Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 06:45 PM EDT

PDB ID	:	2MS3
BMRB ID	:	25102
Title	:	The NMR structure of the rubredoxin domain of the NO Reductase Flavorubredoxin from Escherichia coli
Authors	:	Turner, D.L.; Silva, E.; Lamosa, P.M.; Teixeira, M.
Deposited on	:	2014-07-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

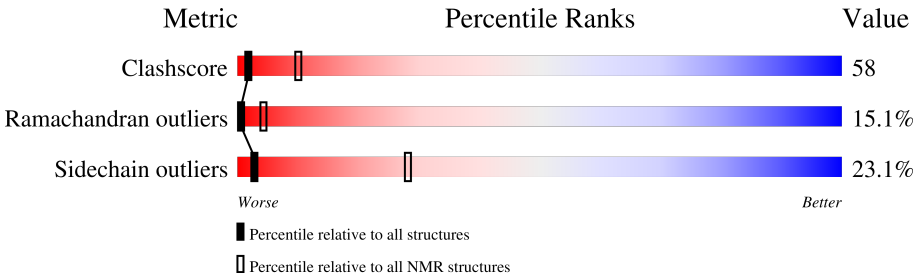
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 60%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	57	19% 53% 19% • 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 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:2-A:54 (53)	0.57	7

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 847 atoms, of which 409 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Anaerobic nitric oxide reductase flavorubredoxin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	57	846	275	409	69	87	6	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 19% 53% 19% • 7%

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: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 33% 46% 12% • 7%

4.2.2 Score per residue for model 2

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 23% 47% 21% • 7%

4.2.3 Score per residue for model 3

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 18% 49% 21% 5% 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 V33 P34 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.4 Score per residue for model 4

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 16% 42% 28% 7% 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 D35 N36 F37 L38 E41 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.5 Score per residue for model 5

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 26% 46% 19% • 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 W11 I12 Y13 D14 P15 A16 K17 G18 M21 Q22 D23 G27 T28 P29 W30 S31 E32 V33 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.6 Score per residue for model 6

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 21% 49% 19% • 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 Y13 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 W30 S31 E32 V33 P34 F37 L38 C39 P40 E41 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

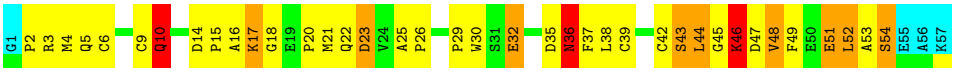
Chain A: 28% 42% 18% 5% 7%

G1 P2 R3 M4 Q5 C6 C9 Q10 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 P29 W30 S31 E32 V33 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.8 Score per residue for model 8

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

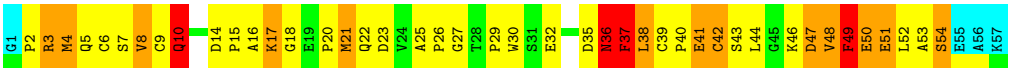
Chain A: 26% 46% 16% 5% 7%



4.2.9 Score per residue for model 9

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

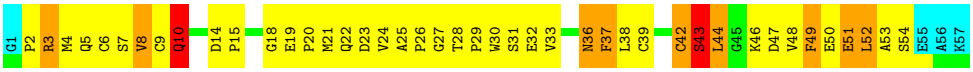
Chain A: 18% 46% 23% 7% 7%



4.2.10 Score per residue for model 10

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

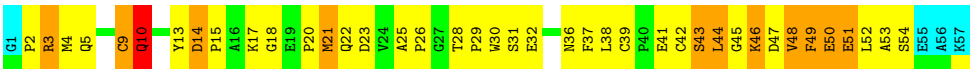
Chain A: 18% 56% 16% • 7%



4.2.11 Score per residue for model 11

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

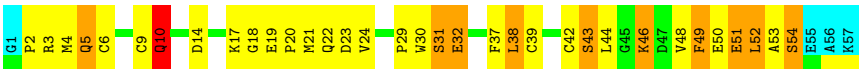
Chain A: 23% 49% 19% • 7%



4.2.12 Score per residue for model 12

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 33% 40% 18% • 7%



4.2.13 Score per residue for model 13

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 23% 49% 19% • 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 W11 I12 Y13 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 P29 W30 S31 E32 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.14 Score per residue for model 14

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 21% 46% 23% • 7%

G1 P2 R3 M4 Q5 C6 C9 Q10 Y13 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 D35 N36 F37 L38 C39 P40 E41 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.15 Score per residue for model 15

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 18% 53% 21% • 7%

G1 P2 R3 M4 Q5 C6 C9 Q10 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 V33 P34 D35 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.16 Score per residue for model 16

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 19% 47% 23% • 7%

G1 P2 R3 M4 Q5 C6 C9 Q10 Y13 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 V33 P34 D35 N36 F37 L38 C39 P40 E41 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.17 Score per residue for model 17

• Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 19% 51% 21% • 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 W11 I12 Y13 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.18 Score per residue for model 18

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 21% 49% 19% • 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 Y13 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 P26 G27 T28 P29 W30 S31 E32 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.19 Score per residue for model 19

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 26% 42% 23% • 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 D35 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

4.2.20 Score per residue for model 20

- Molecule 1: Anaerobic nitric oxide reductase flavorubredoxin

Chain A: 16% 49% 25% • 7%

G1 P2 R3 M4 Q5 C6 S7 V8 C9 Q10 Y13 D14 P15 A16 K17 G18 E19 P20 M21 Q22 D23 V24 A25 P26 G27 T28 P29 W30 S31 E32 V33 P34 D35 N36 F37 L38 C39 C42 S43 L44 G45 K46 D47 V48 F49 E50 E51 L52 A53 S54 E55 A56 K57

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, simulated annealing.*

Of the 200 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**
DYANA	structure solution	
DYANA	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	422
Number of shifts mapped to atoms	422
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	410	382	376	45±7
All	All	8220	7640	7520	905

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:PHE:O	1:A:38:LEU:HD23	0.93	1.62	5	10
1:A:8:VAL:HG21	1:A:44:LEU:CD1	0.83	2.04	10	2
1:A:51:GLU:C	1:A:52:LEU:HD13	0.82	1.95	5	1
1:A:2:PRO:CB	1:A:52:LEU:HD23	0.82	2.05	20	1
1:A:2:PRO:HB3	1:A:52:LEU:HD23	0.81	1.52	20	1
1:A:15:PRO:HG3	1:A:53:ALA:HB1	0.81	1.50	8	3
1:A:37:PHE:C	1:A:38:LEU:HD22	0.81	1.96	11	1
1:A:44:LEU:HD23	1:A:49:PHE:CD1	0.79	2.12	1	3
1:A:47:ASP:O	1:A:48:VAL:HG23	0.78	1.79	16	7
1:A:44:LEU:HD13	1:A:48:VAL:HB	0.77	1.55	13	1
1:A:29:PRO:HG2	1:A:32:GLU:CB	0.76	2.10	10	11
1:A:42:CYS:SG	1:A:42:CYS:O	0.75	2.45	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD21	1:A:48:VAL:HB	0.75	1.55	15	10
1:A:2:PRO:CB	1:A:52:LEU:HD22	0.75	2.11	4	4
1:A:4:MET:SD	1:A:53:ALA:HB2	0.74	2.22	20	2
1:A:25:ALA:HB1	1:A:26:PRO:HD2	0.73	1.61	17	15
1:A:36:ASN:O	1:A:38:LEU:HD22	0.73	1.83	10	1
1:A:4:MET:CE	1:A:30:TRP:CE3	0.71	2.73	4	2
1:A:38:LEU:HD22	1:A:44:LEU:O	0.71	1.86	14	7
1:A:42:CYS:O	1:A:43:SER:C	0.70	2.30	10	15
1:A:4:MET:HE1	1:A:30:TRP:CG	0.69	2.22	16	17
1:A:52:LEU:HD13	1:A:52:LEU:N	0.69	2.01	5	1
1:A:7:SER:O	1:A:8:VAL:HG23	0.69	1.85	10	2
1:A:33:VAL:HG12	1:A:46:LYS:HE2	0.68	1.64	5	3
1:A:38:LEU:HD12	1:A:44:LEU:O	0.68	1.87	11	1
1:A:29:PRO:HG2	1:A:32:GLU:HB2	0.68	1.66	1	11
1:A:51:GLU:C	1:A:52:LEU:HD12	0.68	2.09	1	1
1:A:2:PRO:HB3	1:A:52:LEU:HD12	0.67	1.64	15	2
1:A:30:TRP:CH2	1:A:46:LYS:CD	0.67	2.78	5	7
1:A:13:TYR:CD2	1:A:13:TYR:O	0.67	2.48	6	2
1:A:4:MET:CE	1:A:30:TRP:CG	0.66	2.78	17	18
1:A:29:PRO:HG2	1:A:32:GLU:HB3	0.66	1.66	20	6
1:A:29:PRO:HG2	1:A:32:GLU:CG	0.65	2.21	15	1
1:A:44:LEU:HD23	1:A:49:PHE:HD1	0.65	1.50	1	3
1:A:2:PRO:HG2	1:A:53:ALA:C	0.65	2.11	19	9
1:A:4:MET:HE3	1:A:30:TRP:CE3	0.64	2.26	4	1
1:A:4:MET:CE	1:A:30:TRP:CD2	0.64	2.80	20	4
1:A:48:VAL:HG12	1:A:48:VAL:O	0.63	1.94	8	3
1:A:2:PRO:HB3	1:A:52:LEU:HD22	0.63	1.69	4	4
1:A:44:LEU:HD22	1:A:48:VAL:CB	0.63	2.24	20	1
1:A:2:PRO:HG2	1:A:53:ALA:CA	0.63	2.24	9	5
1:A:51:GLU:O	1:A:52:LEU:HD12	0.62	1.93	1	2
1:A:36:ASN:O	1:A:37:PHE:C	0.62	2.37	10	9
1:A:4:MET:HE1	1:A:30:TRP:CD2	0.62	2.30	9	2
1:A:51:GLU:O	1:A:51:GLU:CG	0.62	2.48	9	3
1:A:4:MET:SD	1:A:30:TRP:CE3	0.61	2.94	12	5
1:A:22:GLN:OE1	1:A:37:PHE:CD1	0.61	2.54	12	1
1:A:39:CYS:O	1:A:43:SER:N	0.61	2.34	14	13
1:A:37:PHE:C	1:A:37:PHE:CD1	0.61	2.74	4	3
1:A:2:PRO:O	1:A:15:PRO:HG2	0.60	1.96	6	4
1:A:3:ARG:N	1:A:3:ARG:CD	0.60	2.63	13	8
1:A:29:PRO:HG2	1:A:32:GLU:HG3	0.60	1.72	15	1
1:A:42:CYS:O	1:A:43:SER:CB	0.60	2.48	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:VAL:O	1:A:49:PHE:C	0.60	2.40	12	16
1:A:37:PHE:C	1:A:38:LEU:HD23	0.60	2.16	6	3
1:A:44:LEU:HD22	1:A:48:VAL:HB	0.60	1.71	8	2
1:A:42:CYS:O	1:A:42:CYS:SG	0.59	2.60	10	13
1:A:37:PHE:O	1:A:38:LEU:HD22	0.59	1.97	11	1
1:A:9:CYS:HB3	1:A:42:CYS:HB3	0.59	1.73	9	11
1:A:8:VAL:HG21	1:A:44:LEU:HD11	0.59	1.75	2	1
1:A:43:SER:O	1:A:44:LEU:CB	0.59	2.50	17	7
1:A:44:LEU:CD2	1:A:48:VAL:HG11	0.58	2.27	20	1
1:A:8:VAL:HG21	1:A:44:LEU:HD13	0.58	1.72	10	1
1:A:22:GLN:OE1	1:A:37:PHE:CD2	0.58	2.56	15	4
1:A:22:GLN:O	1:A:23:ASP:CB	0.58	2.52	14	16
1:A:6:CYS:SG	1:A:44:LEU:HD22	0.57	2.39	4	1
1:A:39:CYS:N	1:A:43:SER:O	0.57	2.34	14	9
1:A:30:TRP:CZ2	1:A:46:LYS:HD2	0.56	2.35	9	12
1:A:20:PRO:O	1:A:21:MET:HE1	0.56	2.00	12	2
1:A:36:ASN:O	1:A:38:LEU:CD2	0.56	2.52	9	7
1:A:50:GLU:O	1:A:51:GLU:CB	0.56	2.53	4	11
1:A:20:PRO:HB2	1:A:21:MET:HE3	0.56	1.77	16	4
1:A:30:TRP:CZ2	1:A:46:LYS:CD	0.56	2.88	20	4
1:A:42:CYS:O	1:A:44:LEU:N	0.56	2.37	20	10
1:A:30:TRP:CH2	1:A:46:LYS:HD2	0.56	2.35	7	7
1:A:30:TRP:CH2	1:A:46:LYS:HD3	0.56	2.36	4	8
1:A:2:PRO:CB	1:A:52:LEU:HD12	0.56	2.30	14	2
1:A:47:ASP:O	1:A:48:VAL:CG2	0.56	2.54	17	9
1:A:46:LYS:HZ2	1:A:46:LYS:HA	0.56	1.60	19	1
1:A:4:MET:HE1	1:A:30:TRP:CE3	0.55	2.36	20	2
1:A:8:VAL:CG2	1:A:44:LEU:HD13	0.55	2.31	10	1
1:A:9:CYS:O	1:A:10:GLN:CB	0.55	2.55	10	13
1:A:45:GLY:O	1:A:46:LYS:CB	0.55	2.54	20	1
1:A:2:PRO:CD	1:A:54:SER:O	0.55	2.55	10	12
1:A:35:ASP:O	1:A:36:ASN:CB	0.54	2.53	2	7
1:A:42:CYS:SG	1:A:43:SER:N	0.54	2.80	9	4
1:A:8:VAL:CG1	1:A:42:CYS:SG	0.54	2.95	4	2
1:A:4:MET:HE3	1:A:30:TRP:CG	0.54	2.37	18	1
1:A:38:LEU:O	1:A:39:CYS:C	0.54	2.45	10	6
1:A:2:PRO:O	1:A:15:PRO:CG	0.54	2.56	18	4
1:A:8:VAL:CG2	1:A:44:LEU:CD1	0.54	2.84	10	2
1:A:4:MET:HE3	1:A:30:TRP:CD2	0.53	2.39	4	1
1:A:41:GLU:O	1:A:42:CYS:HB3	0.53	2.03	6	1
1:A:2:PRO:O	1:A:15:PRO:CD	0.53	2.57	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PRO:O	1:A:21:MET:CE	0.53	2.56	12	2
1:A:4:MET:SD	1:A:30:TRP:CD2	0.52	3.02	2	3
1:A:4:MET:CE	1:A:30:TRP:CB	0.52	2.86	17	5
1:A:46:LYS:O	1:A:46:LYS:CG	0.52	2.56	12	1
1:A:42:CYS:O	1:A:43:SER:O	0.52	2.26	18	4
1:A:22:GLN:O	1:A:24:VAL:HG23	0.52	2.05	15	1
1:A:39:CYS:CB	1:A:43:SER:O	0.52	2.58	17	1
1:A:2:PRO:HG2	1:A:53:ALA:O	0.51	2.05	2	5
1:A:9:CYS:O	1:A:10:GLN:O	0.51	2.28	14	2
1:A:2:PRO:CB	1:A:52:LEU:CD2	0.51	2.89	9	2
1:A:45:GLY:O	1:A:46:LYS:CG	0.51	2.59	20	1
1:A:2:PRO:HB3	1:A:52:LEU:CD2	0.51	2.36	17	2
1:A:46:LYS:N	1:A:46:LYS:NZ	0.51	2.59	19	1
1:A:7:SER:O	1:A:8:VAL:CG2	0.51	2.59	6	7
1:A:16:ALA:O	1:A:17:LYS:CD	0.50	2.59	5	11
1:A:20:PRO:HG2	1:A:21:MET:HE2	0.50	1.82	18	2
1:A:50:GLU:C	1:A:51:GLU:CG	0.50	2.79	2	6
1:A:15:PRO:O	1:A:26:PRO:CB	0.50	2.60	16	2
1:A:28:THR:HG23	1:A:29:PRO:HD2	0.50	1.82	10	2
1:A:8:VAL:CG2	1:A:44:LEU:HD11	0.50	2.36	2	1
1:A:44:LEU:HD11	1:A:48:VAL:HB	0.50	1.82	3	1
1:A:30:TRP:CZ2	1:A:46:LYS:HD3	0.50	2.42	6	1
1:A:30:TRP:CZ2	1:A:46:LYS:NZ	0.50	2.73	15	1
1:A:3:ARG:CB	1:A:13:TYR:O	0.50	2.59	16	1
1:A:19:GLU:O	1:A:22:GLN:N	0.50	2.45	2	5
1:A:6:CYS:SG	1:A:44:LEU:CD1	0.49	3.00	9	1
1:A:46:LYS:HZ2	1:A:46:LYS:CA	0.49	2.20	19	1
1:A:38:LEU:HD22	1:A:45:GLY:HA2	0.49	1.84	3	1
1:A:36:ASN:HD22	1:A:37:PHE:N	0.49	2.04	13	1
1:A:39:CYS:O	1:A:43:SER:HA	0.49	2.08	7	7
1:A:15:PRO:O	1:A:26:PRO:CA	0.49	2.60	16	3
1:A:38:LEU:CD2	1:A:44:LEU:O	0.49	2.61	9	6
1:A:30:TRP:CE2	1:A:46:LYS:NZ	0.49	2.80	15	1
1:A:47:ASP:C	1:A:48:VAL:CG2	0.49	2.81	11	5
1:A:4:MET:HA	1:A:51:GLU:CB	0.48	2.38	15	4
1:A:40:PRO:O	1:A:41:GLU:CB	0.48	2.61	9	2
1:A:20:PRO:CB	1:A:21:MET:CE	0.48	2.91	19	1
1:A:5:GLN:NE2	1:A:51:GLU:CD	0.48	2.66	13	2
1:A:50:GLU:O	1:A:51:GLU:CG	0.48	2.61	13	5
1:A:14:ASP:O	1:A:18:GLY:N	0.48	2.46	18	17
1:A:21:MET:SD	1:A:21:MET:N	0.48	2.86	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ALA:O	1:A:54:SER:O	0.48	2.32	9	4
1:A:13:TYR:O	1:A:13:TYR:CD1	0.48	2.66	11	6
1:A:44:LEU:HD23	1:A:46:LYS:H	0.48	1.69	16	1
1:A:15:PRO:O	1:A:27:GLY:N	0.48	2.46	14	11
1:A:14:ASP:OD2	1:A:17:LYS:CG	0.48	2.62	5	1
1:A:6:CYS:SG	1:A:10:GLN:N	0.48	2.87	2	3
1:A:29:PRO:O	1:A:32:GLU:N	0.48	2.47	9	11
1:A:20:PRO:HD2	1:A:21:MET:HE3	0.47	1.85	13	2
1:A:48:VAL:O	1:A:49:PHE:O	0.47	2.32	9	6
1:A:4:MET:CE	1:A:30:TRP:HB2	0.47	2.39	17	1
1:A:49:PHE:O	1:A:50:GLU:O	0.47	2.33	9	6
1:A:5:GLN:NE2	1:A:51:GLU:OE1	0.47	2.48	6	4
1:A:13:TYR:O	1:A:15:PRO:HD3	0.47	2.10	6	1
1:A:15:PRO:CG	1:A:53:ALA:HB1	0.47	2.37	7	1
1:A:29:PRO:C	1:A:31:SER:N	0.46	2.68	16	7
1:A:9:CYS:SG	1:A:10:GLN:N	0.46	2.88	5	3
1:A:20:PRO:HB2	1:A:21:MET:CE	0.46	2.40	19	2
1:A:53:ALA:C	1:A:54:SER:HG	0.46	2.11	16	1
1:A:33:VAL:O	1:A:46:LYS:NZ	0.46	2.49	1	1
1:A:3:ARG:N	1:A:52:LEU:O	0.46	2.48	11	2
1:A:45:GLY:O	1:A:47:ASP:N	0.46	2.48	8	4
1:A:44:LEU:HD12	1:A:49:PHE:CE1	0.46	2.46	18	1
1:A:47:ASP:C	1:A:48:VAL:HG23	0.46	2.31	8	6
1:A:6:CYS:SG	1:A:7:SER:N	0.46	2.89	6	1
1:A:21:MET:CE	1:A:21:MET:N	0.46	2.79	6	1
1:A:19:GLU:N	1:A:20:PRO:CD	0.46	2.79	15	5
1:A:34:PRO:O	1:A:46:LYS:NZ	0.46	2.49	6	1
1:A:44:LEU:HD21	1:A:48:VAL:CB	0.46	2.41	11	2
1:A:39:CYS:C	1:A:41:GLU:N	0.46	2.69	14	1
1:A:4:MET:CG	1:A:53:ALA:HB2	0.46	2.41	18	1
1:A:37:PHE:O	1:A:46:LYS:CD	0.46	2.64	19	1
1:A:6:CYS:SG	1:A:44:LEU:HD12	0.46	2.51	9	1
1:A:40:PRO:O	1:A:41:GLU:OE2	0.46	2.34	16	1
1:A:47:ASP:CG	1:A:48:VAL:N	0.45	2.70	10	2
1:A:42:CYS:SG	1:A:44:LEU:HD12	0.45	2.51	8	1
1:A:44:LEU:HD23	1:A:46:LYS:N	0.45	2.26	16	1
1:A:41:GLU:O	1:A:42:CYS:CB	0.45	2.64	6	1
1:A:4:MET:CG	1:A:52:LEU:O	0.45	2.64	6	7
1:A:45:GLY:C	1:A:47:ASP:N	0.45	2.69	17	6
1:A:38:LEU:CD1	1:A:44:LEU:O	0.45	2.62	11	1
1:A:43:SER:O	1:A:44:LEU:HB2	0.45	2.09	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ALA:C	1:A:17:LYS:CD	0.45	2.85	17	9
1:A:51:GLU:OE1	1:A:52:LEU:N	0.45	2.49	7	2
1:A:44:LEU:HD22	1:A:48:VAL:CG2	0.45	2.41	20	1
1:A:4:MET:HE1	1:A:30:TRP:CD1	0.45	2.47	16	1
1:A:5:GLN:NE2	1:A:51:GLU:OE2	0.44	2.49	3	2
1:A:7:SER:C	1:A:8:VAL:HG23	0.44	2.32	6	6
1:A:6:CYS:HB2	1:A:49:PHE:CE1	0.44	2.47	6	1
1:A:4:MET:HE3	1:A:30:TRP:CB	0.44	2.42	19	4
1:A:22:GLN:NE2	1:A:37:PHE:CE1	0.44	2.85	14	1
1:A:17:LYS:O	1:A:20:PRO:CD	0.44	2.64	15	1
1:A:45:GLY:O	1:A:46:LYS:C	0.44	2.54	8	4
1:A:2:PRO:C	1:A:52:LEU:O	0.44	2.56	20	1
1:A:52:LEU:N	1:A:52:LEU:CD1	0.44	2.72	5	1
1:A:3:ARG:NE	1:A:3:ARG:H	0.44	2.11	20	1
1:A:4:MET:SD	1:A:13:TYR:CD1	0.44	3.10	20	1
1:A:44:LEU:HD21	1:A:48:VAL:HG11	0.44	1.88	20	1
1:A:48:VAL:O	1:A:48:VAL:CG1	0.44	2.64	8	1
1:A:19:GLU:C	1:A:21:MET:H	0.44	2.16	14	2
1:A:3:ARG:CD	1:A:3:ARG:N	0.44	2.81	1	1
1:A:6:CYS:SG	1:A:6:CYS:O	0.44	2.76	14	2
1:A:2:PRO:HB2	1:A:52:LEU:C	0.44	2.33	17	2
1:A:53:ALA:O	1:A:54:SER:CB	0.44	2.65	10	1
1:A:51:GLU:C	1:A:52:LEU:CD1	0.44	2.79	5	1
1:A:19:GLU:O	1:A:22:GLN:CB	0.44	2.66	6	1
1:A:38:LEU:HD12	1:A:44:LEU:C	0.44	2.33	11	1
1:A:50:GLU:O	1:A:51:GLU:HB3	0.44	2.12	16	2
1:A:44:LEU:HD22	1:A:48:VAL:HG21	0.44	1.89	20	1
1:A:29:PRO:CG	1:A:32:GLU:HB2	0.44	2.42	20	1
1:A:20:PRO:HG3	1:A:26:PRO:HD3	0.43	1.90	10	2
1:A:2:PRO:HB2	1:A:53:ALA:N	0.43	2.28	11	1
1:A:36:ASN:O	1:A:38:LEU:HG	0.43	2.13	14	1
1:A:34:PRO:C	1:A:36:ASN:N	0.43	2.71	16	3
1:A:42:CYS:SG	1:A:43:SER:O	0.43	2.77	6	1
1:A:3:ARG:CA	1:A:52:LEU:O	0.43	2.66	4	1
1:A:29:PRO:HG2	1:A:32:GLU:OE1	0.43	2.14	8	1
1:A:28:THR:CG2	1:A:29:PRO:HD2	0.43	2.44	17	3
1:A:39:CYS:N	1:A:43:SER:HA	0.43	2.28	13	2
1:A:9:CYS:O	1:A:10:GLN:HB3	0.43	2.13	15	2
1:A:20:PRO:C	1:A:21:MET:SD	0.43	2.97	3	1
1:A:39:CYS:C	1:A:41:GLU:H	0.43	2.16	14	1
1:A:9:CYS:O	1:A:10:GLN:C	0.42	2.58	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ARG:O	1:A:51:GLU:CD	0.42	2.57	15	2
1:A:9:CYS:SG	1:A:41:GLU:CB	0.42	3.07	14	2
1:A:20:PRO:HD2	1:A:21:MET:CE	0.42	2.44	14	3
1:A:26:PRO:O	1:A:27:GLY:C	0.42	2.57	4	2
1:A:3:ARG:N	1:A:3:ARG:HD3	0.42	2.29	20	1
1:A:32:GLU:O	1:A:33:VAL:C	0.42	2.58	3	3
1:A:19:GLU:O	1:A:24:VAL:O	0.42	2.38	14	5
1:A:51:GLU:CA	1:A:52:LEU:HD13	0.42	2.44	5	1
1:A:20:PRO:O	1:A:21:MET:SD	0.42	2.77	8	2
1:A:22:GLN:C	1:A:23:ASP:OD1	0.42	2.58	8	2
1:A:34:PRO:O	1:A:36:ASN:N	0.42	2.52	15	1
1:A:44:LEU:HD22	1:A:48:VAL:CG1	0.42	2.44	20	1
1:A:44:LEU:CD2	1:A:48:VAL:HB	0.42	2.45	12	2
1:A:38:LEU:HD23	1:A:44:LEU:O	0.42	2.15	13	1
1:A:46:LYS:NZ	1:A:46:LYS:CA	0.42	2.82	19	1
1:A:19:GLU:C	1:A:21:MET:N	0.42	2.73	2	1
1:A:51:GLU:C	1:A:52:LEU:HD23	0.42	2.35	2	2
1:A:33:VAL:O	1:A:34:PRO:O	0.42	2.38	6	2
1:A:22:GLN:NE2	1:A:37:PHE:CE2	0.42	2.87	4	1
1:A:3:ARG:O	1:A:52:LEU:CB	0.42	2.68	9	1
1:A:8:VAL:HB	1:A:42:CYS:SG	0.42	2.55	9	1
1:A:35:ASP:C	1:A:37:PHE:N	0.42	2.73	15	1
1:A:39:CYS:O	1:A:43:SER:CA	0.42	2.67	7	4
1:A:35:ASP:O	1:A:36:ASN:OD1	0.42	2.38	9	3
1:A:17:LYS:O	1:A:20:PRO:HD3	0.42	2.15	15	1
1:A:6:CYS:HB3	1:A:44:LEU:HD22	0.42	1.92	17	1
1:A:46:LYS:N	1:A:46:LYS:HZ3	0.42	2.12	19	1
1:A:25:ALA:HB1	1:A:26:PRO:CD	0.42	2.45	11	2
1:A:14:ASP:OD2	1:A:17:LYS:NZ	0.42	2.53	7	1
1:A:23:ASP:C	1:A:24:VAL:CG2	0.42	2.89	20	1
1:A:47:ASP:O	1:A:48:VAL:HG22	0.41	2.14	11	1
1:A:20:PRO:N	1:A:24:VAL:O	0.41	2.53	1	1
1:A:5:GLN:CG	1:A:12:ILE:HG12	0.41	2.45	13	2
1:A:3:ARG:N	1:A:3:ARG:HD2	0.41	2.30	16	2
1:A:4:MET:HE2	1:A:30:TRP:CE3	0.41	2.51	20	1
1:A:44:LEU:CD1	1:A:48:VAL:HB	0.41	2.46	3	1
1:A:25:ALA:CB	1:A:26:PRO:HD2	0.41	2.41	9	2
1:A:3:ARG:O	1:A:51:GLU:CB	0.41	2.68	14	1
1:A:36:ASN:O	1:A:37:PHE:O	0.41	2.38	4	3
1:A:49:PHE:O	1:A:50:GLU:C	0.41	2.59	4	1
1:A:43:SER:O	1:A:43:SER:OG	0.41	2.37	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD22	1:A:48:VAL:HG11	0.41	1.93	20	1
1:A:2:PRO:HD3	1:A:54:SER:O	0.41	2.16	2	1
1:A:37:PHE:O	1:A:38:LEU:CD2	0.41	2.59	3	1
1:A:33:VAL:HG12	1:A:46:LYS:CE	0.41	2.43	6	1
1:A:29:PRO:CG	1:A:32:GLU:CB	0.41	2.93	20	1
1:A:25:ALA:O	1:A:28:THR:OG1	0.41	2.36	11	1
1:A:10:GLN:OE1	1:A:10:GLN:C	0.41	2.59	15	1
1:A:4:MET:SD	1:A:51:GLU:HA	0.41	2.56	17	1
1:A:40:PRO:O	1:A:41:GLU:HB2	0.41	2.15	16	2
1:A:53:ALA:O	1:A:54:SER:C	0.41	2.59	9	1
1:A:39:CYS:HB3	1:A:42:CYS:C	0.41	2.36	14	1
1:A:10:GLN:HG3	1:A:10:GLN:O	0.41	2.16	15	1
1:A:8:VAL:HG11	1:A:42:CYS:SG	0.41	2.55	4	2
1:A:22:GLN:O	1:A:22:GLN:OE1	0.41	2.39	4	1
1:A:45:GLY:O	1:A:47:ASP:OD1	0.41	2.39	5	1
1:A:14:ASP:HB2	1:A:17:LYS:CD	0.40	2.46	13	1
1:A:3:ARG:HG3	1:A:12:ILE:CG2	0.40	2.46	17	1
1:A:44:LEU:HD21	1:A:48:VAL:CG1	0.40	2.46	2	1
1:A:7:SER:C	1:A:8:VAL:CG2	0.40	2.90	18	2
1:A:19:GLU:C	1:A:24:VAL:O	0.40	2.60	10	1
1:A:4:MET:HA	1:A:51:GLU:HB2	0.40	1.94	1	1
1:A:3:ARG:O	1:A:51:GLU:OE2	0.40	2.39	7	1
1:A:36:ASN:ND2	1:A:36:ASN:C	0.40	2.74	13	1
1:A:30:TRP:CH2	1:A:49:PHE:CD2	0.40	3.10	2	1
1:A:10:GLN:O	1:A:10:GLN:CG	0.40	2.70	15	1
1:A:47:ASP:OD1	1:A:48:VAL:N	0.40	2.53	2	1
1:A:2:PRO:CG	1:A:54:SER:O	0.40	2.70	8	1
1:A:22:GLN:O	1:A:23:ASP:CG	0.40	2.60	12	1
1:A:22:GLN:O	1:A:23:ASP:HB2	0.40	2.16	15	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	53/57 (93%)	34±2 (65±4%)	11±2 (20±4%)	8±1 (15±3%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1060/1140 (93%)	688 (65%)	212 (20%)	160 (15%)	0 4

All 21 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	43	SER	18
1	A	10	GLN	17
1	A	54	SER	17
1	A	51	GLU	16
1	A	48	VAL	14
1	A	49	PHE	12
1	A	8	VAL	11
1	A	44	LEU	9
1	A	36	ASN	9
1	A	50	GLU	6
1	A	41	GLU	5
1	A	37	PHE	5
1	A	42	CYS	4
1	A	23	ASP	4
1	A	46	LYS	4
1	A	18	GLY	2
1	A	26	PRO	2
1	A	34	PRO	2
1	A	45	GLY	1
1	A	20	PRO	1
1	A	24	VAL	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	47/49 (96%)	36±2 (77±4%)	11±2 (23±4%)	3 28
All	All	940/980 (96%)	723 (77%)	217 (23%)	3 28

All 30 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	3	ARG	20
1	A	10	GLN	17
1	A	17	LYS	17
1	A	5	GLN	16
1	A	6	CYS	14
1	A	21	MET	14
1	A	52	LEU	14
1	A	46	LYS	13
1	A	36	ASN	11
1	A	31	SER	9
1	A	32	GLU	8
1	A	23	ASP	7
1	A	43	SER	6
1	A	38	LEU	6
1	A	49	PHE	5
1	A	42	CYS	5
1	A	51	GLU	5
1	A	47	ASP	4
1	A	4	MET	4
1	A	14	ASP	4
1	A	39	CYS	3
1	A	44	LEU	3
1	A	22	GLN	2
1	A	37	PHE	2
1	A	7	SER	2
1	A	9	CYS	2
1	A	19	GLU	1
1	A	50	GLU	1
1	A	41	GLU	1
1	A	54	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 60% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	422
Number of shifts mapped to atoms	422
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	48	0.13 ± 0.74	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 60%, i.e. 400 atoms were assigned a chemical shift out of a possible 671. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	147/254 (58%)	102/102 (100%)	0/106 (0%)	45/46 (98%)
Sidechain	225/364 (62%)	221/236 (94%)	0/119 (0%)	4/9 (44%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	28/53 (53%)	26/26 (100%)	0/25 (0%)	2/2 (100%)
Overall	400/671 (60%)	349/364 (96%)	0/250 (0%)	51/57 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 419 atoms were assigned a chemical shift out of a possible 716. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	158/275 (57%)	110/111 (99%)	0/114 (0%)	48/50 (96%)
Sidechain	233/388 (60%)	229/251 (91%)	0/127 (0%)	4/10 (40%)
Aromatic	28/53 (53%)	26/26 (100%)	0/25 (0%)	2/2 (100%)
Overall	419/716 (59%)	365/388 (94%)	0/266 (0%)	54/62 (87%)

7.1.4 Statistically unusual chemical shifts (i)

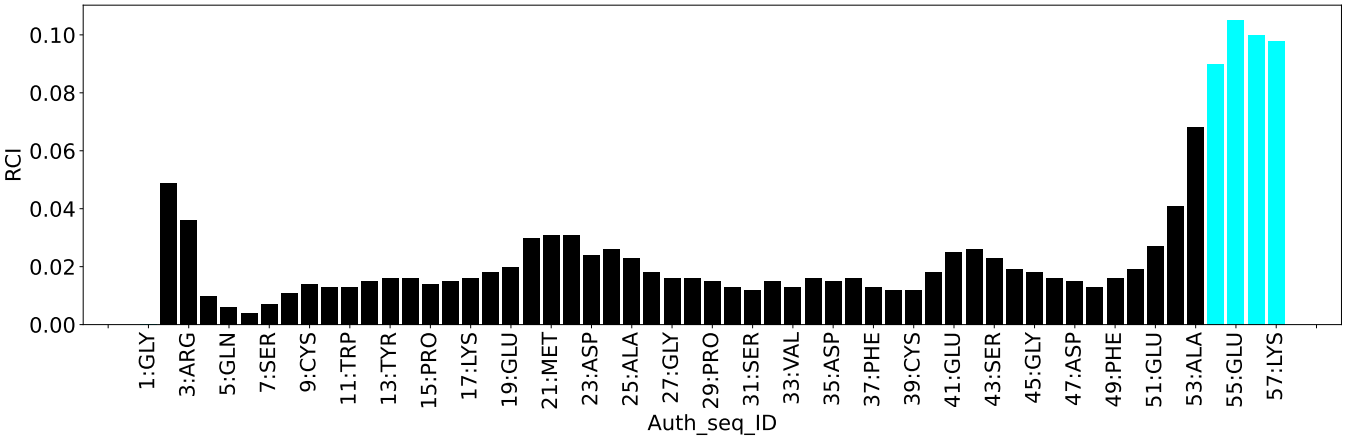
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	28	THR	HG1	6.86	0.08 – 2.19	27.1

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
1:GLY
3:ARG
5:GLN
7:SER
9:CYS
11:TRP
13:TYR
15:PRO
17:LYS
19:GLU
21:MET
23:ASP
25:ALA
27:GLY
29:PRO
31:SER
33:VAL
35:ASP
37:PHE
39:CYS
41:GLU
43:SER
45:GLY
47:ASP
49:PHE
51:GLU
53:ALA
55:GLU
57:LYS
Auth_seq_ID