



Full wwPDB NMR Structure Validation Report ⓘ

Aug 8, 2020 – 10:19 PM BST

PDB ID : 6S10
Title : NMR solution structure of a ProQ homolog from Legionella pneumophila
Authors : Immer, C.; Hacker, C.; Woehnert, J.
Deposited on : 2019-06-18

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 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 : 2.13.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

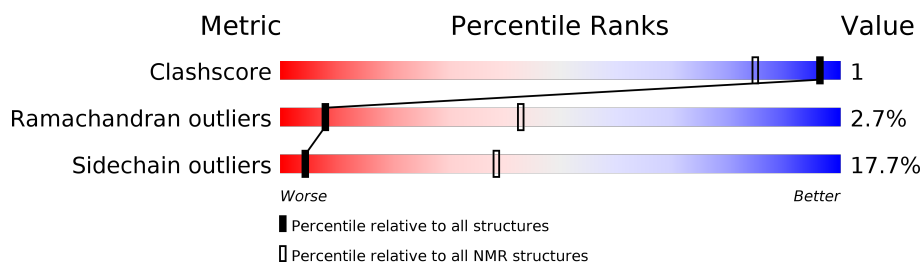
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	122	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:11-A:114 (104)	0.34	19

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1990 atoms, of which 989 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA chaperone ProQ.

Mol	Chain	Residues	Atoms						Trace
1	A	122	Total	C	H	N	O	S	0
			1990	641	989	168	191	1	

There are 2 discrepancies between the modelled and reference sequences:

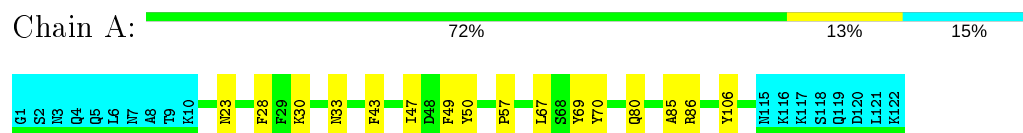
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A131MWN1
A	2	SER	-	expression tag	UNP A0A131MWN1

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: RNA chaperone ProQ

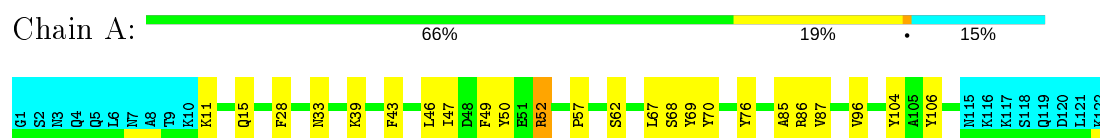


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

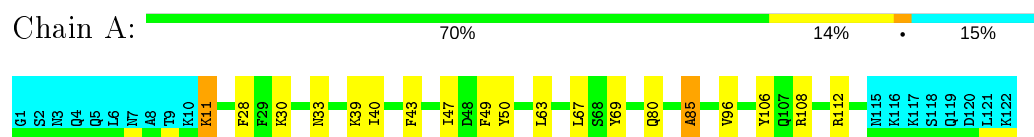
4.2.1 Score per residue for model 1

- Molecule 1: RNA chaperone ProQ



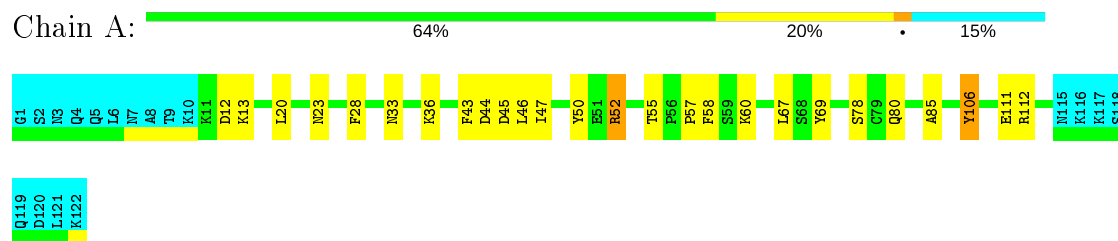
4.2.2 Score per residue for model 2

- Molecule 1: RNA chaperone ProQ



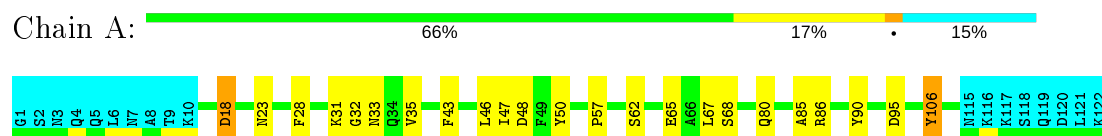
4.2.3 Score per residue for model 3

- Molecule 1: RNA chaperone ProQ



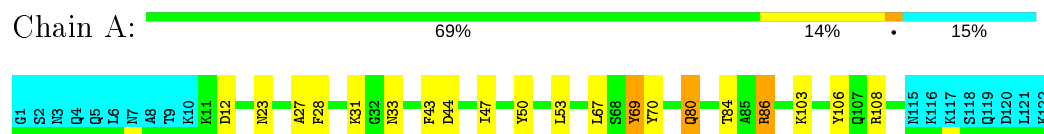
4.2.4 Score per residue for model 4

- Molecule 1: RNA chaperone ProQ



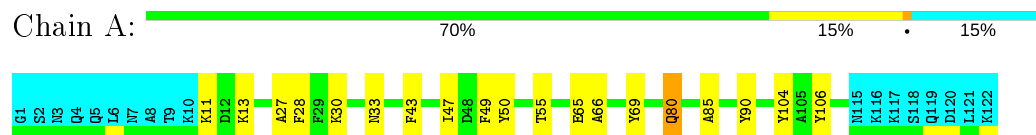
4.2.5 Score per residue for model 5

- Molecule 1: RNA chaperone ProQ



4.2.6 Score per residue for model 6

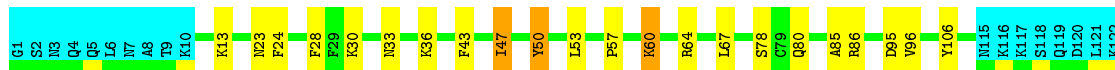
- Molecule 1: RNA chaperone ProQ





4.2.8 Score per residue for model 8

- Molecule 1: RNA chaperone ProQ



4.2.9 Score per residue for model 9

- Molecule 1: RNA chaperone ProQ



4.2.10 Score per residue for model 10

- Molecule 1: RNA chaperone ProQ



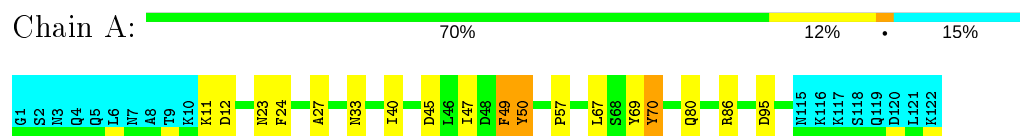
4.2.11 Score per residue for model 11

- Molecule 1: RNA chaperone ProQ



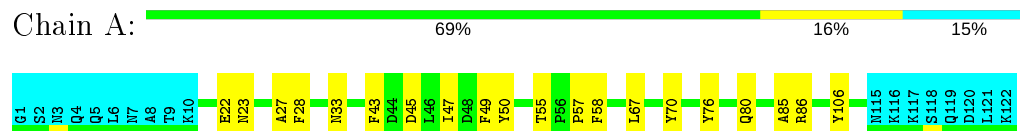
4.2.12 Score per residue for model 12

- Molecule 1: RNA chaperone ProQ



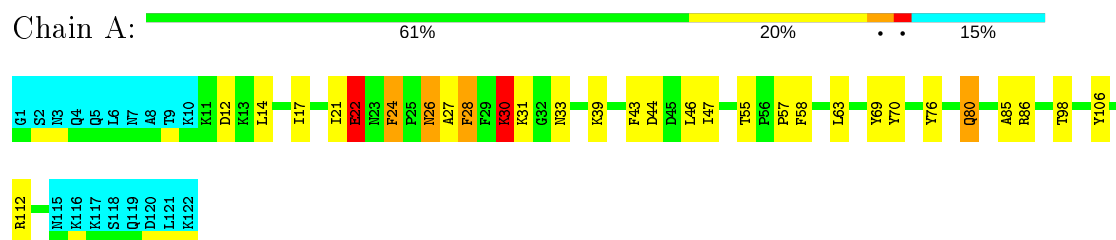
4.2.13 Score per residue for model 13

- Molecule 1: RNA chaperone ProQ



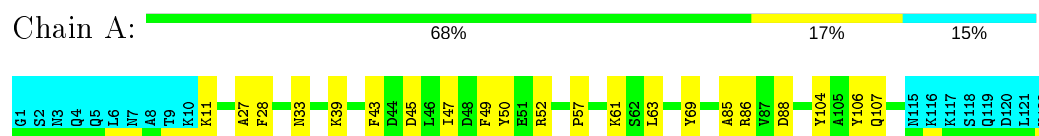
4.2.14 Score per residue for model 14

- Molecule 1: RNA chaperone ProQ



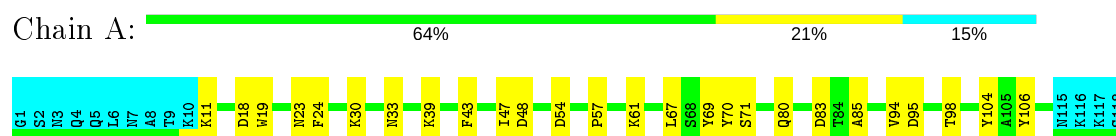
4.2.15 Score per residue for model 15

- Molecule 1: RNA chaperone ProQ



4.2.16 Score per residue for model 16

- Molecule 1: RNA chaperone ProQ

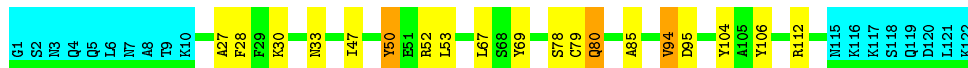




4.2.17 Score per residue for model 17

- Molecule 1: RNA chaperone ProQ

Chain A: 70% 13% 15%



4.2.18 Score per residue for model 18

- Molecule 1: RNA chaperone ProQ

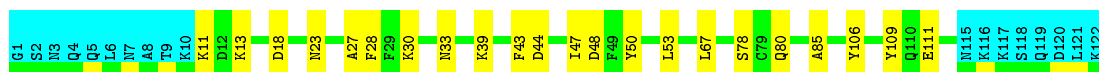
Chain A: 65% 20% 15%



4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: RNA chaperone ProQ

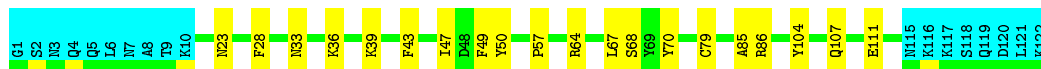
Chain A: 67% 18% 15%



4.2.20 Score per residue for model 20

- Molecule 1: RNA chaperone ProQ

Chain A: 69% 16% 15%



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	refinement	
CYANA	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	1459
Number of shifts mapped to atoms	1459
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

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	0.70±0.05	0±1/886 (0.0± 0.1%)	1.03±0.09	1±2/1201 (0.1± 0.2%)
All	All	0.70	3/17720 (0.0%)	1.04	28/24020 (0.1%)

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	1.2±1.2
All	All	0	24

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	30	LYS	CA-CB	10.73	1.77	1.53	14	1
1	A	30	LYS	CB-CG	8.23	1.74	1.52	14	1
1	A	30	LYS	N-CA	5.28	1.56	1.46	14	1

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	22	GLU	N-CA-CB	-12.01	88.99	110.60	14	1
1	A	30	LYS	CA-CB-CG	9.04	133.29	113.40	14	1
1	A	30	LYS	N-CA-CB	8.40	125.73	110.60	14	1
1	A	22	GLU	C-N-CA	8.00	141.70	121.70	14	1
1	A	22	GLU	N-CA-C	7.87	132.24	111.00	14	1
1	A	22	GLU	CA-C-N	-7.63	100.42	117.20	14	1
1	A	86	ARG	NE-CZ-NH2	-6.54	117.03	120.30	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	LEU	CB-CG-CD1	6.50	122.05	111.00	17	4
1	A	24	PHE	N-CA-C	-6.32	93.93	111.00	14	1
1	A	86	ARG	NE-CZ-NH1	6.15	123.38	120.30	7	1
1	A	24	PHE	CB-CA-C	5.94	122.27	110.40	14	1
1	A	94	VAL	CB-CA-C	5.85	122.52	111.40	18	4
1	A	21	ILE	C-N-CA	5.61	135.73	121.70	14	1
1	A	69	TYR	CB-CG-CD1	-5.61	117.64	121.00	14	1
1	A	90	TYR	CB-CG-CD2	-5.55	117.67	121.00	4	2
1	A	52	ARG	NE-CZ-NH2	-5.53	117.53	120.30	3	2
1	A	106	TYR	CB-CG-CD2	-5.48	117.71	121.00	3	1
1	A	86	ARG	CD-NE-CZ	5.29	131.01	123.60	11	1
1	A	18	ASP	CB-CG-OD2	5.09	122.88	118.30	4	2

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	86	ARG	Sidechain	4
1	A	76	TYR	Sidechain	3
1	A	50	TYR	Sidechain	3
1	A	112	ARG	Sidechain	3
1	A	108	ARG	Sidechain	2
1	A	52	ARG	Sidechain	2
1	A	109	TYR	Sidechain	1
1	A	28	PHE	Sidechain	1
1	A	70	TYR	Sidechain	1
1	A	113	TYR	Sidechain	1
1	A	69	TYR	Sidechain	1
1	A	106	TYR	Sidechain	1
1	A	22	GLU	Mainchain	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	862	844	844	1±2
All	All	17240	16880	16880	26

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LYS:CG	1:A:30:LYS:CB	1.57	1.74	14	1
1:A:30:LYS:CB	1:A:30:LYS:CA	1.55	1.77	14	1
1:A:30:LYS:CD	1:A:30:LYS:CB	0.73	2.66	14	1
1:A:30:LYS:HA	1:A:30:LYS:CB	0.59	2.12	14	1
1:A:30:LYS:CB	1:A:30:LYS:C	0.59	2.69	14	1
1:A:85:ALA:H	1:A:96:VAL:HG12	0.54	1.61	8	4
1:A:85:ALA:N	1:A:96:VAL:HG12	0.51	2.21	10	2
1:A:24:PHE:C	1:A:26:ASN:H	0.51	2.08	14	1
1:A:32:GLY:O	1:A:35:VAL:HG22	0.49	2.07	4	1
1:A:20:LEU:HB2	1:A:46:LEU:HD21	0.46	1.87	3	1
1:A:13:LYS:O	1:A:66:ALA:HB1	0.45	2.11	6	1
1:A:14:LEU:HD22	1:A:70:TYR:CE1	0.45	2.47	14	1
1:A:17:ILE:HD13	1:A:70:TYR:CG	0.44	2.47	14	1
1:A:17:ILE:HG21	1:A:70:TYR:CD2	0.44	2.47	14	1
1:A:24:PHE:CZ	1:A:49:PHE:CD1	0.44	3.06	12	1
1:A:43:PHE:CE2	1:A:64:ARG:HB2	0.42	2.49	10	1
1:A:17:ILE:HD13	1:A:70:TYR:CD1	0.42	2.49	18	1
1:A:47:ILE:HD11	1:A:60:LYS:HE2	0.42	1.92	8	1
1:A:11:LYS:HE2	1:A:11:LYS:HA	0.42	1.91	11	1
1:A:46:LEU:O	1:A:46:LEU:HD13	0.41	2.16	1	1
1:A:30:LYS:HG2	1:A:31:LYS:HG3	0.41	1.93	14	1
1:A:46:LEU:HD13	1:A:46:LEU:C	0.40	2.37	1	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	104/122 (85%)	96±2 (92±2%)	6±2 (5±2%)	3±1 (3±1%)	8	43
All	All	2080/2440 (85%)	1910 (92%)	113 (5%)	57 (3%)	8	43

All 6 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	80	GLN	16
1	A	85	ALA	15
1	A	57	PRO	13
1	A	27	ALA	8
1	A	11	LYS	4
1	A	31	LYS	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	93/109 (85%)	77±2 (82±2%)	16±2 (18±2%)	4	38
All	All	1860/2180 (85%)	1531 (82%)	329 (18%)	4	38

All 58 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	33	ASN	20
1	A	47	ILE	20
1	A	106	TYR	18
1	A	43	PHE	17
1	A	50	TYR	16
1	A	28	PHE	15
1	A	67	LEU	15
1	A	23	ASN	12
1	A	49	PHE	11
1	A	69	TYR	10
1	A	86	ARG	9
1	A	30	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	95	ASP	8
1	A	104	TYR	8
1	A	39	LYS	8
1	A	70	TYR	8
1	A	80	GLN	7
1	A	55	THR	7
1	A	48	ASP	6
1	A	44	ASP	6
1	A	58	PHE	5
1	A	68	SER	5
1	A	12	ASP	5
1	A	45	ASP	5
1	A	11	LYS	5
1	A	98	THR	4
1	A	111	GLU	4
1	A	13	LYS	4
1	A	78	SER	4
1	A	52	ARG	3
1	A	60	LYS	3
1	A	84	THR	3
1	A	63	LEU	3
1	A	62	SER	3
1	A	40	ILE	3
1	A	24	PHE	3
1	A	107	GLN	3
1	A	31	LYS	3
1	A	36	LYS	3
1	A	64	ARG	2
1	A	112	ARG	2
1	A	18	ASP	2
1	A	15	GLN	2
1	A	65	GLU	2
1	A	61	LYS	2
1	A	79	CYS	2
1	A	22	GLU	2
1	A	46	LEU	2
1	A	87	VAL	1
1	A	19	TRP	1
1	A	94	VAL	1
1	A	35	VAL	1
1	A	88	ASP	1
1	A	103	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	26	ASN	1
1	A	83	ASP	1
1	A	54	ASP	1
1	A	71	SER	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 [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Lpp1663_BMRB.str*

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	1459
Number of shifts mapped to atoms	1459
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	118	-0.28 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	0.17 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	115	-0.23 ± 0.16	None needed (< 0.5 ppm)
^{15}N	108	0.09 ± 0.42	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 86%, i.e. 1160 atoms were assigned a chemical shift out of a possible 1350. 14 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	487/506 (96%)	193/201 (96%)	201/208 (97%)	93/97 (96%)
Sidechain	558/706 (79%)	349/418 (83%)	205/253 (81%)	4/35 (11%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	115/138 (83%)	60/72 (83%)	55/65 (85%)	0/1 (0%)
Overall	1160/1350 (86%)	602/691 (87%)	461/526 (88%)	97/133 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1335 atoms were assigned a chemical shift out of a possible 1577. 16 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	564/596 (95%)	223/237 (94%)	233/244 (95%)	108/115 (94%)
Sidechain	656/843 (78%)	411/499 (82%)	239/299 (80%)	6/45 (13%)
Aromatic	115/138 (83%)	60/72 (83%)	55/65 (85%)	0/1 (0%)
Overall	1335/1577 (85%)	694/808 (86%)	527/608 (87%)	114/161 (71%)

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	23	ASN	HB3	0.57	4.41 – 1.11	-6.6
1	A	24	PHE	HB3	0.57	4.85 – 1.05	-6.3
1	A	23	ASN	HB2	1.06	4.36 – 1.26	-5.6
1	A	24	PHE	HB2	1.05	4.85 – 1.15	-5.3

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:

