Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 07:24 PM EDT

PDB ID	:	2KGT
BMRB ID	:	16219
Title	:	Solution structure of SH3 domain of PTK6
Authors	:	Lee, W.; Ko, S.
Deposited on	:	2009-03-18

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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

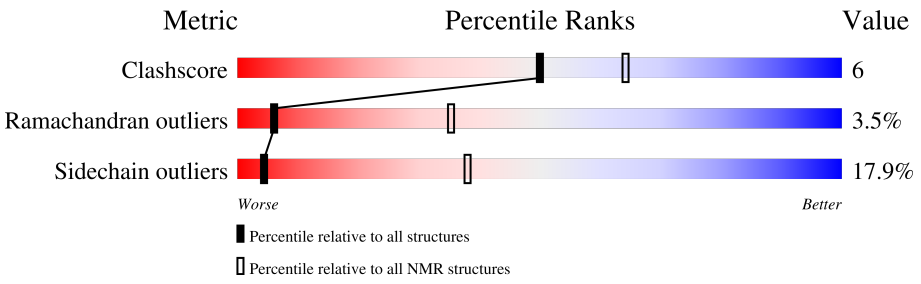
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 78%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	72	61% 21% 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:12-A:70 (59)	0.75	1

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1138 atoms, of which 548 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrosine-protein kinase 6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	72	1138	376	548	104	109	1	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Tyrosine-protein kinase 6

Chain A: 61% 21% 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 V14 G15 L16 W17 D18 R22 L27 S28 F29 R30 A31 G32 D33 V34 F35 L49 L50 Y66 L67 E71 T72

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 (medoid)

• Molecule 1: Tyrosine-protein kinase 6

Chain A: 61% 19% • 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 K12 G15 R22 T23 D24 L27 F35 W45 L49 L50 D51 E52 A53 V57 A58 L67 E71 T72

4.2.2 Score per residue for model 2

• Molecule 1: Tyrosine-protein kinase 6

Chain A: 58% 17% 7% 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 K12 Y13 V14 G15 L16 W17 D18 R22 T23 F29 R30 A31 G32 D33 V34 F35 K40 L49 L50 Y66 R70 E71 T72

4.2.3 Score per residue for model 3

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 58% 22% • 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 K12 Y13 V14 G15 L16 W17 D18 F19 K20 S21 L27 S28 F29 F35 K40 W45 L50 V57 G60 L67 E71 T72

4.2.4 Score per residue for model 4

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 60% 21% • 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 V14 G15 L16 W17 S21 R22 T23 D24 L27 R30 A31 G32 D33 K40 L50 Q59 Y66 L67 A68 E69 R70 E71 T72

4.2.5 Score per residue for model 5

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 58% 17% 7% 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 V14 G15 L16 W17 D18 S21 R22 T23 L27 S28 F29 R30 A31 G32 D33 R39 W45 L49 L50 V57 E71 T72

4.2.6 Score per residue for model 6

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 65% 15% • 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 G15 D18 S21 R22 F29 D33 V34 F35 L49 L50 L67 A68 E69 R70 E71 T72

4.2.7 Score per residue for model 7

- Molecule 1: Tyrosine-protein kinase 6

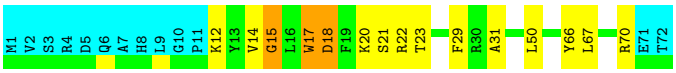
Chain A: 61% 18% • 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 V14 G15 L16 W17 D18 L27 S28 F29 D33 V34 F35 H36 V37 W46 L49 L50 V57 L67 A68 E69 R70 E71 T72

4.2.8 Score per residue for model 8

- Molecule 1: Tyrosine-protein kinase 6

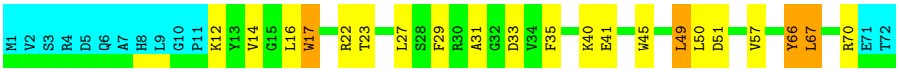
Chain A: 61% 17% • 18%



4.2.9 Score per residue for model 9

- Molecule 1: Tyrosine-protein kinase 6

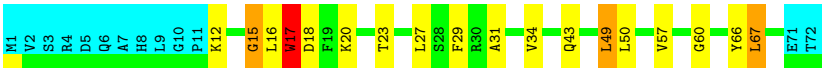
Chain A: 53% 24% 6% 18%



4.2.10 Score per residue for model 10

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 57% 19% • • 18%



4.2.11 Score per residue for model 11

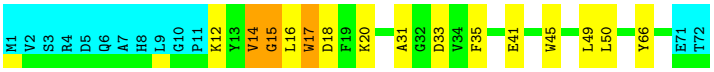
- Molecule 1: Tyrosine-protein kinase 6

Chain A: 67% 14% • 18%

4.2.12 Score per residue for model 12

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 61% 17% • 18%



4.2.13 Score per residue for model 13

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 65% 11% 6% 18%

4.2.14 Score per residue for model 14

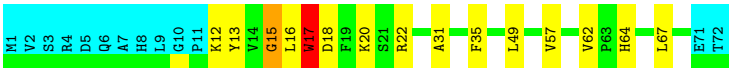
- Molecule 1: Tyrosine-protein kinase 6

Chain A: 64% 17% • 18%

4.2.15 Score per residue for model 15

- Molecule 1: Tyrosine-protein kinase 6

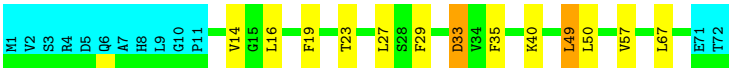
Chain A: 61% 18% •• 18%



4.2.16 Score per residue for model 16

- Molecule 1: Tyrosine-protein kinase 6

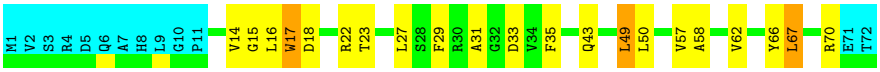
Chain A: 64% 15% • 18%



4.2.17 Score per residue for model 17

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 53% 25% • 18%



4.2.18 Score per residue for model 18

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 67% 8% 7% 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 K12 Y13 V14 G15 L16 W17 D18 A31 G32 D33 V34 F35 K40 Y66 L67 E71 T72

4.2.19 Score per residue for model 19

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 49% 31% • 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 K12 Y13 V14 G15 L16 W17 D18 F19 K20 S21 R22 T23 D24 E25 E26 L27 A31 F35 E41 W45 T48 L49 L50 A58 Q59 G60 Y61 V62 N65 Y66 L67 A68 E69 R70 E71 T72

4.2.20 Score per residue for model 20

- Molecule 1: Tyrosine-protein kinase 6

Chain A: 67% 11% • 18%

M1 V2 S3 R4 D5 Q6 A7 H8 L9 G10 P11 K12 Y13 V14 D18 R22 F29 D33 V34 F35 L49 L50 A56 Y66 E71 T72

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	**Classification**	**Version**
CYANA	structure solution	2.2.5
CYANA	refinement	2.2.5

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	768
Number of shifts mapped to atoms	768
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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	491	454	454	6±2
All	All	9820	9080	9080	114

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD12	1:A:49:LEU:HD23	0.83	1.50	17	1
1:A:27:LEU:HD22	1:A:49:LEU:HD23	0.66	1.67	5	2
1:A:67:LEU:C	1:A:67:LEU:HD22	0.66	2.11	18	1
1:A:49:LEU:HB2	1:A:58:ALA:HB3	0.65	1.68	1	2
1:A:27:LEU:CD2	1:A:49:LEU:HD23	0.63	2.23	16	3
1:A:14:VAL:HG23	1:A:33:ASP:O	0.63	1.94	2	8
1:A:35:PHE:CE1	1:A:67:LEU:HD22	0.62	2.30	7	1
1:A:35:PHE:CE2	1:A:49:LEU:HD13	0.60	2.32	6	2
1:A:15:GLY:O	1:A:16:LEU:HD22	0.60	1.97	12	3
1:A:15:GLY:HA3	1:A:67:LEU:HD22	0.59	1.73	14	1
1:A:17:TRP:HA	1:A:31:ALA:HB2	0.58	1.75	11	13
1:A:27:LEU:CD1	1:A:49:LEU:HD23	0.58	2.26	17	1
1:A:49:LEU:CB	1:A:58:ALA:HB3	0.58	2.29	1	1
1:A:15:GLY:O	1:A:16:LEU:HD12	0.57	1.99	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD21	1:A:60:GLY:O	0.56	2.01	3	3
1:A:16:LEU:HD13	1:A:35:PHE:CZ	0.55	2.37	15	1
1:A:15:GLY:C	1:A:67:LEU:HD22	0.54	2.22	10	1
1:A:35:PHE:CE2	1:A:67:LEU:HD22	0.54	2.38	1	2
1:A:16:LEU:HD23	1:A:35:PHE:CE2	0.54	2.38	17	1
1:A:62:VAL:HG11	1:A:67:LEU:CD1	0.53	2.33	17	1
1:A:16:LEU:HD23	1:A:67:LEU:HG	0.53	1.78	4	1
1:A:13:TYR:HB3	1:A:67:LEU:HD13	0.52	1.82	3	2
1:A:15:GLY:C	1:A:16:LEU:HD22	0.52	2.24	2	3
1:A:29:PHE:CD1	1:A:49:LEU:HD21	0.52	2.38	2	3
1:A:16:LEU:HD21	1:A:27:LEU:HB2	0.52	1.80	7	1
1:A:16:LEU:HD23	1:A:35:PHE:CE1	0.52	2.40	2	1
1:A:16:LEU:HD23	1:A:29:PHE:CE1	0.51	2.40	16	1
1:A:29:PHE:HB2	1:A:49:LEU:HD11	0.51	1.81	10	2
1:A:16:LEU:HD13	1:A:66:TYR:CD1	0.51	2.40	12	2
1:A:35:PHE:CZ	1:A:67:LEU:HD21	0.51	2.40	9	1
1:A:27:LEU:HD22	1:A:49:LEU:HD12	0.50	1.83	11	1
1:A:35:PHE:HB3	1:A:49:LEU:HD22	0.49	1.84	16	2
1:A:16:LEU:HD21	1:A:27:LEU:HD13	0.48	1.85	16	2
1:A:14:VAL:HG12	1:A:70:ARG:CG	0.48	2.38	9	4
1:A:67:LEU:HD13	1:A:68:ALA:N	0.48	2.23	19	2
1:A:14:VAL:HG12	1:A:70:ARG:HG3	0.48	1.85	9	4
1:A:62:VAL:HG11	1:A:67:LEU:HD12	0.48	1.85	17	1
1:A:13:TYR:HB3	1:A:67:LEU:HD11	0.48	1.86	19	1
1:A:16:LEU:HD13	1:A:66:TYR:CE1	0.47	2.44	12	1
1:A:29:PHE:CD2	1:A:49:LEU:HD11	0.47	2.43	16	1
1:A:12:LYS:NZ	1:A:34:VAL:HG21	0.47	2.25	10	1
1:A:16:LEU:HD22	1:A:29:PHE:CZ	0.46	2.45	9	1
1:A:15:GLY:C	1:A:67:LEU:HD12	0.46	2.30	8	1
1:A:33:ASP:CG	1:A:49:LEU:HD11	0.46	2.31	9	1
1:A:62:VAL:HG23	1:A:67:LEU:HD23	0.46	1.86	15	1
1:A:48:THR:HG23	1:A:58:ALA:O	0.45	2.12	19	1
1:A:27:LEU:HD22	1:A:35:PHE:CE2	0.45	2.47	19	1
1:A:49:LEU:HD12	1:A:50:LEU:N	0.44	2.27	20	1
1:A:22:ARG:HD2	1:A:23:THR:HG23	0.43	1.89	17	1
1:A:27:LEU:HD11	1:A:60:GLY:O	0.43	2.13	19	1
1:A:62:VAL:CG2	1:A:67:LEU:HD23	0.43	2.43	15	1
1:A:27:LEU:HG	1:A:49:LEU:HD23	0.43	1.90	7	1
1:A:67:LEU:C	1:A:67:LEU:CD2	0.43	2.83	18	1
1:A:27:LEU:HD23	1:A:49:LEU:HD23	0.42	1.90	1	1
1:A:67:LEU:O	1:A:67:LEU:HD12	0.42	2.13	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PHE:HE1	1:A:49:LEU:HD13	0.42	1.73	20	1
1:A:37:VAL:HG13	1:A:46:TRP:O	0.42	2.14	7	1
1:A:16:LEU:HD12	1:A:66:TYR:CD1	0.41	2.50	9	1
1:A:14:VAL:HG22	1:A:33:ASP:O	0.41	2.15	16	2
1:A:51:ASP:OD1	1:A:53:ALA:HB3	0.41	2.16	1	1
1:A:16:LEU:HD23	1:A:29:PHE:CZ	0.41	2.51	3	1
1:A:27:LEU:HD12	1:A:49:LEU:HB2	0.41	1.92	10	1
1:A:15:GLY:C	1:A:16:LEU:HD12	0.41	2.36	5	1
1:A:16:LEU:HD23	1:A:29:PHE:HE1	0.40	1.75	16	1
1:A:16:LEU:O	1:A:31:ALA:HB2	0.40	2.16	17	1
1:A:16:LEU:HD21	1:A:62:VAL:HG11	0.40	1.93	19	1
1:A:16:LEU:CD2	1:A:67:LEU:HD23	0.40	2.47	19	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	59/72 (82%)	51±2 (87±3%)	6±2 (10±4%)	2±1 (3±2%)	6	35
All	All	1180/1440 (82%)	1021 (87%)	118 (10%)	41 (3%)	6	35

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	15	GLY	12
1	A	18	ASP	10
1	A	17	TRP	9
1	A	57	VAL	8
1	A	16	LEU	1
1	A	56	ALA	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	47/58 (81%)	39±2 (82±4%)	8±2 (18±4%)	4 38
All	All	940/1160 (81%)	772 (82%)	168 (18%)	4 38

All 34 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	50	LEU	18
1	A	66	TYR	11
1	A	22	ARG	10
1	A	49	LEU	10
1	A	12	LYS	9
1	A	23	THR	9
1	A	29	PHE	9
1	A	33	ASP	9
1	A	67	LEU	9
1	A	45	TRP	7
1	A	18	ASP	7
1	A	21	SER	7
1	A	40	LYS	6
1	A	20	LYS	5
1	A	17	TRP	4
1	A	19	PHE	4
1	A	16	LEU	3
1	A	27	LEU	3
1	A	69	GLU	3
1	A	70	ARG	3
1	A	41	GLU	3
1	A	24	ASP	2
1	A	57	VAL	2
1	A	59	GLN	2
1	A	43	GLN	2
1	A	14	VAL	2
1	A	35	PHE	2
1	A	28	SER	1
1	A	30	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	39	ARG	1
1	A	51	ASP	1
1	A	64	HIS	1
1	A	25	GLU	1
1	A	65	ASN	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 (i)

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 78% 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 (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	768
Number of shifts mapped to atoms	768
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	72	-0.20 ± 0.25	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	65	-0.35 ± 0.26	None needed (< 0.5 ppm)
$^{13}C'$	68	0.15 ± 0.09	None needed (< 0.5 ppm)
^{15}N	68	0.41 ± 0.44	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 78%, i.e. 639 atoms were assigned a chemical shift out of a possible 819. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	294/298 (99%)	121/122 (99%)	116/118 (98%)	57/58 (98%)
Sidechain	317/402 (79%)	222/259 (86%)	95/125 (76%)	0/18 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	28/119 (24%)	24/59 (41%)	0/54 (0%)	4/6 (67%)
Overall	639/819 (78%)	367/440 (83%)	211/297 (71%)	61/82 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 768 atoms were assigned a chemical shift out of a possible 987. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	354/362 (98%)	146/148 (99%)	140/144 (97%)	68/70 (97%)
Sidechain	386/499 (77%)	270/322 (84%)	116/155 (75%)	0/22 (0%)
Aromatic	28/126 (22%)	24/63 (38%)	0/56 (0%)	4/7 (57%)
Overall	768/987 (78%)	440/533 (83%)	256/355 (72%)	72/99 (73%)

7.1.4 Statistically unusual chemical shifts (i)

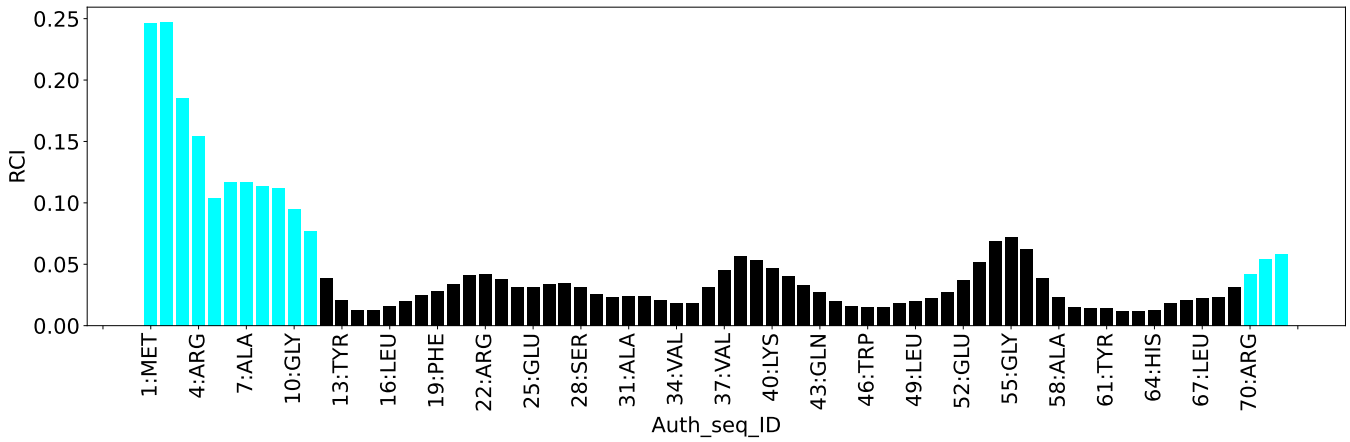
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	64	HIS	HA	2.32	2.49 – 6.71	-5.4
1	A	16	LEU	HB3	-0.37	-0.26 – 3.31	-5.3

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
4:ARG
7:ALA
10:GLY
13:TYR
16:LEU
19:PHE
22:ARG
25:GLU
28:SER
31:ALA
34:VAL
37:VAL
40:LYS
43:GLN
46:TRP
49:LEU
52:GLU
55:GLY
58:ALA
61:TYR
64:HIS
67:LEU
70:ARG
Auth_seq_ID

8 NMR restraints analysis (i)

No restraints data found

9 Distance violation analysis (i)

No distance restraints data found

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value