



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 AM UTC

PDB ID : 1V0V / pdb_00001v0v
Title : Phospholipase D from Streptomyces sp. strain PMF soaked with the substrate dibutylphosphatidylcholine.
Authors : Leiros, I.; McSweeney, S.; Hough, E.
Deposited on : 2004-04-02
Resolution : 1.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

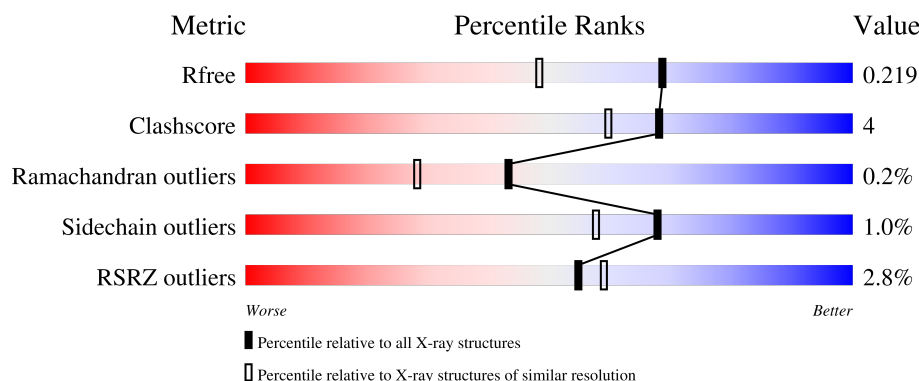
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

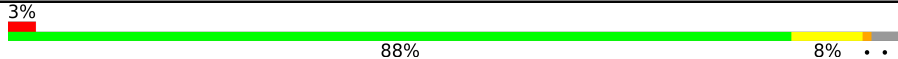
The reported resolution of this entry is 1.70 Å.

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 $\leq 5\%$. 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](#)

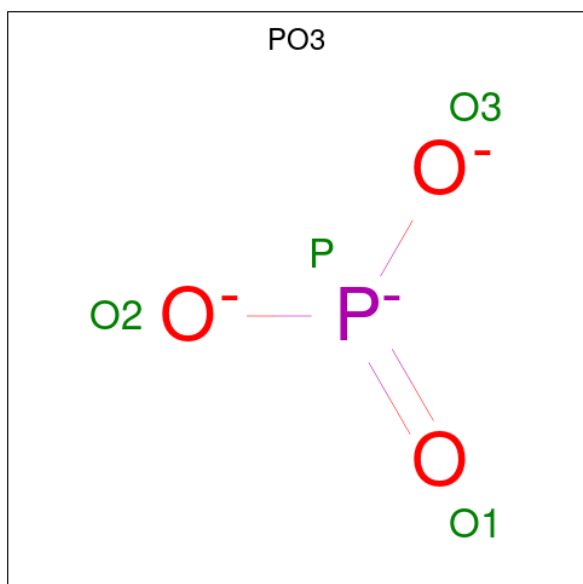
There are 3 unique types of molecules in this entry. The entry contains 4170 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	492	3704	2311	651	728	14	58	0	0

- Molecule 2 is PHOSPHITE ION (CCD ID: PO3) (formula: O_3P).



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

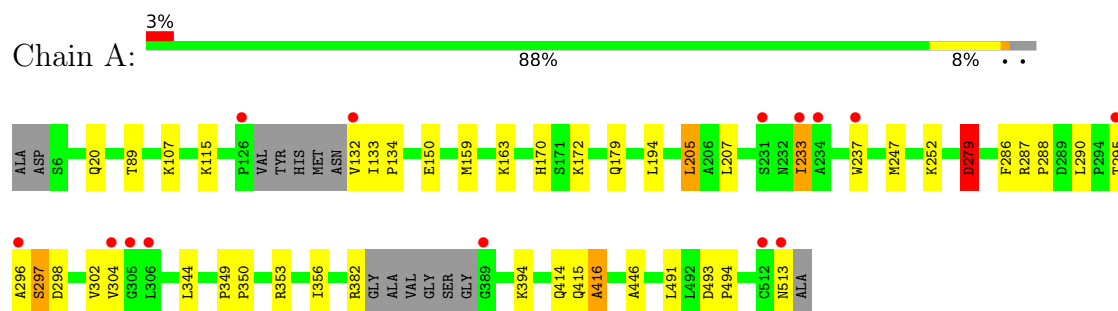
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	462	462	462	0	0

3 Residue-property plots

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 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	57.45Å 56.75Å 68.54Å 90.00° 93.39° 90.00°	Depositor
Resolution (Å)	69.01 – 1.70 68.42 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.7 (69.01-1.70) 90.7 (68.42-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.162 , 0.208 0.173 , 0.219	Depositor DCC
R_{free} test set	2229 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4170	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.30	20/3779 (0.5%)	1.22	18/5145 (0.3%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	GLU	CB-CG	-15.67	1.05	1.52
1	A	170	HIS	CD2-NE2	-14.36	1.22	1.37
1	A	170	HIS	CE1-NE2	13.57	1.46	1.32
1	A	170	HIS	ND1-CE1	12.80	1.45	1.32
1	A	290	LEU	C-N	12.54	1.51	1.33
1	A	416	ALA	C-N	12.27	1.51	1.33
1	A	252	LYS	CD-CE	-11.84	1.17	1.52
1	A	170	HIS	CG-CD2	-10.53	1.24	1.35
1	A	279	ASP	CB-CG	-8.10	1.31	1.52
1	A	107	LYS	CD-CE	-6.94	1.31	1.52
1	A	194	LEU	CA-C	6.62	1.57	1.52
1	A	159	MET	SD-CE	-6.45	1.63	1.79
1	A	382	ARG	NE-CZ	-6.44	1.25	1.33
1	A	415	GLN	CB-CG	-6.08	1.34	1.52
1	A	247	MET	SD-CE	-5.31	1.66	1.79
1	A	115	LYS	CG-CD	-5.23	1.36	1.52
1	A	394	LYS	CG-CD	-5.16	1.36	1.52
1	A	163	LYS	CB-CG	-5.14	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	ALA	CA-CB	-5.09	1.46	1.53
1	A	89	THR	CA-CB	5.02	1.61	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	HIS	CG-CD2-NE2	23.93	131.12	107.20
1	A	150	GLU	CA-CB-CG	11.16	136.42	114.10
1	A	132	VAL	N-CA-CB	10.29	128.99	111.50
1	A	170	HIS	ND1-CG-CD2	-10.15	95.95	106.10
1	A	394	LYS	CB-CG-CD	9.44	133.00	111.30
1	A	382	ARG	NE-CZ-NH2	9.07	127.36	119.20
1	A	382	ARG	NE-CZ-NH1	-8.66	112.84	121.50
1	A	170	HIS	CE1-NE2-CD2	-8.43	100.57	109.00
1	A	170	HIS	ND1-CE1-NE2	-7.93	100.47	108.40
1	A	233	ILE	CG1-CB-CG2	-7.59	87.94	110.70
1	A	382	ARG	CD-NE-CZ	6.71	133.80	124.40
1	A	290	LEU	CA-C-N	-6.65	113.86	120.98
1	A	290	LEU	C-N-CA	-6.65	113.86	120.98
1	A	170	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	170	HIS	N-CA-C	-5.65	105.33	114.09
1	A	414	GLN	N-CA-C	5.46	117.23	111.28
1	A	170	HIS	CB-CG-CD2	5.18	137.94	131.20
1	A	172	LYS	CG-CD-CE	5.11	123.05	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	416	ALA	Mainchain

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	3704	0	3641	26	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	462	0	0	10	0
All	All	4170	0	3641	26	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 4.

All (26) 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:302:VAL:C	1:A:304:VAL:N	2.01	1.16
1:A:279:ASP:HB3	3:A:2294:HOH:O	1.66	0.93
1:A:20:GLN:OE1	3:A:2041:HOH:O	2.06	0.73
1:A:297:SER:HB2	3:A:2310:HOH:O	1.95	0.67
1:A:302:VAL:C	1:A:304:VAL:CA	2.73	0.62
1:A:296:ALA:CB	3:A:2183:HOH:O	2.52	0.56
1:A:179:GLN:NE2	3:A:2222:HOH:O	2.40	0.54
1:A:233:ILE:CG2	1:A:237:TRP:CH2	2.92	0.53
1:A:286:PHE:O	1:A:287:ARG:HD3	2.09	0.52
1:A:297:SER:CA	3:A:2310:HOH:O	2.57	0.52
1:A:491:LEU:C	1:A:491:LEU:HD23	2.35	0.51
1:A:207:LEU:C	1:A:207:LEU:HD12	2.36	0.49
1:A:297:SER:HA	3:A:2310:HOH:O	2.12	0.49
1:A:513:ASN:ND2	3:A:2461:HOH:O	2.47	0.48
1:A:296:ALA:HA	1:A:356:ILE:HD13	1.98	0.46
1:A:205:LEU:C	1:A:205:LEU:HD12	2.41	0.45
1:A:298:ASP:OD1	1:A:298:ASP:N	2.47	0.45
1:A:233:ILE:CG2	1:A:237:TRP:CZ2	3.00	0.44
1:A:233:ILE:HG23	1:A:237:TRP:CH2	2.53	0.44
1:A:133:ILE:HB	1:A:134:PRO:HD3	2.00	0.44
1:A:493:ASP:HB2	1:A:494:PRO:HD3	1.99	0.43
1:A:296:ALA:O	1:A:297:SER:CB	2.68	0.41
1:A:286:PHE:CZ	1:A:288:PRO:HB3	2.54	0.41
1:A:296:ALA:HB1	3:A:2183:HOH:O	2.17	0.41
1:A:353:ARG:NH1	3:A:2354:HOH:O	2.42	0.41
1:A:349:PRO:HB2	1:A:350:PRO:HA	2.02	0.40

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	484/506 (96%)	465 (96%)	18 (4%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER

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	398/406 (98%)	394 (99%)	4 (1%)	68	58

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	A	279	ASP
1	A	295	THR
1	A	344	LEU

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

Mol	Chain	Res	Type
1	A	20	GLN

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Mol	Chain	Res	Type
1	A	179	GLN
1	A	198	HIS
1	A	309	ASN
1	A	409	ASN
1	A	495	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 oligosaccharides 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	-	-	0,3,3	-	-

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	1

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	2.01

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	492/506 (97%)	-0.02	14 (2%) 55 59	10, 19, 34, 46	19 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	PRO	4.7
1	A	132	VAL	4.6
1	A	296	ALA	4.4
1	A	237	TRP	3.4
1	A	295	THR	3.2
1	A	304	VAL	2.9
1	A	306	LEU	2.8
1	A	233	ILE	2.6
1	A	305	GLY	2.4
1	A	512	CYS	2.4
1	A	389	GLY	2.3
1	A	234	ALA	2.2
1	A	513	ASN	2.1
1	A	231	SER	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO3	A	1515	4/4	0.98	0.07	20,21,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.