



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2017 – 01:13 AM EDT

PDB ID : 5CSA
Title : Crystal structure of domains BT-BCCP-AC1-AC5 of yeast acetyl-CoA carboxylase
Authors : Wei, J.; Tong, L.
Deposited on : unknown
Resolution : 3.00 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

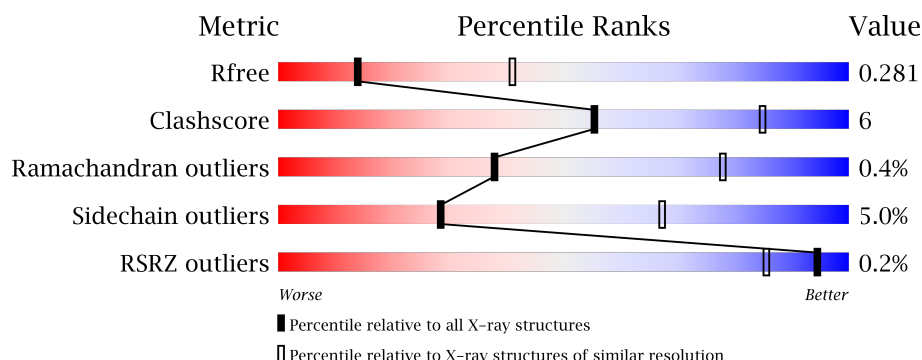
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	932	 78% 14% • 6%
1	B	932	 77% 13% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13699 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	872	Total	C	N	O	S	0	4	0
			6939	4440	1182	1296	21			
1	B	852	Total	C	N	O	S	0	0	0
			6760	4329	1146	1265	20			

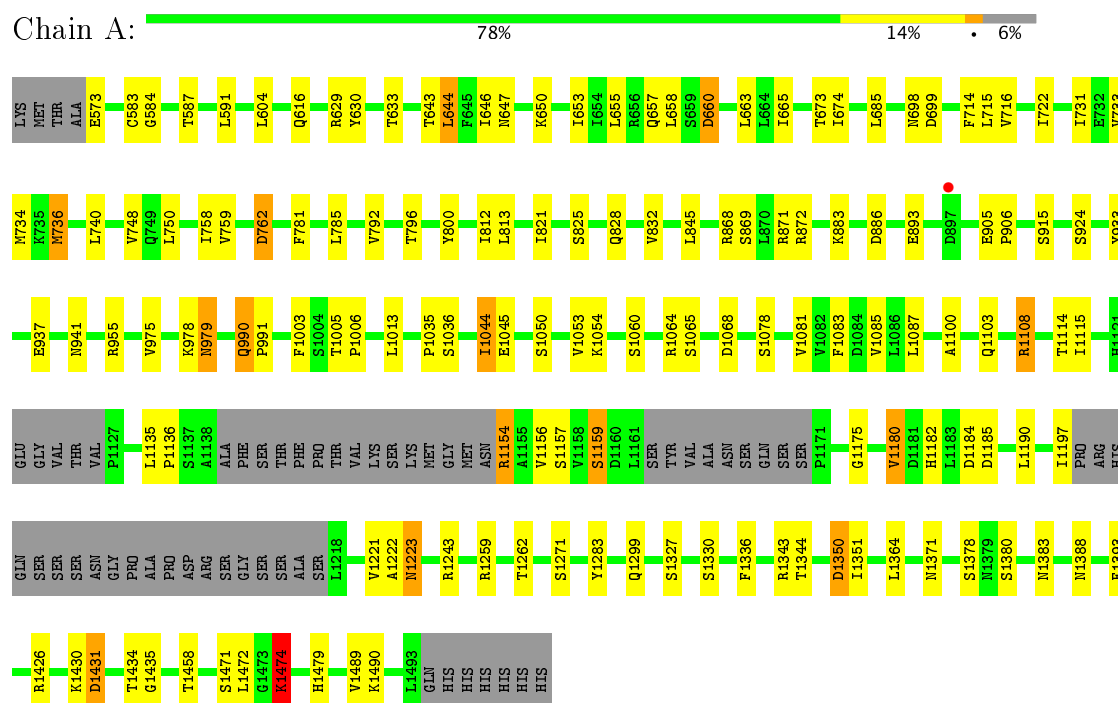
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1495	HIS	-	expression tag	UNP Q00955
A	1496	HIS	-	expression tag	UNP Q00955
A	1497	HIS	-	expression tag	UNP Q00955
A	1498	HIS	-	expression tag	UNP Q00955
A	1499	HIS	-	expression tag	UNP Q00955
A	1500	HIS	-	expression tag	UNP Q00955
B	1495	HIS	-	expression tag	UNP Q00955
B	1496	HIS	-	expression tag	UNP Q00955
B	1497	HIS	-	expression tag	UNP Q00955
B	1498	HIS	-	expression tag	UNP Q00955
B	1499	HIS	-	expression tag	UNP Q00955
B	1500	HIS	-	expression tag	UNP Q00955

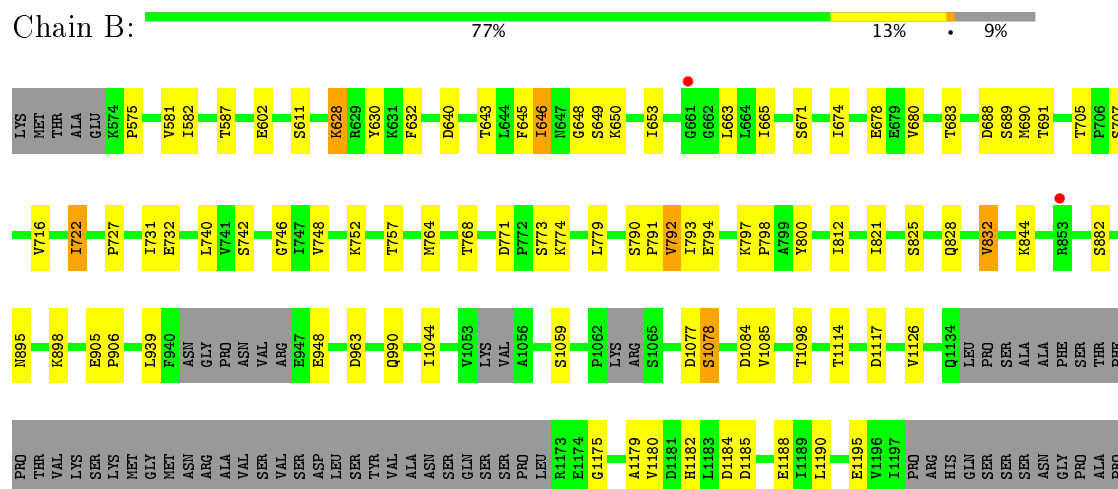
3 Residue-property plots

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.

- Molecule 1: Acetyl-CoA carboxylase



- Molecule 1: Acetyl-CoA carboxylase



ASP	ARG	SER	GLY	SER	SER	ALA	SER	L1218	V1221	A1222	N1223	S1228	R1241	E1252	R1259	S1271	Y1272	P1273	L1305	I1310	V1322	S1327	K1334	T1338	R1343	L1364	I1368	S1380	F1386	S1396	L1408	S1422	A1423	E1424	I1429	K1430	D1431	P1432
Q1433	T1434	G1435	A1436	L1440	Y1450	V1451	I1452	E1455	M1456	Y1457	V1460	K1461	N1462	A1463	E1466	W1467	K1470	S1471	H1479	I1483	V1489	K1490	L1493	GLN	HIS	HIS	HIS	HIS	HIS	HIS	L1493	HIS	HIS	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.33Å 149.67Å 95.44Å 90.00° 118.39° 90.00°	Depositor
Resolution (Å)	42.63 – 3.00 42.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.63-3.00) 97.9 (42.64-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.230 , 0.289 0.224 , 0.281	Depositor DCC
R_{free} test set	2290 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.020 for h,-k,-h-l 0.023 for -h-l,-k,l 0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13699	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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

5.1 Standard geometry

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	0.52	1/7082 (0.0%)	0.68	3/9586 (0.0%)
1	B	0.58	6/6890 (0.1%)	0.66	1/9327 (0.0%)
All	All	0.55	7/13972 (0.1%)	0.67	4/18913 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1450	TYR	CE1-CZ	12.68	1.55	1.38
1	B	1466	GLU	CD-OE1	7.30	1.33	1.25
1	B	602	GLU	CD-OE2	7.02	1.33	1.25
1	B	602	GLU	CD-OE1	7.01	1.33	1.25
1	B	1450	TYR	CZ-OH	5.80	1.47	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1474	LYS	CD-CE-NZ	7.50	128.95	111.70
1	B	1436	ALA	C-N-CD	5.39	139.72	128.40
1	A	660	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	1431	ASP	C-N-CD	5.02	138.95	128.40

There are no chirality outliers.

There are no planarity outliers.

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	6939	0	7077	82	6
1	B	6760	0	6877	87	6
All	All	13699	0	13954	164	6

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 6.

The worst 5 of 164 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:1431:ASP:OD2	1:A:1434:THR:OG1	1.89	0.91
1:B:1461:LYS:HE2	1:B:1467:TRP:CD1	2.10	0.85
1:B:1432:PRO:HG2	1:B:1433:GLN:NE2	1.92	0.85
1:B:1432:PRO:HG2	1:B:1433:GLN:HE21	1.42	0.85
1:B:1431:ASP:OD2	1:B:1434:THR:OG1	2.00	0.79

The worst 5 of 6 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:1474:LYS:CD	1:B:1450:TYR:CE1[2_546]	1.72	0.48
1:A:1474:LYS:CE	1:B:1450:TYR:CE1[2_546]	1.85	0.35
1:A:1474:LYS:CE	1:B:1450:TYR:OH[2_546]	2.05	0.15
1:A:1474:LYS:CE	1:B:1450:TYR:CZ[2_546]	2.09	0.11
1:A:1474:LYS:NZ	1:B:1450:TYR:CE1[2_546]	2.10	0.10

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	866/932 (93%)	792 (92%)	73 (8%)	1 (0%)	55 89
1	B	840/932 (90%)	775 (92%)	60 (7%)	5 (1%)	28 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1706/1864 (92%)	1567 (92%)	133 (8%)	6 (0%)	38 78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	680	VAL
1	A	1378	SER
1	B	939	LEU
1	B	948	GLU
1	B	646	ILE

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	774/821 (94%)	731 (94%)	43 (6%)	25 62
1	B	752/821 (92%)	719 (96%)	33 (4%)	33 72
All	All	1526/1642 (93%)	1450 (95%)	76 (5%)	28 67

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1271	SER
1	A	1474	LYS
1	B	1380	SER
1	A	1330	SER
1	A	1364	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1182	HIS
1	A	1479	HIS
1	B	1384	HIS

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Mol	Chain	Res	Type
1	A	979	ASN
1	B	1371	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](#)

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	872/932 (93%)	-0.41	1 (0%) 95 88	40, 71, 105, 142	0
1	B	852/932 (91%)	-0.37	3 (0%) 92 77	44, 75, 111, 151	0
All	All	1724/1864 (92%)	-0.39	4 (0%) 94 85	40, 73, 109, 151	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	853	ARG	2.7
1	A	897	ASP	2.6
1	B	661	GLY	2.3
1	B	1463	ALA	2.2

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.