



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:11 pm GMT

PDB ID : 1DJG  
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM  
RAT COMPLEXED WITH LANTHANUM  
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.  
Deposited on : 1996-09-25  
Resolution : 2.60 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

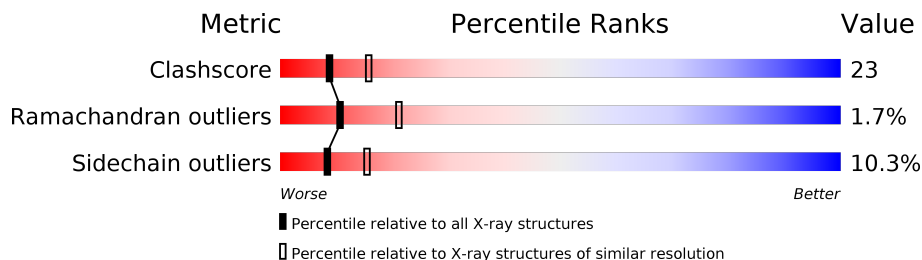
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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  $\geq 3$ , 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	624	
1	B	624	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	5	-	-	X	-

## 2 Entry composition [i](#)

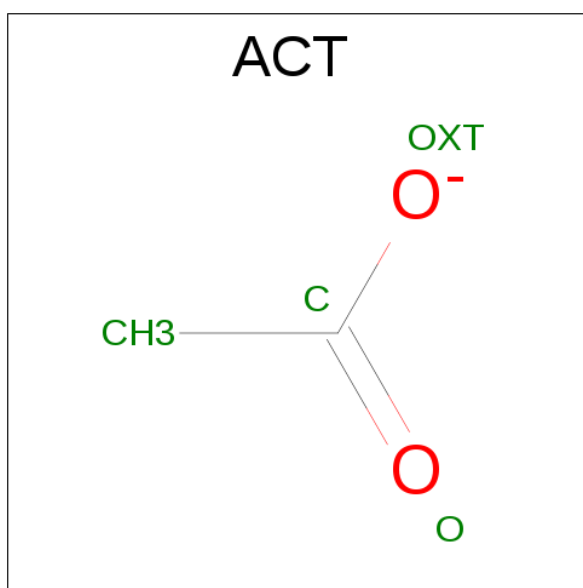
There are 4 unique types of molecules in this entry. The entry contains 9246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	86	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	101	0	0
			4465	2818	776	847	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is LANTHANUM (III) ION (three-letter code: LA) (formula: La).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	La 4	0	0
3	A	4	Total 4	La 4	0	0

- Molecule 4 is water.

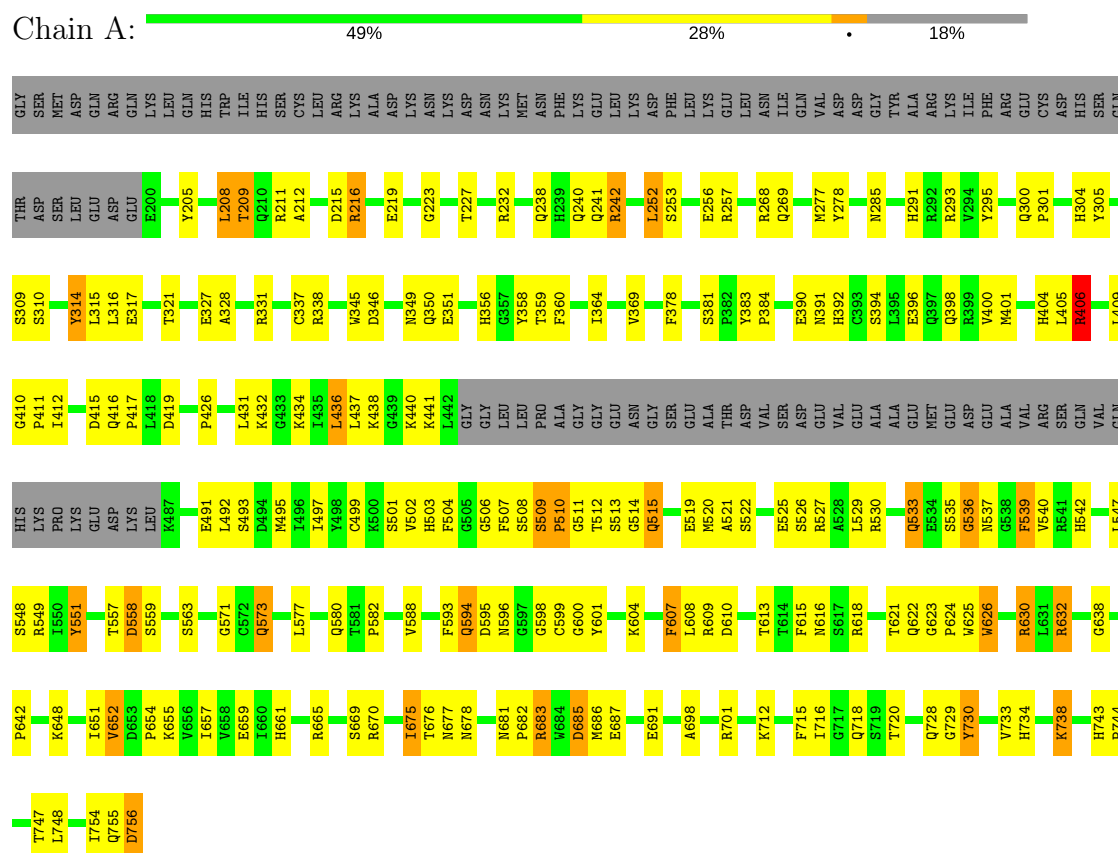
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total 335	O 335	0	0
4	B	373	Total 373	O 373	0	0

### 3 Residue-property plots

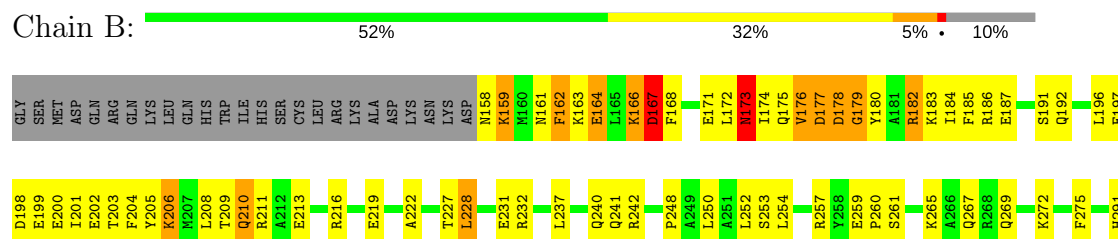
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1



#### • Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1



R292	R293	L405	R406	L409	I412	H304	S309	S310	T313	Y314	L315	L316	Y329	L330	R331	C337	L342	D343	C344	W345	D346	P348	N349	Q350	E351	L405	R406	L409	I412	D415	Q416	P417	L418	V421	T422	T423	S424	L425	P426	S427	L431	K432	L436	L437	G438	G439	K440	K441	L442	L445	LEU	PRO	ALA	GLY	GLY	GLU	ASN	GLY	SER	GLU	K378	K379	ALA	THR	ASP	P384	S388	L389	E390	N391	H392	C393	S394	L395	ALA	ALA	GLU	GLU	GLU	ASP	GLU	ALA	VAL	M401
ARG	SER	GLN	VAL	GLN	HIS	LYS	PRO	LYS	GLU	D484	L488	T489	P490	G491	F492	Q493	D494	N495	G496	G497	G498	C499	K500	P501	A502	R503	T504	Q505	G506	F507	T508	Q509	P510	A511	V512	D513	K514	L515	R516	G517	G518	W519	D520	F521	S522	E523	E524	E525	S526	R527	A528	L529	Q530	E531	S532	K533	N534	G535	V536	N537	S538	S539	P540	I541	V542	D543	P544	K545	N546	S547	L548	S549	T550	F551	P552	V553	D554	G555	P556	I557	V558			
D558	S559	S563	E566	G571	C572	Q573	Q580	T581	P582	G583	F593	Q594	D595	N596	G597	G598	C599	K604	P605	A606	R607	T613	T621	Q622	G623	P624	W625	R630	L631	R632	V633	R634	G638	P642	K643	N647	K648	N649	S650	I651	V652	D653	P654	K655	V656	I657	V658																																					
E659	I660	H661	R665	I675	N678	N681	P682	R683	W684	D685	N686	E687	E691	D696	L697	A698	R701	S709	S710	S711	K712	F715	I716	G717	Q718	S719	I720	Q728	G729	Y730	H734	L735	K738	H743	T747	K751	I752	S753	I754	Q755	D756																																											

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	397.92Å 397.92Å 397.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.5 (10.00-2.60)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.210 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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: ACT, LA

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	0.98	29/4152 (0.7%)	0.88	4/5624 (0.1%)
1	B	1.00	31/4565 (0.7%)	0.90	8/6174 (0.1%)
All	All	0.99	60/8717 (0.7%)	0.89	12/11798 (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	1	0
All	All	1	1

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	730	TYR	CE2-CZ	-10.49	1.25	1.38
1	A	358	TYR	CE1-CZ	-9.51	1.26	1.38
1	A	314	TYR	CE2-CZ	-9.42	1.26	1.38
1	A	551	TYR	CE2-CZ	-9.34	1.26	1.38
1	B	314	TYR	CE1-CZ	-8.98	1.26	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	CYS	CA-CB-SG	8.09	128.56	114.00
1	A	406	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	B	393	CYS	N-CA-C	6.06	127.35	111.00
1	A	509	SER	N-CA-C	5.79	126.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASN	CB-CA-C	5.50	121.39	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	393	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	691	GLU	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	4057	0	3972	173	0
1	B	4465	0	4375	208	0
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	335	0	0	11	0
4	B	373	0	0	18	0
All	All	9246	0	8353	370	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 23.

The worst 5 of 370 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:B:161:ASN:H	1:B:164:GLU:HG3	1.18	1.07
1:A:613:THR:HG22	1:A:615:PHE:H	1.23	1.02
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.24	1.01
1:B:438:LYS:HD2	1:B:520:MET:HE1	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:GLN:NE2	1:B:754:ILE:H	1.64	0.94

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	509/624 (82%)	471 (92%)	31 (6%)	7 (1%)	13	26
1	B	557/624 (89%)	511 (92%)	35 (6%)	11 (2%)	9	17
All	All	1066/1248 (85%)	982 (92%)	66 (6%)	18 (2%)	11	21

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	B	175	GLN
1	B	176	VAL
1	B	177	ASP
1	B	510	PRO

### 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	444/545 (82%)	404 (91%)	40 (9%)	11	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	492/545 (90%)	436 (89%)	56 (11%)	7 12
All	All	936/1090 (86%)	840 (90%)	96 (10%)	8 15

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	166	LYS
1	B	242	ARG
1	B	685	ASP
1	B	167	ASP
1	B	206	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	734	HIS
1	B	241	GLN
1	B	661	HIS
1	A	661	HIS
1	A	718	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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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 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	$\# Z  > 2$
2	ACT	A	5	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
2	ACT	B	5	-	1,3,3	2.07	1 (100%)	0,3,3	0.00	-

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	ACT	A	5	-	-	0/0/0/0	0/0/0/0
2	ACT	B	5	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	ACT	CH3-C	2.07	1.51	1.48
2	A	5	ACT	CH3-C	2.54	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	ACT	2	0

## 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 [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.