



wwPDB X-ray Structure Validation Summary Report

Feb 15, 2017 – 05:03 am GMT

PDB ID : 2BZR
Title : CRYSTAL STRUCTURE OF ACCD5 (RV3280), AN ACYL-COA CARBOXYLASE BETA-SUBUNIT FROM MYCOBACTERIUM TUBERCULOSIS
Authors : Holton, S.J.
Deposited on : 2005-08-22
Resolution : 2.20 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 : 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

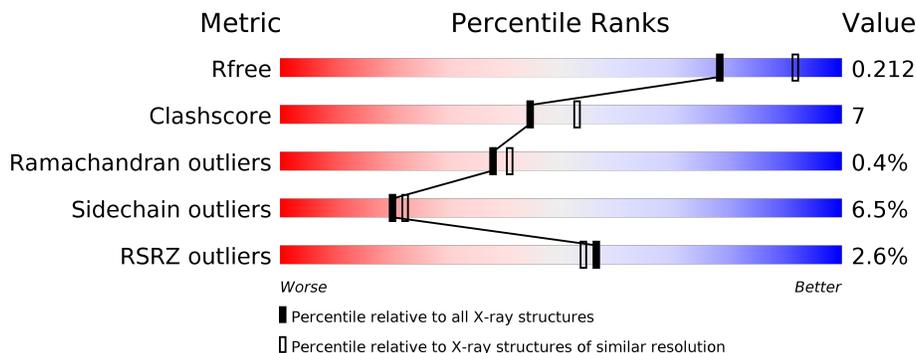
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	548	 3% 76% 14% • 7%
1	B	548	 3% 76% 14% • 8%
1	C	548	 2% 75% 15% • 8%
1	D	548	 2% 77% 13% • 7%
1	E	548	 % 75% 15% • 8%
1	F	548	 2% 77% 12% • 8%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 24961 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 PROPIONYL-COA CARBOXYLASE BETA CHAIN 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	512	3948	2488	684	760	16	0	6	0
1	B	504	3883	2449	669	749	16	0	7	0
1	C	506	3862	2434	670	742	16	0	1	0
1	D	508	3875	2441	674	744	16	0	0	0
1	E	506	3857	2431	670	740	16	0	0	0
1	F	505	3846	2425	666	739	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	512	GLY	ASP	CONFLICT	UNP P96885
B	512	GLY	ASP	CONFLICT	UNP P96885
C	512	GLY	ASP	CONFLICT	UNP P96885
D	512	GLY	ASP	CONFLICT	UNP P96885
E	512	GLY	ASP	CONFLICT	UNP P96885
F	512	GLY	ASP	CONFLICT	UNP P96885

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	280	Total 280	O 280	0	0
2	B	273	Total 273	O 273	0	0
2	C	285	Total 285	O 285	0	0

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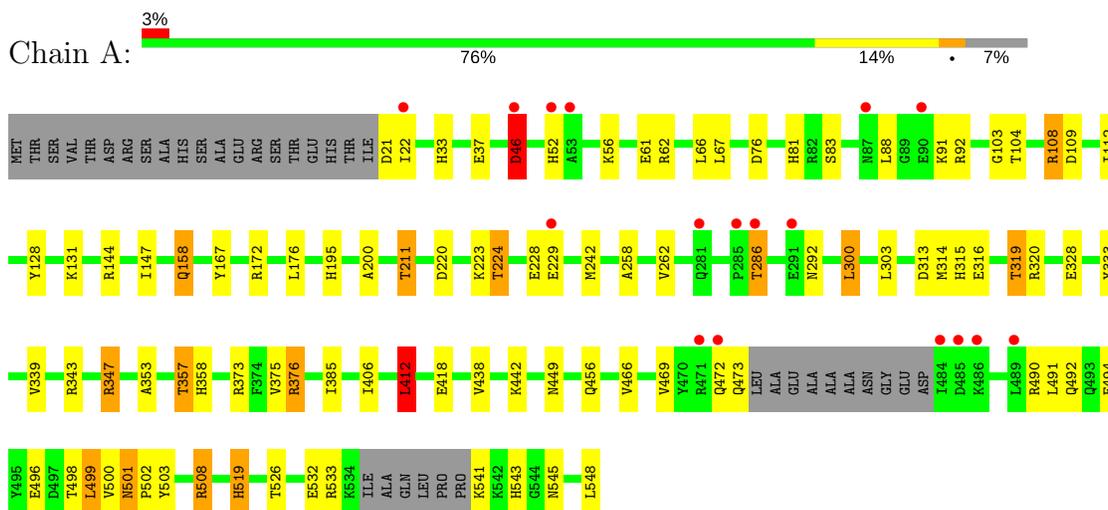
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	271	Total 271	O 271	0	0
2	E	307	Total 307	O 307	0	0
2	F	274	Total 274	O 274	0	0

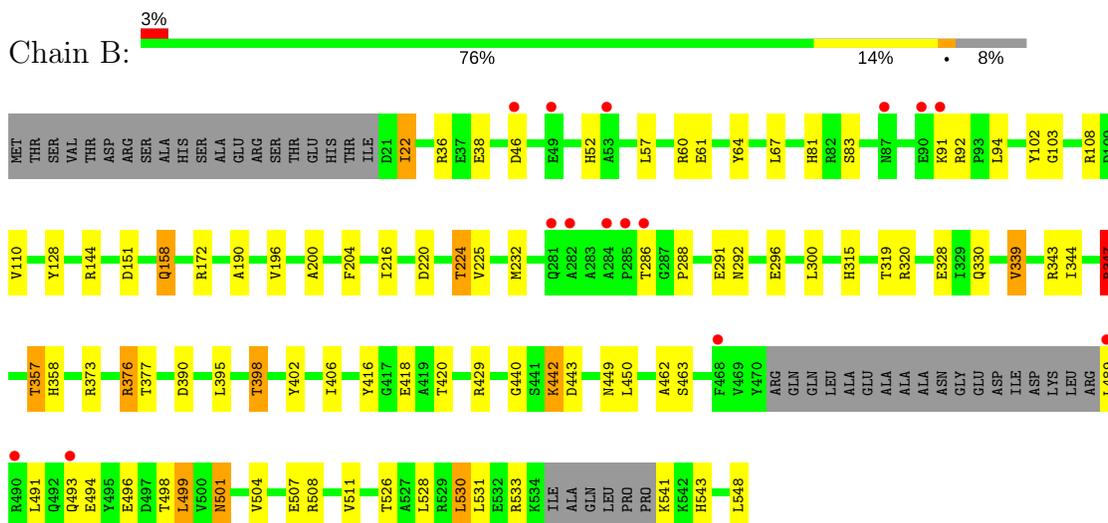
3 Residue-property plots [i](#)

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: PROPIONYL-COA CARBOXYLASE BETA CHAIN 5

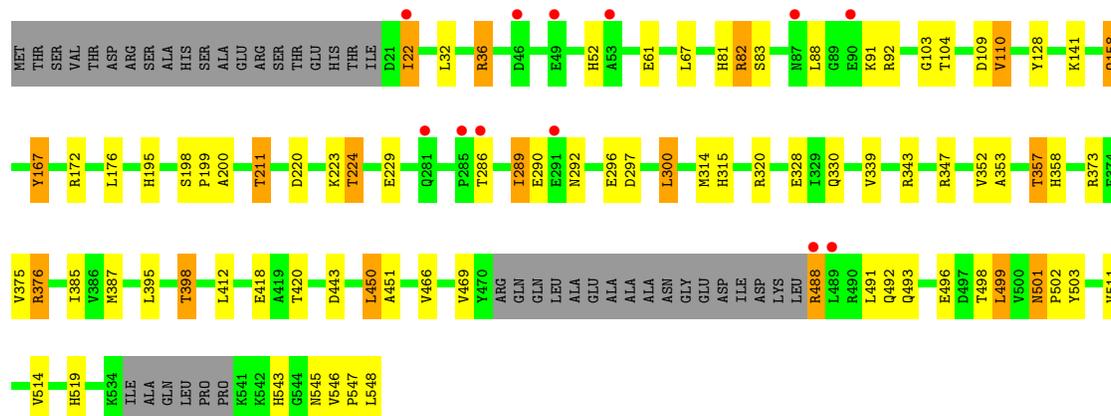


• Molecule 1: PROPIONYL-COA CARBOXYLASE BETA CHAIN 5



• Molecule 1: PROPIONYL-COA CARBOXYLASE BETA CHAIN 5





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.56Å 173.56Å 339.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.09 – 2.20 32.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.09-2.20) 96.4 (32.09-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.176 , 0.211 0.179 , 0.212	Depositor DCC
R_{free} test set	13260 reflections (5.57%)	DCC
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24961	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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	0.85	1/4030 (0.0%)	0.90	11/5464 (0.2%)
1	B	0.83	0/3966	0.88	10/5381 (0.2%)
1	C	0.86	1/3938 (0.0%)	0.89	7/5341 (0.1%)
1	D	0.87	0/3948	0.86	6/5354 (0.1%)
1	E	0.86	0/3930	0.88	10/5330 (0.2%)
1	F	0.83	0/3919	0.84	8/5316 (0.2%)
All	All	0.85	2/23731 (0.0%)	0.87	52/32186 (0.2%)

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	D	0	2
1	E	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	234	GLU	CG-CD	8.19	1.64	1.51
1	A	46	ASP	CB-CG	6.09	1.64	1.51

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ARG	NE-CZ-NH2	-12.85	113.87	120.30
1	E	376	ARG	NE-CZ-NH2	-12.65	113.98	120.30
1	B	376	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	376	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	347	ARG	NE-CZ-NH2	-10.99	114.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	292	ASN	Peptide
1	D	498	THR	Peptide
1	E	154	GLY	Peptide

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	3948	0	3917	66	0
1	B	3883	0	3841	55	0
1	C	3862	0	3827	69	0
1	D	3875	0	3839	64	0
1	E	3857	0	3823	60	0
1	F	3846	0	3810	52	0
2	A	280	0	0	12	1
2	B	273	0	0	8	0
2	C	285	0	0	14	0
2	D	271	0	0	15	0
2	E	307	0	0	13	0
2	F	274	0	0	17	0
All	All	24961	0	23057	347	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 7.

The worst 5 of 347 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:399[B]:ASP:OD1	2:C:2222:HOH:O	1.62	1.15
1:E:154:GLY:HA2	2:E:2095:HOH:O	1.47	1.12
1:C:286:THR:HB	1:C:292:ASN:HD21	1.19	1.04
1:E:286:THR:HB	1:E:292:ASN:HD21	1.23	1.03
1:A:158:GLN:H	1:A:158:GLN:HE21	1.09	0.96

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)
2:A:2160:HOH:O	2:A:2160:HOH:O[7_555]	0.33	1.87

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	512/548 (93%)	494 (96%)	16 (3%)	2 (0%)	38	41
1	B	505/548 (92%)	487 (96%)	15 (3%)	3 (1%)	28	29
1	C	501/548 (91%)	482 (96%)	14 (3%)	5 (1%)	18	16
1	D	502/548 (92%)	479 (95%)	22 (4%)	1 (0%)	51	58
1	E	500/548 (91%)	483 (97%)	17 (3%)	0	100	100
1	F	499/548 (91%)	485 (97%)	13 (3%)	1 (0%)	51	58
All	All	3019/3288 (92%)	2910 (96%)	97 (3%)	12 (0%)	38	41

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	B	22	ILE
1	D	293	LEU
1	C	156	ARG
1	C	492	GLN

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	417/439 (95%)	396 (95%)	21 (5%)	28	34
1	B	410/439 (93%)	382 (93%)	28 (7%)	18	20
1	C	406/439 (92%)	378 (93%)	28 (7%)	18	19
1	D	407/439 (93%)	380 (93%)	27 (7%)	19	21
1	E	405/439 (92%)	380 (94%)	25 (6%)	21	24
1	F	404/439 (92%)	375 (93%)	29 (7%)	17	18
All	All	2449/2634 (93%)	2291 (94%)	158 (6%)	20	22

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	511	VAL
1	D	290	GLU
1	F	398	THR
1	C	531	LEU
1	D	60	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	501	ASN
1	D	158	GLN
1	F	315	HIS
1	C	545	ASN
1	D	52	HIS

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	512/548 (93%)	-0.41	17 (3%) 47 44	11, 20, 45, 73	0
1	B	504/548 (91%)	-0.49	15 (2%) 51 48	12, 21, 43, 64	0
1	C	506/548 (92%)	-0.53	13 (2%) 56 54	12, 20, 46, 66	0
1	D	508/548 (92%)	-0.54	13 (2%) 56 54	11, 19, 47, 71	0
1	E	506/548 (92%)	-0.58	8 (1%) 72 70	12, 19, 41, 62	0
1	F	505/548 (92%)	-0.46	12 (2%) 59 57	14, 21, 43, 64	0
All	All	3041/3288 (92%)	-0.50	78 (2%) 56 54	11, 20, 44, 73	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	286	THR	7.0
1	A	286	THR	6.6
1	D	286	THR	6.3
1	F	286	THR	6.1
1	C	286	THR	5.6

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.