



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4FB8
Title : Crystal Structure of apo Acyl-CoA Carboxylase
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Deposited on : 2012-05-22
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
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

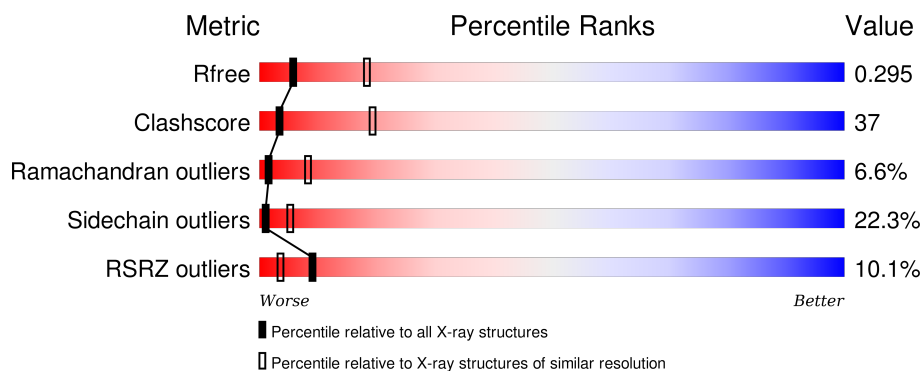
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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	473	<div> <div>11%</div> <div>35%</div> <div>44%</div> <div>11%</div> <div>8%</div> </div>
1	B	473	<div> <div>8%</div> <div>31%</div> <div>46%</div> <div>13%</div> <div>10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6220 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 Probable propionyl-CoA carboxylase beta chain 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3135	1959	577	585	14			
1	B	427	Total	C	N	O	S	0	0	0
			3080	1933	561	572	14			

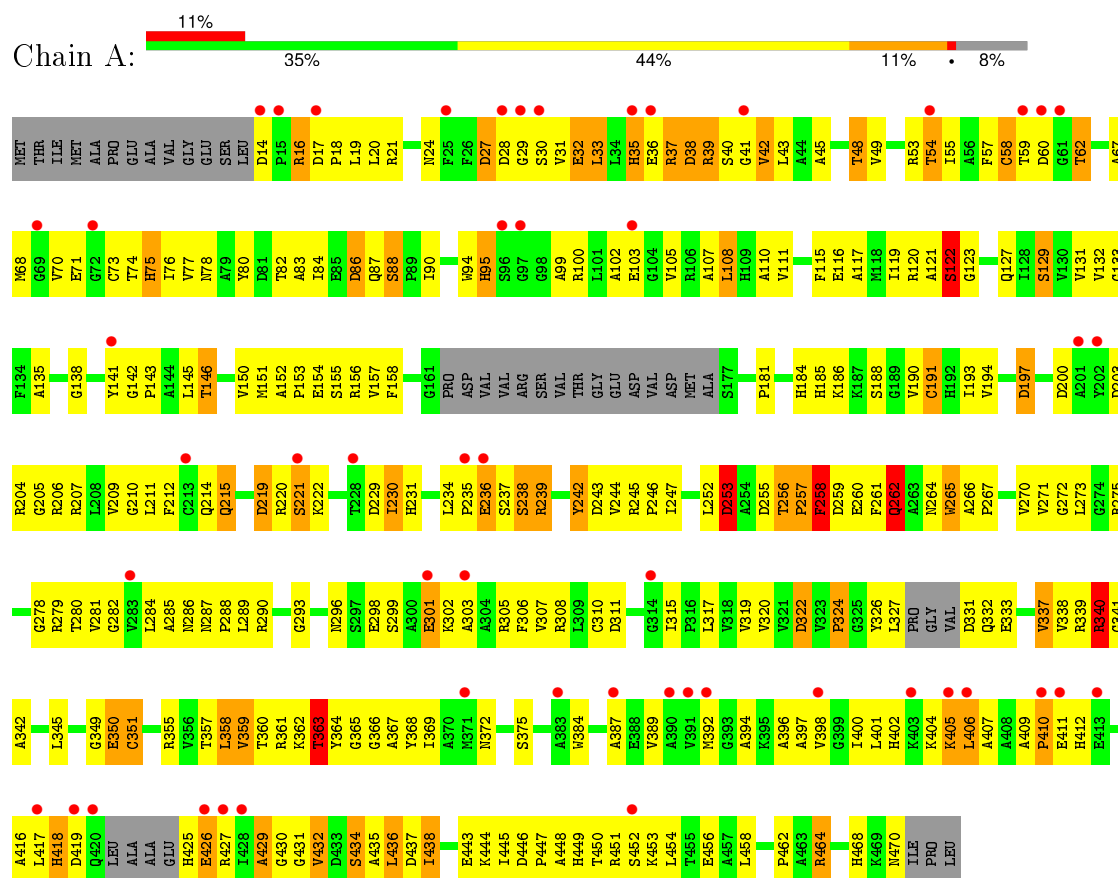
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	3	Total	O	0	0
			3	3		

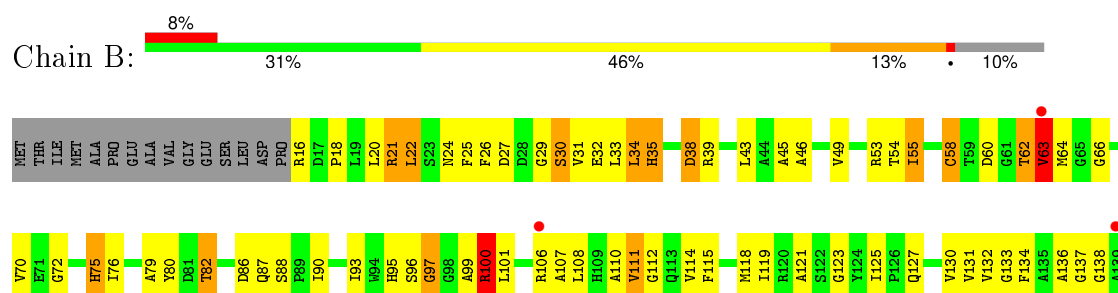
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Probable propionyl-CoA carboxylase beta chain 6



- Molecule 1: Probable propionyl-CoA carboxylase beta chain 6



R464	G393	VAL	P267	D203	A140
R465	A394	ASP	S268	R204	Y141
ARG	R395	Q332	M269	G205	G142
HIS	A396	G335	V270	R206	P143
LYS	V398	G336	V271	R207	A144
ASN	G399	V337	G772	L208	L145
ILE	I400	V338	L273	Y209	T146
PRO	L401	R339	G274	G210	D147
LEU	L402	R340	R275	L211	V148
	H403	G341	L276	F212	
	R404	G342	S277	C213	M151
	K405	K343	G278	Q214	A152
	L406	L344	R279	Q215	P153
	A408	H346	T280	G216	E154
	A409	A347	V281	H217	S155
	P410	F348	G282	D219	R156
	E411	G349	V283	R220	V157
	H412	E350	L284	S221	F158
	H413	C351	A285	K222	V159
	R414	T352	N286	A223	T160
	E415	V353	P287	E224	G161
	A416	P354	P288	A225	P162
	L417	R355	L289	G226	ASP
	H418		R290	D227	VAL
	D419	L358	L291	T228	VAL
	Q420	V359	C294	D229	ARG
	L421	T360	N295	I230	SER
	A422	R361	N296	H231	VAL
	A423	K362	S297	A232	THR
	E424	T363	E298	L233	GLY
	R425	Y364	S299	LEU	GIU
	E426	G365	A300	PRO	ASP
	R427	G366	E301	GLU	VAL
	I428	A367	K302	SER	ASP
	A429	Y368	A303	SER	MET
	G430	I369	L304	ARG	ALA
	G431	A370	R305	ARG	S177
	V432	N371	F306	A241	L178
	D433	S372	V307	Y242	G179
	A435	R373	R308	D243	G180
	L436	S374	L309	V244	P181
	D437	S375	C310	R245	E182
	I438	L376	D311	P246	T183
	V441	N377	A312	I247	H184
	D442	A378	F313	V248	H185
	E443	T379	P316		
	K444	K380	V320		S188
	L445	V381	V321	I251	G189
	A448	P385	D322	L252	V190
	R451	D386	V323	D253	C191
	S452	A387	P324	A254	H192
	R453	E388	G325	D255	I193
	L454	V389	Y326	F258	V194
		A390	L327	D259	A195
		V391	P328	E260	D196
		M392	G329	F261	D197
				Q262	D200
				A263	A201
				N264	Y202

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.28Å 82.36Å 157.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.85 – 3.00 46.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.85-3.00) 93.3 (46.85-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.233 , 0.304 0.234 , 0.295	Depositor DCC
R_{free} test set	1041 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.0	EDS
Estimated twinning fraction	0.479 for K,H,-L 0.429 for k,h,-l	Xtriage
Reported twinning fraction	0.479 for K,H,-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20652 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6220	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 32.14 % 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 9.8635e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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	0.39	0/3191	0.63	0/4337
1	B	0.39	0/3137	0.64	0/4267
All	All	0.39	0/6328	0.63	0/8604

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	THR	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	3135	0	3012	230	1
1	B	3080	0	2982	236	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
All	All	6220	0	5994	447	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 37.

The worst 5 of 447 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:258:PHE:N	1:A:259:ASP:HB2	1.58	1.19
1:A:258:PHE:CD1	1:A:260:GLU:HB3	1.89	1.07
1:A:258:PHE:CA	1:A:259:ASP:HB2	1.85	1.04
1:A:257:PRO:O	1:A:258:PHE:HB2	1.60	0.98
1:A:258:PHE:CE1	1:A:260:GLU:HB3	2.02	0.95

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)
1:A:102:ALA:O	1:A:405:LYS:NZ[2_555]	2.06	0.14

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	427/473 (90%)	321 (75%)	76 (18%)	30 (7%)	1	7
1	B	419/473 (89%)	309 (74%)	84 (20%)	26 (6%)	2	10
All	All	846/946 (89%)	630 (74%)	160 (19%)	56 (7%)	1	8

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	87	GLN
1	A	95	HIS
1	A	122	SER
1	A	253	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	301/362 (83%)	237 (79%)	64 (21%)	1	6
1	B	296/362 (82%)	227 (77%)	69 (23%)	1	4
All	All	597/724 (82%)	464 (78%)	133 (22%)	1	5

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	ILE
1	B	87	GLN
1	B	421	LEU
1	A	452	SER
1	B	38	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN

5.3.3 RNA ⓘ

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	435/473 (91%)	0.65	51 (11%) 6 2	13, 50, 87, 139	0
1	B	427/473 (90%)	0.52	36 (8%) 14 5	6, 44, 89, 123	0
All	All	862/946 (91%)	0.59	87 (10%) 9 3	6, 47, 88, 139	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	GLU	8.5
1	A	428	ILE	7.3
1	A	398	VAL	6.3
1	A	72	GLY	5.6
1	B	429	ALA	5.2

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.