



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 10:18 am BST

PDB ID : 8CR4
Title : Crystal structure of recombinant LasB_{Artif} from *Pseudomonas aeruginosa* AZ-PAE14816
Authors : Kolling, D.; Koehnke, J.
Deposited on : 2023-03-07
Resolution : 0.91 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

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>.

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 : 2.35
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) : 2.35

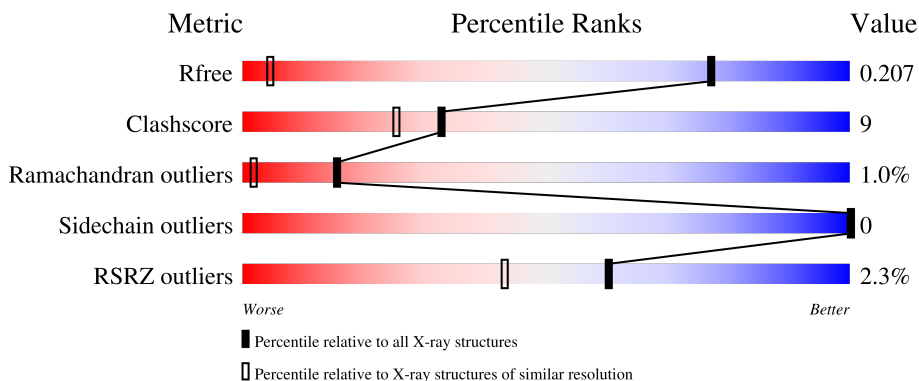
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.91 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	1039 (1.04-0.80)
Clashscore	141614	1108 (1.04-0.80)
Ramachandran outliers	138981	1035 (1.04-0.80)
Sidechain outliers	138945	1036 (1.04-0.80)
RSRZ outliers	127900	1009 (1.04-0.80)

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 $\leq 5\%$. 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	514	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4706 atoms, of which 2085 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 Pro-elastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	298	4367	1436	2085	391	444	11	0	0	0

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-197	MET	-	initiating methionine	UNP Q02RJ6
A	-196	LYS	-	expression tag	UNP Q02RJ6
A	-195	TYR	-	expression tag	UNP Q02RJ6
A	-194	LEU	-	expression tag	UNP Q02RJ6
A	-193	LEU	-	expression tag	UNP Q02RJ6
A	-192	PRO	-	expression tag	UNP Q02RJ6
A	-191	THR	-	expression tag	UNP Q02RJ6
A	-190	ALA	-	expression tag	UNP Q02RJ6
A	-189	ALA	-	expression tag	UNP Q02RJ6
A	-188	ALA	-	expression tag	UNP Q02RJ6
A	-187	GLY	-	expression tag	UNP Q02RJ6
A	-186	LEU	-	expression tag	UNP Q02RJ6
A	-185	LEU	-	expression tag	UNP Q02RJ6
A	-184	LEU	-	expression tag	UNP Q02RJ6
A	-183	LEU	-	expression tag	UNP Q02RJ6
A	-182	ALA	-	expression tag	UNP Q02RJ6
A	-181	ALA	-	expression tag	UNP Q02RJ6
A	-180	GLN	-	expression tag	UNP Q02RJ6
A	-179	PRO	-	expression tag	UNP Q02RJ6
A	-178	ALA	-	expression tag	UNP Q02RJ6
A	-177	MET	-	expression tag	UNP Q02RJ6
A	-176	ALA	-	expression tag	UNP Q02RJ6
A	-175	MET	-	expression tag	UNP Q02RJ6
A	-174	GLY	-	expression tag	UNP Q02RJ6
A	-95	GLN	ARG	conflict	UNP Q02RJ6
A	2	GLN	GLU	conflict	UNP Q02RJ6
A	16	ASN	THR	conflict	UNP Q02RJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	THR	SER	conflict	UNP Q02RJ6
A	51	SER	THR	conflict	UNP Q02RJ6
A	66	ILE	VAL	conflict	UNP Q02RJ6
A	88	LYS	ARG	conflict	UNP Q02RJ6
A	93	ALA	THR	conflict	UNP Q02RJ6
A	120	VAL	MET	conflict	UNP Q02RJ6
A	154	VAL	ILE	conflict	UNP Q02RJ6
A	214	GLY	SER	conflict	UNP Q02RJ6
A	264	THR	ASN	conflict	UNP Q02RJ6
A	265	PHE	TYR	conflict	UNP Q02RJ6
A	282	PRO	SER	conflict	UNP Q02RJ6
A	302	GLU	-	expression tag	UNP Q02RJ6
A	303	ASN	-	expression tag	UNP Q02RJ6
A	304	LEU	-	expression tag	UNP Q02RJ6
A	305	TYR	-	expression tag	UNP Q02RJ6
A	306	PHE	-	expression tag	UNP Q02RJ6
A	307	GLN	-	expression tag	UNP Q02RJ6
A	308	GLY	-	expression tag	UNP Q02RJ6
A	309	LEU	-	expression tag	UNP Q02RJ6
A	310	GLU	-	expression tag	UNP Q02RJ6
A	311	HIS	-	expression tag	UNP Q02RJ6
A	312	HIS	-	expression tag	UNP Q02RJ6
A	313	HIS	-	expression tag	UNP Q02RJ6
A	314	HIS	-	expression tag	UNP Q02RJ6
A	315	HIS	-	expression tag	UNP Q02RJ6
A	316	HIS	-	expression tag	UNP Q02RJ6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	1	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	337	Total 337	O 337	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.41Å 40.46Å 45.38Å 100.52° 98.61° 107.45°	Depositor
Resolution (Å)	21.77 – 0.91 43.54 – 0.91	Depositor EDS
% Data completeness (in resolution range)	90.1 (21.77-0.91) 90.5 (43.54-0.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 0.91Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.195 , 0.206 0.195 , 0.207	Depositor DCC
R_{free} test set	8424 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	9.3	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4706	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, CA

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	0.53	0/2345	0.77	2/3186 (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 outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	MET	CG-SD-CE	-12.21	80.67	100.20
1	A	136	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	SER	Peptide

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	2282	2085	2087	38	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	337	0	0	17	3
All	All	2621	2085	2087	38	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 9.

All (38) 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:47:ASN:O	1:A:49:SER:N	1.97	0.97
1:A:94:SER:OG	4:A:501:HOH:O	1.81	0.94
1:A:49:SER:O	4:A:502:HOH:O	1.86	0.92
1:A:50:LYS:HD2	4:A:504:HOH:O	1.76	0.84
1:A:256:ARG:HD3	4:A:514:HOH:O	1.79	0.82
1:A:229:TYR:CD1	4:A:756:HOH:O	2.34	0.81
1:A:229:TYR:HD1	4:A:756:HOH:O	1.65	0.79
1:A:50:LYS:CD	4:A:504:HOH:O	2.32	0.76
1:A:48:ASP:HA	1:A:50:LYS:HD3	1.69	0.75
1:A:48:ASP:OD1	1:A:50:LYS:HE2	1.93	0.68
1:A:85:ASN:ND2	4:A:507:HOH:O	2.27	0.68
1:A:50:LYS:N	4:A:504:HOH:O	2.23	0.64
1:A:47:ASN:O	1:A:48:ASP:C	2.36	0.64
1:A:48:ASP:HA	1:A:50:LYS:CD	2.28	0.64
1:A:48:ASP:OD1	1:A:50:LYS:HG2	1.99	0.62
1:A:256:ARG:HD3	4:A:776:HOH:O	2.01	0.60
1:A:179:ARG:HD3	4:A:641:HOH:O	2.01	0.59
1:A:45:SER:CB	1:A:48:ASP:OD2	2.51	0.57
1:A:45:SER:HB3	1:A:48:ASP:HB2	1.88	0.55
1:A:45:SER:CB	1:A:48:ASP:HB2	2.37	0.54
1:A:29:ARG:CB	4:A:770:HOH:O	2.58	0.51
1:A:45:SER:HB2	1:A:48:ASP:OD2	2.11	0.51
1:A:48:ASP:OD1	1:A:50:LYS:CE	2.59	0.51
1:A:48:ASP:CG	1:A:50:LYS:HE2	2.32	0.50
1:A:100:LEU:HD13	4:A:705:HOH:O	2.10	0.50
1:A:201:ASP:OD1	4:A:503:HOH:O	2.18	0.50
1:A:48:ASP:O	1:A:50:LYS:HB2	2.11	0.50
1:A:48:ASP:HA	1:A:50:LYS:CE	2.41	0.50
1:A:48:ASP:C	1:A:50:LYS:HB2	2.34	0.48
1:A:228:VAL:HB	4:A:756:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:CD1	4:A:705:HOH:O	2.61	0.47
1:A:139:ALA:HB3	1:A:171:GLY:HA2	1.98	0.46
1:A:45:SER:OG	1:A:48:ASP:OD2	2.31	0.45
1:A:45:SER:OG	1:A:48:ASP:HB2	2.17	0.44
1:A:51:SER:OG	1:A:103:LYS:HE2	2.19	0.43
1:A:48:ASP:HA	1:A:50:LYS:HE2	2.00	0.42
1:A:256:ARG:NH1	4:A:514:HOH:O	2.53	0.41
1:A:48:ASP:CA	1:A:50:LYS:HD3	2.47	0.40

All (3) 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)
4:A:740:HOH:O	4:A:767:HOH:O[1_556]	1.94	0.26
4:A:770:HOH:O	4:A:785:HOH:O[1_545]	2.10	0.10
4:A:769:HOH:O	4:A:775:HOH:O[1_545]	2.17	0.03

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	296/514 (58%)	282 (95%)	11 (4%)	3 (1%)	15 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	50	LYS
1	A	126	ALA

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	231/399 (58%)	231 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 2 ligands modelled in this entry, 2 are 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, 95th 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 ²)	Q<0.9
1	A	298/514 (57%)	-0.03	7 (2%) 60 43	6, 10, 19, 42	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	ASP	9.5
1	A	50	LYS	6.0
1	A	49	SER	5.8
1	A	47	ASN	5.3
1	A	101	TYR	4.0
1	A	194	SER	2.3
1	A	108	ARG	2.2

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](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.