



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:26 pm BST

PDB ID : 2K5G
Title : Solution NMR structure of protein encoded by gene BPP1335 from *Bordetella parapertussis*: Northeast Structural Genomics Target BpR195
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Deposited on : 2008-06-27

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

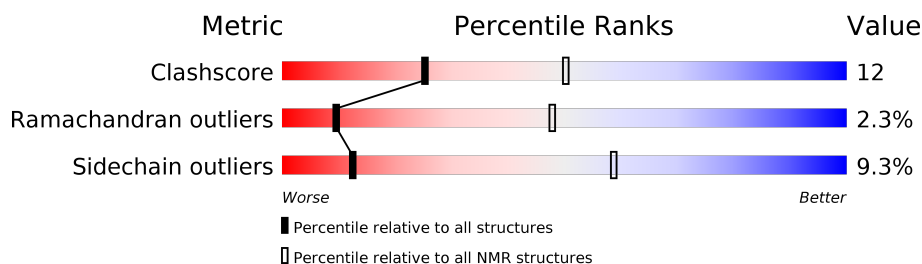
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	191	

2 Ensemble composition and analysis

This entry contains 20 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:19-A:64, A:75-A:107, A:111-A:180 (149)	0.73	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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2958 atoms, of which 1460 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	191	Total	C	H	N	O	S	0
			2958	947	1460	283	265	3	

There are 8 discrepancies between the modelled and reference sequences:

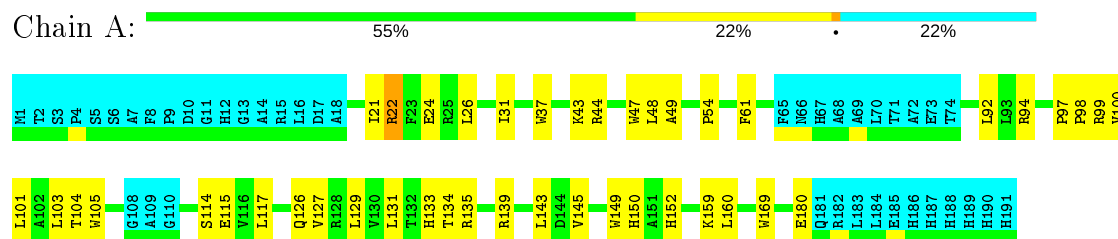
Chain	Residue	Modelled	Actual	Comment	Reference
A	184	LEU	-	expression tag	UNP Q7WAN9
A	185	GLU	-	expression tag	UNP Q7WAN9
A	186	HIS	-	expression tag	UNP Q7WAN9
A	187	HIS	-	expression tag	UNP Q7WAN9
A	188	HIS	-	expression tag	UNP Q7WAN9
A	189	HIS	-	expression tag	UNP Q7WAN9
A	190	HIS	-	expression tag	UNP Q7WAN9
A	191	HIS	-	expression tag	UNP Q7WAN9

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: uncharacterized protein

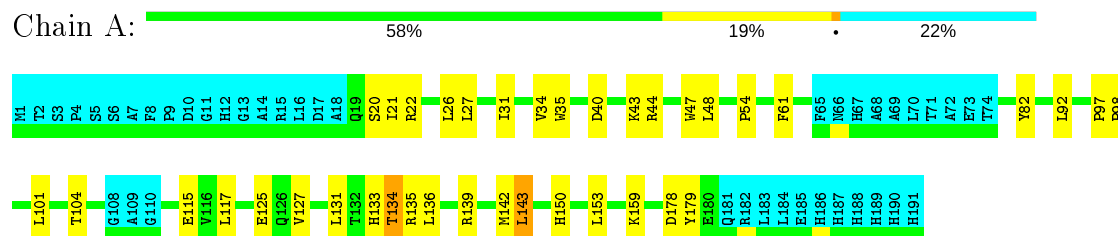


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

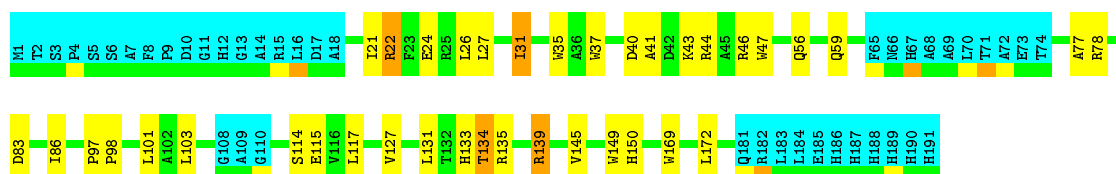
- Molecule 1: uncharacterized protein



4.2.2 Score per residue for model 2

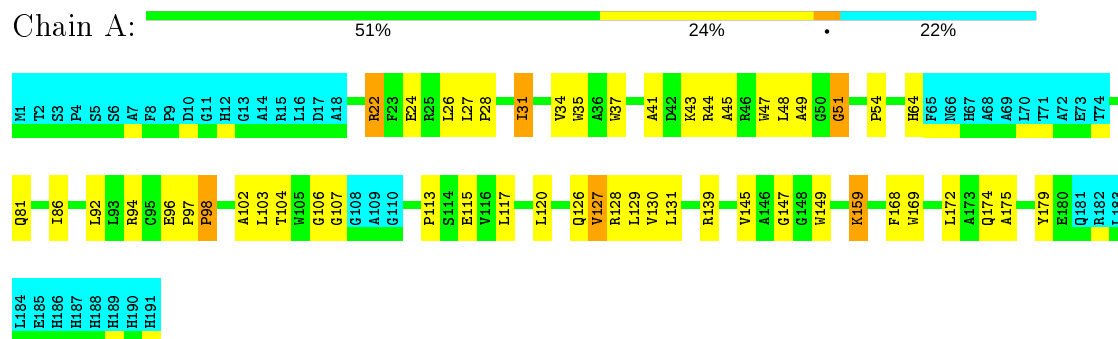
- Molecule 1: uncharacterized protein





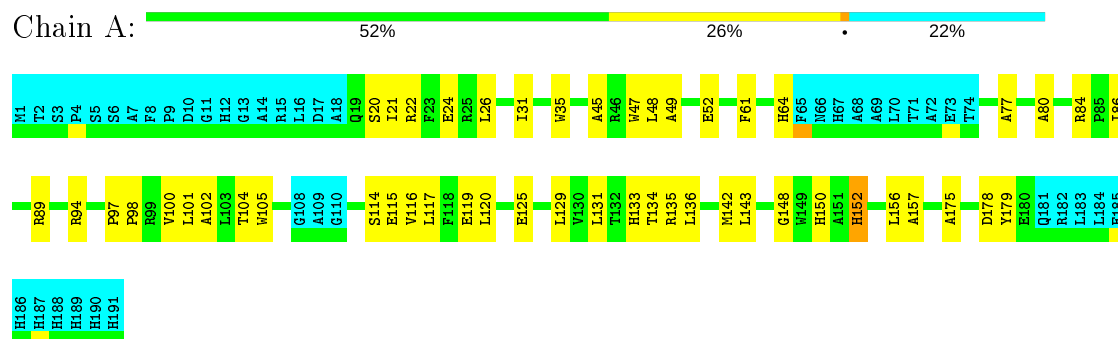
4.2.3 Score per residue for model 3

- Molecule 1: uncharacterized protein



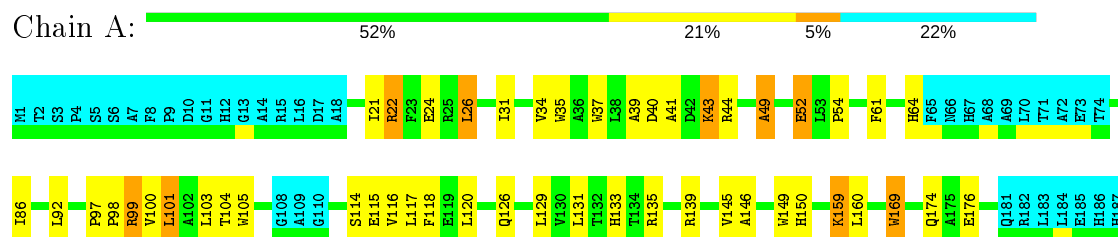
4.2.4 Score per residue for model 4

- Molecule 1: uncharacterized protein



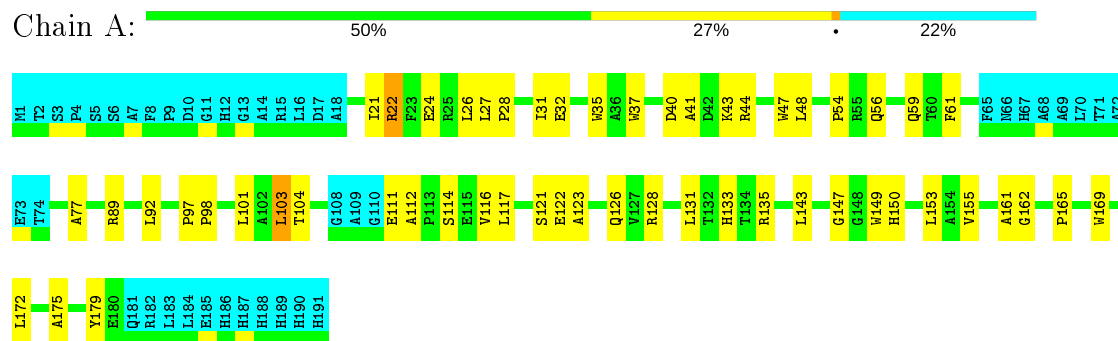
4.2.5 Score per residue for model 5

- Molecule 1: uncharacterized protein



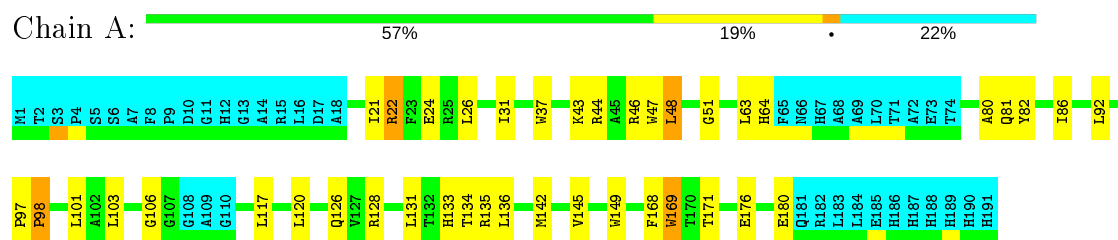
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: uncharacterized protein



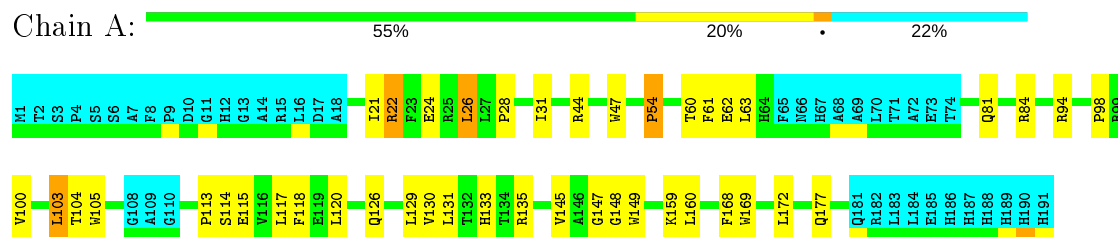
4.2.7 Score per residue for model 7

- Molecule 1: uncharacterized protein



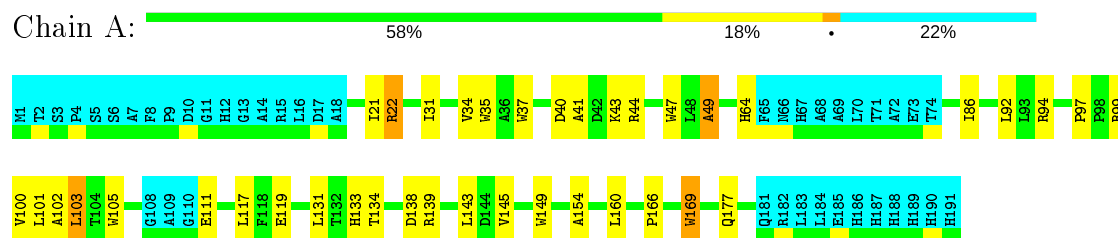
4.2.8 Score per residue for model 8

- Molecule 1: uncharacterized protein



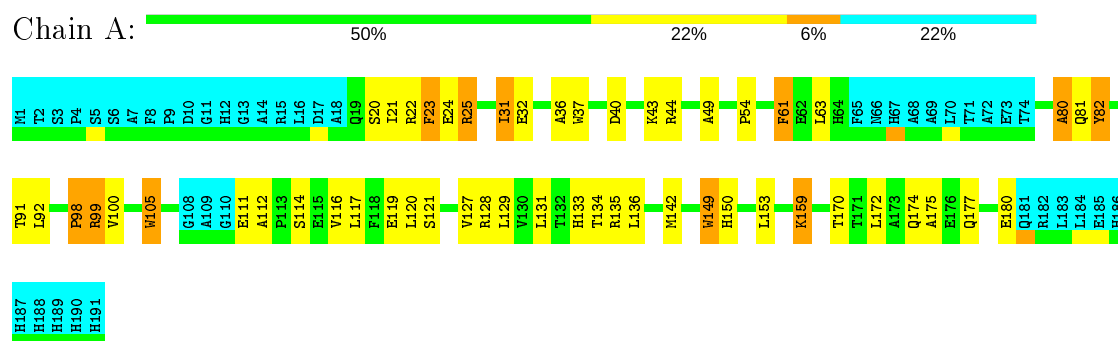
4.2.9 Score per residue for model 9

- Molecule 1: uncharacterized protein



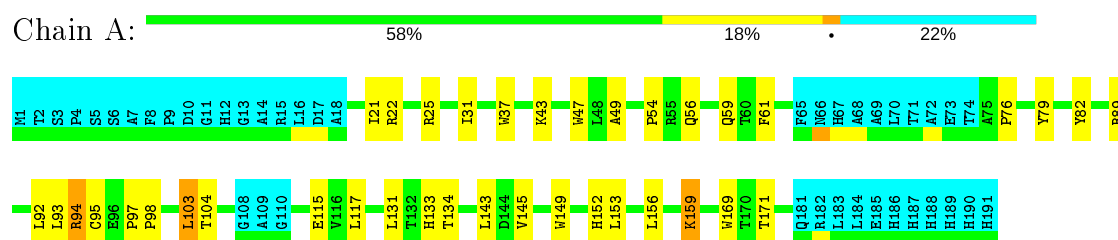
4.2.10 Score per residue for model 10

- Molecule 1: uncharacterized protein



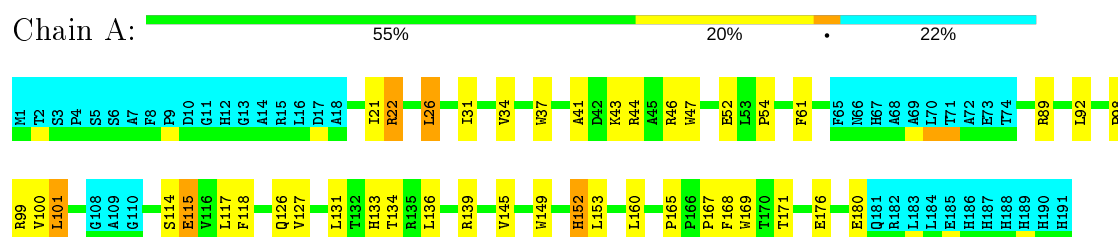
4.2.11 Score per residue for model 11

- Molecule 1: uncharacterized protein



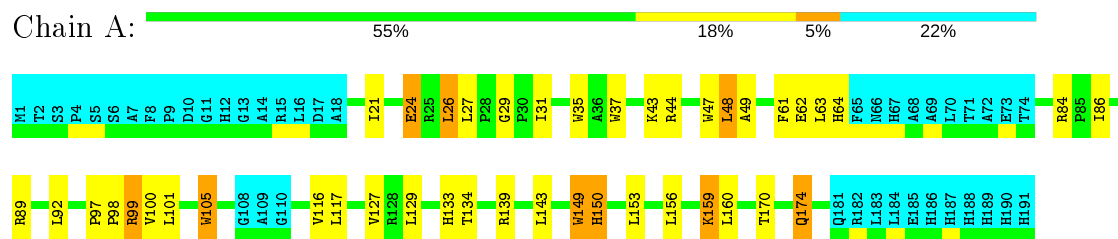
4.2.12 Score per residue for model 12

- Molecule 1: uncharacterized protein



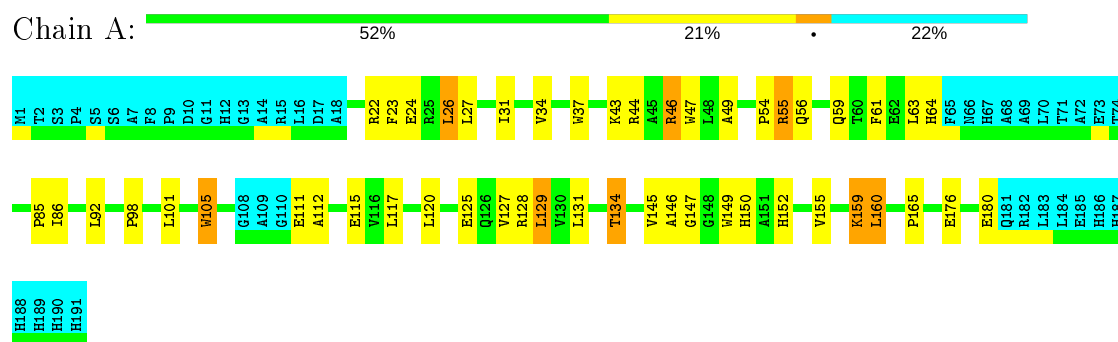
4.2.13 Score per residue for model 13

- Molecule 1: uncharacterized protein



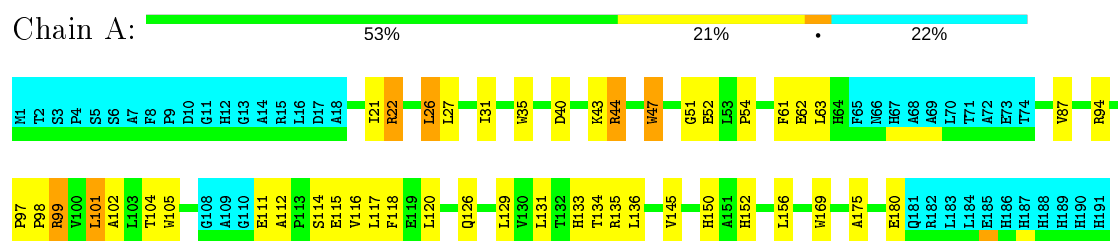
4.2.14 Score per residue for model 14

- Molecule 1: uncharacterized protein



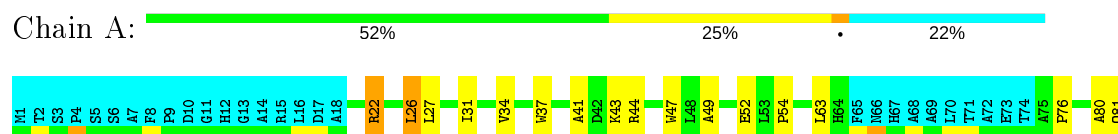
4.2.15 Score per residue for model 15

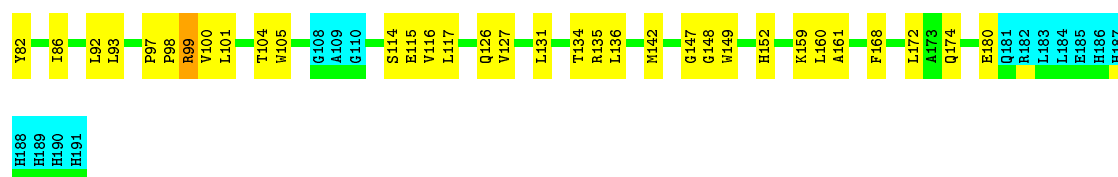
- Molecule 1: uncharacterized protein



4.2.16 Score per residue for model 16

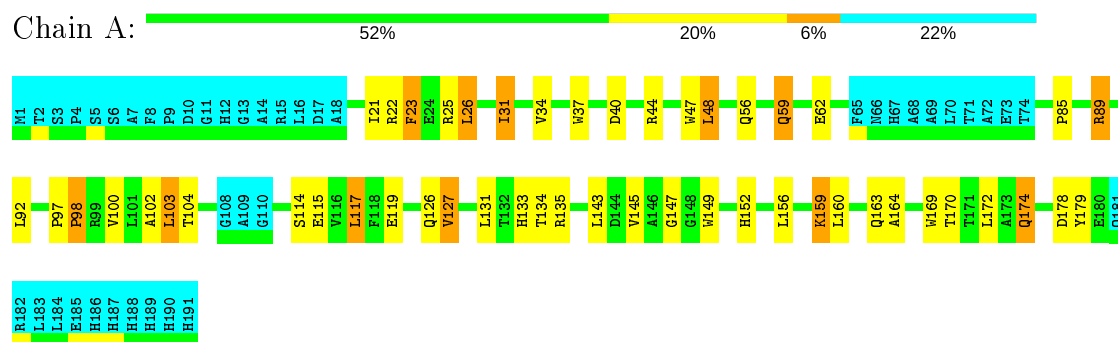
- Molecule 1: uncharacterized protein





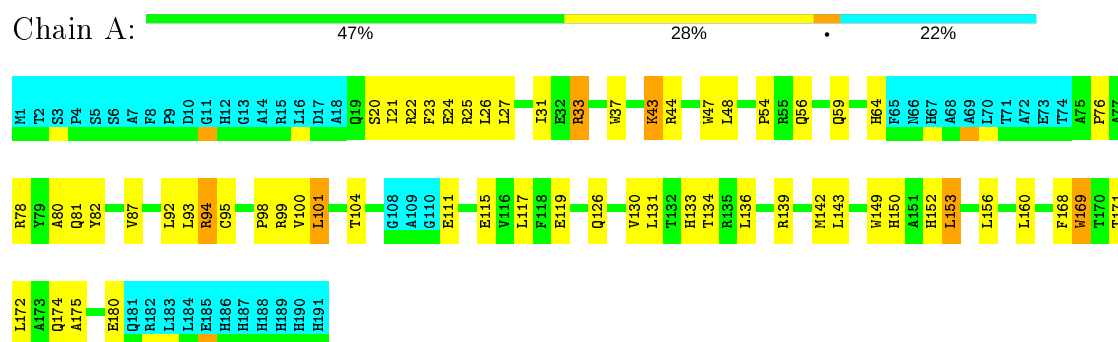
4.2.17 Score per residue for model 17

- Molecule 1: uncharacterized protein



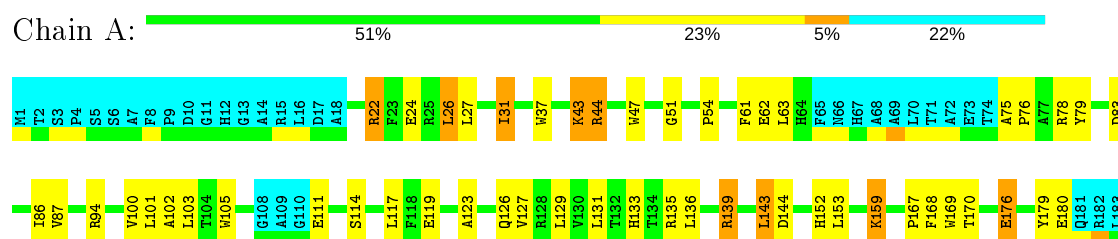
4.2.18 Score per residue for model 18

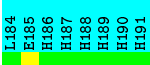
- Molecule 1: uncharacterized protein



4.2.19 Score per residue for model 19

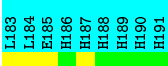
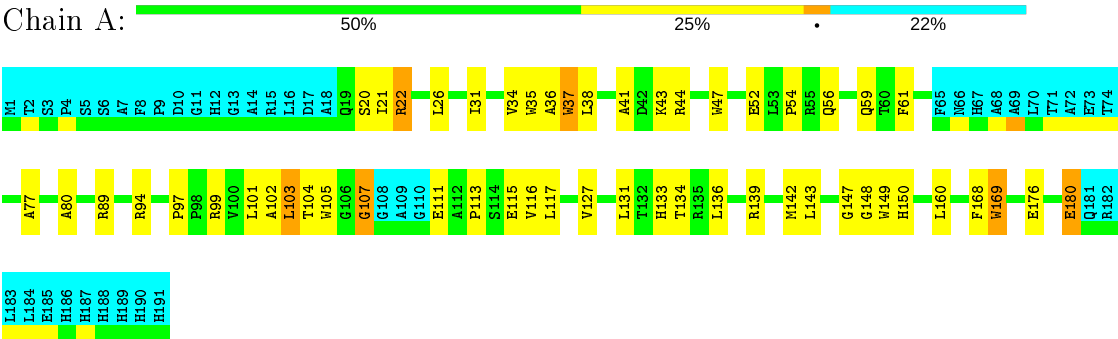
- Molecule 1: uncharacterized protein





4.2.20 Score per residue for model 20

- Molecule 1: uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 100 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
AutoStructure	structure solution	
CNS	refinement	
CYANA	structure solution	
MOLMOL	structure solution	
PSVS	geometry optimization	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2137
Number of shifts mapped to atoms	2137
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	1178	1166	1161	27±6
All	All	23560	23320	23220	538

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:TRP:HB3	1:A:43:LYS:HD3	0.88	1.43	14	3
1:A:44:ARG:HB3	1:A:47:TRP:HD1	0.88	1.26	15	1
1:A:20:SER:HA	1:A:136:LEU:HD12	0.86	1.45	1	4
1:A:21:ILE:HB	1:A:133:HIS:HB3	0.86	1.43	5	15
1:A:114:SER:HA	1:A:135:ARG:HB3	0.86	1.43	4	4
1:A:37:TRP:CE3	1:A:43:LYS:HE3	0.84	2.07	20	1
1:A:100:VAL:HG12	1:A:119:GLU:HA	0.83	1.51	10	6
1:A:41:ALA:HA	1:A:44:ARG:HG2	0.81	1.52	12	4
1:A:44:ARG:HB3	1:A:47:TRP:CD1	0.80	2.12	15	2
1:A:44:ARG:HD3	1:A:47:TRP:CD1	0.76	2.15	19	1
1:A:111:GLU:HG3	1:A:112:ALA:H	0.76	1.40	10	2
1:A:114:SER:HA	1:A:135:ARG:HB2	0.74	1.57	2	5
1:A:136:LEU:HD13	1:A:142:MET:HG2	0.74	1.58	18	6
1:A:41:ALA:HA	1:A:51:GLY:HA3	0.73	1.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LYS:HA	1:A:159:LYS:HE3	0.73	1.59	13	2
1:A:45:ALA:HA	1:A:49:ALA:HA	0.73	1.58	3	2
1:A:49:ALA:HB1	1:A:64:HIS:HB2	0.73	1.61	14	2
1:A:61:PHE:HE2	1:A:92:LEU:HB3	0.72	1.44	13	1
1:A:34:VAL:HG21	1:A:127:VAL:HG21	0.72	1.60	3	2
1:A:147:GLY:HA2	1:A:172:LEU:HD11	0.72	1.62	6	3
1:A:37:TRP:HE1	1:A:160:LEU:HD11	0.69	1.48	18	3
1:A:37:TRP:CD1	1:A:160:LEU:HD21	0.69	2.22	14	3
1:A:26:LEU:HD11	1:A:126:GLN:HB3	0.68	1.66	6	9
1:A:94:ARG:H	1:A:102:ALA:HB3	0.67	1.50	20	4
1:A:139:ARG:H	1:A:139:ARG:HD2	0.67	1.48	13	2
1:A:76:PRO:HD2	1:A:79:TYR:HD2	0.67	1.50	19	2
1:A:56:GLN:HB2	1:A:59:GLN:HG3	0.67	1.66	20	6
1:A:54:PRO:HD3	1:A:61:PHE:HB3	0.67	1.66	11	5
1:A:154:ALA:HB1	1:A:166:PRO:HG2	0.66	1.65	9	1
1:A:37:TRP:HA	1:A:43:LYS:HD2	0.66	1.64	9	4
1:A:152:HIS:O	1:A:156:LEU:HG	0.66	1.91	18	2
1:A:159:LYS:HA	1:A:159:LYS:HE2	0.65	1.66	16	3
1:A:147:GLY:HA3	1:A:176:GLU:HG2	0.65	1.66	20	2
1:A:37:TRP:HB2	1:A:47:TRP:HE1	0.65	1.51	14	1
1:A:99:ARG:HG3	1:A:100:VAL:HG23	0.65	1.69	13	4
1:A:44:ARG:HA	1:A:47:TRP:NE1	0.64	2.08	13	9
1:A:21:ILE:HB	1:A:133:HIS:CB	0.63	2.23	1	2
1:A:34:VAL:HG21	1:A:127:VAL:HG11	0.63	1.70	14	4
1:A:99:ARG:HG3	1:A:100:VAL:HG13	0.62	1.71	18	2
1:A:23:PHE:HE1	1:A:131:LEU:HD13	0.62	1.53	10	1
1:A:22:ARG:HA	1:A:131:LEU:O	0.61	1.94	8	18
1:A:131:LEU:HD13	1:A:153:LEU:HD21	0.61	1.72	12	2
1:A:61:PHE:CE2	1:A:92:LEU:HB3	0.61	2.30	13	1
1:A:41:ALA:CA	1:A:51:GLY:HA3	0.61	2.26	3	1
1:A:104:THR:HA	1:A:115:GLU:HA	0.61	1.73	15	11
1:A:92:LEU:HA	1:A:103:LEU:HA	0.61	1.73	9	3
1:A:44:ARG:NH1	1:A:52:GLU:HA	0.61	2.11	5	1
1:A:44:ARG:HD3	1:A:47:TRP:HD1	0.61	1.53	19	1
1:A:159:LYS:HE3	1:A:159:LYS:HA	0.60	1.73	19	2
1:A:176:GLU:O	1:A:180:GLU:HB2	0.60	1.97	12	5
1:A:54:PRO:HD2	1:A:92:LEU:HD22	0.60	1.73	16	1
1:A:44:ARG:HA	1:A:47:TRP:CD1	0.60	2.32	20	13
1:A:64:HIS:HA	1:A:86:ILE:O	0.59	1.97	14	3
1:A:92:LEU:HD23	1:A:92:LEU:H	0.59	1.57	14	2
1:A:34:VAL:CG2	1:A:127:VAL:HG11	0.59	2.27	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:TRP:NE1	1:A:145:VAL:HG12	0.59	2.12	5	1
1:A:54:PRO:HD2	1:A:92:LEU:HD13	0.59	1.73	6	1
1:A:43:LYS:HD3	1:A:44:ARG:CD	0.59	2.27	19	1
1:A:45:ALA:HA	1:A:49:ALA:CA	0.59	2.27	3	2
1:A:139:ARG:HA	1:A:142:MET:SD	0.59	2.36	1	1
1:A:37:TRP:O	1:A:44:ARG:HG3	0.59	1.98	19	1
1:A:23:PHE:CE1	1:A:131:LEU:HD13	0.59	2.32	10	1
1:A:37:TRP:NE1	1:A:160:LEU:HD11	0.59	2.12	17	2
1:A:123:ALA:HB3	1:A:126:GLN:HG3	0.59	1.74	19	1
1:A:31:ILE:HA	1:A:127:VAL:HG11	0.58	1.75	17	3
1:A:150:HIS:CE1	1:A:175:ALA:HB3	0.57	2.33	10	1
1:A:44:ARG:HD3	1:A:51:GLY:HA2	0.57	1.76	3	1
1:A:111:GLU:HG3	1:A:112:ALA:N	0.57	2.14	15	4
1:A:21:ILE:HG22	1:A:133:HIS:HB3	0.57	1.76	17	1
1:A:93:LEU:HG	1:A:94:ARG:H	0.57	1.58	18	1
1:A:54:PRO:HG3	1:A:61:PHE:HB3	0.57	1.76	14	6
1:A:94:ARG:HB3	1:A:102:ALA:HB3	0.57	1.76	19	2
1:A:41:ALA:HA	1:A:44:ARG:CG	0.57	2.29	12	3
1:A:34:VAL:HA	1:A:160:LEU:HD21	0.57	1.77	5	5
1:A:39:ALA:HA	1:A:44:ARG:NH2	0.57	2.15	5	1
1:A:37:TRP:CE3	1:A:43:LYS:HD2	0.57	2.34	16	2
1:A:139:ARG:HD2	1:A:139:ARG:H	0.56	1.60	3	1
1:A:37:TRP:CE3	1:A:43:LYS:HE2	0.56	2.34	9	2
1:A:24:GLU:HG3	1:A:130:VAL:HG23	0.56	1.77	18	1
1:A:37:TRP:HB3	1:A:43:LYS:CD	0.56	2.30	18	1
1:A:115:GLU:HG3	1:A:134:THR:OG1	0.56	2.01	1	2
1:A:41:ALA:HA	1:A:44:ARG:HB3	0.56	1.77	6	2
1:A:63:LEU:O	1:A:87:VAL:HA	0.56	2.01	19	2
1:A:145:VAL:HB	1:A:149:TRP:CD1	0.56	2.34	3	1
1:A:155:VAL:HG13	1:A:165:PRO:HB3	0.56	1.76	6	2
1:A:78:ARG:NH2	1:A:144:ASP:HA	0.55	2.16	19	1
1:A:44:ARG:HE	1:A:44:ARG:HA	0.55	1.61	19	1
1:A:143:LEU:HG	1:A:179:TYR:HB3	0.55	1.77	1	2
1:A:54:PRO:HG2	1:A:92:LEU:HD22	0.55	1.79	6	3
1:A:47:TRP:CE3	1:A:48:LEU:HB2	0.55	2.37	17	5
1:A:120:LEU:HD21	1:A:129:LEU:HD12	0.55	1.78	10	4
1:A:49:ALA:HB1	1:A:64:HIS:O	0.55	2.01	9	2
1:A:150:HIS:NE2	1:A:175:ALA:HB3	0.55	2.16	18	2
1:A:105:TRP:CD1	1:A:145:VAL:HG12	0.55	2.36	9	2
1:A:37:TRP:HB2	1:A:47:TRP:NE1	0.55	2.16	14	1
1:A:54:PRO:HD2	1:A:92:LEU:HD11	0.54	1.79	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:VAL:HG21	1:A:127:VAL:CG1	0.54	2.33	16	3
1:A:44:ARG:HG3	1:A:49:ALA:O	0.54	2.02	16	1
1:A:169:TRP:CE3	1:A:169:TRP:HA	0.54	2.38	2	1
1:A:159:LYS:HE2	1:A:159:LYS:HA	0.54	1.79	11	1
1:A:146:ALA:HA	1:A:150:HIS:ND1	0.54	2.17	14	1
1:A:145:VAL:HB	1:A:149:TRP:HD1	0.54	1.63	3	1
1:A:92:LEU:H	1:A:92:LEU:HD23	0.54	1.62	5	2
1:A:37:TRP:CE3	1:A:43:LYS:CE	0.54	2.88	20	1
1:A:41:ALA:HB2	1:A:52:GLU:HG2	0.53	1.80	5	1
1:A:75:ALA:HB1	1:A:79:TYR:HB2	0.53	1.78	19	1
1:A:23:PHE:CD1	1:A:131:LEU:HB2	0.53	2.38	17	1
1:A:56:GLN:HB2	1:A:59:GLN:CG	0.53	2.34	20	2
1:A:147:GLY:HA2	1:A:172:LEU:HG	0.53	1.80	8	2
1:A:94:ARG:HD3	1:A:96:GLU:OE1	0.53	2.03	3	1
1:A:37:TRP:O	1:A:44:ARG:HB3	0.53	2.03	14	1
1:A:77:ALA:HA	1:A:80:ALA:HB3	0.52	1.80	20	1
1:A:76:PRO:HG2	1:A:78:ARG:HG2	0.52	1.81	18	1
1:A:37:TRP:CZ2	1:A:156:LEU:HD11	0.52	2.39	13	1
1:A:35:TRP:CZ2	1:A:97:PRO:HB3	0.52	2.39	2	10
1:A:133:HIS:CE1	1:A:145:VAL:HG11	0.52	2.40	2	3
1:A:105:TRP:HB2	1:A:116:VAL:HG23	0.52	1.80	15	3
1:A:48:LEU:HD13	1:A:48:LEU:O	0.52	2.05	3	2
1:A:115:GLU:HG2	1:A:135:ARG:HB2	0.52	1.82	1	1
1:A:43:LYS:HD3	1:A:44:ARG:CG	0.52	2.35	19	1
1:A:47:TRP:CE3	1:A:156:LEU:HB3	0.51	2.40	11	1
1:A:146:ALA:HA	1:A:150:HIS:HD1	0.51	1.65	14	1
1:A:55:ARG:HA	1:A:55:ARG:NE	0.51	2.21	14	1
1:A:40:ASP:O	1:A:44:ARG:HB2	0.51	2.06	10	3
1:A:103:LEU:HD13	1:A:103:LEU:N	0.51	2.21	17	1
1:A:145:VAL:HB	1:A:149:TRP:HB3	0.50	1.81	14	2
1:A:103:LEU:N	1:A:103:LEU:HD13	0.50	2.22	11	4
1:A:47:TRP:HZ3	1:A:152:HIS:HD2	0.50	1.48	11	1
1:A:149:TRP:CE3	1:A:152:HIS:HE1	0.50	2.24	16	1
1:A:149:TRP:HE3	1:A:152:HIS:HE2	0.50	1.48	18	1
1:A:93:LEU:HD12	1:A:94:ARG:HG3	0.50	1.83	11	1
1:A:40:ASP:OD2	1:A:43:LYS:HG2	0.50	2.07	9	5
1:A:149:TRP:HA	1:A:149:TRP:CE3	0.50	2.41	10	2
1:A:134:THR:O	1:A:135:ARG:HB2	0.50	2.07	7	1
1:A:76:PRO:HD2	1:A:79:TYR:CD2	0.50	2.38	19	2
1:A:47:TRP:CZ3	1:A:156:LEU:HG	0.49	2.42	15	1
1:A:25:ARG:HA	1:A:25:ARG:HE	0.49	1.67	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:HIS:CE1	1:A:136:LEU:HD21	0.49	2.42	15	3
1:A:63:LEU:HG	1:A:64:HIS:H	0.49	1.66	14	1
1:A:43:LYS:HD3	1:A:44:ARG:HG2	0.49	1.84	19	1
1:A:113:PRO:O	1:A:135:ARG:HD3	0.49	2.07	8	1
1:A:167:PRO:HB2	1:A:170:THR:HB	0.49	1.85	19	1
1:A:105:TRP:HE1	1:A:145:VAL:HG12	0.49	1.67	5	1
1:A:32:GLU:HG2	1:A:98:PRO:HG2	0.49	1.82	10	1
1:A:139:ARG:O	1:A:142:MET:HG2	0.48	2.09	1	1
1:A:43:LYS:CD	1:A:44:ARG:HG2	0.48	2.38	19	1
1:A:123:ALA:HB3	1:A:126:GLN:HB2	0.48	1.85	6	1
1:A:80:ALA:O	1:A:82:TYR:N	0.48	2.47	10	3
1:A:25:ARG:HA	1:A:25:ARG:NE	0.48	2.24	10	1
1:A:44:ARG:CB	1:A:47:TRP:HD1	0.48	2.12	15	1
1:A:26:LEU:HD11	1:A:126:GLN:HB2	0.48	1.83	8	1
1:A:27:LEU:HD22	1:A:160:LEU:HD12	0.48	1.84	13	1
1:A:37:TRP:CG	1:A:43:LYS:HD3	0.48	2.44	11	1
1:A:148:GLY:O	1:A:150:HIS:N	0.48	2.46	20	1
1:A:116:VAL:HG21	1:A:149:TRP:CZ2	0.48	2.44	16	3
1:A:150:HIS:NE2	1:A:172:LEU:HD12	0.48	2.23	2	1
1:A:114:SER:HA	1:A:135:ARG:CB	0.48	2.39	10	3
1:A:37:TRP:CB	1:A:43:LYS:HD3	0.48	2.33	13	1
1:A:54:PRO:HG2	1:A:92:LEU:HB2	0.48	1.84	18	1
1:A:35:TRP:HA	1:A:38:LEU:HD12	0.48	1.85	20	1
1:A:37:TRP:CD1	1:A:43:LYS:HD2	0.47	2.44	3	1
1:A:102:ALA:HB2	1:A:117:LEU:HD22	0.47	1.86	17	1
1:A:31:ILE:HA	1:A:127:VAL:CG2	0.47	2.39	19	2
1:A:43:LYS:HD3	1:A:44:ARG:HD2	0.47	1.86	19	1
1:A:24:GLU:HA	1:A:129:LEU:O	0.47	2.10	13	3
1:A:159:LYS:CE	1:A:159:LYS:HA	0.47	2.40	5	2
1:A:25:ARG:HD2	1:A:153:LEU:HB3	0.47	1.86	10	1
1:A:131:LEU:HD22	1:A:153:LEU:HD21	0.47	1.87	11	1
1:A:148:GLY:HA2	1:A:168:PHE:CZ	0.46	2.44	8	1
1:A:62:GLU:HA	1:A:89:ARG:HA	0.46	1.87	17	2
1:A:155:VAL:HG13	1:A:165:PRO:CB	0.46	2.40	14	1
1:A:101:LEU:HG	1:A:118:PHE:HB2	0.46	1.87	15	3
1:A:105:TRP:CE3	1:A:105:TRP:HA	0.46	2.45	13	2
1:A:46:ARG:HD3	1:A:46:ARG:O	0.46	2.10	2	1
1:A:54:PRO:CD	1:A:61:PHE:HB3	0.46	2.40	15	1
1:A:23:PHE:HD2	1:A:131:LEU:HD23	0.46	1.69	18	1
1:A:133:HIS:HE1	1:A:145:VAL:HG11	0.46	1.71	2	2
1:A:145:VAL:O	1:A:149:TRP:HB3	0.46	2.10	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ARG:HE	1:A:44:ARG:CA	0.46	2.23	19	1
1:A:24:GLU:HG2	1:A:130:VAL:HG22	0.46	1.87	8	1
1:A:40:ASP:HB3	1:A:43:LYS:HE2	0.46	1.87	15	1
1:A:51:GLY:HA3	1:A:63:LEU:HD23	0.46	1.88	7	1
1:A:80:ALA:O	1:A:81:GLN:HG2	0.46	2.10	18	1
1:A:150:HIS:O	1:A:153:LEU:HB2	0.46	2.10	13	2
1:A:98:PRO:O	1:A:99:ARG:HD2	0.46	2.11	10	1
