Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 07:24 AM EDT

PDB ID	:	2NNZ
BMRB ID	:	7271
Title	:	Solution structure of the hypothetical protein AF2241 from Archaeoglobus fulgidus
Authors	:	Ai, X.; Semesib, A.; Yee, A.; Arrowsmith, C.H.; Li, S.S.C.; Choy, W.Y.; Ontario Centre for Structural Proteomics (OCSP)
Deposited on	:	2006-10-24

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

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

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

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

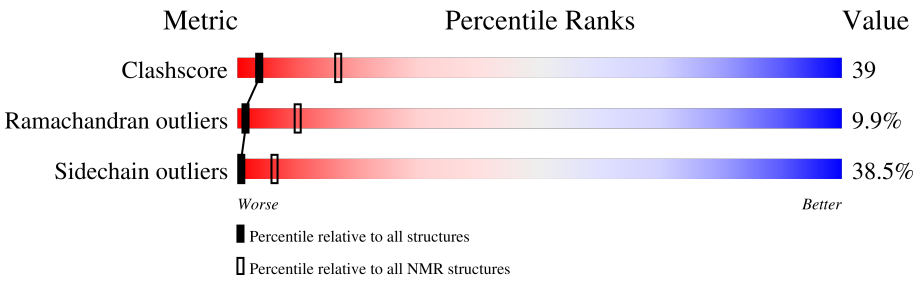
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 86%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	153	27% 31% 18% 10% 14%

2 Ensemble composition and analysis (i)

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: *closest to the average*.

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:8-A:94, A:98-A:111, A:117-A:131 (116)	0.30	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2032 atoms, of which 1011 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	2032	643	1011	173	200	5	0

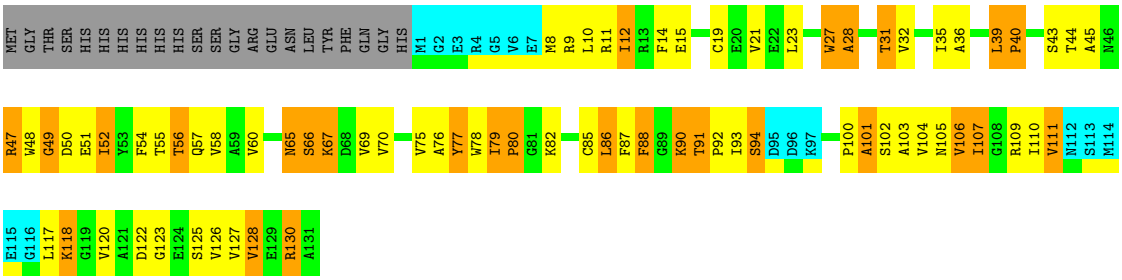
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Hypothetical protein

Chain A: 27% 31% 18% 10% 14%



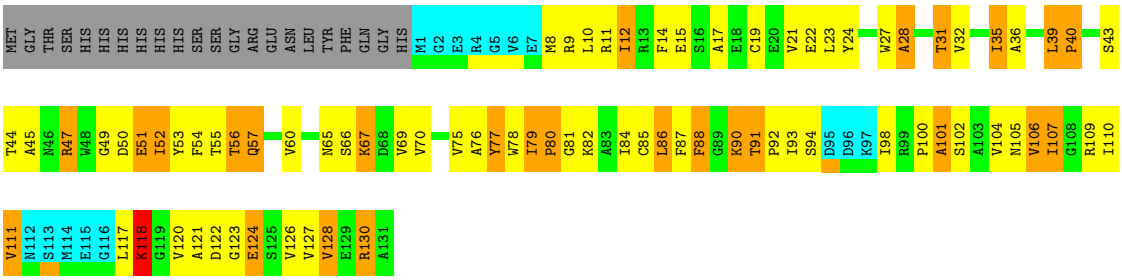
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Hypothetical protein

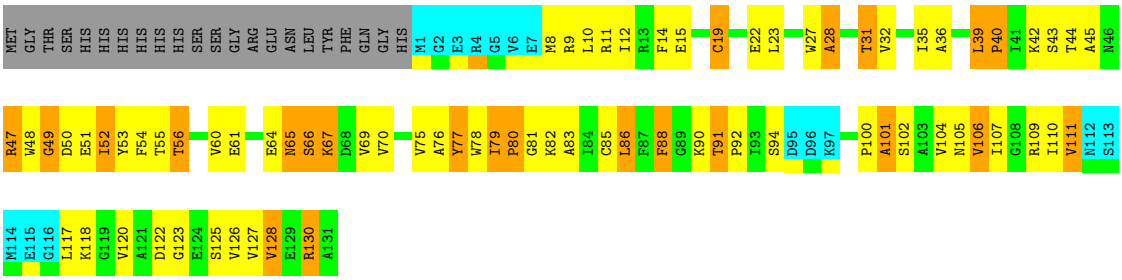
Chain A: 24% 35% 17% • 10% 14%



4.2.2 Score per residue for model 2

- Molecule 1: Hypothetical protein

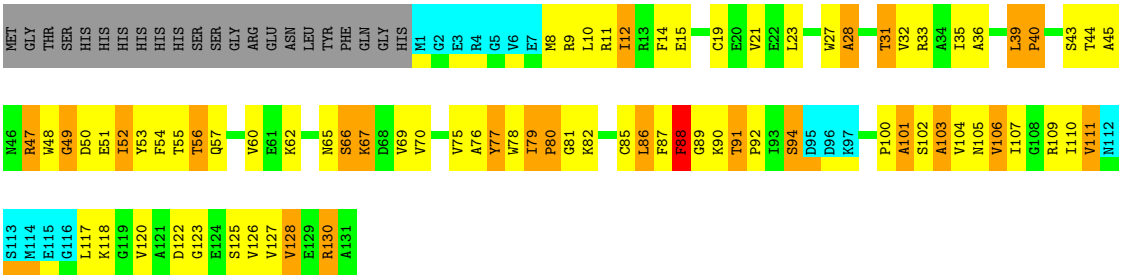
Chain A: 26% 35% 15% 10% 14%



4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein

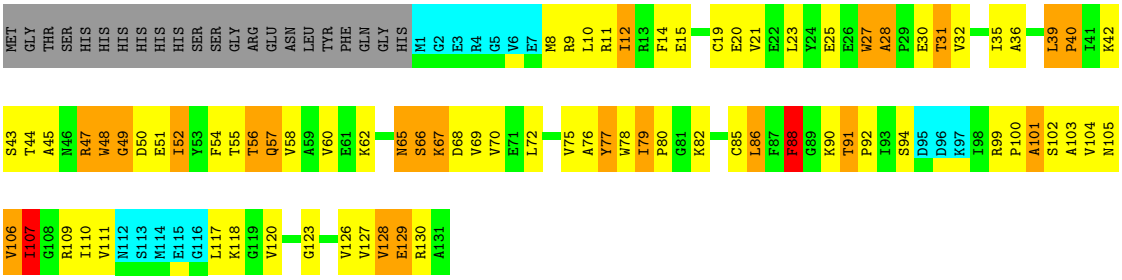
Chain A: 25% 35% 15% • 10% 14%



4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein

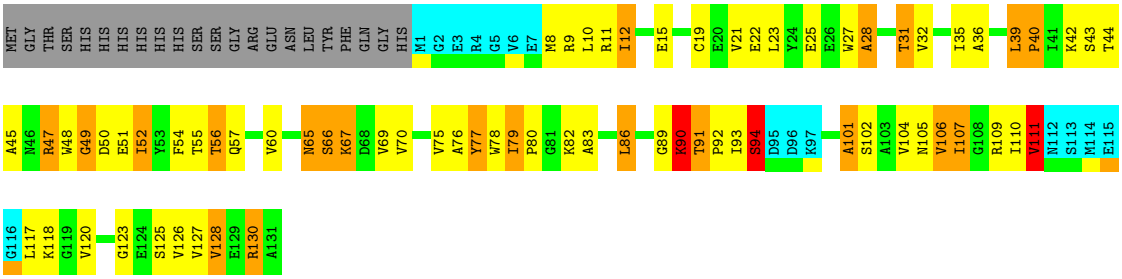
Chain A: 24% 36% 15% • 10% 14%



4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical protein

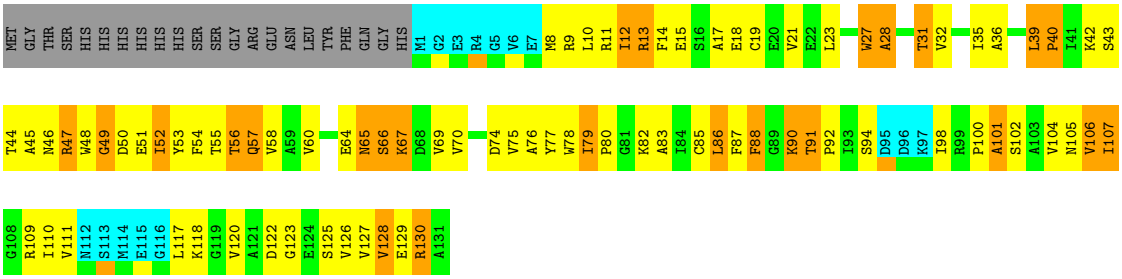
Chain A: 29% 31% 14% • 10% 14%



4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein

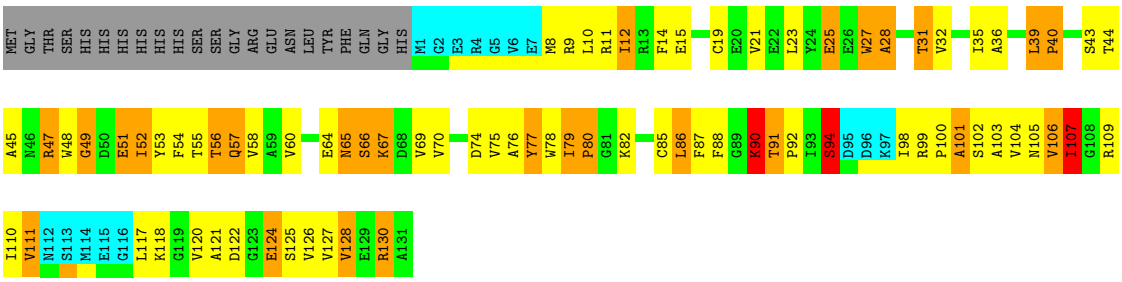
Chain A: 21% 39% 16% 10% 14%



4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein

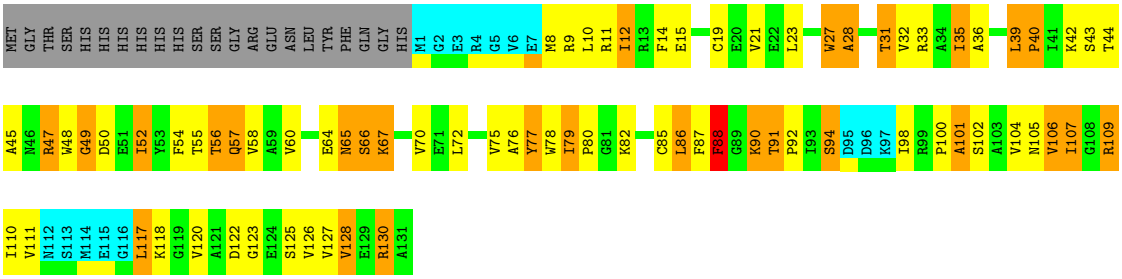
Chain A: 24% 33% 18% • 10% 14%



4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein

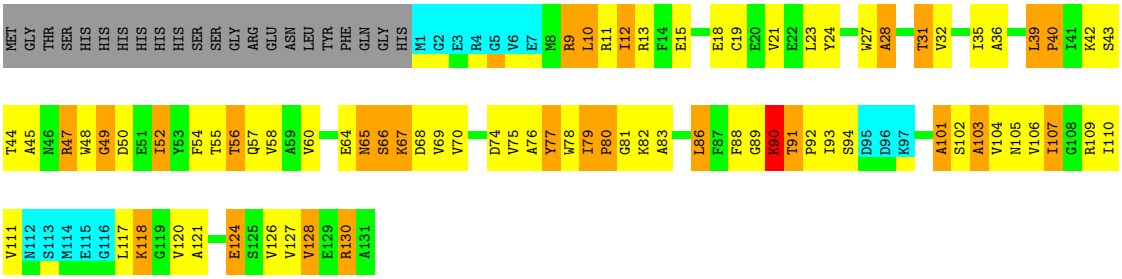
Chain A: 26% 31% 18% • 10% 14%



4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein

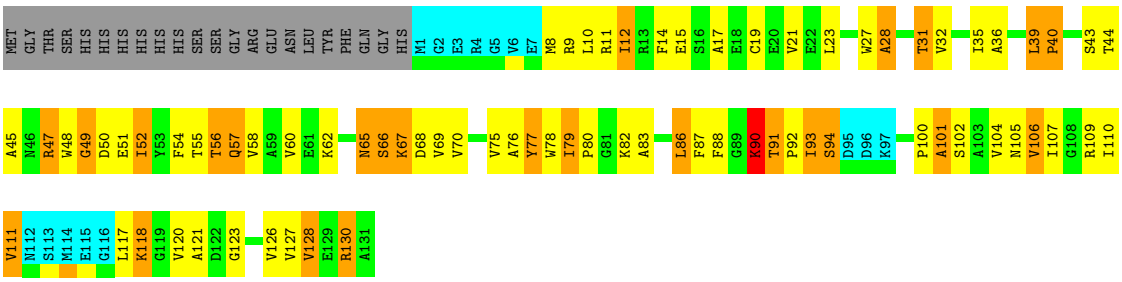
Chain A: 25% 33% 17% • 10% 14%



4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein

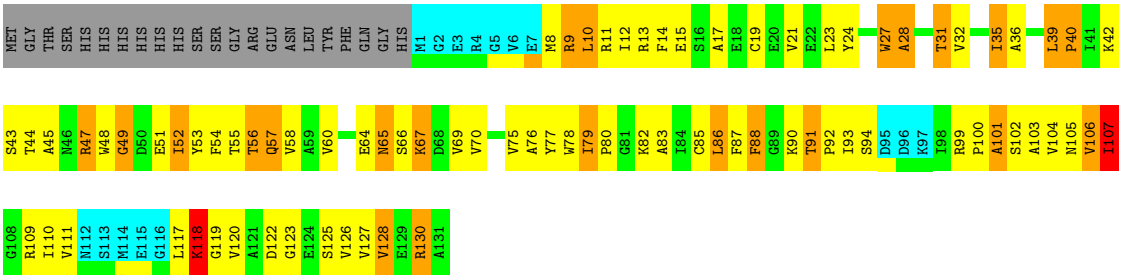
Chain A: 26% 33% 16% • 10% 14%



4.2.11 Score per residue for model 11

- Molecule 1: Hypothetical protein

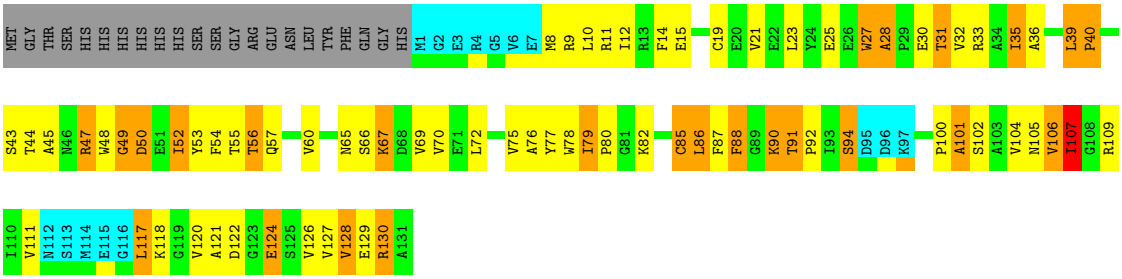
Chain A: 22% 38% 15% • 10% 14%



4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical protein

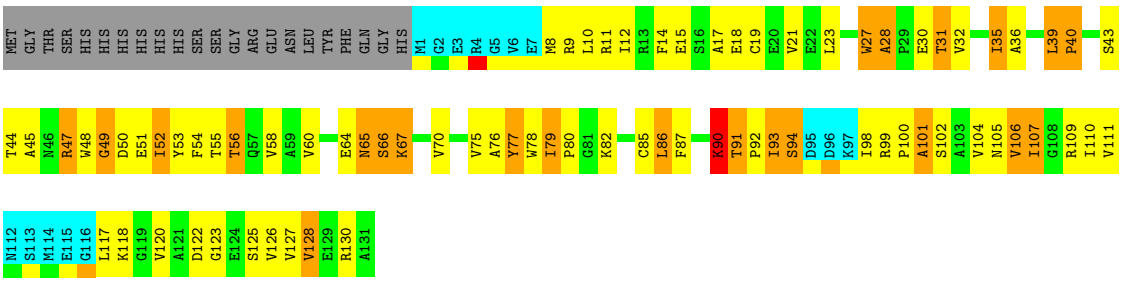
Chain A: 26% 33% 16% • 10% 14%



4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical protein

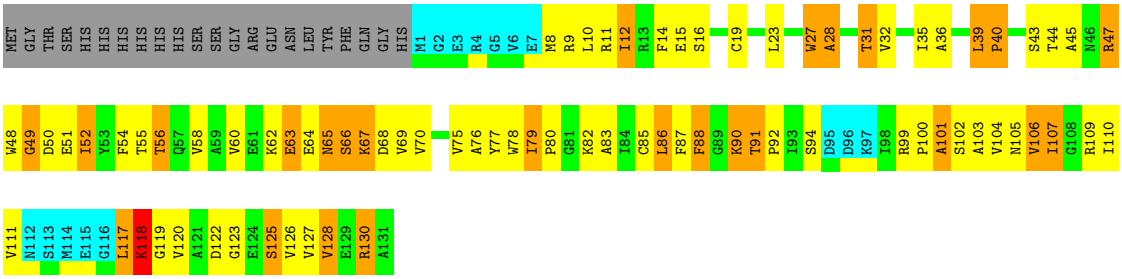
Chain A: 25% 35% 15% • 10% 14%



4.2.14 Score per residue for model 14

• Molecule 1: Hypothetical protein

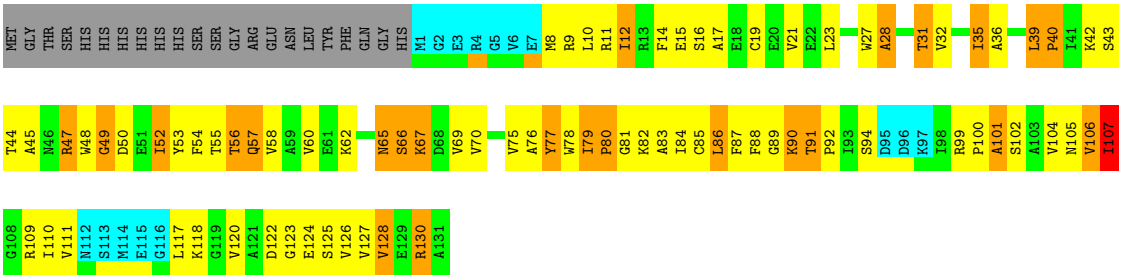
Chain A: 24% 35% 17% • 10% 14%



4.2.15 Score per residue for model 15

• Molecule 1: Hypothetical protein

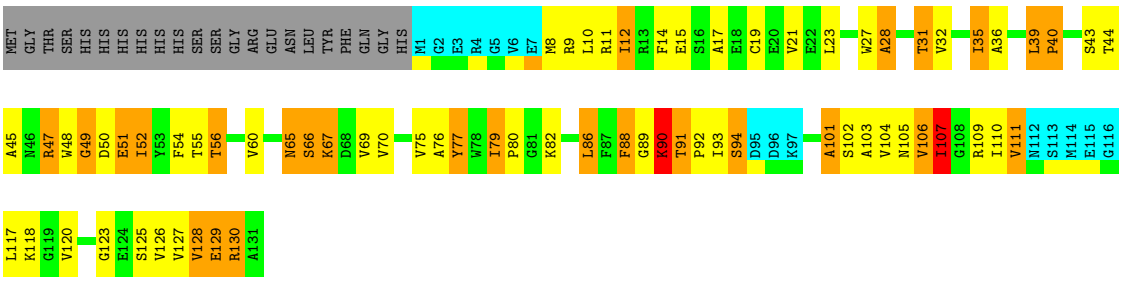
Chain A: 22% 38% 16% • 10% 14%



4.2.16 Score per residue for model 16

• Molecule 1: Hypothetical protein

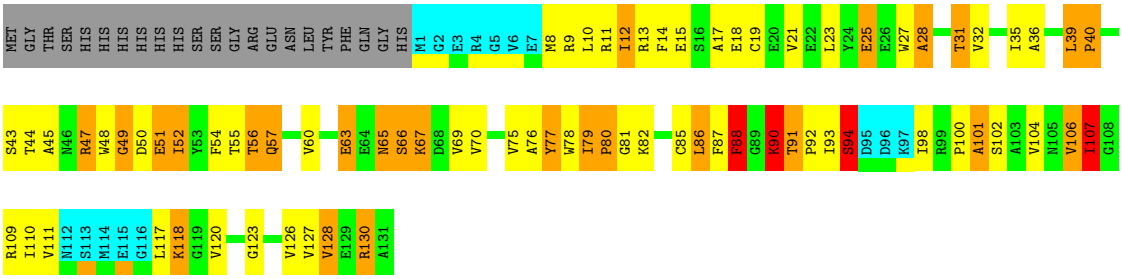
Chain A: 29% 28% 17% • 10% 14%



4.2.17 Score per residue for model 17

- Molecule 1: Hypothetical protein

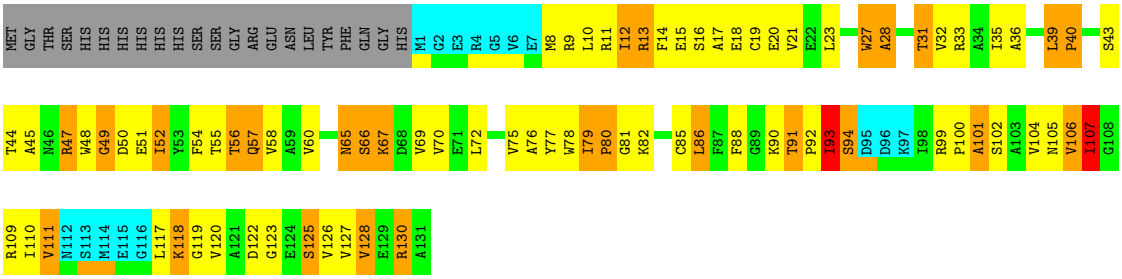
Chain A: 25% 31% 17% • 10% 14%



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Hypothetical protein

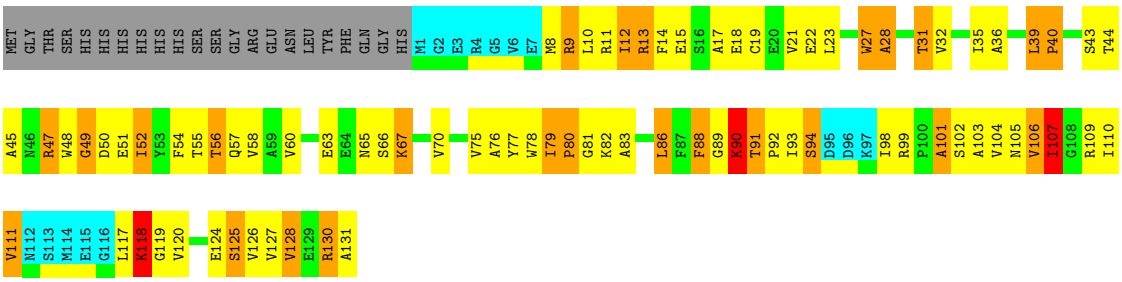
Chain A: 22% 35% 18% • 10% 14%



4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical protein

Chain A: 22% 35% 16% • 10% 14%



4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein

Chain A: 24% 34% 16% • 10% 14%

MET GLY THR SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY HIS M1 G2 E3 R4 G5 V6 E7 M8 R9 L10 R11 I12 E15 C19 E20 V21 E22 L23 Y24 E25 E26 W27 A28 T31 V32 I35 A36 L39 P40 I41 K42 S43 T44

A45 N46 R47 W48 G49 D50 E51 I52 Y53 F54 T55 T56 Q57 V58 A59 V60 E63 E64 N65 S66 K67 D68 V69 V70 D74 V75 A76 Y77 W78 I79 P80 G81 K82 A83 I84 C85 L86 F87 F88 G89 K90 T91 P92 I93 S94 D95 D96 K97 I98 R99 P100 A101 S102 A103 V104 N105 V106 I107

I110 V111 N112 S113 M114 E115 G116 L117 K118 G119 V120 A121 D122 G123 V126 V127 V128 E129 R130 A131

5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	**Classification**	**Version**
CNS	structure solution	1.1
CNS	refinement	1.1

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1452
Number of shifts mapped to atoms	1452
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	909	912	912	72±4
All	All	18180	18240	18240	1430

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:HD13	1:A:117:LEU:HD22	0.90	1.40	3	18
1:A:23:LEU:HD21	1:A:32:VAL:HG22	0.90	1.40	18	17
1:A:39:LEU:HB3	1:A:40:PRO:HD2	0.85	1.48	12	20
1:A:45:ALA:HB1	1:A:47:ARG:NH2	0.85	1.86	10	3
1:A:117:LEU:O	1:A:120:VAL:HG13	0.83	1.73	13	20
1:A:14:PHE:CE2	1:A:126:VAL:HG22	0.81	2.10	17	3
1:A:47:ARG:HD2	1:A:120:VAL:HG23	0.81	1.53	18	16
1:A:45:ALA:HB2	1:A:126:VAL:HG21	0.79	1.54	11	20
1:A:45:ALA:HB2	1:A:126:VAL:CG2	0.78	2.08	17	20
1:A:23:LEU:CD2	1:A:32:VAL:HG13	0.77	2.10	12	20
1:A:31:THR:HG22	1:A:60:VAL:CG2	0.75	2.11	19	18
1:A:67:LYS:HE2	1:A:106:VAL:HG13	0.74	1.60	13	19
1:A:31:THR:HG22	1:A:60:VAL:HG22	0.74	1.59	20	10
1:A:14:PHE:CE1	1:A:126:VAL:HG22	0.73	2.19	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HD21	1:A:32:VAL:CG2	0.72	2.15	18	3
1:A:52:ILE:HG21	1:A:117:LEU:HD21	0.71	1.62	4	5
1:A:86:LEU:HD13	1:A:117:LEU:CD2	0.71	2.15	10	10
1:A:91:THR:HG21	1:A:100:PRO:HA	0.70	1.62	11	14
1:A:39:LEU:HB3	1:A:40:PRO:CD	0.70	2.15	7	20
1:A:75:VAL:HG23	1:A:109:ARG:HA	0.70	1.62	17	19
1:A:27:TRP:CZ2	1:A:31:THR:HG21	0.70	2.21	5	10
1:A:23:LEU:HD21	1:A:32:VAL:HG13	0.70	1.62	4	19
1:A:76:ALA:HB1	1:A:105:ASN:O	0.69	1.86	16	18
1:A:28:ALA:HB3	1:A:31:THR:OG1	0.68	1.87	7	7
1:A:78:TRP:CD1	1:A:104:VAL:HG12	0.67	2.24	13	14
1:A:56:THR:HG21	1:A:128:VAL:HG21	0.67	1.67	20	20
1:A:47:ARG:CD	1:A:120:VAL:HG23	0.67	2.19	8	3
1:A:51:GLU:HG3	1:A:91:THR:HG22	0.66	1.67	4	6
1:A:27:TRP:CH2	1:A:79:ILE:HD11	0.66	2.24	12	4
1:A:68:ASP:OD1	1:A:69:VAL:HG23	0.65	1.92	14	4
1:A:101:ALA:HB3	1:A:104:VAL:HG13	0.64	1.67	16	20
1:A:79:ILE:HB	1:A:80:PRO:HD3	0.64	1.70	15	12
1:A:86:LEU:HD13	1:A:117:LEU:HD23	0.63	1.71	20	2
1:A:86:LEU:CD1	1:A:117:LEU:HD22	0.63	2.23	4	7
1:A:93:ILE:N	1:A:93:ILE:HD13	0.62	2.10	20	4
1:A:39:LEU:CB	1:A:40:PRO:HD2	0.61	2.24	18	20
1:A:36:ALA:O	1:A:39:LEU:CD2	0.61	2.49	4	20
1:A:107:ILE:O	1:A:107:ILE:HD13	0.61	1.95	9	5
1:A:90:LYS:CD	1:A:90:LYS:N	0.61	2.64	14	3
1:A:27:TRP:O	1:A:28:ALA:HB2	0.61	1.95	14	20
1:A:39:LEU:HD22	1:A:130:ARG:CB	0.61	2.26	17	20
1:A:91:THR:OG1	1:A:98:ILE:HG23	0.61	1.94	13	7
1:A:75:VAL:HG22	1:A:110:ILE:CD1	0.61	2.24	6	17
1:A:22:GLU:OE2	1:A:111:VAL:HG13	0.60	1.96	5	1
1:A:27:TRP:NE1	1:A:31:THR:HG21	0.60	2.11	7	9
1:A:27:TRP:CZ2	1:A:77:TYR:CE2	0.59	2.90	16	5
1:A:39:LEU:HD22	1:A:130:ARG:HB3	0.59	1.74	6	9
1:A:78:TRP:CD1	1:A:80:PRO:HD2	0.59	2.33	8	4
1:A:27:TRP:CZ2	1:A:77:TYR:CE1	0.59	2.91	15	5
1:A:31:THR:HG22	1:A:60:VAL:HG21	0.58	1.74	16	6
1:A:47:ARG:HD3	1:A:120:VAL:O	0.58	1.99	1	2
1:A:48:TRP:O	1:A:50:ASP:N	0.57	2.37	4	15
1:A:22:GLU:OE2	1:A:111:VAL:HG21	0.57	2.00	2	1
1:A:91:THR:HG22	1:A:92:PRO:CD	0.57	2.29	12	10
1:A:10:LEU:N	1:A:10:LEU:HD23	0.57	2.15	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:TRP:CE2	1:A:31:THR:HG21	0.57	2.35	5	5
1:A:121:ALA:HB3	1:A:124:GLU:OE1	0.56	1.99	12	4
1:A:56:THR:CG2	1:A:128:VAL:HG21	0.56	2.30	11	20
1:A:47:ARG:HG3	1:A:122:ASP:HA	0.55	1.78	20	12
1:A:66:SER:OG	1:A:79:ILE:HD12	0.55	2.02	10	3
1:A:78:TRP:HD1	1:A:104:VAL:HG12	0.55	1.60	13	4
1:A:43:SER:OG	1:A:126:VAL:HB	0.55	2.01	13	19
1:A:12:ILE:HG22	1:A:12:ILE:O	0.55	2.02	7	20
1:A:101:ALA:HB3	1:A:104:VAL:CG1	0.55	2.32	9	2
1:A:27:TRP:CZ2	1:A:31:THR:CG2	0.54	2.90	15	10
1:A:52:ILE:O	1:A:85:CYS:HA	0.54	2.03	8	13
1:A:76:ALA:HA	1:A:107:ILE:H	0.54	1.62	16	10
1:A:31:THR:CG2	1:A:60:VAL:HG22	0.54	2.31	20	6
1:A:79:ILE:CB	1:A:80:PRO:HD3	0.53	2.32	15	10
1:A:27:TRP:O	1:A:28:ALA:CB	0.53	2.55	9	20
1:A:63:GLU:CG	1:A:63:GLU:O	0.52	2.58	17	2
1:A:76:ALA:CB	1:A:105:ASN:O	0.52	2.57	16	9
1:A:39:LEU:CB	1:A:40:PRO:CD	0.52	2.88	16	20
1:A:27:TRP:O	1:A:27:TRP:CE3	0.52	2.62	11	10
1:A:23:LEU:HD21	1:A:32:VAL:CG1	0.51	2.33	15	10
1:A:60:VAL:O	1:A:60:VAL:HG13	0.51	2.05	14	17
1:A:127:VAL:O	1:A:127:VAL:HG23	0.51	2.06	17	19
1:A:14:PHE:CZ	1:A:126:VAL:HG22	0.51	2.40	15	9
1:A:47:ARG:HD2	1:A:120:VAL:O	0.51	2.06	9	7
1:A:78:TRP:HA	1:A:104:VAL:HG12	0.51	1.83	7	8
1:A:79:ILE:HB	1:A:80:PRO:CD	0.51	2.35	14	7
1:A:52:ILE:CG2	1:A:52:ILE:O	0.51	2.58	15	2
1:A:51:GLU:CD	1:A:91:THR:HG22	0.51	2.25	6	2
1:A:47:ARG:NH1	1:A:120:VAL:HG21	0.51	2.20	10	1
1:A:67:LYS:NZ	1:A:70:VAL:HG11	0.50	2.21	19	20
1:A:25:GLU:OE1	1:A:32:VAL:HG21	0.50	2.06	7	2
1:A:27:TRP:CH2	1:A:77:TYR:CD2	0.50	3.00	1	2
1:A:92:PRO:HB2	1:A:93:ILE:HD12	0.50	1.84	17	5
1:A:88:PHE:HB3	1:A:118:LYS:HG2	0.50	1.84	1	4
1:A:75:VAL:HG22	1:A:110:ILE:HD11	0.50	1.84	13	8
1:A:91:THR:CB	1:A:92:PRO:HD2	0.50	2.37	4	9
1:A:14:PHE:N	1:A:17:ALA:O	0.50	2.44	11	10
1:A:91:THR:HB	1:A:92:PRO:HD2	0.50	1.84	10	15
1:A:47:ARG:CD	1:A:120:VAL:O	0.49	2.59	11	7
1:A:48:TRP:O	1:A:49:GLY:C	0.49	2.50	8	7
1:A:79:ILE:CB	1:A:80:PRO:CD	0.49	2.90	7	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:THR:CB	1:A:92:PRO:CD	0.49	2.91	3	16
1:A:77:TYR:CE1	1:A:78:TRP:O	0.48	2.66	8	6
1:A:90:LYS:CB	1:A:94:SER:HB3	0.48	2.39	8	1
1:A:127:VAL:HG23	1:A:129:GLU:OE2	0.48	2.09	4	2
1:A:48:TRP:CD1	1:A:49:GLY:N	0.47	2.82	20	14
1:A:65:ASN:O	1:A:66:SER:C	0.47	2.51	9	14
1:A:23:LEU:HD13	1:A:107:ILE:HG12	0.47	1.85	14	6
1:A:49:GLY:O	1:A:50:ASP:HB3	0.47	2.10	19	5
1:A:66:SER:N	1:A:105:ASN:OD1	0.47	2.48	8	2
1:A:47:ARG:CZ	1:A:120:VAL:HG21	0.47	2.39	10	1
1:A:74:ASP:O	1:A:87:PHE:CE1	0.47	2.68	7	2
1:A:91:THR:HG22	1:A:92:PRO:HD3	0.47	1.85	12	5
1:A:76:ALA:HB3	1:A:87:PHE:CE2	0.47	2.44	17	3
1:A:47:ARG:NH1	1:A:120:VAL:HB	0.47	2.25	6	2
1:A:79:ILE:O	1:A:81:GLY:N	0.46	2.49	19	8
1:A:52:ILE:O	1:A:52:ILE:CG2	0.46	2.63	8	3
1:A:27:TRP:CD2	1:A:105:ASN:ND2	0.46	2.83	8	2
1:A:87:PHE:CE1	1:A:100:PRO:HB3	0.46	2.46	12	11
1:A:107:ILE:O	1:A:107:ILE:HG23	0.46	2.10	12	8
1:A:39:LEU:O	1:A:40:PRO:C	0.46	2.54	18	20
1:A:54:PHE:C	1:A:54:PHE:CD1	0.46	2.89	8	17
1:A:89:GLY:O	1:A:90:LYS:O	0.46	2.33	9	4
1:A:77:TYR:CE2	1:A:105:ASN:ND2	0.46	2.83	7	1
1:A:47:ARG:NH2	1:A:52:ILE:HG12	0.46	2.26	10	1
1:A:47:ARG:HD3	1:A:121:ALA:O	0.46	2.11	10	1
1:A:52:ILE:O	1:A:52:ILE:HG22	0.45	2.11	16	4
1:A:69:VAL:O	1:A:70:VAL:HG13	0.45	2.11	12	10
1:A:14:PHE:CZ	1:A:126:VAL:CG2	0.45	3.00	4	6
1:A:90:LYS:HB2	1:A:94:SER:HB3	0.45	1.88	7	3
1:A:109:ARG:N	1:A:109:ARG:CD	0.45	2.79	8	1
1:A:76:ALA:HB3	1:A:87:PHE:HE2	0.45	1.71	13	1
1:A:27:TRP:CH2	1:A:77:TYR:CE2	0.44	3.05	1	2
1:A:39:LEU:HD22	1:A:130:ARG:HB2	0.44	1.89	17	6
1:A:78:TRP:CB	1:A:83:ALA:O	0.44	2.66	10	10
1:A:100:PRO:O	1:A:101:ALA:HB2	0.44	2.13	7	7
1:A:54:PHE:CD1	1:A:54:PHE:C	0.44	2.91	18	3
1:A:67:LYS:HG3	1:A:104:VAL:O	0.44	2.12	15	5
1:A:14:PHE:CG	1:A:117:LEU:HD11	0.44	2.47	7	1
1:A:52:ILE:HG22	1:A:52:ILE:O	0.44	2.12	9	1
1:A:36:ALA:O	1:A:39:LEU:HD21	0.44	2.13	4	15
1:A:54:PHE:CE2	1:A:126:VAL:HG11	0.44	2.48	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:THR:CG2	1:A:60:VAL:CG2	0.44	2.95	8	9
1:A:87:PHE:O	1:A:88:PHE:CD2	0.44	2.71	17	3
1:A:54:PHE:CD1	1:A:54:PHE:O	0.43	2.71	4	16
1:A:69:VAL:O	1:A:70:VAL:CG1	0.43	2.66	1	17
1:A:27:TRP:CH2	1:A:77:TYR:CE1	0.43	3.06	15	1
1:A:64:GLU:HG3	1:A:65:ASN:N	0.43	2.28	20	9
1:A:23:LEU:HD23	1:A:32:VAL:HG13	0.43	1.89	19	6
1:A:14:PHE:CD2	1:A:117:LEU:CD1	0.43	3.01	6	1
1:A:27:TRP:CH2	1:A:77:TYR:CD1	0.43	3.07	15	1
1:A:27:TRP:CE2	1:A:105:ASN:OD1	0.43	2.71	1	2
1:A:27:TRP:CH2	1:A:79:ILE:CD1	0.43	2.99	19	1
1:A:67:LYS:NZ	1:A:76:ALA:CB	0.43	2.81	1	3
1:A:75:VAL:HG21	1:A:110:ILE:HG13	0.43	1.91	9	2
1:A:53:TYR:O	1:A:53:TYR:CD1	0.43	2.71	20	8
1:A:67:LYS:HZ3	1:A:70:VAL:HG11	0.43	1.73	13	2
1:A:63:GLU:O	1:A:63:GLU:HG3	0.43	2.13	14	2
1:A:23:LEU:CD1	1:A:107:ILE:HG12	0.43	2.44	17	1
1:A:12:ILE:O	1:A:12:ILE:CG2	0.43	2.66	19	10
1:A:58:VAL:O	1:A:58:VAL:HG13	0.43	2.13	11	13
1:A:56:THR:O	1:A:57:GLN:CB	0.43	2.67	15	15
1:A:48:TRP:CH2	1:A:92:PRO:HA	0.43	2.48	4	1
1:A:90:LYS:CD	1:A:91:THR:N	0.43	2.82	10	1
1:A:93:ILE:HG22	1:A:93:ILE:O	0.43	2.14	16	2
1:A:79:ILE:HD11	1:A:105:ASN:OD1	0.42	2.14	4	2
1:A:14:PHE:CE1	1:A:126:VAL:HG13	0.42	2.49	3	2
1:A:45:ALA:HB1	1:A:47:ARG:HH21	0.42	1.74	6	2
1:A:9:ARG:C	1:A:10:LEU:HD23	0.42	2.34	11	2
1:A:65:ASN:ND2	1:A:105:ASN:HB3	0.42	2.29	9	2
1:A:91:THR:O	1:A:93:ILE:N	0.42	2.52	20	2
1:A:19:CYS:SG	1:A:117:LEU:HD12	0.42	2.54	2	1
1:A:91:THR:HG22	1:A:92:PRO:HD2	0.42	1.91	11	2
1:A:52:ILE:CG2	1:A:117:LEU:HD21	0.42	2.43	12	1
1:A:91:THR:HB	1:A:92:PRO:CD	0.42	2.44	13	5
1:A:77:TYR:O	1:A:77:TYR:CD1	0.42	2.73	2	2
1:A:47:ARG:CG	1:A:122:ASP:HA	0.42	2.44	1	3
1:A:127:VAL:HG23	1:A:127:VAL:O	0.42	2.15	4	1
1:A:118:LYS:CE	1:A:119:GLY:N	0.42	2.82	14	2
1:A:52:ILE:CD1	1:A:120:VAL:HG21	0.42	2.44	13	1
1:A:91:THR:CG2	1:A:92:PRO:CD	0.42	2.98	12	4
1:A:90:LYS:HB2	1:A:94:SER:CB	0.42	2.45	7	2
1:A:67:LYS:HZ1	1:A:104:VAL:HG23	0.42	1.74	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:N	1:A:35:ILE:HD13	0.42	2.30	11	3
1:A:92:PRO:HB2	1:A:93:ILE:HD13	0.42	1.91	13	1
1:A:75:VAL:HG23	1:A:109:ARG:CA	0.41	2.41	10	1
1:A:35:ILE:HD13	1:A:35:ILE:N	0.41	2.31	13	4
1:A:90:LYS:HD2	1:A:91:THR:O	0.41	2.15	15	1
1:A:23:LEU:CD2	1:A:32:VAL:CG1	0.41	2.97	17	1
1:A:40:PRO:HA	1:A:128:VAL:O	0.41	2.16	17	2
1:A:46:ASN:ND2	1:A:53:TYR:CE1	0.41	2.89	6	1
1:A:9:ARG:NH1	1:A:131:ALA:HB2	0.41	2.31	19	1
1:A:63:GLU:HG2	1:A:63:GLU:O	0.41	2.16	19	1
1:A:66:SER:OG	1:A:103:ALA:HB1	0.41	2.16	3	2
1:A:75:VAL:CG2	1:A:110:ILE:CD1	0.41	2.99	5	4
1:A:117:LEU:O	1:A:119:GLY:N	0.41	2.54	18	2
1:A:78:TRP:HB3	1:A:83:ALA:O	0.41	2.15	9	1
1:A:52:ILE:CD1	1:A:120:VAL:CG2	0.41	2.99	11	2
1:A:28:ALA:O	1:A:32:VAL:HG23	0.41	2.16	9	1
1:A:48:TRP:CD1	1:A:51:GLU:HB3	0.41	2.51	14	1
1:A:53:TYR:HA	1:A:84:ILE:O	0.41	2.16	15	1
1:A:47:ARG:NH1	1:A:120:VAL:CG2	0.41	2.84	17	1
1:A:74:ASP:N	1:A:109:ARG:NH2	0.41	2.69	9	1
1:A:27:TRP:CD1	1:A:27:TRP:C	0.41	2.95	20	1
1:A:13:ARG:CG	1:A:127:VAL:CG2	0.40	3.00	18	4
1:A:93:ILE:N	1:A:93:ILE:CD1	0.40	2.81	18	3
1:A:10:LEU:N	1:A:10:LEU:CD2	0.40	2.83	9	1
1:A:22:GLU:OE1	1:A:111:VAL:HG21	0.40	2.15	1	1
1:A:48:TRP:CE3	1:A:49:GLY:N	0.40	2.89	8	1
1:A:79:ILE:HD11	1:A:105:ASN:ND2	0.40	2.31	8	1
1:A:40:PRO:HD3	1:A:129:GLU:CB	0.40	2.46	4	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	115/153 (75%)	84±2 (73±1%)	20±2 (17±2%)	11±2 (10±2%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2300/3060 (75%)	1675 (73%)	397 (17%)	228 (10%)	1 10

All 20 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	28	ALA	20
1	A	39	LEU	20
1	A	40	PRO	20
1	A	49	GLY	20
1	A	66	SER	20
1	A	101	ALA	20
1	A	65	ASN	19
1	A	123	GLY	16
1	A	80	PRO	10
1	A	107	ILE	10
1	A	90	LYS	9
1	A	103	ALA	9
1	A	111	VAL	8
1	A	94	SER	7
1	A	118	LYS	6
1	A	88	PHE	5
1	A	125	SER	5
1	A	89	GLY	2
1	A	93	ILE	1
1	A	92	PRO	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	96/127 (76%)	59±3 (62±3%)	37±3 (38±3%)	0 6
All	All	1920/2540 (76%)	1181 (62%)	739 (38%)	0 6

All 62 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	9	ARG	20
1	A	10	LEU	20
1	A	11	ARG	20
1	A	15	GLU	20
1	A	19	CYS	20
1	A	31	THR	20
1	A	35	ILE	20
1	A	44	THR	20
1	A	47	ARG	20
1	A	52	ILE	20
1	A	55	THR	20
1	A	56	THR	20
1	A	67	LYS	20
1	A	77	TYR	20
1	A	79	ILE	20
1	A	82	LYS	20
1	A	86	LEU	20
1	A	90	LYS	20
1	A	91	THR	20
1	A	94	SER	20
1	A	102	SER	20
1	A	106	VAL	20
1	A	107	ILE	20
1	A	111	VAL	20
1	A	118	LYS	20
1	A	128	VAL	20
1	A	8	MET	18
1	A	21	VAL	18
1	A	130	ARG	18
1	A	12	ILE	16
1	A	88	PHE	16
1	A	51	GLU	11
1	A	125	SER	11
1	A	57	GLN	10
1	A	27	TRP	10
1	A	42	LYS	9
1	A	99	ARG	9
1	A	124	GLU	6
1	A	18	GLU	6
1	A	62	LYS	5
1	A	13	ARG	5
1	A	50	ASP	4
1	A	33	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	72	LEU	4
1	A	129	GLU	4
1	A	93	ILE	4
1	A	30	GLU	3
1	A	25	GLU	3
1	A	117	LEU	3
1	A	85	CYS	3
1	A	16	SER	3
1	A	63	GLU	3
1	A	84	ILE	2
1	A	20	GLU	2
1	A	74	ASP	2
1	A	61	GLU	1
1	A	48	TRP	1
1	A	109	ARG	1
1	A	43	SER	1
1	A	22	GLU	1
1	A	64	GLU	1
1	A	66	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1452
Number of shifts mapped to atoms	1452
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	125	-0.03 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	116	0.22 ± 0.20	None needed (< 0.5 ppm)
$^{13}C'$	115	0.16 ± 0.15	None needed (< 0.5 ppm)
^{15}N	115	0.33 ± 0.48	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1360 atoms were assigned a chemical shift out of a possible 1590. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	562/577 (97%)	230/234 (98%)	223/232 (96%)	109/111 (98%)
Sidechain	782/910 (86%)	534/594 (90%)	245/282 (87%)	3/34 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	16/103 (16%)	13/50 (26%)	0/50 (0%)	3/3 (100%)
Overall	1360/1590 (86%)	777/878 (88%)	468/564 (83%)	115/148 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1452 atoms were assigned a chemical shift out of a possible 1768. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	602/655 (92%)	247/267 (93%)	240/262 (92%)	115/126 (91%)
Sidechain	834/1010 (83%)	569/656 (87%)	261/315 (83%)	4/39 (10%)
Aromatic	16/103 (16%)	13/50 (26%)	0/50 (0%)	3/3 (100%)
Overall	1452/1768 (82%)	829/973 (85%)	501/627 (80%)	122/168 (73%)

7.1.4 Statistically unusual chemical shifts (i)

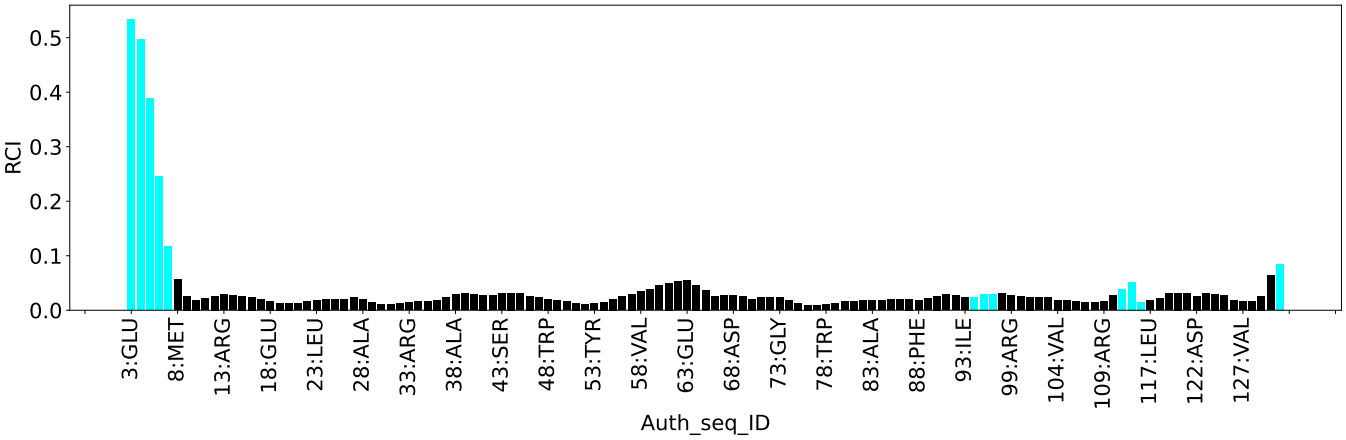
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	70	VAL	HG21	-0.58	-0.58 – 2.19	-5.0
1	A	70	VAL	HG22	-0.58	-0.58 – 2.19	-5.0
1	A	70	VAL	HG23	-0.58	-0.58 – 2.19	-5.0

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
3:GLU
8:MET
13:ARG
18:GLU
23:LEU
28:ALA
33:ARG
38:ALA
43:SER
48:TRP
53:TYR
58:VAL
63:GLU
68:ASP
73:GLY
78:TRP
83:ALA
88:PHE
93:ILE
99:ARG
104:VAL
109:ARG
117:LEU
122:ASP
127:VAL
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1313
Intra-residue (|i-j|=0)	458
Sequential (|i-j|=1)	361
Medium range (|i-j|>1 and |i-j|<5)	129
Long range (|i-j|≥5)	365
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	150
Number of unmapped restraints	0
Number of restraints per residue	9.6
Number of long range restraints per residue[1]	2.4

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.6	0.19
0.2-0.5 (Medium)	0.1	0.22
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	4.7	2.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

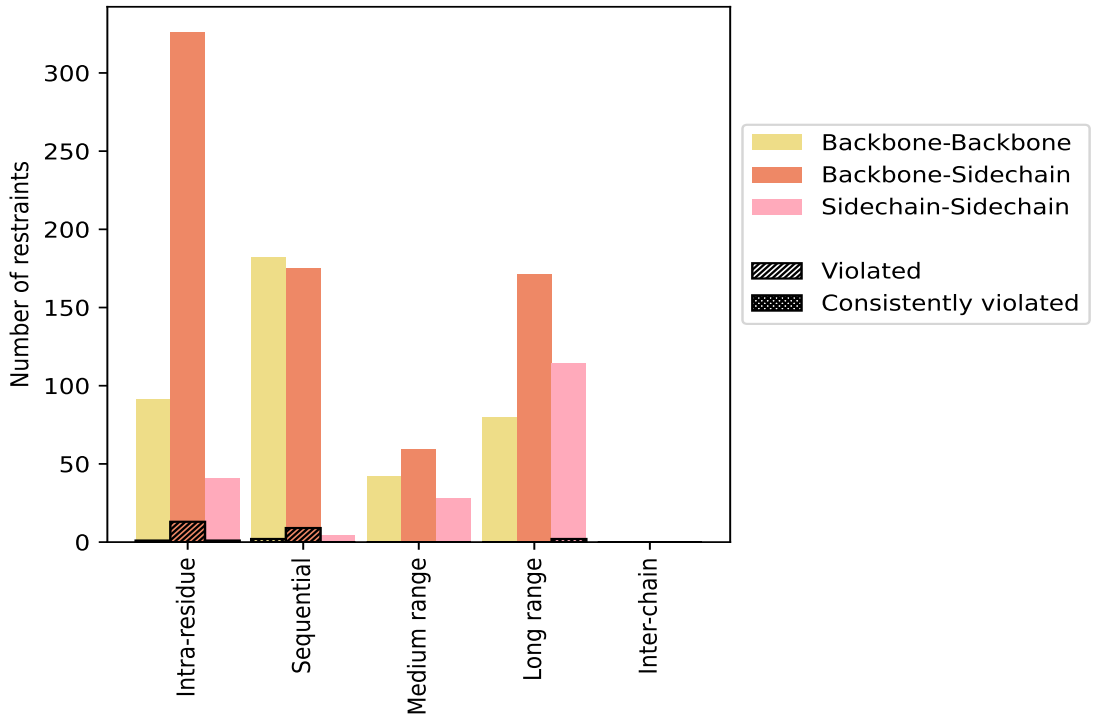
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	458	34.9	15	3.3	1.1	0	0.0	0.0
Backbone-Backbone	91	6.9	1	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	326	24.8	13	4.0	1.0	0	0.0	0.0
Sidechain-Sidechain	41	3.1	1	2.4	0.1	0	0.0	0.0
Sequential (|i-j|=1)	361	27.5	11	3.0	0.8	0	0.0	0.0
Backbone-Backbone	182	13.9	2	1.1	0.2	0	0.0	0.0
Backbone-Sidechain	175	13.3	9	5.1	0.7	0	0.0	0.0
Sidechain-Sidechain	4	0.3	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	129	9.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	42	3.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	59	4.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	28	2.1	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	365	27.8	2	0.5	0.2	0	0.0	0.0
Backbone-Backbone	80	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	171	13.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	114	8.7	2	1.8	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1313	100.0	28	2.1	2.1	0	0.0	0.0
Backbone-Backbone	395	30.1	3	0.8	0.2	0	0.0	0.0
Backbone-Sidechain	731	55.7	22	3.0	1.7	0	0.0	0.0
Sidechain-Sidechain	187	14.2	3	1.6	0.2	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	1	0	0	0	1	0.13	0.13	0.0	0.13
2	1	2	0	0	0	3	0.11	0.11	0.0	0.11
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	1	0	0	0	0	1	0.12	0.12	0.0	0.12
5	1	0	0	0	0	1	0.14	0.14	0.0	0.14
6	2	4	0	0	0	6	0.12	0.14	0.01	0.12
7	1	0	0	0	0	1	0.11	0.11	0.0	0.11
8	1	1	0	0	0	2	0.11	0.11	0.0	0.11
9	3	0	0	0	0	3	0.16	0.21	0.04	0.15
10	1	2	0	0	0	3	0.12	0.13	0.01	0.11
11	0	2	0	1	0	3	0.11	0.11	0.0	0.11

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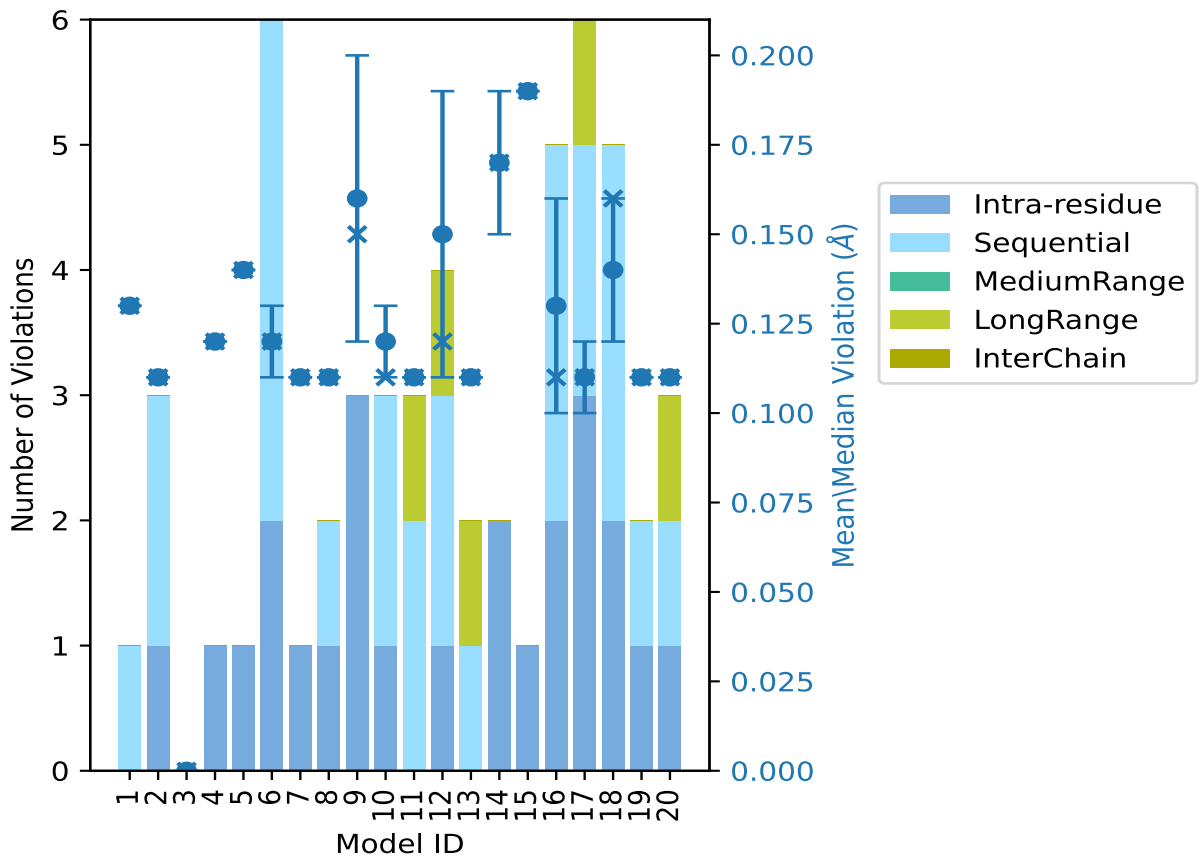
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	2	0	1	0	4	0.15	0.22	0.04	0.12
13	0	1	0	1	0	2	0.11	0.11	0.0	0.11
14	2	0	0	0	0	2	0.17	0.19	0.02	0.17
15	1	0	0	0	0	1	0.19	0.19	0.0	0.19
16	2	3	0	0	0	5	0.13	0.18	0.03	0.11
17	3	2	0	1	0	6	0.11	0.13	0.01	0.11
18	2	3	0	0	0	5	0.14	0.17	0.02	0.16
19	1	1	0	0	0	2	0.11	0.11	0.0	0.11
20	1	1	0	1	0	3	0.11	0.12	0.0	0.11

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

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



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

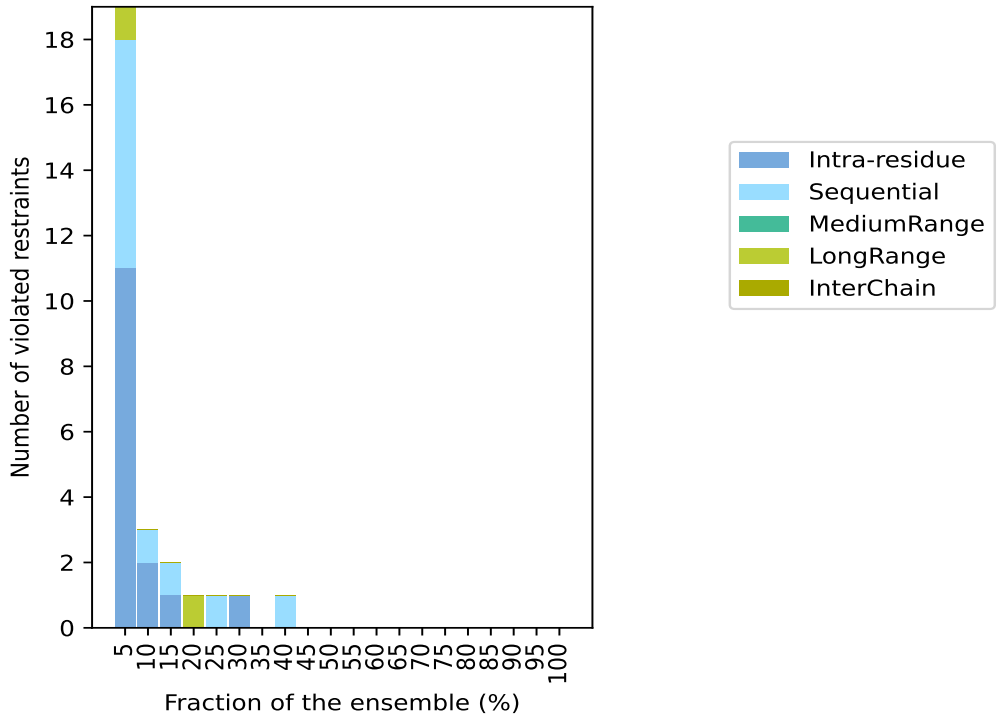
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1285(IR:443, SQ:350, MR:129, LR:363, 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]	%
11	7	0	1	0	19	1	5.0
2	1	0	0	0	3	2	10.0
1	1	0	0	0	2	3	15.0
0	0	0	1	0	1	4	20.0
0	1	0	0	0	1	5	25.0
1	0	0	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	1	0	0	0	1	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

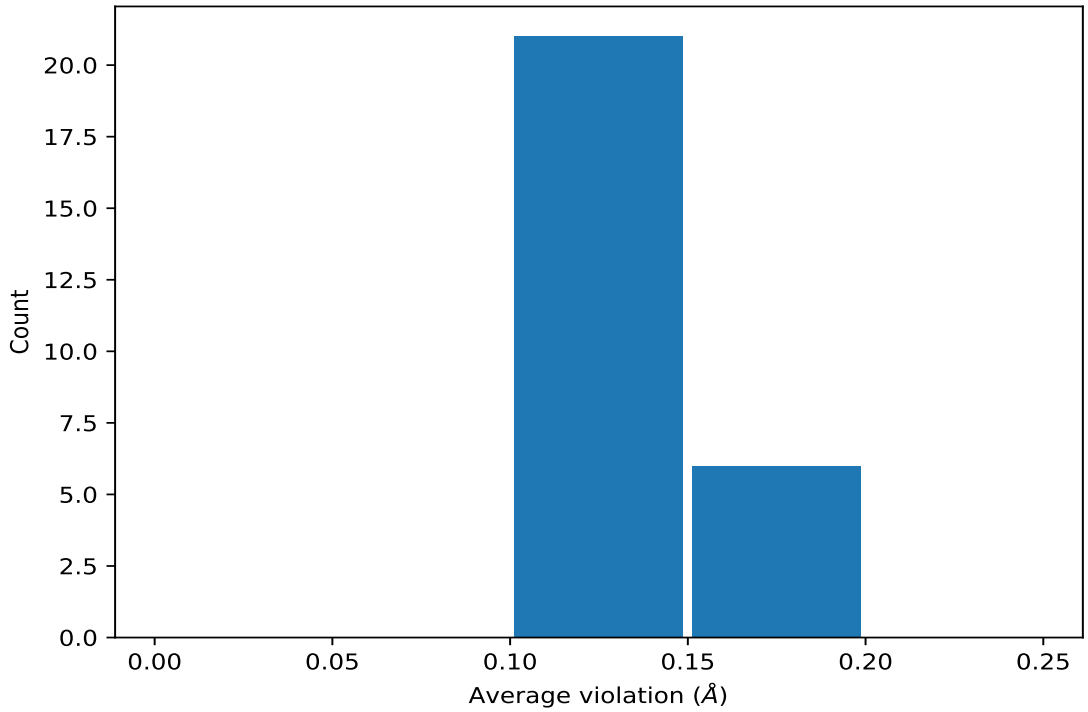
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	8	0.11	0.0	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	8	0.11	0.0	0.11
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	8	0.11	0.0	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	8	0.11	0.0	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	8	0.11	0.0	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	8	0.11	0.0	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD11	6	0.12	0.01	0.12
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD12	6	0.12	0.01	0.12
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD13	6	0.12	0.01	0.12
(1,296)	1:A:37:ASP:H	1:A:38:ALA:H	5	0.11	0.0	0.11
(1,1311)	1:A:54:PHE:HD1	1:A:126:VAL:HB	4	0.11	0.0	0.11
(1,1311)	1:A:54:PHE:HD2	1:A:126:VAL:HB	4	0.11	0.0	0.11
(1,803)	1:A:107:ILE:HD11	1:A:108:GLY:H	3	0.11	0.0	0.11
(1,803)	1:A:107:ILE:HD12	1:A:108:GLY:H	3	0.11	0.0	0.11
(1,803)	1:A:107:ILE:HD13	1:A:108:GLY:H	3	0.11	0.0	0.11
(1,1211)	1:A:101:ALA:HA	1:A:101:ALA:H	3	0.11	0.0	0.11

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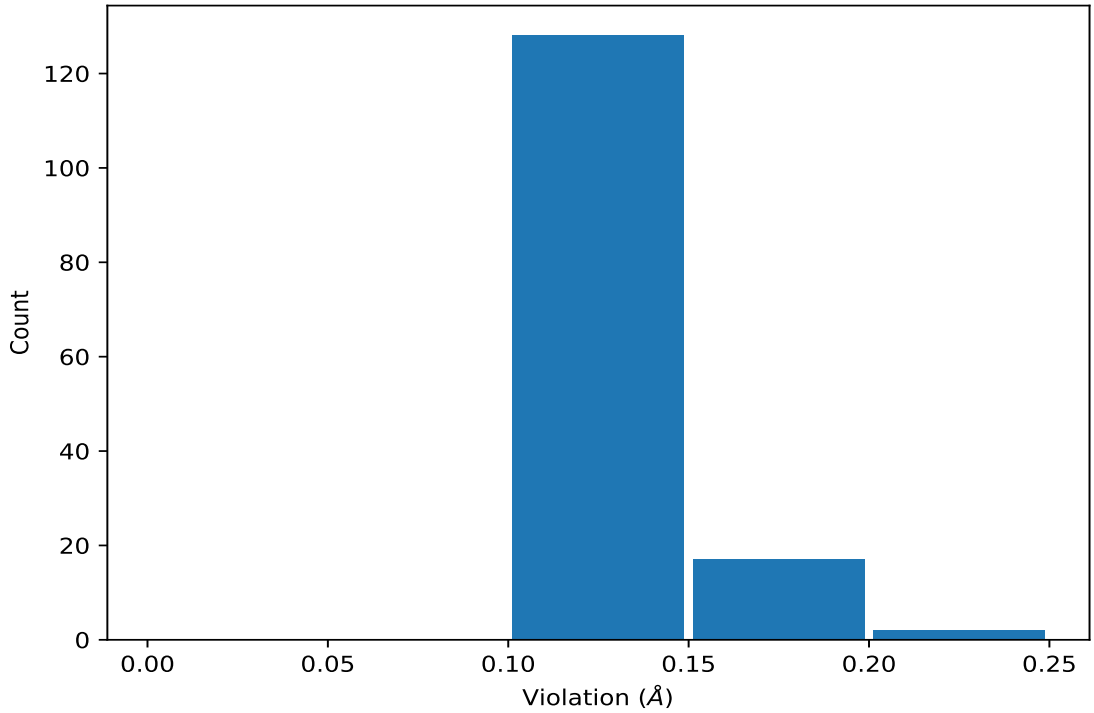
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG11	2	0.19	0.0	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG12	2	0.19	0.0	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG13	2	0.19	0.0	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG21	2	0.19	0.0	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG22	2	0.19	0.0	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG23	2	0.19	0.0	0.19
(1,397)	1:A:47:ARG:HA	1:A:47:ARG:HD2	2	0.14	0.01	0.14
(1,397)	1:A:47:ARG:HA	1:A:47:ARG:HD3	2	0.14	0.01	0.14
(1,1011)	1:A:70:VAL:HG21	1:A:71:GLU:H	2	0.12	0.02	0.12
(1,1011)	1:A:70:VAL:HG22	1:A:71:GLU:H	2	0.12	0.02	0.12
(1,1011)	1:A:70:VAL:HG23	1:A:71:GLU:H	2	0.12	0.02	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,595)	1:A:71:GLU:HB2	1:A:71:GLU:H	12	0.22
(1,19)	1:A:7:GLU:HG2	1:A:7:GLU:H	9	0.21
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG11	14	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG12	14	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG13	14	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG21	14	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG22	14	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG23	14	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG11	15	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG12	15	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG13	15	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG21	15	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG22	15	0.19
(1,10)	1:A:6:VAL:HA	1:A:6:VAL:HG23	15	0.19
(1,102)	1:A:13:ARG:HB2	1:A:13:ARG:H	16	0.18
(1,102)	1:A:13:ARG:HB3	1:A:13:ARG:H	16	0.18
(1,594)	1:A:71:GLU:HB3	1:A:72:LEU:H	18	0.17
(1,596)	1:A:71:GLU:HB2	1:A:72:LEU:H	18	0.16
(1,593)	1:A:71:GLU:HB3	1:A:71:GLU:H	18	0.16
(1,17)	1:A:7:GLU:HB2	1:A:7:GLU:H	9	0.15
(1,1)	1:A:3:GLU:HA	1:A:3:GLU:HG2	14	0.15
(1,1)	1:A:3:GLU:HA	1:A:3:GLU:HG3	14	0.15
(1,625)	1:A:74:ASP:HB3	1:A:75:VAL:H	6	0.14
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD11	5	0.14
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD12	5	0.14
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD13	5	0.14
(1,397)	1:A:47:ARG:HA	1:A:47:ARG:HD2	6	0.14
(1,397)	1:A:47:ARG:HA	1:A:47:ARG:HD3	6	0.14
(1,1011)	1:A:70:VAL:HG21	1:A:71:GLU:H	12	0.14
(1,1011)	1:A:70:VAL:HG22	1:A:71:GLU:H	12	0.14
(1,1011)	1:A:70:VAL:HG23	1:A:71:GLU:H	12	0.14
(1,708)	1:A:85:CYS:HB2	1:A:86:LEU:H	1	0.13
(1,708)	1:A:85:CYS:HB3	1:A:86:LEU:H	1	0.13
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD11	10	0.13
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD12	10	0.13
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD13	10	0.13
(1,397)	1:A:47:ARG:HA	1:A:47:ARG:HD2	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:A:47:ARG:HA	1:A:47:ARG:HD3	17	0.13
(1,103)	1:A:13:ARG:HG2	1:A:14:PHE:H	16	0.13
(1,103)	1:A:13:ARG:HG3	1:A:14:PHE:H	16	0.13
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	6	0.12
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	6	0.12
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	6	0.12
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	6	0.12
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	6	0.12
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	6	0.12
(1,634)	1:A:75:VAL:HB	1:A:75:VAL:H	6	0.12
(1,590)	1:A:71:GLU:HA	1:A:71:GLU:HG3	18	0.12
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD11	4	0.12
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD12	4	0.12
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD13	4	0.12
(1,1311)	1:A:54:PHE:HD1	1:A:126:VAL:HB	20	0.12
(1,1311)	1:A:54:PHE:HD2	1:A:126:VAL:HB	20	0.12
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	2	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	2	0.11
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	2	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	2	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	2	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	2	0.11
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	10	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	10	0.11
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	10	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	10	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	10	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	10	0.11
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	11	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	11	0.11
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	11	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	11	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	11	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	11	0.11
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	12	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	12	0.11
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	12	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	12	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	12	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	12	0.11
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	13	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	13	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	13	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	13	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	13	0.11
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	17	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	17	0.11
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	17	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	17	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	17	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	17	0.11
(1,885)	1:A:128:VAL:HG11	1:A:129:GLU:H	19	0.11
(1,885)	1:A:128:VAL:HG12	1:A:129:GLU:H	19	0.11
(1,885)	1:A:128:VAL:HG13	1:A:129:GLU:H	19	0.11
(1,885)	1:A:128:VAL:HG21	1:A:129:GLU:H	19	0.11
(1,885)	1:A:128:VAL:HG22	1:A:129:GLU:H	19	0.11
(1,885)	1:A:128:VAL:HG23	1:A:129:GLU:H	19	0.11
(1,803)	1:A:107:ILE:HD11	1:A:108:GLY:H	2	0.11
(1,803)	1:A:107:ILE:HD12	1:A:108:GLY:H	2	0.11
(1,803)	1:A:107:ILE:HD13	1:A:108:GLY:H	2	0.11
(1,803)	1:A:107:ILE:HD11	1:A:108:GLY:H	6	0.11
(1,803)	1:A:107:ILE:HD12	1:A:108:GLY:H	6	0.11
(1,803)	1:A:107:ILE:HD13	1:A:108:GLY:H	6	0.11
(1,803)	1:A:107:ILE:HD11	1:A:108:GLY:H	8	0.11
(1,803)	1:A:107:ILE:HD12	1:A:108:GLY:H	8	0.11
(1,803)	1:A:107:ILE:HD13	1:A:108:GLY:H	8	0.11
(1,732)	1:A:88:PHE:HD1	1:A:88:PHE:H	8	0.11
(1,732)	1:A:88:PHE:HD2	1:A:88:PHE:H	8	0.11
(1,713)	1:A:86:LEU:HB3	1:A:86:LEU:H	17	0.11
(1,585)	1:A:70:VAL:HG21	1:A:98:ILE:HD11	17	0.11
(1,585)	1:A:70:VAL:HG21	1:A:98:ILE:HD12	17	0.11
(1,585)	1:A:70:VAL:HG21	1:A:98:ILE:HD13	17	0.11
(1,585)	1:A:70:VAL:HG22	1:A:98:ILE:HD11	17	0.11
(1,585)	1:A:70:VAL:HG22	1:A:98:ILE:HD12	17	0.11
(1,585)	1:A:70:VAL:HG22	1:A:98:ILE:HD13	17	0.11
(1,585)	1:A:70:VAL:HG23	1:A:98:ILE:HD11	17	0.11
(1,585)	1:A:70:VAL:HG23	1:A:98:ILE:HD12	17	0.11
(1,585)	1:A:70:VAL:HG23	1:A:98:ILE:HD13	17	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD11	9	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD12	9	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD13	9	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD11	16	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD12	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD13	16	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD11	19	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD12	19	0.11
(1,415)	1:A:52:ILE:HB	1:A:52:ILE:HD13	19	0.11
(1,296)	1:A:37:ASP:H	1:A:38:ALA:H	6	0.11
(1,296)	1:A:37:ASP:H	1:A:38:ALA:H	10	0.11
(1,296)	1:A:37:ASP:H	1:A:38:ALA:H	16	0.11
(1,296)	1:A:37:ASP:H	1:A:38:ALA:H	17	0.11
(1,296)	1:A:37:ASP:H	1:A:38:ALA:H	20	0.11
(1,277)	1:A:35:ILE:HA	1:A:36:ALA:H	16	0.11
(1,1311)	1:A:54:PHE:HD1	1:A:126:VAL:HB	11	0.11
(1,1311)	1:A:54:PHE:HD2	1:A:126:VAL:HB	11	0.11
(1,1311)	1:A:54:PHE:HD1	1:A:126:VAL:HB	12	0.11
(1,1311)	1:A:54:PHE:HD2	1:A:126:VAL:HB	12	0.11
(1,1311)	1:A:54:PHE:HD1	1:A:126:VAL:HB	13	0.11
(1,1311)	1:A:54:PHE:HD2	1:A:126:VAL:HB	13	0.11
(1,1211)	1:A:101:ALA:HA	1:A:101:ALA:H	2	0.11
(1,1211)	1:A:101:ALA:HA	1:A:101:ALA:H	7	0.11
(1,1211)	1:A:101:ALA:HA	1:A:101:ALA:H	20	0.11
(1,12)	1:A:6:VAL:HB	1:A:7:GLU:H	11	0.11
(1,1149)	1:A:59:ALA:HB1	1:A:59:ALA:H	17	0.11
(1,1149)	1:A:59:ALA:HB2	1:A:59:ALA:H	17	0.11
(1,1149)	1:A:59:ALA:HB3	1:A:59:ALA:H	17	0.11
(1,1011)	1:A:70:VAL:HG21	1:A:71:GLU:H	18	0.11
(1,1011)	1:A:70:VAL:HG22	1:A:71:GLU:H	18	0.11
(1,1011)	1:A:70:VAL:HG23	1:A:71:GLU:H	18	0.11

10 Dihedral-angle violation analysis (i)

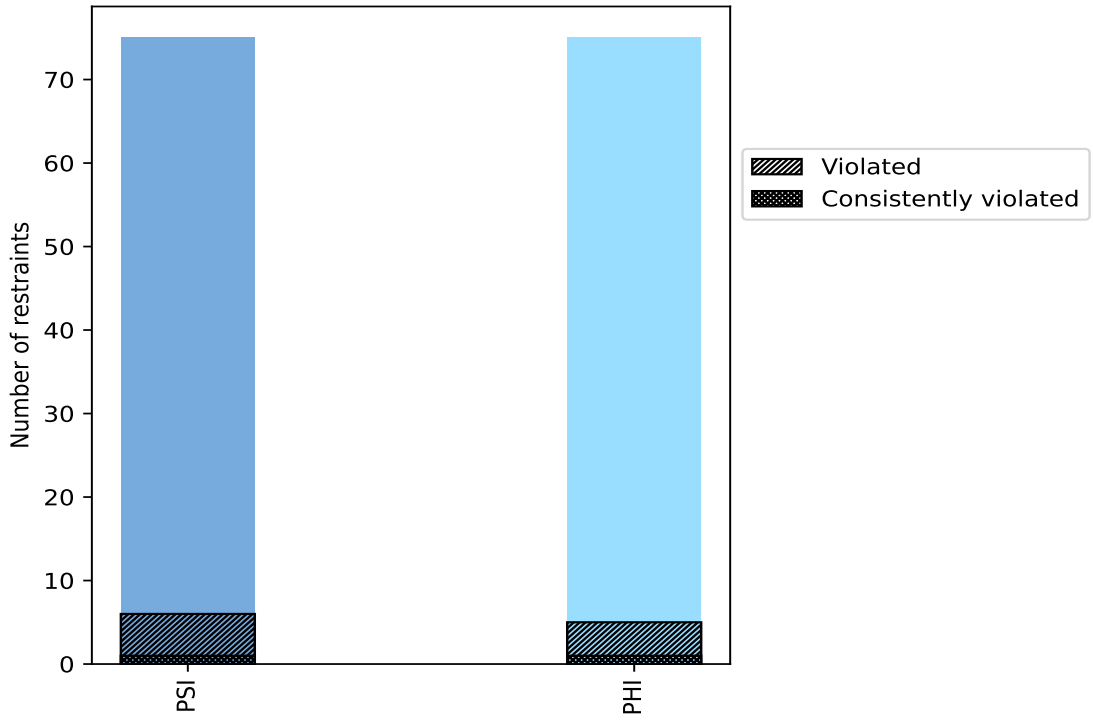
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	75	50.0	6	8.0	4.0	1	1.3	0.7
PHI	75	50.0	5	6.7	3.3	1	1.3	0.7
Total	150	100.0	11	7.3	7.3	2	1.3	1.3

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

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



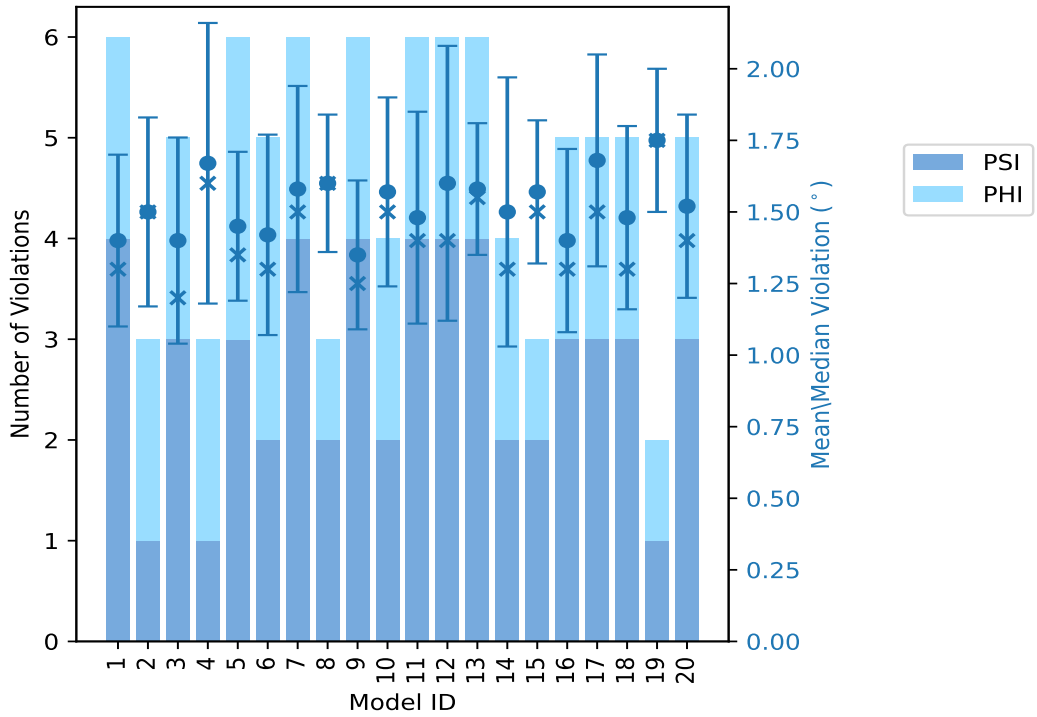
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	4	2	6	1.4	1.8	0.3	1.3
2	1	2	3	1.5	1.9	0.33	1.5
3	3	2	5	1.4	2.1	0.36	1.2
4	1	2	3	1.67	2.3	0.49	1.6
5	3	3	6	1.45	2.0	0.26	1.35
6	2	3	5	1.42	2.1	0.35	1.3
7	4	2	6	1.58	2.1	0.36	1.5
8	2	1	3	1.6	1.9	0.24	1.6
9	4	2	6	1.35	1.8	0.26	1.25
10	2	2	4	1.57	2.1	0.33	1.5
11	4	2	6	1.48	2.0	0.37	1.4
12	4	2	6	1.6	2.3	0.48	1.4
13	4	2	6	1.58	2.0	0.23	1.55
14	2	2	4	1.5	2.3	0.47	1.3
15	2	1	3	1.57	1.9	0.25	1.5
16	3	2	5	1.4	2.0	0.32	1.3
17	3	2	5	1.68	2.2	0.37	1.5
18	3	2	5	1.48	2.0	0.32	1.3
19	1	1	2	1.75	2.0	0.25	1.75
20	3	2	5	1.52	2.0	0.32	1.4

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	2	3	1	5.0
0	1	1	2	10.0
0	0	0	3	15.0
1	0	1	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
1	0	1	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

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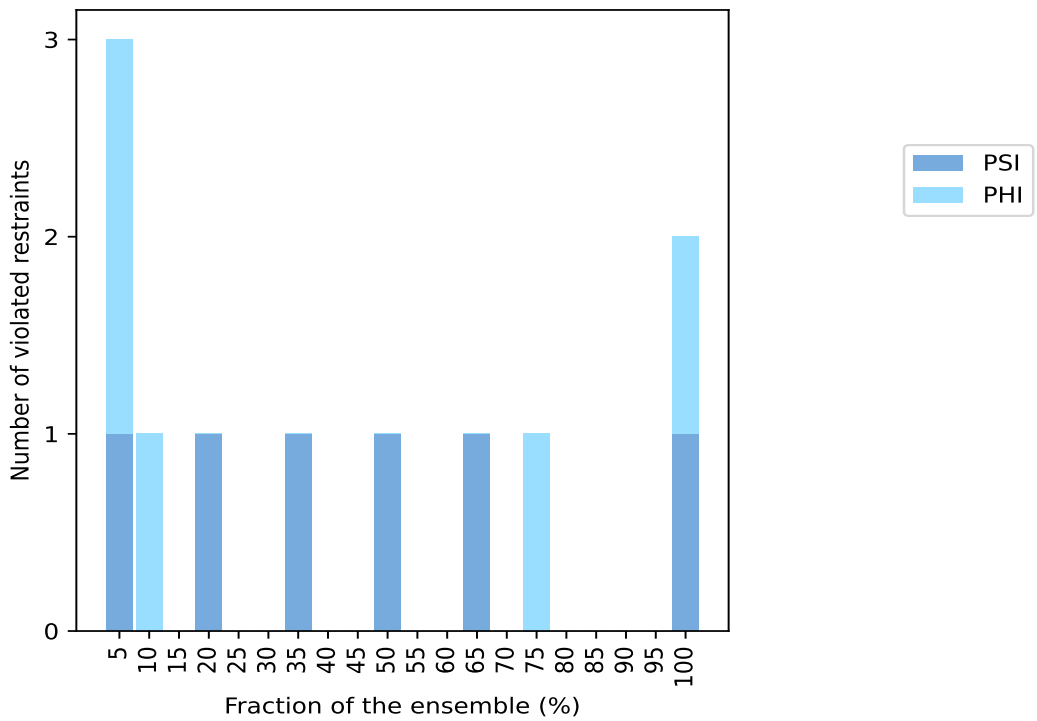
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
1	1	2	20	100.0

[1] Number of models with violations

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

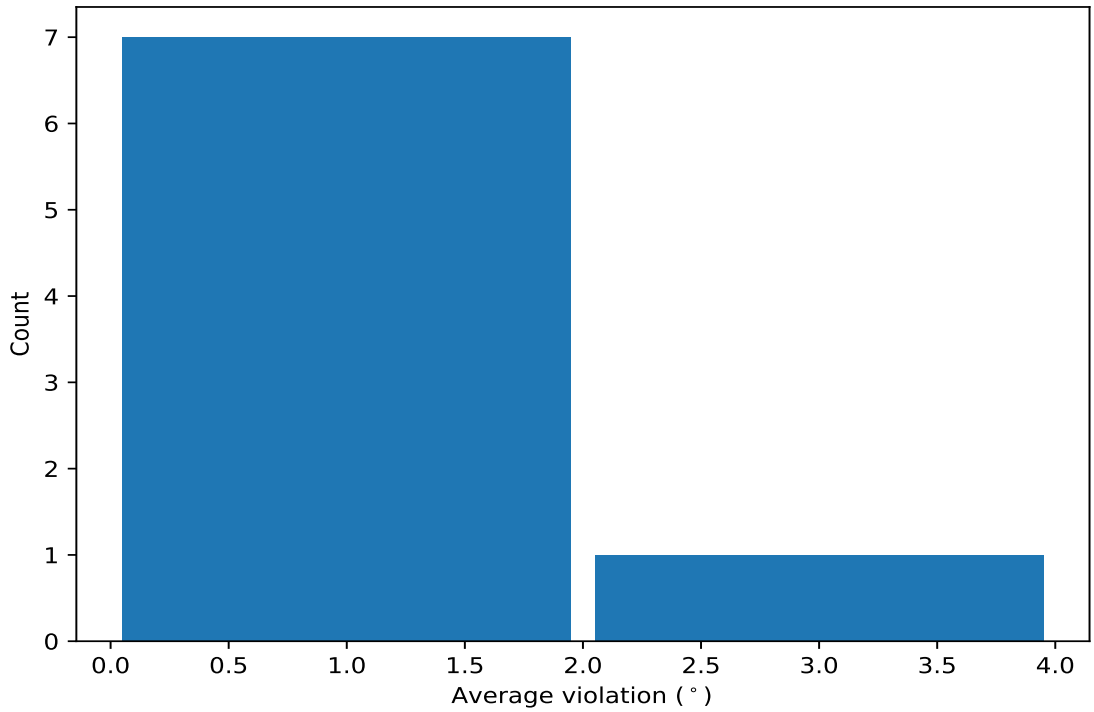


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

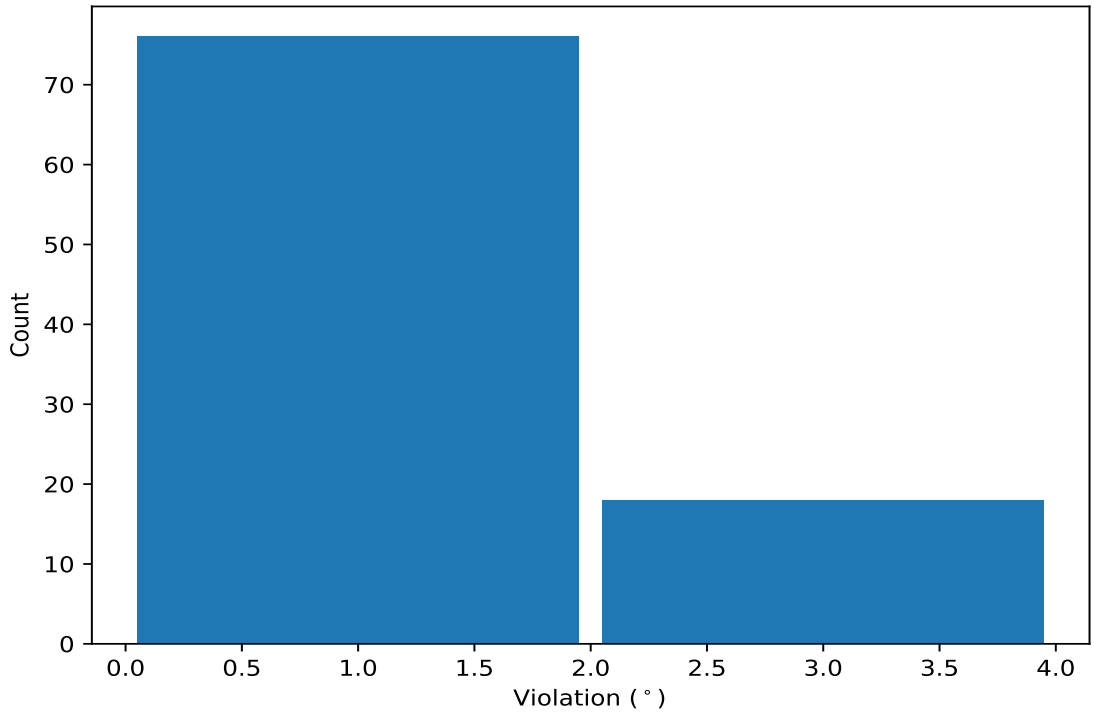
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	20	2.04	0.14	2.0
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	20	1.54	0.28	1.45
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	15	1.23	0.11	1.2
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	13	1.5	0.24	1.5
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	10	1.23	0.17	1.15
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	7	1.27	0.17	1.2
(1,150)	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	1:A:117:LEU:N	4	1.32	0.13	1.3
(1,75)	1:A:115:GLU:C	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	2	1.3	0.0	1.3

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	12	2.3
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	4	2.3
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	14	2.3
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	12	2.2
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	17	2.2
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	3	2.1
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	6	2.1
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	7	2.1
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	10	2.1
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	7	2.0
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	17	2.0
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	5	2.0
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	11	2.0
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	13	2.0
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	16	2.0
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	18	2.0
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	19	2.0
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	20	2.0
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	11	1.9
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	2	1.9
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	8	1.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	15	1.9
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	1	1.8
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	20	1.8
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	1	1.8
(1,101)	1:A:39:LEU:N	1:A:39:LEU:CA	1:A:39:LEU:C	1:A:40:PRO:N	9	1.8
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	18	1.7
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	13	1.7
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	4	1.6
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	8	1.6
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	11	1.6
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	13	1.6
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	9	1.6
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	10	1.6
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	7	1.5
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	12	1.5
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	17	1.5
(1,150)	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	1:A:117:LEU:N	13	1.5
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	2	1.5
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	19	1.5
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	5	1.5
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	7	1.5
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	15	1.5
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	17	1.5
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	13	1.4
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	10	1.4
(1,150)	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	1:A:117:LEU:N	5	1.4
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	1	1.4
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	3	1.4
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	6	1.4
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	14	1.4
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	16	1.4
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	20	1.4
(1,75)	1:A:115:GLU:C	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	5	1.3
(1,75)	1:A:115:GLU:C	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	13	1.3
(1,47)	1:A:71:GLU:C	1:A:72:LEU:N	1:A:72:LEU:CA	1:A:72:LEU:C	18	1.3
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	6	1.3
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	7	1.3
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	9	1.3
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	5	1.3
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	15	1.3
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	8	1.3
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	12	1.3
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	18	1.3
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	16	1.3
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	17	1.2
(1,49)	1:A:74:ASP:C	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	6	1.2
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	1	1.2
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	5	1.2
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	12	1.2
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	14	1.2
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	16	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	20	1.2
(1,150)	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	1:A:117:LEU:N	9	1.2
(1,150)	1:A:116:GLY:N	1:A:116:GLY:CA	1:A:116:GLY:C	1:A:117:LEU:N	11	1.2
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	10	1.2
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	3	1.2
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	3	1.2
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	20	1.2
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	1	1.1
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	11	1.1
(1,89)	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	1:A:26:GLU:N	18	1.1
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	2	1.1
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	3	1.1
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	4	1.1
(1,30)	1:A:43:SER:C	1:A:44:THR:N	1:A:44:THR:CA	1:A:44:THR:C	11	1.1
(1,15)	1:A:25:GLU:C	1:A:26:GLU:N	1:A:26:GLU:CA	1:A:26:GLU:C	9	1.1
(1,142)	1:A:120:VAL:N	1:A:120:VAL:CA	1:A:120:VAL:C	1:A:121:ALA:N	16	1.1
(1,109)	1:A:48:TRP:N	1:A:48:TRP:CA	1:A:48:TRP:C	1:A:49:GLY:N	12	1.1
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	1	1.1
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	6	1.1
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	7	1.1
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	9	1.1
(1,104)	1:A:43:SER:N	1:A:43:SER:CA	1:A:43:SER:C	1:A:44:THR:N	14	1.1