Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:47 am BST

PDB ID	:	6HXJ
Title	:	Structure of ATP citrate lyase from Chlorobium limicola in complex with citrate and coenzyme A.
Authors	:	Verstraete, K.; Verschueren, K.
Deposited on	:	2018-10-17
Resolution	:	2.58 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 following versions of software and data (see references ⓘ) were used in the production of this report:

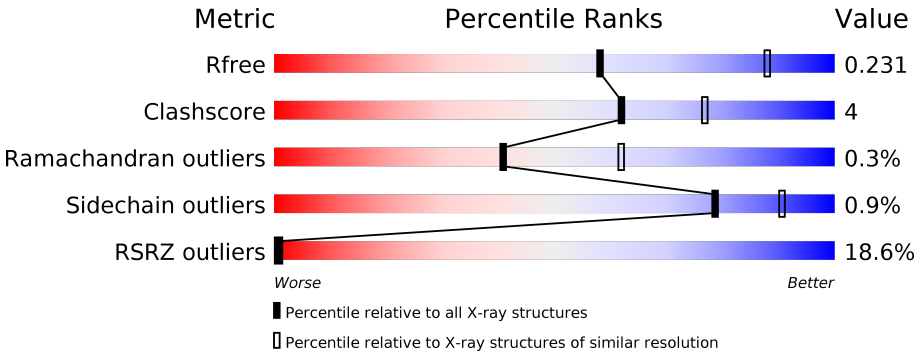
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.58 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	398	31% 72% 12% • 16%
1	C	398	12% 71% 10% 19%
1	E	398	31% 71% 10% 20%
1	G	398	34% 66% 14% • 19%
2	B	617	10% 86% 10% 5%
2	D	617	8% 87% 9% •

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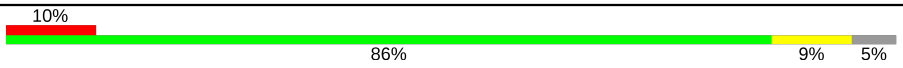
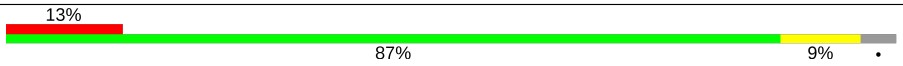
Mol	Chain	Length	Quality of chain
2	F	617	
2	H	617	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TRS	D	1004	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28715 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 ATP-citrate lyase beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2597	1652	440	494	11			
1	C	324	Total	C	N	O	S	0	0	0
			2512	1593	426	483	10			
1	E	320	Total	C	N	O	S	0	0	0
			2480	1575	420	475	10			
1	G	322	Total	C	N	O	S	0	0	0
			2498	1583	424	481	10			

- Molecule 2 is a protein called ATP-citrate lyase alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	589	Total	C	N	O	S	0	0	0
			4464	2832	760	847	25			
2	D	591	Total	C	N	O	S	0	0	0
			4477	2840	763	849	25			
2	F	588	Total	C	N	O	S	0	0	0
			4459	2829	759	846	25			
2	H	591	Total	C	N	O	S	0	0	0
			4477	2840	763	849	25			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	609	GLY	-	expression tag	UNP Q9AJC4
B	610	GLY	-	expression tag	UNP Q9AJC4
B	611	SER	-	expression tag	UNP Q9AJC4
B	612	HIS	-	expression tag	UNP Q9AJC4
B	613	HIS	-	expression tag	UNP Q9AJC4
B	614	HIS	-	expression tag	UNP Q9AJC4
B	615	HIS	-	expression tag	UNP Q9AJC4
B	616	HIS	-	expression tag	UNP Q9AJC4

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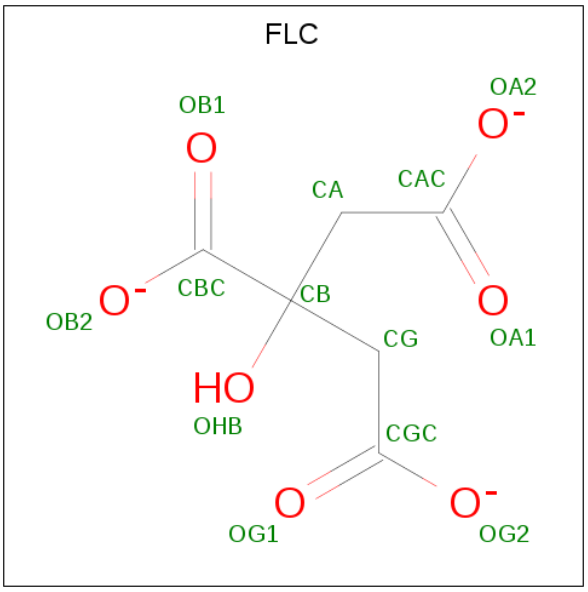
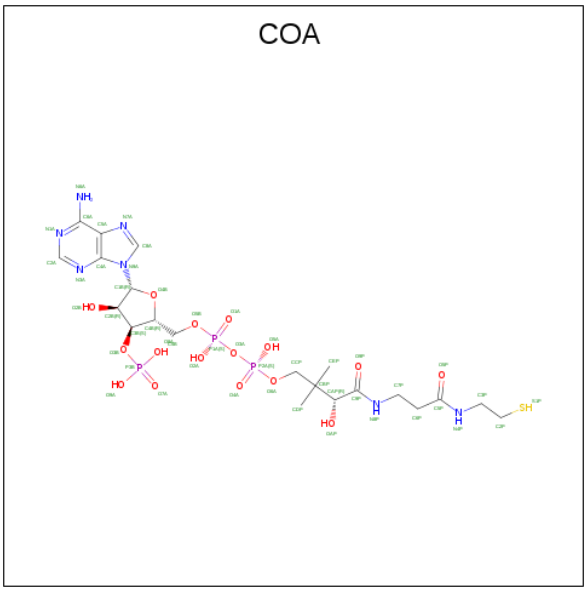
Chain	Residue	Modelled	Actual	Comment	Reference
B	617	HIS	-	expression tag	UNP Q9AJC4
D	609	GLY	-	expression tag	UNP Q9AJC4
D	610	GLY	-	expression tag	UNP Q9AJC4
D	611	SER	-	expression tag	UNP Q9AJC4
D	612	HIS	-	expression tag	UNP Q9AJC4
D	613	HIS	-	expression tag	UNP Q9AJC4
D	614	HIS	-	expression tag	UNP Q9AJC4
D	615	HIS	-	expression tag	UNP Q9AJC4
D	616	HIS	-	expression tag	UNP Q9AJC4
D	617	HIS	-	expression tag	UNP Q9AJC4
F	609	GLY	-	expression tag	UNP Q9AJC4
F	610	GLY	-	expression tag	UNP Q9AJC4
F	611	SER	-	expression tag	UNP Q9AJC4
F	612	HIS	-	expression tag	UNP Q9AJC4
F	613	HIS	-	expression tag	UNP Q9AJC4
F	614	HIS	-	expression tag	UNP Q9AJC4
F	615	HIS	-	expression tag	UNP Q9AJC4
F	616	HIS	-	expression tag	UNP Q9AJC4
F	617	HIS	-	expression tag	UNP Q9AJC4
H	609	GLY	-	expression tag	UNP Q9AJC4
H	610	GLY	-	expression tag	UNP Q9AJC4
H	611	SER	-	expression tag	UNP Q9AJC4
H	612	HIS	-	expression tag	UNP Q9AJC4
H	613	HIS	-	expression tag	UNP Q9AJC4
H	614	HIS	-	expression tag	UNP Q9AJC4
H	615	HIS	-	expression tag	UNP Q9AJC4
H	616	HIS	-	expression tag	UNP Q9AJC4
H	617	HIS	-	expression tag	UNP Q9AJC4

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by author).



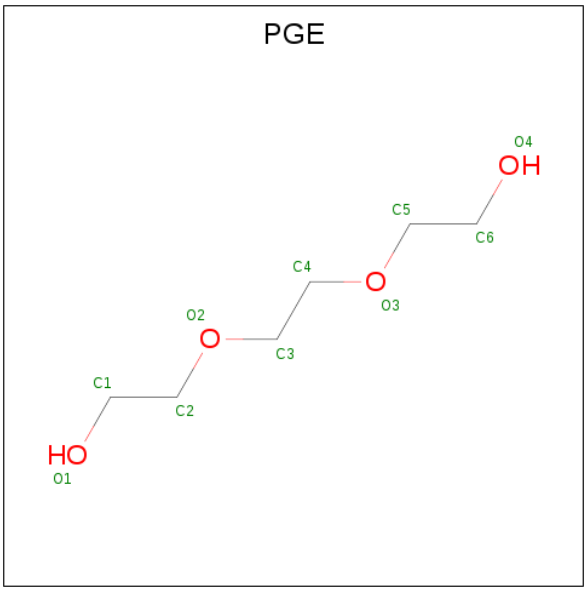
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0
3	E	1	Total C O 13 6 7	0	0
3	F	1	Total C O 13 6 7	0	0
3	G	1	Total C O 13 6 7	0	0
3	H	1	Total C O 13 6 7	0	0

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by author).



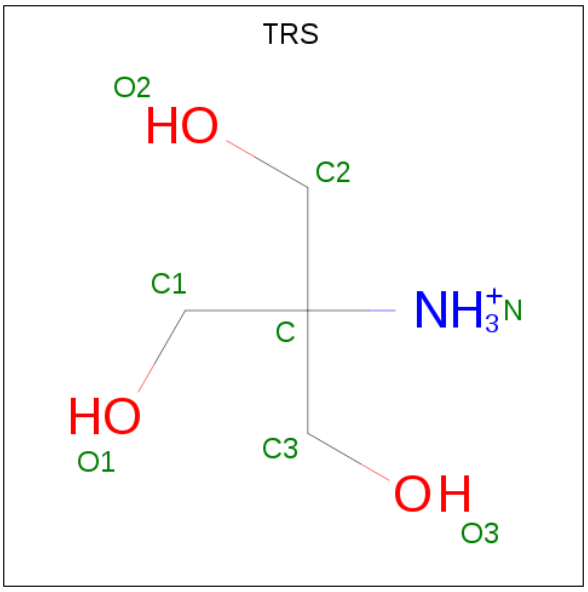
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 37 15 5 14 3	0	0
4	B	1	Total C N O P S 48 21 7 16 3 1	0	0
4	D	1	Total C N O P 31 10 5 13 3	0	0
4	D	1	Total C N O P 41 17 6 15 3	0	0
4	F	1	Total C N O P 31 10 5 13 3	0	0
4	F	1	Total C N O P 42 18 6 15 3	0	0
4	H	1	Total C N O P 31 10 5 13 3	0	0
4	H	1	Total C N O P 40 16 6 15 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



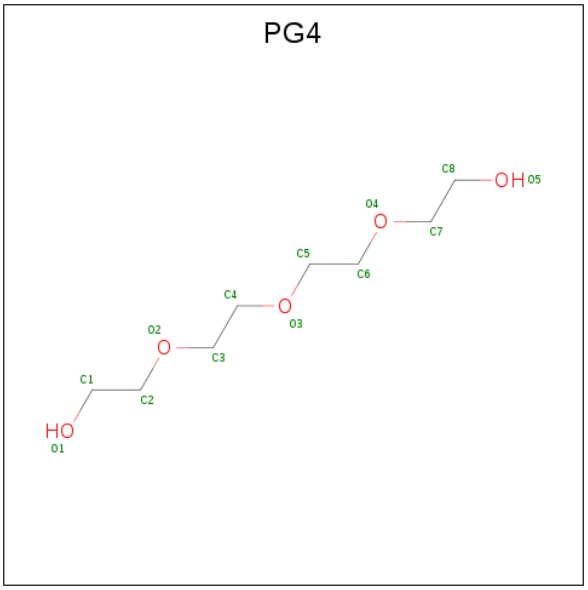
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	H	1	Total C O 10 6 4	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 8 4 1 3	0	0
6	D	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 13 8 5	0	0
7	D	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

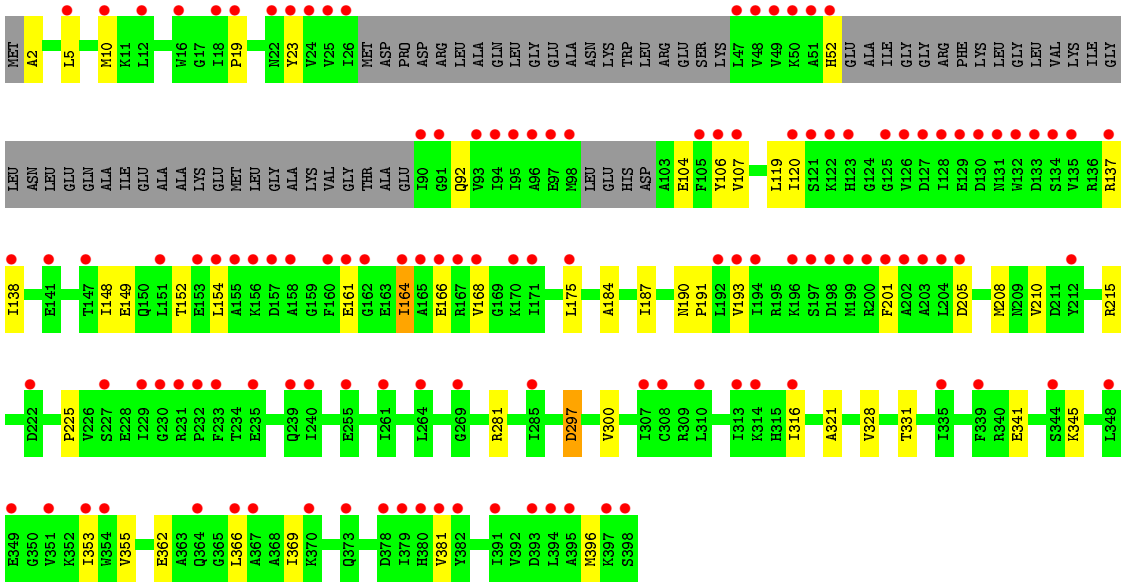
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	3	Total O 3 3	0	0
8	B	61	Total O 61 61	0	0
8	C	15	Total O 15 15	0	0
8	D	58	Total O 58 58	0	0
8	E	5	Total O 5 5	0	0
8	F	60	Total O 60 60	0	0
8	G	2	Total O 2 2	0	0
8	H	50	Total O 50 50	0	0

3 Residue-property plots (i)

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

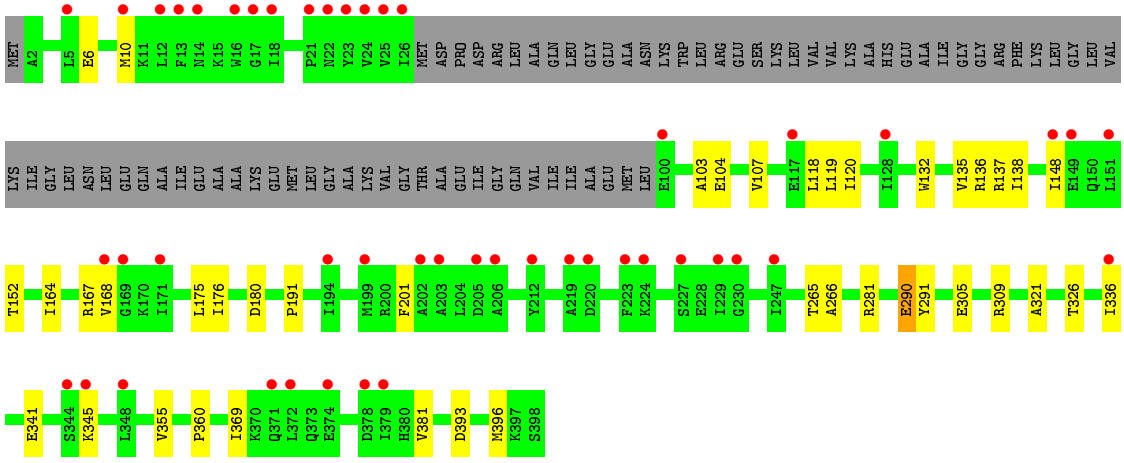
- Molecule 1: ATP-citrate lyase beta-subunit

Chain A:



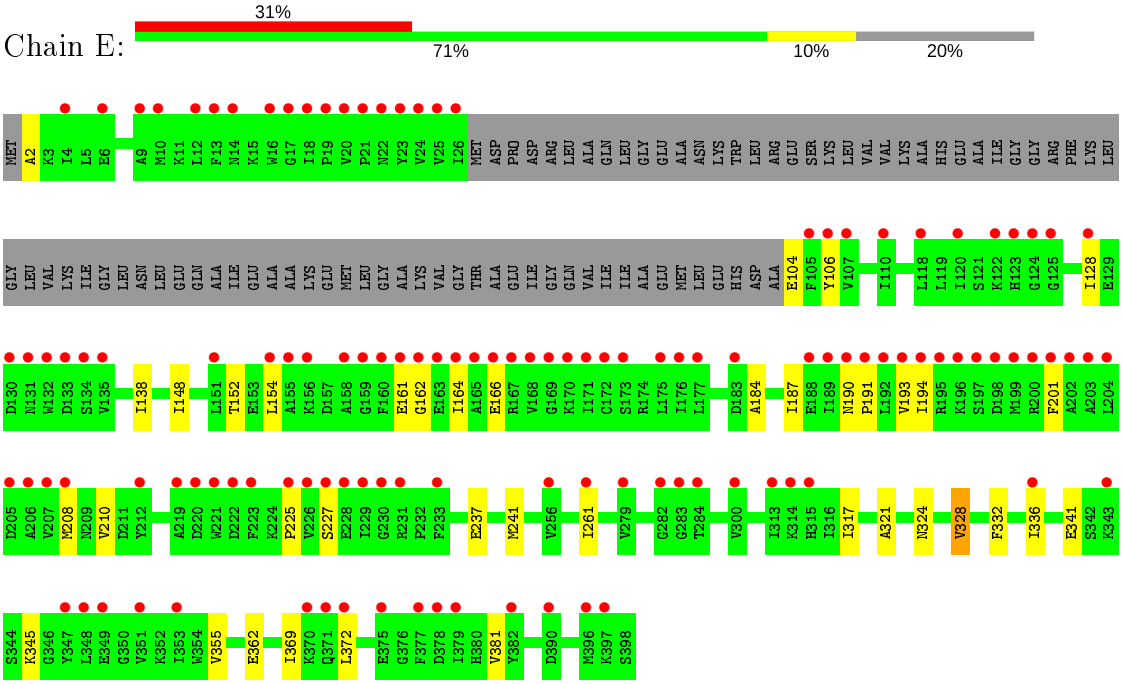
- Molecule 1: ATP-citrate lyase beta-subunit

Chain C:



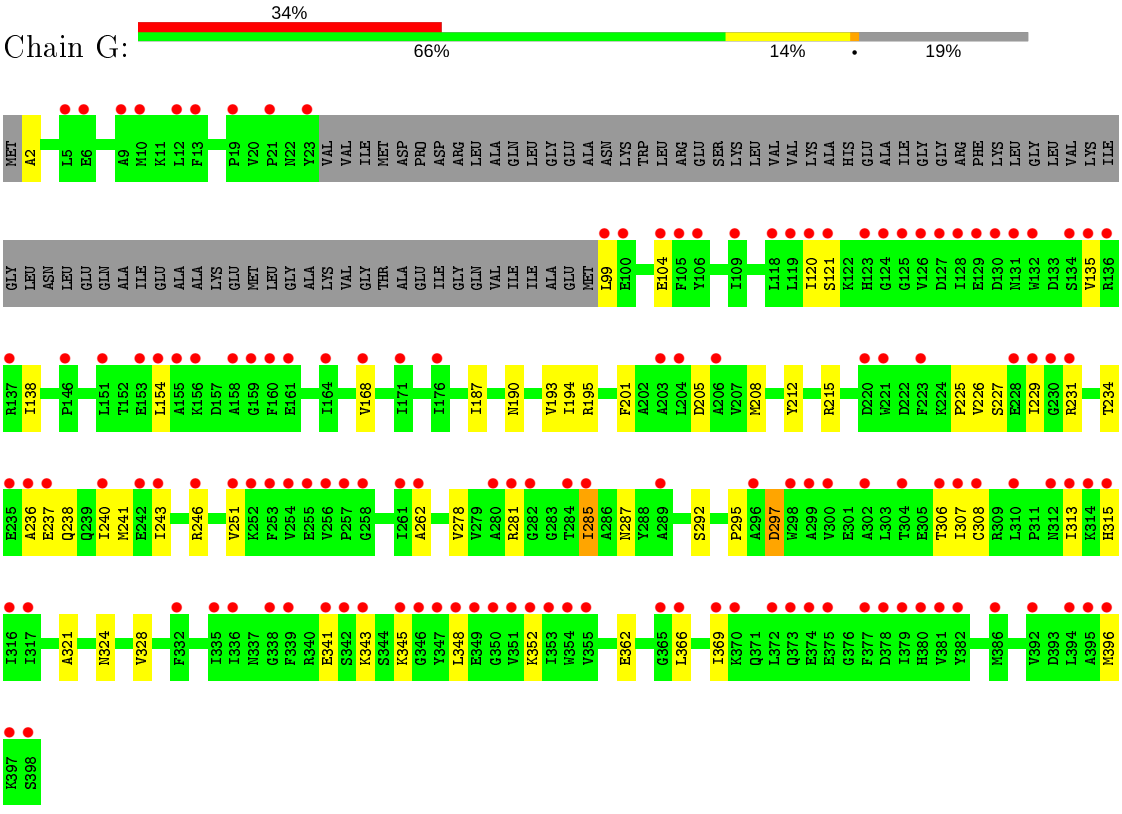
• Molecule 1: ATP-citrate lyase beta-subunit

Chain E:



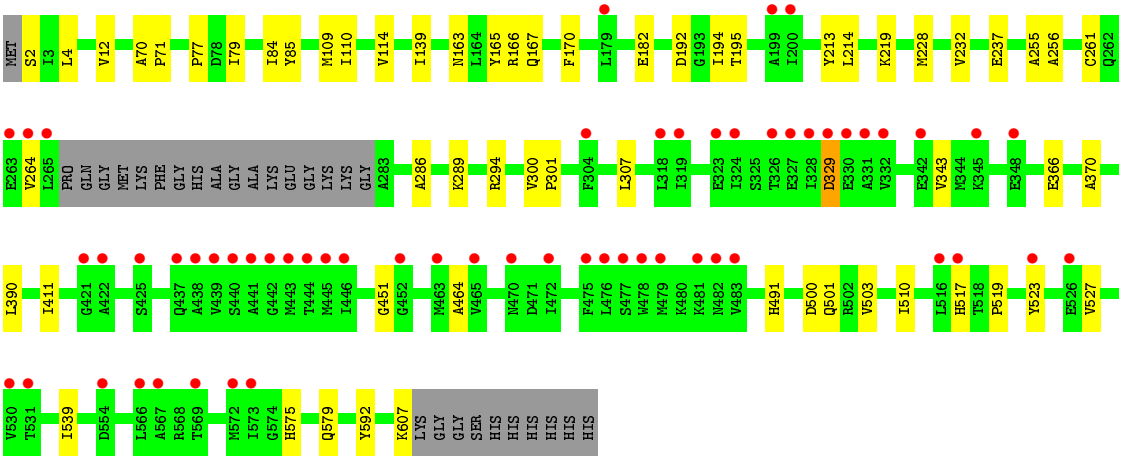
• Molecule 1: ATP-citrate lyase beta-subunit

Chain G:



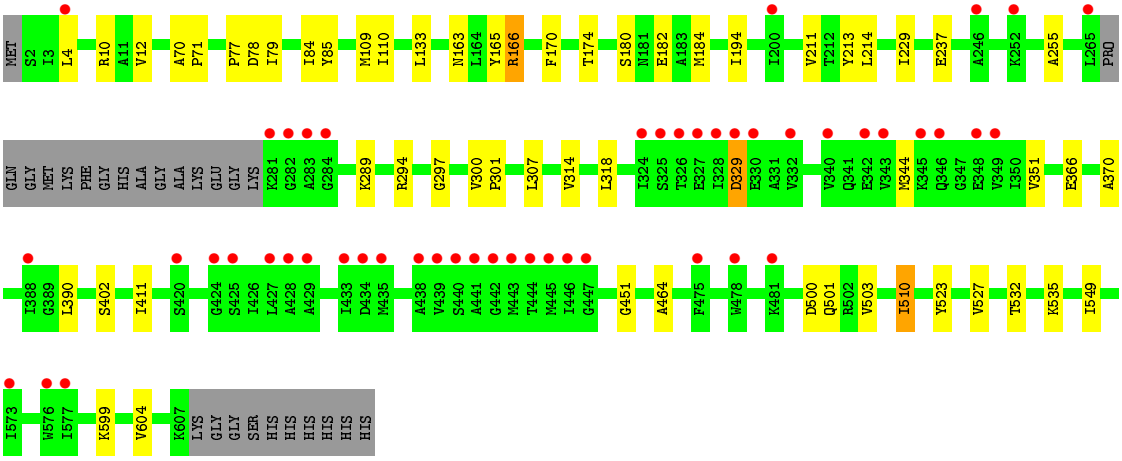
• Molecule 2: ATP-citrate lyase alpha-subunit

Chain B:



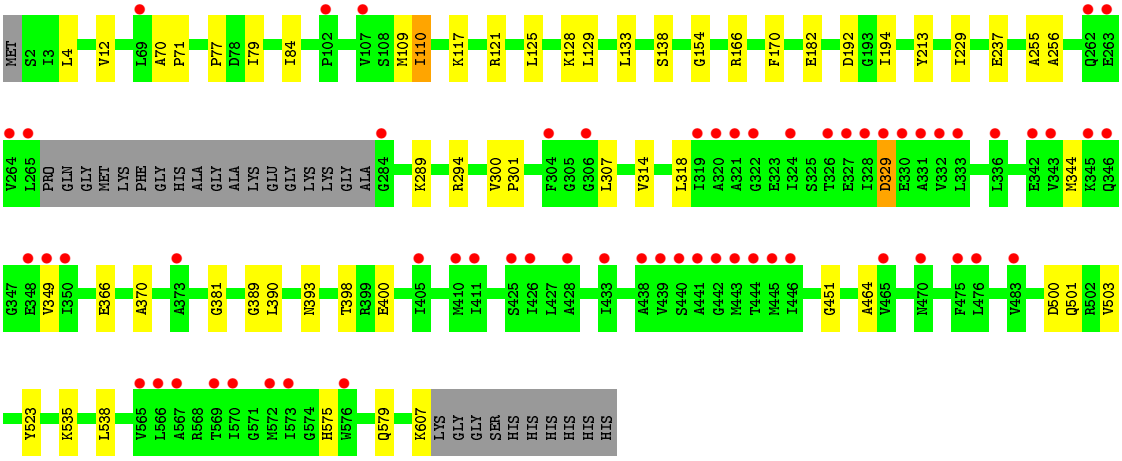
• Molecule 2: ATP-citrate lyase alpha-subunit

Chain D:



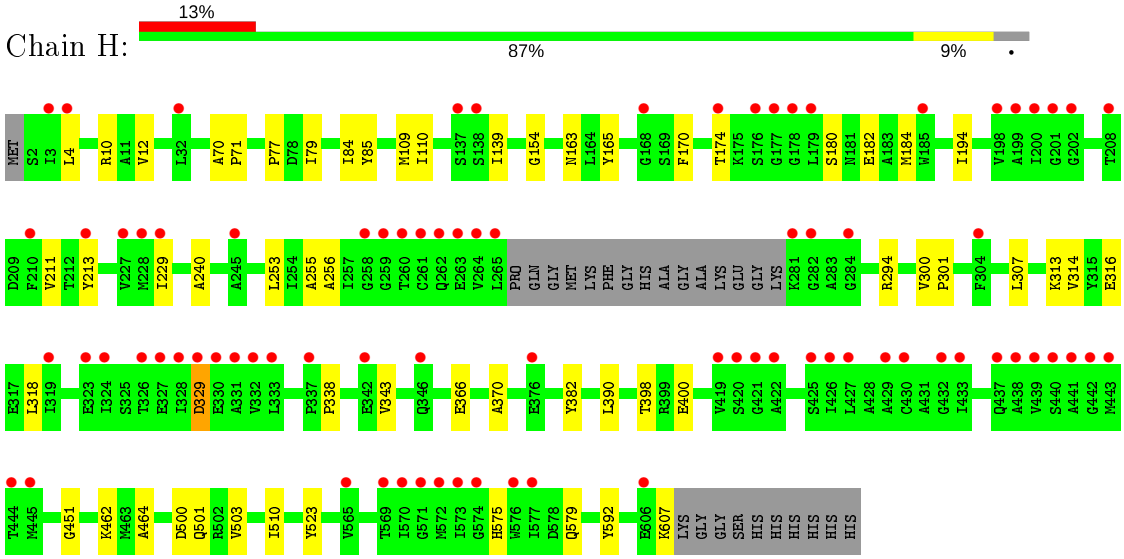
• Molecule 2: ATP-citrate lyase alpha-subunit

Chain F:



• Molecule 2: ATP-citrate lyase alpha-subunit

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.67Å 134.93Å 177.71Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	47.55 – 2.58 47.55 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.55-2.58) 98.6 (47.55-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.183 , 0.216 0.194 , 0.231	Depositor DCC
R_{free} test set	7169 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	67.9	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 80.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28715	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, PG4, PGE, TRS, FLC

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	0.48	0/2642	0.70	0/3569
1	C	0.51	0/2559	0.72	0/3460
1	E	0.49	0/2526	0.71	1/3415 (0.0%)
1	G	0.51	0/2545	0.72	0/3440
2	B	0.53	0/4543	0.70	1/6145 (0.0%)
2	D	0.51	0/4556	0.70	1/6161 (0.0%)
2	F	0.53	0/4538	0.69	1/6138 (0.0%)
2	H	0.53	0/4556	0.70	1/6161 (0.0%)
All	All	0.51	0/28465	0.70	5/38489 (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	C	0	1
2	D	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	77	PRO	C-N-CA	5.83	136.27	121.70
1	E	227	SER	CB-CA-C	5.76	121.05	110.10
2	B	77	PRO	C-N-CA	5.62	135.74	121.70
2	D	77	PRO	C-N-CA	5.57	135.62	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	77	PRO	C-N-CA	5.53	135.52	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ARG	Sidechain
1	C	136	ARG	Sidechain
2	D	166	ARG	Sidechain
2	H	10	ARG	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	2597	0	2584	32	0
1	C	2512	0	2476	23	0
1	E	2480	0	2454	22	0
1	G	2498	0	2458	40	0
2	B	4464	0	4524	38	0
2	D	4477	0	4540	40	0
2	F	4459	0	4519	38	0
2	H	4477	0	4540	32	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	0	0
3	F	13	0	5	0	0
3	G	13	0	5	0	0
3	H	13	0	5	0	0
4	B	85	0	52	2	0
4	D	72	0	33	0	0
4	F	73	0	35	0	0
4	H	71	0	32	0	0
5	B	10	0	14	2	0
5	C	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	14	1	0
5	F	10	0	14	0	0
5	H	10	0	14	2	0
6	B	8	0	12	0	0
6	D	8	0	12	0	0
7	C	13	0	18	1	0
7	D	13	0	18	2	0
8	A	3	0	0	0	0
8	B	61	0	0	1	0
8	C	15	0	0	0	0
8	D	58	0	0	0	0
8	E	5	0	0	0	0
8	F	60	0	0	0	0
8	G	2	0	0	0	0
8	H	50	0	0	0	0
All	All	28715	0	28417	249	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 4.

All (249) 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)
2:D:163:ASN:HB3	2:D:166:ARG:NH2	1.67	1.10
2:D:163:ASN:CB	2:D:166:ARG:NH2	2.22	1.01
1:G:231:ARG:HH12	1:G:234:THR:HG23	1.26	0.98
2:B:166:ARG:NH2	2:B:192:ASP:O	1.97	0.95
2:B:607:LYS:NZ	8:B:1101:HOH:O	1.57	0.95
2:B:592:TYR:HB2	2:D:344:MET:SD	2.10	0.91
2:F:166:ARG:NH1	2:F:192:ASP:O	2.10	0.82
2:F:166:ARG:HD2	2:F:166:ARG:O	1.82	0.79
2:B:163:ASN:HA	2:B:165:TYR:CE1	2.21	0.76
1:G:231:ARG:NH1	1:G:234:THR:HG23	2.00	0.74
2:B:219:LYS:HZ3	5:B:1004:PGE:H32	1.54	0.73
1:E:138:ILE:HG12	1:E:154:LEU:HD22	1.71	0.72
2:D:163:ASN:CB	2:D:166:ARG:HH21	2.04	0.71
1:G:308:CYS:O	1:G:313:ILE:HD13	1.89	0.71
1:G:328:VAL:CG2	1:G:362:GLU:HA	2.21	0.70
1:A:316:ILE:HD12	1:A:353:ILE:HG12	1.74	0.69
2:B:219:LYS:NZ	5:B:1004:PGE:H32	2.08	0.69
2:D:163:ASN:HB3	2:D:166:ARG:HH21	1.51	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:MET:SD	2:H:592:TYR:HB2	2.35	0.67
1:E:2:ALA:HB1	1:E:225:PRO:HB3	1.78	0.66
1:G:226:VAL:HG12	1:G:227:SER:N	2.11	0.66
1:G:328:VAL:HG21	1:G:362:GLU:HA	1.78	0.66
2:D:163:ASN:CB	2:D:166:ARG:HH22	2.10	0.65
2:B:109:MET:HE2	2:B:114:VAL:HG21	1.80	0.64
2:H:462:LYS:HE3	5:H:1004:PGE:H12	1.81	0.63
2:H:462:LYS:HE3	5:H:1004:PGE:C1	2.29	0.63
2:D:4:LEU:HD11	2:D:213:TYR:CE1	2.35	0.62
1:A:107:VAL:HG11	1:A:175:LEU:HD22	1.81	0.62
2:B:232:VAL:HG13	2:B:286:ALA:HB2	1.81	0.62
2:H:398:THR:HG22	2:H:400:GLU:H	1.62	0.62
1:G:138:ILE:HG23	1:G:154:LEU:HD13	1.80	0.62
1:A:148:ILE:O	1:A:152:THR:HG23	2.00	0.61
2:F:110:ILE:HG22	2:F:138:SER:O	2.01	0.60
1:G:226:VAL:HG12	1:G:227:SER:H	1.66	0.60
1:A:138:ILE:HG12	1:A:154:LEU:HD22	1.83	0.60
2:D:4:LEU:HD11	2:D:213:TYR:HE1	1.66	0.59
1:E:321:ALA:HB1	2:F:182:GLU:HB2	1.83	0.59
1:A:297:ASP:OD1	1:A:297:ASP:N	2.34	0.59
1:A:321:ALA:HB1	2:B:182:GLU:HB2	1.85	0.59
2:D:366:GLU:HB3	2:F:501:GLN:HB3	1.85	0.58
2:H:4:LEU:HD11	2:H:213:TYR:HE1	1.67	0.58
2:F:398:THR:HG22	2:F:400:GLU:H	1.68	0.58
1:G:308:CYS:O	1:G:313:ILE:CD1	2.51	0.58
2:H:4:LEU:HD11	2:H:213:TYR:CE1	2.39	0.58
1:C:167:ARG:HG2	1:C:201:PHE:CE1	2.38	0.58
1:C:118:LEU:HB3	1:C:138:ILE:CG2	2.33	0.58
2:F:4:LEU:HD11	2:F:213:TYR:HE1	1.68	0.58
2:B:517:HIS:CE1	2:B:519:PRO:HD3	2.39	0.58
2:D:163:ASN:HB2	2:D:166:ARG:HH22	1.67	0.57
1:E:261:ILE:HD11	1:E:317:ILE:HD11	1.86	0.57
1:A:5:LEU:HD13	1:A:52:HIS:ND1	2.18	0.57
1:A:138:ILE:HG23	1:A:154:LEU:HD13	1.86	0.57
2:B:4:LEU:HD11	2:B:213:TYR:HE1	1.68	0.57
2:F:4:LEU:HD11	2:F:213:TYR:CE1	2.39	0.57
2:B:4:LEU:HD11	2:B:213:TYR:CE1	2.40	0.57
1:A:2:ALA:HB1	1:A:225:PRO:HB3	1.86	0.56
1:G:281:ARG:HB2	1:G:396:MET:HE3	1.86	0.56
1:E:328:VAL:CG2	1:E:362:GLU:HA	2.34	0.56
2:F:125:LEU:HA	2:F:128:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:ASP:N	1:G:297:ASP:OD1	2.38	0.56
2:F:117:LYS:HE3	2:F:121:ARG:NH2	2.21	0.55
2:B:366:GLU:HB3	2:H:501:GLN:HB3	1.88	0.55
2:F:166:ARG:HD2	2:F:166:ARG:C	2.26	0.55
1:C:281:ARG:HD2	1:C:393:ASP:OD1	2.07	0.54
2:B:575:HIS:O	2:B:579:GLN:HG2	2.07	0.54
1:A:119:LEU:HG	1:A:137:ARG:HB3	1.90	0.54
1:C:321:ALA:HB1	2:D:182:GLU:HB2	1.90	0.54
1:A:366:LEU:HA	1:A:369:ILE:HG22	1.90	0.53
1:C:148:ILE:O	1:C:152:THR:HG23	2.08	0.53
1:C:103:ALA:HB2	7:C:1002:PG4:H32	1.91	0.52
1:A:19:PRO:HB3	1:A:201:PHE:O	2.09	0.52
2:H:294:ARG:HD3	2:H:300:VAL:HB	1.92	0.52
2:F:381:GLY:O	2:H:607:LYS:HE2	2.08	0.52
1:G:287:ASN:HD21	1:G:307:ILE:HG12	1.74	0.52
1:A:187:ILE:HG12	1:A:208:MET:HG3	1.92	0.52
1:A:52:HIS:HB2	1:A:92:GLN:HB3	1.92	0.52
2:D:501:GLN:HB3	2:F:366:GLU:HB3	1.91	0.51
2:B:294:ARG:HD3	2:B:300:VAL:HB	1.91	0.51
1:E:148:ILE:O	1:E:152:THR:HG23	2.09	0.51
2:F:464:ALA:HB1	2:F:523:TYR:CE1	2.46	0.51
2:F:535:LYS:HB2	2:F:538:LEU:HG	1.92	0.51
1:A:341:GLU:O	1:A:345:LYS:HG2	2.11	0.51
1:G:341:GLU:O	1:G:345:LYS:HG2	2.11	0.51
2:D:294:ARG:HD3	2:D:300:VAL:HB	1.92	0.50
1:A:107:VAL:CG1	1:A:175:LEU:HD22	2.41	0.50
1:E:328:VAL:O	1:E:332:PHE:HB2	2.12	0.50
1:G:281:ARG:HB2	1:G:396:MET:CE	2.42	0.50
1:G:321:ALA:HB1	2:H:182:GLU:HB2	1.93	0.50
2:B:12:VAL:HB	2:B:79:ILE:HD13	1.93	0.50
2:F:12:VAL:HB	2:F:79:ILE:HD13	1.94	0.50
2:H:12:VAL:HB	2:H:79:ILE:HD13	1.93	0.50
1:C:341:GLU:O	1:C:345:LYS:HG2	2.12	0.49
2:F:294:ARG:HD3	2:F:300:VAL:HB	1.93	0.49
2:F:70:ALA:HB3	2:F:71:PRO:HD3	1.94	0.49
1:G:226:VAL:CG1	1:G:227:SER:H	2.25	0.49
1:E:328:VAL:HG21	1:E:362:GLU:HA	1.94	0.49
1:A:106:TYR:HD1	1:A:190:ASN:HB2	1.78	0.49
2:B:464:ALA:HB1	2:B:523:TYR:CE1	2.47	0.49
1:G:121:SER:HB2	1:G:135:VAL:HG22	1.94	0.49
1:A:10:MET:HB3	1:A:23:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ARG:HG2	1:C:201:PHE:HE1	1.78	0.49
1:G:2:ALA:HB1	1:G:225:PRO:HB3	1.95	0.49
2:H:85:TYR:CD1	2:H:110:ILE:HG12	2.48	0.49
1:C:355:VAL:HB	1:C:381:VAL:HB	1.94	0.48
2:F:229:ILE:HD11	2:F:307:LEU:HD21	1.95	0.48
2:D:532:THR:HA	2:D:535:LYS:O	2.13	0.48
2:D:211:VAL:HA	2:D:214:LEU:HD12	1.94	0.48
2:D:464:ALA:HB1	2:D:523:TYR:CE1	2.49	0.48
2:D:229:ILE:HD11	2:D:307:LEU:HD21	1.95	0.48
2:H:464:ALA:HB1	2:H:523:TYR:CE1	2.48	0.48
1:E:341:GLU:O	1:E:345:LYS:HG2	2.14	0.48
1:G:240:ILE:HG23	1:G:251:VAL:HG22	1.96	0.48
1:E:138:ILE:HG12	1:E:154:LEU:CD2	2.39	0.47
1:E:355:VAL:HB	1:E:381:VAL:HB	1.95	0.47
1:A:149:GLU:H	1:A:149:GLU:CD	2.17	0.47
2:B:2:SER:N	2:B:167:GLN:HE22	2.12	0.47
1:G:226:VAL:CG1	1:G:227:SER:N	2.77	0.47
1:C:305:GLU:O	1:C:309:ARG:HG2	2.15	0.47
2:D:12:VAL:HB	2:D:79:ILE:HD13	1.96	0.47
1:E:104:GLU:HB3	1:E:193:VAL:HG12	1.97	0.47
2:B:163:ASN:HA	2:B:165:TYR:HE1	1.75	0.47
1:E:194:ILE:HD13	1:E:201:PHE:CE1	2.49	0.47
1:E:187:ILE:HG12	1:E:208:MET:HG3	1.97	0.47
1:G:366:LEU:HA	1:G:369:ILE:HG22	1.97	0.47
1:A:328:VAL:CG2	1:A:362:GLU:HA	2.45	0.46
1:G:194:ILE:HD13	1:G:201:PHE:CE1	2.49	0.46
2:D:510:ILE:HD13	2:D:549:ILE:CD1	2.46	0.46
2:B:261:CYS:HB3	2:B:264:VAL:HG12	1.97	0.46
2:D:85:TYR:CD2	2:D:110:ILE:HG12	2.50	0.46
1:G:243:ILE:HA	1:G:246:ARG:HD2	1.97	0.46
2:B:85:TYR:CD2	2:B:110:ILE:HG12	2.50	0.46
1:C:336:ILE:HG12	1:C:369:ILE:HD12	1.98	0.46
1:G:287:ASN:ND2	1:G:307:ILE:HG12	2.30	0.46
2:B:214:LEU:HD11	2:B:228:MET:HE1	1.97	0.46
2:B:237:GLU:HB2	2:B:289:LYS:HD3	1.98	0.46
1:C:120:ILE:HD11	1:C:168:VAL:CG1	2.46	0.46
2:D:163:ASN:CG	2:D:166:ARG:HH21	2.19	0.46
1:E:237:GLU:O	1:E:241:MET:HG3	2.16	0.46
2:H:500:ASP:HB3	2:H:503:VAL:HG13	1.97	0.46
1:A:190:ASN:O	1:A:205:ASP:HB2	2.15	0.45
2:D:10:ARG:HD3	2:D:78:ASP:CG	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:VAL:HG22	1:E:362:GLU:HA	1.97	0.45
2:B:500:ASP:HB3	2:B:503:VAL:HG13	1.97	0.45
1:E:184:ALA:HA	1:E:210:VAL:HA	1.97	0.45
2:F:370:ALA:HB3	2:F:390:LEU:HD22	1.98	0.45
2:F:575:HIS:O	2:F:579:GLN:HG2	2.16	0.45
2:B:501:GLN:HB3	2:H:366:GLU:HB3	1.96	0.45
1:G:292:SER:O	1:G:295:PRO:HG3	2.16	0.45
2:B:343:VAL:HG21	2:F:349:VAL:HG23	1.98	0.45
1:G:104:GLU:HG2	1:G:193:VAL:HG12	1.98	0.45
2:D:500:ASP:HB3	2:D:503:VAL:HG13	1.98	0.45
1:E:161:GLU:O	1:E:164:ILE:HG13	2.17	0.45
2:F:389:GLY:O	2:F:393:ASN:HB2	2.17	0.45
1:G:99:LEU:HD21	1:G:195:ARG:CZ	2.46	0.45
2:H:70:ALA:HB3	2:H:71:PRO:HD3	1.98	0.45
2:F:314:VAL:O	2:F:318:LEU:HG	2.17	0.45
2:D:370:ALA:HB3	2:D:390:LEU:HD22	1.98	0.45
1:G:120:ILE:HD11	1:G:168:VAL:HG11	1.99	0.44
1:C:119:LEU:HD23	1:C:135:VAL:HG11	1.98	0.44
2:F:166:ARG:CD	2:F:166:ARG:C	2.85	0.44
2:F:170:PHE:O	2:F:194:ILE:HA	2.18	0.44
2:D:599:LYS:HZ2	7:D:1005:PG4:H72	1.83	0.44
2:D:70:ALA:HB3	2:D:71:PRO:HD3	1.98	0.44
2:B:84:ILE:HB	2:B:109:MET:HG2	2.00	0.44
2:F:125:LEU:HD12	2:F:128:LYS:HD2	1.98	0.44
2:H:255:ALA:O	2:H:301:PRO:HD2	2.18	0.44
1:A:328:VAL:HG22	1:A:362:GLU:HA	1.99	0.44
1:E:324:ASN:O	2:F:154:GLY:HA2	2.18	0.44
1:G:240:ILE:HD13	1:G:243:ILE:HD11	1.99	0.44
1:G:324:ASN:O	2:H:154:GLY:HA2	2.18	0.44
2:H:170:PHE:O	2:H:194:ILE:HA	2.18	0.44
2:H:84:ILE:HB	2:H:109:MET:HG2	2.00	0.44
1:G:315:HIS:HE1	1:G:352:LYS:HD2	1.82	0.44
2:H:575:HIS:O	2:H:579:GLN:HG2	2.18	0.44
1:G:343:LYS:HG3	1:G:348:LEU:HB2	2.00	0.44
2:B:592:TYR:HD1	2:D:351:VAL:HG11	1.82	0.43
1:G:190:ASN:O	1:G:205:ASP:HB3	2.18	0.43
2:H:370:ALA:HB3	2:H:390:LEU:HD22	1.99	0.43
2:B:70:ALA:HB3	2:B:71:PRO:HD3	2.00	0.43
1:C:107:VAL:HG11	1:C:175:LEU:HD22	2.01	0.43
2:B:256:ALA:HB2	2:B:307:LEU:HD13	2.00	0.43
1:G:236:ALA:HB1	1:G:306:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:ALA:HB1	1:G:307:ILE:HG23	1.99	0.43
2:H:163:ASN:HA	2:H:165:TYR:CE1	2.54	0.43
2:D:84:ILE:HB	2:D:109:MET:HG2	2.00	0.43
2:D:237:GLU:HB2	2:D:289:LYS:HD3	1.99	0.43
1:G:187:ILE:HG12	1:G:208:MET:HG3	2.00	0.43
2:H:174:THR:HG22	2:H:229:ILE:HB	2.00	0.43
2:B:110:ILE:HD11	4:B:1002:COA:H133	1.99	0.43
2:F:255:ALA:O	2:F:301:PRO:HD2	2.18	0.43
1:A:107:VAL:CG1	1:A:175:LEU:CD2	2.96	0.43
2:D:255:ALA:O	2:D:301:PRO:HD2	2.19	0.43
1:A:355:VAL:HB	1:A:381:VAL:HB	2.00	0.43
1:E:336:ILE:HG23	1:E:372:LEU:HD21	2.01	0.43
1:A:300:VAL:HG21	1:A:331:THR:HG22	2.01	0.43
2:F:109:MET:HE2	2:F:133:LEU:HD11	2.01	0.43
1:C:118:LEU:HB3	1:C:138:ILE:HG23	2.01	0.42
2:D:163:ASN:HB2	2:D:166:ARG:NH2	2.16	0.42
1:C:104:GLU:HB3	1:C:191:PRO:HB3	2.01	0.42
2:F:256:ALA:HB2	2:F:307:LEU:HD13	2.01	0.42
1:G:234:THR:OG1	1:G:237:GLU:HB2	2.19	0.42
1:C:6:GLU:O	1:C:10:MET:HG2	2.19	0.42
2:H:313:LYS:O	2:H:316:GLU:HG2	2.20	0.42
1:C:266:ALA:HB2	1:C:291:TYR:CZ	2.55	0.42
2:D:109:MET:HE2	2:D:133:LEU:HD11	2.01	0.42
1:A:152:THR:HG22	1:A:166:GLU:HA	2.02	0.42
2:H:256:ALA:HB2	2:H:307:LEU:HD13	2.00	0.42
2:B:370:ALA:HB3	2:B:390:LEU:HD22	2.01	0.42
2:D:599:LYS:NZ	7:D:1005:PG4:H72	2.34	0.42
2:D:170:PHE:O	2:D:194:ILE:HA	2.20	0.42
2:H:338:PRO:HG2	2:H:343:VAL:CG2	2.50	0.42
2:B:170:PHE:O	2:B:194:ILE:HA	2.20	0.42
1:C:132:TRP:HE1	1:C:137:ARG:HH21	1.67	0.42
2:F:500:ASP:HB3	2:F:503:VAL:HG13	2.00	0.42
2:H:85:TYR:CE1	2:H:110:ILE:HG12	2.54	0.42
2:F:125:LEU:O	2:F:128:LYS:HG2	2.20	0.42
2:F:128:LYS:HG3	2:F:129:LEU:HG	2.02	0.41
2:F:237:GLU:HB2	2:F:289:LYS:HD3	2.02	0.41
2:F:607:LYS:HE3	2:H:382:TYR:CD1	2.55	0.41
2:D:174:THR:HG22	2:D:229:ILE:HB	2.02	0.41
1:G:238:GLN:HA	1:G:241:MET:HE3	2.01	0.41
2:H:314:VAL:O	2:H:318:LEU:HG	2.20	0.41
1:A:184:ALA:HA	1:A:210:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:180:SER:O	2:H:184:MET:HG3	2.20	0.41
1:E:162:GLY:O	1:E:166:GLU:HG2	2.21	0.41
2:B:255:ALA:O	2:B:301:PRO:HD2	2.20	0.41
2:B:491:HIS:HB2	2:B:539:ILE:HD11	2.01	0.41
2:D:510:ILE:HD13	2:D:549:ILE:HD13	2.02	0.41
2:F:84:ILE:HB	2:F:109:MET:HG2	2.03	0.41
1:A:161:GLU:O	1:A:164:ILE:HD12	2.20	0.41
1:A:281:ARG:HB3	1:A:396:MET:HG3	2.02	0.41
1:C:176:ILE:O	1:C:180:ASP:HB2	2.20	0.41
1:G:278:VAL:HG11	1:G:285:ILE:HG23	2.02	0.41
2:H:211:VAL:HG12	2:H:240:ALA:HA	2.03	0.41
1:C:326:THR:O	1:C:360:PRO:HD2	2.21	0.41
1:G:212:TYR:CZ	1:G:215:ARG:HD3	2.56	0.41
1:A:120:ILE:HD11	1:A:168:VAL:HG11	2.03	0.41
2:D:163:ASN:HA	2:D:165:TYR:CE1	2.56	0.41
2:D:180:SER:O	2:D:184:MET:HG3	2.21	0.41
2:D:297:GLY:HA2	5:D:1006:PGE:H62	2.02	0.41
2:B:110:ILE:CD1	4:B:1002:COA:H133	2.51	0.40
1:C:281:ARG:HB3	1:C:396:MET:HG3	2.02	0.40
1:C:265:THR:O	1:C:290:GLU:HA	2.21	0.40
1:A:104:GLU:HG2	1:A:193:VAL:HG12	2.02	0.40
1:A:190:ASN:HA	1:A:191:PRO:HA	1.79	0.40
2:B:167:GLN:OE1	2:B:195:THR:HA	2.22	0.40
2:B:85:TYR:CE2	2:B:110:ILE:HG12	2.56	0.40
2:D:314:VAL:O	2:D:318:LEU:HG	2.20	0.40
1:E:106:TYR:HD1	1:E:190:ASN:HA	1.86	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	328/398 (82%)	311 (95%)	17 (5%)	0	100	100
1	C	320/398 (80%)	304 (95%)	16 (5%)	0	100	100
1	E	316/398 (79%)	297 (94%)	18 (6%)	1 (0%)	41	62
1	G	318/398 (80%)	295 (93%)	22 (7%)	1 (0%)	41	62
2	B	585/617 (95%)	572 (98%)	11 (2%)	2 (0%)	41	62
2	D	587/617 (95%)	573 (98%)	12 (2%)	2 (0%)	41	62
2	F	584/617 (95%)	570 (98%)	12 (2%)	2 (0%)	41	62
2	H	587/617 (95%)	574 (98%)	11 (2%)	2 (0%)	41	62
All	All	3625/4060 (89%)	3496 (96%)	119 (3%)	10 (0%)	41	62

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	329	ASP
2	F	329	ASP
2	D	329	ASP
2	F	451	GLY
2	H	329	ASP
1	G	229	ILE
1	E	191	PRO
2	H	451	GLY
2	B	451	GLY
2	D	451	GLY

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	272/319 (85%)	270 (99%)	2 (1%)	84	93
1	C	263/319 (82%)	261 (99%)	2 (1%)	81	92
1	E	260/319 (82%)	257 (99%)	3 (1%)	71	86
1	G	261/319 (82%)	259 (99%)	2 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	471/490 (96%)	466 (99%)	5 (1%)	73 88
2	D	472/490 (96%)	466 (99%)	6 (1%)	69 85
2	F	471/490 (96%)	469 (100%)	2 (0%)	91 97
2	H	472/490 (96%)	468 (99%)	4 (1%)	81 92
All	All	2942/3236 (91%)	2916 (99%)	26 (1%)	78 90

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ILE
1	A	297	ASP
2	B	139	ILE
2	B	329	ASP
2	B	411	ILE
2	B	510	ILE
2	B	527	VAL
1	C	164	ILE
1	C	290	GLU
2	D	329	ASP
2	D	402	SER
2	D	411	ILE
2	D	510	ILE
2	D	527	VAL
2	D	604	VAL
1	E	128	ILE
1	E	328	VAL
1	E	369	ILE
2	F	110	ILE
2	F	329	ASP
1	G	285	ILE
1	G	297	ASP
2	H	139	ILE
2	H	253	LEU
2	H	329	ASP
2	H	510	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

25 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	$\#\|Z\| > 2$
6	TRS	B	1005	-	7,7,7	0.19	0	9,9,9	0.33	0
5	PGE	F	1004	-	9,9,9	0.32	0	8,8,8	0.25	0
3	FLC	H	1003	-	3,12,12	0.31	0	3,17,17	2.68	2 (66%)
6	TRS	D	1004	-	7,7,7	0.33	0	9,9,9	0.42	0
4	COA	H	1001	-	28,33,50	1.00	1 (3%)	35,52,75	0.98	2 (5%)
5	PGE	C	1003	-	9,9,9	0.30	0	8,8,8	0.21	0
3	FLC	E	1001	-	3,12,12	0.42	0	3,17,17	1.34	1 (33%)
5	PGE	H	1004	-	9,9,9	0.22	0	8,8,8	0.18	0
4	COA	B	1001	-	34,39,50	0.67	0	40,61,75	0.93	2 (5%)
7	PG4	C	1002	-	12,12,12	0.19	0	11,11,11	0.28	0
3	FLC	G	1001	-	3,12,12	0.54	0	3,17,17	1.48	0
4	COA	D	1002	-	35,43,50	0.65	1 (2%)	45,67,75	0.68	1 (2%)
3	FLC	D	1003	-	3,12,12	0.37	0	3,17,17	2.00	1 (33%)
4	COA	F	1002	-	36,44,50	0.65	0	45,68,75	0.70	1 (2%)
5	PGE	D	1006	-	9,9,9	0.27	0	8,8,8	0.41	0
4	COA	F	1001	-	28,33,50	0.88	0	35,52,75	0.90	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PGE	B	1004	-	9,9,9	0.37	0	8,8,8	0.39	0
4	COA	D	1001	-	28,33,50	1.08	2 (7%)	35,52,75	0.96	2 (5%)
4	COA	B	1002	-	41,50,50	0.59	1 (2%)	52,75,75	1.09	4 (7%)
3	FLC	F	1003	-	3,12,12	0.40	0	3,17,17	2.21	1 (33%)
3	FLC	A	1001	-	3,12,12	0.43	0	3,17,17	0.64	0
4	COA	H	1002	-	35,42,50	0.64	1 (2%)	45,66,75	0.79	2 (4%)
3	FLC	C	1001	-	3,12,12	0.39	0	3,17,17	0.95	0
3	FLC	B	1003	-	3,12,12	0.38	0	3,17,17	2.84	1 (33%)
7	PG4	D	1005	-	12,12,12	0.27	0	11,11,11	0.40	0

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
6	TRS	B	1005	-	-	3/9/9/9	-
5	PGE	F	1004	-	-	2/7/7/7	-
3	FLC	H	1003	-	-	0/6/16/16	-
6	TRS	D	1004	-	-	3/9/9/9	-
4	COA	H	1001	-	-	9/17/37/64	0/3/3/3
5	PGE	C	1003	-	-	3/7/7/7	-
3	FLC	E	1001	-	-	0/6/16/16	-
5	PGE	H	1004	-	-	3/7/7/7	-
4	COA	B	1001	-	-	10/27/47/64	0/3/3/3
7	PG4	C	1002	-	-	2/10/10/10	-
3	FLC	G	1001	-	-	0/6/16/16	-
4	COA	D	1002	-	-	11/36/56/64	0/3/3/3
3	FLC	D	1003	-	-	0/6/16/16	-
4	COA	F	1002	-	-	10/37/57/64	0/3/3/3
5	PGE	D	1006	-	-	4/7/7/7	-
4	COA	F	1001	-	-	3/17/37/64	0/3/3/3
5	PGE	B	1004	-	-	6/7/7/7	-
4	COA	D	1001	-	-	6/17/37/64	0/3/3/3
4	COA	B	1002	-	-	13/44/64/64	0/3/3/3
3	FLC	F	1003	-	-	0/6/16/16	-
3	FLC	A	1001	-	-	0/6/16/16	-
4	COA	H	1002	-	-	11/33/54/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	C	1001	-	-	0/6/16/16	-
3	FLC	B	1003	-	-	0/6/16/16	-
7	PG4	D	1005	-	-	5/10/10/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1001	COA	P2A-O4A	3.54	1.62	1.50
4	H	1001	COA	P3B-O3B	2.31	1.63	1.59
4	D	1001	COA	P3B-O3B	2.29	1.63	1.59
4	H	1002	COA	P3B-O3B	2.13	1.63	1.59
4	D	1002	COA	P3B-O3B	2.11	1.63	1.59
4	B	1002	COA	P3B-O3B	2.10	1.63	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1002	COA	O6A-P2A-O4A	5.12	129.09	109.07
3	B	1003	FLC	CB-CG-CGC	4.58	122.32	114.98
3	H	1003	FLC	CB-CA-CAC	4.03	121.44	114.98
3	F	1003	FLC	CB-CG-CGC	3.55	120.68	114.98
3	D	1003	FLC	CB-CA-CAC	3.40	120.42	114.98
4	B	1001	COA	CCP-CBP-CAP	3.38	115.83	110.10
4	B	1002	COA	C5A-C6A-N6A	2.55	124.23	120.35
4	B	1001	COA	C5A-C6A-N6A	2.42	124.02	120.35
4	D	1001	COA	O6A-P2A-O5A	2.32	116.50	107.64
4	D	1001	COA	C5A-C6A-N6A	2.28	123.82	120.35
4	H	1002	COA	CBP-CAP-C9P	2.27	118.13	113.70
4	B	1002	COA	CDP-CBP-CAP	2.26	112.74	108.82
4	B	1002	COA	O5A-P2A-O6A	-2.25	97.31	107.75
4	F	1002	COA	C5A-C6A-N6A	2.24	123.75	120.35
3	H	1003	FLC	CB-CG-CGC	2.24	118.56	114.98
4	F	1001	COA	C5A-C6A-N6A	2.22	123.73	120.35
4	D	1002	COA	C5A-C6A-N6A	2.20	123.70	120.35
4	H	1002	COA	C5A-C6A-N6A	2.17	123.65	120.35
3	E	1001	FLC	CB-CG-CGC	2.14	118.41	114.98
4	H	1001	COA	C5A-C6A-N6A	2.07	123.50	120.35
4	H	1001	COA	O5A-P2A-O4A	2.01	118.56	110.68

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1005	TRS	C1-C-C3-O3
6	B	1005	TRS	C2-C-C3-O3
6	B	1005	TRS	N-C-C3-O3
4	H	1001	COA	C3B-O3B-P3B-O7A
4	H	1001	COA	C5B-O5B-P1A-O1A
4	H	1001	COA	C5B-O5B-P1A-O2A
4	H	1001	COA	P1A-O3A-P2A-O6A
4	B	1001	COA	C5B-O5B-P1A-O1A
4	B	1001	COA	CCP-O6A-P2A-O3A
4	D	1002	COA	C5B-O5B-P1A-O2A
4	D	1002	COA	CCP-O6A-P2A-O3A
4	D	1002	COA	CCP-O6A-P2A-O4A
4	D	1002	COA	CCP-O6A-P2A-O5A
4	D	1002	COA	CDP-CBP-CCP-O6A
4	D	1002	COA	CEP-CBP-CCP-O6A
4	D	1002	COA	CAP-CBP-CCP-O6A
4	F	1002	COA	C5B-O5B-P1A-O2A
4	F	1002	COA	CCP-O6A-P2A-O3A
4	F	1002	COA	CCP-O6A-P2A-O4A
4	F	1002	COA	CCP-O6A-P2A-O5A
4	F	1002	COA	CDP-CBP-CCP-O6A
4	F	1002	COA	CEP-CBP-CCP-O6A
4	F	1002	COA	CAP-CBP-CCP-O6A
4	F	1001	COA	P1A-O3A-P2A-O6A
4	B	1002	COA	C5B-O5B-P1A-O1A
4	B	1002	COA	N8P-C9P-CAP-CBP
4	B	1002	COA	N8P-C9P-CAP-OAP
4	H	1002	COA	C5B-O5B-P1A-O2A
4	H	1002	COA	CCP-O6A-P2A-O3A
4	H	1002	COA	CCP-O6A-P2A-O4A
4	H	1002	COA	CCP-O6A-P2A-O5A
4	H	1002	COA	CDP-CBP-CCP-O6A
4	H	1002	COA	CEP-CBP-CCP-O6A
4	H	1002	COA	CAP-CBP-CCP-O6A
4	H	1002	COA	N8P-C9P-CAP-OAP
4	H	1001	COA	C3B-C4B-C5B-O5B
4	H	1001	COA	O4B-C4B-C5B-O5B
5	H	1004	PGE	O1-C1-C2-O2
7	C	1002	PG4	O4-C7-C8-O5
5	B	1004	PGE	O2-C3-C4-O3
5	B	1004	PGE	O3-C5-C6-O4
7	D	1005	PG4	O2-C3-C4-O3
6	D	1004	TRS	C1-C-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	1002	COA	O9P-C9P-CAP-OAP
5	D	1006	PGE	O3-C5-C6-O4
4	B	1002	COA	O9P-C9P-CAP-CBP
4	B	1001	COA	C4B-C5B-O5B-P1A
4	B	1001	COA	P2A-O3A-P1A-O5B
4	B	1001	COA	P1A-O3A-P2A-O6A
4	D	1002	COA	P2A-O3A-P1A-O5B
4	F	1002	COA	P2A-O3A-P1A-O5B
4	D	1001	COA	P2A-O3A-P1A-O5B
4	H	1002	COA	P2A-O3A-P1A-O5B
7	D	1005	PG4	C6-C5-O3-C4
5	F	1004	PGE	C3-C4-O3-C5
5	D	1006	PGE	C1-C2-O2-C3
4	D	1001	COA	C4B-C5B-O5B-P1A
4	H	1001	COA	P1A-O3A-P2A-O5A
5	F	1004	PGE	C1-C2-O2-C3
5	H	1004	PGE	C3-C4-O3-C5
5	H	1004	PGE	C6-C5-O3-C4
5	B	1004	PGE	C3-C4-O3-C5
5	D	1006	PGE	C6-C5-O3-C4
4	B	1001	COA	C5B-O5B-P1A-O3A
4	D	1002	COA	C5B-O5B-P1A-O3A
4	F	1002	COA	C5B-O5B-P1A-O3A
4	B	1002	COA	C5B-O5B-P1A-O3A
4	H	1002	COA	C5B-O5B-P1A-O3A
5	C	1003	PGE	C6-C5-O3-C4
5	D	1006	PGE	C3-C4-O3-C5
6	D	1004	TRS	N-C-C2-O2
7	C	1002	PG4	C4-C3-O2-C2
4	B	1001	COA	C5B-O5B-P1A-O2A
4	B	1001	COA	CCP-O6A-P2A-O4A
4	D	1002	COA	C5B-O5B-P1A-O1A
4	F	1002	COA	C5B-O5B-P1A-O1A
4	B	1002	COA	C5B-O5B-P1A-O2A
4	H	1002	COA	C5B-O5B-P1A-O1A
7	D	1005	PG4	C1-C2-O2-C3
5	C	1003	PGE	C4-C3-O2-C2
4	B	1001	COA	OAP-CAP-CBP-CCP
5	B	1004	PGE	C1-C2-O2-C3
4	B	1002	COA	CAP-CBP-CCP-O6A
4	D	1002	COA	O9P-C9P-N8P-C7P
4	B	1002	COA	CEP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
5	B	1004	PGE	C6-C5-O3-C4
4	F	1001	COA	C4B-C5B-O5B-P1A
4	H	1001	COA	C4B-C5B-O5B-P1A
7	D	1005	PG4	O3-C5-C6-O4
6	D	1004	TRS	C3-C-C2-O2
4	D	1001	COA	P1A-O3A-P2A-O4A
4	B	1001	COA	OAP-CAP-CBP-CEP
4	B	1002	COA	P2A-O3A-P1A-O1A
4	B	1002	COA	P2A-O3A-P1A-O5B
4	D	1001	COA	C3B-O3B-P3B-O7A
4	B	1002	COA	CDP-CBP-CCP-O6A
4	H	1001	COA	C5B-O5B-P1A-O3A
4	D	1001	COA	C3B-O3B-P3B-O8A
5	C	1003	PGE	O3-C5-C6-O4
7	D	1005	PG4	C8-C7-O4-C6
4	D	1001	COA	C5B-O5B-P1A-O1A
4	F	1001	COA	P1A-O3A-P2A-O4A
5	B	1004	PGE	C4-C3-O2-C2
4	B	1002	COA	C4B-C5B-O5B-P1A

There are no ring outliers.

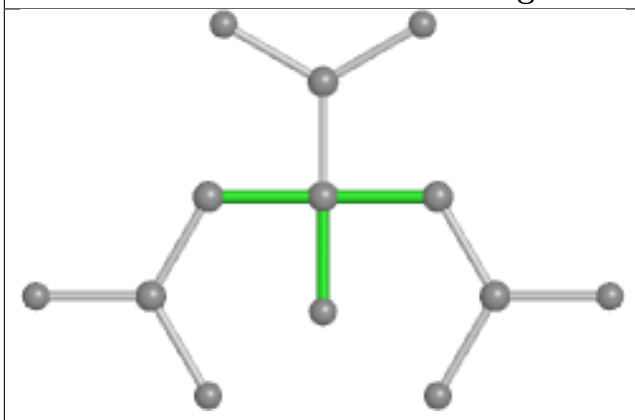
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1004	PGE	2	0
7	C	1002	PG4	1	0
5	D	1006	PGE	1	0
5	B	1004	PGE	2	0
4	B	1002	COA	2	0
7	D	1005	PG4	2	0

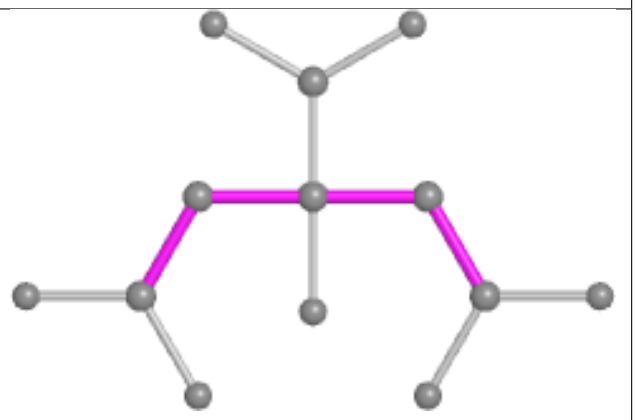
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

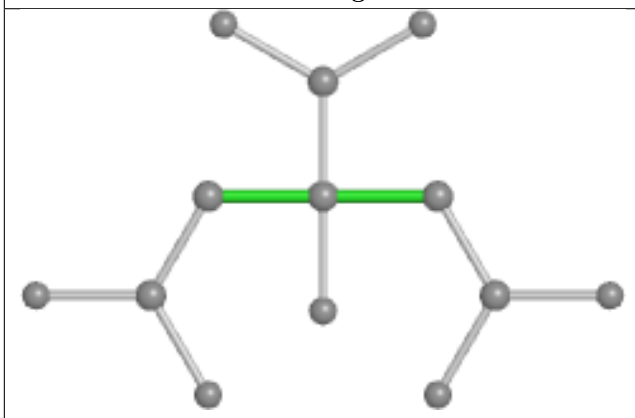
Ligand FLC H 1003



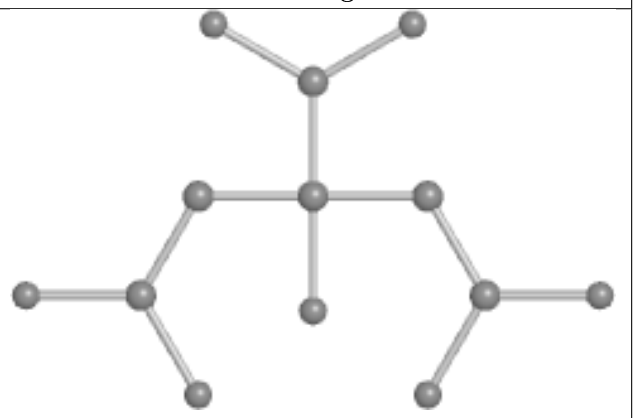
Bond lengths



Bond angles

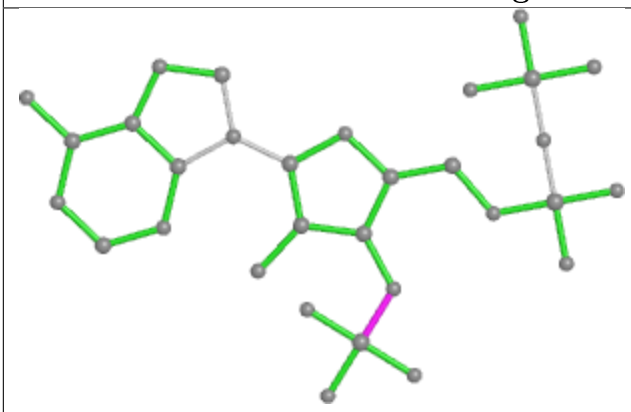


Torsions

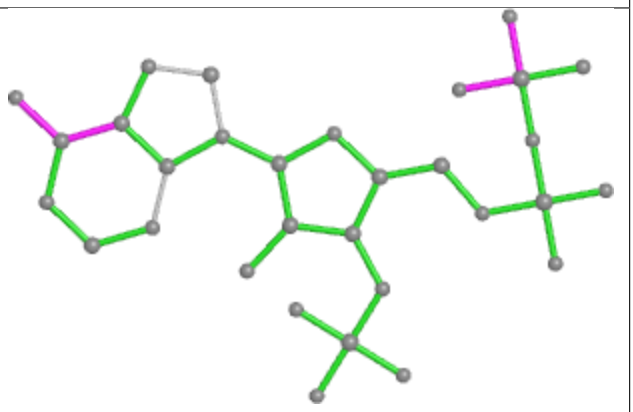


Rings

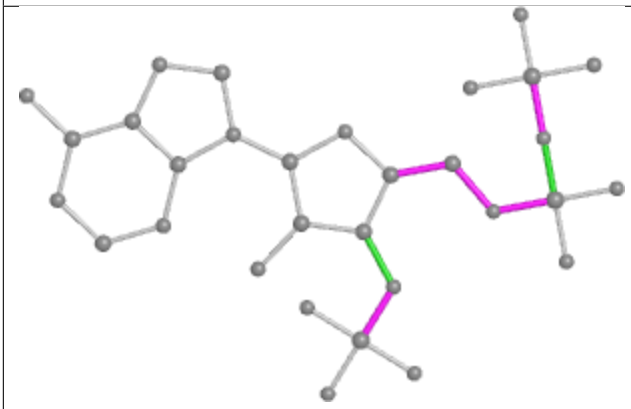
Ligand COA H 1001



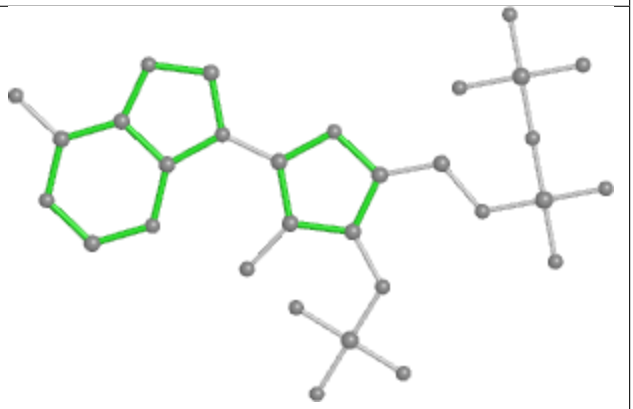
Bond lengths



Bond angles

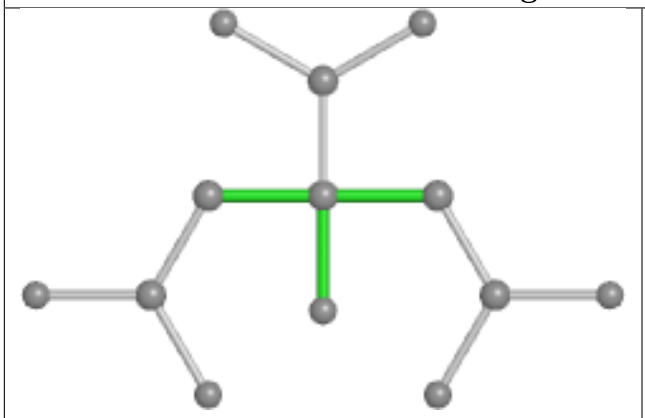


Torsions

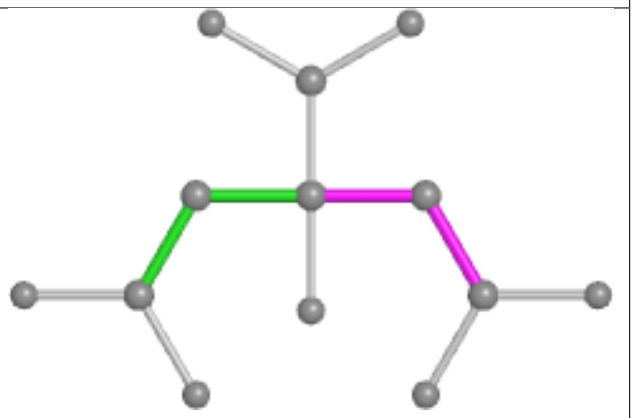


Rings

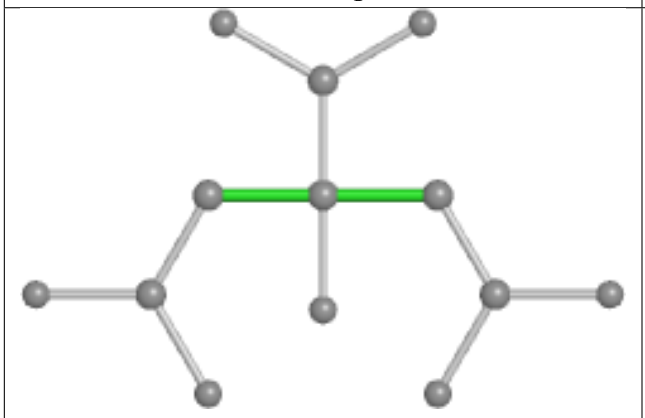
Ligand FLC E 1001



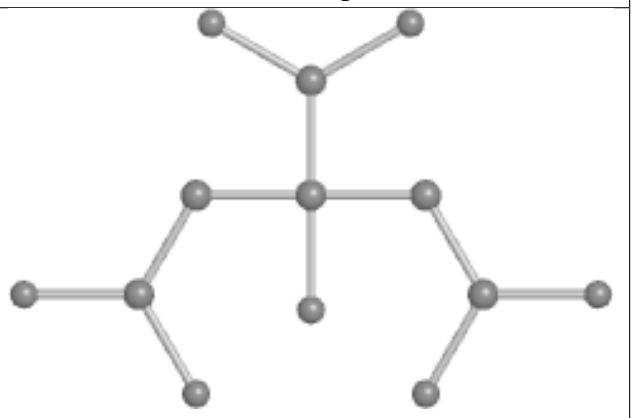
Bond lengths



Bond angles

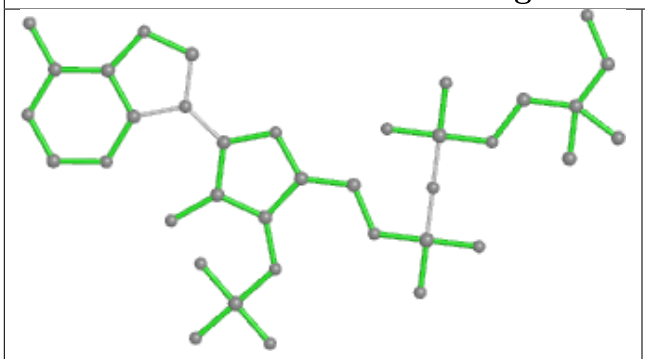


Torsions



Rings

Ligand COA B 1001



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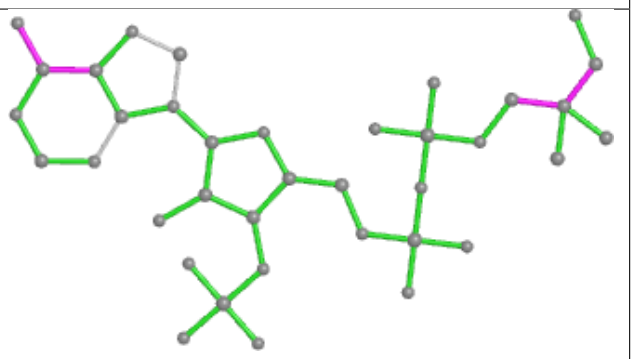
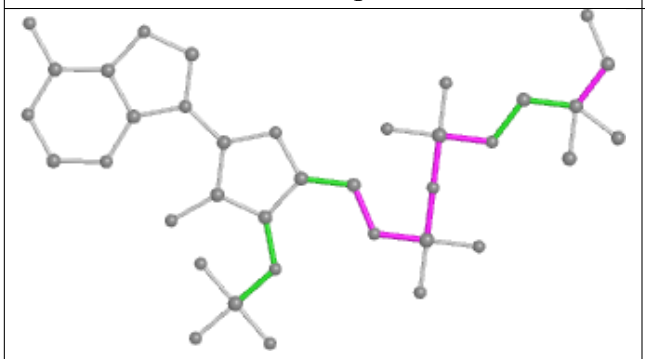
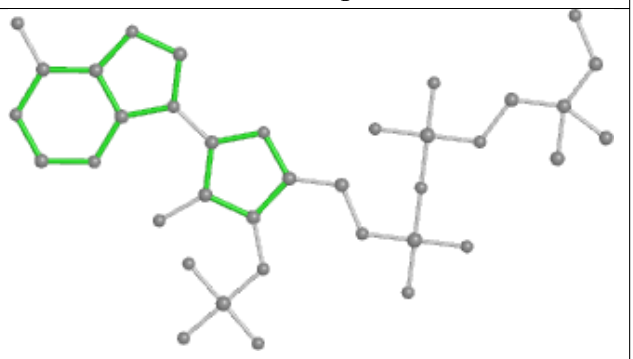


Bond angles

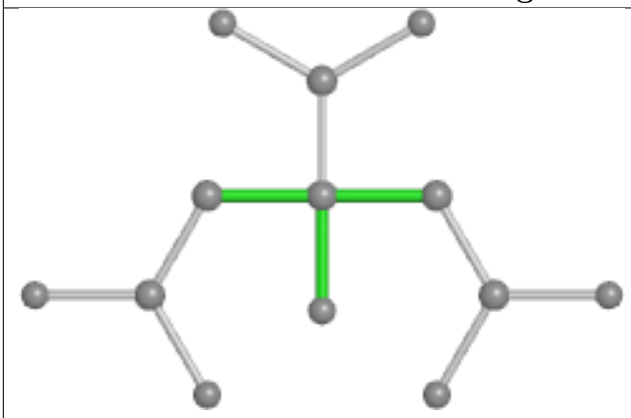


Torsions

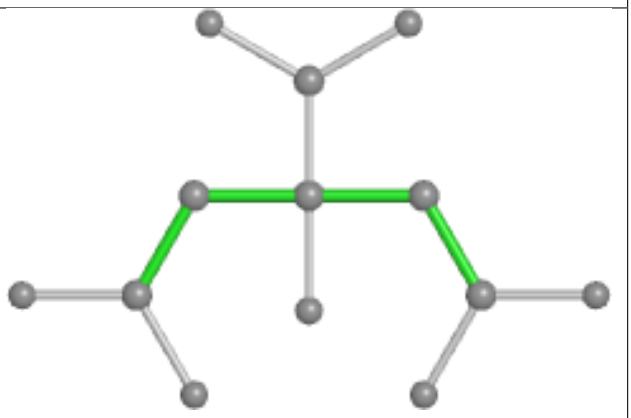


Rings

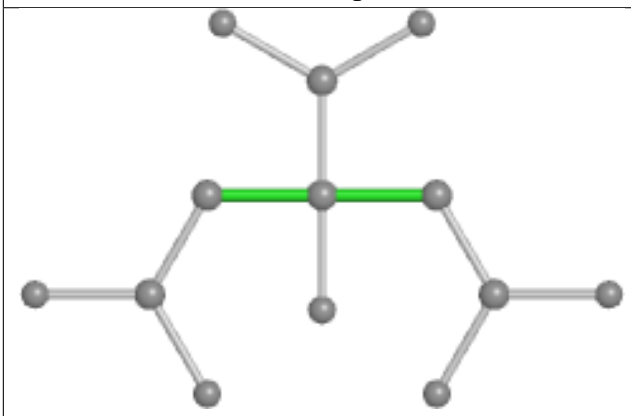
Ligand FLC G 1001



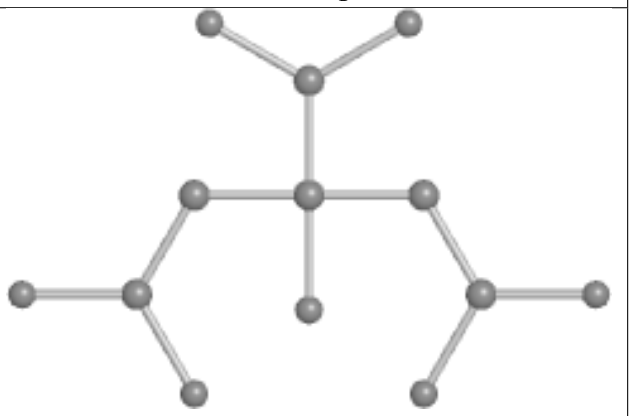
Bond lengths



Bond angles

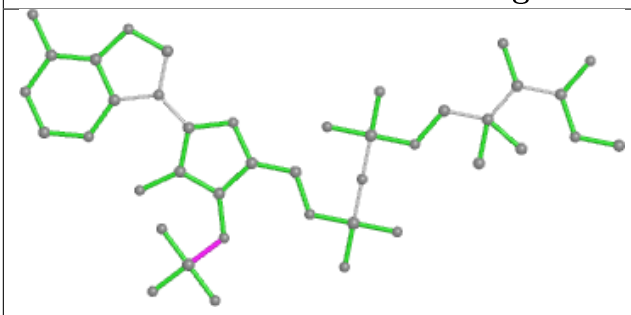


Torsions

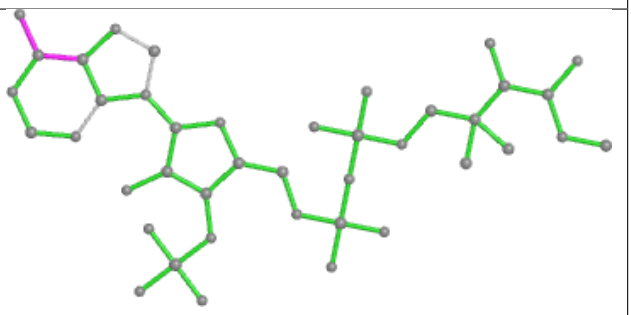


Rings

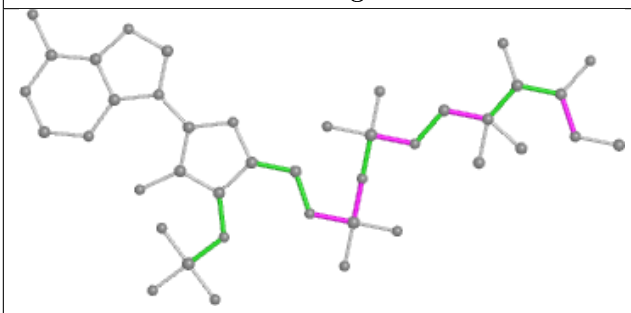
Ligand COA D 1002



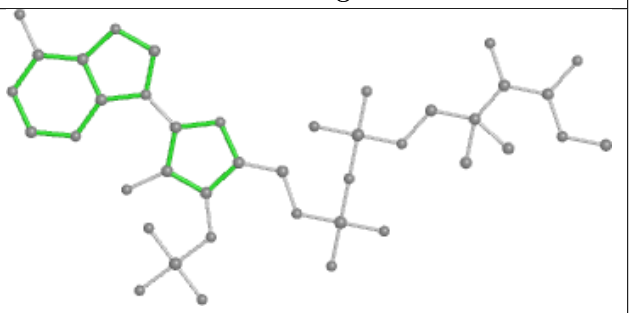
Bond lengths



Bond angles

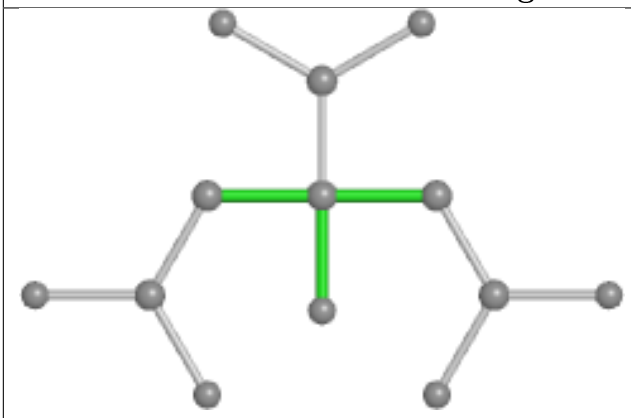


Torsions

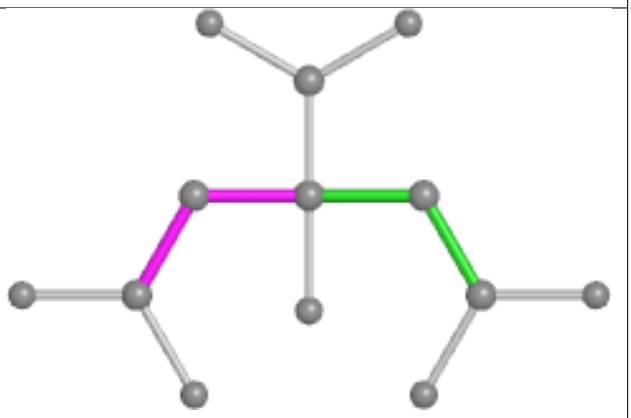


Rings

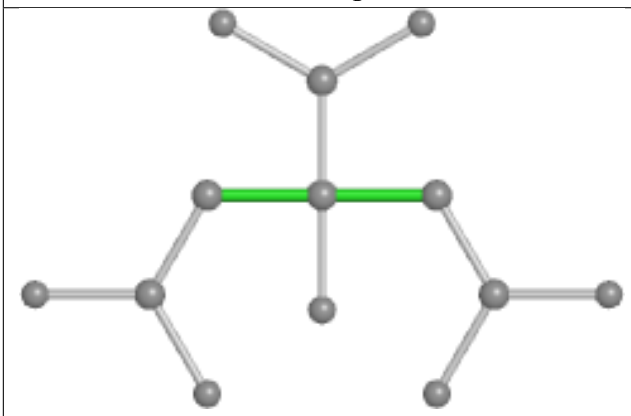
Ligand FLC D 1003



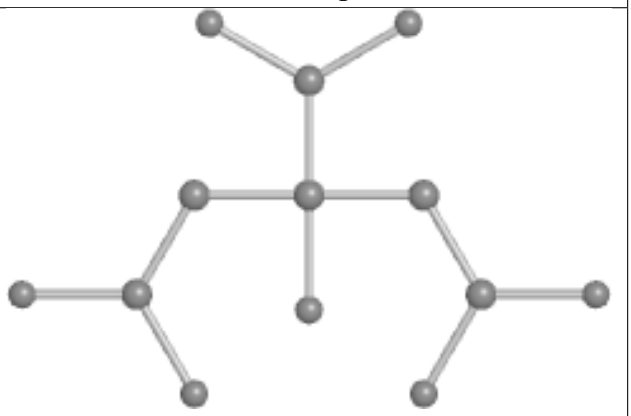
Bond lengths



Bond angles

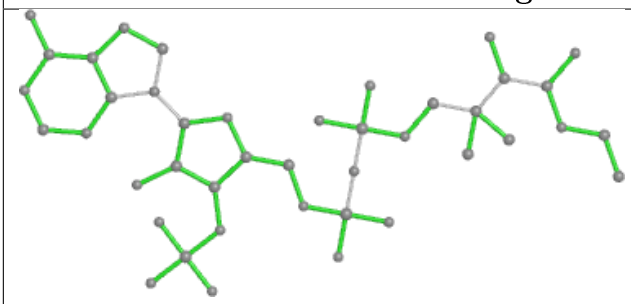


Torsions

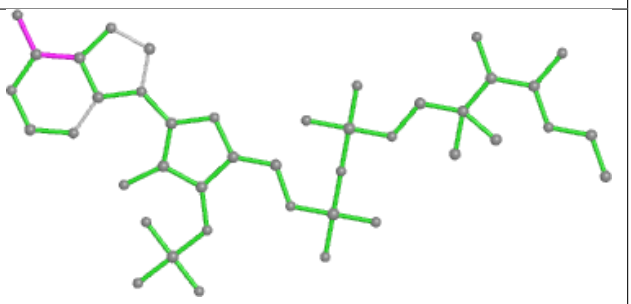


Rings

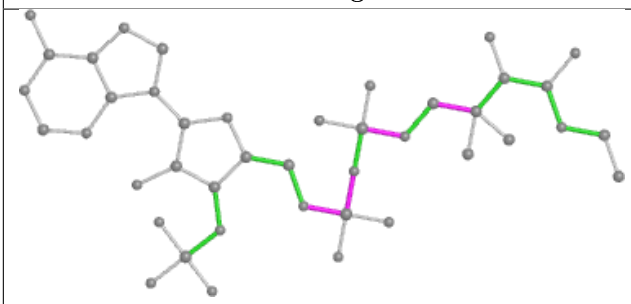
Ligand COA F 1002



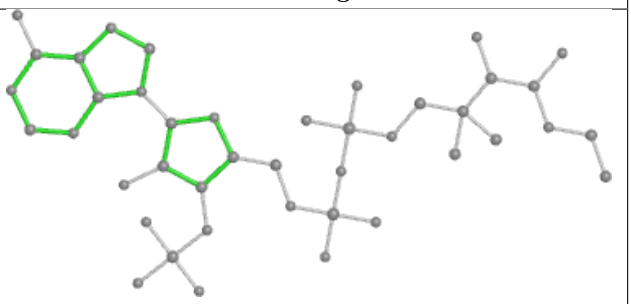
Bond lengths



Bond angles

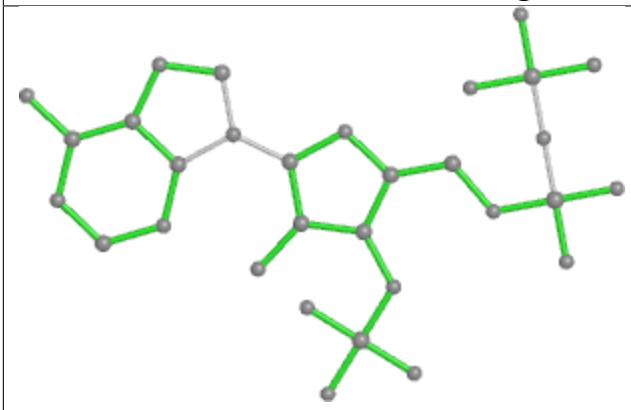


Torsions

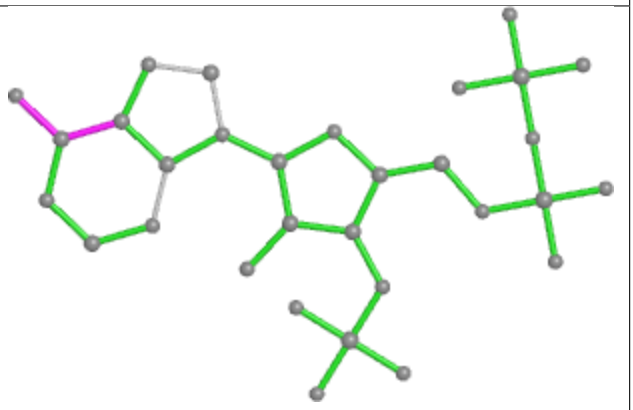


Rings

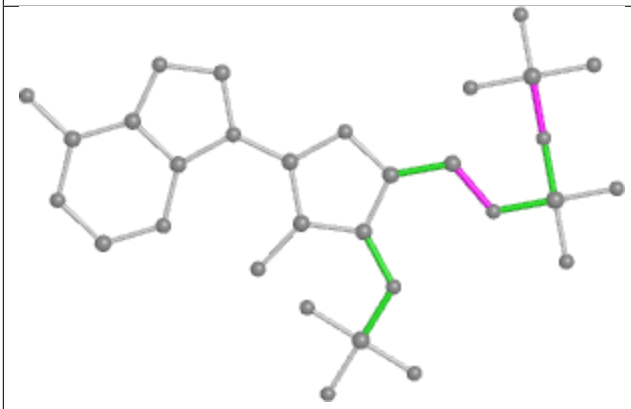
Ligand COA F 1001



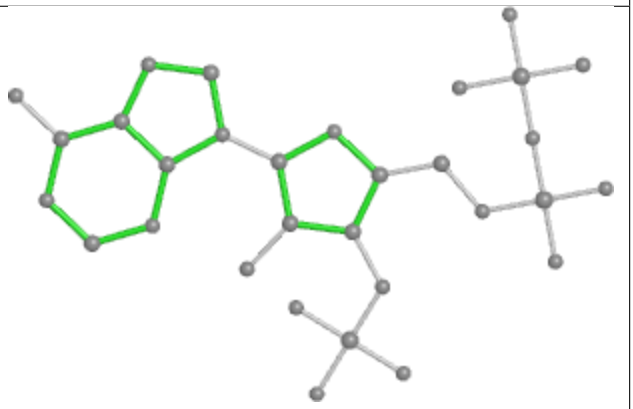
Bond lengths



Bond angles

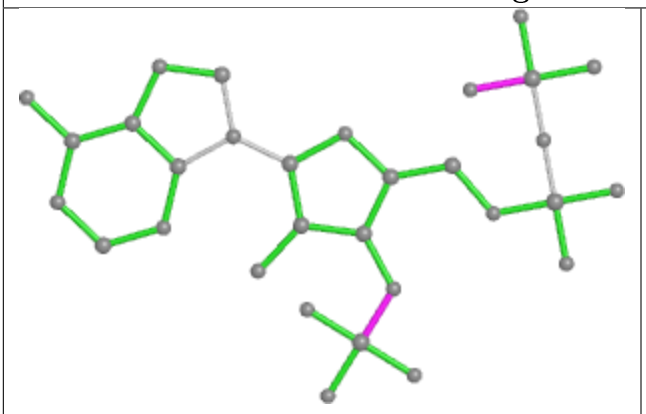


Torsions

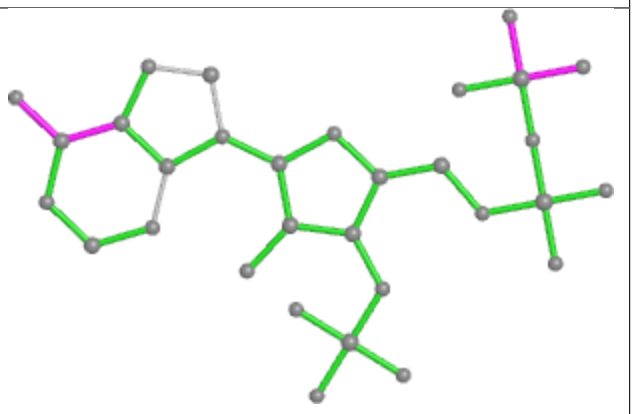


Rings

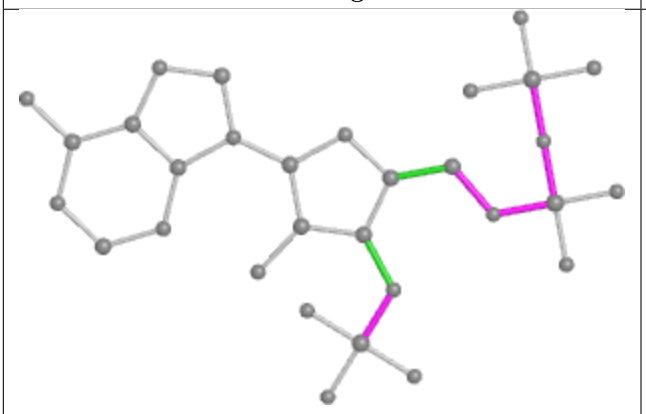
Ligand COA D 1001



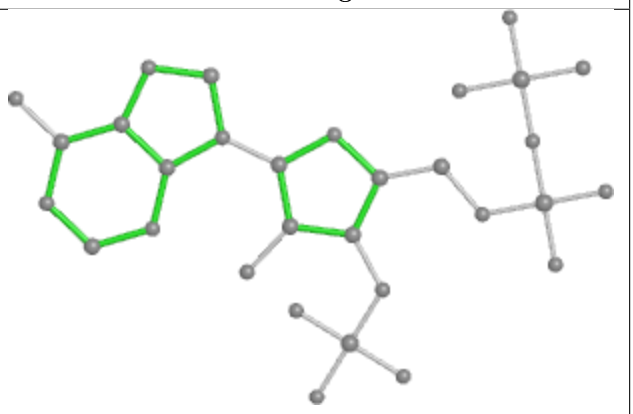
Bond lengths



Bond angles

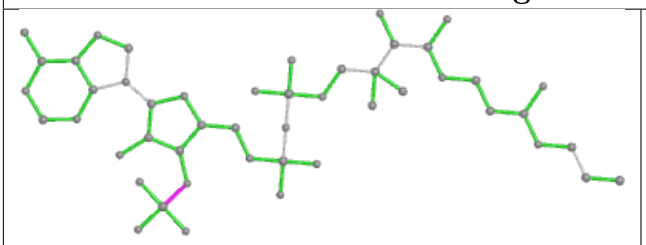


Torsions

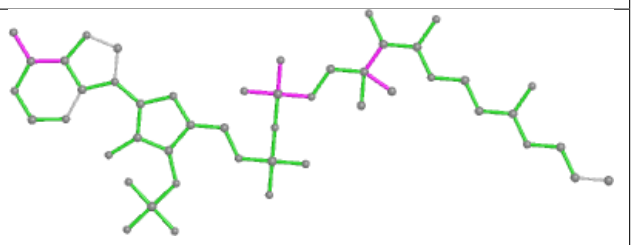


Rings

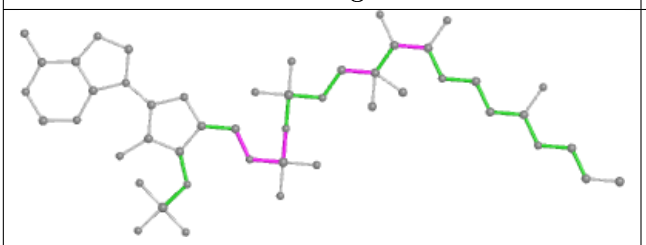
Ligand COA B 1002



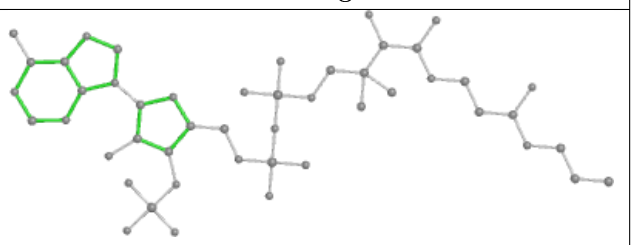
Bond lengths



Bond angles

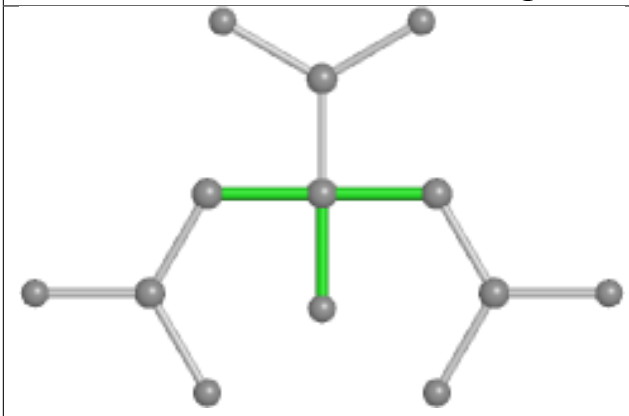


Torsions

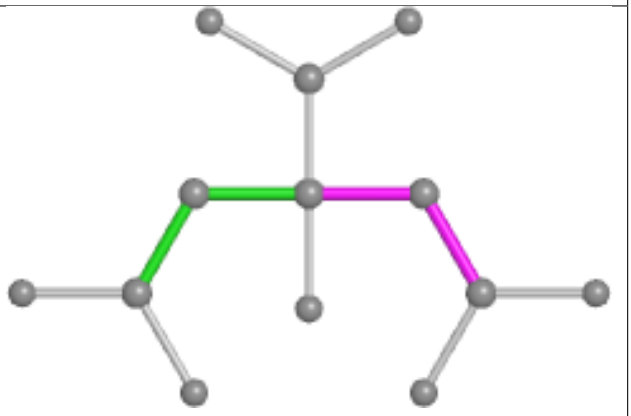


Rings

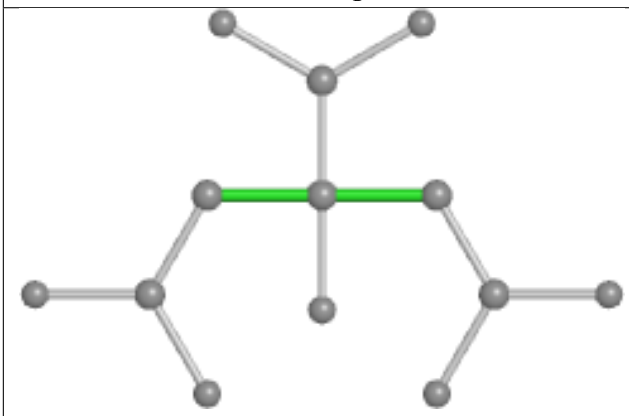
Ligand FLC F 1003



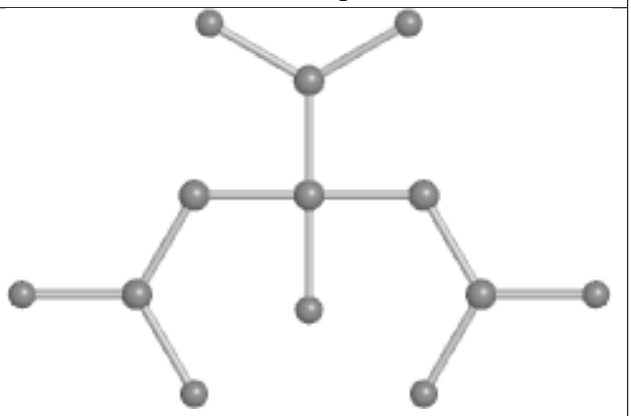
Bond lengths



Bond angles

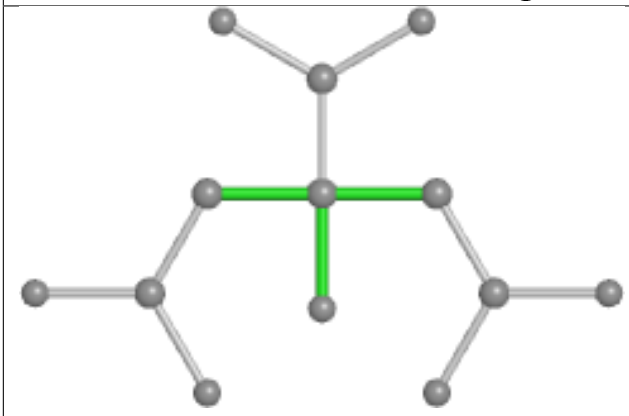


Torsions

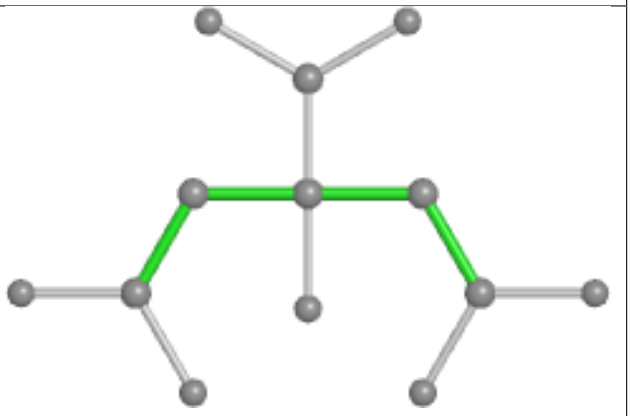


Rings

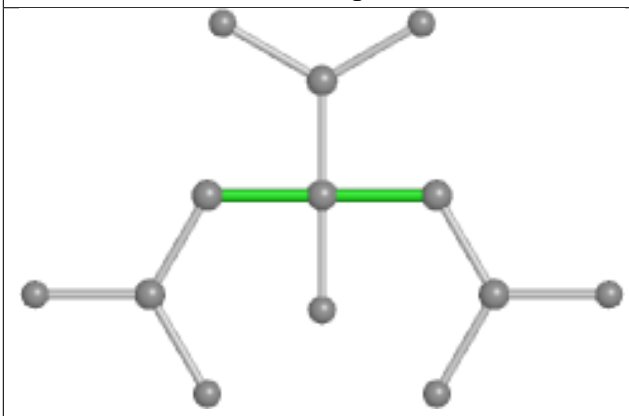
Ligand FLC A 1001



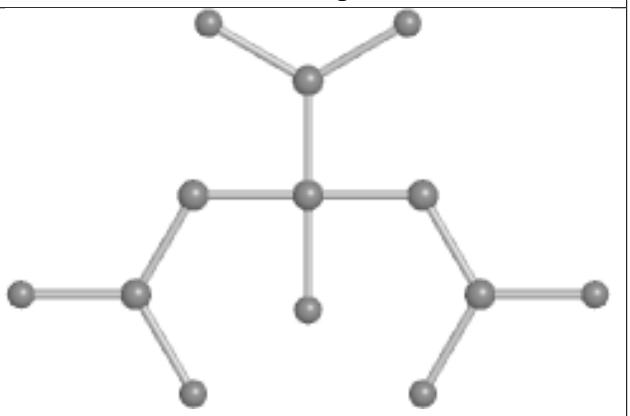
Bond lengths



Bond angles

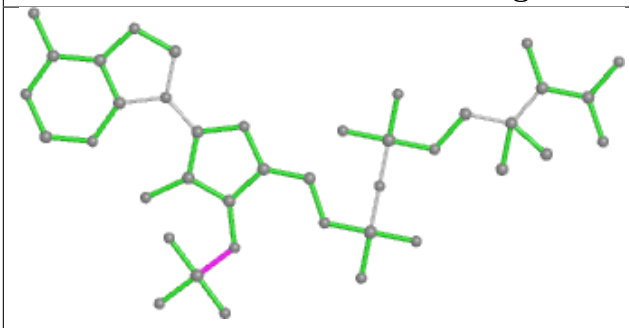


Torsions

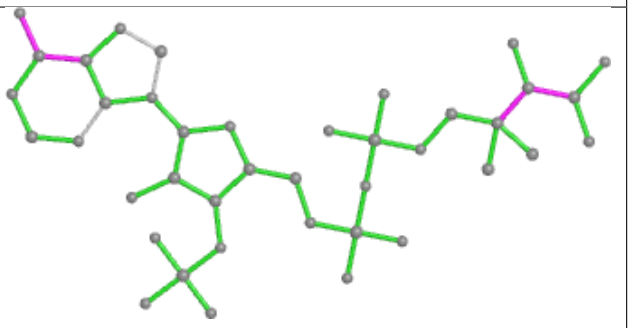


Rings

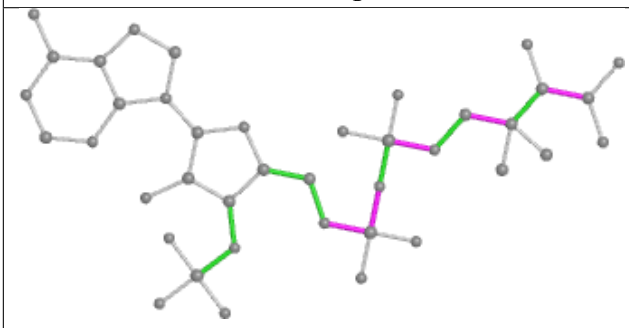
Ligand COA H 1002



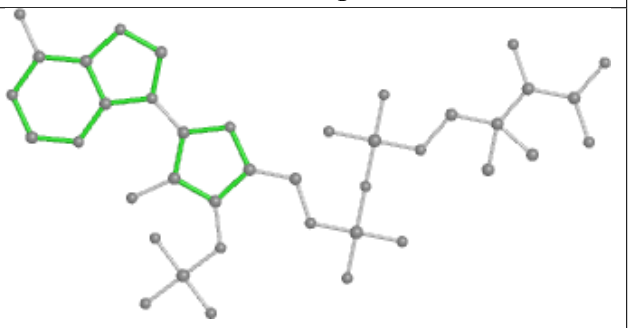
Bond lengths



Bond angles

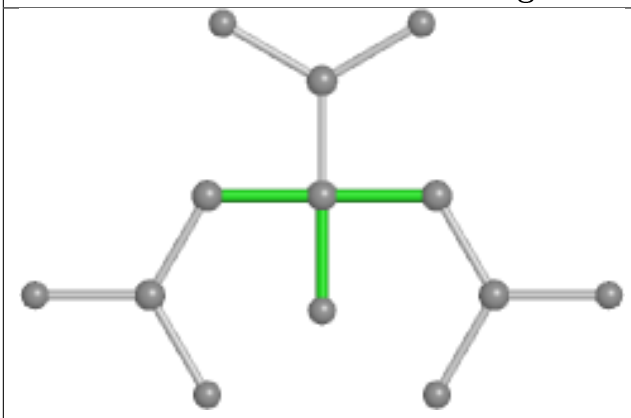


Torsions

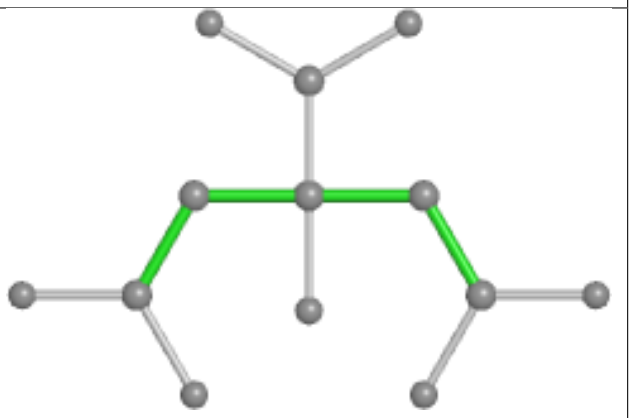


Rings

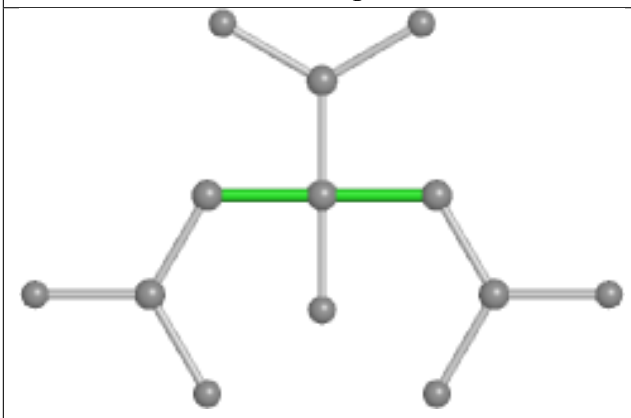
Ligand FLC C 1001



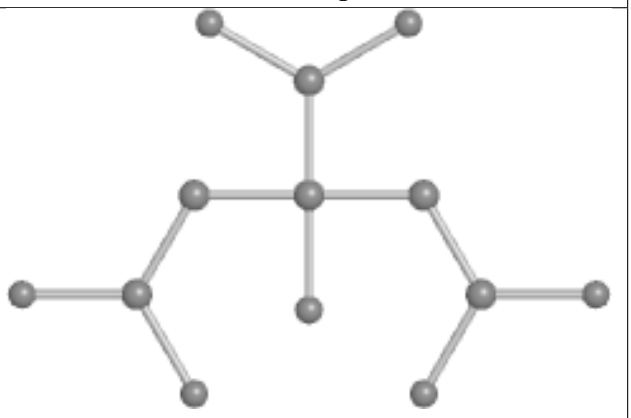
Bond lengths



Bond angles

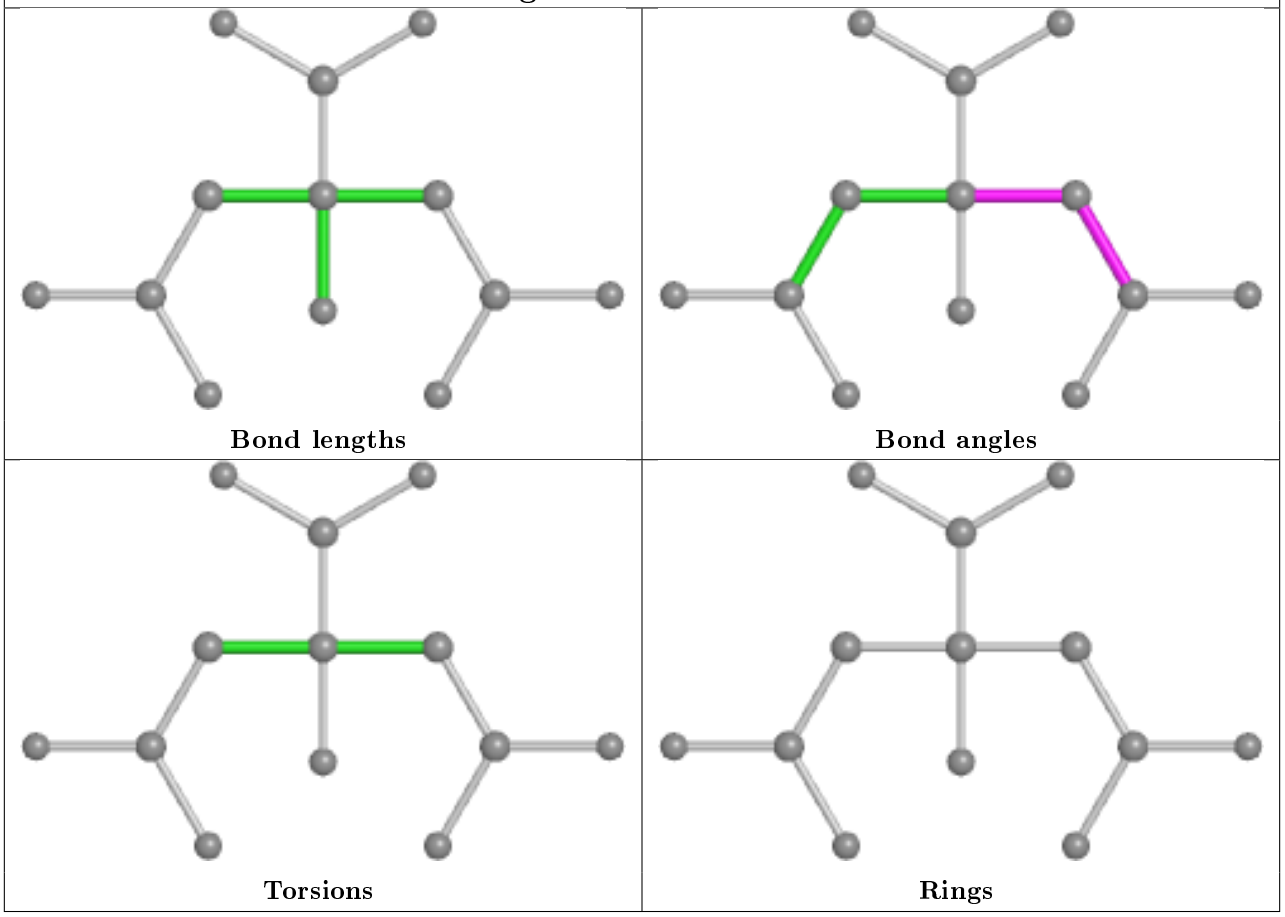


Torsions



Rings

Ligand FLC B 1003



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	336/398 (84%)	1.82	124 (36%)	0	0	76, 112, 155, 183	0
1	C	324/398 (81%)	0.94	47 (14%)	2	1	65, 96, 129, 155	0
1	E	320/398 (80%)	2.09	122 (38%)	0	0	73, 120, 157, 182	0
1	G	322/398 (80%)	2.09	136 (42%)	0	0	80, 120, 158, 177	0
2	B	589/617 (95%)	0.83	59 (10%)	7	5	43, 74, 120, 184	0
2	D	591/617 (95%)	0.88	50 (8%)	10	8	45, 76, 116, 189	0
2	F	588/617 (95%)	0.87	61 (10%)	6	5	44, 75, 119, 172	0
2	H	591/617 (95%)	0.93	81 (13%)	3	2	41, 77, 147, 212	0
All	All	3661/4060 (90%)	1.18	680 (18%)	1	0	41, 87, 146, 212	0

All (680) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	265	LEU	12.4
1	E	194	ILE	11.8
1	E	193	VAL	11.3
1	G	229	ILE	11.0
1	G	372	LEU	10.2
1	E	25	VAL	9.8
1	G	316	ILE	9.8
2	F	330	GLU	9.6
2	D	328	ILE	9.6
2	H	332	VAL	9.5
1	E	19	PRO	9.4
1	E	192	LEU	9.1
1	E	204	LEU	9.0
1	G	354	TRP	8.8
1	G	348	LEU	8.7
2	F	328	ILE	8.6

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Mol	Chain	Res	Type	RSRZ
1	E	106	TYR	8.6
1	E	23	TYR	8.4
1	E	18	ILE	8.4
1	G	377	PHE	8.2
1	E	199	MET	8.1
1	E	206	ALA	8.0
1	E	26	ILE	7.9
2	H	328	ILE	7.9
1	G	228	GLU	7.8
2	F	329	ASP	7.8
1	A	348	LEU	7.7
2	D	330	GLU	7.7
1	G	396	MET	7.6
1	E	222	ASP	7.4
1	G	398	SER	7.3
1	E	24	VAL	7.3
1	A	154	LEU	7.2
1	E	201	PHE	7.2
2	B	328	ILE	7.2
1	G	132	TRP	7.1
1	E	12	LEU	7.1
1	A	132	TRP	7.1
2	B	265	LEU	7.0
1	A	229	ILE	6.9
1	A	128	ILE	6.9
2	B	263	GLU	6.8
2	H	331	ALA	6.7
1	A	90	ILE	6.7
2	H	330	GLU	6.7
1	G	154	LEU	6.7
1	E	190	ASN	6.7
1	E	122	LYS	6.6
1	G	130	ASP	6.6
1	E	164	ILE	6.6
1	E	20	VAL	6.6
1	E	132	TRP	6.5
2	H	262	GLN	6.4
1	A	204	LEU	6.4
1	A	261	ILE	6.4
1	E	130	ASP	6.4
1	E	223	PHE	6.4
1	E	207	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	26	ILE	6.2
1	E	172	CYS	6.2
1	G	350	GLY	6.2
1	E	21	PRO	6.1
1	G	379	ILE	6.1
1	G	380	HIS	6.1
1	A	194	ILE	6.1
1	G	252	LYS	6.0
1	A	133	ASP	6.0
1	E	13	PHE	6.0
1	A	95	ILE	6.0
2	B	331	ALA	6.0
2	F	331	ALA	5.9
1	C	25	VAL	5.9
1	A	48	VAL	5.8
1	G	315	HIS	5.7
1	E	125	GLY	5.7
1	G	369	ILE	5.7
1	E	4	ILE	5.6
1	A	199	MET	5.6
1	E	189	ILE	5.5
2	B	326	THR	5.5
1	E	205	ASP	5.5
1	G	352	LYS	5.5
2	D	329	ASP	5.5
1	E	10	MET	5.5
1	A	160	PHE	5.5
1	G	236	ALA	5.5
2	F	332	VAL	5.5
1	A	130	ASP	5.4
1	G	119	LEU	5.4
2	H	281	LYS	5.4
1	A	203	ALA	5.4
1	G	351	VAL	5.4
1	E	22	ASN	5.4
1	E	220	ASP	5.4
1	A	233	PHE	5.3
1	A	5	LEU	5.3
1	A	398	SER	5.3
1	G	338	GLY	5.3
1	E	198	ASP	5.3
2	F	327	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	107	VAL	5.3
1	E	175	LEU	5.2
1	E	203	ALA	5.2
1	E	123	HIS	5.2
1	E	131	ASN	5.1
1	G	127	ASP	5.1
1	G	105	PHE	5.1
1	G	307	ILE	5.1
1	G	313	ILE	5.1
1	A	201	PHE	5.1
1	E	196	LYS	5.1
1	A	25	VAL	5.0
1	A	105	PHE	5.0
1	E	397	LYS	5.0
2	D	343	VAL	5.0
1	G	128	ILE	5.0
1	G	242	GLU	4.9
2	H	260	THR	4.9
2	H	324	ILE	4.9
1	G	382	TYR	4.9
1	E	105	PHE	4.9
1	E	158	ALA	4.9
1	E	163	GLU	4.9
1	A	126	VAL	4.9
1	G	257	PRO	4.9
1	G	341	GLU	4.8
1	A	24	VAL	4.8
1	E	133	ASP	4.8
1	A	49	VAL	4.8
2	D	327	GLU	4.8
1	A	198	ASP	4.8
1	E	191	PRO	4.8
1	G	392	VAL	4.8
1	G	160	PHE	4.8
1	C	23	TYR	4.7
1	A	351	VAL	4.7
1	G	397	LYS	4.7
2	D	440	SER	4.7
2	D	281	LYS	4.7
1	E	159	GLY	4.6
1	A	96	ALA	4.6
1	E	353	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	298	TRP	4.4
1	E	347	TYR	4.4
1	E	202	ALA	4.4
1	A	230	GLY	4.4
2	F	265	LEU	4.4
1	G	126	VAL	4.4
1	C	24	VAL	4.3
1	G	120	ILE	4.3
1	C	12	LEU	4.3
1	E	197	SER	4.3
1	E	195	ARG	4.3
1	A	344	SER	4.3
1	A	168	VAL	4.3
1	G	129	GLU	4.3
2	D	265	LEU	4.2
2	B	530	VAL	4.2
1	A	131	ASN	4.2
1	E	200	ARG	4.2
1	E	166	GLU	4.2
1	G	349	GLU	4.2
1	G	346	GLY	4.2
2	D	441	ALA	4.2
2	H	438	ALA	4.2
1	G	135	VAL	4.2
1	G	230	GLY	4.2
2	H	264	VAL	4.2
1	A	235	GLU	4.2
1	E	160	PHE	4.2
1	A	353	ILE	4.1
1	A	397	LYS	4.1
2	F	326	THR	4.1
1	E	226	VAL	4.1
1	G	204	LEU	4.1
2	D	332	VAL	4.1
1	E	168	VAL	4.1
2	B	475	PHE	4.0
1	E	124	GLY	4.0
1	G	284	THR	4.0
1	G	339	PHE	4.0
1	G	366	LEU	4.0
1	G	256	VAL	4.0
1	E	188	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	255	GLU	4.0
1	G	253	PHE	4.0
1	A	307	ILE	4.0
1	G	158	ALA	4.0
1	A	205	ASP	4.0
1	A	202	ALA	4.0
1	G	302	ALA	4.0
1	E	379	ILE	3.9
2	H	329	ASP	3.9
1	E	6	GLU	3.9
1	A	127	ASP	3.9
2	F	306	GLY	3.9
1	A	107	VAL	3.9
1	G	168	VAL	3.9
1	A	47	LEU	3.9
1	G	131	ASN	3.9
1	G	12	LEU	3.9
1	G	280	ALA	3.9
1	G	223	PHE	3.9
1	G	285	ILE	3.9
2	H	333	LEU	3.9
1	A	151	LEU	3.8
1	C	230	GLY	3.8
1	E	221	TRP	3.8
1	A	135	VAL	3.8
1	C	5	LEU	3.8
1	A	349	GLU	3.8
1	E	208	MET	3.8
1	G	231	ARG	3.8
1	E	382	TYR	3.8
1	A	157	ASP	3.8
1	A	94	ILE	3.8
1	A	316	ILE	3.7
1	E	225	PRO	3.7
2	D	325	SER	3.7
1	G	203	ALA	3.7
1	G	312	ASN	3.7
1	A	120	ILE	3.7
1	E	348	LEU	3.7
1	A	19	PRO	3.7
1	G	254	VAL	3.7
2	H	444	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	3.7
1	C	206	ALA	3.7
1	E	118	LEU	3.7
2	D	444	THR	3.7
2	F	444	THR	3.7
1	A	106	TYR	3.6
2	B	318	LEU	3.6
2	B	332	VAL	3.6
2	D	326	THR	3.6
2	H	569	THR	3.6
2	H	572	MET	3.6
2	F	336	LEU	3.6
1	E	336	ILE	3.6
1	G	164	ILE	3.6
1	G	123	HIS	3.6
1	A	310	LEU	3.6
1	E	135	VAL	3.6
2	D	475	PHE	3.6
1	E	9	ALA	3.6
2	B	478	TRP	3.6
1	A	222	ASP	3.6
1	C	219	ALA	3.6
1	G	136	ARG	3.5
1	A	138	ILE	3.5
2	H	573	ILE	3.5
1	A	175	LEU	3.5
1	G	394	LEU	3.5
1	G	355	VAL	3.5
2	D	346	GLN	3.5
2	H	229	ILE	3.5
1	C	223	PHE	3.5
1	A	197	SER	3.5
1	E	227	SER	3.5
1	G	237	GLU	3.5
1	C	205	ASP	3.5
1	A	240	ILE	3.4
1	G	335	ILE	3.4
1	A	196	LYS	3.4
1	A	308	CYS	3.4
2	D	439	VAL	3.4
1	G	332	PHE	3.4
1	E	219	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	440	SER	3.4
2	B	481	LYS	3.4
2	H	443	MET	3.4
1	G	261	ILE	3.4
2	B	443	MET	3.4
1	E	284	THR	3.4
2	H	342	GLU	3.4
1	A	255	GLU	3.3
1	E	110	ILE	3.3
2	B	330	GLU	3.3
2	B	444	THR	3.3
2	D	345	LYS	3.3
2	H	168	GLY	3.3
2	B	440	SER	3.3
1	A	129	GLU	3.3
1	E	283	GLY	3.3
1	A	192	LEU	3.3
1	A	23	TYR	3.3
2	B	463	MET	3.3
1	G	206	ALA	3.3
1	A	167	ARG	3.3
1	G	100	GLU	3.3
1	A	93	VAL	3.3
1	A	379	ILE	3.3
2	H	319	ILE	3.3
1	C	378	ASP	3.3
1	E	161	GLU	3.3
1	G	21	PRO	3.2
1	E	372	LEU	3.2
1	G	308	CYS	3.2
1	C	344	SER	3.2
1	A	193	VAL	3.2
2	D	478	TRP	3.2
1	G	171	ILE	3.2
2	F	349	VAL	3.2
2	D	442	GLY	3.2
1	A	158	ALA	3.2
1	A	227	SER	3.2
1	A	285	ILE	3.2
2	B	319	ILE	3.2
1	E	151	LEU	3.2
2	F	345	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	120	ILE	3.2
1	A	166	GLU	3.2
1	E	16	TRP	3.2
2	B	421	GLY	3.2
1	G	23	TYR	3.1
1	G	296	ALA	3.1
2	H	326	THR	3.1
2	F	565	VAL	3.1
2	H	327	GLU	3.1
1	G	159	GLY	3.1
2	F	475	PHE	3.1
2	H	199	ALA	3.1
1	A	125	GLY	3.1
1	G	347	TYR	3.1
2	H	304	PHE	3.1
1	A	164	ILE	3.1
1	C	21	PRO	3.1
1	E	396	MET	3.1
2	D	443	MET	3.1
2	H	439	VAL	3.1
1	C	379	ILE	3.1
2	B	348	GLU	3.0
1	E	229	ILE	3.0
1	E	162	GLY	3.0
2	H	201	GLY	3.0
2	H	571	GLY	3.0
1	C	227	SER	3.0
1	C	212	TYR	3.0
1	G	281	ARG	3.0
2	B	446	ILE	3.0
1	E	230	GLY	3.0
2	B	441	ALA	3.0
2	D	446	ILE	3.0
2	H	282	GLY	3.0
2	H	346	GLN	3.0
1	G	374	GLU	3.0
1	A	18	ILE	3.0
1	E	128	ILE	3.0
2	F	350	ILE	3.0
1	C	148	ILE	3.0
1	E	176	ILE	3.0
1	A	122	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	378	ASP	2.9
1	G	317	ILE	2.9
2	B	342	GLU	2.9
1	G	342	SER	2.9
2	H	425	SER	2.9
1	G	124	GLY	2.9
2	H	263	GLU	2.9
1	G	151	LEU	2.9
1	E	377	PHE	2.9
1	A	134	SER	2.9
1	E	155	ALA	2.9
2	D	429	ALA	2.9
2	B	323	GLU	2.9
2	H	137	SER	2.9
1	G	221	TRP	2.9
1	A	366	LEU	2.9
1	G	155	ALA	2.9
2	H	440	SER	2.9
1	G	258	GLY	2.9
2	F	284	GLY	2.9
2	H	284	GLY	2.9
1	A	373	GLN	2.9
1	C	348	LEU	2.9
2	F	442	GLY	2.8
2	F	465	VAL	2.8
2	H	419	VAL	2.8
1	G	137	ARG	2.8
1	A	171	ILE	2.8
1	E	171	ILE	2.8
2	D	324	ILE	2.8
2	F	441	ALA	2.8
1	A	354	TRP	2.8
1	C	16	TRP	2.8
2	B	329	ASP	2.8
2	B	483	VAL	2.8
1	A	232	PRO	2.8
1	C	224	LYS	2.8
1	A	165	ALA	2.8
1	G	299	ALA	2.8
1	A	394	LEU	2.8
1	E	343	LYS	2.8
1	A	339	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	482	ASN	2.8
2	D	573	ILE	2.8
2	H	426	ILE	2.8
2	D	428	ALA	2.8
2	D	282	GLY	2.8
2	D	445	MET	2.8
1	E	183	ASP	2.8
2	B	517	HIS	2.8
1	C	100	GLU	2.8
1	C	13	PHE	2.8
2	F	324	ILE	2.8
1	G	118	LEU	2.8
2	B	516	LEU	2.8
2	H	176	SER	2.8
1	G	246	ARG	2.8
1	E	212	TYR	2.7
2	H	174	THR	2.7
1	G	121	SER	2.7
1	A	26	ILE	2.7
1	A	137	ARG	2.7
2	B	324	ILE	2.7
2	D	246	ALA	2.7
1	A	121	SER	2.7
1	G	6	GLU	2.7
2	F	102	PRO	2.7
2	F	443	MET	2.7
1	E	165	ALA	2.7
2	F	569	THR	2.7
1	E	173	SER	2.7
1	G	125	GLY	2.7
2	H	261	CYS	2.7
2	F	346	GLN	2.7
1	G	153	GLU	2.7
1	G	146	PRO	2.7
2	H	227	VAL	2.7
1	A	231	ARG	2.7
1	E	282	GLY	2.7
1	A	16	TRP	2.7
2	H	576	TRP	2.7
1	A	381	VAL	2.6
2	B	477	SER	2.6
2	D	438	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	373	ALA	2.6
2	F	425	SER	2.6
2	B	531	THR	2.6
1	G	243	ILE	2.6
2	D	433	ILE	2.6
1	G	378	ASP	2.6
2	F	426	ILE	2.6
1	A	50	LYS	2.6
2	D	283	ALA	2.6
1	G	353	ILE	2.6
2	B	572	MET	2.6
1	G	9	ALA	2.6
1	C	194	ILE	2.6
2	B	304	PHE	2.6
2	F	572	MET	2.6
1	G	106	TYR	2.6
2	B	523	TYR	2.6
2	H	138	SER	2.6
2	F	333	LEU	2.6
2	F	570	ILE	2.6
1	G	375	GLU	2.6
1	G	386	MET	2.6
1	E	134	SER	2.6
1	A	395	ALA	2.6
1	G	381	VAL	2.6
2	D	340	VAL	2.6
1	G	310	LEU	2.6
1	G	373	GLN	2.6
2	F	262	GLN	2.6
1	E	390	ASP	2.6
1	A	382	TYR	2.6
1	G	99	LEU	2.5
2	F	476	LEU	2.5
2	H	179	LEU	2.5
1	A	239	GLN	2.5
1	G	134	SER	2.5
2	B	445	MET	2.5
2	H	442	GLY	2.5
1	G	304	THR	2.5
2	H	437	GLN	2.5
2	H	429	ALA	2.5
1	A	153	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	372	LEU	2.5
2	B	566	LEU	2.5
1	A	269	GLY	2.5
1	G	343	LYS	2.5
1	A	98	MET	2.5
2	H	198	VAL	2.5
1	G	336	ILE	2.5
1	G	235	GLU	2.5
2	H	422	ALA	2.5
1	C	220	ASP	2.5
2	D	434	ASP	2.5
1	A	162	GLY	2.5
1	C	14	ASN	2.5
2	F	343	VAL	2.5
1	C	117	GLU	2.5
1	G	13	PHE	2.5
2	F	342	GLU	2.5
2	H	323	GLU	2.5
2	B	442	GLY	2.5
2	D	284	GLY	2.5
2	H	178	GLY	2.5
2	B	425	SER	2.5
1	G	109	ILE	2.5
1	A	264	LEU	2.4
2	H	3	ILE	2.4
2	H	200	ILE	2.4
2	B	472	ILE	2.4
2	F	433	ILE	2.4
2	H	570	ILE	2.4
2	H	606	GLU	2.4
1	E	231	ARG	2.4
2	H	202	GLY	2.4
1	A	155	ALA	2.4
1	G	5	LEU	2.4
1	A	335	ILE	2.4
1	C	336	ILE	2.4
2	B	470	ASN	2.4
2	H	430	CYS	2.4
1	E	300	VAL	2.4
2	D	348	GLU	2.4
2	H	445	MET	2.4
1	E	315	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	22	ASN	2.4
2	B	345	LYS	2.4
1	G	10	MET	2.4
2	D	420	SER	2.4
2	F	566	LEU	2.3
2	D	349	VAL	2.3
2	F	483	VAL	2.3
1	C	374	GLU	2.3
1	E	375	GLU	2.3
1	E	233	PHE	2.3
1	C	202	ALA	2.3
1	E	156	LYS	2.3
1	G	365	GLY	2.3
1	G	220	ASP	2.3
2	F	263	GLU	2.3
2	B	437	GLN	2.3
2	F	405	ILE	2.3
2	B	422	ALA	2.3
1	G	370	LYS	2.3
1	G	19	PRO	2.3
1	A	97	GLU	2.3
1	A	161	GLU	2.3
1	G	289	ALA	2.3
2	D	424	GLY	2.3
2	D	425	SER	2.3
2	F	567	ALA	2.3
2	H	441	ALA	2.3
1	A	170	LYS	2.3
1	A	364	GLN	2.3
1	E	314	LYS	2.3
1	A	123	HIS	2.3
2	F	410	MET	2.3
2	H	228	MET	2.3
1	A	391	ILE	2.3
1	E	14	ASN	2.3
1	E	261	ILE	2.3
2	F	322	GLY	2.3
1	A	370	LYS	2.3
2	F	438	ALA	2.3
2	B	569	THR	2.3
2	B	476	LEU	2.3
2	H	376	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	439	VAL	2.3
1	A	314	LYS	2.3
2	H	177	GLY	2.3
1	C	247	ILE	2.3
1	G	395	ALA	2.3
2	H	185	TRP	2.3
2	H	210	PHE	2.3
2	D	447	GLY	2.2
1	C	18	ILE	2.2
2	F	428	ALA	2.2
2	F	446	ILE	2.2
1	G	104	GLU	2.2
2	H	4	LEU	2.2
2	H	427	LEU	2.2
1	E	279	VAL	2.2
1	G	300	VAL	2.2
1	G	240	ILE	2.2
2	D	576	TRP	2.2
1	A	91	GLY	2.2
2	H	258	GLY	2.2
2	F	439	VAL	2.2
1	C	229	ILE	2.2
2	B	438	ALA	2.2
2	D	342	GLU	2.2
2	D	435	MET	2.2
1	A	380	HIS	2.2
1	C	171	ILE	2.2
1	E	313	ILE	2.2
2	B	567	ALA	2.2
2	D	427	LEU	2.2
2	H	421	GLY	2.2
1	C	168	VAL	2.2
1	E	349	GLU	2.2
1	E	371	GLN	2.2
1	G	262	ALA	2.2
2	B	200	ILE	2.2
2	B	573	ILE	2.2
1	A	12	LEU	2.2
2	H	32	LEU	2.2
1	C	345	LYS	2.2
1	E	351	VAL	2.2
2	F	107	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	321	ALA	2.2
1	G	306	THR	2.2
2	H	574	GLY	2.2
1	A	156	LYS	2.1
2	D	481	LYS	2.1
1	A	393	ASP	2.1
1	C	169	GLY	2.1
1	E	167	ARG	2.1
2	F	411	ILE	2.1
2	H	208	THR	2.1
2	H	433	ILE	2.1
2	H	577	ILE	2.1
1	E	177	LEU	2.1
1	G	156	LYS	2.1
2	H	420	SER	2.1
2	B	479	MET	2.1
1	G	282	GLY	2.1
1	G	314	LYS	2.1
2	F	304	PHE	2.1
2	F	470	ASN	2.1
1	E	17	GLY	2.1
1	A	51	ALA	2.1
1	C	371	GLN	2.1
2	D	577	ILE	2.1
2	F	573	ILE	2.1
2	H	337	PRO	2.1
1	C	151	LEU	2.1
2	F	69	LEU	2.1
1	A	313	ILE	2.1
1	G	176	ILE	2.1
2	F	319	ILE	2.1
1	G	161	GLU	2.1
2	B	452	GLY	2.1
2	F	445	MET	2.1
1	A	147	THR	2.1
1	E	370	LYS	2.1
1	G	345	LYS	2.1
2	B	554	ASP	2.1
2	H	432	GLY	2.1
1	E	228	GLU	2.1
1	A	367	ALA	2.1
1	C	203	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	212	TYR	2.1
1	C	128	ILE	2.1
1	A	22	ASN	2.1
1	A	141	GLU	2.1
1	C	17	GLY	2.1
1	A	200	ARG	2.1
2	B	199	ALA	2.0
2	F	320	ALA	2.0
2	H	245	ALA	2.0
1	E	256	VAL	2.0
1	G	251	VAL	2.0
2	B	264	VAL	2.0
2	D	200	ILE	2.0
2	H	213	TYR	2.0
1	C	149	GLU	2.0
1	C	10	MET	2.0
2	B	327	GLU	2.0
2	F	264	VAL	2.0
1	E	169	GLY	2.0
2	B	179	LEU	2.0
2	D	388	ILE	2.0
2	H	259	GLY	2.0
2	B	526	GLU	2.0
2	F	348	GLU	2.0
2	F	576	TRP	2.0
1	A	52	HIS	2.0
2	D	252	LYS	2.0
2	B	465	VAL	2.0
2	H	565	VAL	2.0
1	E	154	LEU	2.0
2	D	4	LEU	2.0
1	E	170	LYS	2.0
1	A	10	MET	2.0
1	C	199	MET	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 carbohydrates in this entry.

6.4 Ligands (i)

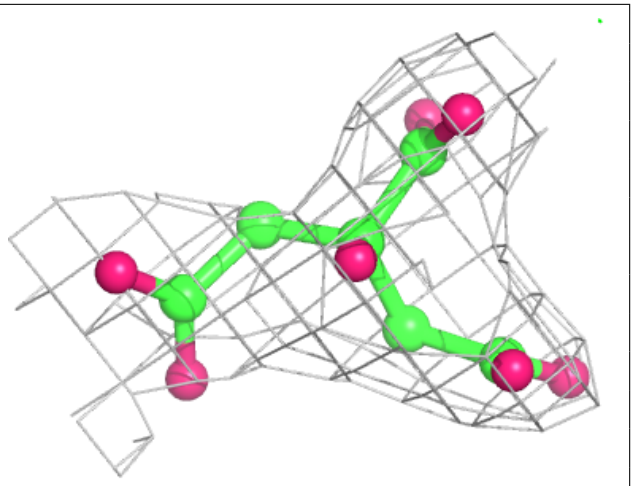
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

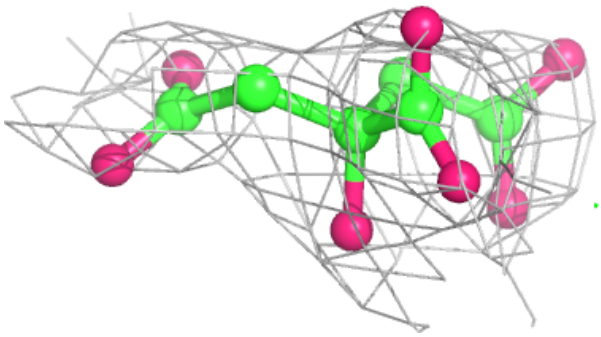
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	C	1003	10/10	0.68	0.31	94,106,111,111	0
5	PGE	B	1004	10/10	0.76	0.22	106,112,116,117	0
5	PGE	F	1004	10/10	0.80	0.29	99,100,104,104	0
6	TRS	D	1004	8/8	0.80	0.43	100,109,112,114	0
3	FLC	E	1001	13/13	0.81	0.21	114,116,131,131	0
5	PGE	D	1006	10/10	0.84	0.16	98,110,115,116	0
6	TRS	B	1005	8/8	0.86	0.24	83,92,96,97	0
5	PGE	H	1004	10/10	0.87	0.28	89,94,97,99	0
4	COA	F	1002	42/48	0.87	0.19	95,107,146,149	0
4	COA	H	1002	40/48	0.87	0.15	111,123,163,164	0
4	COA	D	1001	31/48	0.88	0.16	91,122,166,168	0
4	COA	F	1001	31/48	0.88	0.14	92,113,163,165	0
4	COA	B	1001	37/48	0.89	0.22	92,131,159,160	0
4	COA	D	1002	41/48	0.90	0.16	96,104,149,151	0
3	FLC	C	1001	13/13	0.91	0.16	91,105,111,111	0
7	PG4	C	1002	13/13	0.92	0.17	80,83,91,92	0
7	PG4	D	1005	13/13	0.92	0.18	83,90,96,98	0
3	FLC	H	1003	13/13	0.93	0.21	67,76,89,89	0
3	FLC	G	1001	13/13	0.93	0.21	98,109,121,123	0
3	FLC	A	1001	13/13	0.93	0.20	97,104,108,111	0
4	COA	H	1001	31/48	0.94	0.15	63,86,140,141	0
4	COA	B	1002	48/48	0.95	0.15	74,85,111,114	0
3	FLC	B	1003	13/13	0.95	0.15	70,75,91,94	0
3	FLC	F	1003	13/13	0.95	0.22	75,78,84,86	0
3	FLC	D	1003	13/13	0.96	0.18	69,83,98,100	0

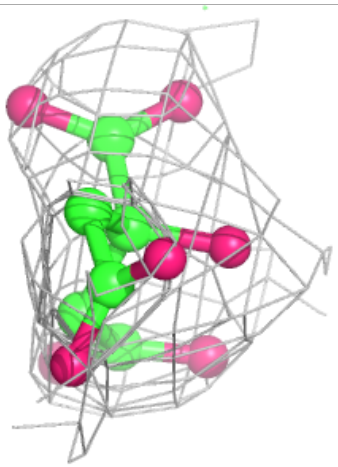
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FLC E 1001:

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

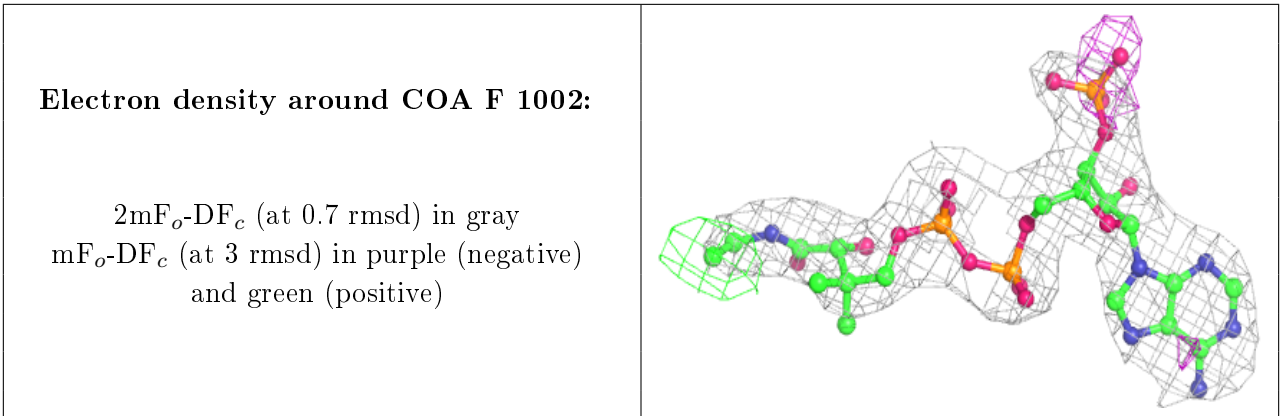






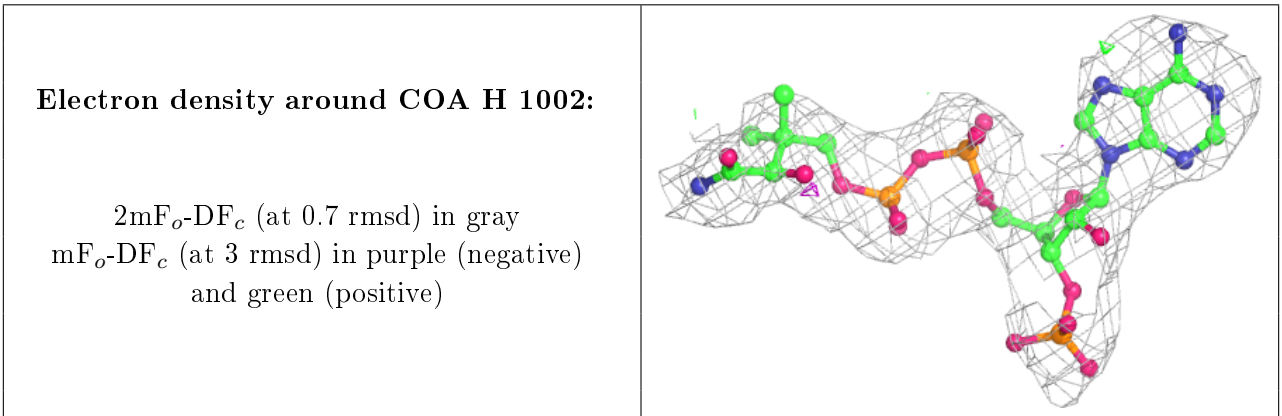
Electron density around COA F 1002:

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



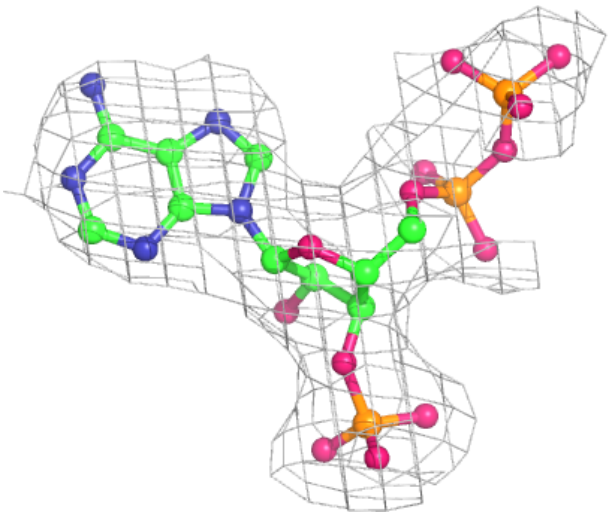
Electron density around COA H 1002:

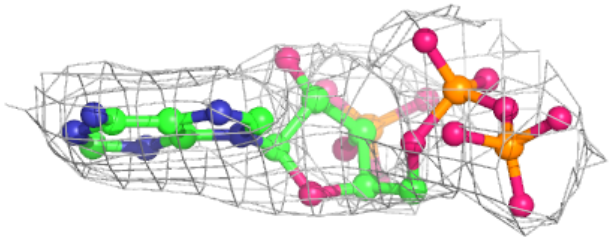
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

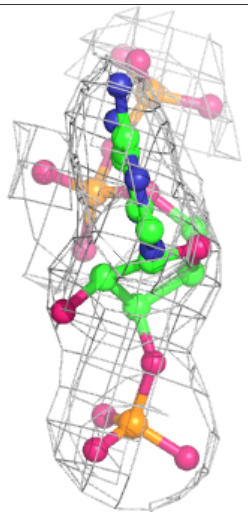


Electron density around COA D 1001:

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

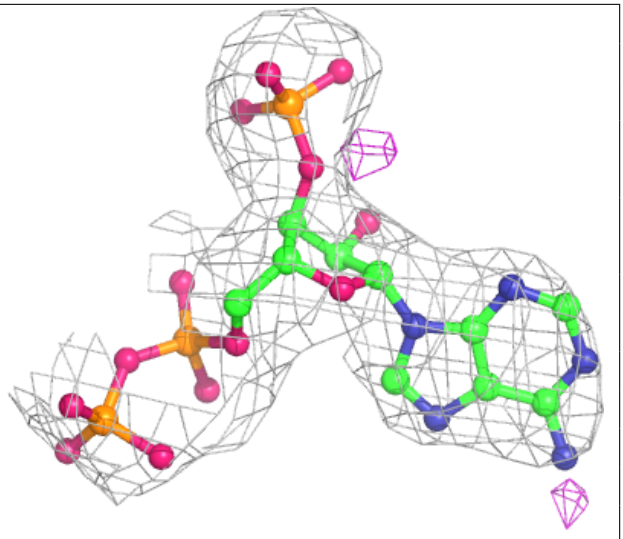


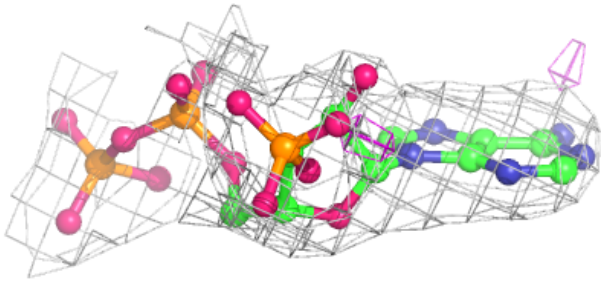


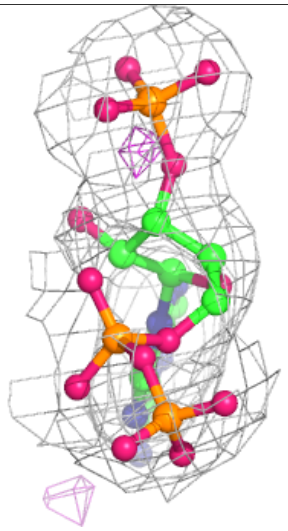


Electron density around COA F 1001:

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

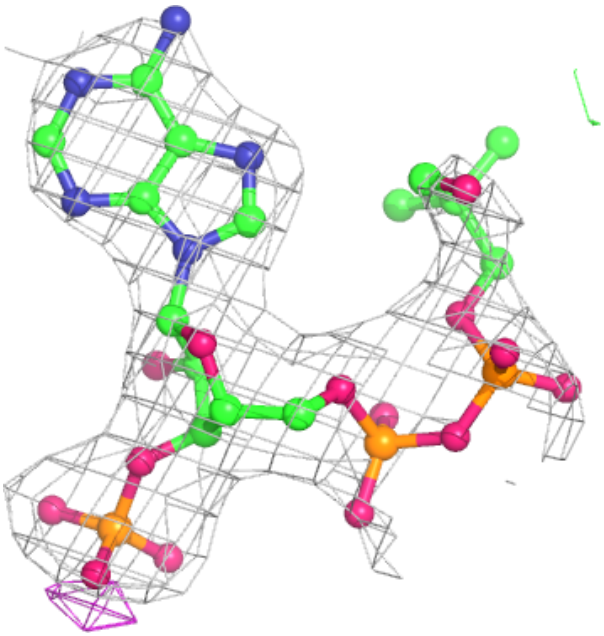


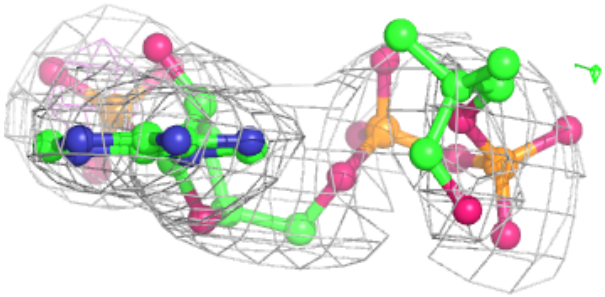


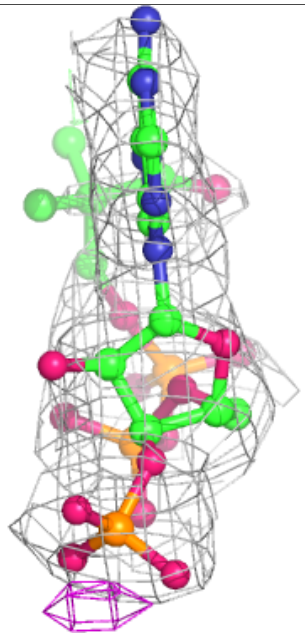


Electron density around COA B 1001:

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

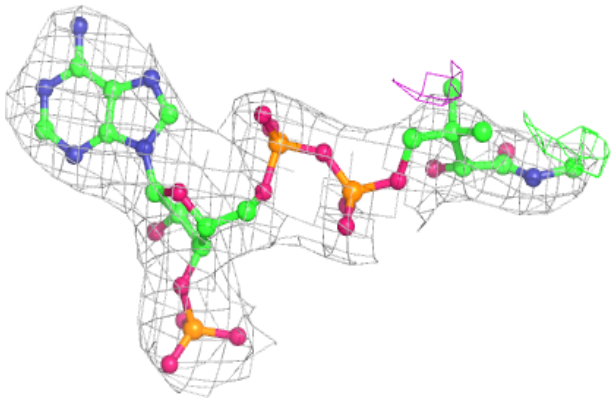


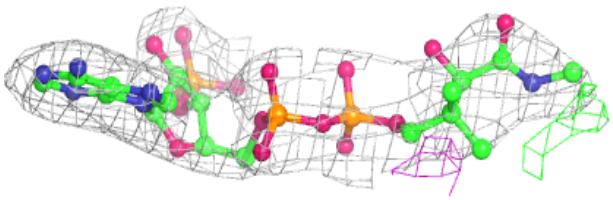


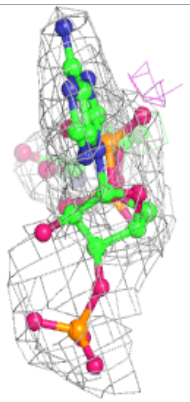


Electron density around COA D 1002:

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

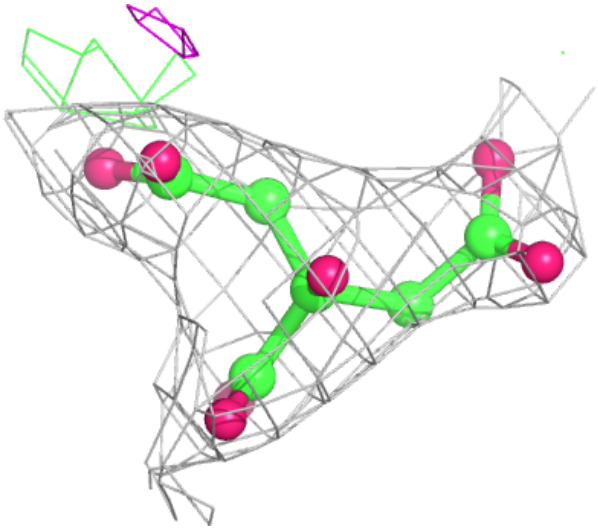


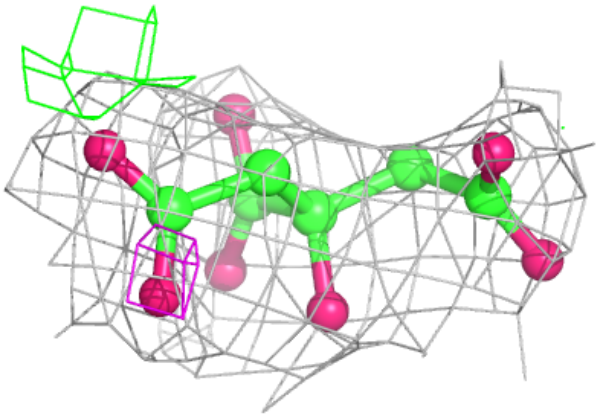


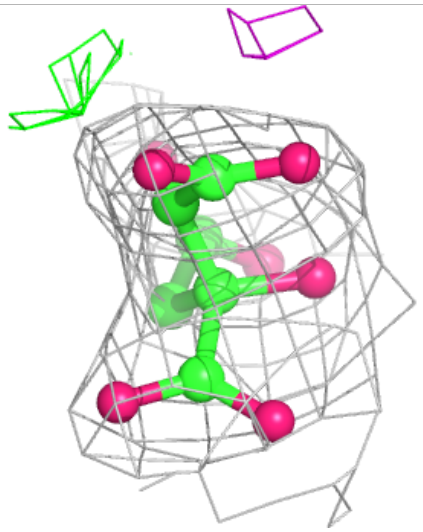


Electron density around FLC C 1001:

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

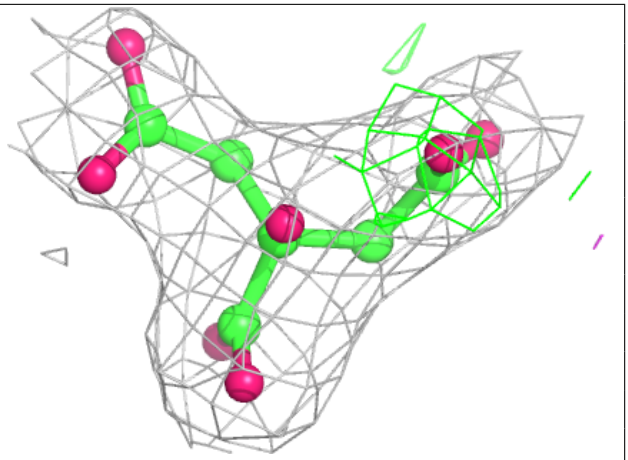


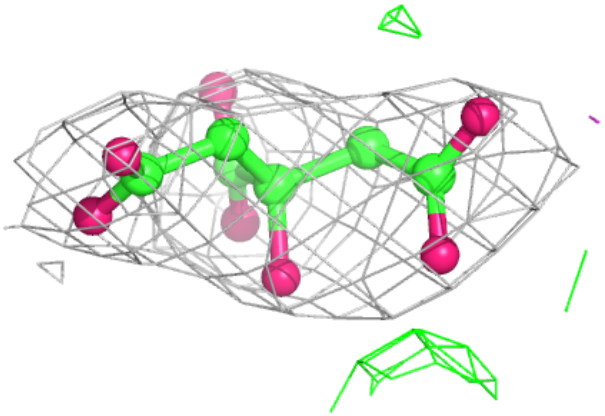


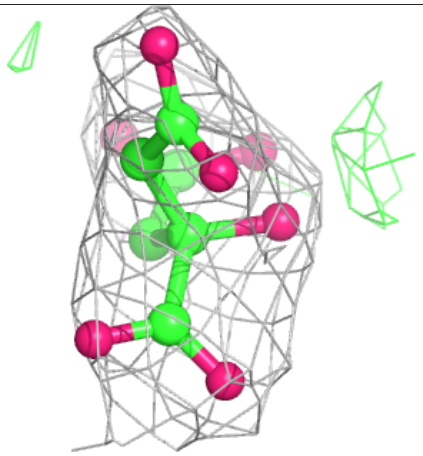


Electron density around FLC H 1003:

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

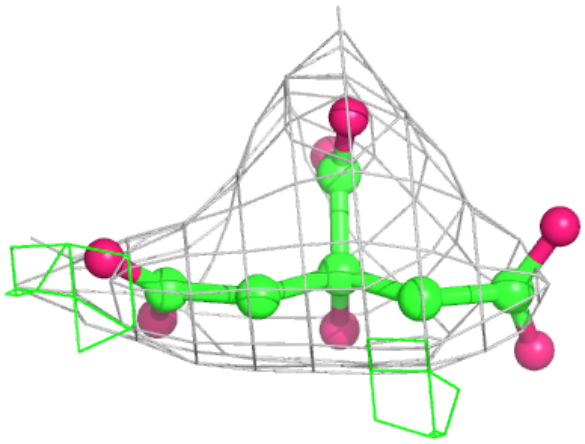


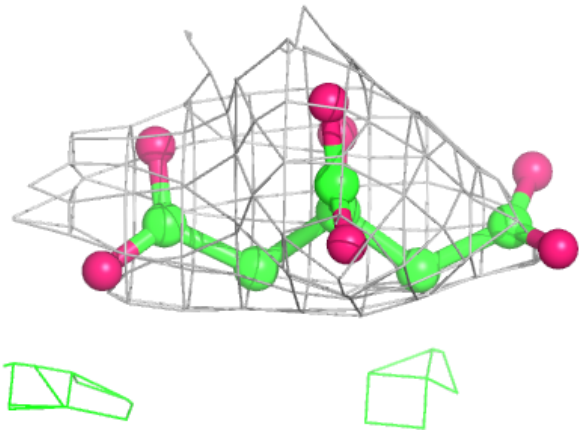


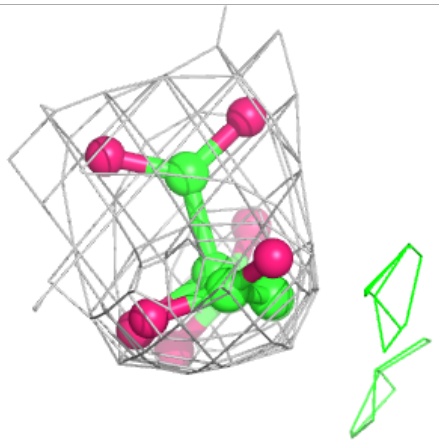


Electron density around FLC G 1001:

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

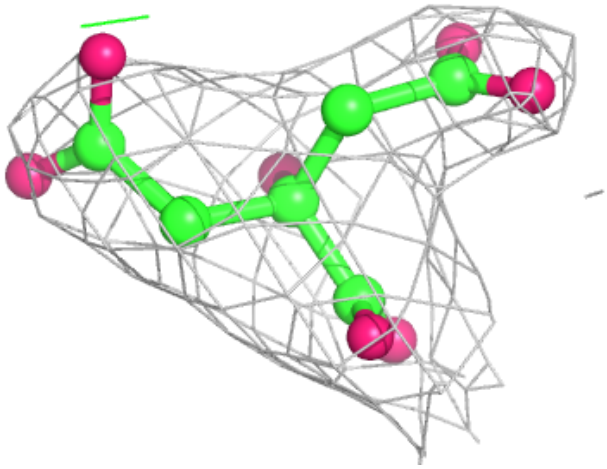


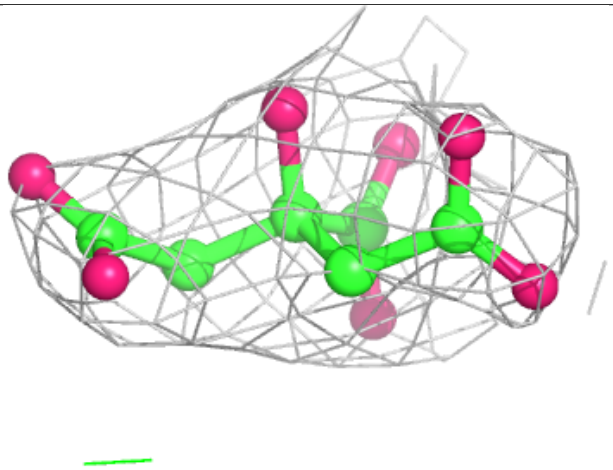


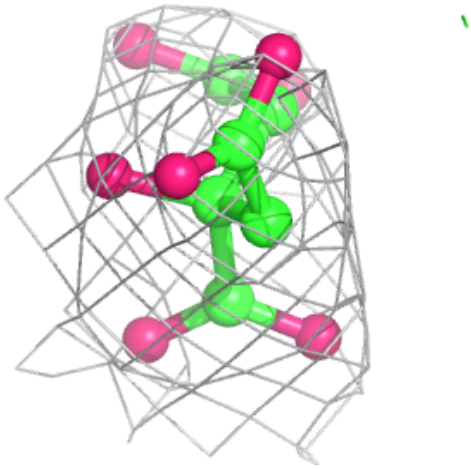


Electron density around FLC A 1001:

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

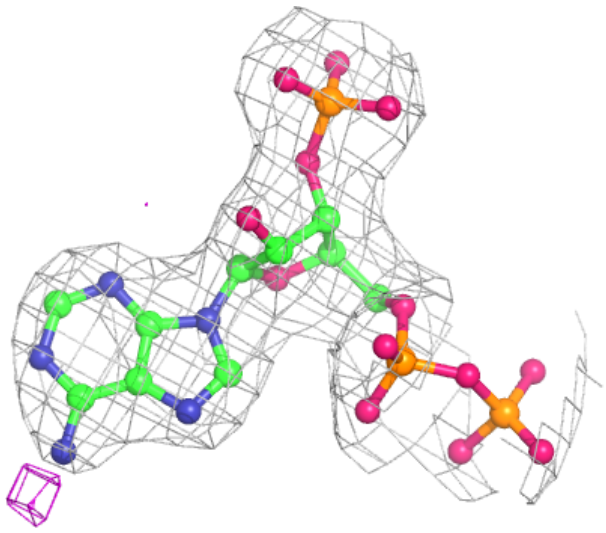


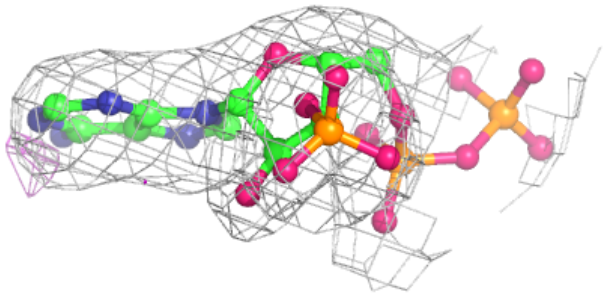


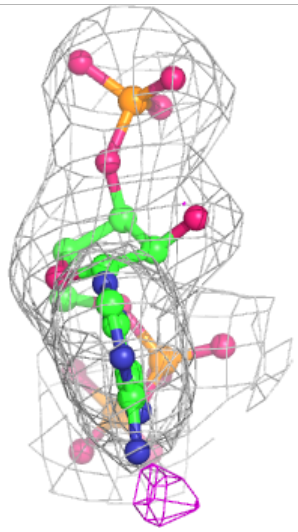


Electron density around COA H 1001:

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

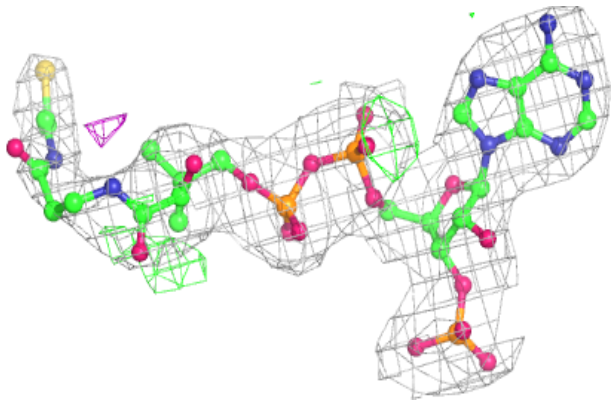


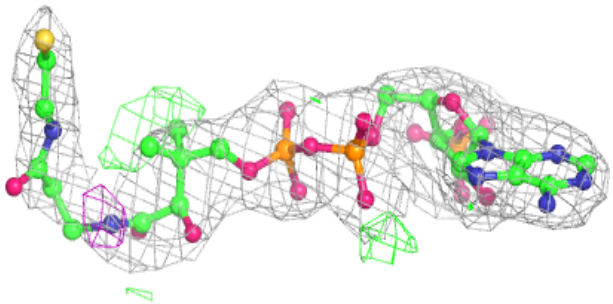


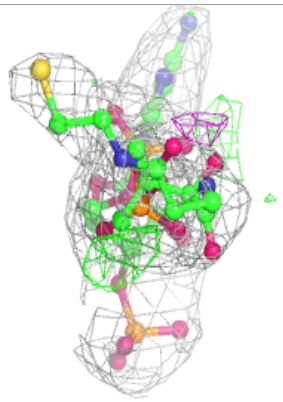


Electron density around COA B 1002:

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

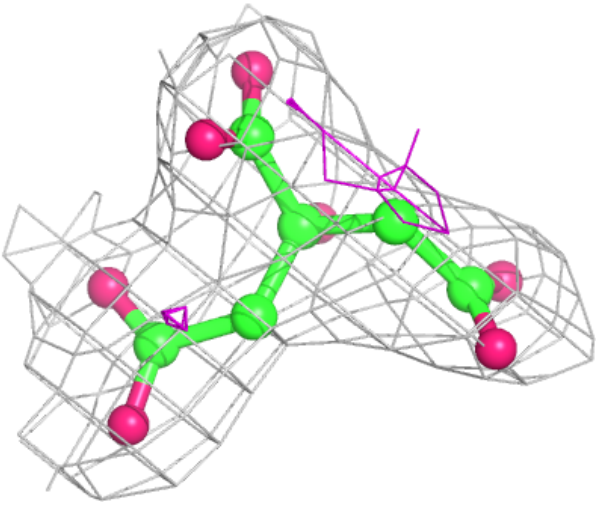


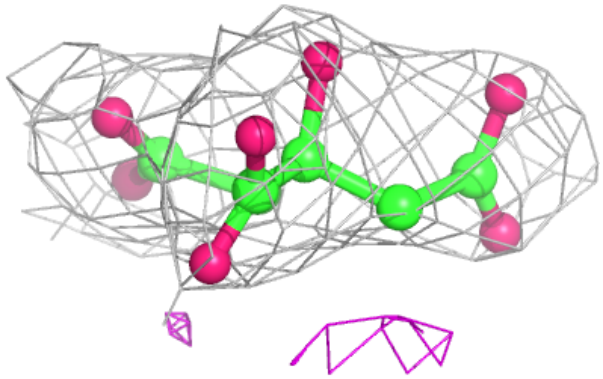


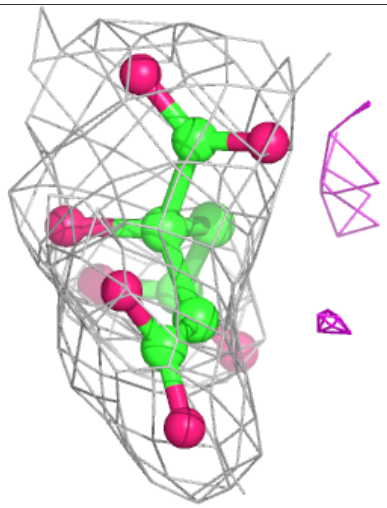


Electron density around FLC B 1003:

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

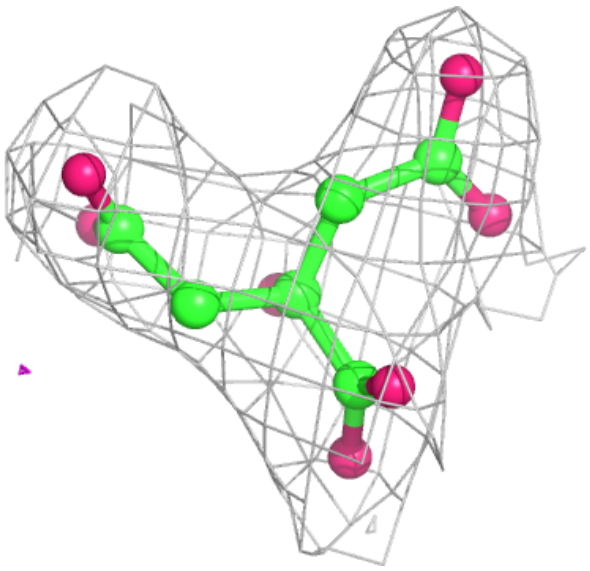


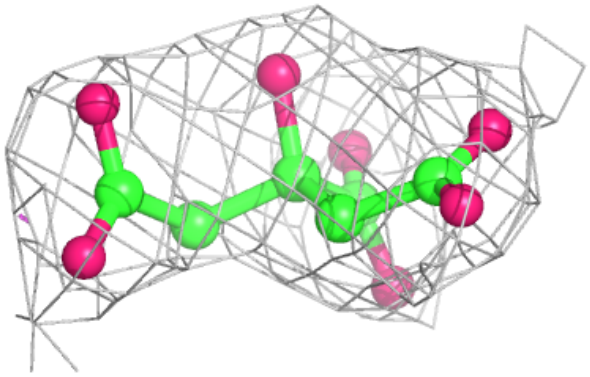


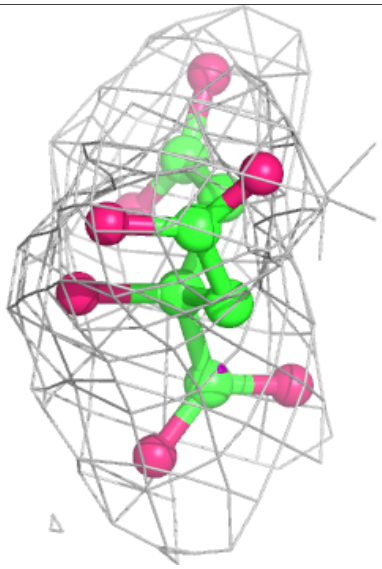


Electron density around FLC F 1003:

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

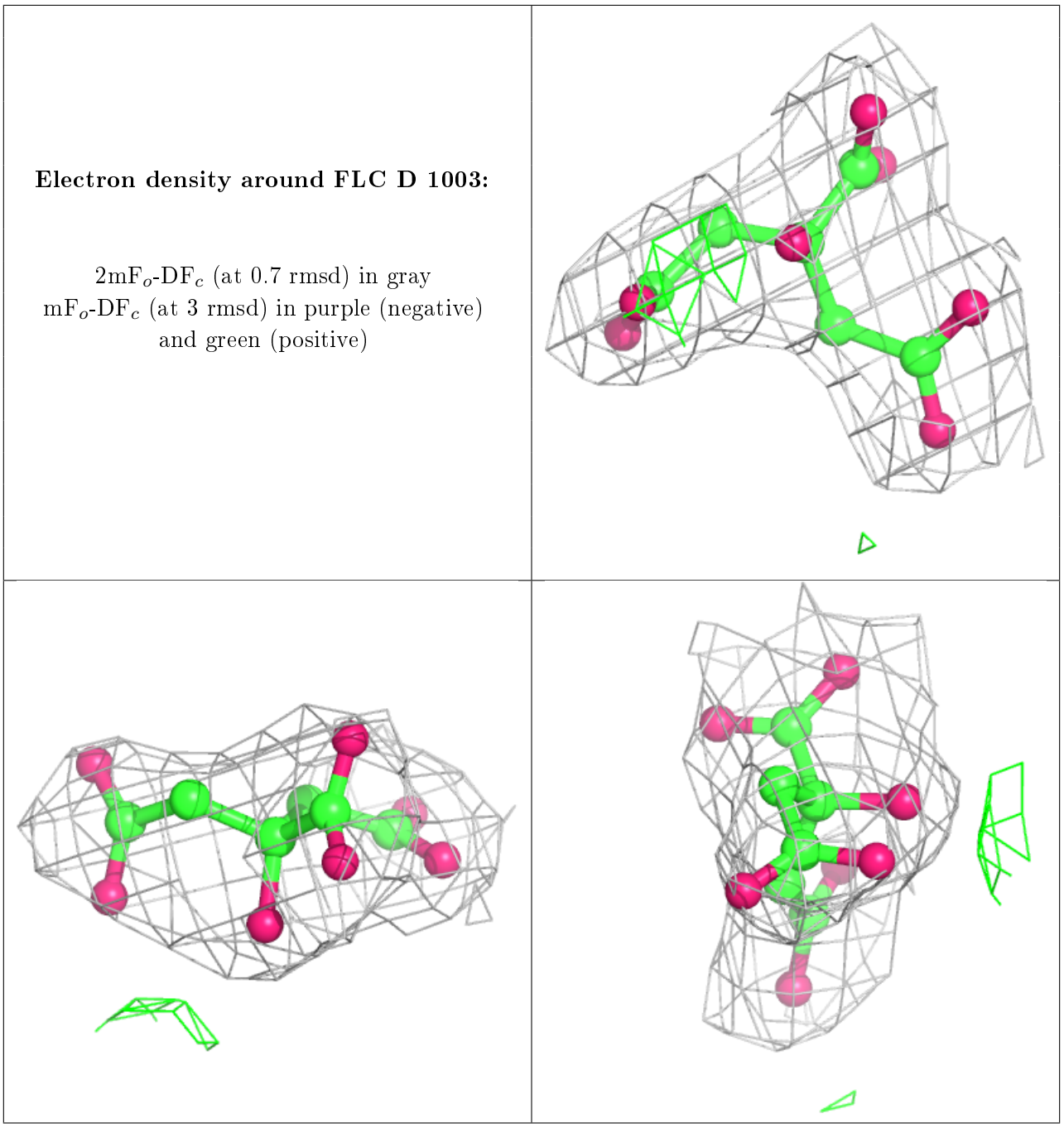






Electron density around FLC D 1003:

$2mF_o$-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

There are no such residues in this entry.