



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6AUN / pdb_00006aun
Title : calcium-independent phospholipase A2 beta
Authors : Malley, K.; Koroleva, O.; Miller, I.; Sanishvili, R.; Jenkins, C.M.; Gross, R.W.;
Korolev, S.
Deposited on : 2017-09-01
Resolution : 3.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

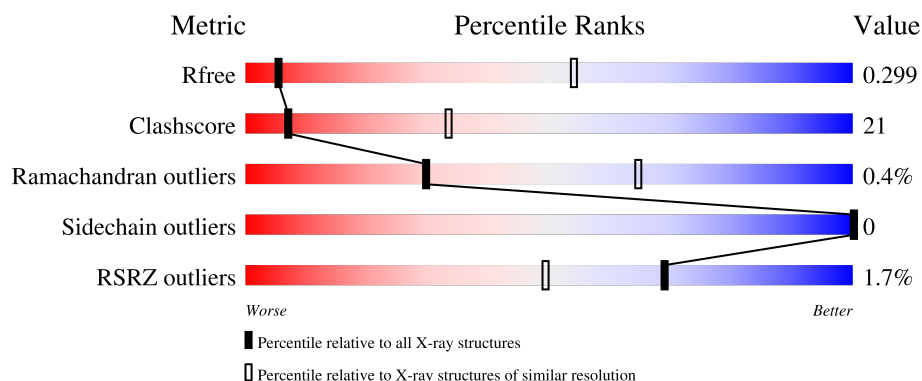
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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	752	
1	B	752	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9396 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 PLA2G6, iPLA2beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	0	0
			4698	2942	835	882	39			
1	B	618	Total	C	N	O	S	0	0	0
			4698	2942	835	882	39			

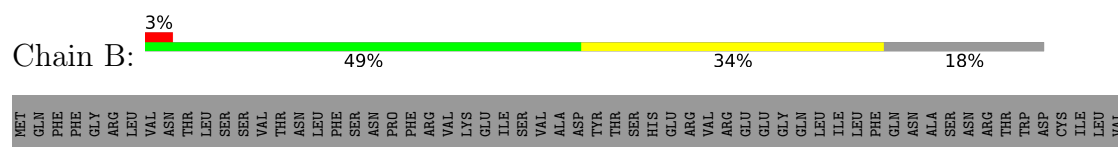
3 Residue-property plots

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: PLA2G6, iPLA2beta



• Molecule 1: PLA2G6, iPLA2beta



L745	TRP	A585	F495	P409	C308	G220	ARG	SER
M748	GLU	A586	E502	S415	T313	L221	GLU	PRO
L749	LEU	P587	E502	M416	S314	T222	CYS	ARG
P752	ALA	T588	P505	L422	A315	P223	ASN	ASN
	LYS	Y589	P505	L426	A316	L224	HIS	PRO
	THR	F590	E508	L427	G317	C227	HIS	HIS
	VAL	R591	F509	L428	N318	C228	SER	SER
	PHE	P592	L510	C428	T319	Q229	ARG	GLY
	GLY	R595	K511	L429	A320		ILE	PHE
	ALA	F596	K511	L430	L321	K232	LEU	ARG
	K671	L597	T521	D430	H322		SER	LEU
		D522	D522			N235	CYS	PHE
	V678	V523	V523	G433	V325	V236	ALA	GLN
		K524	K524	V434	M526		ASN	LEU
	T682	L601	K525	V435	R327	L240	S146	LEU
	R687	L602	P526	G436	N328			GLU
	A688	A603	K527	L437	R329	A244	M149	GLU
	V689	N604	V528	V438	F330		E150	ALA
	D690	N605	M529	I439	D331	P251	E151	ASP
	R691	P606	L530	I440	C332		G152	ALA
	A692	T607	T531	E447	M334	I256	C153	L81
	R693	L608	G532		V335	A259		P92
	A694	D609	T533	S450	V335	N260	F93	P93
	V695	M611	L534	G451	A341		F94	F94
	S696	T612	R537	V452		K265	TYR	TYR
	E697	E613	Q538	A453	G347	G266	GLU	GLU
	M698	I614	L542	T454		C267	SER	SER
	I701	H615	H543	K455	L354	A268	VAL	VAL
	Q702	Q619	L544	D456	H355	S165	GLN	GLN
	Y703		F545	L457	L356	E269	VAL	VAL
	F704		R546	F458	A357	I167	LEU	LEU
	R705	R623	N547	V461	I358	L168	HIS	HIS
	L706	K629	Y548	A462	M363	V169	V104	V104
	N707	V630	D549	G463	E364	E170	E105	E105
	P708	K631		T464	M365		V106	V106
	Q709	K632	E552	S465	I366	Q173	L107	L107
	L710	L633	V553	T466	N380	C175	Q108	Q108
	L716	L639	I554	G467				
	D717	G640	R555	G468		K185	D112	D112
	E718	T641	N562	I469	E384		LEU	LEU
	D721	G642	I563	L470	T385		ILE	ILE
		R643	N564	A471	P386	T188	ARG	ARG
	W729	V647	L565	I474	M389	A189	SER	SER
	E730	P648	K566	L475		F190	HIS	HIS
	T731		P567	H476	S394	H191	P118	P118
	E732		P568	S477		Y192	S119	S119
	V733	C651	A572	M480	L397	H292	W120	W120
	Y734	VAL	D573	A481		V293	T121	T121
	I735	ASP	Q574	Y482	M401	A294	V122	V122
	Y736	VAL	L575		P402	D197	T123	T123
	E737	PHE			A403	N198	H124	H124
	H738	ARG	R578	V486	I403	A297	L125	L125
	R739	PRO		Y487	S404	N299	A126	A126
	E740	SER	S583	K491	ARG	A300	V127	V127
		ASN	G584		ALA		E128	E128
	K744	PRO			ARG	L304	LEU	LEU
					ALA		GLY	GLY
					LYS		ILE	ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	266.06Å 266.06Å 79.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.11 – 3.95 39.11 – 3.95	Depositor EDS
% Data completeness (in resolution range)	86.4 (39.11-3.95) 80.7 (39.11-3.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.257 , 0.310 0.249 , 0.299	Depositor DCC
R_{free} test set	2461 reflections (8.62%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	9396	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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](#)

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	0.24	0/4782	0.65	4/6465 (0.1%)
1	B	0.26	1/4782 (0.0%)	0.62	4/6465 (0.1%)
All	All	0.25	1/9564 (0.0%)	0.64	8/12930 (0.1%)

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	6
1	B	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	552	GLU	C-N	5.71	1.36	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	PRO	N-CA-CB	8.39	110.36	101.88
1	B	93	PRO	N-CA-CB	7.60	110.15	102.17
1	A	92	PRO	N-CA-CB	7.27	110.13	103.08
1	B	92	PRO	N-CA-CB	7.00	109.87	103.08
1	A	409	PRO	N-CA-CB	6.74	110.42	103.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	MET	Peptide
1	A	452	VAL	Peptide
1	A	548	TYR	Peptide
1	A	562	ASN	Peptide
1	A	591	ARG	Peptide

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	4698	0	4595	199	0
1	B	4698	0	4595	210	0
All	All	9396	0	9190	390	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 21.

The worst 5 of 390 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:464:THR:HG21	1:A:604:ASN:HA	1.53	0.90
1:B:464:THR:HG21	1:B:604:ASN:HA	1.56	0.88
1:A:562:ASN:O	1:A:564:ASN:N	2.07	0.86
1:A:288:ALA:HB1	1:A:292:HIS:HB2	1.58	0.84
1:B:260:MET:HB3	1:B:294:ALA:HB1	1.62	0.81

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	606/752 (81%)	509 (84%)	94 (16%)	3 (0%)	24	60
1	B	606/752 (81%)	500 (82%)	104 (17%)	2 (0%)	36	69
All	All	1212/1504 (81%)	1009 (83%)	198 (16%)	5 (0%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	563	ILE
1	A	554	ILE
1	B	739	ARG
1	A	564	ASN
1	B	572	ALA

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	495/646 (77%)	495 (100%)	0	100	100
1	B	495/646 (77%)	495 (100%)	0	100	100
All	All	990/1292 (77%)	990 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	570	GLN
1	B	646	GLN
1	B	738	HIS
1	A	646	GLN
1	B	280	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	618/752 (82%)	-0.52	0 100 100	22, 53, 106, 135	0
1	B	618/752 (82%)	-0.14	21 (3%) 48 34	19, 68, 148, 182	0
All	All	1236/1504 (82%)	-0.33	21 (1%) 69 49	19, 60, 142, 182	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	ALA	4.3
1	B	193	ALA	4.1
1	B	160	CYS	3.9
1	B	127	VAL	3.6
1	B	126	ALA	3.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.