



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 13, 2021 – 05:06 am GMT

PDB ID : 7NM2  
Title : Solution structure of MLKL executioner domain in complex with a fragment  
Authors : Ruebbelke, M.; Bauer, M.; Hamilton, J.; Binder, F.; Nar, H.; Zeeb, M.  
Deposited on : 2021-02-23

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

MolProbity : 4.02b-467  
Mogul : 1.8.4 (270009), 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 : 2.23.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

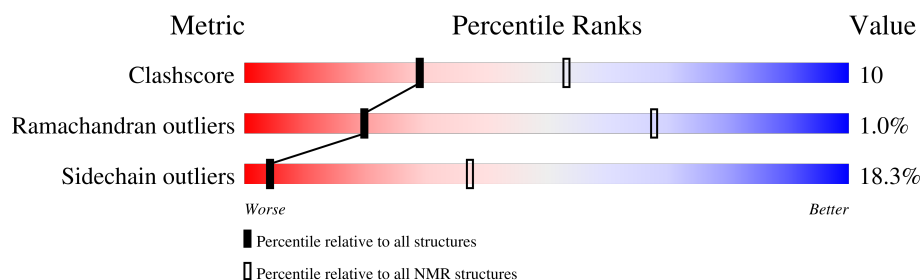
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 76%.

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  $\geq 3$ , 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	157	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:47, A:53-A:89, A:96-A:124, A:132-A:148 (129)	0.35	15

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2608 atoms, of which 1315 are hydrogens and 0 are deuteriums.

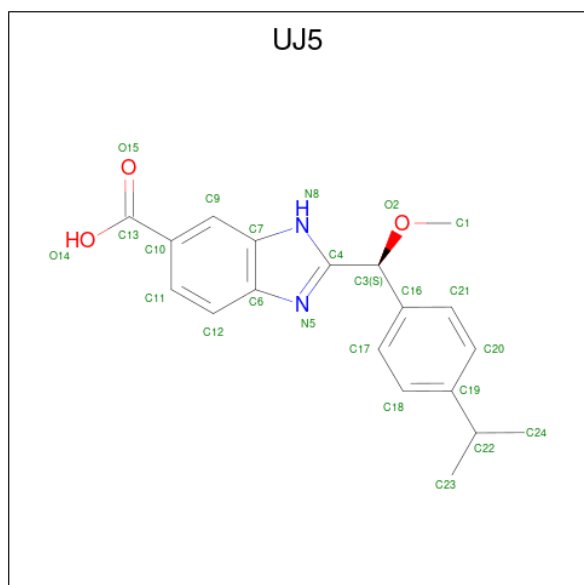
- Molecule 1 is a protein called Mixed lineage kinase domain-like protein.

Mol	Chain	Residues	Atoms						Trace
1	A	157	Total	C	H	N	O	S	0
			2564	786	1295	239	235	9	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8NB16
A	-1	SER	-	expression tag	UNP Q8NB16
A	0	PRO	-	expression tag	UNP Q8NB16
A	1	GLY	-	expression tag	UNP Q8NB16

- Molecule 2 is 2-[(S)-methoxy-(4-propan-2-ylphenyl)methyl]-3 H-benzimidazole-5-carboxylic acid (three-letter code: UJ5) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



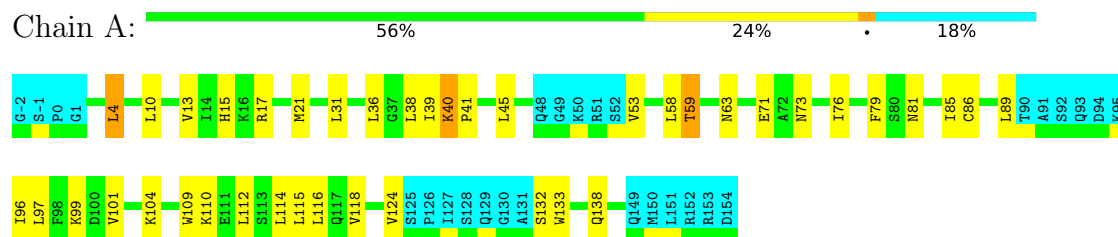
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	
			44	19	20	2	3	

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Mixed lineage kinase domain-like protein

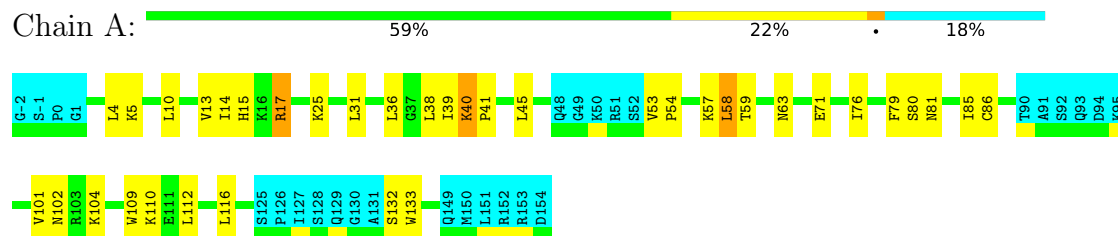


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

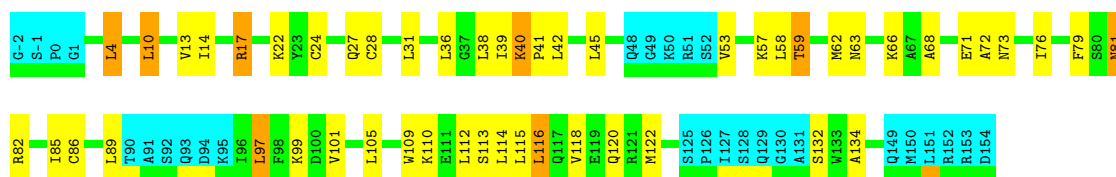
- Molecule 1: Mixed lineage kinase domain-like protein



#### 4.2.2 Score per residue for model 2

- Molecule 1: Mixed lineage kinase domain-like protein

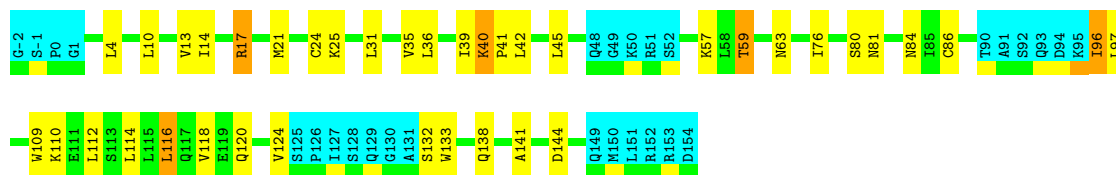




### 4.2.3 Score per residue for model 3

- Molecule 1: Mixed lineage kinase domain-like protein

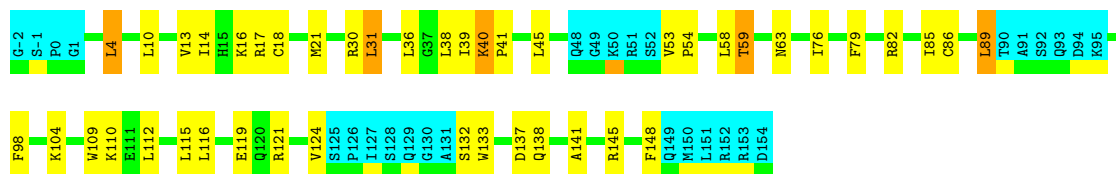
Chain A: 57% 22% 18%



### 4.2.4 Score per residue for model 4

- Molecule 1: Mixed lineage kinase domain-like protein

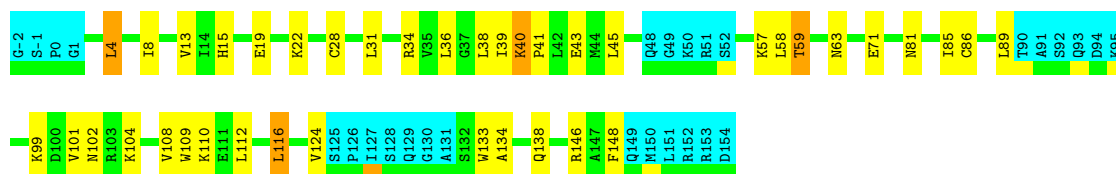
Chain A: 54% 25% 18%



### 4.2.5 Score per residue for model 5

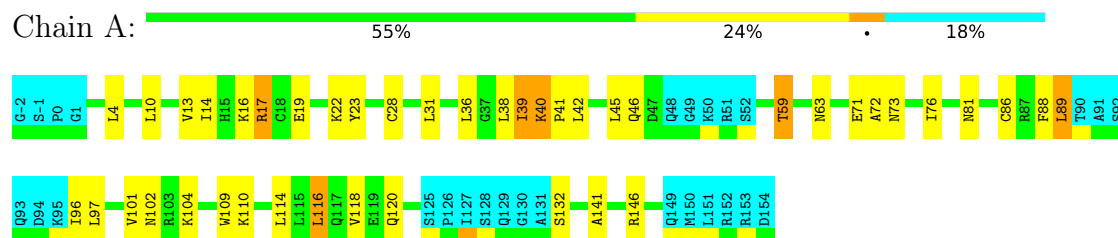
- Molecule 1: Mixed lineage kinase domain-like protein

Chain A: 57% 23% 18%



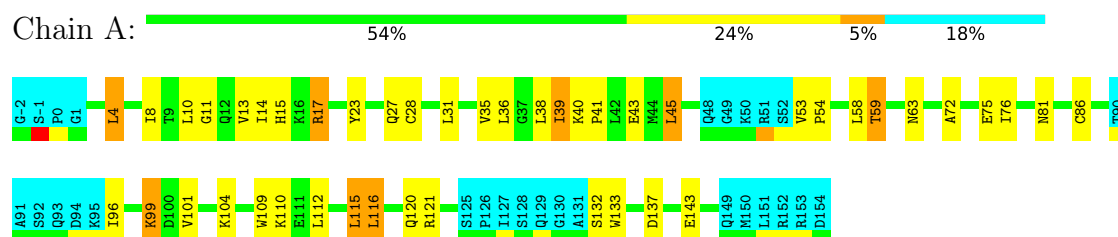
### 4.2.6 Score per residue for model 6

- Molecule 1: Mixed lineage kinase domain-like protein



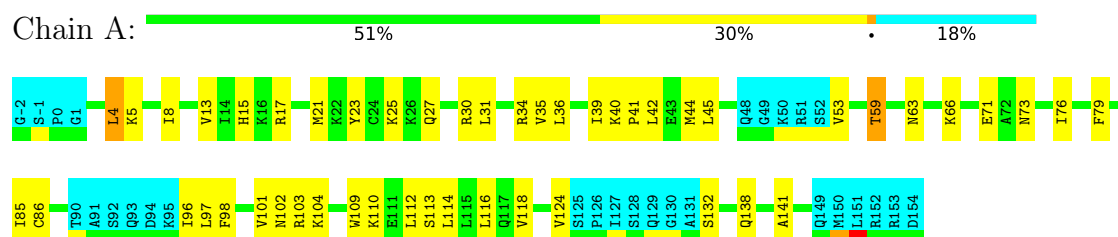
#### 4.2.7 Score per residue for model 7

- Molecule 1: Mixed lineage kinase domain-like protein



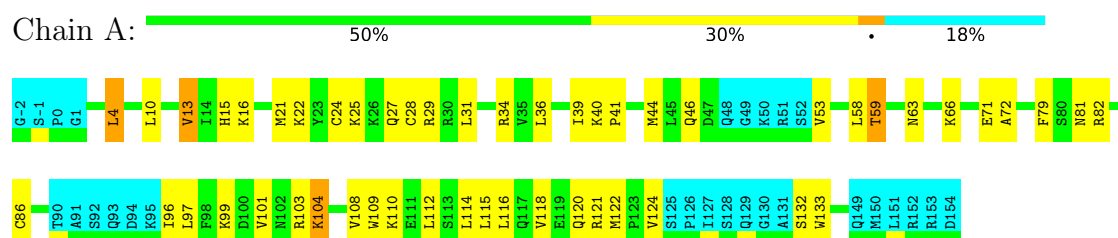
#### 4.2.8 Score per residue for model 8

- Molecule 1: Mixed lineage kinase domain-like protein



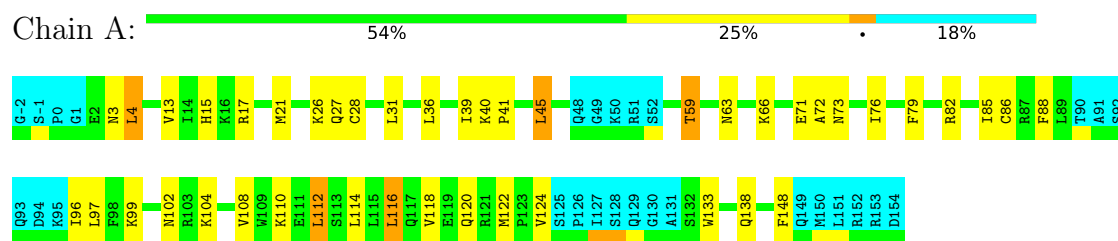
#### 4.2.9 Score per residue for model 9

- Molecule 1: Mixed lineage kinase domain-like protein



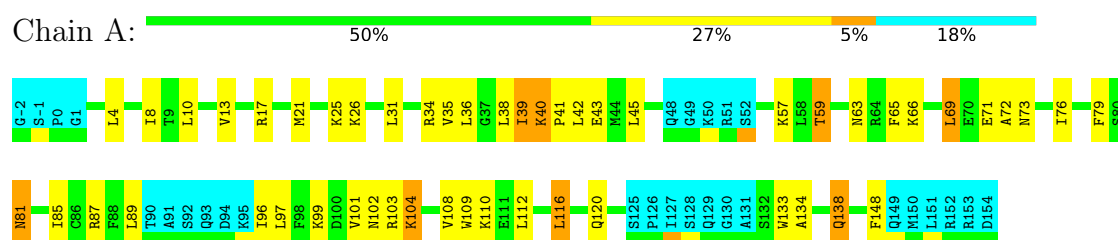
### 4.2.10 Score per residue for model 10

- Molecule 1: Mixed lineage kinase domain-like protein



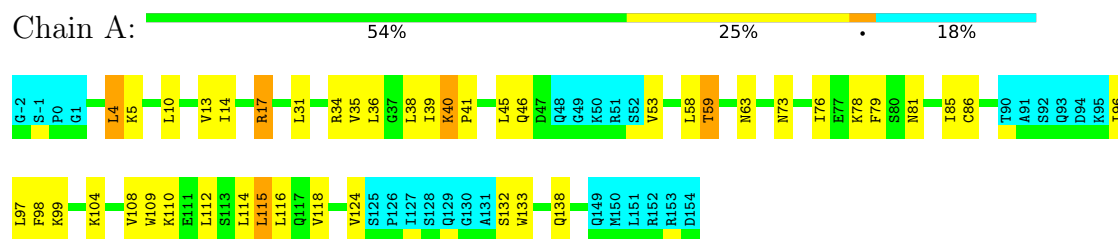
### 4.2.11 Score per residue for model 11

- Molecule 1: Mixed lineage kinase domain-like protein



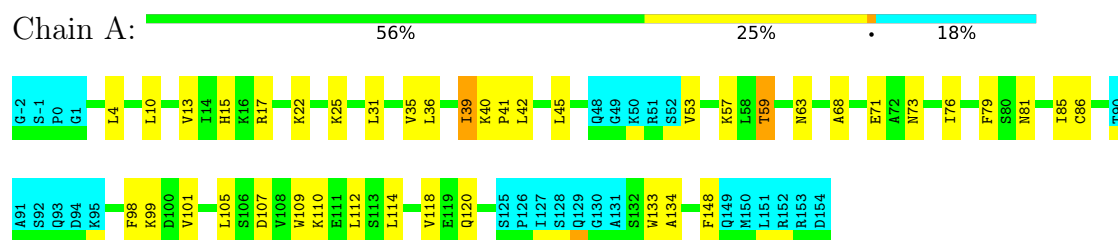
### 4.2.12 Score per residue for model 12

