



Full wwPDB NMR Structure Validation Report ⓘ

Feb 17, 2018 – 08:50 am GMT

PDB ID : 4A1M
Title : NMR Structure of protoporphyrin-IX bound murine p22HBP
Authors : Goodfellow, B.J.; Dias, J.S.; Macedo, A.L.; Ferreira, G.C.; Peterson, F.C.; Volkman, B.F.; Duarte, I.C.N.
Deposited on : 2011-09-15

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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

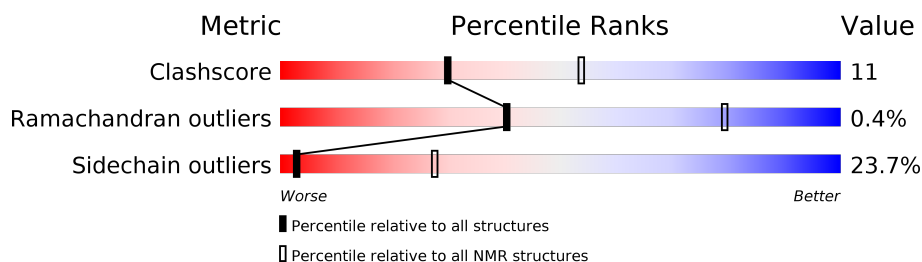
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	195	 53% 29% • 12% 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:18-A:73, A:78-A:172, A:181-A:190 (161)	0.42	1

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2814 atoms, of which 1381 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HEME-BINDING PROTEIN 1.

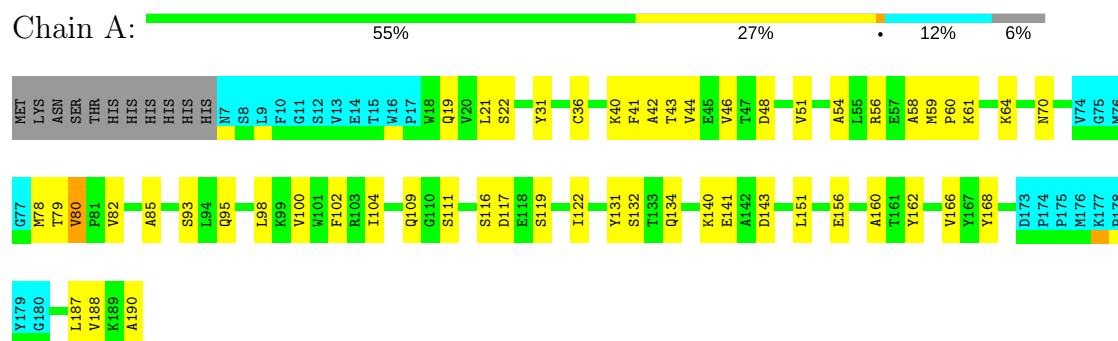
Mol	Chain	Residues	Atoms						Trace
1	A	184	Total	C	H	N	O	S	0
			2814	911	1381	236	279	7	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP Q9R257
A	-3	LYS	-	expression tag	UNP Q9R257
A	-2	ASN	-	expression tag	UNP Q9R257
A	-1	SER	-	expression tag	UNP Q9R257
A	0	THR	-	expression tag	UNP Q9R257
A	1	HIS	-	expression tag	UNP Q9R257
A	2	HIS	-	expression tag	UNP Q9R257
A	3	HIS	-	expression tag	UNP Q9R257
A	4	HIS	-	expression tag	UNP Q9R257
A	5	HIS	-	expression tag	UNP Q9R257
A	6	HIS	-	expression tag	UNP Q9R257

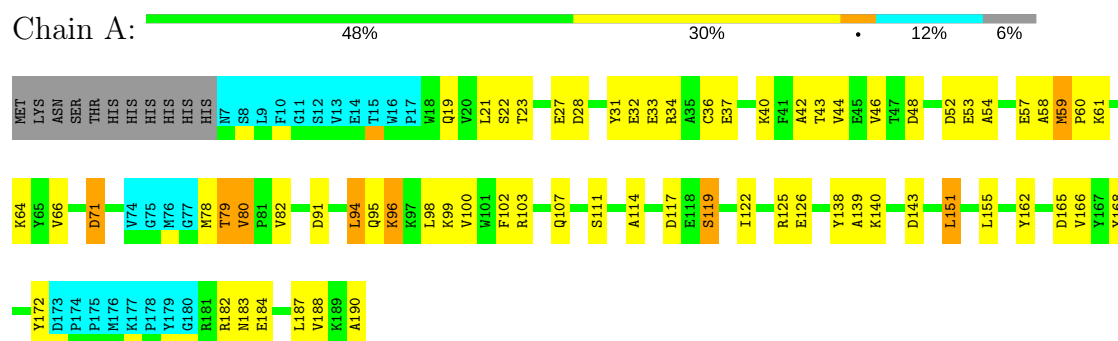
4.2.2 Score per residue for model 2

• Molecule 1: HEME-BINDING PROTEIN 1



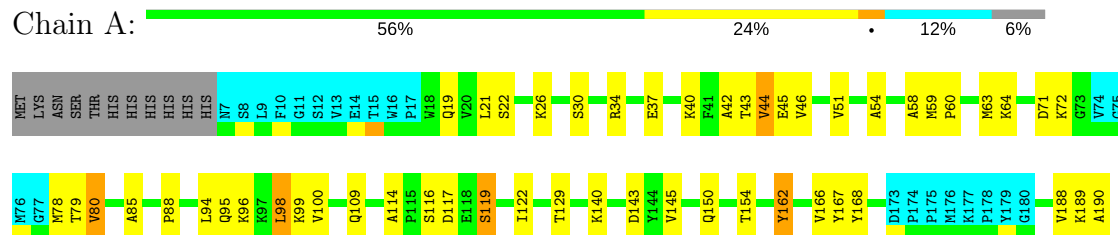
4.2.3 Score per residue for model 3

- Molecule 1: HEME-BINDING PROTEIN 1



4.2.4 Score per residue for model 4

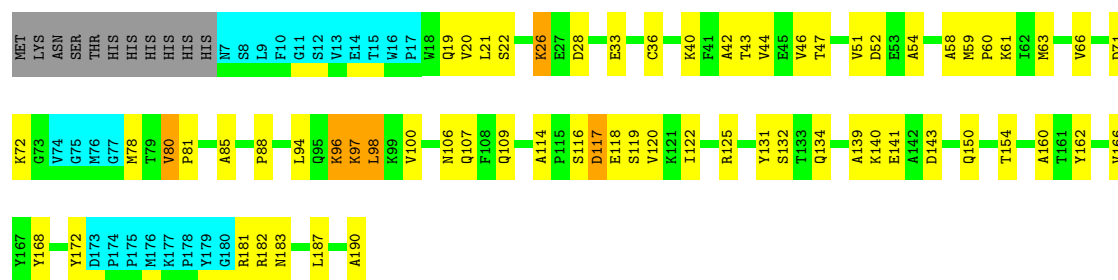
- Molecule 1: HEME-BINDING PROTEIN 1



4.2.5 Score per residue for model 5

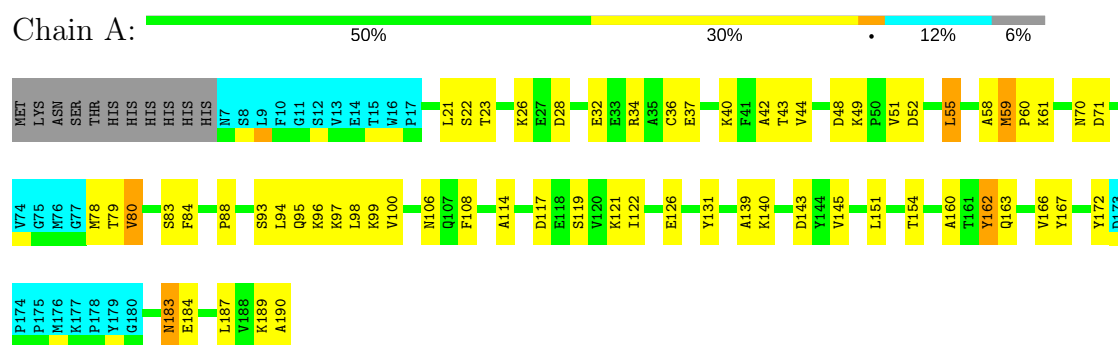
- Molecule 1: HEME-BINDING PROTEIN 1





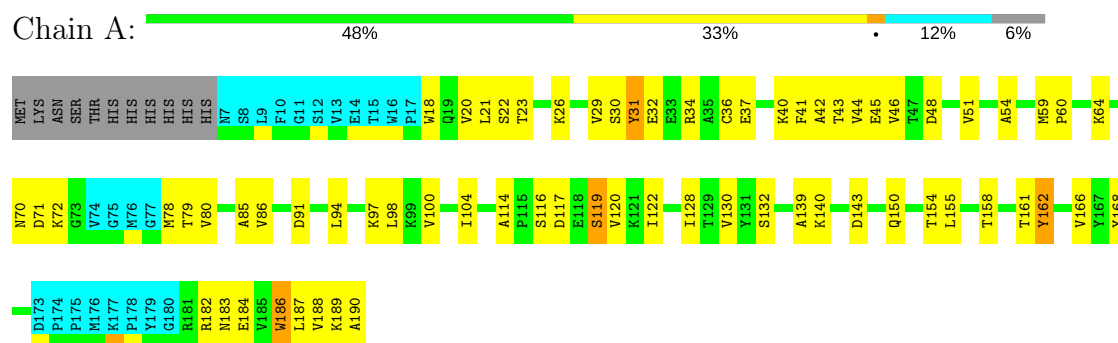
4.2.6 Score per residue for model 6

- Molecule 1: HEME-BINDING PROTEIN 1



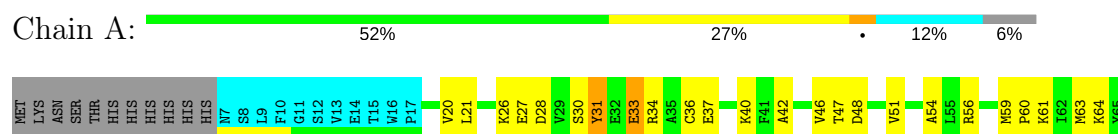
4.2.7 Score per residue for model 7

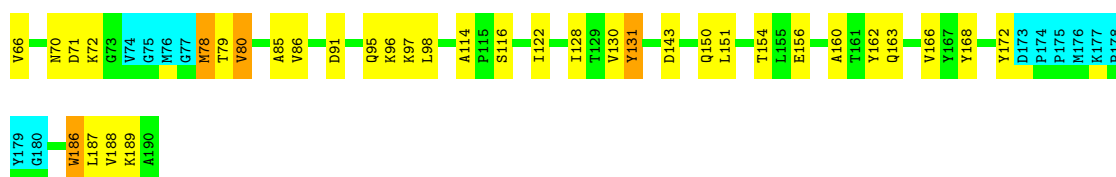
- Molecule 1: HEME-BINDING PROTEIN 1



4.2.8 Score per residue for model 8

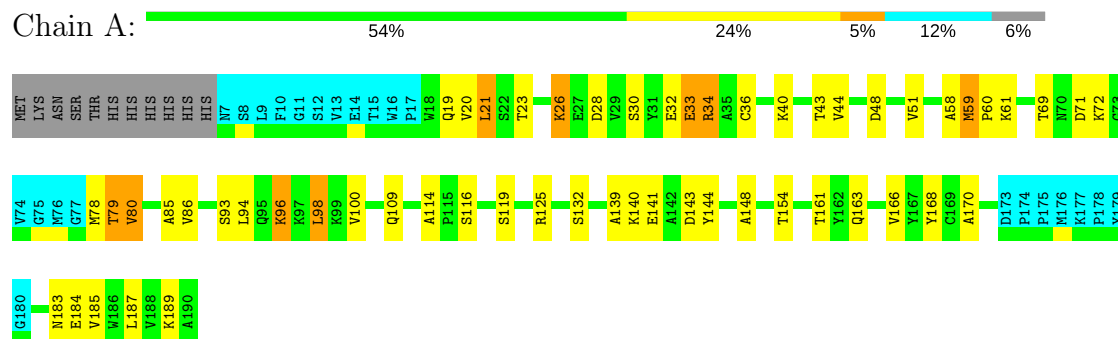
- Molecule 1: HEME-BINDING PROTEIN 1





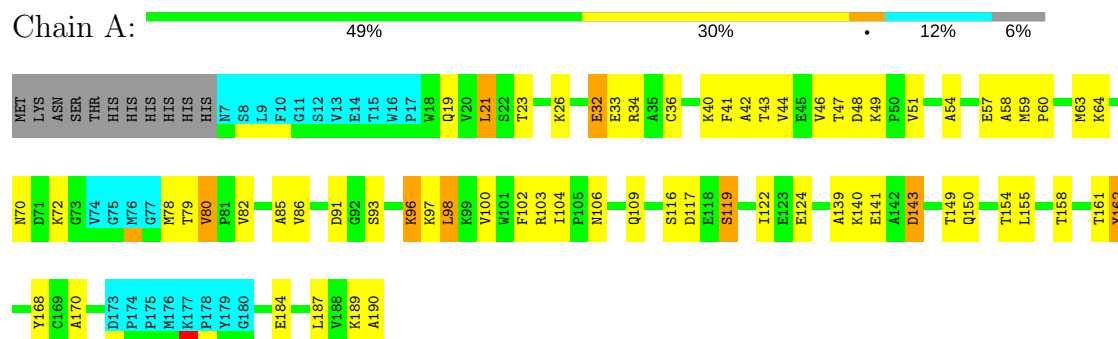
4.2.9 Score per residue for model 9

- Molecule 1: HEME-BINDING PROTEIN 1



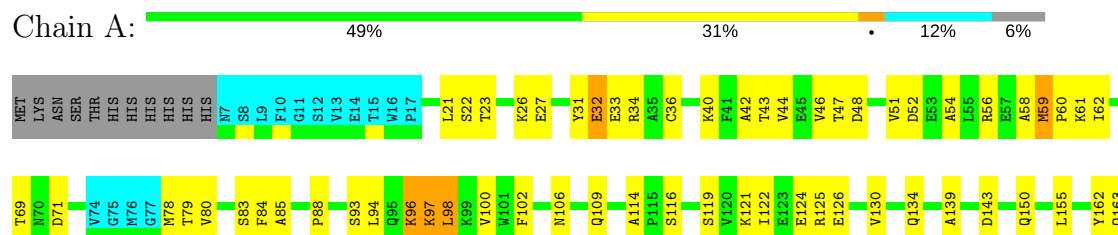
4.2.10 Score per residue for model 10

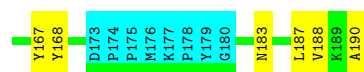
- Molecule 1: HEME-BINDING PROTEIN 1



4.2.11 Score per residue for model 11

- Molecule 1: HEME-BINDING PROTEIN 1

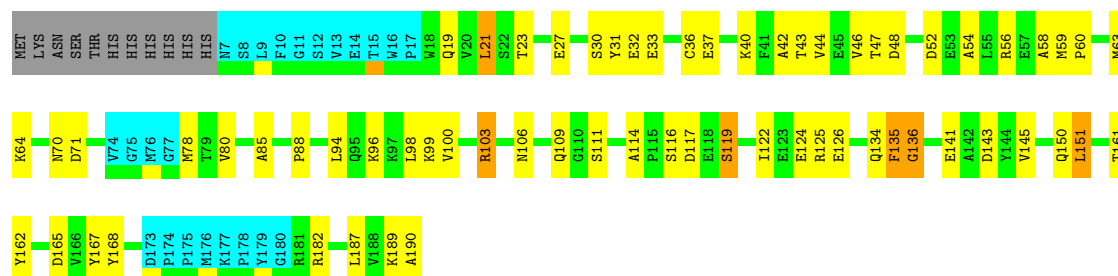




4.2.12 Score per residue for model 12

- Molecule 1: HEME-BINDING PROTEIN 1

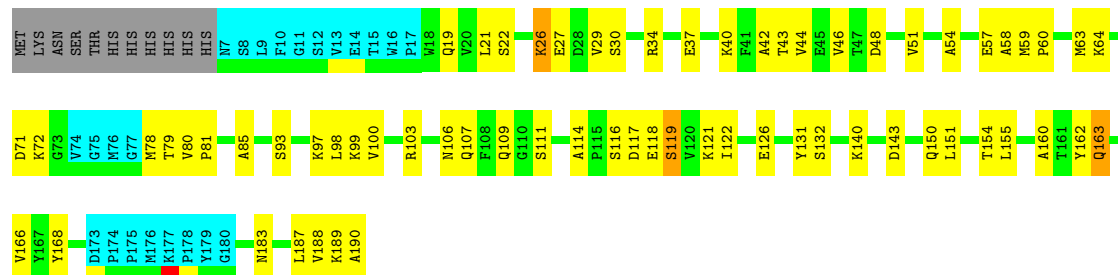
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: HEME-BINDING PROTEIN 1

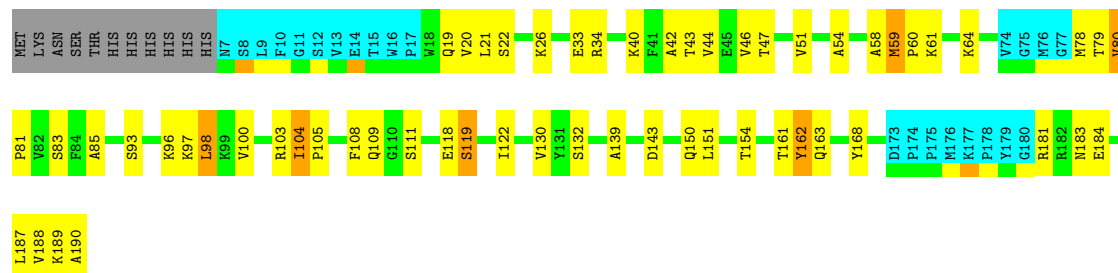
Chain A:



4.2.14 Score per residue for model 14

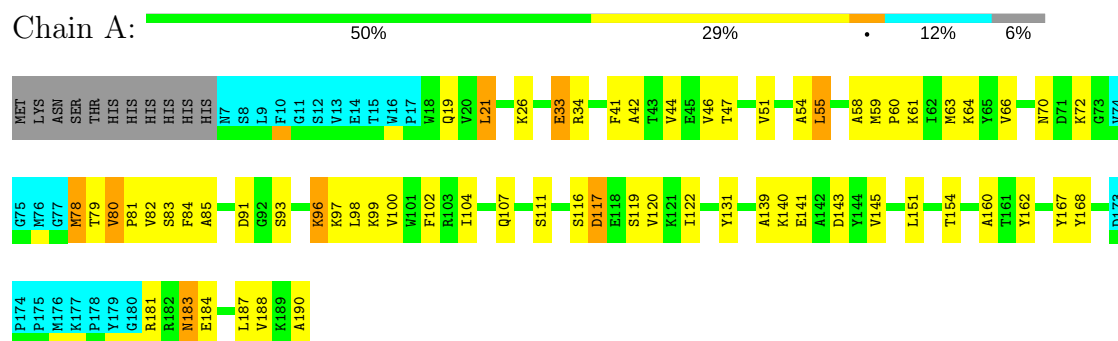
- Molecule 1: HEME-BINDING PROTEIN 1

Chain A:



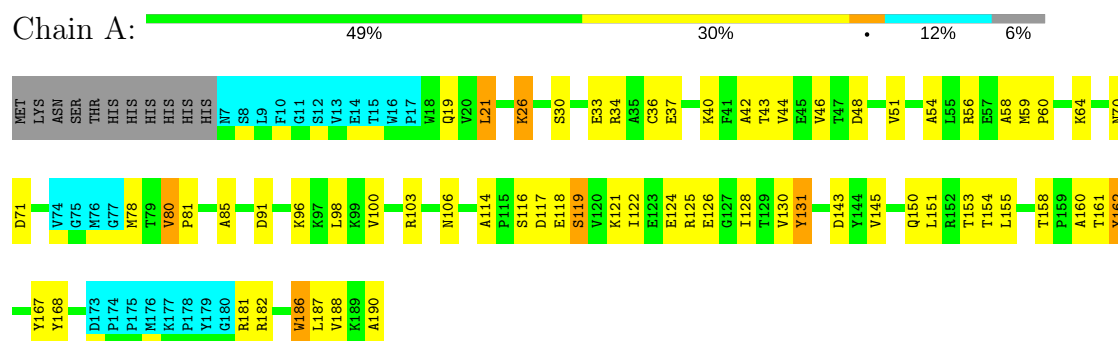
4.2.15 Score per residue for model 15

• Molecule 1: HEME-BINDING PROTEIN 1



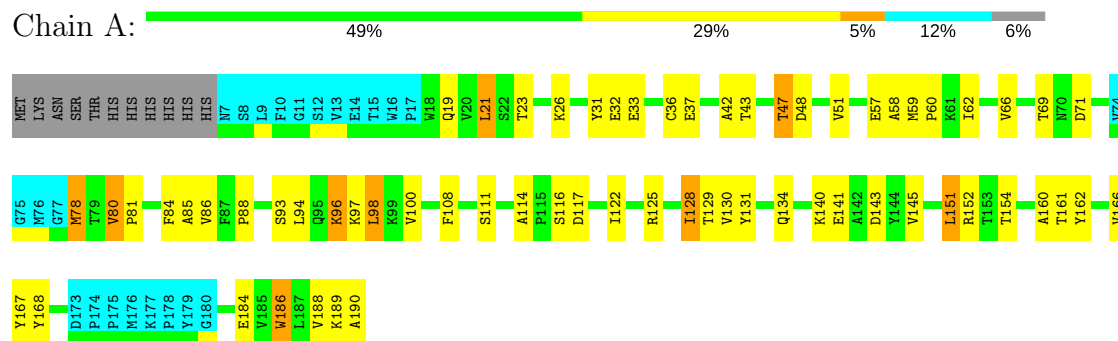
4.2.16 Score per residue for model 16

• Molecule 1: HEME-BINDING PROTEIN 1



4.2.17 Score per residue for model 17

• Molecule 1: HEME-BINDING PROTEIN 1



4.2.18 Score per residue for model 18

- Molecule 1: HEME-BINDING PROTEIN 1



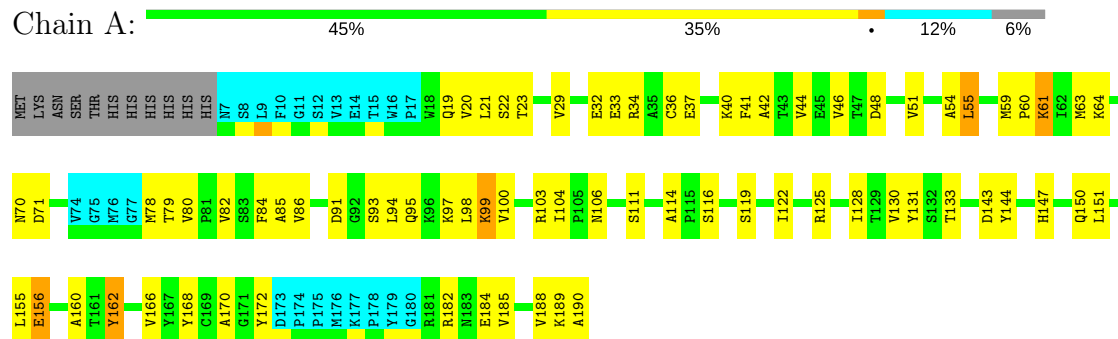
4.2.19 Score per residue for model 19

- Molecule 1: HEME-BINDING PROTEIN 1



4.2.20 Score per residue for model 20

- Molecule 1: HEME-BINDING PROTEIN 1



5 Refinement protocol and experimental data overview

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure solution	2.1

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)	4a1m_cs.str
Number of chemical shift lists	1
Total number of shifts	1903
Number of shifts mapped to atoms	1903
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	1261	1220	1220	27±5
All	All	25220	24400	24400	542

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:LEU:HD23	1:A:187:LEU:HD12	0.98	1.30	2	7
1:A:51:VAL:HG13	1:A:98:LEU:HD13	0.78	1.55	17	11
1:A:44:VAL:HG22	1:A:100:VAL:HB	0.69	1.63	1	3
1:A:85:ALA:HB2	1:A:168:TYR:CZ	0.68	2.23	14	3
1:A:98:LEU:HD13	1:A:99:LYS:N	0.66	2.05	20	1
1:A:51:VAL:HG12	1:A:98:LEU:HD23	0.66	1.66	20	1
1:A:26:LYS:HB2	1:A:154:THR:HG23	0.65	1.68	4	11
1:A:85:ALA:HB2	1:A:168:TYR:CE1	0.65	2.27	13	12
1:A:44:VAL:HG23	1:A:119:SER:O	0.64	1.92	5	6
1:A:44:VAL:HG12	1:A:119:SER:O	0.64	1.92	13	9
1:A:162:TYR:C	1:A:190:ALA:HB2	0.64	2.13	16	16
1:A:21:LEU:HD23	1:A:33:GLU:CG	0.64	2.22	17	2
1:A:42:ALA:HB2	1:A:122:ILE:HD13	0.64	1.68	20	15
1:A:71:ASP:HB3	1:A:114:ALA:HB3	0.63	1.70	3	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:HIS:CD2	1:A:185:VAL:HG21	0.63	2.28	18	1
1:A:21:LEU:HD23	1:A:33:GLU:HG2	0.63	1.71	17	1
1:A:131:TYR:OH	1:A:160:ALA:HB1	0.63	1.93	17	10
1:A:145:VAL:HG22	1:A:167:TYR:OH	0.63	1.92	17	8
1:A:162:TYR:O	1:A:190:ALA:HB2	0.63	1.93	17	2
1:A:33:GLU:OE2	1:A:129:THR:HG23	0.63	1.94	17	1
1:A:51:VAL:HG13	1:A:98:LEU:CD1	0.62	2.25	5	14
1:A:21:LEU:HD21	1:A:33:GLU:HG2	0.62	1.71	16	1
1:A:117:ASP:HB3	1:A:120:VAL:HG12	0.61	1.72	5	2
1:A:130:VAL:HG12	1:A:188:VAL:HA	0.61	1.72	7	8
1:A:47:THR:HG22	1:A:97:LYS:HG3	0.60	1.71	10	4
1:A:44:VAL:HG21	1:A:61:LYS:HD3	0.60	1.72	9	4
1:A:42:ALA:HB2	1:A:122:ILE:CD1	0.60	2.27	20	19
1:A:20:VAL:HG22	1:A:34:ARG:HB3	0.59	1.74	7	1
1:A:151:LEU:CD2	1:A:187:LEU:HD12	0.59	2.27	18	4
1:A:85:ALA:HB2	1:A:168:TYR:CE2	0.59	2.31	16	6
1:A:46:VAL:HG11	1:A:54:ALA:HA	0.59	1.74	1	14
1:A:23:THR:HG22	1:A:32:GLU:CG	0.59	2.28	10	5
1:A:170:ALA:HB3	1:A:184:GLU:HB3	0.58	1.75	20	1
1:A:88:PRO:HA	1:A:94:LEU:HD23	0.58	1.75	19	7
1:A:66:VAL:HG23	1:A:78:MET:HG3	0.58	1.75	8	2
1:A:128:ILE:HD12	1:A:130:VAL:HG13	0.58	1.75	17	6
1:A:148:ALA:O	1:A:187:LEU:HD11	0.58	1.98	9	1
1:A:71:ASP:CB	1:A:114:ALA:HB3	0.58	2.29	6	8
1:A:84:PHE:CD1	1:A:98:LEU:HD11	0.57	2.34	11	2
1:A:31:TYR:CE2	1:A:155:LEU:HD23	0.57	2.33	7	1
1:A:133:THR:CG2	1:A:151:LEU:HD11	0.57	2.29	20	1
1:A:58:ALA:CB	1:A:100:VAL:HG21	0.57	2.30	2	16
1:A:59:MET:CE	1:A:82:VAL:HG11	0.56	2.30	20	3
1:A:80:VAL:HG11	1:A:103:ARG:O	0.56	2.00	13	1
1:A:139:ALA:HB1	1:A:143:ASP:HB3	0.56	1.76	19	1
1:A:23:THR:HG22	1:A:32:GLU:HB2	0.56	1.77	3	2
1:A:23:THR:HG22	1:A:32:GLU:HG3	0.56	1.76	9	8
1:A:82:VAL:HG22	1:A:102:PHE:CD1	0.56	2.35	15	2
1:A:21:LEU:O	1:A:21:LEU:HD12	0.56	2.01	10	2
1:A:131:TYR:CZ	1:A:160:ALA:HB1	0.56	2.36	16	3
1:A:54:ALA:HB3	1:A:98:LEU:HG	0.56	1.78	20	1
1:A:20:VAL:HG22	1:A:34:ARG:HG3	0.56	1.76	9	1
1:A:170:ALA:HB3	1:A:184:GLU:HG3	0.55	1.77	9	1
1:A:21:LEU:HD12	1:A:21:LEU:O	0.55	2.02	9	1
1:A:71:ASP:CG	1:A:114:ALA:HB3	0.55	2.22	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:TYR:HB3	1:A:151:LEU:HD21	0.55	1.78	8	3
1:A:139:ALA:HB3	1:A:183:ASN:OD1	0.55	2.01	5	5
1:A:44:VAL:HG22	1:A:119:SER:O	0.55	2.02	19	1
1:A:55:LEU:HD11	1:A:84:PHE:CE1	0.55	2.37	20	2
1:A:170:ALA:HB3	1:A:184:GLU:CB	0.55	2.32	10	1
1:A:66:VAL:HG23	1:A:78:MET:HG2	0.55	1.78	5	2
1:A:104:ILE:HG22	1:A:105:PRO:HD2	0.55	1.79	14	1
1:A:170:ALA:HB3	1:A:184:GLU:CG	0.55	2.32	9	1
1:A:55:LEU:HD11	1:A:84:PHE:CE2	0.54	2.37	6	1
1:A:44:VAL:HG11	1:A:61:LYS:CD	0.54	2.33	20	1
1:A:44:VAL:CG1	1:A:120:VAL:HG22	0.53	2.34	18	2
1:A:151:LEU:HD12	1:A:187:LEU:CD1	0.53	2.33	16	1
1:A:51:VAL:HG13	1:A:98:LEU:HD12	0.53	1.80	13	2
1:A:29:VAL:HG13	1:A:154:THR:HG21	0.53	1.80	13	2
1:A:54:ALA:CB	1:A:98:LEU:HD22	0.53	2.34	15	5
1:A:133:THR:CG2	1:A:185:VAL:HG23	0.53	2.33	18	1
1:A:151:LEU:HD23	1:A:187:LEU:HB2	0.53	1.80	13	1
1:A:86:VAL:O	1:A:166:VAL:HG13	0.53	2.03	8	1
1:A:155:LEU:O	1:A:158:THR:HG22	0.53	2.03	16	2
1:A:79:THR:O	1:A:80:VAL:HG13	0.52	2.05	9	6
1:A:44:VAL:CG2	1:A:120:VAL:HG22	0.52	2.35	19	1
1:A:58:ALA:HB3	1:A:100:VAL:HG21	0.52	1.79	19	10
1:A:168:TYR:CE1	1:A:188:VAL:HG22	0.52	2.39	3	1
1:A:21:LEU:HD12	1:A:22:SER:HB3	0.52	1.81	13	11
1:A:26:LYS:CB	1:A:154:THR:HG23	0.52	2.35	15	6
1:A:139:ALA:HB1	1:A:143:ASP:CB	0.52	2.34	19	2
1:A:155:LEU:HD13	1:A:162:TYR:OH	0.52	2.04	13	3
1:A:31:TYR:CZ	1:A:155:LEU:HD23	0.52	2.39	3	3
1:A:33:GLU:CD	1:A:129:THR:HG23	0.52	2.25	17	1
1:A:166:VAL:HG13	1:A:188:VAL:CG1	0.51	2.34	4	3
1:A:66:VAL:HG23	1:A:78:MET:CG	0.51	2.35	5	1
1:A:80:VAL:HG23	1:A:102:PHE:CZ	0.51	2.40	10	2
1:A:59:MET:N	1:A:60:PRO:HD2	0.51	2.19	4	20
1:A:29:VAL:HG13	1:A:147:HIS:NE2	0.51	2.21	20	1
1:A:86:VAL:HB	1:A:94:LEU:HD12	0.51	1.82	9	1
1:A:98:LEU:CD1	1:A:100:VAL:HG23	0.51	2.36	20	1
1:A:21:LEU:HD21	1:A:33:GLU:HB3	0.51	1.82	11	4
1:A:151:LEU:O	1:A:155:LEU:HD12	0.50	2.06	16	2
1:A:85:ALA:HB2	1:A:168:TYR:CD2	0.50	2.42	20	3
1:A:88:PRO:CA	1:A:94:LEU:HD23	0.50	2.36	17	4
1:A:82:VAL:HG22	1:A:102:PHE:CE1	0.49	2.43	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:HG22	1:A:81:PRO:HD2	0.49	1.84	14	6
1:A:55:LEU:HD11	1:A:84:PHE:CZ	0.49	2.42	15	3
1:A:31:TYR:HB3	1:A:151:LEU:HD11	0.49	1.84	18	2
1:A:47:THR:HG22	1:A:97:LYS:CG	0.49	2.37	10	2
1:A:46:VAL:HB	1:A:54:ALA:HB1	0.49	1.85	20	3
1:A:166:VAL:O	1:A:187:LEU:HD23	0.49	2.08	8	3
1:A:135:PHE:O	1:A:136:GLY:C	0.49	2.51	12	1
1:A:59:MET:HE1	1:A:82:VAL:HG11	0.48	1.85	20	1
1:A:166:VAL:O	1:A:187:LEU:HD12	0.48	2.09	13	2
1:A:162:TYR:CE1	1:A:187:LEU:HD21	0.48	2.43	11	1
1:A:21:LEU:HD11	1:A:33:GLU:OE1	0.47	2.09	15	2
1:A:151:LEU:HD23	1:A:187:LEU:CD1	0.47	2.35	18	1
1:A:44:VAL:HG21	1:A:58:ALA:CB	0.47	2.38	1	2
1:A:144:TYR:CD2	1:A:185:VAL:HG22	0.47	2.44	20	2
1:A:47:THR:HG22	1:A:97:LYS:HG2	0.47	1.85	11	3
1:A:26:LYS:HB3	1:A:154:THR:HG23	0.47	1.86	13	1
1:A:51:VAL:HG11	1:A:86:VAL:HG12	0.47	1.85	10	2
1:A:166:VAL:HG13	1:A:188:VAL:CG2	0.47	2.40	2	2
1:A:20:VAL:HG13	1:A:33:GLU:O	0.46	2.10	14	2
1:A:54:ALA:HB1	1:A:98:LEU:HD22	0.46	1.86	3	4
1:A:86:VAL:HB	1:A:94:LEU:HD22	0.46	1.88	20	2
1:A:139:ALA:HB3	1:A:183:ASN:ND2	0.46	2.25	9	3
1:A:59:MET:CB	1:A:60:PRO:CD	0.46	2.94	7	17
1:A:62:ILE:O	1:A:66:VAL:HG12	0.46	2.11	17	1
1:A:47:THR:HG23	1:A:97:LYS:HG3	0.46	1.88	17	1
1:A:44:VAL:HG11	1:A:61:LYS:HD2	0.45	1.88	20	1
1:A:170:ALA:HB3	1:A:184:GLU:HB2	0.45	1.86	10	1
1:A:66:VAL:HG21	1:A:78:MET:O	0.45	2.12	19	1
1:A:128:ILE:CD1	1:A:130:VAL:HG13	0.45	2.40	8	2
1:A:144:TYR:HA	1:A:147:HIS:CE1	0.45	2.47	18	1
1:A:85:ALA:HB2	1:A:168:TYR:CD1	0.44	2.47	13	6
1:A:147:HIS:CD2	1:A:148:ALA:N	0.44	2.86	18	1
1:A:44:VAL:HG21	1:A:58:ALA:HB1	0.44	1.88	1	1
1:A:20:VAL:HG23	1:A:33:GLU:O	0.44	2.12	5	3
1:A:41:PHE:HA	1:A:104:ILE:HD12	0.44	1.88	20	5
1:A:166:VAL:CG2	1:A:188:VAL:HG22	0.44	2.43	17	1
1:A:94:LEU:HD11	1:A:167:TYR:OH	0.44	2.12	11	1
1:A:133:THR:HG21	1:A:151:LEU:HD11	0.44	1.87	20	1
1:A:21:LEU:HD21	1:A:33:GLU:CG	0.44	2.40	16	1
1:A:186:TRP:N	1:A:186:TRP:CD1	0.44	2.85	8	2
1:A:98:LEU:HD11	1:A:100:VAL:HG23	0.44	1.87	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:THR:HG22	1:A:32:GLU:CB	0.44	2.41	3	1
1:A:186:TRP:CD1	1:A:186:TRP:N	0.44	2.86	7	2
1:A:54:ALA:HB3	1:A:98:LEU:HD22	0.44	1.90	5	2
1:A:80:VAL:HG23	1:A:81:PRO:HD2	0.43	1.90	13	1
1:A:86:VAL:HG12	1:A:98:LEU:HD12	0.43	1.90	9	1
1:A:21:LEU:HD11	1:A:33:GLU:HG3	0.43	1.90	3	2
1:A:51:VAL:HG21	1:A:94:LEU:CD1	0.43	2.44	18	1
1:A:21:LEU:HD12	1:A:22:SER:N	0.43	2.28	5	1
1:A:166:VAL:HG13	1:A:188:VAL:HB	0.43	1.90	3	1
1:A:59:MET:N	1:A:60:PRO:CD	0.42	2.82	4	1
1:A:94:LEU:HD22	1:A:94:LEU:H	0.42	1.74	1	2
1:A:20:VAL:HG22	1:A:34:ARG:HG2	0.42	1.91	20	1
1:A:21:LEU:HD21	1:A:33:GLU:HG3	0.42	1.90	3	2
1:A:155:LEU:HD22	1:A:158:THR:HG21	0.42	1.90	7	1
1:A:21:LEU:HD12	1:A:33:GLU:HB3	0.42	1.91	12	1
1:A:51:VAL:CG1	1:A:98:LEU:HD23	0.41	2.41	20	1
1:A:54:ALA:HB3	1:A:98:LEU:HD13	0.41	1.92	1	1
1:A:62:ILE:HG21	1:A:102:PHE:CD1	0.41	2.51	11	1
1:A:98:LEU:HD13	1:A:98:LEU:C	0.41	2.34	20	1
1:A:133:THR:HG22	1:A:185:VAL:HG23	0.41	1.93	18	1
1:A:80:VAL:HG21	1:A:103:ARG:O	0.41	2.16	12	1
1:A:86:VAL:O	1:A:166:VAL:HG23	0.41	2.15	7	1
1:A:98:LEU:HD21	1:A:100:VAL:HG23	0.41	1.92	7	1
1:A:98:LEU:O	1:A:98:LEU:HD23	0.41	2.16	10	1
1:A:161:THR:HG23	1:A:190:ALA:HB3	0.41	1.93	12	1
1:A:155:LEU:O	1:A:156:GLU:C	0.40	2.59	20	1
1:A:26:LYS:HB2	1:A:154:THR:HG22	0.40	1.92	16	1
1:A:163:GLN:NE2	1:A:188:VAL:HG12	0.40	2.32	13	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	160/195 (82%)	152±1 (95±1%)	7±1 (4±1%)	1±1 (0±0%)	40	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3200/3900 (82%)	3043 (95%)	144 (4%)	13 (0%)	40 79

All 2 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	96	LYS	12
1	A	136	GLY	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	133/163 (82%)	102±4 (76±3%)	32±4 (24±3%)	3 27
All	All	2660/3260 (82%)	2030 (76%)	630 (24%)	3 27

All 94 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	78	MET	19
1	A	80	VAL	18
1	A	40	LYS	18
1	A	143	ASP	18
1	A	116	SER	17
1	A	43	THR	16
1	A	36	CYS	16
1	A	19	GLN	16
1	A	48	ASP	15
1	A	117	ASP	14
1	A	37	GLU	13
1	A	140	LYS	12
1	A	150	GLN	12
1	A	79	THR	12
1	A	34	ARG	12
1	A	189	LYS	12
1	A	64	LYS	12

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Mol	Chain	Res	Type	Models (Total)
1	A	119	SER	11
1	A	96	LYS	11
1	A	93	SER	11
1	A	99	LYS	10
1	A	109	GLN	10
1	A	72	LYS	10
1	A	111	SER	9
1	A	163	GLN	9
1	A	125	ARG	9
1	A	21	LEU	9
1	A	162	TYR	8
1	A	63	MET	8
1	A	30	SER	8
1	A	91	ASP	8
1	A	70	ASN	8
1	A	126	GLU	8
1	A	141	GLU	8
1	A	103	ARG	8
1	A	95	GLN	7
1	A	61	LYS	7
1	A	172	TYR	7
1	A	106	ASN	7
1	A	52	ASP	7
1	A	98	LEU	7
1	A	59	MET	7
1	A	97	LYS	7
1	A	28	ASP	7
1	A	134	GLN	6
1	A	161	THR	6
1	A	56	ARG	6
1	A	27	GLU	6
1	A	121	LYS	6
1	A	182	ARG	6
1	A	26	LYS	6
1	A	184	GLU	6
1	A	132	SER	6
1	A	124	GLU	5
1	A	183	ASN	4
1	A	107	GLN	4
1	A	83	SER	4
1	A	118	GLU	4
1	A	181	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	187	LEU	4
1	A	186	TRP	4
1	A	33	GLU	4
1	A	156	GLU	4
1	A	57	GLU	4
1	A	151	LEU	3
1	A	108	PHE	3
1	A	49	LYS	3
1	A	55	LEU	3
1	A	31	TYR	3
1	A	152	ARG	3
1	A	165	ASP	3
1	A	45	GLU	3
1	A	69	THR	3
1	A	47	THR	2
1	A	138	TYR	2
1	A	94	LEU	2
1	A	131	TYR	2
1	A	32	GLU	2
1	A	129	THR	1
1	A	153	THR	1
1	A	185	VAL	1
1	A	18	TRP	1
1	A	149	THR	1
1	A	128	ILE	1
1	A	188	VAL	1
1	A	53	GLU	1
1	A	71	ASP	1
1	A	44	VAL	1
1	A	104	ILE	1
1	A	86	VAL	1
1	A	135	PHE	1
1	A	155	LEU	1
1	A	90	GLU	1
1	A	22	SER	1

6.3.3 RNA ⓘ

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 84% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: 4a1m_cs.str

Chemical shift list name: *deposit2_1.bmr.b.csh*

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	1903
Number of shifts mapped to atoms	1903
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	167	-0.37 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	151	-0.31 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	145	0.01 ± 0.12	None needed (< 0.5 ppm)
^{15}N	154	0.44 ± 0.23	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 84%, i.e. 1616 atoms were assigned a chemical shift out of a possible 1934. 21 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	750/787 (95%)	308/313 (98%)	297/322 (92%)	145/152 (95%)
Sidechain	747/978 (76%)	477/574 (83%)	261/360 (72%)	9/44 (20%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	119/169 (70%)	77/88 (88%)	39/77 (51%)	3/4 (75%)
Overall	1616/1934 (84%)	862/975 (88%)	597/759 (79%)	157/200 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1721 atoms were assigned a chemical shift out of a possible 2193. 22 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	795/894 (89%)	329/355 (93%)	312/368 (85%)	154/171 (90%)
Sidechain	794/1101 (72%)	508/649 (78%)	277/406 (68%)	9/46 (20%)
Aromatic	132/198 (67%)	85/103 (83%)	43/90 (48%)	4/5 (80%)
Overall	1721/2193 (78%)	922/1107 (83%)	632/864 (73%)	167/222 (75%)

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	103	ARG	HD3	1.22	4.36 – 1.86	-7.6
1	A	103	ARG	HG2	-0.44	2.92 – 0.22	-7.4
1	A	103	ARG	HG3	-0.52	3.00 – 0.10	-7.1
1	A	183	ASN	HB3	0.58	4.41 – 1.11	-6.6
1	A	176	MET	CG	38.63	38.33 – 25.73	5.2
1	A	130	VAL	HG11	-0.53	2.13 – -0.47	-5.2
1	A	130	VAL	HG12	-0.53	2.13 – -0.47	-5.2
1	A	130	VAL	HG13	-0.53	2.13 – -0.47	-5.2
1	A	81	PRO	HB2	0.31	3.82 – 0.32	-5.0

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:

