



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:14 am GMT

PDB ID : 1GC0
Title : CRYSTAL STRUCTURE OF THE PYRIDOXAL-5'-PHOSPHATE
DEPENDENT L-METHIONINE GAMMA-LYASE FROM PSEUDOMONAS
PUTIDA
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Deposited on : 2000-07-06
Resolution : 1.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

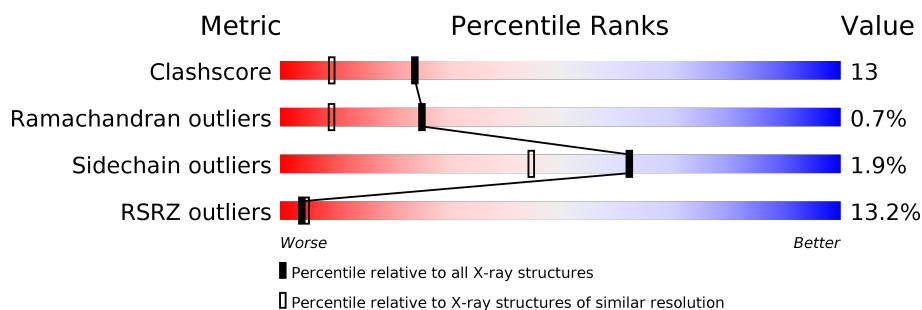
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

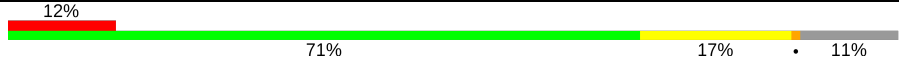



The reported resolution of this entry is 1.70 Å.

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))
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	398	
1	B	398	
1	C	398	
1	D	398	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12053 atoms, of which 0 are hydrogens and 0 are deuteriums.

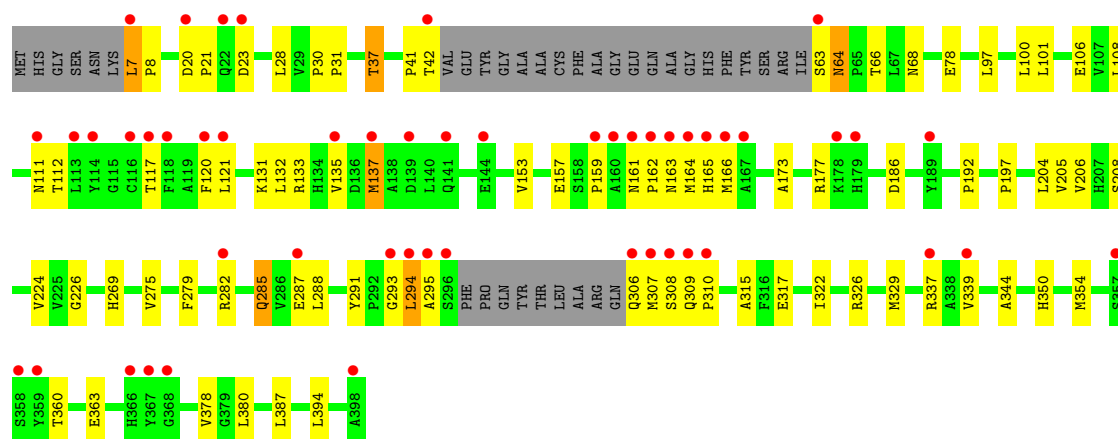
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHIONINE GAMMA-LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	P	S	0	0	0
			2681	1690	474	501	1	15			
1	B	357	Total	C	N	O	P	S	0	0	0
			2695	1699	475	505	1	15			
1	C	363	Total	C	N	O	P	S	0	0	0
			2734	1721	483	513	1	16			
1	D	356	Total	C	N	O	P	S	0	0	0
			2685	1692	475	502	1	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	362	Total	O	0	0
			362	362		
2	B	310	Total	O	0	0
			310	310		
2	C	324	Total	O	0	0
			324	324		
2	D	262	Total	O	0	0
			262	262		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.86Å 81.03Å 81.28Å 70.56° 63.17° 63.38°	Depositor
Resolution (Å)	71.46 – 1.70 71.55 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (71.46-1.70) 85.0 (71.55-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 1.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.210 , 0.236 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,h-k,h-l 0.478 for -h,-h+l,-h+k 0.477 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12053	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, 0.333 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: LLP

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	0.28	0/2710	0.59	1/3677 (0.0%)
1	B	0.29	0/2724	0.58	1/3696 (0.0%)
1	C	0.28	0/2763	0.58	1/3748 (0.0%)
1	D	0.28	0/2714	0.59	1/3682 (0.0%)
All	All	0.29	0/10911	0.59	4/14803 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	SER	N-CA-C	-5.80	95.33	111.00
1	D	208	SER	N-CA-C	-5.65	95.74	111.00
1	C	208	SER	N-CA-C	-5.61	95.85	111.00
1	A	208	SER	N-CA-C	-5.51	96.12	111.00

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	2681	0	2658	65	0
1	B	2695	0	2672	61	0
1	C	2734	0	2710	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2685	0	2660	73	0
2	A	362	0	0	14	0
2	B	310	0	0	15	0
2	C	324	0	0	9	0
2	D	262	0	0	15	0
All	All	12053	0	10700	269	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 13.

The worst 5 of 269 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:121:LEU:HB3	1:C:132:LEU:HD21	1.43	1.00
1:C:111:ASN:H	1:C:137:MET:HE2	1.33	0.93
1:A:313:MET:HG3	2:A:628:HOH:O	1.72	0.90
1:D:313:MET:HG3	2:D:581:HOH:O	1.75	0.86
1:C:380:LEU:HG	2:C:679:HOH:O	1.77	0.85

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	348/398 (87%)	334 (96%)	12 (3%)	2 (1%)	28	12
1	B	350/398 (88%)	339 (97%)	10 (3%)	1 (0%)	44	25
1	C	356/398 (89%)	345 (97%)	9 (2%)	2 (1%)	28	12
1	D	349/398 (88%)	335 (96%)	9 (3%)	5 (1%)	13	2
All	All	1403/1592 (88%)	1353 (96%)	40 (3%)	10 (1%)	25	9

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	PRO
1	D	114	TYR
1	D	162	PRO
1	A	114	TYR
1	C	294	LEU

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	274/306 (90%)	271 (99%)	3 (1%)	78	68
1	B	276/306 (90%)	271 (98%)	5 (2%)	64	47
1	C	280/306 (92%)	274 (98%)	6 (2%)	59	40
1	D	274/306 (90%)	267 (97%)	7 (3%)	51	31
All	All	1104/1224 (90%)	1083 (98%)	21 (2%)	62	45

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	37	THR
1	C	137	MET
1	D	285	GLN
1	C	7	LEU
1	D	341	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	ASN
1	C	274	GLN
1	D	290	HIS
1	C	68	ASN
1	C	269	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	211	1	24,24,25	1.54	5 (20%)	28,32,34	2.23	11 (39%)
1	LLP	B	211	1	24,24,25	1.52	5 (20%)	28,32,34	2.22	11 (39%)
1	LLP	C	211	1	24,24,25	1.52	5 (20%)	28,32,34	2.22	11 (39%)
1	LLP	D	211	1	24,24,25	1.54	5 (20%)	28,32,34	2.22	11 (39%)

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
1	LLP	A	211	1	-	0/15/17/19	0/1/1/1
1	LLP	B	211	1	-	0/15/17/19	0/1/1/1
1	LLP	C	211	1	-	0/15/17/19	0/1/1/1
1	LLP	D	211	1	-	0/15/17/19	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	LLP	O3-C3	-2.21	1.31	1.37
1	C	211	LLP	O3-C3	-2.18	1.32	1.37
1	A	211	LLP	O3-C3	-2.15	1.32	1.37
1	D	211	LLP	O3-C3	-2.04	1.32	1.37
1	B	211	LLP	C4-C3	2.17	1.44	1.40

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	LLP	C5-C6-N1	-3.94	117.20	123.87
1	B	211	LLP	C5-C6-N1	-3.92	117.24	123.87
1	D	211	LLP	C5-C6-N1	-3.89	117.28	123.87
1	A	211	LLP	C5-C6-N1	-3.86	117.34	123.87
1	A	211	LLP	C5'-C5-C6	-3.58	113.17	119.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	211	LLP	2	0
1	D	211	LLP	1	0

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 [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	354/398 (88%)	0.91	46 (12%) 4 5	8, 16, 35, 42	0
1	B	356/398 (89%)	0.89	42 (11%) 5 6	8, 16, 35, 42	0
1	C	362/398 (90%)	1.03	51 (14%) 3 4	8, 17, 37, 47	0
1	D	355/398 (89%)	0.96	49 (13%) 3 4	8, 16, 35, 42	0
All	All	1427/1592 (89%)	0.95	188 (13%) 4 4	8, 16, 36, 47	0

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	TYR	11.1
1	D	114	TYR	10.4
1	C	114	TYR	9.6
1	A	116	CYS	8.4
1	D	166	MET	8.2

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	LLP	B	211	24/25	0.88	0.18	-	9,19,22,23	0
1	LLP	D	211	24/25	0.90	0.16	-	10,19,22,23	0
1	LLP	A	211	24/25	0.90	0.17	-	10,20,23,24	0
1	LLP	C	211	24/25	0.91	0.13	-	9,20,22,23	0

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.