wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 05:04 AM EST

PDB ID	:	1QAT
Title	:	1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODIESTERASE 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
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 (i)) were used in the production of this report:

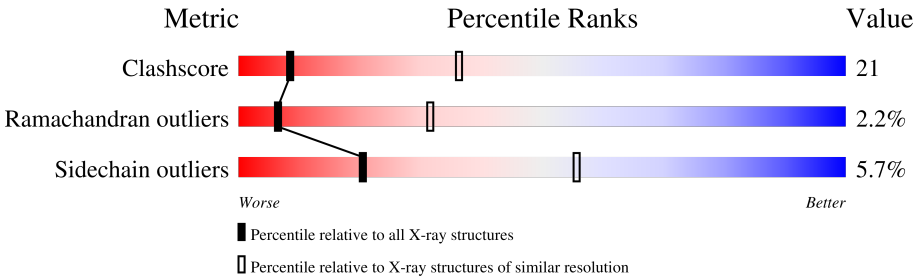
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 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	A	622	45% 34% · 18%
1	B	622	46% 32% · 18%

2 Entry composition (i)

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	A	2	Total	Sm	0	0
			2	2		
2	B	3	Total	Sm	0	0
			3	3		

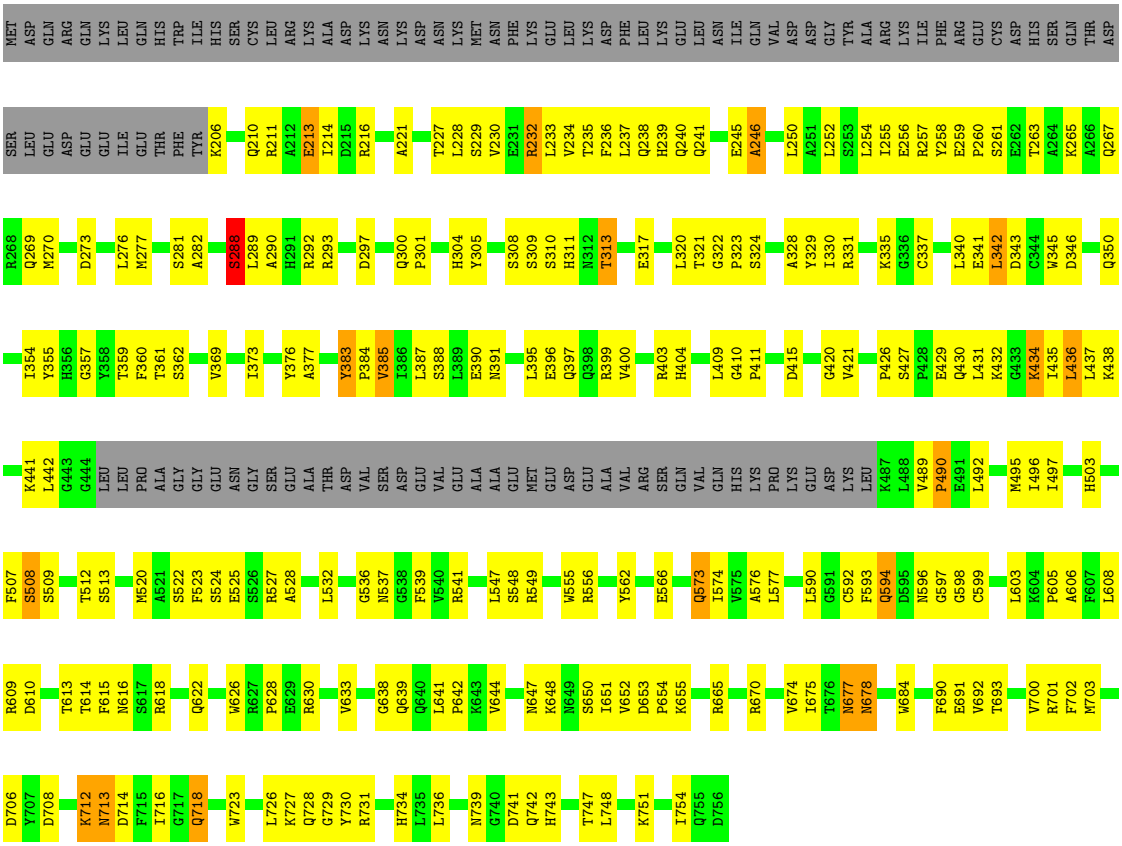
3 Residue-property plots (i)

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.

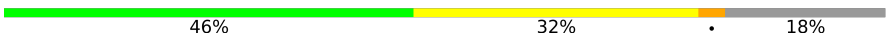
• Molecule 1: PHOSPHOLIPASE C DELTA-1

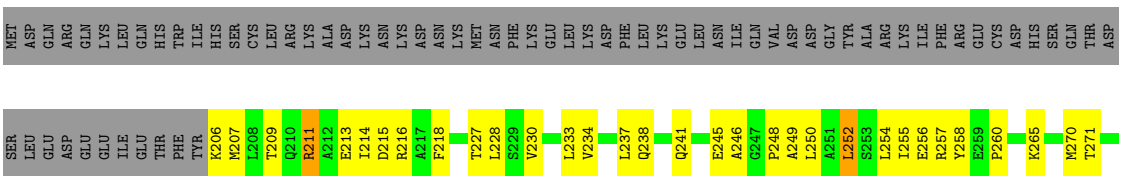
Chain A:

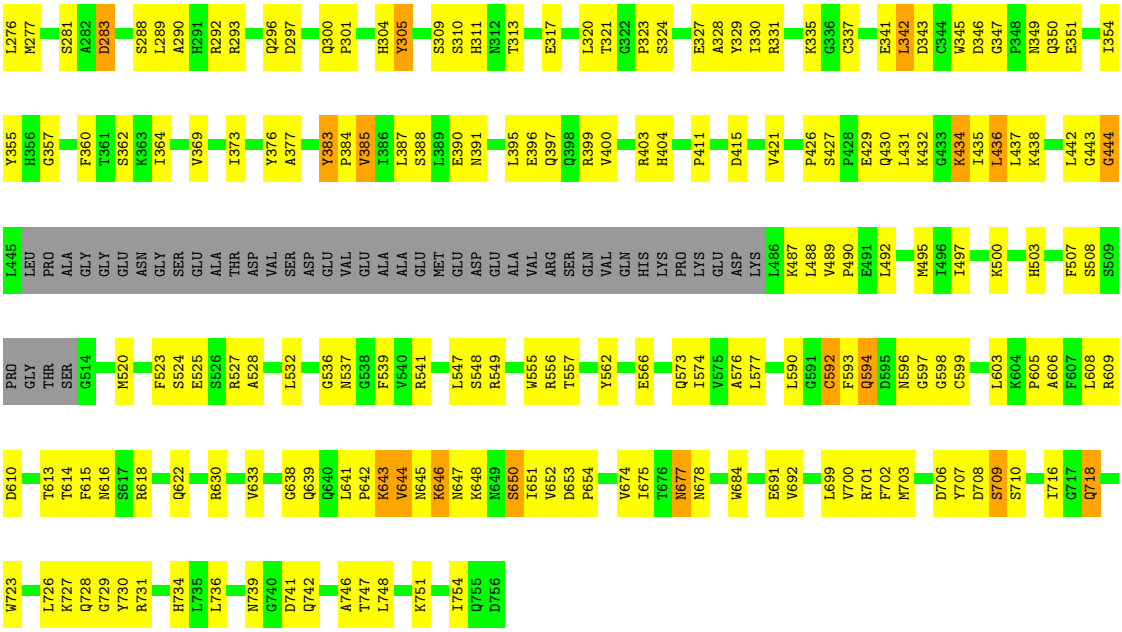


• Molecule 1: PHOSPHOLIPASE C DELTA-1

Chain B:






L276 M277 S281 A282 D283 S288 L289 A290 H291 R292 R293 Q296 D297 Q300 P301 H304 Y305 S309 S310 H311 N312 T313 E317 L320 T321 G322 P323 S324 E327 A328 Y329 I330 R331 K335 G336 C337 E341 L342 D343 C344 W345 D346 G347 P348 N349 Q350 E351 I354
Y355 H356 G357 F360 T361 S362 K363 I364 V369 I373 Y376 A377 Y383 P384 V385 I386 L387 S388 L389 E390 N391 L395 E396 Q397 Q398 R399 V400 R403 H404 P411 D415 V421 P426 S427 P428 E429 Q430 L431 K432 G433 K434 I435 L436 L437 K438 L442 G443 G444
L445 LEU PRO ALA GLY GLY GLU ASN GLY SER GLU ALA THR ASP VAL SER ASP GLU VAL GLU ALA ALA GLU MET GLU ASP GLU ALA VAL ARG SER GLN VAL GLN HIS LYS PRO LYS GLU ASP LYS L486 K487 L488 V489 P490 E491 L492 M495 I496 I497 K500 H503 F507 S508 S509
PRO GLY THR SER G514 M520 F523 S524 E525 S526 R527 A528 L532 G536 N537 G538 F539 V540 R541 L547 S548 R549 W555 R556 T557 Y562 E566 Q573 I574 V575 A576 L577 L590 G591 C592 F593 Q594 D595 N596 G597 G598 C599 L603 K604 P605 A606 F607 L608 R609
D610 T613 T614 F615 N616 S617 R618 Q622 R630 V633 G638 Q639 Q640 L641 P642 K643 V644 N645 K646 N647 K648 N649 S650 I651 V652 D653 P654 V674 I675 T676 N677 N678 W684 E691 V692 L699 V700 R701 F702 M703 D706 Y707 D708 S709 S710 I716 G717 Q718
W723 L726 K727 Q728 G729 Y730 R731 H734 L735 L736 N739 G740 D741 Q742 A746 T747 L748 K751 I754 Q755 D756

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 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

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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%)	6	31
1	B	501/622 (80%)	452 (90%)	38 (8%)	11 (2%)	6	31
All	All	1006/1244 (81%)	909 (90%)	75 (8%)	22 (2%)	6	31

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 (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	A	441/544 (81%)	416 (94%)	25 (6%)	20	56
1	B	437/544 (80%)	412 (94%)	25 (6%)	20	56
All	All	878/1088 (81%)	828 (94%)	50 (6%)	20	56

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

Mol	Chain	Res	Type
1	B	252	LEU
1	B	434	LYS
1	B	718	GLN
1	B	254	LEU
1	B	342	LEU

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

Mol	Chain	Res	Type
1	B	349	ASN
1	B	503	HIS
1	B	728	GLN
1	B	391	ASN
1	B	515	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.