



Full wwPDB NMR Structure Validation Report ⓘ

Apr 6, 2026 – 01:09 AM UTC

PDB ID : 2K3R / pdb_00002k3r
BMRB ID : 15776
Title : Pfu Rpp21 structure and assignments
Authors : Amero, C.D.; Foster, M.P.; Boomershine, W.P.; Xu, Y.
Deposited on : 2008-05-15

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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

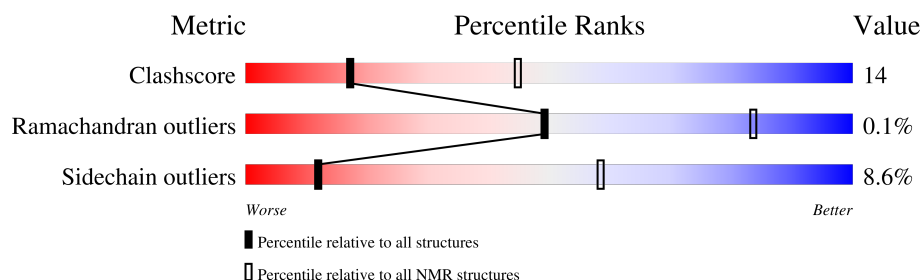
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	123	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:16-A:103 (88)	0.62	7

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1610 atoms, of which 839 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribonuclease P protein component 4.

Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1609	503	839	147	114	6	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	GLY	-	expression tag	UNP Q8U0H6
A	119	GLY	-	expression tag	UNP Q8U0H6
A	120	LEU	-	expression tag	UNP Q8U0H6
A	121	VAL	-	expression tag	UNP Q8U0H6
A	122	PRO	-	expression tag	UNP Q8U0H6
A	123	ARG	-	expression tag	UNP Q8U0H6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

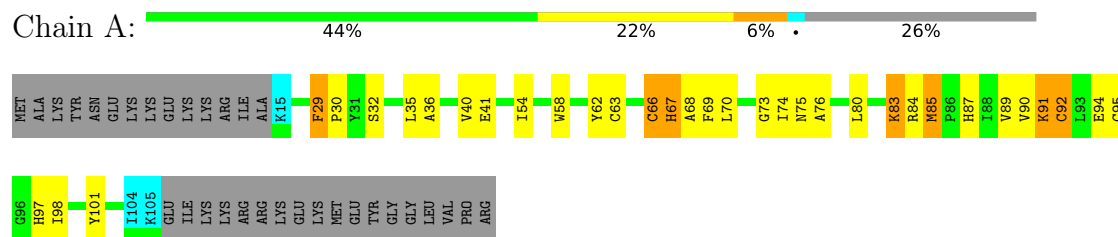
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: Ribonuclease P protein component 4

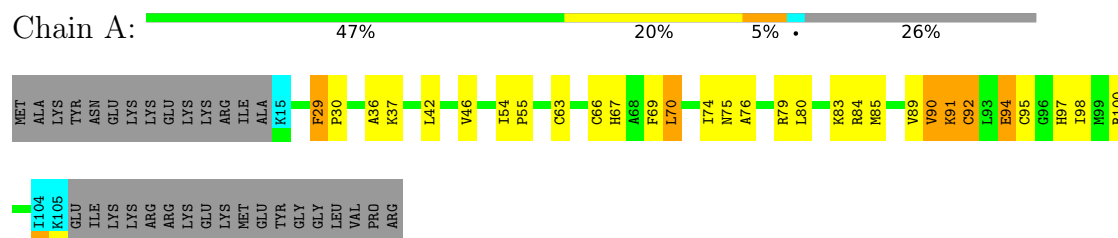


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

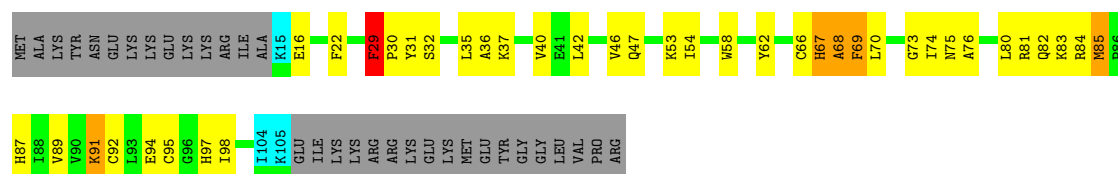
- Molecule 1: Ribonuclease P protein component 4



4.2.2 Score per residue for model 2

- Molecule 1: Ribonuclease P protein component 4

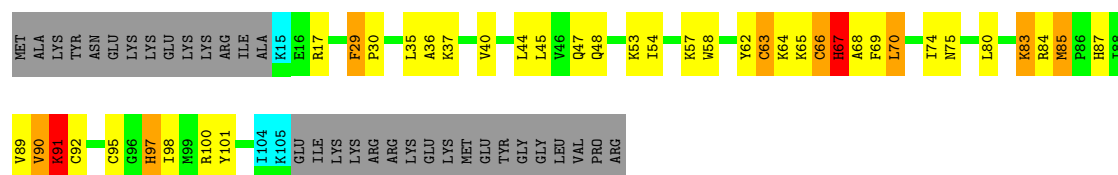




4.2.3 Score per residue for model 3

- Molecule 1: Ribonuclease P protein component 4

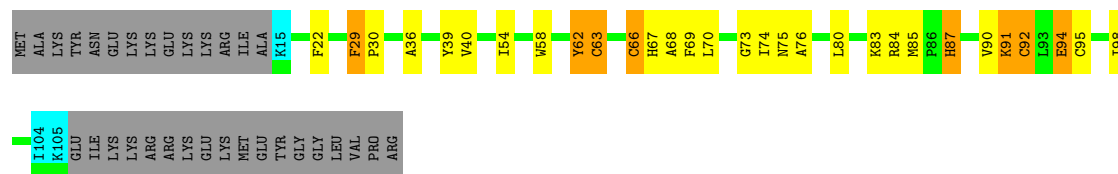
Chain A: 39% 24% 7% 26%



4.2.4 Score per residue for model 4

- Molecule 1: Ribonuclease P protein component 4

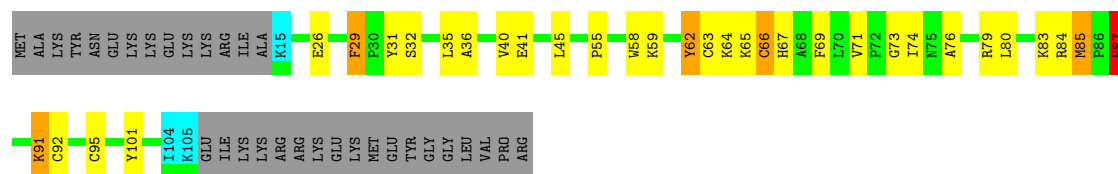
Chain A: 47% 18% 7% 26%



4.2.5 Score per residue for model 5

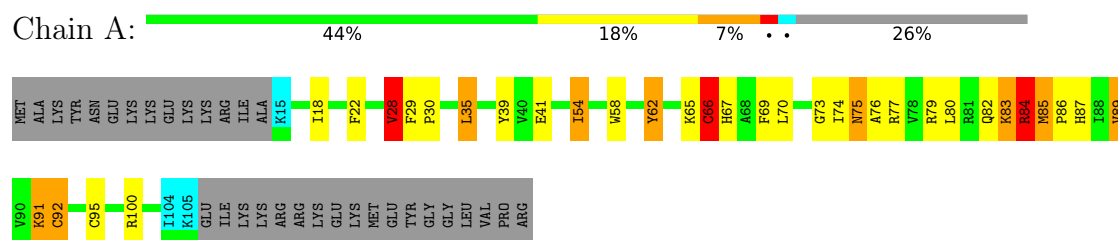
- Molecule 1: Ribonuclease P protein component 4

Chain A: 45% 22% 26%



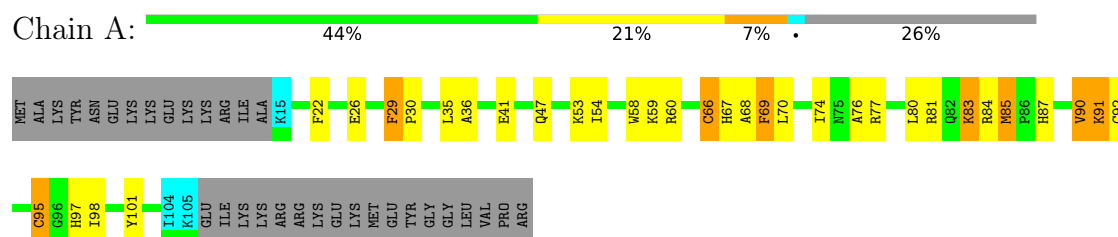
4.2.6 Score per residue for model 6

- Molecule 1: Ribonuclease P protein component 4



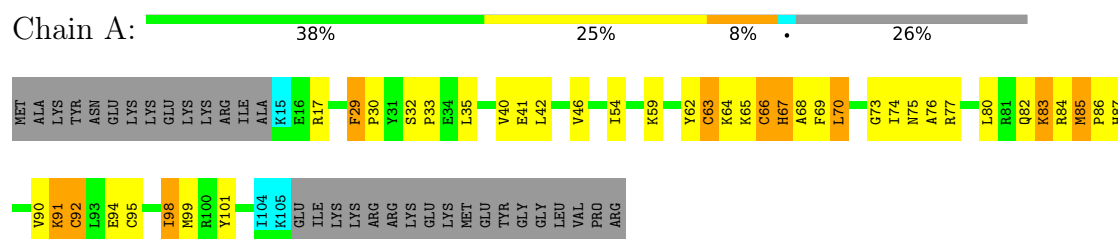
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Ribonuclease P protein component 4



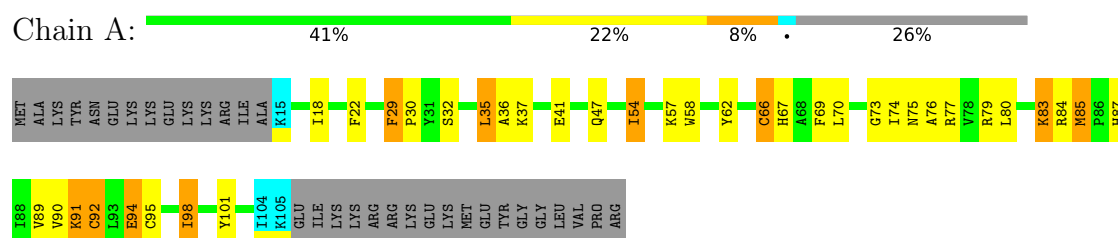
4.2.8 Score per residue for model 8

- Molecule 1: Ribonuclease P protein component 4



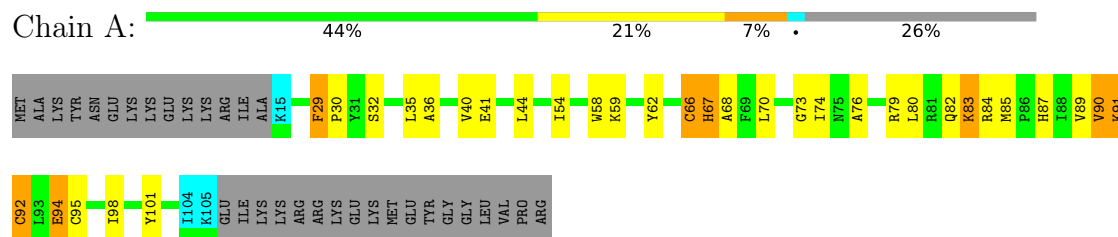
4.2.9 Score per residue for model 9

- Molecule 1: Ribonuclease P protein component 4



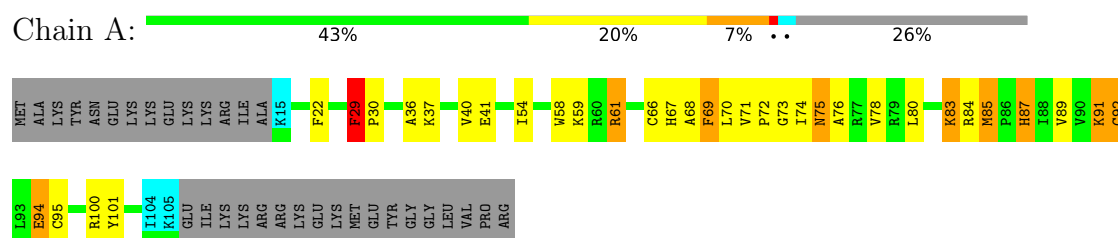
4.2.10 Score per residue for model 10

- Molecule 1: Ribonuclease P protein component 4



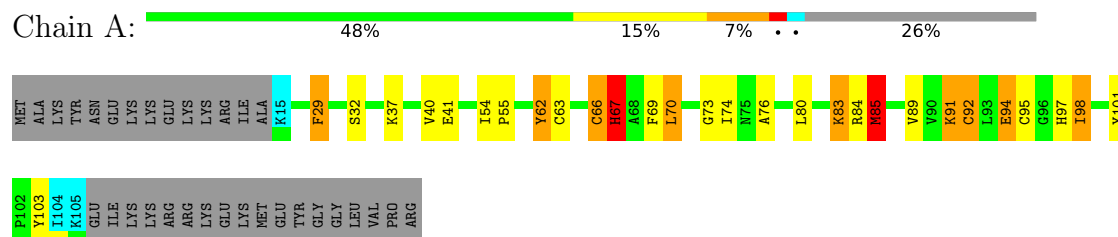
4.2.11 Score per residue for model 11

- Molecule 1: Ribonuclease P protein component 4



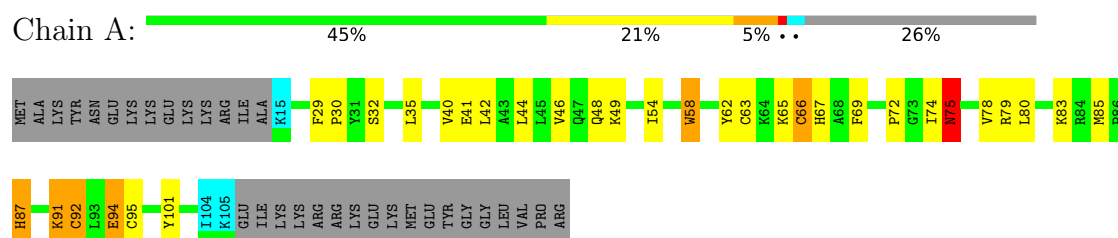
4.2.12 Score per residue for model 12

- Molecule 1: Ribonuclease P protein component 4



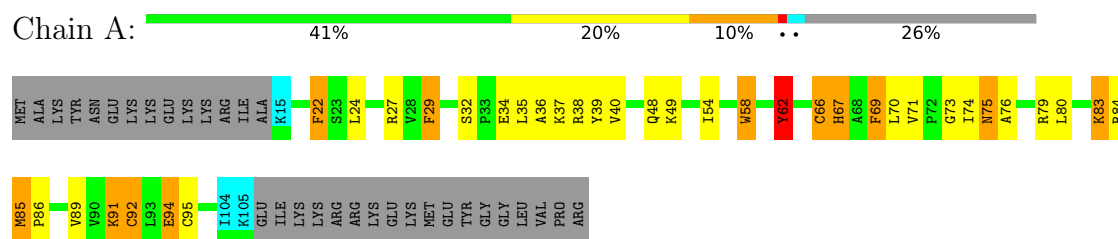
4.2.13 Score per residue for model 13

- Molecule 1: Ribonuclease P protein component 4



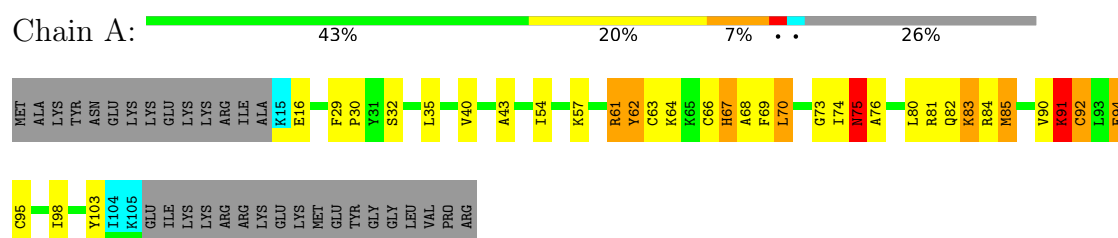
4.2.14 Score per residue for model 14

- Molecule 1: Ribonuclease P protein component 4



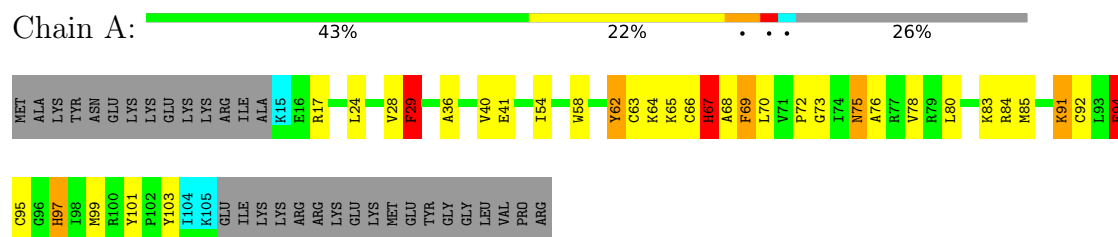
4.2.15 Score per residue for model 15

- Molecule 1: Ribonuclease P protein component 4



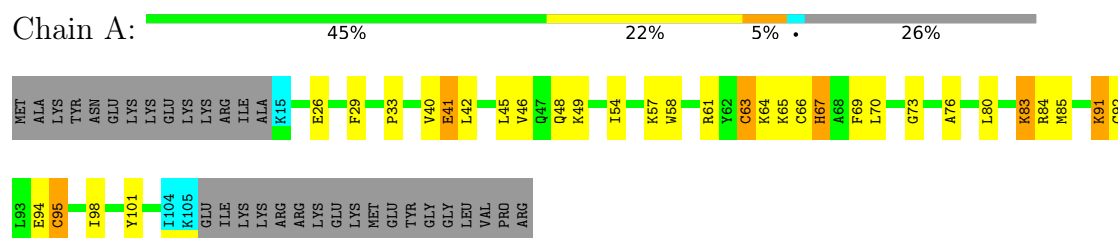
4.2.16 Score per residue for model 16

- Molecule 1: Ribonuclease P protein component 4



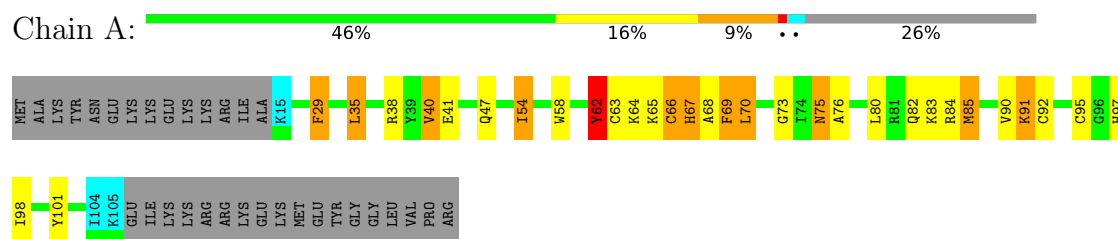
4.2.17 Score per residue for model 17

- Molecule 1: Ribonuclease P protein component 4



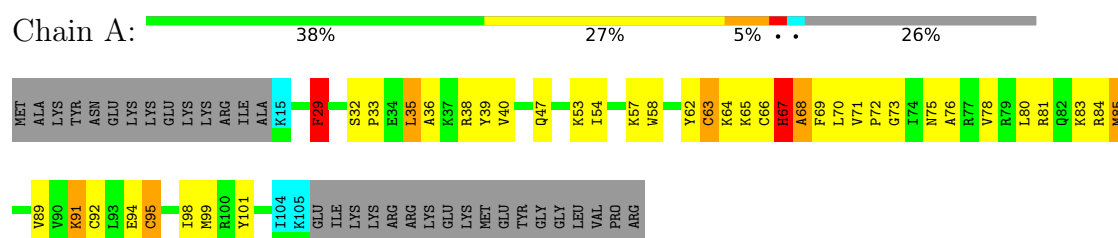
4.2.18 Score per residue for model 18

- Molecule 1: Ribonuclease P protein component 4



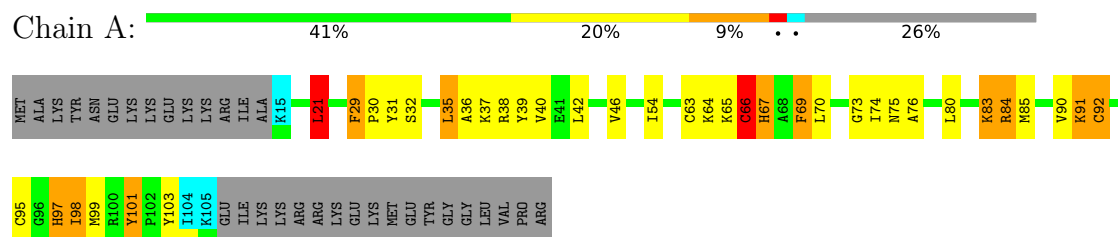
4.2.19 Score per residue for model 19

- Molecule 1: Ribonuclease P protein component 4



4.2.20 Score per residue for model 20

- Molecule 1: Ribonuclease P protein component 4



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure solution	
X-PLOR NIH	geometry optimization	
NMRView	structure solution	
CARA	structure solution	

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	1003
Number of shifts mapped to atoms	983
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	0.62±0.01	0±0/763 (0.0± 0.0%)	1.17±0.03	2±1/1025 (0.2± 0.1%)
All	All	0.62	0/15260 (0.0%)	1.17	48/20500 (0.2%)

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	14.1±3.0
All	All	0	281

There are no bond-length outliers.

All unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	85	MET	O-C-N	-6.07	117.63	121.27	12	1
1	A	83	LYS	CA-C-N	-5.97	113.38	122.21	14	12
1	A	83	LYS	C-N-CA	-5.97	113.38	122.21	14	12
1	A	97	HIS	CE1-NE2-CD2	-5.83	103.17	109.00	16	2
1	A	66	CYS	N-CA-CB	5.78	118.71	110.16	20	4
1	A	97	HIS	CA-CB-CG	-5.52	108.28	113.80	12	6
1	A	66	CYS	CB-CA-C	-5.42	101.64	110.85	6	2
1	A	67	HIS	CA-CB-CG	-5.41	108.39	113.80	3	5
1	A	87	HIS	CA-CB-CG	-5.28	108.52	113.80	13	1
1	A	87	HIS	CE1-NE2-CD2	-5.12	103.88	109.00	11	2
1	A	84	ARG	N-CA-C	-5.09	101.81	109.60	6	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	29	PHE	Sidechain	20
1	A	69	PHE	Sidechain,Mainchain	19
1	A	84	ARG	Mainchain,Peptide,Sidechain	19
1	A	67	HIS	Mainchain,Sidechain	18
1	A	62	TYR	Sidechain,Mainchain	15
1	A	35	LEU	Mainchain	12
1	A	66	CYS	Mainchain	12
1	A	41	GLU	Mainchain,Sidechain	12
1	A	87	HIS	Sidechain	9
1	A	90	VAL	Mainchain	7
1	A	22	PHE	Sidechain	7
1	A	79	ARG	Sidechain	5
1	A	68	ALA	Mainchain	5
1	A	39	TYR	Sidechain,Mainchain	5
1	A	59	LYS	Mainchain	5
1	A	82	GLN	Mainchain	5
1	A	94	GLU	Sidechain	5
1	A	97	HIS	Sidechain	4
1	A	81	ARG	Sidechain	4
1	A	77	ARG	Sidechain	4
1	A	58	TRP	Mainchain	4
1	A	103	TYR	Sidechain	4
1	A	31	TYR	Sidechain	3
1	A	17	ARG	Mainchain	3
1	A	57	LYS	Mainchain	3
1	A	26	GLU	Mainchain	3
1	A	86	PRO	Mainchain	3
1	A	95	CYS	Mainchain	3
1	A	33	PRO	Mainchain	3
1	A	63	CYS	Mainchain	3
1	A	98	ILE	Mainchain	3
1	A	61	ARG	Sidechain	3
1	A	83	LYS	Mainchain	2
1	A	85	MET	Mainchain,Peptide	2
1	A	91	LYS	Mainchain	2
1	A	101	TYR	Sidechain	2
1	A	55	PRO	Mainchain	2
1	A	92	CYS	Mainchain	2
1	A	75	ASN	Mainchain	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	16	GLU	Mainchain	1
1	A	28	VAL	Mainchain	1
1	A	89	VAL	Mainchain	1
1	A	60	ARG	Sidechain	1
1	A	70	LEU	Mainchain	1
1	A	21	LEU	Mainchain	1

6.2 Too-close contacts [i](#)

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	744	802	799	21±3
All	All	14900	16040	15980	423

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:VAL:HG11	1:A:67:HIS:O	0.83	1.72	14	4
1:A:66:CYS:SG	1:A:68:ALA:HB3	0.79	2.17	16	1
1:A:54:ILE:HG21	1:A:58:TRP:H	0.78	1.39	17	7
1:A:66:CYS:SG	1:A:95:CYS:N	0.77	2.56	2	10
1:A:53:LYS:C	1:A:54:ILE:HD12	0.74	2.07	19	4
1:A:65:LYS:HB3	1:A:95:CYS:SG	0.72	2.24	13	10
1:A:29:PHE:CE2	1:A:74:ILE:HG21	0.69	2.22	14	1
1:A:91:LYS:N	1:A:91:LYS:HD3	0.66	2.06	4	20
1:A:91:LYS:HD2	1:A:98:ILE:HD13	0.66	1.68	18	12
1:A:63:CYS:SG	1:A:64:LYS:N	0.66	2.68	18	8
1:A:80:LEU:N	1:A:80:LEU:HD12	0.64	2.08	10	20
1:A:47:GLN:HE21	1:A:54:ILE:HD11	0.64	1.52	9	1
1:A:63:CYS:SG	1:A:65:LYS:N	0.64	2.70	17	2
1:A:66:CYS:SG	1:A:68:ALA:CB	0.63	2.85	16	1
1:A:35:LEU:HD23	1:A:38:ARG:HH21	0.61	1.55	20	3
1:A:66:CYS:N	1:A:95:CYS:SG	0.61	2.74	19	6
1:A:47:GLN:NE2	1:A:54:ILE:HD11	0.60	2.12	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:CYS:SG	1:A:94:GLU:CB	0.60	2.89	15	1
1:A:66:CYS:SG	1:A:94:GLU:HB2	0.59	2.37	15	6
1:A:40:VAL:HG21	1:A:68:ALA:HA	0.59	1.74	18	3
1:A:24:LEU:HD23	1:A:27:ARG:HH21	0.58	1.59	14	1
1:A:30:PRO:HA	1:A:74:ILE:HG23	0.57	1.75	4	13
1:A:47:GLN:HE21	1:A:54:ILE:HD13	0.57	1.59	7	4
1:A:65:LYS:C	1:A:95:CYS:SG	0.57	2.88	19	4
1:A:87:HIS:CE1	1:A:89:VAL:HG13	0.57	2.34	6	1
1:A:63:CYS:CB	1:A:66:CYS:SG	0.57	2.93	16	1
1:A:40:VAL:HG22	1:A:58:TRP:CH2	0.56	2.36	11	4
1:A:89:VAL:HB	1:A:98:ILE:HD11	0.56	1.78	1	4
1:A:92:CYS:O	1:A:95:CYS:SG	0.55	2.65	12	7
1:A:47:GLN:NE2	1:A:54:ILE:HD13	0.55	2.17	7	3
1:A:66:CYS:SG	1:A:94:GLU:CD	0.55	2.89	13	1
1:A:29:PHE:CD2	1:A:74:ILE:HG21	0.55	2.36	14	5
1:A:54:ILE:HD12	1:A:57:LYS:HD3	0.54	1.79	9	1
1:A:58:TRP:CH2	1:A:61:ARG:NH1	0.54	2.75	11	1
1:A:68:ALA:HB2	1:A:94:GLU:OE1	0.54	2.02	2	1
1:A:40:VAL:HG11	1:A:67:HIS:C	0.54	2.28	4	6
1:A:89:VAL:HG12	1:A:100:ARG:HG2	0.54	1.78	3	3
1:A:65:LYS:CB	1:A:95:CYS:SG	0.54	2.96	18	8
1:A:32:SER:HB2	1:A:35:LEU:HD12	0.53	1.78	19	2
1:A:54:ILE:CG2	1:A:58:TRP:H	0.53	2.16	4	5
1:A:89:VAL:HG23	1:A:91:LYS:NZ	0.53	2.19	2	3
1:A:90:VAL:C	1:A:98:ILE:HD12	0.53	2.29	7	6
1:A:29:PHE:CE1	1:A:36:ALA:HB1	0.52	2.39	19	3
1:A:75:ASN:HD22	1:A:75:ASN:H	0.52	1.46	6	2
1:A:75:ASN:H	1:A:75:ASN:HD22	0.52	1.47	18	3
1:A:29:PHE:CE2	1:A:69:PHE:O	0.51	2.63	11	3
1:A:83:LYS:C	1:A:85:MET:H	0.51	2.13	16	17
1:A:87:HIS:NE2	1:A:89:VAL:HG13	0.51	2.20	6	1
1:A:29:PHE:CE2	1:A:75:ASN:CG	0.51	2.89	2	2
1:A:29:PHE:HA	1:A:36:ALA:HB2	0.51	1.82	7	8
1:A:92:CYS:SG	1:A:94:GLU:HG2	0.51	2.46	4	3
1:A:29:PHE:CZ	1:A:69:PHE:O	0.50	2.63	7	2
1:A:66:CYS:SG	1:A:92:CYS:HB2	0.50	2.45	13	2
1:A:91:LYS:CD	1:A:98:ILE:HD13	0.50	2.37	1	2
1:A:66:CYS:HB3	1:A:68:ALA:HB3	0.50	1.83	3	2
1:A:45:LEU:HD23	1:A:45:LEU:C	0.50	2.31	5	1
1:A:79:ARG:NE	1:A:91:LYS:HZ1	0.50	2.04	10	1
1:A:44:LEU:HD22	1:A:67:HIS:CG	0.50	2.42	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:GLY:N	1:A:76:ALA:O	0.50	2.45	18	16
1:A:70:LEU:HD12	1:A:75:ASN:HD21	0.49	1.66	15	2
1:A:79:ARG:HG3	1:A:91:LYS:HZ1	0.49	1.68	5	1
1:A:29:PHE:CE1	1:A:75:ASN:CG	0.49	2.91	9	6
1:A:42:LEU:O	1:A:46:VAL:HG23	0.49	2.07	17	6
1:A:76:ALA:HA	1:A:91:LYS:O	0.48	2.08	7	3
1:A:64:LYS:HD2	1:A:99:MET:SD	0.48	2.48	16	1
1:A:89:VAL:HG23	1:A:91:LYS:HZ3	0.48	1.67	2	1
1:A:84:ARG:C	1:A:85:MET:SD	0.48	2.96	20	1
1:A:32:SER:OG	1:A:35:LEU:HD12	0.48	2.08	9	1
1:A:72:PRO:HB3	1:A:78:VAL:HG12	0.48	1.86	16	4
1:A:66:CYS:CB	1:A:68:ALA:HB3	0.47	2.39	19	1
1:A:37:LYS:HD3	1:A:37:LYS:C	0.47	2.35	2	6
1:A:70:LEU:C	1:A:70:LEU:HD13	0.47	2.35	17	3
1:A:48:GLN:HG3	1:A:49:LYS:N	0.47	2.24	17	3
1:A:64:LYS:NZ	1:A:99:MET:SD	0.47	2.84	19	1
1:A:92:CYS:CB	1:A:95:CYS:HB2	0.46	2.39	17	1
1:A:54:ILE:HD12	1:A:58:TRP:H	0.46	1.70	18	1
1:A:18:ILE:HG21	1:A:54:ILE:HD13	0.46	1.86	6	1
1:A:54:ILE:HD12	1:A:57:LYS:HB3	0.46	1.87	9	1
1:A:91:LYS:N	1:A:91:LYS:CD	0.46	2.79	5	13
1:A:40:VAL:CG1	1:A:67:HIS:O	0.46	2.64	3	2
1:A:65:LYS:CG	1:A:95:CYS:SG	0.45	3.04	3	3
1:A:37:LYS:HD2	1:A:66:CYS:O	0.45	2.11	20	1
1:A:63:CYS:HB3	1:A:66:CYS:HB2	0.45	1.87	13	1
1:A:63:CYS:N	1:A:70:LEU:HD23	0.45	2.27	4	3
1:A:18:ILE:HG21	1:A:54:ILE:CD1	0.45	2.41	6	1
1:A:70:LEU:C	1:A:70:LEU:CD1	0.45	2.90	18	1
1:A:29:PHE:CE1	1:A:75:ASN:HB3	0.45	2.47	3	1
1:A:54:ILE:HD12	1:A:54:ILE:N	0.45	2.25	7	1
1:A:29:PHE:CD1	1:A:36:ALA:HB1	0.45	2.47	11	3
1:A:40:VAL:HB	1:A:67:HIS:O	0.45	2.11	8	5
1:A:63:CYS:HB3	1:A:66:CYS:SG	0.45	2.50	16	1
1:A:35:LEU:HD23	1:A:38:ARG:NH2	0.44	2.25	20	1
1:A:80:LEU:N	1:A:80:LEU:CD1	0.44	2.78	10	4
1:A:94:GLU:N	1:A:94:GLU:CD	0.44	2.76	10	5
1:A:80:LEU:HD12	1:A:80:LEU:H	0.44	1.72	2	1
1:A:32:SER:HB3	1:A:35:LEU:HD12	0.44	1.88	8	1
1:A:61:ARG:CG	1:A:69:PHE:CD1	0.44	3.00	11	1
1:A:63:CYS:SG	1:A:66:CYS:N	0.44	2.82	17	1
1:A:62:TYR:C	1:A:62:TYR:CD1	0.44	2.96	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:ALA:HB2	1:A:92:CYS:HB2	0.44	1.88	4	1
1:A:66:CYS:C	1:A:68:ALA:N	0.44	2.76	18	2
1:A:87:HIS:NE2	1:A:100:ARG:NH1	0.43	2.66	6	1
1:A:66:CYS:C	1:A:68:ALA:H	0.43	2.20	15	1
1:A:98:ILE:HD12	1:A:99:MET:N	0.43	2.28	8	2
1:A:21:LEU:CD1	1:A:21:LEU:C	0.43	2.92	20	1
1:A:28:VAL:HG13	1:A:35:LEU:HB2	0.43	1.90	6	1
1:A:65:LYS:HG2	1:A:95:CYS:SG	0.43	2.53	6	1
1:A:83:LYS:C	1:A:85:MET:N	0.43	2.76	11	5
1:A:90:VAL:O	1:A:98:ILE:HD12	0.43	2.14	15	1
1:A:66:CYS:HB3	1:A:68:ALA:CB	0.42	2.44	3	1
1:A:21:LEU:C	1:A:21:LEU:HD13	0.42	2.39	20	1
1:A:44:LEU:HD22	1:A:67:HIS:HB3	0.42	1.90	10	1
1:A:29:PHE:CE2	1:A:75:ASN:HB3	0.42	2.48	11	1
1:A:62:TYR:HB2	1:A:67:HIS:O	0.42	2.15	14	1
1:A:29:PHE:CE1	1:A:74:ILE:CG2	0.42	3.02	12	2
1:A:68:ALA:HB3	1:A:94:GLU:OE1	0.42	2.15	15	1
1:A:66:CYS:SG	1:A:94:GLU:C	0.42	3.03	2	1
1:A:34:GLU:HG2	1:A:38:ARG:NH1	0.42	2.30	14	1
1:A:66:CYS:SG	1:A:92:CYS:CB	0.42	3.07	20	1
1:A:36:ALA:O	1:A:40:VAL:HG23	0.42	2.14	4	1
1:A:57:LYS:O	1:A:61:ARG:NE	0.42	2.52	15	1
1:A:29:PHE:CE1	1:A:69:PHE:O	0.42	2.73	18	2
1:A:87:HIS:CD2	1:A:87:HIS:N	0.42	2.88	5	1
1:A:85:MET:O	1:A:87:HIS:CD2	0.41	2.73	2	1
1:A:58:TRP:O	1:A:62:TYR:CD2	0.41	2.73	6	1
1:A:41:GLU:O	1:A:45:LEU:HD13	0.41	2.14	17	1
1:A:83:LYS:C	1:A:84:ARG:O	0.41	2.61	6	1
1:A:70:LEU:CD1	1:A:70:LEU:C	0.41	2.94	8	1
1:A:40:VAL:HG22	1:A:58:TRP:HH2	0.41	1.72	11	1
1:A:22:PHE:CE1	1:A:69:PHE:CE1	0.41	3.09	14	1
1:A:91:LYS:HD2	1:A:98:ILE:CD1	0.41	2.46	4	1
1:A:29:PHE:HZ	1:A:71:VAL:H	0.41	1.59	5	1
1:A:66:CYS:SG	1:A:92:CYS:HB3	0.41	2.55	6	1
1:A:40:VAL:O	1:A:43:ALA:N	0.41	2.54	15	1
1:A:24:LEU:O	1:A:28:VAL:HG12	0.41	2.15	16	1
1:A:94:GLU:CD	1:A:94:GLU:N	0.41	2.79	1	1
1:A:37:LYS:CD	1:A:66:CYS:O	0.41	2.68	3	1
1:A:44:LEU:CD2	1:A:67:HIS:CG	0.41	3.03	10	1
1:A:48:GLN:CG	1:A:49:LYS:N	0.41	2.83	17	3
1:A:94:GLU:CD	1:A:94:GLU:H	0.40	2.24	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:PRO:HA	1:A:74:ILE:CG2	0.40	2.47	4	1
1:A:45:LEU:HD12	1:A:48:GLN:HE21	0.40	1.75	3	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	88/123 (72%)	85±1 (96±1%)	3±1 (4±1%)	0±0 (0±0%)	49	83
All	All	1760/2460 (72%)	1696 (96%)	62 (4%)	2 (0%)	49	83

All 2 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	55	PRO	1
1	A	82	GLN	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	80/111 (72%)	73±2 (91±2%)	7±2 (9±2%)	12	58
All	All	1600/2220 (72%)	1462 (91%)	138 (9%)	12	58

All 19 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	91	LYS	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	92	CYS	17
1	A	70	LEU	14
1	A	85	MET	13
1	A	101	TYR	13
1	A	54	ILE	12
1	A	94	GLU	9
1	A	75	ASN	8
1	A	32	SER	7
1	A	62	TYR	7
1	A	29	PHE	4
1	A	71	VAL	3
1	A	44	LEU	2
1	A	63	CYS	2
1	A	87	HIS	2
1	A	98	ILE	2
1	A	28	VAL	1
1	A	40	VAL	1
1	A	21	LEU	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 69% 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	1003
Number of shifts mapped to atoms	983
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 20 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	PRO	HA	4.42	0.02	1
1	A	122	PRO	HB2	1.98	0.02	2
1	A	122	PRO	HB3	2.24	0.02	2
1	A	122	PRO	C	175.6	0.3	1
1	A	122	PRO	CA	63.7	0.3	1
1	A	122	PRO	CB	32.8	0.3	1
1	A	122	PRO	CD	51.7	0.3	1
1	A	122	PRO	CG	27.8	0.3	1
1	A	123	ARG	H	7.79	0.02	1
1	A	123	ARG	HA	4.2	0.02	1
1	A	123	ARG	HB2	1.74	0.02	2
1	A	123	ARG	HB3	1.91	0.02	2
1	A	123	ARG	HD3	3.25	0.02	1
1	A	123	ARG	HG2	1.37	0.02	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	ARG	HG3	1.65	0.02	2
1	A	123	ARG	CA	57.9	0.3	1
1	A	123	ARG	CB	32.4	0.3	1
1	A	123	ARG	CD	44.3	0.3	1
1	A	123	ARG	CG	27.9	0.3	1
1	A	123	ARG	N	126.3	0.3	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	-0.68 ± 0.22	Should be applied
$^{13}\text{C}_\beta$	78	-0.22 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	62	-0.09 ± 0.17	None needed (< 0.5 ppm)
^{15}N	71	0.22 ± 0.55	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 72%, i.e. 983 atoms were assigned a chemical shift out of a possible 1372. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	359/430 (83%)	150/172 (87%)	139/176 (79%)	70/82 (85%)
Sidechain	554/831 (67%)	363/540 (67%)	188/244 (77%)	3/47 (6%)
Aromatic	70/111 (63%)	35/53 (66%)	34/51 (67%)	1/7 (14%)
Overall	983/1372 (72%)	548/765 (72%)	361/471 (77%)	74/136 (54%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 983 atoms were assigned a chemical shift out of a possible 1426. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	359/445 (81%)	150/178 (84%)	139/182 (76%)	70/85 (82%)
Sidechain	554/870 (64%)	363/565 (64%)	188/256 (73%)	3/49 (6%)
Aromatic	70/111 (63%)	35/53 (66%)	34/51 (67%)	1/7 (14%)
Overall	983/1426 (69%)	548/796 (69%)	361/489 (74%)	74/141 (52%)

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	22	PHE	HB2	0.44	1.20 – 4.80	-7.1
1	A	57	LYS	HG2	0.12	0.13 – 2.61	-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:

