WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 10:11 PM EDT

PDB ID	:	2KKM
BMRB ID	:	16365
Title	:	Solution NMR structure of yeast protein YOR252W [residues 38-178]: Northeast Structural Genomics Consortium target YT654
Authors	:	Cort, J.R.; Yee, A.; Liu, C.; Arrowsmith, C.H.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-06-26

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 ⓘ symbol.

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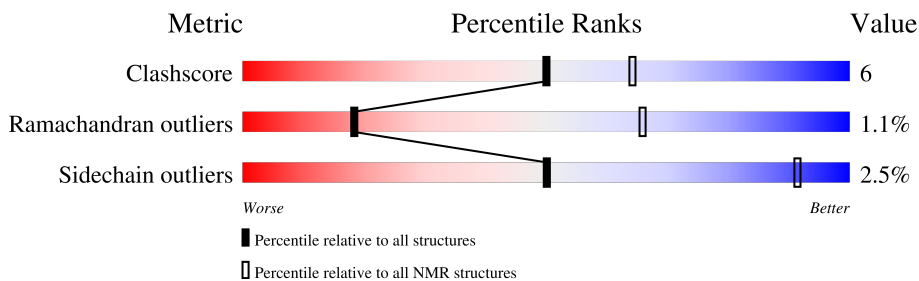http://www.wwpdb.org/validation/2017/FAQs#types.

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 78%.

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		6
Ramachandran outliers		1.1%
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	144	67% 10% 21% •

2   Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *no criteria*.

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:18-A:65, A:75-A:137 (111)	1.06	18

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2353 atoms, of which 1181 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	141	2353	728	1181	224	216	4	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q08687
A	-1	SER	-	expression tag	UNP Q08687
A	0	HIS	-	expression tag	UNP Q08687

4 Residue-property plots ⓘ

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.

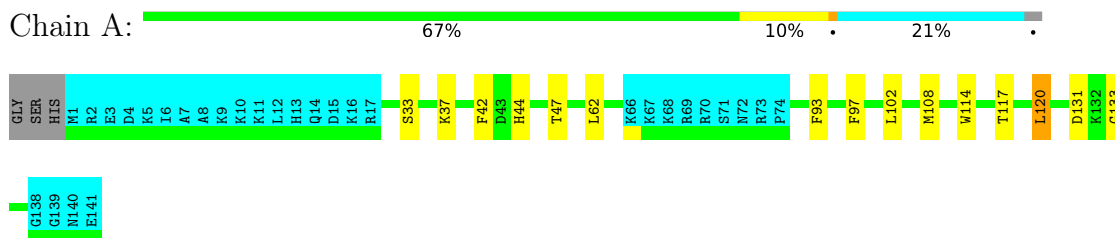• Molecule 1: Translation machinery-associated protein 16
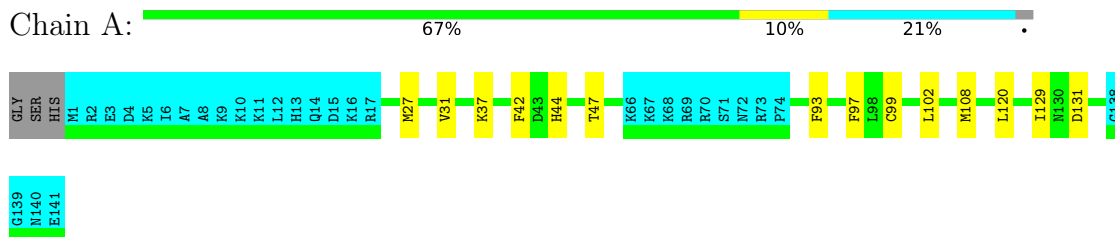
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

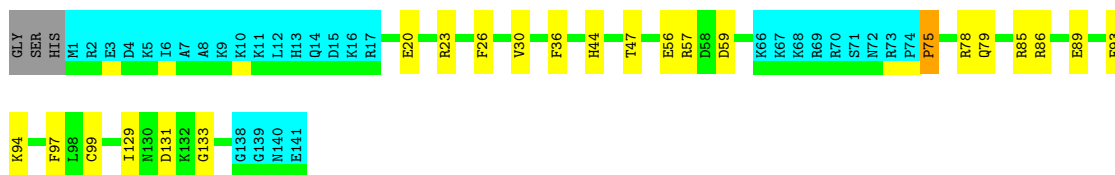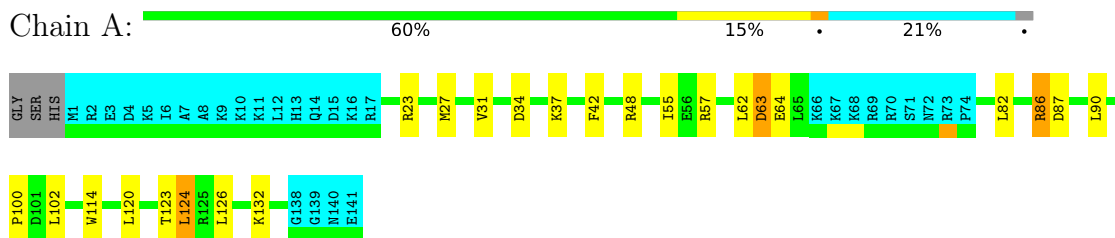### 4.2.1 Score per residue for model 1

• Molecule 1: Translation machinery-associated protein 16

4.2.2 Score per residue for model 2

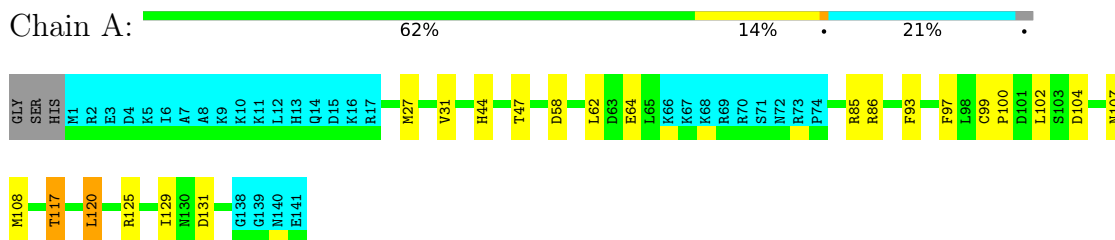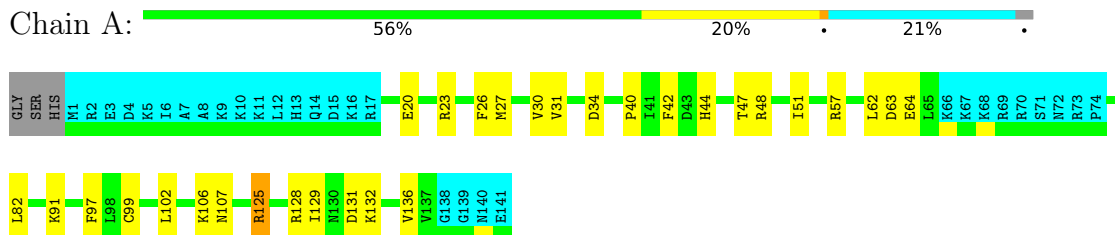• Molecule 1: Translation machinery-associated protein 16

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 E20 R23 F26 V30 F36 H44 T47 E56 R57 D58 D59 K66 K67 K68 R69 R70 S71 N72 R73 P74 P75 R78 Q79 R85 R86 E89 F93

K94 F97 L98 C99 I129 N130 D131 K132 G133 G138 G139 N140 E141

4.2.3 Score per residue for model 3

- Molecule 1: Translation machinery-associated protein 16

Chain A: 60%   15% • 21% •

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 R23 M27 V31 D34 K37 F42 R48 I55 E56 R57 L62 D63 E64 L65 K66 K67 K68 R69 R70 S71 N72 R73 P74 L82 R86 D87 L90

P100 D101 L102 W114 L120 T123 L124 R125 L126 K132 G138 G139 N140 E141

4.2.4 Score per residue for model 4

- Molecule 1: Translation machinery-associated protein 16

Chain A: 62%   14% • 21% •

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 M27 V31 H44 T47 D58 L62 D63 E64 L65 K66 K67 K68 R69 R70 S71 N72 R73 P74 R85 R86 F93 F97 L98 C99 P100 D101 L102 S103 D104 N107

M108 T117 L120 R125 I129 N130 D131 G138 G139 N140 E141

4.2.5 Score per residue for model 5

- Molecule 1: Translation machinery-associated protein 16

Chain A: 56%   20% • 21% •

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 E20 R23 F26 M27 V30 V31 D34 P40 I41 F42 D43 H44 T47 R48 I51 R57 L62 D63 E64 L65 K66 K67 K68 R69 R70 S71 N72 R73 P74

L82 K91 F97 L98 C99 L102 K106 N107 R125 R128 I129 N130 D131 K132 V136 V137 G138 G139 N140 E141

4.2.6 Score per residue for model 6

- Molecule 1: Translation machinery-associated protein 16

Chain A: 62% 12% • 21% •

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 M27 V31 P40 I41 F42 D43 R48 K66 K67 K68 R69 R70 S71 N72 R73 P74 P75 S76 R85 F93 F97 L98 C99 L102 S103 M108 R112 N113 W114

T117 L120 I129 K132 G138 G139 N140 E141

4.2.7 Score per residue for model 7

• Molecule 1: Translation machinery-associated protein 16

Chain A: 71% 6% 21% •

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 S33 K37 H46 E49 K66 K67 K68 R69 R70 S71 N72 R73 P74 R85 E89 L111 R128 V136 V137 G138 G139 N140 E141

4.2.8 Score per residue for model 8

• Molecule 1: Translation machinery-associated protein 16

Chain A: 60% 17% • 21% •

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 V18 H19 E20 R23 V31 D34 G38 Q39 P40 I41 H44 T47 E64 L65 K66 K67 K68 R69 R70 S71 N72 R73 P74 P75 S76 V80 L81 L82 Q83 Q84 R85 R86

A105 R112 T117 L120 N130 D131 K132 G133 E134 G138 G139 N140 E141

4.2.9 Score per residue for model 9

• Molecule 1: Translation machinery-associated protein 16

Chain A: 62% 15% • 21% •

GLY SER HIS M1 R2 E3 D4 K5 I6 A7 A8 K9 K10 K11 L12 H13 Q14 D15 K16 R17 R23 M27 S33 K37 H44 T47 I51 I55 K66 K67 K68 R69 R70 S71 N72 R73 P74 P75 R78 R86 P100 D101 L102 N107 M108 L111

W114 L120 L124 R125 L126 I127 R128 I129 G138 G139 N140 E141

4.2.10 Score per residue for model 10

• Molecule 1: Translation machinery-associated protein 16

Chain A:

4.2.11 Score per residue for model 11
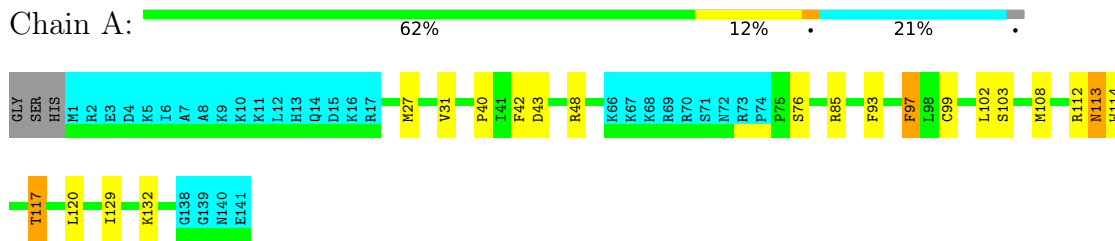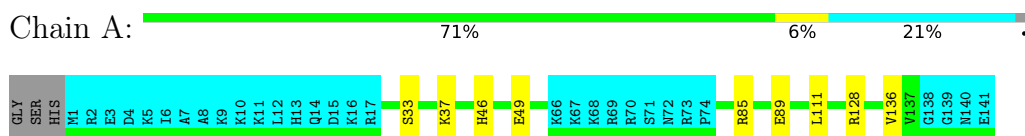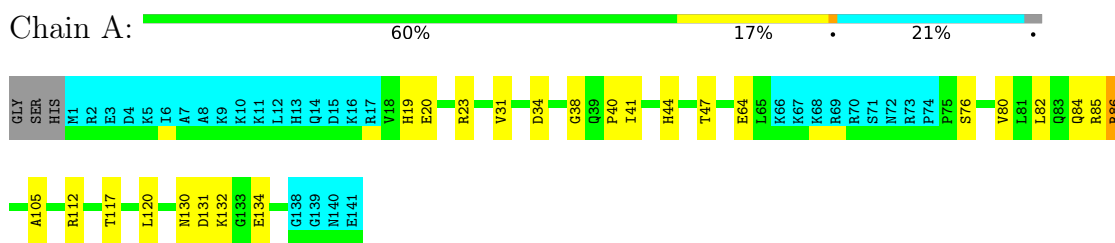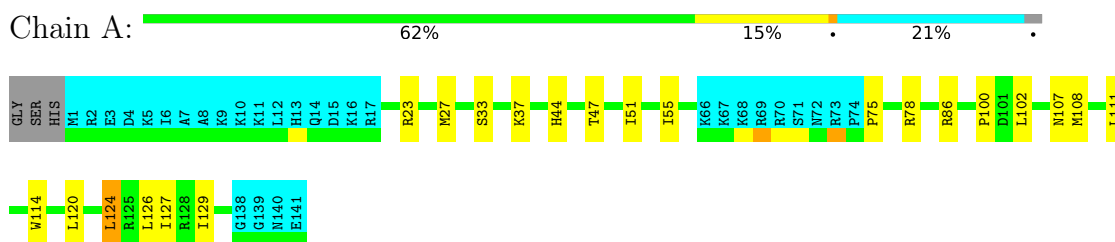
• Molecule 1: Translation machinery-associated protein 16

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Translation machinery-associated protein 16

Chain A:

4.2.13 Score per residue for model 13

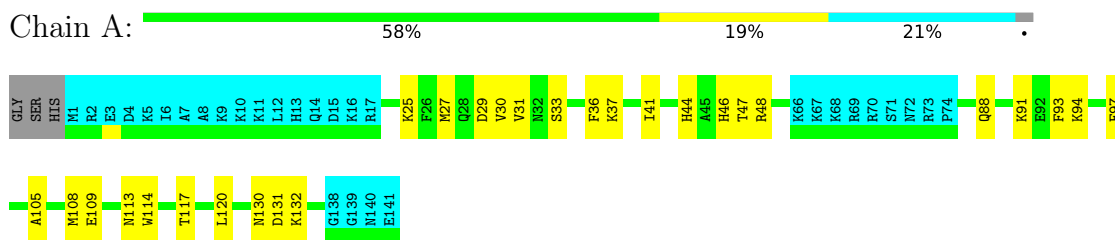• Molecule 1: Translation machinery-associated protein 16
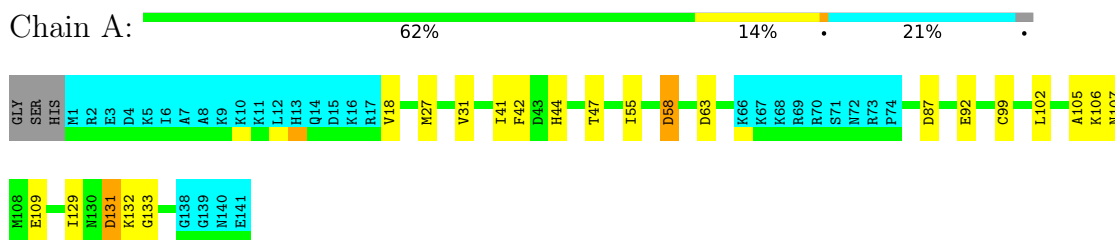
Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: Translation machinery-associated protein 16

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: Translation machinery-associated protein 16

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: Translation machinery-associated protein 16

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: Translation machinery-associated protein 16

Chain A:

4.2.18   Score per residue for model 18 (medoid)

• Molecule 1: Translation machinery-associated protein 16
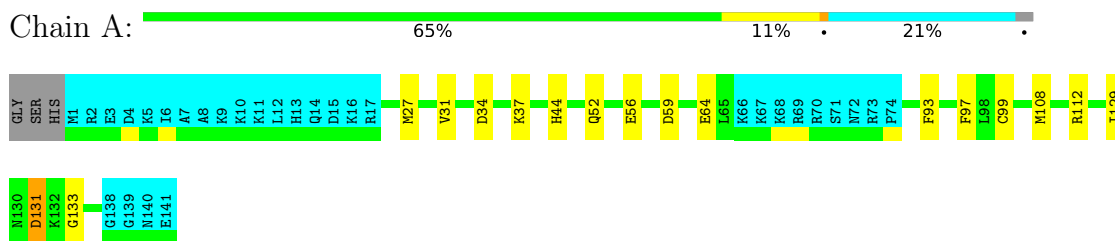
4.2.19   Score per residue for model 19

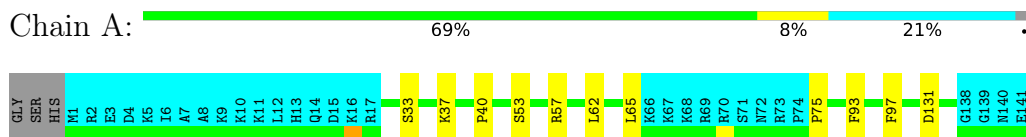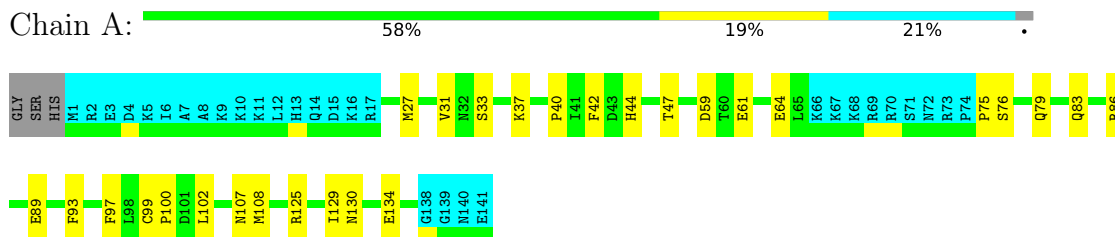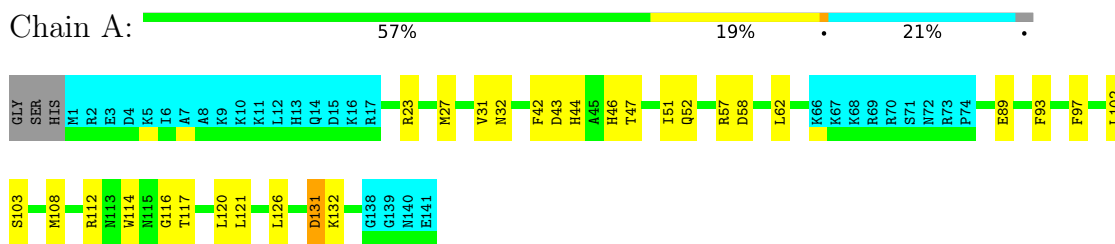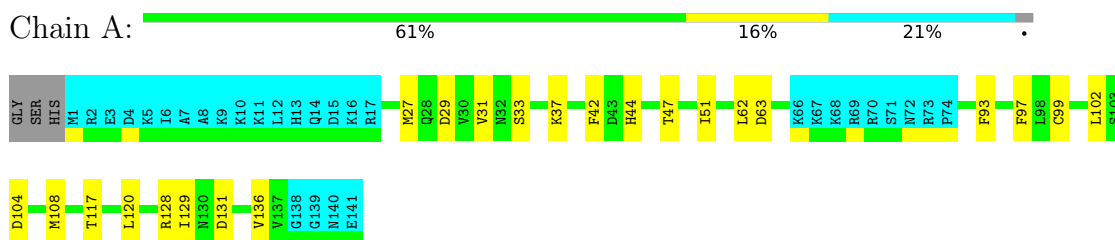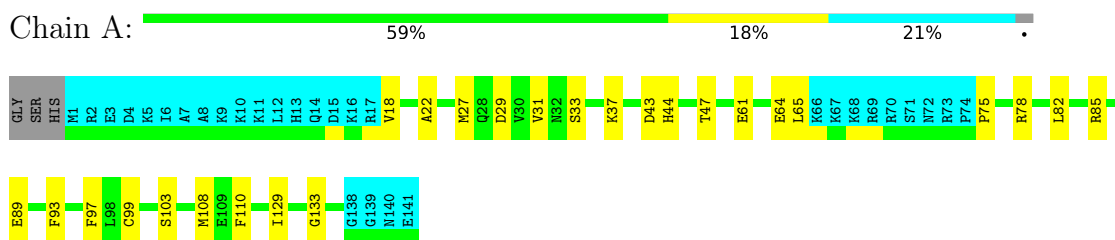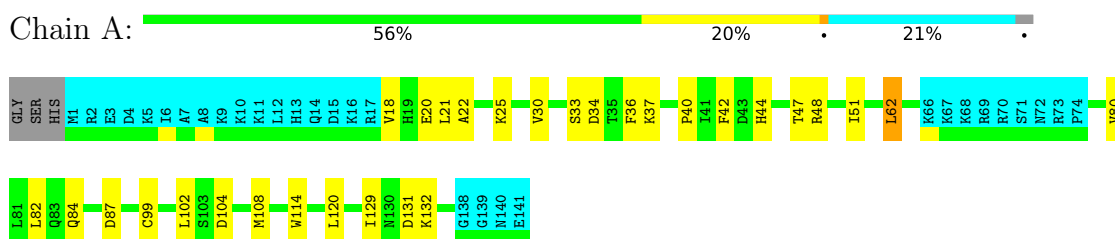• Molecule 1: Translation machinery-associated protein 16
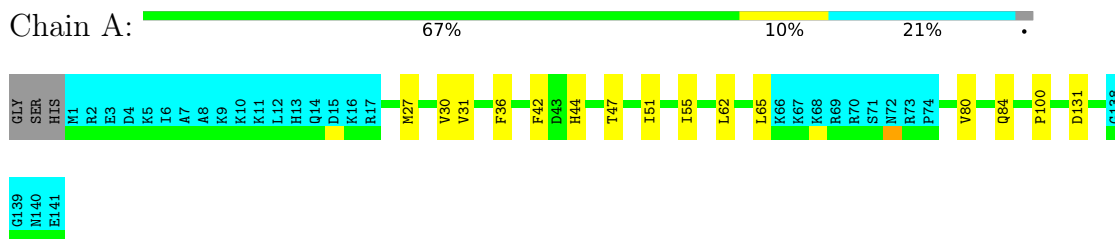
4.2.20   Score per residue for model 20

• Molecule 1: Translation machinery-associated protein 16
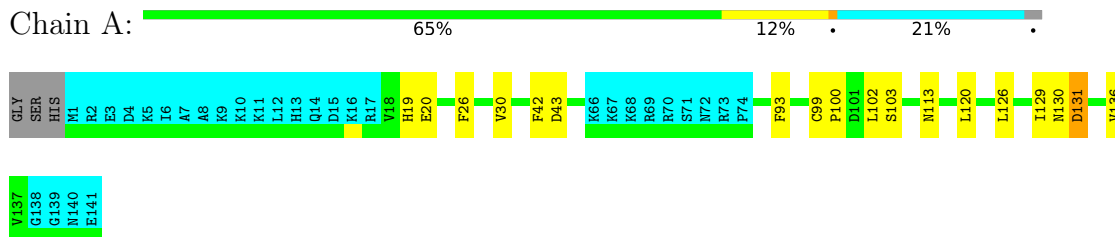
5 Refinement protocol and experimental data overview ⓘ

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

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *combination of lowest energy, fewest restraint violations, and favorable geometry.*

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

Software name	Classification	Version
AutoStructure	structure solution	
AutoStructure	refinement	
X-PLOR NIH	refinement	
PSVS	refinement	
CNS	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	1422
Number of shifts mapped to atoms	1422
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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	920	905	902	11±3
All	All	18400	18100	18040	217

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:48:ARG:HG3	1:A:132:LYS:HB3	0.94	1.35	3	2
1:A:130:ASN:HB3	1:A:134:GLU:HB2	0.83	1.50	8	2
1:A:93:PHE:HA	1:A:97:PHE:HB2	0.81	1.52	4	9
1:A:34:ASP:HA	1:A:37:LYS:HB2	0.80	1.51	3	2
1:A:117:THR:HB	1:A:120:LEU:HB2	0.73	1.60	4	4
1:A:31:VAL:HG23	1:A:112:ARG:HG3	0.71	1.62	8	1
1:A:75:PRO:HB2	1:A:78:ARG:HB2	0.68	1.65	9	2
1:A:42:PHE:HB2	1:A:102:LEU:HG	0.67	1.66	5	7
1:A:56:GLU:HA	1:A:86:ARG:HH21	0.66	1.51	2	1
1:A:43:ASP:HA	1:A:103:SER:HB3	0.66	1.68	14	3
1:A:94:LYS:HA	1:A:130:ASN:OD1	0.64	1.93	10	1
1:A:44:HIS:HB3	1:A:133:GLY:HA3	0.64	1.69	11	5
1:A:93:PHE:CE2	1:A:131:ASP:HA	0.63	2.28	20	2
1:A:99:CYS:HB2	1:A:129:ILE:HD12	0.63	1.70	15	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:HA	1:A:23:ARG:NH1	0.62	2.10	5	1
1:A:102:LEU:HA	1:A:108:MET:SD	0.62	2.34	4	1
1:A:30:VAL:HG12	1:A:36:PHE:HB2	0.61	1.70	2	4
1:A:100:PRO:HA	1:A:126:LEU:HA	0.61	1.73	3	3
1:A:65:LEU:HD22	1:A:75:PRO:HG2	0.60	1.71	12	1
1:A:44:HIS:O	1:A:47:THR:HB	0.58	1.99	1	14
1:A:117:THR:OG1	1:A:120:LEU:HB2	0.58	1.99	14	1
1:A:53:SER:O	1:A:57:ARG:HG3	0.57	1.99	12	1
1:A:27:MET:O	1:A:31:VAL:HG23	0.57	1.99	10	11
1:A:62:LEU:HB2	1:A:82:LEU:HD12	0.55	1.77	3	1
1:A:62:LEU:HD12	1:A:65:LEU:HD12	0.55	1.77	12	2
1:A:33:SER:O	1:A:37:LYS:HB2	0.55	2.02	9	9
1:A:48:ARG:HD3	1:A:132:LYS:HB3	0.55	1.77	17	3
1:A:104:ASP:O	1:A:108:MET:HG2	0.55	2.02	15	2
1:A:86:ARG:HH11	1:A:86:ARG:HB3	0.53	1.63	8	1
1:A:27:MET:SD	1:A:102:LEU:HD21	0.51	2.45	9	2
1:A:48:ARG:HH11	1:A:132:LYS:HB3	0.51	1.65	10	1
1:A:114:TRP:HA	1:A:120:LEU:HD13	0.51	1.82	9	5
1:A:86:ARG:O	1:A:90:LEU:HG	0.51	2.06	3	1
1:A:107:ASN:ND2	1:A:125:ARG:HB2	0.51	2.21	4	1
1:A:32:ASN:HD21	1:A:112:ARG:HG3	0.51	1.65	14	1
1:A:58:ASP:OD1	1:A:86:ARG:HD2	0.50	2.06	4	1
1:A:31:VAL:HG23	1:A:112:ARG:HG2	0.50	1.82	18	1
1:A:31:VAL:HG22	1:A:42:PHE:CE1	0.50	2.42	19	2
1:A:88:GLN:HA	1:A:91:LYS:HD2	0.50	1.83	10	1
1:A:99:CYS:SG	1:A:100:PRO:HD2	0.50	2.47	13	1
1:A:93:PHE:HD1	1:A:97:PHE:HB2	0.50	1.67	1	1
1:A:57:ARG:HD3	1:A:57:ARG:O	0.50	2.06	2	1
1:A:20:GLU:HA	1:A:23:ARG:NH2	0.49	2.23	2	1
1:A:128:ARG:CB	1:A:136:VAL:HB	0.49	2.38	7	1
1:A:85:ARG:O	1:A:89:GLU:HG2	0.49	2.08	2	3
1:A:131:ASP:OD2	1:A:132:LYS:HG3	0.48	2.09	14	3
1:A:23:ARG:HD3	1:A:51:ILE:HD12	0.48	1.85	9	1
1:A:23:ARG:NH2	1:A:51:ILE:HG12	0.48	2.24	14	1
1:A:86:ARG:HB3	1:A:86:ARG:NH1	0.48	2.23	8	1
1:A:47:THR:O	1:A:51:ILE:HG13	0.48	2.09	14	2
1:A:42:PHE:HB2	1:A:102:LEU:HB3	0.48	1.84	17	2
1:A:117:THR:HG23	1:A:120:LEU:HB2	0.47	1.86	6	1
1:A:120:LEU:O	1:A:120:LEU:HD23	0.47	2.09	17	6
1:A:55:ILE:HG23	1:A:86:ARG:HB2	0.47	1.85	3	1
1:A:83:GLN:O	1:A:86:ARG:HG2	0.47	2.09	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:LYS:O	1:A:109:GLU:HB3	0.47	2.08	11	1
1:A:75:PRO:HG2	1:A:79:GLN:HB2	0.47	1.87	13	1
1:A:25:LYS:HB2	1:A:114:TRP:HZ3	0.47	1.70	10	2
1:A:121:LEU:HD12	1:A:126:LEU:HD11	0.46	1.86	14	1
1:A:34:ASP:HA	1:A:37:LYS:HB3	0.46	1.85	17	1
1:A:27:MET:O	1:A:31:VAL:HG22	0.46	2.10	18	1
1:A:41:ILE:HD11	1:A:105:ALA:HA	0.45	1.88	10	1
1:A:18:VAL:O	1:A:22:ALA:HB3	0.45	2.12	16	2
1:A:94:LYS:HD3	1:A:94:LYS:O	0.45	2.11	2	1
1:A:26:PHE:O	1:A:30:VAL:HG23	0.45	2.12	5	3
1:A:31:VAL:CG2	1:A:112:ARG:HG2	0.45	2.41	18	1
1:A:127:ILE:HG13	1:A:129:ILE:HG13	0.44	1.88	9	1
1:A:36:PHE:HB3	1:A:42:PHE:CZ	0.44	2.47	19	1
1:A:89:GLU:OE1	1:A:89:GLU:HA	0.44	2.12	13	1
1:A:61:GLU:O	1:A:64:GLU:HB2	0.44	2.12	13	1
1:A:47:THR:O	1:A:51:ILE:HG12	0.44	2.12	17	2
1:A:93:PHE:CD1	1:A:97:PHE:HB2	0.43	2.49	6	1
1:A:65:LEU:HB3	1:A:75:PRO:HG2	0.43	1.90	16	1
1:A:20:GLU:HB3	1:A:21:LEU:HD22	0.43	1.89	17	1
1:A:20:GLU:O	1:A:23:ARG:HG2	0.43	2.13	8	1
1:A:41:ILE:CD1	1:A:105:ALA:HA	0.43	2.43	8	1
1:A:52:GLN:O	1:A:56:GLU:HG3	0.43	2.13	18	1
1:A:108:MET:SD	1:A:111:LEU:HD12	0.43	2.54	9	1
1:A:57:ARG:HH11	1:A:57:ARG:HB3	0.43	1.74	5	1
1:A:31:VAL:HG21	1:A:108:MET:SD	0.43	2.53	16	1
1:A:105:ALA:O	1:A:109:GLU:HG2	0.43	2.14	10	1
1:A:89:GLU:O	1:A:93:PHE:HD1	0.43	1.96	14	1
1:A:108:MET:O	1:A:112:ARG:HG3	0.42	2.13	6	2
1:A:102:LEU:HD12	1:A:108:MET:SD	0.42	2.54	1	1
1:A:44:HIS:HA	1:A:47:THR:OG1	0.42	2.13	2	1
1:A:58:ASP:HB2	1:A:85:ARG:HH22	0.42	1.74	4	1
1:A:40:PRO:O	1:A:108:MET:HG2	0.42	2.15	13	1
1:A:91:LYS:C	1:A:91:LYS:HD3	0.42	2.33	5	1
1:A:27:MET:SD	1:A:100:PRO:HG2	0.42	2.54	19	2
1:A:113:ASN:HD22	1:A:113:ASN:N	0.42	2.13	6	1
1:A:107:ASN:HB2	1:A:125:ARG:HB2	0.42	1.91	13	1
1:A:129:ILE:HG22	1:A:130:ASN:O	0.42	2.15	13	1
1:A:128:ARG:HB2	1:A:136:VAL:HB	0.42	1.90	15	2
1:A:82:LEU:HD12	1:A:85:ARG:HD2	0.42	1.92	8	1
1:A:106:LYS:HB3	1:A:125:ARG:NH2	0.41	2.30	5	1
1:A:130:ASN:HB2	1:A:136:VAL:CG2	0.41	2.44	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ARG:HB3	1:A:57:ARG:NH1	0.41	2.30	5	1
1:A:107:ASN:OD1	1:A:124:LEU:HD23	0.41	2.16	9	1
1:A:41:ILE:HD12	1:A:105:ALA:HA	0.41	1.90	11	1
1:A:23:ARG:HH12	1:A:93:PHE:HE2	0.41	1.57	14	1
1:A:46:HIS:HA	1:A:49:GLU:HB2	0.41	1.92	7	1
1:A:80:VAL:O	1:A:84:GLN:HG3	0.41	2.15	8	3
1:A:97:PHE:HD2	1:A:99:CYS:SG	0.41	2.38	5	1
1:A:128:ARG:HB3	1:A:136:VAL:HB	0.41	1.92	7	1
1:A:120:LEU:HD23	1:A:123:THR:OG1	0.41	2.15	3	1
1:A:107:ASN:ND2	1:A:125:ARG:HE	0.41	2.14	5	1
1:A:55:ILE:HG22	1:A:86:ARG:HE	0.41	1.75	9	1
1:A:55:ILE:O	1:A:58:ASP:HB3	0.41	2.15	11	1
1:A:61:GLU:O	1:A:65:LEU:HG	0.41	2.16	16	1
1:A:31:VAL:HB	1:A:112:ARG:NH1	0.40	2.31	8	1
1:A:117:THR:HB	1:A:120:LEU:HG	0.40	1.93	15	1
1:A:51:ILE:O	1:A:55:ILE:HG13	0.40	2.15	19	1
1:A:120:LEU:O	1:A:124:LEU:HB2	0.40	2.15	3	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/144 (77%)	103±2 (93±2%)	7±2 (6±2%)	1±1 (1±1%)	18	66
All	All	2220/2880 (77%)	2056 (93%)	139 (6%)	25 (1%)	18	66

All 7 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	131	ASP	13
1	A	40	PRO	5
1	A	76	SER	3
1	A	75	PRO	1
1	A	38	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	116	GLY	1
1	A	103	SER	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	102/130 (78%)	100±2 (98±2%)	2±2 (2±2%)	50	91
All	All	2040/2600 (78%)	1990 (98%)	50 (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	59	ASP	3
1	A	87	ASP	3
1	A	82	LEU	3
1	A	113	ASN	3
1	A	29	ASP	3
1	A	120	LEU	2
1	A	57	ARG	2
1	A	86	ARG	2
1	A	124	LEU	2
1	A	117	THR	2
1	A	34	ASP	2
1	A	19	HIS	2
1	A	46	HIS	2
1	A	108	MET	2
1	A	58	ASP	2
1	A	23	ARG	1
1	A	63	ASP	1
1	A	104	ASP	1
1	A	125	ARG	1
1	A	85	ARG	1
1	A	97	PHE	1
1	A	111	LEU	1
1	A	18	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	92	GLU	1
1	A	107	ASN	1
1	A	52	GLN	1
1	A	43	ASP	1
1	A	78	ARG	1
1	A	110	PHE	1
1	A	62	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 78% for the well-defined parts and 69% 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	1422
Number of shifts mapped to atoms	1422
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	127	-0.44 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	122	0.40 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	113	-0.33 ± 0.16	None needed (< 0.5 ppm)
^{15}N	116	0.11 ± 0.29	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1248 atoms were assigned a chemical shift out of a possible 1603. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	522/554 (94%)	213/224 (95%)	208/222 (94%)	101/108 (94%)
Sidechain	685/923 (74%)	455/590 (77%)	217/285 (76%)	13/48 (27%)

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W O R L D W I D E
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PROTEIN DATA BANK

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	41/126 (33%)	22/63 (35%)	18/56 (32%)	1/7 (14%)
Overall	1248/1603 (78%)	690/877 (79%)	443/563 (79%)	115/163 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1421 atoms were assigned a chemical shift out of a possible 2060. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	595/704 (85%)	239/285 (84%)	240/282 (85%)	116/137 (85%)
Sidechain	785/1222 (64%)	513/776 (66%)	256/372 (69%)	16/74 (22%)
Aromatic	41/134 (31%)	22/67 (33%)	18/58 (31%)	1/9 (11%)
Overall	1421/2060 (69%)	774/1128 (69%)	514/712 (72%)	133/220 (60%)

### 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	131	ASP	HB2	0.73	1.41 − 4.01	-7.6
1	A	116	GLY	HA2	1.26	2.15 − 5.77	-7.5
1	A	51	ILE	HD11	-1.31	-0.72 − 2.09	-7.1
1	A	51	ILE	HD12	-1.31	-0.72 − 2.09	-7.1
1	A	51	ILE	HD13	-1.31	-0.72 − 2.09	-7.1
1	A	30	VAL	HG11	-0.57	-0.48 − 2.12	-5.4
1	A	30	VAL	HG12	-0.57	-0.48 − 2.12	-5.4
1	A	30	VAL	HG13	-0.57	-0.48 − 2.12	-5.4
1	A	131	ASP	HA	3.02	3.04 − 6.12	-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:
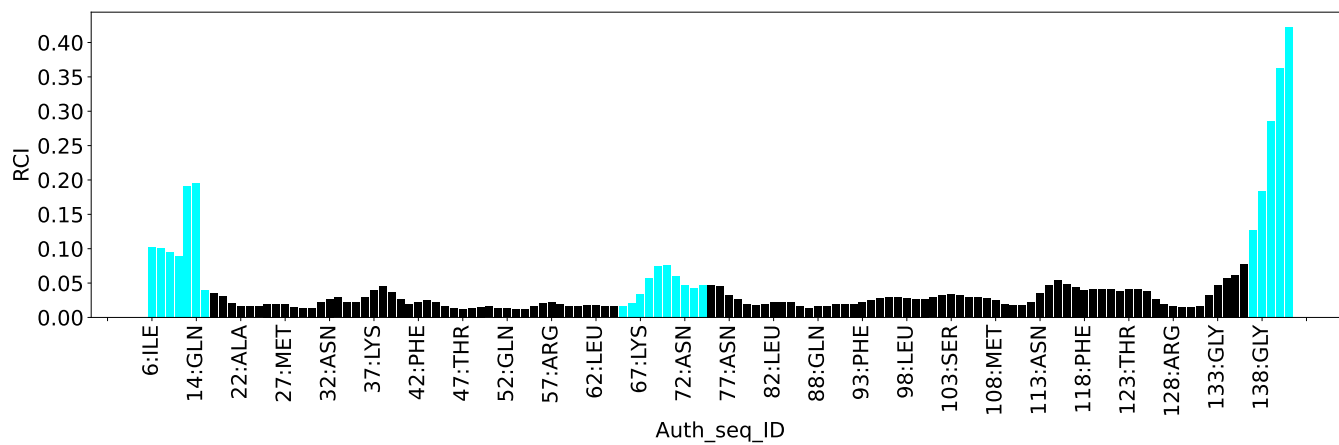
8 NMR restraints analysis ⓘ

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	837
Intra-residue ($|i-j|$=0)	0
Sequential ($|i-j|$=1)	187
Medium range ($|i-j|$>1 and $|i-j|$<5)	259
Long range ($|i-j|$≥5)	319
Inter-chain	0
Hydrogen bond restraints	72
Disulfide bond restraints	0
Total dihedral-angle restraints	145
Number of unmapped restraints	0
Number of restraints per residue	6.8
Number of long range restraints per residue[1]	2.3

[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)	0.7	0.2
0.2-0.5 (Medium)	0.6	0.48
>0.5 (Large)	1.0	1.56

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
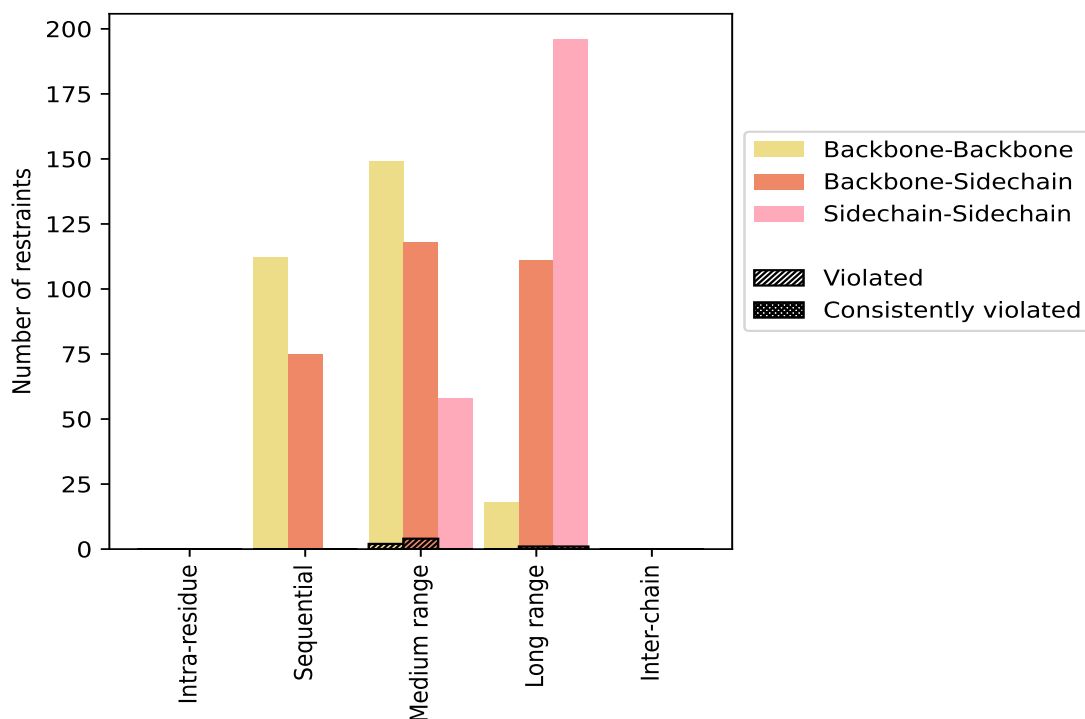
9 Distance violation analysis ⓘ

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)	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
Sequential (|i-j|=1)	187	22.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	112	13.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	75	9.0	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
Medium range (|i-j|>1 & |i-j|<5)	259	30.9	4	1.5	0.5	0	0.0	0.0
Backbone-Backbone	83	9.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	118	14.1	4	3.4	0.5	0	0.0	0.0
Sidechain-Sidechain	58	6.9	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	319	38.1	2	0.6	0.2	0	0.0	0.0
Backbone-Backbone	12	1.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	111	13.3	1	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	196	23.4	1	0.5	0.1	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	72	8.6	2	2.8	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	837	100.0	8	1.0	1.0	0	0.0	0.0
Backbone-Backbone	279	33.3	2	0.7	0.2	0	0.0	0.0
Backbone-Sidechain	304	36.3	5	1.6	0.6	0	0.0	0.0
Sidechain-Sidechain	254	30.3	1	0.4	0.1	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	0	0	2	0	0	2	0.22	0.26	0.04	0.22
2	0	0	3	0	0	3	0.59	0.89	0.32	0.74
3	0	0	3	0	0	3	0.62	0.95	0.36	0.78
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	2	0	0	2	0.6	0.63	0.03	0.6
6	0	0	4	0	0	4	0.14	0.21	0.04	0.11
7	0	0	3	0	0	3	0.93	1.35	0.56	1.29
8	0	0	2	0	0	2	1.17	1.23	0.06	1.17
9	0	0	1	0	0	1	0.18	0.18	0.0	0.18
10	0	0	2	0	0	2	0.26	0.33	0.07	0.26
11	0	0	2	0	0	2	0.64	0.71	0.06	0.64

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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	0	2	1	0	3	0.81	1.23	0.5	1.08
13	0	0	2	0	0	2	0.44	0.48	0.04	0.44
14	0	0	2	0	0	2	0.75	0.83	0.08	0.75
15	0	0	2	1	0	3	0.22	0.35	0.1	0.2
16	0	0	2	0	0	2	1.18	1.24	0.06	1.18
17	0	0	2	1	0	3	1.04	1.56	0.65	1.43
18	0	0	2	0	0	2	0.29	0.33	0.05	0.29
19	0	0	2	1	0	3	0.28	0.41	0.12	0.3
20	0	0	2	0	0	2	0.3	0.33	0.04	0.3

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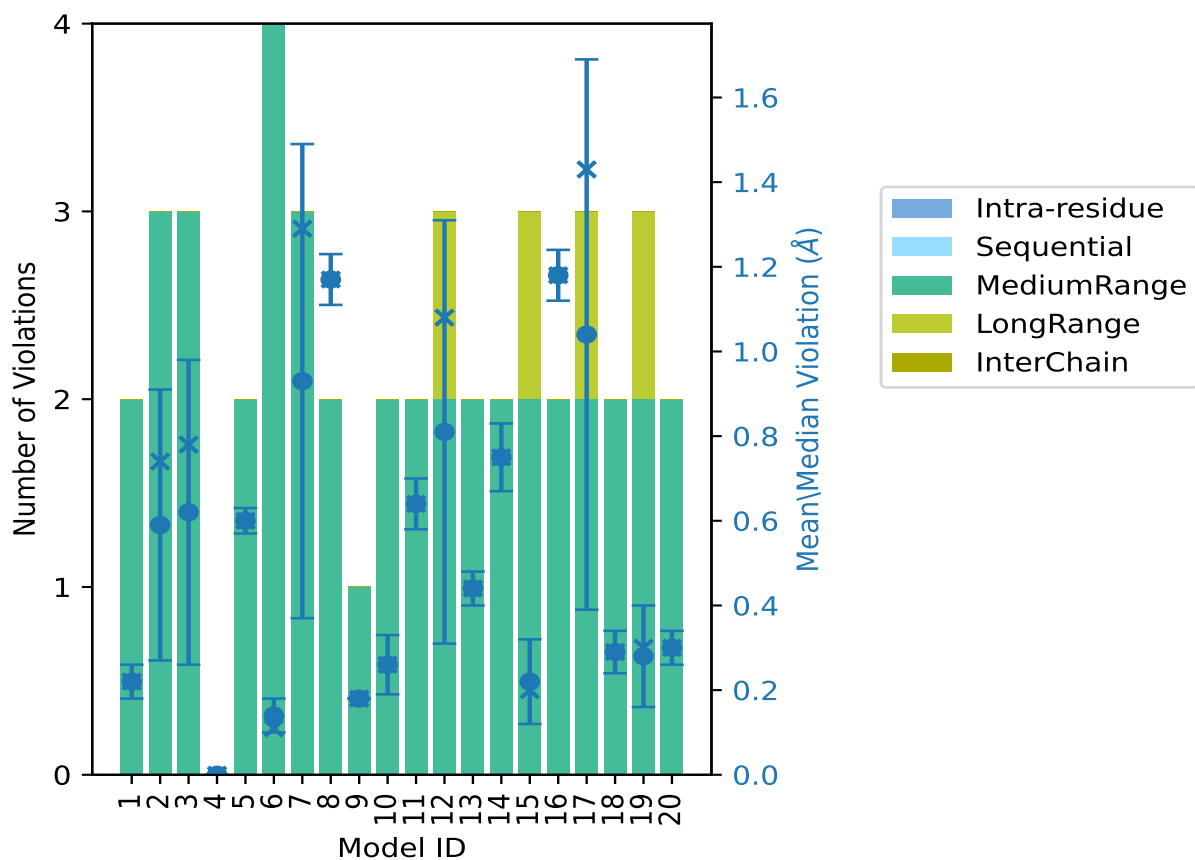
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

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, 759(IR:0, SQ:187, MR:255, LR:317, 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]	%
0	0	3	0	0	3	1	5.0
0	0	1	2	0	3	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	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 (i)
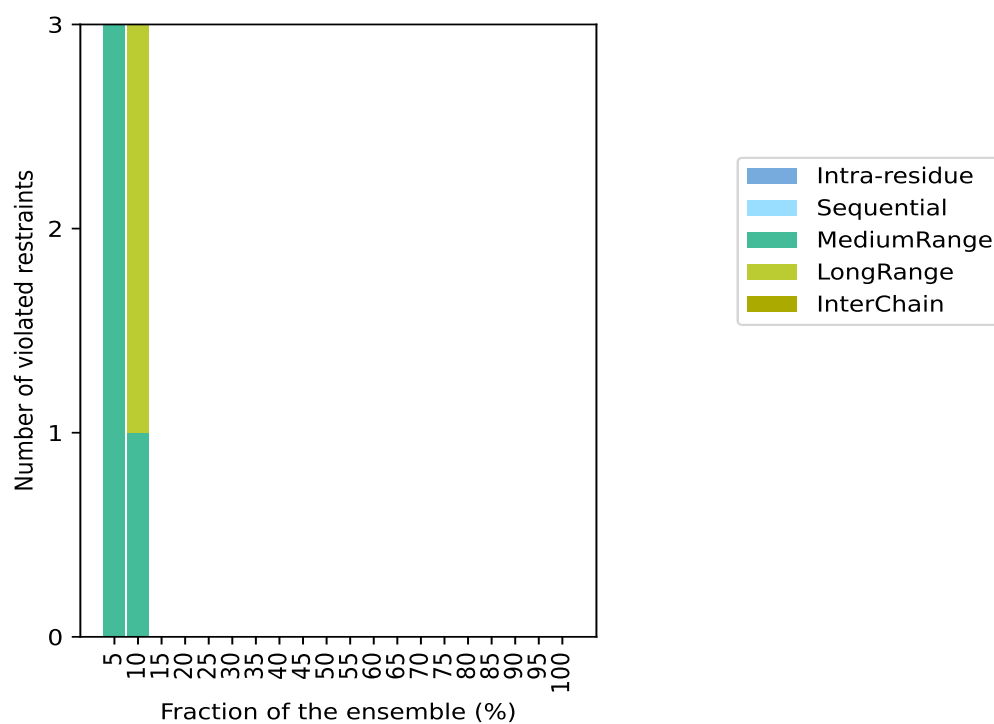
9.4 Most violated distance restraints in the ensemble (i)

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
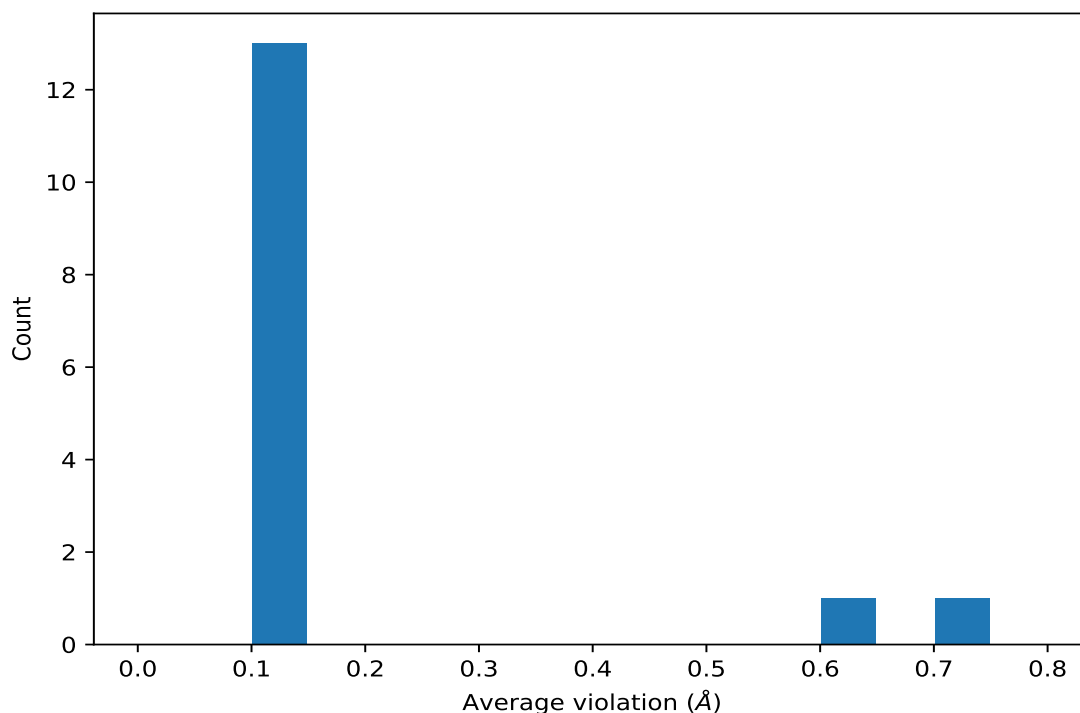
9.4.2 Table: Most violated distance restraints ⓘ

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	19	0.71	0.43	0.63
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	18	0.63	0.41	0.57
(1,467)	1:A:45:ALA:HA	1:A:49:GLU:HB2	2	0.12	0.02	0.12
(1,467)	1:A:45:ALA:HA	1:A:49:GLU:HB3	2	0.12	0.02	0.12
(1,399)	1:A:75:PRO:HB2	1:A:80:VAL:H	2	0.12	0.0	0.12
(1,399)	1:A:75:PRO:HB3	1:A:80:VAL:H	2	0.12	0.0	0.12
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD11	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD12	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD13	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD11	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD12	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD13	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD11	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD12	2	0.12	0.01	0.12
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD13	2	0.12	0.01	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.
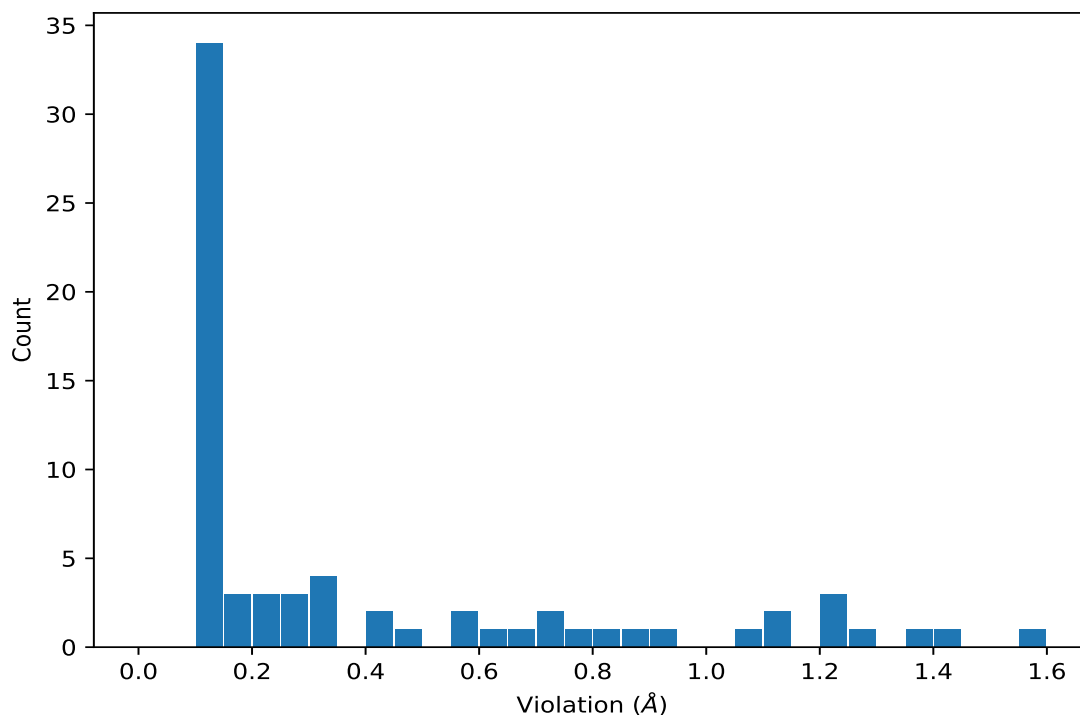
9.5.2 Table : All distance violations ⓘ

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)
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	17	1.56
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	17	1.43
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	7	1.35
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	7	1.29
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	16	1.24
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	8	1.23
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	12	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	16	1.13
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	8	1.11
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	12	1.08
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	3	0.95
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	2	0.89
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	14	0.83
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	3	0.78
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	2	0.74
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	11	0.71
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	14	0.67
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	5	0.63
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	11	0.58
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	5	0.56
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	13	0.48
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	19	0.41
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	13	0.41
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	15	0.35
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	10	0.33
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	18	0.33
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	20	0.33
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	19	0.3
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	1	0.26
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	20	0.26
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	18	0.24
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	6	0.21
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	15	0.2
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	1	0.19
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	10	0.19
(2,12)	1:A:20:GLU:O	1:A:24:VAL:H	9	0.18
(1,439)	1:A:21:LEU:HA	1:A:23:ARG:HB2	2	0.15
(1,439)	1:A:21:LEU:HA	1:A:23:ARG:HB3	2	0.15
(1,467)	1:A:45:ALA:HA	1:A:49:GLU:HB2	7	0.14
(1,467)	1:A:45:ALA:HA	1:A:49:GLU:HB3	7	0.14
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD11	17	0.13
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD12	17	0.13
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD13	17	0.13
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD11	17	0.13
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD12	17	0.13
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD13	17	0.13
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD11	17	0.13
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD12	17	0.13
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD13	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:A:75:PRO:HB2	1:A:80:VAL:H	15	0.12
(1,399)	1:A:75:PRO:HB3	1:A:80:VAL:H	15	0.12
(1,399)	1:A:75:PRO:HB2	1:A:80:VAL:H	19	0.12
(1,399)	1:A:75:PRO:HB3	1:A:80:VAL:H	19	0.12
(1,268)	1:A:84:GLN:HB2	1:A:86:ARG:H	3	0.12
(1,268)	1:A:84:GLN:HB3	1:A:86:ARG:H	3	0.12
(2,11)	1:A:20:GLU:O	1:A:24:VAL:N	6	0.11
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD11	12	0.11
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD12	12	0.11
(1,595)	1:A:41:ILE:HG21	1:A:102:LEU:HD13	12	0.11
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD11	12	0.11
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD12	12	0.11
(1,595)	1:A:41:ILE:HG22	1:A:102:LEU:HD13	12	0.11
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD11	12	0.11
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD12	12	0.11
(1,595)	1:A:41:ILE:HG23	1:A:102:LEU:HD13	12	0.11
(1,467)	1:A:45:ALA:HA	1:A:49:GLU:HB2	6	0.11
(1,467)	1:A:45:ALA:HA	1:A:49:GLU:HB3	6	0.11
(1,284)	1:A:18:VAL:HG21	1:A:22:ALA:H	6	0.11
(1,284)	1:A:18:VAL:HG22	1:A:22:ALA:H	6	0.11
(1,284)	1:A:18:VAL:HG23	1:A:22:ALA:H	6	0.11

10   Dihedral-angle violation analysis ⓘ

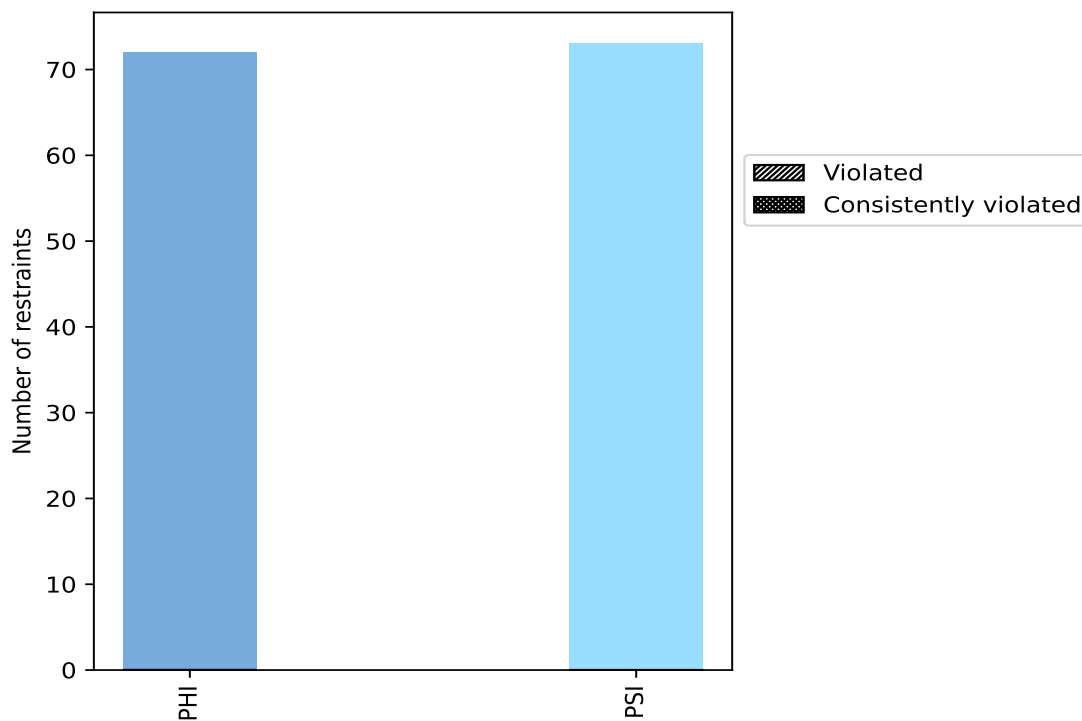## 10.1   Summary of dihedral-angle violations ⓘ

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	$\%^2$	$\%^1$
PHI	72	49.7	0	0.0	0.0	0	0.0	0.0
PSI	73	50.3	0	0.0	0.0	0	0.0	0.0
Total	145	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 ⓘ

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

10.2　Dihedral-angle violation statistics for each model ⓘ

No violations found

10.3　Dihedral-angle violation statistics for the ensemble ⓘ

No violations found

10.4　Most violated dihedral-angle restraints in the ensemble ⓘ

No violations found

10.5　All violated dihedral-angle restraints ⓘ

No violations found