Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 06:30 AM EDT

PDB ID	:	2MLF
BMRB ID	:	19817
Title	:	NMR structure of the dilated cardiomyopathy mutation G159D in troponin C bound to the anchoring region of troponin I
Authors	:	Baryshnikova, O.K.; Robertson, I.M.; Mercier, P.; Sykes, B.D.
Deposited on	:	2014-02-26

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:

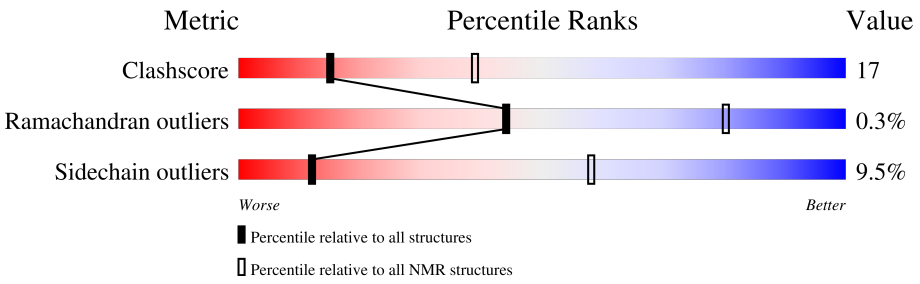
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 77%.

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	C	72	47% 42% • 10%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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	C:94-C:158 (65)	1.13	6

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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1135 atoms, of which 546 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	C	72	1133	362	546	88	132	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	MET	-	initiating methionine	UNP P63316
C	159	ASP	GLY	engineered mutation	UNP P63316

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	C	2	2	2

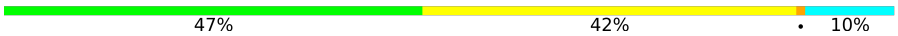
4 Residue-property plots (i)

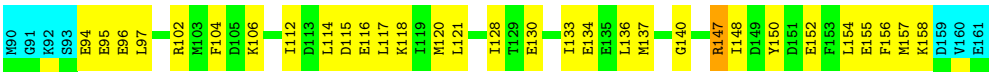
4.1 Average score per residue in the NMR ensemble

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: Troponin C, slow skeletal and cardiac muscles

Chain C:





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

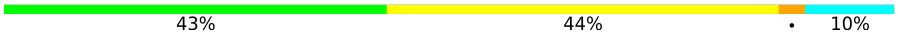
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

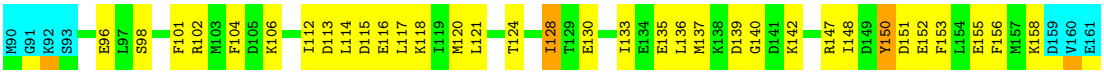
Chain C:

4.2.2 Score per residue for model 2

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:

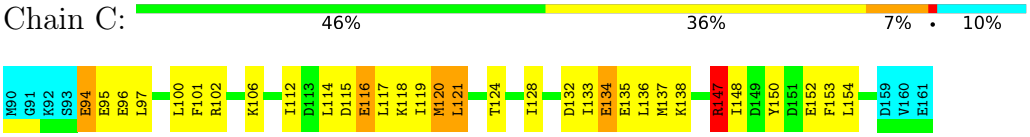




4.2.3 Score per residue for model 3

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

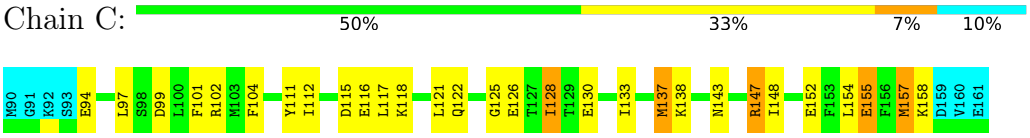
Chain C:



4.2.4 Score per residue for model 4

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

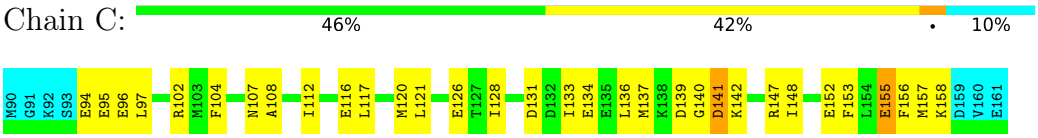
Chain C:



4.2.5 Score per residue for model 5

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

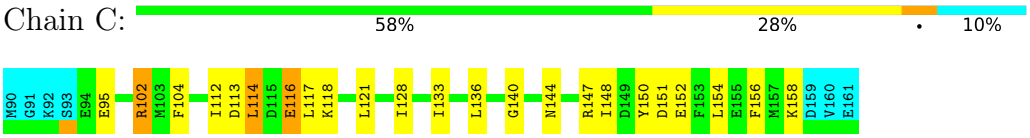
Chain C:



4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

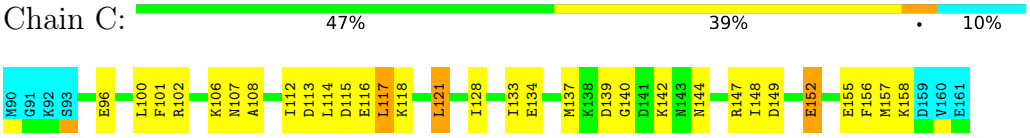
Chain C:



4.2.7 Score per residue for model 7

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:



4.2.8 Score per residue for model 8

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 46% 35% 8% • 10%

M90 G91 K92 S93 E94 E95 E96 L97 S98 D99 R102 M103 F104 D105 K106 N107 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 T124 I128 T129 E130 I133 D141 N144 R147 I148 D149 Y150 D151 E152 F153 L154 E155 F156 M157 K158 D159 V160 E161

4.2.9 Score per residue for model 9

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 60% 31% 10%

M90 G91 K92 S93 L97 R102 M103 F104 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 E126 T127 I128 I133 E134 R147 I148 D149 Y150 D151 E152 F153 L154 M157 K158 D159 V160 E161

4.2.10 Score per residue for model 10

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 51% 36% • 10%

M90 G91 K92 S93 E94 E95 E96 L97 S98 D99 R102 M103 F104 D105 K106 Y111 I112 D113 L114 D115 E116 M120 L121 I128 L136 M137 K138 D139 G140 D141 K142 R147 I148 D149 Y150 D151 E152 E155 F156 M157 K158 D159 V160 E161

4.2.11 Score per residue for model 11

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 46% 36% 7% • 10%

M90 G91 K92 S93 E94 E95 E96 L97 L100 F101 R102 K106 Y111 I112 D113 E116 L117 K118 I119 M120 L121 Q122 A123 T124 G125 E126 T127 I128 T129 E130 I133 E134 G140 R147 I148 D149 Y150 D151 E152 F153 L154 E155 F156 M157 K158 D159 V160 E161

4.2.12 Score per residue for model 12

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 46% 40% • 10%

M90 G91 K92 S93 E94 E95 E96 L97 F101 R102 K106 I112 D115 E116 L117 K118 I119 M120 L121 T127 I128 T129 E130 D131 D132 I133 E134 E135 L136 M137 G140 D141 K142 N143 N144 R147 I148 D149 E152 E155 F156 M157 K158 D159 V160 E161

4.2.13 Score per residue for model 13

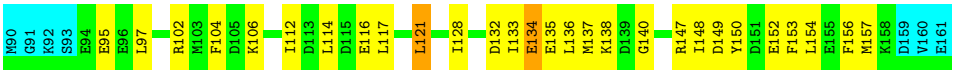
- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 51% 29% 10% 10%

4.2.14 Score per residue for model 14

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 51% 36% • 10%



4.2.15 Score per residue for model 15

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 51% 36% • 10%

4.2.16 Score per residue for model 16

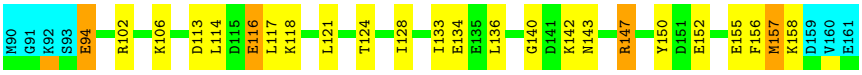
- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C: 57% 32% • 10%

4.2.17 Score per residue for model 17

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

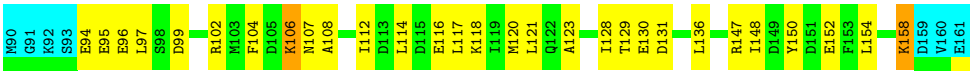
Chain C: 57% 28% 6% 10%



4.2.18 Score per residue for model 18

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

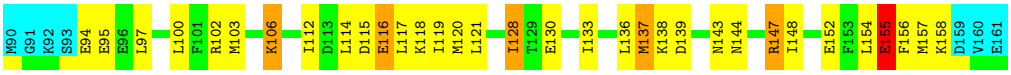
Chain C:



4.2.19 Score per residue for model 19

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:



4.2.20 Score per residue for model 20

- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	geometry optimization	
ProcheckNMR	refinement	
TALOS	refinement	
X-PLOR NIH	refinement	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	735
Number of shifts mapped to atoms	735
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality (i)

6.1 Standard geometry (i)

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

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	C	1.56±0.02	6±1/541 (1.2± 0.2%)	1.17±0.02	0±0/724 (0.0± 0.0%)
All	All	1.56	128/10820 (1.2%)	1.17	0/14480 (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	C	0.0±0.0	1.9±0.2
All	All	0	39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	116	GLU	CD-OE2	-9.48	1.15	1.25	16	20
1	C	152	GLU	CD-OE2	-8.74	1.16	1.25	10	20
1	C	116	GLU	CD-OE1	-8.41	1.16	1.25	8	20
1	C	152	GLU	CD-OE1	-8.10	1.16	1.25	15	20
1	C	135	GLU	CD-OE2	-5.91	1.19	1.25	2	4
1	C	126	GLU	CD-OE2	-5.70	1.19	1.25	11	5
1	C	155	GLU	CD-OE2	-5.68	1.19	1.25	8	3
1	C	94	GLU	CD-OE2	-5.63	1.19	1.25	3	5
1	C	130	GLU	CD-OE2	-5.60	1.19	1.25	18	4
1	C	96	GLU	CD-OE2	-5.58	1.19	1.25	7	7
1	C	95	GLU	CD-OE2	-5.57	1.19	1.25	10	10
1	C	134	GLU	CD-OE2	-5.39	1.19	1.25	11	5
1	C	134	GLU	CD-OE1	-5.33	1.19	1.25	12	2
1	C	155	GLU	CD-OE1	-5.31	1.19	1.25	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	96	GLU	CD-OE1	-5.04	1.20	1.25	2	1

There are no bond-angle outliers.

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	C	102	ARG	Sidechain	20
1	C	147	ARG	Sidechain	19

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	C	535	495	495	17±4
All	All	10740	9900	9900	345

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:97:LEU:HD13	1:C:154:LEU:HD22	1.00	1.31	4	4
1:C:117:LEU:HD21	1:C:136:LEU:HD23	0.92	1.37	5	4
1:C:117:LEU:HD22	1:C:133:ILE:HG23	0.91	1.43	2	7
1:C:117:LEU:HD11	1:C:136:LEU:HD23	0.90	1.42	6	3
1:C:117:LEU:HD23	1:C:133:ILE:HG23	0.88	1.45	17	4
1:C:97:LEU:HD22	1:C:157:MET:HB3	0.86	1.45	9	1
1:C:150:TYR:CE2	1:C:154:LEU:HD11	0.73	2.19	20	4
1:C:97:LEU:HD11	1:C:158:LYS:HA	0.71	1.60	1	1
1:C:137:MET:HA	1:C:148:ILE:HD11	0.70	1.63	7	3
1:C:106:LYS:HG3	1:C:119:ILE:HD12	0.69	1.62	19	1
1:C:100:LEU:HD13	1:C:157:MET:SD	0.69	2.26	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:99:ASP:HA	1:C:102:ARG:CZ	0.67	2.19	15	2
1:C:117:LEU:HD21	1:C:136:LEU:HD22	0.66	1.65	15	2
1:C:118:LYS:HB3	1:C:133:ILE:HD11	0.66	1.67	11	1
1:C:104:PHE:HA	1:C:120:MET:SD	0.66	2.31	5	5
1:C:106:LYS:HD2	1:C:119:ILE:HG21	0.66	1.66	3	1
1:C:97:LEU:HD21	1:C:157:MET:SD	0.66	2.30	8	1
1:C:97:LEU:HD23	1:C:157:MET:SD	0.66	2.30	19	1
1:C:94:GLU:HA	1:C:97:LEU:HD12	0.65	1.68	12	5
1:C:121:LEU:HD13	1:C:128:ILE:CG1	0.65	2.21	18	2
1:C:117:LEU:HD23	1:C:121:LEU:CD2	0.64	2.23	14	1
1:C:112:ILE:HB	1:C:148:ILE:HB	0.64	1.69	5	15
1:C:137:MET:O	1:C:148:ILE:HD11	0.64	1.93	16	2
1:C:150:TYR:CZ	1:C:154:LEU:HD21	0.63	2.28	15	4
1:C:114:LEU:HD12	1:C:133:ILE:HG21	0.62	1.70	9	1
1:C:121:LEU:HD13	1:C:128:ILE:HG13	0.62	1.71	18	2
1:C:137:MET:CG	1:C:148:ILE:HD11	0.62	2.25	14	1
1:C:117:LEU:HD22	1:C:133:ILE:CG2	0.61	2.22	2	2
1:C:117:LEU:HD23	1:C:133:ILE:CG2	0.61	2.25	3	1
1:C:117:LEU:CD2	1:C:121:LEU:HD11	0.61	2.25	18	1
1:C:121:LEU:HG	1:C:128:ILE:HD11	0.61	1.72	13	1
1:C:118:LYS:HA	1:C:121:LEU:HD12	0.61	1.72	18	1
1:C:112:ILE:CG2	1:C:117:LEU:HD11	0.60	2.26	7	1
1:C:121:LEU:HG	1:C:133:ILE:HG12	0.60	1.73	7	1
1:C:97:LEU:HD22	1:C:157:MET:SD	0.60	2.36	15	3
1:C:114:LEU:HD12	1:C:133:ILE:HG22	0.60	1.73	17	2
1:C:116:GLU:O	1:C:119:ILE:HG22	0.59	1.96	3	1
1:C:114:LEU:HD21	1:C:130:GLU:CB	0.59	2.27	2	1
1:C:121:LEU:CG	1:C:128:ILE:HD11	0.59	2.27	13	1
1:C:130:GLU:HA	1:C:133:ILE:HD12	0.59	1.73	19	3
1:C:117:LEU:HG	1:C:121:LEU:HD23	0.59	1.74	16	1
1:C:97:LEU:HD13	1:C:154:LEU:O	0.58	1.98	1	1
1:C:121:LEU:HD12	1:C:128:ILE:HG13	0.58	1.74	6	5
1:C:118:LYS:HB3	1:C:133:ILE:HD13	0.58	1.75	12	2
1:C:97:LEU:CD2	1:C:157:MET:HB2	0.58	2.28	12	1
1:C:121:LEU:HD21	1:C:128:ILE:HD12	0.57	1.75	19	1
1:C:147:ARG:HB3	1:C:147:ARG:CZ	0.57	2.30	1	2
1:C:97:LEU:CD1	1:C:154:LEU:HD22	0.57	2.21	4	1
1:C:137:MET:HG3	1:C:148:ILE:HD11	0.56	1.75	14	2
1:C:140:GLY:HA3	1:C:156:PHE:CE1	0.56	2.35	5	3
1:C:140:GLY:HA3	1:C:156:PHE:CZ	0.56	2.36	2	7
1:C:121:LEU:HD21	1:C:128:ILE:HG13	0.56	1.78	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:121:LEU:HD12	1:C:128:ILE:HD11	0.55	1.76	8	2
1:C:117:LEU:HD23	1:C:120:MET:SD	0.55	2.41	9	1
1:C:142:LYS:HD3	1:C:155:GLU:HG3	0.55	1.79	17	1
1:C:121:LEU:O	1:C:124:THR:HB	0.55	2.01	11	3
1:C:147:ARG:CZ	1:C:147:ARG:HB2	0.55	2.31	3	1
1:C:142:LYS:CE	1:C:155:GLU:HG3	0.55	2.31	12	1
1:C:111:TYR:HB3	1:C:147:ARG:HD3	0.55	1.78	4	1
1:C:115:ASP:HA	1:C:118:LYS:HG2	0.55	1.79	8	3
1:C:117:LEU:O	1:C:121:LEU:HD22	0.55	2.01	13	2
1:C:112:ILE:HD12	1:C:148:ILE:HB	0.55	1.77	6	1
1:C:100:LEU:HD12	1:C:103:MET:CE	0.54	2.32	19	1
1:C:97:LEU:HD22	1:C:157:MET:CE	0.54	2.33	15	1
1:C:100:LEU:HA	1:C:103:MET:HE2	0.54	1.79	16	1
1:C:117:LEU:HD23	1:C:121:LEU:HD11	0.54	1.79	18	1
1:C:142:LYS:HE3	1:C:155:GLU:HG3	0.54	1.80	12	1
1:C:97:LEU:CD2	1:C:157:MET:SD	0.53	2.96	19	3
1:C:117:LEU:HD11	1:C:136:LEU:CD2	0.53	2.31	14	1
1:C:150:TYR:CE2	1:C:154:LEU:HD21	0.53	2.38	8	1
1:C:113:ASP:HB2	1:C:116:GLU:HG3	0.53	1.80	13	3
1:C:99:ASP:O	1:C:102:ARG:HG2	0.53	2.04	20	2
1:C:117:LEU:CD2	1:C:133:ILE:HG23	0.52	2.28	2	2
1:C:115:ASP:HA	1:C:118:LYS:HE2	0.52	1.82	3	1
1:C:121:LEU:CD2	1:C:128:ILE:HG13	0.52	2.35	5	1
1:C:114:LEU:HD21	1:C:130:GLU:HB2	0.52	1.81	2	1
1:C:121:LEU:HG	1:C:128:ILE:HG13	0.51	1.82	3	2
1:C:117:LEU:O	1:C:120:MET:HG2	0.51	2.05	3	2
1:C:128:ILE:HG23	1:C:132:ASP:HB3	0.51	1.83	20	1
1:C:140:GLY:HA3	1:C:156:PHE:CE2	0.51	2.41	10	5
1:C:155:GLU:O	1:C:158:LYS:HG3	0.51	2.06	4	1
1:C:155:GLU:O	1:C:158:LYS:HG2	0.51	2.05	11	2
1:C:118:LYS:HG2	1:C:133:ILE:HD13	0.51	1.83	17	1
1:C:121:LEU:HD12	1:C:128:ILE:HD12	0.51	1.83	4	1
1:C:141:ASP:OD1	1:C:148:ILE:HD13	0.50	2.05	5	1
1:C:121:LEU:CB	1:C:128:ILE:CG1	0.50	2.89	11	1
1:C:97:LEU:HD22	1:C:157:MET:CB	0.50	2.31	9	1
1:C:121:LEU:HB3	1:C:128:ILE:HG13	0.50	1.83	10	3
1:C:130:GLU:HA	1:C:133:ILE:HB	0.50	1.82	19	1
1:C:99:ASP:HA	1:C:102:ARG:HD3	0.50	1.84	10	1
1:C:117:LEU:HD11	1:C:136:LEU:HD13	0.50	1.83	18	1
1:C:128:ILE:CG2	1:C:132:ASP:HB3	0.50	2.37	14	3
1:C:121:LEU:HG	1:C:128:ILE:CD1	0.50	2.37	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:128:ILE:HG21	1:C:133:ILE:HG13	0.50	1.83	4	1
1:C:140:GLY:HA3	1:C:156:PHE:CD1	0.50	2.42	5	1
1:C:155:GLU:HA	1:C:158:LYS:HD3	0.49	1.83	2	2
1:C:142:LYS:HD3	1:C:155:GLU:CG	0.49	2.37	17	2
1:C:117:LEU:HD23	1:C:121:LEU:HD21	0.49	1.83	14	1
1:C:100:LEU:HB3	1:C:157:MET:HE1	0.49	1.84	7	1
1:C:136:LEU:HD13	1:C:136:LEU:C	0.49	2.28	13	3
1:C:97:LEU:HD13	1:C:154:LEU:HD23	0.49	1.85	8	1
1:C:97:LEU:HD12	1:C:154:LEU:HD22	0.49	1.83	14	1
1:C:121:LEU:HG	1:C:128:ILE:HG21	0.49	1.82	7	1
1:C:106:LYS:HA	1:C:106:LYS:HE3	0.49	1.83	18	1
1:C:121:LEU:HA	1:C:124:THR:OG1	0.49	2.08	13	1
1:C:121:LEU:HD13	1:C:128:ILE:CB	0.48	2.37	18	1
1:C:115:ASP:HA	1:C:118:LYS:HE3	0.48	1.84	7	1
1:C:118:LYS:HG2	1:C:133:ILE:CD1	0.48	2.38	3	3
1:C:121:LEU:HD12	1:C:128:ILE:CD1	0.48	2.38	4	2
1:C:113:ASP:HB3	1:C:116:GLU:HG3	0.48	1.85	8	2
1:C:155:GLU:HA	1:C:158:LYS:HE3	0.48	1.85	19	1
1:C:97:LEU:HB3	1:C:157:MET:SD	0.48	2.48	10	2
1:C:104:PHE:HB3	1:C:112:ILE:HD13	0.48	1.86	14	7
1:C:117:LEU:HD13	1:C:133:ILE:HG23	0.47	1.83	8	2
1:C:137:MET:CA	1:C:148:ILE:HD11	0.47	2.38	7	2
1:C:148:ILE:HD13	1:C:156:PHE:CE2	0.47	2.44	7	2
1:C:107:ASN:O	1:C:108:ALA:HB3	0.47	2.09	5	3
1:C:106:LYS:NZ	1:C:116:GLU:HA	0.47	2.24	11	1
1:C:117:LEU:HA	1:C:120:MET:HE3	0.47	1.87	12	1
1:C:137:MET:HB2	1:C:148:ILE:HD11	0.47	1.87	19	1
1:C:121:LEU:HB3	1:C:128:ILE:CG1	0.47	2.39	11	1
1:C:104:PHE:CD2	1:C:153:PHE:CE1	0.47	3.02	2	1
1:C:104:PHE:HB3	1:C:112:ILE:CD1	0.47	2.40	9	1
1:C:101:PHE:CZ	1:C:112:ILE:HG13	0.47	2.44	2	2
1:C:117:LEU:HD22	1:C:133:ILE:HG12	0.47	1.87	1	1
1:C:118:LYS:HG2	1:C:133:ILE:HD11	0.47	1.87	1	1
1:C:136:LEU:C	1:C:136:LEU:HD13	0.46	2.31	2	1
1:C:101:PHE:CE2	1:C:112:ILE:HG13	0.46	2.45	4	1
1:C:114:LEU:O	1:C:118:LYS:HG3	0.46	2.10	6	1
1:C:153:PHE:HA	1:C:156:PHE:CD1	0.46	2.45	5	1
1:C:135:GLU:HA	1:C:138:LYS:CG	0.46	2.41	3	1
1:C:117:LEU:HB3	1:C:133:ILE:HG23	0.46	1.87	19	1
1:C:117:LEU:CD2	1:C:121:LEU:HD21	0.45	2.41	14	1
1:C:114:LEU:HD13	1:C:130:GLU:HB3	0.45	1.88	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:115:ASP:O	1:C:118:LYS:HG2	0.45	2.11	12	3
1:C:106:LYS:HA	1:C:106:LYS:CE	0.45	2.40	18	1
1:C:100:LEU:CD1	1:C:157:MET:SD	0.45	3.03	20	1
1:C:97:LEU:HD12	1:C:154:LEU:CD2	0.45	2.42	14	1
1:C:120:MET:O	1:C:124:THR:HG23	0.45	2.11	8	1
1:C:121:LEU:CD2	1:C:121:LEU:N	0.45	2.79	11	1
1:C:103:MET:O	1:C:106:LYS:NZ	0.45	2.48	8	2
1:C:101:PHE:CE1	1:C:112:ILE:HG13	0.45	2.47	16	2
1:C:155:GLU:HA	1:C:158:LYS:CG	0.45	2.41	5	1
1:C:118:LYS:HB3	1:C:133:ILE:CD1	0.44	2.42	12	2
1:C:139:ASP:O	1:C:142:LYS:NZ	0.44	2.43	7	3
1:C:104:PHE:HA	1:C:120:MET:CE	0.44	2.42	9	1
1:C:120:MET:O	1:C:123:ALA:HB3	0.44	2.12	18	1
1:C:106:LYS:HE3	1:C:106:LYS:HA	0.44	1.89	19	1
1:C:96:GLU:O	1:C:100:LEU:HD23	0.44	2.12	3	1
1:C:122:GLN:HA	1:C:126:GLU:O	0.44	2.13	11	1
1:C:137:MET:HG2	1:C:148:ILE:HD11	0.44	1.89	1	1
1:C:115:ASP:HA	1:C:118:LYS:CG	0.44	2.43	8	1
1:C:106:LYS:HE2	1:C:120:MET:HG3	0.44	1.90	10	1
1:C:101:PHE:CD1	1:C:112:ILE:HD11	0.44	2.48	12	1
1:C:111:TYR:HB3	1:C:147:ARG:HB3	0.44	1.87	11	1
1:C:117:LEU:CD2	1:C:136:LEU:HD23	0.43	2.27	5	1
1:C:117:LEU:HA	1:C:120:MET:HE2	0.43	1.90	19	1
1:C:117:LEU:CD2	1:C:136:LEU:HD22	0.43	2.41	15	1
1:C:95:GLU:HG2	1:C:96:GLU:N	0.43	2.29	20	2
1:C:121:LEU:HD22	1:C:128:ILE:HG13	0.43	1.90	18	1
1:C:104:PHE:HB3	1:C:112:ILE:CG2	0.43	2.44	18	2
1:C:97:LEU:HD22	1:C:154:LEU:HA	0.43	1.89	19	1
1:C:117:LEU:HD21	1:C:136:LEU:CD2	0.43	2.26	5	1
1:C:148:ILE:HG23	1:C:152:GLU:HB3	0.43	1.90	7	1
1:C:115:ASP:O	1:C:119:ILE:HG13	0.43	2.14	15	1
1:C:94:GLU:HB3	1:C:150:TYR:OH	0.43	2.14	17	1
1:C:112:ILE:CD1	1:C:153:PHE:CD1	0.42	3.02	3	2
1:C:121:LEU:HG	1:C:128:ILE:CG1	0.42	2.43	14	1
1:C:99:ASP:HA	1:C:102:ARG:NE	0.42	2.29	20	1
1:C:117:LEU:HD23	1:C:121:LEU:CD1	0.42	2.44	18	1
1:C:104:PHE:CB	1:C:112:ILE:HD13	0.42	2.44	2	2
1:C:112:ILE:O	1:C:147:ARG:HA	0.42	2.14	13	1
1:C:122:GLN:HA	1:C:125:GLY:O	0.42	2.15	4	1
1:C:114:LEU:HA	1:C:133:ILE:CG2	0.42	2.44	20	1
1:C:121:LEU:CG	1:C:133:ILE:HG12	0.42	2.42	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:119:ILE:HA	1:C:122:GLN:HB2	0.42	1.92	15	1
1:C:118:LYS:CB	1:C:133:ILE:CD1	0.42	2.98	19	1
1:C:137:MET:HB3	1:C:148:ILE:HD11	0.42	1.91	5	1
1:C:113:ASP:O	1:C:117:LEU:HD12	0.42	2.15	13	1
1:C:141:ASP:HA	1:C:152:GLU:HB3	0.42	1.91	13	1
1:C:106:LYS:HG3	1:C:116:GLU:HA	0.42	1.90	11	1
1:C:121:LEU:CD1	1:C:128:ILE:HG13	0.41	2.43	2	1
1:C:106:LYS:HB2	1:C:116:GLU:HG2	0.41	1.92	3	1
1:C:97:LEU:HD23	1:C:157:MET:CG	0.41	2.45	4	1
1:C:121:LEU:N	1:C:121:LEU:HD22	0.41	2.30	11	1
1:C:137:MET:CE	1:C:148:ILE:HG12	0.41	2.44	12	1
1:C:158:LYS:NZ	1:C:158:LYS:HB2	0.41	2.30	19	1
1:C:130:GLU:O	1:C:134:GLU:HG3	0.41	2.15	11	1
1:C:150:TYR:O	1:C:154:LEU:HG	0.41	2.14	20	3
1:C:136:LEU:HD13	1:C:136:LEU:O	0.41	2.16	13	1
1:C:158:LYS:NZ	1:C:158:LYS:HA	0.41	2.30	18	1
1:C:151:ASP:O	1:C:155:GLU:HG2	0.41	2.15	2	1
1:C:155:GLU:O	1:C:158:LYS:CG	0.41	2.68	4	1
1:C:104:PHE:HB3	1:C:112:ILE:HG23	0.41	1.92	6	1
1:C:106:LYS:CG	1:C:116:GLU:HA	0.41	2.45	19	1
1:C:114:LEU:HD23	1:C:146:GLY:O	0.41	2.15	1	1
1:C:117:LEU:HD23	1:C:121:LEU:HD23	0.41	1.91	4	1
1:C:121:LEU:HD12	1:C:128:ILE:CG1	0.41	2.45	9	1
1:C:138:LYS:CG	1:C:139:ASP:N	0.41	2.83	10	1
1:C:134:GLU:O	1:C:138:LYS:HG3	0.41	2.16	14	1
1:C:114:LEU:CA	1:C:133:ILE:HG21	0.41	2.46	20	1
1:C:134:GLU:O	1:C:138:LYS:HG2	0.41	2.15	3	2
1:C:153:PHE:HA	1:C:156:PHE:CD2	0.41	2.51	8	1
1:C:106:LYS:HD3	1:C:119:ILE:HB	0.41	1.92	11	1
1:C:121:LEU:HD23	1:C:133:ILE:HG12	0.41	1.93	5	1
1:C:111:TYR:CE2	1:C:149:ASP:HB2	0.41	2.50	10	1
1:C:101:PHE:CE2	1:C:150:TYR:HA	0.41	2.51	2	1
1:C:121:LEU:CB	1:C:128:ILE:HG13	0.41	2.46	11	1
1:C:113:ASP:HB2	1:C:116:GLU:CG	0.41	2.46	13	1
1:C:149:ASP:HB3	1:C:152:GLU:HG3	0.40	1.93	11	1
1:C:118:LYS:HG3	1:C:119:ILE:N	0.40	2.31	19	1
1:C:97:LEU:HD13	1:C:154:LEU:CD2	0.40	2.45	8	1
1:C:114:LEU:CD1	1:C:133:ILE:HG21	0.40	2.44	9	1
1:C:137:MET:CB	1:C:148:ILE:HD11	0.40	2.46	19	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	C	65/72 (90%)	63±1 (97±2%)	2±1 (3±2%)	0±0 (0±1%)	44	80
All	All	1300/1440 (90%)	1256 (97%)	40 (3%)	4 (0%)	44	80

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	126	GLU	2
1	C	128	ILE	1
1	C	130	GLU	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	C	59/65 (91%)	53±2 (91±4%)	6±2 (9±4%)	12	58
All	All	1180/1300 (91%)	1068 (91%)	112 (9%)	12	58

All 36 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	C	106	LYS	10
1	C	114	LEU	8
1	C	147	ARG	7
1	C	144	ASN	7
1	C	115	ASP	6
1	C	121	LEU	6
1	C	128	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	C	143	ASN	5
1	C	131	ASP	5
1	C	157	MET	4
1	C	158	LYS	4
1	C	149	ASP	4
1	C	113	ASP	3
1	C	99	ASP	3
1	C	138	LYS	3
1	C	129	THR	3
1	C	134	GLU	2
1	C	94	GLU	2
1	C	137	MET	2
1	C	141	ASP	2
1	C	102	ARG	2
1	C	151	ASP	2
1	C	117	LEU	2
1	C	118	LYS	2
1	C	130	GLU	2
1	C	98	SER	1
1	C	124	THR	1
1	C	150	TYR	1
1	C	120	MET	1
1	C	107	ASN	1
1	C	100	LEU	1
1	C	127	THR	1
1	C	122	GLN	1
1	C	139	ASP	1
1	C	155	GLU	1
1	C	105	ASP	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 76% 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	735
Number of shifts mapped to atoms	735
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	71	-0.14 ± 0.23	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	67	0.01 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	71	0.45 ± 0.26	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 77%, i.e. 678 atoms were assigned a chemical shift out of a possible 880. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	264/329 (80%)	134/134 (100%)	65/130 (50%)	65/65 (100%)
Sidechain	399/493 (81%)	259/312 (83%)	136/166 (82%)	4/15 (27%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	15/58 (26%)	15/28 (54%)	0/30 (0%)	0/0 (—%)
Overall	678/880 (77%)	408/474 (86%)	201/326 (62%)	69/80 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 735 atoms were assigned a chemical shift out of a possible 963. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	287/365 (79%)	145/149 (97%)	71/144 (49%)	71/72 (99%)
Sidechain	433/540 (80%)	281/342 (82%)	148/182 (81%)	4/16 (25%)
Aromatic	15/58 (26%)	15/28 (54%)	0/30 (0%)	0/0 (—%)
Overall	735/963 (76%)	441/519 (85%)	219/356 (62%)	75/88 (85%)

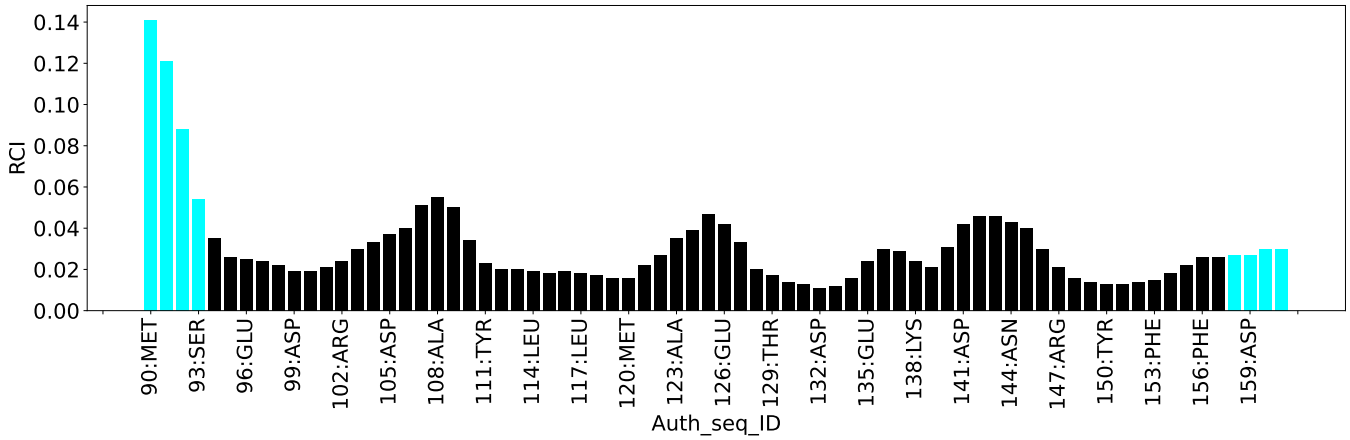
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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 C:



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	1074
Intra-residue (|i-j|=0)	319
Sequential (|i-j|=1)	304
Medium range (|i-j|>1 and |i-j|<5)	231
Long range (|i-j|≥5)	220
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	72
Number of unmapped restraints	1
Number of restraints per residue	15.9
Number of long range restraints per residue[1]	3.1

[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)	4.5	0.2
0.2-0.5 (Medium)	1.0	0.42
>0.5 (Large)	0.1	0.52

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

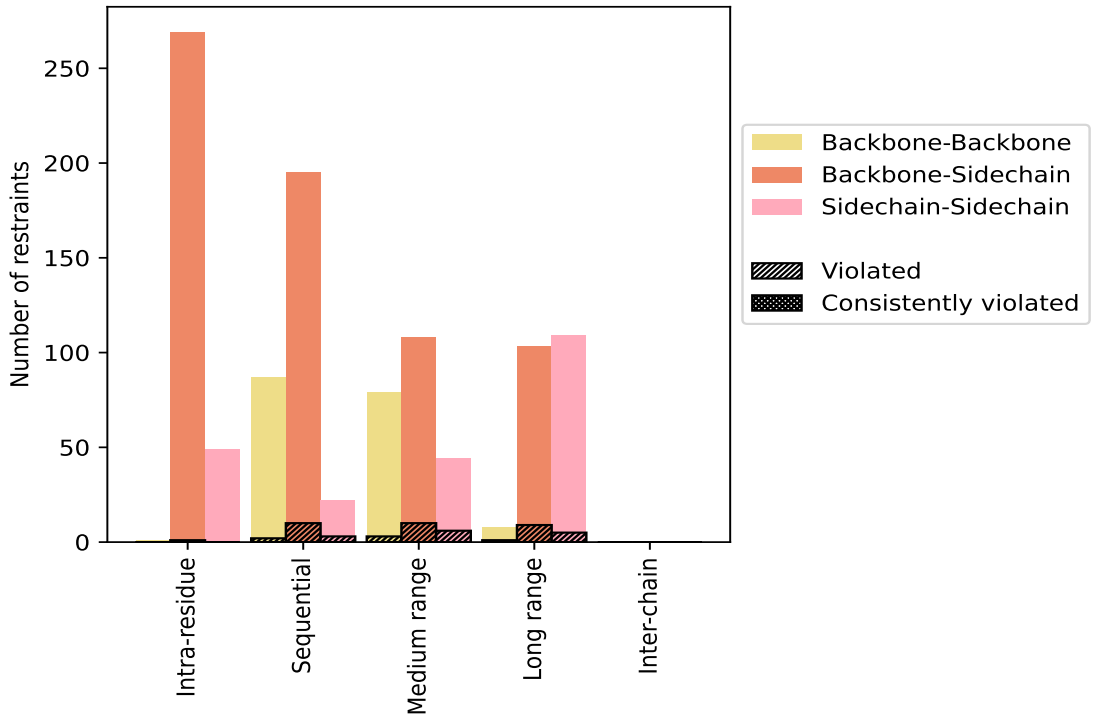
9.1 Summary of distance violations (i)

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)	319	29.7	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	269	25.0	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	49	4.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	304	28.3	15	4.9	1.4	0	0.0	0.0
Backbone-Backbone	87	8.1	2	2.3	0.2	0	0.0	0.0
Backbone-Sidechain	195	18.2	10	5.1	0.9	0	0.0	0.0
Sidechain-Sidechain	22	2.0	3	13.6	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	231	21.5	19	8.2	1.8	0	0.0	0.0
Backbone-Backbone	79	7.4	3	3.8	0.3	0	0.0	0.0
Backbone-Sidechain	108	10.1	10	9.3	0.9	0	0.0	0.0
Sidechain-Sidechain	44	4.1	6	13.6	0.6	0	0.0	0.0
Long range (|i-j|≥5)	220	20.5	15	6.8	1.4	0	0.0	0.0
Backbone-Backbone	8	0.7	1	12.5	0.1	0	0.0	0.0
Backbone-Sidechain	103	9.6	9	8.7	0.8	0	0.0	0.0
Sidechain-Sidechain	109	10.1	5	4.6	0.5	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	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	1074	100.0	50	4.7	4.7	0	0.0	0.0
Backbone-Backbone	175	16.3	6	3.4	0.6	0	0.0	0.0
Backbone-Sidechain	675	62.8	30	4.4	2.8	0	0.0	0.0
Sidechain-Sidechain	224	20.9	14	6.2	1.3	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	6	0	0	7	0.16	0.23	0.04	0.14
2	0	1	1	4	0	6	0.17	0.23	0.05	0.16
3	0	3	4	0	0	7	0.24	0.52	0.12	0.21
4	0	2	2	1	0	5	0.14	0.17	0.02	0.14
5	0	2	3	1	0	6	0.15	0.22	0.04	0.15
6	0	3	1	0	0	4	0.24	0.51	0.16	0.16
7	0	1	1	1	0	3	0.2	0.27	0.07	0.23
8	0	2	3	3	0	8	0.14	0.21	0.03	0.13
9	1	1	1	1	0	4	0.15	0.24	0.05	0.12
10	0	1	1	0	0	2	0.14	0.17	0.03	0.14
11	0	5	3	3	0	11	0.18	0.42	0.08	0.15

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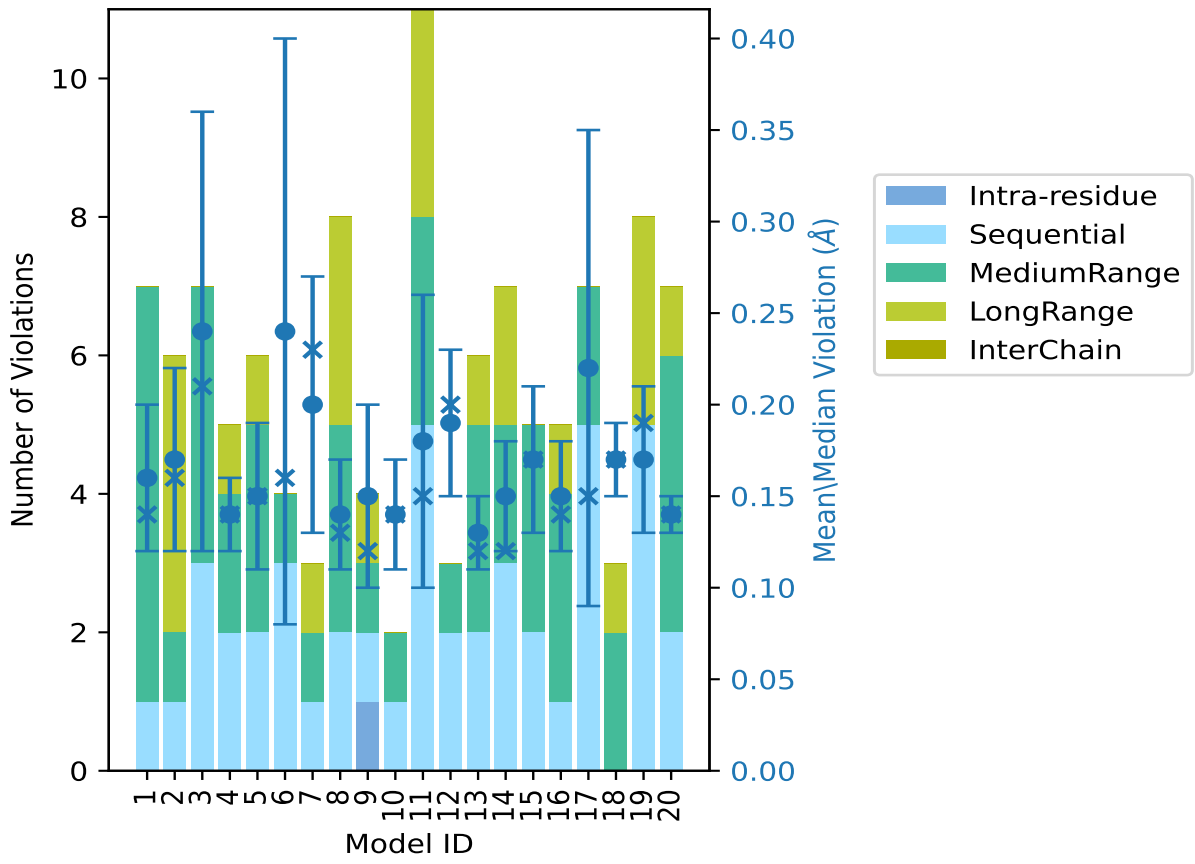
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	1	0	0	3	0.19	0.24	0.04	0.2
13	0	2	3	1	0	6	0.13	0.17	0.02	0.12
14	0	3	2	2	0	7	0.15	0.2	0.03	0.12
15	0	2	3	0	0	5	0.17	0.24	0.04	0.17
16	0	1	3	1	0	5	0.15	0.21	0.03	0.14
17	0	5	2	0	0	7	0.22	0.51	0.13	0.15
18	0	0	2	1	0	3	0.17	0.19	0.02	0.17
19	0	5	0	3	0	8	0.17	0.23	0.04	0.19
20	0	2	4	1	0	7	0.14	0.15	0.01	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

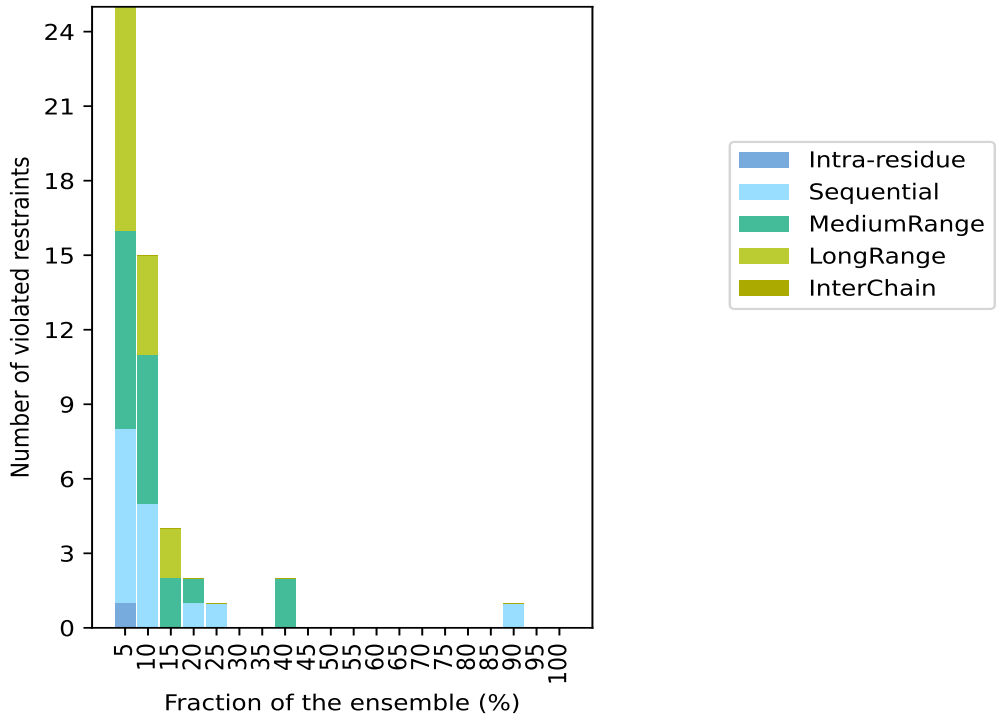
9.3 Distance violation statistics for the ensemble (i)

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, 1024(IR:318, SQ:289, MR:212, LR:205, 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]	%
1	7	8	9	0	25	1	5.0
0	5	6	4	0	15	2	10.0
0	0	2	2	0	4	3	15.0
0	1	1	0	0	2	4	20.0
0	1	0	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	2	0	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	1	0	0	0	1	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

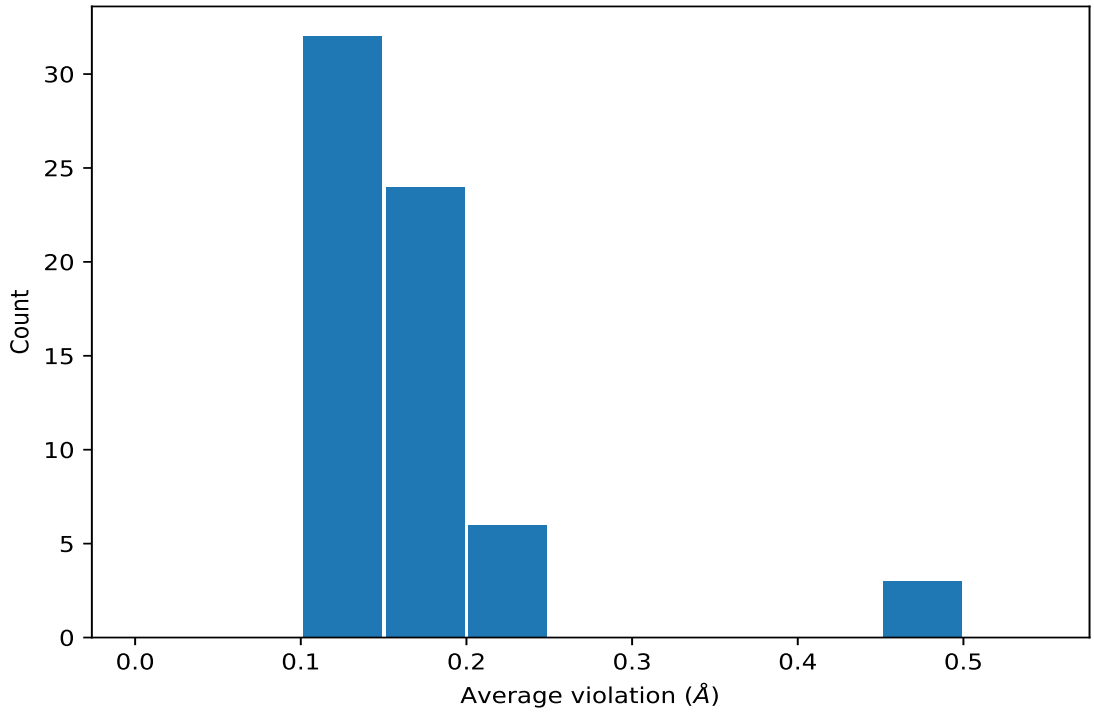
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	18	0.18	0.04	0.17
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	18	0.18	0.04	0.17
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	8	0.2	0.06	0.2
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	8	0.2	0.06	0.2
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	8	0.2	0.06	0.2
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	8	0.16	0.04	0.16
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	8	0.16	0.04	0.16
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	8	0.16	0.04	0.16
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB2	5	0.15	0.03	0.16
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB3	5	0.15	0.03	0.16
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG21	4	0.49	0.04	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG22	4	0.49	0.04	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG23	4	0.49	0.04	0.51
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD2	4	0.18	0.05	0.18
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD3	4	0.18	0.05	0.18
(1,518)	1:C:97:LEU:HB3	1:C:157:MET:H	3	0.14	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD11	3	0.13	0.02	0.12
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD12	3	0.13	0.02	0.12
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD13	3	0.13	0.02	0.12
(1,827)	1:C:153:PHE:HD1	1:C:156:PHE:HZ	3	0.12	0.01	0.12
(1,827)	1:C:153:PHE:HD2	1:C:156:PHE:HZ	3	0.12	0.01	0.12
(1,590)	1:C:105:ASP:H	1:C:108:ALA:H	3	0.12	0.01	0.12
(1,528)	1:C:121:LEU:HD11	1:C:124:THR:H	2	0.2	0.03	0.2
(1,528)	1:C:121:LEU:HD12	1:C:124:THR:H	2	0.2	0.03	0.2
(1,528)	1:C:121:LEU:HD13	1:C:124:THR:H	2	0.2	0.03	0.2
(1,829)	1:C:150:TYR:HE1	1:C:154:LEU:HA	2	0.18	0.04	0.18
(1,829)	1:C:150:TYR:HE2	1:C:154:LEU:HA	2	0.18	0.04	0.18
(1,97)	1:C:128:ILE:HG12	1:C:133:ILE:HA	2	0.18	0.03	0.18
(1,97)	1:C:128:ILE:HG13	1:C:133:ILE:HA	2	0.18	0.03	0.18
(1,193)	1:C:114:LEU:HG	1:C:115:ASP:HB3	2	0.18	0.06	0.18
(1,1002)	1:C:136:LEU:HD11	1:C:137:MET:HG2	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD11	1:C:137:MET:HG3	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD12	1:C:137:MET:HG2	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD12	1:C:137:MET:HG3	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD13	1:C:137:MET:HG2	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD13	1:C:137:MET:HG3	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD21	1:C:137:MET:HG2	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD21	1:C:137:MET:HG3	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD22	1:C:137:MET:HG2	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD22	1:C:137:MET:HG3	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD23	1:C:137:MET:HG2	2	0.17	0.01	0.17
(1,1002)	1:C:136:LEU:HD23	1:C:137:MET:HG3	2	0.17	0.01	0.17
(1,496)	1:C:142:LYS:H	1:C:143:ASN:H	2	0.15	0.01	0.15
(1,420)	1:C:128:ILE:HG21	1:C:131:ASP:H	2	0.15	0.03	0.15
(1,420)	1:C:128:ILE:HG22	1:C:131:ASP:H	2	0.15	0.03	0.15
(1,420)	1:C:128:ILE:HG23	1:C:131:ASP:H	2	0.15	0.03	0.15
(1,842)	1:C:91:GLY:H	1:C:92:LYS:HB2	2	0.15	0.03	0.15
(1,842)	1:C:91:GLY:H	1:C:92:LYS:HB3	2	0.15	0.03	0.15
(1,830)	1:C:100:LEU:HB2	1:C:153:PHE:HD1	2	0.14	0.0	0.14
(1,830)	1:C:100:LEU:HB2	1:C:153:PHE:HD2	2	0.14	0.0	0.14
(1,922)	1:C:111:TYR:HE1	1:C:147:ARG:HD2	2	0.14	0.02	0.14
(1,922)	1:C:111:TYR:HE1	1:C:147:ARG:HD3	2	0.14	0.02	0.14
(1,922)	1:C:111:TYR:HE2	1:C:147:ARG:HD2	2	0.14	0.02	0.14
(1,922)	1:C:111:TYR:HE2	1:C:147:ARG:HD3	2	0.14	0.02	0.14
(1,578)	1:C:113:ASP:H	1:C:117:LEU:HA	2	0.13	0.02	0.13
(1,928)	1:C:113:ASP:H	1:C:147:ARG:HB2	2	0.12	0.01	0.12
(1,928)	1:C:113:ASP:H	1:C:147:ARG:HB3	2	0.12	0.01	0.12
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG21	2	0.12	0.01	0.12

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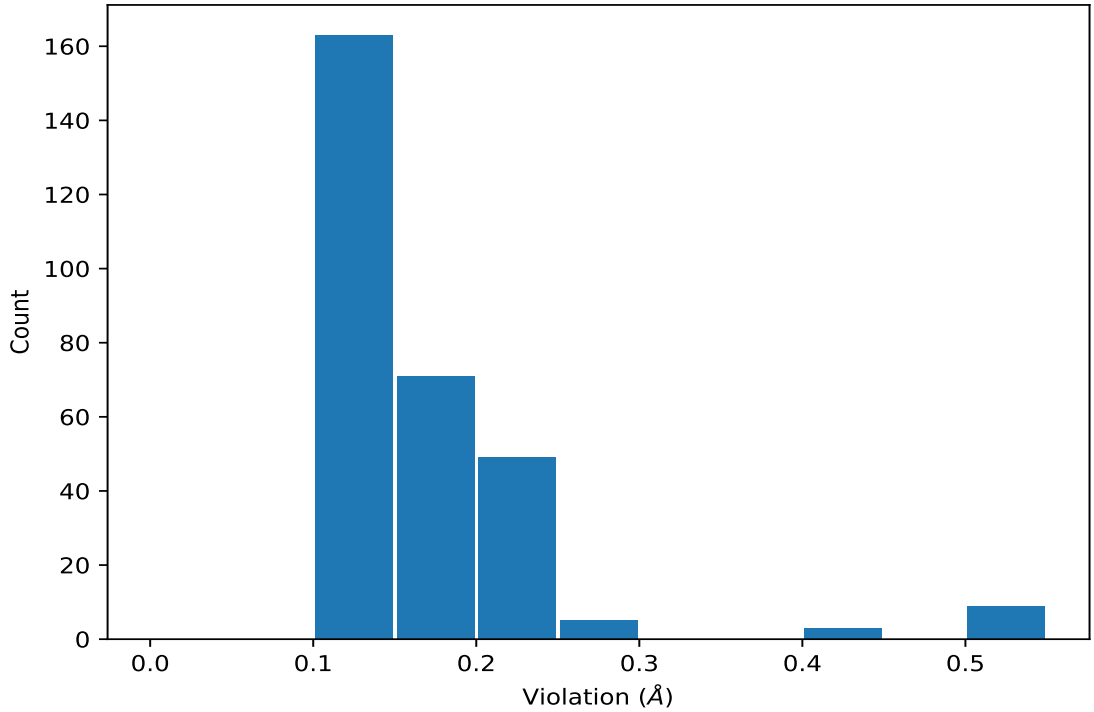
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG22	2	0.12	0.01	0.12
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG23	2	0.12	0.01	0.12
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG21	2	0.12	0.01	0.12
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG22	2	0.12	0.01	0.12
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG23	2	0.12	0.01	0.12
(1,98)	1:C:133:ILE:HA	1:C:136:LEU:HG	2	0.12	0.0	0.12
(1,405)	1:C:136:LEU:HG	1:C:137:MET:H	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG21	3	0.52
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG22	3	0.52
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG23	3	0.52
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG21	6	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG22	6	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG23	6	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG21	17	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG22	17	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG23	17	0.51
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG21	11	0.42
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG22	11	0.42
(1,321)	1:C:123:ALA:H	1:C:124:THR:HG23	11	0.42
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	17	0.3
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	17	0.3
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	17	0.3
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	7	0.27
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	7	0.27
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	3	0.24
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	3	0.24
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	3	0.24
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	9	0.24
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	9	0.24
(1,528)	1:C:121:LEU:HD11	1:C:124:THR:H	15	0.24
(1,528)	1:C:121:LEU:HD12	1:C:124:THR:H	15	0.24
(1,528)	1:C:121:LEU:HD13	1:C:124:THR:H	15	0.24
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD2	12	0.24
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD3	12	0.24
(1,971)	1:C:126:GLU:HB2	1:C:128:ILE:H	7	0.23
(1,971)	1:C:126:GLU:HB3	1:C:128:ILE:H	7	0.23
(1,902)	1:C:103:MET:HB3	1:C:120:MET:HB2	2	0.23
(1,902)	1:C:103:MET:HB3	1:C:120:MET:HB3	2	0.23
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	2	0.23
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	2	0.23
(1,299)	1:C:156:PHE:HD1	1:C:158:LYS:H	1	0.23
(1,299)	1:C:156:PHE:HD2	1:C:158:LYS:H	1	0.23
(1,193)	1:C:114:LEU:HG	1:C:115:ASP:HB3	19	0.23
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD2	3	0.23
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD3	3	0.23
(1,829)	1:C:150:TYR:HE1	1:C:154:LEU:HA	5	0.22
(1,829)	1:C:150:TYR:HE2	1:C:154:LEU:HA	5	0.22
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	17	0.22
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	17	0.22
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	11	0.22
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	11	0.22
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	11	0.22
(1,97)	1:C:128:ILE:HG12	1:C:133:ILE:HA	19	0.21
(1,97)	1:C:128:ILE:HG13	1:C:133:ILE:HA	19	0.21
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	16	0.21
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	16	0.21
(1,350)	1:C:128:ILE:HD11	1:C:129:THR:H	8	0.21
(1,350)	1:C:128:ILE:HD12	1:C:129:THR:H	8	0.21
(1,350)	1:C:128:ILE:HD13	1:C:129:THR:H	8	0.21
(1,234)	1:C:118:LYS:H	1:C:119:ILE:HD11	3	0.21
(1,234)	1:C:118:LYS:H	1:C:119:ILE:HD12	3	0.21
(1,234)	1:C:118:LYS:H	1:C:119:ILE:HD13	3	0.21
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	3	0.2
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	3	0.2
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	3	0.2
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	14	0.2
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	14	0.2
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	14	0.2
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	1	0.2
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	1	0.2
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	12	0.2
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	12	0.2
(1,984)	1:C:133:ILE:HG21	1:C:134:GLU:HG2	19	0.19
(1,984)	1:C:133:ILE:HG21	1:C:134:GLU:HG3	19	0.19
(1,984)	1:C:133:ILE:HG22	1:C:134:GLU:HG2	19	0.19
(1,984)	1:C:133:ILE:HG22	1:C:134:GLU:HG3	19	0.19
(1,984)	1:C:133:ILE:HG23	1:C:134:GLU:HG2	19	0.19
(1,984)	1:C:133:ILE:HG23	1:C:134:GLU:HG3	19	0.19
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB2	19	0.19
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB3	19	0.19
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	11	0.19
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	11	0.19
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	11	0.19
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	18	0.19
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	18	0.19
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	18	0.19
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	5	0.19
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	5	0.19
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	19	0.19
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	19	0.19
(1,1002)	1:C:136:LEU:HD11	1:C:137:MET:HG2	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:C:136:LEU:HD11	1:C:137:MET:HG3	14	0.18
(1,1002)	1:C:136:LEU:HD12	1:C:137:MET:HG2	14	0.18
(1,1002)	1:C:136:LEU:HD12	1:C:137:MET:HG3	14	0.18
(1,1002)	1:C:136:LEU:HD13	1:C:137:MET:HG2	14	0.18
(1,1002)	1:C:136:LEU:HD13	1:C:137:MET:HG3	14	0.18
(1,1002)	1:C:136:LEU:HD21	1:C:137:MET:HG2	14	0.18
(1,1002)	1:C:136:LEU:HD21	1:C:137:MET:HG3	14	0.18
(1,1002)	1:C:136:LEU:HD22	1:C:137:MET:HG2	14	0.18
(1,1002)	1:C:136:LEU:HD22	1:C:137:MET:HG3	14	0.18
(1,1002)	1:C:136:LEU:HD23	1:C:137:MET:HG2	14	0.18
(1,1002)	1:C:136:LEU:HD23	1:C:137:MET:HG3	14	0.18
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB2	11	0.17
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB3	11	0.17
(1,842)	1:C:91:GLY:H	1:C:92:LYS:HB2	14	0.17
(1,842)	1:C:91:GLY:H	1:C:92:LYS:HB3	14	0.17
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	15	0.17
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	15	0.17
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	15	0.17
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	4	0.17
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	4	0.17
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	10	0.17
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	10	0.17
(1,528)	1:C:121:LEU:HD11	1:C:124:THR:H	18	0.17
(1,528)	1:C:121:LEU:HD12	1:C:124:THR:H	18	0.17
(1,528)	1:C:121:LEU:HD13	1:C:124:THR:H	18	0.17
(1,468)	1:C:143:ASN:H	1:C:144:ASN:H	11	0.17
(1,420)	1:C:128:ILE:HG21	1:C:131:ASP:H	13	0.17
(1,420)	1:C:128:ILE:HG22	1:C:131:ASP:H	13	0.17
(1,420)	1:C:128:ILE:HG23	1:C:131:ASP:H	13	0.17
(1,159)	1:C:135:GLU:HG2	1:C:138:LYS:HD2	15	0.17
(1,159)	1:C:135:GLU:HG2	1:C:138:LYS:HD3	15	0.17
(1,922)	1:C:111:TYR:HE1	1:C:147:ARG:HD2	2	0.16
(1,922)	1:C:111:TYR:HE1	1:C:147:ARG:HD3	2	0.16
(1,922)	1:C:111:TYR:HE2	1:C:147:ARG:HD2	2	0.16
(1,922)	1:C:111:TYR:HE2	1:C:147:ARG:HD3	2	0.16
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB2	6	0.16
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB3	6	0.16
(1,568)	1:C:102:ARG:H	1:C:153:PHE:HD1	8	0.16
(1,568)	1:C:102:ARG:H	1:C:153:PHE:HD2	8	0.16
(1,496)	1:C:142:LYS:H	1:C:143:ASN:H	15	0.16
(1,1002)	1:C:136:LEU:HD11	1:C:137:MET:HG2	4	0.16
(1,1002)	1:C:136:LEU:HD11	1:C:137:MET:HG3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:C:136:LEU:HD12	1:C:137:MET:HG2	4	0.16
(1,1002)	1:C:136:LEU:HD12	1:C:137:MET:HG3	4	0.16
(1,1002)	1:C:136:LEU:HD13	1:C:137:MET:HG2	4	0.16
(1,1002)	1:C:136:LEU:HD13	1:C:137:MET:HG3	4	0.16
(1,1002)	1:C:136:LEU:HD21	1:C:137:MET:HG2	4	0.16
(1,1002)	1:C:136:LEU:HD21	1:C:137:MET:HG3	4	0.16
(1,1002)	1:C:136:LEU:HD22	1:C:137:MET:HG2	4	0.16
(1,1002)	1:C:136:LEU:HD22	1:C:137:MET:HG3	4	0.16
(1,1002)	1:C:136:LEU:HD23	1:C:137:MET:HG2	4	0.16
(1,1002)	1:C:136:LEU:HD23	1:C:137:MET:HG3	4	0.16
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD11	20	0.15
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD12	20	0.15
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD13	20	0.15
(1,700)	1:C:122:GLN:H	1:C:128:ILE:HD11	2	0.15
(1,700)	1:C:122:GLN:H	1:C:128:ILE:HD12	2	0.15
(1,700)	1:C:122:GLN:H	1:C:128:ILE:HD13	2	0.15
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	5	0.15
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	5	0.15
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	5	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	3	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	3	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	6	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	6	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	13	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	13	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	17	0.15
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	17	0.15
(1,578)	1:C:113:ASP:H	1:C:117:LEU:HA	20	0.15
(1,518)	1:C:97:LEU:HB3	1:C:157:MET:H	11	0.15
(1,421)	1:C:131:ASP:H	1:C:133:ILE:HD11	20	0.15
(1,421)	1:C:131:ASP:H	1:C:133:ILE:HD12	20	0.15
(1,421)	1:C:131:ASP:H	1:C:133:ILE:HD13	20	0.15
(1,191)	1:C:128:ILE:HG21	1:C:131:ASP:HB2	1	0.15
(1,191)	1:C:128:ILE:HG21	1:C:131:ASP:HB3	1	0.15
(1,191)	1:C:128:ILE:HG22	1:C:131:ASP:HB2	1	0.15
(1,191)	1:C:128:ILE:HG22	1:C:131:ASP:HB3	1	0.15
(1,191)	1:C:128:ILE:HG23	1:C:131:ASP:HB2	1	0.15
(1,191)	1:C:128:ILE:HG23	1:C:131:ASP:HB3	1	0.15
(1,97)	1:C:128:ILE:HG12	1:C:133:ILE:HA	16	0.14
(1,97)	1:C:128:ILE:HG13	1:C:133:ILE:HA	16	0.14
(1,830)	1:C:100:LEU:HB2	1:C:153:PHE:HD1	18	0.14
(1,830)	1:C:100:LEU:HB2	1:C:153:PHE:HD2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,830)	1:C:100:LEU:HB2	1:C:153:PHE:HD1	19	0.14
(1,830)	1:C:100:LEU:HB2	1:C:153:PHE:HD2	19	0.14
(1,829)	1:C:150:TYR:HE1	1:C:154:LEU:HA	1	0.14
(1,829)	1:C:150:TYR:HE2	1:C:154:LEU:HA	1	0.14
(1,827)	1:C:153:PHE:HD1	1:C:156:PHE:HZ	20	0.14
(1,827)	1:C:153:PHE:HD2	1:C:156:PHE:HZ	20	0.14
(1,705)	1:C:121:LEU:HG	1:C:128:ILE:H	4	0.14
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	2	0.14
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	2	0.14
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	2	0.14
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	5	0.14
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	5	0.14
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	5	0.14
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	1	0.14
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	1	0.14
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	1	0.14
(1,496)	1:C:142:LYS:H	1:C:143:ASN:H	12	0.14
(1,286)	1:C:106:LYS:HB2	1:C:117:LEU:H	11	0.14
(1,286)	1:C:106:LYS:HB3	1:C:117:LEU:H	11	0.14
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD2	16	0.14
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD3	16	0.14
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG21	11	0.13
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG22	11	0.13
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG23	11	0.13
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG21	11	0.13
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG22	11	0.13
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG23	11	0.13
(1,928)	1:C:113:ASP:H	1:C:147:ARG:HB2	8	0.13
(1,928)	1:C:113:ASP:H	1:C:147:ARG:HB3	8	0.13
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB2	17	0.13
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB3	17	0.13
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	4	0.13
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	4	0.13
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	4	0.13
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	20	0.13
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	20	0.13
(1,590)	1:C:105:ASP:H	1:C:108:ALA:H	8	0.13
(1,518)	1:C:97:LEU:HB3	1:C:157:MET:H	8	0.13
(1,518)	1:C:97:LEU:HB3	1:C:157:MET:H	13	0.13
(1,1016)	1:C:137:MET:HG2	1:C:141:ASP:H	16	0.13
(1,1016)	1:C:137:MET:HG3	1:C:141:ASP:H	16	0.13
(1,98)	1:C:133:ILE:HA	1:C:136:LEU:HG	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:C:120:MET:H	1:C:121:LEU:HD11	19	0.12
(1,943)	1:C:120:MET:H	1:C:121:LEU:HD12	19	0.12
(1,943)	1:C:120:MET:H	1:C:121:LEU:HD13	19	0.12
(1,943)	1:C:120:MET:H	1:C:121:LEU:HD21	19	0.12
(1,943)	1:C:120:MET:H	1:C:121:LEU:HD22	19	0.12
(1,943)	1:C:120:MET:H	1:C:121:LEU:HD23	19	0.12
(1,928)	1:C:113:ASP:H	1:C:147:ARG:HB2	14	0.12
(1,928)	1:C:113:ASP:H	1:C:147:ARG:HB3	14	0.12
(1,867)	1:C:97:LEU:HD11	1:C:157:MET:HB2	9	0.12
(1,867)	1:C:97:LEU:HD11	1:C:157:MET:HB3	9	0.12
(1,867)	1:C:97:LEU:HD12	1:C:157:MET:HB2	9	0.12
(1,867)	1:C:97:LEU:HD12	1:C:157:MET:HB3	9	0.12
(1,867)	1:C:97:LEU:HD13	1:C:157:MET:HB2	9	0.12
(1,867)	1:C:97:LEU:HD13	1:C:157:MET:HB3	9	0.12
(1,867)	1:C:97:LEU:HD21	1:C:157:MET:HB2	9	0.12
(1,867)	1:C:97:LEU:HD21	1:C:157:MET:HB3	9	0.12
(1,867)	1:C:97:LEU:HD22	1:C:157:MET:HB2	9	0.12
(1,867)	1:C:97:LEU:HD22	1:C:157:MET:HB3	9	0.12
(1,867)	1:C:97:LEU:HD23	1:C:157:MET:HB2	9	0.12
(1,867)	1:C:97:LEU:HD23	1:C:157:MET:HB3	9	0.12
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB2	14	0.12
(1,844)	1:C:92:LYS:H	1:C:93:SER:HB3	14	0.12
(1,842)	1:C:91:GLY:H	1:C:92:LYS:HB2	17	0.12
(1,842)	1:C:91:GLY:H	1:C:92:LYS:HB3	17	0.12
(1,827)	1:C:153:PHE:HD1	1:C:156:PHE:HZ	9	0.12
(1,827)	1:C:153:PHE:HD2	1:C:156:PHE:HZ	9	0.12
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD11	19	0.12
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD12	19	0.12
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD13	19	0.12
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD11	8	0.12
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD12	8	0.12
(1,663)	1:C:124:THR:H	1:C:128:ILE:HD13	8	0.12
(1,653)	1:C:96:GLU:H	1:C:97:LEU:HG	17	0.12
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	11	0.12
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	11	0.12
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	15	0.12
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	15	0.12
(1,617)	1:C:128:ILE:HD11	1:C:133:ILE:H	14	0.12
(1,617)	1:C:128:ILE:HD12	1:C:133:ILE:H	14	0.12
(1,617)	1:C:128:ILE:HD13	1:C:133:ILE:H	14	0.12
(1,590)	1:C:105:ASP:H	1:C:108:ALA:H	1	0.12
(1,475)	1:C:108:ALA:H	1:C:111:TYR:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:C:128:ILE:HG21	1:C:131:ASP:H	8	0.12
(1,420)	1:C:128:ILE:HG22	1:C:131:ASP:H	8	0.12
(1,420)	1:C:128:ILE:HG23	1:C:131:ASP:H	8	0.12
(1,405)	1:C:136:LEU:HG	1:C:137:MET:H	20	0.12
(1,193)	1:C:114:LEU:HG	1:C:115:ASP:HB3	11	0.12
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD2	6	0.12
(1,160)	1:C:135:GLU:HG3	1:C:138:LYS:HD3	6	0.12
(1,14)	1:C:117:LEU:HG	1:C:120:MET:HE1	13	0.12
(1,14)	1:C:117:LEU:HG	1:C:120:MET:HE2	13	0.12
(1,14)	1:C:117:LEU:HG	1:C:120:MET:HE3	13	0.12
(1,98)	1:C:133:ILE:HA	1:C:136:LEU:HG	16	0.11
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG21	3	0.11
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG22	3	0.11
(1,949)	1:C:120:MET:HB2	1:C:124:THR:HG23	3	0.11
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG21	3	0.11
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG22	3	0.11
(1,949)	1:C:120:MET:HB3	1:C:124:THR:HG23	3	0.11
(1,922)	1:C:111:TYR:HE1	1:C:147:ARG:HD2	11	0.11
(1,922)	1:C:111:TYR:HE1	1:C:147:ARG:HD3	11	0.11
(1,922)	1:C:111:TYR:HE2	1:C:147:ARG:HD2	11	0.11
(1,922)	1:C:111:TYR:HE2	1:C:147:ARG:HD3	11	0.11
(1,827)	1:C:153:PHE:HD1	1:C:156:PHE:HZ	10	0.11
(1,827)	1:C:153:PHE:HD2	1:C:156:PHE:HZ	10	0.11
(1,780)	1:C:111:TYR:HD1	1:C:147:ARG:HG2	5	0.11
(1,780)	1:C:111:TYR:HD1	1:C:147:ARG:HG3	5	0.11
(1,780)	1:C:111:TYR:HD2	1:C:147:ARG:HG2	5	0.11
(1,780)	1:C:111:TYR:HD2	1:C:147:ARG:HG3	5	0.11
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD11	7	0.11
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD12	7	0.11
(1,710)	1:C:142:LYS:H	1:C:148:ILE:HD13	7	0.11
(1,696)	1:C:128:ILE:HD11	1:C:132:ASP:H	1	0.11
(1,696)	1:C:128:ILE:HD12	1:C:132:ASP:H	1	0.11
(1,696)	1:C:128:ILE:HD13	1:C:132:ASP:H	1	0.11
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD1	8	0.11
(1,640)	1:C:152:GLU:H	1:C:153:PHE:HD2	8	0.11
(1,590)	1:C:105:ASP:H	1:C:108:ALA:H	4	0.11
(1,584)	1:C:106:LYS:H	1:C:117:LEU:H	2	0.11
(1,582)	1:C:106:LYS:H	1:C:106:LYS:HE2	9	0.11
(1,582)	1:C:106:LYS:H	1:C:106:LYS:HE3	9	0.11
(1,578)	1:C:113:ASP:H	1:C:117:LEU:HA	13	0.11
(1,405)	1:C:136:LEU:HG	1:C:137:MET:H	13	0.11
(1,1000)	1:C:136:LEU:HD11	1:C:137:MET:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:C:136:LEU:HD12	1:C:137:MET:HA	5	0.11
(1,1000)	1:C:136:LEU:HD13	1:C:137:MET:HA	5	0.11
(1,1000)	1:C:136:LEU:HD21	1:C:137:MET:HA	5	0.11
(1,1000)	1:C:136:LEU:HD22	1:C:137:MET:HA	5	0.11
(1,1000)	1:C:136:LEU:HD23	1:C:137:MET:HA	5	0.11

10 Dihedral-angle violation analysis (i)

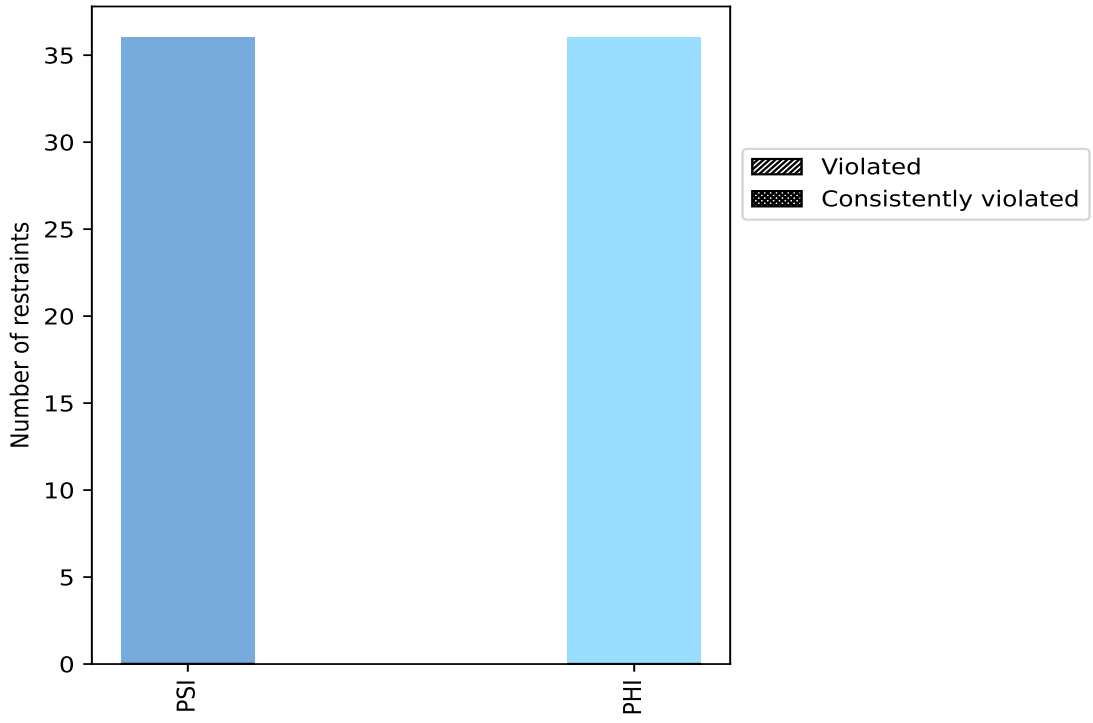
10.1 Summary of dihedral-angle violations (i)

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]
PSI	36	50.0	0	0.0	0.0	0	0.0	0.0
PHI	36	50.0	0	0.0	0.0	0	0.0	0.0
Total	72	100.0	0	0.0	0.0	0	0.0	0.0

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

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



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

10.2 Dihedral-angle violation statistics for each model (i)

No violations found

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

No violations found

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

No violations found

10.5 All violated dihedral-angle restraints (i)

No violations found