



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2023 – 04:09 PM EDT

PDB ID : 2QJK  
Title : Crystal Structure Analysis of mutant rhodobacter sphaeroides bc1 with stigmatellin and antimycin  
Authors : Esser, L.  
Deposited on : 2007-07-07  
Resolution : 3.10 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](mailto: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 : 2.35  
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) : 2.35

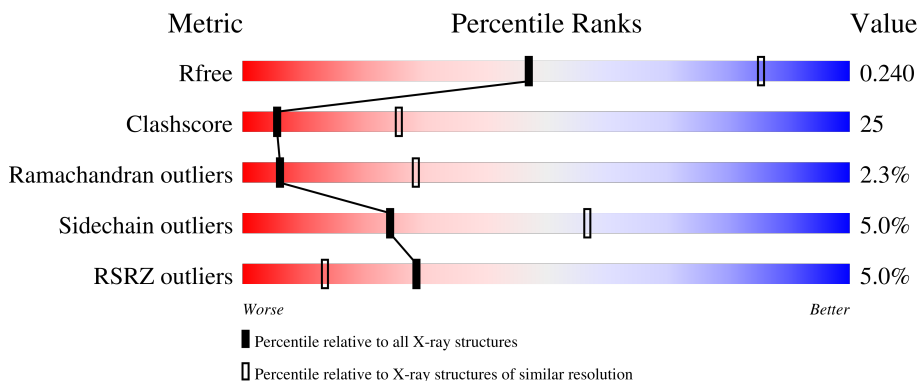
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.




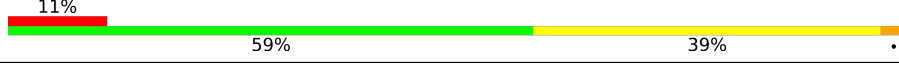
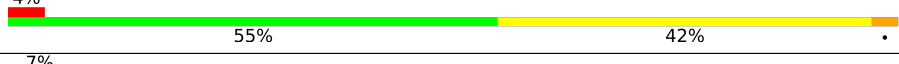








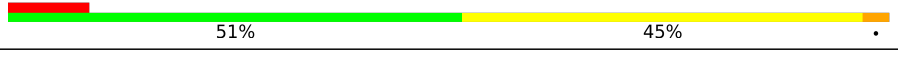

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	428	 4% 54% 42%
1	D	428	 4% 54% 44%
1	G	428	 3% 52% 44%
1	J	428	 4% 50% 47%
1	M	428	 4% 49% 47%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	428	
2	B	256	
2	E	256	
2	H	256	
2	K	256	
2	N	256	
2	Q	256	
3	C	179	
3	F	179	
3	I	179	
3	L	179	
3	O	179	
3	R	179	

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
10	FES	C	200	-	-	X	-
10	FES	F	200	-	-	X	-
10	FES	I	200	-	-	X	-
10	FES	L	200	-	-	X	-
10	FES	O	200	-	-	X	-
10	FES	R	200	-	-	X	-
4	BGL	M	431	-	-	-	X
7	LOP	J	504	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 42048 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 Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	428	3440	2322	548	555	15	0	0	0
1	D	428	3440	2322	548	555	15	0	0	0
1	G	428	3440	2322	548	555	15	0	0	0
1	J	428	3440	2322	548	555	15	0	0	0
1	M	428	3440	2322	548	555	15	0	0	0
1	P	428	3440	2322	548	555	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	ARG	SER	engineered mutation	UNP Q02761
D	287	ARG	SER	engineered mutation	UNP Q02761
G	287	ARG	SER	engineered mutation	UNP Q02761
J	287	ARG	SER	engineered mutation	UNP Q02761
M	287	ARG	SER	engineered mutation	UNP Q02761
P	287	ARG	SER	engineered mutation	UNP Q02761

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	256	1953	1240	326	374	13	0	0	0
2	E	256	1953	1240	326	374	13	0	0	0
2	H	256	1953	1240	326	374	13	0	0	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	N	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	Q	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

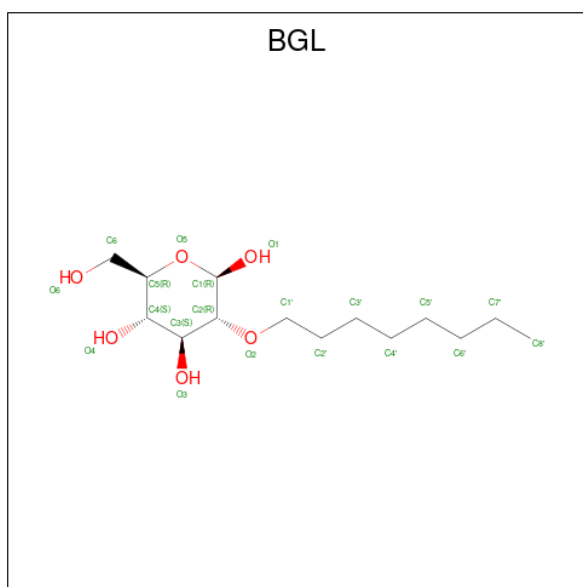
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	F	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	I	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	L	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	O	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	R	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			

There are 6 discrepancies between the modelled and reference sequences:

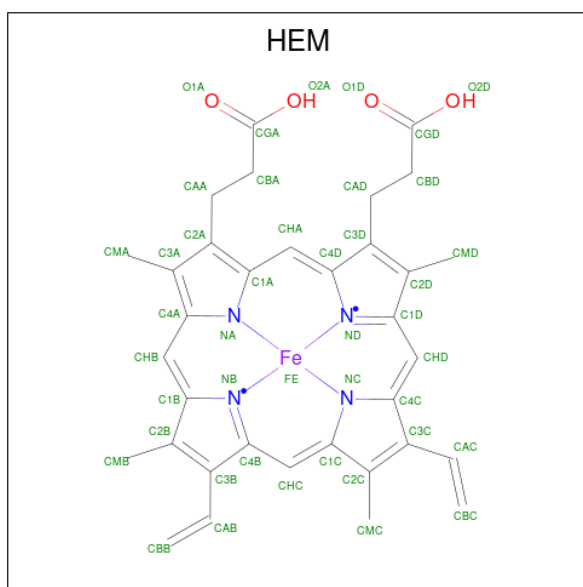
Chain	Residue	Modelled	Actual	Comment	Reference
C	135	SER	VAL	engineered mutation	UNP Q02762
F	135	SER	VAL	engineered mutation	UNP Q02762
I	135	SER	VAL	engineered mutation	UNP Q02762
L	135	SER	VAL	engineered mutation	UNP Q02762
O	135	SER	VAL	engineered mutation	UNP Q02762
R	135	SER	VAL	engineered mutation	UNP Q02762

- Molecule 4 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			20	14 6		
4	D	1	Total	C O	0	0
			20	14 6		
4	G	1	Total	C O	0	0
			20	14 6		
4	J	1	Total	C O	0	0
			20	14 6		
4	M	1	Total	C O	0	0
			20	14 6		
4	Q	1	Total	C O	0	0
			20	14 6		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



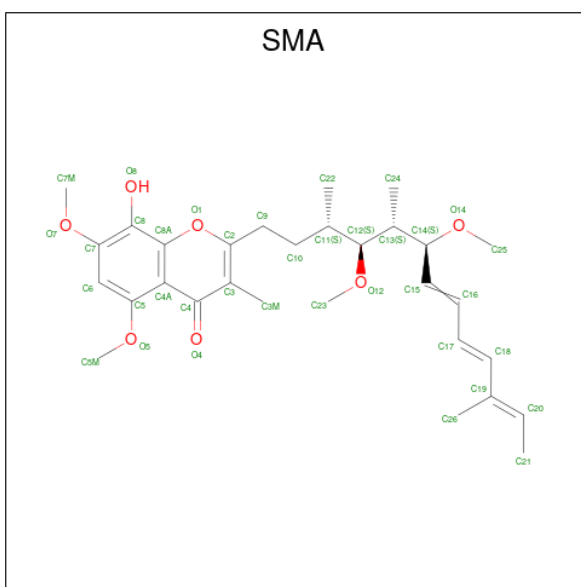
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

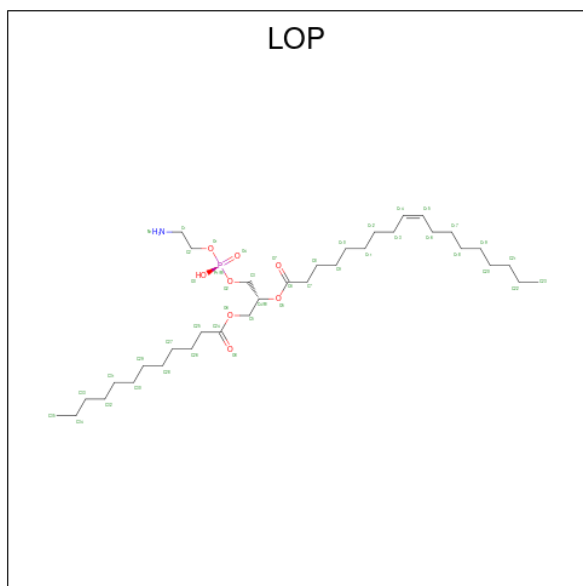
- Molecule 6 is STIGMATELLIN A (three-letter code: SMA) (formula: C<sub>30</sub>H<sub>42</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			37	30 7		
6	D	1	Total	C O	0	0
			37	30 7		
6	G	1	Total	C O	0	0
			37	30 7		
6	J	1	Total	C O	0	0
			37	30 7		
6	M	1	Total	C O	0	0
			37	30 7		
6	P	1	Total	C O	0	0
			37	30 7		

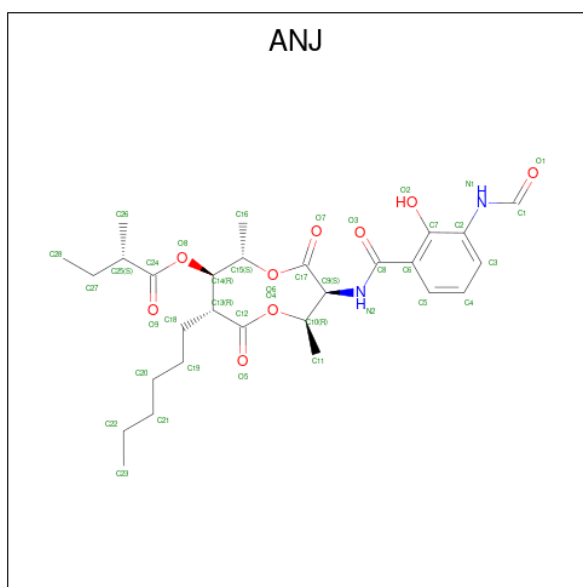
- Molecule 7 is (1R)-2-[[[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code:

LOP) (formula: C<sub>35</sub>H<sub>68</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	M	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 8 is (2R,3S,6S,7R,8R)-3-{{3-(FORMYLAMINO)-2-HYDROXYBENZOYL}AMINO O}-8-HEXYL-2,6-DIMETHYL-4,9-DIOXO-1,5-DIOXONAN-7-YL (2S)-2-METHYLBUTANOATE (three-letter code: ANJ) (formula: C<sub>28</sub>H<sub>40</sub>N<sub>2</sub>O<sub>9</sub>).

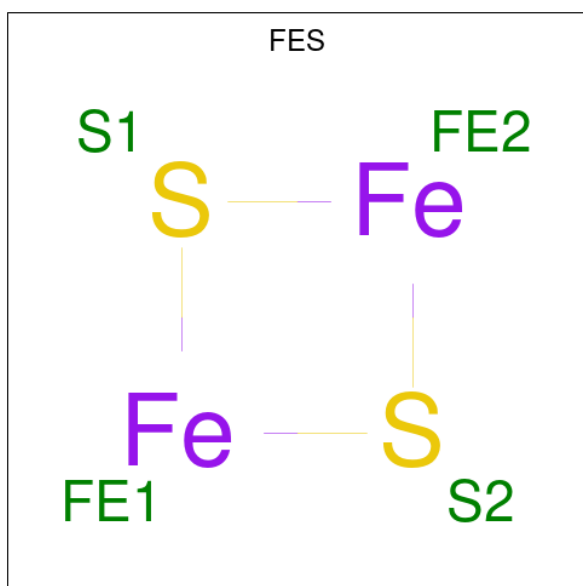


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	Total	C	N	O	0	0
			39	28	2	9		
8	D	1	Total	C	N	O	0	0
			39	28	2	9		
8	G	1	Total	C	N	O	0	0
			39	28	2	9		
8	J	1	Total	C	N	O	0	0
			39	28	2	9		
8	M	1	Total	C	N	O	0	0
			39	28	2	9		
8	P	1	Total	C	N	O	0	0
			39	28	2	9		

- Molecule 9 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
9	B	1	Total	Sr	0	0
			1	1		
9	E	1	Total	Sr	0	0
			1	1		
9	H	1	Total	Sr	0	0
			1	1		
9	K	1	Total	Sr	0	0
			1	1		
9	N	1	Total	Sr	0	0
			1	1		
9	Q	1	Total	Sr	0	0
			1	1		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

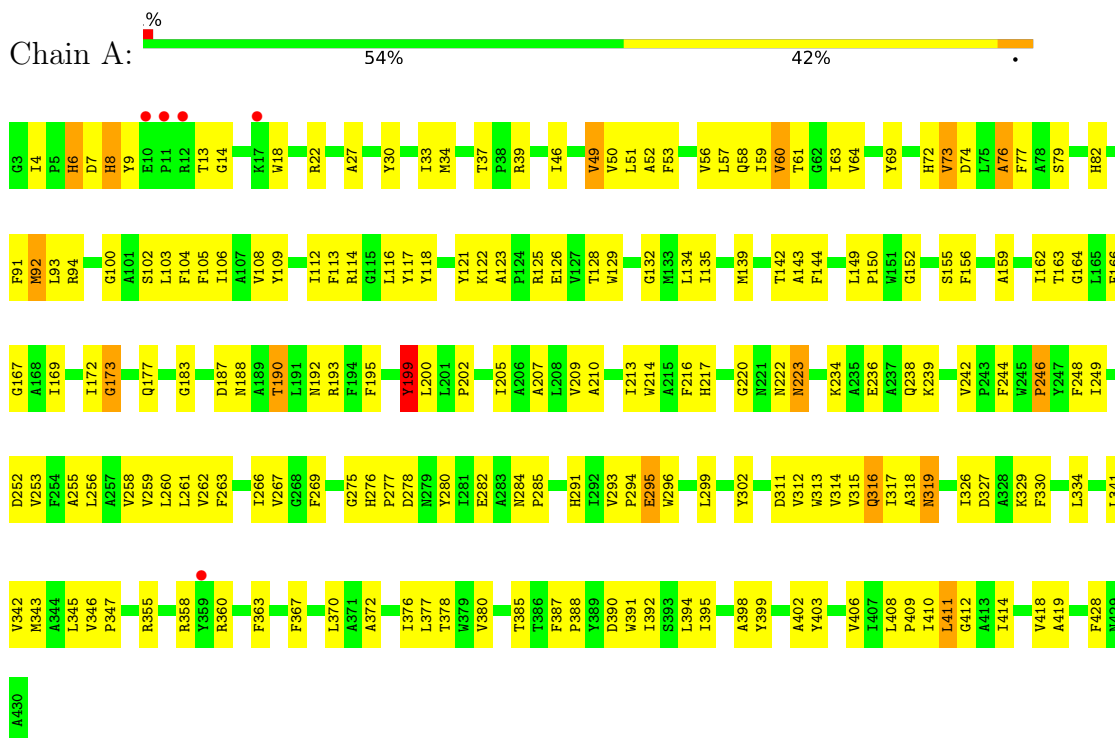


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	Fe	S	0	0
			4	2	2		
10	F	1	Total	Fe	S	0	0
			4	2	2		
10	I	1	Total	Fe	S	0	0
			4	2	2		
10	L	1	Total	Fe	S	0	0
			4	2	2		
10	O	1	Total	Fe	S	0	0
			4	2	2		
10	R	1	Total	Fe	S	0	0
			4	2	2		

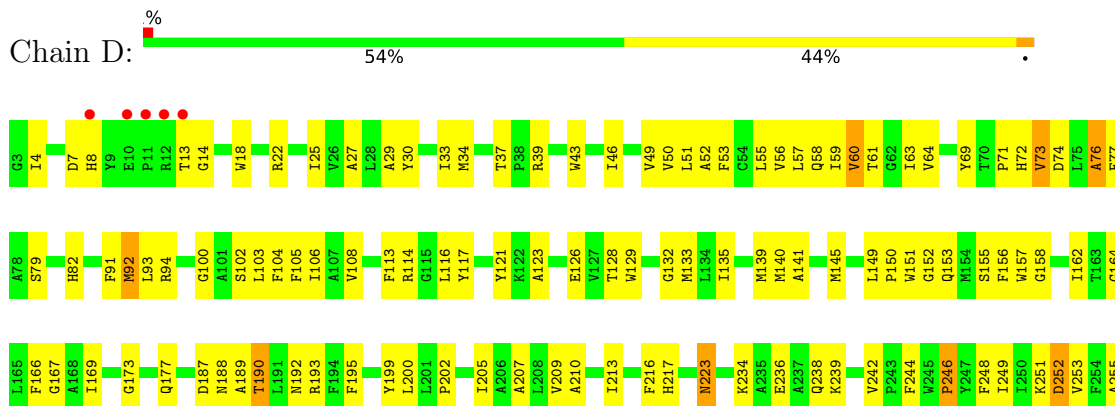
### 3 Residue-property plots i

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.

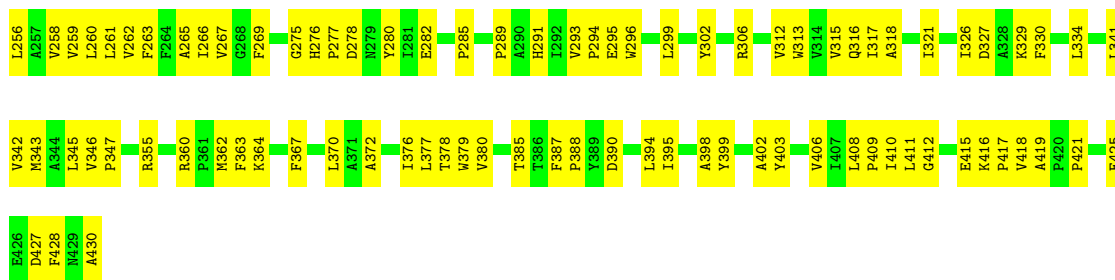
- Molecule 1: Cytochrome b



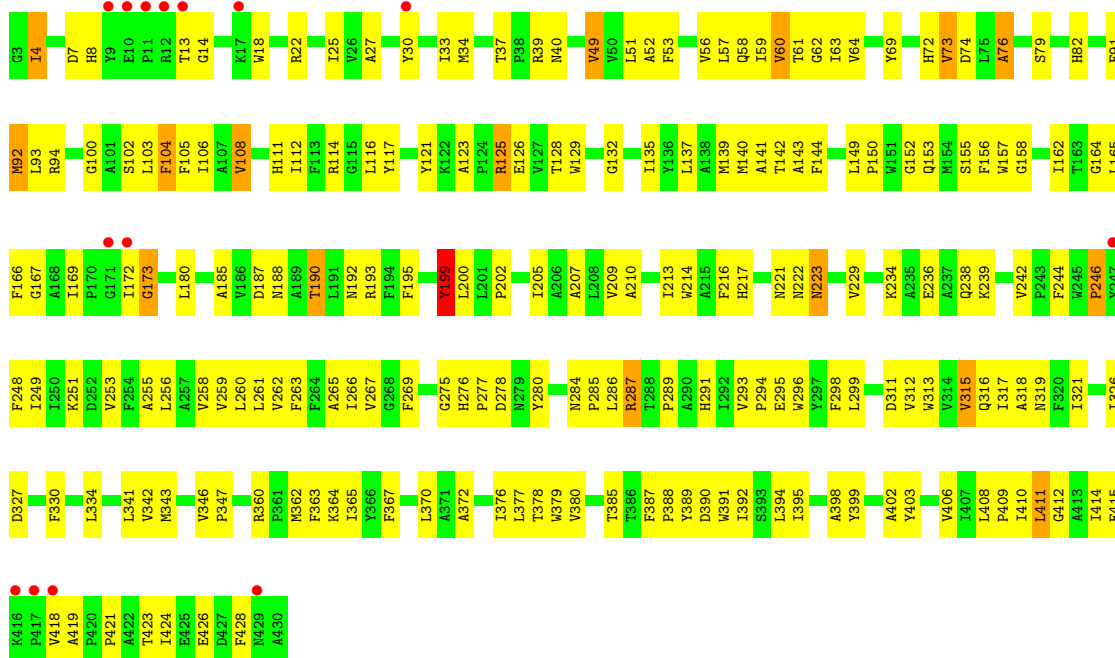
- Molecule 1: Cytochrome b



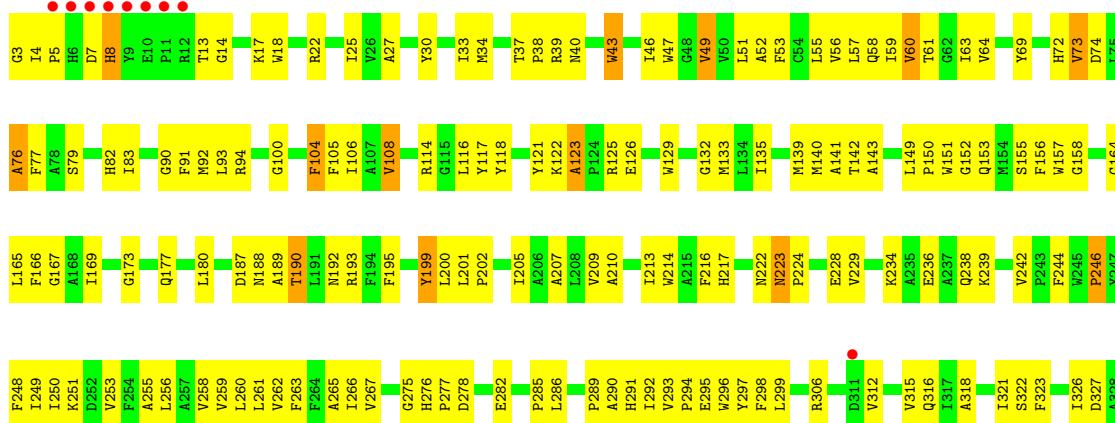


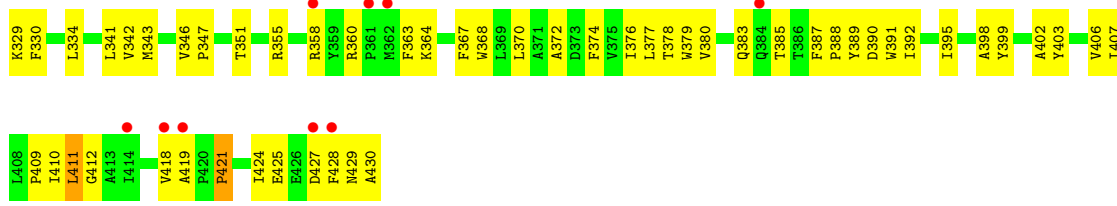


• Molecule 1: Cytochrome b

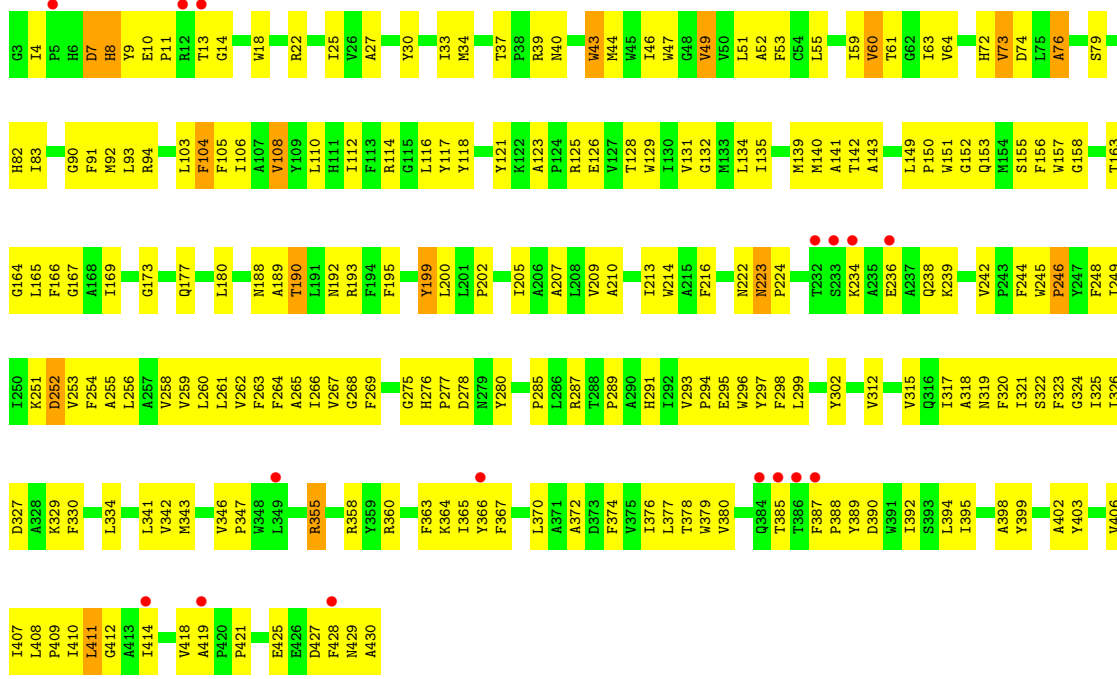


• Molecule 1: Cytochrome b

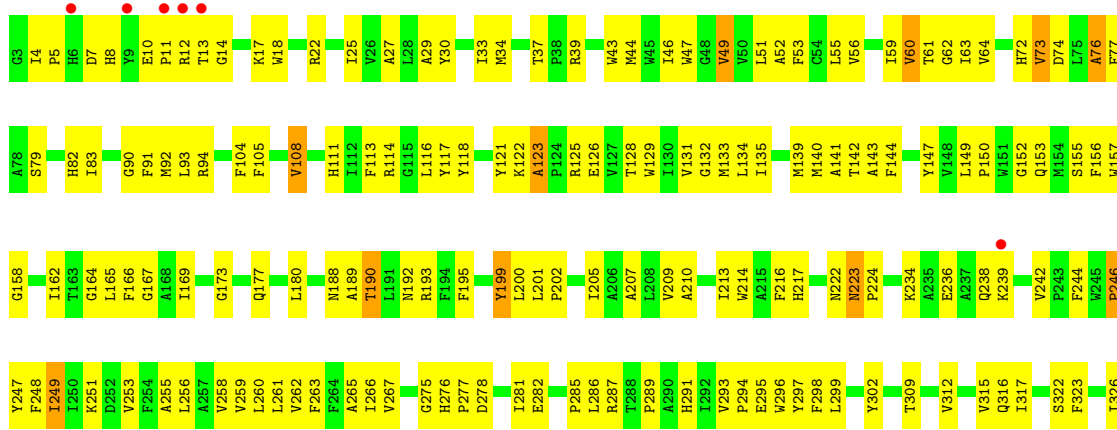


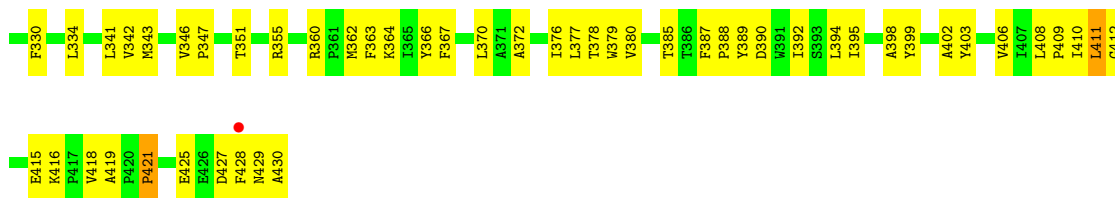


● Molecule 1: Cytochrome b

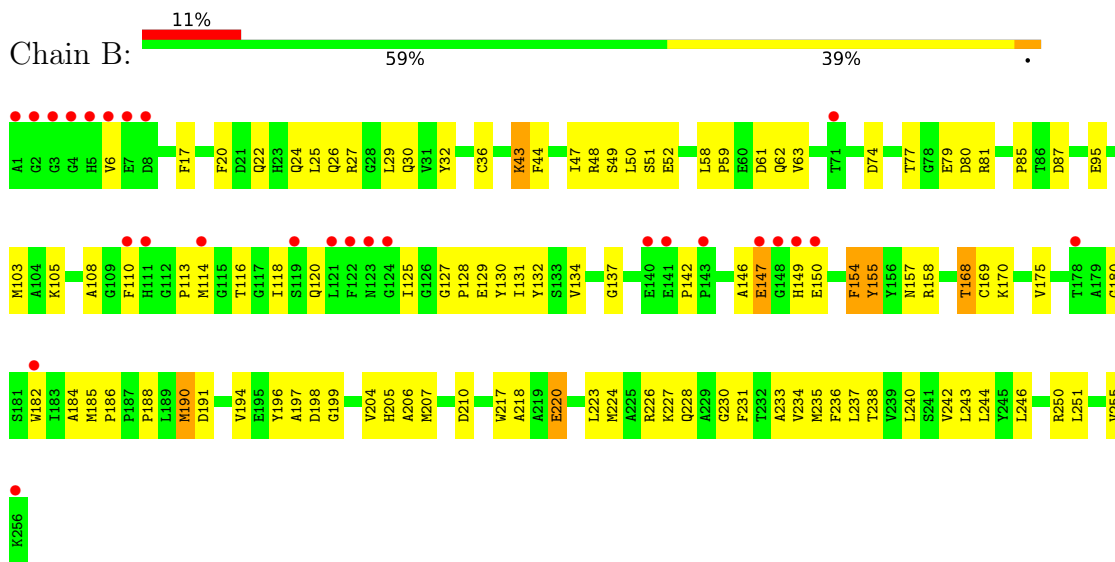


● Molecule 1: Cytochrome b

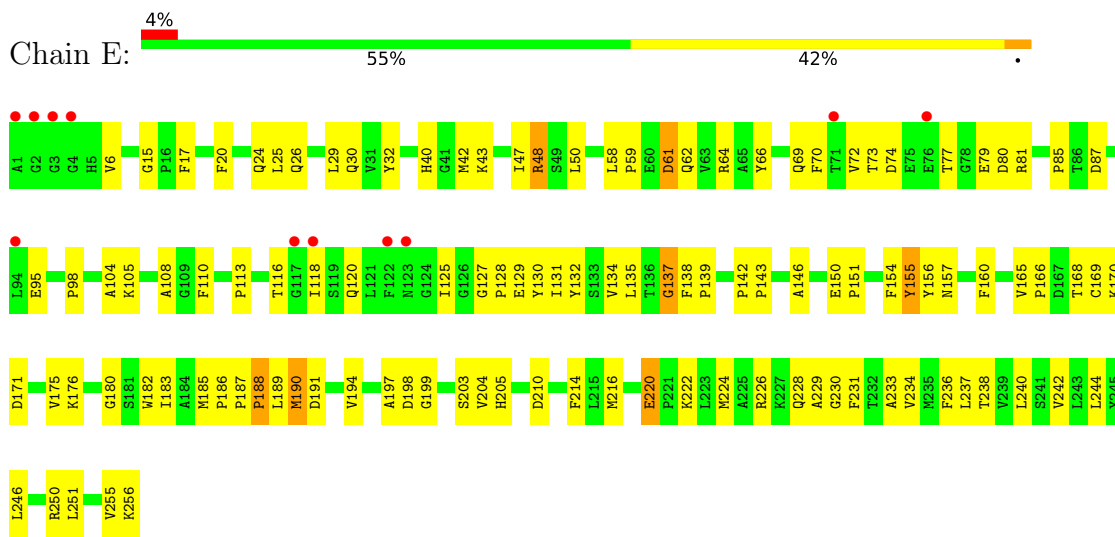




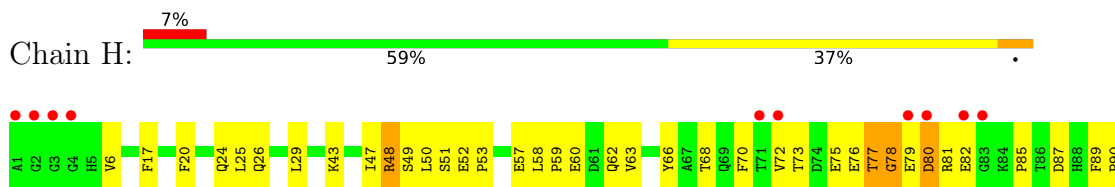
• Molecule 2: Cytochrome c1

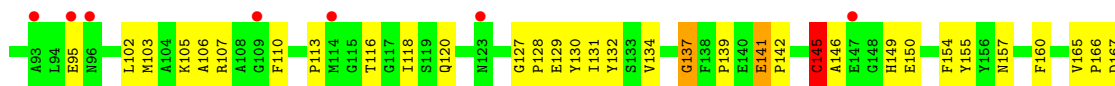


• Molecule 2: Cytochrome c1

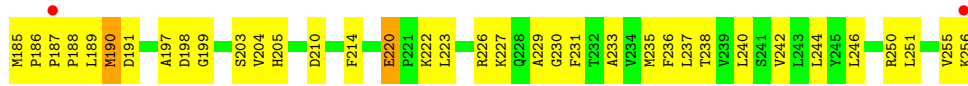
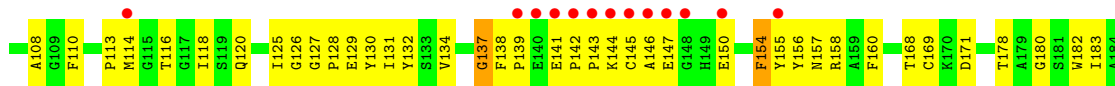
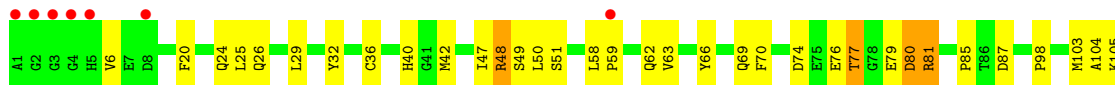


• Molecule 2: Cytochrome c1

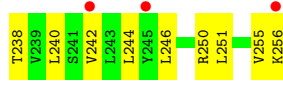
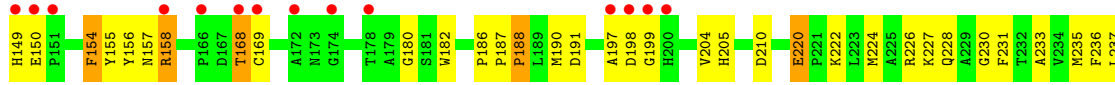
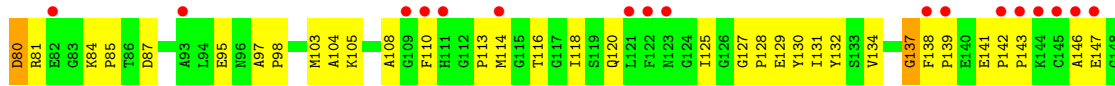
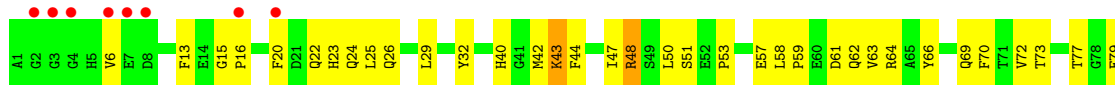




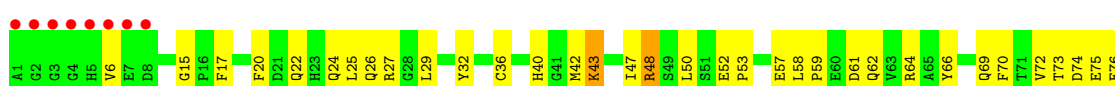
• Molecule 2: Cytochrome c1

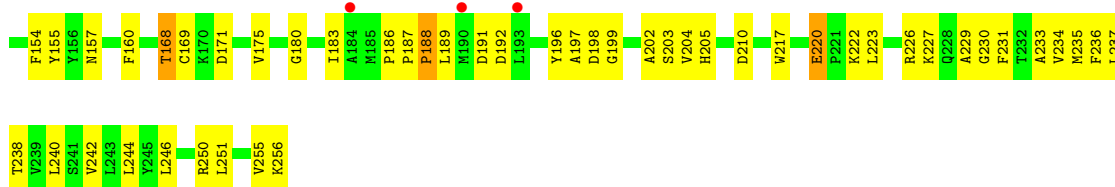


• Molecule 2: Cytochrome c1

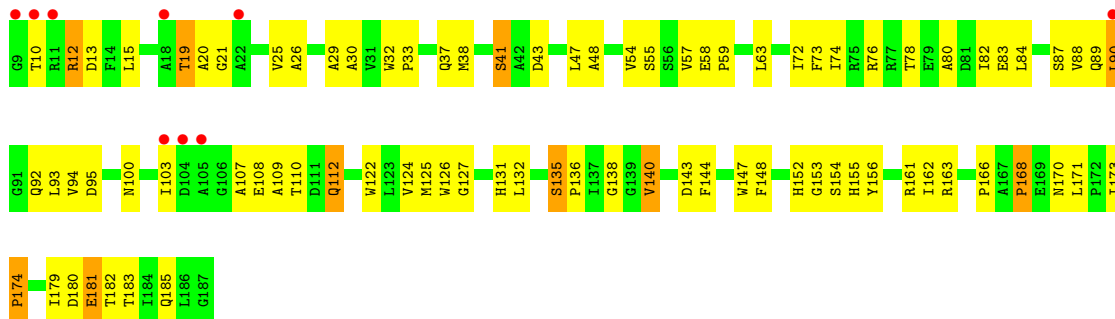


• Molecule 2: Cytochrome c1

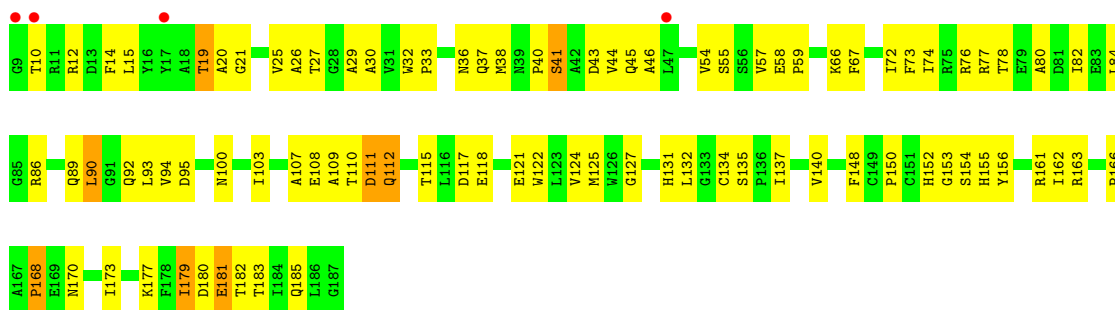




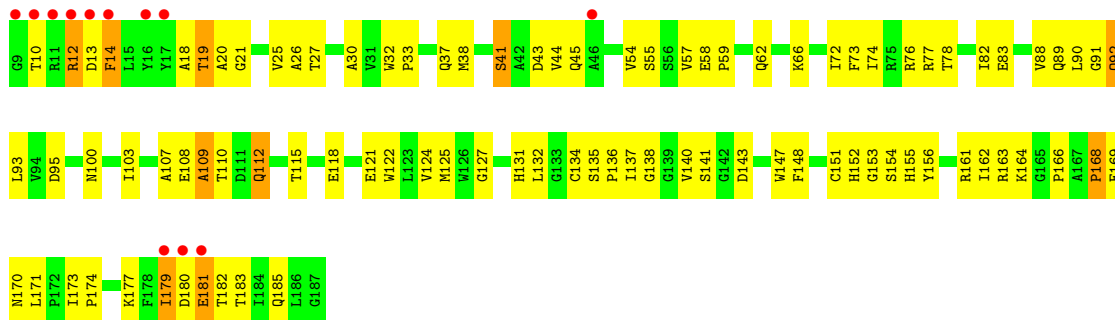
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



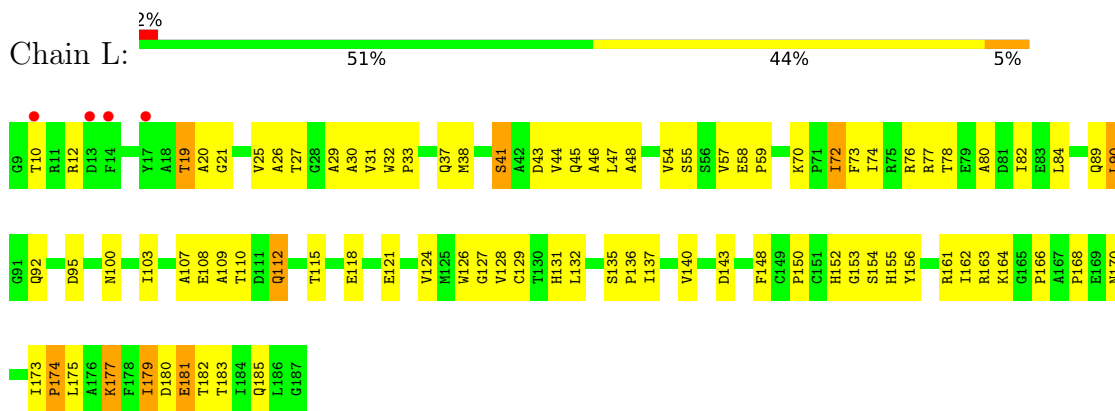
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



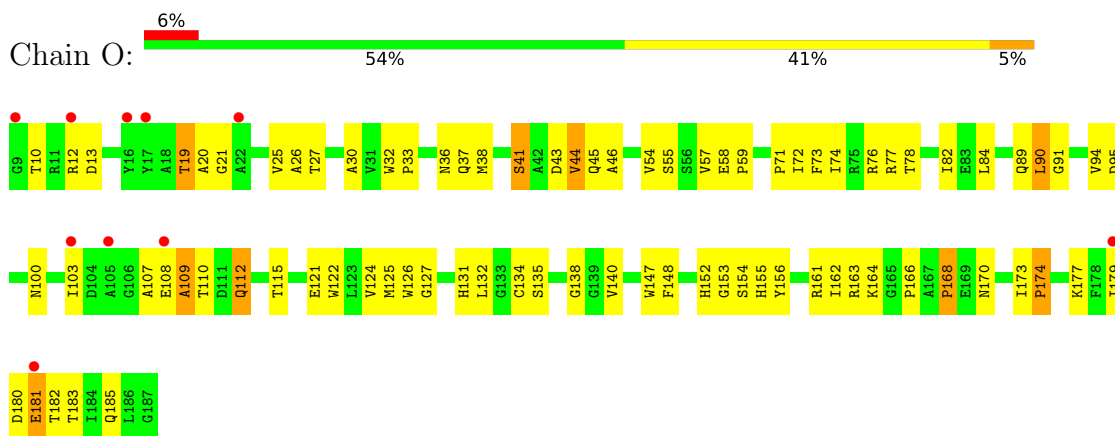
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



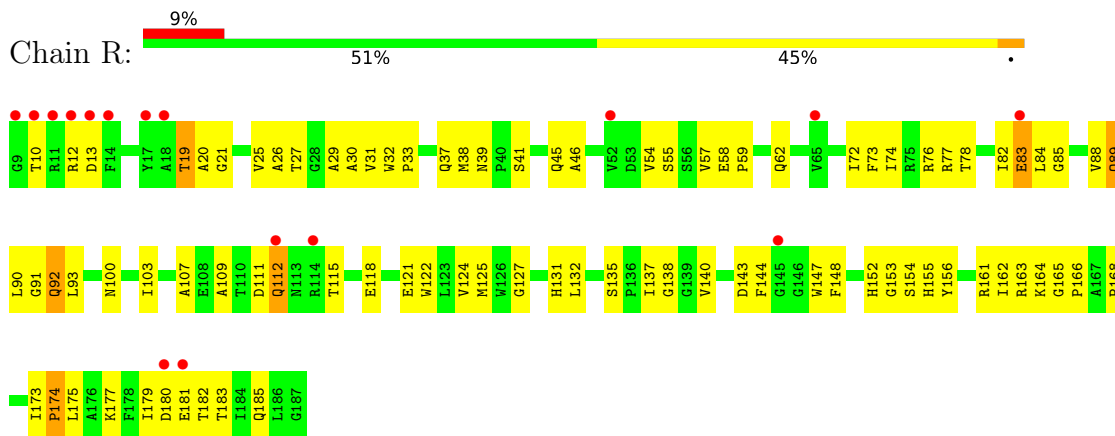
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	352.29Å 147.40Å 160.76Å 90.00° 104.13° 90.00°	Depositor
Resolution (Å)	18.00 – 3.10 44.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (18.00-3.10) 96.1 (44.00-3.05)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.06Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.266 0.223 , 0.240	Depositor DCC
$R_{free}$ test set	5751 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	42048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FES, SMA, LOP, ANJ, SR, HEM, BGL

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	0.59	0/3570	0.73	0/4897
1	D	0.59	0/3570	0.73	1/4897 (0.0%)
1	G	0.57	0/3570	0.72	0/4897
1	J	0.58	0/3570	0.73	0/4897
1	M	0.56	0/3570	0.73	0/4897
1	P	0.57	0/3570	0.72	0/4897
2	B	0.50	0/2010	0.71	1/2733 (0.0%)
2	E	0.50	0/2010	0.70	0/2733
2	H	0.52	0/2010	0.72	1/2733 (0.0%)
2	K	0.48	0/2010	0.69	1/2733 (0.0%)
2	N	0.49	0/2010	0.71	0/2733
2	Q	0.47	0/2010	0.70	0/2733
3	C	0.66	1/1370 (0.1%)	0.86	4/1866 (0.2%)
3	F	0.70	1/1370 (0.1%)	0.83	1/1866 (0.1%)
3	I	0.66	1/1370 (0.1%)	0.86	4/1866 (0.2%)
3	L	0.70	2/1370 (0.1%)	0.82	2/1866 (0.1%)
3	O	0.67	2/1370 (0.1%)	0.83	4/1866 (0.2%)
3	R	0.63	2/1370 (0.1%)	0.83	2/1866 (0.1%)
All	All	0.58	9/41700 (0.0%)	0.74	21/56976 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	J	0	1
1	P	0	1
All	All	0	4



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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	181	GLU	CB-CG	-13.28	1.26	1.52
3	F	181	GLU	CB-CG	-12.17	1.29	1.52
3	L	181	GLU	CB-CG	-11.99	1.29	1.52
3	C	181	GLU	CB-CG	-10.97	1.31	1.52
3	I	181	GLU	CB-CG	-10.23	1.32	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	181	GLU	OE1-CD-OE2	9.52	134.72	123.30
3	C	181	GLU	CG-CD-OE2	-8.83	100.64	118.30
3	R	181	GLU	OE1-CD-OE2	7.79	132.65	123.30
3	L	181	GLU	OE1-CD-OE2	7.71	132.55	123.30
2	H	145	CYS	CA-CB-SG	-7.66	100.22	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
1	G	199	TYR	Sidechain
1	J	199	TYR	Sidechain
1	P	199	TYR	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3428	190	0
1	D	3440	0	3428	199	0
1	G	3440	0	3428	209	0
1	J	3440	0	3428	215	0
1	M	3440	0	3428	217	0
1	P	3440	0	3428	203	0
2	B	1953	0	1848	89	0
2	E	1953	0	1848	94	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1953	0	1848	83	0
2	K	1953	0	1848	92	0
2	N	1953	0	1848	95	0
2	Q	1953	0	1848	105	0
3	C	1340	0	1303	82	0
3	F	1340	0	1303	77	0
3	I	1340	0	1303	79	0
3	L	1340	0	1303	71	0
3	O	1340	0	1303	65	0
3	R	1340	0	1303	71	0
4	A	20	0	28	1	0
4	D	20	0	28	2	0
4	G	20	0	28	2	0
4	J	20	0	28	0	0
4	M	20	0	28	2	0
4	Q	20	0	28	0	0
5	A	86	0	60	7	0
5	B	43	0	30	6	0
5	D	86	0	60	14	0
5	E	43	0	30	2	0
5	G	86	0	60	12	0
5	H	43	0	30	1	0
5	J	86	0	60	12	0
5	K	43	0	30	2	0
5	M	86	0	60	6	0
5	N	43	0	30	0	0
5	P	86	0	60	17	0
5	Q	43	0	30	1	0
6	A	37	0	42	6	0
6	D	37	0	42	3	0
6	G	37	0	42	6	0
6	J	37	0	42	4	0
6	M	37	0	42	3	0
6	P	37	0	42	4	0
7	A	45	0	67	5	0
7	D	45	0	67	3	0
7	G	45	0	67	4	0
7	J	45	0	67	3	0
7	M	45	0	67	7	0
7	P	45	0	67	4	0
8	A	39	0	40	7	0
8	D	39	0	39	7	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	39	0	39	7	0
8	J	39	0	40	7	0
8	M	39	0	39	6	0
8	P	39	0	39	7	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
9	H	1	0	0	0	0
9	K	1	0	0	0	0
9	N	1	0	0	0	0
9	Q	1	0	0	0	0
10	C	4	0	0	2	0
10	F	4	0	0	2	0
10	I	4	0	0	2	0
10	L	4	0	0	2	0
10	O	4	0	0	2	0
10	R	4	0	0	3	0
All	All	42048	0	41072	2117	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 25.

The worst 5 of 2117 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:B:103:MET:HE3	5:B:301:HEM:HAA2	1.33	1.09
2:K:250:ARG:CZ	3:L:12:ARG:HB3	1.85	1.04
1:J:236:GLU:HA	1:J:239:LYS:HD3	1.37	1.03
3:C:143:ASP:HA	3:L:89:GLN:HE21	1.24	1.01
1:M:200:LEU:HD22	1:P:63:ILE:HD13	1.41	1.01

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	426/428 (100%)	366 (86%)	54 (13%)	6 (1%)	11	40
1	D	426/428 (100%)	365 (86%)	57 (13%)	4 (1%)	17	52
1	G	426/428 (100%)	368 (86%)	53 (12%)	5 (1%)	13	44
1	J	426/428 (100%)	361 (85%)	58 (14%)	7 (2%)	9	37
1	M	426/428 (100%)	364 (85%)	54 (13%)	8 (2%)	8	33
1	P	426/428 (100%)	364 (85%)	54 (13%)	8 (2%)	8	33
2	B	254/256 (99%)	210 (83%)	38 (15%)	6 (2%)	6	27
2	E	254/256 (99%)	210 (83%)	37 (15%)	7 (3%)	5	25
2	H	254/256 (99%)	205 (81%)	42 (16%)	7 (3%)	5	25
2	K	254/256 (99%)	205 (81%)	41 (16%)	8 (3%)	4	23
2	N	254/256 (99%)	210 (83%)	36 (14%)	8 (3%)	4	23
2	Q	254/256 (99%)	212 (84%)	34 (13%)	8 (3%)	4	23
3	C	177/179 (99%)	143 (81%)	28 (16%)	6 (3%)	3	21
3	F	177/179 (99%)	148 (84%)	23 (13%)	6 (3%)	3	21
3	I	177/179 (99%)	145 (82%)	24 (14%)	8 (4%)	2	15
3	L	177/179 (99%)	144 (81%)	29 (16%)	4 (2%)	6	28
3	O	177/179 (99%)	148 (84%)	22 (12%)	7 (4%)	3	17
3	R	177/179 (99%)	143 (81%)	28 (16%)	6 (3%)	3	21
All	All	5142/5178 (99%)	4311 (84%)	712 (14%)	119 (2%)	6	28

5 of 119 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
3	C	109	ALA
1	D	73	VAL
1	D	76	ALA
3	F	45	GLN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/353 (100%)	333 (94%)	20 (6%)	20	52
1	D	353/353 (100%)	340 (96%)	13 (4%)	34	66
1	G	353/353 (100%)	332 (94%)	21 (6%)	19	50
1	J	353/353 (100%)	338 (96%)	15 (4%)	30	62
1	M	353/353 (100%)	338 (96%)	15 (4%)	30	62
1	P	353/353 (100%)	337 (96%)	16 (4%)	27	60
2	B	203/203 (100%)	195 (96%)	8 (4%)	32	65
2	E	203/203 (100%)	197 (97%)	6 (3%)	41	71
2	H	203/203 (100%)	192 (95%)	11 (5%)	22	53
2	K	203/203 (100%)	197 (97%)	6 (3%)	41	71
2	N	203/203 (100%)	197 (97%)	6 (3%)	41	71
2	Q	203/203 (100%)	198 (98%)	5 (2%)	47	75
3	C	138/138 (100%)	129 (94%)	9 (6%)	17	47
3	F	138/138 (100%)	127 (92%)	11 (8%)	12	40
3	I	138/138 (100%)	125 (91%)	13 (9%)	8	32
3	L	138/138 (100%)	128 (93%)	10 (7%)	14	44
3	O	138/138 (100%)	127 (92%)	11 (8%)	12	40
3	R	138/138 (100%)	126 (91%)	12 (9%)	10	36
All	All	4164/4164 (100%)	3956 (95%)	208 (5%)	24	57

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	49	VAL
1	M	7	ASP
3	R	89	GLN
1	J	108	VAL
2	K	171	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	192	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	Q	22	GLN
1	M	429	ASN
3	O	112	GLN
3	R	36	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 6 are monoatomic - leaving 48 for Mogul analysis.

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
5	HEM	A	501	1	41,50,50	1.54	6 (14%)	45,82,82	1.08	1 (2%)
6	SMA	J	503	-	38,38,38	1.89	6 (15%)	48,52,52	2.04	12 (25%)
6	SMA	A	1	-	38,38,38	1.94	7 (18%)	48,52,52	2.32	13 (27%)
4	BGL	M	431	-	20,20,20	1.71	2 (10%)	24,25,25	0.67	0
5	HEM	K	301	2	41,50,50	1.62	5 (12%)	45,82,82	1.14	3 (6%)
7	LOP	D	503	-	44,44,44	0.56	0	47,49,49	1.31	6 (12%)
5	HEM	A	502	1	41,50,50	1.85	8 (19%)	45,82,82	1.19	3 (6%)
4	BGL	A	431	-	20,20,20	1.59	2 (10%)	24,25,25	1.07	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SMA	D	2	-	38,38,38	2.26	9 (23%)	48,52,52	2.01	13 (27%)
7	LOP	M	504	-	44,44,44	0.63	0	47,49,49	1.33	6 (12%)
5	HEM	E	301	2	41,50,50	1.58	6 (14%)	45,82,82	1.15	1 (2%)
6	SMA	M	503	-	38,38,38	2.11	8 (21%)	48,52,52	2.12	13 (27%)
7	LOP	A	503	-	44,44,44	0.55	0	47,49,49	1.26	6 (12%)
4	BGL	G	431	-	20,20,20	1.75	1 (5%)	24,25,25	0.86	0
10	FES	C	200	3	0,4,4	-	-	-	-	-
5	HEM	P	501	1	41,50,50	1.71	6 (14%)	45,82,82	1.11	1 (2%)
4	BGL	Q	257	-	20,20,20	1.43	2 (10%)	24,25,25	1.01	1 (4%)
5	HEM	N	301	2	41,50,50	1.46	4 (9%)	45,82,82	1.12	2 (4%)
7	LOP	G	504	-	44,44,44	0.63	0	47,49,49	1.21	3 (6%)
8	ANJ	G	505	-	40,40,40	1.62	10 (25%)	36,54,54	1.82	8 (22%)
5	HEM	G	501	1	41,50,50	1.69	6 (14%)	45,82,82	1.07	1 (2%)
10	FES	R	200	3	0,4,4	-	-	-	-	-
5	HEM	D	501	1	41,50,50	1.66	7 (17%)	45,82,82	1.10	2 (4%)
5	HEM	J	501	1	41,50,50	1.57	5 (12%)	45,82,82	1.07	2 (4%)
4	BGL	D	431	-	20,20,20	1.38	1 (5%)	24,25,25	1.15	2 (8%)
10	FES	F	200	3	0,4,4	-	-	-	-	-
8	ANJ	D	504	-	40,40,40	1.77	13 (32%)	36,54,54	1.65	8 (22%)
5	HEM	B	301	2	41,50,50	1.59	6 (14%)	45,82,82	1.13	1 (2%)
10	FES	O	200	3	0,4,4	-	-	-	-	-
5	HEM	J	502	1	41,50,50	1.64	7 (17%)	45,82,82	1.11	2 (4%)
5	HEM	D	502	1	41,50,50	1.59	7 (17%)	45,82,82	1.20	3 (6%)
8	ANJ	P	505	-	40,40,40	1.71	11 (27%)	36,54,54	1.67	8 (22%)
7	LOP	J	504	-	44,44,44	0.68	1 (2%)	47,49,49	1.17	2 (4%)
6	SMA	P	503	-	38,38,38	1.97	8 (21%)	48,52,52	1.73	8 (16%)
5	HEM	M	502	1	41,50,50	1.66	8 (19%)	45,82,82	1.16	2 (4%)
5	HEM	H	301	2	41,50,50	1.72	7 (17%)	45,82,82	1.21	3 (6%)
5	HEM	G	502	1	41,50,50	1.75	8 (19%)	45,82,82	1.11	3 (6%)
10	FES	L	200	3	0,4,4	-	-	-	-	-
8	ANJ	M	505	-	40,40,40	1.77	11 (27%)	36,54,54	1.79	9 (25%)
8	ANJ	J	505	-	40,40,40	1.86	11 (27%)	36,54,54	1.66	6 (16%)
5	HEM	M	501	1	41,50,50	1.52	5 (12%)	45,82,82	1.13	2 (4%)
5	HEM	Q	301	2	41,50,50	1.54	6 (14%)	45,82,82	1.17	1 (2%)
7	LOP	P	504	-	44,44,44	0.62	0	47,49,49	1.28	5 (10%)
8	ANJ	A	504	-	40,40,40	1.74	13 (32%)	36,54,54	1.72	7 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SMA	G	503	-	38,38,38	1.93	8 (21%)	48,52,52	2.31	12 (25%)
4	BGL	J	431	-	20,20,20	1.55	2 (10%)	24,25,25	1.01	3 (12%)
5	HEM	P	502	1	41,50,50	1.69	8 (19%)	45,82,82	1.15	1 (2%)
10	FES	I	200	3	0,4,4	-	-	-	-	-

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
5	HEM	A	501	1	-	7/12/54/54	-
6	SMA	J	503	-	-	9/34/34/34	0/2/2/2
6	SMA	A	1	-	-	8/34/34/34	0/2/2/2
4	BGL	M	431	-	-	0/11/31/31	0/1/1/1
5	HEM	K	301	2	-	6/12/54/54	-
7	LOP	D	503	-	-	5/48/48/48	-
5	HEM	A	502	1	-	5/12/54/54	-
4	BGL	A	431	-	-	0/11/31/31	0/1/1/1
6	SMA	D	2	-	-	6/34/34/34	0/2/2/2
7	LOP	M	504	-	-	8/48/48/48	-
5	HEM	E	301	2	-	4/12/54/54	-
6	SMA	M	503	-	-	10/34/34/34	0/2/2/2
7	LOP	A	503	-	-	11/48/48/48	-
4	BGL	G	431	-	-	0/11/31/31	0/1/1/1
10	FES	C	200	3	-	-	0/1/1/1
5	HEM	P	501	1	-	8/12/54/54	-
4	BGL	Q	257	-	-	0/11/31/31	0/1/1/1
5	HEM	N	301	2	-	5/12/54/54	-
7	LOP	G	504	-	-	11/48/48/48	-
8	ANJ	G	505	-	-	5/40/55/55	0/1/2/2
5	HEM	G	501	1	-	5/12/54/54	-
10	FES	R	200	3	-	-	0/1/1/1
5	HEM	D	501	1	-	4/12/54/54	-
5	HEM	J	501	1	-	5/12/54/54	-
4	BGL	D	431	-	-	0/11/31/31	0/1/1/1
10	FES	F	200	3	-	-	0/1/1/1
8	ANJ	D	504	-	-	4/40/55/55	0/1/2/2

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	B	301	2	-	5/12/54/54	-
10	FES	O	200	3	-	-	0/1/1/1
5	HEM	J	502	1	-	4/12/54/54	-
5	HEM	D	502	1	-	4/12/54/54	-
8	ANJ	P	505	-	-	6/40/55/55	0/1/2/2
7	LOP	J	504	-	-	10/48/48/48	-
6	SMA	P	503	-	-	7/34/34/34	0/2/2/2
5	HEM	M	502	1	-	6/12/54/54	-
5	HEM	H	301	2	-	7/12/54/54	-
5	HEM	G	502	1	-	7/12/54/54	-
10	FES	L	200	3	-	-	0/1/1/1
8	ANJ	M	505	-	-	4/40/55/55	0/1/2/2
8	ANJ	J	505	-	-	4/40/55/55	0/1/2/2
5	HEM	M	501	1	-	7/12/54/54	-
5	HEM	Q	301	2	-	8/12/54/54	-
7	LOP	P	504	-	-	5/48/48/48	-
8	ANJ	A	504	-	-	5/40/55/55	0/1/2/2
6	SMA	G	503	-	-	7/34/34/34	0/2/2/2
4	BGL	J	431	-	-	0/11/31/31	0/1/1/1
5	HEM	P	502	1	-	5/12/54/54	-
10	FES	I	200	3	-	-	0/1/1/1

The worst 5 of 241 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	503	SMA	O7-C7	6.92	1.48	1.37
6	D	2	SMA	O5-C5	6.74	1.47	1.37
4	G	431	BGL	C1-C2	6.66	1.58	1.52
6	P	503	SMA	O5-C5	6.46	1.47	1.37
6	D	2	SMA	O7-C7	6.04	1.46	1.37

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	503	SMA	O7-C7-C8	7.75	122.36	114.54
6	A	1	SMA	O7-C7-C8	6.89	121.49	114.54
6	M	503	SMA	O7-C7-C8	6.74	121.34	114.54
6	A	1	SMA	C5M-O5-C5	-6.29	108.04	117.53

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	SMA	O7-C7-C8	6.00	120.59	114.54

There are no chirality outliers.

5 of 227 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	HEM	C2B-C3B-CAB-CBB
5	B	301	HEM	C2B-C3B-CAB-CBB
5	E	301	HEM	C2B-C3B-CAB-CBB
5	G	501	HEM	C2B-C3B-CAB-CBB
5	H	301	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

45 monomers are involved in 193 short contacts:

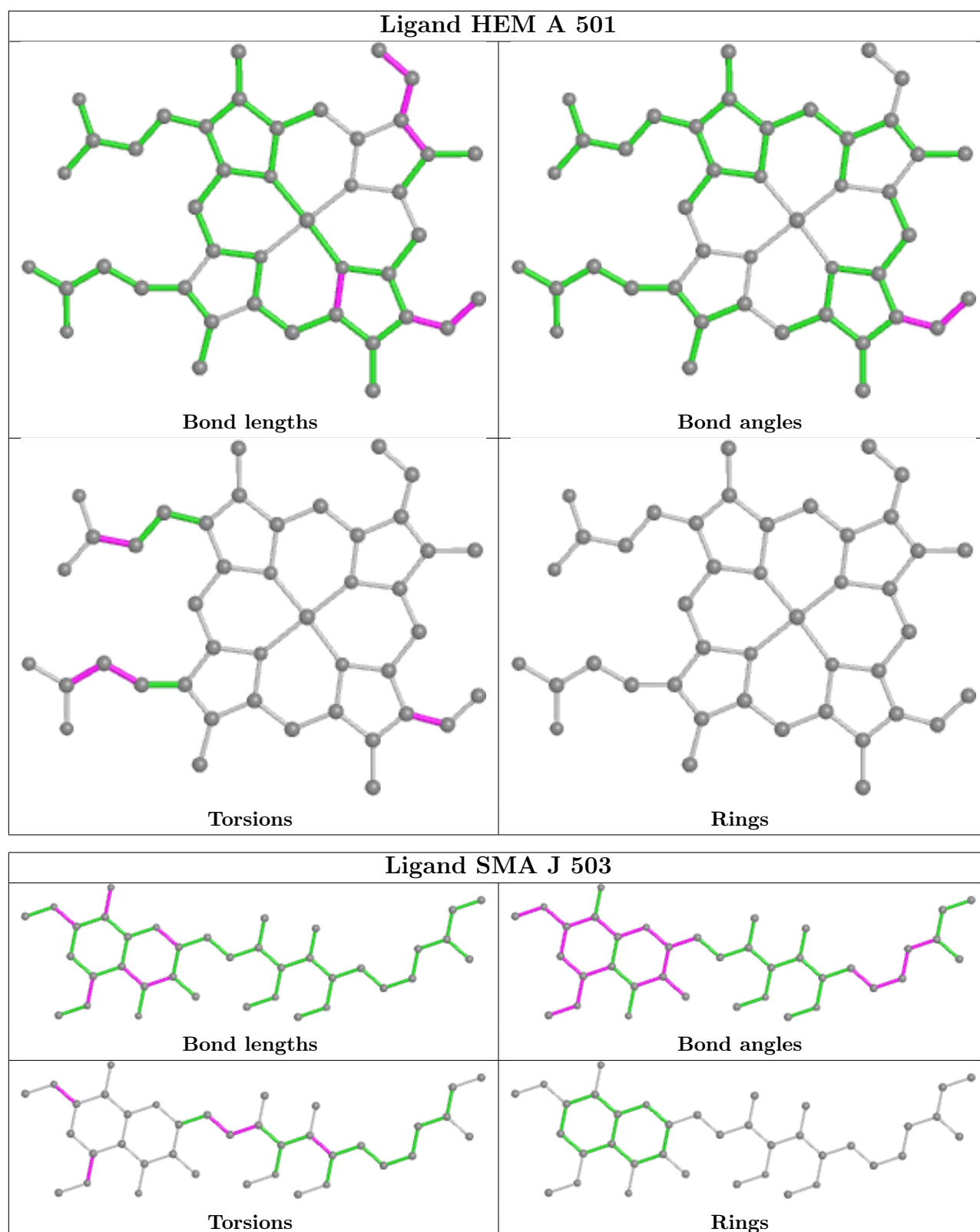
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	HEM	6	0
6	J	503	SMA	4	0
6	A	1	SMA	6	0
4	M	431	BGL	2	0
5	K	301	HEM	2	0
7	D	503	LOP	3	0
5	A	502	HEM	1	0
4	A	431	BGL	1	0
6	D	2	SMA	3	0
7	M	504	LOP	7	0
5	E	301	HEM	2	0
6	M	503	SMA	3	0
7	A	503	LOP	5	0
4	G	431	BGL	2	0
10	C	200	FES	2	0
5	P	501	HEM	11	0
7	G	504	LOP	4	0
8	G	505	ANJ	7	0
5	G	501	HEM	8	0
10	R	200	FES	3	0
5	D	501	HEM	6	0
5	J	501	HEM	7	0
4	D	431	BGL	2	0
10	F	200	FES	2	0
8	D	504	ANJ	7	0

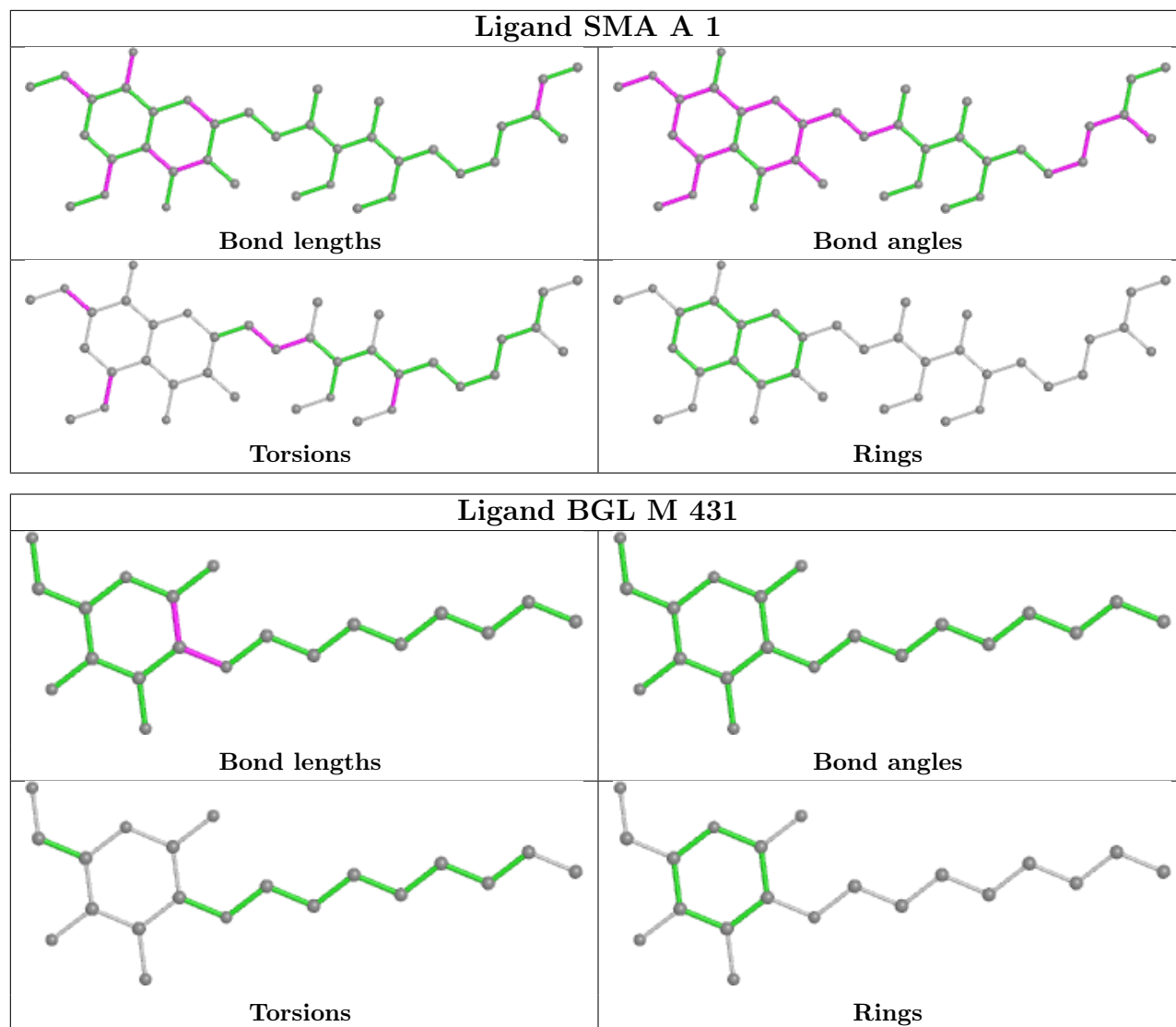
*Continued on next page...*

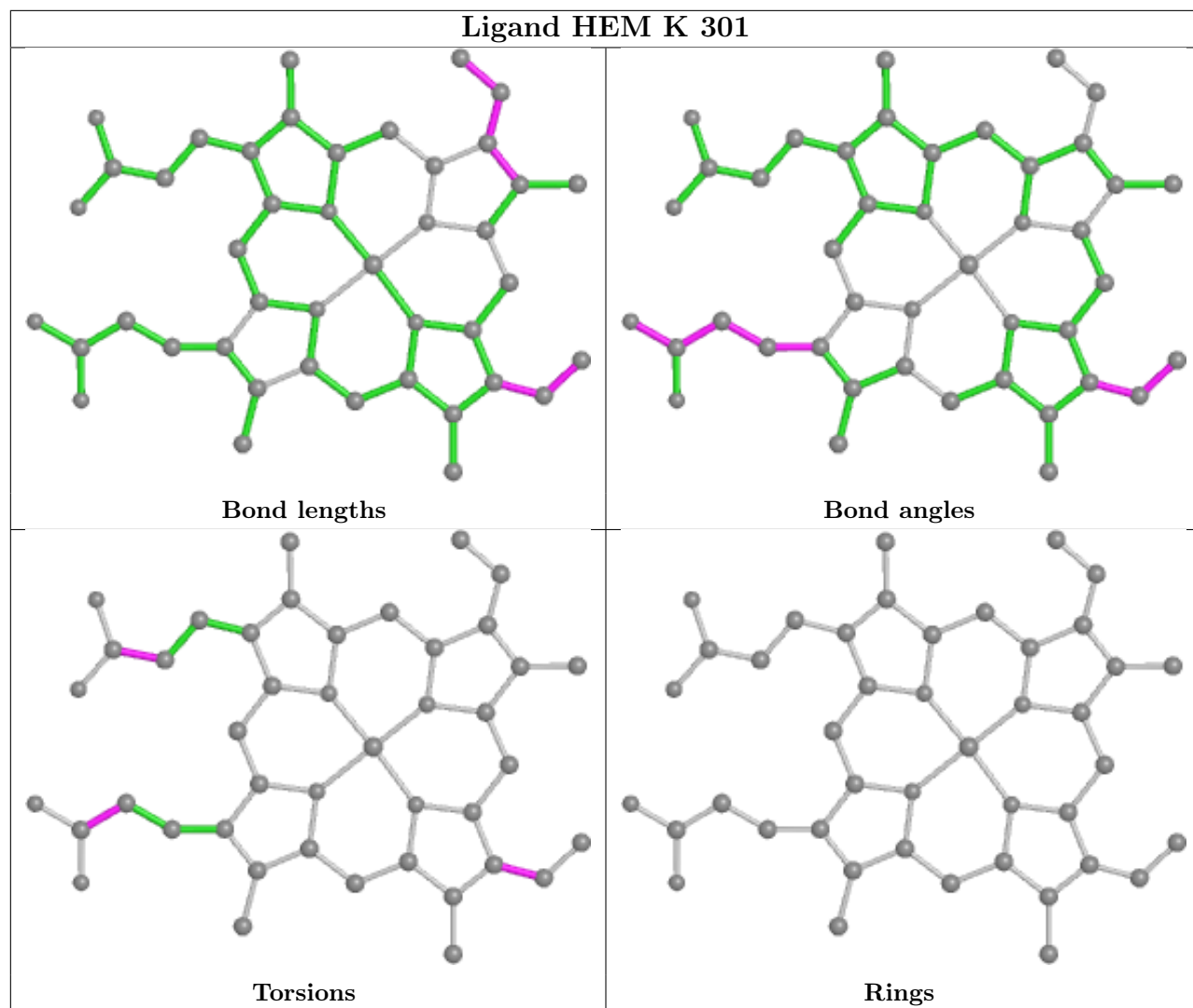
*Continued from previous page...*

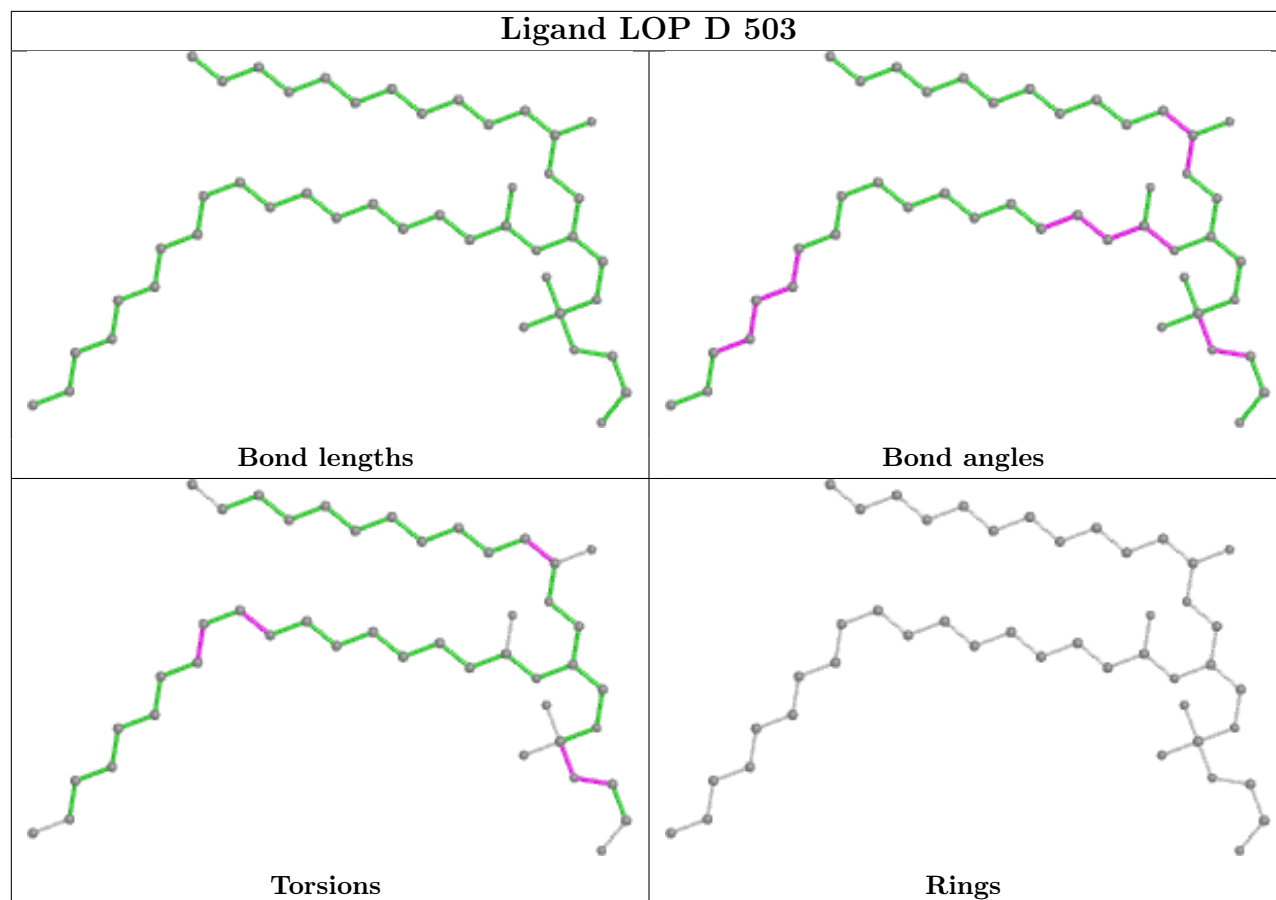
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	HEM	6	0
10	O	200	FES	2	0
5	J	502	HEM	5	0
5	D	502	HEM	8	0
8	P	505	ANJ	7	0
7	J	504	LOP	3	0
6	P	503	SMA	4	0
5	M	502	HEM	1	0
5	H	301	HEM	1	0
5	G	502	HEM	4	0
10	L	200	FES	2	0
8	M	505	ANJ	6	0
8	J	505	ANJ	7	0
5	M	501	HEM	5	0
5	Q	301	HEM	1	0
7	P	504	LOP	4	0
8	A	504	ANJ	7	0
6	G	503	SMA	6	0
5	P	502	HEM	6	0
10	I	200	FES	2	0

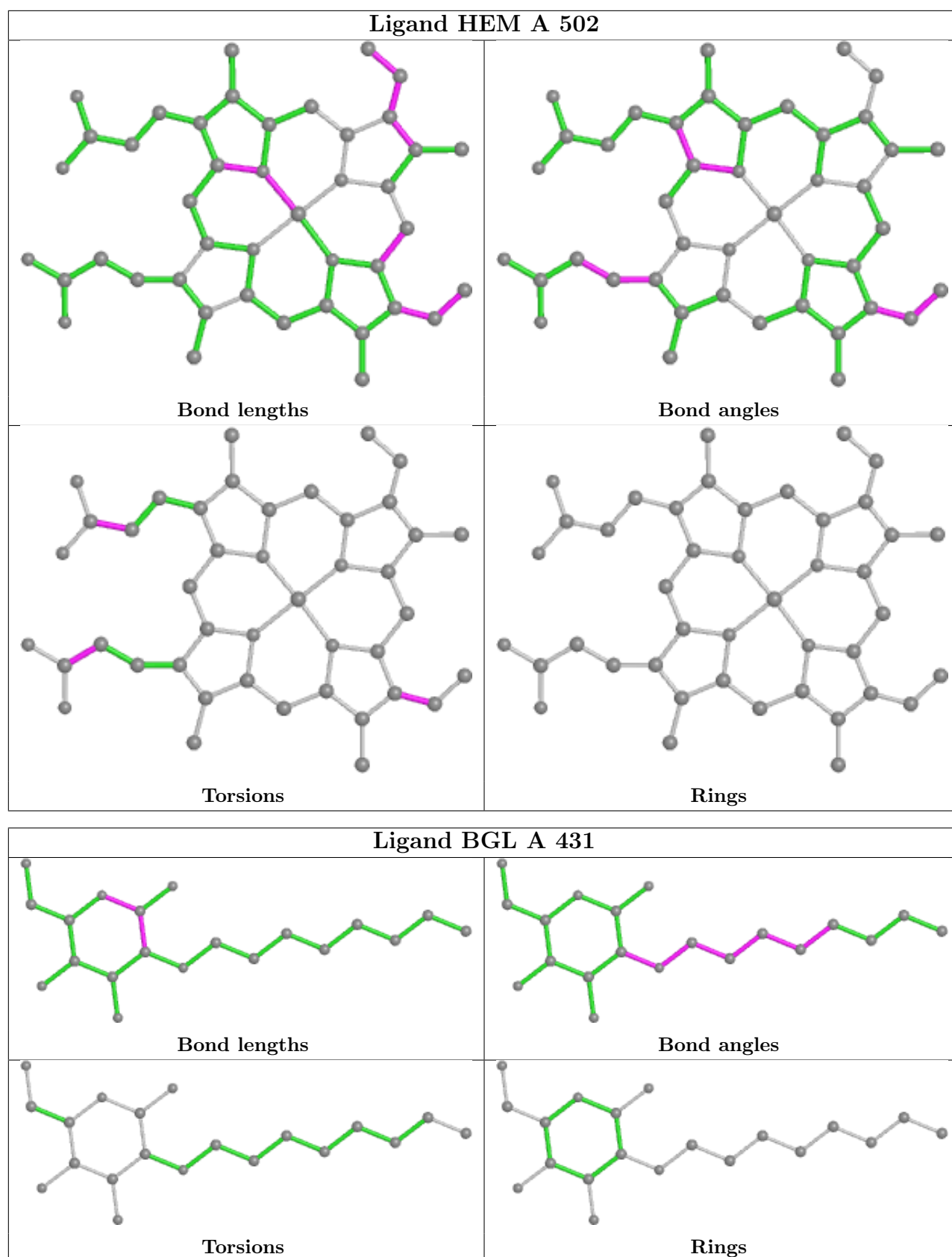
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



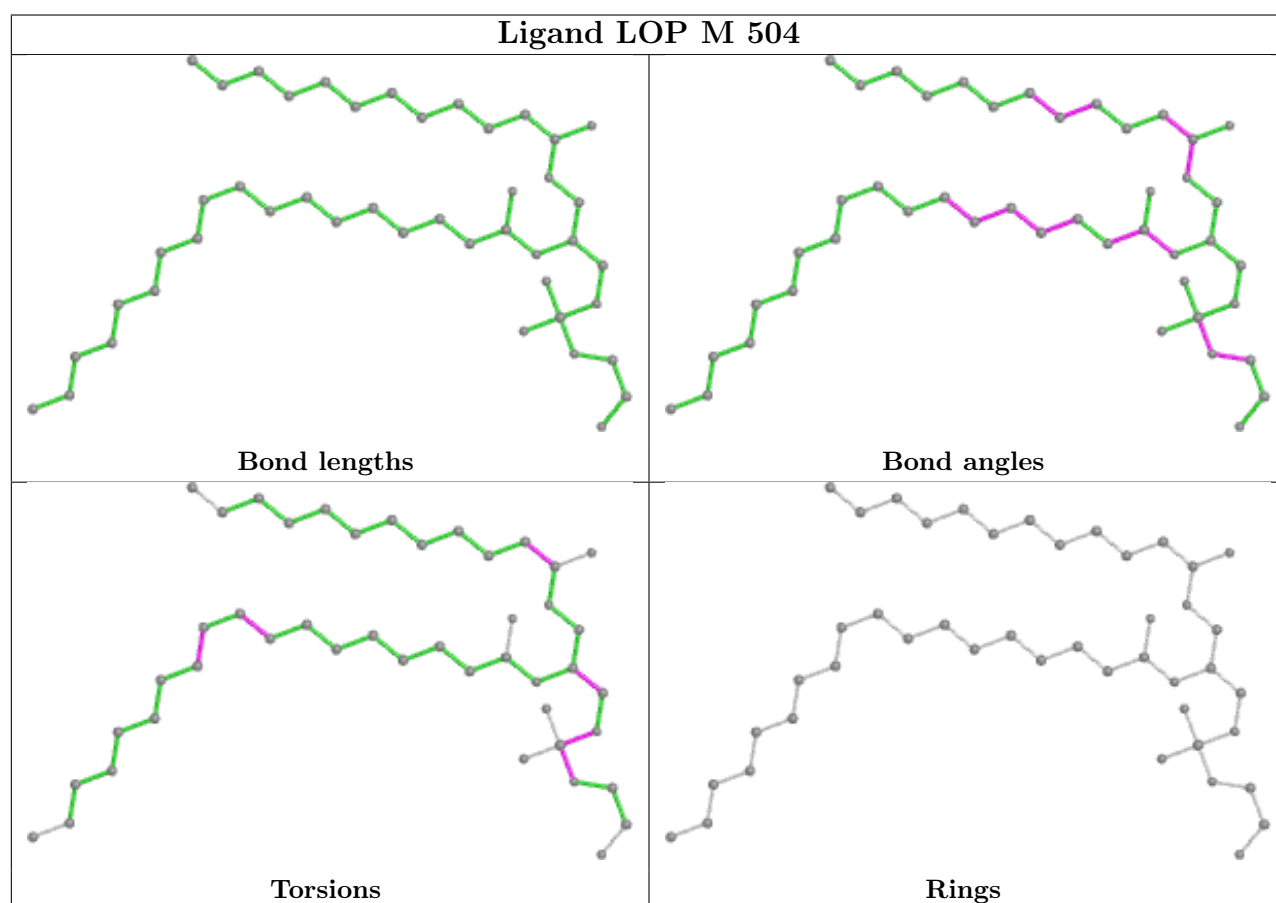
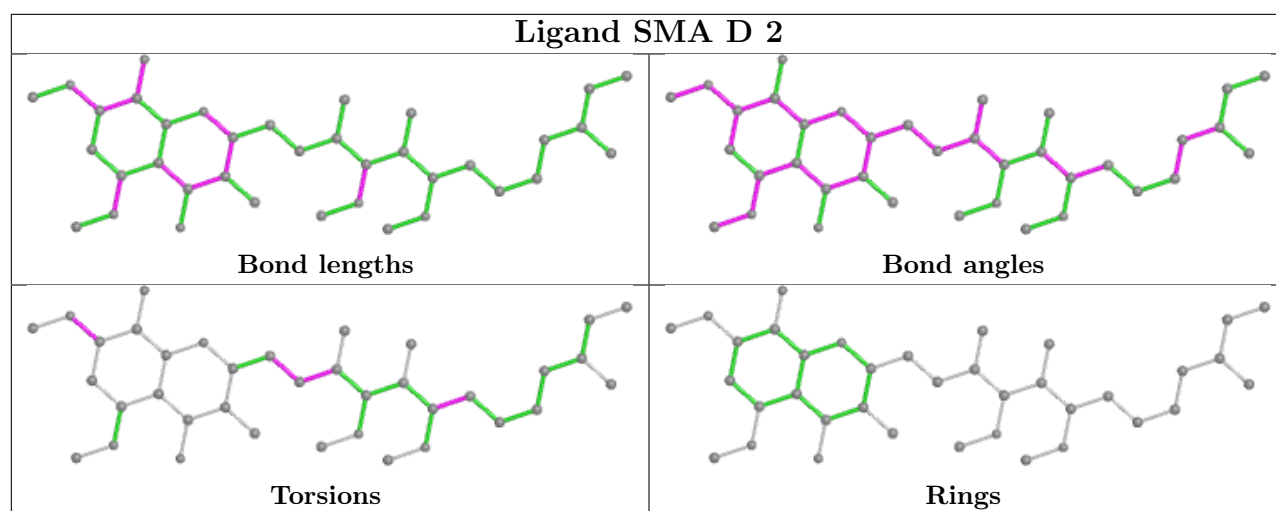


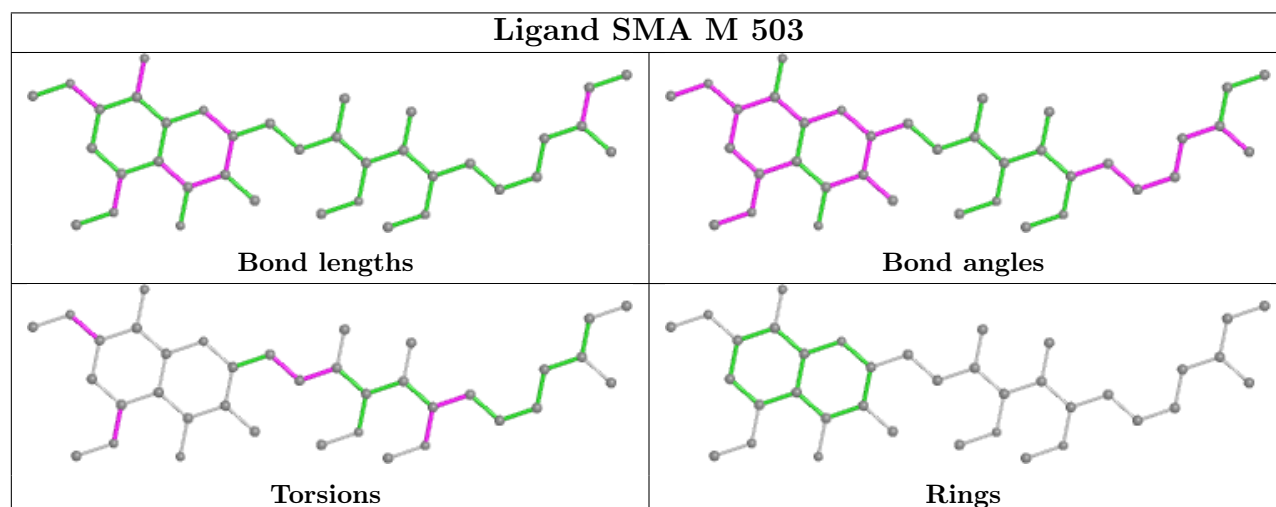
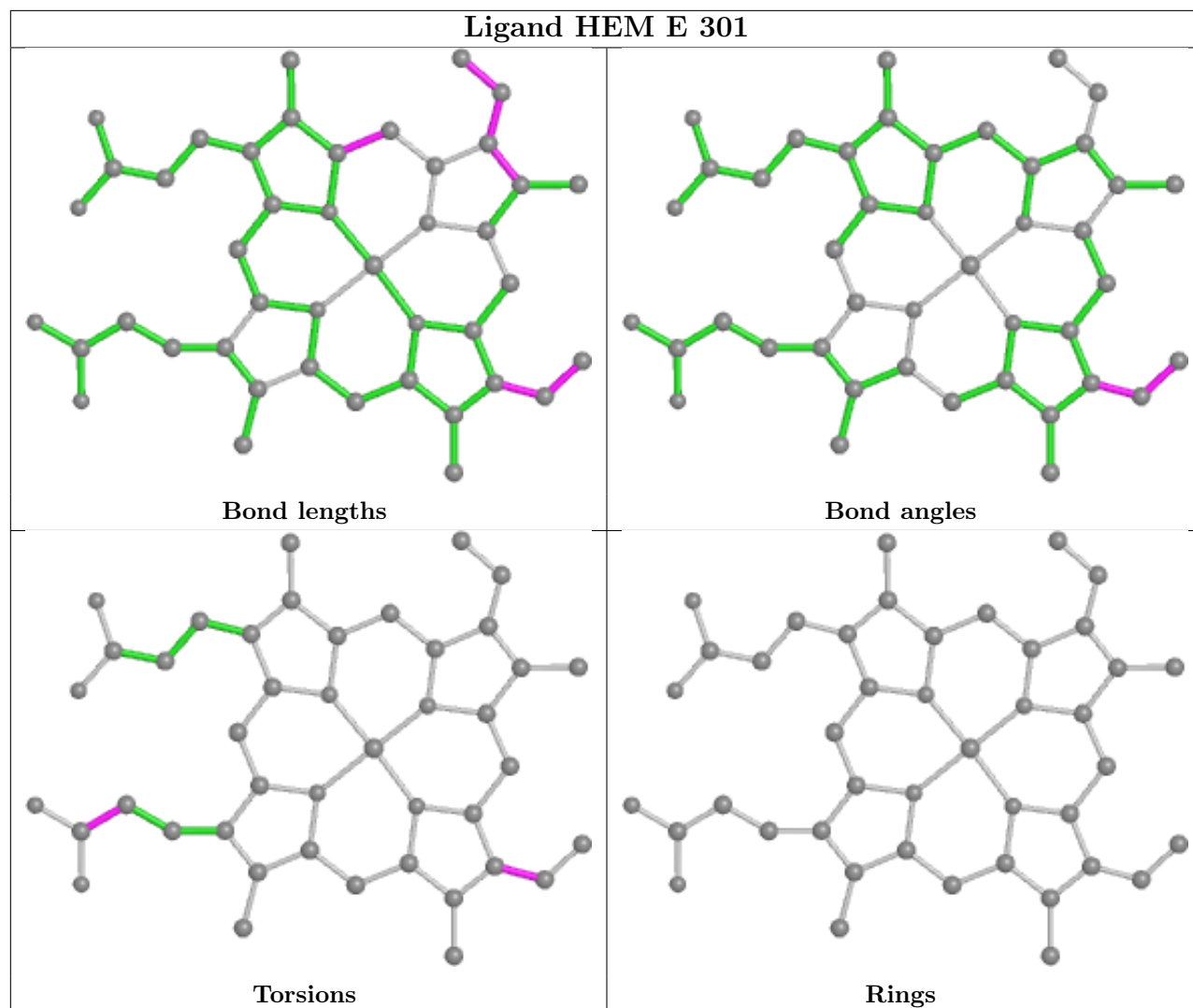


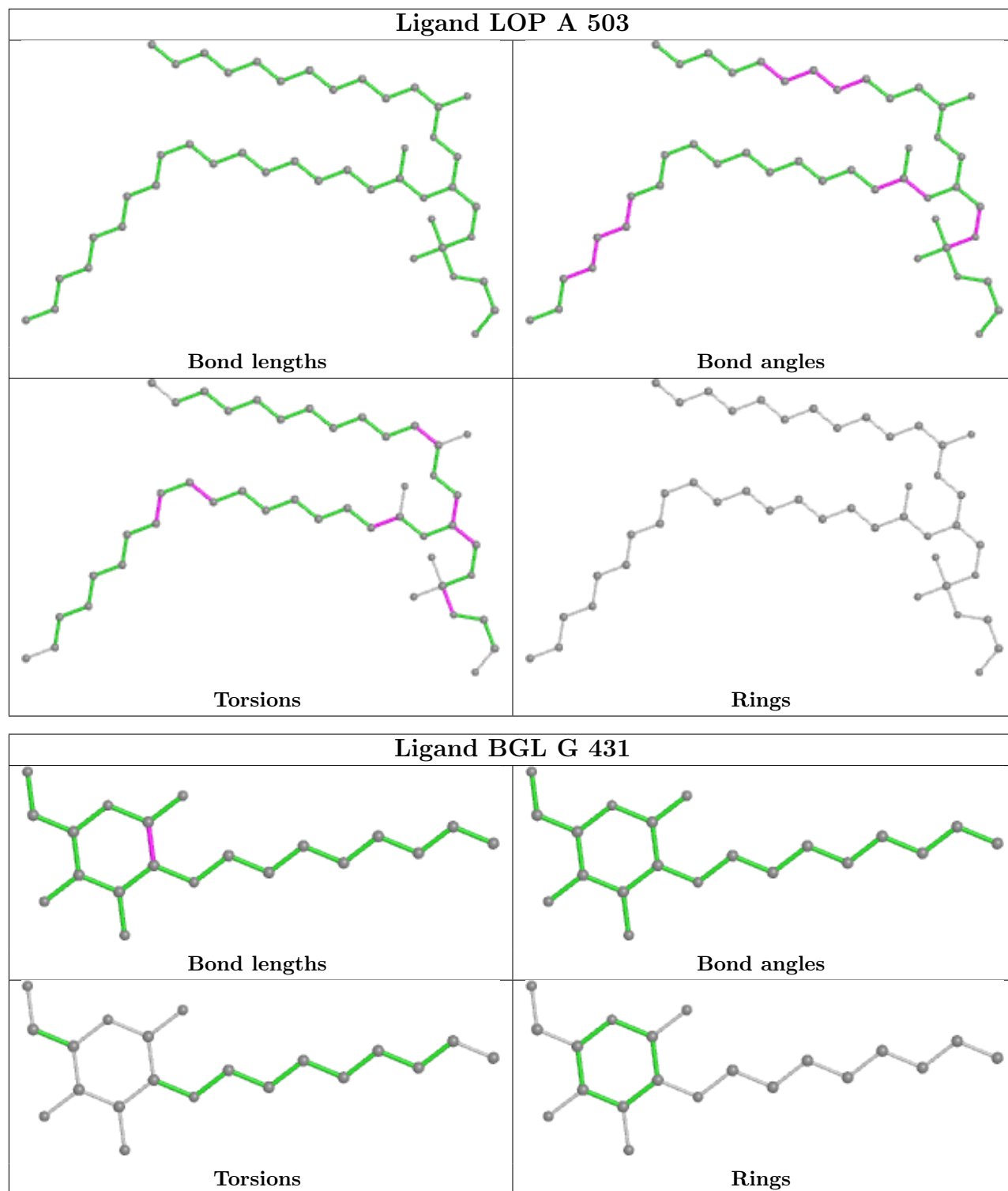


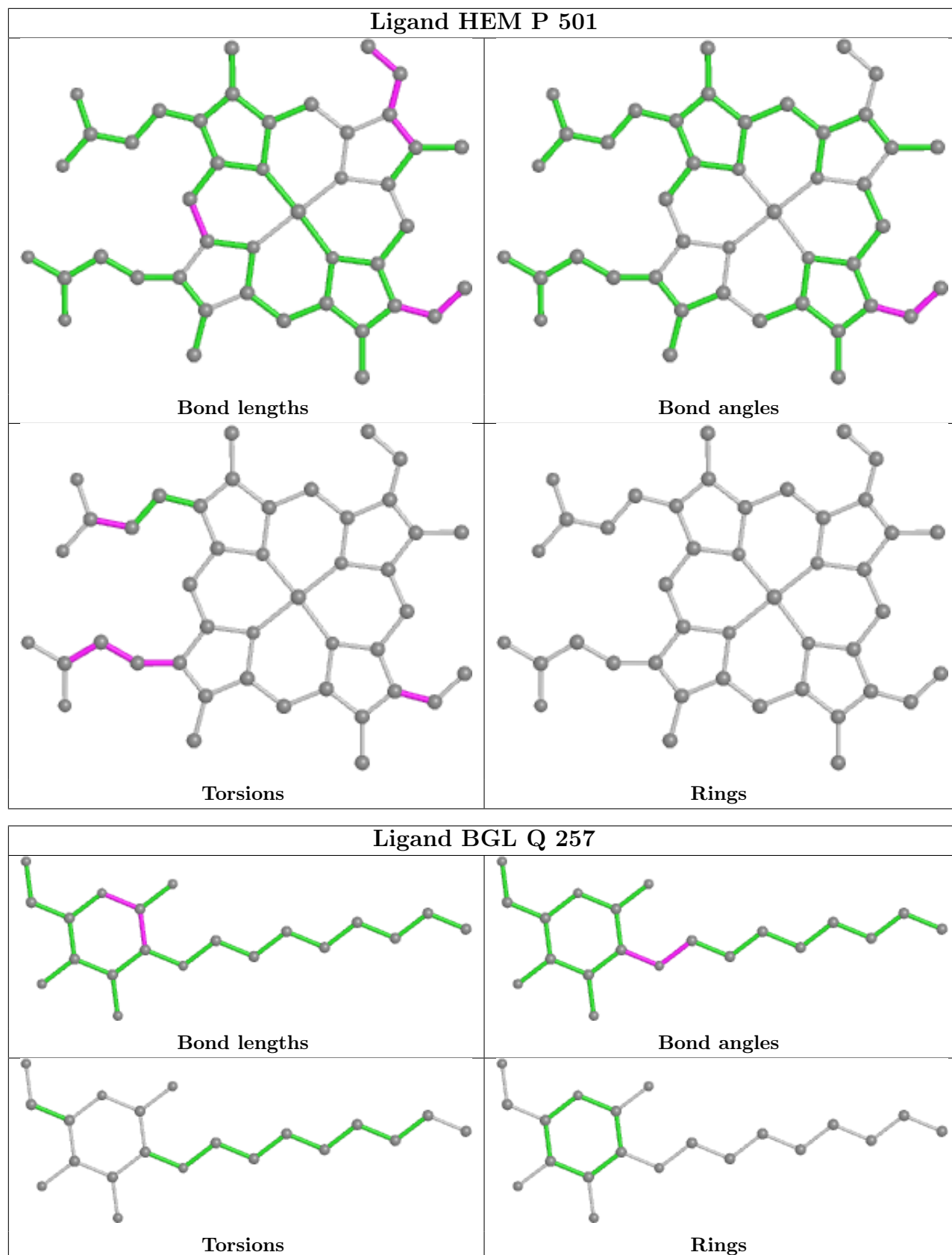


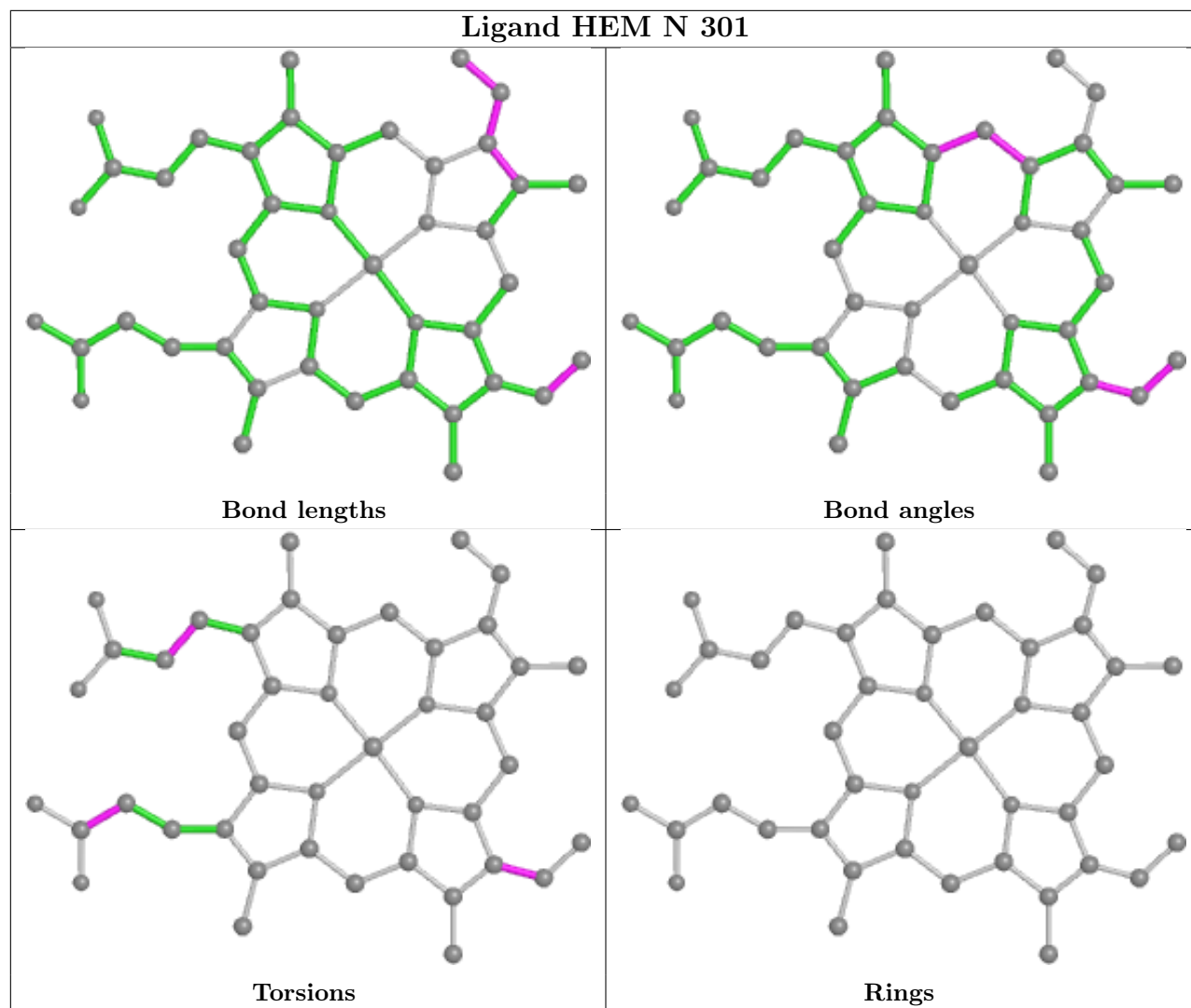


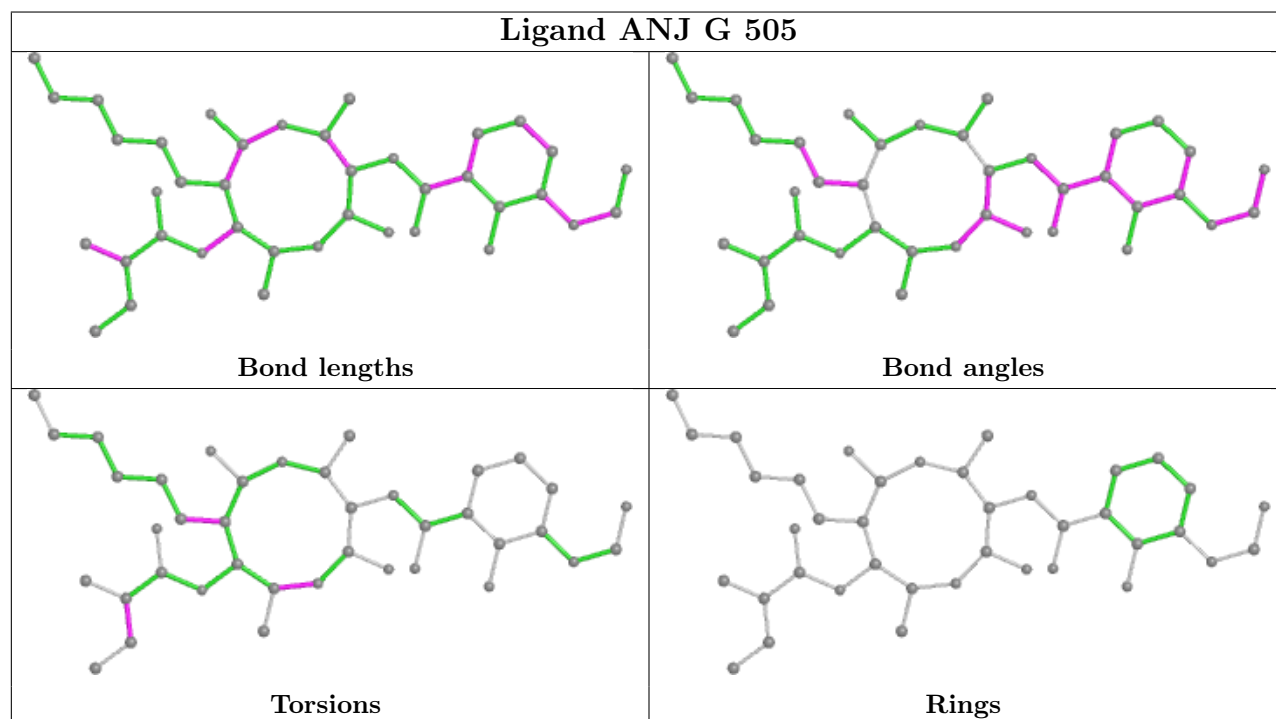
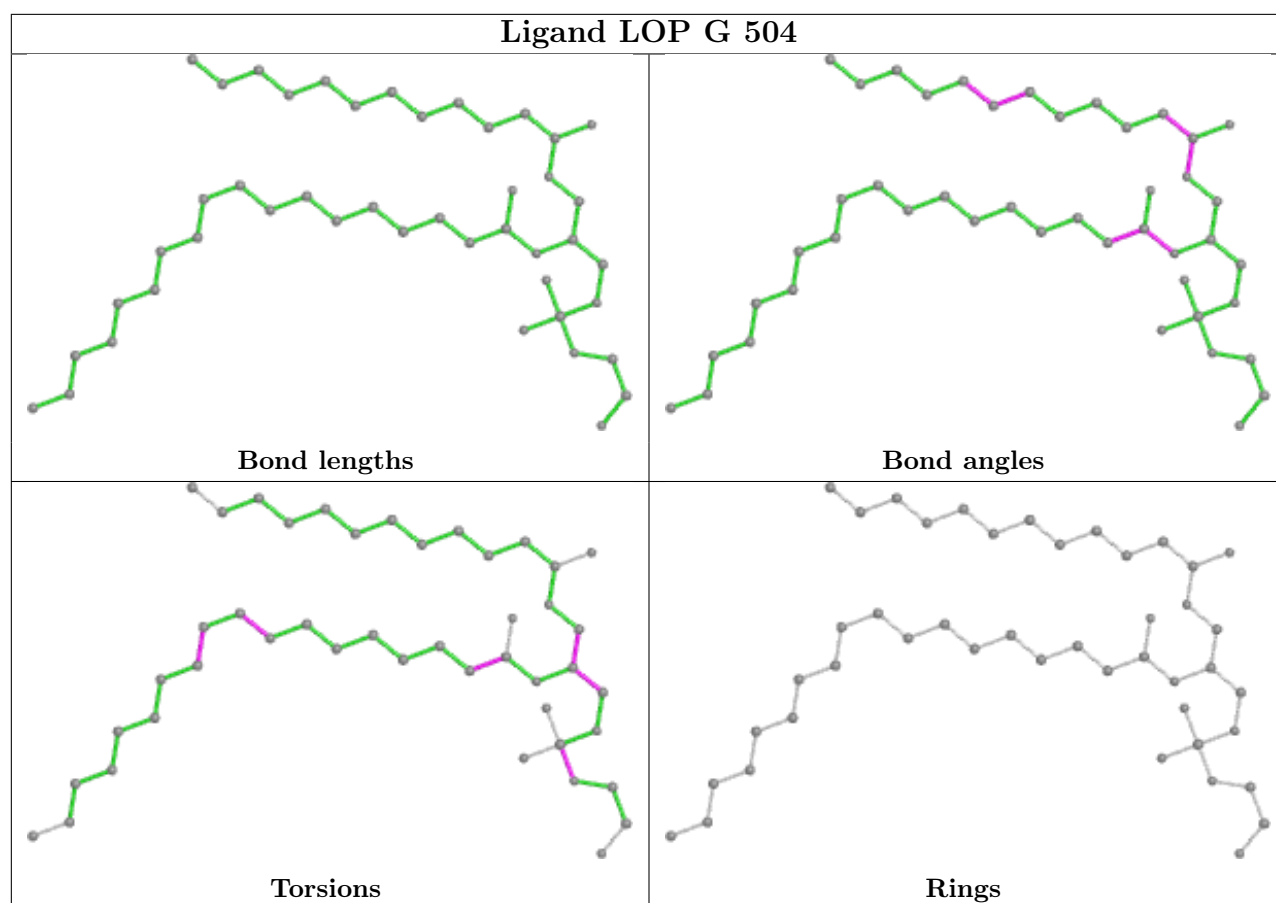


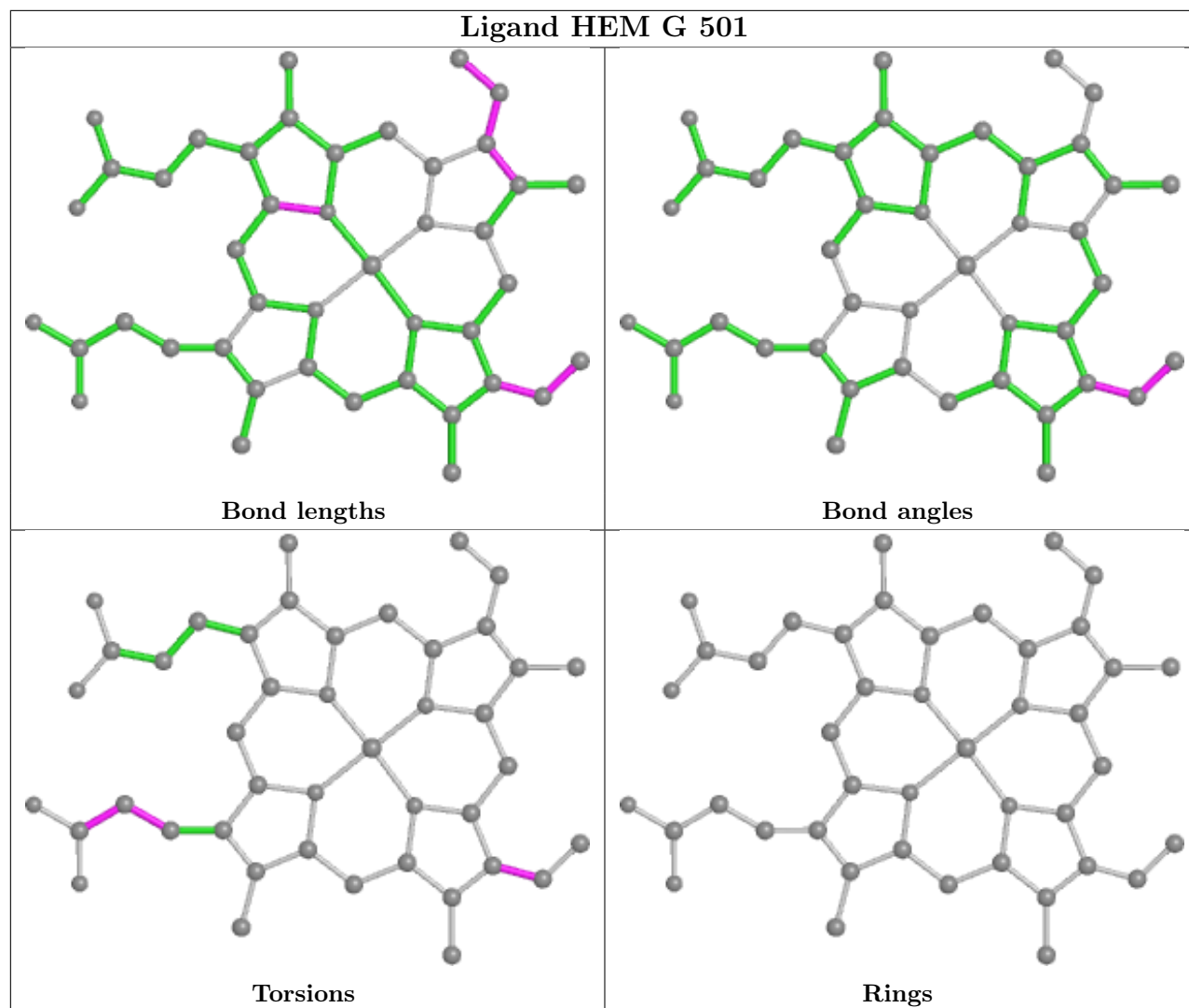


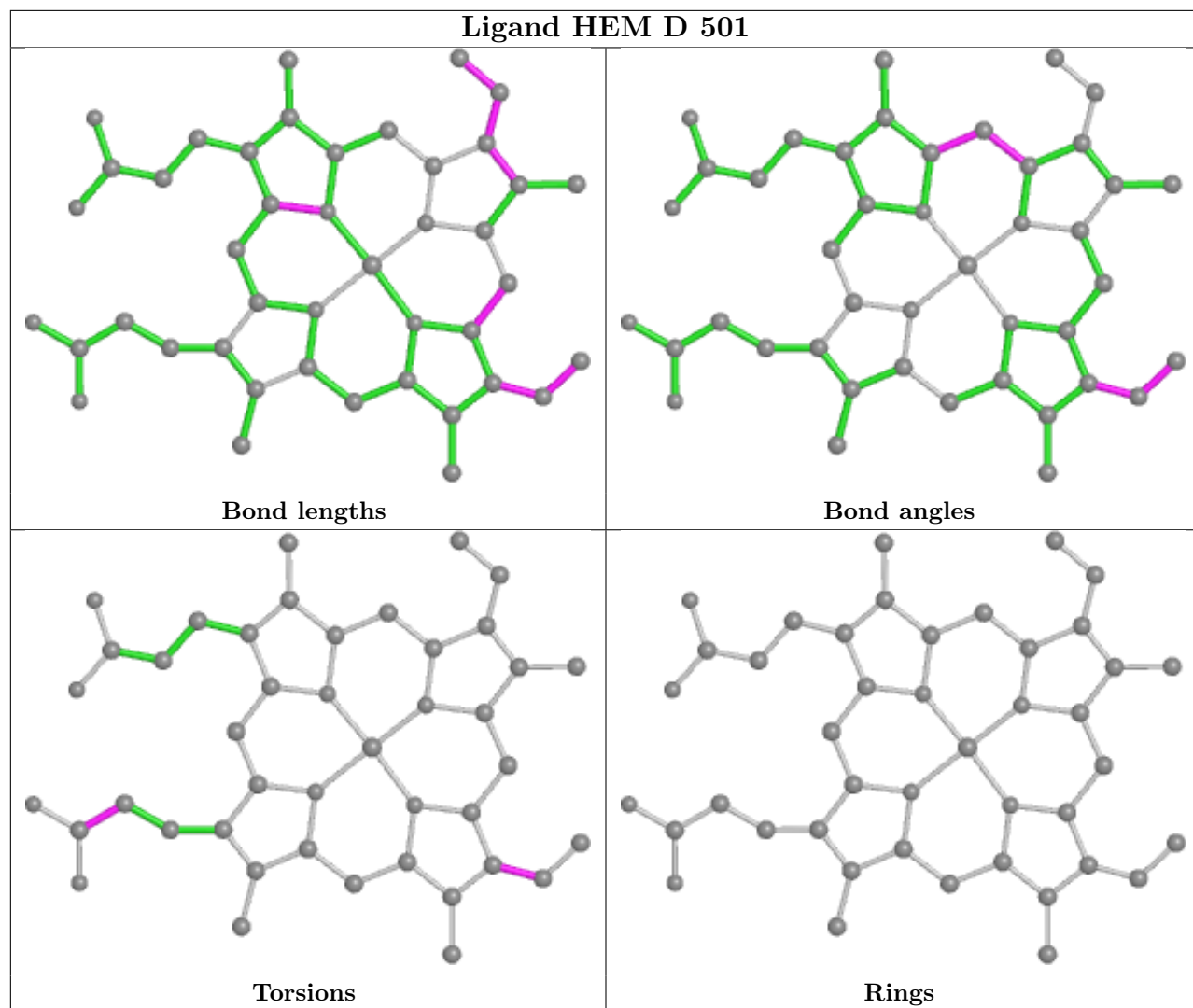




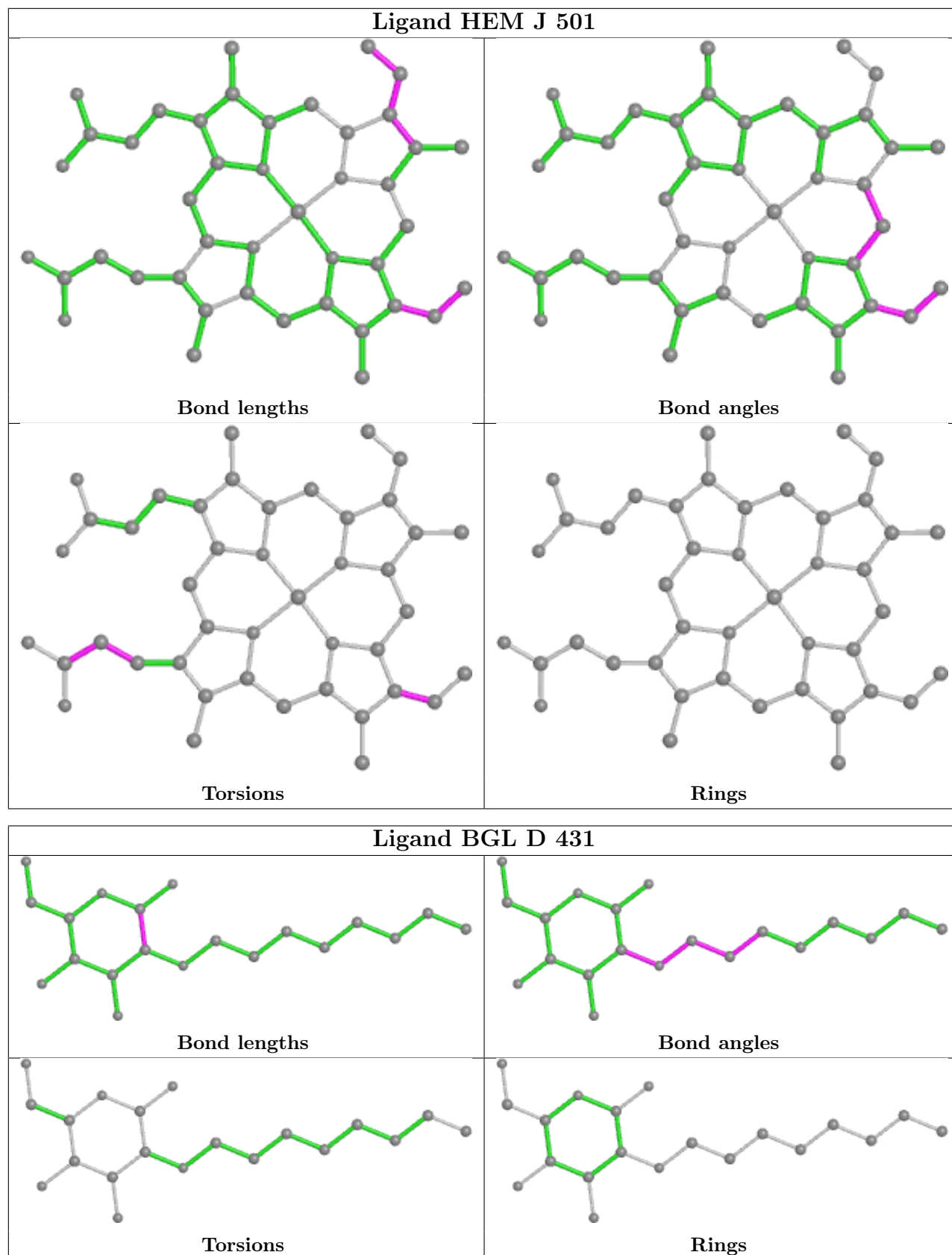


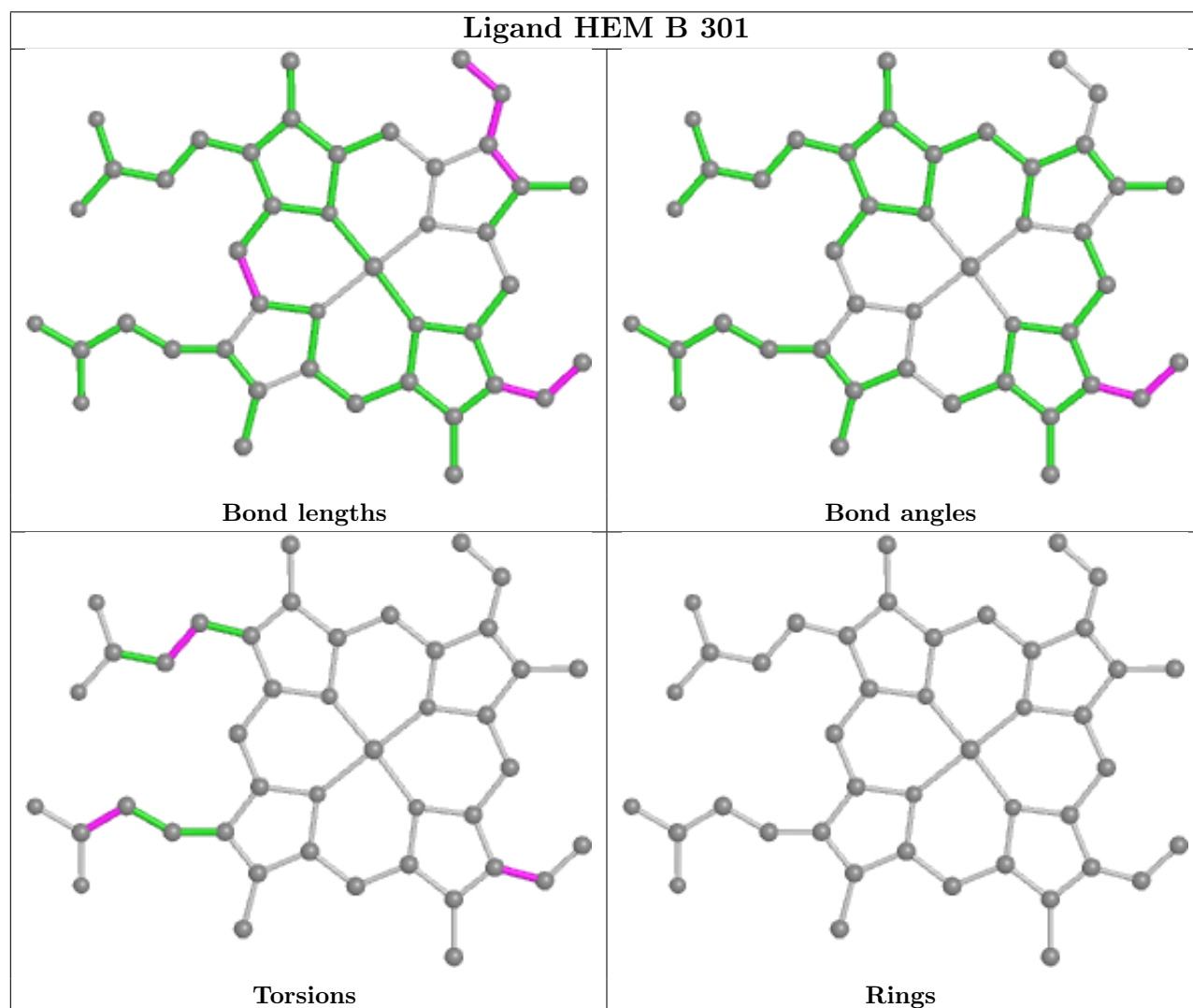
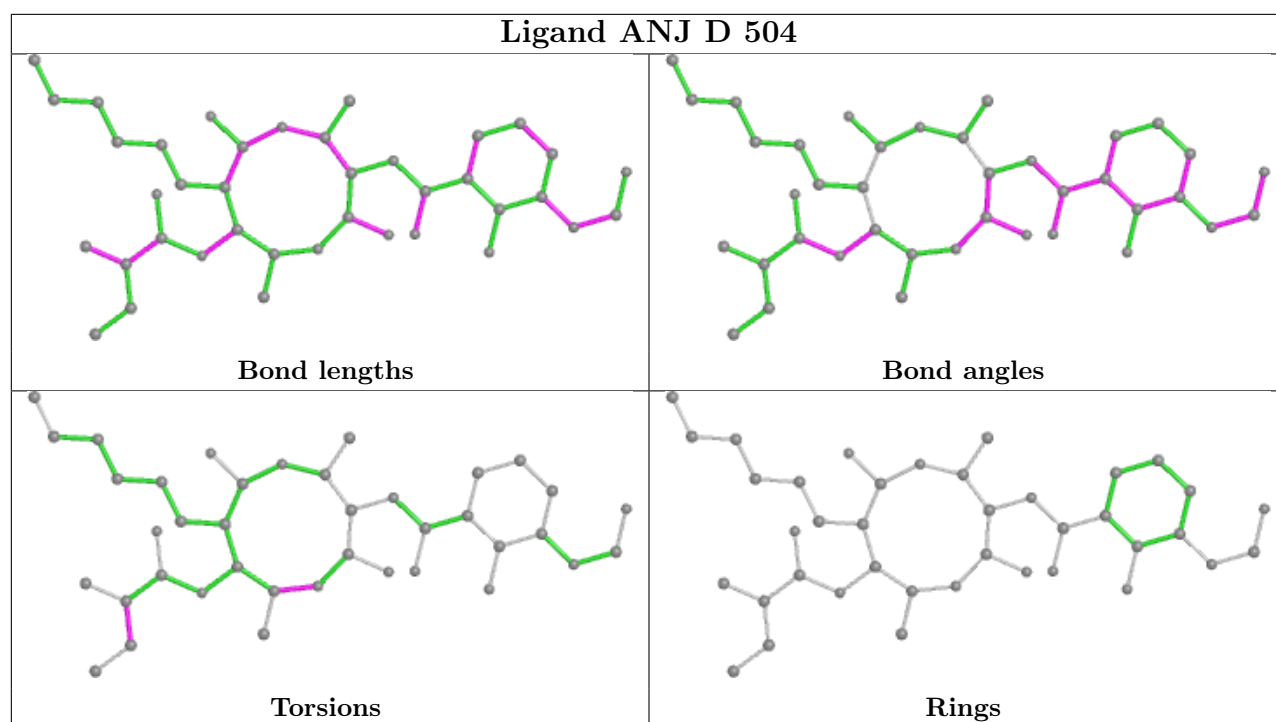


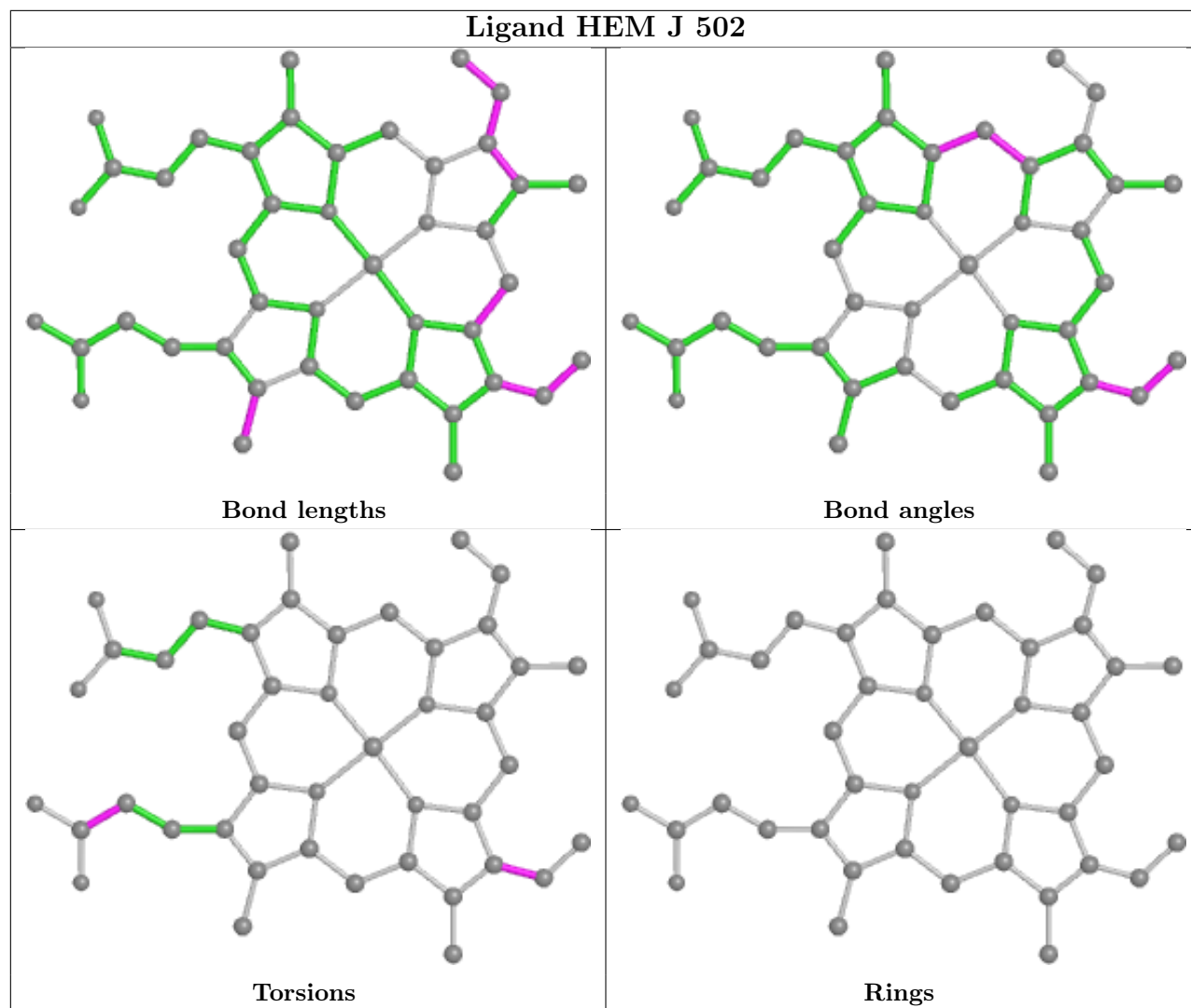


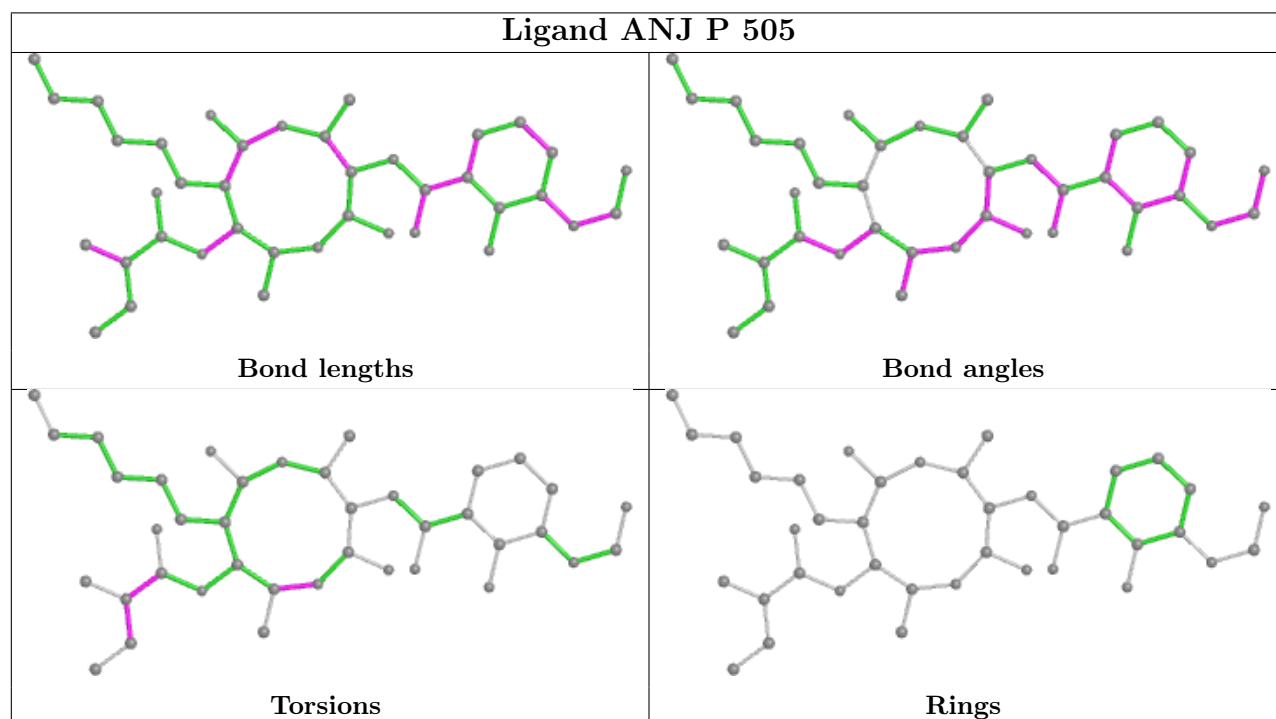
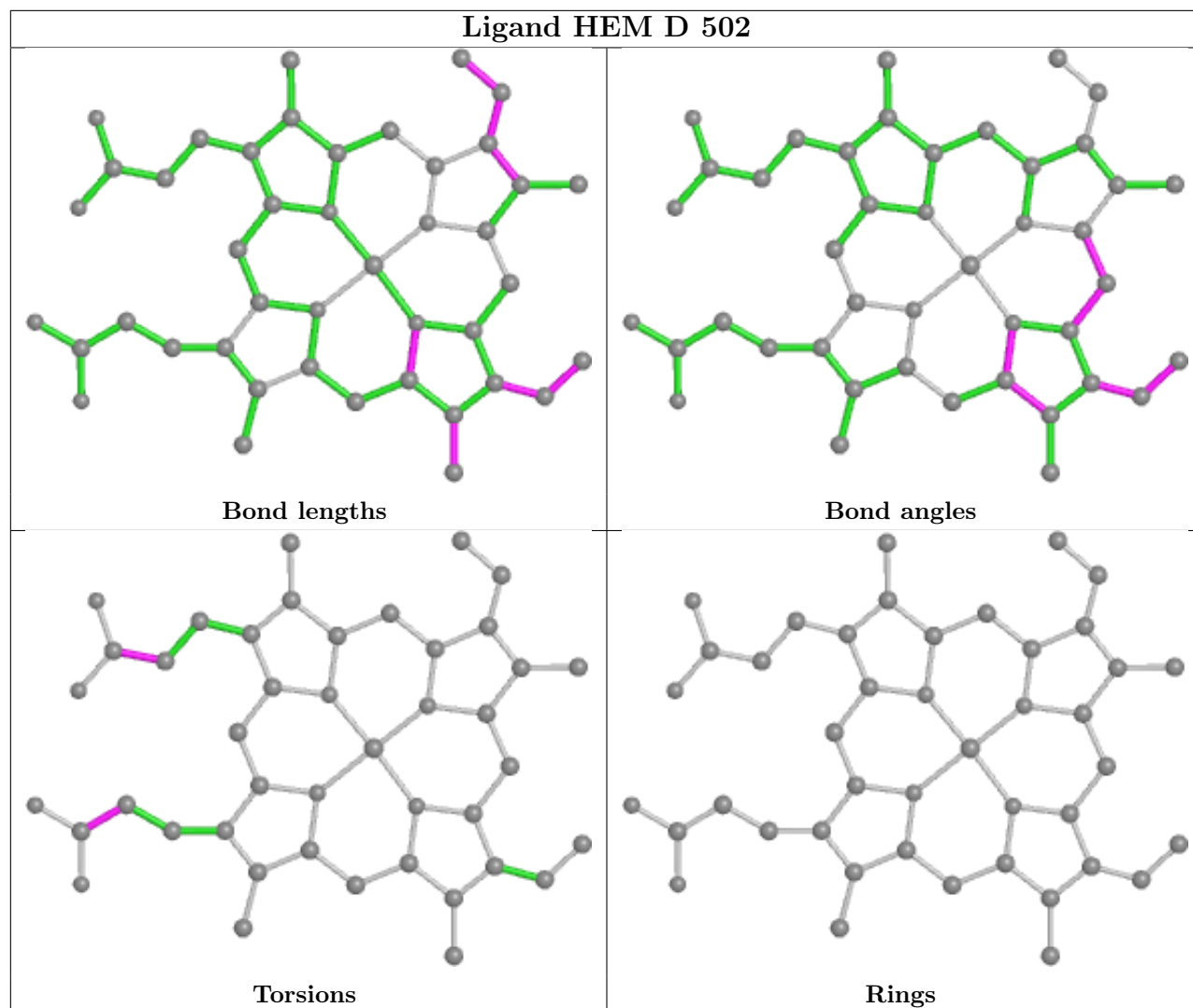


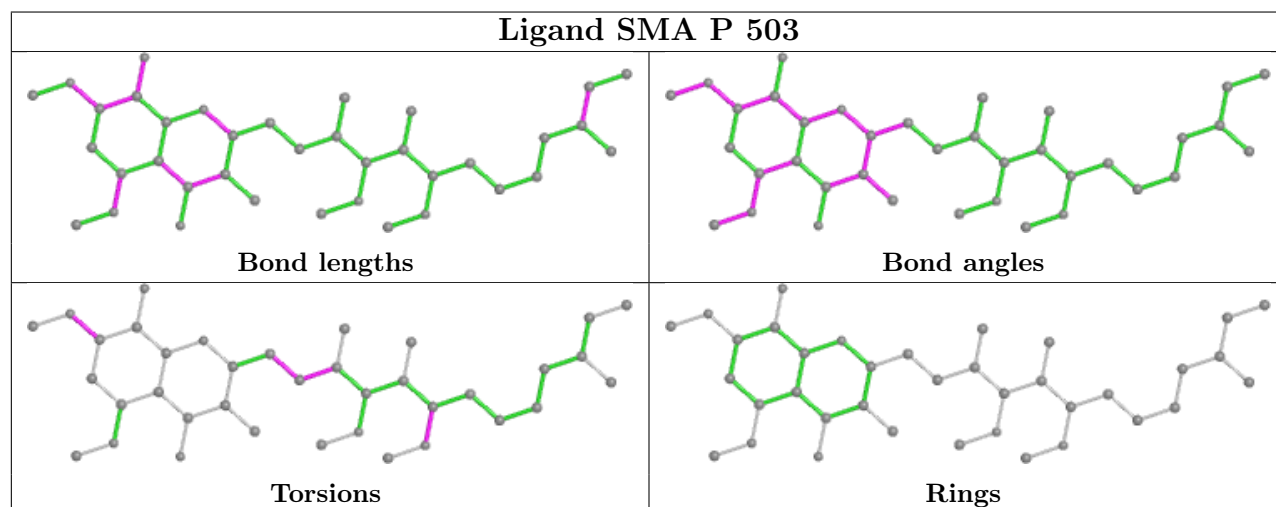
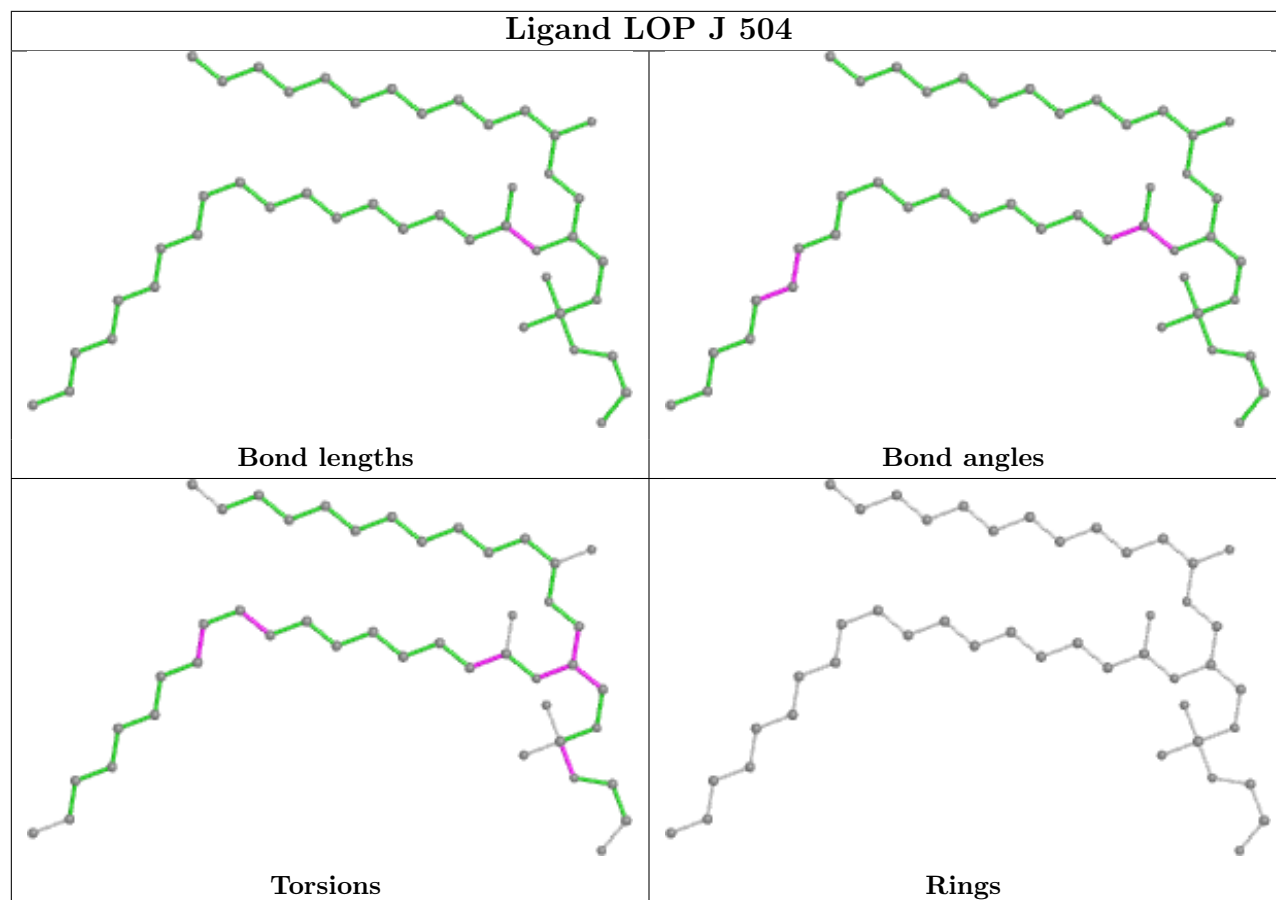


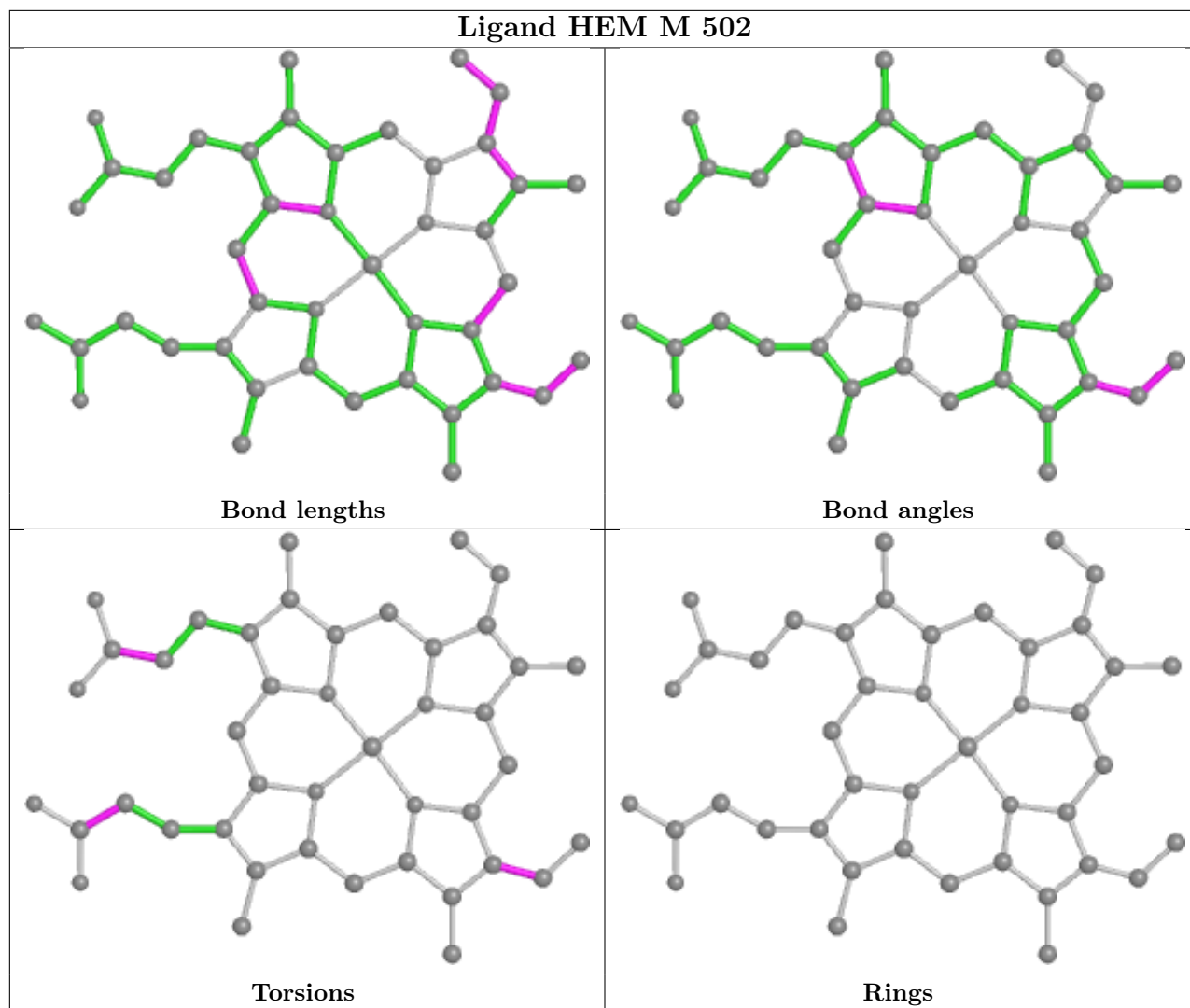


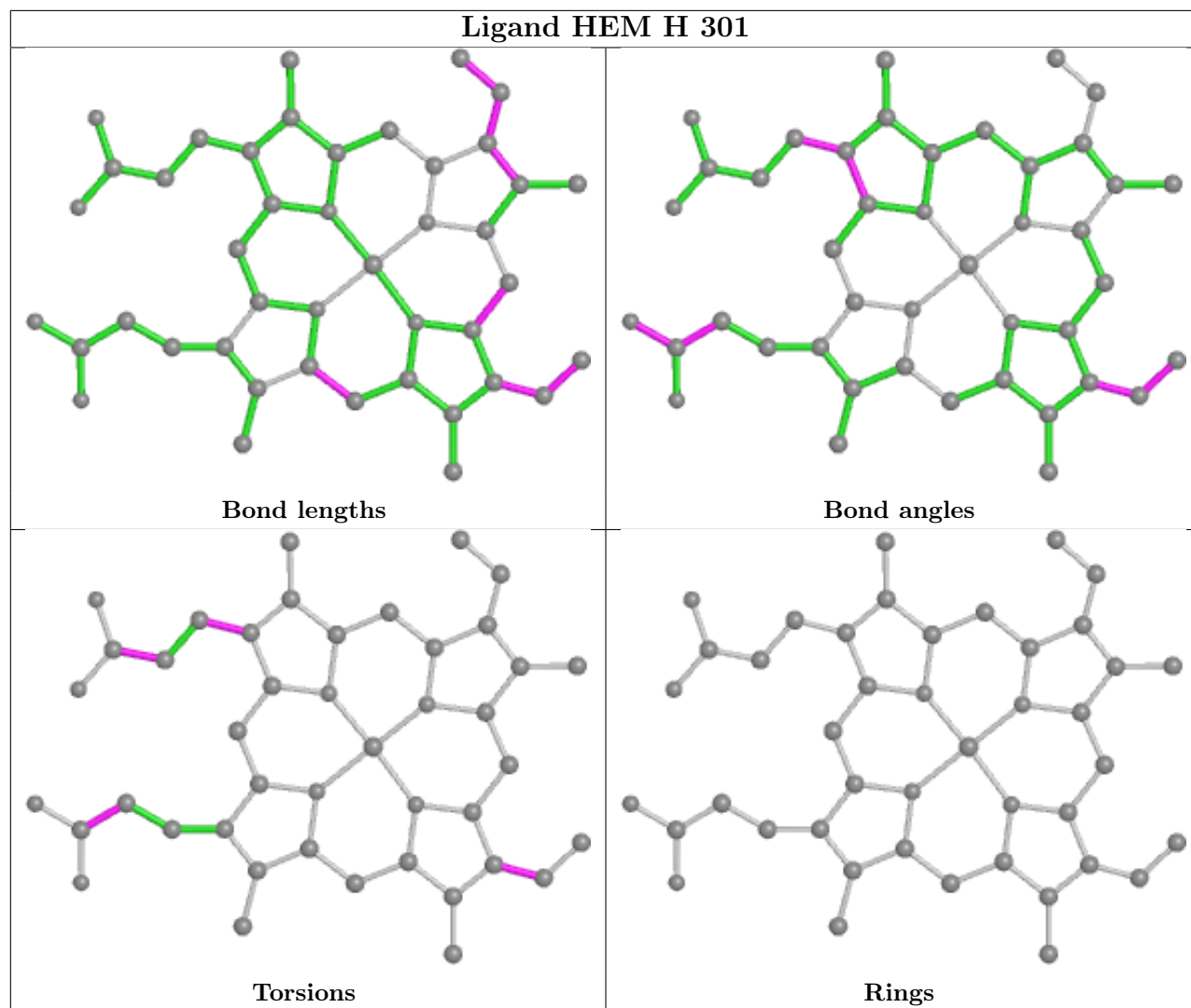


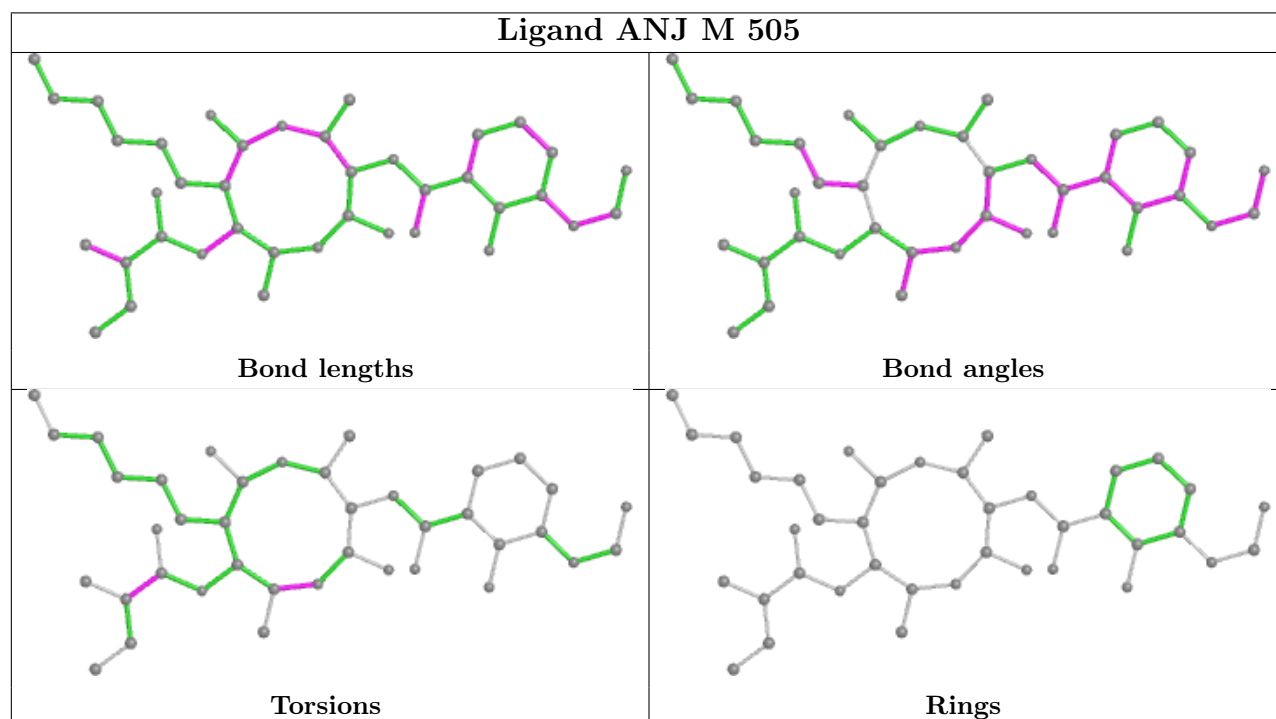
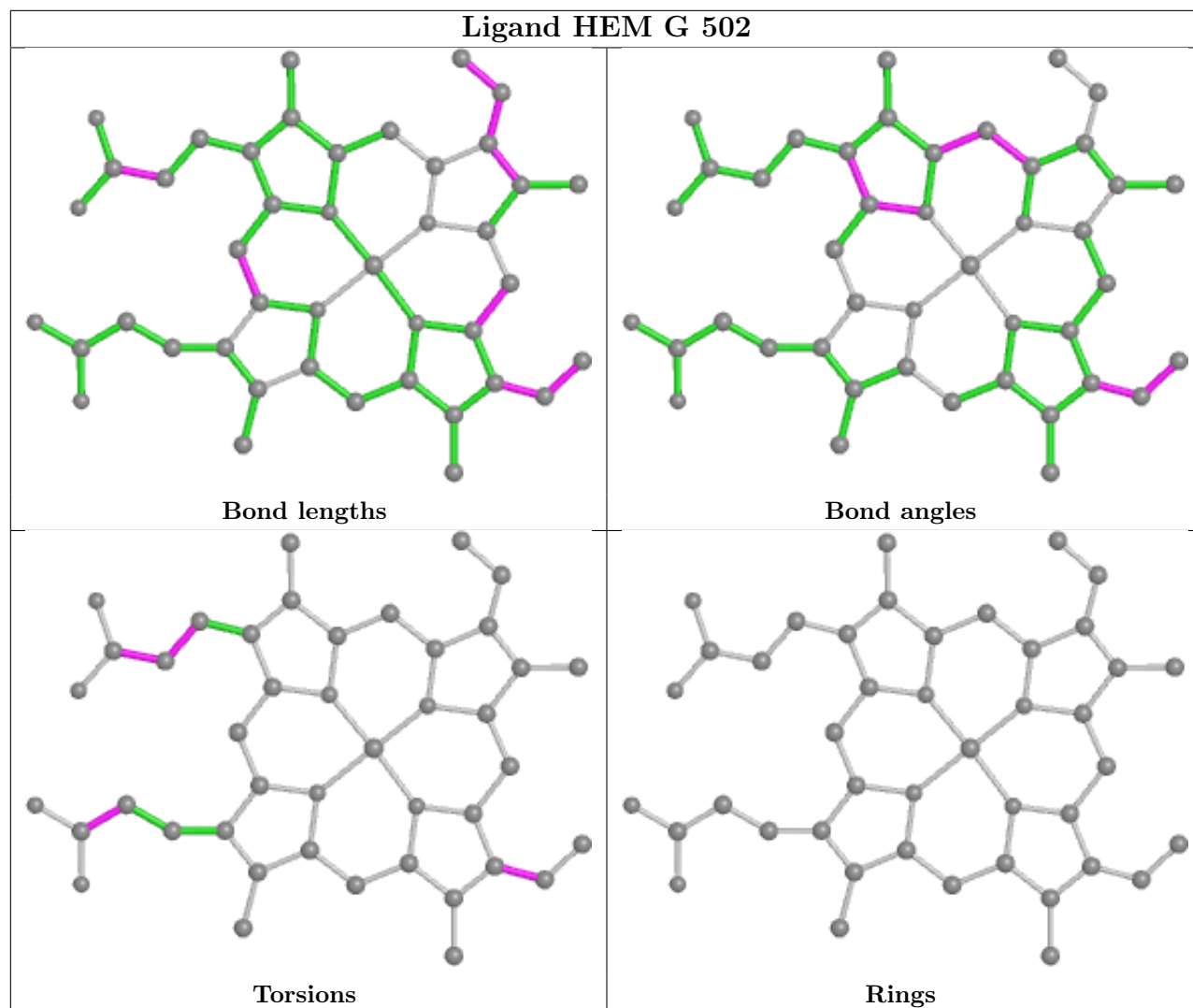




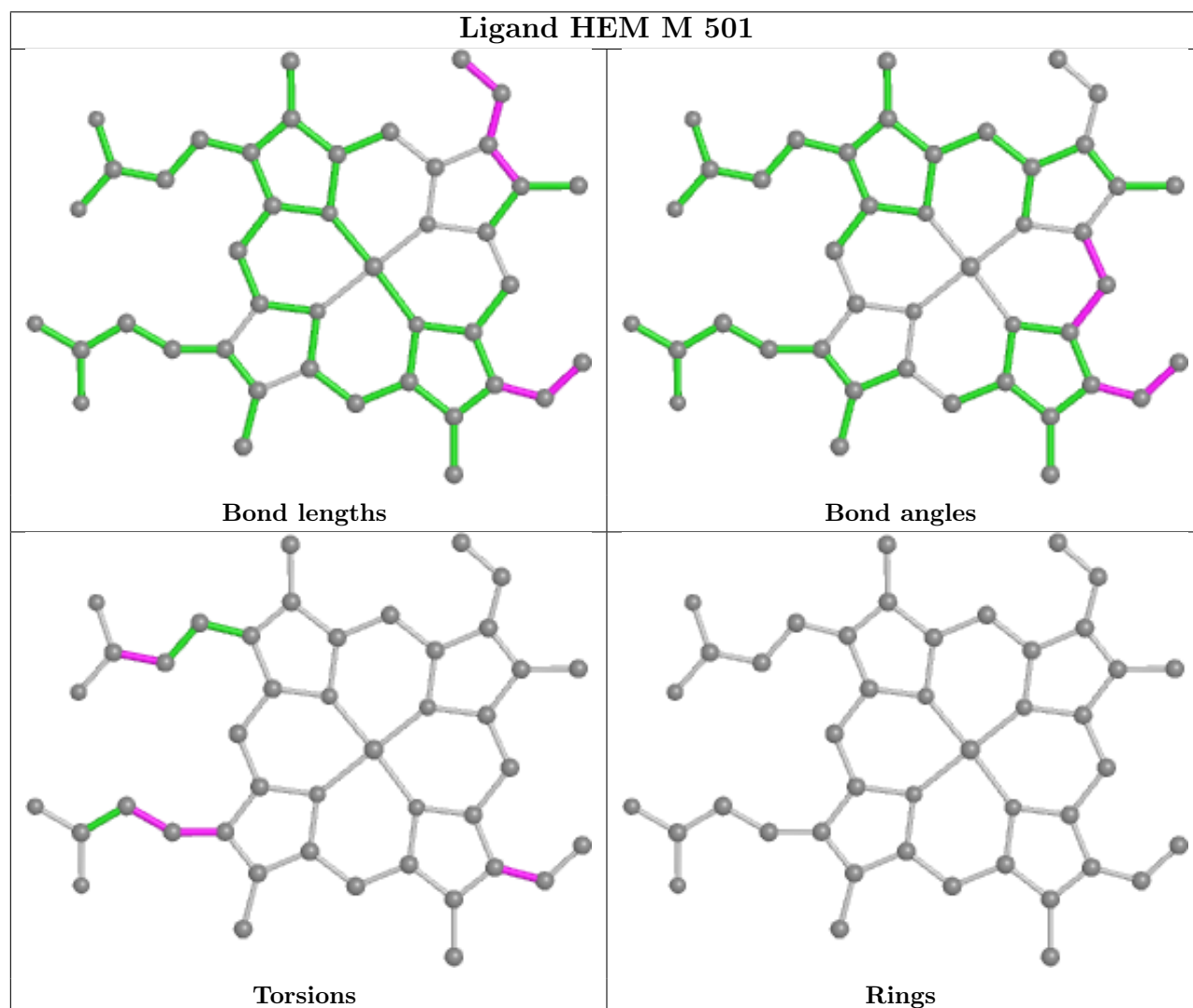
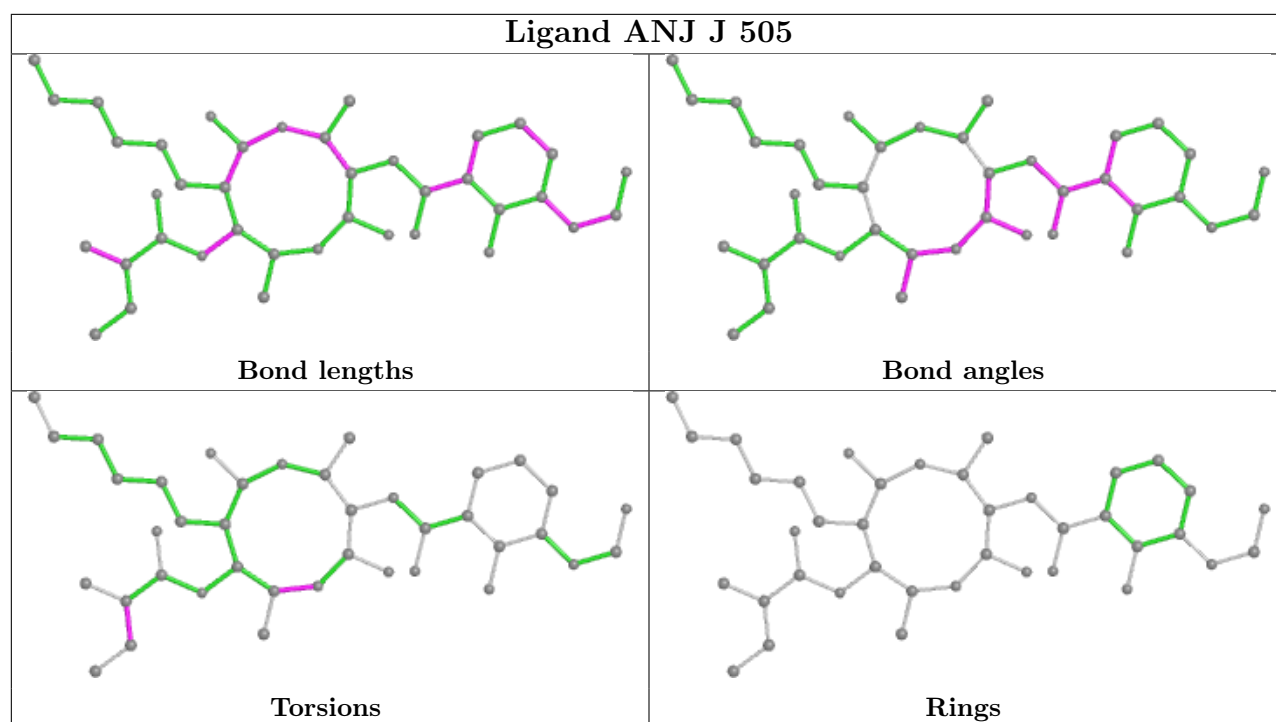


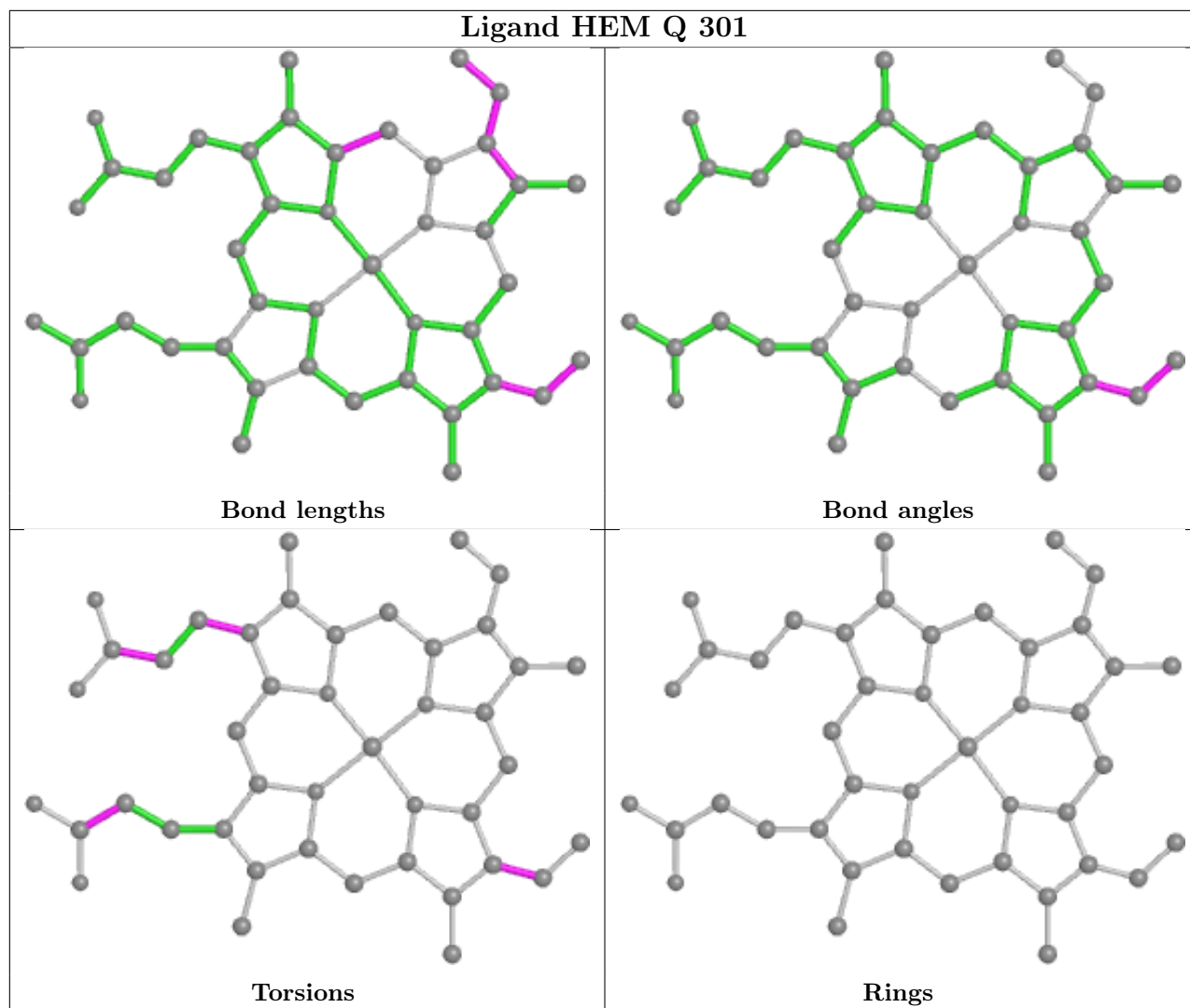


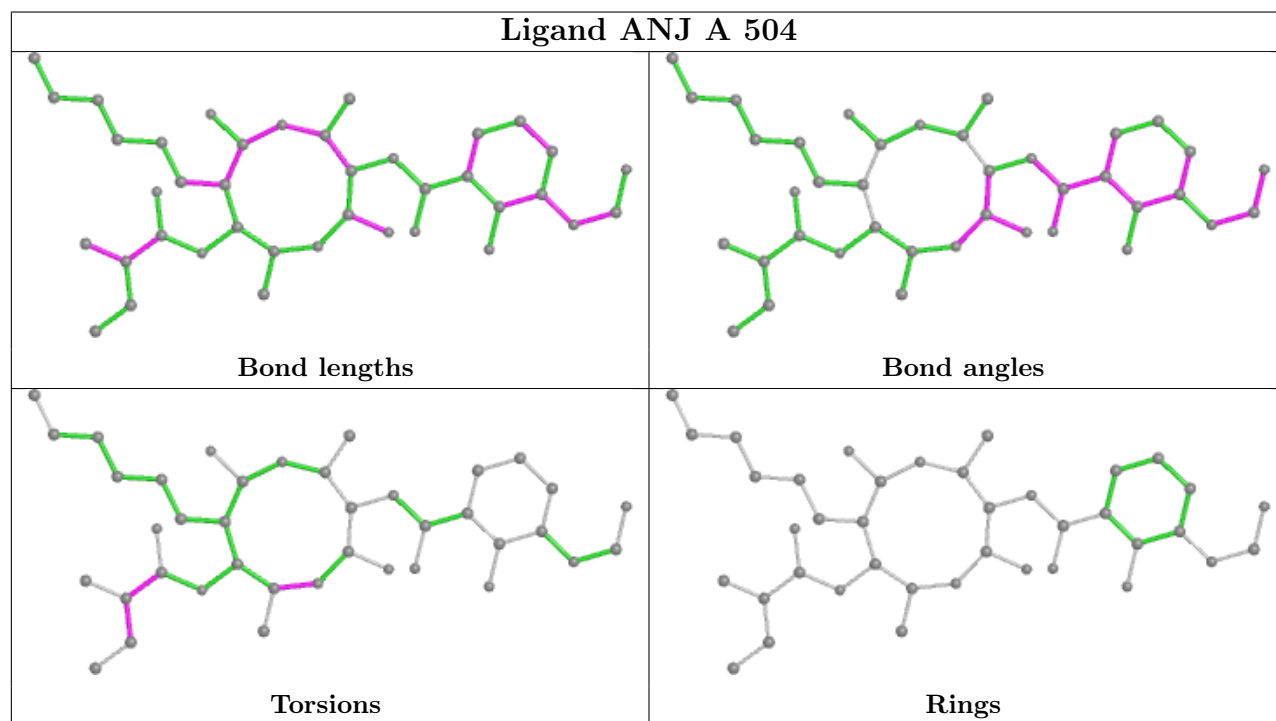
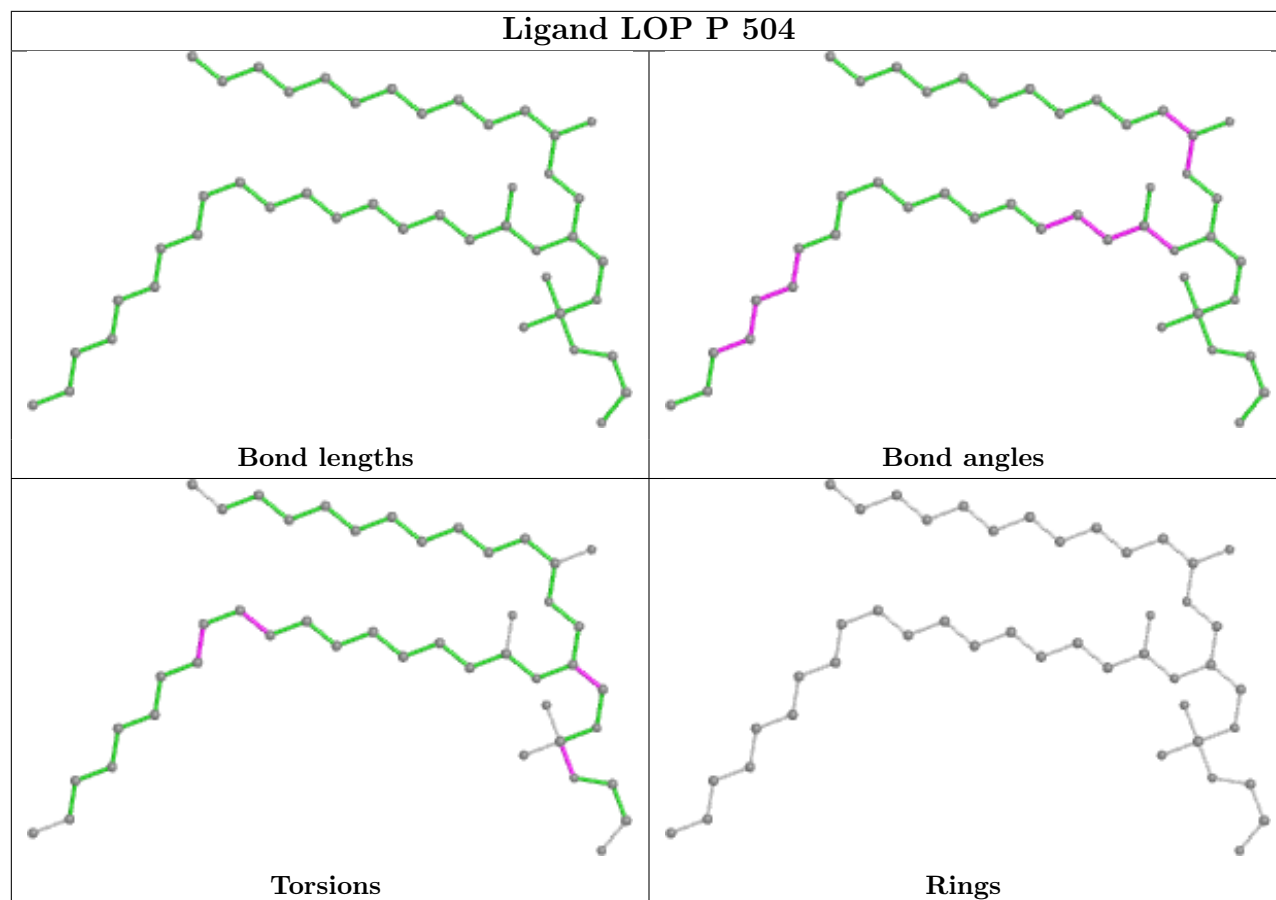


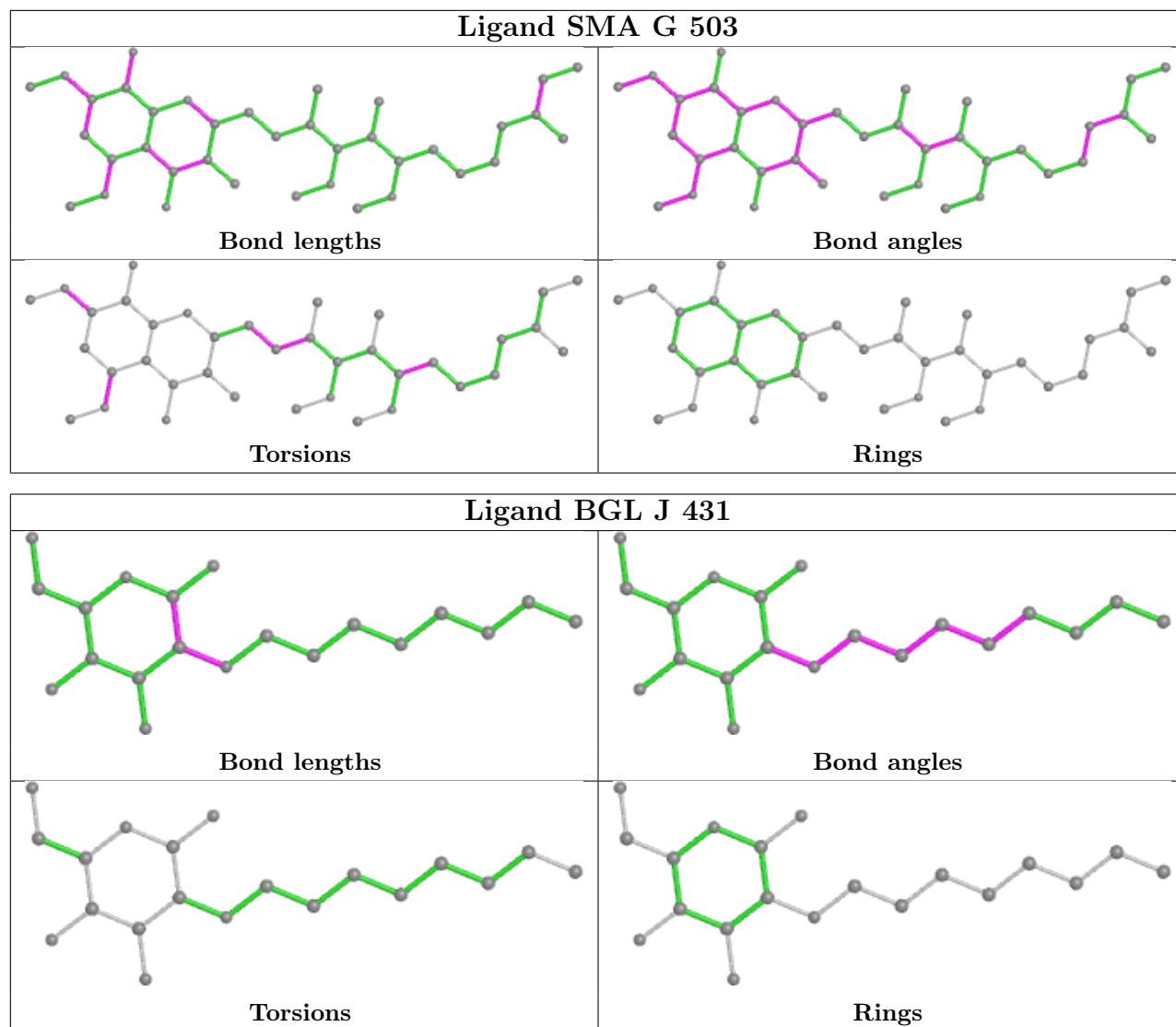


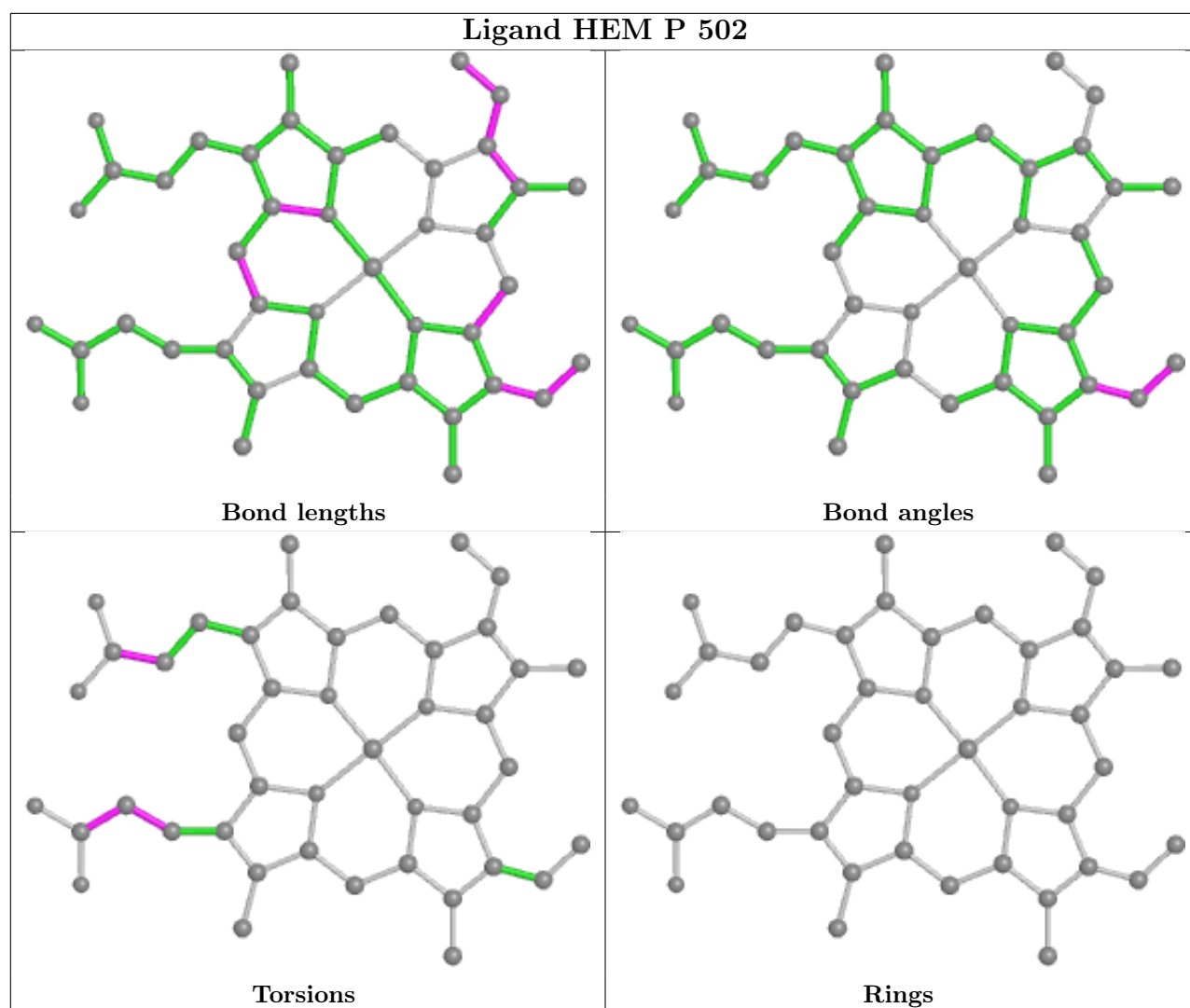












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	428/428 (100%)	-0.33	5 (1%) 79 61	31, 60, 105, 139	0
1	D	428/428 (100%)	-0.34	5 (1%) 79 61	33, 59, 109, 147	0
1	G	428/428 (100%)	-0.20	14 (3%) 46 24	34, 63, 113, 153	0
1	J	428/428 (100%)	-0.18	18 (4%) 36 18	36, 65, 113, 164	0
1	M	428/428 (100%)	-0.19	16 (3%) 41 21	41, 71, 117, 157	0
1	P	428/428 (100%)	-0.29	7 (1%) 72 51	40, 64, 116, 162	0
2	B	256/256 (100%)	0.33	27 (10%) 6 2	54, 90, 138, 176	0
2	E	256/256 (100%)	0.06	11 (4%) 35 17	47, 89, 141, 172	0
2	H	256/256 (100%)	0.15	17 (6%) 18 7	41, 88, 139, 179	0
2	K	256/256 (100%)	0.12	22 (8%) 10 4	49, 95, 141, 173	0
2	N	256/256 (100%)	0.66	42 (16%) 1 1	64, 104, 148, 177	0
2	Q	256/256 (100%)	0.21	22 (8%) 10 4	59, 99, 148, 174	0
3	C	179/179 (100%)	-0.23	9 (5%) 28 13	38, 67, 125, 186	0
3	F	179/179 (100%)	-0.20	4 (2%) 62 41	42, 70, 127, 184	0
3	I	179/179 (100%)	-0.07	12 (6%) 17 7	44, 70, 124, 183	0
3	L	179/179 (100%)	-0.25	4 (2%) 62 41	39, 68, 129, 183	0
3	O	179/179 (100%)	-0.06	10 (5%) 24 11	44, 75, 131, 184	0
3	R	179/179 (100%)	0.36	16 (8%) 9 3	49, 86, 130, 181	0
All	All	5178/5178 (100%)	-0.07	261 (5%) 28 13	31, 75, 132, 186	0

The worst 5 of 261 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	GLY	12.7
2	B	4	GLY	11.5
2	E	3	GLY	10.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	R	9	GLY	10.3
2	Q	4	GLY	10.3

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	BGL	M	431	20/20	0.67	0.66	120,124,128,129	0
9	SR	N	257	1/1	0.74	0.07	153,153,153,153	0
7	LOP	G	504	45/45	0.78	0.35	91,111,130,131	0
7	LOP	J	504	45/45	0.79	0.60	105,143,157,158	0
4	BGL	G	431	20/20	0.80	0.48	93,98,109,109	0
7	LOP	M	504	45/45	0.83	0.36	91,121,132,133	0
7	LOP	P	504	45/45	0.84	0.38	63,98,114,118	0
4	BGL	Q	257	20/20	0.84	0.21	94,99,103,103	0
4	BGL	J	431	20/20	0.86	0.17	94,99,103,104	0
4	BGL	A	431	20/20	0.86	0.32	90,98,102,104	0
9	SR	Q	258	1/1	0.87	0.07	139,139,139,139	0
9	SR	K	257	1/1	0.88	0.07	134,134,134,134	0
7	LOP	D	503	45/45	0.89	0.28	49,102,111,113	0
4	BGL	D	431	20/20	0.89	0.21	79,86,88,89	0
7	LOP	A	503	45/45	0.90	0.25	62,89,101,105	0
5	HEM	N	301	43/43	0.91	0.24	71,81,87,89	0
8	ANJ	J	505	39/39	0.92	0.23	88,96,102,104	0
9	SR	B	257	1/1	0.92	0.04	136,136,136,136	0
9	SR	E	257	1/1	0.92	0.05	111,111,111,111	0
6	SMA	M	503	37/37	0.93	0.20	50,68,78,80	0
8	ANJ	M	505	39/39	0.93	0.24	82,96,101,103	0

*Continued on next page...*

*Continued from previous page...*

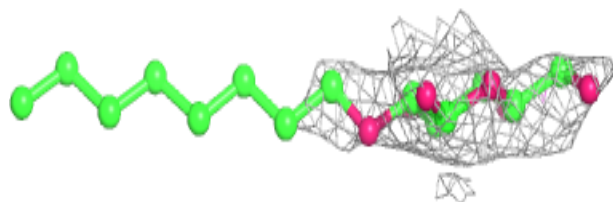
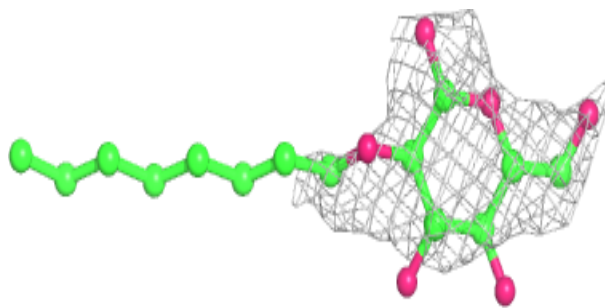
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ANJ	P	505	39/39	0.93	0.24	63,74,89,96	0
8	ANJ	A	504	39/39	0.93	0.21	57,73,93,96	0
6	SMA	A	1	37/37	0.94	0.20	34,49,61,66	0
6	SMA	J	503	37/37	0.94	0.23	42,60,69,72	0
8	ANJ	D	504	39/39	0.94	0.21	57,69,84,85	0
8	ANJ	G	505	39/39	0.94	0.26	52,75,95,98	0
9	SR	H	257	1/1	0.95	0.06	106,106,106,106	0
6	SMA	G	503	37/37	0.95	0.22	37,47,64,67	0
5	HEM	J	501	43/43	0.96	0.22	74,84,95,99	0
6	SMA	D	2	37/37	0.96	0.19	32,44,52,54	0
5	HEM	M	501	43/43	0.96	0.23	73,78,88,91	0
5	HEM	B	301	43/43	0.96	0.21	54,59,74,78	0
5	HEM	Q	301	43/43	0.96	0.23	64,75,81,82	0
6	SMA	P	503	37/37	0.96	0.22	33,47,68,70	0
5	HEM	H	301	43/43	0.97	0.20	39,50,58,60	0
5	HEM	A	501	43/43	0.97	0.21	39,56,61,62	0
5	HEM	K	301	43/43	0.97	0.17	49,60,74,75	0
5	HEM	D	501	43/43	0.97	0.20	50,56,68,73	0
5	HEM	E	301	43/43	0.97	0.23	55,63,79,80	0
5	HEM	G	501	43/43	0.97	0.24	58,71,84,91	0
5	HEM	D	502	43/43	0.98	0.17	16,29,46,53	0
5	HEM	P	501	43/43	0.98	0.22	58,67,79,85	0
5	HEM	P	502	43/43	0.98	0.18	25,36,48,59	0
5	HEM	J	502	43/43	0.98	0.18	27,37,52,60	0
5	HEM	G	502	43/43	0.98	0.17	22,34,45,51	0
5	HEM	A	502	43/43	0.98	0.17	14,29,45,49	0
5	HEM	M	502	43/43	0.98	0.19	49,54,64,66	0
10	FES	C	200	4/4	0.99	0.15	33,36,40,42	0
10	FES	F	200	4/4	0.99	0.18	42,42,42,45	0
10	FES	I	200	4/4	0.99	0.14	45,47,48,50	0
10	FES	L	200	4/4	0.99	0.17	32,34,36,39	0
10	FES	O	200	4/4	0.99	0.15	40,43,43,50	0
10	FES	R	200	4/4	0.99	0.17	56,57,58,59	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.

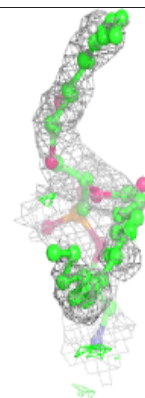
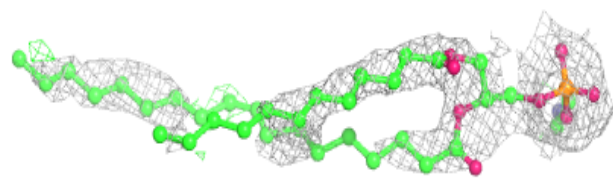
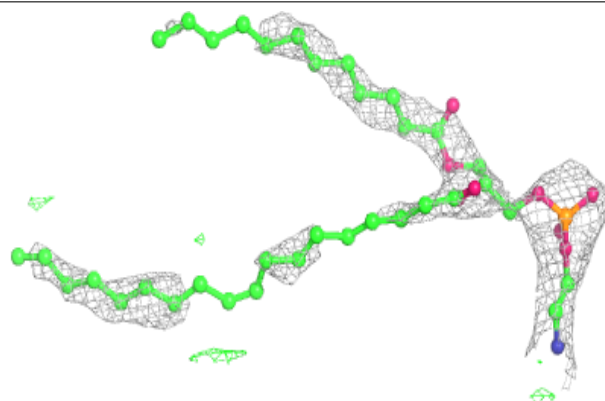


**Electron density around BGL M 431:**

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

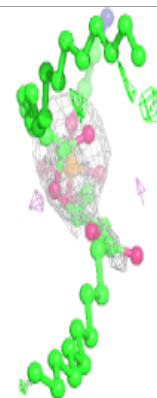
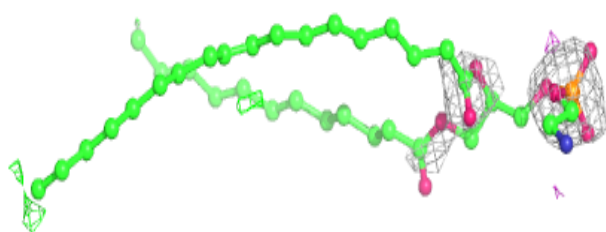
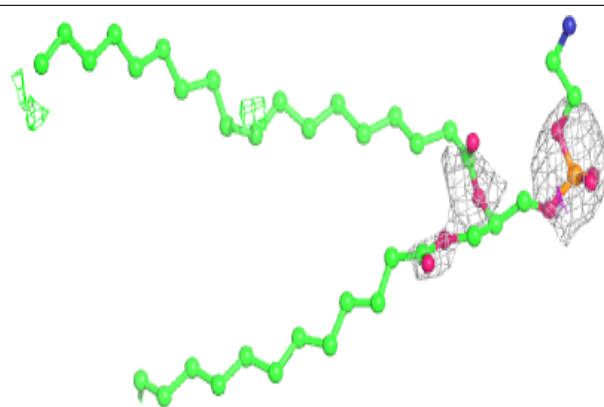
**Electron density around LOP G 504:**

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

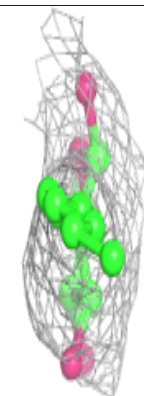
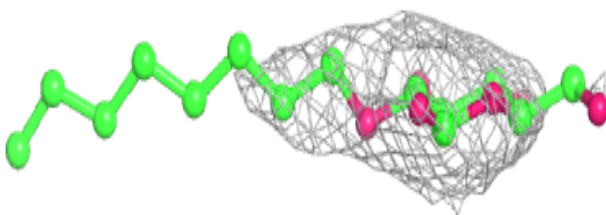
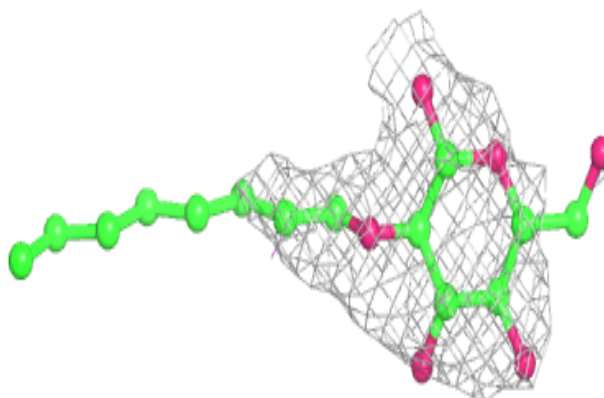


**Electron density around LOP J 504:**

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

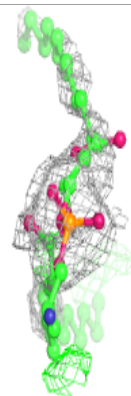
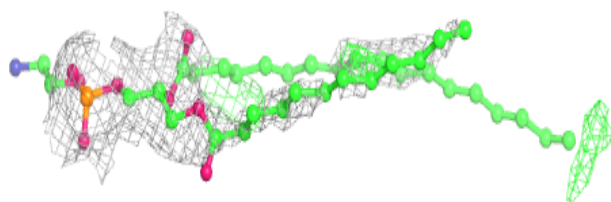
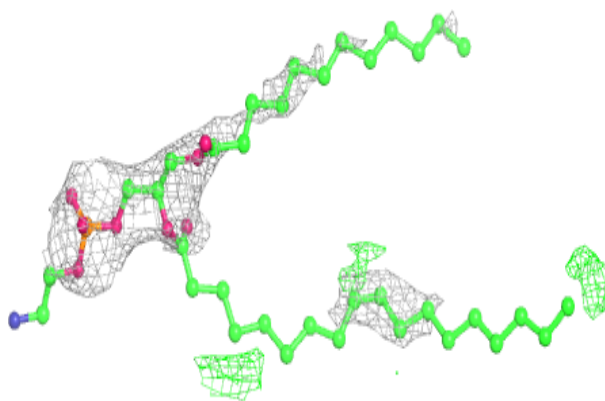
**Electron density around BGL G 431:**

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

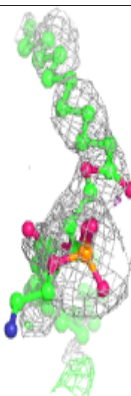
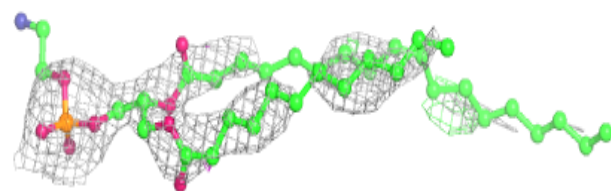
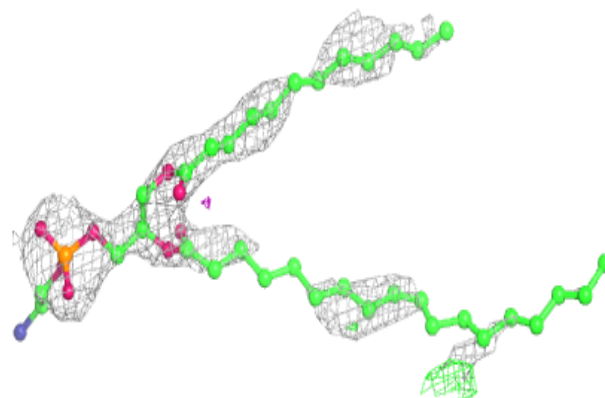


**Electron density around LOP M 504:**

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

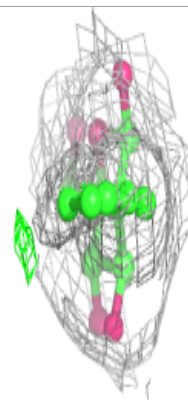
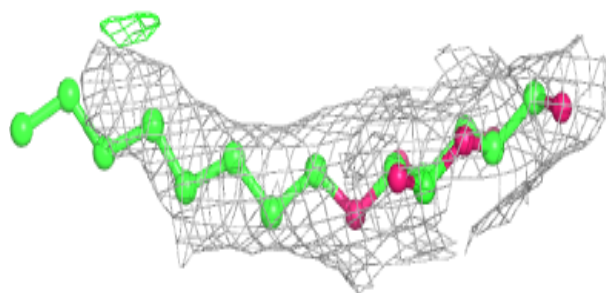
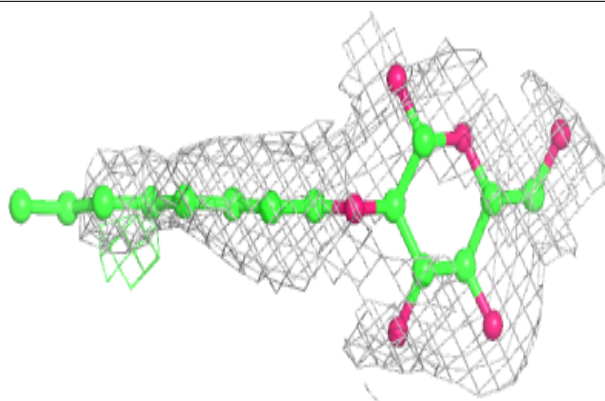
**Electron density around LOP P 504:**

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

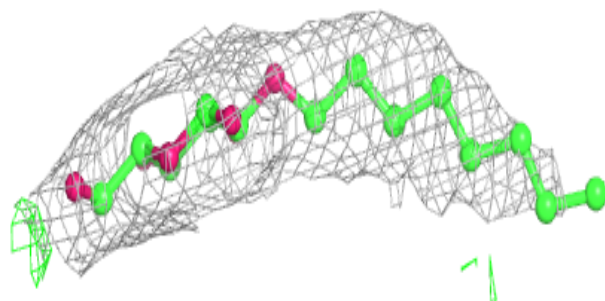
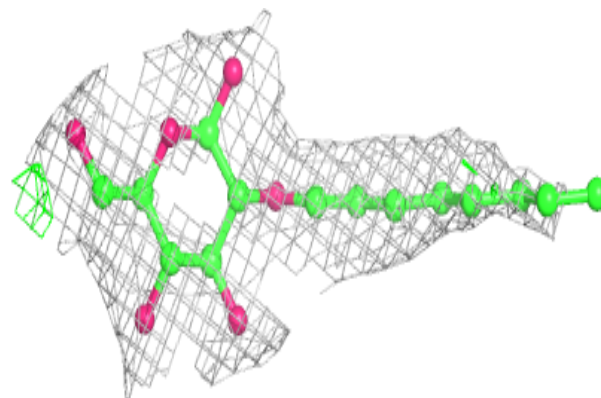


**Electron density around BGL Q 257:**

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

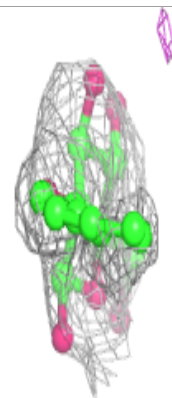
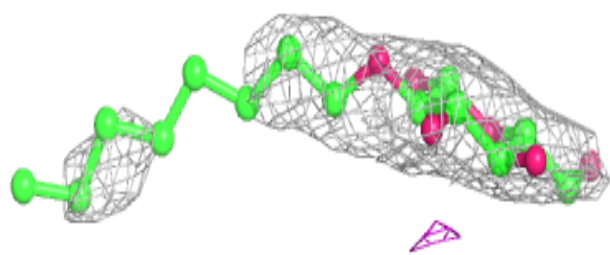
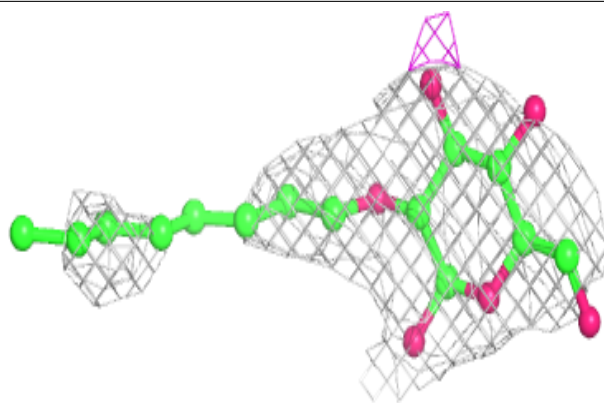
**Electron density around BGL J 431:**

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

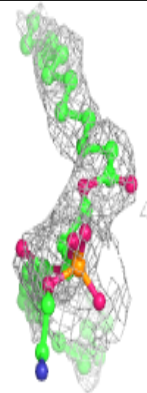
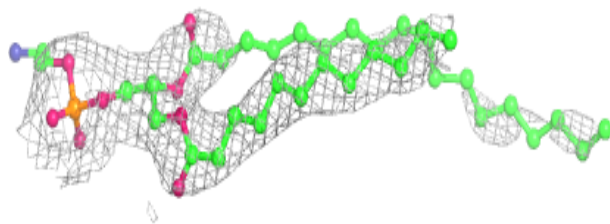
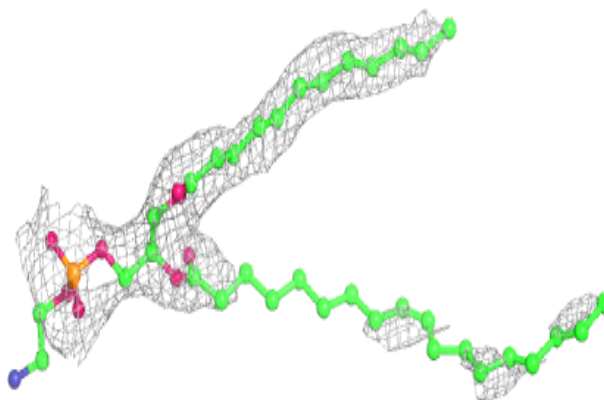


**Electron density around BGL A 431:**

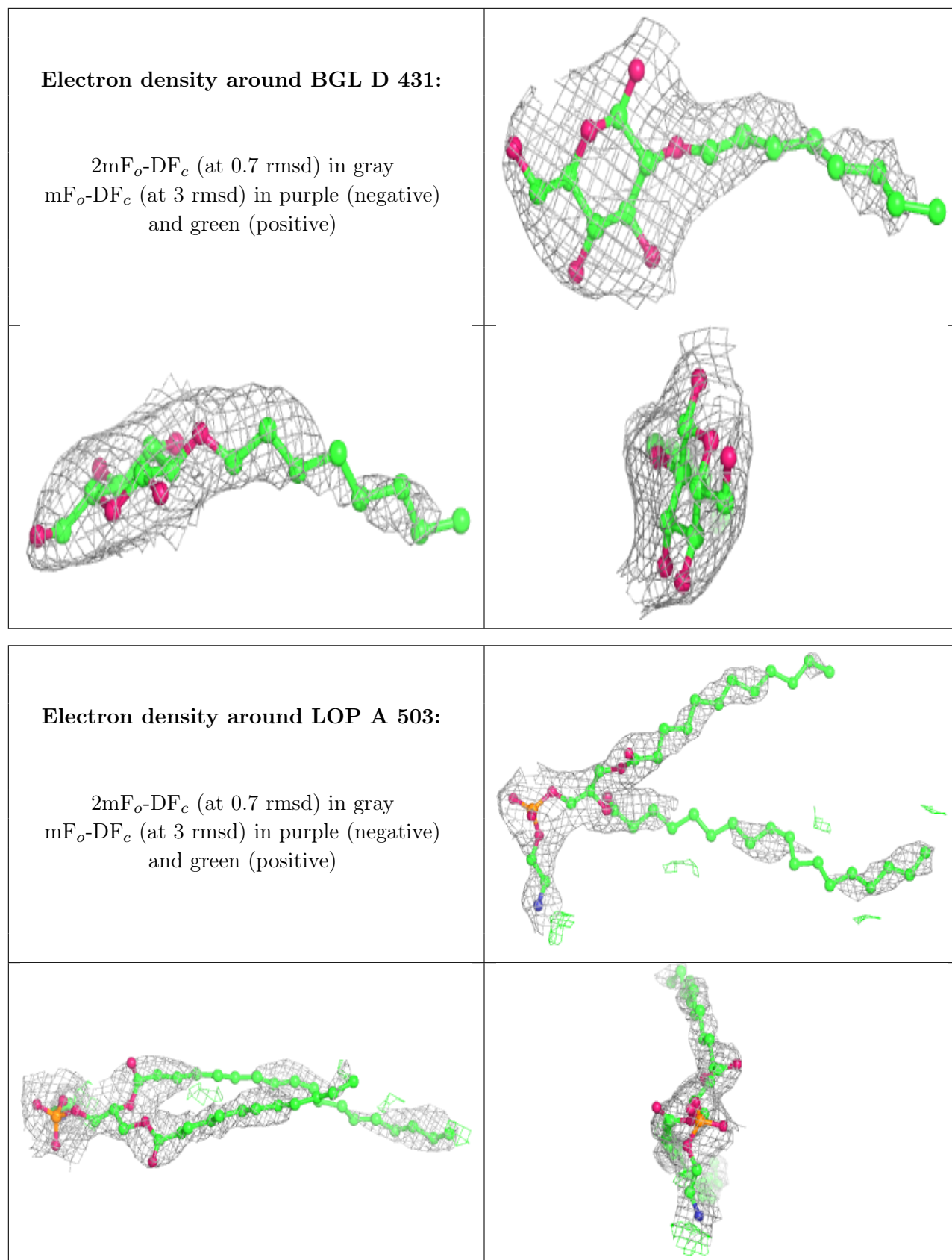
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LOP D 503:**

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

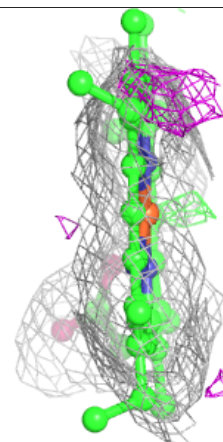
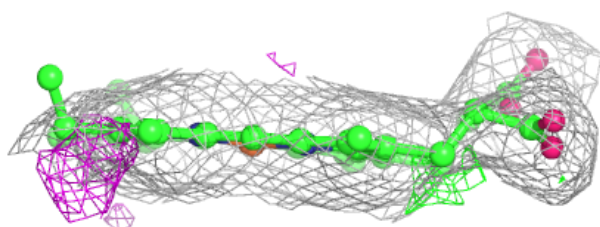
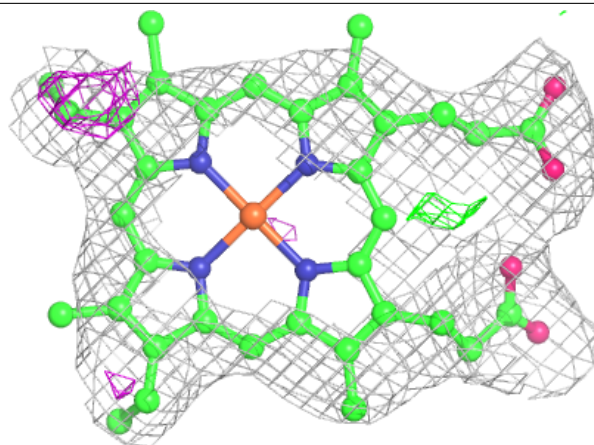




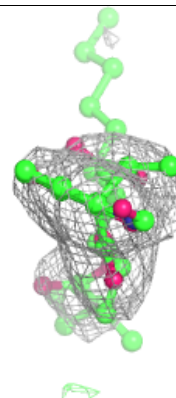
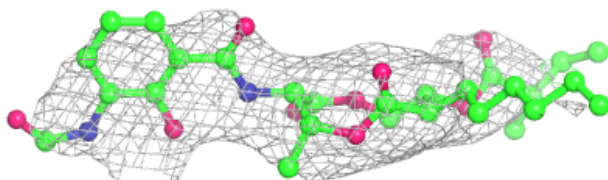
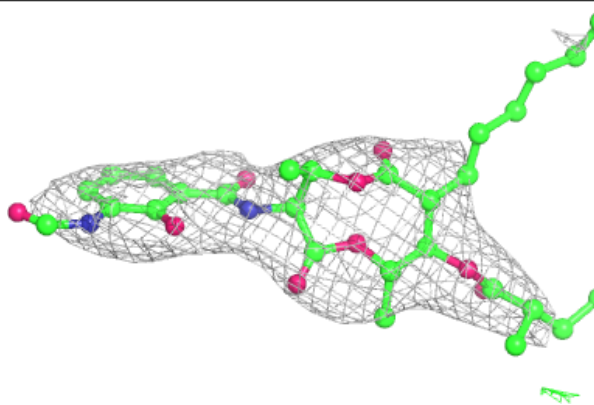


**Electron density around HEM N 301:**

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

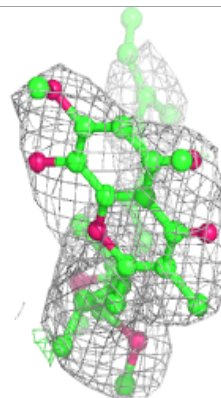
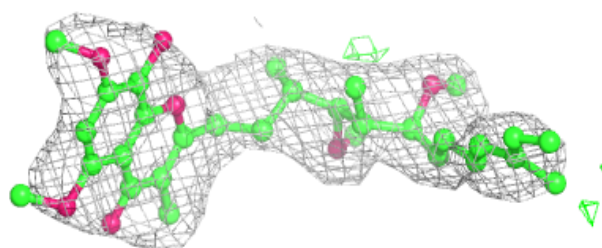
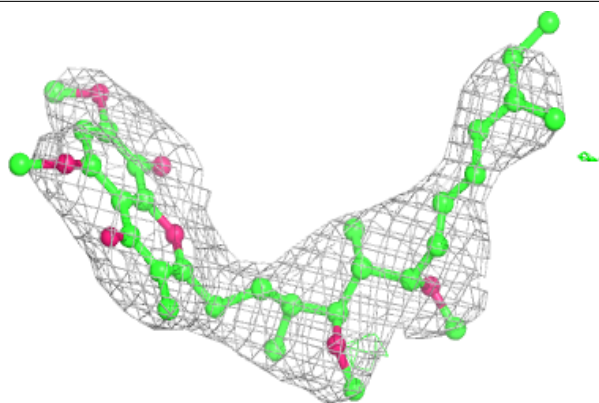
**Electron density around ANJ J 505:**

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

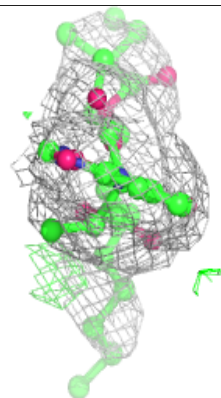
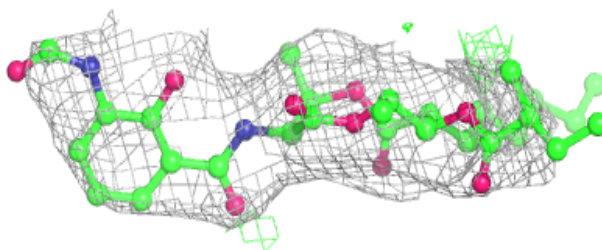
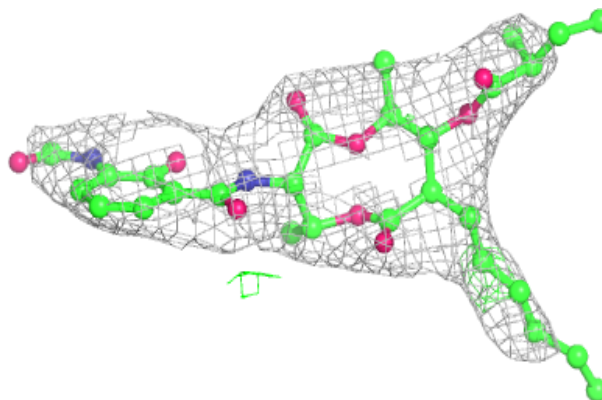


**Electron density around SMA M 503:**

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

**Electron density around ANJ M 505:**

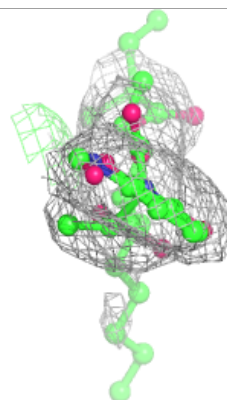
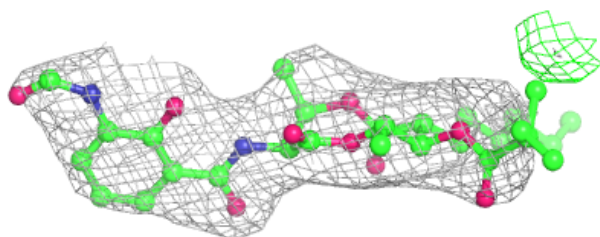
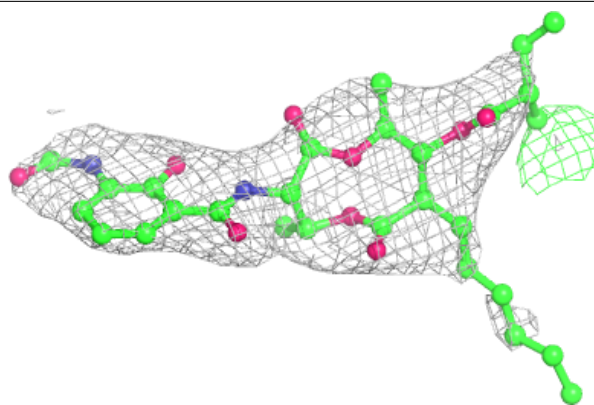
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



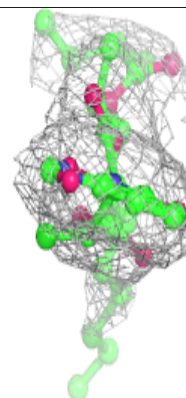
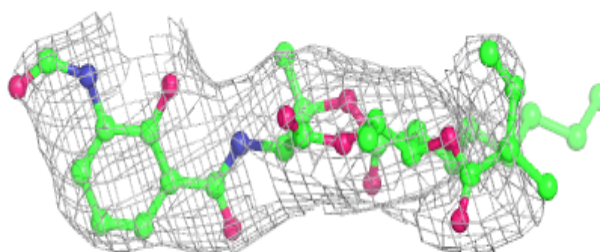
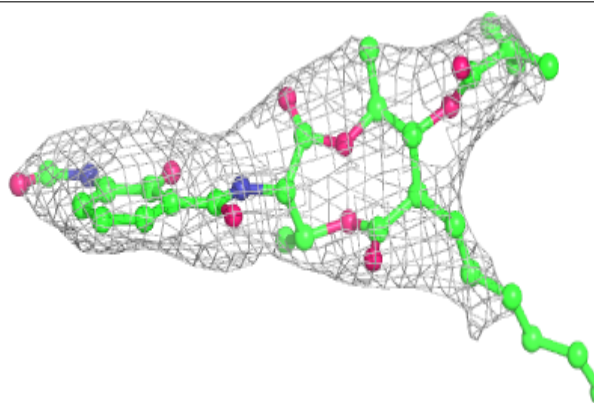


**Electron density around ANJ P 505:**

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

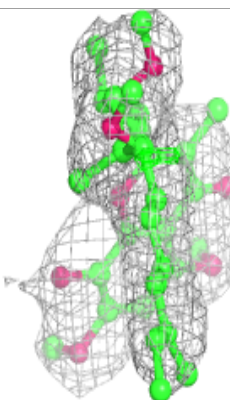
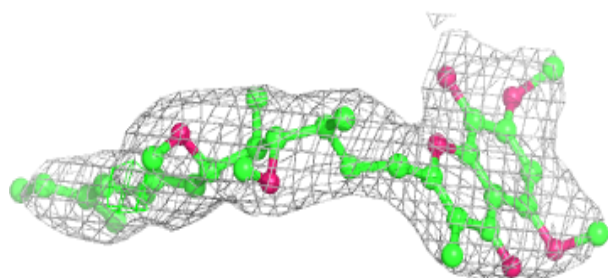
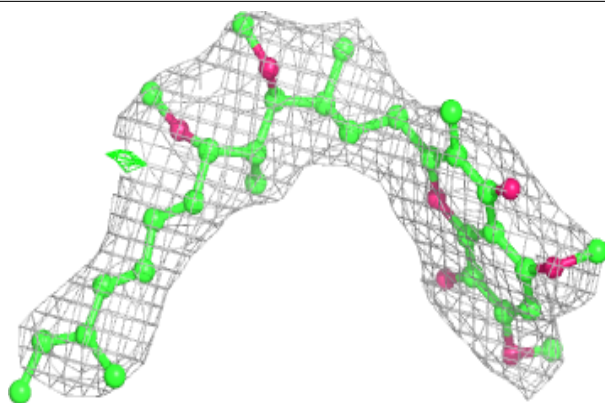
**Electron density around ANJ A 504:**

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

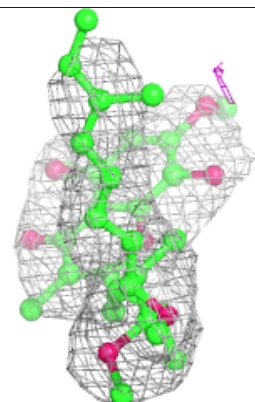
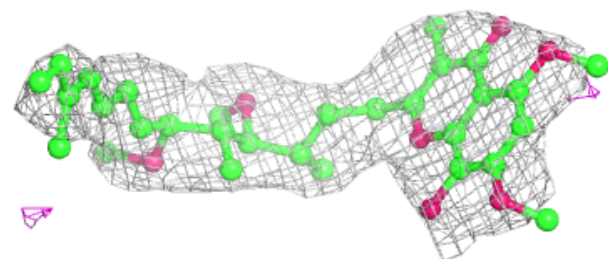
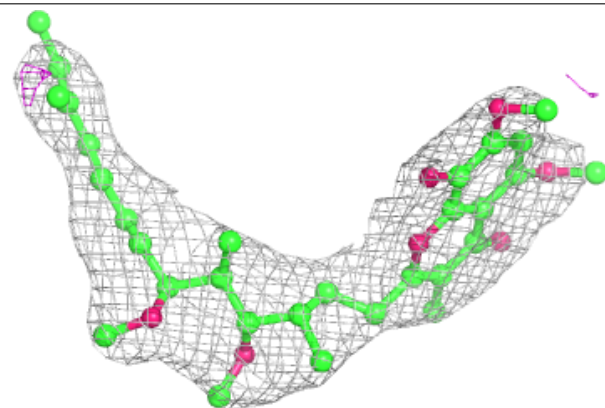


**Electron density around SMA A 1:**

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

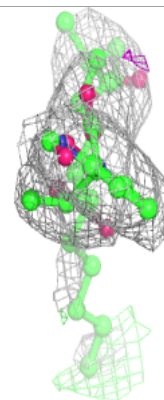
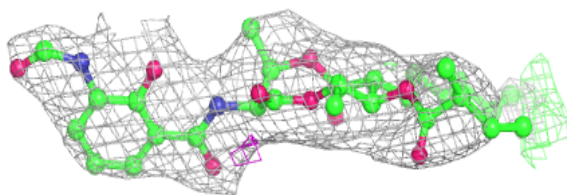
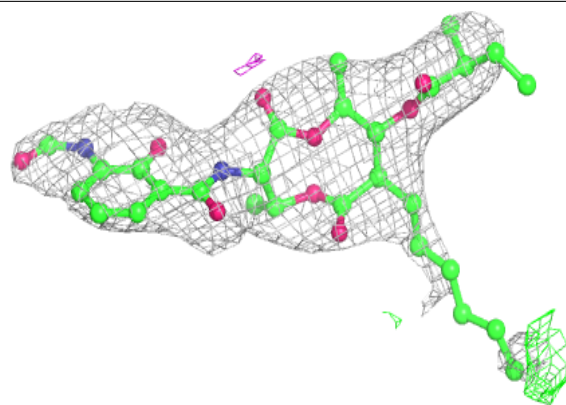
**Electron density around SMA J 503:**

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

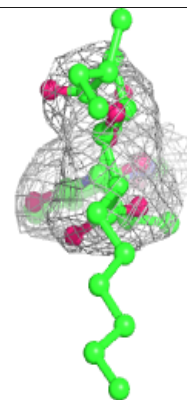
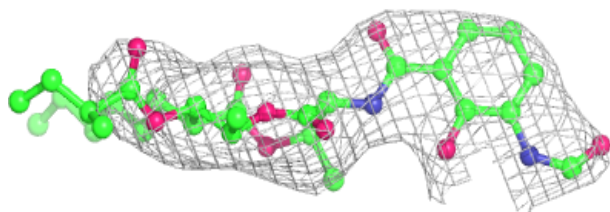
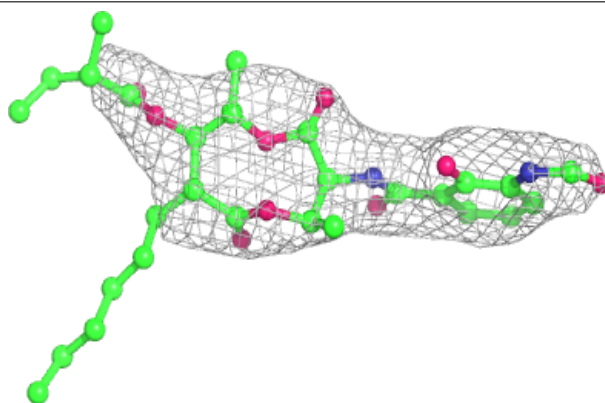


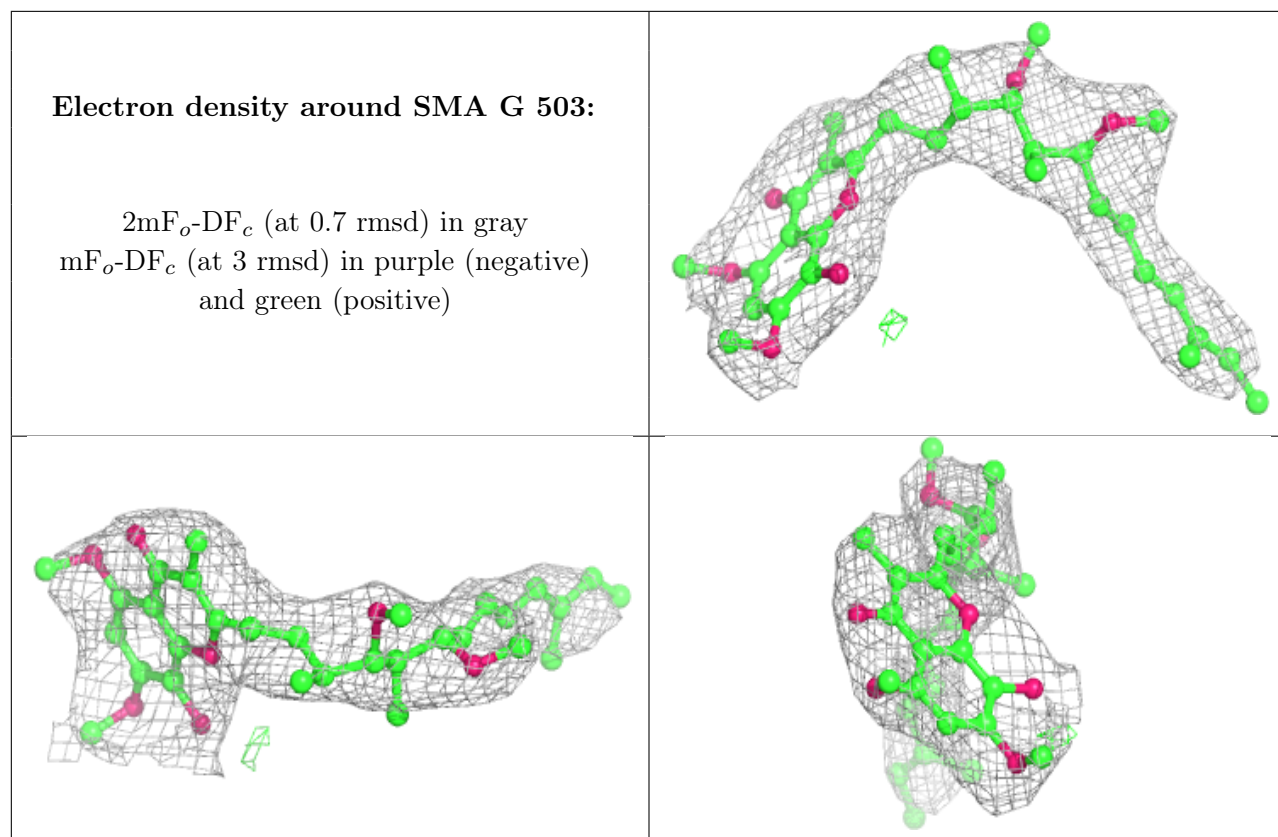
**Electron density around ANJ D 504:**

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

**Electron density around ANJ G 505:**

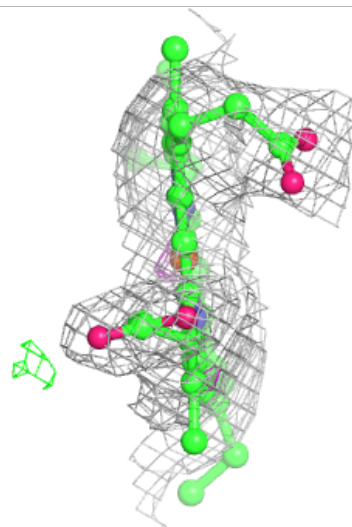
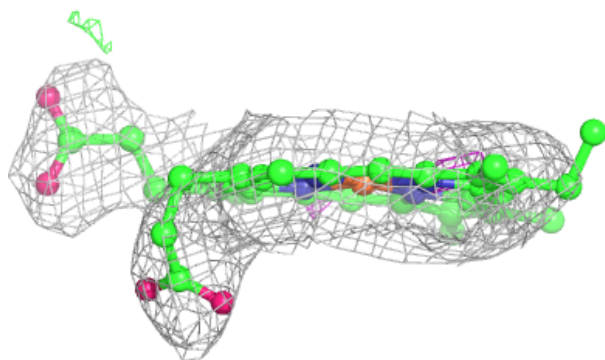
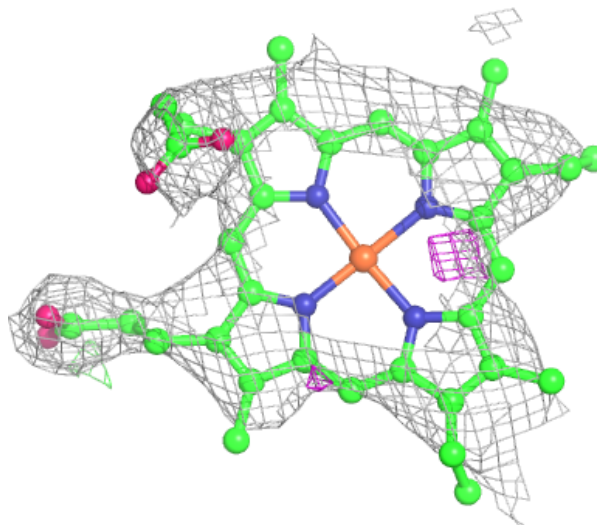
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM J 501:**

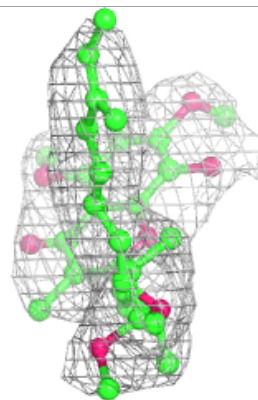
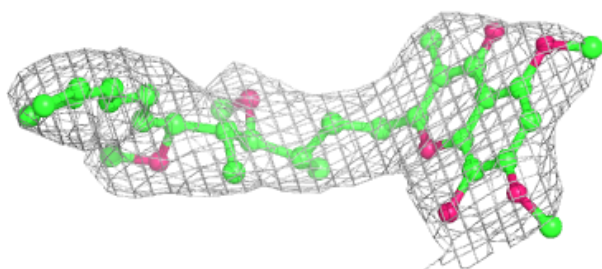
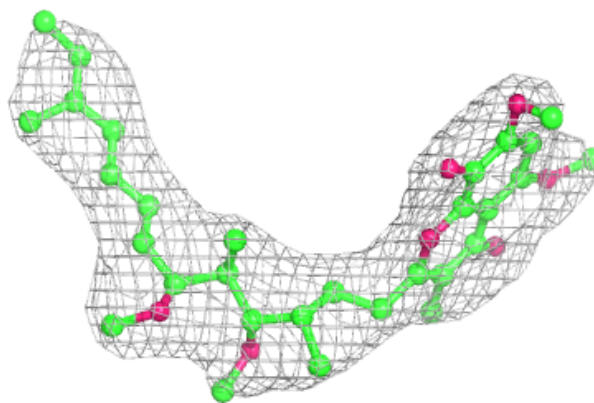
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





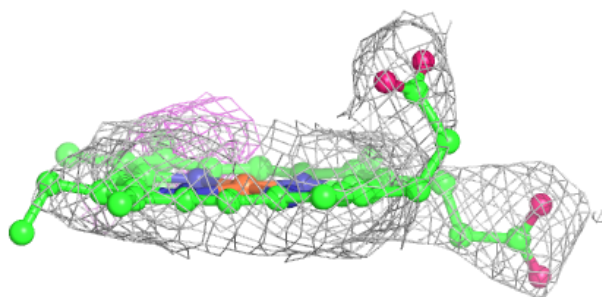
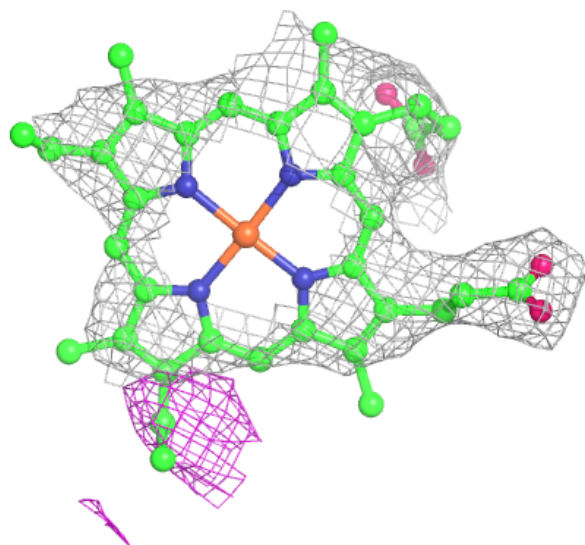
**Electron density around SMA D 2:**

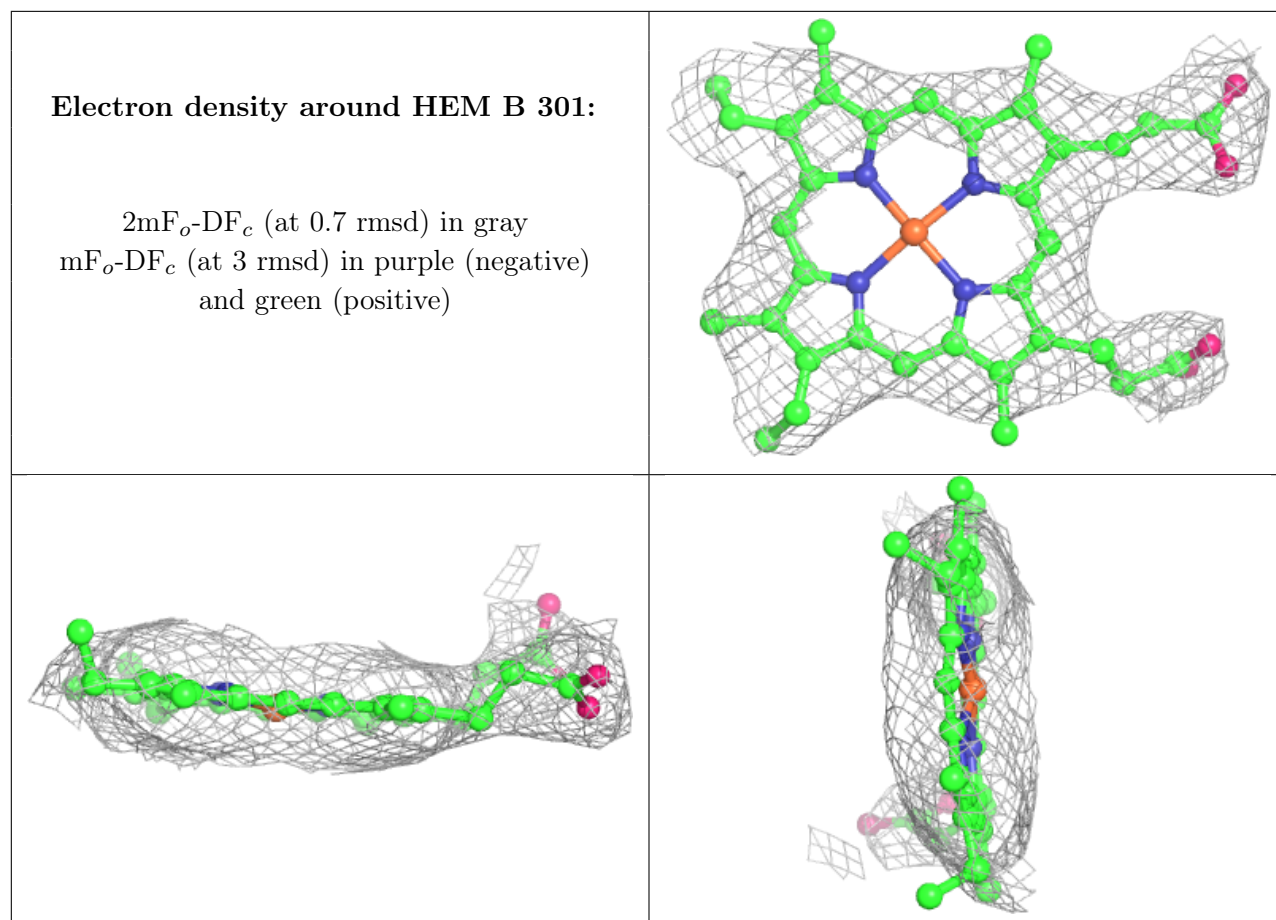
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM M 501:**

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

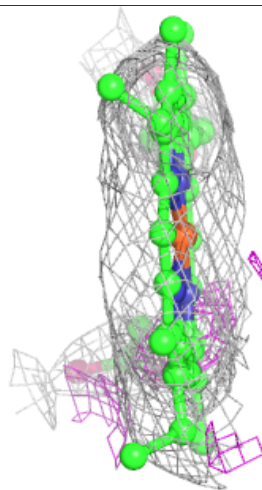
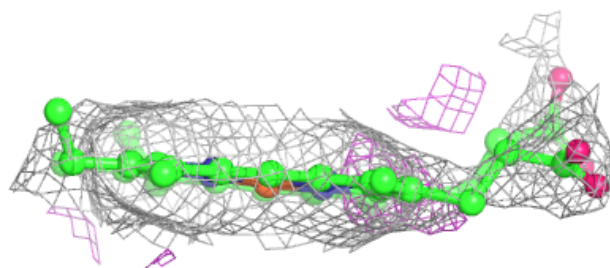
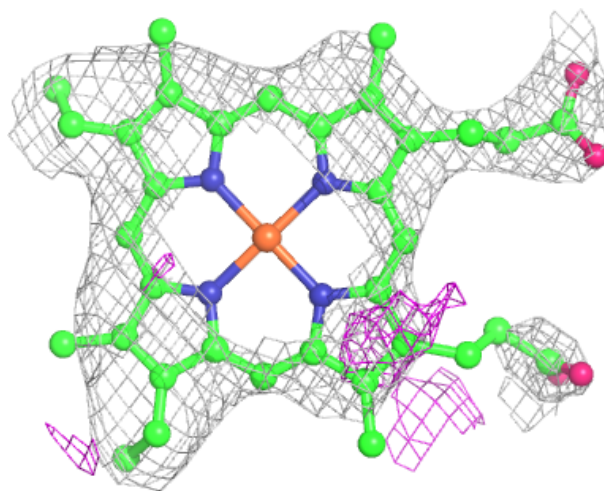






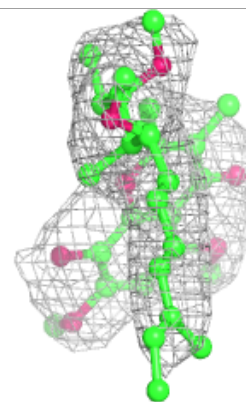
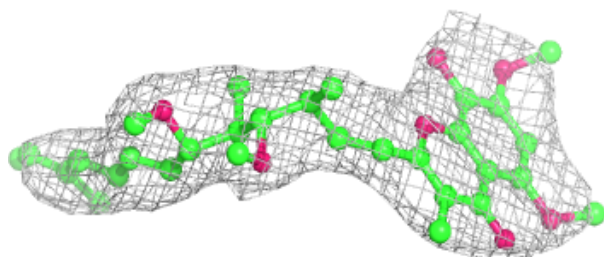
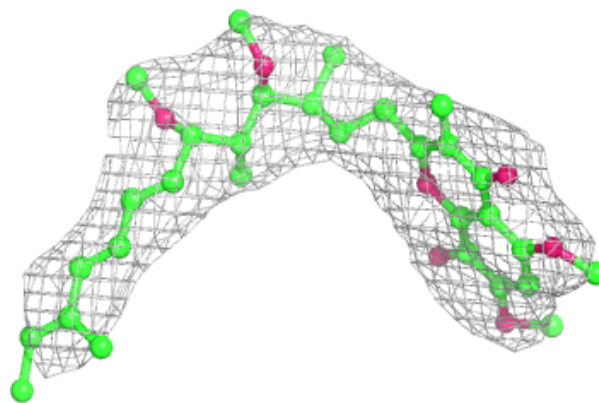
**Electron density around HEM Q 301:**

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

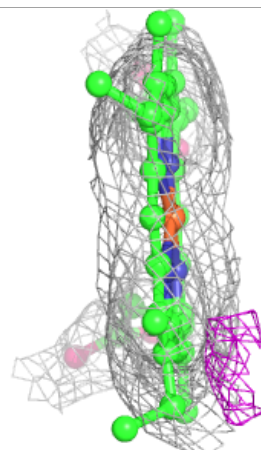
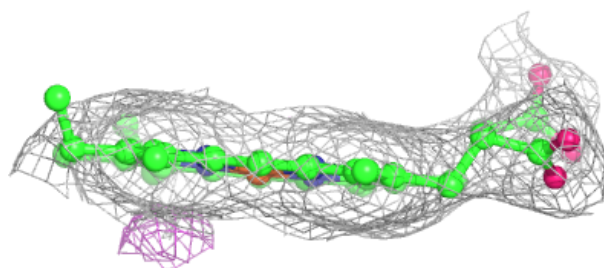
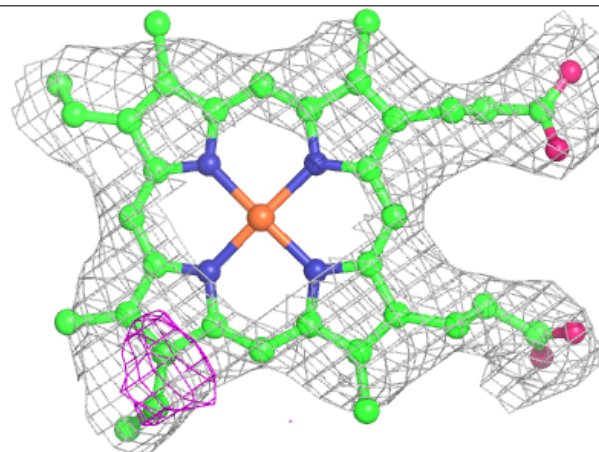


**Electron density around SMA P 503:**

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

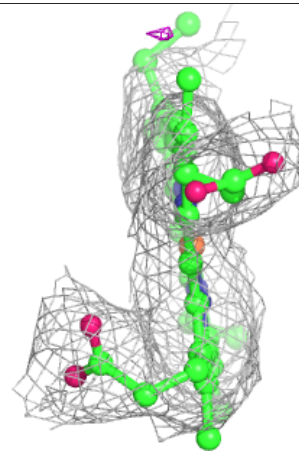
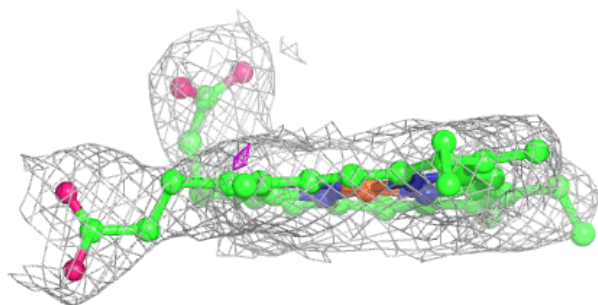
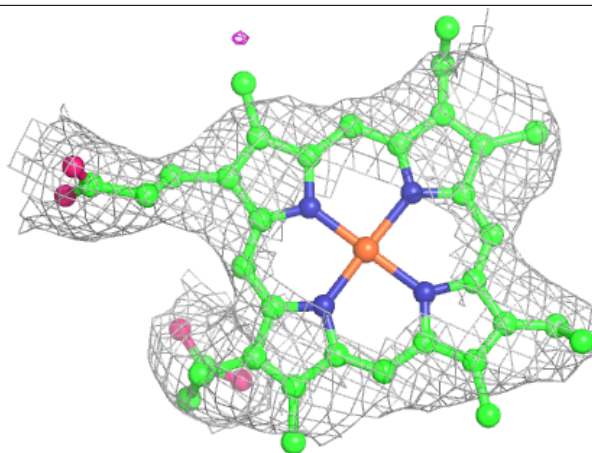
**Electron density around HEM H 301:**

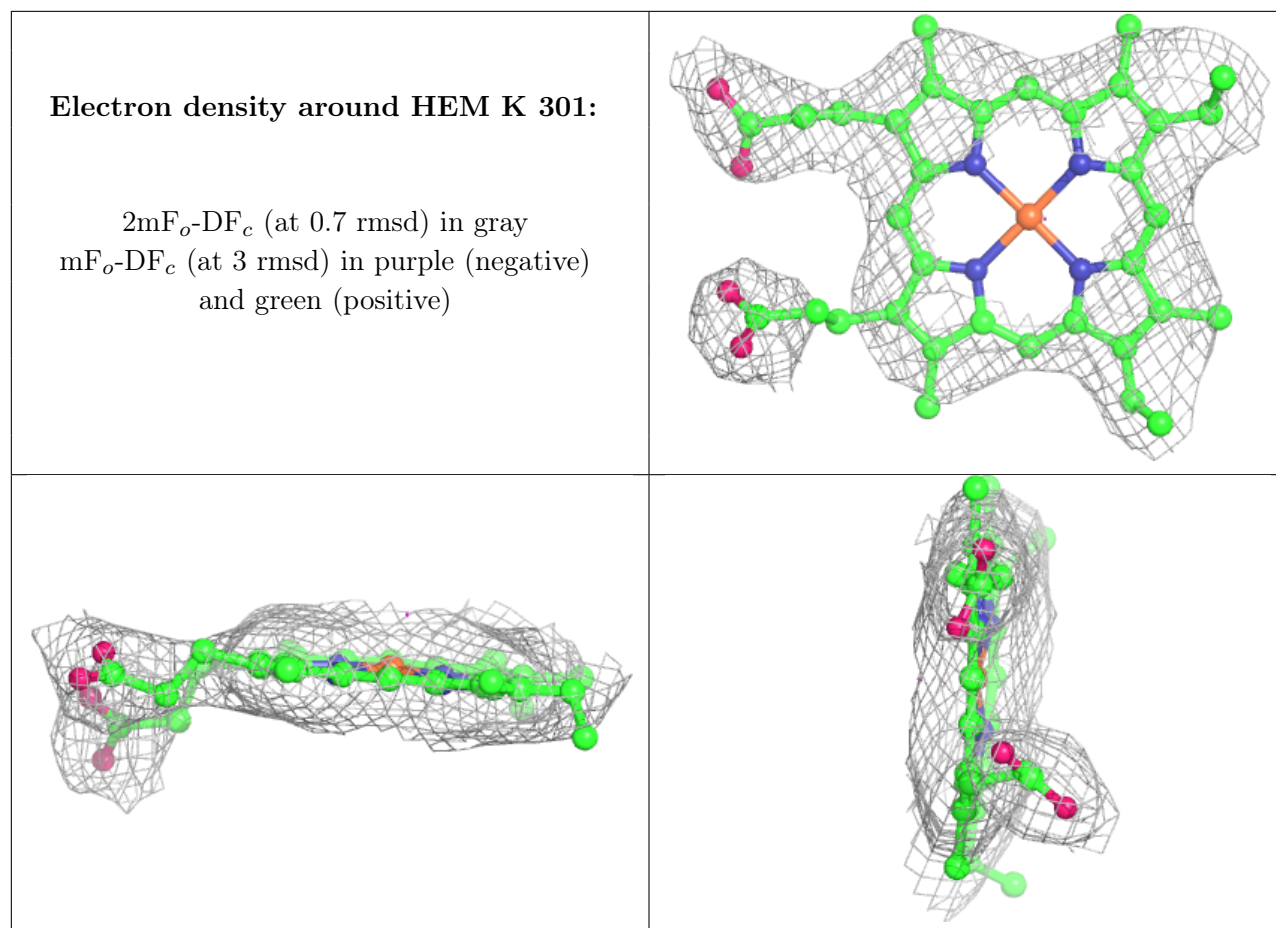
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 501:**

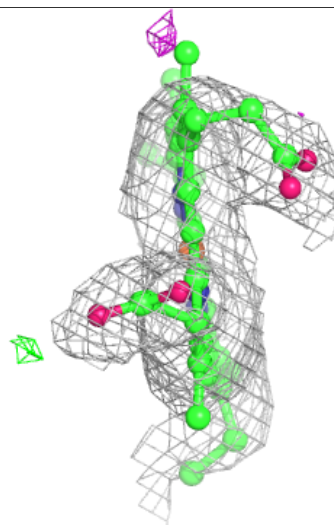
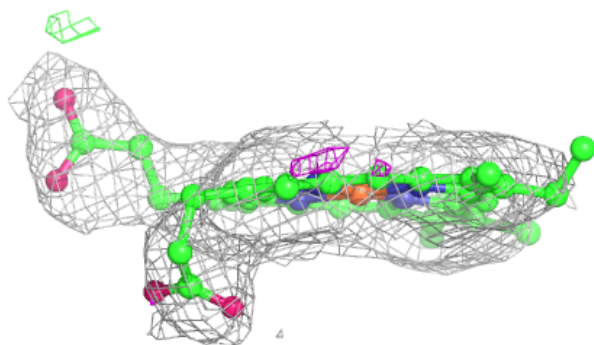
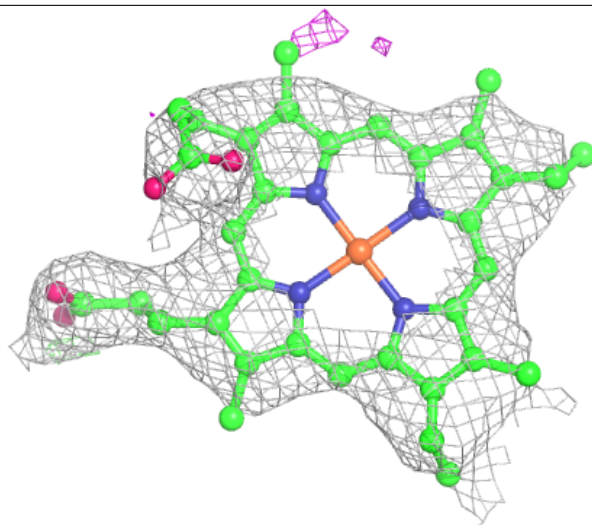
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM D 501:**

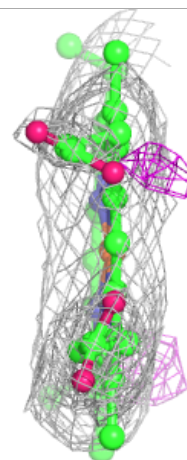
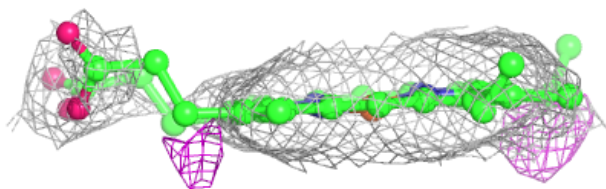
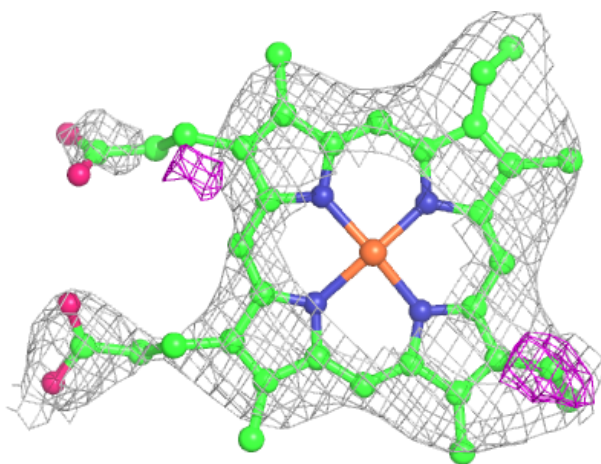
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

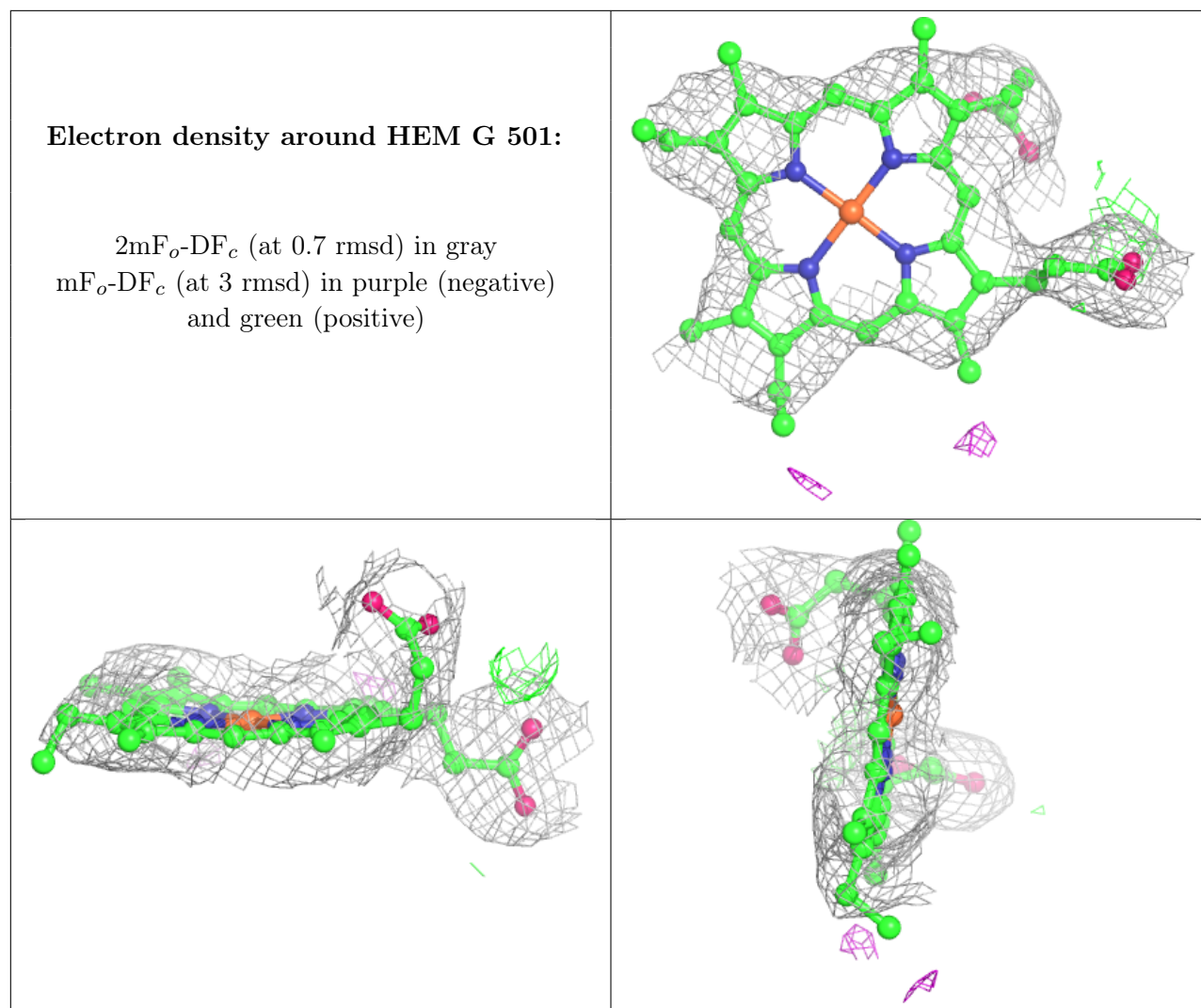




**Electron density around HEM E 301:**

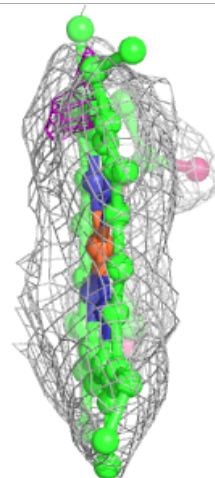
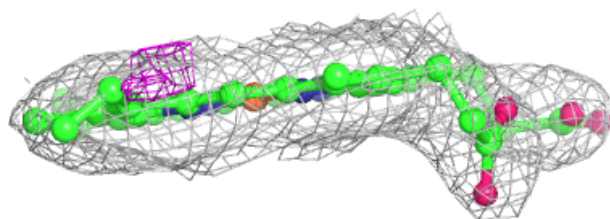
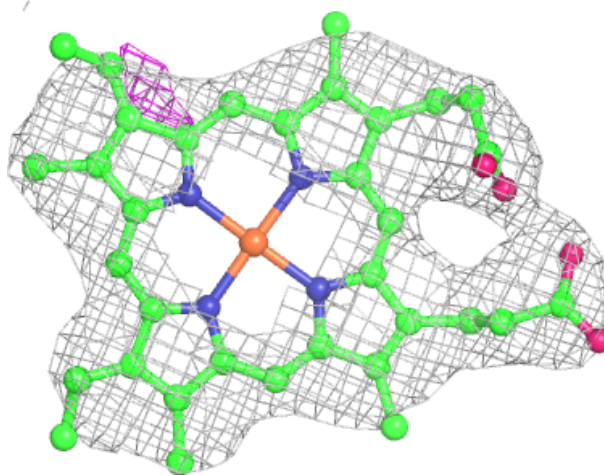
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM D 502:**

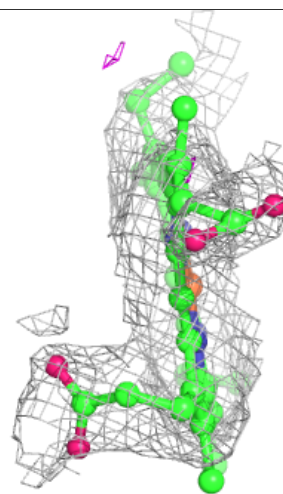
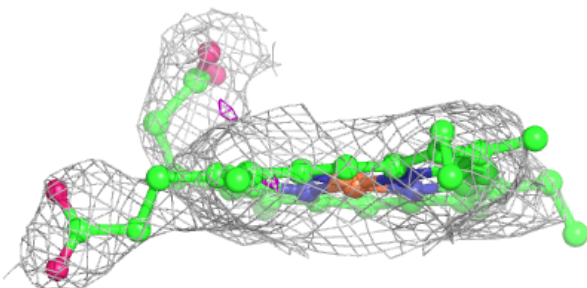
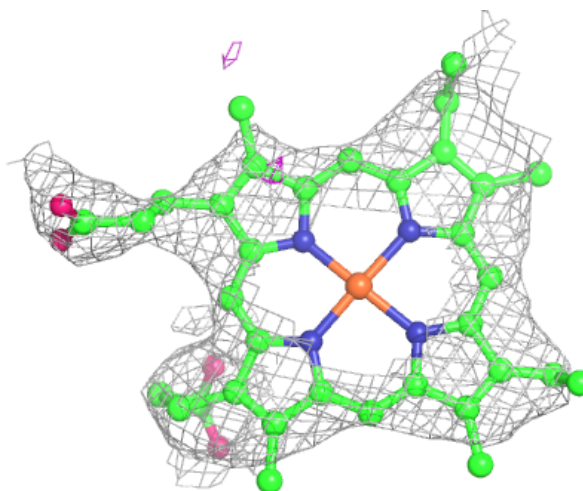
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





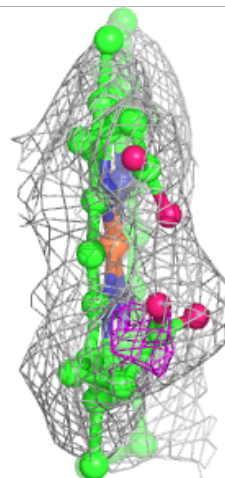
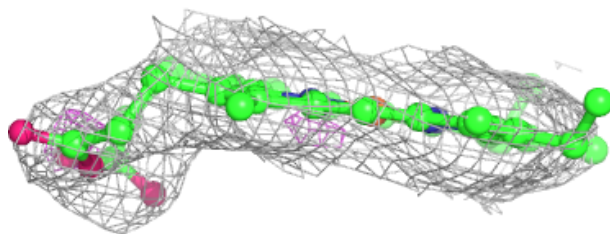
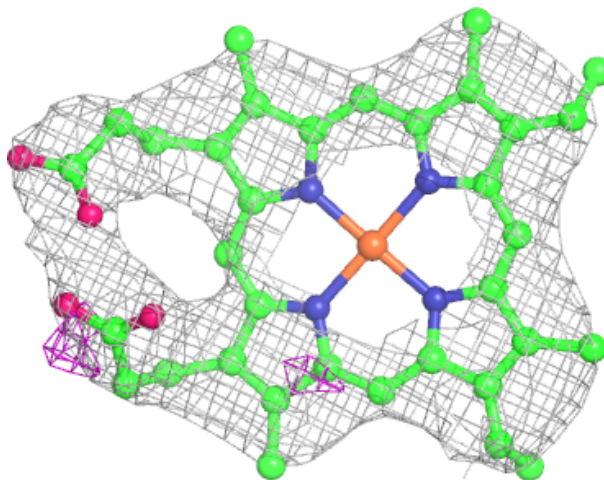
**Electron density around HEM P 501:**

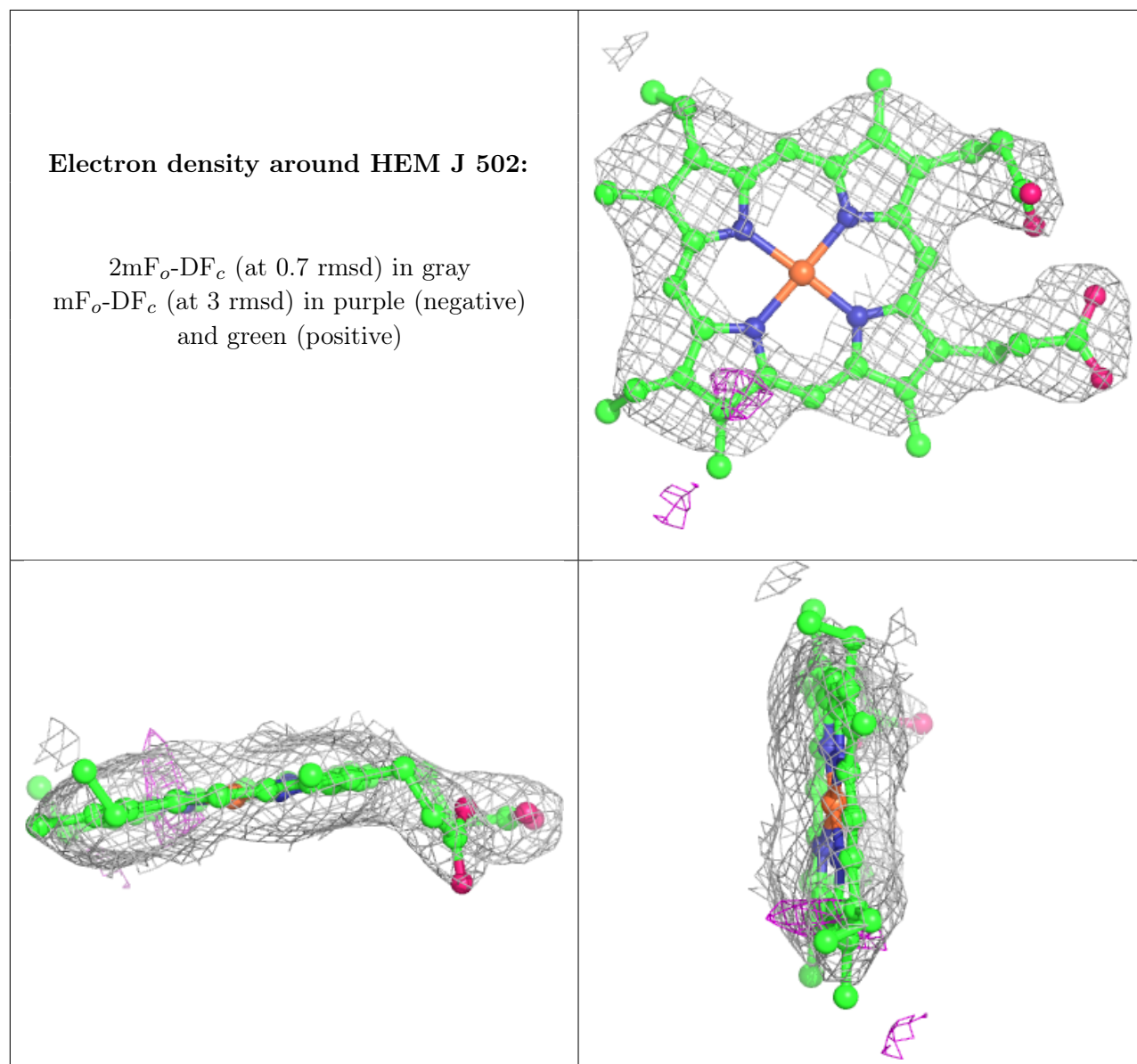
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM P 502:**

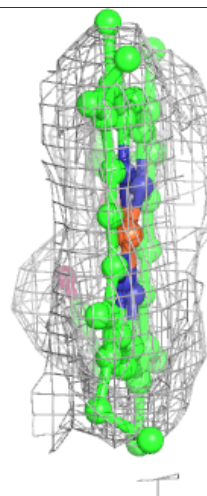
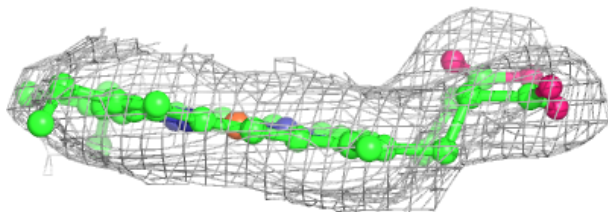
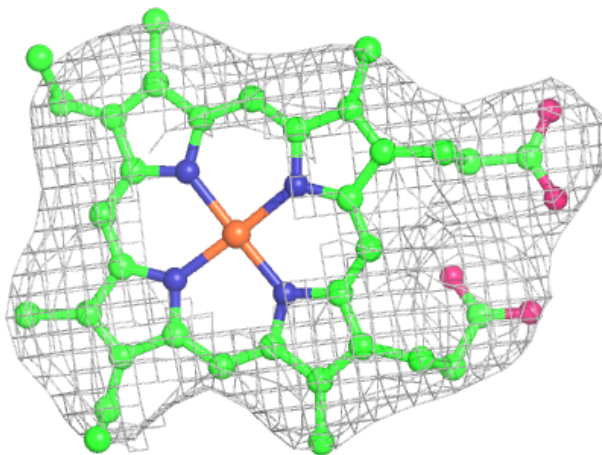
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





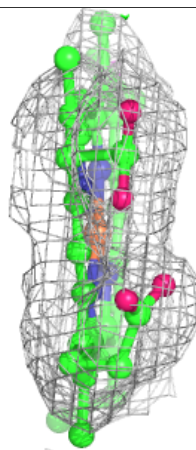
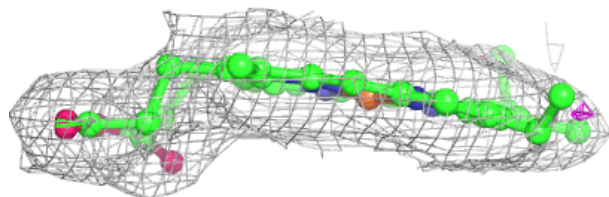
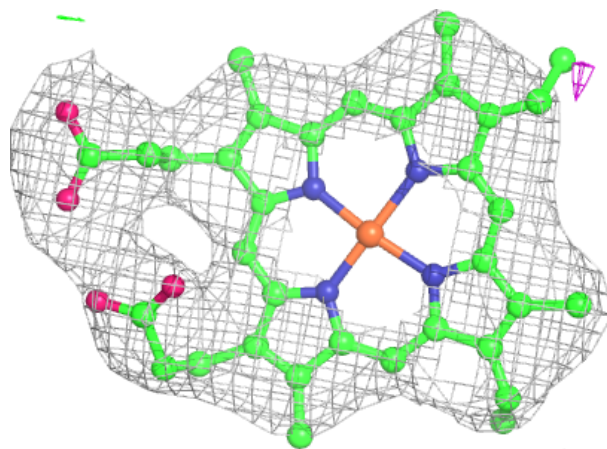
**Electron density around HEM G 502:**

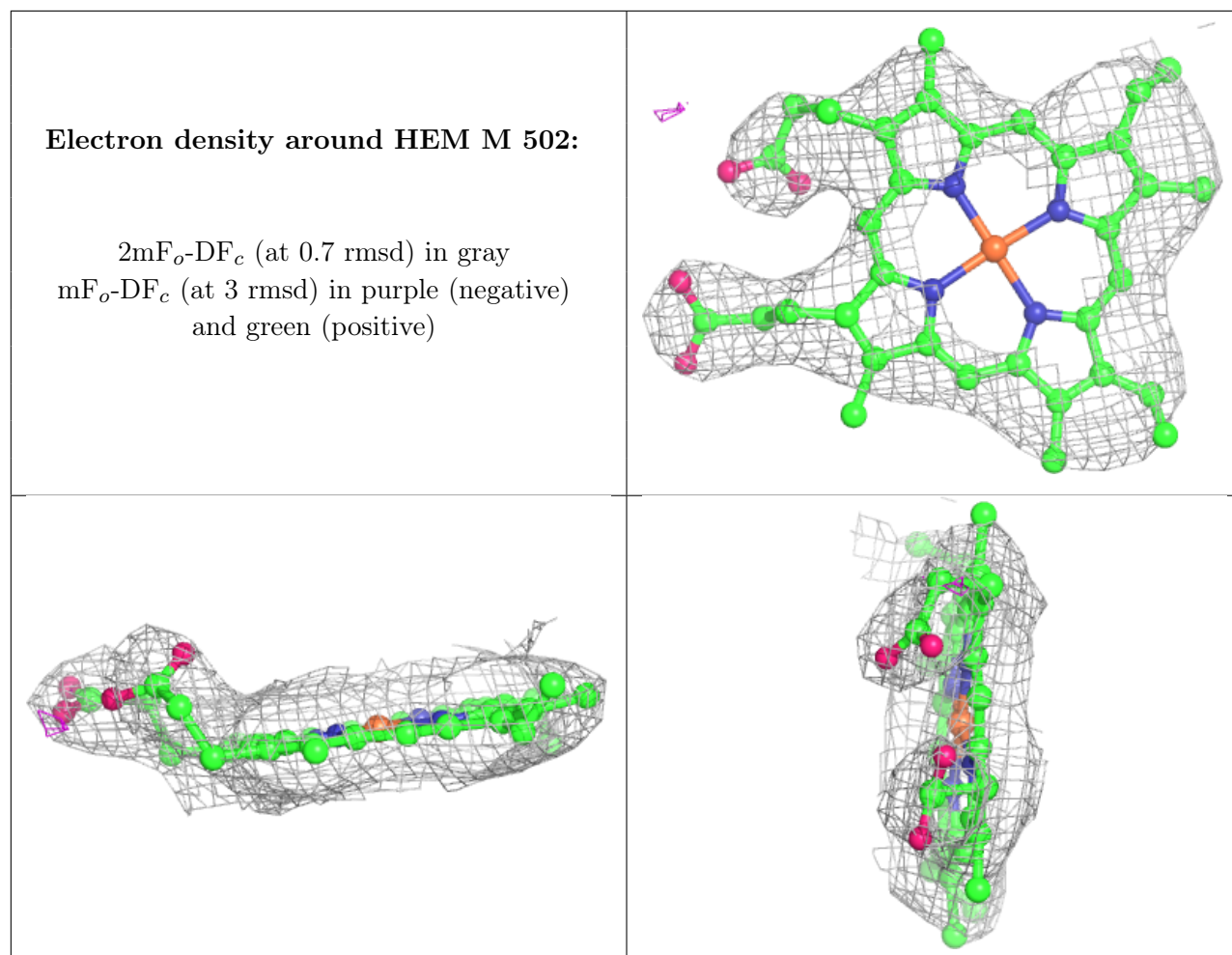
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 502:**

$2mF_o-DF_c$  (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.