



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:36 PM GMT

PDB ID : 4USX
Title : The Structure of the C-terminal YadA-like domain of BPSL2063 from Burkholderia pseudomallei
Authors : Perletti, L.; Gourlay, L.J.; Peano, C.; Pietrelli, A.; DeBellis, G.; Deantonio, C.; Santoro, C.; Sblattero, D.; Bolognesi, M.
Deposited on : 2014-07-16
Resolution : 1.80 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
<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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

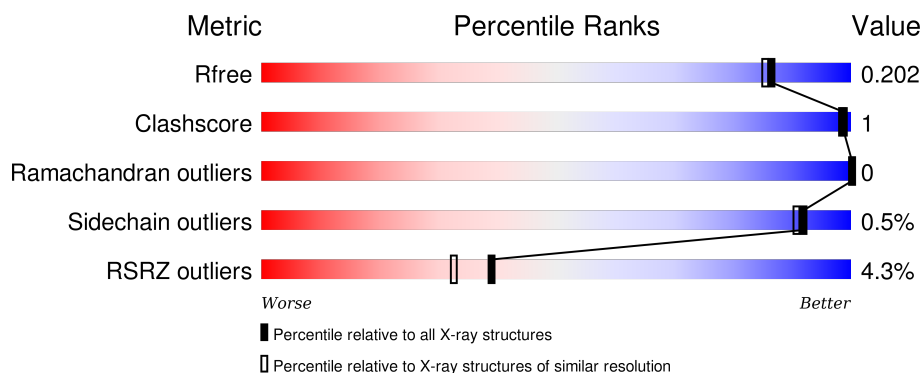
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 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	371	<div> <div>2%</div> <div>55%</div> <div>44%</div> </div>
1	B	371	<div> <div>4%</div> <div>56%</div> <div>43%</div> </div>
1	C	371	<div> <div>2%</div> <div>56%</div> <div>42%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	1892	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4746 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 TRIMERIC AUTOTRANSPORTER ADHESIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1415	860	247	307	1			
1	B	211	Total	C	N	O	S	0	0	0
			1431	870	250	310	1			
1	C	214	Total	C	N	O	S	0	1	0
			1445	875	254	315	1			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	641	MET	-	EXPRESSION TAG	UNP Q63TA4
A	642	ALA	-	EXPRESSION TAG	UNP Q63TA4
A	643	SER	-	EXPRESSION TAG	UNP Q63TA4
A	644	MET	-	EXPRESSION TAG	UNP Q63TA4
A	645	THR	-	EXPRESSION TAG	UNP Q63TA4
A	646	GLY	-	EXPRESSION TAG	UNP Q63TA4
A	647	GLY	-	EXPRESSION TAG	UNP Q63TA4
A	648	GLN	-	EXPRESSION TAG	UNP Q63TA4
A	649	GLN	-	EXPRESSION TAG	UNP Q63TA4
A	650	MET	-	EXPRESSION TAG	UNP Q63TA4
A	651	GLY	-	EXPRESSION TAG	UNP Q63TA4
A	652	ARG	-	EXPRESSION TAG	UNP Q63TA4
A	653	GLY	-	EXPRESSION TAG	UNP Q63TA4
A	654	SER	-	EXPRESSION TAG	UNP Q63TA4
A	655	MET	-	EXPRESSION TAG	UNP Q63TA4
A	656	ALA	-	EXPRESSION TAG	UNP Q63TA4
A	993	ASN	-	EXPRESSION TAG	UNP Q63TA4
A	994	SER	-	EXPRESSION TAG	UNP Q63TA4
A	995	SER	-	EXPRESSION TAG	UNP Q63TA4
A	996	SER	-	EXPRESSION TAG	UNP Q63TA4
A	997	VAL	-	EXPRESSION TAG	UNP Q63TA4
A	998	ASP	-	EXPRESSION TAG	UNP Q63TA4
A	999	LYS	-	EXPRESSION TAG	UNP Q63TA4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1000	LEU	-	EXPRESSION TAG	UNP Q63TA4
A	1001	ALA	-	EXPRESSION TAG	UNP Q63TA4
A	1002	ALA	-	EXPRESSION TAG	UNP Q63TA4
A	1003	ALA	-	EXPRESSION TAG	UNP Q63TA4
A	1004	LEU	-	EXPRESSION TAG	UNP Q63TA4
A	1005	GLU	-	EXPRESSION TAG	UNP Q63TA4
A	1006	HIS	-	EXPRESSION TAG	UNP Q63TA4
A	1007	HIS	-	EXPRESSION TAG	UNP Q63TA4
A	1008	HIS	-	EXPRESSION TAG	UNP Q63TA4
A	1009	HIS	-	EXPRESSION TAG	UNP Q63TA4
A	1010	HIS	-	EXPRESSION TAG	UNP Q63TA4
A	1011	HIS	-	EXPRESSION TAG	UNP Q63TA4
B	641	MET	-	EXPRESSION TAG	UNP Q63TA4
B	642	ALA	-	EXPRESSION TAG	UNP Q63TA4
B	643	SER	-	EXPRESSION TAG	UNP Q63TA4
B	644	MET	-	EXPRESSION TAG	UNP Q63TA4
B	645	THR	-	EXPRESSION TAG	UNP Q63TA4
B	646	GLY	-	EXPRESSION TAG	UNP Q63TA4
B	647	GLY	-	EXPRESSION TAG	UNP Q63TA4
B	648	GLN	-	EXPRESSION TAG	UNP Q63TA4
B	649	GLN	-	EXPRESSION TAG	UNP Q63TA4
B	650	MET	-	EXPRESSION TAG	UNP Q63TA4
B	651	GLY	-	EXPRESSION TAG	UNP Q63TA4
B	652	ARG	-	EXPRESSION TAG	UNP Q63TA4
B	653	GLY	-	EXPRESSION TAG	UNP Q63TA4
B	654	SER	-	EXPRESSION TAG	UNP Q63TA4
B	655	MET	-	EXPRESSION TAG	UNP Q63TA4
B	656	ALA	-	EXPRESSION TAG	UNP Q63TA4
B	993	ASN	-	EXPRESSION TAG	UNP Q63TA4
B	994	SER	-	EXPRESSION TAG	UNP Q63TA4
B	995	SER	-	EXPRESSION TAG	UNP Q63TA4
B	996	SER	-	EXPRESSION TAG	UNP Q63TA4
B	997	VAL	-	EXPRESSION TAG	UNP Q63TA4
B	998	ASP	-	EXPRESSION TAG	UNP Q63TA4
B	999	LYS	-	EXPRESSION TAG	UNP Q63TA4
B	1000	LEU	-	EXPRESSION TAG	UNP Q63TA4
B	1001	ALA	-	EXPRESSION TAG	UNP Q63TA4
B	1002	ALA	-	EXPRESSION TAG	UNP Q63TA4
B	1003	ALA	-	EXPRESSION TAG	UNP Q63TA4
B	1004	LEU	-	EXPRESSION TAG	UNP Q63TA4
B	1005	GLU	-	EXPRESSION TAG	UNP Q63TA4
B	1006	HIS	-	EXPRESSION TAG	UNP Q63TA4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1007	HIS	-	EXPRESSION TAG	UNP Q63TA4
B	1008	HIS	-	EXPRESSION TAG	UNP Q63TA4
B	1009	HIS	-	EXPRESSION TAG	UNP Q63TA4
B	1010	HIS	-	EXPRESSION TAG	UNP Q63TA4
B	1011	HIS	-	EXPRESSION TAG	UNP Q63TA4
C	641	MET	-	EXPRESSION TAG	UNP Q63TA4
C	642	ALA	-	EXPRESSION TAG	UNP Q63TA4
C	643	SER	-	EXPRESSION TAG	UNP Q63TA4
C	644	MET	-	EXPRESSION TAG	UNP Q63TA4
C	645	THR	-	EXPRESSION TAG	UNP Q63TA4
C	646	GLY	-	EXPRESSION TAG	UNP Q63TA4
C	647	GLY	-	EXPRESSION TAG	UNP Q63TA4
C	648	GLN	-	EXPRESSION TAG	UNP Q63TA4
C	649	GLN	-	EXPRESSION TAG	UNP Q63TA4
C	650	MET	-	EXPRESSION TAG	UNP Q63TA4
C	651	GLY	-	EXPRESSION TAG	UNP Q63TA4
C	652	ARG	-	EXPRESSION TAG	UNP Q63TA4
C	653	GLY	-	EXPRESSION TAG	UNP Q63TA4
C	654	SER	-	EXPRESSION TAG	UNP Q63TA4
C	655	MET	-	EXPRESSION TAG	UNP Q63TA4
C	656	ALA	-	EXPRESSION TAG	UNP Q63TA4
C	993	ASN	-	EXPRESSION TAG	UNP Q63TA4
C	994	SER	-	EXPRESSION TAG	UNP Q63TA4
C	995	SER	-	EXPRESSION TAG	UNP Q63TA4
C	996	SER	-	EXPRESSION TAG	UNP Q63TA4
C	997	VAL	-	EXPRESSION TAG	UNP Q63TA4
C	998	ASP	-	EXPRESSION TAG	UNP Q63TA4
C	999	LYS	-	EXPRESSION TAG	UNP Q63TA4
C	1000	LEU	-	EXPRESSION TAG	UNP Q63TA4
C	1001	ALA	-	EXPRESSION TAG	UNP Q63TA4
C	1002	ALA	-	EXPRESSION TAG	UNP Q63TA4
C	1003	ALA	-	EXPRESSION TAG	UNP Q63TA4
C	1004	LEU	-	EXPRESSION TAG	UNP Q63TA4
C	1005	GLU	-	EXPRESSION TAG	UNP Q63TA4
C	1006	HIS	-	EXPRESSION TAG	UNP Q63TA4
C	1007	HIS	-	EXPRESSION TAG	UNP Q63TA4
C	1008	HIS	-	EXPRESSION TAG	UNP Q63TA4
C	1009	HIS	-	EXPRESSION TAG	UNP Q63TA4
C	1010	HIS	-	EXPRESSION TAG	UNP Q63TA4
C	1011	HIS	-	EXPRESSION TAG	UNP Q63TA4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total 4	Mg 4	0	0
2	A	1	Total 1	Mg 1	0	0
2	C	2	Total 2	Mg 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total 184	O 184	0	0
3	B	150	Total 150	O 150	0	0
3	C	114	Total 114	O 114	0	0

SER	ASP	GLY	GLY	ARG	SER	ASN	VAL	SER	VAL	GLY	ALA	PRO	GLY	ALA	GLU	ARG	GLN	THR	ASN	VAL	ALA	ALA	GLY	THR	GLN	ALA	THR	ASP	ALA	VAL	ASN	LEU	GLY	GLN	MET	ASN	GLY	ALA	ASN	SER	SER	SER	VAL	ASP	LYS	LEU	ALA	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 58.85Å 74.41Å 90.00° 104.65° 90.00°	Depositor
Resolution (Å)	39.69 – 1.80 39.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.69-1.80) 93.9 (39.69-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.169 , 0.204 0.165 , 0.202	Depositor DCC
R_{free} test set	2341 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 48582 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4746	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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: MG

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	0.37	0/1435	0.51	0/1966
1	B	0.37	0/1448	0.50	0/1985
1	C	0.40	0/1465	0.55	1/2006 (0.0%)
All	All	0.38	0/4348	0.52	1/5957 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	795	GLN	CA-CB-CG	-5.38	101.56	113.40

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	1415	0	1370	5	0
1	B	1431	0	1388	2	0
1	C	1445	0	1395	4	0
2	A	1	0	0	0	0
2	B	4	0	0	0	0
2	C	2	0	0	0	0
3	A	184	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	150	0	0	0	0
3	C	114	0	0	0	0
All	All	4746	0	4153	7	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 1.

The worst 5 of 7 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:C:795:GLN:HG3	1:C:796:ALA:N	2.10	0.67
1:A:847:ILE:HD11	1:C:849:GLY:HA2	1.88	0.55
1:A:841:GLN:HG3	1:C:853:TYR:CE2	2.44	0.53
1:C:800:LEU:HD23	1:C:814:THR:HB	1.90	0.53
1:A:817:ILE:HG21	1:B:827:VAL:HG12	1.91	0.52

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	205/371 (55%)	203 (99%)	2 (1%)	0	100	100
1	B	207/371 (56%)	204 (99%)	3 (1%)	0	100	100
1	C	211/371 (57%)	207 (98%)	4 (2%)	0	100	100
All	All	623/1113 (56%)	614 (99%)	9 (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	147/259 (57%)	147 (100%)	0	100	100
1	B	148/259 (57%)	147 (99%)	1 (1%)	88	86
1	C	149/259 (58%)	148 (99%)	1 (1%)	88	86
All	All	444/777 (57%)	442 (100%)	2 (0%)	92	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	749	THR
1	C	795	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	795	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

Of 7 ligands modelled in this entry, 7 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	208/371 (56%)	-0.32	7 (3%) 49 43	11, 17, 42, 50	0
1	B	211/371 (56%)	-0.24	14 (6%) 22 17	11, 17, 47, 57	0
1	C	214/371 (57%)	-0.25	6 (2%) 56 51	10, 17, 40, 57	0
All	All	633/1113 (56%)	-0.27	27 (4%) 39 32	10, 17, 43, 57	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	874	ALA	5.4
1	B	889	ALA	4.3
1	C	878	GLY	4.0
1	B	883	TYR	3.9
1	A	889	ALA	3.7

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(\AA^2)	Q<0.9
2	MG	B	1892	1/1	0.99	0.10	4.25	24,24,24,24	0
2	MG	C	1894	1/1	0.99	0.07	0.43	23,23,23,23	0
2	MG	A	1892	1/1	0.99	0.06	-1.29	21,21,21,21	0
2	MG	B	1891	1/1	0.99	0.05	-1.73	20,20,20,20	0
2	MG	C	1893	1/1	0.99	0.06	-1.91	21,21,21,21	0
2	MG	B	1893	1/1	0.95	0.14	-	28,28,28,28	0
2	MG	B	1894	1/1	0.88	0.10	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.