



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 06:29 PM UTC

PDB ID : 2M6L / pdb_00002m6l
BMRB ID : 19143
Title : Solution structure of the Escherichia coli holo ferric enterobactin binding protein
Authors : Chu, B.C.H.; Otten, R.; Krewulak, K.D.; Mulder, F.A.A.; Vogel, H.J.
Deposited on : 2013-04-05

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

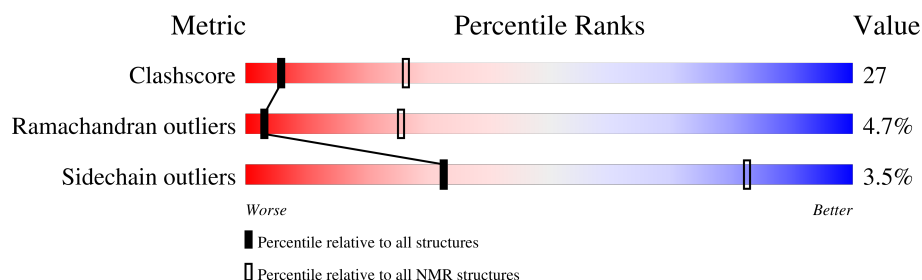
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 35%.

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	315	

2 Ensemble composition and analysis

This entry contains 30 models. Model 12 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:24-A:315 (292)	0.10	12

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 6 single-model clusters were found.

Cluster number	Models
1	1, 6, 8, 9, 10, 12, 18, 19, 23, 24, 27, 29
2	5, 11, 16, 21, 26
3	2, 17, 20, 25
4	13, 14, 15
Single-model clusters	3; 4; 7; 22; 28; 30

3 Entry composition

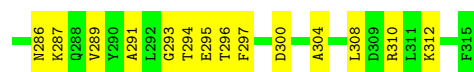
There is only 1 type of molecule in this entry. The entry contains 4462 atoms, of which 2235 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ferrienterobactin-binding periplasmic protein.

Mol	Chain	Residues	Atoms						Trace
1	A	292	Total	C	H	N	O	S	0
			4462	1405	2235	386	433	3	

There are 23 discrepancies between the modelled and reference sequences:

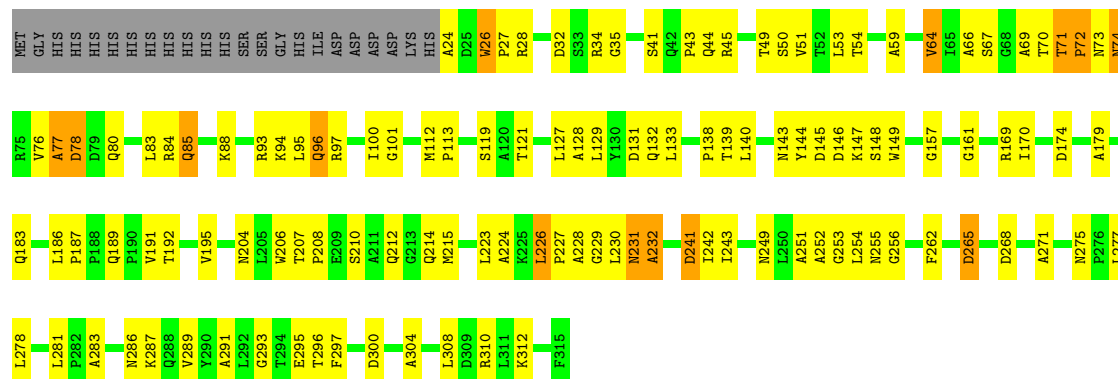
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0AEL6
A	2	GLY	-	expression tag	UNP P0AEL6
A	3	HIS	-	expression tag	UNP P0AEL6
A	4	HIS	-	expression tag	UNP P0AEL6
A	5	HIS	-	expression tag	UNP P0AEL6
A	6	HIS	-	expression tag	UNP P0AEL6
A	7	HIS	-	expression tag	UNP P0AEL6
A	8	HIS	-	expression tag	UNP P0AEL6
A	9	HIS	-	expression tag	UNP P0AEL6
A	10	HIS	-	expression tag	UNP P0AEL6
A	11	HIS	-	expression tag	UNP P0AEL6
A	12	HIS	-	expression tag	UNP P0AEL6
A	13	SER	-	expression tag	UNP P0AEL6
A	14	SER	-	expression tag	UNP P0AEL6
A	15	GLY	-	expression tag	UNP P0AEL6
A	16	HIS	-	expression tag	UNP P0AEL6
A	17	ILE	-	expression tag	UNP P0AEL6
A	18	ASP	-	expression tag	UNP P0AEL6
A	19	ASP	-	expression tag	UNP P0AEL6
A	20	ASP	-	expression tag	UNP P0AEL6
A	21	ASP	-	expression tag	UNP P0AEL6
A	22	LYS	-	expression tag	UNP P0AEL6
A	23	HIS	-	expression tag	UNP P0AEL6



4.2.2 Score per residue for model 2

- Molecule 1: Ferrienterobactin-binding periplasmic protein

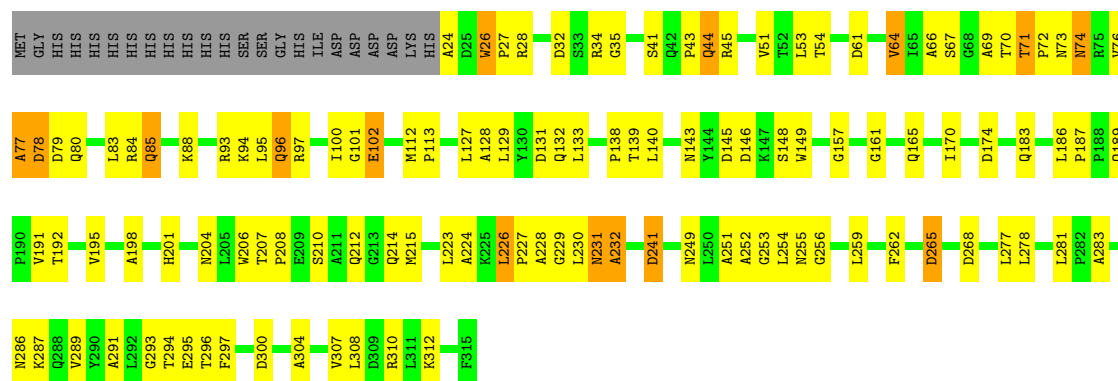
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Ferrienterobactin-binding periplasmic protein

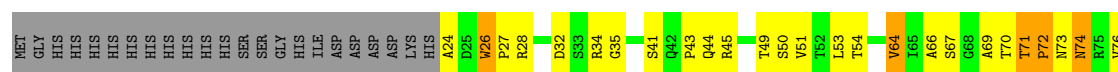
Chain A:

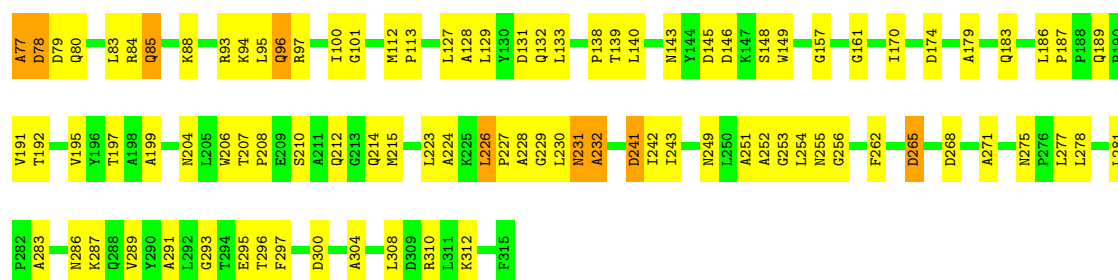


4.2.4 Score per residue for model 4

- Molecule 1: Ferrienterobactin-binding periplasmic protein

Chain A:

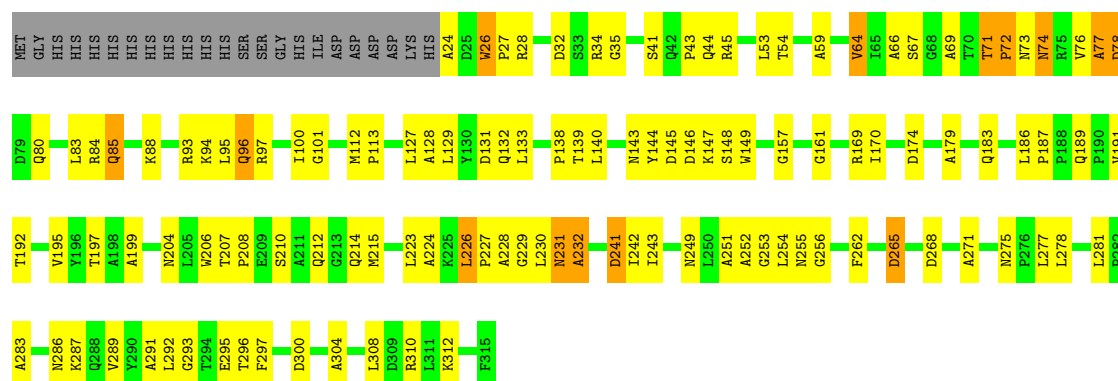




4.2.5 Score per residue for model 5

- Molecule 1: Ferrienterobactin-binding periplasmic protein

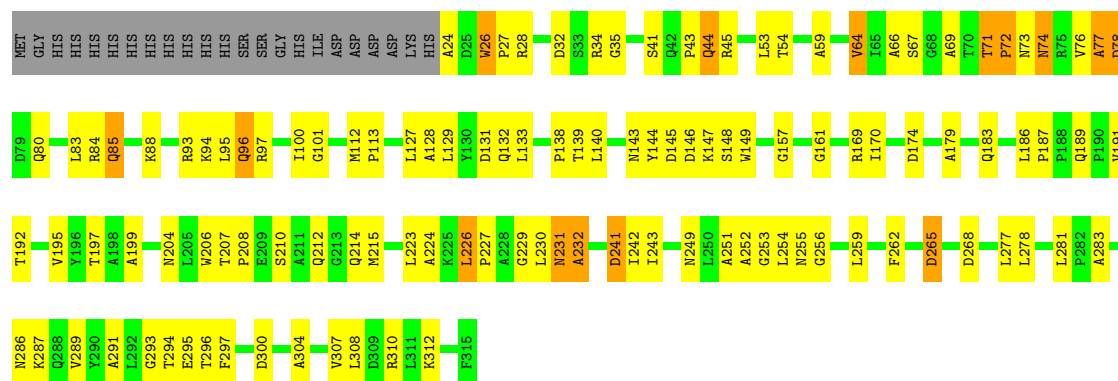
Chain A: 55% 34% 7%

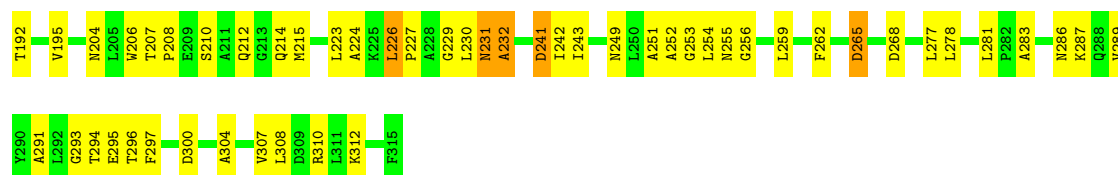


4.2.6 Score per residue for model 6

- Molecule 1: Ferrienterobactin-binding periplasmic protein

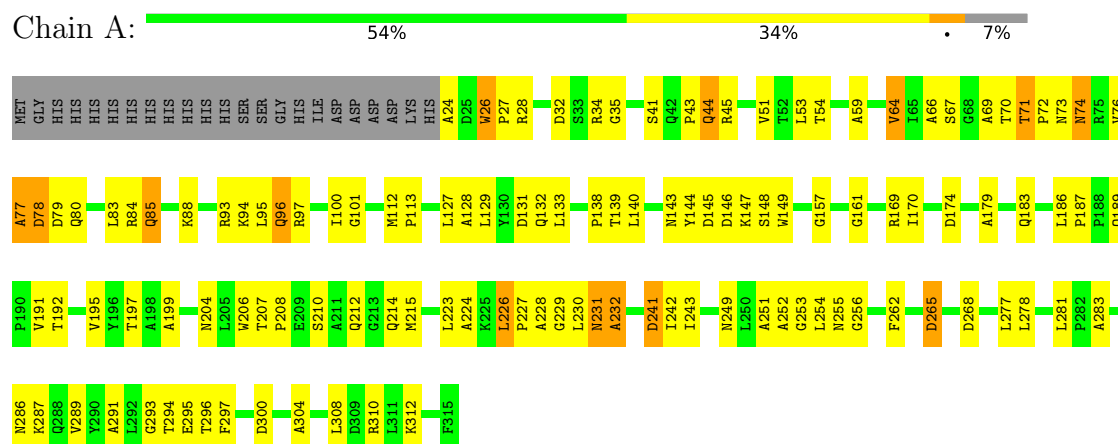
Chain A: 55% 33% 5% 7%





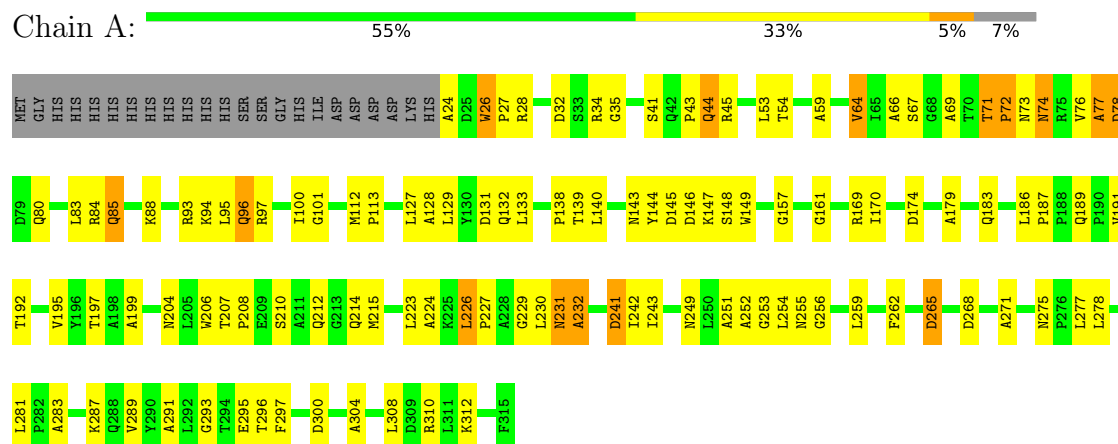
4.2.10 Score per residue for model 10

- Molecule 1: Ferrienterobactin-binding periplasmic protein



4.2.11 Score per residue for model 11

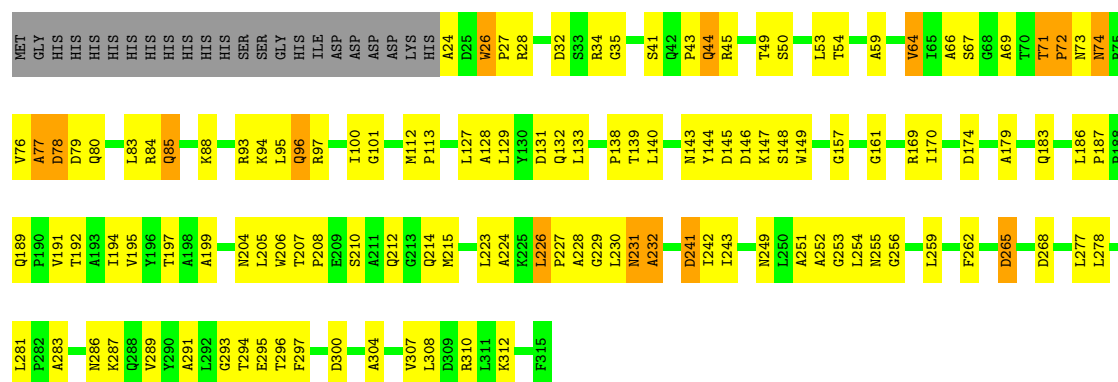
- Molecule 1: Ferrienterobactin-binding periplasmic protein



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Ferrienterobactin-binding periplasmic protein

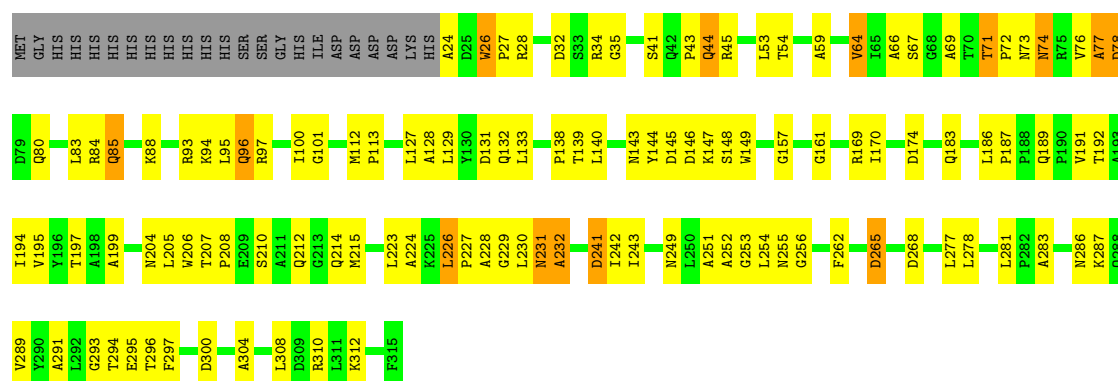




4.2.13 Score per residue for model 13

- Molecule 1: Ferrienterobactin-binding periplasmic protein

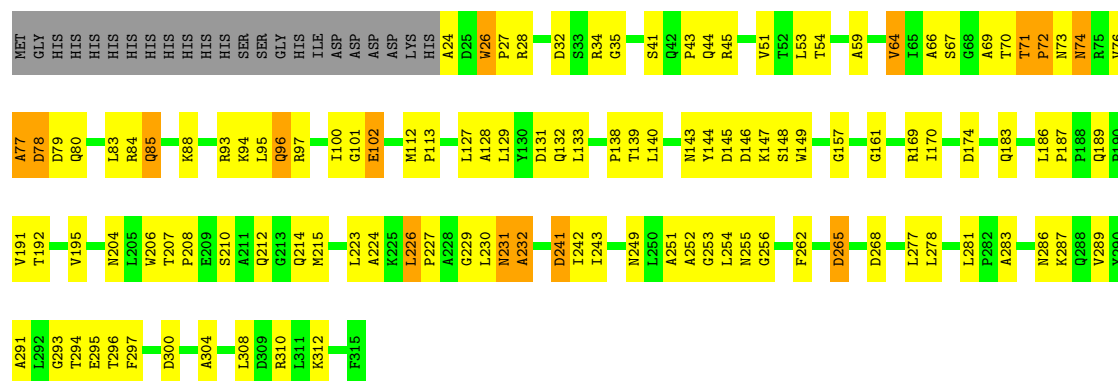
Chain A: 55% 33% 7%



4.2.14 Score per residue for model 14

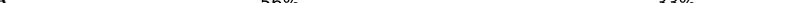
- Molecule 1: Ferrienterobactin-binding periplasmic protein

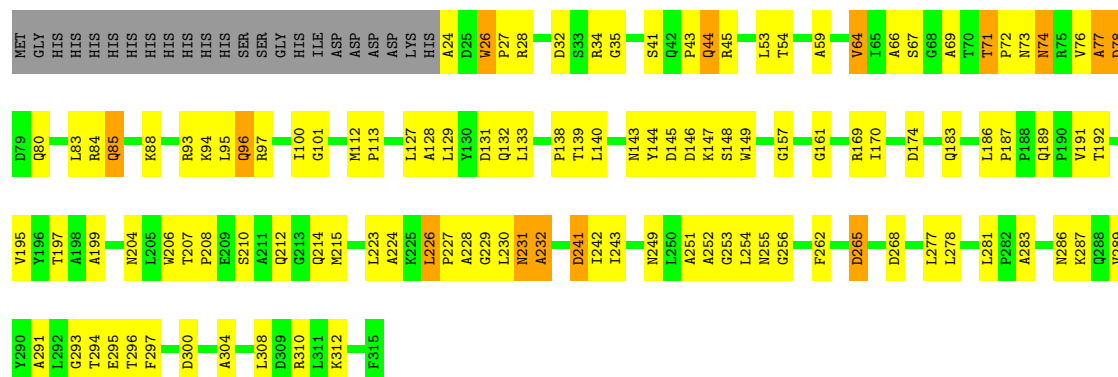
Chain A: 55% 33% 5% 7%



4.2.15 Score per residue for model 15

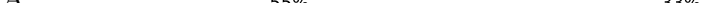
- Molecule 1: Ferrienterobactin-binding periplasmic protein

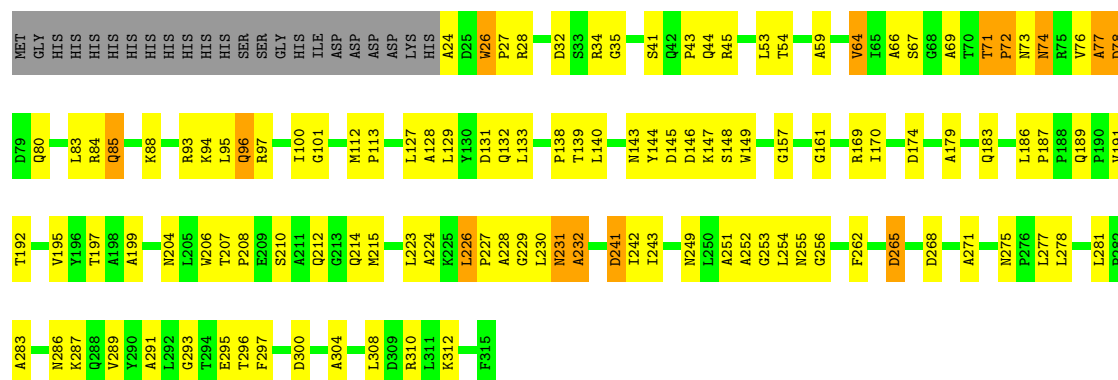
Chain A:  56% 33% 7%



4.2.16 Score per residue for model 16

- Molecule 1: Ferrienterobactin-binding periplasmic protein

Chain A:  55% 33% 7%

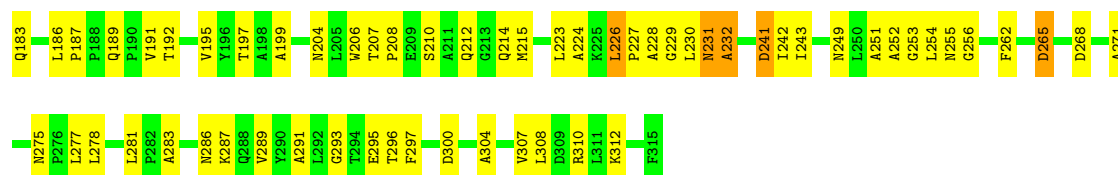


4.2.17 Score per residue for model 17

- Molecule 1: Ferrienterobactin-binding periplasmic protein

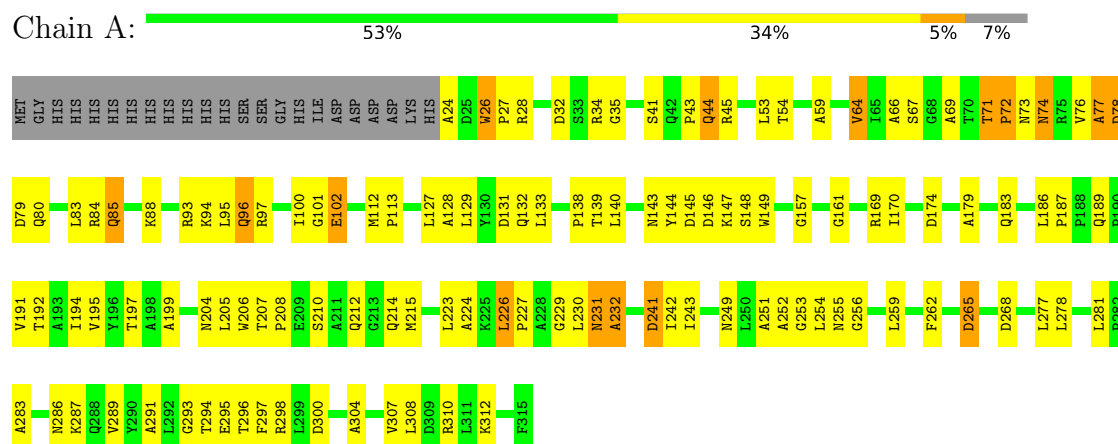
Chain A: 53% 35% 5% 7%





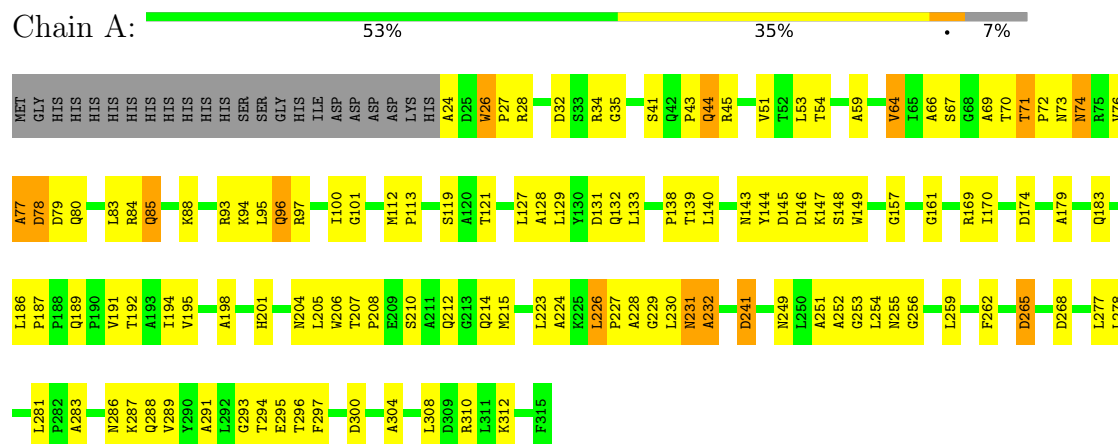
4.2.18 Score per residue for model 18

- Molecule 1: Ferrienterobactin-binding periplasmic protein



4.2.19 Score per residue for model 19

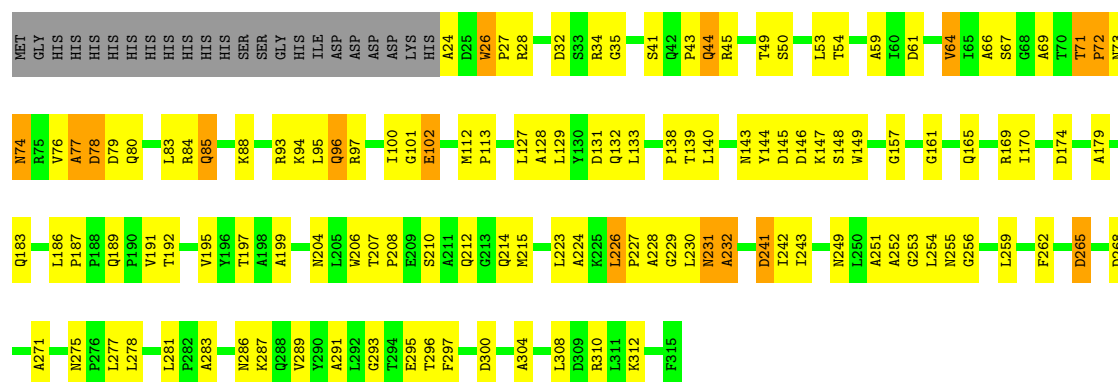
- Molecule 1: Ferrienterobactin-binding periplasmic protein



4.2.20 Score per residue for model 20

- Molecule 1: Ferrienterobactin-binding periplasmic protein

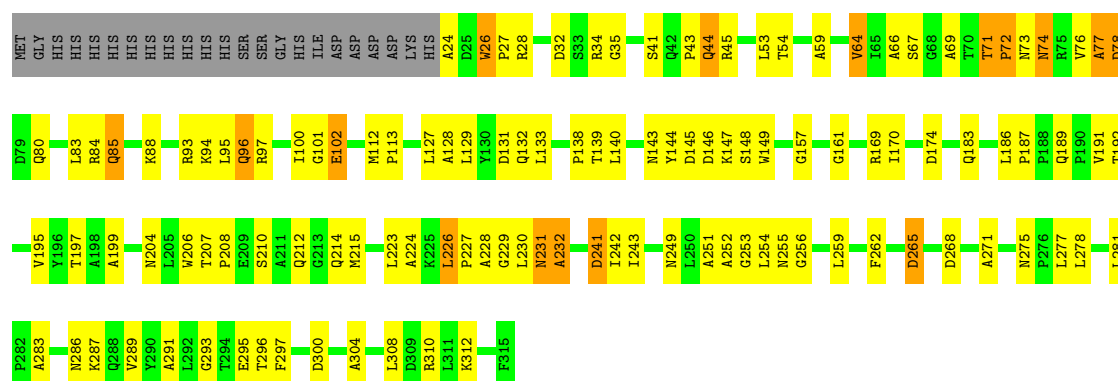




4.2.21 Score per residue for model 21

- Molecule 1: Ferrienterobactin-binding periplasmic protein

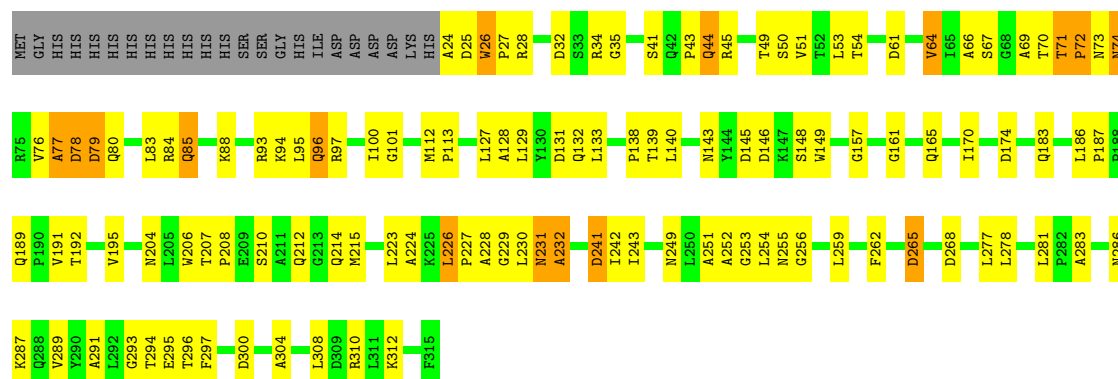
Chain A: 



4.2.22 Score per residue for model 22

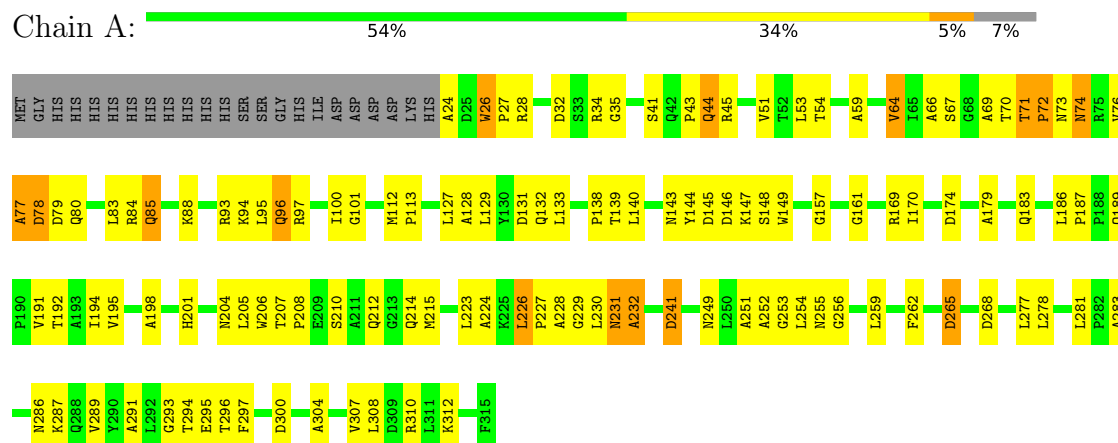
- Molecule 1: Ferrienterobactin-binding periplasmic protein

Chain A: 



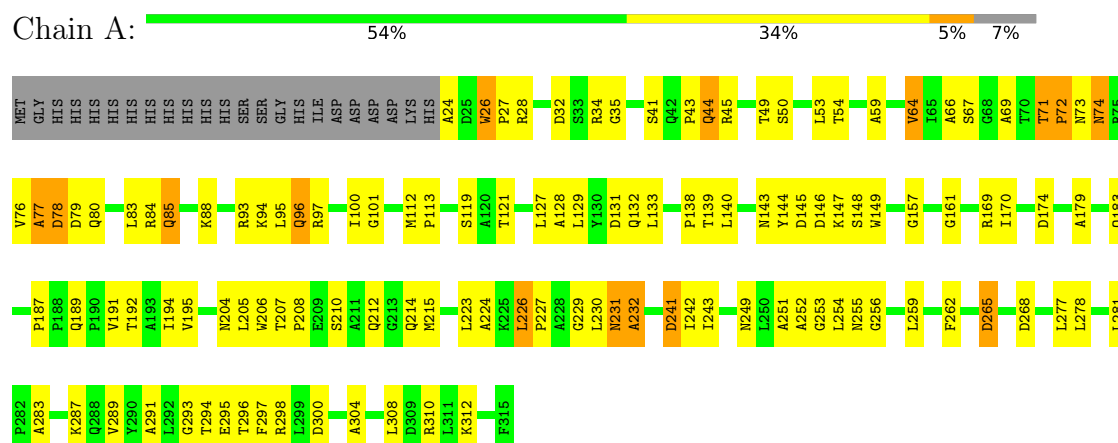
4.2.23 Score per residue for model 23

- Molecule 1: Ferrienterobactin-binding periplasmic protein



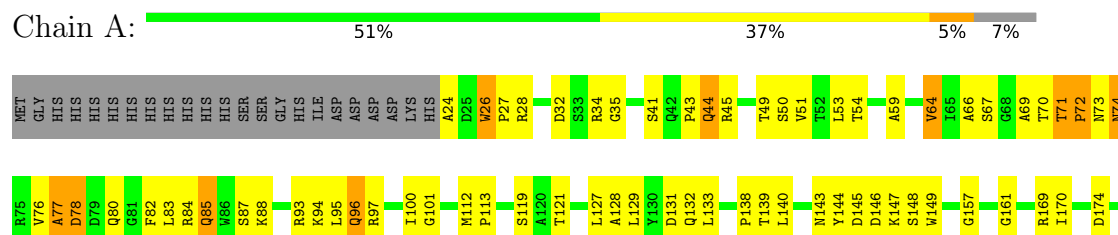
4.2.24 Score per residue for model 24

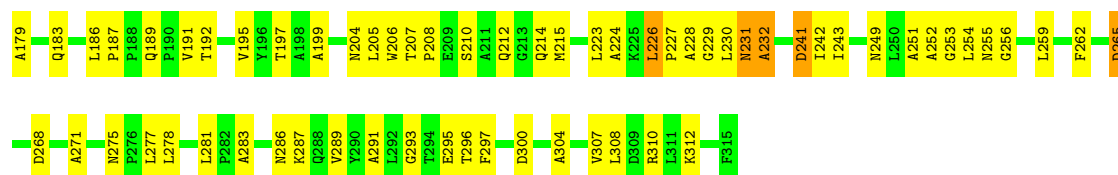
- Molecule 1: Ferrienterobactin-binding periplasmic protein



4.2.25 Score per residue for model 25

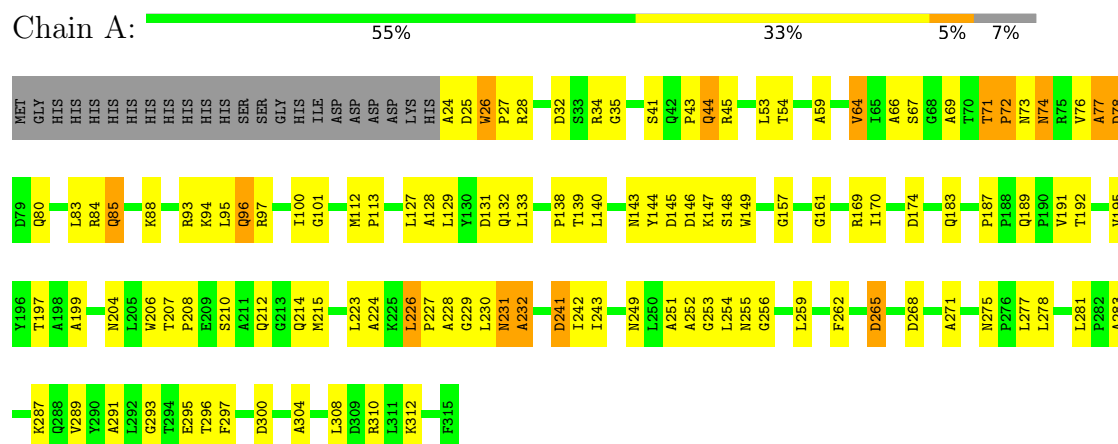
- Molecule 1: Ferrienterobactin-binding periplasmic protein





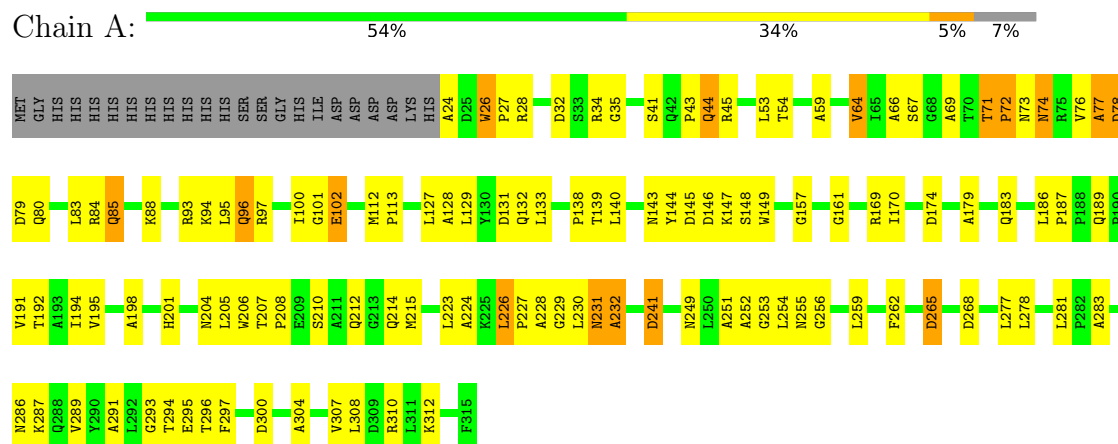
4.2.26 Score per residue for model 26

- Molecule 1: Ferrienterobactin-binding periplasmic protein



4.2.27 Score per residue for model 27

- Molecule 1: Ferrienterobactin-binding periplasmic protein



4.2.28 Score per residue for model 28

- Molecule 1: Ferrienterobactin-binding periplasmic protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 30 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
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1393
Number of shifts mapped to atoms	1349
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

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	2227	2235	2229	119±3
All	All	66810	67050	66870	3578

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:LEU:N	1:A:226:LEU:HD12	0.82	1.89	3	30
1:A:226:LEU:HD12	1:A:226:LEU:H	0.71	1.46	22	30
1:A:296:THR:O	1:A:296:THR:HG22	0.69	1.86	30	30
1:A:95:LEU:O	1:A:96:GLN:CB	0.69	2.41	26	30
1:A:43:PRO:O	1:A:45:ARG:N	0.66	2.28	30	30
1:A:227:PRO:C	1:A:229:GLY:H	0.64	2.00	27	30
1:A:128:ALA:O	1:A:131:ASP:OD1	0.64	2.16	26	30
1:A:183:GLN:NE2	1:A:312:LYS:NZ	0.64	2.46	30	30
1:A:212:GLN:NE2	1:A:297:PHE:CD1	0.62	2.67	15	30
1:A:24:ALA:N	1:A:28:ARG:NH1	0.62	2.48	10	30
1:A:226:LEU:N	1:A:226:LEU:CD1	0.61	2.62	28	30
1:A:183:GLN:NE2	1:A:312:LYS:HZ2	0.60	1.94	5	27
1:A:139:THR:C	1:A:140:LEU:HD12	0.60	2.21	6	30
1:A:149:TRP:CD1	1:A:215:MET:SD	0.60	2.94	30	30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ALA:O	1:A:100:ILE:HD12	0.60	1.97	4	30
1:A:145:ASP:OD1	1:A:146:ASP:N	0.59	2.35	4	30
1:A:149:TRP:CG	1:A:215:MET:SD	0.59	2.95	3	30
1:A:149:TRP:CD2	1:A:215:MET:SD	0.59	2.95	8	24
1:A:73:ASN:O	1:A:74:ASN:CB	0.58	2.52	21	30
1:A:149:TRP:CE2	1:A:215:MET:SD	0.58	2.97	6	24
1:A:223:LEU:HD22	1:A:223:LEU:N	0.57	2.11	30	1
1:A:100:ILE:HG22	1:A:101:GLY:N	0.57	2.14	18	30
1:A:85:GLN:NE2	1:A:88:LYS:NZ	0.57	2.53	10	30
1:A:223:LEU:CD2	1:A:223:LEU:N	0.57	2.68	20	29
1:A:223:LEU:N	1:A:223:LEU:CD2	0.57	2.67	30	1
1:A:84:ARG:O	1:A:85:GLN:CB	0.56	2.52	21	30
1:A:93:ARG:O	1:A:94:LYS:HB2	0.56	2.00	26	30
1:A:227:PRO:O	1:A:229:GLY:N	0.56	2.38	27	30
1:A:157:GLY:O	1:A:161:GLY:N	0.55	2.39	22	30
1:A:189:GLN:N	1:A:189:GLN:OE1	0.55	2.40	8	30
1:A:71:THR:O	1:A:73:ASN:N	0.55	2.40	21	30
1:A:223:LEU:N	1:A:223:LEU:HD22	0.55	2.17	24	29
1:A:183:GLN:NE2	1:A:312:LYS:HZ1	0.55	2.00	25	24
1:A:131:ASP:OD1	1:A:132:GLN:N	0.55	2.40	24	30
1:A:143:ASN:ND2	1:A:145:ASP:OD1	0.54	2.40	22	30
1:A:67:SER:O	1:A:97:ARG:O	0.54	2.25	18	30
1:A:191:VAL:HG22	1:A:192:THR:N	0.54	2.18	6	30
1:A:278:LEU:HD12	1:A:278:LEU:N	0.54	2.18	30	30
1:A:283:ALA:O	1:A:287:LYS:N	0.54	2.41	19	30
1:A:189:GLN:O	1:A:189:GLN:NE2	0.53	2.41	21	30
1:A:83:LEU:CD1	1:A:83:LEU:N	0.53	2.71	20	30
1:A:227:PRO:C	1:A:229:GLY:N	0.53	2.66	27	30
1:A:191:VAL:CG2	1:A:192:THR:N	0.53	2.72	3	30
1:A:230:LEU:C	1:A:232:ALA:H	0.53	2.11	30	30
1:A:100:ILE:CG2	1:A:101:GLY:N	0.53	2.72	8	30
1:A:83:LEU:N	1:A:83:LEU:HD12	0.53	2.18	13	30
1:A:74:ASN:ND2	1:A:294:THR:OG1	0.52	2.43	22	18
1:A:143:ASN:ND2	1:A:146:ASP:CG	0.52	2.67	8	26
1:A:226:LEU:HD23	1:A:249:ASN:ND2	0.52	2.19	30	30
1:A:198:ALA:O	1:A:201:HIS:CE1	0.52	2.62	19	7
1:A:170:ILE:O	1:A:174:ASP:N	0.52	2.42	22	30
1:A:230:LEU:O	1:A:232:ALA:N	0.52	2.43	19	30
1:A:73:ASN:O	1:A:73:ASN:OD1	0.52	2.28	17	30
1:A:102:GLU:N	1:A:102:GLU:CD	0.52	2.67	18	7
1:A:277:LEU:CD2	1:A:277:LEU:N	0.52	2.73	21	30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:254:LEU:HD12	1:A:254:LEU:N	0.52	2.19	24	30
1:A:212:GLN:NE2	1:A:297:PHE:O	0.51	2.42	4	14
1:A:149:TRP:N	1:A:214:GLN:OE1	0.51	2.43	30	6
1:A:189:GLN:N	1:A:189:GLN:CD	0.51	2.68	3	30
1:A:85:GLN:NE2	1:A:88:LYS:HZ1	0.51	2.03	13	28
1:A:291:ALA:O	1:A:310:ARG:CZ	0.51	2.59	1	30
1:A:76:VAL:O	1:A:77:ALA:O	0.51	2.28	29	30
1:A:78:ASP:C	1:A:80:GLN:N	0.51	2.68	8	30
1:A:277:LEU:N	1:A:277:LEU:HD22	0.50	2.20	4	30
1:A:265:ASP:OD1	1:A:310:ARG:NH2	0.50	2.45	28	30
1:A:296:THR:O	1:A:296:THR:CG2	0.50	2.59	26	30
1:A:71:THR:CB	1:A:72:PRO:CD	0.50	2.90	26	30
1:A:26:TRP:CB	1:A:27:PRO:CD	0.49	2.90	26	30
1:A:195:VAL:O	1:A:204:ASN:O	0.49	2.30	19	30
1:A:73:ASN:O	1:A:74:ASN:ND2	0.49	2.45	27	30
1:A:32:ASP:OD1	1:A:34:ARG:N	0.49	2.45	7	30
1:A:64:VAL:CG2	1:A:66:ALA:O	0.49	2.60	30	30
1:A:252:ALA:O	1:A:253:GLY:C	0.49	2.53	26	30
1:A:32:ASP:OD1	1:A:32:ASP:C	0.49	2.54	22	7
1:A:32:ASP:C	1:A:32:ASP:OD1	0.49	2.55	24	23
1:A:262:PHE:CE1	1:A:293:GLY:O	0.48	2.66	30	30
1:A:206:TRP:NE1	1:A:210:SER:OG	0.48	2.45	4	30
1:A:78:ASP:C	1:A:80:GLN:H	0.48	2.16	22	30
1:A:127:LEU:HD12	1:A:127:LEU:N	0.48	2.24	22	30
1:A:143:ASN:CG	1:A:145:ASP:OD1	0.47	2.57	30	30
1:A:59:ALA:HB1	1:A:169:ARG:NH1	0.47	2.24	30	27
1:A:224:ALA:CB	1:A:255:ASN:OD1	0.47	2.62	3	30
1:A:32:ASP:OD1	1:A:35:GLY:O	0.47	2.32	4	30
1:A:73:ASN:O	1:A:74:ASN:HB2	0.47	2.09	21	30
1:A:157:GLY:O	1:A:161:GLY:CA	0.47	2.63	24	30
1:A:148:SER:C	1:A:214:GLN:OE1	0.47	2.58	30	30
1:A:82:PHE:CZ	1:A:87:SER:OG	0.47	2.65	25	1
1:A:208:PRO:C	1:A:210:SER:N	0.46	2.73	13	30
1:A:295:GLU:C	1:A:297:PHE:H	0.46	2.18	30	30
1:A:187:PRO:O	1:A:189:GLN:OE1	0.46	2.33	21	30
1:A:300:ASP:O	1:A:304:ALA:CB	0.46	2.63	14	30
1:A:93:ARG:O	1:A:94:LYS:CB	0.46	2.63	22	30
1:A:292:LEU:O	1:A:296:THR:OG1	0.46	2.32	5	1
1:A:224:ALA:HB2	1:A:255:ASN:OD1	0.46	2.10	22	29
1:A:230:LEU:C	1:A:232:ALA:N	0.45	2.74	30	30
1:A:78:ASP:O	1:A:80:GLN:N	0.45	2.49	22	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LYS:O	1:A:214:GLN:OE1	0.45	2.34	18	22
1:A:253:GLY:O	1:A:254:LEU:C	0.45	2.59	7	30
1:A:183:GLN:HE21	1:A:312:LYS:HZ1	0.45	1.54	17	3
1:A:140:LEU:HD12	1:A:140:LEU:N	0.45	2.27	29	30
1:A:51:VAL:HG21	1:A:70:THR:HG23	0.45	1.89	22	13
1:A:129:LEU:O	1:A:133:LEU:N	0.45	2.42	6	30
1:A:286:ASN:OD1	1:A:286:ASN:O	0.45	2.34	4	24
1:A:102:GLU:O	1:A:102:GLU:CD	0.45	2.60	27	2
1:A:143:ASN:HD22	1:A:146:ASP:CG	0.45	2.20	30	2
1:A:304:ALA:O	1:A:308:LEU:CB	0.44	2.65	21	30
1:A:95:LEU:O	1:A:96:GLN:HB3	0.44	2.12	26	19
1:A:251:ALA:C	1:A:253:GLY:H	0.44	2.21	3	30
1:A:144:TYR:O	1:A:147:LYS:O	0.44	2.36	8	25
1:A:231:ASN:O	1:A:232:ALA:C	0.44	2.60	6	30
1:A:253:GLY:O	1:A:256:GLY:N	0.44	2.51	7	30
1:A:78:ASP:C	1:A:78:ASP:OD1	0.44	2.60	18	30
1:A:179:ALA:O	1:A:183:GLN:N	0.44	2.49	30	23
1:A:278:LEU:N	1:A:278:LEU:CD1	0.44	2.81	24	30
1:A:73:ASN:O	1:A:74:ASN:CG	0.43	2.61	21	24
1:A:297:PHE:CE2	1:A:298:ARG:CZ	0.43	3.01	18	2
1:A:32:ASP:CG	1:A:35:GLY:O	0.43	2.61	1	30
1:A:170:ILE:O	1:A:174:ASP:CG	0.43	2.62	26	26
1:A:144:TYR:O	1:A:214:GLN:NE2	0.43	2.49	15	11
1:A:73:ASN:C	1:A:74:ASN:CG	0.42	2.85	24	30
1:A:119:SER:OG	1:A:121:THR:O	0.42	2.37	19	8
1:A:143:ASN:OD1	1:A:145:ASP:OD1	0.42	2.37	12	19
1:A:127:LEU:N	1:A:127:LEU:CD1	0.42	2.83	22	30
1:A:271:ALA:O	1:A:275:ASN:CG	0.42	2.63	16	11
1:A:53:LEU:O	1:A:54:THR:C	0.42	2.63	8	30
1:A:49:THR:OG1	1:A:50:SER:N	0.42	2.52	2	9
1:A:76:VAL:C	1:A:77:ALA:O	0.42	2.63	19	15
1:A:268:ASP:OD1	1:A:268:ASP:C	0.42	2.63	23	30
1:A:242:ILE:CG1	1:A:243:ILE:N	0.42	2.82	20	23
1:A:61:ASP:CB	1:A:165:GLN:NE2	0.42	2.83	3	4
1:A:112:MET:N	1:A:113:PRO:CD	0.42	2.82	8	30
1:A:226:LEU:HD13	1:A:230:LEU:HD21	0.42	1.91	29	9
1:A:194:ILE:HG22	1:A:205:LEU:HD12	0.42	1.92	24	10
1:A:189:GLN:O	1:A:189:GLN:CD	0.42	2.63	24	23
1:A:241:ASP:OD1	1:A:241:ASP:C	0.41	2.63	3	30
1:A:131:ASP:OD1	1:A:131:ASP:N	0.41	2.53	1	30
1:A:197:THR:HG22	1:A:199:ALA:H	0.41	1.75	26	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:286:ASN:ND2	1:A:288:GLN:CG	0.41	2.83	19	1
1:A:83:LEU:HD23	1:A:300:ASP:CB	0.41	2.44	19	18
1:A:242:ILE:CG1	1:A:243:ILE:H	0.41	2.28	20	11
1:A:43:PRO:O	1:A:44:GLN:C	0.41	2.64	24	24
1:A:79:ASP:OD1	1:A:79:ASP:N	0.41	2.53	4	15
1:A:300:ASP:O	1:A:304:ALA:N	0.41	2.44	21	18
1:A:259:LEU:C	1:A:259:LEU:HD23	0.41	2.41	21	20
1:A:102:GLU:O	1:A:102:GLU:OE1	0.41	2.38	14	1
1:A:95:LEU:O	1:A:96:GLN:HB2	0.41	2.12	26	3
1:A:149:TRP:NE1	1:A:215:MET:SD	0.41	2.94	24	6
1:A:296:THR:HG23	1:A:307:VAL:HG21	0.41	1.92	29	10
1:A:25:ASP:C	1:A:26:TRP:CD1	0.41	2.99	26	2
1:A:79:ASP:N	1:A:79:ASP:OD1	0.40	2.54	12	2
1:A:205:LEU:HD23	1:A:206:TRP:N	0.40	2.31	25	1
1:A:300:ASP:O	1:A:304:ALA:HB2	0.40	2.17	28	1
1:A:301:TYR:CE2	1:A:305:MET:CE	0.40	3.04	30	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	290/315 (92%)	246±0 (85±0%)	30±1 (10±0%)	14±1 (5±0%)	3	25
All	All	8700/9450 (92%)	7379 (85%)	912 (10%)	409 (5%)	3	25

All 15 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	41	SER	30
1	A	44	GLN	30
1	A	74	ASN	30
1	A	77	ALA	30
1	A	78	ASP	30
1	A	85	GLN	30

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Mol	Chain	Res	Type	Models (Total)
1	A	96	GLN	30
1	A	138	PRO	30
1	A	231	ASN	30
1	A	232	ALA	30
1	A	241	ASP	30
1	A	265	ASP	30
1	A	72	PRO	25
1	A	228	ALA	23
1	A	79	ASP	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	232/253 (92%)	224±1 (96±0%)	8±1 (4±0%)	32	82
All	All	6960/7590 (92%)	6713 (96%)	247 (4%)	32	82

All 9 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	26	TRP	30
1	A	64	VAL	30
1	A	71	THR	30
1	A	207	THR	30
1	A	226	LEU	30
1	A	281	LEU	30
1	A	289	VAL	30
1	A	186	LEU	28
1	A	102	GLU	9

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 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 35% for the well-defined parts and 35% 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	1393
Number of shifts mapped to atoms	1349
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 44 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	SER	H	8.489	.	1
1	A	13	SER	C	174.7	.	1
1	A	13	SER	CA	58.63	.	1
1	A	13	SER	CB	64.52	.	1
1	A	13	SER	N	118.6	.	1
1	A	15	GLY	H	8.391	.	1
1	A	15	GLY	C	173.7	.	1
1	A	15	GLY	CA	45.59	.	1
1	A	15	GLY	N	111.0	.	1
1	A	16	HIS	H	8.201	.	1
1	A	16	HIS	C	174.6	.	1
1	A	16	HIS	CA	55.87	.	1
1	A	16	HIS	CB	29.86	.	1
1	A	16	HIS	N	119.6	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	ILE	H	8.155	.	1
1	A	17	ILE	C	175.8	.	1
1	A	17	ILE	CA	61.48	.	1
1	A	17	ILE	CB	39.23	.	1
1	A	17	ILE	N	123.8	.	1
1	A	18	ASP	H	8.426	.	1
1	A	18	ASP	C	175.9	.	1
1	A	18	ASP	CA	54.64	.	1
1	A	18	ASP	CB	41.45	.	1
1	A	18	ASP	N	124.6	.	1
1	A	19	ASP	H	8.28	.	1
1	A	19	ASP	C	176.3	.	1
1	A	19	ASP	CA	54.9	.	1
1	A	19	ASP	CB	41.32	.	1
1	A	19	ASP	N	120.9	.	1
1	A	20	ASP	H	8.199	.	1
1	A	20	ASP	C	176.6	.	1
1	A	20	ASP	CA	54.79	.	1
1	A	20	ASP	CB	41.1	.	1
1	A	20	ASP	N	120.9	.	1
1	A	22	LYS	H	8.059	.	1
1	A	22	LYS	C	176.8	.	1
1	A	22	LYS	CA	56.67	.	1
1	A	22	LYS	CB	32.71	.	1
1	A	22	LYS	N	121.2	.	1
1	A	23	HIS	H	8.334	.	1
1	A	23	HIS	C	174.8	.	1
1	A	23	HIS	CA	55.92	.	1
1	A	23	HIS	CB	29.08	.	1
1	A	23	HIS	N	119.4	.	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
$^{13}\text{C}_\alpha$	294	-0.43 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	270	0.22 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	287	-0.18 ± 0.10	None needed (< 0.5 ppm)
^{15}N	271	0.41 ± 0.26	None needed (< 0.5 ppm)

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 35%, i.e. 1349 atoms were assigned a chemical shift out of a possible 3895. 0 out of 48 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1087/1451 (75%)	262/589 (44%)	563/584 (96%)	262/278 (94%)
Sidechain	262/2214 (12%)	0/1450 (0%)	262/684 (38%)	0/80 (0%)
Aromatic	0/230 (0%)	0/111 (0%)	0/105 (0%)	0/14 (0%)
Overall	1349/3895 (35%)	262/2150 (12%)	825/1373 (60%)	262/372 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 1349 atoms were assigned a chemical shift out of a possible 3895. 0 out of 48 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1087/1451 (75%)	262/589 (44%)	563/584 (96%)	262/278 (94%)
Sidechain	262/2214 (12%)	0/1450 (0%)	262/684 (38%)	0/80 (0%)
Aromatic	0/230 (0%)	0/111 (0%)	0/105 (0%)	0/14 (0%)
Overall	1349/3895 (35%)	262/2150 (12%)	825/1373 (60%)	262/372 (70%)

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	211	ALA	CB	31.73	10.19 – 27.75	7.3
1	A	44	GLN	H	11.22	5.39 – 11.05	5.3
1	A	104	SER	H	5.43	5.45 – 11.10	-5.0

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:

