Full wwPDB NMR Structure Validation Report

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PDB ID	:	2L50
BMRB ID	:	17261
Title	:	Solution structure of apo S100A16
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Deposited on	:	2010-10-22

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 ⓘ 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 ⓘ) were used in the production of this report:

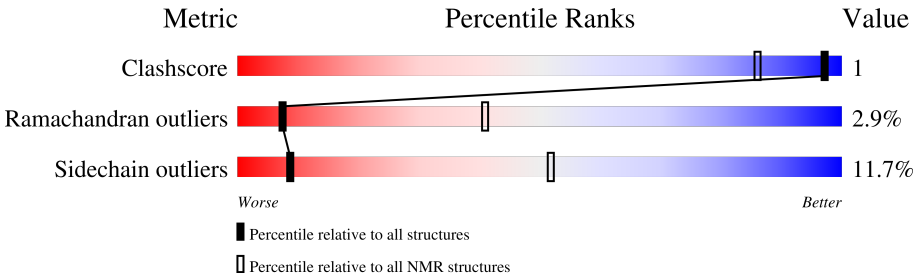
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 68%.

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	102	76% 8% 16%
1	B	102	76% 9% 15%

2 Ensemble composition and analysis

This entry contains 30 models. Model 2 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:5-A:23, A:33-A:99, B:108-B:126, B:136-B:203 (173)	1.07	2

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

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

The models can be grouped into 3 clusters and 7 single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 8, 9, 11, 13, 15, 18, 20, 21, 24, 25, 27, 28
2	2, 6, 10, 16, 19, 26
3	17, 22
Single-model clusters	4; 7; 12; 14; 23; 29; 30

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3278 atoms, of which 1636 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A16.

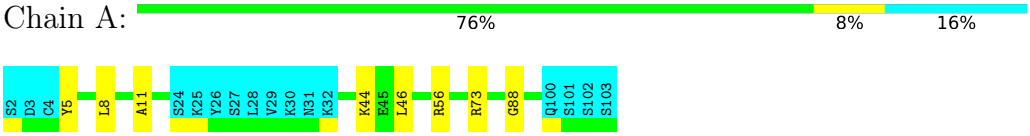
Mol	Chain	Residues	Atoms						Trace
1	A	102	Total	C	H	N	O	S	0
			1639	517	818	139	162	3	
1	B	102	Total	C	H	N	O	S	0
			1639	517	818	139	162	3	

4 Residue-property plots

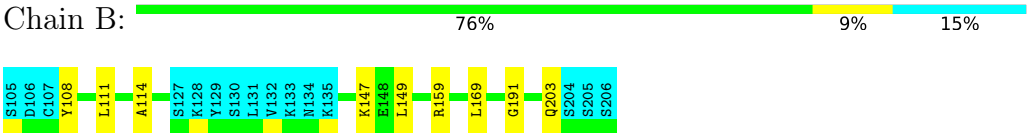
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Protein S100-A16



• Molecule 1: Protein S100-A16

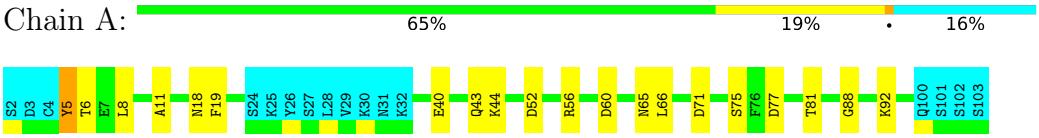


4.2 Scores per residue for each member of the ensemble

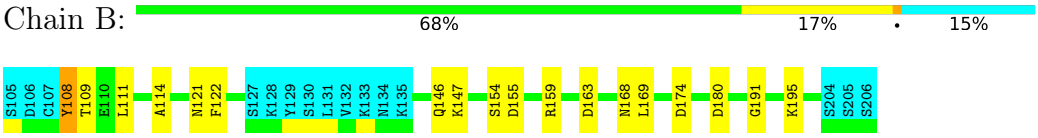
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Protein S100-A16



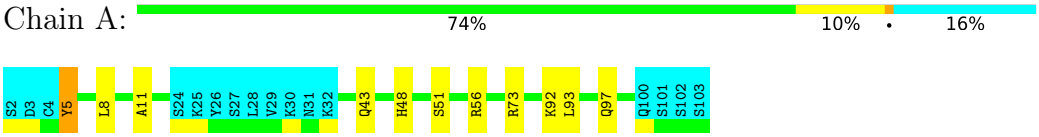
• Molecule 1: Protein S100-A16



4.2.2 Score per residue for model 2 (medoid)

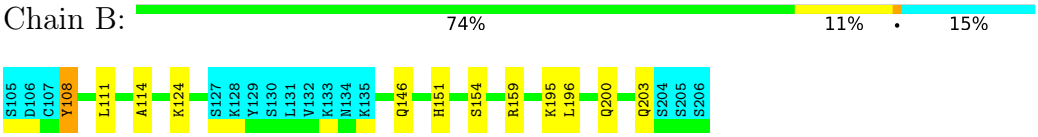
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

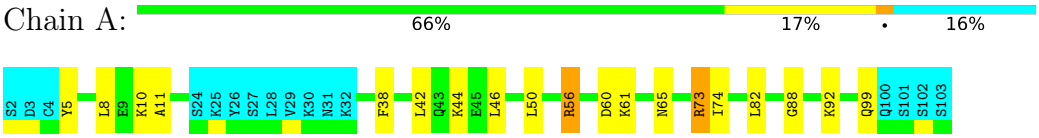
Chain B:



4.2.3 Score per residue for model 3

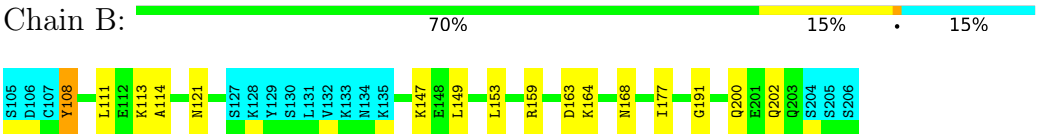
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

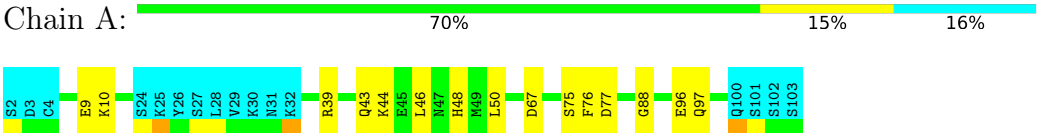
Chain B:



4.2.4 Score per residue for model 4

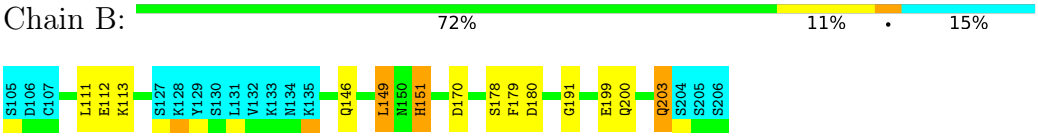
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

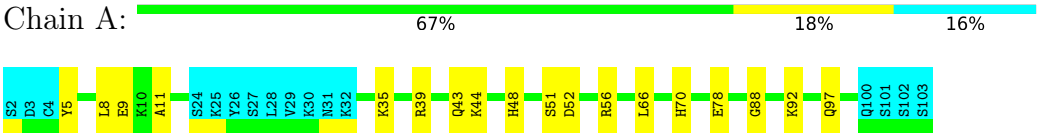
Chain B:



4.2.5 Score per residue for model 5

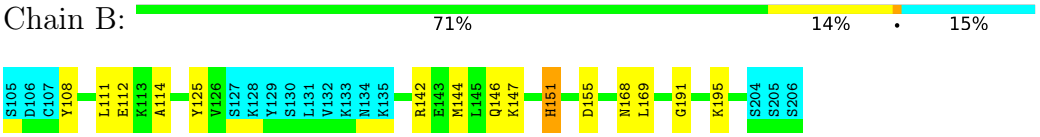
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

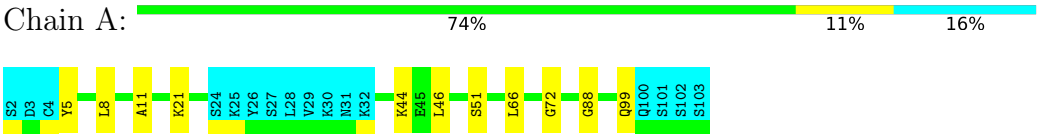
Chain B:



4.2.6 Score per residue for model 6

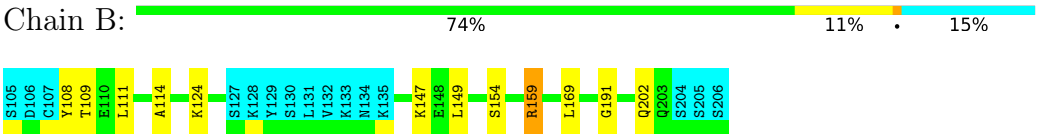
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

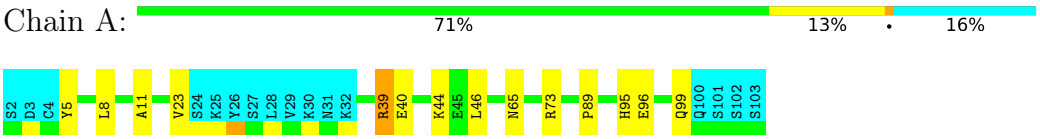
Chain B:



4.2.7 Score per residue for model 7

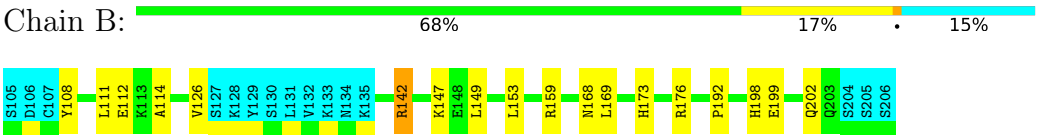
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

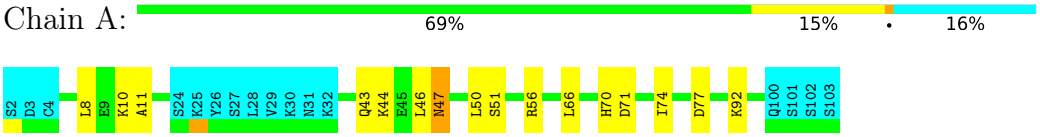
Chain B:



4.2.8 Score per residue for model 8

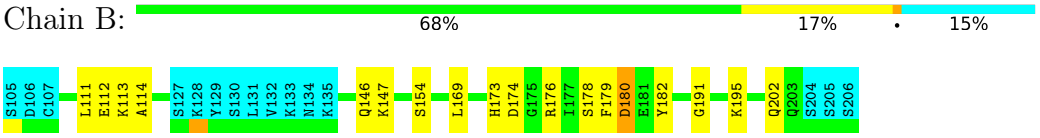
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

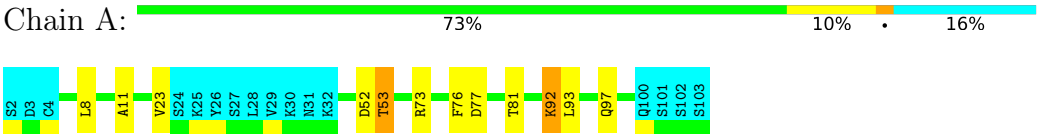
Chain B:



4.2.9 Score per residue for model 9

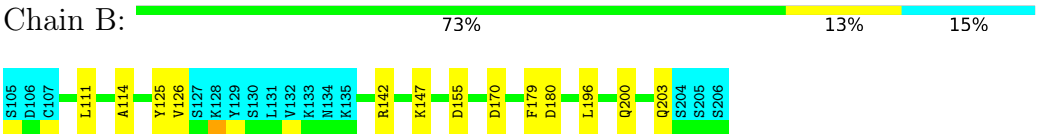
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

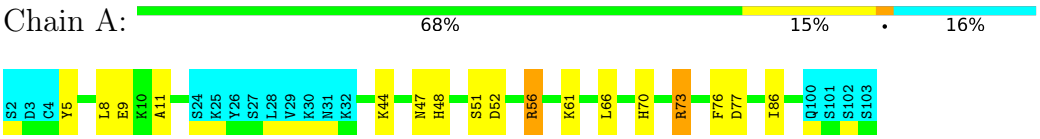
Chain B:



4.2.10 Score per residue for model 10

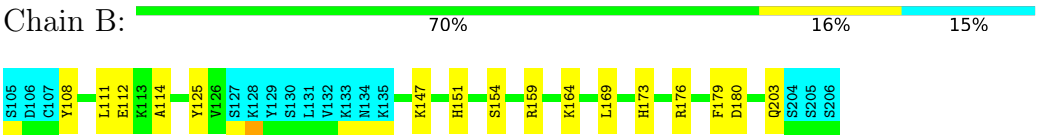
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

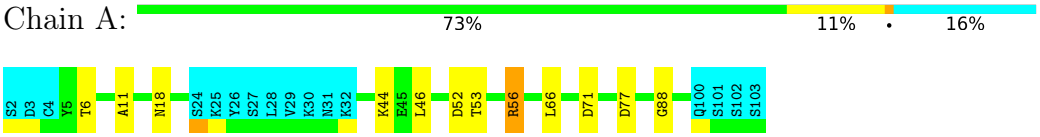
Chain B:



4.2.11 Score per residue for model 11

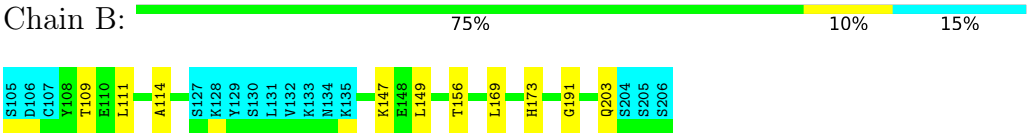
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

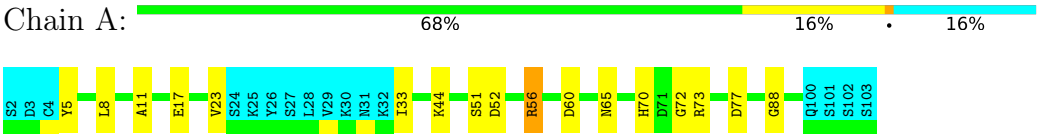
Chain B:



4.2.12 Score per residue for model 12

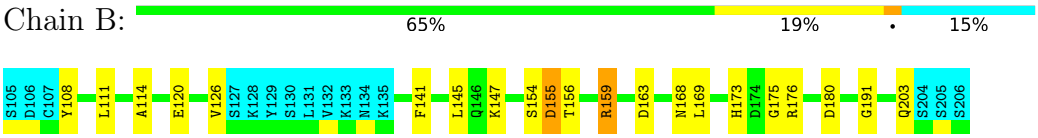
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

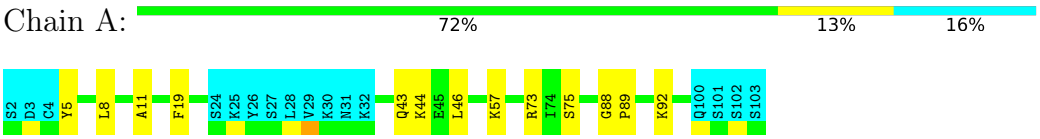
Chain B:



4.2.13 Score per residue for model 13

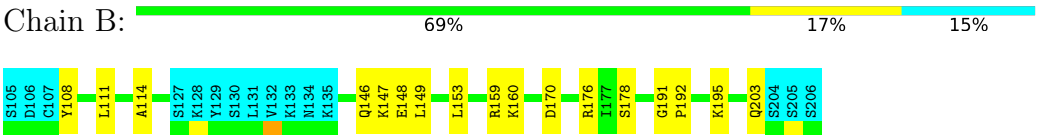
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

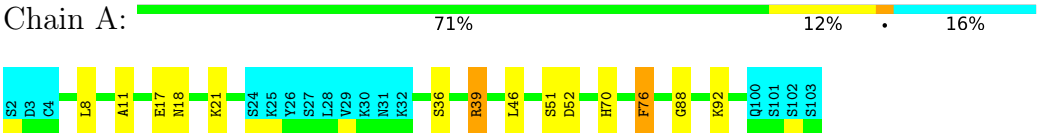
Chain B:



4.2.14 Score per residue for model 14

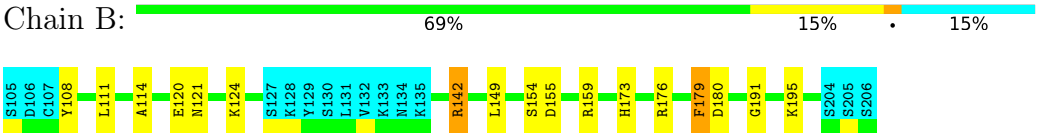
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

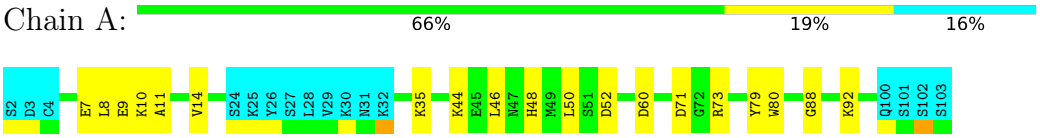
Chain B:



4.2.15 Score per residue for model 15

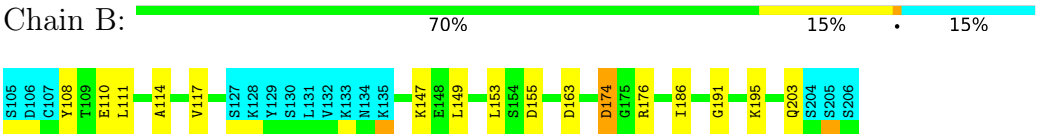
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

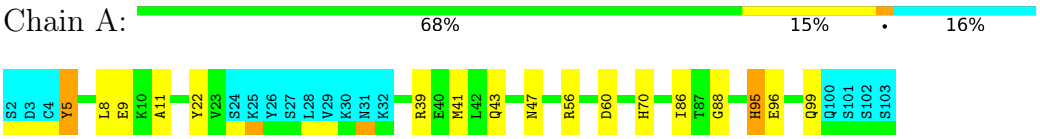
Chain B:



4.2.16 Score per residue for model 16

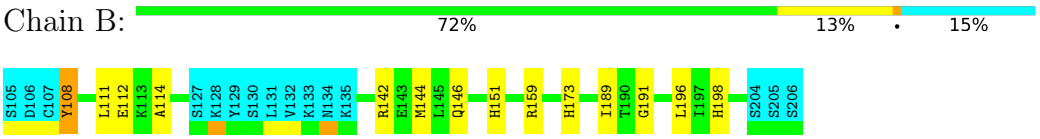
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

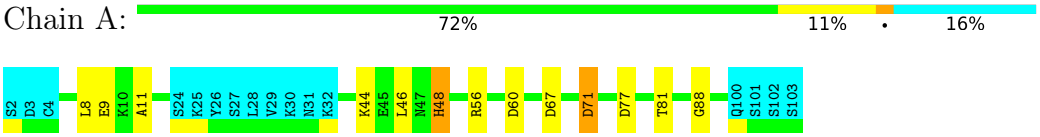
Chain B:



4.2.17 Score per residue for model 17

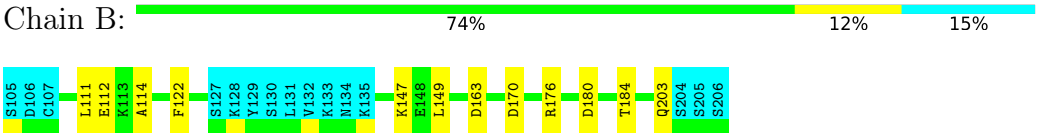
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

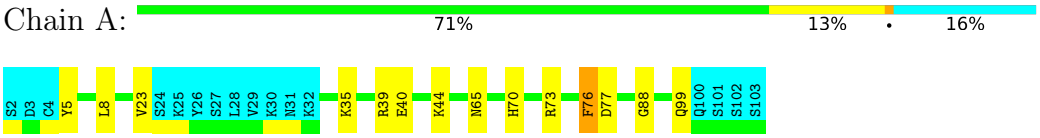
Chain B:



4.2.18 Score per residue for model 18

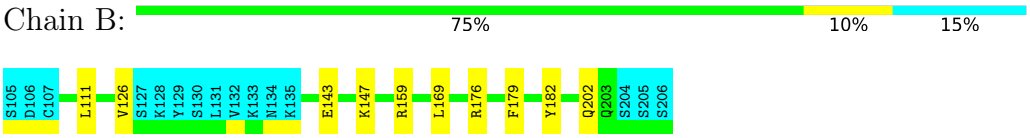
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

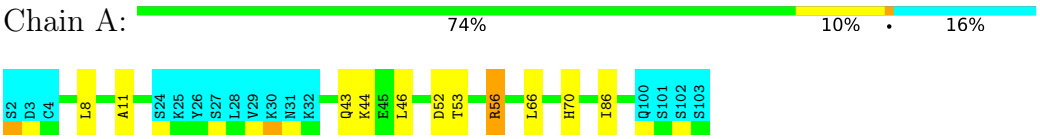
Chain B:



4.2.19 Score per residue for model 19

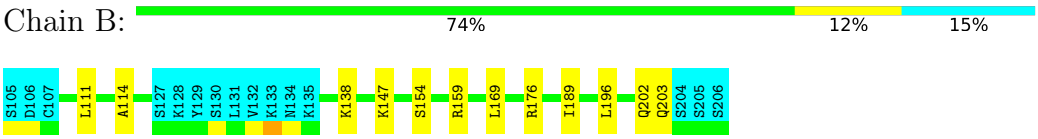
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

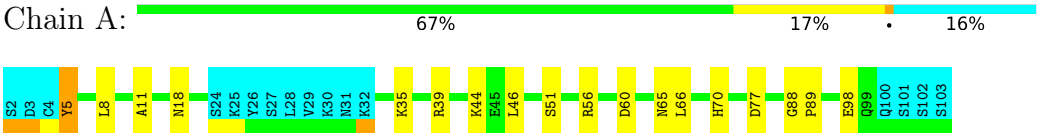
Chain B:



4.2.20 Score per residue for model 20

• Molecule 1: Protein S100-A16

Chain A:



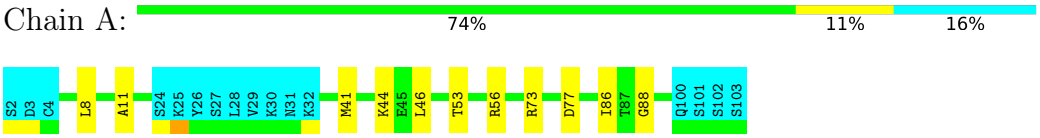
• Molecule 1: Protein S100-A16

Chain B:

4.2.21 Score per residue for model 21

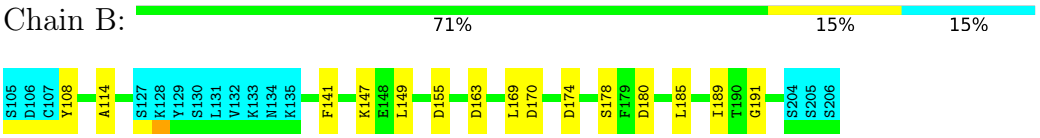
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

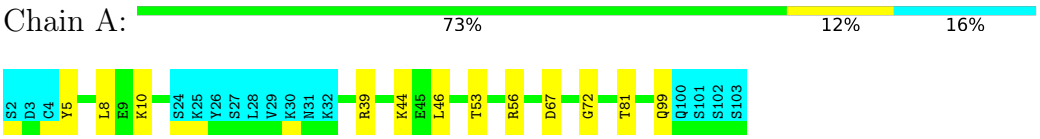
Chain B:



4.2.22 Score per residue for model 22

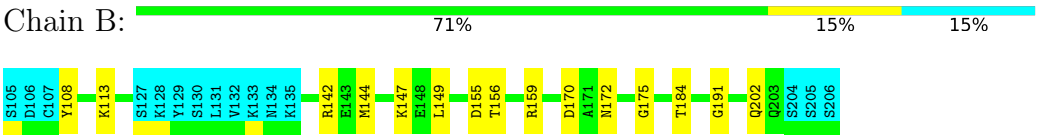
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

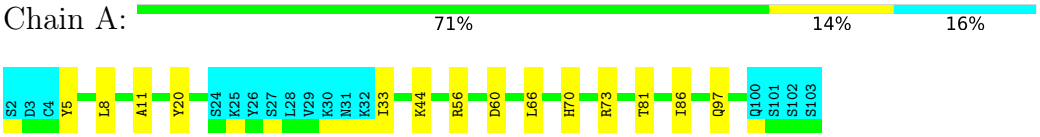
Chain B:



4.2.23 Score per residue for model 23

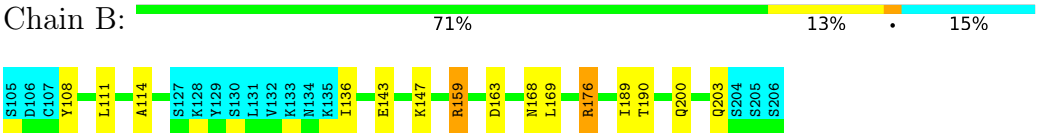
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

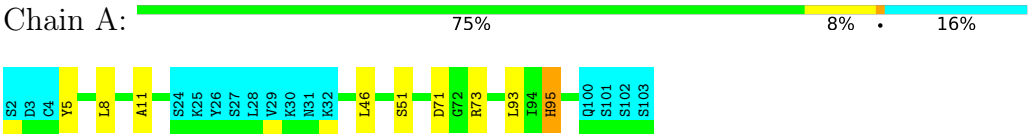
Chain B:



4.2.24 Score per residue for model 24

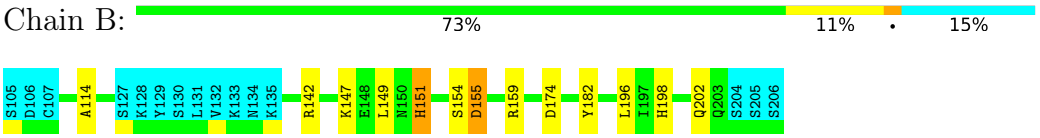
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

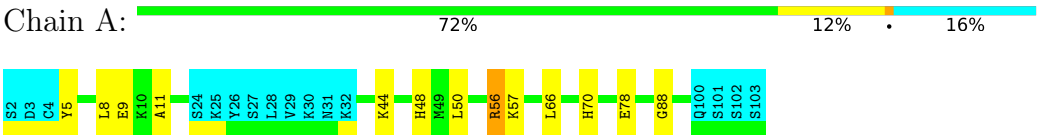
Chain B:



4.2.25 Score per residue for model 25

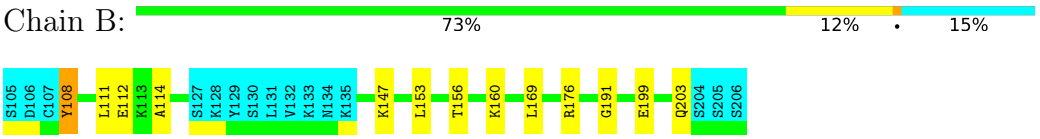
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

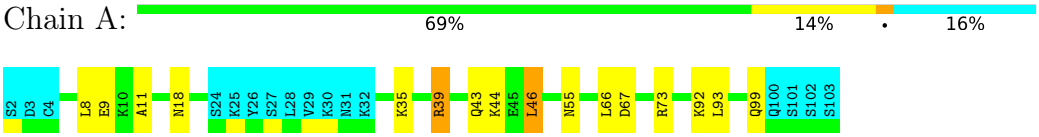
Chain B:



4.2.26 Score per residue for model 26

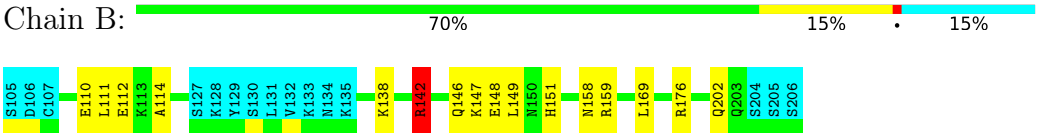
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

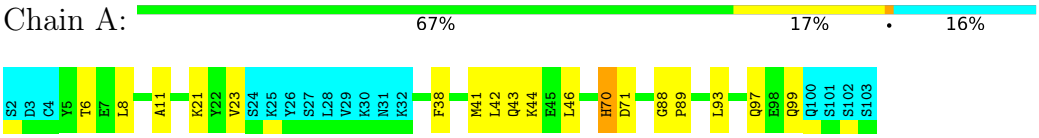
Chain B:



4.2.27 Score per residue for model 27

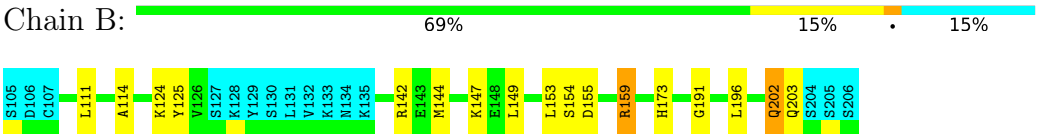
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

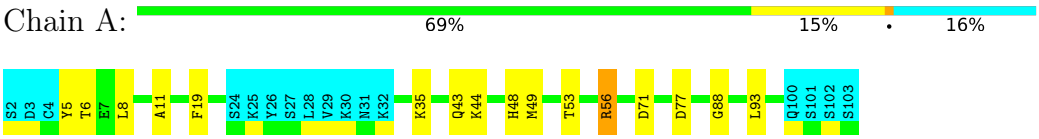
Chain B:



4.2.28 Score per residue for model 28

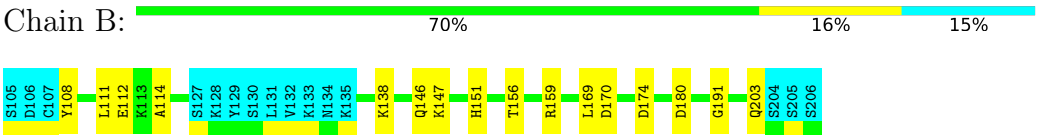
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

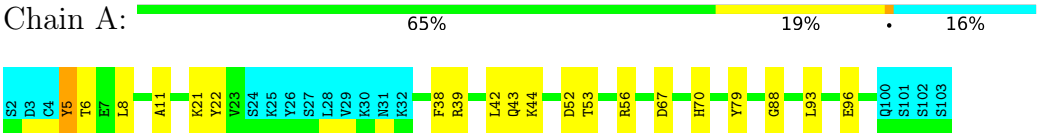
Chain B:



4.2.29 Score per residue for model 29

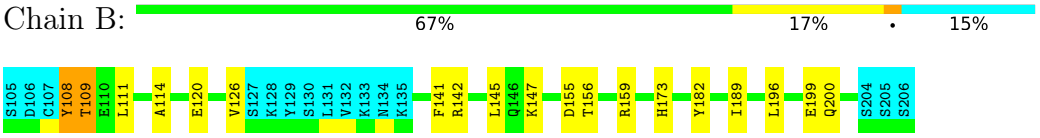
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

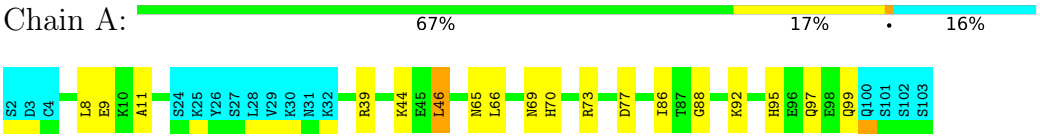
Chain B:



4.2.30 Score per residue for model 30

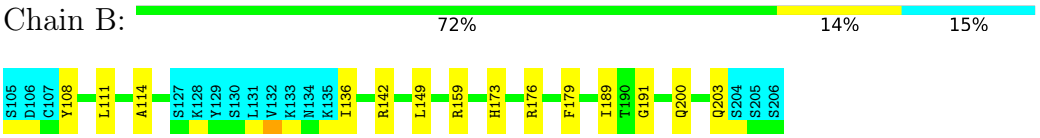
• Molecule 1: Protein S100-A16

Chain A:



• Molecule 1: Protein S100-A16

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 350 calculated structures, 30 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Amber	structure solution	10.0
CYANA	structure solution	2.1
ProcheckNMR	structure solution	
TALOS	structure solution	
WHAT IF	structure solution	
WHAT IF	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	1904
Number of shifts mapped to atoms	1904
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.01	0±0/712 (0.0± 0.0%)	1.08±0.04	2±1/960 (0.2± 0.1%)
1	B	0.67±0.01	0±0/721 (0.0± 0.0%)	1.08±0.03	2±1/972 (0.2± 0.1%)
All	All	0.67	0/42990 (0.0%)	1.08	105/57960 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.3±1.2
1	B	0.0±0.0	1.5±1.3
All	All	0	84

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	73	ARG	NE-CZ-NH1	11.95	126.28	120.30	3	8
1	A	39	ARG	NE-CZ-NH2	-8.96	115.82	120.30	7	3
1	B	142	ARG	NE-CZ-NH2	-8.60	116.00	120.30	7	6
1	A	39	ARG	NE-CZ-NH1	8.53	124.57	120.30	7	7
1	A	56	ARG	NE-CZ-NH1	8.33	124.47	120.30	21	14
1	B	159	ARG	NE-CZ-NH2	-7.13	116.73	120.30	12	6
1	B	159	ARG	NE-CZ-NH1	7.05	123.83	120.30	30	14
1	A	56	ARG	NE-CZ-NH2	-7.04	116.78	120.30	12	4
1	A	73	ARG	NE-CZ-NH2	-7.00	116.80	120.30	23	3
1	B	142	ARG	NE-CZ-NH1	6.83	123.72	120.30	7	7
1	B	176	ARG	NE-CZ-NH1	6.71	123.66	120.30	7	8
1	B	108	TYR	CB-CG-CD2	-6.34	117.19	121.00	25	3
1	B	122	PHE	CB-CG-CD2	-6.12	116.52	120.80	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	19	PHE	CB-CG-CD2	-6.01	116.59	120.80	1	3
1	A	73	ARG	CD-NE-CZ	5.99	131.99	123.60	3	1
1	A	76	PHE	CB-CG-CD1	-5.58	116.89	120.80	14	2
1	B	199	GLU	CB-CA-C	5.56	121.52	110.40	29	2
1	A	96	GLU	CB-CA-C	5.53	121.46	110.40	29	2
1	B	179	PHE	CB-CG-CD1	-5.48	116.97	120.80	14	1
1	A	20	TYR	CB-CG-CD2	-5.37	117.78	121.00	23	1
1	A	5	TYR	CB-CG-CD2	-5.21	117.88	121.00	16	2
1	B	125	TYR	CB-CG-CD2	-5.21	117.88	121.00	27	2
1	B	113	LYS	N-CA-CB	-5.04	101.52	110.60	20	1
1	A	39	ARG	CD-NE-CZ	5.03	130.64	123.60	18	1
1	B	202	GLN	C-N-CA	5.02	134.25	121.70	27	1
1	A	92	LYS	CA-CB-CG	5.00	124.40	113.40	9	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	179	PHE	Sidechain,Peptide	8
1	B	159	ARG	Sidechain	7
1	A	56	ARG	Sidechain	6
1	A	73	ARG	Peptide,Sidechain	5
1	A	76	PHE	Sidechain	5
1	B	176	ARG	Sidechain	5
1	B	108	TYR	Sidechain	4
1	A	72	GLY	Peptide	3
1	A	39	ARG	Sidechain	3
1	A	95	HIS	Sidechain	3
1	B	142	ARG	Sidechain	3
1	B	155	ASP	Peptide	3
1	B	154	SER	Peptide	3
1	B	182	TYR	Sidechain	3
1	A	5	TYR	Sidechain	2
1	B	198	HIS	Sidechain	2
1	A	51	SER	Peptide	2
1	B	175	GLY	Peptide	2
1	A	79	TYR	Sidechain	2
1	A	70	HIS	Peptide,Sidechain	2
1	A	46	LEU	Peptide	2
1	B	173	HIS	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	52	ASP	Peptide	1
1	B	125	TYR	Sidechain	1
1	A	33	ILE	Peptide	1
1	B	174	ASP	Peptide	1
1	A	22	TYR	Sidechain	1
1	A	98	GLU	Peptide	1
1	B	151	HIS	Sidechain	1
1	B	109	THR	Peptide	1

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	699	695	695	2±1
1	B	708	703	703	2±1
All	All	42210	41940	41940	54

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ALA:HB1	1:B:114:ALA:HB1	0.72	1.61	12	27
1:A:11:ALA:HB1	1:B:114:ALA:CB	0.50	2.36	15	3
1:A:11:ALA:CB	1:B:114:ALA:HB1	0.47	2.38	12	3
1:A:21:LYS:HE3	1:A:22:TYR:CE1	0.47	2.44	29	1
1:B:155:ASP:CG	1:B:156:THR:H	0.47	2.14	29	1
1:A:52:ASP:CG	1:A:53:THR:H	0.45	2.15	29	1
1:B:151:HIS:H	1:B:151:HIS:CD2	0.45	2.28	5	2
1:A:14:VAL:HG21	1:B:110:GLU:HG2	0.45	1.88	15	1
1:A:7:GLU:HG2	1:B:117:VAL:HG21	0.43	1.90	15	1
1:A:38:PHE:CZ	1:A:42:LEU:HD11	0.43	2.48	3	2
1:B:141:PHE:CE2	1:B:145:LEU:HD11	0.43	2.49	20	2
1:B:141:PHE:CZ	1:B:185:LEU:HB3	0.43	2.48	21	1
1:A:35:LYS:HE2	1:A:78:GLU:OE2	0.42	2.15	5	1
1:B:125:TYR:CE2	1:B:144:MET:HG3	0.42	2.49	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:PHE:CE2	1:A:42:LEU:HD11	0.42	2.49	29	1
1:B:141:PHE:CE1	1:B:145:LEU:HD11	0.42	2.49	12	1
1:A:48:HIS:CD2	1:B:108:TYR:HA	0.41	2.50	15	1
1:A:80:TRP:CZ2	1:B:186:ILE:HG21	0.41	2.50	15	1
1:A:48:HIS:CD2	1:A:48:HIS:H	0.41	2.33	17	1
1:A:38:PHE:CZ	1:A:82:LEU:HB3	0.40	2.51	3	1
1:A:52:ASP:CG	1:A:53:THR:N	0.40	2.75	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	86/102 (84%)	76±2 (88±3%)	8±2 (9±3%)	2±1 (3±1%)	8	42
1	B	87/102 (85%)	75±3 (87±3%)	9±3 (10±3%)	3±1 (3±1%)	7	40
All	All	5190/6120 (85%)	4530 (87%)	509 (10%)	151 (3%)	7	41

All 33 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	88	GLY	20
1	B	191	GLY	19
1	B	108	TYR	15
1	A	5	TYR	14
1	B	203	GLN	9
1	B	155	ASP	7
1	A	52	ASP	6
1	B	154	SER	6
1	A	23	VAL	5
1	B	126	VAL	5
1	A	71	ASP	5
1	A	51	SER	4
1	A	89	PRO	4
1	B	192	PRO	3

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Mol	Chain	Res	Type	Models (Total)
1	A	47	ASN	3
1	B	174	ASP	3
1	A	53	THR	3
1	A	50	LEU	2
1	B	178	SER	2
1	B	156	THR	2
1	B	136	ILE	2
1	B	149	LEU	1
1	B	180	ASP	1
1	A	75	SER	1
1	A	35	LYS	1
1	B	172	ASN	1
1	A	33	ILE	1
1	B	153	LEU	1
1	A	70	HIS	1
1	B	173	HIS	1
1	A	49	MET	1
1	A	6	THR	1
1	B	109	THR	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	76/92 (83%)	67±2 (88±3%)	9±2 (12±3%)	8	51
1	B	77/92 (84%)	68±2 (89±3%)	9±2 (11±3%)	9	52
All	All	4590/5520 (83%)	4053 (88%)	537 (12%)	9	52

All 93 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	8	LEU	28
1	B	111	LEU	27
1	A	44	LYS	25
1	B	147	LYS	25
1	A	46	LEU	18

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Mol	Chain	Res	Type	Models (Total)
1	B	169	LEU	16
1	B	149	LEU	16
1	A	77	ASP	13
1	A	43	GLN	12
1	A	66	LEU	12
1	A	70	HIS	12
1	A	92	LYS	11
1	B	180	ASP	11
1	B	202	GLN	11
1	B	112	GLU	10
1	B	146	GLN	9
1	A	99	GLN	9
1	A	9	GLU	9
1	B	173	HIS	9
1	A	60	ASP	8
1	B	151	HIS	8
1	A	65	ASN	7
1	B	163	ASP	7
1	B	195	LYS	7
1	A	48	HIS	7
1	A	93	LEU	7
1	A	97	GLN	7
1	B	196	LEU	7
1	B	200	GLN	7
1	B	203	GLN	7
1	B	170	ASP	7
1	B	168	ASN	6
1	A	86	ILE	6
1	B	189	ILE	6
1	A	18	ASN	5
1	A	81	THR	5
1	A	10	LYS	5
1	B	153	LEU	5
1	A	67	ASP	5
1	A	5	TYR	4
1	A	6	THR	4
1	A	71	ASP	4
1	B	121	ASN	4
1	B	124	LYS	4
1	A	56	ARG	4
1	B	113	LYS	4
1	A	35	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	B	138	LYS	4
1	A	40	GLU	3
1	B	108	TYR	3
1	B	109	THR	3
1	B	174	ASP	3
1	A	50	LEU	3
1	A	51	SER	3
1	A	21	LYS	3
1	A	53	THR	3
1	B	120	GLU	3
1	B	156	THR	3
1	A	41	MET	3
1	A	95	HIS	3
1	B	144	MET	3
1	A	75	SER	2
1	A	61	LYS	2
1	A	73	ARG	2
1	A	74	ILE	2
1	B	164	LYS	2
1	B	178	SER	2
1	A	96	GLU	2
1	B	199	GLU	2
1	B	154	SER	2
1	A	17	GLU	2
1	B	155	ASP	2
1	B	176	ARG	2
1	A	57	LYS	2
1	B	148	GLU	2
1	B	160	LYS	2
1	B	184	THR	2
1	B	143	GLU	2
1	B	159	ARG	2
1	B	177	ILE	1
1	A	47	ASN	1
1	B	182	TYR	1
1	A	36	SER	1
1	A	52	ASP	1
1	A	39	ARG	1
1	B	190	THR	1
1	B	198	HIS	1
1	A	78	GLU	1
1	A	55	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	B	110	GLU	1
1	B	142	ARG	1
1	B	158	ASN	1
1	A	69	ASN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 68% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1904
Number of shifts mapped to atoms	1904
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	200	1.99 ± 0.05	Should be checked
$^{13}C_{\beta}$	190	2.92 ± 0.05	Should be checked
$^{13}C'$	194	2.22 ± 0.15	Should be applied
^{15}N	194	0.24 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 68%, i.e. 1661 atoms were assigned a chemical shift out of a possible 2435. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	853/871 (98%)	346/354 (98%)	338/346 (98%)	169/171 (99%)
Sidechain	806/1366 (59%)	426/884 (48%)	378/431 (88%)	2/51 (4%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/198 (1%)	2/98 (2%)	0/92 (0%)	0/8 (0%)
Overall	1661/2435 (68%)	774/1336 (58%)	716/869 (82%)	171/230 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 1900 atoms were assigned a chemical shift out of a possible 2812. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	988/1026 (96%)	400/416 (96%)	394/408 (97%)	194/202 (96%)
Sidechain	910/1570 (58%)	478/1014 (47%)	430/496 (87%)	2/60 (3%)
Aromatic	2/216 (1%)	2/106 (2%)	0/102 (0%)	0/8 (0%)
Overall	1900/2812 (68%)	880/1536 (57%)	824/1006 (82%)	196/270 (73%)

7.1.4 Statistically unusual chemical shifts (i)

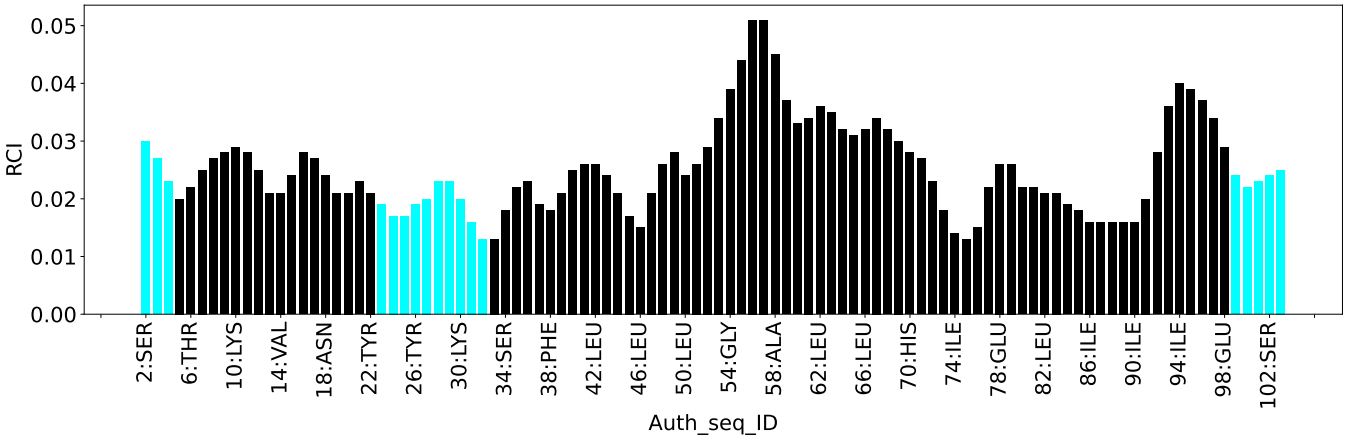
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	6	THR	HG1	6.12	0.08 – 2.19	23.6
1	B	109	THR	HG1	6.12	0.08 – 2.19	23.6
1	A	87	THR	HG1	2.74	0.08 – 2.19	7.6
1	B	190	THR	HG1	2.74	0.08 – 2.19	7.6
1	A	84	GLY	HA3	1.68	2.08 – 5.71	-6.1
1	B	187	GLY	HA3	1.68	2.08 – 5.71	-6.1

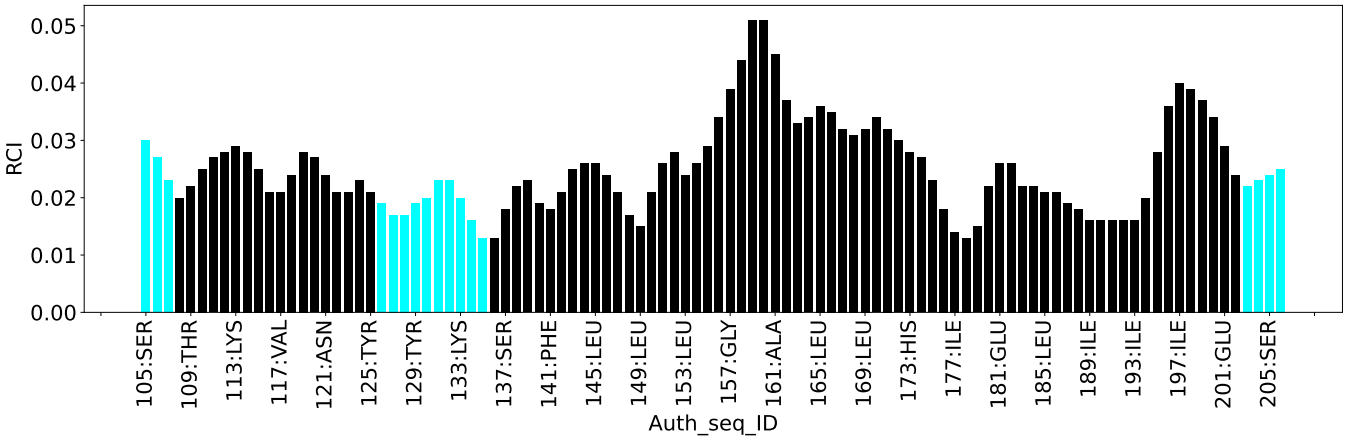
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2420
Intra-residue (|i-j|=0)	977
Sequential (|i-j|=1)	558
Medium range (|i-j|>1 and |i-j|<5)	448
Long range (|i-j|≥5)	268
Inter-chain	169
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	1.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.6	0.19
0.2-0.5 (Medium)	0.0	0.22
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

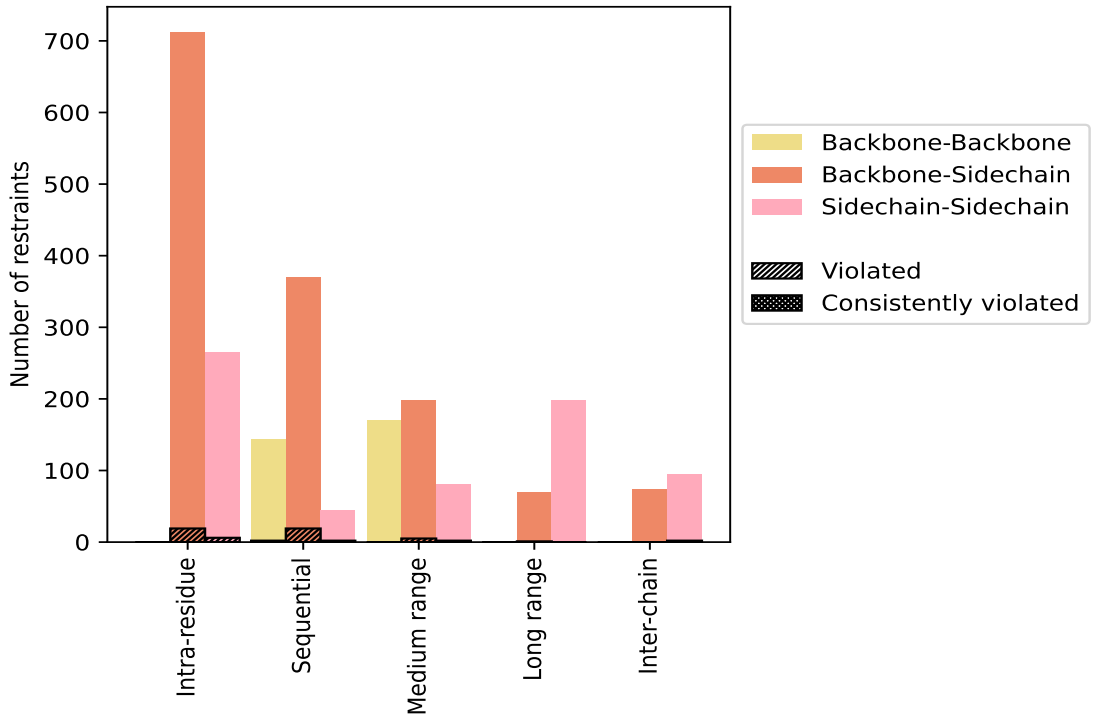
9.1 Summary of distance violations (i)

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)	977	40.4	25	2.6	1.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	712	29.4	19	2.7	0.8	0	0.0	0.0
Sidechain-Sidechain	265	11.0	6	2.3	0.2	0	0.0	0.0
Sequential (|i-j|=1)	558	23.1	23	4.1	1.0	0	0.0	0.0
Backbone-Backbone	144	6.0	2	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	370	15.3	19	5.1	0.8	0	0.0	0.0
Sidechain-Sidechain	44	1.8	2	4.5	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	448	18.5	7	1.6	0.3	0	0.0	0.0
Backbone-Backbone	170	7.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	198	8.2	5	2.5	0.2	0	0.0	0.0
Sidechain-Sidechain	80	3.3	2	2.5	0.1	0	0.0	0.0
Long range (|i-j|≥5)	268	11.1	1	0.4	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	70	2.9	1	1.4	0.0	0	0.0	0.0
Sidechain-Sidechain	198	8.2	0	0.0	0.0	0	0.0	0.0
Inter-chain	169	7.0	2	1.2	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	74	3.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	95	3.9	2	2.1	0.1	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	2420	100.0	58	2.4	2.4	0	0.0	0.0
Backbone-Backbone	314	13.0	2	0.6	0.1	0	0.0	0.0
Backbone-Sidechain	1424	58.8	44	3.1	1.8	0	0.0	0.0
Sidechain-Sidechain	682	28.2	12	1.8	0.5	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	0	0	0	0	2	0.15	0.15	0.0	0.15
2	2	6	0	0	0	8	0.13	0.15	0.02	0.13
3	3	1	1	0	1	6	0.12	0.14	0.01	0.12
4	2	3	0	0	0	5	0.16	0.17	0.02	0.16
5	2	5	0	0	1	8	0.13	0.18	0.02	0.14
6	1	1	0	0	0	2	0.15	0.15	0.0	0.15
7	2	3	1	0	0	6	0.12	0.15	0.02	0.12
8	1	2	0	0	0	3	0.12	0.15	0.02	0.11
9	3	1	0	0	0	4	0.15	0.19	0.03	0.15
10	3	9	0	0	0	12	0.14	0.22	0.03	0.13
11	0	1	1	0	0	2	0.11	0.11	0.0	0.11

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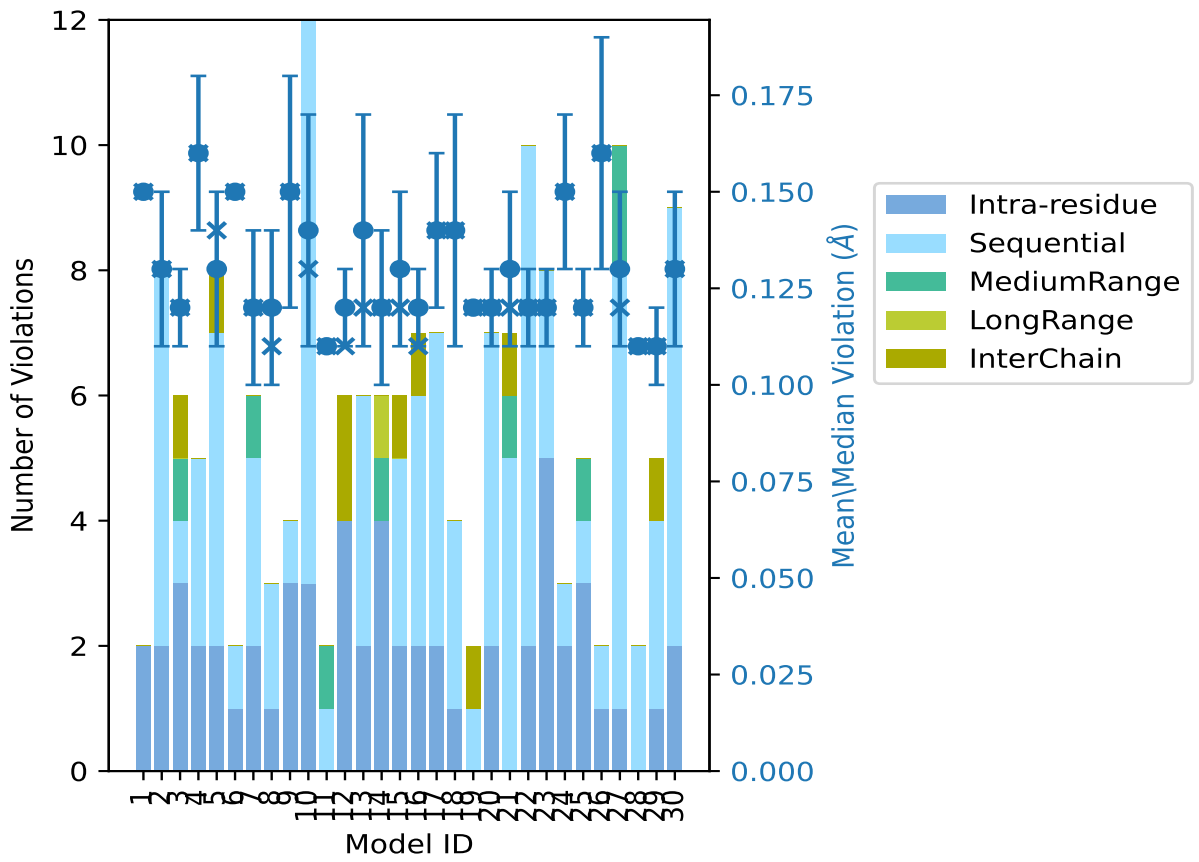
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	4	0	0	0	2	6	0.12	0.13	0.01	0.11
13	2	4	0	0	0	6	0.14	0.18	0.03	0.12
14	4	0	1	1	0	6	0.12	0.14	0.02	0.12
15	2	3	0	0	1	6	0.13	0.18	0.02	0.12
16	2	4	0	0	1	7	0.12	0.14	0.01	0.11
17	2	5	0	0	0	7	0.14	0.17	0.02	0.14
18	1	3	0	0	0	4	0.14	0.17	0.03	0.14
19	0	1	0	0	1	2	0.12	0.12	0.0	0.12
20	2	5	0	0	0	7	0.12	0.15	0.01	0.12
21	0	5	1	0	1	7	0.13	0.17	0.02	0.12
22	2	8	0	0	0	10	0.12	0.15	0.01	0.12
23	5	3	0	0	0	8	0.12	0.14	0.01	0.12
24	2	1	0	0	0	3	0.15	0.18	0.02	0.15
25	3	1	1	0	0	5	0.12	0.13	0.01	0.12
26	1	1	0	0	0	2	0.16	0.19	0.03	0.16
27	1	7	2	0	0	10	0.13	0.18	0.02	0.12
28	0	2	0	0	0	2	0.11	0.11	0.0	0.11
29	1	3	0	0	1	5	0.11	0.13	0.01	0.11
30	2	7	0	0	0	9	0.13	0.16	0.02	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



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

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2362(IR:952, SQ:535, MR:441, LR:267, IC:167) 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]	%
15	8	6	1	0	30	1	3.3
4	2	1	0	0	7	2	6.7
2	4	0	0	0	6	3	10.0
1	2	0	0	1	4	4	13.3
0	0	0	0	1	1	5	16.7
1	1	0	0	0	2	6	20.0

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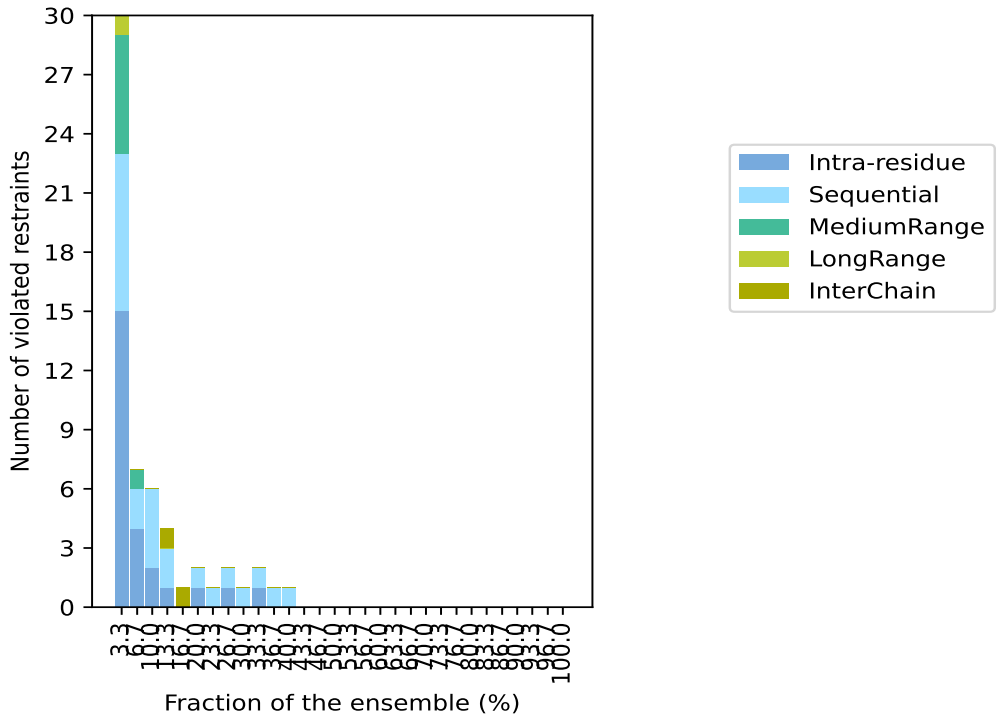
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	0	0	0	1	7	23.3
1	1	0	0	0	2	8	26.7
0	1	0	0	0	1	9	30.0
1	1	0	0	0	2	10	33.3
0	1	0	0	0	1	11	36.7
0	1	0	0	0	1	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	30	100.0

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

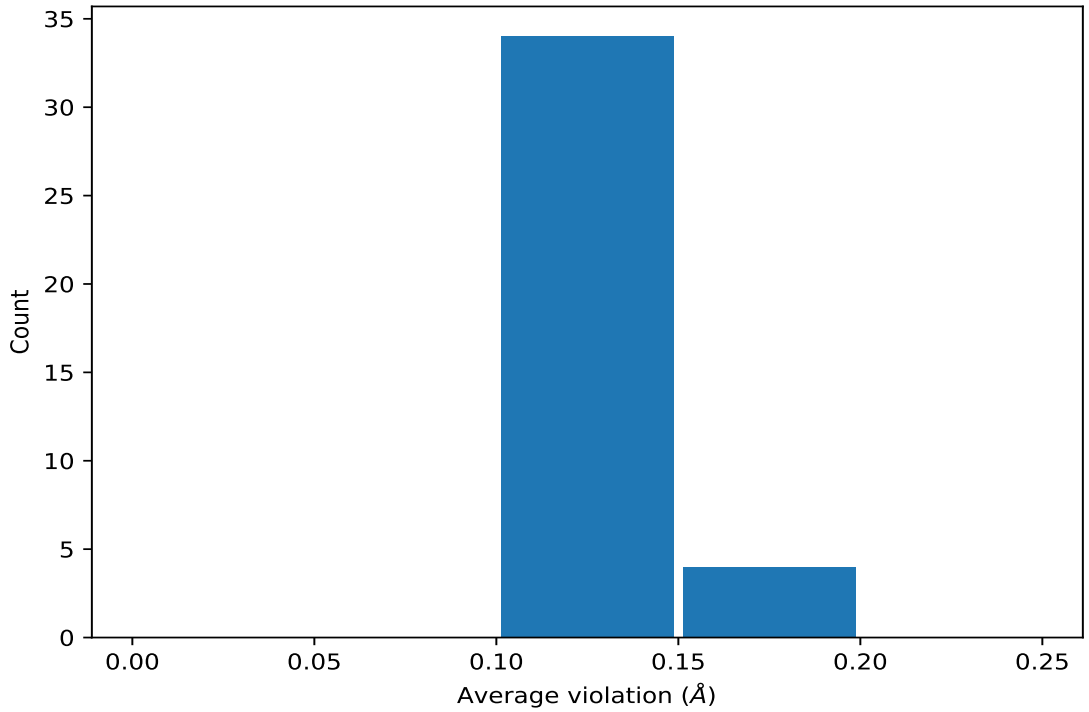
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	12	0.15	0.02	0.15
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	11	0.14	0.03	0.15
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	10	0.14	0.02	0.14
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	10	0.11	0.0	0.11
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	9	0.12	0.01	0.11
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	8	0.14	0.02	0.14
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	8	0.12	0.02	0.12
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	7	0.13	0.01	0.13
(1,1275)	1:A:24:SER:HB2	1:A:25:LYS:HB2	6	0.16	0.03	0.16
(1,1275)	1:A:24:SER:HB3	1:A:25:LYS:HB2	6	0.16	0.03	0.16
(1,77)	1:A:10:LYS:H	1:A:10:LYS:HD2	6	0.13	0.01	0.12
(1,817)	1:A:11:ALA:HB1	1:B:110:GLU:HG3	5	0.11	0.0	0.11
(1,817)	1:A:11:ALA:HB2	1:B:110:GLU:HG3	5	0.11	0.0	0.11
(1,817)	1:A:11:ALA:HB3	1:B:110:GLU:HG3	5	0.11	0.0	0.11
(1,2414)	1:B:127:SER:HB2	1:B:128:LYS:HB2	4	0.15	0.02	0.15
(1,2414)	1:B:127:SER:HB3	1:B:128:LYS:HB2	4	0.15	0.02	0.15

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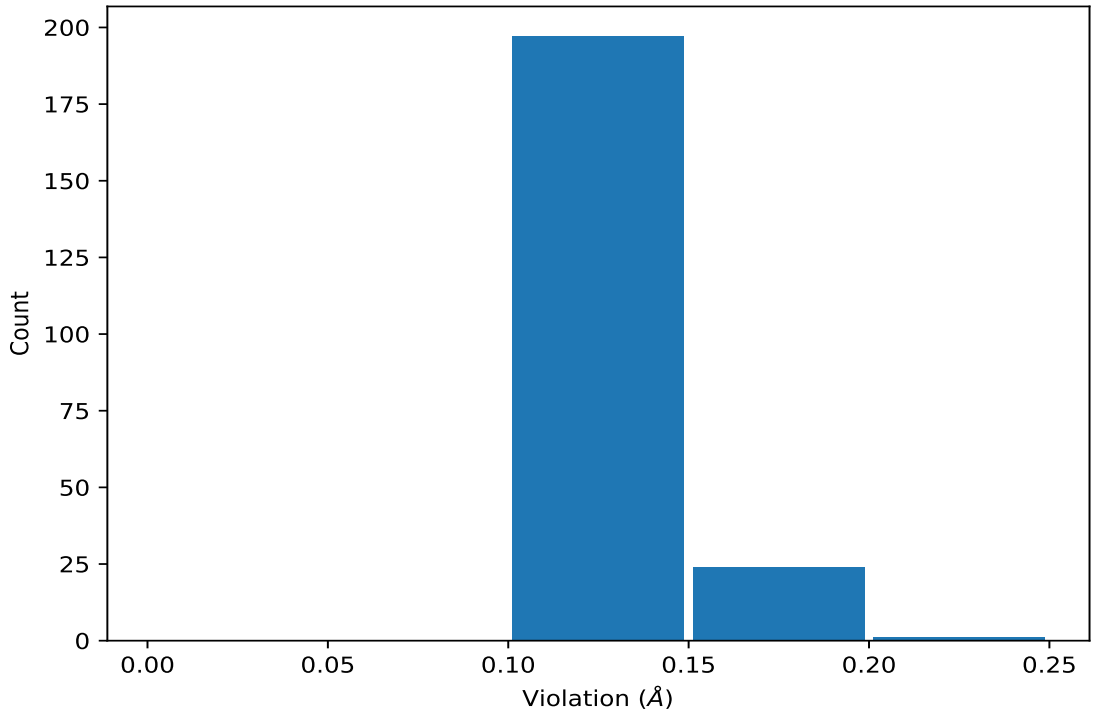
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1371)	1:B:113:LYS:H	1:B:113:LYS:HD2	4	0.12	0.02	0.12
(1,1547)	1:B:106:ASP:HB3	1:B:107:CYS:H	4	0.12	0.01	0.12
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB1	4	0.11	0.0	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB2	4	0.11	0.0	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB3	4	0.11	0.0	0.11
(1,1450)	1:B:159:ARG:H	1:B:159:ARG:HD2	3	0.16	0.01	0.15
(1,262)	1:A:3:ASP:HB3	1:A:4:CYS:H	3	0.13	0.02	0.14
(1,145)	1:A:61:LYS:HG2	1:A:62:LEU:H	3	0.12	0.0	0.12
(1,1432)	1:B:164:LYS:HG2	1:B:165:LEU:H	3	0.12	0.01	0.12
(1,2412)	1:B:173:HIS:HA	1:B:173:HIS:HE1	3	0.12	0.01	0.11
(1,973)	1:A:48:HIS:HD2	1:A:49:MET:H	3	0.11	0.0	0.11
(1,1933)	1:B:160:LYS:HG2	1:B:161:ALA:H	2	0.16	0.02	0.16
(1,164)	1:A:56:ARG:H	1:A:56:ARG:HD2	2	0.15	0.0	0.15
(1,48)	1:A:101:SER:H	1:A:101:SER:HB2	2	0.14	0.0	0.14
(1,48)	1:A:101:SER:H	1:A:101:SER:HB3	2	0.14	0.0	0.14
(1,1973)	1:B:133:LYS:HA	1:B:133:LYS:HD2	2	0.14	0.0	0.14
(1,1973)	1:B:133:LYS:HA	1:B:133:LYS:HD3	2	0.14	0.0	0.14
(1,1342)	1:B:204:SER:H	1:B:204:SER:HB2	2	0.14	0.01	0.14
(1,1342)	1:B:204:SER:H	1:B:204:SER:HB3	2	0.14	0.01	0.14
(1,1345)	1:B:203:GLN:H	1:B:204:SER:H	2	0.12	0.0	0.12
(1,1784)	1:B:161:ALA:HA	1:B:164:LYS:HB2	2	0.12	0.0	0.12
(1,1784)	1:B:161:ALA:HA	1:B:164:LYS:HB3	2	0.12	0.0	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)
(1,1437)	1:B:164:LYS:HG3	1:B:165:LEU:H	10	0.22
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	9	0.19
(1,1275)	1:A:24:SER:HB2	1:A:25:LYS:HB2	26	0.19
(1,1275)	1:A:24:SER:HB3	1:A:25:LYS:HB2	26	0.19
(1,2414)	1:B:127:SER:HB2	1:B:128:LYS:HB2	27	0.18
(1,2414)	1:B:127:SER:HB3	1:B:128:LYS:HB2	27	0.18
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	13	0.18
(1,1933)	1:B:160:LYS:HG2	1:B:161:ALA:H	24	0.18
(1,162)	1:A:56:ARG:H	1:A:56:ARG:HD3	15	0.18
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	5	0.18
(1,1275)	1:A:24:SER:HB2	1:A:25:LYS:HB2	10	0.18
(1,1275)	1:A:24:SER:HB3	1:A:25:LYS:HB2	10	0.18
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	4	0.17
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	9	0.17
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	4	0.17
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	21	0.17
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	13	0.17
(1,1450)	1:B:159:ARG:H	1:B:159:ARG:HD2	10	0.17
(1,1275)	1:A:24:SER:HB2	1:A:25:LYS:HB2	17	0.17
(1,1275)	1:A:24:SER:HB3	1:A:25:LYS:HB2	17	0.17
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	4	0.16
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	4	0.16
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	18	0.16
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	30	0.16
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	2	0.15
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	24	0.15
(1,262)	1:A:3:ASP:HB3	1:A:4:CYS:H	8	0.15
(1,2414)	1:B:127:SER:HB2	1:B:128:LYS:HB2	7	0.15
(1,2414)	1:B:127:SER:HB3	1:B:128:LYS:HB2	7	0.15
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	2	0.15
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	6	0.15
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	30	0.15
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	17	0.15
(1,164)	1:A:56:ARG:H	1:A:56:ARG:HD2	22	0.15
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	2	0.15
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	17	0.15
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	20	0.15
(1,1450)	1:B:159:ARG:H	1:B:159:ARG:HD2	6	0.15
(1,1450)	1:B:159:ARG:H	1:B:159:ARG:HD2	22	0.15
(1,1371)	1:B:113:LYS:H	1:B:113:LYS:HD2	1	0.15
(1,1275)	1:A:24:SER:HB2	1:A:25:LYS:HB2	7	0.15
(1,1275)	1:A:24:SER:HB3	1:A:25:LYS:HB2	7	0.15
(1,1275)	1:A:24:SER:HB2	1:A:25:LYS:HB2	27	0.15
(1,1275)	1:A:24:SER:HB3	1:A:25:LYS:HB2	27	0.15
(1,77)	1:A:10:LYS:H	1:A:10:LYS:HD2	1	0.14
(1,77)	1:A:10:LYS:H	1:A:10:LYS:HD2	30	0.14
(1,715)	1:A:30:LYS:HA	1:A:30:LYS:HD2	5	0.14
(1,715)	1:A:30:LYS:HA	1:A:30:LYS:HD3	5	0.14
(1,48)	1:A:101:SER:H	1:A:101:SER:HB2	3	0.14
(1,48)	1:A:101:SER:H	1:A:101:SER:HB3	3	0.14
(1,48)	1:A:101:SER:H	1:A:101:SER:HB2	14	0.14
(1,48)	1:A:101:SER:H	1:A:101:SER:HB3	14	0.14
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	5	0.14
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	30	0.14
(1,262)	1:A:3:ASP:HB3	1:A:4:CYS:H	27	0.14
(1,2414)	1:B:127:SER:HB2	1:B:128:LYS:HB2	17	0.14
(1,2414)	1:B:127:SER:HB3	1:B:128:LYS:HB2	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2412)	1:B:173:HIS:HA	1:B:173:HIS:HE1	23	0.14
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	2	0.14
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	14	0.14
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	15	0.14
(1,1973)	1:B:133:LYS:HA	1:B:133:LYS:HD2	5	0.14
(1,1973)	1:B:133:LYS:HA	1:B:133:LYS:HD3	5	0.14
(1,1973)	1:B:133:LYS:HA	1:B:133:LYS:HD2	16	0.14
(1,1973)	1:B:133:LYS:HA	1:B:133:LYS:HD3	16	0.14
(1,164)	1:A:56:ARG:H	1:A:56:ARG:HD2	10	0.14
(1,1342)	1:B:204:SER:H	1:B:204:SER:HB2	14	0.14
(1,1342)	1:B:204:SER:H	1:B:204:SER:HB3	14	0.14
(1,77)	1:A:10:LYS:H	1:A:10:LYS:HD2	20	0.13
(1,538)	1:A:40:GLU:HG2	1:A:41:MET:H	16	0.13
(1,389)	1:A:29:VAL:H	1:A:29:VAL:HB	13	0.13
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	5	0.13
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	10	0.13
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	12	0.13
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	23	0.13
(1,1933)	1:B:160:LYS:HG2	1:B:161:ALA:H	29	0.13
(1,1886)	1:B:138:LYS:HG2	1:B:138:LYS:HE2	25	0.13
(1,1886)	1:B:138:LYS:HG2	1:B:138:LYS:HE3	25	0.13
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	10	0.13
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	20	0.13
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	21	0.13
(1,1780)	1:B:160:LYS:HB2	1:B:160:LYS:HE2	10	0.13
(1,1780)	1:B:160:LYS:HB2	1:B:160:LYS:HE3	10	0.13
(1,1780)	1:B:160:LYS:HB3	1:B:160:LYS:HE2	10	0.13
(1,1780)	1:B:160:LYS:HB3	1:B:160:LYS:HE3	10	0.13
(1,1547)	1:B:106:ASP:HB3	1:B:107:CYS:H	27	0.13
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	10	0.13
(1,145)	1:A:61:LYS:HG2	1:A:62:LEU:H	30	0.13
(1,1432)	1:B:164:LYS:HG2	1:B:165:LEU:H	30	0.13
(1,1371)	1:B:113:LYS:H	1:B:113:LYS:HD2	23	0.13
(1,1342)	1:B:204:SER:H	1:B:204:SER:HB2	26	0.13
(1,1342)	1:B:204:SER:H	1:B:204:SER:HB3	26	0.13
(1,817)	1:A:11:ALA:HB1	1:B:110:GLU:HG3	3	0.12
(1,817)	1:A:11:ALA:HB2	1:B:110:GLU:HG3	3	0.12
(1,817)	1:A:11:ALA:HB3	1:B:110:GLU:HG3	3	0.12
(1,77)	1:A:10:LYS:H	1:A:10:LYS:HD2	18	0.12
(1,77)	1:A:10:LYS:H	1:A:10:LYS:HD2	23	0.12
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	12	0.12
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	23	0.12
(1,737)	1:A:56:ARG:HA	1:A:56:ARG:HD3	25	0.12
(1,626)	1:A:35:LYS:HG2	1:A:35:LYS:HE2	25	0.12
(1,626)	1:A:35:LYS:HG2	1:A:35:LYS:HE3	25	0.12
(1,51)	1:A:100:GLN:H	1:A:101:SER:H	10	0.12
(1,343)	1:A:29:VAL:H	1:A:29:VAL:HG21	16	0.12
(1,343)	1:A:29:VAL:H	1:A:29:VAL:HG22	16	0.12
(1,343)	1:A:29:VAL:H	1:A:29:VAL:HG23	16	0.12
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	13	0.12
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	21	0.12
(1,2414)	1:B:127:SER:HB2	1:B:128:LYS:HB2	20	0.12
(1,2414)	1:B:127:SER:HB3	1:B:128:LYS:HB2	20	0.12
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	15	0.12
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	22	0.12
(1,2133)	1:B:203:GLN:HB2	1:B:203:GLN:HE21	3	0.12
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	17	0.12
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	24	0.12
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	9	0.12
(1,1784)	1:B:161:ALA:HA	1:B:164:LYS:HB2	7	0.12
(1,1784)	1:B:161:ALA:HA	1:B:164:LYS:HB3	7	0.12
(1,1692)	1:B:132:VAL:HG11	1:B:133:LYS:H	15	0.12
(1,1692)	1:B:132:VAL:HG12	1:B:133:LYS:H	15	0.12
(1,1692)	1:B:132:VAL:HG13	1:B:133:LYS:H	15	0.12
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	13	0.12
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	19	0.12
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	22	0.12
(1,1547)	1:B:106:ASP:HB3	1:B:107:CYS:H	5	0.12
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	21	0.12
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	27	0.12
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	2	0.12
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	21	0.12
(1,145)	1:A:61:LYS:HG2	1:A:62:LEU:H	4	0.12
(1,145)	1:A:61:LYS:HG2	1:A:62:LEU:H	22	0.12
(1,1432)	1:B:164:LYS:HG2	1:B:165:LEU:H	22	0.12
(1,1345)	1:B:203:GLN:H	1:B:204:SER:H	27	0.12
(1,973)	1:A:48:HIS:HD2	1:A:49:MET:H	3	0.11
(1,973)	1:A:48:HIS:HD2	1:A:49:MET:H	7	0.11
(1,973)	1:A:48:HIS:HD2	1:A:49:MET:H	11	0.11
(1,914)	1:A:100:GLN:HB2	1:A:100:GLN:HE21	3	0.11
(1,832)	1:A:58:ALA:HB1	1:A:62:LEU:H	21	0.11
(1,832)	1:A:58:ALA:HB2	1:A:62:LEU:H	21	0.11
(1,832)	1:A:58:ALA:HB3	1:A:62:LEU:H	21	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,817)	1:A:11:ALA:HB1	1:B:110:GLU:HG3	12	0.11
(1,817)	1:A:11:ALA:HB2	1:B:110:GLU:HG3	12	0.11
(1,817)	1:A:11:ALA:HB3	1:B:110:GLU:HG3	12	0.11
(1,817)	1:A:11:ALA:HB1	1:B:110:GLU:HG3	15	0.11
(1,817)	1:A:11:ALA:HB2	1:B:110:GLU:HG3	15	0.11
(1,817)	1:A:11:ALA:HB3	1:B:110:GLU:HG3	15	0.11
(1,817)	1:A:11:ALA:HB1	1:B:110:GLU:HG3	16	0.11
(1,817)	1:A:11:ALA:HB2	1:B:110:GLU:HG3	16	0.11
(1,817)	1:A:11:ALA:HB3	1:B:110:GLU:HG3	16	0.11
(1,817)	1:A:11:ALA:HB1	1:B:110:GLU:HG3	29	0.11
(1,817)	1:A:11:ALA:HB2	1:B:110:GLU:HG3	29	0.11
(1,817)	1:A:11:ALA:HB3	1:B:110:GLU:HG3	29	0.11
(1,77)	1:A:10:LYS:H	1:A:10:LYS:HD2	12	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB1	5	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB2	5	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB3	5	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB1	12	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB2	12	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB3	12	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB1	19	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB2	19	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB3	19	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB1	21	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB2	21	0.11
(1,714)	1:A:7:GLU:HG3	1:B:114:ALA:HB3	21	0.11
(1,674)	1:A:57:LYS:HG2	1:A:58:ALA:H	29	0.11
(1,468)	1:A:45:GLU:HA	1:A:47:ASN:HD22	11	0.11
(1,424)	1:A:39:ARG:HG3	1:A:41:MET:H	3	0.11
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	2	0.11
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	16	0.11
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	18	0.11
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	22	0.11
(1,323)	1:A:64:GLN:HB3	1:A:65:ASN:H	27	0.11
(1,262)	1:A:3:ASP:HB3	1:A:4:CYS:H	22	0.11
(1,2412)	1:B:173:HIS:HA	1:B:173:HIS:HE1	7	0.11
(1,2412)	1:B:173:HIS:HA	1:B:173:HIS:HE1	9	0.11
(1,240)	1:A:57:LYS:HG3	1:A:58:ALA:H	28	0.11
(1,2334)	1:B:141:PHE:HD1	1:B:145:LEU:HB3	27	0.11
(1,2334)	1:B:141:PHE:HD2	1:B:145:LEU:HB3	27	0.11
(1,2154)	1:B:164:LYS:HG3	1:B:164:LYS:HD2	14	0.11
(1,2154)	1:B:164:LYS:HG3	1:B:164:LYS:HD3	14	0.11
(1,2036)	1:B:138:LYS:HD2	1:B:166:ILE:HA	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1995)	1:B:159:ARG:HA	1:B:159:ARG:HD3	7	0.11
(1,1926)	1:B:124:LYS:HA	1:B:124:LYS:HE2	20	0.11
(1,1926)	1:B:124:LYS:HA	1:B:124:LYS:HE3	20	0.11
(1,1836)	1:B:110:GLU:H	1:B:110:GLU:HG2	29	0.11
(1,1803)	1:B:143:GLU:HG2	1:B:144:MET:H	16	0.11
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	2	0.11
(1,180)	1:A:98:GLU:HG2	1:A:99:GLN:H	23	0.11
(1,1784)	1:B:161:ALA:HA	1:B:164:LYS:HB2	14	0.11
(1,1784)	1:B:161:ALA:HA	1:B:164:LYS:HB3	14	0.11
(1,1730)	1:B:156:THR:HB	1:B:157:GLY:H	10	0.11
(1,1682)	1:B:146:GLN:HA	1:B:146:GLN:HG3	8	0.11
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	2	0.11
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	5	0.11
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	17	0.11
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	20	0.11
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	23	0.11
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	29	0.11
(1,1608)	1:B:167:GLN:HB3	1:B:168:ASN:H	30	0.11
(1,1548)	1:B:105:SER:HB3	1:B:107:CYS:H	25	0.11
(1,1547)	1:B:106:ASP:HB3	1:B:107:CYS:H	8	0.11
(1,1547)	1:B:106:ASP:HB3	1:B:107:CYS:H	22	0.11
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	15	0.11
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	22	0.11
(1,1525)	1:B:160:LYS:HG3	1:B:161:ALA:H	28	0.11
(1,150)	1:A:61:LYS:HG3	1:A:62:LEU:H	10	0.11
(1,1467)	1:B:128:LYS:H	1:B:128:LYS:HG3	13	0.11
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	16	0.11
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	23	0.11
(1,1465)	1:B:201:GLU:HG2	1:B:202:GLN:H	30	0.11
(1,1448)	1:B:159:ARG:H	1:B:159:ARG:HD3	27	0.11
(1,1432)	1:B:164:LYS:HG2	1:B:165:LEU:H	25	0.11
(1,1371)	1:B:113:LYS:H	1:B:113:LYS:HD2	12	0.11
(1,1371)	1:B:113:LYS:H	1:B:113:LYS:HD2	30	0.11
(1,1345)	1:B:203:GLN:H	1:B:204:SER:H	10	0.11
(1,1275)	1:A:24:SER:HB2	1:A:25:LYS:HB2	20	0.11
(1,1275)	1:A:24:SER:HB3	1:A:25:LYS:HB2	20	0.11
(1,1156)	1:A:38:PHE:HD1	1:A:42:LEU:HB3	27	0.11
(1,1156)	1:A:38:PHE:HD2	1:A:42:LEU:HB3	27	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