Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2017 – 11:41 pm GMT

PDB ID	:	2L55
Title	:	Solution structure of the C-terminal domain of SilB from Cupriavidus metallidurans
Authors	:	Bersch, B.; Derfoufi, K.; Vandenbussche, G.
Deposited on	:	2010-10-25

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

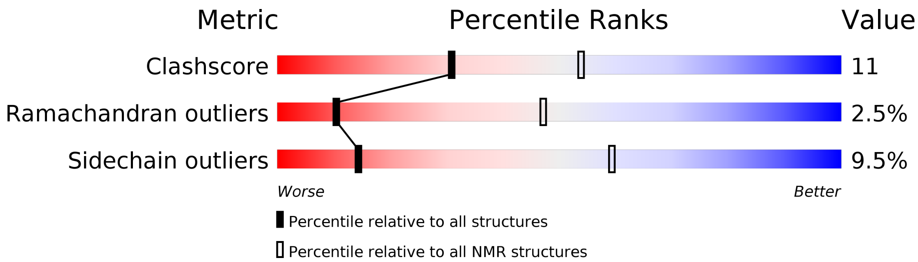
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 92%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	82	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:75 (74)	0.35	16

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1210 atoms, of which 609 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system.

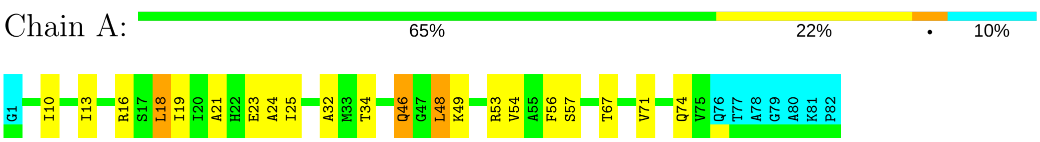
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	82	1210	379	609	111	108	3	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system

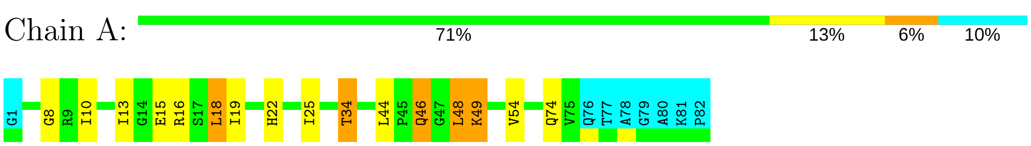


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

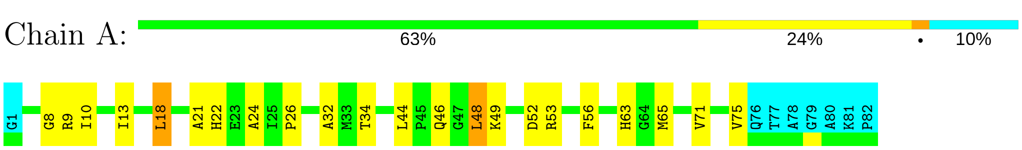
4.2.1 Score per residue for model 1

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



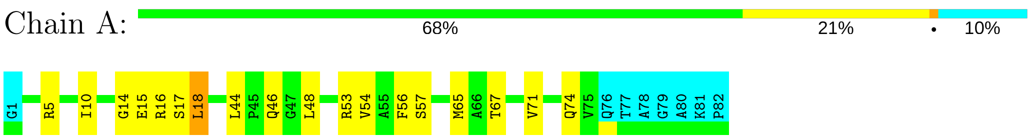
4.2.2 Score per residue for model 2

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



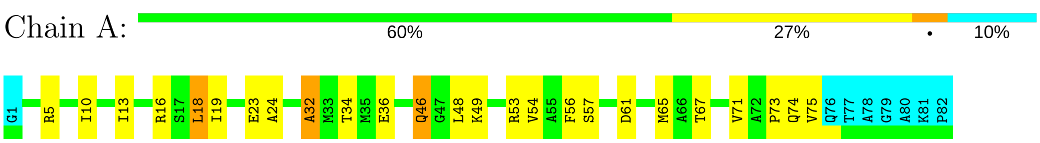
4.2.3 Score per residue for model 3

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



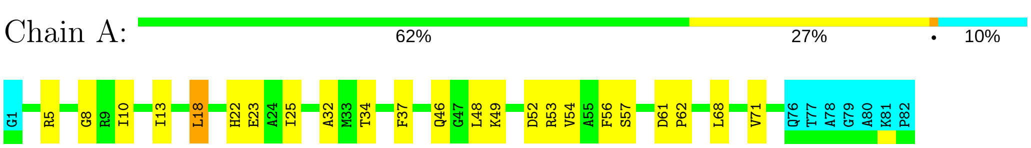
4.2.4 Score per residue for model 4

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



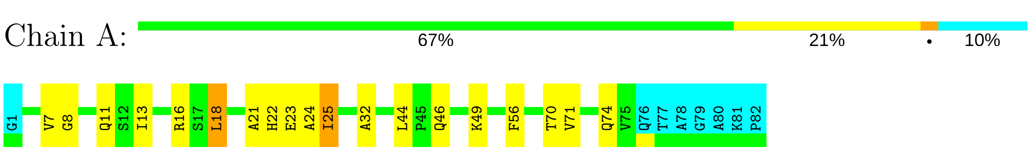
4.2.5 Score per residue for model 5

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



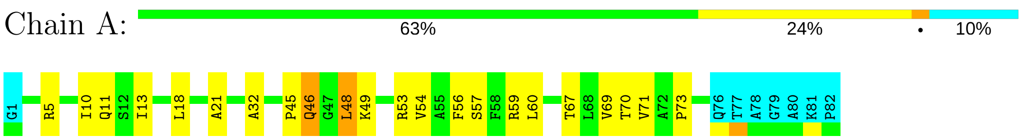
4.2.6 Score per residue for model 6

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



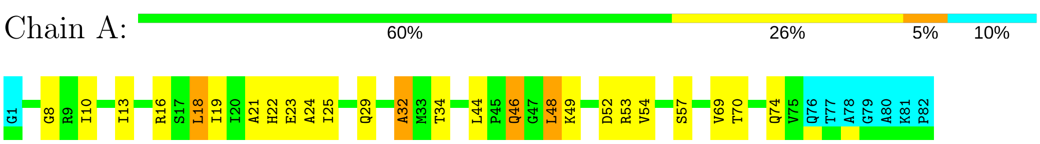
4.2.7 Score per residue for model 7

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



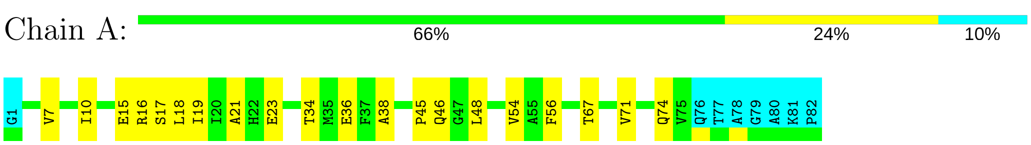
4.2.8 Score per residue for model 8

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



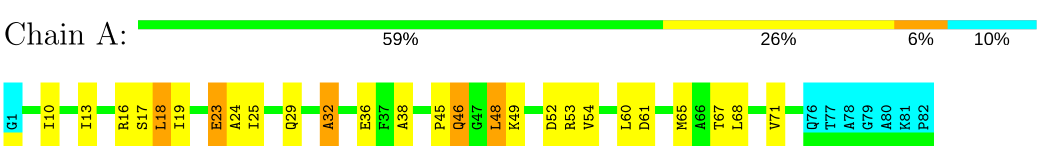
4.2.9 Score per residue for model 9

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



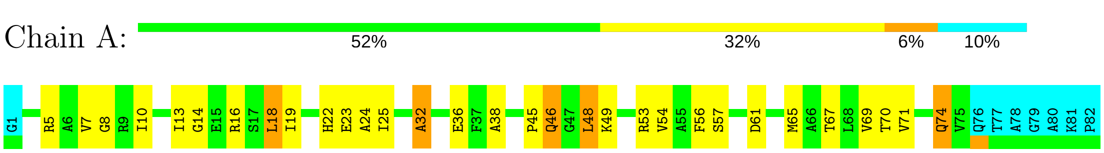
4.2.10 Score per residue for model 10

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



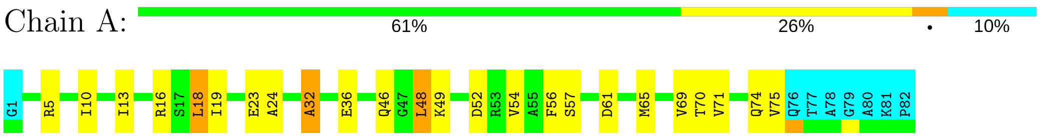
4.2.11 Score per residue for model 11

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



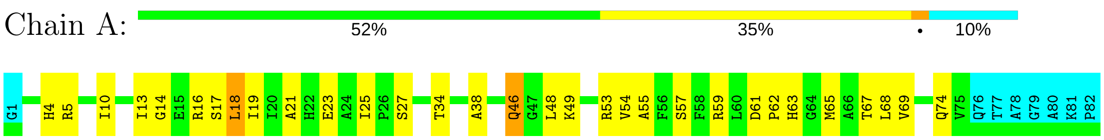
4.2.12 Score per residue for model 12

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



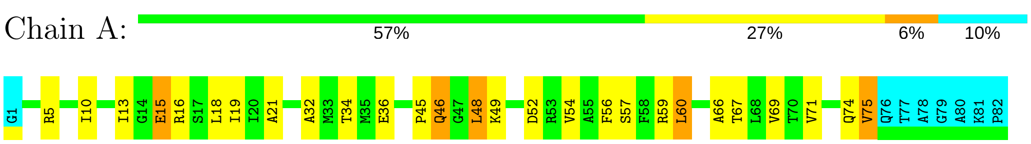
4.2.13 Score per residue for model 13

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



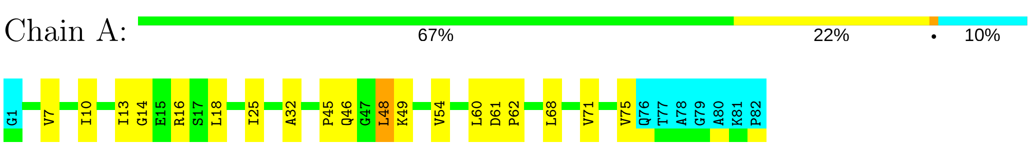
4.2.14 Score per residue for model 14

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



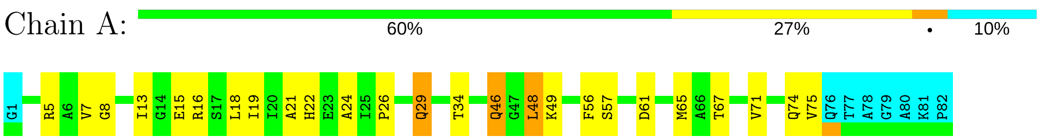
4.2.15 Score per residue for model 15

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



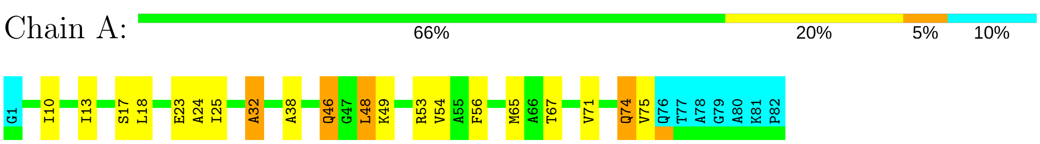
4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



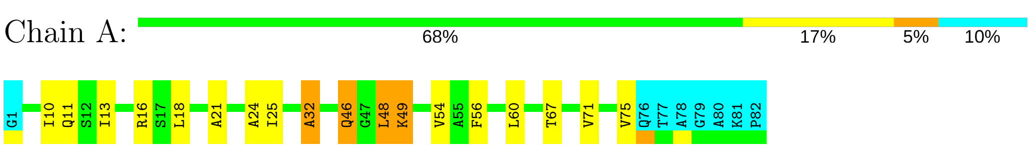
4.2.17 Score per residue for model 17

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



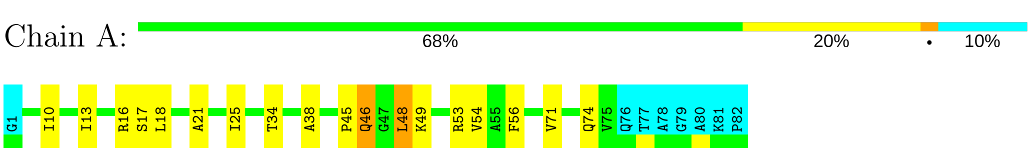
4.2.18 Score per residue for model 18

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



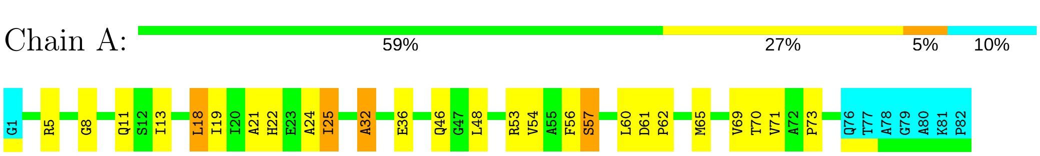
4.2.19 Score per residue for model 19

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



4.2.20 Score per residue for model 20

• Molecule 1: SilB,Silver efflux protein, MFP component of the three components proton antiporter metal efflux system



5 Refinement protocol and experimental data overview (i)

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

Of the 1000 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
UNIO08	structure solution	
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)	BMRB entry 17266
Number of chemical shift lists	1
Total number of shifts	969
Number of shifts mapped to atoms	969
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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)

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 (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	550	556	553	12±4
All	All	11000	11120	11060	244

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ASP:HB2	1:A:65:MET:HB2	0.78	1.54	11	4
1:A:13:ILE:HD11	1:A:49:LYS:HA	0.74	1.60	6	14
1:A:56:PHE:HB3	1:A:71:VAL:HG23	0.74	1.59	2	15
1:A:46:GLN:HA	1:A:46:GLN:HE21	0.73	1.44	4	1
1:A:17:SER:HB3	1:A:38:ALA:HA	0.69	1.63	10	3
1:A:19:ILE:HA	1:A:36:GLU:HA	0.69	1.64	11	7
1:A:18:LEU:HD21	1:A:44:LEU:HG	0.69	1.64	8	5
1:A:13:ILE:HA	1:A:18:LEU:HB3	0.67	1.64	20	3
1:A:13:ILE:HG23	1:A:18:LEU:HD22	0.65	1.68	2	5
1:A:19:ILE:HG22	1:A:34:THR:HG22	0.65	1.66	16	6
1:A:5:ARG:HG2	1:A:57:SER:HB2	0.64	1.68	12	2
1:A:37:PHE:HB3	1:A:68:LEU:HG	0.64	1.70	5	1
1:A:48:LEU:HD23	1:A:71:VAL:HG11	0.62	1.70	2	8
1:A:15:GLU:HG3	1:A:16:ARG:HG2	0.62	1.72	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:GLY:HA3	1:A:22:HIS:HA	0.60	1.72	20	8
1:A:15:GLU:HG3	1:A:16:ARG:HG3	0.59	1.71	9	2
1:A:7:VAL:HB	1:A:74:GLN:HE22	0.59	1.58	9	3
1:A:54:VAL:HG12	1:A:73:PRO:HA	0.57	1.75	7	3
1:A:5:ARG:HG2	1:A:57:SER:HB3	0.57	1.76	4	2
1:A:69:VAL:HG23	1:A:70:THR:H	0.56	1.61	20	4
1:A:5:ARG:HD3	1:A:57:SER:OG	0.56	2.00	11	1
1:A:45:PRO:HD2	1:A:48:LEU:HD21	0.55	1.76	10	7
1:A:57:SER:C	1:A:69:VAL:HG22	0.55	2.22	11	4
1:A:46:GLN:NE2	1:A:46:GLN:H	0.55	2.00	13	10
1:A:59:ARG:HG3	1:A:69:VAL:HG21	0.55	1.79	14	3
1:A:11:GLN:HE21	1:A:21:ALA:HB2	0.55	1.62	18	4
1:A:46:GLN:H	1:A:46:GLN:NE2	0.54	2.01	7	1
1:A:21:ALA:HA	1:A:34:THR:HA	0.54	1.79	9	7
1:A:10:ILE:HD11	1:A:54:VAL:HG21	0.53	1.79	9	12
1:A:10:ILE:HD11	1:A:54:VAL:CG2	0.53	2.34	5	6
1:A:5:ARG:HA	1:A:57:SER:HA	0.52	1.82	16	1
1:A:7:VAL:HB	1:A:74:GLN:NE2	0.52	2.20	9	2
1:A:13:ILE:CD1	1:A:49:LYS:HA	0.51	2.33	6	4
1:A:24:ALA:O	1:A:26:PRO:HD3	0.51	2.06	16	2
1:A:48:LEU:HB3	1:A:54:VAL:HG11	0.51	1.83	1	3
1:A:7:VAL:O	1:A:23:GLU:HG3	0.50	2.06	9	1
1:A:49:LYS:HG3	1:A:52:ASP:OD2	0.50	2.06	5	1
1:A:10:ILE:HB	1:A:49:LYS:O	0.49	2.07	4	8
1:A:24:ALA:HA	1:A:32:ALA:N	0.49	2.23	10	8
1:A:13:ILE:HG12	1:A:18:LEU:HD13	0.49	1.85	20	1
1:A:13:ILE:CD1	1:A:49:LYS:HD3	0.49	2.38	13	2
1:A:14:GLY:H	1:A:18:LEU:HB3	0.48	1.67	11	3
1:A:14:GLY:HA3	1:A:17:SER:O	0.48	2.07	3	2
1:A:49:LYS:HG2	1:A:52:ASP:OD2	0.48	2.09	8	5
1:A:57:SER:HB3	1:A:69:VAL:CG2	0.47	2.39	12	1
1:A:69:VAL:HG23	1:A:70:THR:N	0.47	2.24	11	4
1:A:5:ARG:HD2	1:A:57:SER:HB3	0.47	1.86	5	2
1:A:9:ARG:HG3	1:A:53:ARG:HG3	0.47	1.87	2	1
1:A:46:GLN:CA	1:A:46:GLN:HE21	0.47	2.19	4	1
1:A:53:ARG:HG2	1:A:74:GLN:NE2	0.47	2.24	13	1
1:A:74:GLN:HG3	1:A:75:VAL:N	0.47	2.23	14	1
1:A:54:VAL:HA	1:A:74:GLN:H	0.46	1.69	19	1
1:A:74:GLN:CG	1:A:75:VAL:N	0.46	2.78	16	1
1:A:19:ILE:CG2	1:A:34:THR:HG22	0.45	2.41	16	2
1:A:48:LEU:HD22	1:A:71:VAL:HG13	0.45	1.88	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ILE:HD12	1:A:49:LYS:HD3	0.45	1.87	15	2
1:A:60:LEU:HD22	1:A:66:ALA:HA	0.45	1.87	14	1
1:A:59:ARG:HG3	1:A:69:VAL:CG2	0.44	2.42	14	1
1:A:18:LEU:CD2	1:A:44:LEU:HG	0.44	2.37	8	1
1:A:24:ALA:HA	1:A:32:ALA:H	0.44	1.71	8	1
1:A:54:VAL:CA	1:A:74:GLN:HG2	0.44	2.42	1	1
1:A:29:GLN:HE21	1:A:29:GLN:N	0.43	2.11	16	1
1:A:63:HIS:HB3	1:A:65:MET:HG3	0.43	1.91	2	1
1:A:4:HIS:HB3	1:A:27:SER:HB3	0.43	1.91	13	1
1:A:65:MET:HA	1:A:65:MET:CE	0.43	2.44	17	2
1:A:61:ASP:OD2	1:A:65:MET:HB2	0.43	2.14	16	1
1:A:17:SER:CB	1:A:38:ALA:HA	0.43	2.44	19	1
1:A:17:SER:OG	1:A:38:ALA:HA	0.43	2.14	19	1
1:A:54:VAL:HB	1:A:71:VAL:CG2	0.42	2.44	10	1
1:A:38:ALA:HB3	1:A:67:THR:HG23	0.42	1.90	11	2
1:A:57:SER:HB2	1:A:69:VAL:CG2	0.42	2.45	11	1
1:A:61:ASP:HB3	1:A:62:PRO:CD	0.42	2.44	15	4
1:A:61:ASP:CG	1:A:65:MET:HG2	0.42	2.34	4	1
1:A:5:ARG:HD3	1:A:57:SER:HB3	0.42	1.91	13	2
1:A:63:HIS:HB2	1:A:65:MET:HG3	0.42	1.91	13	1
1:A:74:GLN:HG2	1:A:75:VAL:N	0.42	2.30	16	1
1:A:54:VAL:C	1:A:74:GLN:HG2	0.41	2.36	12	1
1:A:15:GLU:HG2	1:A:16:ARG:HG3	0.41	1.92	14	1
1:A:24:ALA:O	1:A:25:ILE:HB	0.41	2.16	6	1
1:A:5:ARG:O	1:A:25:ILE:HG23	0.40	2.16	20	1
1:A:55:ALA:HB2	1:A:74:GLN:HG3	0.40	1.93	13	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	74/82 (90%)	66±2 (89±2%)	6±2 (8±2%)	2±1 (2±1%)	10	47
All	All	1480/1640 (90%)	1320 (89%)	123 (8%)	37 (2%)	10	47

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	32	ALA	14
1	A	25	ILE	12
1	A	23	GLU	9
1	A	75	VAL	2

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	55/59 (93%)	50±1 (90±3%)	5±1 (10±3%)	14	59
All	All	1100/1180 (93%)	995 (90%)	105 (10%)	14	59

All 17 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	46	GLN	20
1	A	18	LEU	19
1	A	48	LEU	17
1	A	16	ARG	11
1	A	67	THR	9
1	A	53	ARG	4
1	A	74	GLN	4
1	A	60	LEU	3
1	A	29	GLN	3
1	A	68	LEU	3
1	A	34	THR	3
1	A	49	LYS	2
1	A	15	GLU	2
1	A	70	THR	2
1	A	57	SER	1
1	A	23	GLU	1
1	A	75	VAL	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 carbohydrates 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 (i)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17266

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	969
Number of shifts mapped to atoms	969
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	81	0.30 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	72	-0.11 ± 0.25	None needed (< 0.5 ppm)
$^{13}C'$	73	0.45 ± 0.20	None needed (< 0.5 ppm)
^{15}N	73	0.23 ± 0.43	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 803 atoms were assigned a chemical shift out of a possible 874. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	349/356 (98%)	140/141 (99%)	142/148 (96%)	67/67 (100%)
Sidechain	398/455 (87%)	243/269 (90%)	147/166 (89%)	8/20 (40%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	56/63 (89%)	27/33 (82%)	22/23 (96%)	7/7 (100%)
Overall	803/874 (92%)	410/443 (93%)	311/337 (92%)	82/94 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 850 atoms were assigned a chemical shift out of a possible 952. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	380/394 (96%)	153/156 (98%)	154/164 (94%)	73/74 (99%)
Sidechain	414/495 (84%)	252/293 (86%)	153/180 (85%)	9/22 (41%)
Aromatic	56/63 (89%)	27/33 (82%)	22/23 (96%)	7/7 (100%)
Overall	850/952 (89%)	432/482 (90%)	329/367 (90%)	89/103 (86%)

7.1.4 Statistically unusual chemical shifts (i)

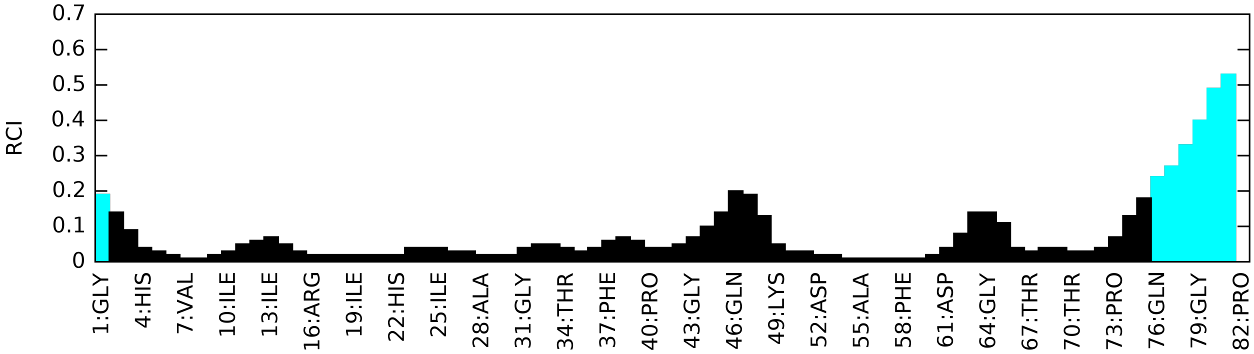
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	28	ALA	HB1	-0.19	2.61 – 0.11	-6.2
1	A	28	ALA	HB3	-0.19	2.61 – 0.11	-6.2
1	A	28	ALA	HB2	-0.19	2.61 – 0.11	-6.2
1	A	4	HIS	HB3	0.91	5.00 – 1.10	-5.5
1	A	22	HIS	NE2	257.57	255.67 – 109.17	5.1

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1:GLY
4:HIS
7:VAL
10:ILE
13:ILE
16:ARG
19:ILE
22:HIS
25:ILE
28:ALA
31:GLY
34:THR
37:PHE
40:PRO
43:GLY
46:GLN
49:LYS
52:ASP
55:ALA
58:PHE
61:ASP
64:GLY
67:THR
70:THR
73:PRO
76:GLN
79:GLY
82:PRO