



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 10:18 PM UTC

PDB ID : 4H0M / pdb_00004h0m
Title : X-Ray Crystal Structure of Phycocyanin from *Synechococcus elongatus* sp. PCC 7942
Authors : Marx, A.; Adir, N.
Deposited on : 2012-09-09
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

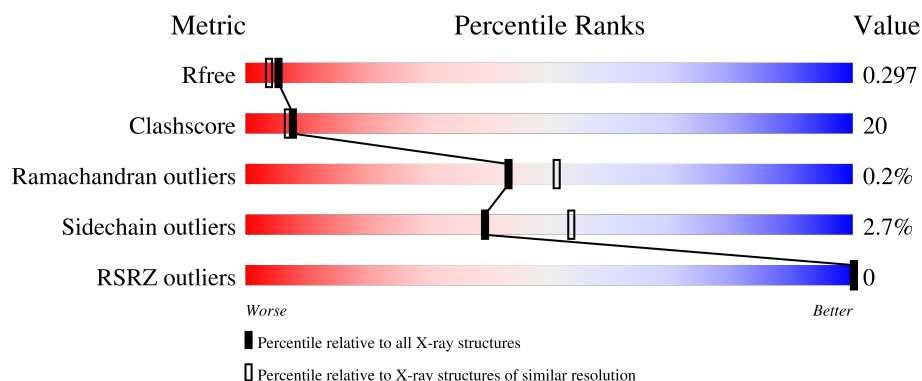
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

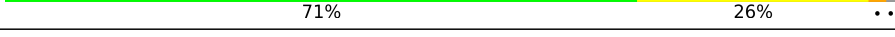
The reported resolution of this entry is 2.20 Å.

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



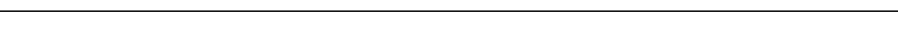
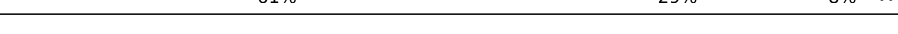
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	163	 66% 31% ..
1	C	163	 65% 32% ..
1	E	163	 74% 23% ...
1	G	163	 71% 26% ..
1	I	163	 74% 24% ..

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Mol	Chain	Length	Quality of chain
1	K	163	
1	M	163	
1	O	163	
1	Q	163	
1	S	163	
1	U	163	
1	W	163	
2	B	173	
2	D	173	
2	F	173	
2	H	173	
2	J	173	
2	L	173	
2	N	173	
2	P	173	
2	R	173	
2	T	173	
2	V	173	
2	X	173	

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
2	MEN	J	72	-	-	X	-
2	MEN	N	72	-	-	X	-
2	MEN	T	72	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32152 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 C-phycocyanin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	C	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	E	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	G	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	I	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	K	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	M	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	O	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	Q	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	S	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	U	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			
1	W	162	Total	C	N	O	S	0	0	0
			1213	766	204	242	1			

- Molecule 2 is a protein called C-phycocyanin beta chain.

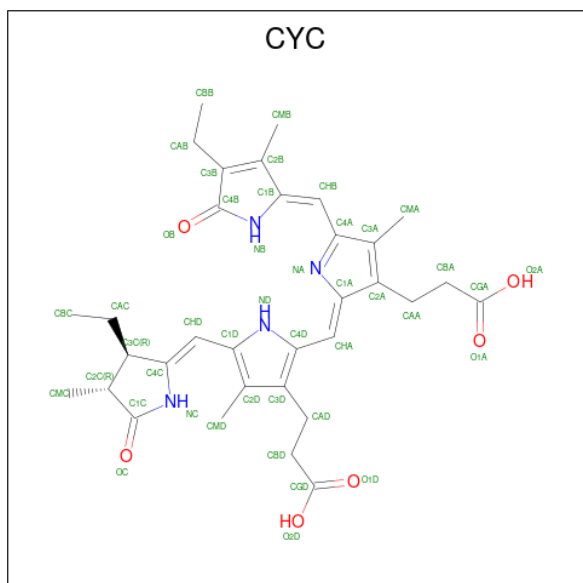
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	D	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	H	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	J	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	L	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	N	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	P	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	R	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	T	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	V	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			
2	X	172	Total	C	N	O	S	0	0	0
			1273	789	228	250	6			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: 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		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	Q	1	Total	C	N	O	0	0
			43	33	4	6		
3	R	1	Total	C	N	O	0	0
			43	33	4	6		
3	R	1	Total	C	N	O	0	0
			43	33	4	6		
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
3	V	1	Total	C	N	O	0	0
			43	33	4	6		
3	V	1	Total	C	N	O	0	0
			43	33	4	6		
3	W	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	41	Total	O	0	0
			41	41		
4	C	31	Total	O	0	0
			31	31		
4	D	38	Total	O	0	0
			38	38		
4	E	46	Total	O	0	0
			46	46		

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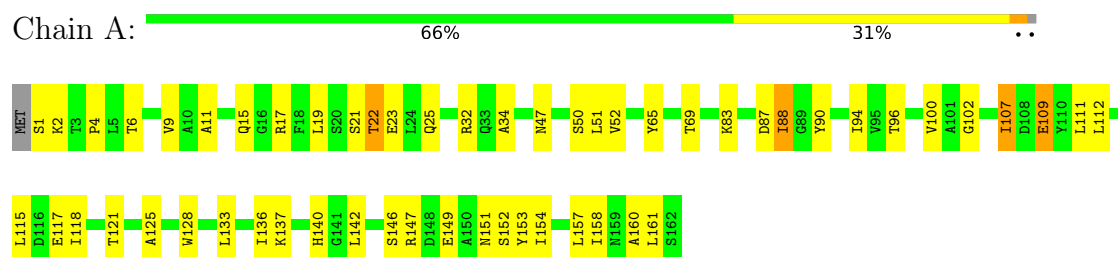
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	19	Total 19	O 19	0	0
4	G	30	Total 30	O 30	0	0
4	H	17	Total 17	O 17	0	0
4	I	34	Total 34	O 34	0	0
4	J	25	Total 25	O 25	0	0
4	K	33	Total 33	O 33	0	0
4	L	20	Total 20	O 20	0	0
4	M	37	Total 37	O 37	0	0
4	N	23	Total 23	O 23	0	0
4	O	35	Total 35	O 35	0	0
4	P	27	Total 27	O 27	0	0
4	Q	38	Total 38	O 38	0	0
4	R	25	Total 25	O 25	0	0
4	S	47	Total 47	O 47	0	0
4	T	21	Total 21	O 21	0	0
4	U	41	Total 41	O 41	0	0
4	V	31	Total 31	O 31	0	0
4	W	40	Total 40	O 40	0	0
4	X	32	Total 32	O 32	0	0

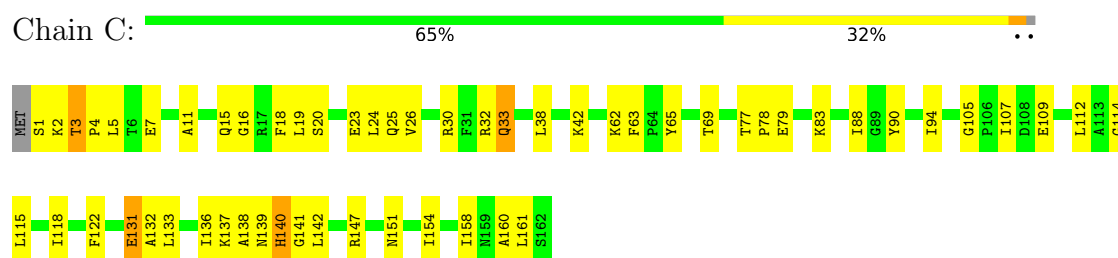
3 Residue-property plots

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.

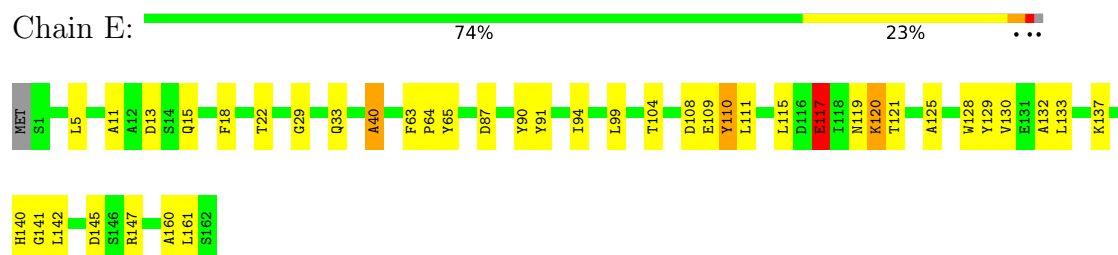
- Molecule 1: C-phycocyanin alpha chain



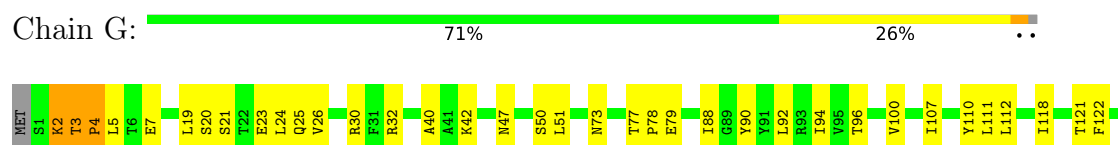
- Molecule 1: C-phycocyanin alpha chain

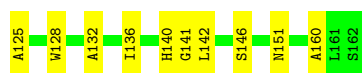


- Molecule 1: C-phycocyanin alpha chain



- Molecule 1: C-phycocyanin alpha chain





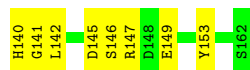
- Molecule 1: C-phycoerythrin alpha chain

Chain I: 74% 24% ..



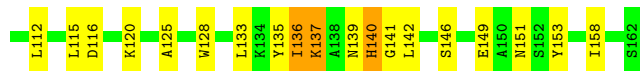
- Molecule 1: C-phycoerythrin alpha chain

Chain K: 74% 23% ..



- Molecule 1: C-phycoerythrin alpha chain

Chain M: 65% 29% 6% .



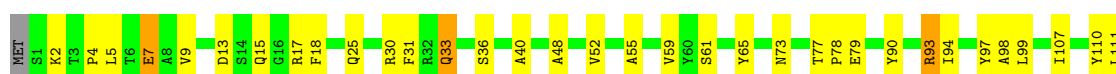
- Molecule 1: C-phycoerythrin alpha chain

Chain O: 76% 19% ..



- Molecule 1: C-phycoerythrin alpha chain

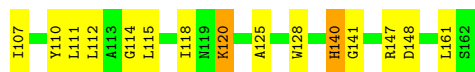
Chain Q: 72% 25% ..





- Molecule 1: C-phycocyanin alpha chain

Chain S: 68% 29% ..



- Molecule 1: C-phycocyanin alpha chain

Chain U: 80% 20% .



- Molecule 1: C-phycocyanin alpha chain

Chain W: 69% 29% ..



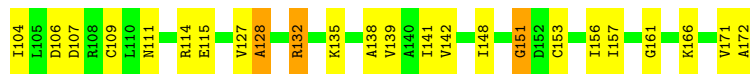
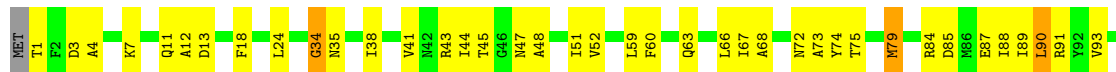
- Molecule 2: C-phycocyanin beta chain

Chain B: 62% 34% ...

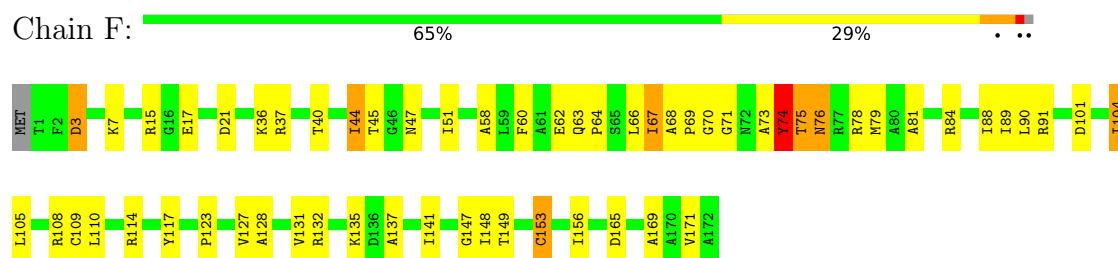


- Molecule 2: C-phycocyanin beta chain

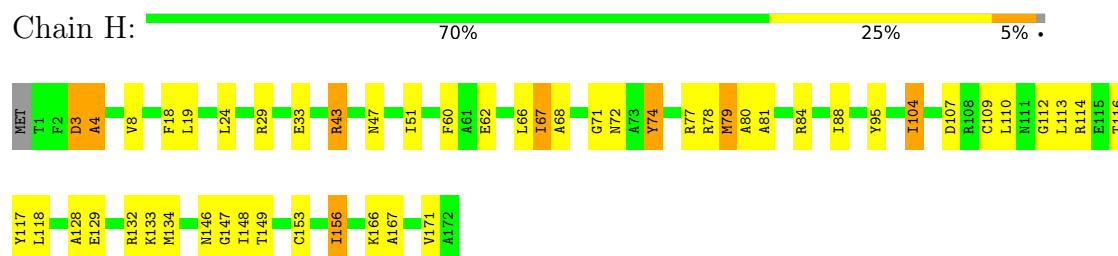
Chain D: 63% 33% ..



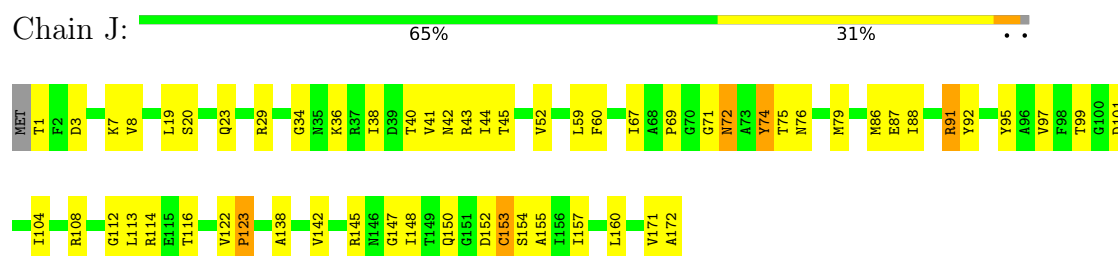
- Molecule 2: C-phycocyanin beta chain



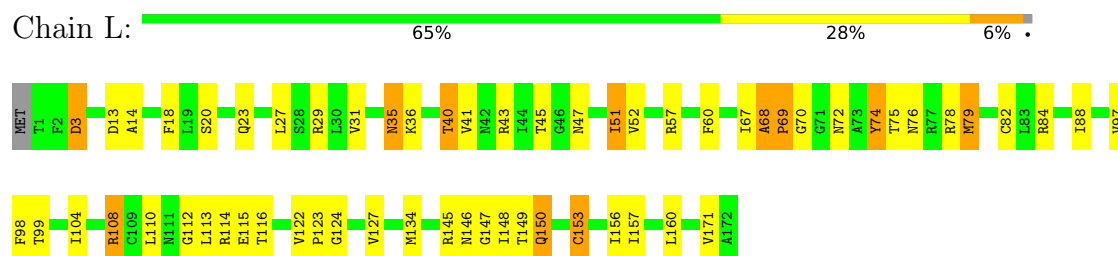
- Molecule 2: C-phycocyanin beta chain



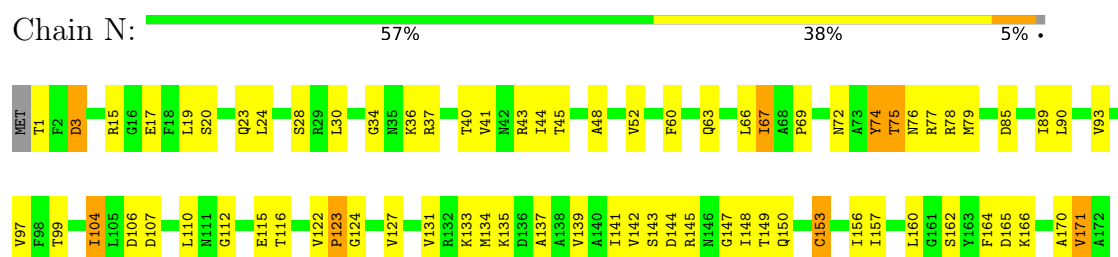
- Molecule 2: C-phycocyanin beta chain



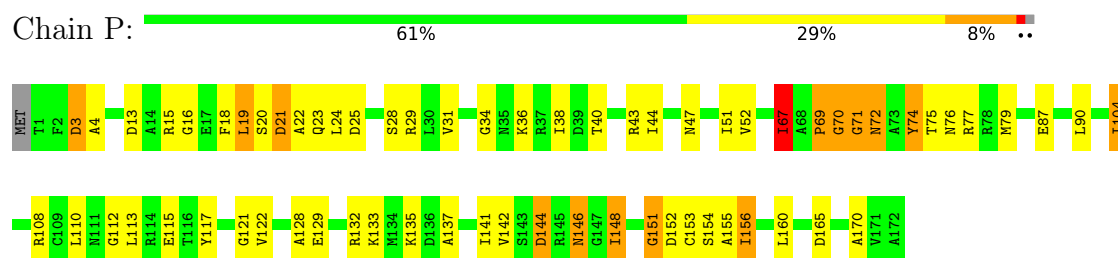
- Molecule 2: C-phycocyanin beta chain



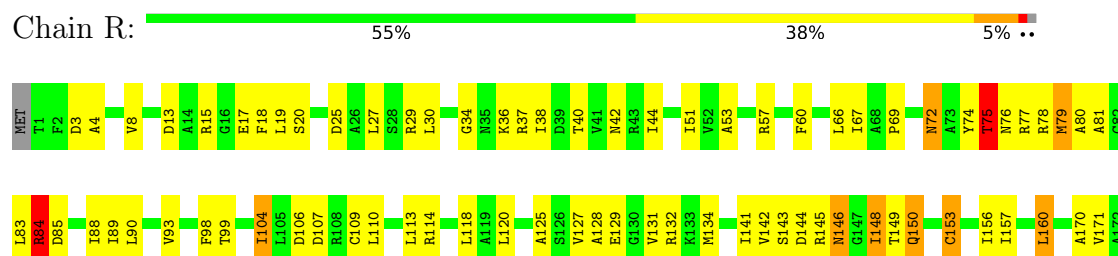
- Molecule 2: C-phycocyanin beta chain



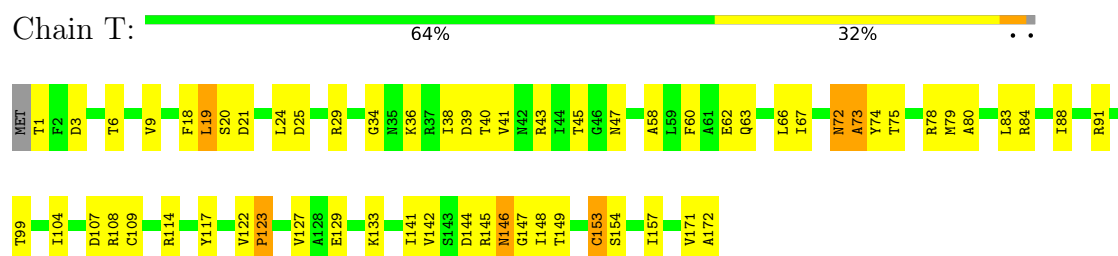
- Molecule 2: C-phycocyanin beta chain



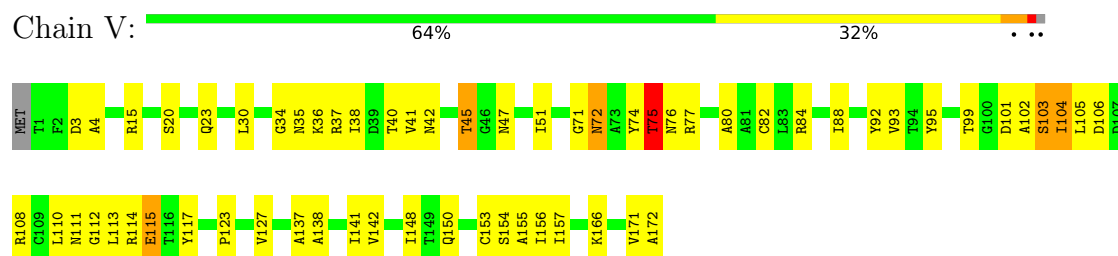
- Molecule 2: C-phycocyanin beta chain



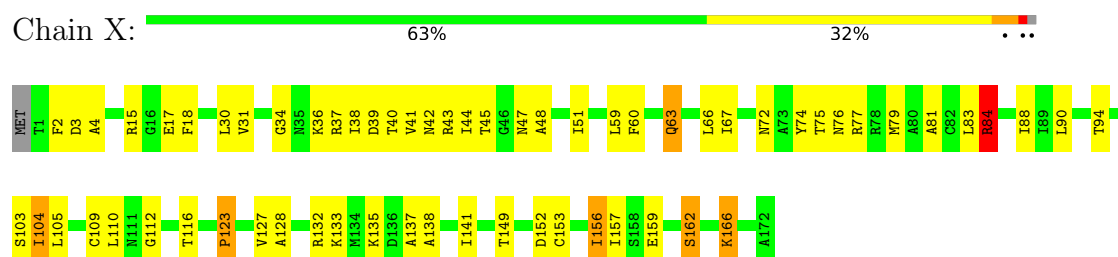
- Molecule 2: C-phycocyanin beta chain



- Molecule 2: C-phycocyanin beta chain



- Molecule 2: C-phycocyanin beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.84Å 113.52Å 184.44Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.00-2.20) 87.3 (40.00-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.295 0.243 , 0.297	Depositor DCC
R_{free} test set	11202 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 1.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32152	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2934e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CYC, MEN

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	1.10	6/1237 (0.5%)	0.97	6/1681 (0.4%)
1	C	1.20	5/1237 (0.4%)	1.06	6/1681 (0.4%)
1	E	1.16	8/1237 (0.6%)	0.95	3/1681 (0.2%)
1	G	1.07	2/1237 (0.2%)	0.97	3/1681 (0.2%)
1	I	1.19	12/1237 (1.0%)	0.96	2/1681 (0.1%)
1	K	1.04	3/1237 (0.2%)	0.98	7/1681 (0.4%)
1	M	1.02	2/1237 (0.2%)	0.99	10/1681 (0.6%)
1	O	1.05	1/1237 (0.1%)	0.99	6/1681 (0.4%)
1	Q	1.07	5/1237 (0.4%)	1.01	6/1681 (0.4%)
1	S	1.26	11/1237 (0.9%)	0.98	1/1681 (0.1%)
1	U	0.97	0/1237	0.90	2/1681 (0.1%)
1	W	1.01	2/1237 (0.2%)	0.99	7/1681 (0.4%)
2	B	1.29	12/1276 (0.9%)	1.15	10/1724 (0.6%)
2	D	1.19	10/1276 (0.8%)	1.07	11/1724 (0.6%)
2	F	1.09	8/1276 (0.6%)	0.98	4/1724 (0.2%)
2	H	1.09	2/1276 (0.2%)	1.01	10/1724 (0.6%)
2	J	1.24	9/1276 (0.7%)	1.02	4/1724 (0.2%)
2	L	1.26	10/1276 (0.8%)	1.11	12/1724 (0.7%)
2	N	1.17	6/1276 (0.5%)	1.04	11/1724 (0.6%)
2	P	1.27	11/1276 (0.9%)	1.15	9/1724 (0.5%)
2	R	1.35	17/1276 (1.3%)	1.14	10/1724 (0.6%)
2	T	1.21	7/1276 (0.5%)	1.09	13/1724 (0.8%)
2	V	1.09	3/1276 (0.2%)	1.03	4/1724 (0.2%)
2	X	1.27	13/1276 (1.0%)	1.11	8/1724 (0.5%)
All	All	1.16	165/30156 (0.5%)	1.03	165/40860 (0.4%)

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	113	LEU	C-N	10.51	1.47	1.33
2	J	29	ARG	C-N	-10.14	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	64	PRO	C-N	9.81	1.47	1.33
2	B	78	ARG	C-O	-9.75	1.12	1.24
2	P	74	TYR	C-O	-9.59	1.12	1.24

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	HIS	CB-CA-C	-15.06	87.23	110.88
1	W	141	GLY	N-CA-C	-10.00	101.17	115.27
2	B	76	ASN	N-CA-C	9.75	122.81	111.11
1	G	141	GLY	N-CA-C	-9.30	103.12	115.21
2	P	74	TYR	O-C-N	-9.15	112.42	122.12

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	1213	0	1183	38	0
1	C	1213	0	1183	47	0
1	E	1213	0	1183	31	0
1	G	1213	0	1183	41	0
1	I	1213	0	1183	33	0
1	K	1213	0	1183	38	0
1	M	1213	0	1183	49	0
1	O	1213	0	1183	38	0
1	Q	1213	0	1183	44	0
1	S	1213	0	1183	48	0
1	U	1213	0	1183	37	0
1	W	1213	0	1183	42	0
2	B	1273	0	1275	73	0
2	D	1273	0	1276	61	0
2	F	1273	0	1276	71	0
2	H	1273	0	1275	62	0
2	J	1273	0	1276	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1273	0	1276	57	0
2	N	1273	0	1275	100	0
2	P	1273	0	1275	71	0
2	R	1273	0	1274	65	0
2	T	1273	0	1274	60	0
2	V	1273	0	1276	59	0
2	X	1273	0	1275	47	0
3	A	43	0	37	1	0
3	B	86	0	71	18	0
3	C	43	0	37	3	0
3	D	86	0	74	17	0
3	E	43	0	37	2	0
3	F	86	0	74	13	0
3	G	43	0	37	2	0
3	H	86	0	73	5	0
3	I	43	0	37	4	0
3	J	86	0	76	14	0
3	K	43	0	37	5	0
3	L	86	0	74	12	0
3	M	43	0	37	1	0
3	N	86	0	74	9	0
3	O	43	0	37	1	0
3	P	86	0	73	15	0
3	Q	43	0	37	1	0
3	R	86	0	74	7	0
3	S	43	0	37	3	0
3	T	86	0	71	17	0
3	U	43	0	37	1	0
3	V	86	0	75	17	0
3	W	43	0	37	2	0
3	X	86	0	72	8	0
4	A	41	0	0	2	0
4	B	41	0	0	2	0
4	C	31	0	0	1	0
4	D	38	0	0	3	0
4	E	46	0	0	4	0
4	F	19	0	0	1	0
4	G	30	0	0	3	0
4	H	17	0	0	3	0
4	I	34	0	0	4	0
4	J	25	0	0	2	0
4	K	33	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	20	0	0	0	0
4	M	37	0	0	0	0
4	N	23	0	0	3	0
4	O	35	0	0	5	0
4	P	27	0	0	1	0
4	Q	38	0	0	4	0
4	R	25	0	0	2	0
4	S	47	0	0	2	0
4	T	21	0	0	2	0
4	U	41	0	0	1	0
4	V	31	0	0	0	0
4	W	40	0	0	4	0
4	X	32	0	0	1	0
All	All	32152	0	30824	1230	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 20.

The worst 5 of 1230 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:F:153:CYS:SG	3:F:202:CYC:HAC2	1.28	1.66
2:D:153:CYS:SG	3:D:202:CYC:HAC2	1.12	1.62
2:J:153:CYS:SG	3:J:202:CYC:HAC2	1.38	1.59
2:V:153:CYS:SG	3:V:202:CYC:HAC2	1.60	1.40
2:N:72:MEN:CE2	2:N:123:PRO:HD2	1.52	1.39

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	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
1	C	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
1	E	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
1	G	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
1	I	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
1	K	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
1	M	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
1	O	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
1	Q	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
1	S	160/163 (98%)	158 (99%)	2 (1%)	0	100	100
1	U	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
1	W	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	B	169/173 (98%)	166 (98%)	2 (1%)	1 (1%)	21	23
2	D	169/173 (98%)	161 (95%)	8 (5%)	0	100	100
2	F	169/173 (98%)	165 (98%)	2 (1%)	2 (1%)	10	8
2	H	169/173 (98%)	165 (98%)	4 (2%)	0	100	100
2	J	169/173 (98%)	166 (98%)	2 (1%)	1 (1%)	21	23
2	L	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
2	N	169/173 (98%)	164 (97%)	5 (3%)	0	100	100
2	P	169/173 (98%)	160 (95%)	8 (5%)	1 (1%)	21	23
2	R	169/173 (98%)	165 (98%)	4 (2%)	0	100	100
2	T	169/173 (98%)	166 (98%)	2 (1%)	1 (1%)	21	23
2	V	169/173 (98%)	164 (97%)	2 (1%)	3 (2%)	6	4
2	X	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	3948/4032 (98%)	3832 (97%)	107 (3%)	9 (0%)	43	51

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	74	TYR
2	V	103	SER
2	V	104	ILE
2	P	71	GLY
2	V	75	THR

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	122/123 (99%)	121 (99%)	1 (1%)	73	85
1	C	122/123 (99%)	119 (98%)	3 (2%)	42	56
1	E	122/123 (99%)	120 (98%)	2 (2%)	55	71
1	G	122/123 (99%)	120 (98%)	2 (2%)	55	71
1	I	122/123 (99%)	120 (98%)	2 (2%)	55	71
1	K	122/123 (99%)	119 (98%)	3 (2%)	42	56
1	M	122/123 (99%)	118 (97%)	4 (3%)	33	45
1	O	122/123 (99%)	118 (97%)	4 (3%)	33	45
1	Q	122/123 (99%)	118 (97%)	4 (3%)	33	45
1	S	122/123 (99%)	118 (97%)	4 (3%)	33	45
1	U	122/123 (99%)	121 (99%)	1 (1%)	73	85
1	W	122/123 (99%)	119 (98%)	3 (2%)	42	56
2	B	127/128 (99%)	122 (96%)	5 (4%)	28	39
2	D	127/128 (99%)	126 (99%)	1 (1%)	73	85
2	F	127/128 (99%)	124 (98%)	3 (2%)	43	58
2	H	127/128 (99%)	122 (96%)	5 (4%)	28	39
2	J	127/128 (99%)	124 (98%)	3 (2%)	43	58
2	L	127/128 (99%)	125 (98%)	2 (2%)	55	71
2	N	127/128 (99%)	124 (98%)	3 (2%)	43	58
2	P	127/128 (99%)	122 (96%)	5 (4%)	28	39
2	R	127/128 (99%)	119 (94%)	8 (6%)	16	19
2	T	127/128 (99%)	125 (98%)	2 (2%)	55	71
2	V	127/128 (99%)	121 (95%)	6 (5%)	23	31
2	X	127/128 (99%)	122 (96%)	5 (4%)	28	39
All	All	2988/3012 (99%)	2907 (97%)	81 (3%)	39	53

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	148	ILE
2	V	111	ASN
2	R	160	LEU
2	T	145	ARG
1	W	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	25	GLN
2	X	63	GLN
1	O	15	GLN
2	X	47	ASN
2	V	35	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	MEN	P	72	2	7,8,9	1.80	3 (42%)	4,9,11	1.22	1 (25%)
2	MEN	R	72	2	7,8,9	4.42	2 (28%)	4,9,11	2.77	3 (75%)
2	MEN	V	72	2	7,8,9	3.42	4 (57%)	4,9,11	2.79	2 (50%)
2	MEN	N	72	2	7,8,9	0.47	0	4,9,11	0.53	0
2	MEN	J	72	2	7,8,9	1.49	1 (14%)	4,9,11	1.87	2 (50%)
2	MEN	B	72	2	7,8,9	1.23	1 (14%)	4,9,11	0.50	0
2	MEN	D	72	2	7,8,9	0.99	0	4,9,11	0.55	0
2	MEN	H	72	2	7,8,9	1.44	1 (14%)	4,9,11	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	T	72	2	7,8,9	1.22	0	4,9,11	1.46	1 (25%)
2	MEN	X	72	2	7,8,9	0.84	0	4,9,11	0.81	0
2	MEN	F	72	2	7,8,9	0.97	0	4,9,11	0.45	0
2	MEN	L	72	2	7,8,9	0.52	0	4,9,11	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	P	72	2	-	4/7/8/10	-
2	MEN	R	72	2	-	4/7/8/10	-
2	MEN	V	72	2	-	3/7/8/10	-
2	MEN	N	72	2	-	4/7/8/10	-
2	MEN	J	72	2	-	0/7/8/10	-
2	MEN	B	72	2	-	2/7/8/10	-
2	MEN	D	72	2	-	4/7/8/10	-
2	MEN	H	72	2	-	4/7/8/10	-
2	MEN	T	72	2	-	4/7/8/10	-
2	MEN	X	72	2	-	2/7/8/10	-
2	MEN	F	72	2	-	4/7/8/10	-
2	MEN	L	72	2	-	6/7/8/10	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	72	MEN	CE2-ND2	-10.40	1.27	1.45
2	V	72	MEN	CB-CG	-5.52	1.39	1.51
2	V	72	MEN	CB-CA	-5.47	1.42	1.53
2	R	72	MEN	CG-ND2	-4.44	1.14	1.34
2	H	72	MEN	CB-CG	3.51	1.59	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	72	MEN	CB-CG-ND2	-4.76	109.32	115.53
2	R	72	MEN	OD1-CG-CB	-4.06	115.59	121.54
2	R	72	MEN	CB-CG-ND2	3.03	119.48	115.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	72	MEN	CE2-ND2-CG	-2.85	100.94	121.92
2	P	72	MEN	CE2-ND2-CG	2.44	139.90	121.92

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	CB-CG-ND2-CE2
2	B	72	MEN	OD1-CG-ND2-CE2
2	D	72	MEN	CB-CG-ND2-CE2
2	D	72	MEN	OD1-CG-ND2-CE2
2	F	72	MEN	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	72	MEN	2	0
2	R	72	MEN	1	0
2	V	72	MEN	1	0
2	N	72	MEN	22	0
2	J	72	MEN	10	0
2	D	72	MEN	2	0
2	T	72	MEN	13	0
2	X	72	MEN	1	0
2	L	72	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 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	L	202	2	46,46,46	2.51	17 (36%)	63,67,67	3.58	32 (50%)
3	CYC	P	201	2	46,46,46	2.22	14 (30%)	63,67,67	3.33	26 (41%)
3	CYC	R	201	2	46,46,46	2.26	14 (30%)	63,67,67	3.23	25 (39%)
3	CYC	E	201	1	46,46,46	2.20	16 (34%)	63,67,67	3.21	26 (41%)
3	CYC	T	201	2	46,46,46	2.18	14 (30%)	63,67,67	3.21	24 (38%)
3	CYC	B	202	2	46,46,46	3.20	17 (36%)	63,67,67	3.81	33 (52%)
3	CYC	X	202	2	46,46,46	3.19	20 (43%)	63,67,67	4.03	32 (50%)
3	CYC	H	202	2	46,46,46	2.20	14 (30%)	63,67,67	3.59	31 (49%)
3	CYC	Q	201	1	46,46,46	2.31	18 (39%)	63,67,67	3.22	28 (44%)
3	CYC	T	202	2	46,46,46	3.65	17 (36%)	63,67,67	3.87	32 (50%)
3	CYC	W	201	1	46,46,46	2.25	16 (34%)	63,67,67	3.27	24 (38%)
3	CYC	N	202	2	46,46,46	3.16	18 (39%)	63,67,67	3.34	34 (53%)
3	CYC	X	201	2	46,46,46	2.28	14 (30%)	63,67,67	3.30	27 (42%)
3	CYC	A	201	1	46,46,46	2.18	17 (36%)	63,67,67	3.34	27 (42%)
3	CYC	O	201	1	46,46,46	2.26	17 (36%)	63,67,67	3.17	25 (39%)
3	CYC	J	202	2	46,46,46	2.59	17 (36%)	63,67,67	3.70	30 (47%)
3	CYC	D	202	2	46,46,46	3.93	15 (32%)	63,67,67	3.95	32 (50%)
3	CYC	R	202	2	46,46,46	2.21	16 (34%)	63,67,67	3.35	31 (49%)
3	CYC	F	201	2	46,46,46	2.19	14 (30%)	63,67,67	3.20	23 (36%)
3	CYC	N	201	2	46,46,46	2.30	16 (34%)	63,67,67	3.25	29 (46%)
3	CYC	J	201	2	46,46,46	2.27	16 (34%)	63,67,67	3.33	28 (44%)
3	CYC	S	201	1	46,46,46	2.20	15 (32%)	63,67,67	3.23	26 (41%)
3	CYC	L	201	-	46,46,46	2.33	15 (32%)	63,67,67	3.25	27 (42%)
3	CYC	V	201	-	46,46,46	2.32	14 (30%)	63,67,67	3.29	27 (42%)
3	CYC	K	201	1	46,46,46	2.23	15 (32%)	63,67,67	3.23	26 (41%)
3	CYC	C	201	1	46,46,46	2.22	14 (30%)	63,67,67	3.23	27 (42%)
3	CYC	B	201	2	46,46,46	2.38	15 (32%)	63,67,67	3.28	24 (38%)
3	CYC	H	201	2	46,46,46	2.29	17 (36%)	63,67,67	3.30	26 (41%)
3	CYC	I	201	1	46,46,46	2.32	17 (36%)	63,67,67	3.28	28 (44%)
3	CYC	G	201	1	46,46,46	2.27	17 (36%)	63,67,67	3.25	27 (42%)
3	CYC	F	202	2	46,46,46	2.59	18 (39%)	63,67,67	3.60	29 (46%)
3	CYC	U	201	1	46,46,46	2.20	17 (36%)	63,67,67	3.28	24 (38%)
3	CYC	M	201	1	46,46,46	2.32	15 (32%)	63,67,67	3.27	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYC	V	202	2	46,46,46	2.77	17 (36%)	63,67,67	3.62	28 (44%)
3	CYC	D	201	2	46,46,46	2.26	15 (32%)	63,67,67	3.34	25 (39%)
3	CYC	P	202	2	46,46,46	2.80	14 (30%)	63,67,67	3.45	31 (49%)

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	L	202	2	-	10/26/74/74	0/4/4/4
3	CYC	P	201	2	-	6/26/74/74	0/4/4/4
3	CYC	R	201	2	-	8/26/74/74	0/4/4/4
3	CYC	E	201	1	-	11/26/74/74	0/4/4/4
3	CYC	T	201	2	-	7/26/74/74	0/4/4/4
3	CYC	B	202	2	-	10/26/74/74	0/4/4/4
3	CYC	X	202	2	-	9/26/74/74	0/4/4/4
3	CYC	H	202	2	-	8/26/74/74	0/4/4/4
3	CYC	Q	201	1	-	9/26/74/74	0/4/4/4
3	CYC	T	202	2	-	11/26/74/74	0/4/4/4
3	CYC	W	201	1	-	13/26/74/74	0/4/4/4
3	CYC	N	202	2	-	11/26/74/74	0/4/4/4
3	CYC	X	201	2	-	8/26/74/74	0/4/4/4
3	CYC	A	201	1	-	10/26/74/74	0/4/4/4
3	CYC	O	201	1	-	12/26/74/74	0/4/4/4
3	CYC	J	202	2	-	9/26/74/74	0/4/4/4
3	CYC	D	202	2	-	11/26/74/74	0/4/4/4
3	CYC	R	202	2	-	8/26/74/74	0/4/4/4
3	CYC	F	201	2	-	10/26/74/74	0/4/4/4
3	CYC	N	201	2	-	10/26/74/74	0/4/4/4
3	CYC	J	201	2	-	8/26/74/74	0/4/4/4
3	CYC	S	201	1	-	10/26/74/74	0/4/4/4
3	CYC	L	201	-	-	9/26/74/74	0/4/4/4
3	CYC	V	201	-	-	7/26/74/74	0/4/4/4
3	CYC	K	201	1	-	12/26/74/74	0/4/4/4
3	CYC	C	201	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	B	201	2	-	6/26/74/74	0/4/4/4
3	CYC	H	201	2	-	9/26/74/74	0/4/4/4
3	CYC	I	201	1	-	10/26/74/74	0/4/4/4
3	CYC	G	201	1	-	11/26/74/74	0/4/4/4
3	CYC	F	202	2	-	9/26/74/74	0/4/4/4
3	CYC	U	201	1	-	9/26/74/74	0/4/4/4
3	CYC	M	201	1	-	7/26/74/74	0/4/4/4
3	CYC	V	202	2	-	8/26/74/74	0/4/4/4
3	CYC	D	201	2	-	8/26/74/74	0/4/4/4
3	CYC	P	202	2	-	9/26/74/74	0/4/4/4

The worst 5 of 572 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	202	CYC	CBD-CGD	-20.80	1.02	1.50
3	T	202	CYC	CBD-CGD	-18.88	1.06	1.50
3	B	202	CYC	CBD-CGD	-14.28	1.17	1.50
3	X	202	CYC	CBD-CGD	-14.04	1.18	1.50
3	P	202	CYC	CBD-CGD	-12.54	1.21	1.50

The worst 5 of 1001 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	CYC	CAD-CBD-CGD	15.84	155.68	113.67
3	D	202	CYC	C3B-C4B-NB	13.57	117.59	106.77
3	L	201	CYC	C3B-C4B-NB	13.37	117.43	106.77
3	P	202	CYC	C3B-C4B-NB	13.28	117.36	106.77
3	W	201	CYC	C3B-C4B-NB	13.25	117.34	106.77

There are no chirality outliers.

5 of 333 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	201	CYC	C4C-C3C-CAC-CBC
3	B	201	CYC	NA-C4A-CHB-C1B
3	B	201	CYC	C3A-C4A-CHB-C1B

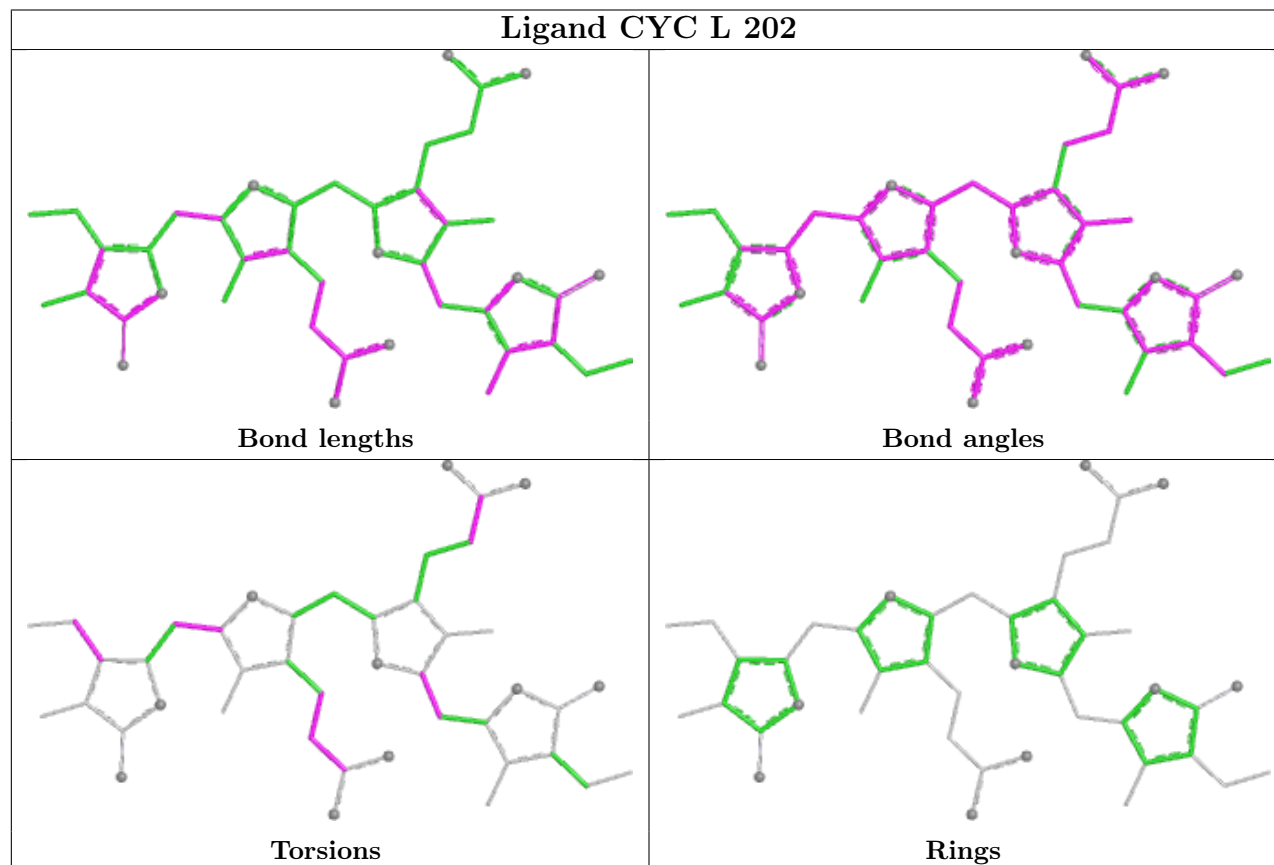
There are no ring outliers.

36 monomers are involved in 178 short contacts:

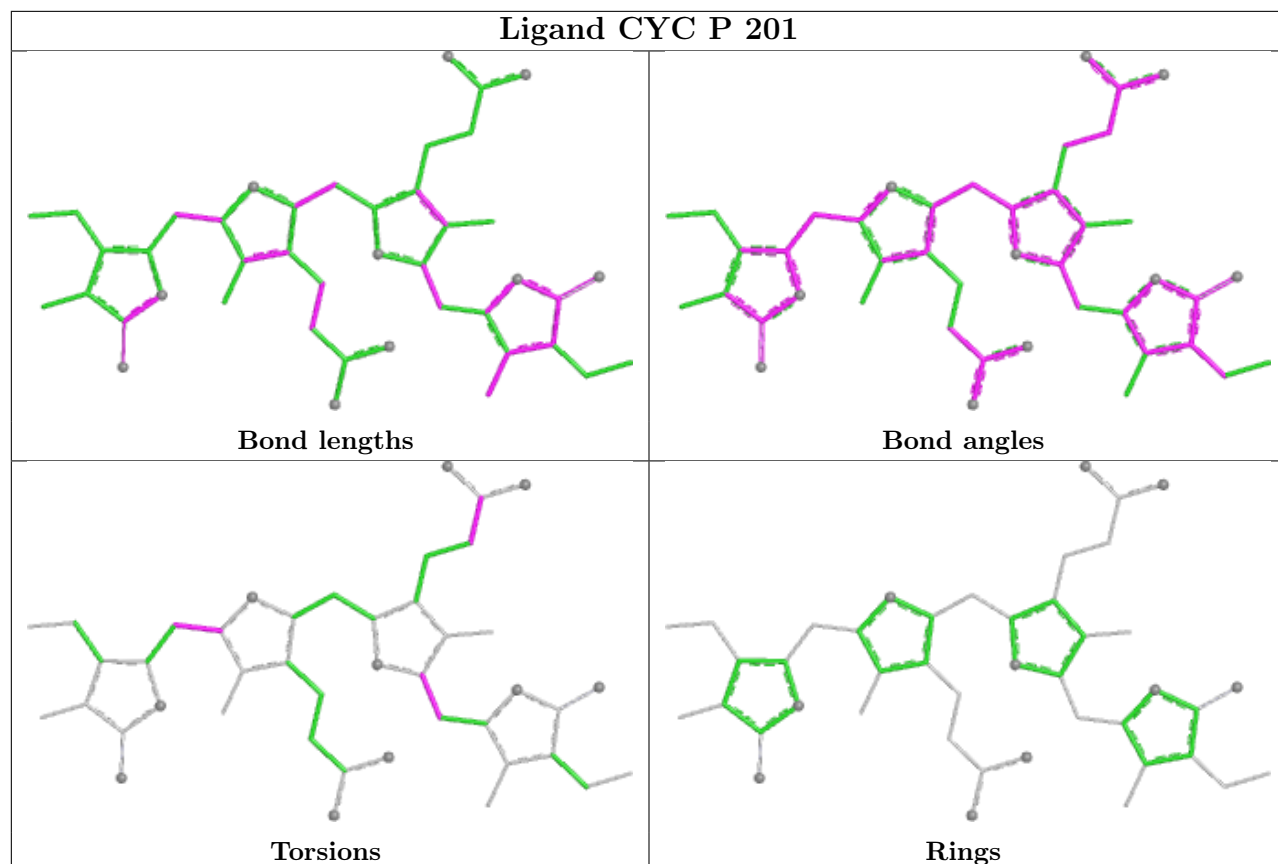
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	202	CYC	6	0
3	P	201	CYC	2	0
3	R	201	CYC	2	0
3	E	201	CYC	2	0
3	T	201	CYC	12	0
3	B	202	CYC	14	0
3	X	202	CYC	6	0
3	H	202	CYC	2	0
3	Q	201	CYC	1	0
3	T	202	CYC	5	0
3	W	201	CYC	2	0
3	N	202	CYC	4	0
3	X	201	CYC	2	0
3	A	201	CYC	1	0
3	O	201	CYC	1	0
3	J	202	CYC	7	0
3	D	202	CYC	14	0
3	R	202	CYC	5	0
3	F	201	CYC	2	0
3	N	201	CYC	5	0
3	J	201	CYC	7	0
3	S	201	CYC	3	0
3	L	201	CYC	6	0
3	V	201	CYC	6	0
3	K	201	CYC	5	0
3	C	201	CYC	3	0
3	B	201	CYC	4	0
3	H	201	CYC	3	0
3	I	201	CYC	4	0
3	G	201	CYC	2	0
3	F	202	CYC	11	0
3	U	201	CYC	1	0
3	M	201	CYC	1	0
3	V	202	CYC	11	0
3	D	201	CYC	3	0
3	P	202	CYC	13	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

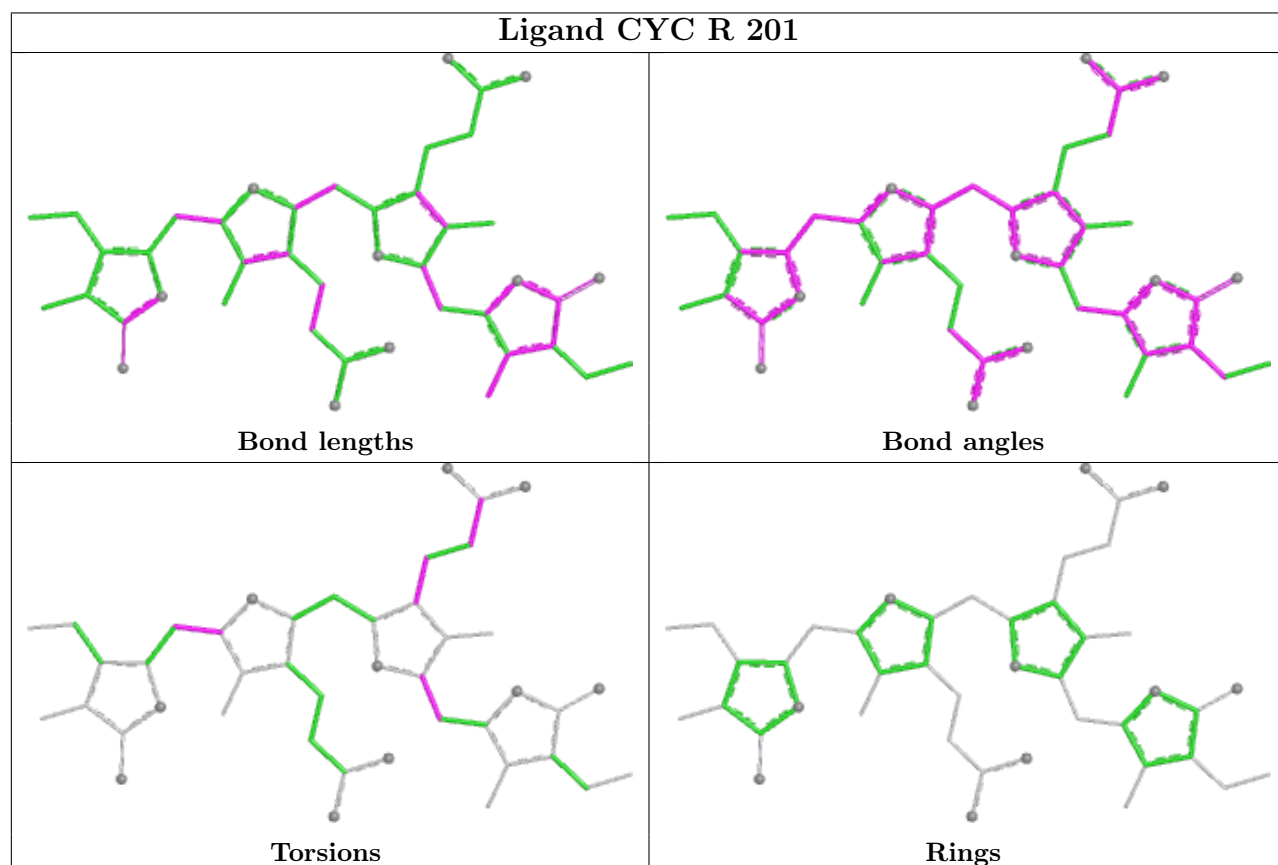
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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



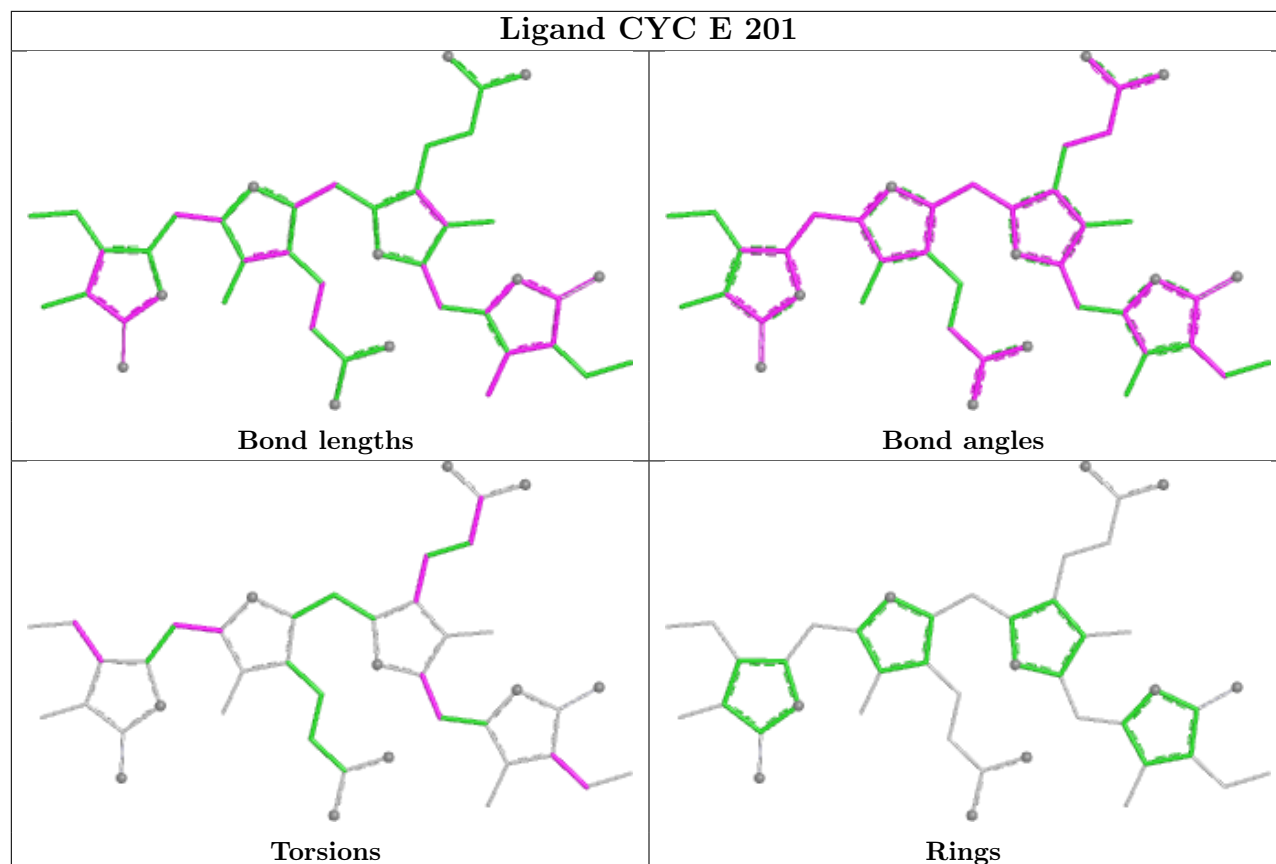
Ligand CYC P 201



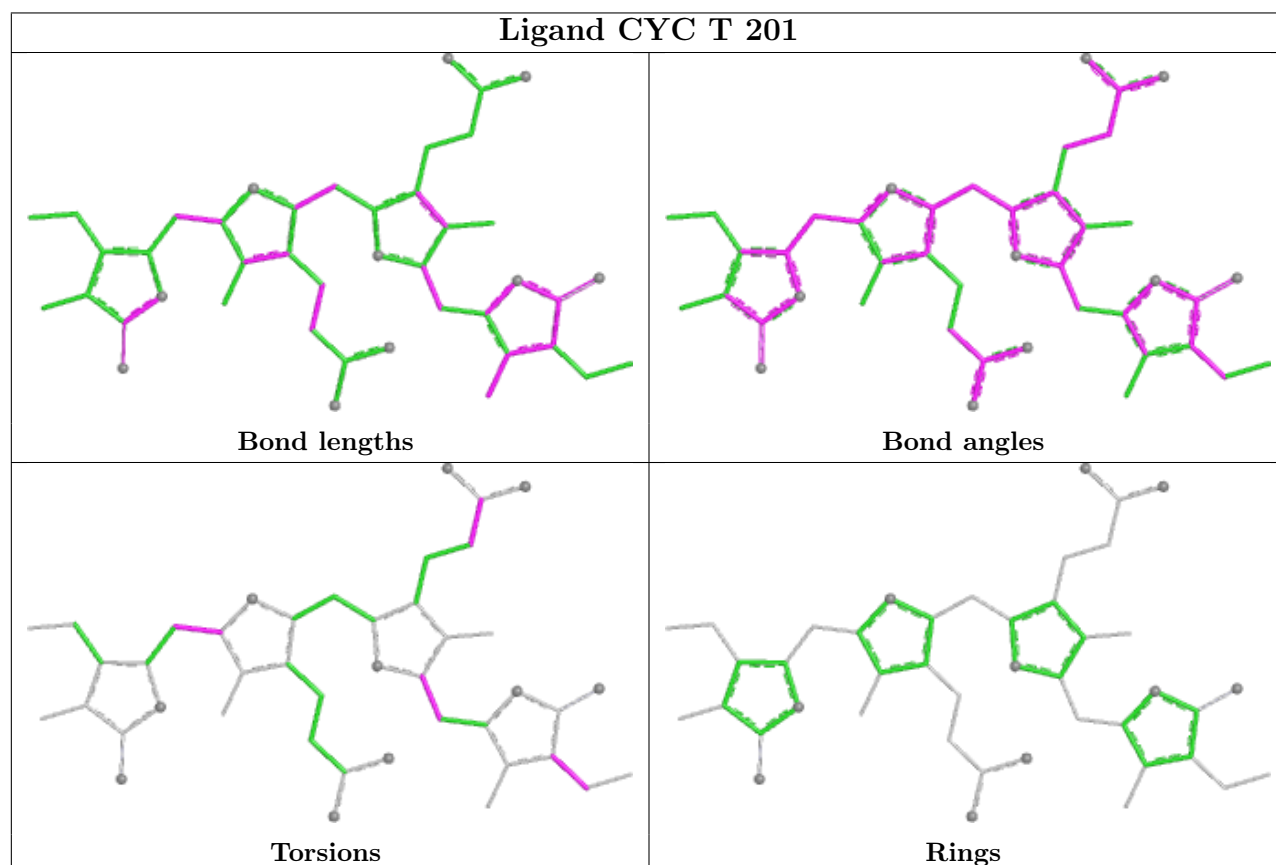
Ligand CYC R 201

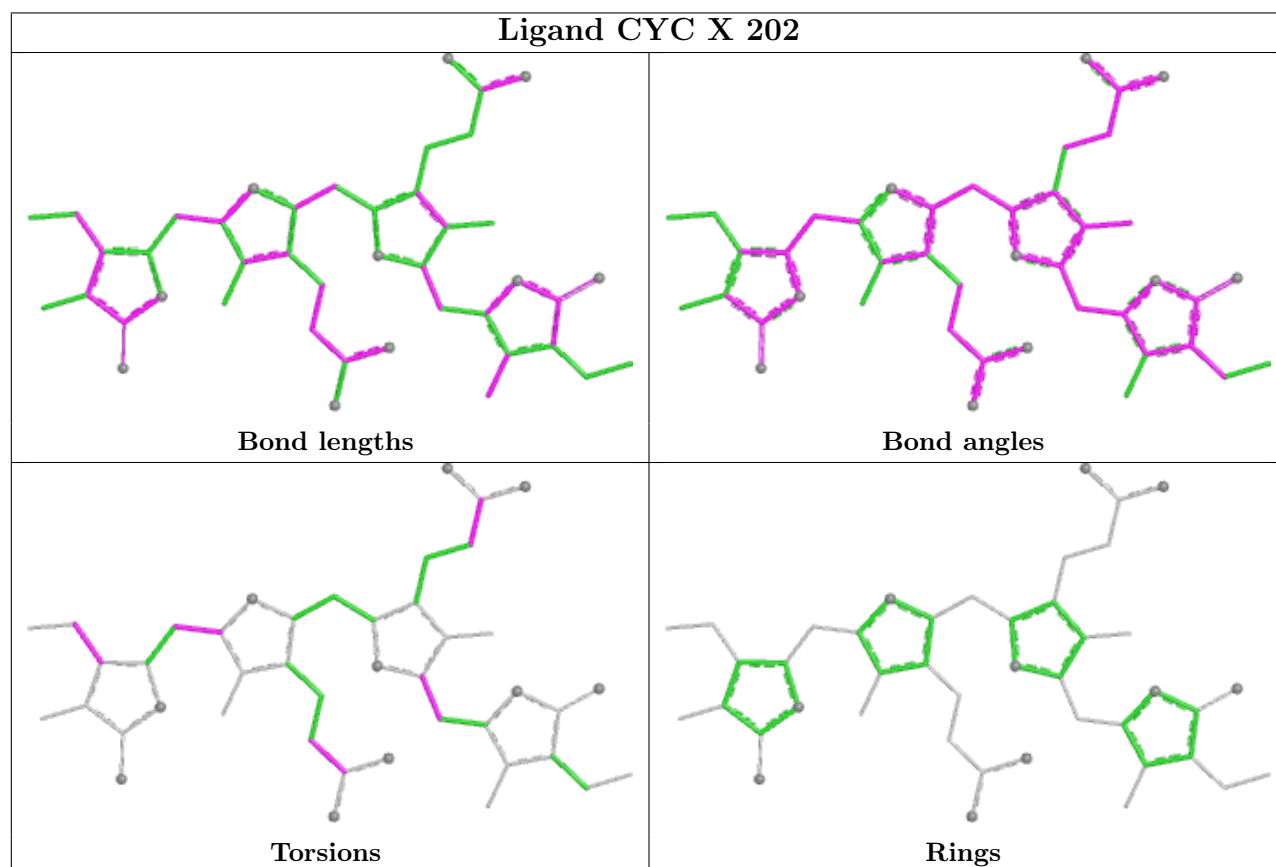
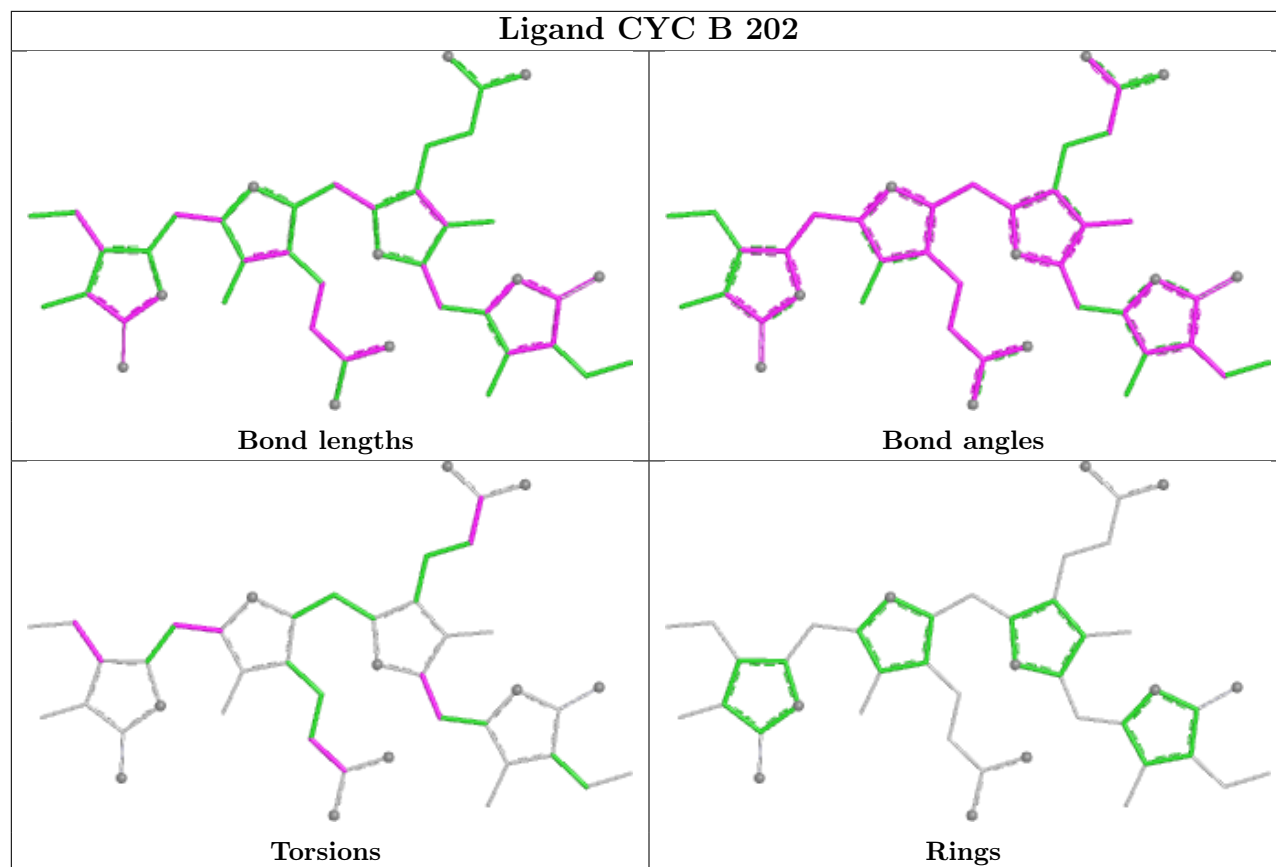


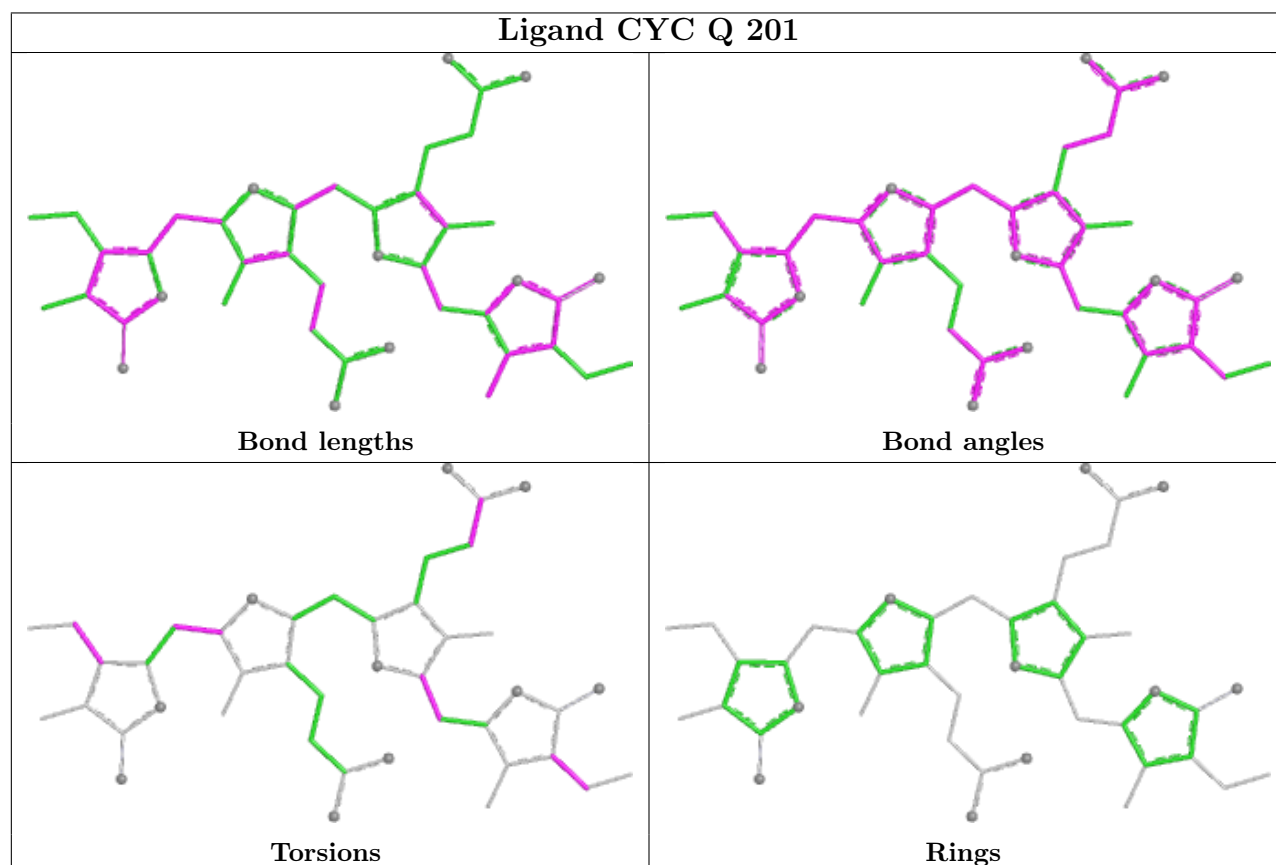
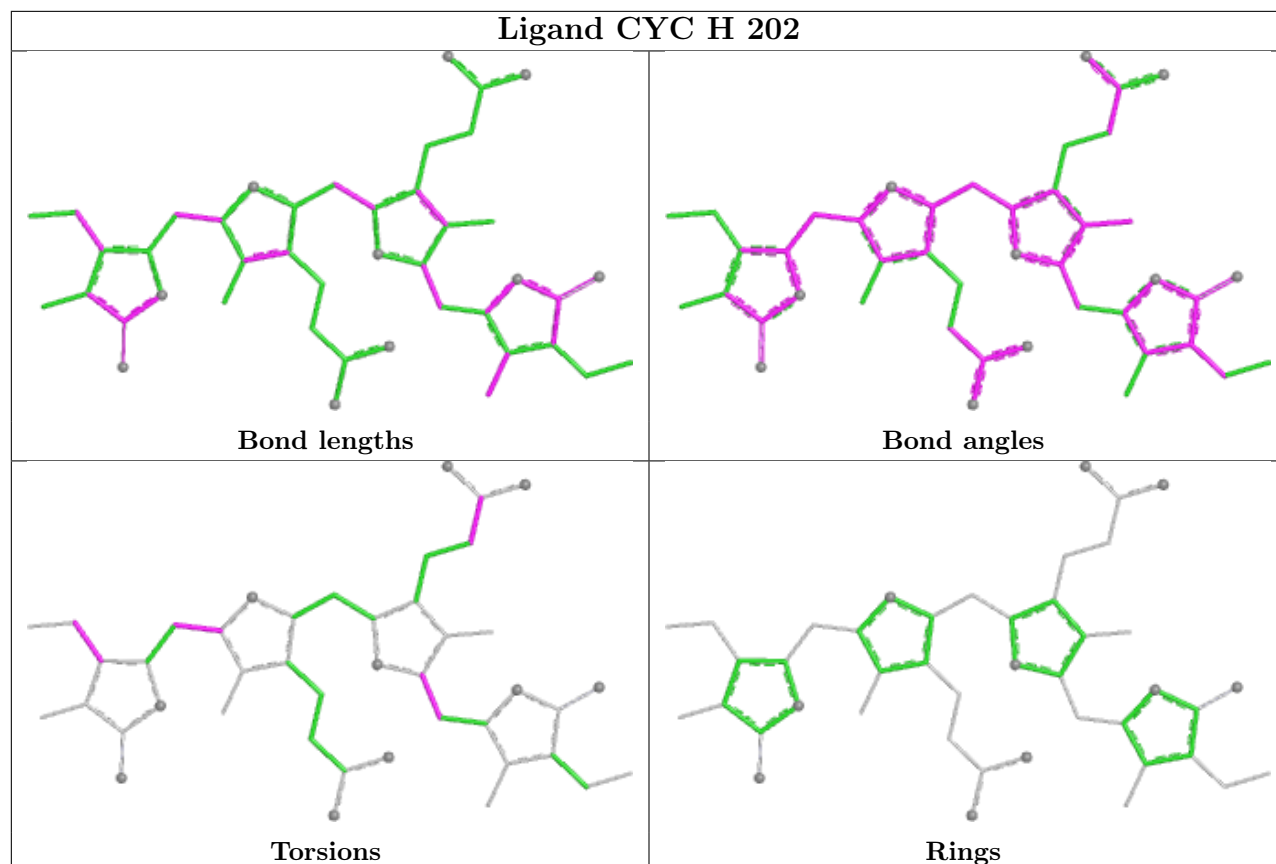
Ligand CYC E 201

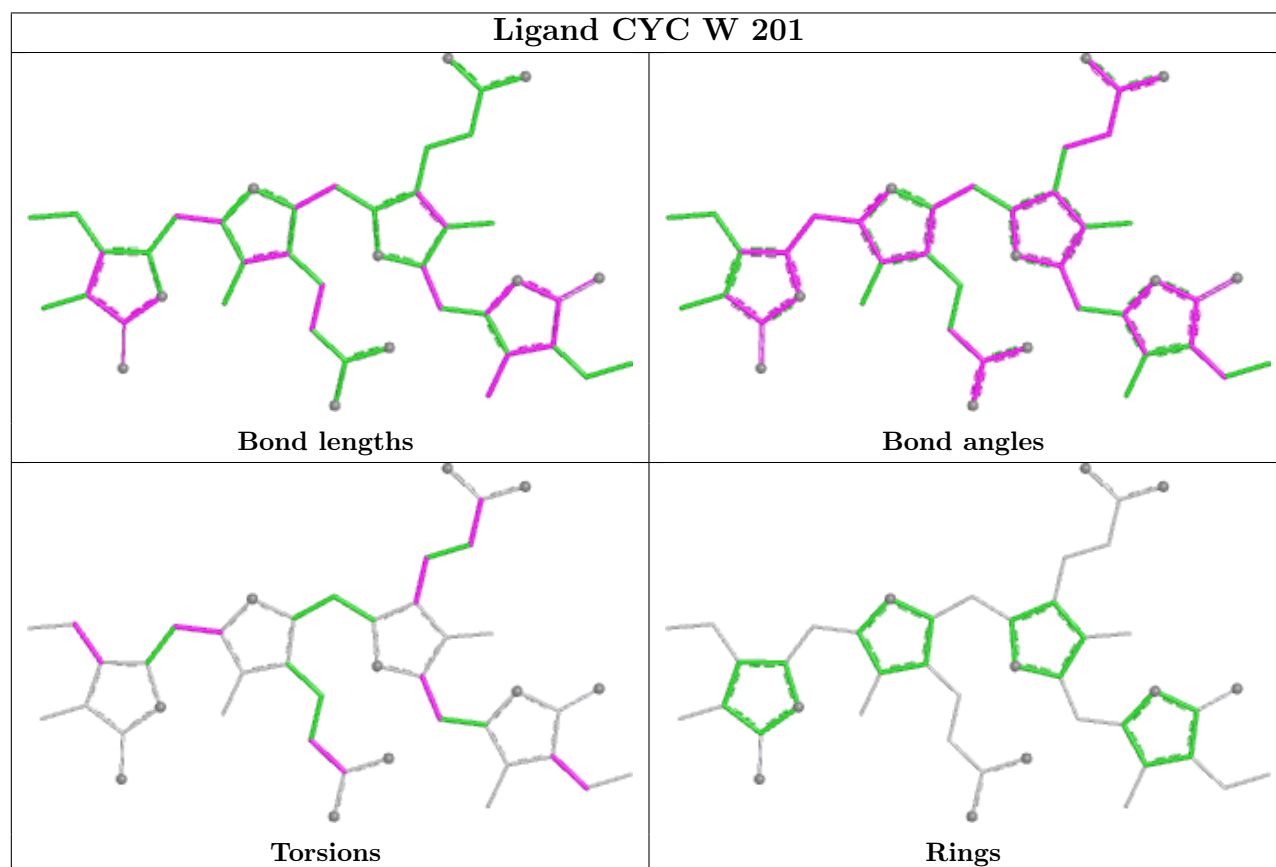
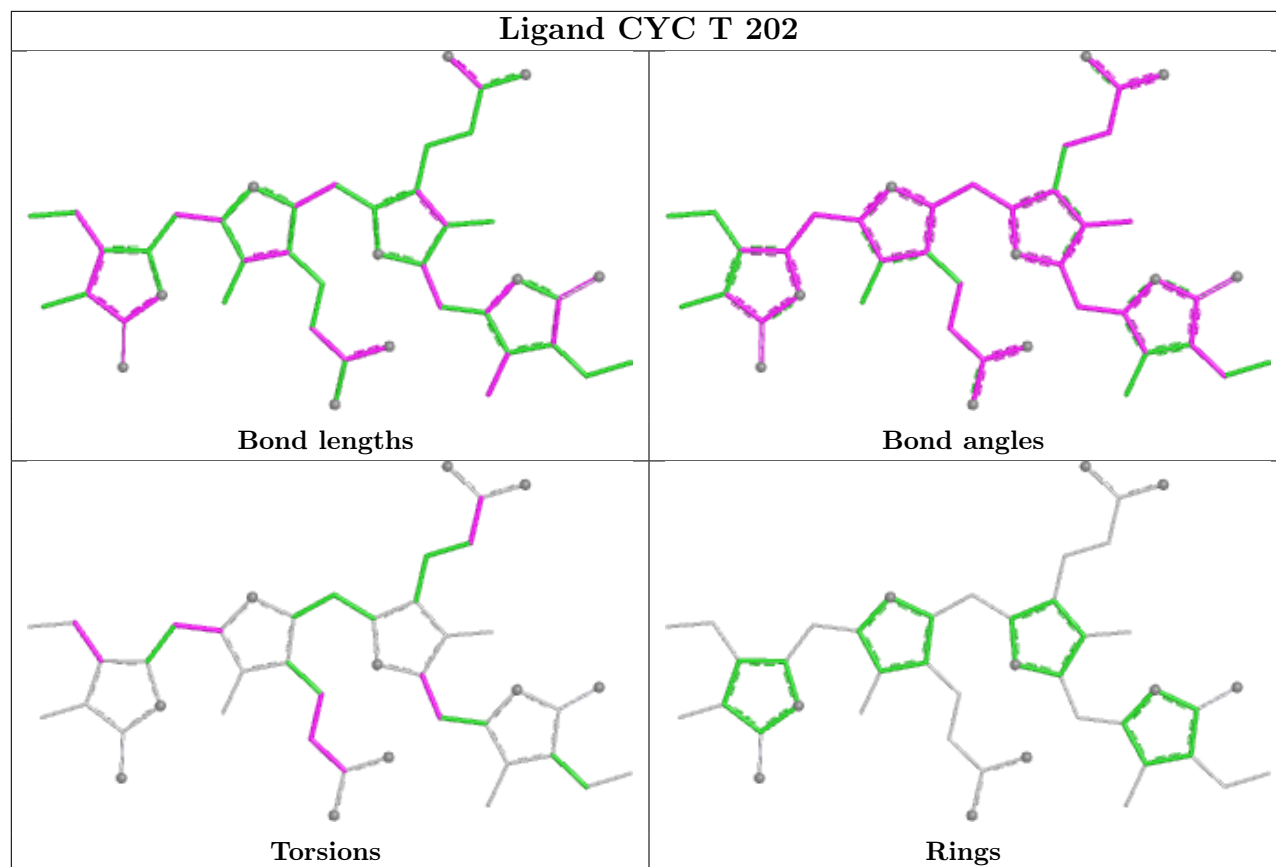


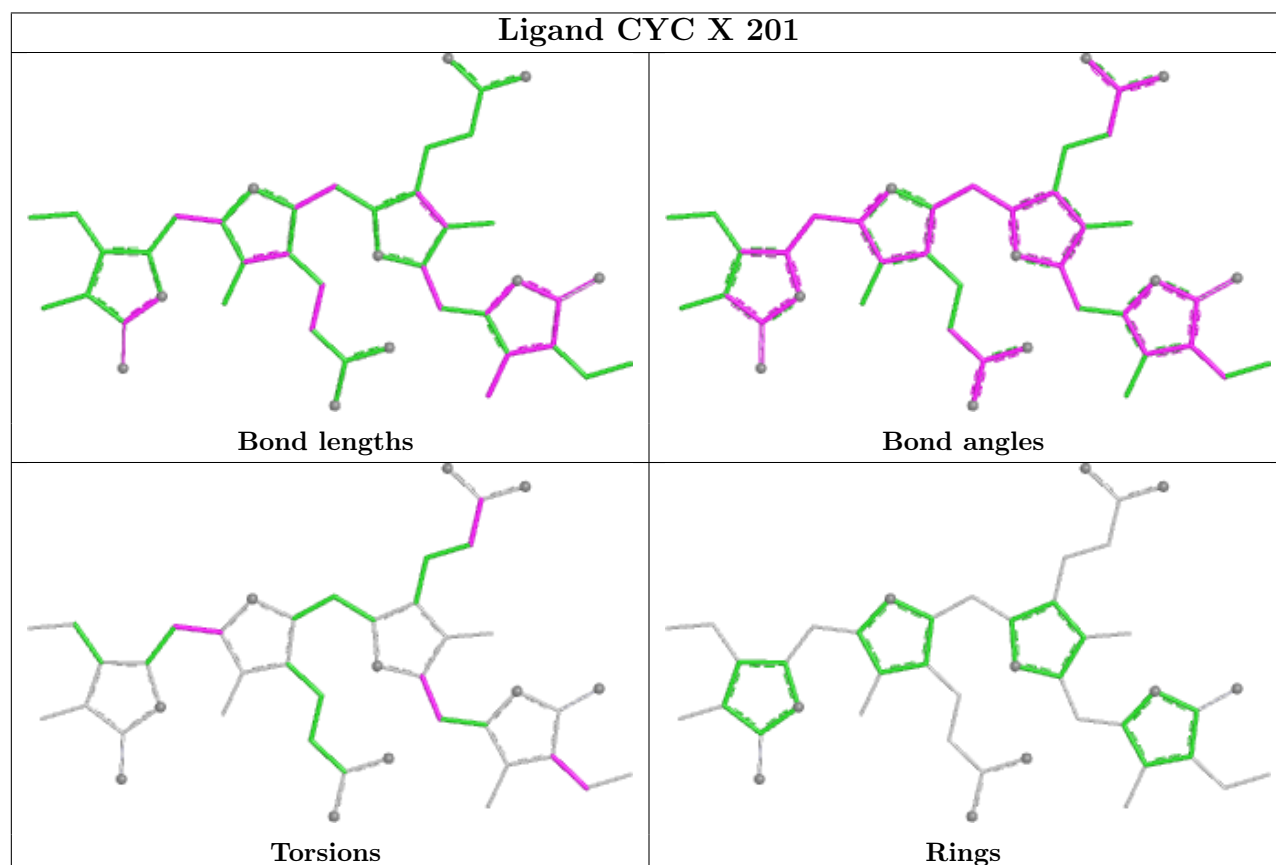
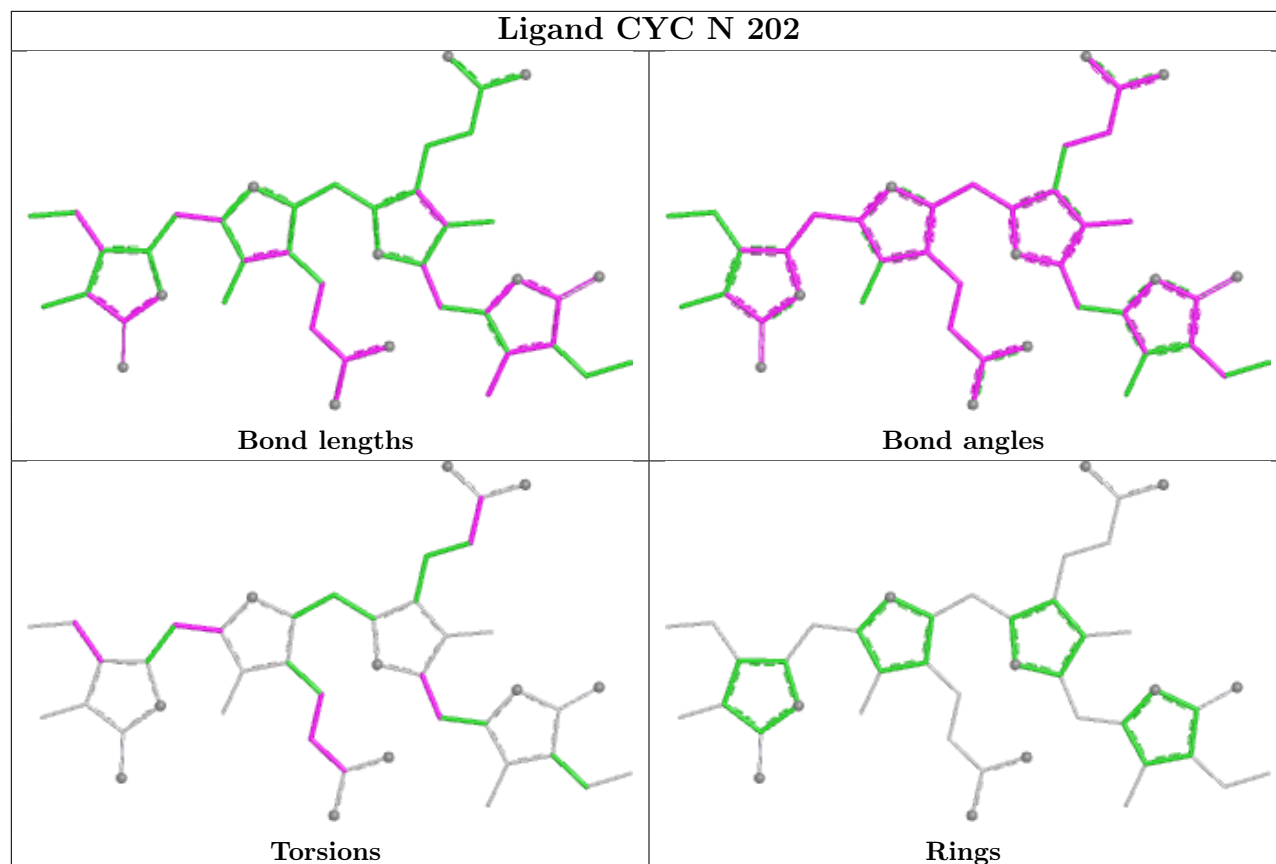
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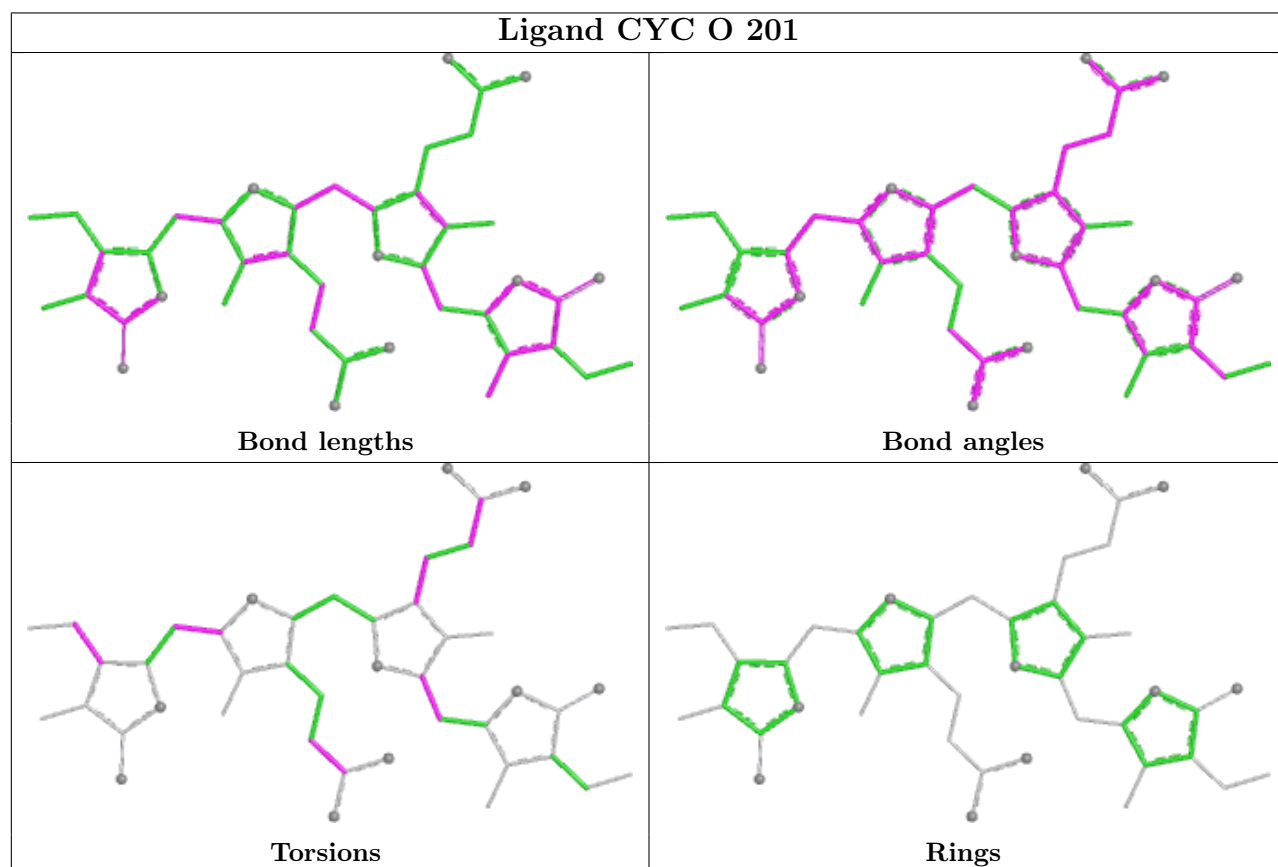
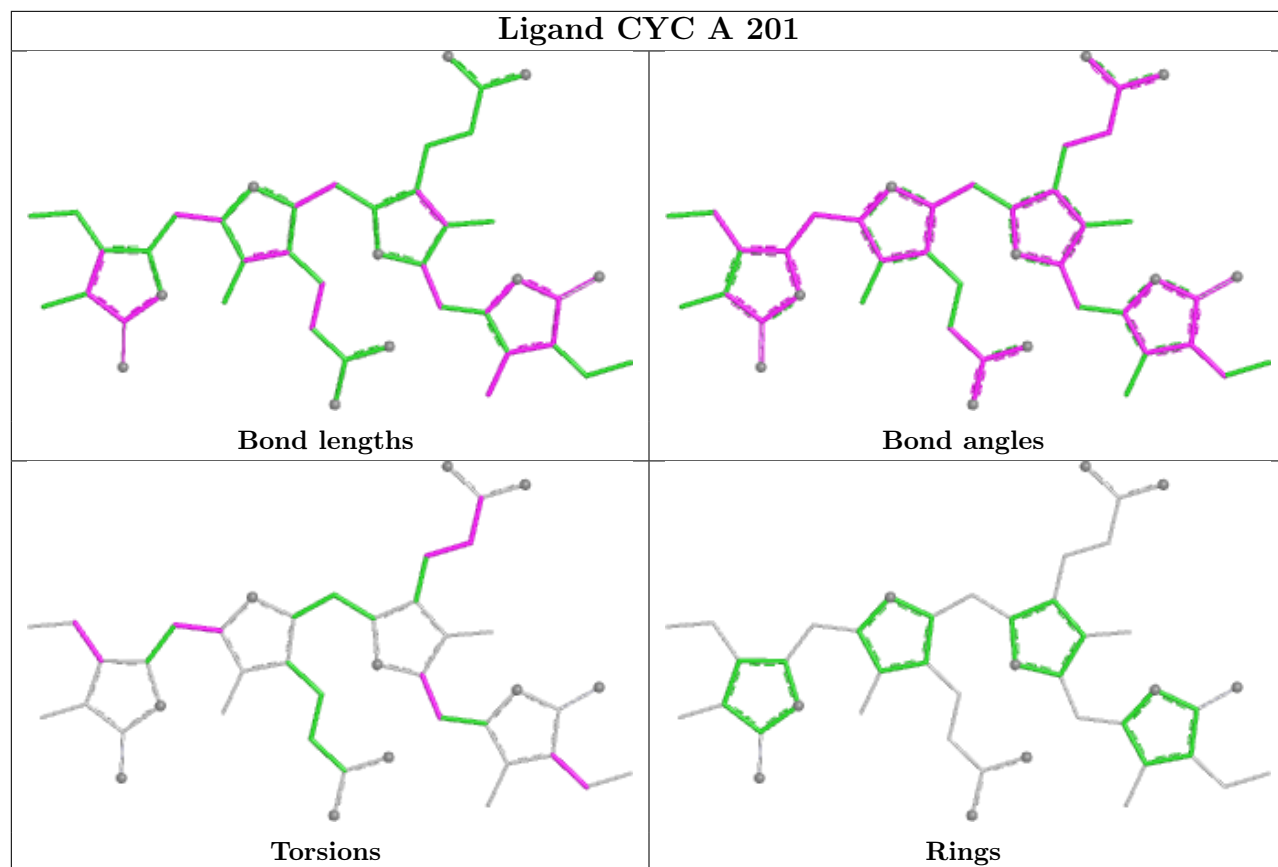




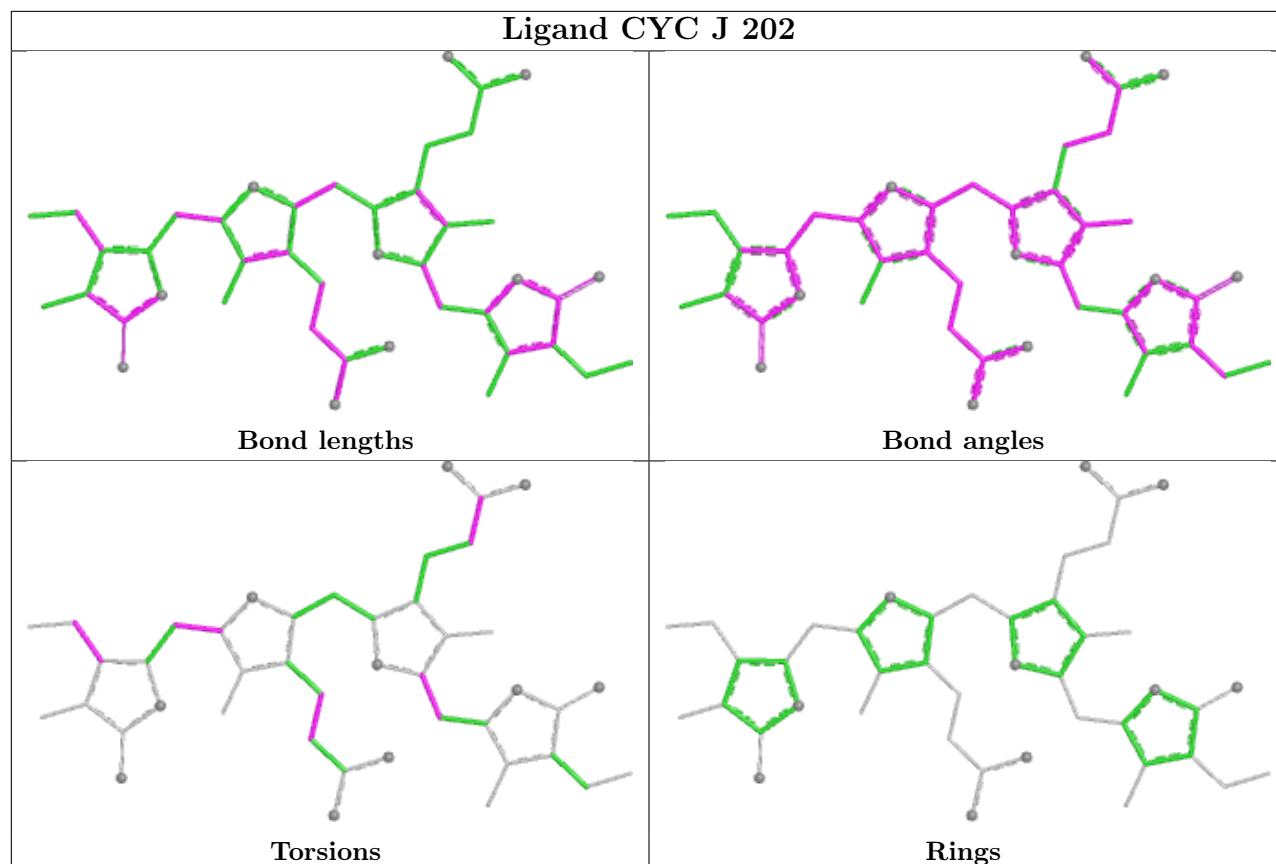




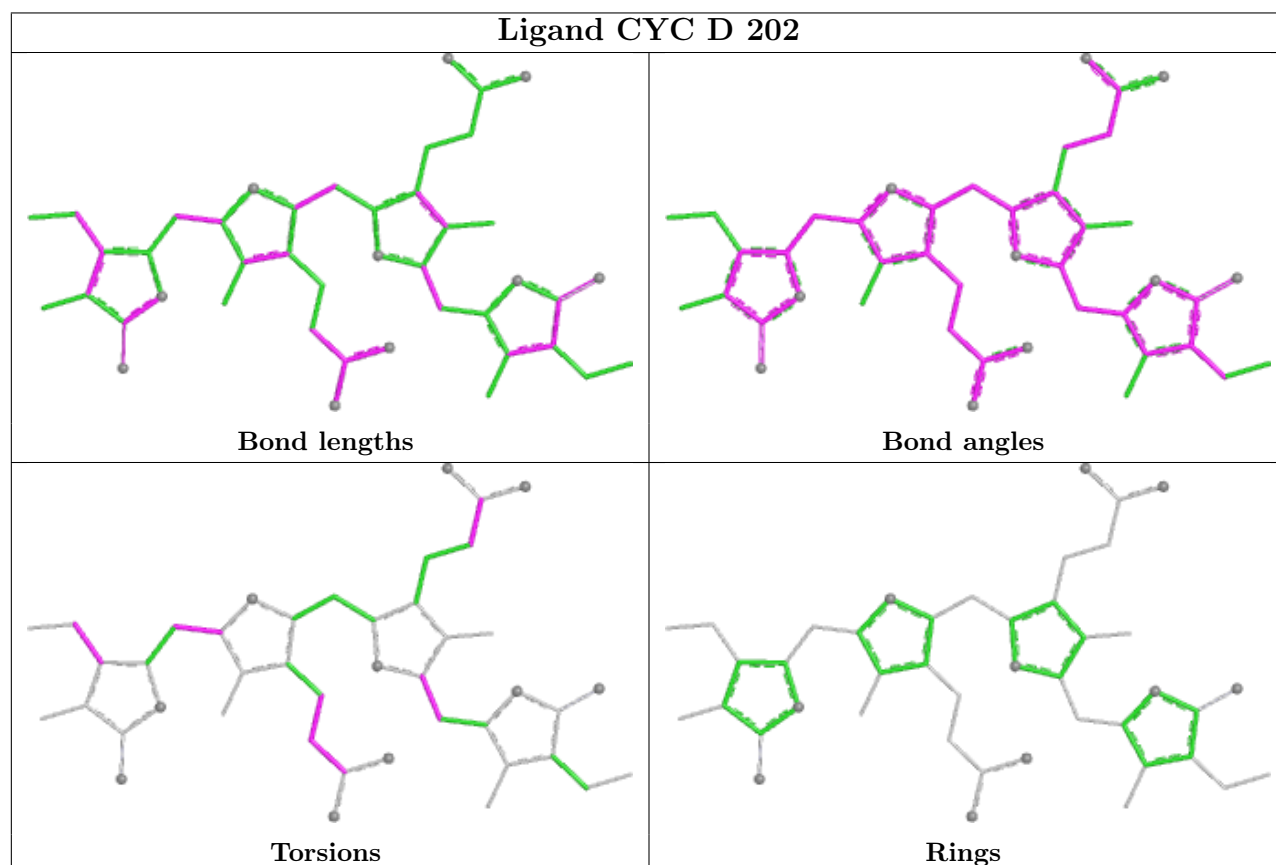




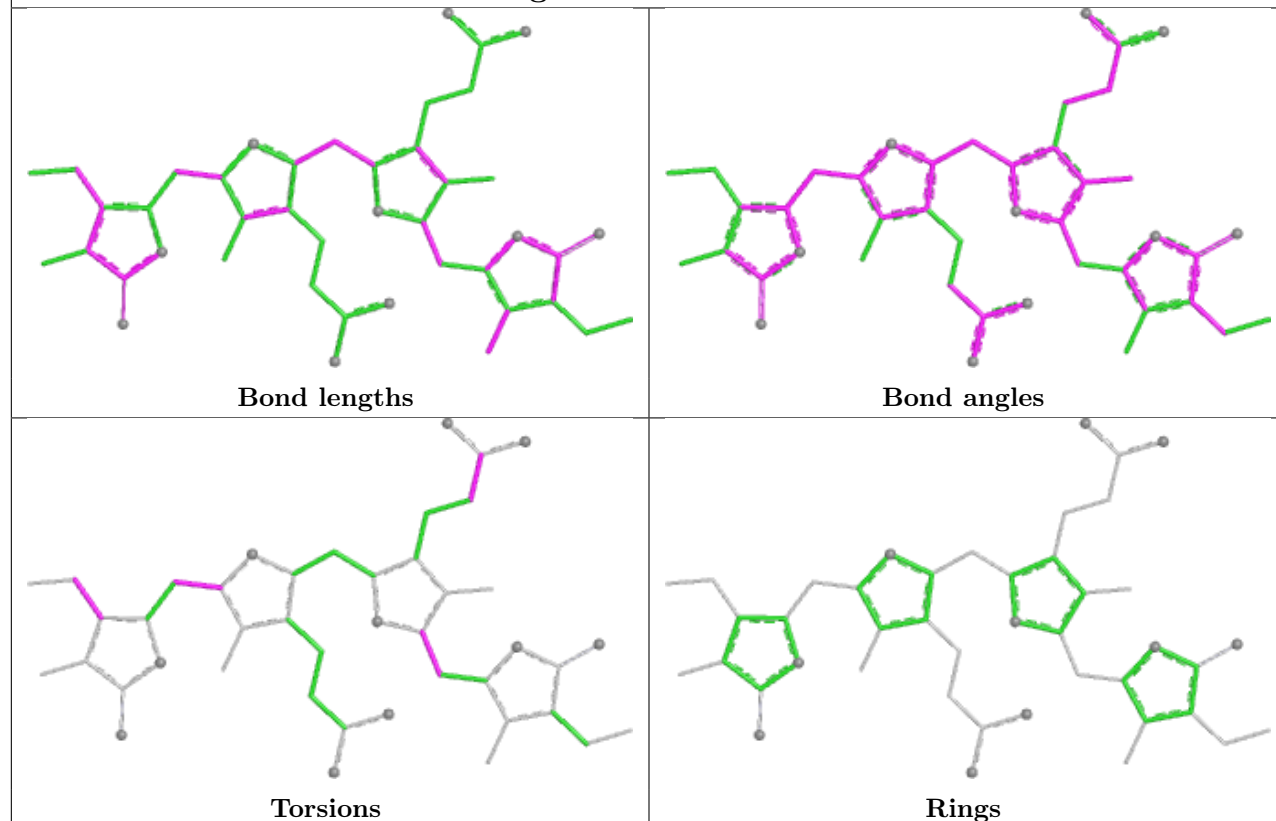
Ligand CYC J 202



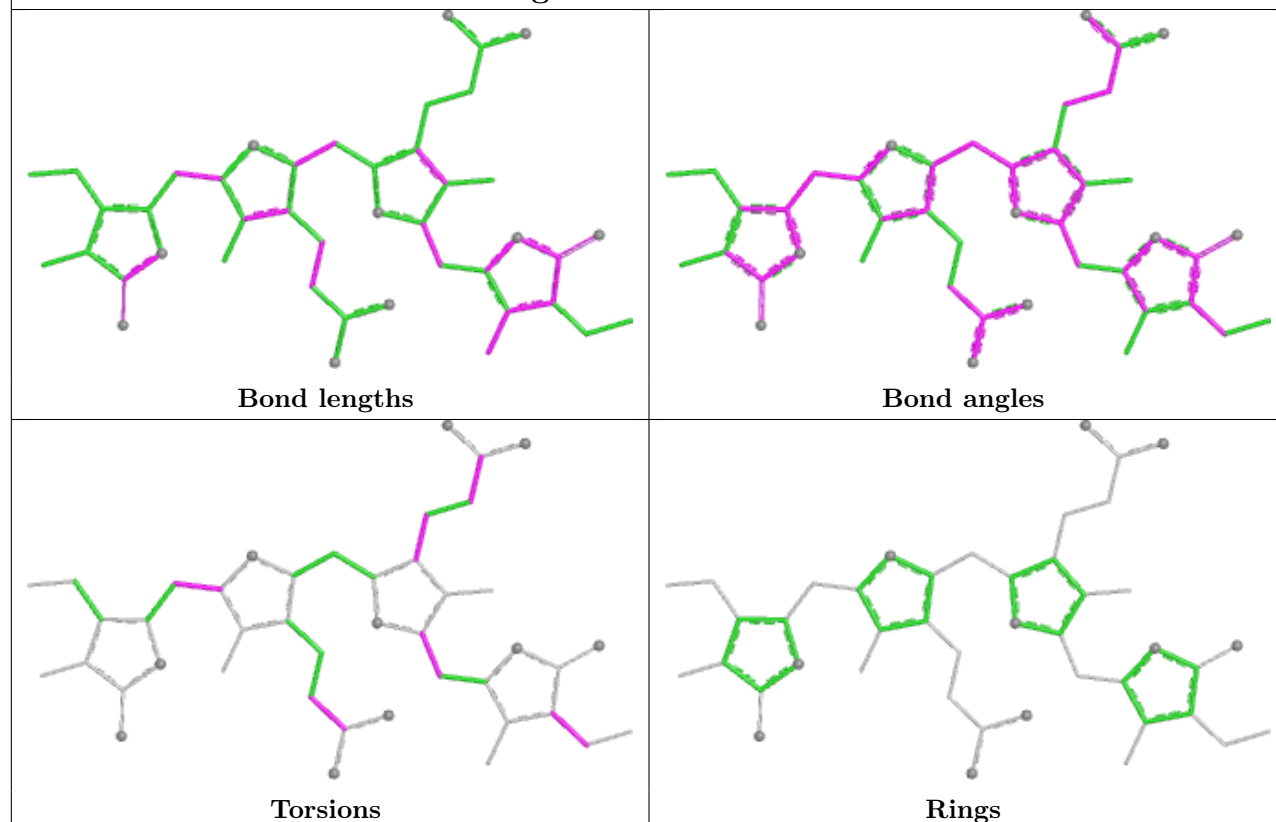
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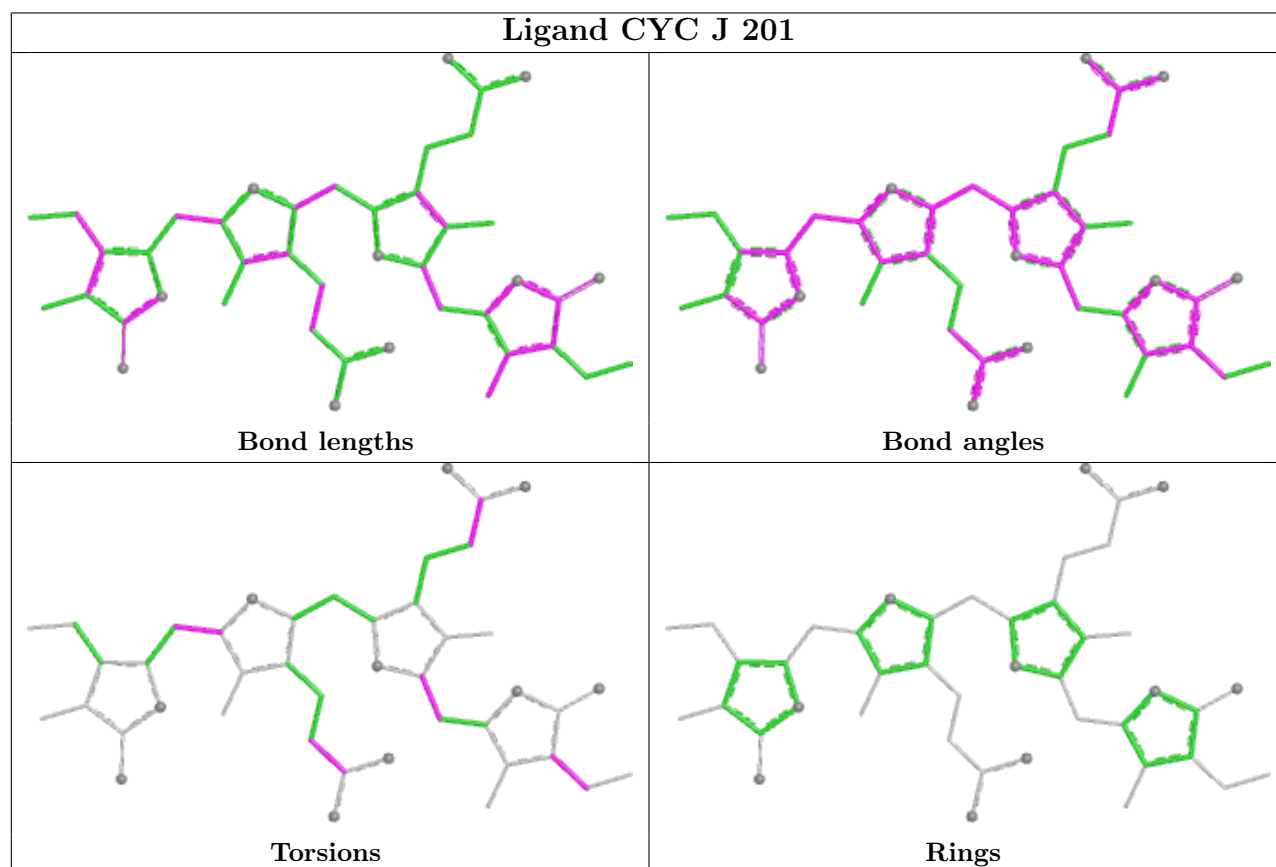
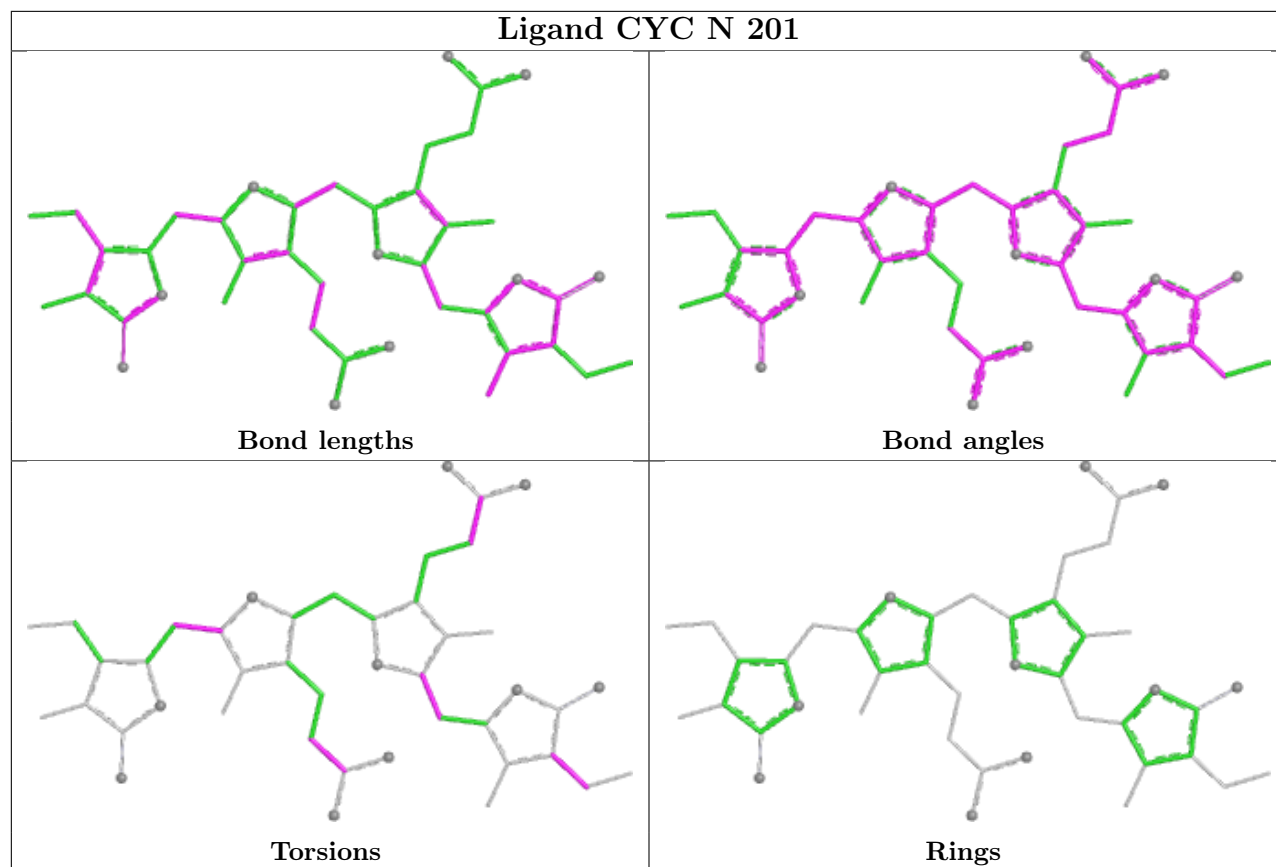


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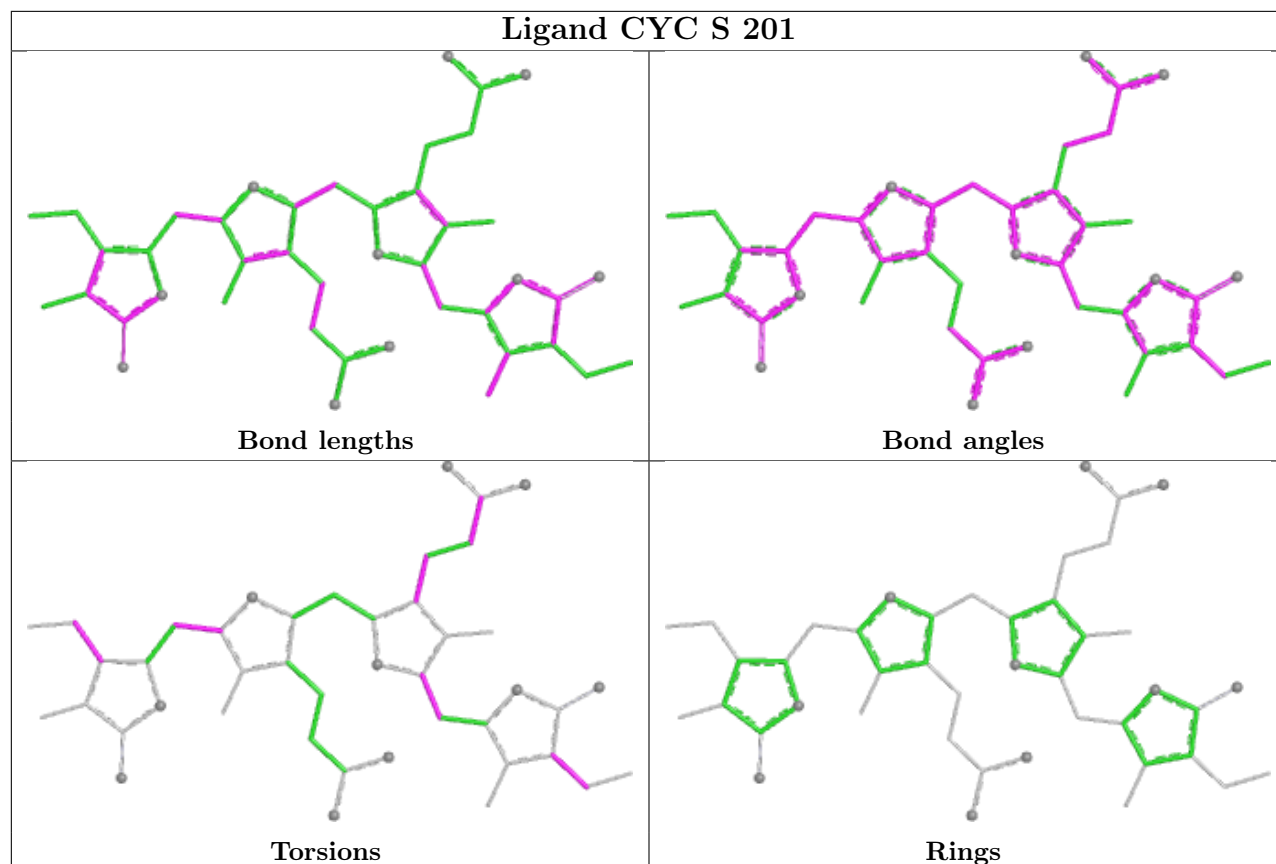


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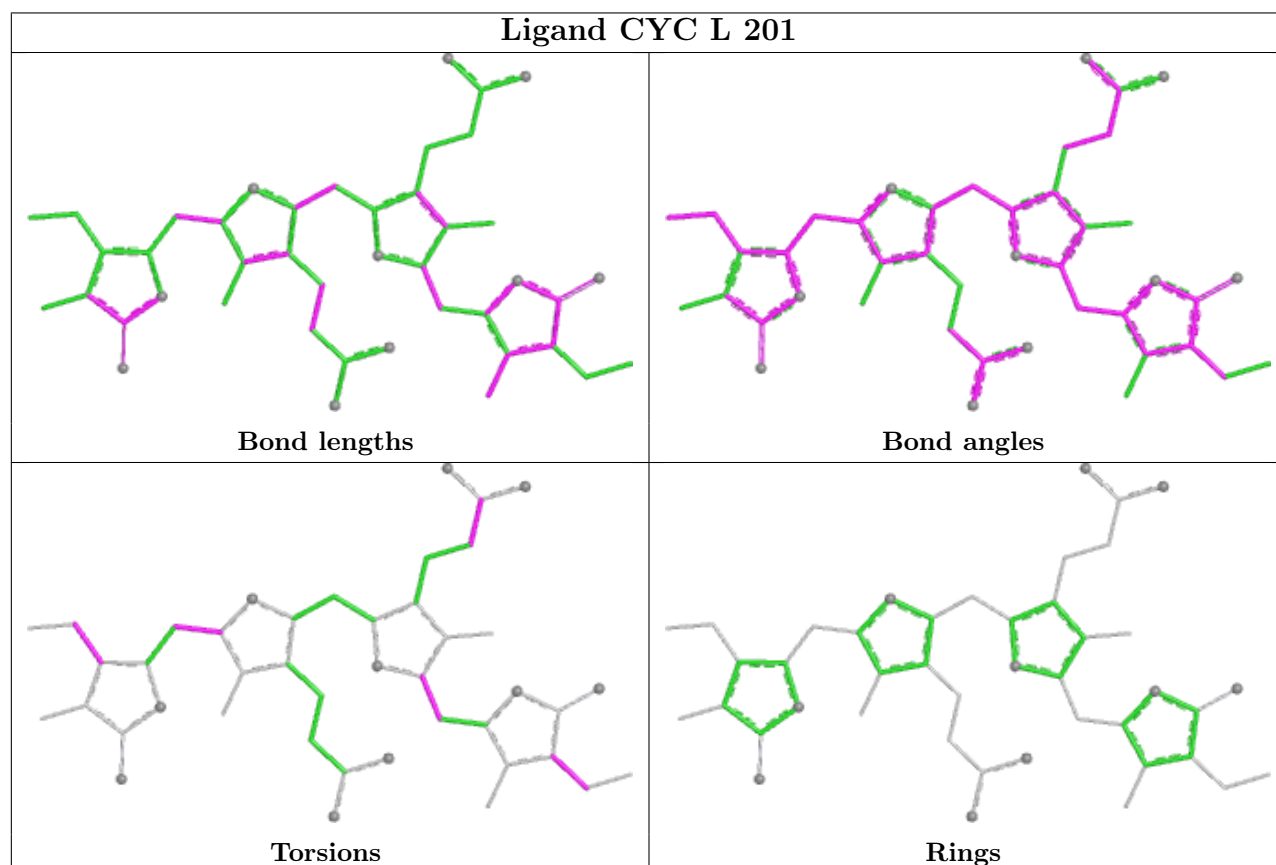


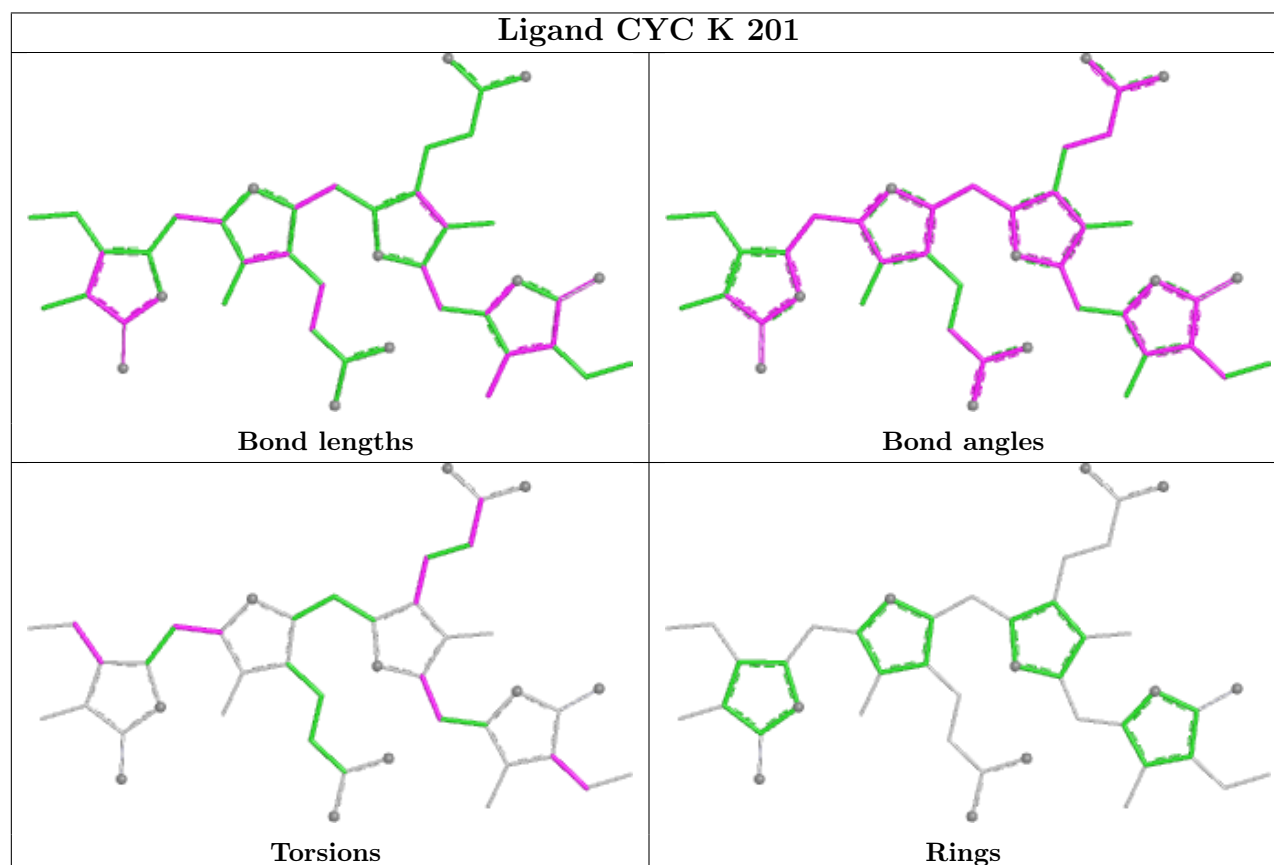
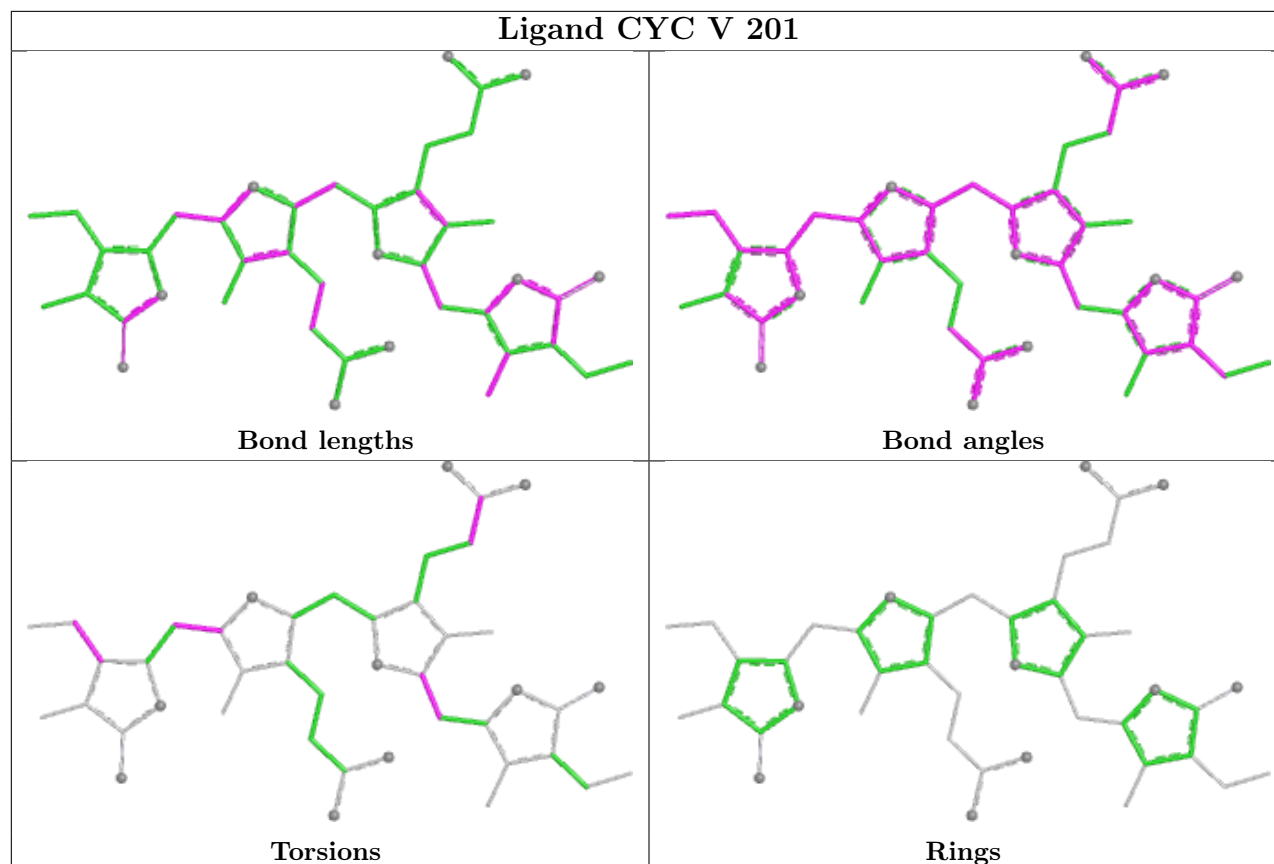


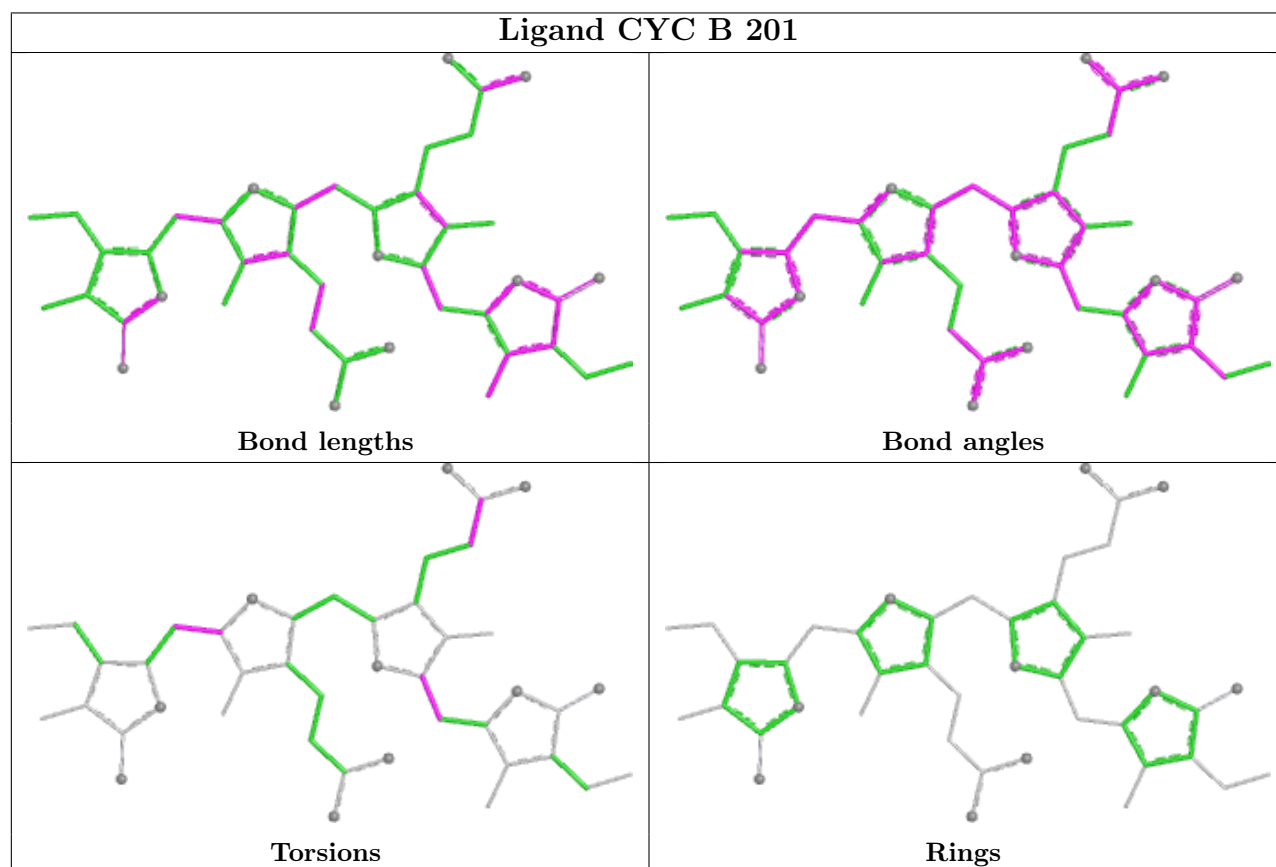
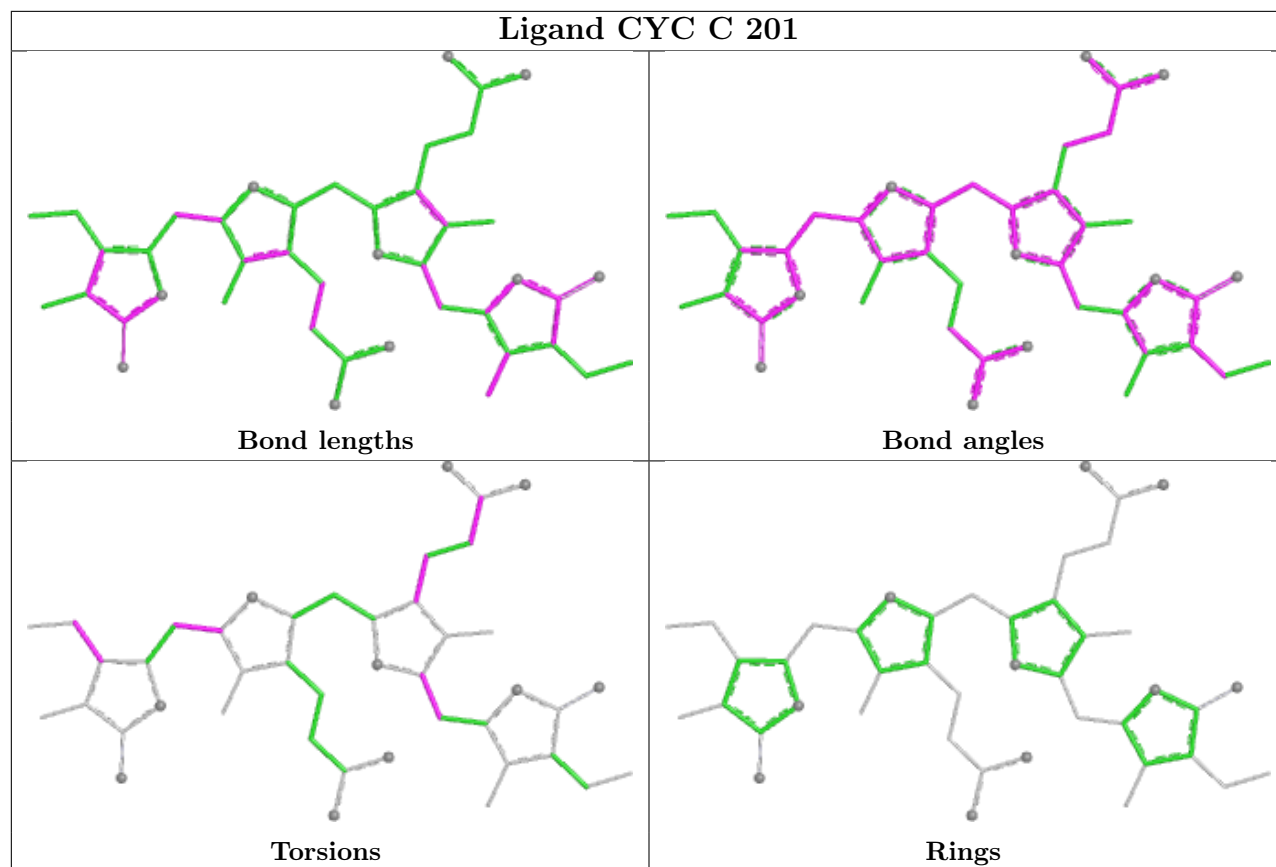
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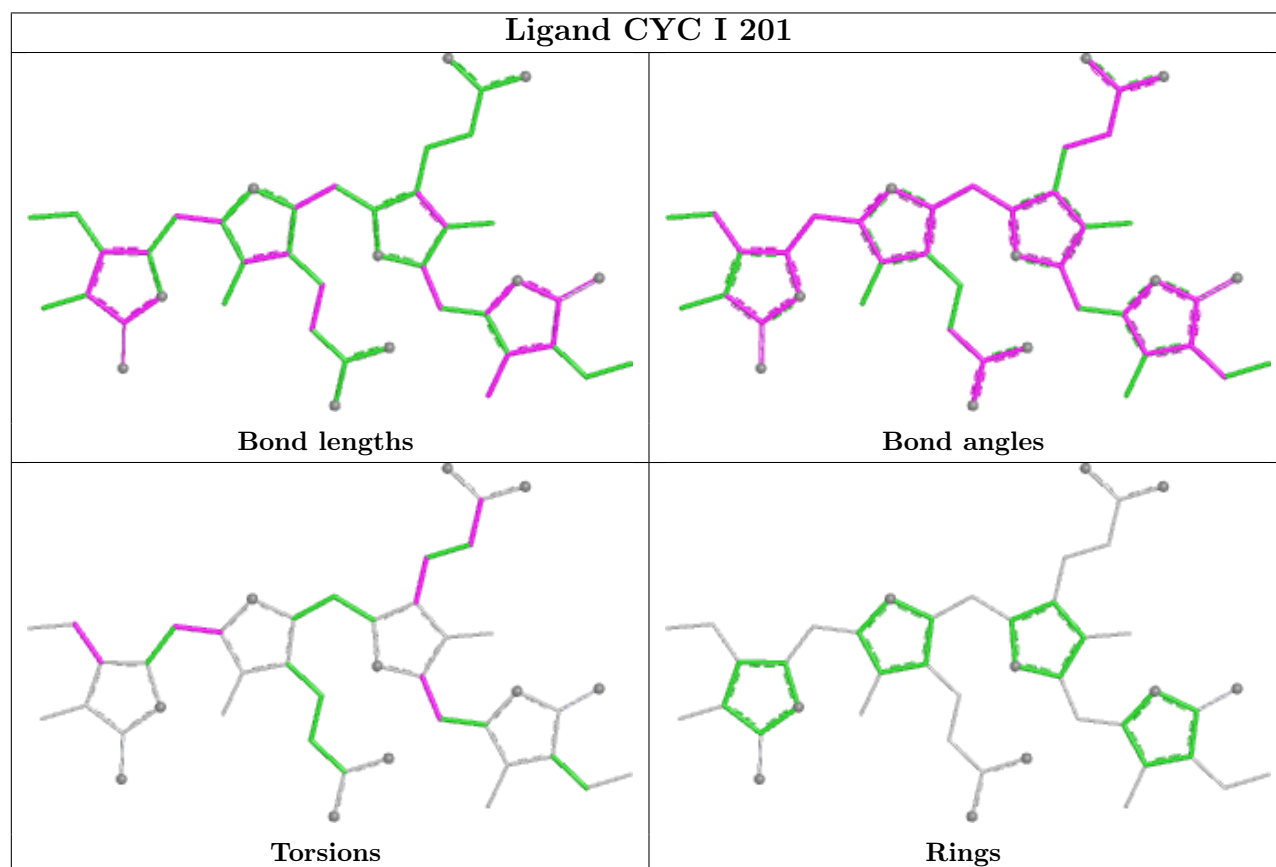
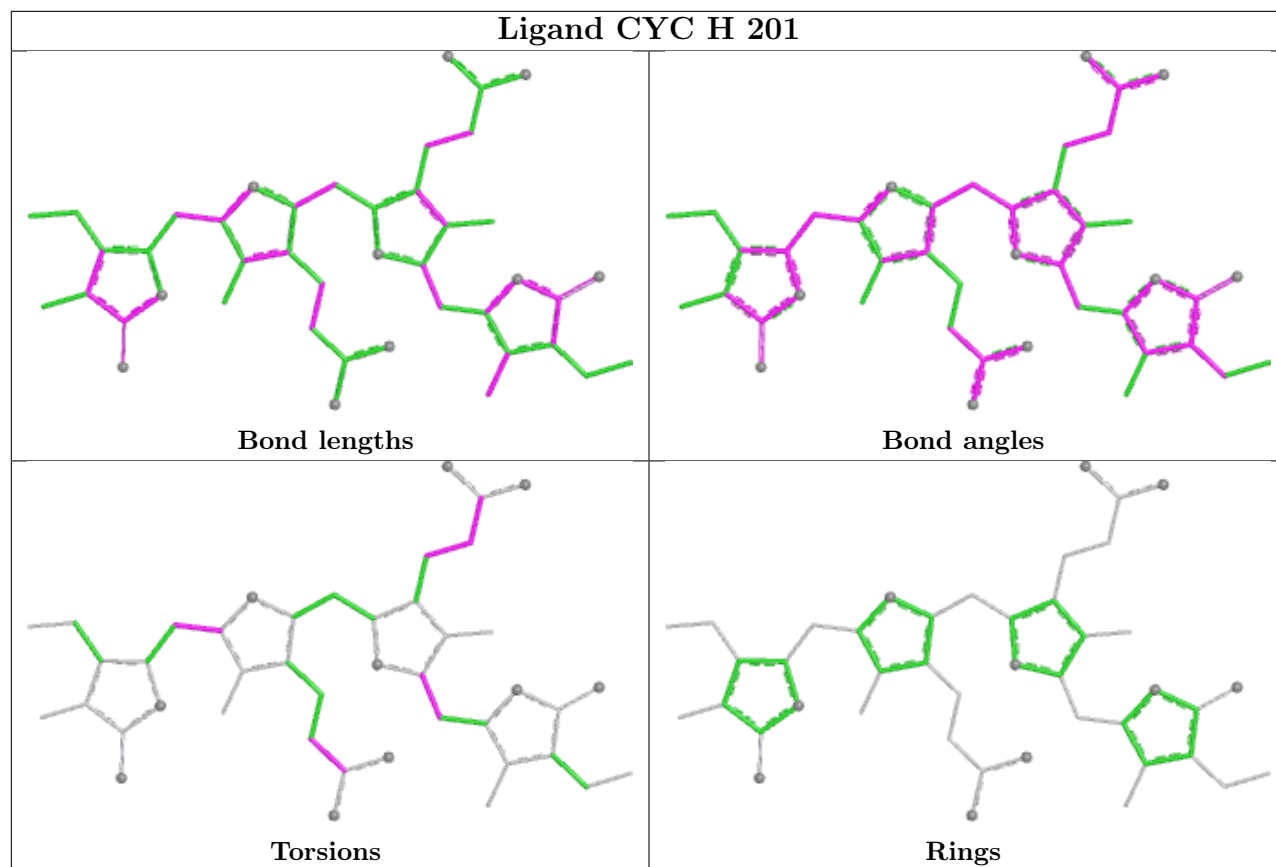


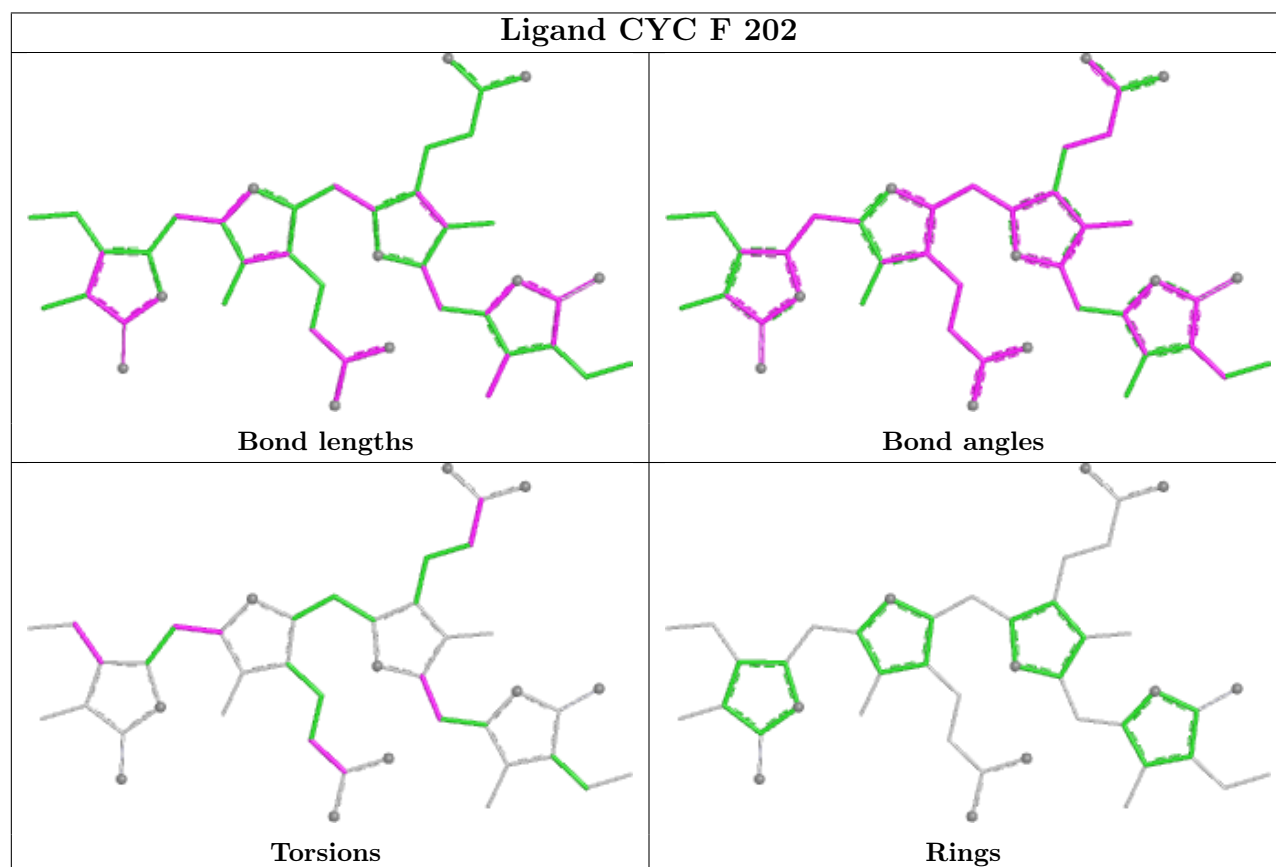
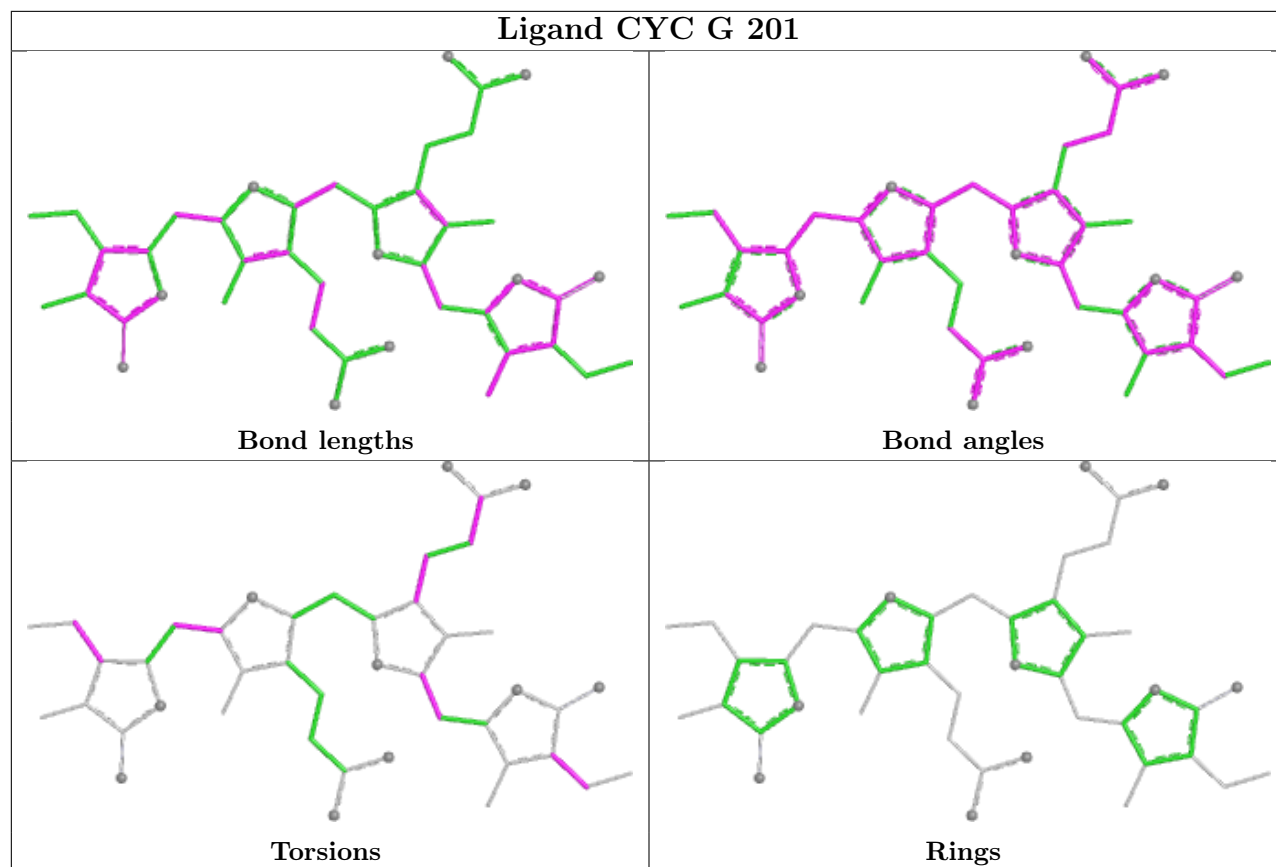
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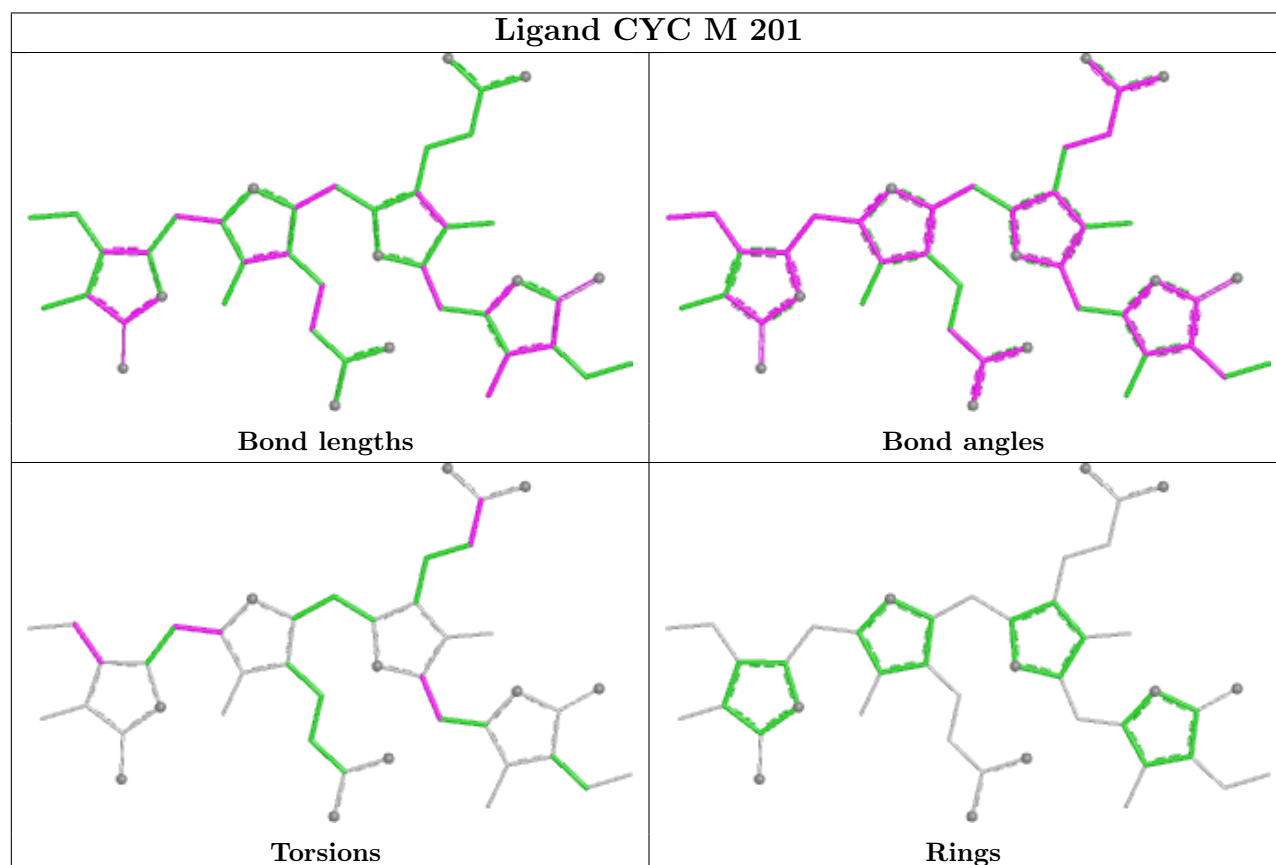
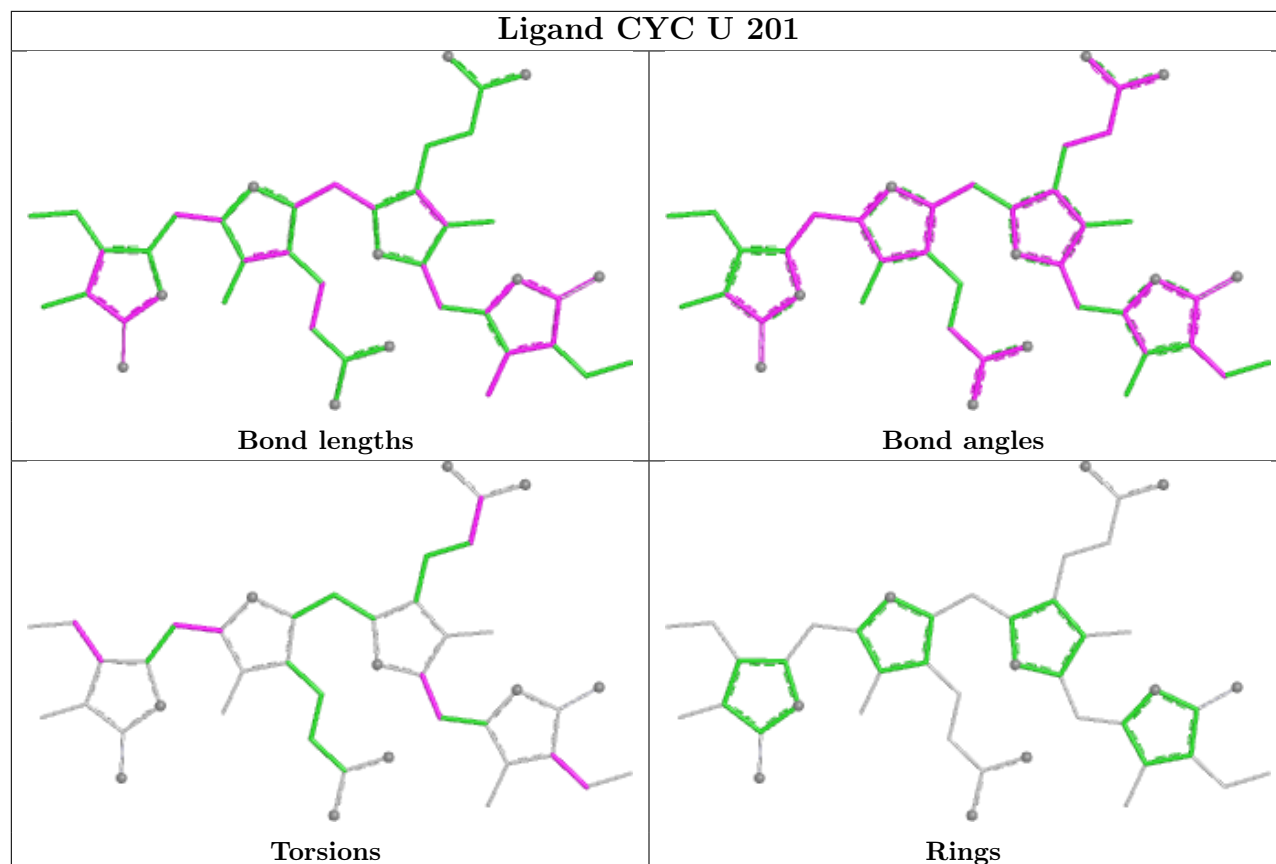


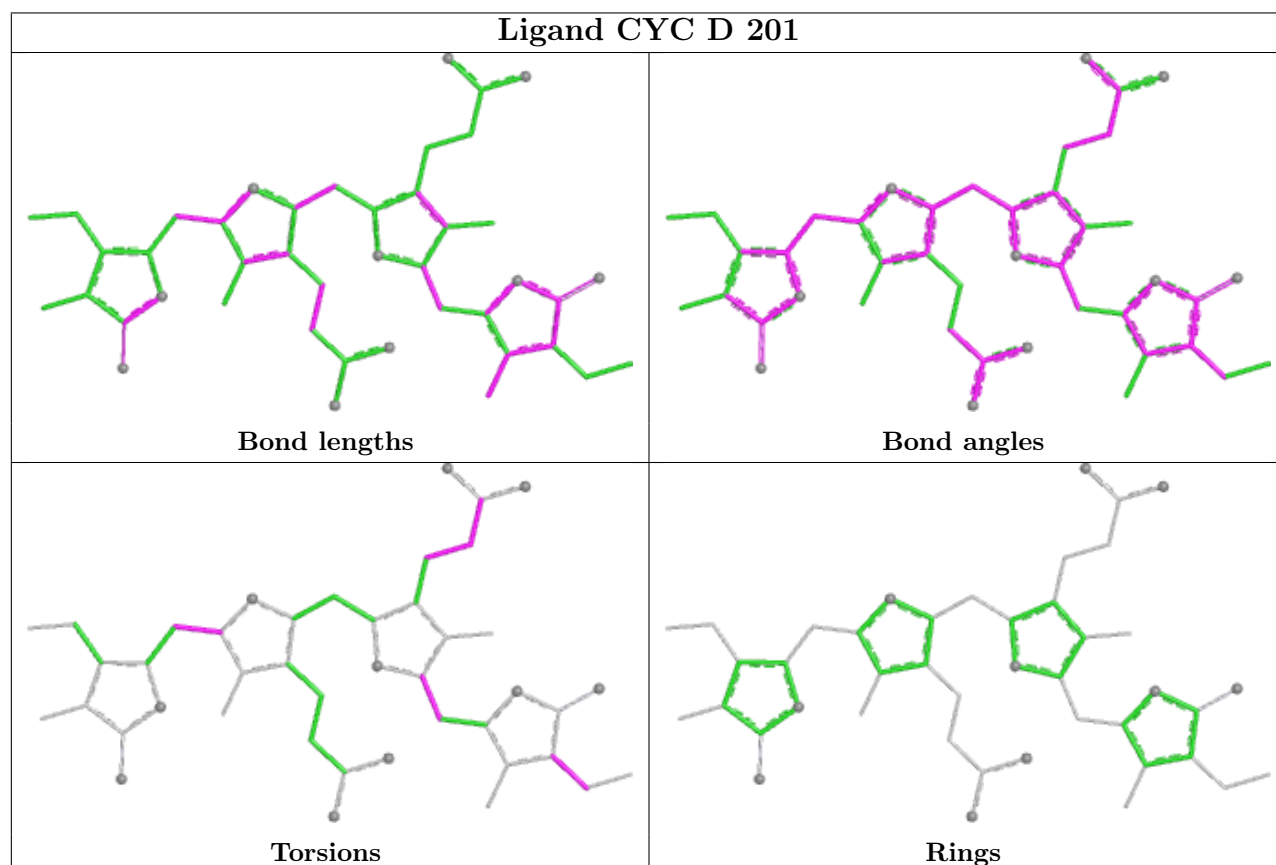
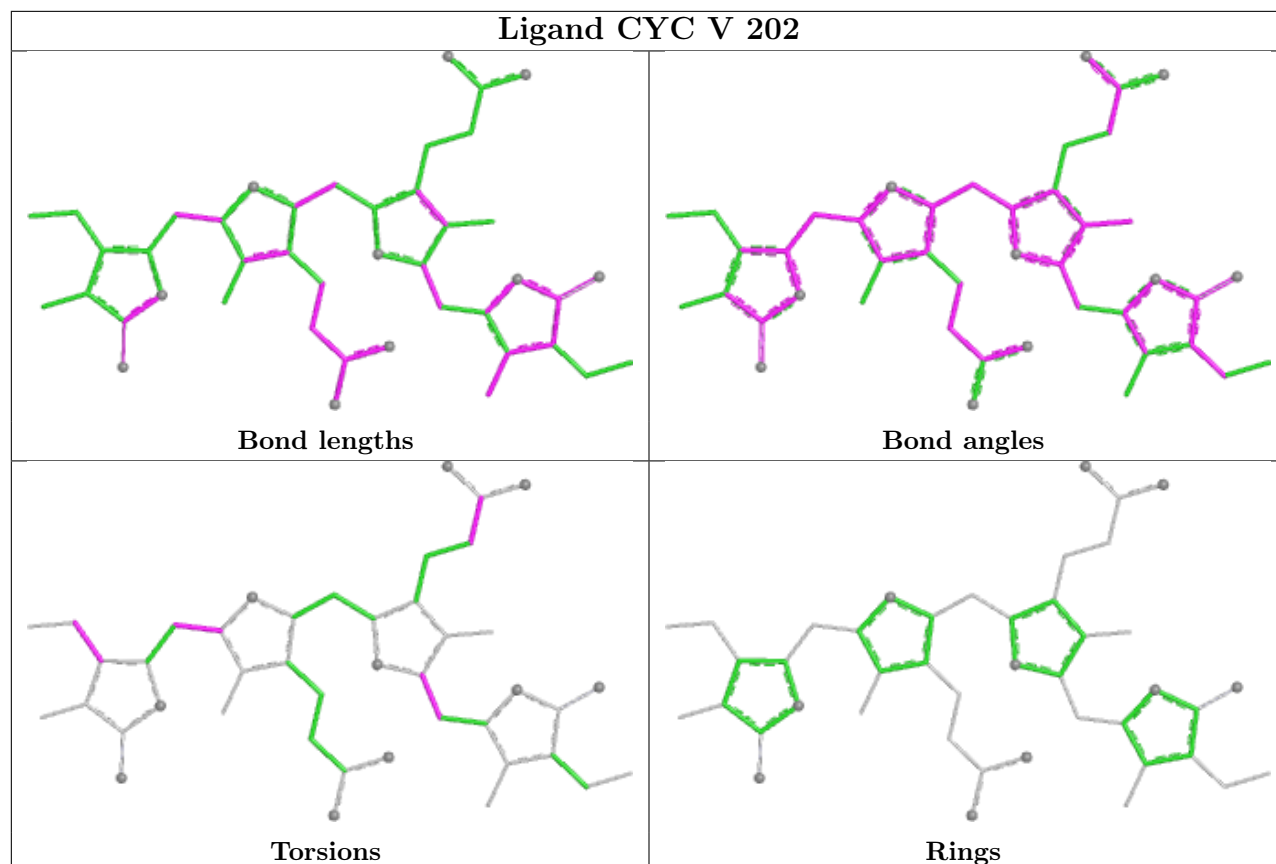


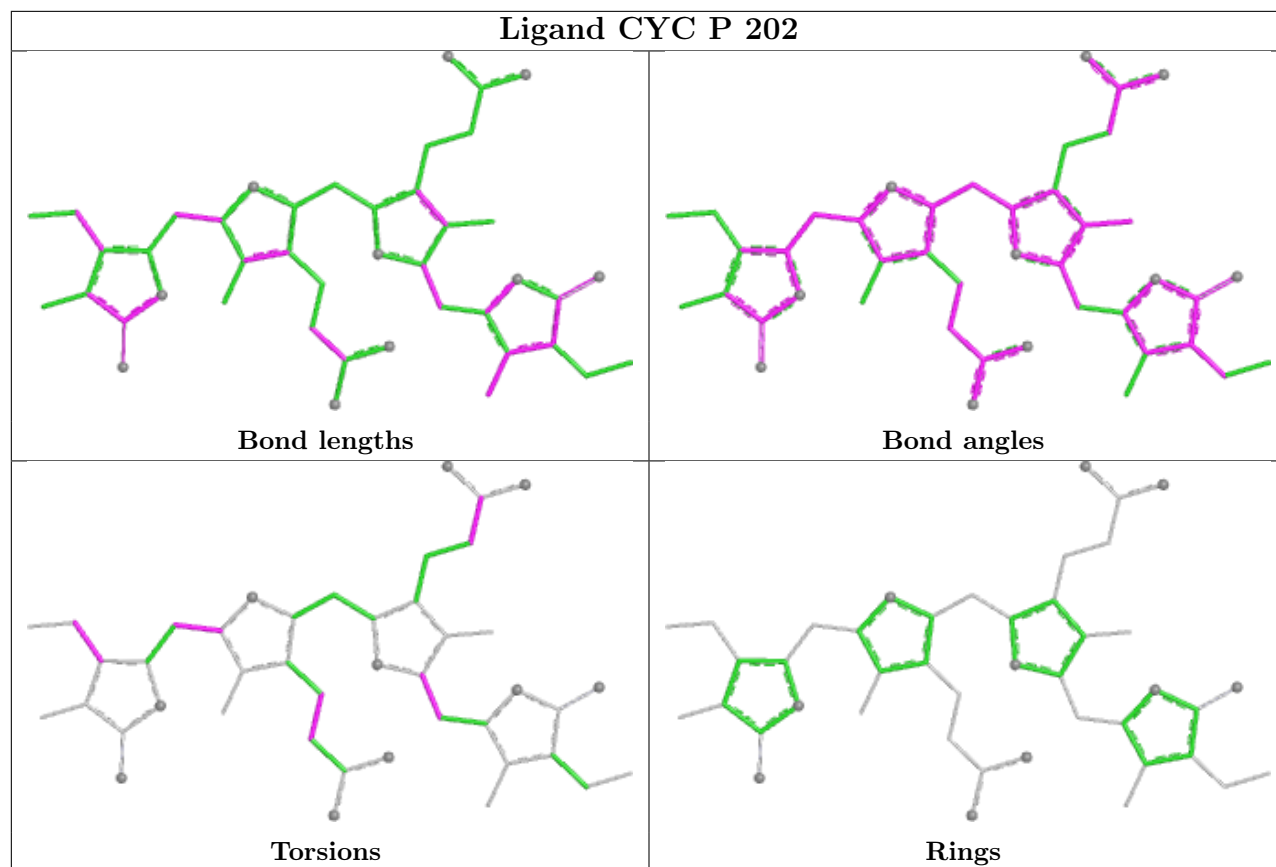












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	162/163 (99%)	-1.46	0 100 100	3, 11, 25, 35	0
1	C	162/163 (99%)	-1.41	0 100 100	5, 14, 27, 56	0
1	E	162/163 (99%)	-1.44	0 100 100	5, 12, 26, 57	0
1	G	162/163 (99%)	-1.43	0 100 100	5, 14, 29, 40	0
1	I	162/163 (99%)	-1.45	0 100 100	3, 12, 28, 55	0
1	K	162/163 (99%)	-1.43	0 100 100	3, 13, 27, 65	0
1	M	162/163 (99%)	-1.40	0 100 100	6, 13, 30, 51	0
1	O	162/163 (99%)	-1.45	0 100 100	4, 13, 25, 37	0
1	Q	162/163 (99%)	-1.40	0 100 100	4, 13, 30, 65	0
1	S	162/163 (99%)	-1.45	0 100 100	3, 12, 23, 38	0
1	U	162/163 (99%)	-1.48	0 100 100	3, 12, 21, 30	0
1	W	162/163 (99%)	-1.40	0 100 100	4, 14, 28, 41	0
2	B	171/173 (98%)	-1.40	0 100 100	3, 14, 31, 53	0
2	D	171/173 (98%)	-1.39	0 100 100	4, 14, 30, 55	0
2	F	171/173 (98%)	-1.38	0 100 100	5, 16, 34, 48	0
2	H	171/173 (98%)	-1.35	0 100 100	7, 18, 36, 53	0
2	J	171/173 (98%)	-1.35	0 100 100	6, 16, 36, 50	0
2	L	171/173 (98%)	-1.37	0 100 100	5, 16, 35, 51	0
2	N	171/173 (98%)	-1.37	0 100 100	5, 15, 35, 54	0
2	P	171/173 (98%)	-1.38	0 100 100	6, 15, 34, 61	0
2	R	171/173 (98%)	-1.35	0 100 100	6, 17, 40, 53	0
2	T	171/173 (98%)	-1.40	0 100 100	5, 16, 34, 51	0
2	V	171/173 (98%)	-1.43	0 100 100	5, 13, 29, 45	0
2	X	171/173 (98%)	-1.40	0 100 100	5, 14, 33, 43	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3996/4032 (99%)	-1.41	0 100 100	3, 14, 33, 65	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	MEN	H	72	9/10	0.98	0.04	20,20,32,32	0
2	MEN	R	72	9/10	0.98	0.04	15,19,28,28	0
2	MEN	V	72	9/10	0.98	0.05	20,21,27,27	0
2	MEN	B	72	9/10	0.99	0.03	15,19,20,20	0
2	MEN	J	72	9/10	0.99	0.05	15,19,27,29	0
2	MEN	L	72	9/10	0.99	0.04	20,20,23,30	0
2	MEN	N	72	9/10	0.99	0.06	15,19,24,24	0
2	MEN	P	72	9/10	0.99	0.04	20,20,31,34	0
2	MEN	D	72	9/10	0.99	0.04	18,19,25,28	0
2	MEN	T	72	9/10	0.99	0.04	20,20,30,30	0
2	MEN	F	72	9/10	0.99	0.04	26,28,35,37	0
2	MEN	X	72	9/10	0.99	0.04	19,21,23,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A	201	43/43	0.99	0.04	5,11,18,23	0
3	CYC	B	201	43/43	0.99	0.03	8,14,25,27	0
3	CYC	B	202	43/43	0.99	0.03	5,15,31,40	0

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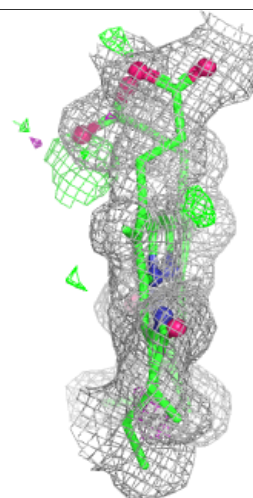
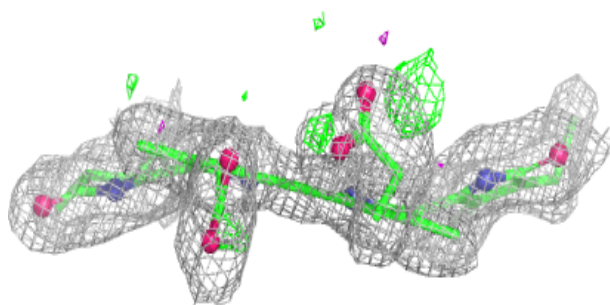
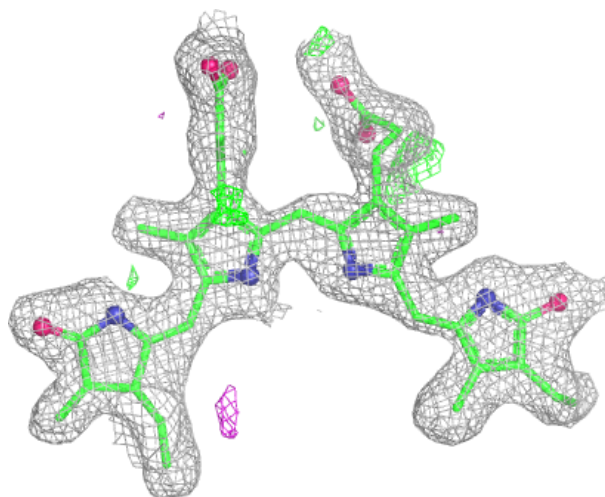
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CYC	C	201	43/43	0.99	0.03	5,10,15,21	0
3	CYC	D	201	43/43	0.99	0.03	11,14,19,22	0
3	CYC	D	202	43/43	0.99	0.04	4,17,31,39	0
3	CYC	E	201	43/43	0.99	0.03	3,9,13,15	0
3	CYC	F	201	43/43	0.99	0.03	13,18,22,25	0
3	CYC	F	202	43/43	0.99	0.04	4,21,35,43	0
3	CYC	G	201	43/43	0.99	0.03	5,15,18,18	0
3	CYC	H	201	43/43	0.99	0.03	14,18,22,24	0
3	CYC	H	202	43/43	0.99	0.03	4,15,32,41	0
3	CYC	I	201	43/43	0.99	0.03	5,10,13,15	0
3	CYC	J	201	43/43	0.99	0.03	6,19,24,27	0
3	CYC	J	202	43/43	0.99	0.04	4,13,34,45	0
3	CYC	K	201	43/43	0.99	0.03	2,10,16,20	0
3	CYC	L	201	43/43	0.99	0.03	6,16,25,31	0
3	CYC	L	202	43/43	0.99	0.03	2,18,35,46	0
3	CYC	M	201	43/43	0.99	0.03	7,12,17,23	0
3	CYC	N	201	43/43	0.99	0.03	8,17,28,32	0
3	CYC	N	202	43/43	0.99	0.04	4,17,31,38	0
3	CYC	O	201	43/43	0.99	0.03	5,11,14,20	0
3	CYC	P	201	43/43	0.99	0.03	8,17,25,26	0
3	CYC	P	202	43/43	0.99	0.04	5,16,33,41	0
3	CYC	Q	201	43/43	0.99	0.03	5,10,13,14	0
3	CYC	R	201	43/43	0.99	0.04	16,18,24,25	0
3	CYC	R	202	43/43	0.99	0.04	9,20,32,39	0
3	CYC	S	201	43/43	0.99	0.03	3,7,12,16	0
3	CYC	T	201	43/43	0.99	0.04	15,19,26,29	0
3	CYC	T	202	43/43	0.99	0.04	7,18,32,39	0
3	CYC	U	201	43/43	0.99	0.03	6,9,14,17	0
3	CYC	V	201	43/43	0.99	0.03	3,11,20,23	0
3	CYC	V	202	43/43	0.99	0.03	7,17,32,41	0
3	CYC	W	201	43/43	0.99	0.03	7,12,16,18	0
3	CYC	X	201	43/43	0.99	0.03	8,15,18,22	0
3	CYC	X	202	43/43	0.99	0.04	6,18,29,40	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.

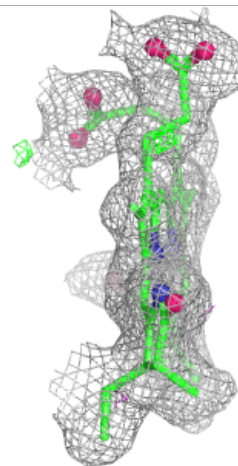
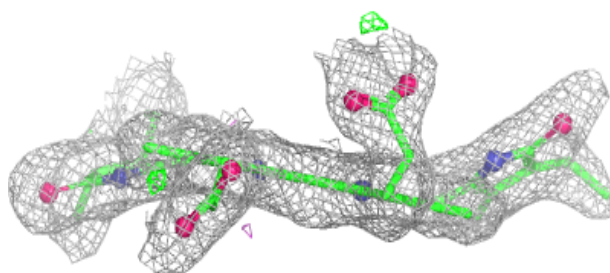
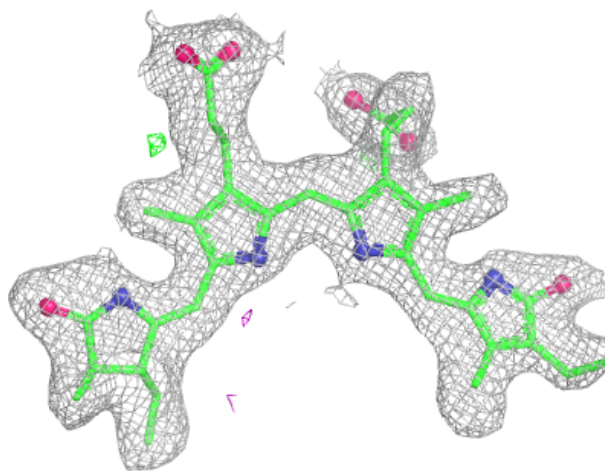
Electron density around CYC A 201:

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



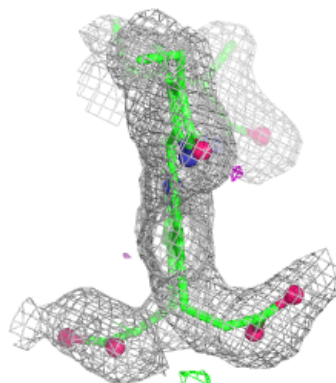
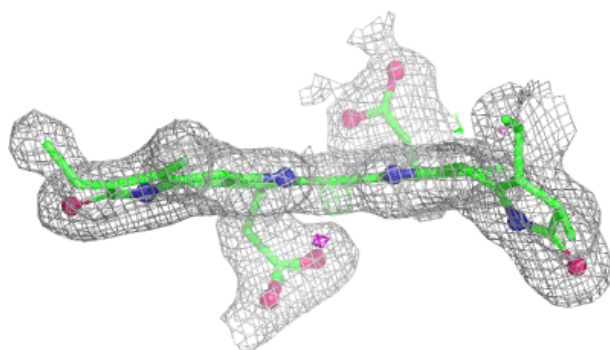
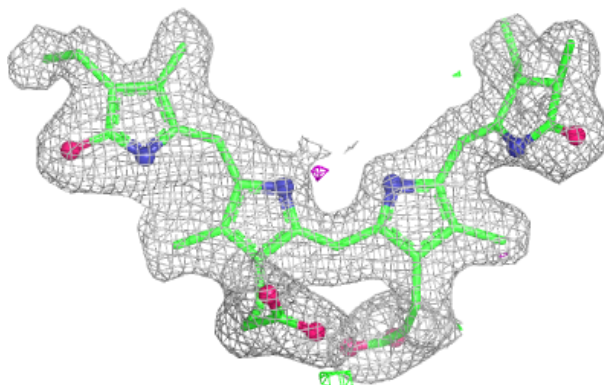
Electron density around CYC B 201:

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



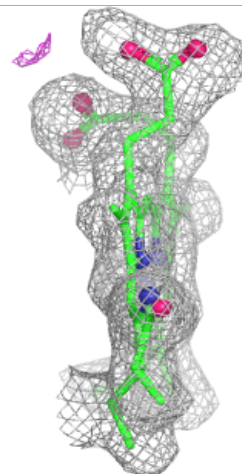
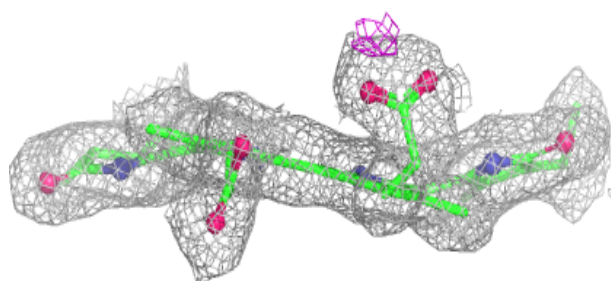
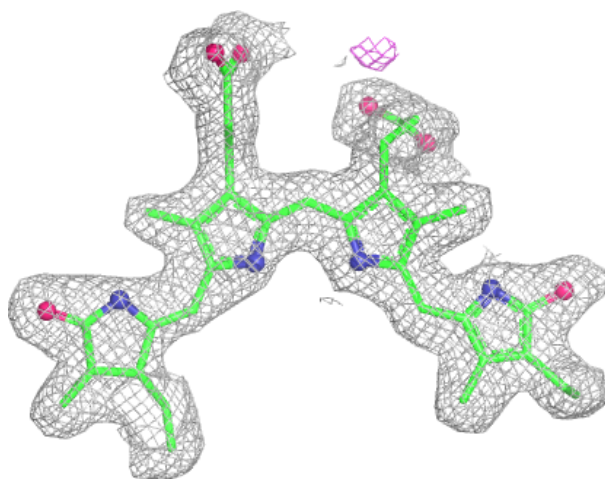
Electron density around CYC B 202:

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



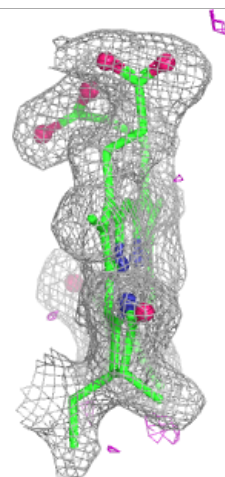
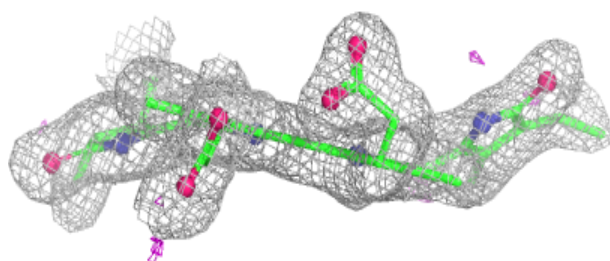
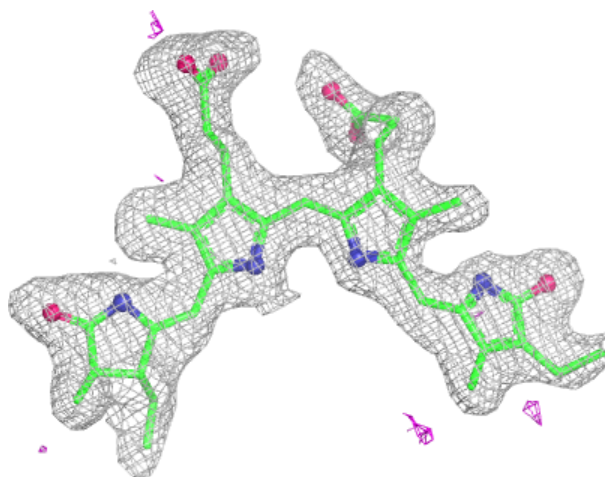
Electron density around CYC C 201:

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



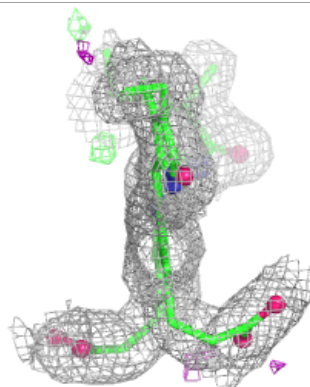
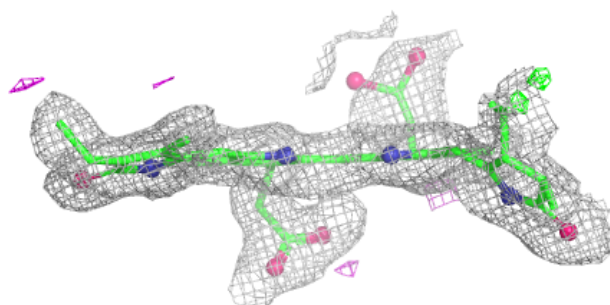
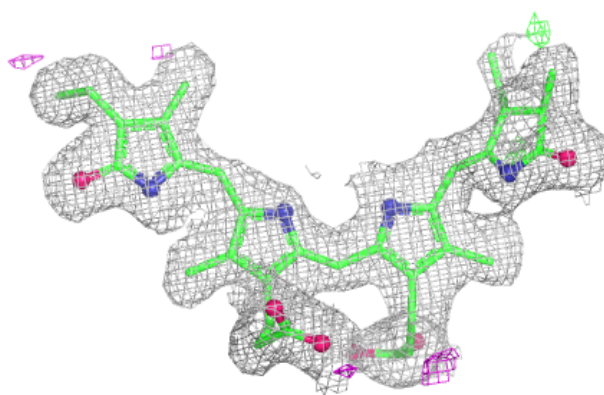
Electron density around CYC D 201:

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



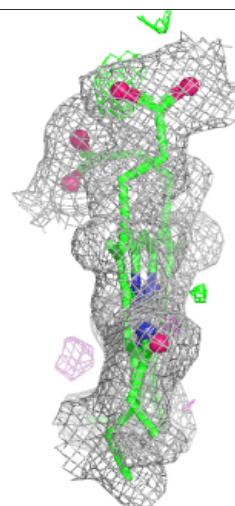
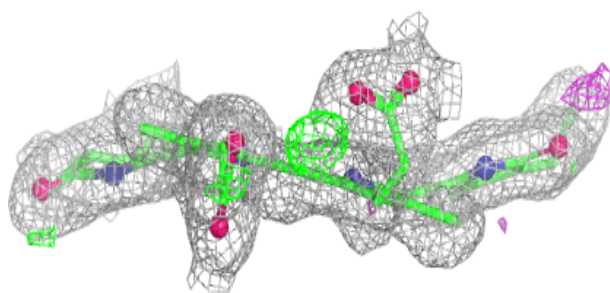
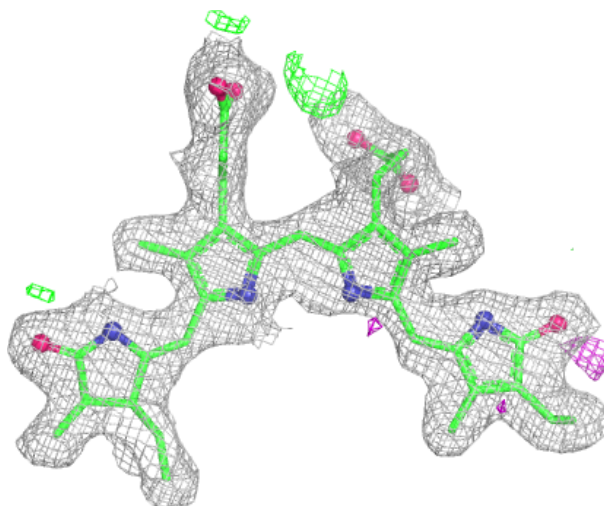
Electron density around CYC D 202:

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



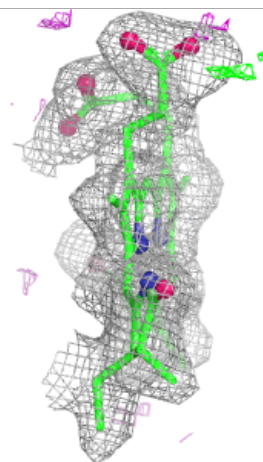
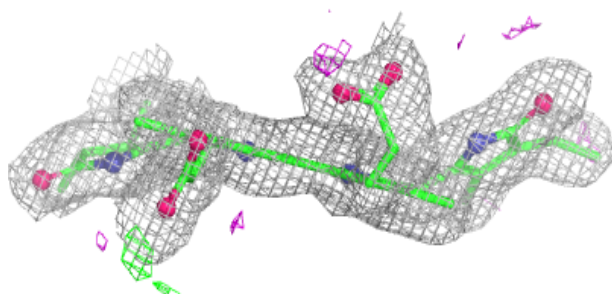
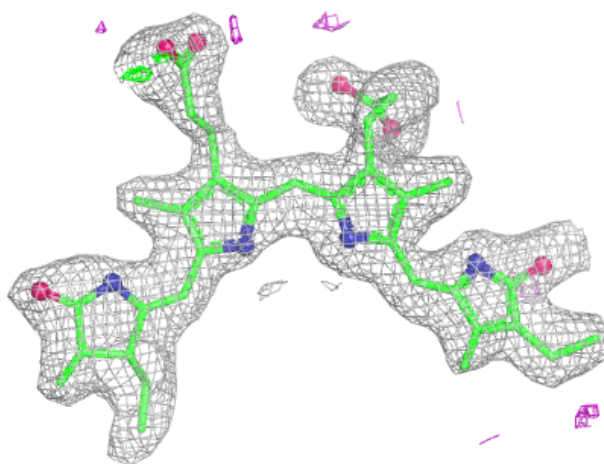
Electron density around CYC E 201:

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



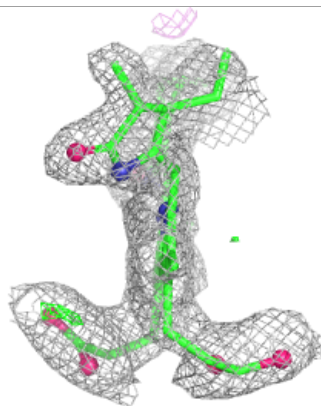
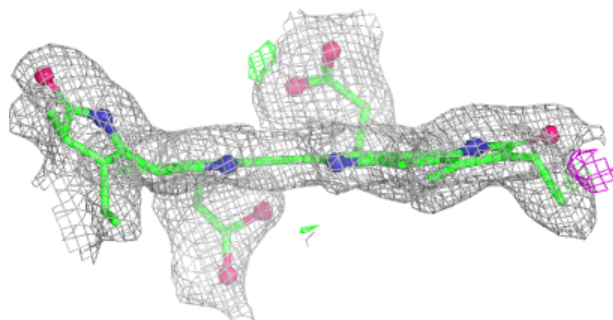
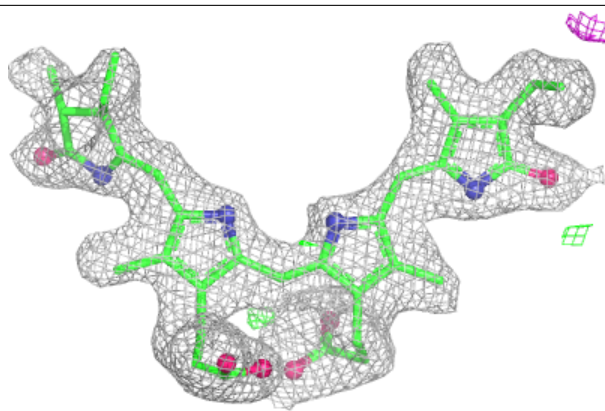
Electron density around CYC F 201:

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



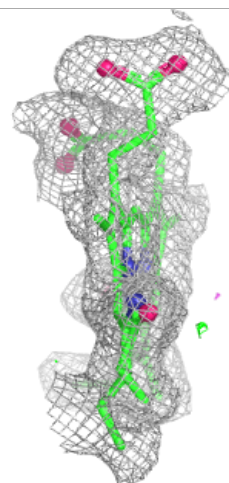
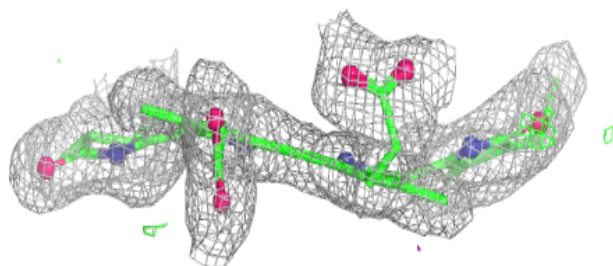
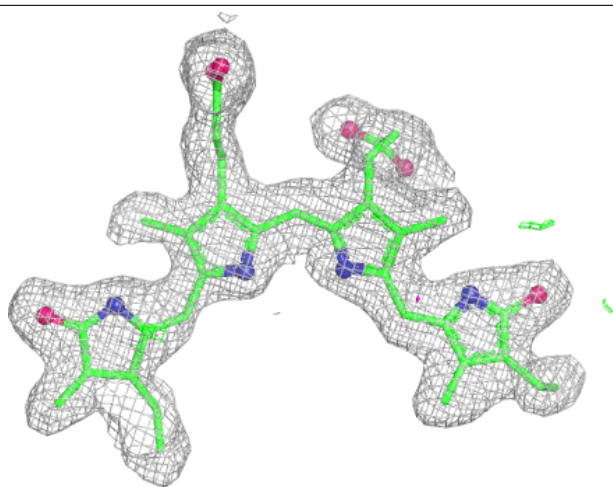
Electron density around CYC F 202:

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



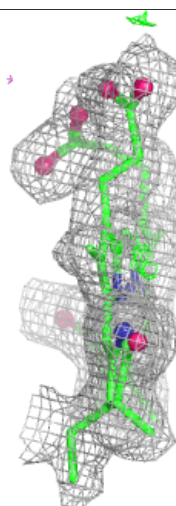
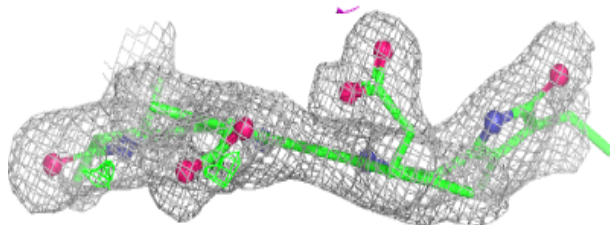
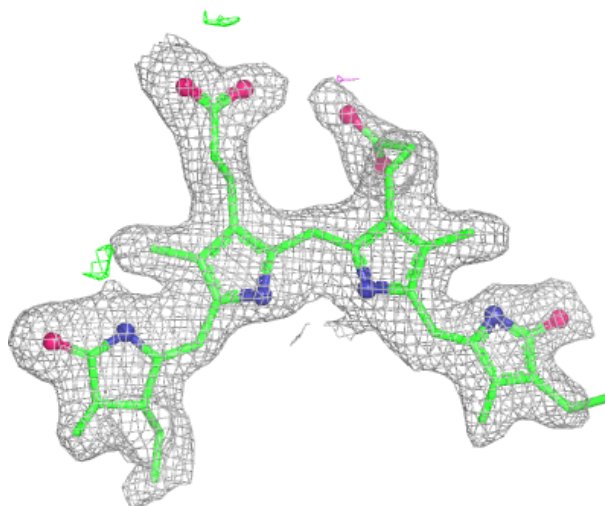
Electron density around CYC G 201:

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



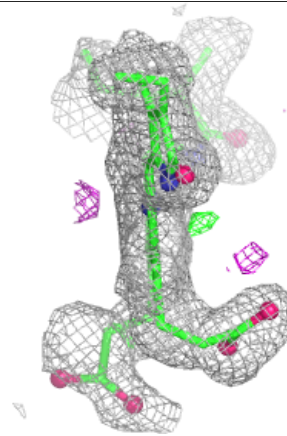
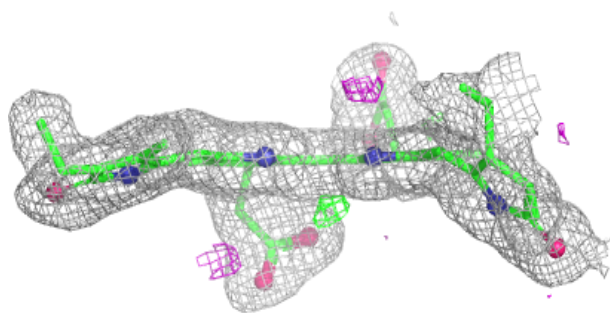
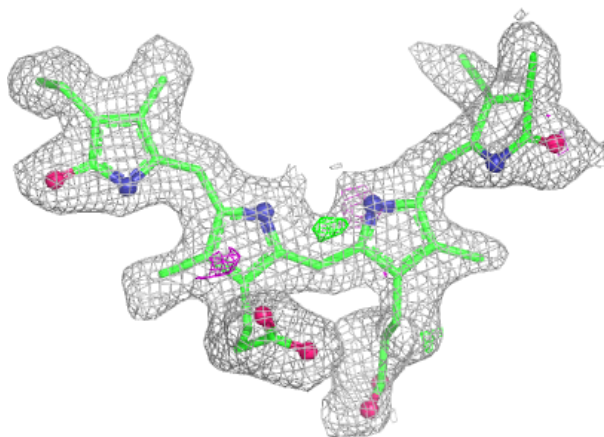
Electron density around CYC H 201:

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



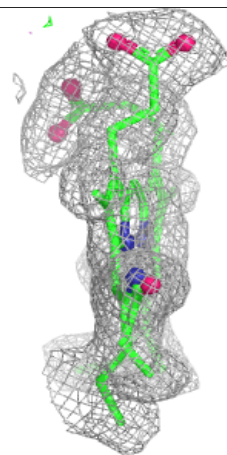
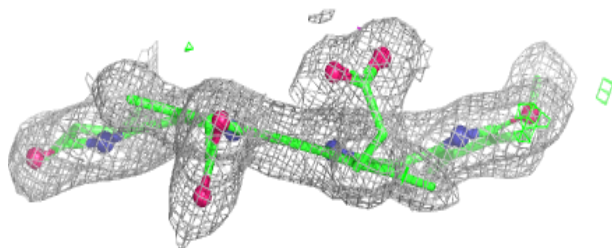
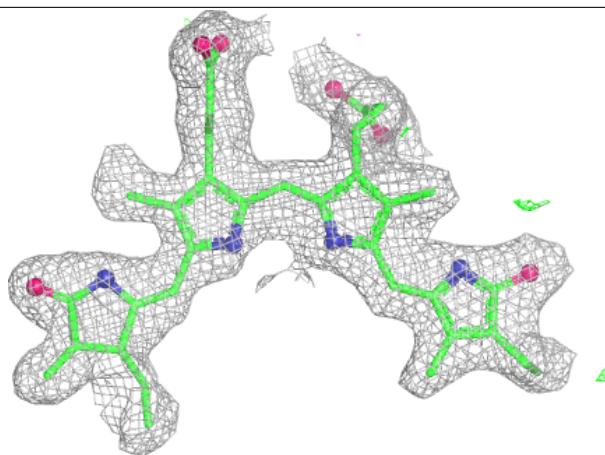
Electron density around CYC H 202:

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



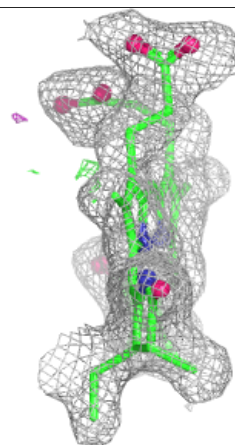
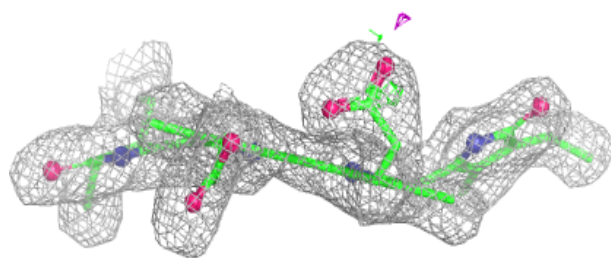
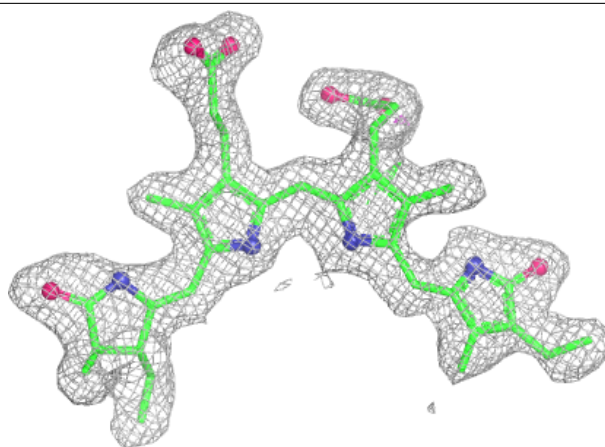
Electron density around CYC I 201:

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



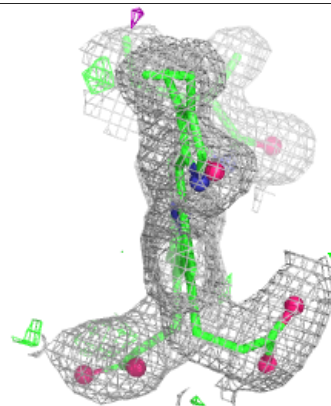
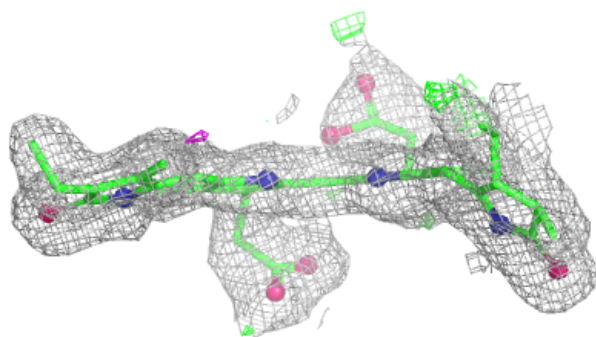
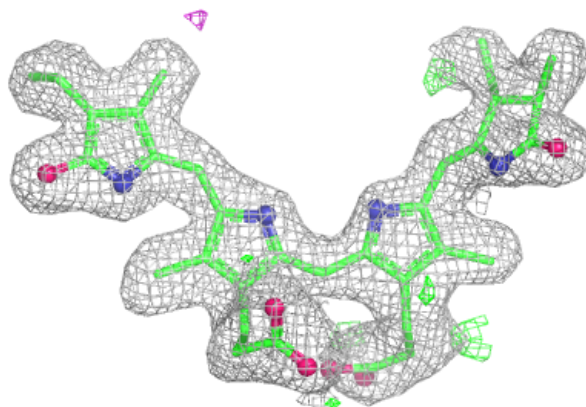
Electron density around CYC J 201:

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



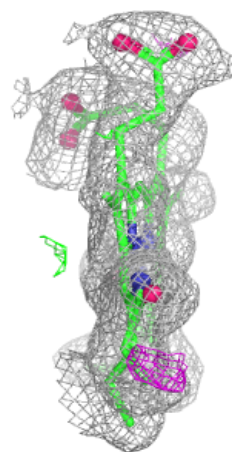
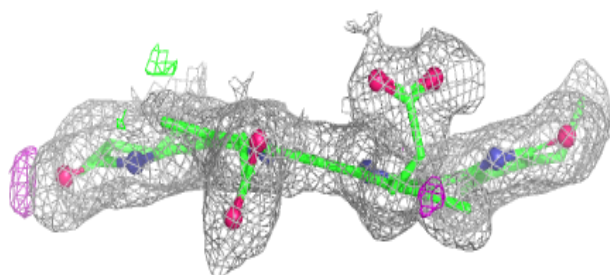
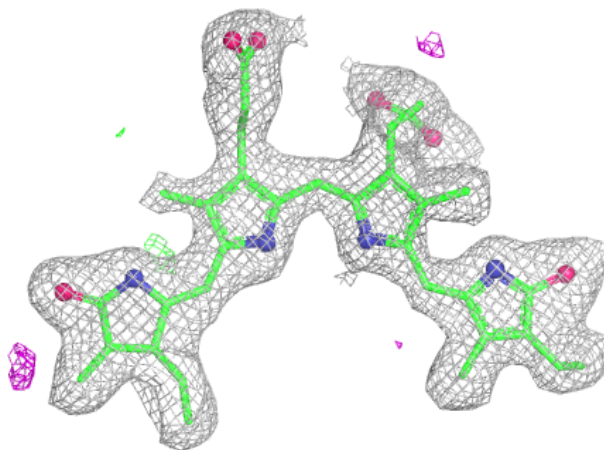
Electron density around CYC J 202:

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



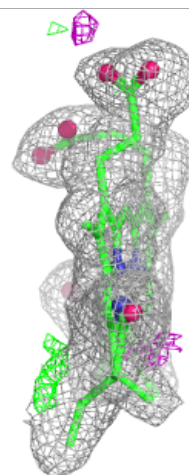
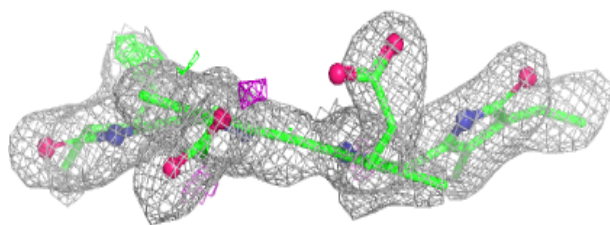
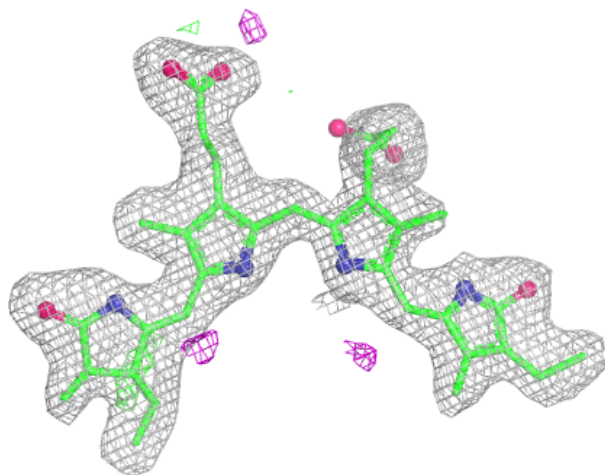
Electron density around CYC K 201:

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



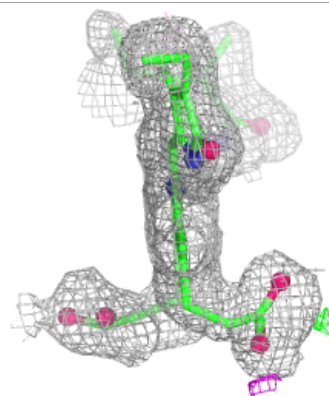
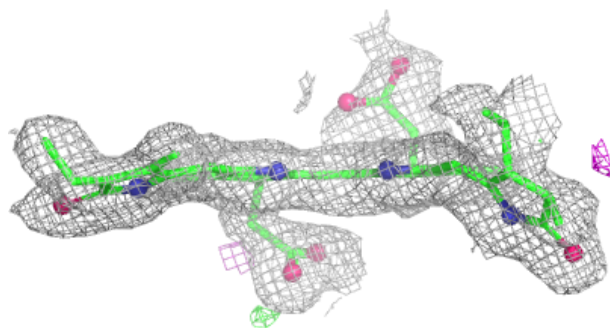
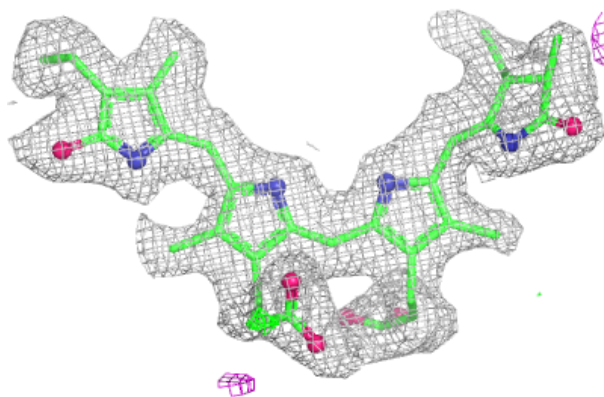
Electron density around CYC L 201:

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



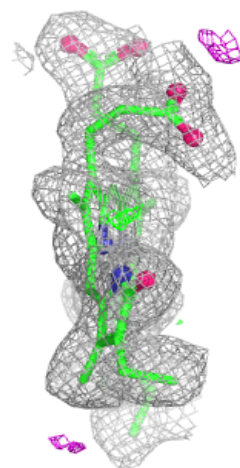
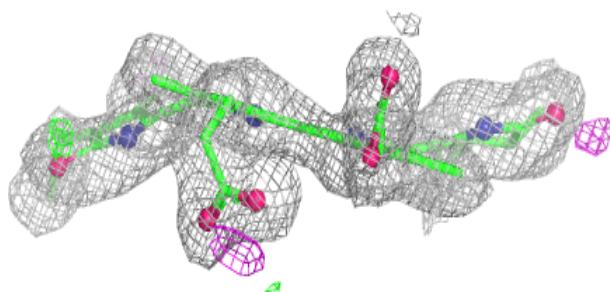
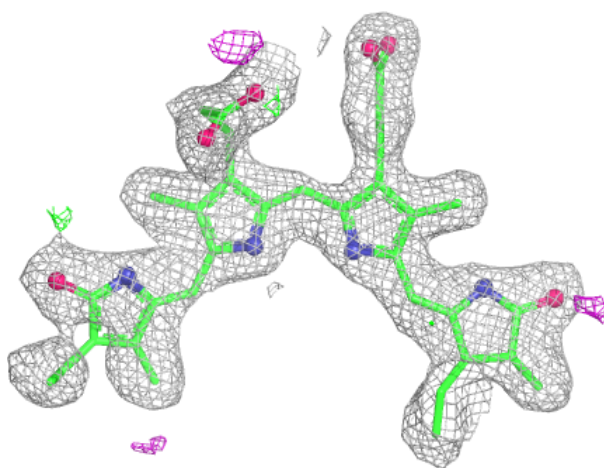
Electron density around CYC L 202:

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



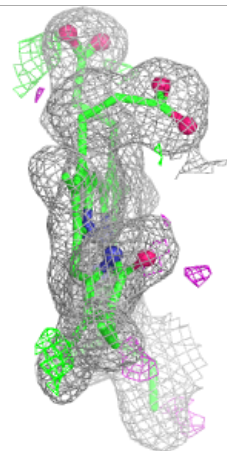
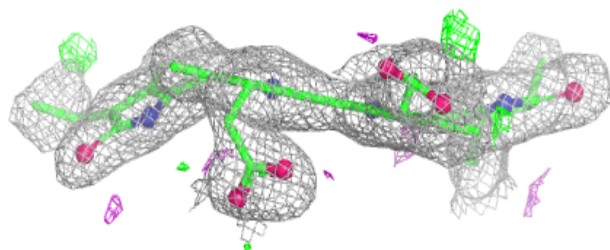
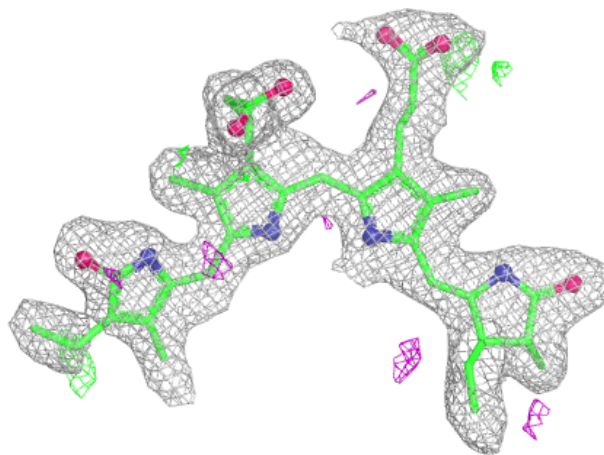
Electron density around CYC M 201:

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



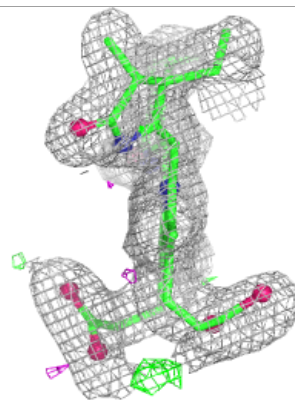
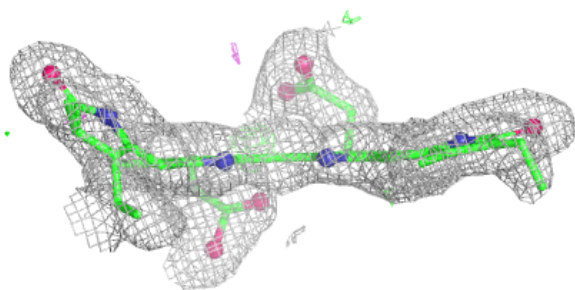
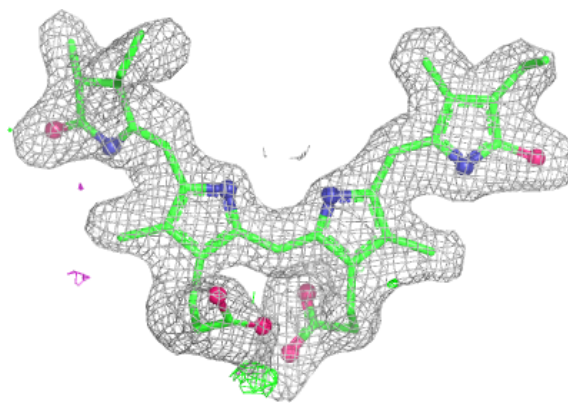
Electron density around CYC N 201:

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



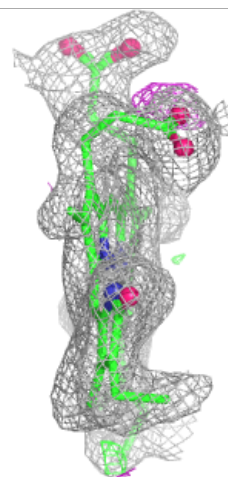
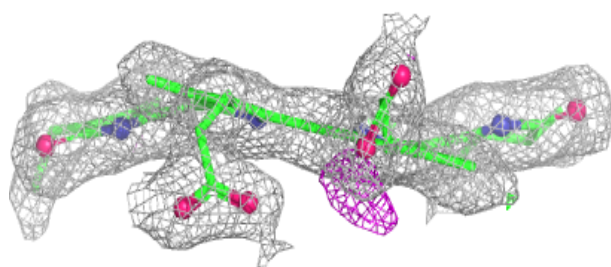
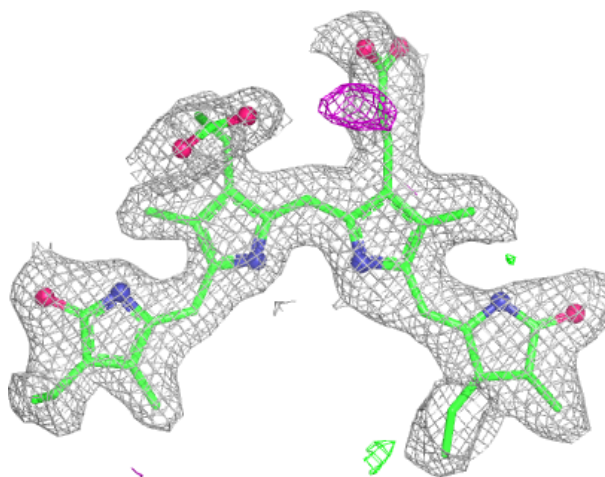
Electron density around CYC N 202:

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



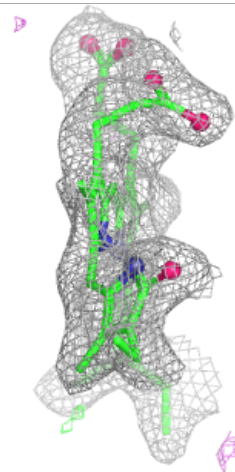
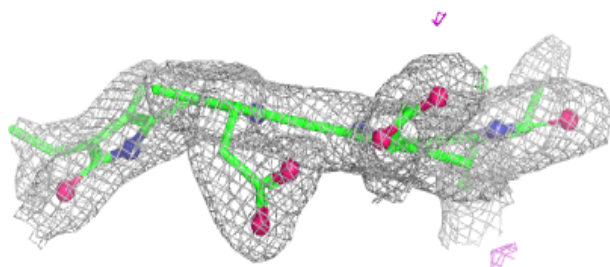
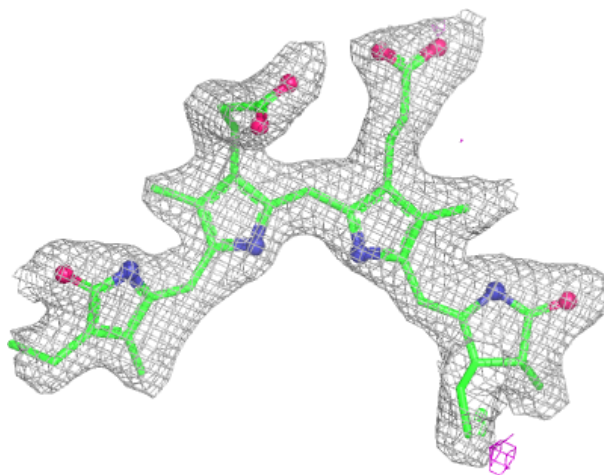
Electron density around CYC O 201:

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



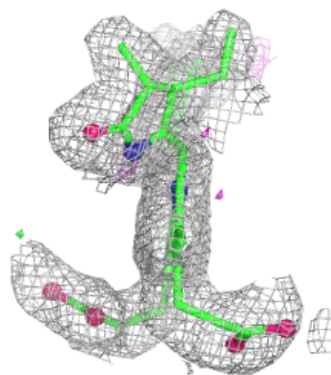
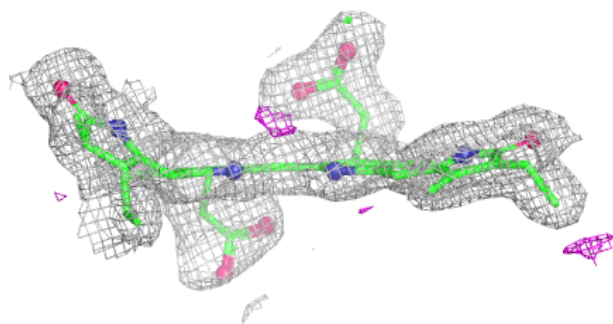
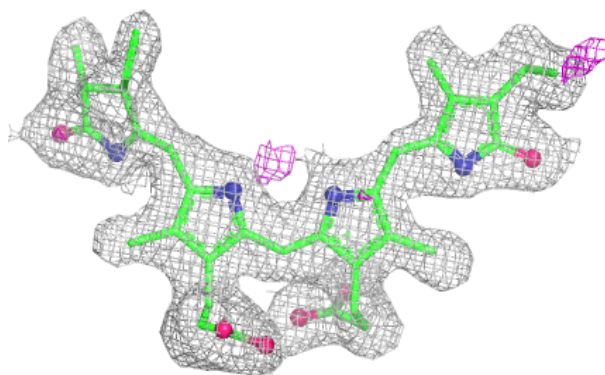
Electron density around CYC P 201:

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



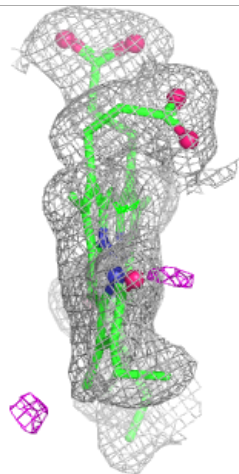
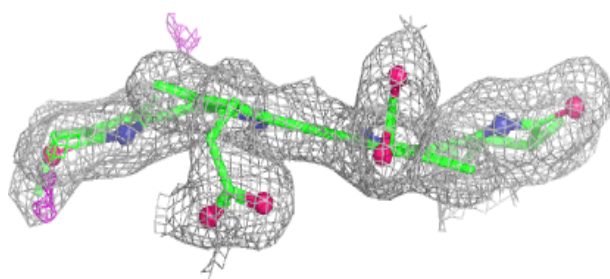
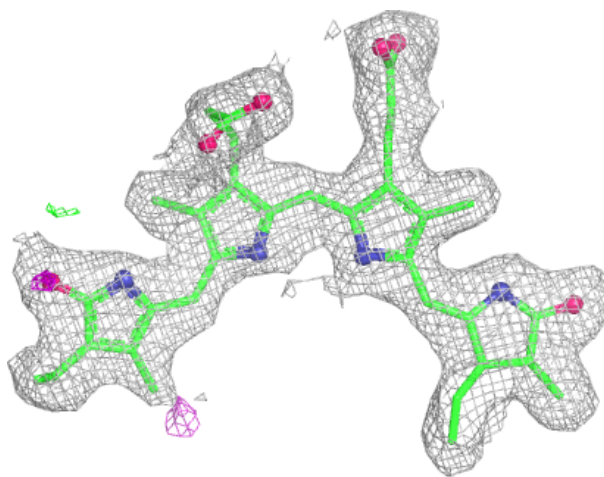
Electron density around CYC P 202:

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



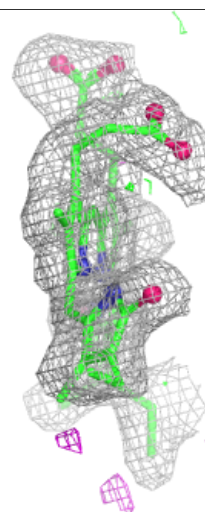
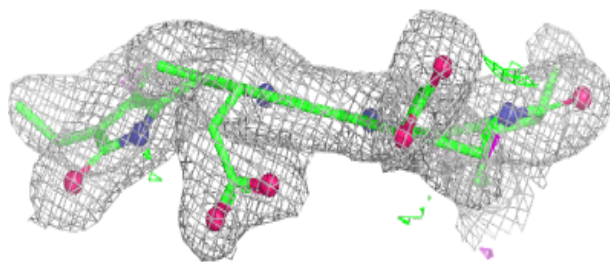
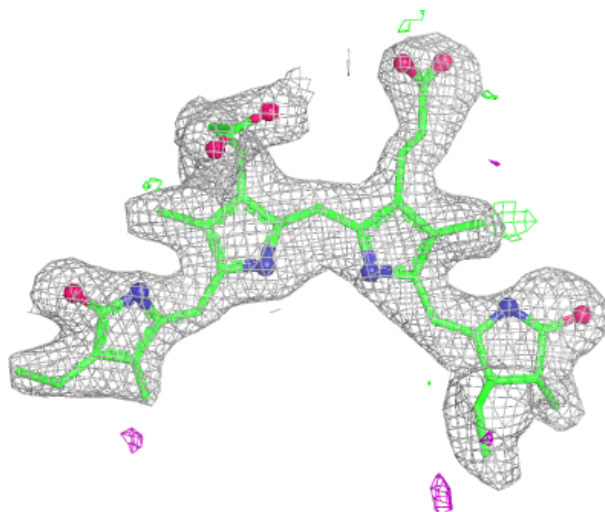
Electron density around CYC Q 201:

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



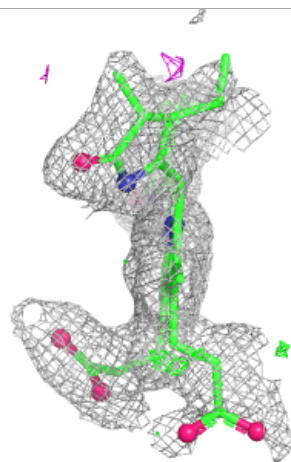
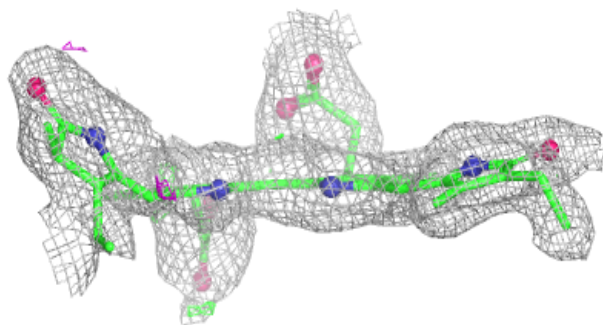
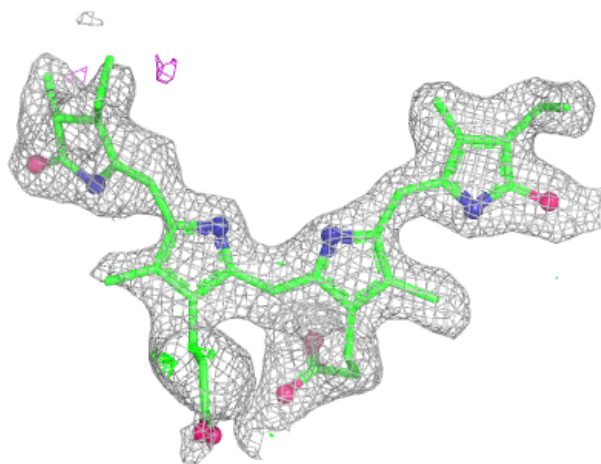
Electron density around CYC R 201:

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



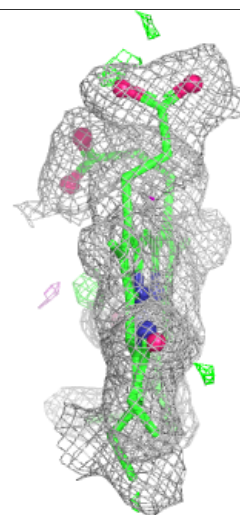
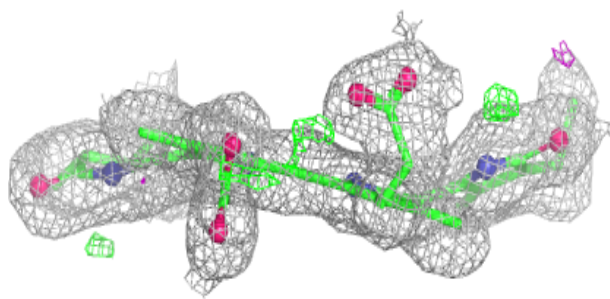
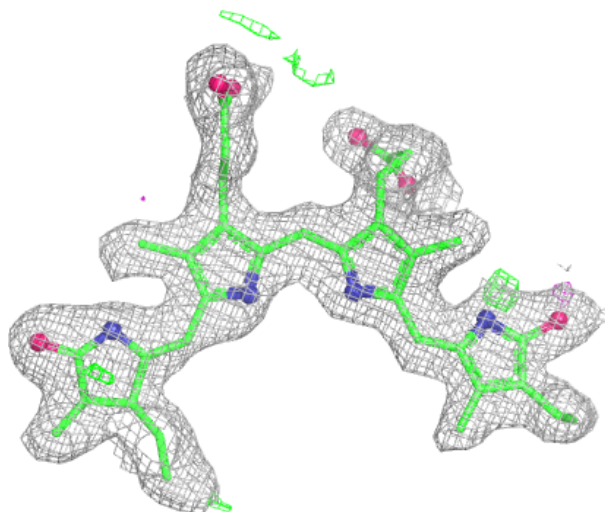
Electron density around CYC R 202:

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



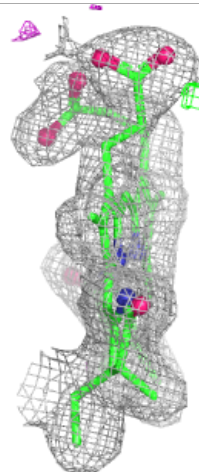
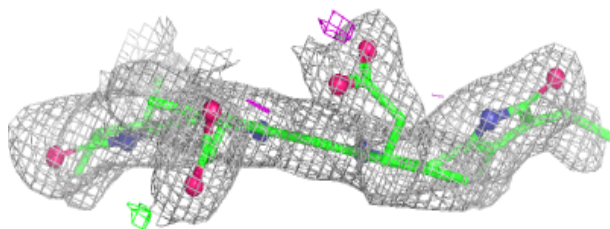
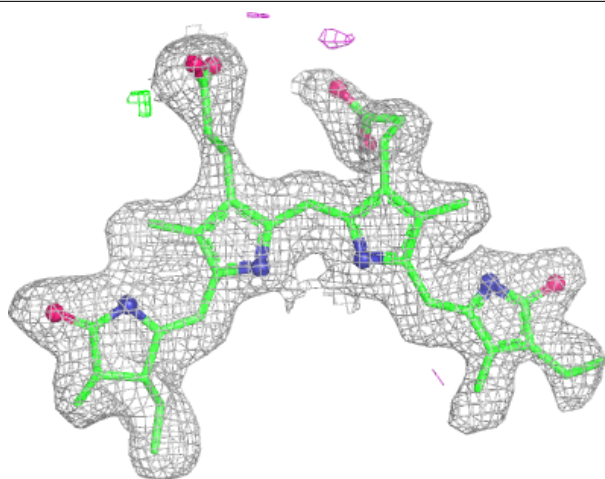
Electron density around CYC S 201:

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



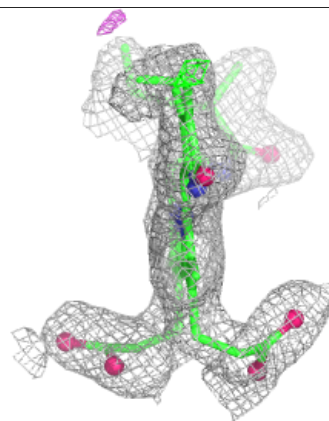
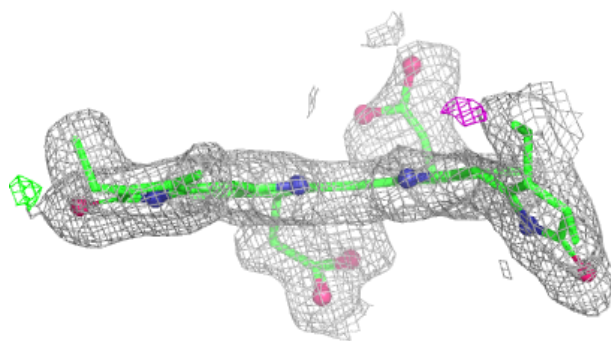
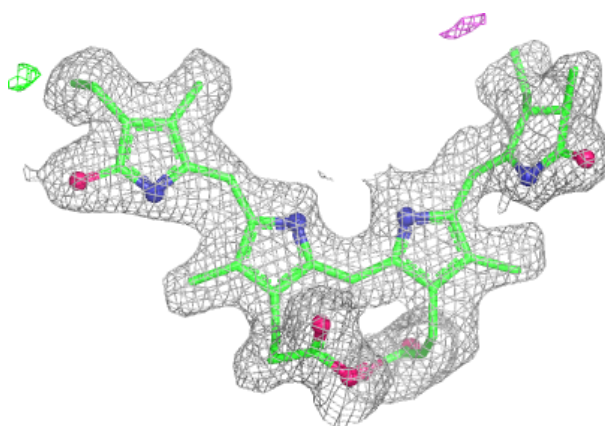
Electron density around CYC T 201:

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



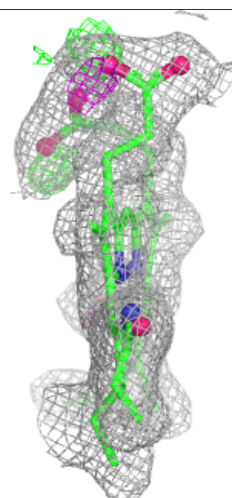
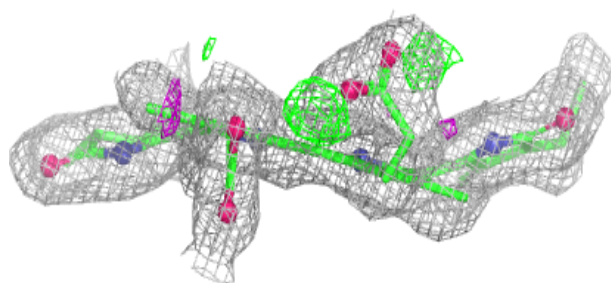
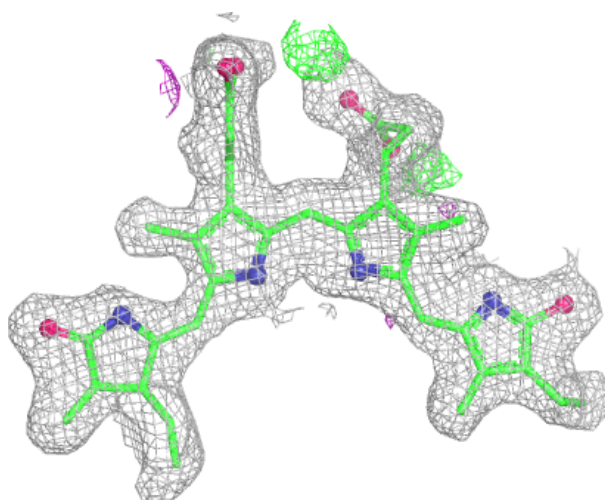
Electron density around CYC T 202:

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



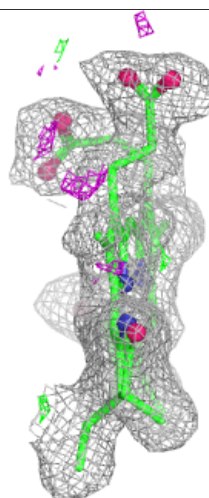
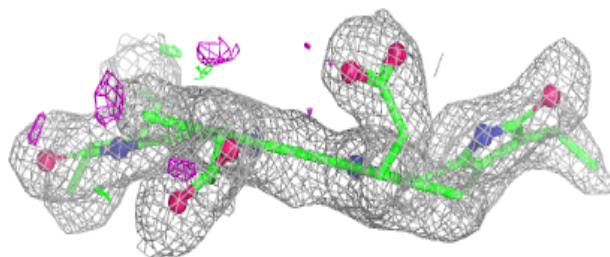
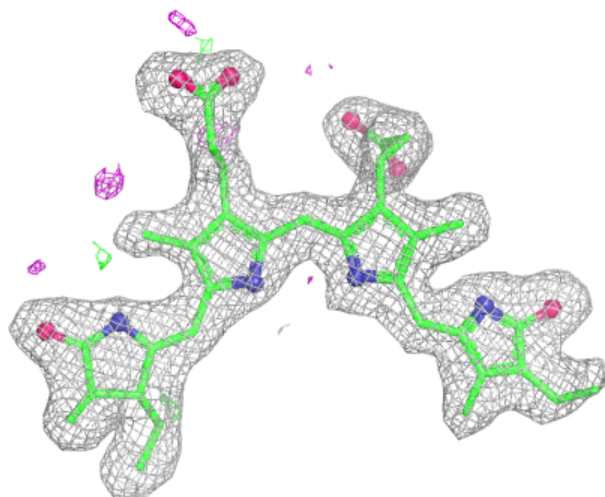
Electron density around CYC U 201:

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



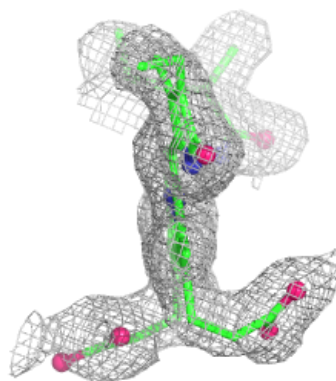
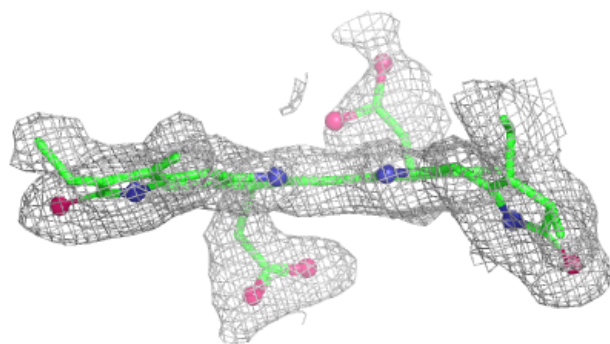
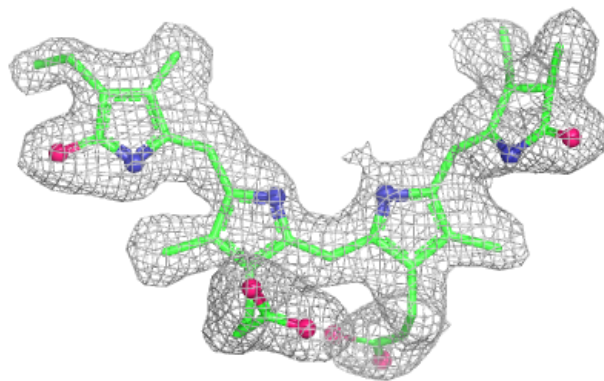
Electron density around CYC V 201:

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



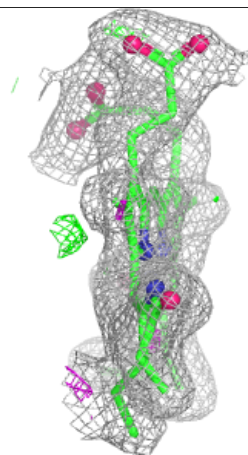
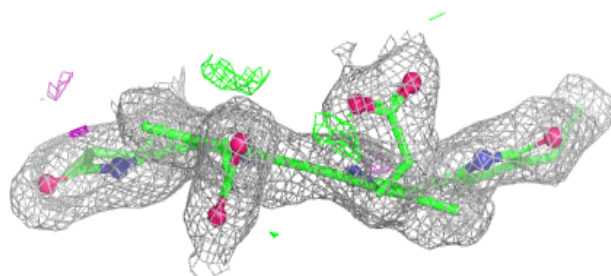
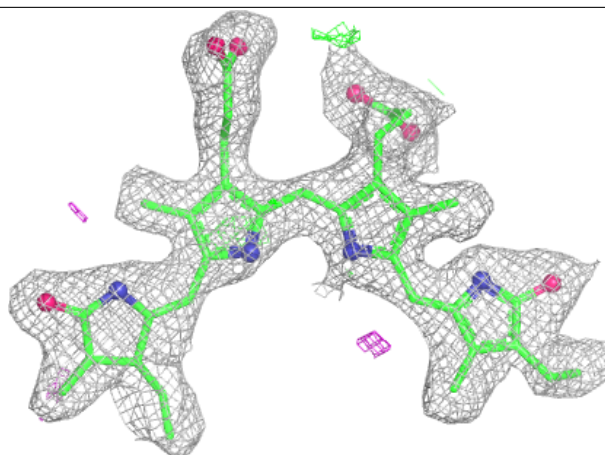
Electron density around CYC V 202:

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



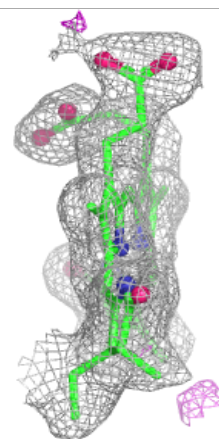
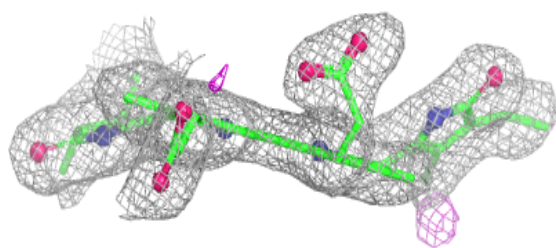
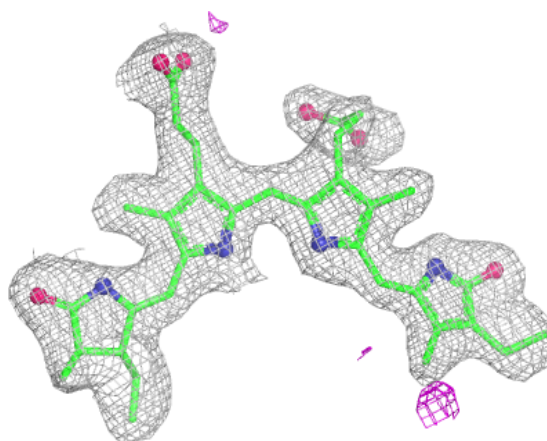
Electron density around CYC W 201:

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



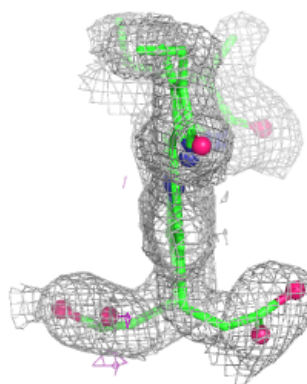
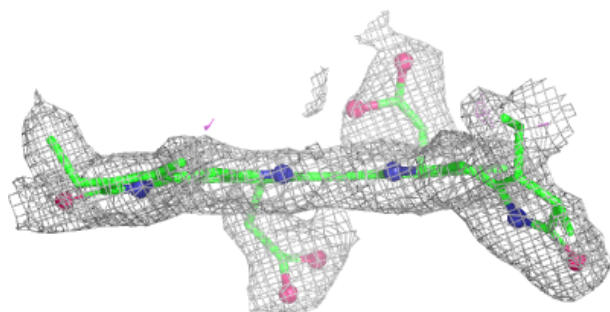
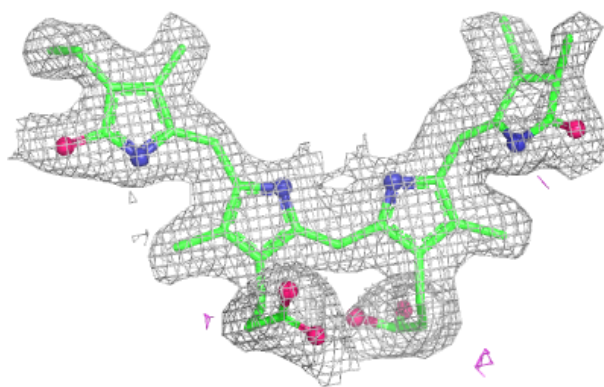
Electron density around CYC X 201:

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



Electron density around CYC X 202:

$2mF_o-DF_c$ (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.