1:A:61:PHE:O	1:A:89:ARG:HA	0.45	2.10	12	4
1:A:26:LEU:HD13	1:A:27:LEU:N	0.45	2.26	3	9
1:A:43:LYS:HB2	1:A:43:LYS:NZ	0.45	2.26	5	1
1:A:134:THR:HG22	1:A:135:ARG:H	0.45	1.71	10	1
1:A:44:ARG:HH12	1:A:52:GLU:HA	0.45	1.71	5	1
1:A:84:ARG:O	1:A:86:ILE:HG13	0.45	2.11	13	1
1:A:121:SER:HB2	1:A:128:ARG:CG	0.45	2.42	10	1
1:A:114:SER:HB3	1:A:134:THR:O	0.45	2.12	12	1
1:A:62:GLU:HG2	1:A:89:ARG:HB3	0.45	1.89	13	1
1:A:23:PHE:HD1	1:A:131:LEU:CB	0.45	2.25	17	1
1:A:81:GLN:HG3	1:A:84:ARG:CZ	0.45	2.42	8	1
1:A:120:LEU:CD2	1:A:129:LEU:HB2	0.45	2.42	15	3
1:A:95:CYS:HA	1:A:101:LEU:HA	0.45	1.89	18	1
1:A:23:PHE:CD1	1:A:131:LEU:CB	0.44	3.00	17	1
1:A:43:LYS:HG3	1:A:44:ARG:HG2	0.44	1.89	19	1
1:A:107:GLY:HA2	1:A:113:PRO:HG3	0.44	1.89	20	1
1:A:37:TRP:CD1	1:A:43:LYS:HD3	0.44	2.48	6	1
1:A:105:TRP:O	1:A:114:SER:HB2	0.44	2.13	8	1
1:A:177:GLN:HA	1:A:177:GLN:OE1	0.44	2.13	9	1
1:A:37:TRP:HE3	1:A:43:LYS:HE3	0.44	1.65	20	1
1:A:95:CYS:O	1:A:97:PRO:HD3	0.44	2.13	11	1
1:A:44:ARG:HA	1:A:44:ARG:NE	0.44	2.27	19	1
1:A:20:SER:HB3	1:A:133:HIS:O	0.44	2.12	1	2
1:A:143:LEU:HD21	1:A:179:TYR:HB2	0.44	1.88	4	2
1:A:40:ASP:OD2	1:A:43:LYS:HB2	0.44	2.13	5	1
1:A:24:GLU:HA	1:A:130:VAL:HA	0.43	1.90	3	1
1:A:120:LEU:HA	1:A:128:ARG:O	0.43	2.13	7	1
1:A:100:VAL:HG23	1:A:118:PHE:O	0.43	2.13	8	1
1:A:28:PRO:HD2	1:A:160:LEU:HB3	0.43	1.90	8	1
1:A:150:HIS:HE1	1:A:172:LEU:HA	0.43	1.74	10	1
1:A:105:TRP:C	1:A:105:TRP:CD1	0.43	2.92	10	1
1:A:116:VAL:HG11	1:A:149:TRP:CH2	0.43	2.48	6	1
1:A:34:VAL:HA	1:A:37:TRP:NE1	0.43	2.28	14	1
1:A:44:ARG:HB3	1:A:47:TRP:NE1	0.43	2.29	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:HD12	1:A:153:LEU:HD21	0.43	1.90	1	1
1:A:80:ALA:O	1:A:84:ARG:HG2	0.43	2.14	4	1
1:A:34:VAL:HG21	1:A:127:VAL:CG2	0.43	2.43	17	1
1:A:51:GLY:HA2	1:A:62:GLU:O	0.43	2.13	19	1
1:A:116:VAL:HG11	1:A:149:TRP:CZ2	0.43	2.49	10	2
1:A:41:ALA:CA	1:A:44:ARG:HG2	0.43	2.35	12	1
1:A:97:PRO:HA	1:A:98:PRO:HA	0.42	1.69	16	4
1:A:37:TRP:HA	1:A:43:LYS:CD	0.42	2.41	9	2
1:A:149:TRP:O	1:A:152:HIS:HD2	0.42	1.97	12	1
1:A:146:ALA:HA	1:A:150:HIS:CE1	0.42	2.49	5	1
1:A:170:THR:O	1:A:174:GLN:HB2	0.42	2.14	17	2
1:A:61:PHE:CE2	1:A:63:LEU:HG	0.42	2.50	15	1
1:A:115:GLU:HG2	1:A:134:THR:HB	0.42	1.90	2	1
1:A:34:VAL:HA	1:A:37:TRP:HE1	0.42	1.73	14	1
1:A:63:LEU:HG	1:A:64:HIS:N	0.42	2.29	14	1
1:A:153:LEU:HD13	1:A:156:LEU:HD12	0.42	1.90	18	1
1:A:156:LEU:HD12	1:A:157:ALA:N	0.42	2.29	4	1
1:A:59:GLN:O	1:A:92:LEU:HD23	0.42	2.13	17	1
1:A:131:LEU:HD11	1:A:149:TRP:HE1	0.42	1.75	8	1
1:A:154:ALA:HB1	1:A:166:PRO:CG	0.42	2.41	9	1
1:A:46:ARG:HE	1:A:46:ARG:HA	0.42	1.75	14	1
1:A:37:TRP:CH2	1:A:156:LEU:HD13	0.42	2.50	18	1
1:A:44:ARG:HG3	1:A:47:TRP:CZ2	0.42	2.50	1	1
1:A:104:THR:HB	1:A:114:SER:O	0.42	2.15	5	1
1:A:37:TRP:CZ3	1:A:43:LYS:HE2	0.42	2.50	9	2
1:A:76:PRO:HD3	1:A:169:TRP:HZ2	0.42	1.73	18	1
1:A:168:PHE:HA	1:A:171:THR:HG22	0.42	1.92	18	1
1:A:169:TRP:HA	1:A:169:TRP:HE3	0.41	1.74	2	1
1:A:56:GLN:HB3	1:A:59:GLN:NE2	0.41	2.30	17	1
1:A:91:THR:HG22	1:A:92:LEU:O	0.41	2.15	10	1
1:A:37:TRP:CE3	1:A:43:LYS:CD	0.41	3.03	16	1
1:A:106:GLY:C	1:A:113:PRO:HB3	0.41	2.36	3	1
1:A:43:LYS:HZ3	1:A:43:LYS:HB2	0.41	1.75	5	1
1:A:37:TRP:CD2	1:A:43:LYS:HD2	0.41	2.51	7	1
1:A:115:GLU:O	1:A:133:HIS:HA	0.41	2.15	12	1
1:A:20:SER:CA	1:A:136:LEU:HD12	0.41	2.32	1	1
1:A:36:ALA:HB3	1:A:37:TRP:CE3	0.41	2.50	20	2
1:A:93:LEU:CD1	1:A:94:ARG:HG3	0.41	2.45	11	1
1:A:49:ALA:HB3	1:A:63:LEU:HD12	0.41	1.92	10	2
1:A:29:GLY:O	1:A:127:VAL:HG23	0.41	2.16	13	1
1:A:175:ALA:O	1:A:178:ASP:HB2	0.41	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:TRP:HZ3	1:A:152:HIS:HD1	0.41	1.57	4	1
1:A:22:ARG:HD3	1:A:22:ARG:N	0.41	2.30	5	1
1:A:54:PRO:HD2	1:A:92:LEU:CD1	0.41	2.45	12	1
1:A:22:ARG:N	1:A:22:ARG:HD3	0.41	2.31	15	1
1:A:27:LEU:HB2	1:A:127:VAL:HG13	0.40	1.92	1	1
1:A:76:PRO:HD3	1:A:169:TRP:CZ2	0.40	2.51	18	1
1:A:31:ILE:HA	1:A:127:VAL:HG22	0.40	1.92	19	1
1:A:175:ALA:O	1:A:179:TYR:HD1	0.40	1.99	3	2
1:A:121:SER:HB2	1:A:128:ARG:HG2	0.40	1.93	10	1
1:A:34:VAL:CG2	1:A:127:VAL:HG21	0.40	2.47	17	1
1:A:121:SER:HB2	1:A:128:ARG:HB2	0.40	1.93	6	1
1:A:23:PHE:CE1	1:A:131:LEU:HB2	0.40	2.51	17	1
1:A:37:TRP:NE1	1:A:160:LEU:HD21	0.40	2.31	17	1
1:A:48:LEU:O	1:A:49:ALA:HB3	0.40	2.17	4	1
1:A:64:HIS:CD2	1:A:87:VAL:HG22	0.40	2.51	18	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	149/191 (78%)	131±3 (88±2%)	14±3 (10±2%)	3±1 (2±1%)	9	48
All	All	2980/3820 (78%)	2623 (88%)	289 (10%)	68 (2%)	9	48

All 16 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	31	ILE	20
1	A	98	PRO	16
1	A	99	ARG	5
1	A	81	GLN	3
1	A	125	GLU	3
1	A	49	ALA	3
1	A	77	ALA	3

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Mol	Chain	Res	Type	Models (Total)
1	A	169	TRP	3
1	A	51	GLY	2
1	A	107	GLY	2
1	A	149	TRP	2
1	A	148	GLY	2
1	A	106	GLY	1
1	A	80	ALA	1
1	A	94	ARG	1
1	A	76	PRO	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	115/146 (79%)	104±2 (91±1%)	11±2 (9±1%)	12 59
All	All	2300/2920 (79%)	2086 (91%)	214 (9%)	12 59

All 56 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	117	LEU	20
1	A	101	LEU	15
1	A	22	ARG	13
1	A	134	THR	12
1	A	26	LEU	12
1	A	103	LEU	11
1	A	169	TRP	10
1	A	159	LYS	9
1	A	24	GLU	7
1	A	143	LEU	7
1	A	174	GLN	6
1	A	52	GLU	6
1	A	105	TRP	5
1	A	180	GLU	5
1	A	48	LEU	5
1	A	152	HIS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	139	ARG	4
1	A	111	GLU	4
1	A	171	THR	3
1	A	25	ARG	3
1	A	150	HIS	3
1	A	43	LYS	3
1	A	127	VAL	2
1	A	46	ARG	2
1	A	23	PHE	2
1	A	94	ARG	2
1	A	128	ARG	2
1	A	62	GLU	2
1	A	89	ARG	2
1	A	99	ARG	2
1	A	44	ARG	2
1	A	176	GLU	2
1	A	82	TYR	2
1	A	63	LEU	2
1	A	59	GLN	1
1	A	64	HIS	1
1	A	60	THR	1
1	A	129	LEU	1
1	A	81	GLN	1
1	A	37	TRP	1
1	A	92	LEU	1
1	A	149	TRP	1
1	A	138	ASP	1
1	A	160	LEU	1
1	A	61	PHE	1
1	A	54	PRO	1
1	A	104	THR	1
1	A	47	TRP	1
1	A	55	ARG	1
1	A	32	GLU	1
1	A	33	ARG	1
1	A	78	ARG	1
1	A	122	GLU	1
1	A	115	GLU	1
1	A	153	LEU	1
1	A	93	LEU	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 carbohydrates 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 88% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: input_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	2137
Number of shifts mapped to atoms	2137
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	174	-0.02 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	160	0.01 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	148	0.05 ± 0.19	None needed (< 0.5 ppm)
^{15}N	161	0.39 ± 0.31	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 1651 atoms were assigned a chemical shift out of a possible 1870. 28 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	705/721 (98%)	286/286 (100%)	282/298 (95%)	137/137 (100%)
Sidechain	808/977 (83%)	498/575 (87%)	303/350 (87%)	7/52 (13%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	138/172 (80%)	78/88 (89%)	54/68 (79%)	6/16 (38%)
Overall	1651/1870 (88%)	862/949 (91%)	639/716 (89%)	150/205 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1885 atoms were assigned a chemical shift out of a possible 2360. 31 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	819/927 (88%)	336/368 (91%)	322/382 (84%)	161/177 (91%)
Sidechain	910/1179 (77%)	561/695 (81%)	341/424 (80%)	8/60 (13%)
Aromatic	156/254 (61%)	90/130 (69%)	60/92 (65%)	6/32 (19%)
Overall	1885/2360 (80%)	987/1193 (83%)	723/898 (81%)	175/269 (65%)

7.1.4 Statistically unusual chemical shifts ⓘ

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	149	TRP	HE1	-1.28	12.85 – 7.35	-20.7
1	A	171	THR	CB	39.36	78.10 – 61.30	-18.1
1	A	66	ASN	CB	9.26	47.13 – 30.23	-17.4
1	A	170	THR	CB	40.51	78.10 – 61.30	-17.4
1	A	69	ALA	CB	47.05	28.03 – 9.93	15.5
1	A	48	LEU	HB2	-0.83	3.32 – -0.08	-7.2
1	A	97	PRO	HA	2.27	6.05 – 2.75	-6.4
1	A	43	LYS	HB2	0.48	3.03 – 0.53	-5.2
1	A	131	LEU	HD12	-0.67	2.16 – -0.64	-5.1
1	A	131	LEU	HD11	-0.67	2.16 – -0.64	-5.1
1	A	131	LEU	HD13	-0.67	2.16 – -0.64	-5.1
1	A	49	ALA	HB2	0.09	2.61 – 0.11	-5.1
1	A	49	ALA	HB3	0.09	2.61 – 0.11	-5.1
1	A	49	ALA	HB1	0.09	2.61 – 0.11	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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.

Random coil index (RCI) for chain A:

