



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 03:21 AM BST

PDB ID : 2MLK
Title : Three-dimensional structure of the C-terminal DNA-binding domain of RstA protein from *Klebsiella pneumoniae*
Authors : Fang, P.; Chen, S.; Cheng, Y.; Chang, C.; Yu, T.; Huang, T.
Deposited on : 2014-03-02

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

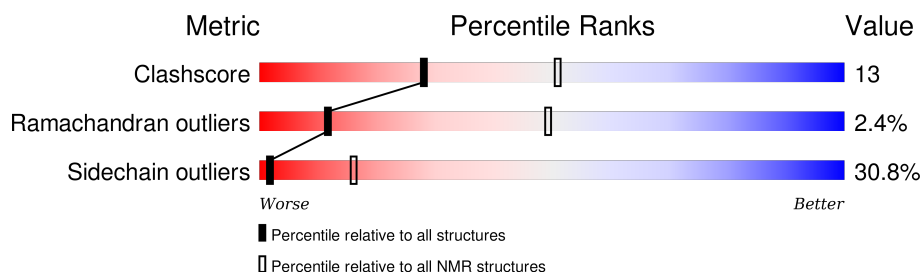
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	119	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 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:136-A:234 (99)	0.49	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1738 atoms, of which 873 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RstA.

Mol	Chain	Residues	Atoms						Trace
1	A	110	Total	C	H	N	O	S	0
			1738	546	873	156	161	2	

There are 10 discrepancies between the modelled and reference sequences:

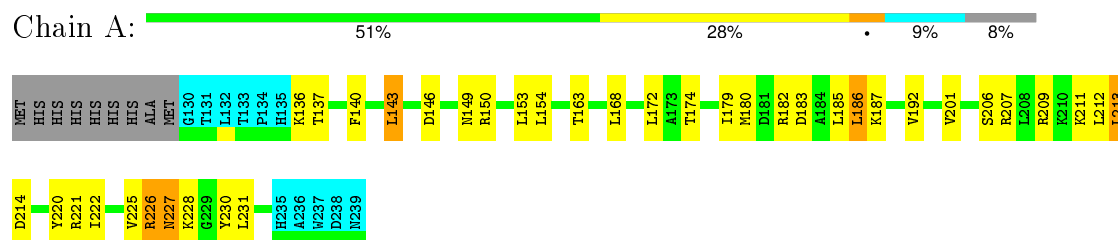
Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MET	-	EXPRESSION TAG	UNP U5MDD9
A	122	HIS	-	EXPRESSION TAG	UNP U5MDD9
A	123	HIS	-	EXPRESSION TAG	UNP U5MDD9
A	124	HIS	-	EXPRESSION TAG	UNP U5MDD9
A	125	HIS	-	EXPRESSION TAG	UNP U5MDD9
A	126	HIS	-	EXPRESSION TAG	UNP U5MDD9
A	127	HIS	-	EXPRESSION TAG	UNP U5MDD9
A	128	ALA	-	EXPRESSION TAG	UNP U5MDD9
A	129	MET	-	EXPRESSION TAG	UNP U5MDD9
A	130	GLY	-	EXPRESSION TAG	UNP U5MDD9

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: RstA

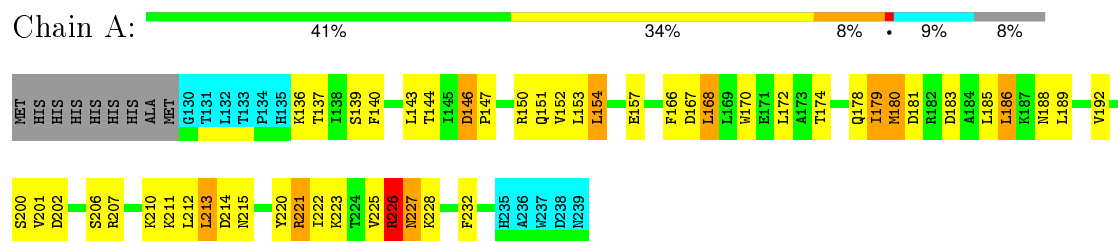


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

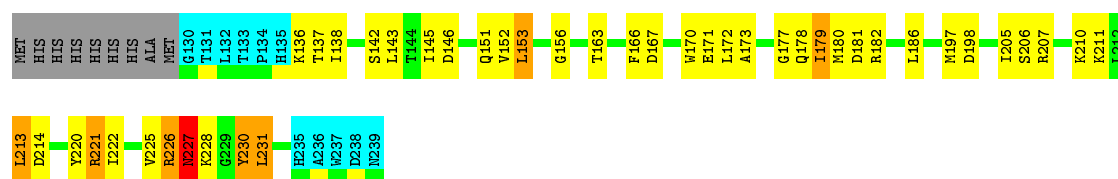
- Molecule 1: RstA



4.2.2 Score per residue for model 2

- Molecule 1: RstA

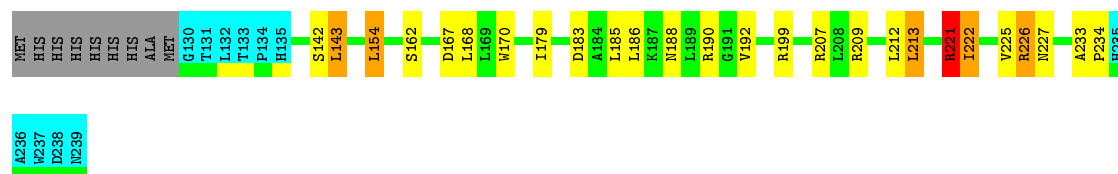




4.2.3 Score per residue for model 3

- Molecule 1: RstA

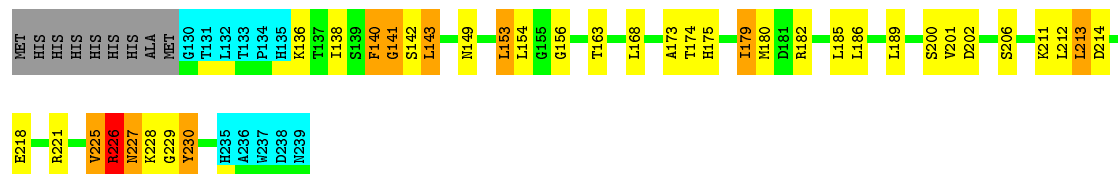
Chain A: 61% 17% 9% 8%



4.2.4 Score per residue for model 4

- Molecule 1: RstA

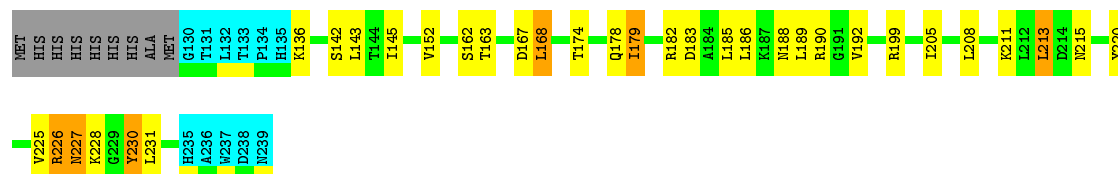
Chain A: 52% 23% 8% 9% 8%



4.2.5 Score per residue for model 5

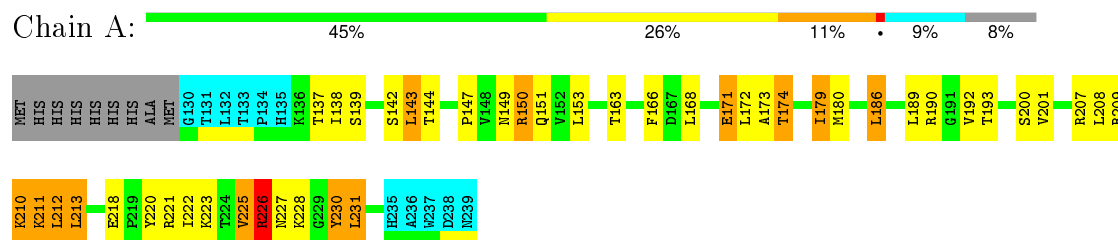
- Molecule 1: RstA

Chain A: 55% 23% 5% 9% 8%



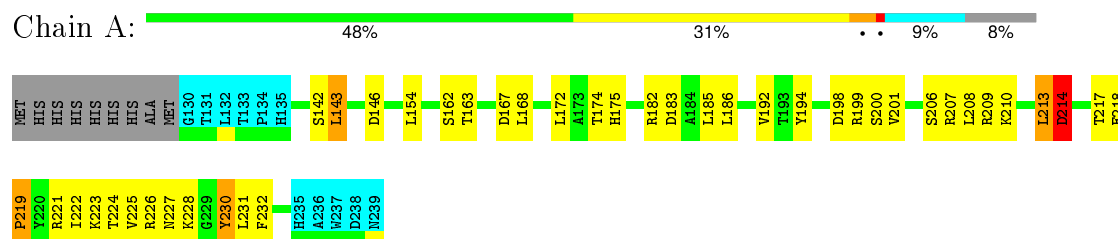
4.2.6 Score per residue for model 6

- Molecule 1: RstA



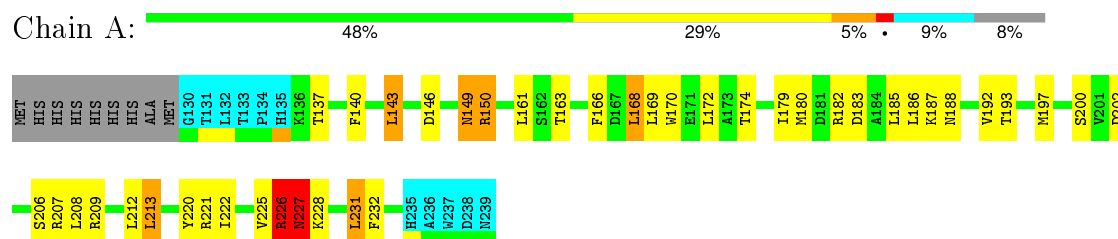
4.2.7 Score per residue for model 7

- Molecule 1: RstA



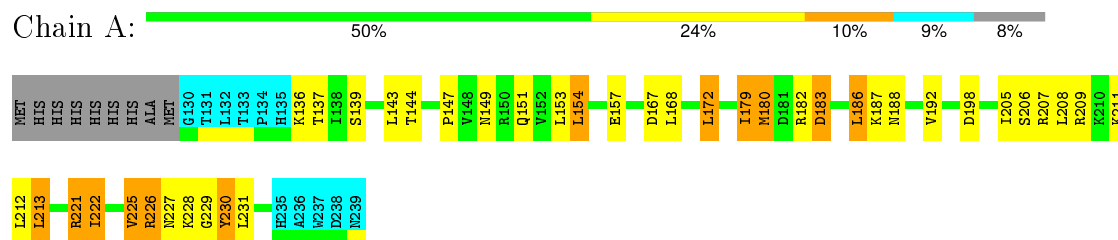
4.2.8 Score per residue for model 8

- Molecule 1: RstA



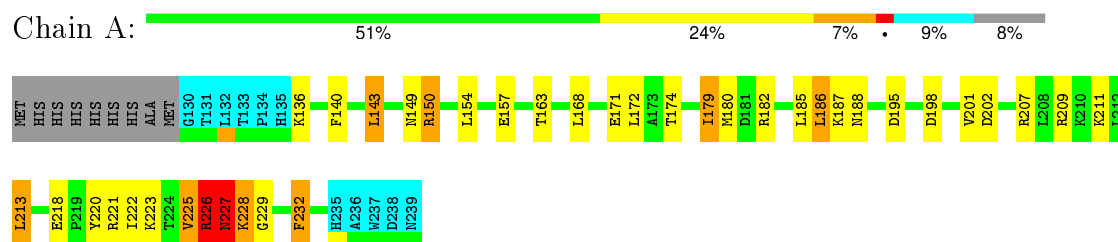
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: RstA



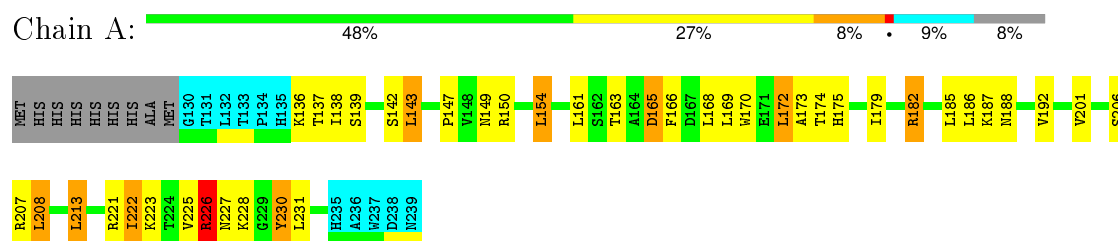
4.2.10 Score per residue for model 10

- Molecule 1: RstA



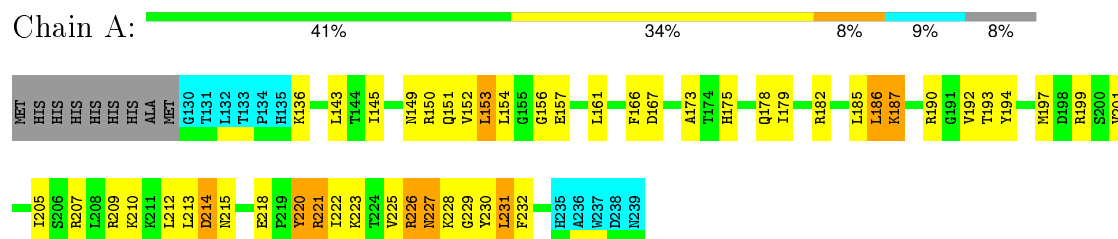
4.2.11 Score per residue for model 11

- Molecule 1: RstA



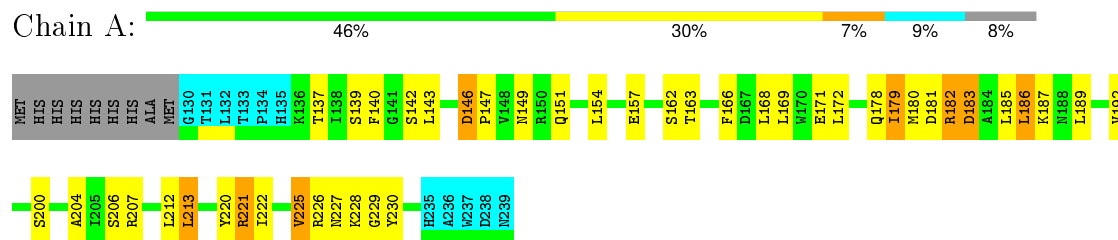
4.2.12 Score per residue for model 12

- Molecule 1: RstA



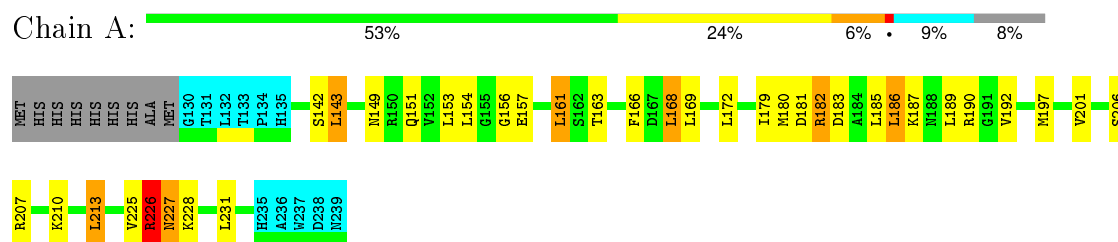
4.2.13 Score per residue for model 13

- Molecule 1: RstA



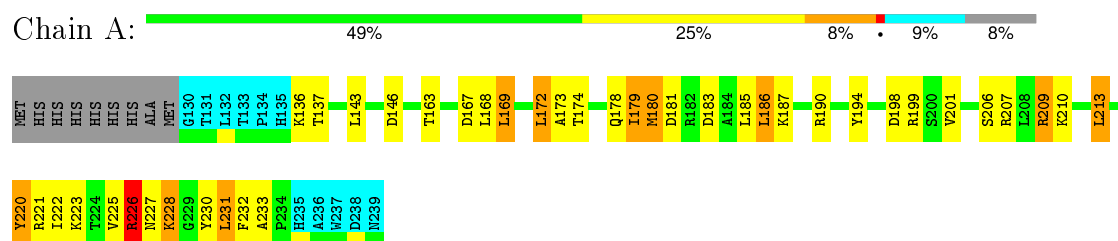
4.2.14 Score per residue for model 14

- Molecule 1: RstA



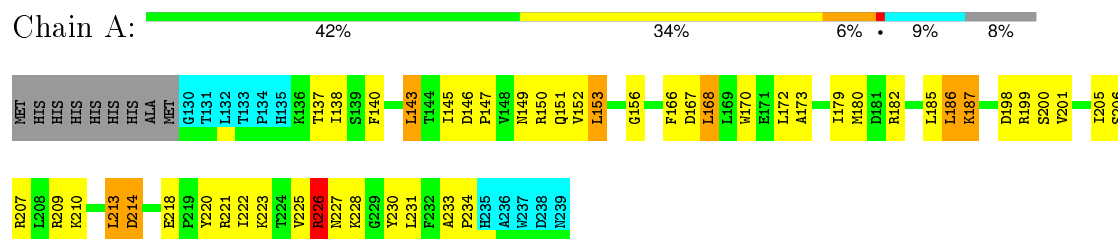
4.2.15 Score per residue for model 15

- Molecule 1: RstA



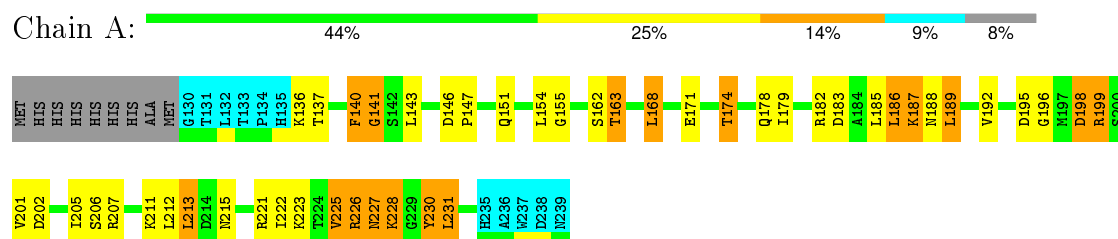
4.2.16 Score per residue for model 16

- Molecule 1: RstA



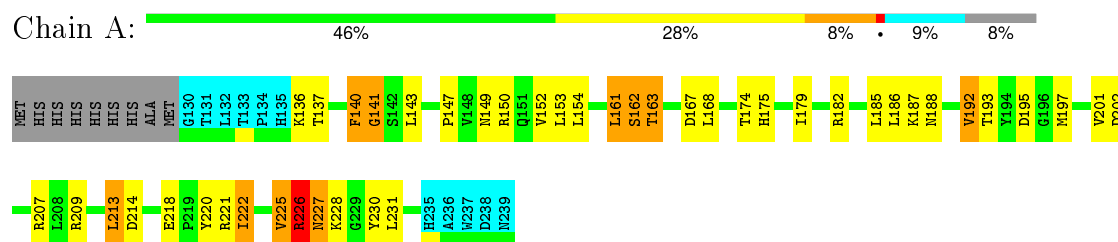
4.2.17 Score per residue for model 17

- Molecule 1: RstA



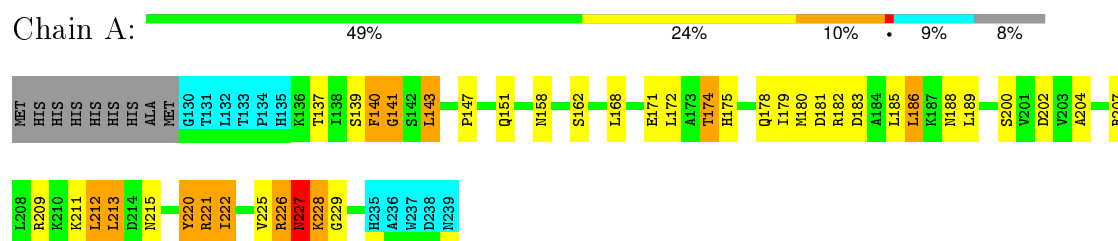
4.2.18 Score per residue for model 18

- Molecule 1: RstA



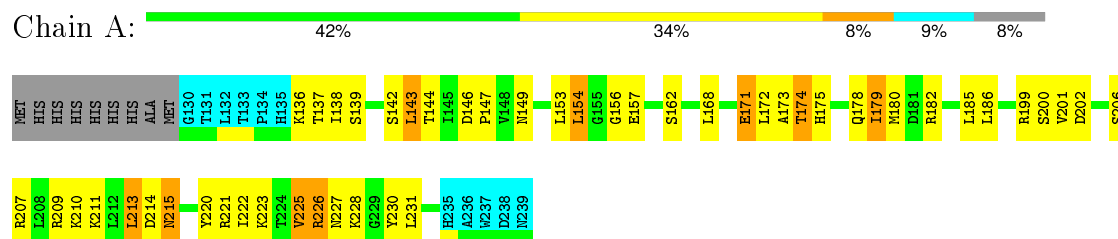
4.2.19 Score per residue for model 19

- Molecule 1: RstA



4.2.20 Score per residue for model 20

- Molecule 1: RstA



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 150 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
CYANA	structure solution	
CYANA	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)	2mlk_cs.str
Number of chemical shift lists	1
Total number of shifts	1173
Number of shifts mapped to atoms	1173
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

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.

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	777	799	799	20±5
All	All	15540	15980	15980	397

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:ILE:HG23	1:A:222:ILE:O	0.90	1.64	19	2
1:A:186:LEU:HD13	1:A:187:LYS:N	0.90	1.81	13	1
1:A:168:LEU:HD13	1:A:185:LEU:HD21	0.89	1.44	8	2
1:A:143:LEU:HD12	1:A:154:LEU:HD12	0.87	1.46	14	2
1:A:168:LEU:HD12	1:A:189:LEU:HD11	0.78	1.55	1	2
1:A:143:LEU:HD12	1:A:212:LEU:HD21	0.77	1.53	19	2
1:A:186:LEU:HD22	1:A:186:LEU:O	0.77	1.79	13	1
1:A:186:LEU:HD23	1:A:187:LYS:N	0.76	1.95	17	4
1:A:225:VAL:HG11	1:A:231:LEU:HD12	0.76	1.56	17	4
1:A:154:LEU:HD13	1:A:212:LEU:HD11	0.72	1.61	3	2
1:A:168:LEU:HD21	1:A:185:LEU:HD21	0.72	1.62	5	9
1:A:222:ILE:CG2	1:A:222:ILE:O	0.71	2.37	19	1
1:A:222:ILE:HG22	1:A:230:TYR:CE1	0.70	2.22	2	3
1:A:168:LEU:HD11	1:A:185:LEU:HD21	0.69	1.64	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:ILE:HG21	1:A:230:TYR:CZ	0.69	2.23	16	2
1:A:168:LEU:HD23	1:A:208:LEU:HD22	0.65	1.67	6	1
1:A:186:LEU:C	1:A:186:LEU:HD22	0.65	2.10	13	1
1:A:175:HIS:O	1:A:175:HIS:CG	0.64	2.50	19	1
1:A:168:LEU:HD23	1:A:189:LEU:HD11	0.63	1.70	17	1
1:A:143:LEU:HD13	1:A:220:TYR:CE1	0.63	2.28	8	1
1:A:209:ARG:O	1:A:213:LEU:N	0.63	2.32	12	10
1:A:140:PHE:O	1:A:141:GLY:C	0.62	2.35	4	4
1:A:185:LEU:HD22	1:A:230:TYR:CE2	0.62	2.29	4	1
1:A:168:LEU:HD12	1:A:204:ALA:HB1	0.62	1.71	19	2
1:A:185:LEU:HD23	1:A:201:VAL:HG13	0.61	1.70	7	3
1:A:168:LEU:CD2	1:A:185:LEU:HD11	0.61	2.24	3	1
1:A:172:LEU:HD21	1:A:230:TYR:CE2	0.61	2.30	11	1
1:A:168:LEU:HG	1:A:189:LEU:HD11	0.61	1.72	13	1
1:A:186:LEU:HD12	1:A:187:LYS:N	0.61	2.10	14	2
1:A:186:LEU:HB3	1:A:201:VAL:HG23	0.61	1.73	14	3
1:A:179:ILE:CD1	1:A:225:VAL:HG21	0.61	2.26	11	3
1:A:192:VAL:HG11	1:A:194:TYR:CE2	0.60	2.31	7	1
1:A:143:LEU:CD1	1:A:212:LEU:HD21	0.60	2.24	19	3
1:A:169:LEU:HD22	1:A:220:TYR:OH	0.60	1.96	8	1
1:A:168:LEU:HG	1:A:185:LEU:HD11	0.59	1.74	11	3
1:A:168:LEU:CD2	1:A:189:LEU:HD11	0.59	2.27	17	1
1:A:205:ILE:HG23	1:A:230:TYR:CZ	0.59	2.32	2	4
1:A:143:LEU:HD21	1:A:152:VAL:HB	0.58	1.73	1	2
1:A:179:ILE:HD12	1:A:180:MET:N	0.58	2.13	19	4
1:A:139:SER:HB3	1:A:144:THR:HG23	0.58	1.74	9	4
1:A:143:LEU:HD12	1:A:154:LEU:HD13	0.58	1.75	11	2
1:A:165:ASP:OD2	1:A:208:LEU:HD12	0.58	1.97	11	1
1:A:220:TYR:CD2	1:A:222:ILE:HD11	0.58	2.34	15	1
1:A:205:ILE:HD13	1:A:230:TYR:CE1	0.57	2.34	16	1
1:A:192:VAL:HG23	1:A:194:TYR:H	0.57	1.59	12	1
1:A:172:LEU:HD13	1:A:230:TYR:CE2	0.57	2.34	15	3
1:A:168:LEU:HD21	1:A:185:LEU:HD11	0.57	1.76	3	1
1:A:154:LEU:HD22	1:A:212:LEU:HD23	0.57	1.75	4	1
1:A:225:VAL:CG1	1:A:231:LEU:HD12	0.57	2.29	17	1
1:A:154:LEU:HD13	1:A:212:LEU:CD1	0.57	2.30	3	2
1:A:179:ILE:HD11	1:A:228:LYS:O	0.56	1.99	19	10
1:A:222:ILE:HG22	1:A:230:TYR:OH	0.56	2.00	11	1
1:A:220:TYR:CE2	1:A:222:ILE:HD12	0.56	2.36	16	1
1:A:221:ARG:HD3	1:A:233:ALA:HB3	0.56	1.77	15	1
1:A:172:LEU:HD11	1:A:232:PHE:CZ	0.56	2.36	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:LEU:CD1	1:A:189:LEU:HD11	0.56	2.29	1	3
1:A:168:LEU:CD1	1:A:185:LEU:HD11	0.56	2.31	20	1
1:A:212:LEU:HD13	1:A:220:TYR:CD2	0.56	2.34	8	1
1:A:145:ILE:HG12	1:A:152:VAL:HG12	0.56	1.76	12	3
1:A:168:LEU:CD1	1:A:185:LEU:HD21	0.55	2.32	20	2
1:A:220:TYR:O	1:A:221:ARG:C	0.55	2.44	10	7
1:A:222:ILE:HG22	1:A:230:TYR:CE2	0.55	2.36	7	1
1:A:205:ILE:HG23	1:A:230:TYR:CE2	0.55	2.36	2	1
1:A:186:LEU:HA	1:A:189:LEU:HD12	0.55	1.78	17	1
1:A:183:ASP:HA	1:A:186:LEU:HD11	0.55	1.78	14	1
1:A:222:ILE:O	1:A:222:ILE:HG23	0.54	2.01	8	2
1:A:213:LEU:O	1:A:213:LEU:CG	0.54	2.56	16	5
1:A:186:LEU:C	1:A:186:LEU:HD13	0.54	2.21	13	1
1:A:168:LEU:HD13	1:A:189:LEU:HD11	0.54	1.79	6	2
1:A:213:LEU:O	1:A:214:ASP:C	0.54	2.45	7	2
1:A:225:VAL:O	1:A:227:ASN:N	0.54	2.41	4	20
1:A:154:LEU:HD22	1:A:212:LEU:CD2	0.54	2.32	4	2
1:A:192:VAL:HG23	1:A:194:TYR:N	0.54	2.18	12	1
1:A:168:LEU:HD22	1:A:208:LEU:CD2	0.53	2.32	7	2
1:A:185:LEU:HD22	1:A:230:TYR:CE1	0.53	2.38	13	1
1:A:168:LEU:HD12	1:A:189:LEU:HD21	0.53	1.79	14	1
1:A:185:LEU:HD23	1:A:201:VAL:CG1	0.53	2.33	15	2
1:A:153:LEU:HD11	1:A:156:GLY:O	0.53	2.04	14	2
1:A:168:LEU:CD2	1:A:185:LEU:HD21	0.53	2.34	1	3
1:A:179:ILE:HD11	1:A:225:VAL:HG21	0.53	1.78	11	1
1:A:137:THR:HG22	1:A:147:PRO:HD2	0.53	1.79	20	10
1:A:210:LYS:HG3	1:A:211:LYS:N	0.53	2.18	6	1
1:A:205:ILE:HG21	1:A:230:TYR:CE2	0.52	2.38	16	1
1:A:213:LEU:O	1:A:213:LEU:HG	0.52	2.04	16	10
1:A:179:ILE:HD13	1:A:180:MET:N	0.52	2.19	10	6
1:A:143:LEU:HD12	1:A:154:LEU:CD1	0.52	2.34	20	1
1:A:153:LEU:HD21	1:A:156:GLY:HA2	0.52	1.80	16	4
1:A:177:GLY:O	1:A:231:LEU:HD21	0.52	2.05	2	1
1:A:138:ILE:HD12	1:A:173:ALA:HB1	0.52	1.80	2	1
1:A:172:LEU:C	1:A:172:LEU:HD12	0.51	2.26	15	1
1:A:221:ARG:O	1:A:222:ILE:HG22	0.51	2.05	9	1
1:A:168:LEU:O	1:A:168:LEU:HD12	0.51	2.05	8	2
1:A:209:ARG:NH2	1:A:222:ILE:HD12	0.51	2.19	6	1
1:A:143:LEU:HD12	1:A:212:LEU:CD1	0.51	2.34	3	1
1:A:138:ILE:HD12	1:A:173:ALA:CB	0.51	2.36	20	5
1:A:182:ARG:O	1:A:186:LEU:HD12	0.51	2.06	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:LEU:CG	1:A:185:LEU:HD21	0.50	2.36	1	1
1:A:225:VAL:HG23	1:A:229:GLY:N	0.50	2.22	13	4
1:A:213:LEU:HG	1:A:213:LEU:O	0.50	2.05	8	6
1:A:231:LEU:HD23	1:A:232:PHE:H	0.50	1.65	15	3
1:A:169:LEU:HA	1:A:172:LEU:HD23	0.50	1.83	15	1
1:A:212:LEU:HD13	1:A:220:TYR:CE2	0.50	2.40	8	1
1:A:231:LEU:HD23	1:A:232:PHE:N	0.50	2.22	15	2
1:A:232:PHE:C	1:A:232:PHE:CD1	0.49	2.84	10	1
1:A:145:ILE:HG13	1:A:152:VAL:HG12	0.49	1.83	5	1
1:A:201:VAL:HG12	1:A:205:ILE:HD11	0.49	1.84	16	1
1:A:143:LEU:CD1	1:A:212:LEU:HD11	0.49	2.38	6	1
1:A:183:ASP:HA	1:A:186:LEU:HD21	0.49	1.82	19	4
1:A:172:LEU:HD12	1:A:172:LEU:O	0.49	2.07	15	2
1:A:161:LEU:HD13	1:A:208:LEU:CD1	0.49	2.37	8	1
1:A:179:ILE:HD11	1:A:229:GLY:HA3	0.49	1.84	4	1
1:A:222:ILE:HG22	1:A:230:TYR:CD1	0.49	2.43	6	1
1:A:210:LYS:O	1:A:213:LEU:HD13	0.49	2.08	16	1
1:A:183:ASP:HA	1:A:186:LEU:HD22	0.49	1.84	15	1
1:A:205:ILE:HG23	1:A:230:TYR:OH	0.49	2.07	17	1
1:A:221:ARG:O	1:A:222:ILE:CG2	0.48	2.61	9	2
1:A:152:VAL:HG21	1:A:161:LEU:CD1	0.48	2.37	18	1
1:A:169:LEU:HD21	1:A:208:LEU:HG	0.48	1.84	8	1
1:A:213:LEU:CG	1:A:213:LEU:O	0.48	2.60	8	9
1:A:172:LEU:HD11	1:A:222:ILE:HD13	0.48	1.84	8	1
1:A:149:ASN:O	1:A:150:ARG:C	0.48	2.52	11	5
1:A:137:THR:HG21	1:A:146:ASP:OD2	0.48	2.08	2	4
1:A:214:ASP:O	1:A:218:GLU:C	0.48	2.52	16	1
1:A:186:LEU:C	1:A:186:LEU:CD2	0.48	2.81	13	1
1:A:172:LEU:CD1	1:A:222:ILE:HD11	0.48	2.38	9	1
1:A:169:LEU:HD23	1:A:172:LEU:HD23	0.47	1.85	13	1
1:A:168:LEU:HD21	1:A:185:LEU:HG	0.47	1.86	19	1
1:A:139:SER:CB	1:A:144:THR:HG23	0.47	2.39	1	1
1:A:168:LEU:HD22	1:A:208:LEU:HD22	0.47	1.85	7	2
1:A:201:VAL:HG12	1:A:205:ILE:CD1	0.47	2.40	16	1
1:A:154:LEU:HD21	1:A:214:ASP:OD2	0.46	2.10	1	1
1:A:168:LEU:HD23	1:A:208:LEU:HD11	0.46	1.88	9	1
1:A:154:LEU:HD13	1:A:154:LEU:C	0.46	2.30	17	1
1:A:181:ASP:O	1:A:185:LEU:N	0.46	2.48	15	1
1:A:222:ILE:HD13	1:A:222:ILE:C	0.46	2.30	19	1
1:A:149:ASN:C	1:A:150:ARG:HG2	0.46	2.31	8	1
1:A:161:LEU:HD13	1:A:169:LEU:CD1	0.46	2.41	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:ILE:CD1	1:A:173:ALA:HB2	0.46	2.41	12	1
1:A:183:ASP:O	1:A:186:LEU:CD1	0.46	2.64	13	1
1:A:233:ALA:HB1	1:A:234:PRO:HD2	0.46	1.88	16	2
1:A:213:LEU:O	1:A:215:ASN:N	0.45	2.49	20	1
1:A:220:TYR:CZ	1:A:222:ILE:HD12	0.45	2.46	16	1
1:A:226:ARG:O	1:A:227:ASN:C	0.45	2.54	19	18
1:A:192:VAL:HG12	1:A:193:THR:H	0.45	1.72	8	3
1:A:143:LEU:HD12	1:A:154:LEU:HD22	0.45	1.88	10	1
1:A:208:LEU:O	1:A:212:LEU:HD12	0.45	2.12	8	1
1:A:182:ARG:O	1:A:186:LEU:HG	0.45	2.12	14	2
1:A:154:LEU:CD2	1:A:212:LEU:HD22	0.45	2.42	12	1
1:A:226:ARG:O	1:A:228:LYS:N	0.44	2.50	4	6
1:A:222:ILE:CD1	1:A:222:ILE:C	0.44	2.86	19	1
1:A:161:LEU:HD13	1:A:208:LEU:HD11	0.44	1.90	8	1
1:A:186:LEU:CB	1:A:201:VAL:HG21	0.44	2.42	17	1
1:A:222:ILE:HG22	1:A:222:ILE:O	0.44	2.13	15	1
1:A:185:LEU:HD23	1:A:201:VAL:HG11	0.44	1.90	15	1
1:A:172:LEU:HD11	1:A:222:ILE:CD1	0.44	2.43	8	1
1:A:168:LEU:HG	1:A:185:LEU:HD21	0.44	1.90	1	1
1:A:198:ASP:O	1:A:199:ARG:C	0.43	2.57	15	3
1:A:149:ASN:O	1:A:150:ARG:HG2	0.43	2.13	6	1
1:A:138:ILE:HD12	1:A:173:ALA:HB3	0.43	1.89	20	4
1:A:171:GLU:O	1:A:174:THR:HG22	0.43	2.14	6	4
1:A:222:ILE:HG22	1:A:230:TYR:HE2	0.43	1.74	7	1
1:A:179:ILE:HD12	1:A:180:MET:H	0.43	1.74	19	1
1:A:168:LEU:CG	1:A:189:LEU:HD11	0.42	2.42	13	1
1:A:225:VAL:HG22	1:A:229:GLY:C	0.42	2.35	12	2
1:A:230:TYR:C	1:A:230:TYR:CD1	0.42	2.93	11	1
1:A:154:LEU:HD23	1:A:212:LEU:HD22	0.42	1.89	12	1
1:A:143:LEU:HD23	1:A:144:THR:N	0.42	2.29	1	1
1:A:168:LEU:HG	1:A:189:LEU:HD21	0.42	1.90	19	1
1:A:143:LEU:HD12	1:A:212:LEU:HD11	0.42	1.91	3	1
1:A:218:GLU:HB3	1:A:219:PRO:HD2	0.42	1.91	7	1
1:A:154:LEU:HD22	1:A:155:GLY:N	0.42	2.30	17	1
1:A:172:LEU:HG	1:A:173:ALA:N	0.42	2.29	15	1
1:A:162:SER:O	1:A:163:THR:C	0.42	2.58	17	2
1:A:171:GLU:HA	1:A:174:THR:HG22	0.41	1.92	10	1
1:A:225:VAL:HG22	1:A:229:GLY:O	0.41	2.14	12	1
1:A:186:LEU:HB3	1:A:201:VAL:HG21	0.41	1.91	12	1
1:A:183:ASP:O	1:A:186:LEU:CD2	0.41	2.68	17	1
1:A:186:LEU:HD23	1:A:201:VAL:HG21	0.41	1.93	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:192:VAL:HG23	1:A:193:THR:N	0.41	2.30	12	1
1:A:179:ILE:HB	1:A:231:LEU:HD12	0.41	1.93	12	1
1:A:186:LEU:HD12	1:A:197:MET:O	0.41	2.16	12	1
1:A:186:LEU:HD12	1:A:196:GLY:O	0.41	2.16	17	1
1:A:186:LEU:C	1:A:186:LEU:HD23	0.40	2.35	17	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	99/119 (83%)	83±2 (84±2%)	13±2 (14±2%)	2±1 (2±1%)	12	49
All	All	1980/2380 (83%)	1663 (84%)	269 (14%)	48 (2%)	12	49

All 8 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	226	ARG	20
1	A	227	ASN	10
1	A	222	ILE	5
1	A	141	GLY	4
1	A	221	ARG	4
1	A	214	ASP	3
1	A	194	TYR	1
1	A	219	PRO	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	84/101 (83%)	58±4 (69±5%)	26±4 (31±5%)	2	16
All	All	1680/2020 (83%)	1163 (69%)	517 (31%)	2	16

All 69 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	143	LEU	19
1	A	213	LEU	19
1	A	186	LEU	18
1	A	207	ARG	18
1	A	182	ARG	16
1	A	163	THR	13
1	A	206	SER	13
1	A	174	THR	12
1	A	179	ILE	12
1	A	231	LEU	12
1	A	136	LYS	12
1	A	221	ARG	11
1	A	172	LEU	11
1	A	228	LYS	11
1	A	226	ARG	10
1	A	167	ASP	10
1	A	211	LYS	10
1	A	151	GLN	10
1	A	188	ASN	10
1	A	223	LYS	10
1	A	142	SER	10
1	A	200	SER	9
1	A	140	PHE	9
1	A	192	VAL	9
1	A	178	GLN	9
1	A	230	TYR	9
1	A	166	PHE	9
1	A	149	ASN	8
1	A	153	LEU	8
1	A	225	VAL	8
1	A	202	ASP	8
1	A	210	LYS	8
1	A	146	ASP	7
1	A	157	GLU	7
1	A	162	SER	7
1	A	187	LYS	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	215	ASN	6
1	A	168	LEU	6
1	A	220	TYR	6
1	A	150	ARG	6
1	A	154	LEU	6
1	A	170	TRP	6
1	A	180	MET	6
1	A	190	ARG	6
1	A	175	HIS	6
1	A	199	ARG	6
1	A	183	ASP	5
1	A	227	ASN	5
1	A	181	ASP	5
1	A	198	ASP	5
1	A	214	ASP	5
1	A	218	GLU	5
1	A	222	ILE	4
1	A	197	MET	4
1	A	171	GLU	4
1	A	195	ASP	3
1	A	232	PHE	3
1	A	212	LEU	3
1	A	209	ARG	3
1	A	161	LEU	3
1	A	139	SER	3
1	A	165	ASP	1
1	A	208	LEU	1
1	A	169	LEU	1
1	A	201	VAL	1
1	A	158	ASN	1
1	A	189	LEU	1
1	A	224	THR	1
1	A	217	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: 2mlk_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1173
Number of shifts mapped to atoms	1173
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	104	-0.10 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	95	0.23 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	101	0.10 ± 0.12	None needed (< 0.5 ppm)
^{15}N	102	-0.31 ± 0.40	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 930 atoms were assigned a chemical shift out of a possible 1232. 3 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	466/489 (95%)	187/195 (96%)	186/198 (94%)	93/96 (97%)
Sidechain	438/673 (65%)	279/390 (72%)	158/246 (64%)	1/37 (3%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	26/70 (37%)	18/37 (49%)	8/31 (26%)	0/2 (0%)
Overall	930/1232 (75%)	484/622 (78%)	352/475 (74%)	94/135 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 993 atoms were assigned a chemical shift out of a possible 1359. 3 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	503/542 (93%)	202/216 (94%)	201/220 (91%)	100/106 (94%)
Sidechain	462/721 (64%)	294/418 (70%)	167/265 (63%)	1/38 (3%)
Aromatic	28/96 (29%)	19/51 (37%)	9/40 (22%)	0/5 (0%)
Overall	993/1359 (73%)	515/685 (75%)	377/525 (72%)	101/149 (68%)

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	221	ARG	HG3	-0.63	3.00 – 0.10	-7.5
1	A	221	ARG	HD3	1.28	4.36 – 1.86	-7.3
1	A	221	ARG	HG2	-0.04	2.92 – 0.22	-6.0
1	A	221	ARG	HD2	1.75	4.27 – 1.97	-5.9
1	A	174	THR	HG21	-0.05	2.29 – -0.01	-5.2
1	A	174	THR	HG22	-0.05	2.29 – -0.01	-5.2
1	A	174	THR	HG23	-0.05	2.29 – -0.01	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

