Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LC4
BMRB ID	:	17598
Title	:	Solution Structure of PilP from Pseudomonas aeruginosa
Authors	:	Howell, P.; Tammam, S.; Chong, P.; Forman-Kay, J.D.
Deposited on	:	2011-04-22

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:

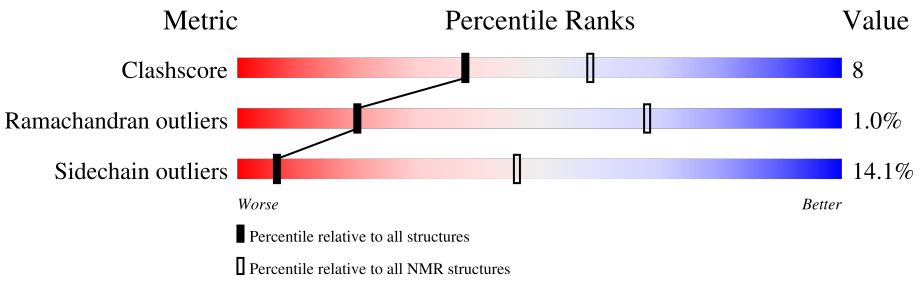
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 85%.

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	111	55% 15% 30%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:22-A:99 (78)	0.51	6

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1747 atoms, of which 872 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PilP protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	111	1747	546	872	166	162	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	LEU	-	expression tag	UNP Q51354
A	105	GLU	-	expression tag	UNP Q51354
A	106	HIS	-	expression tag	UNP Q51354
A	107	HIS	-	expression tag	UNP Q51354
A	108	HIS	-	expression tag	UNP Q51354
A	109	HIS	-	expression tag	UNP Q51354
A	110	HIS	-	expression tag	UNP Q51354
A	111	HIS	-	expression tag	UNP Q51354

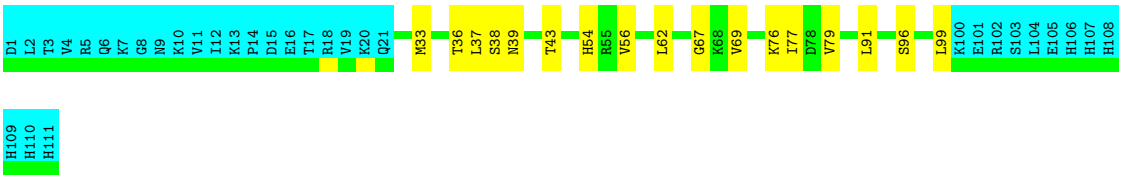
4 Residue-property plots (i)

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: PilP protein

Chain A: 55% 15% 30%



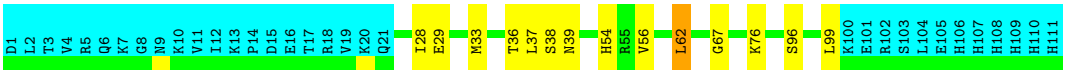
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PilP protein

Chain A: 58% 12% • 30%



4.2.2 Score per residue for model 2

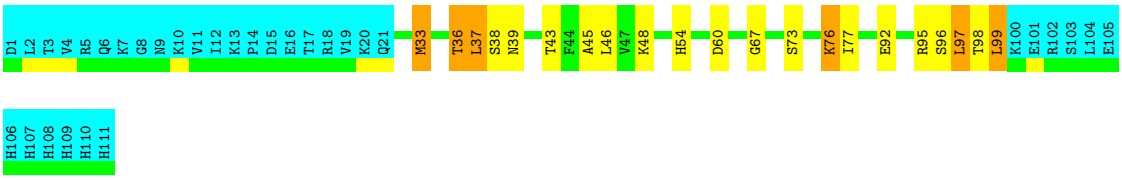
• Molecule 1: PilP protein

Chain A: 49% 20% • 30%

4.2.3 Score per residue for model 3

- Molecule 1: PilP protein

Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: PilP protein

Chain A:

4.2.5 Score per residue for model 5

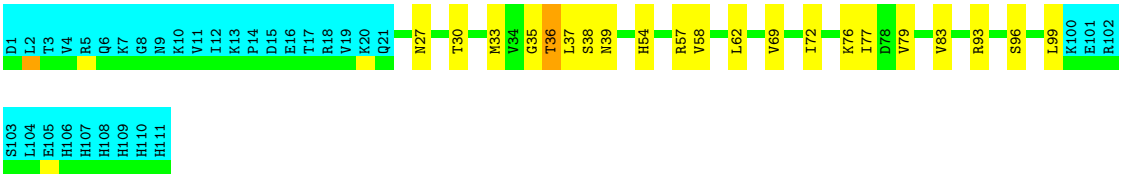
- Molecule 1: PilP protein

Chain A:

4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: PilP protein

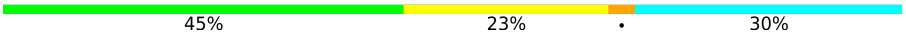
Chain A:

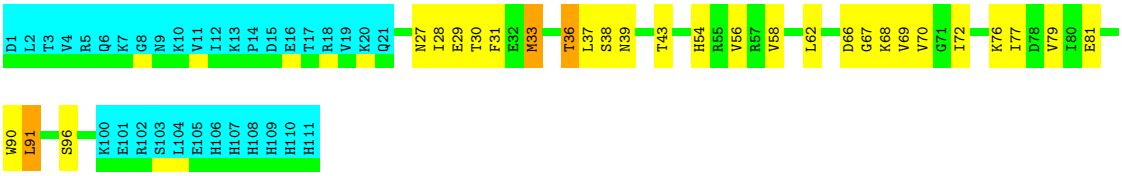


4.2.7 Score per residue for model 7

- Molecule 1: PilP protein

Chain A:

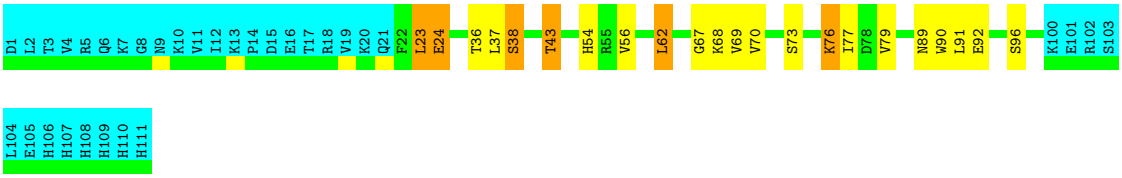




4.2.8 Score per residue for model 8

- Molecule 1: PilP protein

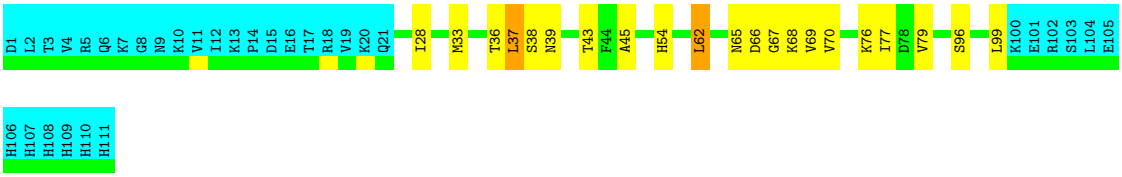
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: PilP protein

Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: PilP protein

Chain A: 49% 18% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 F22 L23 N27 I28 E29 T30 F31 V34 G35 T36 L37 S38 T43 K48 H54 D60 V69 I72 S73 K76 I77 D78 V79 I82 W90 L91 S96

L97 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.11 Score per residue for model 11

- Molecule 1: PilP protein

Chain A: 60% 8% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 T36 L37 S38 A45 H54 V58 I72 K76 I77 G88 S96 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.12 Score per residue for model 12

- Molecule 1: PilP protein

Chain A: 56% 14% 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 E32 T36 L37 S38 N39 A40 Q41 G42 T43 F44 A45 H54 L62 G67 S73 K76 I77 W90 L91 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110

H111

4.2.13 Score per residue for model 13

- Molecule 1: PilP protein

Chain A: 49% 19% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 F22 L23 I28 T36 L37 S38 N39 T43 L46 H54 R55 V56 L62 N65 D66 G67 K68 V69 I72 K76 I77 D78 V79 N89 W90 L91 S96 L97

T98 L99 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.14 Score per residue for model 14

- Molecule 1: PilP protein

Chain A: 54% 15% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 F22 L23 E24 T36 L37 S38 A45 K48 H54 L62 G67 K68 V69 K76 I77 D78 V79 I82 W90 S96 L99 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.15 Score per residue for model 15

- Molecule 1: PilP protein

Chain A: 59% 9% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 M33 T36 L37 S38 H54 R55 V56 L62 V69 K76 I77 D78 V79 S96 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.16 Score per residue for model 16

- Molecule 1: PilP protein

Chain A: 47% 20% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 F22 L23 M33 V34 G35 T36 L37 S38 N39 A40 Q41 G42 T43 F44 A45 L46 H54 R55 V56 L62 G67 K68 V69 V70 G71 I72 K76 I77 D78 V79 W90 L91 S96 L99 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.17 Score per residue for model 17

- Molecule 1: PilP protein

Chain A: 52% 16% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 F22 L23 I28 V34 G35 T36 L37 S38 N39 H54 L62 V69 I72 I77 D78 V79 I82 D85 W90 L91 S96 L99 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.18 Score per residue for model 18

- Molecule 1: PilP protein

Chain A: 50% 18% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 I28 M33 T36 L37 S38 N39 A40 Q41 G42 T43 H54 R55 V56 L62 G67 K68 V69 K76 I77 D78 V79 I80 E81 W90 S96 L97 T98 L99 K100 E101

R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.19 Score per residue for model 19

- Molecule 1: PilP protein

Chain A: 50% 19% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 I28 E29 M33 L37 S38 N39 T43 F44 A45 H54 R55 V56 L62 N65 D66 G67 K68 V69 S73 K76 I77 D78 V79 I80 E81 S96 L97 T98 L99

K100 E101 R102 S103 L104 E105 H106 H107 H108 H109 H110 H111

4.2.20 Score per residue for model 20

- Molecule 1: PilP protein

Chain A: 56% 14% • 30%

D1 L2 T3 V4 R5 Q6 K7 G8 N9 K10 V11 I12 K13 P14 D15 E16 T17 R18 V19 K20 Q21 E24 I28 M33 T36 N39 H54 L62 G67 K68 V69 V70 K76 V79 L91 S96 L99 K100 E101 R102 S103 L104 E105 H106 H107 H108 H109

H110 H111

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
TALOS	geometry optimization	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1215
Number of shifts mapped to atoms	1215
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	592	589	589	10±4
All	All	11840	11780	11780	191

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:VAL:HG21	1:A:62:LEU:HD23	0.74	1.58	8	3
1:A:45:ALA:HB1	1:A:77:ILE:HD13	0.72	1.59	12	5
1:A:23:LEU:HD11	1:A:54:HIS:CE1	0.68	2.23	14	2
1:A:56:VAL:HG21	1:A:62:LEU:HD22	0.65	1.66	1	2
1:A:23:LEU:HD12	1:A:31:PHE:CE1	0.65	2.27	10	1
1:A:90:TRP:O	1:A:91:LEU:HD22	0.63	1.94	8	6
1:A:28:ILE:HD13	1:A:62:LEU:O	0.62	1.95	20	7
1:A:36:THR:CG2	1:A:77:ILE:HD11	0.62	2.25	18	8
1:A:33:MET:HG3	1:A:99:LEU:HD22	0.62	1.72	16	1
1:A:33:MET:CG	1:A:99:LEU:HD22	0.62	2.25	16	1
1:A:23:LEU:HD11	1:A:54:HIS:NE2	0.61	2.10	10	2
1:A:33:MET:CE	1:A:36:THR:HG23	0.61	2.25	16	4
1:A:37:LEU:HD13	1:A:38:SER:N	0.61	2.11	8	18
1:A:76:LYS:O	1:A:77:ILE:HD13	0.60	1.96	16	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HG23	1:A:77:ILE:CD1	0.60	2.27	17	3
1:A:45:ALA:HB1	1:A:77:ILE:CD1	0.59	2.27	9	3
1:A:56:VAL:HG11	1:A:62:LEU:HD13	0.59	1.75	4	3
1:A:23:LEU:HD21	1:A:54:HIS:ND1	0.58	2.13	10	1
1:A:33:MET:HE1	1:A:36:THR:HG23	0.57	1.76	16	1
1:A:28:ILE:HG21	1:A:81:GLU:OE2	0.56	2.00	7	1
1:A:79:VAL:CG2	1:A:97:LEU:HD11	0.56	2.29	19	1
1:A:47:VAL:HG11	1:A:62:LEU:HD21	0.56	1.77	4	1
1:A:85:ASP:OD1	1:A:91:LEU:HD23	0.56	2.01	17	1
1:A:77:ILE:O	1:A:97:LEU:HD12	0.56	2.00	13	5
1:A:56:VAL:HG21	1:A:62:LEU:CD2	0.55	2.32	15	4
1:A:76:LYS:HB3	1:A:98:THR:HG22	0.55	1.79	3	1
1:A:79:VAL:HG23	1:A:81:GLU:OE1	0.55	2.02	5	1
1:A:79:VAL:HG22	1:A:97:LEU:HD11	0.55	1.79	19	1
1:A:33:MET:HG2	1:A:99:LEU:HD12	0.54	1.78	9	2
1:A:72:ILE:HG23	1:A:77:ILE:HD12	0.54	1.78	6	6
1:A:30:THR:HG23	1:A:31:PHE:CD1	0.53	2.38	7	1
1:A:33:MET:HE2	1:A:36:THR:HG23	0.52	1.81	15	2
1:A:36:THR:HG21	1:A:77:ILE:HD11	0.51	1.82	10	3
1:A:36:THR:HG22	1:A:45:ALA:HA	0.51	1.81	4	4
1:A:58:VAL:HG23	1:A:72:ILE:HD12	0.51	1.82	7	4
1:A:69:VAL:HA	1:A:79:VAL:HG12	0.50	1.83	9	14
1:A:33:MET:SD	1:A:99:LEU:HD12	0.50	2.47	20	2
1:A:31:PHE:CD2	1:A:62:LEU:HD23	0.50	2.42	2	1
1:A:62:LEU:HD12	1:A:62:LEU:O	0.50	2.07	8	2
1:A:28:ILE:HG21	1:A:81:GLU:HG2	0.50	1.83	18	1
1:A:45:ALA:C	1:A:46:LEU:HD23	0.49	2.27	16	2
1:A:38:SER:OG	1:A:43:THR:HG23	0.49	2.06	8	1
1:A:28:ILE:HG22	1:A:65:ASN:OD1	0.49	2.08	9	3
1:A:35:GLY:HA2	1:A:99:LEU:HD21	0.49	1.85	6	1
1:A:27:ASN:O	1:A:30:THR:HG22	0.48	2.08	10	2
1:A:68:LYS:HE3	1:A:70:VAL:HG12	0.48	1.85	2	6
1:A:82:ILE:HG22	1:A:90:TRP:CE3	0.48	2.44	10	4
1:A:34:VAL:HG11	1:A:48:LYS:HB2	0.46	1.86	10	2
1:A:37:LEU:HD13	1:A:38:SER:H	0.46	1.70	2	3
1:A:45:ALA:O	1:A:46:LEU:HD23	0.45	2.12	16	1
1:A:83:VAL:HG21	1:A:93:ARG:HH11	0.44	1.71	6	1
1:A:34:VAL:O	1:A:99:LEU:HD11	0.44	2.12	16	1
1:A:33:MET:HE3	1:A:36:THR:HG23	0.43	1.90	7	2
1:A:28:ILE:HG21	1:A:81:GLU:OE1	0.43	2.14	19	2
1:A:56:VAL:HG21	1:A:62:LEU:HD12	0.43	1.90	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:VAL:HG11	1:A:72:ILE:HD11	0.42	1.90	4	1
1:A:28:ILE:HG21	1:A:81:GLU:CD	0.42	2.35	2	1
1:A:36:THR:HG21	1:A:73:SER:O	0.42	2.14	3	1
1:A:90:TRP:C	1:A:91:LEU:HD22	0.42	2.35	12	1
1:A:46:LEU:HD22	1:A:55:ARG:HG2	0.41	1.92	13	1
1:A:33:MET:CE	1:A:77:ILE:HD11	0.41	2.46	16	1
1:A:37:LEU:HD13	1:A:37:LEU:C	0.41	2.36	18	11
1:A:27:ASN:HB2	1:A:30:THR:HG23	0.41	1.91	6	1
1:A:33:MET:HE1	1:A:99:LEU:HD12	0.40	1.92	3	1
1:A:28:ILE:CD1	1:A:62:LEU:HD13	0.40	2.46	19	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/111 (70%)	70±2 (90±2%)	7±2 (9±3%)	1±1 (1±1%)	20	68
All	All	1560/2220 (70%)	1398 (90%)	146 (9%)	16 (1%)	20	68

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

Mol	Chain	Res	Type	Models (Total)
1	A	67	GLY	14
1	A	60	ASP	1
1	A	88	GLY	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	62/94 (66%)	53±2 (86±3%)	9±2 (14±3%)	6 46
All	All	1240/1880 (66%)	1065 (86%)	175 (14%)	6 46

All 30 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	54	HIS	20
1	A	96	SER	19
1	A	36	THR	17
1	A	76	LYS	15
1	A	39	ASN	14
1	A	62	LEU	13
1	A	43	THR	13
1	A	99	LEU	11
1	A	91	LEU	6
1	A	33	MET	5
1	A	29	GLU	4
1	A	41	GLN	4
1	A	23	LEU	4
1	A	73	SER	4
1	A	37	LEU	3
1	A	24	GLU	3
1	A	48	LYS	2
1	A	92	GLU	2
1	A	95	ARG	2
1	A	97	LEU	2
1	A	66	ASP	2
1	A	38	SER	2
1	A	64	ARG	1
1	A	87	GLU	1
1	A	57	ARG	1
1	A	89	ASN	1
1	A	60	ASP	1
1	A	32	GLU	1
1	A	78	ASP	1
1	A	55	ARG	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 85% for the well-defined parts and 79% 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	1215
Number of shifts mapped to atoms	1215
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	107	0.08 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	93	0.17 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	99	0.13 ± 0.27	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 85%, i.e. 884 atoms were assigned a chemical shift out of a possible 1039. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	318/399 (80%)	165/167 (99%)	78/156 (50%)	75/76 (99%)
Sidechain	502/572 (88%)	343/372 (92%)	156/177 (88%)	3/23 (13%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	64/68 (94%)	32/34 (94%)	31/32 (97%)	1/2 (50%)
Overall	884/1039 (85%)	540/573 (94%)	265/365 (73%)	79/101 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1215 atoms were assigned a chemical shift out of a possible 1531. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	423/563 (75%)	217/233 (93%)	107/222 (48%)	99/108 (92%)
Sidechain	728/858 (85%)	492/553 (89%)	229/265 (86%)	7/40 (18%)
Aromatic	64/110 (58%)	32/58 (55%)	31/44 (70%)	1/8 (12%)
Overall	1215/1531 (79%)	741/844 (88%)	367/531 (69%)	107/156 (69%)

