Full wwPDB NMR Structure Validation Report (i)

Oct 16, 2021 – 10:55 PM EDT

PDB ID	:	1R4Y
Title	:	SOLUTION STRUCTURE OF THE DELETION MUTANT DELTA(7-22) OF THE CYTOTOXIC RIBONUCLEASE ALPHA-SARCIN
Authors	:	Garcia-Mayoral, M.F.; Garcia-Ortega, L.; Lillo, M.P.; Santoro, J.; Martinez Del Pozo, A.; Gavilanes, J.G.; Rico, M.; Bruix, M.
Deposited on	:	2003-10-09

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

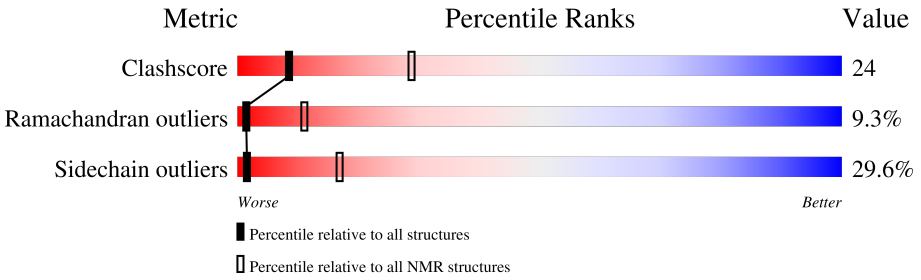
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 was not calculated.

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	136	31% 53% 9% 7%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:2-A:122, A:132-A:136 (126)	0.34	18

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2091 atoms, of which 1021 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribonuclease alpha-sarcin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	136	2091	675	1021	189	202	4	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	LEU	engineered mutation	UNP P00655
A	?	-	ASN	deletion	UNP P00655
A	?	-	ASP	deletion	UNP P00655
A	?	-	GLN	deletion	UNP P00655
A	?	-	LYS	deletion	UNP P00655
A	?	-	ASN	deletion	UNP P00655
A	?	-	PRO	deletion	UNP P00655
A	?	-	LYS	deletion	UNP P00655
A	?	-	THR	deletion	UNP P00655
A	?	-	ASN	deletion	UNP P00655
A	?	-	LYS	deletion	UNP P00655
A	?	-	TYR	deletion	UNP P00655
A	?	-	GLU	deletion	UNP P00655
A	?	-	THR	deletion	UNP P00655
A	?	-	LYS	deletion	UNP P00655
A	8	GLY	ARG	engineered mutation	UNP P00655

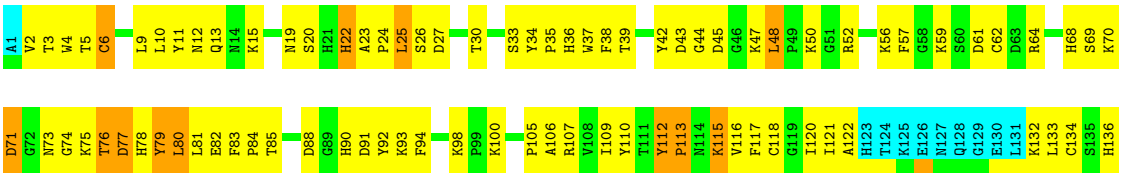
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Ribonuclease alpha-sarcin

Chain A: 31% 53% 9% 7%



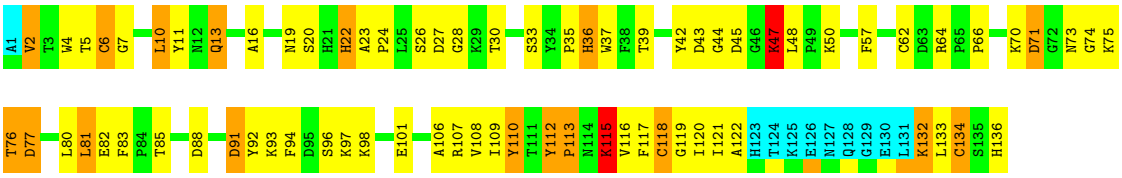
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Ribonuclease alpha-sarcin

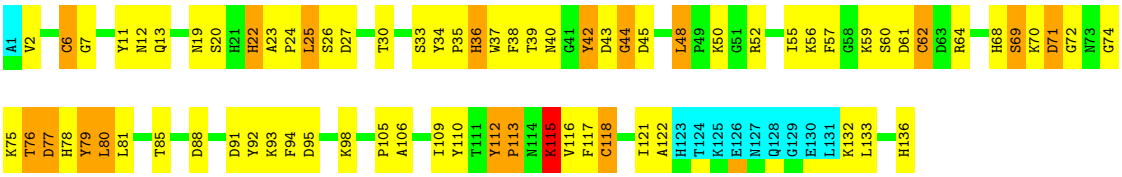
Chain A: 38% 40% 12% • 7%



4.2.2 Score per residue for model 2

• Molecule 1: Ribonuclease alpha-sarcin

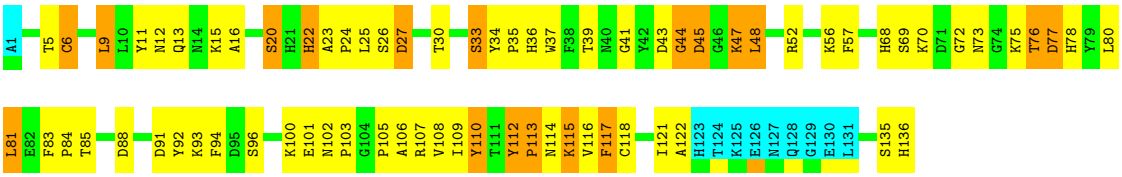
Chain A: 38% 41% 12% • 7%



4.2.3 Score per residue for model 3

- Molecule 1: Ribonuclease alpha-sarcin

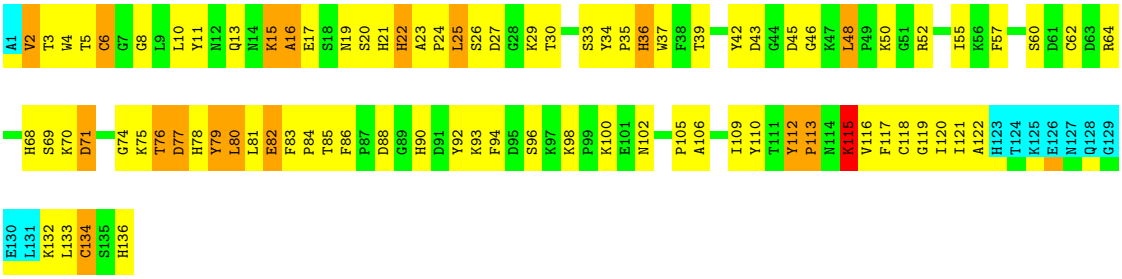
Chain A: 40% 40% 13% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Ribonuclease alpha-sarcin

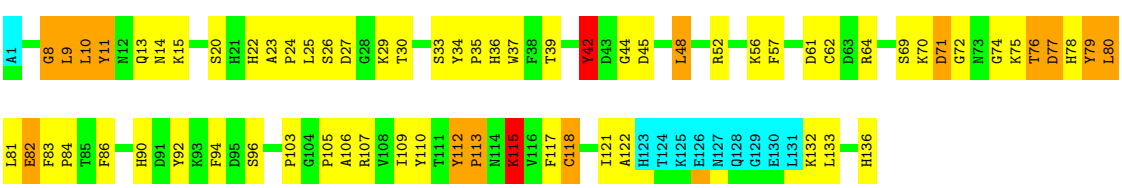
Chain A: 30% 49% 12% • 7%



4.2.5 Score per residue for model 5

- Molecule 1: Ribonuclease alpha-sarcin

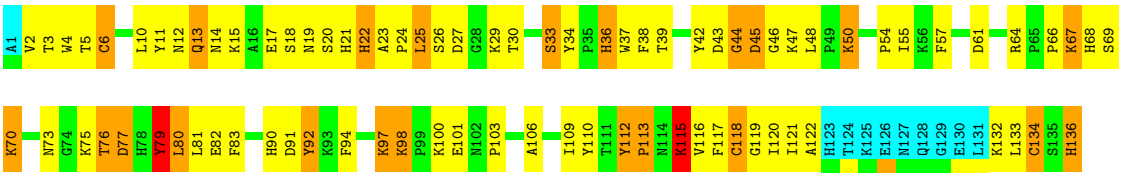
Chain A: 43% 38% 10% • 7%



4.2.6 Score per residue for model 6

- Molecule 1: Ribonuclease alpha-sarcin

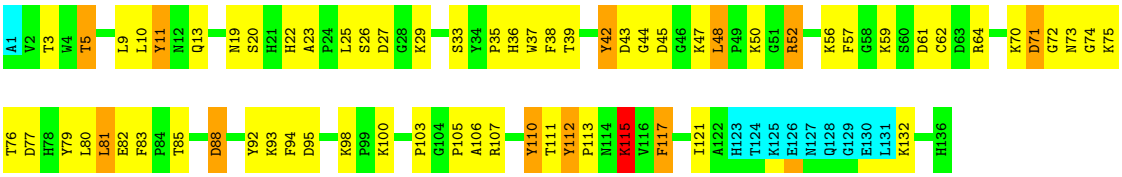
Chain A: 32% 43% 16% • 7%



4.2.7 Score per residue for model 7

- Molecule 1: Ribonuclease alpha-sarcin

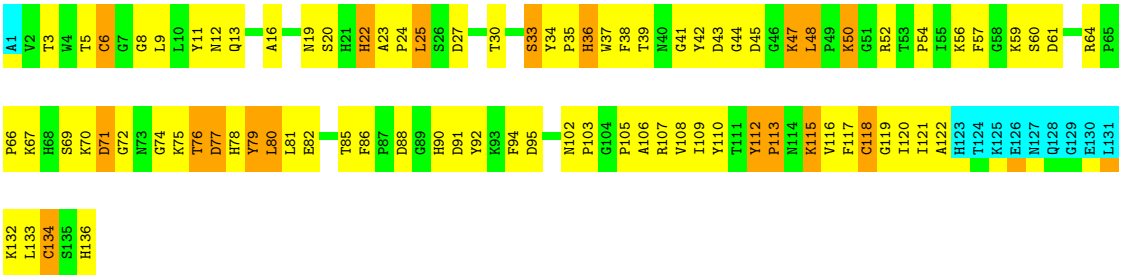
Chain A: 43% 40% 8% • 7%



4.2.8 Score per residue for model 8

- Molecule 1: Ribonuclease alpha-sarcin

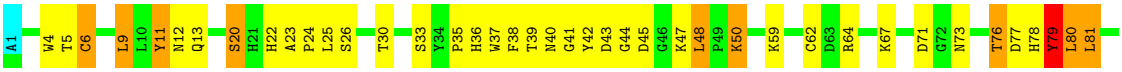
Chain A: 30% 49% 13% 7%

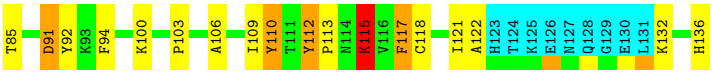


4.2.9 Score per residue for model 9

- Molecule 1: Ribonuclease alpha-sarcin

Chain A: 49% 32% 10% • 7%

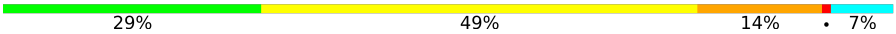


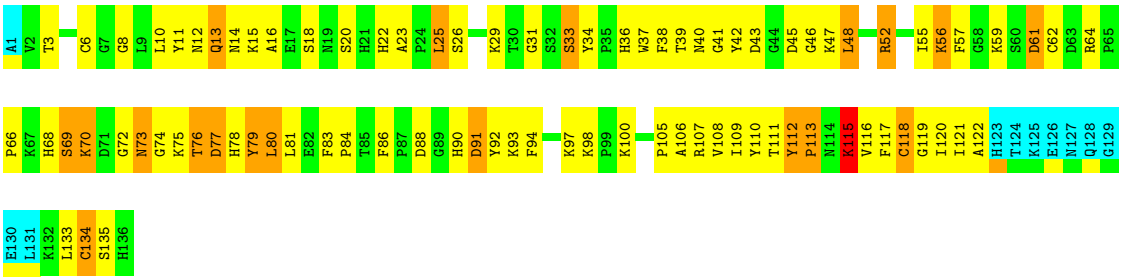


4.2.10 Score per residue for model 10

- Molecule 1: Ribonuclease alpha-sarcin

Chain A:

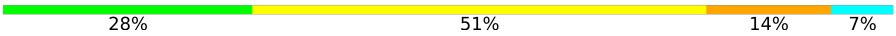


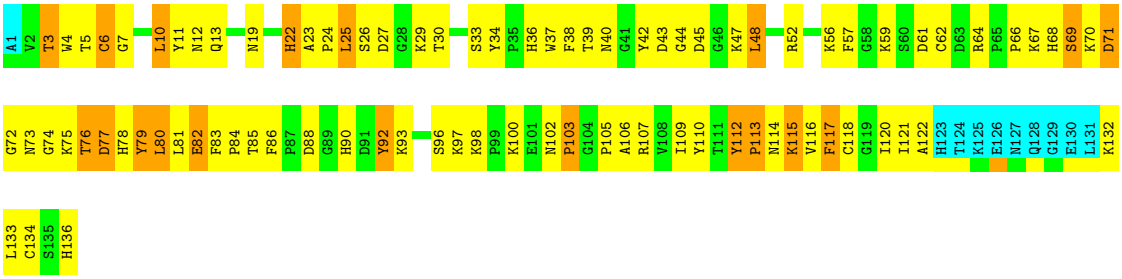


4.2.11 Score per residue for model 11

- Molecule 1: Ribonuclease alpha-sarcin

Chain A:

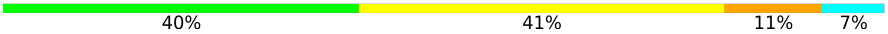


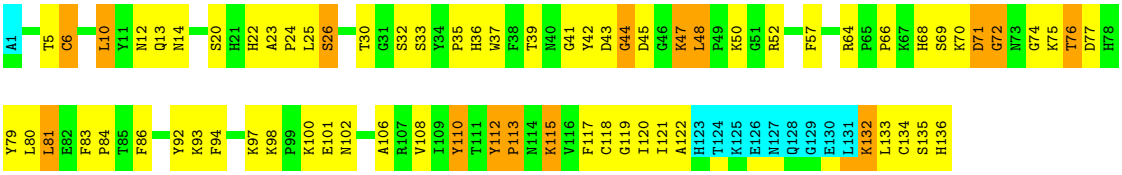


4.2.12 Score per residue for model 12

- Molecule 1: Ribonuclease alpha-sarcin

Chain A:

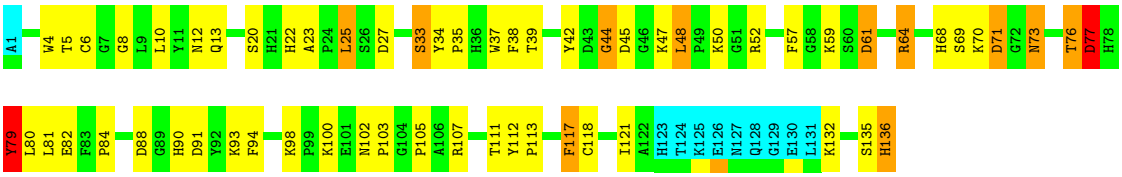




4.2.13 Score per residue for model 13

- Molecule 1: Ribonuclease alpha-sarcin

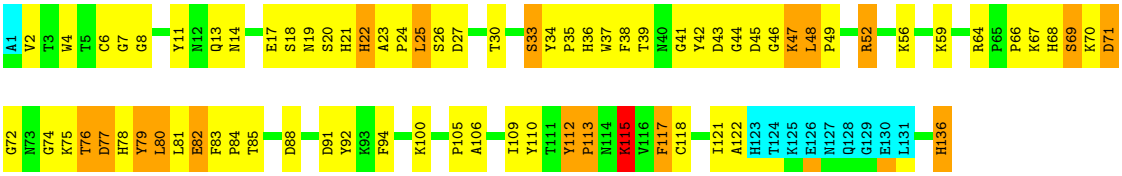
Chain A: 48% 35% 8% • 7%



4.2.14 Score per residue for model 14

- Molecule 1: Ribonuclease alpha-sarcin

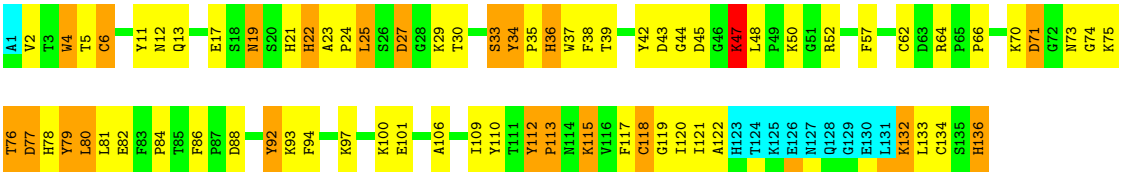
Chain A: 37% 43% 12% • 7%



4.2.15 Score per residue for model 15

- Molecule 1: Ribonuclease alpha-sarcin

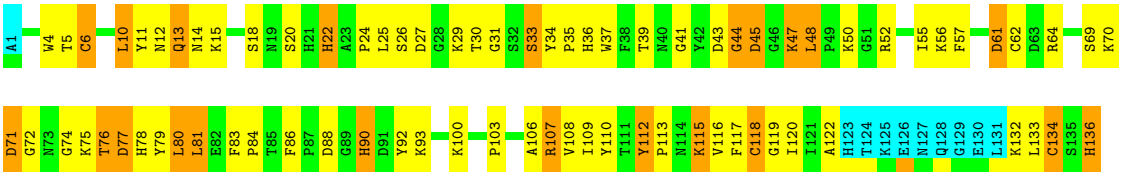
Chain A: 39% 38% 15% • 7%



4.2.16 Score per residue for model 16

- Molecule 1: Ribonuclease alpha-sarcin

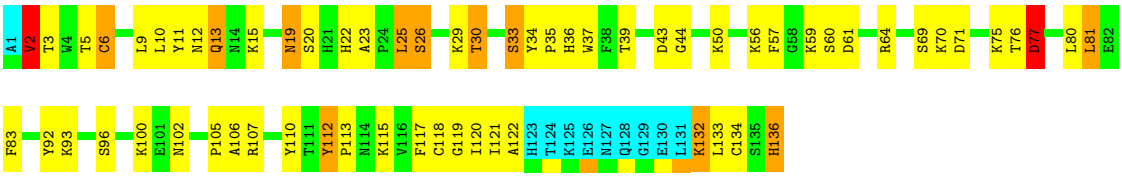
Chain A: 35% 41% 16% 7%



4.2.17 Score per residue for model 17

- Molecule 1: Ribonuclease alpha-sarcin

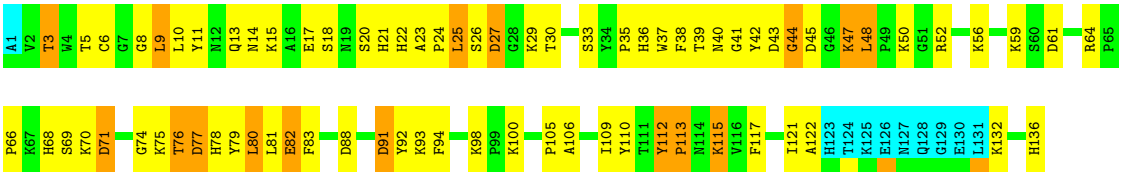
Chain A: 46% 38% 8% • 7%



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Ribonuclease alpha-sarcin

Chain A: 37% 44% 12% 7%



4.2.19 Score per residue for model 19

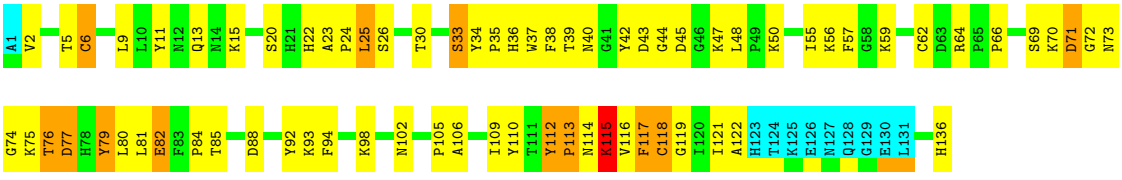
- Molecule 1: Ribonuclease alpha-sarcin

Chain A: 44% 40% 8% 7%

4.2.20 Score per residue for model 20

- Molecule 1: Ribonuclease alpha-sarcin

Chain A: 40% 43% 9% • 7%



4.2.21 Score per residue for model 21

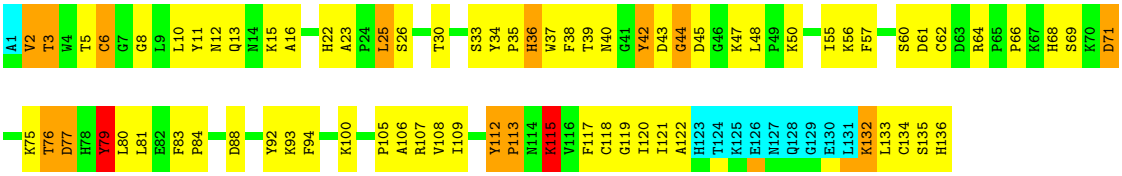
- Molecule 1: Ribonuclease alpha-sarcin

Chain A: 49% 32% 12% • 7%

4.2.22 Score per residue for model 22

- Molecule 1: Ribonuclease alpha-sarcin

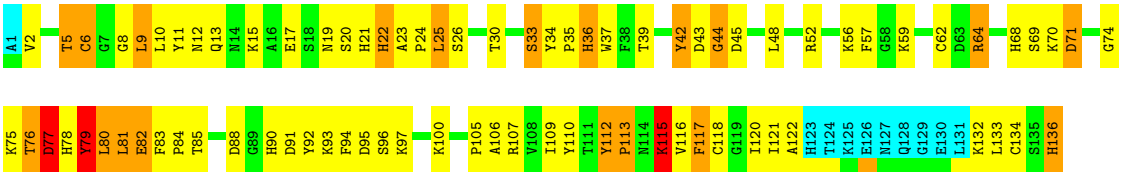
Chain A: 38% 43% 10% • 7%



4.2.23 Score per residue for model 23

- Molecule 1: Ribonuclease alpha-sarcin

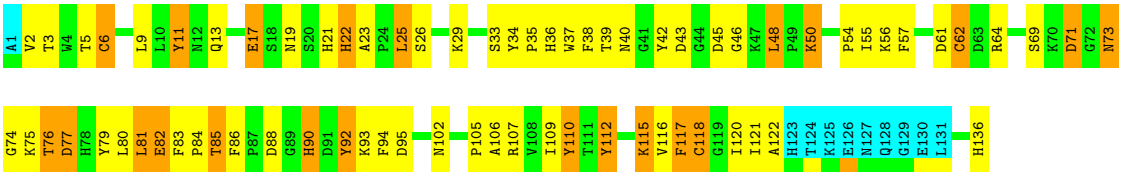
Chain A: 33% 43% 14% • 7%



4.2.24 Score per residue for model 24

- Molecule 1: Ribonuclease alpha-sarcin

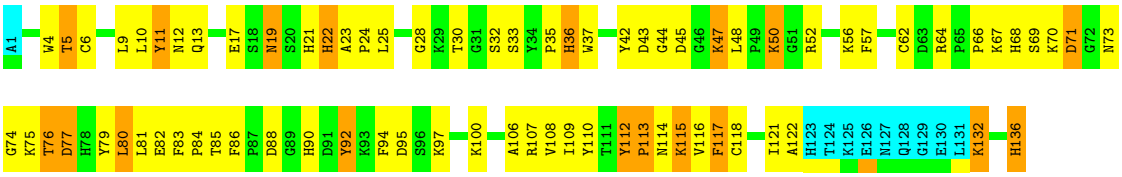
Chain A: 40% 37% 16% 7%



4.2.25 Score per residue for model 25

- Molecule 1: Ribonuclease alpha-sarcin

Chain A: 37% 43% 13% 7%



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 25 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
DYANA	structure solution	1.5
DYANA	refinement	1.5
Amber	refinement	7

No chemical shift data was provided.

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	0.71±0.08	0±0/1027 (0.0± 0.0%)	1.02±0.16	2±2/1389 (0.1± 0.2%)
All	All	0.72	2/25675 (0.0%)	1.03	39/34725 (0.1%)

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	0.6±0.9
All	All	0	14

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	62	CYS	CB-SG	-5.70	1.72	1.81	24	1
1	A	11	TYR	CE2-CZ	5.16	1.45	1.38	21	1

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	42	TYR	CB-CG-CD1	-9.40	115.36	121.00	21	4
1	A	64	ARG	NE-CZ-NH1	8.48	124.54	120.30	21	2
1	A	88	ASP	CB-CG-OD2	-7.53	111.52	118.30	3	6
1	A	76	THR	CA-CB-CG2	6.84	121.98	112.40	13	2
1	A	42	TYR	CB-CG-CD2	6.28	124.77	121.00	13	4
1	A	11	TYR	CB-CG-CD1	-6.23	117.26	121.00	21	1
1	A	34	TYR	CG-CD2-CE2	-6.13	116.40	121.30	15	1
1	A	94	PHE	CB-CG-CD2	-6.05	116.56	120.80	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	4	TRP	CD1-NE1-CE2	5.88	114.29	109.00	21	2
1	A	91	ASP	CB-CG-OD1	-5.72	113.15	118.30	1	4
1	A	91	ASP	CB-CG-OD2	-5.61	113.25	118.30	9	1
1	A	77	ASP	CB-CG-OD2	-5.58	113.28	118.30	13	1
1	A	112	TYR	CB-CG-CD1	-5.32	117.81	121.00	21	1
1	A	45	ASP	CB-CG-OD1	-5.32	113.52	118.30	16	2
1	A	27	ASP	CB-CG-OD1	-5.20	113.62	118.30	15	2
1	A	34	TYR	CZ-CE2-CD2	5.19	124.47	119.80	15	1
1	A	79	TYR	CB-CG-CD1	5.17	124.10	121.00	13	1
1	A	135	SER	CB-CA-C	5.16	119.90	110.10	13	1
1	A	90	HIS	CB-CA-C	5.14	120.68	110.40	13	1
1	A	94	PHE	CB-CG-CD1	-5.12	117.21	120.80	21	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	110	TYR	Sidechain	6
1	A	11	TYR	Sidechain	5
1	A	34	TYR	Sidechain	1
1	A	92	TYR	Sidechain	1
1	A	112	TYR	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	992	946	939	46±14
All	All	24800	23650	23475	1161

