WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 12:27 AM EDT

PDB ID	:	2L06
BMRB ID	:	17031
Title	:	Solution NMR structure of the PBS linker polypeptide domain (fragment 254-400) of phycobilisome linker protein ApcE from Synechocystis sp. PCC 6803. Northeast Structural Genomics Consortium Target SgR209C
Authors	:	Ramelot, T.A.; Yang, Y.; Cort, J.R.; Hamilton, K.; Ciccosanti, C.; Lee, D.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-06-30

The following versions of software and data (see references ⓘ) 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 ⓘ

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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.8%
Sidechain outliers		2.5%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures
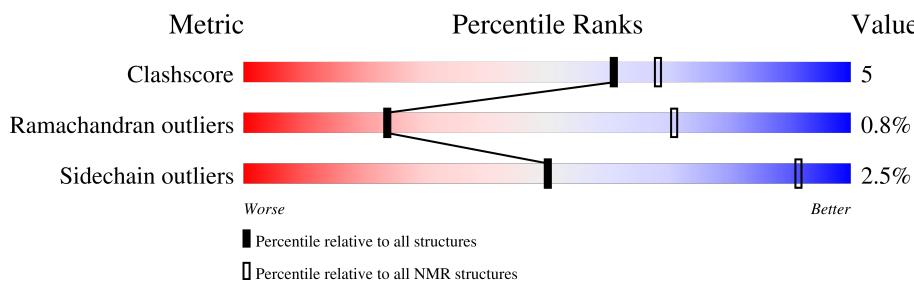
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	155	76% • 20%
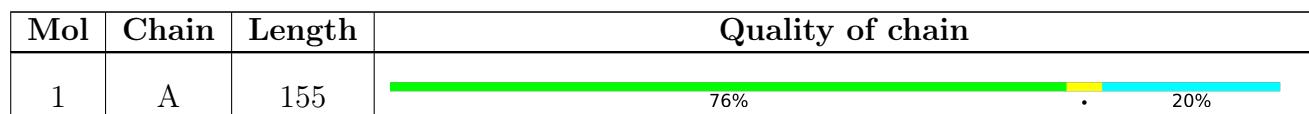
2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 13 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:14-A:38, A:45-A:143 (124)	1.10	13

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

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

The models can be grouped into 4 clusters and 4 single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 2517 atoms, of which 1253 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Phycobilisome LCM core-membrane linker polypeptide.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	155	2517	806	1253	227	229	2	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	GLU	-	expression tag	UNP Q55544
A	150	HIS	-	expression tag	UNP Q55544
A	151	HIS	-	expression tag	UNP Q55544
A	152	HIS	-	expression tag	UNP Q55544
A	153	HIS	-	expression tag	UNP Q55544
A	154	HIS	-	expression tag	UNP Q55544
A	155	HIS	-	expression tag	UNP Q55544

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: Phycobilisome LCM core-membrane linker polypeptide

Chain A:
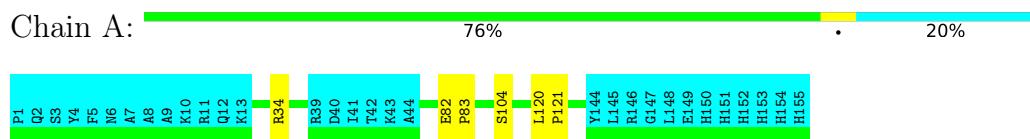
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:
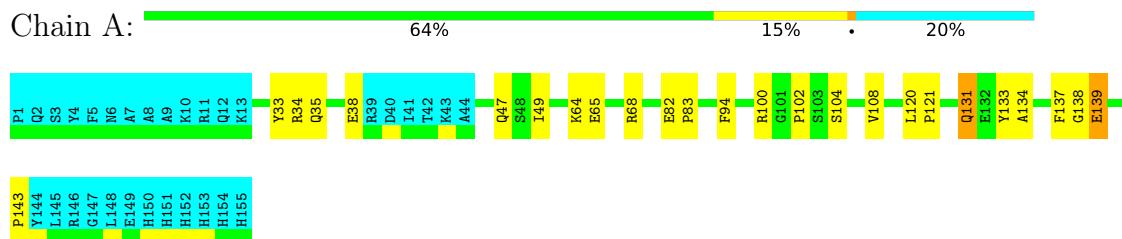
4.2.2 Score per residue for model 2

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:

H150 H151 H152 H153 H154 H155
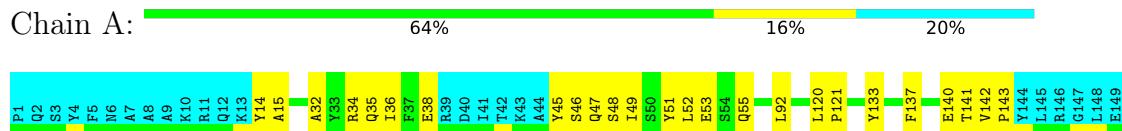
4.2.3 Score per residue for model 3

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 67%   11% ·   20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 R39 D40 I41 T42 K43 A44 Y45 S48 T49 S50 Y51 L52 E53 S54 Q55 E65 R69 L75 Q79 F84 I85 E91 F94 S104 V108 L120 P121 E139 Y144 L145 R146 G147 L148

E149 H150 H151 H152 H153 H154 H155
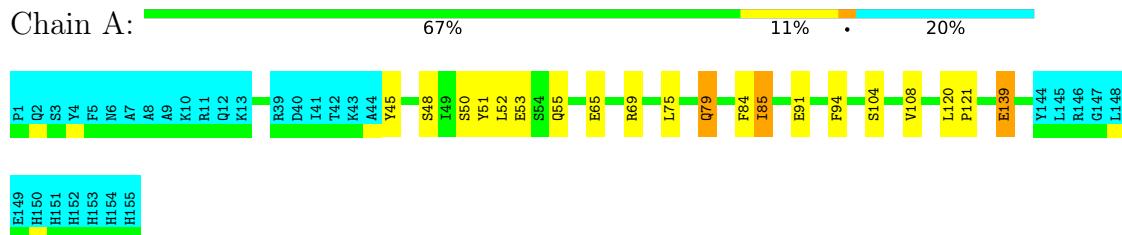
4.2.4 Score per residue for model 4

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 72%   8% ·   20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 R34 Q35 E38 R39 D40 I41 T42 K43 A44 Y45 E82 P83 F84 G99 S104 V108 L120 P121 E139 P143 Y144 L145 R146 G147 L148 E149 H150 H151 H152 H153 H154 H155
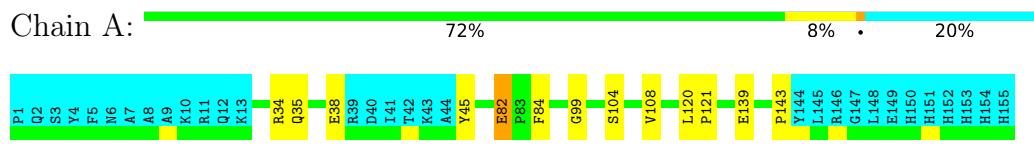
4.2.5 Score per residue for model 5

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 66%   13% ·   20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 R39 D40 I41 T42 K43 A44 Y51 Q55 F66 L70 A71 K72 E82 P83 F84 I85 P102 S103 S104 V108 L120 P121 Y133 A134 D135 Y136 F137 G138 E139 E140 T141 V142 P143 Y144 L145 R146 G147

L148 E149 H150 H151 H152 H153 H154 H155
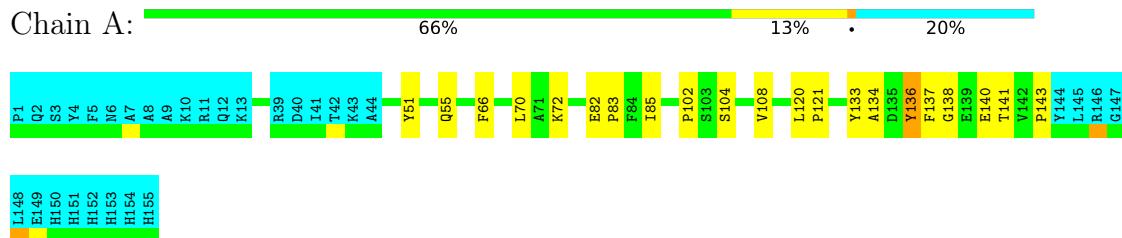
4.2.6 Score per residue for model 6

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 65%   14% ·   20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 K17 P18 G19 L20 S21 Y33 R34 E38 R39 D40 I41 T42 K43 A44 Y45 S46 I49 K64 F81 E82 P83 L98 S104 R105 E106 E107 V108 L120 P121 L127 V128 D129 F137 Y144 L145

R146 G147 L148 E149 H150 H151 H152 H153 H154 H155

4.2.7 Score per residue for model 7

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:

62% 17% • 20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 Y14 A15 M16 E24 V28 A32 Y33 R34 Q35 I36 F37 E38 R39 D40 I41 T42 K43 A44 Y45 S46 Y51 Q55 K64 E65 F66 V67 L70 Y76 E82 P83 S104 V108 L120 P121

E139 E140 P143 Y144 L145 R146 G147 L148 E149 H150 H151 H152 H153 H154 H155
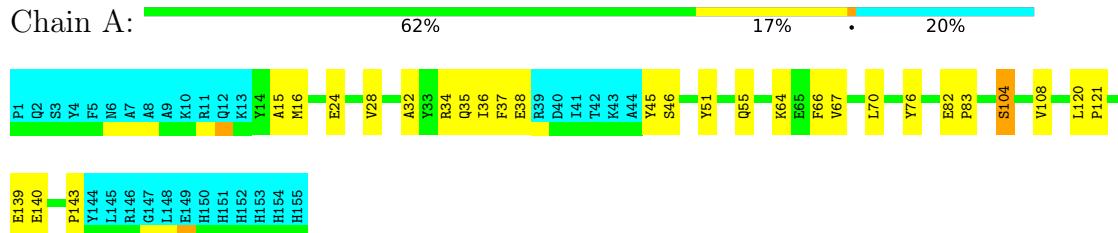
4.2.8 Score per residue for model 8

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:

68% 12% 20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 M16 S21 E24 F37 E38 R39 D40 I41 T42 K43 A44 Y51 Q55 V56 R69 L75 Y76 R77 F81 L90 F94 R100 L120 P121 A122 L123 Y144 L145 R146 G147 L148 E149 H150

H151 H152 H153 H154 H155
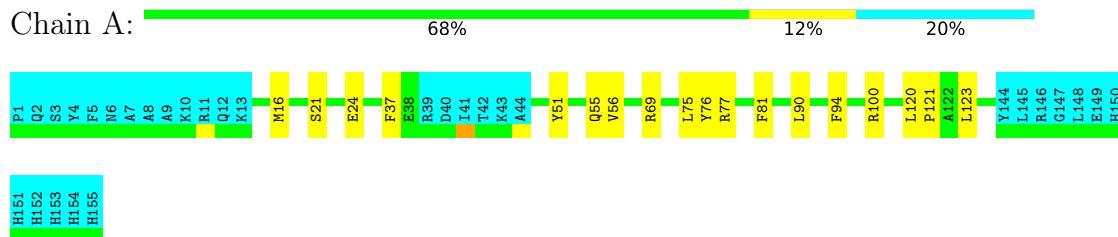
4.2.9 Score per residue for model 9

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:

69% 11% 20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 E24 V28 I36 R39 D40 I41 T42 K43 A44 M63 V67 R68 R69 K72 E82 P83 F94 R95 H96 S104 E107 V108 L120 P121 P143 Y144 L145 R146 G147 L148 E149 H150 H151 H152

H153 H154 H155
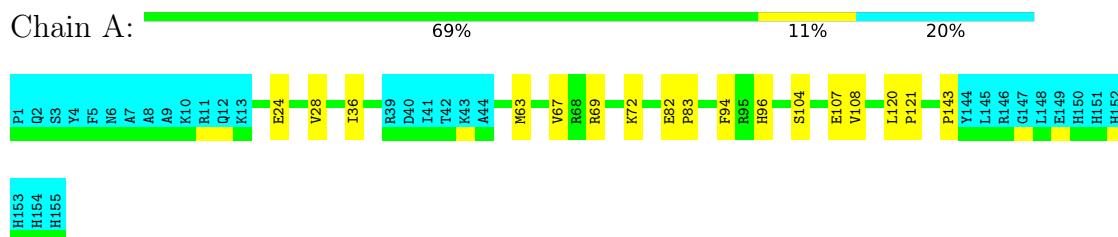
4.2.10 Score per residue for model 10

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:

71% 9% 20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 Y14 A15 M16 Q35 I36 R39 D40 I41 T42 K43 A44 V56 K64 R69 E82 P83 N86 A134 G138 E139 P143 Y144 L145 R146 G147 L148 E149 H150 H151 H152 H153 H154 H155

4.2.11 Score per residue for model 11

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 68%   11%   •   20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 M16 K25 I29 R39 D40 I41 T42 K43 A44 Y45 S46 Q47 S48 I49 S50 E53 M63 K64 K72 Y76 F80 E91 V115 G119 L120 P121 A134 Y144 L145 R146 G147 L148 E149

H150 H151 H152 H153 H154 H155
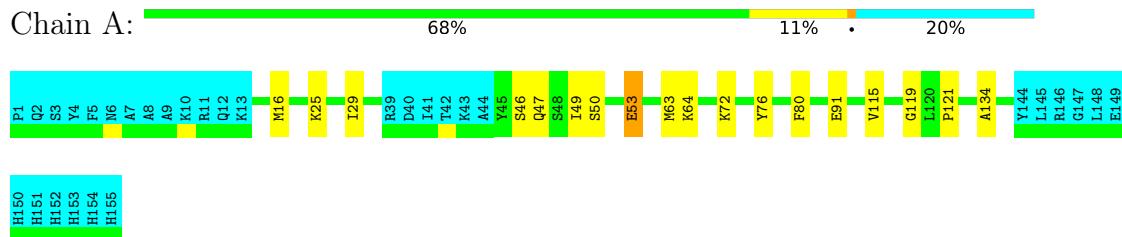
4.2.12 Score per residue for model 12

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 70%   10%   20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 K17 E24 V28 R34 R39 D40 I41 T42 K43 A44 S48 L52 E53 R57 M63 K72 L75 Q79 G99 D125 E140 T141 V142 P143 Y144 L145 R146 G147 L148 E149 H150 H151

H152 H153 H154 H155
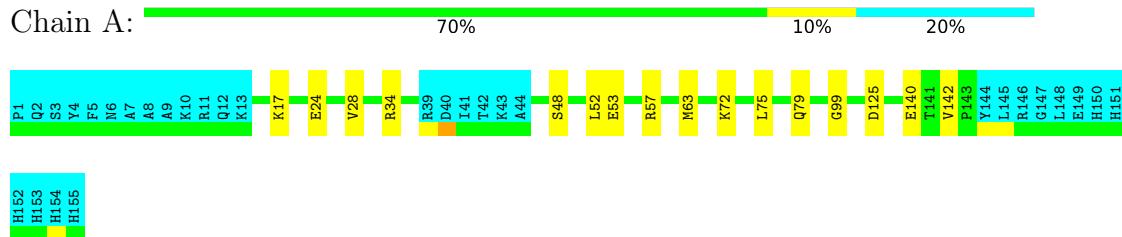
4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 70%   10%   •   20%

P1 Q2 S3 Y4 F5 N6 A7 A8 A9 K10 R11 Q12 K13 K17 L20 E24 R34 E38 R39 D40 I41 T42 K43 A44 E65 R69 L70 A71 L75 Y76 R77 K78 Q79 E82 P83 R95 E132 Y144 L145 R146 G147 L148 E149 H150 H151 H152 H153 H154

H155
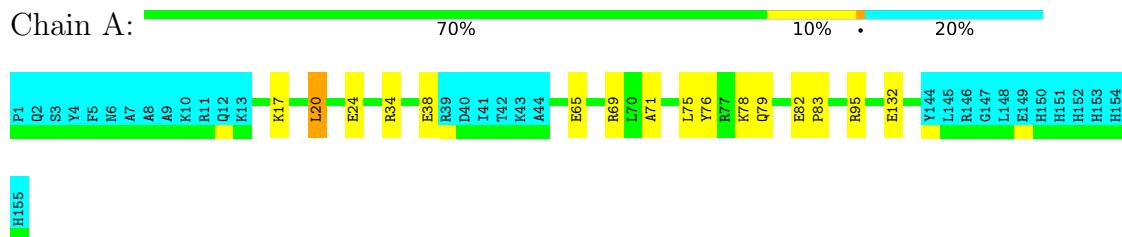
4.2.14 Score per residue for model 14

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A: 66%   14%   •   20%

4.2.15 Score per residue for model 15

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:
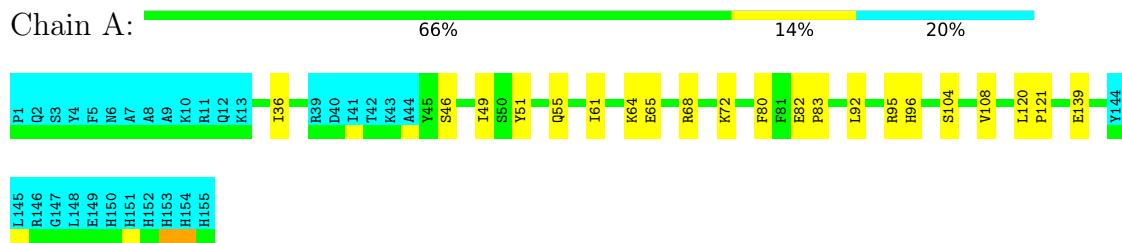
4.2.16 Score per residue for model 16

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:
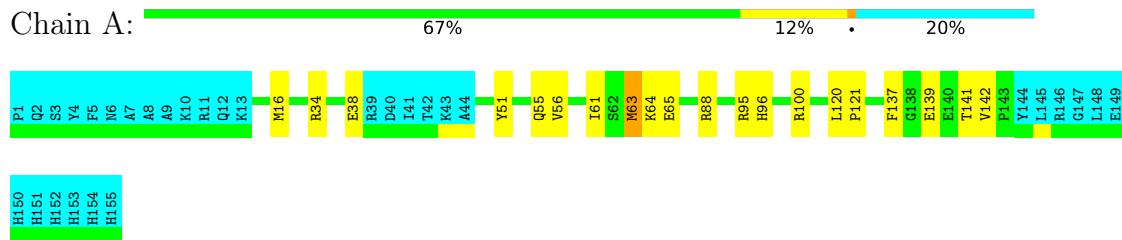
### 4.2.17 Score per residue for model 17

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:
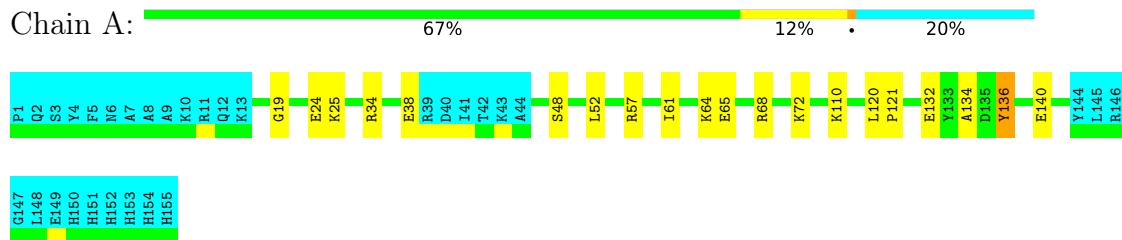
### 4.2.18 Score per residue for model 18

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:
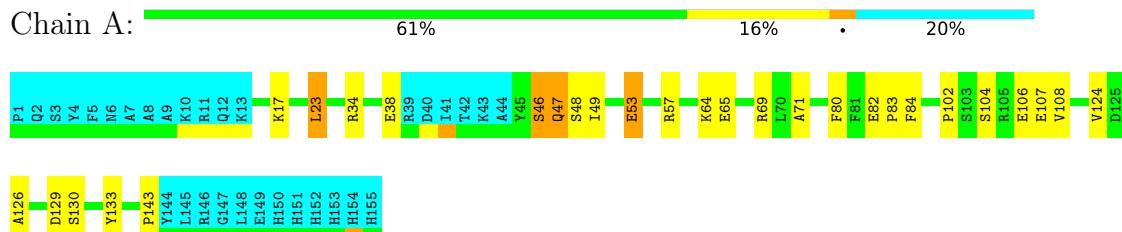
4.2.19 Score per residue for model 19

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:

4.2.20 Score per residue for model 20

• Molecule 1: Phycobilisome LCM core-membrane linker polypeptide

Chain A:
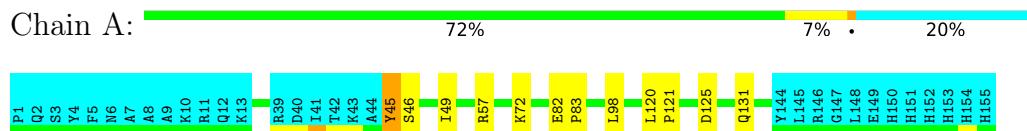
5 Refinement protocol and experimental data overview ⓘ

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

Of the 125 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.25
X-PLOR NIH	refinement	2.25

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	1833
Number of shifts mapped to atoms	1833
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 ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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	997	991	990	9±3
All	All	19940	19820	19800	182

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:133:TYR:HA	1:A:137:PHE:HD2	0.67	1.49	2	1
1:A:131:GLN:HE21	1:A:131:GLN:HA	0.65	1.51	1	1
1:A:47:GLN:HG3	1:A:48:SER:H	0.63	1.53	18	1
1:A:34:ARG:O	1:A:38:GLU:HA	0.62	1.94	13	10
1:A:64:LYS:HE2	1:A:134:ALA:HA	0.62	1.69	11	2
1:A:65:GLU:O	1:A:69:ARG:HG2	0.62	1.95	13	2
1:A:77:ARG:HG2	1:A:120:LEU:HD23	0.60	1.74	8	1
1:A:64:LYS:HB2	1:A:139:GLU:HB2	0.59	1.71	10	3
1:A:16:MET:HB2	1:A:63:MET:HB2	0.59	1.75	11	1
1:A:46:SER:HA	1:A:49:ILE:HB	0.59	1.72	18	3
1:A:79:GLN:HE21	1:A:79:GLN:HA	0.58	1.58	3	1
1:A:65:GLU:HA	1:A:68:ARG:HG2	0.57	1.75	1	1
1:A:104:SER:HB2	1:A:107:GLU:HB3	0.55	1.78	9	1
1:A:36:ILE:HA	1:A:96:HIS:CE1	0.54	2.37	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:17:LYS:HB2	1:A:20:LEU:HB3	0.54	1.78	13	2
1:A:120:LEU:N	1:A:121:PRO:HD2	0.54	2.17	3	11
1:A:17:LYS:HG3	1:A:20:LEU:HB3	0.53	1.78	14	1
1:A:51:TYR:O	1:A:55:GLN:HG2	0.53	2.03	15	4
1:A:61:ILE:HB	1:A:65:GLU:HB2	0.53	1.80	16	3
1:A:15:ALA:HA	1:A:140:GLU:O	0.53	2.03	7	2
1:A:32:ALA:O	1:A:36:ILE:HG12	0.52	2.04	7	2
1:A:104:SER:HB2	1:A:106:GLU:OE1	0.51	2.05	6	1
1:A:53:GLU:O	1:A:57:ARG:HB2	0.51	2.04	18	1
1:A:65:GLU:HB3	1:A:69:ARG:HH21	0.51	1.65	19	1
1:A:51:TYR:O	1:A:55:GLN:HG3	0.51	2.06	5	3
1:A:104:SER:HB2	1:A:107:GLU:CB	0.51	2.35	9	1
1:A:72:LYS:HG3	1:A:121:PRO:HB3	0.50	1.83	5	1
1:A:64:LYS:HE2	1:A:129:ASP:HA	0.50	1.82	6	1
1:A:133:TYR:HA	1:A:137:PHE:CD2	0.50	2.37	2	1
1:A:45:TYR:HB3	1:A:75:LEU:HD23	0.49	1.84	3	1
1:A:17:LYS:O	1:A:20:LEU:HD12	0.49	2.08	6	2
1:A:25:LYS:HD3	1:A:57:ARG:HA	0.49	1.84	17	1
1:A:25:LYS:O	1:A:29:ILE:HG13	0.49	2.08	19	2
1:A:72:LYS:HE3	1:A:125:ASP:HB3	0.49	1.83	20	1
1:A:21:SER:HB2	1:A:24:GLU:OE1	0.48	2.09	8	1
1:A:64:LYS:HE3	1:A:129:ASP:HA	0.48	1.86	18	1
1:A:66:PHE:O	1:A:70:LEU:HG	0.47	2.09	19	4
1:A:74:PRO:O	1:A:78:LYS:HB2	0.47	2.09	19	1
1:A:16:MET:SD	1:A:56:VAL:HG22	0.47	2.49	16	3
1:A:63:MET:SD	1:A:142:VAL:HG22	0.47	2.49	16	2
1:A:75:LEU:O	1:A:79:GLN:HG2	0.47	2.08	13	2
1:A:137:PHE:HD2	1:A:141:THR:HB	0.47	1.70	16	1
1:A:33:TYR:CZ	1:A:49:ILE:HG23	0.47	2.45	1	2
1:A:94:PHE:HB3	1:A:100:ARG:O	0.47	2.10	8	2
1:A:54:SER:HA	1:A:57:ARG:CG	0.47	2.40	19	1
1:A:64:LYS:HE3	1:A:128:VAL:O	0.47	2.09	14	1
1:A:82:GLU:HB3	1:A:84:PHE:HD2	0.47	1.69	4	1
1:A:82:GLU:HB2	1:A:83:PRO:HD3	0.47	1.86	6	3
1:A:98:LEU:HD11	1:A:127:LEU:HD22	0.47	1.86	6	1
1:A:46:SER:CA	1:A:49:ILE:HB	0.46	2.40	18	1
1:A:132:GLU:O	1:A:136:TYR:HB2	0.46	2.10	17	1
1:A:104:SER:O	1:A:108:VAL:HG23	0.46	2.11	7	9
1:A:106:GLU:H	1:A:106:GLU:CD	0.46	2.14	18	1
1:A:72:LYS:HD2	1:A:125:ASP:HB2	0.46	1.88	12	1
1:A:48:SER:O	1:A:52:LEU:HG	0.46	2.10	3	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:37:PHE:HE1	1:A:76:TYR:HB2	0.46	1.70	7	1
1:A:24:GLU:O	1:A:28:VAL:HG23	0.45	2.11	14	4
1:A:23:LEU:HD22	1:A:23:LEU:C	0.45	2.31	18	1
1:A:71:ALA:HA	1:A:76:TYR:CD2	0.45	2.46	13	1
1:A:80:PHE:HA	1:A:84:PHE:HD2	0.45	1.72	18	1
1:A:102:PRO:HB2	1:A:108:VAL:HG22	0.45	1.89	5	3
1:A:82:GLU:HB3	1:A:83:PRO:HD3	0.45	1.88	18	6
1:A:25:LYS:HD2	1:A:57:ARG:O	0.45	2.12	19	1
1:A:37:PHE:HA	1:A:76:TYR:CE1	0.45	2.47	8	1
1:A:54:SER:HA	1:A:57:ARG:HG3	0.45	1.88	19	1
1:A:36:ILE:HA	1:A:96:HIS:NE2	0.45	2.27	15	1
1:A:45:TYR:CG	1:A:49:ILE:HD11	0.44	2.47	20	1
1:A:65:GLU:HG3	1:A:68:ARG:HE	0.44	1.72	1	1
1:A:133:TYR:O	1:A:136:TYR:HB2	0.44	2.12	5	1
1:A:84:PHE:O	1:A:85:ILE:HB	0.44	2.12	3	1
1:A:104:SER:O	1:A:107:GLU:HB3	0.44	2.13	18	1
1:A:78:LYS:HG3	1:A:82:GLU:HG2	0.44	1.90	13	1
1:A:121:PRO:O	1:A:125:ASP:HB2	0.43	2.12	14	1
1:A:126:ALA:O	1:A:130:SER:HB2	0.43	2.12	18	1
1:A:133:TYR:HA	1:A:137:PHE:CD1	0.43	2.49	1	1
1:A:37:PHE:HA	1:A:76:TYR:HE1	0.43	1.72	8	1
1:A:139:GLU:H	1:A:139:GLU:CD	0.43	2.16	3	1
1:A:65:GLU:HB3	1:A:69:ARG:NH1	0.43	2.29	3	1
1:A:95:ARG:HA	1:A:100:ARG:O	0.43	2.13	16	1
1:A:37:PHE:O	1:A:38:GLU:HB3	0.43	2.13	7	1
1:A:134:ALA:O	1:A:138:GLY:HA2	0.43	2.14	10	1
1:A:130:SER:HB3	1:A:133:TYR:CD2	0.43	2.49	18	1
1:A:80:PHE:HE1	1:A:92:LEU:HB3	0.43	1.74	15	1
1:A:76:TYR:O	1:A:80:PHE:HB2	0.42	2.14	11	1
1:A:82:GLU:N	1:A:83:PRO:HD2	0.42	2.29	5	1
1:A:45:TYR:CD1	1:A:49:ILE:HD11	0.42	2.50	20	1
1:A:50:SER:O	1:A:53:GLU:HG2	0.42	2.15	3	1
1:A:36:ILE:HD11	1:A:143:PRO:HG2	0.42	1.91	10	1
1:A:120:LEU:HB3	1:A:121:PRO:HD3	0.42	1.91	17	4
1:A:72:LYS:HG3	1:A:121:PRO:HA	0.42	1.92	11	1
1:A:67:VAL:HG21	1:A:143:PRO:HD2	0.41	1.90	9	1
1:A:17:LYS:HE2	1:A:140:GLU:OE2	0.41	2.15	12	1
1:A:79:GLN:O	1:A:80:PHE:HB2	0.41	2.15	14	1
1:A:45:TYR:HB3	1:A:49:ILE:HD12	0.41	1.93	19	1
1:A:139:GLU:CD	1:A:139:GLU:H	0.41	2.19	1	1
1:A:90:LEU:HD12	1:A:123:LEU:HD21	0.41	1.92	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ARG:O	1:A:72:LYS:HG3	0.41	2.16	17	1
1:A:20:LEU:HD23	1:A:24:GLU:HB2	0.41	1.92	13	1
1:A:80:PHE:HA	1:A:84:PHE:CD2	0.41	2.51	18	1
1:A:115:VAL:O	1:A:119:GLY:HA2	0.41	2.16	11	1
1:A:14:TYR:HB2	1:A:142:VAL:HB	0.41	1.93	2	1
1:A:82:GLU:H	1:A:83:PRO:HD2	0.41	1.76	20	1
1:A:104:SER:HB2	1:A:107:GLU:HB2	0.40	1.92	18	1
1:A:95:ARG:O	1:A:99:GLY:HA2	0.40	2.16	19	1
1:A:68:ARG:O	1:A:72:LYS:HG2	0.40	2.16	15	1
1:A:71:ALA:CB	1:A:124:VAL:HG11	0.40	2.47	18	1
1:A:69:ARG:HD3	1:A:72:LYS:HE2	0.40	1.93	9	1
1:A:50:SER:HA	1:A:53:GLU:HB3	0.40	1.92	11	1
1:A:132:GLU:CD	1:A:132:GLU:H	0.40	2.20	13	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	124/155 (80%)	117±2 (94±2%)	6±2 (5±2%)	1±1 (1±1%)	24	71
All	All	2480/3100 (80%)	2337 (94%)	123 (5%)	20 (1%)	24	71

All 9 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	46	SER	5
1	A	47	GLN	4
1	A	143	PRO	4
1	A	81	PHE	2
1	A	85	ILE	1
1	A	82	GLU	1
1	A	18	PRO	1
1	A	83	PRO	1
1	A	19	GLY	1

6.3.2 Protein sidechains ⓘ

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	106/132 (80%)	103±1 (98±1%)	3±1 (2±1%)	50	91
All	All	2120/2640 (80%)	2067 (98%)	53 (2%)	50	91

All 30 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	139	GLU	4
1	A	53	GLU	4
1	A	45	TYR	4
1	A	140	GLU	3
1	A	20	LEU	3
1	A	69	ARG	3
1	A	131	GLN	2
1	A	91	GLU	2
1	A	94	PHE	2
1	A	35	GLN	2
1	A	136	TYR	2
1	A	63	MET	2
1	A	57	ARG	2
1	A	47	GLN	2
1	A	92	LEU	1
1	A	79	GLN	1
1	A	85	ILE	1
1	A	141	THR	1
1	A	21	SER	1
1	A	137	PHE	1
1	A	16	MET	1
1	A	104	SER	1
1	A	86	ASN	1
1	A	95	ARG	1
1	A	88	ARG	1
1	A	24	GLU	1
1	A	110	LYS	1
1	A	17	LYS	1
1	A	23	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	98	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1833
Number of shifts mapped to atoms	1833
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	145	-0.62 ± 0.12	Should be checked
$^{13}C_\beta$	137	0.21 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	128	-0.36 ± 0.10	None needed (< 0.5 ppm)
^{15}N	136	0.65 ± 0.17	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1575 atoms were assigned a chemical shift out of a possible 1733. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	599/615 (97%)	248/249 (100%)	234/248 (94%)	117/118 (99%)
Sidechain	860/958 (90%)	577/622 (93%)	267/293 (91%)	16/43 (37%)

Continued on next page...

Continued from previous page...

	Total	**¹H**	**¹³C**	**¹⁵N**
Aromatic	116/160 (72%)	59/76 (78%)	57/82 (70%)	0/2 (0%)
Overall	1575/1733 (91%)	884/947 (93%)	558/623 (90%)	133/163 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1831 atoms were assigned a chemical shift out of a possible 2194. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**¹H**	**¹³C**	**¹⁵N**
Backbone	695/769 (90%)	286/311 (92%)	273/310 (88%)	136/148 (92%)
Sidechain	1012/1189 (85%)	676/770 (88%)	316/361 (88%)	20/58 (34%)
Aromatic	124/236 (53%)	63/113 (56%)	61/109 (56%)	0/14 (0%)
Overall	1831/2194 (83%)	1025/1194 (86%)	650/780 (83%)	156/220 (71%)

### 7.1.4   Statistically unusual chemical shifts ⓘ

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

List Id	**Chain**	**Res**	**Type**	**Atom**	**Shift, *ppm***	**Expected range, *ppm***	**Z-score**
1	A	143	PRO	HA	1.97	$2.78 - 6.00$	-7.5
1	A	83	PRO	HB2	0.33	$0.37 - 3.78$	-5.1

7.1.5   Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:
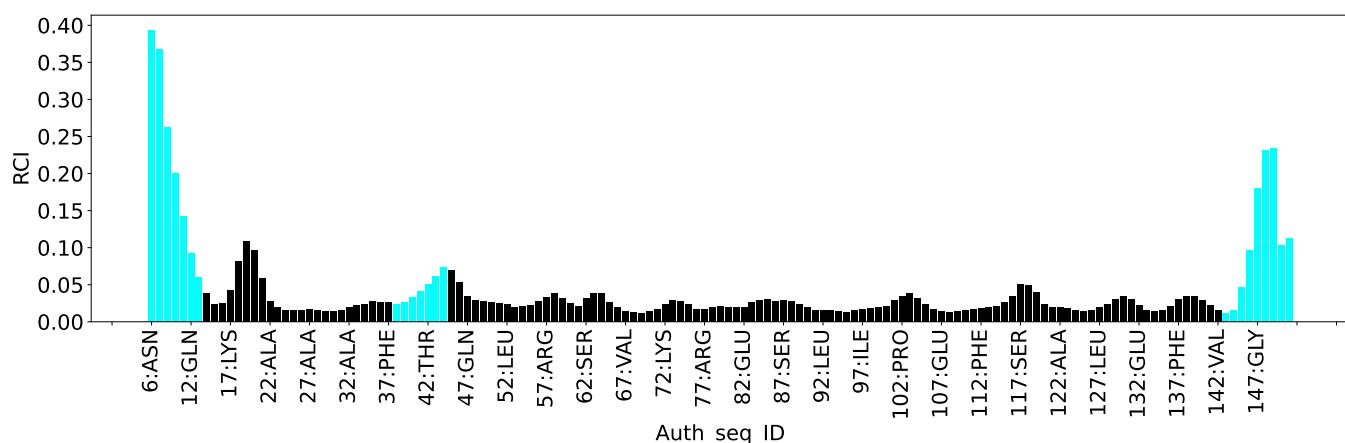
8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1906
Intra-residue ($|i-j|=0$)	497
Sequential ($|i-j|=1$)	465
Medium range ($|i-j|>1$ and $|i-j|<5$)	399
Long range ($|i-j|\geq 5$)	429
Inter-chain	0
Hydrogen bond restraints	116
Disulfide bond restraints	0
Total dihedral-angle restraints	196
Number of unmapped restraints	0
Number of restraints per residue	13.6
Number of long range restraints per residue[1]	2.8

[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 ⓘ

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model ⓘ

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	3.2	0.2
0.2-0.5 (Medium)	0.8	0.41
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.1	3.9
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9   Distance violation analysis ⓘ

9.1   Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	497	26.1	15	3.0	0.8	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	399	20.9	15	3.8	0.8	0	0.0	0.0
Sidechain-Sidechain	98	5.1	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	465	24.4	11	2.4	0.6	0	0.0	0.0
Backbone-Backbone	124	6.5	3	2.4	0.2	0	0.0	0.0
Backbone-Sidechain	280	14.7	7	2.5	0.4	0	0.0	0.0
Sidechain-Sidechain	61	3.2	1	1.6	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	399	20.9	12	3.0	0.6	0	0.0	0.0
Backbone-Backbone	108	5.7	2	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	159	8.3	2	1.3	0.1	0	0.0	0.0
Sidechain-Sidechain	132	6.9	8	6.1	0.4	0	0.0	0.0
Long range (|i-j|≥5)	429	22.5	12	2.8	0.6	0	0.0	0.0
Backbone-Backbone	9	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	159	8.3	2	1.3	0.1	0	0.0	0.0
Sidechain-Sidechain	261	13.7	10	3.8	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	116	6.1	1	0.9	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1906	100.0	51	2.7	2.7	0	0.0	0.0
Backbone-Backbone	357	18.7	6	1.7	0.3	0	0.0	0.0
Backbone-Sidechain	997	52.3	26	2.6	1.4	0	0.0	0.0
Sidechain-Sidechain	552	29.0	19	3.4	1.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations ⓘ
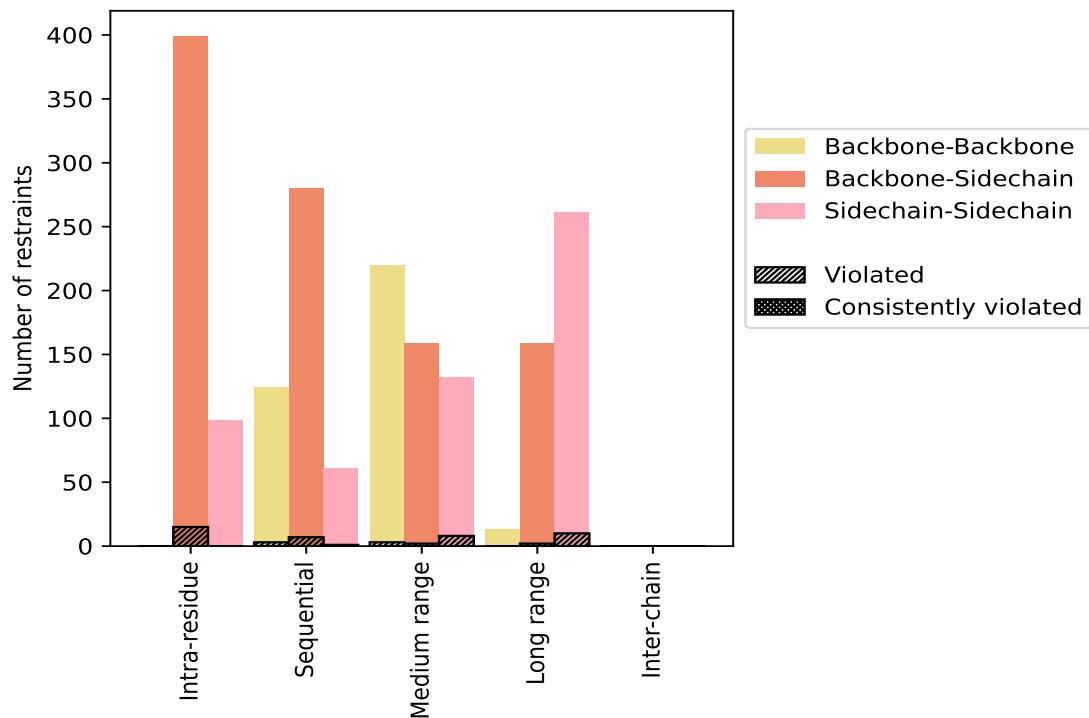
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model ⓘ

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	0	0	1	0	2	0.28	0.41	0.12	0.28
2	1	2	1	1	0	5	0.14	0.2	0.03	0.12
3	0	0	1	1	0	2	0.18	0.22	0.04	0.18
4	2	1	1	0	0	4	0.15	0.2	0.03	0.14
5	1	1	3	1	0	6	0.16	0.2	0.03	0.16
6	2	0	1	1	0	4	0.25	0.32	0.07	0.26
7	0	1	0	2	0	3	0.15	0.19	0.03	0.14
8	0	0	2	1	0	3	0.19	0.23	0.04	0.21
9	0	1	1	1	0	3	0.17	0.27	0.07	0.13
10	0	1	0	0	0	1	0.17	0.17	0.0	0.17
11	0	1	0	1	0	2	0.14	0.17	0.03	0.14

Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	2	1	2	2	0	7	0.2	0.33	0.08	0.17
14	2	3	4	1	0	10	0.18	0.35	0.08	0.15
15	1	1	1	1	0	4	0.18	0.4	0.12	0.12
16	0	1	0	0	0	1	0.11	0.11	0.0	0.11
17	0	3	0	0	0	3	0.15	0.18	0.03	0.15
18	5	1	0	0	0	6	0.15	0.24	0.05	0.12
19	3	1	1	1	0	6	0.13	0.15	0.01	0.13
20	2	3	2	1	0	8	0.15	0.22	0.03	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)
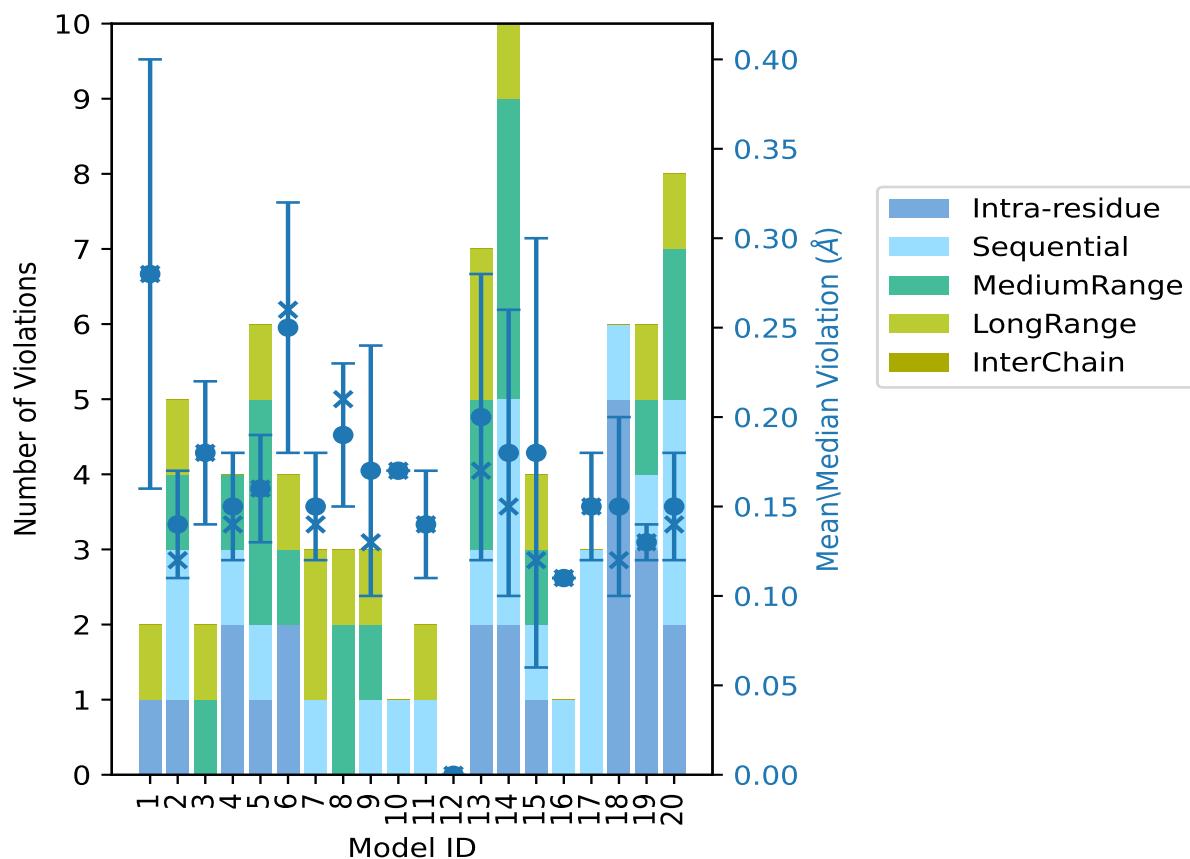
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3   Distance violation statistics for the ensemble ⓘ

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, 1740(IR:482, SQ:454, MR:387, LR:417, 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]	%
10	5	8	10	0	33	1	5.0
3	4	1	0	0	8	2	10.0
2	0	3	2	0	7	3	15.0
0	1	0	0	0	1	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	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	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 ⓘ
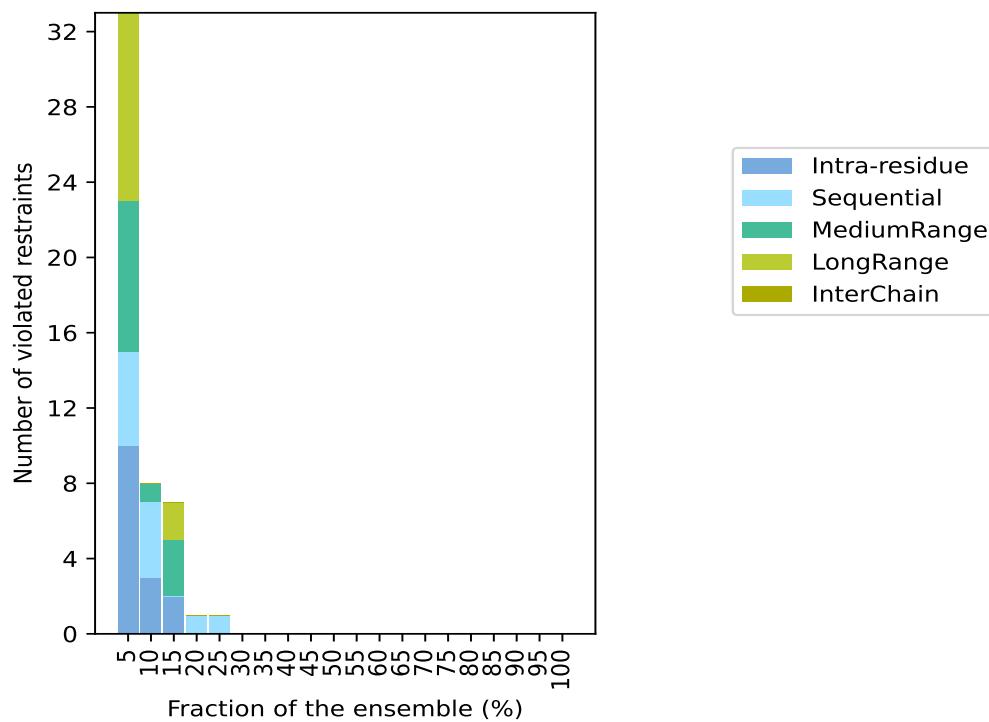
9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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
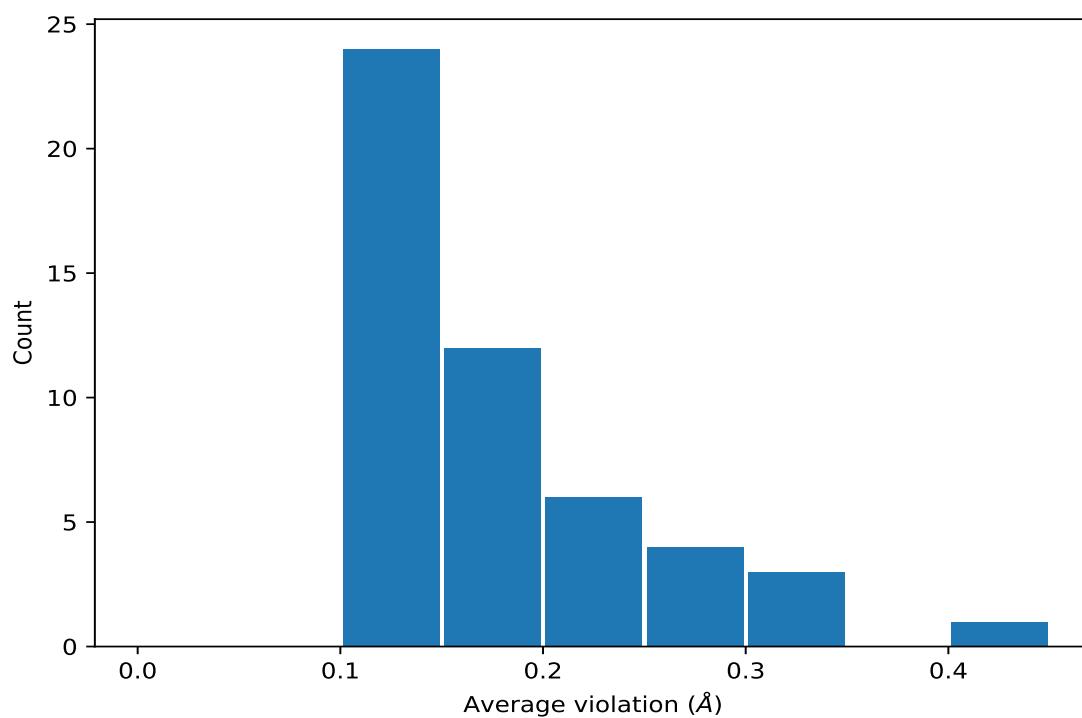
9.4.2   Table: Most violated distance restraints ⓘ

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)
(1,1)	1:A:10:LYS:HA	1:A:11:ARG:H	5	0.14	0.02	0.14
(1,455)	1:A:39:ARG:HB2	1:A:40:ASP:H	4	0.14	0.02	0.12
(1,455)	1:A:39:ARG:HB3	1:A:40:ASP:H	4	0.14	0.02	0.12
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD21	3	0.33	0.02	0.33
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD22	3	0.33	0.02	0.33
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD23	3	0.33	0.02	0.33
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE2	3	0.26	0.04	0.28
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE3	3	0.26	0.04	0.28
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE2	3	0.26	0.04	0.28
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE3	3	0.26	0.04	0.28
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE1	3	0.21	0.02	0.22
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE2	3	0.21	0.02	0.22
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE1	3	0.21	0.02	0.22
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE2	3	0.21	0.02	0.22
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE1	3	0.21	0.02	0.22
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE2	3	0.21	0.02	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1762)	1:A:145:LEU:H	1:A:145:LEU:HG	3	0.18	0.02	0.18
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB2	3	0.14	0.02	0.15
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB3	3	0.14	0.02	0.15
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB2	3	0.14	0.02	0.15
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB3	3	0.14	0.02	0.15
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB2	3	0.14	0.02	0.15
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB3	3	0.14	0.02	0.15
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG21	3	0.14	0.02	0.13
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG22	3	0.14	0.02	0.13
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG23	3	0.14	0.02	0.13
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG21	3	0.14	0.02	0.13
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG22	3	0.14	0.02	0.13
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG23	3	0.14	0.02	0.13
(1,411)	1:A:36:ILE:HD11	1:A:96:HIS:HD2	3	0.13	0.02	0.11
(1,411)	1:A:36:ILE:HD12	1:A:96:HIS:HD2	3	0.13	0.02	0.11
(1,411)	1:A:36:ILE:HD13	1:A:96:HIS:HD2	3	0.13	0.02	0.11
(1,1790)	1:A:149:GLU:H	1:A:149:GLU:HG2	2	0.4	0.0	0.4
(1,1781)	1:A:148:LEU:HG	1:A:149:GLU:H	2	0.18	0.02	0.18
(1,1774)	1:A:148:LEU:HA	1:A:149:GLU:H	2	0.18	0.03	0.18
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD21	2	0.16	0.04	0.16
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD22	2	0.16	0.04	0.16
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD23	2	0.16	0.04	0.16
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD21	2	0.16	0.04	0.16
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD22	2	0.16	0.04	0.16
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD23	2	0.16	0.04	0.16
(1,473)	1:A:41:ILE:HD11	1:A:42:THR:H	2	0.16	0.06	0.16
(1,473)	1:A:41:ILE:HD12	1:A:42:THR:H	2	0.16	0.06	0.16
(1,473)	1:A:41:ILE:HD13	1:A:42:THR:H	2	0.16	0.06	0.16
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD21	2	0.13	0.0	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD22	2	0.13	0.0	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD23	2	0.13	0.0	0.13
(1,232)	1:A:23:LEU:H	1:A:23:LEU:HG	2	0.12	0.0	0.12
(1,1743)	1:A:144:TYR:HB2	1:A:145:LEU:H	2	0.12	0.0	0.12
(1,1743)	1:A:144:TYR:HB3	1:A:145:LEU:H	2	0.12	0.0	0.12

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

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
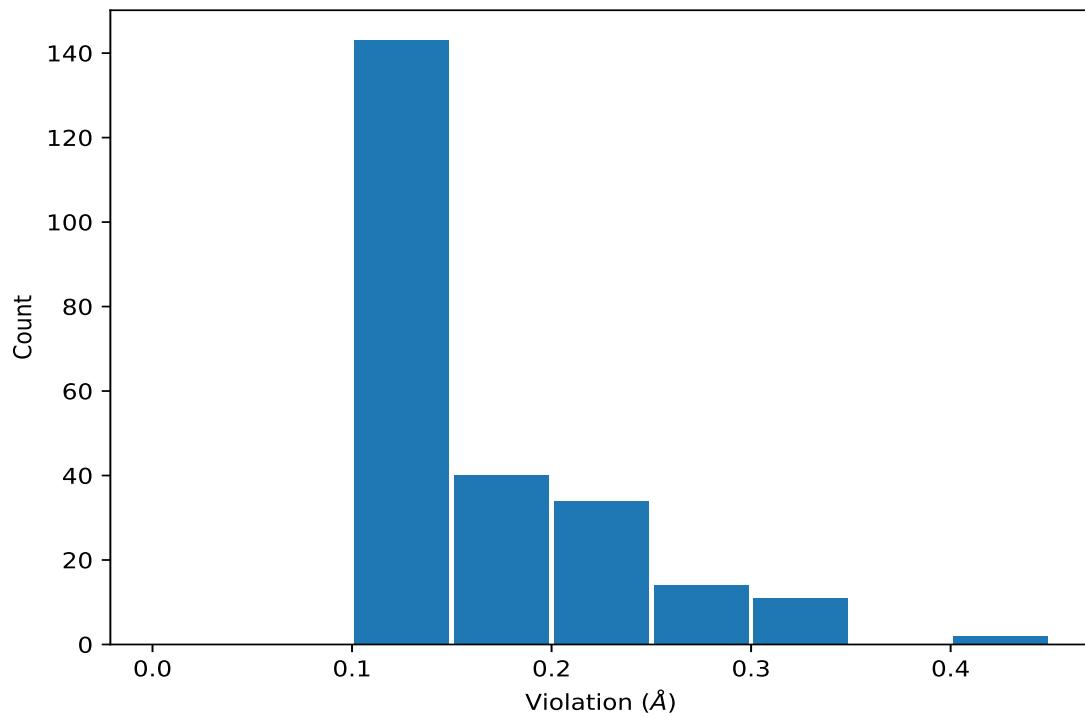
9.5.2 Table : All distance violations ⓘ

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)
(1,1790)	1:A:149:GLU:H	1:A:149:GLU:HG2	1	0.41
(1,1790)	1:A:149:GLU:H	1:A:149:GLU:HG2	15	0.4
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD21	14	0.35
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD22	14	0.35
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD23	14	0.35
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD21	13	0.33
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD22	13	0.33
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD23	13	0.33
(1,36)	1:A:13:LYS:H	1:A:13:LYS:HG2	6	0.32
(1,36)	1:A:13:LYS:H	1:A:13:LYS:HG3	6	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD21	6	0.31
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD22	6	0.31
(1,157)	1:A:20:LEU:HA	1:A:20:LEU:HD23	6	0.31
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE2	14	0.29
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE3	14	0.29
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE2	14	0.29
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE3	14	0.29
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE2	13	0.28
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE3	13	0.28
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE2	13	0.28
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE3	13	0.28
(1,18)	1:A:12:GLN:HG2	1:A:13:LYS:H	9	0.27
(1,18)	1:A:12:GLN:HG3	1:A:13:LYS:H	9	0.27
(1,543)	1:A:47:GLN:HG2	1:A:48:SER:HB2	13	0.25
(1,543)	1:A:47:GLN:HG2	1:A:48:SER:HB3	13	0.25
(1,543)	1:A:47:GLN:HG3	1:A:48:SER:HB2	13	0.25
(1,543)	1:A:47:GLN:HG3	1:A:48:SER:HB3	13	0.25
(1,211)	1:A:23:LEU:HA	1:A:23:LEU:HD21	18	0.24
(1,211)	1:A:23:LEU:HA	1:A:23:LEU:HD22	18	0.24
(1,211)	1:A:23:LEU:HA	1:A:23:LEU:HD23	18	0.24
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE1	8	0.23
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE2	8	0.23
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE1	8	0.23
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE2	8	0.23
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE1	8	0.23
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE2	8	0.23
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE1	3	0.22
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE2	3	0.22
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE1	3	0.22
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE2	3	0.22
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE1	3	0.22
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE2	3	0.22
(1,473)	1:A:41:ILE:HD11	1:A:42:THR:H	20	0.22
(1,473)	1:A:41:ILE:HD12	1:A:42:THR:H	20	0.22
(1,473)	1:A:41:ILE:HD13	1:A:42:THR:H	20	0.22
(1,472)	1:A:41:ILE:HB	1:A:45:TYR:HE1	8	0.21
(1,472)	1:A:41:ILE:HB	1:A:45:TYR:HE2	8	0.21
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE2	6	0.21
(1,162)	1:A:20:LEU:HB2	1:A:25:LYS:HE3	6	0.21
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE2	6	0.21
(1,162)	1:A:20:LEU:HB3	1:A:25:LYS:HE3	6	0.21
(1,1781)	1:A:148:LEU:HG	1:A:149:GLU:H	2	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:A:148:LEU:HA	1:A:149:GLU:H	14	0.2
(1,1762)	1:A:145:LEU:H	1:A:145:LEU:HG	4	0.2
(1,1678)	1:A:133:TYR:HA	1:A:137:PHE:H	5	0.2
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD21	14	0.2
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD22	14	0.2
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD23	14	0.2
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD21	14	0.2
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD22	14	0.2
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD23	14	0.2
(1,830)	1:A:67:VAL:HG21	1:A:143:PRO:HG2	7	0.19
(1,830)	1:A:67:VAL:HG21	1:A:143:PRO:HG3	7	0.19
(1,830)	1:A:67:VAL:HG22	1:A:143:PRO:HG2	7	0.19
(1,830)	1:A:67:VAL:HG22	1:A:143:PRO:HG3	7	0.19
(1,830)	1:A:67:VAL:HG23	1:A:143:PRO:HG2	7	0.19
(1,830)	1:A:67:VAL:HG23	1:A:143:PRO:HG3	7	0.19
(1,1705)	1:A:136:TYR:H	1:A:138:GLY:H	5	0.19
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE1	20	0.18
(1,502)	1:A:42:THR:HG21	1:A:45:TYR:HE2	20	0.18
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE1	20	0.18
(1,502)	1:A:42:THR:HG22	1:A:45:TYR:HE2	20	0.18
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE1	20	0.18
(1,502)	1:A:42:THR:HG23	1:A:45:TYR:HE2	20	0.18
(1,455)	1:A:39:ARG:HB2	1:A:40:ASP:H	17	0.18
(1,455)	1:A:39:ARG:HB3	1:A:40:ASP:H	17	0.18
(1,1762)	1:A:145:LEU:H	1:A:145:LEU:HG	18	0.18
(1,968)	1:A:80:PHE:HB2	1:A:92:LEU:HD11	5	0.17
(1,968)	1:A:80:PHE:HB2	1:A:92:LEU:HD12	5	0.17
(1,968)	1:A:80:PHE:HB2	1:A:92:LEU:HD13	5	0.17
(1,968)	1:A:80:PHE:HB3	1:A:92:LEU:HD11	5	0.17
(1,968)	1:A:80:PHE:HB3	1:A:92:LEU:HD12	5	0.17
(1,968)	1:A:80:PHE:HB3	1:A:92:LEU:HD13	5	0.17
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG21	14	0.17
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG22	14	0.17
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG23	14	0.17
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG21	14	0.17
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG22	14	0.17
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG23	14	0.17
(1,1781)	1:A:148:LEU:HG	1:A:149:GLU:H	10	0.17
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB2	13	0.17
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB3	13	0.17
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB2	13	0.17
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB3	13	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB2	13	0.17
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB3	13	0.17
(1,1)	1:A:10:LYS:HA	1:A:11:ARG:H	11	0.17
(1,411)	1:A:36:ILE:HD11	1:A:96:HIS:HD2	1	0.16
(1,411)	1:A:36:ILE:HD12	1:A:96:HIS:HD2	1	0.16
(1,411)	1:A:36:ILE:HD13	1:A:96:HIS:HD2	1	0.16
(1,1)	1:A:10:LYS:HA	1:A:11:ARG:H	20	0.16
(1,1774)	1:A:148:LEU:HA	1:A:149:GLU:H	17	0.15
(1,1762)	1:A:145:LEU:H	1:A:145:LEU:HG	19	0.15
(1,1746)	1:A:144:TYR:HE1	1:A:146:ARG:HG2	2	0.15
(1,1746)	1:A:144:TYR:HE1	1:A:146:ARG:HG3	2	0.15
(1,1746)	1:A:144:TYR:HE2	1:A:146:ARG:HG2	2	0.15
(1,1746)	1:A:144:TYR:HE2	1:A:146:ARG:HG3	2	0.15
(1,1728)	1:A:141:THR:H	1:A:141:THR:HB	5	0.15
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB2	6	0.15
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB3	6	0.15
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB2	6	0.15
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB3	6	0.15
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB2	6	0.15
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB3	6	0.15
(1,935)	1:A:77:ARG:HD2	1:A:78:LYS:H	7	0.14
(1,935)	1:A:77:ARG:HD3	1:A:78:LYS:H	7	0.14
(1,551)	1:A:49:ILE:HA	1:A:49:ILE:HD11	20	0.14
(1,551)	1:A:49:ILE:HA	1:A:49:ILE:HD12	20	0.14
(1,551)	1:A:49:ILE:HA	1:A:49:ILE:HD13	20	0.14
(1,526)	1:A:45:TYR:HE1	1:A:75:LEU:HD11	8	0.14
(1,526)	1:A:45:TYR:HE1	1:A:75:LEU:HD12	8	0.14
(1,526)	1:A:45:TYR:HE1	1:A:75:LEU:HD13	8	0.14
(1,526)	1:A:45:TYR:HE2	1:A:75:LEU:HD11	8	0.14
(1,526)	1:A:45:TYR:HE2	1:A:75:LEU:HD12	8	0.14
(1,526)	1:A:45:TYR:HE2	1:A:75:LEU:HD13	8	0.14
(1,1234)	1:A:97:ILE:HG21	1:A:129:ASP:H	19	0.14
(1,1234)	1:A:97:ILE:HG22	1:A:129:ASP:H	19	0.14
(1,1234)	1:A:97:ILE:HG23	1:A:129:ASP:H	19	0.14
(1,1)	1:A:10:LYS:HA	1:A:11:ARG:H	4	0.14
(1,994)	1:A:82:GLU:H	1:A:82:GLU:HG2	18	0.13
(1,994)	1:A:82:GLU:H	1:A:82:GLU:HG3	18	0.13
(1,987)	1:A:81:PHE:H	1:A:83:PRO:HD2	4	0.13
(1,987)	1:A:81:PHE:H	1:A:83:PRO:HD3	4	0.13
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG21	9	0.13
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG22	9	0.13
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG23	9	0.13

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG21	9	0.13
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG22	9	0.13
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG23	9	0.13
(1,455)	1:A:39:ARG:HB2	1:A:40:ASP:H	19	0.13
(1,455)	1:A:39:ARG:HB3	1:A:40:ASP:H	19	0.13
(1,310)	1:A:29:ILE:HD11	1:A:53:GLU:HG2	3	0.13
(1,310)	1:A:29:ILE:HD12	1:A:53:GLU:HG2	3	0.13
(1,310)	1:A:29:ILE:HD13	1:A:53:GLU:HG2	3	0.13
(1,24)	1:A:13:LYS:HA	1:A:13:LYS:HE2	20	0.13
(1,24)	1:A:13:LYS:HA	1:A:13:LYS:HE3	20	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD21	4	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD22	4	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD23	4	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD21	19	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD22	19	0.13
(1,1761)	1:A:145:LEU:H	1:A:145:LEU:HD23	19	0.13
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD21	13	0.13
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD22	13	0.13
(1,139)	1:A:17:LYS:HD2	1:A:20:LEU:HD23	13	0.13
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD21	13	0.13
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD22	13	0.13
(1,139)	1:A:17:LYS:HD3	1:A:20:LEU:HD23	13	0.13
(1,1198)	1:A:95:ARG:HD2	1:A:145:LEU:HD21	13	0.13
(1,1198)	1:A:95:ARG:HD2	1:A:145:LEU:HD22	13	0.13
(1,1198)	1:A:95:ARG:HD2	1:A:145:LEU:HD23	13	0.13
(1,1198)	1:A:95:ARG:HD3	1:A:145:LEU:HD21	13	0.13
(1,1198)	1:A:95:ARG:HD3	1:A:145:LEU:HD22	13	0.13
(1,1198)	1:A:95:ARG:HD3	1:A:145:LEU:HD23	13	0.13
(1,1)	1:A:10:LYS:HA	1:A:11:ARG:H	14	0.13
(1,960)	1:A:79:GLN:H	1:A:79:GLN:HE21	18	0.12
(1,960)	1:A:79:GLN:H	1:A:79:GLN:HE22	18	0.12
(1,779)	1:A:64:LYS:HD2	1:A:139:GLU:HA	7	0.12
(1,779)	1:A:64:LYS:HD3	1:A:139:GLU:HA	7	0.12
(1,532)	1:A:46:SER:HB2	1:A:49:ILE:HD11	20	0.12
(1,532)	1:A:46:SER:HB2	1:A:49:ILE:HD12	20	0.12
(1,532)	1:A:46:SER:HB2	1:A:49:ILE:HD13	20	0.12
(1,532)	1:A:46:SER:HB3	1:A:49:ILE:HD11	20	0.12
(1,532)	1:A:46:SER:HB3	1:A:49:ILE:HD12	20	0.12
(1,532)	1:A:46:SER:HB3	1:A:49:ILE:HD13	20	0.12
(1,528)	1:A:45:TYR:H	1:A:45:TYR:HB2	19	0.12
(1,528)	1:A:45:TYR:H	1:A:45:TYR:HB3	19	0.12
(1,482)	1:A:41:ILE:HG21	1:A:42:THR:H	20	0.12

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:A:41:ILE:HG22	1:A:42:THR:H	20	0.12
(1,482)	1:A:41:ILE:HG23	1:A:42:THR:H	20	0.12
(1,455)	1:A:39:ARG:HB2	1:A:40:ASP:H	14	0.12
(1,455)	1:A:39:ARG:HB3	1:A:40:ASP:H	14	0.12
(1,455)	1:A:39:ARG:HB2	1:A:40:ASP:H	15	0.12
(1,455)	1:A:39:ARG:HB3	1:A:40:ASP:H	15	0.12
(1,232)	1:A:23:LEU:H	1:A:23:LEU:HG	14	0.12
(1,1743)	1:A:144:TYR:HB2	1:A:145:LEU:H	18	0.12
(1,1743)	1:A:144:TYR:HB3	1:A:145:LEU:H	18	0.12
(1,1311)	1:A:105:ARG:HD2	1:A:109:GLN:HE22	19	0.12
(1,1311)	1:A:105:ARG:HD3	1:A:109:GLN:HE22	19	0.12
(1,1134)	1:A:92:LEU:HA	1:A:95:ARG:HD2	5	0.12
(1,1134)	1:A:92:LEU:HA	1:A:95:ARG:HD3	5	0.12
(1,1)	1:A:10:LYS:HA	1:A:11:ARG:H	2	0.12
(2,25)	1:A:45:TYR:H	1:A:42:THR:O	14	0.11
(1,963)	1:A:79:GLN:H	1:A:80:PHE:H	16	0.11
(1,487)	1:A:41:ILE:HG21	1:A:49:ILE:HG21	20	0.11
(1,487)	1:A:41:ILE:HG21	1:A:49:ILE:HG22	20	0.11
(1,487)	1:A:41:ILE:HG21	1:A:49:ILE:HG23	20	0.11
(1,487)	1:A:41:ILE:HG22	1:A:49:ILE:HG21	20	0.11
(1,487)	1:A:41:ILE:HG22	1:A:49:ILE:HG22	20	0.11
(1,487)	1:A:41:ILE:HG22	1:A:49:ILE:HG23	20	0.11
(1,487)	1:A:41:ILE:HG23	1:A:49:ILE:HG21	20	0.11
(1,487)	1:A:41:ILE:HG23	1:A:49:ILE:HG22	20	0.11
(1,487)	1:A:41:ILE:HG23	1:A:49:ILE:HG23	20	0.11
(1,473)	1:A:41:ILE:HD11	1:A:42:THR:H	17	0.11
(1,473)	1:A:41:ILE:HD12	1:A:42:THR:H	17	0.11
(1,473)	1:A:41:ILE:HD13	1:A:42:THR:H	17	0.11
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG21	15	0.11
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG22	15	0.11
(1,456)	1:A:39:ARG:HB2	1:A:41:ILE:HG23	15	0.11
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG21	15	0.11
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG22	15	0.11
(1,456)	1:A:39:ARG:HB3	1:A:41:ILE:HG23	15	0.11
(1,411)	1:A:36:ILE:HD11	1:A:96:HIS:HD2	9	0.11
(1,411)	1:A:36:ILE:HD12	1:A:96:HIS:HD2	9	0.11
(1,411)	1:A:36:ILE:HD13	1:A:96:HIS:HD2	9	0.11
(1,411)	1:A:36:ILE:HD11	1:A:96:HIS:HD2	15	0.11
(1,411)	1:A:36:ILE:HD12	1:A:96:HIS:HD2	15	0.11
(1,411)	1:A:36:ILE:HD13	1:A:96:HIS:HD2	15	0.11
(1,232)	1:A:23:LEU:H	1:A:23:LEU:HG	2	0.11
(1,1743)	1:A:144:TYR:HB2	1:A:145:LEU:H	5	0.11

Continued on next page...

Continued from previous page...

| Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	1:A:144:TYR:HB3	1:A:145:LEU:H	5	0.11
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB2	14	0.11
(1,168)	1:A:20:LEU:HD11	1:A:24:GLU:HB3	14	0.11
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB2	14	0.11
(1,168)	1:A:20:LEU:HD12	1:A:24:GLU:HB3	14	0.11
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB2	14	0.11
(1,168)	1:A:20:LEU:HD13	1:A:24:GLU:HB3	14	0.11
(1,1374)	1:A:109:GLN:H	1:A:109:GLN:HG2	13	0.11
(1,1361)	1:A:109:GLN:HA	1:A:109:GLN:HG3	18	0.11
(1,1236)	1:A:97:ILE:HG21	1:A:133:TYR:HD1	11	0.11
(1,1236)	1:A:97:ILE:HG21	1:A:133:TYR:HD2	11	0.11
(1,1236)	1:A:97:ILE:HG22	1:A:133:TYR:HD1	11	0.11
(1,1236)	1:A:97:ILE:HG22	1:A:133:TYR:HD2	11	0.11
(1,1236)	1:A:97:ILE:HG23	1:A:133:TYR:HD1	11	0.11
(1,1236)	1:A:97:ILE:HG23	1:A:133:TYR:HD2	11	0.11
(1,107)	1:A:16:MET:HE1	1:A:28:VAL:HG11	2	0.11
(1,107)	1:A:16:MET:HE1	1:A:28:VAL:HG12	2	0.11
(1,107)	1:A:16:MET:HE1	1:A:28:VAL:HG13	2	0.11
(1,107)	1:A:16:MET:HE2	1:A:28:VAL:HG11	2	0.11
(1,107)	1:A:16:MET:HE2	1:A:28:VAL:HG12	2	0.11
(1,107)	1:A:16:MET:HE2	1:A:28:VAL:HG13	2	0.11
(1,107)	1:A:16:MET:HE3	1:A:28:VAL:HG11	2	0.11
(1,107)	1:A:16:MET:HE3	1:A:28:VAL:HG12	2	0.11
(1,107)	1:A:16:MET:HE3	1:A:28:VAL:HG13	2	0.11

10 Dihedral-angle violation analysis ⓘ

10.1 Summary of dihedral-angle violations ⓘ

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	98	50.0	12	12.2	6.1	0	0.0	0.0
PHI	98	50.0	3	3.1	1.5	0	0.0	0.0
Total	196	100.0	15	7.7	7.7	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 ⓘ
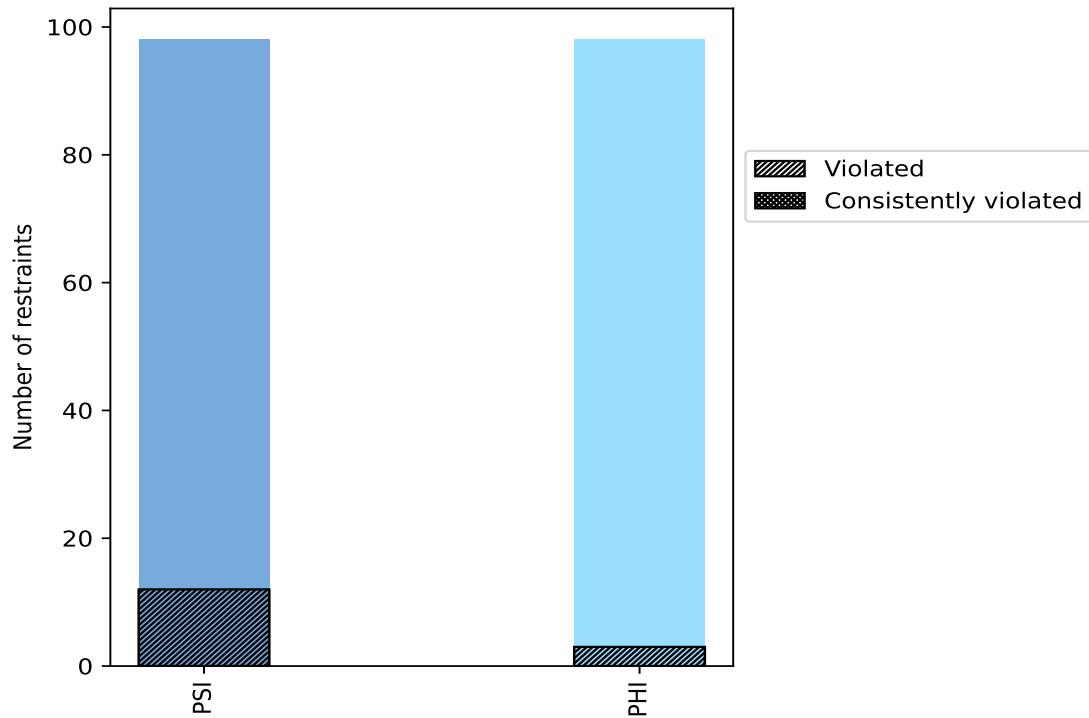

Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	1	1	2	1.35	1.6	0.25	1.35
3	1	0	1	1.1	1.1	0.0	1.1
4	2	1	3	2.07	2.3	0.17	2.0
5	2	1	3	1.3	1.5	0.14	1.2
6	0	0	0	0.0	0.0	0.0	0.0
7	2	0	2	1.7	1.7	0.0	1.7
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	2.3	2.3	0.0	2.3
11	1	0	1	1.3	1.3	0.0	1.3
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	2	0	2	1.2	1.3	0.1	1.2
15	1	2	3	2.3	3.9	1.14	1.7
16	1	0	1	1.3	1.3	0.0	1.3
17	0	1	1	2.8	2.8	0.0	2.8
18	0	0	0	0.0	0.0	0.0	0.0
19	2	0	2	1.8	2.4	0.6	1.8
20	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ
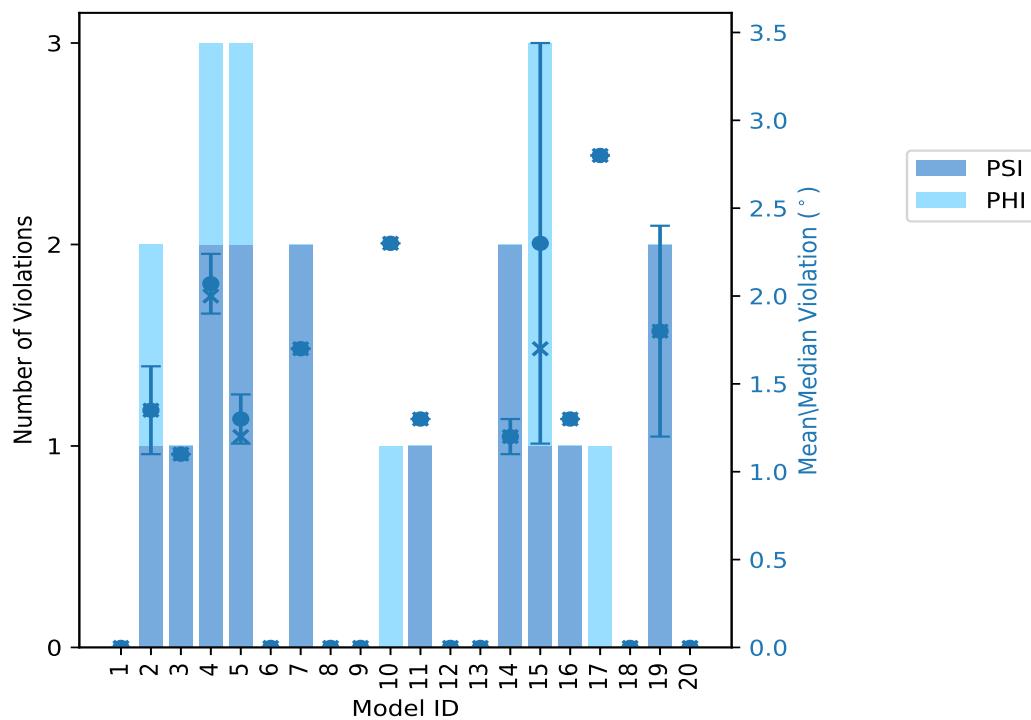
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
10	1	11	1	5.0
1	0	1	2	10.0
1	2	3	3	15.0
0	0	0	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

Continued on next page...

Continued from previous page...

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

[1] Number of models with violations

10.3.1　Bar graph : Dihedral-angle Violation statistics for the ensemble (i)
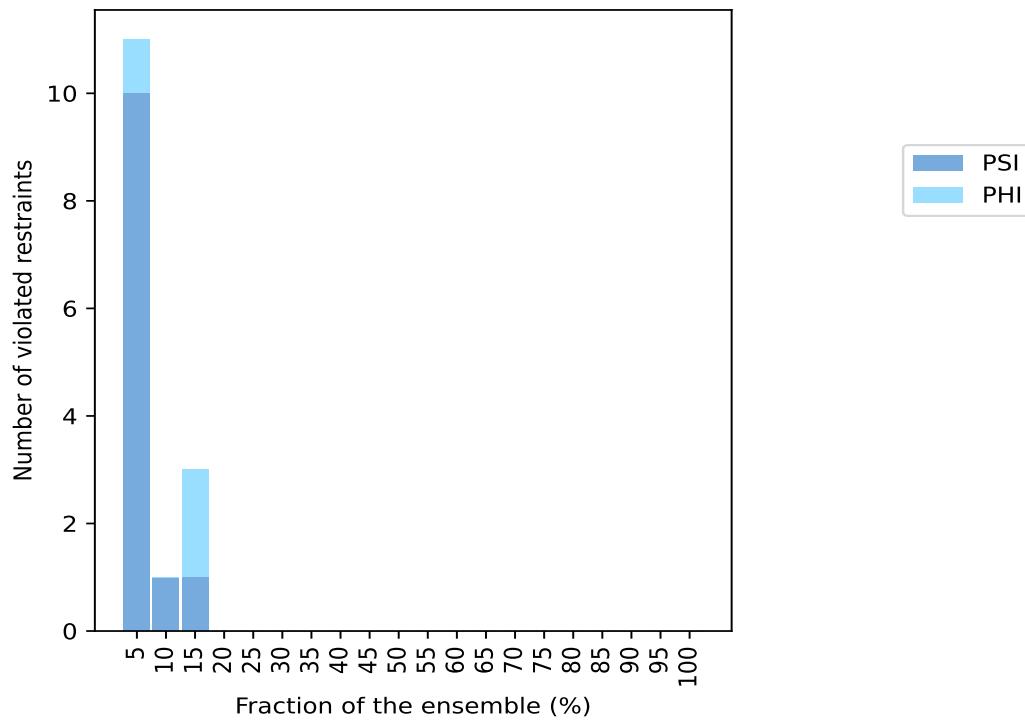
## 10.4　Most violated dihedral-angle restraints in the ensemble (i)

10.4.1　Histogram : Distribution of mean dihedral-angle violations (i)

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

in the ensemble
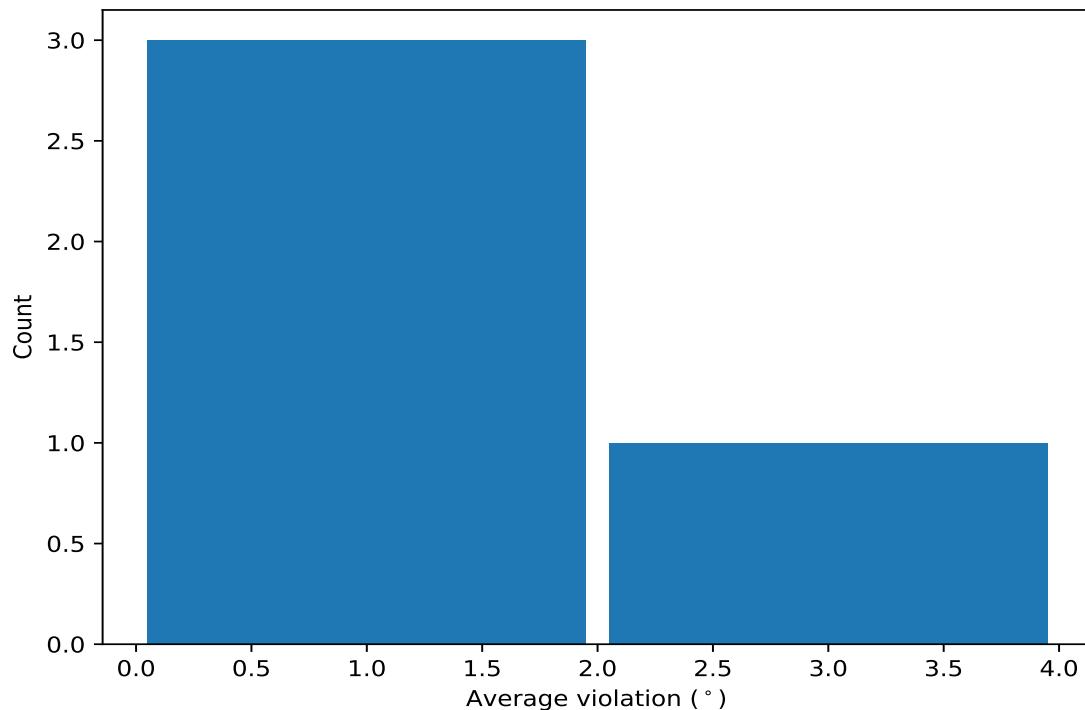
10.4.2   Table: Most violated dihedral-angle restraints ⓘ

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
(1,41)	1:A:35:GLN:C	1:A:36:ILE:N	1:A:36:ILE:CA	1:A:36:ILE:C	3	2.17	0.46	2.0
(1,183)	1:A:134:ALA:C	1:A:135:ASP:N	1:A:135:ASP:CA	1:A:135:ASP:C	3	1.8	0.36	1.6
(1,188)	1:A:137:PHE:N	1:A:137:PHE:CA	1:A:137:PHE:C	1:A:138:GLY:N	3	1.33	0.26	1.2
(1,124)	1:A:95:ARG:N	1:A:95:ARG:CA	1:A:95:ARG:C	1:A:96:HIS:N	2	1.85	0.55	1.85

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5   All violated dihedral-angle restraints ⓘ

10.5.1   Histogram : Distribution of violations ⓘ

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 (°)
(1,100)	1:A:76:TYR:N	1:A:76:TYR:CA	1:A:76:TYR:C	1:A:77:ARG:N	15	3.9
(1,41)	1:A:35:GLN:C	1:A:36:ILE:N	1:A:36:ILE:CA	1:A:36:ILE:C	17	2.8
(1,124)	1:A:95:ARG:N	1:A:95:ARG:CA	1:A:95:ARG:C	1:A:96:HIS:N	19	2.4
(1,183)	1:A:134:ALA:C	1:A:135:ASP:N	1:A:135:ASP:CA	1:A:135:ASP:C	10	2.3
(1,108)	1:A:87:SER:N	1:A:87:SER:CA	1:A:87:SER:C	1:A:88:ARG:N	4	2.3
(1,41)	1:A:35:GLN:C	1:A:36:ILE:N	1:A:36:ILE:CA	1:A:36:ILE:C	4	2.0
(1,130)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:GLY:N	4	1.9
(1,6)	1:A:16:MET:N	1:A:16:MET:CA	1:A:16:MET:C	1:A:17:LYS:N	7	1.7
(1,41)	1:A:35:GLN:C	1:A:36:ILE:N	1:A:36:ILE:CA	1:A:36:ILE:C	15	1.7
(1,188)	1:A:137:PHE:N	1:A:137:PHE:CA	1:A:137:PHE:C	1:A:138:GLY:N	7	1.7
(1,183)	1:A:134:ALA:C	1:A:135:ASP:N	1:A:135:ASP:CA	1:A:135:ASP:C	2	1.6
(1,183)	1:A:134:ALA:C	1:A:135:ASP:N	1:A:135:ASP:CA	1:A:135:ASP:C	5	1.5
(1,40)	1:A:35:GLN:N	1:A:35:GLN:CA	1:A:35:GLN:C	1:A:36:ILE:N	14	1.3
(1,193)	1:A:140:GLU:C	1:A:141:THR:N	1:A:141:THR:CA	1:A:141:THR:C	15	1.3
(1,190)	1:A:139:GLU:N	1:A:139:GLU:CA	1:A:139:GLU:C	1:A:140:GLU:N	16	1.3
(1,124)	1:A:95:ARG:N	1:A:95:ARG:CA	1:A:95:ARG:C	1:A:96:HIS:N	11	1.3
(1,188)	1:A:137:PHE:N	1:A:137:PHE:CA	1:A:137:PHE:C	1:A:138:GLY:N	5	1.2
(1,184)	1:A:135:ASP:N	1:A:135:ASP:CA	1:A:135:ASP:C	1:A:136:TYR:N	5	1.2
(1,172)	1:A:128:VAL:N	1:A:128:VAL:CA	1:A:128:VAL:C	1:A:129:ASP:N	19	1.2
(1,2)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	1:A:15:ALA:N	2	1.1
(1,188)	1:A:137:PHE:N	1:A:137:PHE:CA	1:A:137:PHE:C	1:A:138:GLY:N	3	1.1
(1,102)	1:A:77:ARG:N	1:A:77:ARG:CA	1:A:77:ARG:C	1:A:78:LYS:N	14	1.1