7.1.4 Statistically unusual chemical shifts (i)

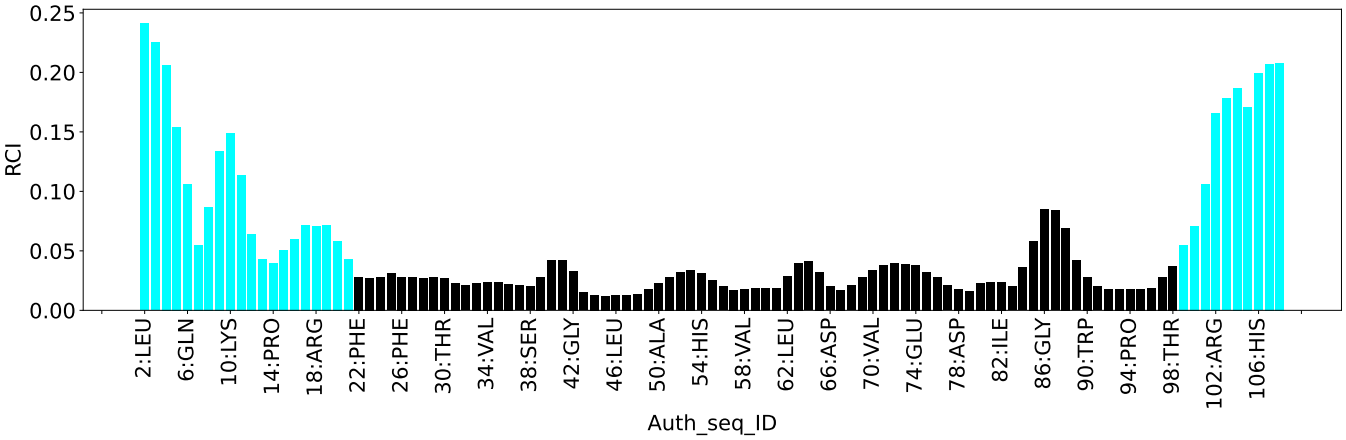
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	54	HIS	HE1	0.42	5.13 – 10.76	-13.4
1	A	54	HIS	CE1	120.36	126.08 – 149.12	-7.5
1	A	7	LYS	CD	21.03	23.50 – 34.42	-7.3
1	A	7	LYS	CE	35.78	37.57 – 46.21	-7.1

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
0.25
0.20
0.15
0.10
0.05
0.00
2:LEU
6:GLN
10:LYS
14:PRO
18:ARG
22:PHE
26:PHE
30:THR
34:VAL
38:SER
42:GLY
46:LEU
50:ALA
54:HIS
58:VAL
62:LEU
66:ASP
70:VAL
74:GLU
78:ASP
82:ILE
86:GLY
90:TRP
94:PRO
98:THR
102:ARG
106:HIS
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	1332
Intra-residue (|i-j|=0)	304
Sequential (|i-j|=1)	413
Medium range (|i-j|>1 and |i-j|<5)	162
Long range (|i-j|≥5)	383
Inter-chain	0
Hydrogen bond restraints	70
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.0
Number of long range restraints per residue[1]	4.0

[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)	2.8	0.2
0.2-0.5 (Medium)	0.8	0.37
>0.5 (Large)	0.1	0.7

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)

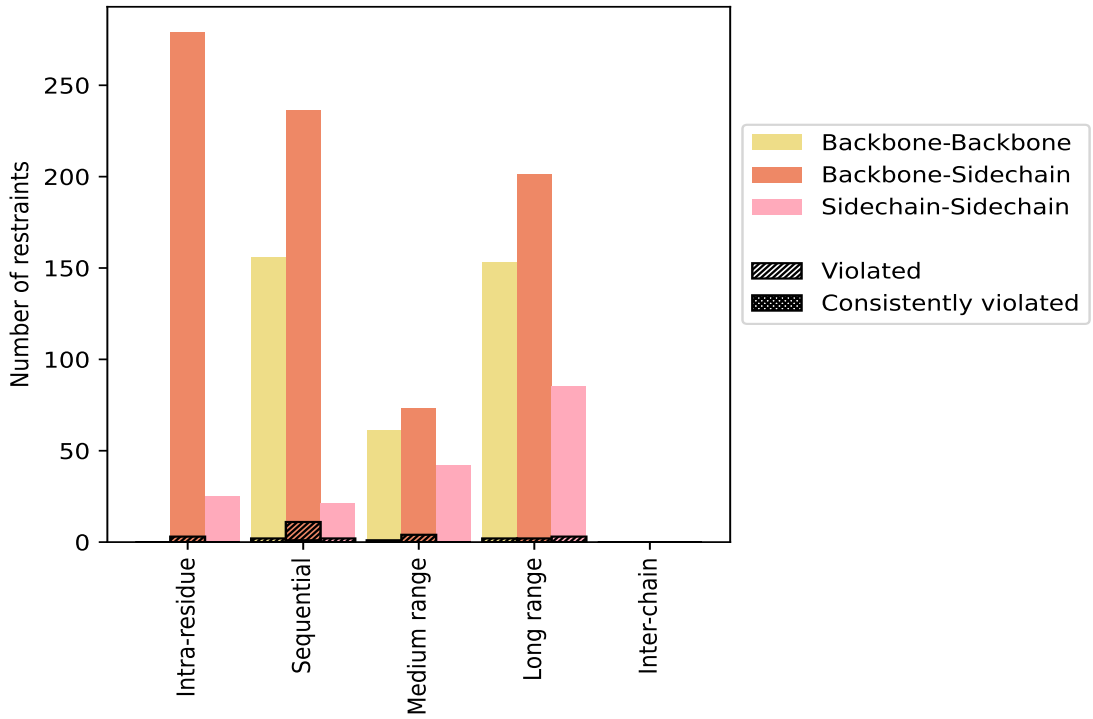
9.1 Summary of distance violations (i)

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)	304	22.8	3	1.0	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	279	20.9	3	1.1	0.2	0	0.0	0.0
Sidechain-Sidechain	25	1.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	413	31.0	15	3.6	1.1	1	0.2	0.1
Backbone-Backbone	156	11.7	2	1.3	0.2	0	0.0	0.0
Backbone-Sidechain	236	17.7	11	4.7	0.8	1	0.4	0.1
Sidechain-Sidechain	21	1.6	2	9.5	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	162	12.2	5	3.1	0.4	0	0.0	0.0
Backbone-Backbone	47	3.5	1	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	73	5.5	4	5.5	0.3	0	0.0	0.0
Sidechain-Sidechain	42	3.2	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	383	28.8	5	1.3	0.4	0	0.0	0.0
Backbone-Backbone	97	7.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	201	15.1	2	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	85	6.4	3	3.5	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	70	5.3	2	2.9	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1332	100.0	30	2.3	2.3	1	0.1	0.1
Backbone-Backbone	370	27.8	5	1.4	0.4	0	0.0	0.0
Backbone-Sidechain	789	59.2	20	2.5	1.5	1	0.1	0.1
Sidechain-Sidechain	173	13.0	5	2.9	0.4	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	0.21	0.21	0.0	0.21
2	0	2	0	0	0	2	0.22	0.26	0.04	0.22
3	0	1	0	1	0	2	0.16	0.21	0.05	0.16
4	0	2	0	0	0	2	0.16	0.21	0.05	0.16
5	0	2	0	0	0	2	0.16	0.19	0.04	0.16
6	0	2	0	1	0	3	0.2	0.3	0.08	0.18
7	0	2	0	0	0	2	0.22	0.26	0.04	0.22
8	0	2	0	0	0	2	0.16	0.2	0.04	0.16
9	0	4	0	0	0	4	0.18	0.26	0.05	0.16
10	0	2	0	1	0	3	0.22	0.31	0.07	0.2
11	1	3	0	0	0	4	0.22	0.37	0.09	0.2

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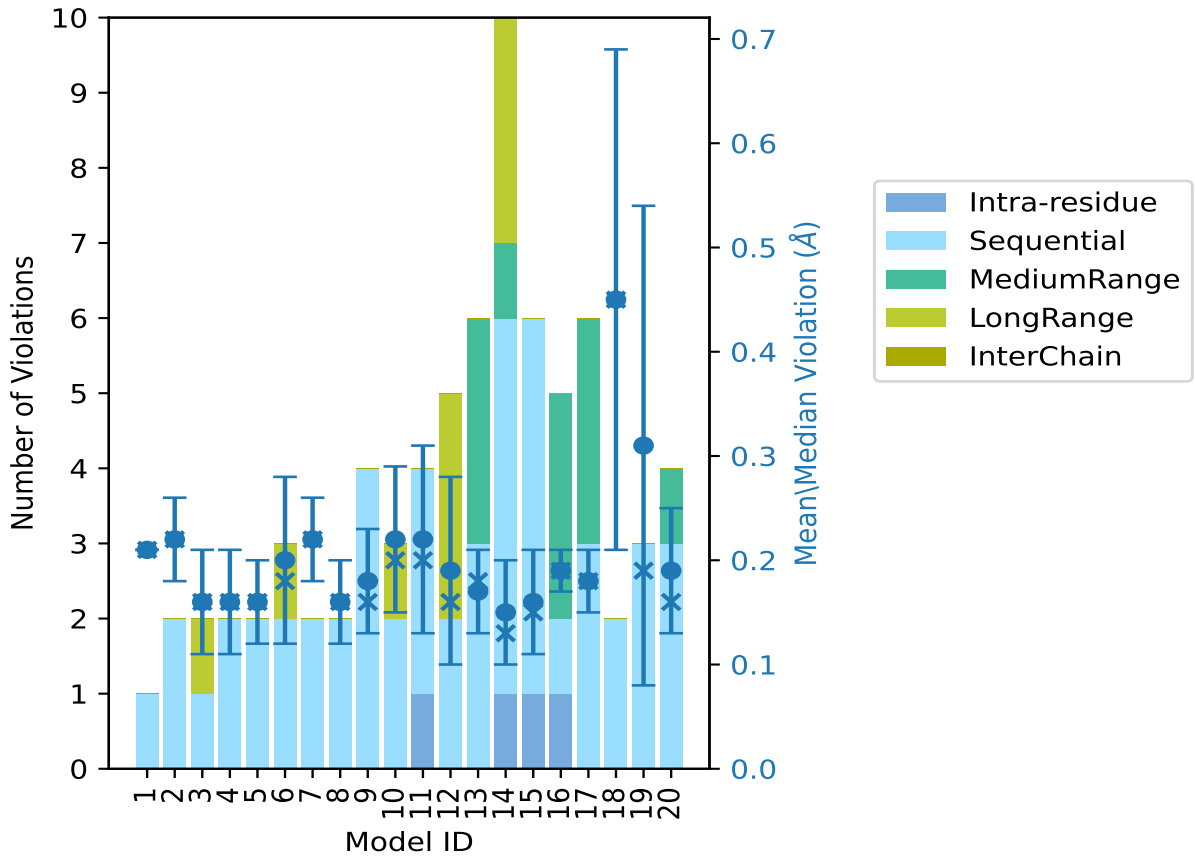
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	0	3	0	5	0.19	0.35	0.09	0.16
13	0	3	3	0	0	6	0.17	0.22	0.04	0.18
14	1	5	1	3	0	10	0.15	0.29	0.05	0.13
15	1	5	0	0	0	6	0.16	0.26	0.05	0.15
16	1	1	3	0	0	5	0.19	0.23	0.02	0.19
17	0	3	3	0	0	6	0.18	0.22	0.03	0.18
18	0	2	0	0	0	2	0.45	0.7	0.24	0.45
19	0	3	0	0	0	3	0.31	0.63	0.23	0.19
20	0	3	1	0	0	4	0.19	0.29	0.06	0.16

[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

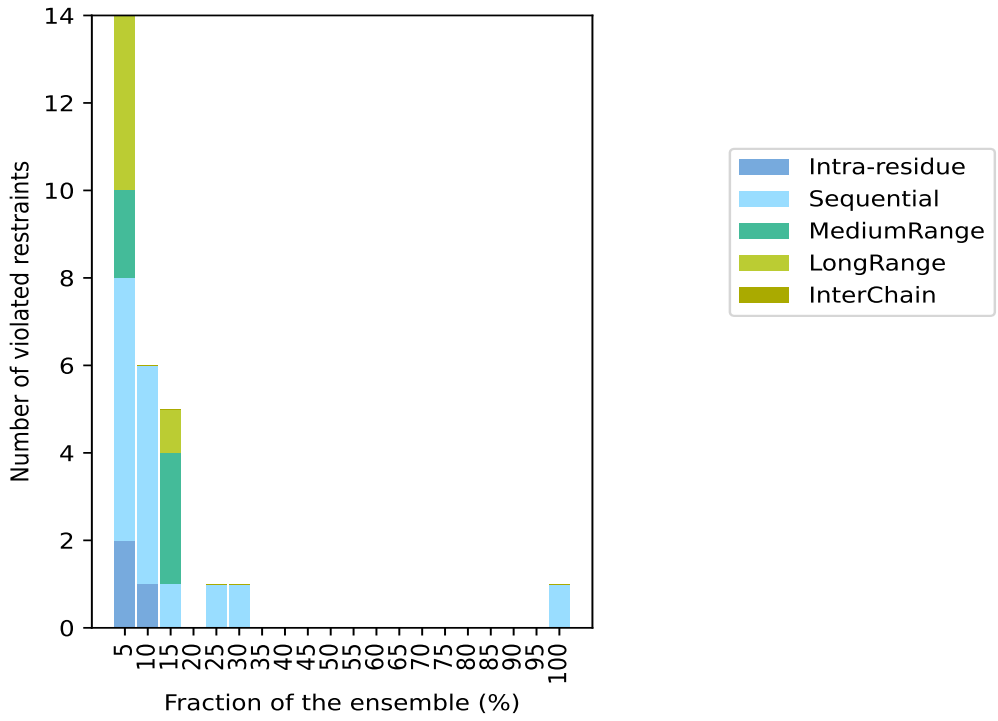
9.3 Distance violation statistics for the ensemble (i)

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, 1234(IR:301, SQ:398, MR:157, LR:378, 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]	%
2	6	2	4	0	14	1	5.0
1	5	0	0	0	6	2	10.0
0	1	3	1	0	5	3	15.0
0	0	0	0	0	0	4	20.0
0	1	0	0	0	1	5	25.0
0	1	0	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	1	0	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

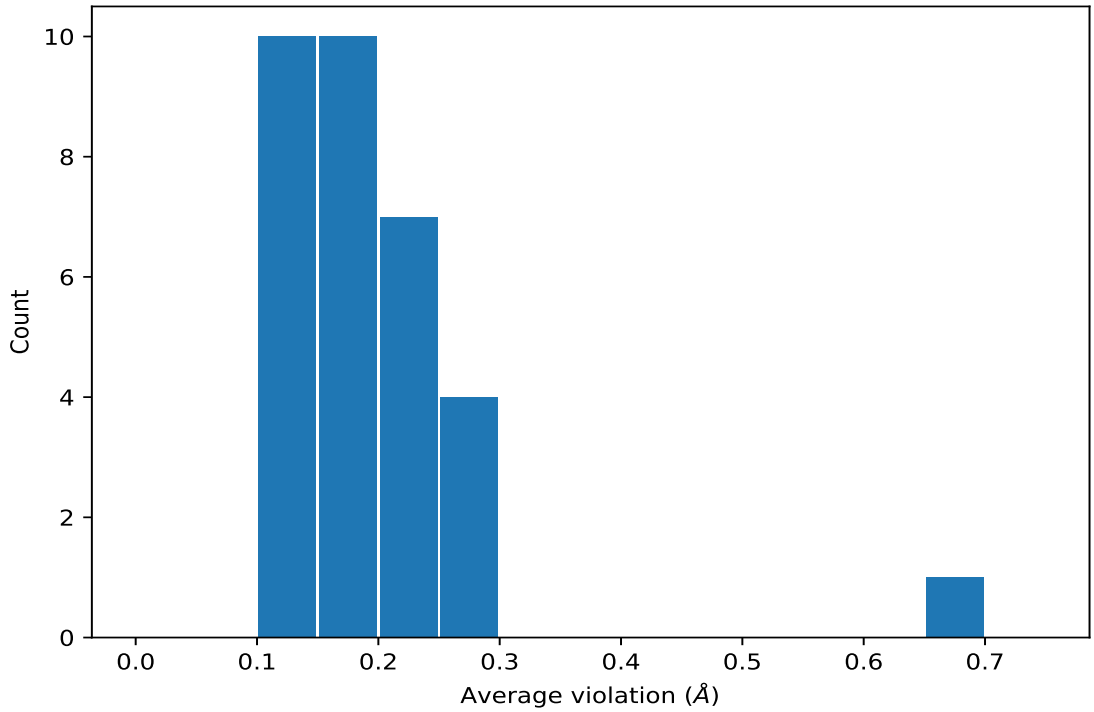
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	20	0.2	0.01	0.2
(1,238)	1:A:11:VAL:HB	1:A:12:ILE:H	6	0.29	0.04	0.26
(1,682)	1:A:73:SER:HB2	1:A:74:GLU:H	5	0.13	0.0	0.13
(1,1006)	1:A:23:LEU:HD11	1:A:25:GLY:H	3	0.22	0.0	0.22
(1,1006)	1:A:23:LEU:HD12	1:A:25:GLY:H	3	0.22	0.0	0.22
(1,1006)	1:A:23:LEU:HD13	1:A:25:GLY:H	3	0.22	0.0	0.22
(1,1006)	1:A:23:LEU:HD21	1:A:25:GLY:H	3	0.22	0.0	0.22
(1,1006)	1:A:23:LEU:HD22	1:A:25:GLY:H	3	0.22	0.0	0.22
(1,1006)	1:A:23:LEU:HD23	1:A:25:GLY:H	3	0.22	0.0	0.22
(1,80)	1:A:23:LEU:HD21	1:A:25:GLY:H	3	0.18	0.01	0.17
(1,80)	1:A:23:LEU:HD22	1:A:25:GLY:H	3	0.18	0.01	0.17
(1,80)	1:A:23:LEU:HD23	1:A:25:GLY:H	3	0.18	0.01	0.17
(1,566)	1:A:23:LEU:HD11	1:A:25:GLY:H	3	0.18	0.0	0.18
(1,566)	1:A:23:LEU:HD12	1:A:25:GLY:H	3	0.18	0.0	0.18
(1,566)	1:A:23:LEU:HD13	1:A:25:GLY:H	3	0.18	0.0	0.18
(1,1127)	1:A:55:ARG:HG2	1:A:56:VAL:H	3	0.12	0.0	0.12

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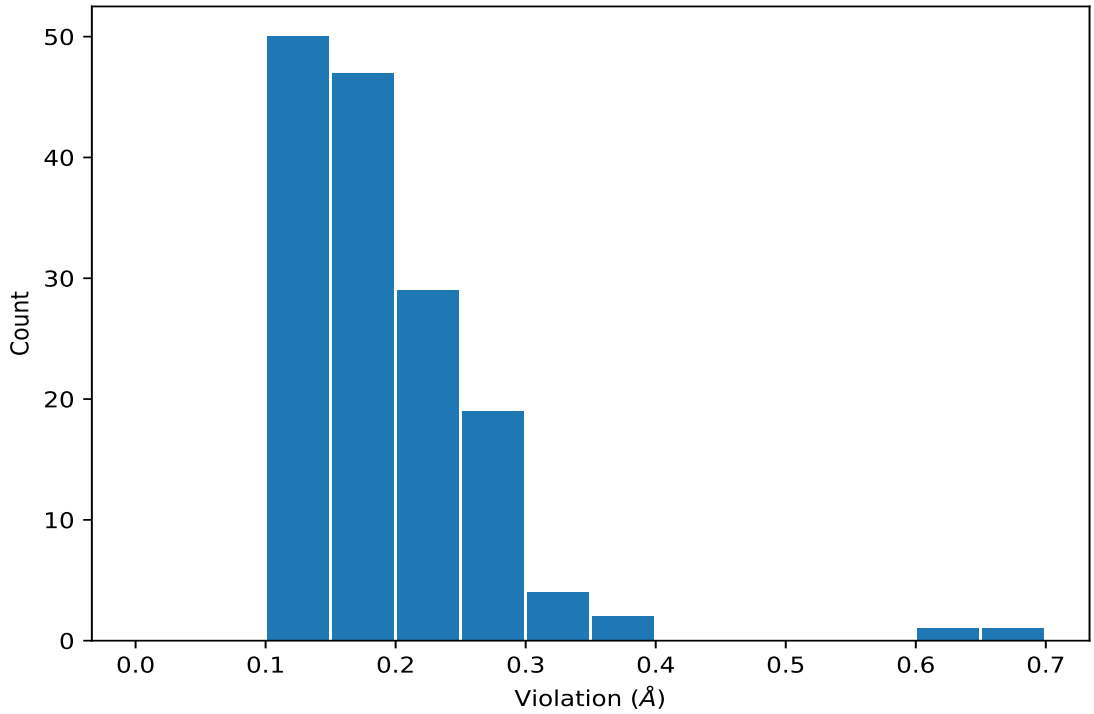
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1127)	1:A:55:ARG:HG3	1:A:56:VAL:H	3	0.12	0.0	0.12
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD11	3	0.11	0.0	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD12	3	0.11	0.0	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD13	3	0.11	0.0	0.11
(1,235)	1:A:18:ARG:HA	1:A:19:VAL:H	2	0.66	0.03	0.66
(1,579)	1:A:53:VAL:HG21	1:A:54:HIS:HD2	2	0.3	0.01	0.3
(1,579)	1:A:53:VAL:HG22	1:A:54:HIS:HD2	2	0.3	0.01	0.3
(1,579)	1:A:53:VAL:HG23	1:A:54:HIS:HD2	2	0.3	0.01	0.3
(1,1242)	1:A:95:ARG:HB2	1:A:96:SER:H	2	0.17	0.0	0.17
(1,1242)	1:A:95:ARG:HB3	1:A:96:SER:H	2	0.17	0.0	0.17
(1,1241)	1:A:95:ARG:H	1:A:95:ARG:HG2	2	0.16	0.01	0.16
(1,1241)	1:A:95:ARG:H	1:A:95:ARG:HG3	2	0.16	0.01	0.16
(1,513)	1:A:64:ARG:H	1:A:65:ASN:HD22	2	0.12	0.01	0.12
(1,817)	1:A:53:VAL:HG11	1:A:54:HIS:H	2	0.12	0.01	0.12
(1,817)	1:A:53:VAL:HG12	1:A:54:HIS:H	2	0.12	0.01	0.12
(1,817)	1:A:53:VAL:HG13	1:A:54:HIS:H	2	0.12	0.01	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)
(1,235)	1:A:18:ARG:HA	1:A:19:VAL:H	18	0.7
(1,235)	1:A:18:ARG:HA	1:A:19:VAL:H	19	0.63
(1,238)	1:A:11:VAL:HB	1:A:12:ILE:H	11	0.37
(1,835)	1:A:20:LYS:HA	1:A:21:GLN:H	12	0.35
(1,579)	1:A:53:VAL:HG21	1:A:54:HIS:HD2	10	0.31
(1,579)	1:A:53:VAL:HG22	1:A:54:HIS:HD2	10	0.31
(1,579)	1:A:53:VAL:HG23	1:A:54:HIS:HD2	10	0.31
(1,238)	1:A:11:VAL:HB	1:A:12:ILE:H	6	0.3
(1,579)	1:A:53:VAL:HG21	1:A:54:HIS:HD2	14	0.29
(1,579)	1:A:53:VAL:HG22	1:A:54:HIS:HD2	14	0.29
(1,579)	1:A:53:VAL:HG23	1:A:54:HIS:HD2	14	0.29
(1,1076)	1:A:37:LEU:HD11	1:A:38:SER:HB2	20	0.29
(1,1076)	1:A:37:LEU:HD11	1:A:38:SER:HB3	20	0.29
(1,1076)	1:A:37:LEU:HD12	1:A:38:SER:HB2	20	0.29
(1,1076)	1:A:37:LEU:HD12	1:A:38:SER:HB3	20	0.29
(1,1076)	1:A:37:LEU:HD13	1:A:38:SER:HB2	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	1:A:37:LEU:HD13	1:A:38:SER:HB3	20	0.29
(1,1076)	1:A:37:LEU:HD21	1:A:38:SER:HB2	20	0.29
(1,1076)	1:A:37:LEU:HD21	1:A:38:SER:HB3	20	0.29
(1,1076)	1:A:37:LEU:HD22	1:A:38:SER:HB2	20	0.29
(1,1076)	1:A:37:LEU:HD22	1:A:38:SER:HB3	20	0.29
(1,1076)	1:A:37:LEU:HD23	1:A:38:SER:HB2	20	0.29
(1,1076)	1:A:37:LEU:HD23	1:A:38:SER:HB3	20	0.29
(1,238)	1:A:11:VAL:HB	1:A:12:ILE:H	2	0.26
(1,238)	1:A:11:VAL:HB	1:A:12:ILE:H	7	0.26
(1,238)	1:A:11:VAL:HB	1:A:12:ILE:H	9	0.26
(1,238)	1:A:11:VAL:HB	1:A:12:ILE:H	15	0.26
(1,1006)	1:A:23:LEU:HD11	1:A:25:GLY:H	16	0.23
(1,1006)	1:A:23:LEU:HD12	1:A:25:GLY:H	16	0.23
(1,1006)	1:A:23:LEU:HD13	1:A:25:GLY:H	16	0.23
(1,1006)	1:A:23:LEU:HD21	1:A:25:GLY:H	16	0.23
(1,1006)	1:A:23:LEU:HD22	1:A:25:GLY:H	16	0.23
(1,1006)	1:A:23:LEU:HD23	1:A:25:GLY:H	16	0.23
(1,1006)	1:A:23:LEU:HD11	1:A:25:GLY:H	13	0.22
(1,1006)	1:A:23:LEU:HD12	1:A:25:GLY:H	13	0.22
(1,1006)	1:A:23:LEU:HD13	1:A:25:GLY:H	13	0.22
(1,1006)	1:A:23:LEU:HD21	1:A:25:GLY:H	13	0.22
(1,1006)	1:A:23:LEU:HD22	1:A:25:GLY:H	13	0.22
(1,1006)	1:A:23:LEU:HD23	1:A:25:GLY:H	13	0.22
(1,1006)	1:A:23:LEU:HD11	1:A:25:GLY:H	17	0.22
(1,1006)	1:A:23:LEU:HD12	1:A:25:GLY:H	17	0.22
(1,1006)	1:A:23:LEU:HD13	1:A:25:GLY:H	17	0.22
(1,1006)	1:A:23:LEU:HD21	1:A:25:GLY:H	17	0.22
(1,1006)	1:A:23:LEU:HD22	1:A:25:GLY:H	17	0.22
(1,1006)	1:A:23:LEU:HD23	1:A:25:GLY:H	17	0.22
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	1	0.21
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	3	0.21
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	4	0.21
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	18	0.21
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	8	0.2
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	9	0.2
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	10	0.2
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	11	0.2
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	12	0.2
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	13	0.2
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	17	0.2
(1,80)	1:A:23:LEU:HD21	1:A:25:GLY:H	16	0.19
(1,80)	1:A:23:LEU:HD22	1:A:25:GLY:H	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:A:23:LEU:HD23	1:A:25:GLY:H	16	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	2	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	5	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	7	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	14	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	15	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	16	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	19	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	20	0.19
(1,426)	1:A:89:ASN:H	1:A:89:ASN:HB3	11	0.19
(1,654)	1:A:69:VAL:HA	1:A:70:VAL:HB	6	0.18
(1,566)	1:A:23:LEU:HD11	1:A:25:GLY:H	13	0.18
(1,566)	1:A:23:LEU:HD12	1:A:25:GLY:H	13	0.18
(1,566)	1:A:23:LEU:HD13	1:A:25:GLY:H	13	0.18
(1,566)	1:A:23:LEU:HD11	1:A:25:GLY:H	17	0.18
(1,566)	1:A:23:LEU:HD12	1:A:25:GLY:H	17	0.18
(1,566)	1:A:23:LEU:HD13	1:A:25:GLY:H	17	0.18
(1,80)	1:A:23:LEU:HD21	1:A:25:GLY:H	13	0.17
(1,80)	1:A:23:LEU:HD22	1:A:25:GLY:H	13	0.17
(1,80)	1:A:23:LEU:HD23	1:A:25:GLY:H	13	0.17
(1,80)	1:A:23:LEU:HD21	1:A:25:GLY:H	17	0.17
(1,80)	1:A:23:LEU:HD22	1:A:25:GLY:H	17	0.17
(1,80)	1:A:23:LEU:HD23	1:A:25:GLY:H	17	0.17
(1,566)	1:A:23:LEU:HD11	1:A:25:GLY:H	16	0.17
(1,566)	1:A:23:LEU:HD12	1:A:25:GLY:H	16	0.17
(1,566)	1:A:23:LEU:HD13	1:A:25:GLY:H	16	0.17
(1,1242)	1:A:95:ARG:HB2	1:A:96:SER:H	14	0.17
(1,1242)	1:A:95:ARG:HB3	1:A:96:SER:H	14	0.17
(1,1242)	1:A:95:ARG:HB2	1:A:96:SER:H	17	0.17
(1,1242)	1:A:95:ARG:HB3	1:A:96:SER:H	17	0.17
(2,29)	1:A:77:ILE:H	1:A:97:LEU:O	12	0.16
(1,1241)	1:A:95:ARG:H	1:A:95:ARG:HG2	16	0.16
(1,1241)	1:A:95:ARG:H	1:A:95:ARG:HG3	16	0.16
(1,586)	1:A:16:GLU:H	1:A:17:THR:HG21	15	0.15
(1,586)	1:A:16:GLU:H	1:A:17:THR:HG22	15	0.15
(1,586)	1:A:16:GLU:H	1:A:17:THR:HG23	15	0.15
(1,577)	1:A:23:LEU:HB3	1:A:54:HIS:HD2	10	0.15
(1,1241)	1:A:95:ARG:H	1:A:95:ARG:HG2	15	0.15
(1,1241)	1:A:95:ARG:H	1:A:95:ARG:HG3	15	0.15
(1,1015)	1:A:23:LEU:HD11	1:A:53:VAL:H	14	0.15
(1,1015)	1:A:23:LEU:HD12	1:A:53:VAL:H	14	0.15
(1,1015)	1:A:23:LEU:HD13	1:A:53:VAL:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:A:23:LEU:HD21	1:A:53:VAL:H	14	0.15
(1,1015)	1:A:23:LEU:HD22	1:A:53:VAL:H	14	0.15
(1,1015)	1:A:23:LEU:HD23	1:A:53:VAL:H	14	0.15
(1,411)	1:A:15:ASP:HA	1:A:18:ARG:H	20	0.14
(1,24)	1:A:54:HIS:H	1:A:54:HIS:HE1	14	0.14
(1,817)	1:A:53:VAL:HG11	1:A:54:HIS:H	9	0.13
(1,817)	1:A:53:VAL:HG12	1:A:54:HIS:H	9	0.13
(1,817)	1:A:53:VAL:HG13	1:A:54:HIS:H	9	0.13
(1,682)	1:A:73:SER:HB2	1:A:74:GLU:H	9	0.13
(1,682)	1:A:73:SER:HB2	1:A:74:GLU:H	13	0.13
(1,682)	1:A:73:SER:HB2	1:A:74:GLU:H	15	0.13
(1,682)	1:A:73:SER:HB2	1:A:74:GLU:H	20	0.13
(1,513)	1:A:64:ARG:H	1:A:65:ASN:HD22	11	0.13
(1,682)	1:A:73:SER:HB2	1:A:74:GLU:H	5	0.12
(1,408)	1:A:54:HIS:HD2	1:A:55:ARG:H	14	0.12
(1,134)	1:A:50:ALA:HB1	1:A:52:GLY:H	14	0.12
(1,134)	1:A:50:ALA:HB2	1:A:52:GLY:H	14	0.12
(1,134)	1:A:50:ALA:HB3	1:A:52:GLY:H	14	0.12
(1,1127)	1:A:55:ARG:HG2	1:A:56:VAL:H	8	0.12
(1,1127)	1:A:55:ARG:HG3	1:A:56:VAL:H	8	0.12
(1,1127)	1:A:55:ARG:HG2	1:A:56:VAL:H	17	0.12
(1,1127)	1:A:55:ARG:HG3	1:A:56:VAL:H	17	0.12
(1,1018)	1:A:23:LEU:HD11	1:A:54:HIS:HD2	14	0.12
(1,1018)	1:A:23:LEU:HD12	1:A:54:HIS:HD2	14	0.12
(1,1018)	1:A:23:LEU:HD13	1:A:54:HIS:HD2	14	0.12
(1,1018)	1:A:23:LEU:HD21	1:A:54:HIS:HD2	14	0.12
(1,1018)	1:A:23:LEU:HD22	1:A:54:HIS:HD2	14	0.12
(1,1018)	1:A:23:LEU:HD23	1:A:54:HIS:HD2	14	0.12
(2,21)	1:A:71:GLY:O	1:A:78:ASP:H	12	0.11
(1,982)	1:A:19:VAL:HG11	1:A:20:LYS:H	15	0.11
(1,982)	1:A:19:VAL:HG12	1:A:20:LYS:H	15	0.11
(1,982)	1:A:19:VAL:HG13	1:A:20:LYS:H	15	0.11
(1,982)	1:A:19:VAL:HG21	1:A:20:LYS:H	15	0.11
(1,982)	1:A:19:VAL:HG22	1:A:20:LYS:H	15	0.11
(1,982)	1:A:19:VAL:HG23	1:A:20:LYS:H	15	0.11
(1,976)	1:A:18:ARG:HG2	1:A:19:VAL:H	19	0.11
(1,976)	1:A:18:ARG:HG3	1:A:19:VAL:H	19	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD11	3	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD12	3	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD13	3	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD11	6	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD12	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD13	6	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD11	12	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD12	12	0.11
(1,845)	1:A:68:LYS:H	1:A:80:ILE:HD13	12	0.11
(1,817)	1:A:53:VAL:HG11	1:A:54:HIS:H	14	0.11
(1,817)	1:A:53:VAL:HG12	1:A:54:HIS:H	14	0.11
(1,817)	1:A:53:VAL:HG13	1:A:54:HIS:H	14	0.11
(1,725)	1:A:47:VAL:HB	1:A:54:HIS:HB2	14	0.11
(1,513)	1:A:64:ARG:H	1:A:65:ASN:HD22	4	0.11
(1,1127)	1:A:55:ARG:HG2	1:A:56:VAL:H	13	0.11
(1,1127)	1:A:55:ARG:HG3	1:A:56:VAL:H	13	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