



Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 08:03 PM UTC

PDB ID : 2LMD / pdb_00002lmd
BMRB ID : 18112
Title : Minimal Constraints Solution NMR Structure of Prospero Homeobox protein 1 from Homo sapiens, Northeast Structural Genomics Consortium Target HR4660B
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Deposited on : 2011-11-29

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

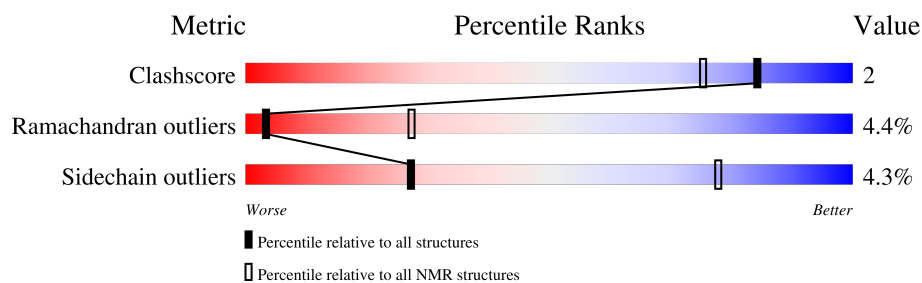
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 58%.

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	174	

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:20-A:167 (148)	1.77	4

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2888 atoms, of which 1431 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Prospero homeobox protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			2888	935	1431	250	261	11	

There are 11 discrepancies between the modelled and reference sequences:

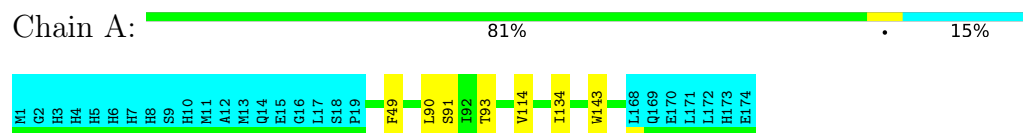
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q92786
A	2	GLY	-	expression tag	UNP Q92786
A	3	HIS	-	expression tag	UNP Q92786
A	4	HIS	-	expression tag	UNP Q92786
A	5	HIS	-	expression tag	UNP Q92786
A	6	HIS	-	expression tag	UNP Q92786
A	7	HIS	-	expression tag	UNP Q92786
A	8	HIS	-	expression tag	UNP Q92786
A	9	SER	-	expression tag	UNP Q92786
A	10	HIS	-	expression tag	UNP Q92786
A	11	MET	-	expression tag	UNP Q92786

4 Residue-property plots

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: Prospero homeobox protein 1

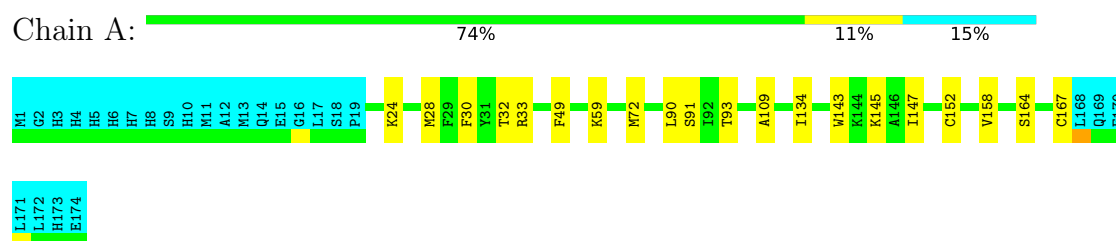


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

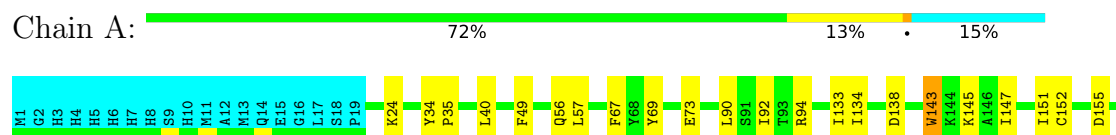
4.2.1 Score per residue for model 1

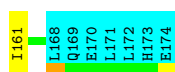
- Molecule 1: Prospero homeobox protein 1



4.2.2 Score per residue for model 2

- Molecule 1: Prospero homeobox protein 1

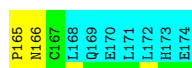




4.2.3 Score per residue for model 3

- Molecule 1: Prospero homeobox protein 1

Chain A: 72% 13% 15%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Prospero homeobox protein 1

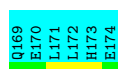
Chain A: 70% 14% 15%



4.2.5 Score per residue for model 5

- Molecule 1: Prospero homeobox protein 1

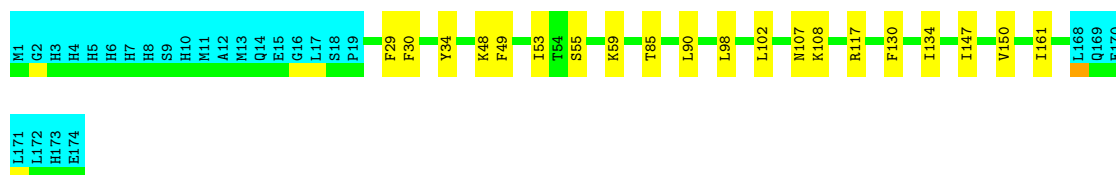
Chain A: 72% 11% 15%



4.2.6 Score per residue for model 6

- Molecule 1: Prospero homeobox protein 1

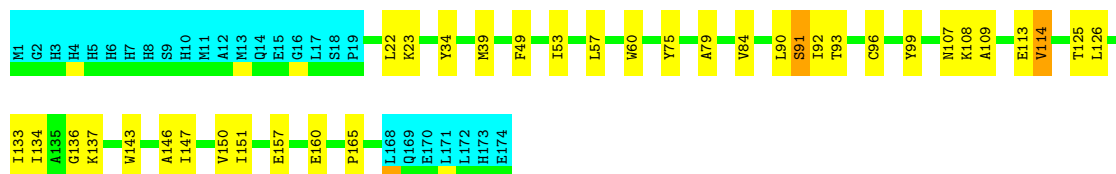
Chain A: 74% 11% 15%



4.2.7 Score per residue for model 7

- Molecule 1: Prospero homeobox protein 1

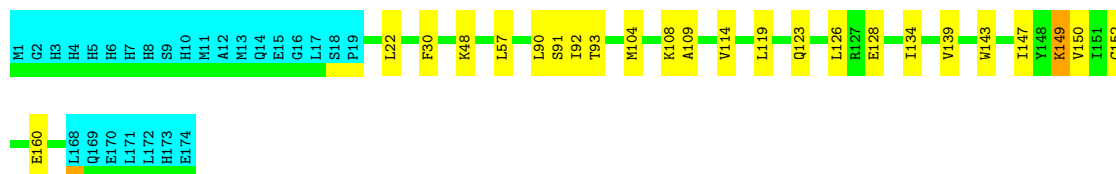
Chain A: 64% 20% 15%



4.2.8 Score per residue for model 8

- Molecule 1: Prospero homeobox protein 1

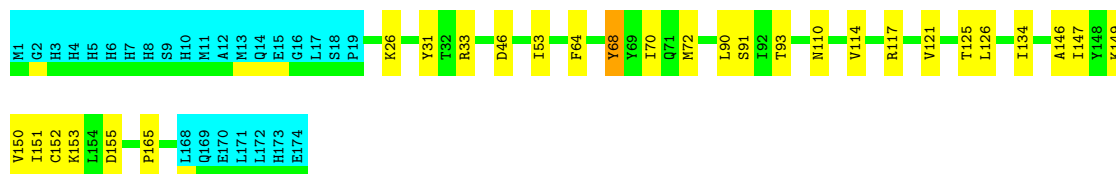
Chain A: 71% 13% 15%



4.2.9 Score per residue for model 9

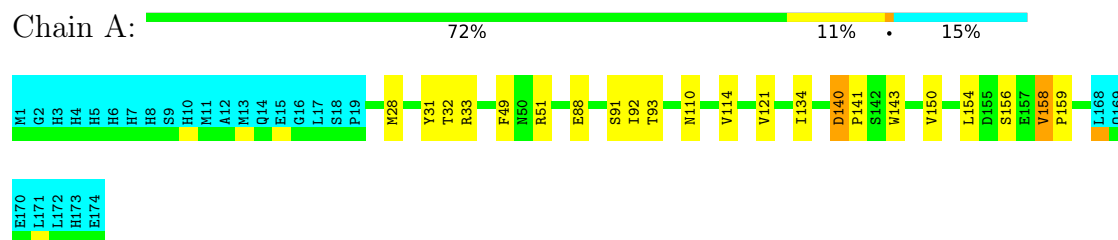
- Molecule 1: Prospero homeobox protein 1

Chain A: 69% 16% 15%



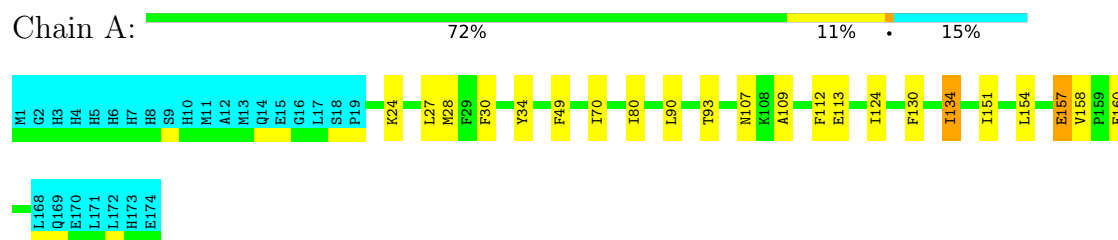
4.2.10 Score per residue for model 10

- Molecule 1: Prospero homeobox protein 1



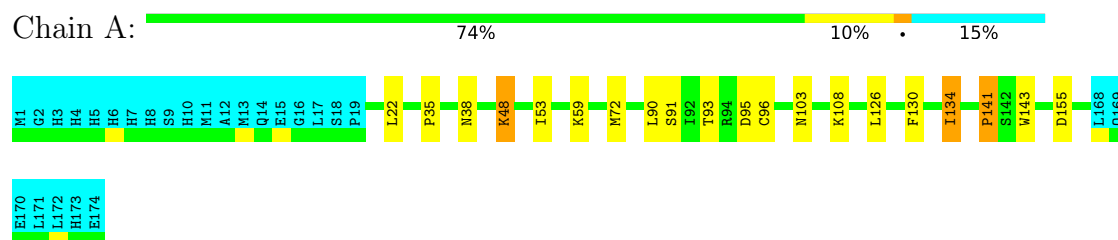
4.2.11 Score per residue for model 11

- Molecule 1: Prospero homeobox protein 1



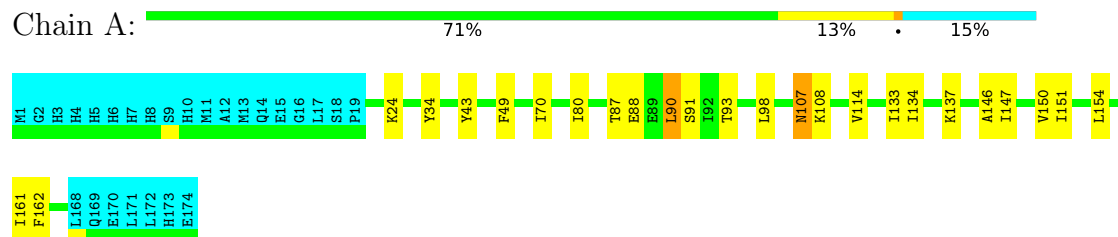
4.2.12 Score per residue for model 12

- Molecule 1: Prospero homeobox protein 1



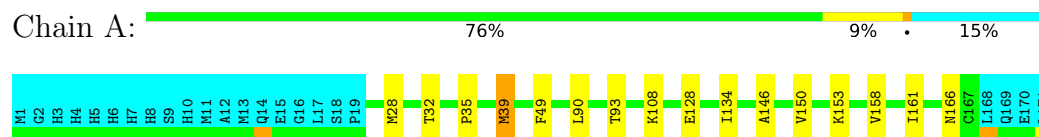
4.2.13 Score per residue for model 13

- Molecule 1: Prospero homeobox protein 1



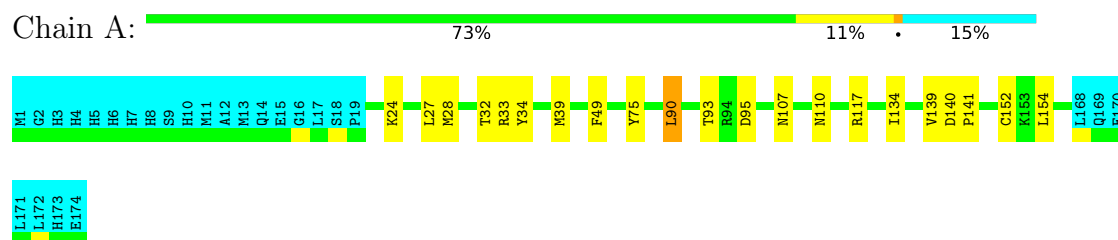
4.2.14 Score per residue for model 14

- Molecule 1: Prospero homeobox protein 1



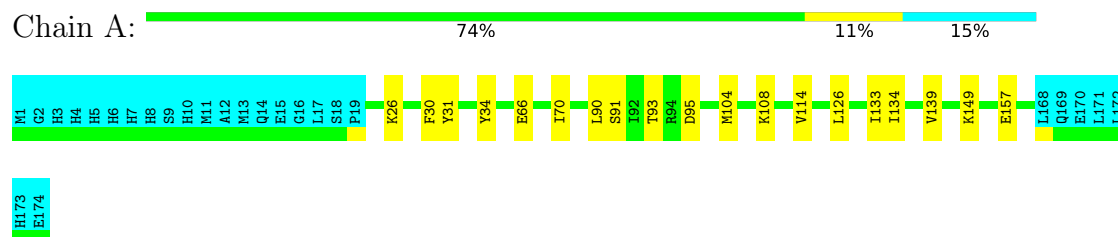
4.2.15 Score per residue for model 15

- Molecule 1: Prospero homeobox protein 1



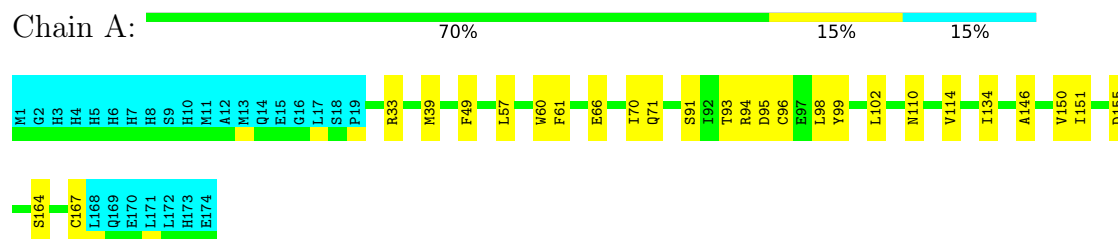
4.2.16 Score per residue for model 16

- Molecule 1: Prospero homeobox protein 1



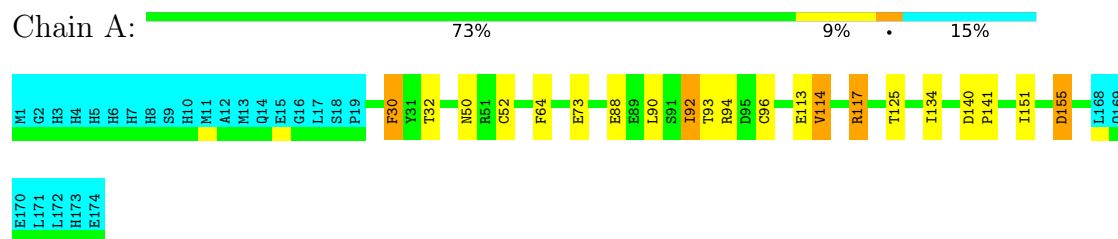
4.2.17 Score per residue for model 17

- Molecule 1: Prospero homeobox protein 1



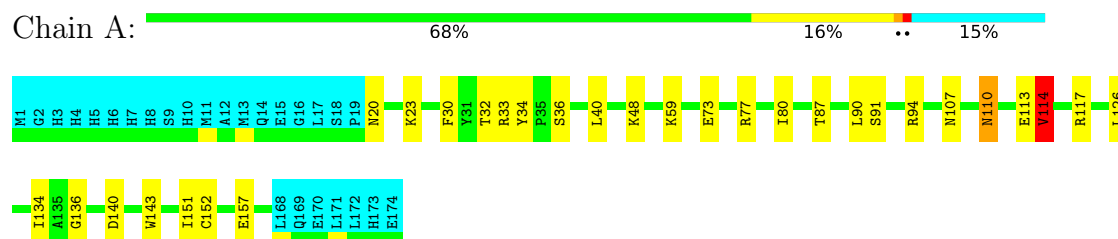
4.2.18 Score per residue for model 18

- Molecule 1: Prospero homeobox protein 1



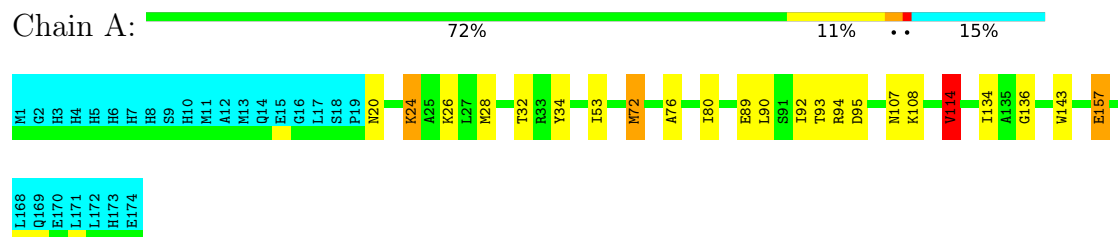
4.2.19 Score per residue for model 19

- Molecule 1: Prospero homeobox protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Prospero homeobox protein 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	
CNS	geometry optimization	
CYANA	refinement	3.0
CYANA	geometry optimization	3.0
CYANA	structure solution	3.0
TALOS+	geometry optimization	
PALES	geometry optimization	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1366
Number of shifts mapped to atoms	1366
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.27±0.03	1±1/1275 (0.1± 0.1%)	1.10±0.03	0±0/1719 (0.0± 0.0%)
All	All	1.27	19/25500 (0.1%)	1.10	3/34380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	107	ASN	CA-C	6.30	1.55	1.52	20	1
1	A	114	VAL	CA-CB	6.23	1.62	1.54	20	4
1	A	80	ILE	CA-CB	5.58	1.60	1.54	13	3
1	A	70	ILE	CA-CB	5.43	1.61	1.54	11	4
1	A	158	VAL	C-N	5.40	1.37	1.33	1	1
1	A	133	ILE	CA-CB	5.22	1.60	1.54	5	3
1	A	147	ILE	CA-CB	5.13	1.60	1.54	13	2
1	A	158	VAL	CA-C	5.05	1.58	1.52	10	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	114	VAL	N-CA-CB	6.74	120.64	111.21	19	2
1	A	67	PHE	CA-CB-CG	5.64	119.44	113.80	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	112	PHE	Peptide	1

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	1243	1232	1230	6±2
All	All	24860	24640	24600	116

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:GLU:HG3	1:A:150:VAL:HG21	0.63	1.69	5	1
1:A:149:LYS:HA	1:A:152:CYS:SG	0.61	2.36	9	3
1:A:33:ARG:HA	1:A:152:CYS:SG	0.60	2.36	5	3
1:A:39:MET:SD	1:A:61:PHE:HZ	0.58	2.22	17	1
1:A:164:SER:HB3	1:A:167:CYS:SG	0.57	2.39	17	1
1:A:107:ASN:HB2	1:A:110:ASN:HB2	0.57	1.76	19	1
1:A:117:ARG:HD3	1:A:155:ASP:HB3	0.57	1.76	18	1
1:A:104:MET:SD	1:A:108:LYS:HE3	0.55	2.42	16	1
1:A:28:MET:HG3	1:A:158:VAL:HG11	0.54	1.79	10	2
1:A:32:THR:HG21	1:A:39:MET:SD	0.54	2.43	14	1
1:A:91:SER:HB3	1:A:126:LEU:HD22	0.53	1.80	8	4
1:A:139:VAL:HG23	1:A:143:TRP:HB3	0.53	1.81	8	1
1:A:39:MET:SD	1:A:39:MET:C	0.52	2.92	17	4
1:A:35:PRO:HD3	1:A:152:CYS:SG	0.52	2.45	2	1
1:A:33:ARG:HE	1:A:121:VAL:HG11	0.51	1.65	3	1
1:A:31:TYR:HA	1:A:33:ARG:NH2	0.51	2.20	10	1
1:A:125:THR:HB	1:A:151:ILE:HG21	0.50	1.83	9	3
1:A:24:LYS:HE3	1:A:28:MET:SD	0.50	2.45	20	1
1:A:92:ILE:HG23	1:A:123:GLN:HG3	0.50	1.82	4	1
1:A:33:ARG:NH2	1:A:121:VAL:HG21	0.49	2.22	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:ASN:HB2	1:A:110:ASN:HB3	0.49	1.84	15	1
1:A:33:ARG:HG2	1:A:155:ASP:HB2	0.49	1.84	17	1
1:A:133:ILE:HA	1:A:137:LYS:HA	0.49	1.84	13	1
1:A:75:TYR:HB3	1:A:90:LEU:HB3	0.48	1.84	3	2
1:A:117:ARG:HG2	1:A:155:ASP:HB3	0.47	1.85	9	1
1:A:20:ASN:HA	1:A:23:LYS:HD3	0.47	1.87	19	1
1:A:133:ILE:HG12	1:A:138:ASP:HB3	0.46	1.84	2	1
1:A:23:LYS:HG3	1:A:109:ALA:HB1	0.46	1.87	7	1
1:A:88:GLU:HA	1:A:92:ILE:HB	0.46	1.87	4	2
1:A:72:MET:HE1	1:A:91:SER:OG	0.46	2.11	1	1
1:A:133:ILE:HG13	1:A:138:ASP:HB3	0.46	1.88	5	1
1:A:158:VAL:N	1:A:159:PRO:HD3	0.46	2.25	10	1
1:A:152:CYS:HA	1:A:155:ASP:HB2	0.45	1.87	2	1
1:A:137:LYS:HB3	1:A:143:TRP:HB3	0.45	1.86	5	1
1:A:24:LYS:HE3	1:A:162:PHE:HB2	0.45	1.88	13	1
1:A:141:PRO:HD2	1:A:143:TRP:CD1	0.45	2.47	12	1
1:A:140:ASP:HA	1:A:143:TRP:CD1	0.45	2.47	10	1
1:A:90:LEU:HB2	1:A:126:LEU:HD21	0.44	1.89	16	3
1:A:32:THR:HA	1:A:156:SER:HA	0.44	1.88	10	1
1:A:104:MET:SD	1:A:108:LYS:HD3	0.44	2.53	8	1
1:A:146:ALA:O	1:A:150:VAL:HG13	0.44	2.12	14	6
1:A:143:TRP:O	1:A:147:ILE:HG12	0.44	2.13	7	4
1:A:93:THR:O	1:A:94:ARG:HG3	0.44	2.13	3	1
1:A:124:ILE:HD12	1:A:154:LEU:HD11	0.43	1.89	4	2
1:A:40:LEU:HD11	1:A:57:LEU:HD13	0.43	1.90	2	1
1:A:26:LYS:HD2	1:A:107:ASN:ND2	0.43	2.28	3	1
1:A:64:PHE:O	1:A:68:TYR:HB2	0.43	2.14	9	1
1:A:98:LEU:O	1:A:102:LEU:HG	0.43	2.13	6	2
1:A:32:THR:HB	1:A:39:MET:SD	0.43	2.53	4	1
1:A:26:LYS:NZ	1:A:26:LYS:HB3	0.43	2.28	4	1
1:A:27:LEU:HD21	1:A:109:ALA:O	0.43	2.13	11	1
1:A:87:THR:HA	1:A:90:LEU:HG	0.43	1.90	19	2
1:A:91:SER:HB2	1:A:98:LEU:HD13	0.43	1.91	13	1
1:A:48:LYS:H	1:A:48:LYS:HD2	0.43	1.73	12	1
1:A:33:ARG:NE	1:A:152:CYS:SG	0.43	2.92	15	1
1:A:24:LYS:HE2	1:A:28:MET:SD	0.42	2.54	11	1
1:A:164:SER:HB2	1:A:167:CYS:HB2	0.42	1.92	1	1
1:A:79:ALA:HA	1:A:84:VAL:HB	0.42	1.91	7	1
1:A:33:ARG:NE	1:A:121:VAL:HG11	0.42	2.29	9	1
1:A:124:ILE:O	1:A:128:GLU:HG2	0.42	2.15	3	1
1:A:75:TYR:HB3	1:A:90:LEU:HD12	0.42	1.92	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:GLU:O	1:A:70:ILE:HG12	0.42	2.14	17	2
1:A:76:ALA:O	1:A:80:ILE:HG12	0.42	2.15	20	1
1:A:92:ILE:HD12	1:A:123:GLN:HG2	0.42	1.91	8	1
1:A:28:MET:O	1:A:32:THR:HG23	0.41	2.14	15	1
1:A:147:ILE:O	1:A:150:VAL:HG22	0.41	2.15	8	2
1:A:36:SER:O	1:A:40:LEU:HB2	0.41	2.14	19	1
1:A:88:GLU:HA	1:A:92:ILE:HG21	0.41	1.91	10	1
1:A:150:VAL:O	1:A:154:LEU:HG	0.41	2.15	13	2
1:A:55:SER:O	1:A:59:LYS:HG2	0.41	2.16	6	1
1:A:24:LYS:NZ	1:A:28:MET:SD	0.41	2.83	1	1
1:A:69:TYR:O	1:A:73:GLU:HB2	0.41	2.16	2	1
1:A:22:LEU:HD13	1:A:60:TRP:CD2	0.41	2.51	7	1
1:A:75:TYR:HB3	1:A:90:LEU:HD13	0.41	1.92	15	1
1:A:73:GLU:HG2	1:A:77:ARG:HE	0.41	1.75	19	1
1:A:89:GLU:HA	1:A:94:ARG:NH2	0.41	2.30	20	1
1:A:130:PHE:O	1:A:134:ILE:HG22	0.41	2.15	12	2
1:A:113:GLU:O	1:A:114:VAL:HG22	0.41	2.16	19	1
1:A:93:THR:HA	1:A:119:LEU:HB3	0.40	1.92	8	1
1:A:30:PHE:HA	1:A:64:PHE:CE1	0.40	2.52	18	1
1:A:72:MET:N	1:A:72:MET:SD	0.40	2.93	20	1
1:A:94:ARG:HB3	1:A:96:CYS:SG	0.40	2.56	18	1
1:A:117:ARG:HD2	1:A:154:LEU:O	0.40	2.16	15	1
1:A:117:ARG:H	1:A:117:ARG:HD2	0.40	1.76	6	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	148/174 (85%)	126±4 (85±3%)	16±4 (11±3%)	6±2 (4±1%)	3	27
All	All	2960/3480 (85%)	2513 (85%)	318 (11%)	129 (4%)	3	27

All 30 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	93	THR	15
1	A	49	PHE	13
1	A	114	VAL	11
1	A	30	PHE	8
1	A	34	TYR	8
1	A	91	SER	7
1	A	95	ASP	7
1	A	140	ASP	6
1	A	141	PRO	5
1	A	108	LYS	5
1	A	32	THR	4
1	A	107	ASN	4
1	A	110	ASN	4
1	A	94	ARG	3
1	A	165	PRO	3
1	A	96	CYS	3
1	A	136	GLY	3
1	A	109	ALA	2
1	A	31	TYR	2
1	A	113	GLU	2
1	A	35	PRO	2
1	A	155	ASP	2
1	A	92	ILE	2
1	A	157	GLU	2
1	A	166	ASN	1
1	A	111	ASP	1
1	A	29	PHE	1
1	A	137	LYS	1
1	A	90	LEU	1
1	A	139	VAL	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	137/160 (86%)	131±2 (96±1%)	6±2 (4±1%)	27	78
All	All	2740/3200 (86%)	2621 (96%)	119 (4%)	27	78

All 49 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	134	ILE	20
1	A	90	LEU	12
1	A	151	ILE	6
1	A	157	GLU	6
1	A	26	LYS	4
1	A	57	LEU	4
1	A	48	LYS	4
1	A	59	LYS	3
1	A	24	LYS	3
1	A	143	TRP	3
1	A	22	LEU	3
1	A	114	VAL	3
1	A	72	MET	3
1	A	145	LYS	2
1	A	92	ILE	2
1	A	99	TYR	2
1	A	128	GLU	2
1	A	149	LYS	2
1	A	153	LYS	2
1	A	107	ASN	2
1	A	161	ILE	2
1	A	117	ARG	2
1	A	94	ARG	1
1	A	137	LYS	1
1	A	41	LYS	1
1	A	65	ARG	1
1	A	85	THR	1
1	A	130	PHE	1
1	A	31	TYR	1
1	A	46	ASP	1
1	A	53	ILE	1
1	A	68	TYR	1
1	A	51	ARG	1
1	A	160	GLU	1
1	A	38	ASN	1
1	A	103	ASN	1
1	A	43	TYR	1
1	A	88	GLU	1
1	A	39	MET	1
1	A	108	LYS	1
1	A	166	ASN	1
1	A	27	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	139	VAL	1
1	A	71	GLN	1
1	A	50	ASN	1
1	A	73	GLU	1
1	A	113	GLU	1
1	A	20	ASN	1
1	A	34	TYR	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 oligosaccharides 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 58% for the well-defined parts and 55% 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	1366
Number of shifts mapped to atoms	1366
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	-0.37 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	112	1.35 ± 0.10	Should be checked
$^{13}\text{C}'$	141	-0.40 ± 0.10	None needed (< 0.5 ppm)
^{15}N	144	1.13 ± 0.22	Should be applied

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 58%, i.e. 1243 atoms were assigned a chemical shift out of a possible 2137. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	626/732 (86%)	232/293 (79%)	263/296 (89%)	131/143 (92%)
Sidechain	517/1164 (44%)	345/751 (46%)	172/361 (48%)	0/52 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	100/241 (41%)	50/116 (43%)	48/119 (40%)	2/6 (33%)
Overall	1243/2137 (58%)	627/1160 (54%)	483/776 (62%)	133/201 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 1366 atoms were assigned a chemical shift out of a possible 2497. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	684/862 (79%)	251/346 (73%)	289/348 (83%)	144/168 (86%)
Sidechain	582/1330 (44%)	389/861 (45%)	193/415 (47%)	0/54 (0%)
Aromatic	100/305 (33%)	50/148 (34%)	48/135 (36%)	2/22 (9%)
Overall	1366/2497 (55%)	690/1355 (51%)	530/898 (59%)	146/244 (60%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	138	ASP	HB3	0.16	1.32 – 4.00	-9.3
1	A	18	SER	H	11.63	5.45 – 11.10	5.9

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. 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:

