Full wwPDB NMR Structure Validation Report

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PDB ID	:	2MSV
BMRB ID	:	25135
Title	:	Solution structure of the MLKL N-terminal domain
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Deposited on	:	2014-08-07

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

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

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

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

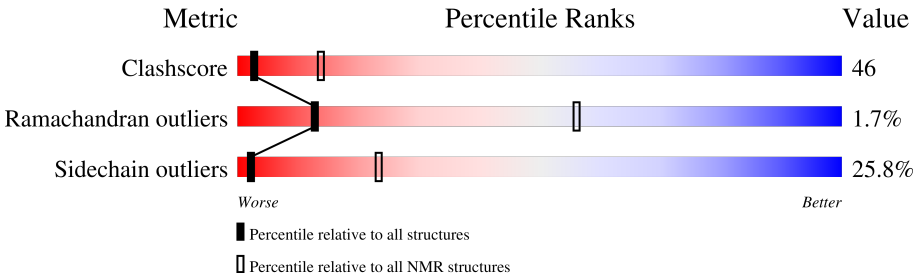
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 91%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	166	24% 48% 10% 10% 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:47, A:55-A:145 (137)	0.38	18

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2548 atoms, of which 1291 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	154	2548	780	1291	236	232	9	0

There are 13 discrepancies between the modelled and reference sequences:

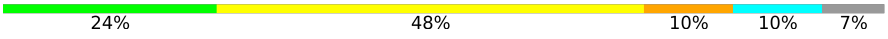
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLY	-	expression tag	UNP Q8NB16
A	-10	SER	-	expression tag	UNP Q8NB16
A	-9	PRO	-	expression tag	UNP Q8NB16
A	-8	GLY	-	expression tag	UNP Q8NB16
A	-7	ILE	-	expression tag	UNP Q8NB16
A	-6	SER	-	expression tag	UNP Q8NB16
A	-5	GLY	-	expression tag	UNP Q8NB16
A	-4	GLY	-	expression tag	UNP Q8NB16
A	-3	GLY	-	expression tag	UNP Q8NB16
A	-2	GLY	-	expression tag	UNP Q8NB16
A	-1	GLY	-	expression tag	UNP Q8NB16
A	0	ILE	-	expression tag	UNP Q8NB16
A	1	LEU	MET	engineered mutation	UNP Q8NB16

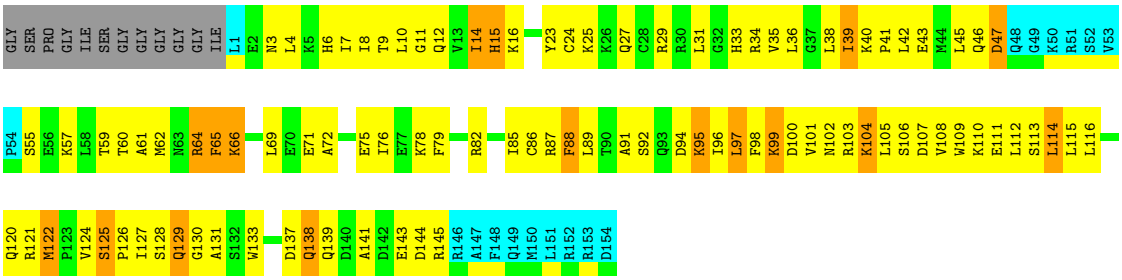
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Mixed lineage kinase domain-like protein

Chain A: 

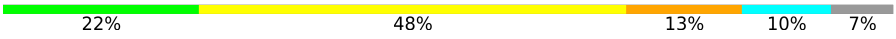


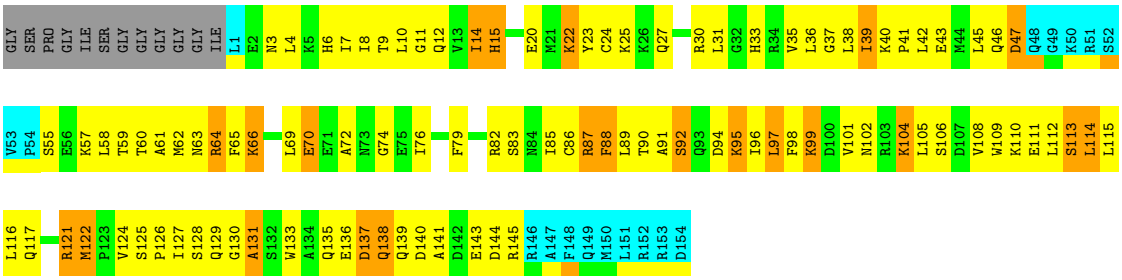
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Mixed lineage kinase domain-like protein

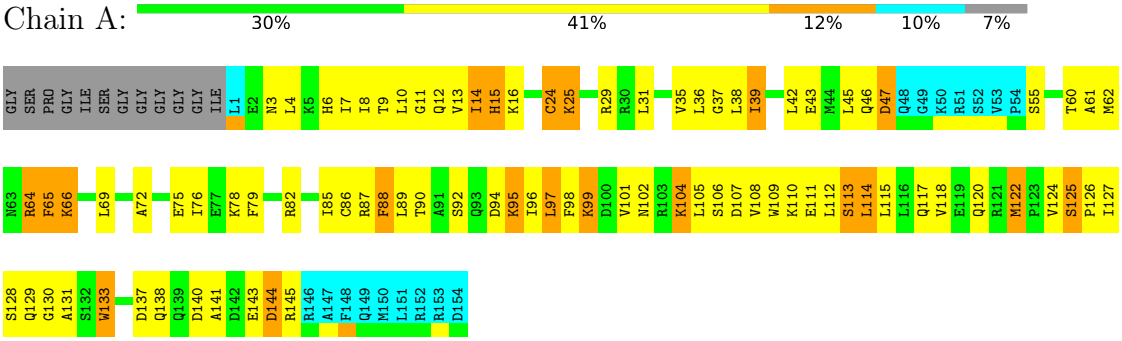
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Mixed lineage kinase domain-like protein

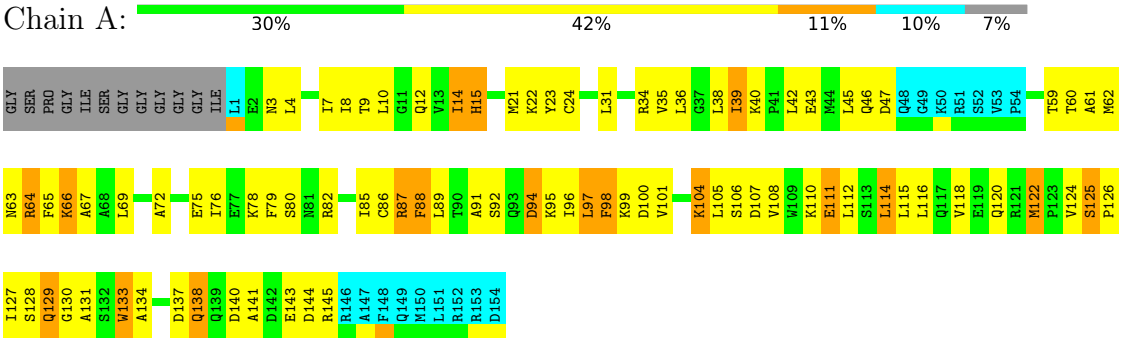
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Mixed lineage kinase domain-like protein

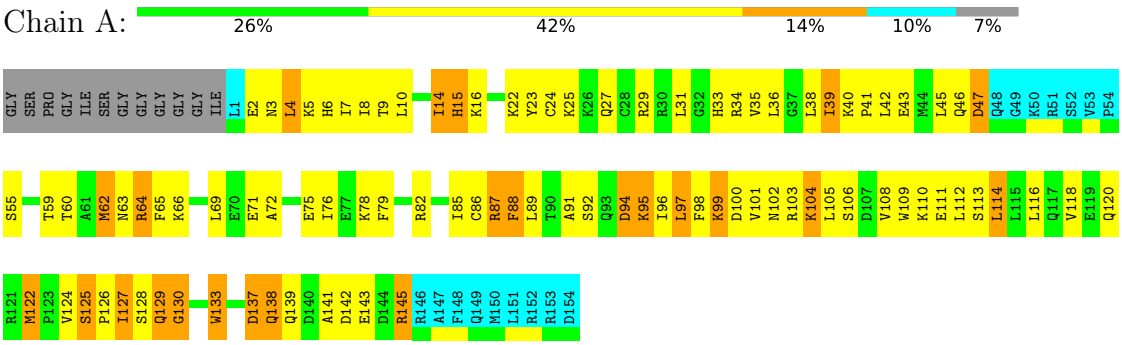
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Mixed lineage kinase domain-like protein

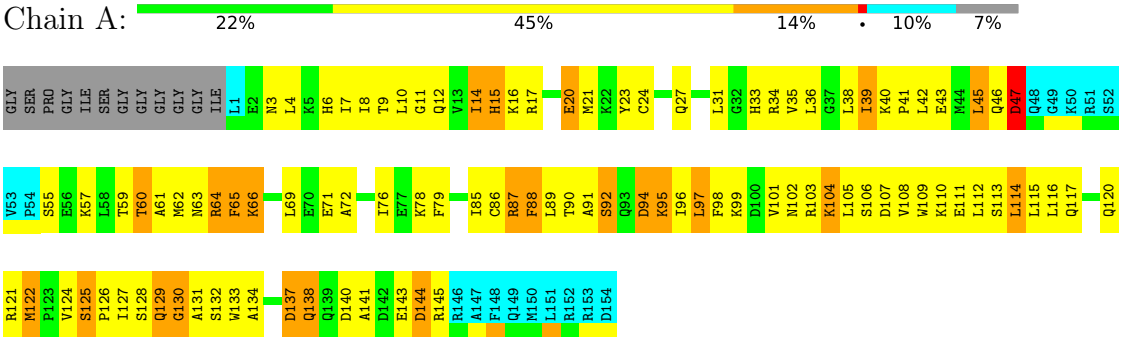
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Mixed lineage kinase domain-like protein

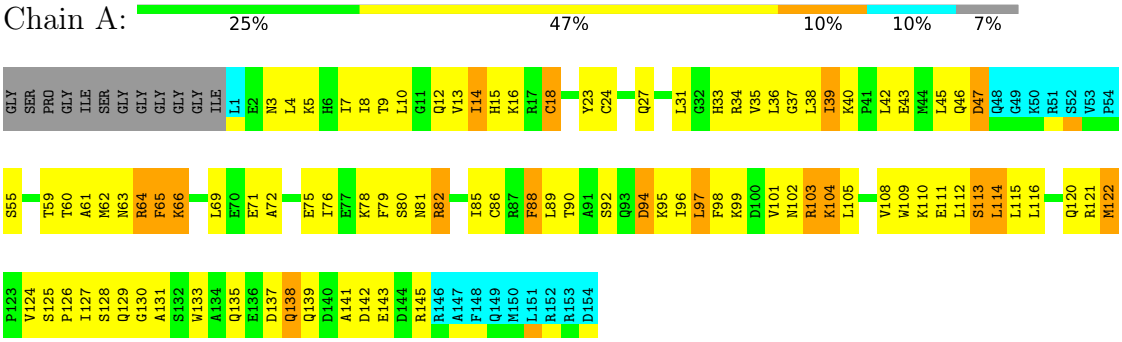
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Mixed lineage kinase domain-like protein

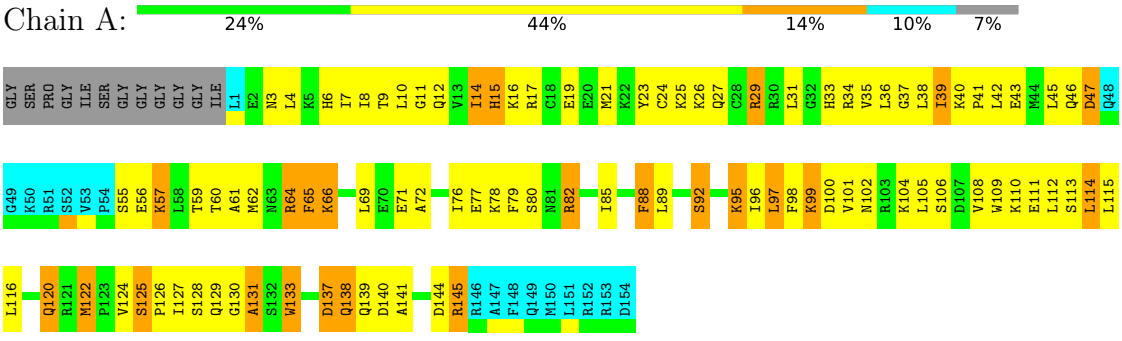
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Mixed lineage kinase domain-like protein

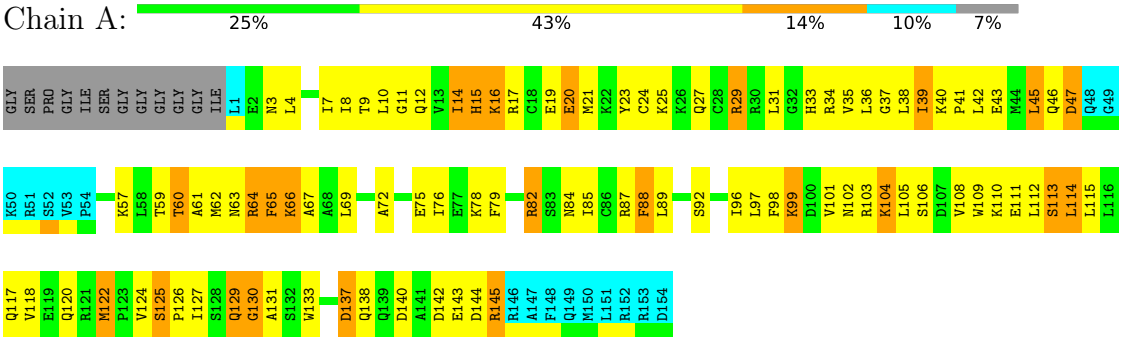
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Mixed lineage kinase domain-like protein

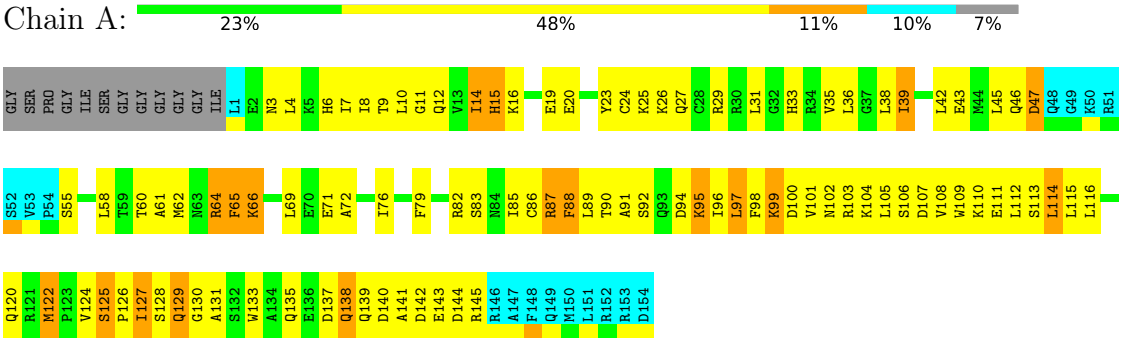
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Mixed lineage kinase domain-like protein

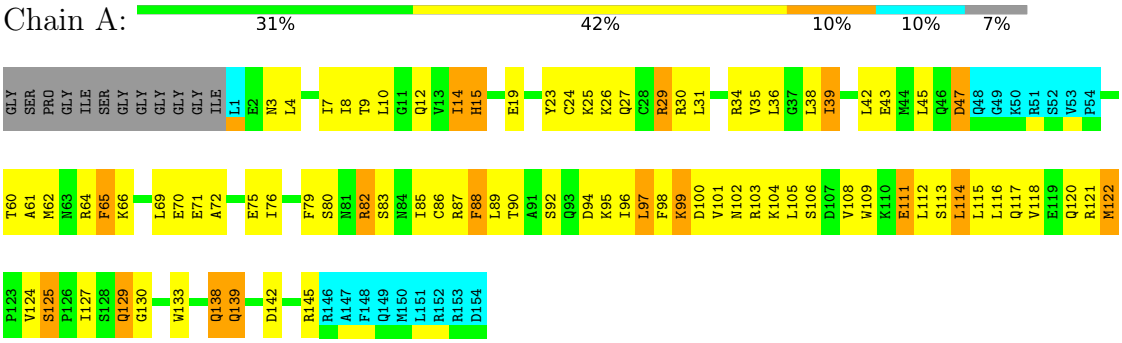
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Mixed lineage kinase domain-like protein

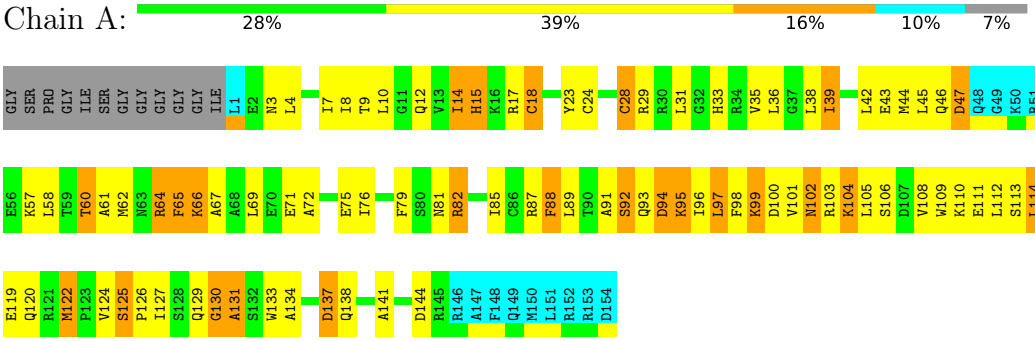
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Mixed lineage kinase domain-like protein

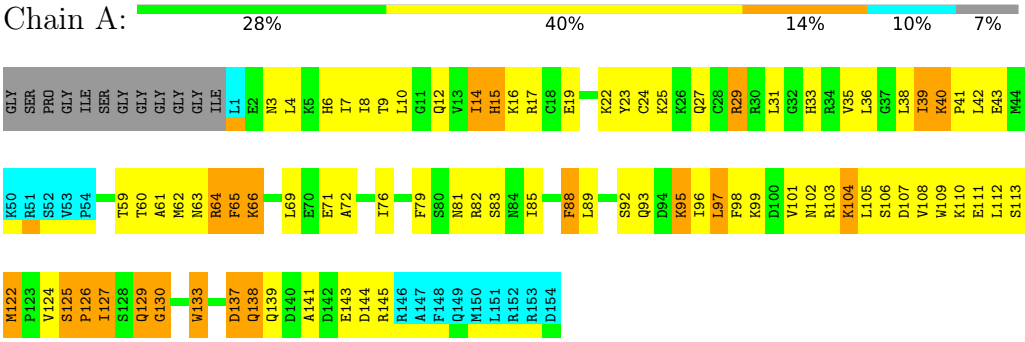
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Mixed lineage kinase domain-like protein

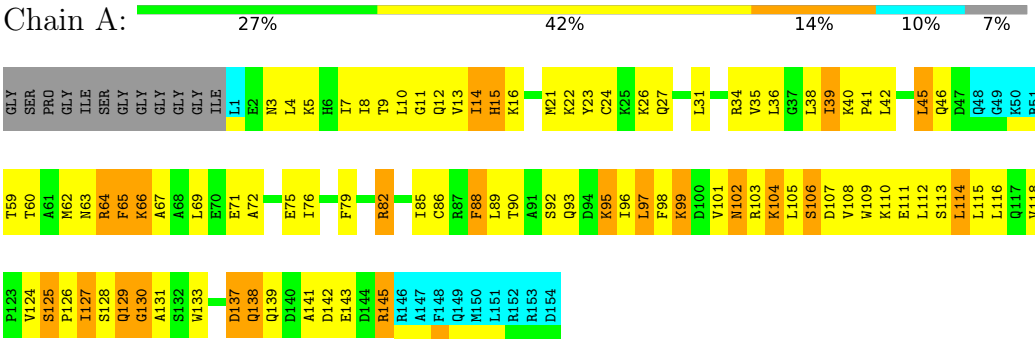
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Mixed lineage kinase domain-like protein

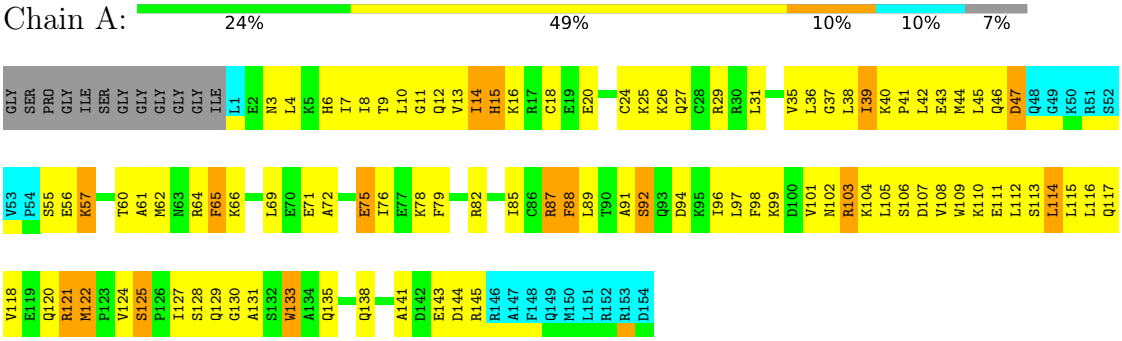
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Mixed lineage kinase domain-like protein

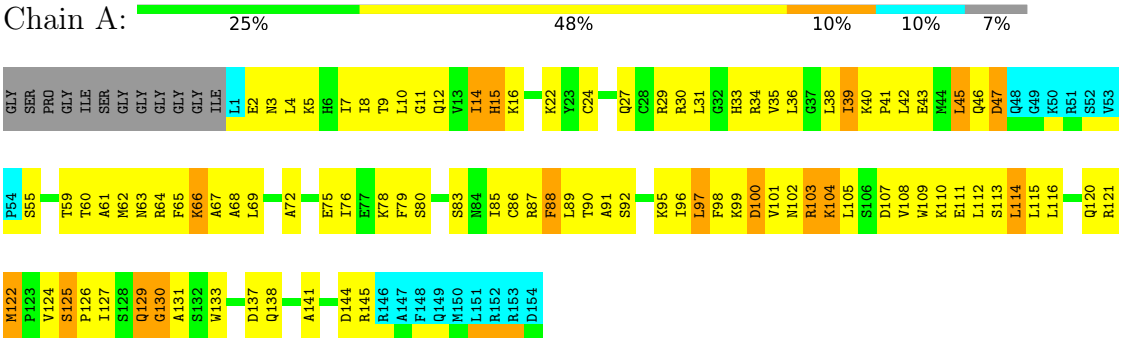
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Mixed lineage kinase domain-like protein

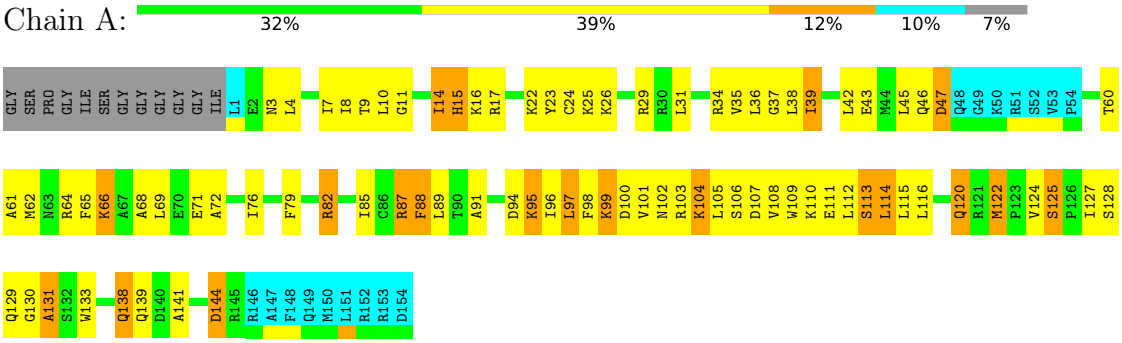
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Mixed lineage kinase domain-like protein

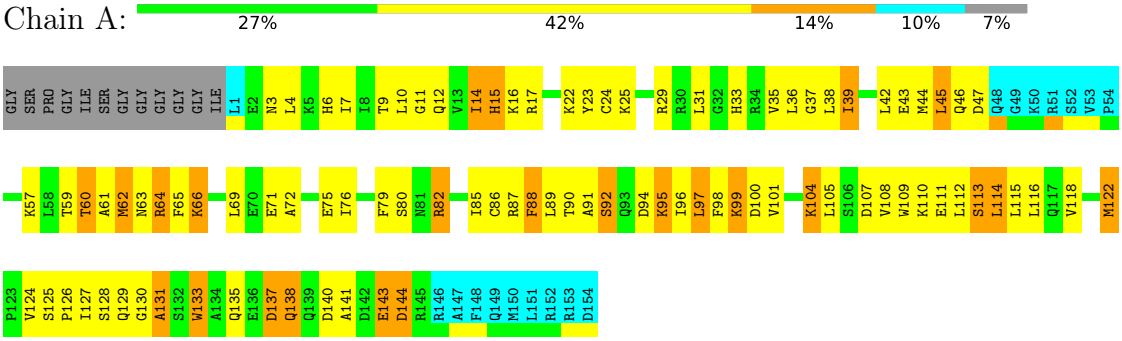
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Mixed lineage kinase domain-like protein

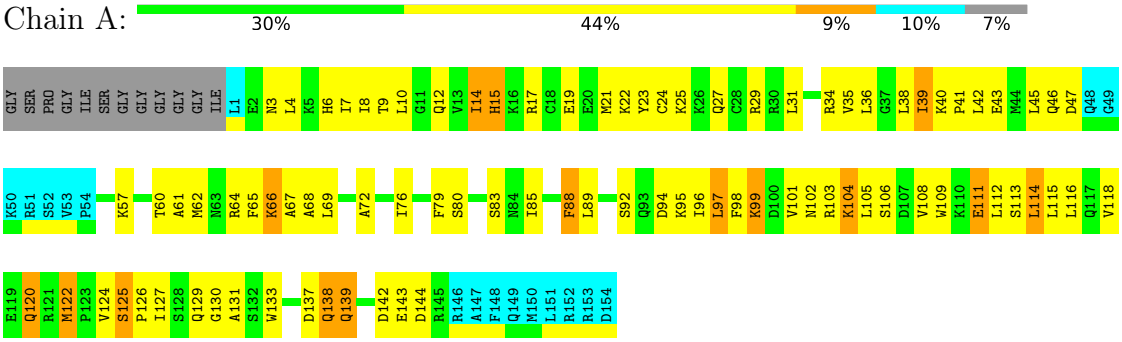
Chain A:



4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: Mixed lineage kinase domain-like protein

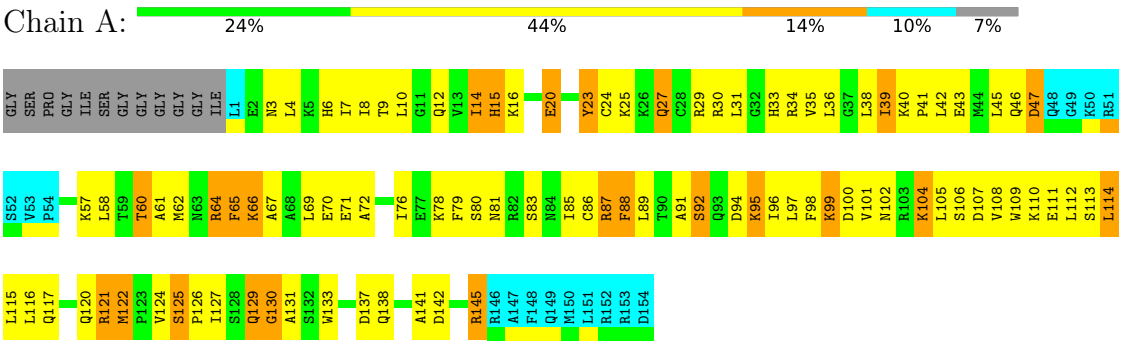
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Mixed lineage kinase domain-like protein

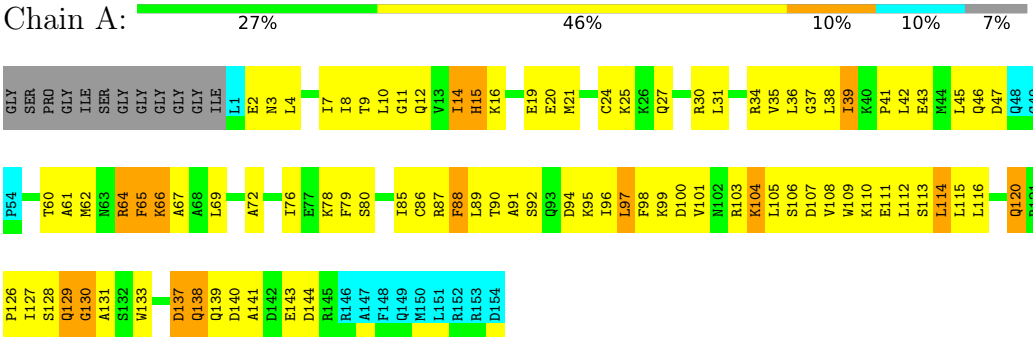
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Mixed lineage kinase domain-like protein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 5000 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
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1994
Number of shifts mapped to atoms	1994
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	1113	1137	1134	103±9
All	All	22260	22740	22680	2054

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD21	1:A:72:ALA:HB1	1.08	1.25	6	20
1:A:72:ALA:HB2	1:A:101:VAL:HG11	1.04	1.27	9	20
1:A:7:ILE:HG23	1:A:69:LEU:HD11	0.95	1.36	13	15
1:A:38:LEU:HD23	1:A:129:GLN:HG3	0.93	1.39	13	9
1:A:114:LEU:HD13	1:A:115:LEU:N	0.90	1.82	12	16
1:A:7:ILE:HG21	1:A:65:PHE:CE2	0.87	2.05	15	20
1:A:137:ASP:OD1	1:A:138:GLN:N	0.86	2.08	3	1
1:A:31:LEU:HD21	1:A:72:ALA:CB	0.83	2.04	5	20
1:A:38:LEU:HD23	1:A:129:GLN:CG	0.83	2.03	13	4
1:A:7:ILE:HG21	1:A:65:PHE:CD2	0.81	2.09	13	20
1:A:65:PHE:HA	1:A:108:VAL:HG11	0.81	1.50	18	20
1:A:3:ASN:O	1:A:7:ILE:HD12	0.80	1.75	8	20
1:A:71:GLU:CG	1:A:101:VAL:HG22	0.79	2.07	11	8
1:A:23:TYR:CD1	1:A:85:ILE:HG21	0.78	2.12	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:ILE:HG22	1:A:129:GLN:HG2	0.76	1.57	20	7
1:A:38:LEU:CD1	1:A:105:LEU:HD21	0.75	2.10	3	20
1:A:104:LYS:O	1:A:108:VAL:HG23	0.75	1.81	7	20
1:A:35:VAL:HG22	1:A:105:LEU:HD11	0.74	1.56	11	20
1:A:31:LEU:HD13	1:A:98:PHE:CD2	0.74	2.18	16	8
1:A:31:LEU:HD23	1:A:76:ILE:HD11	0.73	1.59	6	20
1:A:65:PHE:CD2	1:A:112:LEU:CD2	0.73	2.71	16	20
1:A:64:ARG:HG3	1:A:108:VAL:HG13	0.73	1.58	15	3
1:A:114:LEU:O	1:A:118:VAL:HG23	0.73	1.84	14	10
1:A:31:LEU:HD13	1:A:98:PHE:CE2	0.73	2.18	16	3
1:A:111:GLU:HA	1:A:114:LEU:HD12	0.73	1.61	15	16
1:A:4:LEU:HD13	1:A:46:GLN:HB3	0.72	1.61	14	14
1:A:45:LEU:HD22	1:A:46:GLN:N	0.72	1.99	13	1
1:A:72:ALA:CB	1:A:101:VAL:HG11	0.72	2.13	9	17
1:A:39:ILE:HA	1:A:42:LEU:HD12	0.71	1.61	1	20
1:A:79:PHE:CD2	1:A:97:LEU:HD13	0.71	2.21	5	5
1:A:15:HIS:CG	1:A:36:LEU:HD11	0.71	2.21	16	19
1:A:88:PHE:CE2	1:A:97:LEU:HG	0.71	2.20	17	15
1:A:65:PHE:CA	1:A:108:VAL:HG11	0.70	2.15	15	20
1:A:7:ILE:HD11	1:A:62:MET:O	0.70	1.86	16	20
1:A:61:ALA:HB2	1:A:115:LEU:HD12	0.70	1.62	10	15
1:A:87:ARG:O	1:A:91:ALA:HB3	0.69	1.88	5	12
1:A:88:PHE:CE2	1:A:89:LEU:HD23	0.68	2.24	18	20
1:A:86:CYS:O	1:A:90:THR:HG22	0.67	1.89	15	10
1:A:4:LEU:HD22	1:A:46:GLN:HG2	0.67	1.65	17	7
1:A:8:ILE:HD11	1:A:46:GLN:HG2	0.67	1.67	4	17
1:A:45:LEU:HD23	1:A:120:GLN:CD	0.67	2.09	14	10
1:A:110:LYS:HD3	1:A:127:ILE:HD11	0.67	1.64	6	1
1:A:31:LEU:CD2	1:A:72:ALA:HB1	0.67	2.12	5	18
1:A:24:CYS:SG	1:A:97:LEU:HD21	0.67	2.30	11	13
1:A:88:PHE:CZ	1:A:97:LEU:HG	0.67	2.24	18	15
1:A:31:LEU:O	1:A:35:VAL:HG23	0.67	1.90	14	19
1:A:114:LEU:HD22	1:A:114:LEU:O	0.66	1.90	15	16
1:A:4:LEU:CD2	1:A:42:LEU:HD13	0.66	2.20	3	6
1:A:31:LEU:HD22	1:A:98:PHE:CD2	0.66	2.26	13	4
1:A:31:LEU:HD22	1:A:98:PHE:CG	0.66	2.26	13	8
1:A:96:ILE:HG23	1:A:141:ALA:HB2	0.65	1.68	4	9
1:A:4:LEU:HD21	1:A:42:LEU:HD22	0.65	1.68	11	2
1:A:127:ILE:HG22	1:A:129:GLN:CG	0.65	2.22	8	6
1:A:101:VAL:O	1:A:105:LEU:N	0.65	2.30	11	20
1:A:38:LEU:HD23	1:A:129:GLN:CD	0.64	2.12	7	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD23	1:A:120:GLN:NE2	0.64	2.06	6	6
1:A:105:LEU:HD23	1:A:105:LEU:O	0.64	1.93	7	18
1:A:23:TYR:CD2	1:A:85:ILE:HG21	0.64	2.28	17	5
1:A:111:GLU:HA	1:A:114:LEU:HD23	0.63	1.68	14	3
1:A:45:LEU:HD21	1:A:122:MET:HG2	0.63	1.70	14	16
1:A:24:CYS:SG	1:A:97:LEU:HD22	0.63	2.34	18	3
1:A:95:LYS:O	1:A:141:ALA:HB1	0.63	1.94	6	7
1:A:127:ILE:HG22	1:A:129:GLN:H	0.62	1.53	11	1
1:A:38:LEU:HD23	1:A:129:GLN:HE21	0.62	1.54	9	3
1:A:45:LEU:HD23	1:A:120:GLN:HG2	0.62	1.71	16	2
1:A:127:ILE:HD12	1:A:131:ALA:HB2	0.62	1.70	7	15
1:A:72:ALA:HB2	1:A:101:VAL:CG1	0.62	2.17	9	9
1:A:45:LEU:HD13	1:A:45:LEU:H	0.62	1.55	13	1
1:A:45:LEU:HD21	1:A:122:MET:CG	0.62	2.23	1	19
1:A:38:LEU:HD12	1:A:105:LEU:HD21	0.62	1.71	2	10
1:A:71:GLU:HG3	1:A:101:VAL:HG22	0.62	1.71	16	9
1:A:31:LEU:HD23	1:A:76:ILE:CD1	0.61	2.24	5	8
1:A:88:PHE:CE2	1:A:97:LEU:HD22	0.61	2.29	16	5
1:A:114:LEU:HD22	1:A:114:LEU:C	0.61	2.16	12	15
1:A:79:PHE:CD2	1:A:97:LEU:HD23	0.61	2.30	2	2
1:A:38:LEU:HD11	1:A:105:LEU:HD21	0.61	1.69	3	6
1:A:127:ILE:CD1	1:A:131:ALA:HB2	0.61	2.25	19	13
1:A:114:LEU:C	1:A:114:LEU:HD22	0.61	2.16	13	1
1:A:130:GLY:O	1:A:133:TRP:NE1	0.60	2.35	13	20
1:A:71:GLU:HG2	1:A:101:VAL:HG22	0.60	1.74	11	7
1:A:127:ILE:HG21	1:A:131:ALA:HB2	0.59	1.71	13	1
1:A:7:ILE:HG23	1:A:69:LEU:CD1	0.59	2.21	13	4
1:A:79:PHE:HB3	1:A:85:ILE:HD11	0.59	1.75	18	20
1:A:42:LEU:O	1:A:46:GLN:N	0.59	2.36	13	4
1:A:45:LEU:HG	1:A:122:MET:CB	0.59	2.28	13	1
1:A:24:CYS:SG	1:A:85:ILE:HD12	0.59	2.37	13	5
1:A:13:VAL:HG22	1:A:16:LYS:HE2	0.59	1.75	13	3
1:A:14:ILE:HD11	1:A:69:LEU:O	0.58	1.99	14	19
1:A:110:LYS:HG2	1:A:127:ILE:HD11	0.58	1.75	4	6
1:A:88:PHE:CE2	1:A:89:LEU:CD2	0.58	2.87	11	20
1:A:96:ILE:HG21	1:A:137:ASP:HB3	0.57	1.75	20	10
1:A:25:LYS:O	1:A:29:ARG:N	0.57	2.33	19	10
1:A:3:ASN:C	1:A:7:ILE:HD12	0.57	2.20	9	19
1:A:116:LEU:HD13	1:A:122:MET:HE2	0.57	1.76	11	17
1:A:96:ILE:HB	1:A:99:LYS:CB	0.57	2.29	15	20
1:A:88:PHE:CE2	1:A:97:LEU:CD2	0.57	2.87	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HB	1:A:99:LYS:HB3	0.57	1.75	4	12
1:A:127:ILE:HD12	1:A:131:ALA:CB	0.57	2.29	18	10
1:A:35:VAL:CG2	1:A:105:LEU:HD11	0.57	2.29	11	6
1:A:113:SER:HB2	1:A:124:VAL:HG11	0.57	1.77	6	4
1:A:42:LEU:HD21	1:A:109:TRP:CH2	0.57	2.34	13	1
1:A:113:SER:OG	1:A:124:VAL:HG11	0.56	1.99	13	1
1:A:125:SER:O	1:A:127:ILE:N	0.56	2.38	5	20
1:A:45:LEU:HG	1:A:122:MET:HB2	0.56	1.78	13	1
1:A:130:GLY:O	1:A:133:TRP:CD1	0.55	2.60	12	19
1:A:12:GLN:HE21	1:A:39:ILE:HD11	0.55	1.61	12	17
1:A:4:LEU:HD23	1:A:42:LEU:HD13	0.54	1.77	3	5
1:A:79:PHE:O	1:A:85:ILE:HD11	0.54	2.03	19	2
1:A:109:TRP:CD1	1:A:127:ILE:HA	0.54	2.38	11	1
1:A:14:ILE:HD12	1:A:69:LEU:CD2	0.54	2.32	11	2
1:A:105:LEU:HD23	1:A:105:LEU:C	0.54	2.23	7	18
1:A:96:ILE:HD11	1:A:138:GLN:CB	0.54	2.32	8	17
1:A:110:LYS:O	1:A:114:LEU:HB3	0.54	2.03	17	16
1:A:96:ILE:HD11	1:A:138:GLN:HB3	0.53	1.79	15	7
1:A:31:LEU:CD2	1:A:76:ILE:HD11	0.53	2.32	5	16
1:A:4:LEU:HD13	1:A:46:GLN:CB	0.53	2.33	14	8
1:A:45:LEU:HD21	1:A:122:MET:SD	0.53	2.43	13	1
1:A:8:ILE:HA	1:A:39:ILE:HD12	0.53	1.80	13	12
1:A:40:LYS:HB2	1:A:41:PRO:HD3	0.53	1.81	18	7
1:A:24:CYS:CB	1:A:97:LEU:HD23	0.53	2.32	16	4
1:A:45:LEU:HD23	1:A:120:GLN:OE1	0.53	2.03	9	4
1:A:64:ARG:HB3	1:A:108:VAL:HG13	0.53	1.80	7	17
1:A:8:ILE:HG22	1:A:12:GLN:NE2	0.52	2.18	6	1
1:A:79:PHE:CG	1:A:97:LEU:HD23	0.52	2.40	12	2
1:A:98:PHE:O	1:A:98:PHE:CD2	0.52	2.63	8	7
1:A:14:ILE:HD12	1:A:69:LEU:HD22	0.52	1.79	11	1
1:A:27:GLN:OE1	1:A:141:ALA:HB2	0.52	2.05	13	3
1:A:7:ILE:CG2	1:A:65:PHE:CE2	0.52	2.92	16	14
1:A:109:TRP:CD1	1:A:127:ILE:HD13	0.52	2.40	11	1
1:A:27:GLN:OE1	1:A:97:LEU:HD12	0.52	2.04	10	1
1:A:8:ILE:HD13	1:A:46:GLN:NE2	0.52	2.20	2	7
1:A:14:ILE:HD13	1:A:69:LEU:HD23	0.52	1.82	14	5
1:A:38:LEU:HD22	1:A:109:TRP:CG	0.52	2.40	11	1
1:A:45:LEU:H	1:A:45:LEU:CD1	0.52	2.17	13	1
1:A:38:LEU:CD2	1:A:129:GLN:HG3	0.51	2.35	3	7
1:A:98:PHE:CG	1:A:98:PHE:O	0.51	2.62	3	2
1:A:57:LYS:O	1:A:115:LEU:HD13	0.51	2.04	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD12	1:A:35:VAL:HG23	0.51	1.82	12	5
1:A:111:GLU:HA	1:A:114:LEU:CD2	0.51	2.36	14	4
1:A:38:LEU:HD21	1:A:133:TRP:HZ2	0.51	1.65	13	1
1:A:14:ILE:O	1:A:18:CYS:HB2	0.51	2.05	6	2
1:A:110:LYS:HE3	1:A:127:ILE:HD11	0.51	1.83	7	1
1:A:40:LYS:CB	1:A:41:PRO:HD3	0.51	2.36	13	5
1:A:27:GLN:CD	1:A:97:LEU:HD12	0.51	2.27	10	1
1:A:79:PHE:CE2	1:A:97:LEU:HD23	0.50	2.41	2	1
1:A:12:GLN:NE2	1:A:39:ILE:HD11	0.50	2.21	12	13
1:A:114:LEU:C	1:A:114:LEU:HD12	0.50	2.26	4	4
1:A:88:PHE:CD1	1:A:88:PHE:C	0.50	2.84	10	11
1:A:114:LEU:HD13	1:A:114:LEU:C	0.50	2.26	6	16
1:A:38:LEU:HD11	1:A:133:TRP:CH2	0.50	2.42	16	3
1:A:27:GLN:O	1:A:98:PHE:CE1	0.49	2.65	15	9
1:A:38:LEU:CD1	1:A:105:LEU:CD2	0.49	2.90	18	13
1:A:106:SER:OG	1:A:133:TRP:CZ3	0.49	2.65	10	4
1:A:98:PHE:CE2	1:A:102:ASN:HB3	0.49	2.42	13	4
1:A:65:PHE:N	1:A:108:VAL:HG11	0.49	2.23	7	11
1:A:96:ILE:HG21	1:A:137:ASP:HB2	0.49	1.83	3	1
1:A:127:ILE:HG13	1:A:131:ALA:HB2	0.49	1.85	11	1
1:A:98:PHE:CE2	1:A:102:ASN:ND2	0.49	2.81	12	1
1:A:116:LEU:CD1	1:A:122:MET:HE1	0.49	2.38	13	1
1:A:62:MET:CG	1:A:112:LEU:HD11	0.48	2.38	15	18
1:A:7:ILE:O	1:A:11:GLY:N	0.48	2.46	7	12
1:A:111:GLU:CA	1:A:114:LEU:HD12	0.48	2.38	6	15
1:A:42:LEU:O	1:A:46:GLN:HG3	0.48	2.08	13	1
1:A:98:PHE:CE1	1:A:137:ASP:OD2	0.48	2.66	20	6
1:A:31:LEU:HD22	1:A:98:PHE:CB	0.48	2.38	15	3
1:A:7:ILE:HG13	1:A:66:LYS:HA	0.48	1.84	15	13
1:A:122:MET:CE	1:A:124:VAL:HG21	0.48	2.39	11	5
1:A:102:ASN:OD1	1:A:103:ARG:N	0.48	2.47	6	8
1:A:7:ILE:HG13	1:A:66:LYS:CA	0.48	2.39	15	17
1:A:43:GLU:O	1:A:47:ASP:CB	0.48	2.62	3	19
1:A:109:TRP:CE2	1:A:113:SER:HB3	0.48	2.44	2	16
1:A:36:LEU:O	1:A:40:LYS:N	0.48	2.47	13	6
1:A:8:ILE:HG23	1:A:39:ILE:HG13	0.47	1.86	6	1
1:A:4:LEU:HD21	1:A:42:LEU:HD13	0.47	1.85	19	1
1:A:13:VAL:HG22	1:A:16:LYS:CE	0.47	2.40	2	1
1:A:4:LEU:HD13	1:A:46:GLN:HB2	0.47	1.85	13	1
1:A:94:ASP:O	1:A:95:LYS:HB2	0.47	2.09	9	2
1:A:66:LYS:HE2	1:A:67:ALA:HB2	0.47	1.87	20	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD21	1:A:122:MET:CB	0.47	2.39	6	9
1:A:102:ASN:O	1:A:106:SER:CB	0.47	2.63	12	7
1:A:100:ASP:O	1:A:104:LYS:HB3	0.47	2.10	4	5
1:A:134:ALA:O	1:A:137:ASP:OD1	0.47	2.33	3	1
1:A:61:ALA:HA	1:A:64:ARG:NE	0.47	2.25	16	1
1:A:108:VAL:O	1:A:112:LEU:N	0.47	2.48	16	12
1:A:23:TYR:CE1	1:A:82:ARG:CB	0.46	2.98	6	6
1:A:88:PHE:CD1	1:A:88:PHE:O	0.46	2.69	5	4
1:A:34:ARG:CD	1:A:133:TRP:CD1	0.46	2.98	19	4
1:A:88:PHE:O	1:A:92:SER:N	0.46	2.47	18	15
1:A:98:PHE:O	1:A:98:PHE:CG	0.46	2.68	8	6
1:A:35:VAL:HG22	1:A:105:LEU:CD1	0.46	2.36	11	1
1:A:31:LEU:O	1:A:31:LEU:HD12	0.46	2.11	13	2
1:A:27:GLN:NE2	1:A:97:LEU:HD12	0.46	2.26	18	1
1:A:9:THR:CG2	1:A:10:LEU:N	0.46	2.78	3	20
1:A:23:TYR:CE2	1:A:82:ARG:CB	0.46	2.98	11	1
1:A:18:CYS:HB3	1:A:76:ILE:HD13	0.46	1.88	14	1
1:A:138:GLN:HG3	1:A:139:GLN:N	0.46	2.26	1	10
1:A:140:ASP:O	1:A:144:ASP:HB2	0.46	2.11	7	2
1:A:31:LEU:HB2	1:A:98:PHE:CD2	0.46	2.46	3	1
1:A:14:ILE:CD1	1:A:72:ALA:HB3	0.46	2.41	6	1
1:A:122:MET:HG3	1:A:122:MET:O	0.46	2.11	19	6
1:A:79:PHE:CD2	1:A:97:LEU:CD1	0.46	2.99	20	3
1:A:37:GLY:C	1:A:129:GLN:HG2	0.46	2.32	6	7
1:A:31:LEU:HD23	1:A:76:ILE:CG1	0.46	2.40	5	1
1:A:110:LYS:CG	1:A:127:ILE:HD11	0.46	2.41	11	2
1:A:38:LEU:HD21	1:A:133:TRP:CZ2	0.46	2.45	13	1
1:A:64:ARG:O	1:A:68:ALA:HB2	0.46	2.11	18	2
1:A:61:ALA:O	1:A:64:ARG:HG2	0.46	2.11	18	1
1:A:109:TRP:CD1	1:A:127:ILE:HG23	0.45	2.46	9	1
1:A:140:ASP:O	1:A:144:ASP:CB	0.45	2.64	1	5
1:A:31:LEU:HD21	1:A:72:ALA:CA	0.45	2.42	5	2
1:A:98:PHE:CZ	1:A:137:ASP:OD1	0.45	2.70	12	8
1:A:106:SER:HB2	1:A:133:TRP:CZ3	0.45	2.46	3	6
1:A:31:LEU:HB2	1:A:98:PHE:CE2	0.45	2.46	12	2
1:A:61:ALA:CB	1:A:112:LEU:HD13	0.45	2.42	15	9
1:A:117:GLN:HB3	1:A:124:VAL:HG23	0.45	1.89	8	1
1:A:28:CYS:SG	1:A:29:ARG:N	0.45	2.89	11	1
1:A:27:GLN:HE22	1:A:141:ALA:HB2	0.45	1.70	12	1
1:A:117:GLN:NE2	1:A:124:VAL:HB	0.45	2.27	8	2
1:A:116:LEU:CD2	1:A:120:GLN:NE2	0.45	2.80	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:PHE:CE2	1:A:89:LEU:HD21	0.45	2.47	20	1
1:A:98:PHE:CZ	1:A:137:ASP:OD2	0.45	2.70	5	5
1:A:35:VAL:HA	1:A:38:LEU:HD12	0.45	1.88	11	1
1:A:127:ILE:CG2	1:A:129:GLN:OE1	0.45	2.65	18	1
1:A:94:ASP:O	1:A:95:LYS:CB	0.45	2.65	20	8
1:A:98:PHE:CD2	1:A:98:PHE:O	0.45	2.69	12	4
1:A:68:ALA:CB	1:A:108:VAL:HG21	0.45	2.41	16	1
1:A:110:LYS:HE2	1:A:127:ILE:HD11	0.44	1.87	14	1
1:A:117:GLN:O	1:A:121:ARG:HA	0.44	2.12	1	5
1:A:65:PHE:CD2	1:A:112:LEU:HD23	0.44	2.47	13	12
1:A:106:SER:HB3	1:A:133:TRP:CZ3	0.44	2.46	11	4
1:A:98:PHE:CE1	1:A:137:ASP:OD1	0.44	2.71	8	5
1:A:71:GLU:HG2	1:A:104:LYS:NZ	0.44	2.27	19	1
1:A:23:TYR:CZ	1:A:82:ARG:CB	0.44	3.00	16	1
1:A:79:PHE:CE2	1:A:97:LEU:HA	0.44	2.47	19	1
1:A:40:LYS:CB	1:A:41:PRO:CD	0.44	2.95	15	5
1:A:71:GLU:CB	1:A:101:VAL:HG22	0.44	2.43	7	1
1:A:21:MET:HG3	1:A:76:ILE:HG23	0.44	1.88	5	1
1:A:56:GLU:O	1:A:59:THR:HG22	0.44	2.12	7	1
1:A:98:PHE:CE2	1:A:137:ASP:OD1	0.44	2.71	1	1
1:A:96:ILE:HG12	1:A:141:ALA:CB	0.44	2.43	6	7
1:A:87:ARG:O	1:A:91:ALA:CB	0.44	2.66	9	3
1:A:124:VAL:HG12	1:A:125:SER:N	0.44	2.28	4	12
1:A:38:LEU:HD22	1:A:109:TRP:CB	0.44	2.43	11	1
1:A:36:LEU:HD23	1:A:39:ILE:HD13	0.44	1.90	16	1
1:A:59:THR:O	1:A:63:ASN:N	0.44	2.50	4	10
1:A:98:PHE:CD2	1:A:102:ASN:OD1	0.44	2.71	1	2
1:A:102:ASN:OD1	1:A:134:ALA:HB2	0.44	2.12	11	1
1:A:75:GLU:O	1:A:79:PHE:CD2	0.43	2.71	4	7
1:A:16:LYS:O	1:A:20:GLU:CG	0.43	2.66	8	3
1:A:4:LEU:O	1:A:8:ILE:HG13	0.43	2.13	10	11
1:A:109:TRP:CZ2	1:A:113:SER:HB2	0.43	2.48	17	4
1:A:30:ARG:O	1:A:34:ARG:HG2	0.43	2.13	15	1
1:A:57:LYS:O	1:A:60:THR:HG22	0.43	2.14	17	5
1:A:109:TRP:CE2	1:A:113:SER:CB	0.43	3.01	8	3
1:A:96:ILE:HB	1:A:99:LYS:HB2	0.43	1.90	14	2
1:A:117:GLN:HG3	1:A:124:VAL:HG23	0.43	1.90	19	2
1:A:23:TYR:HD2	1:A:85:ILE:HG21	0.43	1.67	17	4
1:A:122:MET:SD	1:A:124:VAL:HG22	0.43	2.53	12	1
1:A:23:TYR:CE1	1:A:82:ARG:HB3	0.43	2.49	4	7
1:A:64:ARG:O	1:A:68:ALA:CB	0.43	2.67	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:GLN:CG	1:A:140:ASP:CB	0.43	2.97	7	1
1:A:114:LEU:HD13	1:A:115:LEU:H	0.43	1.70	13	1
1:A:116:LEU:HD13	1:A:122:MET:HE1	0.42	1.91	13	1
1:A:38:LEU:CD2	1:A:129:GLN:OE1	0.42	2.67	18	1
1:A:88:PHE:CZ	1:A:97:LEU:N	0.42	2.87	15	1
1:A:37:GLY:O	1:A:41:PRO:CD	0.42	2.67	7	2
1:A:116:LEU:CB	1:A:122:MET:CE	0.42	2.97	13	1
1:A:98:PHE:CE2	1:A:137:ASP:OD2	0.42	2.72	1	4
1:A:38:LEU:HD11	1:A:105:LEU:CD2	0.42	2.44	5	4
1:A:127:ILE:CD1	1:A:131:ALA:CB	0.42	2.98	5	2
1:A:95:LYS:O	1:A:96:ILE:CG1	0.42	2.67	20	2
1:A:8:ILE:HG23	1:A:39:ILE:HD12	0.42	1.90	5	1
1:A:122:MET:CE	1:A:124:VAL:CG2	0.42	2.98	20	5
1:A:31:LEU:HB2	1:A:98:PHE:CZ	0.42	2.49	5	1
1:A:35:VAL:O	1:A:39:ILE:HG23	0.42	2.14	6	2
1:A:45:LEU:HD11	1:A:122:MET:SD	0.42	2.55	14	1
1:A:134:ALA:HA	1:A:137:ASP:OD2	0.42	2.14	3	1
1:A:70:GLU:O	1:A:74:GLY:N	0.42	2.50	1	1
1:A:27:GLN:NE2	1:A:97:LEU:CD1	0.42	2.83	14	3
1:A:114:LEU:C	1:A:114:LEU:CD2	0.42	2.88	11	4
1:A:100:ASP:O	1:A:104:LYS:HG3	0.42	2.15	10	1
1:A:109:TRP:CE2	1:A:113:SER:HB2	0.42	2.50	18	1
1:A:27:GLN:O	1:A:98:PHE:CZ	0.41	2.73	7	1
1:A:31:LEU:O	1:A:35:VAL:CG2	0.41	2.68	9	2
1:A:38:LEU:HD23	1:A:129:GLN:OE1	0.41	2.15	18	1
1:A:127:ILE:HG23	1:A:129:GLN:OE1	0.41	2.15	18	1
1:A:23:TYR:CZ	1:A:82:ARG:HB2	0.41	2.50	12	1
1:A:140:ASP:O	1:A:144:ASP:N	0.41	2.54	3	3
1:A:8:ILE:HD11	1:A:46:GLN:CG	0.41	2.41	4	2
1:A:134:ALA:O	1:A:138:GLN:HG3	0.41	2.15	5	1
1:A:24:CYS:SG	1:A:97:LEU:HD11	0.41	2.55	6	1
1:A:38:LEU:HA	1:A:129:GLN:NE2	0.41	2.30	18	1
1:A:127:ILE:O	1:A:129:GLN:N	0.41	2.52	10	1
1:A:116:LEU:HD22	1:A:120:GLN:HG3	0.41	1.93	11	1
1:A:122:MET:HE3	1:A:124:VAL:HG21	0.41	1.91	13	1
1:A:38:LEU:HD23	1:A:129:GLN:NE2	0.41	2.29	7	2
1:A:88:PHE:CZ	1:A:89:LEU:HD23	0.41	2.51	10	1
1:A:69:LEU:O	1:A:72:ALA:N	0.41	2.53	9	1
1:A:125:SER:CB	1:A:126:PRO:CD	0.41	2.99	9	1
1:A:104:LYS:HG2	1:A:105:LEU:N	0.41	2.29	16	2
1:A:122:MET:CE	1:A:124:VAL:HG22	0.41	2.45	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:MET:HE1	1:A:79:PHE:C	0.41	2.36	20	1
1:A:127:ILE:CG2	1:A:129:GLN:HG2	0.41	2.45	3	1
1:A:129:GLN:N	1:A:129:GLN:OE1	0.41	2.53	13	1
1:A:125:SER:CB	1:A:126:PRO:HD2	0.41	2.46	3	3
1:A:34:ARG:HD3	1:A:133:TRP:CD1	0.41	2.50	8	1
1:A:37:GLY:O	1:A:41:PRO:HD3	0.41	2.16	20	2
1:A:96:ILE:CD1	1:A:138:GLN:HB3	0.41	2.46	19	3
1:A:14:ILE:CD1	1:A:69:LEU:HD23	0.41	2.45	11	1
1:A:102:ASN:ND2	1:A:133:TRP:CB	0.41	2.83	12	1
1:A:34:ARG:NE	1:A:133:TRP:CD1	0.41	2.89	4	1
1:A:13:VAL:HA	1:A:16:LYS:CD	0.41	2.46	6	1
1:A:96:ILE:CD1	1:A:138:GLN:CB	0.41	2.98	8	2
1:A:11:GLY:O	1:A:36:LEU:CD2	0.41	2.69	9	2
1:A:79:PHE:CE1	1:A:88:PHE:CD2	0.41	3.09	19	1
1:A:101:VAL:HA	1:A:104:LYS:HD2	0.41	1.93	1	1
1:A:111:GLU:O	1:A:115:LEU:HG	0.41	2.16	15	1
1:A:14:ILE:CD1	1:A:69:LEU:CD2	0.40	2.98	11	1
1:A:88:PHE:CD2	1:A:89:LEU:HD23	0.40	2.51	11	1
1:A:22:LYS:O	1:A:23:TYR:CD1	0.40	2.75	18	2
1:A:34:ARG:HG2	1:A:133:TRP:CD1	0.40	2.51	20	2
1:A:8:ILE:CD1	1:A:46:GLN:NE2	0.40	2.84	15	2
1:A:66:LYS:HA	1:A:69:LEU:HD12	0.40	1.92	16	1
1:A:34:ARG:HD3	1:A:133:TRP:CG	0.40	2.51	5	1
1:A:114:LEU:CD1	1:A:115:LEU:HG	0.40	2.46	8	1
1:A:8:ILE:HD11	1:A:46:GLN:CD	0.40	2.36	13	1
1:A:127:ILE:HD13	1:A:131:ALA:HB2	0.40	1.93	5	1
1:A:55:SER:HG	1:A:119:GLU:HG3	0.40	1.76	11	1
1:A:113:SER:HG	1:A:124:VAL:HG11	0.40	1.75	13	1
1:A:109:TRP:CD1	1:A:129:GLN:OE1	0.40	2.75	18	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	137/166 (83%)	120±2 (88±1%)	15±2 (11±2%)	2±1 (2±1%)	13 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2740/3320 (83%)	2398 (88%)	295 (11%)	47 (2%)	13 56

All 7 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	126	PRO	14
1	A	97	LEU	12
1	A	130	GLY	9
1	A	131	ALA	6
1	A	127	ILE	4
1	A	24	CYS	1
1	A	47	ASP	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	124/144 (86%)	92±3 (74±3%)	32±3 (26±3%)	2 23
All	All	2480/2880 (86%)	1841 (74%)	639 (26%)	2 23

All 81 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	14	ILE	20
1	A	15	HIS	20
1	A	39	ILE	20
1	A	60	THR	20
1	A	66	LYS	20
1	A	88	PHE	20
1	A	114	LEU	20
1	A	122	MET	19
1	A	125	SER	17
1	A	104	LYS	16
1	A	138	GLN	16
1	A	64	ARG	15

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Mol	Chain	Res	Type	Models (Total)
1	A	47	ASP	14
1	A	95	LYS	14
1	A	99	LYS	13
1	A	128	SER	13
1	A	65	PHE	13
1	A	33	HIS	12
1	A	107	ASP	12
1	A	6	HIS	11
1	A	87	ARG	11
1	A	92	SER	11
1	A	78	LYS	11
1	A	82	ARG	11
1	A	129	GLN	11
1	A	55	SER	10
1	A	94	ASP	10
1	A	137	ASP	10
1	A	145	ARG	9
1	A	80	SER	9
1	A	16	LYS	9
1	A	103	ARG	9
1	A	22	LYS	8
1	A	144	ASP	8
1	A	142	ASP	8
1	A	17	ARG	8
1	A	20	GLU	7
1	A	83	SER	7
1	A	121	ARG	7
1	A	133	TRP	7
1	A	29	ARG	7
1	A	19	GLU	7
1	A	113	SER	6
1	A	45	LEU	6
1	A	26	LYS	6
1	A	100	ASP	6
1	A	120	GLN	6
1	A	25	LYS	5
1	A	135	GLN	5
1	A	75	GLU	5
1	A	102	ASN	5
1	A	21	MET	5
1	A	97	LEU	5
1	A	30	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	34	ARG	4
1	A	81	ASN	4
1	A	57	LYS	3
1	A	70	GLU	3
1	A	86	CYS	3
1	A	111	GLU	3
1	A	2	GLU	3
1	A	5	LYS	3
1	A	71	GLU	3
1	A	139	GLN	3
1	A	93	GLN	3
1	A	62	MET	2
1	A	18	CYS	2
1	A	27	GLN	2
1	A	143	GLU	2
1	A	136	GLU	1
1	A	98	PHE	1
1	A	4	LEU	1
1	A	132	SER	1
1	A	77	GLU	1
1	A	84	ASN	1
1	A	140	ASP	1
1	A	28	CYS	1
1	A	40	LYS	1
1	A	106	SER	1
1	A	56	GLU	1
1	A	23	TYR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1994
Number of shifts mapped to atoms	1994
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	153	-0.46 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	147	0.12 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	145	-0.39 ± 0.15	None needed (< 0.5 ppm)
^{15}N	149	0.18 ± 0.26	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 91%, i.e. 1774 atoms were assigned a chemical shift out of a possible 1959. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	673/684 (98%)	274/276 (99%)	266/274 (97%)	133/134 (99%)
Sidechain	1021/1178 (87%)	694/756 (92%)	311/363 (86%)	16/59 (27%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	80/97 (82%)	40/48 (83%)	38/41 (93%)	2/8 (25%)
Overall	1774/1959 (91%)	1008/1080 (93%)	615/678 (91%)	151/201 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1994 atoms were assigned a chemical shift out of a possible 2227. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	755/768 (98%)	308/310 (99%)	298/308 (97%)	149/150 (99%)
Sidechain	1153/1352 (85%)	783/867 (90%)	352/411 (86%)	18/74 (24%)
Aromatic	86/107 (80%)	44/53 (83%)	40/46 (87%)	2/8 (25%)
Overall	1994/2227 (90%)	1135/1230 (92%)	690/765 (90%)	169/232 (73%)

7.1.4 Statistically unusual chemical shifts (i)

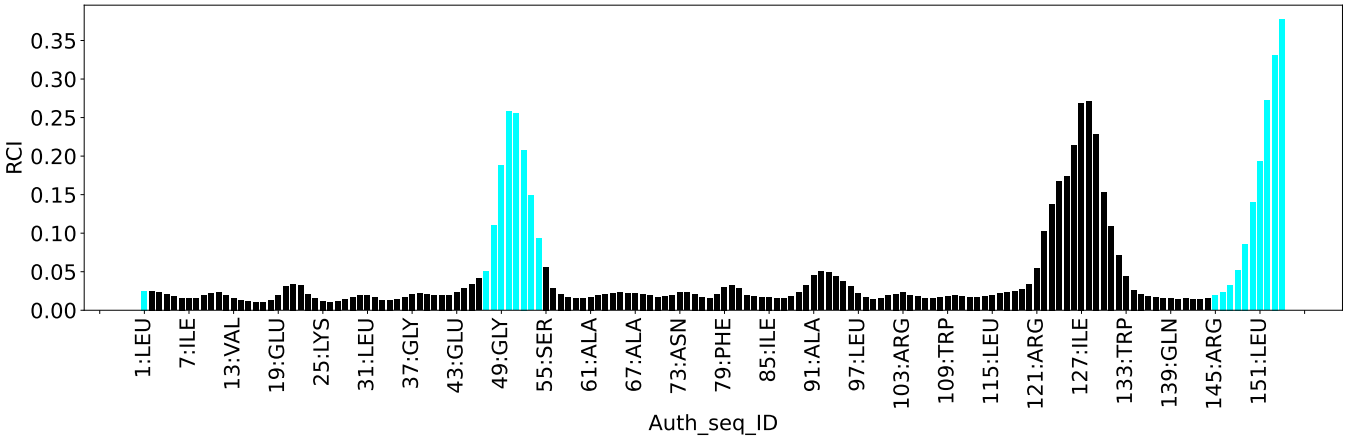
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	34	ARG	HD3	0.27	1.81 – 4.39	-11.0
1	A	113	SER	HB3	2.48	2.49 – 5.20	-5.0

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1:LEU
7:ILE
13:VAL
19:GLU
25:LYS
31:LEU
37:GLY
43:GLU
49:GLY
55:SER
61:ALA
67:ALA
73:ASN
79:PHE
85:ILE
91:ALA
97:LEU
103:ARG
109:TRP
115:LEU
121:ARG
127:ILE
133:TRP
139:GLN
145:ARG
151:LEU
Auth_seq_ID