



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1F0I / pdb_00001f0i
Title : THE FIRST CRYSTAL STRUCTURE OF A PHOSPHOLIPASE D
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Deposited on : 2000-05-16
Resolution : 1.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

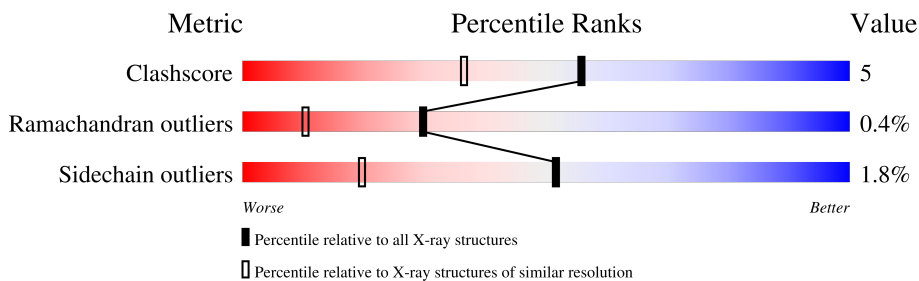
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	504	 87% 10% ..

2 Entry composition [i](#)

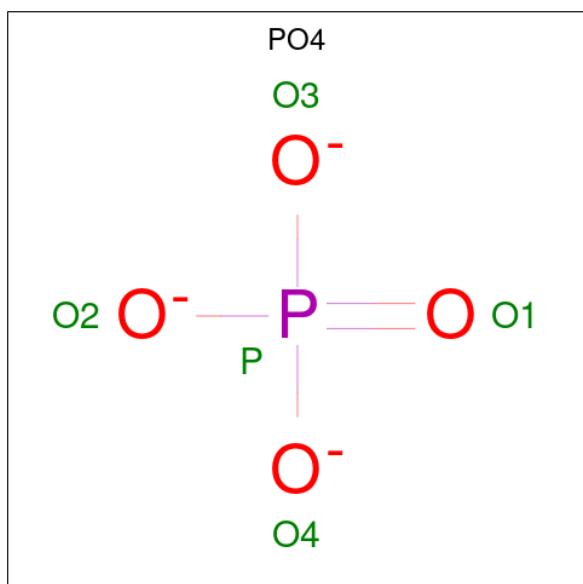
There are 3 unique types of molecules in this entry. The entry contains 4468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	496	Total	C	N	O	S	0	10	0
			3759	2352	657	735	15			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

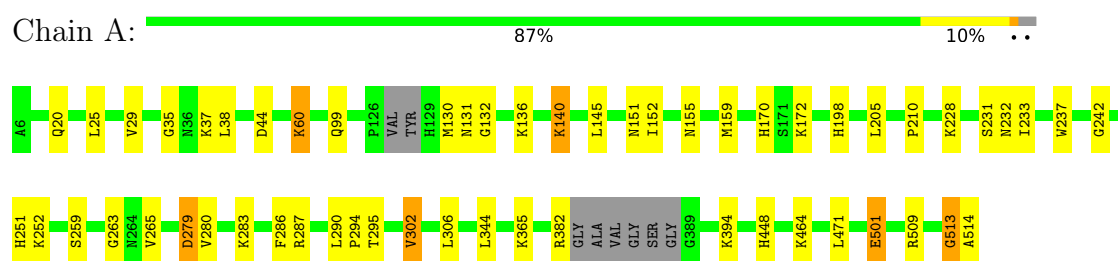
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	692	Total	O	0	7
			699	699		

3 Residue-property plots [i](#)

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. 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. 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: PHOSPHOLIPASE D



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.28 Å 57.42 Å 68.70 Å 90.00° 93.17° 90.00°	Depositor
Resolution (Å)	10.00 – 1.40	Depositor
% Data completeness (in resolution range)	99.2 (10.00-1.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.130 , 0.185	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.78	9/3874 (0.2%)	1.31	25/5269 (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	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	THR	C-N	11.88	1.50	1.33
1	A	501	GLU	C-N	11.30	1.50	1.33
1	A	295	THR	N-CA	8.85	1.57	1.46
1	A	231	SER	C-N	6.79	1.44	1.33
1	A	233	ILE	C-N	6.28	1.43	1.33
1	A	290	LEU	C-N	-5.99	1.25	1.33
1	A	302[A]	VAL	C-N	5.27	1.40	1.33
1	A	302[B]	VAL	C-N	5.27	1.40	1.33
1	A	294	PRO	C-N	5.12	1.40	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ASN	O-C-N	-11.37	108.88	122.87
1	A	232	ASN	CA-C-N	10.91	138.75	120.64
1	A	232	ASN	C-N-CA	10.91	138.75	120.64
1	A	295	THR	O-C-N	10.54	135.76	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ILE	O-C-N	10.31	135.55	122.05
1	A	99	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	A	509	ARG	CD-NE-CZ	8.87	136.82	124.40
1	A	233	ILE	CA-C-N	-8.71	105.90	121.14
1	A	233	ILE	C-N-CA	-8.71	105.90	121.14
1	A	295	THR	N-CA-CB	-7.87	96.58	109.56
1	A	132	GLY	CA-C-N	-7.07	114.68	120.33
1	A	132	GLY	C-N-CA	-7.07	114.68	120.33
1	A	99	GLN	CG-CD-NE2	6.70	126.44	116.40
1	A	509	ARG	NE-CZ-NH1	6.51	128.01	121.50
1	A	44	ASP	CA-CB-CG	6.11	118.70	112.60
1	A	172	LYS	CG-CD-CE	5.95	124.99	111.30
1	A	294	PRO	CA-C-N	-5.93	112.47	121.31
1	A	294	PRO	C-N-CA	-5.93	112.47	121.31
1	A	448	HIS	CA-CB-CG	5.77	119.57	113.80
1	A	251	HIS	CA-CB-CG	-5.48	108.32	113.80
1	A	155	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	287	ARG	CD-NE-CZ	5.24	131.73	124.40
1	A	302[A]	VAL	O-C-N	-5.17	117.60	123.18
1	A	302[B]	VAL	O-C-N	-5.17	117.60	123.18
1	A	198	HIS	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	513	GLY	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	3759	0	3735	35	0
2	A	10	0	0	0	0
3	A	699	0	0	8	0
All	All	4468	0	3735	35	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 5.

