



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MFM  
Title : Crystal Structures and Mutational Analyses of Acyl-CoA Carboxylase Subunit of *Streptomyces coelicolor*  
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Melgar, M.M.  
Deposited on : 2010-04-02  
Resolution : 2.38 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

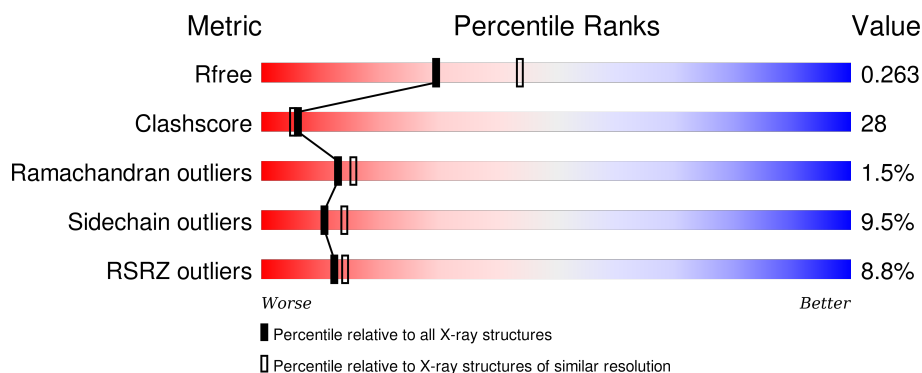
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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))
$R_{free}$	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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  $\geq 3$ , 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	530	<div> <div>11%</div> <div>51%</div> <div>40%</div> <div>8%</div> </div>
1	B	530	<div> <div>11%</div> <div>50%</div> <div>41%</div> <div>7%</div> </div>
1	C	530	<div> <div>7%</div> <div>61%</div> <div>32%</div> <div>5%</div> </div>
1	D	530	<div> <div>8%</div> <div>55%</div> <div>38%</div> <div>5%</div> </div>
1	E	530	<div> <div>6%</div> <div>59%</div> <div>33%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	530	<div><div></div><div>9%</div><div>58%</div><div>35%</div><div>5%</div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23718 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.

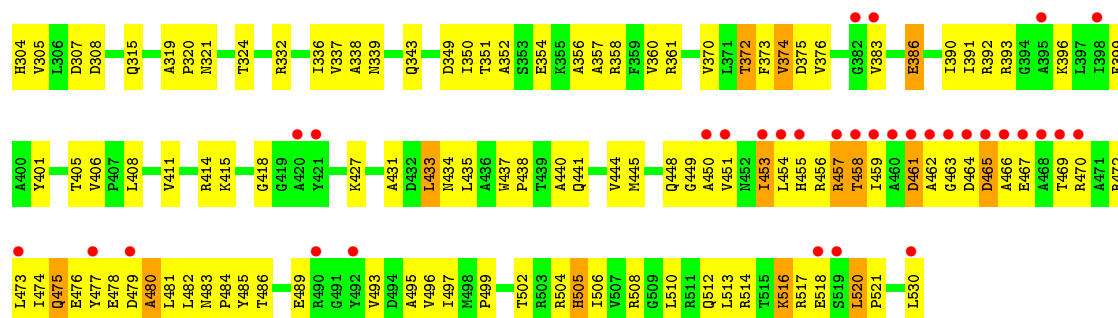
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	F	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	A	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	B	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	D	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	E	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			

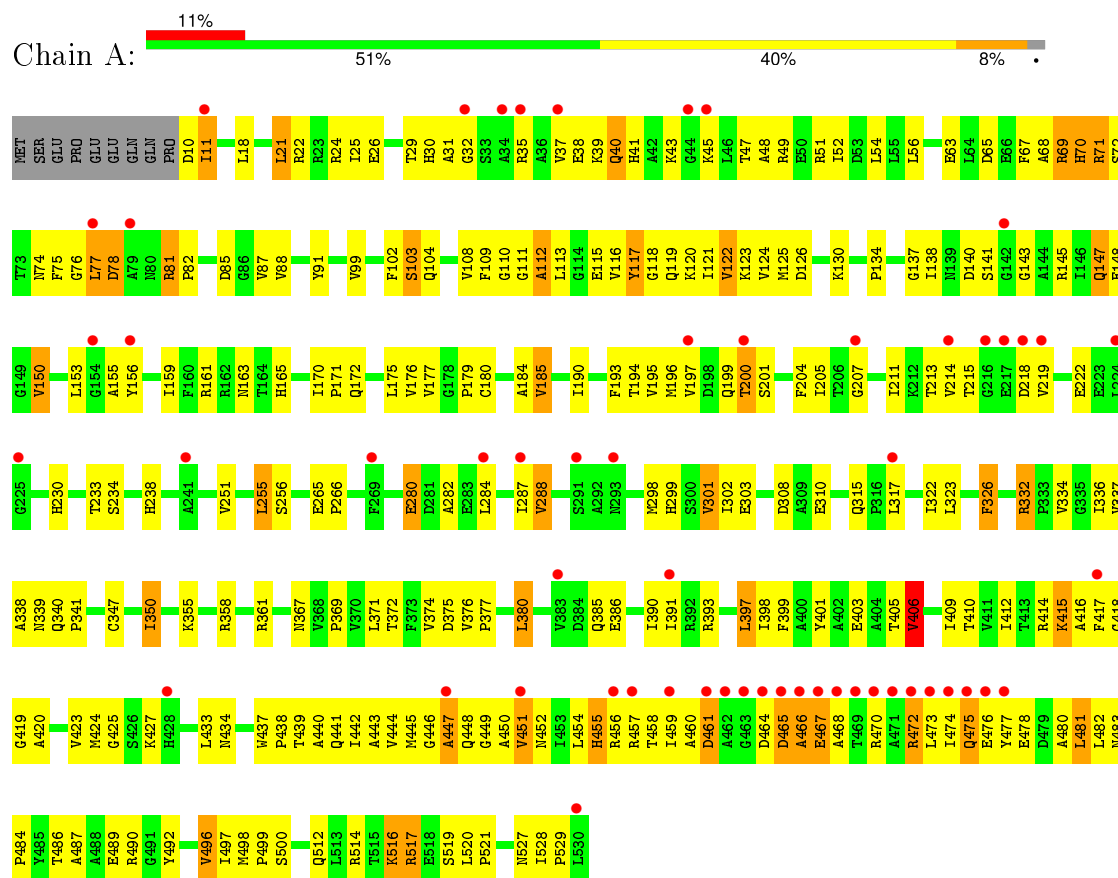
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
F	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
A	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
B	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
D	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
E	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7

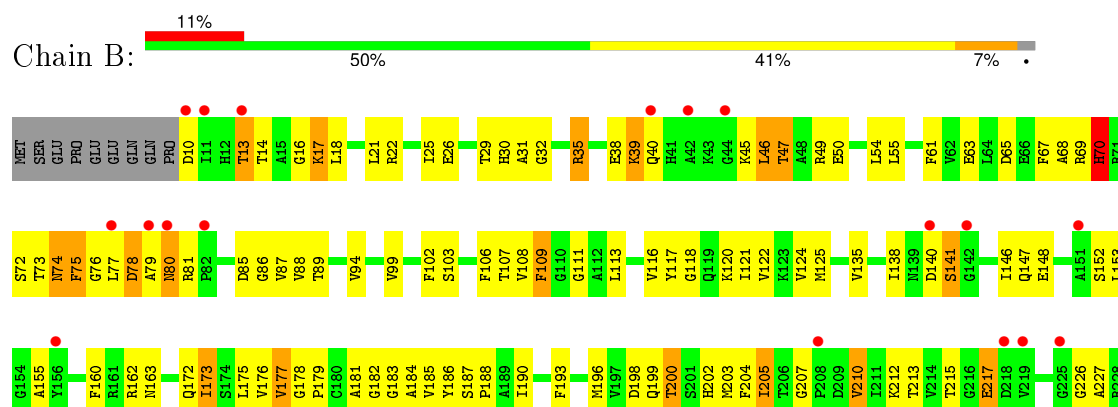




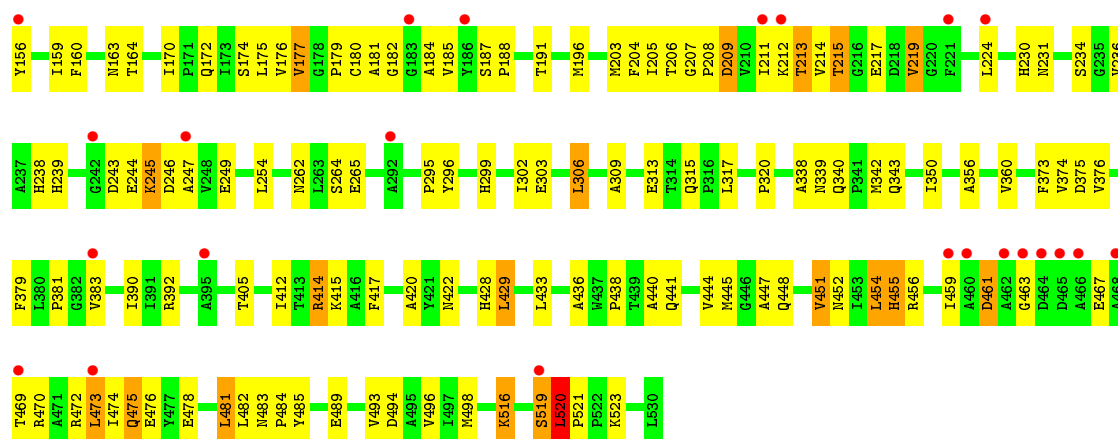
• Molecule 1: Propionyl-CoA carboxylase complex B subunit



• Molecule 1: Propionyl-CoA carboxylase complex B subunit









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.67Å 220.96Å 136.74Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	38.82 – 2.38 45.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.82-2.38) 99.1 (45.00-2.38)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.224 , 0.268 0.213 , 0.263	Depositor DCC
$R_{free}$ test set	9088 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	1.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 182382 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23718	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.90 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2372e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.42	0/4033	0.61	0/5478
1	B	0.44	0/4033	0.62	0/5478
1	C	0.41	0/4033	0.61	1/5478 (0.0%)
1	D	0.44	0/4033	0.62	1/5478 (0.0%)
1	E	0.41	0/4033	0.60	0/5478
1	F	0.41	0/4033	0.60	0/5478
All	All	0.42	0/24198	0.61	2/32868 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	GLY	N-CA-C	-5.39	99.61	113.10
1	C	109	PHE	N-CA-C	-5.01	97.48	111.00

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	3953	0	3882	310	0
1	B	3953	0	3882	299	0
1	C	3953	0	3882	192	0
1	D	3953	0	3882	218	0
1	E	3953	0	3882	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3953	0	3882	213	0
All	All	23718	0	23292	1319	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 28.

The worst 5 of 1319 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:B:337:VAL:HG21	1:B:401:TYR:OH	1.46	1.15
1:E:69:ARG:HH11	1:E:69:ARG:HG3	1.01	1.13
1:B:35:ARG:HH11	1:B:35:ARG:HG2	1.06	1.13
1:C:520:LEU:HD12	1:C:521:PRO:HD2	1.16	1.12
1:A:163:ASN:HB3	1:A:190:ILE:HD11	1.23	1.11

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	519/530 (98%)	470 (91%)	38 (7%)	11 (2%)	9	9
1	B	519/530 (98%)	455 (88%)	52 (10%)	12 (2%)	8	8
1	C	519/530 (98%)	475 (92%)	37 (7%)	7 (1%)	15	19
1	D	519/530 (98%)	472 (91%)	41 (8%)	6 (1%)	16	21
1	E	519/530 (98%)	476 (92%)	39 (8%)	4 (1%)	24	33
1	F	519/530 (98%)	479 (92%)	33 (6%)	7 (1%)	15	19
All	All	3114/3180 (98%)	2827 (91%)	240 (8%)	47 (2%)	13	15

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	520	LEU
1	F	480	ALA
1	B	75	PHE
1	B	306	LEU
1	D	198	ASP

### 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	412/421 (98%)	361 (88%)	51 (12%)	6	6
1	B	412/421 (98%)	371 (90%)	41 (10%)	9	12
1	C	412/421 (98%)	383 (93%)	29 (7%)	19	27
1	D	412/421 (98%)	377 (92%)	35 (8%)	13	18
1	E	412/421 (98%)	370 (90%)	42 (10%)	9	12
1	F	412/421 (98%)	376 (91%)	36 (9%)	13	17
All	All	2472/2526 (98%)	2238 (90%)	234 (10%)	11	14

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	ASP
1	B	217	GLU
1	E	264	SER
1	A	475	GLN
1	B	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	GLN
1	B	299	HIS
1	E	231	ASN
1	B	80	ASN

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Mol	Chain	Res	Type
1	B	339	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	521/530 (98%)	0.68	56 (10%) 8 9	39, 81, 153, 270	0
1	B	521/530 (98%)	0.70	57 (10%) 7 9	35, 81, 154, 242	0
1	C	521/530 (98%)	0.50	38 (7%) 18 20	25, 64, 134, 204	0
1	D	521/530 (98%)	0.57	44 (8%) 14 16	23, 63, 139, 258	0
1	E	521/530 (98%)	0.54	33 (6%) 23 27	26, 65, 137, 192	0
1	F	521/530 (98%)	0.59	47 (9%) 12 13	25, 64, 138, 266	0
All	All	3126/3180 (98%)	0.60	275 (8%) 12 14	23, 70, 143, 270	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	459	ILE	8.5
1	F	460	ALA	8.0
1	D	459	ILE	7.6
1	F	383	VAL	7.5
1	E	466	ALA	7.5

### 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.