



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 07:32 pm GMT

PDB ID : 1V0T
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 : 1.53 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

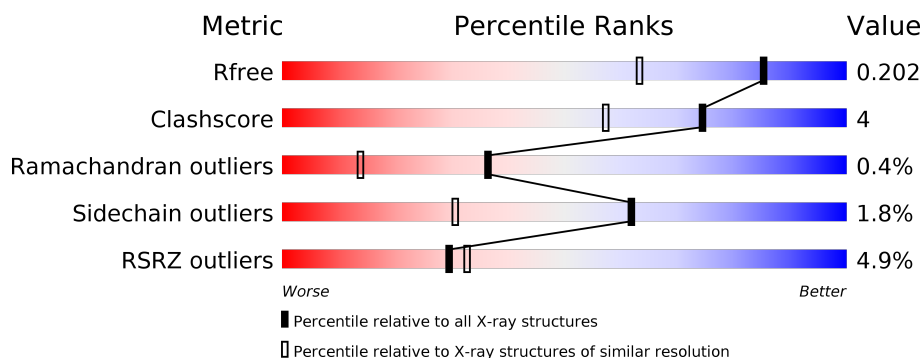
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	2055 (1.56-1.52)
Clashscore	122126	2124 (1.56-1.52)
Ramachandran outliers	120053	2083 (1.56-1.52)
Sidechain outliers	120020	2081 (1.56-1.52)
RSRZ outliers	108989	2027 (1.56-1.52)

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	<div> <div>5%</div> <div>88%</div> <div>7% . .</div> </div>

2 Entry composition [i](#)

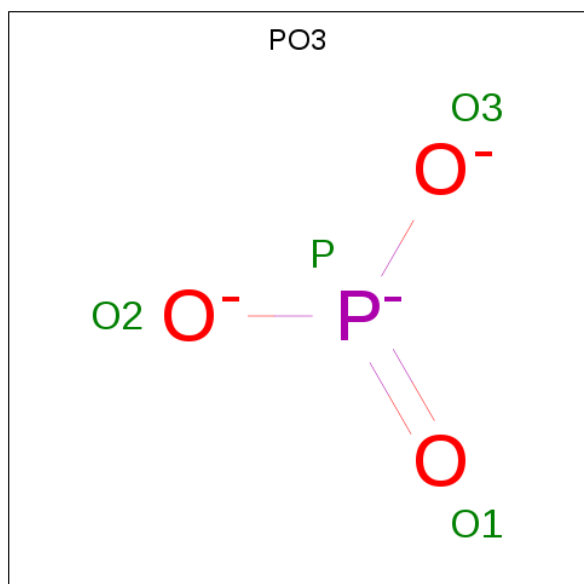
There are 3 unique types of molecules in this entry. The entry contains 4281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	491	Total	C	N	O	S	81	0	0
			3694	2305	650	725	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		

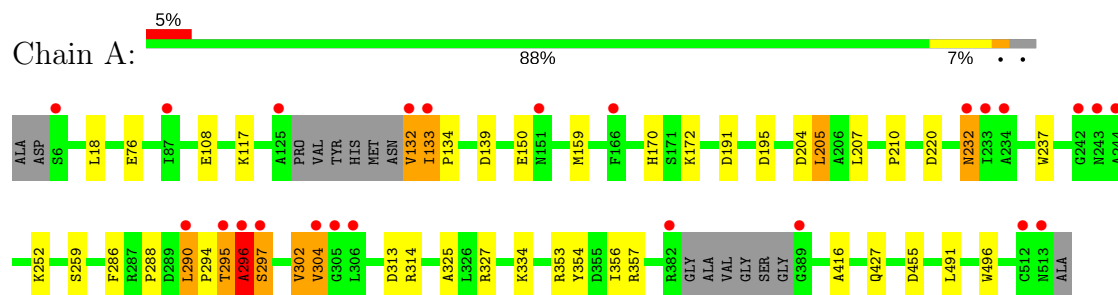
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	583	Total	O	0	0
			583	583		

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	57.16Å 56.94Å 68.81Å 90.00° 93.48° 90.00°	Depositor
Resolution (Å)	69.01 – 1.53 26.71 – 1.53	Depositor EDS
% Data completeness (in resolution range)	95.8 (69.01-1.53) 95.8 (26.71-1.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.156 , 0.188 0.170 , 0.202	Depositor DCC
R_{free} test set	1927 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.7	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	4281	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 7.45% 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	1.03	15/3769 (0.4%)	0.99	22/5132 (0.4%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	VAL	C-N	27.46	1.97	1.34
1	A	290	LEU	C-N	18.92	1.70	1.34
1	A	237	TRP	CG-CD1	-17.88	1.11	1.36
1	A	150	GLU	CB-CG	-17.10	1.19	1.52
1	A	237	TRP	CG-CD2	13.31	1.66	1.43
1	A	117	LYS	CE-NZ	9.91	1.73	1.49
1	A	304	VAL	CA-CB	-8.92	1.36	1.54
1	A	195	ASP	CB-CG	8.02	1.68	1.51
1	A	416	ALA	C-N	7.17	1.50	1.34
1	A	170	HIS	CG-CD2	-5.85	1.25	1.35
1	A	170	HIS	CD2-NE2	-5.75	1.25	1.38
1	A	132	VAL	CA-CB	5.60	1.66	1.54
1	A	170	HIS	CE1-NE2	5.60	1.45	1.32
1	A	252	LYS	CE-NZ	-5.46	1.35	1.49
1	A	334	LYS	CG-CD	5.12	1.69	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	TRP	CB-CG-CD2	-14.06	108.32	126.60
1	A	237	TRP	CB-CG-CD1	12.31	143.01	127.00
1	A	132	VAL	N-CA-CB	11.87	137.60	111.50
1	A	327	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	A	170	HIS	CG-CD2-NE2	9.50	127.24	109.20
1	A	237	TRP	CE2-CD2-CG	-9.34	99.83	107.30
1	A	237	TRP	CG-CD2-CE3	8.22	141.29	133.90
1	A	150	GLU	CA-CB-CG	7.47	129.83	113.40
1	A	353	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	117	LYS	CD-CE-NZ	-6.83	95.99	111.70
1	A	237	TRP	CG-CD1-NE1	6.73	116.83	110.10
1	A	204	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	353	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	313	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	139	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	357	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	327	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	132	VAL	CB-CA-C	-5.57	100.81	111.40
1	A	170	HIS	ND1-CG-CD2	-5.42	98.42	106.00
1	A	455	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	191	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	220	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

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	3694	0	3632	25	0
2	A	4	0	0	0	0
3	A	583	0	0	2	0
All	All	4281	0	3632	25	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 (25) 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	1.70	1.44
1:A:302:VAL:C	1:A:304:VAL:N	1.97	1.18
1:A:295:THR:O	1:A:296:ALA:O	1.80	1.00
1:A:296:ALA:HA	1:A:356:ILE:HD13	1.65	0.77
1:A:290:LEU:C	1:A:294:PRO:CA	2.56	0.73
1:A:76:GLU:CG	3:A:2159:HOH:O	2.42	0.67
1:A:296:ALA:HA	1:A:356:ILE:CD1	2.31	0.60
1:A:295:THR:O	1:A:296:ALA:C	2.40	0.59
1:A:232:ASN:HD22	1:A:232:ASN:C	2.09	0.56
1:A:296:ALA:O	1:A:297:SER:HB3	2.06	0.56
1:A:133:ILE:HG23	1:A:134:PRO:HD3	1.90	0.54
1:A:296:ALA:O	1:A:297:SER:CB	2.57	0.53
1:A:210:PRO:HA	1:A:259:SER:HB2	1.93	0.51
1:A:205:LEU:HD12	1:A:205:LEU:C	2.33	0.48
1:A:133:ILE:CG2	1:A:134:PRO:HD3	2.44	0.47
1:A:286:PHE:CZ	1:A:288:PRO:HB3	2.49	0.47
1:A:491:LEU:HD23	1:A:491:LEU:C	2.38	0.44
1:A:296:ALA:CB	3:A:2214:HOH:O	2.66	0.44
1:A:108:GLU:HA	1:A:108:GLU:OE1	2.18	0.44
1:A:297:SER:HB2	1:A:354:TYR:OH	2.19	0.43
1:A:18:LEU:HD21	1:A:325:ALA:HB2	1.99	0.42
1:A:207:LEU:HD12	1:A:207:LEU:C	2.39	0.42
1:A:427:GLN:HB3	1:A:496:TRP:CH2	2.55	0.42
1:A:296:ALA:C	1:A:297:SER:OG	2.56	0.41
1:A:314:ARG:C	1:A:314:ARG:HD3	2.41	0.41

There are no symmetry-related clashes.

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	485/506 (96%)	470 (97%)	13 (3%)	2 (0%)	36	14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ALA
1	A	297	SER

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	396/406 (98%)	389 (98%)	7 (2%)	62	31

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	133	ILE
1	A	159	MET
1	A	172	LYS
1	A	205	LEU
1	A	232	ASN
1	A	295	THR

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	20	GLN
1	A	114	ASN
1	A	179	GLN
1	A	232	ASN
1	A	409	ASN
1	A	513	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 ⓘ

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	1.97
1	A	290:LEU	C	294:PRO	N	1.70

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	491/506 (97%)	-0.01	24 (4%)	29 33	9, 16, 31, 45	25 (5%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	ALA	8.0
1	A	295	THR	8.0
1	A	125	ALA	6.0
1	A	132	VAL	5.6
1	A	233	ILE	5.1
1	A	305	GLY	4.9
1	A	151	ASN	3.9
1	A	242	GLY	3.7
1	A	166	PHE	3.5
1	A	244	ALA	3.3
1	A	243	ASN	3.2
1	A	232	ASN	3.2
1	A	297	SER	3.2
1	A	304	VAL	3.2
1	A	133	ILE	3.1
1	A	512	CYS	3.0
1	A	234	ALA	3.0
1	A	290	LEU	2.9
1	A	6	SER	2.8
1	A	306	LEU	2.5
1	A	389	GLY	2.2
1	A	87	ILE	2.0
1	A	382	ARG	2.0
1	A	513	ASN	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	0.04	13,14,14,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.