



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:46 PM UTC

PDB ID : 3LXZ / pdb_00003lxz
Title : Structure of probable Glutathione S-transferase(PP0183) from Pseudomonas putida
Authors : Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-02-25
Resolution : 1.76 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

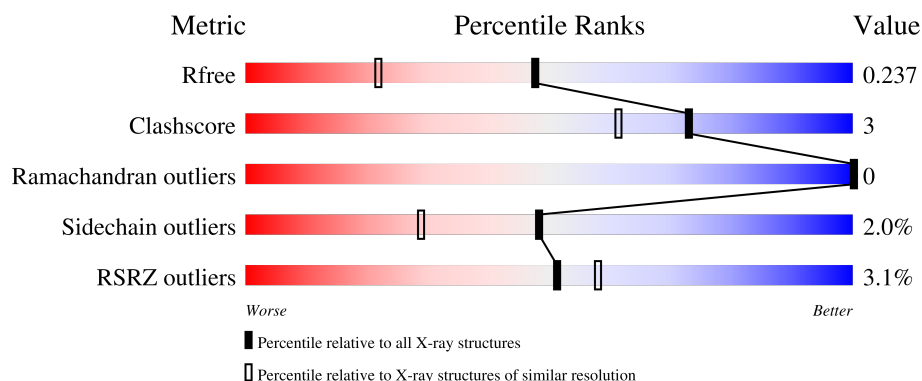
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	229	2% 91% 5%
1	B	229	3% 90% 5%
1	C	229	3% 86% 9% 5%
1	D	229	3% 86% 8% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7538 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 Glutathione S-transferase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	Se	0	1	0
			1699	1101	272	316	2	8			
1	B	217	Total	C	N	O	S	Se	0	5	0
			1729	1120	279	320	2	8			
1	C	218	Total	C	N	O	S	Se	0	6	0
			1747	1127	286	324	2	8			
1	D	217	Total	C	N	O	S	Se	0	3	0
			1710	1105	279	316	2	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	expression tag	UNP Q88RE7
A	1	SER	-	expression tag	UNP Q88RE7
A	221	GLU	-	expression tag	UNP Q88RE7
A	222	GLY	-	expression tag	UNP Q88RE7
A	223	HIS	-	expression tag	UNP Q88RE7
A	224	HIS	-	expression tag	UNP Q88RE7
A	225	HIS	-	expression tag	UNP Q88RE7
A	226	HIS	-	expression tag	UNP Q88RE7
A	227	HIS	-	expression tag	UNP Q88RE7
A	228	HIS	-	expression tag	UNP Q88RE7
B	0	MSE	-	expression tag	UNP Q88RE7
B	1	SER	-	expression tag	UNP Q88RE7
B	221	GLU	-	expression tag	UNP Q88RE7
B	222	GLY	-	expression tag	UNP Q88RE7
B	223	HIS	-	expression tag	UNP Q88RE7
B	224	HIS	-	expression tag	UNP Q88RE7
B	225	HIS	-	expression tag	UNP Q88RE7
B	226	HIS	-	expression tag	UNP Q88RE7
B	227	HIS	-	expression tag	UNP Q88RE7
B	228	HIS	-	expression tag	UNP Q88RE7
C	0	MSE	-	expression tag	UNP Q88RE7

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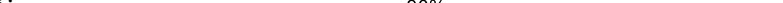
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	-	expression tag	UNP Q88RE7
C	221	GLU	-	expression tag	UNP Q88RE7
C	222	GLY	-	expression tag	UNP Q88RE7
C	223	HIS	-	expression tag	UNP Q88RE7
C	224	HIS	-	expression tag	UNP Q88RE7
C	225	HIS	-	expression tag	UNP Q88RE7
C	226	HIS	-	expression tag	UNP Q88RE7
C	227	HIS	-	expression tag	UNP Q88RE7
C	228	HIS	-	expression tag	UNP Q88RE7
D	0	MSE	-	expression tag	UNP Q88RE7
D	1	SER	-	expression tag	UNP Q88RE7
D	221	GLU	-	expression tag	UNP Q88RE7
D	222	GLY	-	expression tag	UNP Q88RE7
D	223	HIS	-	expression tag	UNP Q88RE7
D	224	HIS	-	expression tag	UNP Q88RE7
D	225	HIS	-	expression tag	UNP Q88RE7
D	226	HIS	-	expression tag	UNP Q88RE7
D	227	HIS	-	expression tag	UNP Q88RE7
D	228	HIS	-	expression tag	UNP Q88RE7

- Molecule 2 is water.

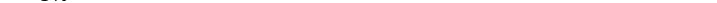
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	148	Total O 148 148	0	0
2	B	181	Total O 181 181	0	0
2	C	170	Total O 170 170	0	0
2	D	154	Total O 154 154	0	0

- Molecule 1: Glutathione S-transferase family protein



- Chain B:  3% 90% 5%



- Chain C:  3% 86% 9% 5%



- Chain D:  3% 86% 8% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.05Å 66.36Å 88.66Å 89.96° 85.27° 87.04°	Depositor
Resolution (Å)	50.00 – 1.76 50.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-1.76) 90.5 (50.00-1.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.229 0.206 , 0.237	Depositor DCC
R_{free} test set	4901 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.064 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7538	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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](#)

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	0.82	0/1726	0.92	0/2318
1	B	0.86	1/1755 (0.1%)	0.91	0/2355
1	C	0.86	0/1773	0.94	2/2377 (0.1%)
1	D	0.85	0/1735	0.91	0/2328
All	All	0.85	1/6989 (0.0%)	0.92	2/9378 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	GLU	C-O	-6.31	1.16	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	LEU	CA-C-N	-5.28	113.19	119.05
1	C	102	LEU	C-N-CA	-5.28	113.19	119.05

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	1699	0	1717	6	0
1	B	1729	0	1755	6	0
1	C	1747	0	1767	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1710	0	1737	12	0
2	A	148	0	0	1	0
2	B	181	0	0	3	0
2	C	170	0	0	2	0
2	D	154	0	0	6	0
All	All	7538	0	6976	45	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 3.

All (45) 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:208:MSE:SE	1:C:212:MSE:HE3	2.21	0.90
1:C:211:PHE:CD2	1:C:212:MSE:HE2	2.08	0.87
1:C:211:PHE:CD2	1:C:212:MSE:CE	2.61	0.83
1:C:211:PHE:HD2	1:C:212:MSE:CE	2.02	0.71
1:C:47:GLY:HA2	2:C:245:HOH:O	1.93	0.68
1:D:126:ARG:NH1	1:D:175:ILE:HD11	2.08	0.68
1:C:211:PHE:HD2	1:C:212:MSE:HE2	1.57	0.65
1:A:126:ARG:HH11	1:A:175:ILE:HD11	1.61	0.64
1:D:126:ARG:HH12	1:D:175:ILE:HD11	1.64	0.62
1:C:211:PHE:CE2	1:C:212:MSE:HE1	2.36	0.61
1:C:214:MSE:HE3	1:C:215:ILE:CD1	2.31	0.61
1:A:185:LYS:HE2	2:A:443:HOH:O	2.01	0.61
1:B:47:GLY:HA2	2:B:281:HOH:O	2.02	0.58
1:D:118:GLU:HG3	2:D:274:HOH:O	2.05	0.56
1:C:214:MSE:HE3	1:C:215:ILE:HD13	1.88	0.56
1:C:211:PHE:CD2	1:C:212:MSE:HE1	2.38	0.55
1:D:47:GLY:HA2	2:D:261:HOH:O	2.06	0.55
1:A:126:ARG:NH1	1:A:175:ILE:HD11	2.23	0.54
1:B:167:ALA:O	1:B:171:LYS:HD3	2.08	0.53
1:B:171:LYS:HD3	1:B:171:LYS:N	2.23	0.52
1:C:166:ASN:HD21	1:C:177:PHE:N	2.08	0.52
1:A:185:LYS:HD3	2:D:248:HOH:O	2.10	0.52
1:C:39[B]:GLN:CD	1:C:39[B]:GLN:H	2.19	0.51
1:C:46:ARG:O	1:C:46:ARG:HG3	2.11	0.50
1:B:190:LEU:C	1:B:190:LEU:HD23	2.37	0.50
1:D:183:GLN:CG	2:D:420:HOH:O	2.59	0.50
1:C:190:LEU:C	1:C:190:LEU:HD23	2.39	0.48
1:D:11:ASN:O	1:D:15:MSE:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:PHE:HB3	1:D:115:MSE:HE3	1.97	0.47
1:A:6:GLY:HA3	1:A:13:TYR:CD1	2.53	0.44
1:C:141:ARG:NH1	2:C:360:HOH:O	2.51	0.44
1:C:44:SER:HB2	1:C:51:VAL:HG21	1.99	0.43
1:C:166:ASN:HD21	1:C:177:PHE:H	1.66	0.43
1:C:166:ASN:ND2	1:C:177:PHE:H	2.16	0.43
1:D:6:GLY:HA3	1:D:13:TYR:CD1	2.52	0.43
1:A:92:LEU:HD13	1:A:146:VAL:HG12	2.01	0.43
1:D:183:GLN:HG2	2:D:420:HOH:O	2.17	0.43
1:D:44:SER:HB2	1:D:51:VAL:HG21	2.02	0.42
1:D:137:LYS:HE3	2:D:651:HOH:O	2.18	0.42
1:B:183:GLN:HG2	2:B:319:HOH:O	2.19	0.41
1:B:171:LYS:HD3	1:B:171:LYS:H	1.86	0.41
1:C:18:LEU:HD23	1:C:156:LEU:HD22	2.02	0.41
1:C:45:PRO:HB2	1:D:135:THR:HG23	2.03	0.41
1:C:112:PHE:N	1:C:112:PHE:CD1	2.89	0.41
2:B:240:HOH:O	1:C:185:LYS:HD3	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	217/229 (95%)	213 (98%)	4 (2%)	0	100	100
1	B	220/229 (96%)	215 (98%)	5 (2%)	0	100	100
1	C	222/229 (97%)	219 (99%)	3 (1%)	0	100	100
1	D	218/229 (95%)	214 (98%)	4 (2%)	0	100	100
All	All	877/916 (96%)	861 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	179/180 (99%)	175 (98%)	4 (2%)	45	26
1	B	184/180 (102%)	178 (97%)	6 (3%)	33	13
1	C	185/180 (103%)	182 (98%)	3 (2%)	55	38
1	D	181/180 (101%)	177 (98%)	4 (2%)	45	26
All	All	729/720 (101%)	712 (98%)	17 (2%)	48	24

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	120	LEU
1	A	180[A]	ASP
1	A	180[B]	ASP
1	B	39	GLN
1	B	49	VAL
1	B	117[A]	VAL
1	B	117[B]	VAL
1	B	201[A]	LEU
1	B	201[B]	LEU
1	C	49	VAL
1	C	189	GLN
1	C	214	MSE
1	D	49	VAL
1	D	120	LEU
1	D	171	LYS
1	D	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	GLN
1	C	56	HIS

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Mol	Chain	Res	Type
1	C	166	ASN
1	C	189	GLN
1	D	189	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 oligosaccharides 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	210/229 (91%)	0.12	4 (1%) 66 73	13, 21, 33, 47	1 (0%)
1	B	209/229 (91%)	-0.06	8 (3%) 44 50	9, 18, 32, 47	5 (2%)
1	C	210/229 (91%)	-0.02	7 (3%) 49 55	9, 18, 30, 49	6 (2%)
1	D	209/229 (91%)	0.04	7 (3%) 49 55	10, 19, 33, 55	3 (1%)
All	All	838/916 (91%)	0.02	26 (3%) 51 58	9, 19, 33, 55	15 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	PHE	4.6
1	B	112	PHE	3.5
1	B	1	SER	3.5
1	D	113	PHE	3.5
1	A	1	SER	3.5
1	A	112	PHE	3.3
1	C	113	PHE	3.2
1	D	112	PHE	3.2
1	C	1	SER	3.1
1	A	218	GLY	2.9
1	B	215	ILE	2.9
1	B	217	SER	2.7
1	D	215	ILE	2.5
1	C	180	ASP	2.5
1	D	1	SER	2.5
1	B	113	PHE	2.5
1	B	114	GLY	2.3
1	D	216	ARG	2.3
1	C	218	GLY	2.2
1	A	117	VAL	2.2
1	D	114	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	171	LYS	2.1
1	D	217	SER	2.1
1	C	174[A]	ASN	2.0
1	C	217	SER	2.0
1	B	216	ARG	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 oligosaccharides 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.