All (35) 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[A]:VAL:HG23	1:A:306:LEU:HG	1.36	1.04
1:A:228:LYS:HE3	3:A:1620:HOH:O	1.61	1.00
1:A:513:GLY:O	1:A:514:ALA:HB2	1.63	0.96
1:A:302[A]:VAL:CG2	1:A:306:LEU:HG	2.12	0.79
1:A:228:LYS:CE	3:A:1620:HOH:O	2.27	0.73
1:A:501:GLU:HA	1:A:501:GLU:OE1	1.88	0.73
1:A:513:GLY:O	1:A:514:ALA:CB	2.33	0.66
1:A:151:ASN:HB2	3:A:1442:HOH:O	1.98	0.64
1:A:210:PRO:HA	1:A:259:SER:HB2	1.81	0.60
1:A:302[A]:VAL:HG23	1:A:306:LEU:CG	2.24	0.59
1:A:302[A]:VAL:CG2	1:A:306:LEU:CG	2.82	0.58
1:A:283:LYS:HD3	3:A:1425:HOH:O	2.04	0.57
1:A:279:ASP:OD1	1:A:280:VAL:HG12	2.04	0.57
1:A:382:ARG:HH12	1:A:394:LYS:NZ	2.02	0.57
1:A:382:ARG:NH2	1:A:394:LYS:HG2	2.20	0.56
1:A:382:ARG:CZ	1:A:394:LYS:HG2	2.36	0.56
1:A:302[A]:VAL:HG22	1:A:306:LEU:HD11	1.89	0.54
1:A:302[A]:VAL:HG22	1:A:306:LEU:CD1	2.38	0.54
1:A:136:LYS:HG2	1:A:140:LYS:HD3	1.90	0.53
1:A:38[B]:LEU:HD22	1:A:265:VAL:HG21	1.90	0.53
1:A:382:ARG:HH12	1:A:394:LYS:CE	2.23	0.51
1:A:145:LEU:HD13	1:A:152:ILE:HD12	1.93	0.50
1:A:302[A]:VAL:CG2	1:A:306:LEU:CD1	2.90	0.49
1:A:25[B]:LEU:HD23	1:A:29:VAL:HB	1.93	0.48
1:A:170:HIS:CG	1:A:471:LEU:HD13	2.48	0.47
1:A:60:LYS:HB2	1:A:60:LYS:HE2	1.48	0.47
1:A:20:GLN:O	1:A:286:PHE:HB2	2.16	0.46
1:A:131:ASN:HB3	1:A:237:TRP:CD2	2.51	0.45
1:A:365[B]:LYS:NZ	3:A:1234:HOH:O	2.49	0.45
1:A:38[B]:LEU:HD23	3:A:1241:HOH:O	2.17	0.44
1:A:464:LYS:HE3	3:A:1295:HOH:O	2.17	0.44
1:A:302[A]:VAL:CG2	1:A:306:LEU:HD11	2.49	0.42
1:A:501:GLU:OE1	1:A:501:GLU:CA	2.59	0.42
1:A:35:GLY:HA2	1:A:263:GLY:O	2.20	0.42
1:A:37:LYS:HE3	3:A:1443:HOH:O	2.20	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	501/504 (99%)	480 (96%)	19 (4%)	2 (0%)	30	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	MET
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	408/402 (102%)	401 (98%)	7 (2%)	53	21

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

Mol	Chain	Res	Type
1	A	60	LYS
1	A	140	LYS
1	A	159	MET
1	A	205	LEU
1	A	252	LYS
1	A	279	ASP
1	A	344	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	309	ASN
1	A	409	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	PO4	A	601	-	4,4,4	0.60	0	6,6,6	0.45	0
2	PO4	A	600	-	4,4,4	0.67	0	6,6,6	0.52	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

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.