- Molecule 1: Mixed lineage kinase domain-like protein



### 4.2.13 Score per residue for model 13

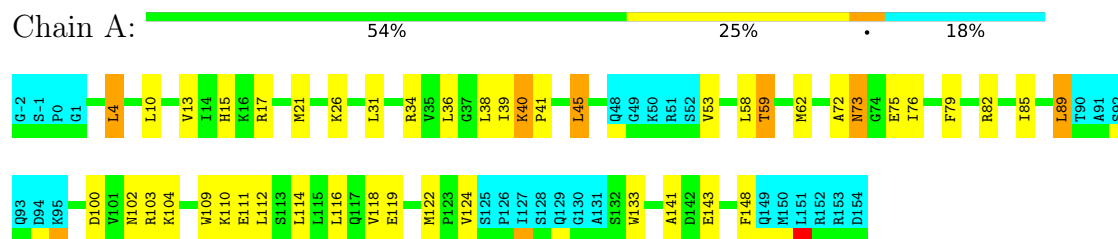
- Molecule 1: Mixed lineage kinase domain-like protein





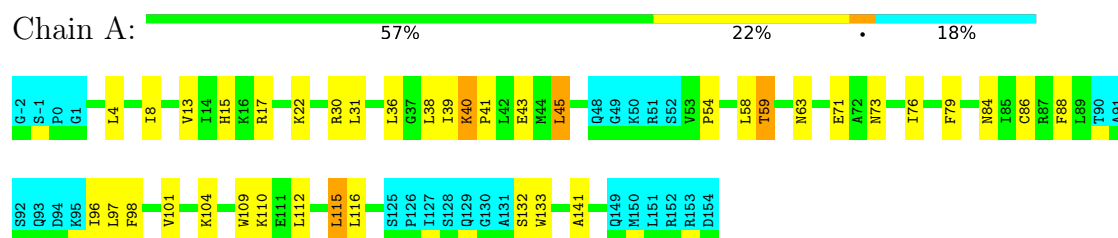
## 4.2.14 Score per residue for model 14

- Molecule 1: Mixed lineage kinase domain-like protein



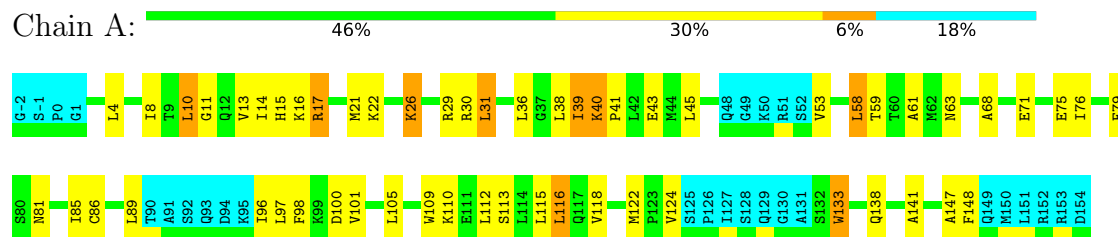
## 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Mixed lineage kinase domain-like protein



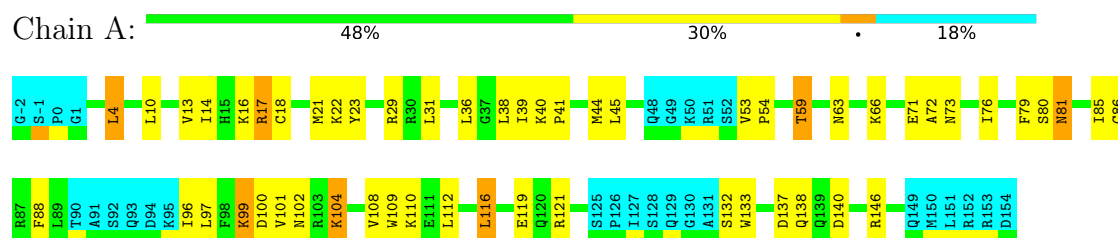
## 4.2.16 Score per residue for model 16

- Molecule 1: Mixed lineage kinase domain-like protein



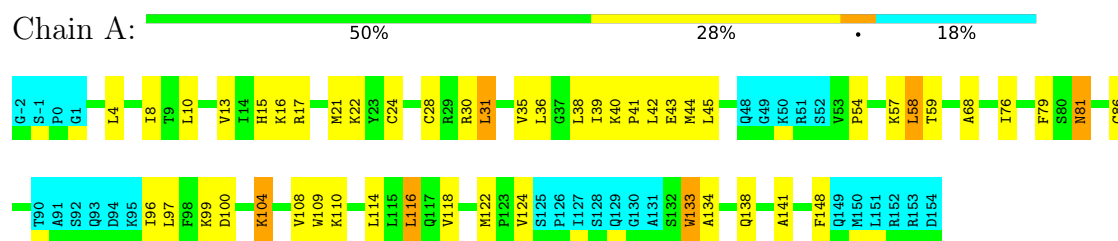
## 4.2.17 Score per residue for model 17

- Molecule 1: Mixed lineage kinase domain-like protein



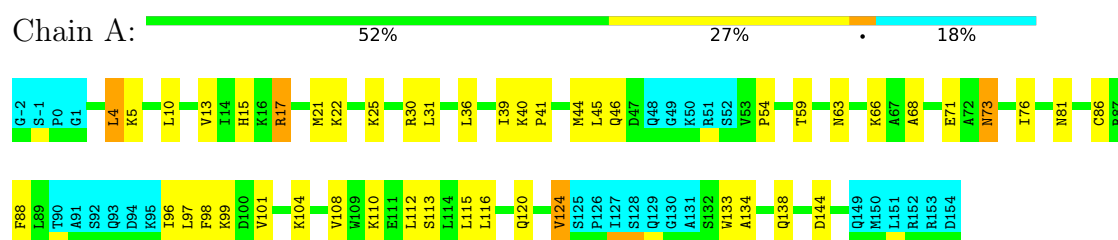
### 4.2.18 Score per residue for model 18

- Molecule 1: Mixed lineage kinase domain-like protein



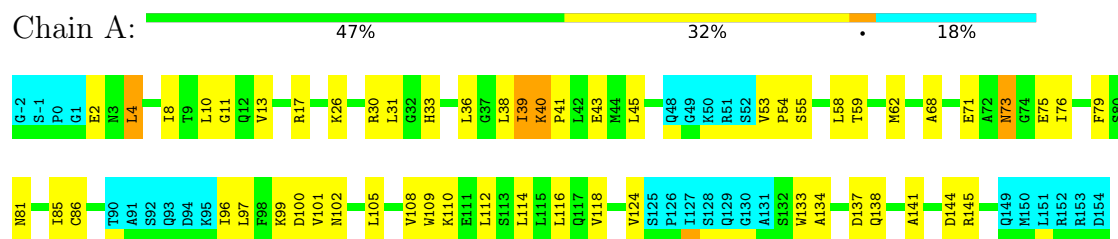
### 4.2.19 Score per residue for model 19

- Molecule 1: Mixed lineage kinase domain-like protein



### 4.2.20 Score per residue for model 20

- Molecule 1: Mixed lineage kinase domain-like protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.9

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1730
Number of shifts mapped to atoms	1730
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UJ5

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	1065	1091	1091	22±5
2	A	24	20	0	2±1
All	All	21780	22220	21820	450

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:ILE:HG23	1:A:76:ILE:HD11	0.96	1.36	6	9
1:A:58:LEU:HD13	1:A:115:LEU:HD11	0.95	1.35	7	2
1:A:89:LEU:HD21	1:A:97:LEU:HD11	0.69	1.62	2	2
1:A:53:VAL:HG21	2:A:201:UJ5:C12	0.66	2.20	13	5
1:A:79:PHE:CE2	1:A:97:LEU:HD22	0.66	2.25	15	5
1:A:99:LYS:HE3	1:A:134:ALA:HB1	0.66	1.67	20	6
1:A:114:LEU:O	1:A:118:VAL:HG23	0.64	1.92	9	7
1:A:42:LEU:HD11	1:A:109:TRP:CZ3	0.64	2.28	3	3
1:A:40:LYS:N	1:A:41:PRO:HD2	0.64	2.08	10	20
1:A:31:LEU:HD11	1:A:72:ALA:HB1	0.63	1.71	2	4
1:A:71:GLU:CG	1:A:101:VAL:HG22	0.63	2.23	6	11

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:TRP:CE3	1:A:112:LEU:HD11	0.63	2.28	16	11
1:A:14:ILE:HG23	1:A:76:ILE:CD1	0.63	2.22	2	7
1:A:31:LEU:HD13	1:A:102:ASN:ND2	0.62	2.09	17	4
1:A:99:LYS:CE	1:A:134:ALA:HB1	0.62	2.24	19	3
1:A:38:LEU:HD22	1:A:109:TRP:CG	0.62	2.30	2	11
1:A:17:ARG:HB3	1:A:76:ILE:HG21	0.61	1.72	1	10
1:A:88:PHE:CD1	1:A:97:LEU:HD23	0.61	2.30	17	4
1:A:58:LEU:HD13	1:A:115:LEU:HD21	0.61	1.73	2	1
1:A:116:LEU:HD23	1:A:120:GLN:CB	0.61	2.26	2	3
1:A:79:PHE:CE2	1:A:97:LEU:HD23	0.60	2.31	8	5
1:A:73:ASN:HA	1:A:76:ILE:HD12	0.60	1.73	2	9
1:A:53:VAL:HG21	2:A:201:UJ5:C6	0.60	2.26	4	6
1:A:31:LEU:HD13	1:A:102:ASN:OD1	0.59	1.96	10	4
1:A:71:GLU:HG2	1:A:101:VAL:HG22	0.59	1.75	5	8
1:A:53:VAL:HG23	1:A:58:LEU:HD23	0.59	1.74	12	1
1:A:17:ARG:HB3	1:A:76:ILE:HD13	0.59	1.75	7	3
1:A:10:LEU:O	1:A:13:VAL:HG12	0.59	1.98	16	12
1:A:54:PRO:HG3	1:A:58:LEU:HD13	0.58	1.76	18	2
1:A:58:LEU:HG	1:A:115:LEU:HD11	0.58	1.75	15	1
1:A:116:LEU:HD23	1:A:120:GLN:HB2	0.58	1.73	2	4
1:A:96:ILE:HD12	1:A:99:LYS:HD3	0.58	1.75	11	5
1:A:53:VAL:HG13	2:A:201:UJ5:C12	0.58	2.29	9	2
1:A:54:PRO:CG	1:A:58:LEU:HD13	0.57	2.29	18	2
1:A:41:PRO:O	1:A:45:LEU:HD23	0.57	2.00	16	6
1:A:113:SER:O	1:A:124:VAL:HG11	0.57	1.98	8	1
1:A:4:LEU:HD11	2:A:201:UJ5:C20	0.57	2.29	5	3
1:A:59:THR:HG23	2:A:201:UJ5:N5	0.57	2.15	5	13
1:A:24:CYS:HB2	1:A:85:ILE:HD12	0.57	1.76	2	1
1:A:79:PHE:O	1:A:85:ILE:HD11	0.57	2.00	2	12
1:A:96:ILE:HD11	1:A:138:GLN:CA	0.57	2.30	11	1
1:A:96:ILE:HD13	1:A:137:ASP:CG	0.57	2.21	7	1
1:A:99:LYS:HE2	1:A:134:ALA:HB1	0.56	1.78	13	2
1:A:27:GLN:CD	1:A:96:ILE:HG23	0.56	2.21	8	1
1:A:62:MET:CE	1:A:112:LEU:HD13	0.56	2.30	20	1
1:A:79:PHE:CD2	1:A:97:LEU:HD23	0.56	2.35	18	3
1:A:109:TRP:CZ3	1:A:112:LEU:HD11	0.55	2.37	1	9
1:A:68:ALA:HB1	1:A:105:LEU:HD23	0.55	1.78	13	4
1:A:96:ILE:HD12	1:A:99:LYS:CD	0.55	2.32	10	2
1:A:53:VAL:HG21	2:A:201:UJ5:C7	0.55	2.31	17	1
1:A:71:GLU:HG3	1:A:101:VAL:HG22	0.54	1.79	13	8
1:A:104:LYS:O	1:A:108:VAL:HG13	0.54	2.01	19	7

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HG12	1:A:141:ALA:HB2	0.54	1.78	6	5
1:A:4:LEU:HD21	2:A:201:UJ5:C21	0.54	2.33	20	2
1:A:96:ILE:HD12	1:A:99:LYS:HD2	0.53	1.79	7	2
1:A:40:LYS:N	1:A:41:PRO:CD	0.53	2.71	10	19
1:A:96:ILE:HD11	1:A:138:GLN:HA	0.53	1.81	11	2
1:A:108:VAL:O	1:A:112:LEU:HD23	0.53	2.03	10	2
1:A:8:ILE:HD12	1:A:43:GLU:CD	0.53	2.23	20	3
1:A:39:ILE:HD13	1:A:40:LYS:N	0.53	2.19	11	3
1:A:53:VAL:HG13	2:A:201:UJ5:C9	0.53	2.33	8	2
1:A:114:LEU:O	1:A:118:VAL:HG13	0.53	2.04	18	4
1:A:58:LEU:HD22	2:A:201:UJ5:C17	0.53	2.34	15	1
1:A:59:THR:HG23	2:A:201:UJ5:N8	0.52	2.20	17	1
1:A:59:THR:HG23	2:A:201:UJ5:C7	0.52	2.35	8	1
1:A:112:LEU:HD12	1:A:113:SER:N	0.51	2.21	16	2
1:A:65:PHE:O	1:A:69:LEU:HD22	0.51	2.05	11	1
1:A:68:ALA:CB	1:A:108:VAL:HG21	0.51	2.35	18	1
1:A:85:ILE:HG22	1:A:89:LEU:HD13	0.51	1.81	14	1
1:A:4:LEU:HD11	2:A:201:UJ5:C17	0.51	2.35	9	1
1:A:31:LEU:O	1:A:35:VAL:HG13	0.51	2.06	13	2
1:A:58:LEU:HD12	1:A:115:LEU:CD1	0.51	2.36	16	1
1:A:116:LEU:HD22	1:A:122:MET:HB3	0.50	1.82	2	1
1:A:8:ILE:HD12	1:A:43:GLU:OE1	0.50	2.06	5	2
1:A:59:THR:HG23	2:A:201:UJ5:C4	0.50	2.36	9	2
1:A:31:LEU:HD12	1:A:98:PHE:CG	0.50	2.42	16	2
1:A:59:THR:HG23	2:A:201:UJ5:C6	0.50	2.36	3	2
1:A:122:MET:CE	1:A:124:VAL:HG12	0.50	2.37	14	5
1:A:42:LEU:HD11	1:A:116:LEU:HD11	0.49	1.83	2	1
1:A:24:CYS:SG	1:A:97:LEU:HD11	0.49	2.47	3	1
1:A:85:ILE:HG22	1:A:89:LEU:HD11	0.49	1.83	5	1
1:A:42:LEU:CD2	1:A:116:LEU:HD11	0.49	2.36	6	1
1:A:13:VAL:HG22	1:A:17:ARG:CD	0.49	2.37	1	1
1:A:38:LEU:HD11	1:A:133:TRP:CH2	0.49	2.43	16	1
1:A:24:CYS:SG	1:A:97:LEU:HD13	0.49	2.47	2	3
1:A:13:VAL:HG22	1:A:17:ARG:HD3	0.49	1.83	16	1
1:A:112:LEU:CD1	1:A:116:LEU:HD12	0.49	2.37	19	1
1:A:8:ILE:HD12	1:A:43:GLU:OE2	0.49	2.07	16	4
1:A:4:LEU:HD22	1:A:46:GLN:HB3	0.49	1.83	12	1
1:A:8:ILE:HD12	1:A:43:GLU:HG3	0.49	1.85	18	1
1:A:88:PHE:CD1	1:A:97:LEU:HD12	0.49	2.42	19	1
1:A:54:PRO:HG2	1:A:58:LEU:HD22	0.49	1.84	18	2
1:A:11:GLY:HA3	1:A:39:ILE:HG21	0.49	1.84	16	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD21	1:A:72:ALA:HB1	0.49	1.83	11	4
1:A:4:LEU:HD11	2:A:201:UJ5:C18	0.48	2.37	12	3
1:A:96:ILE:CG1	1:A:141:ALA:HB2	0.48	2.38	20	2
1:A:104:LYS:O	1:A:108:VAL:HG22	0.48	2.08	18	3
1:A:116:LEU:HD23	1:A:120:GLN:HB3	0.48	1.86	3	1
1:A:53:VAL:HG13	2:A:201:UJ5:C10	0.48	2.39	16	1
1:A:58:LEU:HD12	1:A:115:LEU:HD13	0.48	1.84	16	1
1:A:58:LEU:HD13	1:A:115:LEU:CD2	0.48	2.38	2	1
1:A:116:LEU:HD22	1:A:122:MET:CB	0.48	2.39	2	1
1:A:35:VAL:HA	1:A:38:LEU:HD12	0.48	1.85	7	2
1:A:68:ALA:HB2	1:A:108:VAL:HG11	0.48	1.85	19	1
1:A:4:LEU:HD21	2:A:201:UJ5:C17	0.47	2.39	4	2
1:A:89:LEU:CD2	1:A:97:LEU:HD21	0.47	2.38	6	1
1:A:115:LEU:HD12	1:A:115:LEU:O	0.47	2.09	2	1
1:A:45:LEU:HD21	1:A:122:MET:HG3	0.47	1.84	14	1
1:A:45:LEU:CD2	1:A:116:LEU:HD21	0.47	2.40	11	2
1:A:96:ILE:HG22	1:A:98:PHE:H	0.47	1.69	12	3
1:A:58:LEU:HD21	1:A:62:MET:HE2	0.47	1.87	14	1
1:A:58:LEU:HA	1:A:115:LEU:HD13	0.47	1.85	9	1
1:A:115:LEU:HD22	1:A:119:GLU:OE1	0.47	2.10	4	1
1:A:96:ILE:HG13	1:A:141:ALA:HB2	0.47	1.86	18	2
1:A:17:ARG:CG	1:A:76:ILE:HG21	0.46	2.39	19	1
1:A:89:LEU:HD22	1:A:148:PHE:CD2	0.46	2.45	4	1
1:A:115:LEU:HD12	1:A:116:LEU:N	0.46	2.25	19	2
1:A:31:LEU:O	1:A:35:VAL:HG12	0.46	2.10	18	2
1:A:75:GLU:OE1	1:A:101:VAL:HG21	0.46	2.10	7	1
1:A:112:LEU:HA	1:A:115:LEU:HD23	0.46	1.87	15	2
1:A:61:ALA:CB	1:A:115:LEU:HD21	0.46	2.41	16	1
1:A:89:LEU:HD12	1:A:148:PHE:CD2	0.46	2.45	16	1
1:A:85:ILE:HG22	1:A:89:LEU:CD1	0.45	2.41	5	1
1:A:58:LEU:HD21	2:A:201:UJ5:C18	0.45	2.42	7	1
1:A:113:SER:HB2	1:A:124:VAL:HG11	0.45	1.89	19	1
1:A:96:ILE:HD11	1:A:138:GLN:N	0.45	2.26	11	1
1:A:45:LEU:HD21	1:A:120:GLN:HG2	0.45	1.88	6	1
1:A:31:LEU:HD22	1:A:98:PHE:CG	0.45	2.47	15	2
1:A:116:LEU:HD21	2:A:201:UJ5:C24	0.44	2.42	17	1
1:A:4:LEU:HD12	1:A:46:GLN:OE1	0.44	2.13	19	1
1:A:116:LEU:HD23	1:A:120:GLN:HG3	0.44	1.90	9	1
1:A:42:LEU:HD22	1:A:116:LEU:HD11	0.43	1.87	11	2
1:A:79:PHE:CZ	1:A:97:LEU:HD23	0.43	2.48	2	1
1:A:113:SER:HB2	1:A:124:VAL:HG21	0.43	1.89	16	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:MET:HE1	1:A:112:LEU:HD13	0.43	1.89	20	1
1:A:26:LYS:HE2	1:A:147:ALA:HB2	0.43	1.88	16	1
1:A:24:CYS:SG	1:A:97:LEU:HD22	0.43	2.53	18	1
1:A:31:LEU:HD12	1:A:98:PHE:CD1	0.42	2.49	4	2
1:A:58:LEU:HD12	1:A:58:LEU:O	0.42	2.14	7	1
1:A:31:LEU:HD23	1:A:102:ASN:HB3	0.42	1.92	6	1
1:A:13:VAL:HG22	1:A:16:LYS:HE2	0.41	1.92	9	1
1:A:31:LEU:HD12	1:A:31:LEU:O	0.41	2.15	14	1
1:A:5:LYS:HD3	1:A:8:ILE:HD11	0.41	1.91	8	1
1:A:41:PRO:HG2	1:A:42:LEU:HD12	0.41	1.91	3	1
1:A:17:ARG:HH21	1:A:76:ILE:HG22	0.41	1.75	15	1
1:A:40:LYS:HB3	1:A:41:PRO:HD3	0.41	1.92	19	3
1:A:31:LEU:HD22	1:A:98:PHE:CB	0.41	2.46	8	1
1:A:4:LEU:HD22	1:A:46:GLN:CG	0.41	2.46	12	1
1:A:17:ARG:CB	1:A:76:ILE:HG21	0.41	2.46	7	1
1:A:35:VAL:HG12	1:A:105:LEU:HD13	0.41	1.93	13	1
1:A:31:LEU:O	1:A:31:LEU:HD12	0.41	2.16	20	1
1:A:79:PHE:CZ	1:A:97:LEU:HD22	0.41	2.51	10	1
1:A:38:LEU:HD11	1:A:133:TRP:HH2	0.41	1.76	18	1
1:A:86:CYS:HA	1:A:89:LEU:HD12	0.40	1.93	5	1
1:A:115:LEU:HA	1:A:118:VAL:HG22	0.40	1.93	16	1
1:A:96:ILE:HD13	1:A:137:ASP:OD2	0.40	2.16	17	1
1:A:14:ILE:HG21	1:A:31:LEU:CD1	0.40	2.46	6	1
1:A:88:PHE:CE1	1:A:97:LEU:HD23	0.40	2.51	6	1
1:A:89:LEU:HD13	1:A:148:PHE:CG	0.40	2.52	5	1
1:A:122:MET:HE3	1:A:124:VAL:HG12	0.40	1.93	16	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	129/157 (82%)	120±2 (93±2%)	8±2 (6±2%)	1±1 (1±1%)	20	68
All	All	2580/3140 (82%)	2393 (93%)	162 (6%)	25 (1%)	20	68



All 5 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	21	MET	9
1	A	81	ASN	7
1	A	54	PRO	6
1	A	124	VAL	2
1	A	96	ILE	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	118/140 (84%)	96±2 (82±2%)	22±2 (18±2%)	4	37
All	All	2360/2800 (84%)	1927 (82%)	433 (18%)	4	37

All 72 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	4	LEU	20
1	A	36	LEU	20
1	A	39	ILE	20
1	A	110	LYS	20
1	A	59	THR	18
1	A	63	ASN	17
1	A	116	LEU	17
1	A	133	TRP	17
1	A	17	ARG	14
1	A	45	LEU	13
1	A	15	HIS	12
1	A	40	LYS	12
1	A	104	LYS	12
1	A	81	ASN	12
1	A	132	SER	11
1	A	138	GLN	11
1	A	22	LYS	9
1	A	13	VAL	8
1	A	25	LYS	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	57	LYS	7
1	A	28	CYS	7
1	A	66	LYS	7
1	A	30	ARG	7
1	A	58	LEU	6
1	A	10	LEU	6
1	A	31	LEU	6
1	A	34	ARG	6
1	A	73	ASN	6
1	A	82	ARG	5
1	A	16	LYS	5
1	A	44	MET	5
1	A	26	LYS	5
1	A	100	ASP	5
1	A	27	GLN	4
1	A	124	VAL	4
1	A	121	ARG	4
1	A	103	ARG	4
1	A	5	LYS	3
1	A	80	SER	3
1	A	144	ASP	3
1	A	89	LEU	3
1	A	146	ARG	3
1	A	115	LEU	3
1	A	29	ARG	3
1	A	75	GLU	3
1	A	35	VAL	2
1	A	84	ASN	2
1	A	18	CYS	2
1	A	137	ASP	2
1	A	145	ARG	2
1	A	19	GLU	2
1	A	112	LEU	2
1	A	46	GLN	2
1	A	99	LYS	2
1	A	143	GLU	2
1	A	120	GLN	2
1	A	119	GLU	2
1	A	21	MET	2
1	A	62	MET	1
1	A	97	LEU	1
1	A	23	TYR	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	3	ASN	1
1	A	71	GLU	1
1	A	69	LEU	1
1	A	87	ARG	1
1	A	78	LYS	1
1	A	107	ASP	1
1	A	111	GLU	1
1	A	140	ASP	1
1	A	2	GLU	1
1	A	33	HIS	1
1	A	55	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 monosaccharides in this entry.

## 6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *molecule\_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	1730
Number of shifts mapped to atoms	1730
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	154	$-0.45 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	139	$0.20 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	141	$-0.01 \pm 0.15$	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 76%, i.e. 1317 atoms were assigned a chemical shift out of a possible 1729. 23 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	494/639 (77%)	247/255 (97%)	127/258 (49%)	120/126 (95%)
Sidechain	757/992 (76%)	470/584 (80%)	276/349 (79%)	11/59 (19%)

*Continued on next page...*

Continued from previous page...

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Aromatic	66/98 (67%)	33/53 (62%)	31/40 (78%)	2/5 (40%)
Overall	1317/1729 (76%)	750/892 (84%)	434/647 (67%)	133/190 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1550 atoms were assigned a chemical shift out of a possible 2060. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	590/775 (76%)	295/309 (95%)	154/314 (49%)	141/152 (93%)
Sidechain	894/1187 (75%)	558/702 (79%)	321/411 (78%)	15/74 (20%)
Aromatic	66/98 (67%)	33/53 (62%)	31/40 (78%)	2/5 (40%)
Overall	1550/2060 (75%)	886/1064 (83%)	506/765 (66%)	158/231 (68%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 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:

