



Full wwPDB NMR Structure Validation Report ⓘ

Jun 18, 2022 – 08:05 AM EDT

PDB ID : 7PVC
Title : The structure of Kbp.K from E. coli with potassium bound.
Authors : Smith, B.O.
Deposited on : 2021-10-01

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

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

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

The following versions of software and data (see [references ⓘ](#)) 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)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.29
BMRB Restraints Analysis	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

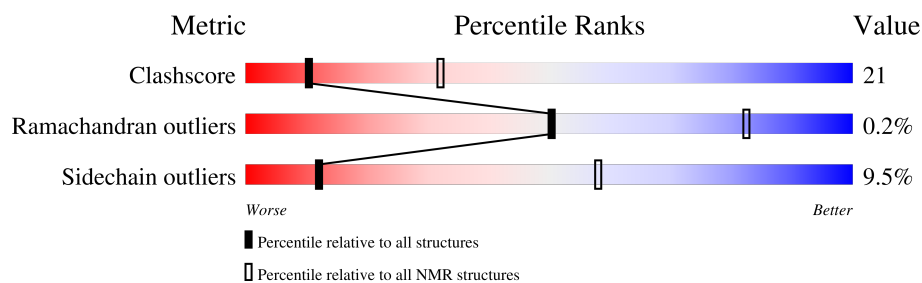
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	157	

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: *closest to the average*.

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:3-A:15, A:25-A:148 (137)	0.29	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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2413 atoms, of which 1204 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potassium binding protein Kbp.

Mol	Chain	Residues	Atoms						Trace
1	A	157	Total	C	H	N	O	S	0
			2412	757	1204	211	238	2	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LEU	-	expression tag	UNP P0ADE6
A	151	GLU	-	expression tag	UNP P0ADE6
A	152	HIS	-	expression tag	UNP P0ADE6
A	153	HIS	-	expression tag	UNP P0ADE6
A	154	HIS	-	expression tag	UNP P0ADE6
A	155	HIS	-	expression tag	UNP P0ADE6
A	156	HIS	-	expression tag	UNP P0ADE6
A	157	HIS	-	expression tag	UNP P0ADE6

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

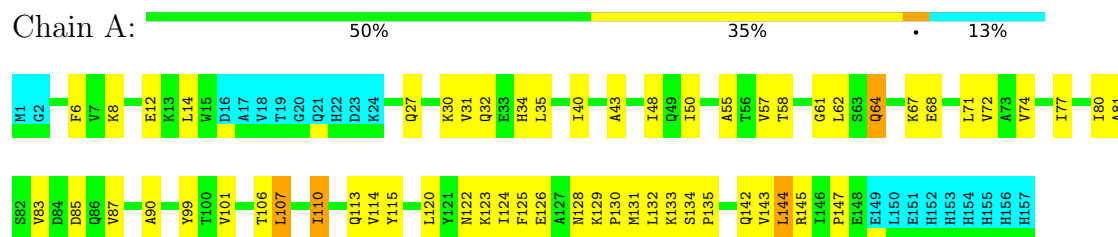
Mol	Chain	Residues	Atoms	
2	A	1	Total	K
			1	1

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: Potassium binding protein Kbp

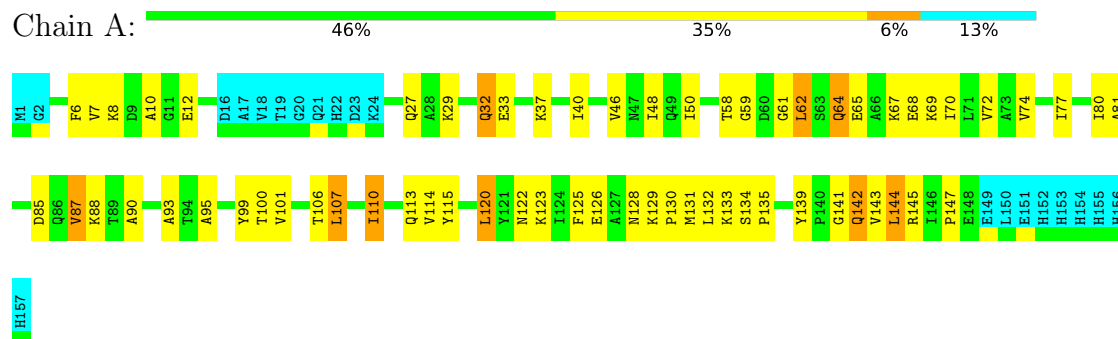


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

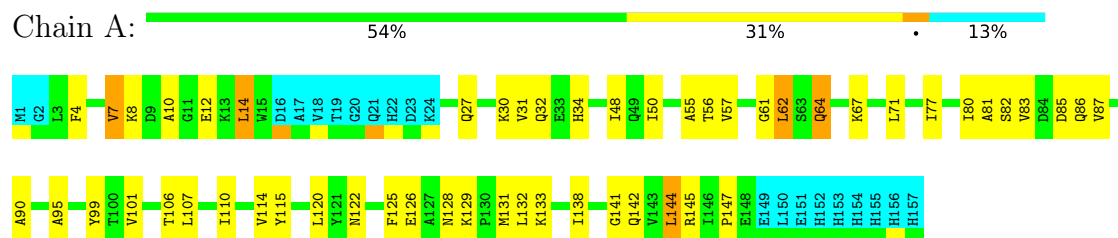
4.2.1 Score per residue for model 1

- Molecule 1: Potassium binding protein Kbp



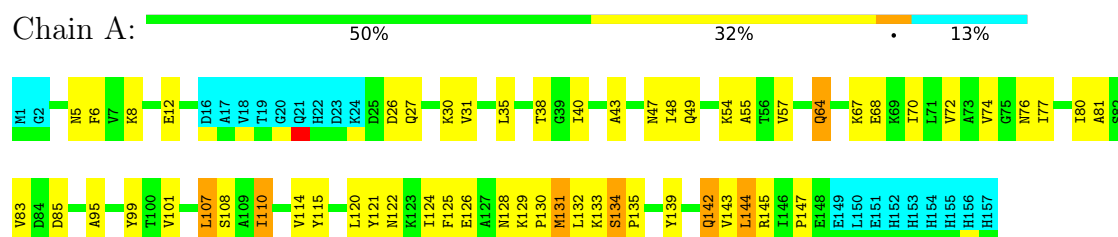
4.2.2 Score per residue for model 2

- Molecule 1: Potassium binding protein Kbp



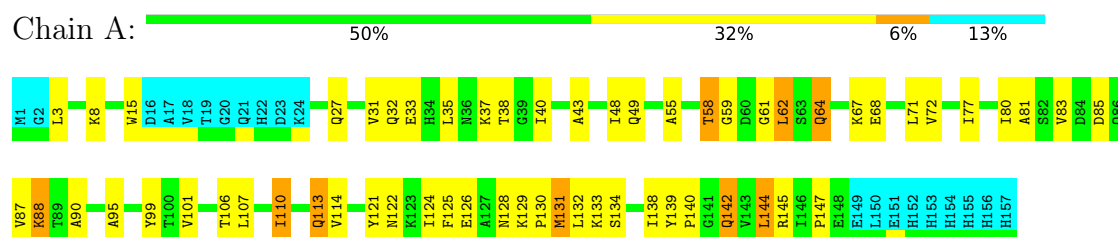
4.2.3 Score per residue for model 3

- Molecule 1: Potassium binding protein Kbp



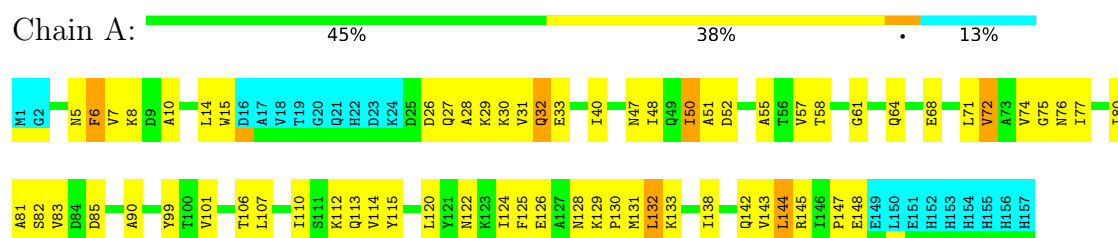
4.2.4 Score per residue for model 4

- Molecule 1: Potassium binding protein Kbp



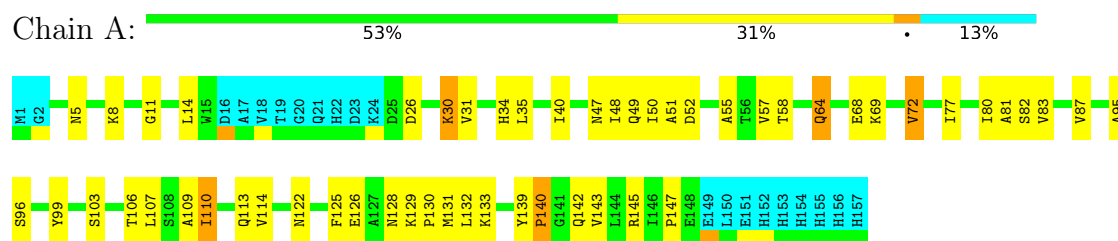
4.2.5 Score per residue for model 5

- Molecule 1: Potassium binding protein Kbp



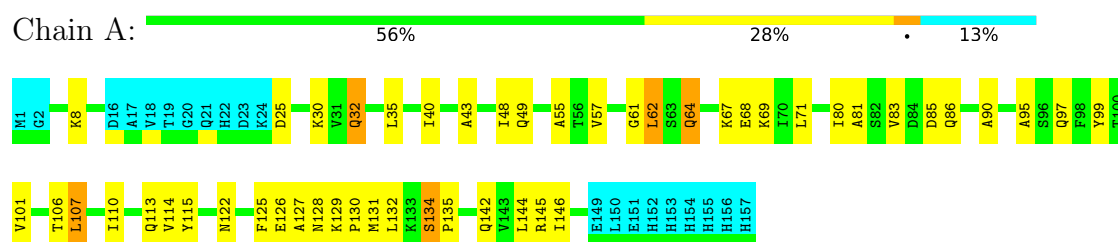
4.2.6 Score per residue for model 6

- Molecule 1: Potassium binding protein Kbp



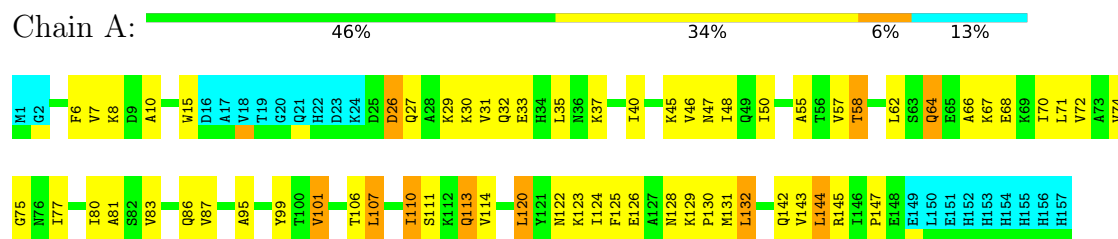
4.2.7 Score per residue for model 7

- Molecule 1: Potassium binding protein Kbp



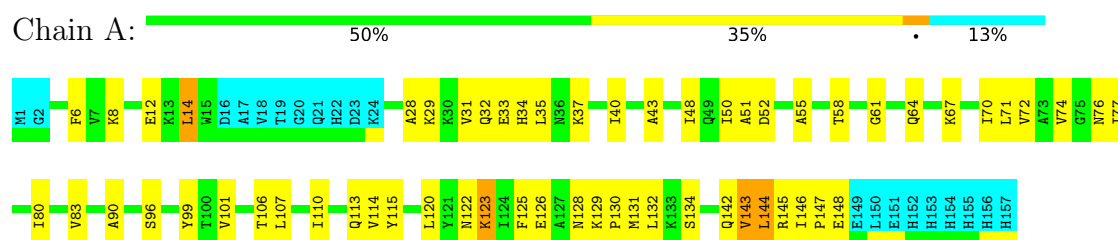
4.2.8 Score per residue for model 8

- Molecule 1: Potassium binding protein Kbp



4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Potassium binding protein Kbp



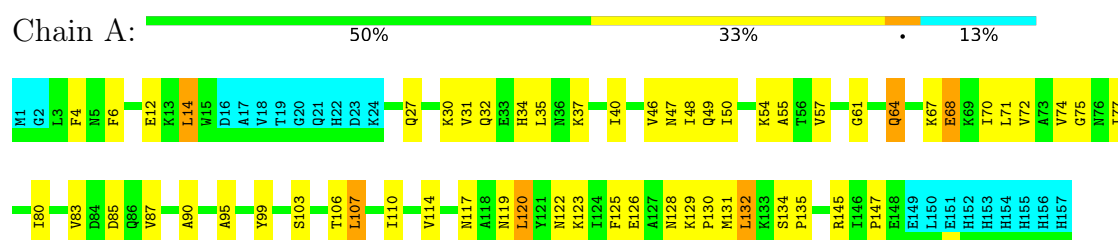
4.2.10 Score per residue for model 10

- Molecule 1: Potassium binding protein Kbp



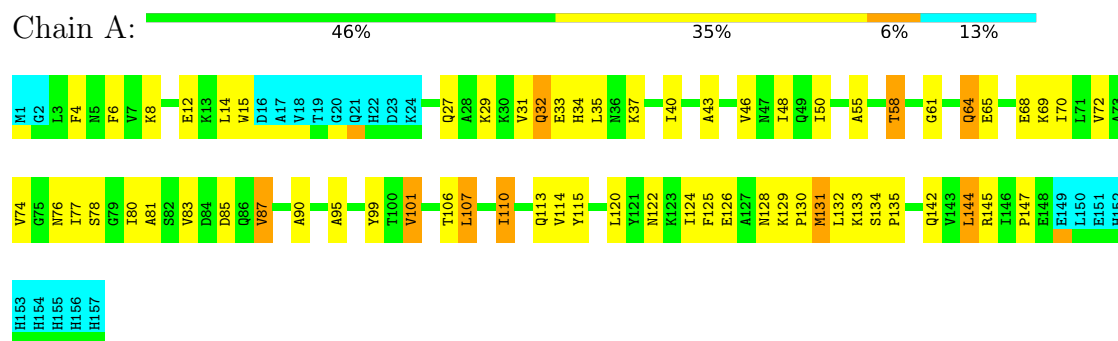
4.2.11 Score per residue for model 11

- Molecule 1: Potassium binding protein Kbp



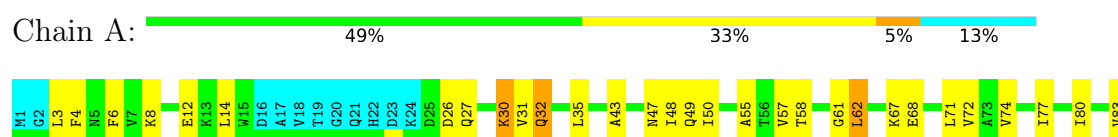
4.2.12 Score per residue for model 12

- Molecule 1: Potassium binding protein Kbp



4.2.13 Score per residue for model 13

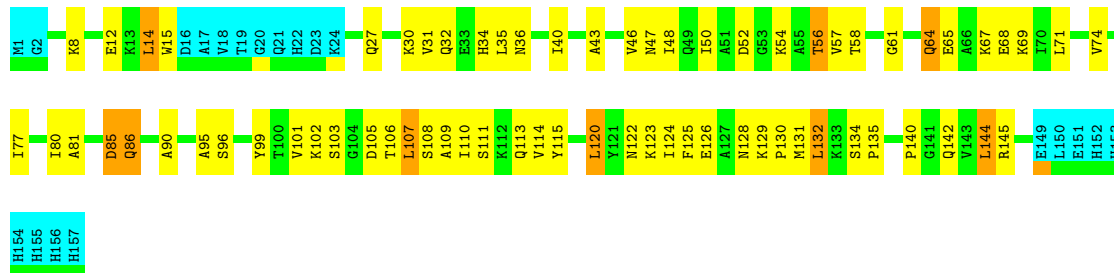
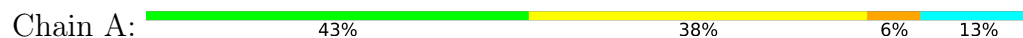
- Molecule 1: Potassium binding protein Kbp





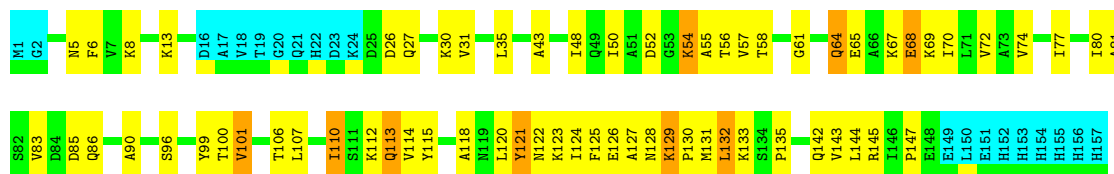
4.2.14 Score per residue for model 14

- Molecule 1: Potassium binding protein Kbp



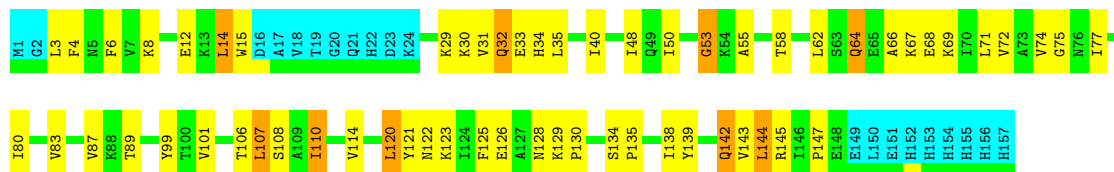
4.2.15 Score per residue for model 15

- Molecule 1: Potassium binding protein Kbp



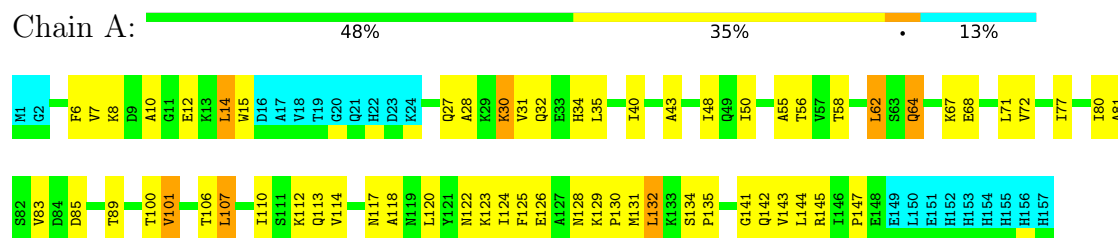
4.2.16 Score per residue for model 16

- Molecule 1: Potassium binding protein Kbp



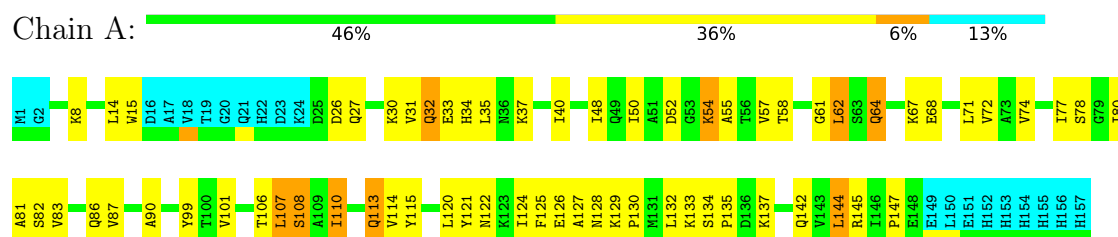
4.2.17 Score per residue for model 17

- Molecule 1: Potassium binding protein Kbp



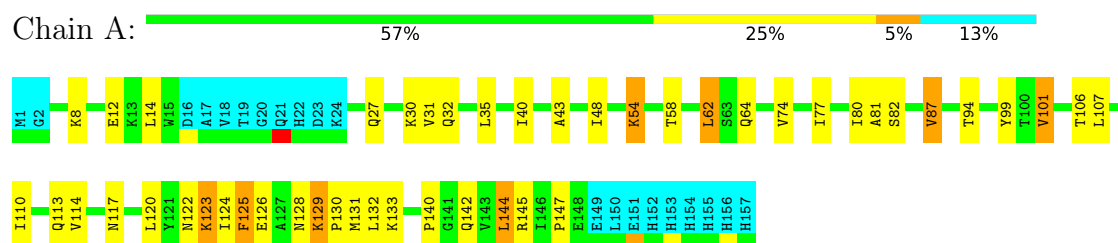
4.2.18 Score per residue for model 18

- Molecule 1: Potassium binding protein Kbp



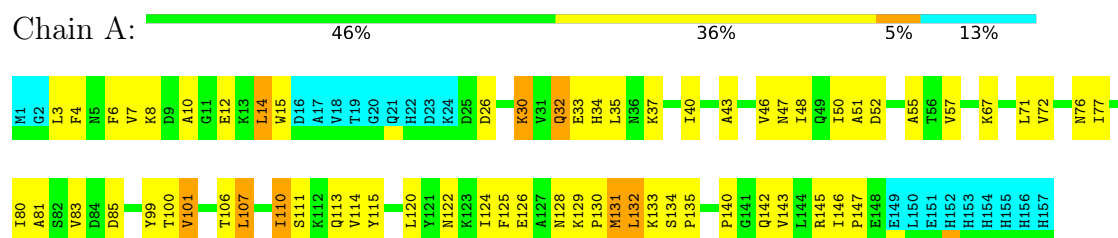
4.2.19 Score per residue for model 19

- Molecule 1: Potassium binding protein Kbp



4.2.20 Score per residue for model 20

- Molecule 1: Potassium binding protein Kbp



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
ARIA	structure calculation	2.3
CNS	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1879
Number of shifts mapped to atoms	1879
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality

6.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.48±0.05	1±1/1059 (0.1± 0.1%)	0.51±0.02	0±0/1434 (0.0± 0.0%)
All	All	0.48	11/21180 (0.1%)	0.51	0/28680 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	115	TYR	CE1-CZ	-8.93	1.26	1.38	13	4
1	A	115	TYR	CE2-CZ	7.98	1.49	1.38	13	3
1	A	125	PHE	CE1-CZ	6.90	1.50	1.37	19	1
1	A	125	PHE	CE2-CZ	-5.89	1.26	1.37	19	1
1	A	6	PHE	CE1-CZ	5.32	1.47	1.37	5	1
1	A	99	TYR	CE2-CZ	5.03	1.45	1.38	13	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	121	TYR	Sidechain	1

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1042	1058	1057	45±6
All	All	20860	21160	21140	891

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:VAL:HG11	1:A:10:ALA:HB3	0.94	1.37	8	5
1:A:35:LEU:HB3	1:A:43:ALA:HB1	0.87	1.47	19	10
1:A:32:GLN:NE2	1:A:48:ILE:HB	0.80	1.90	1	5
1:A:107:LEU:HD23	1:A:135:PRO:HA	0.79	1.55	16	5
1:A:125:PHE:CE1	1:A:129:LYS:HD3	0.78	2.14	2	2
1:A:4:PHE:HB2	1:A:83:VAL:HG12	0.77	1.55	12	2
1:A:6:PHE:CD2	1:A:143:VAL:HG11	0.75	2.15	16	8
1:A:107:LEU:HD13	1:A:121:TYR:HB2	0.73	1.60	18	2
1:A:128:ASN:OD1	1:A:144:LEU:HG	0.72	1.84	1	13
1:A:56:THR:HG22	1:A:86:GLN:NE2	0.72	1.99	14	1
1:A:31:VAL:O	1:A:35:LEU:HG	0.72	1.85	15	6
1:A:40:ILE:HD13	1:A:130:PRO:HD2	0.71	1.63	20	15
1:A:8:LYS:HB3	1:A:81:ALA:HB2	0.70	1.63	14	6
1:A:56:THR:HG22	1:A:86:GLN:CD	0.69	2.06	14	1
1:A:128:ASN:HB3	1:A:131:MET:HE3	0.69	1.64	3	3
1:A:7:VAL:CG1	1:A:10:ALA:HB3	0.68	2.17	5	6
1:A:32:GLN:HA	1:A:35:LEU:HD12	0.68	1.65	4	3
1:A:46:VAL:HG22	1:A:47:ASN:H	0.68	1.46	14	4
1:A:8:LYS:HD3	1:A:81:ALA:HB2	0.67	1.64	20	4
1:A:40:ILE:HB	1:A:43:ALA:HB2	0.67	1.66	19	2
1:A:125:PHE:CZ	1:A:134:SER:HA	0.66	2.25	9	3
1:A:122:ASN:O	1:A:126:GLU:HG3	0.66	1.90	1	18
1:A:99:TYR:CE1	1:A:110:ILE:HB	0.66	2.26	16	17
1:A:64:GLN:NE2	1:A:95:ALA:HA	0.66	2.06	2	6
1:A:128:ASN:O	1:A:131:MET:HG3	0.65	1.91	10	5
1:A:132:LEU:HD12	1:A:133:LYS:N	0.65	2.07	5	9
1:A:126:GLU:HA	1:A:129:LYS:CG	0.64	2.22	17	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:GLN:O	1:A:68:GLU:HG2	0.64	1.92	12	4
1:A:74:VAL:O	1:A:77:ILE:HG12	0.64	1.93	3	13
1:A:55:ALA:O	1:A:83:VAL:HA	0.63	1.93	3	17
1:A:110:ILE:O	1:A:114:VAL:HG22	0.63	1.94	13	20
1:A:67:LYS:O	1:A:71:LEU:HG	0.63	1.93	9	9
1:A:107:LEU:HD11	1:A:124:ILE:HB	0.62	1.71	8	3
1:A:125:PHE:O	1:A:129:LYS:HG2	0.62	1.95	13	15
1:A:6:PHE:CE1	1:A:75:GLY:HA3	0.61	2.30	11	1
1:A:68:GLU:O	1:A:72:VAL:HG23	0.61	1.95	18	10
1:A:6:PHE:HD2	1:A:143:VAL:HG11	0.60	1.57	17	2
1:A:14:LEU:HD23	1:A:77:ILE:HG23	0.60	1.73	9	8
1:A:64:GLN:CD	1:A:95:ALA:HA	0.60	2.17	14	4
1:A:50:ILE:HD12	1:A:80:ILE:HD11	0.60	1.72	8	14
1:A:120:LEU:HG	1:A:123:LYS:HD3	0.59	1.73	10	10
1:A:106:THR:O	1:A:110:ILE:HG23	0.59	1.97	13	19
1:A:107:LEU:HD21	1:A:124:ILE:HB	0.59	1.74	17	2
1:A:107:LEU:HD12	1:A:135:PRO:HA	0.58	1.75	11	5
1:A:145:ARG:O	1:A:147:PRO:HD3	0.57	1.99	9	18
1:A:70:ILE:O	1:A:74:VAL:HG12	0.57	1.98	3	2
1:A:128:ASN:O	1:A:131:MET:HB3	0.57	1.99	19	12
1:A:107:LEU:HB2	1:A:135:PRO:O	0.57	1.99	17	2
1:A:110:ILE:HD11	1:A:124:ILE:HD13	0.57	1.76	15	9
1:A:125:PHE:CE2	1:A:134:SER:HA	0.57	2.34	1	9
1:A:64:GLN:HG3	1:A:93:ALA:HB3	0.57	1.75	1	1
1:A:142:GLN:HG3	1:A:144:LEU:HD13	0.57	1.77	12	2
1:A:101:VAL:HG13	1:A:142:GLN:O	0.56	2.00	15	6
1:A:14:LEU:HB3	1:A:30:LYS:CG	0.56	2.31	17	2
1:A:67:LYS:HG3	1:A:87:VAL:HG13	0.56	1.77	1	2
1:A:107:LEU:CD1	1:A:125:PHE:HB2	0.56	2.31	4	1
1:A:62:LEU:HD11	1:A:87:VAL:HG21	0.56	1.77	19	1
1:A:101:VAL:HG23	1:A:142:GLN:O	0.55	2.01	9	12
1:A:69:LYS:HE2	1:A:129:LYS:O	0.55	2.01	6	2
1:A:27:GLN:O	1:A:31:VAL:HG23	0.55	2.01	18	11
1:A:96:SER:HB3	1:A:146:ILE:O	0.55	2.01	9	1
1:A:107:LEU:HD11	1:A:135:PRO:HB3	0.55	1.79	18	2
1:A:3:LEU:HD13	1:A:4:PHE:N	0.55	2.17	13	3
1:A:99:TYR:O	1:A:143:VAL:HA	0.54	2.02	20	5
1:A:125:PHE:O	1:A:129:LYS:HG3	0.54	2.02	2	2
1:A:46:VAL:HG21	1:A:70:ILE:HG12	0.54	1.78	1	1
1:A:62:LEU:H	1:A:62:LEU:HD13	0.54	1.62	4	4
1:A:14:LEU:HD11	1:A:34:HIS:HB2	0.54	1.80	20	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:PHE:CZ	1:A:129:LYS:HD3	0.54	2.38	7	6
1:A:120:LEU:HG	1:A:123:LYS:CD	0.54	2.32	10	3
1:A:115:TYR:CD1	1:A:120:LEU:HD23	0.54	2.38	14	1
1:A:8:LYS:HA	1:A:80:ILE:O	0.54	2.03	14	15
1:A:33:GLU:O	1:A:37:LYS:HG2	0.54	2.03	4	5
1:A:31:VAL:HG21	1:A:48:ILE:HG21	0.54	1.80	10	3
1:A:29:LYS:O	1:A:33:GLU:HG3	0.53	2.03	5	6
1:A:14:LEU:CD2	1:A:77:ILE:HG23	0.53	2.33	14	8
1:A:127:ALA:O	1:A:145:ARG:HD2	0.53	2.03	15	1
1:A:65:GLU:O	1:A:69:LYS:HB2	0.53	2.03	1	1
1:A:49:GLN:O	1:A:55:ALA:HA	0.53	2.02	13	7
1:A:54:LYS:HA	1:A:82:SER:OG	0.53	2.03	19	2
1:A:114:VAL:HB	1:A:146:ILE:HG21	0.53	1.81	20	1
1:A:115:TYR:HB3	1:A:120:LEU:HD12	0.53	1.81	2	7
1:A:122:ASN:O	1:A:126:GLU:HG2	0.53	2.03	13	2
1:A:6:PHE:CE2	1:A:75:GLY:HA3	0.53	2.38	16	4
1:A:32:GLN:HG2	1:A:48:ILE:CG1	0.53	2.33	8	3
1:A:46:VAL:HG21	1:A:57:VAL:HG23	0.53	1.79	14	1
1:A:57:VAL:CG1	1:A:85:ASP:HA	0.52	2.34	14	7
1:A:124:ILE:HG22	1:A:128:ASN:OD1	0.52	2.02	3	6
1:A:14:LEU:HD22	1:A:77:ILE:HD12	0.52	1.81	13	3
1:A:106:THR:HA	1:A:138:ILE:HD11	0.52	1.82	13	3
1:A:7:VAL:O	1:A:81:ALA:HA	0.52	2.05	17	2
1:A:125:PHE:CE1	1:A:129:LYS:HG2	0.52	2.40	15	3
1:A:139:TYR:CE2	1:A:142:GLN:HG2	0.52	2.40	3	2
1:A:40:ILE:CD1	1:A:130:PRO:HD2	0.52	2.35	12	2
1:A:26:ASP:O	1:A:30:LYS:HD3	0.52	2.05	8	2
1:A:67:LYS:O	1:A:71:LEU:HD13	0.51	2.05	11	2
1:A:126:GLU:HA	1:A:129:LYS:HG3	0.51	1.82	17	13
1:A:30:LYS:N	1:A:30:LYS:HD2	0.51	2.19	11	1
1:A:50:ILE:HD12	1:A:80:ILE:CD1	0.51	2.34	9	2
1:A:6:PHE:CD2	1:A:143:VAL:CG1	0.51	2.91	16	4
1:A:8:LYS:O	1:A:78:SER:HA	0.51	2.05	18	2
1:A:26:ASP:O	1:A:30:LYS:HG2	0.51	2.06	5	4
1:A:57:VAL:HG11	1:A:71:LEU:CD2	0.51	2.36	20	6
1:A:125:PHE:CD1	1:A:129:LYS:HG2	0.50	2.41	15	3
1:A:32:GLN:HG2	1:A:48:ILE:HD13	0.50	1.83	11	5
1:A:115:TYR:OH	1:A:147:PRO:HD2	0.50	2.07	13	4
1:A:14:LEU:CD2	1:A:77:ILE:HD12	0.50	2.37	20	5
1:A:110:ILE:HA	1:A:113:GLN:HG3	0.50	1.83	10	7
1:A:7:VAL:HG11	1:A:141:GLY:O	0.50	2.06	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LEU:HD23	1:A:133:LYS:N	0.50	2.22	1	3
1:A:77:ILE:HB	1:A:80:ILE:CG1	0.50	2.37	16	6
1:A:64:GLN:OE1	1:A:95:ALA:HA	0.50	2.07	7	1
1:A:68:GLU:O	1:A:72:VAL:HG22	0.49	2.07	6	2
1:A:132:LEU:HG	1:A:142:GLN:NE2	0.49	2.22	14	3
1:A:58:THR:C	1:A:87:VAL:HB	0.49	2.28	1	3
1:A:61:GLY:HA2	1:A:90:ALA:HB2	0.49	1.85	15	12
1:A:112:LYS:HB2	1:A:118:ALA:HB2	0.49	1.84	15	2
1:A:126:GLU:HA	1:A:129:LYS:HG2	0.49	1.84	17	2
1:A:72:VAL:O	1:A:76:ASN:HB2	0.49	2.08	3	4
1:A:5:ASN:HA	1:A:82:SER:OG	0.49	2.08	6	2
1:A:109:ALA:O	1:A:113:GLN:HG2	0.49	2.08	6	2
1:A:142:GLN:HG3	1:A:144:LEU:CD1	0.49	2.38	12	1
1:A:107:LEU:HD21	1:A:125:PHE:HB2	0.48	1.83	9	3
1:A:127:ALA:O	1:A:145:ARG:HD3	0.48	2.09	18	2
1:A:111:SER:HA	1:A:114:VAL:CG2	0.48	2.38	8	2
1:A:132:LEU:HG	1:A:142:GLN:HE22	0.48	1.68	14	2
1:A:129:LYS:HB2	1:A:130:PRO:HA	0.48	1.85	10	3
1:A:46:VAL:HG21	1:A:70:ILE:HG21	0.48	1.83	11	2
1:A:67:LYS:HD2	1:A:85:ASP:OD1	0.48	2.09	4	2
1:A:48:ILE:HA	1:A:56:THR:O	0.48	2.09	17	4
1:A:111:SER:O	1:A:115:TYR:HB2	0.48	2.09	14	1
1:A:72:VAL:HG21	1:A:145:ARG:HG2	0.48	1.86	15	1
1:A:139:TYR:CZ	1:A:142:GLN:HG2	0.48	2.43	16	4
1:A:32:GLN:HE21	1:A:48:ILE:HB	0.47	1.69	5	2
1:A:8:LYS:HD2	1:A:81:ALA:HB2	0.47	1.87	5	5
1:A:100:THR:HA	1:A:143:VAL:HA	0.47	1.86	17	4
1:A:69:LYS:HA	1:A:145:ARG:NE	0.47	2.23	15	1
1:A:107:LEU:HB3	1:A:121:TYR:HB2	0.47	1.86	15	1
1:A:26:ASP:O	1:A:30:LYS:HE3	0.47	2.10	6	1
1:A:55:ALA:HB2	1:A:80:ILE:HD12	0.47	1.86	10	2
1:A:120:LEU:CD1	1:A:120:LEU:N	0.47	2.78	15	1
1:A:57:VAL:O	1:A:86:GLN:HB2	0.46	2.10	15	4
1:A:15:TRP:CH2	1:A:77:ILE:HG21	0.46	2.45	14	6
1:A:7:VAL:HG11	1:A:141:GLY:CA	0.46	2.39	2	1
1:A:107:LEU:CD1	1:A:135:PRO:HA	0.46	2.40	3	3
1:A:72:VAL:HG21	1:A:145:ARG:CG	0.46	2.40	13	4
1:A:6:PHE:HD2	1:A:143:VAL:CG1	0.46	2.23	15	2
1:A:62:LEU:HD13	1:A:62:LEU:N	0.46	2.25	4	3
1:A:14:LEU:HB3	1:A:30:LYS:HB3	0.46	1.88	14	4
1:A:107:LEU:CD1	1:A:121:TYR:HB2	0.46	2.38	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:VAL:HG21	1:A:57:VAL:CG2	0.46	2.39	14	1
1:A:35:LEU:HB3	1:A:43:ALA:CB	0.46	2.41	13	3
1:A:11:GLY:HA2	1:A:139:TYR:OH	0.46	2.10	6	1
1:A:32:GLN:HG2	1:A:48:ILE:HG12	0.46	1.86	8	3
1:A:6:PHE:CD2	1:A:75:GLY:HA3	0.46	2.46	16	1
1:A:103:SER:HA	1:A:140:PRO:HG3	0.46	1.88	6	2
1:A:46:VAL:HG21	1:A:57:VAL:HG13	0.45	1.87	11	2
1:A:114:VAL:HG23	1:A:115:TYR:CD2	0.45	2.46	14	1
1:A:58:THR:HG23	1:A:86:GLN:HB2	0.45	1.87	10	2
1:A:64:GLN:HE22	1:A:68:GLU:CD	0.45	2.15	8	1
1:A:102:LYS:HB2	1:A:105:ASP:OD2	0.45	2.11	14	2
1:A:57:VAL:HG13	1:A:87:VAL:HG23	0.45	1.86	18	1
1:A:28:ALA:HA	1:A:31:VAL:HG22	0.45	1.87	10	3
1:A:6:PHE:CZ	1:A:75:GLY:HA3	0.45	2.46	11	1
1:A:69:LYS:HA	1:A:145:ARG:CZ	0.45	2.41	15	1
1:A:132:LEU:HD12	1:A:133:LYS:H	0.45	1.70	2	4
1:A:120:LEU:HB3	1:A:123:LYS:HZ3	0.45	1.72	19	1
1:A:7:VAL:HG22	1:A:8:LYS:N	0.45	2.26	8	2
1:A:117:ASN:HB3	1:A:120:LEU:HD22	0.44	1.89	17	2
1:A:125:PHE:CE2	1:A:129:LYS:HD3	0.44	2.47	1	1
1:A:77:ILE:HB	1:A:80:ILE:HG12	0.44	1.87	16	4
1:A:107:LEU:HD11	1:A:135:PRO:CB	0.44	2.40	18	1
1:A:14:LEU:HG	1:A:30:LYS:HB3	0.44	1.89	13	2
1:A:57:VAL:HG11	1:A:71:LEU:HD23	0.44	1.89	18	1
1:A:126:GLU:HA	1:A:129:LYS:HE2	0.44	1.90	2	1
1:A:57:VAL:CG2	1:A:70:ILE:HG21	0.44	2.43	15	1
1:A:7:VAL:HG13	1:A:10:ALA:HB3	0.44	1.89	2	1
1:A:48:ILE:HD12	1:A:48:ILE:N	0.44	2.27	19	4
1:A:108:SER:HA	1:A:121:TYR:HB3	0.44	1.89	18	3
1:A:38:THR:OG1	1:A:40:ILE:HG12	0.44	2.13	4	2
1:A:3:LEU:HD12	1:A:83:VAL:O	0.44	2.13	4	2
1:A:6:PHE:CD2	1:A:143:VAL:HG21	0.44	2.48	5	1
1:A:14:LEU:HB3	1:A:30:LYS:HG3	0.43	1.90	6	2
1:A:107:LEU:CD2	1:A:125:PHE:HB2	0.43	2.42	9	1
1:A:132:LEU:HG	1:A:142:GLN:HE21	0.43	1.72	12	1
1:A:138:ILE:HA	1:A:142:GLN:OE1	0.43	2.12	2	2
1:A:51:ALA:O	1:A:52:ASP:HB2	0.43	2.12	20	3
1:A:69:LYS:HD2	1:A:129:LYS:O	0.43	2.13	7	1
1:A:129:LYS:HA	1:A:131:MET:N	0.43	2.28	19	1
1:A:76:ASN:OD1	1:A:142:GLN:HA	0.43	2.12	10	2
1:A:128:ASN:HA	1:A:145:ARG:NH1	0.43	2.28	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:O	1:A:37:LYS:HG3	0.43	2.13	1	2
1:A:67:LYS:HG3	1:A:87:VAL:CG1	0.43	2.43	1	1
1:A:64:GLN:HA	1:A:67:LYS:HG2	0.43	1.91	3	1
1:A:72:VAL:HG23	1:A:143:VAL:O	0.43	2.13	8	1
1:A:26:ASP:O	1:A:29:LYS:HB3	0.43	2.14	10	1
1:A:107:LEU:HA	1:A:110:ILE:CG1	0.43	2.43	13	1
1:A:57:VAL:HG12	1:A:85:ASP:HA	0.43	1.90	3	2
1:A:53:GLY:O	1:A:80:ILE:HA	0.43	2.14	16	1
1:A:59:GLY:N	1:A:87:VAL:HB	0.43	2.28	1	1
1:A:139:TYR:O	1:A:142:GLN:HB2	0.43	2.14	16	2
1:A:57:VAL:HG12	1:A:87:VAL:CG2	0.43	2.44	10	3
1:A:65:GLU:O	1:A:69:LYS:HG3	0.43	2.13	14	1
1:A:59:GLY:O	1:A:88:LYS:HG2	0.43	2.13	4	1
1:A:88:LYS:N	1:A:88:LYS:HD3	0.43	2.29	4	1
1:A:28:ALA:N	1:A:50:ILE:HG13	0.43	2.29	5	2
1:A:64:GLN:HG3	1:A:65:GLU:N	0.43	2.29	14	2
1:A:64:GLN:HA	1:A:89:THR:HG21	0.43	1.90	16	1
1:A:57:VAL:O	1:A:57:VAL:HG13	0.42	2.14	14	1
1:A:10:ALA:CB	1:A:141:GLY:HA3	0.42	2.44	1	1
1:A:31:VAL:HG11	1:A:74:VAL:HG23	0.42	1.90	3	1
1:A:4:PHE:O	1:A:82:SER:HA	0.42	2.14	2	1
1:A:57:VAL:HG13	1:A:85:ASP:HA	0.42	1.91	14	1
1:A:65:GLU:O	1:A:69:LYS:HD3	0.42	2.14	15	1
1:A:125:PHE:HD2	1:A:132:LEU:HD13	0.42	1.74	11	1
1:A:27:GLN:O	1:A:31:VAL:HG13	0.42	2.14	5	1
1:A:110:ILE:HA	1:A:113:GLN:CG	0.42	2.45	14	1
1:A:32:GLN:HB2	1:A:48:ILE:HD12	0.42	1.91	4	1
1:A:31:VAL:CG2	1:A:48:ILE:HG21	0.42	2.44	6	1
1:A:32:GLN:O	1:A:35:LEU:HB2	0.42	2.15	4	1
1:A:14:LEU:HD23	1:A:77:ILE:CG2	0.42	2.43	9	2
1:A:35:LEU:HD13	1:A:43:ALA:HB1	0.41	1.91	4	1
1:A:66:ALA:O	1:A:70:ILE:HD12	0.41	2.15	8	1
1:A:128:ASN:OD1	1:A:144:LEU:HA	0.41	2.14	16	1
1:A:67:LYS:NZ	1:A:71:LEU:HD11	0.41	2.30	2	2
1:A:64:GLN:O	1:A:67:LYS:HB3	0.41	2.14	15	2
1:A:45:LYS:HB2	1:A:62:LEU:CD2	0.41	2.44	8	1
1:A:58:THR:C	1:A:87:VAL:HG22	0.41	2.34	4	1
1:A:97:GLN:HB3	1:A:146:ILE:HB	0.41	1.92	7	1
1:A:120:LEU:N	1:A:120:LEU:HD12	0.41	2.30	15	1
1:A:101:VAL:O	1:A:140:PRO:HA	0.41	2.15	4	1
1:A:6:PHE:HE1	1:A:83:VAL:HG12	0.41	1.76	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:HD23	1:A:62:LEU:N	0.41	2.31	18	2
1:A:62:LEU:O	1:A:89:THR:HA	0.41	2.16	17	1
1:A:64:GLN:O	1:A:68:GLU:HG3	0.41	2.15	17	2
1:A:128:ASN:HB3	1:A:131:MET:CE	0.41	2.46	17	1
1:A:12:GLU:HG2	1:A:34:HIS:ND1	0.41	2.31	2	1
1:A:57:VAL:CG2	1:A:74:VAL:HG21	0.41	2.46	13	1
1:A:31:VAL:HG11	1:A:74:VAL:HG13	0.41	1.93	16	1
1:A:66:ALA:O	1:A:69:LYS:HB2	0.41	2.15	16	1
1:A:35:LEU:HD23	1:A:40:ILE:HG13	0.41	1.93	12	1
1:A:124:ILE:HG23	1:A:145:ARG:O	0.41	2.16	14	1
1:A:50:ILE:HD13	1:A:80:ILE:HD11	0.41	1.93	16	1
1:A:134:SER:OG	1:A:137:LYS:HG3	0.41	2.15	18	1
1:A:107:LEU:CB	1:A:121:TYR:HB2	0.40	2.46	4	1
1:A:14:LEU:HB2	1:A:15:TRP:CE3	0.40	2.51	5	1
1:A:28:ALA:O	1:A:31:VAL:HG22	0.40	2.16	5	1
1:A:67:LYS:HB2	1:A:87:VAL:CG1	0.40	2.46	11	1
1:A:52:ASP:C	1:A:54:LYS:H	0.40	2.18	18	2
1:A:120:LEU:CG	1:A:123:LYS:HD3	0.40	2.46	15	1
1:A:67:LYS:CG	1:A:87:VAL:HG13	0.40	2.46	16	1
1:A:48:ILE:N	1:A:48:ILE:HD12	0.40	2.30	20	1
1:A:107:LEU:O	1:A:110:ILE:HG13	0.40	2.15	5	2
1:A:46:VAL:CG2	1:A:57:VAL:HG13	0.40	2.46	11	1
1:A:85:ASP:OD1	1:A:87:VAL:HG12	0.40	2.15	11	1
1:A:14:LEU:CD1	1:A:34:HIS:HB2	0.40	2.46	18	1
1:A:120:LEU:HB3	1:A:123:LYS:NZ	0.40	2.31	19	1
1:A:51:ALA:O	1:A:52:ASP:HB3	0.40	2.16	9	1
1:A:46:VAL:CG2	1:A:70:ILE:HG12	0.40	2.47	1	1
1:A:125:PHE:CE1	1:A:135:PRO:HD3	0.40	2.52	7	1
1:A:134:SER:HB2	1:A:137:LYS:CG	0.40	2.47	13	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	137/157 (87%)	127±2 (93±2%)	10±2 (7±2%)	0±0 (0±0%)	50	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2740/3140 (87%)	2538 (93%)	196 (7%)	6 (0%)	50 82

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	140	PRO	3
1	A	103	SER	1
1	A	85	ASP	1
1	A	53	GLY	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	113/130 (87%)	102±2 (91±2%)	11±2 (9±2%)	12 58
All	All	2260/2600 (87%)	2046 (91%)	214 (9%)	12 58

All 43 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	144	LEU	17
1	A	64	GLN	16
1	A	107	LEU	14
1	A	58	THR	13
1	A	12	GLU	12
1	A	113	GLN	12
1	A	32	GLN	11
1	A	110	ILE	11
1	A	132	LEU	10
1	A	62	LEU	9
1	A	30	LYS	9
1	A	14	LEU	8
1	A	54	LYS	6
1	A	131	MET	6
1	A	101	VAL	6

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Mol	Chain	Res	Type	Models (Total)
1	A	120	LEU	5
1	A	87	VAL	4
1	A	142	GLN	4
1	A	47	ASN	4
1	A	96	SER	3
1	A	129	LYS	3
1	A	88	LYS	2
1	A	5	ASN	2
1	A	134	SER	2
1	A	72	VAL	2
1	A	26	ASP	2
1	A	123	LYS	2
1	A	94	THR	2
1	A	68	GLU	2
1	A	108	SER	2
1	A	7	VAL	1
1	A	50	ILE	1
1	A	112	LYS	1
1	A	25	ASP	1
1	A	143	VAL	1
1	A	13	LYS	1
1	A	37	LYS	1
1	A	119	ASN	1
1	A	36	ASN	1
1	A	52	ASP	1
1	A	56	THR	1
1	A	86	GLN	1
1	A	85	ASP	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 [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 94% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_K*

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	1879
Number of shifts mapped to atoms	1879
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	153	-0.26 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	141	0.04 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	153	-0.18 ± 0.11	None needed (< 0.5 ppm)
^{15}N	141	0.29 ± 0.34	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 94%, i.e. 1526 atoms were assigned a chemical shift out of a possible 1622. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	667/673 (99%)	265/268 (99%)	274/274 (100%)	128/131 (98%)
Sidechain	781/861 (91%)	485/500 (97%)	279/326 (86%)	17/35 (49%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	78/88 (89%)	40/46 (87%)	37/39 (95%)	1/3 (33%)
Overall	1526/1622 (94%)	790/814 (97%)	590/639 (92%)	146/169 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1673 atoms were assigned a chemical shift out of a possible 1873. 1 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	741/773 (96%)	294/308 (95%)	306/314 (97%)	141/151 (93%)
Sidechain	852/956 (89%)	530/556 (95%)	304/363 (84%)	18/37 (49%)
Aromatic	80/144 (56%)	41/74 (55%)	38/53 (72%)	1/17 (6%)
Overall	1673/1873 (89%)	865/938 (92%)	648/730 (89%)	160/205 (78%)

7.1.4 Statistically unusual chemical shifts ⓘ

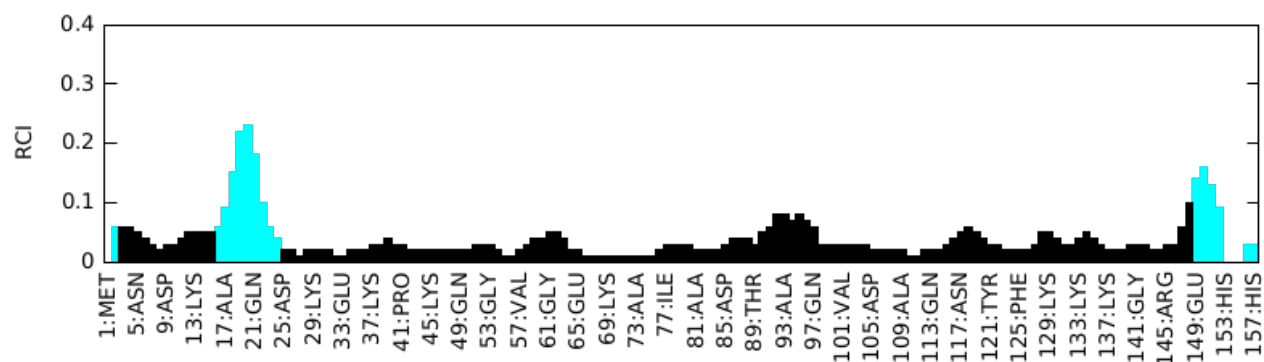
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	75	GLY	HA3	0.74	5.80 – 2.00	-8.3
1	A	27	GLN	HG3	0.24	3.75 – 0.85	-7.1
1	A	142	GLN	HB3	0.24	3.37 – 0.67	-6.6

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:



Restraints validation did not run