



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:45 pm BST

PDB ID : 2F9I
Title : Crystal Structure of the carboxyltransferase subunit of ACC from Staphylococcus aureus
Authors : Bilder, P.W.
Deposited on : 2005-12-05
Resolution : 1.98 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 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	:	2.11
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)	:	2.11

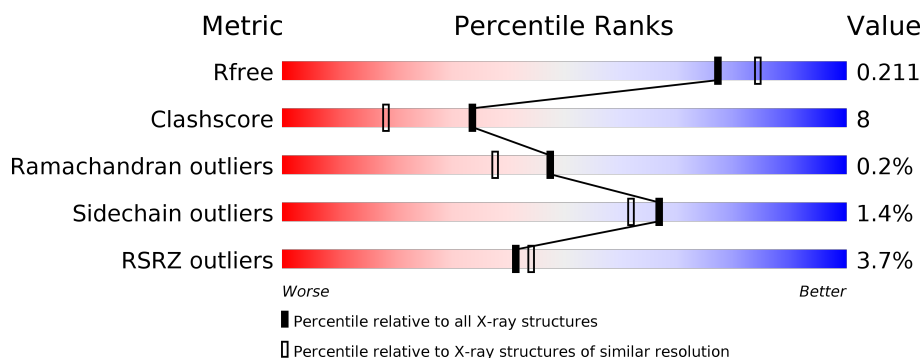
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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	327	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>•• 6%</div> </div> </div>
1	C	327	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•• 9%</div> </div> </div>
2	B	285	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• 9%</div> </div> </div>
2	D	285	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>• 11%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9270 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-coenzyme A carboxylase carboxyl transferase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	45	0	0
			2407	1523	417	459	8			
1	C	297	Total	C	N	O	S	48	0	0
			2289	1447	396	438	8			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	CLONING ARTIFACT	GB 49244968
A	-11	HIS	-	EXPRESSION TAG	GB 49244968
A	-10	HIS	-	EXPRESSION TAG	GB 49244968
A	-9	HIS	-	EXPRESSION TAG	GB 49244968
A	-8	HIS	-	EXPRESSION TAG	GB 49244968
A	-7	HIS	-	EXPRESSION TAG	GB 49244968
A	-6	HIS	-	EXPRESSION TAG	GB 49244968
A	-5	LEU	-	CLONING ARTIFACT	GB 49244968
A	-4	VAL	-	CLONING ARTIFACT	GB 49244968
A	-3	PRO	-	CLONING ARTIFACT	GB 49244968
A	-2	ARG	-	CLONING ARTIFACT	GB 49244968
A	-1	GLY	-	CLONING ARTIFACT	GB 49244968
A	0	SER	-	CLONING ARTIFACT	GB 49244968
C	-12	MET	-	CLONING ARTIFACT	GB 49244968
C	-11	HIS	-	EXPRESSION TAG	GB 49244968
C	-10	HIS	-	EXPRESSION TAG	GB 49244968
C	-9	HIS	-	EXPRESSION TAG	GB 49244968
C	-8	HIS	-	EXPRESSION TAG	GB 49244968
C	-7	HIS	-	EXPRESSION TAG	GB 49244968
C	-6	HIS	-	EXPRESSION TAG	GB 49244968
C	-5	LEU	-	CLONING ARTIFACT	GB 49244968
C	-4	VAL	-	CLONING ARTIFACT	GB 49244968
C	-3	PRO	-	CLONING ARTIFACT	GB 49244968
C	-2	ARG	-	CLONING ARTIFACT	GB 49244968

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	CLONING ARTIFACT	GB 49244968
C	0	SER	-	CLONING ARTIFACT	GB 49244968

- Molecule 2 is a protein called acetyl-coenzyme A carboxylase carboxyl transferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	20	0	0
			2009	1263	344	385	17			
2	D	255	Total	C	N	O	S	26	0	0
			1980	1246	339	378	17			

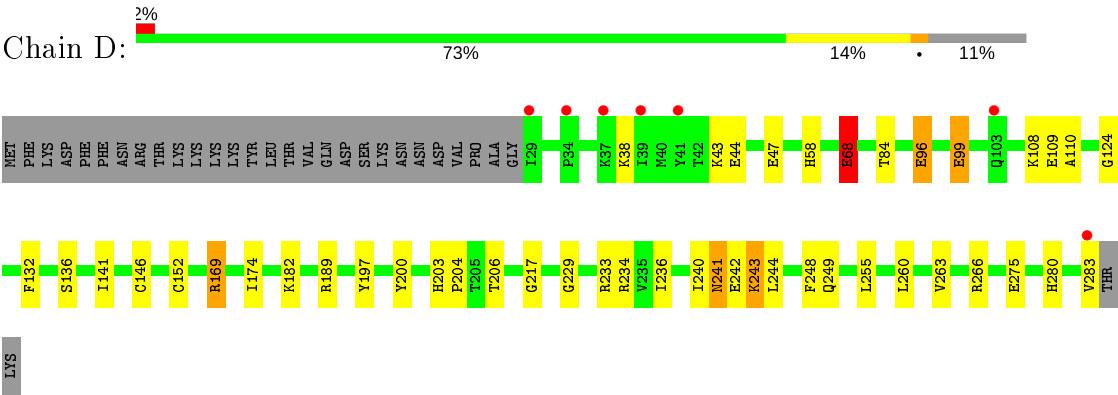
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	155	Total	O	0	0
			155	155		
4	C	163	Total	O	0	0
			163	163		
4	D	132	Total	O	0	0
			132	132		

● Molecule 2: acetyl-coenzyme A carboxylase carboxyl transferase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.98Å 50.86Å 149.64Å 90.00° 113.51° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 49.43 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-1.98) 97.5 (49.43-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 1.98Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, R_{free}	0.186 , 0.213 0.185 , 0.211	Depositor DCC
R_{free} test set	9030 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9270	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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](#)

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

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	2.10	29/2446 (1.2%)	1.34	33/3292 (1.0%)
1	C	1.79	30/2326 (1.3%)	1.66	49/3134 (1.6%)
2	B	1.17	12/2041 (0.6%)	1.03	13/2741 (0.5%)
2	D	1.14	11/2011 (0.5%)	1.02	19/2701 (0.7%)
All	All	1.64	82/8824 (0.9%)	1.31	114/11868 (1.0%)

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	4
1	C	1	7
2	B	0	3
2	D	0	2
All	All	1	16

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	GLU	CD-OE2	-52.02	0.68	1.25
1	A	232	LYS	CE-NZ	-33.86	0.64	1.49
1	A	-4	VAL	CB-CG2	32.45	2.21	1.52
1	A	-4	VAL	CB-CG1	26.37	2.08	1.52
1	C	291	GLU	CD-OE2	23.22	1.51	1.25

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	CB-CG-OD2	-32.68	88.89	118.30
1	C	36	LEU	CB-CG-CD1	-30.23	59.61	111.00
1	C	116	ASP	CB-CG-OD1	27.09	142.68	118.30
2	B	234	ARG	NE-CZ-NH2	-21.89	109.36	120.30
1	C	291	GLU	CG-CD-OE2	-21.06	76.18	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	1	MET	CA

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ILE	Mainchain
1	A	16	GLU	Mainchain
1	A	253	GLN	Sidechain
1	A	34	ASP	Sidechain
2	B	99	GLU	Sidechain

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	2407	0	2419	53	0
1	C	2289	0	2273	34	0
2	B	2009	0	2017	43	0
2	D	1980	0	1992	33	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	133	0	0	5	0
4	B	155	0	0	8	0
4	C	163	0	0	6	0
4	D	132	0	0	6	0
All	All	9270	0	8701	144	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 8.

The worst 5 of 144 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:C:36:LEU:CG	1:C:36:LEU:CD2	1.76	1.56
1:C:34:ASP:C	1:C:34:ASP:CA	1.74	1.53
1:C:36:LEU:CD1	1:C:36:LEU:CG	1.97	1.38
1:C:232:LYS:NZ	1:C:232:LYS:CE	2.05	1.19
1:A:274:GLN:HG2	4:A:413:HOH:O	1.66	0.96

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	305/327 (93%)	290 (95%)	14 (5%)	1 (0%)	41	29
1	C	293/327 (90%)	278 (95%)	15 (5%)	0	100	100
2	B	258/285 (90%)	252 (98%)	5 (2%)	1 (0%)	34	22
2	D	253/285 (89%)	248 (98%)	5 (2%)	0	100	100
All	All	1109/1224 (91%)	1068 (96%)	39 (4%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	27	ALA
1	A	31	GLU

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	252/274 (92%)	246 (98%)	6 (2%)	49	41
1	C	235/274 (86%)	232 (99%)	3 (1%)	69	64
2	B	221/247 (90%)	219 (99%)	2 (1%)	78	77
2	D	219/247 (89%)	217 (99%)	2 (1%)	78	77
All	All	927/1042 (89%)	914 (99%)	13 (1%)	67	62

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	LYS
2	B	53	PHE
1	C	232	LYS
1	A	218	TYR
1	C	218	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	280	HIS
1	C	124	ASN
2	D	241	ASN
1	C	83	HIS
1	C	87	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 ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	16:GLU	C	17:SER	N	1.64

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	309/327 (94%)	0.19	16 (5%)	27 29	23, 35, 72, 90	29 (9%)
1	C	297/327 (90%)	0.21	11 (3%)	41 44	23, 34, 79, 94	30 (10%)
2	B	260/285 (91%)	0.01	8 (3%)	49 51	24, 35, 55, 71	12 (4%)
2	D	255/285 (89%)	-0.08	7 (2%)	54 56	25, 35, 53, 63	17 (6%)
All	All	1121/1224 (91%)	0.09	42 (3%)	41 44	23, 35, 65, 94	88 (7%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	PHE	8.0
2	D	29	ILE	6.7
1	C	11	ILE	6.6
2	D	283	VAL	6.4
1	A	9	PHE	5.1

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. 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	B-factors(\AA^2)	Q<0.9
3	ZN	D	602	1/1	0.98	0.07	44,44,44,44	0
3	ZN	B	601	1/1	1.00	0.09	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.