



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6FW4 / pdb_00006fw4
BMRB ID : 25689
Title : Protein-protein interactions and conformational changes : Importance of the hydrophobic cavity of TolA C-terminal domain
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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

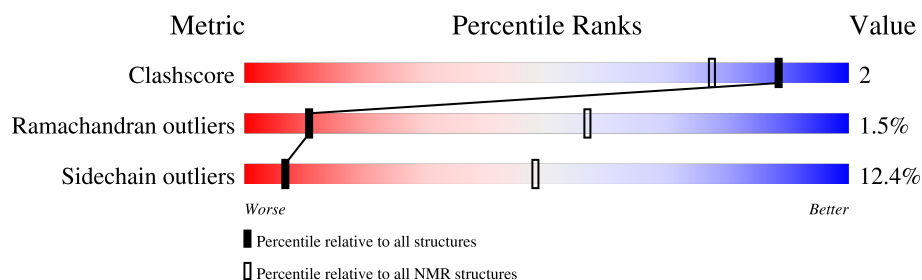
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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	101	 75% 10% • 14%

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:34-A:120 (87)	0.53	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 5 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1578 atoms, of which 806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TolA protein.

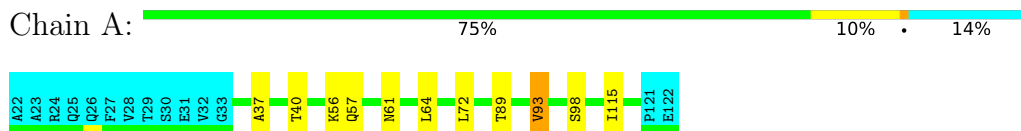
Mol	Chain	Residues	Atoms						Trace
1	A	101	Total	C	H	N	O	S	0
			1578	485	806	140	145	2	

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.

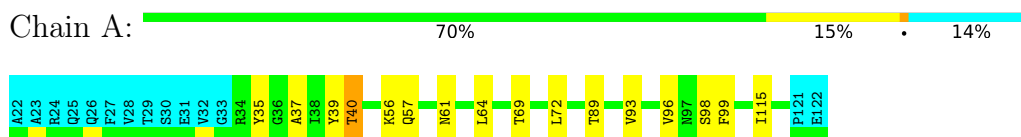
- Molecule 1: TolA protein



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 19. Colouring as in section 4.1 above.

- Molecule 1: TolA protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, molecular dynamics*.

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
Amber	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	1303
Number of shifts mapped to atoms	1182
Number of unparsed shifts	0
Number of shifts with mapping errors	121
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	0.76±0.01	0±0/674 (0.0± 0.0%)	1.36±0.02	1±1/915 (0.2± 0.1%)
All	All	0.76	0/13480 (0.0%)	1.36	28/18300 (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	0.9±0.8
All	All	0	18

There are no bond-length outliers.

5 of 8 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	34	ARG	CA-C-N	5.79	128.03	120.28	10	9
1	A	34	ARG	C-N-CA	5.79	128.03	120.28	10	9
1	A	100	PRO	N-CA-CB	5.53	106.02	102.92	17	1
1	A	120	ALA	N-CA-C	5.49	112.96	108.07	8	1
1	A	44	ARG	NE-CZ-NH2	5.37	124.04	119.20	5	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	35	TYR	Sidechain	8
1	A	39	TYR	Sidechain	7
1	A	82	ASP	Peptide	3

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	666	706	706	3±1
All	All	13320	14120	14120	51

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 2.

5 of 6 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:VAL:HG21	1:A:99:PHE:CZ	0.62	2.29	1	10
1:A:89:THR:O	1:A:93:VAL:HG23	0.61	1.94	10	20
1:A:101:LEU:H	1:A:101:LEU:HD23	0.53	1.64	17	2
1:A:37:ALA:HA	1:A:40:THR:HG22	0.47	1.86	8	16
1:A:101:LEU:H	1:A:101:LEU:HD22	0.44	1.73	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	87/101 (86%)	80±2 (92±2%)	5±2 (6±2%)	1±1 (1±1%)	11	57
All	All	1740/2020 (86%)	1605 (92%)	109 (6%)	26 (1%)	11	57

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	98	SER	20
1	A	120	ALA	4
1	A	83	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	102	PRO	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	74/85 (87%)	65±1 (88±2%)	9±1 (12±2%)	7	48
All	All	1480/1700 (87%)	1296 (88%)	184 (12%)	7	48

5 of 20 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	57	GLN	20
1	A	64	LEU	20
1	A	72	LEU	20
1	A	115	ILE	20
1	A	56	LYS	19

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](#)

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: *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	1303
Number of shifts mapped to atoms	1182
Number of unparsed shifts	0
Number of shifts with mapping errors	121
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 121) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	ALA	H	8.221	0.020	1
1	A	1	ALA	HA	4.094	0.020	1
1	A	1	ALA	HB1	1.243	0.020	1
1	A	1	ALA	HB2	1.243	0.020	1
1	A	1	ALA	HB3	1.243	0.020	1
1	A	1	ALA	C	178.703	0.3	1
1	A	1	ALA	CA	52.535	0.3	1
1	A	1	ALA	CB	18.396	0.3	1
1	A	1	ALA	N	128.788	0.3	1
1	A	2	GLU	H	8.447	0.020	1
1	A	2	GLU	HA	3.995	0.020	1
1	A	2	GLU	HB2	1.593	0.020	1
1	A	2	GLU	HB3	1.593	0.020	1
1	A	2	GLU	HG2	1.866	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	GLU	HG3	1.983	0.020	2
1	A	2	GLU	C	176.644	0.3	1
1	A	2	GLU	CA	56.649	0.3	1
1	A	2	GLU	CB	29.102	0.3	1
1	A	2	GLU	CG	35.481	0.3	1
1	A	2	GLU	N	119.356	0.3	1
1	A	3	PHE	H	7.959	0.020	1
1	A	3	PHE	HA	4.435	0.020	1
1	A	3	PHE	HB2	3.03	0.020	2
1	A	3	PHE	HB3	2.886	0.020	2
1	A	3	PHE	HD1	7.02	0.020	1
1	A	3	PHE	HD2	7.02	0.020	1
1	A	3	PHE	HE1	7.137	0.020	1
1	A	3	PHE	HE2	7.137	0.020	1
1	A	3	PHE	C	175.831	0.3	1
1	A	3	PHE	CA	57.28	0.3	1
1	A	3	PHE	CB	38.622	0.3	1
1	A	3	PHE	CD1	131.987	0.3	1
1	A	3	PHE	CD2	131.987	0.3	1
1	A	3	PHE	CE1	131.327	0.3	1
1	A	3	PHE	CE2	131.327	0.3	1
1	A	3	PHE	N	120.515	0.3	1
1	A	6	LEU	H	7.924	0.020	1
1	A	6	LEU	HA	4.118	0.020	1
1	A	6	LEU	HB2	1.527	0.020	2
1	A	6	LEU	HB3	1.408	0.020	2
1	A	6	LEU	HG	1.261	0.020	1
1	A	6	LEU	HD11	0.777	0.020	2
1	A	6	LEU	HD12	0.777	0.020	2
1	A	6	LEU	HD13	0.777	0.020	2
1	A	6	LEU	HD21	0.702	0.020	2
1	A	6	LEU	HD22	0.702	0.020	2
1	A	6	LEU	HD23	0.702	0.020	2
1	A	6	LEU	C	177.24	0.3	1
1	A	6	LEU	CA	54.988	0.3	1
1	A	6	LEU	CB	41.568	0.3	1
1	A	6	LEU	CG	26.118	0.3	1
1	A	6	LEU	CD1	22.711	0.3	1
1	A	6	LEU	CD2	24.415	0.3	1
1	A	6	LEU	N	120.587	0.3	1
1	A	7	ASN	H	8.094	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ASN	HA	4.528	0.020	1
1	A	7	ASN	HB2	2.637	0.020	2
1	A	7	ASN	HB3	2.519	0.020	2
1	A	7	ASN	HD21	7.267	0.020	1
1	A	7	ASN	HD22	6.423	0.020	1
1	A	7	ASN	C	174.801	0.3	1
1	A	7	ASN	CA	52.807	0.3	1
1	A	7	ASN	CB	38.503	0.3	1
1	A	7	ASN	N	118.479	0.3	1
1	A	7	ASN	ND2	111.427	0.3	1
1	A	8	ASP	H	8.112	0.020	1
1	A	8	ASP	HA	4.447	0.020	1
1	A	8	ASP	HB2	2.519	0.020	2
1	A	8	ASP	HB3	2.472	0.020	2
1	A	8	ASP	C	176.373	0.3	1
1	A	8	ASP	CA	53.679	0.3	1
1	A	8	ASP	CB	40.423	0.3	1
1	A	8	ASP	N	120.817	0.3	1
1	A	9	ILE	H	7.788	0.020	1
1	A	9	ILE	HA	3.905	0.020	1
1	A	9	ILE	HB	1.588	0.020	1
1	A	9	ILE	HG12	1.01	0.020	2
1	A	9	ILE	HG13	0.877	0.020	2
1	A	9	ILE	HG21	0.826	0.020	1
1	A	9	ILE	HG22	0.826	0.020	1
1	A	9	ILE	HG23	0.826	0.020	1
1	A	9	ILE	HD11	0.594	0.020	1
1	A	9	ILE	HD12	0.594	0.020	1
1	A	9	ILE	HD13	0.594	0.020	1
1	A	9	ILE	C	176.373	0.3	1
1	A	9	ILE	CA	61.208	0.3	1
1	A	9	ILE	CB	37.722	0.3	1
1	A	9	ILE	CG1	26.271	0.3	1
1	A	9	ILE	CG2	16.685	0.3	1
1	A	9	ILE	CD1	12.547	0.3	1
1	A	9	ILE	N	120.073	0.3	1
1	A	10	PHE	HZ	7.115	0.020	1
1	A	10	PHE	CZ	130.376	0.3	1
1	A	11	GLY	H	8.118	0.020	1
1	A	11	GLY	HA2	3.804	0.020	1
1	A	11	GLY	HA3	3.804	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	GLY	C	174.178	0.3	1
1	A	11	GLY	CA	44.96	0.3	1
1	A	11	GLY	N	110.211	0.3	1
1	A	12	SER	H	8.1	0.020	1
1	A	12	SER	HA	4.336	0.020	1
1	A	12	SER	HB2	3.778	0.020	1
1	A	12	SER	HB3	3.778	0.020	1
1	A	12	SER	C	174.611	0.3	1
1	A	12	SER	CA	57.793	0.3	1
1	A	12	SER	CB	63.188	0.3	1
1	A	12	SER	N	115.85	0.3	1
1	A	18	GLN	H	8.219	0.020	1
1	A	18	GLN	HA	4.129	0.020	1
1	A	18	GLN	HB2	1.972	0.020	2
1	A	18	GLN	HB3	1.901	0.020	2
1	A	18	GLN	HG2	2.275	0.020	1
1	A	18	GLN	HG3	2.275	0.020	1
1	A	18	GLN	HE21	7.368	0.020	1
1	A	18	GLN	HE22	6.763	0.020	1
1	A	18	GLN	C	176.888	0.3	1
1	A	18	GLN	CA	56.362	0.3	1
1	A	18	GLN	CB	28.233	0.3	1
1	A	18	GLN	CG	33.095	0.3	1
1	A	18	GLN	N	121.877	0.3	1
1	A	18	GLN	NE2	112.763	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
$^{13}\text{C}_\alpha$	106	0.44 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	98	0.81 ± 0.10	Should be checked
$^{13}\text{C}'$	103	0.21 ± 0.16	None needed (< 0.5 ppm)
^{15}N	103	-0.48 ± 0.34	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1034 atoms were assigned a chemical shift out of a possible 1207. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	404/433 (93%)	162/176 (92%)	165/174 (95%)	77/83 (93%)
Sidechain	598/736 (81%)	425/480 (89%)	167/222 (75%)	6/34 (18%)
Aromatic	32/38 (84%)	18/18 (100%)	14/20 (70%)	0/0 (—%)
Overall	1034/1207 (86%)	605/674 (90%)	346/416 (83%)	83/117 (71%)

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	118	THR	CG2	27.28	16.06 – 27.03	5.2

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:

