



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 04:51 PM EDT

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 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

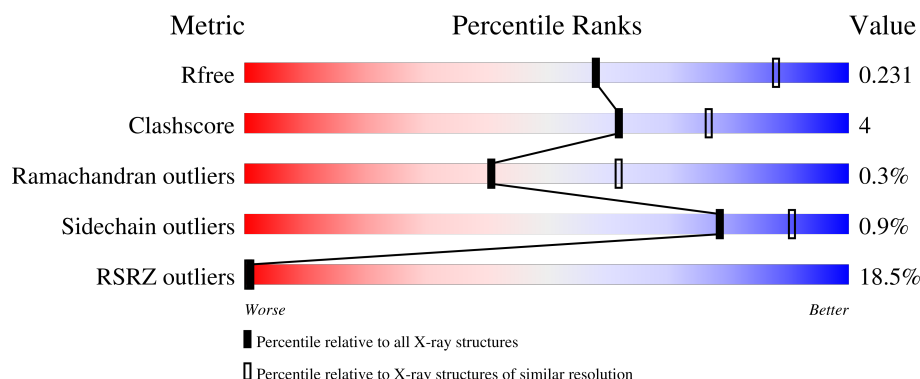
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 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	398	
1	C	398	
1	E	398	
1	G	398	
2	B	617	

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Mol	Chain	Length	Quality of chain
2	D	617	
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:

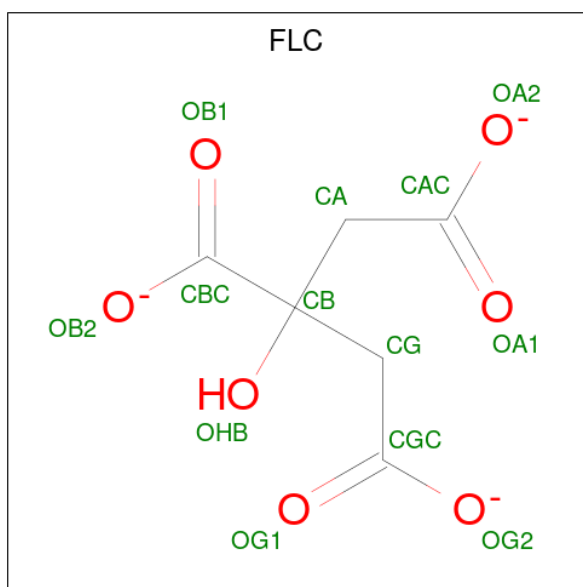
Chain	Residue	Modelled	Actual	Comment	Reference
B	609	GLY	-	expression tag	UNP Q9AJC4
B	610	GLY	-	expression tag	UNP Q9AJC4
B	611	SER	-	expression tag	UNP Q9AJC4
B	612	HIS	-	expression tag	UNP Q9AJC4
B	613	HIS	-	expression tag	UNP Q9AJC4
B	614	HIS	-	expression tag	UNP Q9AJC4
B	615	HIS	-	expression tag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

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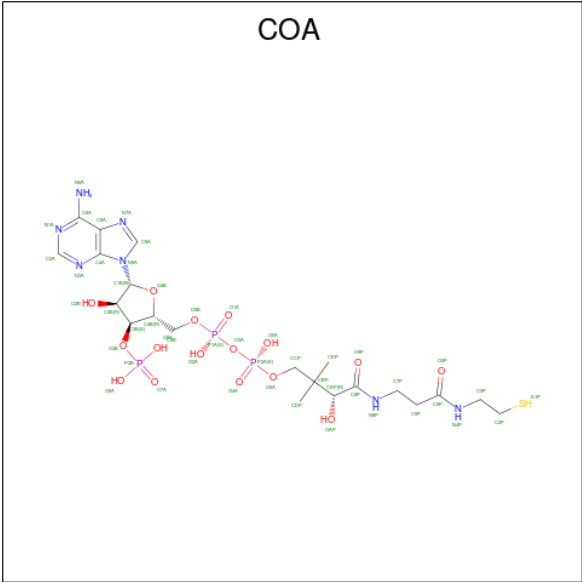
Chain	Residue	Modelled	Actual	Comment	Reference
B	617	HIS	-	expression tag	UNP Q9AJC4
D	609	GLY	-	expression tag	UNP Q9AJC4
D	610	GLY	-	expression tag	UNP Q9AJC4
D	611	SER	-	expression tag	UNP Q9AJC4
D	612	HIS	-	expression tag	UNP Q9AJC4
D	613	HIS	-	expression tag	UNP Q9AJC4
D	614	HIS	-	expression tag	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: C₆H₅O₇) (labeled as "Ligand of Interest" by depositor).



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

- 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 depositor).



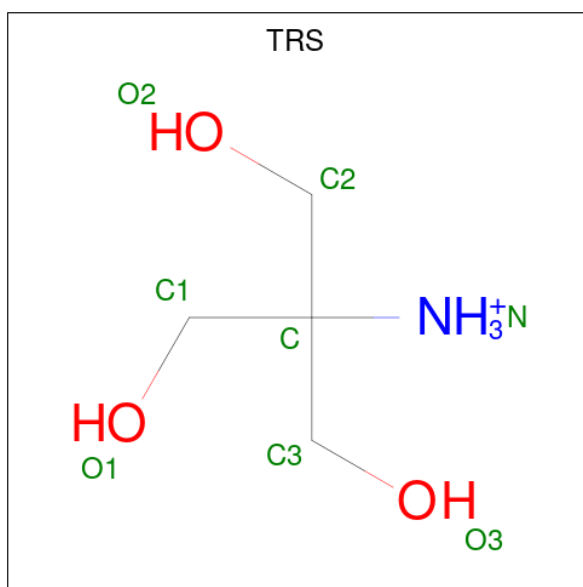
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 37	C 15	N 5	O 14	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 16	P 3 S 1	0	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	D	1	Total 41	C 17	N 6	O 15	P 3	0	0
4	F	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	F	1	Total 42	C 18	N 6	O 15	P 3	0	0
4	H	1	Total 31	C 10	N 5	O 13	P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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



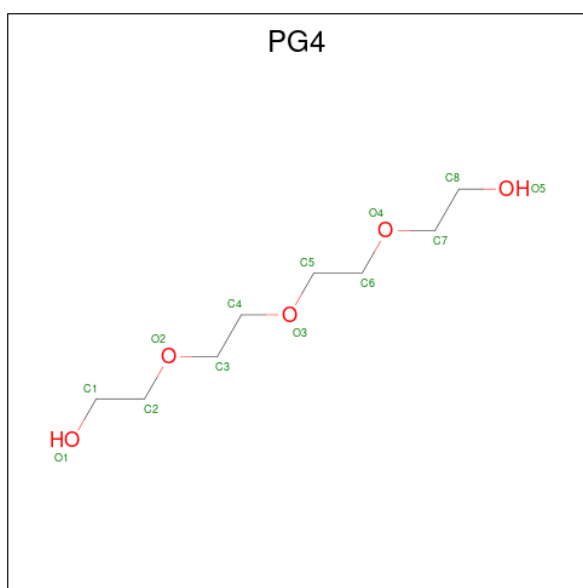
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	F	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

- 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	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		

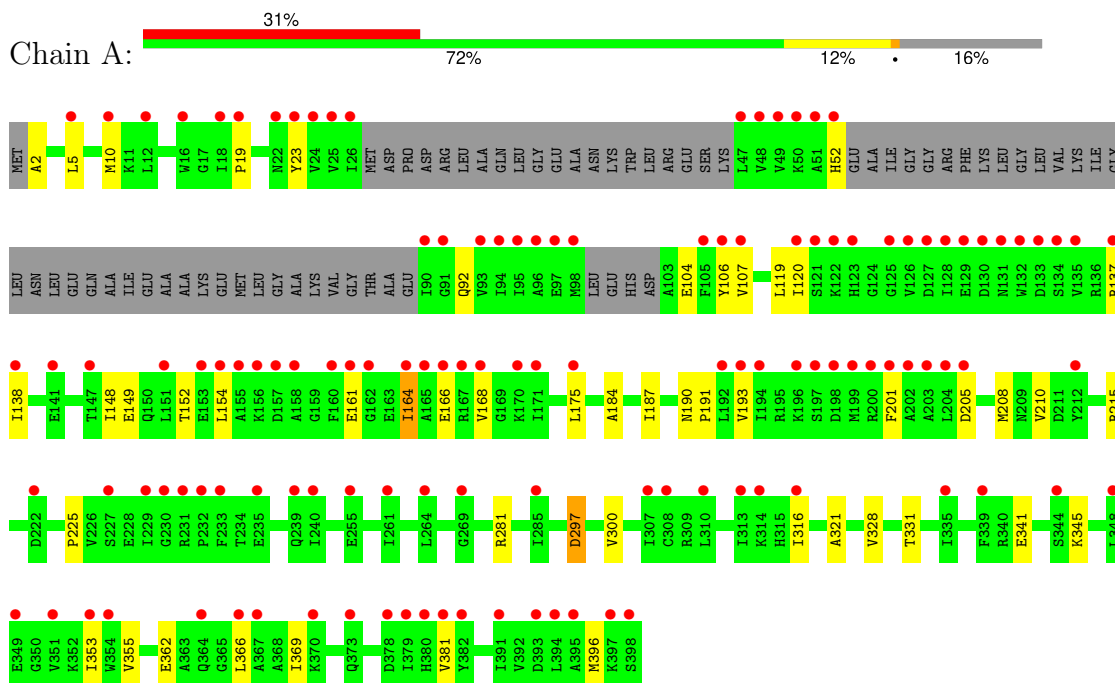
- Molecule 8 is water.

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

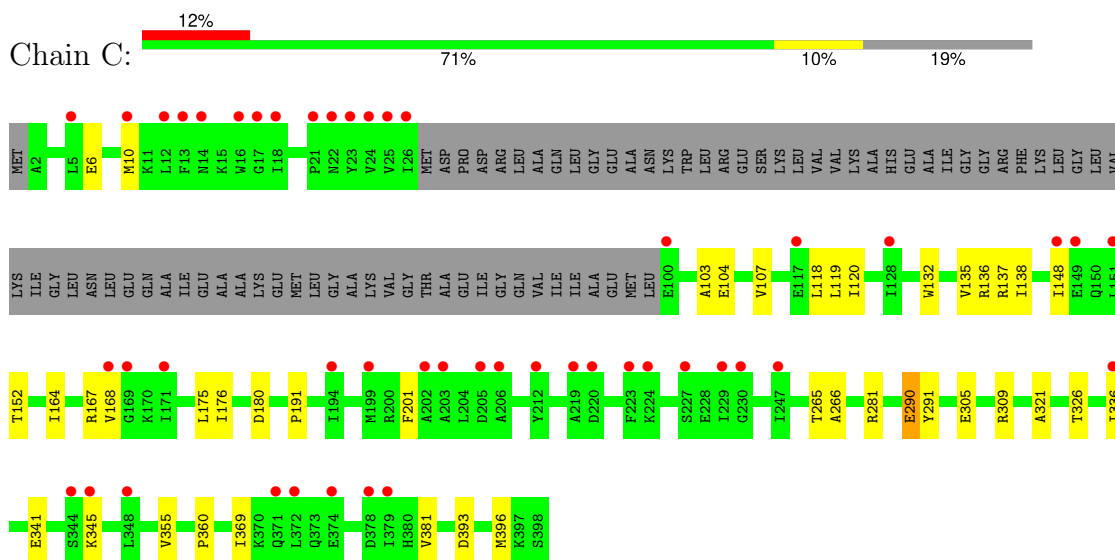
3 Residue-property plots

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: ATP-citrate lyase beta-subunit

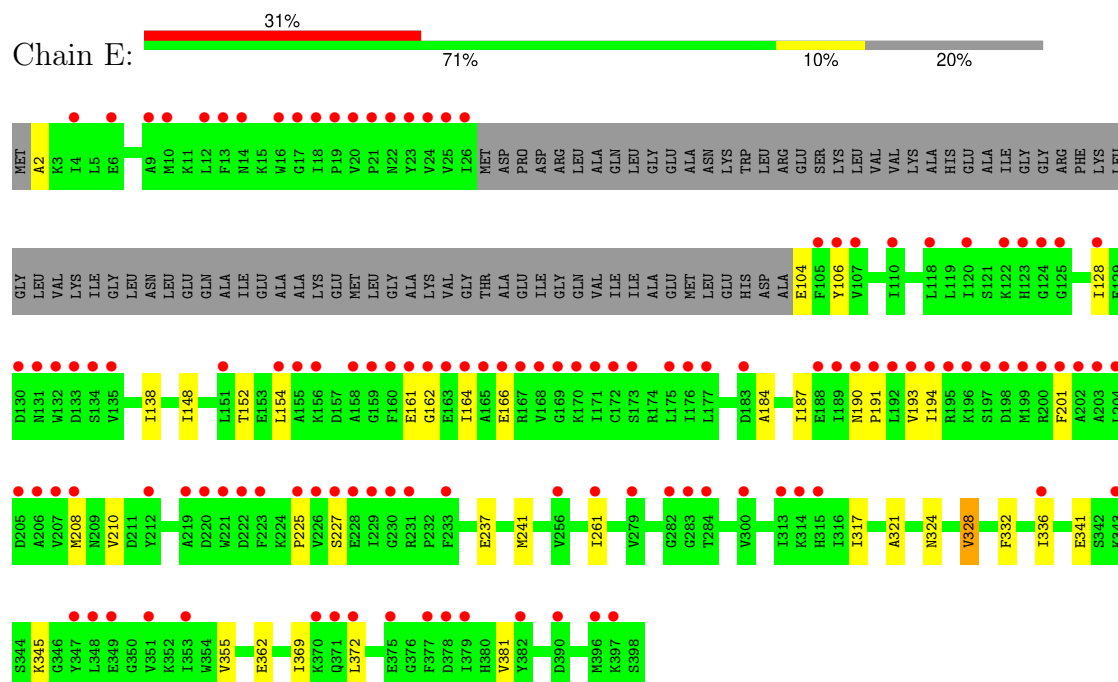


• Molecule 1: ATP-citrate lyase beta-subunit



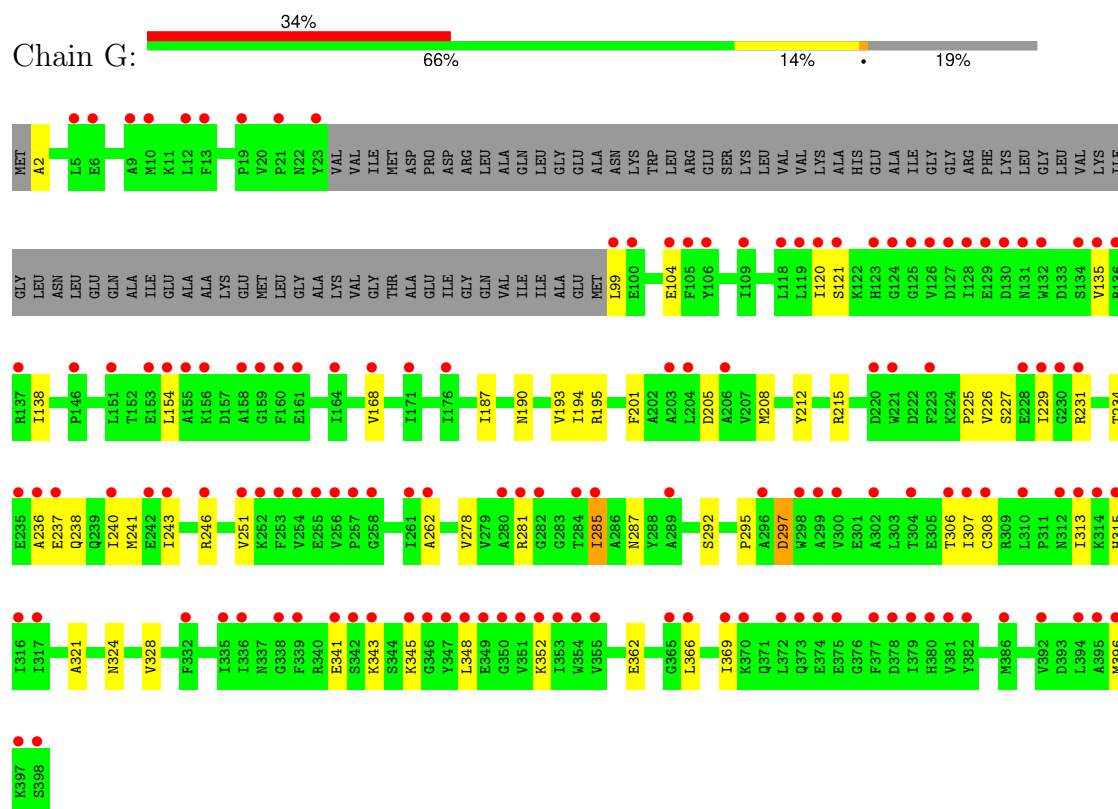
• Molecule 1: ATP-citrate lyase beta-subunit

