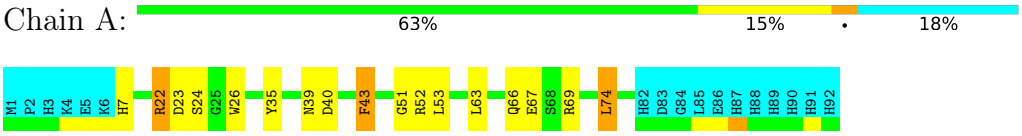
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein

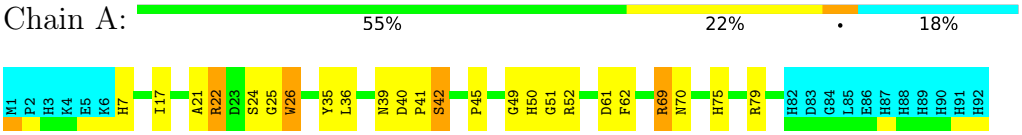
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein

Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein

Chain A: 66% 13% • • 18%

M1 P2 H3 K4 E5 K6 L9 A21 R22 D23 Y35 N39 D40 P41 S42 F43 D61 F62 E67 S68 R69 L80 R81 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein

Chain A: 62% 17% • • 18%

M1 P2 H3 K4 E5 K6 H7 P8 L9 I17 A21 R22 W26 Y35 L36 A37 K38 N39 D40 P41 Q66 R69 N70 H75 L80 R81 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein

Chain A: 54% 24% • • 18%

M1 P2 H3 K4 E5 K6 H7 I17 V20 A21 R22 D23 S24 G25 W26 Y35 L36 N39 D40 D44 P45 R46 H50 Q55 F62 E67 S68 R69 N70 K73 L74 H75 S76 E77 L80 R81 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein

Chain A: 58% 16% 8% 18%

M1 P2 H3 K4 E5 K6 Q10 T14 R22 D23 S24 G25 W26 Y35 N39 P45 G49 H50 G51 R52 L53 L60 D61 F62 L63 Q66 E67 S68 R69 L80 R81 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein

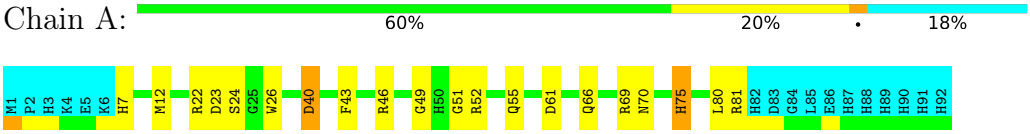
Chain A: 60% 14% • • 18%

M1 P2 H3 K4 E5 K6 A21 R22 D23 Y35 L36 N39 D40 D44 P45 R46 N47 W48 G49 R52 M56 D61 F62 L63 E67 S68 R69 R79 H82 D83 G84 L85 E86 H87 H88 H89 H90 H91 H92

4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein

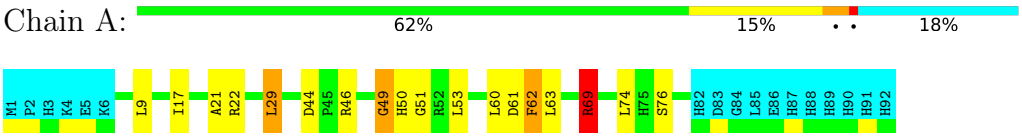
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein

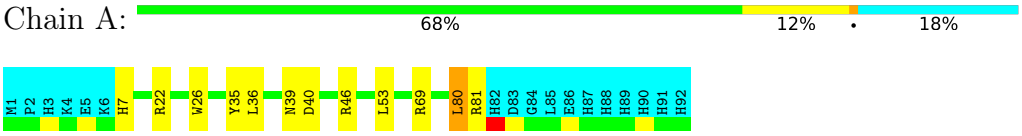
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein

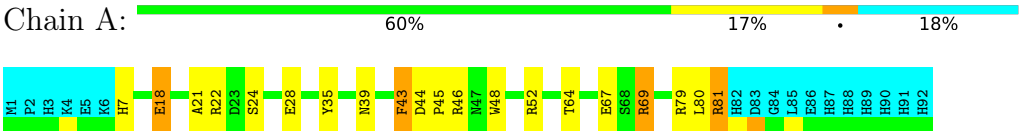
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein

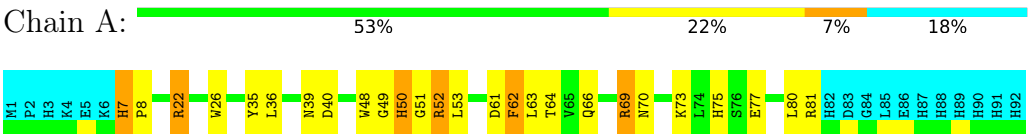
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein

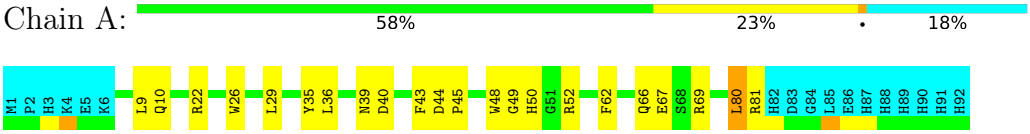
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein

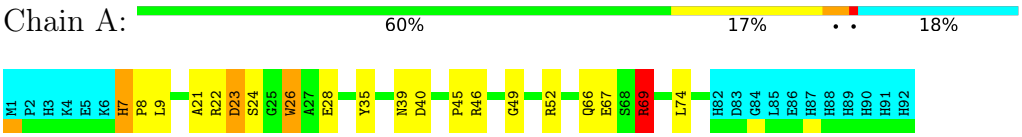
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein

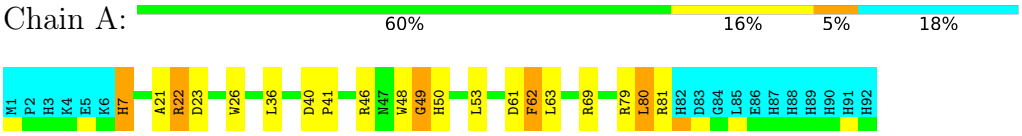
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein

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
X-PLOR NIH	structure solution	2.20
CNS	refinement	1.2
PSVS	refinement	1.4
PdbStat	structure solution	5.1
CYANA	structure solution	2.1

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	1100
Number of shifts mapped to atoms	1100
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality (i)

6.1 Standard geometry (i)

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	1.10±0.01	0±0/609 (0.0± 0.0%)	0.87±0.02	0±0/822 (0.0± 0.1%)
All	All	1.10	0/12180 (0.0%)	0.88	5/16440 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.3±1.2
All	All	0	46

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	69	ARG	NE-CZ-NH1	7.22	123.91	120.30	9	4
1	A	22	ARG	NE-CZ-NH1	5.30	122.95	120.30	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	69	ARG	Sidechain	16
1	A	22	ARG	Sidechain	12
1	A	46	ARG	Sidechain	7
1	A	52	ARG	Sidechain	6
1	A	79	ARG	Sidechain	4
1	A	81	ARG	Sidechain	1

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	595	582	582	13±5
All	All	11900	11640	11640	257

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLY:O	1:A:53:LEU:N	0.65	2.29	11	2
1:A:7:HIS:N	1:A:8:PRO:CD	0.57	2.67	4	5
1:A:35:TYR:CE2	1:A:39:ASN:ND2	0.57	2.73	9	10
1:A:22:ARG:CG	1:A:22:ARG:HH11	0.56	2.13	8	1
1:A:46:ARG:HH11	1:A:46:ARG:HG3	0.56	1.60	12	1
1:A:69:ARG:HH11	1:A:69:ARG:CG	0.56	2.12	9	5
1:A:35:TYR:CZ	1:A:39:ASN:ND2	0.56	2.74	5	8
1:A:26:TRP:H	1:A:79:ARG:NH2	0.56	1.99	7	1
1:A:47:ASN:O	1:A:52:ARG:NH2	0.56	2.39	12	1
1:A:69:ARG:NH1	1:A:69:ARG:HG3	0.55	2.16	16	1
1:A:70:ASN:ND2	1:A:75:HIS:CD2	0.55	2.75	13	2
1:A:70:ASN:ND2	1:A:75:HIS:NE2	0.55	2.54	7	1
1:A:26:TRP:CH2	1:A:66:GLN:NE2	0.55	2.75	13	6
1:A:22:ARG:O	1:A:24:SER:N	0.55	2.40	6	2
1:A:22:ARG:HH11	1:A:22:ARG:HG3	0.54	1.62	8	2
1:A:70:ASN:ND2	1:A:75:HIS:CE1	0.54	2.76	1	1
1:A:35:TYR:CE1	1:A:39:ASN:ND2	0.54	2.76	1	2
1:A:22:ARG:HG2	1:A:22:ARG:HH11	0.54	1.63	12	2
1:A:60:LEU:O	1:A:62:PHE:N	0.53	2.40	4	3
1:A:69:ARG:HG3	1:A:69:ARG:HH11	0.53	1.62	16	1
1:A:69:ARG:HH11	1:A:69:ARG:HG2	0.53	1.63	9	3
1:A:48:TRP:CD2	1:A:56:MET:SD	0.53	3.02	1	1
1:A:45:PRO:O	1:A:49:GLY:N	0.52	2.41	11	4
1:A:48:TRP:CE3	1:A:56:MET:SD	0.52	3.02	12	1
1:A:43:PHE:CG	1:A:44:ASP:N	0.52	2.78	16	1
1:A:69:ARG:N	1:A:69:ARG:HD3	0.52	2.20	12	1
1:A:48:TRP:CZ3	1:A:56:MET:SD	0.51	3.03	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ASP:O	1:A:63:LEU:N	0.51	2.43	17	5
1:A:44:ASP:O	1:A:48:TRP:CD1	0.51	2.64	16	1
1:A:29:LEU:HD23	1:A:76:SER:OG	0.51	2.04	14	1
1:A:7:HIS:H	1:A:7:HIS:CD2	0.51	2.24	20	1
1:A:46:ARG:N	1:A:46:ARG:CD	0.50	2.73	12	2
1:A:69:ARG:HG2	1:A:69:ARG:NH1	0.50	2.21	3	3
1:A:40:ASP:OD1	1:A:43:PHE:N	0.50	2.45	13	2
1:A:69:ARG:N	1:A:69:ARG:CD	0.50	2.75	14	1
1:A:67:GLU:OE1	1:A:67:GLU:N	0.50	2.45	19	4
1:A:18:GLU:OE1	1:A:18:GLU:N	0.49	2.46	16	1
1:A:26:TRP:CZ2	1:A:66:GLN:OE1	0.49	2.65	18	2
1:A:60:LEU:O	1:A:62:PHE:CD2	0.49	2.65	4	2
1:A:36:LEU:O	1:A:40:ASP:N	0.49	2.45	20	13
1:A:61:ASP:O	1:A:62:PHE:CG	0.49	2.66	12	2
1:A:61:ASP:O	1:A:62:PHE:CD1	0.49	2.66	17	2
1:A:69:ARG:NH1	1:A:69:ARG:HG2	0.49	2.23	17	4
1:A:35:TYR:CD1	1:A:39:ASN:ND2	0.48	2.81	1	1
1:A:77:GLU:N	1:A:77:GLU:OE1	0.48	2.46	10	3
1:A:17:ILE:O	1:A:21:ALA:N	0.48	2.45	14	6
1:A:23:ASP:OD1	1:A:24:SER:N	0.48	2.46	5	1
1:A:7:HIS:NE2	1:A:12:MET:SD	0.48	2.82	13	1
1:A:21:ALA:O	1:A:23:ASP:N	0.48	2.47	12	4
1:A:64:THR:OG1	1:A:81:ARG:NE	0.47	2.47	2	2
1:A:20:VAL:C	1:A:22:ARG:H	0.47	2.12	10	1
1:A:22:ARG:HG3	1:A:22:ARG:NH1	0.47	2.25	17	1
1:A:49:GLY:O	1:A:51:GLY:N	0.47	2.47	14	2
1:A:22:ARG:HH11	1:A:22:ARG:CG	0.47	2.21	17	1
1:A:80:LEU:O	1:A:81:ARG:CB	0.47	2.63	17	1
1:A:75:HIS:CG	1:A:77:GLU:OE2	0.47	2.68	17	1
1:A:9:LEU:HD12	1:A:9:LEU:N	0.47	2.25	3	6
1:A:50:HIS:O	1:A:50:HIS:ND1	0.47	2.47	7	1
1:A:35:TYR:CE2	1:A:39:ASN:OD1	0.47	2.68	6	2
1:A:23:ASP:O	1:A:25:GLY:N	0.47	2.48	11	1
1:A:40:ASP:OD2	1:A:43:PHE:N	0.47	2.48	13	1
1:A:69:ARG:CG	1:A:69:ARG:NH1	0.46	2.78	5	3
1:A:67:GLU:N	1:A:67:GLU:OE1	0.46	2.48	1	2
1:A:10:GLN:NE2	1:A:14:THR:OG1	0.46	2.49	11	1
1:A:61:ASP:OD1	1:A:62:PHE:N	0.46	2.49	3	4
1:A:80:LEU:HD13	1:A:81:ARG:N	0.46	2.24	15	3
1:A:22:ARG:O	1:A:23:ASP:O	0.46	2.34	2	1
1:A:50:HIS:O	1:A:52:ARG:N	0.46	2.47	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:PHE:CZ	1:A:48:TRP:NE1	0.46	2.84	18	1
1:A:35:TYR:O	1:A:39:ASN:ND2	0.46	2.49	8	2
1:A:22:ARG:NH1	1:A:23:ASP:OD1	0.46	2.49	12	1
1:A:35:TYR:CE1	1:A:39:ASN:OD1	0.46	2.69	15	1
1:A:61:ASP:O	1:A:62:PHE:CD2	0.45	2.69	12	1
1:A:37:ALA:O	1:A:41:PRO:N	0.45	2.49	9	1
1:A:46:ARG:HH11	1:A:46:ARG:CG	0.45	2.25	12	1
1:A:22:ARG:CG	1:A:22:ARG:NH1	0.45	2.80	8	1
1:A:9:LEU:HD22	1:A:9:LEU:N	0.45	2.27	9	1
1:A:60:LEU:O	1:A:62:PHE:CD1	0.44	2.70	11	1
1:A:47:ASN:OD1	1:A:48:TRP:CD1	0.44	2.70	12	1
1:A:53:LEU:HD12	1:A:53:LEU:N	0.44	2.27	20	3
1:A:70:ASN:OD1	1:A:75:HIS:N	0.44	2.50	17	1
1:A:67:GLU:CD	1:A:67:GLU:N	0.44	2.70	16	3
1:A:73:LYS:O	1:A:75:HIS:ND1	0.44	2.50	10	1
1:A:46:ARG:O	1:A:48:TRP:N	0.44	2.51	16	1
1:A:26:TRP:N	1:A:26:TRP:CD1	0.44	2.86	18	1
1:A:69:ARG:HG2	1:A:69:ARG:HH11	0.44	1.71	10	2
1:A:44:ASP:O	1:A:47:ASN:ND2	0.44	2.51	12	1
1:A:61:ASP:C	1:A:62:PHE:CD1	0.44	2.91	20	1
1:A:28:GLU:OE1	1:A:28:GLU:N	0.44	2.49	5	2
1:A:74:LEU:O	1:A:74:LEU:HD12	0.44	2.13	6	1
1:A:9:LEU:N	1:A:9:LEU:CD2	0.44	2.80	9	1
1:A:35:TYR:CD2	1:A:39:ASN:ND2	0.43	2.86	1	1
1:A:46:ARG:HD3	1:A:46:ARG:N	0.43	2.28	2	1
1:A:69:ARG:NH1	1:A:69:ARG:CG	0.43	2.81	17	2
1:A:20:VAL:O	1:A:22:ARG:N	0.43	2.51	10	1
1:A:21:ALA:O	1:A:22:ARG:O	0.43	2.36	10	1
1:A:24:SER:O	1:A:26:TRP:N	0.43	2.51	1	2
1:A:51:GLY:C	1:A:53:LEU:H	0.43	2.17	17	1
1:A:55:GLN:N	1:A:55:GLN:CD	0.43	2.72	10	3
1:A:46:ARG:HD3	1:A:46:ARG:H	0.43	1.73	2	1
1:A:61:ASP:C	1:A:63:LEU:H	0.43	2.17	4	3
1:A:61:ASP:OD1	1:A:61:ASP:N	0.43	2.51	8	2
1:A:24:SER:OG	1:A:25:GLY:N	0.43	2.49	11	1
1:A:21:ALA:C	1:A:23:ASP:H	0.43	2.17	5	1
1:A:43:PHE:CD2	1:A:44:ASP:N	0.43	2.86	16	1
1:A:35:TYR:CG	1:A:39:ASN:ND2	0.42	2.87	1	1
1:A:9:LEU:N	1:A:9:LEU:CD1	0.42	2.82	19	2
1:A:61:ASP:N	1:A:61:ASP:OD1	0.42	2.51	5	1
1:A:51:GLY:O	1:A:55:GLN:NE2	0.42	2.52	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ASP:OD1	1:A:44:ASP:N	0.42	2.52	10	1
1:A:21:ALA:HB1	1:A:24:SER:O	0.42	2.15	16	1
1:A:53:LEU:N	1:A:53:LEU:CD1	0.42	2.82	14	2
1:A:46:ARG:C	1:A:48:TRP:N	0.42	2.71	16	1
1:A:26:TRP:CH2	1:A:66:GLN:CD	0.42	2.93	5	2
1:A:61:ASP:C	1:A:62:PHE:CD2	0.42	2.92	12	1
1:A:41:PRO:O	1:A:42:SER:CB	0.41	2.68	7	1
1:A:68:SER:HG	1:A:77:GLU:CD	0.41	2.17	4	1
1:A:49:GLY:O	1:A:50:HIS:O	0.41	2.39	17	1
1:A:26:TRP:CH2	1:A:66:GLN:OE1	0.41	2.74	6	1
1:A:44:ASP:O	1:A:48:TRP:NE1	0.41	2.53	16	1
1:A:69:ARG:CG	1:A:69:ARG:HH11	0.41	2.27	17	1
1:A:61:ASP:C	1:A:63:LEU:N	0.41	2.74	12	3
1:A:25:GLY:O	1:A:26:TRP:O	0.41	2.38	7	1
1:A:48:TRP:O	1:A:49:GLY:O	0.41	2.39	20	1
1:A:67:GLU:N	1:A:67:GLU:CD	0.41	2.74	11	2
1:A:50:HIS:C	1:A:52:ARG:H	0.41	2.18	3	2
1:A:51:GLY:C	1:A:53:LEU:N	0.41	2.73	14	1
1:A:49:GLY:C	1:A:51:GLY:N	0.41	2.74	7	1
1:A:49:GLY:C	1:A:51:GLY:H	0.41	2.20	7	1
1:A:46:ARG:N	1:A:46:ARG:HD2	0.41	2.31	12	1
1:A:22:ARG:NH1	1:A:22:ARG:CG	0.41	2.83	17	1
1:A:21:ALA:C	1:A:23:ASP:N	0.41	2.71	20	1
1:A:28:GLU:N	1:A:28:GLU:CD	0.40	2.75	16	1
1:A:64:THR:N	1:A:81:ARG:O	0.40	2.54	17	1
1:A:68:SER:O	1:A:70:ASN:N	0.40	2.55	10	1
1:A:48:TRP:CD1	1:A:48:TRP:N	0.40	2.89	17	1
1:A:70:ASN:OD1	1:A:73:LYS:O	0.40	2.40	17	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	75/92 (82%)	65±3 (87±4%)	7±3 (9±4%)	3±2 (5±2%)	4 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1500/1840 (82%)	1301 (87%)	131 (9%)	68 (5%)	4 28

All 19 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	62	PHE	10
1	A	22	ARG	9
1	A	26	TRP	8
1	A	23	ASP	7
1	A	24	SER	6
1	A	49	GLY	6
1	A	50	HIS	4
1	A	61	ASP	3
1	A	25	GLY	2
1	A	43	PHE	2
1	A	52	ARG	2
1	A	44	ASP	2
1	A	7	HIS	1
1	A	42	SER	1
1	A	21	ALA	1
1	A	69	ARG	1
1	A	81	ARG	1
1	A	45	PRO	1
1	A	41	PRO	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	64/80 (80%)	61±1 (96±2%)	3±1 (4±2%)	34 82
All	All	1280/1600 (80%)	1227 (96%)	53 (4%)	34 82

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	69	ARG	12
1	A	80	LEU	11
1	A	7	HIS	10
1	A	40	ASP	4
1	A	63	LEU	3
1	A	74	LEU	3
1	A	56	MET	2
1	A	29	LEU	2
1	A	42	SER	1
1	A	46	ARG	1
1	A	75	HIS	1
1	A	18	GLU	1
1	A	22	ARG	1
1	A	52	ARG	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 91% 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	1100
Number of shifts mapped to atoms	1100
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	91	-0.32 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	85	0.14 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	85	-0.05 ± 0.09	None needed (< 0.5 ppm)
^{15}N	86	-0.40 ± 0.45	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 91%, i.e. 932 atoms were assigned a chemical shift out of a possible 1024. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	370/374 (99%)	152/152 (100%)	146/150 (97%)	72/72 (100%)
Sidechain	503/566 (89%)	341/366 (93%)	150/172 (87%)	12/28 (43%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	59/84 (70%)	30/43 (70%)	27/36 (75%)	2/5 (40%)
Overall	932/1024 (91%)	523/561 (93%)	323/358 (90%)	86/105 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1096 atoms were assigned a chemical shift out of a possible 1264. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	445/458 (97%)	183/186 (98%)	176/184 (96%)	86/88 (98%)
Sidechain	592/666 (89%)	401/430 (93%)	179/206 (87%)	12/30 (40%)
Aromatic	59/140 (42%)	30/75 (40%)	27/52 (52%)	2/13 (15%)
Overall	1096/1264 (87%)	614/691 (89%)	382/442 (86%)	100/131 (76%)

7.1.4 Statistically unusual chemical shifts (i)

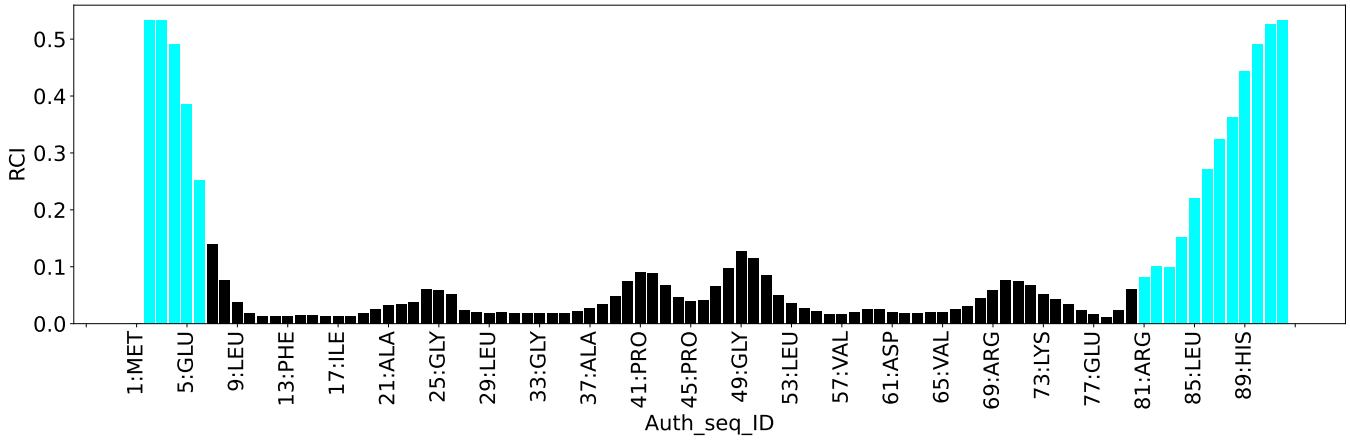
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	64	THR	HG1	6.89	0.08 – 2.19	27.3
1	A	79	ARG	HD3	0.93	1.81 – 4.39	-8.4
1	A	79	ARG	HD2	1.85	1.97 – 4.26	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
1:MET
5:GLU
9:LEU
13:PHE
17:ILE
21:ALA
25:GLY
29:LEU
33:GLY
37:ALA
41:PRO
45:PRO
49:GLY
53:LEU
57:VAL
61:ASP
65:VAL
69:ARG
73:LYS
77:GLU
81:ARG
85:LEU
89:HIS
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	921
Intra-residue (|i-j|=0)	207
Sequential (|i-j|=1)	238
Medium range (|i-j|>1 and |i-j|<5)	85
Long range (|i-j|≥5)	333
Inter-chain	0
Hydrogen bond restraints	58
Disulfide bond restraints	0
Total dihedral-angle restraints	104
Number of unmapped restraints	0
Number of restraints per residue	11.1
Number of long range restraints per residue[1]	3.8

[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)	4.2	0.2
0.2-0.5 (Medium)	1.9	0.47
>0.5 (Large)	0.1	0.75

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)	0.8	3.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

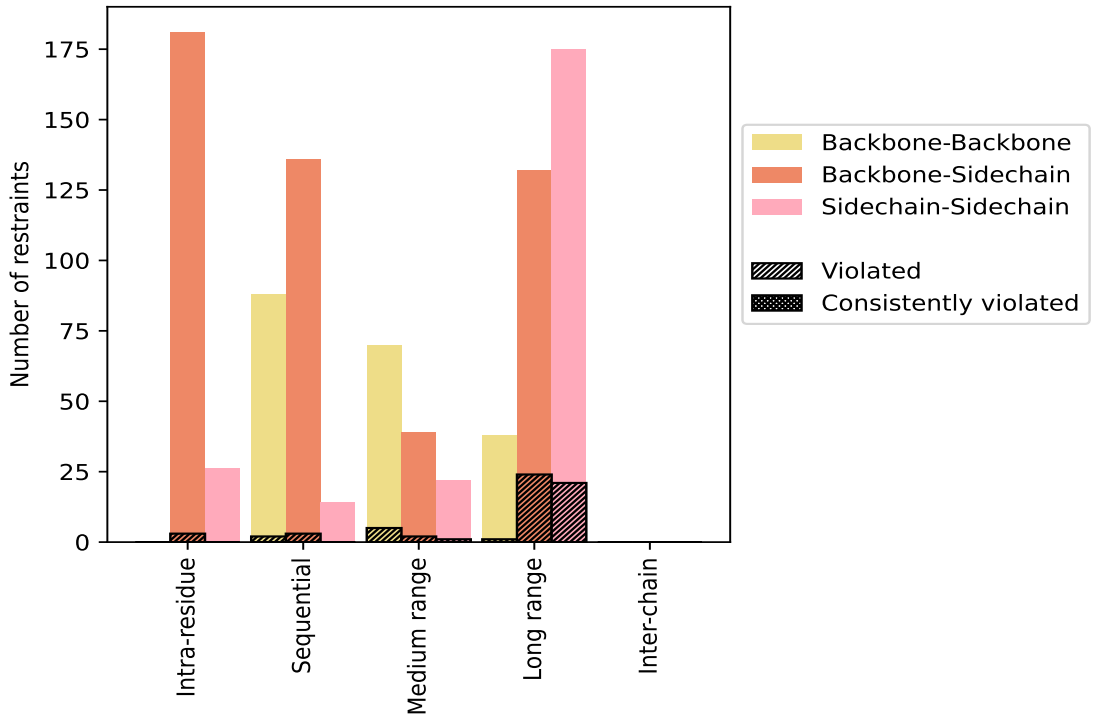
9.1 Summary of distance violations (i)

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)	207	22.5	3	1.4	0.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	181	19.7	3	1.7	0.3	0	0.0	0.0
Sidechain-Sidechain	26	2.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	238	25.8	5	2.1	0.5	0	0.0	0.0
Backbone-Backbone	88	9.6	2	2.3	0.2	0	0.0	0.0
Backbone-Sidechain	136	14.8	3	2.2	0.3	0	0.0	0.0
Sidechain-Sidechain	14	1.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	85	9.2	3	3.5	0.3	0	0.0	0.0
Backbone-Backbone	24	2.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	39	4.2	2	5.1	0.2	0	0.0	0.0
Sidechain-Sidechain	22	2.4	1	4.5	0.1	0	0.0	0.0
Long range (|i-j|≥5)	333	36.2	45	13.5	4.9	0	0.0	0.0
Backbone-Backbone	26	2.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	132	14.3	24	18.2	2.6	0	0.0	0.0
Sidechain-Sidechain	175	19.0	21	12.0	2.3	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	58	6.3	6	10.3	0.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	921	100.0	62	6.7	6.7	0	0.0	0.0
Backbone-Backbone	196	21.3	8	4.1	0.9	0	0.0	0.0
Backbone-Sidechain	488	53.0	32	6.6	3.5	0	0.0	0.0
Sidechain-Sidechain	237	25.7	22	9.3	2.4	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	1	1	2	0	4	0.22	0.42	0.12	0.17
2	1	0	1	5	0	7	0.27	0.54	0.16	0.22
3	0	0	2	6	0	8	0.17	0.34	0.08	0.13
4	1	0	2	3	0	6	0.24	0.72	0.22	0.14
5	0	1	1	4	0	6	0.15	0.22	0.04	0.14
6	0	0	0	5	0	5	0.22	0.38	0.09	0.21
7	0	1	0	4	0	5	0.15	0.25	0.05	0.13
8	0	1	0	3	0	4	0.23	0.32	0.08	0.22
9	0	1	1	0	0	2	0.15	0.18	0.03	0.15
10	0	0	1	5	0	6	0.3	0.75	0.23	0.18
11	0	0	3	3	0	6	0.17	0.28	0.06	0.15

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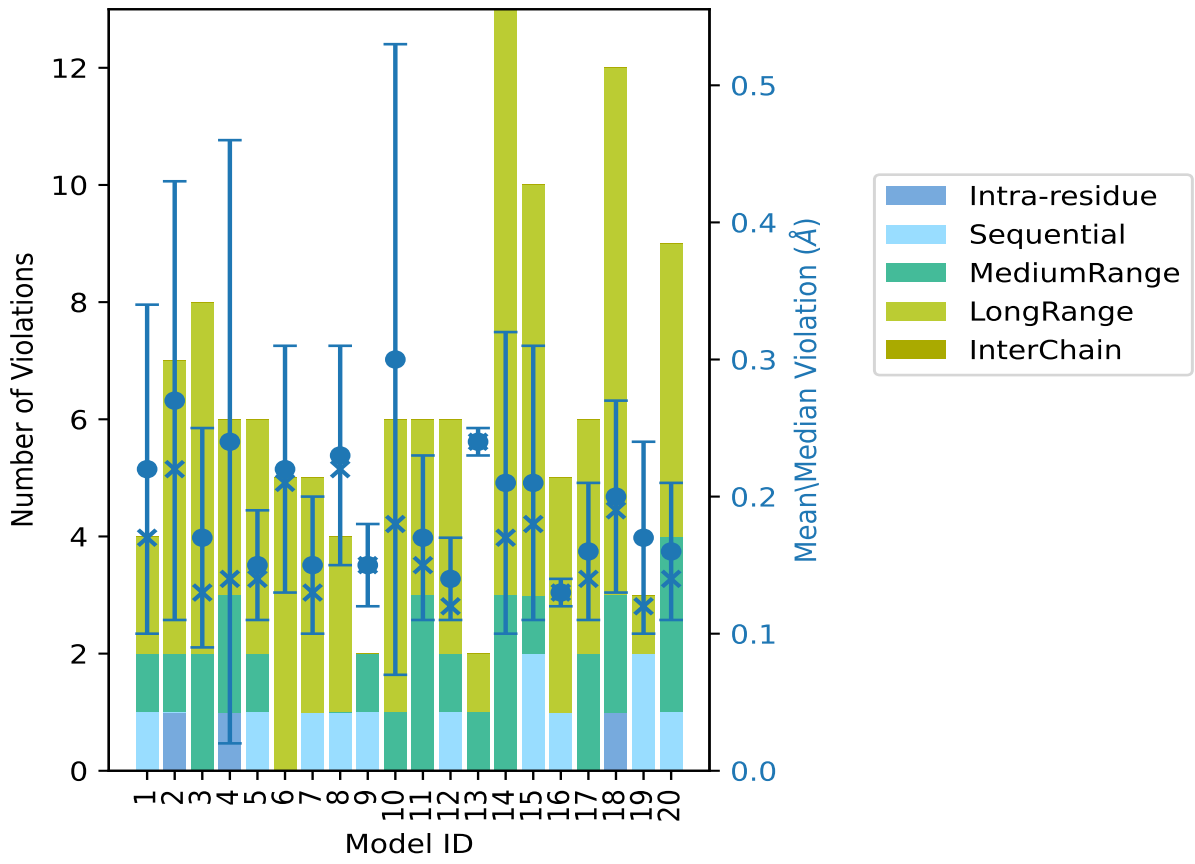
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	1	1	4	0	6	0.14	0.21	0.03	0.12
13	0	0	1	1	0	2	0.24	0.25	0.01	0.24
14	0	0	3	10	0	13	0.21	0.47	0.11	0.17
15	0	2	1	7	0	10	0.21	0.41	0.1	0.18
16	0	1	0	4	0	5	0.13	0.15	0.01	0.13
17	0	0	2	4	0	6	0.16	0.26	0.05	0.14
18	1	0	2	9	0	12	0.2	0.35	0.07	0.19
19	0	2	0	1	0	3	0.17	0.27	0.07	0.12
20	0	1	3	5	0	9	0.16	0.26	0.05	0.14

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

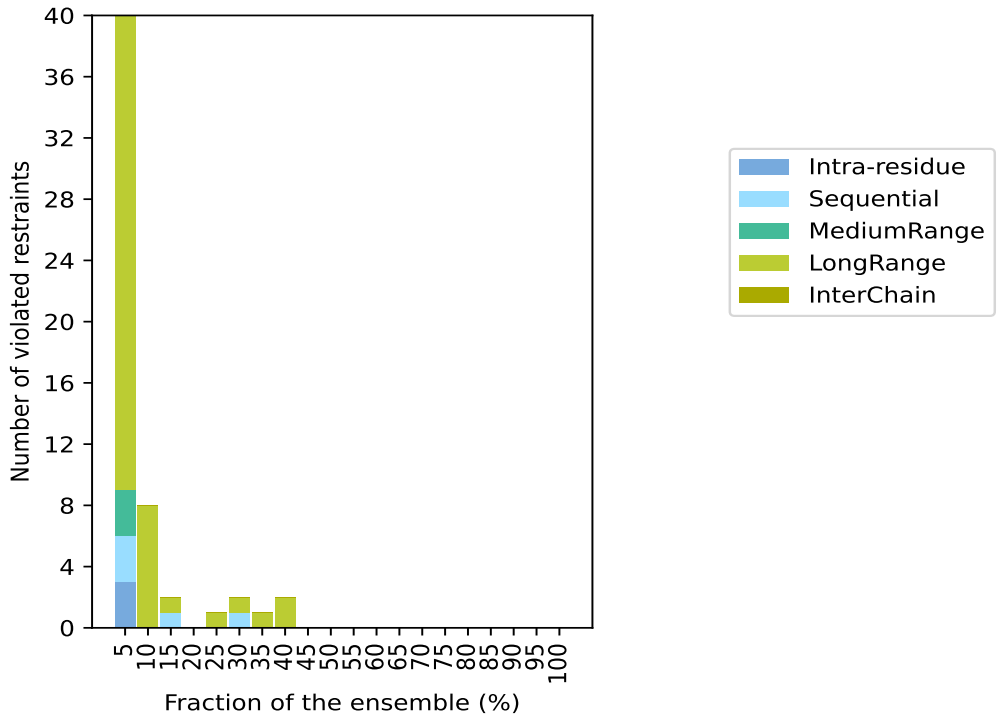
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 807(IR:204, SQ:233, MR:82, LR:288, 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]	%
3	3	3	31	0	40	1	5.0
0	0	0	8	0	8	2	10.0
0	1	0	1	0	2	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	1	0	1	5	25.0
0	1	0	1	0	2	6	30.0
0	0	0	1	0	1	7	35.0
0	0	0	2	0	2	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	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

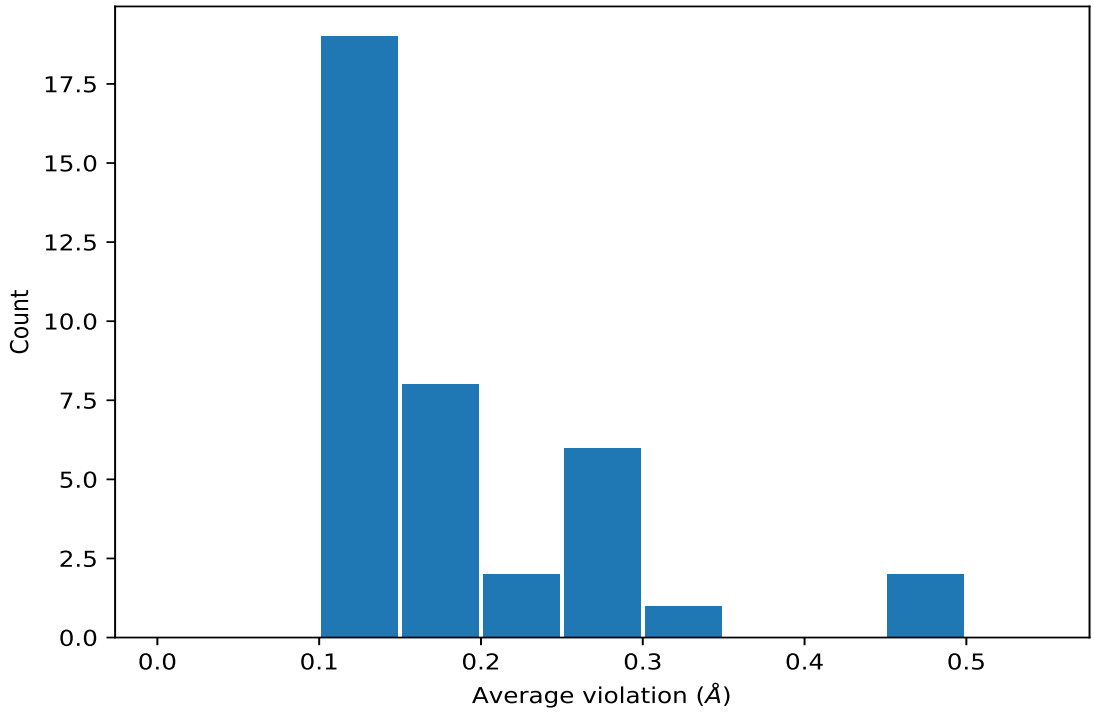
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	10	0.16	0.05	0.15
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	8	0.33	0.16	0.37
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	8	0.26	0.1	0.26
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	8	0.26	0.1	0.26
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	8	0.26	0.1	0.26
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	7	0.49	0.16	0.41
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	7	0.49	0.16	0.41
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	7	0.15	0.05	0.13
(1,756)	1:A:67:GLU:HG3	1:A:76:SER:HA	6	0.22	0.04	0.24
(1,861)	1:A:91:HIS:HA	1:A:92:HIS:H	6	0.12	0.0	0.12
(1,247)	1:A:21:ALA:HA	1:A:27:ALA:HB1	5	0.23	0.04	0.24
(1,679)	1:A:63:LEU:HB2	1:A:78:ILE:HB	3	0.18	0.04	0.21
(2,39)	1:A:54:SER:H	1:A:51:GLY:O	3	0.13	0.01	0.13
(1,855)	1:A:87:HIS:HB2	1:A:88:HIS:H	3	0.12	0.01	0.12
(1,855)	1:A:87:HIS:HB3	1:A:88:HIS:H	3	0.12	0.01	0.12
(1,361)	1:A:29:LEU:HD11	1:A:78:ILE:H	2	0.26	0.02	0.26

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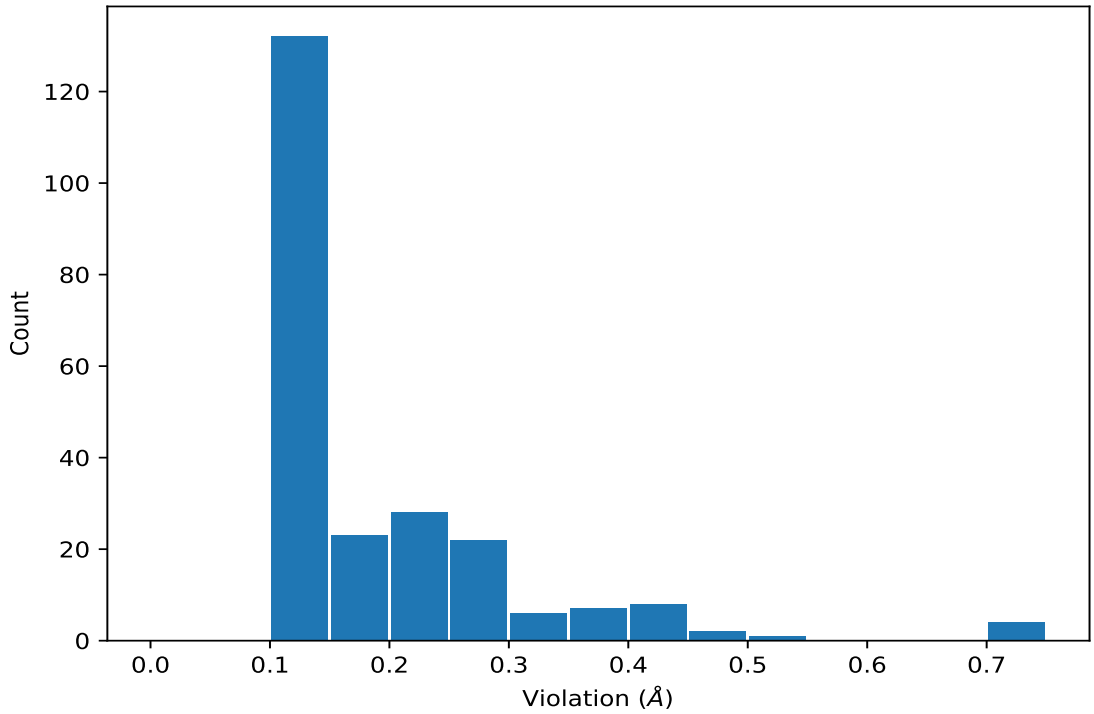
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,361)	1:A:29:LEU:HD12	1:A:78:ILE:H	2	0.26	0.02	0.26
(1,361)	1:A:29:LEU:HD13	1:A:78:ILE:H	2	0.26	0.02	0.26
(1,695)	1:A:63:LEU:H	1:A:81:ARG:HD2	2	0.16	0.04	0.16
(1,695)	1:A:63:LEU:H	1:A:81:ARG:HD3	2	0.16	0.04	0.16
(1,671)	1:A:63:LEU:HA	1:A:81:ARG:HB2	2	0.16	0.01	0.16
(1,232)	1:A:20:VAL:HG21	1:A:27:ALA:HB1	2	0.16	0.05	0.16
(1,232)	1:A:20:VAL:HG22	1:A:27:ALA:HB1	2	0.16	0.05	0.16
(1,232)	1:A:20:VAL:HG23	1:A:27:ALA:HB1	2	0.16	0.05	0.16
(1,358)	1:A:29:LEU:HD11	1:A:77:GLU:HA	2	0.15	0.03	0.15
(1,358)	1:A:29:LEU:HD12	1:A:77:GLU:HA	2	0.15	0.03	0.15
(1,358)	1:A:29:LEU:HD13	1:A:77:GLU:HA	2	0.15	0.03	0.15
(1,746)	1:A:67:GLU:HB2	1:A:74:LEU:HB2	2	0.15	0.0	0.15
(1,746)	1:A:67:GLU:HB3	1:A:74:LEU:HB2	2	0.15	0.0	0.15
(1,357)	1:A:29:LEU:HD11	1:A:76:SER:HB2	2	0.12	0.0	0.12
(1,357)	1:A:29:LEU:HD12	1:A:76:SER:HB2	2	0.12	0.0	0.12
(1,357)	1:A:29:LEU:HD13	1:A:76:SER:HB2	2	0.12	0.0	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD11	2	0.12	0.0	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD12	2	0.12	0.0	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD13	2	0.12	0.0	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD21	2	0.12	0.0	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD22	2	0.12	0.0	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD23	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	10	0.75
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	10	0.75
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	4	0.72
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	4	0.72
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	2	0.54
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	10	0.47
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	14	0.47
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	1	0.42
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	14	0.41
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	14	0.41
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	15	0.41
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	15	0.41
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	2	0.4
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	2	0.4
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	2	0.4
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	2	0.38
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	6	0.38
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	6	0.38
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	15	0.36
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	15	0.36
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	15	0.36
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD1	18	0.35
(1,84)	1:A:12:MET:HE1	1:A:43:PHE:HD2	18	0.35
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	3	0.34
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	3	0.34
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	3	0.34
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	8	0.32
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	8	0.29
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	8	0.29
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	8	0.29
(1,361)	1:A:29:LEU:HD11	1:A:78:ILE:H	18	0.28
(1,361)	1:A:29:LEU:HD12	1:A:78:ILE:H	18	0.28
(1,361)	1:A:29:LEU:HD13	1:A:78:ILE:H	18	0.28
(1,247)	1:A:21:ALA:HA	1:A:27:ALA:HB1	11	0.28
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	18	0.27
(1,247)	1:A:21:ALA:HA	1:A:27:ALA:HB1	19	0.27
(1,756)	1:A:67:GLU:HG3	1:A:76:SER:HA	3	0.26
(1,756)	1:A:67:GLU:HG3	1:A:76:SER:HA	14	0.26
(1,756)	1:A:67:GLU:HG3	1:A:76:SER:HA	20	0.26
(1,694)	1:A:63:LEU:H	1:A:81:ARG:HB2	17	0.26
(1,694)	1:A:63:LEU:H	1:A:81:ARG:HB3	17	0.26
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	13	0.25
(1,840)	1:A:85:LEU:HA	1:A:85:LEU:HD21	18	0.25
(1,840)	1:A:85:LEU:HA	1:A:85:LEU:HD22	18	0.25
(1,840)	1:A:85:LEU:HA	1:A:85:LEU:HD23	18	0.25
(1,361)	1:A:29:LEU:HD11	1:A:78:ILE:H	14	0.25
(1,361)	1:A:29:LEU:HD12	1:A:78:ILE:H	14	0.25
(1,361)	1:A:29:LEU:HD13	1:A:78:ILE:H	14	0.25
(1,282)	1:A:26:TRP:HE1	1:A:79:ARG:HD3	7	0.25
(1,554)	1:A:48:TRP:HE3	1:A:53:LEU:HA	6	0.24
(1,247)	1:A:21:ALA:HA	1:A:27:ALA:HB1	13	0.24
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	20	0.24
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	20	0.24
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	20	0.24
(1,326)	1:A:28:GLU:HB3	1:A:31:ALA:H	14	0.23
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	2	0.22
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:A:63:LEU:HB2	1:A:78:ILE:HB	5	0.22
(1,756)	1:A:67:GLU:HG3	1:A:76:SER:HA	10	0.21
(1,756)	1:A:67:GLU:HG3	1:A:76:SER:HA	15	0.21
(1,679)	1:A:63:LEU:HB2	1:A:78:ILE:HB	6	0.21
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	12	0.21
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	12	0.21
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	12	0.21
(1,156)	1:A:16:ALA:HB1	1:A:32:VAL:HG11	18	0.21
(1,156)	1:A:16:ALA:HB1	1:A:32:VAL:HG12	18	0.21
(1,156)	1:A:16:ALA:HB1	1:A:32:VAL:HG13	18	0.21
(1,695)	1:A:63:LEU:H	1:A:81:ARG:HD2	17	0.2
(1,695)	1:A:63:LEU:H	1:A:81:ARG:HD3	17	0.2
(1,655)	1:A:62:PHE:HA	1:A:81:ARG:HB2	15	0.2
(1,619)	1:A:58:LYS:HA	1:A:65:VAL:HG11	15	0.2
(1,619)	1:A:58:LYS:HA	1:A:65:VAL:HG12	15	0.2
(1,619)	1:A:58:LYS:HA	1:A:65:VAL:HG13	15	0.2
(1,247)	1:A:21:ALA:HA	1:A:27:ALA:HB1	18	0.2
(1,232)	1:A:20:VAL:HG21	1:A:27:ALA:HB1	14	0.2
(1,232)	1:A:20:VAL:HG22	1:A:27:ALA:HB1	14	0.2
(1,232)	1:A:20:VAL:HG23	1:A:27:ALA:HB1	14	0.2
(1,744)	1:A:67:GLU:HB2	1:A:74:LEU:HA	5	0.19
(1,744)	1:A:67:GLU:HB3	1:A:74:LEU:HA	5	0.19
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	9	0.18
(1,687)	1:A:63:LEU:HD21	1:A:80:LEU:H	11	0.18
(1,687)	1:A:63:LEU:HD22	1:A:80:LEU:H	11	0.18
(1,687)	1:A:63:LEU:HD23	1:A:80:LEU:H	11	0.18
(1,358)	1:A:29:LEU:HD11	1:A:77:GLU:HA	18	0.18
(1,358)	1:A:29:LEU:HD12	1:A:77:GLU:HA	18	0.18
(1,358)	1:A:29:LEU:HD13	1:A:77:GLU:HA	18	0.18
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	1	0.17
(1,671)	1:A:63:LEU:HA	1:A:81:ARG:HB2	14	0.17
(1,367)	1:A:29:LEU:HD21	1:A:57:VAL:H	15	0.17
(1,367)	1:A:29:LEU:HD22	1:A:57:VAL:H	15	0.17
(1,367)	1:A:29:LEU:HD23	1:A:57:VAL:H	15	0.17
(1,356)	1:A:29:LEU:HD11	1:A:76:SER:HB3	15	0.17
(1,356)	1:A:29:LEU:HD12	1:A:76:SER:HB3	15	0.17
(1,356)	1:A:29:LEU:HD13	1:A:76:SER:HB3	15	0.17
(1,247)	1:A:21:ALA:HA	1:A:27:ALA:HB1	1	0.17
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	11	0.16
(2,17)	1:A:20:VAL:H	1:A:16:ALA:O	14	0.16
(1,849)	1:A:86:GLU:HB2	1:A:87:HIS:HA	8	0.16
(1,849)	1:A:86:GLU:HB3	1:A:87:HIS:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	20	0.16
(1,756)	1:A:67:GLU:HG3	1:A:76:SER:HA	16	0.15
(1,746)	1:A:67:GLU:HB2	1:A:74:LEU:HB2	5	0.15
(1,746)	1:A:67:GLU:HB3	1:A:74:LEU:HB2	5	0.15
(1,746)	1:A:67:GLU:HB2	1:A:74:LEU:HB2	10	0.15
(1,746)	1:A:67:GLU:HB3	1:A:74:LEU:HB2	10	0.15
(1,745)	1:A:67:GLU:HB2	1:A:74:LEU:HB3	12	0.15
(1,745)	1:A:67:GLU:HB3	1:A:74:LEU:HB3	12	0.15
(1,724)	1:A:65:VAL:HG21	1:A:76:SER:HB2	20	0.15
(1,724)	1:A:65:VAL:HG21	1:A:76:SER:HB3	20	0.15
(1,724)	1:A:65:VAL:HG22	1:A:76:SER:HB2	20	0.15
(1,724)	1:A:65:VAL:HG22	1:A:76:SER:HB3	20	0.15
(1,724)	1:A:65:VAL:HG23	1:A:76:SER:HB2	20	0.15
(1,724)	1:A:65:VAL:HG23	1:A:76:SER:HB3	20	0.15
(1,682)	1:A:63:LEU:HD11	1:A:78:ILE:HB	16	0.15
(1,682)	1:A:63:LEU:HD12	1:A:78:ILE:HB	16	0.15
(1,682)	1:A:63:LEU:HD13	1:A:78:ILE:HB	16	0.15
(1,671)	1:A:63:LEU:HA	1:A:81:ARG:HB2	4	0.15
(1,185)	1:A:17:ILE:HG21	1:A:27:ALA:HB1	8	0.15
(1,185)	1:A:17:ILE:HG22	1:A:27:ALA:HB1	8	0.15
(1,185)	1:A:17:ILE:HG23	1:A:27:ALA:HB1	8	0.15
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	20	0.14
(2,49)	1:A:68:SER:H	1:A:75:HIS:O	17	0.14
(2,39)	1:A:54:SER:H	1:A:51:GLY:O	3	0.14
(1,855)	1:A:87:HIS:HB2	1:A:88:HIS:H	20	0.14
(1,855)	1:A:87:HIS:HB3	1:A:88:HIS:H	20	0.14
(1,759)	1:A:67:GLU:HG2	1:A:76:SER:HA	18	0.14
(1,757)	1:A:67:GLU:HG2	1:A:74:LEU:HD11	14	0.14
(1,757)	1:A:67:GLU:HG2	1:A:74:LEU:HD12	14	0.14
(1,757)	1:A:67:GLU:HG2	1:A:74:LEU:HD13	14	0.14
(1,412)	1:A:33:GLY:HA3	1:A:53:LEU:HD11	11	0.14
(1,412)	1:A:33:GLY:HA3	1:A:53:LEU:HD12	11	0.14
(1,412)	1:A:33:GLY:HA3	1:A:53:LEU:HD13	11	0.14
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	4	0.13
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	17	0.13
(2,39)	1:A:54:SER:H	1:A:51:GLY:O	11	0.13
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	12	0.13
(1,767)	1:A:68:SER:HB2	1:A:75:HIS:HB2	18	0.13
(1,767)	1:A:68:SER:HB3	1:A:75:HIS:HB2	18	0.13
(1,695)	1:A:63:LEU:H	1:A:81:ARG:HD2	10	0.13
(1,695)	1:A:63:LEU:H	1:A:81:ARG:HD3	10	0.13
(1,670)	1:A:63:LEU:HA	1:A:81:ARG:HB3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:A:43:PHE:HD1	1:A:48:TRP:HE1	16	0.13
(1,510)	1:A:43:PHE:HD2	1:A:48:TRP:HE1	16	0.13
(1,251)	1:A:21:ALA:HB1	1:A:26:TRP:H	20	0.13
(1,251)	1:A:21:ALA:HB2	1:A:26:TRP:H	20	0.13
(1,251)	1:A:21:ALA:HB3	1:A:26:TRP:H	20	0.13
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	6	0.13
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	6	0.13
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	6	0.13
(1,223)	1:A:20:VAL:HG11	1:A:31:ALA:HB1	7	0.13
(1,223)	1:A:20:VAL:HG12	1:A:31:ALA:HB1	7	0.13
(1,223)	1:A:20:VAL:HG13	1:A:31:ALA:HB1	7	0.13
(1,220)	1:A:20:VAL:HB	1:A:31:ALA:HB1	3	0.13
(1,167)	1:A:17:ILE:HA	1:A:27:ALA:HB1	18	0.13
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	7	0.13
(1,137)	1:A:15:SER:HB3	1:A:35:TYR:HE1	3	0.13
(1,137)	1:A:15:SER:HB3	1:A:35:TYR:HE2	3	0.13
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	5	0.12
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	17	0.12
(1,861)	1:A:91:HIS:HA	1:A:92:HIS:H	5	0.12
(1,861)	1:A:91:HIS:HA	1:A:92:HIS:H	12	0.12
(1,861)	1:A:91:HIS:HA	1:A:92:HIS:H	15	0.12
(1,861)	1:A:91:HIS:HA	1:A:92:HIS:H	16	0.12
(1,861)	1:A:91:HIS:HA	1:A:92:HIS:H	19	0.12
(1,855)	1:A:87:HIS:HB2	1:A:88:HIS:H	19	0.12
(1,855)	1:A:87:HIS:HB3	1:A:88:HIS:H	19	0.12
(1,770)	1:A:68:SER:H	1:A:74:LEU:HB2	12	0.12
(1,770)	1:A:68:SER:H	1:A:74:LEU:HB3	12	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD11	3	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD12	3	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD13	3	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD21	3	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD22	3	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD23	3	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD11	5	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD12	5	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD13	5	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD21	5	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD22	5	0.12
(1,762)	1:A:67:GLU:H	1:A:74:LEU:HD23	5	0.12
(1,740)	1:A:67:GLU:HA	1:A:74:LEU:HD11	3	0.12
(1,740)	1:A:67:GLU:HA	1:A:74:LEU:HD12	3	0.12
(1,740)	1:A:67:GLU:HA	1:A:74:LEU:HD13	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:A:67:GLU:HA	1:A:74:LEU:HD21	3	0.12
(1,740)	1:A:67:GLU:HA	1:A:74:LEU:HD22	3	0.12
(1,740)	1:A:67:GLU:HA	1:A:74:LEU:HD23	3	0.12
(1,679)	1:A:63:LEU:HB2	1:A:78:ILE:HB	12	0.12
(1,561)	1:A:51:GLY:H	1:A:52:ARG:H	9	0.12
(1,556)	1:A:48:TRP:HZ3	1:A:56:MET:HB2	6	0.12
(1,556)	1:A:48:TRP:HZ3	1:A:56:MET:HB3	6	0.12
(1,542)	1:A:46:ARG:H	1:A:46:ARG:HD2	2	0.12
(1,542)	1:A:46:ARG:H	1:A:46:ARG:HD3	2	0.12
(1,417)	1:A:33:GLY:H	1:A:53:LEU:HD21	14	0.12
(1,417)	1:A:33:GLY:H	1:A:53:LEU:HD22	14	0.12
(1,417)	1:A:33:GLY:H	1:A:53:LEU:HD23	14	0.12
(1,358)	1:A:29:LEU:HD11	1:A:77:GLU:HA	14	0.12
(1,358)	1:A:29:LEU:HD12	1:A:77:GLU:HA	14	0.12
(1,358)	1:A:29:LEU:HD13	1:A:77:GLU:HA	14	0.12
(1,357)	1:A:29:LEU:HD11	1:A:76:SER:HB2	4	0.12
(1,357)	1:A:29:LEU:HD12	1:A:76:SER:HB2	4	0.12
(1,357)	1:A:29:LEU:HD13	1:A:76:SER:HB2	4	0.12
(1,357)	1:A:29:LEU:HD11	1:A:76:SER:HB2	14	0.12
(1,357)	1:A:29:LEU:HD12	1:A:76:SER:HB2	14	0.12
(1,357)	1:A:29:LEU:HD13	1:A:76:SER:HB2	14	0.12
(1,157)	1:A:16:ALA:HB2	1:A:32:VAL:HA	16	0.12
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	10	0.11
(2,51)	1:A:73:LYS:H	1:A:70:ASN:O	14	0.11
(2,41)	1:A:56:MET:H	1:A:52:ARG:O	20	0.11
(2,39)	1:A:54:SER:H	1:A:51:GLY:O	18	0.11
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	3	0.11
(2,35)	1:A:48:TRP:H	1:A:45:PRO:O	11	0.11
(1,861)	1:A:91:HIS:HA	1:A:92:HIS:H	1	0.11
(1,855)	1:A:87:HIS:HB2	1:A:88:HIS:H	7	0.11
(1,855)	1:A:87:HIS:HB3	1:A:88:HIS:H	7	0.11
(1,844)	1:A:85:LEU:H	1:A:85:LEU:HB2	4	0.11
(1,844)	1:A:85:LEU:H	1:A:85:LEU:HB3	4	0.11
(1,755)	1:A:67:GLU:HG3	1:A:74:LEU:HD21	17	0.11
(1,755)	1:A:67:GLU:HG3	1:A:74:LEU:HD22	17	0.11
(1,755)	1:A:67:GLU:HG3	1:A:74:LEU:HD23	17	0.11
(1,645)	1:A:60:LEU:HD21	1:A:61:ASP:H	15	0.11
(1,645)	1:A:60:LEU:HD22	1:A:61:ASP:H	15	0.11
(1,645)	1:A:60:LEU:HD23	1:A:61:ASP:H	15	0.11
(1,640)	1:A:60:LEU:HB2	1:A:63:LEU:HG	15	0.11
(1,640)	1:A:60:LEU:HB3	1:A:63:LEU:HG	15	0.11
(1,562)	1:A:52:ARG:HA	1:A:55:GLN:HB2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:A:52:ARG:HA	1:A:55:GLN:HB3	20	0.11
(1,290)	1:A:26:TRP:HH2	1:A:66:GLN:HG2	18	0.11
(1,275)	1:A:26:TRP:HA	1:A:79:ARG:HD2	2	0.11
(1,275)	1:A:26:TRP:HA	1:A:79:ARG:HD3	2	0.11
(1,232)	1:A:20:VAL:HG21	1:A:27:ALA:HB1	7	0.11
(1,232)	1:A:20:VAL:HG22	1:A:27:ALA:HB1	7	0.11
(1,232)	1:A:20:VAL:HG23	1:A:27:ALA:HB1	7	0.11

10 Dihedral-angle violation analysis (i)

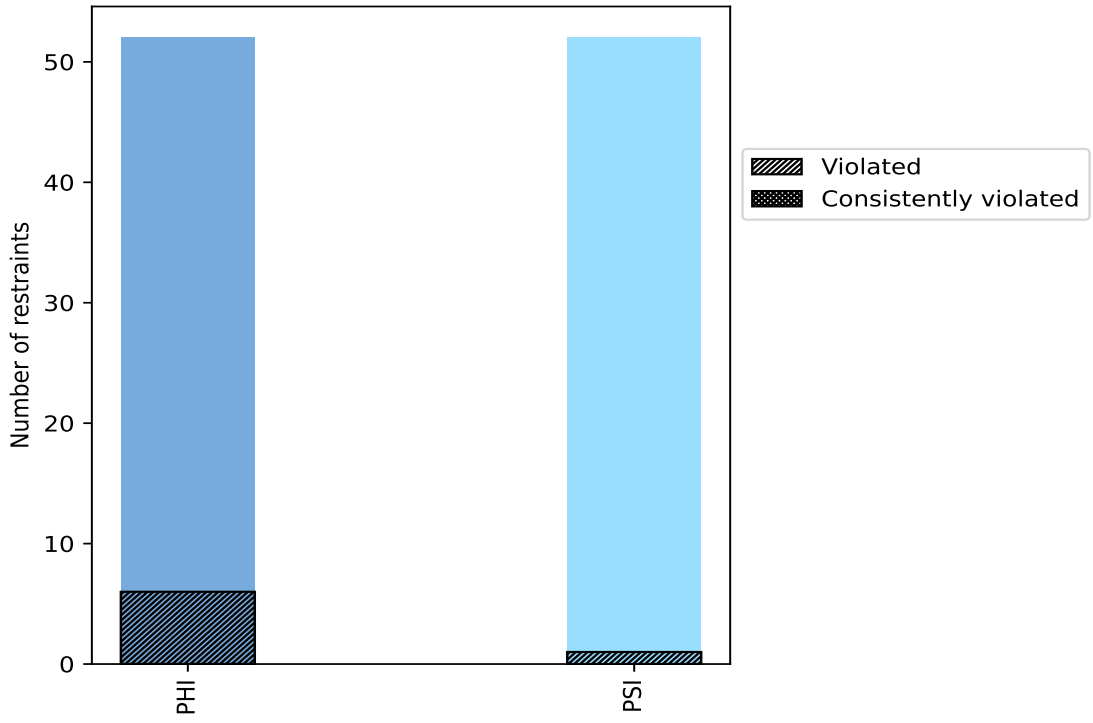
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	52	50.0	6	11.5	5.8	0	0.0	0.0
PSI	52	50.0	1	1.9	1.0	0	0.0	0.0
Total	104	100.0	7	6.7	6.7	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)



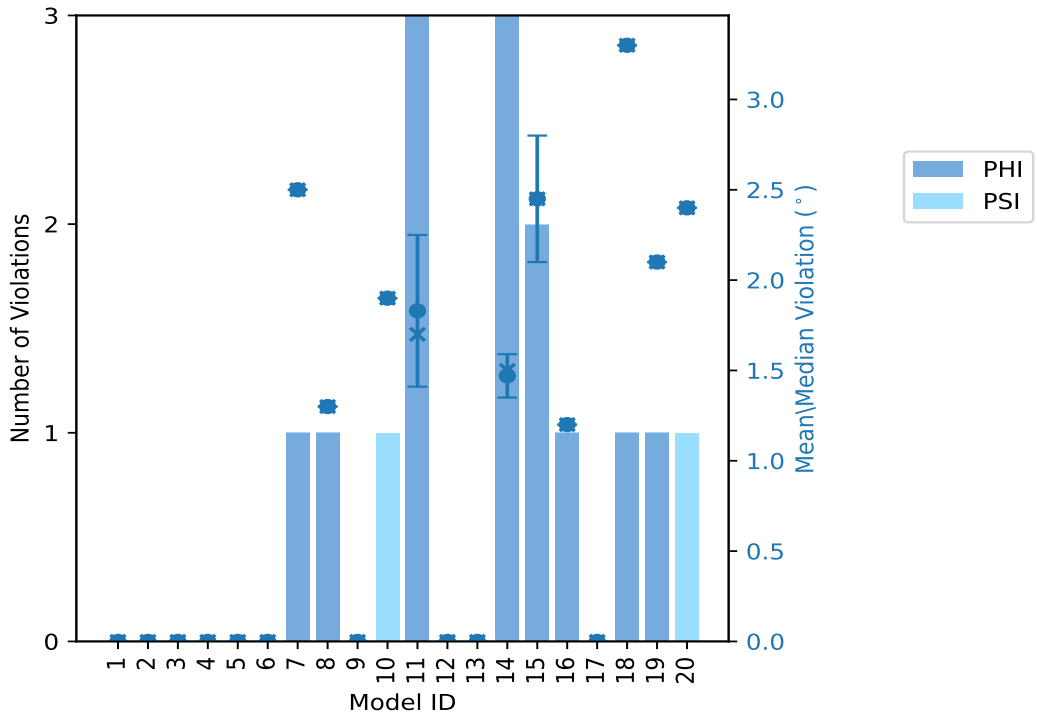
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
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	0	0	0	0.0	0.0	0.0	0.0
7	1	0	1	2.5	2.5	0.0	2.5
8	1	0	1	1.3	1.3	0.0	1.3
9	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	1.9	1.9	0.0	1.9
11	3	0	3	1.83	2.4	0.42	1.7
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	3	0	3	1.47	1.6	0.12	1.5
15	2	0	2	2.45	2.8	0.35	2.45
16	1	0	1	1.2	1.2	0.0	1.2
17	0	0	0	0.0	0.0	0.0	0.0
18	1	0	1	3.3	3.3	0.0	3.3
19	1	0	1	2.1	2.1	0.0	2.1
20	0	1	1	2.4	2.4	0.0	2.4

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
2	0	2	1	5.0
2	1	3	2	10.0
1	0	1	3	15.0
1	0	1	4	20.0
0	0	0	5	25.0
0	0	0	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

