



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 12:39 PM UTC

PDB ID : 2KQ2 / pdb_00002kq2
BMRB ID : 16578
Title : Solution NMR structure of the apo form of a ribonuclease H domain of protein DSY1790 from *Desulfitobacterium hafniense*, Northeast Structural Genomics target DhR1A
Authors : Mills, J.L.; Eletsky, A.; Hua, J.; Belote, R.L.; Buchwald, W.A.; Ciccocanti, C.; Janjua, H.; Nair, R.; Rost, B.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2009-10-24

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

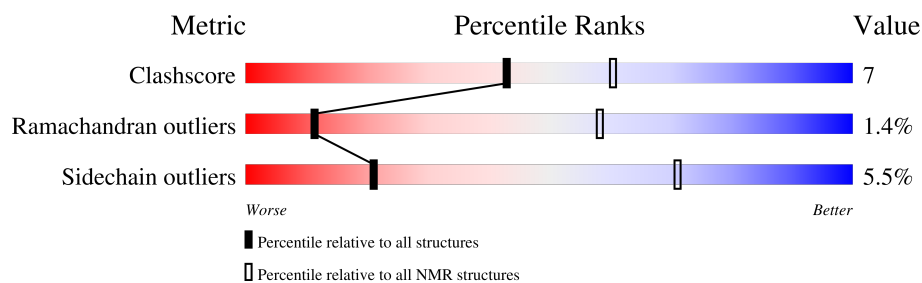
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	147	

2 Ensemble composition and analysis

This entry contains 20 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:3-A:74, A:107-A:137 (103)	2.74	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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2305 atoms, of which 1125 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribonuclease H-related protein.

Mol	Chain	Residues	Atoms						Trace
1	A	147	Total	C	H	N	O	S	0
			2305	750	1125	207	219	4	

There are 9 discrepancies between the modelled and reference sequences:

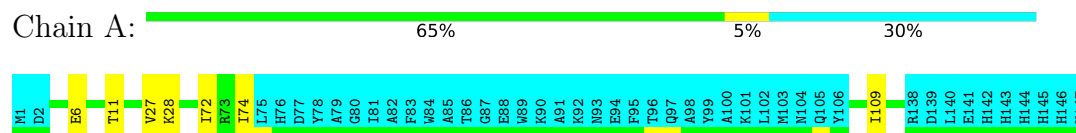
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B8FYYP4
A	140	LEU	-	expression tag	UNP B8FYYP4
A	141	GLU	-	expression tag	UNP B8FYYP4
A	142	HIS	-	expression tag	UNP B8FYYP4
A	143	HIS	-	expression tag	UNP B8FYYP4
A	144	HIS	-	expression tag	UNP B8FYYP4
A	145	HIS	-	expression tag	UNP B8FYYP4
A	146	HIS	-	expression tag	UNP B8FYYP4
A	147	HIS	-	expression tag	UNP B8FYYP4

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: Ribonuclease H-related protein

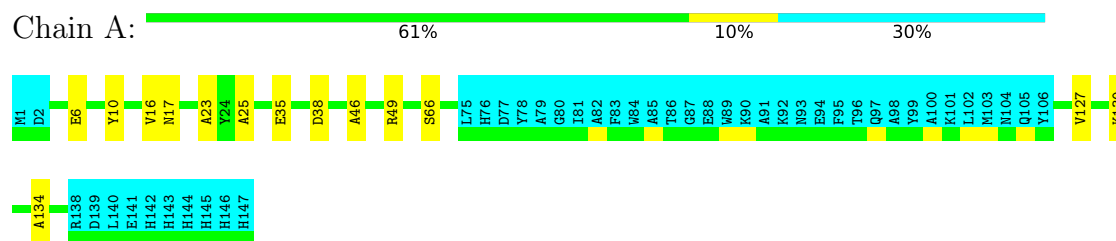


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

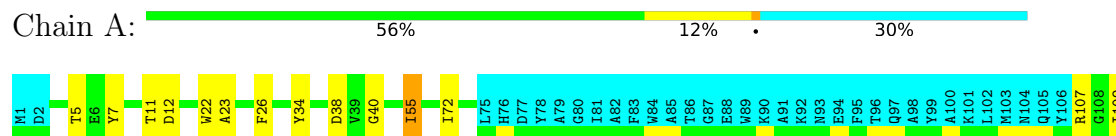
4.2.1 Score per residue for model 1

- Molecule 1: Ribonuclease H-related protein



4.2.2 Score per residue for model 2 (medoid)

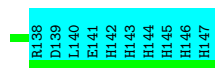
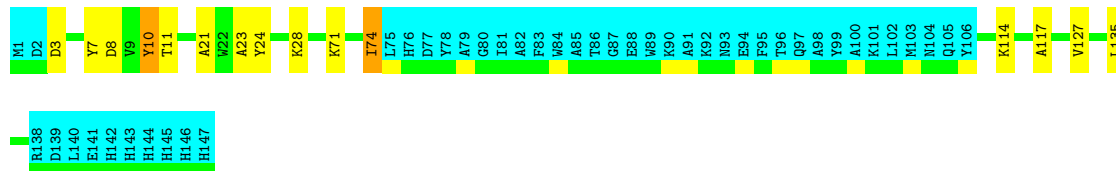
- Molecule 1: Ribonuclease H-related protein





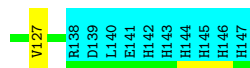
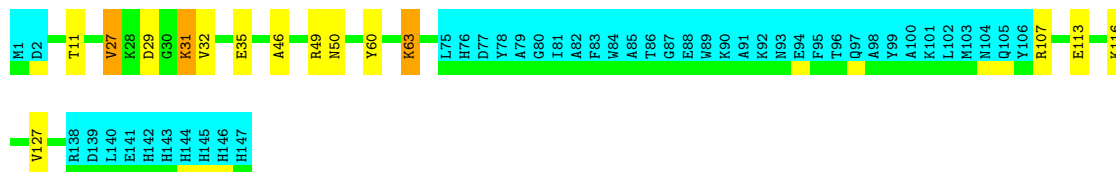
4.2.3 Score per residue for model 3

- Molecule 1: Ribonuclease H-related protein



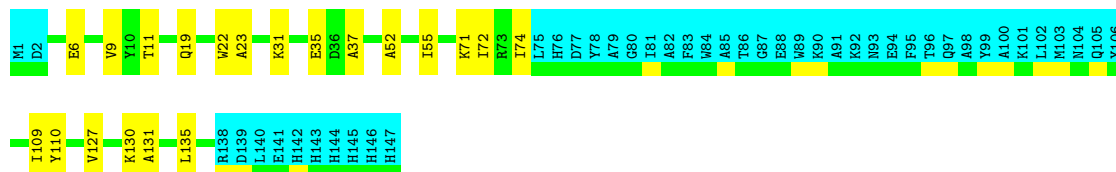
4.2.4 Score per residue for model 4

- Molecule 1: Ribonuclease H-related protein



4.2.5 Score per residue for model 5

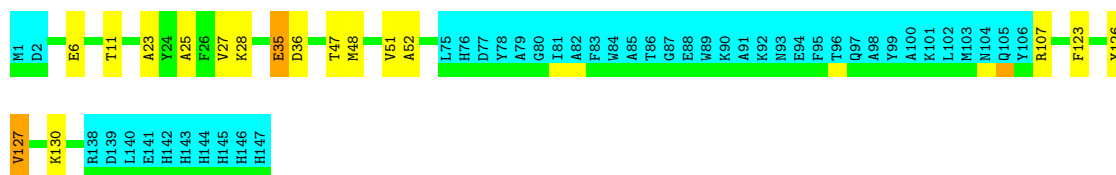
- Molecule 1: Ribonuclease H-related protein



4.2.6 Score per residue for model 6

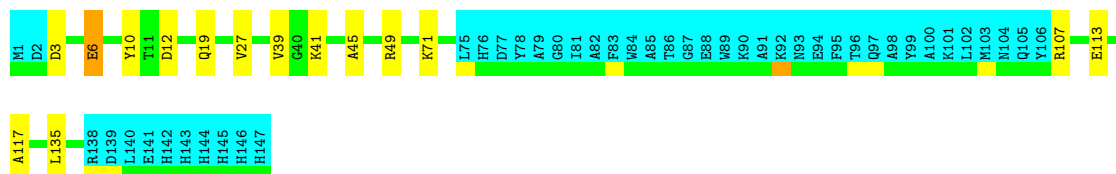
- Molecule 1: Ribonuclease H-related protein





4.2.7 Score per residue for model 7

- Molecule 1: Ribonuclease H-related protein



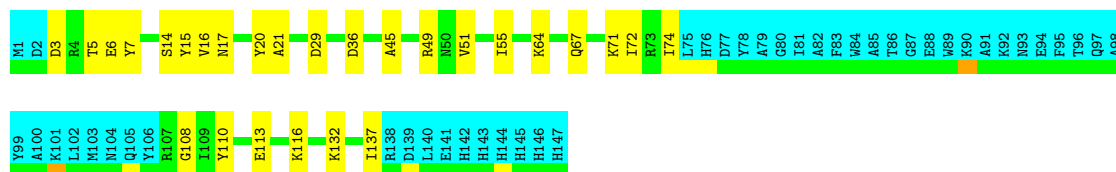
4.2.8 Score per residue for model 8

- Molecule 1: Ribonuclease H-related protein



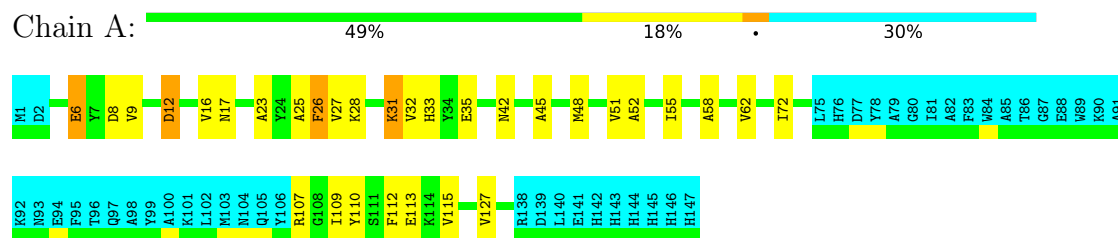
4.2.9 Score per residue for model 9

- Molecule 1: Ribonuclease H-related protein



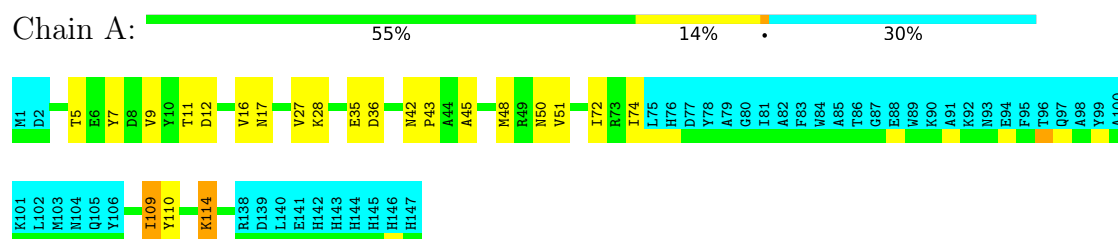
4.2.10 Score per residue for model 10

- Molecule 1: Ribonuclease H-related protein



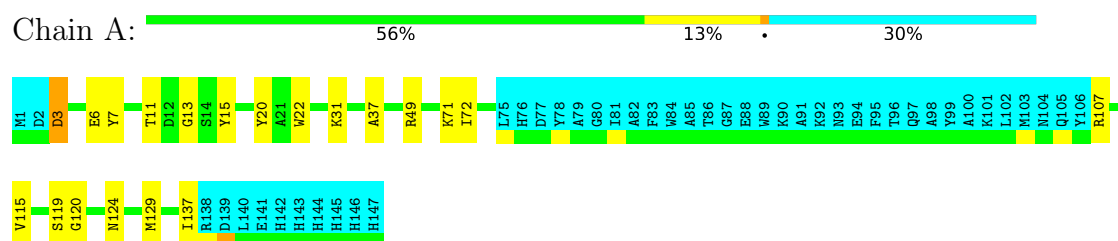
4.2.11 Score per residue for model 11

- Molecule 1: Ribonuclease H-related protein



4.2.12 Score per residue for model 12

- Molecule 1: Ribonuclease H-related protein



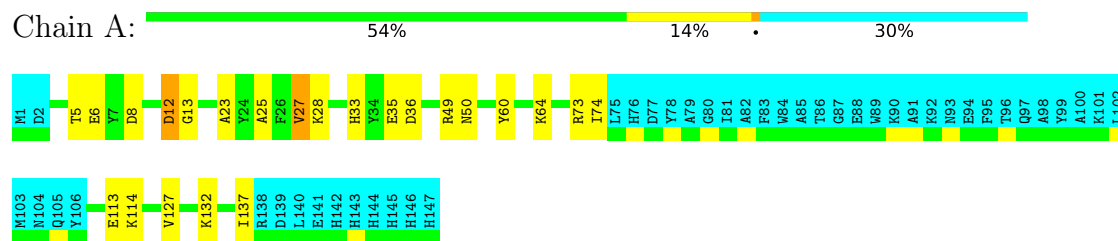
4.2.13 Score per residue for model 13

- Molecule 1: Ribonuclease H-related protein



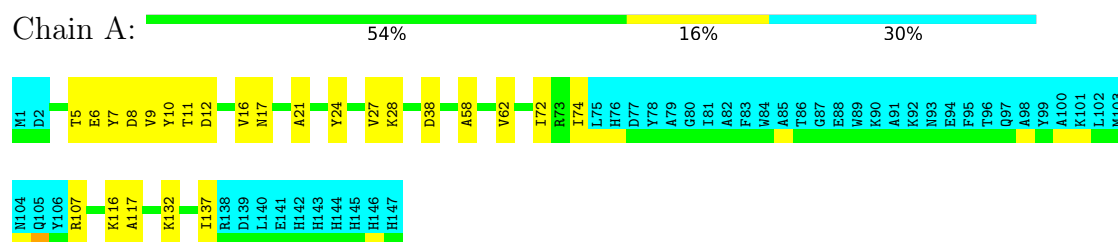
4.2.14 Score per residue for model 14

- Molecule 1: Ribonuclease H-related protein



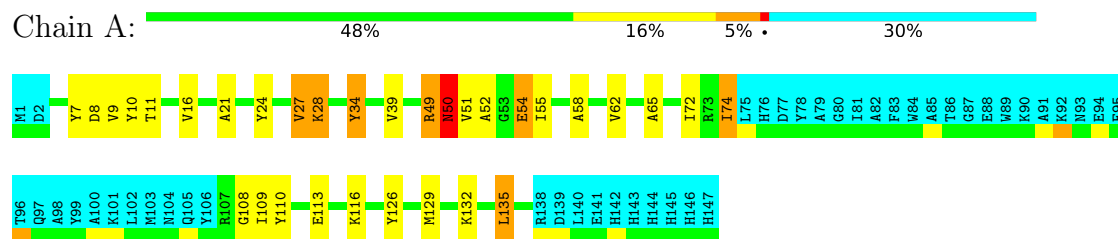
4.2.15 Score per residue for model 15

- Molecule 1: Ribonuclease H-related protein



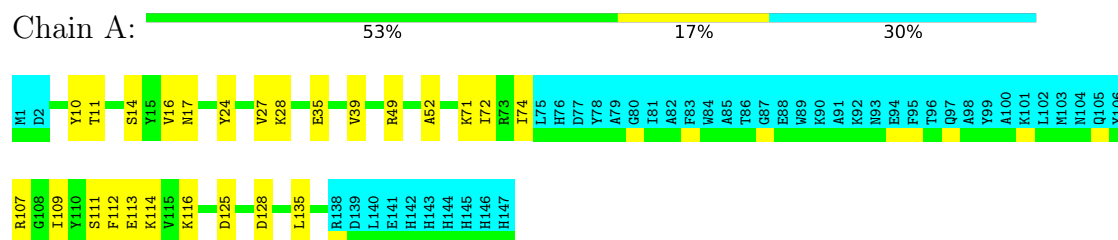
4.2.16 Score per residue for model 16

- Molecule 1: Ribonuclease H-related protein



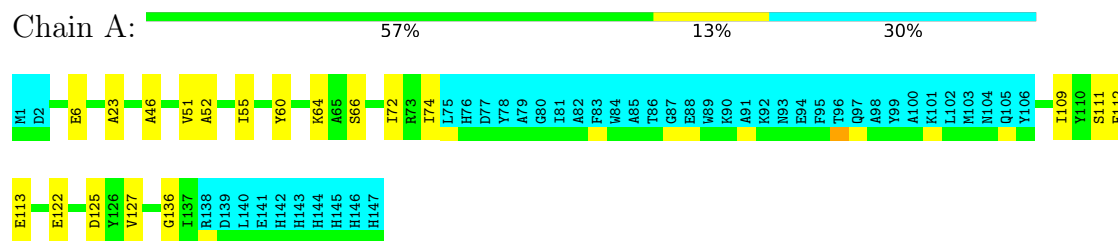
4.2.17 Score per residue for model 17

- Molecule 1: Ribonuclease H-related protein



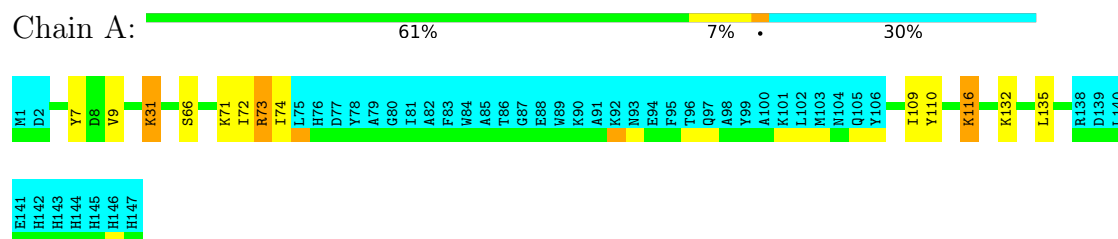
4.2.18 Score per residue for model 18

- Molecule 1: Ribonuclease H-related protein



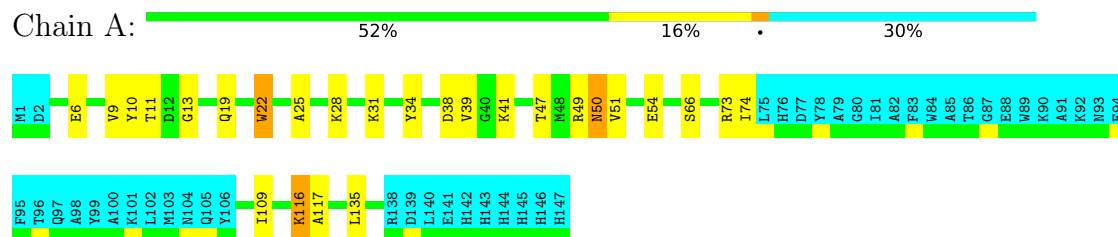
4.2.19 Score per residue for model 19

- Molecule 1: Ribonuclease H-related protein



4.2.20 Score per residue for model 20

- Molecule 1: Ribonuclease H-related protein



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CSI	structure solution	
TALOS	structure solution	
CYANA	structure solution	
CNS	refinement	
MOLMOL	refinement	
PSVS	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	1364
Number of shifts mapped to atoms	1364
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	800	780	778	10±4
All	All	16000	15600	15560	208

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ASP:HB2	1:A:29:ASP:HB3	0.85	1.48	9	1
1:A:19:GLN:HB3	1:A:135:LEU:HG	0.83	1.51	20	1
1:A:11:THR:HA	1:A:116:LYS:HG2	0.76	1.55	17	1
1:A:60:TYR:HA	1:A:63:LYS:HG2	0.75	1.56	4	1
1:A:9:VAL:HB	1:A:74:ILE:HG22	0.73	1.57	11	1
1:A:48:MET:HA	1:A:48:MET:HE3	0.73	1.60	6	2
1:A:7:TYR:HB2	1:A:72:ILE:HG22	0.72	1.59	15	7
1:A:71:LYS:HA	1:A:109:ILE:HG23	0.72	1.60	17	2
1:A:66:SER:HB2	1:A:109:ILE:HD11	0.70	1.64	19	1
1:A:23:ALA:HB1	1:A:127:VAL:HG22	0.68	1.64	3	5
1:A:25:ALA:HB2	1:A:127:VAL:HG21	0.67	1.65	6	1
1:A:11:THR:HG21	1:A:24:TYR:HA	0.67	1.66	15	2
1:A:66:SER:HB3	1:A:109:ILE:HD11	0.64	1.68	18	1
1:A:74:ILE:HD13	1:A:110:TYR:HB2	0.64	1.70	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ALA:HB2	1:A:52:ALA:HB3	0.63	1.68	18	1
1:A:8:ASP:HB2	1:A:10:TYR:HE2	0.62	1.55	16	1
1:A:8:ASP:OD2	1:A:26:PHE:HB2	0.61	1.95	10	1
1:A:22:TRP:CD1	1:A:38:ASP:HB3	0.61	2.30	20	1
1:A:8:ASP:HB2	1:A:10:TYR:CE2	0.61	2.31	16	1
1:A:74:ILE:HD13	1:A:74:ILE:H	0.60	1.57	3	1
1:A:72:ILE:HG12	1:A:110:TYR:HA	0.60	1.73	5	1
1:A:11:THR:HG22	1:A:24:TYR:HA	0.60	1.74	3	1
1:A:13:GLY:HA2	1:A:115:VAL:HA	0.60	1.73	12	1
1:A:35:GLU:HB2	1:A:127:VAL:HG22	0.59	1.74	6	1
1:A:31:LYS:HA	1:A:31:LYS:HE3	0.59	1.74	19	1
1:A:74:ILE:HB	1:A:111:SER:O	0.59	1.97	8	1
1:A:116:LYS:HD3	1:A:116:LYS:O	0.59	1.97	20	1
1:A:109:ILE:HD13	1:A:109:ILE:H	0.58	1.59	11	1
1:A:25:ALA:HB2	1:A:127:VAL:HG11	0.58	1.75	10	2
1:A:3:ASP:HB3	1:A:29:ASP:HB2	0.58	1.75	8	1
1:A:132:LYS:HB3	1:A:137:ILE:HB	0.58	1.75	8	2
1:A:128:ASP:O	1:A:132:LYS:HG2	0.57	1.99	8	1
1:A:114:LYS:HE3	1:A:114:LYS:H	0.57	1.60	11	1
1:A:109:ILE:HD12	1:A:109:ILE:H	0.57	1.60	19	3
1:A:23:ALA:HB1	1:A:127:VAL:HG12	0.57	1.77	6	1
1:A:107:ARG:HA	1:A:107:ARG:NE	0.56	2.16	8	1
1:A:49:ARG:HB3	1:A:52:ALA:HB3	0.56	1.77	17	1
1:A:10:TYR:HB2	1:A:25:ALA:HB3	0.55	1.78	1	1
1:A:8:ASP:HB3	1:A:10:TYR:CE2	0.55	2.37	3	1
1:A:23:ALA:HB1	1:A:127:VAL:CG1	0.55	2.32	6	1
1:A:15:TYR:HB3	1:A:20:TYR:HD1	0.55	1.61	12	2
1:A:39:VAL:HG23	1:A:41:LYS:HG3	0.55	1.79	20	1
1:A:42:ASN:HB2	1:A:45:ALA:HB3	0.54	1.79	10	2
1:A:19:GLN:HB3	1:A:135:LEU:HD22	0.54	1.79	5	1
1:A:12:ASP:HB3	1:A:23:ALA:HB3	0.54	1.79	14	1
1:A:28:LYS:HB3	1:A:28:LYS:NZ	0.54	2.17	16	1
1:A:12:ASP:CG	1:A:117:ALA:HA	0.54	2.27	7	1
1:A:114:LYS:HE3	1:A:114:LYS:N	0.54	2.17	11	1
1:A:72:ILE:HD11	1:A:110:TYR:HD1	0.54	1.61	11	1
1:A:22:TRP:CZ2	1:A:38:ASP:HB3	0.53	2.38	2	1
1:A:49:ARG:HB2	1:A:52:ALA:HB3	0.53	1.79	16	1
1:A:8:ASP:O	1:A:27:VAL:HG13	0.53	2.04	16	3
1:A:36:ASP:HB3	1:A:51:VAL:HG22	0.53	1.78	6	1
1:A:60:TYR:HA	1:A:63:LYS:CG	0.53	2.32	4	1
1:A:7:TYR:CD1	1:A:28:LYS:HB2	0.53	2.38	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:THR:CA	1:A:116:LYS:HG2	0.53	2.32	17	1
1:A:6:GLU:O	1:A:28:LYS:HE2	0.52	2.03	10	1
1:A:72:ILE:HG12	1:A:109:ILE:O	0.52	2.05	18	1
1:A:26:PHE:HB2	1:A:34:TYR:HB2	0.52	1.81	8	2
1:A:41:LYS:HE2	1:A:41:LYS:HA	0.52	1.81	7	1
1:A:23:ALA:HB1	1:A:127:VAL:HB	0.52	1.79	10	2
1:A:22:TRP:CD1	1:A:22:TRP:H	0.52	2.23	20	1
1:A:19:GLN:HG3	1:A:135:LEU:HD13	0.52	1.82	7	1
1:A:122:GLU:HA	1:A:125:ASP:HB3	0.52	1.81	18	1
1:A:51:VAL:O	1:A:55:ILE:HG12	0.52	2.05	16	4
1:A:52:ALA:HA	1:A:55:ILE:HB	0.52	1.82	10	1
1:A:16:VAL:HG22	1:A:17:ASN:HD22	0.52	1.65	10	5
1:A:8:ASP:HB3	1:A:28:LYS:HB2	0.51	1.82	10	1
1:A:27:VAL:HA	1:A:32:VAL:HA	0.51	1.80	10	1
1:A:126:TYR:HA	1:A:129:MET:HE2	0.51	1.81	16	1
1:A:22:TRP:CD1	1:A:22:TRP:N	0.51	2.78	20	1
1:A:72:ILE:HG13	1:A:109:ILE:O	0.51	2.05	17	2
1:A:11:THR:HG22	1:A:12:ASP:H	0.51	1.65	11	1
1:A:12:ASP:HB2	1:A:124:ASN:HB2	0.51	1.83	2	1
1:A:133:SER:HA	1:A:137:ILE:HG22	0.50	1.80	2	1
1:A:28:LYS:O	1:A:31:LYS:HE2	0.50	2.06	10	1
1:A:9:VAL:HG21	1:A:72:ILE:HD13	0.50	1.84	10	1
1:A:15:TYR:HB3	1:A:20:TYR:HB3	0.50	1.83	13	1
1:A:13:GLY:HA3	1:A:114:LYS:HA	0.50	1.83	14	1
1:A:11:THR:HA	1:A:127:VAL:HG11	0.50	1.84	4	1
1:A:10:TYR:O	1:A:11:THR:HG22	0.50	2.07	17	1
1:A:3:ASP:HB2	1:A:28:LYS:CD	0.49	2.37	8	1
1:A:43:PRO:HA	1:A:46:ALA:HB3	0.49	1.84	8	1
1:A:21:ALA:HB2	1:A:39:VAL:HG12	0.49	1.84	16	1
1:A:116:LYS:H	1:A:116:LYS:HD2	0.49	1.66	19	2
1:A:10:TYR:CE2	1:A:27:VAL:HG11	0.49	2.42	7	1
1:A:58:ALA:O	1:A:62:VAL:HG23	0.49	2.07	16	4
1:A:66:SER:HA	1:A:109:ILE:HD11	0.49	1.83	20	1
1:A:39:VAL:HG23	1:A:41:LYS:HE3	0.48	1.84	7	1
1:A:29:ASP:HB3	1:A:31:LYS:HE2	0.48	1.83	4	1
1:A:55:ILE:HD13	1:A:55:ILE:H	0.48	1.67	2	1
1:A:45:ALA:O	1:A:49:ARG:HB2	0.48	2.08	7	1
1:A:60:TYR:CA	1:A:63:LYS:HG2	0.48	2.35	4	1
1:A:38:ASP:HA	1:A:134:ALA:CB	0.47	2.39	1	1
1:A:120:GLY:HA2	1:A:124:ASN:ND2	0.47	2.24	12	1
1:A:132:LYS:HD2	1:A:137:ILE:HD12	0.47	1.86	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LYS:HG2	1:A:137:ILE:HB	0.47	1.85	9	1
1:A:7:TYR:CE1	1:A:28:LYS:HG2	0.47	2.44	11	1
1:A:47:THR:HA	1:A:52:ALA:HB2	0.47	1.86	6	1
1:A:72:ILE:O	1:A:110:TYR:HA	0.47	2.10	9	1
1:A:7:TYR:CD2	1:A:65:ALA:HB2	0.47	2.43	16	1
1:A:72:ILE:HG12	1:A:110:TYR:CD1	0.47	2.45	16	1
1:A:109:ILE:H	1:A:109:ILE:HD12	0.47	1.70	16	1
1:A:71:LYS:N	1:A:71:LYS:HD2	0.47	2.25	19	1
1:A:49:ARG:HG3	1:A:50:ASN:N	0.47	2.25	16	1
1:A:122:GLU:HA	1:A:125:ASP:CB	0.47	2.40	18	1
1:A:122:GLU:CD	1:A:122:GLU:H	0.46	2.19	2	1
1:A:62:VAL:HG22	1:A:110:TYR:CD1	0.46	2.45	16	1
1:A:31:LYS:HD2	1:A:31:LYS:C	0.46	2.36	4	1
1:A:42:ASN:CB	1:A:45:ALA:HB3	0.46	2.41	11	1
1:A:27:VAL:HB	1:A:32:VAL:HG22	0.46	1.87	4	1
1:A:107:ARG:HA	1:A:110:TYR:CE1	0.46	2.46	13	1
1:A:113:GLU:O	1:A:114:LYS:HD2	0.46	2.11	17	1
1:A:9:VAL:HB	1:A:73:ARG:O	0.46	2.11	20	1
1:A:36:ASP:HB3	1:A:51:VAL:HG13	0.45	1.88	9	1
1:A:16:VAL:HG13	1:A:132:LYS:HE3	0.45	1.88	16	1
1:A:64:LYS:HA	1:A:67:GLN:HE21	0.45	1.71	9	1
1:A:46:ALA:HA	1:A:49:ARG:O	0.45	2.11	1	1
1:A:3:ASP:HB3	1:A:7:TYR:CE1	0.45	2.46	3	1
1:A:15:TYR:HB3	1:A:20:TYR:CD1	0.45	2.44	12	1
1:A:74:ILE:HG22	1:A:111:SER:HA	0.44	1.87	17	1
1:A:72:ILE:HD11	1:A:111:SER:N	0.44	2.27	18	1
1:A:9:VAL:O	1:A:74:ILE:HA	0.44	2.12	16	2
1:A:9:VAL:HB	1:A:74:ILE:HD11	0.44	1.90	5	1
1:A:22:TRP:O	1:A:37:ALA:HA	0.44	2.13	5	1
1:A:16:VAL:HG22	1:A:17:ASN:ND2	0.44	2.27	1	3
1:A:38:ASP:HB2	1:A:51:VAL:HG21	0.43	1.90	20	1
1:A:36:ASP:HB2	1:A:51:VAL:HB	0.43	1.90	11	1
1:A:120:GLY:HA2	1:A:124:ASN:HD22	0.43	1.74	12	1
1:A:39:VAL:HG11	1:A:135:LEU:HD22	0.43	1.91	16	1
1:A:131:ALA:O	1:A:135:LEU:HG	0.43	2.13	5	1
1:A:26:PHE:HD2	1:A:33:HIS:HB2	0.43	1.73	10	1
1:A:49:ARG:HG3	1:A:50:ASN:H	0.43	1.73	20	1
1:A:46:ALA:O	1:A:49:ARG:HG3	0.43	2.14	4	1
1:A:9:VAL:O	1:A:73:ARG:HB3	0.43	2.14	19	1
1:A:72:ILE:HD11	1:A:110:TYR:CD1	0.42	2.47	11	1
1:A:74:ILE:HD12	1:A:112:PHE:HE1	0.42	1.74	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ILE:HG12	1:A:112:PHE:O	0.42	2.14	18	1
1:A:123:PHE:HA	1:A:126:TYR:CD2	0.42	2.49	6	1
1:A:21:ALA:HB2	1:A:135:LEU:HD21	0.42	1.91	3	1
1:A:116:LYS:C	1:A:116:LYS:HD3	0.42	2.39	15	1
1:A:41:LYS:HB2	1:A:49:ARG:NH1	0.42	2.29	7	1
1:A:12:ASP:HB2	1:A:117:ALA:HB3	0.42	1.91	15	1
1:A:21:ALA:HB1	1:A:38:ASP:O	0.42	2.14	15	1
1:A:52:ALA:HA	1:A:55:ILE:HG12	0.42	1.92	5	1
1:A:123:PHE:HA	1:A:126:TYR:HD2	0.42	1.74	6	1
1:A:22:TRP:HZ2	1:A:49:ARG:HG3	0.42	1.74	12	1
1:A:39:VAL:HG12	1:A:135:LEU:HD23	0.42	1.92	17	1
1:A:71:LYS:HE2	1:A:108:GLY:O	0.41	2.15	13	1
1:A:12:ASP:HB3	1:A:128:ASP:HB2	0.41	1.91	2	1
1:A:45:ALA:O	1:A:49:ARG:HG3	0.41	2.15	9	1
1:A:60:TYR:O	1:A:64:LYS:HG3	0.41	2.16	14	1
1:A:3:ASP:HB2	1:A:28:LYS:HD2	0.41	1.92	8	1
1:A:34:TYR:CE2	1:A:54:GLU:HG3	0.41	2.50	16	1
1:A:31:LYS:HD2	1:A:31:LYS:O	0.41	2.16	4	1
1:A:11:THR:HG23	1:A:127:VAL:HG11	0.41	1.92	5	1
1:A:12:ASP:HA	1:A:115:VAL:O	0.41	2.15	10	1
1:A:126:TYR:O	1:A:130:LYS:HG3	0.41	2.15	6	1
1:A:107:ARG:HD2	1:A:107:ARG:O	0.41	2.16	15	1
1:A:6:GLU:CD	1:A:73:ARG:HD3	0.41	2.41	14	1
1:A:71:LYS:HD2	1:A:108:GLY:O	0.41	2.15	9	1
1:A:116:LYS:HD2	1:A:116:LYS:N	0.41	2.30	19	1
1:A:10:TYR:CZ	1:A:25:ALA:HB3	0.41	2.51	20	1
1:A:132:LYS:HD3	1:A:135:LEU:HD12	0.41	1.93	19	1
1:A:14:SER:HB2	1:A:21:ALA:O	0.40	2.15	9	1
1:A:125:ASP:HA	1:A:128:ASP:HB3	0.40	1.93	17	1
1:A:60:TYR:O	1:A:64:LYS:HG2	0.40	2.16	8	1
1:A:66:SER:HB3	1:A:109:ILE:CD1	0.40	2.45	18	1
1:A:11:THR:CG2	1:A:24:TYR:HA	0.40	2.47	17	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	103/147 (70%)	94±2 (92±2%)	7±2 (7±2%)	1±1 (1±1%)	11	58
All	All	2060/2940 (70%)	1886 (92%)	146 (7%)	28 (1%)	11	58

All 13 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	6	GLU	10
1	A	50	ASN	5
1	A	48	MET	2
1	A	108	GLY	2
1	A	40	GLY	1
1	A	11	THR	1
1	A	43	PRO	1
1	A	3	ASP	1
1	A	37	ALA	1
1	A	49	ARG	1
1	A	14	SER	1
1	A	13	GLY	1
1	A	117	ALA	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	78/114 (68%)	74±2 (94±2%)	4±2 (6±2%)	21	71
All	All	1560/2280 (68%)	1474 (94%)	86 (6%)	21	71

All 37 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	35	GLU	9
1	A	27	VAL	7
1	A	28	LYS	7
1	A	5	THR	6
1	A	31	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	113	GLU	5
1	A	116	LYS	4
1	A	130	LYS	3
1	A	71	LYS	3
1	A	74	ILE	3
1	A	3	ASP	3
1	A	114	LYS	2
1	A	12	ASP	2
1	A	34	TYR	2
1	A	54	GLU	2
1	A	66	SER	1
1	A	55	ILE	1
1	A	122	GLU	1
1	A	10	TYR	1
1	A	63	LYS	1
1	A	127	VAL	1
1	A	6	GLU	1
1	A	26	PHE	1
1	A	110	TYR	1
1	A	109	ILE	1
1	A	119	SER	1
1	A	33	HIS	1
1	A	36	ASP	1
1	A	49	ARG	1
1	A	50	ASN	1
1	A	135	LEU	1
1	A	107	ARG	1
1	A	60	TYR	1
1	A	64	LYS	1
1	A	73	ARG	1
1	A	22	TRP	1
1	A	47	THR	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 [i](#)

There are no oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 69% 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	1364
Number of shifts mapped to atoms	1364
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	127	-0.10 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	115	0.22 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	126	0.85 ± 0.38	Should be applied

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 78%, i.e. 1056 atoms were assigned a chemical shift out of a possible 1360. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	400/522 (77%)	204/214 (95%)	98/206 (48%)	98/102 (96%)
Sidechain	578/699 (83%)	399/454 (88%)	177/216 (82%)	2/29 (7%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	78/139 (56%)	49/65 (75%)	28/69 (41%)	1/5 (20%)
Overall	1056/1360 (78%)	652/733 (89%)	303/491 (62%)	101/136 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1364 atoms were assigned a chemical shift out of a possible 1983. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	516/744 (69%)	263/304 (87%)	127/294 (43%)	126/146 (86%)
Sidechain	713/973 (73%)	492/631 (78%)	218/303 (72%)	3/39 (8%)
Aromatic	135/266 (51%)	83/127 (65%)	49/118 (42%)	3/21 (14%)
Overall	1364/1983 (69%)	838/1062 (79%)	394/715 (55%)	132/206 (64%)

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	82	ALA	H	5.29	5.31 – 11.08	-5.0

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:

