



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:46 PM GMT

PDB ID : 1V0U
Title : PHOSPHOLIPASE D FROM STREPTOMYCES SP. STRAIN PMF
SOAKED WITH THE PRODUCT GLYCEROPHOSPHATE.
Authors : Leiros, I.; Mcsweeney, S.; Hough, E.
Deposited on : 2004-04-02
Resolution : 1.42 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

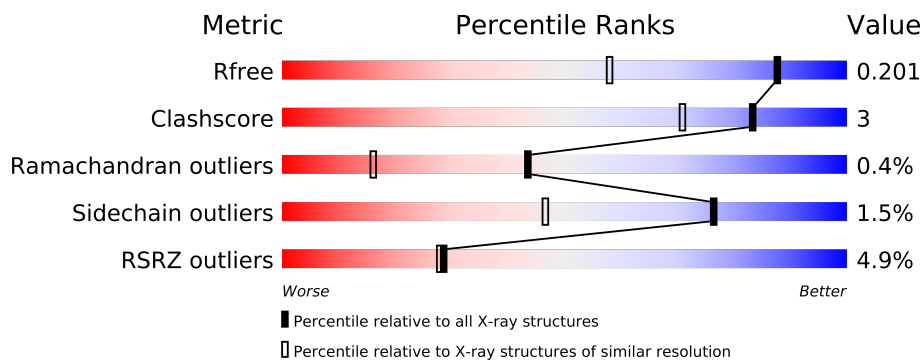
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance


The reported resolution of this entry is 1.42 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))
R_{free}	66092	1110 (1.44-1.40)
Clashscore	79885	1263 (1.44-1.40)
Ramachandran outliers	78287	1226 (1.44-1.40)
Sidechain outliers	78261	1225 (1.44-1.40)
RSRZ outliers	66119	1110 (1.44-1.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	506	

2 Entry composition i

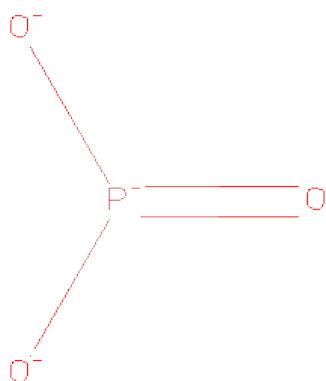
There are 3 unique types of molecules in this entry. The entry contains 4304 atoms, of which 0 are hydrogen and 0 are deuterium.

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 D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3692	2303	649	726	14	75	0	0

- Molecule 2 is PHOSPHITE ION (three-letter code: PO3) (formula: O₃P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	4	3	1	0	0

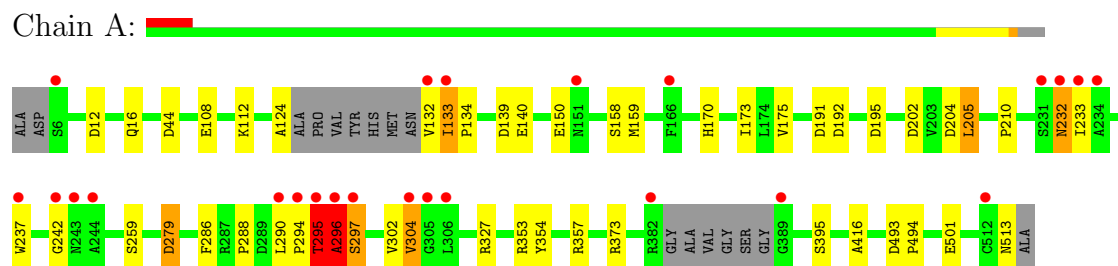
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	608	Total	O	0	0
			608	608		

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.

• Molecule 1: PHOSPHOLIPASE D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.39Å 57.04Å 68.76Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	69.01 – 1.42 23.63 – 1.42	Depositor EDS
% Data completeness (in resolution range)	93.8 (69.01-1.42) 93.8 (23.63-1.42)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.166 , 0.186 0.180 , 0.201	Depositor DCC
R_{free} test set	2408 reflections (3.14%)	DCC
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 79180 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4304	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO3

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	0.77	11/3765 (0.3%)	1.02	26/5122 (0.5%)

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	3	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	GLU	CB-CG	-15.27	1.23	1.52
1	A	501	GLU	CG-CD	12.50	1.70	1.51
1	A	295	THR	CA-CB	-11.31	1.24	1.53
1	A	233	ILE	CB-CG1	-8.21	1.31	1.54
1	A	279	ASP	CB-CG	-7.39	1.36	1.51
1	A	416	ALA	C-N	6.34	1.48	1.34
1	A	140	GLU	CG-CD	5.80	1.60	1.51
1	A	170	HIS	CE1-NE2	5.78	1.46	1.32
1	A	170	HIS	CD2-NE2	-5.66	1.25	1.38
1	A	195	ASP	CB-CG	5.40	1.63	1.51
1	A	170	HIS	CG-CD2	-5.20	1.26	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	THR	CA-CB-CG2	26.46	149.44	112.40
1	A	295	THR	CB-CA-C	-12.44	78.02	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	VAL	N-CA-CB	11.09	135.91	111.50
1	A	233	ILE	CA-CB-CG1	10.26	130.50	111.00
1	A	170	HIS	CG-CD2-NE2	9.86	127.94	109.20
1	A	327	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	A	150	GLU	CA-CB-CG	6.84	128.45	113.40
1	A	237	TRP	CE3-CZ3-CH2	-6.36	114.20	121.20
1	A	132	VAL	CB-CA-C	-6.18	99.66	111.40
1	A	353	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	373	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	304	VAL	N-CA-CB	-5.67	99.02	111.50
1	A	170	HIS	ND1-CG-CD2	-5.66	98.07	106.00
1	A	202	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	191	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	353	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	295	THR	N-CA-CB	5.45	120.65	110.30
1	A	204	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	139	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	12	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	327	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	297	SER	N-CA-C	-5.25	96.83	111.00
1	A	357	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	501	GLU	CB-CG-CD	-5.09	100.46	114.20
1	A	192	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	44	ASP	CB-CG-OD1	5.04	122.84	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	233	ILE	CB
1	A	295	THR	CA,CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3692	0	3628	21	0
2	A	4	0	0	0	0
3	A	608	0	0	5	1
All	All	4304	0	3628	21	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:290:LEU:C	1:A:294:PRO:N	2.02	1.14
1:A:302:VAL:C	1:A:304:VAL:N	2.07	1.08
1:A:108:GLU:OE1	3:A:2227:HOH:O	2.01	0.78
1:A:297:SER:HB2	1:A:354:TYR:OH	1.95	0.67
1:A:232:ASN:HD22	1:A:232:ASN:C	2.06	0.59
1:A:513:ASN:ND2	3:A:2606:HOH:O	2.36	0.57
1:A:108:GLU:OE2	1:A:112:LYS:HE3	2.08	0.54
1:A:295:THR:O	1:A:296:ALA:O	2.26	0.53
1:A:290:LEU:CA	1:A:294:PRO:N	2.72	0.51
1:A:108:GLU:HG2	3:A:2175:HOH:O	2.11	0.50
1:A:286:PHE:CZ	1:A:288:PRO:HB3	2.49	0.48
1:A:210:PRO:HA	1:A:259:SER:HB2	1.96	0.47
1:A:205:LEU:HD12	1:A:205:LEU:C	2.36	0.45
1:A:133:ILE:HG13	1:A:134:PRO:HD3	1.99	0.45
1:A:124:ALA:HB2	1:A:158:SER:OG	2.18	0.43
1:A:302:VAL:C	1:A:304:VAL:CA	2.85	0.41
1:A:493:ASP:HB2	1:A:494:PRO:HD3	2.01	0.41
1:A:294:PRO:HG3	3:A:2467:HOH:O	2.20	0.41
1:A:173:ILE:HG22	1:A:175:VAL:HG23	2.03	0.41
1:A:108:GLU:OE2	1:A:112:LYS:CE	2.68	0.41
1:A:16:GLN:NE2	3:A:2034:HOH:O	2.54	0.41

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	Distance(Å)	Clash(Å)
3:A:2018:HOH:O	3:A:2306:HOH:O[2_646]	2.03	0.17

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	480/506 (95%)	462 (96%)	16 (3%)	2 (0%)	43 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ALA
1	A	242	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	397/406 (98%)	391 (98%)	6 (2%)	76 46

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ILE
1	A	159	MET
1	A	205	LEU
1	A	232	ASN
1	A	279	ASP
1	A	395	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	20	GLN
1	A	114	ASN
1	A	232	ASN
1	A	409	ASN
1	A	513	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is modelled in this entry.

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	PO3	A	1515	1	1,3,3	4.71	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	PO3	A	1515	1	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1515	PO3	P-O1	4.71	1.52	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	490/506 (96%)	0.03	24 (4%)	28 28	9, 16, 30, 42	23 (4%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	ALA	7.7
1	A	132	VAL	7.2
1	A	233	ILE	6.1
1	A	305	GLY	5.2
1	A	237	TRP	4.5
1	A	295	THR	4.5
1	A	242	GLY	4.2
1	A	297	SER	4.1
1	A	133	ILE	3.9
1	A	512	CYS	3.9
1	A	304	VAL	3.8
1	A	234	ALA	3.6
1	A	243	ASN	3.5
1	A	232	ASN	3.4
1	A	244	ALA	2.9
1	A	6	SER	2.8
1	A	382	ARG	2.7
1	A	389	GLY	2.5
1	A	290	LEU	2.4
1	A	294	PRO	2.4
1	A	306	LEU	2.3
1	A	151	ASN	2.2
1	A	166	PHE	2.1
1	A	231	SER	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO3	A	1515	4/4	0.05	-1.13	13,13,14,17	0

6.5 Other polymers

There are no such residues in this entry.