



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 09:19 PM UTC

PDB ID : 2LH0 / pdb_00002lh0
BMRB ID : 17832
Title : NMR structure of the histone-interacting N-terminal homodimeric region of Rtt106
Authors : Hu, Q.; Cui, G.; Mer, G.
Deposited on : 2011-08-04

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

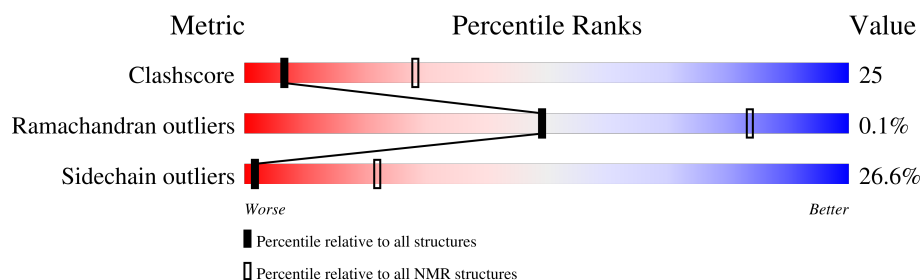
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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	70	
1	B	70	

2 Ensemble composition and analysis

This entry contains 20 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:11-A:39, B:83-B:109 (56)	0.60	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2284 atoms, of which 1144 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone chaperone RTT106.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1142	356	572	97	115	2	
1	B	70	Total	C	H	N	O	S	0
			1142	356	572	97	115	2	

There are 12 discrepancies between the modelled and reference sequences:

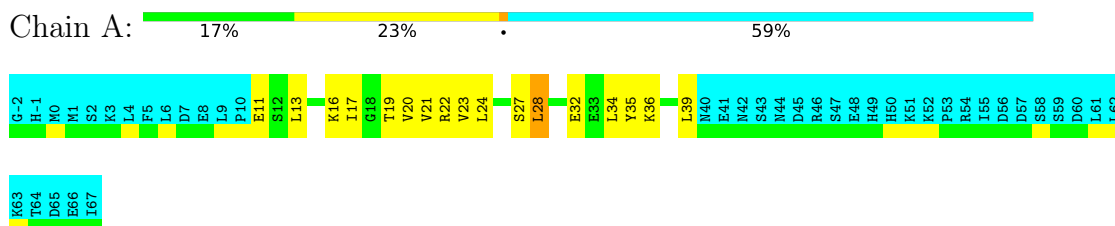
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P40161
A	-1	HIS	-	expression tag	UNP P40161
A	0	MET	-	expression tag	UNP P40161
A	48	GLU	GLY	variant	UNP P40161
A	49	HIS	ARG	variant	UNP P40161
A	57	ASP	VAL	variant	UNP P40161
B	68	GLY	-	expression tag	UNP P40161
B	69	HIS	-	expression tag	UNP P40161
B	70	MET	-	expression tag	UNP P40161
B	118	GLU	GLY	variant	UNP P40161
B	119	HIS	ARG	variant	UNP P40161
B	127	ASP	VAL	variant	UNP P40161

4 Residue-property plots [i](#)

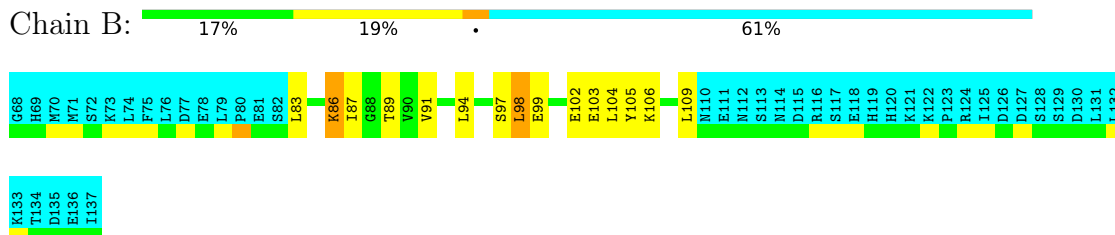
4.1 Average score per residue in the NMR ensemble

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: Histone chaperone RTT106



- Molecule 1: Histone chaperone RTT106

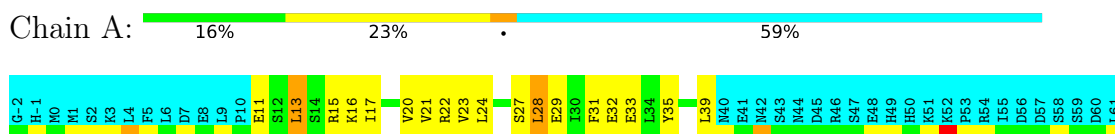


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Histone chaperone RTT106





- Molecule 1: Histone chaperone RTT106

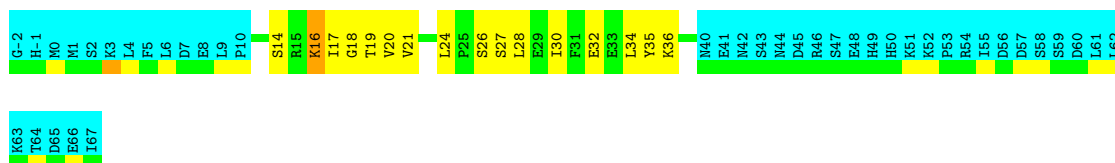
Chain B: 14% 21% 61%



4.2.2 Score per residue for model 2

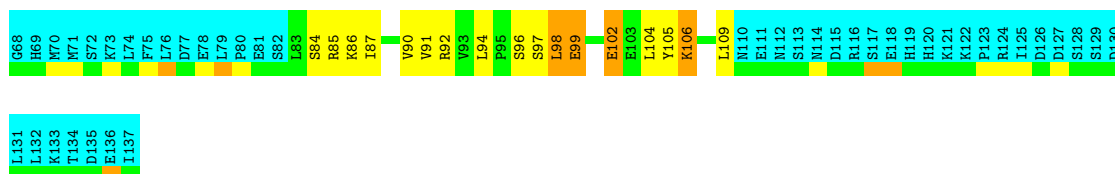
- Molecule 1: Histone chaperone RTT106

Chain A: 19% 21% 59%



- Molecule 1: Histone chaperone RTT106

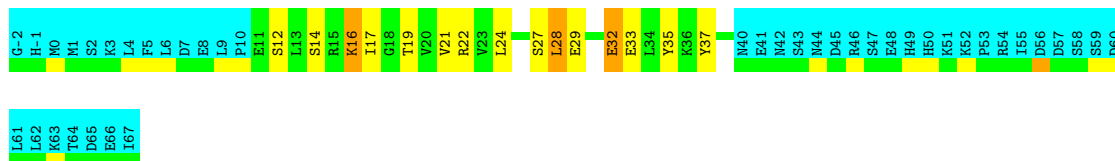
Chain B: 14% 19% 6% 61%



4.2.3 Score per residue for model 3

- Molecule 1: Histone chaperone RTT106

Chain A: 20% 17% 59%

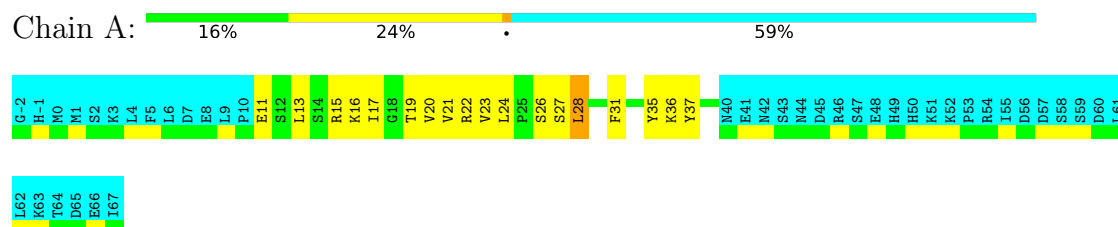


- Molecule 1: Histone chaperone RTT106

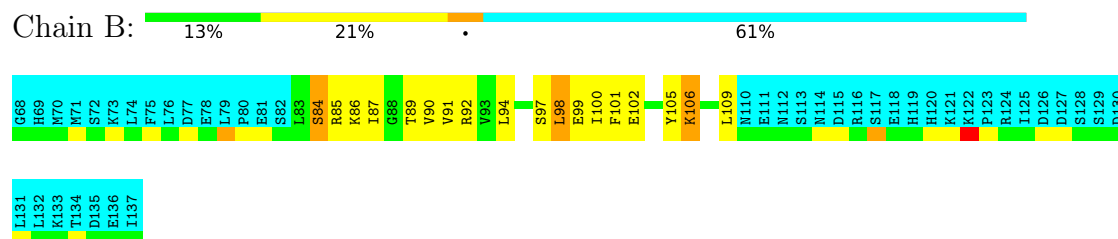


4.2.4 Score per residue for model 4

- Molecule 1: Histone chaperone RTT106

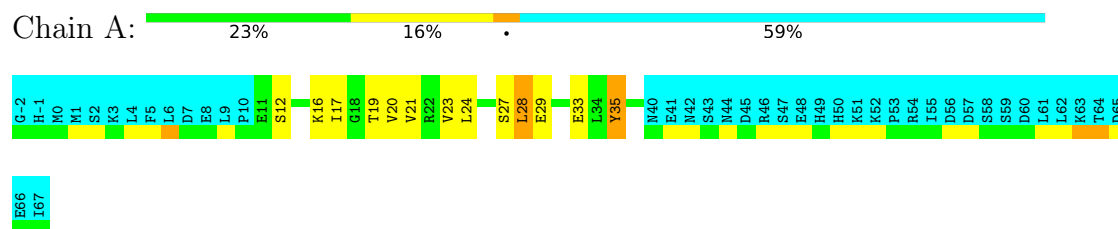


- Molecule 1: Histone chaperone RTT106

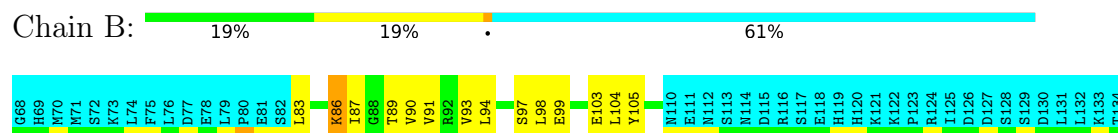


4.2.5 Score per residue for model 5

- Molecule 1: Histone chaperone RTT106



- Molecule 1: Histone chaperone RTT106



D135
E136
I137

4.2.6 Score per residue for model 6

- Molecule 1: Histone chaperone RTT106

Chain A: 17% 20% . 59%

G-2 H-1 M0 M1 S2 K3 L4 F5 L6 D7 E8 E9 P10 P11 S12 L13 S14 I17 V20 V21 V22 V23 L24 S27 L28 L29 E29 E30 F31 E32 Y35 K36 L39 M40 E41 M42 M43 M44 M45 S47 E48 H49 H50 K51 K52 P53 R54 I55 D56 D57 S58 S59 D60 L61 L62

K63
T64
D65
E66
I67

- Molecule 1: Histone chaperone RTT106

Chain B: 14% 19% 6% 61%

G68 H69 M70 M71 S72 K73 L74 F75 L76 D77 E78 E79 L79 P80 P81 S82 L83 S84 R85 K86 I87 T88 G88 T89 V90 V91 R92 R93 L94 S97 L98 S99 F99 I100 E102 E103 L104 Y105 K106 L109 M110 E111 M112 S113 M114 D115 R116 S117 E118 H119 H120 K121 P123 P124 R125 I126 D127 S128 L129

D130
L131
L132
K133
T134
D135
E136
I137

4.2.7 Score per residue for model 7

- Molecule 1: Histone chaperone RTT106

Chain A: 21% 17% . 59%

G-2 H-1 M0 M1 S2 K3 L4 F5 L6 D7 E8 E9 P10 P11 S12 L13 S14 K16 K17 G18 T19 V20 V21 V22 V23 L24 F25 S26 S27 L28 E32 E33 L34 Y35 M40 E41 M42 S43 M44 D45 M46 S47 E48 H49 H50 K51 K52 P53 R54 I55 D56 D57 S58 S59 D60 L61 L62 K63

T64
D65
E66
I67

- Molecule 1: Histone chaperone RTT106

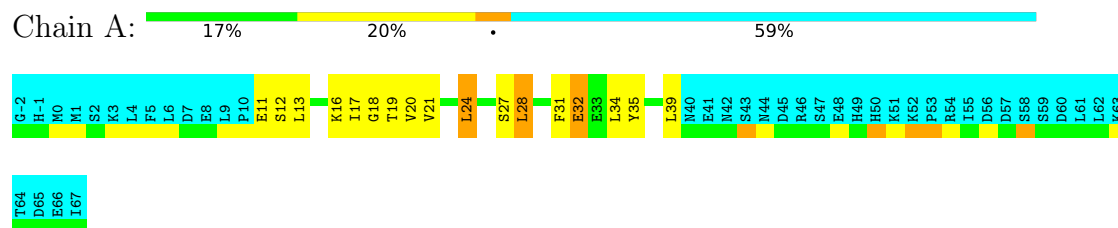
Chain B: 16% 21% . 61%

G68 H69 M70 M71 S72 K73 L74 F75 L76 D77 E78 E79 L79 P80 P81 S82 L83 S84 R85 K86 I87 T88 G88 T89 V90 V91 R92 R93 L94 P95 S96 S97 L98 E102 E103 L104 Y105 K106 M110 E111 M112 S113 M114 D115 R116 S117 E118 H119 H120 K121 P123 P124 R125 I126 D127 S128 L129 L131

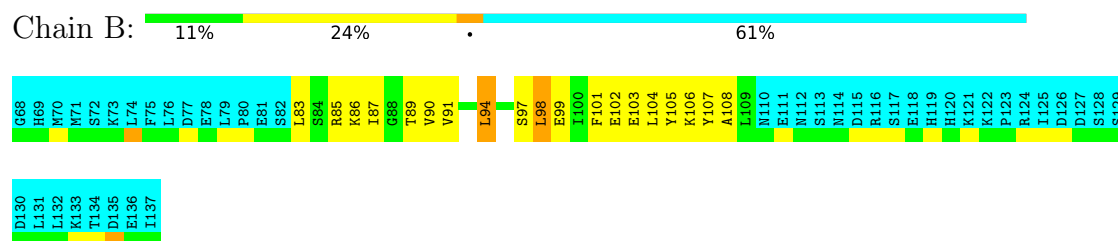
L132
K133
T134
D135
E136
I137

4.2.8 Score per residue for model 8

- Molecule 1: Histone chaperone RTT106

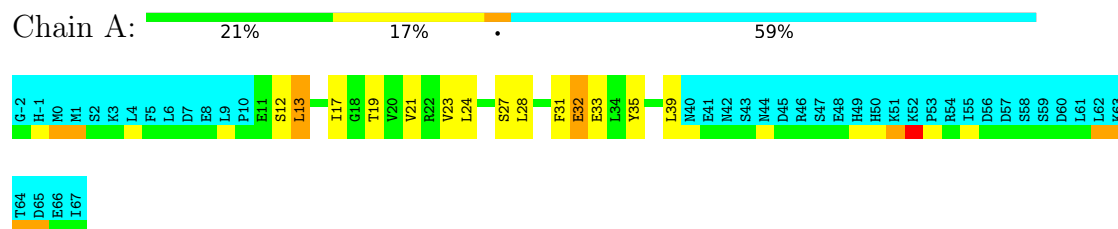


- Molecule 1: Histone chaperone RTT106

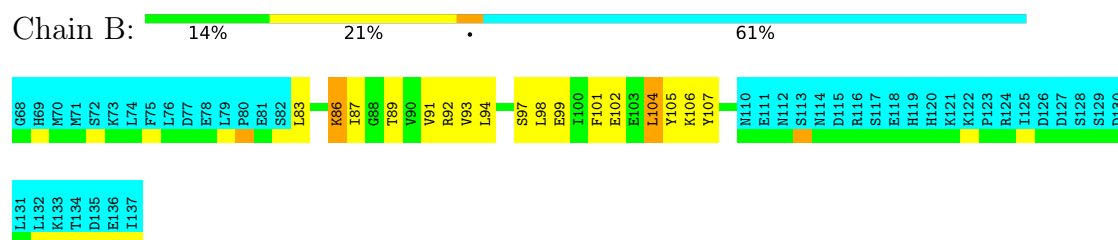


4.2.9 Score per residue for model 9

- Molecule 1: Histone chaperone RTT106



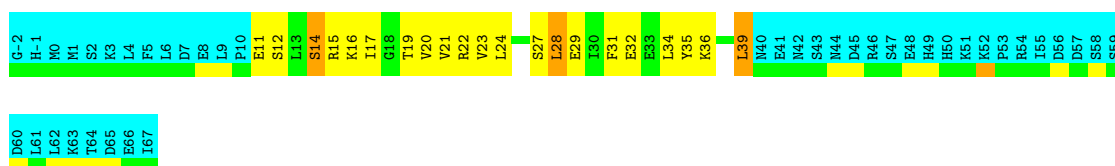
- Molecule 1: Histone chaperone RTT106



4.2.10 Score per residue for model 10

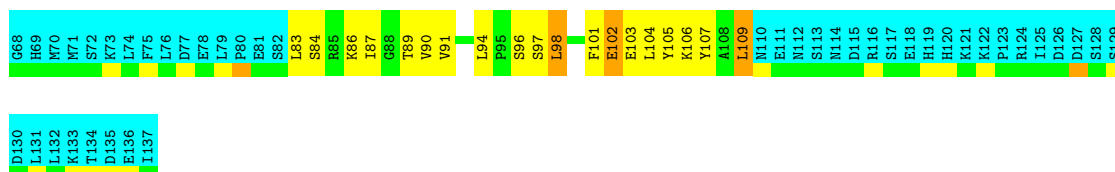
- Molecule 1: Histone chaperone RTT106





• Molecule 1: Histone chaperone RTT106

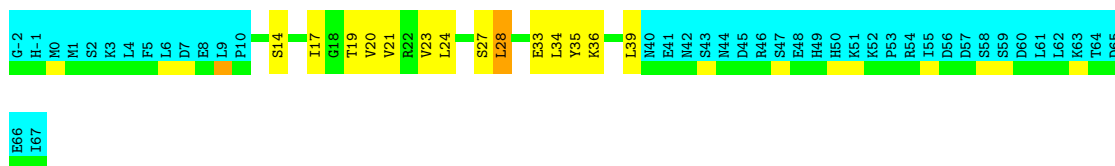
Chain B: 11% 23% . 61%



4.2.11 Score per residue for model 11

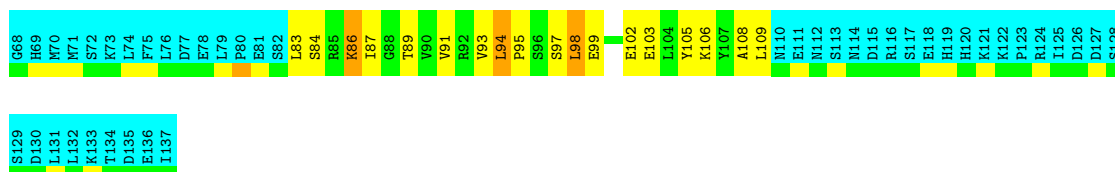
• Molecule 1: Histone chaperone RTT106

Chain A: 21% 19% . 59%



• Molecule 1: Histone chaperone RTT106

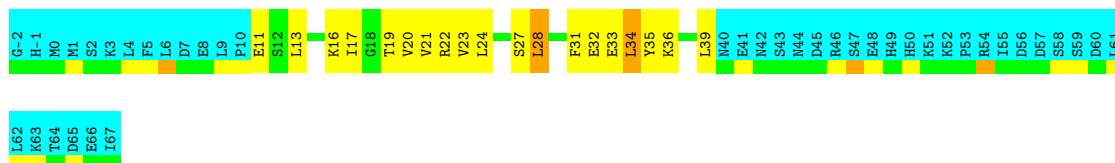
Chain B: 13% 21% . 61%



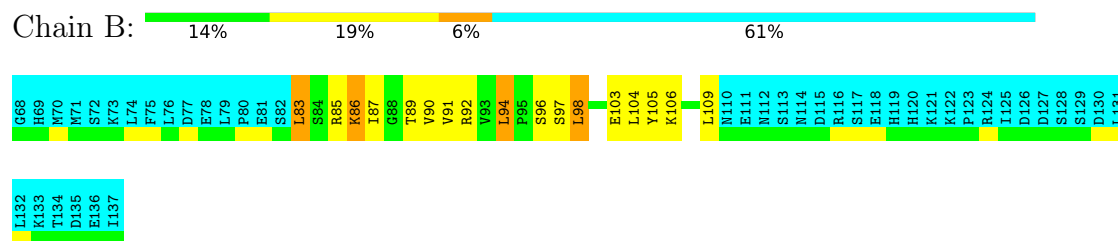
4.2.12 Score per residue for model 12

• Molecule 1: Histone chaperone RTT106

Chain A: 14% 24% . 59%

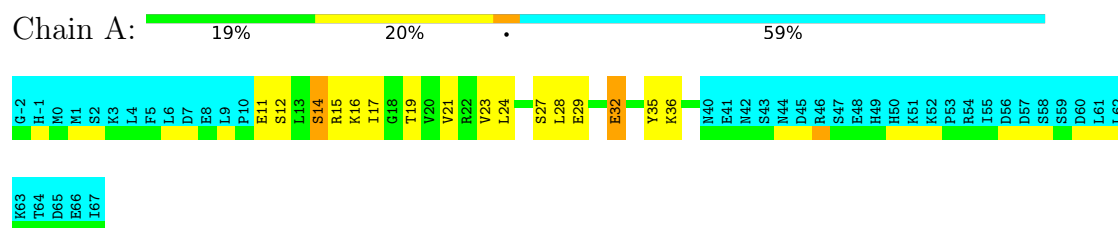


- Molecule 1: Histone chaperone RTT106

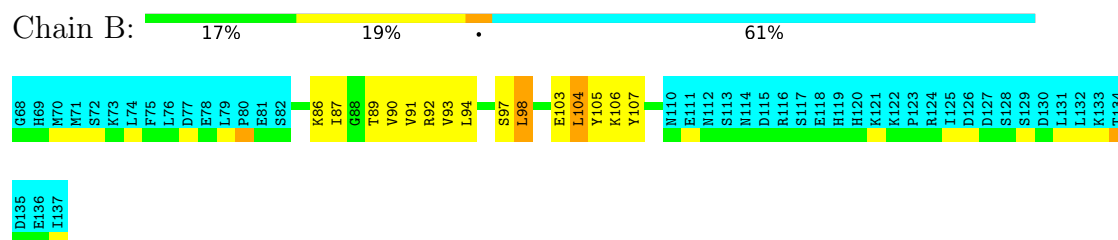


4.2.13 Score per residue for model 13

- Molecule 1: Histone chaperone RTT106

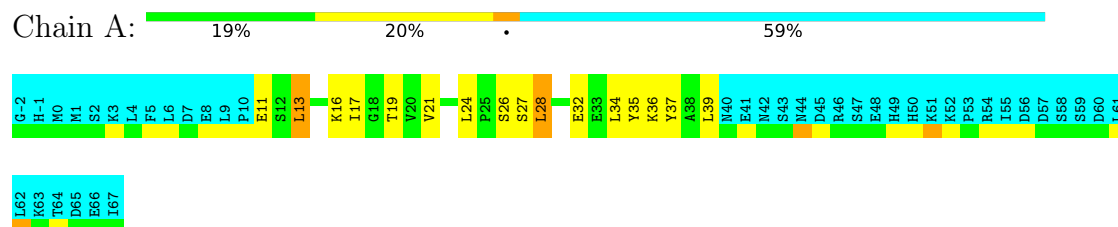


- Molecule 1: Histone chaperone RTT106



4.2.14 Score per residue for model 14

- Molecule 1: Histone chaperone RTT106



- Molecule 1: Histone chaperone RTT106

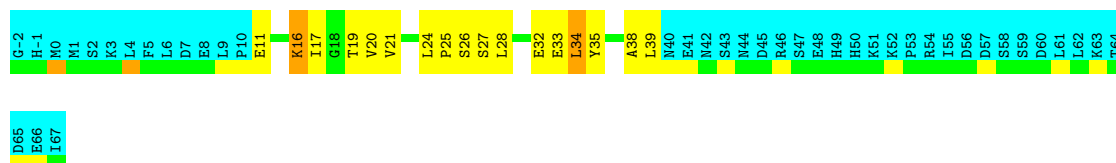




4.2.15 Score per residue for model 15

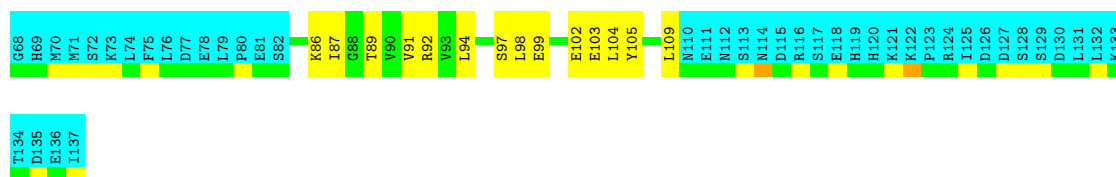
- Molecule 1: Histone chaperone RTT106

Chain A: 17% 21% . 59%



- Molecule 1: Histone chaperone RTT106

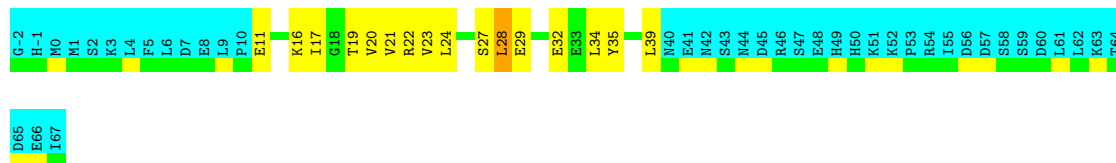
Chain B: 19% 20% . 61%



4.2.16 Score per residue for model 16

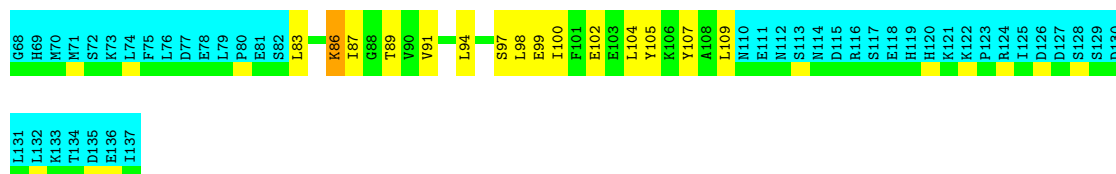
- Molecule 1: Histone chaperone RTT106

Chain A: 19% 21% . 59%



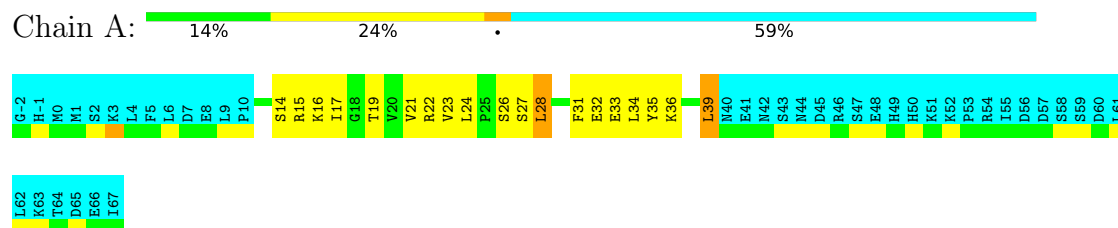
- Molecule 1: Histone chaperone RTT106

Chain B: 17% 20% . 61%

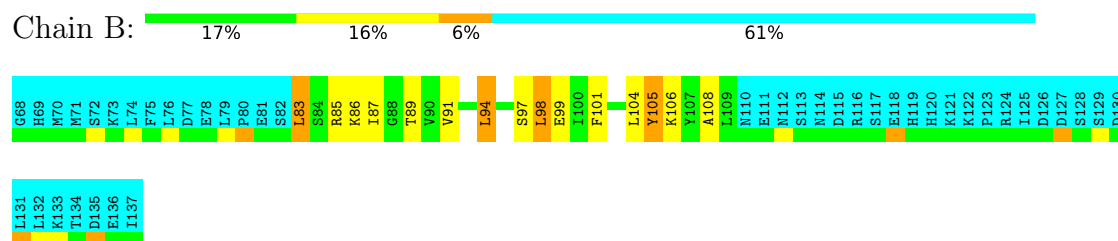


4.2.17 Score per residue for model 17

- Molecule 1: Histone chaperone RTT106

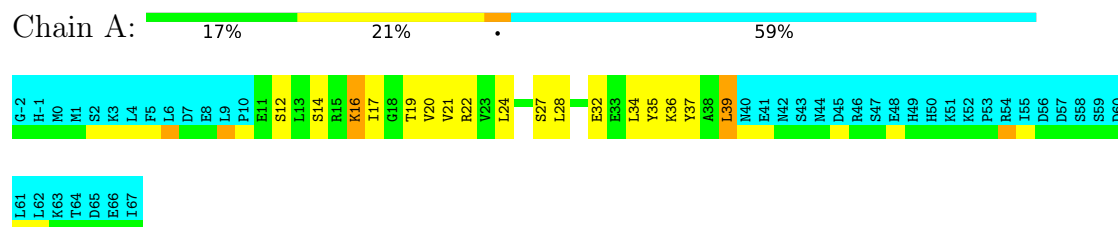


- Molecule 1: Histone chaperone RTT106

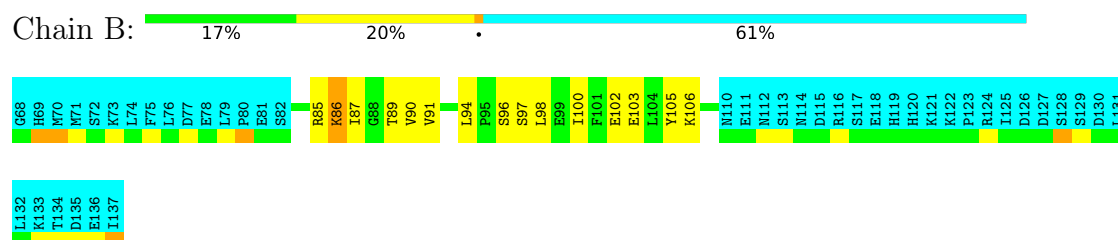


4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Histone chaperone RTT106



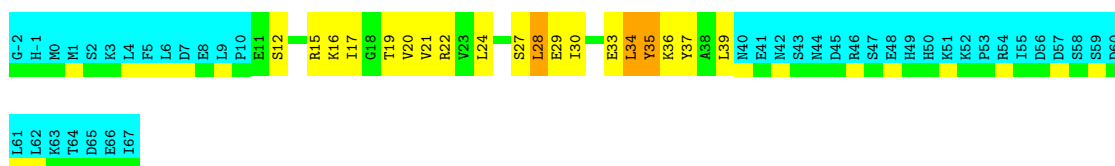
- Molecule 1: Histone chaperone RTT106



4.2.19 Score per residue for model 19

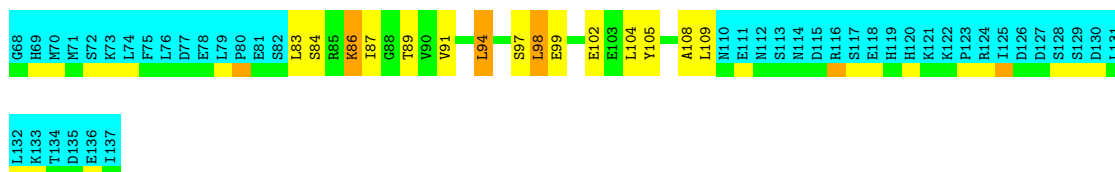
- Molecule 1: Histone chaperone RTT106





- Molecule 1: Histone chaperone RTT106

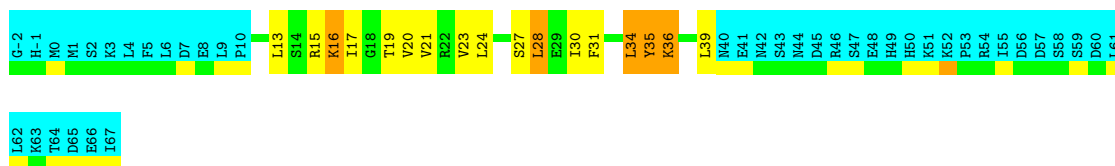
Chain B: 17% 17% . 61%



4.2.20 Score per residue for model 20

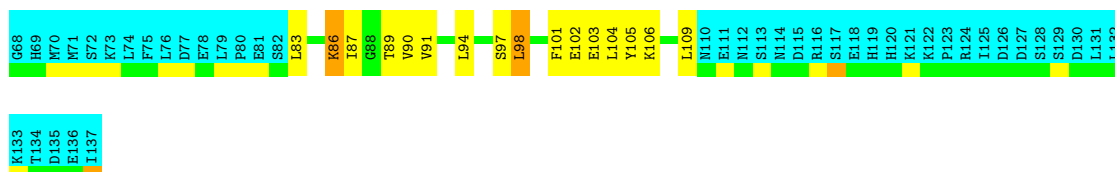
- Molecule 1: Histone chaperone RTT106

Chain A: 17% 17% 7% 59%



- Molecule 1: Histone chaperone RTT106

Chain B: 16% 20% . 61%



5 Refinement protocol and experimental data overview

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

Of the 200 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
CNS	structure solution	1.2
CNS	refinement	1.2

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	803
Number of shifts mapped to atoms	803
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

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	235	249	249	14±3
1	B	220	238	238	14±2
All	All	9100	9740	9740	471

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD13	1:B:94:LEU:HD13	1.03	1.31	8	4
1:A:24:LEU:HD23	1:B:94:LEU:HD13	0.95	1.38	11	4
1:B:91:VAL:HG11	1:B:98:LEU:HD12	0.94	1.37	12	3
1:A:21:VAL:HG11	1:A:28:LEU:HD12	0.90	1.41	19	3
1:A:17:ILE:O	1:A:21:VAL:HG23	0.84	1.72	9	20
1:B:98:LEU:HD13	1:B:99:GLU:N	0.83	1.88	2	1
1:B:91:VAL:CG1	1:B:98:LEU:HD12	0.83	2.03	12	3
1:B:94:LEU:HD23	1:B:97:SER:CB	0.82	2.04	19	9
1:B:87:ILE:O	1:B:91:VAL:HG23	0.82	1.74	20	20
1:A:28:LEU:HD13	1:A:29:GLU:N	0.82	1.89	1	1
1:A:21:VAL:CG1	1:A:28:LEU:HD12	0.80	2.06	19	3
1:B:94:LEU:HD12	1:B:97:SER:CB	0.80	2.05	14	2
1:B:86:LYS:O	1:B:89:THR:HG22	0.79	1.77	6	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD12	1:A:27:SER:CB	0.78	2.08	14	1
1:A:34:LEU:HD22	1:A:34:LEU:O	0.78	1.77	15	3
1:A:23:VAL:HG12	1:B:94:LEU:HD11	0.77	1.54	5	1
1:B:94:LEU:HD13	1:B:97:SER:CB	0.77	2.10	16	2
1:A:23:VAL:CG1	1:B:94:LEU:HD11	0.77	2.10	5	2
1:B:94:LEU:HD12	1:B:97:SER:HB2	0.76	1.56	15	7
1:A:21:VAL:HG22	1:A:28:LEU:CD1	0.76	2.11	4	2
1:B:104:LEU:O	1:B:104:LEU:HD22	0.75	1.80	13	1
1:A:24:LEU:HD13	1:A:27:SER:CB	0.75	2.12	7	5
1:A:24:LEU:HD23	1:A:27:SER:CB	0.72	2.15	13	7
1:B:104:LEU:HD12	1:B:105:TYR:N	0.71	2.00	17	2
1:A:24:LEU:HD12	1:A:27:SER:OG	0.71	1.86	12	1
1:B:98:LEU:O	1:B:98:LEU:HD12	0.70	1.87	17	5
1:A:24:LEU:HD13	1:B:94:LEU:CD1	0.69	2.18	17	3
1:A:13:LEU:HD22	1:A:17:ILE:HD11	0.69	1.65	14	3
1:A:16:LYS:O	1:A:19:THR:HG22	0.68	1.88	17	11
1:A:23:VAL:HG12	1:B:94:LEU:HD21	0.68	1.64	4	2
1:A:24:LEU:HD12	1:A:27:SER:HB2	0.68	1.64	2	6
1:B:104:LEU:HD13	1:B:105:TYR:N	0.67	2.05	13	1
1:B:91:VAL:HG13	1:B:98:LEU:HD12	0.67	1.64	15	1
1:B:86:LYS:O	1:B:90:VAL:HG23	0.67	1.89	20	6
1:A:24:LEU:HD23	1:B:94:LEU:CD1	0.67	2.17	11	2
1:A:34:LEU:HD13	1:A:35:TYR:N	0.67	2.05	15	3
1:A:28:LEU:HD12	1:A:28:LEU:O	0.66	1.89	20	5
1:A:24:LEU:HB2	1:B:94:LEU:HD22	0.64	1.69	8	5
1:B:94:LEU:HD12	1:B:97:SER:HB3	0.64	1.69	14	1
1:A:24:LEU:CD2	1:B:94:LEU:HD13	0.64	2.20	11	4
1:B:84:SER:HA	1:B:87:ILE:HD12	0.64	1.69	14	4
1:A:24:LEU:HD12	1:A:27:SER:HB3	0.63	1.71	14	2
1:A:16:LYS:O	1:A:20:VAL:HG23	0.62	1.94	4	4
1:A:21:VAL:HG11	1:A:28:LEU:HD22	0.62	1.71	17	1
1:A:21:VAL:HG13	1:A:28:LEU:HD22	0.62	1.70	2	2
1:A:24:LEU:HD12	1:B:94:LEU:HB2	0.62	1.72	4	4
1:B:87:ILE:HG22	1:B:91:VAL:CG2	0.62	2.25	15	8
1:A:21:VAL:HG13	1:A:28:LEU:HD13	0.62	1.71	6	2
1:A:39:LEU:HD11	1:B:108:ALA:HB1	0.62	1.70	8	3
1:B:104:LEU:HD22	1:B:104:LEU:C	0.61	2.20	13	1
1:A:24:LEU:HD13	1:B:94:LEU:HD23	0.61	1.73	15	1
1:A:24:LEU:CD1	1:B:94:LEU:HD13	0.60	2.26	18	3
1:A:24:LEU:HD13	1:B:94:LEU:CD2	0.60	2.26	15	2
1:B:94:LEU:HD23	1:B:97:SER:HB3	0.59	1.72	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:SER:HA	1:A:17:ILE:HD12	0.59	1.73	10	1
1:A:28:LEU:HD22	1:A:28:LEU:C	0.59	2.23	1	1
1:A:34:LEU:HD22	1:A:34:LEU:C	0.58	2.22	15	3
1:B:93:VAL:O	1:B:94:LEU:HD22	0.58	1.99	9	3
1:A:24:LEU:HD23	1:A:27:SER:HB2	0.58	1.75	13	3
1:A:35:TYR:O	1:A:39:LEU:HD12	0.58	1.98	10	2
1:A:24:LEU:HD13	1:A:27:SER:HB3	0.58	1.73	9	2
1:A:34:LEU:HD13	1:A:34:LEU:C	0.58	2.24	15	2
1:A:31:PHE:CZ	1:B:91:VAL:HG22	0.57	2.34	12	1
1:A:24:LEU:HD13	1:A:27:SER:HB2	0.57	1.74	5	2
1:B:98:LEU:C	1:B:98:LEU:HD22	0.57	2.24	2	1
1:A:24:LEU:HD22	1:B:94:LEU:HB2	0.57	1.76	18	3
1:A:21:VAL:CG1	1:A:28:LEU:HD22	0.57	2.29	3	2
1:A:23:VAL:O	1:A:24:LEU:HD12	0.57	1.99	10	3
1:A:24:LEU:HD22	1:A:27:SER:HB2	0.56	1.76	20	3
1:A:34:LEU:HD12	1:A:35:TYR:N	0.56	2.16	2	1
1:A:23:VAL:O	1:A:24:LEU:HD22	0.56	2.01	12	3
1:A:20:VAL:HG21	1:B:97:SER:OG	0.55	2.02	6	4
1:A:23:VAL:CG1	1:B:94:LEU:HD21	0.54	2.32	9	2
1:B:94:LEU:HD23	1:B:97:SER:HB2	0.54	1.79	19	2
1:B:94:LEU:HD22	1:B:97:SER:HB2	0.54	1.78	10	2
1:B:104:LEU:C	1:B:104:LEU:HD23	0.54	2.28	8	1
1:B:94:LEU:HD13	1:B:97:SER:HB2	0.53	1.79	10	1
1:B:93:VAL:HG12	1:B:94:LEU:CD2	0.53	2.34	7	2
1:B:94:LEU:HD13	1:B:97:SER:HB3	0.53	1.81	16	1
1:B:104:LEU:HD13	1:B:104:LEU:C	0.53	2.29	13	1
1:B:83:LEU:C	1:B:83:LEU:HD12	0.53	2.28	19	2
1:B:91:VAL:HG22	1:B:98:LEU:CD1	0.53	2.33	10	1
1:A:27:SER:HA	1:A:30:ILE:HD12	0.53	1.79	19	3
1:A:23:VAL:C	1:A:24:LEU:HD22	0.53	2.29	12	2
1:A:20:VAL:HG11	1:B:97:SER:CB	0.52	2.34	11	2
1:A:34:LEU:C	1:A:34:LEU:HD13	0.52	2.30	19	1
1:A:24:LEU:HD12	1:B:94:LEU:HD13	0.52	1.79	20	1
1:A:23:VAL:HG12	1:A:24:LEU:CD2	0.52	2.34	11	4
1:A:21:VAL:HG11	1:A:28:LEU:CD2	0.51	2.34	17	1
1:B:98:LEU:HD22	1:B:98:LEU:O	0.51	2.05	2	1
1:A:39:LEU:HD23	1:B:109:LEU:HG	0.51	1.81	20	1
1:A:24:LEU:HD22	1:A:27:SER:CB	0.51	2.35	7	3
1:A:28:LEU:HD22	1:A:28:LEU:O	0.51	2.05	1	1
1:A:24:LEU:HD23	1:A:27:SER:HB3	0.51	1.81	8	3
1:A:21:VAL:HG13	1:A:28:LEU:CD2	0.51	2.36	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:VAL:HG11	1:B:97:SER:OG	0.51	2.06	11	5
1:B:93:VAL:C	1:B:94:LEU:HD22	0.51	2.31	7	2
1:A:31:PHE:CD2	1:B:101:PHE:CD2	0.50	3.00	4	6
1:B:98:LEU:HD13	1:B:98:LEU:C	0.50	2.31	2	1
1:B:97:SER:HA	1:B:100:ILE:HD12	0.50	1.83	3	3
1:A:39:LEU:HD21	1:B:108:ALA:O	0.50	2.06	8	1
1:A:24:LEU:HB2	1:B:94:LEU:HD12	0.50	1.82	10	1
1:A:28:LEU:HD12	1:A:28:LEU:C	0.50	2.32	15	1
1:A:39:LEU:HD21	1:B:108:ALA:HB1	0.50	1.84	17	1
1:A:13:LEU:HD23	1:A:16:LYS:HE2	0.49	1.82	7	1
1:B:105:TYR:C	1:B:105:TYR:CD1	0.49	2.90	6	9
1:B:106:LYS:HA	1:B:109:LEU:HD12	0.49	1.83	2	1
1:B:93:VAL:O	1:B:94:LEU:HD12	0.49	2.08	5	2
1:A:28:LEU:HD13	1:A:28:LEU:C	0.49	2.33	1	1
1:A:35:TYR:C	1:A:35:TYR:CD1	0.49	2.91	12	6
1:B:91:VAL:HG22	1:B:98:LEU:HD13	0.49	1.84	10	1
1:A:34:LEU:O	1:A:34:LEU:HD23	0.48	2.08	7	3
1:B:91:VAL:HG11	1:B:98:LEU:HD22	0.48	1.84	8	1
1:A:24:LEU:HD22	1:A:27:SER:HB3	0.48	1.85	7	1
1:A:27:SER:OG	1:B:90:VAL:HG11	0.48	2.09	1	4
1:A:31:PHE:CD2	1:B:101:PHE:CE2	0.47	3.03	17	2
1:A:17:ILE:HG22	1:A:21:VAL:CG2	0.47	2.40	18	1
1:A:25:PRO:HA	1:A:28:LEU:HD23	0.46	1.86	15	1
1:A:39:LEU:HD11	1:B:108:ALA:CB	0.46	2.40	8	1
1:A:35:TYR:CD1	1:A:35:TYR:C	0.46	2.93	16	8
1:A:17:ILE:O	1:A:20:VAL:HG12	0.46	2.11	6	2
1:A:27:SER:OG	1:B:90:VAL:HG21	0.46	2.10	2	2
1:B:105:TYR:O	1:B:109:LEU:HD12	0.46	2.11	6	1
1:B:97:SER:O	1:B:100:ILE:HD12	0.46	2.11	6	1
1:A:24:LEU:CD1	1:B:94:LEU:HD23	0.46	2.39	15	1
1:B:105:TYR:CD1	1:B:106:LYS:N	0.45	2.84	18	2
1:A:31:PHE:CZ	1:B:98:LEU:CD1	0.45	3.00	10	1
1:B:104:LEU:HD23	1:B:104:LEU:O	0.45	2.12	16	2
1:B:105:TYR:CE1	1:B:106:LYS:CG	0.45	3.00	6	1
1:B:94:LEU:HD22	1:B:97:SER:CB	0.45	2.42	16	1
1:B:107:TYR:CD1	1:B:107:TYR:C	0.44	2.96	8	5
1:B:94:LEU:HD11	1:B:97:SER:HB2	0.44	1.89	6	1
1:A:23:VAL:HG12	1:A:24:LEU:HD23	0.44	1.90	11	1
1:B:105:TYR:CG	1:B:106:LYS:N	0.44	2.85	18	1
1:B:105:TYR:CZ	1:B:106:LYS:CG	0.44	3.00	20	1
1:B:102:GLU:O	1:B:105:TYR:CD2	0.44	2.71	15	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:105:TYR:CD1	1:B:105:TYR:C	0.44	2.95	13	6
1:A:20:VAL:HG11	1:B:97:SER:HB2	0.44	1.89	11	1
1:A:23:VAL:C	1:A:24:LEU:HD12	0.44	2.38	10	1
1:A:20:VAL:HG21	1:B:97:SER:CB	0.44	2.43	15	2
1:A:31:PHE:CE1	1:B:98:LEU:HD13	0.44	2.48	20	1
1:A:34:LEU:CD1	1:B:87:ILE:HD13	0.44	2.43	12	1
1:A:32:GLU:O	1:A:35:TYR:CD2	0.43	2.71	7	12
1:A:23:VAL:HG12	1:A:24:LEU:HD22	0.43	1.90	6	1
1:B:83:LEU:HD23	1:B:86:LYS:HD2	0.43	1.89	17	1
1:A:24:LEU:HD23	1:B:94:LEU:HD21	0.43	1.89	1	2
1:B:91:VAL:HG22	1:B:98:LEU:HD12	0.43	1.89	4	1
1:A:39:LEU:HG	1:B:109:LEU:HD23	0.43	1.90	10	1
1:A:31:PHE:CE1	1:B:91:VAL:HG22	0.43	2.48	12	1
1:A:21:VAL:HG13	1:A:28:LEU:HD23	0.43	1.89	15	1
1:A:28:LEU:HD13	1:A:29:GLU:H	0.43	1.71	1	1
1:B:102:GLU:O	1:B:105:TYR:CE2	0.42	2.72	4	2
1:A:37:TYR:CD1	1:A:37:TYR:C	0.42	2.97	3	5
1:A:24:LEU:CD2	1:B:94:LEU:CD2	0.42	2.98	14	2
1:B:102:GLU:O	1:B:105:TYR:CD1	0.42	2.73	10	1
1:B:104:LEU:HD23	1:B:104:LEU:C	0.42	2.40	16	1
1:B:87:ILE:HG22	1:B:91:VAL:HG23	0.42	1.91	6	3
1:B:98:LEU:HD12	1:B:98:LEU:C	0.42	2.39	17	1
1:A:21:VAL:HG22	1:A:28:LEU:HD12	0.42	1.90	5	1
1:A:31:PHE:CE1	1:B:98:LEU:HD11	0.42	2.49	6	1
1:A:38:ALA:O	1:B:109:LEU:HD21	0.41	2.15	15	1
1:A:32:GLU:O	1:A:35:TYR:CE2	0.41	2.74	12	3
1:A:32:GLU:O	1:A:35:TYR:CD1	0.41	2.74	17	1
1:A:24:LEU:HD21	1:B:93:VAL:CG1	0.41	2.46	11	1
1:B:104:LEU:HD12	1:B:104:LEU:C	0.41	2.40	12	1
1:A:31:PHE:HZ	1:B:91:VAL:HG22	0.41	1.75	12	1
1:A:20:VAL:HG13	1:A:21:VAL:N	0.41	2.30	2	2
1:A:24:LEU:CD2	1:A:27:SER:CB	0.41	2.98	3	1
1:A:20:VAL:HG21	1:B:97:SER:HB2	0.41	1.91	8	1
1:A:24:LEU:HD21	1:B:93:VAL:HG12	0.41	1.92	11	1
1:B:105:TYR:CZ	1:B:106:LYS:HG3	0.41	2.51	20	1
1:A:34:LEU:HD12	1:A:34:LEU:C	0.40	2.40	2	1
1:A:36:LYS:HA	1:A:39:LEU:HD12	0.40	1.93	20	1
1:A:17:ILE:HG12	1:B:100:ILE:HG21	0.40	1.92	4	1
1:A:27:SER:HB2	1:B:90:VAL:HG21	0.40	1.94	8	1
1:B:90:VAL:HG13	1:B:91:VAL:N	0.40	2.31	12	1
1:A:21:VAL:CG1	1:A:28:LEU:CD2	0.40	2.99	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	29/70 (41%)	29±0 (99±1%)	0±0 (1±1%)	0±0 (0±0%)	100	100
1	B	27/70 (39%)	27±0 (99±1%)	0±0 (0±1%)	0±0 (0±1%)	44	80
All	All	1120/2800 (40%)	1114 (99%)	5 (0%)	1 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	B	95	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	27/67 (40%)	20±2 (73±7%)	7±2 (27±7%)	1	21
1	B	25/67 (37%)	19±2 (74±9%)	6±2 (26±9%)	2	23
All	All	1040/2680 (39%)	763 (73%)	277 (27%)	2	22

All 34 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	B	98	LEU	19
1	A	28	LEU	18
1	B	86	LYS	12
1	B	106	LYS	12
1	A	36	LYS	12
1	A	11	GLU	11
1	A	22	ARG	11

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Mol	Chain	Res	Type	Models (Total)
1	B	99	GLU	11
1	B	103	GLU	11
1	A	16	LYS	10
1	B	85	ARG	10
1	B	83	LEU	10
1	A	33	GLU	9
1	A	39	LEU	9
1	A	34	LEU	9
1	B	92	ARG	8
1	A	12	SER	8
1	A	13	LEU	7
1	A	15	ARG	7
1	B	109	LEU	7
1	A	32	GLU	7
1	A	29	GLU	7
1	A	19	THR	7
1	A	14	SER	6
1	A	26	SER	6
1	B	104	LEU	6
1	B	96	SER	5
1	B	94	LEU	5
1	B	84	SER	4
1	B	89	THR	4
1	B	102	GLU	3
1	A	35	TYR	3
1	B	105	TYR	2
1	A	24	LEU	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

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 41% 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	803
Number of shifts mapped to atoms	803
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	68	2.32 ± 0.16	Should be checked
$^{13}\text{C}_\beta$	67	2.90 ± 0.10	Should be checked
$^{13}\text{C}'$	66	2.46 ± 0.14	Should be applied
^{15}N	63	0.10 ± 0.45	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 46%, i.e. 384 atoms were assigned a chemical shift out of a possible 826. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	144/278 (52%)	58/112 (52%)	58/112 (52%)	28/54 (52%)
Sidechain	227/492 (46%)	155/324 (48%)	72/152 (47%)	0/16 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	13/56 (23%)	13/26 (50%)	0/30 (0%)	0/0 (—%)
Overall	384/826 (46%)	226/462 (49%)	130/294 (44%)	28/70 (40%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 802 atoms were assigned a chemical shift out of a possible 1964. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	325/692 (47%)	128/278 (46%)	134/280 (48%)	63/134 (47%)
Sidechain	460/1148 (40%)	305/740 (41%)	152/366 (42%)	3/42 (7%)
Aromatic	17/124 (14%)	17/60 (28%)	0/52 (0%)	0/12 (0%)
Overall	802/1964 (41%)	450/1078 (42%)	286/698 (41%)	66/188 (35%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:

