Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 01:05 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

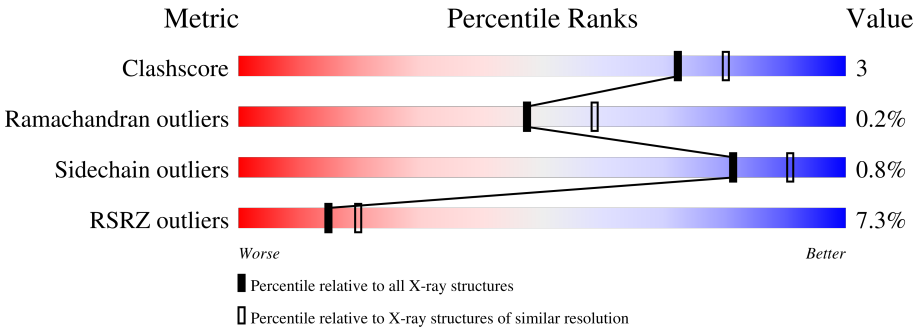
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	3% 92% · ·
1	B	488	2% 90% 5% · 5%
1	C	488	2% 89% 6% 5%
1	D	488	2% 90% 6% ·
1	E	488	8% 84% 10% 5%
1	F	488	6% 82% 12% 5%

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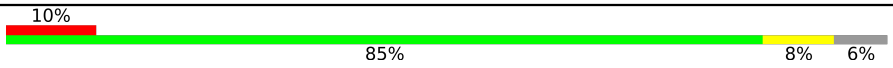
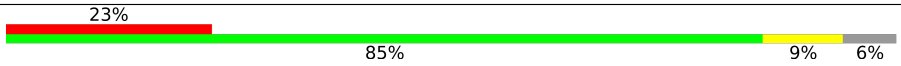
Mol	Chain	Length	Quality of chain
1	G	488	
1	H	488	

2 Entry composition (i)

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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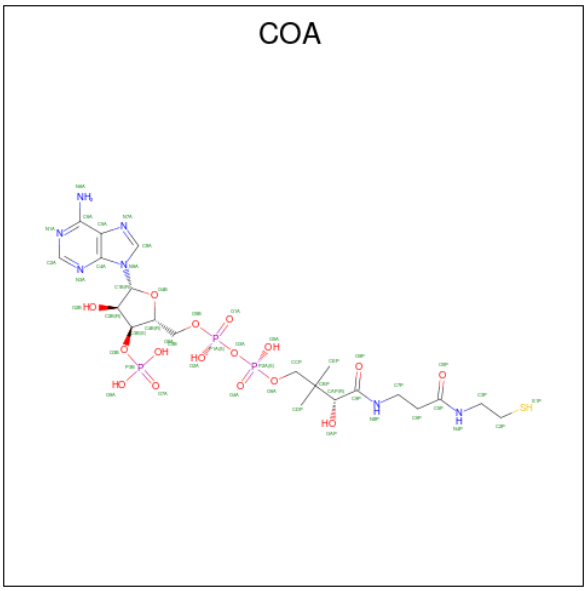
Chain	Residue	Modelled	Actual	Comment	Reference
F	483	HIS	-	expression tag	UNP Q29551
F	484	HIS	-	expression tag	UNP Q29551
F	485	HIS	-	expression tag	UNP Q29551
F	486	HIS	-	expression tag	UNP Q29551
F	487	HIS	-	expression tag	UNP Q29551
F	488	HIS	-	expression tag	UNP Q29551
G	479	LEU	-	expression tag	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	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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.

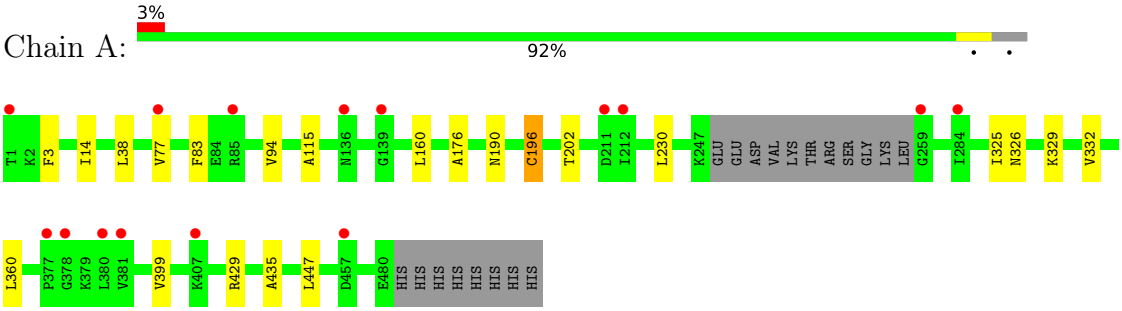
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	60	Total	O	0	0
			60	60		
4	C	65	Total	O	0	0
			65	65		
4	D	58	Total	O	0	0
			58	58		
4	E	53	Total	O	0	0
			53	53		
4	F	44	Total	O	0	0
			44	44		
4	G	43	Total	O	0	0
			43	43		
4	H	26	Total	O	0	0
			26	26		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

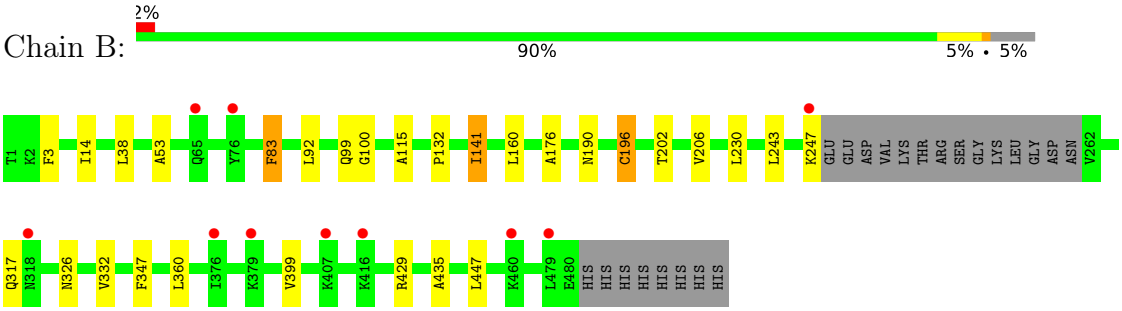
• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

Chain A:



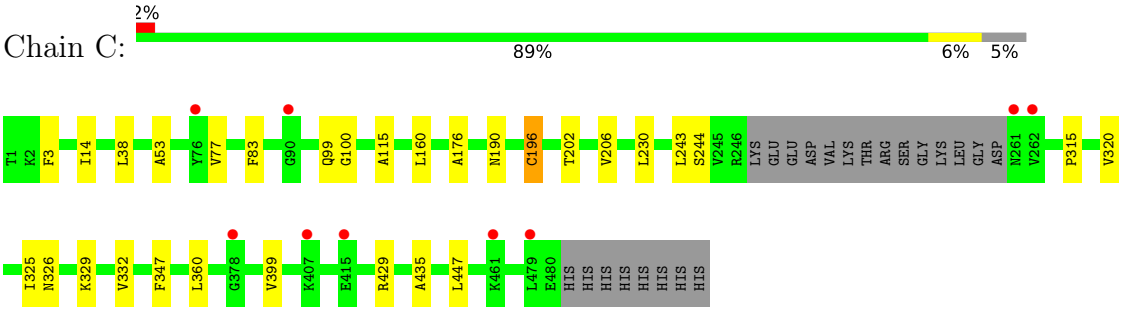
• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

Chain B:



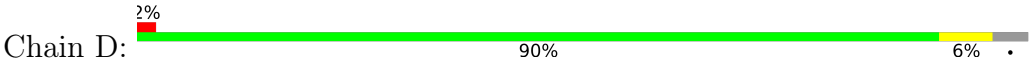
• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

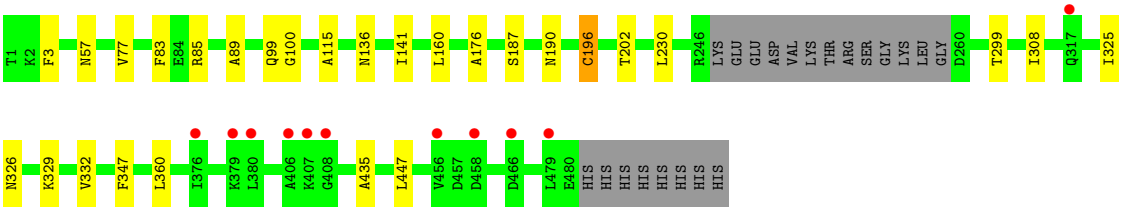
Chain C:



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

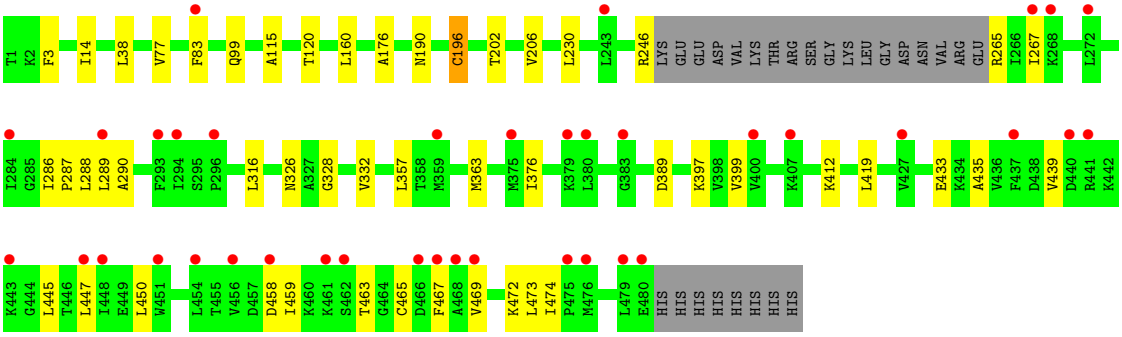
Chain D:





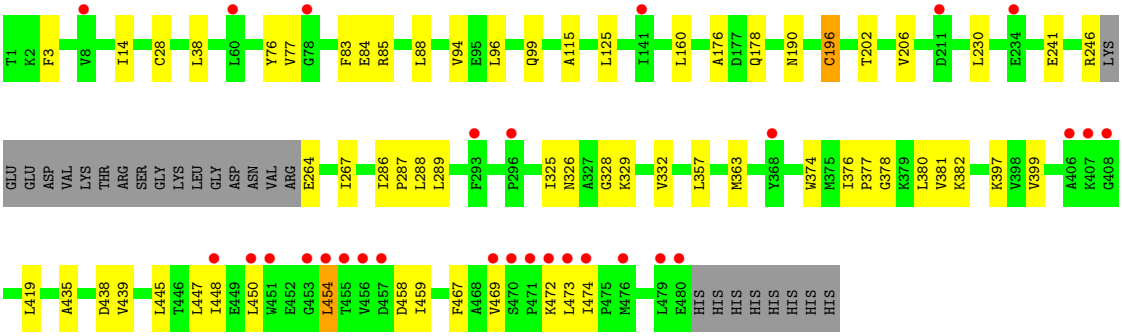
• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

Chain E:



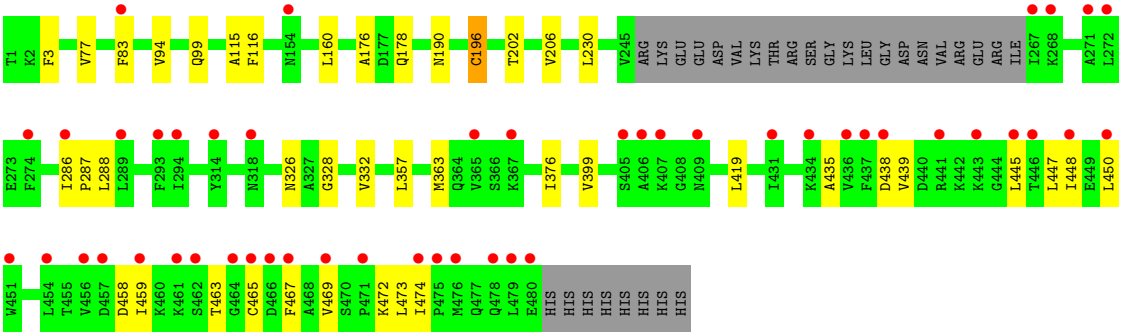
• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

Chain F:



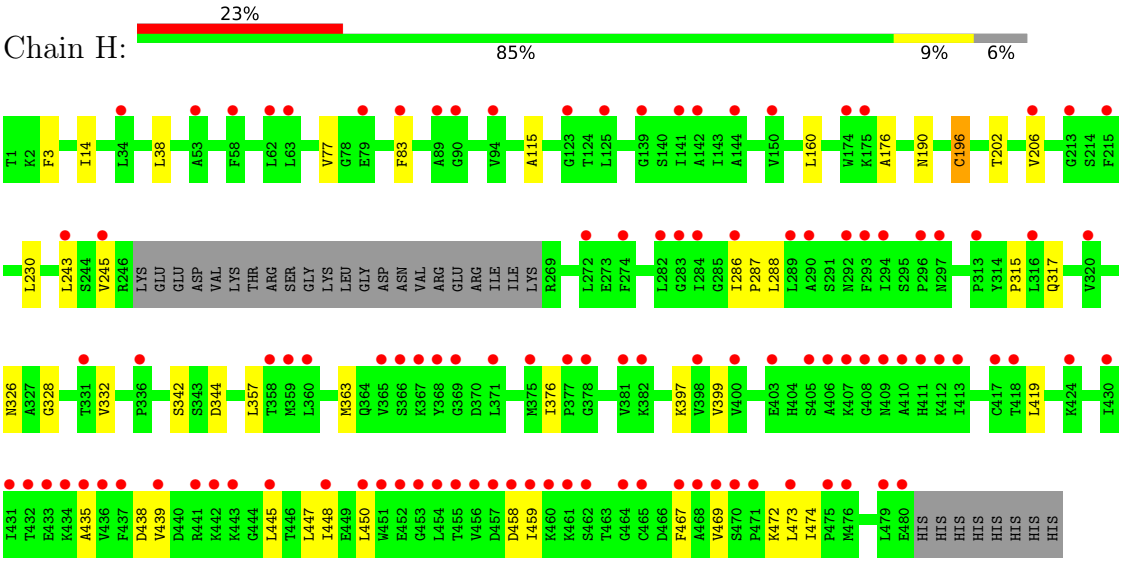
• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase 1, mitochondrial

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 72.6 (21.21-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	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.	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 18.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	28904	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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 (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	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:A:83:PHE:CZ	1:A:94:VAL:HG21	2.24	0.73
1:B:53:ALA:HB2	1:B:83:PHE:CE1	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:E:288:LEU:HD11	1:E:328:GLY:HA3	1.73	0.70
1:H:288:LEU:HD11	1:H: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:D:99:GLN:NE2	4:D:533:HOH:O	2.21	0.57
1:F:447:LEU:HD21	1:F:450:LEU:HD13	1.85	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:B:100:GLY:HA2	1:B:347:PHE:CD2	2.43	0.54
1:F:88:LEU:HD22	1:F:378:GLY:HA2	1.89	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:D:77:VAL:HG22	1:D:83:PHE:CE2	2.42	0.53
1:H:77:VAL:HG22	1:H:83:PHE:CE2	2.43	0.53
1:C:435:ALA:HB1	1:C:447:LEU:CD1	2.38	0.53
1:F:357:LEU:HD11	1:F:399:VAL:HG23	1.90	0.53
1:H:115:ALA:HB1	1:H:160:LEU:HD11	1.90	0.53
1:E:115:ALA:HB1	1:E:160:LEU:HD11	1.91	0.52
1:E:326:ASN:HB3	1:E:332:VAL:HG11	1.91	0.52
1:B:435:ALA:HB1	1:B:447:LEU:CD1	2.39	0.52
1:D:100:GLY:HA2	1:D:347:PHE:CD2	2.45	0.52
1:E:267:ILE:CD1	1:E:289:LEU:HD22	2.39	0.52
1:A:435:ALA:HB1	1:A:447:LEU:CD1	2.40	0.52
1:F:77:VAL:CG2	1:F:83:PHE:CE2	2.92	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:B:196:CYS:O	1:B:202:THR:HG21	2.11	0.51
1:F:115:ALA:HB1	1:F:160:LEU:HD11	1.92	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:E:265:ARG:NH1	1:E:433:GLU:O	2.45	0.50
1:F:196:CYS:O	1:F:202:THR:HG21	2.12	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:F:264:GLU:HA	1:F:267:ILE:HD12	1.94	0.49
1:H:326:ASN:HB3	1:H:332:VAL:HG11	1.93	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:D:115:ALA:HB1	1:D:160:LEU:HD11	1.93	0.49
1:E:412:LYS:NZ	4:E:536:HOH:O	2.44	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:F:472:LYS:O	1:F:474:ILE:HG23	2.14	0.48
1:H:196:CYS:O	1:H:202:THR:HG21	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:E:469:VAL:CG1	1:E:473:LEU:HD22	2.43	0.47
1:G:99:GLN:NE2	4:G:501:HOH:O	2.27	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:D:299:THR:HG23	4:D:522:HOH:O	2.17	0.45
1:F:241:GLU:OE1	1:F:329:LYS:HD2	2.16	0.45
1:G:472:LYS:O	1:G:474:ILE:HG23	2.17	0.45
1:F:76:TYR:CD1	1:F:382:LYS:O	2.70	0.45
1:H:363:MET:HE3	1:H:419:LEU:HD13	1.99	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:B:14:ILE:HD12	1:B:38:LEU:HD21	2.00	0.44
1:G:77:VAL:HG13	1:G:83:PHE:CD2	2.53	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:F:96:LEU:CD1	1:F:374:TRP:HZ3	2.31	0.43
1:G:83:PHE:CD2	1:G:83:PHE:C	2.91	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:A:325:ILE:HD12	1:A:329:LYS:HA	2.02	0.42
1:E:357:LEU:HD12	1:E:397:LYS:O	2.19	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:B:399:VAL:HG22	1:B:429:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ILE:HD12	1:F:38:LEU:HD21	2.02	0.41
1:F:83:PHE:CD2	1:F:83:PHE:C	2.93	0.41
1:G:363:MET:CE	1:G:419:LEU:HD13	2.50	0.41
1:F:325:ILE:HD12	1:F:329:LYS:HA	2.03	0.41
1:F:454:LEU:N	1:F:454:LEU:HD12	2.35	0.41
1:G:116:PHE:O	1:G:160:LEU:HD12	2.21	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:A:399:VAL:HG22	1:A:429:ARG:HB3	2.03	0.41
1:F:99:GLN:NE2	4:F:499:HOH:O	2.50	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:E:286:ILE:N	1:E:287:PRO:CD	2.83	0.41
1:E:363:MET:CE	1:E:419:LEU:HD13	2.51	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:D:141:ILE:O	1:F:377:PRO:HG2	2.22	0.40
1:F:77:VAL:HG21	1:F:83:PHE:CE2	2.56	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:E:14:ILE:HD12	1:E:38:LEU:HD21	2.04	0.40
1:G:438:ASP:OD2	1:G:448:ILE:HG21	2.22	0.40
1:G:463:THR:HG22	1:G:465:CYS:H	1.86	0.40
1:H:286:ILE:N	1:H:287:PRO:CD	2.84	0.40
1:E:176:ALA:HB2	1:E:206:VAL:HG11	2.04	0.40
1:F:76:TYR:OH	1:F:382:LYS:HD2	2.22	0.40
1:H:176:ALA:HB2	1:H:206:VAL:HG11	2.04	0.40

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	465/488 (95%)	456 (98%)	8 (2%)	1 (0%)	47	58
1	B	462/488 (95%)	451 (98%)	10 (2%)	1 (0%)	47	58
1	C	462/488 (95%)	451 (98%)	10 (2%)	1 (0%)	47	58
1	D	463/488 (95%)	453 (98%)	9 (2%)	1 (0%)	47	58
1	E	458/488 (94%)	447 (98%)	10 (2%)	1 (0%)	47	58
1	F	459/488 (94%)	447 (97%)	11 (2%)	1 (0%)	47	58
1	G	455/488 (93%)	444 (98%)	10 (2%)	1 (0%)	47	58
1	H	454/488 (93%)	443 (98%)	10 (2%)	1 (0%)	47	58
All	All	3678/3904 (94%)	3592 (98%)	78 (2%)	8 (0%)	47	58

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/400 (96%)	380 (100%)	2 (0%)	88	95
1	B	380/400 (95%)	375 (99%)	5 (1%)	69	82
1	C	380/400 (95%)	378 (100%)	2 (0%)	88	95
1	D	381/400 (95%)	378 (99%)	3 (1%)	81	91
1	E	376/400 (94%)	374 (100%)	2 (0%)	88	95
1	F	377/400 (94%)	373 (99%)	4 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	373/400 (93%)	370 (99%)	3 (1%)	81 91
1	H	372/400 (93%)	370 (100%)	2 (0%)	88 95
All	All	3021/3200 (94%)	2998 (99%)	23 (1%)	81 91

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

Sometimes 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 (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	F	1305	1	41,50,50	1.72	3 (7%)	52,75,75	1.12	3 (5%)
3	COA	E	1305	1	41,50,50	1.76	3 (7%)	52,75,75	1.10	3 (5%)
3	COA	H	1305	1	41,50,50	1.75	3 (7%)	52,75,75	1.10	3 (5%)
3	COA	G	1305	1	41,50,50	1.72	3 (7%)	52,75,75	1.12	3 (5%)

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	F	1305	1	-	4/44/64/64	0/3/3/3
3	COA	E	1305	1	-	4/44/64/64	0/3/3/3
3	COA	H	1305	1	-	4/44/64/64	0/3/3/3
3	COA	G	1305	1	-	4/44/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1305	COA	O9P-C9P	9.29	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1305	COA	O9P-C9P	9.17	1.41	1.23
3	F	1305	COA	O9P-C9P	9.08	1.41	1.23
3	G	1305	COA	O9P-C9P	8.87	1.41	1.23
3	G	1305	COA	C2A-N3A	4.38	1.39	1.32
3	H	1305	COA	C2A-N3A	4.28	1.39	1.32
3	E	1305	COA	C2A-N3A	4.17	1.38	1.32
3	F	1305	COA	C2A-N3A	4.13	1.38	1.32
3	E	1305	COA	C2A-N1A	2.77	1.39	1.33
3	H	1305	COA	C2A-N1A	2.67	1.38	1.33
3	F	1305	COA	C2A-N1A	2.64	1.38	1.33
3	G	1305	COA	C2A-N1A	2.61	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1305	COA	N3A-C2A-N1A	-5.49	120.09	128.68
3	F	1305	COA	N3A-C2A-N1A	-5.42	120.21	128.68
3	H	1305	COA	N3A-C2A-N1A	-5.39	120.26	128.68
3	E	1305	COA	N3A-C2A-N1A	-5.37	120.28	128.68
3	G	1305	COA	C2P-C3P-N4P	-3.15	105.10	112.31
3	F	1305	COA	C2P-C3P-N4P	-3.04	105.35	112.31
3	E	1305	COA	C2P-C3P-N4P	-3.00	105.46	112.31
3	H	1305	COA	C2P-C3P-N4P	-2.90	105.68	112.31
3	F	1305	COA	P2A-O3A-P1A	-2.60	123.90	132.83
3	H	1305	COA	P2A-O3A-P1A	-2.51	124.21	132.83
3	E	1305	COA	P2A-O3A-P1A	-2.49	124.28	132.83
3	G	1305	COA	P2A-O3A-P1A	-2.45	124.42	132.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1305	COA	C5B-O5B-P1A-O1A
3	E	1305	COA	S1P-C2P-C3P-N4P
3	F	1305	COA	C5B-O5B-P1A-O1A
3	F	1305	COA	S1P-C2P-C3P-N4P
3	G	1305	COA	C5B-O5B-P1A-O1A
3	G	1305	COA	S1P-C2P-C3P-N4P
3	H	1305	COA	C5B-O5B-P1A-O1A
3	H	1305	COA	S1P-C2P-C3P-N4P
3	F	1305	COA	C5B-O5B-P1A-O3A
3	E	1305	COA	C5B-O5B-P1A-O2A

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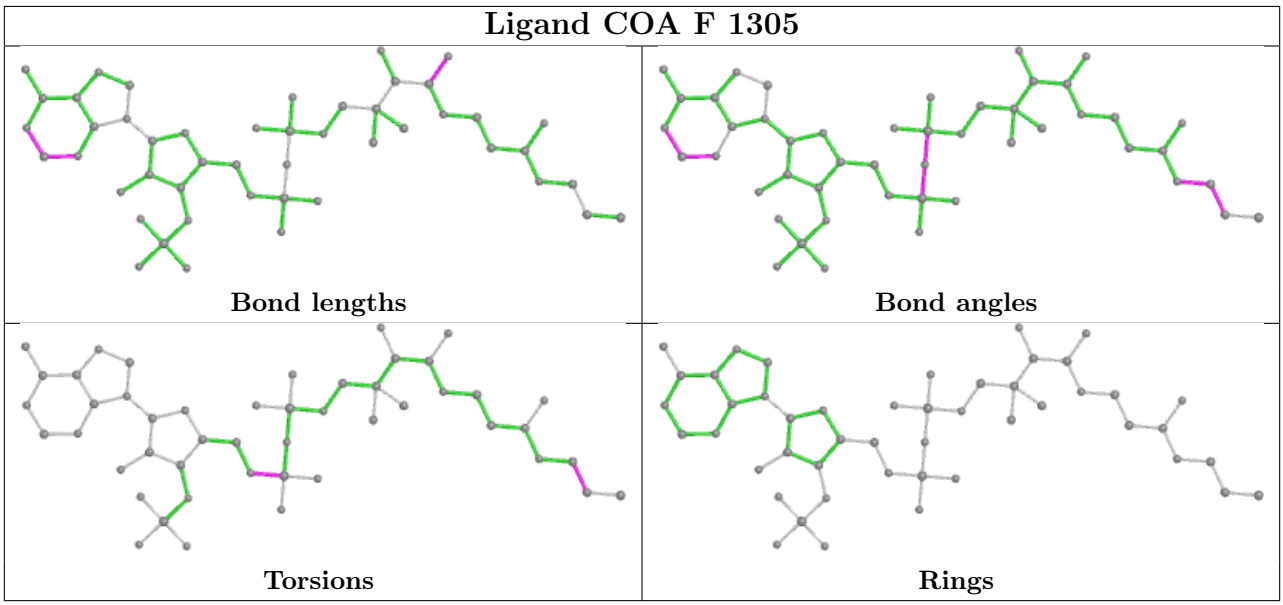
Mol	Chain	Res	Type	Atoms
3	F	1305	COA	C5B-O5B-P1A-O2A
3	G	1305	COA	C5B-O5B-P1A-O2A
3	H	1305	COA	C5B-O5B-P1A-O2A
3	E	1305	COA	C5B-O5B-P1A-O3A
3	G	1305	COA	C5B-O5B-P1A-O3A
3	H	1305	COA	C5B-O5B-P1A-O3A

There are no ring outliers.

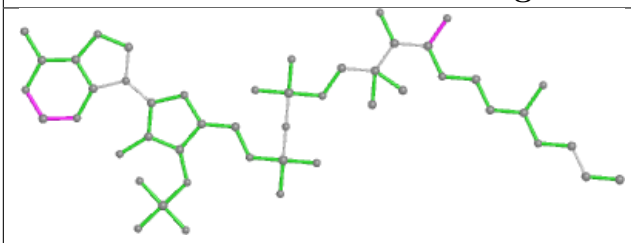
3 monomers are involved in 3 short contacts:

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

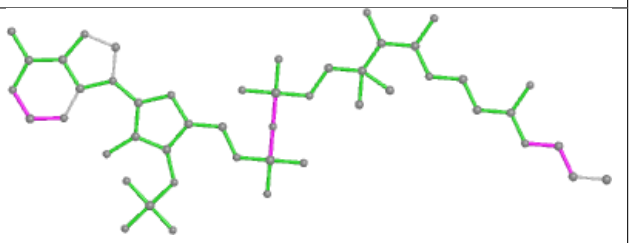
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



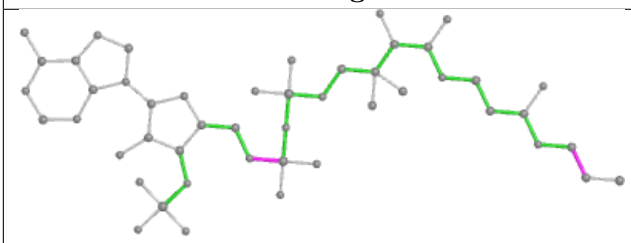
Ligand COA E 1305



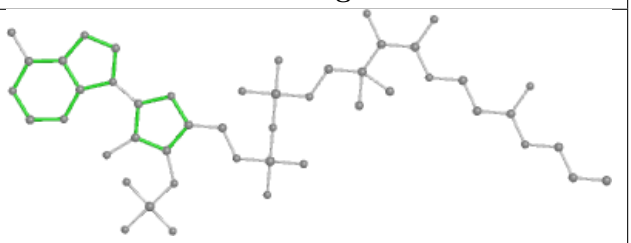
Bond lengths



Bond angles

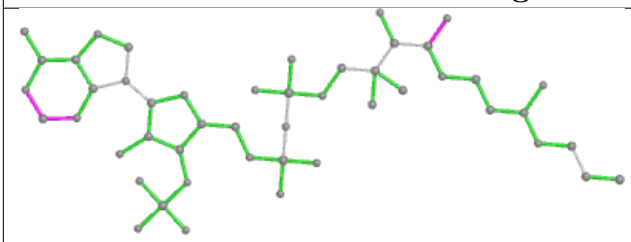


Torsions

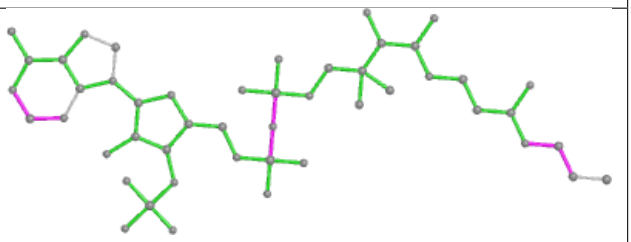


Rings

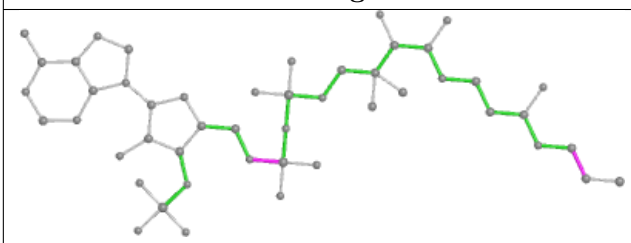
Ligand COA H 1305



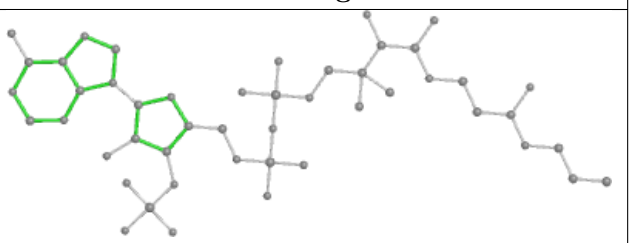
Bond lengths



Bond angles

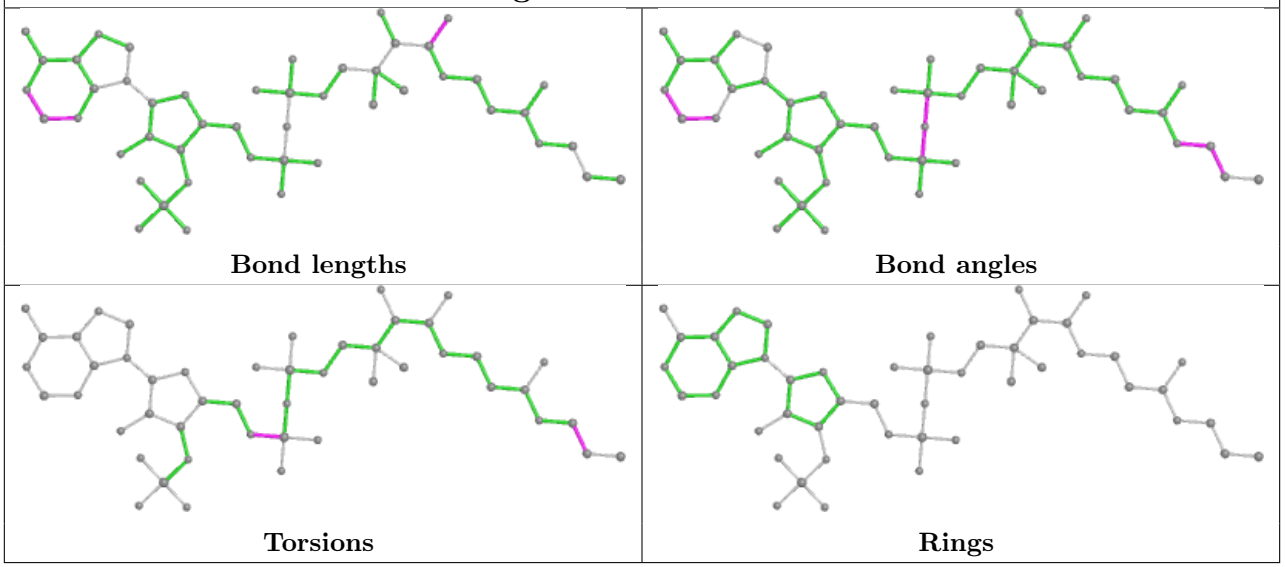


Torsions



Rings

Ligand COA G 1305



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^{th} 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	469/488 (96%)	0.11	15 (3%) 47 54	6, 28, 50, 61	0
1	B	466/488 (95%)	0.09	10 (2%) 63 70	9, 33, 52, 63	0
1	C	466/488 (95%)	0.18	9 (1%) 66 73	10, 35, 51, 60	0
1	D	467/488 (95%)	0.22	11 (2%) 59 66	10, 37, 56, 67	0
1	E	462/488 (94%)	0.49	38 (8%) 11 15	12, 37, 78, 89	0
1	F	463/488 (94%)	0.52	29 (6%) 20 25	16, 41, 75, 87	0
1	G	459/488 (94%)	0.58	49 (10%) 6 8	17, 40, 83, 93	0
1	H	458/488 (93%)	1.35	110 (24%) 0 0	25, 50, 84, 91	0
All	All	3710/3904 (95%)	0.44	271 (7%) 15 20	6, 37, 72, 93	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	469	VAL	9.5
1	H	454	LEU	8.9
1	H	479	LEU	7.2
1	H	293	PHE	6.8
1	H	448	ILE	6.5
1	H	468	ALA	6.4
1	H	435	ALA	6.3
1	H	378	GLY	6.2
1	E	289	LEU	6.2
1	H	445	LEU	6.1
1	H	406	ALA	5.9
1	E	294	ILE	5.7
1	H	410	ALA	5.6
1	G	267	ILE	5.6
1	E	480	GLU	5.6
1	G	457	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	H	467	PHE	5.5
1	E	467	PHE	5.4
1	G	437	PHE	5.2
1	G	454	LEU	5.2
1	H	243	LEU	5.2
1	H	476	MET	5.1
1	H	407	LYS	5.1
1	H	294	ILE	5.1
1	G	469	VAL	5.1
1	H	365	VAL	5.1
1	H	274	PHE	5.0
1	H	413	ILE	5.0
1	B	379	LYS	4.9
1	H	360	LEU	4.7
1	H	284	ILE	4.7
1	G	446	THR	4.6
1	H	289	LEU	4.5
1	H	465	CYS	4.5
1	A	378	GLY	4.4
1	G	448	ILE	4.4
1	G	461	LYS	4.3
1	F	454	LEU	4.3
1	H	456	VAL	4.3
1	H	381	VAL	4.2
1	H	367	LYS	4.2
1	E	456	VAL	4.2
1	G	476	MET	4.1
1	G	451	TRP	4.1
1	H	286	ILE	4.1
1	F	450	LEU	4.1
1	G	467	PHE	4.0
1	G	479	LEU	4.0
1	G	293	PHE	4.0
1	D	456	VAL	4.0
1	G	294	ILE	4.0
1	H	411	HIS	4.0
1	H	400	VAL	3.9
1	H	457	ASP	3.9
1	H	461	LYS	3.9
1	D	479	LEU	3.9
1	H	144	ALA	3.9
1	E	454	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	459	ILE	3.7
1	E	383	GLY	3.7
1	A	377	PRO	3.7
1	A	284	ILE	3.7
1	F	293	PHE	3.6
1	E	448	ILE	3.6
1	H	460	LYS	3.6
1	H	455	THR	3.6
1	H	409	ASN	3.6
1	H	292	ASN	3.5
1	H	480	GLU	3.5
1	F	407	LYS	3.5
1	H	53	ALA	3.5
1	F	455	THR	3.5
1	G	443	LYS	3.5
1	G	289	LEU	3.4
1	E	461	LYS	3.4
1	D	407	LYS	3.3
1	G	456	VAL	3.3
1	A	380	LEU	3.3
1	G	464	GLY	3.3
1	H	272	LEU	3.3
1	G	441	ARG	3.3
1	F	457	ASP	3.3
1	H	450	LEU	3.2
1	H	141	ILE	3.2
1	H	408	GLY	3.2
1	E	466	ASP	3.2
1	H	470	SER	3.2
1	F	456	VAL	3.2
1	G	436	VAL	3.2
1	H	245	VAL	3.2
1	G	459	ILE	3.2
1	B	407	LYS	3.2
1	E	443	LYS	3.2
1	F	453	GLY	3.2
1	H	451	TRP	3.2
1	H	313	PRO	3.2
1	H	418	THR	3.1
1	H	437	PHE	3.1
1	G	450	LEU	3.1
1	G	274	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	469	VAL	3.1
1	F	469	VAL	3.1
1	H	369	GLY	3.1
1	H	453	GLY	3.1
1	E	479	LEU	3.1
1	G	445	LEU	3.1
1	H	464	GLY	3.1
1	E	375	MET	3.1
1	H	359	MET	3.0
1	A	211	ASP	3.0
1	H	174	TRP	3.0
1	H	458	ASP	3.0
1	D	408	GLY	3.0
1	H	475	PRO	3.0
1	D	380	LEU	3.0
1	F	479	LEU	3.0
1	A	77	VAL	3.0
1	A	136	ASN	3.0
1	F	470	SER	3.0
1	H	405	SER	3.0
1	E	475	PRO	3.0
1	F	471	PRO	3.0
1	G	407	LYS	3.0
1	E	462	SER	2.9
1	E	268	LYS	2.9
1	H	320	VAL	2.9
1	E	476	MET	2.9
1	H	89	ALA	2.9
1	F	408	GLY	2.9
1	G	462	SER	2.9
1	E	441	ARG	2.9
1	F	472	LYS	2.9
1	C	378	GLY	2.9
1	H	316	LEU	2.9
1	H	297	ASN	2.9
1	E	284	ILE	2.9
1	A	381	VAL	2.9
1	H	213	GLY	2.9
1	H	371	LEU	2.9
1	E	451	TRP	2.8
1	D	406	ALA	2.8
1	F	473	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	268	LYS	2.8
1	H	331	THR	2.7
1	C	407	LYS	2.7
1	H	462	SER	2.7
1	H	375	MET	2.7
1	G	480	GLU	2.7
1	H	63	LEU	2.7
1	D	317	GLN	2.7
1	A	259	GLY	2.7
1	G	367	LYS	2.6
1	D	458	ASP	2.6
1	G	475	PRO	2.6
1	H	296	PRO	2.6
1	G	409	ASN	2.6
1	F	474	ILE	2.6
1	G	465	CYS	2.6
1	H	433	GLU	2.6
1	H	398	VAL	2.6
1	E	379	LYS	2.6
1	H	439	VAL	2.5
1	E	468	ALA	2.5
1	H	290	ALA	2.5
1	H	366	SER	2.5
1	H	358	THR	2.5
1	G	438	ASP	2.5
1	H	206	VAL	2.5
1	H	430	ILE	2.5
1	H	432	THR	2.5
1	H	452	GLU	2.5
1	H	443	LYS	2.5
1	C	90	GLY	2.5
1	H	139	GLY	2.5
1	H	283	GLY	2.5
1	B	460	LYS	2.5
1	B	376	ILE	2.5
1	H	441	ARG	2.5
1	G	434	LYS	2.5
1	H	434	LYS	2.5
1	F	476	MET	2.5
1	H	79	GLU	2.5
1	H	377	PRO	2.5
1	H	431	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	211	ASP	2.5
1	H	34	LEU	2.5
1	E	437	PHE	2.4
1	G	406	ALA	2.4
1	C	415	GLU	2.4
1	C	461	LYS	2.4
1	H	282	LEU	2.4
1	A	139	GLY	2.4
1	E	427	VAL	2.4
1	H	83	PHE	2.4
1	G	405	SER	2.4
1	D	376	ILE	2.4
1	A	407	LYS	2.4
1	F	78	GLY	2.4
1	H	215	PHE	2.4
1	C	261	ASN	2.4
1	A	212	ILE	2.4
1	G	474	ILE	2.4
1	H	62	LEU	2.4
1	G	365	VAL	2.4
1	E	267	ILE	2.3
1	H	90	GLY	2.3
1	F	60	LEU	2.3
1	G	154	ASN	2.3
1	D	466	ASP	2.3
1	H	336	PRO	2.3
1	H	125	LEU	2.3
1	H	424	LYS	2.3
1	F	368	TYR	2.3
1	B	416	LYS	2.3
1	C	262	VAL	2.3
1	H	442	LYS	2.3
1	F	480	GLU	2.3
1	B	479	LEU	2.3
1	G	314	TYR	2.3
1	D	379	LYS	2.3
1	B	76	TYR	2.3
1	E	400	VAL	2.3
1	H	94	VAL	2.3
1	E	296	PRO	2.3
1	G	272	LEU	2.2
1	H	58	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	8	VAL	2.2
1	F	296	PRO	2.2
1	G	471	PRO	2.2
1	H	471	PRO	2.2
1	F	451	TRP	2.2
1	E	407	LYS	2.2
1	H	175	LYS	2.2
1	H	436	VAL	2.2
1	E	272	LEU	2.2
1	H	368	TYR	2.2
1	G	271	ALA	2.2
1	G	318	ASN	2.2
1	H	142	ALA	2.2
1	G	431	ILE	2.2
1	H	382	LYS	2.2
1	A	85	ARG	2.2
1	F	141	ILE	2.2
1	E	447	LEU	2.2
1	G	466	ASP	2.2
1	A	457	ASP	2.1
1	G	478	GLN	2.1
1	E	458	ASP	2.1
1	H	417	CYS	2.1
1	G	83	PHE	2.1
1	F	234	GLU	2.1
1	H	412	LYS	2.1
1	F	406	ALA	2.1
1	B	65	GLN	2.1
1	E	440	ASP	2.1
1	B	247	LYS	2.1
1	C	76	TYR	2.1
1	C	479	LEU	2.0
1	F	448	ILE	2.0
1	H	403	GLU	2.0
1	E	380	LEU	2.0
1	G	286	ILE	2.0
1	B	318	ASN	2.0
1	A	1	THR	2.0
1	H	150	VAL	2.0
1	E	83	PHE	2.0
1	E	293	PHE	2.0
1	E	243	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	473	LEU	2.0
1	E	359	MET	2.0
1	H	123	GLY	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

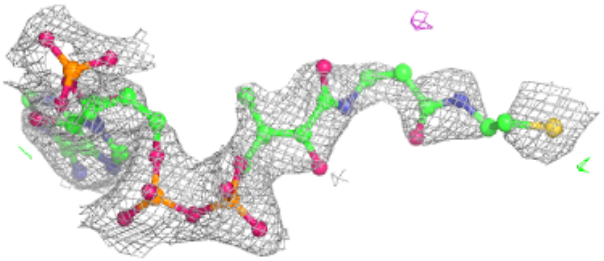
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

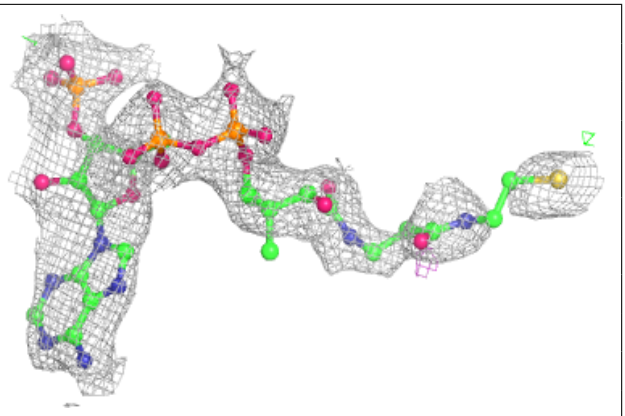
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	COA	H	1305	48/48	0.83	0.22	55,67,77,80	0
3	COA	F	1305	48/48	0.85	0.18	40,51,68,72	0
3	COA	G	1305	48/48	0.88	0.15	29,45,57,59	0
3	COA	E	1305	48/48	0.89	0.15	39,48,65,70	0
2	CL	B	489	1/1	0.98	0.07	37,37,37,37	0
2	CL	D	489	1/1	0.98	0.05	36,36,36,36	0
2	CL	C	489	1/1	0.99	0.10	39,39,39,39	0

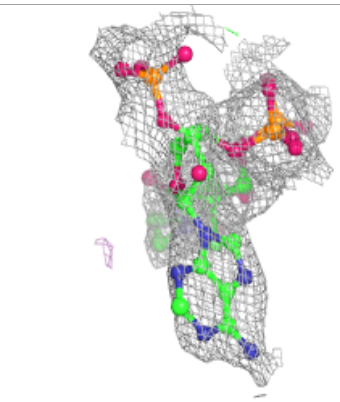
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around COA H 1305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

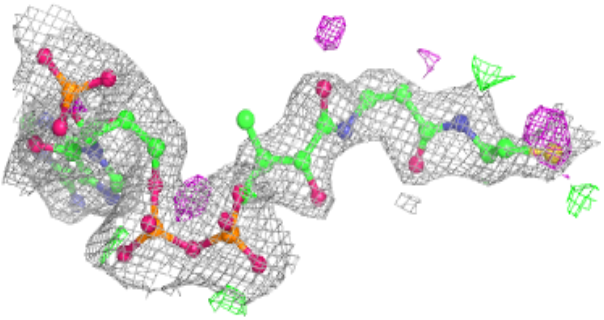


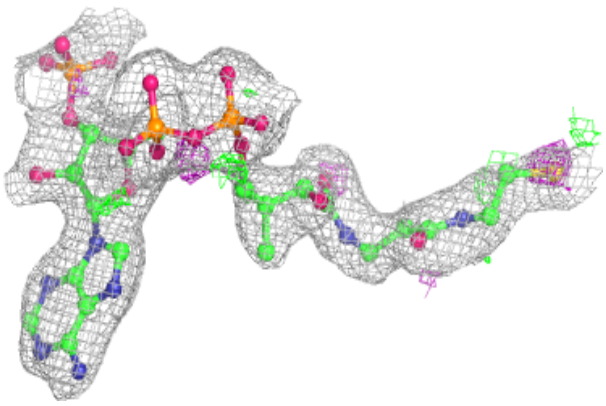


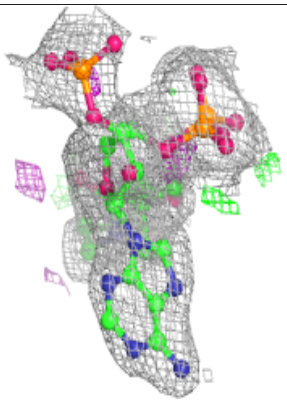


Electron density around COA F 1305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

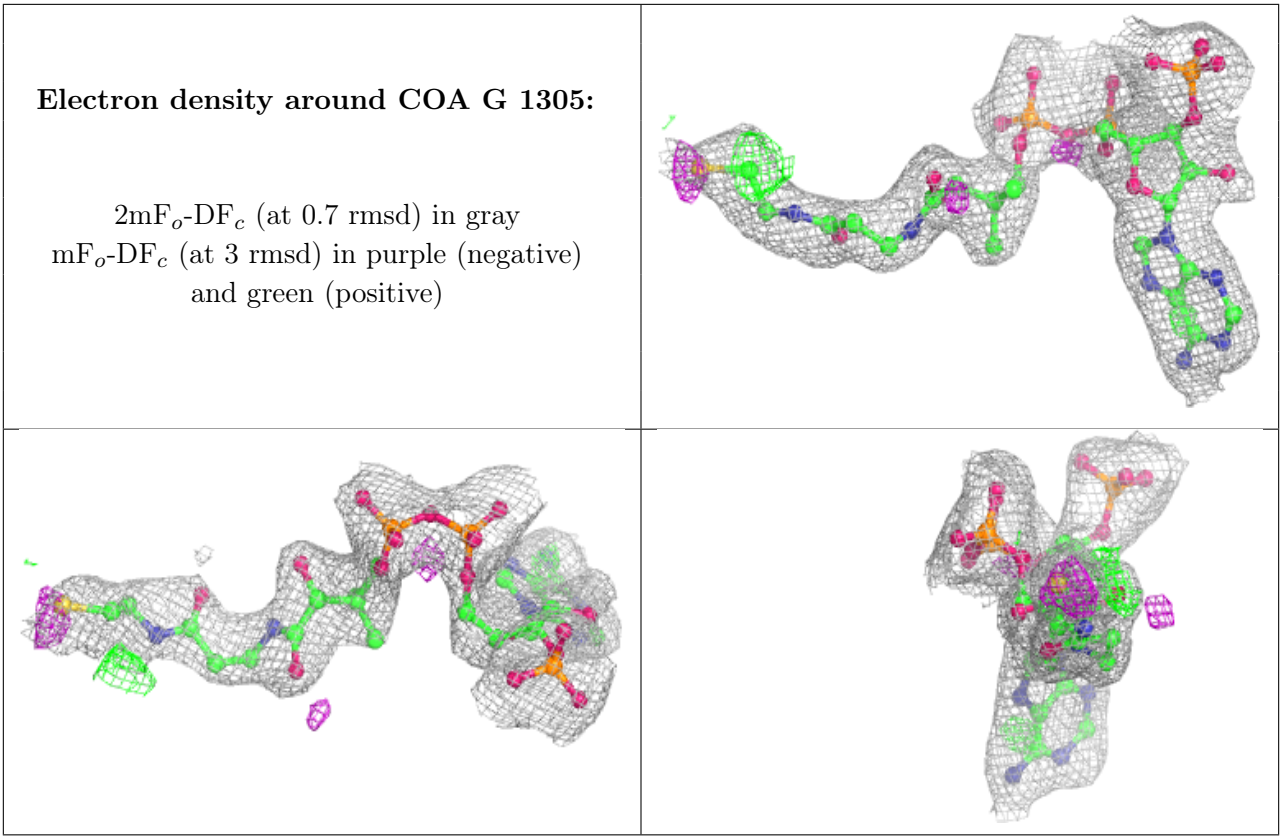






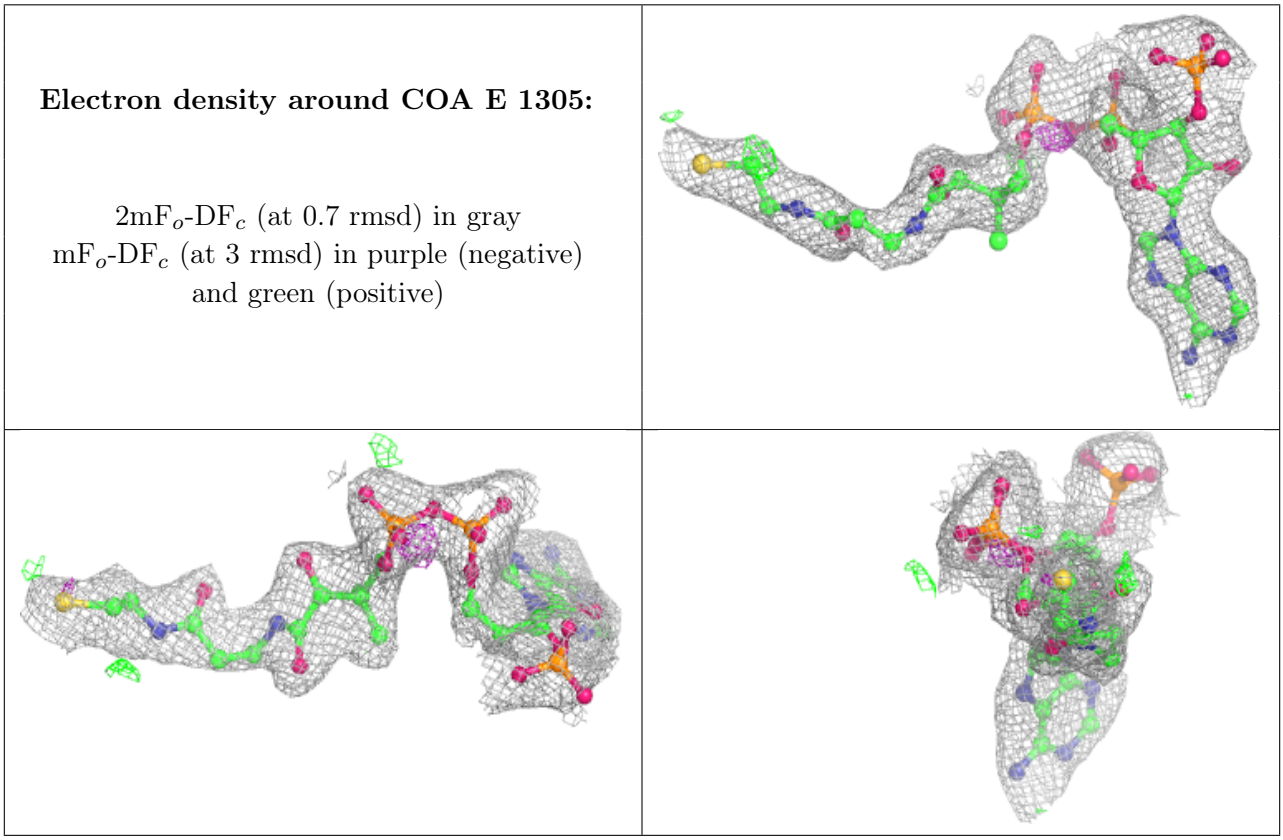
Electron density around COA G 1305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around COA E 1305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.