



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:43 am GMT

PDB ID : 2IUK
Title : Crystal structure of Soybean Lipoxygenase-D
Authors : Youn, B.; Sellhorn, G.E.; Mirchel, R.J.; Gaffney, B.J.; Grimes, H.D.; Kang, C.
Deposited on : 2006-06-05
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

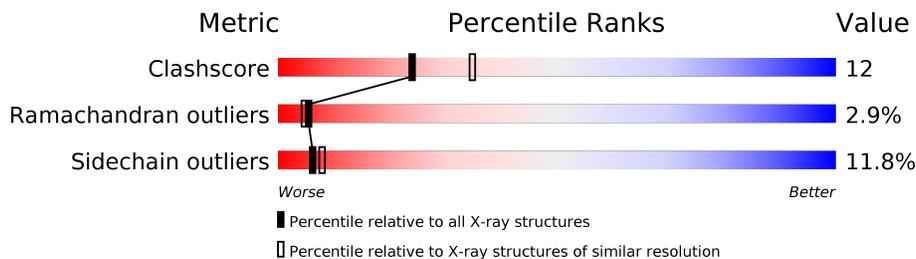
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	864	
1	B	864	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13534 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 SEED LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	835	6649	4272	1115	1251	11	0	0	0
1	B	835	6649	4272	1115	1251	11	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	PHE	LEU	CONFLICT	UNP P24095
A	233	CYS	SER	CONFLICT	UNP P24095
A	240	LEU	ARG	CONFLICT	UNP P24095
A	364	VAL	TRP	CONFLICT	UNP P24095
A	604	HIS	ASP	CONFLICT	UNP P24095
A	695	LYS	MET	CONFLICT	UNP P24095
B	1192	PHE	LEU	CONFLICT	UNP P24095
B	1233	CYS	SER	CONFLICT	UNP P24095
B	1240	LEU	ARG	CONFLICT	UNP P24095
B	1364	VAL	TRP	CONFLICT	UNP P24095
B	1604	HIS	ASP	CONFLICT	UNP P24095
B	1695	LYS	MET	CONFLICT	UNP P24095

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

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

- Molecule 3 is water.

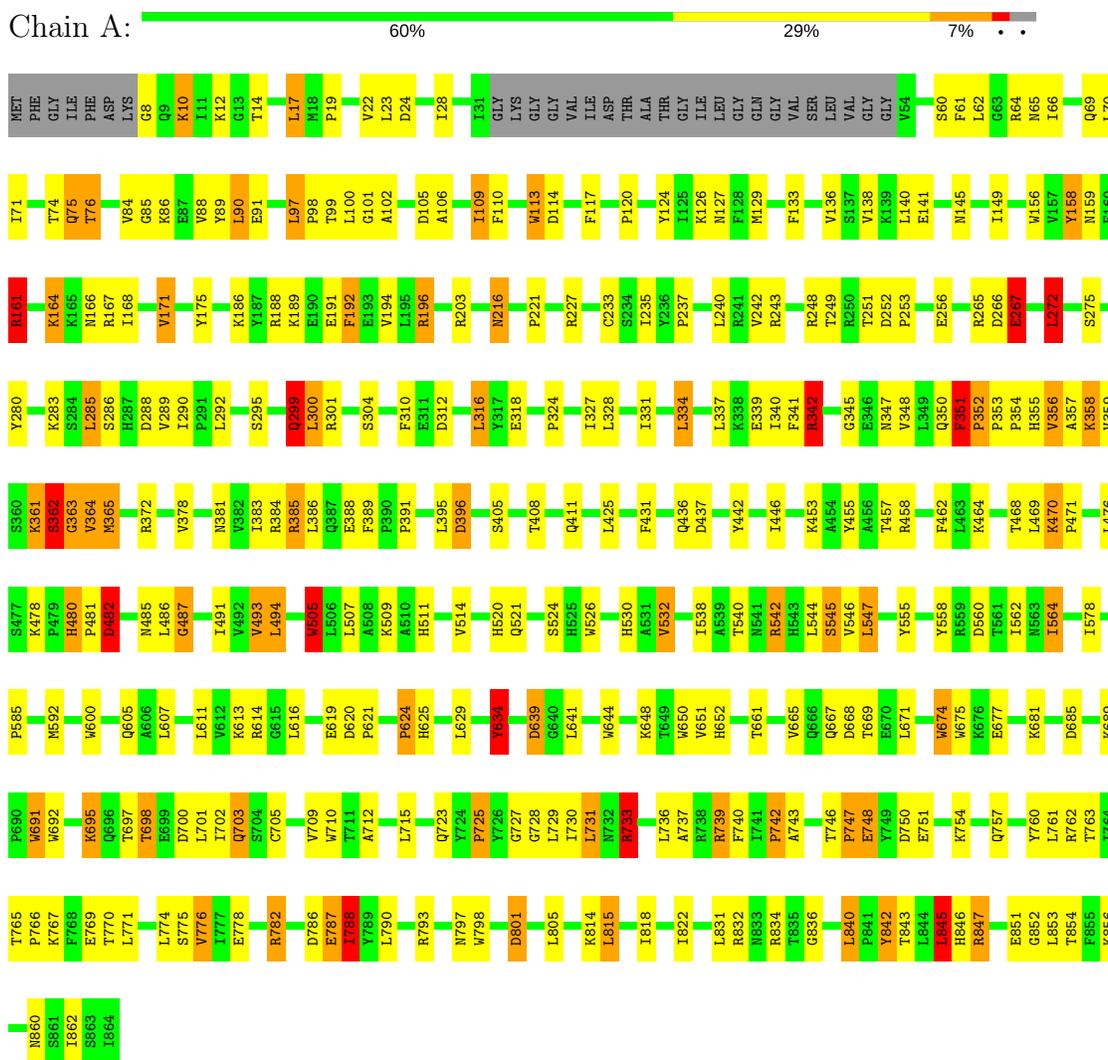
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	113	Total 113	O 113	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: SEED LIPOXYGENASE



- Molecule 1: SEED LIPOXYGENASE



D1773	A1678	G1586	L1486	M1379	Y1262	Y1163	Q1069	MET
V1776	V1679	K1587	G1487	P1380	V1263	K1164	L1070	PHE
I1777	E1680	S1589	P1488	M1381	P1264	P1164	I1071	GLY
E1778	K1681	S1589	V1488	V1382	R1265	Y1175	S1072	ILE
S1781	H1683	M1592	V1494	V1385	L1272	T1180	A1073	PHE
R1782	K1689	V1596	P1496	R1385	K1273	P1181	T1074	ASP
L1790	P1690	Y1597	A1496	S1393	S1274	A1182	Q1075	LYS
W1691	W1600	W1600	G1499	D1396	L1278	G1080	G1080	GLI008
R1793	W1692	V1601	V1500	P1397	L1184	N1081	N1081	K1012
E1794	K1694	P1602	D1501	P1397	L1185	G1082	V1015	V1015
T1795	K1695	L1607	T1503	Y1400	K1186	K1083	L1017	L1017
P1796	L1608	W1504	W1504	K1409	E1191	Y1089	M1018	M1018
W1797	P1608	L1508	E1410	E1410	F1192	F1192	P1019	P1019
W1798	L1611	L1507	Q1411	Q1411	L1195	L1195	K1020	K1020
D1801	I1702	A1508	K1509	I1414	S1315	L1195	D1024	D1024
K1802	Q1703	K1509	K1509	I1414	E1318	G1201	I1028	I1028
K1803	Q1704	V1512	V1512	V1421	I1321	K1202	T1029	T1029
K1809	I1707	S1517	S1517	L1425	K1322	R1208	S1030	S1030
R1810	I1708	Q1521	Q1521	L1425	L1323	R1208	I1031	I1031
L1815	W1709	L1624	L1624	L1425	P1324	D1211	GLY	GLY
E1819	W1710	H1625	L1625	R1429	L1328	Y1212	LYS	LYS
I1822	T1711	G1626	L1626	L1430	L1328	Y1212	GLY	GLY
L1831	A1712	V1630	H1524	F1431	I1331	Y1215	GLY	GLY
R1832	S1713	V1631	W1526	Q1436	S1332	N1216	VAL	VAL
R1833	L1714	E1632	L1527	I1440	P1333	D1222	ILE	ILE
T1835	H1716	D1633	M1528	I1440	L1334	R1227	ASP	ASP
G1836	Q1723	O1634	H1530	L1443	P1335	R1227	THR	THR
P1837	Y1724	L1641	H1530	T1444	K1338	C1233	ALA	ALA
V1838	P1725	L1644	A1531	R1445	E1339	S1234	THR	THR
Q1839	R1733	W1644	M1533	I1446	I1235	I1235	GLY	GLY
Y1842	L1736	I1647	T1540	S1448	F1341	Y1236	LEU	LEU
T1843	W1650	W1650	L1544	P1450	R1342	F1237	GLN	GLN
L1844	V1651	V1651	L1544	R1458	T1343	Y1238	VAL	VAL
L1845	Y1654	Y1654	D1560	R1458	E1346	R1241	SER	SER
H1846	V1655	V1655	T1561	R1458	M1347	V1242	LEU	LEU
R1847	S1656	S1656	D1562	G1467	V1348	R1242	VAL	VAL
S1848	L1657	L1657	I1562	T1468	L1349	R1246	GLY	GLY
S1849	E1748	E1748	M1563	L1469	H1355	E1247	GLY	GLY
E1850	Y1749	Y1749	I1564	K1470	K1358	R1248	V1054	V1054
L1853	D1750	V1665	G1566	P1471	K1358	T1249	I1055	I1055
K1856	E1751	D1668	L1567	E1475	V1359	R1250	D1056	D1056
K1856	M1752	T1669	L1567	L1476	S1360	T1251	T1059	T1059
K1856	V1753	T1669	Q1570	L1476	K1361	D1252	S1060	S1060
K1856	K1754	Q1672	Q1570	S1477	G1362	E1141	F1061	F1061
K1856	A1759	W1674	A1575	H1480	G1363	S1255	L1062	L1062
S1863	W1674	W1674	D1576	P1481	M1364	E1256	G1063	G1063
I1864	W1675	W1675	G1577	D1482	M1364	K1257	R1064	R1064
I1864	K1676	K1676	I1578	G1483	M1365	P1258	M1065	M1065
I1864	T1763	E1677	P1585	D1484	V1370	G1259	I1066	I1066
I1864	T1763	E1677	P1585	N1485	A1371	E1260	S1067	S1067
I1864	T1763	E1677	P1585	N1485	R1372	R1261	M1068	M1068

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.76Å 115.10Å 120.22Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.1 (50.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13534	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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	0.84	3/6822 (0.0%)	1.66	136/9280 (1.5%)
1	B	0.83	1/6822 (0.0%)	1.58	92/9280 (1.0%)
All	All	0.84	4/13644 (0.0%)	1.62	228/18560 (1.2%)

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	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	GLU	CB-CG	6.92	1.65	1.52
1	A	639	ASP	CA-CB	6.04	1.67	1.53
1	A	851	GLU	CG-CD	5.35	1.59	1.51
1	B	1798	TRP	CG-CD2	-5.23	1.34	1.43

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	SER	CA-C-N	-13.93	88.34	116.20
1	A	542	ARG	NE-CZ-NH1	11.85	126.23	120.30
1	A	486	LEU	CA-C-N	-11.70	92.81	116.20
1	A	834	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	B	1793	ARG	NE-CZ-NH1	10.16	125.38	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PHE	Peptide
1	A	362	SER	Mainchain
1	A	480	HIS	Peptide
1	A	487	GLY	Peptide
1	A	97	LEU	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	6649	0	6597	153	0
1	B	6649	0	6597	178	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	121	0	0	5	0
3	B	113	0	0	6	0
All	All	13534	0	13194	331	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 12.

The worst 5 of 331 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:342:ARG:HE	1:A:342:ARG:HA	1.31	0.94
1:A:847:ARG:H	1:A:847:ARG:NE	1.71	0.88
1:B:1020:LYS:H	1:B:1020:LYS:HD3	1.41	0.83
1:B:1371:ALA:HB2	1:B:1471:PRO:HD3	1.59	0.83
1:A:249:THR:HG22	1:A:252:ASP:H	1.43	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	831/864 (96%)	753 (91%)	58 (7%)	20 (2%)	7 7
1	B	831/864 (96%)	726 (87%)	77 (9%)	28 (3%)	4 3
All	All	1662/1728 (96%)	1479 (89%)	135 (8%)	48 (3%)	5 5

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	351	PHE
1	A	383	ILE
1	A	396	ASP
1	A	482	ASP

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	730/750 (97%)	643 (88%)	87 (12%)	6 8
1	B	730/750 (97%)	644 (88%)	86 (12%)	6 8
All	All	1460/1500 (97%)	1287 (88%)	173 (12%)	6 8

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	790	LEU

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Mol	Chain	Res	Type
1	B	1117	PHE
1	B	1790	LEU
1	A	797	ASN
1	B	1020	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	732	ASN
1	B	1075	GLN
1	B	1720	ASN
1	A	797	ASN
1	B	1127	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 carbohydrates 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.