

wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 12:10 AM EST

PDB ID	:	1QAS
Title	:	1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODI-
		ESTERASE DELTA 1
Authors	:	Grobler, J.A.; Hurley, J.H.
Deposited on	:	1996-08-02
Resolution	:	2.40 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 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:

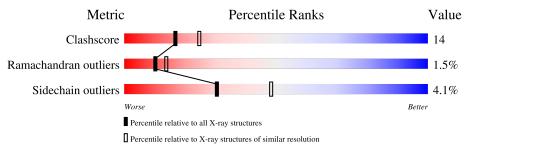
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	622	55%	23%	•	19%		
1	В	622	56%	23%	•	19%		



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8235 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	505	Total 3990	C 2522	11	O 750	S 22	0	0	0
1	В	504	Total 3979	C 2517		0 744	S 22	0	0	0

• Molecule 1 is a protein called PHOSPHOLIPASE C DELTA-1.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	132	Total O 132 132	0	0
2	В	134	Total O 134 134	0	0

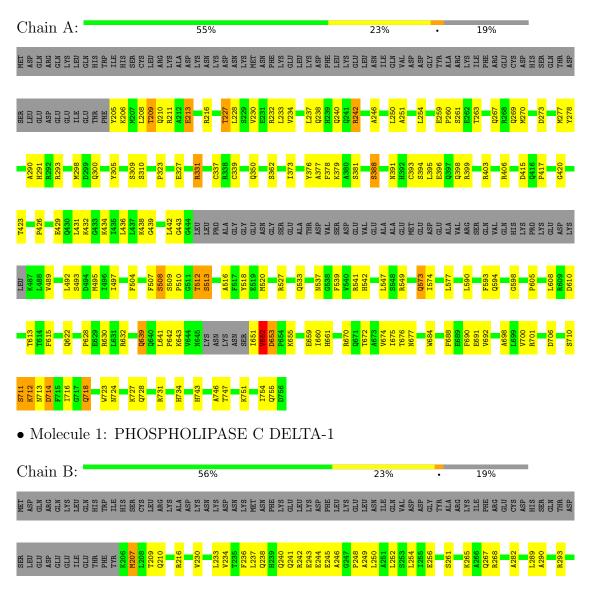


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PHOSPHOLIPASE C DELTA-1



K438 G439 K432 K434 I435 L436 L436 F507 S508 S509 P510 GLY CLHR CG14 G514 A516 F517 F517 F519 F519 T614 F615 P552 A553 <mark>F593</mark> Q594 1520 1573 1574 3525 3526 3526 3527 R54 **9640 1641 1643 1644 1644 1644 1784 1784 1785** N616 S617 S711 K712 N713 1675 T676 N677 F690 E691 V692 L099 V700 R701 <mark>д639</mark> W723 K727 Q728 G729 R731 H734 H734 H734 H734 T734 A746 A746 A756 D714



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	61.10Å 75.40Å 86.90Å	Depositor	
a, b, c, α , β , γ	66.90° 85.40° 89.80°	Depositor	
Resolution (Å)	6.00 - 2.40	Depositor	
% Data completeness	(Not available) (6.00-2.40)	Depositor	
(in resolution range)	(100 available) (0.00-2.40)		
R_{merge}	0.06	Depositor	
R_{sym}	0.06	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.212 , 0.286	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	8235	wwPDB-VP	
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP	



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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.51	0/4083	0.79	5/5531~(0.1%)	
1	В	0.52	0/4070	0.78	5/5511~(0.1%)	
All	All	0.51	0/8153	0.78	10/11042~(0.1%)	

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	331	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	А	331	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	В	331	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	В	331	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	А	331	ARG	CD-NE-CZ	7.38	133.93	123.60

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	А	3990	0	3906	118	0
1	В	3979	0	3903	109	0
2	А	132	0	0	5	0
2	В	134	0	0	7	0
All	All	8235	0	7809	222	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 14.

The worst 5 of 222 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:520:MET:HE3	1:A:549:ARG:HB2	1.47	0.95
1:A:228:LEU:HB2	1:A:270:MET:HB3	1.47	0.94
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.60	0.82
1:A:399:ARG:O	1:A:403:ARG:HG2	1.79	0.82
1:A:573:GLN:H	1:A:573:GLN:HE21	1.31	0.79

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	Favoured Allowed		Percentiles		
1	А	499/622~(80%)	458~(92%)	31~(6%)	10 (2%)	7	9	
1	В	496/622~(80%)	462 (93%)	29~(6%)	5 (1%)	15	23	
All	All	995/1244~(80%)	920~(92%)	60~(6%)	15 (2%)	10	14	

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	513	SER
1	А	711	SER
1	В	711	SER
1	А	508	SER
1	А	512	THR



5.3.2 Protein sidechains (i)

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	А	437/544~(80%)	418 (96%)	19 (4%)	29 46
1	В	435/544 (80%)	418 (96%)	17 (4%)	32 50
All	All	872/1088 (80%)	836 (96%)	36 (4%)	30 48

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	573	GLN
1	В	718	GLN
1	В	622	GLN
1	В	643	LYS
1	А	622	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	728	GLN
1	В	734	HIS
1	В	312	ASN
1	В	671	GLN
1	В	241	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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

