



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4ANR
Title : Crystal structure of soluble lytic Transglycosylase SltB1 from *Pseudomonas aeruginosa*
Authors : Nikolaidis, I.; Izore, T.; Job, V.; Thielens, N.; Breukink, E.; Dessen, A.
Deposited on : 2012-03-22
Resolution : 1.84 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

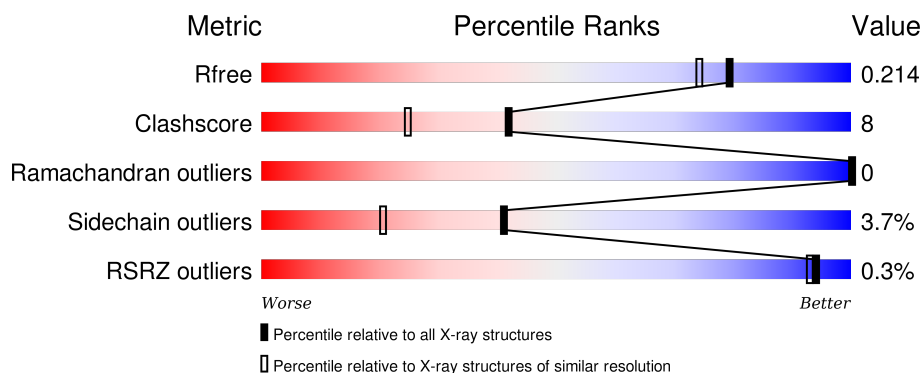
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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 ≥ 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	323	 78% 13% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2554 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 SOLUBLE LYTIC TRANSGLYCOSYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	2	0
			2367	1505	413	440	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP Q9HX24
A	19	GLY	-	EXPRESSION TAG	UNP Q9HX24
A	20	SER	-	EXPRESSION TAG	UNP Q9HX24
A	21	SER	-	EXPRESSION TAG	UNP Q9HX24
A	22	HIS	-	EXPRESSION TAG	UNP Q9HX24
A	23	HIS	-	EXPRESSION TAG	UNP Q9HX24
A	24	HIS	-	EXPRESSION TAG	UNP Q9HX24
A	25	HIS	-	EXPRESSION TAG	UNP Q9HX24
A	26	HIS	-	EXPRESSION TAG	UNP Q9HX24
A	27	HIS	-	EXPRESSION TAG	UNP Q9HX24
A	28	SER	-	EXPRESSION TAG	UNP Q9HX24
A	29	GLN	-	EXPRESSION TAG	UNP Q9HX24
A	30	ASP	-	EXPRESSION TAG	UNP Q9HX24
A	31	PRO	-	EXPRESSION TAG	UNP Q9HX24
A	32	ASN	-	EXPRESSION TAG	UNP Q9HX24
A	33	SER	-	EXPRESSION TAG	UNP Q9HX24
A	34	LEU	-	EXPRESSION TAG	UNP Q9HX24
A	35	VAL	-	EXPRESSION TAG	UNP Q9HX24
A	36	PRO	-	EXPRESSION TAG	UNP Q9HX24
A	37	ARG	-	EXPRESSION TAG	UNP Q9HX24

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total 186	O 186	0	0

• Molecule 1: SOLUBLE LYTIC TRANSGLYCOSYLASE B

R170	E171	F172	L173		Q179		L196	P197		R205		D212		I217	N218		D222	T223	P224		V248		N252		R262		R274		R279	T280	HIS	ASP	ALA	L284		D287		W304		Y316		Q328		R335		S101	R102		E120		F137		V147	M148	D149	A150		P159	P160
Met	Gly	Ser	Ser	His	His	His	His	His	His	Ser	Gln	Asp	Pro	Asn	Ser	Leu	Val	Pro	Arg	Gly	Ser	P40	Q41		E44		D52	Y53		Q59	L60	K70		I73		I77	S78		R83		R91	P92		S101	R102		E120		F137		V147	M148	D149	A150		P159	P160		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.50 Å 91.50 Å 81.30 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.75 – 1.84 45.75 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.75-1.84) 100.0 (45.75-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 1.84 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.178 , 0.211 0.180 , 0.214	Depositor DCC
R_{free} test set	3438 reflections (11.06%)	DCC
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.2	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34515 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2554	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.58	0/2429	0.62	0/3285

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	ASN	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	2367	0	2303	39	2
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	186	0	0	16	1
All	All	2554	0	2303	39	2

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.

All (39) 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:284:LEU:N	3:A:2153:HOH:O	1.71	1.21
1:A:279:ARG:HG3	1:A:279:ARG:HH11	1.41	0.85
1:A:248[A]:VAL:HG13	3:A:2169:HOH:O	1.75	0.85
1:A:40:PRO:HD2	3:A:2001:HOH:O	1.76	0.84
1:A:262:ARG:HD3	3:A:2137:HOH:O	1.78	0.83
1:A:274:ARG:HD3	3:A:2149:HOH:O	1.83	0.78
1:A:91:ARG:HE	1:A:328:GLN:HE22	1.33	0.77
1:A:91:ARG:HE	1:A:328:GLN:NE2	1.85	0.74
1:A:170:ARG:HD3	3:A:2003:HOH:O	1.88	0.73
1:A:148:MET:HE1	1:A:173:LEU:HD21	1.85	0.59
1:A:179:GLN:NE2	1:A:217:ILE:H	2.02	0.57
1:A:70:LYS:HD2	3:A:2012:HOH:O	2.04	0.57
1:A:279:ARG:HG3	1:A:279:ARG:NH1	2.15	0.56
1:A:147:VAL:HA	3:A:2084:HOH:O	2.06	0.56
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.21	0.54
1:A:44:GLU:HB2	3:A:2002:HOH:O	2.08	0.53
1:A:120:GLU:CG	3:A:2061:HOH:O	2.57	0.52
1:A:287:ASP:HB2	3:A:2155:HOH:O	2.10	0.52
1:A:53:TYR:CZ	1:A:170:ARG:HD2	2.46	0.50
1:A:279:ARG:CG	1:A:279:ARG:NH1	2.74	0.48
1:A:40:PRO:CD	3:A:2001:HOH:O	2.49	0.48
1:A:179:GLN:HE22	1:A:217:ILE:H	1.62	0.47
1:A:73:ILE:HD13	1:A:150:ALA:HA	1.97	0.47
1:A:279:ARG:CG	1:A:279:ARG:HH11	2.15	0.47
1:A:262:ARG:NH1	1:A:262:ARG:CG	2.77	0.47
1:A:170:ARG:CD	3:A:2003:HOH:O	2.57	0.46
1:A:159:PRO:HB2	1:A:160:PRO:HD3	1.98	0.45
1:A:102:ARG:HD2	1:A:137:PHE:CE1	2.51	0.44
1:A:218:ASN:O	1:A:222:ASP:HB3	2.16	0.44
1:A:171:GLU:OE1	1:A:205:ARG:HD3	2.17	0.44
1:A:248[A]:VAL:HG23	3:A:2122:HOH:O	2.16	0.44
1:A:212:ASP:HB3	1:A:224:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:HB3	3:A:2006:HOH:O	2.19	0.43
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.86	0.42
1:A:196:LEU:N	1:A:197:PRO:CD	2.83	0.42
1:A:248[B]:VAL:HG12	1:A:304:TRP:CH2	2.55	0.41
1:A:120:GLU:HG2	3:A:2061:HOH:O	2.18	0.41
1:A:91:ARG:N	1:A:92:PRO:HD2	2.36	0.40
1:A:196:LEU:HB2	1:A:197:PRO:HD3	2.03	0.40

All (2) 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:101[A]:SER:OG	1:A:262:ARG:NH1[3_565]	1.91	0.29
1:A:52:ASP:OD1	3:A:2095:HOH:O[6_555]	2.13	0.07

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	295/323 (91%)	291 (99%)	4 (1%)	0	100	100

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	Percentiles	
1	A	244/265 (92%)	235 (96%)	9 (4%)	41	20

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	59	GLN
1	A	77	ILE
1	A	78	SER
1	A	83	ARG
1	A	137	PHE
1	A	262	ARG
1	A	316	TYR
1	A	335	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	179	GLN
1	A	198	GLN
1	A	288	GLN
1	A	328	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](#)

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, 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	297/323 (91%)	-0.34	1 (0%) 94 93	12, 20, 39, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	PRO	2.7

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	CA	A	400	1/1	0.99	0.07	-0.97	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.