Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LGJ
BMRB ID	:	17811
Title	:	Solution structure of MsPTH
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Deposited on	:	2011-07-27

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 (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:

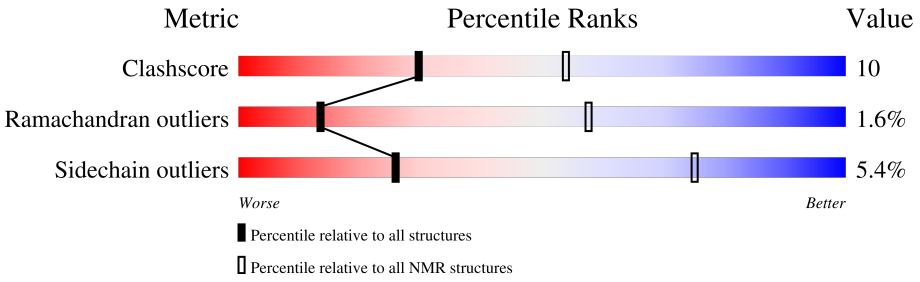
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 82%.

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	191	82% 17% •

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:191 (189)	1.75	3

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 7
2	2, 4, 9
3	5, 10
Single-model clusters	6; 8

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2894 atoms, of which 1464 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-tRNA hydrolase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	191	2894	903	1464	265	258	4	0

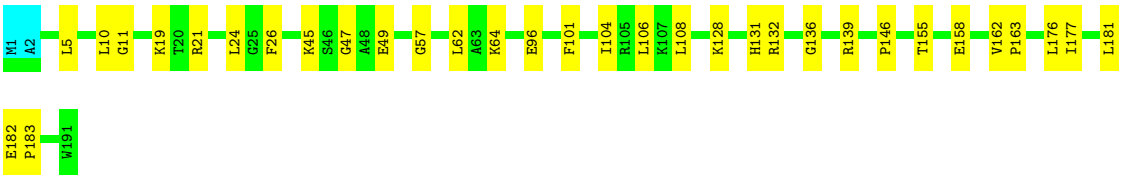
4 Residue-property plots (i)

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: Peptidyl-tRNA hydrolase

Chain A: 82% 17%



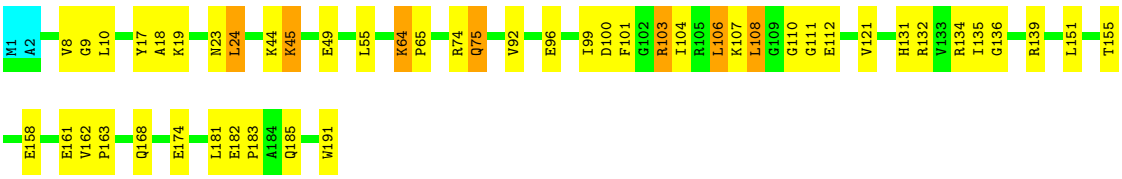
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Peptidyl-tRNA hydrolase

Chain A: 73% 22%



4.2.2 Score per residue for model 2

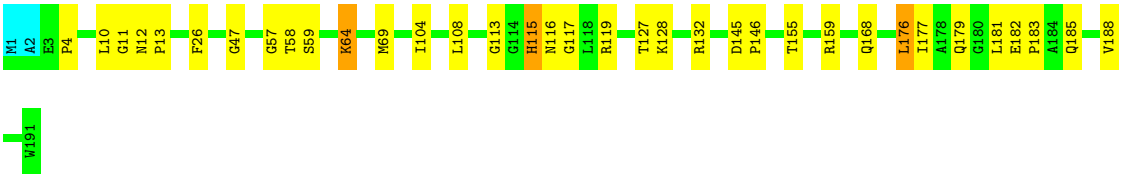
• Molecule 1: Peptidyl-tRNA hydrolase

Chain A: 75% 22%

4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Peptidyl-tRNA hydrolase

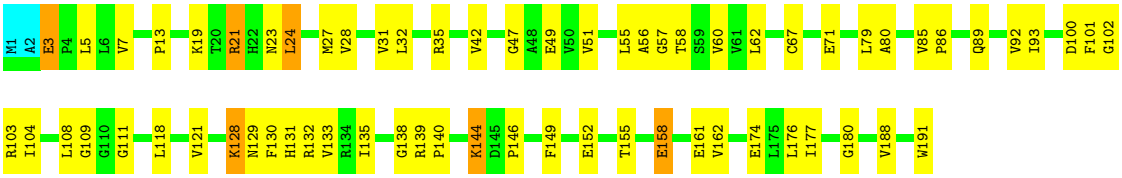
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Peptidyl-tRNA hydrolase

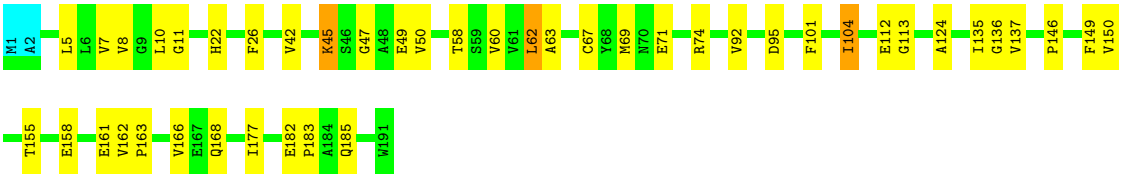
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-tRNA hydrolase

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Peptidyl-tRNA hydrolase

Chain A: 73% 25%

M1 A2 L5 L10 P15 T16 Y17 T20 F26 M27 V28 A29 F40 A48 E49 V50 G57 T58 S59 V60 V61 L62 A63 K64 P65 R74 L79 P87 I90 H94 D95 E96 L97 D100 F101 I104 R105 L106 K128 H131 R132 V133 R134

I135 G136 V137 G138 R139 P140 R143 K144 D145 P146 A147 T155 E158 R159 V162 P163 I177 L181 E182 P183 V188 W191

4.2.7 Score per residue for model 7

- Molecule 1: Peptidyl-tRNA hydrolase

Chain A: 75% 23%

M1 A2 E3 P4 G11 N12 P13 R21 F26 A29 S38 A39 F40 K44 K45 E49 V50 V51 S59 L62 A63 K64 P65 R66 M69 L79 A80 K81 F82 Y83 S84 V85 I90 L97 F101 I104 R105 L106 K107 L108 G117 K128 N129

F130 H131 I135 G136 R139 R143 N153 F154 T155 E158 V162 T173 E174 L175 L176 L181 E182 P183 W191

4.2.8 Score per residue for model 8

- Molecule 1: Peptidyl-tRNA hydrolase

Chain A: 74% 24%

M1 A2 L10 G11 P15 K19 T20 R21 H22 N23 L24 G25 F26 V31 R35 F40 G47 V50 G57 K64 C67 E71 P86 I90 E96 L97 F101 I104 L108 E112 R119 K128 N129 F130 H131 R132 V133 R134 I135

G136 V137 G138 R139 P140 P141 V150 T155 V162 P163 L176 Q179 G180 L181 E182 Q185 V188 W191

4.2.9 Score per residue for model 9

- Molecule 1: Peptidyl-tRNA hydrolase

Chain A: 68% 29%

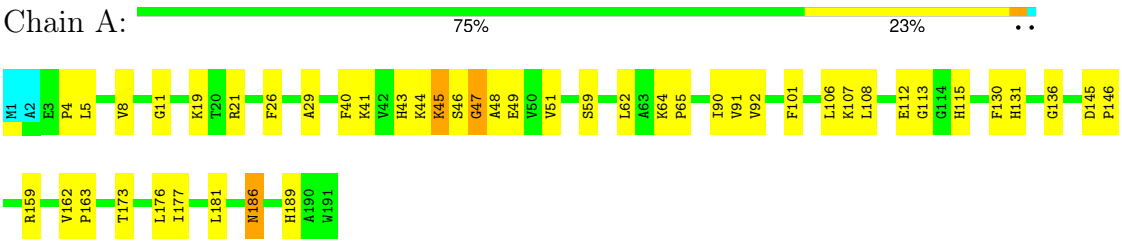
M1 A2 E3 P4 L5 Y17 A18 K19 T20 R21 H22 L32 A33 I36 F40 K41 V42 G47 A48 E49 V50 V51 G57 T58 S59 V60 V61 L62 A63 K64 G73 R74 Q75 V76 G77 V91 H94 D95 E96 L106 K107 L108 G111 G114 H115 L118

V121 L125 H131 V137 P146 A147 A148 F149 V150 L151 T155 E158 R159 V162 P163 V166 L176 I177 A178 Q179 G180 L181 E182 P183 A184 Q185 V188 W191

4.2.10 Score per residue for model 10

- Molecule 1: Peptidyl-tRNA hydrolase

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
TALOS	structure solution	+
CYANA	structure solution	3.0
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	2093
Number of shifts mapped to atoms	2093
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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	1417	1448	1442	29±6
All	All	14170	14480	14420	288

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LYS:HA	1:A:81:LYS:HE2	0.77	1.54	7	1
1:A:11:GLY:HA2	1:A:26:PHE:HB2	0.73	1.60	3	5
1:A:96:GLU:HG3	1:A:134:ARG:HD2	0.71	1.58	2	1
1:A:67:CYS:HB3	1:A:71:GLU:HG3	0.70	1.61	8	1
1:A:4:PRO:HB2	1:A:61:VAL:HG23	0.70	1.61	9	1
1:A:101:PHE:HD2	1:A:137:VAL:HA	0.69	1.46	5	1
1:A:155:THR:HB	1:A:158:GLU:HG2	0.69	1.62	5	1
1:A:19:LYS:HA	1:A:19:LYS:HE2	0.68	1.64	4	1
1:A:69:MET:HB2	1:A:117:GLY:HA2	0.67	1.66	3	1
1:A:96:GLU:HB2	1:A:134:ARG:HB3	0.67	1.64	6	2
1:A:128:LYS:HD2	1:A:128:LYS:H	0.67	1.49	6	2
1:A:93:ILE:HG22	1:A:133:VAL:HB	0.67	1.64	4	1
1:A:21:ARG:HH21	1:A:24:LEU:HG	0.66	1.50	4	1
1:A:49:GLU:HB2	1:A:64:LYS:HB2	0.66	1.65	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:PHE:CD2	1:A:137:VAL:HA	0.66	2.25	5	1
1:A:51:VAL:HG13	1:A:62:LEU:HB3	0.66	1.66	10	2
1:A:45:LYS:HE3	1:A:82:PHE:HB3	0.66	1.66	2	1
1:A:73:GLY:HA3	1:A:121:VAL:HA	0.65	1.68	9	1
1:A:155:THR:HB	1:A:158:GLU:HG3	0.65	1.67	6	1
1:A:176:LEU:HD22	1:A:181:LEU:HA	0.64	1.69	3	2
1:A:97:LEU:H	1:A:97:LEU:HD23	0.64	1.51	6	3
1:A:5:LEU:HD12	1:A:89:GLN:HG2	0.64	1.67	2	1
1:A:101:PHE:HA	1:A:136:GLY:O	0.63	1.94	5	6
1:A:90:ILE:O	1:A:131:HIS:HB3	0.62	1.93	6	3
1:A:162:VAL:HB	1:A:163:PRO:HD3	0.62	1.70	6	4
1:A:182:GLU:HB2	1:A:183:PRO:HD3	0.62	1.71	7	3
1:A:108:LEU:H	1:A:108:LEU:HD23	0.62	1.54	10	4
1:A:173:THR:HA	1:A:176:LEU:HD12	0.62	1.72	10	1
1:A:99:ILE:HD12	1:A:103:ARG:HG2	0.62	1.72	1	1
1:A:8:VAL:HB	1:A:92:VAL:HG22	0.61	1.73	1	3
1:A:42:VAL:HA	1:A:49:GLU:HG2	0.61	1.72	9	1
1:A:106:LEU:HD23	1:A:106:LEU:H	0.60	1.56	10	1
1:A:55:LEU:HD13	1:A:174:GLU:HA	0.60	1.73	1	1
1:A:7:VAL:HB	1:A:62:LEU:HD13	0.60	1.71	4	1
1:A:75:GLN:HE21	1:A:75:GLN:HA	0.60	1.57	1	1
1:A:80:ALA:HA	1:A:83:TYR:CE1	0.59	2.33	7	1
1:A:100:ASP:HA	1:A:138:GLY:HA2	0.59	1.73	6	2
1:A:42:VAL:HA	1:A:49:GLU:HA	0.59	1.72	4	1
1:A:42:VAL:HG22	1:A:49:GLU:HG2	0.58	1.76	5	1
1:A:111:GLY:HA3	1:A:118:LEU:HD13	0.57	1.77	4	2
1:A:176:LEU:HA	1:A:180:GLY:O	0.57	1.98	4	1
1:A:29:ALA:HB1	1:A:62:LEU:HD11	0.57	1.75	2	2
1:A:176:LEU:HD23	1:A:181:LEU:HA	0.57	1.75	10	2
1:A:55:LEU:HG	1:A:60:VAL:HG21	0.57	1.76	4	1
1:A:86:PRO:HD2	1:A:89:GLN:HG3	0.57	1.75	4	1
1:A:49:GLU:HB3	1:A:64:LYS:HE3	0.57	1.76	1	2
1:A:55:LEU:HB2	1:A:174:GLU:HG2	0.57	1.75	2	1
1:A:49:GLU:HG3	1:A:66:ARG:HD2	0.56	1.76	7	1
1:A:91:VAL:HG12	1:A:131:HIS:HB3	0.56	1.75	9	1
1:A:181:LEU:H	1:A:181:LEU:HD23	0.56	1.60	1	4
1:A:67:CYS:HB3	1:A:71:GLU:HB2	0.56	1.77	5	1
1:A:101:PHE:HD2	1:A:158:GLU:HB3	0.55	1.61	2	1
1:A:145:ASP:HB2	1:A:146:PRO:HD2	0.55	1.77	3	2
1:A:13:PRO:HB3	1:A:68:TYR:HA	0.54	1.78	2	1
1:A:21:ARG:HG3	1:A:24:LEU:HD23	0.54	1.78	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:ILE:HG22	1:A:135:ILE:HA	0.54	1.79	4	4
1:A:24:LEU:HD13	1:A:93:ILE:HG12	0.54	1.78	2	1
1:A:44:LYS:HE3	1:A:44:LYS:HA	0.54	1.79	7	1
1:A:58:THR:HB	1:A:177:ILE:HG22	0.54	1.79	3	4
1:A:182:GLU:HB3	1:A:183:PRO:HD3	0.54	1.78	5	1
1:A:155:THR:O	1:A:158:GLU:HG2	0.53	2.02	1	1
1:A:128:LYS:HD2	1:A:129:ASN:N	0.53	2.18	4	1
1:A:144:LYS:HE2	1:A:144:LYS:HA	0.53	1.79	4	1
1:A:101:PHE:HE1	1:A:161:GLU:HB2	0.53	1.64	4	2
1:A:10:LEU:HD21	1:A:69:MET:HA	0.53	1.79	2	1
1:A:7:VAL:HB	1:A:62:LEU:HD22	0.53	1.80	5	1
1:A:22:HIS:CD2	1:A:150:VAL:HA	0.53	2.39	5	1
1:A:97:LEU:O	1:A:139:ARG:HD2	0.53	2.03	7	1
1:A:40:PHE:HB3	1:A:51:VAL:HB	0.53	1.79	7	1
1:A:104:ILE:HD13	1:A:104:ILE:H	0.53	1.64	2	2
1:A:28:VAL:HG12	1:A:32:LEU:HD23	0.53	1.80	4	1
1:A:77:GLY:HA2	1:A:125:LEU:HB3	0.53	1.80	9	1
1:A:111:GLY:HA3	1:A:118:LEU:CD1	0.52	2.34	4	2
1:A:106:LEU:HD22	1:A:181:LEU:HB2	0.52	1.79	7	1
1:A:101:PHE:CE1	1:A:161:GLU:HB2	0.52	2.40	5	2
1:A:20:THR:HG21	1:A:151:LEU:O	0.52	2.03	9	1
1:A:47:GLY:HA3	1:A:75:GLN:HB3	0.52	1.81	9	1
1:A:60:VAL:HG11	1:A:177:ILE:HD13	0.52	1.82	4	2
1:A:125:LEU:HD23	1:A:125:LEU:H	0.51	1.65	2	1
1:A:128:LYS:HD2	1:A:128:LYS:N	0.51	2.20	8	2
1:A:24:LEU:HD12	1:A:25:GLY:N	0.51	2.21	2	1
1:A:8:VAL:O	1:A:92:VAL:HA	0.51	2.04	5	2
1:A:107:LYS:HD3	1:A:134:ARG:HD2	0.51	1.81	1	1
1:A:58:THR:HB	1:A:177:ILE:CG2	0.51	2.35	3	3
1:A:115:HIS:O	1:A:119:ARG:HG2	0.51	2.06	3	1
1:A:4:PRO:HA	1:A:59:SER:O	0.51	2.06	3	4
1:A:5:LEU:HD21	1:A:177:ILE:HG23	0.51	1.83	5	2
1:A:186:ASN:HA	1:A:189:HIS:CE1	0.50	2.41	10	1
1:A:40:PHE:HB3	1:A:50:VAL:O	0.50	2.07	8	2
1:A:140:PRO:HD2	1:A:146:PRO:HB3	0.50	1.82	2	1
1:A:181:LEU:O	1:A:185:GLN:HG2	0.49	2.06	1	1
1:A:121:VAL:HB	1:A:132:ARG:HH22	0.49	1.68	1	1
1:A:155:THR:HB	1:A:158:GLU:CG	0.49	2.35	6	1
1:A:45:LYS:HG2	1:A:83:TYR:CE1	0.49	2.41	2	1
1:A:182:GLU:O	1:A:185:GLN:HG2	0.49	2.07	5	2
1:A:188:VAL:HA	1:A:191:TRP:HD1	0.49	1.67	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:TYR:HE1	1:A:151:LEU:HB3	0.49	1.68	1	1
1:A:20:THR:HG22	1:A:153:ASN:H	0.49	1.68	2	1
1:A:9:GLY:O	1:A:65:PRO:HD2	0.49	2.08	1	1
1:A:168:GLN:NE2	1:A:191:TRP:HB2	0.48	2.22	1	1
1:A:64:LYS:O	1:A:64:LYS:HG2	0.48	2.08	6	1
1:A:87:PRO:HA	1:A:90:ILE:HD12	0.48	1.86	6	1
1:A:95:ASP:HB2	1:A:137:VAL:HG21	0.48	1.85	5	1
1:A:131:HIS:O	1:A:132:ARG:HD2	0.48	2.08	8	2
1:A:182:GLU:O	1:A:185:GLN:HG3	0.48	2.09	3	1
1:A:80:ALA:HA	1:A:85:VAL:HG22	0.48	1.84	4	1
1:A:42:VAL:HB	1:A:49:GLU:HG2	0.48	1.86	4	1
1:A:50:VAL:HG12	1:A:63:ALA:HA	0.48	1.84	5	1
1:A:56:ALA:HB2	1:A:174:GLU:HG2	0.47	1.84	4	1
1:A:29:ALA:HB1	1:A:62:LEU:HD21	0.47	1.86	10	2
1:A:51:VAL:HG13	1:A:62:LEU:HB2	0.47	1.85	4	1
1:A:104:ILE:HD11	1:A:188:VAL:HG21	0.47	1.85	3	2
1:A:168:GLN:OE1	1:A:168:GLN:HA	0.47	2.09	3	1
1:A:97:LEU:O	1:A:139:ARG:HA	0.47	2.10	6	2
1:A:69:MET:HB2	1:A:117:GLY:HA3	0.47	1.87	7	1
1:A:159:ARG:HA	1:A:162:VAL:HG23	0.47	1.86	10	1
1:A:158:GLU:O	1:A:162:VAL:HG23	0.47	2.10	4	2
1:A:115:HIS:HB2	1:A:118:LEU:HG	0.47	1.86	9	1
1:A:17:TYR:HA	1:A:20:THR:HG23	0.47	1.85	6	1
1:A:83:TYR:CD1	1:A:85:VAL:HG22	0.47	2.45	7	1
1:A:146:PRO:HA	1:A:149:PHE:CD1	0.46	2.44	5	1
1:A:106:LEU:HD13	1:A:188:VAL:HG21	0.46	1.86	9	1
1:A:103:ARG:HD2	1:A:103:ARG:H	0.46	1.71	1	1
1:A:21:ARG:HD2	1:A:137:VAL:O	0.46	2.09	8	1
1:A:11:GLY:O	1:A:13:PRO:HD3	0.46	2.10	2	2
1:A:11:GLY:HA3	1:A:65:PRO:O	0.46	2.11	10	1
1:A:44:LYS:O	1:A:45:LYS:HB2	0.46	2.11	1	2
1:A:45:LYS:CE	1:A:82:PHE:HB3	0.46	2.39	2	1
1:A:69:MET:SD	1:A:116:ASN:HB2	0.46	2.50	3	1
1:A:18:ALA:HA	1:A:23:ASN:HD21	0.46	1.71	1	1
1:A:168:GLN:HA	1:A:168:GLN:OE1	0.46	2.11	5	1
1:A:24:LEU:HD22	1:A:25:GLY:N	0.46	2.26	8	1
1:A:146:PRO:HA	1:A:149:PHE:HD2	0.45	1.70	9	2
1:A:50:VAL:HA	1:A:62:LEU:O	0.45	2.11	6	1
1:A:17:TYR:HB3	1:A:22:HIS:CE1	0.45	2.46	9	1
1:A:26:PHE:CD2	1:A:64:LYS:HE2	0.45	2.46	3	1
1:A:51:VAL:CG1	1:A:62:LEU:HB3	0.45	2.40	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:VAL:N	1:A:163:PRO:HD2	0.45	2.26	10	3
1:A:21:ARG:NH2	1:A:24:LEU:HG	0.45	2.24	4	1
1:A:92:VAL:HG21	1:A:121:VAL:HG11	0.45	1.87	4	1
1:A:128:LYS:H	1:A:128:LYS:CD	0.45	2.24	6	1
1:A:21:ARG:HD2	1:A:137:VAL:HB	0.45	1.88	9	1
1:A:5:LEU:HD12	1:A:177:ILE:HG22	0.45	1.89	10	1
1:A:21:ARG:HD3	1:A:101:PHE:CE2	0.45	2.47	4	1
1:A:162:VAL:O	1:A:166:VAL:HG23	0.45	2.12	9	2
1:A:5:LEU:HB2	1:A:60:VAL:HG12	0.45	1.88	9	1
1:A:147:ALA:O	1:A:151:LEU:HG	0.45	2.12	9	1
1:A:27:MET:CE	1:A:27:MET:HA	0.44	2.42	6	1
1:A:69:MET:HB2	1:A:117:GLY:CA	0.44	2.41	7	2
1:A:40:PHE:CD1	1:A:51:VAL:HG23	0.44	2.47	10	2
1:A:21:ARG:HD3	1:A:153:ASN:O	0.44	2.11	7	1
1:A:121:VAL:HB	1:A:132:ARG:NH2	0.44	2.28	1	1
1:A:5:LEU:HD12	1:A:177:ILE:HG23	0.44	1.90	4	1
1:A:99:ILE:HG13	1:A:136:GLY:HA2	0.44	1.88	2	1
1:A:31:VAL:O	1:A:35:ARG:HG2	0.44	2.13	4	2
1:A:40:PHE:HB2	1:A:51:VAL:HB	0.44	1.89	10	1
1:A:46:SER:O	1:A:48:ALA:N	0.44	2.45	10	1
1:A:106:LEU:HD12	1:A:131:HIS:HE1	0.44	1.72	1	1
1:A:3:GLU:O	1:A:3:GLU:HG2	0.44	2.13	4	1
1:A:38:SER:HB3	1:A:51:VAL:CG2	0.44	2.43	7	1
1:A:74:ARG:N	1:A:74:ARG:HD2	0.43	2.28	1	1
1:A:106:LEU:HD21	1:A:181:LEU:HB2	0.43	1.88	6	1
1:A:182:GLU:N	1:A:183:PRO:HD2	0.43	2.28	6	2
1:A:83:TYR:CE1	1:A:85:VAL:HG22	0.43	2.48	7	1
1:A:155:THR:O	1:A:158:GLU:HG3	0.43	2.14	4	1
1:A:26:PHE:CE1	1:A:65:PRO:HD2	0.43	2.49	6	1
1:A:185:GLN:HA	1:A:188:VAL:HG22	0.43	1.91	9	1
1:A:97:LEU:O	1:A:140:PRO:HD3	0.43	2.12	6	1
1:A:96:GLU:OE1	1:A:112:GLU:HB2	0.43	2.14	1	1
1:A:43:HIS:HB3	1:A:50:VAL:HB	0.43	1.89	2	1
1:A:48:ALA:HB2	1:A:79:LEU:HD21	0.43	1.90	6	1
1:A:112:GLU:HG2	1:A:113:GLY:H	0.43	1.73	10	1
1:A:108:LEU:HD12	1:A:108:LEU:O	0.42	2.13	1	2
1:A:43:HIS:O	1:A:47:GLY:HA2	0.42	2.14	10	1
1:A:96:GLU:HB3	1:A:136:GLY:HA2	0.42	1.91	6	1
1:A:44:LYS:HG2	1:A:79:LEU:HD12	0.42	1.90	7	1
1:A:11:GLY:HA3	1:A:26:PHE:HB2	0.42	1.92	8	1
1:A:32:LEU:HD12	1:A:33:ALA:N	0.42	2.30	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:H	1:A:36:ILE:HD12	0.42	1.74	9	1
1:A:155:THR:O	1:A:159:ARG:HG3	0.42	2.14	9	1
1:A:67:CYS:HB3	1:A:71:GLU:HG2	0.42	1.91	4	1
1:A:138:GLY:O	1:A:140:PRO:HD3	0.42	2.15	4	1
1:A:173:THR:HA	1:A:176:LEU:HD13	0.42	1.90	7	1
1:A:104:ILE:HG12	1:A:188:VAL:HG21	0.42	1.92	8	1
1:A:90:ILE:O	1:A:131:HIS:HB2	0.42	2.15	7	1
1:A:46:SER:HB3	1:A:82:PHE:CE2	0.41	2.50	2	1
1:A:109:GLY:O	1:A:132:ARG:HD3	0.41	2.14	4	1
1:A:5:LEU:HD11	1:A:60:VAL:HG12	0.41	1.91	5	2
1:A:22:HIS:CG	1:A:150:VAL:HG23	0.41	2.50	8	1
1:A:27:MET:HA	1:A:27:MET:CE	0.41	2.46	4	1
1:A:86:PRO:O	1:A:90:ILE:HG23	0.41	2.15	8	1
1:A:155:THR:O	1:A:159:ARG:HG2	0.41	2.15	3	1
1:A:101:PHE:HD1	1:A:161:GLU:HB2	0.41	1.75	1	1
1:A:152:GLU:O	1:A:152:GLU:HG3	0.41	2.15	4	1
1:A:91:VAL:HA	1:A:131:HIS:CB	0.41	2.45	10	1
1:A:51:VAL:CG1	1:A:62:LEU:HB2	0.41	2.45	4	1
1:A:74:ARG:HH11	1:A:124:ALA:HB2	0.41	1.75	5	1
1:A:24:LEU:H	1:A:24:LEU:HD12	0.41	1.76	1	1
1:A:102:GLY:O	1:A:103:ARG:HD3	0.41	2.15	4	1
1:A:99:ILE:HD12	1:A:103:ARG:O	0.41	2.16	2	1
1:A:28:VAL:HA	1:A:31:VAL:HG22	0.41	1.93	4	1
1:A:96:GLU:O	1:A:136:GLY:HA2	0.41	2.16	6	1
1:A:97:LEU:HD12	1:A:145:ASP:HB2	0.41	1.92	6	1
1:A:106:LEU:HD12	1:A:106:LEU:O	0.40	2.15	2	1
1:A:145:ASP:OD2	1:A:147:ALA:HB3	0.40	2.16	6	1
1:A:140:PRO:HA	1:A:141:PRO:HD3	0.40	1.78	8	1
1:A:19:LYS:N	1:A:19:LYS:HD2	0.40	2.30	9	1
1:A:119:ARG:N	1:A:119:ARG:HD2	0.40	2.31	8	1
1:A:96:GLU:HA	1:A:96:GLU:OE1	0.40	2.16	9	1
1:A:21:ARG:O	1:A:24:LEU:HG	0.40	2.17	2	1
1:A:127:THR:C	1:A:128:LYS:HD2	0.40	2.37	3	1
1:A:22:HIS:HB3	1:A:150:VAL:HG22	0.40	1.93	9	1
1:A:91:VAL:HA	1:A:131:HIS:HB2	0.40	1.92	10	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	188/191 (98%)	169±3 (90±2%)	16±3 (8±2%)	3±1 (2±1%)	13 57
All	All	1880/1910 (98%)	1693 (90%)	156 (8%)	31 (2%)	13 57

All 14 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	57	GLY	6
1	A	47	GLY	5
1	A	45	LYS	4
1	A	130	PHE	3
1	A	113	GLY	2
1	A	13	PRO	2
1	A	15	PRO	2
1	A	110	GLY	1
1	A	111	GLY	1
1	A	131	HIS	1
1	A	44	LYS	1
1	A	179	GLN	1
1	A	114	GLY	1
1	A	115	HIS	1

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	145/146 (99%)	137±2 (95±1%)	8±2 (5±1%)	26 75
All	All	1450/1460 (99%)	1372 (95%)	78 (5%)	26 75

All 41 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	64	LYS	6
1	A	10	LEU	5
1	A	19	LYS	4
1	A	24	LEU	3
1	A	108	LEU	3
1	A	139	ARG	3
1	A	143	ARG	3
1	A	158	GLU	3
1	A	21	ARG	3
1	A	155	THR	3
1	A	106	LEU	2
1	A	79	LEU	2
1	A	104	ILE	2
1	A	132	ARG	2
1	A	176	LEU	2
1	A	179	GLN	2
1	A	128	LYS	2
1	A	112	GLU	2
1	A	94	HIS	2
1	A	41	LYS	2
1	A	107	LYS	2
1	A	75	GLN	1
1	A	100	ASP	1
1	A	103	ARG	1
1	A	96	GLU	1
1	A	12	ASN	1
1	A	115	HIS	1
1	A	3	GLU	1
1	A	23	ASN	1
1	A	131	HIS	1
1	A	144	LYS	1
1	A	45	LYS	1
1	A	62	LEU	1
1	A	69	MET	1
1	A	58	THR	1
1	A	74	ARG	1
1	A	159	ARG	1
1	A	129	ASN	1
1	A	174	GLU	1
1	A	101	PHE	1
1	A	186	ASN	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 82% for the well-defined parts and 82% 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	2093
Number of shifts mapped to atoms	2093
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	184	-0.15 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	161	-0.10 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	184	0.02 ± 0.10	None needed (< 0.5 ppm)
^{15}N	165	1.00 ± 0.39	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 82%, i.e. 2071 atoms were assigned a chemical shift out of a possible 2528. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	895/944 (95%)	368/389 (95%)	364/378 (96%)	163/177 (92%)
Sidechain	1136/1427 (80%)	792/935 (85%)	344/431 (80%)	0/61 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	40/157 (25%)	20/77 (26%)	20/67 (30%)	0/13 (0%)
Overall	2071/2528 (82%)	1180/1401 (84%)	728/876 (83%)	163/251 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 2090 atoms were assigned a chemical shift out of a possible 2552. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	904/954 (95%)	371/393 (94%)	368/382 (96%)	165/179 (92%)
Sidechain	1146/1441 (80%)	799/945 (85%)	347/435 (80%)	0/61 (0%)
Aromatic	40/157 (25%)	20/77 (26%)	20/67 (30%)	0/13 (0%)
Overall	2090/2552 (82%)	1190/1415 (84%)	735/884 (83%)	165/253 (65%)

7.1.4 Statistically unusual chemical shifts (i)

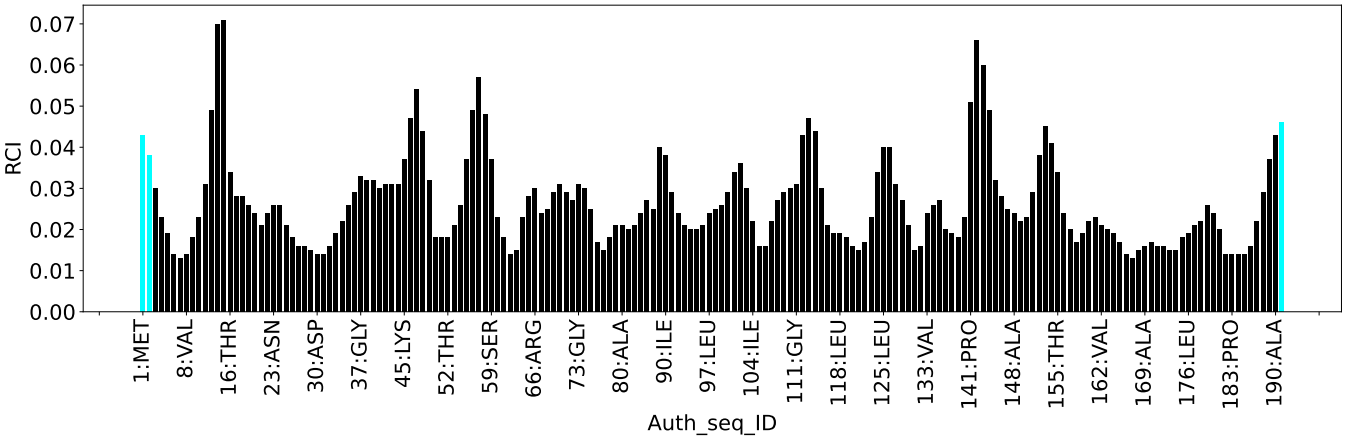
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	11	GLY	HA3	1.54	2.08 – 5.71	-6.5

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:


RCI
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
1:MET
8:VAL
16:THR
23:ASN
30:ASP
37:GLY
45:LYS
52:THR
59:SER
66:ARG
73:GLY
80:ALA
90:ILE
97:LEU
104:ILE
111:GLY
118:LEU
125:LEU
133:VAL
141:PRO
148:ALA
155:THR
162:VAL
169:ALA
176:LEU
183:PRO
190:ALA
Auth_seq_ID