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:TYR:CE1	1:A:81:LEU:HD11	0.95	1.97	4	12
1:A:79:TYR:CZ	1:A:81:LEU:HD11	0.90	2.02	2	7
1:A:37:TRP:CH2	1:A:39:THR:HG22	0.89	2.02	6	24
1:A:79:TYR:CZ	1:A:81:LEU:HD21	0.85	2.07	20	8
1:A:37:TRP:CZ3	1:A:39:THR:HG22	0.83	2.09	4	21
1:A:106:ALA:HB2	1:A:122:ALA:HB2	0.82	1.51	21	1
1:A:79:TYR:CE2	1:A:81:LEU:HD21	0.82	2.10	14	8
1:A:81:LEU:HD22	1:A:110:TYR:CZ	0.81	2.11	17	5
1:A:79:TYR:CE2	1:A:81:LEU:HD11	0.81	2.11	19	5
1:A:35:PRO:HB2	1:A:81:LEU:HD13	0.79	1.53	12	1
1:A:106:ALA:HB1	1:A:120:ILE:CG2	0.78	2.07	12	6
1:A:11:TYR:CZ	1:A:106:ALA:HB3	0.76	2.15	21	15
1:A:25:LEU:HD21	1:A:113:PRO:O	0.76	1.79	10	8
1:A:3:THR:HG21	1:A:10:LEU:HD23	0.75	1.56	19	5
1:A:5:THR:OG1	1:A:10:LEU:HD13	0.75	1.81	23	3
1:A:35:PRO:HB2	1:A:81:LEU:HD11	0.74	1.60	24	5
1:A:121:ILE:HG22	1:A:133:LEU:HD12	0.74	1.59	11	9
1:A:62:CYS:SG	1:A:80:LEU:HD21	0.73	2.23	23	5
1:A:37:TRP:HA	1:A:81:LEU:HD23	0.72	1.62	20	2
1:A:23:ALA:HB1	1:A:35:PRO:HG3	0.71	1.61	24	19
1:A:80:LEU:HD23	1:A:110:TYR:C	0.70	2.07	20	10
1:A:48:LEU:HD22	1:A:52:ARG:HB3	0.70	1.63	10	1
1:A:41:GLY:C	1:A:48:LEU:HD23	0.69	2.08	10	9
1:A:34:TYR:CE2	1:A:36:HIS:CE1	0.69	2.80	6	4
1:A:36:HIS:C	1:A:81:LEU:HD23	0.69	2.08	19	6
1:A:24:PRO:HG2	1:A:30:THR:HG22	0.69	1.65	3	18
1:A:3:THR:HG23	1:A:10:LEU:HD23	0.68	1.64	11	1
1:A:6:CYS:SG	1:A:122:ALA:HB3	0.68	2.28	20	18
1:A:4:TRP:CZ2	1:A:136:HIS:CD2	0.68	2.81	4	4
1:A:6:CYS:HB3	1:A:122:ALA:HB3	0.68	1.65	14	4
1:A:62:CYS:HA	1:A:80:LEU:HD11	0.68	1.64	9	5
1:A:80:LEU:HD22	1:A:109:ILE:CG2	0.67	2.20	6	15
1:A:80:LEU:HD22	1:A:109:ILE:HG22	0.66	1.66	20	5
1:A:25:LEU:HD13	1:A:115:LYS:HE2	0.65	1.67	2	15
1:A:23:ALA:HB2	1:A:83:PHE:CZ	0.65	2.26	5	10
1:A:86:PHE:CD1	1:A:92:TYR:CD1	0.65	2.85	11	4
1:A:35:PRO:CB	1:A:81:LEU:HD11	0.65	2.22	24	1
1:A:86:PHE:CD2	1:A:90:HIS:CE1	0.65	2.85	10	1
1:A:80:LEU:HD22	1:A:109:ILE:HG23	0.64	1.68	1	1
1:A:37:TRP:CD1	1:A:79:TYR:CD2	0.64	2.85	23	7
1:A:25:LEU:HD13	1:A:115:LYS:CE	0.63	2.23	10	11
1:A:76:THR:O	1:A:76:THR:HG23	0.63	1.94	6	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:TYR:CE1	1:A:81:LEU:HD21	0.62	2.29	20	1
1:A:35:PRO:HB2	1:A:81:LEU:HD21	0.62	1.71	7	6
1:A:106:ALA:HB1	1:A:120:ILE:HG21	0.62	1.69	12	5
1:A:37:TRP:CD2	1:A:68:HIS:CD2	0.62	2.88	4	3
1:A:26:SER:O	1:A:81:LEU:HD12	0.62	1.94	17	1
1:A:42:TYR:N	1:A:48:LEU:HD23	0.62	2.10	14	7
1:A:42:TYR:CE1	1:A:48:LEU:HD11	0.62	2.30	25	5
1:A:106:ALA:HA	1:A:122:ALA:HB2	0.61	1.73	14	5
1:A:48:LEU:HD13	1:A:52:ARG:CD	0.61	2.25	14	1
1:A:23:ALA:HB2	1:A:83:PHE:CE2	0.61	2.31	7	5
1:A:25:LEU:HD13	1:A:115:LYS:HE3	0.61	1.73	10	2
1:A:13:GLN:NE2	1:A:117:PHE:CZ	0.60	2.69	10	25
1:A:48:LEU:HD13	1:A:52:ARG:NE	0.60	2.10	7	2
1:A:4:TRP:CH2	1:A:136:HIS:CE1	0.60	2.90	11	2
1:A:81:LEU:HD12	1:A:81:LEU:C	0.60	2.17	12	1
1:A:9:LEU:N	1:A:9:LEU:HD13	0.60	2.11	23	2
1:A:2:VAL:HG13	1:A:136:HIS:CD2	0.60	2.32	24	3
1:A:11:TYR:CE2	1:A:106:ALA:CB	0.59	2.85	6	21
1:A:120:ILE:HG22	1:A:134:CYS:SG	0.59	2.37	6	13
1:A:79:TYR:OH	1:A:81:LEU:HD21	0.59	1.98	6	2
1:A:9:LEU:HD23	1:A:11:TYR:OH	0.59	1.98	5	1
1:A:13:GLN:O	1:A:16:ALA:HB3	0.59	1.97	4	1
1:A:3:THR:CG2	1:A:10:LEU:HD23	0.58	2.28	11	1
1:A:57:PHE:CE1	1:A:133:LEU:HD13	0.58	2.32	6	6
1:A:80:LEU:HD23	1:A:110:TYR:O	0.58	1.98	4	8
1:A:62:CYS:HB3	1:A:80:LEU:HD11	0.58	1.74	20	2
1:A:38:PHE:CE2	1:A:109:ILE:HG21	0.58	2.34	10	3
1:A:34:TYR:CE1	1:A:36:HIS:CE1	0.58	2.92	3	1
1:A:79:TYR:HE2	1:A:81:LEU:HD21	0.57	1.58	14	5
1:A:36:HIS:O	1:A:81:LEU:HD23	0.57	1.98	19	3
1:A:108:VAL:HG23	1:A:117:PHE:CD1	0.57	2.34	22	3
1:A:10:LEU:C	1:A:10:LEU:HD22	0.57	2.20	11	1
1:A:4:TRP:CE2	1:A:136:HIS:CD2	0.57	2.92	4	4
1:A:37:TRP:CE3	1:A:68:HIS:CD2	0.56	2.92	4	1
1:A:116:VAL:HG12	1:A:116:VAL:O	0.56	1.99	6	9
1:A:48:LEU:HD13	1:A:52:ARG:HD2	0.56	1.78	14	1
1:A:38:PHE:CE1	1:A:121:ILE:CD1	0.55	2.89	2	8
1:A:35:PRO:CB	1:A:81:LEU:HD21	0.55	2.31	25	5
1:A:77:ASP:O	1:A:112:TYR:CD1	0.55	2.60	6	18
1:A:81:LEU:C	1:A:81:LEU:HD23	0.55	2.22	16	3
1:A:37:TRP:CZ2	1:A:39:THR:HG22	0.55	2.37	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:HD11	1:A:110:TYR:CZ	0.55	2.37	12	1
1:A:84:PRO:HG2	1:A:92:TYR:CD2	0.54	2.37	21	1
1:A:106:ALA:CB	1:A:122:ALA:HB2	0.54	2.27	21	1
1:A:109:ILE:HG12	1:A:121:ILE:HD13	0.54	1.78	2	3
1:A:42:TYR:HA	1:A:48:LEU:HD23	0.54	1.77	2	2
1:A:42:TYR:CA	1:A:48:LEU:HD23	0.54	2.33	2	2
1:A:26:SER:O	1:A:81:LEU:HD22	0.54	2.03	12	1
1:A:80:LEU:HD21	1:A:118:CYS:SG	0.54	2.43	4	3
1:A:57:PHE:CE2	1:A:133:LEU:HD13	0.53	2.38	10	4
1:A:3:THR:HG21	1:A:10:LEU:HD22	0.53	1.79	22	2
1:A:2:VAL:HG22	1:A:136:HIS:HB2	0.53	1.79	6	4
1:A:92:TYR:O	1:A:94:PHE:CD2	0.53	2.62	6	19
1:A:86:PHE:CE1	1:A:92:TYR:CD1	0.53	2.97	12	1
1:A:48:LEU:HD12	1:A:48:LEU:H	0.52	1.63	15	14
1:A:38:PHE:CZ	1:A:121:ILE:HD13	0.52	2.39	6	7
1:A:82:GLU:CB	1:A:109:ILE:CD1	0.52	2.87	6	11
1:A:48:LEU:HD11	1:A:54:PRO:HG3	0.52	1.80	8	1
1:A:112:TYR:CD1	1:A:112:TYR:C	0.52	2.83	6	20
1:A:38:PHE:CZ	1:A:121:ILE:CD1	0.52	2.92	24	4
1:A:23:ALA:HB2	1:A:83:PHE:CE1	0.52	2.40	3	3
1:A:41:GLY:HA3	1:A:48:LEU:HD23	0.52	1.82	18	5
1:A:35:PRO:CB	1:A:81:LEU:HD13	0.52	2.28	12	1
1:A:112:TYR:CG	1:A:113:PRO:HA	0.51	2.40	11	23
1:A:13:GLN:NE2	1:A:117:PHE:CE1	0.51	2.79	6	7
1:A:92:TYR:CD1	1:A:92:TYR:N	0.51	2.78	11	3
1:A:6:CYS:CB	1:A:122:ALA:HB3	0.51	2.36	21	1
1:A:42:TYR:CZ	1:A:48:LEU:HD11	0.51	2.40	25	1
1:A:57:PHE:CD1	1:A:118:CYS:HB3	0.51	2.41	12	15
1:A:86:PHE:CD1	1:A:92:TYR:CE1	0.51	2.99	15	3
1:A:81:LEU:HD22	1:A:110:TYR:CE2	0.50	2.40	17	1
1:A:61:ASP:OD2	1:A:116:VAL:HG11	0.50	2.06	16	1
1:A:41:GLY:CA	1:A:48:LEU:HD23	0.50	2.36	18	4
1:A:61:ASP:HB2	1:A:111:THR:HG21	0.50	1.82	13	2
1:A:16:ALA:HB1	1:A:120:ILE:HD11	0.50	1.83	22	3
1:A:84:PRO:O	1:A:92:TYR:CE2	0.50	2.64	24	4
1:A:8:GLY:C	1:A:9:LEU:HD13	0.50	2.27	23	3
1:A:76:THR:O	1:A:76:THR:CG2	0.50	2.60	6	5
1:A:11:TYR:CZ	1:A:106:ALA:CB	0.50	2.93	6	4
1:A:117:PHE:CZ	1:A:119:GLY:HA2	0.49	2.42	8	6
1:A:68:HIS:CE1	1:A:70:LYS:O	0.49	2.65	6	2
1:A:16:ALA:CB	1:A:120:ILE:HD11	0.49	2.37	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:PHE:CG	1:A:118:CYS:SG	0.49	3.06	24	7
1:A:78:HIS:H	1:A:78:HIS:CD2	0.49	2.23	15	6
1:A:57:PHE:CD1	1:A:62:CYS:SG	0.49	3.06	2	3
1:A:42:TYR:CD1	1:A:48:LEU:HG	0.49	2.43	7	2
1:A:57:PHE:CE2	1:A:62:CYS:SG	0.49	3.06	23	5
1:A:11:TYR:CE2	1:A:106:ALA:HB3	0.49	2.42	21	5
1:A:110:TYR:CD1	1:A:115:LYS:CG	0.48	2.96	3	13
1:A:37:TRP:CD1	1:A:79:TYR:HB2	0.48	2.43	25	7
1:A:86:PHE:CD2	1:A:90:HIS:NE2	0.48	2.81	4	5
1:A:38:PHE:CE1	1:A:121:ILE:HD13	0.48	2.43	10	1
1:A:20:SER:HB3	1:A:108:VAL:HG11	0.48	1.83	3	1
1:A:34:TYR:CD2	1:A:36:HIS:CD2	0.48	3.01	14	6
1:A:55:ILE:O	1:A:57:PHE:CE2	0.48	2.66	6	4
1:A:72:GLY:O	1:A:79:TYR:CE2	0.48	2.67	14	8
1:A:10:LEU:HD22	1:A:10:LEU:N	0.48	2.22	16	2
1:A:48:LEU:HD12	1:A:48:LEU:N	0.48	2.23	15	2
1:A:37:TRP:CH2	1:A:44:GLY:HA2	0.48	2.44	1	13
1:A:34:TYR:CD1	1:A:84:PRO:HD3	0.48	2.44	23	3
1:A:57:PHE:CD2	1:A:118:CYS:HB3	0.48	2.43	8	2
1:A:11:TYR:CE1	1:A:106:ALA:CB	0.48	2.97	11	1
1:A:37:TRP:CG	1:A:68:HIS:CD2	0.47	3.02	12	1
1:A:117:PHE:CE1	1:A:119:GLY:HA2	0.47	2.45	16	6
1:A:110:TYR:C	1:A:110:TYR:CD1	0.47	2.88	20	8
1:A:20:SER:O	1:A:23:ALA:HB3	0.47	2.09	3	3
1:A:9:LEU:HD22	1:A:9:LEU:H	0.47	1.68	5	3
1:A:16:ALA:O	1:A:108:VAL:HG11	0.47	2.09	3	1
1:A:77:ASP:OD2	1:A:79:TYR:CE1	0.47	2.68	22	1
1:A:42:TYR:CE2	1:A:47:LYS:HA	0.47	2.45	1	6
1:A:42:TYR:CD2	1:A:47:LYS:HA	0.47	2.44	25	2
1:A:83:PHE:CZ	1:A:94:PHE:CD1	0.47	3.02	21	1
1:A:2:VAL:CG1	1:A:136:HIS:CD2	0.47	2.97	24	3
1:A:110:TYR:CD1	1:A:115:LYS:HG3	0.47	2.45	6	11
1:A:80:LEU:HD21	1:A:111:THR:HG22	0.47	1.87	7	1
1:A:48:LEU:HD21	1:A:54:PRO:HG3	0.47	1.85	24	1
1:A:42:TYR:CD2	1:A:66:PRO:HD2	0.47	2.44	25	6
1:A:3:THR:CG2	1:A:10:LEU:HD12	0.47	2.41	7	1
1:A:42:TYR:CD2	1:A:66:PRO:CD	0.47	2.98	22	5
1:A:9:LEU:HD13	1:A:11:TYR:OH	0.47	2.08	9	1
1:A:25:LEU:HD23	1:A:112:TYR:CE2	0.47	2.45	17	1
1:A:81:LEU:CD2	1:A:110:TYR:CZ	0.46	2.98	3	2
1:A:37:TRP:CE3	1:A:68:HIS:NE2	0.46	2.83	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:TYR:CE2	1:A:66:PRO:CD	0.46	2.97	8	2
1:A:38:PHE:CZ	1:A:40:ASN:HA	0.46	2.45	20	1
1:A:120:ILE:N	1:A:120:ILE:HD12	0.46	2.25	16	4
1:A:48:LEU:HD13	1:A:52:ARG:CZ	0.46	2.41	7	1
1:A:34:TYR:CE1	1:A:107:ARG:CZ	0.46	2.99	17	1
1:A:117:PHE:CD1	1:A:117:PHE:C	0.46	2.89	10	4
1:A:83:PHE:CD1	1:A:84:PRO:HD2	0.46	2.45	25	5
1:A:10:LEU:HD22	1:A:10:LEU:H	0.46	1.71	16	3
1:A:112:TYR:CD1	1:A:113:PRO:N	0.46	2.84	6	6
1:A:37:TRP:CA	1:A:81:LEU:HD23	0.46	2.39	20	1
1:A:17:GLU:O	1:A:21:HIS:CD2	0.46	2.68	25	8
1:A:37:TRP:CE3	1:A:39:THR:HG22	0.46	2.44	4	3
1:A:45:ASP:OD2	1:A:67:LYS:CE	0.46	2.64	6	1
1:A:83:PHE:CE2	1:A:92:TYR:CE2	0.46	3.04	25	2
1:A:25:LEU:HD13	1:A:112:TYR:CE2	0.46	2.46	13	1
1:A:81:LEU:HD12	1:A:82:GLU:N	0.46	2.26	24	1
1:A:38:PHE:CE2	1:A:121:ILE:HD13	0.46	2.46	7	1
1:A:85:THR:HG22	1:A:107:ARG:HA	0.46	1.87	11	2
1:A:16:ALA:HA	1:A:85:THR:HG21	0.45	1.88	8	2
1:A:19:ASN:CG	1:A:92:TYR:CZ	0.45	2.89	25	3
1:A:79:TYR:CE2	1:A:81:LEU:CD2	0.45	2.94	14	1
1:A:114:ASN:O	1:A:116:VAL:HG23	0.45	2.10	20	4
1:A:10:LEU:HD13	1:A:10:LEU:N	0.45	2.26	5	1
1:A:42:TYR:CD2	1:A:66:PRO:HG3	0.45	2.45	6	2
1:A:22:HIS:CD2	1:A:22:HIS:N	0.45	2.85	4	12
1:A:19:ASN:ND2	1:A:83:PHE:CE1	0.45	2.85	17	1
1:A:38:PHE:CE2	1:A:40:ASN:HB2	0.45	2.45	10	7
1:A:2:VAL:HG11	1:A:136:HIS:CD2	0.45	2.47	17	1
1:A:35:PRO:HB2	1:A:81:LEU:CD1	0.45	2.37	24	1
1:A:77:ASP:OD2	1:A:79:TYR:CD2	0.45	2.70	6	1
1:A:27:ASP:HB2	1:A:79:TYR:CE2	0.45	2.47	16	1
1:A:34:TYR:CD2	1:A:84:PRO:HD3	0.45	2.47	14	7
1:A:42:TYR:CE2	1:A:66:PRO:HD3	0.45	2.47	14	7
1:A:4:TRP:CE2	1:A:136:HIS:ND1	0.45	2.85	14	3
1:A:9:LEU:HD13	1:A:9:LEU:N	0.45	2.26	5	1
1:A:9:LEU:C	1:A:10:LEU:HD22	0.45	2.31	23	1
1:A:34:TYR:CD1	1:A:36:HIS:CD2	0.45	3.05	23	2
1:A:14:ASN:O	1:A:18:SER:CB	0.45	2.64	6	5
1:A:4:TRP:CZ2	1:A:136:HIS:CE1	0.45	3.05	14	2
1:A:78:HIS:CD2	1:A:78:HIS:H	0.45	2.29	14	1
1:A:38:PHE:CE1	1:A:40:ASN:HA	0.45	2.47	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ILE:CG2	1:A:134:CYS:SG	0.44	3.05	6	3
1:A:37:TRP:CZ2	1:A:44:GLY:HA2	0.44	2.47	7	2
1:A:68:HIS:CE1	1:A:69:SER:O	0.44	2.70	25	5
1:A:4:TRP:CD2	1:A:136:HIS:HB3	0.44	2.48	4	2
1:A:38:PHE:CD2	1:A:40:ASN:HB2	0.44	2.48	10	1
1:A:73:ASN:OD1	1:A:79:TYR:CE1	0.44	2.71	10	1
1:A:68:HIS:HA	1:A:77:ASP:OD2	0.44	2.12	13	1
1:A:37:TRP:CE3	1:A:68:HIS:CE1	0.44	3.05	18	1
1:A:5:THR:OG1	1:A:10:LEU:HD12	0.44	2.12	25	1
1:A:37:TRP:CH2	1:A:39:THR:CG2	0.44	2.91	6	1
1:A:90:HIS:O	1:A:92:TYR:CE1	0.44	2.71	11	3
1:A:85:THR:HA	1:A:92:TYR:CZ	0.44	2.48	24	1
1:A:109:ILE:HD12	1:A:109:ILE:N	0.43	2.28	10	2
1:A:34:TYR:CD1	1:A:84:PRO:HG3	0.43	2.48	24	1
1:A:42:TYR:CE1	1:A:48:LEU:CD1	0.43	3.02	20	2
1:A:2:VAL:HG22	1:A:3:THR:H	0.43	1.72	4	1
1:A:15:LYS:O	1:A:19:ASN:CB	0.43	2.67	4	1
1:A:64:ARG:HD3	1:A:78:HIS:CE1	0.43	2.48	23	1
1:A:110:TYR:CD1	1:A:110:TYR:C	0.43	2.91	16	5
1:A:36:HIS:N	1:A:36:HIS:CD2	0.43	2.86	25	2
1:A:3:THR:HG21	1:A:10:LEU:HD12	0.43	1.91	7	1
1:A:11:TYR:CE2	1:A:106:ALA:HB2	0.43	2.49	25	3
1:A:56:LYS:O	1:A:133:LEU:HD22	0.43	2.13	10	1
1:A:92:TYR:CD2	1:A:94:PHE:HB3	0.43	2.48	6	3
1:A:86:PHE:CZ	1:A:92:TYR:CD1	0.43	3.06	12	1
1:A:73:ASN:ND2	1:A:112:TYR:CZ	0.43	2.87	11	1
1:A:25:LEU:HD22	1:A:115:LYS:HE2	0.43	1.90	23	2
1:A:19:ASN:HA	1:A:22:HIS:CE1	0.42	2.48	11	10
1:A:4:TRP:CE2	1:A:136:HIS:CG	0.42	3.06	4	1
1:A:4:TRP:CD2	1:A:120:ILE:HG13	0.42	2.49	4	1
1:A:13:GLN:OE1	1:A:117:PHE:CZ	0.42	2.72	4	1
1:A:62:CYS:HB3	1:A:80:LEU:HD21	0.42	1.90	19	2
1:A:9:LEU:C	1:A:10:LEU:HD13	0.42	2.35	5	1
1:A:108:VAL:C	1:A:109:ILE:HD12	0.42	2.35	10	4
1:A:55:ILE:O	1:A:57:PHE:CE1	0.42	2.73	24	4
1:A:30:THR:HG21	1:A:35:PRO:HD2	0.42	1.91	22	2
1:A:36:HIS:CD2	1:A:82:GLU:CD	0.42	2.93	6	1
1:A:41:GLY:O	1:A:48:LEU:HD23	0.42	2.15	8	1
1:A:57:PHE:CE1	1:A:62:CYS:SG	0.42	3.13	24	1
1:A:68:HIS:CD2	1:A:72:GLY:O	0.42	2.72	3	1
1:A:38:PHE:CE2	1:A:121:ILE:CD1	0.42	3.02	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:TRP:NE1	1:A:13:GLN:NE2	0.42	2.68	6	2
1:A:90:HIS:CD2	1:A:90:HIS:O	0.42	2.73	6	1
1:A:34:TYR:CE1	1:A:103:PRO:HB3	0.42	2.50	11	1
1:A:37:TRP:CE3	1:A:68:HIS:ND1	0.42	2.88	18	1
1:A:29:LYS:O	1:A:29:LYS:CG	0.42	2.67	6	1
1:A:38:PHE:CD2	1:A:109:ILE:CG2	0.42	3.03	10	1
1:A:37:TRP:CD2	1:A:68:HIS:CG	0.42	3.07	18	1
1:A:36:HIS:CD2	1:A:82:GLU:OE1	0.42	2.73	23	1
1:A:82:GLU:HB2	1:A:109:ILE:HD11	0.42	1.92	25	1
1:A:57:PHE:CD2	1:A:62:CYS:SG	0.42	3.13	22	1
1:A:27:ASP:OD1	1:A:27:ASP:N	0.42	2.53	3	1
1:A:20:SER:CB	1:A:108:VAL:HG11	0.41	2.45	3	1
1:A:76:THR:O	1:A:77:ASP:C	0.41	2.58	25	4
1:A:108:VAL:HG23	1:A:117:PHE:CD2	0.41	2.50	10	1
1:A:19:ASN:OD1	1:A:83:PHE:CD2	0.41	2.73	6	1
1:A:81:LEU:HD11	1:A:110:TYR:CE2	0.41	2.49	12	1
1:A:34:TYR:CE1	1:A:107:ARG:NE	0.41	2.88	16	1
1:A:4:TRP:CE3	1:A:120:ILE:HG13	0.41	2.49	4	1
1:A:25:LEU:HD13	1:A:115:LYS:HD3	0.41	1.92	11	1
1:A:9:LEU:HB2	1:A:11:TYR:CZ	0.41	2.50	23	1
1:A:4:TRP:CE2	1:A:13:GLN:NE2	0.41	2.89	6	1
1:A:37:TRP:CZ3	1:A:39:THR:CG2	0.41	3.04	11	2
1:A:97:LYS:CG	1:A:98:LYS:N	0.41	2.84	6	1
1:A:81:LEU:HG	1:A:110:TYR:CE1	0.41	2.49	12	1
1:A:36:HIS:CD2	1:A:82:GLU:OE2	0.41	2.72	4	1
1:A:10:LEU:O	1:A:11:TYR:CD1	0.41	2.74	21	2
1:A:73:ASN:ND2	1:A:73:ASN:H	0.41	2.13	13	1
1:A:3:THR:CG2	1:A:10:LEU:HD22	0.41	2.45	18	1
1:A:34:TYR:CE2	1:A:107:ARG:CZ	0.41	3.03	22	1
1:A:73:ASN:ND2	1:A:73:ASN:N	0.41	2.68	24	1
1:A:62:CYS:SG	1:A:80:LEU:HD11	0.41	2.56	4	1
1:A:110:TYR:CG	1:A:115:LYS:HG2	0.41	2.51	4	5
1:A:19:ASN:O	1:A:83:PHE:CE2	0.41	2.74	6	1
1:A:27:ASP:HB3	1:A:72:GLY:CA	0.41	2.46	16	2
1:A:82:GLU:HB3	1:A:109:ILE:CD1	0.41	2.46	20	2
1:A:83:PHE:HB3	1:A:108:VAL:HG12	0.41	1.93	25	1
1:A:62:CYS:SG	1:A:80:LEU:CD2	0.41	3.08	22	1
1:A:25:LEU:CD1	1:A:115:LYS:HE2	0.41	2.46	24	1
1:A:57:PHE:CE2	1:A:133:LEU:CD1	0.40	3.04	10	1
1:A:35:PRO:HB2	1:A:81:LEU:CD2	0.40	2.44	25	2
1:A:48:LEU:CB	1:A:49:PRO:CD	0.40	2.99	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:HIS:O	1:A:90:HIS:CD2	0.40	2.75	23	1
1:A:48:LEU:HD13	1:A:54:PRO:HG3	0.40	1.93	6	1
1:A:71:ASP:O	1:A:72:GLY:C	0.40	2.59	12	1
1:A:121:ILE:HG22	1:A:133:LEU:CD1	0.40	2.46	1	1
1:A:9:LEU:HD12	1:A:11:TYR:OH	0.40	2.16	3	1
1:A:25:LEU:HD12	1:A:25:LEU:HA	0.40	1.83	4	1
1:A:4:TRP:CZ2	1:A:117:PHE:CZ	0.40	3.10	11	1
1:A:10:LEU:N	1:A:10:LEU:CD2	0.40	2.85	23	1
1:A:2:VAL:HG22	1:A:3:THR:N	0.40	2.32	24	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	125/136 (92%)	85±4 (68±3%)	28±3 (22±3%)	12±2 (9±2%)	1 11
All	All	3125/3400 (92%)	2137 (68%)	696 (22%)	292 (9%)	1 11

All 30 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	33	SER	25
1	A	77	ASP	25
1	A	75	LYS	23
1	A	71	ASP	21
1	A	74	GLY	19
1	A	113	PRO	19
1	A	25	LEU	17
1	A	105	PRO	17
1	A	44	GLY	16
1	A	47	LYS	13
1	A	50	LYS	12
1	A	115	LYS	12
1	A	103	PRO	10

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Mol	Chain	Res	Type	Models (Total)
1	A	117	PHE	10
1	A	91	ASP	7
1	A	8	GLY	7
1	A	134	CYS	6
1	A	46	GLY	6
1	A	79	TYR	5
1	A	2	VAL	4
1	A	7	GLY	4
1	A	42	TYR	3
1	A	28	GLY	2
1	A	92	TYR	2
1	A	31	GLY	2
1	A	16	ALA	1
1	A	45	ASP	1
1	A	69	SER	1
1	A	72	GLY	1
1	A	70	LYS	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	108/116 (93%)	76±4 (70±3%)	32±4 (30±3%)	1 17
All	All	2700/2900 (93%)	1902 (70%)	798 (30%)	1 17

All 67 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	22	HIS	25
1	A	76	THR	25
1	A	64	ARG	24
1	A	112	TYR	24
1	A	115	LYS	24
1	A	43	ASP	23
1	A	45	ASP	23
1	A	70	LYS	21

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Mol	Chain	Res	Type	Models (Total)
1	A	5	THR	20
1	A	26	SER	20
1	A	71	ASP	20
1	A	80	LEU	20
1	A	6	CYS	19
1	A	93	LYS	19
1	A	69	SER	19
1	A	36	HIS	18
1	A	52	ARG	18
1	A	20	SER	17
1	A	132	LYS	17
1	A	12	ASN	17
1	A	56	LYS	17
1	A	100	LYS	17
1	A	48	LEU	16
1	A	136	HIS	16
1	A	61	ASP	15
1	A	59	LYS	14
1	A	79	TYR	14
1	A	88	ASP	14
1	A	27	ASP	13
1	A	118	CYS	13
1	A	15	LYS	13
1	A	82	GLU	12
1	A	98	LYS	12
1	A	47	LYS	11
1	A	73	ASN	11
1	A	107	ARG	11
1	A	9	LEU	11
1	A	33	SER	11
1	A	29	LYS	11
1	A	50	LYS	11
1	A	81	LEU	10
1	A	85	THR	9
1	A	102	ASN	9
1	A	97	LYS	8
1	A	13	GLN	7
1	A	96	SER	7
1	A	10	LEU	6
1	A	95	ASP	6
1	A	67	LYS	6
1	A	101	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	60	SER	5
1	A	78	HIS	5
1	A	19	ASN	5
1	A	92	TYR	5
1	A	135	SER	4
1	A	3	THR	4
1	A	2	VAL	3
1	A	91	ASP	3
1	A	77	ASP	3
1	A	14	ASN	2
1	A	32	SER	2
1	A	25	LEU	2
1	A	90	HIS	2
1	A	62	CYS	1
1	A	30	THR	1
1	A	17	GLU	1
1	A	120	ILE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided