WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:42 pm GMT

PDB ID	:	2L5O
Title	:	Solution Structure of a Putative Thioredoxin from Neisseria meningitidis
Authors	:	Harris, R.; Foti, R.; Seidel, R.D.; Bonanno, J.B.; Freeman, J.; Bain, K.T.; Sauder, J.M.; Burley, S.K.; Girvin, M.E.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC); New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2010-11-03

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

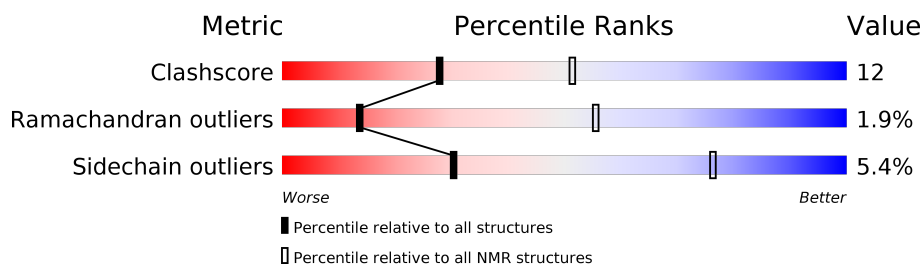|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 was not calculated.

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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		1.9%
Sidechain outliers		5.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	153	64%　　　　21%　　13%　　•

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 20 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:7-A:136 (130)	0.59	20

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 2333 atoms, of which 1153 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative thioredoxin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	150	2333	756	1153	198	222	4	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP Q9JXN4
A	-1	SER	-	EXPRESSION TAG	UNP Q9JXN4
A	0	LEU	-	EXPRESSION TAG	UNP Q9JXN4
A	143	GLU	-	EXPRESSION TAG	UNP Q9JXN4
A	144	GLY	-	EXPRESSION TAG	UNP Q9JXN4
A	145	HIS	-	EXPRESSION TAG	UNP Q9JXN4
A	146	HIS	-	EXPRESSION TAG	UNP Q9JXN4
A	147	HIS	-	EXPRESSION TAG	UNP Q9JXN4
A	148	HIS	-	EXPRESSION TAG	UNP Q9JXN4
A	149	HIS	-	EXPRESSION TAG	UNP Q9JXN4
A	150	HIS	-	EXPRESSION TAG	UNP Q9JXN4

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

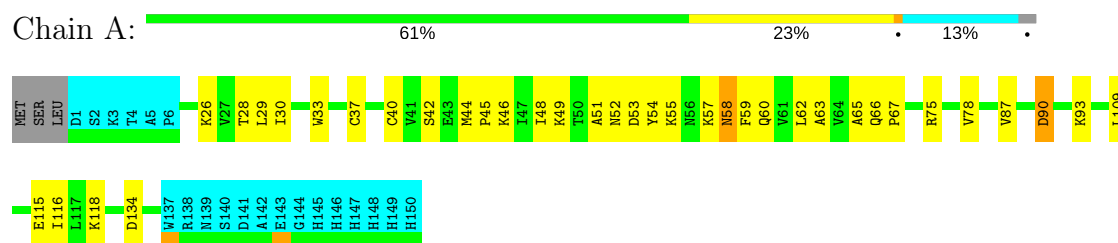- Molecule 1: Putative thioredoxin
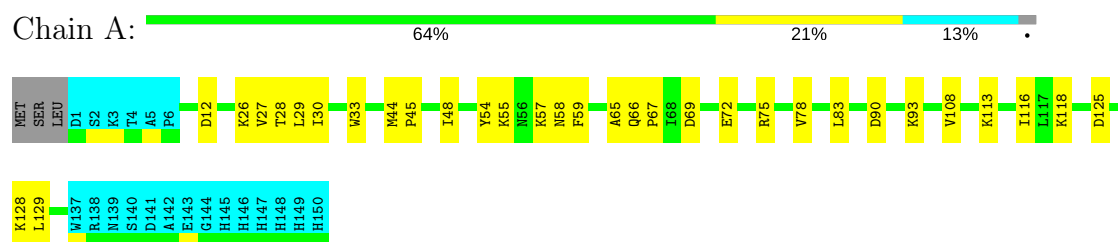
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.
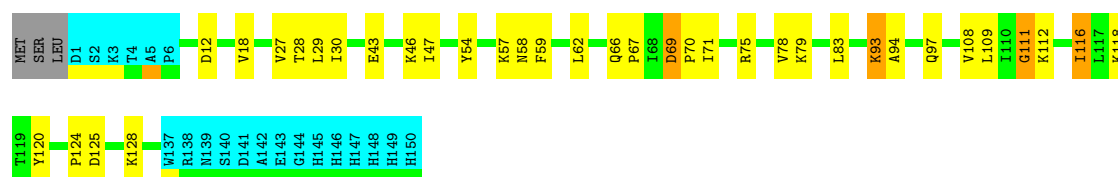
4.2.1 Score per residue for model 1

- Molecule 1: Putative thioredoxin

4.2.2 Score per residue for model 2

- Molecule 1: Putative thioredoxin

4.2.3 Score per residue for model 3

• Molecule 1: Putative thioredoxin

4.2.4 Score per residue for model 4

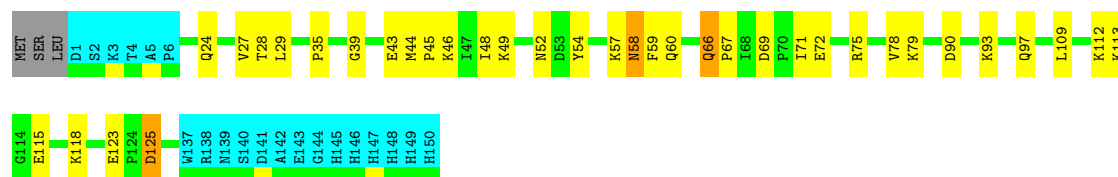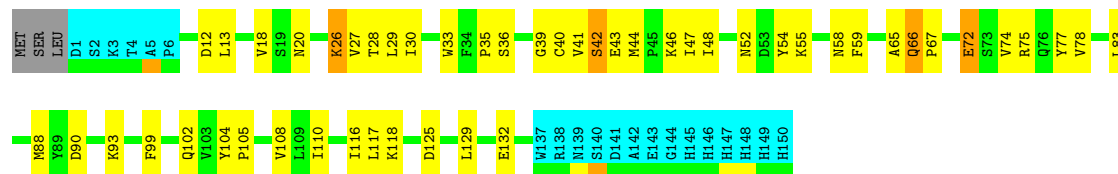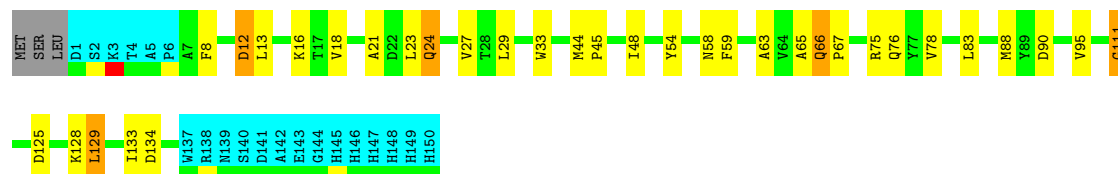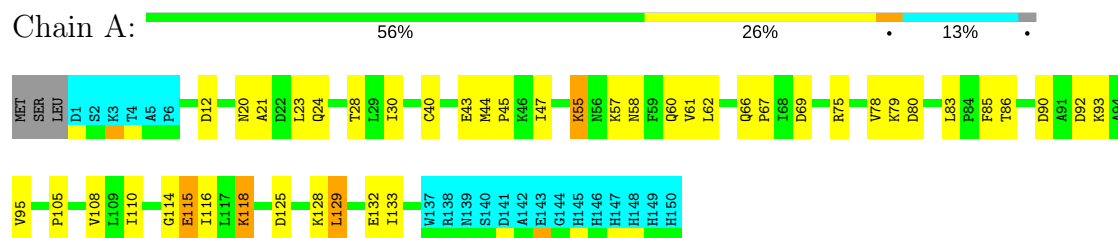• Molecule 1: Putative thioredoxin

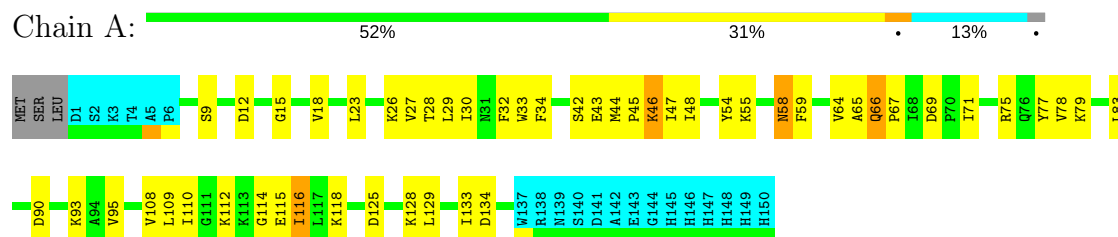### 4.2.5 Score per residue for model 5

• Molecule 1: Putative thioredoxin

4.2.6 Score per residue for model 6

• Molecule 1: Putative thioredoxin
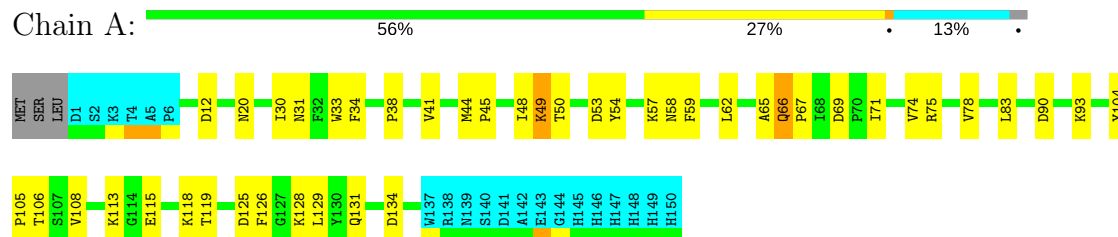
Chain A: 56% 26% • 13% •

MET SER LEU D1 S2 K3 T4 A5 P6 D12 N20 A21 D22 L23 Q24 T28 L29 I30 C40 E43 M44 P45 K46 I47 K55 N56 K57 N58 F59 Q60 V61 L62 Q66 P67 I68 D69 R75 V78 K79 D80 L83 P84 F85 T86 D90 A91 D92 K93 A94

V95 P105 V108 L109 I110 G114 E115 I116 L117 K118 D125 K128 L129 E132 I133 W137 R138 N139 S140 D141 A142 E143 G144 H145 H146 H147 H148 H149 H150

4.2.7 Score per residue for model 7

• Molecule 1: Putative thioredoxin

Chain A: 52% 31% • 13% •

MET SER LEU D1 S2 K3 T4 A5 P6 S9 D12 G15 V18 L23 K26 V27 T28 L29 I30 N31 F32 W33 F34 S42 E43 M44 P45 K46 I47 I48 Y54 K55 N58 F59 V64 A65 Q66 P67 I68 D69 P70 I71 R75 Q76 Y77 V78 K79 L83

D90 K93 A94 V95 V108 L109 I110 G111 K112 K113 G114 E115 I116 L117 K118 D125 K128 L129 I133 D134 W137 R138 N139 S140 D141 A142 E143 G144 H145 H146 H147 H148 H149 H150

4.2.8 Score per residue for model 8

• Molecule 1: Putative thioredoxin

Chain A: 56% 27% • 13% •

MET SER LEU D1 S2 K3 T4 A5 P6 D12 N20 I30 N31 F32 W33 F34 P38 V41 M44 P45 I48 K49 T50 D53 Y54 K57 N58 F59 L62 A65 Q66 P67 I68 D69 P70 I71 V74 R75 V78 L83 D90 K93 Y104

P105 T106 S107 V108 K113 G114 E115 K118 T119 D125 F126 G127 K128 L129 Y130 Q131 D134 W137 R138 N139 S140 D141 A142 E143 G144 H145 H146 H147 H148 H149 H150

4.2.9 Score per residue for model 9

• Molecule 1: Putative thioredoxin

Chain A: 59% 25% • 13% •

MET SER LEU D1 S2 K3 T4 A5 P6 P11 D12 G15 K16 L23 K26 V27 I30 W33 F34 C40 V41 S42 E43 M44 P45 I48 Y54 K55 N56 K57 N58 A65 Q66 P67 I71 E72 R75 D90 F99 V108 L109 I110 G111 G114

E115 I116 L117 K118 E123 K128 L129 Y130 Q131 D134 T135 A136 W137 R138 N139 S140 D141 A142 E143 G144 H145 H146 H147 H148 H149 H150

4.2.10 Score per residue for model 10

• Molecule 1: Putative thioredoxin

Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: Putative thioredoxin
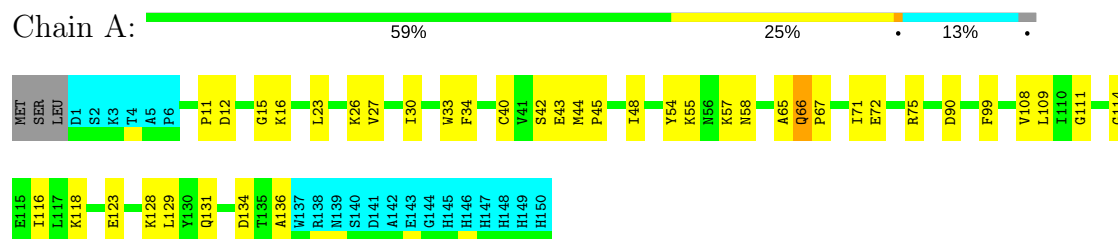
Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Putative thioredoxin

Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: Putative thioredoxin

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: Putative thioredoxin

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: Putative thioredoxin

Chain A:
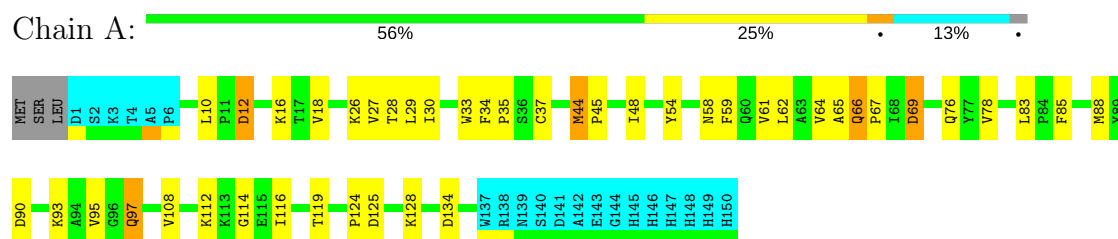
4.2.16 Score per residue for model 16

• Molecule 1: Putative thioredoxin

Chain A:
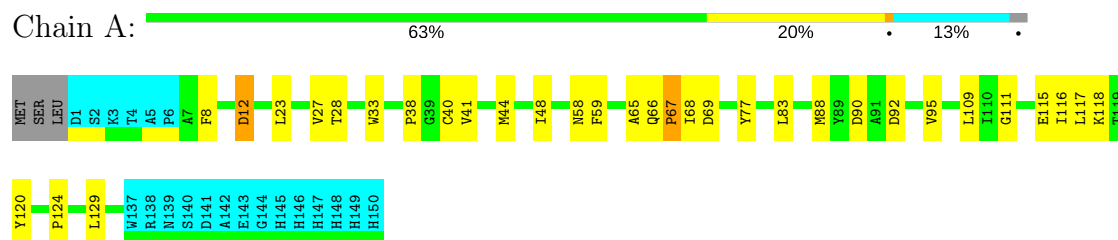
4.2.17 Score per residue for model 17

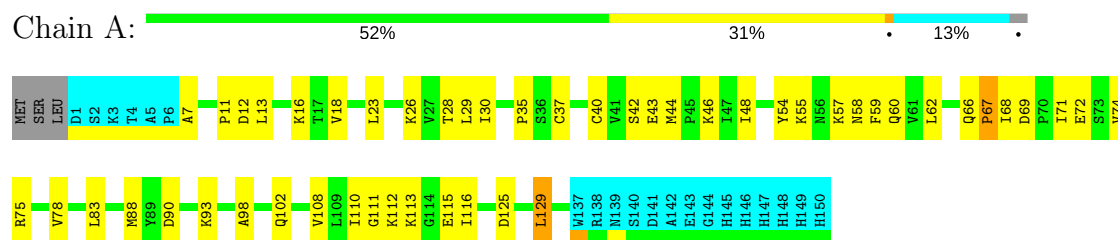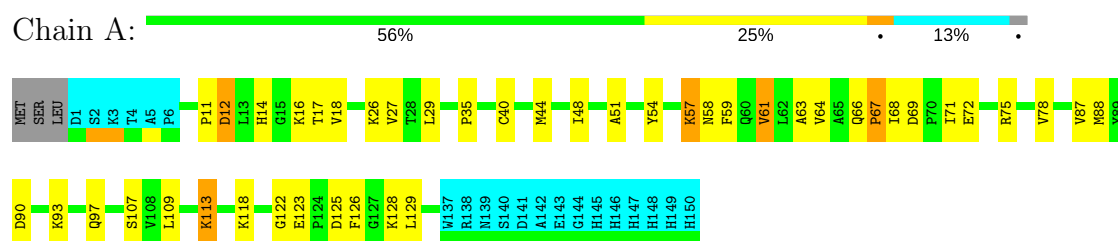• Molecule 1: Putative thioredoxin
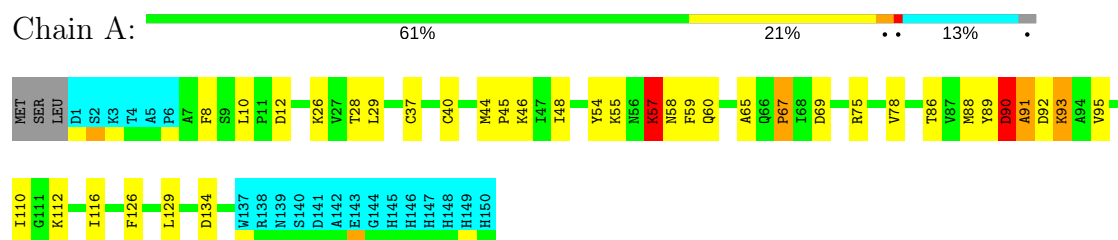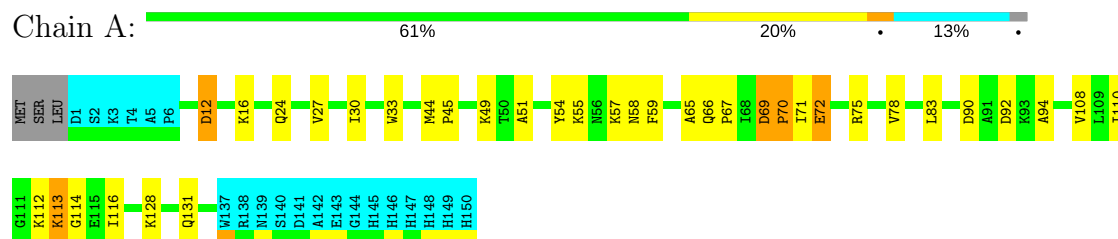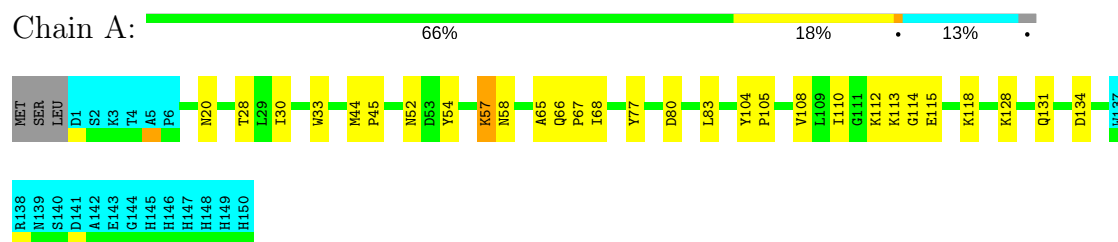
Chain A:
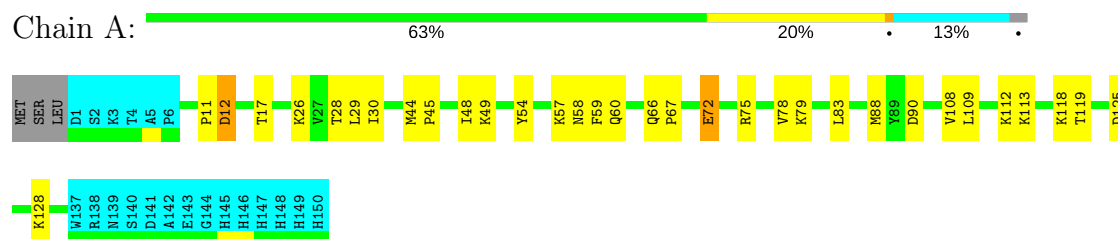
4.2.18 Score per residue for model 18

• Molecule 1: Putative thioredoxin
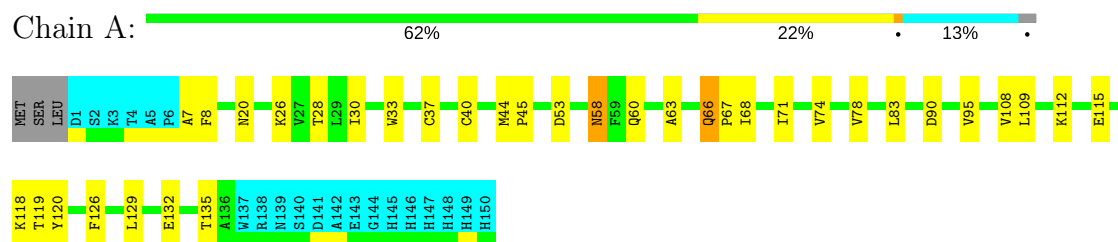
4.2.19 Score per residue for model 19

• Molecule 1: Putative thioredoxin
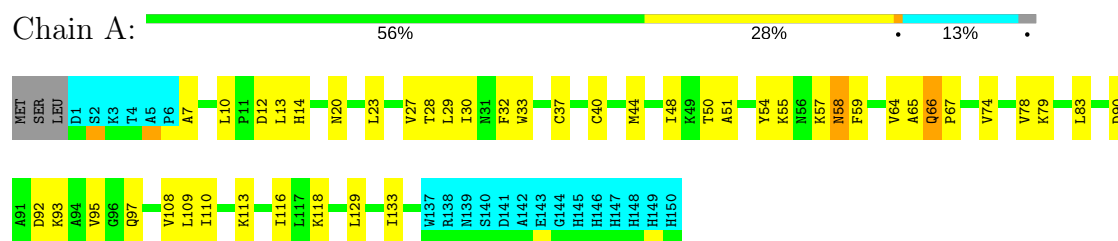
4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: Putative thioredoxin
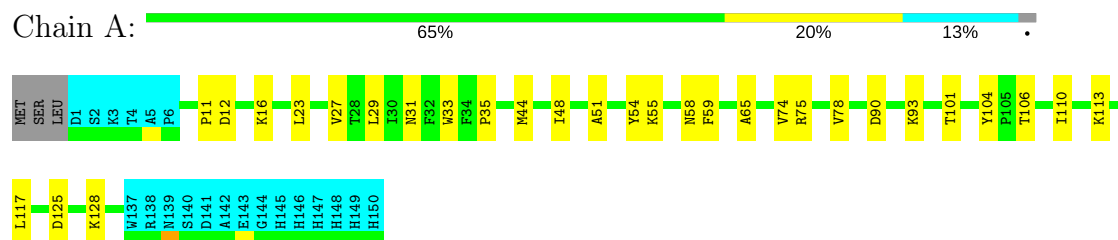
5 Refinement protocol and experimental data overview ⓘ

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

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

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

Software name	Classification	Version
CNS	refinement	1.21

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	90	ASP	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	1012	1012	1011	24±6
All	All	20240	20240	20220	489

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:54:TYR:HB3	1:A:59:PHE:HB3	0.99	1.30	3	14
1:A:78:VAL:HA	1:A:83:LEU:HD23	0.87	1.46	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:PRO:HD3	1:A:91:ALA:HA	0.85	1.44	12	1
1:A:61:VAL:HG11	1:A:85:PHE:HB3	0.84	1.46	15	1
1:A:54:TYR:HA	1:A:57:LYS:HE2	0.84	1.49	14	1
1:A:30:ILE:HB	1:A:108:VAL:HG12	0.79	1.53	6	5
1:A:23:LEU:HD13	1:A:110:ILE:HG21	0.75	1.58	19	2
1:A:64:VAL:HG12	1:A:88:MET:HB2	0.75	1.57	15	1
1:A:40:CYS:HA	1:A:43:GLU:HG2	0.72	1.61	10	1
1:A:39:GLY:O	1:A:43:GLU:HB2	0.71	1.86	3	2
1:A:75:ARG:HA	1:A:78:VAL:HG22	0.70	1.60	6	9
1:A:30:ILE:HB	1:A:108:VAL:CG2	0.70	2.16	18	6
1:A:30:ILE:HG12	1:A:62:LEU:HB2	0.68	1.65	1	2
1:A:90:ASP:OD2	1:A:93:LYS:HA	0.68	1.88	8	4
1:A:29:LEU:HB2	1:A:59:PHE:CZ	0.68	2.23	3	10
1:A:29:LEU:HB2	1:A:59:PHE:HZ	0.67	1.49	2	12
1:A:35:PRO:HG2	1:A:69:ASP:HB3	0.67	1.65	15	1
1:A:125:ASP:HB3	1:A:128:LYS:HG2	0.66	1.67	15	1
1:A:62:LEU:HG	1:A:86:THR:HB	0.65	1.68	6	1
1:A:18:VAL:HB	1:A:88:MET:SD	0.65	2.32	4	2
1:A:44:MET:HB3	1:A:45:PRO:HD3	0.64	1.67	15	9
1:A:28:THR:HG23	1:A:62:LEU:HD13	0.62	1.72	15	2
1:A:34:PHE:HB3	1:A:66:GLN:HE22	0.62	1.55	8	1
1:A:72:GLU:HA	1:A:75:ARG:HG2	0.62	1.69	3	5
1:A:37:CYS:HB3	1:A:40:CYS:SG	0.61	2.35	10	4
1:A:78:VAL:HG13	1:A:83:LEU:HB2	0.61	1.71	10	3
1:A:29:LEU:HB2	1:A:59:PHE:CE2	0.61	2.30	15	1
1:A:79:LYS:HA	1:A:79:LYS:HE3	0.61	1.71	7	1
1:A:30:ILE:HG12	1:A:110:ILE:HD11	0.60	1.73	6	1
1:A:93:LYS:O	1:A:93:LYS:HG2	0.60	1.96	2	1
1:A:113:LYS:HA	1:A:113:LYS:HE3	0.60	1.72	11	1
1:A:109:LEU:HB2	1:A:118:LYS:HB3	0.60	1.73	19	4
1:A:40:CYS:O	1:A:44:MET:HB2	0.60	1.97	6	3
1:A:110:ILE:HG23	1:A:114:GLY:HA2	0.59	1.73	13	1
1:A:35:PRO:HG2	1:A:74:VAL:HA	0.59	1.72	20	2
1:A:26:LYS:O	1:A:112:LYS:HA	0.59	1.96	18	4
1:A:54:TYR:CB	1:A:59:PHE:HB3	0.59	2.27	1	5
1:A:27:VAL:HA	1:A:111:GLY:O	0.59	1.98	5	3
1:A:67:PRO:HD3	1:A:90:ASP:O	0.58	1.98	19	14
1:A:118:LYS:HG3	1:A:132:GLU:OE2	0.58	1.98	4	2
1:A:20:ASN:HA	1:A:23:LEU:HD13	0.58	1.75	6	1
1:A:129:LEU:O	1:A:133:ILE:HG12	0.58	1.98	19	2
1:A:54:TYR:HB3	1:A:59:PHE:CB	0.58	2.23	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:CYS:HA	1:A:44:MET:HG2	0.58	1.73	4	2
1:A:28:THR:HG23	1:A:60:GLN:HG3	0.57	1.76	17	3
1:A:79:LYS:CE	1:A:79:LYS:HA	0.57	2.28	7	1
1:A:30:ILE:HB	1:A:108:VAL:CG1	0.57	2.29	17	4
1:A:109:LEU:HB2	1:A:118:LYS:HB2	0.56	1.77	7	2
1:A:72:GLU:HA	1:A:75:ARG:CG	0.56	2.30	3	4
1:A:118:LYS:HG3	1:A:119:THR:N	0.56	2.15	18	1
1:A:23:LEU:HD21	1:A:62:LEU:HD11	0.56	1.76	10	1
1:A:128:LYS:HB2	1:A:128:LYS:NZ	0.56	2.16	5	1
1:A:33:TRP:O	1:A:65:ALA:HA	0.56	2.01	15	12
1:A:71:ILE:HA	1:A:74:VAL:HG22	0.56	1.77	18	3
1:A:110:ILE:HG23	1:A:115:GLU:HA	0.55	1.77	6	1
1:A:30:ILE:HB	1:A:108:VAL:HG22	0.55	1.78	18	1
1:A:66:GLN:HG2	1:A:68:ILE:HG12	0.55	1.78	18	1
1:A:13:LEU:HD13	1:A:75:ARG:HA	0.55	1.77	10	1
1:A:72:GLU:HA	1:A:75:ARG:HE	0.55	1.61	11	2
1:A:109:LEU:HD21	1:A:129:LEU:HD11	0.55	1.78	9	1
1:A:44:MET:O	1:A:48:ILE:HG12	0.55	2.01	1	15
1:A:90:ASP:O	1:A:92:ASP:N	0.54	2.40	12	1
1:A:99:PHE:HA	1:A:116:ILE:HD11	0.54	1.79	9	1
1:A:66:GLN:HB3	1:A:67:PRO:HD2	0.54	1.79	2	1
1:A:75:ARG:HA	1:A:78:VAL:CG2	0.54	2.33	20	6
1:A:42:SER:HB2	1:A:43:GLU:OE2	0.54	2.03	9	1
1:A:109:LEU:HD11	1:A:129:LEU:HD11	0.54	1.77	16	1
1:A:110:ILE:HG12	1:A:115:GLU:OE2	0.53	2.02	6	1
1:A:23:LEU:HD23	1:A:110:ILE:HD13	0.53	1.78	6	1
1:A:66:GLN:HB2	1:A:67:PRO:HD2	0.53	1.80	16	15
1:A:35:PRO:HD2	1:A:69:ASP:HB2	0.53	1.81	3	2
1:A:67:PRO:HD2	1:A:93:LYS:HG3	0.53	1.80	19	2
1:A:24:GLN:HG2	1:A:113:LYS:HA	0.53	1.81	13	1
1:A:61:VAL:CG1	1:A:85:PHE:HB3	0.52	2.28	15	1
1:A:34:PHE:HB3	1:A:66:GLN:NE2	0.52	2.19	8	1
1:A:66:GLN:HB2	1:A:93:LYS:HG2	0.52	1.81	19	2
1:A:92:ASP:O	1:A:93:LYS:HB2	0.52	2.04	6	2
1:A:118:LYS:HE3	1:A:120:TYR:CE2	0.52	2.40	18	1
1:A:128:LYS:HA	1:A:131:GLN:HE21	0.52	1.64	8	1
1:A:57:LYS:HG3	1:A:58:ASN:OD1	0.52	2.04	3	1
1:A:51:ALA:O	1:A:55:LYS:HB2	0.52	2.03	19	4
1:A:34:PHE:HB3	1:A:66:GLN:OE1	0.52	2.03	7	2
1:A:46:LYS:HB3	1:A:126:PHE:CZ	0.52	2.38	12	1
1:A:54:TYR:HA	1:A:57:LYS:HE3	0.52	1.81	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:79:LYS:HB3	1:A:79:LYS:HZ3	0.52	1.64	6	1
1:A:27:VAL:O	1:A:59:PHE:HA	0.52	2.04	3	5
1:A:27:VAL:HG13	1:A:59:PHE:CD1	0.52	2.40	16	1
1:A:12:ASP:HA	1:A:88:MET:HA	0.51	1.81	12	1
1:A:71:ILE:HA	1:A:74:VAL:CG2	0.51	2.35	10	1
1:A:63:ALA:HB3	1:A:87:VAL:HG12	0.51	1.83	11	1
1:A:71:ILE:O	1:A:75:ARG:HG2	0.51	2.06	9	4
1:A:71:ILE:O	1:A:75:ARG:HG3	0.51	2.06	8	3
1:A:108:VAL:HG12	1:A:119:THR:HG23	0.51	1.83	18	1
1:A:16:LYS:HZ2	1:A:18:VAL:HG12	0.51	1.66	11	1
1:A:57:LYS:O	1:A:58:ASN:HB3	0.51	2.06	1	1
1:A:75:ARG:O	1:A:79:LYS:HB2	0.51	2.06	2	1
1:A:30:ILE:HA	1:A:62:LEU:O	0.50	2.06	1	2
1:A:93:LYS:O	1:A:97:GLN:HG3	0.50	2.07	11	2
1:A:126:PHE:HA	1:A:129:LEU:HB3	0.50	1.84	18	4
1:A:35:PRO:HG2	1:A:69:ASP:CB	0.50	2.35	15	1
1:A:78:VAL:HA	1:A:83:LEU:HD12	0.50	1.83	19	1
1:A:125:ASP:OD1	1:A:128:LYS:HG2	0.50	2.07	17	2
1:A:67:PRO:HD3	1:A:91:ALA:CA	0.50	2.29	12	1
1:A:125:ASP:OD2	1:A:128:LYS:HB3	0.50	2.06	7	2
1:A:67:PRO:O	1:A:68:ILE:HB	0.49	2.06	11	3
1:A:42:SER:O	1:A:46:LYS:HE3	0.49	2.06	7	1
1:A:93:LYS:HB2	1:A:93:LYS:NZ	0.49	2.21	1	1
1:A:57:LYS:HB2	1:A:57:LYS:HZ2	0.49	1.67	12	1
1:A:55:LYS:HA	1:A:59:PHE:O	0.49	2.07	4	3
1:A:13:LEU:HD12	1:A:78:VAL:HG21	0.49	1.82	4	2
1:A:93:LYS:O	1:A:97:GLN:HG2	0.49	2.07	19	1
1:A:71:ILE:O	1:A:74:VAL:HG22	0.49	2.07	8	1
1:A:69:ASP:OD1	1:A:70:PRO:HD2	0.49	2.07	13	2
1:A:52:ASN:HA	1:A:55:LYS:NZ	0.48	2.22	4	1
1:A:71:ILE:HG23	1:A:72:GLU:OE1	0.48	2.08	13	1
1:A:49:LYS:NZ	1:A:49:LYS:HB2	0.48	2.24	8	1
1:A:125:ASP:O	1:A:129:LEU:HB2	0.48	2.08	10	2
1:A:12:ASP:HB3	1:A:16:LYS:O	0.48	2.09	5	1
1:A:40:CYS:HA	1:A:44:MET:HG3	0.48	1.85	16	1
1:A:94:ALA:HA	1:A:97:GLN:HE21	0.48	1.69	2	1
1:A:23:LEU:CD2	1:A:110:ILE:HD13	0.48	2.38	6	1
1:A:79:LYS:NZ	1:A:79:LYS:HB2	0.48	2.24	19	1
1:A:97:GLN:OE1	1:A:97:GLN:HA	0.48	2.08	19	1
1:A:128:LYS:HB3	1:A:128:LYS:NZ	0.48	2.24	2	1
1:A:108:VAL:HG22	1:A:119:THR:HG22	0.48	1.85	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:26:LYS:HG2	1:A:58:ASN:OD1	0.47	2.09	15	2
1:A:48:ILE:HD13	1:A:85:PHE:HE2	0.47	1.68	15	1
1:A:38:PRO:O	1:A:41:VAL:HG12	0.47	2.09	16	2
1:A:47:ILE:HG23	1:A:61:VAL:HG11	0.47	1.84	6	1
1:A:78:VAL:HA	1:A:83:LEU:HD22	0.47	1.84	7	1
1:A:128:LYS:HA	1:A:131:GLN:HG2	0.47	1.85	9	3
1:A:78:VAL:HG11	1:A:87:VAL:HG21	0.47	1.84	11	1
1:A:44:MET:CG	1:A:45:PRO:HD3	0.47	2.39	9	1
1:A:112:LYS:O	1:A:113:LYS:HB2	0.47	2.08	10	1
1:A:30:ILE:HB	1:A:108:VAL:HG23	0.47	1.86	14	4
1:A:11:PRO:HA	1:A:17:THR:HA	0.47	1.86	11	2
1:A:44:MET:N	1:A:45:PRO:HD2	0.47	2.25	5	3
1:A:129:LEU:O	1:A:133:ILE:HG13	0.47	2.10	6	2
1:A:75:ARG:O	1:A:79:LYS:HG2	0.47	2.11	17	1
1:A:30:ILE:CG1	1:A:110:ILE:HD11	0.46	2.41	6	1
1:A:72:GLU:H	1:A:72:GLU:CD	0.46	2.14	11	2
1:A:42:SER:O	1:A:46:LYS:HB3	0.46	2.10	1	1
1:A:33:TRP:NE1	1:A:63:ALA:HB1	0.46	2.25	1	2
1:A:120:TYR:HB3	1:A:124:PRO:HB3	0.46	1.86	2	1
1:A:66:GLN:HB2	1:A:67:PRO:CD	0.46	2.41	10	1
1:A:75:ARG:CA	1:A:78:VAL:HG22	0.46	2.40	5	6
1:A:54:TYR:HA	1:A:57:LYS:HB2	0.46	1.87	11	1
1:A:49:LYS:HZ2	1:A:53:ASP:HB2	0.46	1.71	1	1
1:A:129:LEU:HA	1:A:132:GLU:HG2	0.46	1.86	18	1
1:A:97:GLN:HE21	1:A:97:GLN:HA	0.46	1.71	15	1
1:A:31:ASN:HA	1:A:106:THR:O	0.46	2.11	8	2
1:A:112:LYS:O	1:A:113:LYS:HB3	0.46	2.11	3	1
1:A:91:ALA:C	1:A:93:LYS:H	0.46	2.14	12	1
1:A:90:ASP:OD2	1:A:95:VAL:HG12	0.45	2.11	18	1
1:A:10:LEU:HD13	1:A:92:ASP:HB3	0.45	1.88	12	1
1:A:43:GLU:CD	1:A:46:LYS:HZ1	0.45	2.14	3	1
1:A:34:PHE:O	1:A:37:CYS:HB2	0.45	2.11	15	1
1:A:12:ASP:HA	1:A:88:MET:HG3	0.45	1.89	16	2
1:A:43:GLU:O	1:A:47:ILE:HG12	0.45	2.11	2	2
1:A:27:VAL:HG13	1:A:59:PHE:HA	0.45	1.88	11	1
1:A:16:LYS:C	1:A:16:LYS:HD3	0.45	2.32	5	1
1:A:35:PRO:CG	1:A:74:VAL:HA	0.45	2.41	4	1
1:A:21:ALA:HA	1:A:24:GLN:HE21	0.45	1.72	6	1
1:A:13:LEU:HB3	1:A:75:ARG:HG2	0.45	1.87	5	1
1:A:78:VAL:HG22	1:A:83:LEU:HD22	0.44	1.88	7	2
1:A:23:LEU:HD22	1:A:28:THR:HG21	0.44	1.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:35:PRO:HD3	1:A:74:VAL:HG12	0.44	1.89	10	1
1:A:28:THR:HB	1:A:110:ILE:HB	0.44	1.88	12	6
1:A:64:VAL:HG12	1:A:90:ASP:HB2	0.44	1.88	11	1
1:A:67:PRO:HD2	1:A:93:LYS:HB2	0.44	1.88	7	1
1:A:90:ASP:OD2	1:A:95:VAL:HG22	0.44	2.12	19	6
1:A:125:ASP:HB2	1:A:128:LYS:HE2	0.44	1.89	20	1
1:A:94:ALA:HA	1:A:97:GLN:NE2	0.44	2.28	2	1
1:A:72:GLU:HA	1:A:75:ARG:CD	0.44	2.43	4	1
1:A:125:ASP:CG	1:A:128:LYS:HG2	0.44	2.33	6	1
1:A:55:LYS:O	1:A:55:LYS:HD3	0.44	2.13	20	1
1:A:29:LEU:HD11	1:A:107:SER:HB3	0.44	1.90	11	1
1:A:26:LYS:HB2	1:A:26:LYS:NZ	0.44	2.28	10	1
1:A:37:CYS:O	1:A:40:CYS:HB3	0.44	2.13	19	1
1:A:101:THR:HB	1:A:104:TYR:CE1	0.44	2.47	20	1
1:A:11:PRO:HA	1:A:16:LYS:O	0.44	2.13	9	3
1:A:110:ILE:CG2	1:A:114:GLY:HA2	0.43	2.43	7	1
1:A:23:LEU:HB3	1:A:114:GLY:HA2	0.43	1.90	9	1
1:A:63:ALA:HB3	1:A:87:VAL:HG22	0.43	1.90	1	1
1:A:13:LEU:HD11	1:A:74:VAL:HG12	0.43	1.89	19	1
1:A:23:LEU:HD23	1:A:110:ILE:HG21	0.43	1.90	20	1
1:A:79:LYS:N	1:A:79:LYS:HD2	0.43	2.28	7	1
1:A:12:ASP:HB3	1:A:16:LYS:HB3	0.43	1.90	13	1
1:A:109:LEU:HD21	1:A:120:TYR:HD2	0.43	1.74	2	1
1:A:66:GLN:HG3	1:A:68:ILE:HG12	0.43	1.90	14	1
1:A:112:LYS:O	1:A:115:GLU:HG2	0.43	2.14	3	1
1:A:83:LEU:HD12	1:A:85:PHE:CE2	0.43	2.48	6	1
1:A:28:THR:HA	1:A:60:GLN:O	0.43	2.14	1	4
1:A:120:TYR:CD2	1:A:124:PRO:HB3	0.43	2.49	16	1
1:A:43:GLU:HG2	1:A:105:PRO:HG3	0.43	1.90	6	1
1:A:104:TYR:HB3	1:A:105:PRO:HA	0.43	1.91	4	2
1:A:10:LEU:HD11	1:A:89:TYR:HB3	0.43	1.89	12	1
1:A:109:LEU:HD12	1:A:118:LYS:HB3	0.42	1.90	11	2
1:A:78:VAL:HG12	1:A:83:LEU:HD22	0.42	1.91	5	2
1:A:32:PHE:HA	1:A:64:VAL:O	0.42	2.14	19	2
1:A:132:GLU:O	1:A:135:THR:HB	0.42	2.15	18	1
1:A:67:PRO:N	1:A:90:ASP:HB2	0.42	2.28	12	1
1:A:10:LEU:O	1:A:18:VAL:HG12	0.42	2.13	15	1
1:A:78:VAL:HA	1:A:83:LEU:CD1	0.42	2.44	8	1
1:A:21:ALA:O	1:A:24:GLN:HG3	0.42	2.14	5	1
1:A:78:VAL:HG23	1:A:83:LEU:HB2	0.42	1.90	15	1
1:A:46:LYS:HZ2	1:A:124:PRO:HD2	0.42	1.73	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:THR:O	1:A:54:TYR:HD1	0.42	1.98	19	1
1:A:126:PHE:HA	1:A:129:LEU:CB	0.42	2.44	11	1
1:A:57:LYS:HB2	1:A:57:LYS:NZ	0.42	2.30	12	1
1:A:65:ALA:O	1:A:90:ASP:HA	0.42	2.14	12	1
1:A:111:GLY:O	1:A:112:LYS:HG3	0.42	2.15	10	1
1:A:48:ILE:HA	1:A:85:PHE:CE2	0.42	2.50	15	1
1:A:30:ILE:HD13	1:A:62:LEU:HB2	0.42	1.91	6	1
1:A:12:ASP:HA	1:A:88:MET:HG2	0.42	1.91	17	2
1:A:57:LYS:O	1:A:58:ASN:HB2	0.42	2.14	19	1
1:A:33:TRP:CD1	1:A:63:ALA:HB1	0.42	2.50	18	1
1:A:16:LYS:HE3	1:A:16:LYS:HA	0.42	1.92	13	1
1:A:92:ASP:OD2	1:A:94:ALA:HB2	0.42	2.14	13	1
1:A:41:VAL:HG23	1:A:42:SER:H	0.41	1.76	4	1
1:A:42:SER:O	1:A:46:LYS:HD3	0.41	2.15	4	2
1:A:7:ALA:HA	1:A:20:ASN:OD1	0.41	2.15	19	1
1:A:50:THR:O	1:A:54:TYR:HD2	0.41	1.98	8	1
1:A:18:VAL:HG11	1:A:62:LEU:HD21	0.41	1.91	2	1
1:A:43:GLU:O	1:A:47:ILE:HG13	0.41	2.16	4	1
1:A:109:LEU:HD23	1:A:118:LYS:HB3	0.41	1.93	1	1
1:A:26:LYS:HB2	1:A:58:ASN:O	0.41	2.16	4	1
1:A:58:ASN:OD1	1:A:112:LYS:HE2	0.41	2.15	7	1
1:A:66:GLN:HA	1:A:90:ASP:HB3	0.41	1.91	8	2
1:A:67:PRO:HD2	1:A:93:LYS:CG	0.41	2.45	19	1
1:A:108:VAL:HG22	1:A:119:THR:HG23	0.41	1.92	8	1
1:A:113:LYS:HB3	1:A:115:GLU:OE1	0.41	2.16	14	1
1:A:99:PHE:CE2	1:A:116:ILE:HD12	0.41	2.51	4	1
1:A:109:LEU:HD22	1:A:109:LEU:N	0.41	2.31	2	1
1:A:67:PRO:CA	1:A:90:ASP:HB2	0.40	2.46	12	1
1:A:109:LEU:HD23	1:A:118:LYS:CB	0.40	2.46	17	1
1:A:8:PHE:CE1	1:A:23:LEU:HD11	0.40	2.51	5	1
1:A:55:LYS:HA	1:A:55:LYS:HE3	0.40	1.93	6	1
1:A:51:ALA:HB1	1:A:61:VAL:HG21	0.40	1.93	11	1
1:A:9:SER:HA	1:A:18:VAL:O	0.40	2.16	7	1
1:A:33:TRP:HB2	1:A:40:CYS:SG	0.40	2.56	9	1
1:A:18:VAL:HB	1:A:88:MET:CE	0.40	2.45	10	1
1:A:104:TYR:HA	1:A:105:PRO:C	0.40	2.37	14	1
1:A:23:LEU:HD12	1:A:23:LEU:H	0.40	1.75	6	1
1:A:66:GLN:HB2	1:A:93:LYS:HE2	0.40	1.92	11	1
1:A:8:PHE:HB2	1:A:95:VAL:HG12	0.40	1.93	12	1
1:A:54:TYR:O	1:A:59:PHE:HB3	0.40	2.17	15	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	130/153 (85%)	119±2 (92±2%)	8±2 (6±1%)	3±1 (2±1%)	14	55
All	All	2600/3060 (85%)	2381 (92%)	169 (6%)	50 (2%)	14	55

All 19 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	58	ASN	17
1	A	116	ILE	6
1	A	67	PRO	4
1	A	111	GLY	3
1	A	83	LEU	2
1	A	113	LYS	2
1	A	123	GLU	2
1	A	57	LYS	2
1	A	15	GLY	2
1	A	24	GLN	1
1	A	115	GLU	1
1	A	90	ASP	1
1	A	70	PRO	1
1	A	91	ALA	1
1	A	125	ASP	1
1	A	112	LYS	1
1	A	124	PRO	1
1	A	122	GLY	1
1	A	7	ALA	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	111/131 (85%)	105±2 (95±2%)	6±2 (5±2%)	30	76
All	All	2220/2620 (85%)	2100 (95%)	120 (5%)	30	76

All 43 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	12	ASP	15
1	A	66	GLN	10
1	A	69	ASP	9
1	A	57	LYS	7
1	A	129	LEU	4
1	A	55	LYS	4
1	A	77	TYR	4
1	A	49	LYS	4
1	A	72	GLU	4
1	A	115	GLU	4
1	A	117	LEU	3
1	A	118	LYS	3
1	A	125	ASP	3
1	A	93	LYS	3
1	A	113	LYS	3
1	A	52	ASN	3
1	A	26	LYS	3
1	A	112	LYS	2
1	A	102	GLN	2
1	A	134	ASP	2
1	A	27	VAL	2
1	A	53	ASP	2
1	A	76	GLN	2
1	A	80	ASP	2
1	A	14	HIS	2
1	A	90	ASP	1
1	A	123	GLU	1
1	A	44	MET	1
1	A	10	LEU	1
1	A	61	VAL	1
1	A	46	LYS	1
1	A	97	GLN	1
1	A	16	LYS	1
1	A	20	ASN	1
1	A	86	THR	1
1	A	24	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	36	SER	1
1	A	54	TYR	1
1	A	58	ASN	1
1	A	92	ASP	1
1	A	119	THR	1
1	A	79	LYS	1
1	A	42	SER	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 ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided