

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 10:38 AM EDT

PDB ID	:	6MTW
Title	:	Lysosomal Phospholipase A2 in complex with Zinc
Authors	:	Bouley, R.; Tesmer, J.J.G.
Deposited on		
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 2.00 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.



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6446 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.

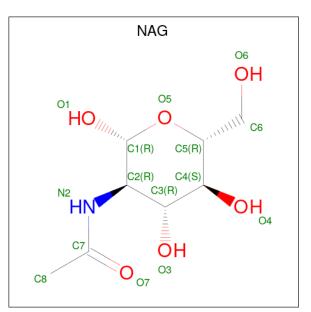
• Molecule 1 is a protein called Group XV phospholipase A2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	376	Total	С	Ν	0	\mathbf{S}	0	0	0
	A		3019	1949	507	550	13	0	0	
1	р	376	Total	С	Ν	0	S	0	0	0
1	D	570	3019	1949	507	550	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8NCC3
В	0	GLY	-	expression tag	UNP Q8NCC3

• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C N O 14 8 1 5	0	0
2	В	1	Total C N O 14 8 1 5	0	0
2	В	1	Total C N O 14 8 1 5	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cl 1 1	0	0
3	В	1	Total Cl 1 1	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	4	Total Zn 4 4	0	0
4	В	4	Total Zn 4 4	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	174	Total O 174 174	0	0
5	В	168	Total O 168 168	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	84.57Å 84.57 Å 321.74 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 - 2.00	Depositor
% Data completeness	98.8 (39.34-2.00)	Depositor
(in resolution range)		-
R_{merge}	0.15	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.53 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.247 , 0.285	Depositor
Wilson B-factor $(Å^2)$	25.5	Xtriage
Anisotropy	0.294	Xtriage
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -h-k,k,-l	Xtriage
Total number of atoms	6446	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 28.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7236e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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 monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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



Mol Type	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	Bo	ond leng	B	Bond angles		
10101	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2				
2	NAG	А	401	1	14,14,15	1.55	2 (14%)	17,19,21	1.54	4 (23%)				
2	NAG	А	402	1	14,14,15	1.63	3 (21%)	17,19,21	1.53	3 (17%)				
2	NAG	В	402	1	14,14,15	1.67	3 (21%)	17,19,21	1.51	4 (23%)				
2	NAG	В	401	1	14,14,15	1.57	2 (14%)	17,19,21	1.53	4 (23%)				

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).

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
2	NAG	А	401	1	-	0/6/23/26	0/1/1/1
2	NAG	А	402	1	-	0/6/23/26	0/1/1/1
2	NAG	В	402	1	-	0/6/23/26	0/1/1/1
2	NAG	В	401	1	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
2	В	401	NAG	C1-C2	3.95	1.58	1.52
2	В	402	NAG	C1-C2	3.43	1.57	1.52
2	А	401	NAG	C1-C2	3.39	1.57	1.52
2	А	402	NAG	C1-C2	3.29	1.57	1.52
2	В	402	NAG	O5-C5	-2.80	1.37	1.43
2	А	402	NAG	O5-C5	-2.51	1.38	1.43
2	А	401	NAG	O5-C5	-2.38	1.38	1.43
2	А	402	NAG	C3-C2	2.21	1.57	1.52
2	В	402	NAG	C3-C2	2.03	1.56	1.52
2	В	401	NAG	O5-C5	-2.03	1.39	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	А	402	NAG	C2-N2-C7	-3.29	118.22	122.90
2	А	401	NAG	C6-C5-C4	-3.08	105.79	113.00
2	В	402	NAG	C2-N2-C7	-3.04	118.58	122.90
2	А	401	NAG	C2-N2-C7	-2.99	118.65	122.90

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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	В	401	NAG	C2-N2-C7	-2.91	118.75	122.90
2	В	401	NAG	C6-C5-C4	-2.88	106.25	113.00
2	В	402	NAG	C1-C2-N2	-2.58	106.08	110.49
2	А	401	NAG	O4-C4-C3	-2.45	104.69	110.35
2	А	402	NAG	C6-C5-C4	-2.33	107.55	113.00
2	В	402	NAG	C6-C5-C4	-2.27	107.68	113.00
2	А	402	NAG	C1-C2-N2	-2.25	106.64	110.49
2	А	401	NAG	C1-C2-N2	-2.22	106.70	110.49
2	В	401	NAG	O4-C4-C3	-2.18	105.30	110.35
2	В	401	NAG	C1-C2-N2	-2.06	106.97	110.49
2	В	402	NAG	O4-C4-C3	-2.05	105.61	110.35

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There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	401	NAG	O5-C5-C6-O6

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)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

