



Full wwPDB NMR Structure Validation Report ⓘ

Jun 2, 2020 – 02:56 pm BST

PDB ID : 5Z4F
Title : An anthrahydroquino-Gama-pyrone synthase Txn09 complexed with SUM
Authors : Song, Y.J.; Cao, C.Y.
Deposited on : 2018-01-11

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 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

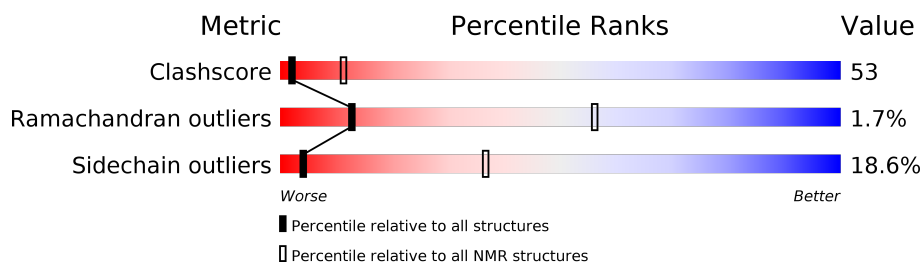
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	158	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 5 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:31, A:45-A:75, A:80-A:91, A:98-A:110, A:114-A:127, A:131-A:137, A:146-A:154 (116)	0.25	5

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 2 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2460 atoms, of which 1196 are hydrogens and 0 are deuteriums.

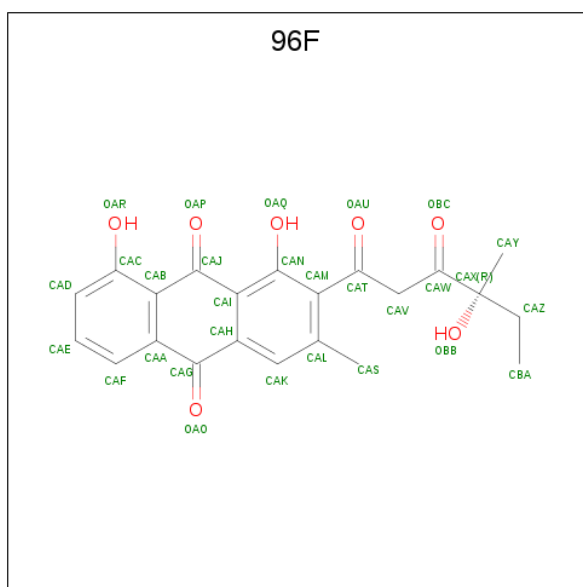
- Molecule 1 is a protein called TxnO9.

Mol	Chain	Residues	Atoms						Trace
1	A	154	Total	C	H	N	O	S	0
			2412	789	1177	220	223	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0K1H313
A	0	SER	-	expression tag	UNP A0A0K1H313
A	155	LEU	-	expression tag	UNP A0A0K1H313
A	156	GLU	-	expression tag	UNP A0A0K1H313

- Molecule 2 is 1,8-dihydroxy-2-[(4R)-4-hydroxy-4-methyl-3-oxohexanoyl]-3-methylanthracene-9,10-dione (three-letter code: 96F) (formula: C₂₂H₂₀O₇).



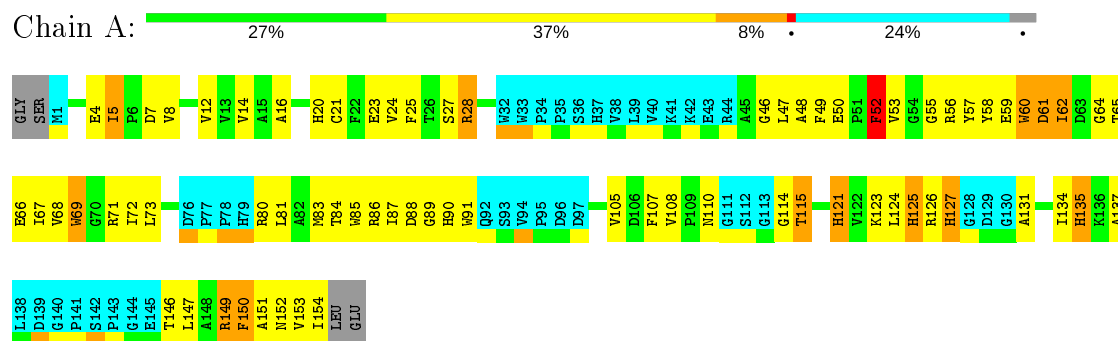
Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			48	22	19	7

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: TxnO9

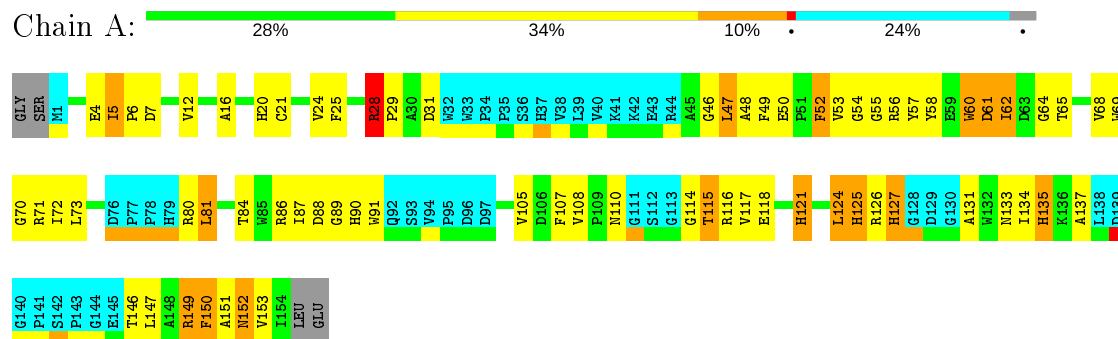


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

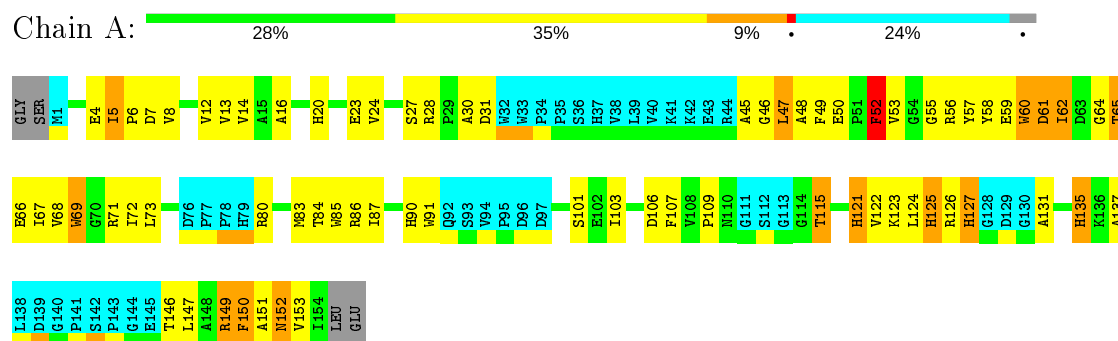
4.2.1 Score per residue for model 1

- Molecule 1: TxnO9



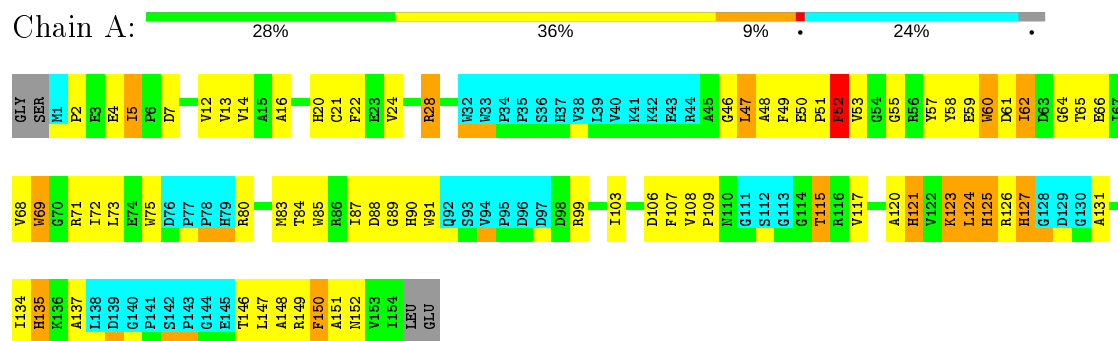
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: TxnO9



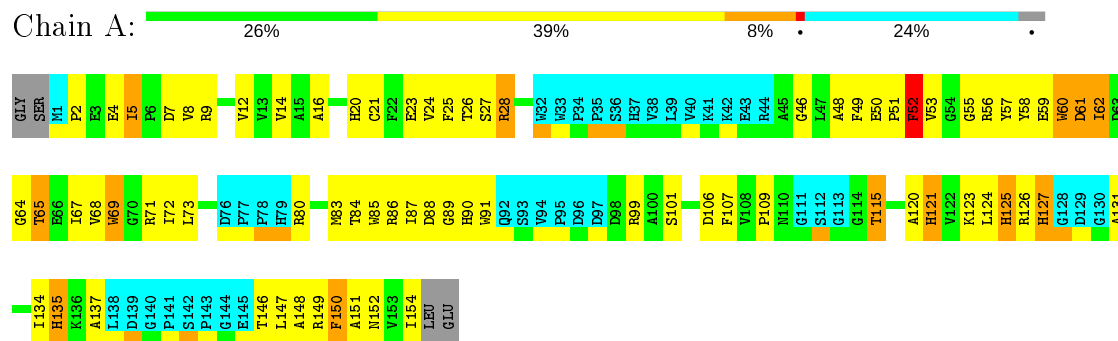
4.2.6 Score per residue for model 6

- Molecule 1: TxnO9



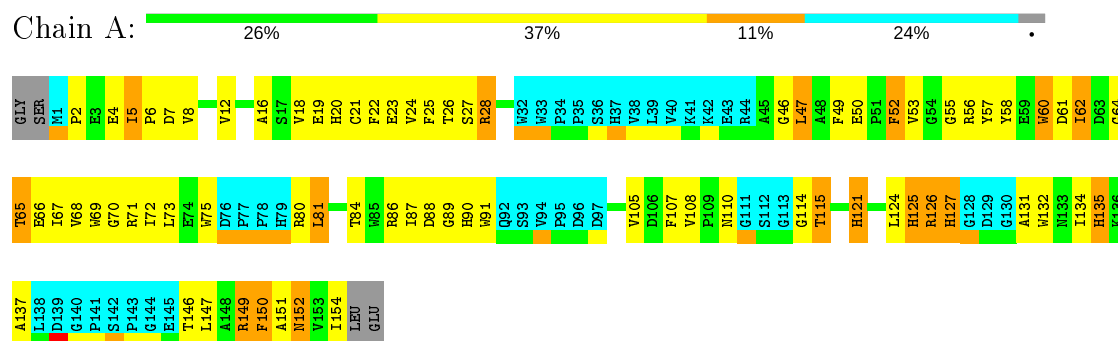
4.2.7 Score per residue for model 7

- Molecule 1: TxnO9



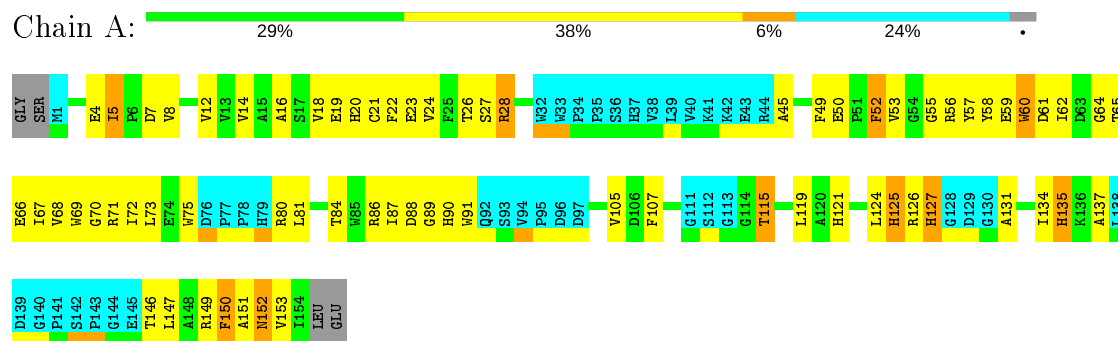
4.2.8 Score per residue for model 8

- Molecule 1: TxnO9



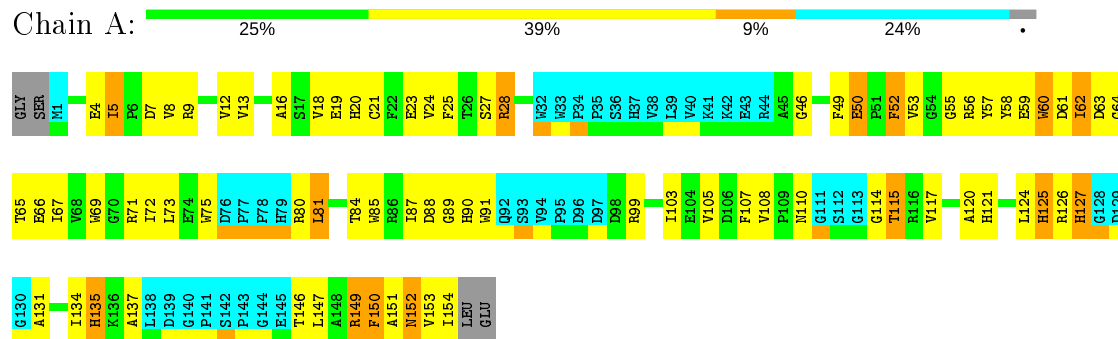
4.2.9 Score per residue for model 9

- Molecule 1: TxnO9



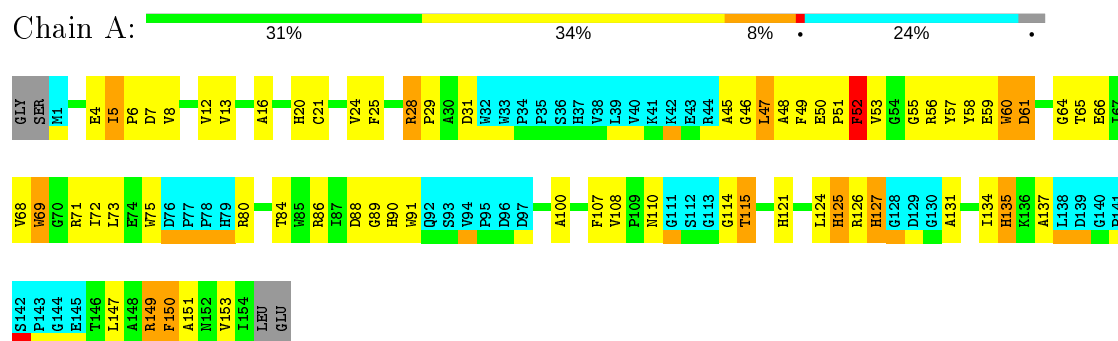
4.2.10 Score per residue for model 10

- Molecule 1: TxnO9



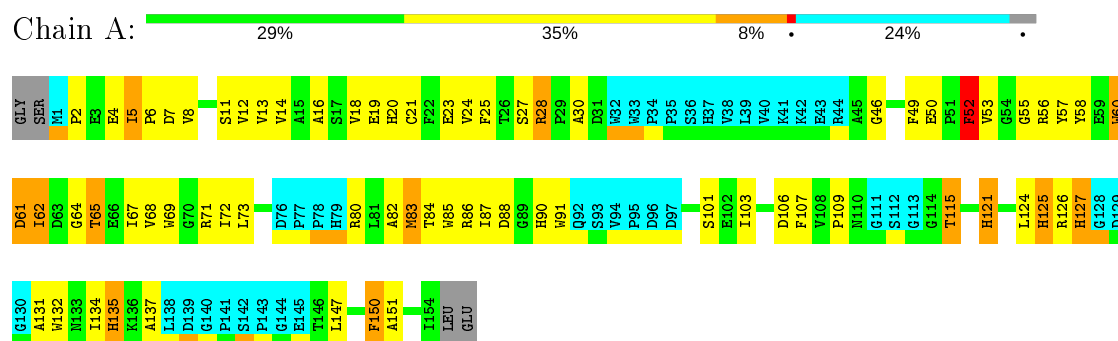
4.2.14 Score per residue for model 14

- Molecule 1: TxnO9



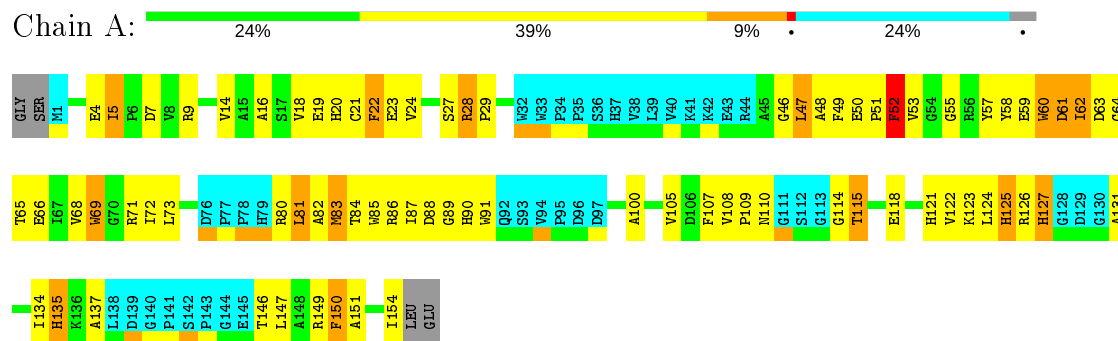
4.2.15 Score per residue for model 15

- Molecule 1: TxnO9



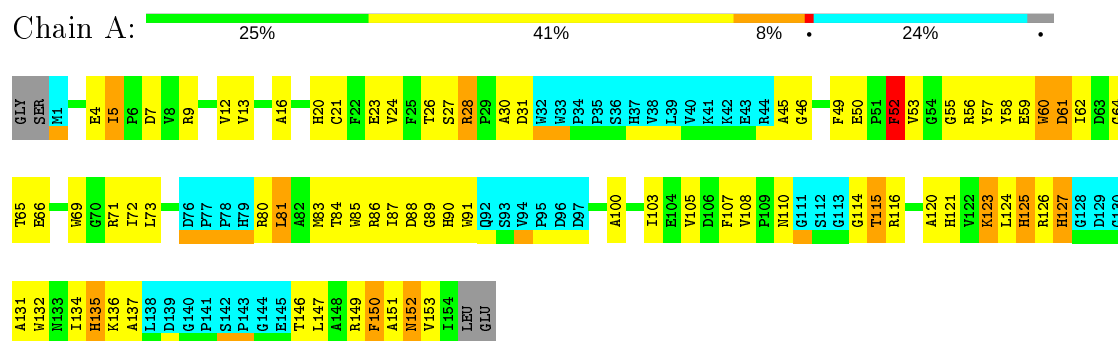
4.2.16 Score per residue for model 16

- Molecule 1: TxnO9



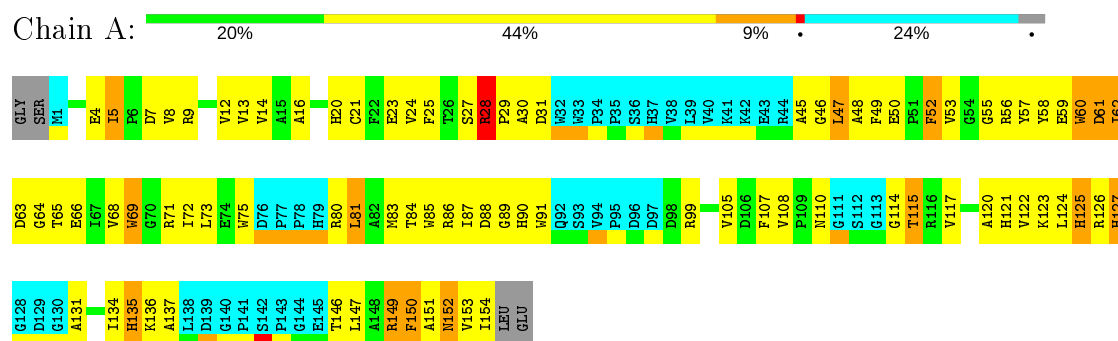
4.2.17 Score per residue for model 17

- Molecule 1: TxnO9



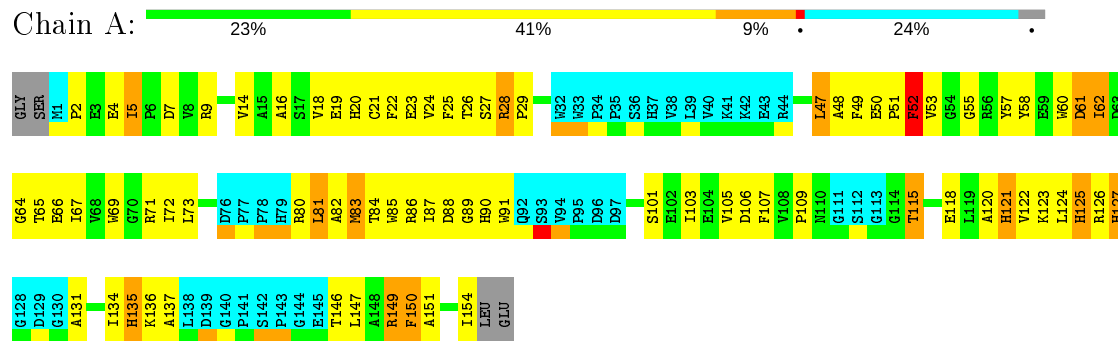
4.2.18 Score per residue for model 18

- Molecule 1: TxnO9



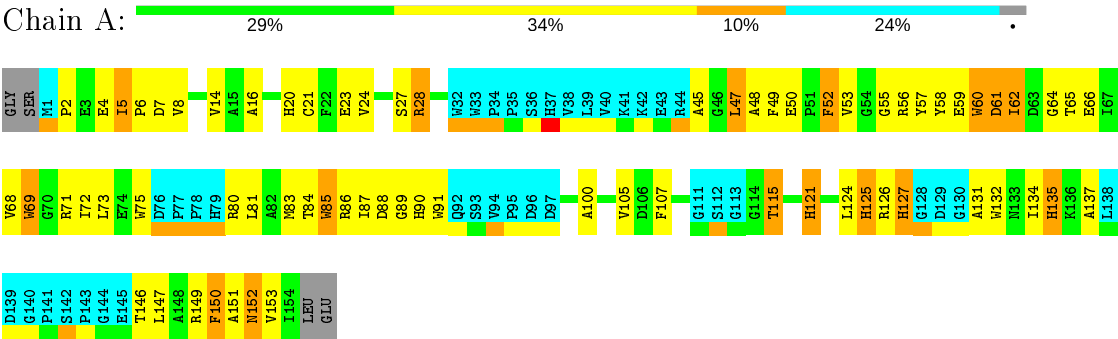
4.2.19 Score per residue for model 19

- Molecule 1: TxnO9



4.2.20 Score per residue for model 20

● Molecule 1: TxnO9



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	refinement	
TALOS	structure calculation	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1702
Number of shifts mapped to atoms	1702
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 96F

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	949	917	911	99±8
2	A	29	19	0	9±2
All	All	19560	18720	18220	1993

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 53.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ALA:HB3	1:A:47:LEU:HD12	0.97	1.36	18	1
1:A:69:TRP:CE3	1:A:70:GLY:N	0.90	2.40	2	1
1:A:47:LEU:N	1:A:47:LEU:HD12	0.88	1.84	6	7
1:A:50:GLU:O	1:A:52:PHE:CE2	0.85	2.29	14	14
1:A:47:LEU:HD12	1:A:47:LEU:N	0.85	1.86	14	6
1:A:50:GLU:O	1:A:52:PHE:CE1	0.85	2.29	7	6
1:A:57:TYR:CZ	1:A:72:ILE:HD11	0.83	2.07	8	20
1:A:147:LEU:HD11	2:A:201:96F:CAK	0.83	2.03	12	18
1:A:53:VAL:HG13	1:A:73:LEU:O	0.81	1.74	10	6
1:A:47:LEU:N	1:A:47:LEU:HD13	0.81	1.91	5	2
1:A:127:HIS:CE1	1:A:131:ALA:HB1	0.80	2.12	4	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ILE:HG21	1:A:91:TRP:O	0.80	1.75	9	2
1:A:147:LEU:HD21	2:A:201:96F:OAO	0.79	1.77	18	16
1:A:121:HIS:ND1	1:A:124:LEU:HD12	0.78	1.92	12	6
1:A:57:TYR:CE1	1:A:72:ILE:HD11	0.76	2.16	18	9
1:A:47:LEU:O	1:A:47:LEU:HD22	0.76	1.79	5	2
1:A:58:TYR:CE1	1:A:68:VAL:HG22	0.76	2.16	20	5
1:A:57:TYR:CE2	1:A:72:ILE:HD11	0.75	2.17	15	11
1:A:52:PHE:CD1	1:A:52:PHE:N	0.75	2.51	2	5
1:A:58:TYR:CE2	1:A:68:VAL:HG22	0.75	2.17	5	3
1:A:52:PHE:N	1:A:52:PHE:CD2	0.74	2.52	4	7
1:A:147:LEU:HD11	2:A:201:96F:CAL	0.74	2.13	13	13
1:A:47:LEU:H	1:A:47:LEU:HD12	0.74	1.40	19	7
1:A:61:ASP:OD1	1:A:62:ILE:HD13	0.74	1.82	10	1
1:A:150:PHE:CD2	1:A:151:ALA:N	0.72	2.57	8	12
1:A:67:ILE:HD13	1:A:91:TRP:O	0.72	1.84	2	4
1:A:4:GLU:C	1:A:5:ILE:HD13	0.72	2.05	7	20
1:A:52:PHE:CD2	1:A:52:PHE:N	0.72	2.53	6	7
1:A:52:PHE:N	1:A:52:PHE:CD1	0.72	2.54	16	1
1:A:91:TRP:CZ2	1:A:137:ALA:HB2	0.72	2.20	6	18
1:A:150:PHE:CD1	1:A:151:ALA:N	0.71	2.58	12	8
1:A:124:LEU:O	1:A:127:HIS:CE1	0.71	2.43	10	20
1:A:49:PHE:CE2	1:A:57:TYR:CD1	0.71	2.79	11	6
1:A:47:LEU:HD12	1:A:47:LEU:H	0.71	1.44	3	4
1:A:49:PHE:CE2	1:A:57:TYR:CD2	0.71	2.79	16	5
1:A:49:PHE:CE1	1:A:57:TYR:CD2	0.71	2.78	20	3
1:A:147:LEU:H	1:A:147:LEU:HD12	0.70	1.47	13	9
1:A:49:PHE:CD1	1:A:57:TYR:CD1	0.70	2.80	2	6
1:A:85:TRP:CD1	1:A:103:ILE:HD12	0.70	2.22	19	6
1:A:49:PHE:CE1	1:A:57:TYR:CD1	0.70	2.79	5	6
1:A:46:GLY:C	1:A:47:LEU:HD13	0.70	2.07	18	2
1:A:49:PHE:CD1	1:A:57:TYR:CD2	0.70	2.80	18	3
1:A:81:LEU:O	1:A:81:LEU:HD12	0.69	1.86	3	2
1:A:147:LEU:HD21	2:A:201:96F:CAG	0.69	2.17	8	15
1:A:49:PHE:CD2	1:A:57:TYR:CD1	0.69	2.80	13	6
1:A:46:GLY:C	1:A:47:LEU:HD12	0.69	2.08	2	2
1:A:71:ARG:C	1:A:72:ILE:HD12	0.69	2.07	18	16
1:A:49:PHE:CE1	1:A:57:TYR:CG	0.68	2.82	2	7
1:A:20:HIS:NE2	1:A:24:VAL:HG21	0.67	2.03	13	14
1:A:71:ARG:NH2	1:A:86:ARG:NH1	0.67	2.41	20	1
1:A:62:ILE:HD13	1:A:62:ILE:N	0.67	2.05	12	4
1:A:62:ILE:HD12	1:A:62:ILE:N	0.67	2.05	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ILE:HD13	1:A:134:ILE:HG23	0.66	1.66	1	2
1:A:52:PHE:CE2	1:A:55:GLY:CA	0.66	2.79	5	14
1:A:59:GLU:N	1:A:69:TRP:HE1	0.66	1.88	4	11
1:A:124:LEU:O	1:A:127:HIS:ND1	0.66	2.29	4	12
1:A:21:CYS:SG	1:A:115:THR:HG21	0.66	2.30	11	16
1:A:8:VAL:HG12	1:A:121:HIS:NE2	0.66	2.06	12	4
1:A:52:PHE:CE1	1:A:55:GLY:CA	0.66	2.79	3	6
1:A:83:MET:N	1:A:83:MET:SD	0.65	2.68	15	3
1:A:62:ILE:N	1:A:62:ILE:HD13	0.65	2.07	19	8
1:A:62:ILE:N	1:A:62:ILE:HD12	0.65	2.07	15	1
1:A:47:LEU:N	1:A:47:LEU:CD1	0.65	2.56	1	7
1:A:71:ARG:CZ	1:A:86:ARG:NH1	0.64	2.61	3	2
1:A:62:ILE:H	1:A:62:ILE:CD1	0.64	2.05	15	8
1:A:65:THR:HG22	1:A:66:GLU:H	0.64	1.52	6	13
1:A:127:HIS:NE2	1:A:131:ALA:HB1	0.64	2.07	14	9
1:A:87:ILE:HD13	1:A:134:ILE:CG2	0.64	2.22	1	15
1:A:56:ARG:NH1	1:A:86:ARG:HH22	0.64	1.90	17	2
1:A:124:LEU:O	1:A:126:ARG:N	0.64	2.31	12	20
1:A:147:LEU:HD12	1:A:147:LEU:H	0.64	1.53	10	11
1:A:135:HIS:ND1	1:A:135:HIS:O	0.63	2.31	2	7
1:A:62:ILE:CD1	1:A:62:ILE:H	0.63	2.06	5	7
1:A:62:ILE:HD12	1:A:62:ILE:H	0.63	1.54	5	1
1:A:62:ILE:H	1:A:62:ILE:HD12	0.63	1.54	7	2
1:A:91:TRP:CE2	1:A:137:ALA:HB2	0.63	2.28	1	18
1:A:58:TYR:CD2	1:A:58:TYR:N	0.63	2.66	12	8
1:A:30:ALA:HB3	1:A:47:LEU:CD1	0.63	2.20	18	1
1:A:135:HIS:O	1:A:135:HIS:ND1	0.63	2.32	1	13
1:A:49:PHE:CD2	1:A:57:TYR:CD2	0.63	2.87	9	5
1:A:47:LEU:CD1	1:A:47:LEU:N	0.62	2.57	12	7
1:A:59:GLU:CB	1:A:69:TRP:HE1	0.62	2.07	13	12
1:A:58:TYR:N	1:A:58:TYR:CD1	0.62	2.67	1	6
1:A:121:HIS:O	1:A:121:HIS:CD2	0.62	2.53	8	4
1:A:26:THR:HG22	1:A:49:PHE:CD2	0.62	2.29	12	5
1:A:49:PHE:CE2	1:A:57:TYR:CG	0.62	2.88	13	10
1:A:69:TRP:CD2	1:A:70:GLY:N	0.62	2.67	2	1
1:A:150:PHE:CZ	2:A:201:96F:CAD	0.62	2.83	14	14
1:A:21:CYS:O	1:A:25:PHE:CD2	0.62	2.53	14	3
1:A:45:ALA:N	1:A:60:TRP:O	0.62	2.32	17	3
1:A:8:VAL:HG22	1:A:121:HIS:NE2	0.62	2.09	14	2
1:A:121:HIS:CD2	1:A:121:HIS:O	0.62	2.53	15	3
1:A:71:ARG:C	1:A:84:THR:O	0.61	2.39	9	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:GLY:CA	1:A:71:ARG:NH2	0.61	2.63	1	1
1:A:85:TRP:CD1	1:A:85:TRP:O	0.61	2.53	11	2
1:A:150:PHE:CE2	2:A:201:96F:CAD	0.61	2.84	16	7
1:A:58:TYR:N	1:A:58:TYR:CD2	0.61	2.68	15	6
1:A:56:ARG:NH1	1:A:86:ARG:NH2	0.61	2.47	17	2
1:A:61:ASP:OD2	1:A:61:ASP:N	0.61	2.34	11	6
1:A:61:ASP:N	1:A:61:ASP:OD1	0.61	2.34	18	2
1:A:150:PHE:CE1	2:A:201:96F:CAD	0.61	2.83	14	6
1:A:56:ARG:NH1	1:A:71:ARG:HH11	0.61	1.94	8	1
1:A:21:CYS:O	1:A:25:PHE:CD1	0.61	2.54	1	5
1:A:85:TRP:O	1:A:85:TRP:CD1	0.61	2.54	20	1
1:A:57:TYR:O	1:A:69:TRP:CE3	0.61	2.53	2	1
1:A:61:ASP:OD1	1:A:61:ASP:N	0.60	2.34	7	4
1:A:69:TRP:O	1:A:85:TRP:CE2	0.60	2.55	16	5
1:A:149:ARG:O	1:A:152:ASN:ND2	0.60	2.35	9	12
1:A:85:TRP:NE1	1:A:103:ILE:HD12	0.60	2.12	12	5
1:A:65:THR:HG22	1:A:66:GLU:N	0.60	2.12	16	12
1:A:147:LEU:N	1:A:147:LEU:HD12	0.60	2.12	6	5
1:A:56:ARG:NE	1:A:58:TYR:OH	0.59	2.35	3	11
1:A:25:PHE:O	1:A:49:PHE:CZ	0.59	2.55	12	6
1:A:57:TYR:C	1:A:58:TYR:CD1	0.59	2.76	2	3
1:A:134:ILE:HD12	1:A:134:ILE:N	0.59	2.11	13	1
1:A:89:GLY:H	1:A:99:ARG:NH1	0.59	1.96	13	1
1:A:121:HIS:CE1	1:A:124:LEU:HD12	0.59	2.32	4	6
1:A:69:TRP:O	1:A:85:TRP:NE1	0.59	2.36	7	5
1:A:16:ALA:O	1:A:115:THR:HG23	0.59	1.97	17	18
1:A:14:VAL:O	1:A:115:THR:N	0.58	2.36	6	10
1:A:60:TRP:CH2	1:A:66:GLU:OE2	0.58	2.56	13	1
1:A:85:TRP:HE1	1:A:87:ILE:CG2	0.58	2.11	3	1
1:A:61:ASP:OD1	1:A:64:GLY:N	0.58	2.36	8	1
1:A:61:ASP:N	1:A:61:ASP:OD2	0.58	2.34	20	1
1:A:116:ARG:NH1	1:A:118:GLU:OE1	0.58	2.36	1	1
1:A:60:TRP:CZ2	1:A:66:GLU:OE2	0.58	2.56	13	2
1:A:20:HIS:NE2	1:A:24:VAL:CG2	0.58	2.67	3	18
1:A:26:THR:HG22	1:A:49:PHE:CD1	0.58	2.33	8	2
1:A:121:HIS:C	1:A:121:HIS:CD2	0.58	2.76	6	1
1:A:87:ILE:HD11	1:A:91:TRP:CD1	0.58	2.33	1	2
1:A:67:ILE:CD1	1:A:91:TRP:O	0.58	2.51	3	6
1:A:88:ASP:OD1	1:A:99:ARG:NH1	0.58	2.36	6	1
1:A:54:GLY:CA	1:A:71:ARG:HH22	0.58	2.12	1	1
1:A:5:ILE:HD13	1:A:5:ILE:N	0.57	2.14	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ASN:HD21	1:A:153:VAL:HG13	0.57	1.59	1	6
1:A:127:HIS:CE1	1:A:131:ALA:CB	0.57	2.87	18	18
1:A:71:ARG:NE	1:A:86:ARG:NH1	0.57	2.53	3	1
1:A:146:THR:HG21	2:A:201:96F:OAQ	0.57	1.99	16	8
1:A:71:ARG:CZ	1:A:86:ARG:HH11	0.57	2.13	3	2
1:A:121:HIS:ND1	1:A:124:LEU:CD1	0.57	2.68	9	6
1:A:54:GLY:O	1:A:71:ARG:NH2	0.57	2.38	1	1
1:A:50:GLU:O	1:A:52:PHE:CZ	0.56	2.58	14	4
1:A:59:GLU:CB	1:A:69:TRP:NE1	0.56	2.68	6	9
1:A:6:PRO:O	1:A:121:HIS:NE2	0.56	2.38	1	6
1:A:5:ILE:N	1:A:5:ILE:HD13	0.56	2.15	10	5
1:A:152:ASN:ND2	1:A:153:VAL:HG13	0.56	2.15	1	6
1:A:52:PHE:CE2	1:A:55:GLY:HA3	0.56	2.35	4	14
1:A:73:LEU:HD21	1:A:84:THR:OG1	0.56	1.99	5	1
1:A:147:LEU:HD12	1:A:147:LEU:N	0.56	2.15	7	3
1:A:71:ARG:CA	1:A:84:THR:O	0.56	2.54	10	17
1:A:71:ARG:NH2	1:A:86:ARG:CZ	0.56	2.69	14	1
1:A:127:HIS:N	1:A:127:HIS:ND1	0.56	2.53	12	7
1:A:46:GLY:O	1:A:60:TRP:N	0.56	2.39	13	14
1:A:103:ILE:HG23	1:A:120:ALA:O	0.56	2.00	6	1
1:A:27:SER:OG	1:A:28:ARG:N	0.55	2.38	2	1
1:A:20:HIS:CE1	1:A:24:VAL:CG2	0.55	2.89	13	5
1:A:16:ALA:O	1:A:115:THR:OG1	0.55	2.25	2	20
1:A:69:TRP:CD1	1:A:69:TRP:C	0.55	2.80	19	4
1:A:61:ASP:CG	1:A:64:GLY:H	0.55	2.05	10	1
1:A:48:ALA:HB3	1:A:58:TYR:HB2	0.55	1.79	4	14
1:A:57:TYR:C	1:A:58:TYR:CD2	0.55	2.81	13	6
1:A:146:THR:HG23	1:A:149:ARG:NH1	0.55	2.17	16	1
1:A:73:LEU:CD2	1:A:84:THR:OG1	0.55	2.55	5	1
1:A:69:TRP:C	1:A:69:TRP:CD2	0.55	2.80	2	1
1:A:28:ARG:CD	1:A:28:ARG:O	0.54	2.55	19	8
1:A:54:GLY:C	1:A:71:ARG:NH2	0.54	2.61	1	1
1:A:16:ALA:HB3	1:A:115:THR:OG1	0.54	2.03	14	9
1:A:62:ILE:CD1	1:A:62:ILE:N	0.54	2.71	12	9
1:A:71:ARG:O	1:A:84:THR:O	0.54	2.26	14	20
1:A:61:ASP:O	1:A:64:GLY:O	0.54	2.26	4	20
1:A:69:TRP:CZ3	1:A:70:GLY:O	0.54	2.61	2	1
1:A:125:HIS:ND1	1:A:125:HIS:O	0.53	2.41	3	5
1:A:124:LEU:C	1:A:126:ARG:N	0.53	2.62	2	20
1:A:80:ARG:CD	1:A:106:ASP:OD2	0.53	2.56	2	5
1:A:61:ASP:OD1	1:A:65:THR:O	0.53	2.26	17	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ARG:CB	1:A:84:THR:O	0.53	2.56	12	15
1:A:75:TRP:CG	1:A:75:TRP:O	0.53	2.61	8	4
1:A:28:ARG:O	1:A:28:ARG:CD	0.53	2.56	3	9
1:A:13:VAL:CG2	1:A:116:ARG:NH2	0.53	2.72	17	1
1:A:91:TRP:CZ2	1:A:137:ALA:HB3	0.53	2.38	14	1
1:A:69:TRP:C	1:A:69:TRP:CD1	0.53	2.82	3	1
1:A:81:LEU:O	1:A:105:VAL:O	0.53	2.27	4	8
1:A:82:ALA:C	1:A:83:MET:SD	0.53	2.87	11	4
1:A:117:VAL:HG21	2:A:201:96F:CAF	0.53	2.34	11	6
1:A:91:TRP:CZ2	1:A:137:ALA:CB	0.52	2.91	14	2
1:A:101:SER:OG	1:A:122:VAL:O	0.52	2.27	5	2
1:A:22:PHE:CE2	1:A:81:LEU:HD21	0.52	2.39	3	2
1:A:56:ARG:CZ	1:A:58:TYR:OH	0.52	2.57	10	2
1:A:62:ILE:HD13	1:A:63:ASP:H	0.52	1.64	10	1
1:A:81:LEU:HD13	1:A:107:PHE:CD1	0.52	2.39	13	1
1:A:71:ARG:N	1:A:84:THR:O	0.52	2.42	10	7
1:A:62:ILE:N	1:A:62:ILE:CD1	0.52	2.73	19	3
1:A:147:LEU:CD2	2:A:201:96F:CAG	0.52	2.88	10	13
1:A:83:MET:SD	1:A:83:MET:N	0.52	2.83	16	1
1:A:110:ASN:O	1:A:114:GLY:N	0.52	2.43	11	12
1:A:52:PHE:CD2	1:A:55:GLY:HA3	0.52	2.40	4	14
1:A:89:GLY:N	1:A:99:ARG:NH1	0.52	2.58	7	1
1:A:7:ASP:O	1:A:7:ASP:OD1	0.52	2.28	4	5
1:A:7:ASP:O	1:A:7:ASP:OD2	0.52	2.28	10	5
1:A:68:VAL:HG13	1:A:68:VAL:O	0.52	2.05	1	3
1:A:7:ASP:OD1	1:A:7:ASP:O	0.52	2.28	18	7
1:A:125:HIS:CG	1:A:125:HIS:O	0.52	2.63	16	11
1:A:7:ASP:OD2	1:A:7:ASP:O	0.51	2.28	19	3
1:A:110:ASN:O	1:A:114:GLY:CA	0.51	2.58	2	11
1:A:67:ILE:HG22	1:A:68:VAL:N	0.51	2.20	8	1
1:A:52:PHE:CE1	1:A:55:GLY:HA3	0.51	2.39	3	6
1:A:89:GLY:O	1:A:134:ILE:HD11	0.51	2.06	13	1
1:A:52:PHE:CD2	1:A:55:GLY:CA	0.51	2.93	20	14
1:A:68:VAL:O	1:A:68:VAL:HG13	0.51	2.04	18	3
1:A:127:HIS:ND1	1:A:127:HIS:N	0.51	2.57	6	3
1:A:72:ILE:CG2	1:A:73:LEU:N	0.51	2.72	5	18
1:A:61:ASP:OD1	1:A:64:GLY:O	0.51	2.29	7	6
1:A:152:ASN:CG	1:A:153:VAL:N	0.51	2.63	2	7
1:A:125:HIS:O	1:A:125:HIS:CG	0.51	2.64	13	7
1:A:121:HIS:O	1:A:121:HIS:CG	0.51	2.64	19	6
1:A:61:ASP:OD2	1:A:64:GLY:O	0.51	2.29	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:TYR:CE1	1:A:68:VAL:CG2	0.51	2.94	4	2
1:A:9:ARG:NH1	1:A:118:GLU:OE2	0.51	2.43	16	1
1:A:23:GLU:O	1:A:27:SER:CB	0.50	2.59	17	14
1:A:146:THR:OG1	2:A:201:96F:CAW	0.50	2.59	5	5
1:A:61:ASP:OD2	1:A:65:THR:O	0.50	2.29	11	5
1:A:30:ALA:CB	1:A:47:LEU:HD12	0.50	2.25	18	1
1:A:72:ILE:HG22	1:A:73:LEU:N	0.50	2.21	13	19
1:A:147:LEU:HD11	2:A:201:96F:CAH	0.50	2.36	18	7
1:A:52:PHE:CD1	1:A:55:GLY:CA	0.50	2.95	16	6
1:A:80:ARG:CD	1:A:106:ASP:OD1	0.50	2.60	12	2
1:A:71:ARG:HH21	1:A:86:ARG:HH11	0.50	1.49	5	1
1:A:30:ALA:HB2	1:A:47:LEU:HD21	0.50	1.83	4	1
1:A:12:VAL:HB	1:A:147:LEU:HD22	0.50	1.83	18	1
1:A:101:SER:OG	1:A:124:LEU:HD12	0.49	2.07	15	2
1:A:121:HIS:CG	1:A:121:HIS:O	0.49	2.64	18	5
1:A:20:HIS:CE1	1:A:24:VAL:HG21	0.49	2.42	4	3
1:A:105:VAL:HG12	1:A:107:PHE:CE2	0.49	2.42	3	4
1:A:16:ALA:N	1:A:115:THR:OG1	0.49	2.46	6	10
1:A:121:HIS:CD2	1:A:124:LEU:HD13	0.49	2.43	6	1
1:A:105:VAL:CG1	1:A:107:PHE:CE1	0.49	2.96	1	8
1:A:8:VAL:HG12	1:A:121:HIS:CD2	0.49	2.43	8	7
1:A:20:HIS:NE2	1:A:154:ILE:HD13	0.48	2.23	12	6
1:A:105:VAL:HG12	1:A:107:PHE:CE1	0.48	2.43	18	8
1:A:88:ASP:CG	1:A:89:GLY:N	0.48	2.66	18	12
1:A:101:SER:OG	1:A:123:LYS:O	0.48	2.31	11	3
1:A:61:ASP:CG	1:A:64:GLY:N	0.48	2.67	10	1
1:A:61:ASP:OD2	1:A:64:GLY:N	0.48	2.46	10	1
1:A:63:ASP:OD2	1:A:64:GLY:N	0.48	2.47	16	1
1:A:150:PHE:CE1	1:A:154:ILE:CD1	0.48	2.95	3	2
1:A:68:VAL:HG21	1:A:86:ARG:NH1	0.48	2.23	7	1
1:A:71:ARG:CZ	1:A:86:ARG:CZ	0.48	2.91	14	1
1:A:134:ILE:CD1	1:A:134:ILE:N	0.48	2.77	13	1
1:A:52:PHE:CD1	1:A:55:GLY:HA3	0.48	2.43	3	6
1:A:56:ARG:NE	1:A:86:ARG:NH2	0.48	2.61	8	1
1:A:7:ASP:HB2	1:A:122:VAL:HG12	0.48	1.85	18	6
1:A:150:PHE:CZ	2:A:201:96F:CAE	0.48	2.97	1	9
1:A:9:ARG:NH1	1:A:118:GLU:OE1	0.48	2.46	19	1
1:A:18:VAL:HG23	1:A:19:GLU:N	0.48	2.23	11	9
1:A:124:LEU:C	1:A:126:ARG:H	0.48	2.11	13	16
1:A:70:GLY:C	1:A:86:ARG:H	0.48	2.12	12	5
1:A:87:ILE:HD11	1:A:91:TRP:CZ3	0.48	2.44	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:HD11	1:A:107:PHE:CE2	0.48	2.44	19	1
1:A:61:ASP:OD1	1:A:62:ILE:N	0.48	2.47	10	1
1:A:75:TRP:CD2	1:A:75:TRP:O	0.48	2.67	10	1
1:A:91:TRP:CH2	1:A:137:ALA:HB3	0.48	2.44	10	1
1:A:45:ALA:HB3	1:A:60:TRP:HB3	0.48	1.84	14	7
1:A:57:TYR:CB	1:A:69:TRP:CZ2	0.48	2.97	12	4
1:A:52:PHE:HD2	1:A:52:PHE:N	0.48	2.03	4	2
1:A:147:LEU:O	1:A:151:ALA:HB2	0.48	2.08	18	1
1:A:63:ASP:OD1	1:A:64:GLY:N	0.48	2.47	18	1
1:A:52:PHE:CE1	1:A:55:GLY:HA2	0.47	2.44	1	6
1:A:75:TRP:O	1:A:75:TRP:CG	0.47	2.66	9	5
1:A:52:PHE:CE2	1:A:55:GLY:HA2	0.47	2.44	8	13
1:A:110:ASN:N	1:A:114:GLY:O	0.47	2.43	11	4
1:A:23:GLU:O	1:A:27:SER:OG	0.47	2.31	18	6
1:A:73:LEU:HD12	1:A:83:MET:N	0.47	2.24	5	1
1:A:80:ARG:NE	1:A:106:ASP:OD2	0.47	2.47	19	1
1:A:88:ASP:OD1	1:A:89:GLY:N	0.47	2.47	20	5
1:A:146:THR:HG21	2:A:201:96F:OAP	0.47	2.09	4	8
1:A:147:LEU:H	1:A:147:LEU:CD1	0.47	2.21	7	3
1:A:51:PRO:C	1:A:52:PHE:CG	0.47	2.88	19	7
1:A:88:ASP:CG	1:A:89:GLY:H	0.47	2.13	10	3
1:A:62:ILE:H	1:A:62:ILE:HD13	0.47	1.70	12	3
1:A:146:THR:OG1	2:A:201:96F:OBC	0.47	2.32	7	1
1:A:66:GLU:O	1:A:66:GLU:OE1	0.47	2.32	11	1
1:A:85:TRP:O	1:A:85:TRP:CG	0.47	2.67	11	1
1:A:16:ALA:O	1:A:115:THR:CG2	0.47	2.62	18	7
1:A:124:LEU:N	1:A:124:LEU:CD2	0.47	2.77	3	2
1:A:68:VAL:O	1:A:68:VAL:CG1	0.47	2.63	1	2
1:A:91:TRP:CZ2	1:A:134:ILE:HA	0.47	2.44	14	3
1:A:91:TRP:CE2	1:A:137:ALA:HB3	0.47	2.45	14	1
1:A:85:TRP:CG	1:A:85:TRP:O	0.47	2.68	20	3
1:A:14:VAL:HG23	1:A:151:ALA:CB	0.46	2.40	18	1
1:A:123:LYS:N	1:A:123:LYS:HD2	0.46	2.25	17	1
1:A:62:ILE:HD13	1:A:62:ILE:H	0.46	1.71	19	3
1:A:68:VAL:CG1	1:A:68:VAL:O	0.46	2.63	18	1
1:A:24:VAL:HG21	1:A:154:ILE:HD11	0.46	1.88	11	1
1:A:25:PHE:O	1:A:49:PHE:CE2	0.46	2.68	4	1
1:A:50:GLU:CB	1:A:52:PHE:CZ	0.46	2.99	13	1
1:A:149:ARG:O	1:A:153:VAL:HG23	0.46	2.11	17	1
1:A:16:ALA:O	1:A:114:GLY:C	0.46	2.54	11	3
1:A:20:HIS:C	1:A:20:HIS:CD2	0.46	2.89	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:TRP:CD2	1:A:85:TRP:O	0.46	2.68	3	1
1:A:20:HIS:CD2	1:A:20:HIS:C	0.46	2.89	19	11
1:A:150:PHE:CE2	1:A:154:ILE:CD1	0.46	2.98	16	2
1:A:20:HIS:NE2	1:A:154:ILE:CD1	0.46	2.78	12	3
1:A:5:ILE:CD1	1:A:5:ILE:N	0.46	2.79	12	6
1:A:75:TRP:O	1:A:75:TRP:CD2	0.46	2.68	20	3
2:A:201:96F:CAS	2:A:201:96F:CAV	0.46	2.94	9	1
1:A:9:ARG:HG3	1:A:120:ALA:HB2	0.45	1.88	11	8
1:A:67:ILE:CG2	1:A:68:VAL:N	0.45	2.79	8	1
1:A:56:ARG:HH11	1:A:71:ARG:NH1	0.45	2.10	8	1
1:A:85:TRP:CE2	1:A:103:ILE:CD1	0.45	3.00	12	1
1:A:49:PHE:CD1	1:A:57:TYR:CE2	0.45	3.04	18	1
1:A:80:ARG:NE	1:A:106:ASP:OD1	0.45	2.49	7	1
1:A:66:GLU:O	1:A:66:GLU:CD	0.45	2.55	9	1
1:A:147:LEU:HD21	2:A:201:96F:CAK	0.45	2.42	13	1
1:A:123:LYS:HD2	1:A:123:LYS:N	0.45	2.27	6	1
1:A:66:GLU:C	1:A:66:GLU:OE1	0.45	2.54	9	1
1:A:60:TRP:CE2	1:A:66:GLU:HB2	0.45	2.47	11	1
1:A:146:THR:CG2	2:A:201:96F:OAP	0.45	2.64	4	5
1:A:54:GLY:C	1:A:71:ARG:HH22	0.45	2.14	1	1
1:A:61:ASP:OD1	1:A:64:GLY:C	0.45	2.55	17	3
1:A:105:VAL:CG1	1:A:107:PHE:CE2	0.45	3.00	20	4
1:A:52:PHE:N	1:A:52:PHE:HD2	0.45	2.06	13	3
1:A:88:ASP:OD2	1:A:89:GLY:N	0.45	2.48	9	3
1:A:58:TYR:CD1	1:A:68:VAL:HG22	0.45	2.47	12	3
1:A:135:HIS:C	1:A:135:HIS:ND1	0.45	2.70	12	8
2:A:201:96F:OAP	2:A:201:96F:OAR	0.45	2.35	19	10
2:A:201:96F:OAR	2:A:201:96F:OAP	0.45	2.35	5	7
1:A:47:LEU:O	1:A:47:LEU:CD2	0.45	2.65	18	2
1:A:85:TRP:HE1	1:A:101:SER:H	0.45	1.55	11	1
1:A:135:HIS:ND1	1:A:135:HIS:C	0.45	2.69	20	3
1:A:63:ASP:OD1	1:A:63:ASP:C	0.44	2.55	18	1
1:A:124:LEU:C	1:A:127:HIS:CE1	0.44	2.91	10	3
1:A:61:ASP:OD2	1:A:64:GLY:C	0.44	2.56	3	3
1:A:56:ARG:NE	1:A:86:ARG:HH21	0.44	2.11	8	1
1:A:55:GLY:O	1:A:71:ARG:CG	0.44	2.66	14	1
1:A:66:GLU:OE1	1:A:66:GLU:C	0.44	2.55	11	1
1:A:52:PHE:CE1	1:A:56:ARG:N	0.44	2.86	2	2
1:A:61:ASP:OD1	1:A:61:ASP:C	0.44	2.54	10	1
1:A:60:TRP:CE3	1:A:66:GLU:CD	0.44	2.92	13	1
1:A:150:PHE:CD2	1:A:150:PHE:C	0.43	2.90	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:TRP:CZ3	1:A:70:GLY:C	0.43	2.91	2	1
1:A:147:LEU:O	1:A:151:ALA:CB	0.43	2.65	5	17
1:A:25:PHE:O	1:A:49:PHE:CE1	0.43	2.71	12	1
1:A:14:VAL:HG13	1:A:115:THR:OG1	0.43	2.13	18	1
1:A:150:PHE:C	1:A:150:PHE:CD2	0.43	2.92	15	2
1:A:52:PHE:CE2	1:A:56:ARG:N	0.43	2.84	4	7
1:A:59:GLU:N	1:A:69:TRP:NE1	0.43	2.65	13	5
1:A:50:GLU:CG	1:A:52:PHE:CE1	0.43	3.01	4	1
1:A:81:LEU:N	1:A:81:LEU:HD12	0.43	2.28	19	1
1:A:75:TRP:CD1	1:A:75:TRP:N	0.43	2.87	13	2
1:A:11:SER:O	1:A:12:VAL:HG23	0.43	2.14	15	1
1:A:85:TRP:HE1	1:A:87:ILE:HG22	0.43	1.73	3	1
1:A:12:VAL:CG1	1:A:13:VAL:N	0.43	2.82	10	8
1:A:150:PHE:CD1	1:A:150:PHE:C	0.43	2.92	5	1
1:A:123:LYS:CD	1:A:123:LYS:N	0.43	2.82	6	2
1:A:55:GLY:H	1:A:72:ILE:HB	0.42	1.74	17	7
1:A:56:ARG:HH11	1:A:71:ARG:HH11	0.42	1.54	8	1
1:A:58:TYR:CD2	1:A:68:VAL:HG22	0.42	2.47	16	3
1:A:29:PRO:HG3	1:A:49:PHE:CE2	0.42	2.49	18	1
1:A:57:TYR:CB	1:A:69:TRP:CH2	0.42	3.02	15	1
1:A:146:THR:HG1	2:A:201:96F:CAW	0.42	2.26	7	1
1:A:91:TRP:CE2	1:A:137:ALA:CB	0.42	3.02	19	7
1:A:117:VAL:CG1	2:A:201:96F:OAO	0.42	2.67	3	3
1:A:56:ARG:CB	1:A:58:TYR:OH	0.42	2.67	15	2
1:A:50:GLU:HB2	1:A:52:PHE:CZ	0.42	2.50	16	8
1:A:58:TYR:CE2	1:A:68:VAL:CG2	0.42	2.98	14	3
1:A:71:ARG:NH2	1:A:86:ARG:NE	0.42	2.67	14	1
1:A:52:PHE:HD1	1:A:52:PHE:N	0.42	2.05	3	2
1:A:63:ASP:OD2	1:A:63:ASP:C	0.42	2.55	16	1
1:A:20:HIS:CD2	1:A:154:ILE:HD13	0.42	2.49	4	2
1:A:57:TYR:HB2	1:A:69:TRP:CH2	0.42	2.50	15	2
1:A:5:ILE:N	1:A:5:ILE:CD1	0.42	2.83	15	1
1:A:52:PHE:N	1:A:52:PHE:HD1	0.42	2.07	1	1
1:A:72:ILE:HD12	1:A:72:ILE:N	0.42	2.29	18	1
1:A:6:PRO:O	1:A:8:VAL:HG13	0.42	2.15	14	1
1:A:150:PHE:CG	1:A:151:ALA:N	0.42	2.87	19	1
1:A:67:ILE:CG1	1:A:68:VAL:N	0.42	2.83	3	1
1:A:91:TRP:CZ2	1:A:133:ASN:O	0.41	2.72	1	1
1:A:16:ALA:C	1:A:115:THR:HG1	0.41	2.16	15	1
1:A:49:PHE:CZ	1:A:57:TYR:HB3	0.41	2.50	10	1
1:A:62:ILE:HD13	1:A:63:ASP:N	0.41	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLU:N	1:A:50:GLU:CD	0.41	2.74	10	1
1:A:73:LEU:N	1:A:83:MET:HA	0.41	2.30	7	2
1:A:105:VAL:HG22	1:A:119:LEU:HG	0.41	1.92	9	1
1:A:85:TRP:CD1	1:A:103:ILE:CD1	0.41	3.01	19	1
1:A:81:LEU:HD13	1:A:83:MET:CE	0.41	2.45	16	1
1:A:12:VAL:HG12	1:A:13:VAL:N	0.41	2.30	6	1
1:A:148:ALA:O	1:A:152:ASN:CG	0.41	2.59	6	2
1:A:51:PRO:C	1:A:52:PHE:CD2	0.41	2.93	12	2
1:A:56:ARG:CD	1:A:86:ARG:HH21	0.41	2.28	12	1
1:A:89:GLY:HA2	1:A:134:ILE:HD11	0.41	1.92	18	1
1:A:124:LEU:N	1:A:124:LEU:HD22	0.41	2.29	3	1
1:A:20:HIS:NE2	1:A:24:VAL:HG23	0.41	2.30	3	1
1:A:84:THR:CG2	1:A:85:TRP:N	0.41	2.83	10	1
1:A:65:THR:CG2	1:A:66:GLU:N	0.41	2.83	18	2
1:A:146:THR:OG1	2:A:201:96F:CAV	0.41	2.69	18	1
1:A:132:TRP:O	1:A:136:LYS:N	0.41	2.51	17	1
1:A:50:GLU:CD	1:A:52:PHE:CE1	0.41	2.94	4	1
1:A:121:HIS:ND1	1:A:124:LEU:HD22	0.41	2.31	8	1
1:A:60:TRP:NE1	1:A:66:GLU:HB2	0.41	2.31	18	2
1:A:59:GLU:HB2	1:A:69:TRP:NE1	0.41	2.31	6	1
1:A:25:PHE:O	1:A:49:PHE:CD1	0.41	2.74	18	1
1:A:125:HIS:O	1:A:125:HIS:ND1	0.41	2.53	8	2
1:A:59:GLU:CD	1:A:59:GLU:C	0.41	2.78	12	1
1:A:51:PRO:C	1:A:52:PHE:CD1	0.41	2.94	2	1
1:A:127:HIS:CD2	1:A:131:ALA:HB1	0.40	2.50	7	2
1:A:91:TRP:CH2	1:A:137:ALA:CB	0.40	3.04	10	1
1:A:85:TRP:CZ2	1:A:124:LEU:HD11	0.40	2.51	11	1
1:A:22:PHE:CZ	1:A:81:LEU:HD22	0.40	2.51	2	1
1:A:6:PRO:O	1:A:121:HIS:CE1	0.40	2.74	5	1
1:A:13:VAL:CG1	1:A:13:VAL:O	0.40	2.70	6	1
1:A:87:ILE:CD1	1:A:134:ILE:HG23	0.40	2.44	1	1
1:A:87:ILE:HG21	1:A:134:ILE:HG21	0.40	1.93	3	1
1:A:147:LEU:N	1:A:147:LEU:CD1	0.40	2.82	6	1
1:A:91:TRP:NE1	1:A:137:ALA:CB	0.40	2.85	12	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	115/158 (73%)	109±1 (94±1%)	5±1 (4±1%)	2±1 (2±0%)	13	56
All	All	2300/3160 (73%)	2172 (94%)	90 (4%)	38 (2%)	13	56

All 4 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	125	HIS	20
1	A	52	PHE	13
1	A	28	ARG	3
1	A	65	THR	2

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	97/132 (73%)	79±2 (81±2%)	18±2 (19±2%)	4	37
All	All	1940/2640 (73%)	1580 (81%)	360 (19%)	4	37

All 31 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	5	ILE	20
1	A	90	HIS	20
1	A	150	PHE	20
1	A	52	PHE	20
1	A	127	HIS	20
1	A	60	TRP	20
1	A	135	HIS	20
1	A	115	THR	19
1	A	62	ILE	18
1	A	28	ARG	18
1	A	61	ASP	16
1	A	149	ARG	14

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Mol	Chain	Res	Type	Models (Total)
1	A	47	LEU	14
1	A	53	VAL	13
1	A	108	VAL	12
1	A	152	ASN	12
1	A	121	HIS	10
1	A	69	TRP	10
1	A	81	LEU	10
1	A	83	MET	9
1	A	12	VAL	9
1	A	123	LYS	8
1	A	65	THR	7
1	A	22	PHE	7
1	A	85	TRP	4
1	A	50	GLU	3
1	A	124	LEU	2
1	A	99	ARG	2
1	A	66	GLU	1
1	A	67	ILE	1
1	A	126	ARG	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.

LIGAND-GEOMETRY INFOmissingINFO

6.6 Other polymers ⓘ

There are no such molecules in this entry.

6.7 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *txn38-sum-20171226-shifts-upload.txt*

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	1702
Number of shifts mapped to atoms	1702
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	19

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	146	0.02 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	130	-0.14 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	133	0.13 ± 0.20	None needed (< 0.5 ppm)
^{15}N	137	0.86 ± 0.46	None needed (imprecise)

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 84%, i.e. 1247 atoms were assigned a chemical shift out of a possible 1481. 18 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	564/570 (99%)	226/227 (100%)	227/232 (98%)	111/111 (100%)
Sidechain	542/721 (75%)	335/420 (80%)	205/265 (77%)	2/36 (6%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	141/190 (74%)	77/98 (79%)	61/74 (82%)	3/18 (17%)
Overall	1247/1481 (84%)	638/745 (86%)	493/571 (86%)	116/165 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1519 atoms were assigned a chemical shift out of a possible 1916. 19 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	697/746 (93%)	281/296 (95%)	279/308 (91%)	137/142 (96%)
Sidechain	663/940 (71%)	420/553 (76%)	240/345 (70%)	3/42 (7%)
Aromatic	159/230 (69%)	87/118 (74%)	69/88 (78%)	3/24 (12%)
Overall	1519/1916 (79%)	788/967 (81%)	588/741 (79%)	143/208 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	57	TYR	CD1	109.44	139.11 – 126.41	-18.4
1	A	57	TYR	CD2	109.44	140.11 – 125.31	-15.7
1	A	52	PHE	CZ	108.01	137.04 – 121.44	-13.6
1	A	121	HIS	HD2	10.91	9.28 – 4.78	8.6
1	A	91	TRP	CH2	107.94	133.06 – 114.56	-8.6
1	A	69	TRP	CD1	112.60	136.18 – 116.78	-7.2
1	A	91	TRP	CE3	108.52	129.06 – 111.96	-7.0
1	A	60	TRP	CE3	109.22	129.06 – 111.96	-6.6
1	A	32	TRP	CE3	109.43	129.06 – 111.96	-6.5
1	A	102	GLU	CG	44.02	42.24 – 29.94	6.4
1	A	51	PRO	HA	2.38	6.05 – 2.75	-6.1
1	A	132	TRP	CE3	110.19	129.06 – 111.96	-6.0
1	A	105	VAL	HG12	-0.70	2.13 – -0.47	-5.9
1	A	105	VAL	HG13	-0.70	2.13 – -0.47	-5.9
1	A	105	VAL	HG11	-0.70	2.13 – -0.47	-5.9
1	A	32	TRP	CZ2	123.05	121.76 – 106.66	5.9
1	A	33	TRP	CD1	115.45	136.18 – 116.78	-5.7
1	A	91	TRP	CZ2	122.22	121.76 – 106.66	5.3
1	A	107	PHE	CE2	124.62	136.81 – 124.71	-5.1

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.

Random coil index (RCI) for chain A:

