Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 01:23 PM JST

PDB ID	:	7CJV
BMRB ID	:	36359
Title	:	Solution structure of monomeric superoxide dismutase 1 with an additional mutation H46W in a dilute environment
Authors	:	Iwakawa, N.; Morimoto, D.; Walinda, E.; Danielsson, J.; Shirakawa, M.; Sugase, K.
Deposited on	:	2020-07-14

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:

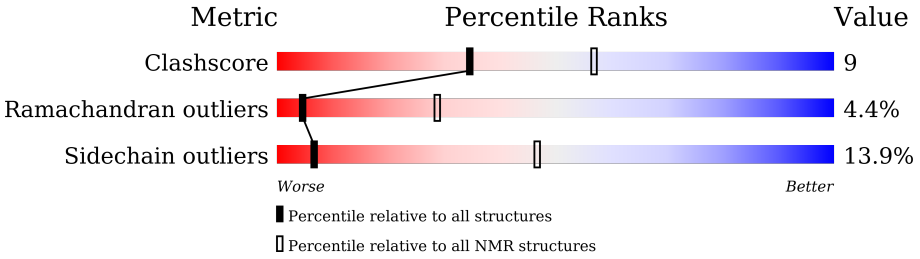
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 95%.

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	110	70% 21% 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:1-A:90, A:101-A:110 (100)	0.40	8

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1555 atoms, of which 778 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Monomeric Human Cu,Zn Superoxide dismutase.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	110	1555	485	778	139	153	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: Monomeric Human Cu,Zn Superoxide dismutase

Chain A: 70% 21% 9%

A1 A4 G12 P13 V14 F20 E21 V29 L38 T39 E40 G41 L42 F45 W46 V47 H48 N56 S68 I69 E70 D71 I74 S75 L76 I82 R85 T86 L87 V88 E91 K92 A93 G94 A95 G96 A97 G98 S99 R100 Q110

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: Monomeric Human Cu,Zn Superoxide dismutase

Chain A: 67% 22% • 9%

A1 A4 L8 G12 F20 V29 L38 T39 E40 G41 L42 H43 G44 F45 W46 V47 H48 G55 N56 V57 V67 S68 I69 E70 D71 I74 S75 L76 I82 L87 E91 K92 A93 G94 A95 G96 A97 G98 S99 R100 G104 V105 I106 Q110

4.2.2 Score per residue for model 2

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

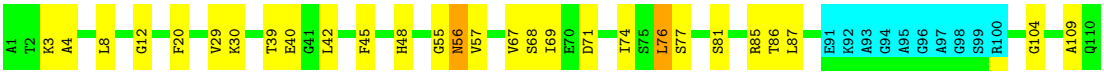
Chain A: 62% 28% • 9%

A1 A4 L8 K9 G12 P13 V14 Q15 G16 F20 E21 V29 I35 L38 L42 F45 W46 V47 H48 G55 N56 V57 T58 A59 D60 S68 I69 E70 D71 I74 S75 L76 I82 R85 T86 L87 V88 V89 H90 E91 K92 A93 G94 A95 G96 A97 G98 S99 R100 S103 I106 Q110

4.2.3 Score per residue for model 3

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

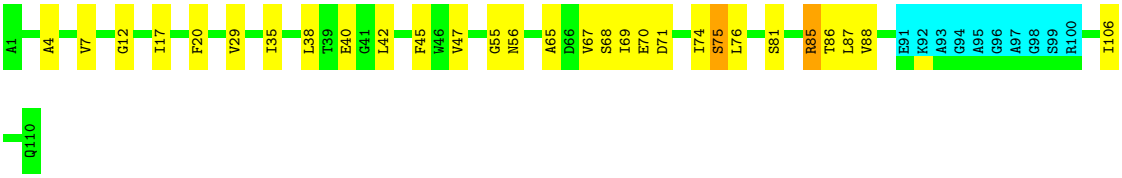
Chain A: 65% 24% • 9%



4.2.4 Score per residue for model 4

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

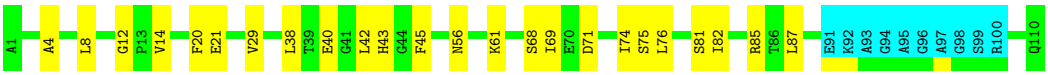
Chain A: 65% 25% • 9%



4.2.5 Score per residue for model 5

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

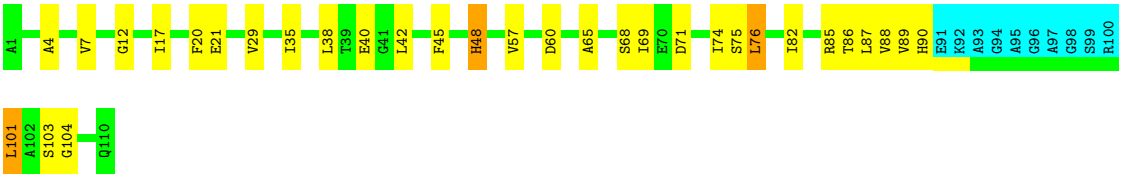
Chain A: 69% 22% 9%



4.2.6 Score per residue for model 6

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

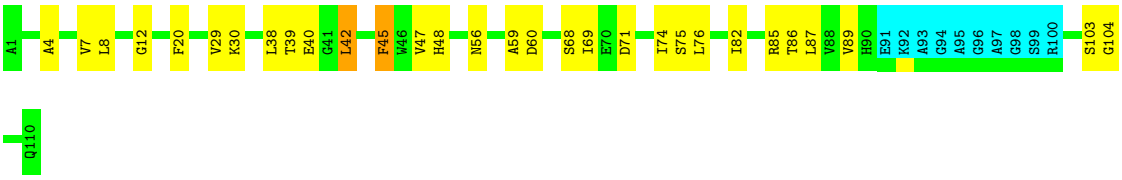
Chain A: 62% 26% • 9%



4.2.7 Score per residue for model 7

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

Chain A: 64% 25% • 9%



4.2.8 Score per residue for model 8 (medoid)

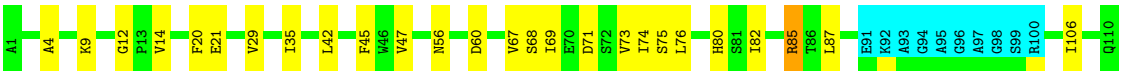
- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

Chain A: 69% 21% • 9%

4.2.9 Score per residue for model 9

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

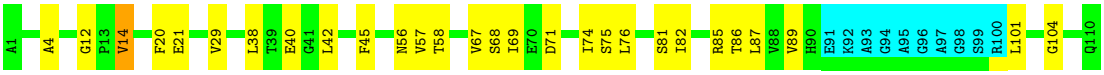
Chain A: 67% 23% • 9%



4.2.10 Score per residue for model 10

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

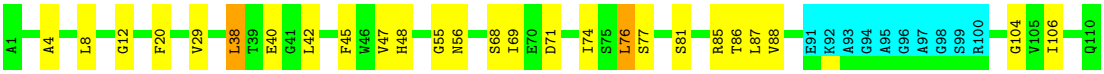
Chain A: 65% 25% • 9%



4.2.11 Score per residue for model 11

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

Chain A: 67% 22% • 9%



4.2.12 Score per residue for model 12

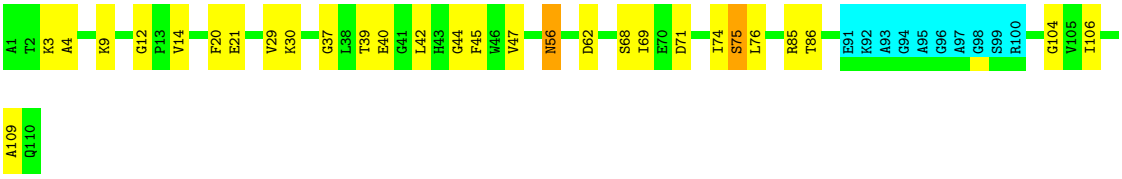
• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

Chain A: 61% 28% • 9%

4.2.13 Score per residue for model 13

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

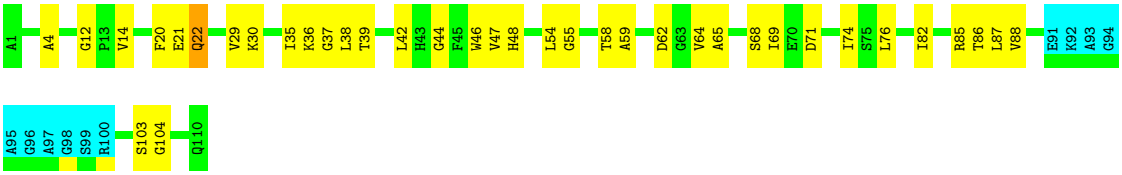
Chain A: 65% 25% • 9%



4.2.14 Score per residue for model 14

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

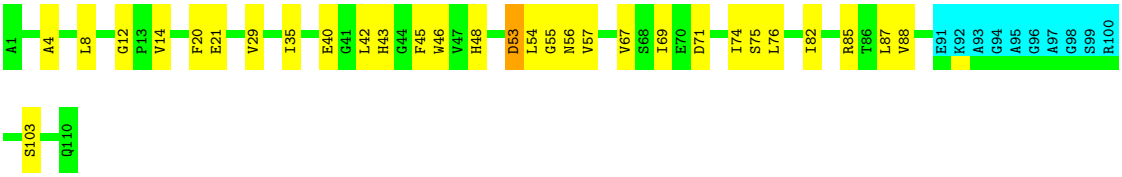
Chain A: 57% 33% • 9%



4.2.15 Score per residue for model 15

• Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

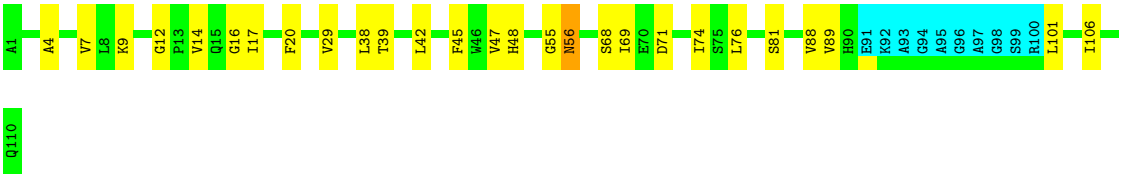
Chain A: 64% 26% • 9%



4.2.16 Score per residue for model 16

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

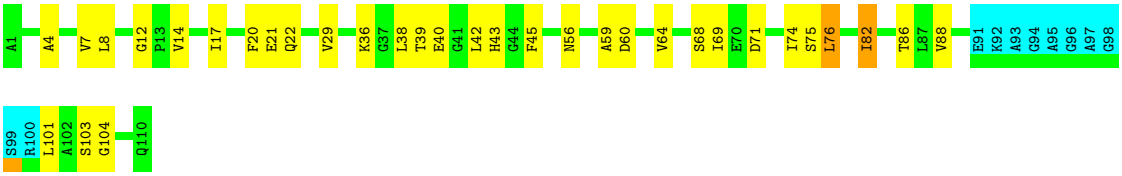
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

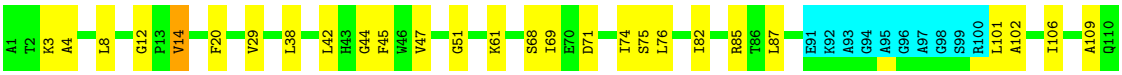
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

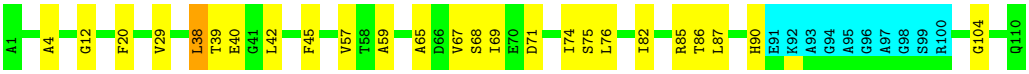
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

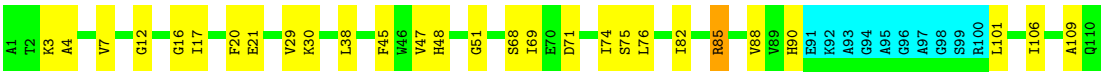
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Monomeric Human Cu,Zn Superoxide dismutase

Chain A:



5 Refinement protocol and experimental data overview (i)

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

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**
CYANA	structure calculation	3.98.5
TALOS	structure calculation	
MOLMOL	refinement	2K.2

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	1285
Number of shifts mapped to atoms	1285
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

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	715	717	719	13±3
All	All	14300	14340	14380	253

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:VAL:HG22	1:A:87:LEU:HD12	0.77	1.56	14	2
1:A:8:LEU:HD11	1:A:87:LEU:HD23	0.73	1.58	3	5
1:A:7:VAL:HG22	1:A:17:ILE:HD12	0.71	1.59	4	3
1:A:29:VAL:HG11	1:A:74:ILE:HD11	0.69	1.64	3	20
1:A:57:VAL:HG11	1:A:67:VAL:HG22	0.68	1.63	15	1
1:A:89:VAL:HG13	1:A:101:LEU:HB2	0.63	1.71	6	3
1:A:42:LEU:HD12	1:A:56:ASN:HB2	0.63	1.69	13	3
1:A:8:LEU:HD13	1:A:45:PHE:CE2	0.63	2.28	1	1
1:A:14:VAL:HG22	1:A:37:GLY:O	0.62	1.95	14	2
1:A:4:ALA:HB3	1:A:20:PHE:HB2	0.62	1.72	13	20
1:A:29:VAL:HG11	1:A:74:ILE:CD1	0.61	2.26	11	19
1:A:22:GLN:OE1	1:A:76:LEU:HD12	0.60	1.96	17	1
1:A:57:VAL:CG1	1:A:67:VAL:HG22	0.60	2.26	15	2
1:A:14:VAL:HG21	1:A:101:LEU:HD12	0.60	1.73	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LEU:HD22	1:A:56:ASN:ND2	0.60	2.11	12	1
1:A:42:LEU:HD12	1:A:56:ASN:CB	0.59	2.28	2	3
1:A:47:VAL:HG21	1:A:106:ILE:HD11	0.58	1.76	1	1
1:A:47:VAL:CG2	1:A:106:ILE:HD11	0.58	2.29	1	4
1:A:8:LEU:HD13	1:A:45:PHE:CZ	0.57	2.34	1	1
1:A:48:HIS:HB2	1:A:88:VAL:HG22	0.57	1.77	12	9
1:A:47:VAL:HA	1:A:87:LEU:HD12	0.56	1.76	7	1
1:A:86:THR:HG23	1:A:104:GLY:O	0.55	2.00	10	9
1:A:88:VAL:HG12	1:A:103:SER:CB	0.55	2.32	2	2
1:A:35:ILE:HB	1:A:65:ALA:HB3	0.55	1.79	6	2
1:A:14:VAL:HG11	1:A:101:LEU:HB3	0.55	1.79	18	1
1:A:87:LEU:HD23	1:A:88:VAL:N	0.54	2.17	6	2
1:A:7:VAL:HG23	1:A:17:ILE:CD1	0.54	2.32	17	1
1:A:3:LYS:HB2	1:A:109:ALA:HB3	0.54	1.79	20	4
1:A:8:LEU:HD21	1:A:87:LEU:CD2	0.54	2.33	15	4
1:A:8:LEU:CD1	1:A:87:LEU:HD23	0.53	2.32	3	3
1:A:8:LEU:HD12	1:A:45:PHE:CZ	0.53	2.38	18	1
1:A:20:PHE:HB3	1:A:76:LEU:HD21	0.53	1.81	17	1
1:A:39:THR:C	1:A:59:ALA:HB3	0.53	2.23	17	2
1:A:35:ILE:HD13	1:A:57:VAL:HG11	0.52	1.81	6	1
1:A:39:THR:O	1:A:59:ALA:HB3	0.52	2.04	17	3
1:A:43:HIS:O	1:A:57:VAL:HG22	0.52	2.04	15	1
1:A:89:VAL:HG13	1:A:101:LEU:CB	0.52	2.34	6	2
1:A:57:VAL:HG13	1:A:67:VAL:HG22	0.51	1.82	19	4
1:A:42:LEU:HD12	1:A:56:ASN:CG	0.51	2.25	3	3
1:A:8:LEU:HB3	1:A:102:ALA:HB1	0.51	1.81	18	1
1:A:7:VAL:HG13	1:A:17:ILE:CD1	0.51	2.35	16	3
1:A:35:ILE:HD11	1:A:67:VAL:HG23	0.51	1.83	15	1
1:A:51:GLY:O	1:A:74:ILE:HG23	0.51	2.05	20	2
1:A:47:VAL:CG2	1:A:87:LEU:HD12	0.51	2.33	14	1
1:A:53:ASP:O	1:A:54:LEU:HD23	0.50	2.07	15	1
1:A:47:VAL:CG1	1:A:106:ILE:HD11	0.50	2.36	2	6
1:A:8:LEU:HD23	1:A:104:GLY:HA3	0.50	1.83	1	1
1:A:8:LEU:HD11	1:A:87:LEU:HD22	0.50	1.83	18	1
1:A:51:GLY:C	1:A:74:ILE:HG23	0.49	2.26	20	1
1:A:8:LEU:HD21	1:A:87:LEU:HD23	0.49	1.83	7	3
1:A:35:ILE:HG22	1:A:38:LEU:HD21	0.49	1.82	14	1
1:A:22:GLN:OE1	1:A:29:VAL:HG22	0.49	2.07	14	1
1:A:16:GLY:O	1:A:17:ILE:HD13	0.49	2.07	16	2
1:A:47:VAL:HG22	1:A:87:LEU:CD1	0.48	2.38	7	2
1:A:7:VAL:HG13	1:A:17:ILE:HD11	0.48	1.85	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ILE:HG22	1:A:82:ILE:HG21	0.48	1.84	14	14
1:A:53:ASP:C	1:A:54:LEU:HD23	0.47	2.29	15	1
1:A:8:LEU:HD22	1:A:45:PHE:CZ	0.47	2.45	12	1
1:A:45:PHE:CZ	1:A:89:VAL:HG22	0.47	2.44	7	1
1:A:38:LEU:HD22	1:A:43:HIS:CG	0.47	2.44	17	2
1:A:47:VAL:CG1	1:A:50:ALA:HB3	0.46	2.39	12	1
1:A:88:VAL:HG12	1:A:103:SER:HA	0.46	1.88	17	3
1:A:74:ILE:CG2	1:A:82:ILE:HG21	0.46	2.41	14	13
1:A:16:GLY:HA3	1:A:35:ILE:HG23	0.46	1.86	12	2
1:A:8:LEU:HD12	1:A:103:SER:C	0.46	2.31	7	1
1:A:35:ILE:CG2	1:A:38:LEU:HD21	0.45	2.41	14	1
1:A:36:LYS:HG3	1:A:64:VAL:HG23	0.45	1.87	17	1
1:A:85:ARG:HB2	1:A:106:ILE:HD12	0.45	1.89	9	3
1:A:20:PHE:CB	1:A:76:LEU:HD21	0.45	2.41	17	1
1:A:46:TRP:CZ3	1:A:54:LEU:HD12	0.45	2.47	12	2
1:A:45:PHE:CD1	1:A:89:VAL:HG13	0.45	2.46	7	1
1:A:42:LEU:H	1:A:42:LEU:HD22	0.44	1.72	1	2
1:A:7:VAL:HG13	1:A:17:ILE:HG12	0.44	1.88	6	1
1:A:35:ILE:CD1	1:A:67:VAL:HG23	0.44	2.42	15	3
1:A:29:VAL:HG13	1:A:76:LEU:CD2	0.43	2.43	11	2
1:A:46:TRP:C	1:A:87:LEU:HD12	0.43	2.33	15	1
1:A:42:LEU:HD22	1:A:56:ASN:CG	0.43	2.34	12	1
1:A:47:VAL:HG13	1:A:47:VAL:O	0.43	2.13	12	1
1:A:74:ILE:HD12	1:A:82:ILE:CD1	0.43	2.44	19	2
1:A:7:VAL:HG22	1:A:17:ILE:CD1	0.43	2.37	4	1
1:A:29:VAL:HG22	1:A:76:LEU:HD23	0.42	1.89	12	3
1:A:36:LYS:HD3	1:A:64:VAL:HG23	0.42	1.92	14	1
1:A:7:VAL:HG23	1:A:17:ILE:HD11	0.41	1.92	17	1
1:A:74:ILE:O	1:A:82:ILE:HG23	0.41	2.16	17	1
1:A:7:VAL:O	1:A:8:LEU:HD13	0.40	2.15	7	1
1:A:59:ALA:HB2	1:A:65:ALA:HB2	0.40	1.92	14	1
1:A:8:LEU:N	1:A:8:LEU:HD22	0.40	2.31	17	2
1:A:38:LEU:HD23	1:A:65:ALA:HB3	0.40	1.93	19	1
1:A:45:PHE:CE2	1:A:89:VAL:HG22	0.40	2.51	7	1
1:A:38:LEU:HD22	1:A:38:LEU:N	0.40	2.32	14	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	98/110 (89%)	80±2 (81±2%)	14±2 (14±2%)	4±1 (4±1%)	4 29
All	All	1960/2200 (89%)	1596 (81%)	278 (14%)	86 (4%)	4 29

