Full wwPDB NMR Structure Validation Report

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PDB ID	:	2LN8
BMRB ID	:	18153
Title	:	The solution structure of theromacin
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Deposited on	:	2011-12-20

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:

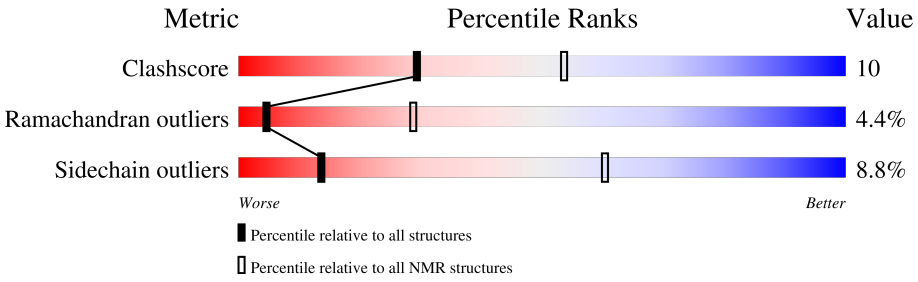
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 56%.

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	75	65% 16% • 15%

2 Ensemble composition and analysis

This entry contains 10 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:1-A:9, A:21-A:75 (64)	1.47	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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 5, 6, 7, 9
2	3, 4, 8, 10
Single-model clusters	1

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 585 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Theromacin.

Mol	Chain	Residues	Atoms					Trace
1	A	75	Total	C	N	O	S	0
			585	353	112	110	10	

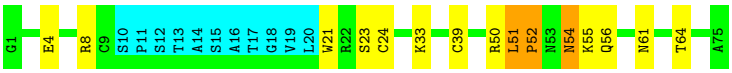
4 Residue-property plots

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: Theromacin

Chain A: 



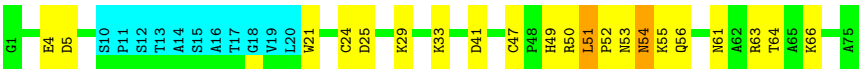
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Theromacin

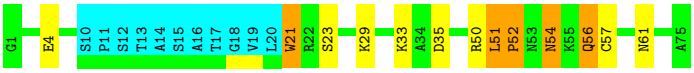
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Theromacin

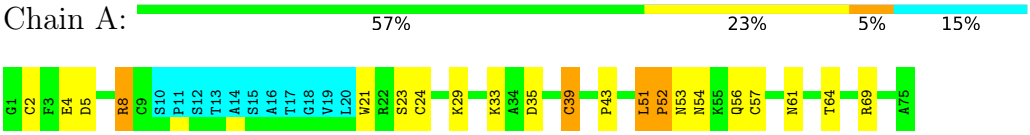
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Theromacin

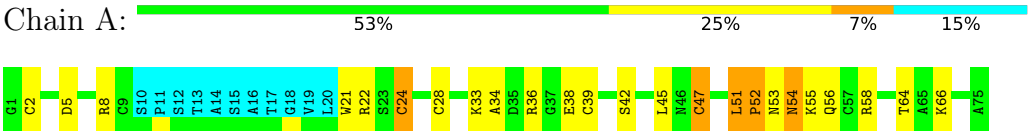
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Theromacin

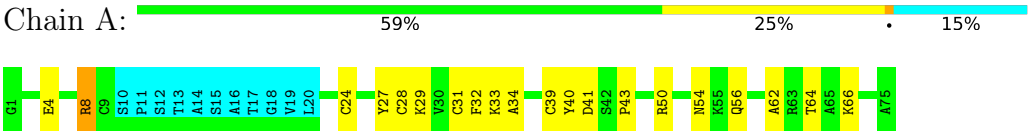
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Theromacin

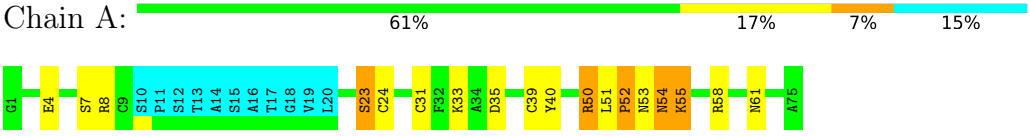
Chain A:



4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Theromacin

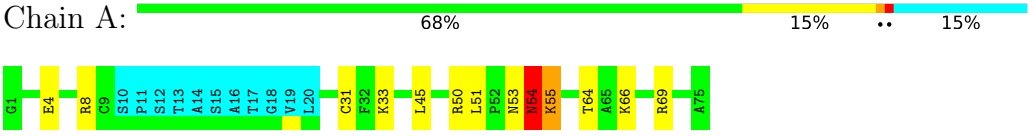
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Theromacin

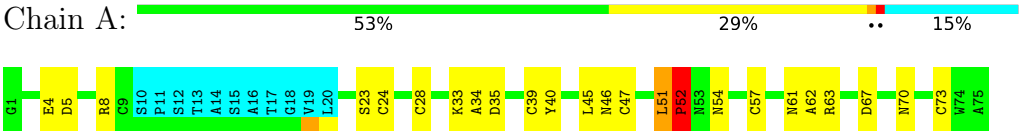
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Theromacin

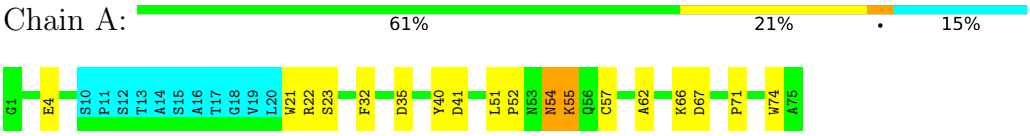
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Theromacin

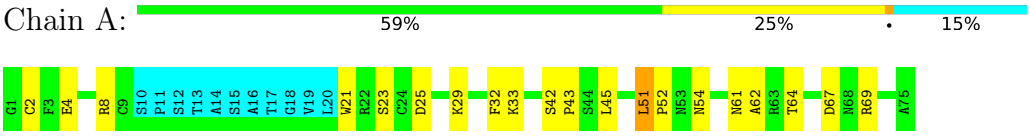
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Theromacin

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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
NMRPipe	structure solution	
NMRView	structure solution	
CYANA	structure solution	
CYANA	refinement	
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	501
Number of shifts mapped to atoms	192
Number of unparsed shifts	0
Number of shifts with mapping errors	309
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	56%

6 Model quality

6.1 Standard geometry

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	0.94±0.03	0±0/531 (0.0± 0.0%)	0.91±0.03	0±0/717 (0.0± 0.0%)
All	All	0.94	0/5310 (0.0%)	0.91	1/7170 (0.0%)

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	0.3±0.6
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	52	PRO	CA-N-CD	-6.09	102.97	111.50	8	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	A	8	ARG	Sidechain	1
1	A	69	ARG	Sidechain	1
1	A	50	ARG	Sidechain	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	517	0	469	10±4
All	All	5170	0	4689	101

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:CYS:SG	1:A:51:LEU:HB3	0.73	2.23	8	2
1:A:47:CYS:SG	1:A:51:LEU:HD22	0.70	2.26	1	1
1:A:24:CYS:HB3	1:A:39:CYS:SG	0.69	2.28	6	4
1:A:28:CYS:HB3	1:A:34:ALA:HB3	0.66	1.66	8	3
1:A:5:ASP:HB3	1:A:54:ASN:ND2	0.59	2.12	3	1
1:A:54:ASN:HD22	1:A:55:LYS:N	0.58	1.96	6	3
1:A:54:ASN:HA	1:A:56:GLN:OE1	0.58	1.98	1	1
1:A:2:CYS:SG	1:A:51:LEU:HB3	0.57	2.39	10	1
1:A:4:GLU:HB2	1:A:51:LEU:HD11	0.57	1.75	2	1
1:A:4:GLU:H	1:A:51:LEU:HD12	0.57	1.60	9	1
1:A:4:GLU:O	1:A:8:ARG:HG2	0.56	2.00	10	2
1:A:2:CYS:HB3	1:A:54:ASN:HB2	0.55	1.77	3	1
1:A:50:ARG:HA	1:A:50:ARG:NE	0.55	2.17	5	1
1:A:29:LYS:O	1:A:33:LYS:HA	0.55	2.02	3	5
1:A:38:GLU:OE2	1:A:58:ARG:HD2	0.54	2.03	4	1
1:A:4:GLU:O	1:A:8:ARG:HB2	0.54	2.02	5	1
1:A:50:ARG:O	1:A:52:PRO:HD3	0.54	2.03	1	1
1:A:33:LYS:O	1:A:63:ARG:HG2	0.54	2.03	8	1
1:A:51:LEU:N	1:A:52:PRO:HD2	0.53	2.19	2	3
1:A:21:TRP:CZ2	1:A:52:PRO:HA	0.52	2.40	3	2
1:A:4:GLU:OE1	1:A:51:LEU:HG	0.51	2.06	1	1
1:A:5:ASP:HA	1:A:8:ARG:HG2	0.51	1.83	8	1
1:A:50:ARG:HD2	1:A:50:ARG:O	0.50	2.07	6	1
1:A:21:TRP:CH2	1:A:50:ARG:HA	0.50	2.42	1	1
1:A:25:ASP:O	1:A:29:LYS:HB2	0.49	2.07	1	1
1:A:35:ASP:HB2	1:A:61:ASN:HB2	0.49	1.83	6	4
1:A:5:ASP:N	1:A:54:ASN:HD21	0.49	2.05	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:CYS:SG	1:A:57:CYS:SG	0.49	3.11	8	1
1:A:41:ASP:HA	1:A:56:GLN:NE2	0.49	2.23	1	1
1:A:33:LYS:N	1:A:33:LYS:HD2	0.48	2.22	6	2
1:A:33:LYS:HE2	1:A:64:THR:HG21	0.48	1.85	4	3
1:A:51:LEU:HB2	1:A:54:ASN:OD1	0.48	2.08	4	1
1:A:32:PHE:HB3	1:A:62:ALA:HB1	0.48	1.86	5	3
1:A:42:SER:HB2	1:A:45:LEU:O	0.48	2.09	10	1
1:A:67:ASP:HB3	1:A:73:CYS:SG	0.47	2.49	8	1
1:A:54:ASN:O	1:A:56:GLN:HG2	0.47	2.09	4	1
1:A:66:LYS:HE3	1:A:67:ASP:O	0.47	2.09	9	1
1:A:33:LYS:HD2	1:A:64:THR:HG21	0.46	1.88	5	3
1:A:4:GLU:OE1	1:A:52:PRO:HA	0.46	2.11	8	1
1:A:51:LEU:HB2	1:A:54:ASN:HB3	0.46	1.87	1	1
1:A:51:LEU:HD22	1:A:54:ASN:HB3	0.46	1.86	7	1
1:A:2:CYS:HB3	1:A:54:ASN:OD1	0.45	2.10	4	1
1:A:21:TRP:HD1	1:A:54:ASN:O	0.45	1.93	1	1
1:A:24:CYS:HA	1:A:27:TYR:HB3	0.45	1.89	5	1
1:A:2:CYS:HA	1:A:51:LEU:HD22	0.44	1.88	3	1
1:A:54:ASN:O	1:A:56:GLN:HG3	0.44	2.12	2	1
1:A:5:ASP:H	1:A:54:ASN:HD21	0.44	1.53	1	1
1:A:34:ALA:HA	1:A:62:ALA:HA	0.44	1.88	8	1
1:A:49:HIS:N	1:A:51:LEU:HD21	0.44	2.28	1	1
1:A:45:LEU:HD13	1:A:45:LEU:O	0.44	2.13	8	1
1:A:2:CYS:CB	1:A:54:ASN:HB2	0.43	2.43	3	1
1:A:51:LEU:CB	1:A:54:ASN:HB3	0.43	2.44	1	1
1:A:5:ASP:HA	1:A:8:ARG:HB2	0.43	1.90	3	1
1:A:4:GLU:H	1:A:51:LEU:CD2	0.43	2.27	10	1
1:A:5:ASP:H	1:A:54:ASN:ND2	0.42	2.12	1	1
1:A:41:ASP:O	1:A:43:PRO:HD3	0.42	2.14	5	1
1:A:51:LEU:HD13	1:A:54:ASN:HB3	0.42	1.91	9	1
1:A:25:ASP:O	1:A:29:LYS:HG2	0.42	2.13	10	1
1:A:71:PRO:HA	1:A:74:TRP:CD2	0.42	2.50	9	1
1:A:51:LEU:O	1:A:53:ASN:N	0.41	2.53	3	1
1:A:49:HIS:H	1:A:51:LEU:HD21	0.41	1.74	1	1
1:A:50:ARG:C	1:A:52:PRO:HD2	0.41	2.35	2	1
1:A:52:PRO:HD2	1:A:53:ASN:H	0.41	1.76	6	1
1:A:21:TRP:NE1	1:A:51:LEU:O	0.41	2.50	1	1
1:A:54:ASN:HD21	1:A:56:GLN:HE21	0.41	1.58	3	1
1:A:53:ASN:O	1:A:55:LYS:N	0.41	2.54	7	1
1:A:67:ASP:OD1	1:A:69:ARG:HG3	0.41	2.15	10	1
1:A:21:TRP:HE1	1:A:52:PRO:C	0.41	2.19	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ASN:HB2	1:A:73:CYS:SG	0.41	2.56	8	1
1:A:61:ASN:O	1:A:63:ARG:HG3	0.41	2.15	1	1
1:A:8:ARG:HD3	1:A:23:SER:OG	0.41	2.16	6	1
1:A:40:TYR:OH	1:A:58:ARG:NH2	0.41	2.54	6	1
1:A:51:LEU:H	1:A:51:LEU:HD23	0.41	1.76	8	1
1:A:42:SER:OG	1:A:56:GLN:HB3	0.40	2.16	4	1
1:A:4:GLU:H	1:A:51:LEU:HD11	0.40	1.76	8	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	62/75 (83%)	53±2 (86±4%)	6±3 (10±4%)	3±1 (4±2%)	4	29
All	All	620/750 (83%)	534 (86%)	59 (10%)	27 (4%)	4	29

All 11 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	52	PRO	6
1	A	23	SER	5
1	A	51	LEU	4
1	A	55	LYS	3
1	A	24	CYS	2
1	A	43	PRO	2
1	A	21	TRP	1
1	A	50	ARG	1
1	A	45	LEU	1
1	A	54	ASN	1
1	A	46	ASN	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	58/66 (88%)	53±2 (91±4%)	5±2 (9±4%)	13	60
All	All	580/660 (88%)	529 (91%)	51 (9%)	13	60

All 24 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	ASN	9
1	A	66	LYS	4
1	A	57	CYS	3
1	A	51	LEU	3
1	A	31	CYS	3
1	A	40	TYR	3
1	A	53	ASN	2
1	A	55	LYS	2
1	A	21	TRP	2
1	A	56	GLN	2
1	A	4	GLU	2
1	A	39	CYS	2
1	A	8	ARG	2
1	A	22	ARG	2
1	A	5	ASP	1
1	A	36	ARG	1
1	A	45	LEU	1
1	A	47	CYS	1
1	A	69	ARG	1
1	A	52	PRO	1
1	A	35	ASP	1
1	A	41	ASP	1
1	A	23	SER	1
1	A	61	ASN	1

6.3.3 RNA (i)

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 56% for the well-defined parts and 52% 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	501
Number of shifts mapped to atoms	192
Number of unparsed shifts	0
Number of shifts with mapping errors	309
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 309 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	PHE	H	9.333	.	1
1	A	3	PHE	HA	4.396	.	1
1	A	3	PHE	HB3	2.765	.	2
1	A	3	PHE	HB2	2.884	.	2
1	A	3	PHE	HD2	6.895	.	3
1	A	3	PHE	HE2	7.278	.	3
1	A	3	PHE	HZ	7.348	.	1
1	A	4	GLU	H	8.551	.	1
1	A	4	GLU	HA	3.742	.	1
1	A	4	GLU	HB3	1.804	.	2
1	A	4	GLU	HB2	2.154	.	2
1	A	4	GLU	HG3	2.255	.	2
1	A	4	GLU	HG2	2.256	.	2
1	A	5	ASP	H	8.341	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	ASP	HA	4.324	.	1
1	A	5	ASP	HB3	2.568	.	2
1	A	5	ASP	HB2	2.711	.	2
1	A	6	TRP	H	7.798	.	1
1	A	6	TRP	HA	4.318	.	1
1	A	6	TRP	HB3	3.147	.	2
1	A	6	TRP	HB2	3.421	.	2
1	A	6	TRP	HD1	7.117	.	1
1	A	6	TRP	HE1	9.662	.	1
1	A	6	TRP	HZ2	7.237	.	1
1	A	7	SER	H	8.493	.	1
1	A	7	SER	HA	3.257	.	1
1	A	7	SER	HB3	3.485	.	2
1	A	7	SER	HB2	3.564	.	2
1	A	8	ARG	H	7.607	.	1
1	A	8	ARG	HA	4.017	.	1
1	A	8	ARG	HB3	1.406	.	2
1	A	8	ARG	HB2	1.525	.	2
1	A	9	CYS	H	7.504	.	1
1	A	9	CYS	HA	4.705	.	1
1	A	9	CYS	HB3	2.546	.	2
1	A	9	CYS	HB2	3.025	.	2
1	A	10	SER	H	7.187	.	1
1	A	10	SER	HA	4.611	.	1
1	A	10	SER	HB3	2.78	.	2
1	A	10	SER	HB2	3.15	.	2
1	A	17	THR	H	7.868	.	1
1	A	17	THR	HA	4.295	.	1
1	A	18	GLY	H	8.207	.	1
1	A	18	GLY	HA3	3.865	.	2
1	A	18	GLY	HA2	4.09	.	2
1	A	19	VAL	H	7.848	.	1
1	A	19	VAL	HA	4.088	.	1
1	A	19	VAL	HB	2.038	.	1
1	A	19	VAL	HG21	0.858	.	2
1	A	19	VAL	HG22	0.858	.	2
1	A	19	VAL	HG23	0.858	.	2
1	A	20	LEU	H	8.252	.	1
1	A	20	LEU	HA	4.293	.	1
1	A	20	LEU	HB3	1.487	.	2
1	A	20	LEU	HB2	1.589	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	21	TRP	H	8.069	.	1
1	A	21	TRP	HA	4.427	.	1
1	A	21	TRP	HB2	3.142	.	2
1	A	21	TRP	HD1	7.538	.	1
1	A	21	TRP	HE1	9.46	.	1
1	A	21	TRP	HZ2	7.337	.	1
1	A	22	ARG	H	7.403	.	1
1	A	22	ARG	HA	4.185	.	1
1	A	22	ARG	HB2	1.563	.	2
1	A	23	SER	H	8.057	.	1
1	A	23	SER	HA	3.963	.	1
1	A	23	SER	HB2	4.188	.	2
1	A	24	CYS	H	7.837	.	1
1	A	24	CYS	HA	3.981	.	1
1	A	24	CYS	HB3	2.676	.	2
1	A	24	CYS	HB2	2.826	.	2
1	A	25	ASP	H	8.634	.	1
1	A	25	ASP	HA	4.077	.	1
1	A	25	ASP	HB3	2.479	.	2
1	A	25	ASP	HB2	2.8	.	2
1	A	26	SER	H	7.813	.	1
1	A	26	SER	HA	4.101	.	1
1	A	26	SER	HB2	3.886	.	2
1	A	27	TYR	H	8.69	.	1
1	A	27	TYR	HA	3.965	.	1
1	A	27	TYR	HB3	2.873	.	2
1	A	27	TYR	HB2	3.056	.	2
1	A	27	TYR	HD2	7.055	.	3
1	A	27	TYR	HE1	6.787	.	3
1	A	27	TYR	HE2	6.773	.	3
1	A	28	CYS	H	8.579	.	1
1	A	28	CYS	HA	4.242	.	1
1	A	28	CYS	HB3	2.371	.	2
1	A	28	CYS	HB2	2.633	.	2
1	A	29	LYS	H	8.257	.	1
1	A	29	LYS	HA	4.083	.	1
1	A	29	LYS	HB2	1.817	.	2
1	A	29	LYS	HG2	1.273	.	2
1	A	29	LYS	HD2	1.389	.	2
1	A	30	VAL	H	8.675	.	1
1	A	30	VAL	HA	3.752	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	VAL	HB	1.983	.	1
1	A	30	VAL	HG11	0.731	.	2
1	A	30	VAL	HG12	0.731	.	2
1	A	30	VAL	HG13	0.731	.	2
1	A	30	VAL	HG21	0.988	.	2
1	A	30	VAL	HG22	0.988	.	2
1	A	30	VAL	HG23	0.988	.	2
1	A	31	CYS	H	8.447	.	1
1	A	31	CYS	HA	4.353	.	1
1	A	31	CYS	HB3	1.916	.	2
1	A	31	CYS	HB2	2.457	.	2
1	A	32	PHE	H	6.854	.	1
1	A	32	PHE	HA	4.655	.	1
1	A	32	PHE	HB3	2.82	.	2
1	A	32	PHE	HB2	3.477	.	2
1	A	32	PHE	HD2	7.25	.	3
1	A	32	PHE	HE2	7.117	.	3
1	A	33	LYS	H	7.13	.	1
1	A	33	LYS	HA	4.332	.	1
1	A	33	LYS	HB3	1.881	.	2
1	A	33	LYS	HB2	2.111	.	2
1	A	33	LYS	HG2	1.443	.	2
1	A	33	LYS	HD2	1.68	.	2
1	A	34	ALA	H	7.372	.	1
1	A	34	ALA	HB1	1.04	.	1
1	A	34	ALA	HB2	1.04	.	1
1	A	34	ALA	HB3	1.04	.	1
1	A	35	ASP	H	7.909	.	1
1	A	35	ASP	HA	4.476	.	1
1	A	35	ASP	HB3	2.406	.	2
1	A	35	ASP	HB2	2.774	.	2
1	A	36	ARG	H	7.258	.	1
1	A	36	ARG	HA	4.647	.	1
1	A	36	ARG	HB3	1.893	.	2
1	A	36	ARG	HB2	2.154	.	2
1	A	36	ARG	HG3	1.099	.	2
1	A	36	ARG	HG2	1.31	.	2
1	A	37	GLY	H	9.375	.	1
1	A	37	GLY	HA3	3.53	.	2
1	A	37	GLY	HA2	5.264	.	2
1	A	38	GLU	H	9.246	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	GLU	HA	4.623	.	1
1	A	38	GLU	HB3	1.776	.	2
1	A	38	GLU	HB2	1.898	.	2
1	A	38	GLU	HG2	2.088	.	2
1	A	39	CYS	HA	5.437	.	1
1	A	39	CYS	HB3	2.551	.	2
1	A	39	CYS	HB2	3.058	.	2
1	A	40	TYR	H	8.979	.	1
1	A	40	TYR	HA	4.901	.	1
1	A	40	TYR	HB2	2.905	.	2
1	A	40	TYR	HD2	7.04	.	3
1	A	40	TYR	HE2	6.599	.	3
1	A	41	ASP	H	8.574	.	1
1	A	41	ASP	HA	4.509	.	1
1	A	41	ASP	HB2	2.504	.	2
1	A	42	SER	H	7.997	.	1
1	A	42	SER	HA	4.828	.	1
1	A	42	SER	HB3	3.601	.	2
1	A	42	SER	HB2	3.863	.	2
1	A	44	SER	H	8.073	.	1
1	A	44	SER	HA	4.426	.	1
1	A	45	LEU	H	7.845	.	1
1	A	45	LEU	HA	4.181	.	1
1	A	45	LEU	HB2	1.613	.	2
1	A	48	PRO	HD3	3.904	.	2
1	A	48	PRO	HD2	3.784	.	2
1	A	49	HIS	H	7.269	.	1
1	A	49	HIS	HA	4.433	.	1
1	A	49	HIS	HB3	2.714	.	2
1	A	49	HIS	HB2	2.953	.	2
1	A	51	LEU	H	8.2	.	1
1	A	51	LEU	HA	4.259	.	1
1	A	51	LEU	HB2	1.52	.	2
1	A	51	LEU	HD21	0.379	.	2
1	A	51	LEU	HD11	0.379	.	2
1	A	51	LEU	HD12	0.379	.	2
1	A	51	LEU	HD13	0.379	.	2
1	A	51	LEU	HD22	0.379	.	2
1	A	51	LEU	HD23	0.379	.	2
1	A	52	PRO	HA	4.291	.	1
1	A	52	PRO	HB3	1.995	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	PRO	HB2	2.281	.	2
1	A	52	PRO	HD3	2.608	.	2
1	A	52	PRO	HD2	3.36	.	2
1	A	53	ASN	H	7.358	.	1
1	A	53	ASN	HA	4.484	.	1
1	A	53	ASN	HB2	3.057	.	2
1	A	53	ASN	HD21	7.402	.	2
1	A	53	ASN	HD22	7.736	.	2
1	A	54	ASN	H	8.305	.	1
1	A	54	ASN	HA	5.025	.	1
1	A	54	ASN	HB3	2.719	.	2
1	A	54	ASN	HB2	3.151	.	2
1	A	54	ASN	HD21	6.793	.	2
1	A	54	ASN	HD22	7.318	.	2
1	A	55	LYS	H	7.922	.	1
1	A	55	LYS	HA	4.533	.	1
1	A	55	LYS	HB3	1.343	.	2
1	A	55	LYS	HB2	1.805	.	2
1	A	55	LYS	HG2	1.528	.	2
1	A	56	GLN	H	8.542	.	1
1	A	56	GLN	HA	4.327	.	1
1	A	56	GLN	HB3	1.531	.	2
1	A	56	GLN	HB2	1.89	.	2
1	A	56	GLN	HG3	2.093	.	2
1	A	56	GLN	HG2	2.226	.	2
1	A	56	GLN	HE21	7.336	.	2
1	A	56	GLN	HE22	8.018	.	2
1	A	57	CYS	H	7.763	.	1
1	A	57	CYS	HA	4.97	.	1
1	A	57	CYS	HB3	2.795	.	2
1	A	57	CYS	HB2	3.061	.	2
1	A	58	ARG	H	9.525	.	1
1	A	58	ARG	HA	4.797	.	1
1	A	58	ARG	HB2	1.815	.	2
1	A	58	ARG	HG3	1.479	.	2
1	A	58	ARG	HG2	1.57	.	2
1	A	58	ARG	HD3	2.643	.	2
1	A	58	ARG	HD2	2.843	.	2
1	A	59	CYS	H	8.827	.	1
1	A	59	CYS	HA	5.257	.	1
1	A	59	CYS	HB2	2.463	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	ILE	H	8.644	.	1
1	A	60	ILE	HA	4.195	.	1
1	A	60	ILE	HB	1.796	.	1
1	A	60	ILE	HG13	1.142	.	2
1	A	60	ILE	HG12	1.311	.	2
1	A	60	ILE	HG21	0.85	.	1
1	A	60	ILE	HG22	0.85	.	1
1	A	60	ILE	HG23	0.85	.	1
1	A	60	ILE	HD11	0.613	.	1
1	A	60	ILE	HD12	0.613	.	1
1	A	60	ILE	HD13	0.613	.	1
1	A	61	ASN	H	9.202	.	1
1	A	61	ASN	HA	4.273	.	1
1	A	61	ASN	HB3	2.654	.	2
1	A	61	ASN	HB2	3.047	.	2
1	A	61	ASN	HD21	6.764	.	2
1	A	61	ASN	HD22	7.707	.	2
1	A	62	ALA	H	8.103	.	1
1	A	62	ALA	HA	3.659	.	1
1	A	62	ALA	HB1	1.295	.	1
1	A	62	ALA	HB2	1.295	.	1
1	A	62	ALA	HB3	1.295	.	1
1	A	63	ARG	H	7.753	.	1
1	A	63	ARG	HA	4.452	.	1
1	A	63	ARG	HB3	1.689	.	2
1	A	63	ARG	HB2	1.945	.	2
1	A	63	ARG	HG3	1.506	.	2
1	A	63	ARG	HG2	2.112	.	2
1	A	63	ARG	HD2	3.155	.	2
1	A	64	THR	H	7.954	.	1
1	A	64	THR	HA	4.694	.	1
1	A	64	THR	HB	4.377	.	1
1	A	64	THR	HG21	1.011	.	1
1	A	64	THR	HG22	1.011	.	1
1	A	64	THR	HG23	1.011	.	1
1	A	65	ALA	H	8.1	.	1
1	A	65	ALA	HA	4.488	.	1
1	A	65	ALA	HB1	1.432	.	1
1	A	65	ALA	HB2	1.432	.	1
1	A	65	ALA	HB3	1.432	.	1
1	A	66	LYS	H	8.413	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	66	LYS	HA	2.855	.	1
1	A	66	LYS	HB2	1.436	.	2
1	A	66	LYS	HG3	0.435	.	2
1	A	66	LYS	HG2	0.881	.	2
1	A	66	LYS	HE2	2.796	.	2
1	A	67	ASP	H	7.881	.	1
1	A	67	ASP	HA	4.478	.	1
1	A	67	ASP	HB3	2.632	.	2
1	A	67	ASP	HB2	3.018	.	2
1	A	68	ASN	H	8.257	.	1
1	A	68	ASN	HA	4.588	.	1
1	A	68	ASN	HB3	2.794	.	2
1	A	68	ASN	HB2	2.808	.	2
1	A	69	ARG	H	8.306	.	1
1	A	69	ARG	HA	4.346	.	1
1	A	69	ARG	HB2	1.942	.	2
1	A	69	ARG	HG3	1.685	.	2
1	A	69	ARG	HD2	3.19	.	2
1	A	70	ASN	H	7.291	.	1
1	A	70	ASN	HA	4.926	.	1
1	A	70	ASN	HB3	2.529	.	2
1	A	70	ASN	HB2	3.005	.	2
1	A	70	ASN	HD21	6.925	.	2
1	A	70	ASN	HD22	8.059	.	2
1	A	71	PRO	HB3	1.704	.	2
1	A	71	PRO	HB2	1.871	.	2
1	A	71	PRO	HD3	3.739	.	2
1	A	71	PRO	HD2	3.93	.	2
1	A	72	THR	H	7.929	.	1
1	A	72	THR	HA	4.179	.	1
1	A	72	THR	HB	4.107	.	1
1	A	72	THR	HG21	1.208	.	1
1	A	72	THR	HG22	1.208	.	1
1	A	72	THR	HG23	1.208	.	1
1	A	73	CYS	H	8.137	.	1
1	A	73	CYS	HB3	2.778	.	2
1	A	73	CYS	HB2	3.134	.	2
1	A	74	TRP	H	7.311	.	1
1	A	74	TRP	HA	4.663	.	1
1	A	74	TRP	HB3	3.227	.	2
1	A	74	TRP	HB2	3.391	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	TRP	HD1	7.125	.	1
1	A	74	TRP	HE1	9.897	.	1
1	A	74	TRP	HZ2	7.323	.	1
1	A	75	ALA	H	7.9	.	1
1	A	75	ALA	HA	4.158	.	1
1	A	75	ALA	HB1	1.287	.	1
1	A	75	ALA	HB2	1.287	.	1
1	A	75	ALA	HB3	1.287	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	64	0.05 ± 0.26	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	61	-0.08 ± 0.23	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	59	0.54 ± 0.59	None needed (imprecise)

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 56%, i.e. 467 atoms were assigned a chemical shift out of a possible 840. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	222/314 (71%)	109/126 (87%)	59/128 (46%)	54/60 (90%)
Sidechain	223/446 (50%)	162/281 (58%)	56/133 (42%)	5/32 (16%)
Aromatic	22/80 (28%)	19/40 (48%)	0/37 (0%)	3/3 (100%)
Overall	467/840 (56%)	290/447 (65%)	115/298 (39%)	62/95 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 501 atoms were assigned a chemical shift out of a possible 955. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	243/368 (66%)	120/148 (81%)	64/150 (43%)	59/70 (84%)
Sidechain	236/507 (47%)	170/323 (53%)	61/152 (40%)	5/32 (16%)
Aromatic	22/80 (28%)	19/40 (48%)	0/37 (0%)	3/3 (100%)

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	Total	^{1}H	^{13}C	^{15}N
Overall	501/955 (52%)	309/511 (60%)	125/339 (37%)	67/105 (64%)

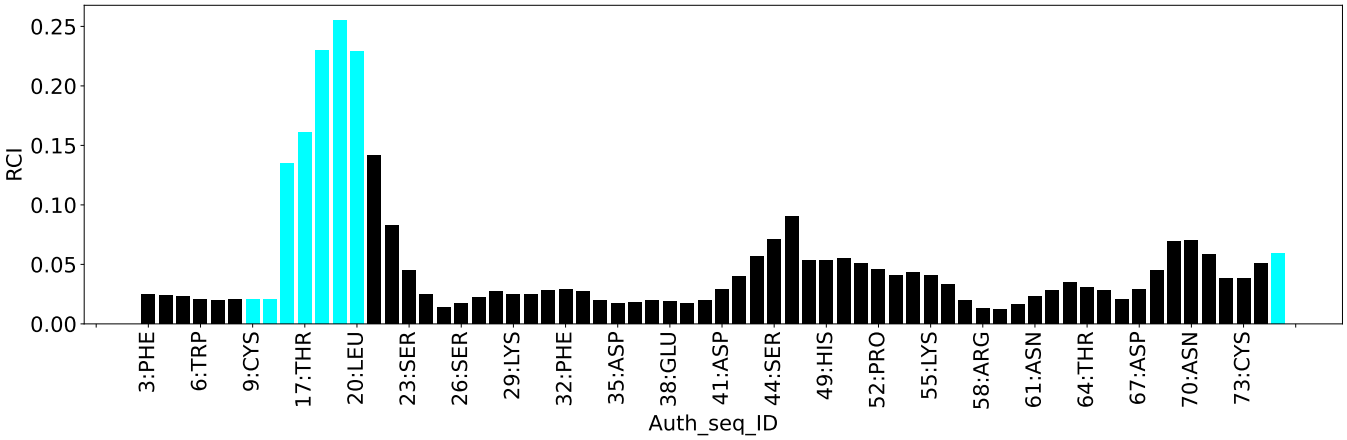
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

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	466
Intra-residue (|i-j|=0)	95
Sequential (|i-j|=1)	169
Medium range (|i-j|>1 and |i-j|<5)	70
Long range (|i-j|≥5)	117
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	15
Total dihedral-angle restraints	0
Number of unmapped restraints	451
Number of restraints per residue	6.2
Number of long range restraints per residue[1]	1.8

[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.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis (i)

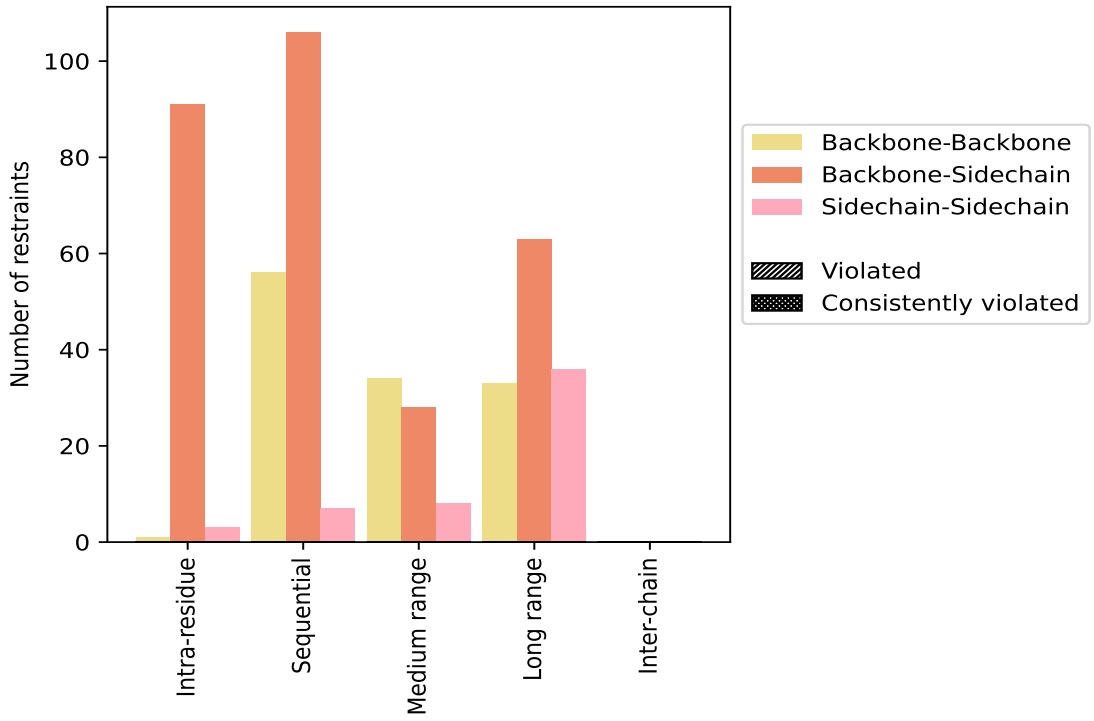
9.1 Summary of distance violations (i)

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)	95	20.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	91	19.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	3	0.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	169	36.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	56	12.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	106	22.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	1.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	70	15.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	34	7.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	28	6.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	1.7	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	117	25.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	33	7.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	63	13.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	21	4.5	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	15	3.2	0	0.0	0.0	0	0.0	0.0
Total	466	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	124	26.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	288	61.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	54	11.6	0	0.0	0.0	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

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found