



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:24 PM EDT

PDB ID : 7SZT / pdb_00007szt
Title : Crystal structure of Gdx-Clo from Small Multidrug Resistance family of transporters in low pH (protonated state)
Authors : Kermani, A.A.; Stockbridge, R.B.; Burata, O.E.
Deposited on : 2021-11-29
Resolution : 2.32 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 2.32 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5966 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.

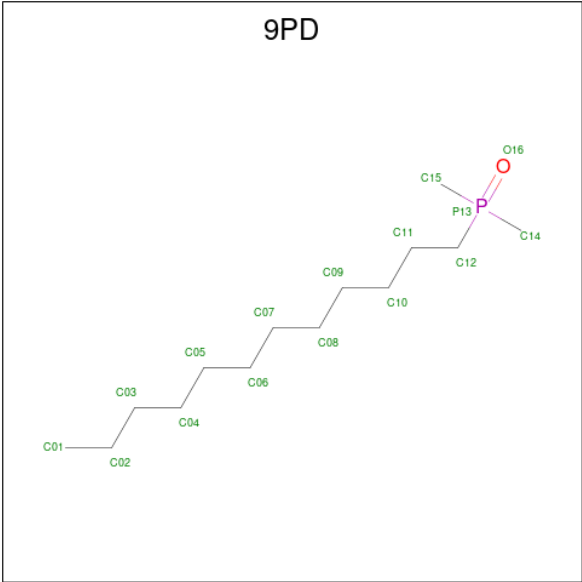
- Molecule 1 is a protein called Multidrug resistance protein, SMR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	2	0
			814	559	121	129	5			
1	B	104	Total	C	N	O	S	0	0	0
			792	541	119	127	5			
1	C	104	Total	C	N	O	S	0	1	0
			803	550	120	128	5			
1	D	104	Total	C	N	O	S	0	0	0
			792	541	119	127	5			

- Molecule 2 is a protein called L10 monobody.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	88	Total	C	N	O	0	0	0
			679	439	105	135			
2	F	89	Total	C	N	O	0	0	0
			691	448	106	137			
2	H	87	Total	C	N	O	0	0	0
			677	441	103	133			
2	G	89	Total	C	N	O	0	0	0
			691	448	106	137			

- Molecule 3 is Dodecyldimethylphosphine oxide (CCD ID: 9PD) (formula: C₁₄H₃₁OP).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	14	1	1		
3	F	1	Total	C	O	P	0	0
			11	9	1	1		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.70Å 74.32Å 107.43Å 93.56° 89.71° 109.92°	Depositor
Resolution (Å)	32.68 – 2.32	Depositor
% Data completeness (in resolution range)	41.8 (32.68-2.32)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.251 , 0.294	Depositor
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.052	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.417 for h,-h-k,-l	Xtriage
Total number of atoms	5966	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 5.92% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

2 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	9PD	A	201	-	14,15,15	1.36	2 (14%)	14,17,17	1.05	1 (7%)
3	9PD	F	301	-	9,10,15	1.65	2 (22%)	9,12,17	1.33	1 (11%)

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	9PD	A	201	-	-	6/13/13/13	-
3	9PD	F	301	-	-	3/8/8/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	9PD	P13-C14	3.45	1.86	1.78
3	F	301	9PD	P13-C15	3.44	1.86	1.78
3	A	201	9PD	P13-C15	3.38	1.86	1.78
3	F	301	9PD	P13-C14	3.21	1.86	1.78

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	9PD	O16-P13-C14	-2.98	108.57	113.32
3	A	201	9PD	O16-P13-C15	-2.69	109.03	113.32

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	301	9PD	C09-C10-C11-C12
3	A	201	9PD	C03-C04-C05-C06
3	A	201	9PD	C08-C09-C10-C11
3	A	201	9PD	C09-C10-C11-C12
3	A	201	9PD	C10-C11-C12-P13
3	F	301	9PD	C07-C08-C09-C10

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Mol	Chain	Res	Type	Atoms
3	A	201	9PD	C06-C07-C08-C09
3	A	201	9PD	C07-C08-C09-C10
3	F	301	9PD	C06-C07-C08-C09

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

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5.4 Ligands [i](#)

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5.5 Other polymers [i](#)

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