



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 02:53 AM UTC

PDB ID : 1DE3 / pdb_00001de3
Title : SOLUTION STRUCTURE OF THE CYTOTOXIC RIBONUCLEASE
ALPHA-SARCIN
Authors : Perez-Canadillas, J.M.; Campos-Olivas, R.; Santoro, J.; Lacadena, J.; Mar-
tinez del Pozo, A.; Gavilanes, J.G.; Rico, M.; Bruix, M.
Deposited on : 1999-11-12

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	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

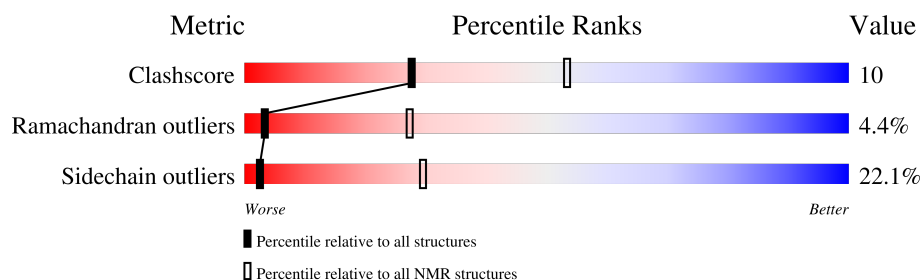
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	150	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 4 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:58, A:67-A:150 (141)	0.61	4

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

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

NmrClust was unable to cluster the ensemble.

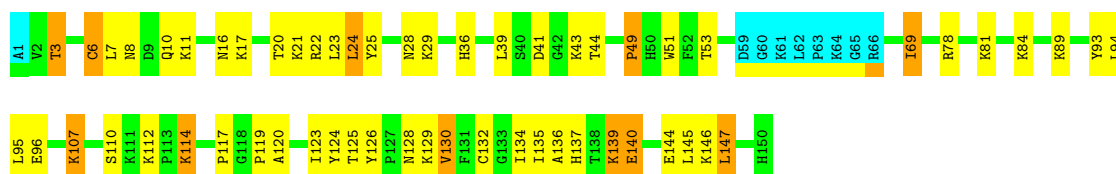
Error message: Inconsistent models

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2355 atoms, of which 1155 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RIBONUCLEASE ALPHA-SARCIN.

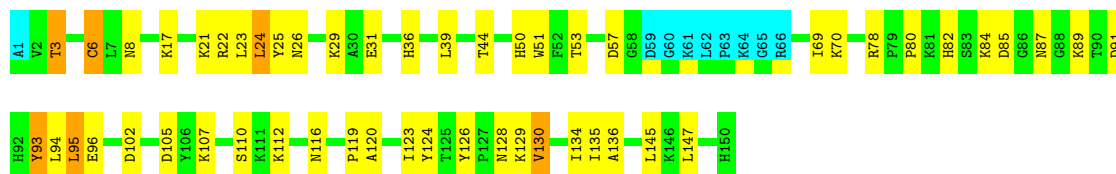
Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2355	755	1155	214	227	4	



4.2.3 Score per residue for model 3

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN

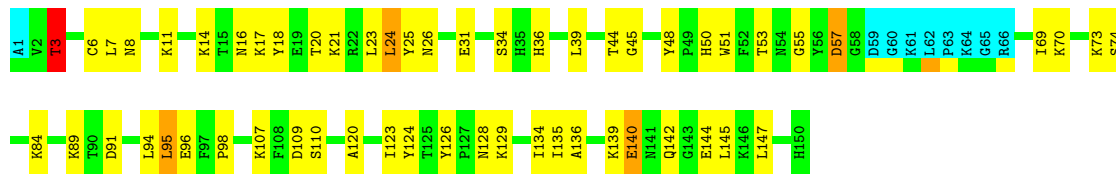
Chain A: 59% 31% 6%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN

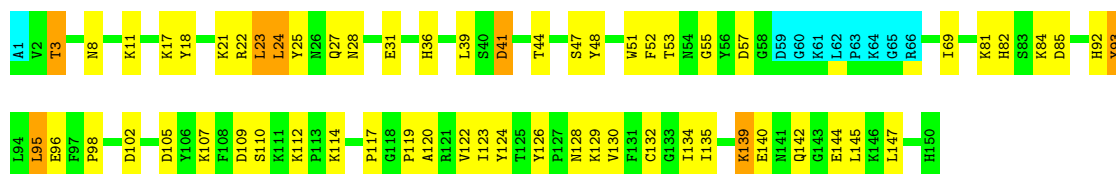
Chain A: 57% 34% 6%



4.2.5 Score per residue for model 5

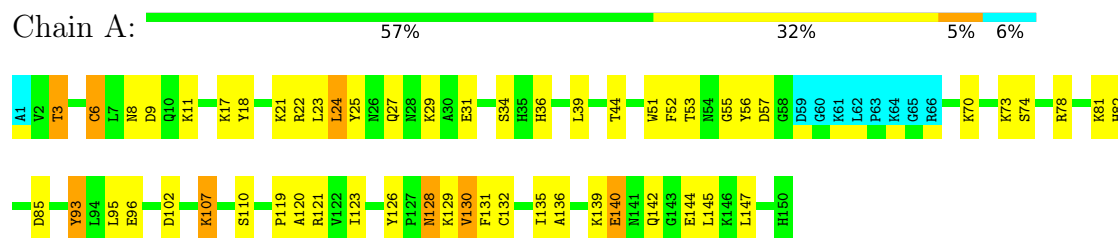
- Molecule 1: RIBONUCLEASE ALPHA-SARCIN

Chain A: 54% 35% 5% 6%



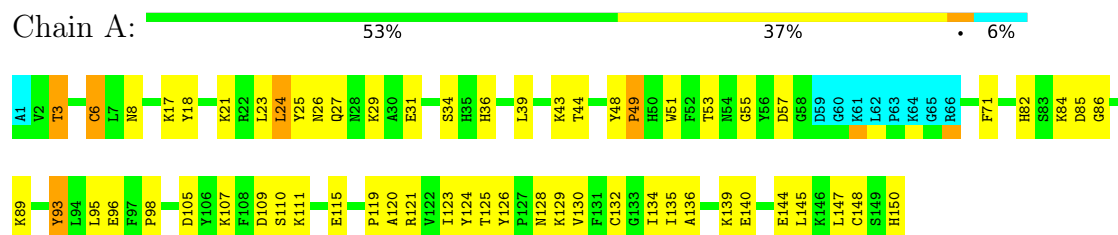
4.2.6 Score per residue for model 6

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



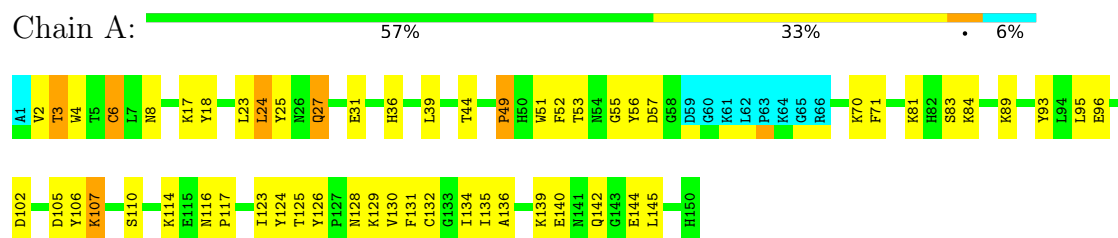
4.2.7 Score per residue for model 7

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



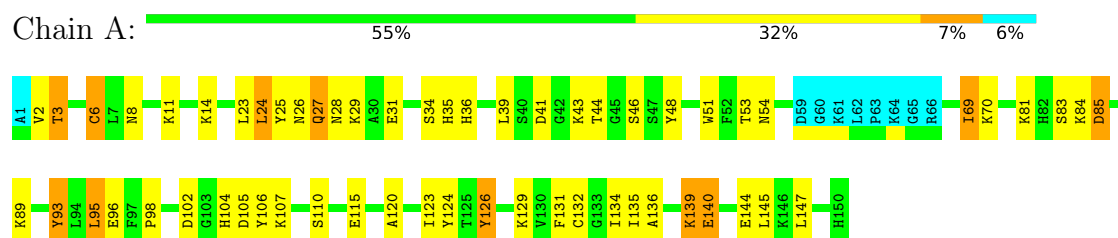
4.2.8 Score per residue for model 8

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



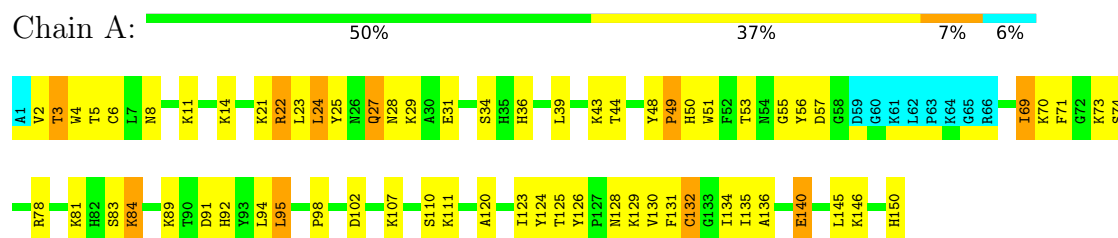
4.2.9 Score per residue for model 9

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



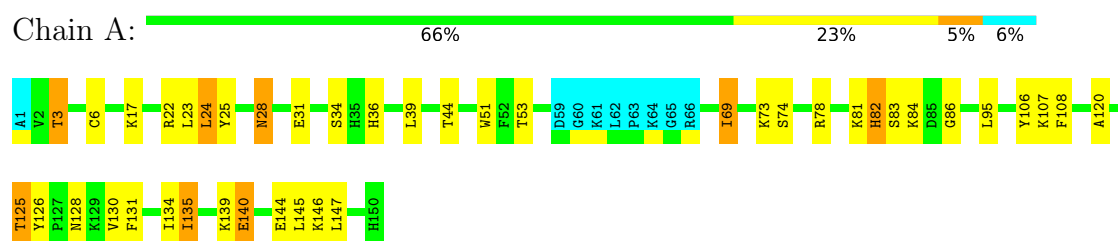
4.2.10 Score per residue for model 10

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



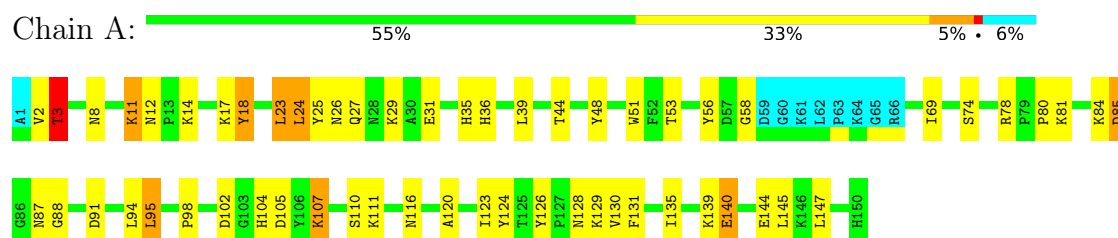
4.2.11 Score per residue for model 11

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



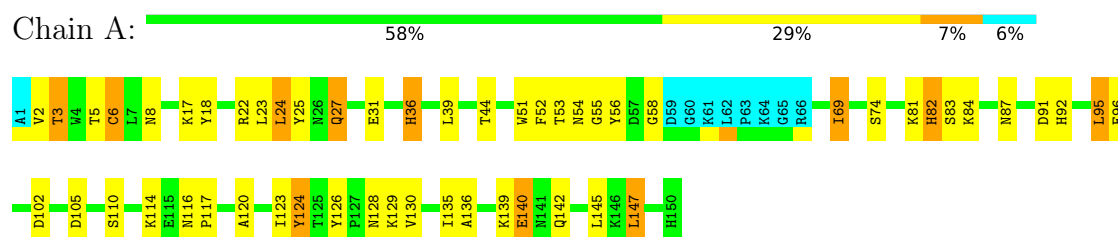
4.2.12 Score per residue for model 12

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



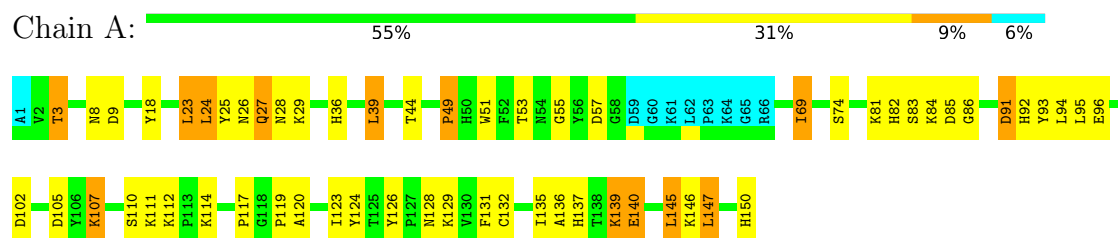
4.2.13 Score per residue for model 13

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



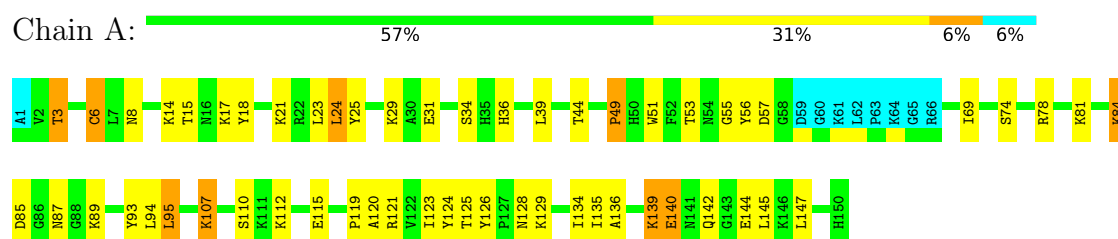
4.2.14 Score per residue for model 14

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



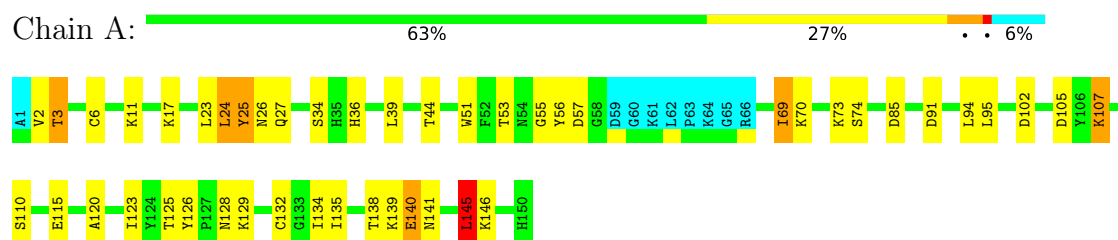
4.2.15 Score per residue for model 15

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



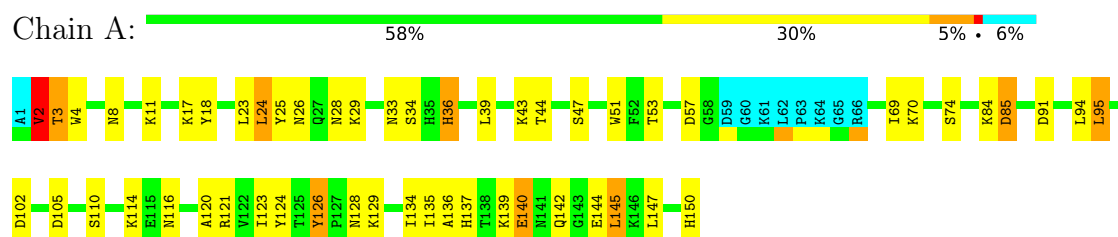
4.2.16 Score per residue for model 16

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



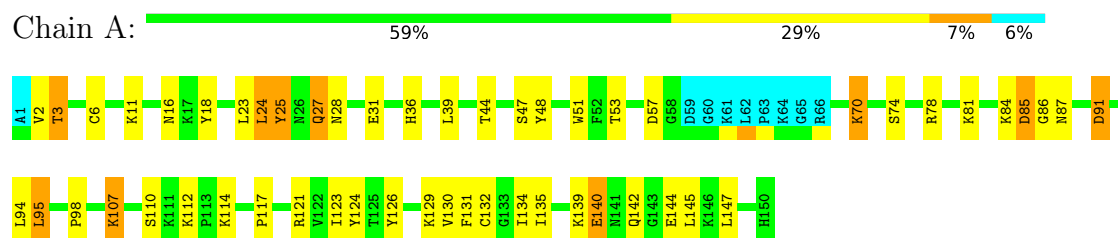
4.2.17 Score per residue for model 17

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



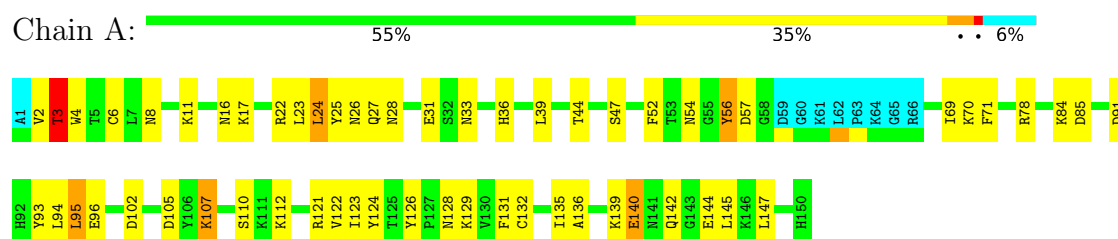
4.2.18 Score per residue for model 18

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



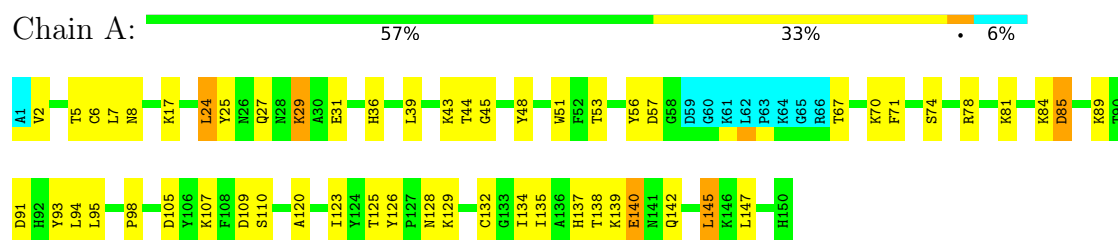
4.2.19 Score per residue for model 19

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



4.2.20 Score per residue for model 20

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



5 Refinement protocol and experimental data overview

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

Of the 47 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
GROMOS	structure solution	97
GROMOS	refinement	97

No chemical shift data was provided.

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	1.01±0.01	1±1/1172 (0.1± 0.1%)	1.25±0.02	1±1/1585 (0.0± 0.0%)
All	All	1.01	29/23440 (0.1%)	1.25	12/31700 (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	1.8±1.0
All	All	0	35

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	150	HIS	CG-ND1	-5.58	1.32	1.38	10	3
1	A	92	HIS	CG-ND1	-5.47	1.32	1.38	5	4
1	A	104	HIS	CG-ND1	-5.41	1.32	1.38	12	2
1	A	50	HIS	CD2-NE2	-5.39	1.31	1.37	10	3
1	A	137	HIS	CD2-NE2	-5.37	1.31	1.37	2	1
1	A	36	HIS	CG-ND1	-5.34	1.32	1.38	13	2
1	A	82	HIS	CG-ND1	-5.32	1.32	1.38	14	5
1	A	50	HIS	CG-ND1	-5.31	1.32	1.38	10	1
1	A	104	HIS	CD2-NE2	-5.28	1.32	1.37	9	2
1	A	35	HIS	CG-ND1	-5.27	1.32	1.38	9	1
1	A	150	HIS	CD2-NE2	-5.20	1.32	1.37	17	1
1	A	35	HIS	CD2-NE2	-5.20	1.32	1.37	12	1
1	A	137	HIS	CG-ND1	-5.14	1.32	1.38	20	2
1	A	82	HIS	CD2-NE2	-5.09	1.32	1.37	6	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(°)	Ideal(°)	Models	
								Worst	Total
1	A	85	ASP	CA-CB-CG	6.57	119.17	112.60	20	5
1	A	91	ASP	CA-CB-CG	6.28	118.88	112.60	14	1
1	A	87	ASN	OD1-CG-ND2	-5.63	116.97	122.60	15	1
1	A	33	ASN	CA-CB-CG	-5.30	107.30	112.60	17	1
1	A	137	HIS	CB-CG-CD2	-5.23	124.41	131.20	14	1
1	A	3	THR	CA-CB-CG2	5.15	119.26	110.50	12	3

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	34	SER	Mainchain	8
1	A	93	TYR	Sidechain	7
1	A	49	PRO	Mainchain	6
1	A	28	ASN	Mainchain	4
1	A	56	TYR	Sidechain	3
1	A	29	LYS	Mainchain	2
1	A	25	TYR	Sidechain	2
1	A	131	PHE	Sidechain	1
1	A	81	LYS	Mainchain	1
1	A	124	TYR	Sidechain	1

6.2 Too-close contacts ⓘ

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	1135	1083	1075	21±4
All	All	22700	21660	21500	429

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:49:PRO:HB2	1:A:95:LEU:HD13	0.87	1.44	10	6
1:A:3:THR:HG23	1:A:24:LEU:HD23	0.82	1.51	17	19
1:A:95:LEU:HD11	1:A:124:TYR:CZ	0.75	2.16	8	6
1:A:8:ASN:HD21	1:A:136:ALA:HB1	0.69	1.48	2	11
1:A:135:ILE:HD12	1:A:145:LEU:HD22	0.69	1.64	8	8
1:A:135:ILE:HD13	1:A:145:LEU:HD22	0.66	1.67	5	4
1:A:135:ILE:HG22	1:A:147:LEU:HA	0.65	1.69	11	14
1:A:51:TRP:CZ3	1:A:53:THR:HG22	0.64	2.28	13	7
1:A:39:LEU:HD11	1:A:129:LYS:HD2	0.61	1.71	8	19
1:A:70:LYS:O	1:A:147:LEU:HD22	0.61	1.95	20	5
1:A:25:TYR:CZ	1:A:120:ALA:HB3	0.61	2.30	11	17
1:A:95:LEU:HD11	1:A:124:TYR:OH	0.61	1.94	7	6
1:A:95:LEU:HD12	1:A:124:TYR:O	0.61	1.95	9	8
1:A:95:LEU:HD12	1:A:95:LEU:C	0.60	2.21	10	5
1:A:123:ILE:HD11	1:A:135:ILE:HD11	0.60	1.72	17	5
1:A:24:LEU:HD22	1:A:25:TYR:N	0.60	2.12	19	19
1:A:69:ILE:HG21	1:A:135:ILE:HG21	0.59	1.74	11	4
1:A:95:LEU:C	1:A:95:LEU:HD12	0.58	2.23	15	1
1:A:95:LEU:HD13	1:A:124:TYR:CE2	0.58	2.33	12	10
1:A:2:VAL:HG12	1:A:4:TRP:CD1	0.58	2.34	17	1
1:A:78:ARG:HH21	1:A:125:THR:HG21	0.57	1.60	11	1
1:A:69:ILE:HD11	1:A:145:LEU:O	0.56	2.00	9	10
1:A:48:TYR:CD2	1:A:98:PRO:HD3	0.56	2.35	12	1
1:A:96:GLU:OE2	1:A:123:ILE:HD11	0.56	2.00	1	7
1:A:51:TRP:CH2	1:A:53:THR:HG22	0.56	2.36	7	14
1:A:39:LEU:HB3	1:A:126:TYR:CD2	0.55	2.36	8	3
1:A:94:LEU:HD22	1:A:123:ILE:HG22	0.55	1.78	15	11
1:A:124:TYR:CD2	1:A:129:LYS:HG2	0.55	2.36	7	2
1:A:114:LYS:NZ	1:A:117:PRO:HD3	0.55	2.17	18	6
1:A:39:LEU:HD22	1:A:126:TYR:HD1	0.54	1.62	20	6
1:A:6:CYS:SG	1:A:136:ALA:HB3	0.54	2.43	13	9
1:A:48:TYR:CD1	1:A:98:PRO:HD3	0.53	2.39	18	5
1:A:39:LEU:HD22	1:A:126:TYR:CD1	0.52	2.39	19	17
1:A:27:GLN:HG3	1:A:131:PHE:CZ	0.52	2.39	8	2
1:A:4:TRP:CD1	1:A:27:GLN:HB2	0.52	2.40	19	3
1:A:82:HIS:CD2	1:A:86:GLY:HA2	0.52	2.40	11	1
1:A:52:PHE:HB2	1:A:96:GLU:HB2	0.52	1.79	5	5
1:A:39:LEU:HD22	1:A:126:TYR:CD2	0.52	2.39	9	2
1:A:95:LEU:H	1:A:95:LEU:HD12	0.51	1.65	19	4
1:A:128:ASN:HB3	1:A:130:VAL:HG23	0.51	1.82	6	7
1:A:87:ASN:O	1:A:91:ASP:HB2	0.50	2.07	18	3
1:A:123:ILE:HD11	1:A:135:ILE:HG12	0.50	1.84	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LEU:HD12	1:A:95:LEU:H	0.50	1.67	5	6
1:A:5:THR:HG21	1:A:22:ARG:HD2	0.50	1.83	10	1
1:A:69:ILE:HG21	1:A:135:ILE:CG2	0.49	2.37	17	2
1:A:3:THR:HG23	1:A:24:LEU:CD2	0.49	2.33	17	3
1:A:39:LEU:HB3	1:A:126:TYR:CD1	0.49	2.42	13	15
1:A:93:TYR:CE2	1:A:95:LEU:HB3	0.49	2.42	2	1
1:A:25:TYR:CE1	1:A:120:ALA:HB3	0.48	2.43	2	3
1:A:8:ASN:OD1	1:A:23:LEU:HD22	0.48	2.08	5	3
1:A:71:PHE:CD2	1:A:147:LEU:HD13	0.48	2.44	7	1
1:A:39:LEU:HD23	1:A:95:LEU:HD21	0.48	1.84	15	3
1:A:7:LEU:HB3	1:A:20:THR:HG22	0.47	1.86	2	2
1:A:95:LEU:HD11	1:A:126:TYR:CB	0.47	2.40	19	1
1:A:27:GLN:HG3	1:A:131:PHE:CE2	0.47	2.44	10	5
1:A:124:TYR:HD2	1:A:129:LYS:HG2	0.47	1.70	13	1
1:A:53:THR:O	1:A:56:TYR:CD2	0.46	2.67	10	4
1:A:122:VAL:O	1:A:123:ILE:HD13	0.46	2.10	5	2
1:A:93:TYR:CE1	1:A:95:LEU:HG	0.45	2.47	9	2
1:A:135:ILE:HD12	1:A:135:ILE:O	0.45	2.10	19	1
1:A:48:TYR:CD2	1:A:98:PRO:HG3	0.45	2.46	20	3
1:A:135:ILE:HD12	1:A:145:LEU:HB3	0.45	1.87	1	1
1:A:41:ASP:HB2	1:A:93:TYR:CZ	0.45	2.46	9	2
1:A:93:TYR:CE1	1:A:95:LEU:HB3	0.45	2.47	8	1
1:A:71:PHE:CD1	1:A:147:LEU:HD13	0.45	2.47	20	2
1:A:96:GLU:OE2	1:A:135:ILE:HD11	0.45	2.11	8	4
1:A:131:PHE:CD1	1:A:131:PHE:C	0.45	2.95	19	1
1:A:69:ILE:HG23	1:A:147:LEU:HB2	0.44	1.88	11	1
1:A:120:ALA:HB2	1:A:136:ALA:HB2	0.44	1.89	2	1
1:A:39:LEU:HD21	1:A:129:LYS:HE3	0.44	1.88	7	1
1:A:39:LEU:HD22	1:A:126:TYR:HD2	0.44	1.72	9	2
1:A:5:THR:HG23	1:A:24:LEU:HB3	0.44	1.88	20	1
1:A:34:SER:HB2	1:A:124:TYR:CZ	0.44	2.46	7	2
1:A:71:PHE:HA	1:A:147:LEU:HD22	0.44	1.89	7	1
1:A:52:PHE:CE2	1:A:54:ASN:ND2	0.44	2.85	13	1
1:A:49:PRO:CB	1:A:95:LEU:HD13	0.44	2.35	2	1
1:A:95:LEU:HD11	1:A:126:TYR:HB2	0.44	1.89	19	3
1:A:39:LEU:HB3	1:A:126:TYR:CE1	0.44	2.47	11	4
1:A:71:PHE:CZ	1:A:123:ILE:HG21	0.44	2.48	10	4
1:A:24:LEU:HD22	1:A:24:LEU:C	0.43	2.38	7	7
1:A:93:TYR:OH	1:A:95:LEU:HD23	0.43	2.13	9	2
1:A:45:GLY:HA3	1:A:109:ASP:O	0.43	2.13	4	2
1:A:94:LEU:HD21	1:A:132:CYS:SG	0.43	2.54	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:O	1:A:138:THR:HG22	0.43	2.14	20	1
1:A:95:LEU:HD13	1:A:124:TYR:CD2	0.43	2.49	9	1
1:A:80:PRO:HB2	1:A:93:TYR:HA	0.42	1.91	3	1
1:A:69:ILE:HD13	1:A:135:ILE:HG21	0.42	1.91	4	1
1:A:27:GLN:HE21	1:A:28:ASN:N	0.42	2.12	18	1
1:A:56:TYR:CE2	1:A:80:PRO:HD2	0.42	2.49	12	1
1:A:93:TYR:CE2	1:A:95:LEU:HG	0.42	2.49	19	2
1:A:71:PHE:CD1	1:A:132:CYS:HB3	0.42	2.49	10	1
1:A:124:TYR:CE2	1:A:129:LYS:HE2	0.42	2.50	8	1
1:A:96:GLU:OE1	1:A:135:ILE:HD11	0.42	2.15	7	1
1:A:6:CYS:HB3	1:A:136:ALA:HB3	0.41	1.90	10	1
1:A:11:LYS:HD3	1:A:18:TYR:CD2	0.41	2.50	12	1
1:A:138:THR:HG23	1:A:146:LYS:HB2	0.41	1.91	16	1
1:A:7:LEU:HD23	1:A:21:LYS:O	0.41	2.15	4	1
1:A:5:THR:HG21	1:A:22:ARG:HD3	0.41	1.90	13	1
1:A:82:HIS:CD2	1:A:86:GLY:HA3	0.41	2.50	7	1
1:A:54:ASN:ND2	1:A:94:LEU:HD12	0.41	2.30	19	1
1:A:9:ASP:HB3	1:A:139:LYS:HA	0.41	1.92	14	1
1:A:3:THR:CG2	1:A:24:LEU:HD23	0.41	2.45	16	1
1:A:96:GLU:CG	1:A:121:ARG:HD2	0.41	2.46	6	1
1:A:96:GLU:CB	1:A:123:ILE:HD13	0.41	2.45	7	1
1:A:108:PHE:CD1	1:A:108:PHE:C	0.41	2.99	11	1
1:A:114:LYS:HZ1	1:A:117:PRO:HD3	0.41	1.75	13	1
1:A:71:PHE:CG	1:A:132:CYS:HB3	0.40	2.51	20	1
1:A:51:TRP:CZ2	1:A:53:THR:HA	0.40	2.52	7	1
1:A:93:TYR:CZ	1:A:95:LEU:HB3	0.40	2.52	7	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	140/150 (93%)	105±3 (75±2%)	29±4 (21±3%)	6±2 (4±1%)	3	27
All	All	2800/3000 (93%)	2101 (75%)	576 (21%)	123 (4%)	3	27

All 23 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	140	GLU	18
1	A	139	LYS	15
1	A	107	LYS	12
1	A	2	VAL	10
1	A	130	VAL	9
1	A	119	PRO	8
1	A	125	THR	8
1	A	69	ILE	7
1	A	47	SER	5
1	A	106	TYR	4
1	A	147	LEU	4
1	A	105	ASP	4
1	A	83	SER	4
1	A	84	LYS	3
1	A	58	GLY	2
1	A	86	GLY	2
1	A	145	LEU	2
1	A	148	CYS	1
1	A	131	PHE	1
1	A	88	GLY	1
1	A	87	ASN	1
1	A	39	LEU	1
1	A	91	ASP	1

6.3.2 Protein sidechains ⓘ

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	126/132 (95%)	98±3 (78±3%)	28±3 (22±3%)	2	29
All	All	2520/2640 (95%)	1962 (78%)	558 (22%)	2	29

All 66 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	24	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	36	HIS	20
1	A	44	THR	20
1	A	3	THR	19
1	A	23	LEU	19
1	A	110	SER	19
1	A	84	LYS	17
1	A	31	GLU	16
1	A	95	LEU	16
1	A	140	GLU	16
1	A	6	CYS	15
1	A	57	ASP	15
1	A	107	LYS	15
1	A	17	LYS	15
1	A	144	GLU	14
1	A	134	ILE	14
1	A	74	SER	13
1	A	81	LYS	13
1	A	128	ASN	13
1	A	85	ASP	13
1	A	132	CYS	12
1	A	102	ASP	12
1	A	142	GLN	11
1	A	11	LYS	11
1	A	18	TYR	11
1	A	26	ASN	10
1	A	78	ARG	10
1	A	29	LYS	10
1	A	105	ASP	9
1	A	89	LYS	9
1	A	27	GLN	9
1	A	21	LYS	8
1	A	91	ASP	8
1	A	139	LYS	7
1	A	22	ARG	7
1	A	112	LYS	7
1	A	70	LYS	7
1	A	43	LYS	6
1	A	16	ASN	5
1	A	116	ASN	5
1	A	14	LYS	5
1	A	73	LYS	5
1	A	145	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	121	ARG	5
1	A	146	LYS	4
1	A	111	LYS	4
1	A	115	GLU	4
1	A	41	ASP	3
1	A	28	ASN	3
1	A	8	ASN	3
1	A	114	LYS	2
1	A	109	ASP	2
1	A	93	TYR	2
1	A	126	TYR	2
1	A	83	SER	2
1	A	10	GLN	1
1	A	9	ASP	1
1	A	46	SER	1
1	A	54	ASN	1
1	A	135	ILE	1
1	A	12	ASN	1
1	A	82	HIS	1
1	A	15	THR	1
1	A	141	ASN	1
1	A	2	VAL	1
1	A	33	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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

No chemical shift data were provided