



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:12 pm BST

PDB ID : 6BL6
Title : Crystallization of lipid A transporter MsbA from Salmonella typhimurium
Authors : Padayatti, P.S.; Stanfield, R.L.; Zhang, Q.; Wilson, I.A.; Lee, S.C.
Deposited on : 2017-11-09
Resolution : 2.80 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 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 : 2.11
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) : 2.11

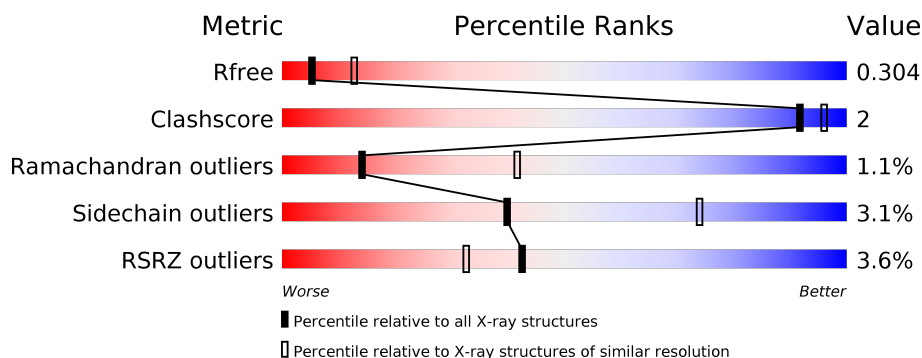
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	576	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	576	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8894 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 Lipid A export ATP-binding/permease protein MsbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4447	2823	770	827	27			
1	B	575	Total	C	N	O	S	0	0	0
			4447	2823	770	827	27			

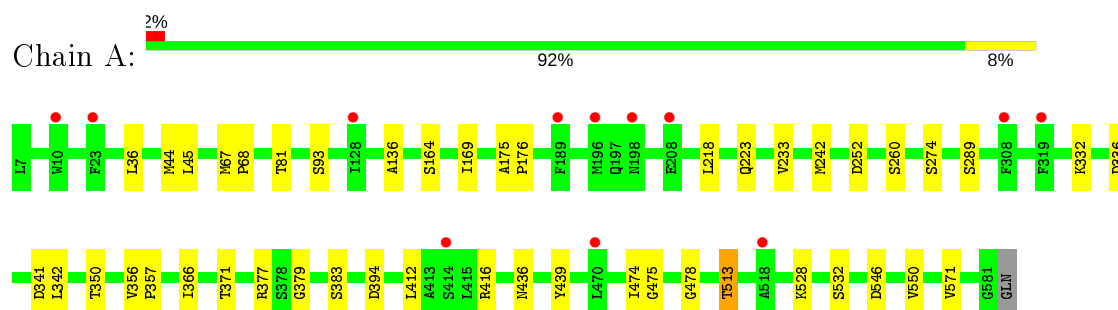
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ALA	LYS	engineered mutation	UNP P63359
B	58	ALA	LYS	engineered mutation	UNP P63359

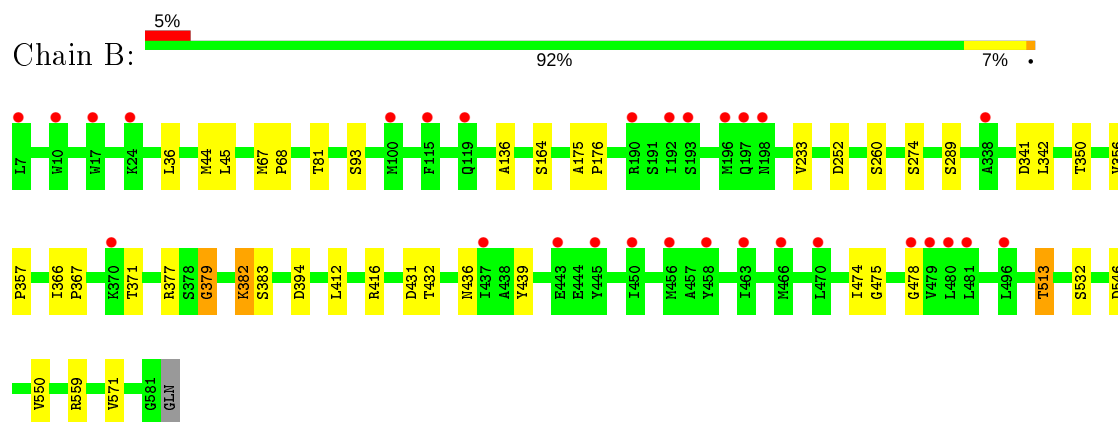
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Lipid A export ATP-binding/permease protein MsbA



- Molecule 1: Lipid A export ATP-binding/permease protein MsbA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.05Å 154.82Å 228.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.80 47.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.9 (50.01-2.80) 82.9 (47.04-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.270 , 0.301 0.277 , 0.304	Depositor DCC
R_{free} test set	2963 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8894	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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

5.1 Standard geometry

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	0.47	0/4514	0.70	0/6101
1	B	0.47	0/4514	0.69	0/6101
All	All	0.47	0/9028	0.69	0/12202

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

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	4447	0	4571	15	0
1	B	4447	0	4571	15	0
All	All	8894	0	9142	28	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 2.

All (28) 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:175:ALA:HB3	1:B:176:PRO:HD3	1.80	0.63
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLY:O	1:B:382:LYS:NZ	2.34	0.60
1:A:412:LEU:HD22	1:A:416:ARG:CZ	2.32	0.60
1:B:412:LEU:HD22	1:B:416:ARG:CZ	2.31	0.60
1:A:550:VAL:HG11	1:A:571:VAL:HG23	1.85	0.58
1:B:550:VAL:HG11	1:B:571:VAL:HG23	1.87	0.55
1:A:342:LEU:HD23	1:A:366:ILE:HD12	1.89	0.55
1:B:342:LEU:HD23	1:B:366:ILE:HD12	1.90	0.54
1:B:350:THR:HG22	1:B:357:PRO:HA	1.90	0.54
1:A:350:THR:HG22	1:A:357:PRO:HA	1.89	0.53
1:B:474:ILE:HG22	1:B:478:GLY:HA2	1.90	0.53
1:A:474:ILE:HG22	1:A:478:GLY:HA2	1.91	0.52
1:A:336:ASP:OD1	1:B:559:ARG:NH1	2.43	0.52
1:A:45:LEU:HD11	1:A:289:SER:HB3	1.93	0.51
1:B:45:LEU:HD11	1:B:289:SER:HB3	1.94	0.48
1:A:93:SER:HB2	1:A:136:ALA:HB1	1.96	0.48
1:A:67:MET:HB3	1:A:68:PRO:HD3	1.97	0.47
1:B:93:SER:HB2	1:B:136:ALA:HB1	1.96	0.46
1:B:67:MET:HB3	1:B:68:PRO:HD3	1.97	0.46
1:B:93:SER:CB	1:B:136:ALA:HB1	2.48	0.43
1:A:36:LEU:HB3	1:A:81:THR:HG21	2.01	0.43
1:B:36:LEU:HB3	1:B:81:THR:HG21	2.00	0.43
1:A:93:SER:CB	1:A:136:ALA:HB1	2.48	0.43
1:A:332:LYS:HD2	1:B:367:PRO:HB3	2.01	0.42
1:A:169:ILE:HA	1:A:169:ILE:HD13	1.95	0.41
1:B:431:ASP:OD1	1:B:432:THR:N	2.53	0.40
1:A:218:LEU:HD23	1:A:223:GLN:HE21	1.86	0.40

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	573/576 (100%)	535 (93%)	31 (5%)	7 (1%)	13	39
1	B	573/576 (100%)	537 (94%)	30 (5%)	6 (1%)	15	44
All	All	1146/1152 (100%)	1072 (94%)	61 (5%)	13 (1%)	14	41

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	THR
1	B	513	THR
1	A	356	VAL
1	B	356	VAL
1	A	164	SER
1	A	439	TYR
1	B	164	SER
1	B	379	GLY
1	B	439	TYR
1	A	379	GLY
1	A	528	LYS
1	A	475	GLY
1	B	475	GLY

5.3.2 Protein sidechains ⓘ

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	485/486 (100%)	470 (97%)	15 (3%)	40	74
1	B	485/486 (100%)	470 (97%)	15 (3%)	40	74
All	All	970/972 (100%)	940 (97%)	30 (3%)	40	74

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	MET
1	A	233	VAL
1	A	242	MET

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Mol	Chain	Res	Type
1	A	252	ASP
1	A	260	SER
1	A	274	SER
1	A	341	ASP
1	A	371	THR
1	A	377	ARG
1	A	383	SER
1	A	394	ASP
1	A	436	ASN
1	A	513	THR
1	A	532	SER
1	A	546	ASP
1	B	44	MET
1	B	233	VAL
1	B	252	ASP
1	B	260	SER
1	B	274	SER
1	B	341	ASP
1	B	371	THR
1	B	377	ARG
1	B	382	LYS
1	B	383	SER
1	B	394	ASP
1	B	436	ASN
1	B	513	THR
1	B	532	SER
1	B	546	ASP

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

Mol	Chain	Res	Type
1	A	477	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	575/576 (99%)	0.26	12 (2%) 63 54	76, 109, 150, 194	0
1	B	575/576 (99%)	0.37	29 (5%) 28 19	78, 120, 171, 226	0
All	All	1150/1152 (99%)	0.32	41 (3%) 42 32	76, 114, 160, 226	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	TRP	4.5
1	A	10	TRP	4.3
1	B	470	LEU	4.2
1	B	17	TRP	3.6
1	B	481	LEU	3.6
1	B	478	GLY	3.4
1	A	23	PHE	3.4
1	B	479	VAL	3.2
1	B	445	TYR	3.2
1	B	456	MET	3.1
1	A	189	PHE	3.0
1	B	190	ARG	2.9
1	B	463	ILE	2.9
1	B	196	MET	2.6
1	B	119	GLN	2.6
1	B	338	ALA	2.6
1	A	208	GLU	2.5
1	A	308	PHE	2.5
1	B	115	PHE	2.5
1	B	7	LEU	2.5
1	A	470	LEU	2.5
1	B	192	ILE	2.5
1	A	198	ASN	2.5
1	B	466	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	319	PHE	2.4
1	B	496	LEU	2.4
1	B	443	GLU	2.3
1	B	370	LYS	2.3
1	B	100	MET	2.3
1	B	437	ILE	2.3
1	B	198	ASN	2.3
1	B	458	TYR	2.2
1	B	450	ILE	2.1
1	A	518	ALA	2.1
1	B	24	LYS	2.1
1	A	128	ILE	2.1
1	B	193	SER	2.0
1	A	196	MET	2.0
1	B	480	LEU	2.0
1	A	414	SER	2.0
1	B	197	GLN	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 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.