



wwPDB X-ray Structure Validation Summary Report

Jan 24, 2021 – 12:27 PM EST

PDB ID : 2POD
Title : Crystal structure of a member of enolase superfamily from Burkholderia pseudomallei K96243
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Deposited on : 2007-04-26
Resolution : 2.34 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

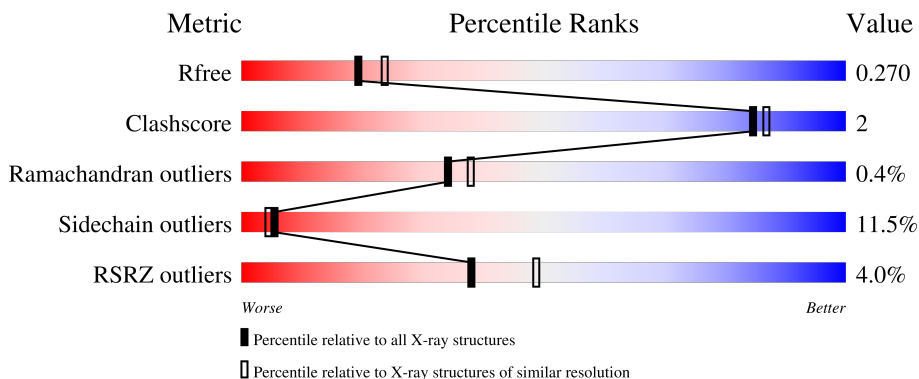
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	410	 2% 80% 12% 8%
1	B	410	 6% 77% 14% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6132 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 Mandelate racemase / muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	379	2987	1900	516	557	6	8	0	1	0
1	B	380	2991	1901	514	562	6	8	0	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP Q63IJ7
A	0	SER	-	cloning artifact	UNP Q63IJ7
A	1	LEU	-	cloning artifact	UNP Q63IJ7
A	81	MSE	MET	modified residue	UNP Q63IJ7
A	173	MSE	MET	modified residue	UNP Q63IJ7
A	213	MSE	MET	modified residue	UNP Q63IJ7
A	216	MSE	MET	modified residue	UNP Q63IJ7
A	249	MSE	MET	modified residue	UNP Q63IJ7
A	291	MSE	MET	modified residue	UNP Q63IJ7
A	309	MSE	MET	modified residue	UNP Q63IJ7
A	383	MSE	MET	modified residue	UNP Q63IJ7
A	401	GLU	-	cloning artifact	UNP Q63IJ7
A	402	GLY	-	cloning artifact	UNP Q63IJ7
A	403	HIS	-	cloning artifact	UNP Q63IJ7
A	404	HIS	-	cloning artifact	UNP Q63IJ7
A	405	HIS	-	cloning artifact	UNP Q63IJ7
A	406	HIS	-	cloning artifact	UNP Q63IJ7
A	407	HIS	-	cloning artifact	UNP Q63IJ7
A	408	HIS	-	cloning artifact	UNP Q63IJ7
B	-1	MSE	-	cloning artifact	UNP Q63IJ7
B	0	SER	-	cloning artifact	UNP Q63IJ7
B	1	LEU	-	cloning artifact	UNP Q63IJ7
B	81	MSE	MET	modified residue	UNP Q63IJ7
B	173	MSE	MET	modified residue	UNP Q63IJ7
B	213	MSE	MET	modified residue	UNP Q63IJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	216	MSE	MET	modified residue	UNP Q63IJ7
B	249	MSE	MET	modified residue	UNP Q63IJ7
B	291	MSE	MET	modified residue	UNP Q63IJ7
B	309	MSE	MET	modified residue	UNP Q63IJ7
B	383	MSE	MET	modified residue	UNP Q63IJ7
B	401	GLU	-	cloning artifact	UNP Q63IJ7
B	402	GLY	-	cloning artifact	UNP Q63IJ7
B	403	HIS	-	cloning artifact	UNP Q63IJ7
B	404	HIS	-	cloning artifact	UNP Q63IJ7
B	405	HIS	-	cloning artifact	UNP Q63IJ7
B	406	HIS	-	cloning artifact	UNP Q63IJ7
B	407	HIS	-	cloning artifact	UNP Q63IJ7
B	408	HIS	-	cloning artifact	UNP Q63IJ7

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0

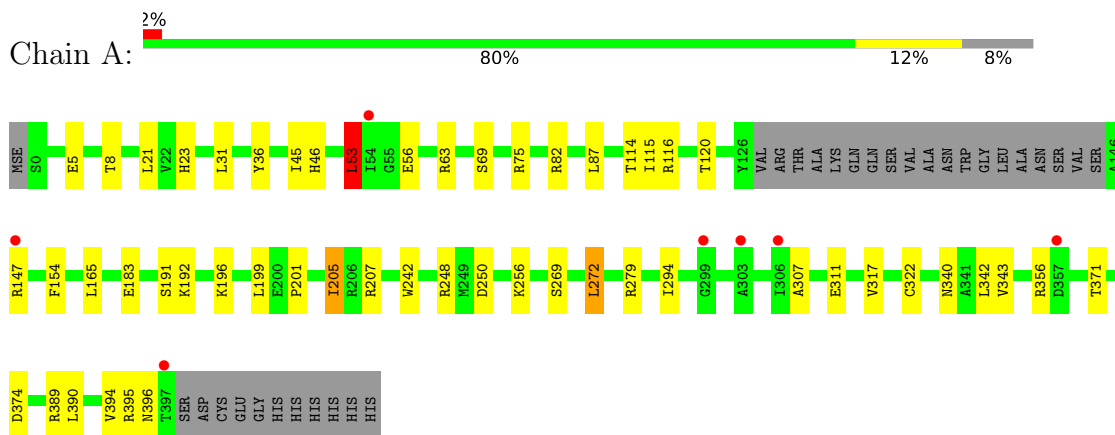
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	88	Total O 88 88	0	0
3	B	64	Total O 64 64	0	0

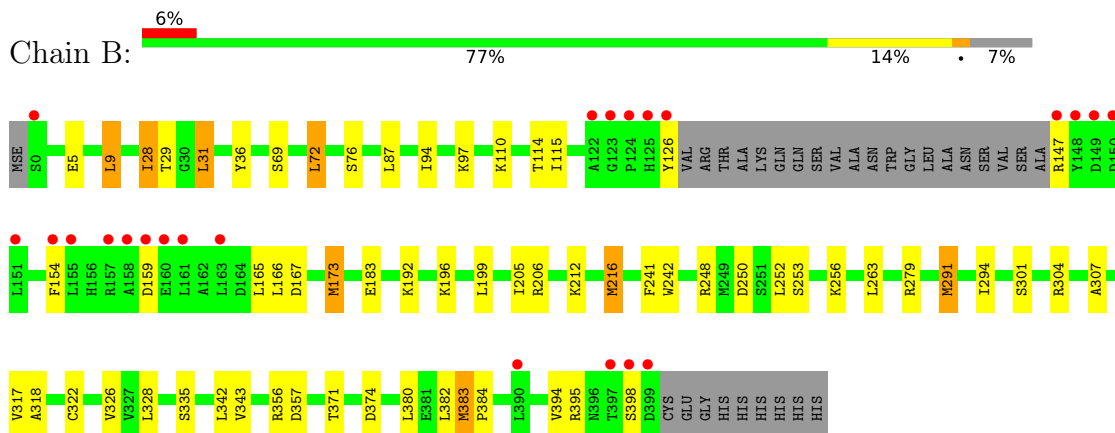
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Mandelate racemase / muconate lactonizing enzyme



- Molecule 1: Mandelate racemase / muconate lactonizing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.77Å 146.77Å 85.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.34 46.41 – 2.34	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.34) 90.7 (46.41-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.209 , 0.275 0.205 , 0.270	Depositor DCC
R_{free} test set	1077 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtrriage
Anisotropy	0.431	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6132	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: NA

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	0/3056	0.63	1/4144 (0.0%)
1	B	0.40	0/3060	0.63	1/4150 (0.0%)
All	All	0.40	0/6116	0.63	2/8294 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	9	LEU	CA-CB-CG	5.25	127.37	115.30

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	2987	0	2931	12	0
1	B	2991	0	2927	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	88	0	0	0	0
3	B	64	0	0	0	0
All	All	6132	0	5858	27	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.

The worst 5 of 27 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:8:THR:OG1	1:A:46:HIS:HE1	1.86	0.58
1:B:216:MSE:HE2	1:B:241:PHE:HB3	1.89	0.55
1:B:28:ILE:HD11	1:B:94:ILE:HA	1.89	0.54
1:A:75:ARG:HB3	1:B:76[A]:SER:HB3	1.92	0.50
1:A:307:ALA:HA	1:A:317:VAL:HG21	1.92	0.50

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	376/410 (92%)	364 (97%)	11 (3%)	1 (0%)	41	47
1	B	377/410 (92%)	357 (95%)	18 (5%)	2 (0%)	29	31
All	All	753/820 (92%)	721 (96%)	29 (4%)	3 (0%)	34	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	TYR
1	B	36	TYR
1	B	322	CYS

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	312/328 (95%)	278 (89%)	34 (11%)	6	5
1	B	314/328 (96%)	276 (88%)	38 (12%)	5	4
All	All	626/656 (95%)	554 (88%)	72 (12%)	5	4

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	ARG
1	B	110	LYS
1	B	343	VAL
1	A	396	ASN
1	B	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	B	344	GLN
1	B	16	ASN
1	A	125	HIS
1	B	125	HIS

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	371/410 (90%)	0.04	7 (1%) 66 75	32, 47, 71, 104	0
1	B	372/410 (90%)	0.26	23 (6%) 20 28	34, 50, 75, 109	0
All	All	743/820 (90%)	0.15	30 (4%) 38 49	32, 48, 74, 109	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	TYR	6.5
1	B	147	ARG	5.7
1	B	123	GLY	5.0
1	A	147	ARG	4.5
1	B	398	SER	4.3

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
2	NA	A	409	1/1	0.78	0.15	73,73,73,73	0
2	NA	B	409	1/1	0.86	0.12	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.