



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 11:29 PM JST

PDB ID : 7Y44  
Title : Re-refinement of damage free X-ray structure of bovine cytochrome c oxidase at 1.9 angstrom resolution  
Authors : Tsukihara, T.; Hirata, K.; Ago, H.  
Deposited on : 2022-06-14  
Resolution : 1.90 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>.

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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 : 2.36  
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) : 2.36

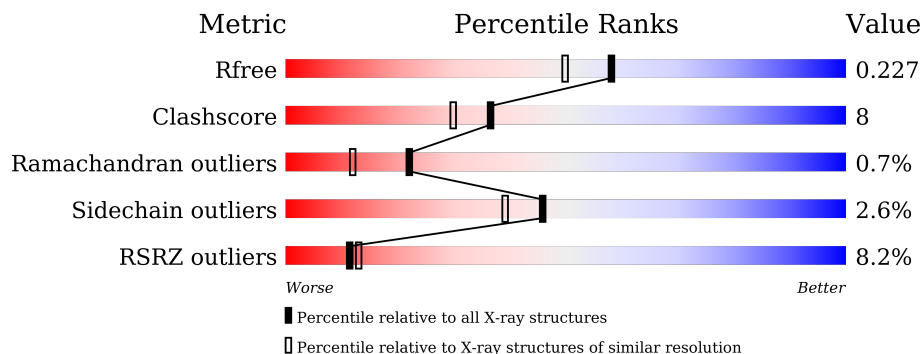
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	

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Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
20	EDO	A	612	-	-	X	-
20	EDO	N	613	-	-	X	-
20	EDO	S	107	-	-	X	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
21	DMU	A	616	-	-	-	X
21	DMU	B	306	-	-	-	X
21	DMU	D	202	-	-	-	X
21	DMU	K	102	-	-	-	X
21	DMU	K	103	-	-	-	X
21	DMU	K	105	-	-	-	X
21	DMU	X	101	-	-	-	X
26	CDL	C	304	-	-	X	-
26	CDL	G	101	-	-	X	-
27	CHD	W	101	-	-	-	X
27	CHD	X	105	-	-	-	X
7	TPO	G	11	-	-	-	X
9	SAC	V	1	-	-	-	X

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 34120 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	10	0
			4051	2710	623	681	37			
1	N	514	Total	C	N	O	S	0	7	0
			4046	2708	623	678	37			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	Total	C	N	O	S	0	3	0
			1834	1190	281	344	19			
2	O	227	Total	C	N	O	S	0	4	0
			1844	1200	283	342	19			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	Total	C	N	O	S	0	3	0
			2117	1416	336	350	15			
3	P	259	Total	C	N	O	S	0	2	0
			2115	1415	336	350	14			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	Total	C	N	O	S	0	1	0
			1201	783	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			860	549	147	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	1	0
			750	465	134	146	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

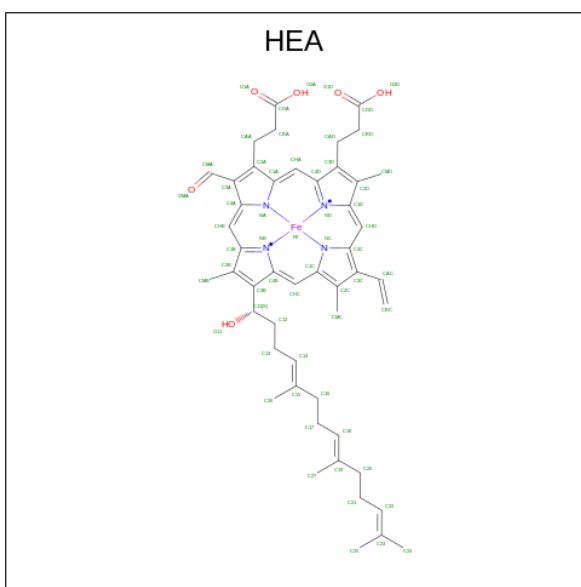
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			383	256	64	60	3			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	A	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

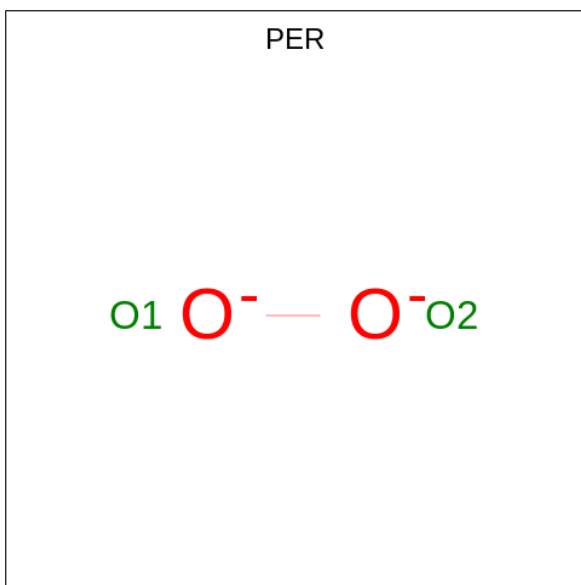
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).



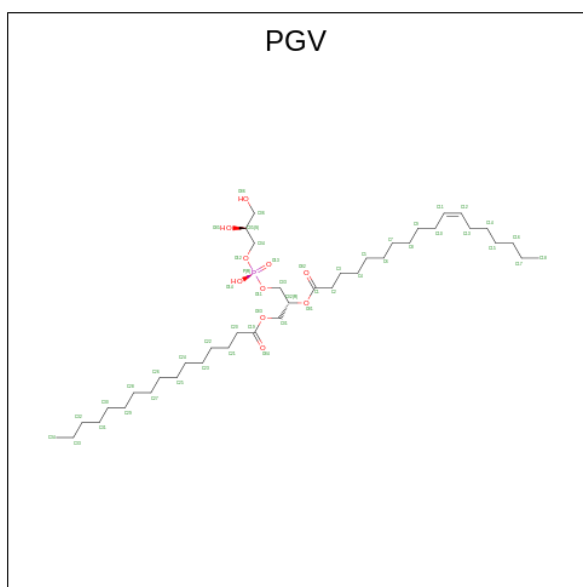
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



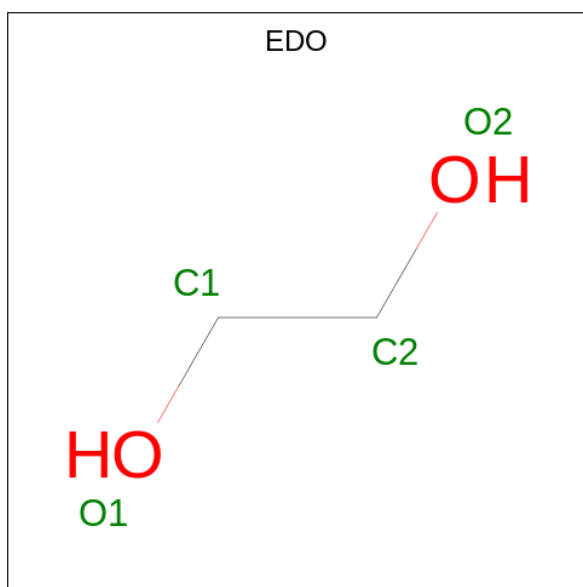
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			P
19	A	1	51	40	10	1	0	0
19	A	1	51	40	10	1	0	0
19	C	1	51	40	10	1	0	0
19	C	1	51	40	10	1	0	0
19	N	1	51	40	10	1	0	0
19	P	1	51	40	10	1	0	0
19	P	1	51	40	10	1	0	0
19	P	1	51	40	10	1	0	0

- Molecule 20 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	A	1	Total C O 4 2 2	0	0
20	B	1	Total C O 4 2 2	0	0
20	B	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	C	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0

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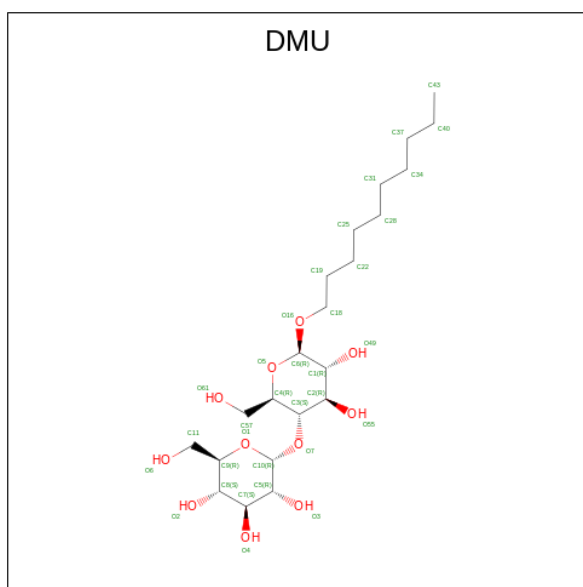
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	F	1	Total	C	O	0	0
			4	2	2		
20	G	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	O	1	Total	C	O	0	0
			4	2	2		
20	O	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	Y	1	Total 4	C 2	O 2	0	0

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



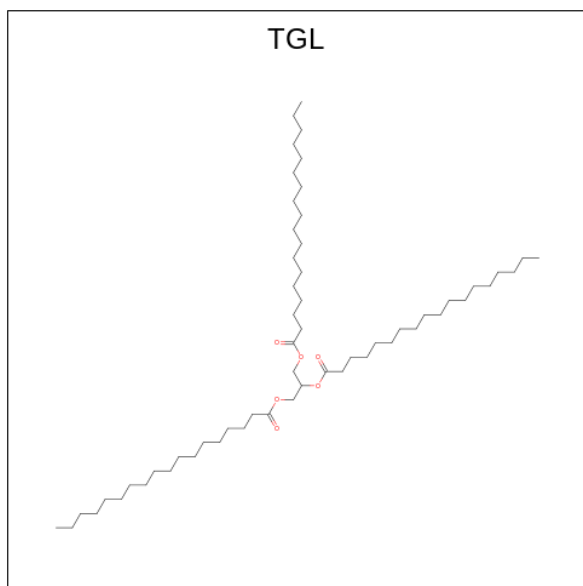
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			33	22	11		
21	B	1	Total	C	O	0	0
			33	22	11		
21	C	1	Total	C	O	0	0
			33	22	11		
21	D	1	Total	C	O	0	0
			33	22	11		
21	G	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	L	1	Total	C	O	0	0
			33	22	11		
21	M	1	Total	C	O	0	0
			33	22	11		
21	O	1	Total	C	O	0	0
			33	22	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P	1	Total	C	O	0	0
			33	22	11		
21	P	1	Total	C	O	0	0
			33	22	11		
21	Q	1	Total	C	O	0	0
			33	22	11		
21	T	1	Total	C	O	0	0
			33	22	11		
21	X	1	Total	C	O	0	0
			33	22	11		
21	X	1	Total	C	O	0	0
			22	16	6		
21	X	1	Total	C	O	0	0
			22	16	6		
21	X	1	Total	C	O	0	0
			22	16	6		
21	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula:  $C_{57}H_{110}O_6$ ).



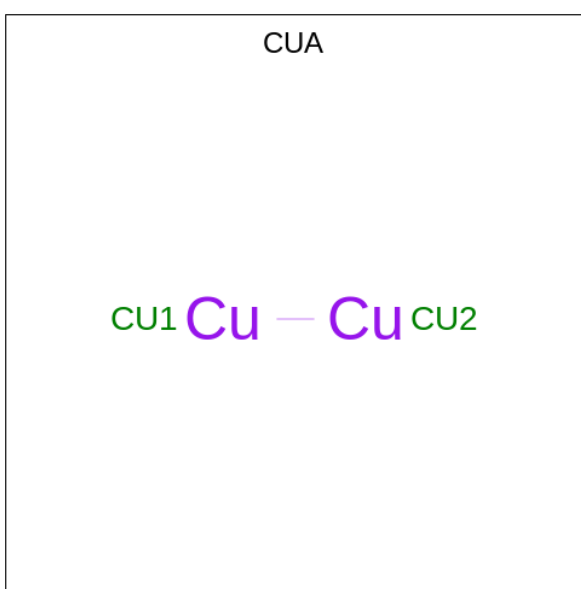
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		
22	D	1	Total	C	O	0	0
			63	57	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	L	1	Total	C	O	0	0
			63	57	6		
22	O	1	Total	C	O	0	0
			63	57	6		
22	Q	1	Total	C	O	0	0
			63	57	6		
22	Y	1	Total	C	O	0	0
			63	57	6		

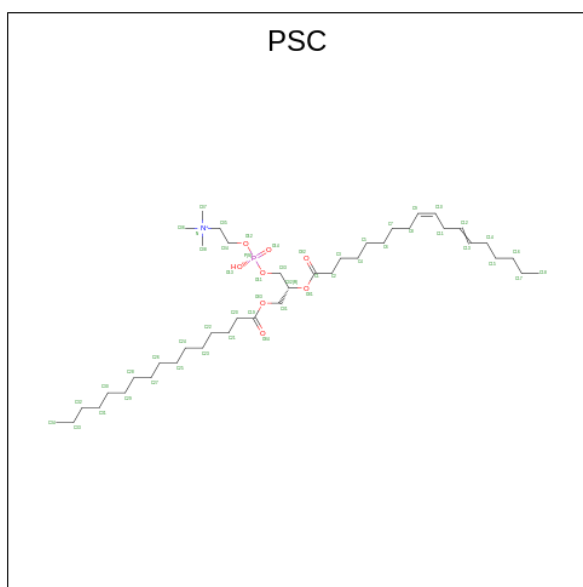
- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

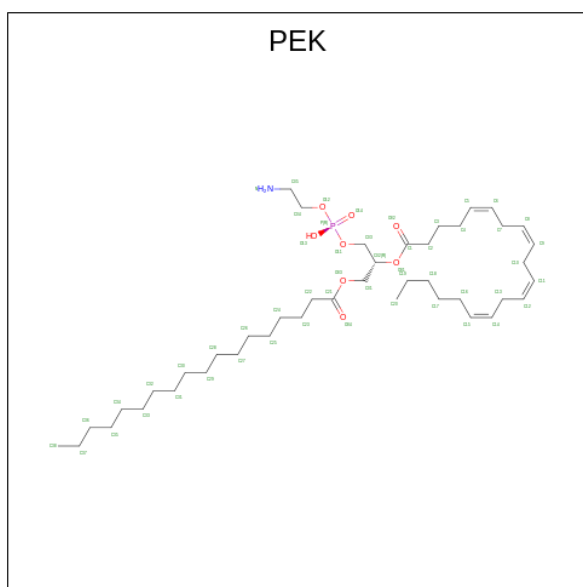
- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	B	1	52	42	1	8	1	0	0
24	N	1	52	42	1	8	1	0	0

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



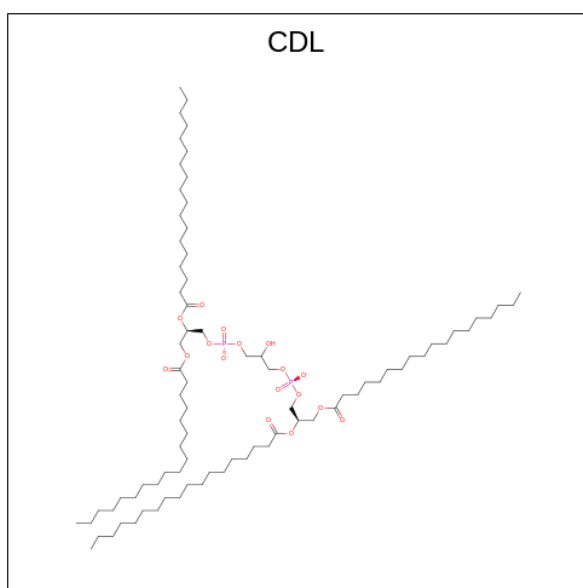
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
25	C	1	53	43	1	8	1	0	0

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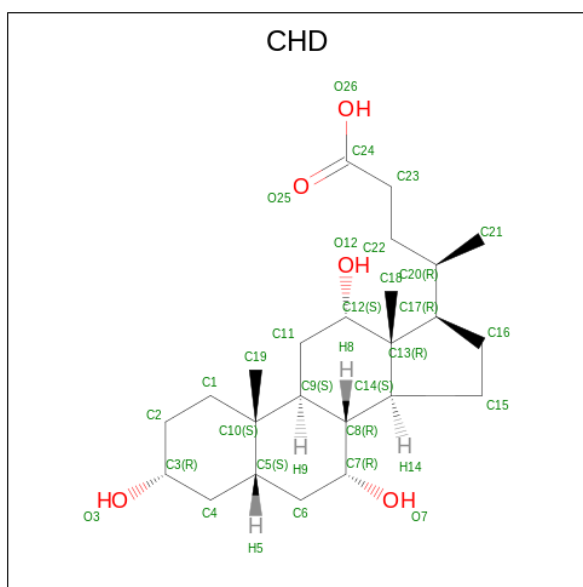
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 29 24 5	0	0
27	C	1	Total C O 29 24 5	0	0
27	G	1	Total C O 29 24 5	0	0
27	J	1	Total C O 29 24 5	0	0
27	L	1	Total C O 29 24 5	0	0
27	P	1	Total C O 29 24 5	0	0
27	P	1	Total C O 29 24 5	0	0
27	T	1	Total C O 29 24 5	0	0
27	W	1	Total C O 29 24 5	0	0
27	X	1	Total C O 29 24 5	0	0
27	Y	1	Total C O 29 24 5	0	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

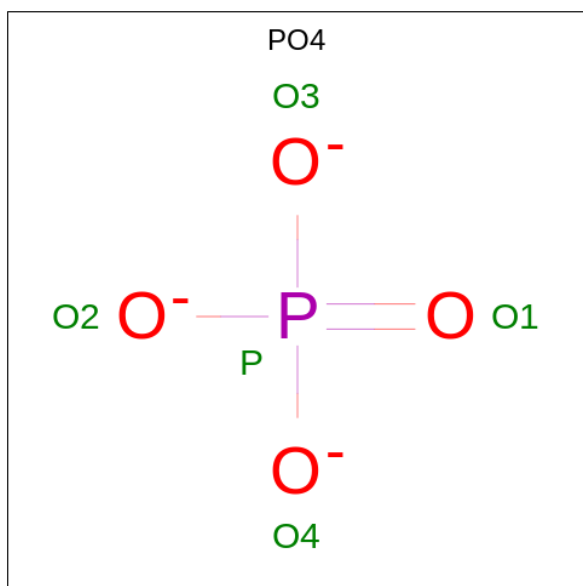
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	F	1	Total Zn 1 1	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	S	1	Total	Zn	0	0
			1	1		

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	H	1	Total	O	P	0	0
			5	4	1		
29	U	1	Total	O	P	0	0
			5	4	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	263	Total	O	0	0
			263	263		
30	B	176	Total	O	0	2
			176	176		
30	C	128	Total	O	0	0
			128	128		
30	D	154	Total	O	0	0
			154	154		
30	E	124	Total	O	0	0
			124	124		
30	F	114	Total	O	0	0
			114	114		

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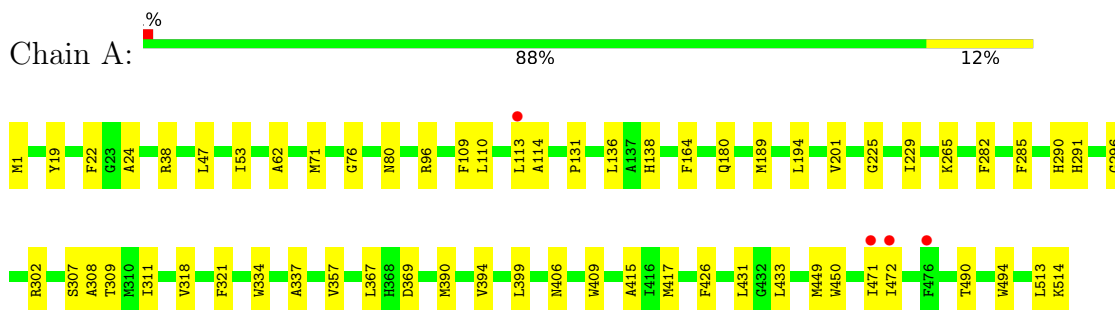
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	G	69	Total O 69 69	0	0
30	H	69	Total O 69 69	0	0
30	I	60	Total O 60 60	0	0
30	J	33	Total O 33 33	0	0
30	K	32	Total O 32 32	0	0
30	L	31	Total O 31 31	0	0
30	M	29	Total O 29 29	0	0
30	N	239	Total O 239 239	0	0
30	O	154	Total O 154 154	0	0
30	P	131	Total O 131 131	0	0
30	Q	91	Total O 91 91	0	0
30	R	93	Total O 93 93	0	0
30	S	108	Total O 108 108	0	0
30	T	61	Total O 61 61	0	0
30	U	50	Total O 50 50	0	0
30	V	41	Total O 41 41	0	0
30	W	39	Total O 39 39	0	0
30	X	31	Total O 31 31	0	0
30	Y	31	Total O 31 31	0	0
30	Z	24	Total O 24 24	0	0

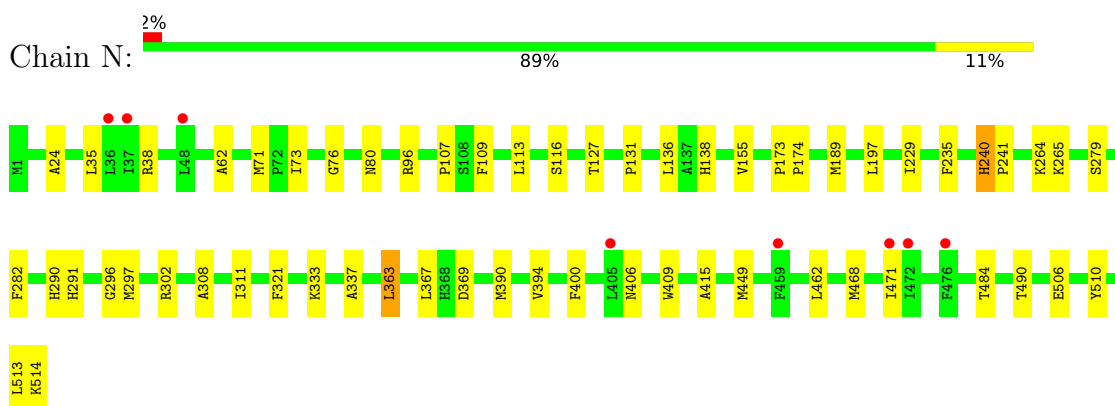
### 3 Residue-property plots [i](#)

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.

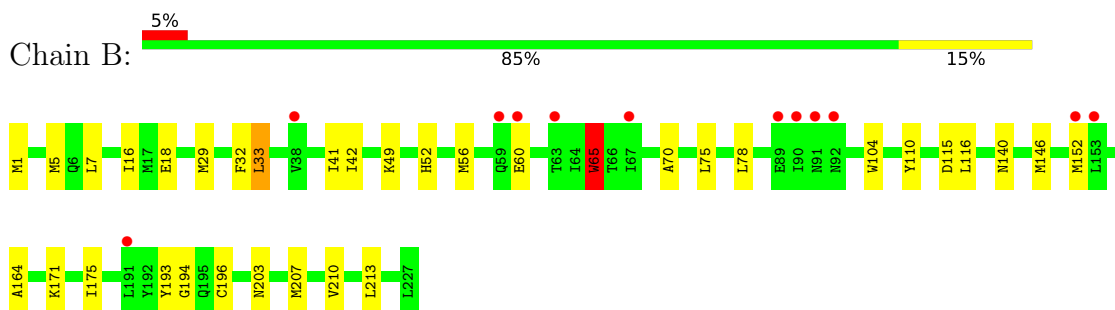
- Molecule 1: Cytochrome c oxidase subunit 1



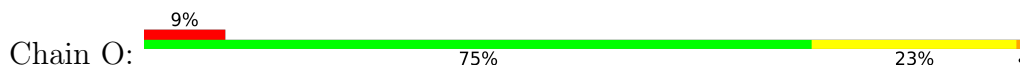
- Molecule 1: Cytochrome c oxidase subunit 1

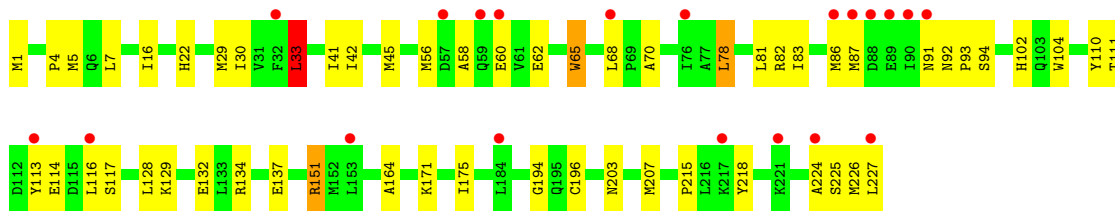


- Molecule 2: Cytochrome c oxidase subunit 2

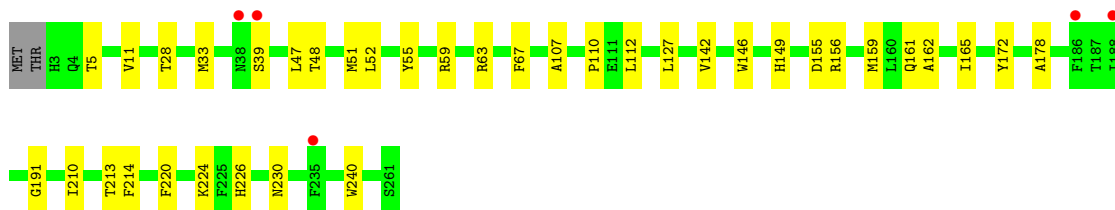
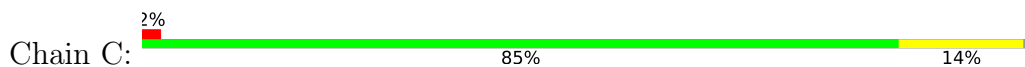


- Molecule 2: Cytochrome c oxidase subunit 2

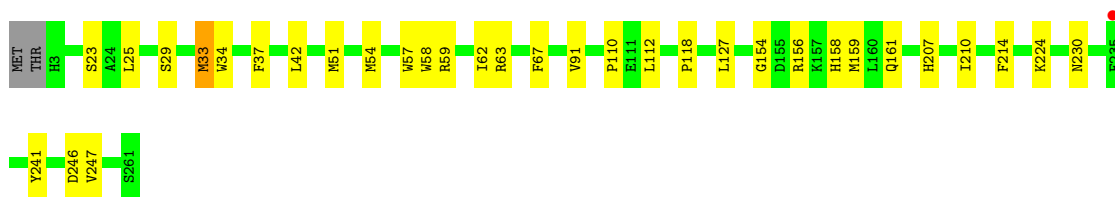
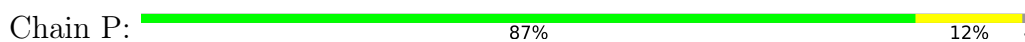




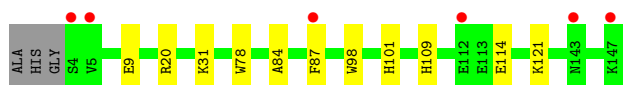
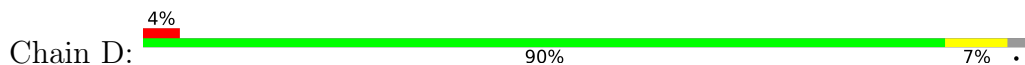
● Molecule 3: Cytochrome c oxidase subunit 3



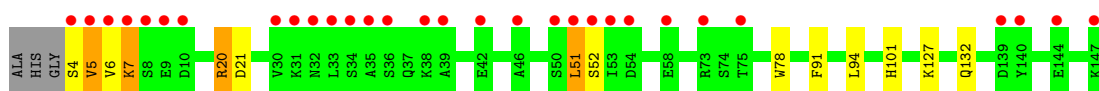
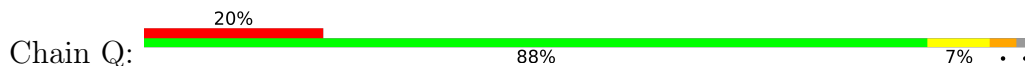
● Molecule 3: Cytochrome c oxidase subunit 3



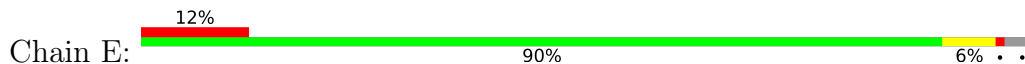
● Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



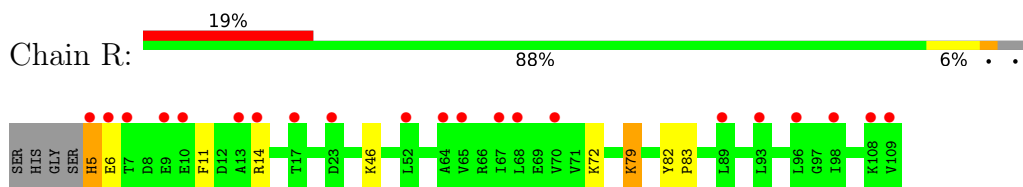
● Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



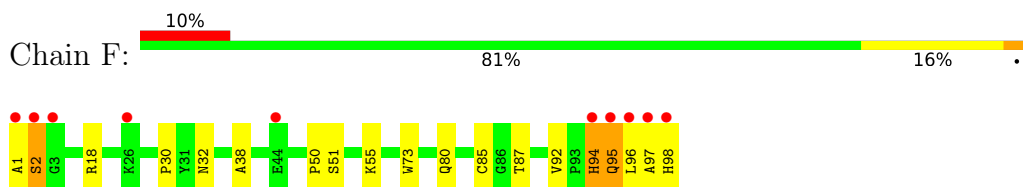
● Molecule 5: Cytochrome c oxidase subunit 5A



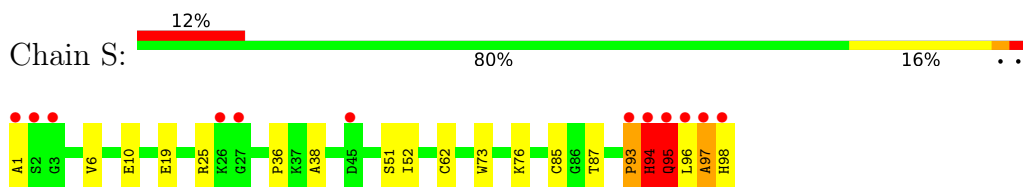
- Molecule 5: Cytochrome c oxidase subunit 5A



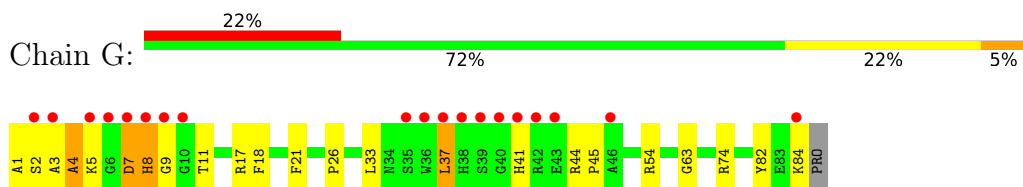
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



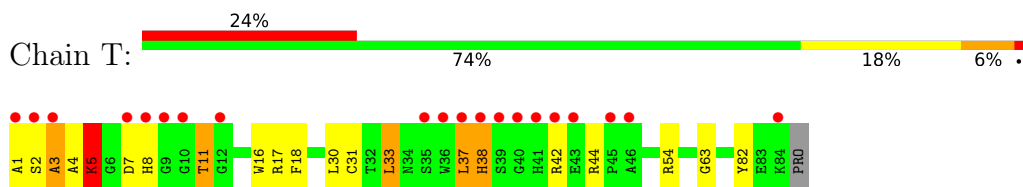
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



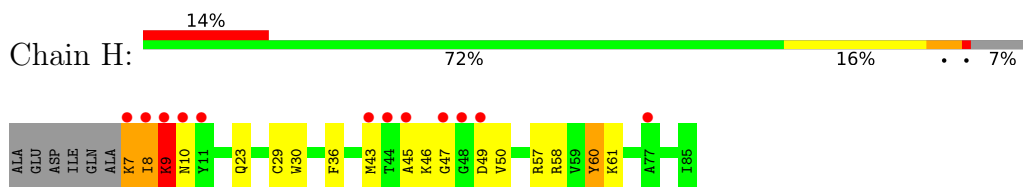
- Molecule 7: Cytochrome c oxidase subunit 6A2



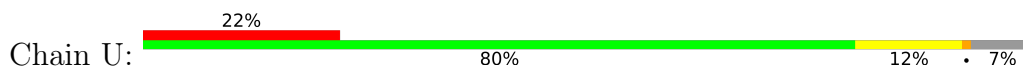
- Molecule 7: Cytochrome c oxidase subunit 6A2



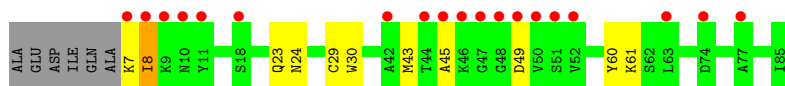
- Molecule 8: Cytochrome c oxidase subunit 6B1



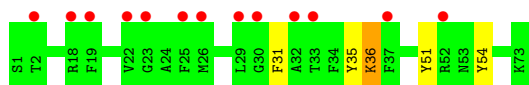
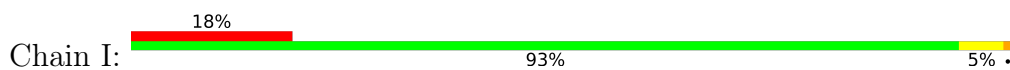
- Molecule 8: Cytochrome c oxidase subunit 6B1



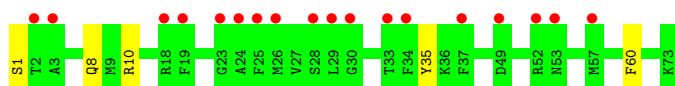




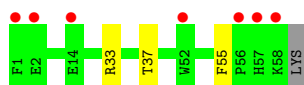
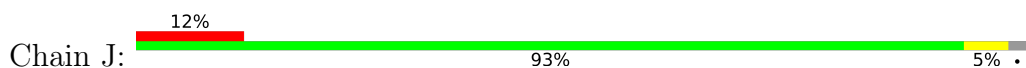
- Molecule 9: Cytochrome c oxidase subunit 6C



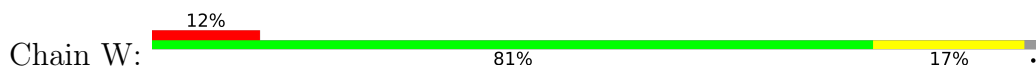
- Molecule 9: Cytochrome c oxidase subunit 6C



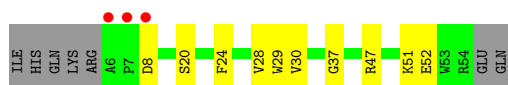
- Molecule 10: Cytochrome c oxidase subunit 7A1



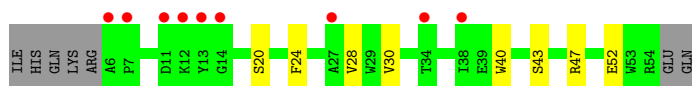
- Molecule 10: Cytochrome c oxidase subunit 7A1



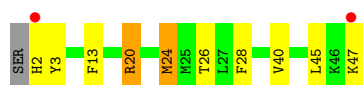
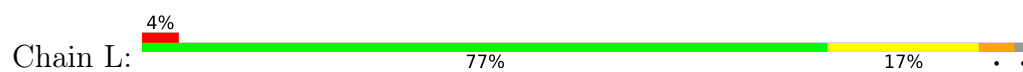
- Molecule 11: Cytochrome c oxidase subunit 7B



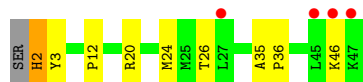
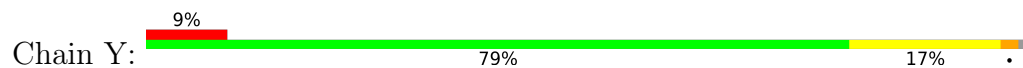
- Molecule 11: Cytochrome c oxidase subunit 7B



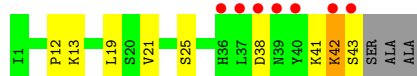
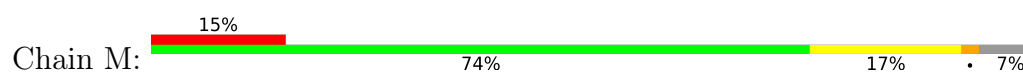
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



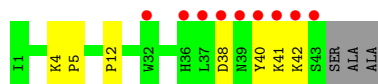
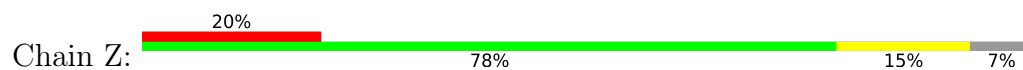
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.60Å 204.51Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.31 – 1.90 27.31 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.0 (27.31-1.90) 95.3 (27.31-1.89)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 1.89Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.185 , 0.227 0.185 , 0.227	Depositor DCC
$R_{free}$ test set	25229 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 79.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: PSC, CU, PGV, CHD, PER, DMU, CDL, EDO, CUA, MG, FME, NA, PEK, HEA, TGL, PO4, TPO, SAC, ZN