All 8 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	12	GLY	20
1	A	75	SER	16
1	A	85	ARG	16
1	A	38	LEU	9
1	A	55	GLY	9
1	A	14	VAL	9
1	A	44	GLY	4
1	A	81	SER	3

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	75/79 (95%)	65±2 (86±2%)	10±2 (14±2%)	7 47
All	All	1500/1580 (95%)	1292 (86%)	208 (14%)	7 47

All 33 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	69	ILE	20
1	A	71	ASP	20

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Mol	Chain	Res	Type	Models (Total)
1	A	76	LEU	20
1	A	68	SER	19
1	A	45	PHE	17
1	A	40	GLU	12
1	A	21	GLU	11
1	A	42	LEU	10
1	A	56	ASN	9
1	A	30	LYS	6
1	A	38	LEU	6
1	A	39	THR	5
1	A	87	LEU	5
1	A	9	LYS	5
1	A	58	THR	5
1	A	60	ASP	5
1	A	48	HIS	4
1	A	90	HIS	4
1	A	81	SER	4
1	A	61	LYS	3
1	A	77	SER	2
1	A	75	SER	2
1	A	101	LEU	2
1	A	103	SER	2
1	A	62	ASP	2
1	A	70	GLU	1
1	A	86	THR	1
1	A	85	ARG	1
1	A	73	VAL	1
1	A	80	HIS	1
1	A	22	GLN	1
1	A	53	ASP	1
1	A	82	ILE	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 95% for the well-defined parts and 94% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1285
Number of shifts mapped to atoms	1285
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 6 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	LEU	HD11	0.748	.	1
1	A	54	LEU	HD12	0.748	.	1
1	A	54	LEU	HD13	0.748	.	1
1	A	101	LEU	HD11	0.840	.	1
1	A	101	LEU	HD12	0.840	.	1
1	A	101	LEU	HD13	0.840	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	110	-0.11 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	90	-0.14 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	106	0.31 ± 0.11	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	105	-0.74 ± 0.33	Should be applied

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 95%, i.e. 1188 atoms were assigned a chemical shift out of a possible 1248. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	507/513 (99%)	214/215 (100%)	196/200 (98%)	97/98 (99%)
Sidechain	631/663 (95%)	433/438 (99%)	192/210 (91%)	6/15 (40%)
Aromatic	50/72 (69%)	25/38 (66%)	23/28 (82%)	2/6 (33%)
Overall	1188/1248 (95%)	672/691 (97%)	411/438 (94%)	105/119 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 1279 atoms were assigned a chemical shift out of a possible 1354. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	556/566 (98%)	235/238 (99%)	216/220 (98%)	105/108 (97%)
Sidechain	673/716 (94%)	462/472 (98%)	205/225 (91%)	6/19 (32%)
Aromatic	50/72 (69%)	25/38 (66%)	23/28 (82%)	2/6 (33%)
Overall	1279/1354 (94%)	722/748 (97%)	444/473 (94%)	113/133 (85%)

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.

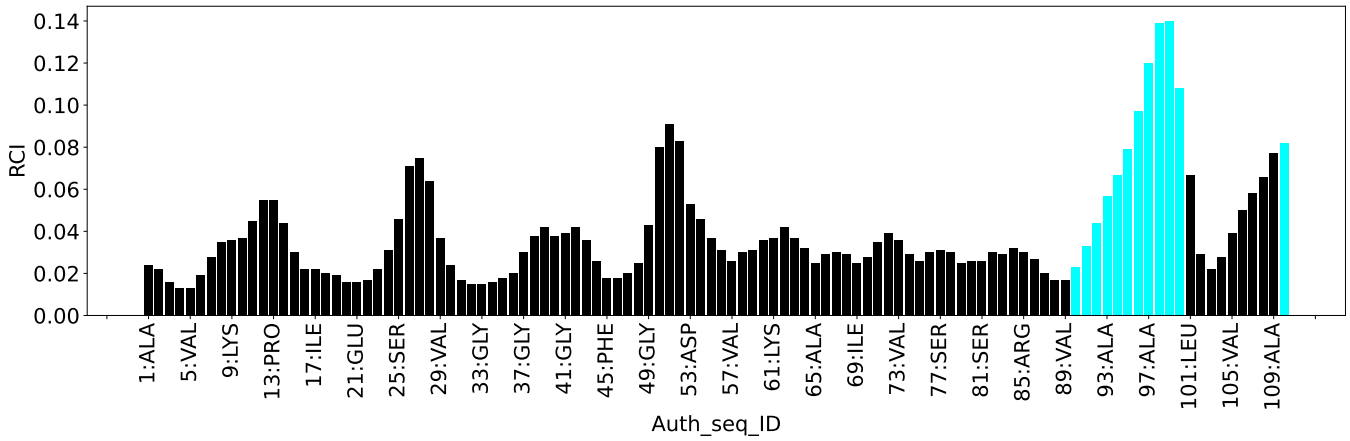
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	19	ASN	HB3	0.33	1.12 – 4.38	-7.4

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:



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	1692
Intra-residue (|i-j|=0)	349
Sequential (|i-j|=1)	432
Medium range (|i-j|>1 and |i-j|<5)	146
Long range (|i-j|≥5)	765
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.4
Number of long range restraints per residue[1]	7.0

[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)	3.4	0.2
0.2-0.5 (Medium)	2.0	0.44
>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.There are no dihedral-angle violations

9 Distance violation analysis (i)

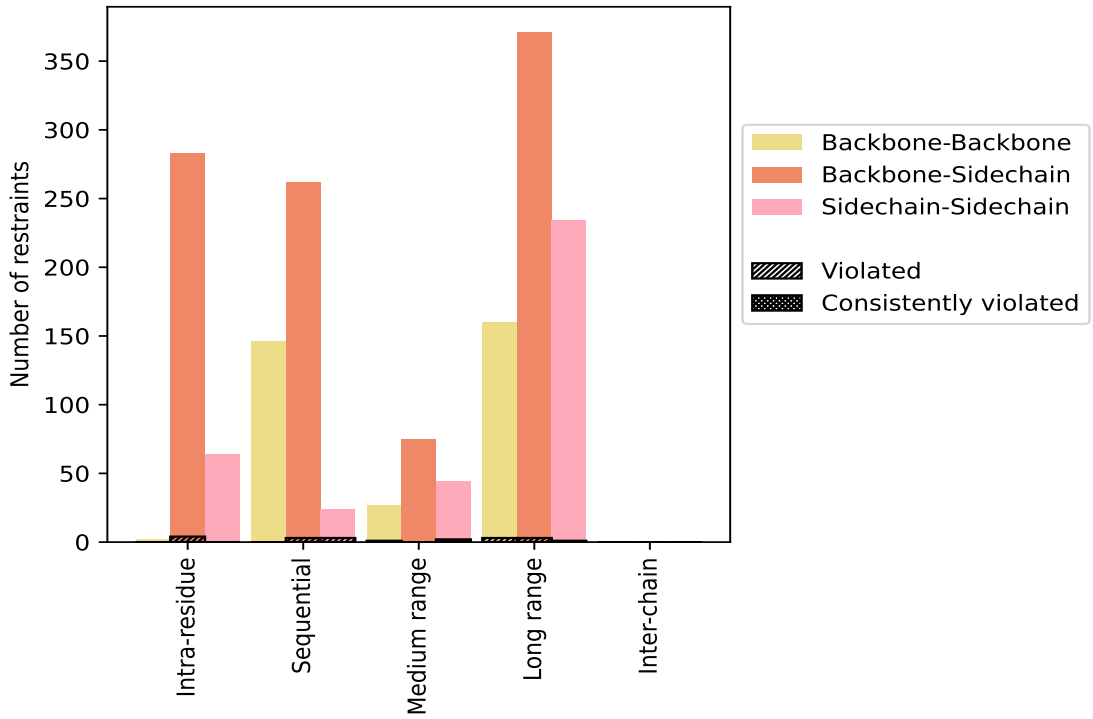
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	349	20.6	4	1.1	0.2	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	283	16.7	4	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	64	3.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	432	25.5	6	1.4	0.4	0	0.0	0.0
Backbone-Backbone	146	8.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	262	15.5	3	1.1	0.2	0	0.0	0.0
Sidechain-Sidechain	24	1.4	3	12.5	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	146	8.6	3	2.1	0.2	1	0.7	0.1
Backbone-Backbone	27	1.6	1	3.7	0.1	0	0.0	0.0
Backbone-Sidechain	75	4.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	44	2.6	2	4.5	0.1	1	2.3	0.1
Long range (|i-j|≥5)	765	45.2	7	0.9	0.4	0	0.0	0.0
Backbone-Backbone	160	9.5	3	1.9	0.2	0	0.0	0.0
Backbone-Sidechain	371	21.9	3	0.8	0.2	0	0.0	0.0
Sidechain-Sidechain	234	13.8	1	0.4	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	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	1692	100.0	20	1.2	1.2	1	0.1	0.1
Backbone-Backbone	335	19.8	4	1.2	0.2	0	0.0	0.0
Backbone-Sidechain	991	58.6	10	1.0	0.6	0	0.0	0.0
Sidechain-Sidechain	366	21.6	6	1.6	0.4	1	0.3	0.1

[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	1	1	1	1	0	4	0.22	0.42	0.13	0.18
2	1	2	1	1	0	5	0.2	0.39	0.11	0.14
3	1	3	2	1	0	7	0.2	0.42	0.1	0.16
4	1	1	1	1	0	4	0.23	0.43	0.12	0.18
5	1	3	1	1	0	6	0.17	0.24	0.06	0.16
6	1	1	1	2	0	5	0.17	0.26	0.07	0.12
7	2	1	1	1	0	5	0.18	0.25	0.05	0.16
8	1	2	1	1	0	5	0.19	0.41	0.12	0.11
9	2	1	1	2	0	6	0.16	0.25	0.06	0.12
10	2	2	1	2	0	7	0.16	0.24	0.05	0.14
11	1	1	2	1	0	5	0.21	0.41	0.11	0.15

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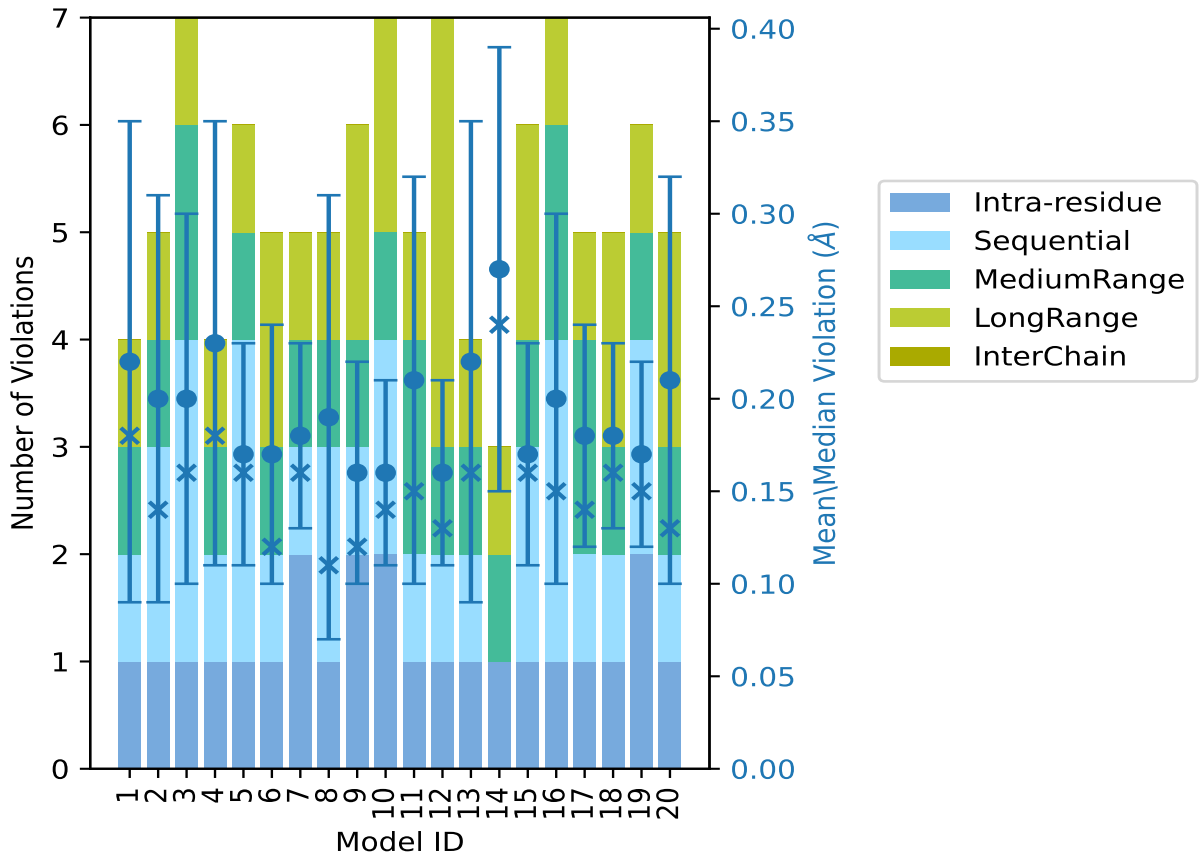
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	1	1	4	0	7	0.16	0.26	0.05	0.13
13	1	1	1	1	0	4	0.22	0.44	0.13	0.16
14	1	0	1	1	0	3	0.27	0.43	0.12	0.24
15	1	2	1	2	0	6	0.17	0.25	0.06	0.16
16	1	3	2	1	0	7	0.2	0.42	0.1	0.15
17	1	1	2	1	0	5	0.18	0.26	0.06	0.14
18	1	1	1	2	0	5	0.18	0.24	0.05	0.16
19	2	2	1	1	0	6	0.17	0.25	0.05	0.15
20	1	1	1	2	0	5	0.21	0.42	0.11	0.13

[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

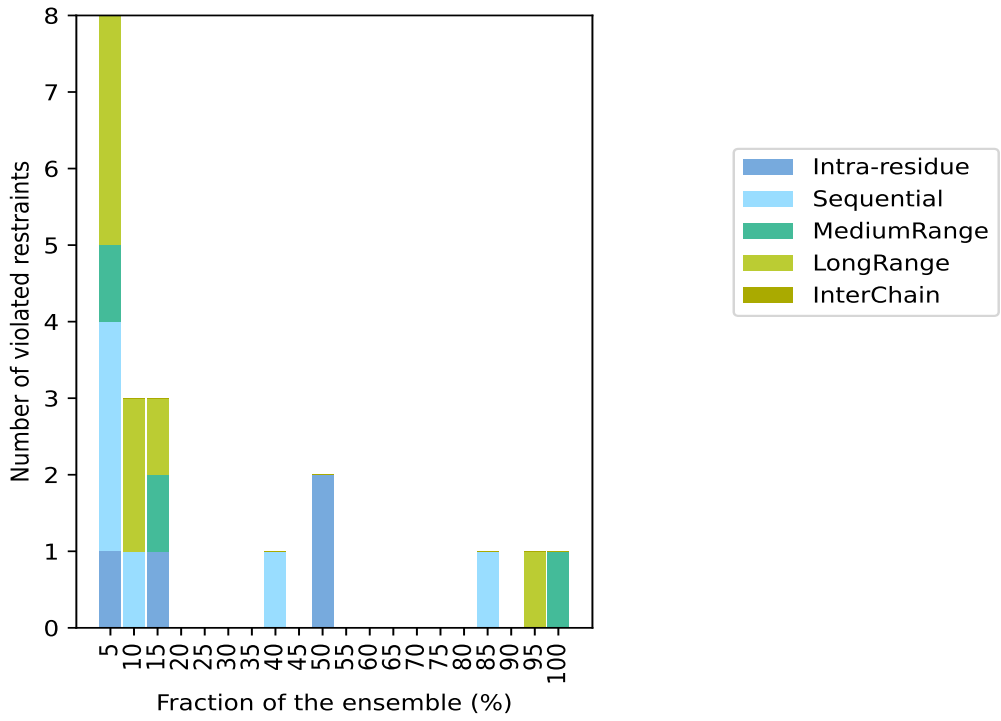
9.3 Distance violation statistics for the ensemble (i)

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, 1672(IR:345, SQ:426, MR:143, LR:758, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	3	1	3	0	8	1	5.0
0	1	0	2	0	3	2	10.0
1	0	1	1	0	3	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	1	0	0	0	1	8	40.0
0	0	0	0	0	0	9	45.0
2	0	0	0	0	2	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	1	0	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	0	1	0	0	1	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

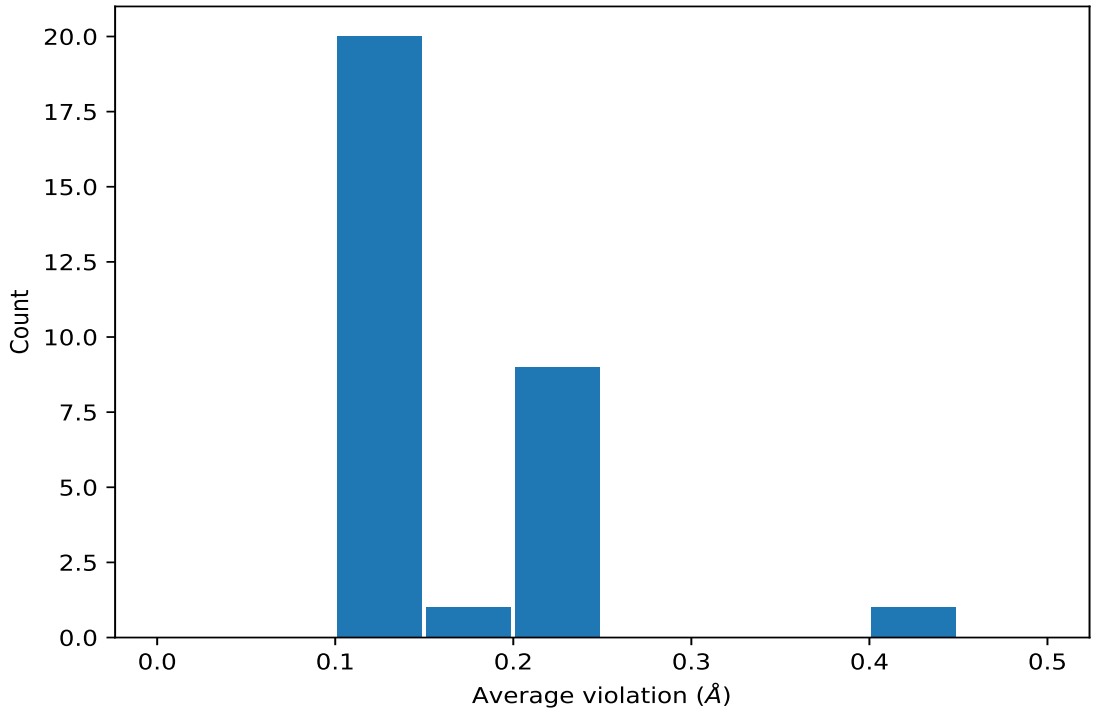
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	20	0.24	0.01	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	20	0.24	0.01	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	20	0.24	0.01	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	20	0.24	0.01	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	20	0.24	0.01	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	20	0.24	0.01	0.24
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	19	0.13	0.01	0.12
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	17	0.13	0.01	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	17	0.13	0.01	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	17	0.13	0.01	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	17	0.13	0.01	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	17	0.13	0.01	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	17	0.13	0.01	0.13
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	10	0.42	0.01	0.42
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	10	0.24	0.01	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	10	0.24	0.01	0.24

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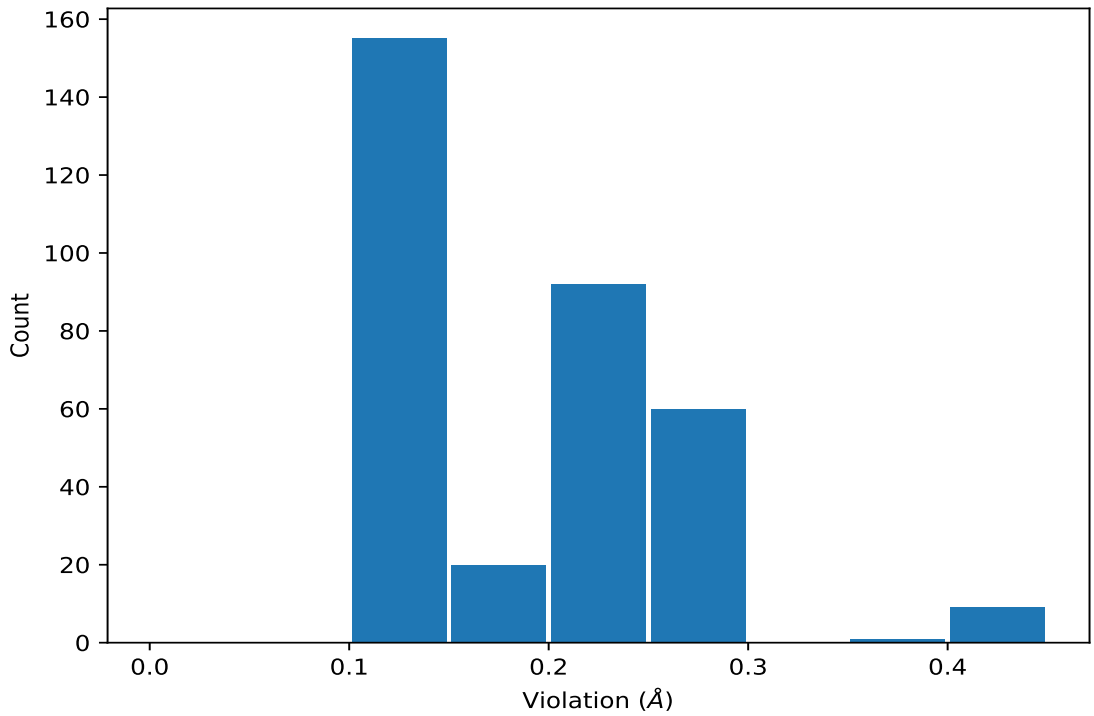
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	10	0.24	0.01	0.24
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	8	0.12	0.01	0.11
(1,1082)	1:A:77:SER:H	1:A:81:SER:H	3	0.15	0.0	0.15
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG11	3	0.14	0.02	0.13
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG12	3	0.14	0.02	0.13
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG13	3	0.14	0.02	0.13
(1,978)	1:A:43:HIS:HB2	1:A:58:THR:H	3	0.11	0.0	0.11
(1,749)	1:A:35:ILE:HB	1:A:36:LYS:H	2	0.19	0.0	0.19
(1,1441)	1:A:42:LEU:HD11	1:A:56:ASN:H	2	0.15	0.01	0.15
(1,1441)	1:A:42:LEU:HD12	1:A:56:ASN:H	2	0.15	0.01	0.15
(1,1441)	1:A:42:LEU:HD13	1:A:56:ASN:H	2	0.15	0.01	0.15
(1,1441)	1:A:42:LEU:HD21	1:A:56:ASN:H	2	0.15	0.01	0.15
(1,1441)	1:A:42:LEU:HD22	1:A:56:ASN:H	2	0.15	0.01	0.15
(1,1441)	1:A:42:LEU:HD23	1:A:56:ASN:H	2	0.15	0.01	0.15
(1,986)	1:A:43:HIS:H	1:A:56:ASN:H	2	0.11	0.0	0.11

[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)
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	13	0.44
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	4	0.43
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	14	0.43
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	1	0.42
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	3	0.42
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	16	0.42
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	20	0.42
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	8	0.41
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	11	0.41
(1,949)	1:A:42:LEU:H	1:A:42:LEU:HG	2	0.39
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	3	0.27
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	3	0.27
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	3	0.27
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	3	0.27
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	3	0.27
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	6	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	6	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	6	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	6	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	6	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	6	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	12	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	12	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	12	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	12	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	12	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	12	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	17	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	17	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	17	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	17	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	17	0.26
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	17	0.26
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	1	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	1	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	1	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	1	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	1	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	1	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	2	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	2	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	2	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	2	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	2	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	2	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	7	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	7	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	7	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	7	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	7	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	7	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	9	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	9	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	9	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	9	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	9	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	15	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	15	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	15	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	15	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	15	0.25
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	15	0.25
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	17	0.25
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	17	0.25
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	17	0.25
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	19	0.25
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	19	0.25
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	19	0.25
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	4	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	4	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	4	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	4	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	4	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	4	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	5	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	5	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	5	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	5	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	5	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	5	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	10	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	10	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	10	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	10	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	10	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	10	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	11	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	11	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	11	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	11	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	11	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	11	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	14	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	14	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	14	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	14	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	14	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	18	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	18	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	18	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	18	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	18	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	18	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	19	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	19	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	19	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	19	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	19	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	19	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	20	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	20	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	20	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	20	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	20	0.24
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	20	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	5	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	5	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	5	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	6	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	6	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	6	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	7	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	7	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	7	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	18	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	18	0.24
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	18	0.24
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	8	0.23
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	8	0.23
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	8	0.23
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	8	0.23
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	8	0.23
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	8	0.23
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	16	0.23
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	16	0.23
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	16	0.23
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	16	0.23
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	16	0.23
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	9	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	9	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	9	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	10	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	10	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	10	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	15	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	15	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	15	0.23
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD21	12	0.22
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD22	12	0.22
(1,153)	1:A:42:LEU:H	1:A:42:LEU:HD23	12	0.22
(1,1527)	1:A:56:ASN:HB2	1:A:57:VAL:HB	15	0.21
(1,1527)	1:A:56:ASN:HB3	1:A:57:VAL:HB	15	0.21
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD11	13	0.2
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD12	13	0.2
(1,1575)	1:A:71:ASP:HB2	1:A:74:ILE:HD13	13	0.2
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD11	13	0.2
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD12	13	0.2
(1,1575)	1:A:71:ASP:HB3	1:A:74:ILE:HD13	13	0.2
(1,749)	1:A:35:ILE:HB	1:A:36:LYS:H	3	0.19
(1,749)	1:A:35:ILE:HB	1:A:36:LYS:H	5	0.19
(1,1549)	1:A:61:LYS:HG2	1:A:62:ASP:H	16	0.19
(1,1549)	1:A:61:LYS:HG3	1:A:62:ASP:H	16	0.19
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG11	7	0.16
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG12	7	0.16
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG13	7	0.16
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	18	0.16
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	18	0.16
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	18	0.16
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	18	0.16
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	18	0.16
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	18	0.16
(1,1441)	1:A:42:LEU:HD11	1:A:56:ASN:H	12	0.16
(1,1441)	1:A:42:LEU:HD12	1:A:56:ASN:H	12	0.16
(1,1441)	1:A:42:LEU:HD13	1:A:56:ASN:H	12	0.16
(1,1441)	1:A:42:LEU:HD21	1:A:56:ASN:H	12	0.16
(1,1441)	1:A:42:LEU:HD22	1:A:56:ASN:H	12	0.16
(1,1441)	1:A:42:LEU:HD23	1:A:56:ASN:H	12	0.16
(1,1082)	1:A:77:SER:H	1:A:81:SER:H	3	0.16
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	16	0.15
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	7	0.15
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	7	0.15
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	7	0.15
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	7	0.15
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	7	0.15
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	19	0.15
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	19	0.15
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	19	0.15
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	19	0.15
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	19	0.15
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	19	0.15
(1,1082)	1:A:77:SER:H	1:A:81:SER:H	11	0.15
(1,1082)	1:A:77:SER:H	1:A:81:SER:H	16	0.15
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	10	0.14
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	18	0.14
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	19	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	2	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	2	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	2	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	2	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	2	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	2	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	5	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	5	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	5	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	5	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	5	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	5	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	10	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	10	0.14
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	10	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	10	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	10	0.14
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	10	0.14
(1,1441)	1:A:42:LEU:HD11	1:A:56:ASN:H	17	0.14
(1,1441)	1:A:42:LEU:HD12	1:A:56:ASN:H	17	0.14
(1,1441)	1:A:42:LEU:HD13	1:A:56:ASN:H	17	0.14
(1,1441)	1:A:42:LEU:HD21	1:A:56:ASN:H	17	0.14
(1,1441)	1:A:42:LEU:HD22	1:A:56:ASN:H	17	0.14
(1,1441)	1:A:42:LEU:HD23	1:A:56:ASN:H	17	0.14
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	3	0.13
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	12	0.13
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	14	0.13
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	20	0.13
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG11	10	0.13
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG12	10	0.13
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG13	10	0.13
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	10	0.13
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	19	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	4	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	4	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	4	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	4	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	4	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	4	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	9	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	9	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	9	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	9	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	9	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	9	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	11	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	11	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	11	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	11	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	11	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	11	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	13	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	13	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	13	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	13	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	13	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	13	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	16	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	16	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	16	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	16	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	16	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	16	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	20	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	20	0.13
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	20	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	20	0.13
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	20	0.13
(1,978)	1:A:43:HIS:HB2	1:A:58:THR:H	18	0.12
(1,919)	1:A:46:TRP:H	1:A:89:VAL:H	20	0.12
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	4	0.12
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	6	0.12
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	7	0.12
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	9	0.12
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	13	0.12
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	15	0.12
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG11	19	0.12
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG12	19	0.12
(1,815)	1:A:88:VAL:H	1:A:88:VAL:HG13	19	0.12
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	17	0.12
(1,1581)	1:A:74:ILE:HB	1:A:76:LEU:HD11	17	0.12
(1,1581)	1:A:74:ILE:HB	1:A:76:LEU:HD12	17	0.12
(1,1581)	1:A:74:ILE:HB	1:A:76:LEU:HD13	17	0.12
(1,1581)	1:A:74:ILE:HB	1:A:76:LEU:HD21	17	0.12
(1,1581)	1:A:74:ILE:HB	1:A:76:LEU:HD22	17	0.12
(1,1581)	1:A:74:ILE:HB	1:A:76:LEU:HD23	17	0.12
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	6	0.12
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	6	0.12
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	6	0.12
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	6	0.12
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	6	0.12
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	6	0.12
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	12	0.12
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	12	0.12
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	12	0.12
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	12	0.12
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	12	0.12
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	12	0.12
(1,986)	1:A:43:HIS:H	1:A:56:ASN:H	9	0.11
(1,986)	1:A:43:HIS:H	1:A:56:ASN:H	12	0.11
(1,978)	1:A:43:HIS:HB2	1:A:58:THR:H	10	0.11
(1,978)	1:A:43:HIS:HB2	1:A:58:THR:H	12	0.11
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	1	0.11
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	2	0.11
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	5	0.11
(1,885)	1:A:29:VAL:H	1:A:74:ILE:HG12	8	0.11
(1,792)	1:A:73:VAL:H	1:A:73:VAL:HB	9	0.11
(1,777)	1:A:68:SER:H	1:A:69:ILE:HB	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:A:36:LYS:HA	1:A:65:ALA:HA	6	0.11
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	2	0.11
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	3	0.11
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	5	0.11
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	8	0.11
(1,36)	1:A:45:PHE:HB3	1:A:46:TRP:HZ3	16	0.11
(1,344)	1:A:46:TRP:HZ3	1:A:57:VAL:HG21	15	0.11
(1,344)	1:A:46:TRP:HZ3	1:A:57:VAL:HG22	15	0.11
(1,344)	1:A:46:TRP:HZ3	1:A:57:VAL:HG23	15	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	3	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	3	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	3	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	3	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	3	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	3	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	8	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	8	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	8	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	8	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	8	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	8	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD11	15	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD12	15	0.11
(1,1571)	1:A:68:SER:HB2	1:A:69:ILE:HD13	15	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD11	15	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD12	15	0.11
(1,1571)	1:A:68:SER:HB3	1:A:69:ILE:HD13	15	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value