



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID : 4EXM  
Title : The crystal structure of an engineered phage lysin containing the binding domain of pesticin and the killing domain of T4-lysozyme  
Authors : Seddiki, N.; Noinaj, N.; Fairman, J.W.; Lukacik, P.; Barnard, T.J.; Buchanan, S.K.  
Deposited on : 2012-04-30  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

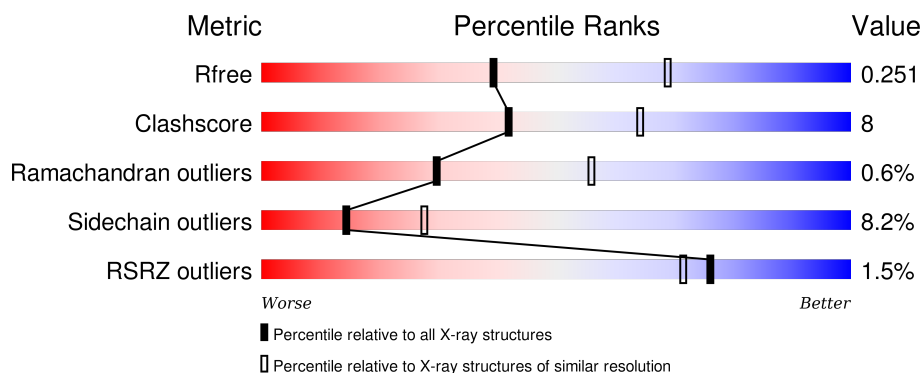
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	<div> <div>2%</div> <div>63% 19% • 16%</div> </div>
1	B	347	<div> <div>%</div> <div>65% 18% • 16%</div> </div>
1	C	347	<div> <div>%</div> <div>70% 22% • 5%</div> </div>
1	D	347	<div> <div>2%</div> <div>68% 25% • 5%</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9875 atoms, of which 0 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.

- Molecule 1 is a protein called Pesticin, Lysozyme Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2269	1429	401	431	8			
1	B	291	Total	C	N	O	S	0	0	0
			2292	1444	401	439	8			
1	C	331	Total	C	N	O	S	0	0	0
			2633	1657	461	505	10			
1	D	331	Total	C	N	O	S	0	0	0
			2606	1640	456	500	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP Q57159
A	-11	HIS	-	EXPRESSION TAG	UNP Q57159
A	-10	HIS	-	EXPRESSION TAG	UNP Q57159
A	-9	HIS	-	EXPRESSION TAG	UNP Q57159
A	-8	HIS	-	EXPRESSION TAG	UNP Q57159
A	-7	HIS	-	EXPRESSION TAG	UNP Q57159
A	-6	HIS	-	EXPRESSION TAG	UNP Q57159
A	-5	HIS	-	EXPRESSION TAG	UNP Q57159
A	-4	HIS	-	EXPRESSION TAG	UNP Q57159
A	-3	HIS	-	EXPRESSION TAG	UNP Q57159
A	-2	HIS	-	EXPRESSION TAG	UNP Q57159
A	-1	GLU	-	EXPRESSION TAG	UNP Q57159
A	0	ASN	-	EXPRESSION TAG	UNP Q57159
A	1	LEU	-	EXPRESSION TAG	UNP Q57159
A	2	TYR	-	EXPRESSION TAG	UNP Q57159
A	3	PHE	-	EXPRESSION TAG	UNP Q57159
A	4	GLN	-	EXPRESSION TAG	UNP Q57159
A	5	SER	-	EXPRESSION TAG	UNP Q57159
A	182	ARG	GLY	ENGINEERED MUTATION	UNP P00720
A	224	THR	CYS	ENGINEERED MUTATION	UNP P00720
A	267	ALA	CYS	ENGINEERED MUTATION	UNP P00720

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Chain	Residue	Modelled	Actual	Comment	Reference
A	307	ILE	ARG	ENGINEERED MUTATION	UNP P00720
B	-12	MET	-	EXPRESSION TAG	UNP Q57159
B	-11	HIS	-	EXPRESSION TAG	UNP Q57159
B	-10	HIS	-	EXPRESSION TAG	UNP Q57159
B	-9	HIS	-	EXPRESSION TAG	UNP Q57159
B	-8	HIS	-	EXPRESSION TAG	UNP Q57159
B	-7	HIS	-	EXPRESSION TAG	UNP Q57159
B	-6	HIS	-	EXPRESSION TAG	UNP Q57159
B	-5	HIS	-	EXPRESSION TAG	UNP Q57159
B	-4	HIS	-	EXPRESSION TAG	UNP Q57159
B	-3	HIS	-	EXPRESSION TAG	UNP Q57159
B	-2	HIS	-	EXPRESSION TAG	UNP Q57159
B	-1	GLU	-	EXPRESSION TAG	UNP Q57159
B	0	ASN	-	EXPRESSION TAG	UNP Q57159
B	1	LEU	-	EXPRESSION TAG	UNP Q57159
B	2	TYR	-	EXPRESSION TAG	UNP Q57159
B	3	PHE	-	EXPRESSION TAG	UNP Q57159
B	4	GLN	-	EXPRESSION TAG	UNP Q57159
B	5	SER	-	EXPRESSION TAG	UNP Q57159
B	182	ARG	GLY	ENGINEERED MUTATION	UNP P00720
B	224	THR	CYS	ENGINEERED MUTATION	UNP P00720
B	267	ALA	CYS	ENGINEERED MUTATION	UNP P00720
B	307	ILE	ARG	ENGINEERED MUTATION	UNP P00720
C	-12	MET	-	EXPRESSION TAG	UNP Q57159
C	-11	HIS	-	EXPRESSION TAG	UNP Q57159
C	-10	HIS	-	EXPRESSION TAG	UNP Q57159
C	-9	HIS	-	EXPRESSION TAG	UNP Q57159
C	-8	HIS	-	EXPRESSION TAG	UNP Q57159
C	-7	HIS	-	EXPRESSION TAG	UNP Q57159
C	-6	HIS	-	EXPRESSION TAG	UNP Q57159
C	-5	HIS	-	EXPRESSION TAG	UNP Q57159
C	-4	HIS	-	EXPRESSION TAG	UNP Q57159
C	-3	HIS	-	EXPRESSION TAG	UNP Q57159
C	-2	HIS	-	EXPRESSION TAG	UNP Q57159
C	-1	GLU	-	EXPRESSION TAG	UNP Q57159
C	0	ASN	-	EXPRESSION TAG	UNP Q57159
C	1	LEU	-	EXPRESSION TAG	UNP Q57159
C	2	TYR	-	EXPRESSION TAG	UNP Q57159
C	3	PHE	-	EXPRESSION TAG	UNP Q57159
C	4	GLN	-	EXPRESSION TAG	UNP Q57159
C	5	SER	-	EXPRESSION TAG	UNP Q57159
C	182	ARG	GLY	ENGINEERED MUTATION	UNP P00720

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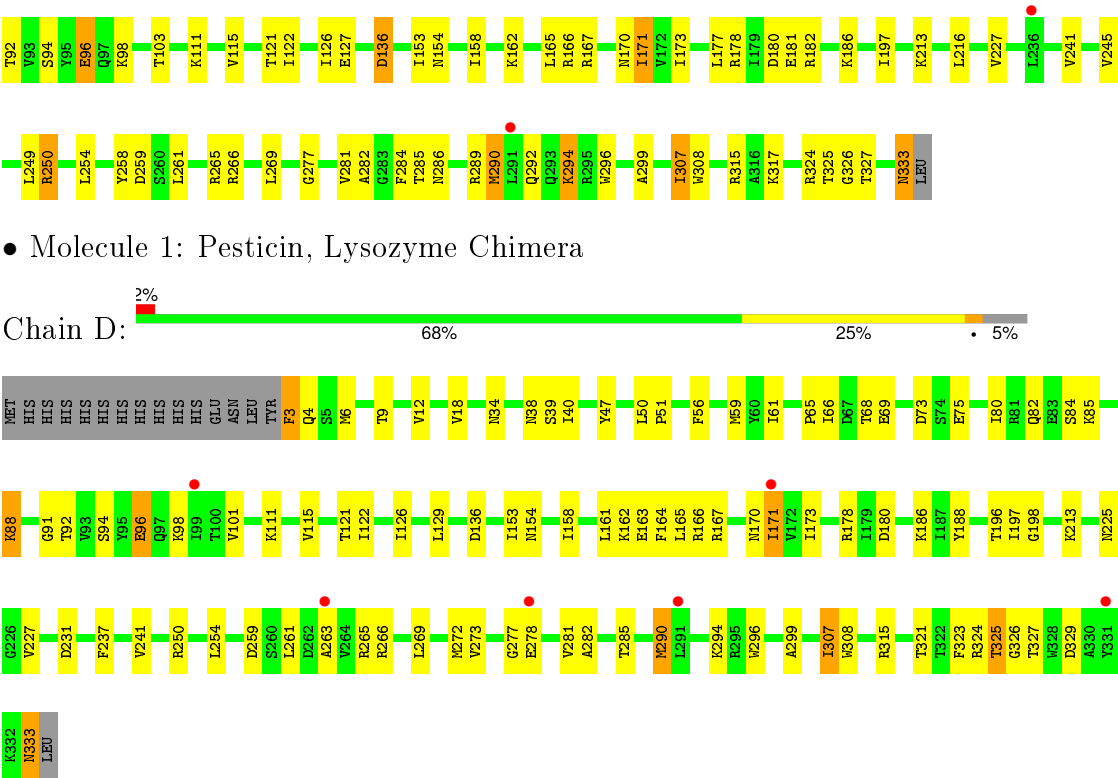
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Chain	Residue	Modelled	Actual	Comment	Reference
C	224	THR	CYS	ENGINEERED MUTATION	UNP P00720
C	267	ALA	CYS	ENGINEERED MUTATION	UNP P00720
C	307	ILE	ARG	ENGINEERED MUTATION	UNP P00720
D	-12	MET	-	EXPRESSION TAG	UNP Q57159
D	-11	HIS	-	EXPRESSION TAG	UNP Q57159
D	-10	HIS	-	EXPRESSION TAG	UNP Q57159
D	-9	HIS	-	EXPRESSION TAG	UNP Q57159
D	-8	HIS	-	EXPRESSION TAG	UNP Q57159
D	-7	HIS	-	EXPRESSION TAG	UNP Q57159
D	-6	HIS	-	EXPRESSION TAG	UNP Q57159
D	-5	HIS	-	EXPRESSION TAG	UNP Q57159
D	-4	HIS	-	EXPRESSION TAG	UNP Q57159
D	-3	HIS	-	EXPRESSION TAG	UNP Q57159
D	-2	HIS	-	EXPRESSION TAG	UNP Q57159
D	-1	GLU	-	EXPRESSION TAG	UNP Q57159
D	0	ASN	-	EXPRESSION TAG	UNP Q57159
D	1	LEU	-	EXPRESSION TAG	UNP Q57159
D	2	TYR	-	EXPRESSION TAG	UNP Q57159
D	3	PHE	-	EXPRESSION TAG	UNP Q57159
D	4	GLN	-	EXPRESSION TAG	UNP Q57159
D	5	SER	-	EXPRESSION TAG	UNP Q57159
D	182	ARG	GLY	ENGINEERED MUTATION	UNP P00720
D	224	THR	CYS	ENGINEERED MUTATION	UNP P00720
D	267	ALA	CYS	ENGINEERED MUTATION	UNP P00720
D	307	ILE	ARG	ENGINEERED MUTATION	UNP P00720

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	28	Total O 28 28	0	0
2	B	27	Total O 27 27	0	0
2	C	9	Total O 9 9	0	0
2	D	11	Total O 11 11	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.43Å 108.43Å 109.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.80 – 2.60 47.38 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.80-2.60) 99.9 (47.38-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1038)	Depositor
R, $R_{free}$	0.199 , 0.251 0.197 , 0.251	Depositor DCC
$R_{free}$ test set	2239 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.7	EDS
Estimated twinning fraction	0.015 for -h,-k,l 0.479 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44745 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/2304	0.51	0/3116
1	B	0.34	0/2328	0.51	0/3146
1	C	0.32	0/2674	0.51	0/3606
1	D	0.32	0/2646	0.51	0/3572
All	All	0.33	0/9952	0.51	0/13440

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	A	2269	0	2212	38	0
1	B	2292	0	2253	34	0
1	C	2633	0	2645	51	0
1	D	2606	0	2604	52	0
2	A	28	0	0	3	0
2	B	27	0	0	4	0
2	C	9	0	0	1	0
2	D	11	0	0	0	0
All	All	9875	0	9714	164	0

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 8.

The worst 5 of 164 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:B:138:LEU:HB3	1:B:158:ILE:HG13	1.53	0.91
1:B:314:ASN:ND2	2:B:425:HOH:O	2.04	0.90
1:B:92:THR:O	2:B:410:HOH:O	1.95	0.84
1:A:138:LEU:HB3	1:A:158:ILE:HG13	1.60	0.83
1:C:265:ARG:NH2	1:C:324:ARG:O	2.15	0.80

There are no symmetry-related clashes.

## 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	A	287/347 (83%)	269 (94%)	18 (6%)	0	100	100
1	B	287/347 (83%)	270 (94%)	15 (5%)	2 (1%)	26	51
1	C	329/347 (95%)	307 (93%)	19 (6%)	3 (1%)	21	42
1	D	329/347 (95%)	304 (92%)	22 (7%)	3 (1%)	21	42
All	All	1232/1388 (89%)	1150 (93%)	74 (6%)	8 (1%)	30	56

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	GLY
1	C	34	ASN
1	C	285	THR
1	D	34	ASN
1	D	285	THR

### 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	Percentiles	
1	A	237/306 (78%)	218 (92%)	19 (8%)	15	29
1	B	244/306 (80%)	227 (93%)	17 (7%)	19	37
1	C	288/306 (94%)	263 (91%)	25 (9%)	13	24
1	D	282/306 (92%)	257 (91%)	25 (9%)	12	23
All	All	1051/1224 (86%)	965 (92%)	86 (8%)	14	27

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	ASN
1	C	127	GLU
1	D	250	ARG
1	C	61	ILE
1	C	75	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4	GLN
1	D	4	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 carbohydrates 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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	291/347 (83%)	-0.18	7 (2%) 62 56	46, 77, 133, 171	0
1	B	291/347 (83%)	-0.18	4 (1%) 78 74	44, 78, 140, 162	0
1	C	331/347 (95%)	-0.10	2 (0%) 90 88	56, 90, 136, 153	0
1	D	331/347 (95%)	-0.10	6 (1%) 71 66	54, 89, 134, 167	0
All	All	1244/1388 (89%)	-0.14	19 (1%) 76 71	44, 85, 137, 171	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	LEU	4.0
1	A	227	VAL	3.9
1	B	328	TRP	3.5
1	D	291	LEU	3.4
1	D	331	TYR	3.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.