Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:36 PM GMT

PDB ID	:	1PTD
Title	:	PHOSPHATIDYLINOSITOL-SPECIFIC PHOSPHOLIPASE C
Authors	:	Heinz, D.W.; Ryan, M.; Bullock, T.L.; Griffith, O.H.
Deposited on	:	1995-05-24
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

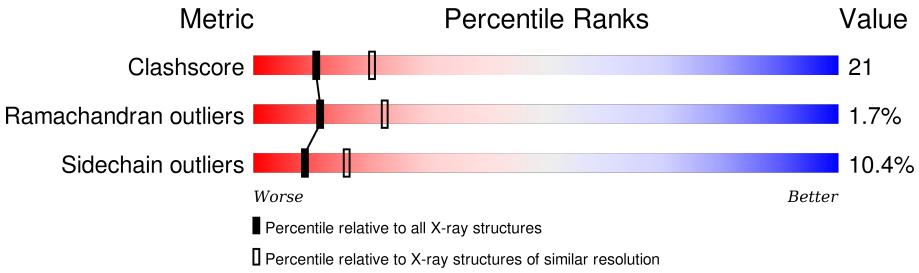
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 >=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 <=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	298	57% 35% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2474 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 PHOSPHATIDYLINOSITOL-SPECIFIC PHOSPHOLIPASE C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2422	1548	400	467	7	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	52	52	52	0	0

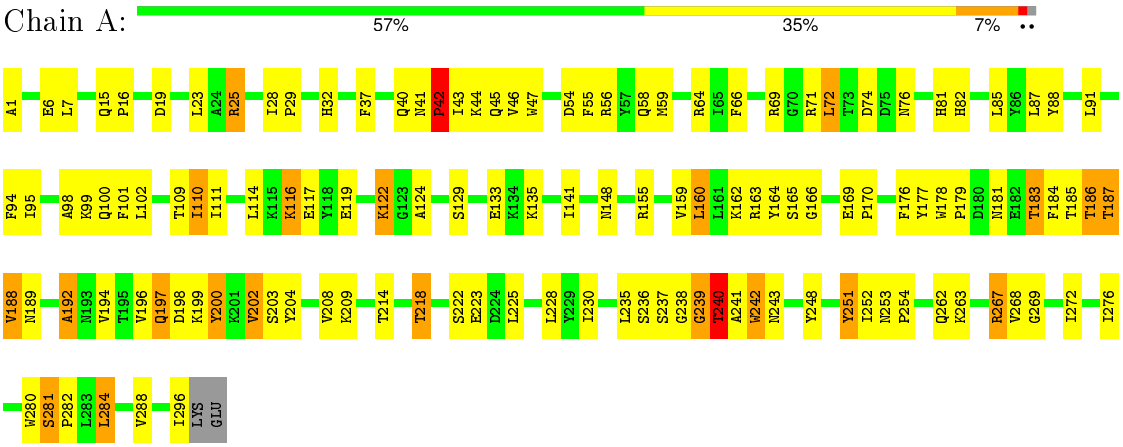
3 Residue-property plots (i)

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: PHOSPHATIDYLINOSITOL-SPECIFIC PHOSPHOLIPASE C

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.20Å 45.60Å 160.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	86.0 (8.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.187 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2474	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.83	0/2486	1.01	5/3373 (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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	183	THR	N-CA-C	-5.79	95.37	111.00
1	A	165	SER	N-CA-C	5.38	125.52	111.00
1	A	228	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	200	TYR	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	TYR	Sidechain

5.2 Too-close contacts

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	2422	0	2340	101	1
2	A	52	0	0	11	0
All	All	2474	0	2340	101	1

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.

All (101) 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:1:ALA:HB3	1:A:16:PRO:HA	1.57	0.84
1:A:238:GLY:O	1:A:243:ASN:HB3	1.80	0.80
1:A:40:GLN:HA	1:A:45:GLN:HE21	1.46	0.80
1:A:281:SER:CB	1:A:282:PRO:HD3	2.13	0.78
1:A:94:PHE:HZ	1:A:110:ILE:HD11	1.50	0.76
1:A:135:LYS:HE2	2:A:746:HOH:O	1.86	0.76
1:A:188:VAL:HG22	1:A:194:VAL:CG2	2.16	0.75
1:A:189:ASN:HB2	2:A:749:HOH:O	1.84	0.75
1:A:40:GLN:HA	1:A:45:GLN:NE2	2.02	0.74
1:A:197:GLN:NE2	1:A:199:LYS:H	1.84	0.74
1:A:254:PRO:HG3	1:A:280:TRP:HB3	1.69	0.74
1:A:69:ARG:HB3	1:A:117:GLU:HB2	1.72	0.72
1:A:183:THR:HG23	1:A:199:LYS:HE3	1.71	0.72
1:A:281:SER:OG	1:A:282:PRO:HD3	1.90	0.71
1:A:116:LYS:HB2	2:A:707:HOH:O	1.90	0.70
1:A:242:TRP:CE3	1:A:242:TRP:HA	2.26	0.69
1:A:94:PHE:CZ	1:A:110:ILE:HD11	2.28	0.69
1:A:166:GLY:N	2:A:706:HOH:O	2.24	0.69
1:A:41:ASN:HB2	1:A:44:LYS:HD2	1.73	0.69
1:A:94:PHE:HZ	1:A:110:ILE:CD1	2.08	0.67
1:A:43:ILE:O	1:A:47:TRP:HD1	1.78	0.66
1:A:197:GLN:HE22	1:A:199:LYS:H	1.45	0.65
1:A:237:SER:N	2:A:718:HOH:O	2.31	0.63
1:A:242:TRP:HE3	1:A:242:TRP:HA	1.64	0.63
1:A:177:TYR:CD2	1:A:179:PRO:HD3	2.35	0.61
1:A:46:VAL:HG23	1:A:47:TRP:CD1	2.35	0.61
1:A:214:THR:O	1:A:218:THR:HG23	2.01	0.61
1:A:230:ILE:HG23	1:A:272:ILE:HD13	1.83	0.61
1:A:41:ASN:HD22	1:A:44:LYS:HD2	1.67	0.60
1:A:281:SER:HB3	1:A:282:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD13	1:A:162:LYS:HG2	1.84	0.59
1:A:183:THR:HG22	1:A:197:GLN:HG2	1.83	0.58
1:A:129:SER:O	1:A:133:GLU:HG3	2.02	0.58
1:A:56:ARG:NH1	1:A:101:PHE:HA	2.19	0.58
1:A:272:ILE:N	1:A:272:ILE:HD12	2.20	0.57
1:A:248:TYR:O	1:A:252:ILE:HG13	2.04	0.57
1:A:41:ASN:O	1:A:44:LYS:HB2	2.04	0.57
1:A:122:LYS:H	1:A:122:LYS:HD3	1.70	0.57
1:A:72:LEU:HD13	1:A:124:ALA:HB1	1.88	0.56
1:A:239:GLY:O	1:A:241:ALA:N	2.39	0.55
1:A:267:ARG:HD3	2:A:743:HOH:O	2.07	0.55
1:A:185:THR:HA	1:A:194:VAL:O	2.08	0.54
1:A:284:LEU:O	1:A:288:VAL:HG23	2.07	0.54
1:A:183:THR:CG2	1:A:199:LYS:HE3	2.37	0.54
1:A:239:GLY:C	1:A:241:ALA:H	2.10	0.53
1:A:19:ASP:OD1	1:A:155:ARG:NH1	2.42	0.52
1:A:204:TYR:O	1:A:208:VAL:HG23	2.10	0.52
1:A:181:ASN:OD1	1:A:199:LYS:HA	2.10	0.51
1:A:253:ASN:HB2	1:A:254:PRO:HD3	1.92	0.51
1:A:188:VAL:HG22	1:A:194:VAL:HG22	1.90	0.51
1:A:32:HIS:HB2	1:A:272:ILE:HG22	1.92	0.51
1:A:46:VAL:HB	1:A:240:THR:H	1.76	0.50
1:A:183:THR:HG23	1:A:199:LYS:CE	2.40	0.50
1:A:184:PHE:CZ	1:A:196:VAL:HB	2.45	0.50
1:A:176:PHE:CD2	1:A:188:VAL:HG13	2.47	0.50
1:A:28:ILE:HG22	1:A:29:PRO:O	2.11	0.50
1:A:202:VAL:HG13	1:A:203:SER:N	2.26	0.49
1:A:268:VAL:O	1:A:268:VAL:HG12	2.11	0.49
1:A:230:ILE:HG23	1:A:272:ILE:CD1	2.43	0.49
1:A:204:TYR:CE1	1:A:208:VAL:HG21	2.48	0.48
1:A:25:ARG:HG3	1:A:225:LEU:HD22	1.95	0.48
1:A:95:ILE:O	1:A:99:LYS:HG3	2.14	0.48
1:A:42:PRO:O	1:A:45:GLN:HB2	2.14	0.47
1:A:281:SER:CB	1:A:282:PRO:CD	2.89	0.47
1:A:119:GLU:HG2	2:A:736:HOH:O	2.15	0.47
1:A:204:TYR:OH	1:A:251:TYR:HB3	2.16	0.46
1:A:6:GLU:HB2	1:A:16:PRO:HG3	1.98	0.46
1:A:177:TYR:CE2	1:A:179:PRO:HD3	2.51	0.45
1:A:40:GLN:O	1:A:42:PRO:HD3	2.17	0.44
1:A:192:ALA:HB3	2:A:749:HOH:O	2.18	0.44
1:A:222:SER:HA	1:A:267:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HA	1:A:46:VAL:HG22	1.99	0.44
1:A:269:GLY:HA2	2:A:743:HOH:O	2.17	0.44
1:A:82:HIS:HB2	1:A:87:LEU:HD21	1.99	0.44
1:A:95:ILE:HG22	1:A:99:LYS:HE3	2.00	0.44
1:A:200:TYR:HB2	1:A:236:SER:OG	2.18	0.44
1:A:183:THR:CG2	1:A:197:GLN:HG2	2.48	0.43
1:A:54:ASP:O	1:A:58:GLN:HG3	2.19	0.43
1:A:15:GLN:N	1:A:16:PRO:HD2	2.32	0.43
1:A:276:ILE:O	1:A:276:ILE:HG23	2.18	0.43
1:A:122:LYS:CD	1:A:122:LYS:H	2.29	0.43
1:A:7:LEU:HG	1:A:296:ILE:HD11	2.01	0.43
1:A:116:LYS:HE2	1:A:164:TYR:HA	2.01	0.42
1:A:41:ASN:ND2	1:A:44:LYS:HD2	2.33	0.42
1:A:74:ASP:C	1:A:76:ASN:H	2.21	0.42
1:A:23:LEU:HA	1:A:23:LEU:HD23	1.83	0.42
1:A:281:SER:OG	1:A:282:PRO:CD	2.62	0.42
1:A:267:ARG:CD	2:A:743:HOH:O	2.67	0.42
1:A:1:ALA:CB	1:A:16:PRO:HA	2.40	0.42
1:A:64:ARG:HD2	1:A:109:THR:O	2.19	0.42
1:A:178:TRP:HA	1:A:184:PHE:CZ	2.55	0.42
1:A:28:ILE:CG2	1:A:64:ARG:HB2	2.50	0.41
1:A:169:GLU:HA	1:A:170:PRO:HD2	1.93	0.41
1:A:59:MET:HG3	1:A:66:PHE:CZ	2.55	0.41
1:A:98:ALA:O	1:A:102:LEU:HD12	2.21	0.41
1:A:111:ILE:HA	1:A:159:VAL:O	2.20	0.41
1:A:163:ARG:HD3	2:A:741:HOH:O	2.21	0.41
1:A:186:THR:HG22	1:A:187:THR:H	1.86	0.41
1:A:37:PHE:HE1	1:A:55:PHE:CE2	2.39	0.40
1:A:71:ARG:NE	1:A:119:GLU:O	2.46	0.40
1:A:88:TYR:N	1:A:88:TYR:CD1	2.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:NZ	1:A:262:GLN:NE2[3_646]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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	294/298 (99%)	259 (88%)	30 (10%)	5 (2%)	11 22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	THR
1	A	281	SER
1	A	42	PRO
1	A	192	ALA
1	A	239	GLY

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	268/270 (99%)	240 (90%)	28 (10%)	9 16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	42	PRO
1	A	72	LEU
1	A	81	HIS
1	A	85	LEU
1	A	91	LEU

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	110	ILE
1	A	114	LEU
1	A	116	LYS
1	A	122	LYS
1	A	141	ILE
1	A	148	ASN
1	A	160	LEU
1	A	186	THR
1	A	187	THR
1	A	188	VAL
1	A	197	GLN
1	A	202	VAL
1	A	209	LYS
1	A	218	THR
1	A	223	GLU
1	A	235	LEU
1	A	240	THR
1	A	242	TRP
1	A	263	LYS
1	A	267	ARG
1	A	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	41	ASN
1	A	45	GLN
1	A	82	HIS
1	A	148	ASN
1	A	197	GLN
1	A	221	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 will therefore be empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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