



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:08 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 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

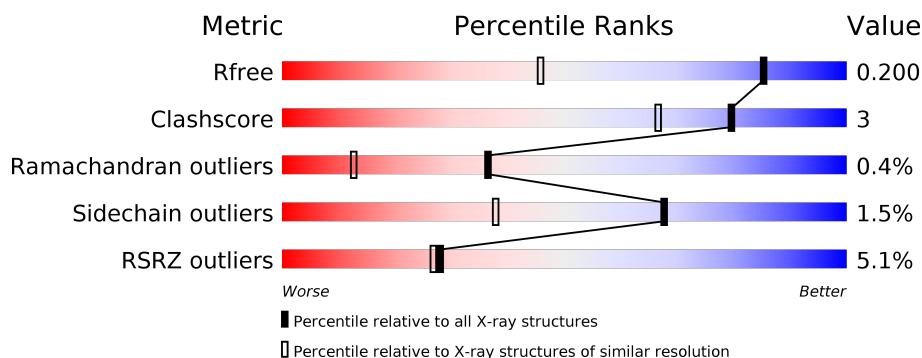
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 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}	111664	2084 (1.44-1.40)
Clashscore	122126	2190 (1.44-1.40)
Ramachandran outliers	120053	2138 (1.44-1.40)
Sidechain outliers	120020	2137 (1.44-1.40)
RSRZ outliers	108989	2035 (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. 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.

Mol	Chain	Length	Quality of chain
1	A	506	

2 Entry composition [i](#)

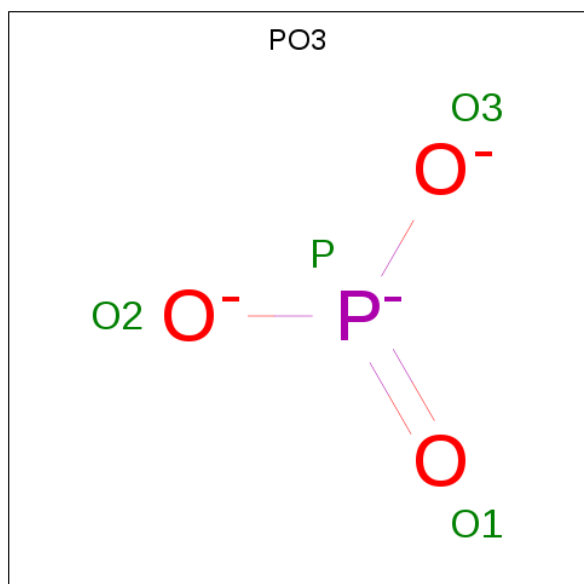
There are 3 unique types of molecules in this entry. The entry contains 4304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D.

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

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



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

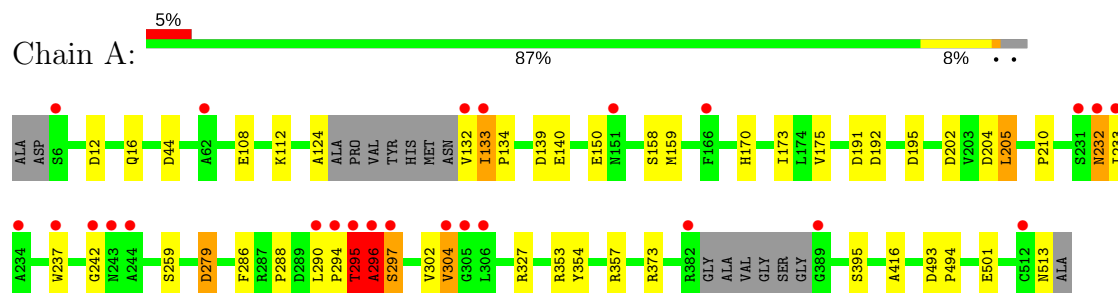
- Molecule 3 is water.

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

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 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.

• 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 0.178 , 0.200	Depositor DCC
R_{free} test set	2408 reflections (3.04%)	wwPDB-VP
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 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 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	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

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 3.

All (21) 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: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	Interatomic distance (Å)	Clash overlap (Å)
3:A:2018:HOH:O	3:A:2306:HOH:O[2_646]	2.03	0.17

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	480/506 (95%)	462 (96%)	16 (3%)	2 (0%)	36	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ALA
1	A	242	GLY

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	397/406 (98%)	391 (98%)	6 (2%)	67	38

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
1	A	20	GLN
1	A	114	ASN
1	A	232	ASN
1	A	409	ASN
1	A	513	ASN

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](#)

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	0,3,3	0.00	-	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

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	302:VAL	C	304:VAL	N	2.07
1	A	290:LEU	C	294:PRO	N	2.02

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%)	0.01	25 (5%) 28 27	9, 16, 30, 42	23 (4%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	ALA	8.7
1	A	132	VAL	7.9
1	A	233	ILE	6.8
1	A	295	THR	5.8
1	A	305	GLY	5.0
1	A	242	GLY	4.9
1	A	234	ALA	4.3
1	A	237	TRP	4.3
1	A	512	CYS	4.1
1	A	297	SER	4.0
1	A	232	ASN	3.8
1	A	243	ASN	3.8
1	A	133	ILE	3.5
1	A	304	VAL	3.2
1	A	244	ALA	3.0
1	A	6	SER	2.8
1	A	382	ARG	2.7
1	A	389	GLY	2.5
1	A	231	SER	2.4
1	A	151	ASN	2.3
1	A	294	PRO	2.3
1	A	306	LEU	2.1
1	A	62	ALA	2.1
1	A	166	PHE	2.0
1	A	290	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO3	A	1515	4/4	0.99	0.05	13,13,14,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.