Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 06:48 AM EDT

PDB ID	:	2MJF
BMRB ID	:	19626
Title	:	Solution structure of the complex between the yeast Rsa1 and Hit1 proteins
Authors	:	Quinternet, M.; Roth, B.; Back, R.; Jacquemin, C.; Manival, X.
Deposited on	:	2014-01-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

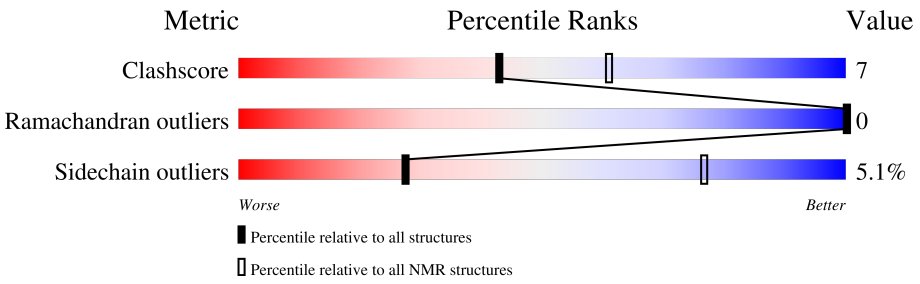
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	40	60% 15% 25%
2	B	95	69% 11% 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:8-A:37, B:43-B:81, B:96-B:132 (106)	0.50	13

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, 11, 12, 13, 14, 15, 17, 18, 20
2	2, 10, 16, 19
Single-model clusters	1

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2174 atoms, of which 1087 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome assembly 1 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	40	624	202	304	51	66	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q08932
A	2	PRO	-	expression tag	UNP Q08932
A	3	HIS	-	expression tag	UNP Q08932
A	4	MET	-	expression tag	UNP Q08932

- Molecule 2 is a protein called Protein HIT1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	95	1550	487	783	129	148	3	0

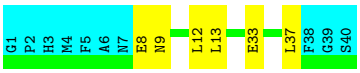
4 Residue-property plots (i)

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.

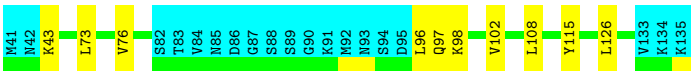
• Molecule 1: Ribosome assembly 1 protein

Chain A: 60% 15% 25%



• Molecule 2: Protein HIT1

Chain B: 69% 11% 20%



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: Ribosome assembly 1 protein

Chain A: 48% 28% 25%

• Molecule 2: Protein HIT1

Chain B: 62% 18% 20%

4.2.2 Score per residue for model 2

- Molecule 1: Ribosome assembly 1 protein

Chain A: 60% 12% • 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 L12 L13 D14 E18 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 65% 14% • 20%

M41 N42 K43 D51 Q55 L73 V76 S81 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 N92 N93 S94 D95 L96 Q97 K98 E99 V102 N103 Y104 L108 I119 V133 K134 K135

4.2.3 Score per residue for model 3

- Molecule 1: Ribosome assembly 1 protein

Chain A: 58% 18% 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 L12 L13 D14 F15 L19 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 58% 19% • 20%

M41 N42 K43 E59 E62 L63 L64 K65 Y66 V69 K70 F71 H72 L73 V76 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 N92 N93 S94 D95 L96 Q97 K98 V102 L108 E117 A118 I119 F122 L126 L130 V133 K134 K135

4.2.4 Score per residue for model 4

- Molecule 1: Ribosome assembly 1 protein

Chain A: 55% 18% • 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 L12 L13 D14 F15 I16 R17 L24 L37 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 62% 16% • 20%

M41 N42 K43 Y54 S57 A58 E59 L60 Q61 E62 F71 H72 L73 V76 Y77 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 N92 N93 S94 D95 L96 Q97 K98 V102 L108 I119 F122 L126 V133 K134 K135

4.2.5 Score per residue for model 5

- Molecule 1: Ribosome assembly 1 protein

Chain A: 52% 22% 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 L12 L13 D14 E18 L25 E33 L37 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 59% 20% • 20%

M41 N42 K43 K48 D51 Q55 F71 H72 L73 A74 K75 V76 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 M92 N93 S94 D95 L96 Q97 K98 V102 N103 Y104 L105 L108 R109 N116 I119 E120 Q124 V133 K134 K135

4.2.6 Score per residue for model 6

- Molecule 1: Ribosome assembly 1 protein

Chain A: 55% 18% • 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 S10 Q11 L12 L13 D14 F15 I16 R17 L24 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 58% 19% • 20%

M41 N42 K43 T44 L45 K46 D51 D52 I53 Y54 Q55 N56 L73 V76 Y77 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 M92 N93 S94 D95 L96 Q97 K98 V102 L105 N106 R109 Y115 L126 L130 V133 K134 K135

4.2.7 Score per residue for model 7

- Molecule 1: Ribosome assembly 1 protein

Chain A: 55% 20% 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 L12 L13 R17 L24 E33 L37 F38 G39 S40

- Molecule 2: Protein HIT1

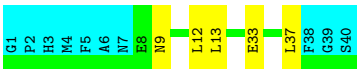
Chain B: 62% 16% • 20%

M41 N42 K43 T44 Y54 Q61 L73 A74 K75 V76 Y77 R78 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 M92 N93 S94 D95 L96 Q97 L105 L108 R109 Y110 Y115 I119 E120 V133 K134 K135

4.2.8 Score per residue for model 8

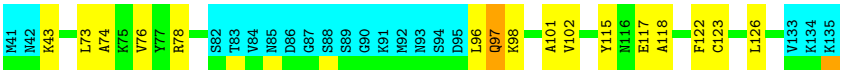
- Molecule 1: Ribosome assembly 1 protein

Chain A: 62% 12% 25%



- Molecule 2: Protein HIT1

Chain B: 63% 16% • 20%



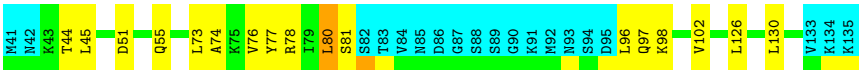
4.2.9 Score per residue for model 9

- Molecule 1: Ribosome assembly 1 protein

Chain A: 48% 28% 25%

- Molecule 2: Protein HIT1

Chain B: 62% 17% • 20%



4.2.10 Score per residue for model 10

- Molecule 1: Ribosome assembly 1 protein

Chain A: 42% 30% • 25%

- Molecule 2: Protein HIT1

Chain B: 64% 15% • 20%

4.2.11 Score per residue for model 11

- Molecule 1: Ribosome assembly 1 protein

Chain A: 55% 18% • 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 S10 Q11 L12 L13 E28 E33 L37 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 69% 11% 20%

M41 N42 K43 L73 V76 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 M92 N93 S94 D95 L96 Q97 L108 I119 Q124 D128 K129 L130 V133 K134 K135

4.2.12 Score per residue for model 12

- Molecule 1: Ribosome assembly 1 protein

Chain A: 58% 18% 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 L12 L13 D14 F15 E33 L37 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 63% 16% • 20%

M41 N42 K43 E59 E62 L73 A74 K75 V76 Y77 R78 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 M92 N93 S94 D95 L96 Q97 K98 V102 N103 Y104 L108 Y115 I119 L126 V133 K134 K135

4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Ribosome assembly 1 protein

Chain A: 60% 15% 25%

G1 P2 H3 M4 F5 A6 N7 E8 N9 L12 L13 E33 L37 F38 G39 S40

- Molecule 2: Protein HIT1

Chain B: 60% 18% • 20%

M41 N42 K43 E59 E62 Y66 V69 L73 V76 S82 T83 V84 N85 D86 G87 S88 S89 G90 K91 M92 N93 S94 D95 L96 Q97 K98 V102 L108 Y115 N116 E117 A118 Q124 I125 L126 L127 D128 K129 L130 V133 K134 K135

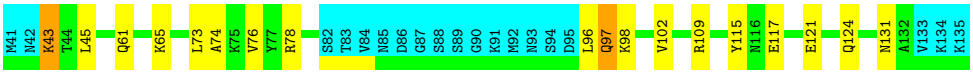
4.2.14 Score per residue for model 14

- Molecule 1: Ribosome assembly 1 protein

Chain A: 52% 18% 5% 25%

- Molecule 2: Protein HIT1

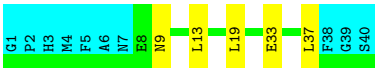
Chain B: 61% 17% • 20%



4.2.15 Score per residue for model 15

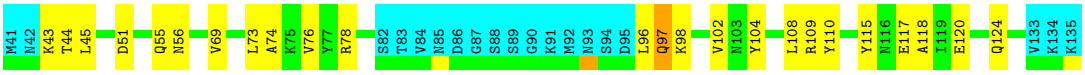
- Molecule 1: Ribosome assembly 1 protein

Chain A: 62% 12% 25%



- Molecule 2: Protein HIT1

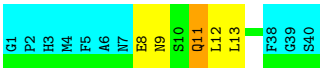
Chain B: 55% 24% • 20%



4.2.16 Score per residue for model 16

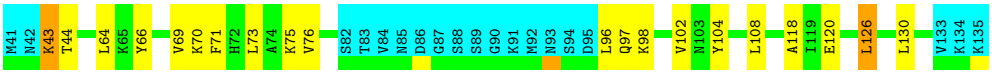
- Molecule 1: Ribosome assembly 1 protein

Chain A: 62% 10% • 25%



- Molecule 2: Protein HIT1

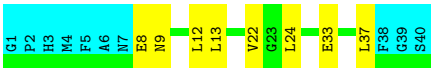
Chain B: 59% 19% • 20%



4.2.17 Score per residue for model 17

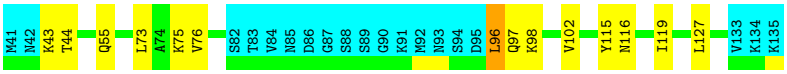
- Molecule 1: Ribosome assembly 1 protein

Chain A: 55% 20% 25%



- Molecule 2: Protein HIT1

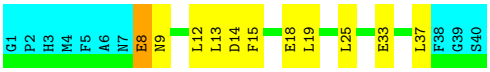
Chain B: 65% 14% • 20%



4.2.18 Score per residue for model 18

- Molecule 1: Ribosome assembly 1 protein

Chain A: 48% 25% • 25%



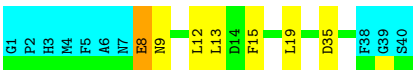
- Molecule 2: Protein HIT1

Chain B: 62% 16% • 20%

4.2.19 Score per residue for model 19

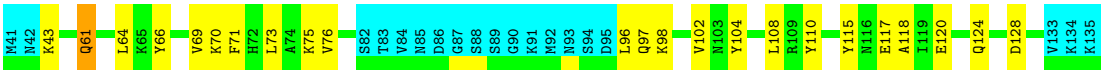
- Molecule 1: Ribosome assembly 1 protein

Chain A: 58% 15% • 25%



- Molecule 2: Protein HIT1

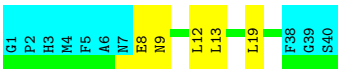
Chain B: 56% 23% • 20%



4.2.20 Score per residue for model 20

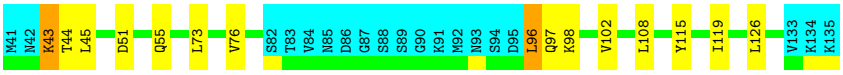
- Molecule 1: Ribosome assembly 1 protein

Chain A:



- Molecule 2: Protein HIT1

Chain B:



5 Refinement protocol and experimental data overview (i)

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
CARA	structure solution	
CARA	structure solution	
CARA	structure solution	
CARA	structure solution	
CNS	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	1715
Number of shifts mapped to atoms	1715
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	245	238	238	5±2
2	B	630	647	645	9±2
All	All	17500	17700	17660	251

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
2:B:69:VAL:HG11	2:B:118:ALA:HB3	0.76	1.57	16	6
1:A:9:ASN:O	1:A:13:LEU:HG	0.71	1.86	5	20
1:A:12:LEU:HD13	2:B:126:LEU:HD12	0.62	1.71	8	1
2:B:71:PHE:O	2:B:75:LYS:HG3	0.58	1.98	16	2
1:A:22:VAL:HG23	1:A:24:LEU:HD13	0.58	1.76	10	3
1:A:12:LEU:HD23	2:B:126:LEU:HD12	0.57	1.76	13	2
1:A:15:PHE:CD2	2:B:126:LEU:HD11	0.56	2.35	1	2
2:B:43:LYS:N	2:B:43:LYS:HD2	0.56	2.15	3	1
2:B:108:LEU:HB3	2:B:119:ILE:HG21	0.56	1.77	1	7
1:A:8:GLU:O	1:A:12:LEU:HG	0.56	2.01	9	6
1:A:19:LEU:HD23	2:B:45:LEU:HD21	0.55	1.77	9	4
2:B:73:LEU:O	2:B:76:VAL:HG22	0.54	2.01	7	19
1:A:12:LEU:HD11	2:B:123:CYS:HA	0.54	1.78	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:66:TYR:O	2:B:69:VAL:HG22	0.54	2.03	16	5
2:B:59:GLU:HA	2:B:62:GLU:OE1	0.54	2.03	13	1
1:A:8:GLU:O	1:A:12:LEU:HD13	0.54	2.03	10	12
2:B:97:GLN:HE21	2:B:97:GLN:HA	0.53	1.63	13	5
2:B:51:ASP:O	2:B:55:GLN:HG2	0.53	2.03	5	8
2:B:104:TYR:O	2:B:108:LEU:HG	0.53	2.04	19	7
2:B:108:LEU:C	2:B:115:TYR:HB2	0.53	2.25	7	3
1:A:24:LEU:HD13	2:B:54:TYR:CE2	0.52	2.39	4	3
1:A:33:GLU:O	1:A:37:LEU:HG	0.51	2.05	18	11
2:B:124:GLN:O	2:B:128:ASP:HB2	0.51	2.05	11	4
2:B:105:LEU:O	2:B:109:ARG:HG2	0.51	2.05	6	2
1:A:8:GLU:HG2	1:A:9:ASN:N	0.50	2.21	19	2
2:B:98:LYS:O	2:B:102:VAL:HG23	0.50	2.07	19	17
2:B:61:GLN:HE21	2:B:61:GLN:HA	0.50	1.66	19	2
2:B:43:LYS:HD2	2:B:43:LYS:H	0.50	1.66	6	10
2:B:74:ALA:O	2:B:78:ARG:HG3	0.50	2.06	18	7
2:B:109:ARG:HH21	2:B:124:GLN:NE2	0.50	2.03	14	1
1:A:9:ASN:HA	1:A:12:LEU:HD12	0.49	1.84	9	2
1:A:30:SER:H	1:A:33:GLU:HG2	0.49	1.67	9	1
2:B:76:VAL:O	2:B:80:LEU:HD22	0.49	2.07	9	1
2:B:110:TYR:HB2	2:B:120:GLU:OE2	0.48	2.08	19	1
1:A:30:SER:HB2	1:A:33:GLU:OE2	0.48	2.09	9	1
1:A:17:ARG:HA	2:B:77:TYR:CD1	0.48	2.44	9	5
2:B:59:GLU:HA	2:B:62:GLU:OE2	0.48	2.09	12	1
1:A:27:TYR:HB3	2:B:70:LYS:HG2	0.48	1.83	1	1
1:A:25:LEU:HD13	2:B:74:ALA:HA	0.47	1.84	5	1
1:A:19:LEU:CB	1:A:25:LEU:HB2	0.47	2.40	9	1
2:B:44:THR:HG22	2:B:55:GLN:NE2	0.47	2.25	17	1
2:B:64:LEU:O	2:B:70:LYS:HD3	0.47	2.10	19	1
2:B:71:PHE:O	2:B:75:LYS:HG2	0.46	2.09	5	1
2:B:43:LYS:HD2	2:B:43:LYS:N	0.46	2.25	6	1
2:B:120:GLU:O	2:B:124:GLN:HG2	0.46	2.09	5	3
2:B:59:GLU:O	2:B:62:GLU:HG2	0.46	2.10	4	3
2:B:109:ARG:HG2	2:B:110:TYR:N	0.46	2.26	15	1
1:A:15:PHE:O	1:A:19:LEU:HG	0.45	2.11	19	6
2:B:61:GLN:O	2:B:65:LYS:HG2	0.45	2.12	14	1
2:B:116:ASN:HB2	2:B:119:ILE:HG12	0.45	1.89	17	2
1:A:31:GLN:HE21	1:A:31:GLN:HA	0.45	1.71	14	1
1:A:37:LEU:HD13	2:B:71:PHE:CD2	0.45	2.47	4	1
1:A:11:GLN:HB3	2:B:130:LEU:HD13	0.45	1.88	16	1
1:A:25:LEU:HD13	1:A:25:LEU:O	0.44	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:SER:H	1:A:33:GLU:CG	0.44	2.25	9	1
1:A:13:LEU:HD22	2:B:101:ALA:HB1	0.44	1.89	8	2
1:A:25:LEU:HA	2:B:70:LYS:HD2	0.44	1.89	1	1
2:B:60:LEU:HD11	2:B:122:PHE:CD1	0.43	2.48	4	1
2:B:117:GLU:O	2:B:121:GLU:HG2	0.43	2.13	14	1
1:A:32:GLN:HE21	1:A:32:GLN:HA	0.43	1.73	10	1
2:B:108:LEU:CB	2:B:119:ILE:HG21	0.43	2.44	7	1
1:A:11:GLN:HE21	1:A:11:GLN:HA	0.43	1.73	16	1
2:B:57:SER:HB2	2:B:60:LEU:CB	0.43	2.43	4	1
2:B:105:LEU:O	2:B:109:ARG:HG3	0.43	2.14	7	1
2:B:64:LEU:O	2:B:70:LYS:HD2	0.43	2.14	16	2
1:A:15:PHE:CE2	2:B:126:LEU:HD11	0.42	2.49	9	2
2:B:57:SER:HB2	2:B:60:LEU:HB3	0.42	1.91	4	1
1:A:25:LEU:HD11	2:B:73:LEU:HB2	0.42	1.92	18	1
2:B:117:GLU:CD	2:B:117:GLU:H	0.42	2.18	15	1
1:A:14:ASP:O	1:A:18:GLU:HG3	0.42	2.14	18	3
2:B:110:TYR:CE2	2:B:120:GLU:HG2	0.41	2.50	7	1
2:B:69:VAL:HG11	2:B:118:ALA:CB	0.41	2.46	15	2
2:B:116:ASN:HB2	2:B:119:ILE:CG1	0.41	2.44	17	1
1:A:37:LEU:HD13	2:B:71:PHE:CG	0.41	2.50	18	1
1:A:8:GLU:HG3	1:A:9:ASN:N	0.41	2.31	3	1
2:B:43:LYS:HD3	2:B:43:LYS:N	0.41	2.31	8	1
1:A:11:GLN:NE2	2:B:130:LEU:HB3	0.41	2.31	6	1
1:A:11:GLN:NE2	2:B:130:LEU:HD22	0.41	2.31	1	1
2:B:59:GLU:O	2:B:63:LEU:HG	0.41	2.16	1	1
2:B:126:LEU:HD13	2:B:130:LEU:HD12	0.41	1.93	13	1
1:A:25:LEU:HD21	2:B:74:ALA:HA	0.41	1.93	1	1
2:B:72:HIS:CG	2:B:108:LEU:HD11	0.41	2.51	3	1
1:A:15:PHE:CD1	2:B:126:LEU:HD21	0.41	2.51	12	1
2:B:118:ALA:O	2:B:122:PHE:HB2	0.40	2.16	8	1
2:B:122:PHE:O	2:B:126:LEU:HB2	0.40	2.16	3	1
2:B:126:LEU:HD22	2:B:130:LEU:CD1	0.40	2.47	3	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	30/40 (75%)	30±1 (99±2%)	0±1 (1±2%)	0±0 (0±0%)	100	100
2	B	76/95 (80%)	74±1 (98±2%)	2±1 (2±2%)	0±0 (0±0%)	100	100
All	All	2120/2700 (79%)	2082 (98%)	38 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	28/35 (80%)	27±1 (98±3%)	1±1 (2±3%)	50	91
2	B	68/85 (80%)	64±2 (94±3%)	4±2 (6±3%)	22	71
All	All	1920/2400 (80%)	1823 (95%)	97 (5%)	27	77

All 26 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)
2	B	96	LEU	17
2	B	43	LYS	15
2	B	97	GLN	9
2	B	115	TYR	9
2	B	44	THR	7
1	A	8	GLU	7
2	B	117	GLU	4
2	B	126	LEU	4
2	B	56	ASN	3
1	A	28	GLU	2
2	B	99	GLU	2
2	B	106	ASN	2
2	B	61	GLN	2
1	A	11	GLN	2
1	A	14	ASP	1
2	B	48	LYS	1
2	B	46	LYS	1
2	B	52	ASP	1
2	B	98	LYS	1

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Mol	Chain	Res	Type	Models (Total)
2	B	80	LEU	1
1	A	32	GLN	1
1	A	31	GLN	1
2	B	131	ASN	1
2	B	120	GLU	1
2	B	75	LYS	1
2	B	127	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 91% 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 (i)

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	1715
Number of shifts mapped to atoms	1715
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	133	-0.54 ± 0.04	Should be checked
$^{13}C_{\beta}$	126	0.14 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	131	-0.45 ± 0.12	None needed (< 0.5 ppm)
^{15}N	131	0.57 ± 0.23	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1418 atoms were assigned a chemical shift out of a possible 1534. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	532/534 (100%)	216/216 (100%)	210/212 (99%)	106/106 (100%)
Sidechain	809/881 (92%)	541/570 (95%)	254/279 (91%)	14/32 (44%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	77/119 (65%)	50/56 (89%)	27/59 (46%)	0/4 (0%)
Overall	1418/1534 (92%)	807/842 (96%)	491/550 (89%)	120/142 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1714 atoms were assigned a chemical shift out of a possible 1877. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	666/681 (98%)	271/277 (98%)	264/270 (98%)	131/134 (98%)
Sidechain	956/1049 (91%)	638/678 (94%)	300/332 (90%)	18/39 (46%)
Aromatic	92/147 (63%)	60/70 (86%)	32/71 (45%)	0/6 (0%)
Overall	1714/1877 (91%)	969/1025 (95%)	596/673 (89%)	149/179 (83%)

7.1.4 Statistically unusual chemical shifts (i)

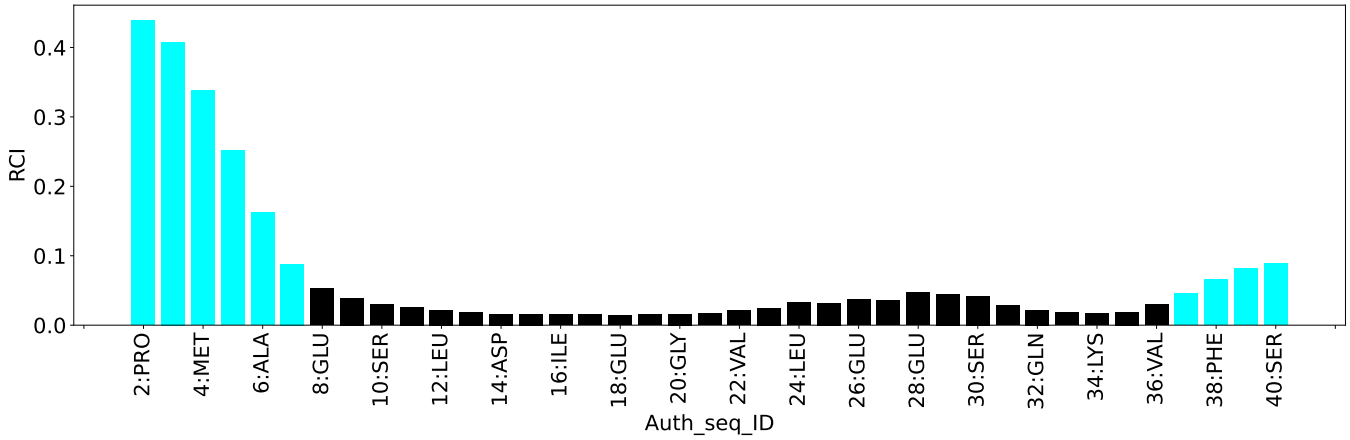
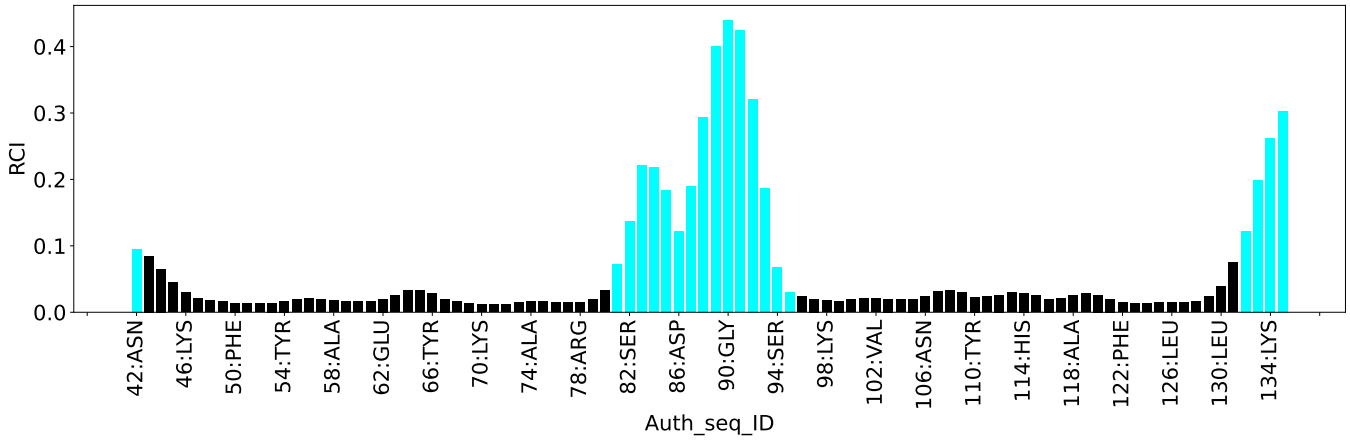
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	20	GLY	HA2	1.74	2.15 – 5.77	-6.1
1	A	32	GLN	HG2	3.90	1.01 – 3.62	6.1
1	A	32	GLN	HG3	3.90	0.91 – 3.68	5.8

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:



Random coil index (RCI) for chain B: