



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 03:21 pm GMT

PDB ID : 8PEA  
Title : OXA-48\_F72L. Epistasis Arises from Shifting the Rate-Limiting Step during Enzyme Evolution  
Authors : Leiros, H.-K.S.; Frohlich, C.  
Deposited on : 2023-06-13  
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

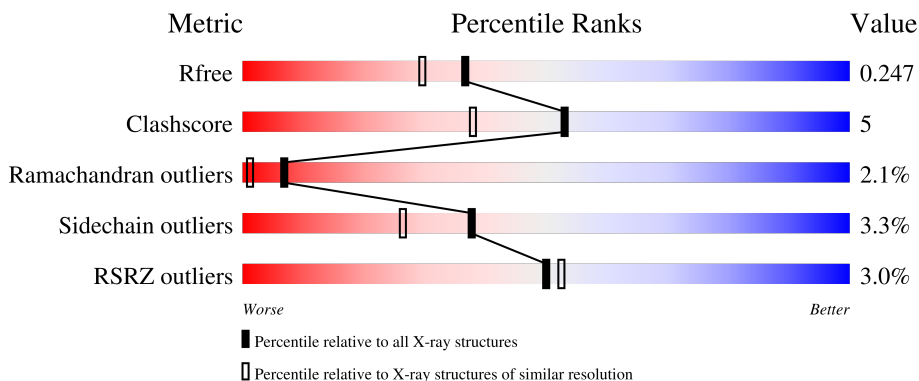
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	265	 3% 80% 10% • 9%
1	B	265	 3% 77% 14% • 9%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4264 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	1977	1257	350	363	7	107	1	0
1	B	242	1991	1266	351	366	8	41	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	LEU	PHE	engineered mutation	UNP Q6XEC0
B	72	LEU	PHE	engineered mutation	UNP Q6XEC0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0

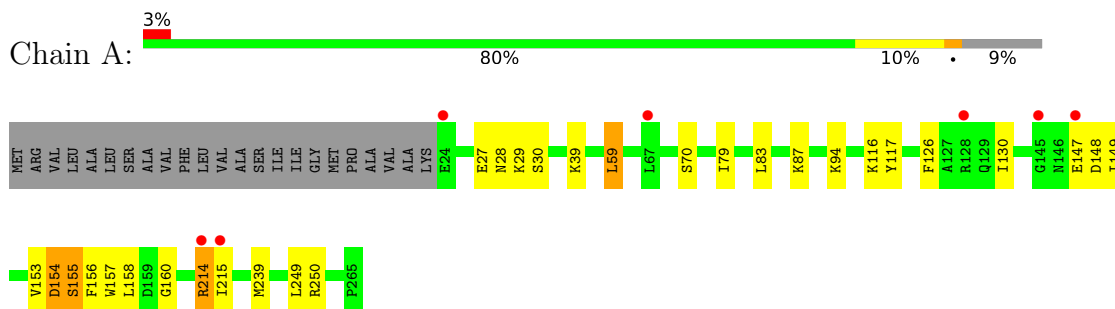
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	148	148	148	0	0
3	B	147	147	147	0	0

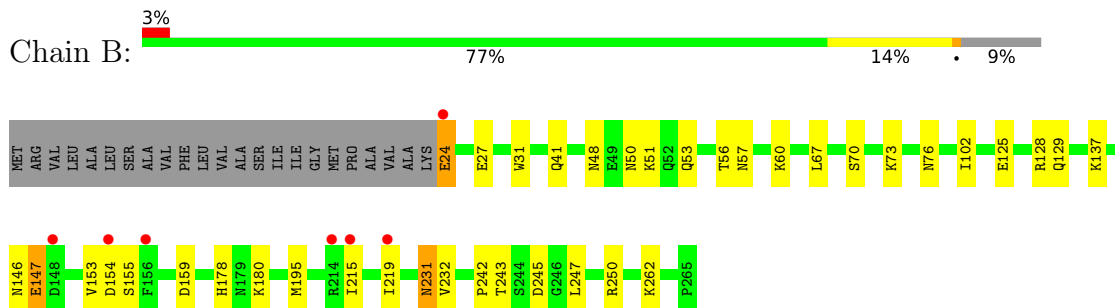
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.68Å 82.82Å 100.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.97 45.51 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.00-1.97) 89.7 (45.51-1.97)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.44 (at 1.97Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.204 , 0.247 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	1603 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.666	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.44	0/2025	0.69	1/2739 (0.0%)
1	B	0.47	0/2039	0.69	1/2757 (0.0%)
All	All	0.46	0/4064	0.69	2/5496 (0.0%)

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 outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	59	LEU	CA-CB-CG	6.09	129.31	115.30
1	B	146	ASN	C-N-CA	5.16	134.61	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	VAL	Peptide
1	A	156	PHE	Peptide

## 5.2 Too-close contacts

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	1977	0	1929	15	0
1	B	1991	0	1948	26	0
2	A	1	0	0	0	0
3	A	148	0	0	1	0
3	B	147	0	0	9	0
All	All	4264	0	3877	41	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 5.

All (41) 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:A:27:GLU:OE2	1:A:29:LYS:NZ	1.98	0.96
1:A:27:GLU:OE1	1:A:59:LEU:HD12	1.86	0.75
1:A:28:ASN:OD1	1:A:30:SER:OG	2.10	0.69
1:B:159:ASP:OD1	3:B:304:HOH:O	2.13	0.67
1:B:129:GLN:OE1	3:B:305:HOH:O	2.14	0.65
1:B:48:ASN:ND2	1:B:51:LYS:HE2	2.14	0.63
1:A:79:ILE:HG22	1:A:130:ILE:HD13	1.81	0.62
1:B:24:GLU:HB3	1:B:53:GLN:HE22	1.65	0.62
1:B:60:LYS:NZ	3:B:312:HOH:O	2.33	0.61
1:B:245:ASP:OD1	3:B:306:HOH:O	2.17	0.60
1:B:67:LEU:HD11	1:B:215:ILE:HD12	1.86	0.57
1:A:116:LYS:HD3	1:A:117:TYR:CZ	2.39	0.57
1:A:70:SER:OG	3:A:401:HOH:O	2.15	0.56
1:B:50:ASN:H	1:B:231:ASN:HD21	1.53	0.56
1:B:129:GLN:NE2	3:B:308:HOH:O	2.20	0.53
1:B:24:GLU:HB3	1:B:53:GLN:NE2	2.22	0.53
1:B:125:GLU:OE2	3:B:305:HOH:O	2.19	0.52
1:A:126:PHE:O	1:A:130:ILE:HG13	2.10	0.51
1:B:125:GLU:OE2	1:B:128:ARG:NH1	2.44	0.50
1:B:178:HIS:O	1:B:180:LYS:HE3	2.12	0.50
1:A:239:MET:HE2	1:A:250:ARG:HG3	1.93	0.50
1:B:147:GLU:HB2	3:B:348:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:HA	1:B:76:ASN:HB2	1.94	0.49
1:B:48:ASN:HD21	1:B:51:LYS:HE2	1.76	0.49
1:B:180:LYS:HA	1:B:180:LYS:HE2	1.95	0.48
1:B:70:SER:OG	3:B:307:HOH:O	2.20	0.47
1:A:214:ARG:HD2	1:A:215:ILE:HG12	1.98	0.46
1:B:147:GLU:OE2	3:B:309:HOH:O	2.21	0.45
1:A:39:LYS:HB2	1:A:39:LYS:HE2	1.75	0.45
1:B:31:TRP:HB2	1:B:57:ASN:HB3	1.97	0.45
1:A:214:ARG:O	1:A:215:ILE:HG12	2.17	0.44
1:B:27:GLU:HA	1:B:56:THR:O	2.18	0.44
1:A:239:MET:HE1	1:A:249:LEU:C	2.39	0.43
1:B:231:ASN:ND2	1:B:232:VAL:H	2.16	0.43
1:A:239:MET:HE1	1:A:249:LEU:HB2	2.01	0.43
1:A:83:LEU:CD1	1:A:130:ILE:HG23	2.49	0.42
1:B:247:LEU:HB3	1:B:250:ARG:NH2	2.34	0.42
1:A:94:LYS:HB2	1:A:94:LYS:HE3	1.79	0.42
1:B:219:ILE:O	1:B:219:ILE:HG13	2.19	0.41
1:B:102:ILE:HD12	1:B:102:ILE:H	1.86	0.41
1:B:231:ASN:HD22	1:B:232:VAL:H	1.69	0.41

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	241/265 (91%)	226 (94%)	8 (3%)	7 (3%)	4	0
1	B	242/265 (91%)	231 (96%)	8 (3%)	3 (1%)	13	4
All	All	483/530 (91%)	457 (95%)	16 (3%)	10 (2%)	7	1

All (10) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	147	GLU
1	A	148	ASP
1	A	154	ASP
1	A	157	TRP
1	A	158	LEU
1	B	147	GLU
1	B	153	VAL
1	A	155	SER
1	B	154	ASP
1	A	160	GLY

### 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	210/228 (92%)	205 (98%)	5 (2%)	49	41
1	B	213/228 (93%)	204 (96%)	9 (4%)	30	17
All	All	423/456 (93%)	409 (97%)	14 (3%)	38	26

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LYS
1	A	149	ILE
1	A	154	ASP
1	A	155	SER
1	A	214	ARG
1	B	24	GLU
1	B	41	GLN
1	B	137	LYS
1	B	155	SER
1	B	195	MET
1	B	231	ASN
1	B	242	PRO
1	B	243	THR
1	B	262	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	B	53	GLN
1	B	231	ASN

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	228/265 (86%)	0.38	7 (3%) 49 51	29, 42, 65, 79	1 (0%)
1	B	237/265 (89%)	0.32	7 (2%) 50 52	29, 40, 63, 83	2 (0%)
All	All	465/530 (87%)	0.35	14 (3%) 50 52	29, 41, 64, 83	3 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	GLU	4.4
1	B	154	ASP	4.1
1	B	148	ASP	4.0
1	A	214	ARG	4.0
1	B	214	ARG	3.9
1	B	156	PHE	3.8
1	A	24	GLU	3.8
1	A	215	ILE	3.7
1	A	147	GLU	3.2
1	B	215	ILE	2.4
1	A	67	LEU	2.2
1	B	219	ILE	2.2
1	A	145	GLY	2.1
1	A	128	ARG	2.0

### 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	A	301	1/1	0.99	0.11	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.