



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
Xtriage (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

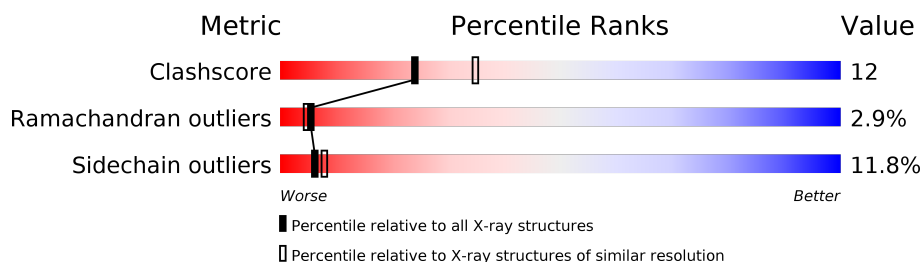
1 Overall quality at a glance

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	 60% 29% 7% . .
1	B	864	 59% 30% 6% . .

2 Entry composition

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
1	A	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			
1	B	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			

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.

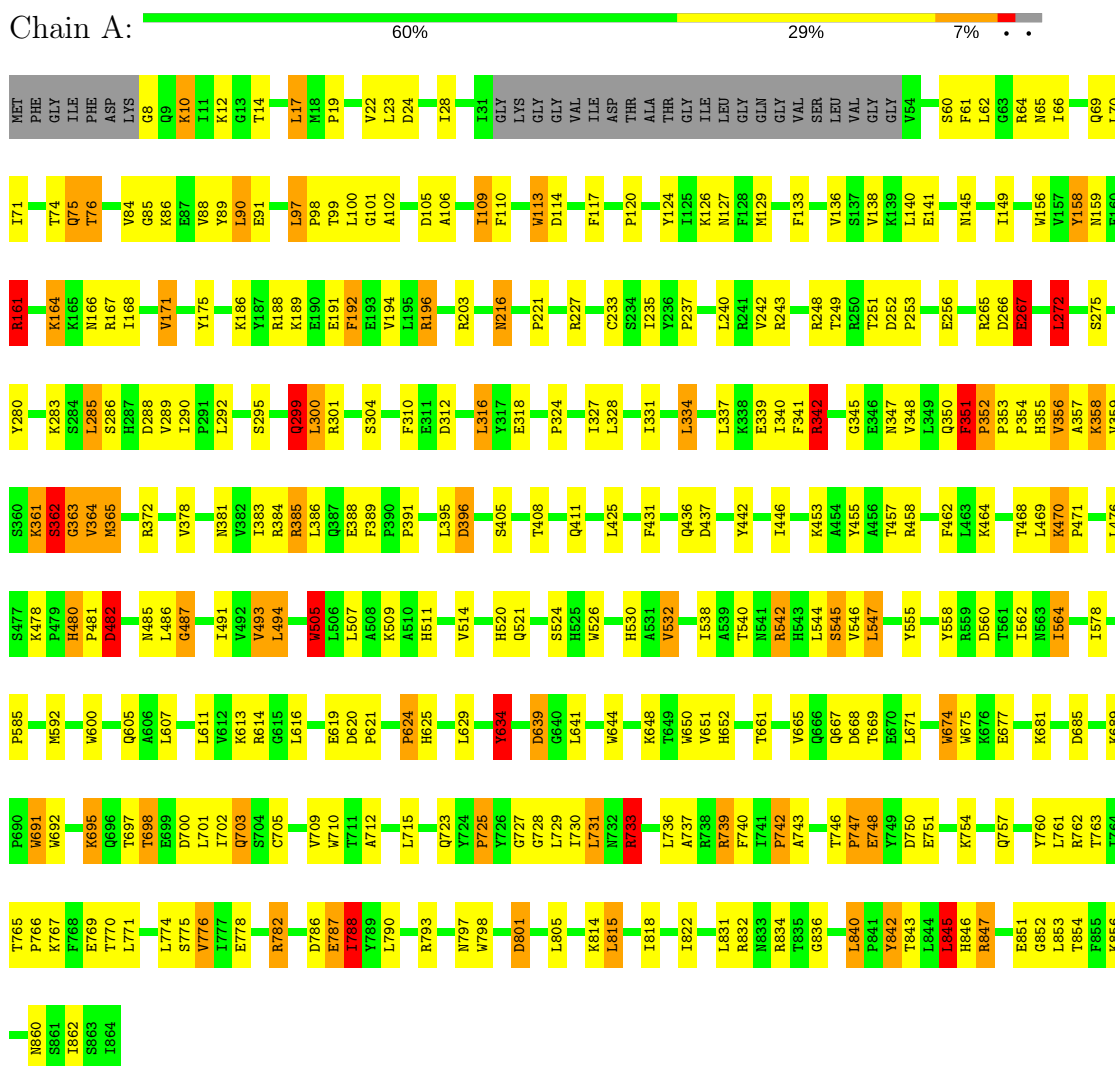
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	113	Total 113	O 113	0	0

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	R1264	R1265	I1071	GLY
E1778	G1682	M1592	V1493	V1382	L1272	Y1175	S1072	ILE
S1781	H1683	V1596	L1494	R1385	K1273	T1180	A1073	PHE
R1782	K1689	Y1597	A1496	S1393	S1274	P1181	T1074	ASP
L1790	P1690	W1600	G1499	D1396	L1278	A1182	Q1075	LYS
W1691	W1691	V1601	V1500	P1397	P1183	P1184	T1076	GLU08
R1793	P1693	V1602	D1501	P1400	L1282	L1185	G1080	K1012
E1794	K1694	S1502	T1503	Y1400	K1283	K1186	N1081	V1015
T1795	K1695	L1607	I1504	K1409	S1284	E1191	G1082	V1016
P1796	P1608	L1506	L1508	E1410	D1288	F1192	N1083	L1017
N1797	L1611	L1507	A1508	Q1411	S1315	L1195	P1098	M1018
W1798	A1617	A1509	K1509	I1414	E1318	G1201	P1097	K1020
D1801	Q1703	P1620	V1512	V1421	I1321	K1202	T1098	D1024
K1803	S1704	P1621	S1517	L1425	K1322	R1208	P1098	I1028
K1809	G1705	P1624	Q1521	R1429	L1323	D1211	G1101	T1029
R1810	I1707	H1625	L1522	L1430	P1324	Y1212	A1102	S1030
L1815	W1709	G1626	V1523	F1431	L1328	Y1215	R1103	I1031
E1819	A1712	L1627	S1524	Q1436	I1331	N1216	Q1104	GLY
I1822	S1713	V1630	W1526	Q1436	S1332	D1222	S1108	VAL
L1831	A1714	E1632	L1527	I1440	P1333	P1222	W1113	ILE
R1832	H1716	D1633	M1528	L1443	L1334	R1227	Y1124	ASP
N1833	Q1723	Y1634	H1530	T1444	P1335	C1233	F1117	THR
T1835	Y1724	L1641	A1531	R1445	K1338	S1234	G1118	ALA
G1836	P1725	W1644	W1532	I1446	E1339	I1235	I1119	THR
P1837	R1733	I1647	M1533	N1447	I1340	I1236	P1120	ILE
V1838	Y1736	W1650	T1540	S1448	F1341	F1237	G1121	LEU
Q1839	L1737	V1651	L1544	P1450	R1342	Y1238	A1122	GLY
Y1842	R1738	V1654	D1560	R1458	E1346	R1241	F1123	GLN
L1844	R1739	Y1654	T1561	G1467	M1347	V1242	Y1124	VAL
L1845	P1742	V1655	I1562	T1468	L1348	F1128	N1127	SER
R1847	Y1748	S1656	N1563	L1469	L1349	M1129	V1127	LEU
S1848	E1749	L1657	T1564	K1470	H1355	F1134	F1128	VAL
S1849	Y1750	V1665	N1565	P1471	K1358	L1135	M1129	GLY
E1850	D1750	V1666	G1566	E1475	R1249	V1138	V1138	D1056
L1853	E1751	D1668	L1567	L1476	S1360	K1139	K1139	T1059
K1856	K1754	T1669	Q1570	S1477	K1361	L1140	L1140	S1060
I1862	A1759	Q1672	A1575	H1480	G1362	E1141	E1141	F1061
S1863	W1674	W1673	D1576	P1481	G1363	D1142	D1142	L1062
I1864	W1675	W1676	G1577	D1482	V1365	K1257	G1063	R1064
	R1762	K1676	I1578	G1483	M1365	P1258	W1156	R1065
	T1763	E1677	P1585	D1484	F1370	G1259	V1157	H1066
					A1371	E1260	Y1158	S1067
					R1372	V1261	F1160	M1068

4 Data and refinement statistics

Xtriage (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.	Xtriage
Total number of atoms	13534	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: 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

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

5.3.1 Protein backbone

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

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 [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.