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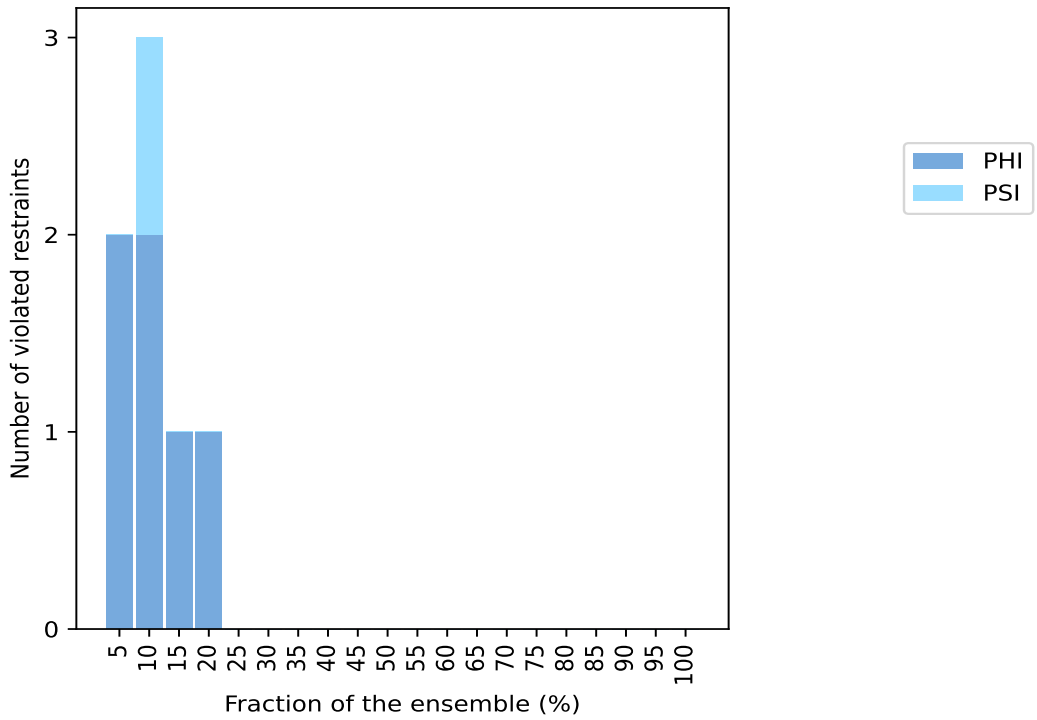
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

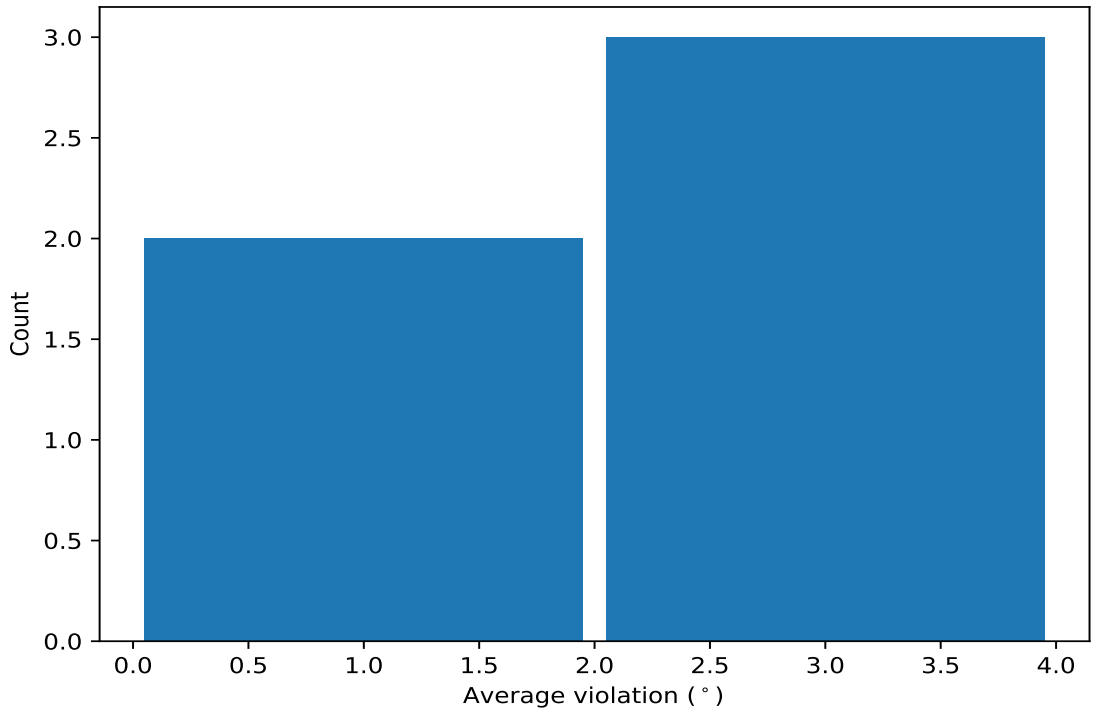


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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.

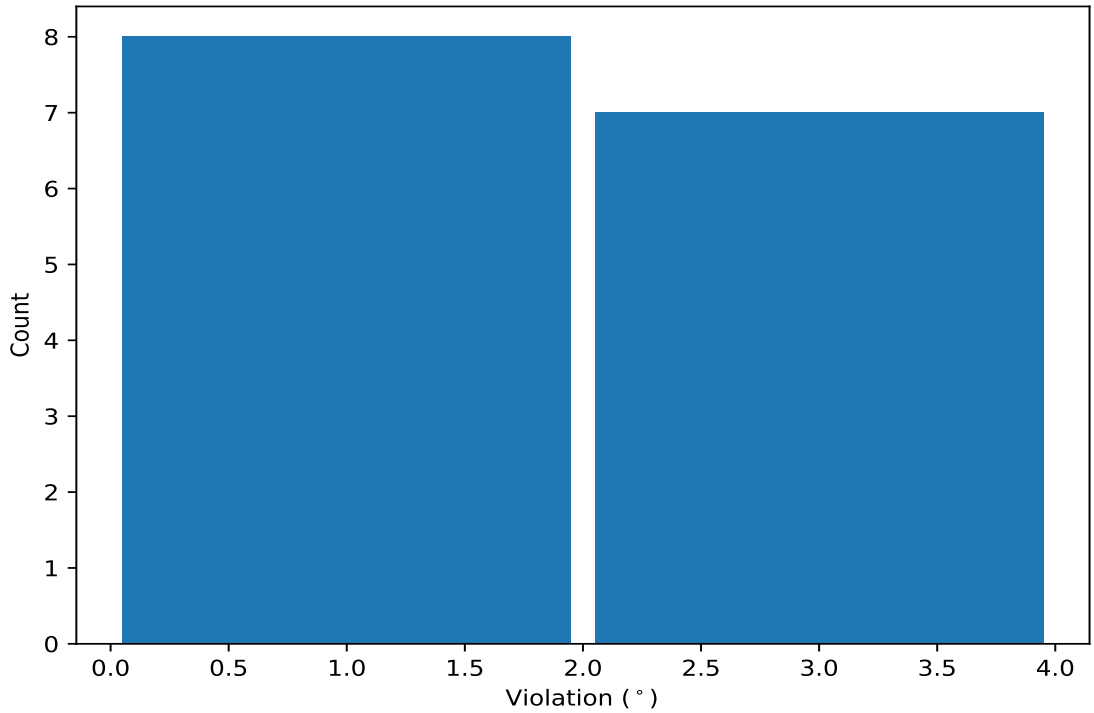
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,85)	1:A:69:ARG:C	1:A:70:ASN:N	1:A:70:ASN:CA	1:A:70:ASN:C	4	1.92	0.69	1.85
(1,57)	1:A:46:ARG:C	1:A:47:ASN:N	1:A:47:ASN:CA	1:A:47:ASN:C	3	2.1	0.33	2.1
(1,97)	1:A:76:SER:C	1:A:77:GLU:N	1:A:77:GLU:CA	1:A:77:GLU:C	2	2.4	0.9	2.4
(1,28)	1:A:21:ALA:N	1:A:21:ALA:CA	1:A:21:ALA:C	1:A:22:ARG:N	2	2.15	0.25	2.15
(1,59)	1:A:47:ASN:C	1:A:48:TRP:N	1:A:48:TRP:CA	1:A:48:TRP:C	2	1.5	0.1	1.5

[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 (°)
(1,97)	1:A:76:SER:C	1:A:77:GLU:N	1:A:77:GLU:CA	1:A:77:GLU:C	18	3.3
(1,85)	1:A:69:ARG:C	1:A:70:ASN:N	1:A:70:ASN:CA	1:A:70:ASN:C	15	2.8
(1,57)	1:A:46:ARG:C	1:A:47:ASN:N	1:A:47:ASN:CA	1:A:47:ASN:C	7	2.5
(1,85)	1:A:69:ARG:C	1:A:70:ASN:N	1:A:70:ASN:CA	1:A:70:ASN:C	11	2.4
(1,28)	1:A:21:ALA:N	1:A:21:ALA:CA	1:A:21:ALA:C	1:A:22:ARG:N	20	2.4
(1,73)	1:A:63:LEU:C	1:A:64:THR:N	1:A:64:THR:CA	1:A:64:THR:C	15	2.1
(1,57)	1:A:46:ARG:C	1:A:47:ASN:N	1:A:47:ASN:CA	1:A:47:ASN:C	19	2.1
(1,28)	1:A:21:ALA:N	1:A:21:ALA:CA	1:A:21:ALA:C	1:A:22:ARG:N	10	1.9
(1,57)	1:A:46:ARG:C	1:A:47:ASN:N	1:A:47:ASN:CA	1:A:47:ASN:C	11	1.7
(1,59)	1:A:47:ASN:C	1:A:48:TRP:N	1:A:48:TRP:CA	1:A:48:TRP:C	14	1.6
(1,97)	1:A:76:SER:C	1:A:77:GLU:N	1:A:77:GLU:CA	1:A:77:GLU:C	14	1.5
(1,59)	1:A:47:ASN:C	1:A:48:TRP:N	1:A:48:TRP:CA	1:A:48:TRP:C	11	1.4
(1,85)	1:A:69:ARG:C	1:A:70:ASN:N	1:A:70:ASN:CA	1:A:70:ASN:C	8	1.3
(1,101)	1:A:78:ILE:C	1:A:79:ARG:N	1:A:79:ARG:CA	1:A:79:ARG:C	14	1.3
(1,85)	1:A:69:ARG:C	1:A:70:ASN:N	1:A:70:ASN:CA	1:A:70:ASN:C	16	1.2