Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:09 pm BST

PDB ID	:	1P2P
Title	:	STRUCTURE OF PORCINE PANCREATIC PHOSPHOLIPASE A2 AT 2.6 ANGSTROMS RESOLUTION AND COMPARISON WITH BOVINE PHOSPHOLIPASE A2
Authors	:	Dijkstra, B.W.; Renetseder, R.; Kalk, K.H.; Hol, W.G.J.; Drenth, J.
Deposited on	:	1983-06-27
Resolution	:	2.60 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:

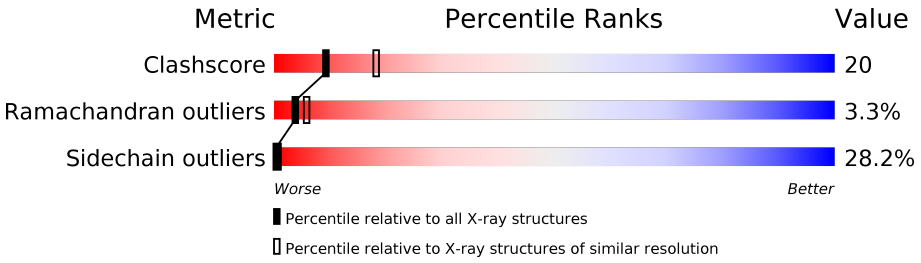
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	124	35% 41% 19% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 978 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 A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			971	596	166	193	16			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

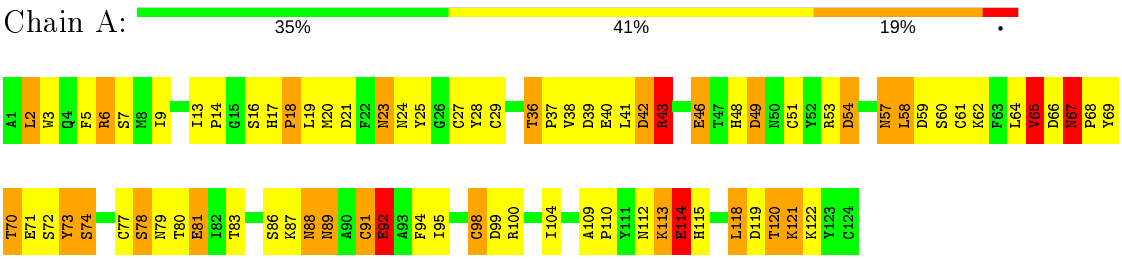
3 Residue-property plots (i)

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. 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 A2

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.82Å 69.82Å 67.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.241 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	978	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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: CA

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	1.23	4/993 (0.4%)	2.12	43/1340 (3.2%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	TRP	NE1-CE2	-7.10	1.28	1.37
1	A	92	GLU	CD-OE2	-5.30	1.19	1.25
1	A	71	GLU	CD-OE2	-5.23	1.19	1.25
1	A	46	GLU	CD-OE2	-5.04	1.20	1.25

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ASP	CB-CG-OD1	16.31	132.98	118.30
1	A	39	ASP	CA-CB-CG	14.27	144.80	113.40
1	A	49	ASP	CB-CG-OD1	11.74	128.87	118.30
1	A	39	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	A	100	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	16	SER	CA-C-O	7.85	136.58	120.10
1	A	74	SER	CA-C-O	7.68	136.23	120.10
1	A	114	GLU	OE1-CD-OE2	7.61	132.43	123.30
1	A	21	ASP	CB-CG-OD1	7.59	125.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ASN	C-N-CD	7.34	143.81	128.40
1	A	16	SER	C-N-CA	7.21	139.73	121.70
1	A	17	HIS	C-N-CD	7.19	143.50	128.40
1	A	51	CYS	CA-CB-SG	-7.04	101.33	114.00
1	A	40	GLU	OE1-CD-OE2	6.99	131.69	123.30
1	A	39	ASP	N-CA-CB	-6.96	98.07	110.60
1	A	77	CYS	CA-CB-SG	-6.96	101.48	114.00
1	A	36	THR	C-N-CD	6.87	142.82	128.40
1	A	119	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	13	ILE	C-N-CD	6.74	142.54	128.40
1	A	59	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	42	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	110	PRO	CA-N-CD	-6.46	102.46	111.50
1	A	40	GLU	CG-CD-OE1	-6.41	105.48	118.30
1	A	81	GLU	OE1-CD-OE2	6.32	130.88	123.30
1	A	54	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	18	PRO	CA-N-CD	-6.19	102.84	111.50
1	A	109	ALA	C-N-CD	5.93	140.85	128.40
1	A	99	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	74	SER	O-C-N	-5.86	113.32	122.70
1	A	91	CYS	CA-CB-SG	-5.84	103.48	114.00
1	A	16	SER	N-CA-CB	-5.82	101.77	110.50
1	A	100	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	23	ASN	N-CA-C	-5.69	95.64	111.00
1	A	114	GLU	CG-CD-OE1	-5.64	107.02	118.30
1	A	65	VAL	CB-CA-C	-5.63	100.71	111.40
1	A	61	CYS	CA-CB-SG	-5.53	104.06	114.00
1	A	28	TYR	CA-CB-CG	-5.42	103.11	113.40
1	A	46	GLU	OE1-CD-OE2	5.34	129.71	123.30
1	A	14	PRO	CA-N-CD	-5.21	104.21	111.50
1	A	81	GLU	CG-CD-OE1	-5.18	107.94	118.30
1	A	27	CYS	N-CA-CB	-5.16	101.31	110.60
1	A	98	CYS	CA-CB-SG	-5.10	104.81	114.00
1	A	65	VAL	O-C-N	5.04	130.76	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	ARG	Sidechain
1	A	6	ARG	Sidechain

5.2 Too-close contacts (i)

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	971	0	886	37	0
2	A	2	0	0	0	0
3	A	5	0	0	0	0
All	All	978	0	886	37	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 20.

All (37) 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:37:PRO:HG3	1:A:43:ARG:HG2	1.75	0.69
1:A:64:LEU:C	1:A:66:ASP:H	1.98	0.66
1:A:73:TYR:HB3	1:A:92:GLU:HB2	1.79	0.65
1:A:19:LEU:O	1:A:23:ASN:HB3	1.98	0.62
1:A:2:LEU:HD13	1:A:6:ARG:HH21	1.65	0.60
1:A:65:VAL:O	1:A:66:ASP:HB2	2.02	0.60
1:A:2:LEU:HD13	1:A:6:ARG:NH2	2.18	0.59
1:A:25:TYR:O	1:A:29:CYS:HB2	2.03	0.58
1:A:113:LYS:NZ	1:A:113:LYS:H	2.04	0.55
1:A:37:PRO:CG	1:A:43:ARG:HG2	2.36	0.55
1:A:112:ASN:HB3	1:A:114:GLU:OE2	2.07	0.55
1:A:64:LEU:O	1:A:70:THR:HG21	2.06	0.55
1:A:73:TYR:O	1:A:88:ASN:ND2	2.39	0.54
1:A:112:ASN:HD22	1:A:115:HIS:CE1	2.27	0.53
1:A:37:PRO:HB2	1:A:42:ASP:HB3	1.93	0.51
1:A:64:LEU:C	1:A:66:ASP:N	2.65	0.51
1:A:5:PHE:O	1:A:9:ILE:HG13	2.12	0.50
1:A:121:LYS:HZ2	1:A:121:LYS:HA	1.78	0.48
1:A:64:LEU:HB3	1:A:70:THR:HG21	1.95	0.48
1:A:73:TYR:CB	1:A:92:GLU:HB2	2.43	0.48
1:A:78:SER:O	1:A:81:GLU:HB2	2.14	0.48
1:A:46:GLU:O	1:A:49:ASP:HB2	2.13	0.47
1:A:58:LEU:HD21	1:A:94:PHE:CE2	2.50	0.47
1:A:48:HIS:HD2	1:A:98:CYS:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HB3	1:A:95:ILE:HD12	1.99	0.45
1:A:91:CYS:O	1:A:95:ILE:HG12	2.17	0.44
1:A:89:ASN:ND2	1:A:92:GLU:OE2	2.51	0.43
1:A:54:ASP:O	1:A:57:ASN:HB2	2.17	0.43
1:A:120:THR:HG22	1:A:121:LYS:N	2.34	0.43
1:A:9:ILE:HB	1:A:18:PRO:CG	2.50	0.42
1:A:113:LYS:HE2	1:A:114:GLU:HG3	2.01	0.42
1:A:9:ILE:HB	1:A:18:PRO:HG2	2.02	0.42
1:A:38:VAL:HG11	1:A:118:LEU:HD11	2.02	0.42
1:A:67:ASN:C	1:A:69:TYR:N	2.73	0.41
1:A:89:ASN:OD1	1:A:91:CYS:N	2.53	0.41
1:A:113:LYS:HZ3	1:A:114:GLU:HG3	1.86	0.41
1:A:64:LEU:HB3	1:A:70:THR:CG2	2.51	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	122/124 (98%)	101 (83%)	17 (14%)	4 (3%)	4 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	74	SER
1	A	120	THR
1	A	104	ILE

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	110/110 (100%)	79 (72%)	31 (28%)	0 1

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	7	SER
1	A	20	MET
1	A	24	ASN
1	A	36	THR
1	A	41	LEU
1	A	43	ARG
1	A	53	ARG
1	A	57	ASN
1	A	58	LEU
1	A	60	SER
1	A	62	LYS
1	A	65	VAL
1	A	67	ASN
1	A	70	THR
1	A	72	SER
1	A	73	TYR
1	A	78	SER
1	A	79	ASN
1	A	80	THR
1	A	83	THR
1	A	86	SER
1	A	87	LYS
1	A	88	ASN
1	A	89	ASN
1	A	92	GLU
1	A	113	LYS
1	A	114	GLU
1	A	118	LEU
1	A	121	LYS

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Mol	Chain	Res	Type
1	A	122	LYS

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	48	HIS
1	A	57	ASN
1	A	79	ASN
1	A	88	ASN
1	A	97	ASN
1	A	112	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.