



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:42 PM GMT

PDB ID : 4PPM
Title : Crystal structure of PigE: a transaminase involved in the biosynthesis of 2-methyl-3-n-amyI-pyrrole (MAP) from *Serratia* sp. FS14
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Deposited on : 2014-02-27
Resolution : 2.30 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 : 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

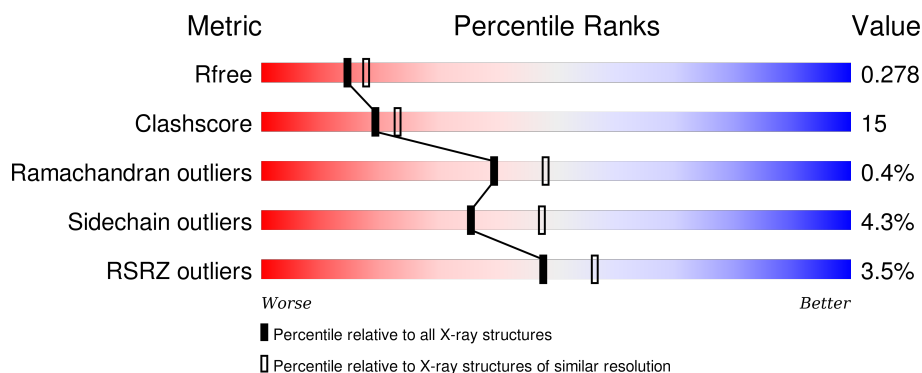
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	861	
1	B	861	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7493 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 Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3563	2265	617	657	24			
1	B	462	Total	C	N	O	S	0	0	0
			3554	2263	615	652	24			

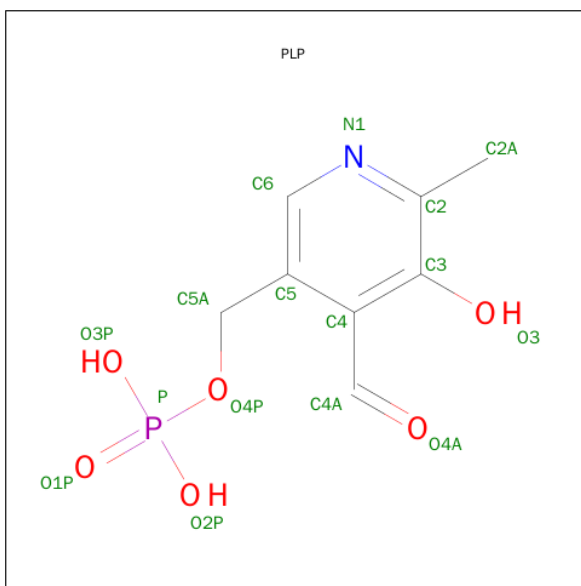
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	LEU	-	EXPRESSION TAG	UNP A0A059ZJX2
A	855	GLU	-	EXPRESSION TAG	UNP A0A059ZJX2
A	856	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
A	857	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
A	858	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
A	859	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
A	860	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
A	861	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
B	854	LEU	-	EXPRESSION TAG	UNP A0A059ZJX2
B	855	GLU	-	EXPRESSION TAG	UNP A0A059ZJX2
B	856	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
B	857	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
B	858	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
B	859	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
B	860	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2
B	861	HIS	-	EXPRESSION TAG	UNP A0A059ZJX2

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

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total	O	0	0
			160	160		
4	B	184	Total	O	0	0
			184	184		



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.10 Å 228.10 Å 67.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.30 19.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.89-2.30) 100.0 (19.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.30 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.238 , 0.272 0.251 , 0.278	Depositor DCC
R_{free} test set	4443 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.5	EDS
Estimated twinning fraction	0.340 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 88591 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: MG, PLP

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	1.41	7/3633 (0.2%)	0.94	19/4920 (0.4%)
1	B	1.36	6/3626 (0.2%)	0.95	20/4912 (0.4%)
All	All	1.39	13/7259 (0.2%)	0.95	39/9832 (0.4%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	GLU	CD-OE2	-5.65	1.19	1.25
1	A	508	GLU	CD-OE1	-5.60	1.19	1.25
1	A	508	GLU	CD-OE2	-5.57	1.19	1.25
1	B	404	PRO	N-CD	5.52	1.55	1.47
1	B	552	PRO	N-CD	5.44	1.55	1.47

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	590	GLY	N-CA-C	6.99	130.58	113.10
1	A	593	ILE	C-N-CD	6.29	141.61	128.40
1	B	725	TYR	C-N-CD	6.16	141.34	128.40
1	A	594	PRO	C-N-CD	6.02	141.04	128.40

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	3563	0	3567	100	0
1	B	3554	0	3558	132	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
4	A	160	0	0	5	0
4	B	184	0	0	6	0
All	All	7493	0	7137	216	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 15.

The worst 5 of 216 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:727:PHE:HB3	1:A:744:GLN:NE2	1.44	1.32
1:A:588:GLU:O	1:A:816:ASN:HB2	1.43	1.14
1:B:388:THR:HG22	4:B:1037:HOH:O	1.55	1.06
1:A:727:PHE:CB	1:A:744:GLN:HE21	1.69	1.05
1:A:727:PHE:HB3	1:A:744:GLN:HE21	0.89	1.04

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	460/861 (53%)	432 (94%)	26 (6%)	2 (0%)	39	48
1	B	458/861 (53%)	440 (96%)	16 (4%)	2 (0%)	39	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	918/1722 (53%)	872 (95%)	42 (5%)	4 (0%)	39 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	645	LYS
1	B	645	LYS
1	A	644	SER
1	B	644	SER

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	372/692 (54%)	360 (97%)	12 (3%)	46 62
1	B	371/692 (54%)	351 (95%)	20 (5%)	27 36
All	All	743/1384 (54%)	711 (96%)	32 (4%)	35 47

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	521	PRO
1	B	550	PHE
1	B	812	PHE
1	B	544	ASP
1	B	572	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	744	GLN
1	B	824	GLN
1	A	805	GLN
1	A	741	GLN

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Mol	Chain	Res	Type
1	A	777	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	PLP	A	902	1	15,15,16	3.09	9 (60%)	21,22,23	2.02	7 (33%)
3	PLP	B	902	1	15,15,16	2.94	7 (46%)	21,22,23	1.70	4 (19%)

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	PLP	A	902	1	-	0/6/6/8	0/1/1/1
3	PLP	B	902	1	-	0/6/6/8	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	PLP	P-O3P	-4.02	1.40	1.54
3	A	902	PLP	P-O2P	-3.88	1.40	1.54
3	B	902	PLP	P-O2P	-3.82	1.41	1.54
3	B	902	PLP	P-O3P	-3.59	1.41	1.54
3	A	902	PLP	P-O1P	-3.39	1.40	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	PLP	C3-C4-C5	-2.70	115.83	118.78
3	A	902	PLP	C6-N1-C2	2.11	123.59	119.28
3	B	902	PLP	C6-N1-C2	2.27	123.90	119.28
3	A	902	PLP	O3P-P-O1P	2.46	118.50	110.58
3	A	902	PLP	C5A-C5-C4	2.54	125.02	121.65

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	464/861 (53%)	-0.22	14 (3%) 54 63	17, 33, 60, 93	0
1	B	462/861 (53%)	-0.14	18 (3%) 43 52	17, 38, 68, 96	0
All	All	926/1722 (53%)	-0.18	32 (3%) 48 56	17, 36, 65, 96	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	765	TRP	7.3
1	B	372	ALA	6.0
1	B	374	PRO	5.2
1	B	766	HIS	5.0
1	A	372	ALA	4.9

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	901	1/1	0.88	0.20	0.47	30,30,30,30	0
3	PLP	A	902	15/16	0.97	0.08	-0.72	21,26,33,35	0
3	PLP	B	902	15/16	0.98	0.09	-0.88	24,29,33,34	0
2	MG	A	901	1/1	0.87	0.06	-1.91	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.