



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5A5X
Title : Crystal Structure of Se-Met MltF from Pseudomonas aeruginosa
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Deposited on : 2015-06-23
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

<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
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

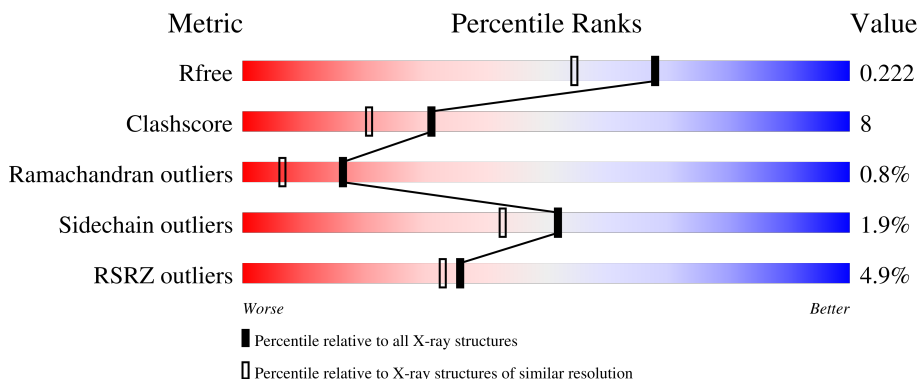
1 Overall quality at a glance

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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 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	453	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>• 7%</div> </div> </div>
2	B	452	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7492 atoms, of which 42 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	Se	0	2	0
			3383	2133	605	636	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	THR	ALA	conflict	UNP Q9HYN1
A	302	LYS	LEU	conflict	UNP Q9HYN1

- Molecule 2 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	417	Total	C	N	O	Se	0	4	0
			3364	2121	600	634	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	MSE	-	expression tag	UNP Q9HYN1
B	302	LYS	LEU	conflict	UNP Q9HYN1

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	317	Total	O	0	0
			317	317		
4	B	358	Total	O	0	0
			358	358		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.99Å 134.98Å 48.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 1.80 43.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.44-1.80) 94.7 (43.44-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.179 , 0.217 0.189 , 0.222	Depositor DCC
R_{free} test set	5054 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7492	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: EDO

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	0.39	0/3450	0.51	0/4647
2	B	0.39	0/3433	0.51	0/4624
All	All	0.39	0/6883	0.51	0/9271

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 [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	3383	0	3343	52	0
2	B	3364	0	3313	57	0
3	A	8	12	12	0	0
3	B	20	30	30	3	0
4	A	317	0	0	7	0
4	B	358	0	0	11	0
All	All	7450	42	6698	109	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 8.

The worst 5 of 109 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)
2:B:113:GLY:HA2	2:B:114:ARG:HB2	1.14	1.13
2:B:154:MSE:HE3	2:B:180:SER:HB3	1.26	1.10
2:B:154:MSE:HE2	2:B:183:VAL:HG21	1.36	1.06
1:A:233:LEU:HD22	1:A:242:MSE:HG2	1.39	1.01
2:B:154:MSE:HE3	2:B:180:SER:CB	2.00	0.92

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	420/453 (93%)	408 (97%)	9 (2%)	3 (1%)	19	9
2	B	419/452 (93%)	405 (97%)	10 (2%)	4 (1%)	13	4
All	All	839/905 (93%)	813 (97%)	19 (2%)	7 (1%)	16	6

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	269	VAL
1	A	117	ASP
1	A	236	GLY
1	A	270	ASP
2	B	270	ASP

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	353/369 (96%)	345 (98%)	8 (2%)	45	34
2	B	350/366 (96%)	344 (98%)	6 (2%)	56	47
All	All	703/735 (96%)	689 (98%)	14 (2%)	52	40

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
2	B	52[A]	SER
2	B	302	LYS
2	B	115	GLU
2	B	209	MSE

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

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	1460	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	A	1458	-	3,3,3	0.45	0	2,2,2	0.44	0
3	EDO	B	1459	-	3,3,3	0.44	0	2,2,2	0.53	0
3	EDO	A	1459	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	B	1462	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	B	1463	-	3,3,3	0.33	0	2,2,2	0.62	0
3	EDO	B	1461	-	3,3,3	0.30	0	2,2,2	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1460	-	-	1/1/1/1	-
3	EDO	A	1458	-	-	0/1/1/1	-
3	EDO	B	1459	-	-	1/1/1/1	-
3	EDO	A	1459	-	-	1/1/1/1	-
3	EDO	B	1462	-	-	0/1/1/1	-
3	EDO	B	1463	-	-	1/1/1/1	-
3	EDO	B	1461	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1460	EDO	O1-C1-C2-O2
3	B	1463	EDO	O1-C1-C2-O2
3	B	1459	EDO	O1-C1-C2-O2
3	A	1459	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1463	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1461	EDO	1	0

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	411/453 (90%)	0.18	23 (5%) 31 29	20, 36, 63, 103	2 (0%)
2	B	408/452 (90%)	0.07	17 (4%) 41 38	12, 33, 56, 89	4 (0%)
All	All	819/905 (90%)	0.13	40 (4%) 36 33	12, 35, 60, 103	6 (0%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	VAL	7.5
2	B	269	VAL	5.8
2	B	270	ASP	4.9
1	A	269	VAL	4.9
2	B	266	TYR	4.5

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, 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	B-factors(\AA^2)	Q<0.9
3	EDO	B	1463	4/4	0.51	0.38	66,80,87,95	0
3	EDO	B	1462	4/4	0.64	0.21	65,78,80,83	0
3	EDO	A	1459	4/4	0.69	0.20	59,71,72,76	0
3	EDO	B	1461	4/4	0.76	0.24	52,63,72,73	0
3	EDO	B	1459	4/4	0.84	0.19	50,69,80,83	0
3	EDO	A	1458	4/4	0.85	0.15	54,65,68,73	0
3	EDO	B	1460	4/4	0.87	0.12	49,58,66,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.