

Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 04:10 PM EDT

PDB ID : 1TGM

Title : Crystal structure of a complex formed between group II phospholipase A2 and

aspirin at 1.86 A resolution

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Deposited on : 2004-05-28

Resolution : 1.86 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 (i) 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

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)

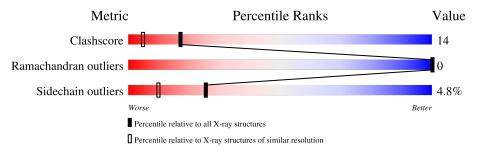
Validation Pipeline (wwPDB-VP) : 2.35

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 1.86 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	121	80%	17%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AIN	A	202	_	-	X	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1098 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.

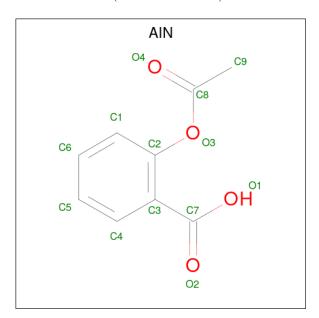
• Molecule 1 is a protein called Phospholipase A2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	121	Total 940	C 588	N 158	O 178	S 16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	SER	LYS	conflict	UNP P59071

• Molecule 2 is 2-(ACETYLOXY)BENZOIC ACID (three-letter code: AIN) (formula: $C_9H_8O_4$).



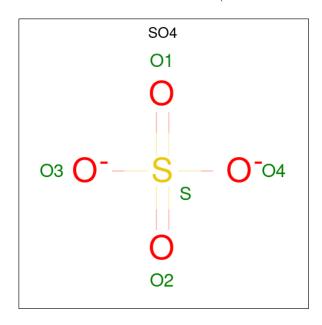
\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 9 4	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	139	Total O 139 139	0	0

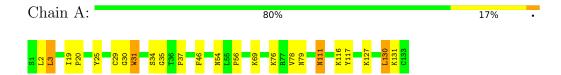


3 Residue-property plots (i)

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 A2





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 43	Depositor	
Cell constants	53.31Å 53.31Å 48.45Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	20.00 - 1.86	Depositor	
% Data completeness	98.5 (20.00-1.86)	Depositor	
(in resolution range)	30.9 (20.00 1.00)	Берозног	
R_{merge}	(Not available)	Depositor	
R_{sym}	0.09	Depositor	
Refinement program	REFMAC 5.0	Depositor	
R, R_{free}	0.197 , 0.224	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1098	wwPDB-VP	
Average B, all atoms (Å ²)	28.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, AIN, SO4

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).

Mal	Chain	Bond	$\mathbf{lengths}$	Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.44	0/960	0.73	0/1289	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	940	0	901	26	0
2	A	13	0	7	7	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	139	0	0	4	0
All	All	1098	0	908	26	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 14.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



A., 1	A., 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} (\mathring{\rm A})$	overlap (Å)
1:A:2:LEU:CD2	2:A:202:AIN:H92	1.83	1.06
1:A:2:LEU:HD21	2:A:202:AIN:C9	1.97	0.95
1:A:2:LEU:HD23	2:A:202:AIN:H92	1.49	0.95
1:A:19:ILE:HD11	2:A:202:AIN:C7	1.99	0.93
1:A:2:LEU:CD2	2:A:202:AIN:C9	2.57	0.75
1:A:37:PRO:HD3	1:A:130:LEU:HD12	1.72	0.71
1:A:116:LYS:HE3	1:A:117:TYR:CZ	2.29	0.67
1:A:2:LEU:HD21	2:A:202:AIN:H93	1.77	0.66
1:A:34:SER:HB3	5:A:318:HOH:O	2.01	0.60
1:A:79:ASN:ND2	5:A:267:HOH:O	2.27	0.60
1:A:37:PRO:CD	1:A:130:LEU:HD12	2.34	0.57
1:A:2:LEU:HD13	1:A:69:LYS:HA	1.89	0.55
1:A:19:ILE:HD12	1:A:19:ILE:N	2.22	0.54
1:A:19:ILE:HD11	2:A:202:AIN:C3	2.38	0.54
1:A:35:GLY:HA2	1:A:127:LYS:C	2.33	0.49
1:A:30:GLY:O	1:A:31:TRP:C	2.53	0.47
1:A:111:ASN:N	1:A:111:ASN:HD22	2.12	0.47
1:A:54:ASN:C	1:A:56:PRO:HD3	2.35	0.46
1:A:2:LEU:CD1	1:A:69:LYS:HA	2.46	0.46
1:A:3:LEU:HD23	5:A:237:HOH:O	2.16	0.45
1:A:76:LYS:NZ	5:A:234:HOH:O	2.50	0.45
1:A:25:TYR:O	1:A:29:CYS:HB2	2.18	0.44
1:A:3:LEU:HD13	1:A:3:LEU:HD13		0.42
1:A:78:VAL:O	1:A:79:ASN:HB2	2.18	0.42
1:A:19:ILE:HA	1:A:20:PRO:HA	1.90	0.41
1:A:46:PHE:CZ	1:A:130:LEU:HB3	2.55	0.41

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	119/121 (98%)	114 (96%)	5 (4%)	0	100	100



There are no Ramachandran outliers to report.

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	Analysed Rotameric		Percentiles		
1	A	104/104 (100%)	99 (95%)	5 (5%)	25 10		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	\mathbf{Type}	
1	A	3	LEU	
1	A	31	TRP	
1	A	111	ASN	
1	A	130	LEU	
1	A	131	LYS	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type	
1	A	111	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 monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	Trimo	Chain	Dag	Timle	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	203	-	4,4,4	0.13	0	6,6,6	0.06	0
2	AIN	A	202	-	13,13,13	1.73	3 (23%)	17,17,17	2.39	3 (17%)

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	AIN	A	202	-	-	2/8/8/8	0/1/1/1	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
2	A	202	AIN	C3-C2	4.60	1.49	1.40
2	A	202	AIN	O3-C8	2.83	1.46	1.35
2	A	202	AIN	O1-C7	-2.60	1.22	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
2	A	202	AIN	C2-O3-C8	6.79	132.12	117.65
2	A	202	AIN	O3-C8-C9	5.68	123.58	110.98
2	A	202	AIN	O3-C8-O4	-2.10	117.68	122.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Mol Chain		Type	Atoms	
2	A	202	AIN	O4-C8-O3-C2	

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\mathbf{Mol}	Chain	Res	Type	Atoms	
2	A	202	AIN	C9-C8-O3-C2	

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	202	AIN	7	0

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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

