



Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 06:00 PM UTC

PDB ID : 1SFV / pdb_00001sfv
Title : PORCINE PANCREAS PHOSPHOLIPASE A2, NMR, MINIMIZED AVERAGE STRUCTURE
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Deposited on : 1996-02-20

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

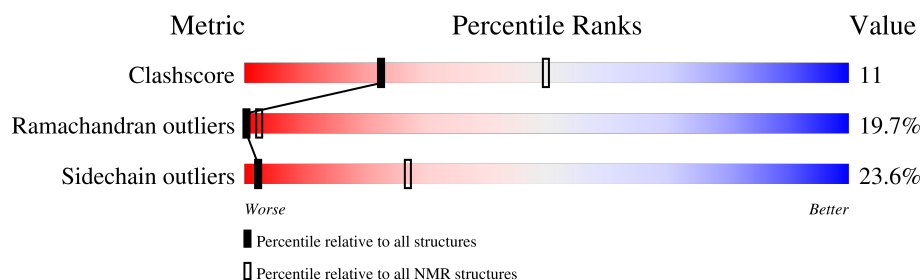
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	124	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 972 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PHOSPHOLIPASE A2.

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

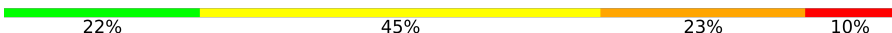
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

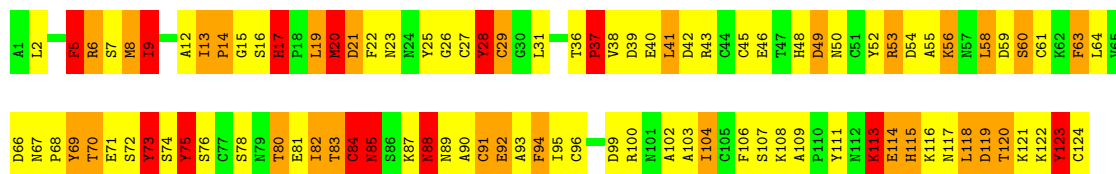
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

4 Residue-property plots [i](#)

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: PHOSPHOLIPASE A2

Chain A: 



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Discover	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 (average) 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	1.73	25/993 (2.5%)	2.52	78/1340 (5.8%)
All	All	1.73	25/993 (2.5%)	2.52	78/1340 (5.8%)

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	Planarity
1	A	0	15
All	All	0	15

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	CYS	C-OXT	7.15	1.37	1.23
1	A	40	GLU	CD-OE1	6.49	1.37	1.25
1	A	81	GLU	CD-OE1	6.48	1.37	1.25
1	A	21	ASP	CG-OD1	6.47	1.37	1.25
1	A	114	GLU	CD-OE2	6.46	1.37	1.25
1	A	54	ASP	CG-OD2	6.46	1.37	1.25
1	A	59	ASP	CG-OD1	6.46	1.37	1.25
1	A	71	GLU	CD-OE2	6.46	1.37	1.25
1	A	46	GLU	CD-OE1	6.44	1.37	1.25
1	A	119	ASP	CG-OD1	6.42	1.37	1.25
1	A	49	ASP	CG-OD2	6.42	1.37	1.25
1	A	66	ASP	CG-OD2	6.39	1.37	1.25
1	A	92	GLU	CD-OE2	6.37	1.37	1.25
1	A	39	ASP	CG-OD2	6.33	1.37	1.25
1	A	80	THR	CA-C	6.10	1.60	1.52
1	A	99	ASP	CG-OD2	6.09	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	LYS	CA-C	6.08	1.60	1.52
1	A	42	ASP	CG-OD2	6.03	1.36	1.25
1	A	14	PRO	N-CA	5.90	1.54	1.47
1	A	17	HIS	ND1-CE1	5.49	1.38	1.32
1	A	7	SER	N-CA	5.33	1.53	1.46
1	A	48	HIS	CG-CD2	5.31	1.41	1.35
1	A	103	ALA	N-CA	5.17	1.52	1.46
1	A	23	ASN	N-CA	5.11	1.52	1.46
1	A	49	ASP	CA-C	5.03	1.59	1.52

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	TYR	N-CA-CB	-12.86	90.50	110.30
1	A	17	HIS	ND1-CE1-NE2	11.70	120.10	108.40
1	A	48	HIS	ND1-CE1-NE2	11.63	120.03	108.40
1	A	115	HIS	ND1-CE1-NE2	11.30	119.70	108.40
1	A	115	HIS	CB-CG-CD2	-10.74	117.23	131.20
1	A	17	HIS	CB-CG-CD2	-10.20	117.94	131.20
1	A	85	ASN	CA-CB-CG	9.92	122.52	112.60
1	A	115	HIS	CE1-NE2-CD2	-9.79	99.22	109.00
1	A	17	HIS	CE1-NE2-CD2	-9.51	99.50	109.00
1	A	71	GLU	N-CA-C	9.32	122.39	111.02
1	A	122	LYS	N-CA-CB	-8.90	97.10	110.01
1	A	48	HIS	CE1-NE2-CD2	-8.61	100.39	109.00
1	A	114	GLU	CB-CA-C	7.74	125.82	110.42
1	A	82	ILE	CB-CA-C	7.64	123.81	111.29
1	A	13	ILE	N-CA-C	-7.61	99.25	107.77
1	A	5	PHE	CA-CB-CG	7.60	121.40	113.80
1	A	94	PHE	CA-CB-CG	7.51	121.31	113.80
1	A	19	LEU	CA-C-N	7.33	135.54	121.54
1	A	19	LEU	C-N-CA	7.33	135.54	121.54
1	A	122	LYS	CA-C-N	7.32	133.12	120.68
1	A	122	LYS	C-N-CA	7.32	133.12	120.68
1	A	20	MET	N-CA-CB	-7.24	98.25	110.49
1	A	84	CYS	N-CA-CB	7.19	122.65	110.49
1	A	116	LYS	N-CA-CB	-6.98	99.03	110.41
1	A	17	HIS	CG-ND1-CE1	-6.85	97.65	109.30
1	A	13	ILE	N-CA-CB	-6.80	102.86	111.23
1	A	9	ILE	CA-CB-CG2	6.77	122.01	110.50
1	A	75	TYR	N-CA-CB	-6.70	99.17	110.49
1	A	31	LEU	CB-CA-C	6.69	123.73	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	93	ALA	N-CA-C	6.39	119.06	111.71
1	A	103	ALA	CA-C-N	6.38	131.68	121.34
1	A	103	ALA	C-N-CA	6.38	131.68	121.34
1	A	49	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	23	ASN	CA-CB-CG	6.37	118.97	112.60
1	A	56	LYS	CB-CA-C	6.30	121.24	110.79
1	A	115	HIS	CG-ND1-CE1	-6.27	98.64	109.30
1	A	48	HIS	CG-ND1-CE1	-6.13	98.87	109.30
1	A	120	THR	CB-CA-C	6.11	122.58	110.42
1	A	114	GLU	N-CA-CB	-5.96	100.41	110.49
1	A	17	HIS	ND1-CG-CD2	5.95	112.05	106.10
1	A	72	SER	N-CA-CB	-5.89	101.02	110.39
1	A	89	ASN	N-CA-C	-5.88	98.28	110.80
1	A	113	LYS	N-CA-C	5.85	118.02	110.65
1	A	7	SER	CA-C-N	5.75	132.10	121.52
1	A	7	SER	C-N-CA	5.75	132.10	121.52
1	A	43	ARG	CB-CA-C	-5.75	101.25	110.79
1	A	17	HIS	N-CA-CB	5.72	118.83	109.90
1	A	104	ILE	N-CA-CB	-5.71	99.84	110.40
1	A	121	LYS	CA-C-N	5.70	127.85	120.44
1	A	121	LYS	C-N-CA	5.70	127.85	120.44
1	A	20	MET	N-CA-C	5.67	122.89	110.80
1	A	6	ARG	N-CA-C	5.64	118.16	111.33
1	A	41	LEU	CB-CA-C	5.63	120.14	110.79
1	A	19	LEU	O-C-N	5.60	130.04	122.59
1	A	78	SER	CA-C-O	5.56	121.17	117.94
1	A	7	SER	N-CA-C	5.53	118.24	111.82
1	A	53	ARG	N-CA-C	5.51	117.72	111.11
1	A	102	ALA	CA-C-O	-5.46	113.35	119.79
1	A	60	SER	N-CA-CB	-5.45	103.34	110.59
1	A	28	TYR	CA-CB-CG	5.43	123.68	113.90
1	A	66	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	69	TYR	CA-CB-CG	5.36	123.55	113.90
1	A	13	ILE	CB-CA-C	5.36	116.94	110.78
1	A	53	ARG	CB-CA-C	5.32	119.32	110.81
1	A	63	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	111	TYR	CB-CG-CD1	-5.29	112.86	120.80
1	A	56	LYS	N-CA-CB	-5.21	102.46	110.12
1	A	40	GLU	N-CA-CB	5.20	117.69	109.94
1	A	63	PHE	CB-CA-C	5.16	120.70	110.42
1	A	6	ARG	CB-CG-CD	5.15	123.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	PRO	N-CA-CB	-5.13	97.87	103.25
1	A	50	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	72	SER	N-CA-C	5.12	117.79	109.86
1	A	82	ILE	CA-CB-CG2	5.12	119.20	110.50
1	A	58	LEU	N-CA-C	5.03	121.50	110.80
1	A	41	LEU	N-CA-CB	-5.02	102.75	110.12
1	A	100	ARG	CA-C-O	-5.02	115.23	120.55

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	14	PRO	Peptide
1	A	20	MET	Peptide
1	A	22	PHE	Sidechain
1	A	25	TYR	Sidechain
1	A	28	TYR	Sidechain
1	A	52	TYR	Sidechain
1	A	64	LEU	Peptide
1	A	69	TYR	Sidechain
1	A	73	TYR	Sidechain
1	A	75	TYR	Sidechain
1	A	76	SER	Peptide
1	A	88	ASN	Peptide
1	A	113	LYS	Peptide
1	A	115	HIS	Sidechain
1	A	123	TYR	Sidechain

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	971	0	886	21
All	All	972	0	886	21

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 11.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:26:GLY:HA2	1:A:118:LEU:HD22	0.70	1.62
1:A:8:MET:SD	1:A:75:TYR:CD2	0.58	2.97
1:A:91:CYS:O	1:A:95:ILE:HD13	0.57	1.99
1:A:13:ILE:HG22	1:A:15:GLY:CA	0.55	2.31
1:A:26:GLY:CA	1:A:118:LEU:HD22	0.53	2.34
1:A:55:ALA:CB	1:A:95:ILE:HD11	0.52	2.34
1:A:83:THR:HG23	1:A:84:CYS:H	0.51	1.64
1:A:5:PHE:CE2	1:A:9:ILE:HD11	0.51	2.41
1:A:12:ALA:HB1	1:A:107:SER:HB2	0.51	1.81
1:A:13:ILE:HG22	1:A:15:GLY:HA3	0.50	1.83
1:A:118:LEU:HD23	1:A:123:TYR:CG	0.50	2.42
1:A:5:PHE:HA	1:A:8:MET:HE2	0.48	1.86
1:A:8:MET:SD	1:A:75:TYR:CG	0.48	3.07
1:A:118:LEU:HG	1:A:123:TYR:CD2	0.47	2.44
1:A:84:CYS:SG	1:A:85:ASN:N	0.45	2.90
1:A:45:CYS:SG	1:A:106:PHE:CZ	0.44	3.11
1:A:17:HIS:CD2	1:A:21:ASP:H	0.42	2.32
1:A:45:CYS:SG	1:A:106:PHE:CE1	0.41	3.14
1:A:55:ALA:HB2	1:A:95:ILE:HD11	0.41	1.92
1:A:60:SER:CB	1:A:90:ALA:HB3	0.41	2.46
1:A:8:MET:SD	1:A:73:TYR:CE2	0.40	3.13

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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%)	73 (60%)	25 (20%)	24 (20%)	0	2
All	All	122/124 (98%)	73 (60%)	25 (20%)	24 (20%)	0	2

All 24 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	16	SER

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Mol	Chain	Res	Type
1	A	19	LEU
1	A	20	MET
1	A	29	CYS
1	A	37	PRO
1	A	49	ASP
1	A	58	LEU
1	A	63	PHE
1	A	67	ASN
1	A	68	PRO
1	A	70	THR
1	A	73	TYR
1	A	74	SER
1	A	80	THR
1	A	82	ILE
1	A	83	THR
1	A	84	CYS
1	A	88	ASN
1	A	91	CYS
1	A	109	ALA
1	A	117	ASN
1	A	118	LEU
1	A	119	ASP
1	A	120	THR

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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%)	84 (76%)	26 (24%)	2	27
All	All	110/110 (100%)	84 (76%)	26 (24%)	2	27

All 26 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	2	LEU
1	A	5	PHE

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Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	MET
1	A	9	ILE
1	A	17	HIS
1	A	27	CYS
1	A	28	TYR
1	A	29	CYS
1	A	36	THR
1	A	37	PRO
1	A	38	VAL
1	A	41	LEU
1	A	53	ARG
1	A	56	LYS
1	A	61	CYS
1	A	70	THR
1	A	85	ASN
1	A	87	LYS
1	A	92	GLU
1	A	94	PHE
1	A	96	CYS
1	A	104	ILE
1	A	108	LYS
1	A	113	LYS
1	A	114	GLU

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided