



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2017 – 01:32 AM EDT

PDB ID : 5CSK
Title : Crystal structure of yeast acetyl-CoA carboxylase, unbiotinylated
Authors : Wei, J.; Tong, L.
Deposited on : unknown
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

<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)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

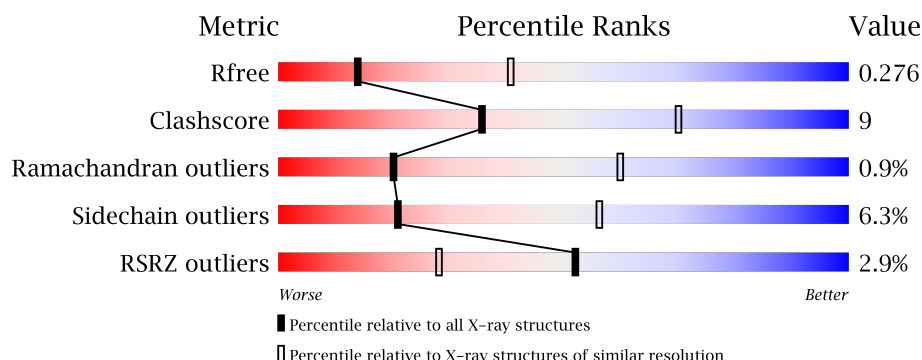
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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.

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

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.

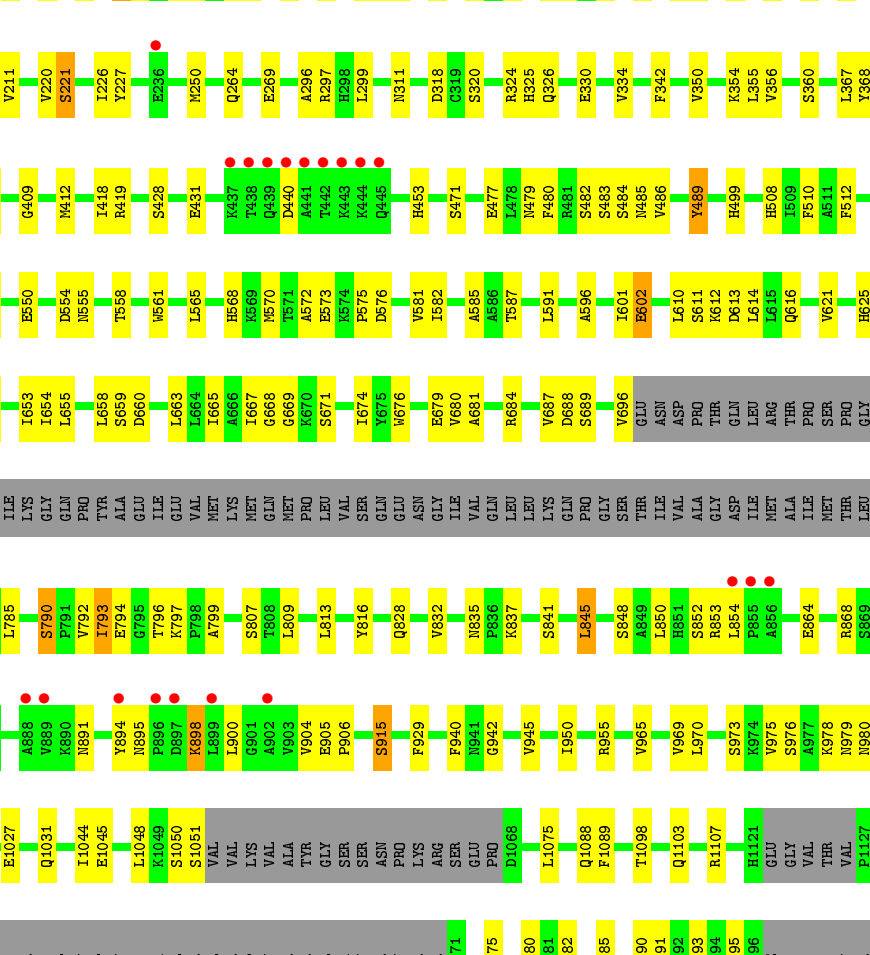
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1996	Total	C	N	O	S	0	0	0
			15828	10063	2733	2980	52			
1	B	2017	Total	C	N	O	S	0	0	0
			15978	10159	2758	3009	52			

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

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 



Position	Amino Acid	Frequency
1	SER	2%
2	GLU	69%
3	ARG	20%
4	THR	10%
5	PHE	2%
6	PRO	69%
7	GLY	20%
8	SER	10%
9	VAL	2%
10	ALA	69%
11	SER	20%
12	LYS	10%
13	GLY	2%
14	VAL	69%
15	THR	20%
16	GLN	10%
17	ASP	2%
18	GLY	69%
19	VAL	20%
20	GLY	10%
21	GLY	2%
22	GLY	69%
23	GLY	20%
24	GLY	10%
25	GLY	2%
26	GLY	69%
27	GLY	20%
28	GLY	10%
29	GLY	2%
30	GLY	69%
31	GLY	20%
32	GLY	10%
33	GLY	2%
34	GLY	69%
35	GLY	20%
36	GLY	10%
37	GLY	2%
38	GLY	69%
39	GLY	20%
40	GLY	10%





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	6821 reflections (5.29%)	DCC
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 , 52.9	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:H	1:A:1735:ILE:HD13	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 [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	1980/2218 (89%)	1771 (89%)	188 (10%)	21 (1%)	17	54
1	B	1997/2218 (90%)	1778 (89%)	203 (10%)	16 (1%)	22	62
All	All	3977/4436 (90%)	3549 (89%)	391 (10%)	37 (1%)	20	60

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 ⓘ

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%)	23	58
1	B	1735/1912 (91%)	1619 (93%)	116 (7%)	19	54
All	All	3453/3824 (90%)	3235 (94%)	218 (6%)	21	56

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

Mol	Chain	Res	Type
1	A	2149	LEU
1	B	673	THR
1	B	1909	ASN
1	A	2187	LYS
1	B	360	SER

Some 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	124	ASN
1	B	453	HIS
1	B	1941	ASN
1	B	152	HIS
1	B	280	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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	38 (1%) 67 46	47, 85, 140, 237	0
1	B	2017/2218 (90%)	-0.05	78 (3%) 40 19	46, 87, 161, 237	0
All	All	4013/4436 (90%)	-0.10	116 (2%) 52 28	46, 86, 150, 237	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	897	ASP	6.7
1	A	856	ALA	6.4
1	B	293	ALA	6.4
1	A	897	ASP	5.8
1	B	2191	LEU	5.7

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 carbohydrates 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.