Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2014 – 06:23 PM GMT

PDB ID	:	1ZYX
Title	:	Crystal structure of the complex of a group IIA phospholipase A2 with a synthetic anti-inflammatory agent licofelone at 1.9A resolution
Authors	:	Singh, N.; Jabeen, T.; Sharma, S.; Bhushan, A.; Singh, T.P.
Deposited on	:	2005-06-13
Resolution	:	1.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

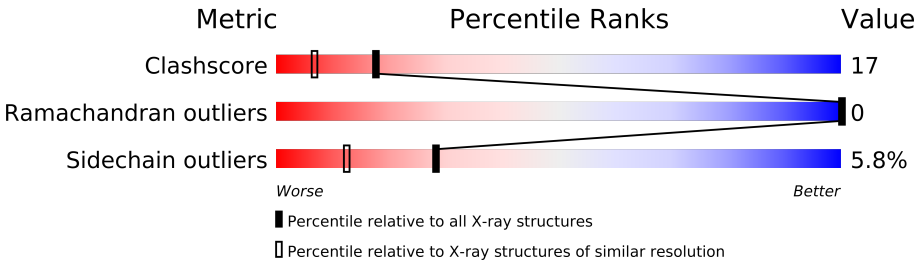
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	121	

2 Entry composition

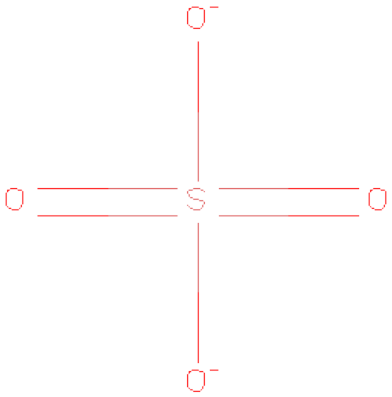
There are 4 unique types of molecules in this entry. The entry contains 1142 atoms, of which 0 are hydrogen and 0 are deuterium.

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 VRV-PL-VIIIa.

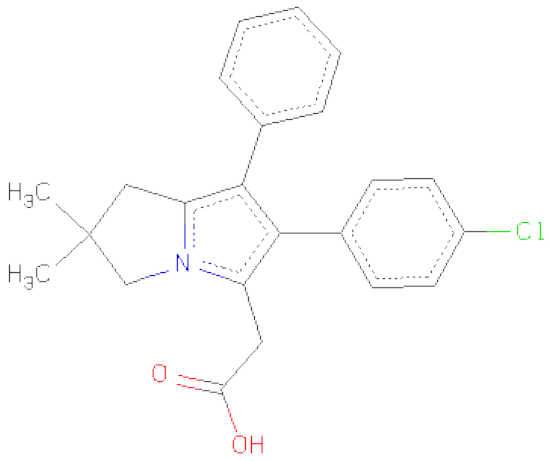
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	121	944	591	159	178	16	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is [6-(4-CHLOROPHENYL)-2,2-DIMETHYL-7-PHENYL-2,3-DIHYDRO-1H-PYRROLIZIN-5-YL]ACETICACID (three-letter code: LCF) (formula: $C_{23}H_{22}ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			27	23	1	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		

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 errors 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.

Note EDS was not executed.

• Molecule 1: Phospholipase A2 VRV-PL-VIIIa

Chain A:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	53.44Å 53.44Å 48.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 1.95	Depositor
% Data completeness (in resolution range)	98.0 (17.97-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.193 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1142	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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: LCF, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/964	0.61	0/1292

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	944	0	907	28	0
2	A	10	0	0	0	0
3	A	27	0	21	8	0
4	A	161	0	0	5	0
All	All	1142	0	928	33	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (33) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:GLU:HG3	1:A:107:ARG:HG3	1.36	1.08
3:A:2001:LCF:H19	3:A:2001:LCF:H17	1.20	1.06
1:A:127:LYS:HD3	1:A:128:GLY:N	1.94	0.81
1:A:19:ILE:HD13	1:A:23:SER:HB3	1.65	0.79
1:A:31:TRP:N	3:A:2001:LCF:H112	2.04	0.73
1:A:7:LYS:O	1:A:11:GLU:HG3	1.89	0.73
1:A:111:ASN:N	1:A:111:ASN:HD22	1.88	0.72
3:A:2001:LCF:H81	3:A:2001:LCF:H23	1.71	0.71
1:A:38:LYS:HA	1:A:38:LYS:HE2	1.74	0.69
3:A:2001:LCF:CL1	4:A:2154:HOH:O	2.49	0.68
1:A:105:CYS:HA	4:A:2133:HOH:O	1.96	0.64
1:A:2:LEU:HD12	4:A:2119:HOH:O	1.99	0.62
1:A:2:LEU:HD13	1:A:69:LYS:HA	1.86	0.58
1:A:38:LYS:HD2	1:A:120:TYR:CE2	2.38	0.57
1:A:114:SER:OG	1:A:116:LYS:HG2	2.05	0.56
1:A:19:ILE:HD13	1:A:23:SER:CB	2.35	0.54
1:A:55:LEU:N	1:A:56:PRO:CD	2.73	0.52
1:A:111:ASN:H	1:A:111:ASN:HD22	1.54	0.51
1:A:127:LYS:HD3	1:A:128:GLY:H	1.75	0.49
1:A:111:ASN:N	1:A:111:ASN:ND2	2.59	0.49
3:A:2001:LCF:H13	3:A:2001:LCF:C4	2.43	0.48
1:A:74:LYS:HB2	1:A:85:GLU:HB2	1.94	0.48
1:A:108:GLN:NE2	4:A:2133:HOH:O	2.40	0.48
1:A:55:LEU:N	1:A:56:PRO:HD3	2.31	0.46
1:A:68:PRO:HA	1:A:95:ILE:HD13	1.97	0.46
1:A:111:ASN:ND2	1:A:111:ASN:H	2.15	0.45
1:A:30:GLY:C	3:A:2001:LCF:H112	2.36	0.45
1:A:22:TYR:O	1:A:29:CYS:HB3	2.18	0.43
3:A:2001:LCF:H23	3:A:2001:LCF:C8	2.45	0.42
1:A:12:GLU:HG3	1:A:107:ARG:CG	2.26	0.42
1:A:31:TRP:CE3	3:A:2001:LCF:H111	2.55	0.41
1:A:104:ILE:HG22	4:A:2133:HOH:O	2.19	0.41
1:A:37:PRO:CD	1:A:130:LEU:HD12	2.51	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

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%)	117 (98%)	2 (2%)	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	Rotameric	Outliers	Percentiles
1	A	104/104 (100%)	98 (94%)	6 (6%)	28 12

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	72	ARG
1	A	79	ASN
1	A	107	ARG
1	A	111	ASN
1	A	130	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	ASN

5.3.3 RNA (i)

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	LCF	A	2001	-	30,30,30	3.26	12 (40%)	45,45,45	2.88	21 (46%)
2	SO4	A	261	-	4,4,4	0.24	0	6,6,6	0.42	0
2	SO4	A	262	-	4,4,4	0.24	0	6,6,6	0.44	0

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
3	LCF	A	2001	-	-	0/12/22/22	0/2/4/4
2	SO4	A	261	-	-	0/0/0/0	0/0/0/0
2	SO4	A	262	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	LCF	C7-C1	11.48	1.56	1.40
3	A	2001	LCF	C6-C5	6.44	1.49	1.40
3	A	2001	LCF	C7-C6	5.59	1.60	1.42
3	A	2001	LCF	C4-C3	-5.33	1.49	1.55
3	A	2001	LCF	C1-N	5.26	1.44	1.36
3	A	2001	LCF	C23-C18	2.65	1.45	1.39
3	A	2001	LCF	C13-C12	2.50	1.44	1.39
3	A	2001	LCF	O1-C9	-2.42	1.21	1.30
3	A	2001	LCF	C14-C13	2.18	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	LCF	C21-CL1	2.17	1.79	1.74
3	A	2001	LCF	C10-C3	-2.16	1.48	1.53
3	A	2001	LCF	C23-C22	2.06	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	LCF	C6-C5-N	8.36	113.77	107.82
3	A	2001	LCF	C2-C3-C4	6.93	112.14	102.42
3	A	2001	LCF	C10-C3-C4	-5.77	98.18	111.15
3	A	2001	LCF	C8-C1-C7	5.36	138.53	130.25
3	A	2001	LCF	C5-N-C1	4.35	111.96	109.47
3	A	2001	LCF	C10-C3-C2	4.33	115.34	110.73
3	A	2001	LCF	C7-C6-C5	-3.87	102.34	107.00
3	A	2001	LCF	C2-N-C1	3.58	135.26	128.77
3	A	2001	LCF	C3-C2-N	-3.27	101.19	104.08
3	A	2001	LCF	C7-C6-C12	3.25	135.41	126.42
3	A	2001	LCF	C3-C4-C5	-3.23	102.07	103.94
3	A	2001	LCF	C16-C17-C12	3.07	124.79	120.56
3	A	2001	LCF	C4-C5-C6	3.05	134.40	131.37
3	A	2001	LCF	C6-C7-C18	2.81	134.18	126.42
3	A	2001	LCF	C22-C21-CL1	2.74	123.86	119.34
3	A	2001	LCF	C18-C7-C1	-2.70	120.42	127.84
3	A	2001	LCF	C14-C13-C12	2.21	123.59	120.56
3	A	2001	LCF	C17-C12-C13	-2.20	113.49	117.58
3	A	2001	LCF	C13-C12-C6	2.19	124.44	120.77
3	A	2001	LCF	C11-C3-C2	-2.05	108.55	110.73
3	A	2001	LCF	C12-C6-C5	-2.03	122.25	127.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.