



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:32 am GMT

PDB ID : 3H0J
Title : Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with compound 2
Authors : Zhang, H.; Tong, L.
Deposited on : 2009-04-09
Resolution : 2.80 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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

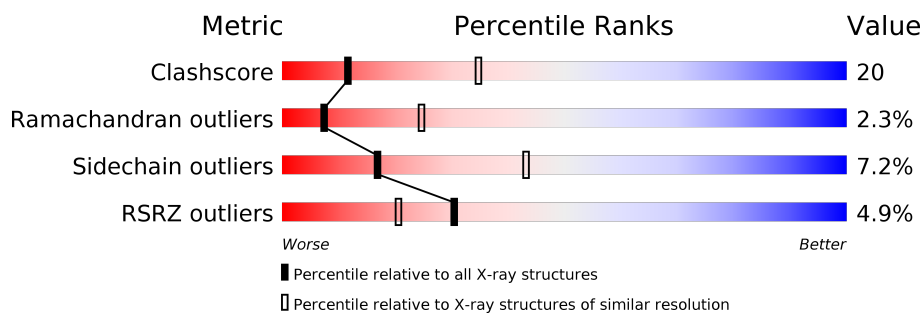
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	769	
1	B	769	
1	C	769	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16200 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	681	Total	C	N	O	S	0	0	0
			5424	3459	930	1016	19			
1	B	675	Total	C	N	O	S	0	0	0
			5376	3427	923	1007	19			
1	C	665	Total	C	N	O	S	0	0	0
			5298	3374	912	993	19			

There are 33 discrepancies between the modelled and reference sequences:

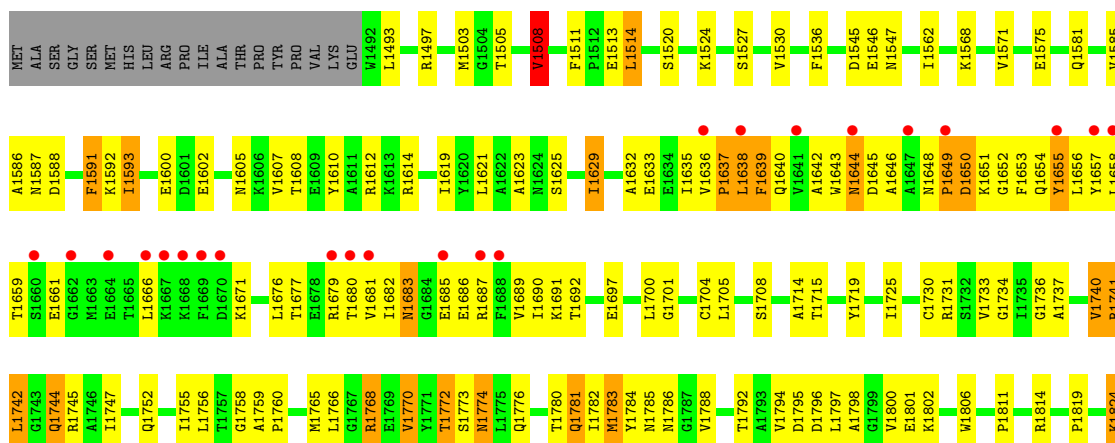
Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	EXPRESSION TAG	UNP Q00955
A	1474	ALA	-	EXPRESSION TAG	UNP Q00955
A	1475	SER	-	EXPRESSION TAG	UNP Q00955
A	2234	LEU	-	EXPRESSION TAG	UNP Q00955
A	2235	GLU	-	EXPRESSION TAG	UNP Q00955
A	2236	HIS	-	EXPRESSION TAG	UNP Q00955
A	2237	HIS	-	EXPRESSION TAG	UNP Q00955
A	2238	HIS	-	EXPRESSION TAG	UNP Q00955
A	2239	HIS	-	EXPRESSION TAG	UNP Q00955
A	2240	HIS	-	EXPRESSION TAG	UNP Q00955
A	2241	HIS	-	EXPRESSION TAG	UNP Q00955
B	1473	MET	-	EXPRESSION TAG	UNP Q00955
B	1474	ALA	-	EXPRESSION TAG	UNP Q00955
B	1475	SER	-	EXPRESSION TAG	UNP Q00955
B	2234	LEU	-	EXPRESSION TAG	UNP Q00955
B	2235	GLU	-	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
B	2240	HIS	-	EXPRESSION TAG	UNP Q00955
B	2241	HIS	-	EXPRESSION TAG	UNP Q00955
C	1473	MET	-	EXPRESSION TAG	UNP Q00955

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	EXPRESSION TAG	UNP Q00955
C	1475	SER	-	EXPRESSION TAG	UNP Q00955
C	2234	LEU	-	EXPRESSION TAG	UNP Q00955
C	2235	GLU	-	EXPRESSION TAG	UNP Q00955
C	2236	HIS	-	EXPRESSION TAG	UNP Q00955
C	2237	HIS	-	EXPRESSION TAG	UNP Q00955
C	2238	HIS	-	EXPRESSION TAG	UNP Q00955
C	2239	HIS	-	EXPRESSION TAG	UNP Q00955
C	2240	HIS	-	EXPRESSION TAG	UNP Q00955
C	2241	HIS	-	EXPRESSION TAG	UNP Q00955

- # B36

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 34	C 31	N 2	O 1	0	0
2	B	1	Total 34	C 31	N 2	O 1	0	0
2	C	1	Total 34	C 31	N 2	O 1	0	0



ASP	LYS	GLU	LYS	LEU	LEU	LYS	THR	LEU	LYS	LEU	GLU	HIS	HIS	HIS	HIS
E2145	K2146	S2147	R2148	K2151	I2152	K2153	R2154	P2160	V2163	D2164	Q2170	T2173	E2177	K2185	I2186
LYS	GLU	LYS	LEU	LEU	LYS	THR	LEU	LYS	LEU	GLU	HIS	HIS	HIS	HIS	HIS
LEU	ALA	PRO	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG
LEU	ALA	PRO	GLU	VAL	HIS	GLN	GLN	ILE	SER	LYS	GLN	LEU	ALA	ASP	ARG
L2089	S2090	L2091	Q2092	F2093	L2096	R2097	P2098	R2099	R2100	S2101	R2102	R2103	V2104	V2108	I2109
LYS	LEU	GLU	SER	SER	PHE	ALA	GLN	ASP	LEU	ALA	LYS	LYS	ILE	ARG	SER
E2114	R2125	R2128	R2129	E2132	I2136	L2139	Q2142	V2143	G2144	L2040	L2041	D2042	T2043	N2044	R2045
ASP	LYS	GLY	LEU	SER	VAL	LYS	LEU	THR	ASP	LYS	ASP	ASP	LYS	ARG	GLU
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
E1929	F1930	I1936	W1953	R1954	G1955	Q1960	E1966	V1967	L1968	A1977	E1919	W1924	H1925	P1926	N1927
ASP	ASP	LYS	ARG	GLU	LEU	SER	LEU	SER	LYS	SER	E1914	A1913	S1912	M1911	P1910
ASP	ASP	LYS	ARG	GLU	LEU	SER	LEU	SER	LYS	SER	E1914	A1913	S1912	M1911	P1910
L1978	Y1988	F1991	T1992	G1993	E1994	L1995	R1996	G1997	G1998	S1999	W2000	V2001	P2005	N2008	M2012
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
L1829	R1844	E1848	E1851	T1852	E1853	S1854	G1855	Y1858	G1872	W1873	A1874	R1883	I1887	V1894	T1898
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.74Å 122.86Å 145.88Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	51.25 – 2.80 51.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.25-2.80) 99.3 (51.25-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.257 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16200	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

Bond lengths and bond angles in the following residue types are not validated in this section: B36

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	0.38	0/5546	0.66	0/7514
1	B	0.36	0/5497	0.65	1/7449 (0.0%)
1	C	0.36	0/5415	0.64	0/7335
All	All	0.37	0/16458	0.65	1/22298 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1791	LEU	CA-CB-CG	5.60	128.17	115.30

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	5424	0	5365	211	0
1	B	5376	0	5316	222	0
1	C	5298	0	5234	220	0
2	A	34	0	28	1	0
2	B	34	0	28	2	0
2	C	34	0	28	1	0
All	All	16200	0	15999	628	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 20.

The worst 5 of 628 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:1494:GLN:HA	1:A:1496:LYS:HE3	1.39	0.99
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.43	0.99
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.61	0.97
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.04	0.97
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.00	0.95

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	677/769 (88%)	608 (90%)	58 (9%)	11 (2%)	11	36
1	B	671/769 (87%)	589 (88%)	63 (9%)	19 (3%)	6	19
1	C	661/769 (86%)	585 (88%)	60 (9%)	16 (2%)	7	23
All	All	2009/2307 (87%)	1782 (89%)	181 (9%)	46 (2%)	7	25

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	B	1643	TRP
1	B	1731	ARG
1	B	1839	GLU
1	B	2142	GLN

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	577/658 (88%)	543 (94%)	34 (6%)	23	54
1	B	572/658 (87%)	522 (91%)	50 (9%)	12	33
1	C	563/658 (86%)	523 (93%)	40 (7%)	17	44
All	All	1712/1974 (87%)	1588 (93%)	124 (7%)	17	43

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1735	ILE
1	B	2001	VAL
1	C	2028	GLN
1	B	1777	LEU
1	B	1852	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1748	GLN
1	B	1944	GLN
1	C	1941	ASN
1	B	1752	GLN
1	B	1909	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B36	A	1	-	39,39,39	2.79	22 (56%)	56,56,56	1.44	8 (14%)
2	B36	B	1	-	39,39,39	3.72	31 (79%)	56,56,56	1.24	4 (7%)
2	B36	C	1	-	39,39,39	3.51	27 (69%)	56,56,56	1.31	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B36	A	1	-	-	0/12/22/22	0/6/6/6
2	B36	B	1	-	-	0/12/22/22	0/6/6/6
2	B36	C	1	-	-	0/12/22/22	0/6/6/6

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	B36	CAQ-CBG	2.08	1.58	1.52
2	B	1	B36	CAU-CBG	2.08	1.59	1.53
2	A	1	B36	CBD-NAV	2.25	1.41	1.37
2	C	1	B36	OAB-CAW	2.27	1.27	1.22
2	A	1	B36	CAP-CBB	2.28	1.43	1.39

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	B36	CBA-CBD-NAV	-3.07	117.21	122.24
2	A	1	B36	OAB-CAW-CAZ	-2.94	118.70	121.59
2	A	1	B36	CBA-CBD-NAV	-2.87	117.55	122.24
2	A	1	B36	CBF-CAZ-CBE	-2.76	117.27	120.95
2	A	1	B36	CAI-CBB-CAP	-2.49	117.92	122.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	B36	1	0
2	B	1	B36	2	0
2	C	1	B36	1	0

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	681/769 (88%)	-0.04	27 (3%)	39 28	24, 43, 89, 107	0
1	B	675/769 (87%)	0.06	36 (5%)	27 18	22, 46, 102, 119	0
1	C	665/769 (86%)	0.09	36 (5%)	26 17	23, 46, 111, 132	0
All	All	2021/2307 (87%)	0.04	99 (4%)	30 20	22, 45, 99, 132	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2037	ARG	5.7
1	C	2082	LEU	5.4
1	B	2082	LEU	5.3
1	B	2143	VAL	5.2
1	C	1679	ARG	4.9

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	B36	A	1	34/34	0.90	0.25	1.63	65,70,74,74	0
2	B36	C	1	34/34	0.93	0.24	1.50	59,61,63,64	0
2	B36	B	1	34/34	0.89	0.23	0.96	63,68,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.