



# wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 34773  
Title : Solution Structure of thanatin-like derivative 5 in complex with E. coli LptA mutant Q62L  
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Deposited on : 2022-11-26

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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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

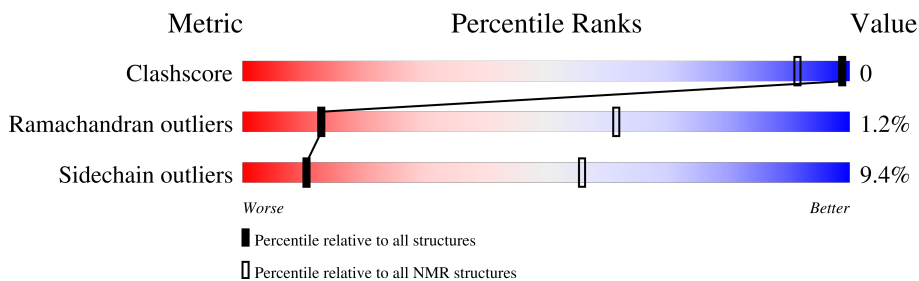
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 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	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  $\geq 3$ , 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	132	
2	B	16	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:76, A:84-A:143, B:208-B:210, B:212-B:213, B:215-B:215, B:217-B:218, B:221-B:221 (112)	1.24	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 3 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2304 atoms, of which 1153 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipopolysaccharide export system protein LptA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	132	2027	636	1009	174	204	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LEU	GLN	engineered mutation	UNP P0ADV1

- Molecule 2 is a protein called Thanatin-like derivative.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	16	277	84	144	25	22	2	0

There are 6 discrepancies between the modelled and reference sequences:

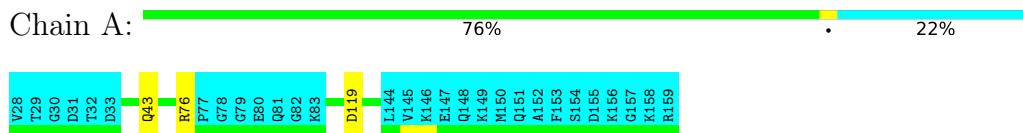
Chain	Residue	Modelled	Actual	Comment	Reference
B	211	LE1	CYS	modified residue	UNP P55788
B	214	DAB	ARG	modified residue	UNP P55788
B	216	4FO	GLY	modified residue	UNP P55788
B	219	DAB	GLN	modified residue	UNP P55788
B	220	DAB	ARG	modified residue	UNP P55788
B	221	TYR	MET	engineered mutation	UNP P55788

## 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: Lipopolysaccharide export system protein LptA



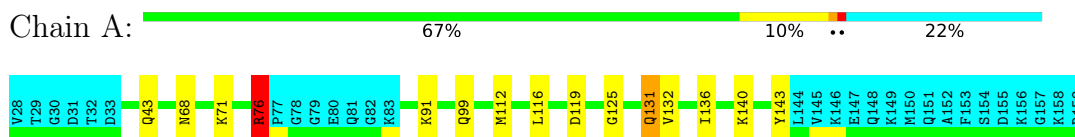
- Molecule 2: Thanatin-like derivative



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

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Lipopolysaccharide export system protein LptA



- Molecule 2: Thanatin-like derivative



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *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
CYANA	structure calculation	3.98
MOE	refinement	2020.09

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	1802
Number of shifts mapped to atoms	1802
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%

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: LE1, DAB, HYP, 4FO

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	0.83±0.02	0±0/814 ( 0.0± 0.0%)	1.42±0.04	2±2/1106 ( 0.2± 0.2%)
2	B	0.78±0.04	0±0/79 ( 0.0± 0.0%)	1.16±0.10	0±0/97 ( 0.1± 0.2%)
All	All	0.82	0/17860 ( 0.0%)	1.40	36/24060 ( 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	1.4±1.3
2	B	0.0±0.0	0.3±0.6
All	All	0	33

There are no bond-length outliers.

5 of 28 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	119	ASP	CA-CB-CG	7.99	120.59	112.60	2	2
1	A	100	ASP	CA-CB-CG	7.55	120.15	112.60	12	1
1	A	54	PHE	CA-CB-CG	7.54	121.34	113.80	2	1
1	A	90	GLY	CA-C-N	6.12	127.67	122.28	7	1
1	A	90	GLY	C-N-CA	6.12	127.67	122.28	7	1

There are no chirality outliers.

5 of 24 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	89	TYR	Sidechain	4
1	A	76	ARG	Sidechain	3
1	A	97	GLN	Peptide	2
1	A	143	TYR	Sidechain	2
2	B	221	TYR	Sidechain	2

## 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	800	788	788	0±0
2	B	82	83	83	0±0
All	All	17640	17420	17420	3

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:VAL:HG22	1:A:131:GLN:HE22	0.51	1.66	7	1
1:A:128:TYR:CE1	1:A:137:LYS:HE3	0.48	2.42	4	1
1:A:116:LEU:H	1:A:116:LEU:HD23	0.42	1.75	1	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	103/132 (78%)	93±3 (90±3%)	9±3 (8±3%)	1±1 (1±1%)	12	60
2	B	8/16 (50%)	7±1 (88±7%)	1±1 (12±7%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2220/2960 (75%)	2001 (90%)	192 (9%)	27 (1%)	13 61

5 of 10 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	119	ASP	5
1	A	132	VAL	5
1	A	125	GLY	4
1	A	133	ASP	3
1	A	57	ASN	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	89/112 (79%)	80±2 (90±2%)	9±2 (10±2%)	10 55
2	B	9/10 (90%)	8±1 (93±8%)	1±1 (7±8%)	17 65
All	All	1960/2440 (80%)	1775 (91%)	185 (9%)	10 56

5 of 61 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	71	LYS	9
1	A	43	GLN	7
1	A	45	LEU	7
1	A	68	ASN	7
1	A	118	LYS	7

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	LE1	B	211	2	3,7,8	0.65±0.05	0±0 (0±0%)
2	DAB	B	219	2	5,6,7	0.61±0.07	0±0 (0±0%)
2	DAB	B	214	2	5,6,7	0.59±0.06	0±0 (0±0%)
2	DAB	B	220	2	5,6,7	0.66±0.05	0±0 (0±0%)
2	4FO	B	216	2	5,6,7	0.62±0.09	0±0 (0±0%)
2	HYP	B	207	2	7,8,9	0.65±0.07	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	LE1	B	211	2	3,10,12	0.99±0.24	0±0 (0±0%)
2	DAB	B	219	2	1,6,8	0.18±0.16	0±0 (0±0%)
2	DAB	B	214	2	1,6,8	0.18±0.11	0±0 (0±0%)
2	DAB	B	220	2	1,6,8	0.39±0.45	0±0 (0±0%)
2	4FO	B	216	2	1,6,8	0.29±0.18	0±0 (0±0%)
2	HYP	B	207	2	5,10,12	1.12±0.23	0±1 (7±11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAB	B	219	2	-	0±0,4,5,7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAB	B	214	2	-	0±0,4,5,7	-
2	DAB	B	220	2	-	0±0,4,5,7	-
2	HYP	B	207	2	-	0±0,0,11,13	0±0,1,1,1
2	LE1	B	211	2	-	0±0,4,8,10	-
2	4FO	B	216	2	-	0±0,4,5,7	-

There are no bond-length outliers.

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
2	B	207	HYP	CG-CB-CA	2.73	106.92	103.75	10	6
2	B	207	HYP	CB-CG-CD	2.08	105.47	103.16	12	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 [i](#)

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

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: starch\_output

#### 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	1802
Number of shifts mapped to atoms	1802
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	132	$-0.08 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	118	$-0.32 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	129	$0.38 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	126	$-0.60 \pm 0.27$	Should be applied

#### 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. 1389 atoms were assigned a chemical shift out of a possible 1516. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	533/563 (95%)	230/230 (100%)	203/224 (91%)	100/109 (92%)
Sidechain	762/839 (91%)	535/545 (98%)	212/264 (80%)	15/30 (50%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	94/114 (82%)	52/55 (95%)	39/56 (70%)	3/3 (100%)
Overall	1389/1516 (92%)	817/830 (98%)	454/544 (83%)	118/142 (83%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

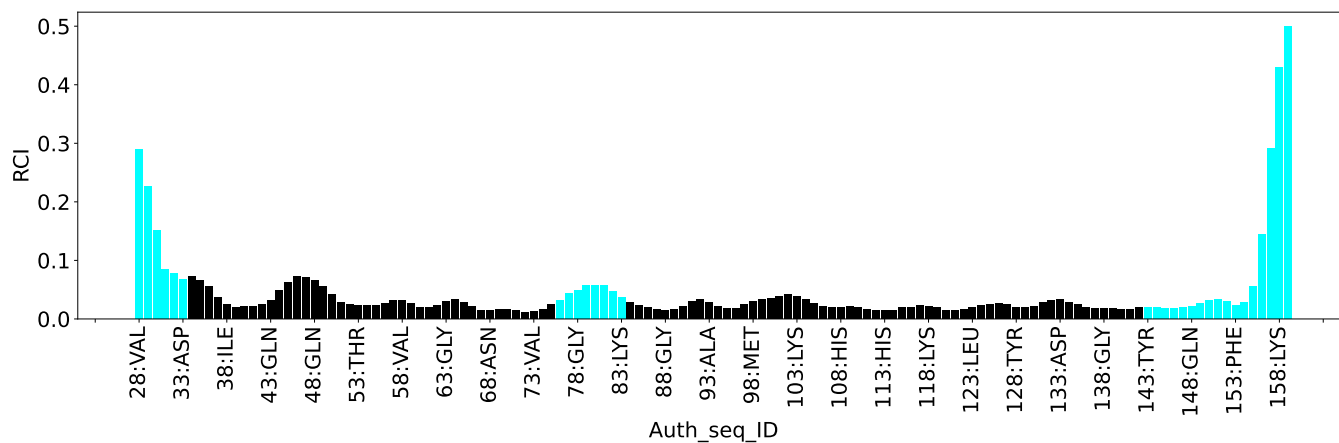
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	142	THR	HG1	9.70	0.08 – 2.19	40.6
1	A	53	THR	HG1	8.42	0.08 – 2.19	34.5
1	A	61	THR	HG1	5.43	0.08 – 2.19	20.4
1	A	124	THR	HG1	4.75	0.08 – 2.19	17.1
1	A	29	THR	HG1	4.02	0.08 – 2.19	13.7
1	A	94	THR	HG1	2.94	0.08 – 2.19	8.5
1	A	153	PHE	CE1	137.52	124.17 – 137.29	5.2
1	A	76	ARG	HE	4.47	4.52 – 10.19	-5.1
1	A	159	ARG	HE	4.47	4.52 – 10.19	-5.1
1	A	113	HIS	CD2	136.77	103.95 – 136.66	5.0
1	A	143	TYR	HD1	5.48	5.49 – 8.39	-5.0

#### 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:



Random coil index (RCI) for chain B:

