



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:42 PM GMT

PDB ID : 1QAT
Title : 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODI-
ESTERASE DELTA COMPLEX WITH SAMARIUM (III) CHLORIDE
Authors : Grobler, J.A.; Hurley, J.H.
Deposited on : 1996-08-02
Resolution : 3.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

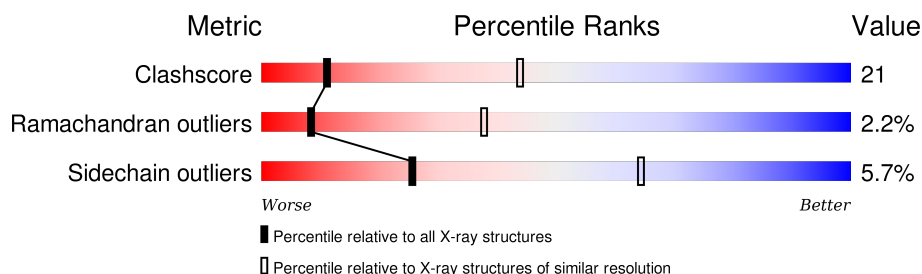
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	 45% 34% • 18%
1	B	622	 46% 32% • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8022 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 PHOSPHOLIPASE C DELTA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4018	2536	704	756	22			
1	B	507	Total	C	N	O	S	0	0	0
			3999	2526	701	750	22			

- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

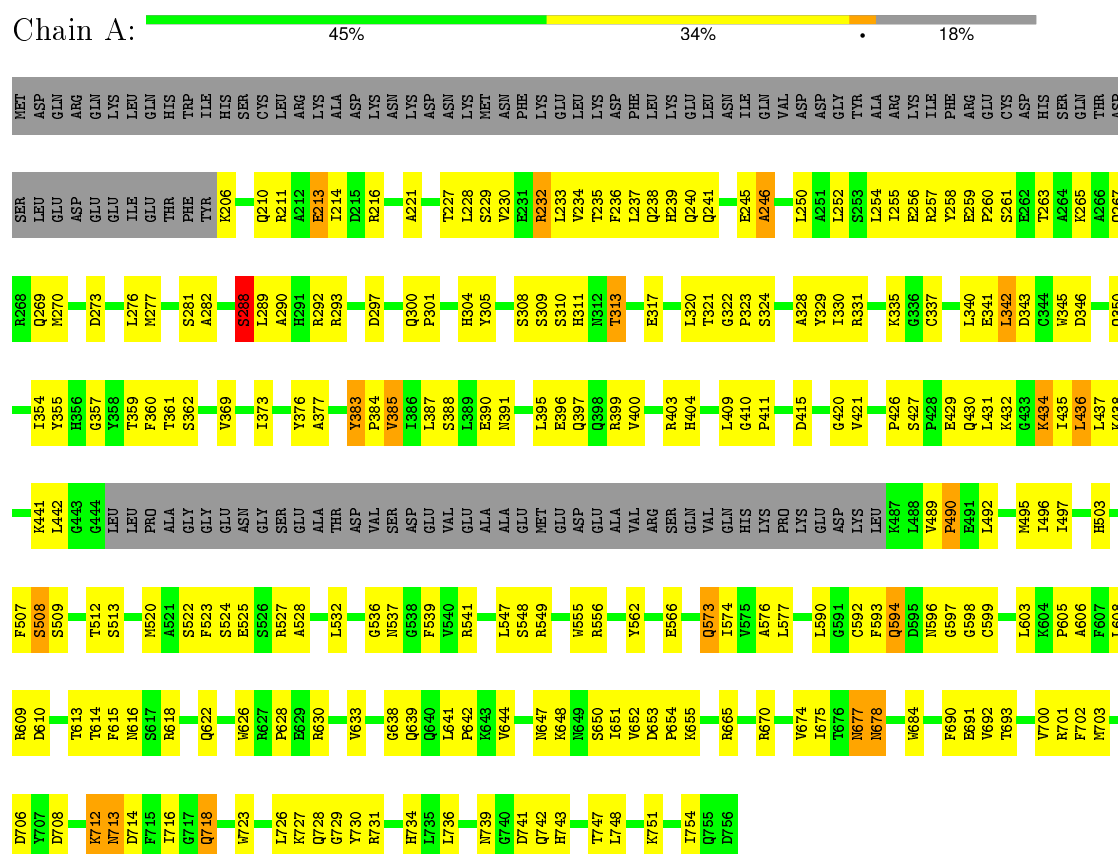
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Sm	0	0
			3	3		
2	A	2	Total	Sm	0	0
			2	2		

3 Residue-property plots

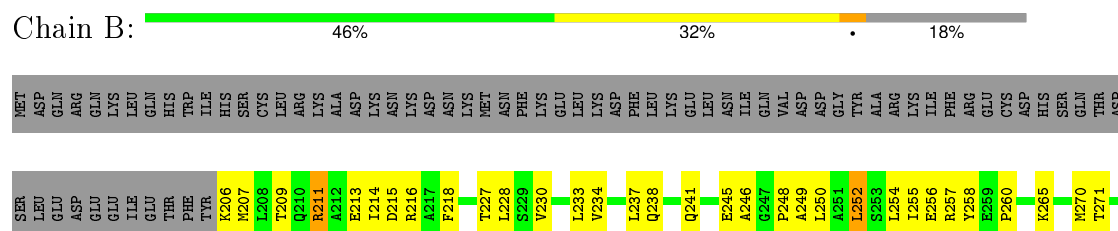
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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



• Molecule 1: PHOSPHOLIPASE C DELTA-1



W723	L726	T727	Q728	G729	Y730	R731	H734	L735	L736	N739	D740	D741	Q742	A746	T747	L748	K751	I754	Q755	D756	L445	PRO	GLY	THR	SER	G514		M520	F523	S524	E525	S526		R527	A528	L532		G536	M537	G538	F539	V540	R541	L547		S548	R549	M555	R556	T557	Y562		E566		Q573	L574	V575	A576	L577	L590		G591	C592	F593	C594	D595	M596	G597	G598	C599	L603		R604	P605	A606	F607	L608	R609	D610	T613	T614	F615	L616	S617		M618	D622		R630	V633		G638	P639	R640		L641	P642	R643	V644	L645	K646	L647	R648	S650		L651	P652	D653	P654	V674	L675	T676		L677	L678	V684		E691		V692	L699	V700	R701	F702	F703	D706		T707	D708	S709	S710	I716		F717	Q718	L276	M277	S281		A282		D283	S288		L289	A290	H291	R292	L293	Q296		D297	Q300		P301	H304		Y305		S309	S310	H311	N312		T313	E317		L320	T321	G322	P323	S324	E327		A328	Y329	L330	R331	K335		G336		C337	E341		L342	D343	C344	V345	D346	G347	P348	N349	Q350	E351	L354
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.60Å 75.10Å 86.40Å 66.40° 85.60° 89.80°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8022	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: SM

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	0.46	0/4111	0.76	3/5568 (0.1%)
1	B	0.46	0/4090	0.76	4/5539 (0.1%)
All	All	0.46	0/8201	0.76	7/11107 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	NE-CZ-NH1	14.31	127.46	120.30
1	A	331	ARG	NE-CZ-NH2	-13.87	113.36	120.30
1	B	331	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	B	331	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	A	331	ARG	CD-NE-CZ	7.13	133.59	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	305	TYR	Sidechain
1	B	383	TYR	Sidechain

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	4018	0	3941	166	0
1	B	3999	0	3916	166	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
All	All	8022	0	7857	330	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 21.

The worst 5 of 330 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:206:LYS:HA	1:A:210:GLN:HG3	1.49	0.93
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.60	0.84
1:A:537:ASN:HD22	1:A:614:THR:HA	1.43	0.81
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.62	0.81
1:B:537:ASN:HD22	1:B:614:THR:HA	1.46	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	Allowed	Outliers	Percentiles	
1	A	505/622 (81%)	457 (90%)	37 (7%)	11 (2%)	8	38
1	B	501/622 (80%)	452 (90%)	38 (8%)	11 (2%)	8	38
All	All	1006/1244 (81%)	909 (90%)	75 (8%)	22 (2%)	8	38

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	THR
1	A	513	SER
1	A	647	ASN
1	B	444	GLY
1	B	644	VAL

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	441/544 (81%)	416 (94%)	25 (6%)	25	64
1	B	437/544 (80%)	412 (94%)	25 (6%)	25	64
All	All	878/1088 (81%)	828 (94%)	50 (6%)	25	64

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	713	ASN
1	B	216	ARG
1	B	643	LYS
1	A	714	ASP
1	B	211	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	743	HIS
1	B	349	ASN
1	B	728	GLN
1	B	210	GLN
1	B	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.