Chain E:



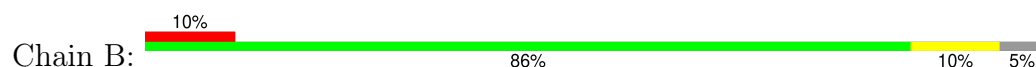
• Molecule 1: ATP-citrate lyase beta-subunit

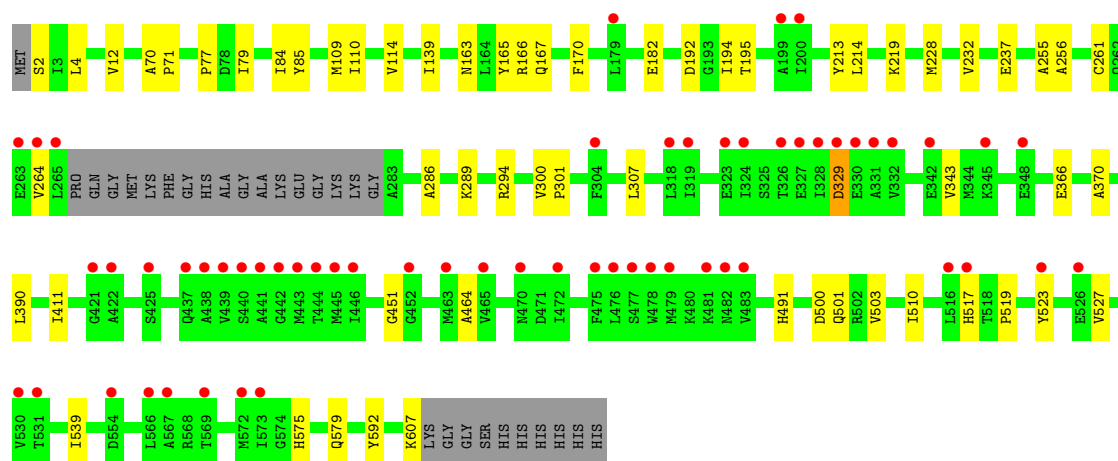
Chain G:



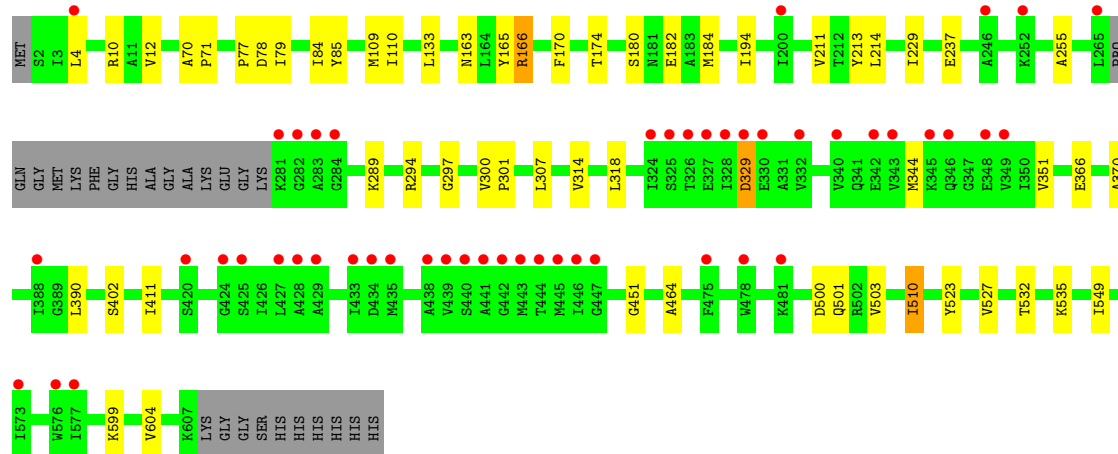
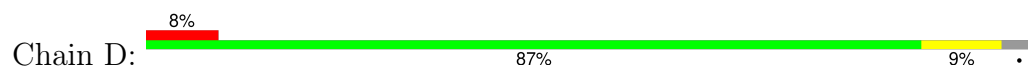
• Molecule 2: ATP-citrate lyase alpha-subunit

Chain B:

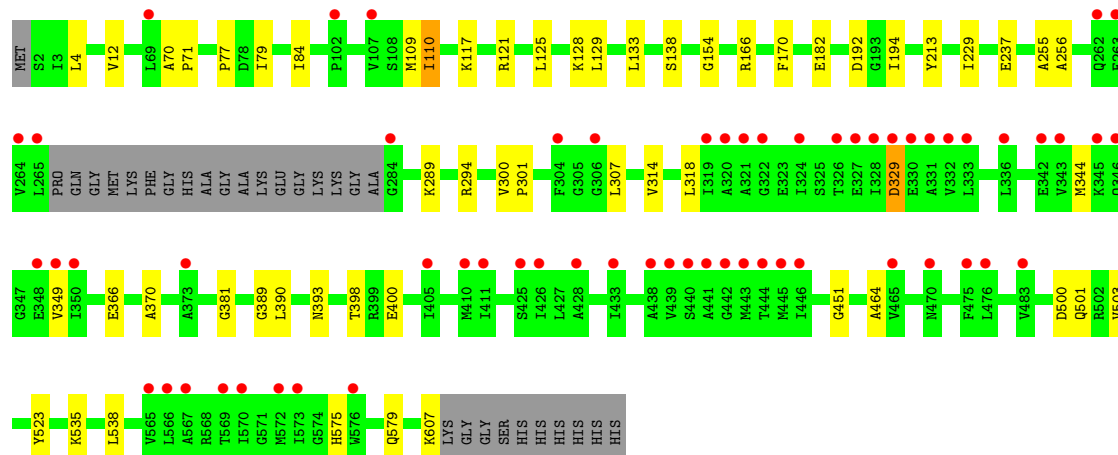
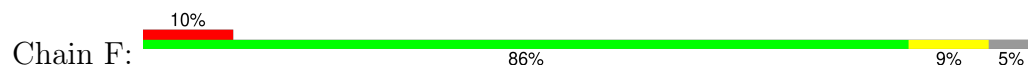




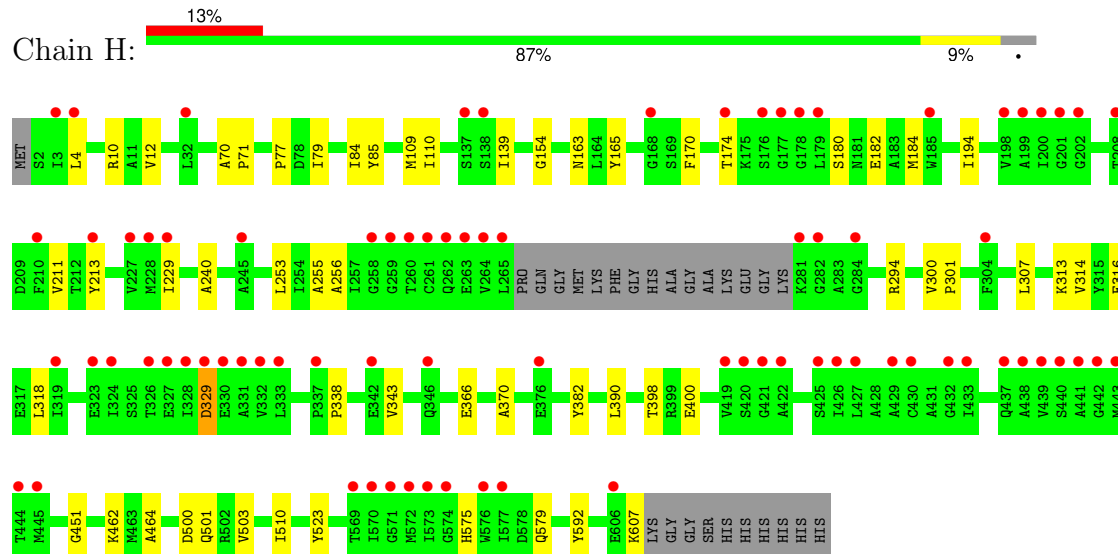
• Molecule 2: ATP-citrate lyase alpha-subunit



• Molecule 2: ATP-citrate lyase alpha-subunit



● Molecule 2: ATP-citrate lyase alpha-subunit



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 80.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, COA, TRS, FLC, PGE

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(°)	Ideal(°)
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(°)	Ideal(°)
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

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.

The worst 5 of 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

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

5 of 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

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	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2942/3236 (91%)	2916 (99%)	26 (1%)	78 90

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	604	VAL
1	E	369	ILE
2	H	329	ASP
1	E	328	VAL
2	F	110	ILE

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	COA	F	1002	-	38,44,50	0.70	0	49,68,75	0.70	1 (2%)
3	FLC	H	1003	-	12,12,12	1.28	1 (8%)	17,17,17	1.46	2 (11%)
4	COA	D	1001	-	28,33,50	1.14	2 (7%)	37,52,75	1.02	3 (8%)
4	COA	B	1002	-	43,50,50	0.62	1 (2%)	56,75,75	1.05	4 (7%)
6	TRS	D	1004	-	7,7,7	0.40	0	9,9,9	0.52	0
6	TRS	B	1005	-	7,7,7	0.21	0	9,9,9	0.37	0
5	PGE	B	1004	-	9,9,9	0.37	0	8,8,8	0.39	0
5	PGE	C	1003	-	9,9,9	0.30	0	8,8,8	0.21	0
4	COA	B	1001	-	35,39,50	0.69	0	44,61,75	0.91	2 (4%)
7	PG4	C	1002	-	12,12,12	0.19	0	11,11,11	0.28	0
4	COA	H	1001	-	28,33,50	1.05	1 (3%)	37,52,75	1.04	1 (2%)
3	FLC	B	1003	-	12,12,12	1.02	0	17,17,17	1.69	5 (29%)
3	FLC	A	1001	-	12,12,12	1.02	0	17,17,17	1.15	1 (5%)
3	FLC	D	1003	-	12,12,12	1.05	0	17,17,17	1.46	3 (17%)
5	PGE	H	1004	-	9,9,9	0.22	0	8,8,8	0.17	0
3	FLC	E	1001	-	12,12,12	1.08	0	17,17,17	1.27	2 (11%)
4	COA	D	1002	-	37,43,50	0.69	1 (2%)	49,67,75	0.68	1 (2%)
4	COA	H	1002	-	36,42,50	0.70	1 (2%)	49,66,75	0.76	2 (4%)
4	COA	F	1001	-	28,33,50	0.93	0	37,52,75	0.94	1 (2%)
5	PGE	D	1006	-	9,9,9	0.27	0	8,8,8	0.40	0
5	PGE	F	1004	-	9,9,9	0.33	0	8,8,8	0.24	0
7	PG4	D	1005	-	12,12,12	0.27	0	11,11,11	0.39	0
3	FLC	G	1001	-	12,12,12	1.11	0	17,17,17	1.34	2 (11%)
3	FLC	C	1001	-	12,12,12	1.10	0	17,17,17	1.05	1 (5%)
3	FLC	F	1003	-	12,12,12	1.13	0	17,17,17	1.56	3 (17%)

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	1002	-	-	10/37/57/64	0/3/3/3
3	FLC	H	1003	-	-	2/16/16/16	-
4	COA	D	1001	-	-	4/17/37/64	0/3/3/3
4	COA	B	1002	-	-	13/44/64/64	0/3/3/3
6	TRS	D	1004	-	-	3/9/9/9	-
6	TRS	B	1005	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	B	1004	-	-	6/7/7/7	-
5	PGE	C	1003	-	-	3/7/7/7	-
4	COA	B	1001	-	-	12/27/47/64	0/3/3/3
7	PG4	C	1002	-	-	2/10/10/10	-
4	COA	H	1001	-	-	9/17/37/64	0/3/3/3
3	FLC	B	1003	-	-	5/16/16/16	-
3	FLC	A	1001	-	-	0/16/16/16	-
3	FLC	D	1003	-	-	2/16/16/16	-
5	PGE	H	1004	-	-	3/7/7/7	-
3	FLC	E	1001	-	-	0/16/16/16	-
4	COA	D	1002	-	-	12/36/56/64	0/3/3/3
4	COA	H	1002	-	-	11/33/54/64	0/3/3/3
4	COA	F	1001	-	-	3/17/37/64	0/3/3/3
5	PGE	D	1006	-	-	4/7/7/7	-
5	PGE	F	1004	-	-	2/7/7/7	-
7	PG4	D	1005	-	-	5/10/10/10	-
3	FLC	G	1001	-	-	0/16/16/16	-
3	FLC	C	1001	-	-	0/16/16/16	-
3	FLC	F	1003	-	-	4/16/16/16	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1001	COA	P2A-O4A	3.69	1.62	1.50
3	H	1003	FLC	OB2-CBC	-2.60	1.21	1.30
4	H	1001	COA	P3B-O3B	2.37	1.63	1.59
4	D	1001	COA	P3B-O3B	2.35	1.63	1.59
4	H	1002	COA	P3B-O3B	2.17	1.63	1.59

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1002	COA	O6A-P2A-O4A	5.09	129.09	108.94
4	B	1001	COA	CCP-CBP-CAP	3.41	115.83	110.08
3	B	1003	FLC	CB-CG-CGC	3.07	122.32	113.92
3	D	1003	FLC	OB1-CBC-CB	-2.76	116.74	122.09
3	B	1003	FLC	CA-CB-CBC	-2.76	103.93	110.03

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

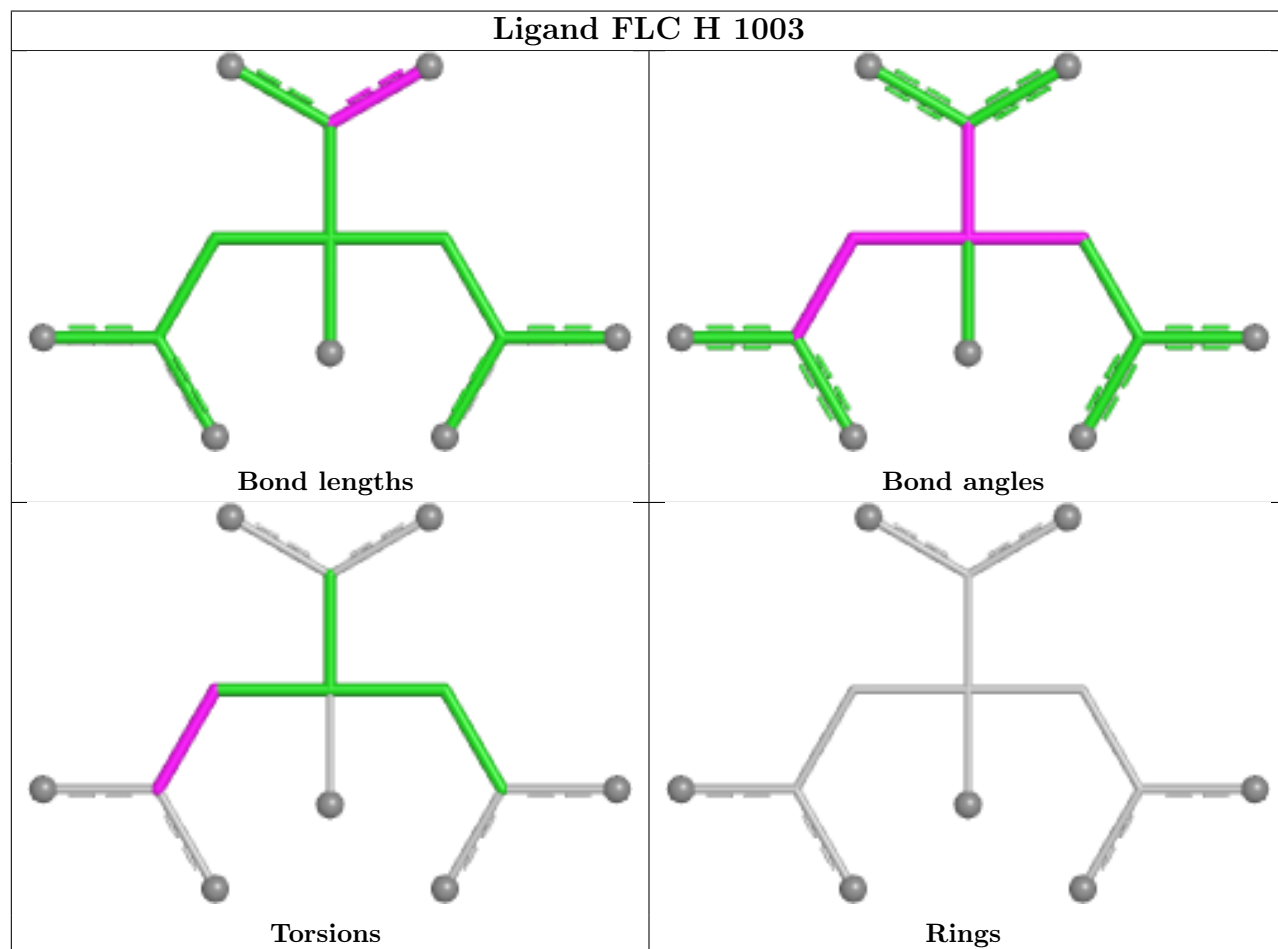
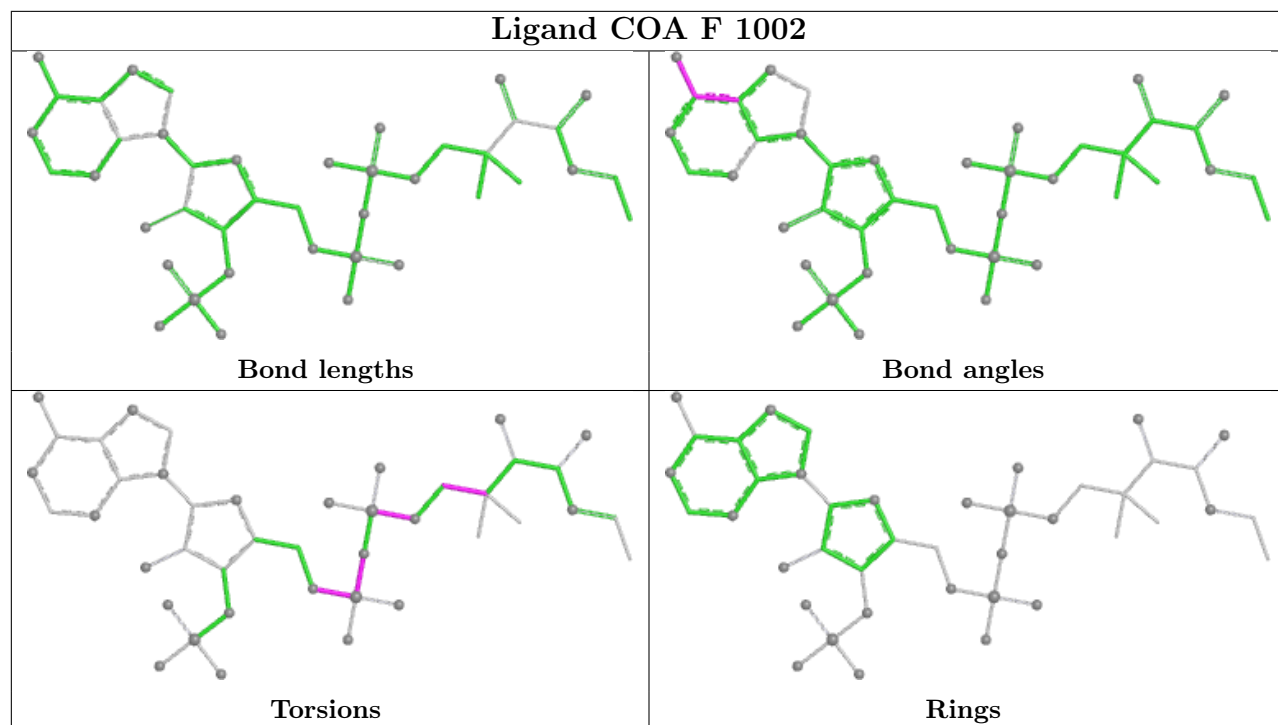
Mol	Chain	Res	Type	Atoms
3	B	1003	FLC	CG-CB-CBC-OB1
4	B	1001	COA	C5B-O5B-P1A-O1A
4	B	1001	COA	C5B-O5B-P1A-O3A
4	B	1001	COA	CCP-O6A-P2A-O3A
4	B	1002	COA	C5B-O5B-P1A-O1A

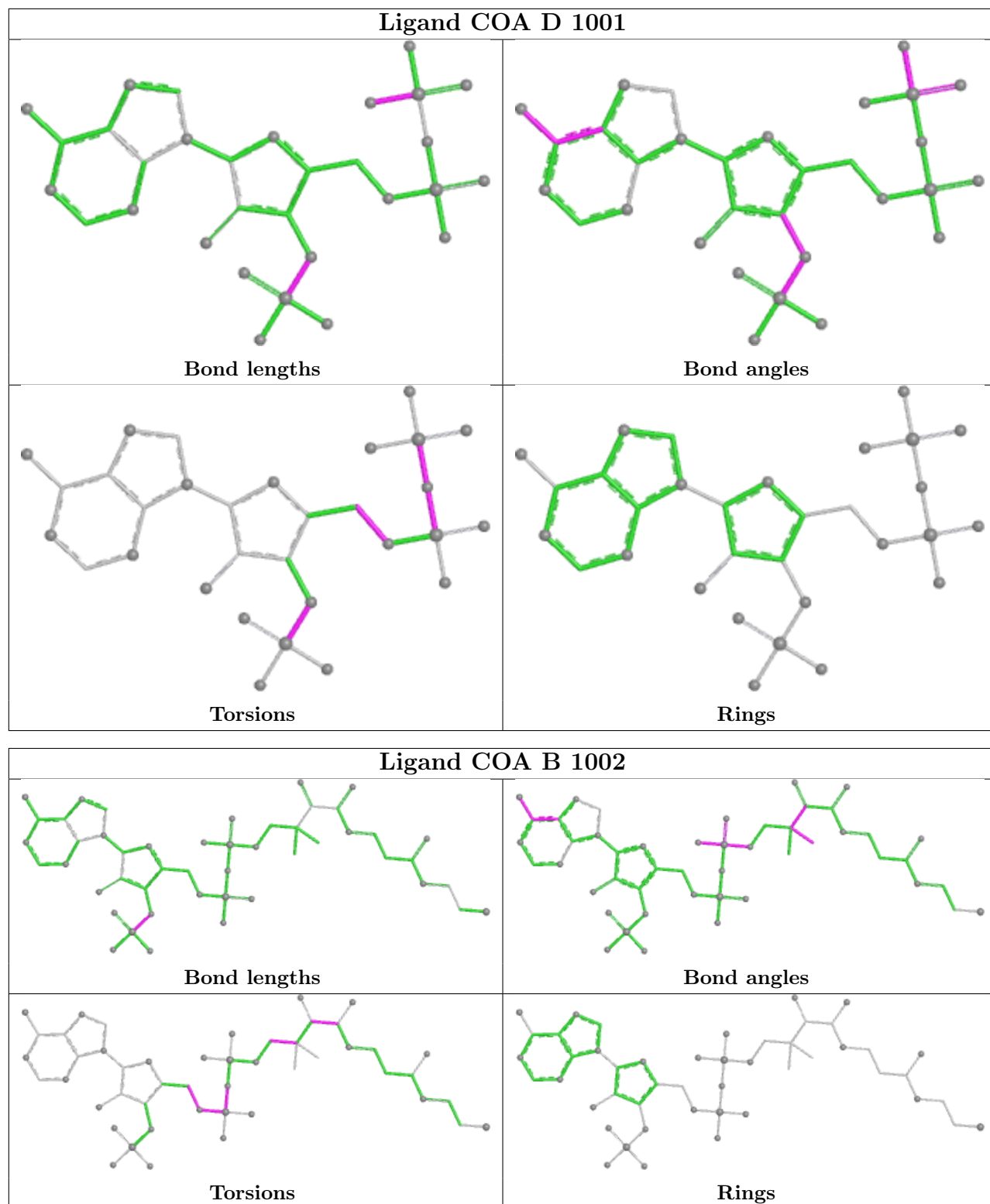
There are no ring outliers.

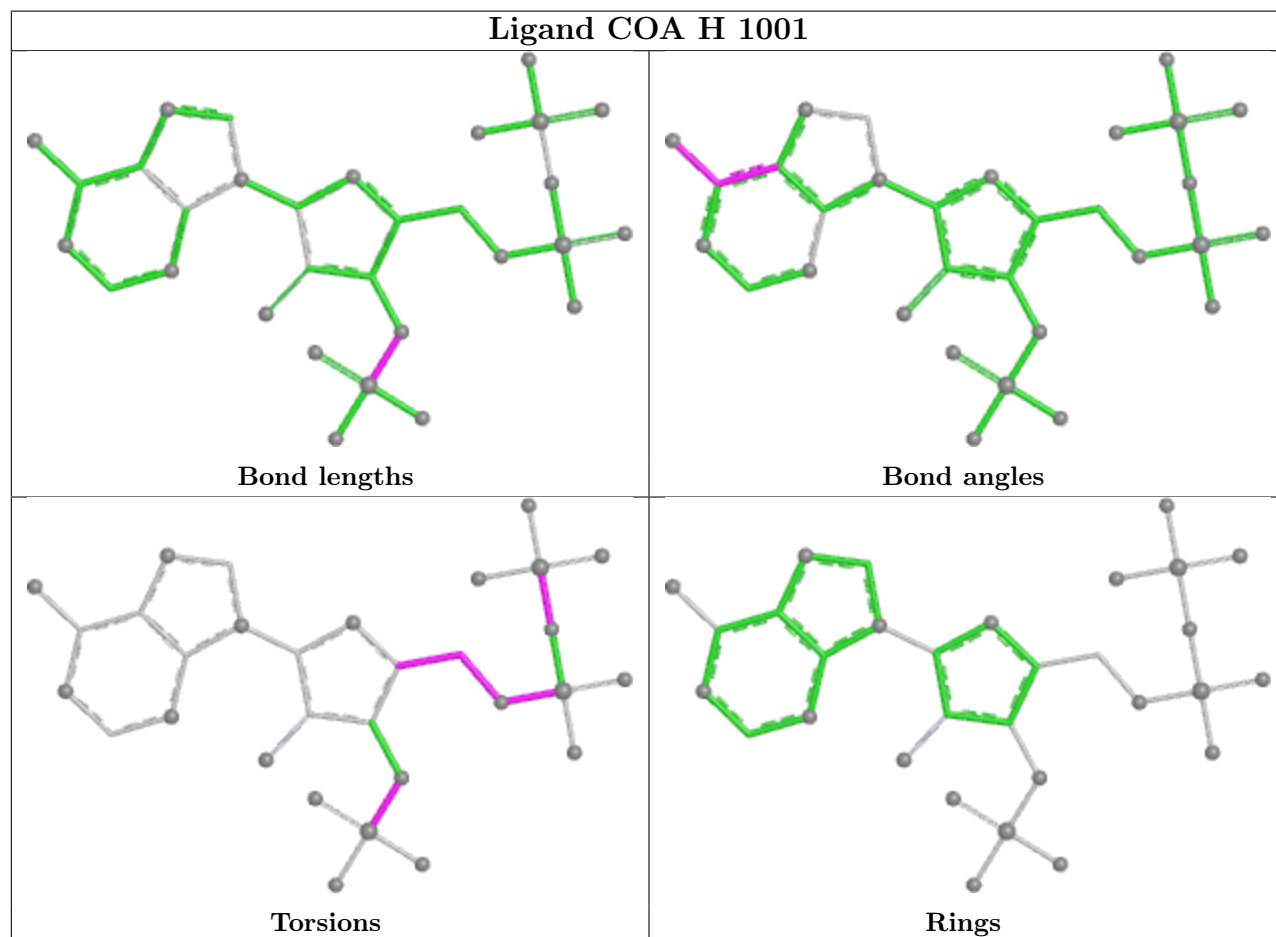
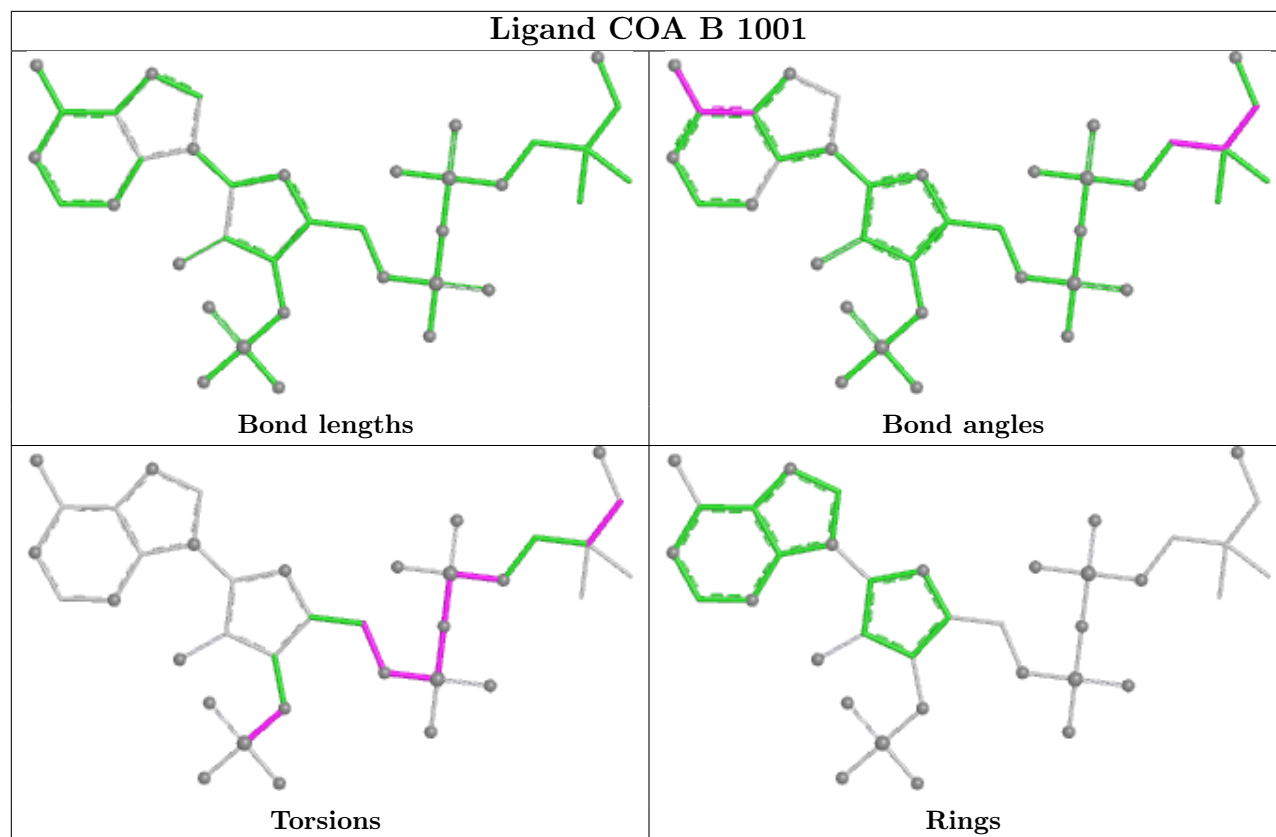
6 monomers are involved in 10 short contacts:

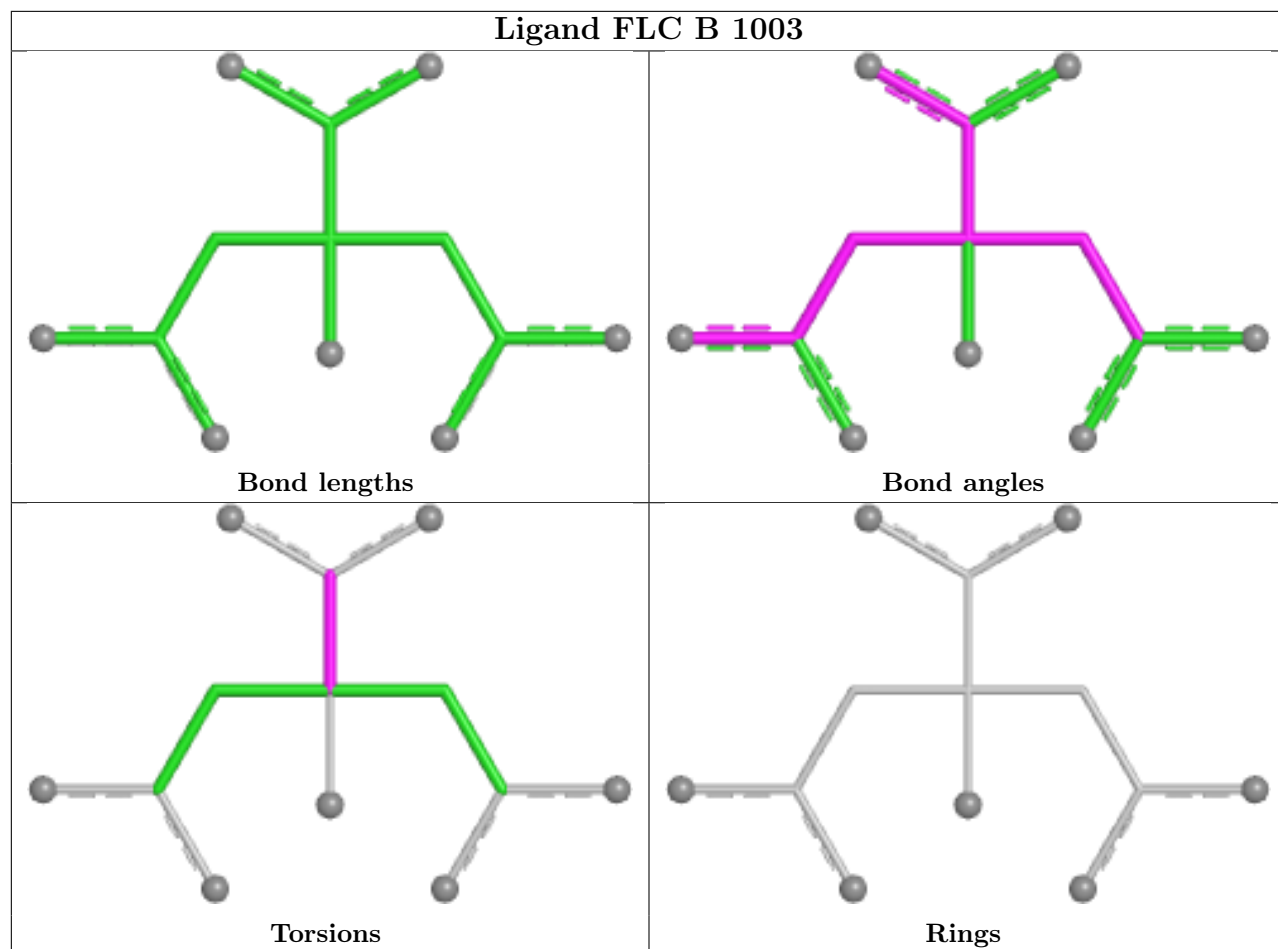
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	COA	2	0
5	B	1004	PGE	2	0
7	C	1002	PG4	1	0
5	H	1004	PGE	2	0
5	D	1006	PGE	1	0
7	D	1005	PG4	2	0

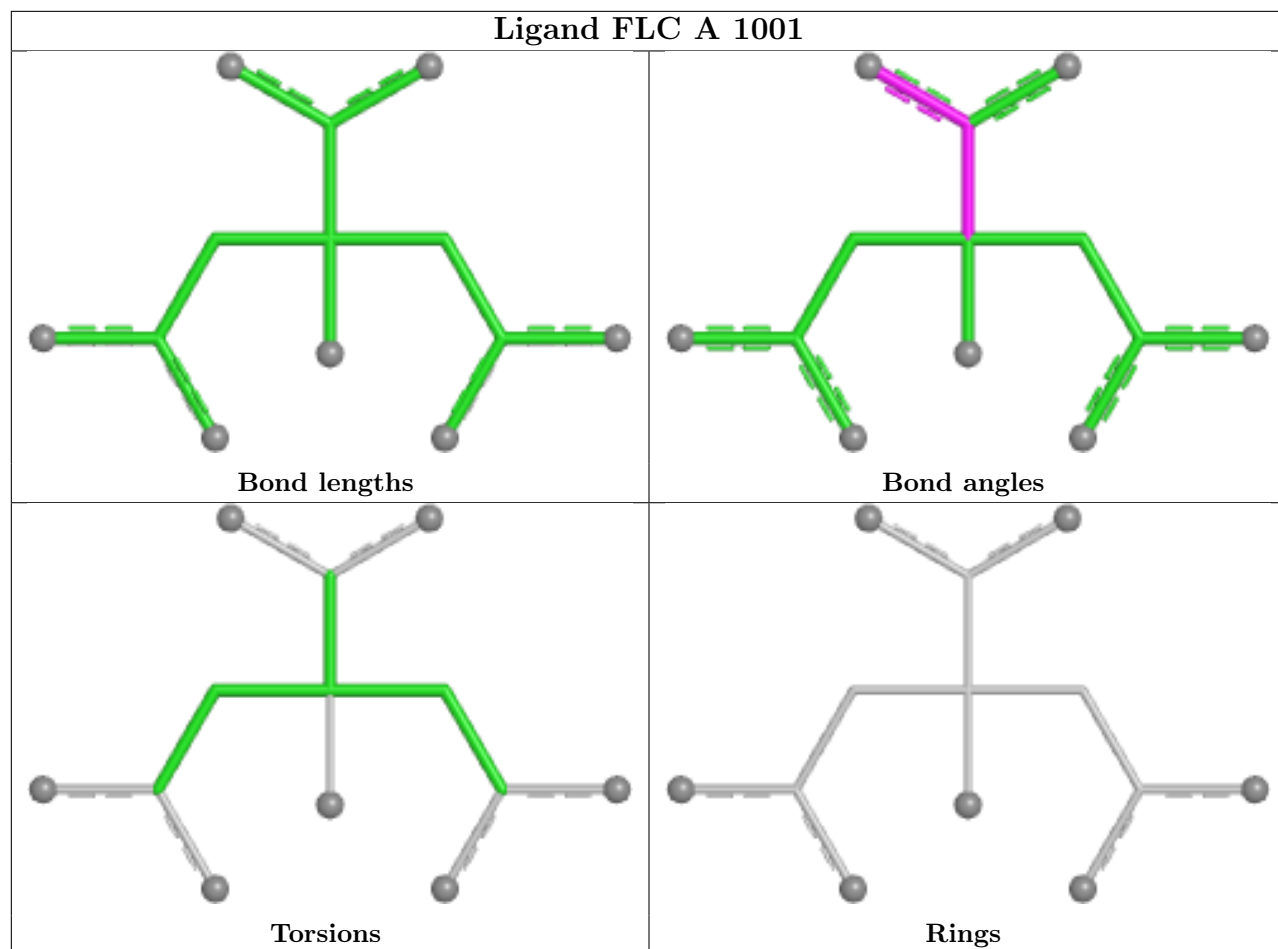
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

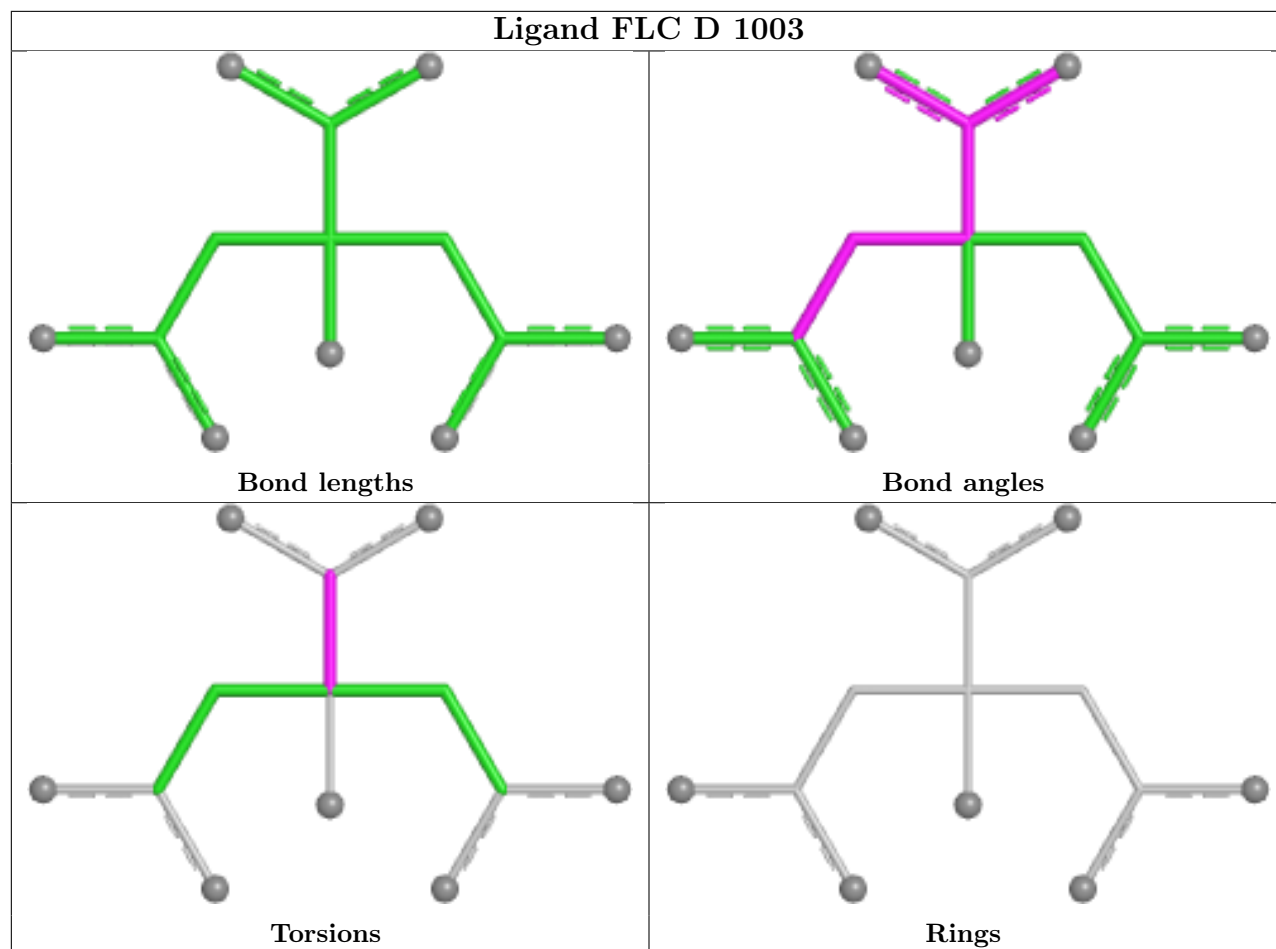


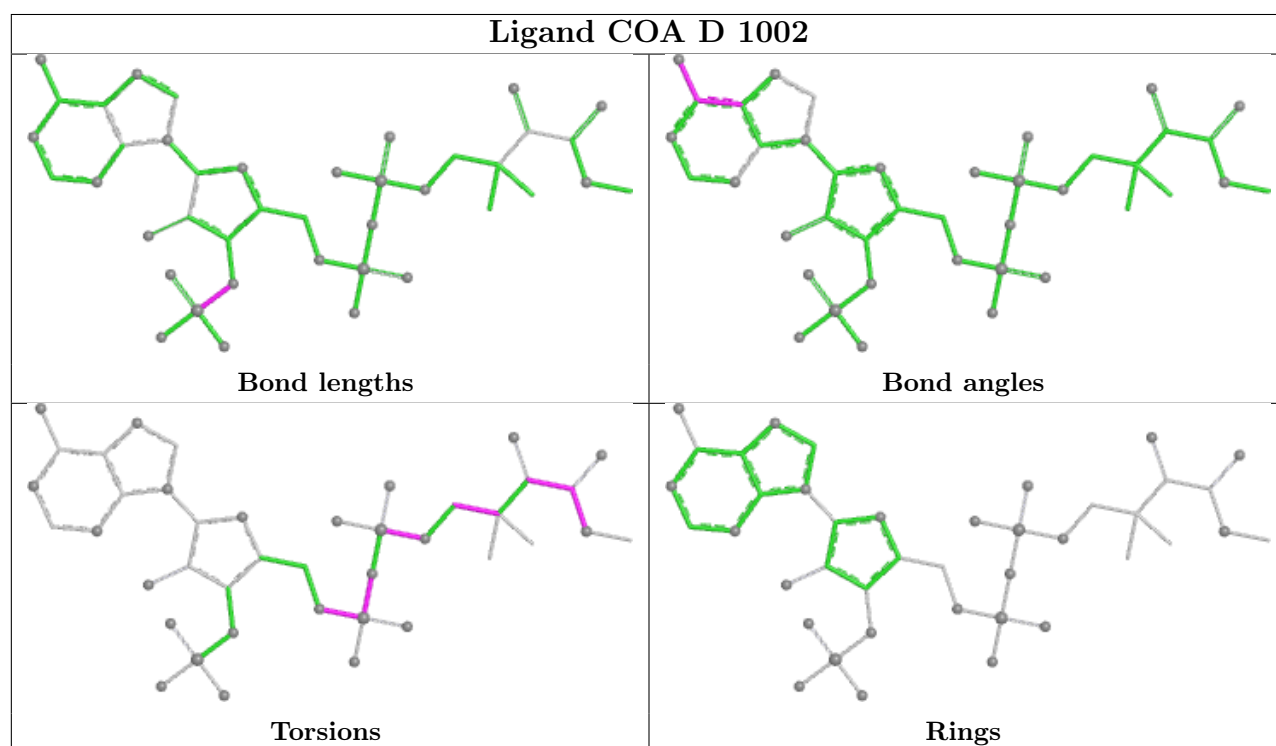
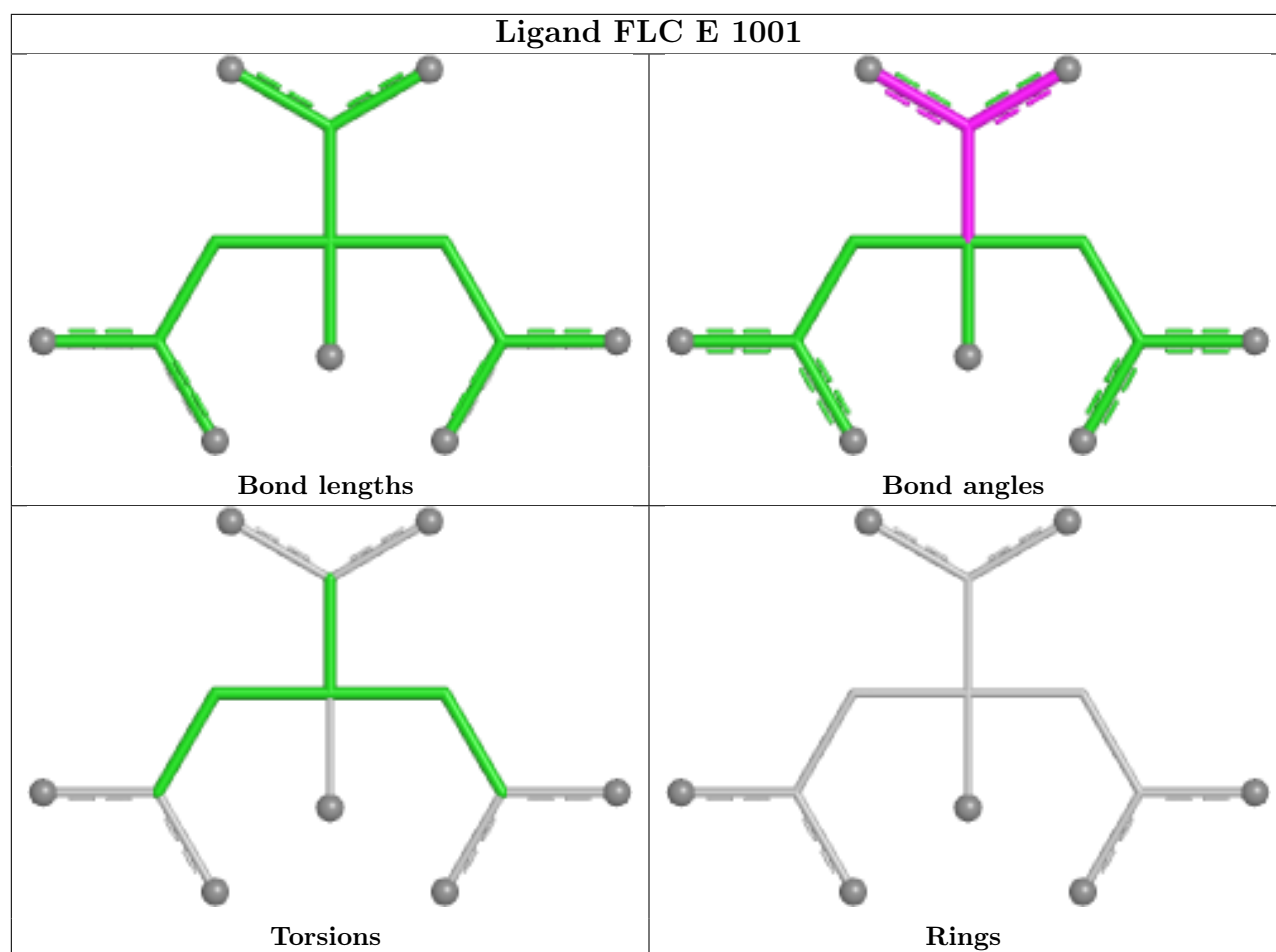


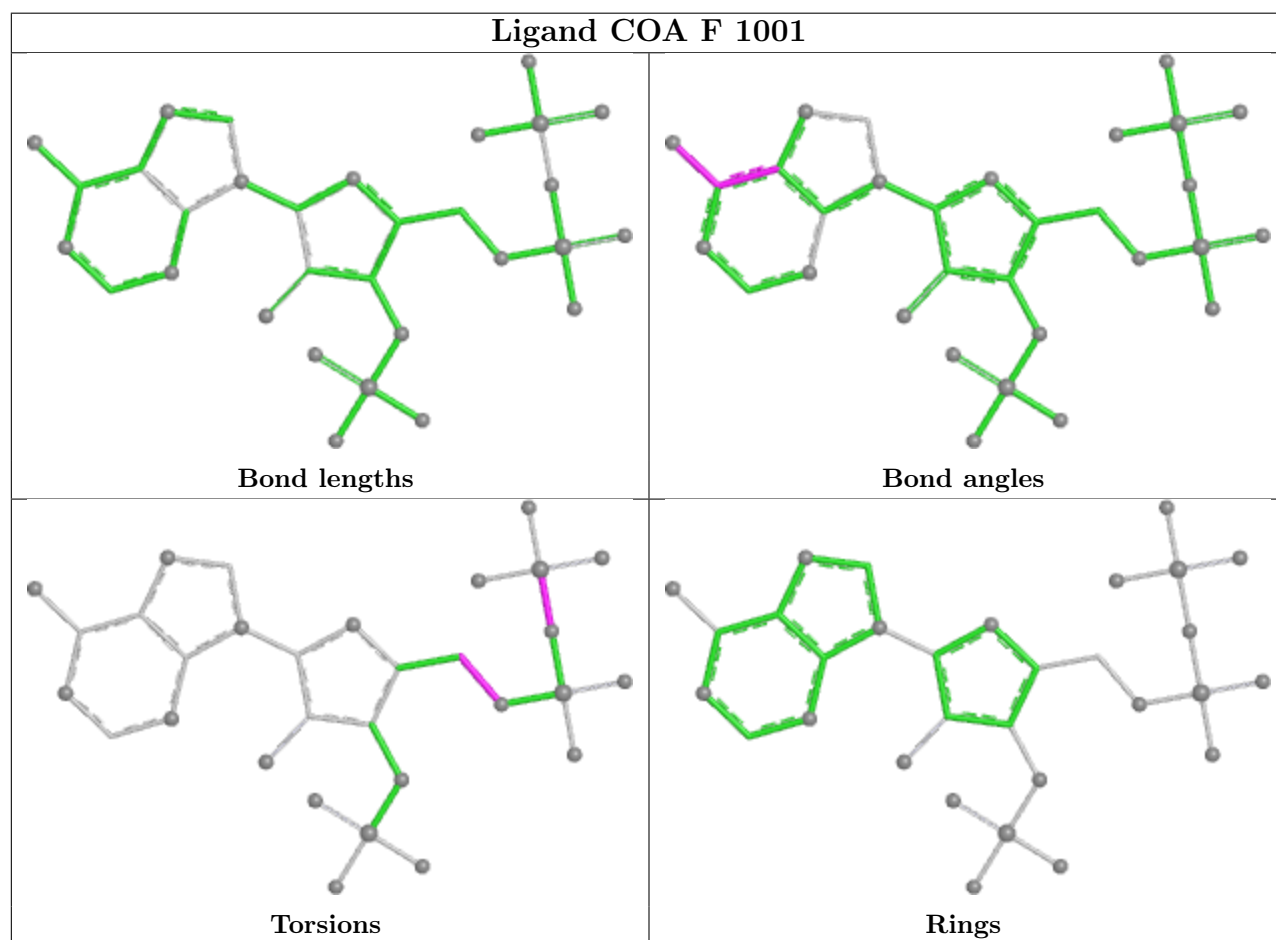
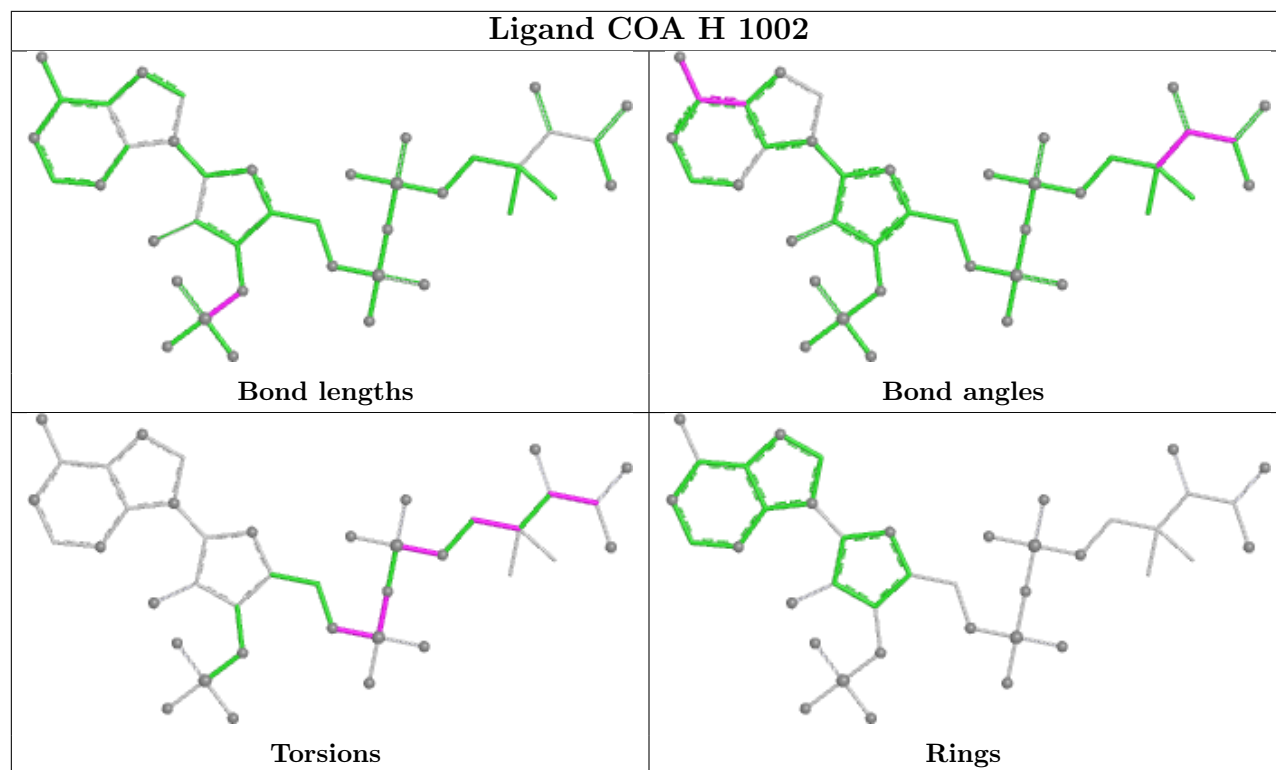


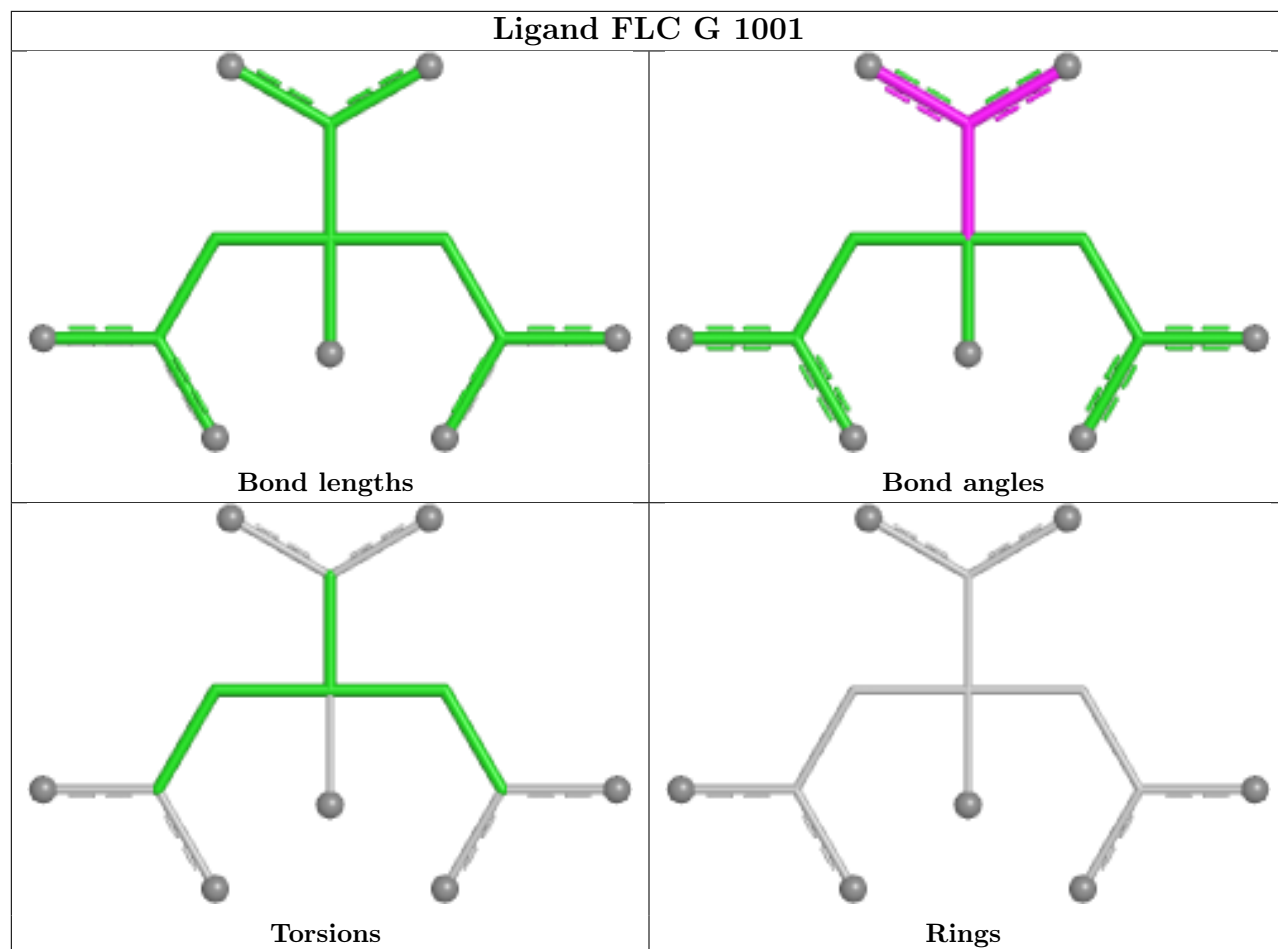


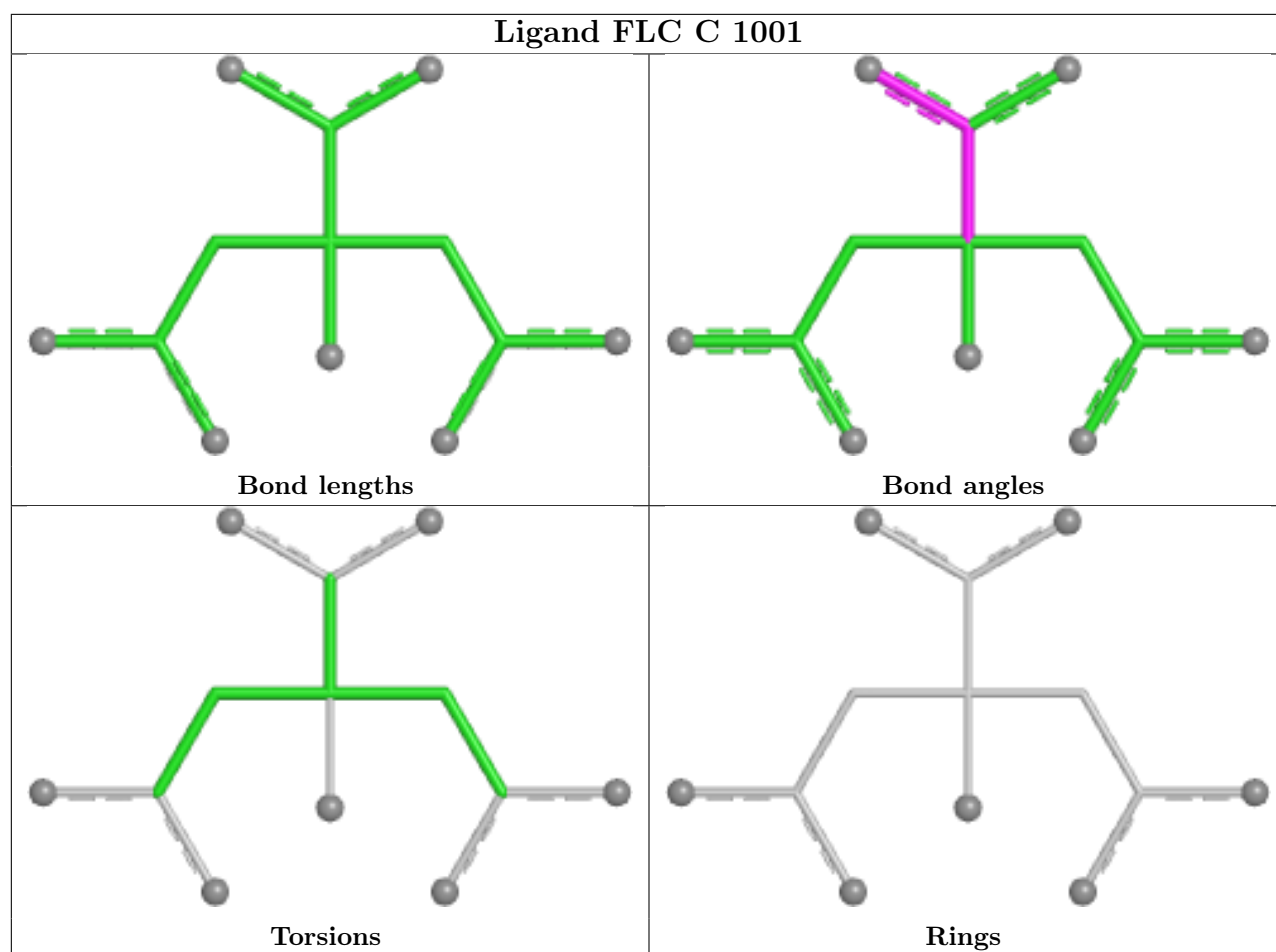


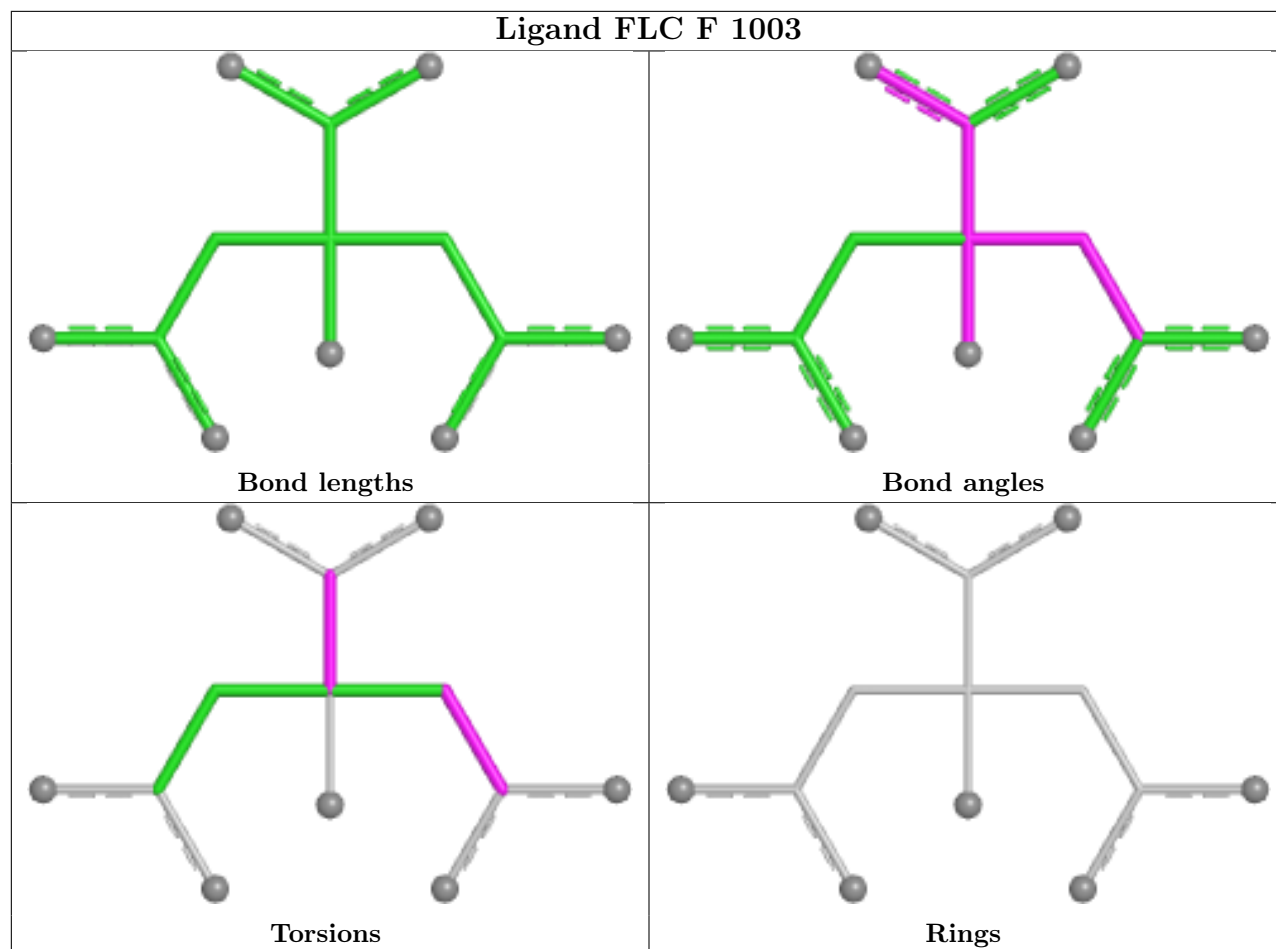












5.7 Other polymers [i](#)

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	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%)	0.82	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	80 (13%) 3 2	41, 77, 147, 212	0
All	All	3661/4060 (90%)	1.18	679 (18%) 1 0	41, 87, 146, 212	0

The worst 5 of 679 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

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

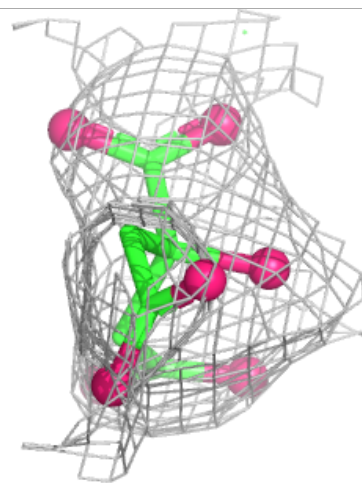
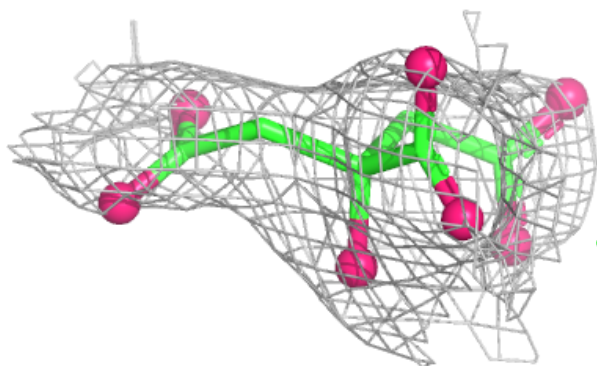
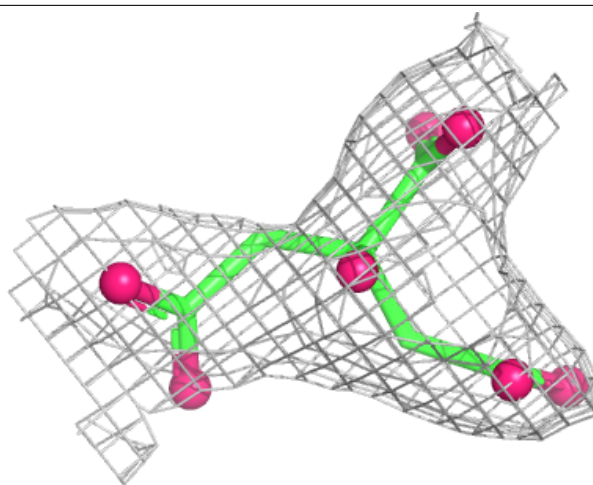
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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	F	1001	31/48	0.88	0.14	92,113,163,165	0
4	COA	D	1001	31/48	0.88	0.16	91,122,166,168	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	A	1001	13/13	0.93	0.20	97,104,108,111	0
3	FLC	G	1001	13/13	0.93	0.21	98,109,121,123	0
3	FLC	H	1003	13/13	0.93	0.21	67,76,89,89	0
4	COA	H	1001	31/48	0.94	0.15	63,86,140,141	0
3	FLC	F	1003	13/13	0.95	0.22	75,78,84,86	0
3	FLC	B	1003	13/13	0.95	0.15	70,75,91,94	0
4	COA	B	1002	48/48	0.95	0.15	74,85,111,114	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.

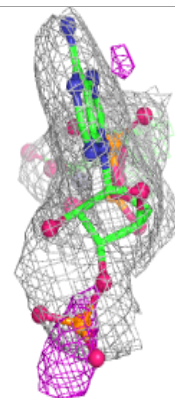
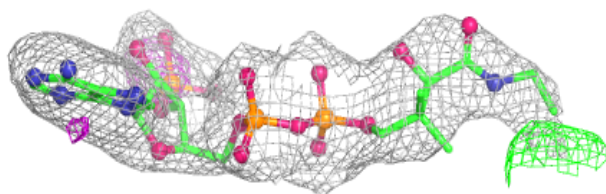
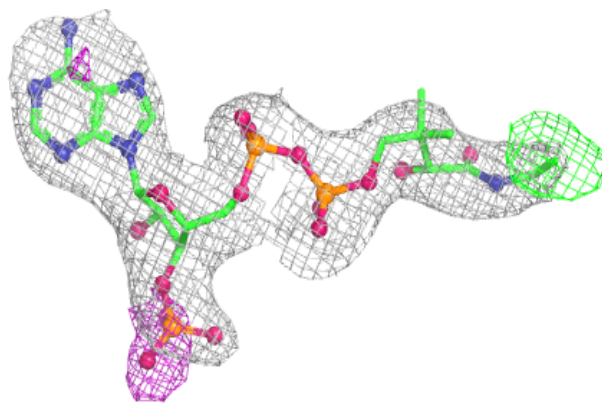
Electron density around FLC E 1001:

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

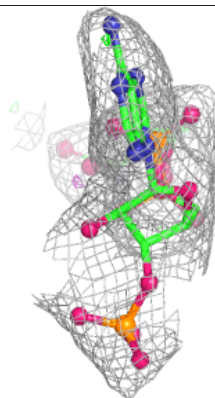
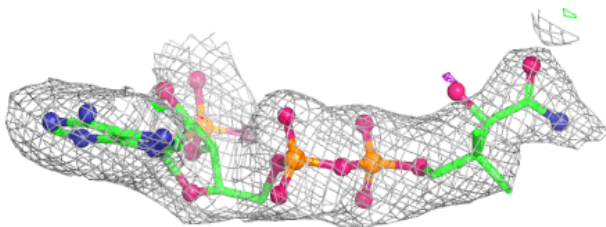
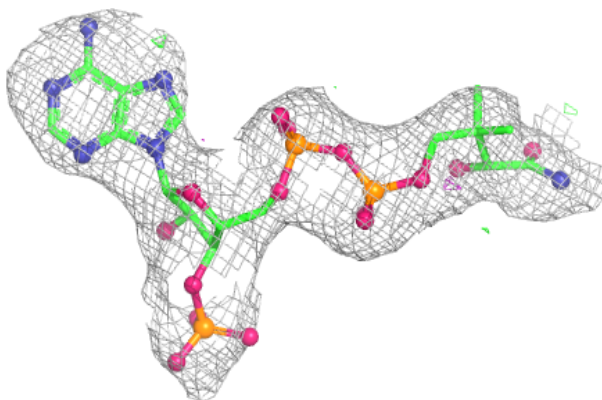


Electron density around COA F 1002:

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

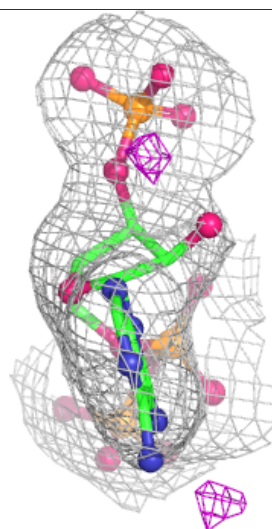
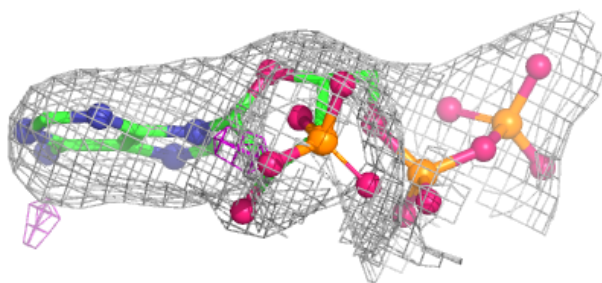
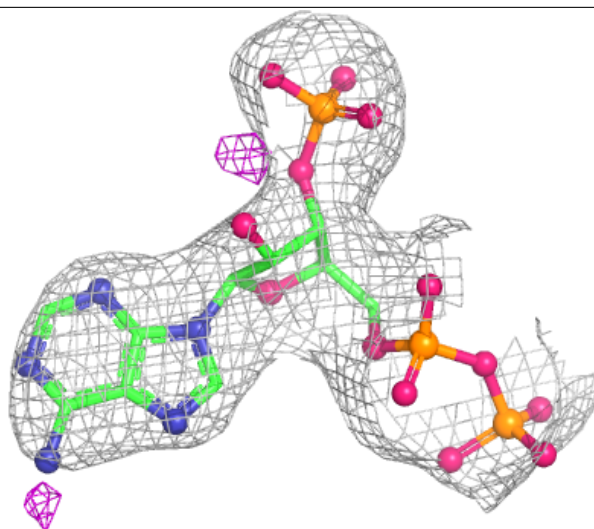
**Electron density around COA H 1002:**

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



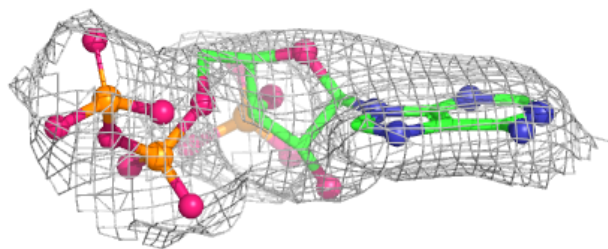
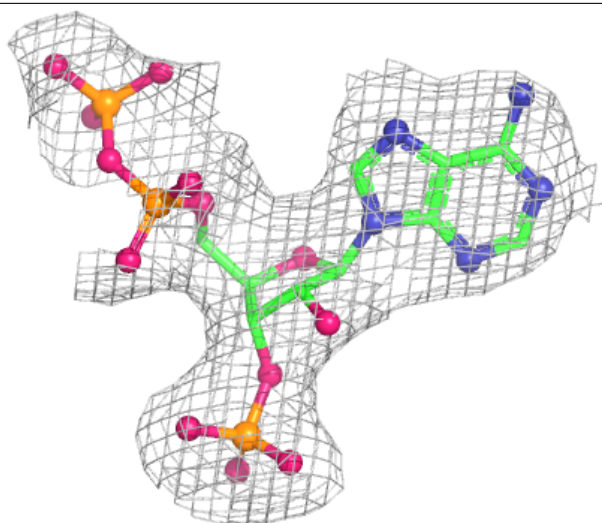
Electron density around COA F 1001:

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



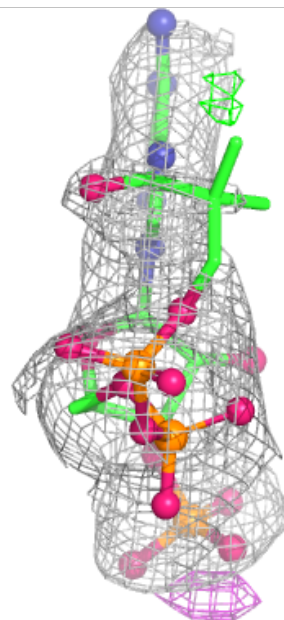
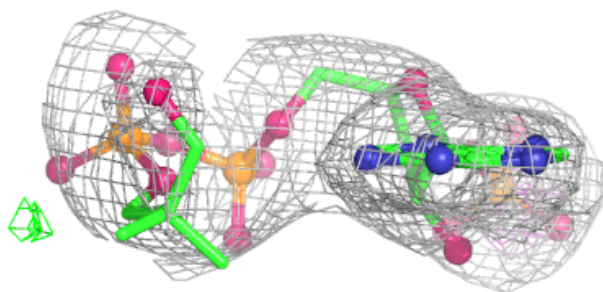
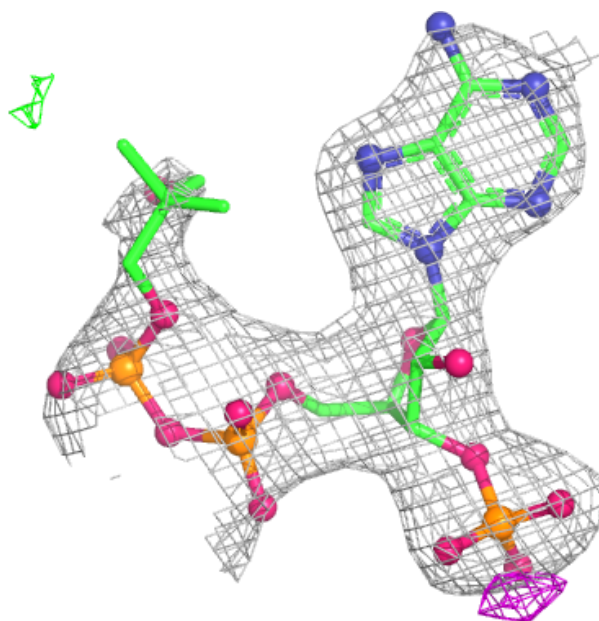
Electron density around COA D 1001:

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



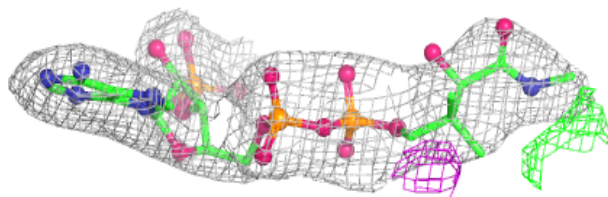
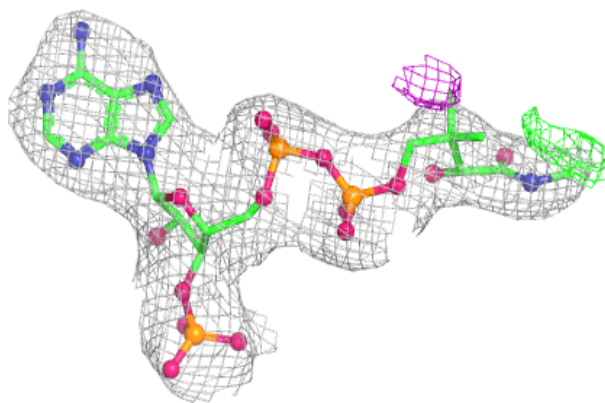
Electron density around COA B 1001:

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



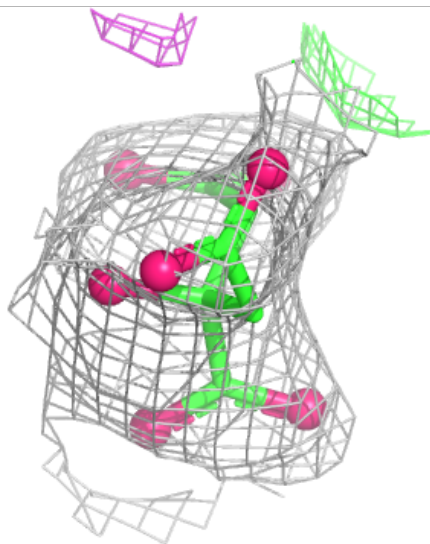
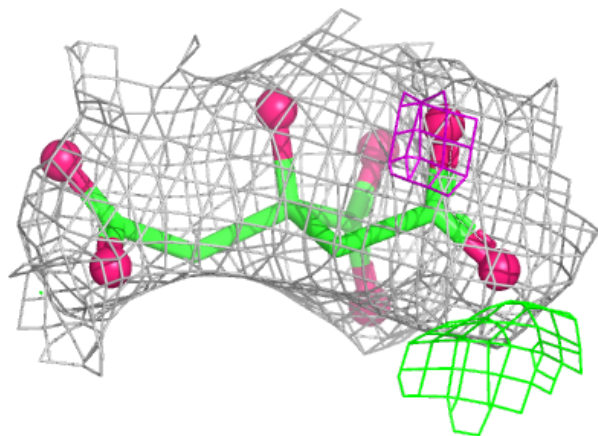
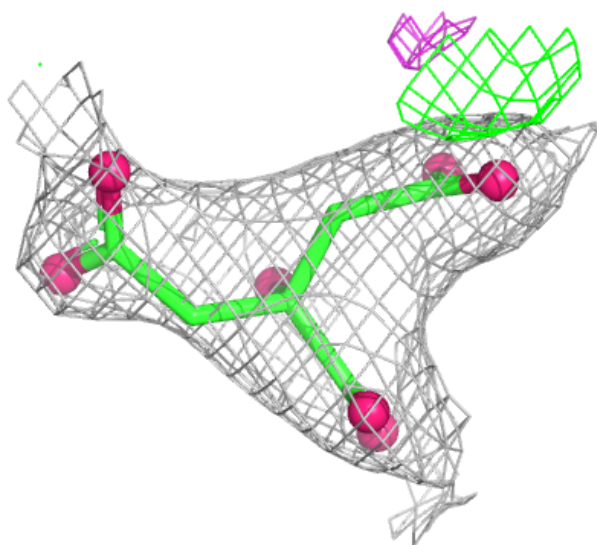
Electron density around COA D 1002:

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



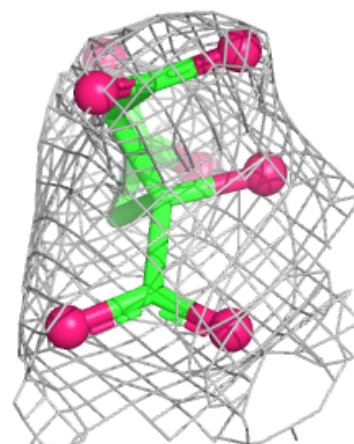
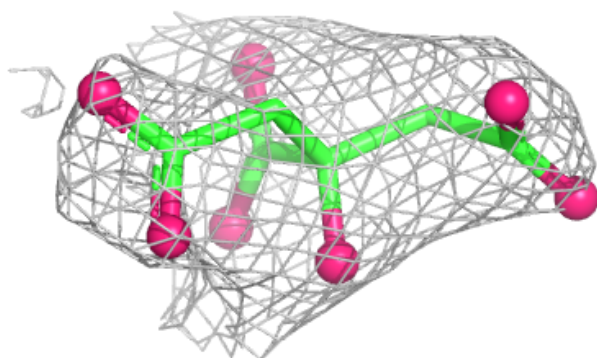
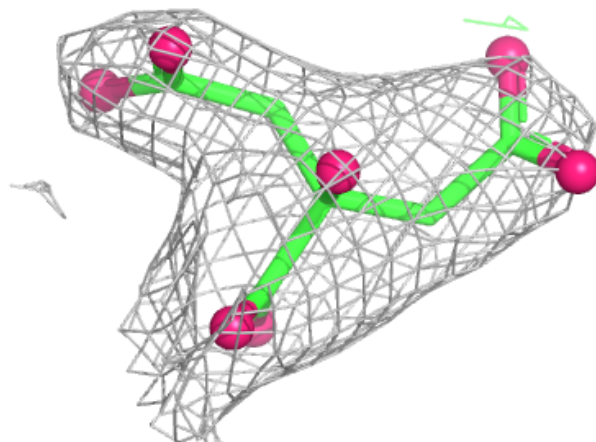
Electron density around FLC C 1001:

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



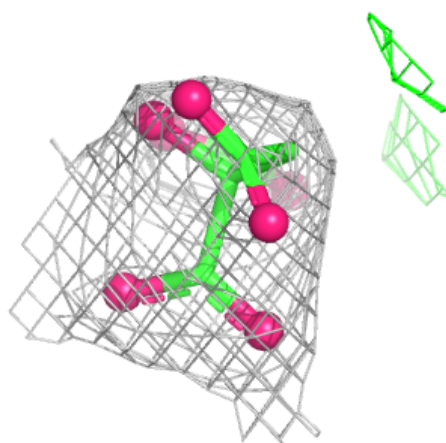
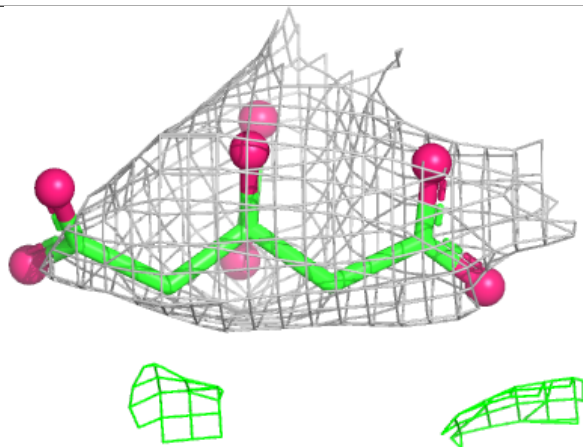
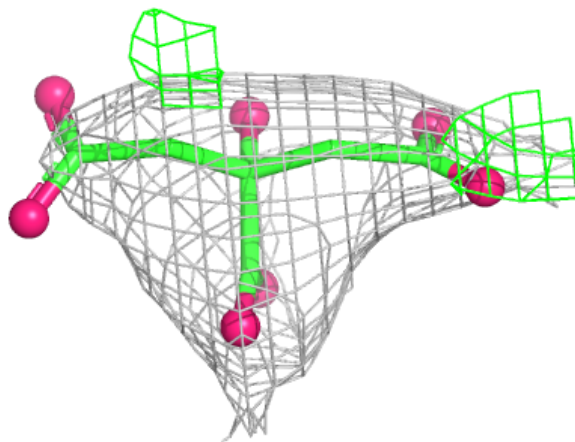
Electron density around FLC A 1001:

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



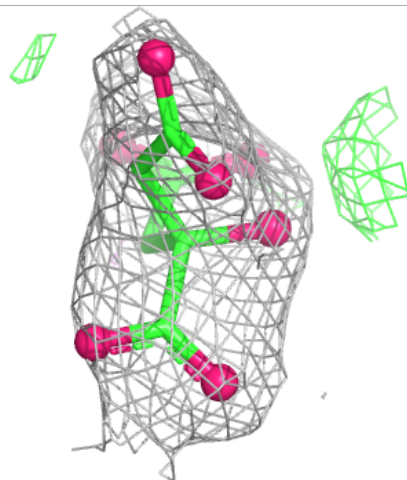
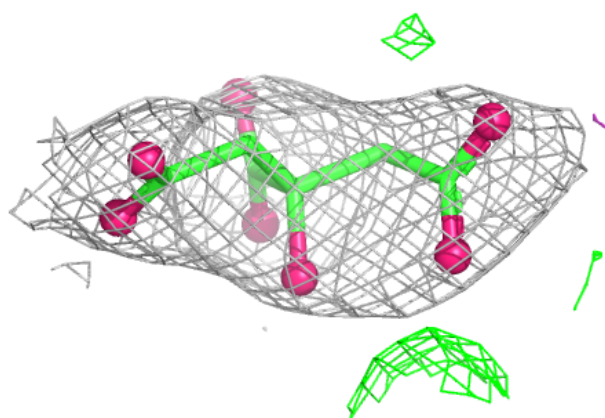
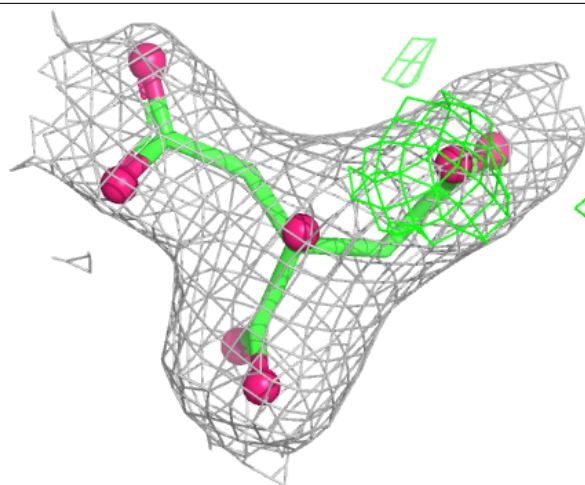
Electron density around FLC G 1001:

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



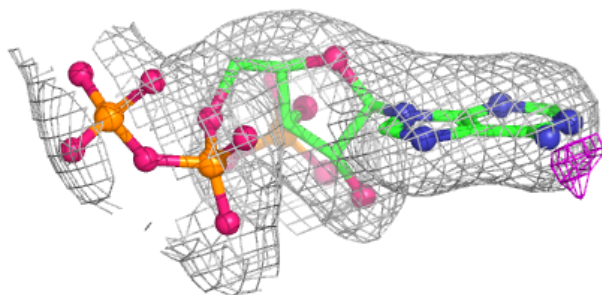
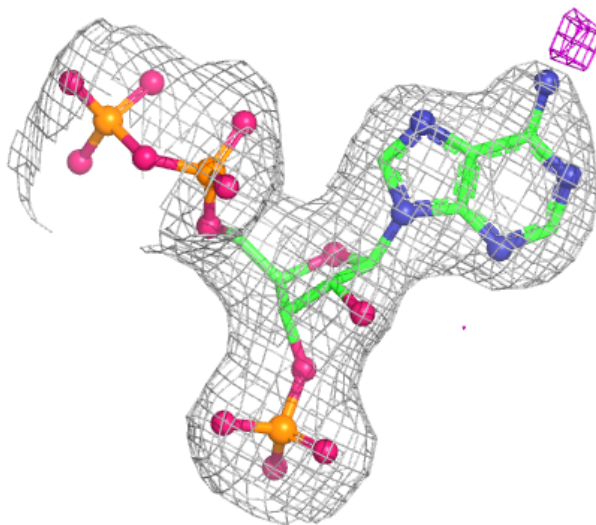
Electron density around FLC H 1003:

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



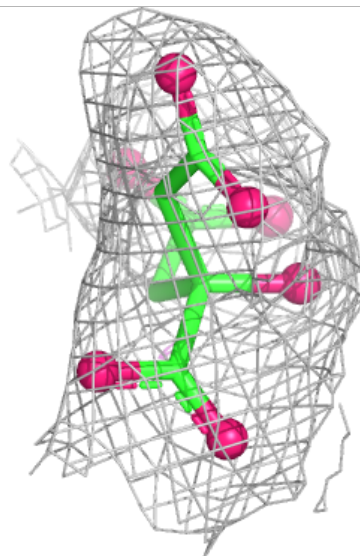
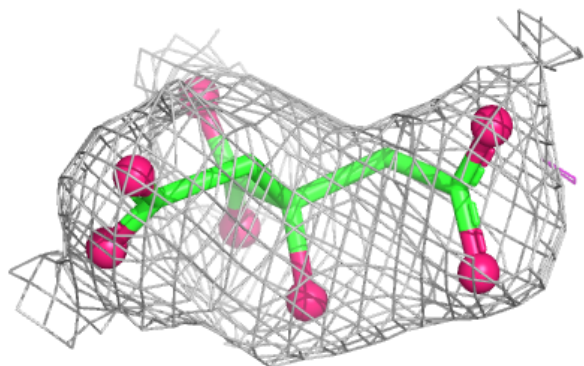
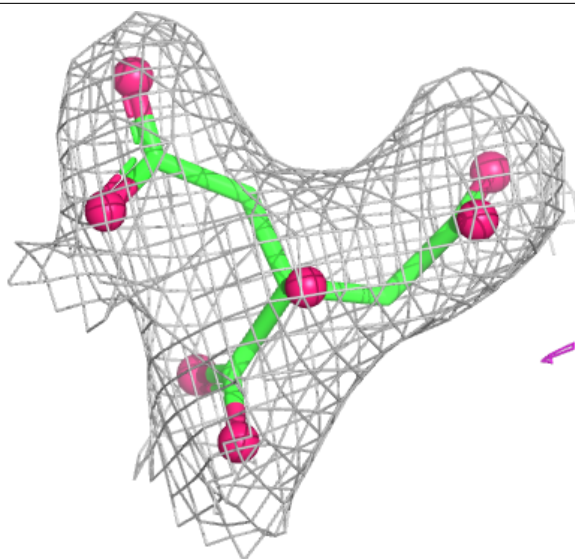
Electron density around COA H 1001:

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



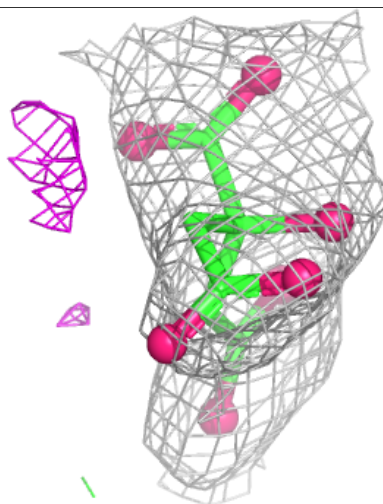
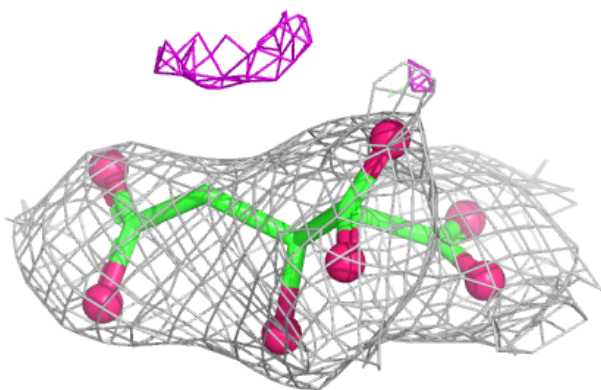
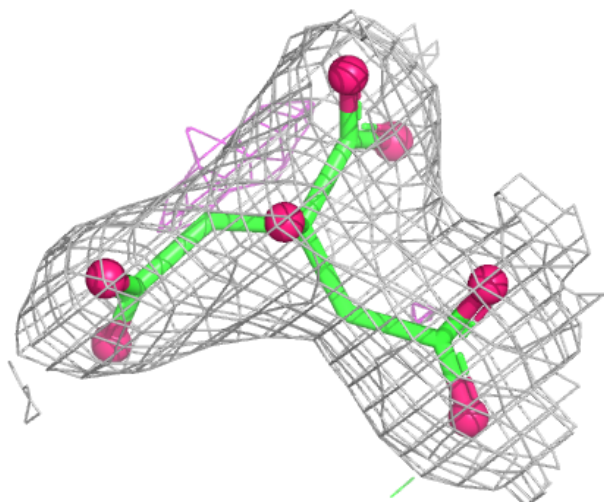
Electron density around FLC F 1003:

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



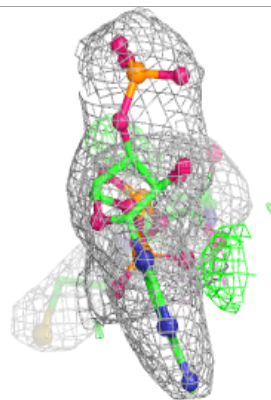
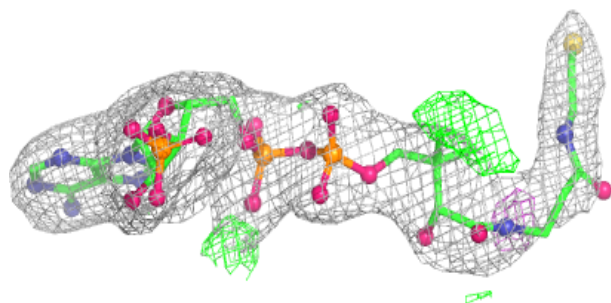
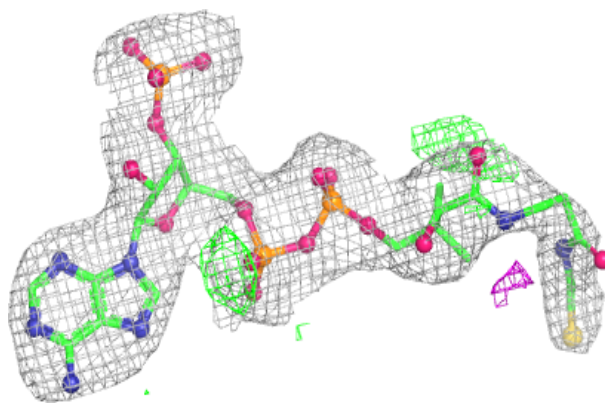
Electron density around FLC B 1003:

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



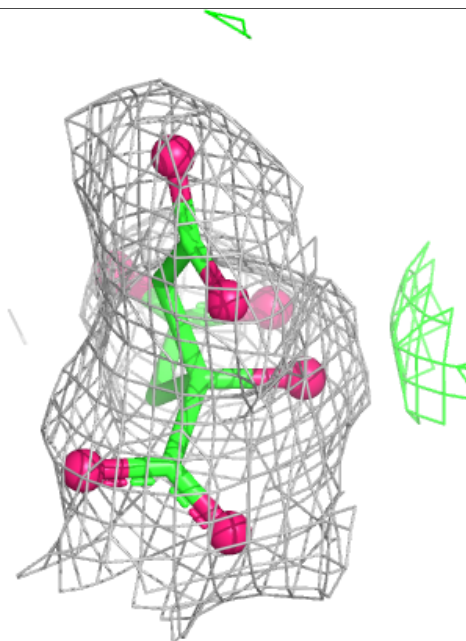
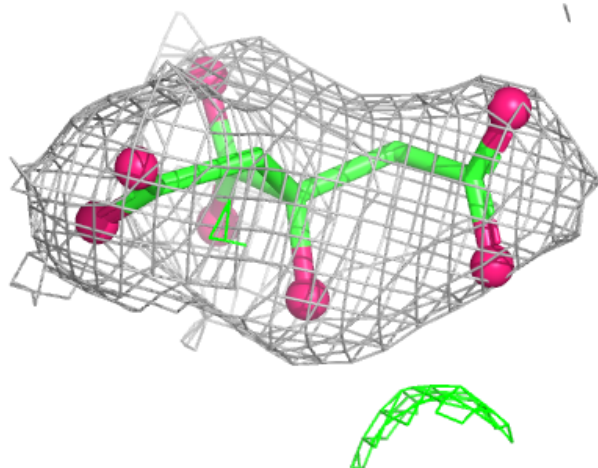
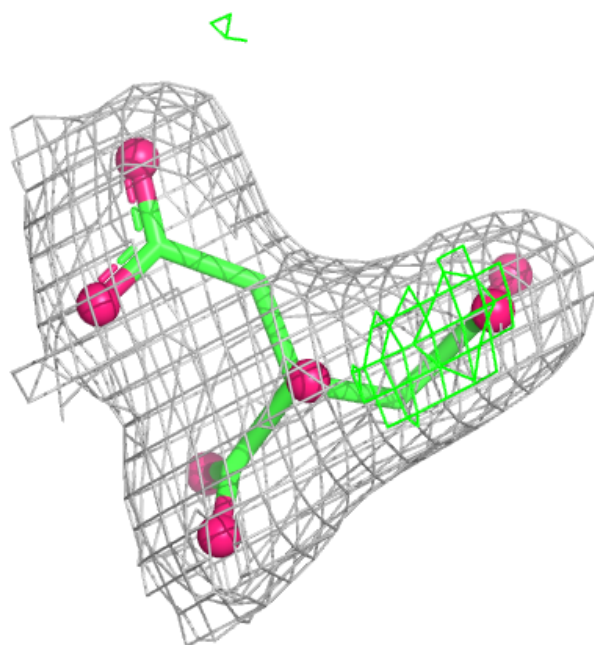
Electron density around COA B 1002:

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



Electron density around FLC 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 [i](#)

There are no such residues in this entry.