



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:28 AM GMT

PDB ID : 3OXO  
Title : Succinyl-CoA:3-ketoacid CoA transferase from pig heart covalently bound to CoA  
Authors : Fraser, M.E.  
Deposited on : 2010-09-21  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

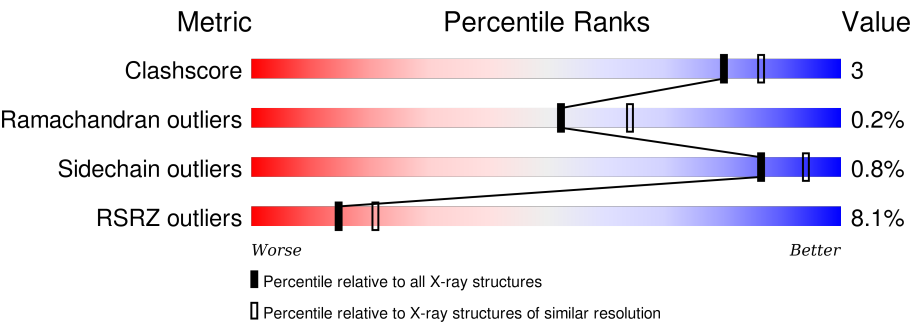
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	488	<div><div>4%</div><div>92%</div><div>• •</div></div>
1	B	488	<div><div>2%</div><div>90%</div><div>5% • 5%</div></div>
1	C	488	<div><div>2%</div><div>89%</div><div>6% 5%</div></div>
1	D	488	<div><div>3%</div><div>90%</div><div>6% •</div></div>
1	E	488	<div><div>9%</div><div>84%</div><div>10% 5%</div></div>
1	F	488	<div><div>7%</div><div>82%</div><div>13% 5%</div></div>
1	G	488	<div><div>11%</div><div>85%</div><div>8% 6%</div></div>

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Mol	Chain	Length	Quality of chain
1	H	488	<div><div></div><div>24%</div><div>85%</div><div>9%</div><div>6%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28904 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 Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3576	2268	613	677	18			
1	B	466	Total	C	N	O	S	0	0	0
			3556	2258	609	671	18			
1	C	466	Total	C	N	O	S	0	0	0
			3555	2256	609	672	18			
1	D	467	Total	C	N	O	S	0	0	0
			3563	2260	610	675	18			
1	E	462	Total	C	N	O	S	0	0	0
			3519	2236	601	664	18			
1	F	463	Total	C	N	O	S	0	0	0
			3528	2241	602	667	18			
1	G	459	Total	C	N	O	S	0	0	0
			3489	2218	592	661	18			
1	H	458	Total	C	N	O	S	0	0	0
			3483	2212	593	660	18			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	LEU	-	EXPRESSION TAG	UNP Q29551
A	480	GLU	-	EXPRESSION TAG	UNP Q29551
A	481	HIS	-	EXPRESSION TAG	UNP Q29551
A	482	HIS	-	EXPRESSION TAG	UNP Q29551
A	483	HIS	-	EXPRESSION TAG	UNP Q29551
A	484	HIS	-	EXPRESSION TAG	UNP Q29551
A	485	HIS	-	EXPRESSION TAG	UNP Q29551
A	486	HIS	-	EXPRESSION TAG	UNP Q29551
A	487	HIS	-	EXPRESSION TAG	UNP Q29551
A	488	HIS	-	EXPRESSION TAG	UNP Q29551
B	479	LEU	-	EXPRESSION TAG	UNP Q29551
B	480	GLU	-	EXPRESSION TAG	UNP Q29551

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	HIS	-	EXPRESSION TAG	UNP Q29551
B	482	HIS	-	EXPRESSION TAG	UNP Q29551
B	483	HIS	-	EXPRESSION TAG	UNP Q29551
B	484	HIS	-	EXPRESSION TAG	UNP Q29551
B	485	HIS	-	EXPRESSION TAG	UNP Q29551
B	486	HIS	-	EXPRESSION TAG	UNP Q29551
B	487	HIS	-	EXPRESSION TAG	UNP Q29551
B	488	HIS	-	EXPRESSION TAG	UNP Q29551
C	479	LEU	-	EXPRESSION TAG	UNP Q29551
C	480	GLU	-	EXPRESSION TAG	UNP Q29551
C	481	HIS	-	EXPRESSION TAG	UNP Q29551
C	482	HIS	-	EXPRESSION TAG	UNP Q29551
C	483	HIS	-	EXPRESSION TAG	UNP Q29551
C	484	HIS	-	EXPRESSION TAG	UNP Q29551
C	485	HIS	-	EXPRESSION TAG	UNP Q29551
C	486	HIS	-	EXPRESSION TAG	UNP Q29551
C	487	HIS	-	EXPRESSION TAG	UNP Q29551
C	488	HIS	-	EXPRESSION TAG	UNP Q29551
D	479	LEU	-	EXPRESSION TAG	UNP Q29551
D	480	GLU	-	EXPRESSION TAG	UNP Q29551
D	481	HIS	-	EXPRESSION TAG	UNP Q29551
D	482	HIS	-	EXPRESSION TAG	UNP Q29551
D	483	HIS	-	EXPRESSION TAG	UNP Q29551
D	484	HIS	-	EXPRESSION TAG	UNP Q29551
D	485	HIS	-	EXPRESSION TAG	UNP Q29551
D	486	HIS	-	EXPRESSION TAG	UNP Q29551
D	487	HIS	-	EXPRESSION TAG	UNP Q29551
D	488	HIS	-	EXPRESSION TAG	UNP Q29551
E	479	LEU	-	EXPRESSION TAG	UNP Q29551
E	480	GLU	-	EXPRESSION TAG	UNP Q29551
E	481	HIS	-	EXPRESSION TAG	UNP Q29551
E	482	HIS	-	EXPRESSION TAG	UNP Q29551
E	483	HIS	-	EXPRESSION TAG	UNP Q29551
E	484	HIS	-	EXPRESSION TAG	UNP Q29551
E	485	HIS	-	EXPRESSION TAG	UNP Q29551
E	486	HIS	-	EXPRESSION TAG	UNP Q29551
E	487	HIS	-	EXPRESSION TAG	UNP Q29551
E	488	HIS	-	EXPRESSION TAG	UNP Q29551
F	479	LEU	-	EXPRESSION TAG	UNP Q29551
F	480	GLU	-	EXPRESSION TAG	UNP Q29551
F	481	HIS	-	EXPRESSION TAG	UNP Q29551
F	482	HIS	-	EXPRESSION TAG	UNP Q29551

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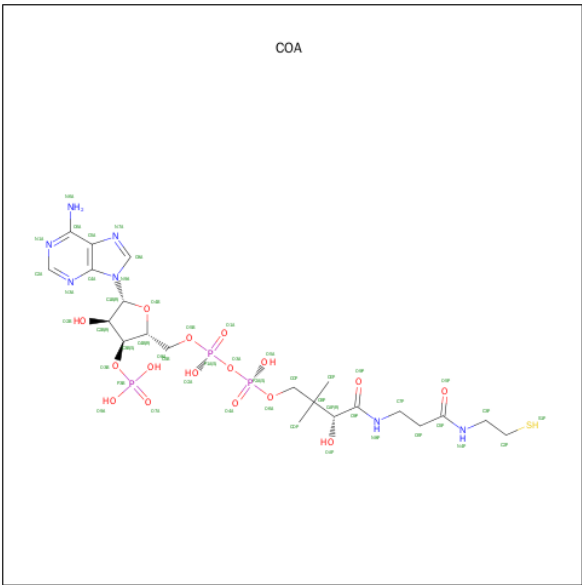
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Chain	Residue	Modelled	Actual	Comment	Reference
F	483	HIS	-	EXPRESSION TAG	UNP Q29551
F	484	HIS	-	EXPRESSION TAG	UNP Q29551
F	485	HIS	-	EXPRESSION TAG	UNP Q29551
F	486	HIS	-	EXPRESSION TAG	UNP Q29551
F	487	HIS	-	EXPRESSION TAG	UNP Q29551
F	488	HIS	-	EXPRESSION TAG	UNP Q29551
G	479	LEU	-	EXPRESSION TAG	UNP Q29551
G	480	GLU	-	EXPRESSION TAG	UNP Q29551
G	481	HIS	-	EXPRESSION TAG	UNP Q29551
G	482	HIS	-	EXPRESSION TAG	UNP Q29551
G	483	HIS	-	EXPRESSION TAG	UNP Q29551
G	484	HIS	-	EXPRESSION TAG	UNP Q29551
G	485	HIS	-	EXPRESSION TAG	UNP Q29551
G	486	HIS	-	EXPRESSION TAG	UNP Q29551
G	487	HIS	-	EXPRESSION TAG	UNP Q29551
G	488	HIS	-	EXPRESSION TAG	UNP Q29551
H	479	LEU	-	EXPRESSION TAG	UNP Q29551
H	480	GLU	-	EXPRESSION TAG	UNP Q29551
H	481	HIS	-	EXPRESSION TAG	UNP Q29551
H	482	HIS	-	EXPRESSION TAG	UNP Q29551
H	483	HIS	-	EXPRESSION TAG	UNP Q29551
H	484	HIS	-	EXPRESSION TAG	UNP Q29551
H	485	HIS	-	EXPRESSION TAG	UNP Q29551
H	486	HIS	-	EXPRESSION TAG	UNP Q29551
H	487	HIS	-	EXPRESSION TAG	UNP Q29551
H	488	HIS	-	EXPRESSION TAG	UNP Q29551

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

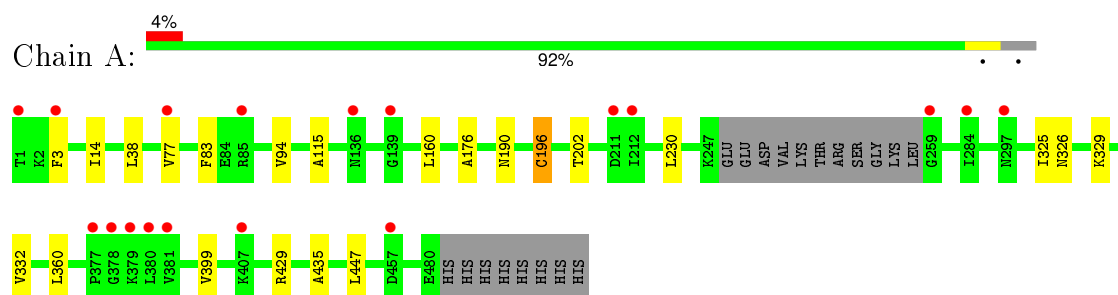
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	60	Total	O	0	0
			60	60		
4	C	65	Total	O	0	0
			65	65		
4	D	58	Total	O	0	0
			58	58		
4	E	53	Total	O	0	0
			53	53		
4	F	44	Total	O	0	0
			44	44		
4	G	43	Total	O	0	0
			43	43		
4	H	26	Total	O	0	0
			26	26		

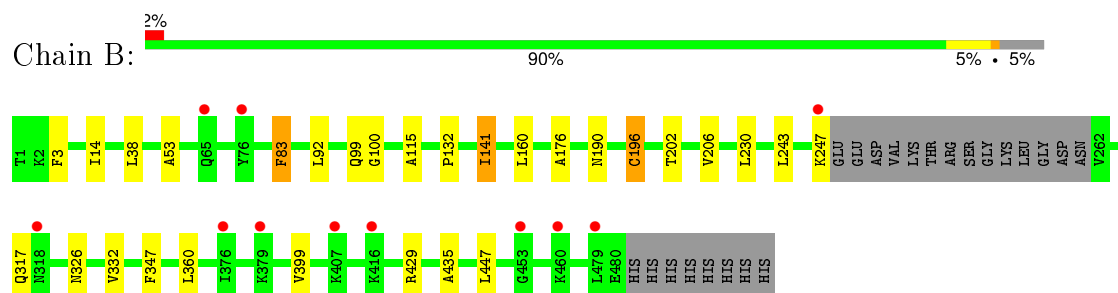
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

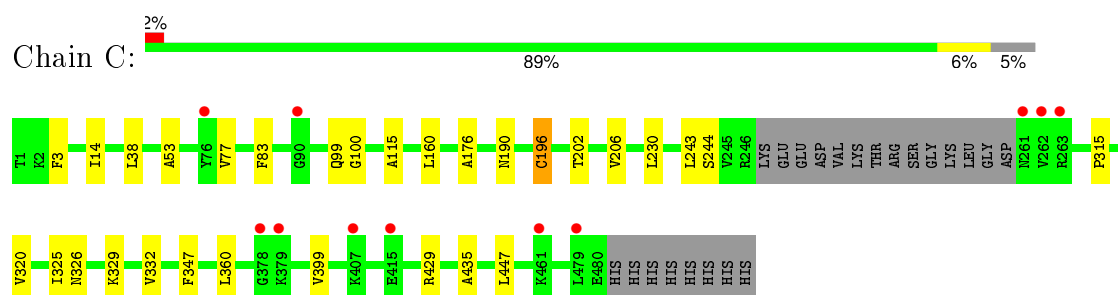
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial



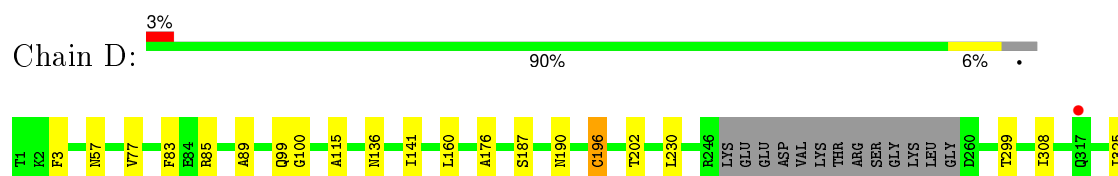
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial



- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial



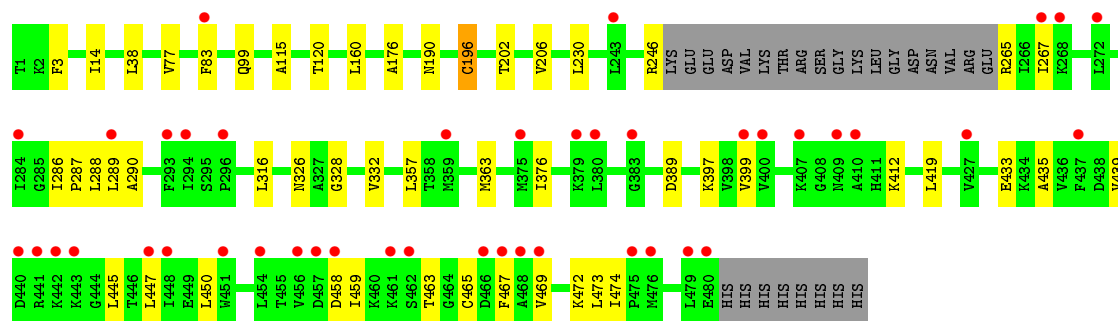
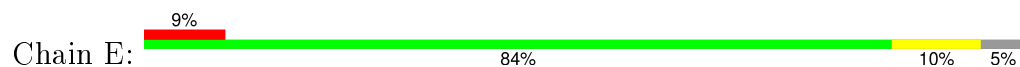
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial



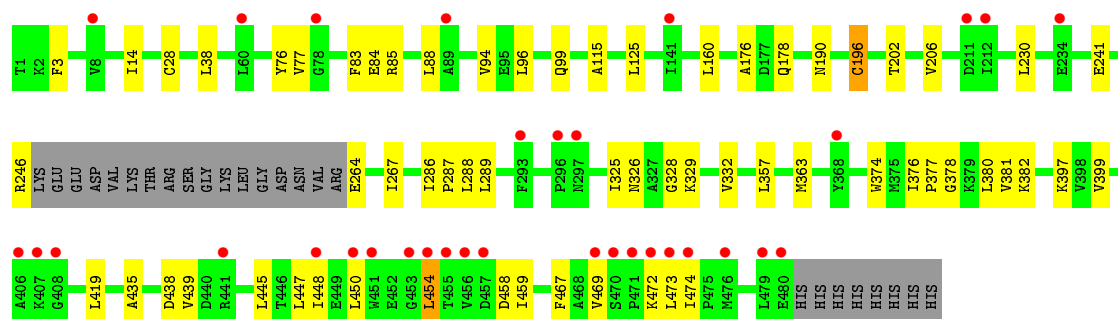
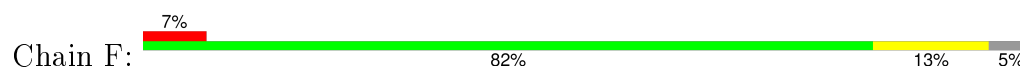




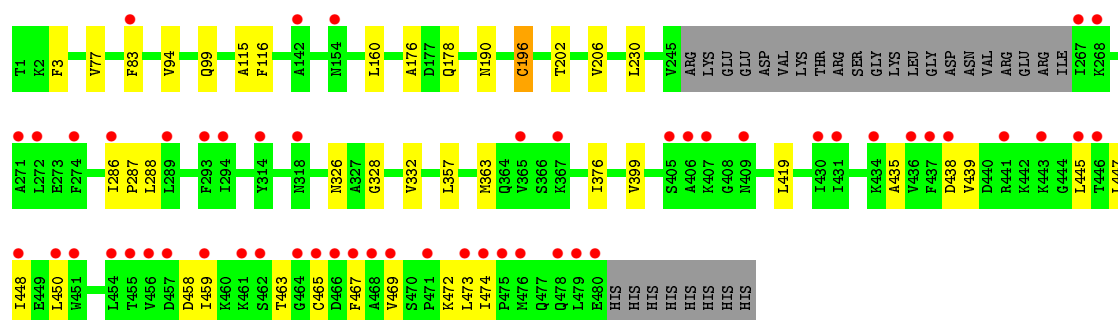
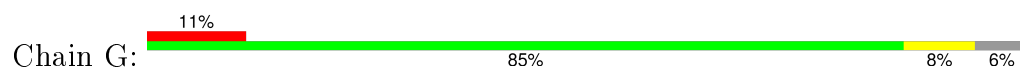
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial



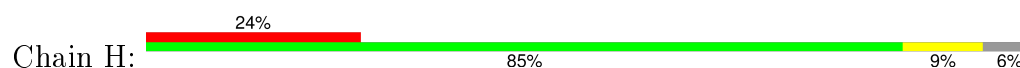
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

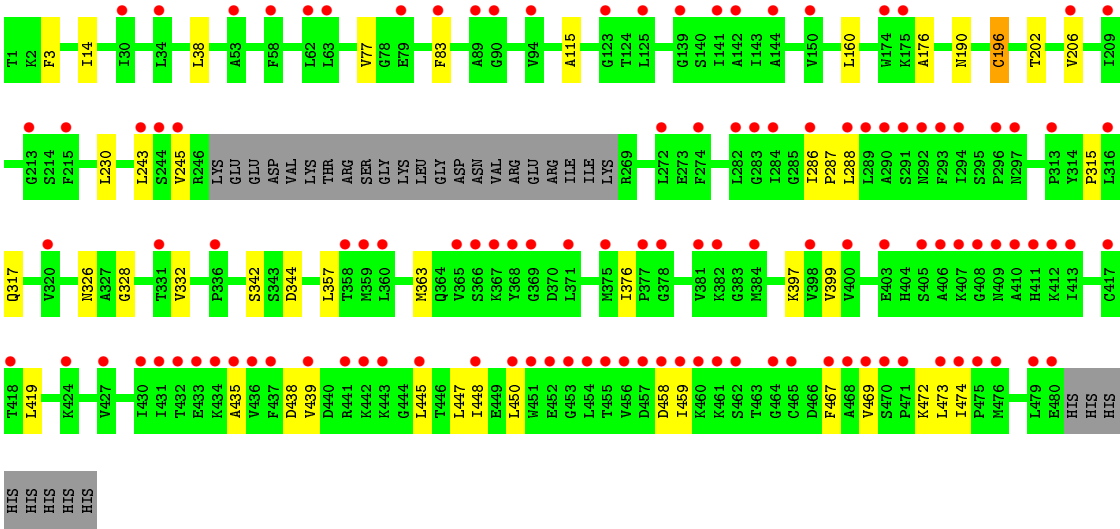


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial



- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.12Å 107.13Å 134.56Å 89.60° 80.21° 75.13°	Depositor
Resolution (Å)	21.20 – 2.30 21.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.4 (21.20-2.30) 72.9 (21.21-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.245 , 0.273 0.252 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 18.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 149071 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<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](#)

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

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	0.37	0/3634	0.51	0/4903
1	B	0.35	0/3614	0.51	0/4876
1	C	0.35	0/3613	0.50	0/4876
1	D	0.34	0/3621	0.49	0/4887
1	E	0.33	0/3577	0.49	0/4827
1	F	0.32	0/3586	0.49	0/4839
1	G	0.32	0/3547	0.49	0/4788
1	H	0.32	0/3541	0.48	0/4780
All	All	0.34	0/28733	0.49	0/38776

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	F	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	F	454	LEU	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	A	3576	0	3644	13	0
1	B	3556	0	3631	20	0
1	C	3555	0	3624	17	0
1	D	3563	0	3628	18	0
1	E	3519	0	3590	33	0
1	F	3528	0	3596	46	0
1	G	3489	0	3553	30	0
1	H	3483	0	3542	28	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	E	48	0	31	1	0
3	F	48	0	31	1	0
3	G	48	0	31	1	0
3	H	48	0	31	0	0
4	A	91	0	0	0	0
4	B	60	0	0	2	0
4	C	65	0	0	1	0
4	D	58	0	0	2	0
4	E	53	0	0	2	0
4	F	44	0	0	1	0
4	G	43	0	0	1	0
4	H	26	0	0	0	0
All	All	28904	0	28932	197	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 3.

All (197) 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:D:85:ARG:HB2	1:H:243:LEU:HD22	1.46	0.96
1:B:99:GLN:NE2	4:B:549:HOH:O	2.01	0.90
1:B:53:ALA:CB	1:B:83:PHE:CD1	2.66	0.78
1:D:136:ASN:HB3	1:F:125:LEU:HD21	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ALA:HB2	1:B:83:PHE:CE1	2.24	0.73
1:A:83:PHE:CZ	1:A:94:VAL:HG21	2.24	0.73
1:E:3:PHE:CE2	1:E:230:LEU:HD23	2.23	0.72
1:C:3:PHE:CE2	1:C:230:LEU:HD23	2.25	0.72
1:F:3:PHE:CE2	1:F:230:LEU:HD23	2.24	0.72
1:B:3:PHE:CE2	1:B:230:LEU:HD23	2.25	0.72
1:D:3:PHE:CE2	1:D:230:LEU:HD23	2.24	0.71
1:A:3:PHE:CE2	1:A:230:LEU:HD23	2.25	0.71
1:H:3:PHE:CE2	1:H:230:LEU:HD23	2.25	0.71
1:G:3:PHE:CE2	1:G:230:LEU:HD23	2.24	0.71
1:H:288:LEU:HD11	1:H:328:GLY:HA3	1.73	0.70
1:E:288:LEU:HD11	1:E:328:GLY:HA3	1.73	0.70
1:F:288:LEU:HD11	1:F:328:GLY:HA3	1.75	0.69
1:G:288:LEU:HD11	1:G:328:GLY:HA3	1.74	0.69
1:H:245:VAL:HG13	1:H:315:PRO:O	1.92	0.69
1:B:53:ALA:HB2	1:B:83:PHE:CD1	2.28	0.68
1:E:99:GLN:NE2	4:E:492:HOH:O	2.01	0.68
1:D:85:ARG:HD3	1:H:243:LEU:HD13	1.77	0.66
1:E:77:VAL:HG22	1:E:83:PHE:CE2	2.32	0.64
1:B:53:ALA:HB3	1:B:83:PHE:HD1	1.64	0.62
1:G:77:VAL:HG22	1:G:83:PHE:CE2	2.35	0.61
1:F:77:VAL:HG21	1:F:381:VAL:HG12	1.81	0.61
1:C:77:VAL:HG13	1:C:83:PHE:CD1	2.35	0.60
1:B:53:ALA:HB3	1:B:83:PHE:CD1	2.36	0.60
1:H:447:LEU:HD21	1:H:450:LEU:HD13	1.83	0.59
1:B:326:ASN:HB3	1:B:332:VAL:HG11	1.84	0.59
1:H:435:ALA:HB1	1:H:447:LEU:HD11	1.84	0.59
1:E:288:LEU:HD22	1:E:326:ASN:ND2	2.18	0.58
1:A:326:ASN:HB3	1:A:332:VAL:HG11	1.85	0.58
1:D:326:ASN:HB3	1:D:332:VAL:HG11	1.86	0.58
1:G:447:LEU:HD21	1:G:450:LEU:HD13	1.84	0.58
1:E:447:LEU:HD21	1:E:450:LEU:HD13	1.85	0.57
1:F:83:PHE:CZ	1:F:94:VAL:HG21	2.40	0.57
1:G:435:ALA:HB1	1:G:447:LEU:HD11	1.86	0.57
1:F:28:CYS:HB2	1:F:325:ILE:HD13	1.86	0.57
1:F:447:LEU:HD21	1:F:450:LEU:HD13	1.85	0.57
1:D:99:GLN:NE2	4:D:533:HOH:O	2.21	0.57
1:C:326:ASN:HB3	1:C:332:VAL:HG11	1.86	0.57
1:G:288:LEU:HD22	1:G:326:ASN:ND2	2.20	0.57
1:E:435:ALA:HB1	1:E:447:LEU:HD11	1.85	0.56
1:G:357:LEU:HD11	1:G:399:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:288:LEU:HD22	1:H:326:ASN:ND2	2.21	0.56
1:E:357:LEU:HD11	1:E:399:VAL:HG23	1.88	0.56
1:F:435:ALA:HB1	1:F:447:LEU:HD11	1.87	0.56
1:H:357:LEU:HD11	1:H:399:VAL:HG23	1.88	0.55
1:G:77:VAL:CG2	1:G:83:PHE:CE2	2.88	0.55
1:F:88:LEU:HD22	1:F:378:GLY:HA2	1.89	0.54
1:B:100:GLY:HA2	1:B:347:PHE:CD2	2.43	0.54
1:F:267:ILE:CD1	1:F:289:LEU:HD22	2.38	0.54
1:D:196:CYS:O	1:D:202:THR:HG21	2.08	0.54
1:B:115:ALA:HB1	1:B:160:LEU:HD11	1.90	0.53
1:H:77:VAL:HG22	1:H:83:PHE:CE2	2.43	0.53
1:D:77:VAL:HG22	1:D:83:PHE:CE2	2.42	0.53
1:C:435:ALA:HB1	1:C:447:LEU:CD1	2.38	0.53
1:H:115:ALA:HB1	1:H:160:LEU:HD11	1.90	0.53
1:F:357:LEU:HD11	1:F:399:VAL:HG23	1.90	0.53
1:E:326:ASN:HB3	1:E:332:VAL:HG11	1.91	0.52
1:E:115:ALA:HB1	1:E:160:LEU:HD11	1.91	0.52
1:D:100:GLY:HA2	1:D:347:PHE:CD2	2.45	0.52
1:B:435:ALA:HB1	1:B:447:LEU:CD1	2.39	0.52
1:E:267:ILE:CD1	1:E:289:LEU:HD22	2.39	0.52
1:F:77:VAL:CG2	1:F:83:PHE:CE2	2.92	0.52
1:A:435:ALA:HB1	1:A:447:LEU:CD1	2.40	0.52
1:F:288:LEU:HD22	1:F:326:ASN:ND2	2.24	0.52
1:F:77:VAL:HG22	1:F:83:PHE:CE2	2.44	0.52
1:F:115:ALA:HB1	1:F:160:LEU:HD11	1.92	0.51
1:B:196:CYS:O	1:B:202:THR:HG21	2.11	0.51
1:D:435:ALA:HB1	1:D:447:LEU:CD1	2.40	0.51
1:C:115:ALA:HB1	1:C:160:LEU:HD11	1.92	0.51
1:E:267:ILE:HD11	1:E:289:LEU:HD22	1.91	0.51
1:G:115:ALA:HB1	1:G:160:LEU:HD11	1.93	0.51
1:C:77:VAL:HG22	1:C:83:PHE:CE1	2.46	0.51
1:C:196:CYS:O	1:C:202:THR:HG21	2.11	0.51
1:E:376:ILE:HA	1:E:419:LEU:HD22	1.94	0.50
1:G:376:ILE:HA	1:G:419:LEU:HD22	1.92	0.50
1:G:469:VAL:CG1	1:G:473:LEU:HD22	2.41	0.50
1:H:469:VAL:CG1	1:H:473:LEU:HD22	2.41	0.50
1:B:132:PRO:HB3	1:B:141:ILE:HD13	1.94	0.50
1:F:196:CYS:O	1:F:202:THR:HG21	2.12	0.50
1:E:265:ARG:NH1	1:E:433:GLU:O	2.45	0.50
1:F:326:ASN:HB3	1:F:332:VAL:HG11	1.94	0.50
1:H:376:ILE:HA	1:H:419:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:326:ASN:HB3	1:H:332:VAL:HG11	1.93	0.49
1:F:264:GLU:HA	1:F:267:ILE:HD12	1.94	0.49
1:D:85:ARG:CD	1:H:243:LEU:HD13	2.42	0.49
1:F:28:CYS:HB2	1:F:325:ILE:CD1	2.42	0.49
1:E:412:LYS:NZ	4:E:536:HOH:O	2.44	0.49
1:D:115:ALA:HB1	1:D:160:LEU:HD11	1.93	0.49
1:G:196:CYS:O	1:G:202:THR:HG21	2.13	0.49
1:B:243:LEU:HD22	1:F:85:ARG:HD3	1.94	0.49
1:F:267:ILE:HD11	1:F:289:LEU:HD22	1.95	0.49
1:F:469:VAL:CG1	1:F:473:LEU:HD22	2.43	0.49
1:G:326:ASN:HB3	1:G:332:VAL:HG11	1.94	0.48
1:A:115:ALA:HB1	1:A:160:LEU:HD11	1.94	0.48
1:H:439:VAL:HG22	1:H:445:LEU:HD23	1.95	0.48
1:H:196:CYS:O	1:H:202:THR:HG21	2.14	0.48
1:F:472:LYS:O	1:F:474:ILE:HG23	2.14	0.48
1:H:342:SER:OG	1:H:344:ASP:OD1	2.26	0.48
1:A:77:VAL:HG22	1:A:83:PHE:CE2	2.50	0.47
1:G:99:GLN:NE2	4:G:501:HOH:O	2.27	0.47
1:E:469:VAL:CG1	1:E:473:LEU:HD22	2.43	0.47
1:E:196:CYS:O	1:E:202:THR:HG21	2.14	0.47
1:G:83:PHE:CZ	1:G:94:VAL:HG21	2.49	0.47
1:E:439:VAL:HG22	1:E:445:LEU:HD23	1.97	0.47
1:C:53:ALA:CB	1:C:83:PHE:CD1	2.98	0.47
1:F:376:ILE:HA	1:F:419:LEU:HD22	1.96	0.47
1:B:317:GLN:OE1	1:F:85:ARG:HG3	2.15	0.47
1:A:196:CYS:O	1:A:202:THR:HG21	2.15	0.46
1:D:89:ALA:HB2	1:H:317:GLN:NE2	2.31	0.46
1:C:399:VAL:HG22	1:C:429:ARG:HB3	1.96	0.46
1:A:77:VAL:CG2	1:A:83:PHE:CE2	2.98	0.46
1:G:459:ILE:HG22	1:G:467:PHE:CE1	2.51	0.46
1:D:325:ILE:HD12	1:D:329:LYS:HA	1.97	0.46
1:C:100:GLY:HA2	1:C:347:PHE:CD2	2.50	0.46
1:F:363:MET:HG3	3:F:1305:COA:H132	1.98	0.45
1:B:176:ALA:CB	1:B:230:LEU:HD21	2.46	0.45
1:F:241:GLU:OE1	1:F:329:LYS:HD2	2.16	0.45
1:D:299:THR:HG23	4:D:522:HOH:O	2.17	0.45
1:G:472:LYS:O	1:G:474:ILE:HG23	2.17	0.45
1:H:363:MET:HE3	1:H:419:LEU:HD13	1.99	0.45
1:F:76:TYR:CD1	1:F:382:LYS:O	2.70	0.45
1:E:363:MET:HE3	1:E:419:LEU:HD13	1.98	0.45
1:E:246:ARG:NH1	1:E:316:LEU:HD21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:472:LYS:O	1:H:474:ILE:HG23	2.17	0.45
1:H:459:ILE:HG22	1:H:467:PHE:CE1	2.52	0.45
1:C:244:SER:O	1:C:315:PRO:HD2	2.17	0.45
1:E:472:LYS:O	1:E:474:ILE:HG23	2.17	0.45
1:G:439:VAL:HG22	1:G:445:LEU:HD23	1.97	0.44
1:F:357:LEU:HD12	1:F:397:LYS:O	2.17	0.44
1:G:77:VAL:HG13	1:G:83:PHE:CD2	2.53	0.44
1:B:14:ILE:HD12	1:B:38:LEU:HD21	2.00	0.44
1:A:176:ALA:CB	1:A:230:LEU:HD21	2.48	0.44
1:E:176:ALA:CB	1:E:230:LEU:HD21	2.47	0.44
1:H:176:ALA:CB	1:H:230:LEU:HD21	2.48	0.44
1:F:176:ALA:CB	1:F:230:LEU:HD21	2.47	0.43
1:E:363:MET:HG3	3:E:1305:COA:H132	2.00	0.43
1:F:439:VAL:HG22	1:F:445:LEU:HD23	1.99	0.43
1:G:438:ASP:CG	1:G:448:ILE:HD13	2.38	0.43
1:H:438:ASP:CG	1:H:448:ILE:HD13	2.39	0.43
1:A:14:ILE:HD12	1:A:38:LEU:HD21	2.00	0.43
1:E:459:ILE:HG22	1:E:467:PHE:CE1	2.54	0.43
1:F:286:ILE:N	1:F:287:PRO:CD	2.82	0.43
1:C:14:ILE:HD12	1:C:38:LEU:HD21	2.00	0.43
1:D:187:SER:HB3	1:D:308:ILE:HD11	2.01	0.43
1:A:83:PHE:HZ	1:A:94:VAL:HG21	1.78	0.43
1:D:176:ALA:CB	1:D:230:LEU:HD21	2.48	0.43
1:G:83:PHE:C	1:G:83:PHE:CD2	2.91	0.43
1:F:96:LEU:CD1	1:F:374:TRP:HZ3	2.31	0.43
1:F:363:MET:HE3	1:F:419:LEU:HD13	2.01	0.43
1:F:438:ASP:CG	1:F:448:ILE:HD13	2.39	0.43
1:F:459:ILE:HG22	1:F:467:PHE:CE1	2.54	0.43
1:H:14:ILE:HD12	1:H:38:LEU:HD21	2.01	0.43
1:E:357:LEU:HD12	1:E:397:LYS:O	2.19	0.42
1:A:325:ILE:HD12	1:A:329:LYS:HA	2.02	0.42
1:C:325:ILE:HD12	1:C:329:LYS:HA	2.01	0.42
1:F:84:GLU:OE2	1:F:380:LEU:HA	2.19	0.42
1:B:92:LEU:N	4:B:514:HOH:O	2.52	0.42
1:C:176:ALA:CB	1:C:230:LEU:HD21	2.50	0.42
1:E:267:ILE:HG23	1:E:290:ALA:HB2	2.01	0.42
1:G:363:MET:HE3	1:G:419:LEU:HD13	2.02	0.42
1:G:176:ALA:CB	1:G:230:LEU:HD21	2.50	0.42
1:G:363:MET:HG3	3:G:1305:COA:H132	2.02	0.42
1:E:267:ILE:HD13	1:E:289:LEU:CB	2.50	0.42
1:F:83:PHE:C	1:F:83:PHE:CD2	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:363:MET:CE	1:G:419:LEU:HD13	2.50	0.41
1:F:14:ILE:HD12	1:F:38:LEU:HD21	2.02	0.41
1:B:399:VAL:HG22	1:B:429:ARG:HB3	2.02	0.41
1:F:325:ILE:HD12	1:F:329:LYS:HA	2.03	0.41
1:G:116:PHE:O	1:G:160:LEU:HD12	2.21	0.41
1:F:454:LEU:N	1:F:454:LEU:HD12	2.35	0.41
1:E:463:THR:HG22	1:E:465:CYS:H	1.86	0.41
1:B:176:ALA:HB2	1:B:206:VAL:HG11	2.02	0.41
1:C:243:LEU:HD11	1:C:320:VAL:HG11	2.02	0.41
1:E:120:THR:OG1	1:E:389:ASP:OD1	2.36	0.41
1:F:176:ALA:HB2	1:F:206:VAL:HG11	2.03	0.41
1:H:357:LEU:HD12	1:H:397:LYS:O	2.21	0.41
1:F:99:GLN:NE2	4:F:499:HOH:O	2.50	0.41
1:A:399:VAL:HG22	1:A:429:ARG:HB3	2.03	0.41
1:E:363:MET:CE	1:E:419:LEU:HD13	2.51	0.41
1:E:286:ILE:N	1:E:287:PRO:CD	2.83	0.41
1:G:286:ILE:N	1:G:287:PRO:CD	2.84	0.41
1:G:176:ALA:HB2	1:G:206:VAL:HG11	2.03	0.40
1:F:77:VAL:HG21	1:F:83:PHE:CE2	2.56	0.40
1:D:141:ILE:O	1:F:377:PRO:HG2	2.22	0.40
1:C:99:GLN:NE2	4:C:554:HOH:O	2.54	0.40
1:C:176:ALA:HB2	1:C:206:VAL:HG11	2.03	0.40
1:G:438:ASP:OD2	1:G:448:ILE:HG21	2.22	0.40
1:H:286:ILE:N	1:H:287:PRO:CD	2.84	0.40
1:E:14:ILE:HD12	1:E:38:LEU:HD21	2.04	0.40
1:G:463:THR:HG22	1:G:465:CYS:H	1.86	0.40
1:E:176:ALA:HB2	1:E:206:VAL:HG11	2.04	0.40
1:H:176:ALA:HB2	1:H:206:VAL:HG11	2.04	0.40
1:F:76:TYR:OH	1:F:382:LYS:HD2	2.22	0.40

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 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	465/488 (95%)	456 (98%)	8 (2%)	1 (0%)	52	64
1	B	462/488 (95%)	451 (98%)	10 (2%)	1 (0%)	52	64
1	C	462/488 (95%)	451 (98%)	10 (2%)	1 (0%)	52	64
1	D	463/488 (95%)	453 (98%)	9 (2%)	1 (0%)	52	64
1	E	458/488 (94%)	447 (98%)	10 (2%)	1 (0%)	52	64
1	F	459/488 (94%)	447 (97%)	11 (2%)	1 (0%)	52	64
1	G	455/488 (93%)	444 (98%)	10 (2%)	1 (0%)	52	64
1	H	454/488 (93%)	443 (98%)	10 (2%)	1 (0%)	52	64
All	All	3678/3904 (94%)	3592 (98%)	78 (2%)	8 (0%)	52	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	B	190	ASN
1	C	190	ASN
1	E	190	ASN
1	F	190	ASN
1	G	190	ASN
1	H	190	ASN
1	D	190	ASN

### 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	382/400 (96%)	380 (100%)	2 (0%)	92	97
1	B	380/400 (95%)	375 (99%)	5 (1%)	76	87
1	C	380/400 (95%)	378 (100%)	2 (0%)	92	97
1	D	381/400 (95%)	378 (99%)	3 (1%)	86	94
1	E	376/400 (94%)	374 (100%)	2 (0%)	92	97
1	F	377/400 (94%)	373 (99%)	4 (1%)	80	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	373/400 (93%)	370 (99%)	3 (1%)	86	94
1	H	372/400 (93%)	370 (100%)	2 (0%)	92	97
All	All	3021/3200 (94%)	2998 (99%)	23 (1%)	86	94

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	CYS
1	A	360	LEU
1	B	83	PHE
1	B	141	ILE
1	B	196	CYS
1	B	247	LYS
1	B	360	LEU
1	C	196	CYS
1	C	360	LEU
1	D	57	ASN
1	D	196	CYS
1	D	360	LEU
1	E	196	CYS
1	E	458	ASP
1	F	178	GLN
1	F	196	CYS
1	F	246	ARG
1	F	458	ASP
1	G	178	GLN
1	G	196	CYS
1	G	458	ASP
1	H	196	CYS
1	H	458	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	157	HIS
1	H	317	GLN

### 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 ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	COA	E	1305	1	40,50,50	1.75	3 (7%)	50,75,75	1.88	4 (8%)
3	COA	F	1305	1	40,50,50	1.71	3 (7%)	50,75,75	1.91	5 (10%)
3	COA	G	1305	1	40,50,50	1.70	3 (7%)	50,75,75	1.92	5 (10%)
3	COA	H	1305	1	40,50,50	1.73	3 (7%)	50,75,75	1.88	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	E	1305	1	-	0/44/64/64	0/3/3/3
3	COA	F	1305	1	-	0/44/64/64	0/3/3/3
3	COA	G	1305	1	-	0/44/64/64	0/3/3/3
3	COA	H	1305	1	-	0/44/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1305	COA	C2A-N1A	2.56	1.38	1.33
3	F	1305	COA	C2A-N1A	2.59	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1305	COA	C2A-N1A	2.61	1.38	1.33
3	E	1305	COA	C2A-N1A	2.72	1.39	1.33
3	F	1305	COA	C2A-N3A	3.71	1.38	1.32
3	E	1305	COA	C2A-N3A	3.74	1.38	1.32
3	H	1305	COA	C2A-N3A	3.85	1.39	1.32
3	G	1305	COA	C2A-N3A	3.94	1.39	1.32
3	G	1305	COA	O9P-C9P	8.99	1.41	1.23
3	F	1305	COA	O9P-C9P	9.20	1.41	1.23
3	H	1305	COA	O9P-C9P	9.29	1.41	1.23
3	E	1305	COA	O9P-C9P	9.42	1.41	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1305	COA	N3A-C2A-N1A	-11.49	120.09	128.89
3	F	1305	COA	N3A-C2A-N1A	-11.34	120.21	128.89
3	H	1305	COA	N3A-C2A-N1A	-11.28	120.26	128.89
3	E	1305	COA	N3A-C2A-N1A	-11.24	120.28	128.89
3	G	1305	COA	C2P-C3P-N4P	-3.68	105.10	112.37
3	F	1305	COA	C2P-C3P-N4P	-3.56	105.35	112.37
3	E	1305	COA	C2P-C3P-N4P	-3.50	105.46	112.37
3	H	1305	COA	C2P-C3P-N4P	-3.39	105.68	112.37
3	F	1305	COA	P2A-O3A-P1A	-3.14	123.90	132.73
3	H	1305	COA	P2A-O3A-P1A	-3.03	124.21	132.73
3	E	1305	COA	P2A-O3A-P1A	-3.01	124.28	132.73
3	G	1305	COA	P2A-O3A-P1A	-2.96	124.42	132.73
3	G	1305	COA	C2B-C1B-N9A	-2.48	110.50	114.29
3	F	1305	COA	C2B-C1B-N9A	-2.44	110.56	114.29
3	E	1305	COA	C2B-C1B-N9A	-2.36	110.69	114.29
3	F	1305	COA	C4A-C5A-N7A	-2.31	107.36	109.48
3	H	1305	COA	C2B-C1B-N9A	-2.30	110.78	114.29
3	G	1305	COA	C4A-C5A-N7A	-2.10	107.54	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1305	COA	1	0
3	F	1305	COA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1305	COA	1	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	469/488 (96%)	0.16	18 (3%)	44	53	6, 28, 50, 61	0
1	B	466/488 (95%)	0.15	11 (2%)	62	71	9, 33, 52, 63	0
1	C	466/488 (95%)	0.24	11 (2%)	62	71	10, 35, 51, 60	0
1	D	467/488 (95%)	0.28	14 (2%)	54	63	10, 37, 56, 67	0
1	E	462/488 (94%)	0.55	43 (9%)	11	16	12, 37, 78, 89	0
1	F	463/488 (94%)	0.59	33 (7%)	19	26	16, 41, 75, 87	0
1	G	459/488 (94%)	0.64	54 (11%)	6	10	17, 40, 83, 93	0
1	H	458/488 (93%)	1.44	118 (25%)	1	1	25, 50, 84, 91	0
All	All	3710/3904 (95%)	0.50	302 (8%)	15	21	6, 37, 72, 93	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	469	VAL	9.9
1	H	454	LEU	9.2
1	H	479	LEU	7.4
1	H	293	PHE	7.0
1	H	448	ILE	6.8
1	H	468	ALA	6.7
1	H	435	ALA	6.5
1	H	378	GLY	6.4
1	H	445	LEU	6.4
1	E	289	LEU	6.3
1	H	406	ALA	6.1
1	E	294	ILE	5.9
1	G	457	ASP	5.8
1	H	410	ALA	5.8
1	G	267	ILE	5.8
1	E	480	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	H	467	PHE	5.7
1	E	467	PHE	5.5
1	G	437	PHE	5.5
1	G	454	LEU	5.4
1	H	243	LEU	5.3
1	H	476	MET	5.3
1	G	469	VAL	5.3
1	H	294	ILE	5.3
1	H	365	VAL	5.2
1	H	407	LYS	5.2
1	H	413	ILE	5.2
1	H	274	PHE	5.2
1	B	379	LYS	5.0
1	H	284	ILE	4.9
1	H	360	LEU	4.9
1	G	446	THR	4.7
1	H	465	CYS	4.7
1	H	289	LEU	4.7
1	A	378	GLY	4.6
1	H	456	VAL	4.5
1	E	456	VAL	4.5
1	G	448	ILE	4.5
1	G	461	LYS	4.5
1	F	454	LEU	4.4
1	H	286	ILE	4.4
1	H	381	VAL	4.4
1	G	451	TRP	4.3
1	F	450	LEU	4.3
1	H	367	LYS	4.3
1	G	467	PHE	4.3
1	G	476	MET	4.3
1	D	456	VAL	4.2
1	G	294	ILE	4.2
1	G	479	LEU	4.2
1	G	293	PHE	4.2
1	H	400	VAL	4.1
1	H	457	ASP	4.1
1	H	411	HIS	4.1
1	H	144	ALA	4.1
1	D	479	LEU	4.0
1	H	461	LYS	4.0
1	H	459	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	454	LEU	3.9
1	A	284	ILE	3.8
1	A	377	PRO	3.8
1	E	383	GLY	3.8
1	E	448	ILE	3.8
1	F	293	PHE	3.7
1	H	455	THR	3.7
1	H	460	LYS	3.7
1	H	409	ASN	3.7
1	H	292	ASN	3.6
1	H	480	GLU	3.6
1	F	455	THR	3.6
1	G	289	LEU	3.6
1	F	407	LYS	3.6
1	H	53	ALA	3.6
1	G	443	LYS	3.5
1	A	380	LEU	3.5
1	E	461	LYS	3.5
1	G	456	VAL	3.5
1	G	464	GLY	3.5
1	H	272	LEU	3.4
1	H	141	ILE	3.4
1	F	456	VAL	3.4
1	F	457	ASP	3.4
1	H	245	VAL	3.4
1	E	466	ASP	3.4
1	D	407	LYS	3.4
1	G	436	VAL	3.4
1	F	453	GLY	3.3
1	G	441	ARG	3.3
1	H	408	GLY	3.3
1	H	451	TRP	3.3
1	H	470	SER	3.3
1	H	418	THR	3.3
1	H	450	LEU	3.3
1	H	453	GLY	3.3
1	H	313	PRO	3.3
1	E	469	VAL	3.3
1	E	479	LEU	3.3
1	G	450	LEU	3.3
1	B	407	LYS	3.2
1	E	443	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	437	PHE	3.2
1	G	459	ILE	3.2
1	H	464	GLY	3.2
1	F	469	VAL	3.2
1	G	274	PHE	3.2
1	H	369	GLY	3.2
1	E	375	MET	3.2
1	G	445	LEU	3.2
1	H	359	MET	3.2
1	A	211	ASP	3.2
1	H	458	ASP	3.2
1	F	479	LEU	3.2
1	A	77	VAL	3.2
1	D	408	GLY	3.1
1	H	174	TRP	3.1
1	E	462	SER	3.1
1	F	470	SER	3.1
1	D	380	LEU	3.1
1	H	475	PRO	3.1
1	H	320	VAL	3.1
1	A	136	ASN	3.1
1	F	471	PRO	3.1
1	H	405	SER	3.1
1	E	284	ILE	3.1
1	F	408	GLY	3.1
1	E	475	PRO	3.1
1	C	378	GLY	3.0
1	E	268	LYS	3.0
1	G	462	SER	3.0
1	H	89	ALA	3.0
1	G	407	LYS	3.0
1	E	476	MET	3.0
1	H	213	GLY	3.0
1	E	441	ARG	3.0
1	H	316	LEU	3.0
1	A	381	VAL	3.0
1	H	297	ASN	3.0
1	H	371	LEU	3.0
1	F	472	LYS	2.9
1	E	451	TRP	2.9
1	D	406	ALA	2.9
1	F	473	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	331	THR	2.9
1	A	259	GLY	2.8
1	C	407	LYS	2.8
1	G	268	LYS	2.8
1	H	296	PRO	2.8
1	G	480	GLU	2.8
1	H	63	LEU	2.8
1	H	375	MET	2.8
1	H	462	SER	2.8
1	D	317	GLN	2.8
1	D	458	ASP	2.7
1	G	367	LYS	2.7
1	G	475	PRO	2.7
1	G	465	CYS	2.7
1	G	409	ASN	2.7
1	H	398	VAL	2.7
1	F	474	ILE	2.7
1	H	439	VAL	2.7
1	E	468	ALA	2.7
1	H	433	GLU	2.7
1	H	366	SER	2.7
1	H	283	GLY	2.7
1	H	358	THR	2.7
1	H	432	THR	2.7
1	H	430	ILE	2.6
1	C	90	GLY	2.6
1	H	452	GLU	2.6
1	B	376	ILE	2.6
1	G	438	ASP	2.6
1	H	139	GLY	2.6
1	H	206	VAL	2.6
1	E	379	LYS	2.6
1	F	211	ASP	2.6
1	H	377	PRO	2.6
1	H	290	ALA	2.6
1	E	437	PHE	2.6
1	G	434	LYS	2.6
1	H	434	LYS	2.6
1	F	476	MET	2.6
1	G	474	ILE	2.6
1	H	431	ILE	2.6
1	H	441	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	415	GLU	2.6
1	G	406	ALA	2.6
1	H	79	GLU	2.5
1	H	83	PHE	2.5
1	B	460	LYS	2.5
1	E	427	VAL	2.5
1	D	376	ILE	2.5
1	H	443	LYS	2.5
1	H	282	LEU	2.5
1	H	215	PHE	2.5
1	C	261	ASN	2.5
1	H	34	LEU	2.5
1	G	365	VAL	2.5
1	C	461	LYS	2.5
1	E	267	ILE	2.5
1	A	139	GLY	2.5
1	F	78	GLY	2.5
1	H	125	LEU	2.5
1	A	212	ILE	2.5
1	H	90	GLY	2.4
1	G	405	SER	2.4
1	G	154	ASN	2.4
1	H	62	LEU	2.4
1	D	466	ASP	2.4
1	H	336	PRO	2.4
1	C	262	VAL	2.4
1	A	407	LYS	2.4
1	F	60	LEU	2.4
1	H	442	LYS	2.4
1	B	479	LEU	2.4
1	F	368	TYR	2.4
1	H	94	VAL	2.4
1	H	424	LYS	2.4
1	E	400	VAL	2.4
1	F	8	VAL	2.4
1	F	480	GLU	2.4
1	E	296	PRO	2.4
1	F	451	TRP	2.4
1	H	58	PHE	2.4
1	B	416	LYS	2.4
1	D	379	LYS	2.4
1	G	272	LEU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	76	TYR	2.3
1	G	314	TYR	2.3
1	F	296	PRO	2.3
1	H	142	ALA	2.3
1	H	368	TYR	2.3
1	H	436	VAL	2.3
1	A	457	ASP	2.3
1	G	431	ILE	2.3
1	H	471	PRO	2.3
1	E	407	LYS	2.3
1	H	175	LYS	2.3
1	E	272	LEU	2.3
1	E	447	LEU	2.3
1	G	471	PRO	2.3
1	G	271	ALA	2.3
1	E	458	ASP	2.3
1	G	466	ASP	2.3
1	G	318	ASN	2.3
1	G	478	GLN	2.2
1	H	382	LYS	2.2
1	F	141	ILE	2.2
1	H	417	CYS	2.2
1	A	85	ARG	2.2
1	G	83	PHE	2.2
1	F	406	ALA	2.2
1	E	440	ASP	2.2
1	F	234	GLU	2.2
1	G	286	ILE	2.2
1	E	399	VAL	2.2
1	E	359	MET	2.2
1	H	150	VAL	2.1
1	C	76	TYR	2.1
1	C	479	LEU	2.1
1	A	1	THR	2.1
1	F	212	ILE	2.1
1	F	448	ILE	2.1
1	B	318	ASN	2.1
1	B	247	LYS	2.1
1	H	412	LYS	2.1
1	E	380	LEU	2.1
1	H	473	LEU	2.1
1	E	457	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	65	GLN	2.1
1	E	410	ALA	2.1
1	H	123	GLY	2.1
1	H	209	ILE	2.1
1	E	83	PHE	2.1
1	E	293	PHE	2.1
1	H	403	GLU	2.1
1	G	142	ALA	2.1
1	F	441	ARG	2.1
1	E	243	LEU	2.1
1	B	453	GLY	2.1
1	F	297	ASN	2.1
1	D	459	ILE	2.1
1	G	430	ILE	2.1
1	E	409	ASN	2.1
1	G	473	LEU	2.1
1	H	384	MET	2.1
1	F	89	ALA	2.1
1	H	30	ILE	2.1
1	H	474	ILE	2.1
1	H	427	VAL	2.1
1	C	263	ARG	2.0
1	C	379	LYS	2.0
1	E	442	LYS	2.0
1	H	291	SER	2.0
1	D	452	GLU	2.0
1	A	379	LYS	2.0
1	D	457	ASP	2.0
1	G	468	ALA	2.0
1	H	288	LEU	2.0
1	A	297	ASN	2.0
1	G	455	THR	2.0
1	A	3	PHE	2.0
1	H	244	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	COA	F	1305	48/48	0.85	0.18	0.11	40,51,68,72	0
3	COA	G	1305	48/48	0.88	0.15	-0.33	29,45,57,59	0
3	COA	H	1305	48/48	0.83	0.22	-0.34	55,67,77,80	0
3	COA	E	1305	48/48	0.89	0.15	-0.65	39,48,65,70	0
2	CL	C	489	1/1	0.99	0.10	-1.26	39,39,39,39	0
2	CL	B	489	1/1	0.98	0.07	-1.66	37,37,37,37	0
2	CL	D	489	1/1	0.98	0.06	-4.00	36,36,36,36	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.