



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 08:46 AM EDT

PDB ID : 5CSK
Title : Crystal structure of yeast acetyl-CoA carboxylase, unbiotinylated
Authors : Wei, J.; Tong, L.
Deposited on : 2015-07-23
Resolution : 3.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

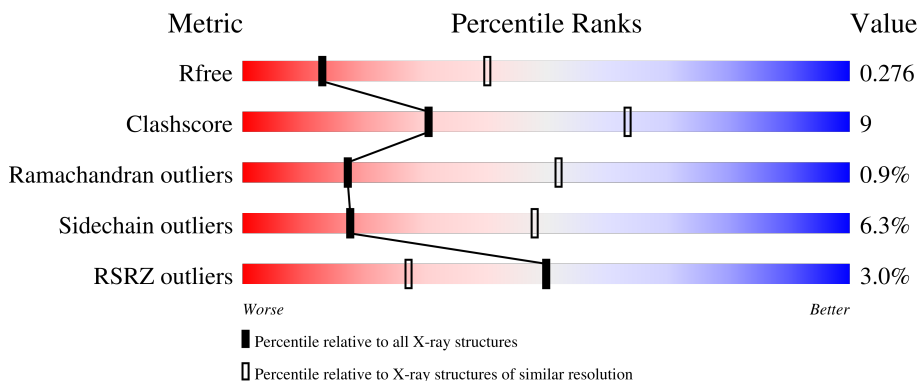
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	2218	 2% 69% 20% 10%
1	B	2218	 4% 68% 20% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31806 atoms, of which 0 are hydrogens and 0 are deuteriums.

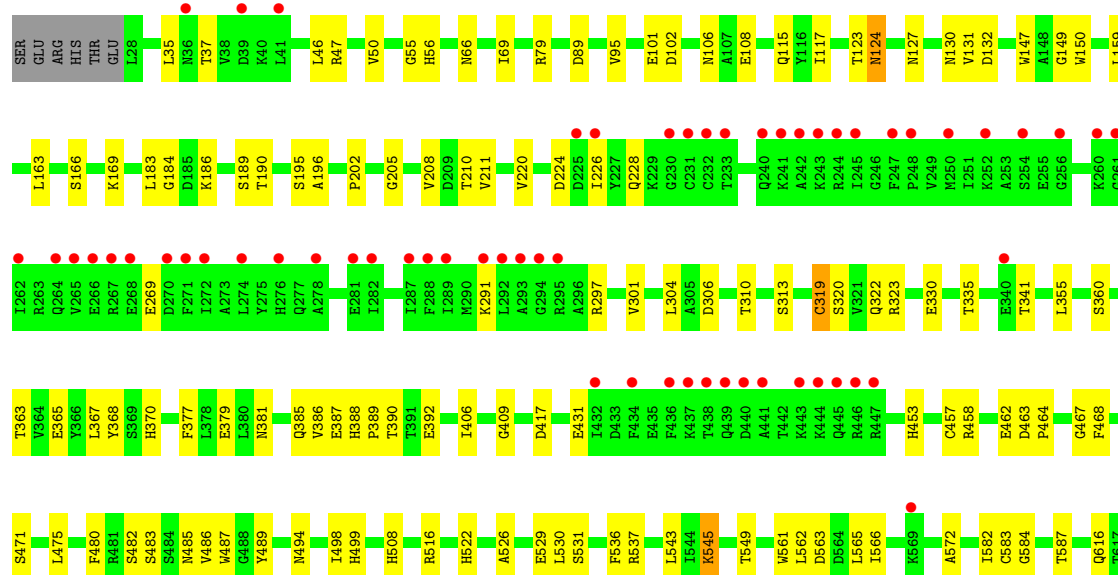
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1996	Total	C	N	O	S	0	0	0
			15828	10063	2733	2980	52			
1	B	2017	Total	C	N	O	S	0	0	0
			15978	10159	2758	3009	52			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2234	HIS	-	expression tag	UNP Q00955
A	2235	HIS	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
B	2234	HIS	-	expression tag	UNP Q00955
B	2235	HIS	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955



THR	D2168	D2169	Q2170	W2174	L2175	E2176	E2177	T2181	L2182	D2183	D2184	K2185	K2186	K2187	G2188	L2189	K2190	E2191	L2191	L2192	P2084	L2085	Y2086	T2089	S2101	R2102	W2103	P1926	N1927	S1928	F1930	L1945	R2119	R2120	R2128	W2131	R2138	L2139	S2140	H2141	G1N	V1L	A2146	W2158	A2161	S2162	V2163													
LEU	D1842	V1843	M1846	T1852	G1855	Y1858	A1874	K1875	V1878	R1883	T1887	L1888	L1889	N1909	E1914	T1915	P1920	W1924	H1925	F1926	N1927	S1928	F1930	L1945	R2119	R2120	R2128	W2131	R2138	L2139	S2140	H2141	G1N	V1L	A2146	W2158	A2161	S2162	V2163																					
LEU	R1741	L1742	G1743	Q1744	R1745	Q1748	G1751	Q1752	A1759	P1760	A1761	K1763	K1764	M1765	L1766	E1769	V1770	Y1771	M1774	L1775	Q1781	L1782	M1783	M1786	G1787	V1788	S1789	K1802	S1808	Y1809	V1810	K1813	V1818	D1825	T1826	W1827	D1828	R1829	P1830	T1836	M1837	D1838	E1839	T1840	Y1841															
HIS	I1619	A1632	E1633	E1634	V1635	P1636	P1637	L1638	F1639	Q1640	V1641	N1648	P1649	D1650	K1651	F1652	F1653	Q1654	L1655	Y1657	L1658	E1664	T1665	K1666	K1667	D1670	V1681	V1682	N1683	F1688	V1689	I1690	K1691	T1692	E1703	A1714	Y1719	T1724	I1725	C1730	R1731	S1732	I1735	G1736	Y1738															
HIS	E1491	W1492	L1493	R1497	Y1498	T1506	Y1507	V1508	Q1517	S1521	T1533	D1534	F1537	I1538	S1539	L1542	I1543	E1544	D1545	E1546	E1549	L1550	P1557	G1558	A1566	F1567	K1568	I1569	V1571	R1580	Q1581	V1584	V1585	I1589	K1592	I1593	G1594	F1603	F1604	N1605	K1606	V1607	I1616																	
HIS	M1371	Y1374	T1375	S1380	I1385	M1388	I1390	F1393	G1406	L1408	E1409	L1415	R1419	S1422	R1426	L1430	D1431	T1434	P1437	R1441	I1444	N1445	V1451	T1454	V1460	K1461	E1466	W1467	F1468	F1469	S1470	S1471	K1474	H1479	L1480	K1490																								
HIS	R1241	L1242	R1243	A1256	S1257	R1259	R1260	T1261	F1263	M1264	Y1272	P1273	F1278	Y1283	N1284	E1285	N1286	E1287	Q1299	L1300	E1301	L1305	I1310	M1317	R1318	V1322	D1333	T1338	I1341	I1342	R1343	T1344	D1350	I1351	S1352	I1353	S1359	L1364	M1365	I1368	L1369	D1370																		
LEU	F876	F877	A878	S882	K883	D886	Y894	E905	P906	K913	Y914	S924	I925	F926	V927	H928	Y933	F940	N941	P950	R955	L967	V975	R979	A980	L981	Q990	P991	S997	P1006	V1011	F1012	L1013	ARG	ARG	GLY	A874	V875																						
LEU	R1026	I1030	R1040	L1044	V1052	V1053	Y1057	G1058	SER	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	F926	N941	P950	R955	L967	V975	R979	A980	L981	Q990	P991	S997	P1006	V1011	F1012	L1013	ARG	ARG	GLY	A874	V875																					
GLY	L618	I624	R629	Y630	PHE	LEU	VAL	GLU	ASN	GLY	GLU	HIS	ILE	ILE	GLY	GLN	PRO	TYR	ALA	ILE	GLU	VAL	MET	LYS	MET	GLN	PRO	LEU	LEU	GLN	PRO	PRO	LEU	LEU	GLN	PRO	PRO	LEU	GLN	GLY	H851	S852	R853	L865	R868	S869	GLN	ASP	THR	GLN	LEU	ARG	THR	ILE	ALA	MET	THR	PRO	PRO	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.88Å 159.88Å 615.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.10 49.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (49.47-3.10) 93.1 (49.42-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.281 0.218 , 0.276	Depositor DCC
R_{free} test set	6831 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31806	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.56	0/16156	0.76	4/21869 (0.0%)
1	B	0.55	0/16306	0.76	10/22069 (0.0%)
All	All	0.56	0/32462	0.76	14/43938 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1419	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	660	ASP	CB-CG-OD1	6.65	124.29	118.30
1	B	1580	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	1571	VAL	CB-CA-C	-5.86	100.27	111.40
1	B	1108	ARG	NE-CZ-NH2	-5.59	117.50	120.30

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	15828	0	15783	289	1
1	B	15978	0	15941	323	0
All	All	31806	0	31724	582	1

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 9.

The worst 5 of 582 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:1735:ILE:HD13	1:A:1735:ILE:H	1.19	1.07
1:B:941:ASN:HD21	1:B:1013:LEU:HA	1.31	0.92
1:B:1040:ARG:NH1	1:B:1081:VAL:O	2.02	0.92
1:A:1243:ARG:NH1	1:A:1283:TYR:O	2.02	0.91
1:A:587:THR:HG22	1:A:663:LEU:HD12	1.53	0.91

All (1) 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:A:440:ASP:OD1	1:A:440:ASP:OD1[7_466]	1.80	0.40

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	1980/2218 (89%)	1771 (89%)	188 (10%)	21 (1%)	14	46
1	B	1997/2218 (90%)	1778 (89%)	203 (10%)	16 (1%)	19	54
All	All	3977/4436 (90%)	3549 (89%)	391 (10%)	37 (1%)	17	52

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	572	ALA
1	A	184	GLY
1	A	573	GLU
1	A	1316	ASP
1	A	1378	SER

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	1718/1912 (90%)	1616 (94%)	102 (6%)	19	50
1	B	1735/1912 (91%)	1619 (93%)	116 (7%)	16	46
All	All	3453/3824 (90%)	3235 (94%)	218 (6%)	18	48

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	483	SER
1	B	1084	ASP
1	B	1875	LYS
1	B	616	GLN
1	B	848	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	HIS
1	B	1909	ASN
1	B	499	HIS
1	B	1786	ASN
1	B	2057	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](#)

There are no ligands in this entry.

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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1996/2218 (89%)	-0.15	39 (1%) 65 44	47, 85, 140, 237	0
1	B	2017/2218 (90%)	-0.05	80 (3%) 38 19	46, 87, 161, 237	0
All	All	4013/4436 (90%)	-0.10	119 (2%) 50 27	46, 86, 150, 237	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	897	ASP	6.9
1	A	856	ALA	6.5
1	B	293	ALA	6.5
1	A	897	ASP	5.9
1	B	2191	LEU	5.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.