



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 05:52 AM UTC

PDB ID : 2V9H / pdb_00002v9h
BMRB ID : 15247
Title : Solution Structure of an Escherichia coli YaeT tandem POTRA domain
Authors : Knowles, T.J.; Jeeves, M.; Bobat, S.; Dancea, F.; McClelland, D.M.; Palmer, T.; Overduin, M.; Henderson, I.R.
Deposited on : 2007-08-23

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

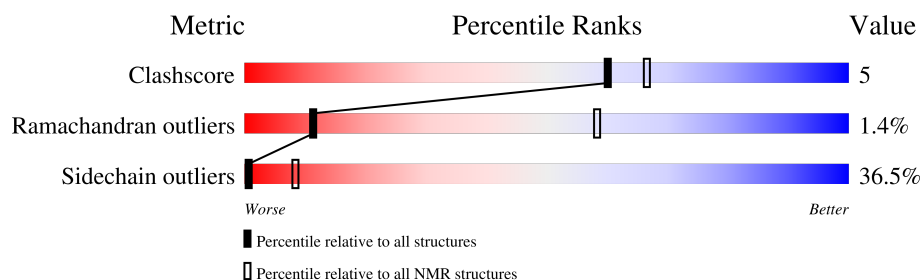
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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	164	

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 3 as representative.

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:23-A:33, A:38-A:89 (63)	0.49	2
2	A:92-A:170 (79)	0.69	9

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 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2383 atoms, of which 1200 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET.

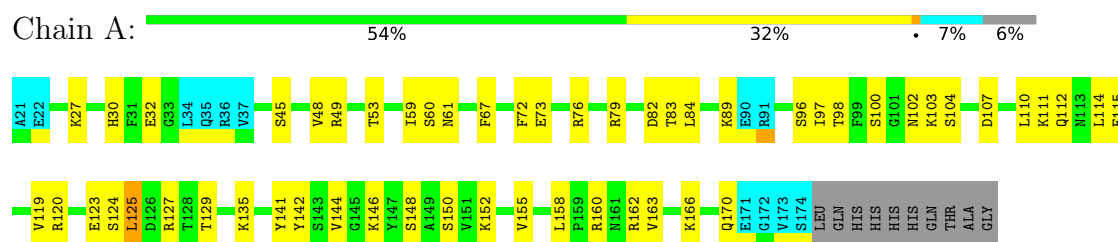
Mol	Chain	Residues	Atoms						Trace
1	A	154	Total	C	H	N	O	S	0
			2383	742	1200	205	234	2	

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: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



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

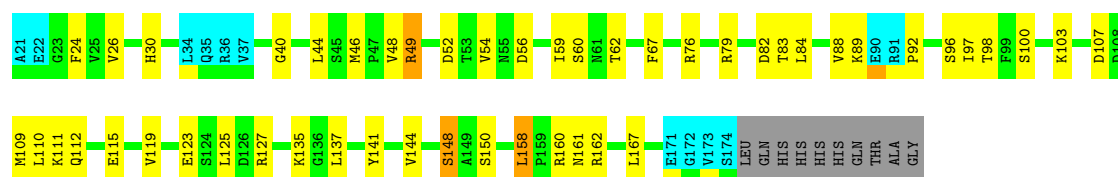
- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



4.2.2 Score per residue for model 2

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

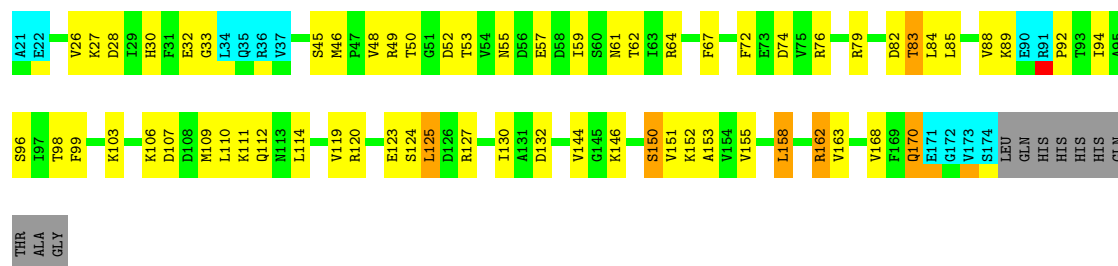




4.2.3 Score per residue for model 3

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

Chain A: 48% 35% 7% 6%



4.2.4 Score per residue for model 4

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

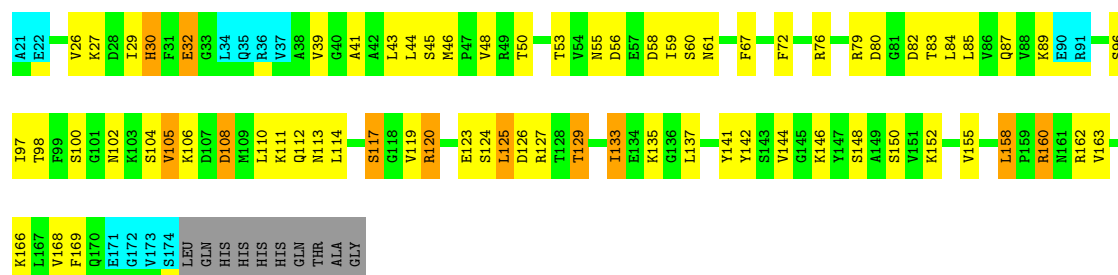
Chain A: 51% 31% 7% 6%



4.2.5 Score per residue for model 5

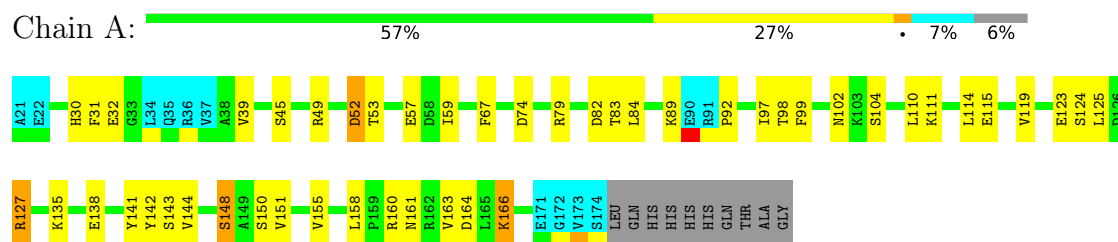
- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

Chain A: 43% 37% 7% 7% 6%



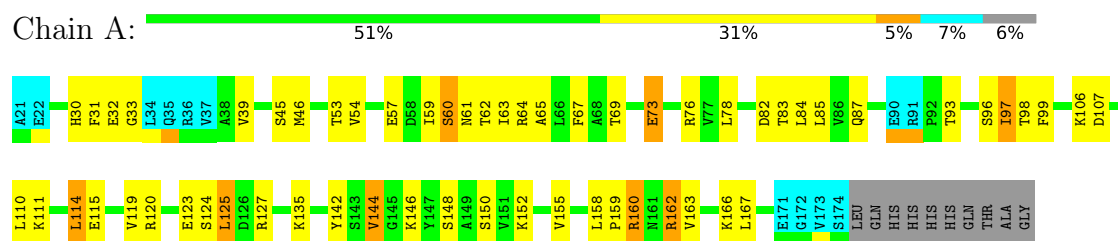
4.2.6 Score per residue for model 6

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



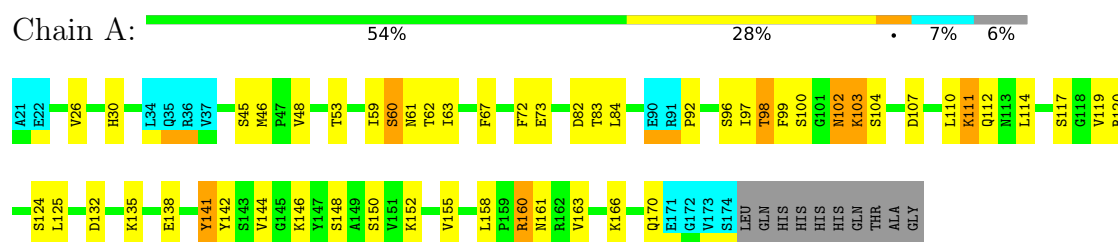
4.2.7 Score per residue for model 7

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



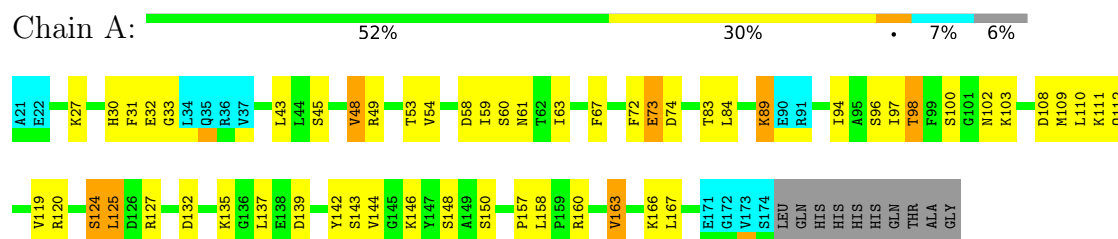
4.2.8 Score per residue for model 8

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



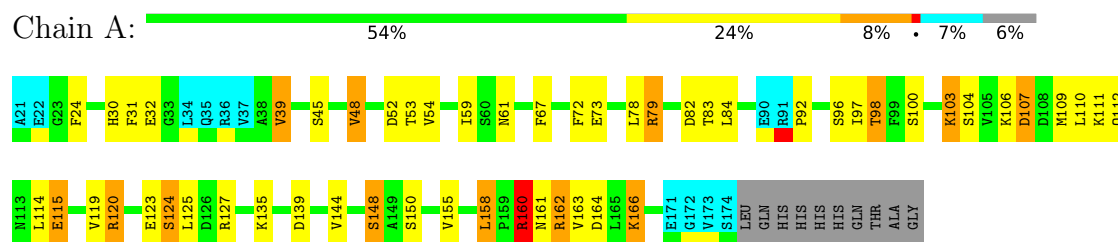
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



4.2.10 Score per residue for model 10

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



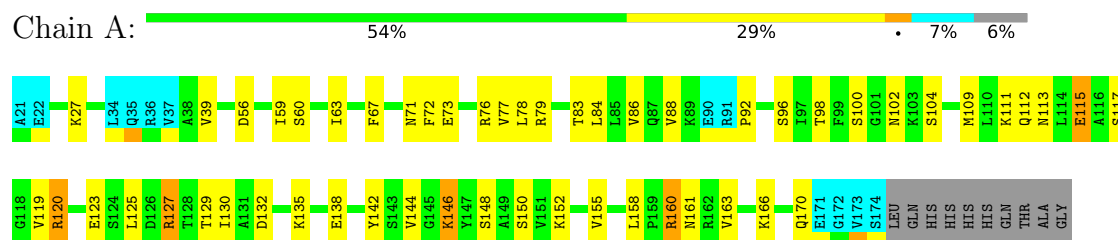
4.2.11 Score per residue for model 11

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



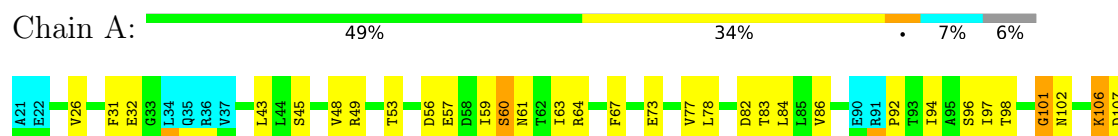
4.2.12 Score per residue for model 12

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



4.2.13 Score per residue for model 13

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

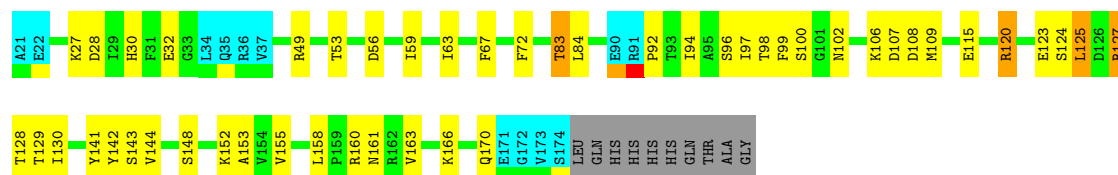




4.2.14 Score per residue for model 14

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

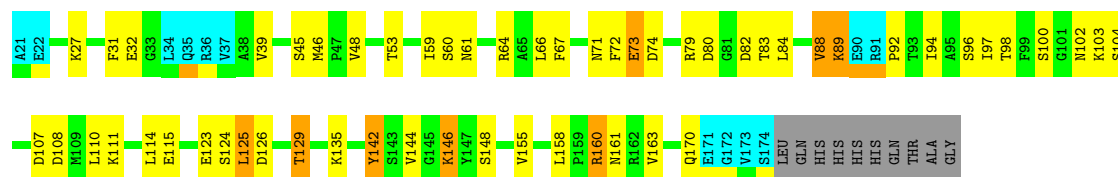
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

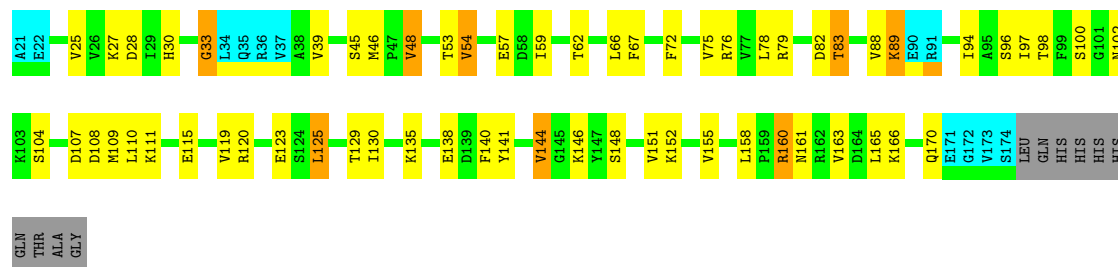
Chain A:



4.2.16 Score per residue for model 16

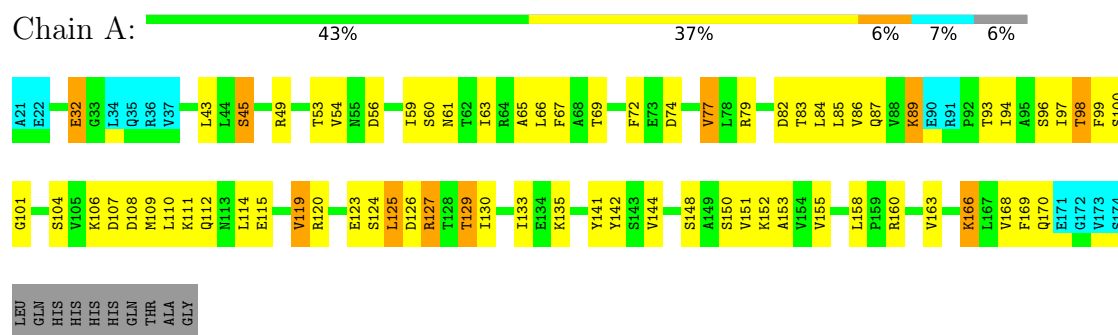
- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET

Chain A:



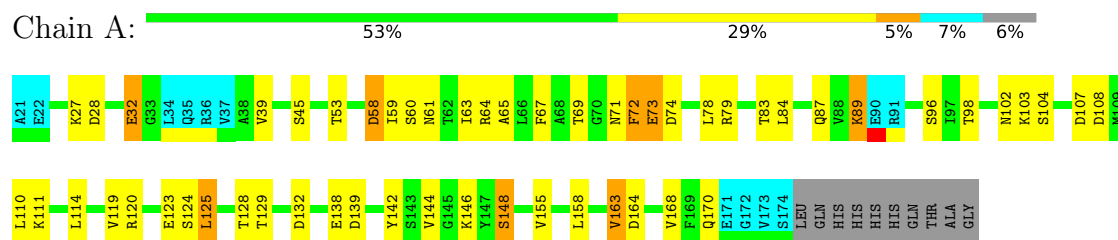
4.2.17 Score per residue for model 17

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



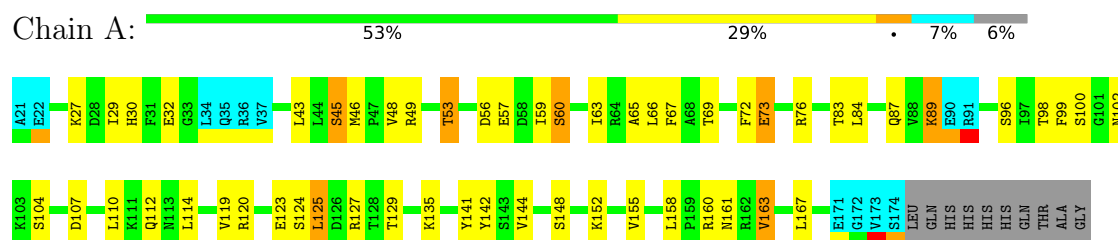
4.2.18 Score per residue for model 18

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



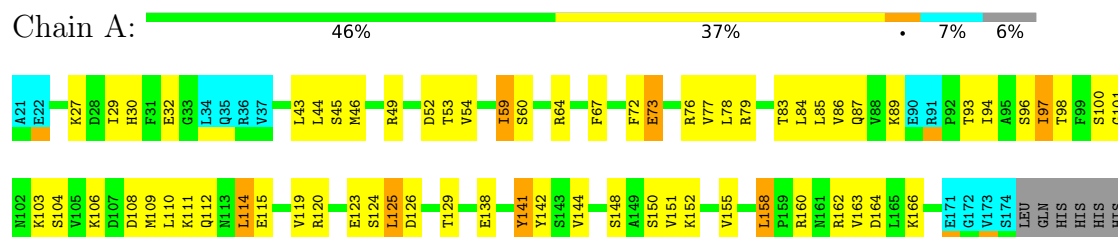
4.2.19 Score per residue for model 19

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



4.2.20 Score per residue for model 20

- Molecule 1: OUTER MEMBRANE PROTEIN ASSEMBLY FACTOR YAET



GLN
THR
ALA
GLY

5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 450 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATIONS*.

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

Software name	Classification	Version
ARIA	refinement	
NMRPipe	structure solution	
Sparky	structure solution	
VNMR	structure solution	
CYANA	structure solution	
CNS	structure solution	

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	1906
Number of shifts mapped to atoms	1888
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	1088	1104	1103	10±4
All	All	21760	22080	22060	198

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ILE:HD11	1:A:79:ARG:HD3	0.70	1.61	20	1
1:A:108:ASP:HA	1:A:111:LYS:HE2	0.69	1.62	5	1
1:A:138:GLU:HG3	1:A:151:VAL:HG23	0.68	1.66	20	4
1:A:93:THR:HB	1:A:162:ARG:HG3	0.68	1.64	7	1
1:A:74:ASP:HB3	1:A:89:LYS:HB2	0.66	1.68	18	6
1:A:115:GLU:HG2	1:A:120:ARG:HG3	0.63	1.69	20	1
1:A:107:ASP:HA	1:A:110:LEU:HD12	0.63	1.68	10	2
1:A:98:THR:HB	1:A:166:LYS:HG3	0.62	1.70	8	2
1:A:125:LEU:HD22	1:A:163:VAL:HG11	0.61	1.71	19	2
1:A:29:ILE:HG21	1:A:46:MET:HE1	0.60	1.73	20	3
1:A:73:GLU:HB3	1:A:124:SER:HB3	0.59	1.74	1	1
1:A:73:GLU:HB3	1:A:124:SER:HB2	0.58	1.75	9	1
1:A:45:SER:HB3	1:A:69:THR:HG21	0.58	1.76	7	3
1:A:115:GLU:HA	1:A:120:ARG:HB3	0.58	1.75	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ASP:HA	1:A:61:ASN:HB2	0.58	1.74	18	4
1:A:93:THR:HB	1:A:162:ARG:HD2	0.58	1.75	20	1
1:A:46:MET:HG2	1:A:62:THR:HG23	0.57	1.76	3	5
1:A:125:LEU:HD22	1:A:163:VAL:HG21	0.57	1.76	5	3
1:A:60:SER:HA	1:A:63:ILE:HD12	0.56	1.76	18	8
1:A:97:ILE:HG21	1:A:114:LEU:HD22	0.56	1.76	1	4
1:A:142:TYR:HA	1:A:146:LYS:HA	0.56	1.76	12	3
1:A:43:LEU:HD22	1:A:49:ARG:HG2	0.56	1.77	19	1
1:A:24:PHE:CE1	1:A:79:ARG:HD2	0.55	2.36	2	2
1:A:32:GLU:HB2	1:A:87:GLN:HG2	0.55	1.76	20	2
1:A:138:GLU:HG3	1:A:151:VAL:HG12	0.55	1.78	13	1
1:A:92:PRO:HA	1:A:161:ASN:O	0.55	2.02	8	6
1:A:31:PHE:HD2	1:A:39:VAL:HG12	0.55	1.62	10	2
1:A:93:THR:HA	1:A:124:SER:HA	0.55	1.78	17	1
1:A:99:PHE:HE1	1:A:111:LYS:HG3	0.54	1.62	6	4
1:A:66:LEU:HB3	1:A:75:VAL:HG21	0.54	1.78	16	1
1:A:108:ASP:HA	1:A:111:LYS:CE	0.54	2.32	5	1
1:A:33:GLY:HA3	1:A:88:VAL:H	0.54	1.59	3	1
1:A:65:ALA:O	1:A:69:THR:HG23	0.54	2.03	7	5
1:A:101:GLY:HA3	1:A:169:PHE:HB2	0.54	1.78	1	3
1:A:103:LYS:H	1:A:103:LYS:HD2	0.53	1.63	8	1
1:A:32:GLU:HB3	1:A:87:GLN:HG2	0.53	1.78	17	2
1:A:28:ASP:HB3	1:A:83:THR:HG23	0.53	1.79	3	3
1:A:66:LEU:HD22	1:A:72:PHE:HE2	0.53	1.63	17	1
1:A:33:GLY:HA3	1:A:88:VAL:HG22	0.53	1.79	16	1
1:A:48:VAL:HG12	1:A:54:VAL:HG11	0.52	1.79	4	1
1:A:73:GLU:HG2	1:A:124:SER:HB2	0.52	1.80	10	2
1:A:125:LEU:HD11	1:A:130:ILE:HD11	0.52	1.81	16	1
1:A:158:LEU:HD11	1:A:162:ARG:HB2	0.51	1.82	20	3
1:A:94:ILE:HG13	1:A:125:LEU:HB2	0.51	1.81	13	1
1:A:115:GLU:HG2	1:A:120:ARG:HB3	0.51	1.82	12	3
1:A:98:THR:HB	1:A:166:LYS:HG2	0.51	1.83	6	2
1:A:130:ILE:HG23	1:A:153:ALA:HB3	0.51	1.83	14	5
1:A:49:ARG:HD2	1:A:52:ASP:HB2	0.51	1.83	2	1
1:A:29:ILE:HD13	1:A:43:LEU:HD21	0.51	1.82	19	1
1:A:41:ALA:HA	1:A:44:LEU:HD12	0.51	1.81	5	1
1:A:48:VAL:HG11	1:A:54:VAL:HG13	0.50	1.83	16	1
1:A:45:SER:HB2	1:A:66:LEU:HD23	0.50	1.82	17	2
1:A:94:ILE:HD11	1:A:125:LEU:HB2	0.49	1.85	15	6
1:A:150:SER:H	1:A:170:GLN:HB2	0.48	1.68	3	1
1:A:77:VAL:HB	1:A:86:VAL:HG22	0.48	1.84	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ASP:HB3	1:A:129:THR:OG1	0.47	2.09	15	4
1:A:127:ARG:HD2	1:A:127:ARG:H	0.47	1.68	17	1
1:A:99:PHE:HB3	1:A:102:ASN:HD21	0.47	1.70	4	1
1:A:130:ILE:HA	1:A:133:ILE:HD12	0.47	1.86	17	1
1:A:48:VAL:HB	1:A:54:VAL:HG11	0.47	1.87	9	1
1:A:77:VAL:HG22	1:A:86:VAL:HG13	0.46	1.86	12	3
1:A:151:VAL:HA	1:A:168:VAL:O	0.46	2.10	17	2
1:A:145:GLY:O	1:A:146:LYS:HG2	0.46	2.10	4	1
1:A:43:LEU:HA	1:A:46:MET:HE3	0.46	1.88	5	1
1:A:30:HIS:O	1:A:85:LEU:HA	0.46	2.11	5	1
1:A:43:LEU:HD22	1:A:49:ARG:HD2	0.46	1.87	13	2
1:A:72:PHE:CD1	1:A:88:VAL:HG21	0.45	2.47	15	1
1:A:32:GLU:HG3	1:A:85:LEU:HD11	0.45	1.87	3	1
1:A:73:GLU:HG2	1:A:89:LYS:HD2	0.45	1.88	15	1
1:A:115:GLU:HG2	1:A:120:ARG:HB2	0.45	1.89	14	1
1:A:46:MET:HE2	1:A:66:LEU:HD11	0.44	1.90	15	1
1:A:100:SER:OG	1:A:166:LYS:HE3	0.44	2.12	1	1
1:A:40:GLY:O	1:A:44:LEU:HG	0.44	2.12	2	1
1:A:117:SER:HB2	1:A:133:ILE:HG12	0.44	1.89	5	1
1:A:77:VAL:O	1:A:78:LEU:HD13	0.43	2.13	20	1
1:A:99:PHE:HD1	1:A:107:ASP:HB2	0.43	1.73	17	2
1:A:127:ARG:HA	1:A:130:ILE:HG12	0.43	1.90	12	2
1:A:106:LYS:O	1:A:110:LEU:HG	0.43	2.13	13	1
1:A:102:ASN:HA	1:A:141:TYR:OH	0.43	2.14	8	1
1:A:98:THR:HB	1:A:166:LYS:HE3	0.43	1.91	11	1
1:A:158:LEU:HD12	1:A:160:ARG:HB2	0.43	1.91	13	1
1:A:119:VAL:HG21	1:A:133:ILE:HD11	0.42	1.91	17	1
1:A:134:GLU:O	1:A:138:GLU:HG2	0.42	2.13	4	1
1:A:102:ASN:HB2	1:A:105:VAL:O	0.42	2.14	11	2
1:A:157:PRO:HA	1:A:163:VAL:HG12	0.42	1.91	9	1
1:A:48:VAL:HG23	1:A:52:ASP:HB3	0.42	1.91	10	1
1:A:73:GLU:O	1:A:126:ASP:HB2	0.42	2.13	20	1
1:A:49:ARG:O	1:A:52:ASP:HB2	0.42	2.15	6	2
1:A:158:LEU:HG	1:A:162:ARG:O	0.42	2.14	5	3
1:A:32:GLU:O	1:A:87:GLN:HA	0.42	2.15	5	1
1:A:160:ARG:HA	1:A:160:ARG:HD2	0.42	1.63	10	1
1:A:127:ARG:HD3	1:A:128:THR:HG23	0.42	1.91	14	1
1:A:140:PHE:O	1:A:144:VAL:HG23	0.42	2.14	4	2
1:A:123:GLU:HG3	1:A:124:SER:N	0.42	2.30	13	1
1:A:137:LEU:HD22	1:A:169:PHE:HZ	0.42	1.75	5	1
1:A:126:ASP:HA	1:A:127:ARG:NH1	0.42	2.30	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:LYS:HA	1:A:103:LYS:HD2	0.42	1.67	10	1
1:A:103:LYS:H	1:A:103:LYS:CD	0.41	2.27	8	1
1:A:27:LYS:HB2	1:A:82:ASP:HB3	0.41	1.93	5	1
1:A:144:VAL:HG13	1:A:145:GLY:H	0.41	1.74	11	1
1:A:74:ASP:HB3	1:A:89:LYS:HB3	0.41	1.92	3	1
1:A:73:GLU:H	1:A:73:GLU:HG3	0.41	1.55	19	1
1:A:97:ILE:HG21	1:A:114:LEU:CD1	0.41	2.46	10	1
1:A:98:THR:HB	1:A:166:LYS:HD3	0.41	1.93	10	1
1:A:73:GLU:OE1	1:A:89:LYS:HE2	0.41	2.16	19	1
1:A:120:ARG:HG3	1:A:123:GLU:HB2	0.41	1.92	5	1
1:A:99:PHE:HE2	1:A:167:LEU:HD13	0.41	1.76	19	1
1:A:29:ILE:HD12	1:A:43:LEU:HD21	0.40	1.92	5	1
1:A:94:ILE:CD1	1:A:125:LEU:HB2	0.40	2.47	14	1
1:A:149:ALA:HA	1:A:170:GLN:O	0.40	2.16	11	1
1:A:104:SER:HB2	1:A:141:TYR:CE1	0.40	2.52	20	1
1:A:94:ILE:CD1	1:A:119:VAL:HG12	0.40	2.46	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	142/164 (87%)	136±2 (96±1%)	4±2 (3±1%)	2±1 (1±1%)	11	58
All	All	2840/3280 (87%)	2728 (96%)	73 (3%)	39 (1%)	11	58

All 7 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	144	VAL	19
1	A	160	ARG	9
1	A	161	ASN	4
1	A	33	GLY	3
1	A	148	SER	2
1	A	159	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	101	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	121/139 (87%)	77±4 (64±4%)	44±4 (36±4%)	1 8
All	All	2420/2780 (87%)	1537 (64%)	883 (36%)	1 8

All 97 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	59	ILE	20
1	A	67	PHE	20
1	A	83	THR	20
1	A	125	LEU	20
1	A	158	LEU	20
1	A	84	LEU	19
1	A	98	THR	19
1	A	148	SER	19
1	A	53	THR	18
1	A	96	SER	18
1	A	119	VAL	17
1	A	45	SER	16
1	A	123	GLU	16
1	A	135	LYS	16
1	A	163	VAL	16
1	A	30	HIS	15
1	A	97	ILE	15
1	A	100	SER	15
1	A	160	ARG	15
1	A	110	LEU	15
1	A	155	VAL	15
1	A	124	SER	14
1	A	127	ARG	14
1	A	150	SER	14

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Mol	Chain	Res	Type	Models (Total)
1	A	120	ARG	14
1	A	102	ASN	13
1	A	107	ASP	13
1	A	111	LYS	13
1	A	114	LEU	13
1	A	152	LYS	13
1	A	27	LYS	12
1	A	32	GLU	12
1	A	112	GLN	12
1	A	146	LYS	12
1	A	170	GLN	12
1	A	141	TYR	12
1	A	72	PHE	12
1	A	76	ARG	11
1	A	82	ASP	11
1	A	48	VAL	11
1	A	89	LYS	11
1	A	79	ARG	11
1	A	104	SER	11
1	A	166	LYS	11
1	A	129	THR	11
1	A	142	TYR	11
1	A	60	SER	10
1	A	109	MET	10
1	A	106	LYS	9
1	A	115	GLU	9
1	A	73	GLU	9
1	A	108	ASP	9
1	A	64	ARG	8
1	A	78	LEU	8
1	A	103	LYS	8
1	A	61	ASN	8
1	A	39	VAL	8
1	A	26	VAL	7
1	A	49	ARG	7
1	A	54	VAL	7
1	A	56	ASP	7
1	A	57	GLU	7
1	A	43	LEU	5
1	A	132	ASP	5
1	A	162	ARG	5
1	A	164	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	71	ASN	4
1	A	85	LEU	4
1	A	143	SER	4
1	A	139	ASP	4
1	A	167	LEU	3
1	A	52	ASP	3
1	A	140	PHE	3
1	A	117	SER	3
1	A	168	VAL	3
1	A	144	VAL	3
1	A	138	GLU	3
1	A	88	VAL	2
1	A	137	LEU	2
1	A	50	THR	2
1	A	55	ASN	2
1	A	80	ASP	2
1	A	113	ASN	2
1	A	63	ILE	2
1	A	105	VAL	1
1	A	133	ILE	1
1	A	62	THR	1
1	A	31	PHE	1
1	A	25	VAL	1
1	A	165	LEU	1
1	A	77	VAL	1
1	A	28	ASP	1
1	A	58	ASP	1
1	A	128	THR	1
1	A	46	MET	1
1	A	87	GLN	1
1	A	44	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [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 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

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	1906
Number of shifts mapped to atoms	1888
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 18 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	175	LEU	H	8.337	0.006	1
1	A	175	LEU	HA	4.35	0.005	1
1	A	175	LEU	HB2	1.546	0.012	2
1	A	175	LEU	HB3	1.543	0.012	2
1	A	175	LEU	HD11	0.843	0.011	2
1	A	175	LEU	HD12	0.843	0.011	2
1	A	175	LEU	HD13	0.843	0.011	2
1	A	175	LEU	HD21	0.839	0.010	2
1	A	175	LEU	HD22	0.839	0.010	2
1	A	175	LEU	HD23	0.839	0.010	2
1	A	175	LEU	HG	1.558	0.007	1
1	A	175	LEU	C	176.39	0.000	1
1	A	175	LEU	CA	55.201	0.035	1
1	A	175	LEU	CB	42.348	0.036	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	175	LEU	CD1	25.118	0.006	2
1	A	175	LEU	CD2	23.351	0.030	2
1	A	175	LEU	CG	27.057	0.014	1
1	A	175	LEU	N	125.032	0.014	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	154	-0.31 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	141	-0.11 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	150	-0.23 ± 0.14	None needed (< 0.5 ppm)
^{15}N	149	-0.34 ± 0.35	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 92%, i.e. 1764 atoms were assigned a chemical shift out of a possible 1911. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	710/713 (100%)	291/291 (100%)	281/284 (99%)	138/138 (100%)
Sidechain	970/1093 (89%)	664/712 (93%)	297/339 (88%)	9/42 (21%)
Aromatic	84/105 (80%)	42/51 (82%)	42/52 (81%)	0/2 (0%)
Overall	1764/1911 (92%)	997/1054 (95%)	620/675 (92%)	147/182 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1888 atoms were assigned a chemical shift out of a possible 2079. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	762/774 (98%)	312/316 (99%)	302/308 (98%)	148/150 (99%)
Sidechain	1042/1200 (87%)	713/780 (91%)	319/371 (86%)	10/49 (20%)
Aromatic	84/105 (80%)	42/51 (82%)	42/52 (81%)	0/2 (0%)
Overall	1888/2079 (91%)	1067/1147 (93%)	663/731 (91%)	158/201 (79%)

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	71	ASN	HB3	0.84	1.12 – 4.38	-5.9
1	A	36	ARG	H	11.50	5.25 – 11.22	5.5
1	A	90	GLU	HB2	3.12	1.00 – 3.05	5.3
1	A	90	GLU	HB3	3.10	0.95 – 3.05	5.3

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:

