

# wwPDB X-ray Structure Validation Summary Report (i)

#### Feb 3, 2024 – 11:07 AM EST

PDB ID	:	1LKT
Title	:	CRYSTAL STRUCTURE OF THE HEAD-BINDING DOMAIN OF PHAGE
		P22 TAILSPIKE PROTEIN
Authors	:	Steinbacher, S.
Deposited on	:	1997-10-17
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp 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:

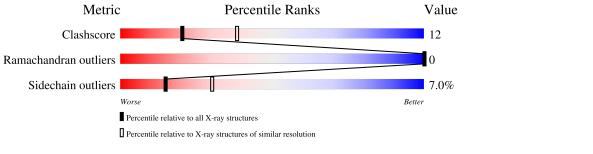
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
$\mathrm{EDS}$	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.60 Å.

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	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	104	69%	27%	•
1	В	104	74%	23%	•
1	С	104	68%	30%	•
1	D	104	67%	28%	5%
1	Е	104	70%	28%	•
1	F	104	66%	32%	·



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7140 atoms, of which 1926 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues			Aton	ns			ZeroOcc	AltConf	Trace
1	А	104	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
	Л	104	974	507	177	136	153	1	0	0	0
1	В	104	Total	С	Η	Ν	Ο	S	0	0	0
	D	104	974	507	177	136	153	1	0	0	0
1	C	104	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
	0	104	974	507	177	136	153	1	0	0	0
1	D	104	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
	D	104	974	507	177	136	153	1	0	0	0
1	Е	104	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
1		104	974	507	177	136	153	1	0	0	0
1	F	104	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
	I.	104	974	507	177	136	153	1		0	0

• Molecule 1 is a protein called TAILSPIKE PROTEIN.

• Molecule 2 is water.

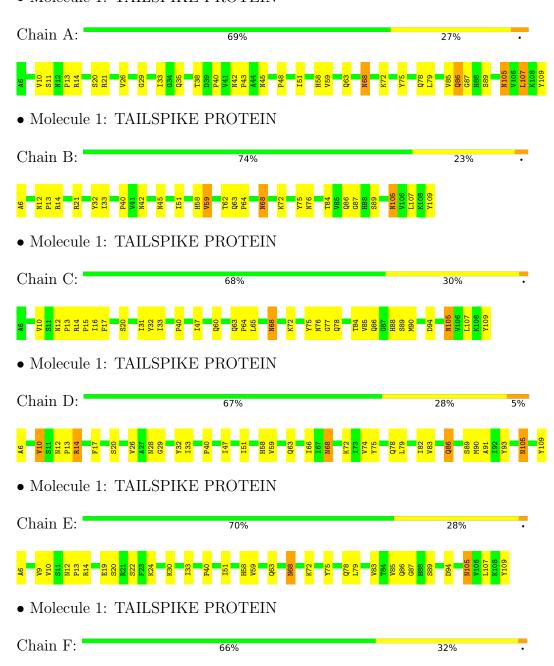
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	75	Total         H         O           225         150         75	0	0
2	В	82	Total         H         O           246         164         82	0	0
2	С	40	Total         H         O           120         80         40	0	0
2	D	103	Total H O 309 206 103	0	0
2	Ε	99	Total         H         O           297         198         99	0	0
2	F	33	Total H O 99 66 33	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.



• Molecule 1: TAILSPIKE PROTEIN







## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	57.30Å 82.10Å 73.80Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.90^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	8.00 - 2.60	Depositor
% Data completeness	96.5 (8.00-2.60)	Depositor
(in resolution range)	50.5 (0.00 2.00)	Depositor
$R_{merge}$	0.08	Depositor
R <sub>sym</sub>	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
$R, R_{free}$	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7140	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	wwPDB-VP



# 5 Model quality (i)

## 5.1 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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles	
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.46	0/812	0.65	0/1109
1	В	0.45	0/812	0.66	0/1109
1	С	0.44	0/812	0.68	0/1109
1	D	0.47	0/812	0.68	0/1109
1	Е	0.46	0/812	0.68	0/1109
1	F	0.45	0/812	0.68	0/1109
All	All	0.45	0/4872	0.67	0/6654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	797	177	798	24	3
1	В	797	177	798	19	1
1	С	797	177	798	18	10
1	D	797	177	798	30	2
1	Е	797	177	798	24	3
1	F	797	177	798	23	6
2	А	75	150	0	4	5
2	В	82	164	0	1	1
2	С	40	80	0	1	0
2	D	103	206	0	5	3

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Mol	3	Non-H	1 0	H(added)	Clashes	Symm-Clashes
2	Е	99	198	0	5	2
2	F	33	66	0	1	0
All	All	5214	1926	4788	119	18

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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 12.

The worst 5 of 119 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:GLY:HA3	1:E:107:LEU:HD22	1.74	0.69
1:E:85:VAL:HA	1:F:6:ALA:HA	1.73	0.69
1:A:33:ILE:H	1:A:63:GLN:NE2	1.90	0.69
1:D:90:MET:SD	2:E:114:HOH:O	2.50	0.68
1:B:40:PRO:HG3	1:B:89:SER:OG	1.94	0.67

The worst 5 of 18 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLN:HE21	$1:C:60:GLN:OE1[2_747]$	1.08	0.52
1:B:21:ARG:HH11	2:E:174:HOH:H2[2_656]	1.13	0.47
1:A:86:GLN:NE2	1:C:60:GLN:OE1[2_747]	1.77	0.43
1:C:85:VAL:H	2:A:125:HOH:O[2_757]	1.17	0.43
1:C:60:GLN:HE21	2:A:145:HOH:H2[2_757]	1.26	0.34

## 5.3 Torsion angles (i)

#### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	А	102/104~(98%)	101 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	В	102/104~(98%)	101 (99%)	1 (1%)	0	100	100
1	$\mathbf{C}$	102/104~(98%)	101 (99%)	1 (1%)	0	100	100
1	D	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
1	Ε	102/104~(98%)	101 (99%)	1 (1%)	0	100	100
1	F	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
All	All	612/624~(98%)	606 (99%)	6 (1%)	0	100	100

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There are no Ramachandran outliers to report.

#### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	P	erce	entiles
1	А	88/88~(100%)	81 (92%)	7 (8%)		12	24
1	В	88/88~(100%)	81 (92%)	7 (8%)		12	24
1	С	88/88~(100%)	82~(93%)	6~(7%)		16	32
1	D	88/88~(100%)	81 (92%)	7 (8%)		12	24
1	Е	88/88~(100%)	83 (94%)	5~(6%)		20	41
1	F	88/88 (100%)	83 (94%)	5~(6%)		20	41
All	All	528/528~(100%)	491 (93%)	37 (7%)		15	30

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ε	20	SER
1	F	86	GLN
1	Е	68	ASN
1	F	10	VAL
1	В	86	GLN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such side chains are listed below:



Mol	Chain	Res	Type
1	Е	12	ASN
1	F	7	ASN
1	Е	45	ASN
1	Е	63	GLN
1	F	46	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

