wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2024 – 03:03 PM EST

PDB ID	:	2SBL
Title	:	THE THREE-DIMENSIONAL STRUCTURE OF AN ARACHIDONIC ACID 15-LIPOXYGENASE
Authors	:	Amzel, L.M.; Boyington, J.C.
Deposited on	:	1993-07-22
Resolution	:	2.60 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 (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:

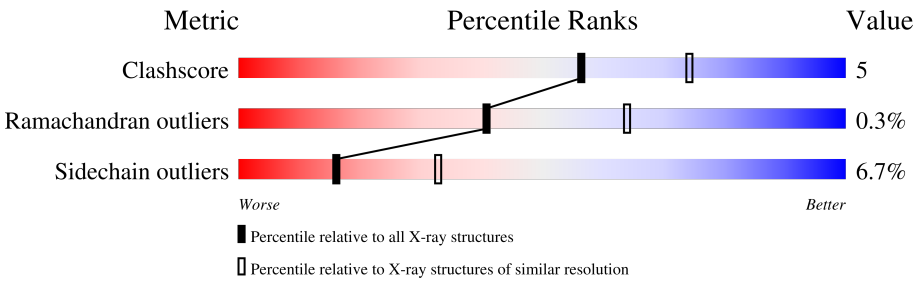
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	839	76% 19% • •
1	B	839	76% 19% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12955 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 LIPOXYGENASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	807	6445	4133	1090	1204	18	0	0	0
1	A	807	6445	4133	1090	1204	18	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	63	63	63	0	0

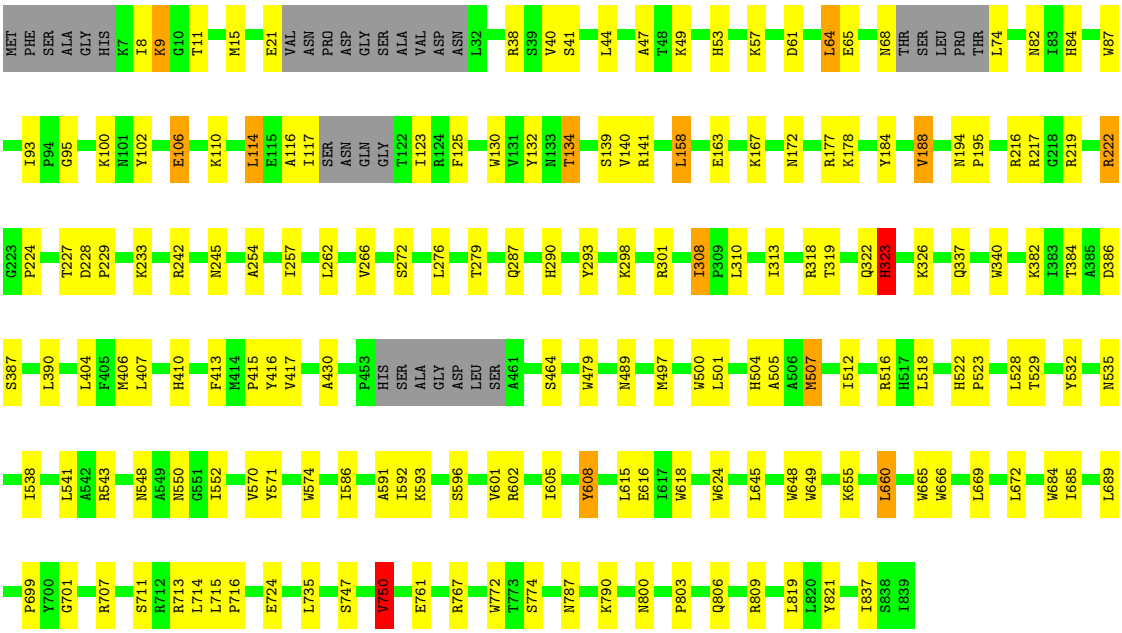
3 Residue-property plots (i)

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.

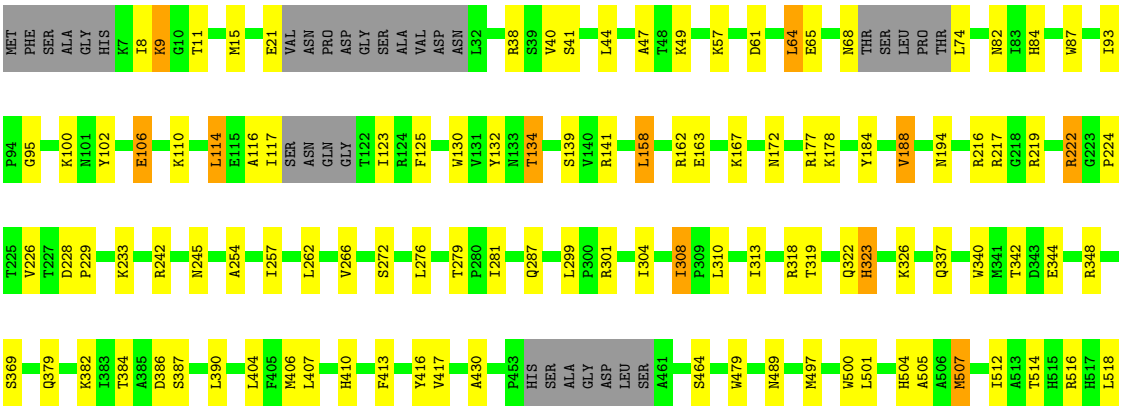
• Molecule 1: LIPOXYGENASE-1

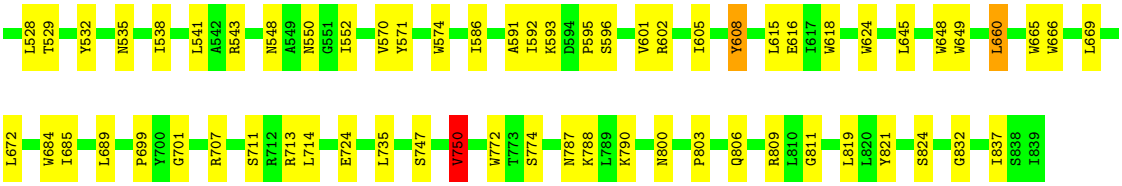
Chain B: 76% 19%



• Molecule 1: LIPOXYGENASE-1

Chain A: 76% 19%




L528 T529 Y532 N535 I538 L541 A542 R543 N548 A549 N550 G551 I552 V570 Y571 W574 I586 A591 I592 K593 D594 P595 S596 V601 R602 I605 Y608 L615 E616 I617 W618 W624 L645 W648 W649 L660 W665 W666 L669
L672 W684 I685 L689 P699 Y700 G701 R707 S711 R712 R713 L714 E724 L735 S747 V750 W772 T773 S774 N787 K788 L789 K790 N800 P803 Q806 R809 L810 G811 L819 L820 Y821 S824 G832 I837 S838 I839

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.50Å 125.60Å 94.70Å 90.00° 102.90° 90.00°	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	X-PLOR 3.1	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12955	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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: FE

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	0.73	0/6606	1.34	81/8973 (0.9%)
1	B	0.73	0/6606	1.34	80/8973 (0.9%)
All	All	0.73	0/13212	1.34	161/17946 (0.9%)

There are no bond length outliers.

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	ARG	NE-CZ-NH2	-14.47	113.06	120.30
1	B	141	ARG	NE-CZ-NH2	-14.43	113.09	120.30
1	B	141	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	A	141	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	A	608	TYR	CB-CG-CD2	-9.38	115.37	121.00

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	6445	0	6397	66	2
1	B	6445	0	6397	69	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	63	0	0	5	0
All	All	12955	0	12794	129	2

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 5.

The worst 5 of 129 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:B:767:ARG:NE	3:B:902:HOH:O	2.02	0.91
1:B:655:LYS:HG2	1:A:226:VAL:HG11	1.55	0.89
1:B:538:ILE:HD11	1:B:837:ILE:HG22	1.77	0.66
1:A:538:ILE:HD11	1:A:837:ILE:HG22	1.77	0.66
1:B:53:HIS:CD2	1:A:281:ILE:CD1	2.83	0.62

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:PRO:O	1:A:595:PRO:CG[4_546]	1.91	0.29
1:B:415:PRO:CB	1:A:595:PRO:CB[4_546]	2.02	0.18

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	797/839 (95%)	764 (96%)	31 (4%)	2 (0%)	41	64
1	B	797/839 (95%)	764 (96%)	31 (4%)	2 (0%)	41	64
All	All	1594/1678 (95%)	1528 (96%)	62 (4%)	4 (0%)	41	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	HIS
1	A	323	HIS
1	B	308	ILE
1	A	308	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	705/730 (97%)	658 (93%)	47 (7%)	16 33
1	B	705/730 (97%)	658 (93%)	47 (7%)	16 33
All	All	1410/1460 (97%)	1316 (93%)	94 (7%)	16 33

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	A	387	SER
1	A	139	SER
1	A	279	THR
1	A	528	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	787	ASN
1	A	800	ASN
1	B	800	ASN
1	A	287	GLN
1	A	322	GLN

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 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 (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.