



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 03:31 PM EDT

PDB ID : 5B13
Title : Crystal structure of phycoerythrin
Authors : Tanaka, Y.; Gai, Z.; Kishimura, H.
Deposited on : 2015-11-18
Resolution : 2.09 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
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

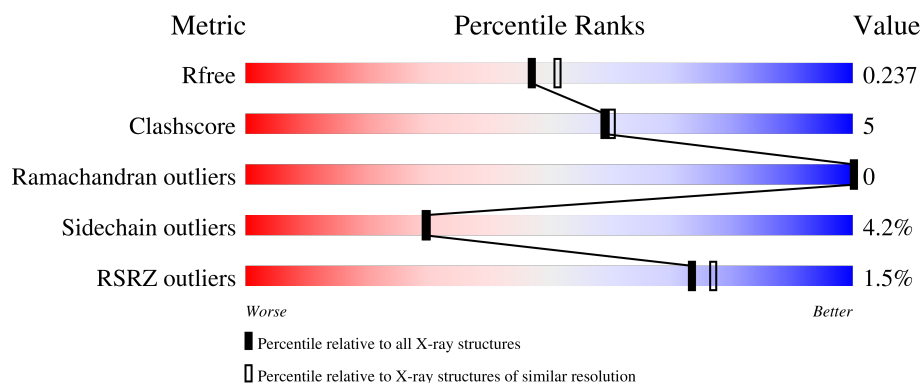
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	164	 91% 8% .
1	B	164	 90% 7% .
1	C	164	 88% 10% .
1	D	164	 88% 10% .
1	E	164	 87% 12% .

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Mol	Chain	Length	Quality of chain
1	F	164	 90%9% .
2	G	177	 2%92%7% .
2	H	177	 3%89%9% .
2	I	177	 %93%7% .
2	J	177	 5%90%10% .
2	K	177	 2%92%8% .
2	L	177	 5%85%14% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18212 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.

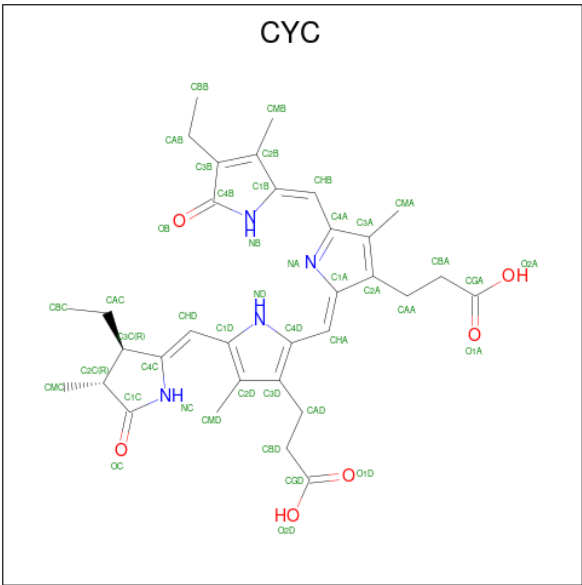
- Molecule 1 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1238	769	217	245	7			
1	B	164	Total	C	N	O	S	0	0	0
			1238	769	217	245	7			
1	C	164	Total	C	N	O	S	0	0	0
			1238	769	217	245	7			
1	D	164	Total	C	N	O	S	0	0	0
			1238	769	217	245	7			
1	E	164	Total	C	N	O	S	0	0	0
			1238	769	217	245	7			
1	F	164	Total	C	N	O	S	0	0	0
			1238	769	217	245	7			

- Molecule 2 is a protein called Phycoerythrin beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	177	Total	C	N	O	S	0	0	0
			1281	789	223	256	13			
2	H	177	Total	C	N	O	S	0	0	0
			1281	789	223	256	13			
2	I	177	Total	C	N	O	S	0	0	0
			1281	789	223	256	13			
2	J	177	Total	C	N	O	S	0	0	0
			1281	789	223	256	13			
2	K	177	Total	C	N	O	S	0	0	0
			1281	789	223	256	13			
2	L	177	Total	C	N	O	S	0	0	0
			1281	789	223	256	13			

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	I	1	Total 43	C 33	N 4	O 6	0	0
3	I	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0

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- The image displays a complex chemical structure, likely a natural product or a synthetic molecule, featuring a central pyrazole core. The structure is composed of several fused and linked rings, including a central pyrazole ring (C4B, C4C, C4D, C4E, C4F, C4G) and a central pyrazole ring (C4B, C4C, C4D, C4E, C4F, C4G). The structure is labeled with atom names (C, N, O) and bond types (single, double, triple). The molecule includes various functional groups, such as carboxylic acid groups (e.g., C4A, C4F, C4G), amide bonds (e.g., C4B, C4C, C4D, C4E, C4F, C4G), and a central pyrazole ring (C4B, C4C, C4D, C4E, C4F, C4G). The structure is highly complex and contains many atoms and bonds, making it difficult to represent with a simple chemical formula. The structure is labeled with atom names (C, N, O) and bond types (single, double, triple). The molecule includes various functional groups, such as carboxylic acid groups (e.g., C4A, C4F, C4G), amide bonds (e.g., C4B, C4C, C4D, C4E, C4F, C4G), and a central pyrazole ring (C4B, C4C, C4D, C4E, C4F, C4G).

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			43	33	4	6		
4	I	1	Total	C	N	O	0	0
			43	33	4	6		
4	J	1	Total	C	N	O	0	0
			43	33	4	6		
4	K	1	Total	C	N	O	0	0
			43	33	4	6		
4	L	1	Total	C	N	O	0	0
			43	33	4	6		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	188	Total	O	0	0
			188	188		
5	G	196	Total	O	0	0
			196	196		
5	B	146	Total	O	0	0
			146	146		
5	C	149	Total	O	0	0
			149	149		
5	D	146	Total	O	0	0
			146	146		
5	E	165	Total	O	0	0
			165	165		
5	F	162	Total	O	0	0
			162	162		
5	H	155	Total	O	0	0
			155	155		
5	I	127	Total	O	0	0
			127	127		
5	J	121	Total	O	0	0
			121	121		
5	K	131	Total	O	0	0
			131	131		
5	L	122	Total	O	0	0
			122	122		

3 Residue-property plots [i](#)


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

- Molecule 1: Phycoerythrin alpha subunit

Chain A:  91% 8% .




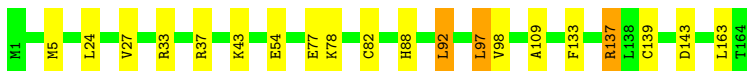
- Molecule 1: Phycoerythrin alpha subunit

Chain B:  90% 7% .




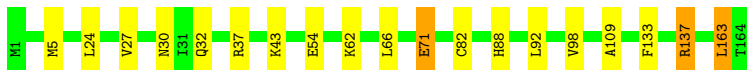
- Molecule 1: Phycoerythrin alpha subunit

Chain C:  88% 10% .




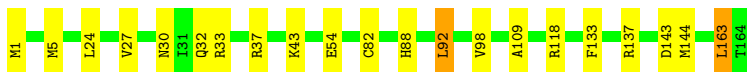
- Molecule 1: Phycoerythrin alpha subunit

Chain D:  88% 10% .




- Molecule 1: Phycoerythrin alpha subunit

Chain E:  87% 12% .

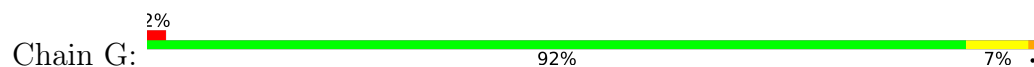


- Molecule 1: Phycoerythrin alpha subunit

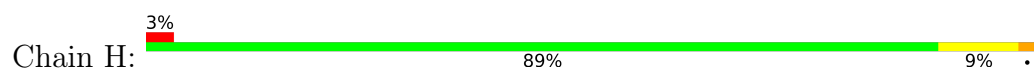
Chain F:  90% 9% .



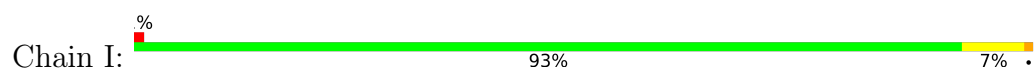
- Molecule 2: Phycoerythrin beta subunit



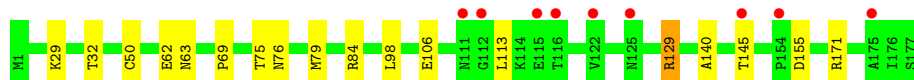
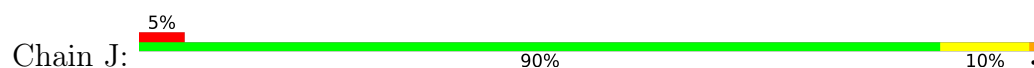
- Molecule 2: Phycoerythrin beta subunit



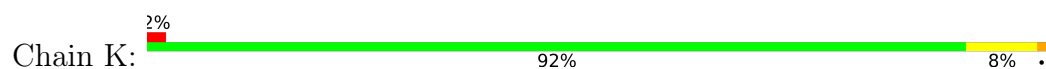
- Molecule 2: Phycoerythrin beta subunit



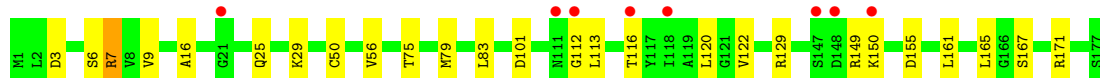
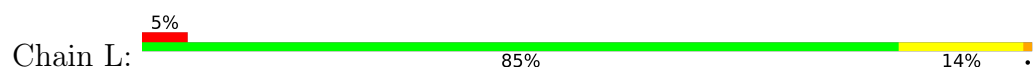
- Molecule 2: Phycoerythrin beta subunit



- Molecule 2: Phycoerythrin beta subunit



- Molecule 2: Phycoerythrin beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.50Å 111.85Å 112.67Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	48.93 – 2.09 48.93 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.93-2.09) 99.5 (48.93-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.236 0.199 , 0.237	Depositor DCC
R_{free} test set	6792 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.007 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.015 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.014 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18212	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: PUB, CYC

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	0.22	0/1259	0.36	0/1704
1	B	0.22	0/1259	0.36	0/1704
1	C	0.23	0/1259	0.38	0/1704
1	D	0.22	0/1259	0.35	0/1704
1	E	0.22	0/1259	0.36	0/1704
1	F	0.22	0/1259	0.37	0/1704
2	G	0.22	0/1295	0.36	0/1750
2	H	0.20	0/1295	0.36	0/1750
2	I	0.22	0/1295	0.36	0/1750
2	J	0.20	0/1295	0.35	0/1750
2	K	0.20	0/1295	0.36	0/1750
2	L	0.22	0/1295	0.36	0/1750
All	All	0.22	0/15324	0.36	0/20724

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1238	0	1204	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1238	0	1204	12	0
1	C	1238	0	1204	15	0
1	D	1238	0	1204	15	0
1	E	1238	0	1204	18	0
1	F	1238	0	1204	13	0
2	G	1281	0	1280	8	0
2	H	1281	0	1280	9	0
2	I	1281	0	1280	7	0
2	J	1281	0	1280	12	0
2	K	1281	0	1280	9	0
2	L	1281	0	1280	13	0
3	A	86	0	74	6	0
3	B	86	0	74	5	0
3	C	86	0	74	9	0
3	D	86	0	74	7	0
3	E	86	0	74	6	0
3	F	86	0	74	4	0
3	G	86	0	74	5	0
3	H	86	0	74	5	0
3	I	86	0	74	4	0
3	J	86	0	73	4	0
3	K	86	0	74	5	0
3	L	86	0	74	6	0
4	G	43	0	38	1	0
4	H	43	0	38	0	0
4	I	43	0	38	1	0
4	J	43	0	38	1	0
4	K	43	0	38	1	0
4	L	43	0	38	1	0
5	A	188	0	0	2	0
5	B	146	0	0	1	0
5	C	149	0	0	1	0
5	D	146	0	0	1	0
5	E	165	0	0	3	0
5	F	162	0	0	2	0
5	G	196	0	0	3	0
5	H	155	0	0	0	0
5	I	127	0	0	3	0
5	J	121	0	0	3	0
5	K	131	0	0	3	0
5	L	122	0	0	3	0
All	All	18212	0	16019	153	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 5.

The worst 5 of 153 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:THR:O	1:E:118:ARG:NH1	2.06	0.89
3:G:202:CYC:HBA1	3:G:202:CYC:HHA	1.65	0.79
1:B:32:GLN:HG3	1:D:32:GLN:HG3	1.67	0.77
1:E:32:GLN:HG3	1:F:32:GLN:HG3	1.68	0.75
3:K:202:CYC:HHA	3:K:202:CYC:HBA1	1.77	0.66

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	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	B	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	C	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	D	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	E	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	F	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
2	G	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
2	H	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
2	I	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
2	J	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	K	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	L	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
All	All	2022/2046 (99%)	1974 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	126/126 (100%)	122 (97%)	4 (3%)	39	41
1	B	126/126 (100%)	120 (95%)	6 (5%)	25	24
1	C	126/126 (100%)	120 (95%)	6 (5%)	25	24
1	D	126/126 (100%)	123 (98%)	3 (2%)	49	53
1	E	126/126 (100%)	123 (98%)	3 (2%)	49	53
1	F	126/126 (100%)	124 (98%)	2 (2%)	62	69
2	G	138/138 (100%)	132 (96%)	6 (4%)	29	29
2	H	138/138 (100%)	127 (92%)	11 (8%)	12	8
2	I	138/138 (100%)	132 (96%)	6 (4%)	29	29
2	J	138/138 (100%)	135 (98%)	3 (2%)	52	57
2	K	138/138 (100%)	132 (96%)	6 (4%)	29	29
2	L	138/138 (100%)	128 (93%)	10 (7%)	14	11
All	All	1584/1584 (100%)	1518 (96%)	66 (4%)	30	30

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	50	CYS
2	L	122	VAL
2	L	165	LEU
1	D	163	LEU
1	D	137	ARG

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

30 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	$\# Z > 2$
3	CYC	J	201	2	42,46,46	4.03	18 (42%)	50,67,67	2.10	9 (18%)
4	PUB	K	203	-	42,46,46	4.05	16 (38%)	37,67,67	2.18	10 (27%)
4	PUB	H	203	-	42,46,46	4.37	18 (42%)	37,67,67	2.58	11 (29%)
3	CYC	A	201	1	42,46,46	4.00	18 (42%)	50,67,67	2.12	9 (18%)
3	CYC	D	202	1	42,46,46	4.01	17 (40%)	50,67,67	2.12	9 (18%)
3	CYC	K	201	2	42,46,46	4.01	18 (42%)	50,67,67	2.14	10 (20%)
4	PUB	L	203	-	42,46,46	4.32	18 (42%)	37,67,67	2.49	10 (27%)
3	CYC	I	202	2	42,46,46	4.00	20 (47%)	50,67,67	1.99	12 (24%)
3	CYC	B	201	1	42,46,46	4.03	17 (40%)	50,67,67	1.85	6 (12%)
4	PUB	G	203	-	42,46,46	4.43	18 (42%)	37,67,67	2.56	9 (24%)
3	CYC	H	201	2	42,46,46	4.02	18 (42%)	50,67,67	2.15	8 (16%)
4	PUB	I	203	-	42,46,46	4.32	19 (45%)	37,67,67	2.27	9 (24%)
3	CYC	F	201	1	42,46,46	4.01	18 (42%)	50,67,67	2.15	8 (16%)
3	CYC	J	202	2	42,46,46	3.98	20 (47%)	50,67,67	1.92	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYC	L	202	2	42,46,46	4.04	19 (45%)	50,67,67	1.92	13 (26%)
3	CYC	A	202	1	42,46,46	3.99	19 (45%)	50,67,67	2.10	9 (18%)
3	CYC	F	202	1	42,46,46	3.99	18 (42%)	50,67,67	2.09	10 (20%)
3	CYC	I	201	2	42,46,46	4.02	19 (45%)	50,67,67	2.12	8 (16%)
3	CYC	C	201	1	42,46,46	4.01	20 (47%)	50,67,67	2.12	6 (12%)
3	CYC	K	202	2	42,46,46	4.05	19 (45%)	50,67,67	1.96	13 (26%)
3	CYC	E	201	1	42,46,46	4.04	17 (40%)	50,67,67	1.97	6 (12%)
3	CYC	B	202	1	42,46,46	3.98	18 (42%)	50,67,67	2.14	9 (18%)
3	CYC	D	201	1	42,46,46	4.02	18 (42%)	50,67,67	2.06	8 (16%)
3	CYC	H	202	2	42,46,46	4.00	19 (45%)	50,67,67	1.81	10 (20%)
3	CYC	C	202	1	42,46,46	3.99	18 (42%)	50,67,67	2.20	9 (18%)
3	CYC	E	202	1	42,46,46	3.99	17 (40%)	50,67,67	2.16	8 (16%)
3	CYC	L	201	2	42,46,46	4.00	18 (42%)	50,67,67	2.16	7 (14%)
4	PUB	J	203	-	42,46,46	4.05	16 (38%)	37,67,67	2.13	9 (24%)
3	CYC	G	201	2	42,46,46	4.01	20 (47%)	50,67,67	2.13	10 (20%)
3	CYC	G	202	2	42,46,46	4.03	20 (47%)	50,67,67	2.01	14 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	J	201	2	-	8/25/74/74	0/4/4/4
4	PUB	K	203	-	-	7/24/74/74	0/4/4/4
4	PUB	H	203	-	-	7/24/74/74	0/4/4/4
3	CYC	A	201	1	-	7/25/74/74	0/4/4/4
3	CYC	D	202	1	-	11/25/74/74	0/4/4/4
3	CYC	K	201	2	-	7/25/74/74	0/4/4/4
4	PUB	L	203	-	-	7/24/74/74	0/4/4/4
3	CYC	I	202	2	-	9/25/74/74	0/4/4/4
3	CYC	B	201	1	-	9/25/74/74	0/4/4/4
4	PUB	G	203	-	-	6/24/74/74	0/4/4/4
3	CYC	H	201	2	-	7/25/74/74	0/4/4/4
4	PUB	I	203	-	-	8/24/74/74	0/4/4/4
3	CYC	F	201	1	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	J	202	2	-	14/25/74/74	0/4/4/4
3	CYC	L	202	2	-	13/25/74/74	0/4/4/4
3	CYC	A	202	1	-	9/25/74/74	0/4/4/4
3	CYC	F	202	1	-	9/25/74/74	0/4/4/4
3	CYC	I	201	2	-	7/25/74/74	0/4/4/4
3	CYC	C	201	1	-	10/25/74/74	0/4/4/4
3	CYC	K	202	2	-	9/25/74/74	0/4/4/4
3	CYC	E	201	1	-	6/25/74/74	0/4/4/4
3	CYC	B	202	1	-	9/25/74/74	0/4/4/4
3	CYC	D	201	1	-	8/25/74/74	0/4/4/4
3	CYC	H	202	2	-	7/25/74/74	0/4/4/4
3	CYC	C	202	1	-	9/25/74/74	0/4/4/4
3	CYC	E	202	1	-	7/25/74/74	0/4/4/4
3	CYC	L	201	2	-	7/25/74/74	0/4/4/4
4	PUB	J	203	-	-	6/24/74/74	0/4/4/4
3	CYC	G	201	2	-	8/25/74/74	0/4/4/4
3	CYC	G	202	2	-	11/25/74/74	0/4/4/4

The worst 5 of 548 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	203	PUB	C1A-NA	15.51	1.56	1.35
4	H	203	PUB	C4D-ND	14.48	1.55	1.35
4	G	203	PUB	C4D-ND	14.25	1.54	1.35
4	I	203	PUB	C4D-ND	14.17	1.54	1.35
4	I	203	PUB	C1A-NA	13.97	1.54	1.35

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	CYC	C4D-CHA-C1A	-11.36	115.23	128.81
3	A	201	CYC	C4D-CHA-C1A	-11.32	115.29	128.81
3	F	201	CYC	C4D-CHA-C1A	-11.30	115.31	128.81
3	C	202	CYC	C4D-CHA-C1A	-11.15	115.49	128.81
4	G	203	PUB	CAD-C3D-C4D	10.84	138.50	121.38

There are no chirality outliers.

5 of 250 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	CYC	NA-C4A-CHB-C1B
3	A	201	CYC	C3A-C4A-CHB-C1B
3	A	202	CYC	NA-C4A-CHB-C1B
3	A	202	CYC	C3A-C4A-CHB-C1B
3	A	202	CYC	NC-C4C-CHD-C1D

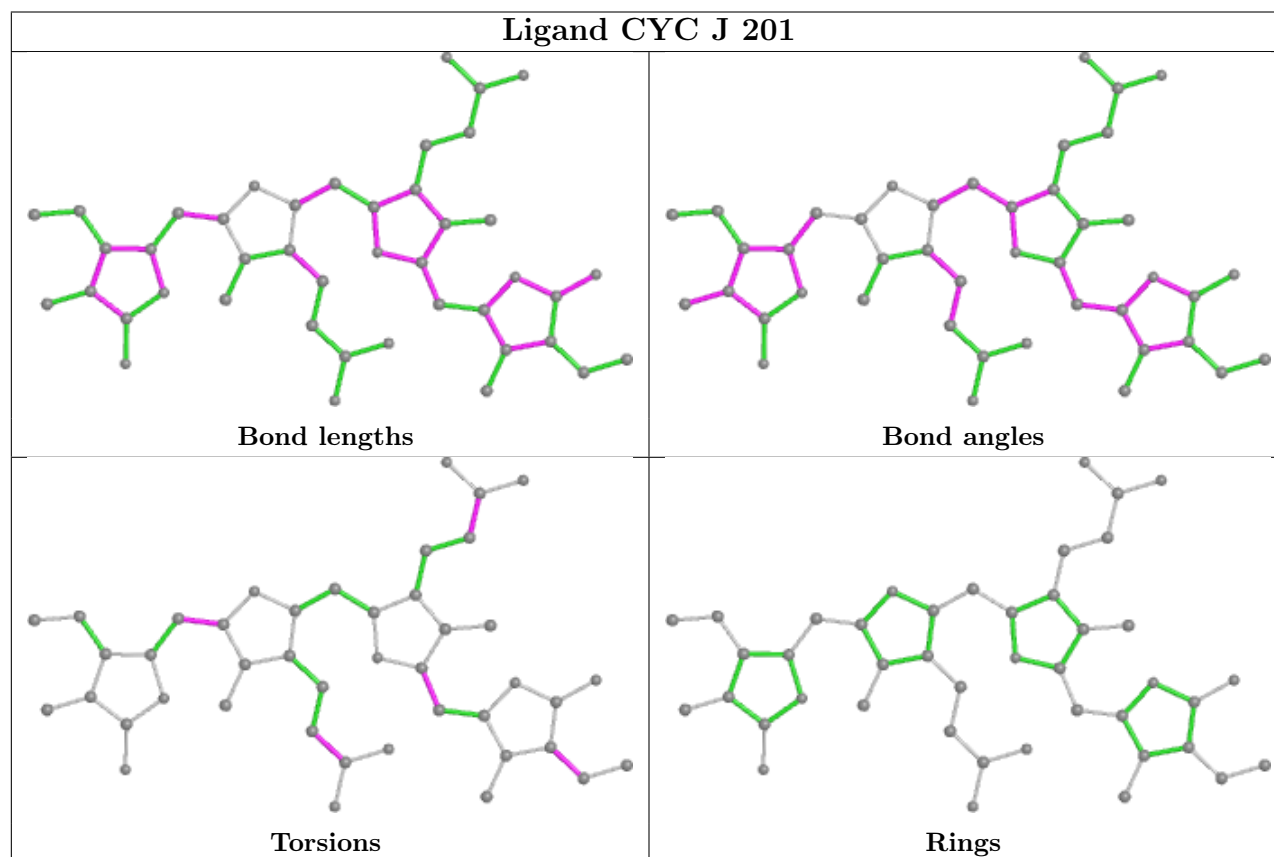
There are no ring outliers.

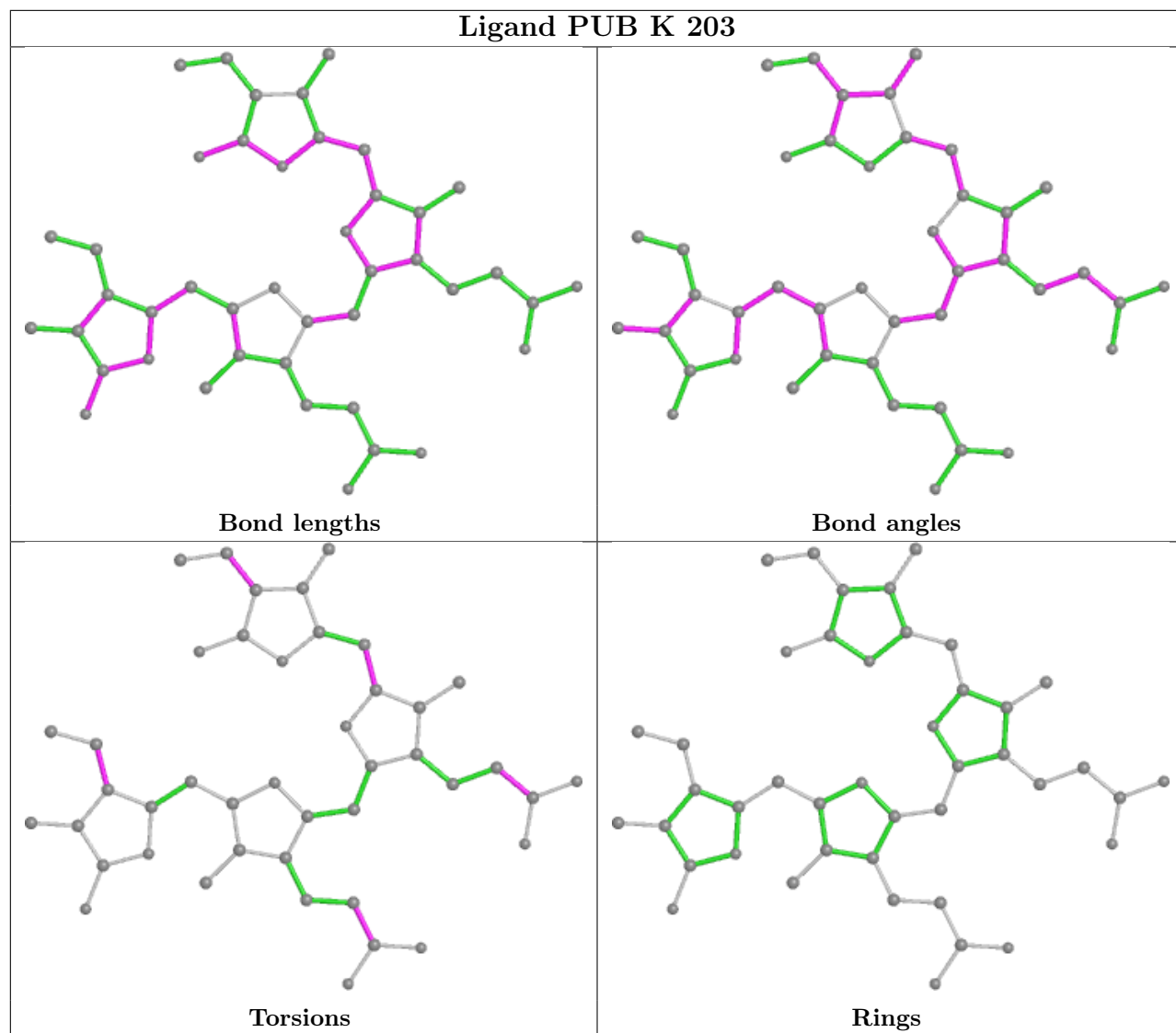
28 monomers are involved in 71 short contacts:

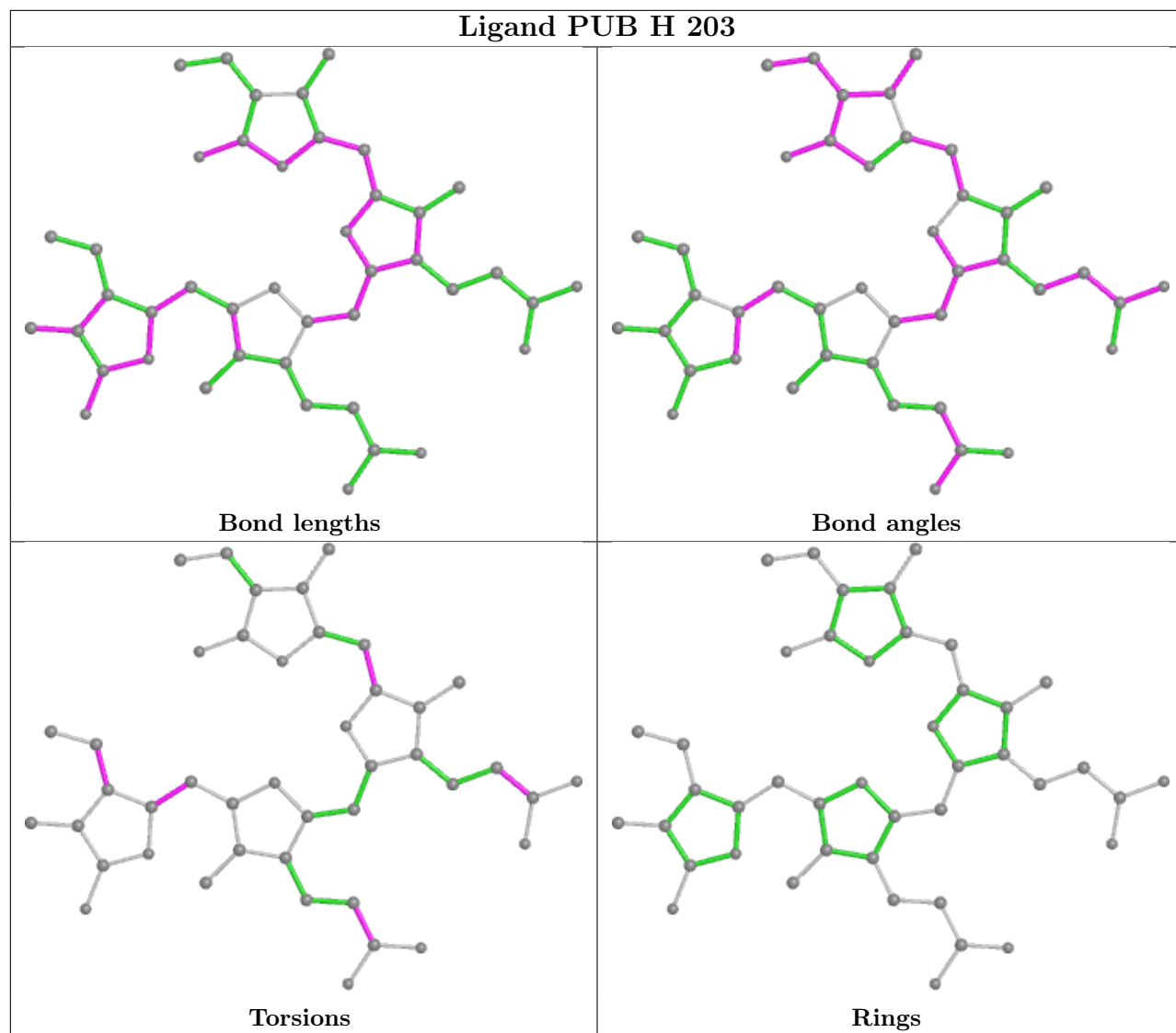
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	201	CYC	3	0
4	K	203	PUB	1	0
3	A	201	CYC	2	0
3	D	202	CYC	5	0
3	K	201	CYC	2	0
4	L	203	PUB	1	0
3	I	202	CYC	2	0
4	G	203	PUB	1	0
3	H	201	CYC	3	0
4	I	203	PUB	1	0
3	F	201	CYC	2	0
3	J	202	CYC	1	0
3	L	202	CYC	3	0
3	A	202	CYC	4	0
3	F	202	CYC	2	0
3	I	201	CYC	2	0
3	C	201	CYC	3	0
3	K	202	CYC	3	0
3	E	201	CYC	1	0
3	B	202	CYC	5	0
3	D	201	CYC	2	0
3	H	202	CYC	2	0
3	C	202	CYC	6	0
3	E	202	CYC	5	0
3	L	201	CYC	3	0
4	J	203	PUB	1	0
3	G	201	CYC	2	0
3	G	202	CYC	3	0

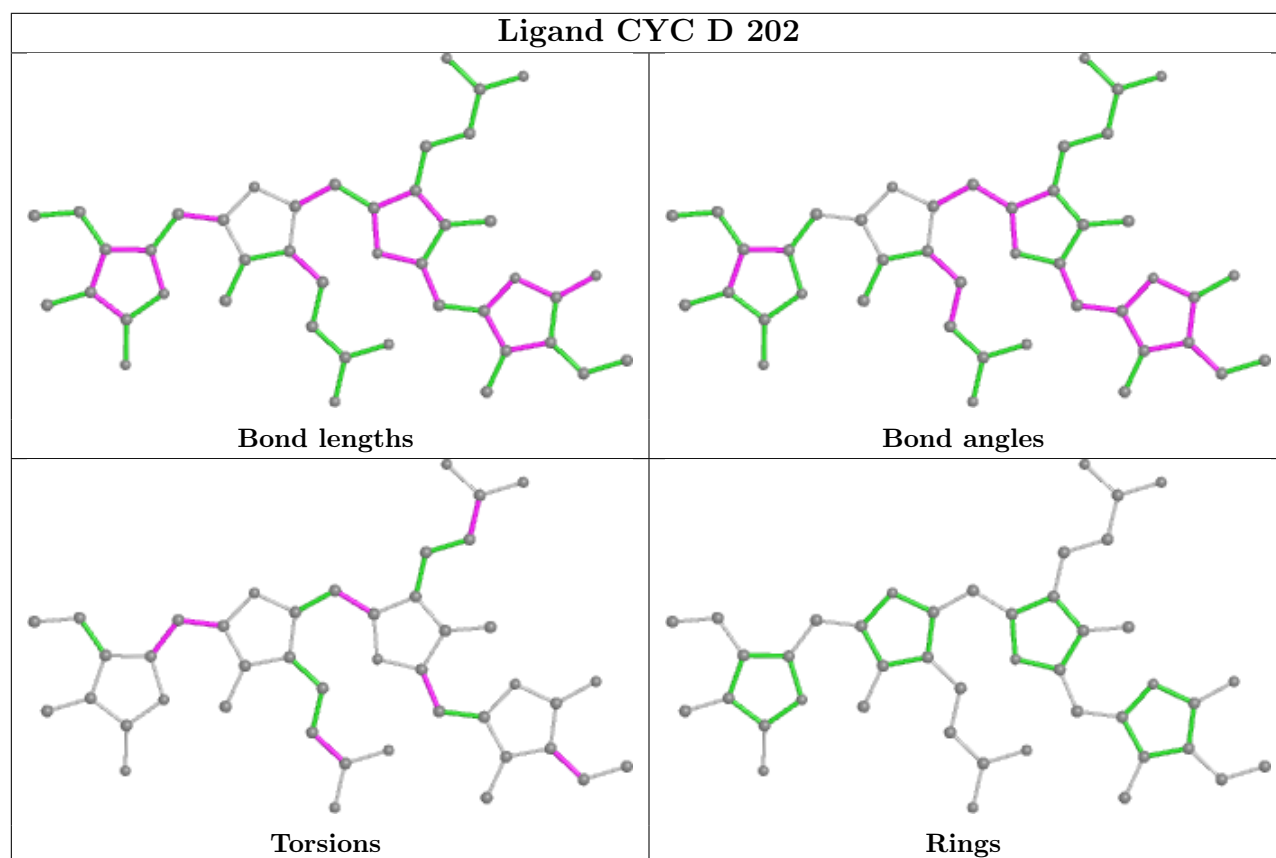
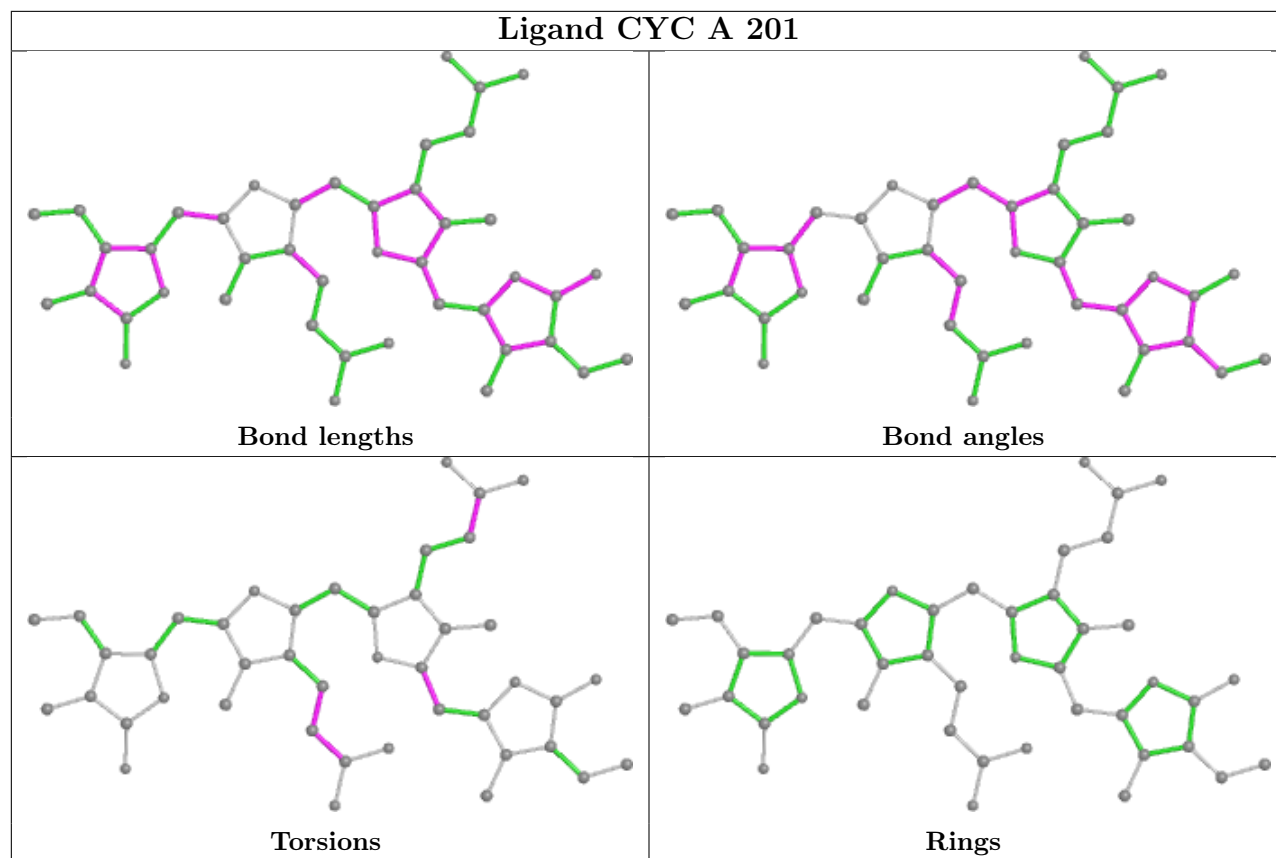
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

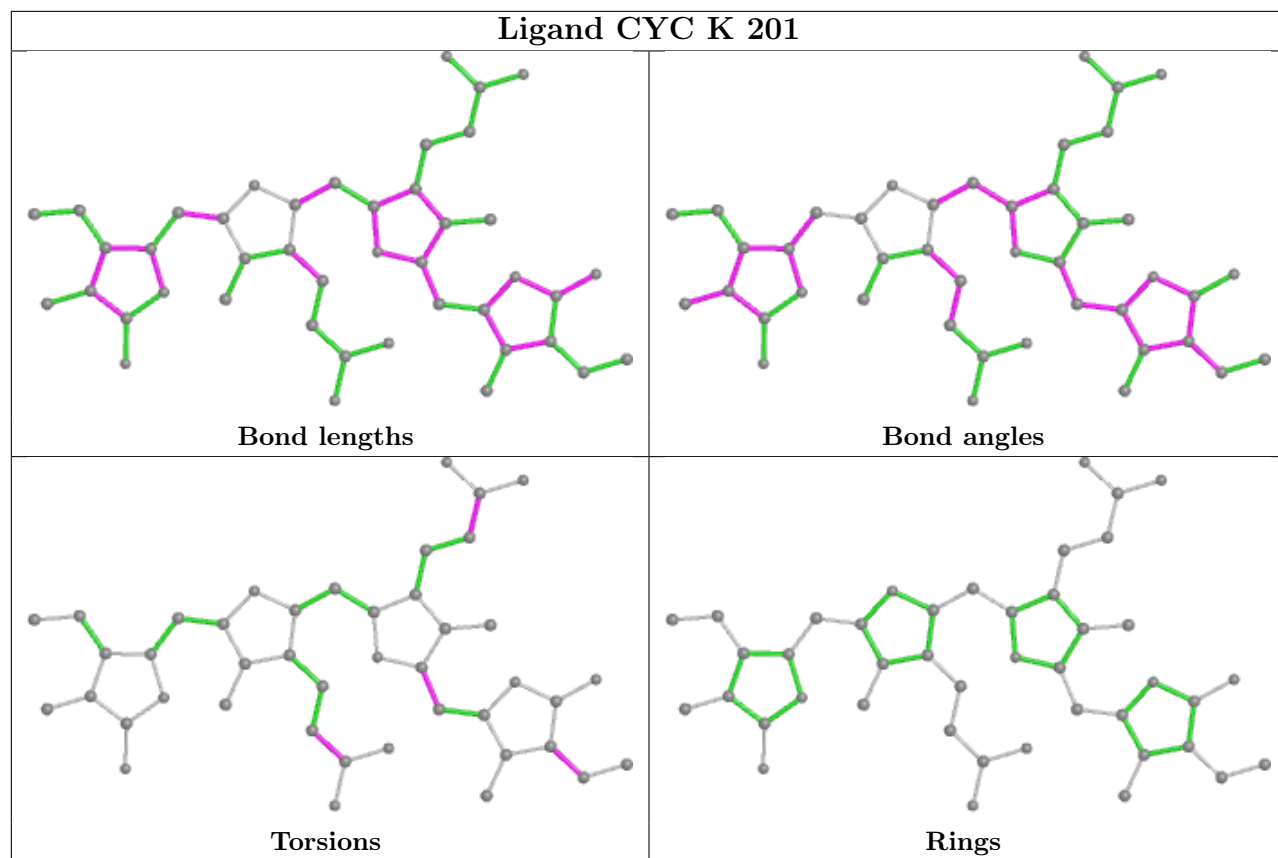
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



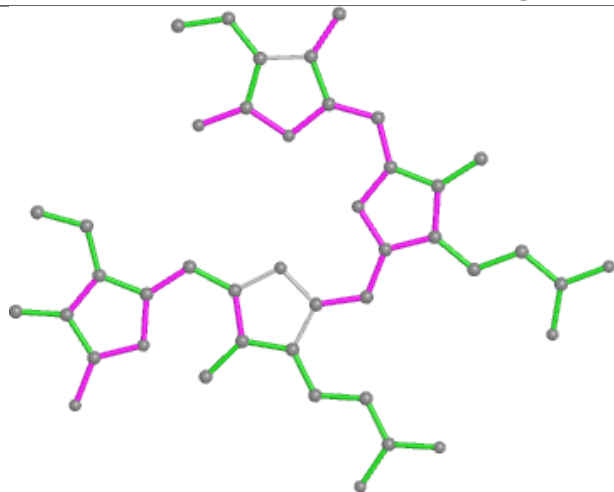




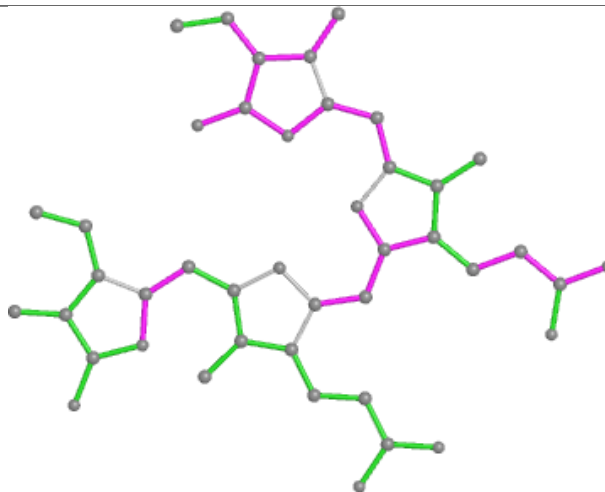




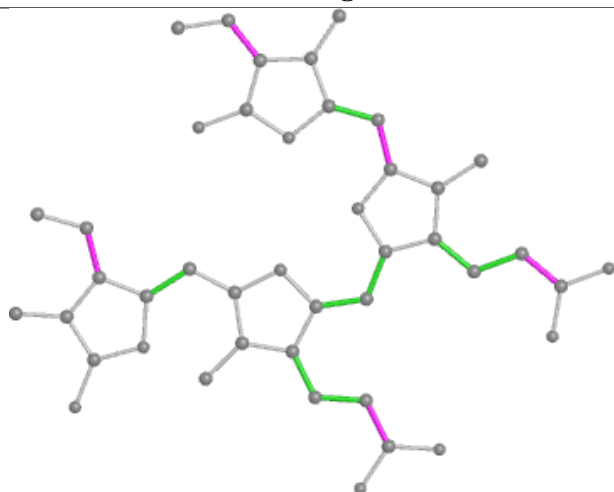
Ligand PUB L 203



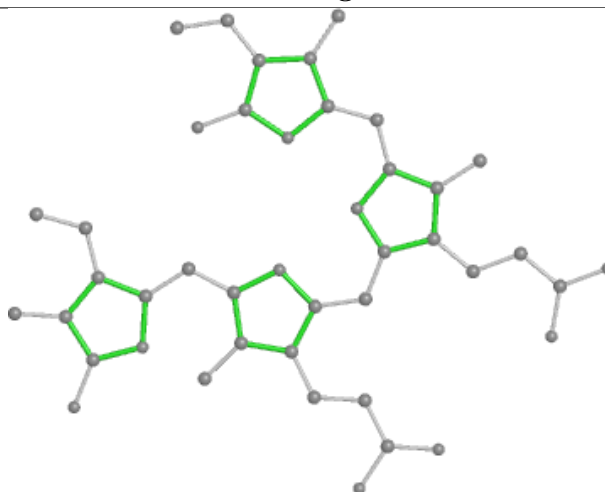
Bond lengths



Bond angles

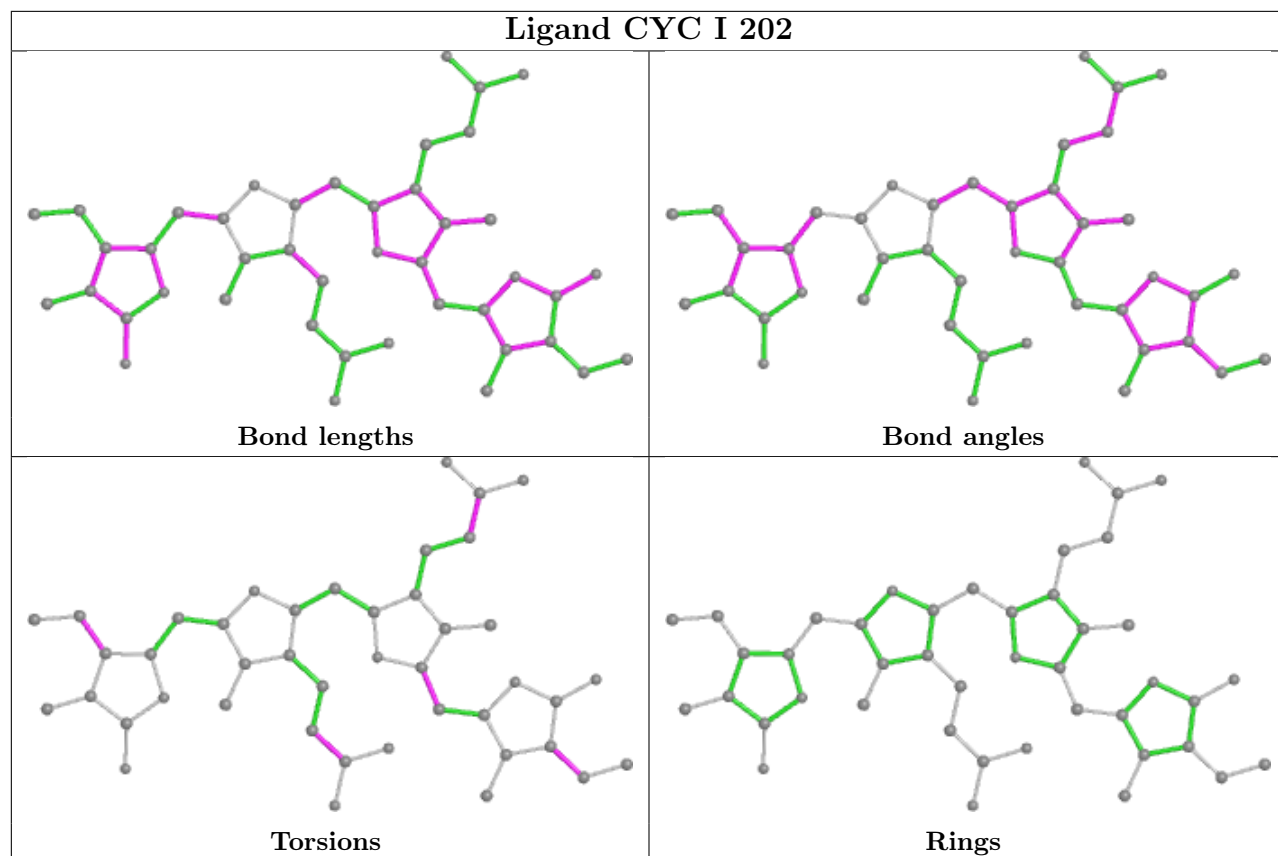


Torsions

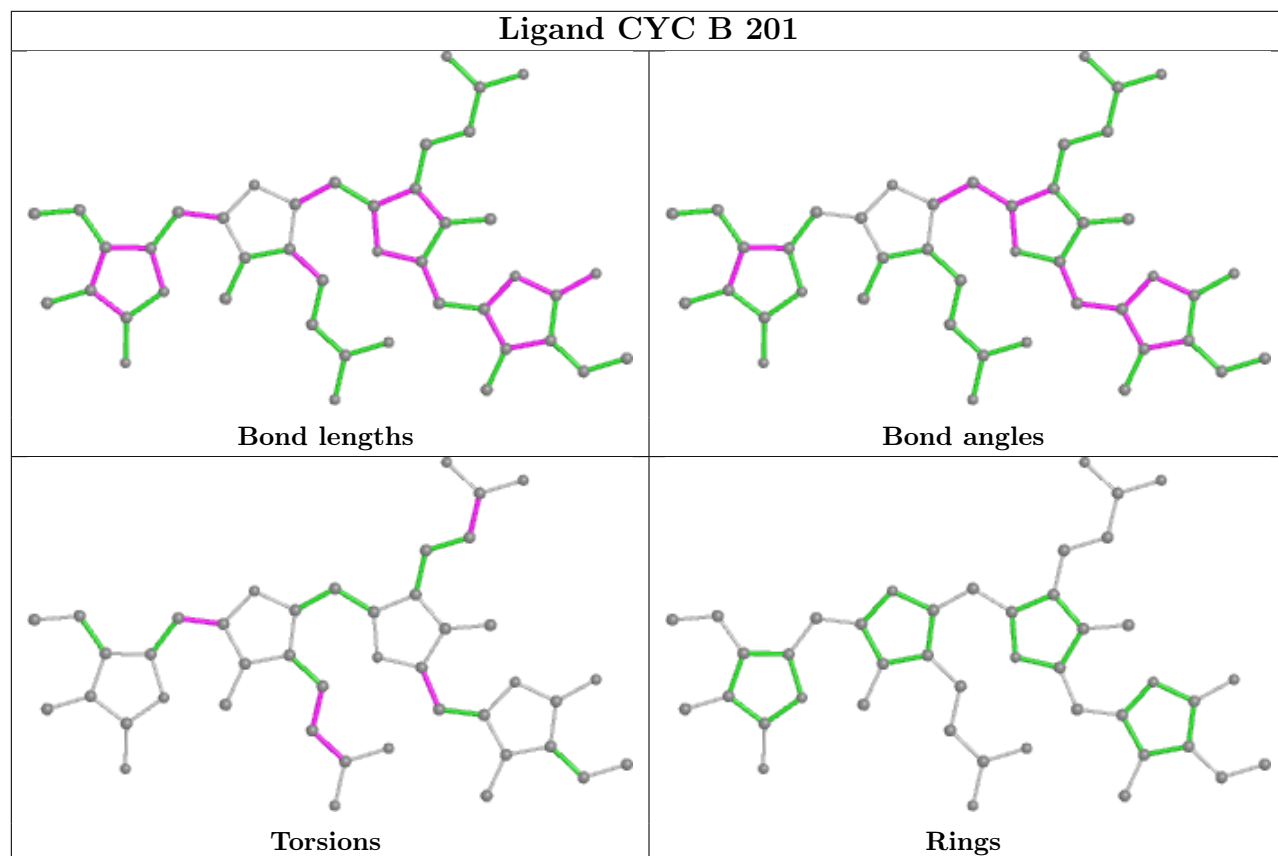


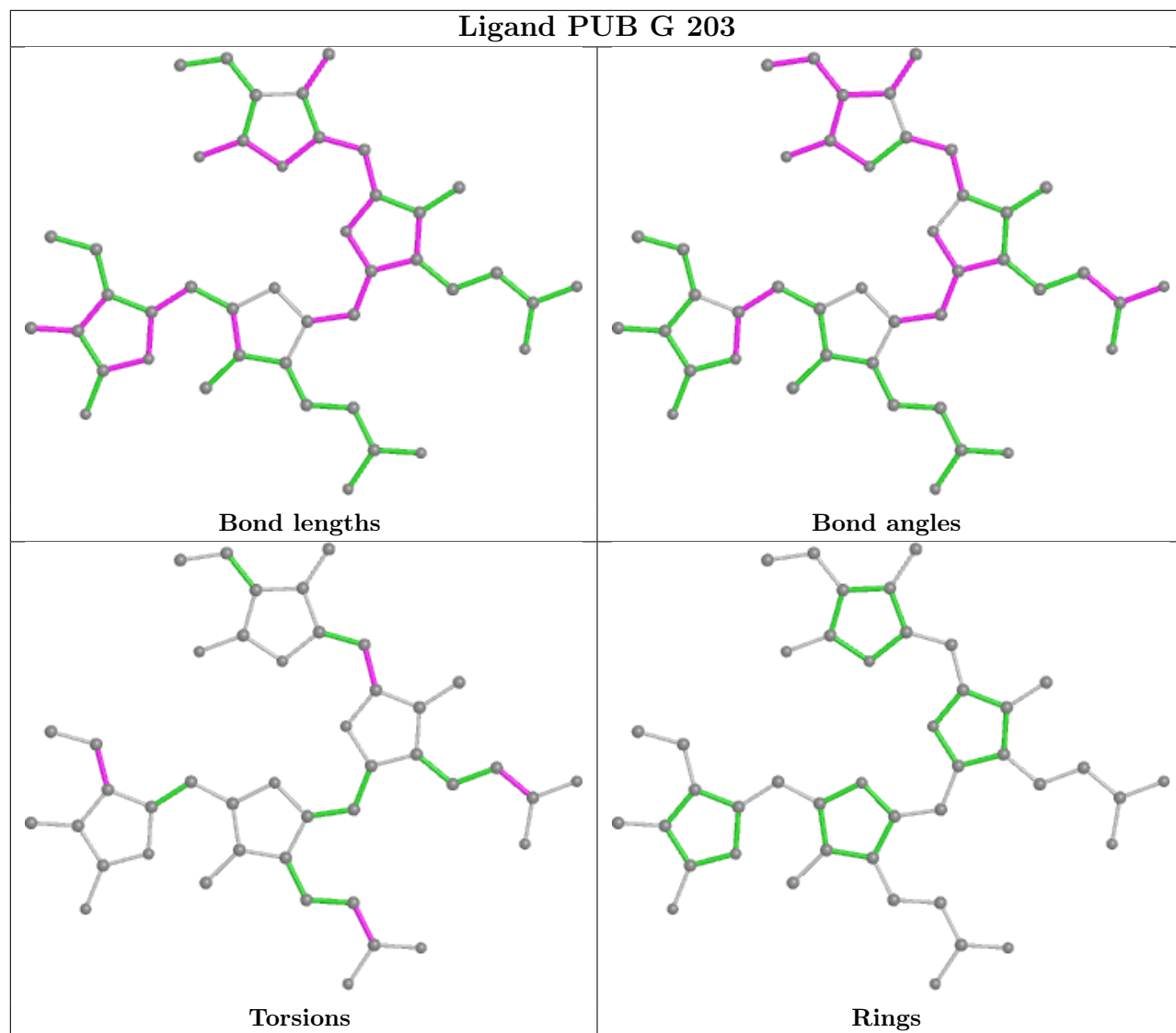
Rings

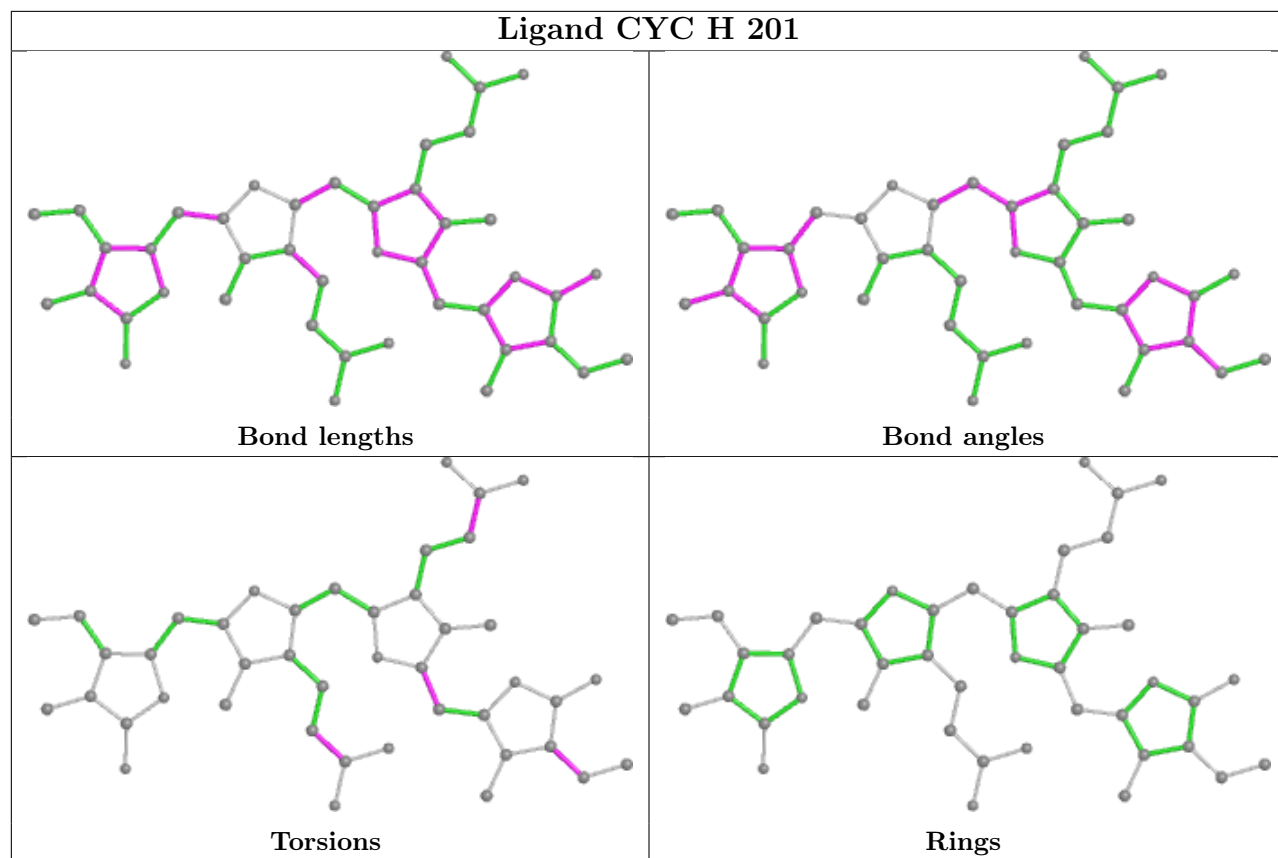
Ligand CYC I 202



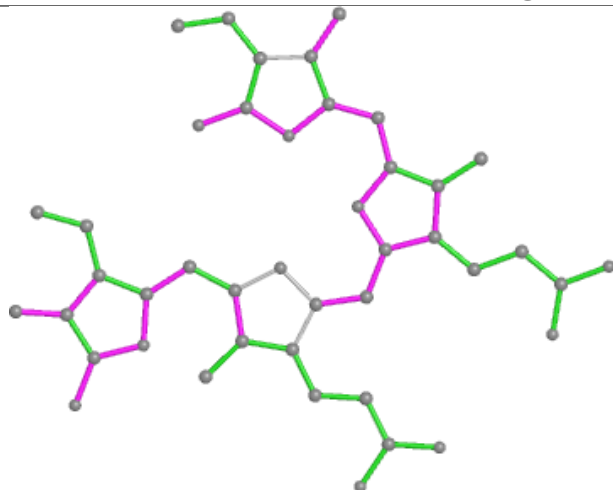
Ligand CYC B 201



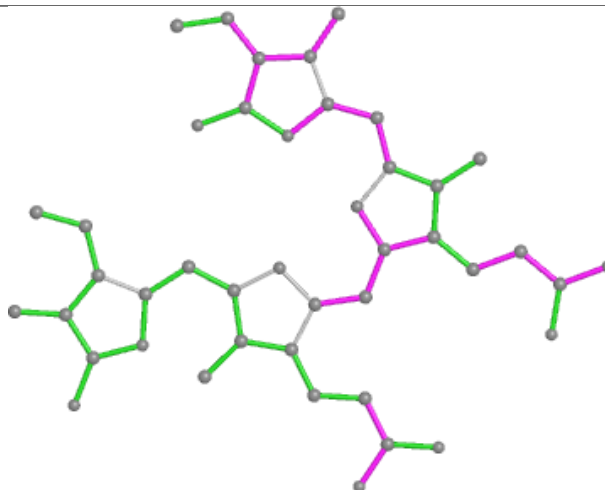




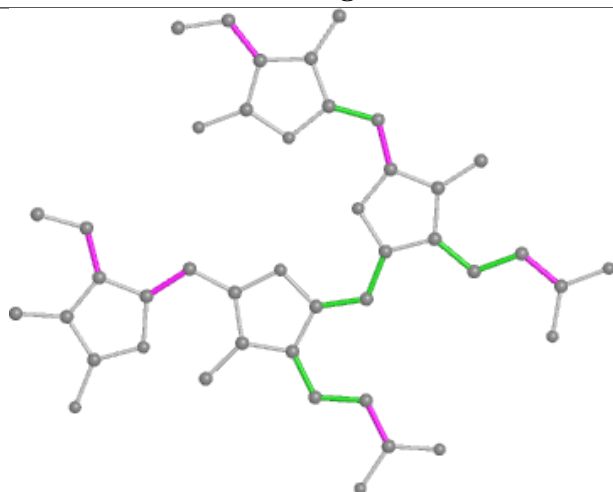
Ligand PUB I 203



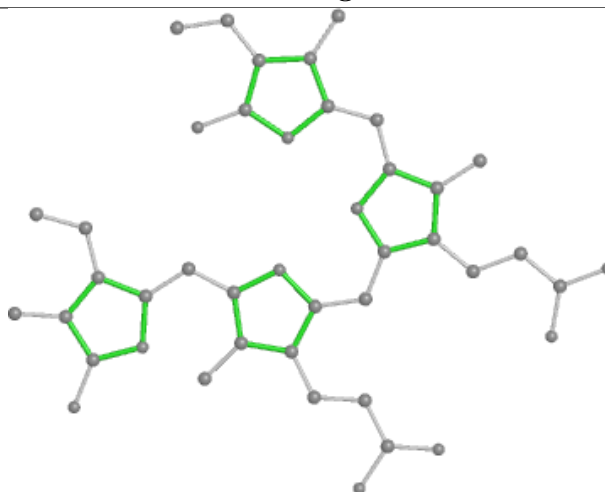
Bond lengths



Bond angles

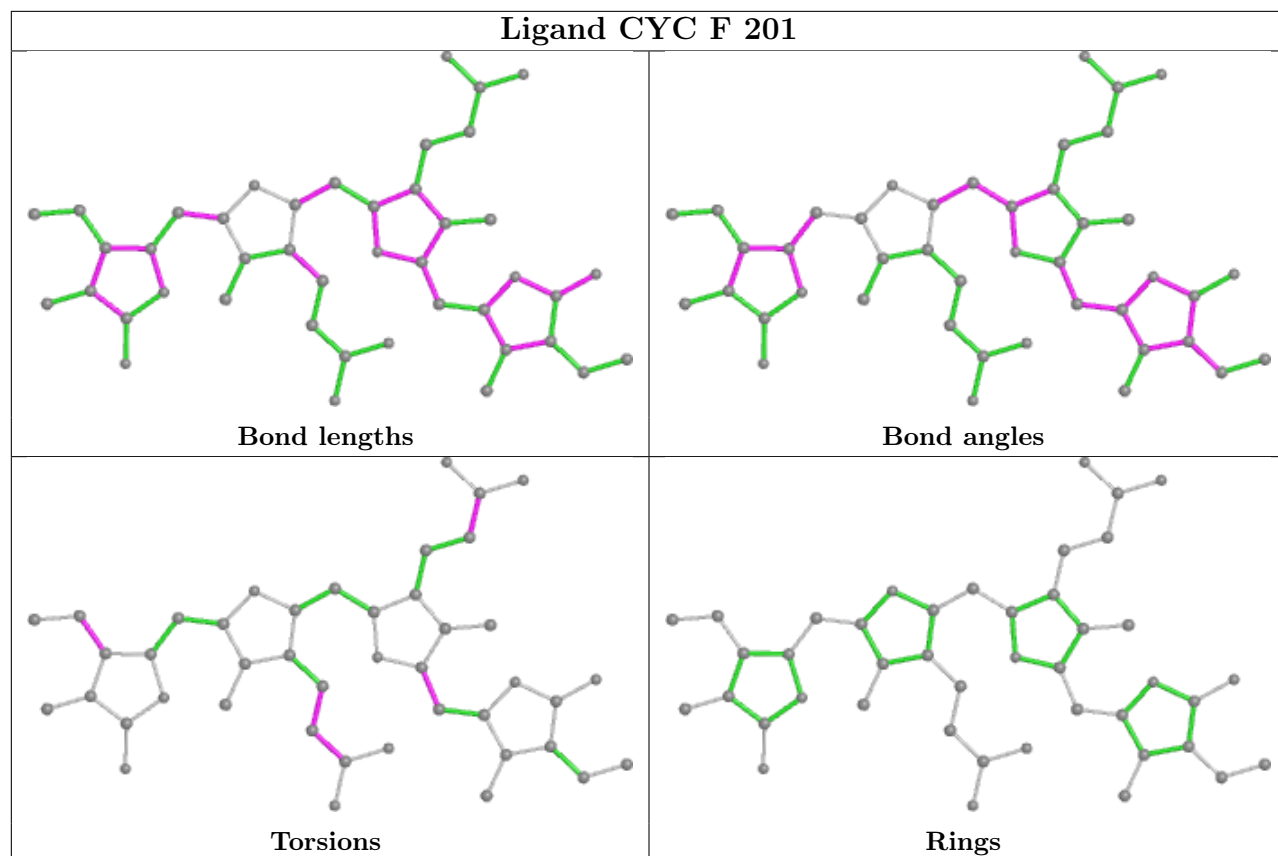


Torsions

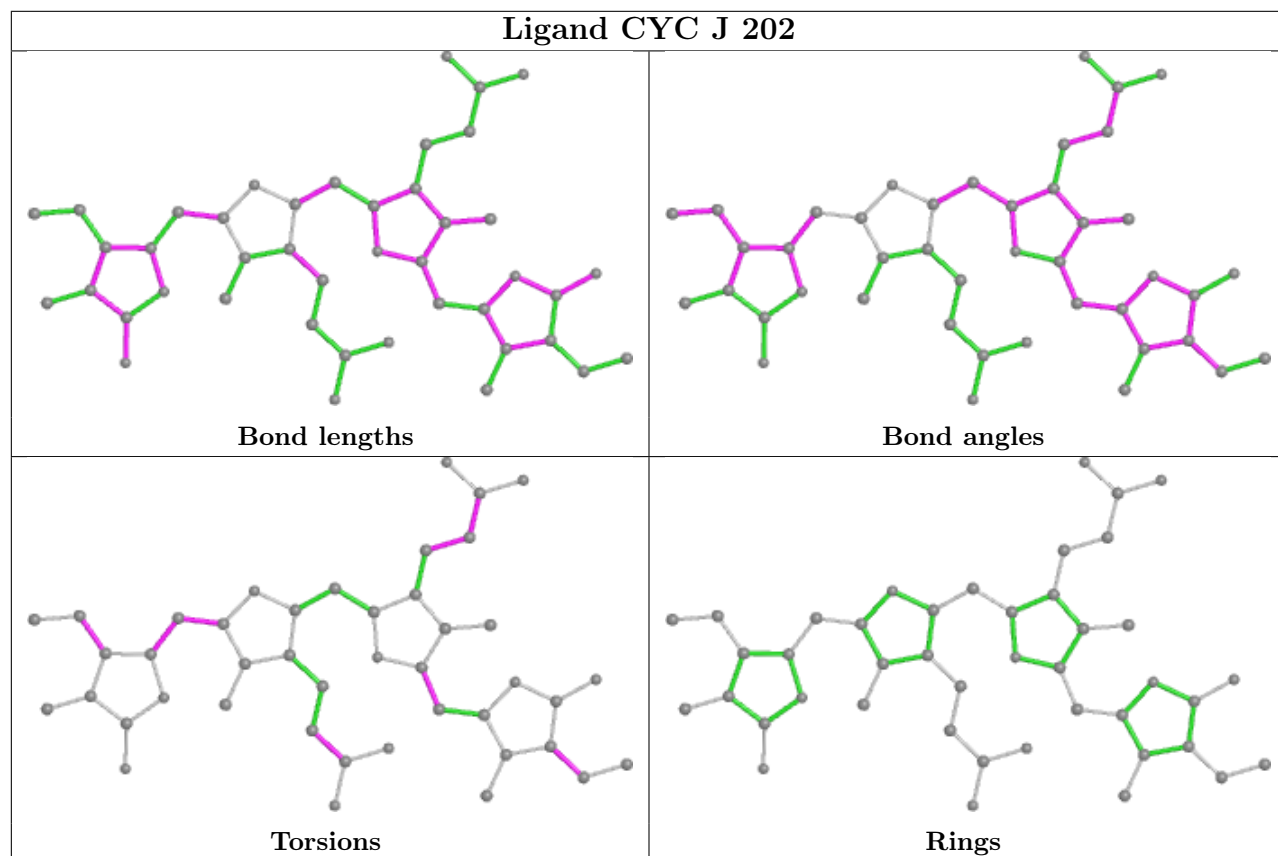


Rings

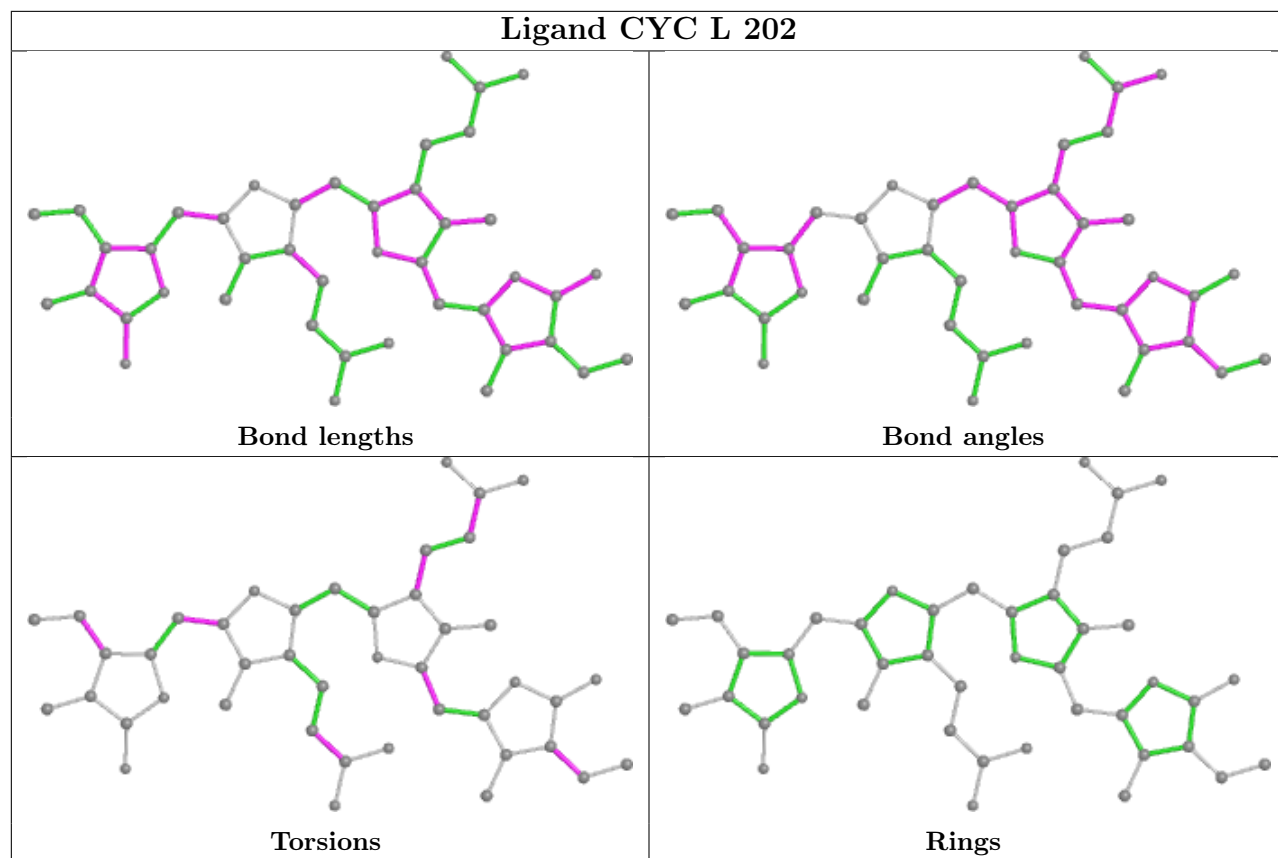
Ligand CYC F 201



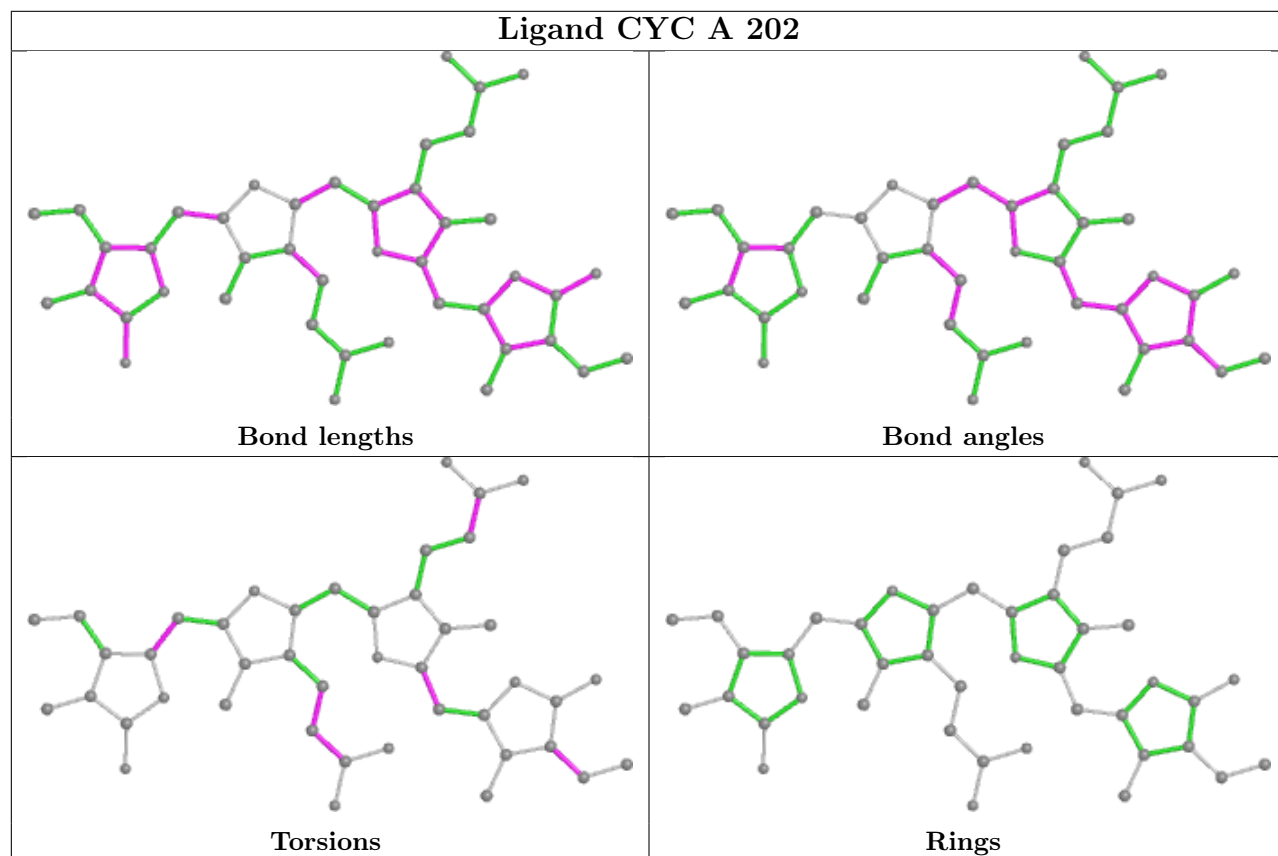
Ligand CYC J 202



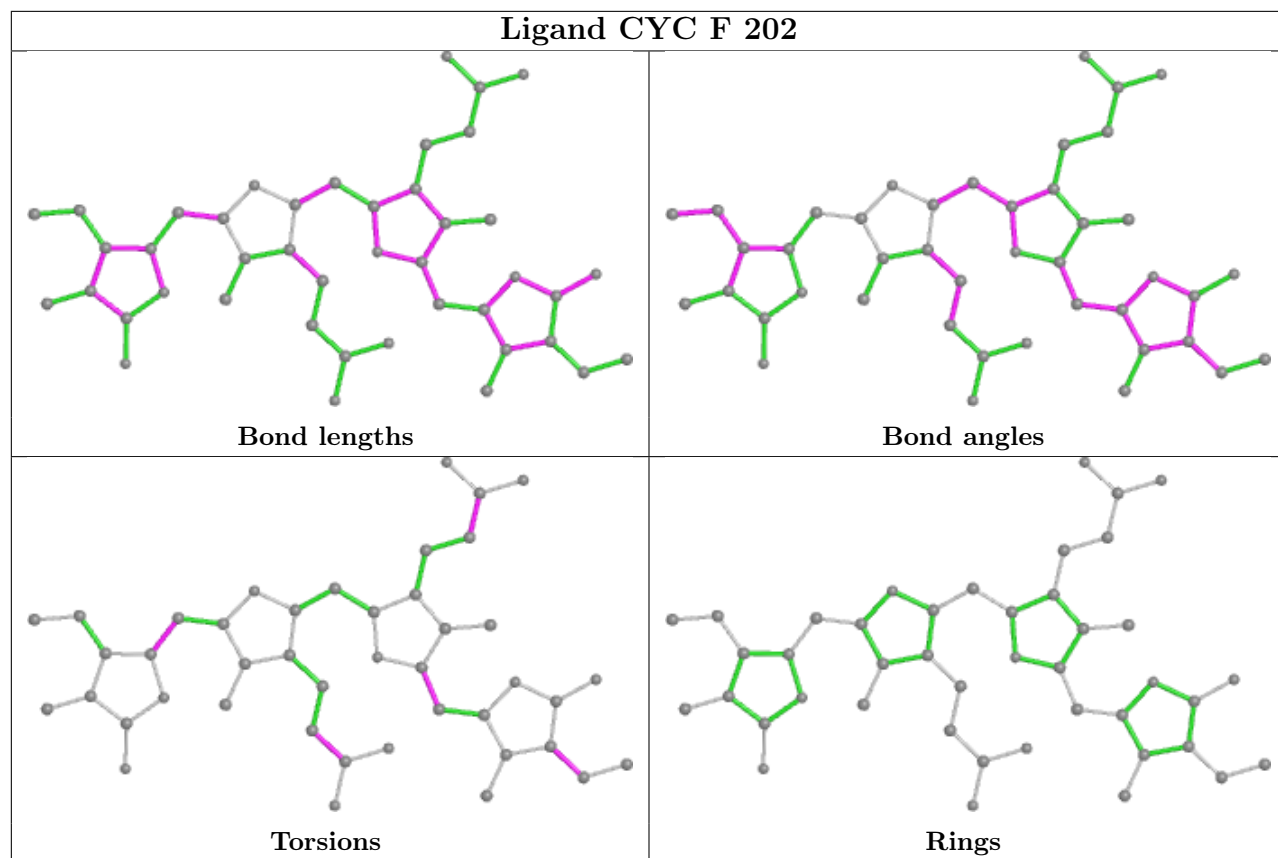
Ligand CYC L 202



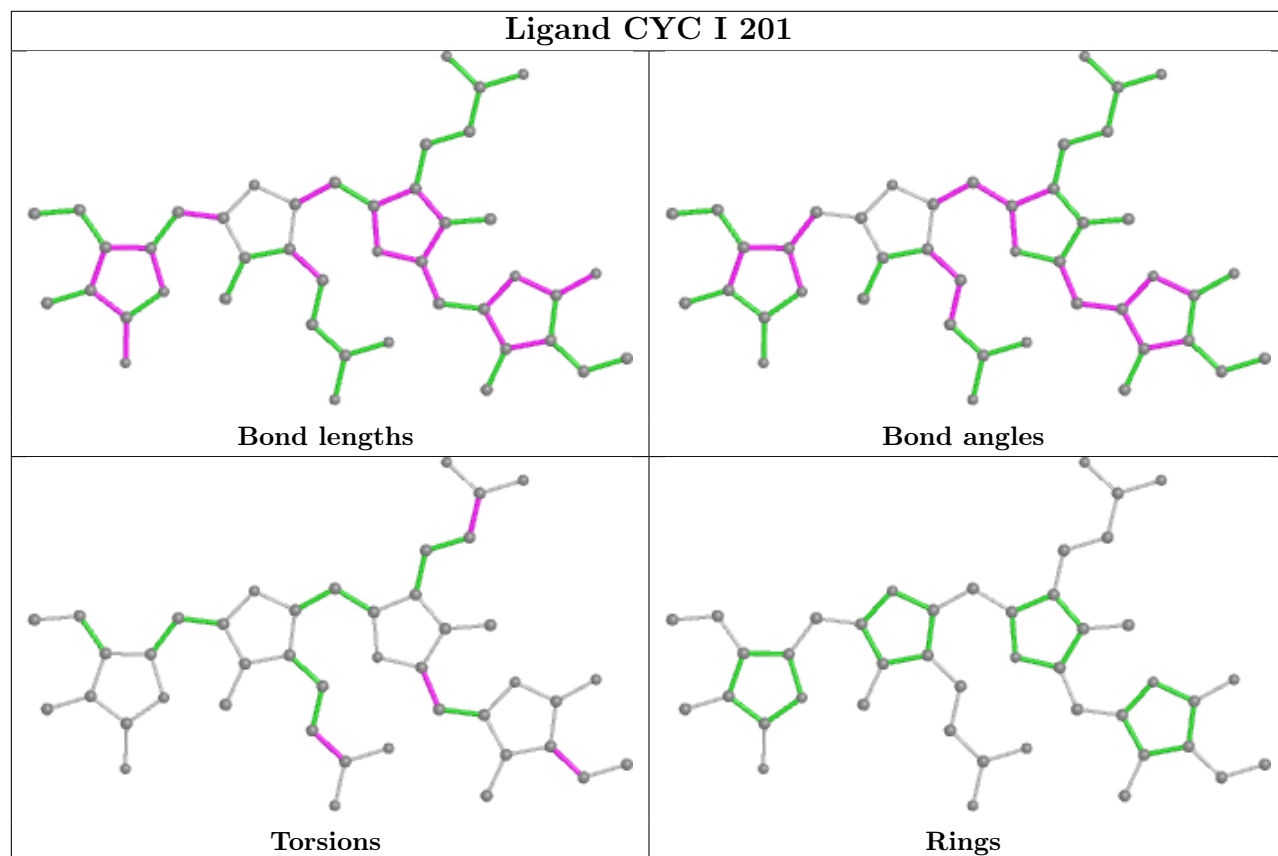
Ligand CYC A 202



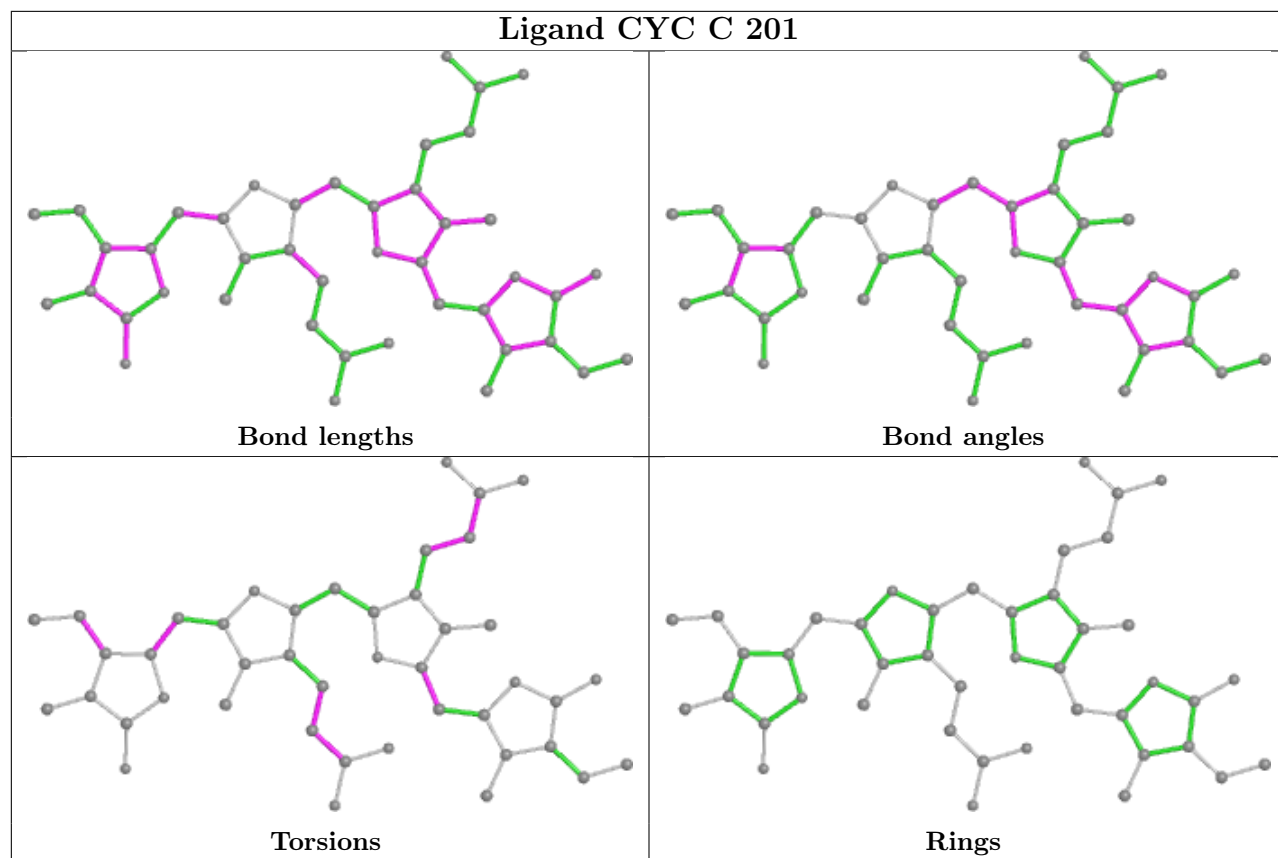
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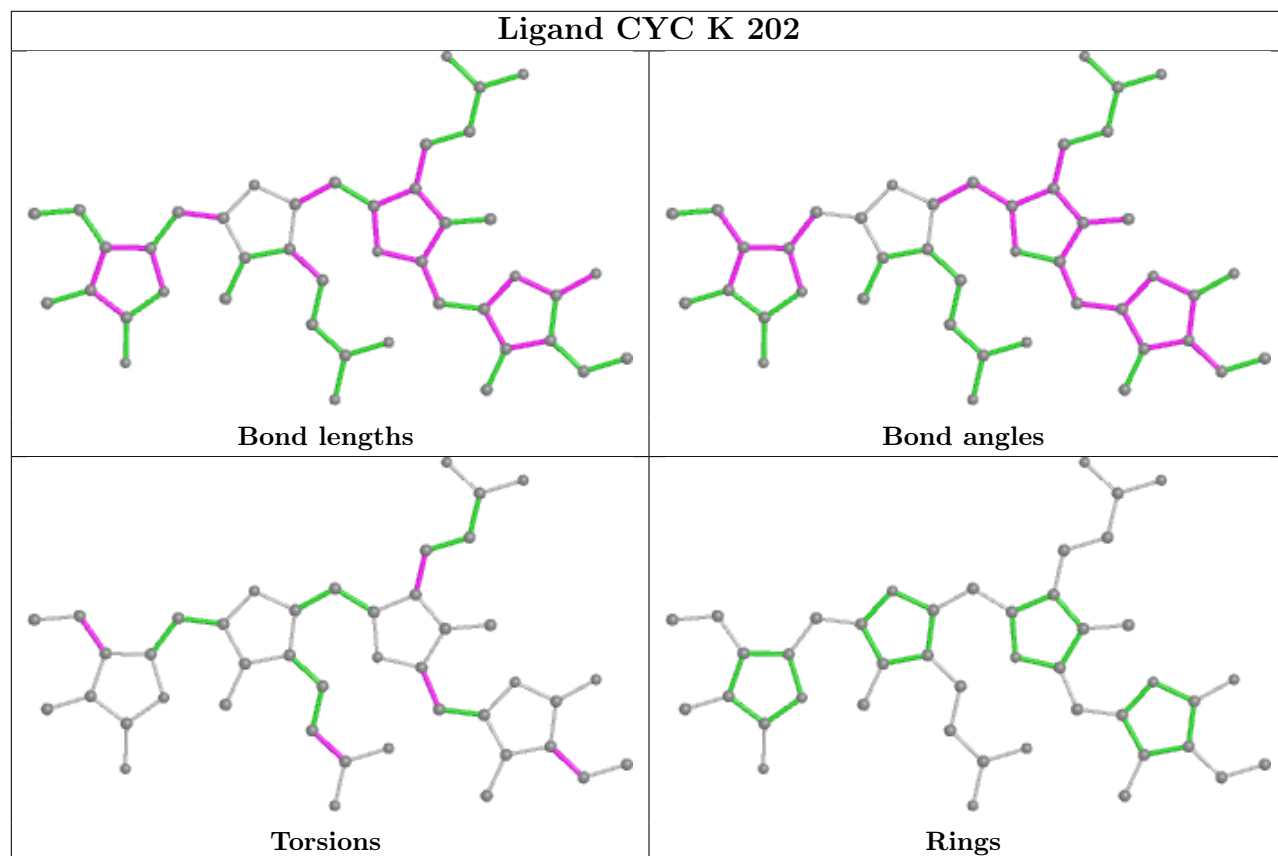
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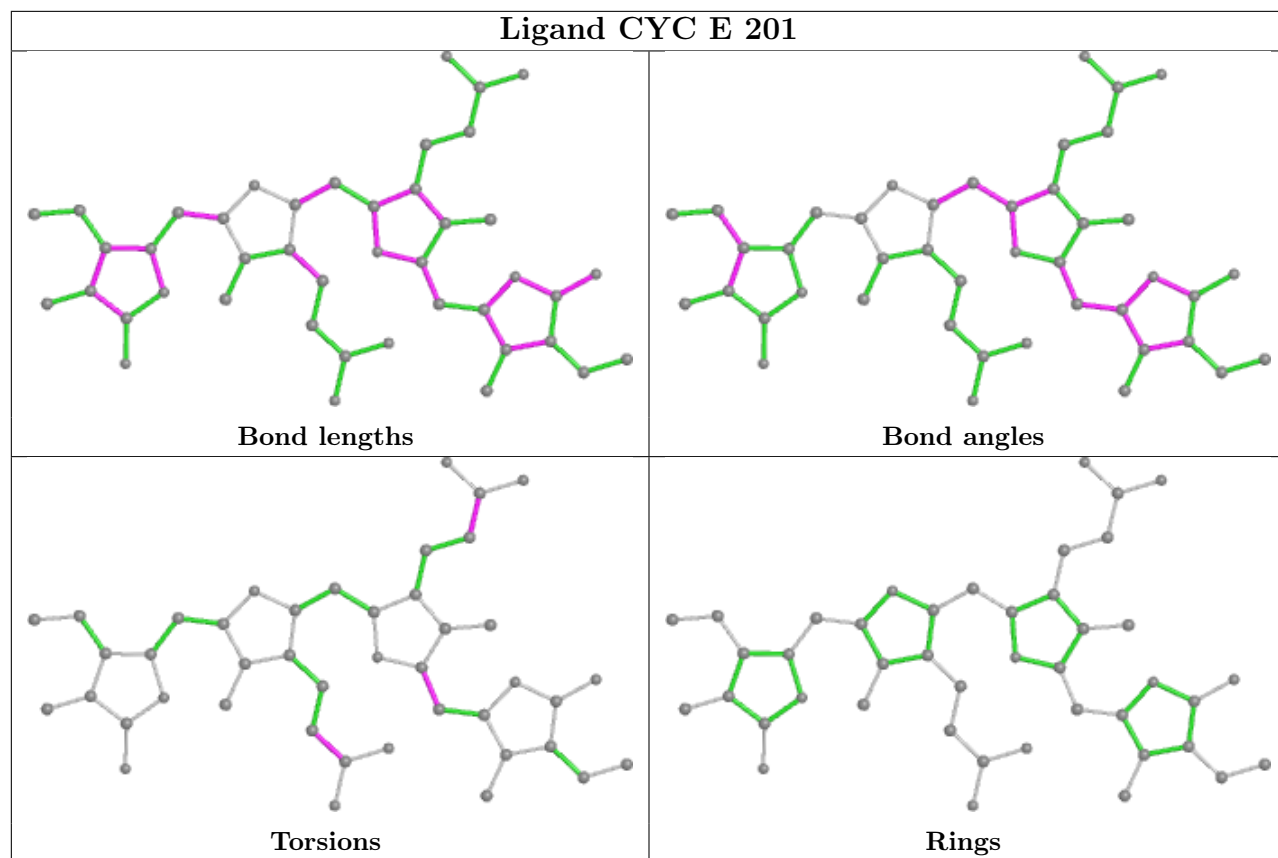
Ligand CYC C 201



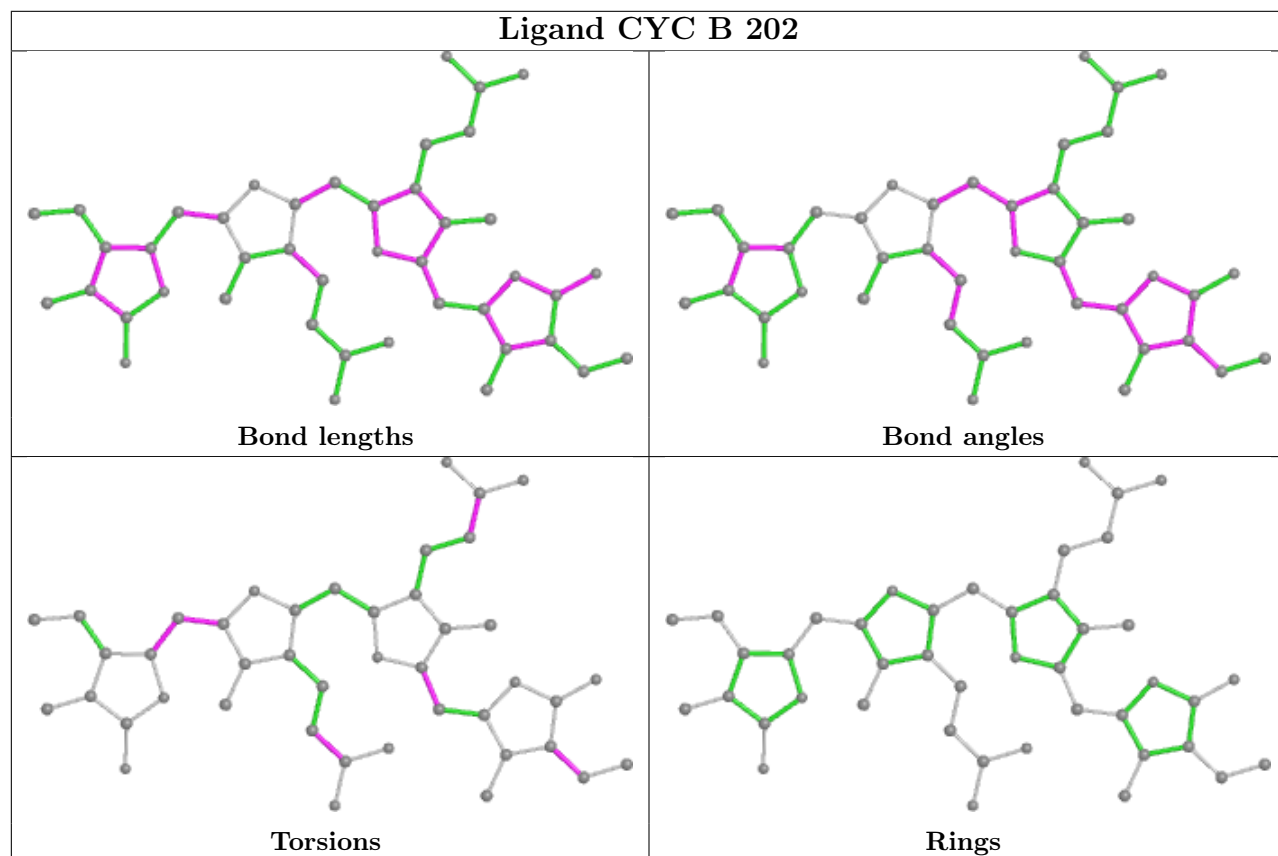
Ligand CYC K 202

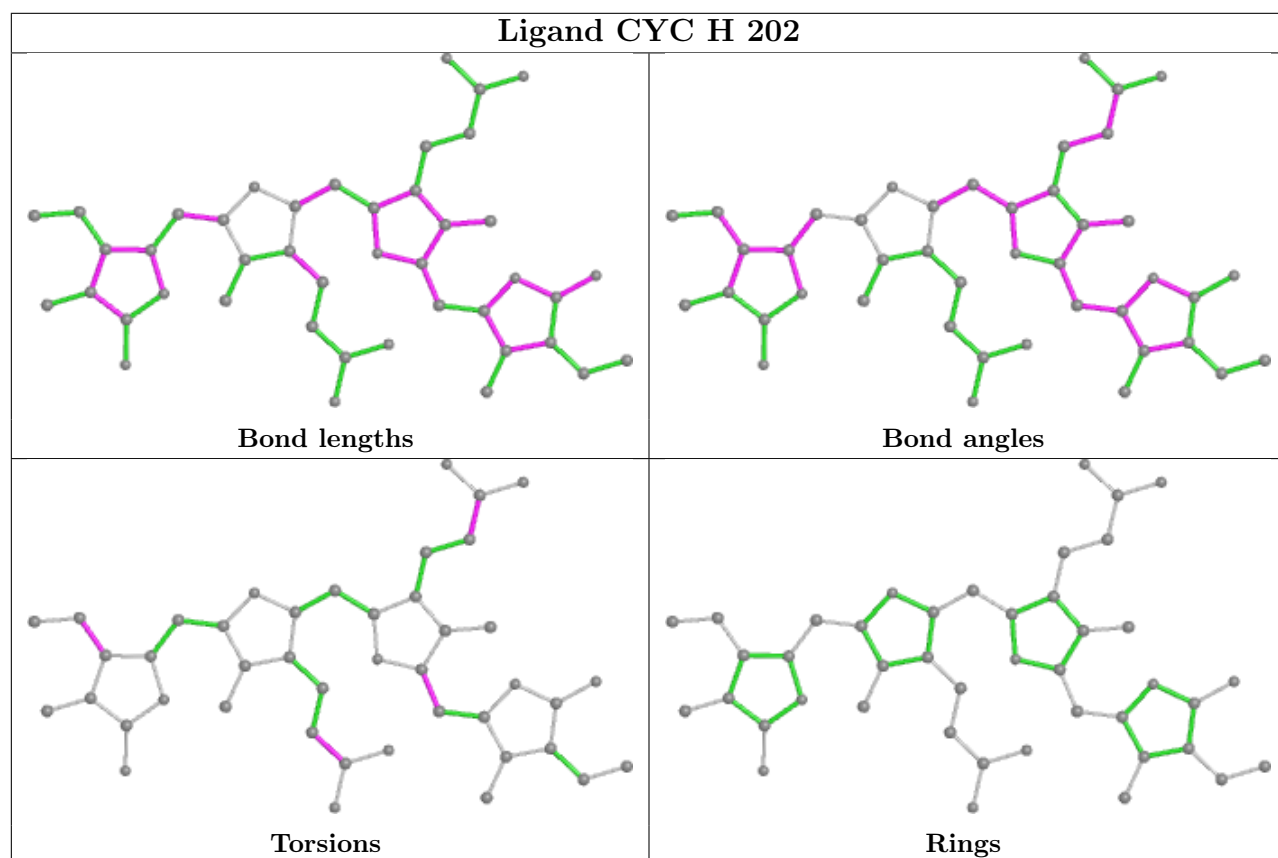
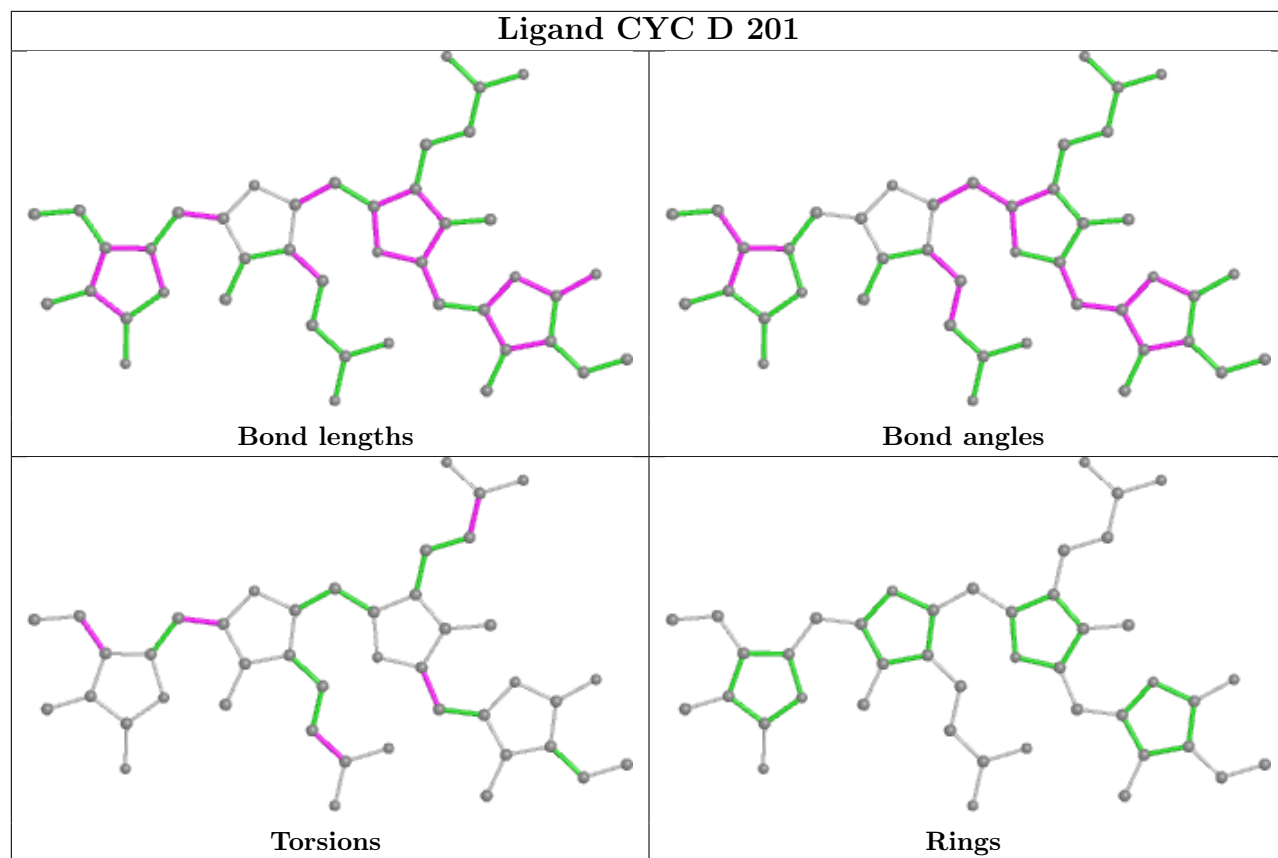


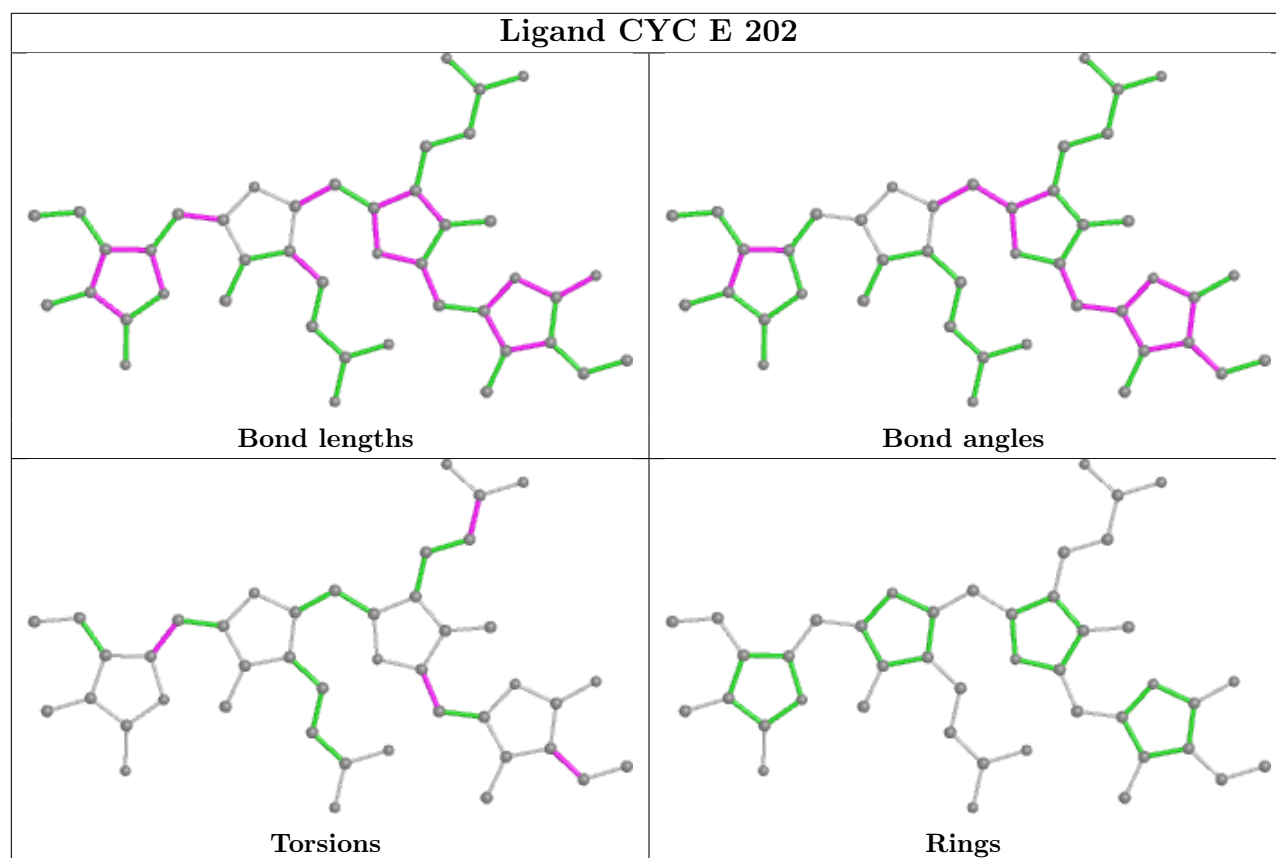
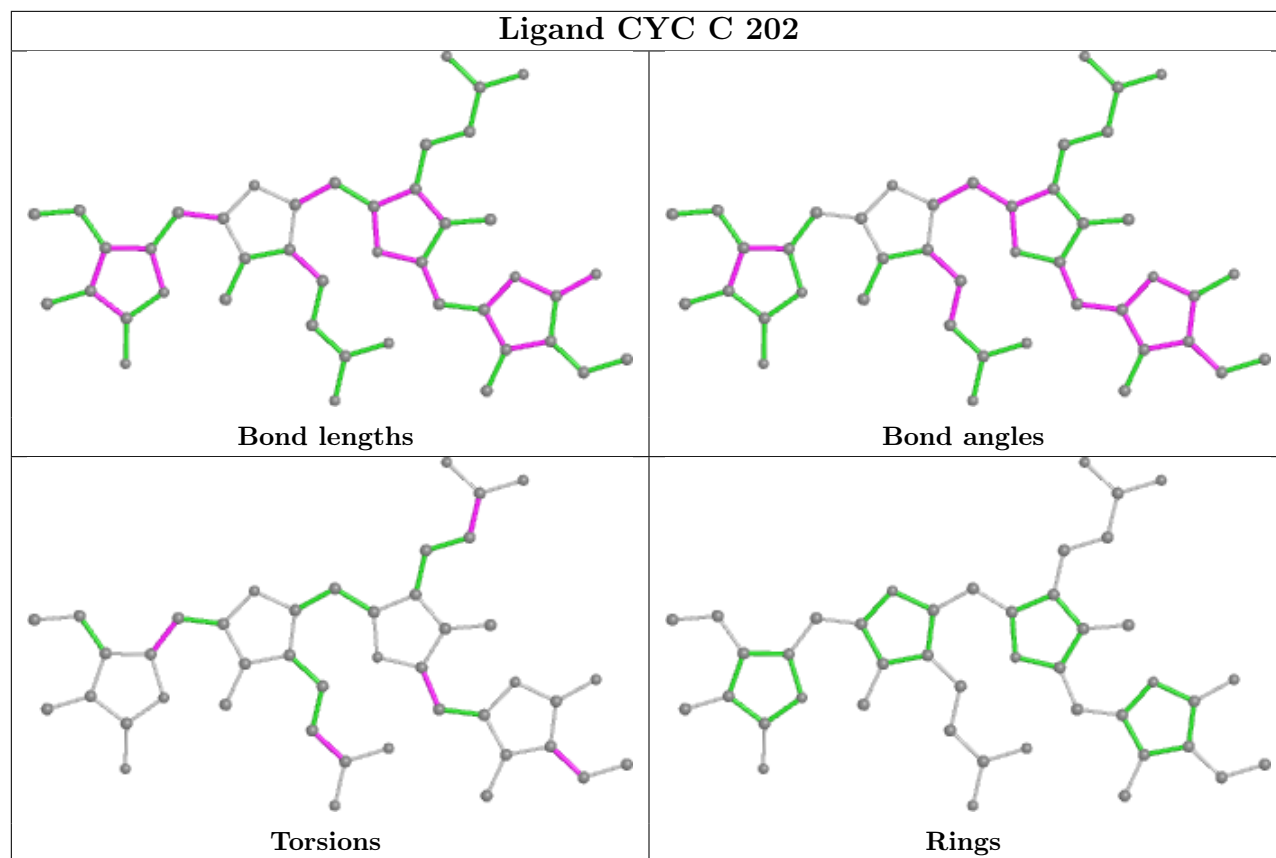
Ligand CYC E 201

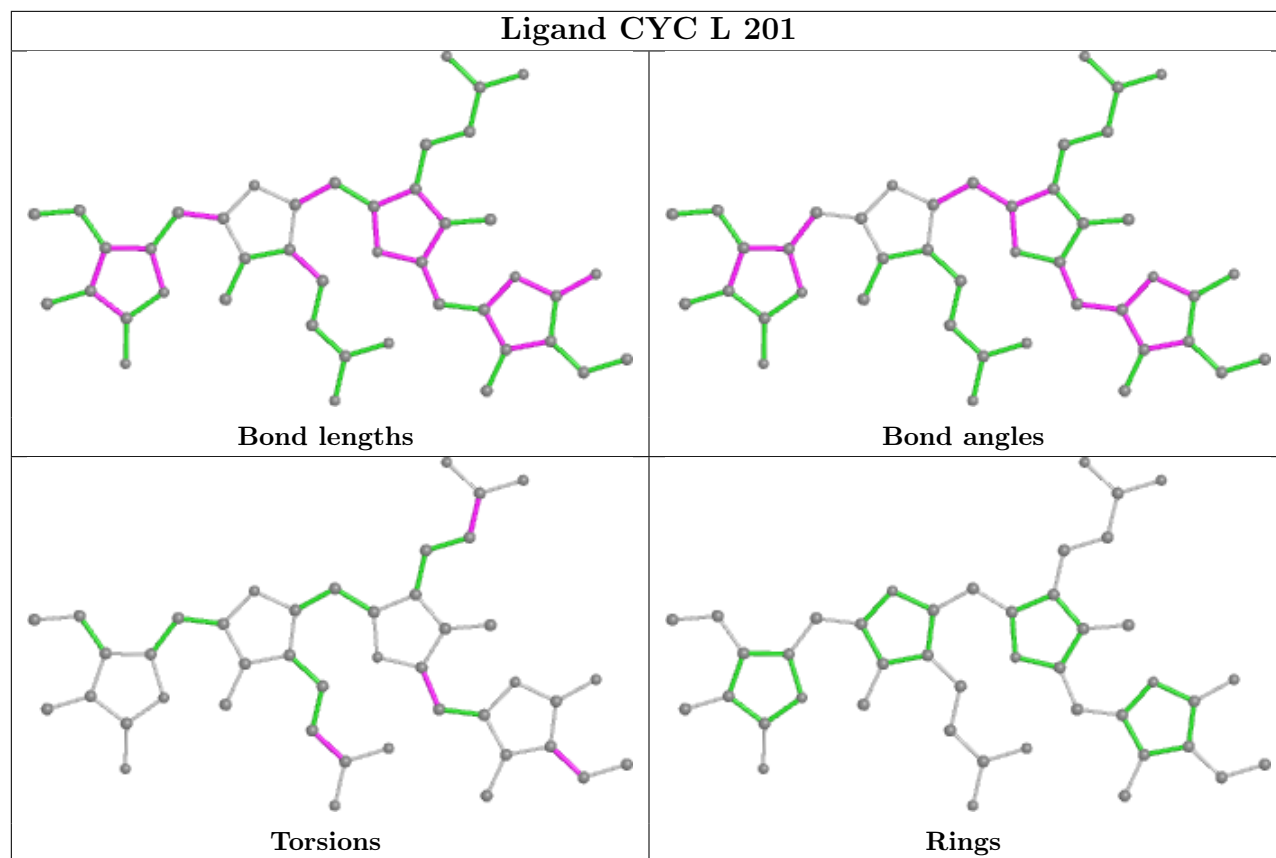


Ligand CYC B 202

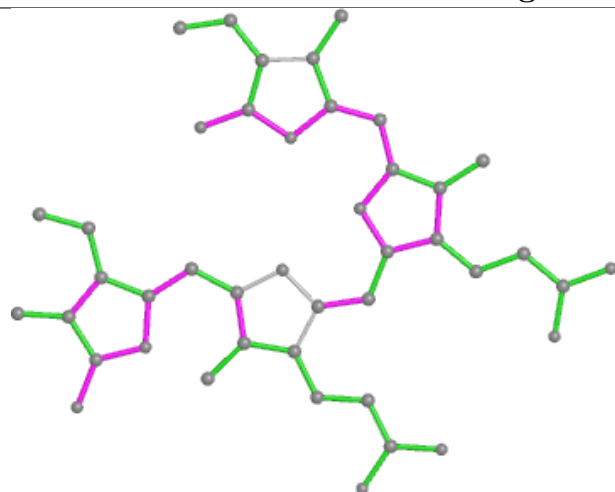




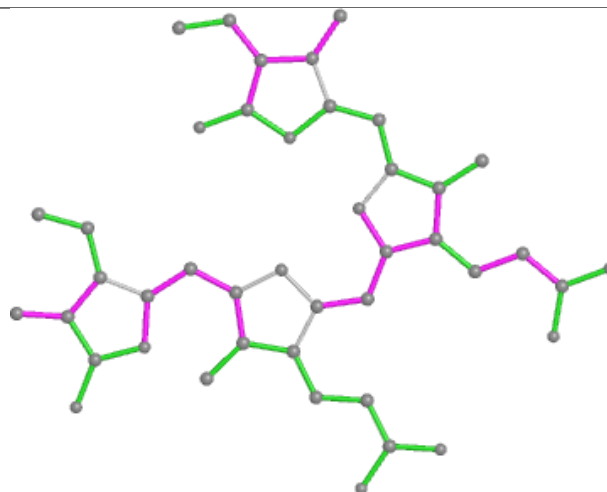




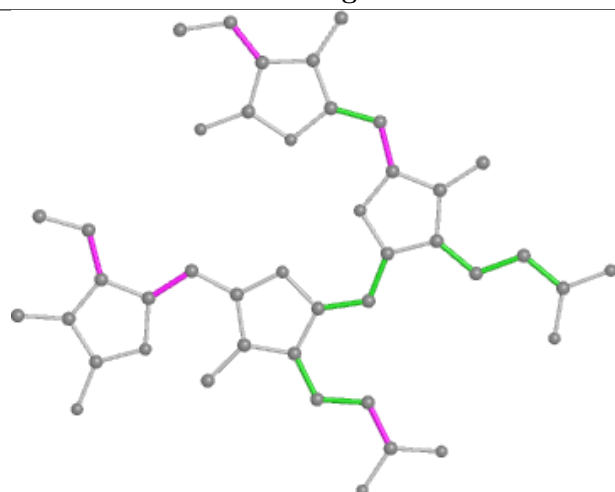
Ligand PUB J 203



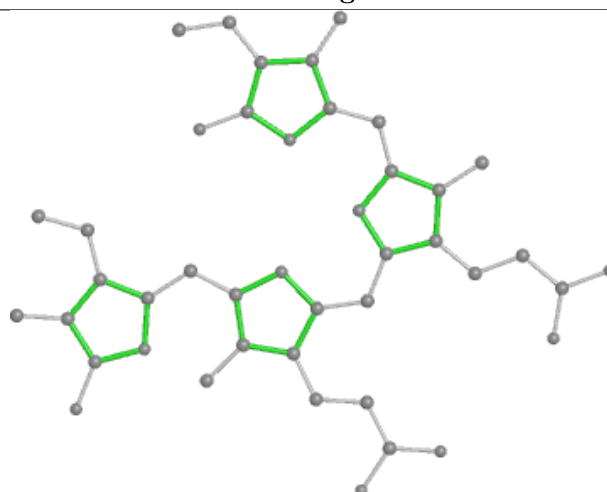
Bond lengths



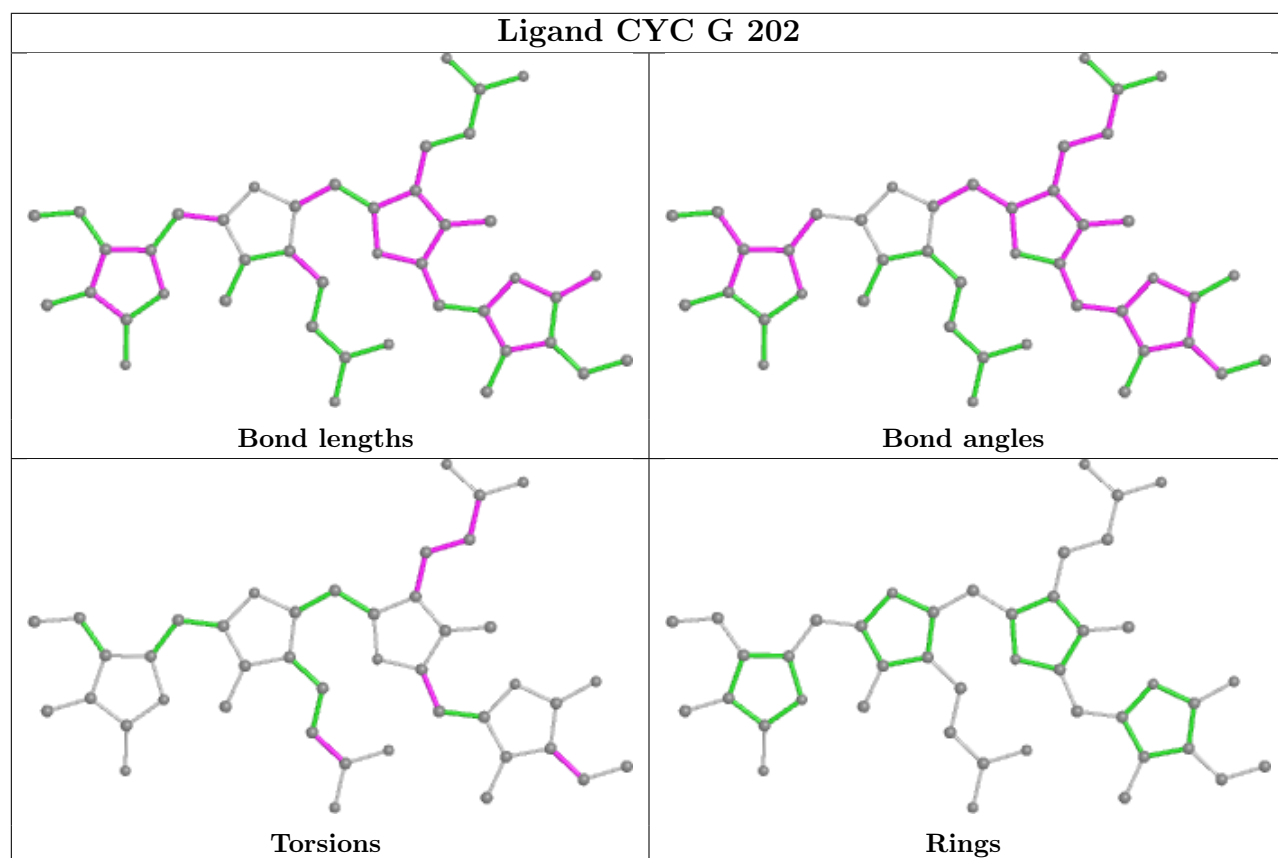
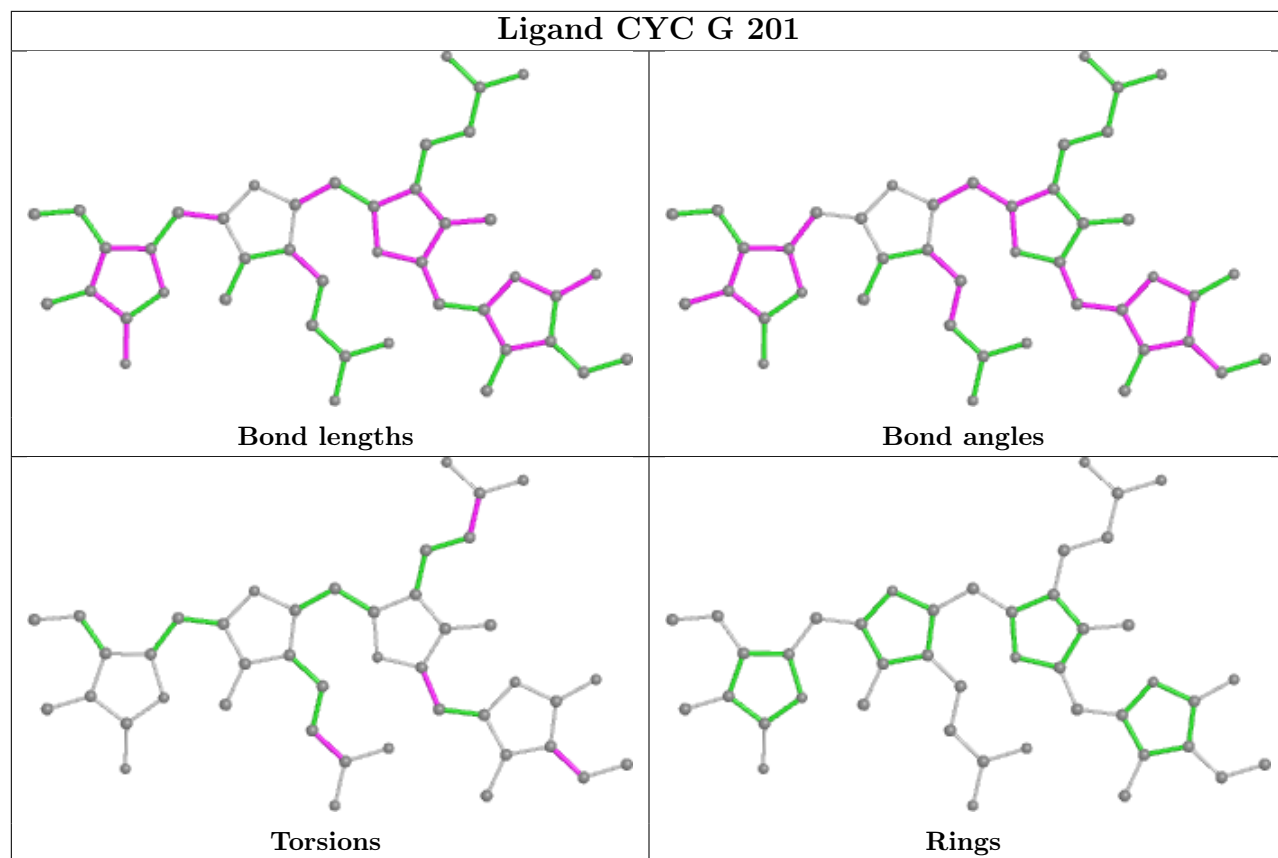
Bond angles



Torsions



Rings



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	164/164 (100%)	-0.23	0 100 100	8, 15, 31, 35	0
1	B	164/164 (100%)	0.00	0 100 100	13, 20, 29, 40	0
1	C	164/164 (100%)	-0.08	0 100 100	10, 20, 35, 40	0
1	D	164/164 (100%)	-0.08	0 100 100	12, 19, 35, 45	0
1	E	164/164 (100%)	-0.11	0 100 100	12, 20, 31, 40	0
1	F	164/164 (100%)	-0.13	0 100 100	12, 20, 29, 37	0
2	G	177/177 (100%)	-0.10	3 (1%) 70 74	11, 18, 33, 42	0
2	H	177/177 (100%)	0.01	5 (2%) 53 59	12, 21, 39, 49	0
2	I	177/177 (100%)	0.03	2 (1%) 80 84	12, 20, 38, 50	0
2	J	177/177 (100%)	0.25	9 (5%) 28 33	15, 27, 41, 49	0
2	K	177/177 (100%)	0.02	4 (2%) 60 65	13, 20, 39, 49	0
2	L	177/177 (100%)	0.09	8 (4%) 33 38	14, 24, 41, 52	0
All	All	2046/2046 (100%)	-0.03	31 (1%) 73 77	8, 20, 37, 52	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	145	THR	3.7
2	H	148	ASP	3.2
2	L	148	ASP	2.9
2	L	116	THR	2.8
2	L	21	GLY	2.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

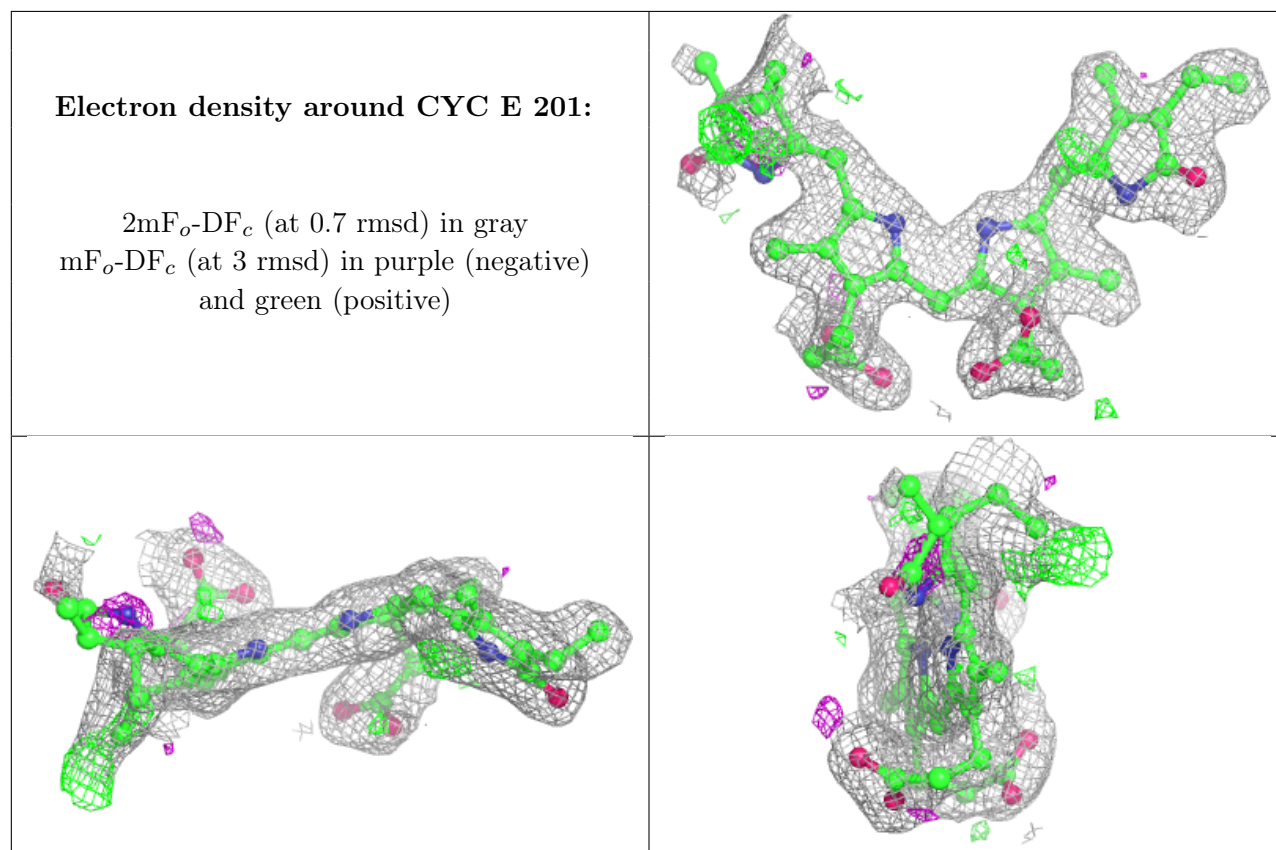
6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	CYC	E	201	43/43	0.83	0.23	14,30,61,62	0
3	CYC	D	201	43/43	0.84	0.21	16,28,52,58	0
3	CYC	J	202	43/43	0.84	0.19	16,26,36,63	0
3	CYC	L	202	43/43	0.85	0.18	18,30,45,52	0
3	CYC	C	201	43/43	0.86	0.23	16,33,48,53	0
3	CYC	H	202	43/43	0.86	0.18	12,24,36,49	0
3	CYC	B	201	43/43	0.87	0.21	21,31,48,55	0
4	PUB	L	203	43/43	0.87	0.16	19,29,46,47	0
3	CYC	G	202	43/43	0.88	0.17	13,22,41,61	0
3	CYC	F	201	43/43	0.88	0.19	19,26,36,52	0
3	CYC	D	202	43/43	0.88	0.16	15,23,33,42	0
3	CYC	C	202	43/43	0.89	0.15	12,24,41,48	0
3	CYC	K	202	43/43	0.89	0.15	17,27,36,49	0
3	CYC	A	201	43/43	0.90	0.17	10,21,28,30	0
3	CYC	I	201	43/43	0.90	0.16	14,24,37,45	0
3	CYC	I	202	43/43	0.90	0.18	8,19,31,40	0
4	PUB	G	203	43/43	0.90	0.16	14,22,37,42	0
4	PUB	J	203	43/43	0.90	0.17	22,34,44,51	0
4	PUB	K	203	43/43	0.90	0.15	16,25,39,45	0
3	CYC	J	201	43/43	0.90	0.17	19,28,46,53	0
3	CYC	L	201	43/43	0.91	0.18	17,24,38,49	0
3	CYC	G	201	43/43	0.91	0.16	11,19,38,45	0
3	CYC	E	202	43/43	0.91	0.16	15,25,38,54	0
4	PUB	H	203	43/43	0.91	0.15	15,23,34,41	0
4	PUB	I	203	43/43	0.91	0.17	18,25,37,48	0
3	CYC	B	202	43/43	0.91	0.17	12,20,34,43	0
3	CYC	F	202	43/43	0.91	0.17	11,19,31,47	0
3	CYC	A	202	43/43	0.91	0.15	13,20,30,38	0
3	CYC	K	201	43/43	0.92	0.15	13,23,36,46	0
3	CYC	H	201	43/43	0.92	0.16	13,23,33,42	0

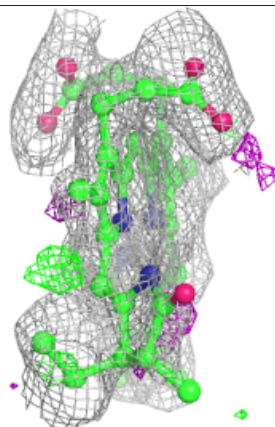
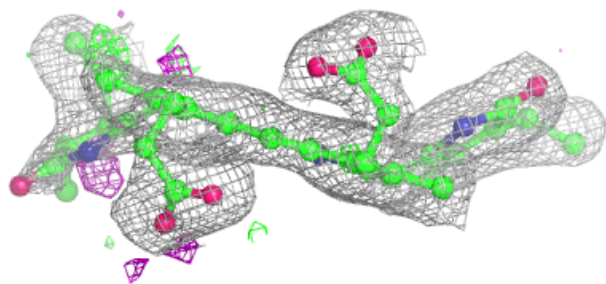
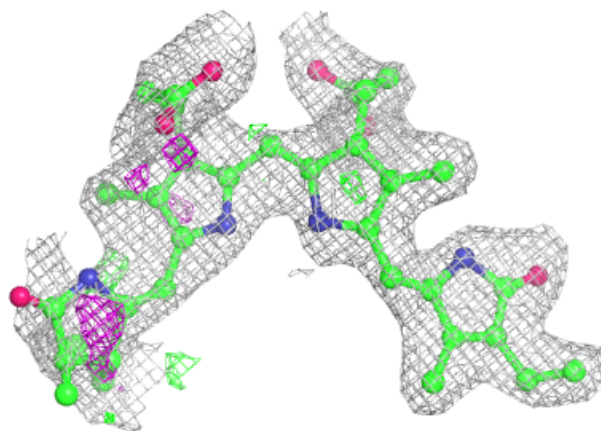
The following is a graphical depiction of the model fit to experimental electron density of all

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.



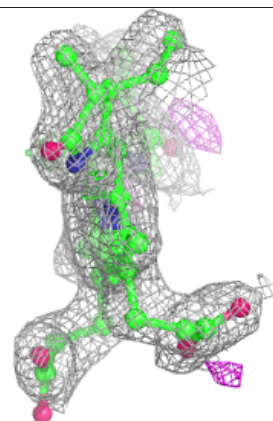
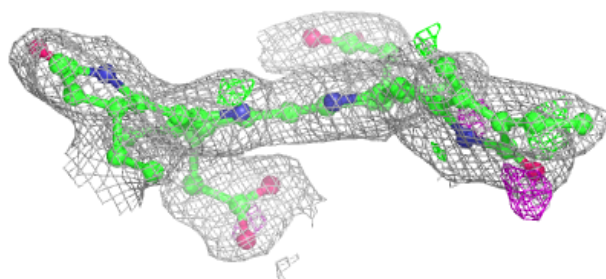
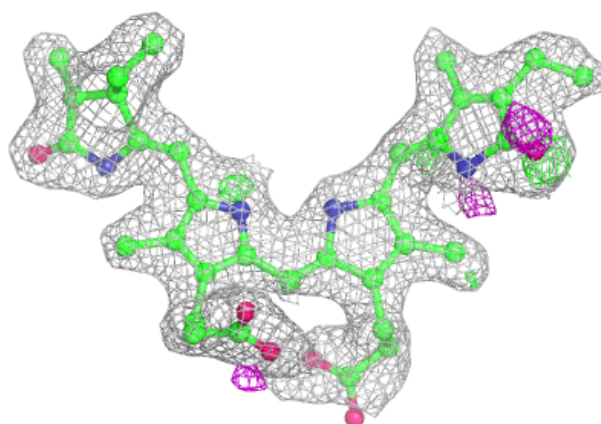
Electron density around CYC D 201:

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

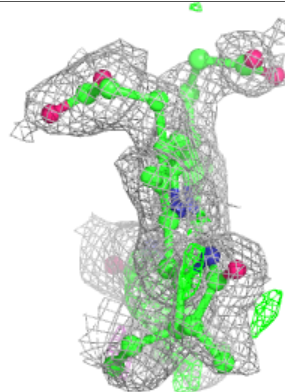
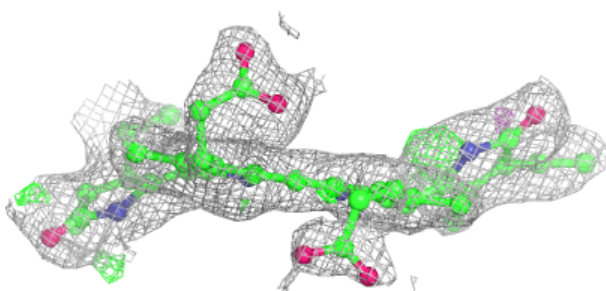
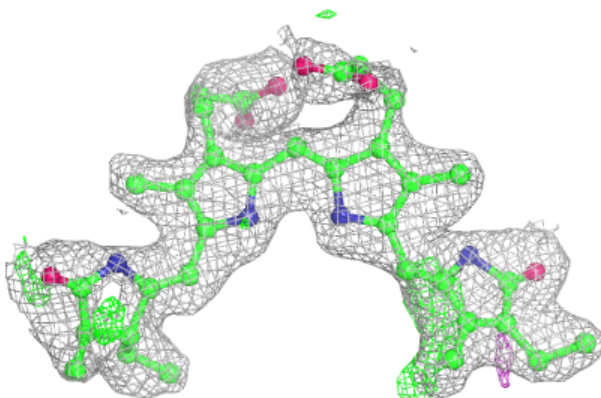


Electron density around CYC J 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

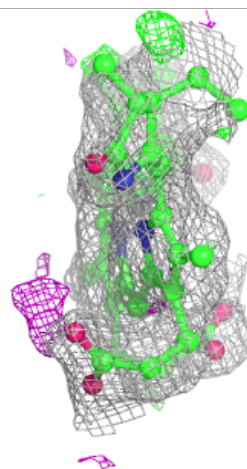
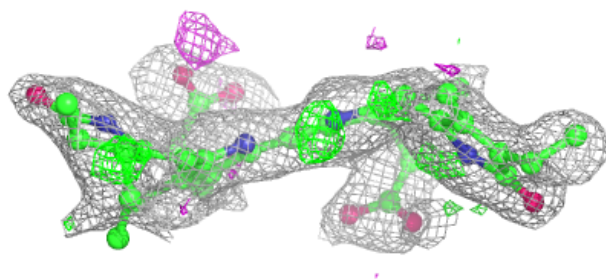
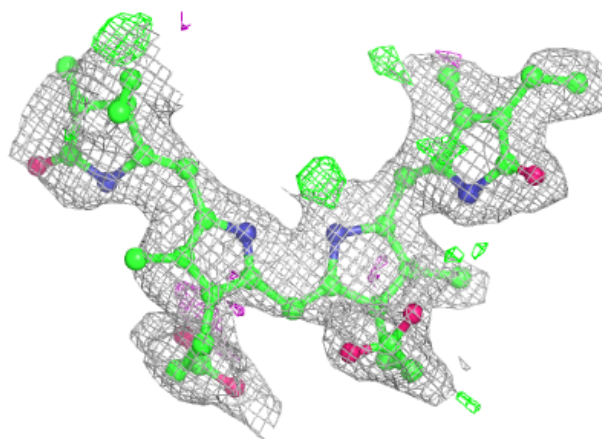
**Electron density around CYC L 202:**

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and green (positive)



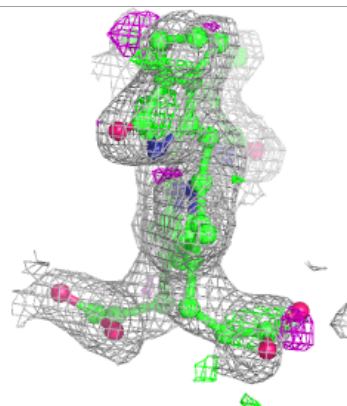
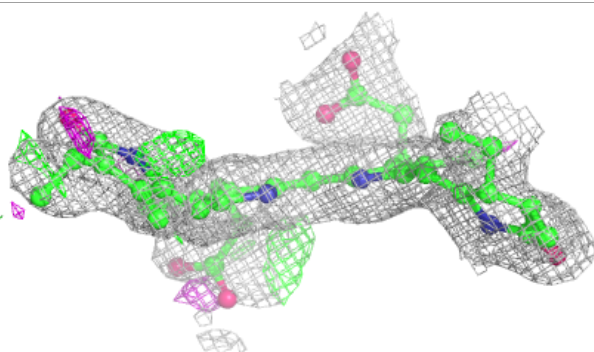
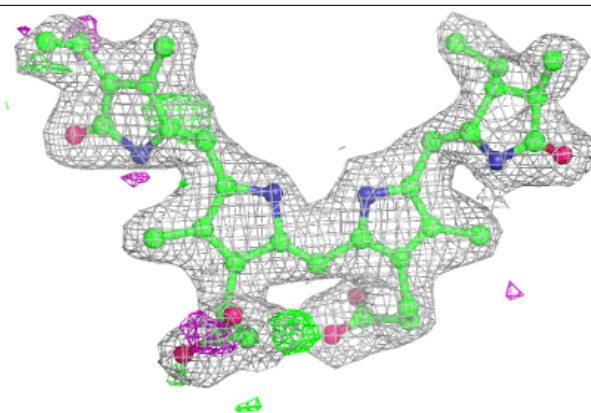
Electron density around CYC C 201:

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and green (positive)

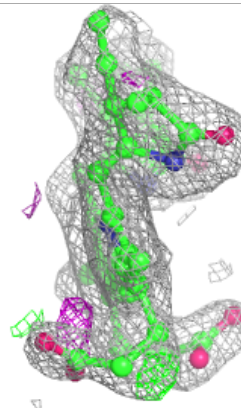
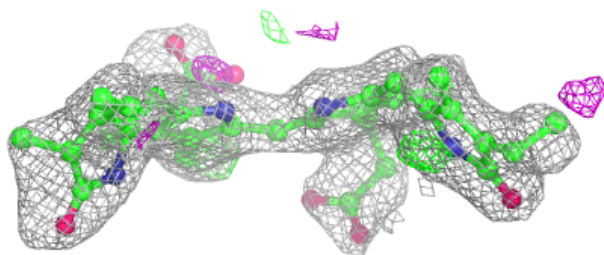
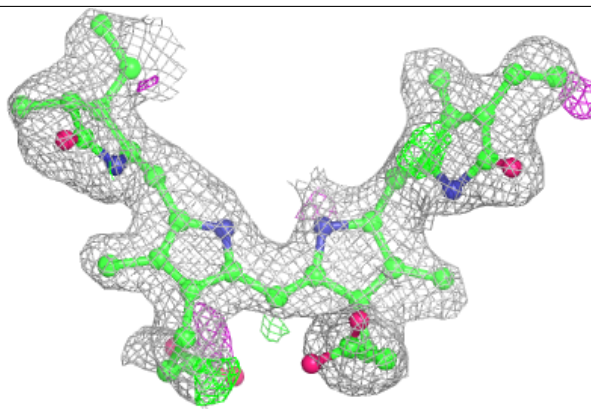


Electron density around CYC H 202:

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and green (positive)

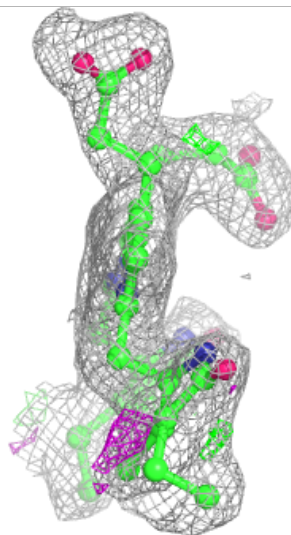
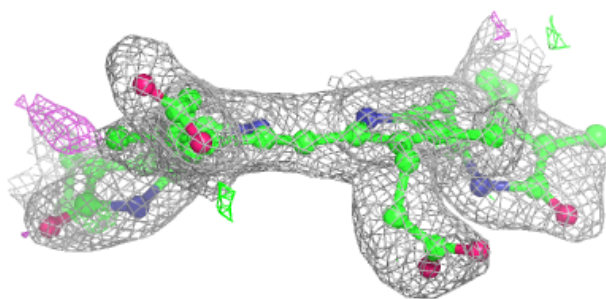
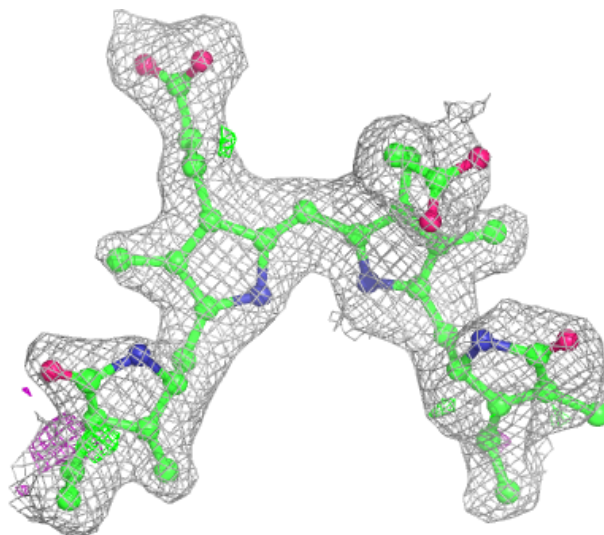
**Electron density around CYC B 201:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



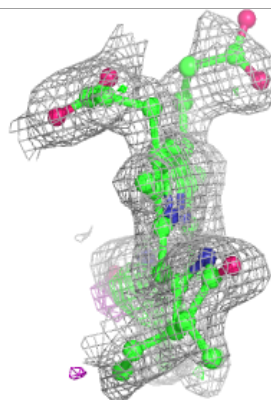
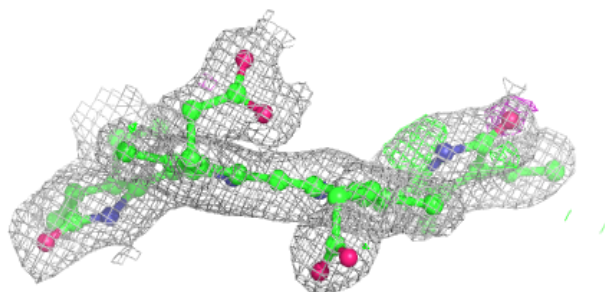
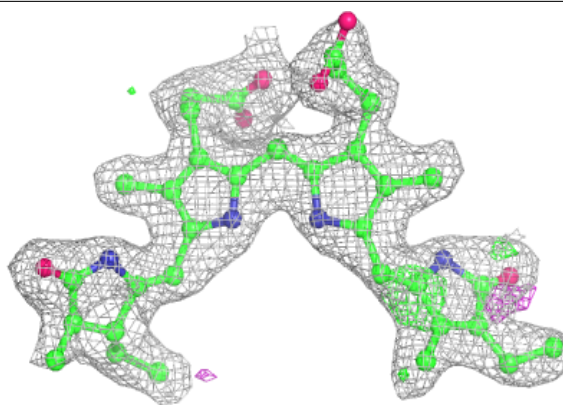
Electron density around PUB L 203:

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and green (positive)

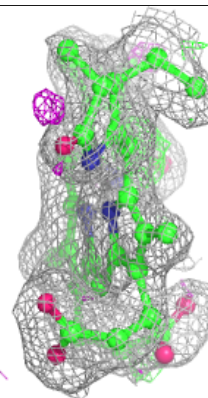
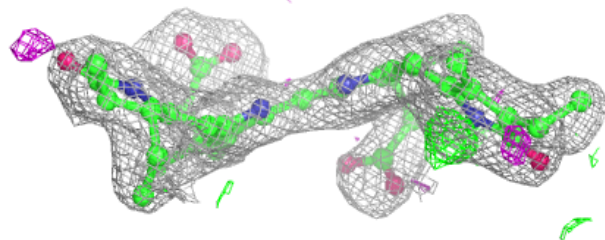
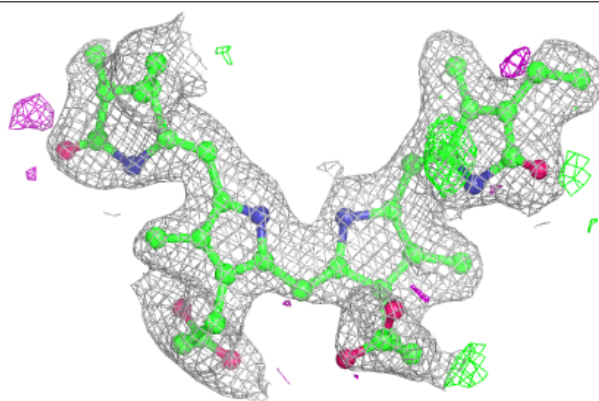


Electron density around CYC G 202:

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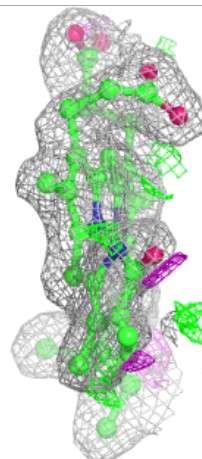
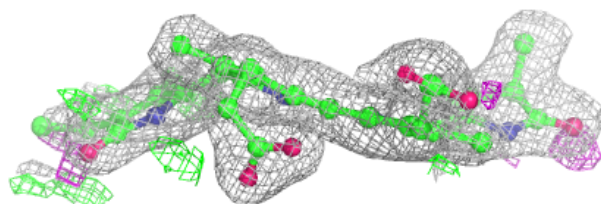
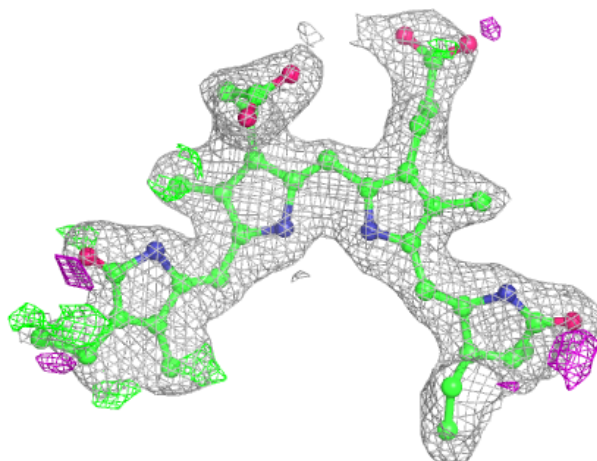
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and green (positive)



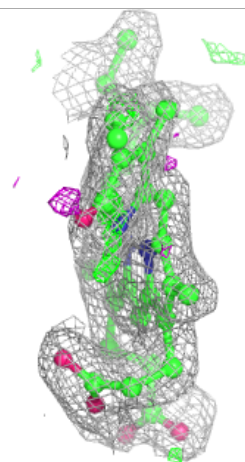
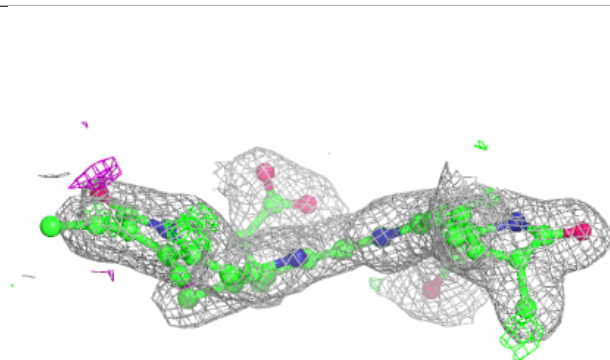
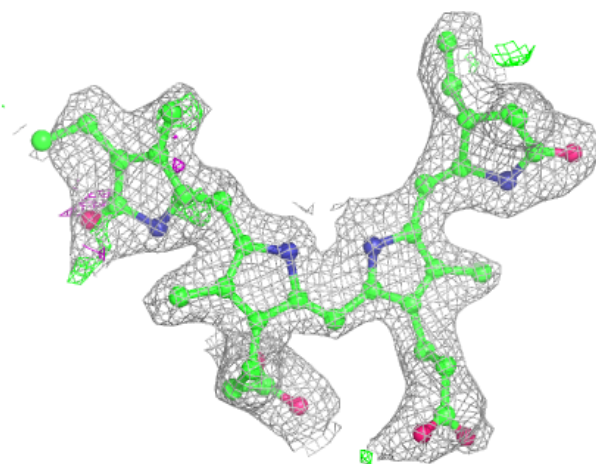
Electron density around CYC D 202:

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and green (positive)



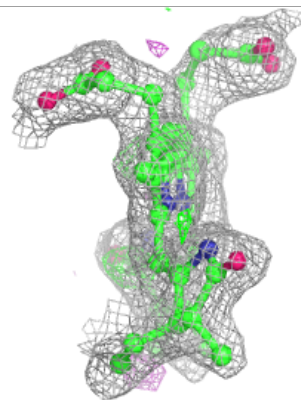
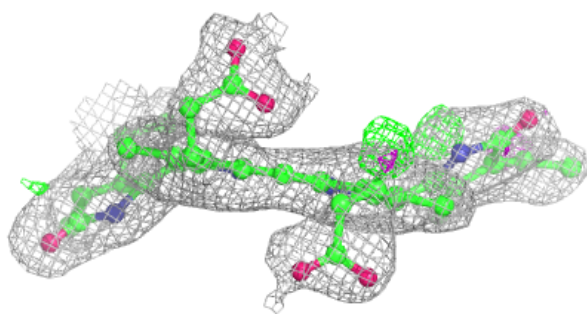
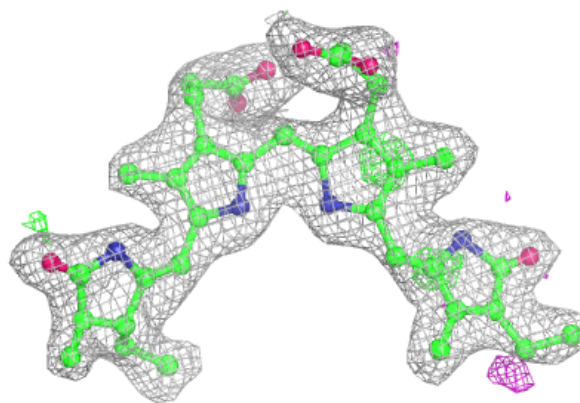
Electron density around CYC C 202:

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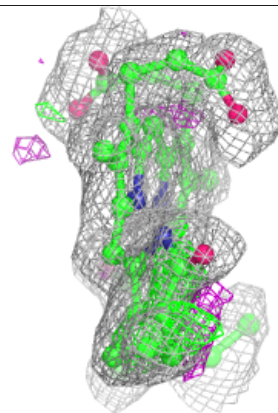
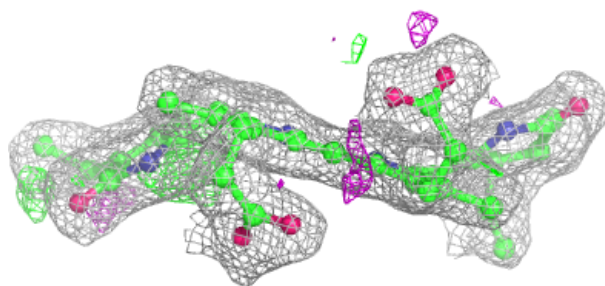
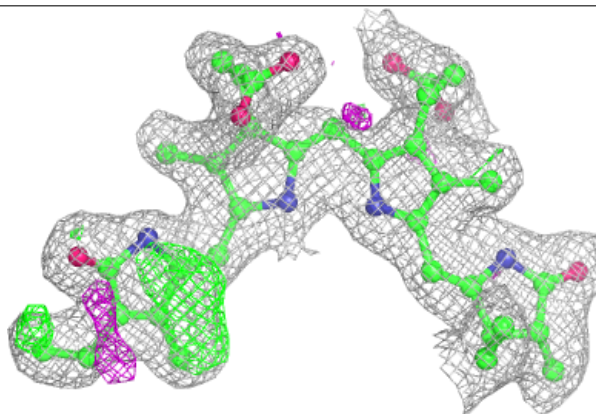


Electron density around CYC K 202:

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and green (positive)

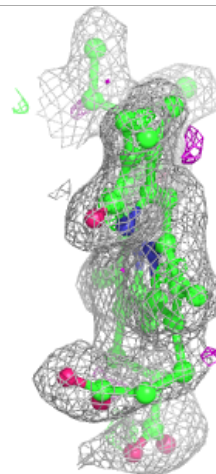
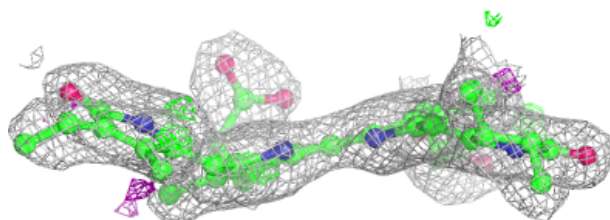
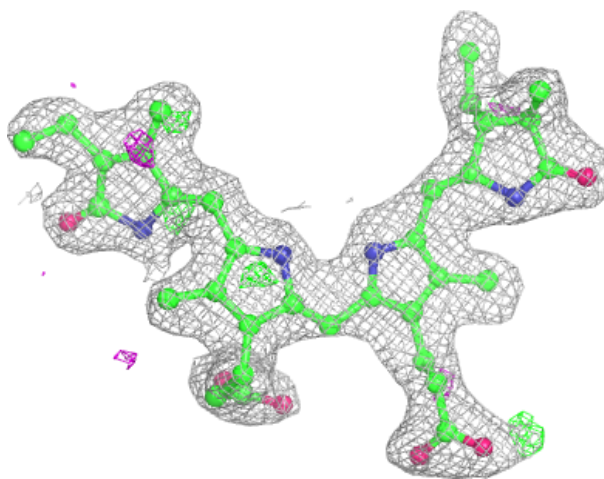
**Electron density around CYC A 201:**

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and green (positive)



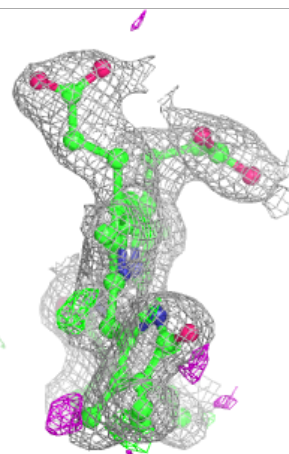
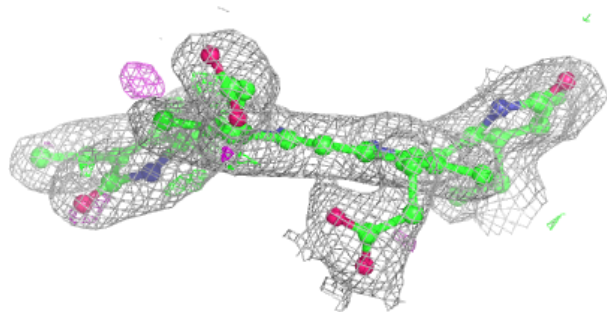
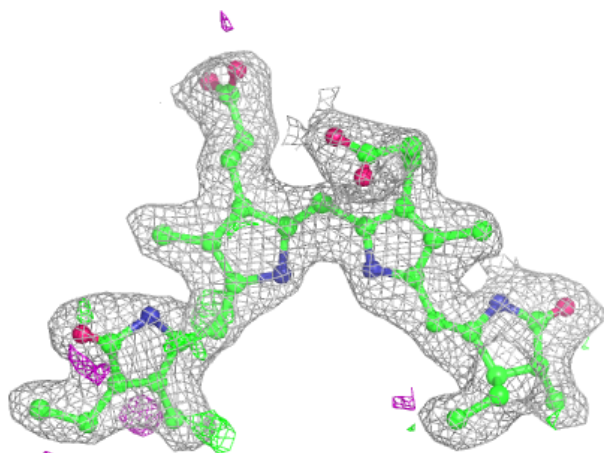
Electron density around CYC I 201:

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and green (positive)



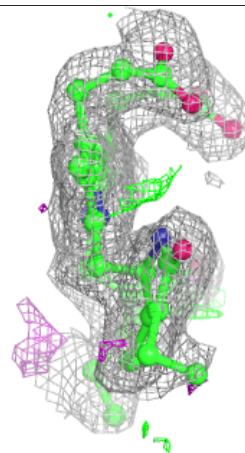
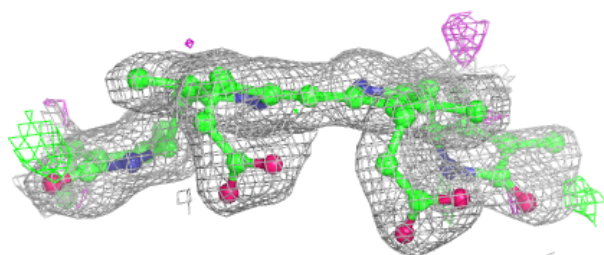
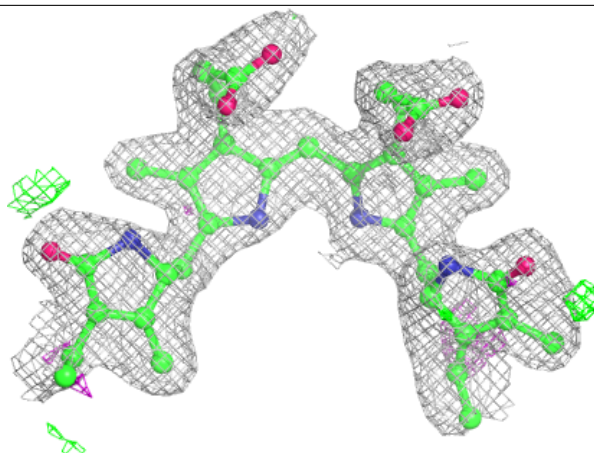
Electron density around CYC I 202:

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and green (positive)



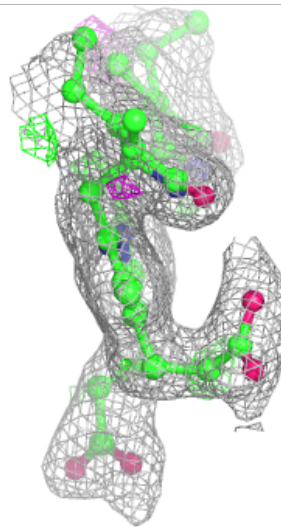
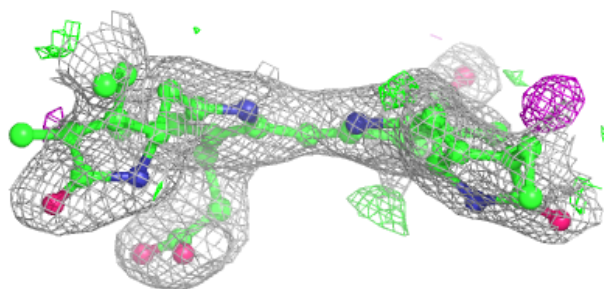
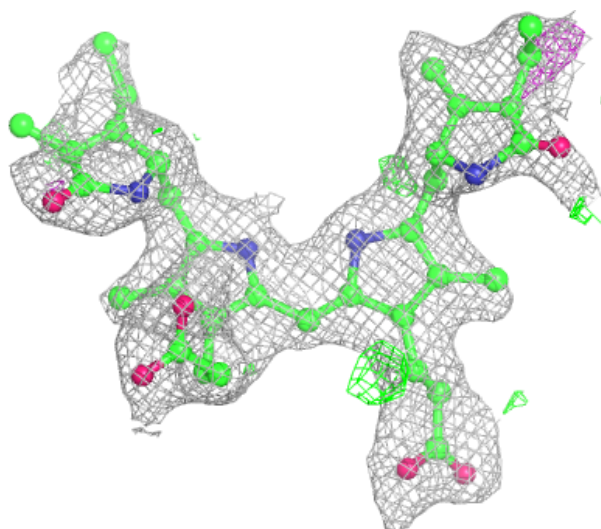
Electron density around PUB G 203:

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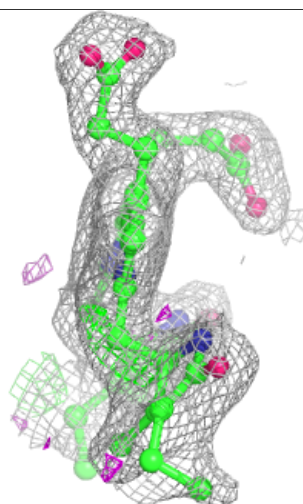
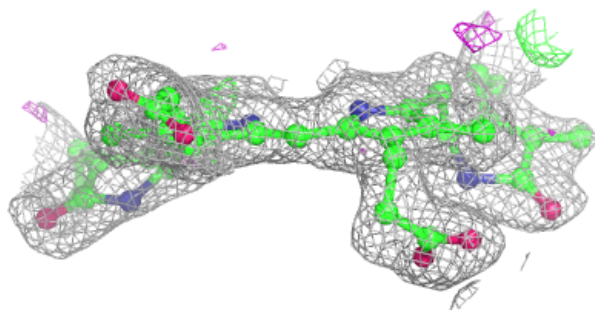
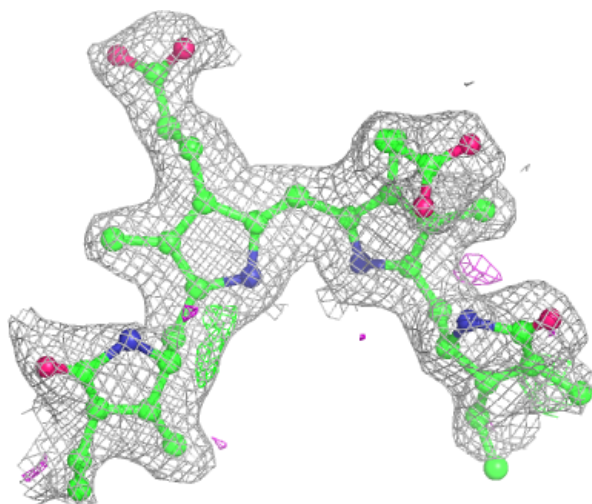
Electron density around PUB J 203:

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and green (positive)



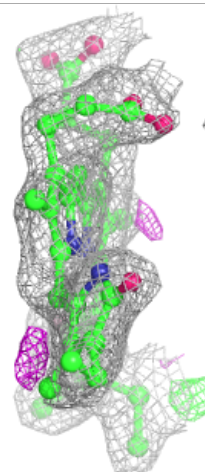
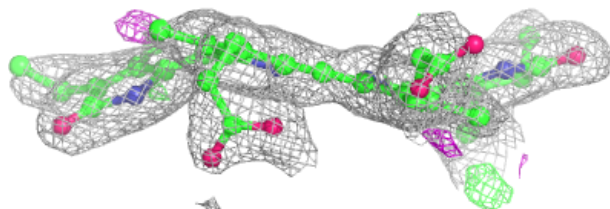
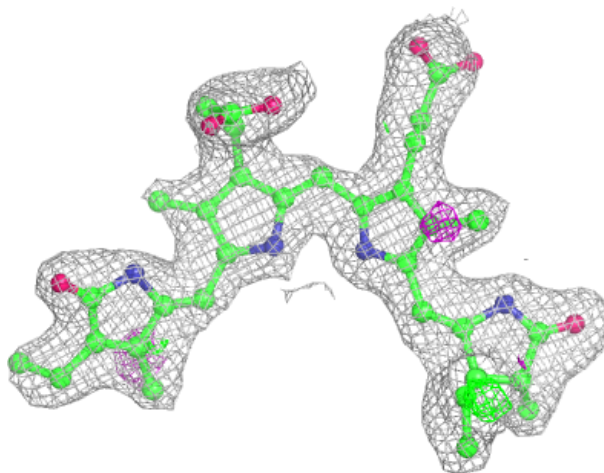
Electron density around PUB K 203:

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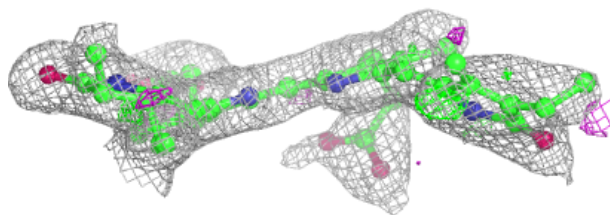
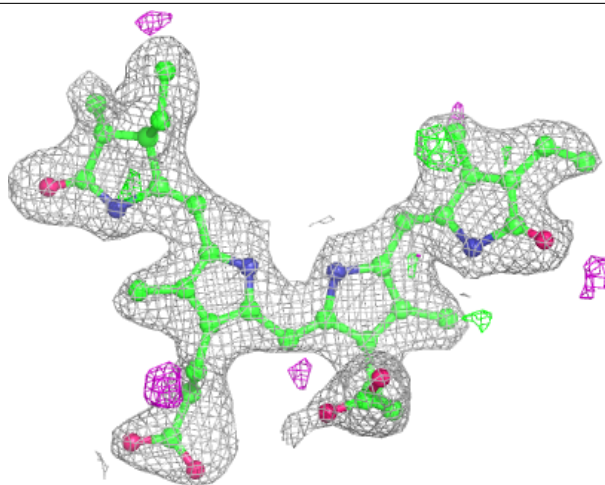
Electron density around CYC J 201:

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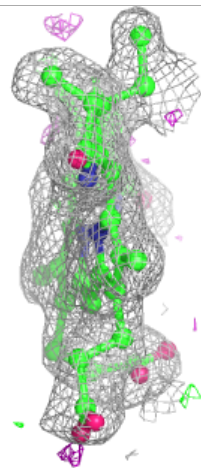
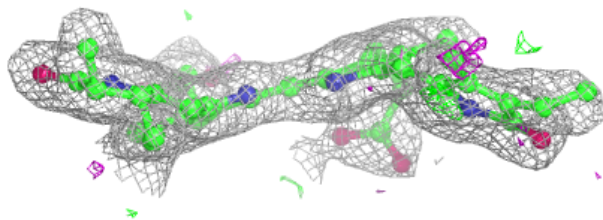
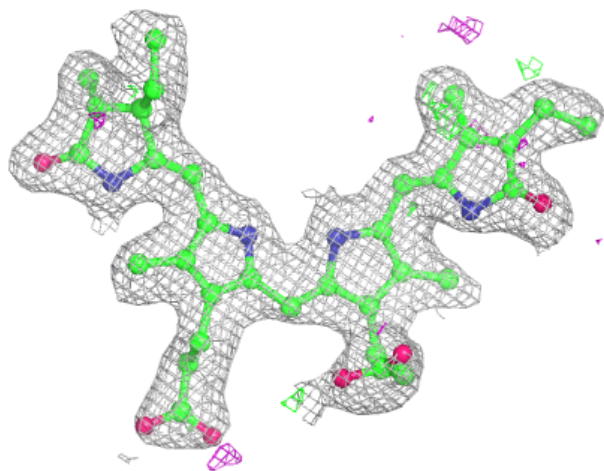
Electron density around CYC L 201:

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and green (positive)



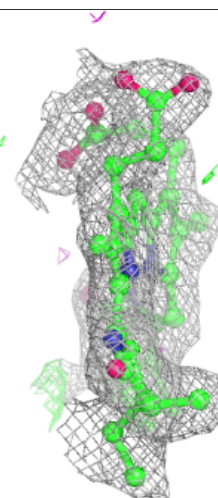
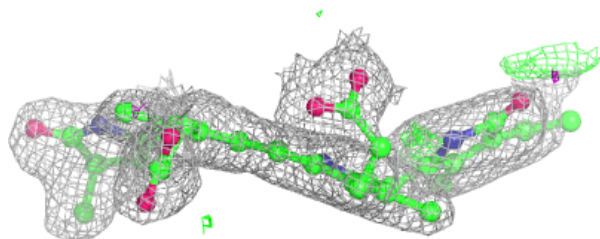
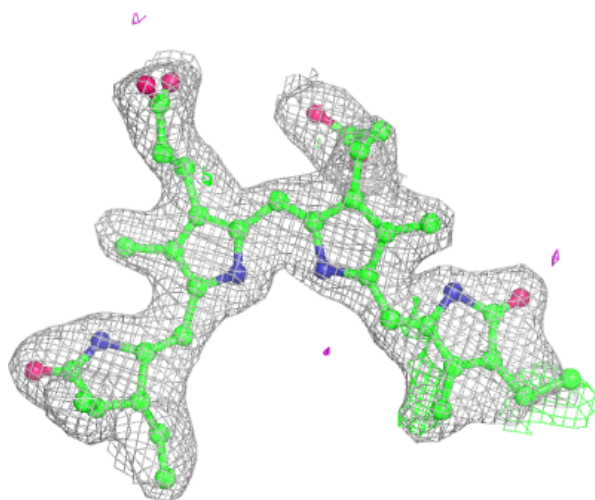
Electron density around CYC G 201:

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and green (positive)



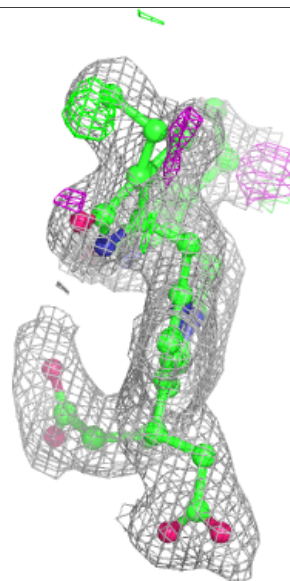
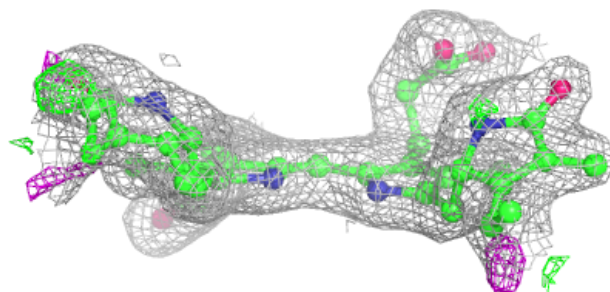
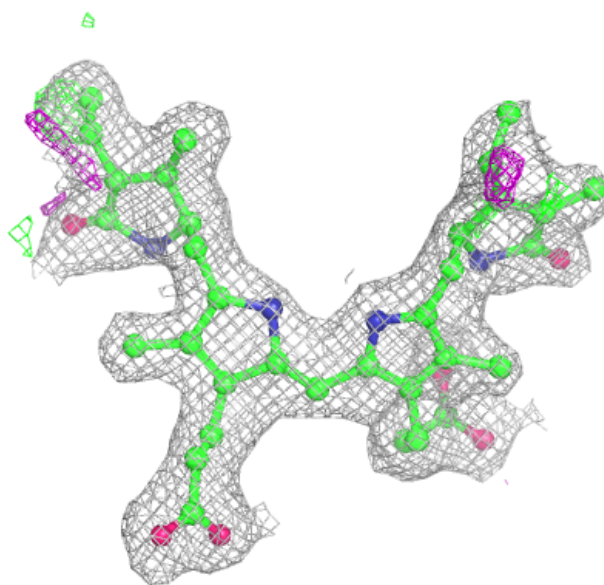
Electron density around CYC E 202:

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



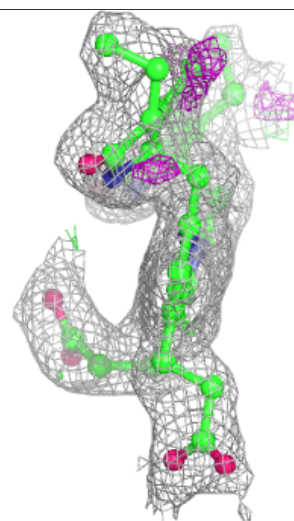
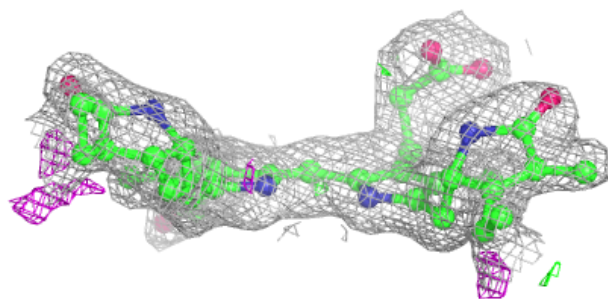
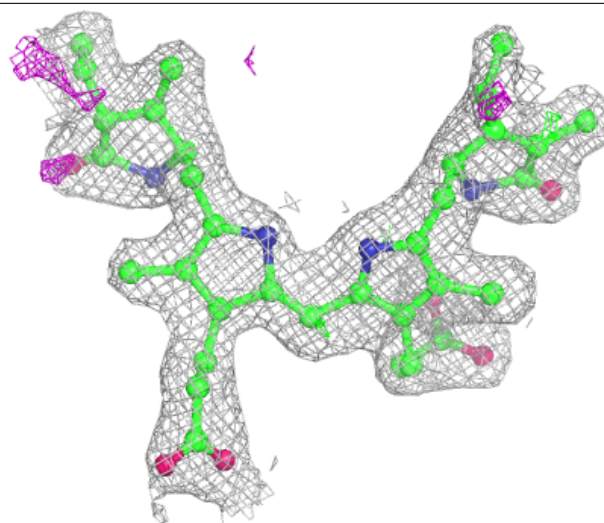
Electron density around PUB H 203:

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



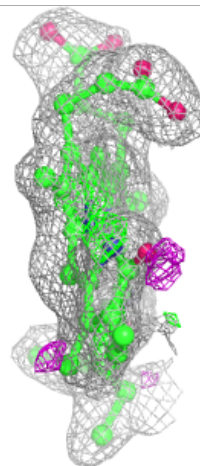
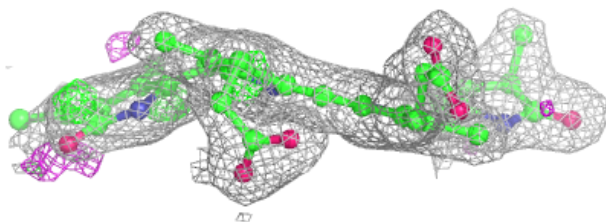
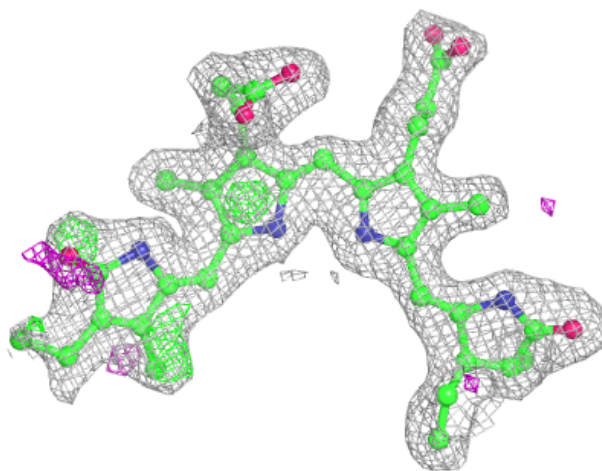
Electron density around PUB I 203:

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



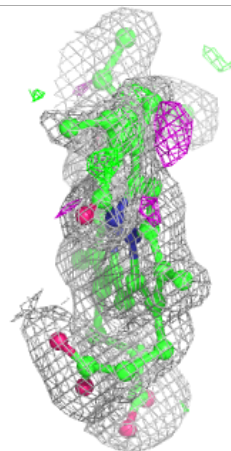
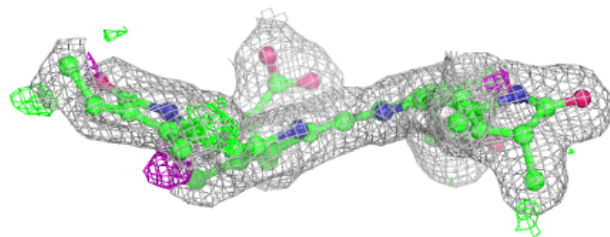
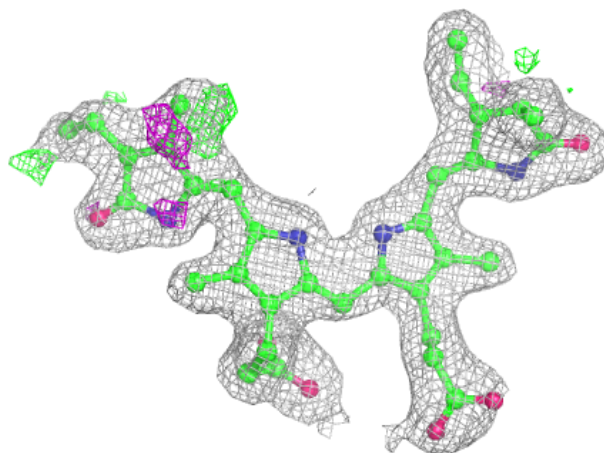
Electron density around CYC B 202:

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



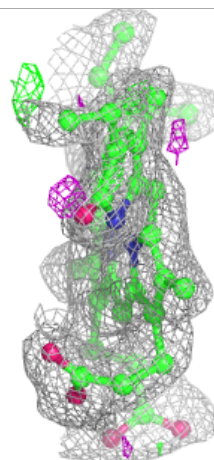
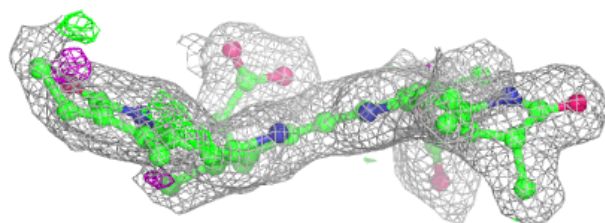
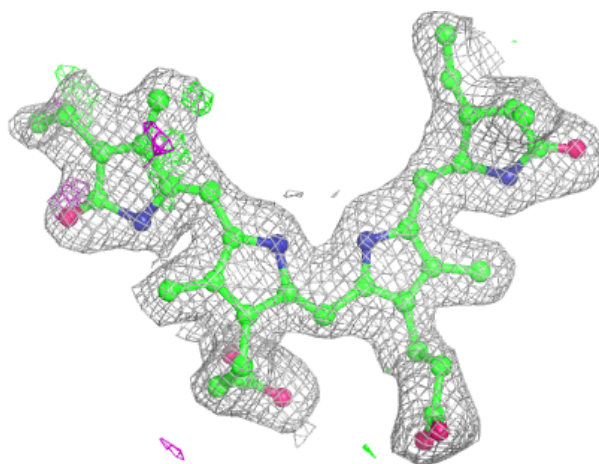
Electron density around CYC F 202:

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



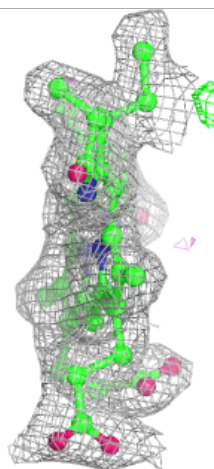
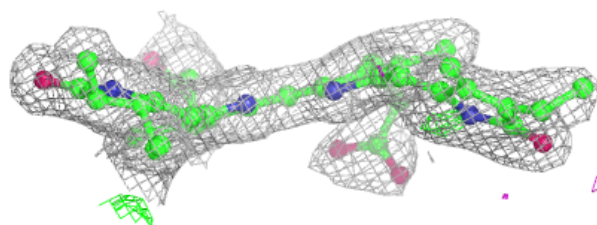
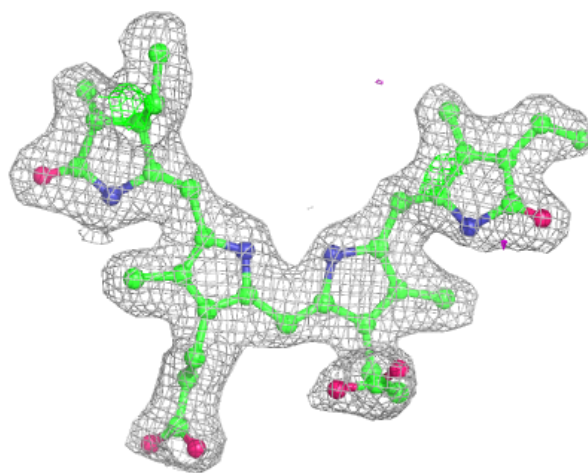
Electron density around CYC A 202:

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



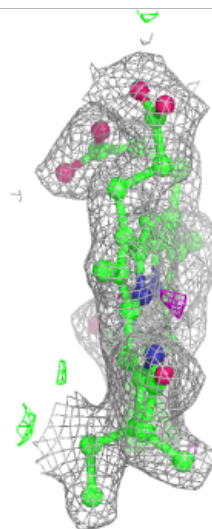
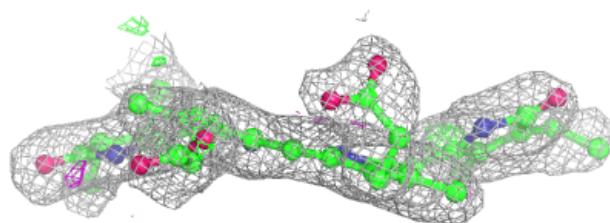
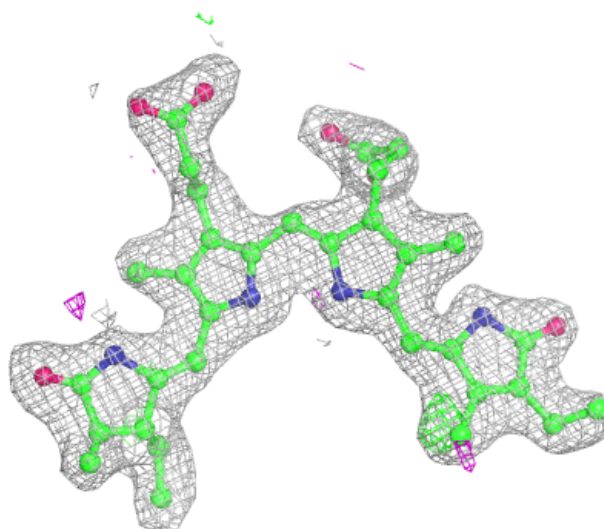
Electron density around CYC K 201:

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



Electron density around CYC H 201:

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.