



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1S62 / pdb_00001s62
Title : Solution structure of the Escherichia coli TolA C-terminal domain
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Deposited on : 2004-01-22

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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

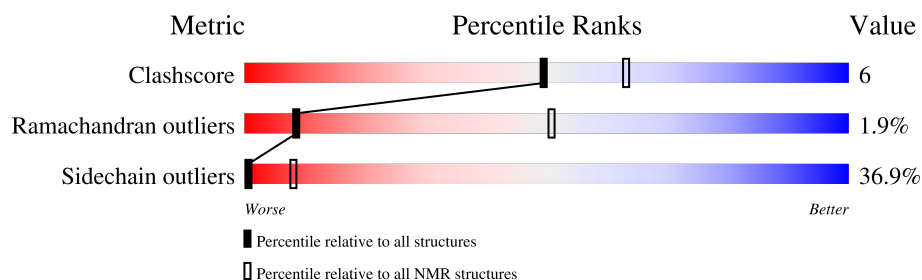
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	106	42% 31% 24% .

2 Ensemble composition and analysis

This entry contains 16 models. Model 3 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:16-A:31, A:40-A:100 (77)	1.01	3

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1516 atoms, of which 759 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TolA protein.

Mol	Chain	Residues	Atoms						Trace
1	A	102	Total	C	H	N	O	S	0
			1516	481	759	129	144	3	

There are 9 discrepancies between the modelled and reference sequences:

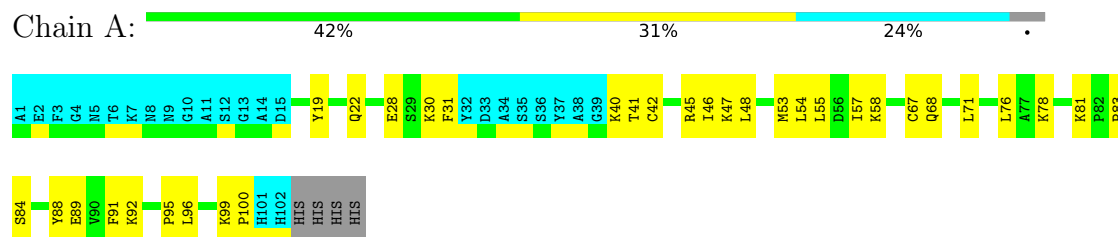
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	cloning artifact	UNP P19934
A	2	GLU	-	cloning artifact	UNP P19934
A	3	PHE	-	cloning artifact	UNP P19934
A	101	HIS	-	expression tag	UNP P19934
A	102	HIS	-	expression tag	UNP P19934
A	103	HIS	-	expression tag	UNP P19934
A	104	HIS	-	expression tag	UNP P19934
A	105	HIS	-	expression tag	UNP P19934
A	106	HIS	-	expression tag	UNP P19934

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

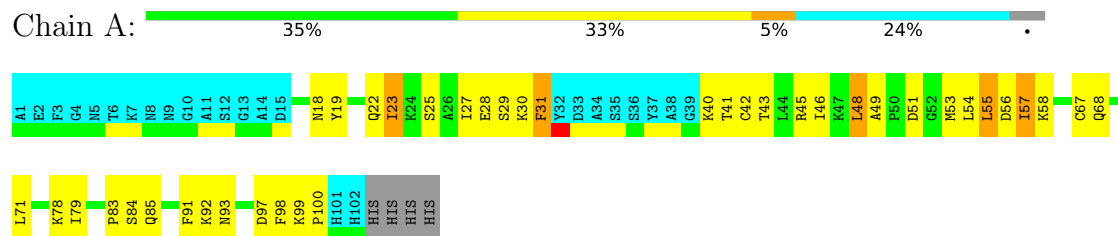


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: TolA protein



4.2.2 Score per residue for model 2

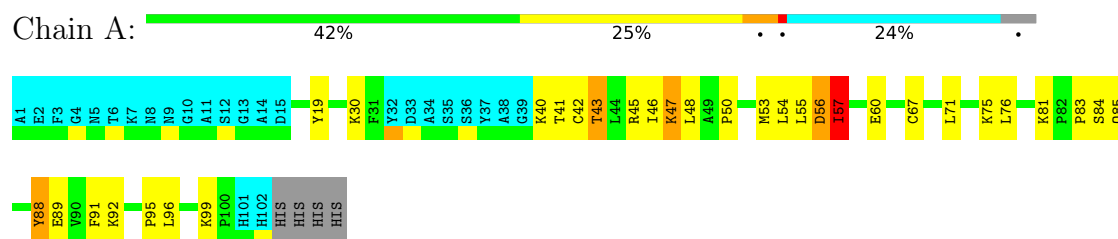
- Molecule 1: TolA protein





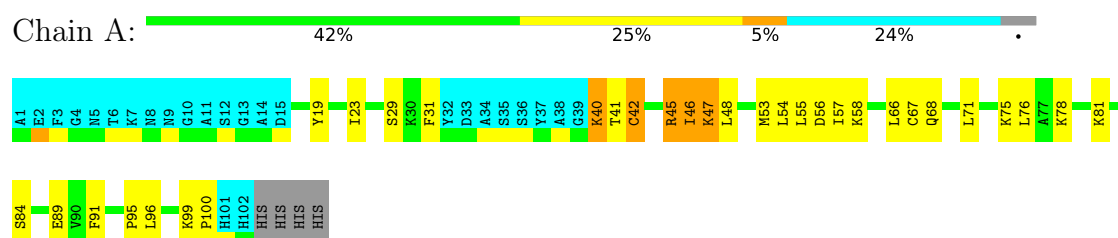
4.2.10 Score per residue for model 10

- Molecule 1: TolA protein



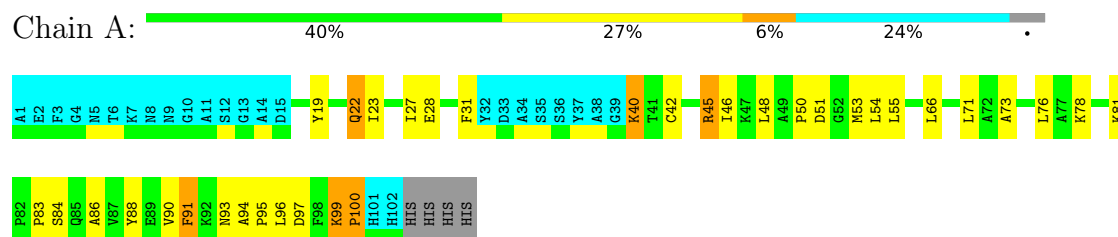
4.2.11 Score per residue for model 11

- Molecule 1: TolA protein



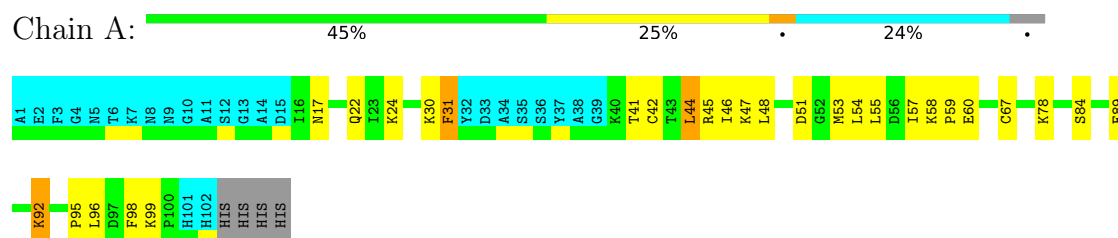
4.2.12 Score per residue for model 12

- Molecule 1: TolA protein



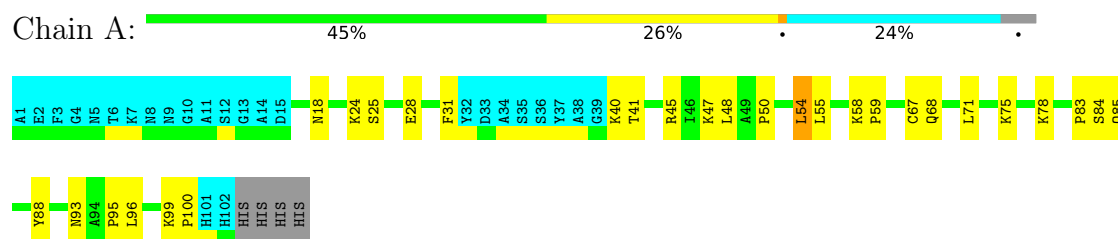
4.2.13 Score per residue for model 13

- Molecule 1: TolA protein



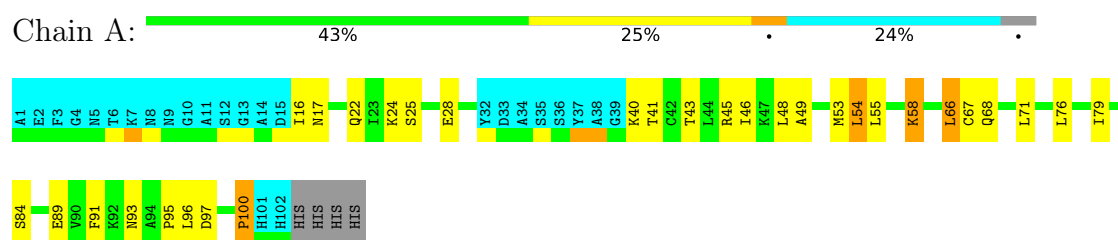
4.2.14 Score per residue for model 14

- Molecule 1: TolA protein



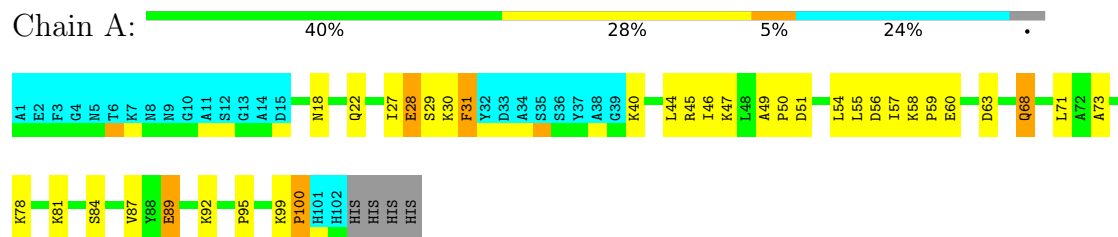
4.2.15 Score per residue for model 15

- Molecule 1: TolA protein



4.2.16 Score per residue for model 16

- Molecule 1: TolA protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *2 step simulated annealing torsion angle dynamics*.

Of the 1000 calculated structures, 16 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
ARIA	structure solution	1.0
TALOS	structure solution	
TALOS	refinement	

No chemical shift data was provided.

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	578	610	610	7±2
All	All	9248	9760	9760	108

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:45:ARG:HA	1:A:95:PRO:HB3	0.74	1.57	4	13
1:A:89:GLU:HA	1:A:92:LYS:HE3	0.72	1.61	16	4
1:A:48:LEU:HD23	1:A:91:PHE:HD2	0.68	1.47	12	1
1:A:43:THR:HA	1:A:97:ASP:HA	0.66	1.66	15	2
1:A:41:THR:HG23	1:A:99:LYS:HG3	0.59	1.74	4	1
1:A:67:CYS:O	1:A:71:LEU:HG	0.58	1.98	11	9
1:A:50:PRO:HA	1:A:91:PHE:HZ	0.58	1.59	12	2
1:A:50:PRO:HA	1:A:91:PHE:CZ	0.57	2.35	12	1
1:A:40:LYS:HB3	1:A:66:LEU:HD22	0.56	1.76	11	2
1:A:30:LYS:HG2	1:A:76:LEU:HB3	0.56	1.78	8	1
1:A:59:PRO:HB3	1:A:67:CYS:HB3	0.56	1.78	2	3
1:A:59:PRO:HB3	1:A:67:CYS:SG	0.54	2.42	8	3
1:A:68:GLN:HA	1:A:71:LEU:HD12	0.54	1.79	3	2
1:A:45:ARG:O	1:A:57:ILE:HA	0.54	2.02	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ALA:HB3	1:A:53:MET:HG3	0.54	1.78	15	1
1:A:45:ARG:HG3	1:A:45:ARG:O	0.53	2.04	12	1
1:A:43:THR:HB	1:A:60:GLU:HB2	0.53	1.81	10	1
1:A:30:LYS:HD2	1:A:76:LEU:HB2	0.52	1.80	5	1
1:A:99:LYS:HB2	1:A:100:PRO:HD2	0.51	1.80	1	3
1:A:42:CYS:HB3	1:A:98:PHE:O	0.51	2.06	1	1
1:A:42:CYS:HB3	1:A:98:PHE:HB3	0.51	1.81	2	1
1:A:47:LYS:HG3	1:A:92:LYS:O	0.51	2.06	16	1
1:A:48:LEU:HG	1:A:54:LEU:HD23	0.51	1.82	14	1
1:A:40:LYS:HB2	1:A:66:LEU:HD23	0.50	1.82	15	1
1:A:48:LEU:O	1:A:92:LYS:HA	0.50	2.07	2	2
1:A:42:CYS:HA	1:A:62:GLY:HA3	0.50	1.84	2	2
1:A:49:ALA:HB1	1:A:50:PRO:HD2	0.49	1.81	6	3
1:A:99:LYS:HG2	1:A:100:PRO:HD2	0.49	1.84	5	1
1:A:82:PRO:HG3	1:A:91:PHE:CZ	0.49	2.43	9	1
1:A:66:LEU:HD11	1:A:100:PRO:HD3	0.48	1.85	8	1
1:A:23:ILE:HG12	1:A:79:ILE:HD12	0.48	1.85	3	1
1:A:50:PRO:HG3	1:A:88:TYR:HE1	0.47	1.68	14	1
1:A:86:ALA:O	1:A:90:VAL:HG23	0.47	2.09	12	1
1:A:25:SER:HA	1:A:28:GLU:OE1	0.47	2.10	4	1
1:A:27:ILE:HG23	1:A:73:ALA:HB1	0.47	1.86	6	1
1:A:59:PRO:HG3	1:A:71:LEU:HD21	0.46	1.87	14	1
1:A:44:LEU:HD11	1:A:98:PHE:HB2	0.46	1.86	13	1
1:A:93:ASN:O	1:A:95:PRO:HD3	0.46	2.11	7	2
1:A:54:LEU:HD12	1:A:75:LYS:HG2	0.45	1.86	14	1
1:A:99:LYS:CG	1:A:100:PRO:HD2	0.45	2.41	5	1
1:A:26:ALA:HB1	1:A:77:ALA:HB1	0.45	1.88	5	1
1:A:40:LYS:O	1:A:100:PRO:HD2	0.45	2.11	6	1
1:A:27:ILE:HG23	1:A:73:ALA:HB3	0.45	1.89	12	2
1:A:47:LYS:HB3	1:A:56:ASP:HB3	0.44	1.89	16	1
1:A:59:PRO:HD3	1:A:71:LEU:HD11	0.44	1.88	16	1
1:A:19:TYR:CE2	1:A:23:ILE:HD11	0.44	2.47	7	1
1:A:90:VAL:HG12	1:A:94:ALA:HB3	0.44	1.89	12	1
1:A:28:GLU:C	1:A:30:LYS:H	0.44	2.21	3	1
1:A:88:TYR:HA	1:A:91:PHE:CE1	0.44	2.47	12	1
1:A:50:PRO:HG3	1:A:88:TYR:HB2	0.44	1.89	10	1
1:A:46:ILE:HD11	1:A:96:LEU:HB2	0.44	1.88	11	1
1:A:54:LEU:HD21	1:A:79:ILE:HD13	0.43	1.89	15	1
1:A:23:ILE:O	1:A:27:ILE:HG13	0.43	2.13	1	1
1:A:45:ARG:HB3	1:A:58:LYS:HD2	0.43	1.90	15	1
1:A:49:ALA:HB2	1:A:55:LEU:HD21	0.43	1.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LYS:HG2	1:A:82:PRO:HD2	0.43	1.90	9	1
1:A:47:LYS:HB3	1:A:47:LYS:HE2	0.43	1.57	2	1
1:A:22:GLN:HG3	1:A:23:ILE:N	0.43	2.28	12	1
1:A:48:LEU:HB2	1:A:91:PHE:O	0.42	2.14	5	2
1:A:42:CYS:HB2	1:A:66:LEU:HD23	0.42	1.92	11	1
1:A:45:ARG:HG3	1:A:60:GLU:HB2	0.42	1.91	2	1
1:A:81:LYS:H	1:A:81:LYS:HG3	0.42	1.35	7	1
1:A:47:LYS:HB2	1:A:56:ASP:HB3	0.41	1.92	10	3
1:A:45:ARG:HB2	1:A:60:GLU:HG3	0.41	1.92	10	1
1:A:88:TYR:HA	1:A:91:PHE:CZ	0.40	2.51	7	1
1:A:88:TYR:O	1:A:92:LYS:HD2	0.40	2.16	5	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	77/106 (73%)	71±2 (92±2%)	5±2 (6±2%)	2±1 (2±1%)	8	51
All	All	1232/1696 (73%)	1133 (92%)	75 (6%)	24 (2%)	8	51

All 5 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	83	PRO	9
1	A	100	PRO	7
1	A	57	ILE	4
1	A	82	PRO	2
1	A	93	ASN	2

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	61/81 (75%)	38±3 (63±5%)	22±3 (37±5%)	1 8
All	All	976/1296 (75%)	616 (63%)	360 (37%)	1 8

All 51 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	54	LEU	16
1	A	55	LEU	16
1	A	84	SER	15
1	A	41	THR	13
1	A	46	ILE	13
1	A	58	LYS	12
1	A	76	LEU	12
1	A	99	LYS	12
1	A	28	GLU	11
1	A	30	LYS	11
1	A	96	LEU	11
1	A	40	LYS	10
1	A	53	MET	10
1	A	78	LYS	10
1	A	81	LYS	10
1	A	22	GLN	9
1	A	42	CYS	9
1	A	19	TYR	8
1	A	48	LEU	8
1	A	68	GLN	8
1	A	47	LYS	7
1	A	75	LYS	7
1	A	25	SER	6
1	A	29	SER	6
1	A	57	ILE	6
1	A	91	PHE	6
1	A	89	GLU	6
1	A	24	LYS	6
1	A	31	PHE	5
1	A	43	THR	5
1	A	45	ARG	5
1	A	51	ASP	5
1	A	85	GLN	5
1	A	16	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	87	VAL	5
1	A	88	TYR	5
1	A	17	ASN	5
1	A	44	LEU	5
1	A	92	LYS	5
1	A	60	GLU	4
1	A	18	ASN	3
1	A	56	ASP	3
1	A	93	ASN	3
1	A	97	ASP	3
1	A	71	LEU	3
1	A	66	LEU	3
1	A	23	ILE	2
1	A	79	ILE	2
1	A	27	ILE	2
1	A	63	ASP	2
1	A	98	PHE	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](#)

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided