



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 3, 2019 – 08:55 PM EST

PDB ID : 6G2D
EMDB ID: : EMD-4342
Title : Citrate-induced acetyl-CoA carboxylase (ACC-Cit) filament at 5.4 Å resolution
Authors : Hunkeler, M.; Hagmann, A.; Stüttfeld, E.; Chami, M.; Stahlberg, H.; Maier, T.
Deposited on : 2018-03-23
Resolution : 5.40 Å (reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

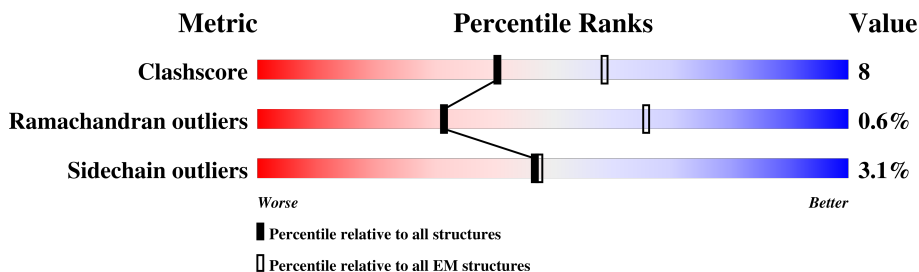
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	2407	
1	C	2407	
1	D	2407	
1	F	2407	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 88169 atoms, of which 43991 are hydrogens and 0 are deuteriums.

In the tables below, 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 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	625	Total	C	H	N	O	S	0	0
			10226	3267	5114	888	922	35		
1	C	2121	Total	C	H	N	O	S	0	0
			33781	10771	16841	2945	3124	100		
1	D	2121	Total	C	H	N	O	S	0	0
			33782	10771	16842	2945	3124	100		
1	F	634	Total	C	H	N	O	S	0	0
			10380	3310	5194	905	936	35		

There are 244 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-60	MET	-	initiating methionine	UNP Q13085
B	-59	ALA	-	expression tag	UNP Q13085
B	-58	HIS	-	expression tag	UNP Q13085
B	-57	HIS	-	expression tag	UNP Q13085
B	-56	HIS	-	expression tag	UNP Q13085
B	-55	HIS	-	expression tag	UNP Q13085
B	-54	HIS	-	expression tag	UNP Q13085
B	-53	HIS	-	expression tag	UNP Q13085
B	-52	HIS	-	expression tag	UNP Q13085
B	-51	HIS	-	expression tag	UNP Q13085
B	-50	HIS	-	expression tag	UNP Q13085
B	-49	HIS	-	expression tag	UNP Q13085
B	-48	GLY	-	expression tag	UNP Q13085
B	-47	SER	-	expression tag	UNP Q13085
B	-46	THR	-	expression tag	UNP Q13085
B	-45	SER	-	expression tag	UNP Q13085
B	-44	GLY	-	expression tag	UNP Q13085
B	-43	SER	-	expression tag	UNP Q13085
B	-42	GLY	-	expression tag	UNP Q13085
B	-41	GLU	-	expression tag	UNP Q13085
B	-40	GLN	-	expression tag	UNP Q13085
B	-39	LYS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	LEU	-	expression tag	UNP Q13085
B	-37	ILE	-	expression tag	UNP Q13085
B	-36	SER	-	expression tag	UNP Q13085
B	-35	GLU	-	expression tag	UNP Q13085
B	-34	GLU	-	expression tag	UNP Q13085
B	-33	ASP	-	expression tag	UNP Q13085
B	-32	LEU	-	expression tag	UNP Q13085
B	-31	GLY	-	expression tag	UNP Q13085
B	-30	SER	-	expression tag	UNP Q13085
B	-29	THR	-	expression tag	UNP Q13085
B	-28	SER	-	expression tag	UNP Q13085
B	-27	GLY	-	expression tag	UNP Q13085
B	-26	SER	-	expression tag	UNP Q13085
B	-25	GLY	-	expression tag	UNP Q13085
B	-24	ASP	-	expression tag	UNP Q13085
B	-23	TYR	-	expression tag	UNP Q13085
B	-22	LYS	-	expression tag	UNP Q13085
B	-21	ASP	-	expression tag	UNP Q13085
B	-20	ASP	-	expression tag	UNP Q13085
B	-19	ASP	-	expression tag	UNP Q13085
B	-18	ASP	-	expression tag	UNP Q13085
B	-17	LYS	-	expression tag	UNP Q13085
B	-16	LEU	-	expression tag	UNP Q13085
B	-15	THR	-	expression tag	UNP Q13085
B	-14	SER	-	expression tag	UNP Q13085
B	-13	LEU	-	expression tag	UNP Q13085
B	-12	TYR	-	expression tag	UNP Q13085
B	-11	LYS	-	expression tag	UNP Q13085
B	-10	LYS	-	expression tag	UNP Q13085
B	-9	ALA	-	expression tag	UNP Q13085
B	-8	GLY	-	expression tag	UNP Q13085
B	-7	LEU	-	expression tag	UNP Q13085
B	-6	GLU	-	expression tag	UNP Q13085
B	-5	ASN	-	expression tag	UNP Q13085
B	-4	LEU	-	expression tag	UNP Q13085
B	-3	TYR	-	expression tag	UNP Q13085
B	-2	PHE	-	expression tag	UNP Q13085
B	-1	GLN	-	expression tag	UNP Q13085
B	0	GLY	-	expression tag	UNP Q13085
C	-60	MET	-	initiating methionine	UNP Q13085
C	-59	ALA	-	expression tag	UNP Q13085
C	-58	HIS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-57	HIS	-	expression tag	UNP Q13085
C	-56	HIS	-	expression tag	UNP Q13085
C	-55	HIS	-	expression tag	UNP Q13085
C	-54	HIS	-	expression tag	UNP Q13085
C	-53	HIS	-	expression tag	UNP Q13085
C	-52	HIS	-	expression tag	UNP Q13085
C	-51	HIS	-	expression tag	UNP Q13085
C	-50	HIS	-	expression tag	UNP Q13085
C	-49	HIS	-	expression tag	UNP Q13085
C	-48	GLY	-	expression tag	UNP Q13085
C	-47	SER	-	expression tag	UNP Q13085
C	-46	THR	-	expression tag	UNP Q13085
C	-45	SER	-	expression tag	UNP Q13085
C	-44	GLY	-	expression tag	UNP Q13085
C	-43	SER	-	expression tag	UNP Q13085
C	-42	GLY	-	expression tag	UNP Q13085
C	-41	GLU	-	expression tag	UNP Q13085
C	-40	GLN	-	expression tag	UNP Q13085
C	-39	LYS	-	expression tag	UNP Q13085
C	-38	LEU	-	expression tag	UNP Q13085
C	-37	ILE	-	expression tag	UNP Q13085
C	-36	SER	-	expression tag	UNP Q13085
C	-35	GLU	-	expression tag	UNP Q13085
C	-34	GLU	-	expression tag	UNP Q13085
C	-33	ASP	-	expression tag	UNP Q13085
C	-32	LEU	-	expression tag	UNP Q13085
C	-31	GLY	-	expression tag	UNP Q13085
C	-30	SER	-	expression tag	UNP Q13085
C	-29	THR	-	expression tag	UNP Q13085
C	-28	SER	-	expression tag	UNP Q13085
C	-27	GLY	-	expression tag	UNP Q13085
C	-26	SER	-	expression tag	UNP Q13085
C	-25	GLY	-	expression tag	UNP Q13085
C	-24	ASP	-	expression tag	UNP Q13085
C	-23	TYR	-	expression tag	UNP Q13085
C	-22	LYS	-	expression tag	UNP Q13085
C	-21	ASP	-	expression tag	UNP Q13085
C	-20	ASP	-	expression tag	UNP Q13085
C	-19	ASP	-	expression tag	UNP Q13085
C	-18	ASP	-	expression tag	UNP Q13085
C	-17	LYS	-	expression tag	UNP Q13085
C	-16	LEU	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	THR	-	expression tag	UNP Q13085
C	-14	SER	-	expression tag	UNP Q13085
C	-13	LEU	-	expression tag	UNP Q13085
C	-12	TYR	-	expression tag	UNP Q13085
C	-11	LYS	-	expression tag	UNP Q13085
C	-10	LYS	-	expression tag	UNP Q13085
C	-9	ALA	-	expression tag	UNP Q13085
C	-8	GLY	-	expression tag	UNP Q13085
C	-7	LEU	-	expression tag	UNP Q13085
C	-6	GLU	-	expression tag	UNP Q13085
C	-5	ASN	-	expression tag	UNP Q13085
C	-4	LEU	-	expression tag	UNP Q13085
C	-3	TYR	-	expression tag	UNP Q13085
C	-2	PHE	-	expression tag	UNP Q13085
C	-1	GLN	-	expression tag	UNP Q13085
C	0	GLY	-	expression tag	UNP Q13085
D	-60	MET	-	initiating methionine	UNP Q13085
D	-59	ALA	-	expression tag	UNP Q13085
D	-58	HIS	-	expression tag	UNP Q13085
D	-57	HIS	-	expression tag	UNP Q13085
D	-56	HIS	-	expression tag	UNP Q13085
D	-55	HIS	-	expression tag	UNP Q13085
D	-54	HIS	-	expression tag	UNP Q13085
D	-53	HIS	-	expression tag	UNP Q13085
D	-52	HIS	-	expression tag	UNP Q13085
D	-51	HIS	-	expression tag	UNP Q13085
D	-50	HIS	-	expression tag	UNP Q13085
D	-49	HIS	-	expression tag	UNP Q13085
D	-48	GLY	-	expression tag	UNP Q13085
D	-47	SER	-	expression tag	UNP Q13085
D	-46	THR	-	expression tag	UNP Q13085
D	-45	SER	-	expression tag	UNP Q13085
D	-44	GLY	-	expression tag	UNP Q13085
D	-43	SER	-	expression tag	UNP Q13085
D	-42	GLY	-	expression tag	UNP Q13085
D	-41	GLU	-	expression tag	UNP Q13085
D	-40	GLN	-	expression tag	UNP Q13085
D	-39	LYS	-	expression tag	UNP Q13085
D	-38	LEU	-	expression tag	UNP Q13085
D	-37	ILE	-	expression tag	UNP Q13085
D	-36	SER	-	expression tag	UNP Q13085
D	-35	GLU	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-34	GLU	-	expression tag	UNP Q13085
D	-33	ASP	-	expression tag	UNP Q13085
D	-32	LEU	-	expression tag	UNP Q13085
D	-31	GLY	-	expression tag	UNP Q13085
D	-30	SER	-	expression tag	UNP Q13085
D	-29	THR	-	expression tag	UNP Q13085
D	-28	SER	-	expression tag	UNP Q13085
D	-27	GLY	-	expression tag	UNP Q13085
D	-26	SER	-	expression tag	UNP Q13085
D	-25	GLY	-	expression tag	UNP Q13085
D	-24	ASP	-	expression tag	UNP Q13085
D	-23	TYR	-	expression tag	UNP Q13085
D	-22	LYS	-	expression tag	UNP Q13085
D	-21	ASP	-	expression tag	UNP Q13085
D	-20	ASP	-	expression tag	UNP Q13085
D	-19	ASP	-	expression tag	UNP Q13085
D	-18	ASP	-	expression tag	UNP Q13085
D	-17	LYS	-	expression tag	UNP Q13085
D	-16	LEU	-	expression tag	UNP Q13085
D	-15	THR	-	expression tag	UNP Q13085
D	-14	SER	-	expression tag	UNP Q13085
D	-13	LEU	-	expression tag	UNP Q13085
D	-12	TYR	-	expression tag	UNP Q13085
D	-11	LYS	-	expression tag	UNP Q13085
D	-10	LYS	-	expression tag	UNP Q13085
D	-9	ALA	-	expression tag	UNP Q13085
D	-8	GLY	-	expression tag	UNP Q13085
D	-7	LEU	-	expression tag	UNP Q13085
D	-6	GLU	-	expression tag	UNP Q13085
D	-5	ASN	-	expression tag	UNP Q13085
D	-4	LEU	-	expression tag	UNP Q13085
D	-3	TYR	-	expression tag	UNP Q13085
D	-2	PHE	-	expression tag	UNP Q13085
D	-1	GLN	-	expression tag	UNP Q13085
D	0	GLY	-	expression tag	UNP Q13085
F	-60	MET	-	initiating methionine	UNP Q13085
F	-59	ALA	-	expression tag	UNP Q13085
F	-58	HIS	-	expression tag	UNP Q13085
F	-57	HIS	-	expression tag	UNP Q13085
F	-56	HIS	-	expression tag	UNP Q13085
F	-55	HIS	-	expression tag	UNP Q13085
F	-54	HIS	-	expression tag	UNP Q13085

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-53	HIS	-	expression tag	UNP Q13085
F	-52	HIS	-	expression tag	UNP Q13085
F	-51	HIS	-	expression tag	UNP Q13085
F	-50	HIS	-	expression tag	UNP Q13085
F	-49	HIS	-	expression tag	UNP Q13085
F	-48	GLY	-	expression tag	UNP Q13085
F	-47	SER	-	expression tag	UNP Q13085
F	-46	THR	-	expression tag	UNP Q13085
F	-45	SER	-	expression tag	UNP Q13085
F	-44	GLY	-	expression tag	UNP Q13085
F	-43	SER	-	expression tag	UNP Q13085
F	-42	GLY	-	expression tag	UNP Q13085
F	-41	GLU	-	expression tag	UNP Q13085
F	-40	GLN	-	expression tag	UNP Q13085
F	-39	LYS	-	expression tag	UNP Q13085
F	-38	LEU	-	expression tag	UNP Q13085
F	-37	ILE	-	expression tag	UNP Q13085
F	-36	SER	-	expression tag	UNP Q13085
F	-35	GLU	-	expression tag	UNP Q13085
F	-34	GLU	-	expression tag	UNP Q13085
F	-33	ASP	-	expression tag	UNP Q13085
F	-32	LEU	-	expression tag	UNP Q13085
F	-31	GLY	-	expression tag	UNP Q13085
F	-30	SER	-	expression tag	UNP Q13085
F	-29	THR	-	expression tag	UNP Q13085
F	-28	SER	-	expression tag	UNP Q13085
F	-27	GLY	-	expression tag	UNP Q13085
F	-26	SER	-	expression tag	UNP Q13085
F	-25	GLY	-	expression tag	UNP Q13085
F	-24	ASP	-	expression tag	UNP Q13085
F	-23	TYR	-	expression tag	UNP Q13085
F	-22	LYS	-	expression tag	UNP Q13085
F	-21	ASP	-	expression tag	UNP Q13085
F	-20	ASP	-	expression tag	UNP Q13085
F	-19	ASP	-	expression tag	UNP Q13085
F	-18	ASP	-	expression tag	UNP Q13085
F	-17	LYS	-	expression tag	UNP Q13085
F	-16	LEU	-	expression tag	UNP Q13085
F	-15	THR	-	expression tag	UNP Q13085
F	-14	SER	-	expression tag	UNP Q13085
F	-13	LEU	-	expression tag	UNP Q13085
F	-12	TYR	-	expression tag	UNP Q13085

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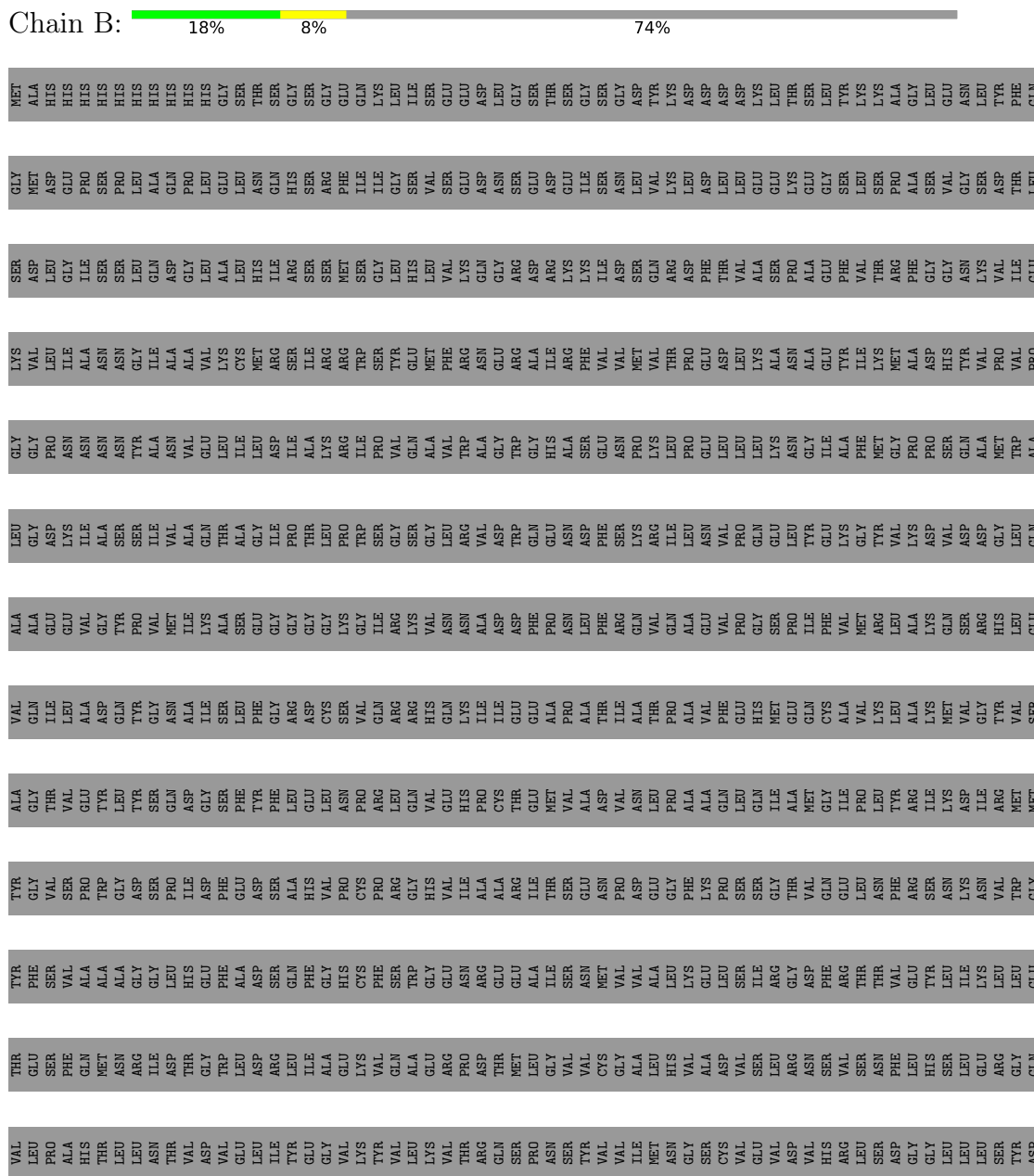
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	LYS	-	expression tag	UNP Q13085
F	-10	LYS	-	expression tag	UNP Q13085
F	-9	ALA	-	expression tag	UNP Q13085
F	-8	GLY	-	expression tag	UNP Q13085
F	-7	LEU	-	expression tag	UNP Q13085
F	-6	GLU	-	expression tag	UNP Q13085
F	-5	ASN	-	expression tag	UNP Q13085
F	-4	LEU	-	expression tag	UNP Q13085
F	-3	TYR	-	expression tag	UNP Q13085
F	-2	PHE	-	expression tag	UNP Q13085
F	-1	GLN	-	expression tag	UNP Q13085
F	0	GLY	-	expression tag	UNP Q13085

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Acetyl-CoA carboxylase 1



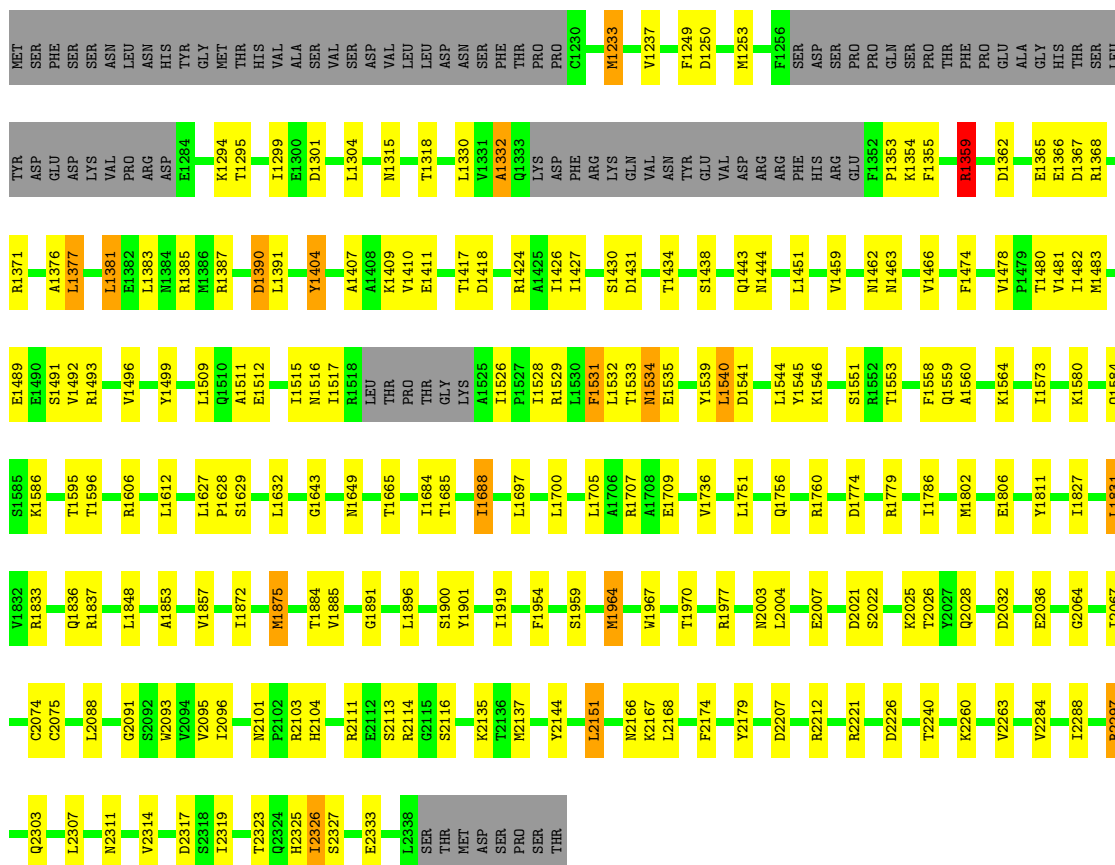
LEU	ALA	GLY	MET	GLU	TRP	D1541	F1421	I1324	G1230	M1164	Q1047	ALA	GLN	ALA	GLN	GLY
ASN	LEU	PRO	PHE	GLY	GLU	I1542	R1424	L1330	V1237	M1165	L1048	THR	SER	THR	SER	SER
ASN	LEU	ASN	HIS	ARG	ASN	S1543	R1424	L1330	V1237	S1166	L1048	THR	THR	ASN	THR	THR
LYS	VAL	VAL	ALA	ASP	MET	L1544	R1428	A1332	F1249	V1166	G1050	ARG	ALA	VAL	GLU	TRR
PRO	LEU	ARG	TRP	ILE	THR	K1546	R1428	O1333	F1249	Q1167	G1050	LYS	ARG	VAL	LEU	TRR
ILE	GLY	VAL	VAL	VAL	GLN		D1431	LYS	M1253	L1171	L1055	LYS	ARG	MET	GLY	TRR
ASP	ASP	ASP	ASP	ILE	ALA	T1549	L1432	ASP	M1253	L1172	D1057	GLU	GLY	LYS	GLY	TRR
SER	GLY	PRO	PRO	GLY	PHE	ASP	L1432	PHE	F1256	K1172	D1057	SER	GLY	MET	GLY	MET
ILE	ASN	LEU	GLU	ASN	LEU	SER	S1438	ARG	F1256	D1173	L1058	ARG	K948	VAL	VAL	GLY
ASP	ASP	ASP	ASP	ASP	PRO	ARG	S1438	LYS	ASP	V1177	L1060	LYS	V960	THR	GLU	GLY
PRO	ILE	ILE	PRO	ILE	SER	THR	L1442	GLN	SER		N1061	THR	H850	LEU	VAL	VAL
THR	THR	THR	TYR	THR	PRO	A1554	Q1443	VAL	PRO	F1180	T1064	ASP	V856	THR	ASP	ASP
LYS	GLY	PRO	LYS	TYR	PRO	Q1559	N1444	ASN	PRO	Q1181	T1064	THR	L857	ALA	ARG	ARG
ASN	ASN	ASN	GLY	ARG	LEU	Q1559	N1444	TYR	GLN	M1181	E1065	THR	D858	VAL	TRR	TRR
THR	GLN	THR	TYR	ILE	PRO	A1560	A1460	GLU	SER	L1184	L1066	GLY	N859	VAL	GLU	GLU
LEU	LEU	GLY	TYR	GLY	SER	TYR	A1460	VAL	PRO		T1067	ARG		SER	LEU	LEU
ASP	GLY	GLY	TYR	SER	ASP	GLY	M1463	ASP	THR	S1187	Q1068	LYS	M864	GLY	THR	THR
MET	PHE	MET	LEU	PHE	MET	ASP	M1463	ARG	PHE	H1188	Q1068	GLU		CYS	CYS	ILE
GLY	GLY	GLY	GLY	GLY	LEU	K1564	V1466	ARG	PRO	PRO	T1073	THR	F874	ILE	ILE	GLY
ASN	ASN	TYR	ASN	TYR	THR		V1466	PHE	GLU	ASN	N1074	THR	L971	HIS	ASN	ASN
THR	GLU	GLU	ILE	GLU	THR	L1568	M1471	HIS	ALA	ARG		VAL	V878	LYS	LYS	LYS
PRO	GLY	PRO	PRO	GLU	THR		M1471	ARG	GLY	GLY	A1077	THR		VAL	THR	THR
GLN	ILE	GLN	GLN	ASP	GLU	P1576	F1474	GLU	HIS	ASN	A1078	LYS	V882	CYS	CYS	CYS
ASP	ILE	ASP	ASP	LEU	LEU	Y1577	F1352	THR	GLY	ILE	L1079	VAL	E883	ARG	VAL	VAL
LEU	SER	TYR	TYR	LEU	VAL	Y1577	T1480	THR	SER	PRO	L1079	ARG	E884	PRO	PHE	PHE
VAL	GLY	LEU	LYS	PHE	LEU	T1579	V1481	LEU	LEU	THR	A1087	GLY	L885	GLY	GLY	GLY
VAL	VAL	VAL	VAL	LEU	ASP	K1580	I1482	F1355	TYR	LEU		ALA	M886	ALA	LYS	LYS
ARG	THR	THR	VAL	ARG	ASP	ASP	V1492	R1359	ASP	ASN	L1090	ALA		ALA	GLY	GLY
ALA	CYS	SER	SER	ALA	GLN	LEU	V1492	R1359	GLU	ARG	L1090	LEU	L889	LEU	ASN	ASN
ARG	ARG	ALA	ALA	SER	GLY	LEU	V1496	A1360	ASP	MET	P1091	ASP	L891	ASP	ASP	ASP
ALA	ALA	LEU	LEU	GLU	GLN	LEU	V1496	A1360	ASP	SER	S1092	THR	L991	THR	LEU	ASN
ASN	ASN	ASN	LEU	GLU	LEU	GLN	V1496	E1365	LYS	MET	S1092	PRO	L991	PRO	PRO	PRO
VAL	VAL	ASN	LEU	LEU	LEU	SER	V1496	E1365	VAL	PHE	E1093	GLY	P892	GLY	GLY	ASN
CYS	CYS	VAL	VAL	ALA	VAL	LYS	L1506	E1366								

[illegible]

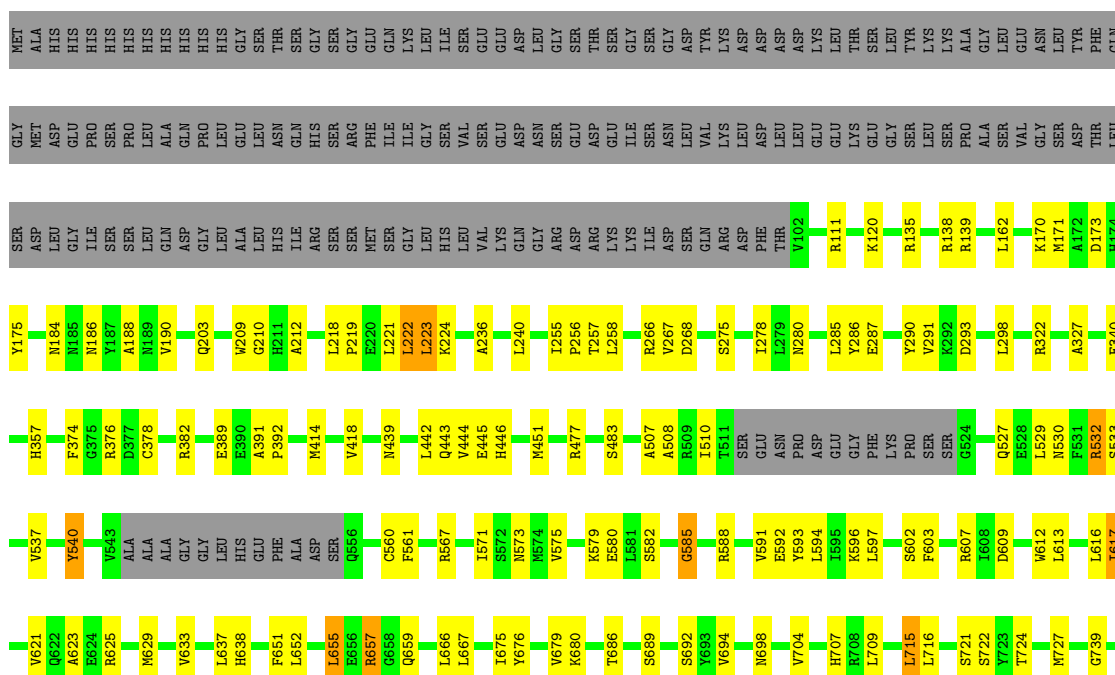
- Molecule 1: Acetyl-CoA carboxylase 1

Chain C: 70% 16% • 12%

[illegible]



- Molecule 1: Acetyl-CoA carboxylase 1



ASP	PHE	F1180	M1074	S938	GLN	ALA	GLY	VAL	THR	TYR	TYR	ALA	ALA	VAL	ALA	LEU	GLY	LYS
ARG	F1181	Q1182	L1079	Q939	THR	ILE	SER	PRO	GLU	SER	PHE	THR	ALA	GLU	ALA	ASP	GLY	VAL
LYS	H1183			N943	ALA	VAL	TYR	ALA	GLU	VAL	VAL	GLU	GLU	GLU	GLU	ASP	ASN	ILE
GLN			R1082	Q1083	LEU	VAL	THR	THR	THR	ALA	ALA	TYR	GLU	GLY	GLY	ALA	ASN	ALA
VAL	PRO		Q1083	S947	ARG	MET	THR	THR	THR	ALA	TRP	TYR	ASP	GLY	ASP	ALA	ASN	ASN
ASN	ASN		A1087	A950	GLY	LYS	TYR	LEU	ASN	ALA	GLY	LEU	GLN	TYR	GLN	SER	ASN	ASN
GLU	ARG			T951	GLU	MET	LYS	ASN	ILE	GLY	SER	TYR	GLY	VAL	VAL	ASN	ASN	ILE
ASN	GLY		L1090	L952	VAL	VAL	GLU	THR	THR	HIS	ILE	GLN	ASN	MET	VAL	VAL	ALA	ALA
ASP	THR		P1091	M963	THR	LEU	GLU	VAL	THR	GLU	ASP	GLY	ILE	ILE	ILE	VAL	VAL	ALA
ARG	PHE		S1092	N964	THR	THR	ASP	VAL	TRP	PHE	PHE	SER	SER	SER	LYS	GLU	VAL	VAL
ARG	PRO		Y1093	N964	ALA	ALA	GLU	GLU	LEU	ALA	ALA	PHE	PHE	PHE	LEU	THR	LEU	LYS
ALA	GLU		E1094	T965	VAL	VAL	TYR	LEU	ASP	TYR	ASP	TYR	GLY	GLY	GLY	GLY	ILE	CYS
HIS	ALA		L1095	Q966	GLU	ARG	ARG	ILE	LEU	SER	PHE	GLY	GLY	GLY	ILE	ASP	ARG	ARG
GLY	GLY		R1096		THR	THR	ILE	TYR	ARG	GLN	ALA	LEU	GLY	ARG	PRO	ILE	ILE	SER
GLU	MET		H1097	V969	SER	SER	ILE	TYR	LEU	GLN	ALA	LEU	GLY	ARG	PRO	ILE	ILE	SER
F1352	THR		M1098	Q970	GLY	GLY	THR	GLU	ILE	PHE	HIS	GLU	GLY	ASP	THR	ALA	ALA	ILE
F1353	PHE		Q1099	L971	CYS	ILE	ILE	GLY	ALA	GLY	VAL	ASN	CYS	GLY	GLY	LEU	LYS	ARG
K1354	SER			V972	ILE	ILE	THR	VAL	GLU	HIS	VAL	ASN	LYS	VAL	TRP	PRO	ARG	ARG
F1355	TYR		S1102		HIS	THR	ASN	TYR	LYS	PHE	CYS	PRO	VAL	ILE	ILE	TRP	ILE	ARG
ASP	ASP			Y975	TYR	TYR	LYS	VAL	VAL	SER	PHE	ARG	GLN	GLY	GLY	VAL	VAL	TYR
R1359	GLU		A1107		VAL	VAL	THR	LEU	GLN	TRP	GLY	GLN	ARG	LEU	LYS	SER	GLY	GLU
A1360	ASN		D1108	Q993	LYS	CYS	THR	LEU	VAL	ALA	ALA	HIS	VAL	VAL	ARG	GLN	ALA	GLU
R1361	HIS		D1109	Y994	ARG	ARG	PHE	VAL	GLU	TRP	HIS	GLU	ASN	ASN	VAL	VAL	ALA	MET
D1367	TYR		H1113	V997	PRO	PRO	GLY	THR	THR	ASN	ILE	HIS	LYS	ASN	TRP	ARG	VAL	PHE
R1368	ARG				ALA	ALA	LYS	GLN	THR	GLU	ALA	CYS	ILE	ALA	ASP	VAL	GLY	ASN
L1373	ASP		C1116	R1014	LEU	LEU	GLU	SER	THR	GLU	ARG	THR	ILE	ASP	ASP	TRP	GLY	ARG
E1384	HIS				ASN	ASN	ASN	PRO	MET	GLU	ARG	ARG	CYS	ILE	ILE	ASN	GLY	GLU
E1385	VAL		L1123	K1018	ASP	PRO	ASP	PRO	LEU	GLU	ILE	GLU	GLU	PHE	PHE	TRP	GLY	ALA
P1375	ALA			S1019	PRO	PRO	GLY	ASN	GLY	ILE	THR	MET	THR	ALA	GLU	LYS	ILE	ALA
L1376	SER		F1137	D1020	GLY	VAL	SER	VAL	VAL	SER	SER	VAL	PRO	ASN	ASN	ASN	VAL	VAL
L1377	VAL		M1021	M1021	CYS	CYS	VAL	TYR	TYR	ASN	GLY	ALA	ALA	ALA	ALA	ASN	ASN	ASN
A1378	SER		H1140	N1022	VAL	VAL	MET	VAL	CYS	MET	MET	THR	THR	PHE	PHE	GLU	VAL	PHE

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	B	0.42	0/5209	0.95	13/7030 (0.2%)
1	C	0.40	1/17302 (0.0%)	0.88	34/23432 (0.1%)
1	D	0.42	2/17302 (0.0%)	0.94	59/23432 (0.3%)
1	F	0.42	0/5284	0.96	12/7131 (0.2%)
All	All	0.41	3/45097 (0.0%)	0.92	118/61025 (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	B	0	8
1	C	0	16
1	D	0	16
1	F	0	10
All	All	0	50

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1526	ILE	C-N	7.03	1.47	1.34
1	D	1527	PRO	CB-CG	-5.58	1.22	1.50
1	C	1138	PHE	CA-C	5.14	1.66	1.52

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	971	LEU	CA-CB-CG	13.49	146.33	115.30
1	D	1526	ILE	C-N-CD	-13.29	91.36	120.60
1	D	585	GLY	N-CA-C	12.22	143.64	113.10
1	D	222	LEU	CA-CB-CG	10.98	140.56	115.30
1	D	1527	PRO	C-N-CA	10.94	149.04	121.70

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1171	LEU	Peptide
1	B	1173	ASP	Peptide
1	B	1249	PHE	Peptide
1	B	1315	ASN	Peptide
1	B	1332	ALA	Peptide

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	B	5112	5114	5134	108	0
1	C	16940	16841	16897	255	0
1	D	16940	16842	16897	282	0
1	F	5186	5194	5214	113	0
All	All	44178	43991	44142	728	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 728 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:1511:ALA:HB3	1:C:1532:LEU:HD12	1.36	1.07
1:C:721:SER:OG	1:D:173:ASP:O	1.92	0.86
1:C:1533:THR:OG1	1:C:1541:ASP:O	1.94	0.84
1:D:357:HIS:ND1	1:D:378:CYS:SG	2.50	0.83
1:C:1387:ARG:O	1:C:1409:LYS:NZ	2.12	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	B	609/2407 (25%)	522 (86%)	81 (13%)	6 (1%)	17	59
1	C	2107/2407 (88%)	1908 (91%)	191 (9%)	8 (0%)	36	77
1	D	2107/2407 (88%)	1901 (90%)	193 (9%)	13 (1%)	27	70
1	F	620/2407 (26%)	521 (84%)	91 (15%)	8 (1%)	13	54
All	All	5443/9628 (56%)	4852 (89%)	556 (10%)	35 (1%)	31	70

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1087	ALA
1	B	1304	LEU
1	B	1365	GLU
1	C	1304	LEU
1	D	1527	PRO

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 PDB entries followed by that with respect to all EM entries.

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	B	571/2108 (27%)	552 (97%)	19 (3%)	41	67
1	C	1855/2108 (88%)	1806 (97%)	49 (3%)	49	73
1	D	1855/2108 (88%)	1800 (97%)	55 (3%)	44	69
1	F	579/2108 (28%)	552 (95%)	27 (5%)	29	59
All	All	4860/8432 (58%)	4710 (97%)	150 (3%)	47	68

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2333	GLU
1	D	954	ARG
1	F	1319	LEU
1	D	439	ASN
1	D	715	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1429	HIS
1	C	2028	GLN
1	F	1181	GLN
1	C	1443	GLN
1	C	1463	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 ⓘ

There are no chain breaks in this entry.