



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 3U9S / pdb_00003u9s
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

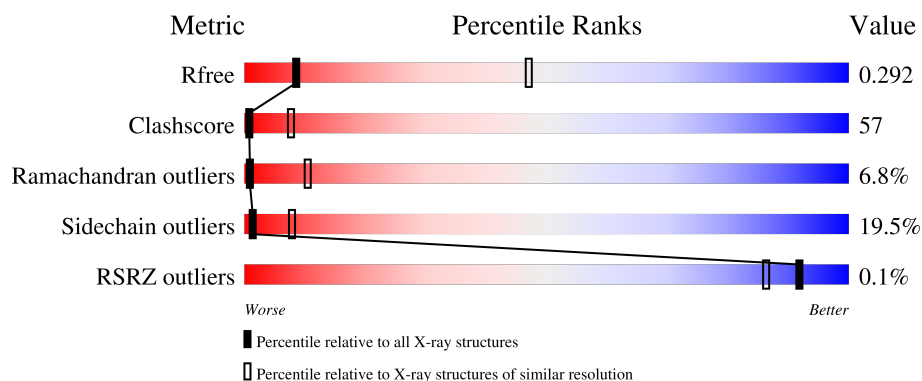
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. 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	655	
1	C	655	
1	E	655	
1	G	655	
1	I	655	

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Mol	Chain	Length	Quality of chain
1	K	655	20%39%15%•24%
2	B	555	32%50%13%••
2	D	555	30%50%16%••
2	F	555	26%52%17%••
2	H	555	31%50%15%••
2	J	555	32%49%15%••
2	L	555	29%51%16%••

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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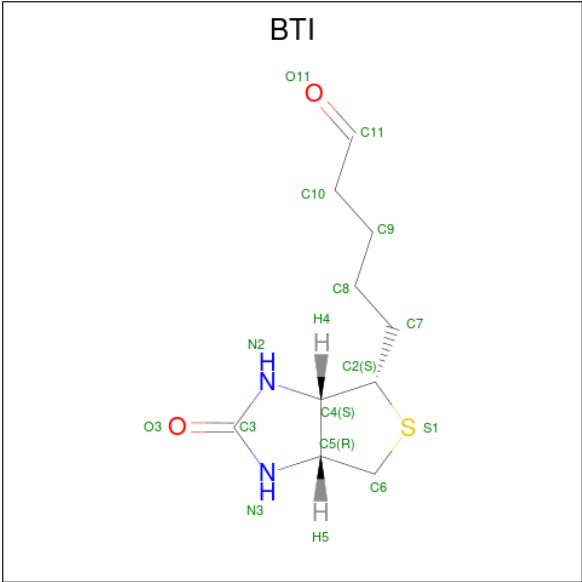
Chain	Residue	Modelled	Actual	Comment	Reference
F	11	SER	-	expression tag	UNP Q9I297
F	12	HIS	-	expression tag	UNP Q9I297
F	13	HIS	-	expression tag	UNP Q9I297
F	14	HIS	-	expression tag	UNP Q9I297
F	15	HIS	-	expression tag	UNP Q9I297
F	16	HIS	-	expression tag	UNP Q9I297
F	17	HIS	-	expression tag	UNP Q9I297
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
F	22	VAL	-	expression tag	UNP Q9I297
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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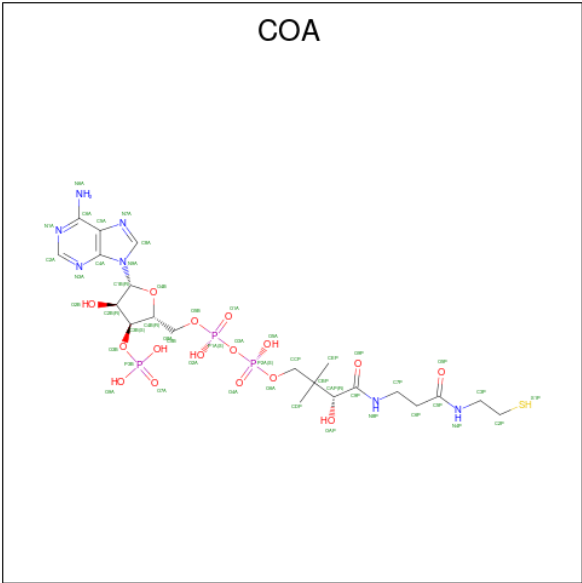
Chain	Residue	Modelled	Actual	Comment	Reference
J	13	HIS	-	expression tag	UNP Q9I297
J	14	HIS	-	expression tag	UNP Q9I297
J	15	HIS	-	expression tag	UNP Q9I297
J	16	HIS	-	expression tag	UNP Q9I297
J	17	HIS	-	expression tag	UNP Q9I297
J	18	SER	-	expression tag	UNP Q9I297
J	19	SER	-	expression tag	UNP Q9I297
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 (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



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 (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



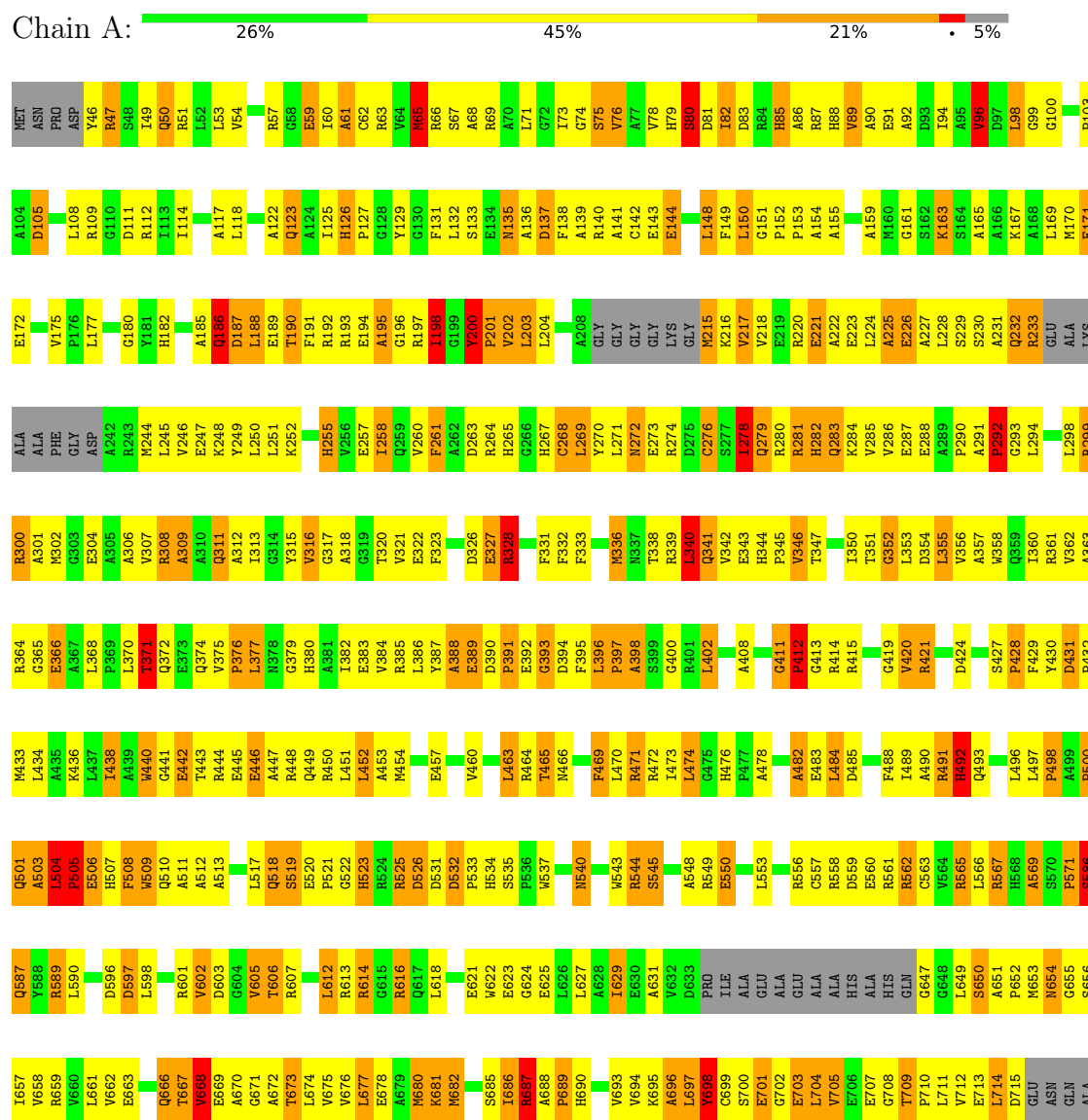
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

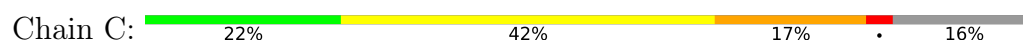
3 Residue-property plots

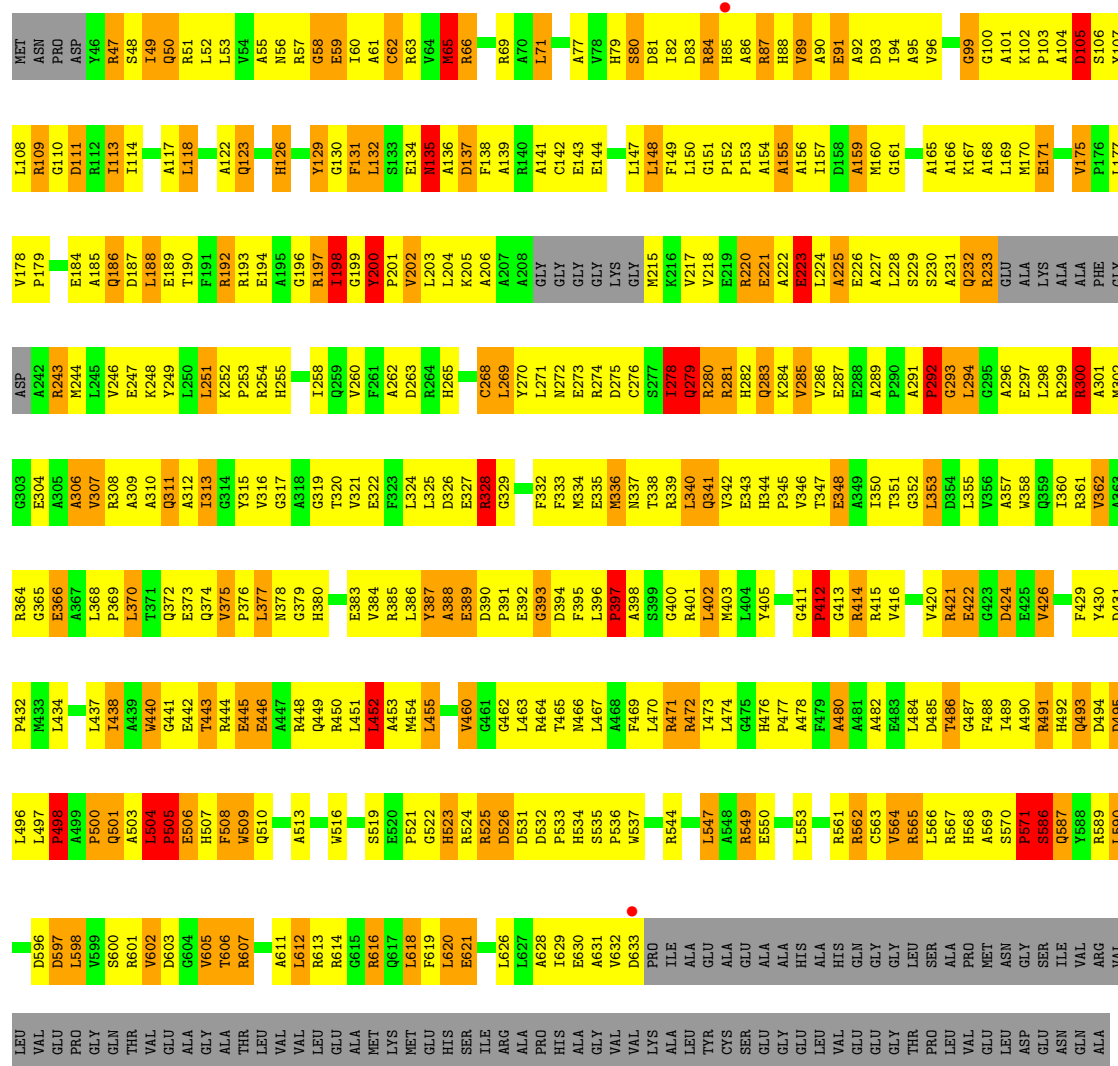
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

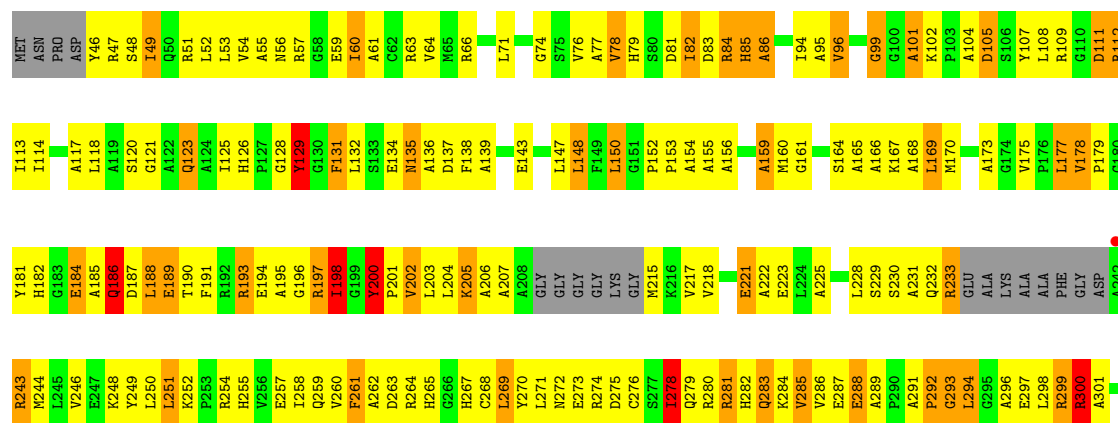
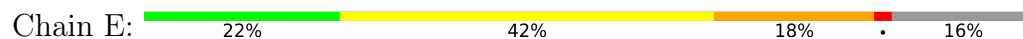


- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit





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

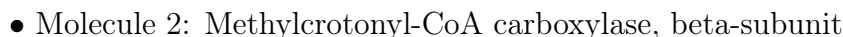


PRO	LEU	ALA	SER	S570	Q501	L434	G365	E304
LEU	VAL	PRO	ALA	P571	A503	A435	E366	
GLU	GLU	ASP	MET	S586	L504	K436	A367	V307
LEU	LEU	ASP	GLY	S587	P505	L437	L368	R308
ASP	ASP	GLY	GLY	Y589	E506	I438		A309
GLU	GLU	SER	SER	L590	F508	T371	T372	A310
ASN	ASN	ILE	ILE	D591	W509	W440	Q373	Q311
GLN	GLN	VAL	VAL	G592	Q510	E442	E374	A312
ALA	ALA	VAL	VAL	D596	A511	T443	V375	I313
		LEU	GLY	ARG	A512	R444	P376	G314
		VAL	LEU	L598	A513	E445	L377	G315
		GLU	VAL	W599	E514	E446	N378	V316
		GLU	GLY	S600	A515	A447	N379	G317
		PRO	THR	R601	W516		G379	A318
		GLY	GLY	G602	Q448	Q449	A381	G319
		GLN	THR	D603	R450	R451	T320	T320
		VAL	VAL	G604	L450	L451	I382	E321
		GLU	GLU	W605	P521	L452	E383	E322
		ALA	ALA	T606	G522	A453	V384	F323
		GLY	GLY	R607	H523	M454	L386	L324
		LEU	LEU	R608	R524	L455	Y387	L325
		THR	THR	A611	R525		A388	E327
		VAL	VAL	L612	D526	T458	D390	R328
		VAL	VAL	R613	D531	S459	D399	G329
		VAL	VAL	R614	D532	V460	P391	G330
		LEU	LEU	G615	P533		E392	F331
		GLY	GLY	H634	H534	L463	G393	F332
		ALA	ALA	Q616	S535	R464	F394	F333
		MET	MET	Q617	P536	T465	F395	M334
		LYS	LYS	L618	R539	N466	L396	E335
		MET	MET	F619	R540	L467	R397	M336
		GLY	GLY	L620	D541	A468	A398	N337
		SER	SER	W621	W622	F469	S399	T338
		ILE	ILE	E623		L470	G400	R339
		ARG	ARG	L626	R544	R471	R401	L340
		ALA	ALA	L627	S545	R472	L402	Q341
		PRO	PRO	A628	A546	I473	M403	V342
		HIS	HIS	T629	A548	L474	L404	E343
		ALA	ALA	E630	R549	F479	R406	H344
		GLY	GLY	A631	E550	A481	V346	P345
		VAL	VAL	W632	L553	A482	T347	V346
		VAL	VAL	D633	M554	E483	G411	T347
		LYS	LYS	ILE	L555	E484	P412	E348
		LEU	LEU	ALA	R556	D485	G413	I350
		TYR	TYR	GLU	C557	T486	R414	T351
		CYS	CYS	ALA	R558	G487	S418	G352
		SER	SER	GLU	D559	F488		L353
		GLY	GLY	ALA	E560	I489	R421	D354
		GLY	GLY	ALA	R561	A490	E422	L355
		GLY	GLY	ALA	R562	R491	A357	V356
		VAL	VAL	ALA	C563	H492	V426	A357
		GLY	GLY	ALA	R564	Q493		W358
		GLN	GLN	HIS	R565		F429	Q359
		GLY	GLY	GLN	L566	L497	Y430	I360
		GLY	GLY	GLY	R567	P498	D431	R361
		THR	THR	LEU	H568	A499	A363	V362
					A569	P500	M433	R364

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

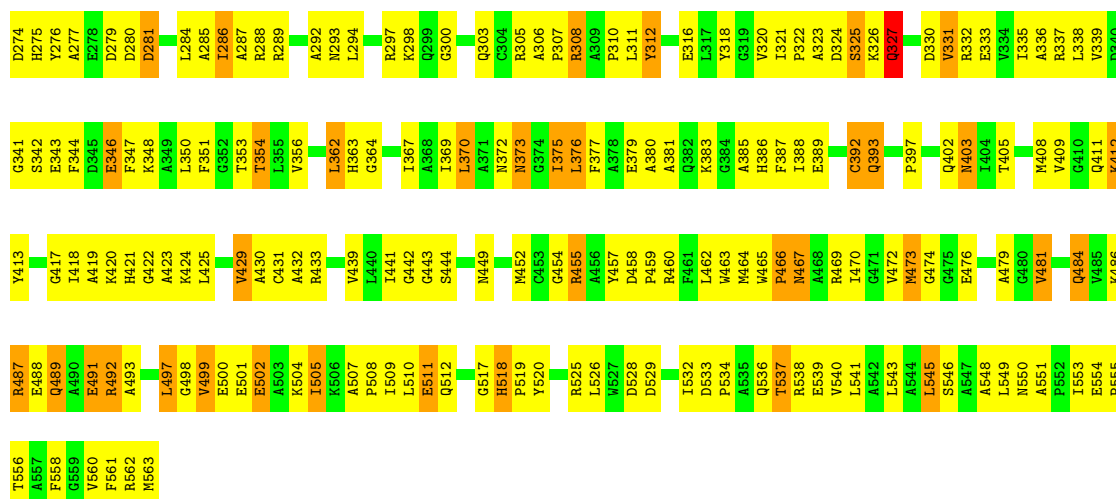
Chain G: 21% 44% 17% • 16%

LEU	VAL	PRO	MET	S570	Q501	L434	G365	E304
LEU	VAL	PRO	MET	P571	A503	A435	E366	
GLU	GLU	ASP	MET	S586	L504	K436	A367	V307
LEU	LEU	ASP	GLY	S587	P505	L437	L368	R308
ASP	ASP	GLY	GLY	Y589	E506	I438		A309
GLU	GLU	SER	SER	L590	F508	T371	T372	A310
ASN	ASN	ILE	ILE	D591	W509	W440	Q373	Q311
GLN	GLN	VAL	VAL	G592	Q510	E442	E374	A312
ALA	ALA	VAL	VAL	D596	A511	T443	V375	I313
		LEU	GLY	ARG	A512	R444	P376	G314
		VAL	LEU	L598	A513	E445	L377	G315
		GLU	VAL	W599	E514	E446	N378	V316
		GLU	GLY	S600	A515	A447	N379	G317
		PRO	THR	R601	W516		G379	A318
		GLY	GLY	G602	Q448	Q449	A381	G319
		GLN	THR	D603	R450	R451	T320	T320
		VAL	VAL	G604	L450	L451	I382	E321
		GLU	GLU	W605	P521	L452	E383	E322
		ALA	ALA	T606	G522	A453	V384	F323
		GLY	GLY	R607	H523	M454	L386	L324
		LEU	LEU	R608	R524	L455	Y387	L325
		THR	THR	A611	R525		A388	E327
		VAL	VAL	L612	D526	T458	D390	R328
		VAL	VAL	R613	D531	S459	D399	G329
		VAL	VAL	R614	D532	V460	P391	G330
		LEU	LEU	G615	P533		E392	F331
		GLY	GLY	H634	H534	L463	G393	F332
		ALA	ALA	Q616	S535	R464	F394	F333
		MET	MET	Q617	P536	T465	F395	M334
		LYS	LYS	L618	R539	N466	L396	E335
		MET	MET	F619	R540	L467	R397	M336
		GLY	GLY	L620	D541	A468	A398	N337
		SER	SER	W621	W622	F469	S399	T338
		ILE	ILE	E623		L470	G400	R339
		ARG	ARG	L626	R544	R471	R401	L340
		ALA	ALA	L627	S545	R472	L402	Q341
		PRO	PRO	A628	A546	I473	M403	V342
		HIS	HIS	T629	A548	L474	L404	E343
		ALA	ALA	E630	R549	F479	R406	H344
		GLY	GLY	A631	E550	A481	V346	P345
		VAL	VAL	W632	L553	A482	T347	V346
		VAL	VAL	D633	M554	E483	G411	T347
		LYS	LYS	ILE	L555	E484	P412	E348
		LEU	LEU	ALA	R556	D485	G413	I350
		TYR	TYR	GLU	C557	T486	R414	T351
		CYS	CYS	ALA	R558	G487	S418	G352
		SER	SER	GLU	D559	F488		L353
		GLY	GLY	ALA	E560	I489	R421	D354
		GLY	GLY	ALA	R561	A490	E422	L355
		GLY	GLY	ALA	R562	R491	A357	V356
		VAL	VAL	ALA	C563	H492	V426	A357
		GLY	GLY	ALA	R564	Q493		W358
		GLN	GLN	HIS	R565		F429	Q359
		GLY	GLY	GLN	L566	L497	Y430	I360
		GLY	GLY	GLY	R567	P498	D431	R361
		THR	THR	LEU	H568	A499	A363	V362
					A569	P500	M433	R364



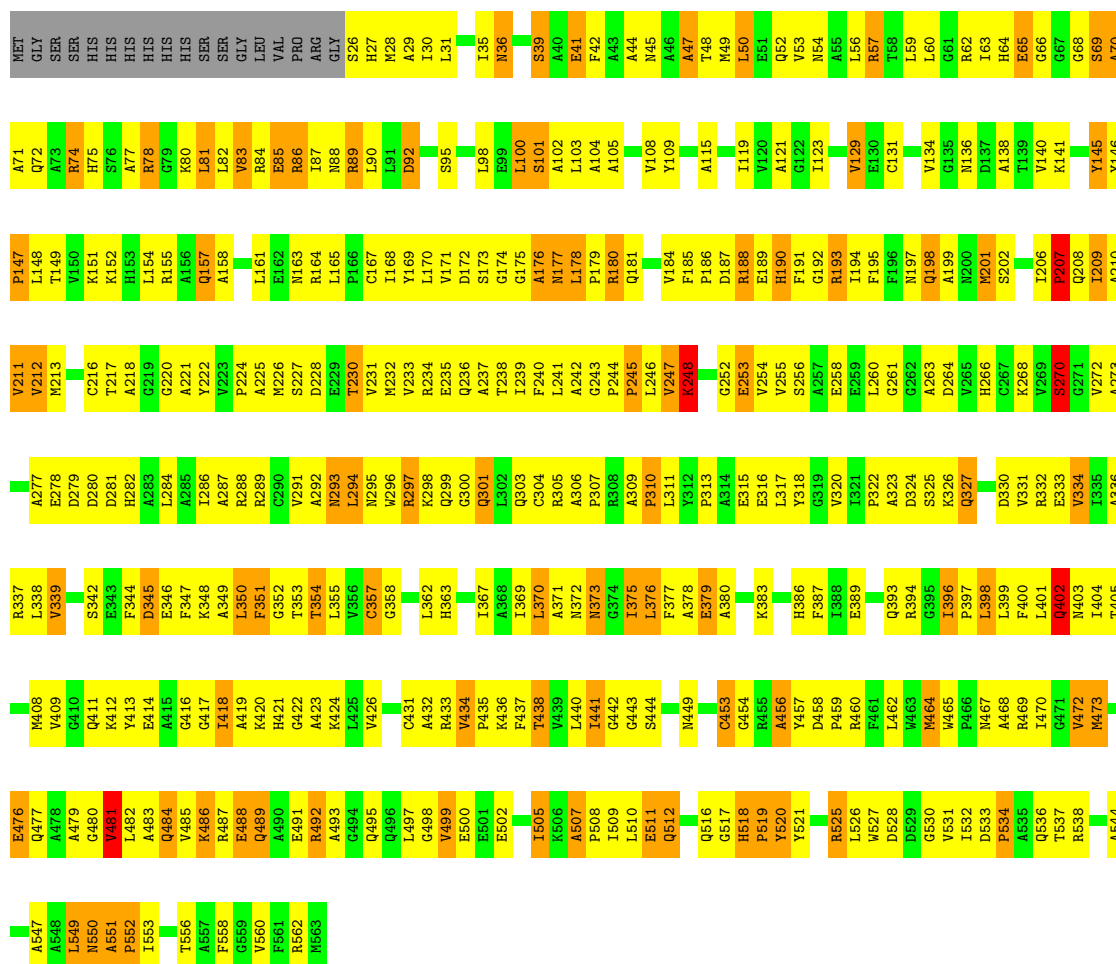
Chain B: 32% 50% 13% ..



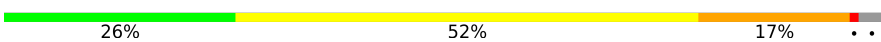


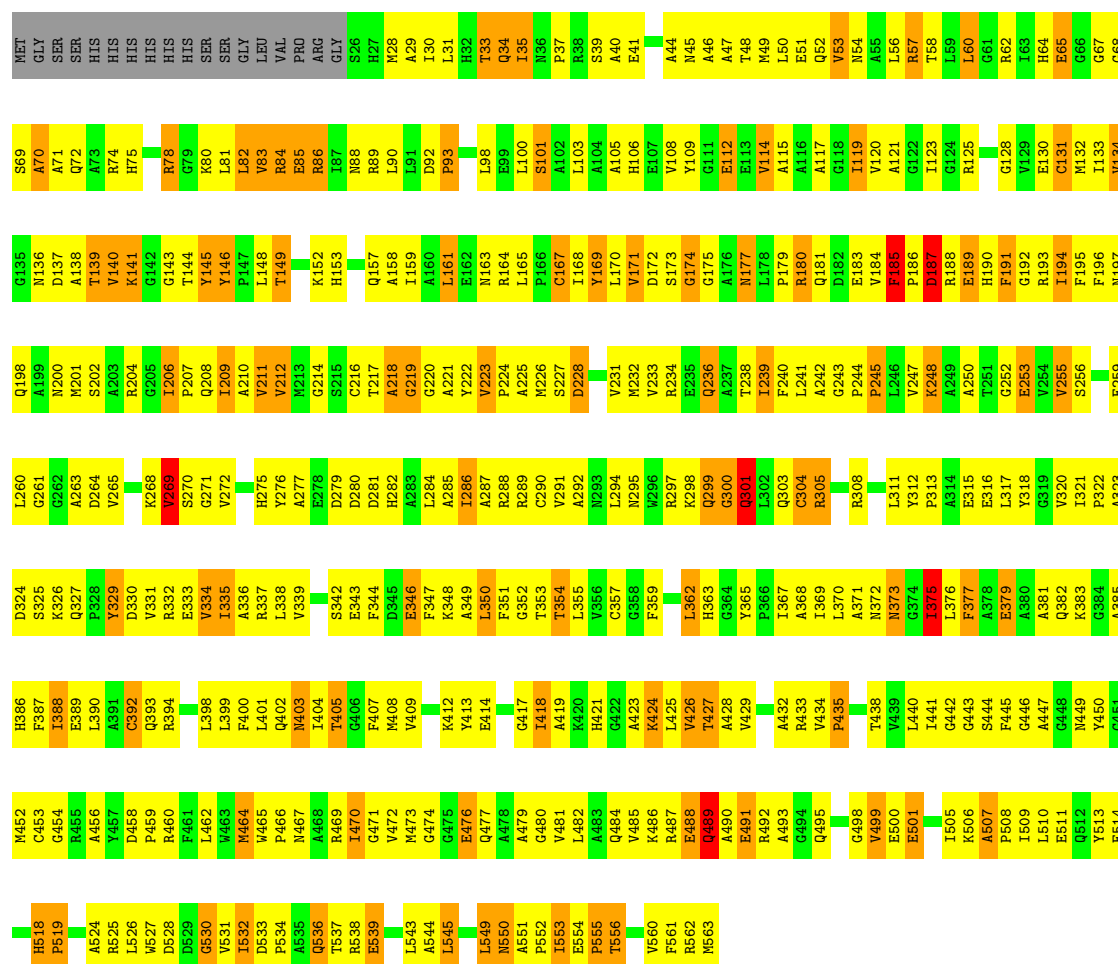
• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

Chain D: 30% 50% 16% ..

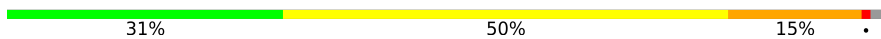


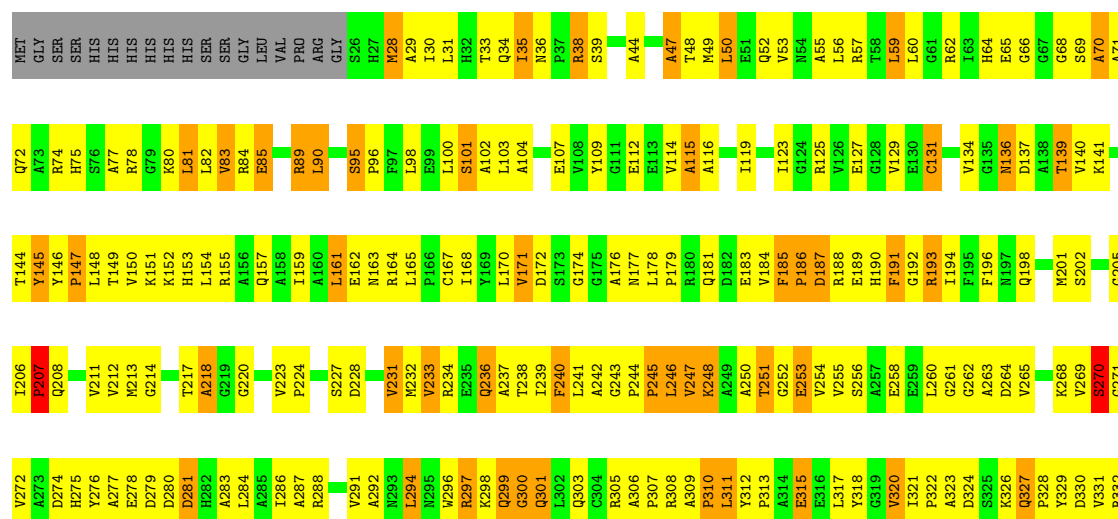
• Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit

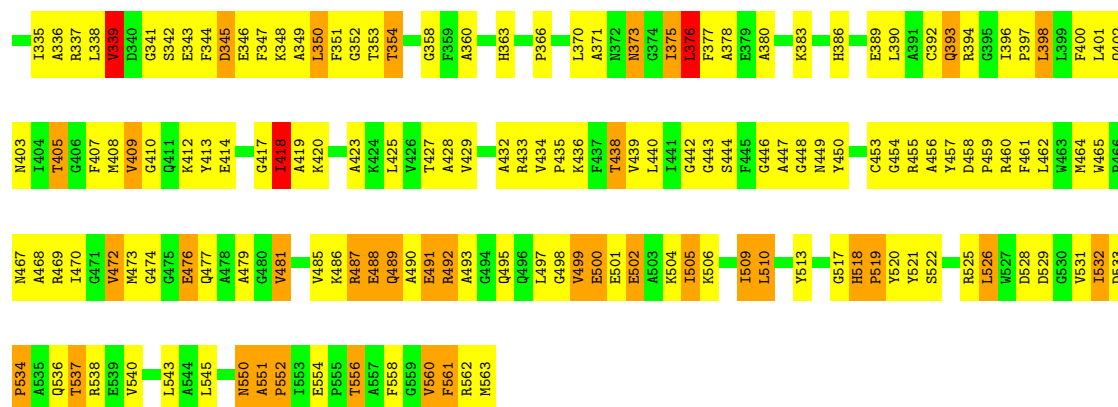
Chain F:  26% 52% 17% ..



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

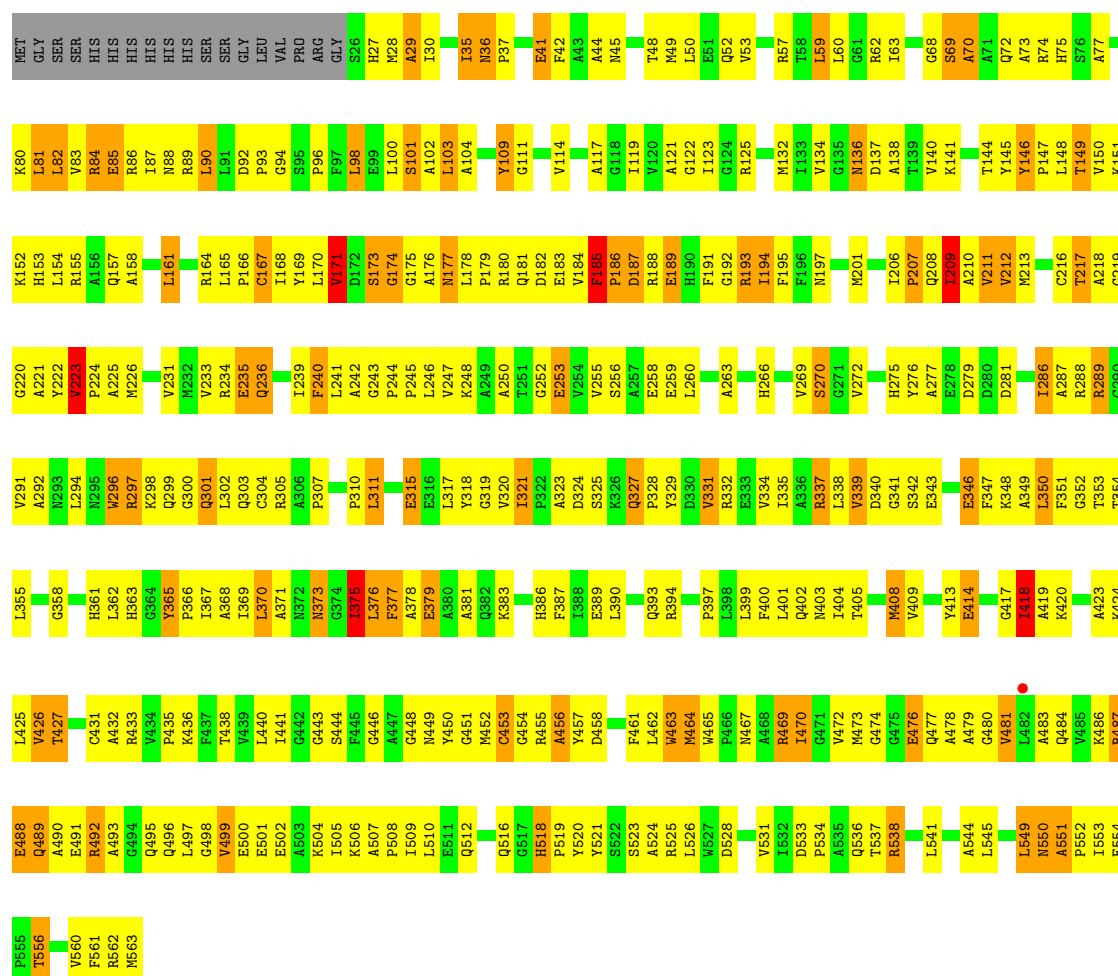
Chain H:  31% 50% 15% ..





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

Chain J: 32% 49% 15% . .



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

Chain L: 29% 51% 16% . .

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																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
W465	L398	L399	L400	L401	Q402	N403	I404	T405	M408	G409	Q410	Q411	K412	Y413	E414	G417	I418	A419	K420	T421	H422	K424	L425	F426	T427	A428	A430	C431	A432	R433	V434	P435	K436	F437	T438	A439	L440	L441	G442	G443	S444	F445	Y449	Y450	Y521	S522	A523	R524	R455	D458	P459	R460	F461	G530	V531	L462	G532	W463	E533	M464																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
W465	L398	L399	L400	L401	Q402	N403	I404	T405	M408	G409	Q410	Q411	K412	Y413	E414	G417	I418	A419	K420	T421	H422	K424	L425	F426	T427	A428	A430	C431	A432	R433	V434	P435	K436	F437	T438	A439	L440	L441	G442	G443	S444	F445	Y449	Y450	Y521	S522	A523	R524	R455	D458	P459	R460	F461	G530	V531	L462	G532	W463	E533	M464																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
V331	R332	E333	V334	I335	D336	R337	L338	V339	D340	E343	F344	D345	E346	F347	K348	A349	L350	R351	G352	T353	T354	G358	L362	H363	G364	Y365	P366	Q367	L368	R369	K370	L371	L372	L373	L374	L375	L376	F377	P378	A379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	S26	A29	I30	L31	H32	T33	N36	P37	S39	A40	E41	F42	A43	A44	M45		T48	M49	L50	E51	Q52	V53	N54	A55	L56	R57	T58	L59	G61	R62	I63	H64	E65	G68	S69	A70	A71																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.292 0.234 , 0.292	Depositor DCC
R_{free} test set	6800 reflections (5.07%)	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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BTI, 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	0.87	3/4866 (0.1%)	1.23	42/6581 (0.6%)
1	C	0.82	0/4362	1.22	39/5897 (0.7%)
1	E	0.80	1/4362 (0.0%)	1.21	35/5897 (0.6%)
1	G	0.83	2/4362 (0.0%)	1.23	40/5897 (0.7%)
1	I	0.82	3/3929 (0.1%)	1.23	37/5315 (0.7%)
1	K	0.89	8/3921 (0.2%)	1.22	28/5307 (0.5%)
2	B	0.88	2/4135 (0.0%)	1.26	30/5605 (0.5%)
2	D	0.85	0/4135	1.26	46/5605 (0.8%)
2	F	0.85	3/4135 (0.1%)	1.27	46/5605 (0.8%)
2	H	0.86	0/4135	1.22	25/5605 (0.4%)
2	J	0.90	2/4135 (0.0%)	1.27	41/5605 (0.7%)
2	L	0.87	2/4135 (0.0%)	1.25	39/5605 (0.7%)
All	All	0.85	26/50612 (0.1%)	1.24	448/68524 (0.7%)

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

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	28	MET	SD-CE	7.71	1.98	1.79
1	K	602	VAL	CA-CB	6.53	1.63	1.54
1	E	632	VAL	CA-CB	6.40	1.61	1.54
2	F	464	MET	SD-CE	6.32	1.95	1.79
1	K	178	VAL	CA-CB	6.27	1.62	1.54

The worst 5 of 448 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	506	GLU	N-CA-C	-16.31	93.10	113.97
1	C	506	GLU	N-CA-C	-14.73	93.60	112.90
1	I	506	GLU	N-CA-C	-13.79	96.53	113.50
1	K	506	GLU	N-CA-C	-13.08	97.01	113.23
1	A	200	TYR	CA-C-N	-12.93	103.68	119.84

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	603	0
1	C	4280	0	4227	567	0
1	E	4280	0	4227	551	0
1	G	4280	0	4227	551	0
1	I	3853	0	3795	501	0
1	K	3844	0	3786	507	0
2	B	4051	0	4023	417	0
2	D	4051	0	4023	443	0
2	F	4051	0	4023	458	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	4051	0	4023	444	0
2	J	4051	0	4023	449	0
2	L	4051	0	4023	448	0
3	A	15	0	15	3	0
3	I	15	0	15	5	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	5697	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 57.

The worst 5 of 5697 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:I:170:MET:HE1	1:I:309:ALA:HB1	1.26	1.18
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
2:J:201:MET:HE3	2:J:208:GLN:HE22	1.10	1.15
1:G:278:ILE:H	1:G:278:ILE:HD12	1.10	1.14

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 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	546/655 (83%)	382 (70%)	113 (21%)	51 (9%)	0	6
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	7
2	B	535/555 (96%)	448 (84%)	63 (12%)	24 (4%)	2	17
2	D	535/555 (96%)	456 (85%)	62 (12%)	17 (3%)	3	24
2	F	535/555 (96%)	439 (82%)	73 (14%)	23 (4%)	2	18
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	23
2	L	535/555 (96%)	438 (82%)	76 (14%)	21 (4%)	2	20
All	All	6447/7260 (89%)	4974 (77%)	1037 (16%)	436 (7%)	1	10

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 ⓘ

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%)	380 (80%)	97 (20%)	1	7
1	C	423/496 (85%)	330 (78%)	93 (22%)	1	5
1	E	423/496 (85%)	327 (77%)	96 (23%)	1	5
1	G	423/496 (85%)	325 (77%)	98 (23%)	1	5
1	I	382/496 (77%)	306 (80%)	76 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	381/496 (77%)	296 (78%)	85 (22%)	1	5
2	B	401/418 (96%)	338 (84%)	63 (16%)	2	15
2	D	401/418 (96%)	323 (80%)	78 (20%)	1	8
2	F	401/418 (96%)	330 (82%)	71 (18%)	2	10
2	H	401/418 (96%)	329 (82%)	72 (18%)	2	10
2	J	401/418 (96%)	345 (86%)	56 (14%)	3	19
2	L	401/418 (96%)	329 (82%)	72 (18%)	2	10
All	All	4915/5484 (90%)	3958 (80%)	957 (20%)	1	8

5 of 957 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	281	ASP
2	L	38	ARG
1	G	495	ASP
1	K	606	THR
2	L	455	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 202 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	232	GLN
2	H	449	ASN
2	L	403	ASN
1	G	372	GLN
2	H	157	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 [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	F	591	-	47,50,50	0.98	3 (6%)	69,75,75	1.43	9 (13%)
4	COA	H	591	-	47,50,50	1.02	3 (6%)	69,75,75	1.43	9 (13%)
4	COA	D	591	-	47,50,50	1.04	4 (8%)	69,75,75	1.48	8 (11%)
4	COA	B	591	-	47,50,50	1.03	4 (8%)	69,75,75	1.45	8 (11%)
4	COA	L	591	-	47,50,50	0.98	3 (6%)	69,75,75	1.51	9 (13%)
4	COA	J	591	-	47,50,50	1.02	3 (6%)	69,75,75	1.42	8 (11%)
3	BTI	A	801	1	15,16,16	1.68	1 (6%)	20,21,21	2.34	7 (35%)
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	F	591	-	-	13/48/64/64	0/3/3/3
4	COA	H	591	-	-	13/48/64/64	0/3/3/3
4	COA	D	591	-	-	12/48/64/64	0/3/3/3
4	COA	B	591	-	-	12/48/64/64	0/3/3/3
4	COA	L	591	-	-	15/48/64/64	0/3/3/3
4	COA	J	591	-	-	14/48/64/64	0/3/3/3
3	BTI	A	801	1	-	5/6/27/27	0/2/2/2
3	BTI	I	801	1	-	5/6/27/27	0/2/2/2

The worst 5 of 22 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
3	A	801	BTI	O3-C3	6.12	1.36	1.23
4	L	591	COA	C5A-N7A	-3.14	1.33	1.39
4	B	591	COA	C5A-N7A	-3.13	1.33	1.39
4	D	591	COA	C5A-N7A	-3.12	1.33	1.39

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	591	COA	C5A-C4A-N3A	-5.47	119.18	126.72
4	L	591	COA	C5A-C4A-N3A	-5.30	119.42	126.72
4	B	591	COA	C5A-C4A-N3A	-5.27	119.47	126.72
4	J	591	COA	C5A-C4A-N3A	-5.14	119.64	126.72
3	A	801	BTI	C4-N2-C3	-4.99	106.36	112.56

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

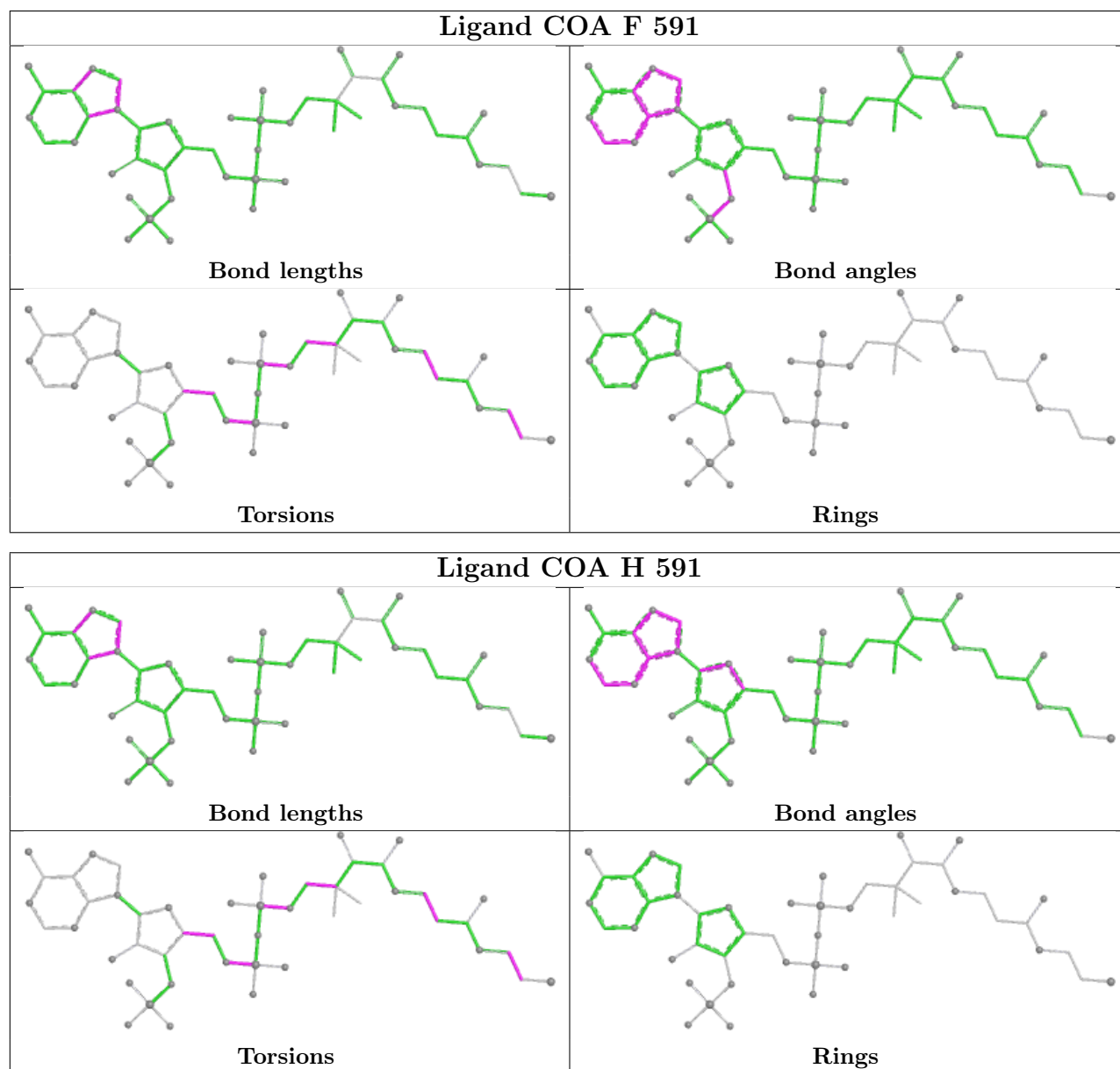
There are no ring outliers.

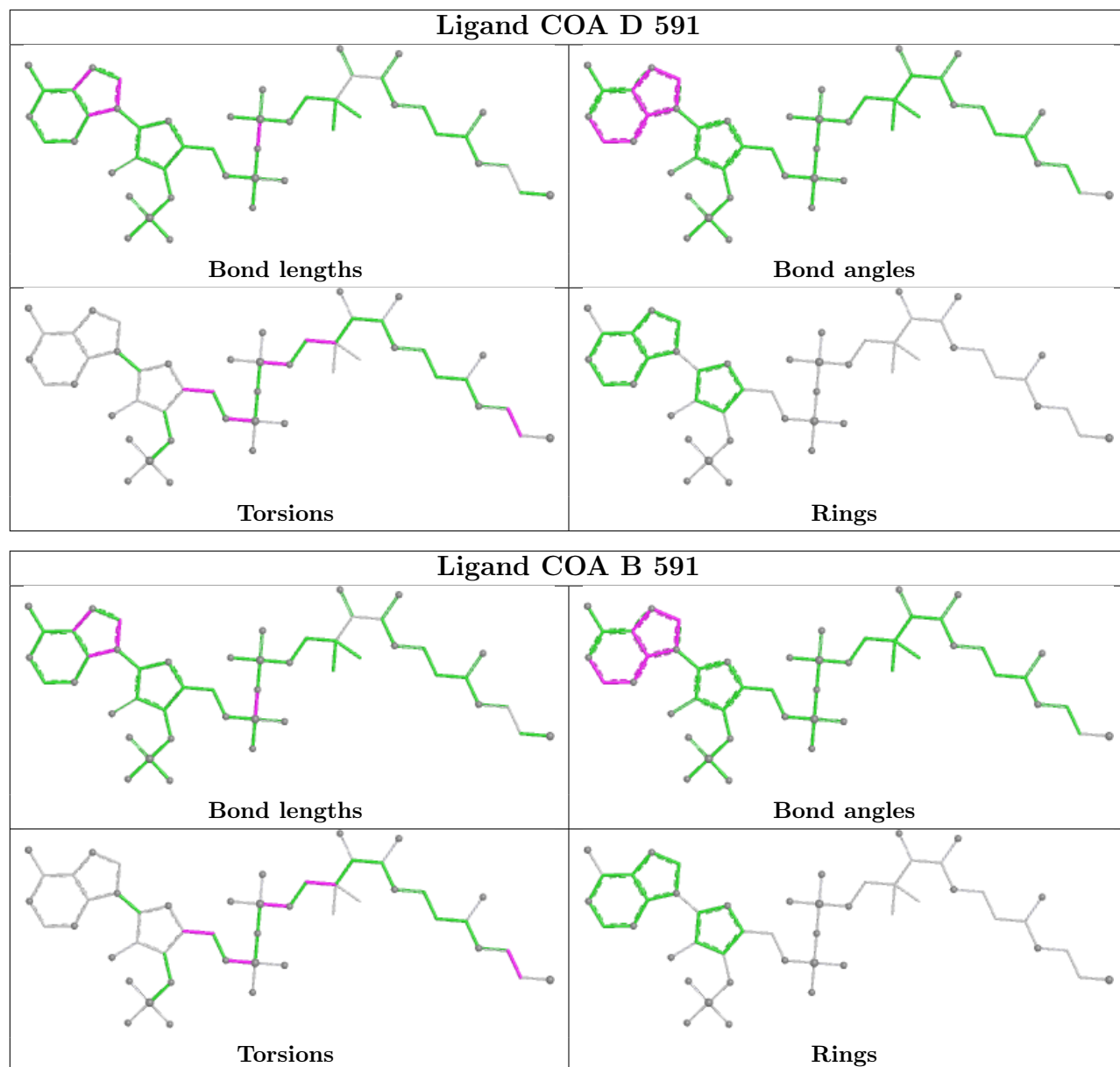
8 monomers are involved in 30 short contacts:

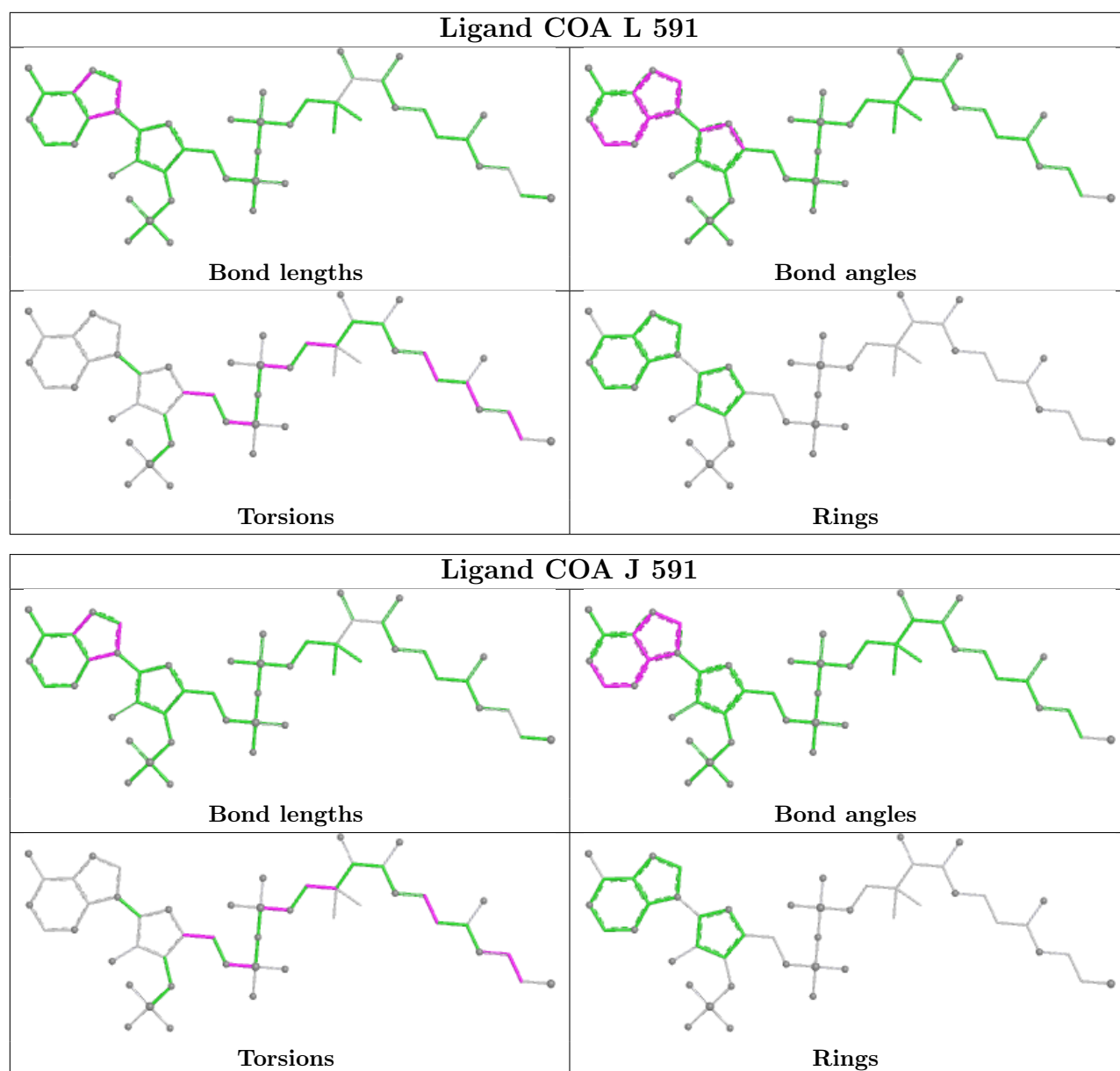
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	591	COA	3	0
4	H	591	COA	6	0
4	D	591	COA	3	0
4	B	591	COA	4	0
4	L	591	COA	2	0
4	J	591	COA	4	0
3	A	801	BTI	3	0
3	I	801	BTI	5	0

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 than 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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	621/655 (94%)	0.05	0 100 100	71, 115, 170, 200	0
1	C	552/655 (84%)	-0.03	2 (0%) 88 72	69, 113, 154, 187	0
1	E	552/655 (84%)	0.01	1 (0%) 91 82	71, 113, 154, 189	0
1	G	552/655 (84%)	0.07	0 100 100	76, 112, 155, 187	0
1	I	498/655 (76%)	0.02	2 (0%) 88 72	73, 113, 146, 193	0
1	K	497/655 (75%)	0.11	2 (0%) 88 72	65, 115, 146, 187	0
2	B	537/555 (96%)	-0.21	0 100 100	60, 87, 140, 169	0
2	D	537/555 (96%)	-0.21	0 100 100	58, 89, 143, 171	0
2	F	537/555 (96%)	-0.19	0 100 100	58, 88, 142, 167	0
2	H	537/555 (96%)	-0.19	0 100 100	59, 88, 138, 169	0
2	J	537/555 (96%)	-0.21	1 (0%) 91 82	55, 88, 142, 168	0
2	L	537/555 (96%)	-0.19	0 100 100	57, 88, 139, 167	0
All	All	6494/7260 (89%)	-0.08	8 (0%) 92 86	55, 103, 153, 200	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	55	ALA	3.0
1	C	633	ASP	2.6
1	I	504	LEU	2.5
2	J	482	LEU	2.2
1	C	85	HIS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

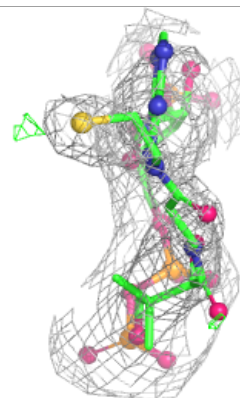
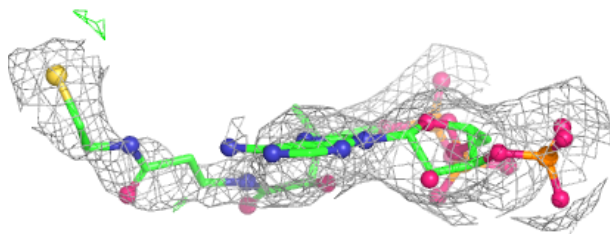
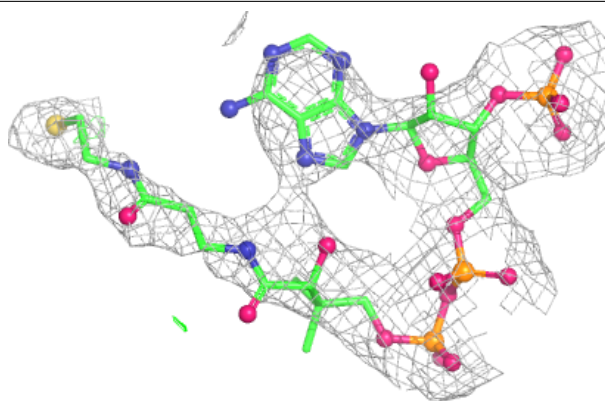
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

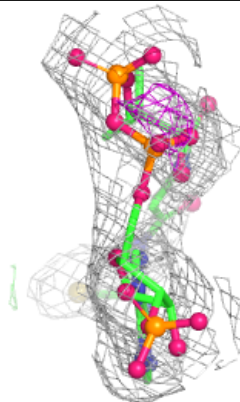
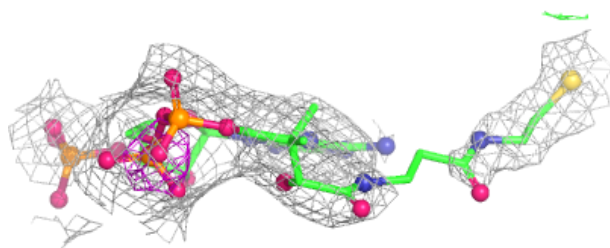
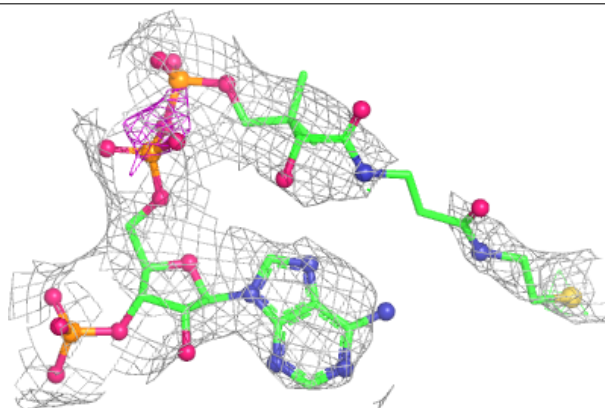
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

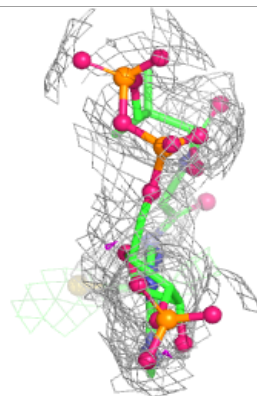
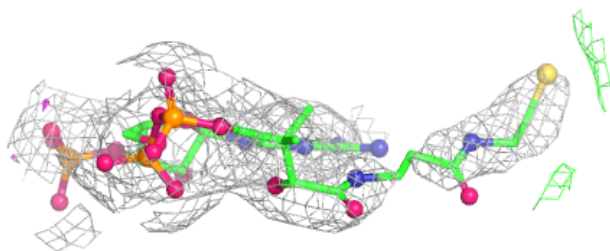
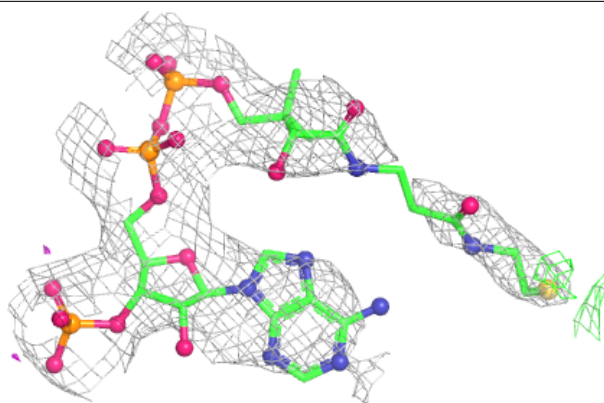
**Electron density around COA D 591:**

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

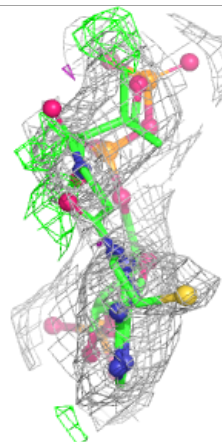
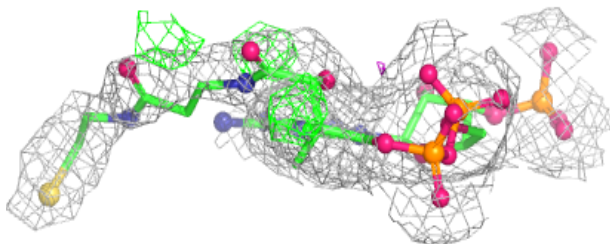
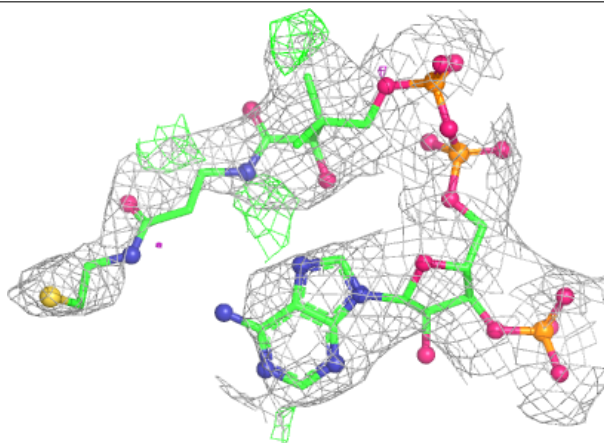


Electron density around COA H 591:

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

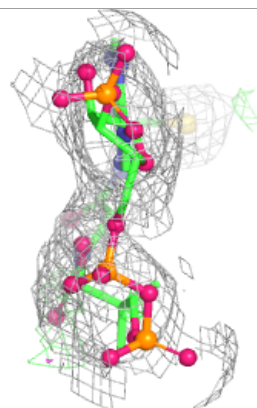
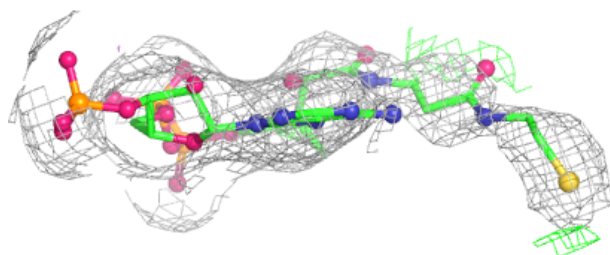
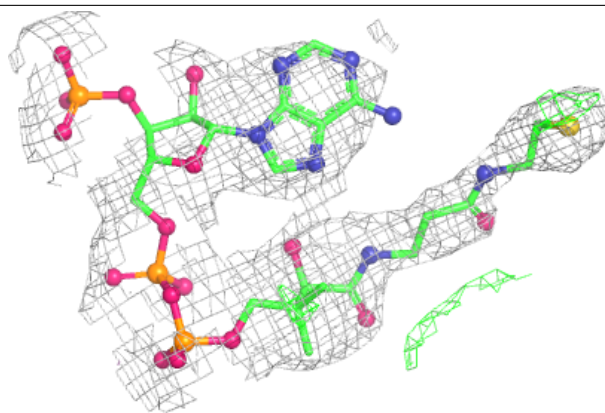
**Electron density around COA J 591:**

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

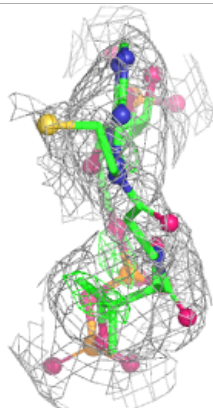
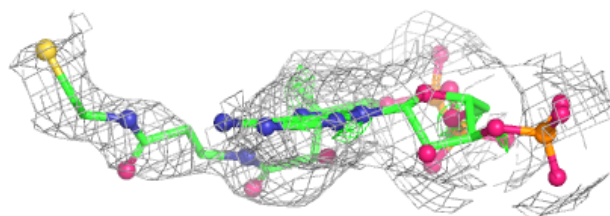
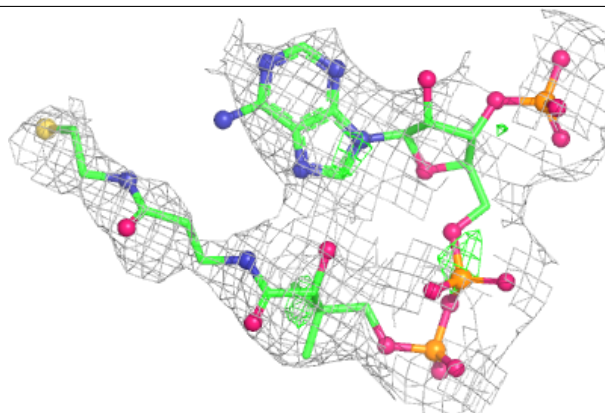


Electron density around COA F 591:

$2mF_o-DF_c$ (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.