wwPDB X-ray Structure Validation Summary Report (i)

Mar 20, 2025 – 02:28 PM EDT

PDB ID	:	3U9S
Title	:	Crystal structure of P. aeruginosa 3-methylcrotonyl-CoA carboxylase (MCC) 750 kD holoenzyme, CoA complex
Authors	:	Huang, C.S.; Tong, L.
Deposited on	:	2011-10-19
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

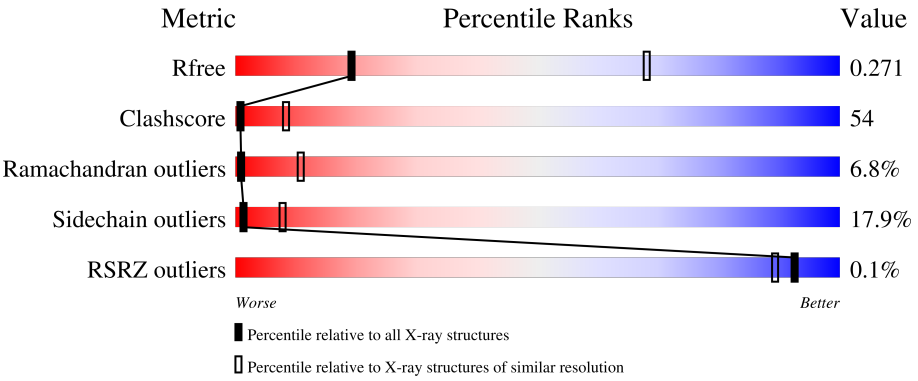
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	655	27% 48% 17% • 5%
1	C	655	24% 44% 14% • 16%
1	E	655	25% 42% 16% • 16%
1	G	655	25% 42% 15% • 16%
1	I	655	23% 40% 12% • 24%

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Mol	Chain	Length	Quality of chain
1	K	655	23% 38% 13% 24%
2	B	555	35% 51% 10%
2	D	555	35% 50% 12%
2	F	555	30% 55% 11%
2	H	555	35% 49% 13%
2	J	555	36% 50% 10%
2	L	555	33% 54% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 49939 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 Methylcrotonyl-CoA carboxylase, alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	0	0
			4778	2978	892	886	22			
1	C	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	E	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	G	552	Total	C	N	O	S	0	0	0
			4280	2666	809	787	18			
1	I	498	Total	C	N	O	S	0	0	0
			3853	2399	731	707	16			
1	K	497	Total	C	N	O	S	0	0	0
			3844	2393	729	706	16			

- Molecule 2 is a protein called Methylcrotonyl-CoA carboxylase, beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	D	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	F	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	H	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	J	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			
2	L	537	Total	C	N	O	S	0	0	0
			4051	2560	728	741	22			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	expression tag	UNP Q9I297

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLY	-	expression tag	UNP Q9I297
B	10	SER	-	expression tag	UNP Q9I297
B	11	SER	-	expression tag	UNP Q9I297
B	12	HIS	-	expression tag	UNP Q9I297
B	13	HIS	-	expression tag	UNP Q9I297
B	14	HIS	-	expression tag	UNP Q9I297
B	15	HIS	-	expression tag	UNP Q9I297
B	16	HIS	-	expression tag	UNP Q9I297
B	17	HIS	-	expression tag	UNP Q9I297
B	18	SER	-	expression tag	UNP Q9I297
B	19	SER	-	expression tag	UNP Q9I297
B	20	GLY	-	expression tag	UNP Q9I297
B	21	LEU	-	expression tag	UNP Q9I297
B	22	VAL	-	expression tag	UNP Q9I297
B	23	PRO	-	expression tag	UNP Q9I297
B	24	ARG	-	expression tag	UNP Q9I297
B	25	GLY	-	expression tag	UNP Q9I297
B	26	SER	-	expression tag	UNP Q9I297
B	27	HIS	-	expression tag	UNP Q9I297
D	8	MET	-	expression tag	UNP Q9I297
D	9	GLY	-	expression tag	UNP Q9I297
D	10	SER	-	expression tag	UNP Q9I297
D	11	SER	-	expression tag	UNP Q9I297
D	12	HIS	-	expression tag	UNP Q9I297
D	13	HIS	-	expression tag	UNP Q9I297
D	14	HIS	-	expression tag	UNP Q9I297
D	15	HIS	-	expression tag	UNP Q9I297
D	16	HIS	-	expression tag	UNP Q9I297
D	17	HIS	-	expression tag	UNP Q9I297
D	18	SER	-	expression tag	UNP Q9I297
D	19	SER	-	expression tag	UNP Q9I297
D	20	GLY	-	expression tag	UNP Q9I297
D	21	LEU	-	expression tag	UNP Q9I297
D	22	VAL	-	expression tag	UNP Q9I297
D	23	PRO	-	expression tag	UNP Q9I297
D	24	ARG	-	expression tag	UNP Q9I297
D	25	GLY	-	expression tag	UNP Q9I297
D	26	SER	-	expression tag	UNP Q9I297
D	27	HIS	-	expression tag	UNP Q9I297
F	8	MET	-	expression tag	UNP Q9I297
F	9	GLY	-	expression tag	UNP Q9I297
F	10	SER	-	expression tag	UNP Q9I297

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Chain	Residue	Modelled	Actual	Comment	Reference
F	11	SER	-	expression tag	UNP Q9I297
F	12	HIS	-	expression tag	UNP Q9I297
F	13	HIS	-	expression tag	UNP Q9I297
F	14	HIS	-	expression tag	UNP Q9I297
F	15	HIS	-	expression tag	UNP Q9I297
F	16	HIS	-	expression tag	UNP Q9I297
F	17	HIS	-	expression tag	UNP Q9I297
F	18	SER	-	expression tag	UNP Q9I297
F	19	SER	-	expression tag	UNP Q9I297
F	20	GLY	-	expression tag	UNP Q9I297
F	21	LEU	-	expression tag	UNP Q9I297
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F	23	PRO	-	expression tag	UNP Q9I297
F	24	ARG	-	expression tag	UNP Q9I297
F	25	GLY	-	expression tag	UNP Q9I297
F	26	SER	-	expression tag	UNP Q9I297
F	27	HIS	-	expression tag	UNP Q9I297
H	8	MET	-	expression tag	UNP Q9I297
H	9	GLY	-	expression tag	UNP Q9I297
H	10	SER	-	expression tag	UNP Q9I297
H	11	SER	-	expression tag	UNP Q9I297
H	12	HIS	-	expression tag	UNP Q9I297
H	13	HIS	-	expression tag	UNP Q9I297
H	14	HIS	-	expression tag	UNP Q9I297
H	15	HIS	-	expression tag	UNP Q9I297
H	16	HIS	-	expression tag	UNP Q9I297
H	17	HIS	-	expression tag	UNP Q9I297
H	18	SER	-	expression tag	UNP Q9I297
H	19	SER	-	expression tag	UNP Q9I297
H	20	GLY	-	expression tag	UNP Q9I297
H	21	LEU	-	expression tag	UNP Q9I297
H	22	VAL	-	expression tag	UNP Q9I297
H	23	PRO	-	expression tag	UNP Q9I297
H	24	ARG	-	expression tag	UNP Q9I297
H	25	GLY	-	expression tag	UNP Q9I297
H	26	SER	-	expression tag	UNP Q9I297
H	27	HIS	-	expression tag	UNP Q9I297
J	8	MET	-	expression tag	UNP Q9I297
J	9	GLY	-	expression tag	UNP Q9I297
J	10	SER	-	expression tag	UNP Q9I297
J	11	SER	-	expression tag	UNP Q9I297
J	12	HIS	-	expression tag	UNP Q9I297

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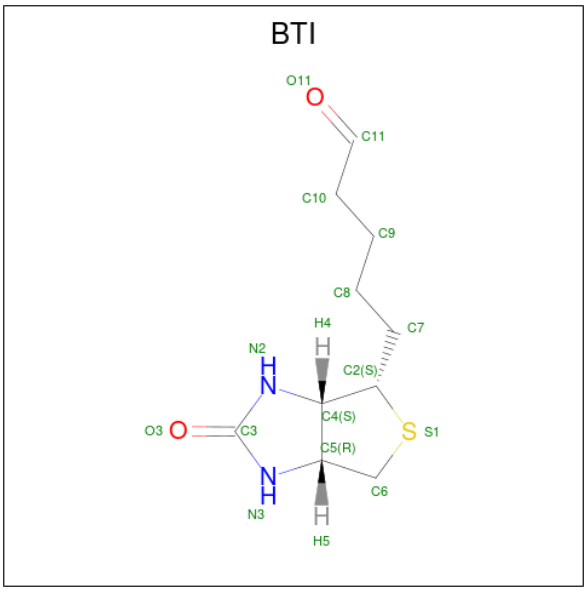
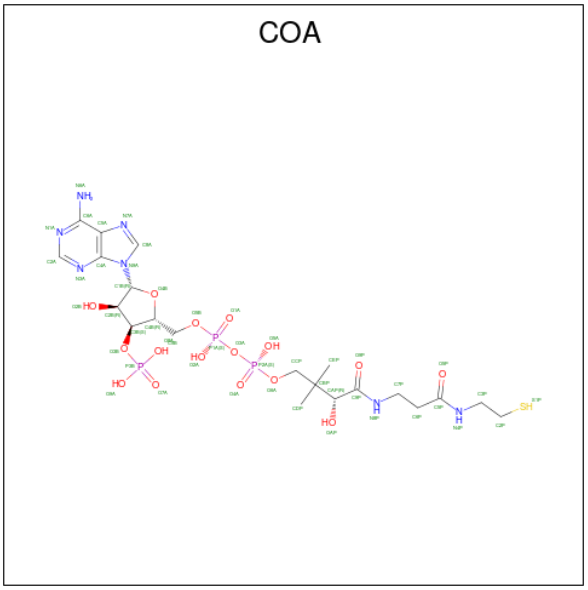
Chain	Residue	Modelled	Actual	Comment	Reference
J	13	HIS	-	expression tag	UNP Q9I297
J	14	HIS	-	expression tag	UNP Q9I297
J	15	HIS	-	expression tag	UNP Q9I297
J	16	HIS	-	expression tag	UNP Q9I297
J	17	HIS	-	expression tag	UNP Q9I297
J	18	SER	-	expression tag	UNP Q9I297
J	19	SER	-	expression tag	UNP Q9I297
J	20	GLY	-	expression tag	UNP Q9I297
J	21	LEU	-	expression tag	UNP Q9I297
J	22	VAL	-	expression tag	UNP Q9I297
J	23	PRO	-	expression tag	UNP Q9I297
J	24	ARG	-	expression tag	UNP Q9I297
J	25	GLY	-	expression tag	UNP Q9I297
J	26	SER	-	expression tag	UNP Q9I297
J	27	HIS	-	expression tag	UNP Q9I297
L	8	MET	-	expression tag	UNP Q9I297
L	9	GLY	-	expression tag	UNP Q9I297
L	10	SER	-	expression tag	UNP Q9I297
L	11	SER	-	expression tag	UNP Q9I297
L	12	HIS	-	expression tag	UNP Q9I297
L	13	HIS	-	expression tag	UNP Q9I297
L	14	HIS	-	expression tag	UNP Q9I297
L	15	HIS	-	expression tag	UNP Q9I297
L	16	HIS	-	expression tag	UNP Q9I297
L	17	HIS	-	expression tag	UNP Q9I297
L	18	SER	-	expression tag	UNP Q9I297
L	19	SER	-	expression tag	UNP Q9I297
L	20	GLY	-	expression tag	UNP Q9I297
L	21	LEU	-	expression tag	UNP Q9I297
L	22	VAL	-	expression tag	UNP Q9I297
L	23	PRO	-	expression tag	UNP Q9I297
L	24	ARG	-	expression tag	UNP Q9I297
L	25	GLY	-	expression tag	UNP Q9I297
L	26	SER	-	expression tag	UNP Q9I297
L	27	HIS	-	expression tag	UNP Q9I297

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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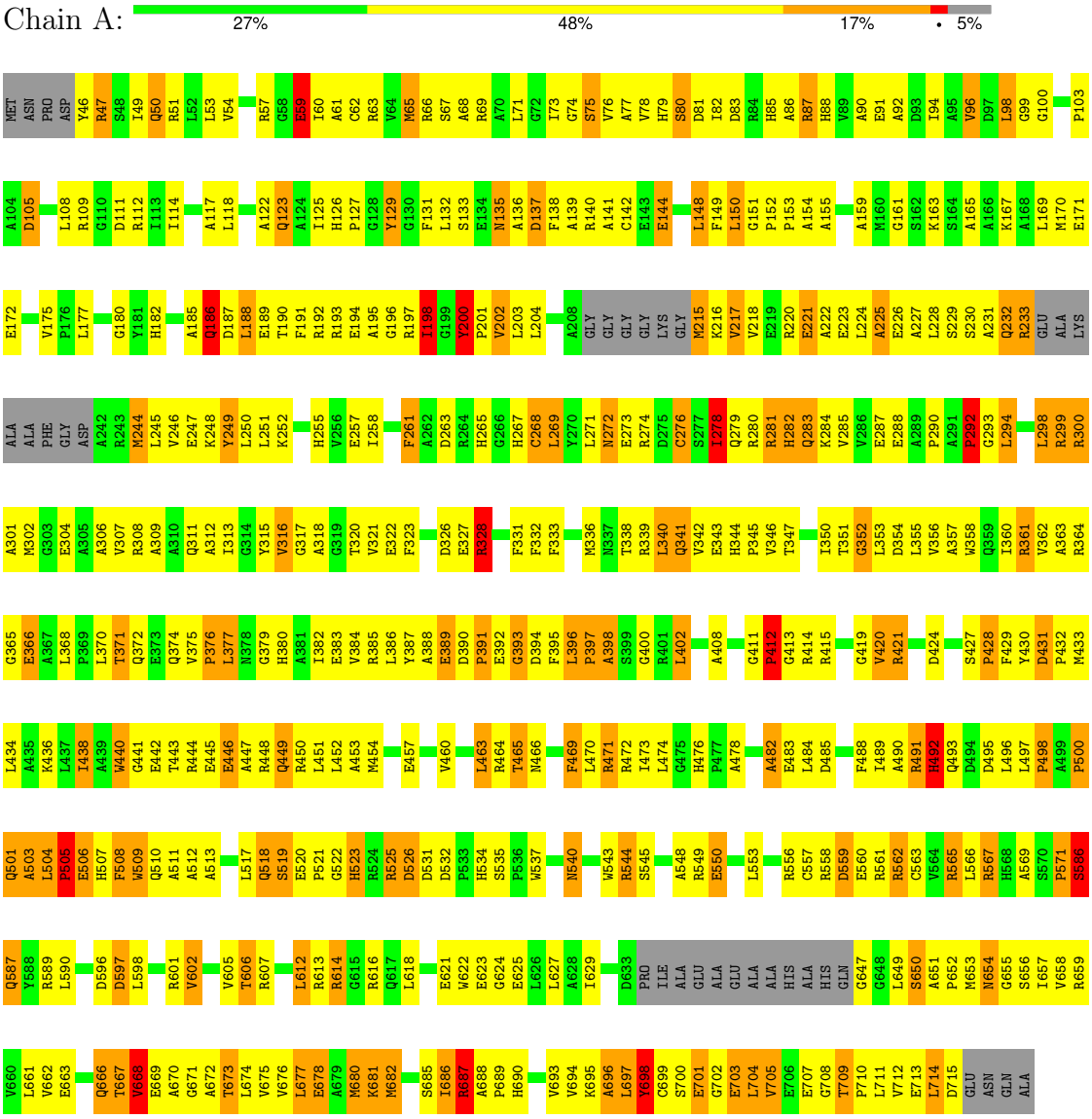
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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.

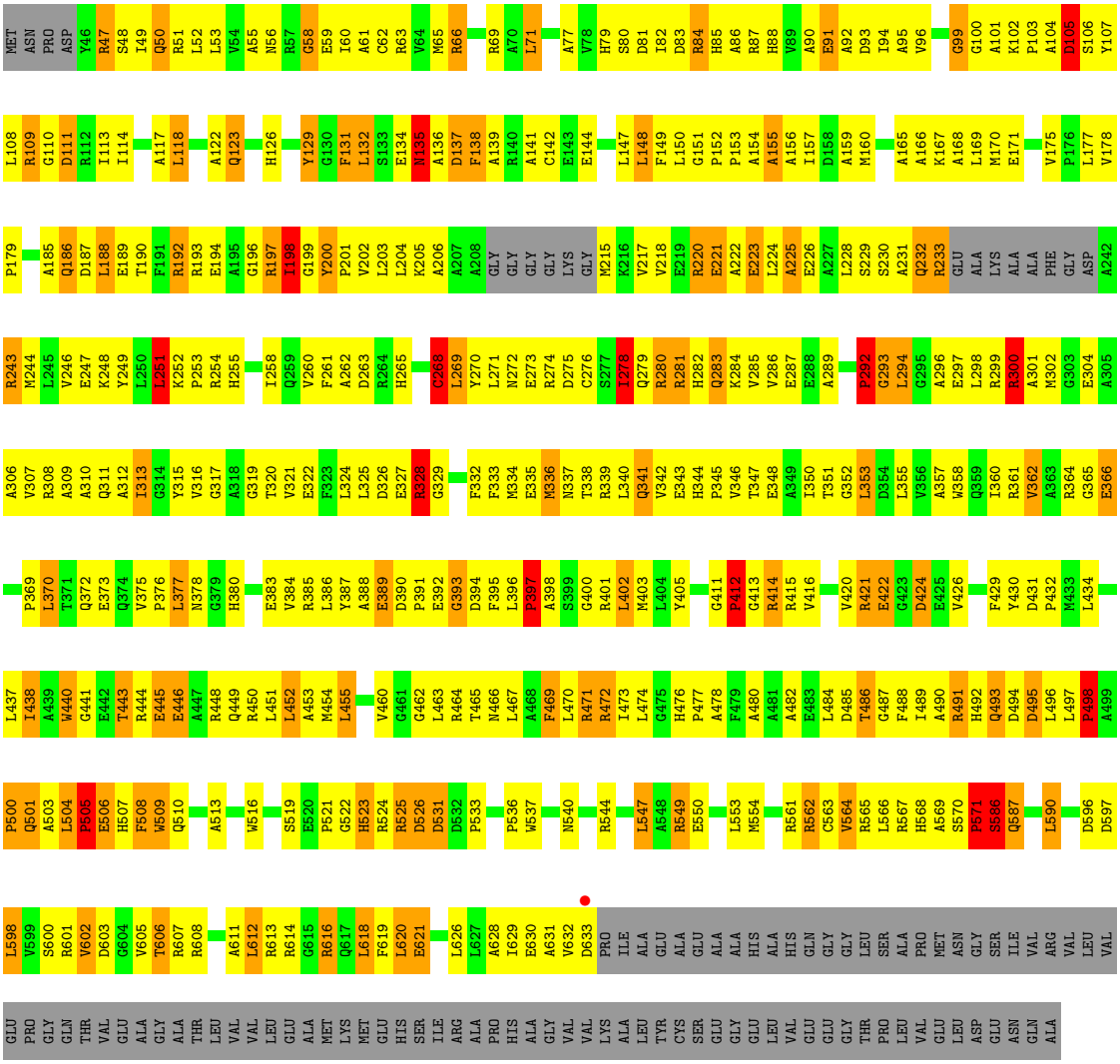
• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

Chain A:



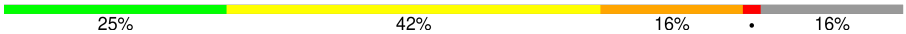
• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

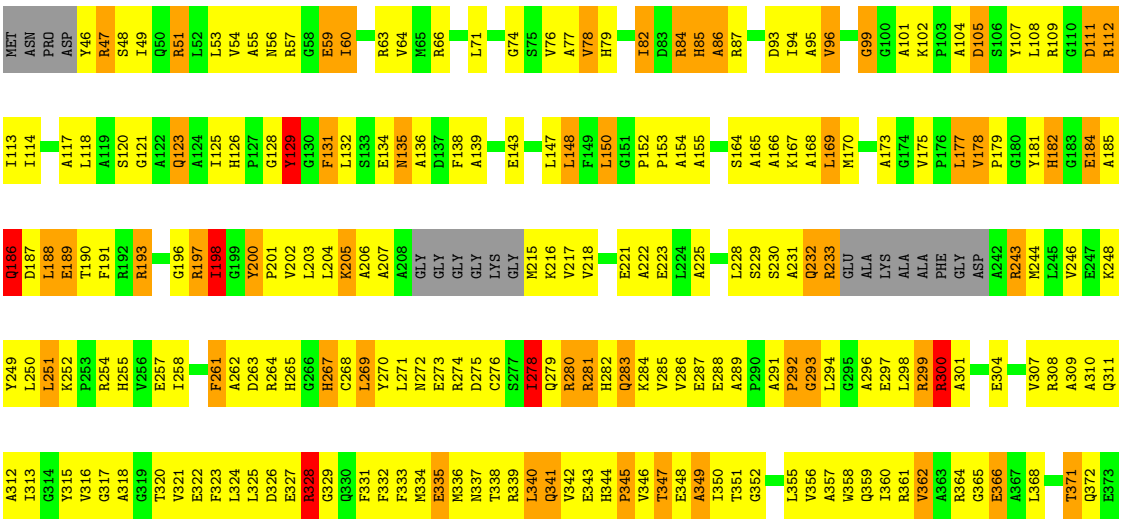
Chain C:

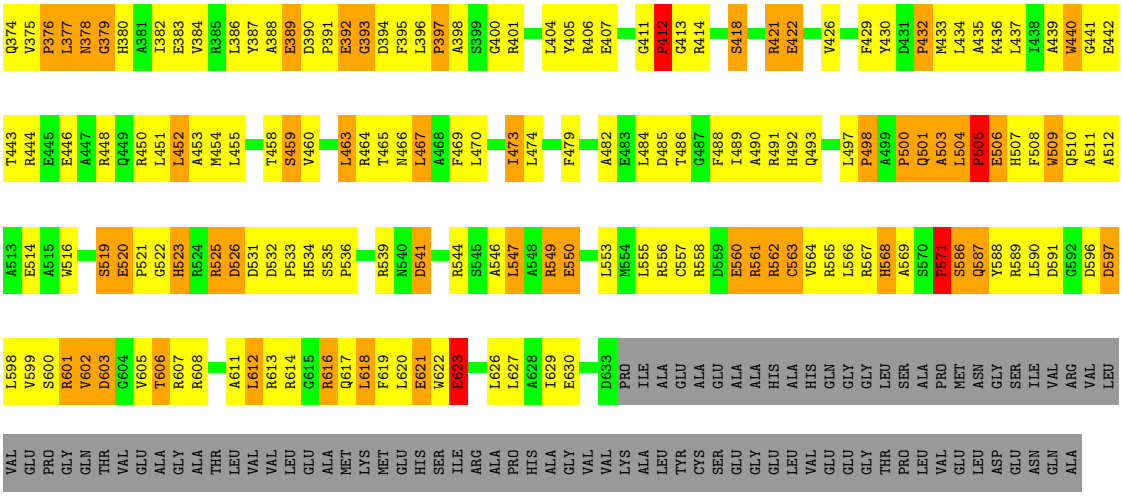


• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

Chain E:

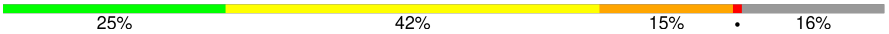


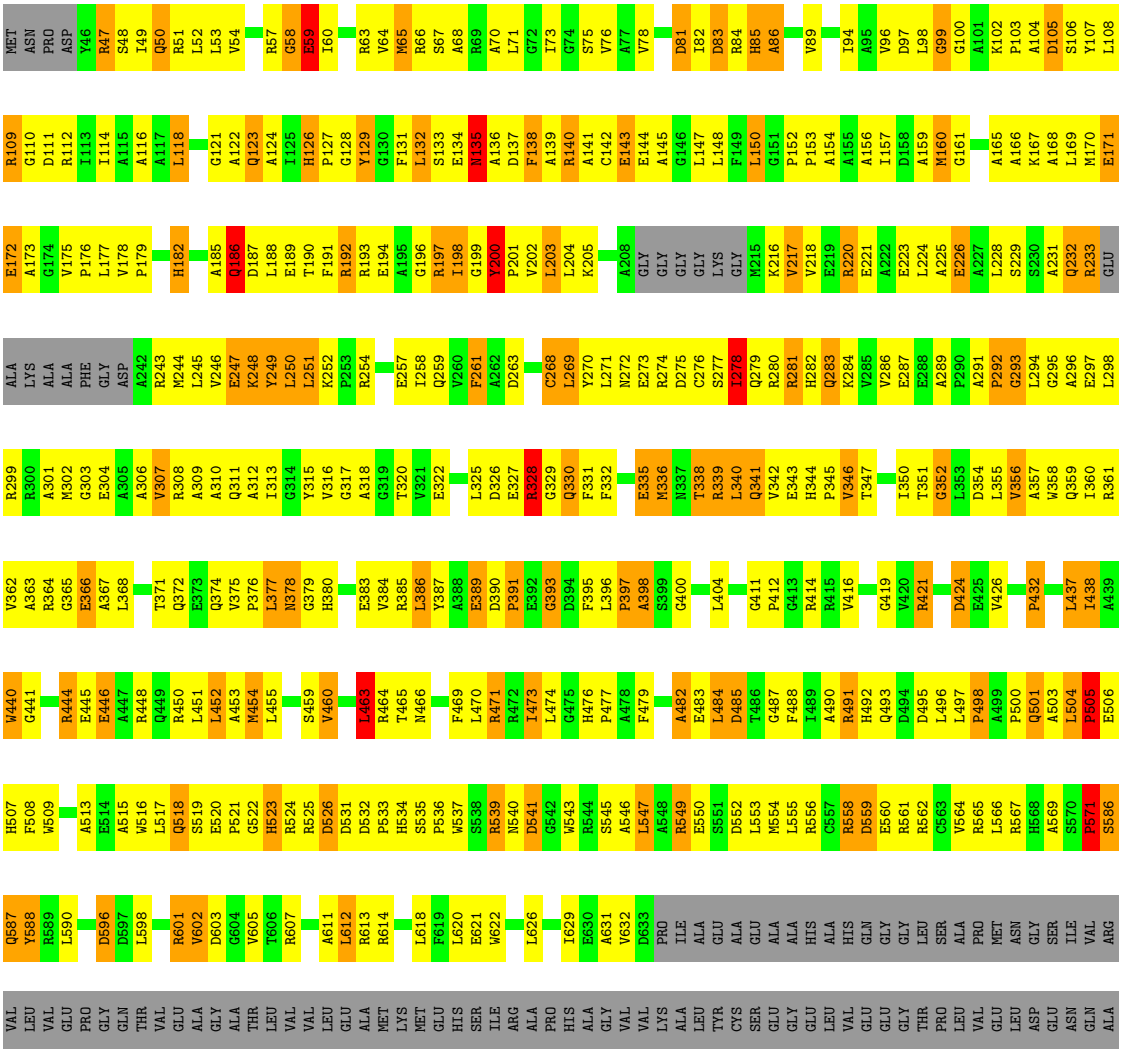




• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

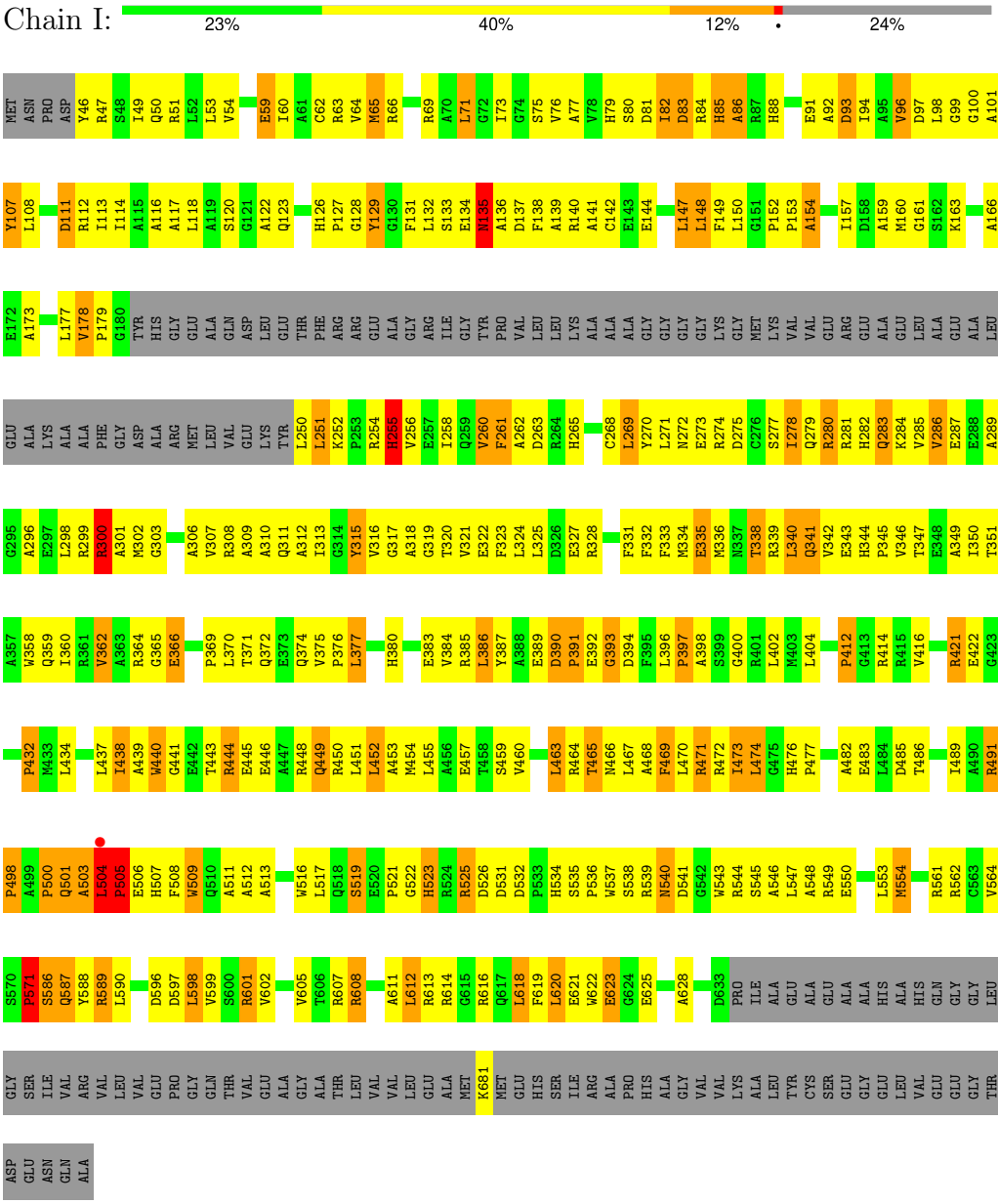
Chain G:





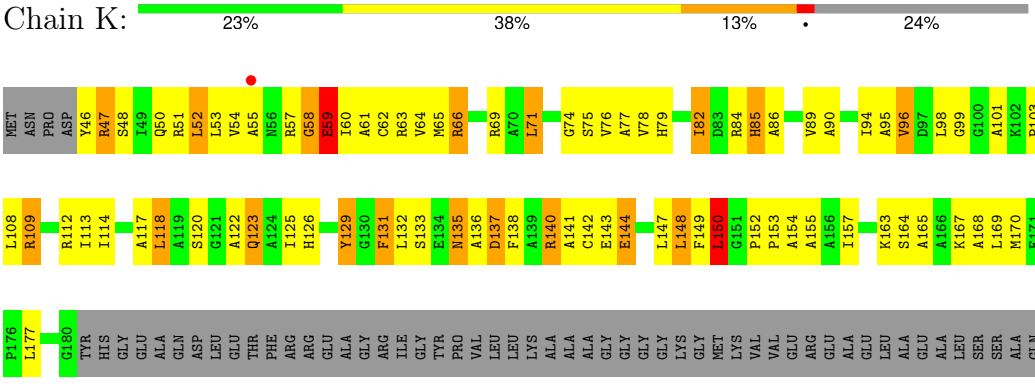
• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

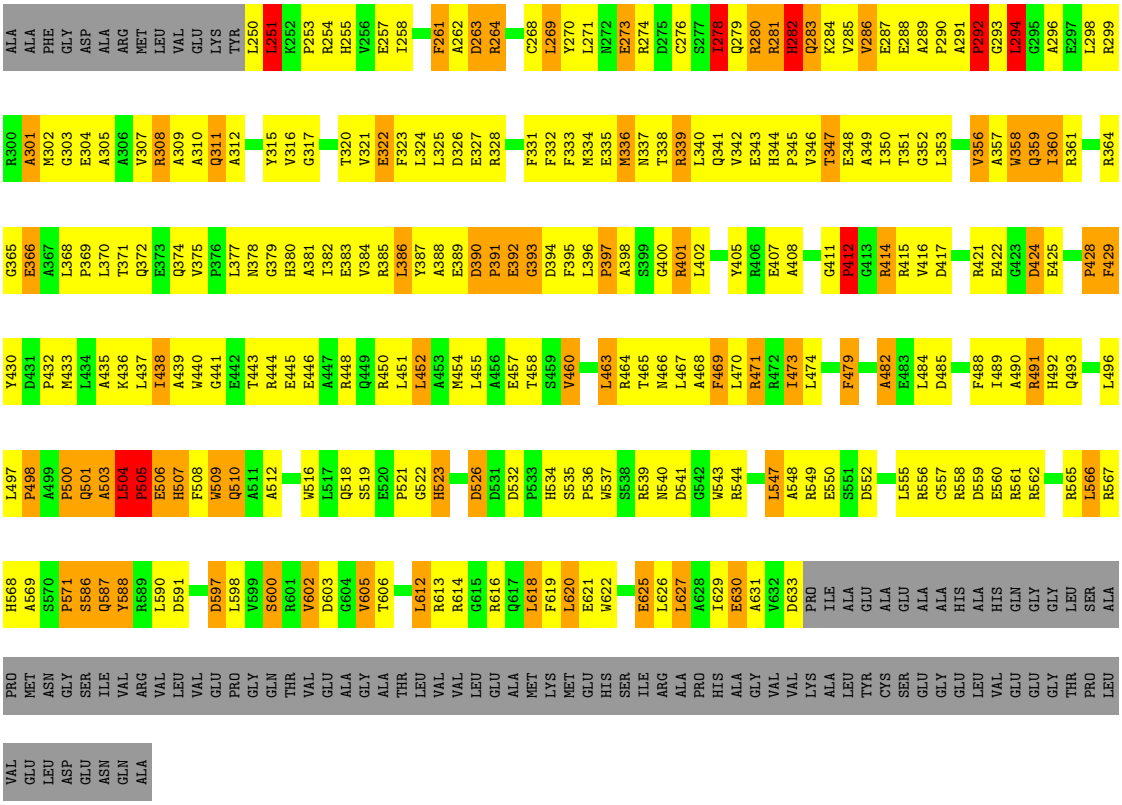
Chain I:



• Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit

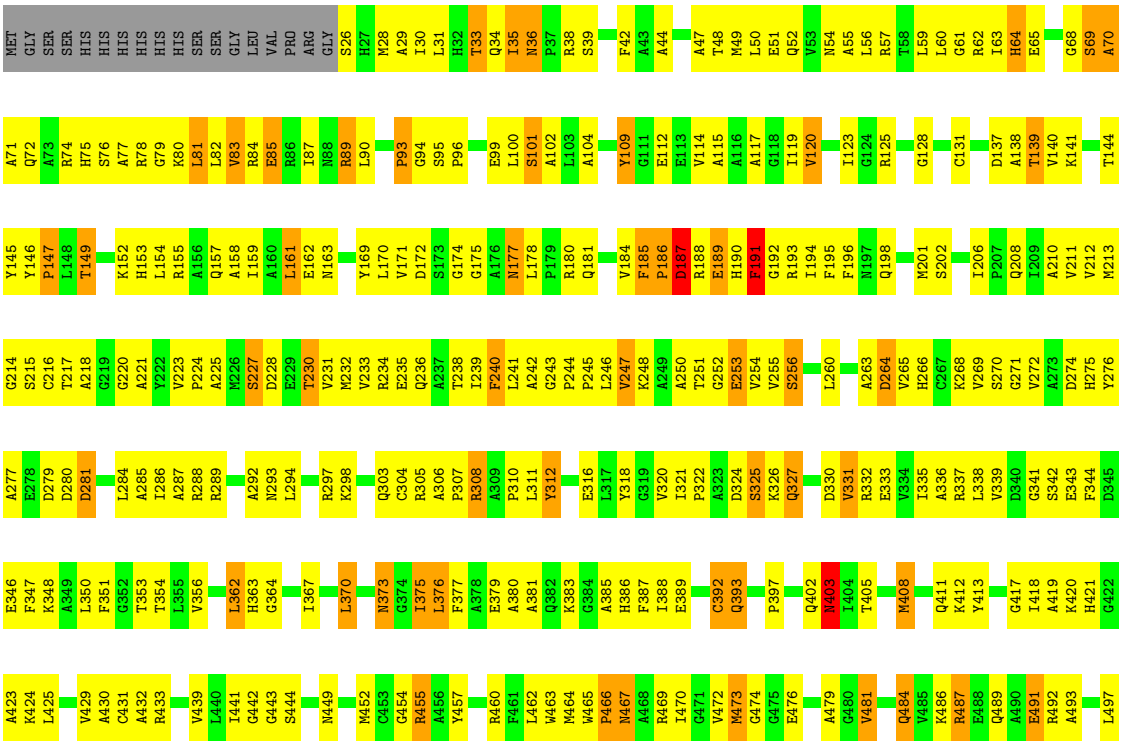
Chain K:

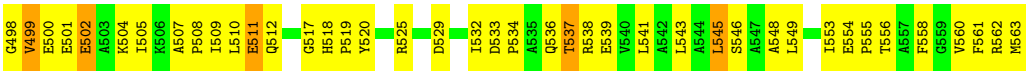




• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

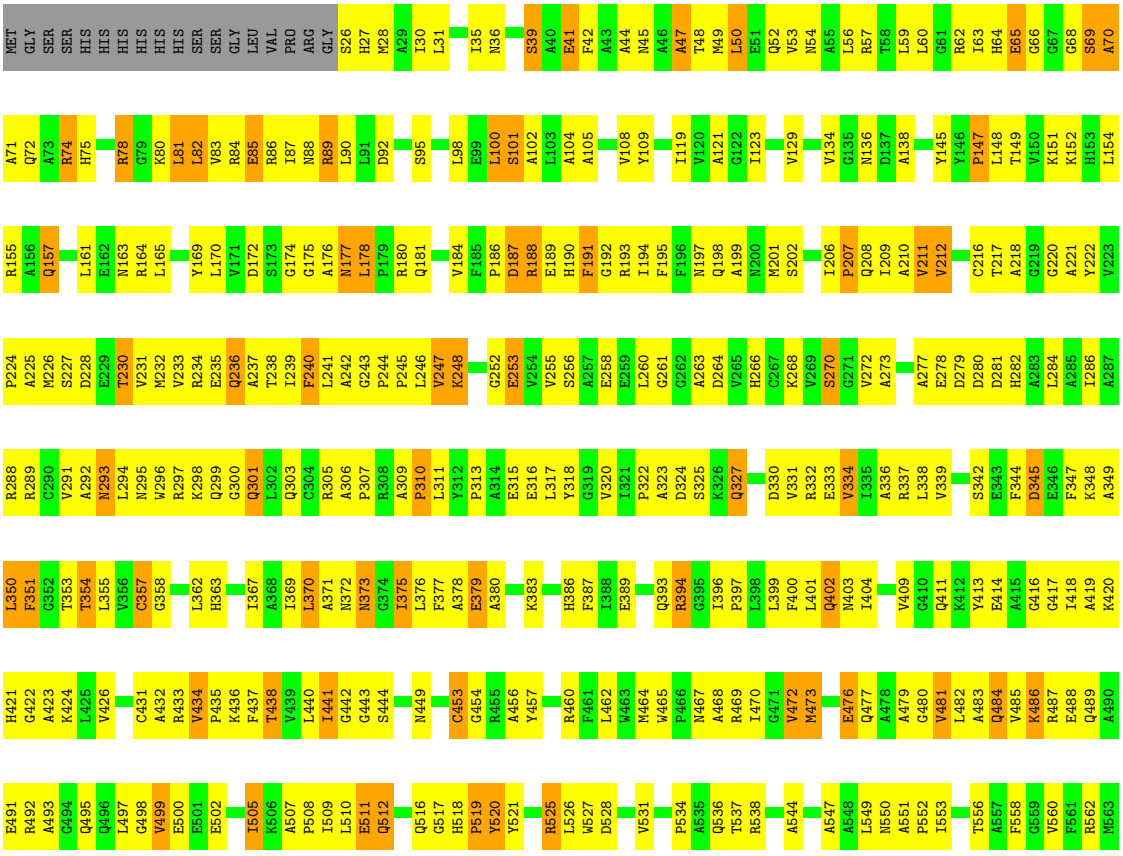
Chain B:





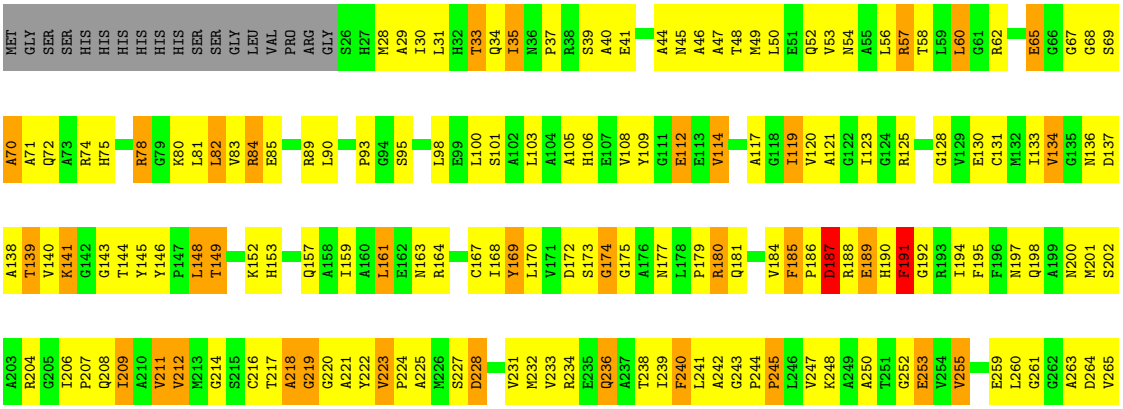
• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

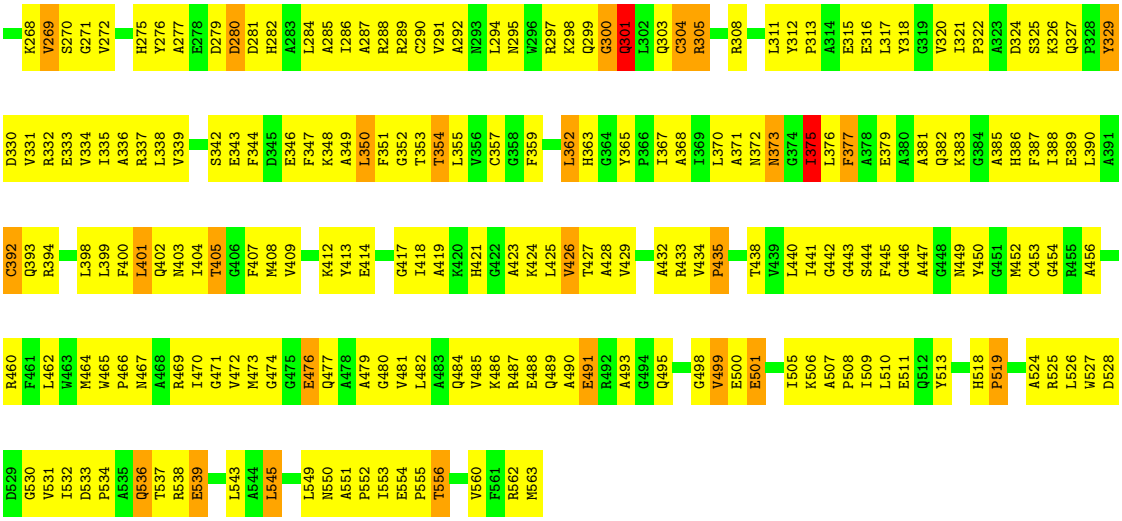
Chain D:



• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

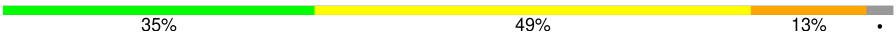
Chain F:

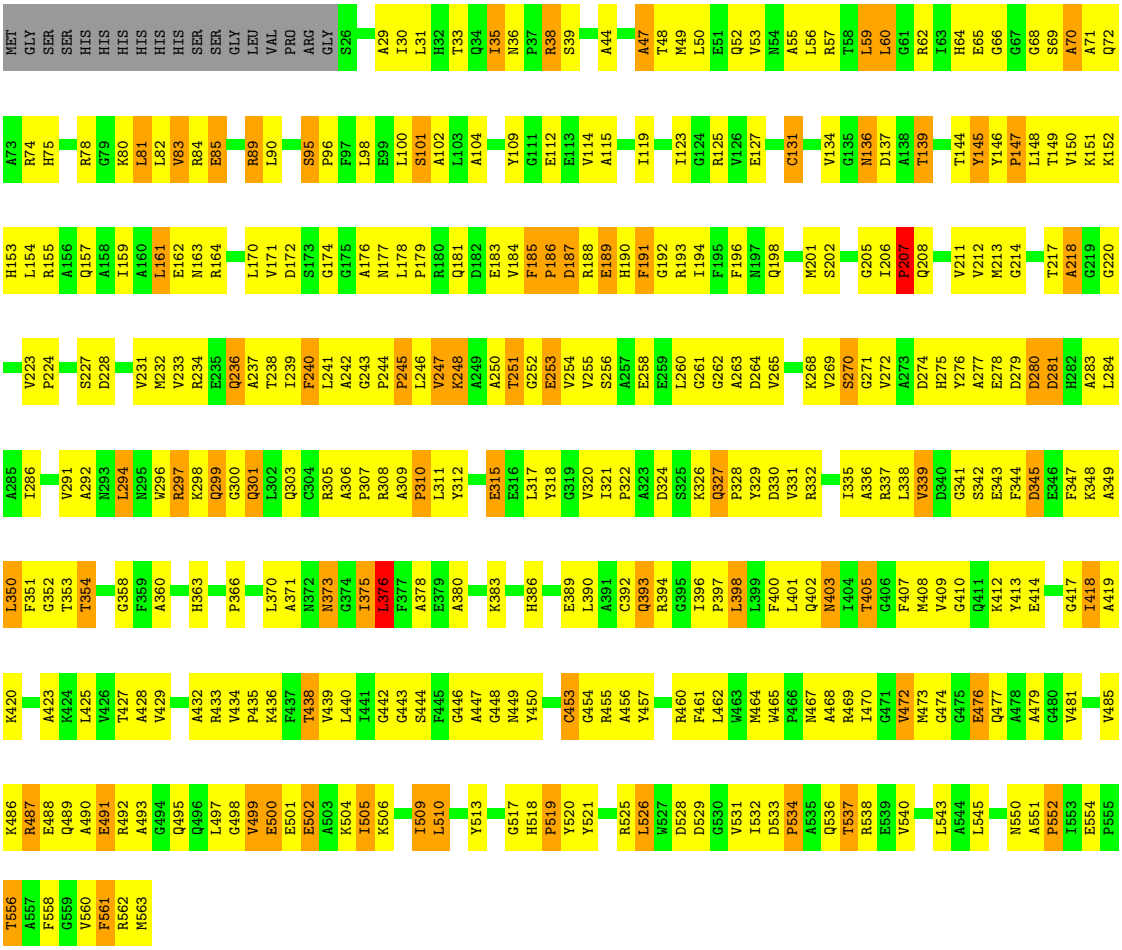




• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

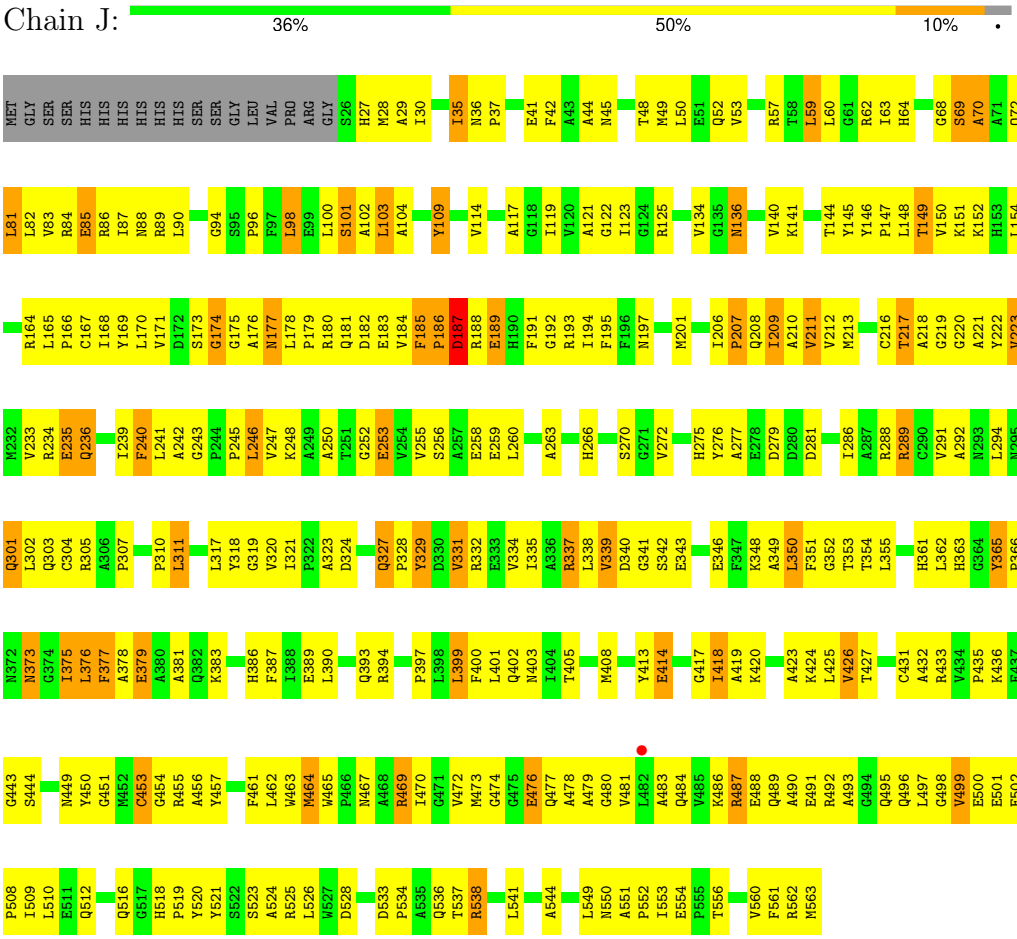
Chain H:





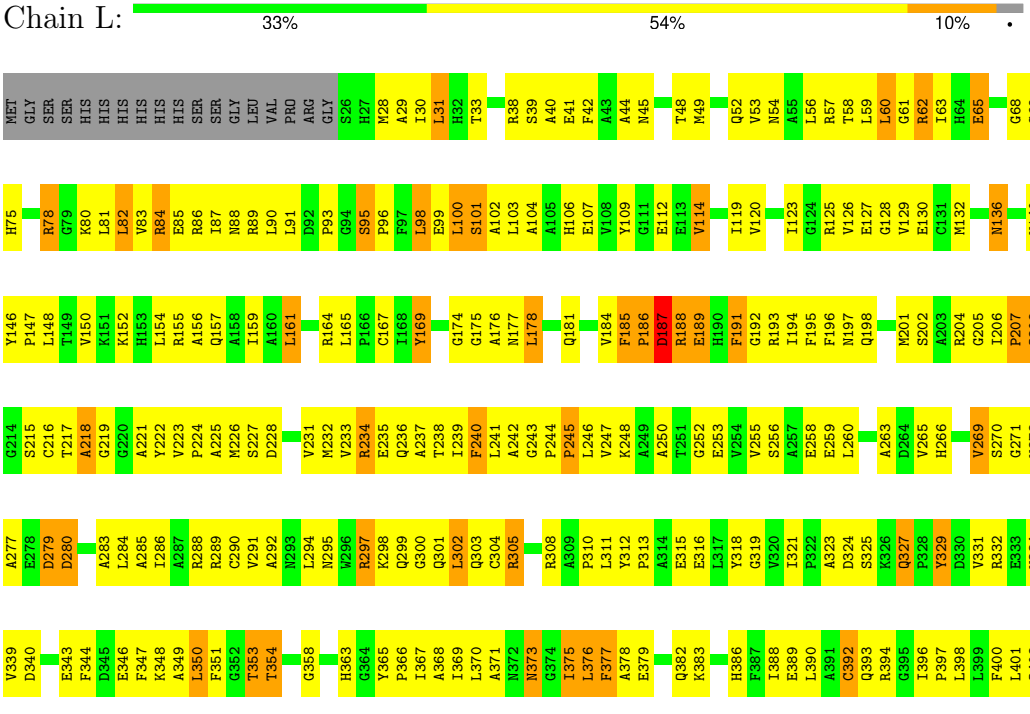
• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain J:



• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain L:




M408 V409 G410 Q411 K412 Y413 E414 G417 I418 A419 K420 H421 K424 L425 V426 V429 A430 C431 A432 R433 V434 P435 K436 F437 T438 V439 L440 I441 G442 G443 S444 F445 N449 Y450 G451 R455 D458 P459 R460 F461 L462 W463 M464 W465 P466 N467 I470 G471 V472 M473 G474 G475 E476
Q477 A478 A479 G480 V481 L482 A483 Q484 V485 K486 R487 E488 E491 R492 A493 L497 G498 V499 E500 E501 I505 K506 A507 P508 I509 L510 Q516 G517 H518 P519 Y520 Y521 A524 R525 L526 W527 D528 V531 I532 Q536 T537 R538 E539 V540 L541 A542 L543 A544 L545 L549 N550 A551
P552 I553 E554 P555 T556 A557 F558 G559 V560 F561 R562 M563

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.51Å 255.34Å 152.67Å 90.00° 95.74° 90.00°	Depositor
Resolution (Å)	48.90 – 3.50 48.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.0 (48.90-3.50) 83.0 (48.90-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.292 0.212 , 0.271	Depositor DCC
R_{free} test set	5856 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 79.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	49939	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: COA, BTI

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	0.68	0/4866	0.87	4/6581 (0.1%)
1	C	0.63	0/4362	0.86	3/5897 (0.1%)
1	E	0.65	1/4362 (0.0%)	0.85	3/5897 (0.1%)
1	G	0.65	0/4362	0.87	0/5897
1	I	0.66	0/3929	0.84	1/5315 (0.0%)
1	K	0.68	0/3921	0.85	2/5307 (0.0%)
2	B	0.67	0/4135	0.86	1/5605 (0.0%)
2	D	0.67	0/4135	0.86	3/5605 (0.1%)
2	F	0.64	0/4135	0.87	3/5605 (0.1%)
2	H	0.67	3/4135 (0.1%)	0.83	1/5605 (0.0%)
2	J	0.68	0/4135	0.87	2/5605 (0.0%)
2	L	0.67	0/4135	0.87	0/5605
All	All	0.66	4/50612 (0.0%)	0.86	23/68524 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	G	0	2
1	I	0	1
2	B	0	1
2	H	0	1
2	J	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	131	CYS	CB-SG	-7.11	1.70	1.82
1	E	563	CYS	CB-SG	5.92	1.92	1.82
2	H	189	GLU	CB-CG	5.11	1.61	1.52
2	H	189	GLU	CG-CD	5.11	1.59	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	399	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	E	506	GLU	N-CA-C	-6.63	93.10	111.00
1	C	506	GLU	N-CA-C	-6.45	93.60	111.00
1	E	566	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	298	LEU	CA-CB-CG	-5.94	101.63	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	698	TYR	Sidechain
2	B	109	TYR	Sidechain
1	E	129	TYR	Sidechain
1	G	129	TYR	Sidechain
1	G	588	TYR	Sidechain

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	4778	0	4730	583	0
1	C	4280	0	4227	535	0
1	E	4280	0	4227	519	0
1	G	4280	0	4227	516	0
1	I	3853	0	3795	477	0
1	K	3844	0	3786	485	0
2	B	4051	0	4023	401	0
2	D	4051	0	4023	425	0
2	F	4051	0	4023	437	0
2	H	4051	0	4023	422	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	4051	0	4023	425	0
2	L	4051	0	4023	419	0
3	A	15	0	15	3	0
3	I	15	0	15	4	0
4	B	48	0	32	4	0
4	D	48	0	32	3	0
4	F	48	0	32	3	0
4	H	48	0	32	6	0
4	J	48	0	32	4	0
4	L	48	0	32	2	0
All	All	49939	0	49352	5408	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 54.

The worst 5 of 5408 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:504:LEU:HB3	1:C:505:PRO:HD2	1.23	1.17
1:G:200:TYR:CE1	1:G:221:GLU:HA	1.82	1.15
1:G:278:ILE:H	1:G:278:ILE:HD12	1.10	1.14
1:K:101:ALA:HB1	1:K:429:PHE:CE1	1.83	1.14
2:F:231:VAL:HG22	2:F:275:HIS:HB2	1.18	1.12

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	613/655 (94%)	427 (70%)	114 (19%)	72 (12%)	0 5
1	C	546/655 (83%)	382 (70%)	113 (21%)	51 (9%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	546/655 (83%)	384 (70%)	109 (20%)	53 (10%)	0 6
1	G	546/655 (83%)	381 (70%)	113 (21%)	52 (10%)	0 6
1	I	493/655 (75%)	353 (72%)	101 (20%)	39 (8%)	1 8
1	K	493/655 (75%)	364 (74%)	88 (18%)	41 (8%)	0 8
2	B	535/555 (96%)	448 (84%)	63 (12%)	24 (4%)	2 18
2	D	535/555 (96%)	456 (85%)	62 (12%)	17 (3%)	3 25
2	F	535/555 (96%)	439 (82%)	73 (14%)	23 (4%)	2 19
2	H	535/555 (96%)	450 (84%)	60 (11%)	25 (5%)	2 17
2	J	535/555 (96%)	452 (84%)	65 (12%)	18 (3%)	3 24
2	L	535/555 (96%)	438 (82%)	76 (14%)	21 (4%)	2 21
All	All	6447/7260 (89%)	4974 (77%)	1037 (16%)	436 (7%)	1 11

5 of 436 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	225	ALA
1	A	230	SER
1	A	294	LEU
1	A	366	GLU

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	477/496 (96%)	384 (80%)	93 (20%)	1 6
1	C	423/496 (85%)	336 (79%)	87 (21%)	1 5
1	E	423/496 (85%)	330 (78%)	93 (22%)	1 4
1	G	423/496 (85%)	329 (78%)	94 (22%)	1 4
1	I	382/496 (77%)	305 (80%)	77 (20%)	1 5
1	K	381/496 (77%)	300 (79%)	81 (21%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	401/418 (96%)	341 (85%)	60 (15%)	2 14
2	D	401/418 (96%)	340 (85%)	61 (15%)	2 14
2	F	401/418 (96%)	339 (84%)	62 (16%)	2 13
2	H	401/418 (96%)	338 (84%)	63 (16%)	2 13
2	J	401/418 (96%)	354 (88%)	47 (12%)	4 21
2	L	401/418 (96%)	341 (85%)	60 (15%)	2 14
All	All	4915/5484 (90%)	4037 (82%)	878 (18%)	1 8

5 of 878 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	85	HIS
2	H	256	SER
2	L	560	VAL
1	K	518	GLN
1	G	172	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	386	HIS
2	J	382	GLN
2	H	449	ASN
1	I	492	HIS
2	J	484	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	COA	B	591	-	43,50,50	0.94	2 (4%)	56,75,75	1.23	2 (3%)
3	BTI	A	801	1	15,16,16	1.68	1 (6%)	20,21,21	2.34	7 (35%)
4	COA	D	591	-	43,50,50	0.94	2 (4%)	56,75,75	1.20	2 (3%)
4	COA	L	591	-	43,50,50	0.86	1 (2%)	56,75,75	1.33	3 (5%)
4	COA	H	591	-	43,50,50	0.93	1 (2%)	56,75,75	1.24	2 (3%)
4	COA	J	591	-	43,50,50	0.93	1 (2%)	56,75,75	1.20	2 (3%)
4	COA	F	591	-	43,50,50	0.89	1 (2%)	56,75,75	1.25	3 (5%)
3	BTI	I	801	1	15,16,16	1.69	1 (6%)	20,21,21	2.30	7 (35%)

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
4	COA	B	591	-	-	12/44/64/64	0/3/3/3
3	BTI	A	801	1	-	5/6/27/27	0/2/2/2
4	COA	D	591	-	-	12/44/64/64	0/3/3/3
4	COA	L	591	-	-	15/44/64/64	0/3/3/3
4	COA	H	591	-	-	13/44/64/64	0/3/3/3
4	COA	J	591	-	-	14/44/64/64	0/3/3/3
4	COA	F	591	-	-	13/44/64/64	0/3/3/3
3	BTI	I	801	1	-	5/6/27/27	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	801	BTI	O3-C3	6.16	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	BTI	O3-C3	6.12	1.36	1.23
4	F	591	COA	O4B-C1B	2.33	1.43	1.40
4	J	591	COA	O4B-C1B	2.33	1.43	1.40
4	H	591	COA	O4B-C1B	2.29	1.43	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	591	COA	C4B-O4B-C1B	-5.82	104.59	109.92
4	H	591	COA	C4B-O4B-C1B	-5.55	104.84	109.92
4	D	591	COA	N3A-C2A-N1A	-5.39	121.36	128.67
4	J	591	COA	N3A-C2A-N1A	-5.23	121.58	128.67
4	L	591	COA	N3A-C2A-N1A	-5.19	121.62	128.67

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	BTI	C11-C10-C9-C8
3	A	801	BTI	S1-C2-C7-C8
3	A	801	BTI	C4-C2-C7-C8
3	I	801	BTI	C11-C10-C9-C8
3	I	801	BTI	S1-C2-C7-C8

There are no ring outliers.

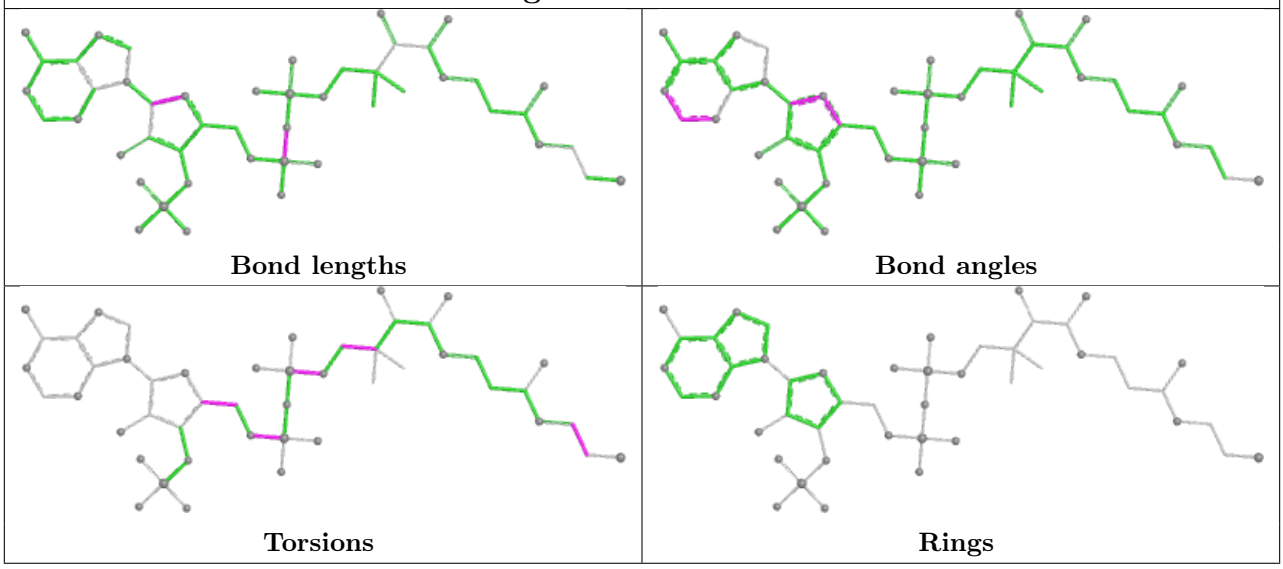
8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	591	COA	4	0
3	A	801	BTI	3	0
4	D	591	COA	3	0
4	L	591	COA	2	0
4	H	591	COA	6	0
4	J	591	COA	4	0
4	F	591	COA	3	0
3	I	801	BTI	4	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 B 591



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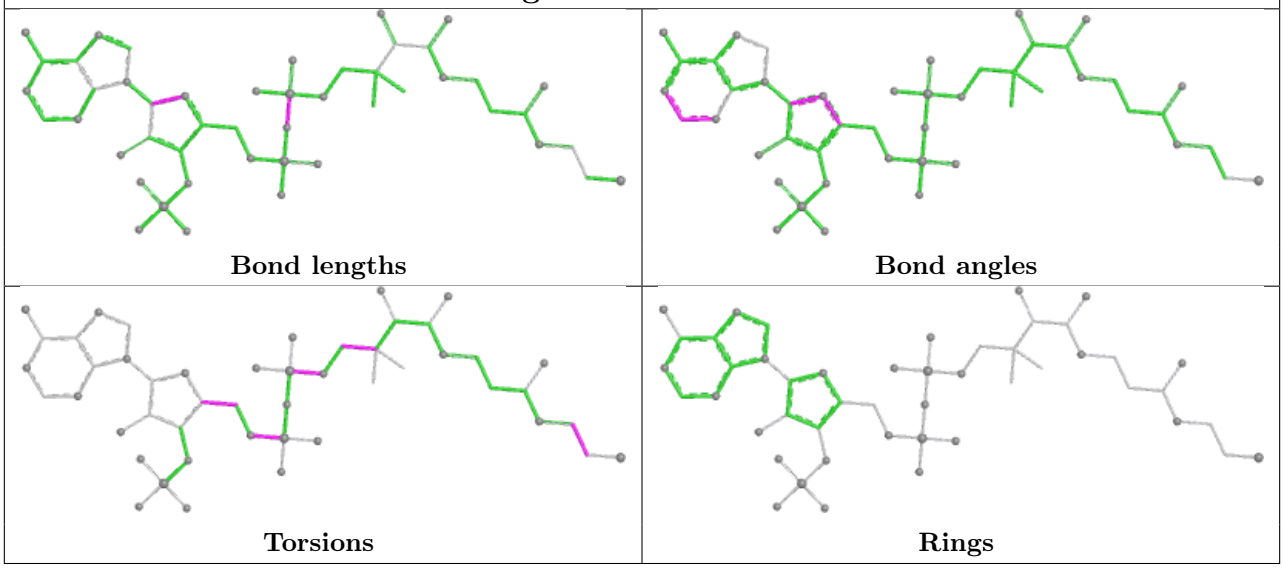

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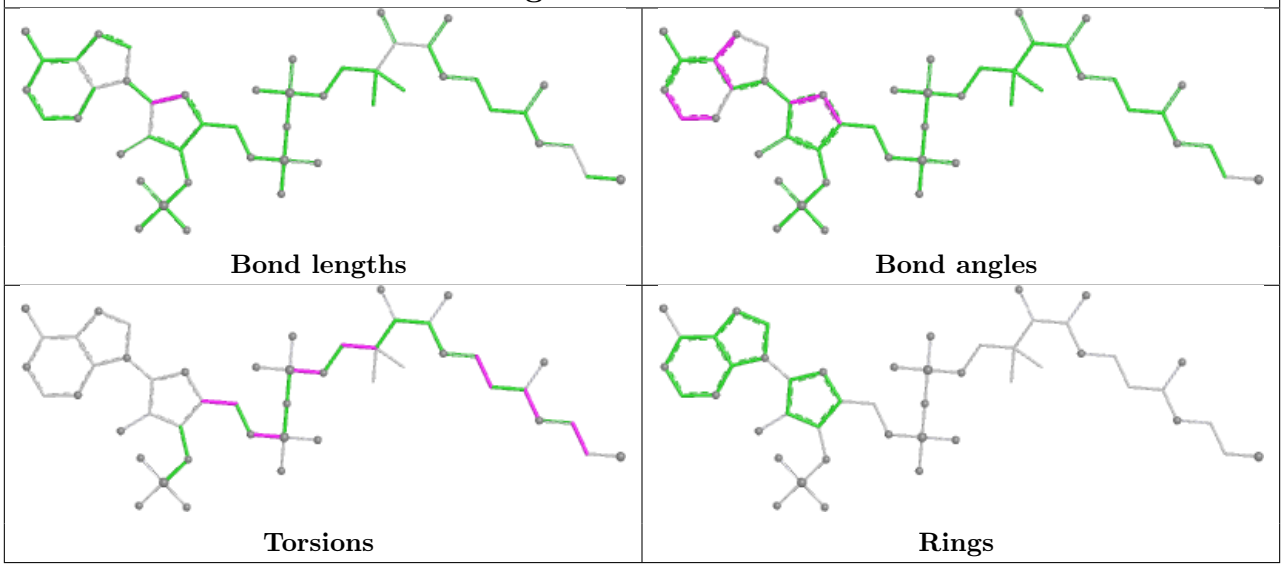

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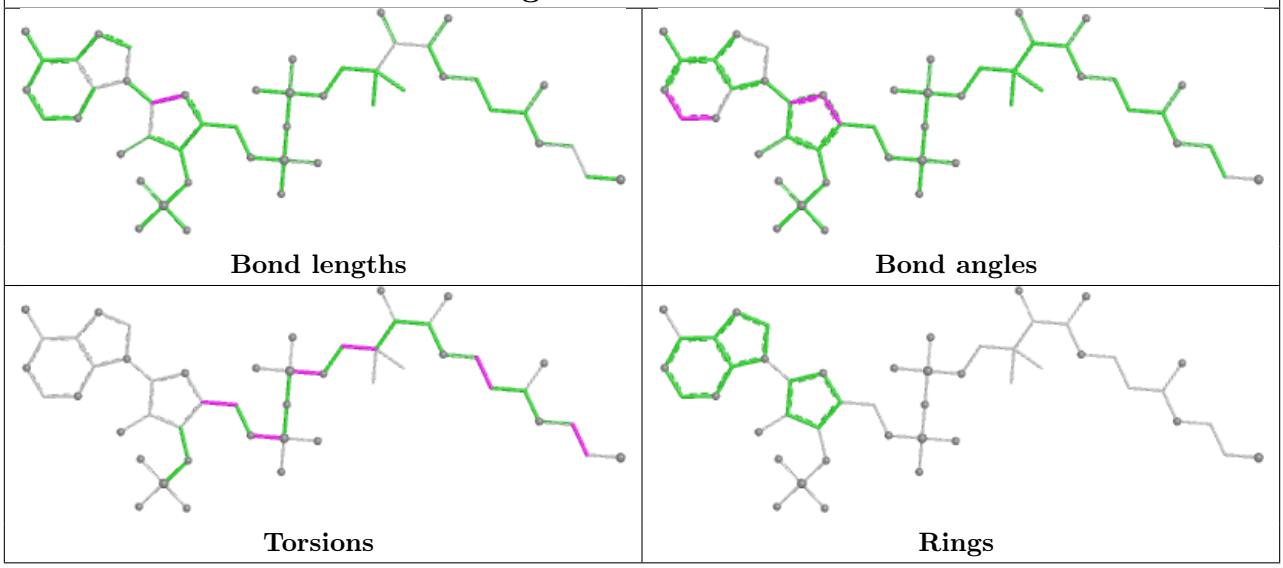
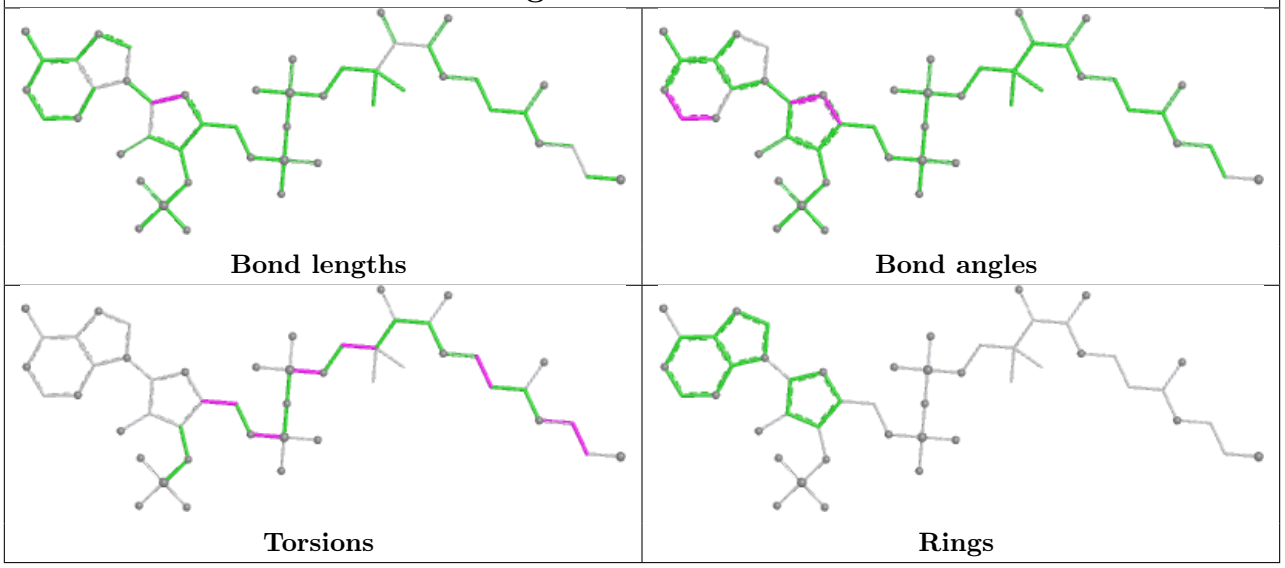
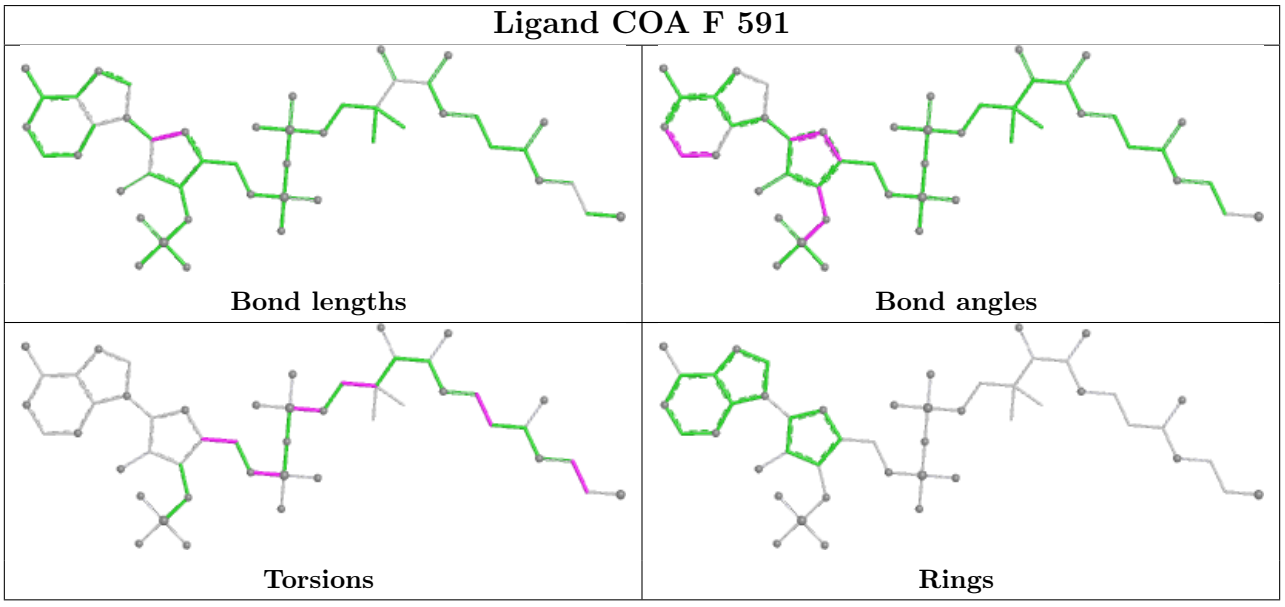


Ligand COA J 591



Ligand COA F 591



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	621/655 (94%)	-0.11	0 100 100	71, 115, 170, 200	0
1	C	552/655 (84%)	-0.20	1 (0%) 92 86	69, 113, 154, 187	0
1	E	552/655 (84%)	-0.16	0 100 100	71, 113, 154, 189	0
1	G	552/655 (84%)	-0.10	0 100 100	76, 112, 155, 187	0
1	I	498/655 (76%)	-0.14	1 (0%) 92 86	73, 113, 146, 193	0
1	K	497/655 (75%)	-0.06	1 (0%) 92 86	65, 115, 146, 187	0
2	B	537/555 (96%)	-0.38	0 100 100	60, 87, 140, 169	0
2	D	537/555 (96%)	-0.38	0 100 100	58, 89, 143, 171	0
2	F	537/555 (96%)	-0.35	0 100 100	58, 88, 142, 167	0
2	H	537/555 (96%)	-0.36	0 100 100	59, 88, 138, 169	0
2	J	537/555 (96%)	-0.37	1 (0%) 92 86	55, 88, 142, 168	0
2	L	537/555 (96%)	-0.36	0 100 100	57, 88, 139, 167	0
All	All	6494/7260 (89%)	-0.25	4 (0%) 92 89	55, 103, 153, 200	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	55	ALA	2.8
1	I	504	LEU	2.5
1	C	633	ASP	2.4
2	J	482	LEU	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

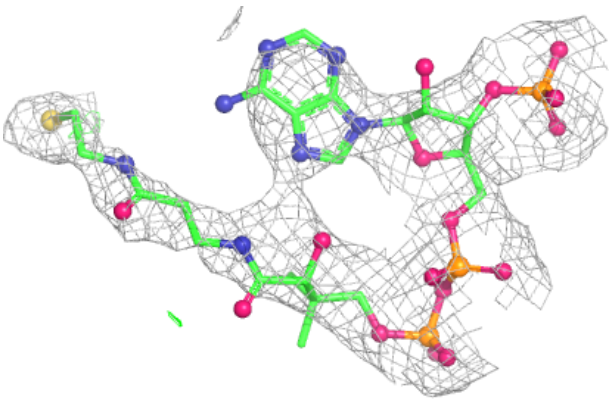
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

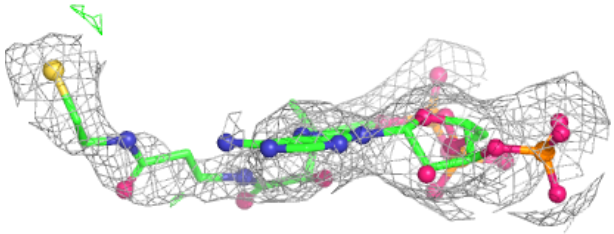
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	COA	B	591	48/48	0.88	0.13	103,129,139,142	0
4	COA	D	591	48/48	0.88	0.11	102,129,142,145	0
4	COA	H	591	48/48	0.90	0.11	102,128,137,139	0
4	COA	J	591	48/48	0.90	0.12	101,127,136,137	0
3	BTI	A	801	15/15	0.91	0.23	140,152,154,155	0
4	COA	F	591	48/48	0.91	0.14	97,124,134,135	0
3	BTI	I	801	15/15	0.92	0.17	142,152,155,158	0
4	COA	L	591	48/48	0.93	0.12	98,125,132,135	0

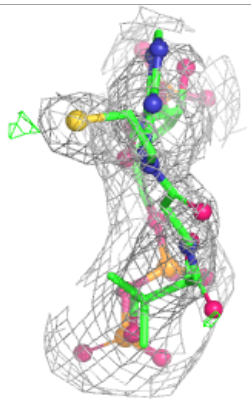
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA B 591:

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

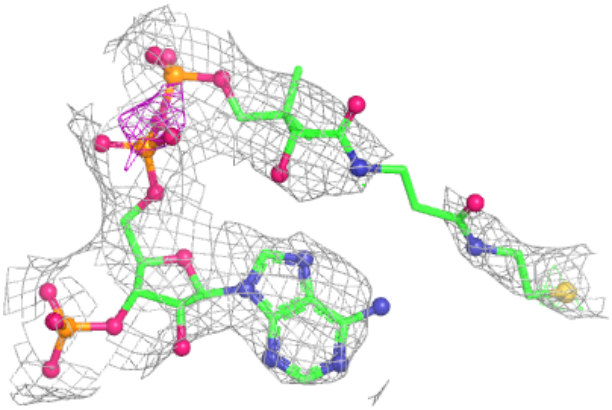


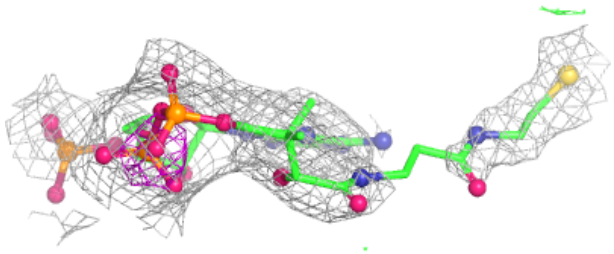


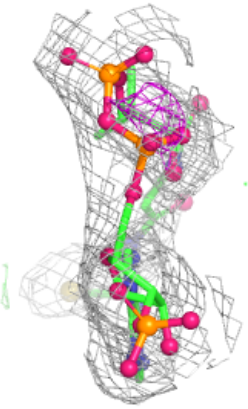


Electron density around COA D 591:

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

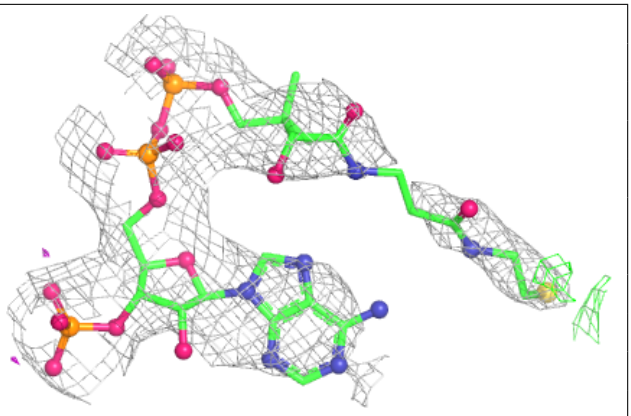


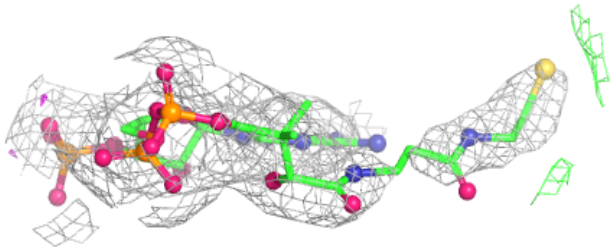


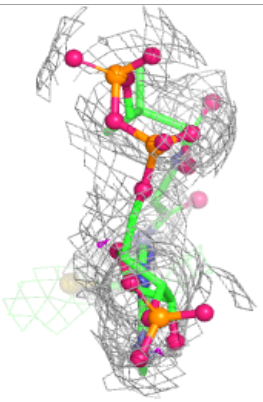


Electron density around COA H 591:

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

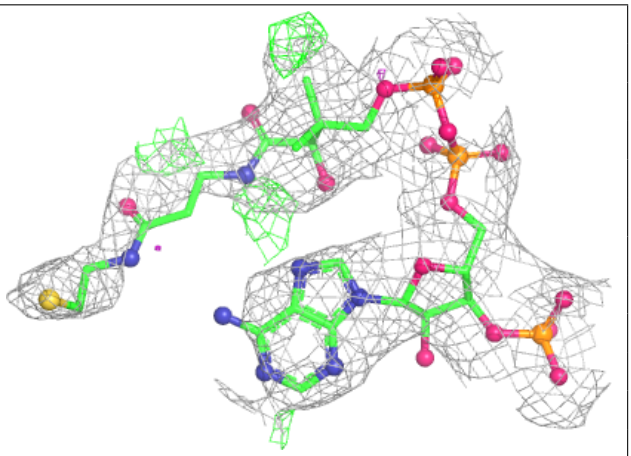


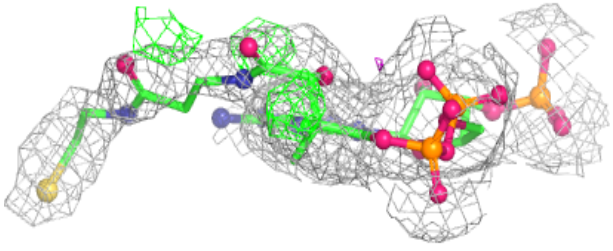


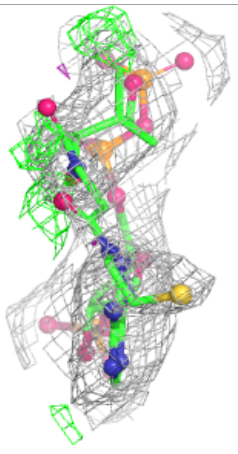


Electron density around COA J 591:

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

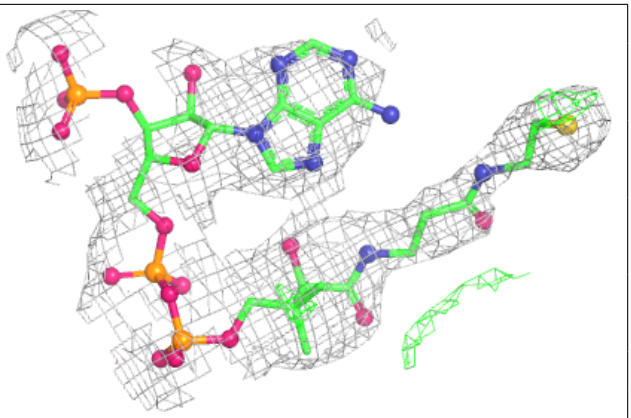


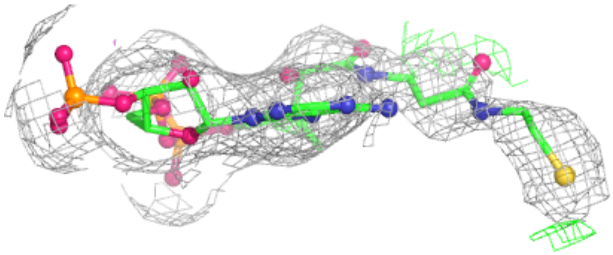


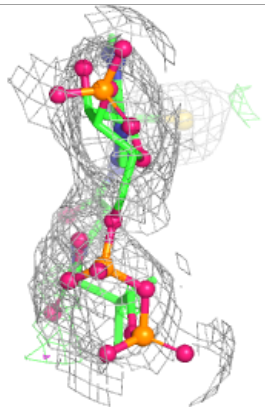


Electron density around COA F 591:

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

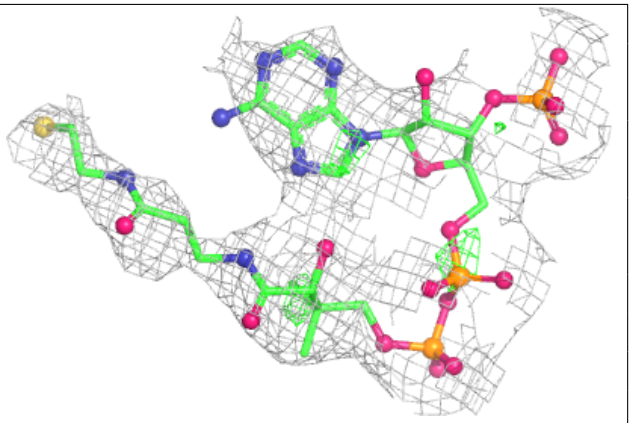


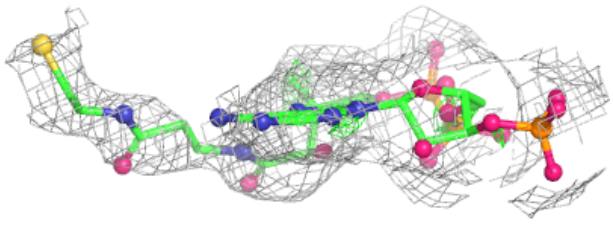


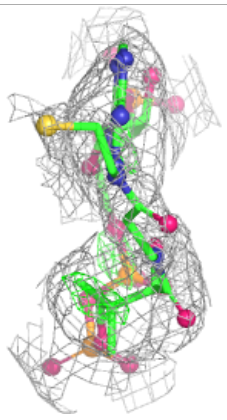


Electron density around COA L 591:

$2mF_o$-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.