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	0.99	2/4233 (0.0%)	0.81	3/5782 (0.1%)
1	N	0.93	1/4211 (0.0%)	0.81	3/5752 (0.1%)
2	B	0.85	0/1885	0.86	3/2567 (0.1%)
2	O	0.75	0/1900	0.81	4/2587 (0.2%)
3	C	0.91	3/2221 (0.1%)	0.71	0/3035
3	P	0.86	0/2213	0.72	0/3025
4	D	0.83	0/1241	0.73	1/1674 (0.1%)
4	Q	0.60	0/1229	0.64	1/1658 (0.1%)
5	E	0.83	0/871	0.74	1/1182 (0.1%)
5	R	0.70	0/882	0.75	0/1196
6	F	0.76	0/772	0.84	1/1048 (0.1%)
6	S	0.74	0/765	0.84	1/1038 (0.1%)
7	G	0.76	0/690	0.76	0/937
7	T	0.64	0/690	0.74	0/937
8	H	0.78	0/682	0.73	1/921 (0.1%)
8	U	0.64	0/682	0.69	0/921
9	I	0.67	0/605	0.74	0/802
9	V	0.54	0/605	0.65	0/802
10	J	0.57	0/471	0.69	0/636
10	W	0.63	0/471	0.68	0/636
11	K	0.68	0/398	0.65	1/546 (0.2%)
11	X	0.51	0/398	0.58	0/546
12	L	0.81	0/401	0.80	1/536 (0.2%)
12	Y	0.71	0/393	0.61	0/526
13	M	0.74	0/345	0.70	0/470
13	Z	0.58	0/345	0.58	0/470
All	All	0.82	6/29599 (0.0%)	0.76	21/40230 (0.1%)

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	N	0	1
6	F	0	1
6	S	0	2
8	H	0	1
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	VAL	CB-CG1	6.74	1.67	1.52
3	C	142	VAL	CB-CG2	6.33	1.66	1.52
3	C	11	VAL	CB-CG2	5.73	1.64	1.52
1	A	357	VAL	CB-CG1	5.29	1.64	1.52
3	C	172	TYR	CD2-CE2	5.16	1.47	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	N	71	MET	CG-SD-CE	-6.93	89.11	100.20
8	H	58	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	N	38	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	O	151	ARG	NE-CZ-NH1	6.80	123.70	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	94	HIS	Peptide
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide

## 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	4051	0	4040	50	0
1	N	4046	0	4040	45	0
2	B	1834	0	1840	28	0
2	O	1844	0	1852	41	0
3	C	2117	0	2034	38	0
3	P	2115	0	2033	42	0
4	D	1201	0	1188	13	0
4	Q	1195	0	1183	16	0
5	E	852	0	845	4	0
5	R	860	0	858	6	0
6	F	750	0	731	20	0
6	S	748	0	728	21	0
7	G	675	0	643	17	0
7	T	675	0	643	21	0
8	H	662	0	623	11	0
8	U	662	0	623	9	0
9	I	601	0	613	4	0
9	V	601	0	613	4	0
10	J	460	0	459	5	0
10	W	460	0	459	6	0
11	K	384	0	366	8	0
11	X	384	0	366	9	0
12	L	383	0	389	15	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0
13	Z	335	0	352	6	0
14	A	129	0	88	4	0
14	N	129	0	88	4	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	102	0	152	9	0
19	C	102	0	152	5	0
19	N	51	0	76	6	0
19	P	153	0	228	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	28	0	42	5	0
20	B	8	0	12	0	0
20	C	8	0	12	1	0
20	F	16	0	24	0	0
20	G	4	0	6	0	0
20	L	8	0	12	0	0
20	M	4	0	6	1	0
20	N	48	0	72	9	0
20	O	8	0	12	0	0
20	P	20	0	30	1	0
20	Q	4	0	6	1	0
20	R	4	0	6	0	0
20	S	24	0	36	5	0
20	W	8	0	12	5	0
20	Y	4	0	6	1	0
21	A	33	0	42	1	0
21	B	33	0	41	0	0
21	C	33	0	42	0	0
21	D	33	0	42	1	0
21	G	33	0	42	1	0
21	K	198	0	252	12	0
21	L	33	0	42	3	0
21	M	33	0	42	1	0
21	O	33	0	42	2	0
21	P	66	0	84	10	0
21	Q	33	0	41	1	0
21	T	33	0	42	2	0
21	X	99	0	135	4	0
21	Z	33	0	42	0	0
22	B	63	0	110	6	0
22	D	63	0	110	10	0
22	L	63	0	108	12	0
22	O	63	0	110	1	0
22	Q	63	0	110	6	0
22	Y	63	0	110	7	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	9	0
24	N	52	0	80	12	0
25	C	159	0	231	20	0
25	G	53	0	77	4	0
25	P	106	0	154	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C	100	0	156	23	0
26	G	100	0	156	21	0
26	P	100	0	156	18	0
26	T	100	0	156	19	0
27	C	58	0	78	1	0
27	G	29	0	39	0	0
27	J	29	0	39	4	0
27	L	29	0	39	1	0
27	P	58	0	78	3	0
27	T	29	0	39	0	0
27	W	29	0	38	1	0
27	X	29	0	39	5	0
27	Y	29	0	39	3	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	263	0	0	2	0
30	B	176	0	0	2	0
30	C	128	0	0	2	0
30	D	154	0	0	2	0
30	E	124	0	0	1	0
30	F	114	0	0	1	0
30	G	69	0	0	4	0
30	H	69	0	0	1	0
30	I	60	0	0	0	0
30	J	33	0	0	1	0
30	K	32	0	0	1	0
30	L	31	0	0	1	0
30	M	29	0	0	0	0
30	N	239	0	0	5	0
30	O	154	0	0	3	0
30	P	131	0	0	3	0
30	Q	91	0	0	4	0
30	R	93	0	0	0	0
30	S	108	0	0	2	0
30	T	61	0	0	0	0
30	U	50	0	0	0	0
30	V	41	0	0	2	0
30	W	39	0	0	1	0
30	X	31	0	0	3	0
30	Y	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Z	24	0	0	0	0
All	All	34120	0	32594	510	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 8.

The worst 5 of 510 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)
18:A:606:PER:O2	18:A:606:PER:O1	1.55	1.23
18:N:606:PER:O2	18:N:606:PER:O1	1.55	1.20
20:N:613:EDO:H21	6:S:36:PRO:HD3	1.38	1.03
25:C:307:PEK:H041	7:G:17:ARG:HH22	1.23	1.03
3:C:67:PHE:HE1	26:C:304:CDL:H1	1.26	0.96

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	522/514 (102%)	508 (97%)	14 (3%)	0	100	100
1	N	519/514 (101%)	505 (97%)	14 (3%)	0	100	100
2	B	228/227 (100%)	220 (96%)	8 (4%)	0	100	100
2	O	229/227 (101%)	219 (96%)	9 (4%)	1 (0%)	34	24
3	C	260/261 (100%)	254 (98%)	6 (2%)	0	100	100
3	P	259/261 (99%)	254 (98%)	5 (2%)	0	100	100
4	D	143/147 (97%)	139 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	22	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	97/98 (99%)	93 (96%)	2 (2%)	2 (2%)	7	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
7	G	81/85 (95%)	71 (88%)	5 (6%)	5 (6%)	1	0
7	T	81/85 (95%)	70 (86%)	7 (9%)	4 (5%)	2	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	5	1
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
All	All	3537/3614 (98%)	3411 (96%)	103 (3%)	23 (1%)	22	12

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE
6	S	94	HIS
7	T	5	LYS

### 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	436/426 (102%)	430 (99%)	6 (1%)	67	65
1	N	433/426 (102%)	426 (98%)	7 (2%)	62	60
2	B	213/210 (101%)	203 (95%)	10 (5%)	26	16
2	O	214/210 (102%)	203 (95%)	11 (5%)	24	14
3	C	227/226 (100%)	224 (99%)	3 (1%)	69	68
3	P	226/226 (100%)	221 (98%)	5 (2%)	52	47
4	D	129/129 (100%)	127 (98%)	2 (2%)	62	60
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	45
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	47
5	R	93/95 (98%)	90 (97%)	3 (3%)	39	30
6	F	82/81 (101%)	80 (98%)	2 (2%)	49	43
6	S	81/81 (100%)	81 (100%)	0	100	100
7	G	67/68 (98%)	64 (96%)	3 (4%)	27	18
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	7
8	U	71/75 (95%)	69 (97%)	2 (3%)	43	36
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	55
9	V	57/57 (100%)	56 (98%)	1 (2%)	59	55
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	51
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	40/40 (100%)	37 (92%)	3 (8%)	13	5
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	14
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	13
13	Z	37/38 (97%)	36 (97%)	1 (3%)	44	38
All	All	3073/3082 (100%)	2991 (97%)	82 (3%)	46	38

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	23	SER

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Mol	Chain	Res	Type
7	T	37	LEU
3	P	159	MET
5	R	5	HIS
8	U	29	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	98	HIS
13	M	36	HIS
6	S	28	GLN
13	M	39	ASN
6	F	94	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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	FME	B	1	2	8,9,10	0.89	0	7,9,11	2.18	4 (57%)
1	FME	A	1	1	8,9,10	0.39	0	7,9,11	1.45	1 (14%)
1	FME	N	1	1	8,9,10	0.44	0	7,9,11	1.08	0
9	SAC	V	1	9	7,8,9	0.57	0	8,9,11	0.86	1 (12%)
7	TPO	G	11	7	8,10,11	1.24	1 (12%)	10,14,16	1.08	0
9	SAC	I	1	9	7,8,9	0.57	0	8,9,11	0.80	0
2	FME	O	1	2	8,9,10	0.78	0	7,9,11	1.84	1 (14%)
7	TPO	T	11	7	8,10,11	1.56	1 (12%)	10,14,16	1.39	1 (10%)

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	FME	B	1	2	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	1/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	3.35	1.61	1.50
7	G	11	TPO	P-O1P	2.46	1.58	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	11	TPO	CG2-CB-CA	3.95	120.96	113.16
2	O	1	FME	CG-CB-CA	-3.84	102.27	112.95
1	A	1	FME	C-CA-N	2.91	114.99	109.73
2	B	1	FME	C-CA-N	-2.84	104.60	109.73
2	B	1	FME	O-C-CA	-2.80	117.45	124.78

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	CG2-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 131 ligands modelled in this entry, 10 are monoatomic - leaving 121 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
25	PEK	C	307	-	52,52,52	0.99	2 (3%)	55,57,57	1.52	9 (16%)
19	PGV	P	305	-	50,50,50	0.82	2 (4%)	53,56,56	1.12	4 (7%)
20	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.11	0
25	PEK	C	302	-	52,52,52	0.97	2 (3%)	55,57,57	1.14	5 (9%)
19	PGV	P	301	-	50,50,50	0.98	2 (4%)	53,56,56	1.28	4 (7%)
20	EDO	N	617	-	3,3,3	0.35	0	2,2,2	1.13	0
23	CUA	B	302	2	0,1,1	-	-	-		
20	EDO	N	620	-	3,3,3	0.41	0	2,2,2	0.33	0
21	DMU	P	316	-	34,34,34	0.79	1 (2%)	45,45,45	2.37	16 (35%)
20	EDO	N	611	-	3,3,3	0.49	0	2,2,2	0.32	0
27	CHD	X	105	-	32,32,32	0.75	0	51,51,51	1.69	14 (27%)
21	DMU	Z	101	-	34,34,34	0.60	1 (2%)	45,45,45	0.97	3 (6%)
21	DMU	X	102	-	22,22,34	0.70	1 (4%)	27,27,45	1.59	6 (22%)
21	DMU	O	305	-	34,34,34	0.56	0	45,45,45	1.70	12 (26%)
20	EDO	Q	202	-	3,3,3	0.40	0	2,2,2	0.59	0
20	EDO	L	105	-	3,3,3	0.50	0	2,2,2	0.20	0
21	DMU	K	101	-	34,34,34	0.54	1 (2%)	45,45,45	1.54	10 (22%)
20	EDO	S	104	-	3,3,3	0.54	0	2,2,2	0.53	0
27	CHD	C	305	-	32,32,32	0.81	1 (3%)	51,51,51	1.40	9 (17%)
20	EDO	M	102	-	3,3,3	0.37	0	2,2,2	0.38	0
20	EDO	W	102	-	3,3,3	0.44	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CHD	Y	102	-	32,32,32	0.72	0	51,51,51	2.16	15 (29%)
20	EDO	P	310	-	3,3,3	0.64	0	2,2,2	0.17	0
20	EDO	F	104	-	3,3,3	0.34	0	2,2,2	0.60	0
22	TGL	Q	201	-	62,62,62	1.07	3 (4%)	65,65,65	0.99	5 (7%)
26	CDL	G	101	-	99,99,99	1.34	12 (12%)	105,111,111	1.46	12 (11%)
20	EDO	A	611	-	3,3,3	0.40	0	2,2,2	0.08	0
22	TGL	L	101	12	62,62,62	1.17	4 (6%)	65,65,65	1.56	7 (10%)
27	CHD	J	101	-	32,32,32	0.62	0	51,51,51	2.38	21 (41%)
19	PGV	N	607	-	50,50,50	0.97	2 (4%)	53,56,56	1.30	7 (13%)
26	CDL	T	102	-	99,99,99	1.30	12 (12%)	105,111,111	1.31	7 (6%)
27	CHD	G	103	-	32,32,32	0.96	2 (6%)	51,51,51	1.52	10 (19%)
20	EDO	B	304	-	3,3,3	0.64	0	2,2,2	0.20	0
20	EDO	W	103	-	3,3,3	0.56	0	2,2,2	0.60	0
21	DMU	K	106	-	34,34,34	0.55	1 (2%)	45,45,45	1.45	6 (13%)
20	EDO	S	106	-	3,3,3	0.68	0	2,2,2	0.67	0
23	CUA	O	302	2	0,1,1	-	-	-	-	-
27	CHD	C	306	-	32,32,32	0.92	0	51,51,51	1.38	7 (13%)
20	EDO	B	305	-	3,3,3	0.47	0	2,2,2	0.43	0
19	PGV	A	608	-	50,50,50	1.06	2 (4%)	53,56,56	1.13	4 (7%)
24	PSC	N	608	-	51,51,51	1.14	3 (5%)	57,59,59	1.54	7 (12%)
20	EDO	P	311	-	3,3,3	0.64	0	2,2,2	0.14	0
21	DMU	K	103	-	34,34,34	0.53	0	45,45,45	1.34	6 (13%)
20	EDO	N	615	-	3,3,3	0.36	0	2,2,2	0.78	0
20	EDO	Y	103	-	3,3,3	0.43	0	2,2,2	0.13	0
19	PGV	A	607	-	50,50,50	1.02	3 (6%)	53,56,56	1.26	4 (7%)
14	HEA	A	602	1,18	57,67,67	1.40	6 (10%)	61,103,103	1.84	20 (32%)
22	TGL	O	301	-	62,62,62	1.11	3 (4%)	65,65,65	1.14	5 (7%)
26	CDL	C	304	-	99,99,99	1.36	12 (12%)	105,111,111	1.43	12 (11%)
20	EDO	G	105	-	3,3,3	0.54	0	2,2,2	0.13	0
21	DMU	X	101	-	34,34,34	0.59	1 (2%)	45,45,45	1.78	10 (22%)
14	HEA	N	601[B]	-	57,67,67	1.34	8 (14%)	61,103,103	1.83	17 (27%)
25	PEK	P	309	-	52,52,52	1.05	2 (3%)	55,57,57	1.49	4 (7%)
20	EDO	P	315	-	3,3,3	0.37	0	2,2,2	1.05	0
20	EDO	P	312	-	3,3,3	0.49	0	2,2,2	1.13	0
27	CHD	W	101	-	32,32,32	0.76	0	51,51,51	2.35	17 (33%)
20	EDO	N	609	-	3,3,3	0.80	0	2,2,2	0.67	0
20	EDO	N	610	-	3,3,3	0.80	0	2,2,2	0.34	0
25	PEK	P	304	-	52,52,52	0.85	2 (3%)	55,57,57	1.23	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	A	614	-	3,3,3	0.57	0	2,2,2	0.09	0
27	CHD	P	308	-	32,32,32	0.70	0	51,51,51	1.35	6 (11%)
21	DMU	X	103	-	22,22,34	0.54	0	27,27,45	0.68	0
20	EDO	C	310	-	3,3,3	0.75	0	2,2,2	0.53	0
29	PO4	H	101	-	4,4,4	0.82	0	6,6,6	0.42	0
20	EDO	P	313	-	3,3,3	0.51	0	2,2,2	0.47	0
20	EDO	S	107	-	3,3,3	0.42	0	2,2,2	0.41	0
21	DMU	D	202	-	34,34,34	0.53	0	45,45,45	1.09	3 (6%)
22	TGL	D	201	-	62,62,62	1.16	4 (6%)	65,65,65	1.04	4 (6%)
20	EDO	O	304	-	3,3,3	0.62	0	2,2,2	0.25	0
27	CHD	L	103	-	32,32,32	0.68	0	51,51,51	2.70	20 (39%)
21	DMU	B	306	-	34,34,34	0.84	1 (2%)	45,45,45	2.60	16 (35%)
21	DMU	K	105	-	34,34,34	0.49	0	45,45,45	1.33	6 (13%)
19	PGV	P	302	-	50,50,50	1.02	2 (4%)	53,56,56	1.26	6 (11%)
14	HEA	N	601[A]	-	57,67,67	1.36	8 (14%)	61,103,103	1.83	16 (26%)
20	EDO	A	612	-	3,3,3	0.37	0	2,2,2	0.30	0
21	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.17	4 (8%)
20	EDO	N	613	-	3,3,3	0.39	0	2,2,2	0.51	0
21	DMU	Q	203	-	34,34,34	0.78	1 (2%)	45,45,45	2.65	18 (40%)
18	PER	A	606	15,14	0,1,1	-	-	-	-	-
21	DMU	P	314	-	34,34,34	0.56	0	45,45,45	1.34	4 (8%)
20	EDO	C	311	-	3,3,3	0.35	0	2,2,2	0.77	0
29	PO4	U	101	-	4,4,4	1.02	0	6,6,6	0.58	0
22	TGL	B	301	-	62,62,62	1.09	3 (4%)	65,65,65	1.25	4 (6%)
20	EDO	A	610	-	3,3,3	0.62	0	2,2,2	0.56	0
19	PGV	C	303	-	50,50,50	0.83	2 (4%)	53,56,56	1.06	4 (7%)
20	EDO	N	614	-	3,3,3	0.60	0	2,2,2	0.15	0
20	EDO	R	201	-	3,3,3	0.38	0	2,2,2	0.40	0
14	HEA	A	601[B]	-	57,67,67	1.62	14 (24%)	61,103,103	1.95	22 (36%)
20	EDO	L	104	-	3,3,3	0.51	0	2,2,2	0.41	0
20	EDO	F	102	-	3,3,3	0.50	0	2,2,2	0.82	0
21	DMU	L	102	-	34,34,34	0.54	0	45,45,45	1.05	2 (4%)
27	CHD	P	307	-	32,32,32	0.73	0	51,51,51	1.43	9 (17%)
14	HEA	N	602	1,18	57,67,67	1.61	9 (15%)	61,103,103	1.89	17 (27%)
18	PER	N	606	15,14	0,1,1	-	-	-	-	-
21	DMU	K	104	-	34,34,34	0.52	0	45,45,45	1.19	6 (13%)
22	TGL	Y	101	-	62,62,62	1.11	3 (4%)	65,65,65	1.41	7 (10%)
24	PSC	B	303	-	51,51,51	1.09	3 (5%)	57,59,59	1.41	5 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.43	0
21	DMU	G	104	-	34,34,34	0.57	0	45,45,45	1.45	8 (17%)
27	CHD	T	101	-	32,32,32	0.85	1 (3%)	51,51,51	1.55	10 (19%)
20	EDO	O	303	-	3,3,3	0.76	0	2,2,2	0.60	0
21	DMU	K	102	-	34,34,34	0.55	1 (2%)	45,45,45	1.40	7 (15%)
20	EDO	S	105	-	3,3,3	0.52	0	2,2,2	0.16	0
19	PGV	C	308	-	50,50,50	1.08	2 (4%)	53,56,56	1.64	8 (15%)
20	EDO	A	615	-	3,3,3	0.88	0	2,2,2	0.59	0
21	DMU	T	103	-	34,34,34	0.56	0	45,45,45	1.23	7 (15%)
25	PEK	C	309	-	52,52,52	1.00	2 (3%)	55,57,57	1.40	6 (10%)
20	EDO	F	105	-	3,3,3	0.50	0	2,2,2	0.70	0
20	EDO	A	613	-	3,3,3	0.78	0	2,2,2	0.18	0
14	HEA	A	601[A]	-	57,67,67	1.62	14 (24%)	61,103,103	1.95	21 (34%)
20	EDO	N	619	-	3,3,3	0.51	0	2,2,2	0.16	0
20	EDO	F	103	-	3,3,3	0.68	0	2,2,2	0.59	0
21	DMU	X	104	-	22,22,34	0.51	0	27,27,45	0.60	0
25	PEK	G	102	-	52,52,52	1.02	2 (3%)	55,57,57	1.07	4 (7%)
26	CDL	P	306	-	99,99,99	1.37	12 (12%)	105,111,111	1.52	17 (16%)
21	DMU	A	616	-	34,34,34	0.47	0	45,45,45	1.07	2 (4%)
21	DMU	C	312	-	34,34,34	0.48	0	45,45,45	1.45	8 (17%)
20	EDO	S	102	-	3,3,3	0.82	0	2,2,2	0.33	0
20	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.81	0
20	EDO	N	618	-	3,3,3	0.35	0	2,2,2	0.48	0
20	EDO	N	612	-	3,3,3	0.53	0	2,2,2	0.12	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	C	307	-	-	28/56/56/56	-
19	PGV	P	305	-	-	5/55/55/55	-
20	EDO	S	103	-	-	0/1/1/1	-
25	PEK	C	302	-	-	15/56/56/56	-
19	PGV	P	301	-	-	8/55/55/55	-
20	EDO	N	617	-	-	1/1/1/1	-
20	EDO	N	620	-	-	1/1/1/1	-
21	DMU	P	316	-	-	14/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	611	-	-	0/1/1/1	-
27	CHD	X	105	-	-	7/9/74/74	0/4/4/4
21	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
21	DMU	X	102	-	-	8/13/33/59	0/1/1/2
21	DMU	O	305	-	-	10/19/59/59	0/2/2/2
20	EDO	Q	202	-	-	1/1/1/1	-
20	EDO	L	105	-	-	0/1/1/1	-
21	DMU	K	101	-	-	7/19/59/59	0/2/2/2
20	EDO	S	104	-	-	1/1/1/1	-
27	CHD	C	305	-	-	5/9/74/74	0/4/4/4
20	EDO	M	102	-	-	1/1/1/1	-
20	EDO	W	102	-	-	1/1/1/1	-
27	CHD	Y	102	-	-	0/9/74/74	0/4/4/4
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	F	104	-	-	1/1/1/1	-
22	TGL	Q	201	-	-	31/65/65/65	-
26	CDL	G	101	-	-	38/110/110/110	-
20	EDO	A	611	-	-	0/1/1/1	-
22	TGL	L	101	12	-	34/65/65/65	-
27	CHD	J	101	-	-	7/9/74/74	0/4/4/4
19	PGV	N	607	-	-	22/55/55/55	-
26	CDL	T	102	-	-	42/110/110/110	-
27	CHD	G	103	-	-	2/9/74/74	0/4/4/4
20	EDO	B	304	-	-	0/1/1/1	-
20	EDO	W	103	-	-	1/1/1/1	-
21	DMU	K	106	-	-	10/19/59/59	0/2/2/2
20	EDO	S	106	-	-	0/1/1/1	-
27	CHD	C	306	-	-	2/9/74/74	0/4/4/4
20	EDO	B	305	-	-	0/1/1/1	-
19	PGV	A	608	-	-	23/55/55/55	-
24	PSC	N	608	-	-	28/55/55/55	-
20	EDO	P	311	-	-	1/1/1/1	-
21	DMU	K	103	-	-	10/19/59/59	0/2/2/2
20	EDO	N	615	-	-	1/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-
19	PGV	A	607	-	-	6/55/55/55	-
14	HEA	A	602	1,18	-	6/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	TGL	O	301	-	-	30/65/65/65	-
26	CDL	C	304	-	-	47/110/110/110	-
20	EDO	G	105	-	-	0/1/1/1	-
21	DMU	X	101	-	-	11/19/59/59	0/2/2/2
14	HEA	N	601[B]	-	-	7/32/76/76	-
25	PEK	P	309	-	-	30/56/56/56	-
20	EDO	P	315	-	-	1/1/1/1	-
20	EDO	P	312	-	-	1/1/1/1	-
27	CHD	W	101	-	-	6/9/74/74	0/4/4/4
20	EDO	N	609	-	-	0/1/1/1	-
20	EDO	N	610	-	-	0/1/1/1	-
25	PEK	P	304	-	-	8/56/56/56	-
20	EDO	A	614	-	-	1/1/1/1	-
27	CHD	P	308	-	-	2/9/74/74	0/4/4/4
21	DMU	X	103	-	-	6/13/33/59	0/1/1/2
20	EDO	C	310	-	-	0/1/1/1	-
20	EDO	P	313	-	-	0/1/1/1	-
20	EDO	S	107	-	-	1/1/1/1	-
21	DMU	D	202	-	-	8/19/59/59	0/2/2/2
22	TGL	D	201	-	-	26/65/65/65	-
20	EDO	O	304	-	-	1/1/1/1	-
27	CHD	L	103	-	-	5/9/74/74	0/4/4/4
21	DMU	B	306	-	-	14/19/59/59	0/2/2/2
21	DMU	K	105	-	-	10/19/59/59	0/2/2/2
19	PGV	P	302	-	-	18/55/55/55	-
14	HEA	N	601[A]	-	-	4/32/76/76	-
20	EDO	A	612	-	-	0/1/1/1	-
21	DMU	M	101	-	-	4/19/59/59	0/2/2/2
20	EDO	N	613	-	-	1/1/1/1	-
21	DMU	Q	203	-	-	17/19/59/59	0/2/2/2
21	DMU	P	314	-	-	7/19/59/59	0/2/2/2
20	EDO	C	311	-	-	1/1/1/1	-
22	TGL	B	301	-	-	27/65/65/65	-
20	EDO	A	610	-	-	0/1/1/1	-
19	PGV	C	303	-	-	14/55/55/55	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601[B]	-	-	6/32/76/76	-
20	EDO	L	104	-	-	1/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
21	DMU	L	102	-	-	9/19/59/59	0/2/2/2
27	CHD	P	307	-	-	5/9/74/74	0/4/4/4
14	HEA	N	602	1,18	-	4/32/76/76	-
21	DMU	K	104	-	-	12/19/59/59	0/2/2/2
22	TGL	Y	101	-	-	29/65/65/65	-
24	PSC	B	303	-	-	26/55/55/55	-
20	EDO	N	616	-	-	1/1/1/1	-
21	DMU	G	104	-	-	9/19/59/59	0/2/2/2
27	CHD	T	101	-	-	2/9/74/74	0/4/4/4
20	EDO	O	303	-	-	0/1/1/1	-
21	DMU	K	102	-	-	11/19/59/59	0/2/2/2
20	EDO	S	105	-	-	0/1/1/1	-
19	PGV	C	308	-	-	20/55/55/55	-
20	EDO	A	615	-	-	0/1/1/1	-
21	DMU	T	103	-	-	8/19/59/59	0/2/2/2
25	PEK	C	309	-	-	22/56/56/56	-
20	EDO	F	105	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	4/32/76/76	-
20	EDO	N	619	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
21	DMU	X	104	-	-	7/13/33/59	0/1/1/2
25	PEK	G	102	-	-	15/56/56/56	-
26	CDL	P	306	-	-	46/110/110/110	-
21	DMU	A	616	-	-	8/19/59/59	0/2/2/2
21	DMU	C	312	-	-	10/19/59/59	0/2/2/2
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-

The worst 5 of 175 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	101	TGL	OG2-CB1	5.27	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	308	PGV	O03-C19	5.25	1.48	1.33
22	Y	101	TGL	OG2-CB1	5.15	1.48	1.34
22	O	301	TGL	OG3-CC1	5.04	1.48	1.33
19	A	608	PGV	O03-C19	5.03	1.48	1.33

The worst 5 of 576 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	306	DMU	O4-C7-C5	-7.29	93.49	110.35
27	J	101	CHD	C10-C9-C8	7.13	119.48	111.82
26	G	101	CDL	OA6-CA5-C11	7.03	126.66	111.50
21	B	306	DMU	C10-O1-C9	6.69	126.82	113.69
27	W	101	CHD	C13-C17-C20	6.59	127.36	119.50

There are no chirality outliers.

5 of 948 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[B]	HEA	C18-C19-C20-C21
19	A	608	PGV	C04-O12-P-O14
19	A	608	PGV	C2-C1-O01-C02
19	A	608	PGV	O04-C19-O03-C01
19	A	608	PGV	C20-C19-O03-C01

There are no ring outliers.

76 monomers are involved in 291 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	307	PEK	13	0
19	P	305	PGV	4	0
25	C	302	PEK	3	0
19	P	301	PGV	3	0
20	N	617	EDO	2	0
21	P	316	DMU	10	0
27	X	105	CHD	5	0
21	X	102	DMU	2	0
21	O	305	DMU	2	0
20	Q	202	EDO	1	0
21	K	101	DMU	3	0
27	C	305	CHD	1	0
20	M	102	EDO	1	0

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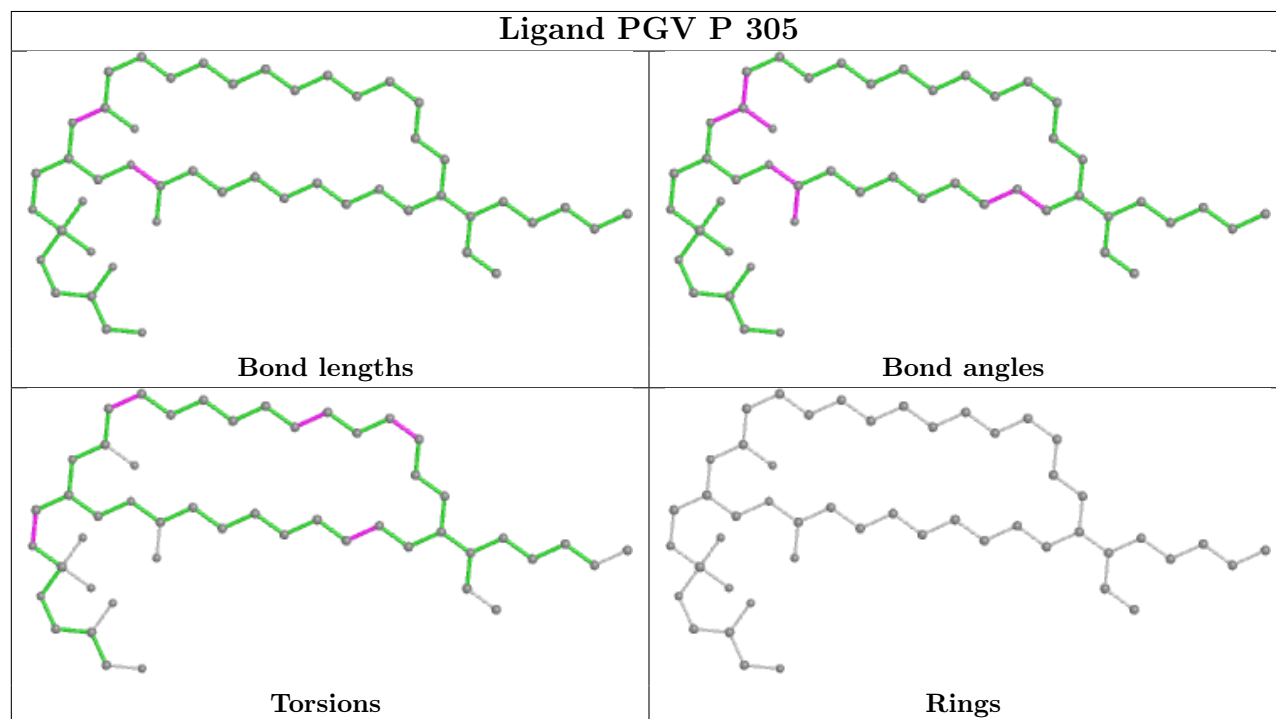
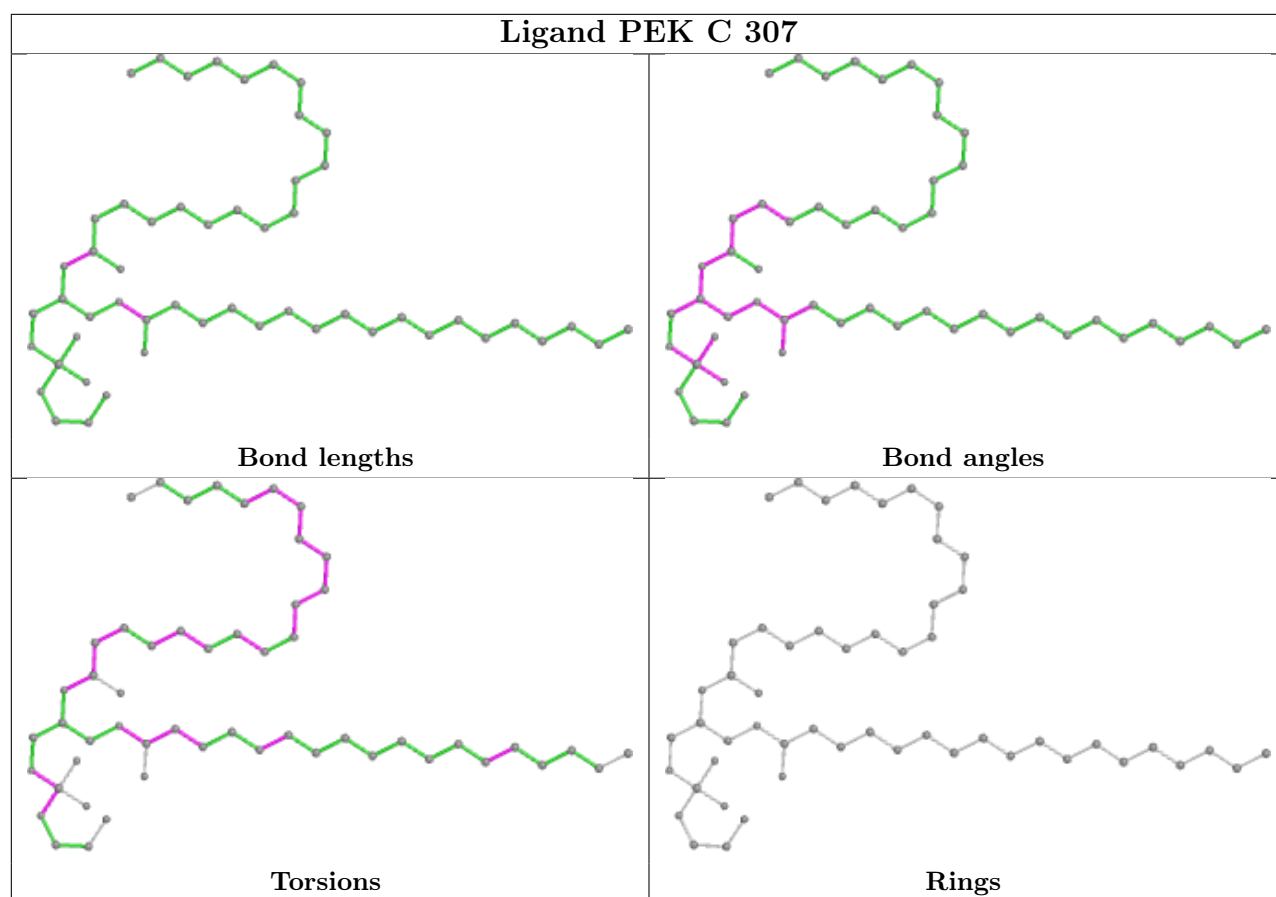
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	W	102	EDO	3	0
27	Y	102	CHD	3	0
22	Q	201	TGL	6	0
26	G	101	CDL	21	0
20	A	611	EDO	1	0
22	L	101	TGL	12	0
27	J	101	CHD	4	0
19	N	607	PGV	6	0
26	T	102	CDL	19	0
20	W	103	EDO	2	0
21	K	106	DMU	1	0
19	A	608	PGV	8	0
24	N	608	PSC	12	0
21	K	103	DMU	3	0
20	Y	103	EDO	1	0
19	A	607	PGV	1	0
14	A	602	HEA	2	0
22	O	301	TGL	1	0
26	C	304	CDL	23	0
21	X	101	DMU	1	0
14	N	601[B]	HEA	1	0
25	P	309	PEK	5	0
20	P	315	EDO	1	0
27	W	101	CHD	1	0
25	P	304	PEK	3	0
27	P	308	CHD	1	0
21	X	103	DMU	1	0
20	S	107	EDO	4	0
21	D	202	DMU	1	0
22	D	201	TGL	10	0
27	L	103	CHD	1	0
21	K	105	DMU	5	0
19	P	302	PGV	2	0
14	N	601[A]	HEA	1	0
20	A	612	EDO	4	0
21	M	101	DMU	1	0
20	N	613	EDO	4	0
21	Q	203	DMU	1	0
18	A	606	PER	1	0
20	C	311	EDO	1	0
22	B	301	TGL	6	0
19	C	303	PGV	2	0

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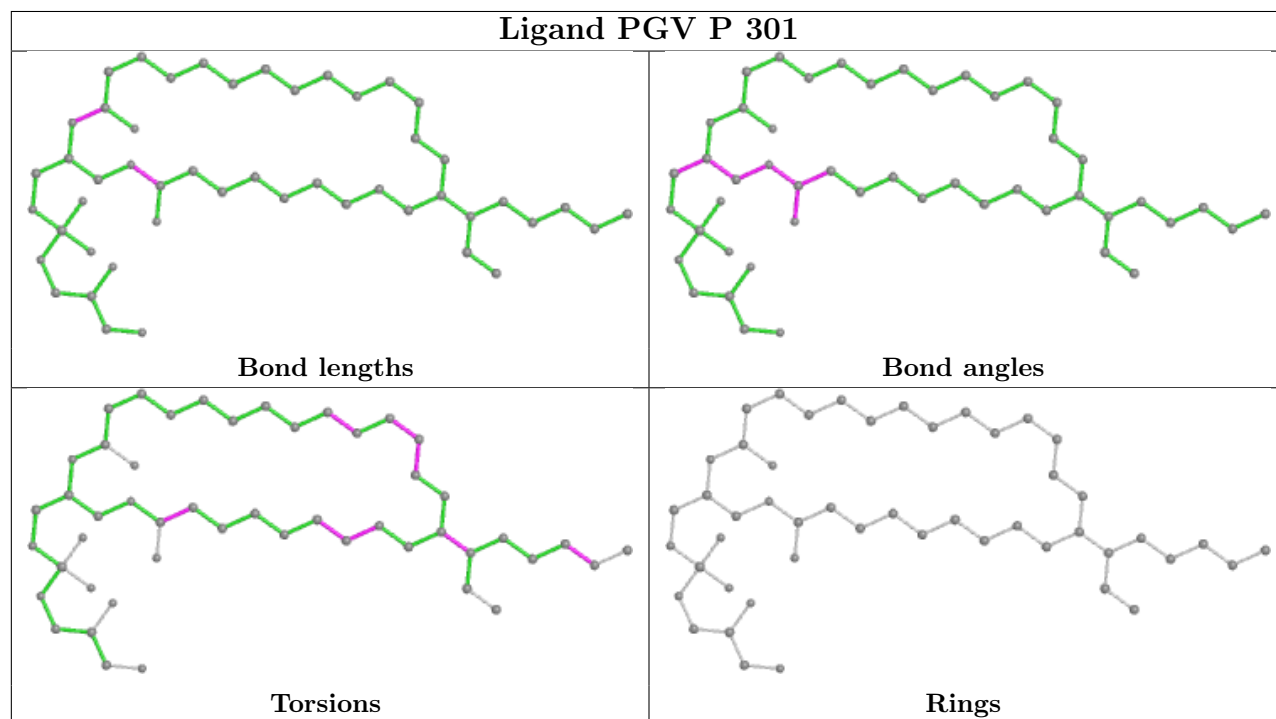
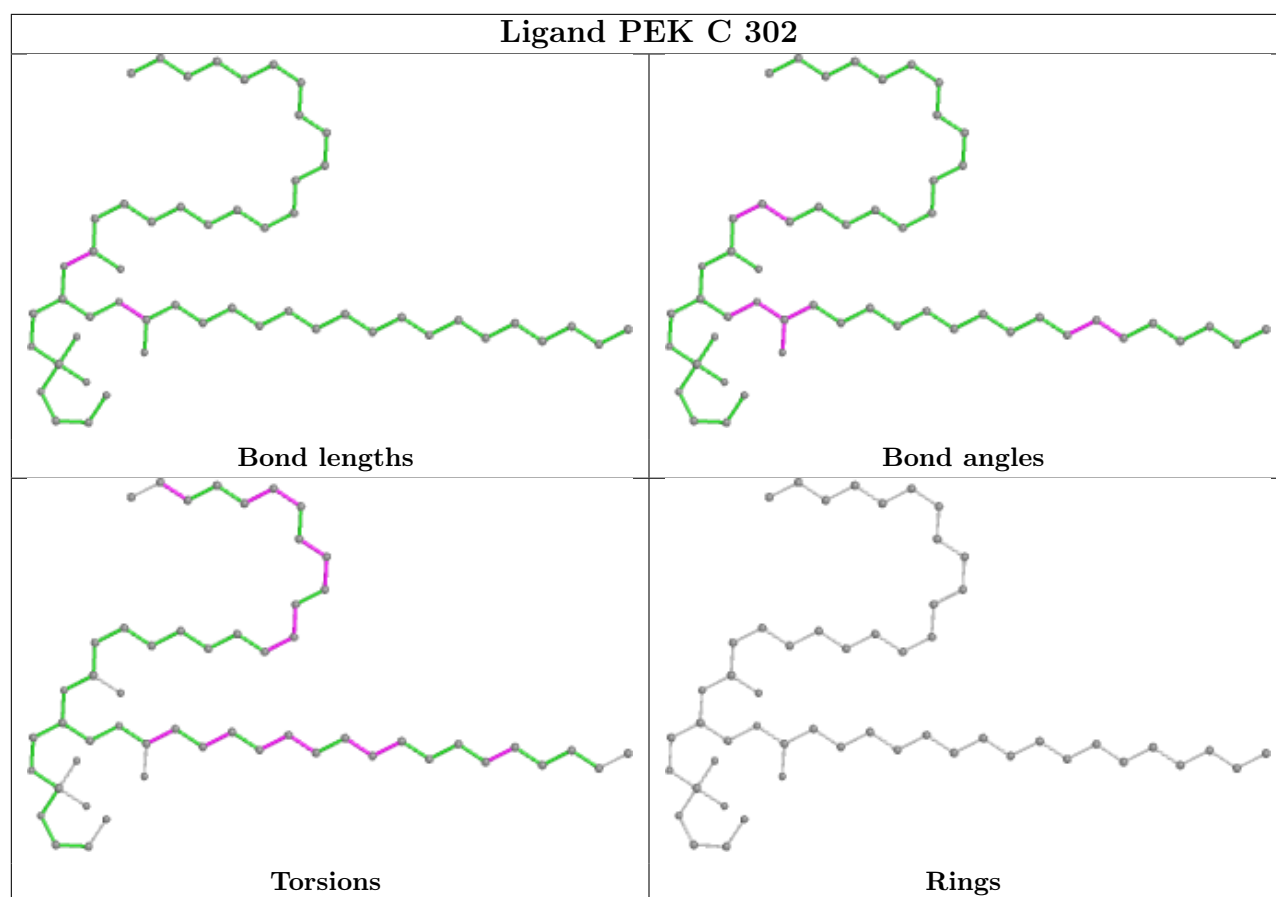
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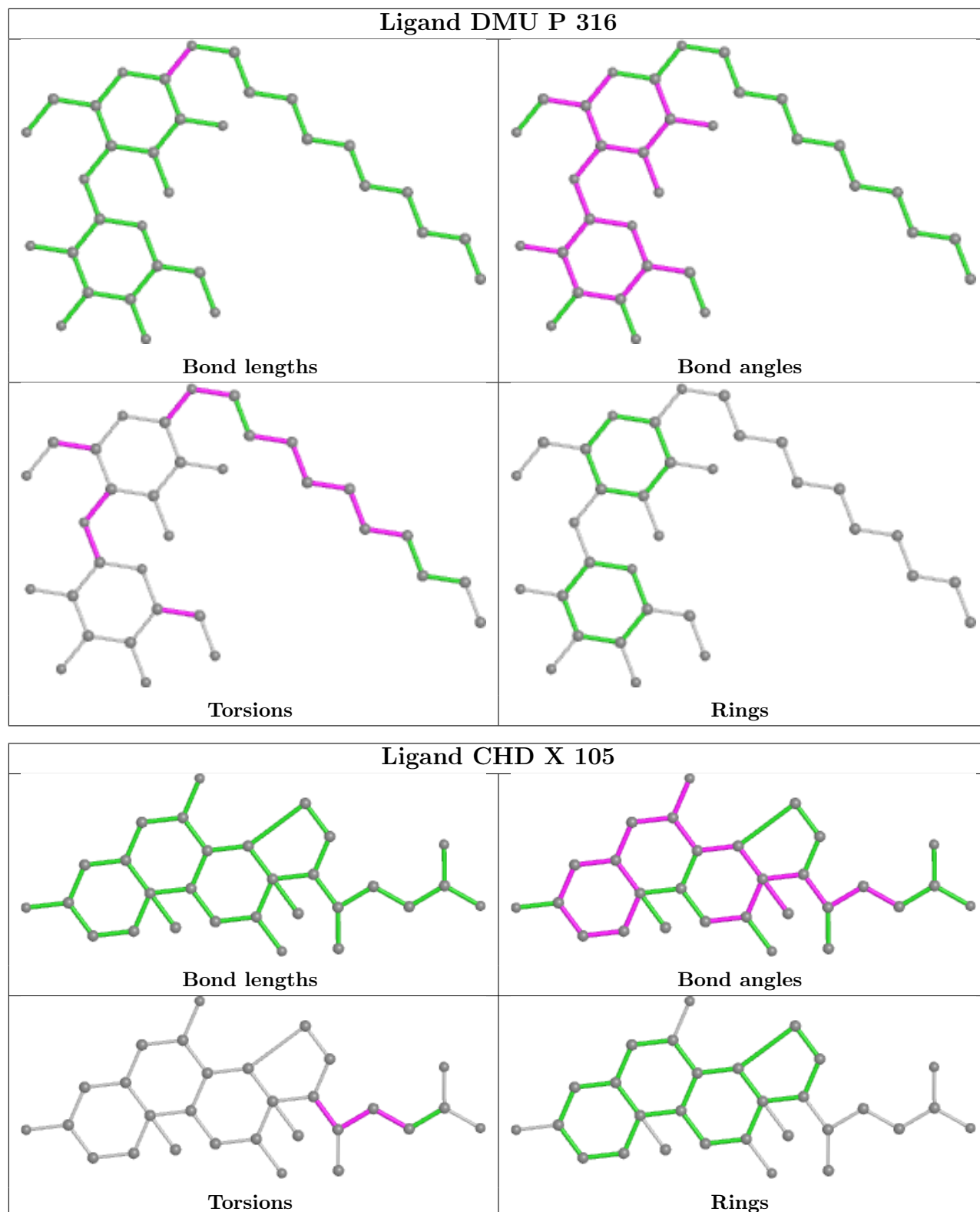
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601[B]	HEA	1	0
21	L	102	DMU	3	0
27	P	307	CHD	2	0
14	N	602	HEA	2	0
18	N	606	PER	1	0
21	K	104	DMU	1	0
22	Y	101	TGL	7	0
24	B	303	PSC	9	0
20	N	616	EDO	1	0
21	G	104	DMU	1	0
21	K	102	DMU	1	0
20	S	105	EDO	1	0
19	C	308	PGV	3	0
21	T	103	DMU	2	0
25	C	309	PEK	4	0
14	A	601[A]	HEA	1	0
25	G	102	PEK	4	0
26	P	306	CDL	18	0
21	A	616	DMU	1	0
20	N	618	EDO	1	0
20	N	612	EDO	1	0

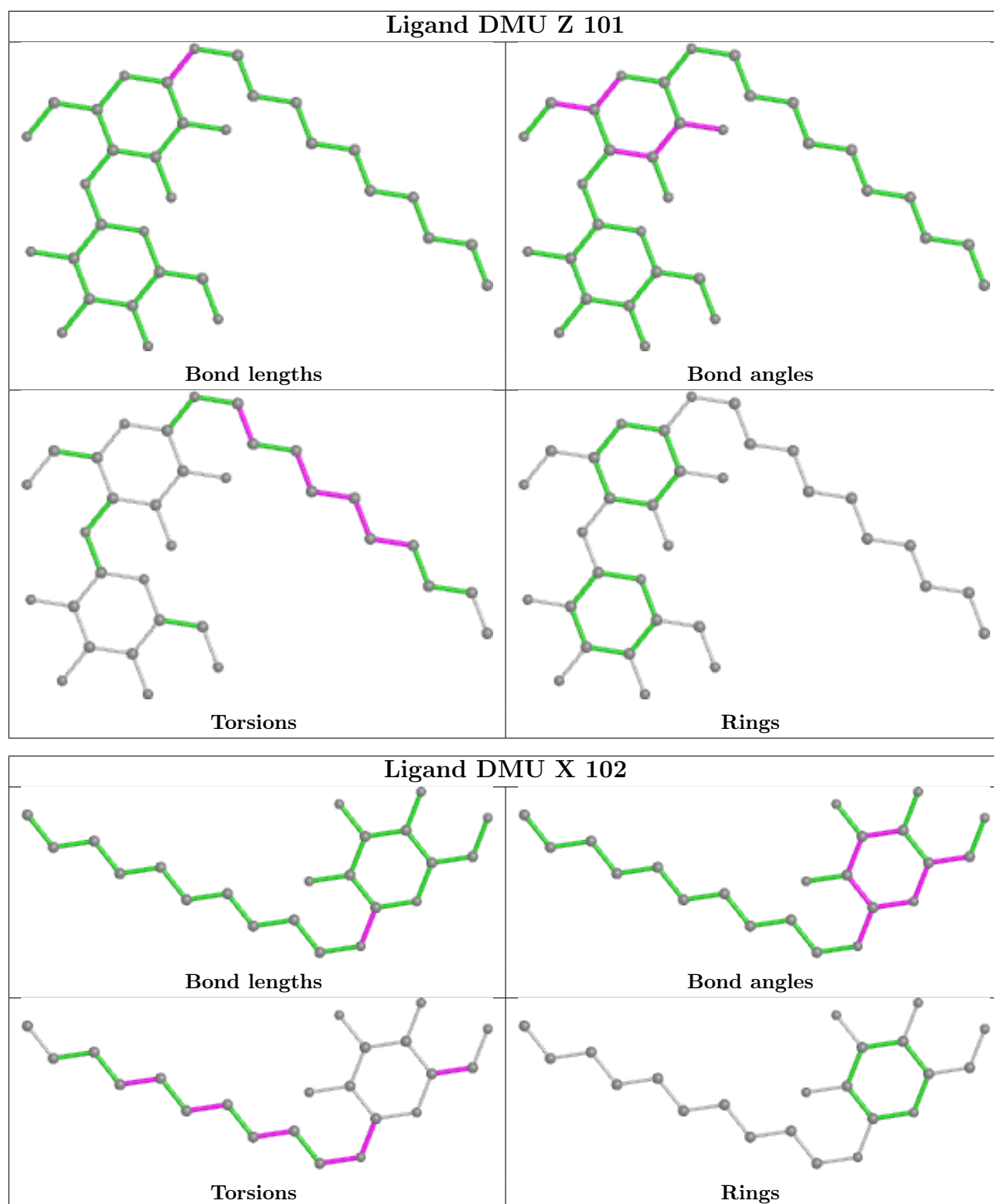
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

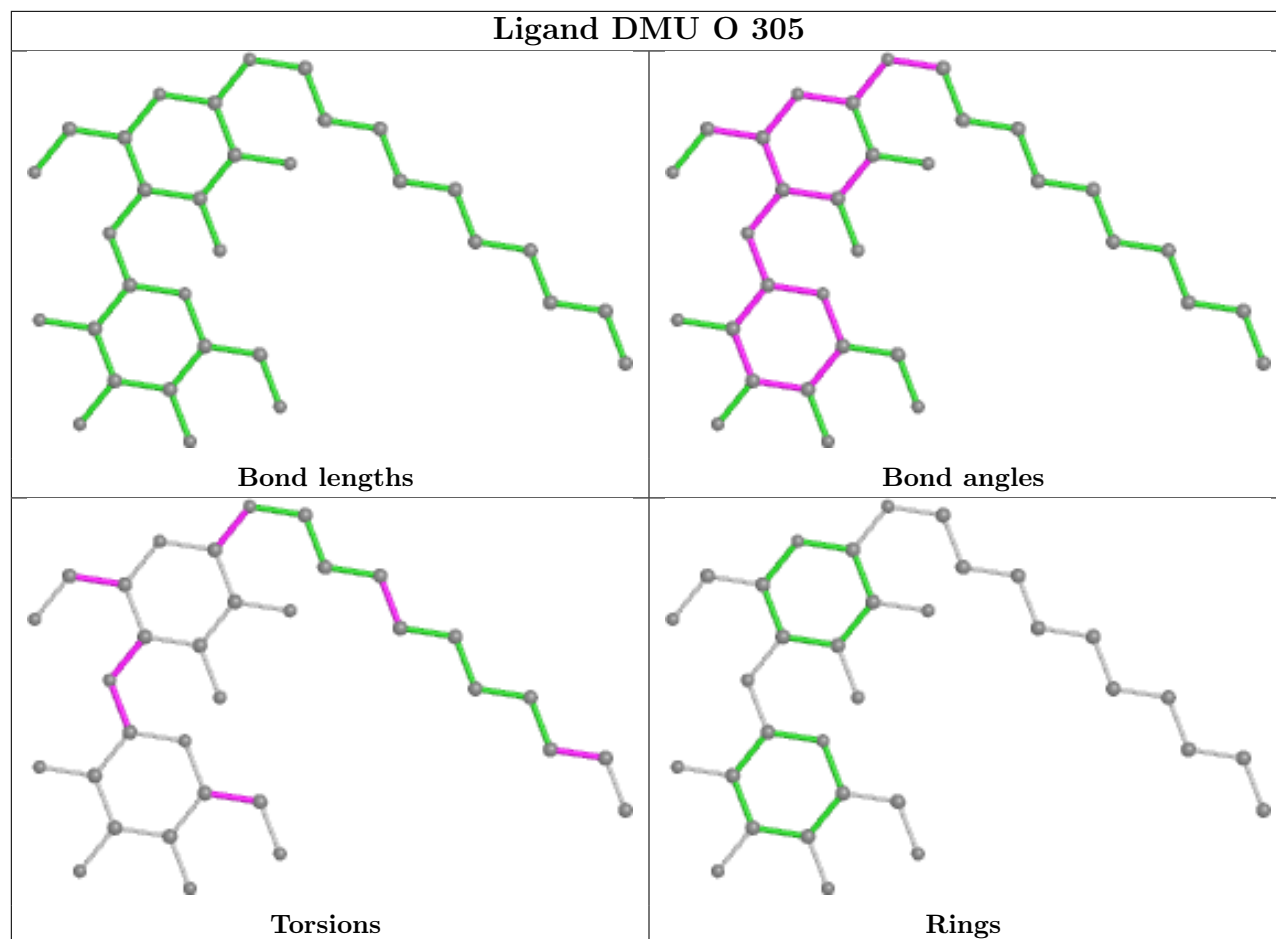


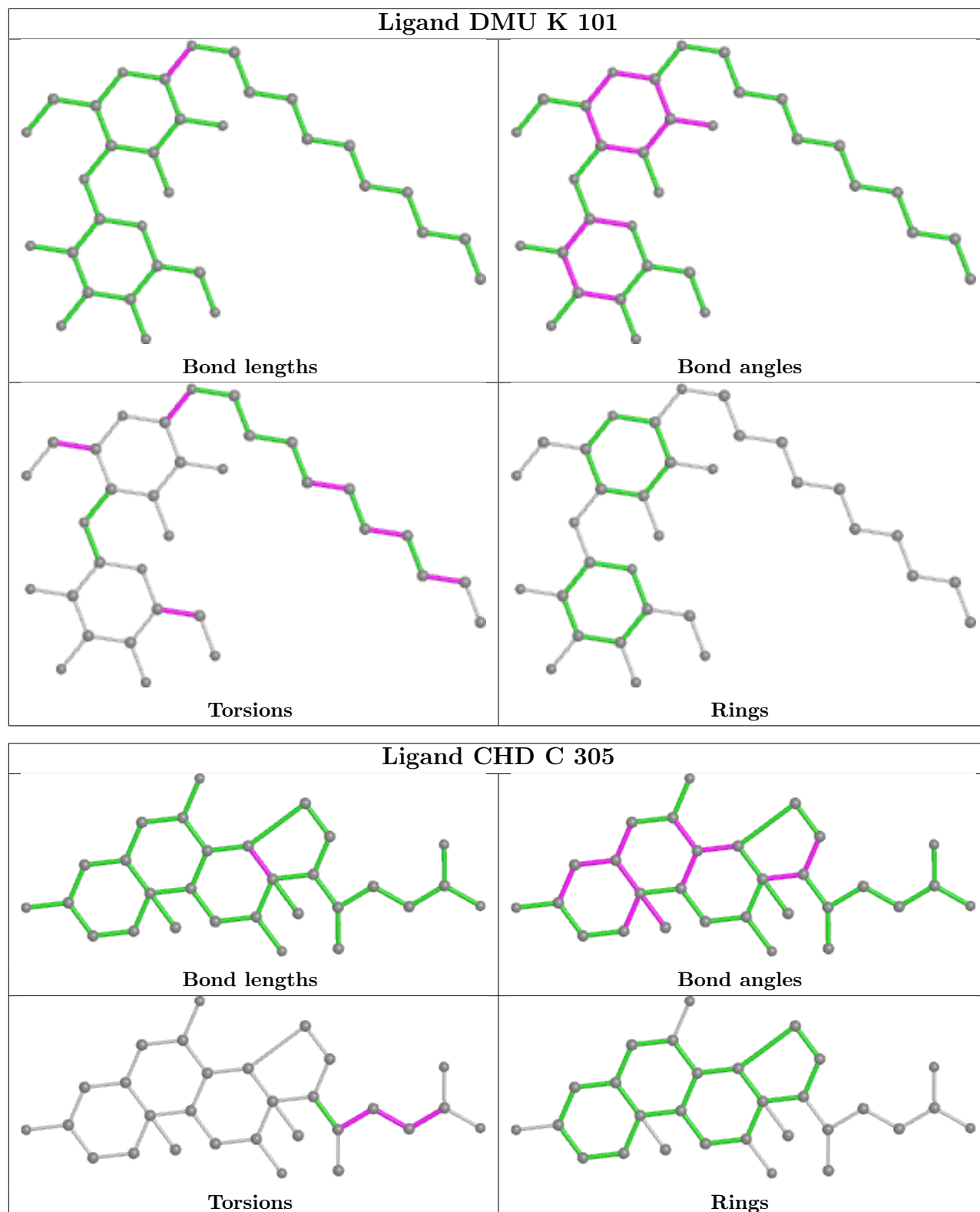


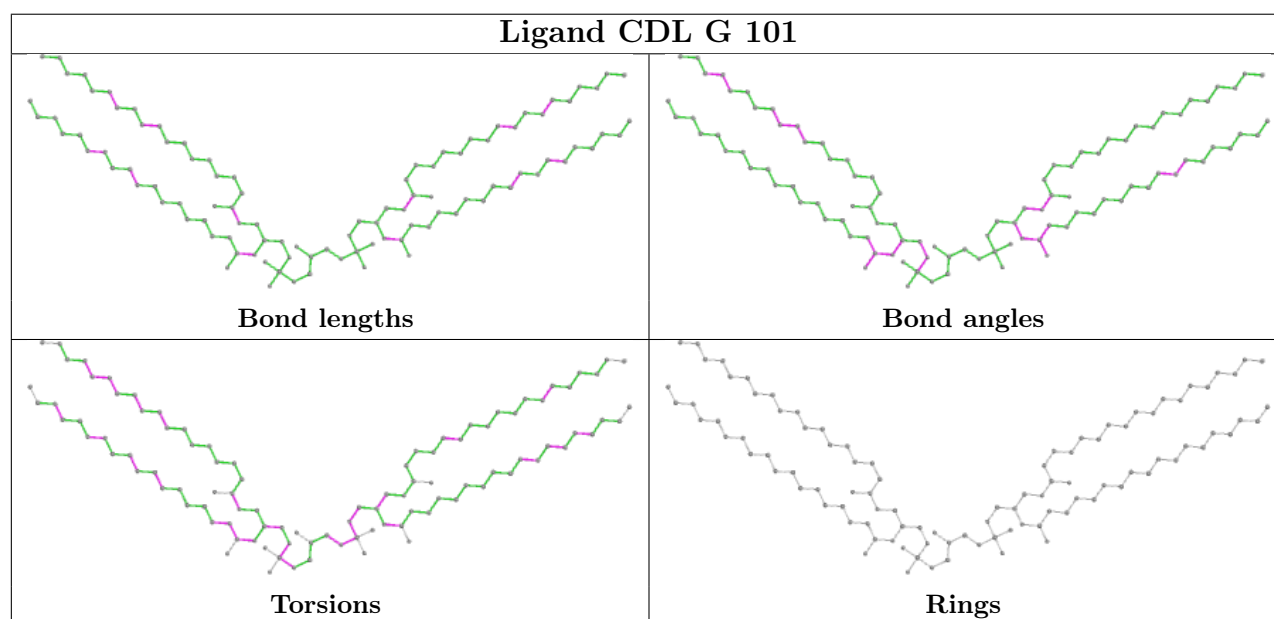
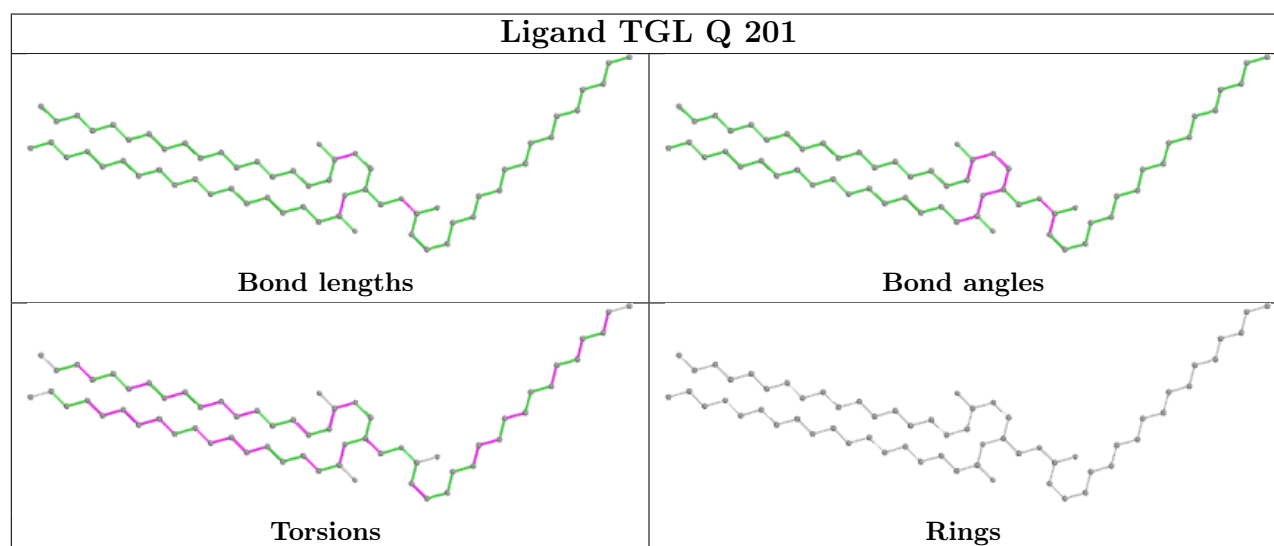
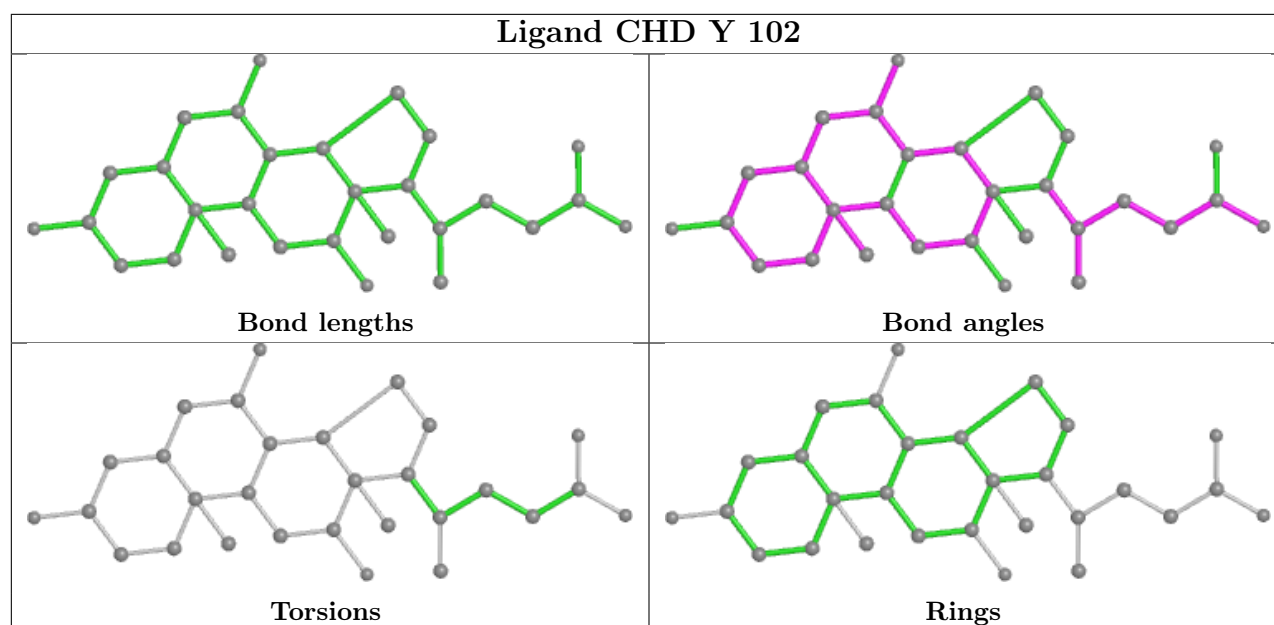


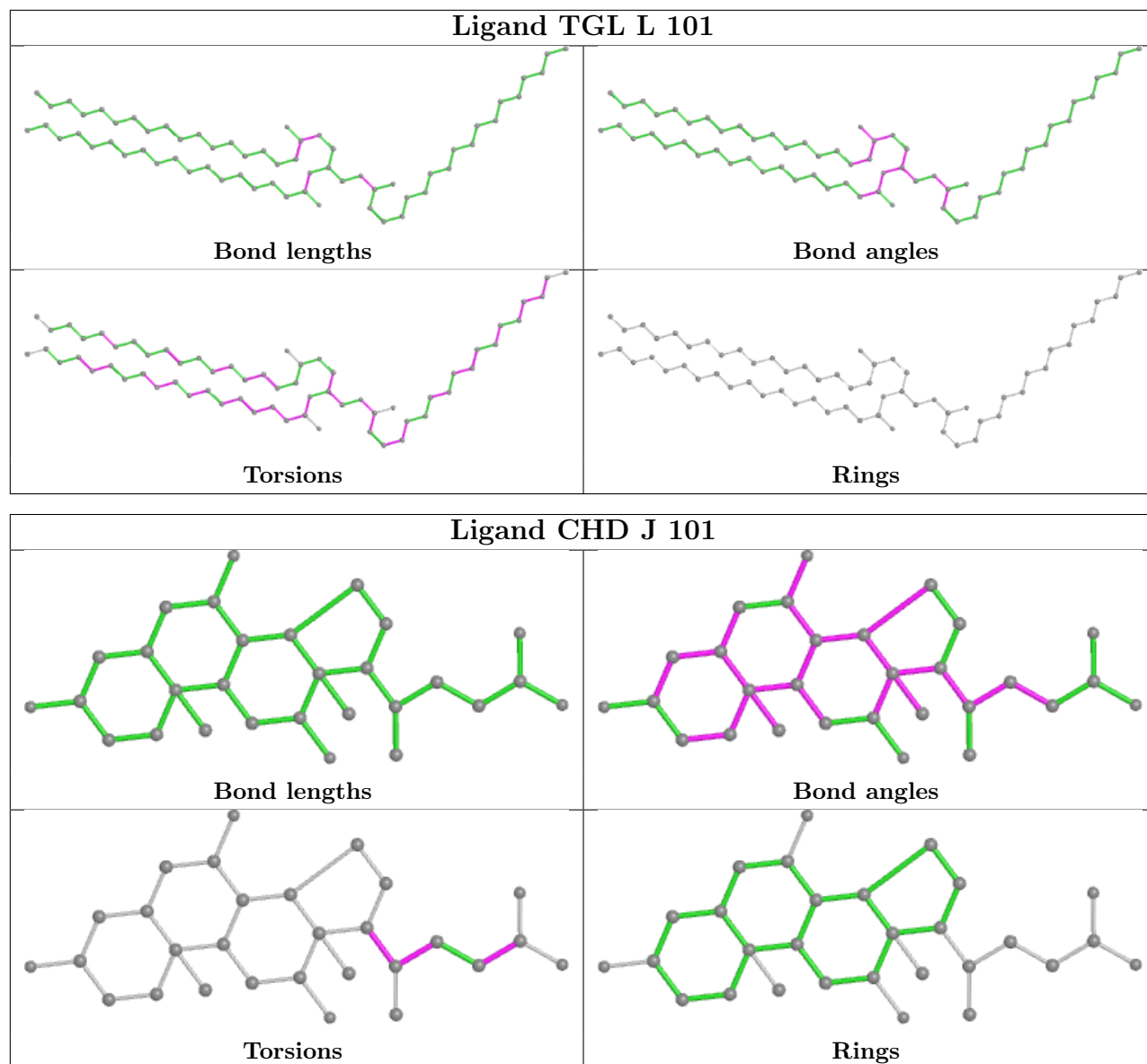


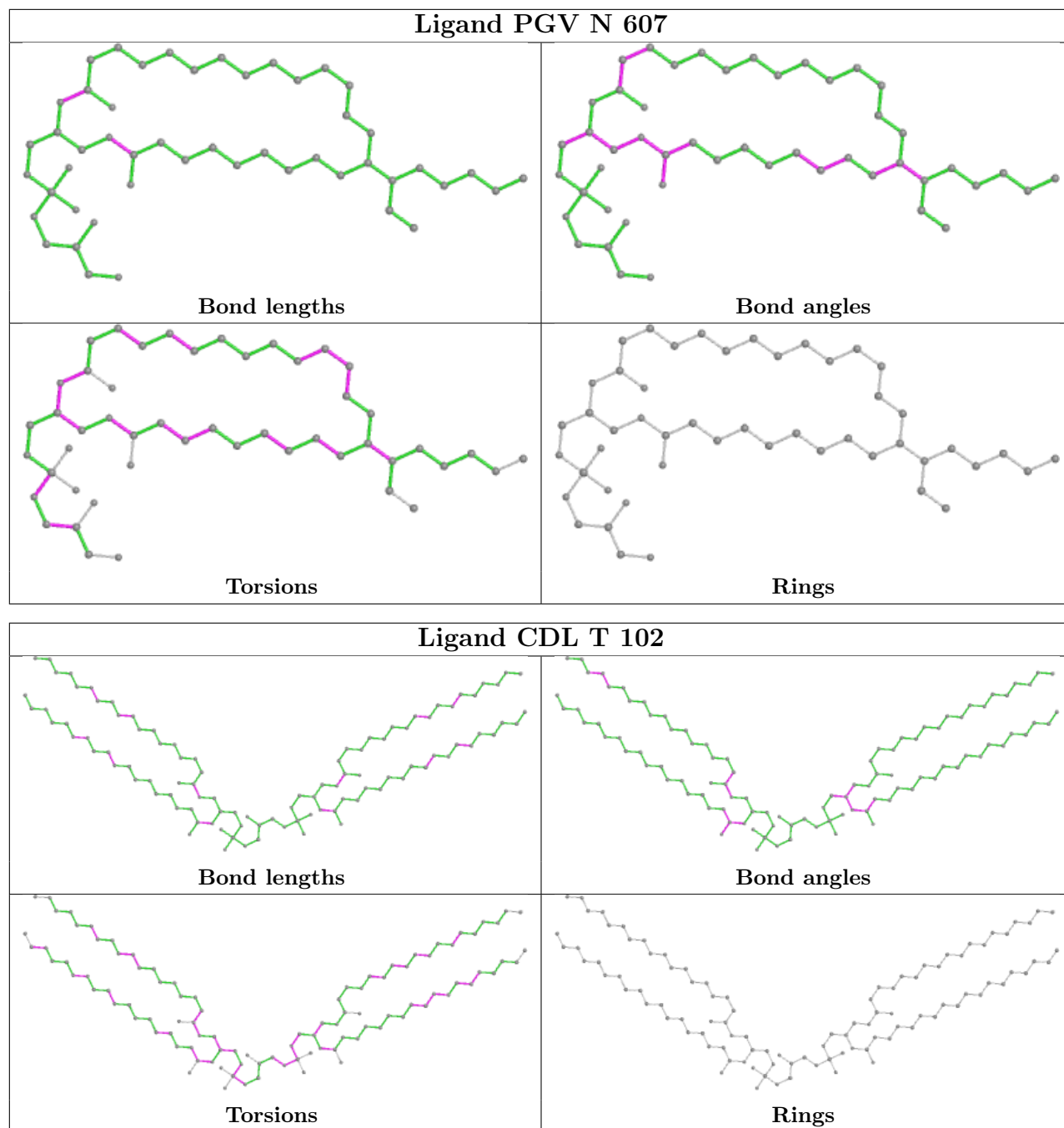




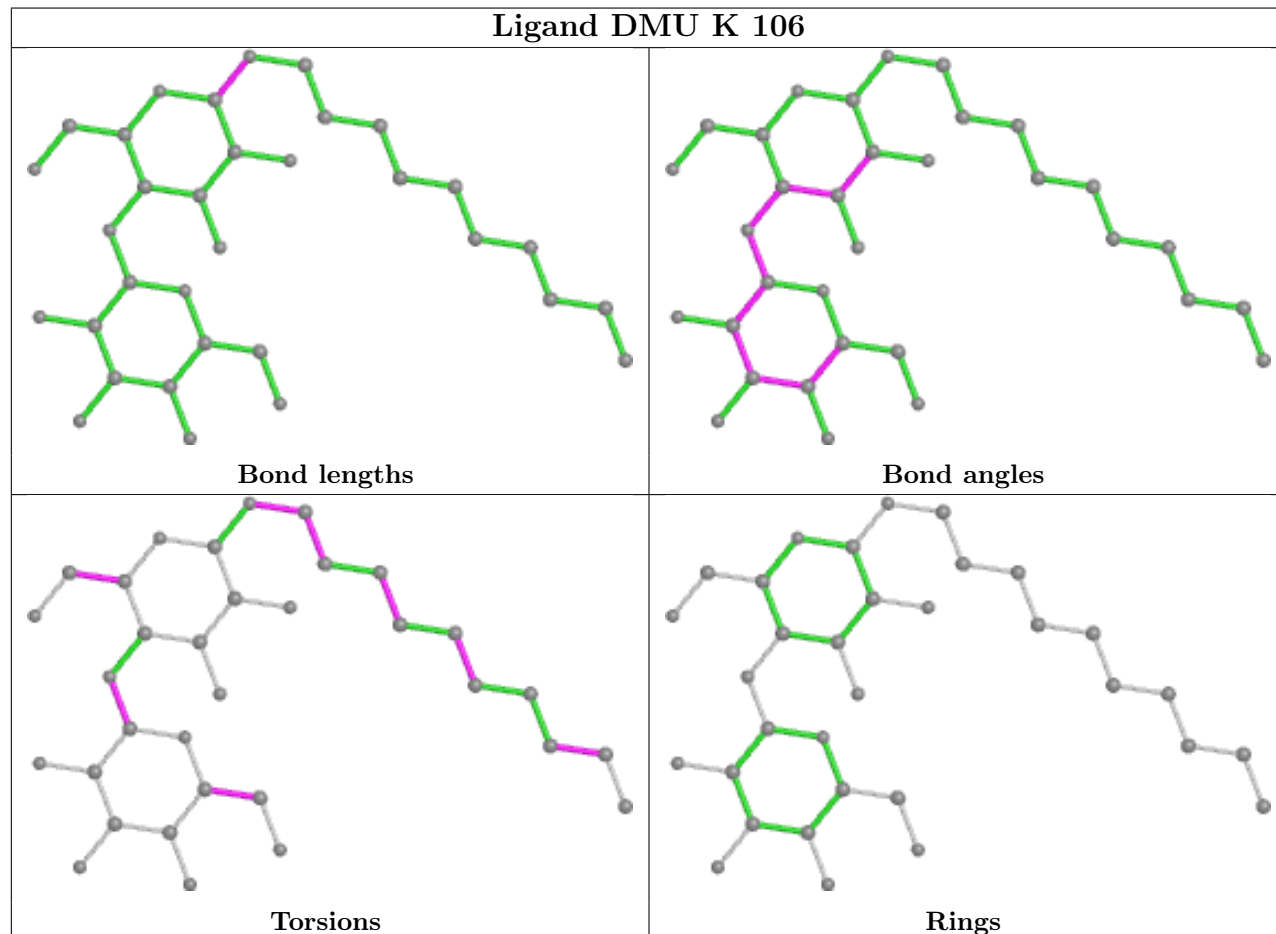
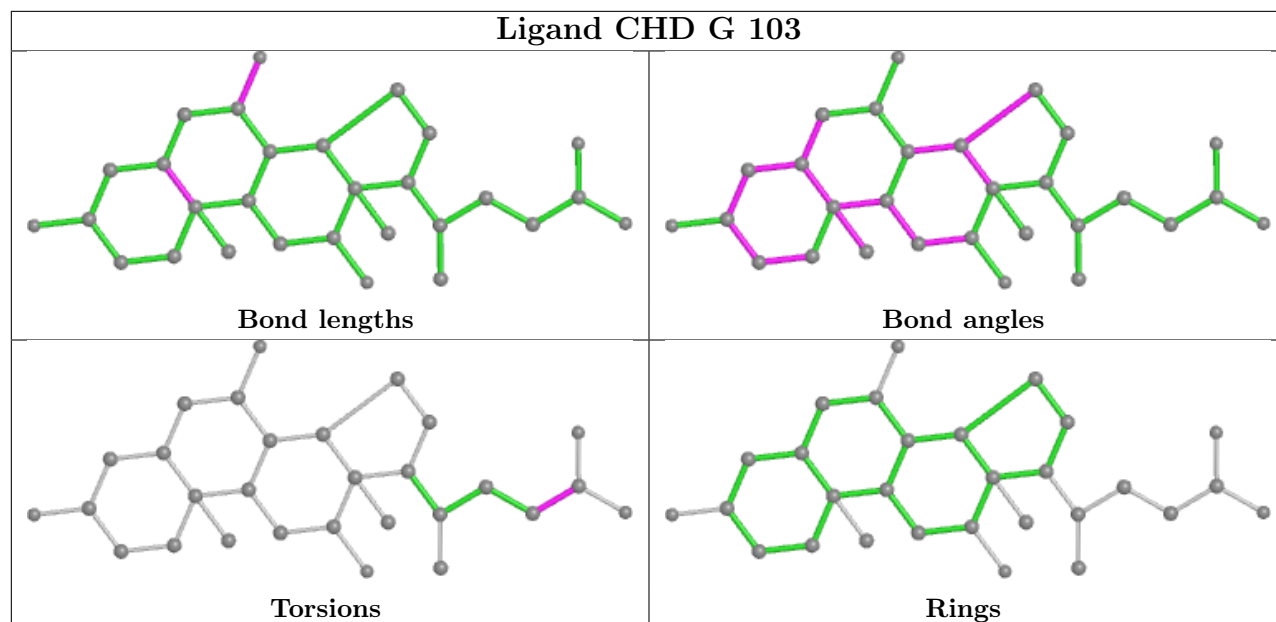


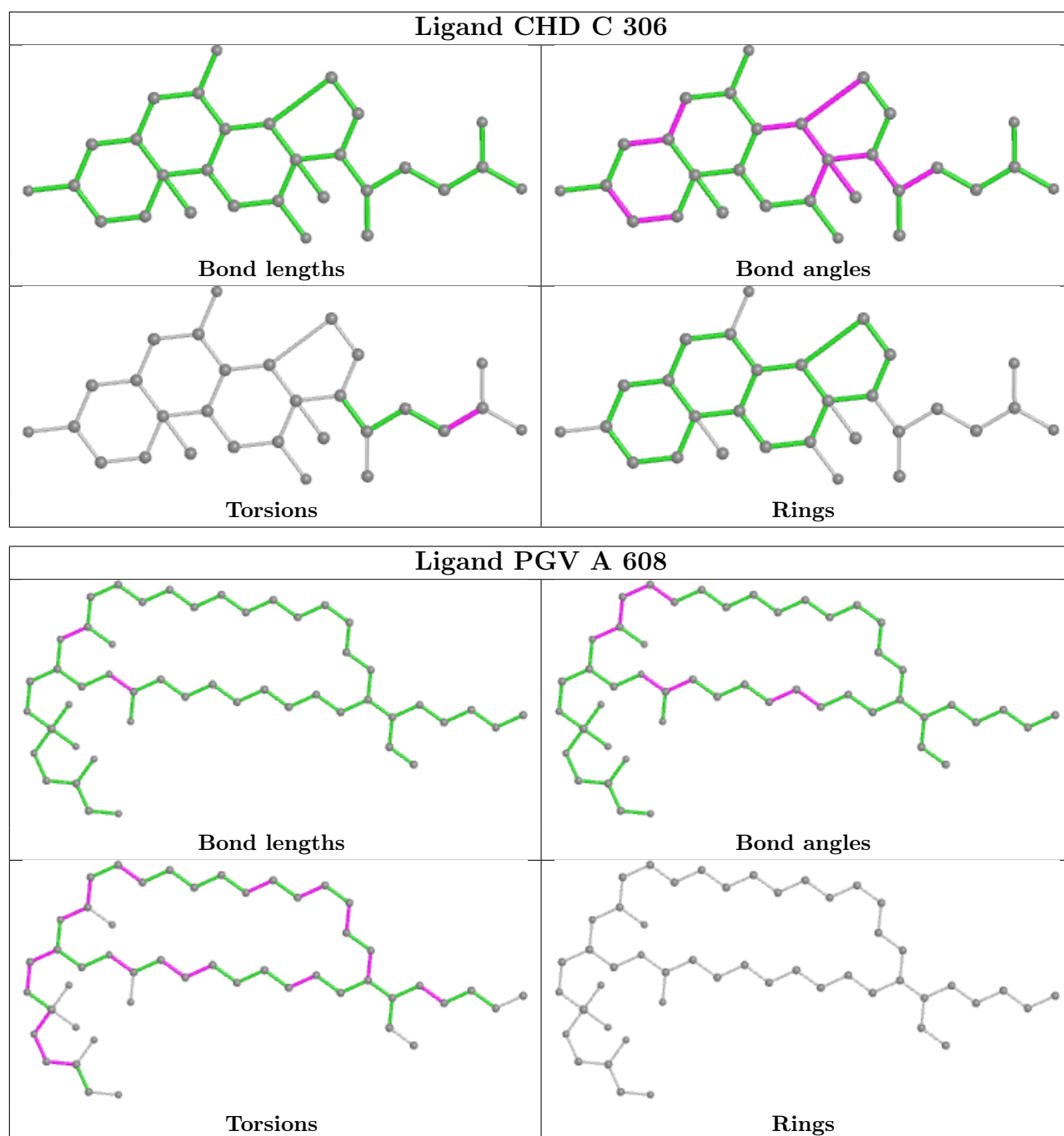


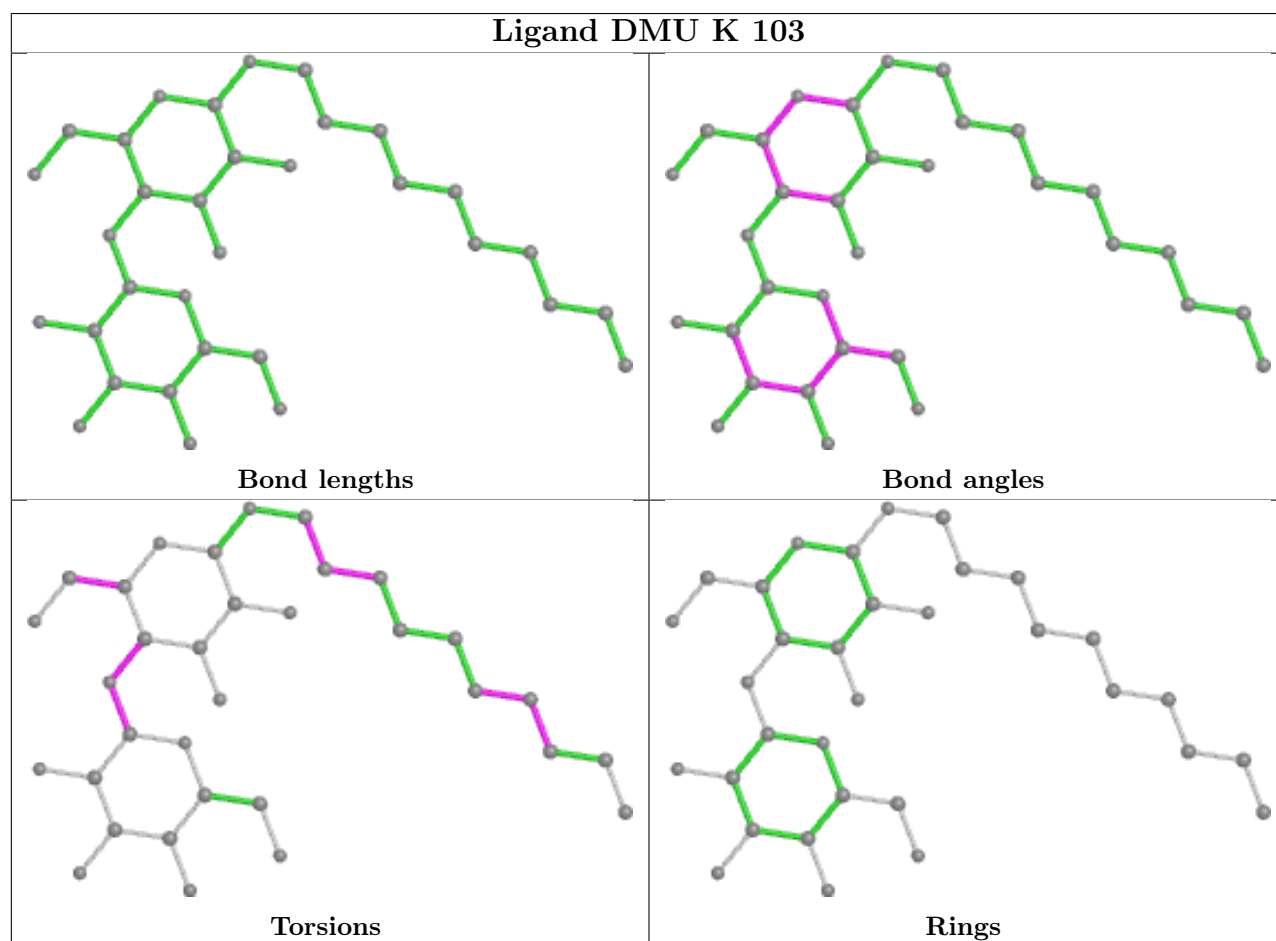
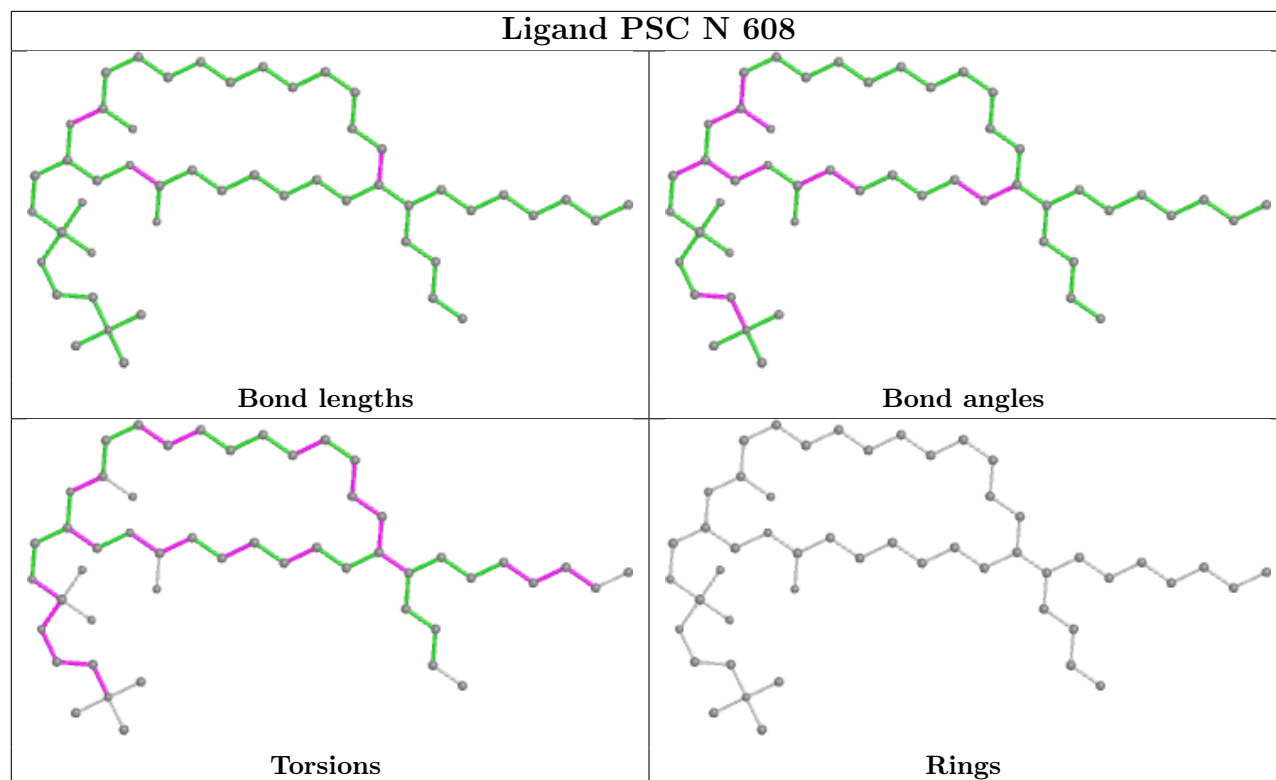


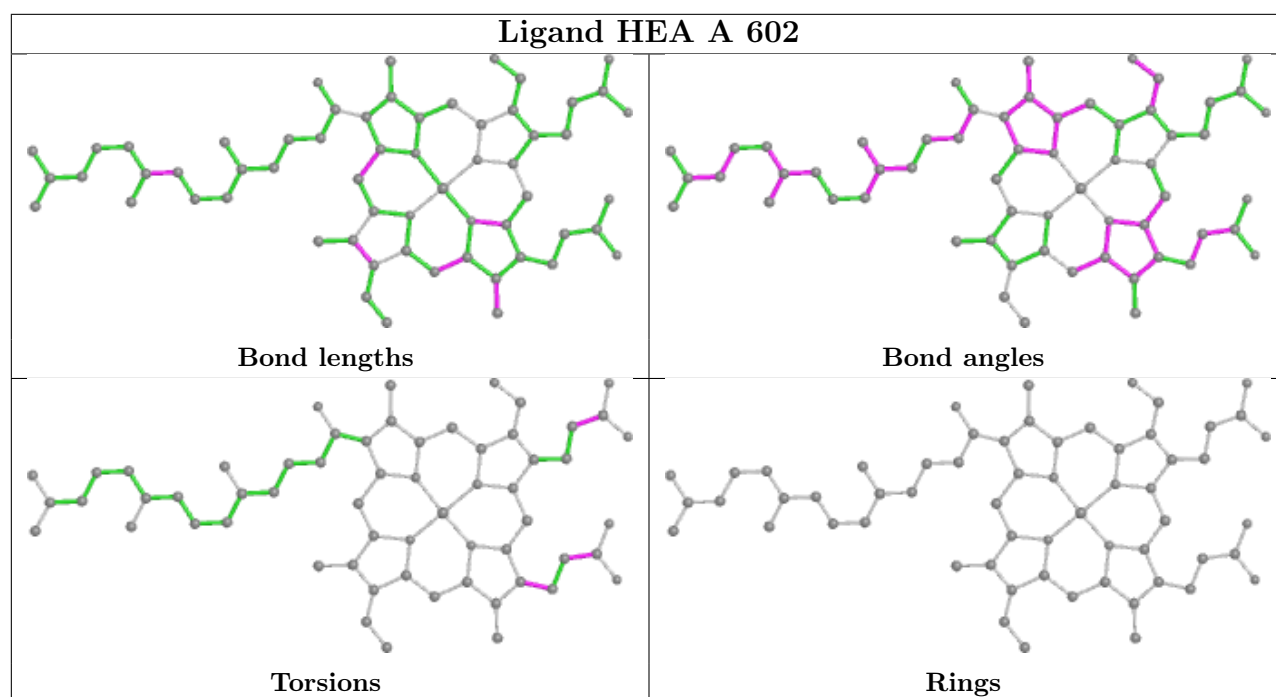
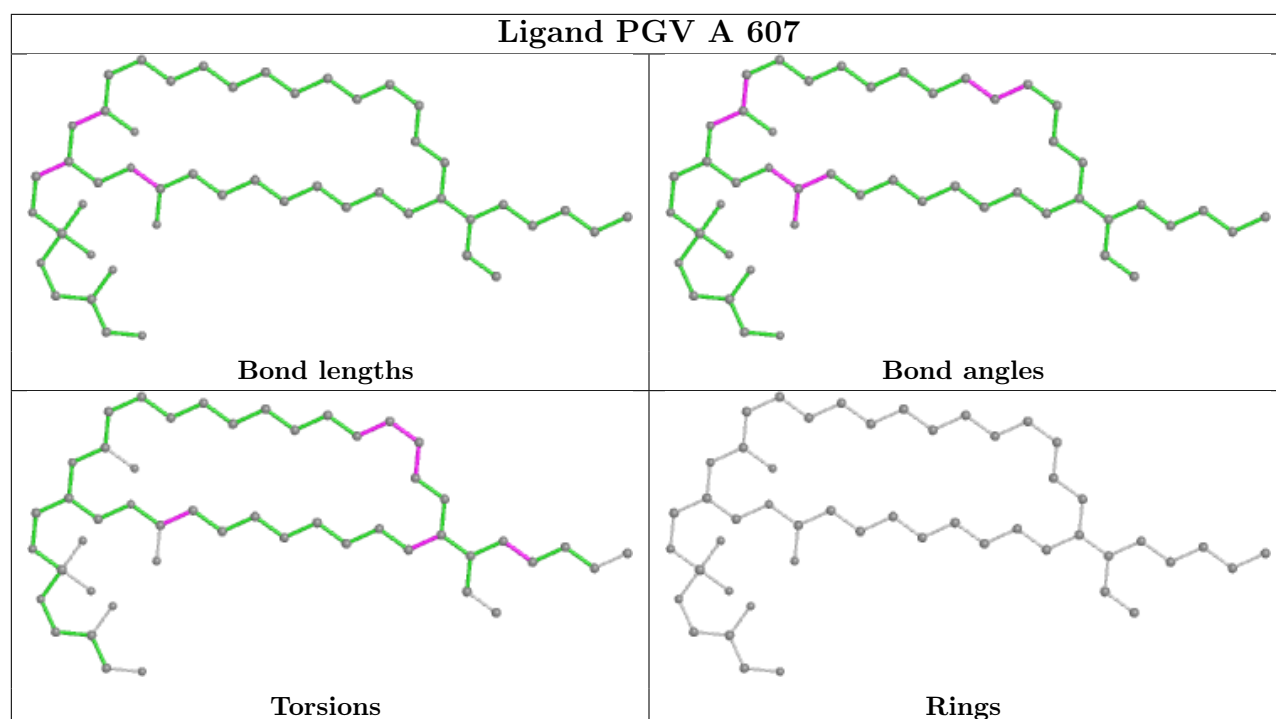


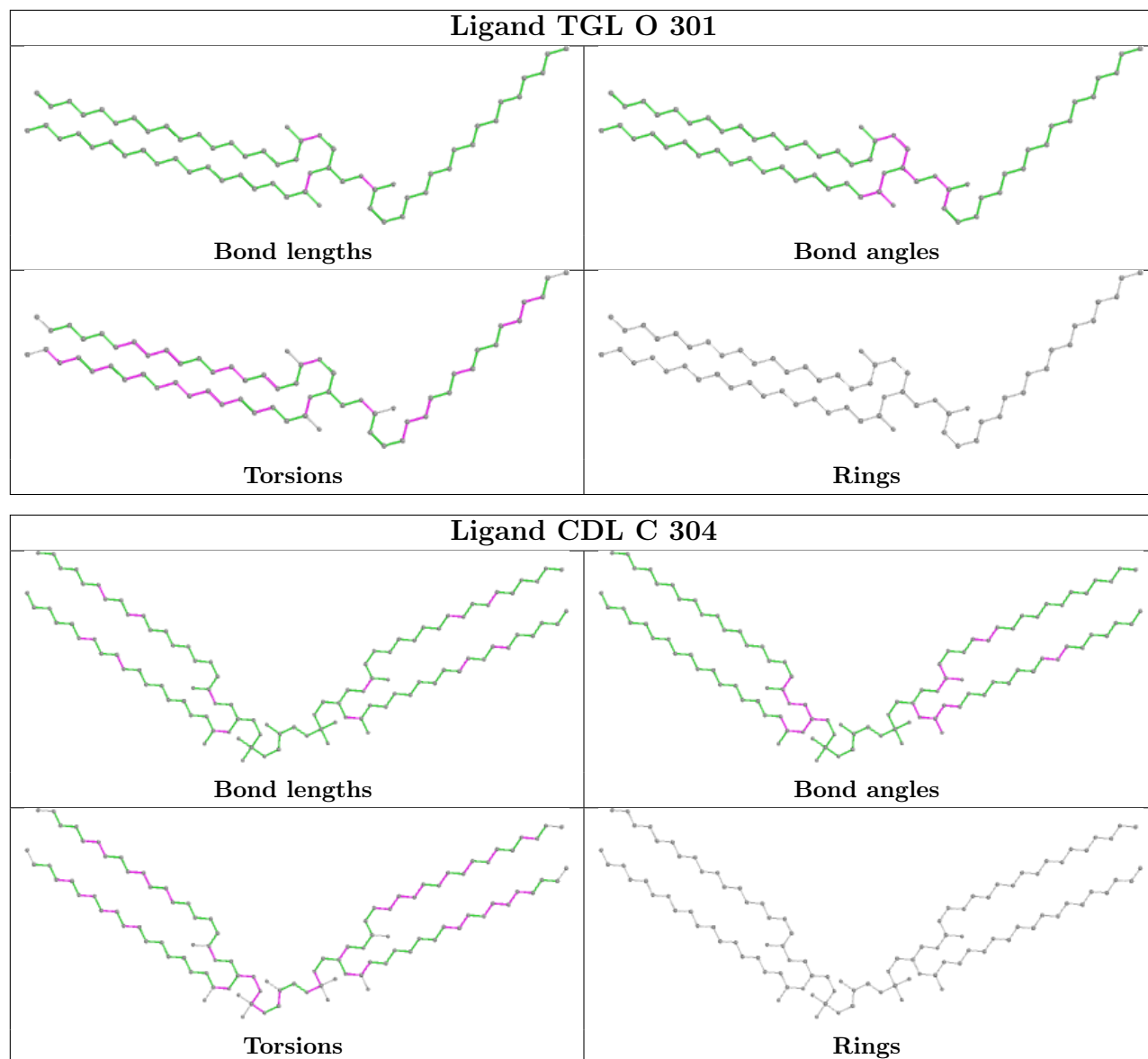


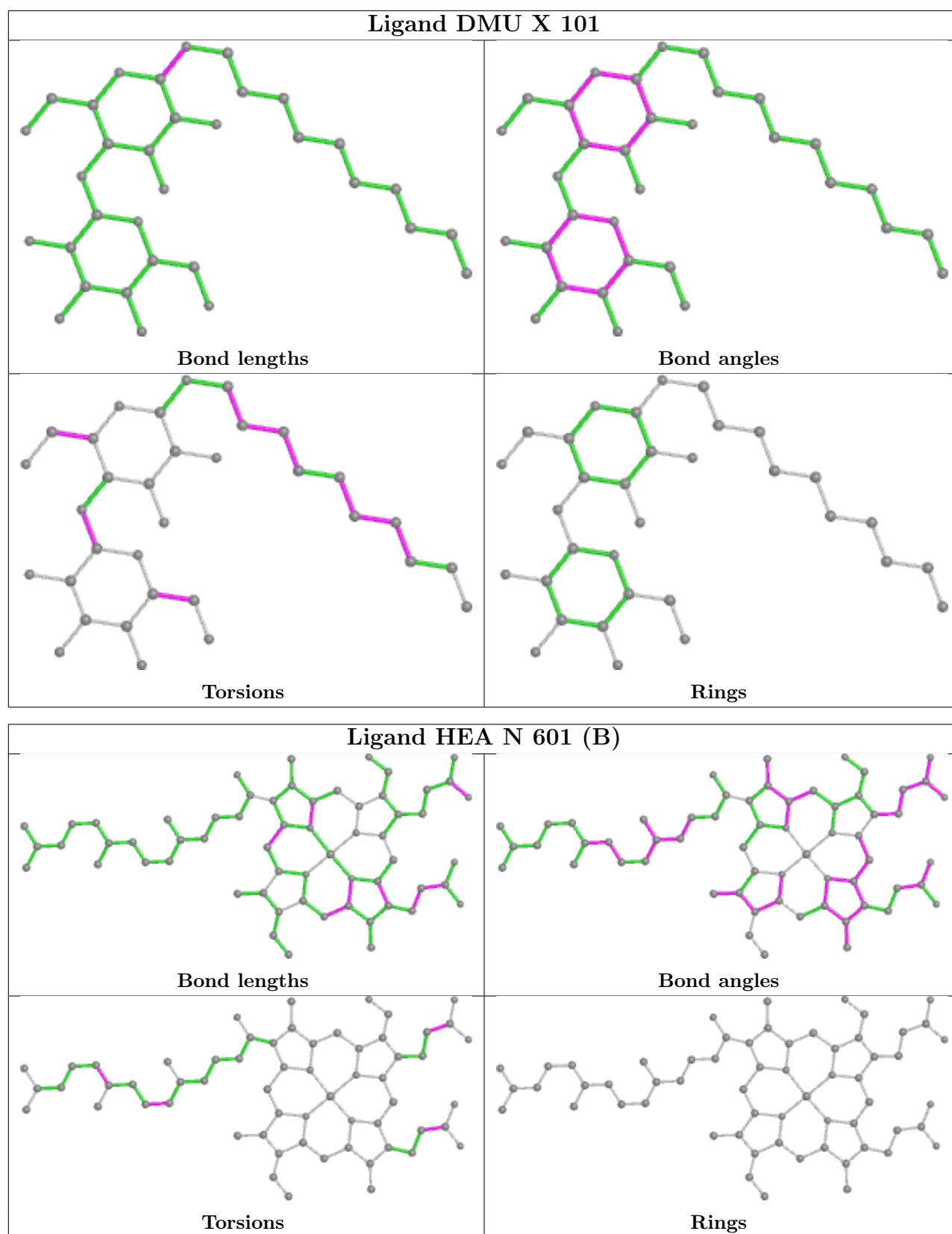


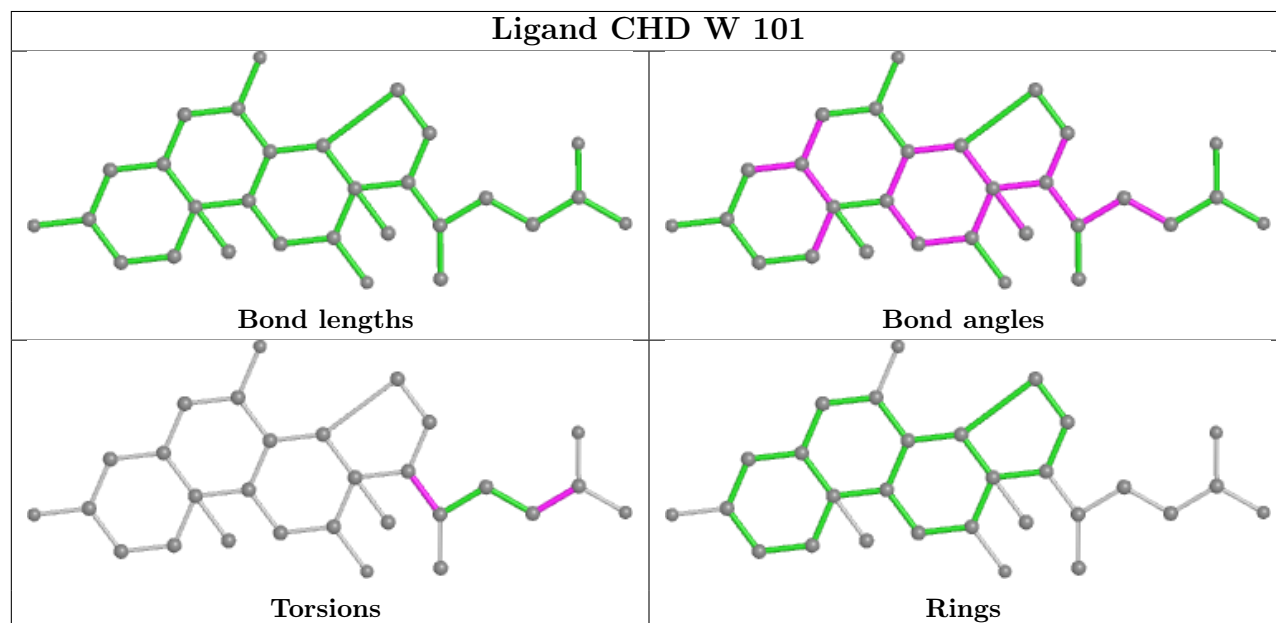
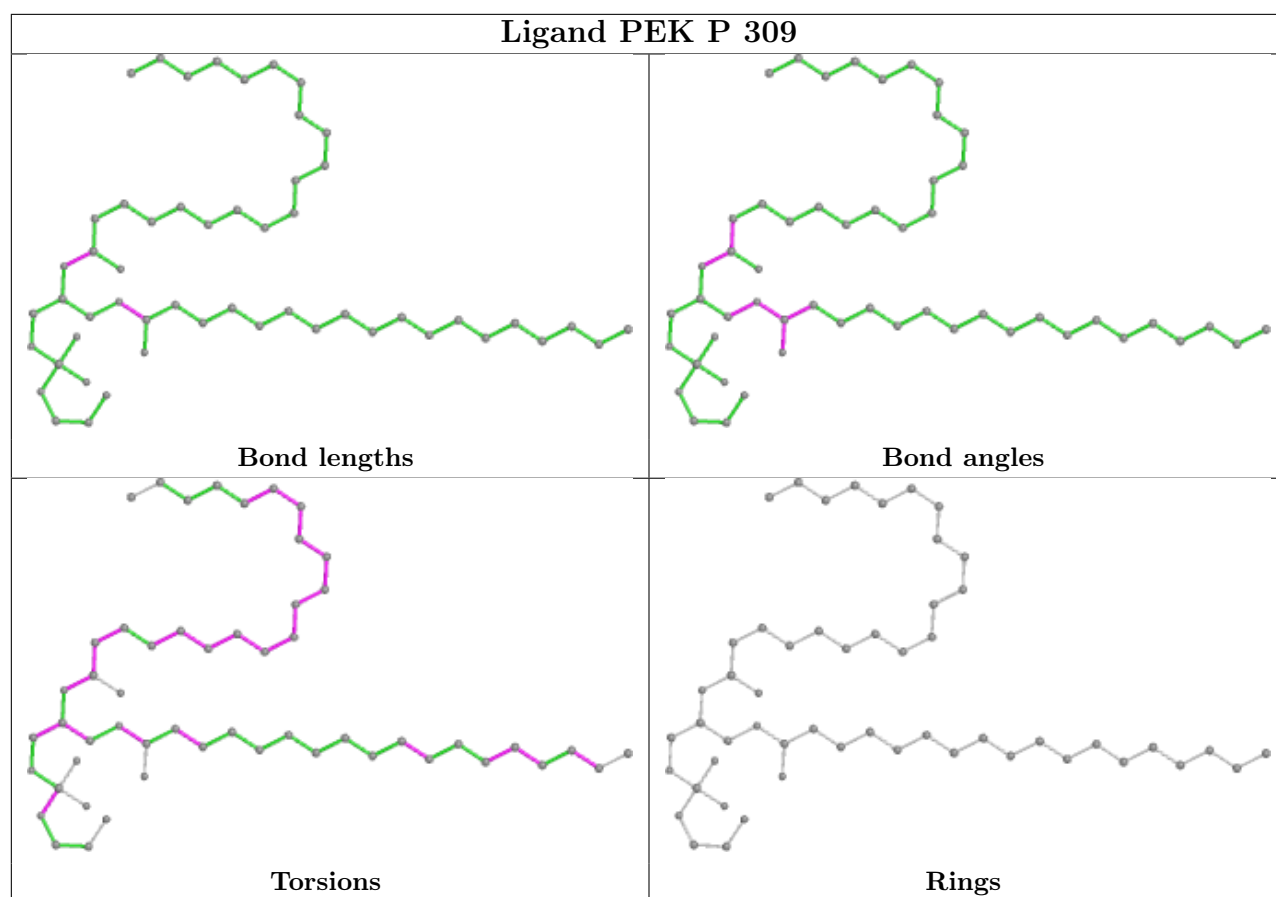


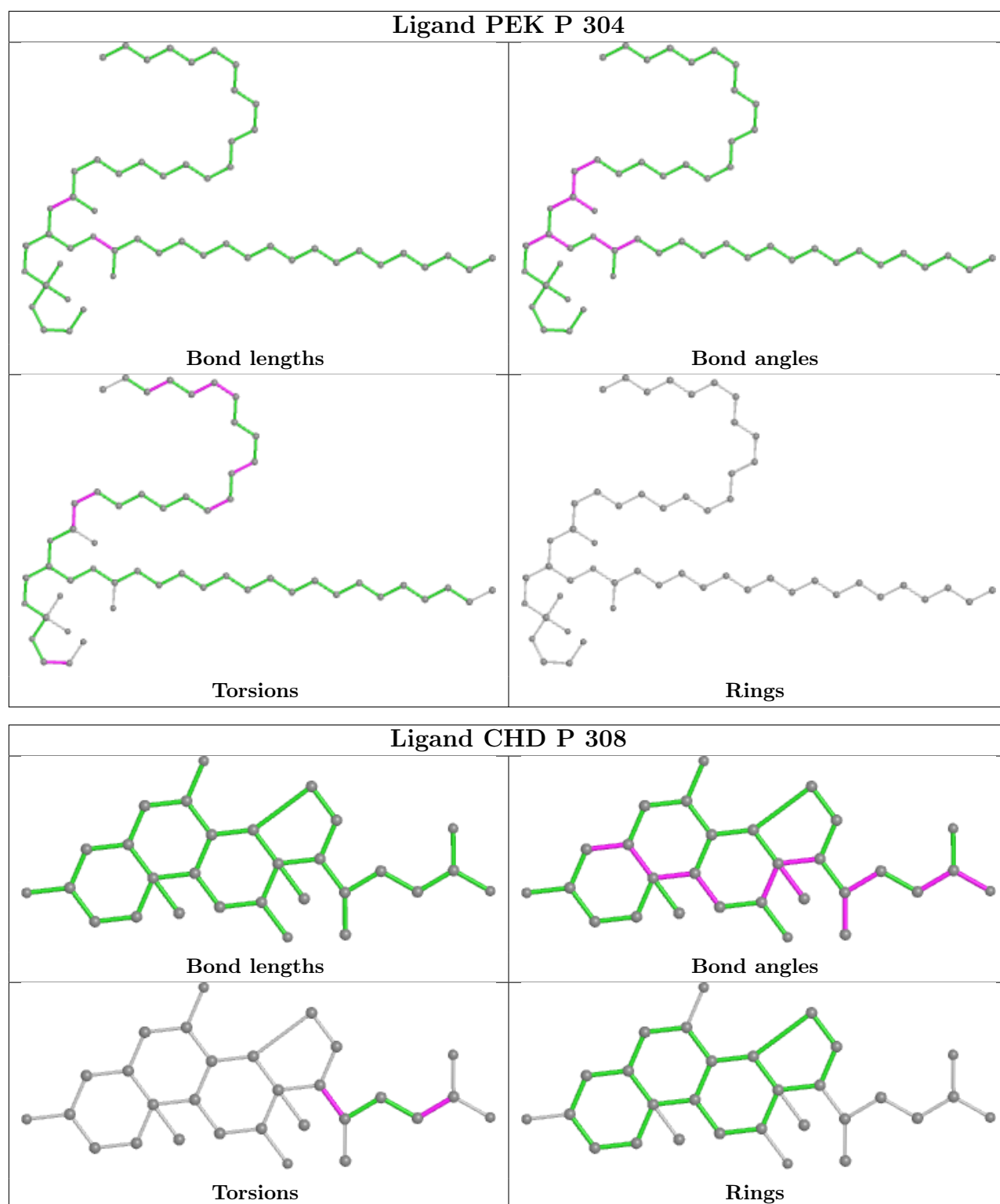




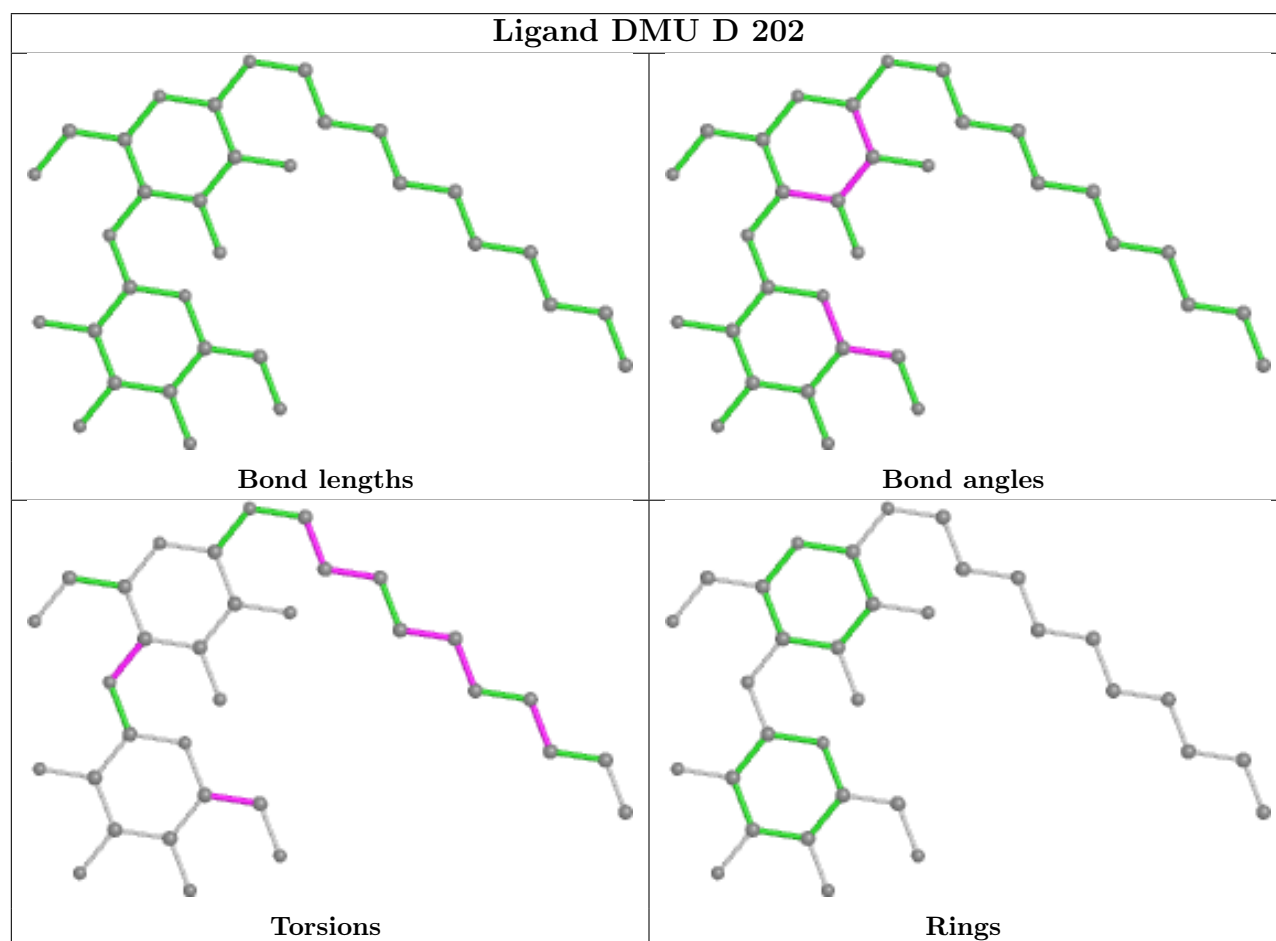
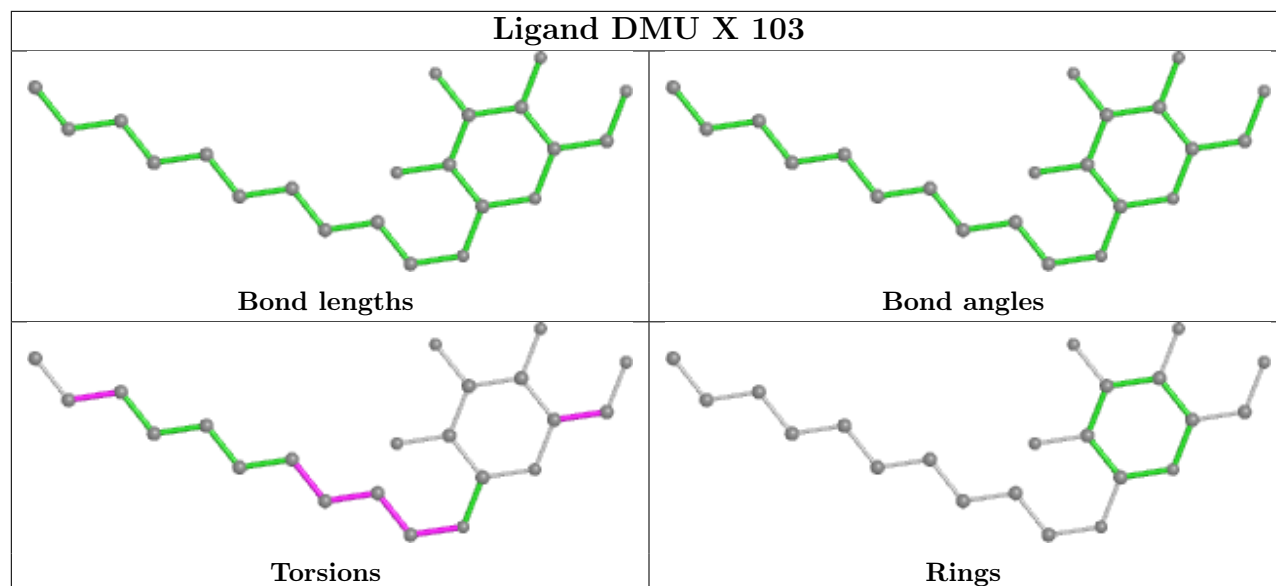


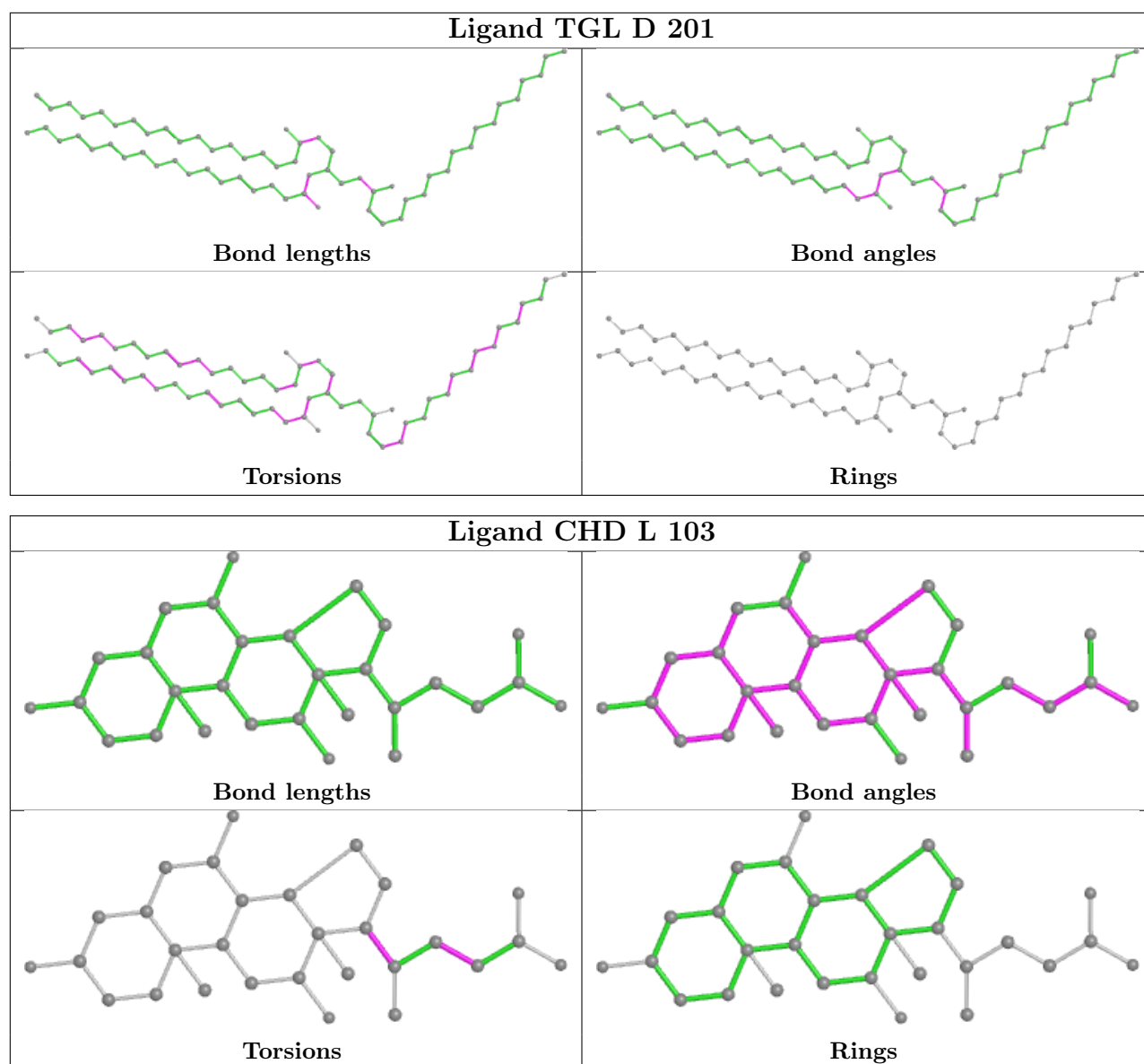


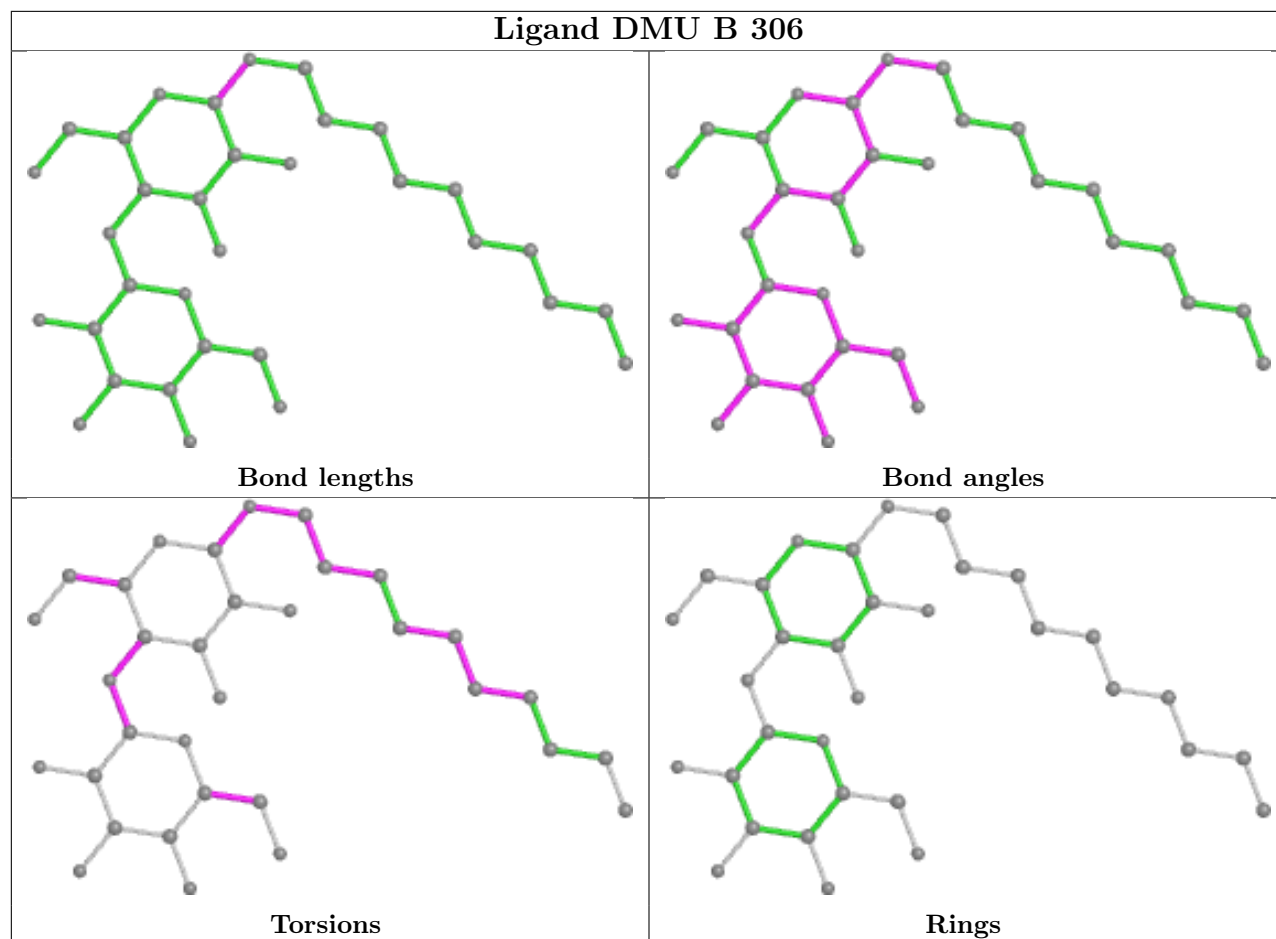


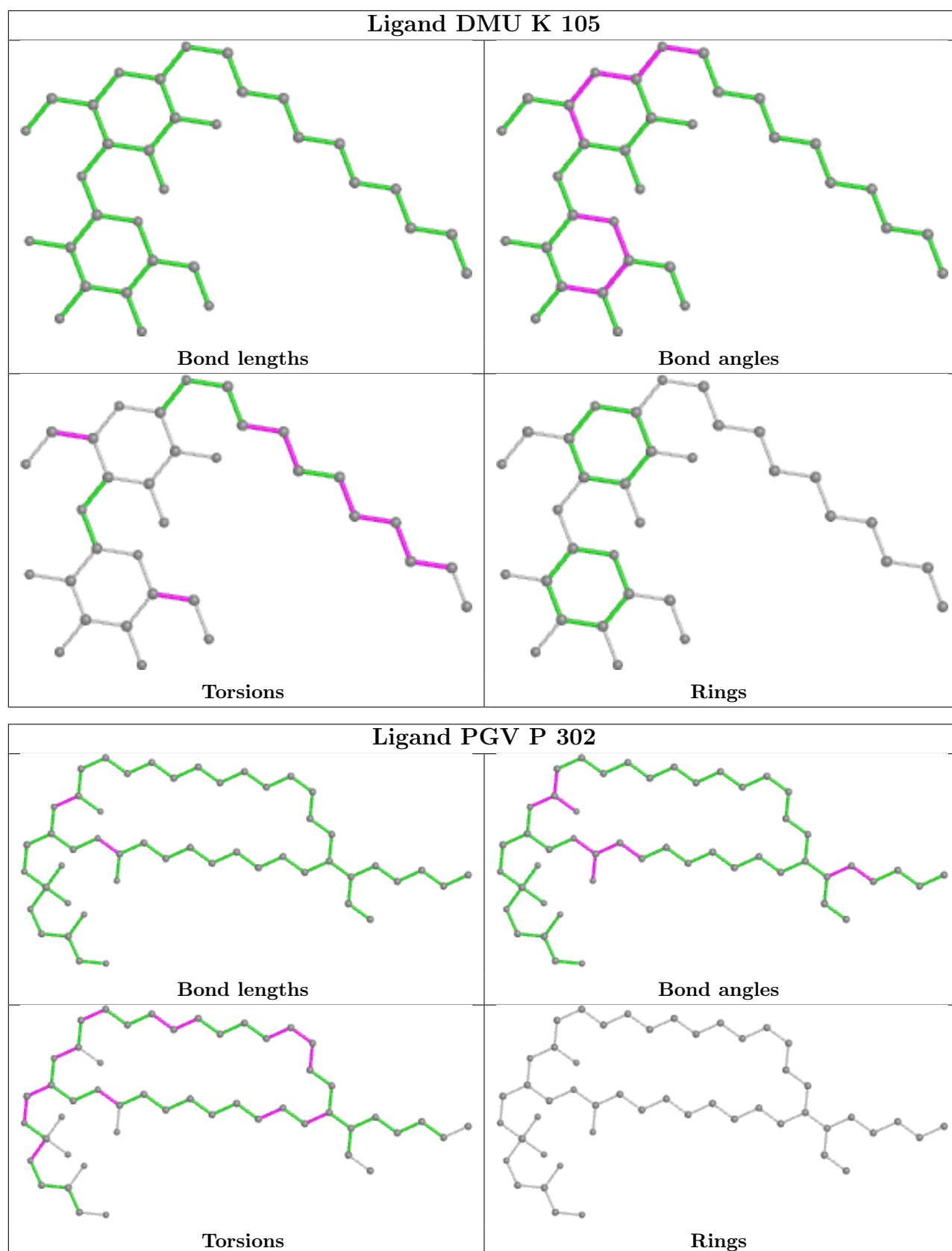


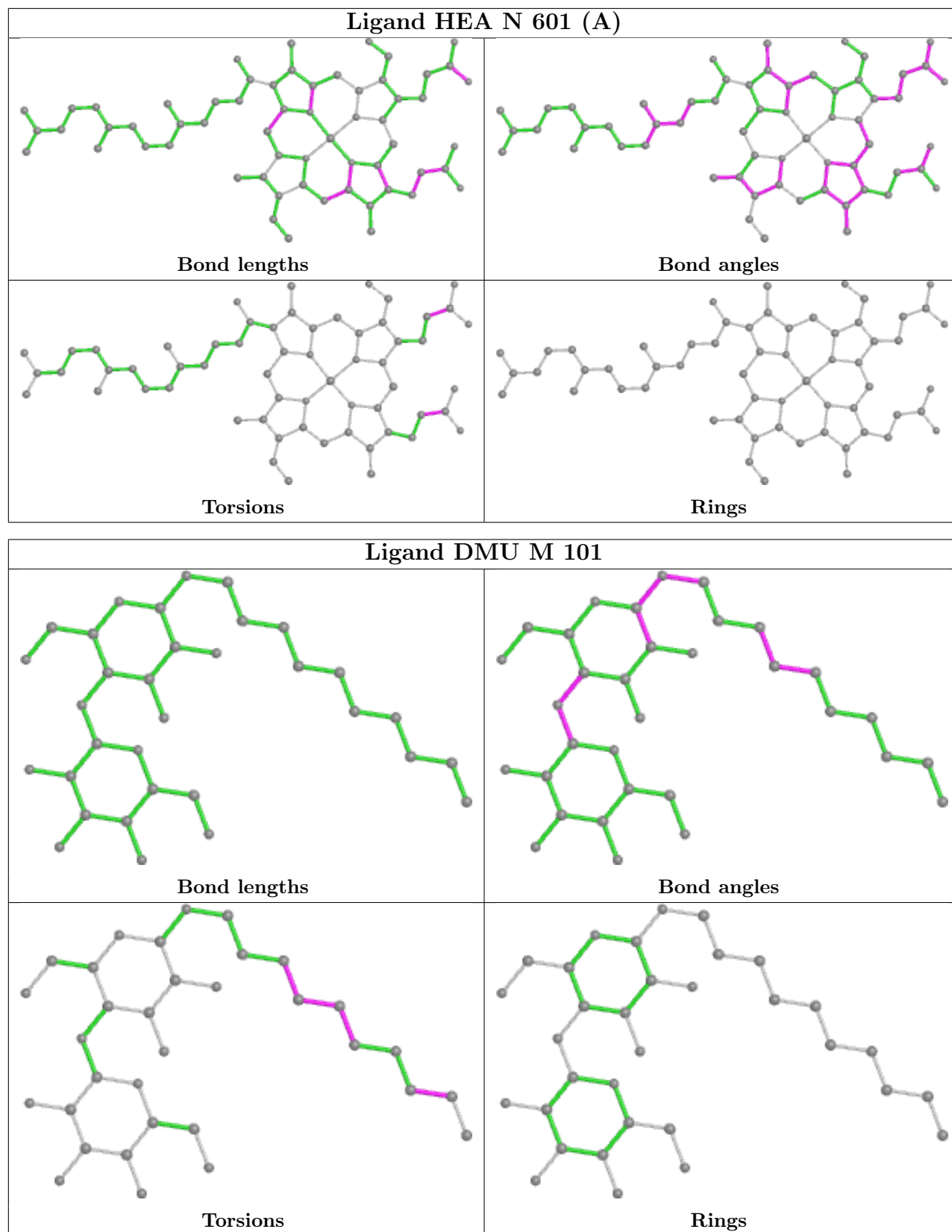


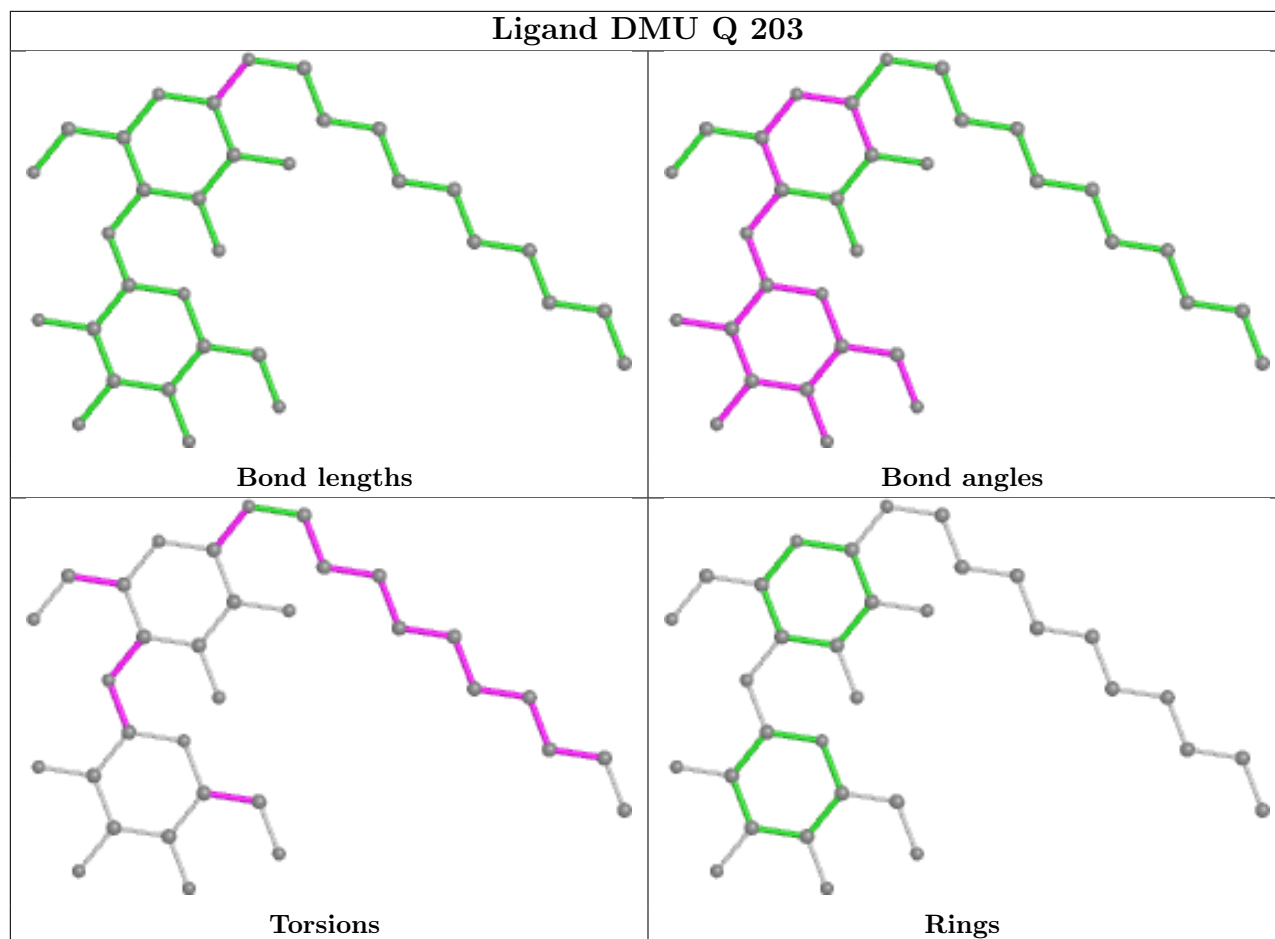


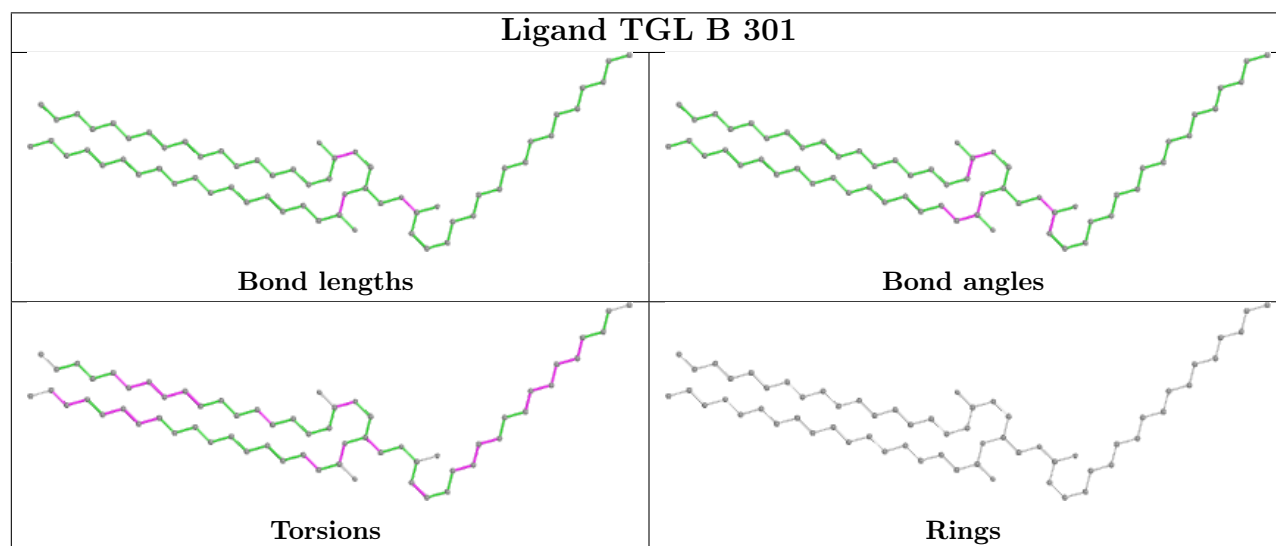
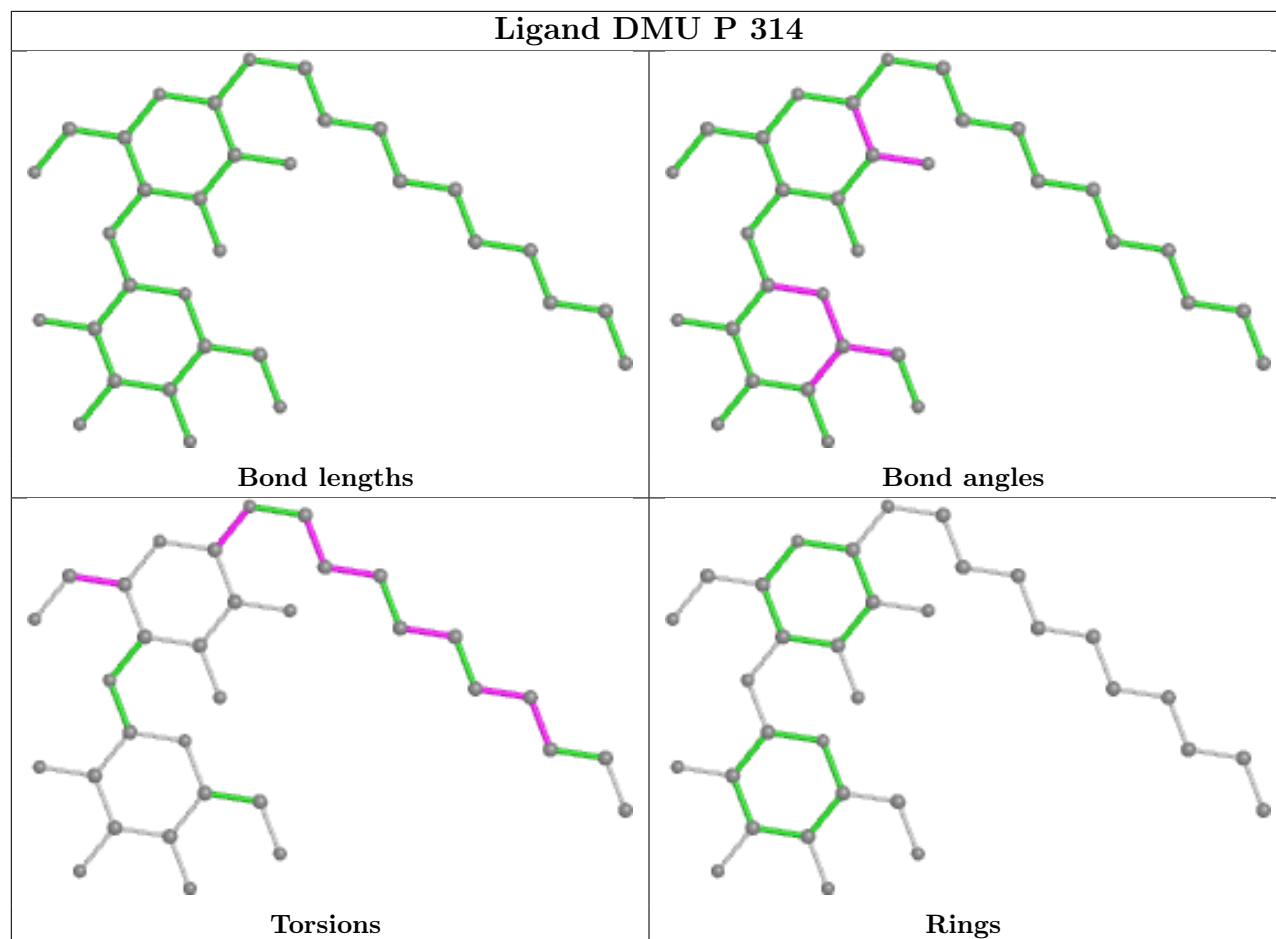


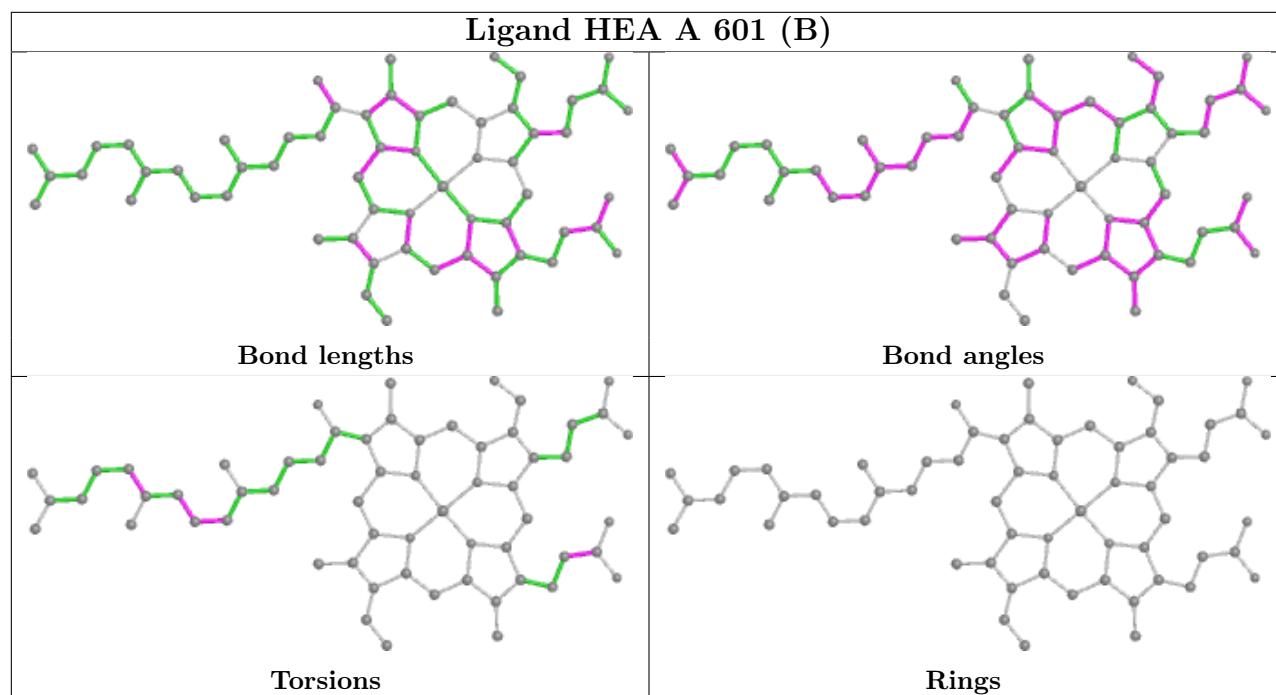
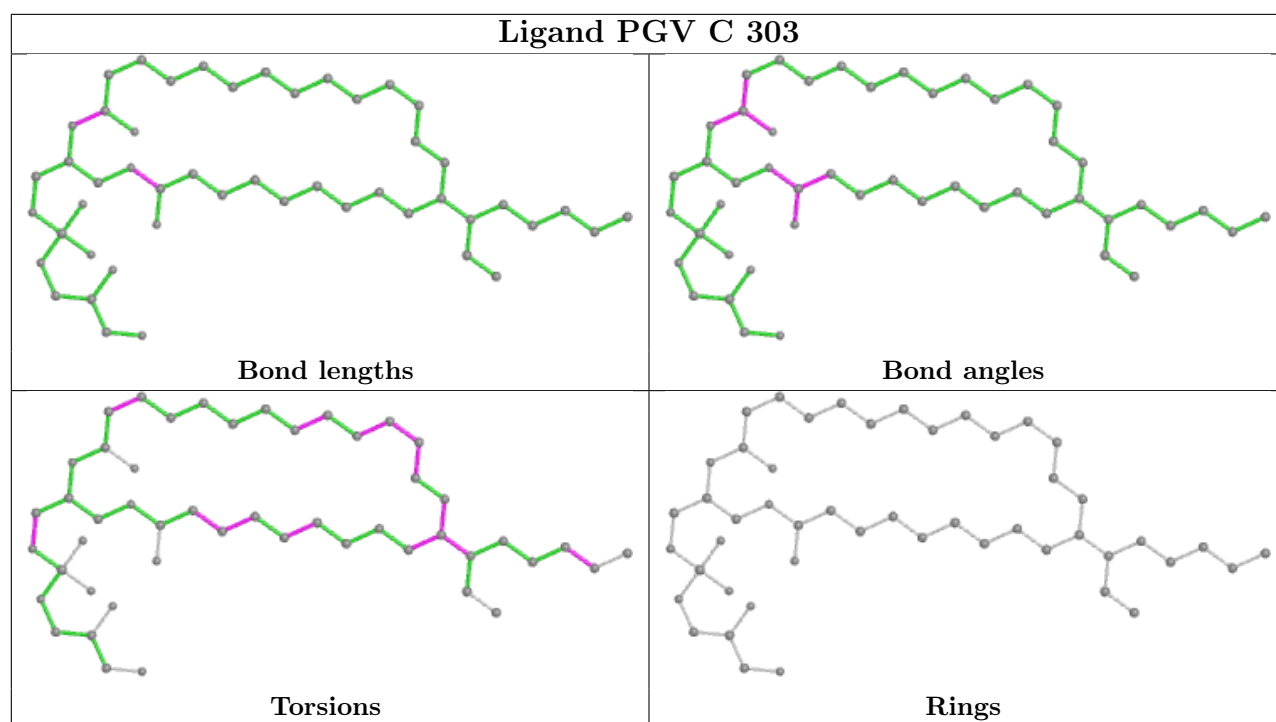




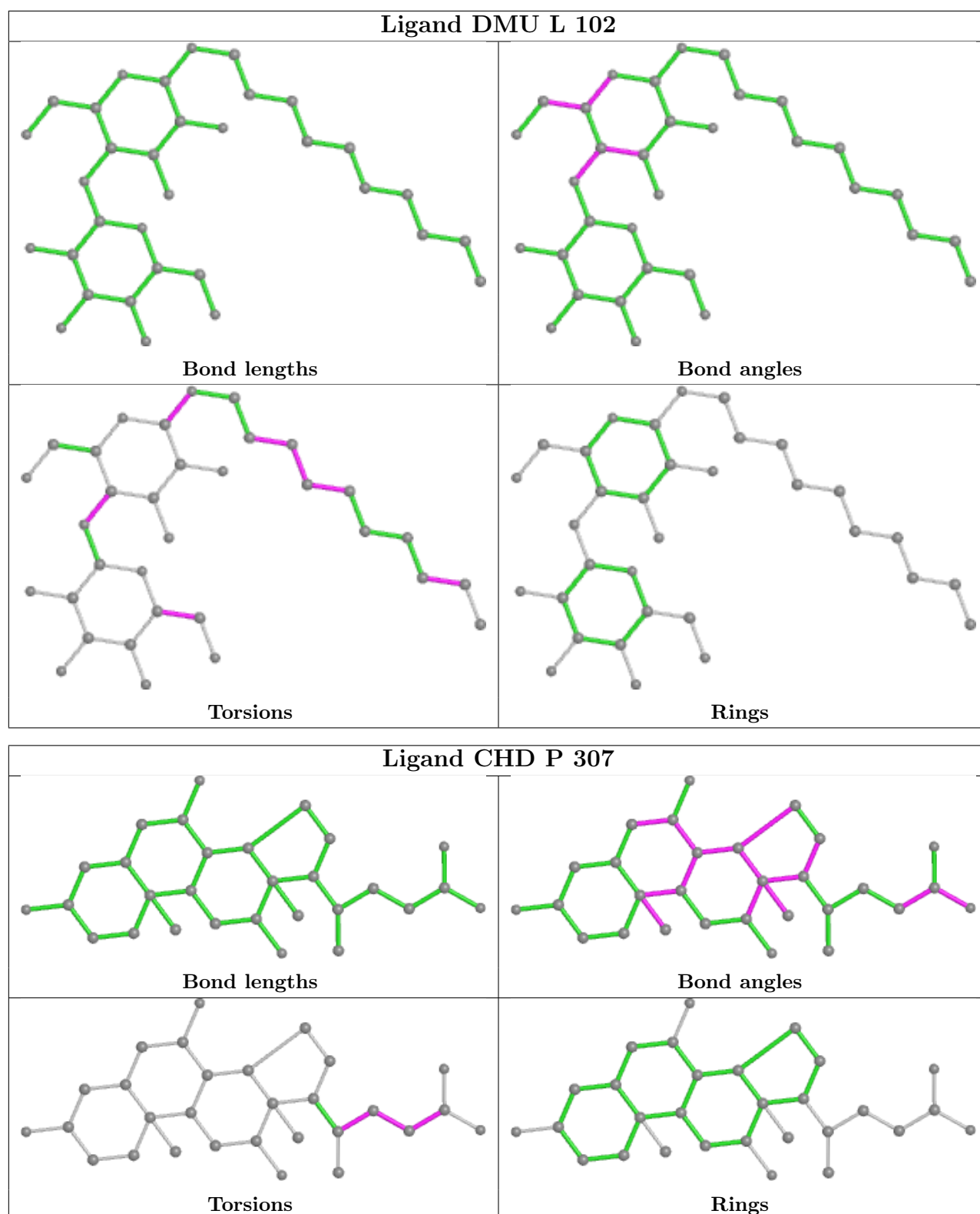


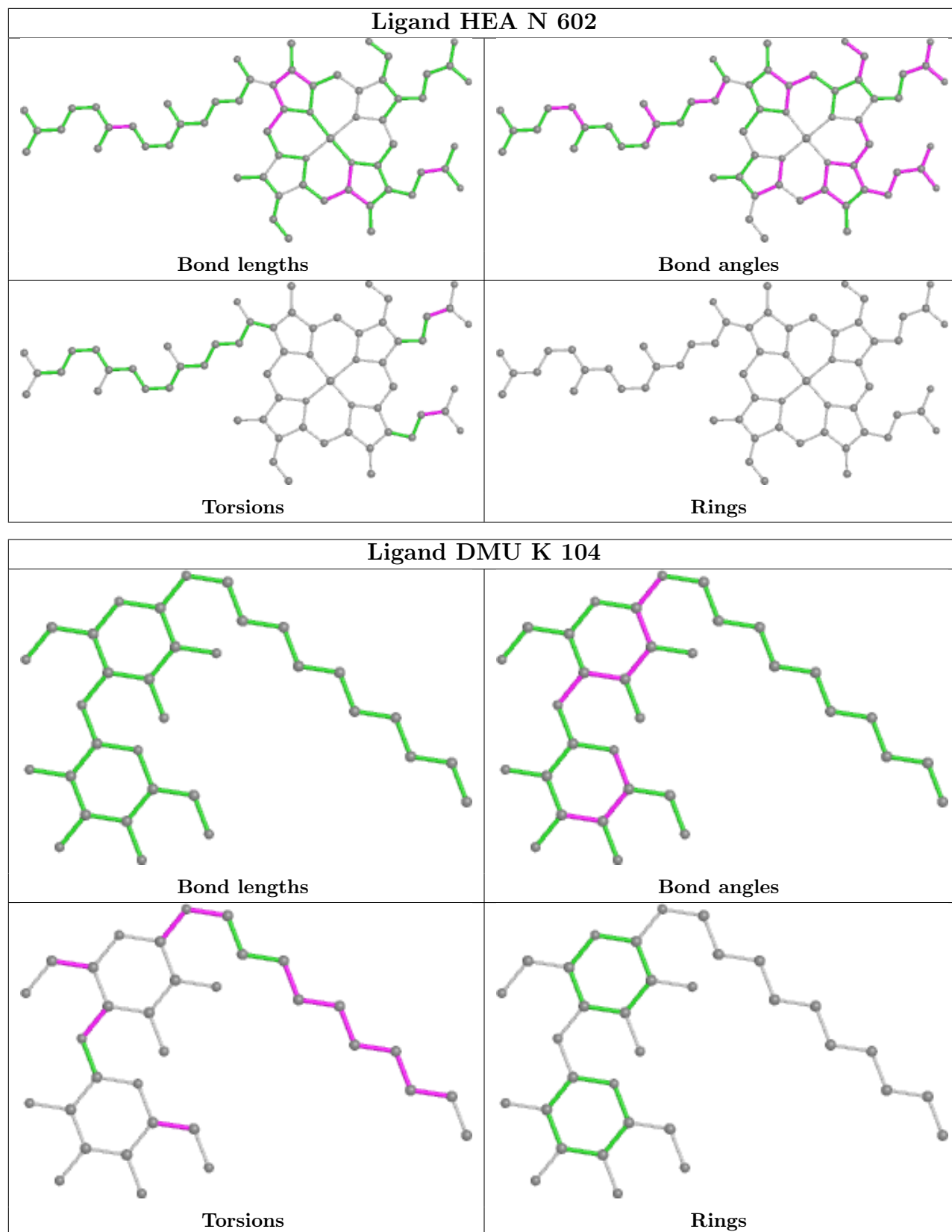


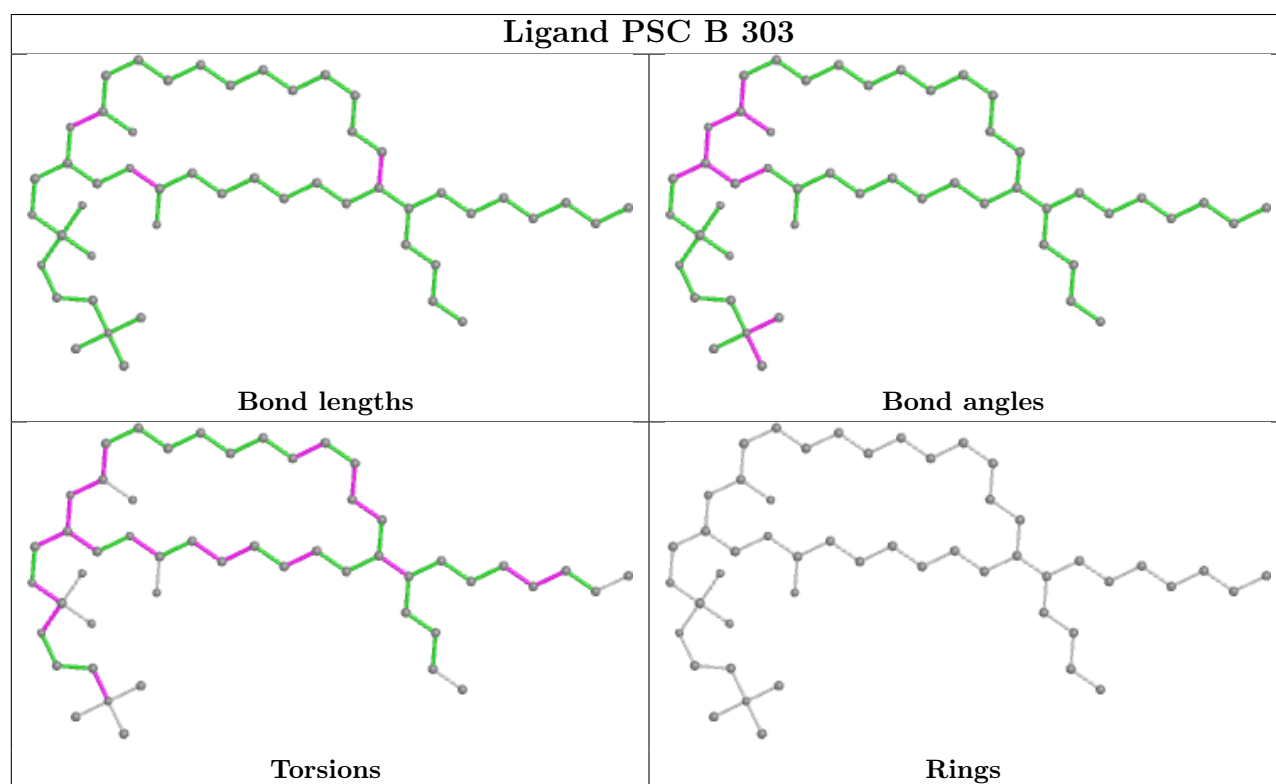
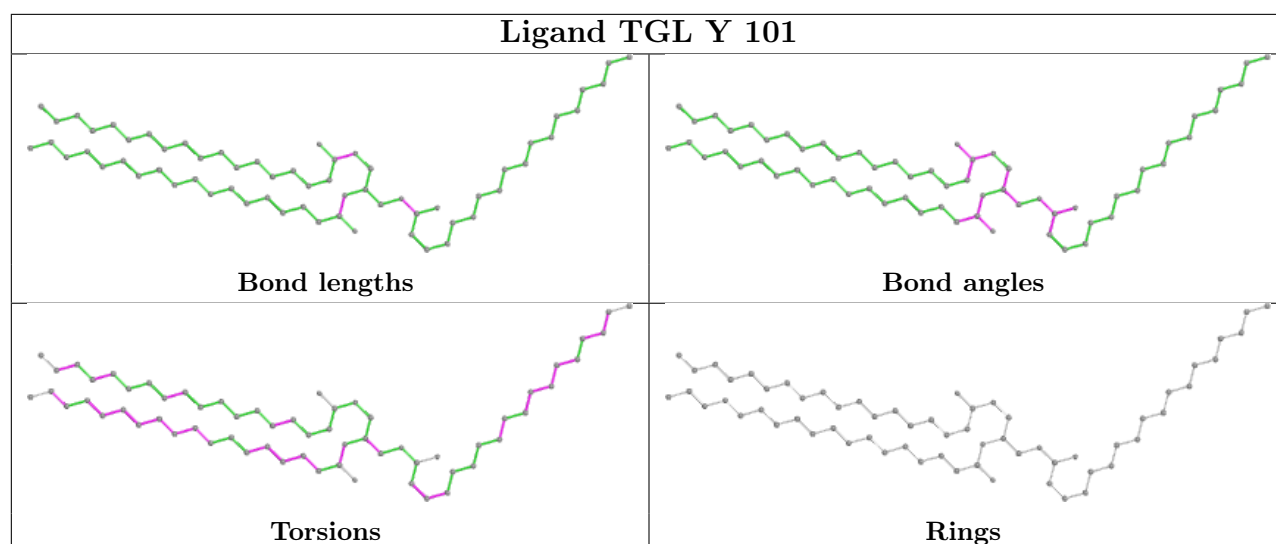


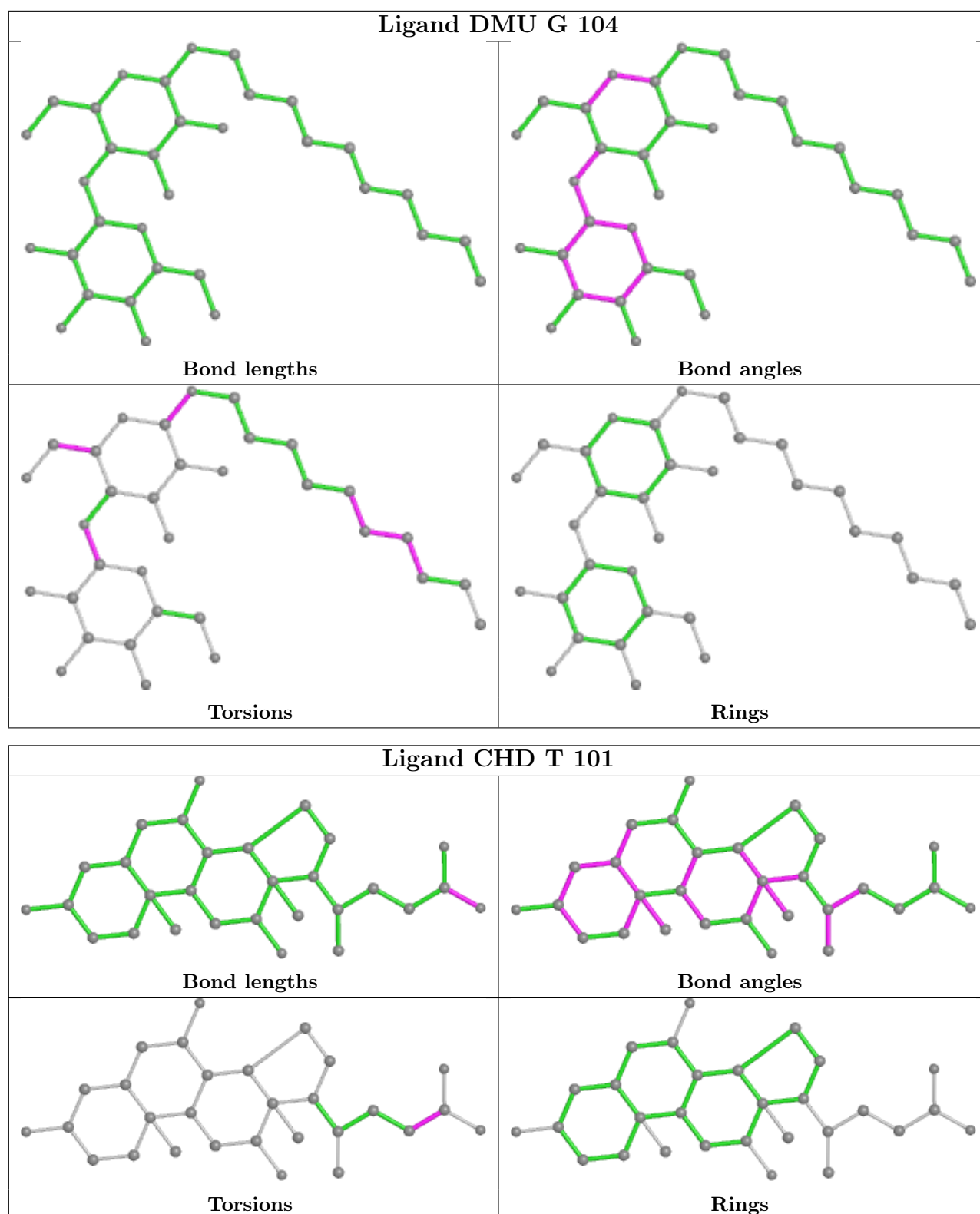


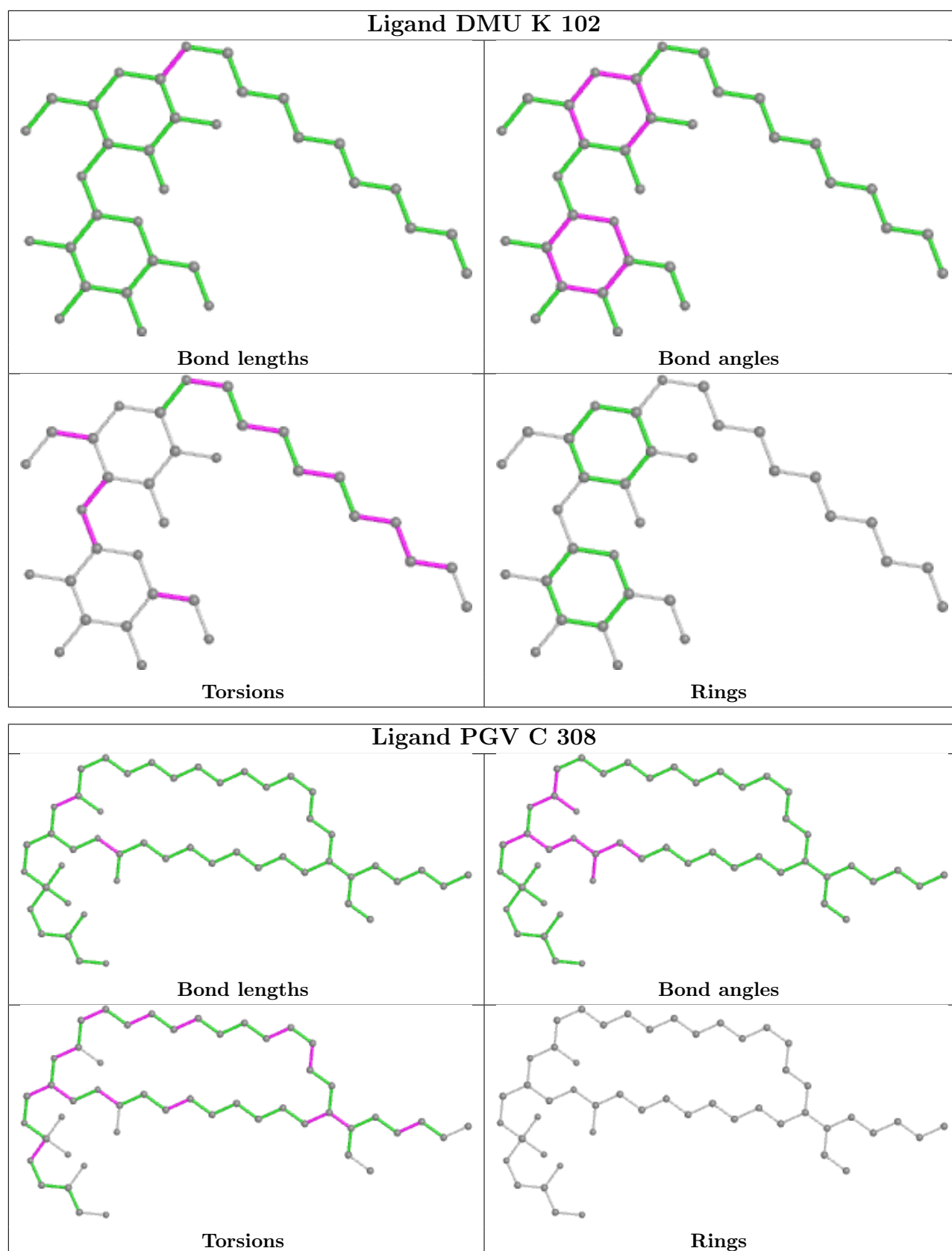


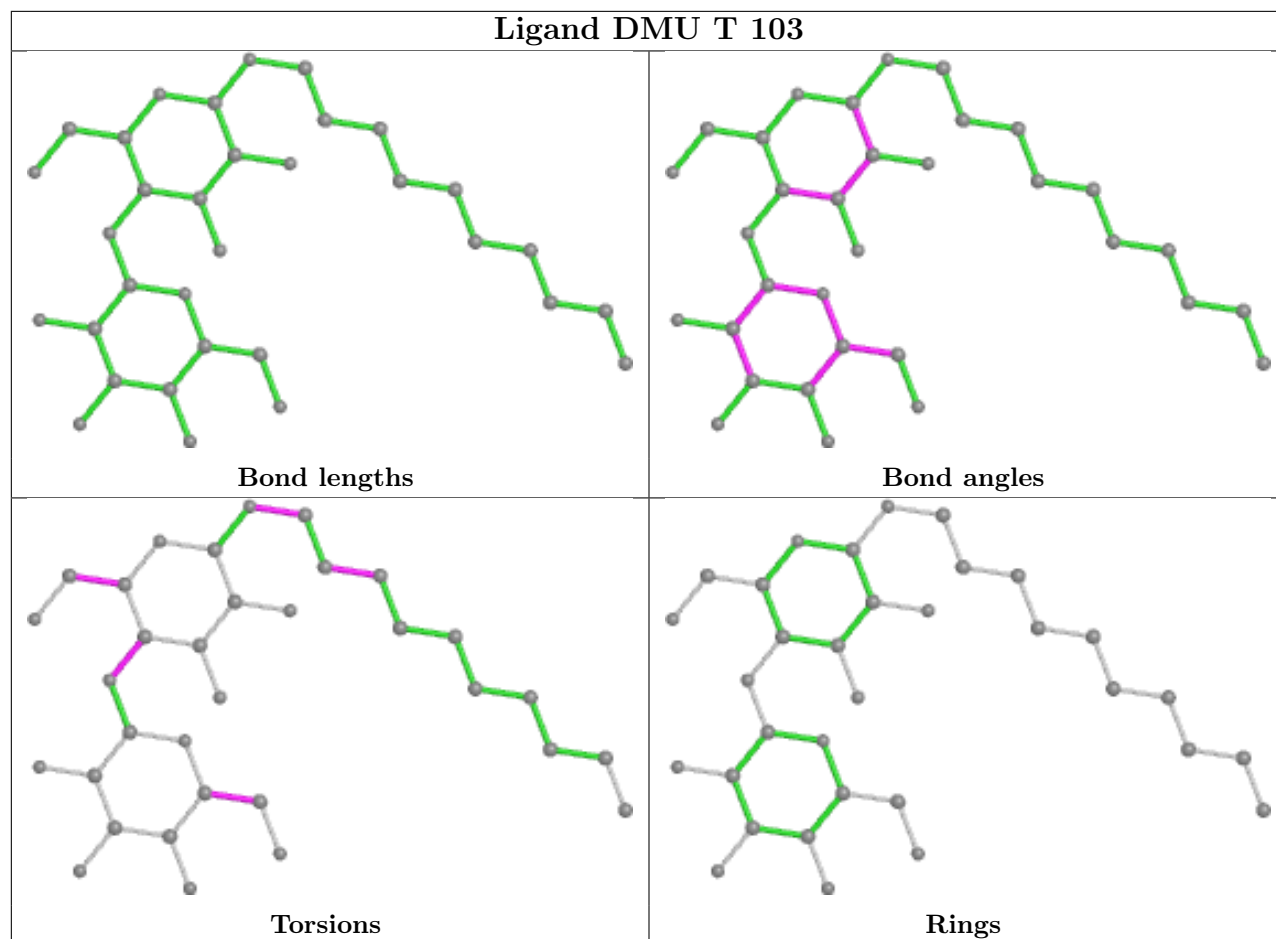


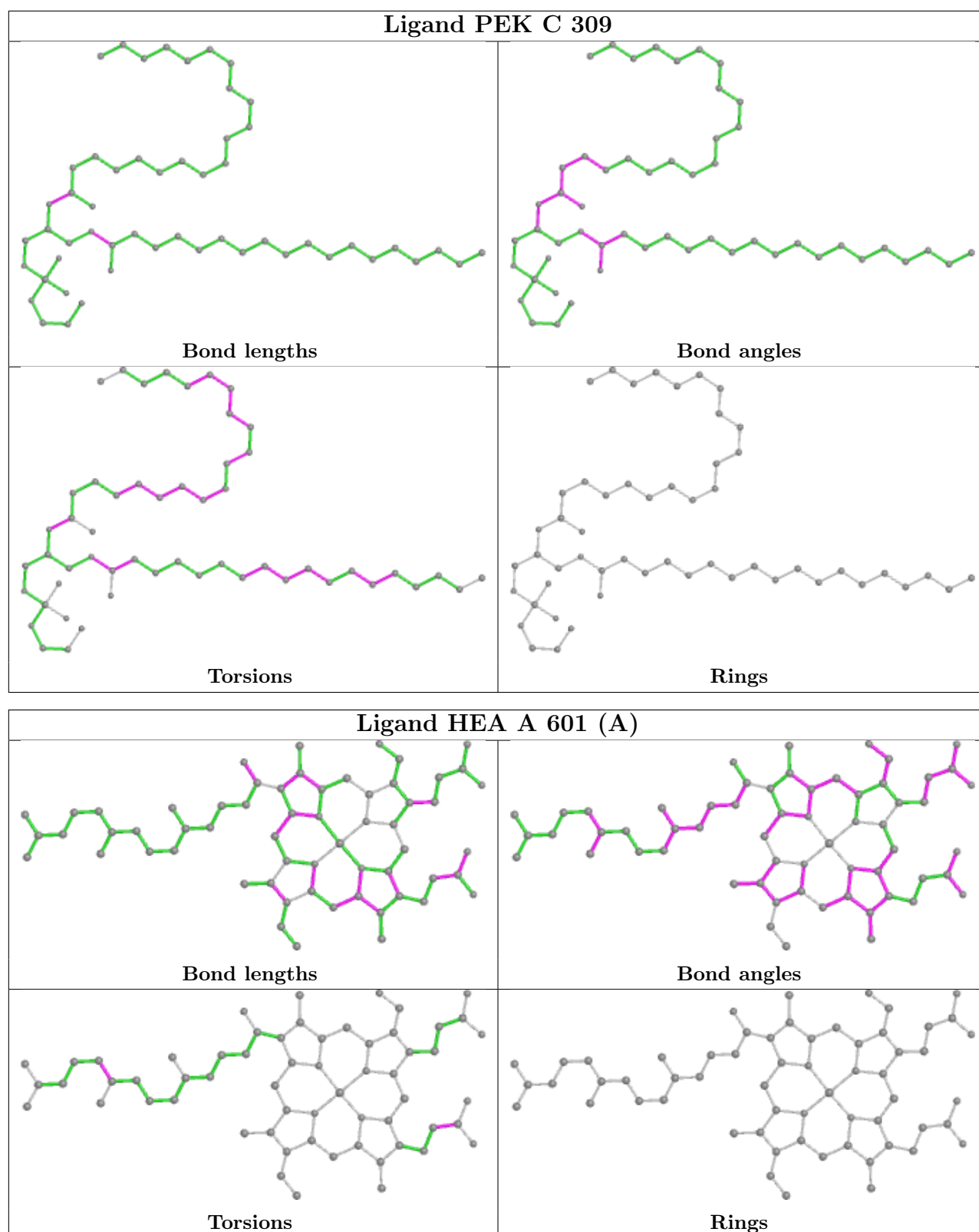


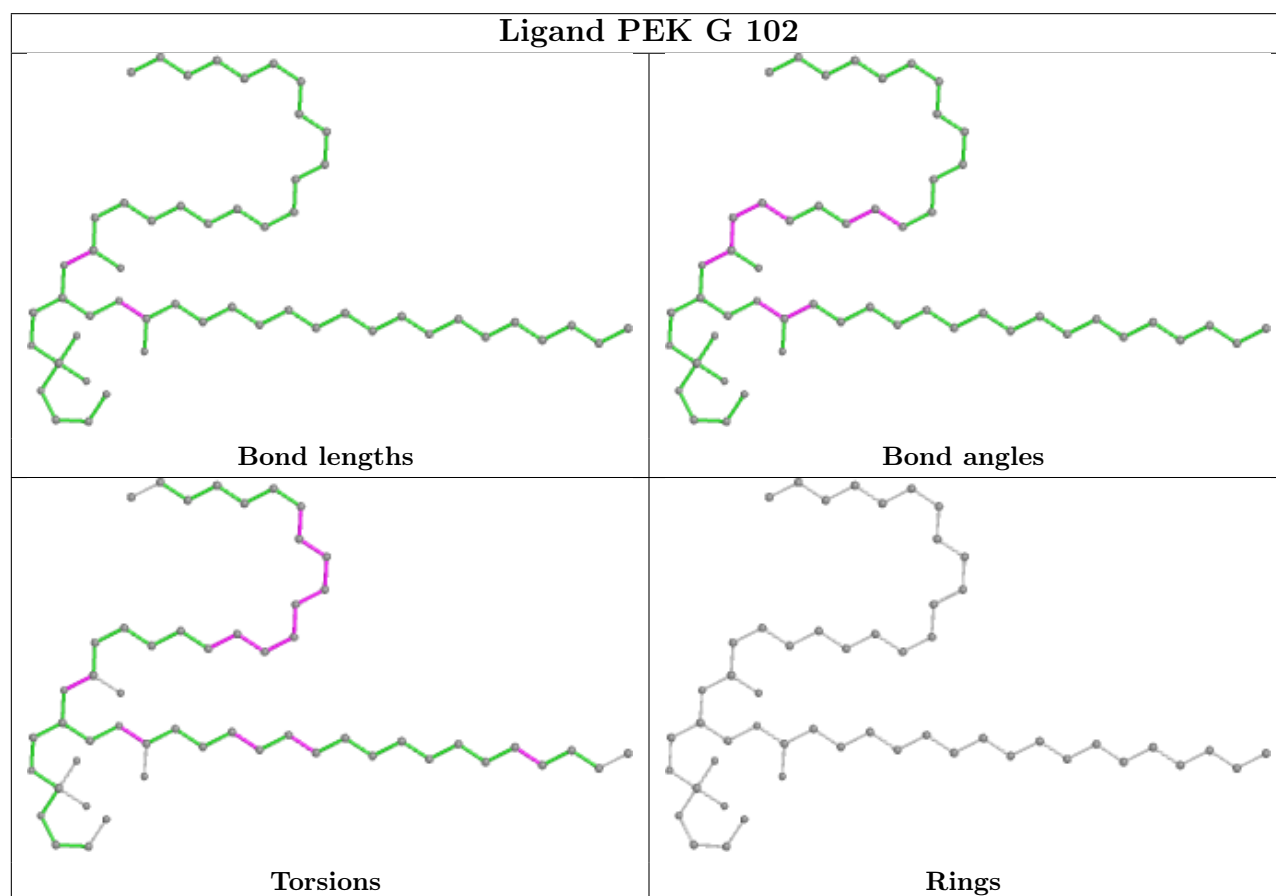
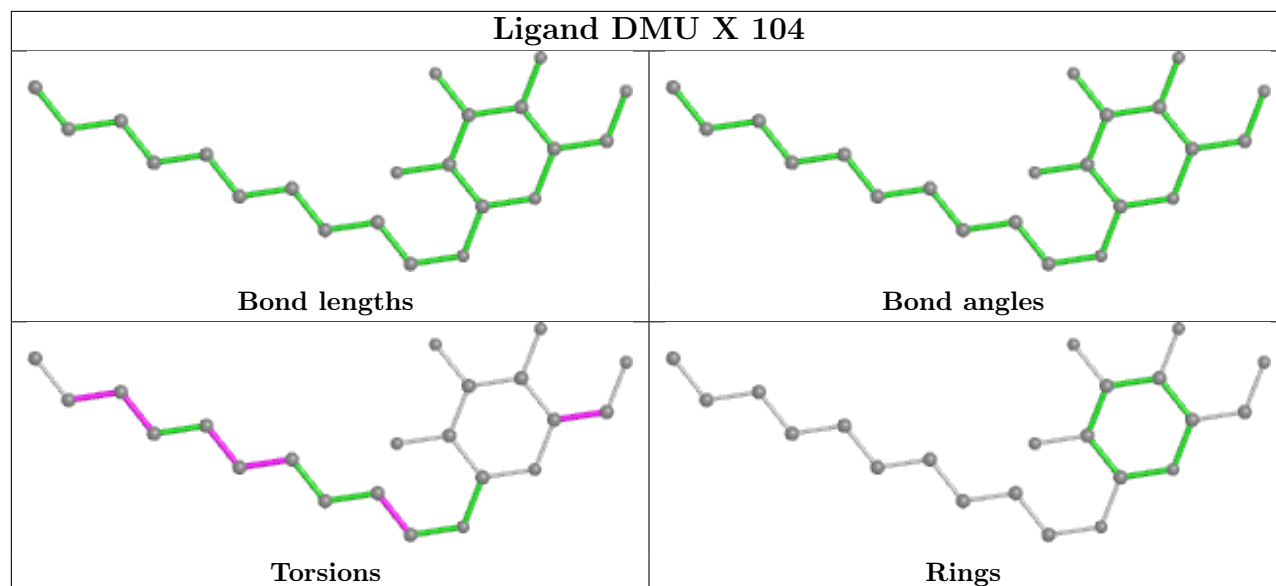




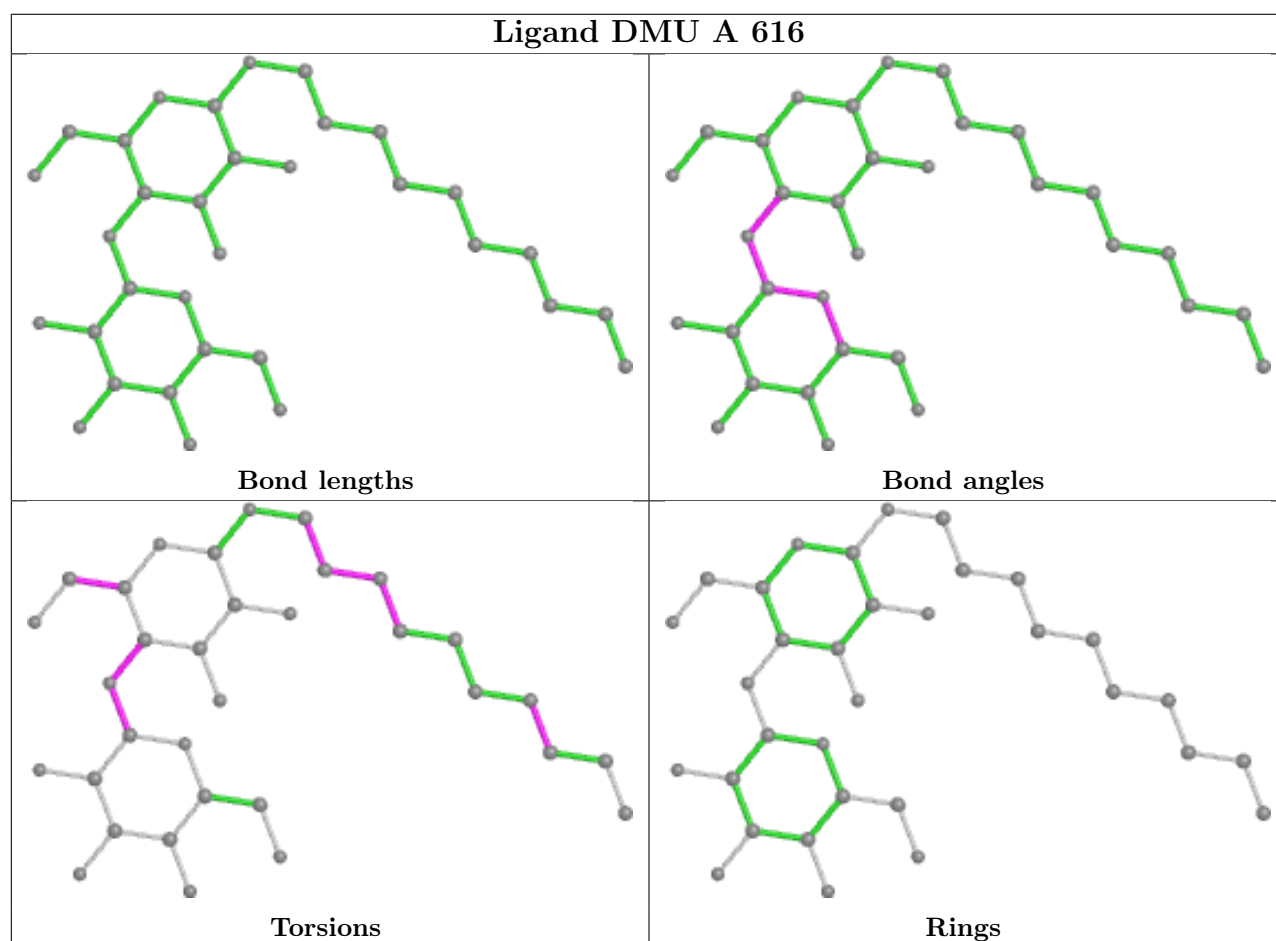
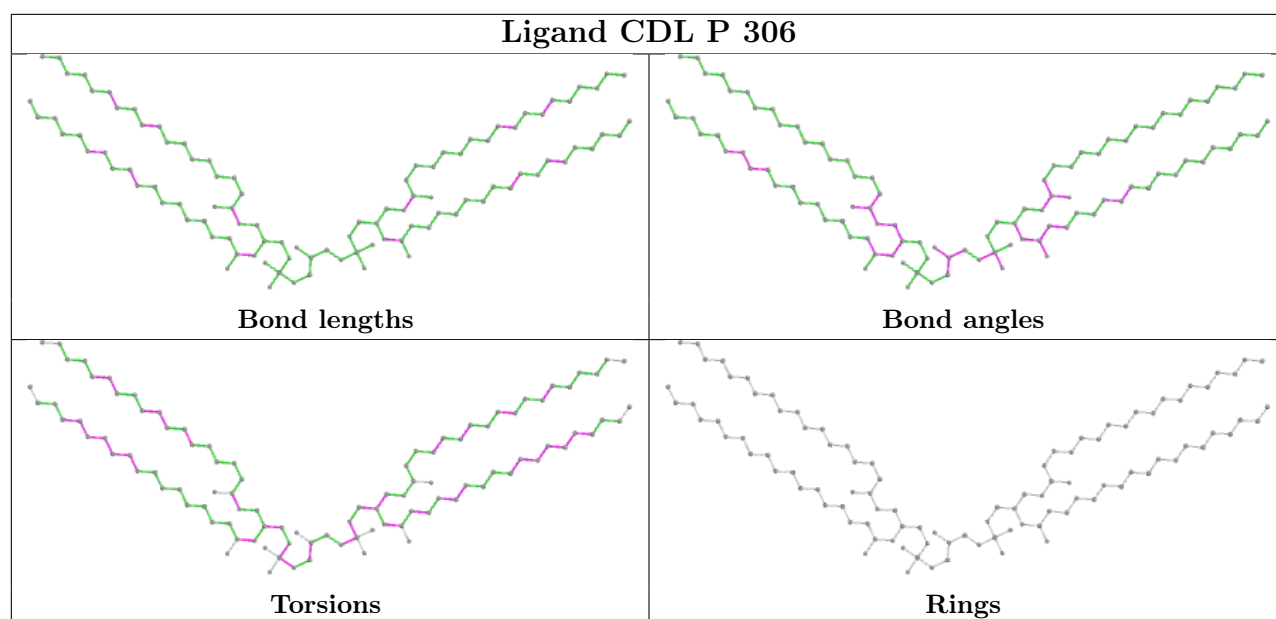


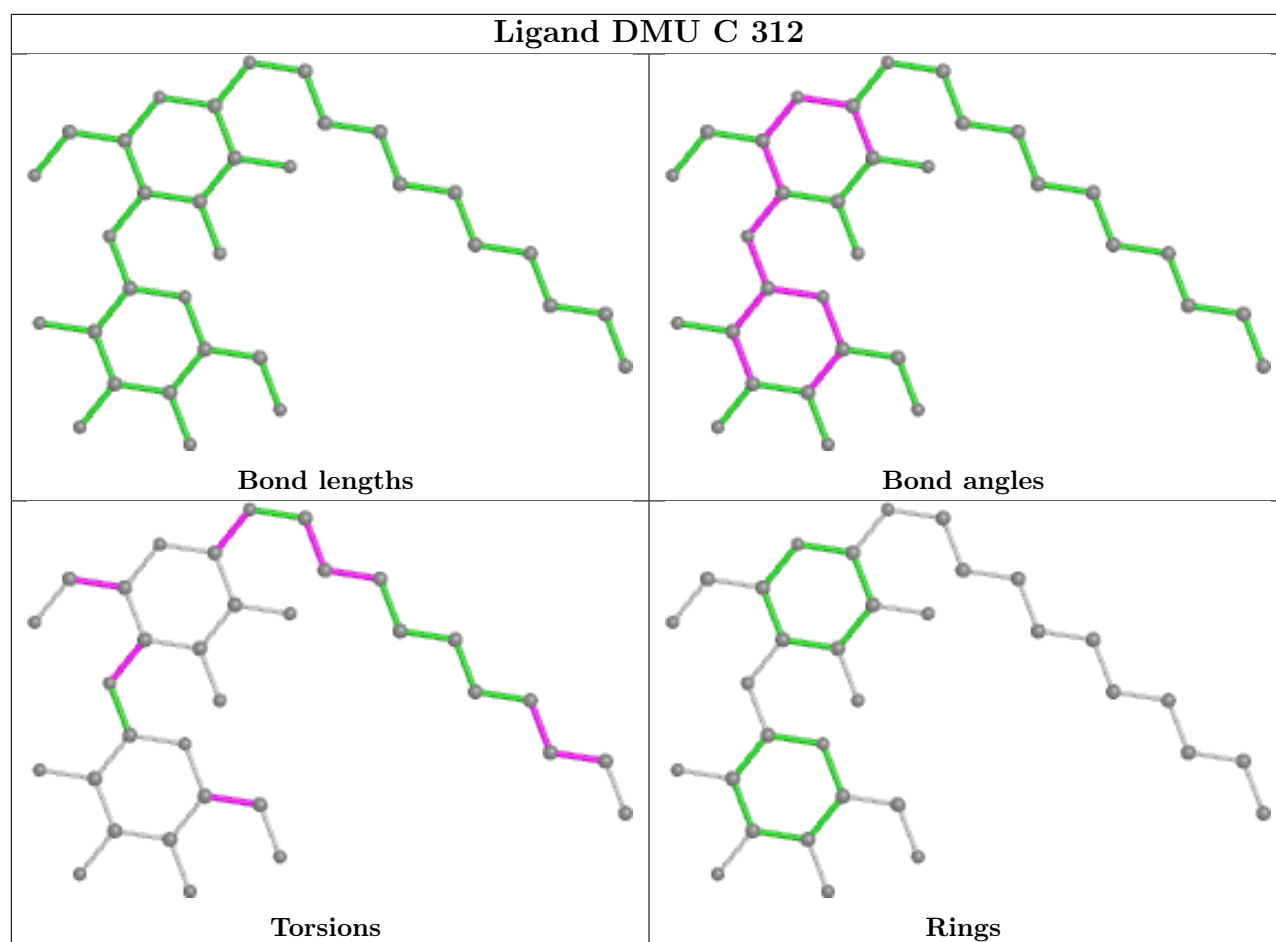












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	513/514 (99%)	-0.12	4 (0%) 86 87	13, 19, 29, 75	0
1	N	513/514 (99%)	-0.07	8 (1%) 72 74	15, 22, 33, 67	0
2	B	226/227 (99%)	0.22	12 (5%) 26 29	17, 26, 52, 93	0
2	O	226/227 (99%)	0.41	20 (8%) 10 11	22, 32, 68, 124	0
3	C	259/261 (99%)	0.01	5 (1%) 66 69	17, 23, 37, 79	0
3	P	259/261 (99%)	-0.04	1 (0%) 92 93	17, 24, 41, 80	0
4	D	144/147 (97%)	0.19	6 (4%) 36 39	19, 28, 50, 95	0
4	Q	144/147 (97%)	1.27	30 (20%) 1 1	26, 42, 87, 227	0
5	E	105/109 (96%)	0.49	13 (12%) 4 4	19, 28, 57, 141	0
5	R	105/109 (96%)	0.99	21 (20%) 1 1	24, 36, 61, 137	0
6	F	98/98 (100%)	0.62	10 (10%) 6 8	18, 29, 105, 151	0
6	S	98/98 (100%)	0.60	12 (12%) 4 4	19, 28, 94, 185	0
7	G	83/85 (97%)	1.03	19 (22%) 0 0	20, 32, 124, 163	0
7	T	83/85 (97%)	1.30	20 (24%) 0 0	20, 34, 114, 165	0
8	H	79/85 (92%)	0.85	12 (15%) 2 2	23, 35, 106, 153	0
8	U	79/85 (92%)	1.05	19 (24%) 0 0	27, 38, 131, 184	0
9	I	72/73 (98%)	0.99	13 (18%) 1 1	26, 39, 70, 87	0
9	V	72/73 (98%)	1.50	18 (25%) 0 0	25, 50, 75, 134	0
10	J	58/59 (98%)	0.64	7 (12%) 4 4	23, 34, 69, 106	0
10	W	58/59 (98%)	0.76	7 (12%) 4 4	24, 37, 78, 157	0
11	K	49/56 (87%)	0.42	3 (6%) 21 24	24, 35, 58, 62	0
11	X	49/56 (87%)	1.07	9 (18%) 1 1	36, 44, 65, 82	0
12	L	46/47 (97%)	0.08	2 (4%) 35 38	20, 26, 47, 94	0
12	Y	46/47 (97%)	0.40	4 (8%) 10 11	23, 32, 69, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.57	7 (16%) 1 1	20, 26, 68, 101	0
13	Z	43/46 (93%)	1.17	9 (20%) 1 1	29, 36, 86, 126	0
All	All	3550/3614 (98%)	0.36	291 (8%) 11 13	13, 27, 67, 227	0

The worst 5 of 291 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	15.1
8	H	8	ILE	12.9
6	F	96	LEU	12.3
4	Q	4	SER	11.6
4	Q	5	VAL	11.0

## 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, 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
9	SAC	V	1	9/10	0.40	0.81	168,196,204,213	0
7	TPO	G	11	11/12	0.62	0.47	102,138,168,184	0
7	TPO	T	11	11/12	0.82	0.31	37,90,131,149	0
9	SAC	I	1	9/10	0.84	0.40	64,103,134,151	0
1	FME	N	1	10/11	0.94	0.19	30,45,72,79	0
1	FME	A	1	10/11	0.96	0.20	30,35,87,99	0
2	FME	B	1	10/11	0.97	0.14	15,24,35,116	0
2	FME	O	1	10/11	0.98	0.19	25,35,45,96	0

## 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
21	DMU	B	306	33/33	-0.00	0.49	46,75,90,95	0
21	DMU	X	101	33/33	0.05	0.55	45,136,220,232	0
21	DMU	P	316	33/33	0.23	0.39	45,72,87,88	0
21	DMU	A	616	33/33	0.28	0.48	56,130,180,189	0
21	DMU	K	102	33/33	0.32	0.45	40,137,212,226	0
21	DMU	D	202	33/33	0.42	0.45	45,120,185,206	0
21	DMU	T	103	33/33	0.45	0.38	43,92,177,189	0
27	CHD	X	105	29/29	0.45	0.55	91,122,143,147	0
21	DMU	G	104	33/33	0.46	0.34	44,93,162,176	0
21	DMU	K	105	33/33	0.50	0.43	45,140,194,202	0
21	DMU	K	104	33/33	0.50	0.38	55,109,174,183	0
21	DMU	Q	203	33/33	0.50	0.37	50,70,87,89	0
21	DMU	K	103	33/33	0.53	0.43	46,125,193,196	0
24	PSC	B	303	52/52	0.54	0.37	29,85,150,174	0
21	DMU	C	312	33/33	0.54	0.26	40,102,147,166	0
27	CHD	J	101	29/29	0.55	0.36	36,97,125,132	0
21	DMU	K	106	33/33	0.56	0.34	37,128,202,207	0
21	DMU	X	103	22/33	0.57	0.24	44,114,175,179	0
27	CHD	W	101	29/29	0.58	0.42	48,87,120,129	0
25	PEK	P	309	53/53	0.59	0.30	31,69,134,199	0
21	DMU	K	101	33/33	0.60	0.28	41,96,158,172	0
25	PEK	G	102	53/53	0.60	0.32	35,84,135,144	0
22	TGL	Y	101	63/63	0.60	0.29	29,62,103,122	0
21	DMU	X	104	22/33	0.61	0.30	50,86,128,134	0
21	DMU	L	102	33/33	0.61	0.31	45,90,142,145	0
26	CDL	T	102	100/100	0.62	0.28	36,85,128,174	0
21	DMU	X	102	22/33	0.62	0.27	51,87,176,183	0
21	DMU	O	305	33/33	0.63	0.35	39,118,177,200	0
27	CHD	L	103	29/29	0.65	0.36	43,92,143,156	0
25	PEK	C	307	53/53	0.65	0.24	30,67,125,163	0
25	PEK	C	309	53/53	0.65	0.34	38,89,140,147	0
21	DMU	P	314	33/33	0.66	0.30	44,95,145,181	0
19	PGV	N	607	51/51	0.67	0.30	29,74,124,175	0
26	CDL	G	101	100/100	0.68	0.24	37,78,128,171	0
21	DMU	M	101	33/33	0.68	0.23	27,38,63,68	0
22	TGL	L	101	63/63	0.69	0.28	23,52,106,155	0
22	TGL	Q	201	63/63	0.70	0.24	34,64,99,123	0
24	PSC	N	608	52/52	0.70	0.29	26,80,141,151	0
21	DMU	Z	101	33/33	0.70	0.27	25,52,70,76	0
27	CHD	Y	102	29/29	0.71	0.36	51,96,128,136	0
19	PGV	C	308	51/51	0.73	0.27	38,73,130,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
19	PGV	A	608	51/51	0.76	0.24	24,62,119,169	0
22	TGL	D	201	63/63	0.76	0.21	25,56,92,141	0
20	EDO	N	619	4/4	0.77	0.16	45,52,58,70	0
26	CDL	P	306	100/100	0.77	0.24	21,78,136,154	0
26	CDL	C	304	100/100	0.79	0.23	15,70,122,136	0
19	PGV	P	302	51/51	0.81	0.19	39,75,131,156	0
20	EDO	S	105	4/4	0.82	0.29	50,56,81,100	0
20	EDO	M	102	4/4	0.82	0.12	44,46,46,67	0
22	TGL	O	301	63/63	0.82	0.18	29,69,101,117	0
22	TGL	B	301	63/63	0.82	0.18	26,59,100,113	0
27	CHD	P	307	29/29	0.83	0.21	37,57,80,101	0
27	CHD	C	305	29/29	0.84	0.25	38,56,79,104	0
20	EDO	P	310	4/4	0.87	0.36	36,41,65,76	0
20	EDO	O	304	4/4	0.88	0.11	40,61,63,67	0
20	EDO	W	103	4/4	0.88	0.11	45,47,50,68	0
20	EDO	P	313	4/4	0.88	0.15	28,43,51,66	0
20	EDO	Y	103	4/4	0.89	0.42	53,59,59,70	0
17	NA	P	303	1/1	0.90	0.11	42,42,42,42	0
20	EDO	A	613	4/4	0.90	0.17	30,42,53,62	0
20	EDO	N	618	4/4	0.91	0.10	49,51,55,101	0
20	EDO	F	105	4/4	0.91	0.19	45,45,75,75	0
29	PO4	U	101	5/5	0.91	0.19	48,52,113,186	0
20	EDO	N	614	4/4	0.92	0.20	38,46,50,53	0
20	EDO	L	105	4/4	0.92	0.14	45,52,55,62	0
27	CHD	P	308	29/29	0.93	0.10	17,25,33,42	0
20	EDO	P	312	4/4	0.93	0.13	40,50,56,61	0
20	EDO	S	107	4/4	0.93	0.18	45,51,52,55	0
25	PEK	P	304	53/53	0.93	0.19	22,39,106,120	0
20	EDO	N	615	4/4	0.93	0.25	28,52,52,53	0
20	EDO	N	617	4/4	0.94	0.26	44,48,53,81	0
25	PEK	C	302	53/53	0.94	0.20	19,37,81,96	0
27	CHD	C	306	29/29	0.94	0.08	18,26,33,37	0
27	CHD	G	103	29/29	0.94	0.10	16,21,28,36	0
20	EDO	R	201	4/4	0.94	0.13	45,45,50,50	0
20	EDO	B	304	4/4	0.94	0.12	31,56,61,72	0
20	EDO	F	103	4/4	0.94	0.08	33,33,38,51	0
20	EDO	N	620	4/4	0.94	0.18	45,47,56,72	0
20	EDO	O	303	4/4	0.94	0.20	20,21,27,32	0
20	EDO	N	610	4/4	0.94	0.15	24,25,31,40	0
20	EDO	F	104	4/4	0.94	0.16	45,45,67,73	0
20	EDO	A	609	4/4	0.94	0.07	34,65,68,70	0
14	HEA	N	601[A]	60/60	0.95	0.15	12,20,30,35	9

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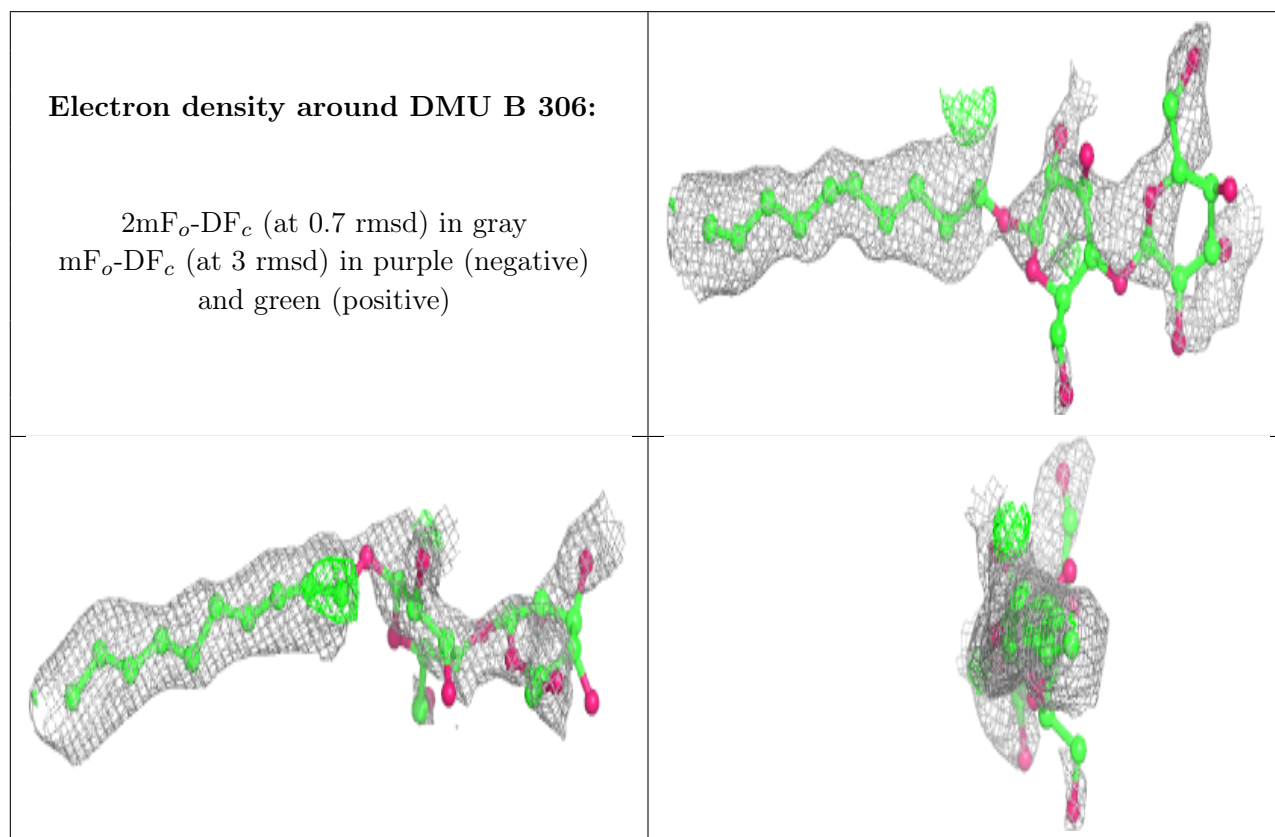
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
20	EDO	P	315	4/4	0.95	0.16	45,45,45,48	0
14	HEA	N	601[B]	60/60	0.95	0.15	12,21,47,59	9
20	EDO	G	105	4/4	0.95	0.23	45,45,45,45	0
20	EDO	S	106	4/4	0.95	0.09	34,35,46,54	0
20	EDO	L	104	4/4	0.95	0.09	45,45,51,58	0
20	EDO	A	614	4/4	0.95	0.13	37,41,48,59	0
20	EDO	A	615	4/4	0.95	0.14	22,26,27,37	0
19	PGV	C	303	51/51	0.95	0.20	15,26,67,85	0
20	EDO	N	613	4/4	0.95	0.16	31,38,40,103	0
20	EDO	P	311	4/4	0.95	0.11	34,36,43,44	0
19	PGV	P	305	51/51	0.95	0.22	13,27,75,97	0
20	EDO	S	103	4/4	0.96	0.10	27,31,36,39	0
20	EDO	S	104	4/4	0.96	0.13	28,37,45,46	0
14	HEA	A	602	60/60	0.96	0.13	11,17,23,27	0
19	PGV	P	301	51/51	0.96	0.22	17,32,72,81	0
20	EDO	N	609	4/4	0.96	0.15	19,25,27,28	0
20	EDO	W	102	4/4	0.96	0.11	52,52,66,80	0
27	CHD	T	101	29/29	0.96	0.08	16,22,26,39	0
20	EDO	A	611	4/4	0.96	0.12	25,31,56,74	0
20	EDO	N	611	4/4	0.96	0.10	31,32,38,47	0
20	EDO	N	612	4/4	0.96	0.17	27,34,37,65	0
29	PO4	H	101	5/5	0.96	0.18	58,61,79,149	0
14	HEA	N	602	60/60	0.96	0.13	13,18,27,30	0
20	EDO	N	616	4/4	0.97	0.09	32,38,39,48	0
14	HEA	A	601[A]	60/60	0.97	0.12	10,16,32,46	9
20	EDO	B	305	4/4	0.97	0.16	17,19,25,30	0
20	EDO	S	102	4/4	0.97	0.11	19,19,19,20	0
20	EDO	C	310	4/4	0.97	0.11	26,31,32,34	0
20	EDO	C	311	4/4	0.97	0.11	23,27,47,49	0
18	PER	N	606	2/2	0.97	0.07	17,17,17,18	0
20	EDO	A	612	4/4	0.97	0.20	24,26,62,82	0
19	PGV	A	607	51/51	0.97	0.20	17,30,63,68	0
14	HEA	A	601[B]	60/60	0.97	0.12	10,16,35,64	9
17	NA	C	301	1/1	0.97	0.13	58,58,58,58	0
16	MG	N	604	1/1	0.98	0.03	16,16,16,16	0
17	NA	N	605	1/1	0.98	0.06	25,25,25,25	0
18	PER	A	606	2/2	0.99	0.06	12,12,12,15	0
20	EDO	Q	202	4/4	0.99	0.09	25,35,53,70	0
17	NA	A	605	1/1	0.99	0.06	20,20,20,20	0
20	EDO	A	610	4/4	0.99	0.12	19,22,22,23	0
16	MG	A	604	1/1	0.99	0.03	13,13,13,13	0
20	EDO	F	102	4/4	0.99	0.11	16,18,21,21	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CU	N	603	1/1	1.00	0.04	18,18,18,18	0
23	CUA	B	302	2/2	1.00	0.03	18,18,18,19	0
28	ZN	F	101	1/1	1.00	0.04	22,22,22,22	0
28	ZN	S	101	1/1	1.00	0.05	22,22,22,22	0
23	CUA	O	302	2/2	1.00	0.04	22,22,22,22	0
15	CU	A	603	1/1	1.00	0.04	17,17,17,17	0

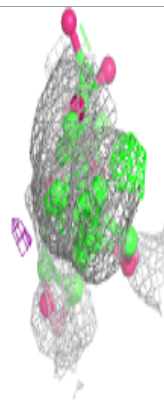
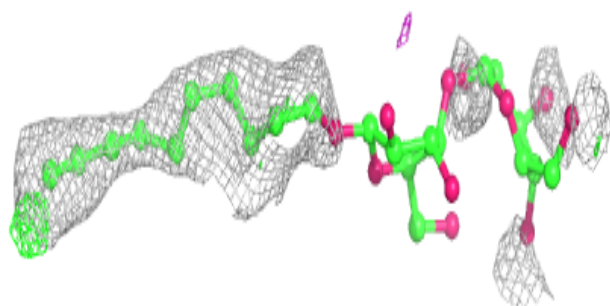
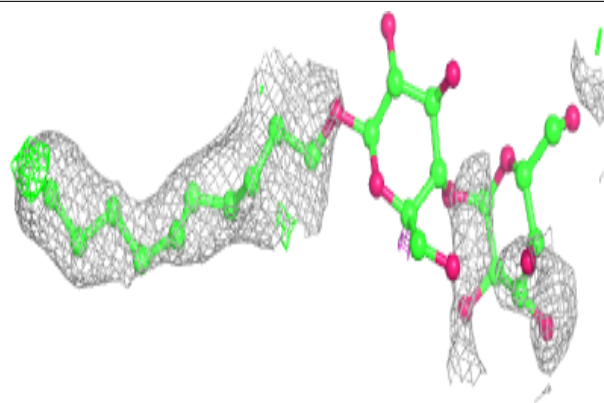
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



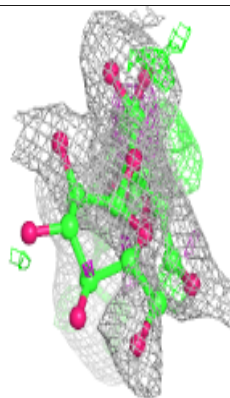
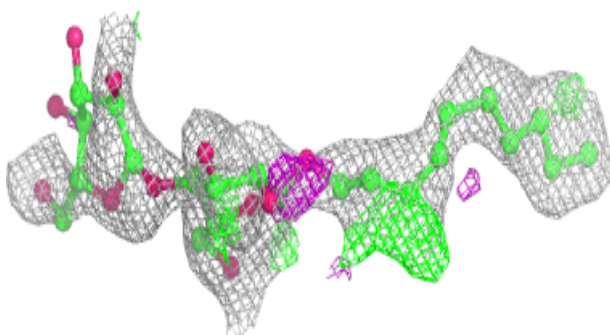
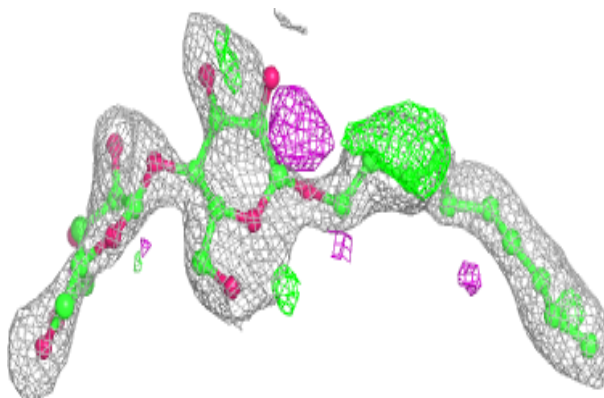


**Electron density around DMU X 101:**

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

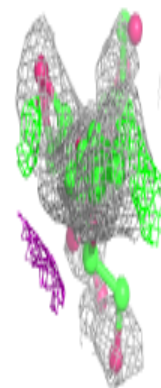
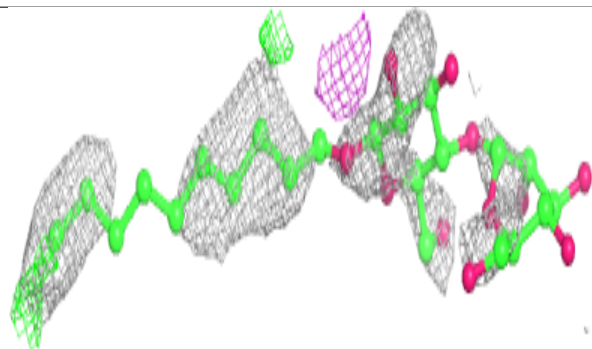
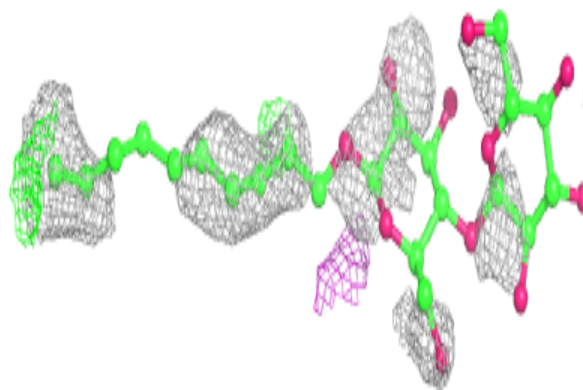
**Electron density around DMU P 316:**

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

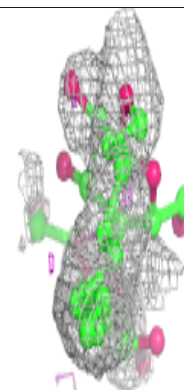
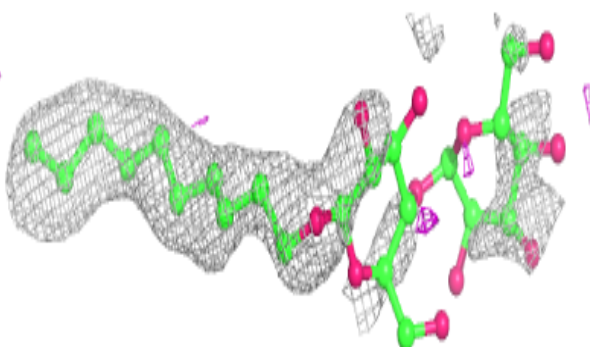
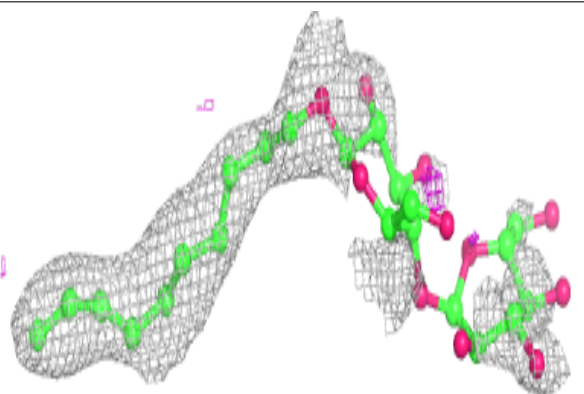


**Electron density around DMU A 616:**

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

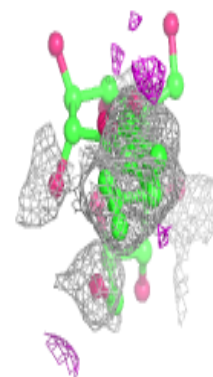
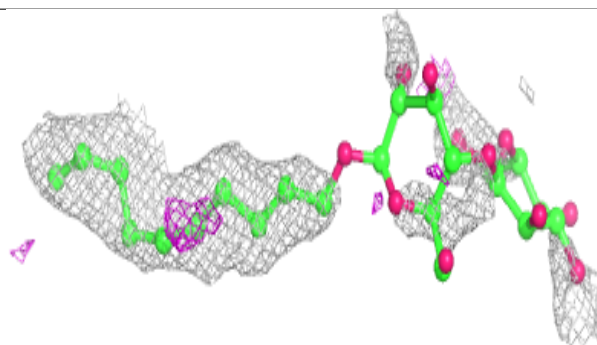
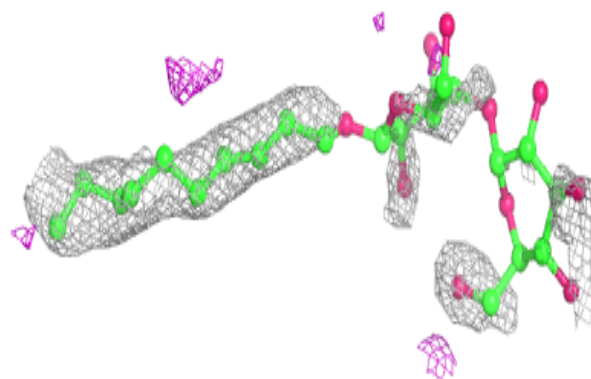
**Electron density around DMU K 102:**

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

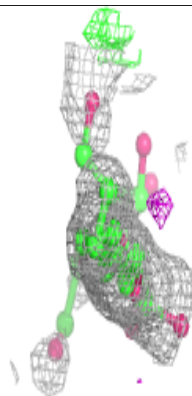
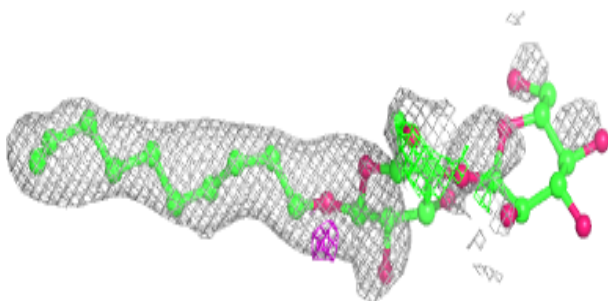
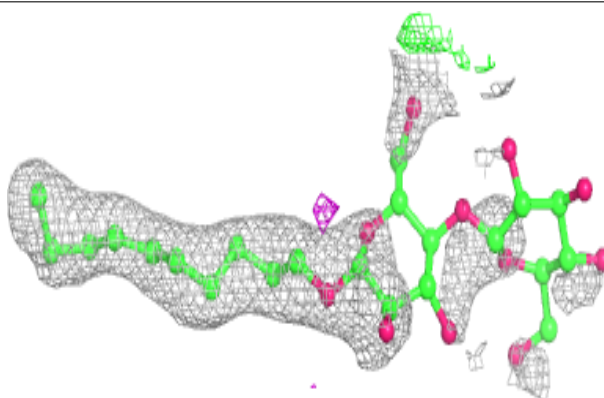


**Electron density around DMU D 202:**

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

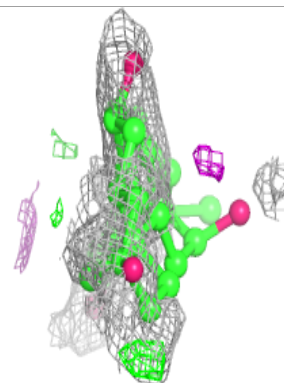
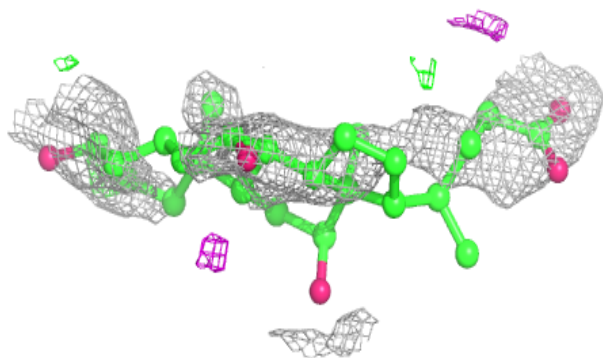
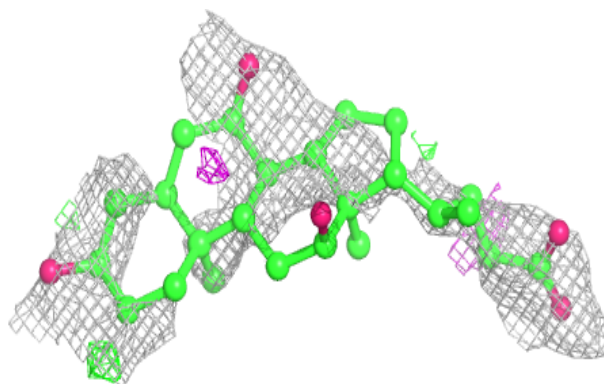
**Electron density around DMU T 103:**

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

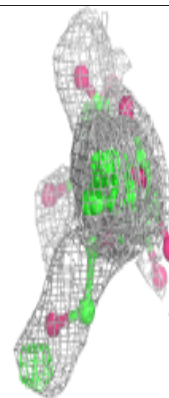
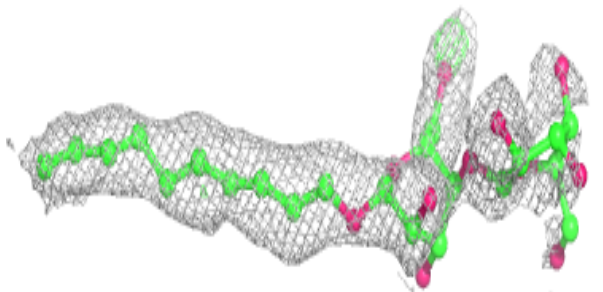
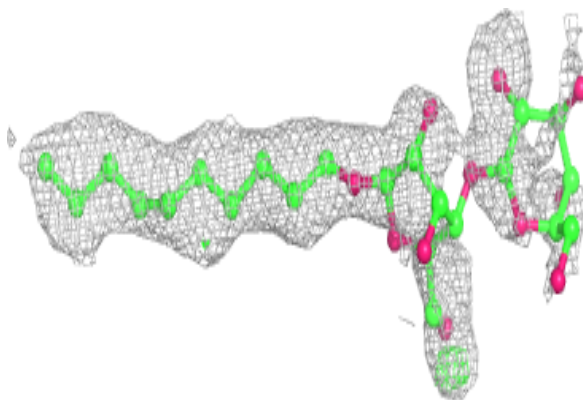


**Electron density around CHD X 105:**

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

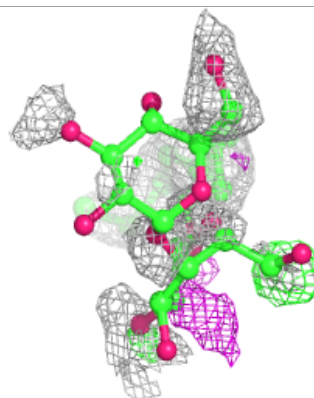
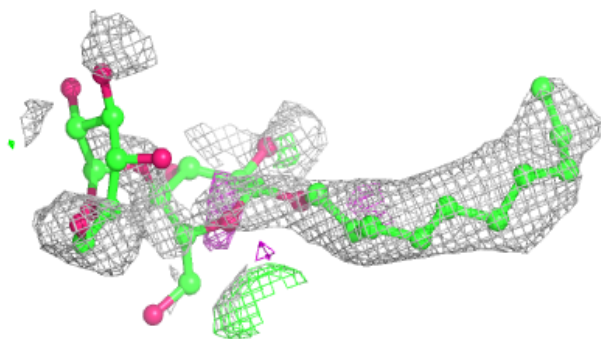
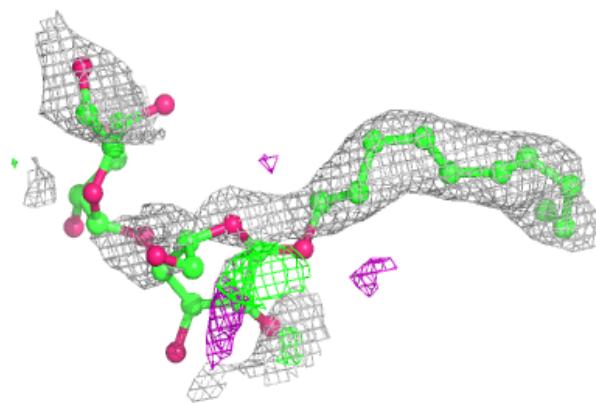
**Electron density around DMU G 104:**

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

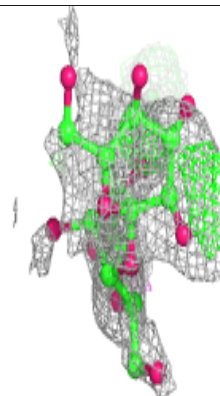
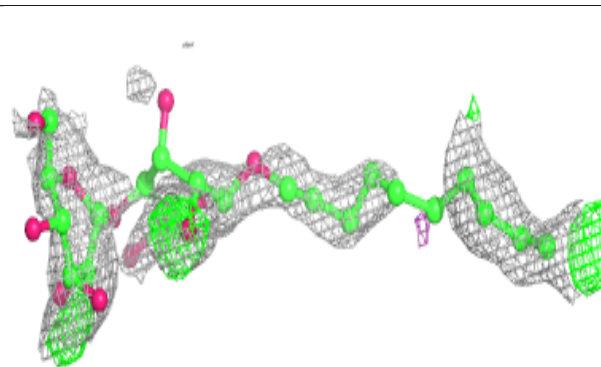
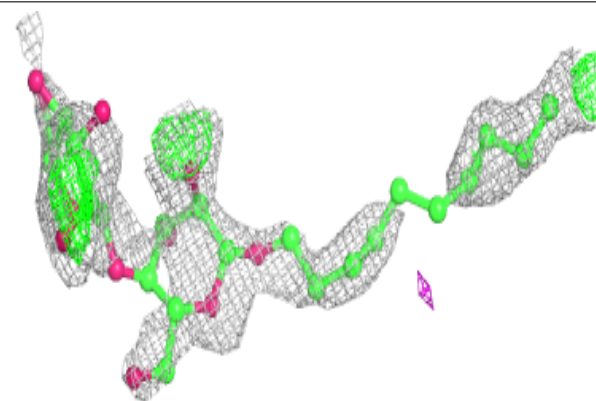


**Electron density around DMU K 105:**

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

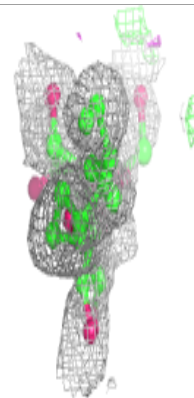
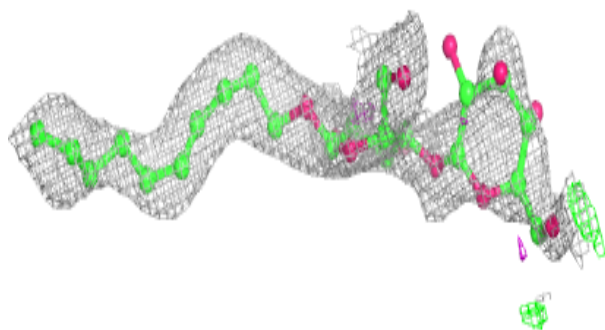
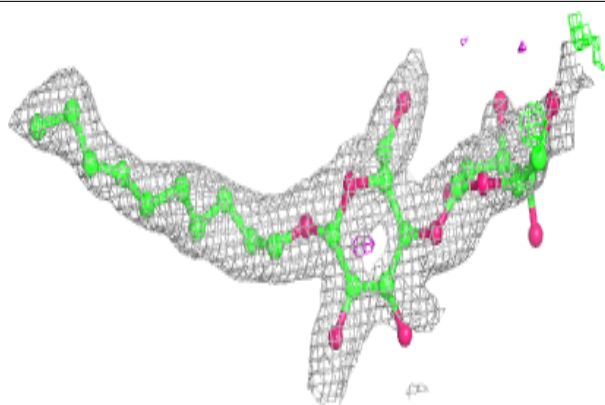
**Electron density around DMU K 104:**

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

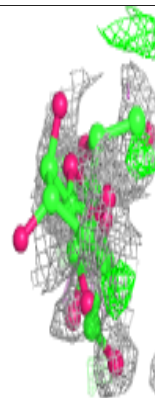
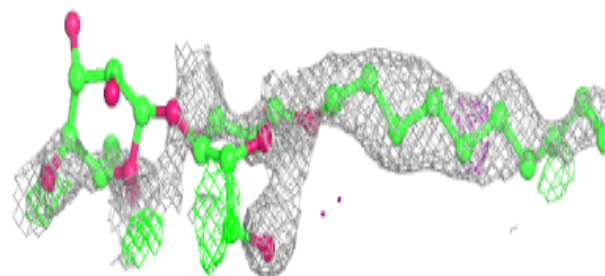
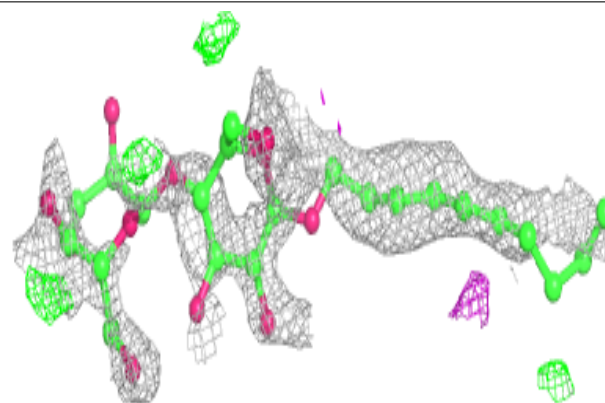


**Electron density around DMU Q 203:**

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

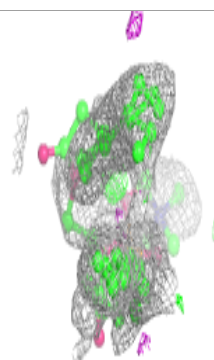
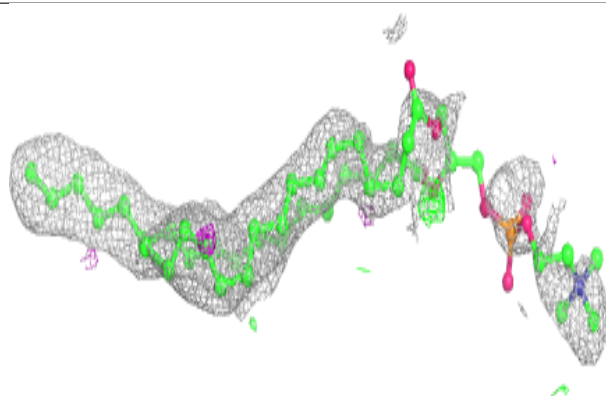
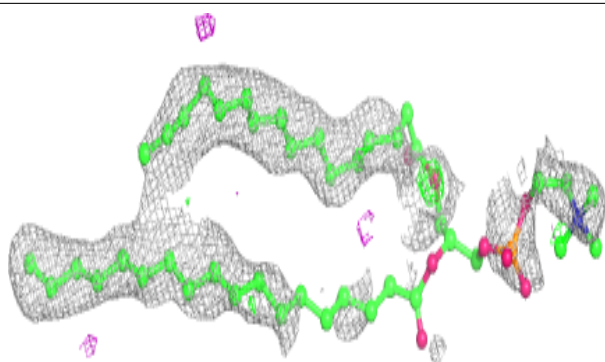
**Electron density around DMU K 103:**

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

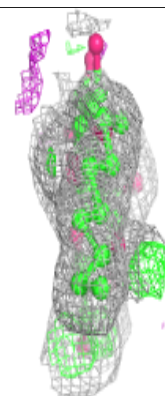
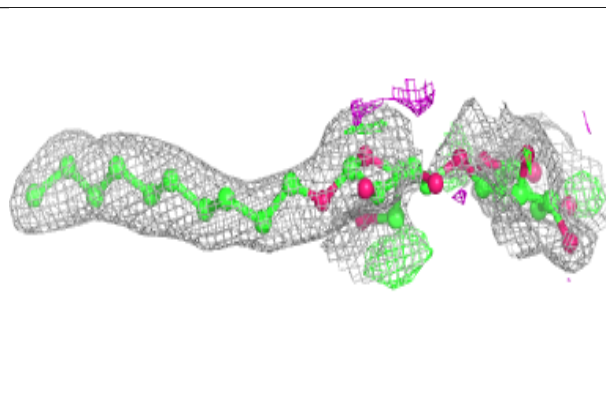
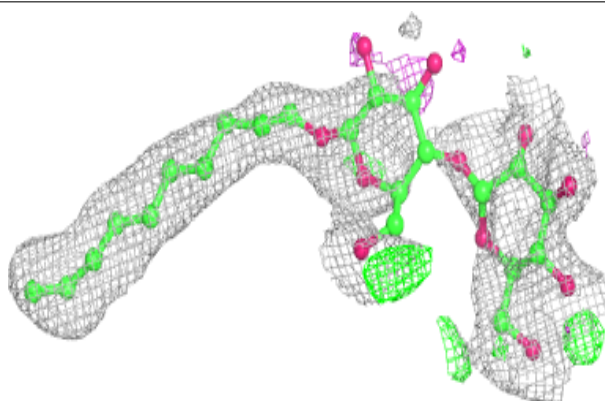


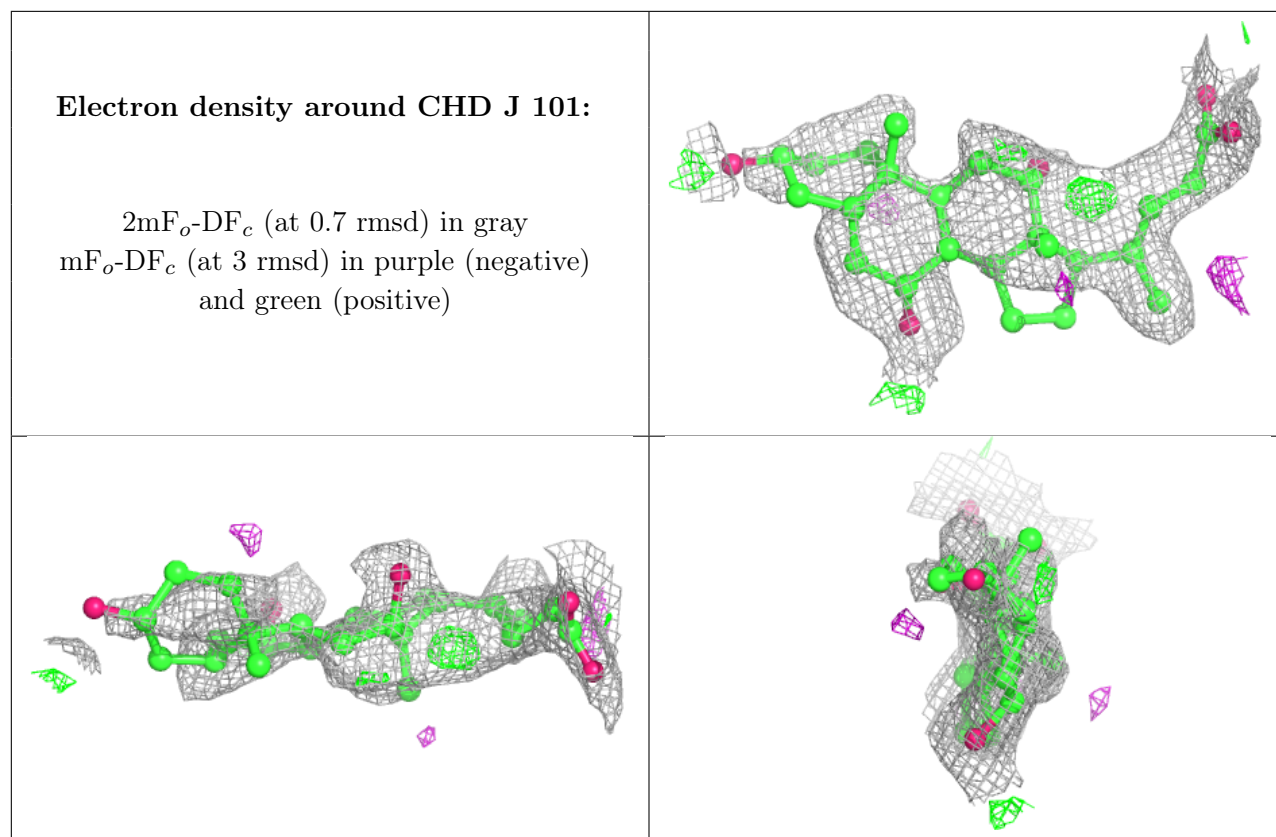
**Electron density around PSC B 303:**

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

**Electron density around DMU C 312:**

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

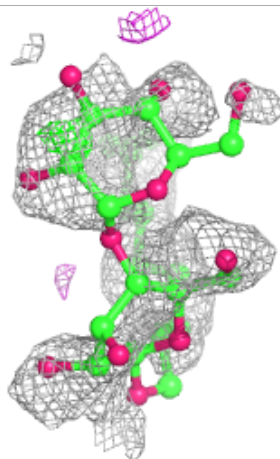
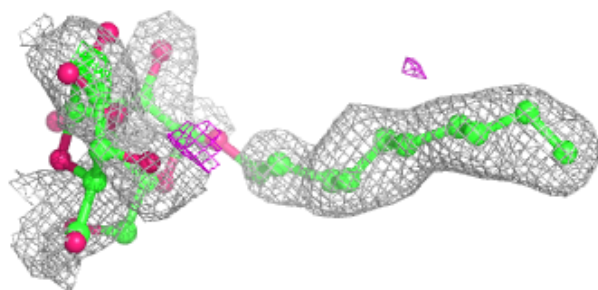
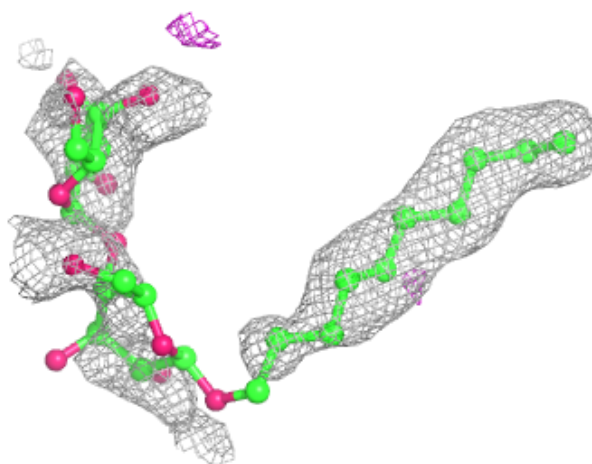






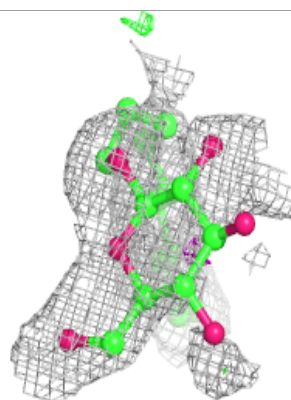
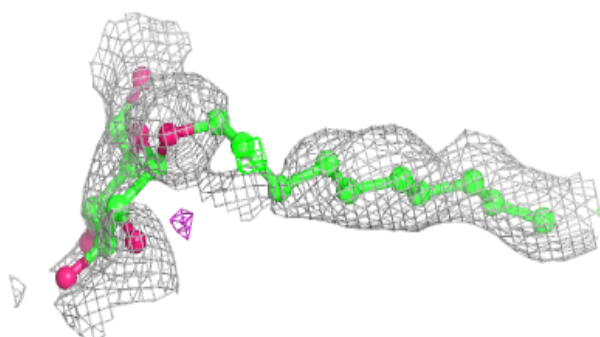
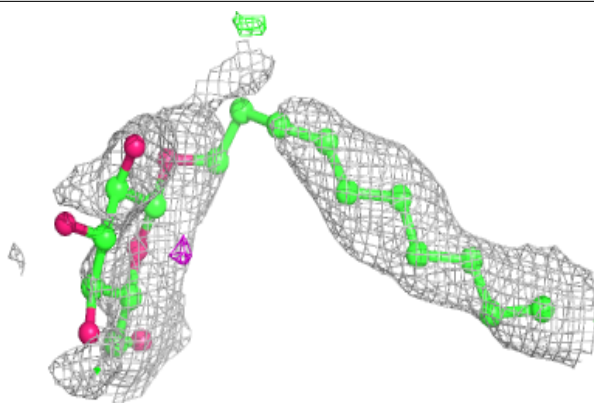
**Electron density around DMU K 106:**

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

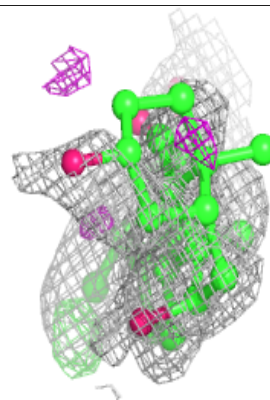
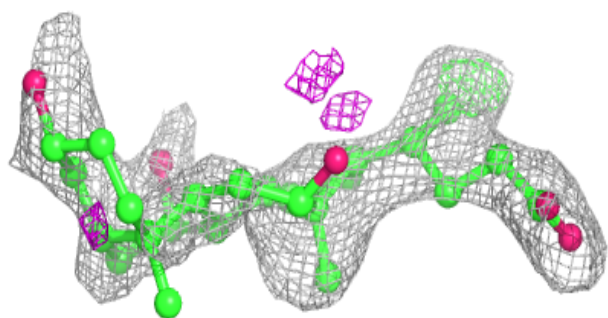
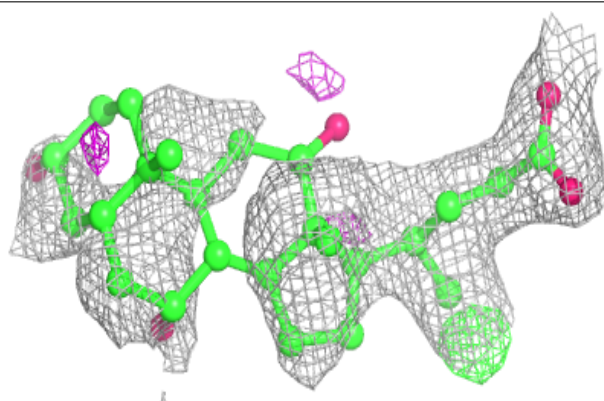


**Electron density around DMU X 103:**

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

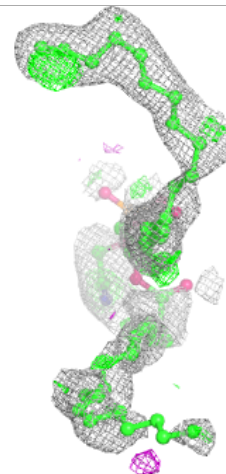
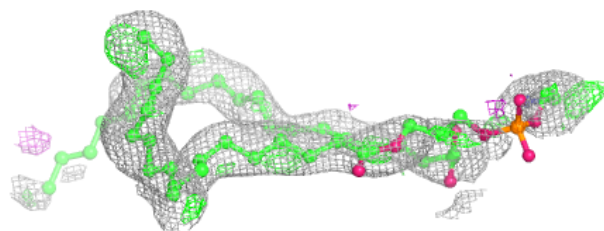
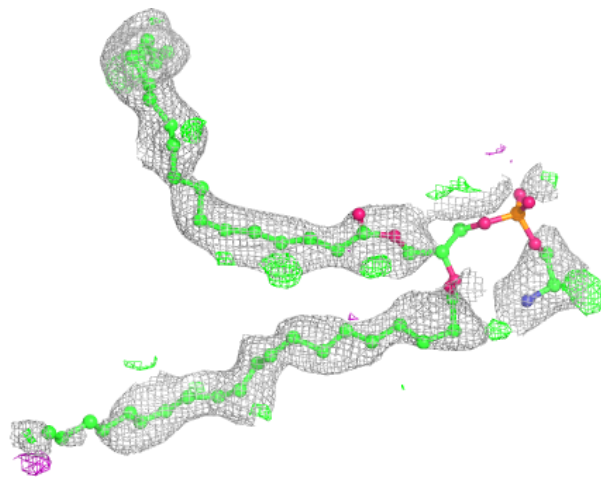
**Electron density around CHD W 101:**

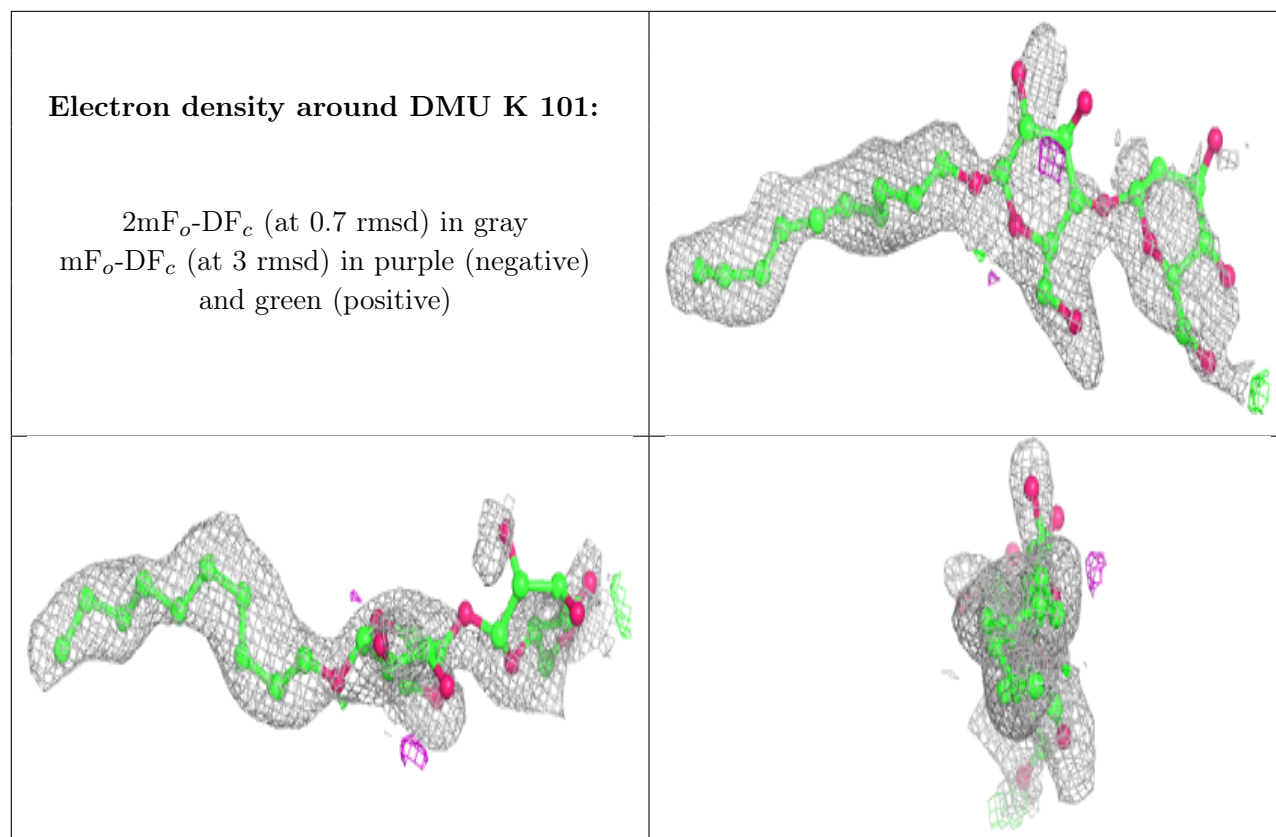
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

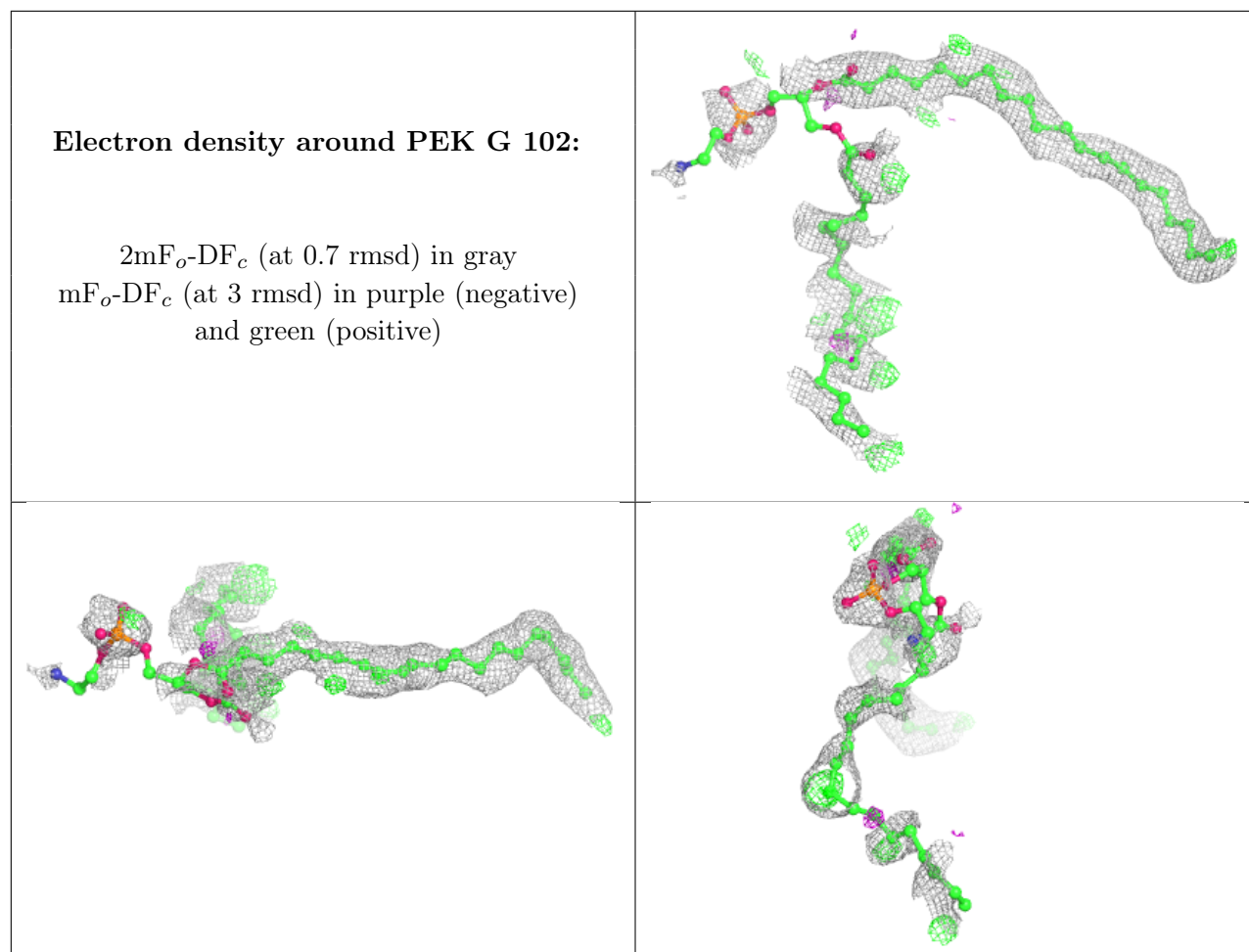


**Electron density around PEK P 309:**

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

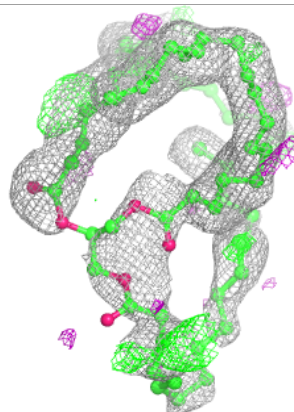
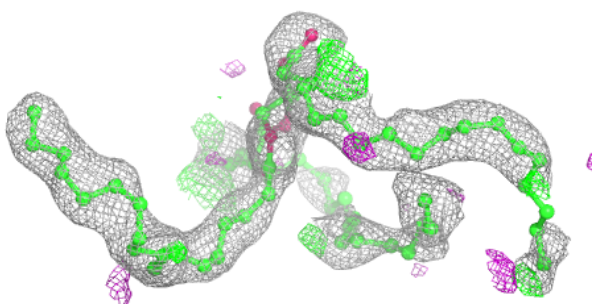
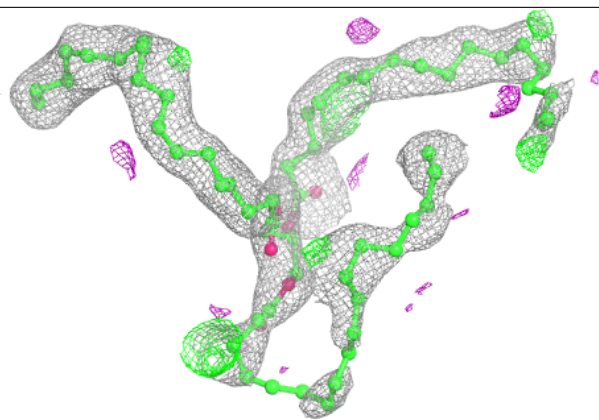




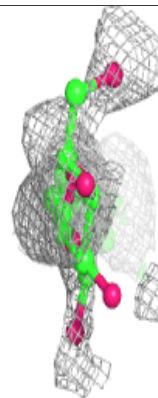
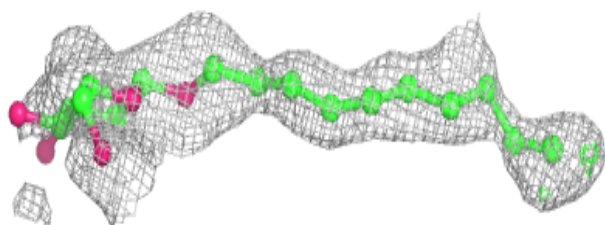
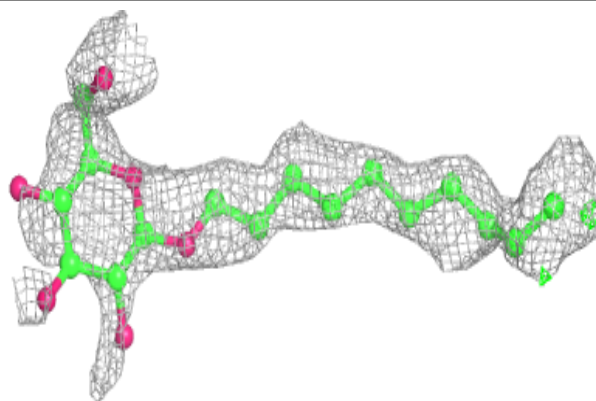


**Electron density around TGL Y 101:**

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

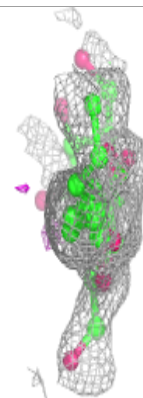
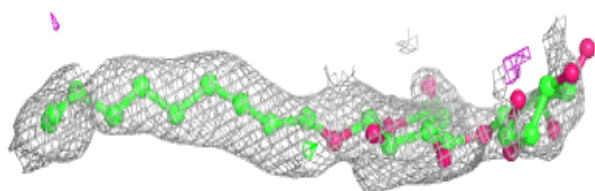
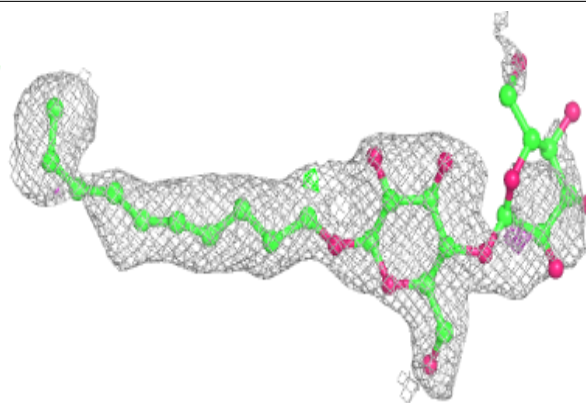
**Electron density around DMU X 104:**

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

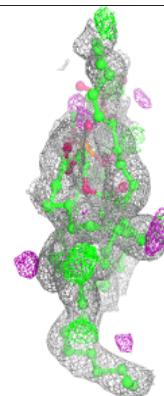
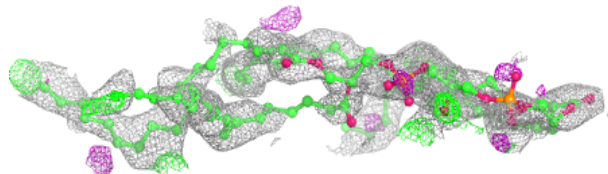
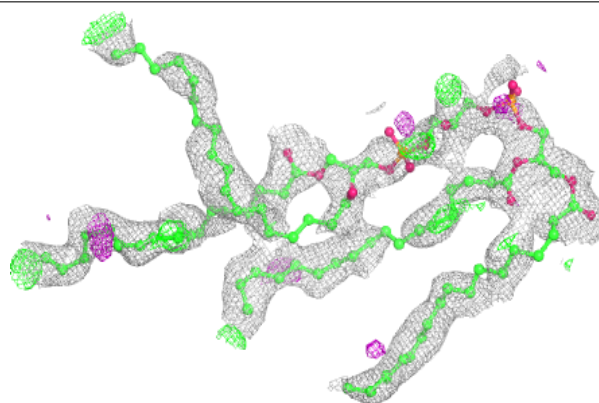


**Electron density around DMU L 102:**

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

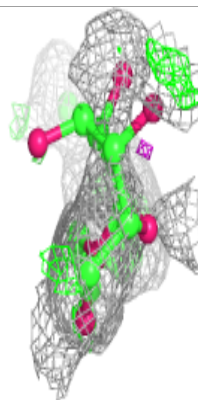
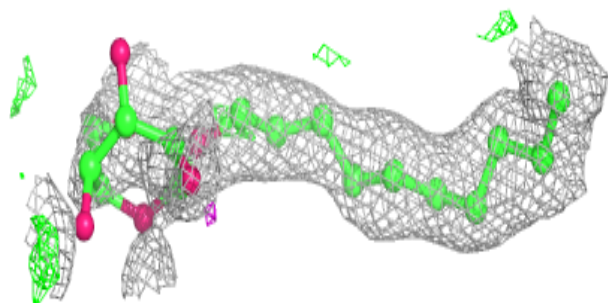
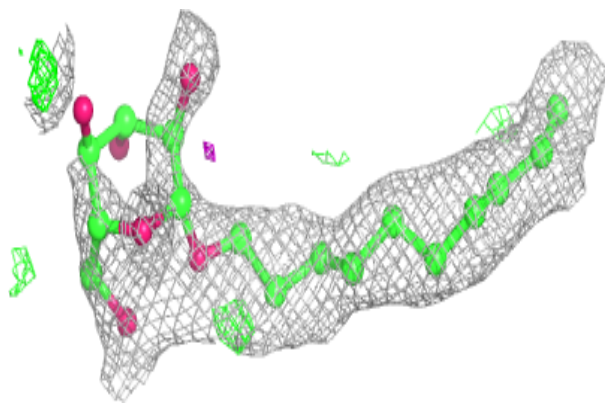
**Electron density around CDL T 102:**

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

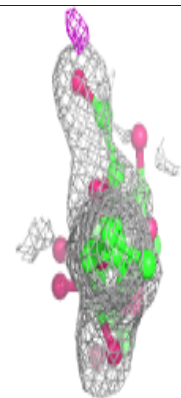
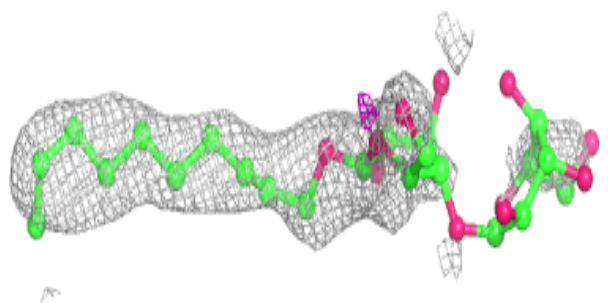
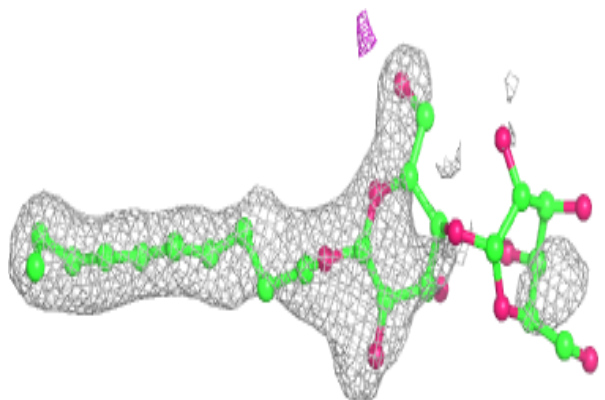


**Electron density around DMU X 102:**

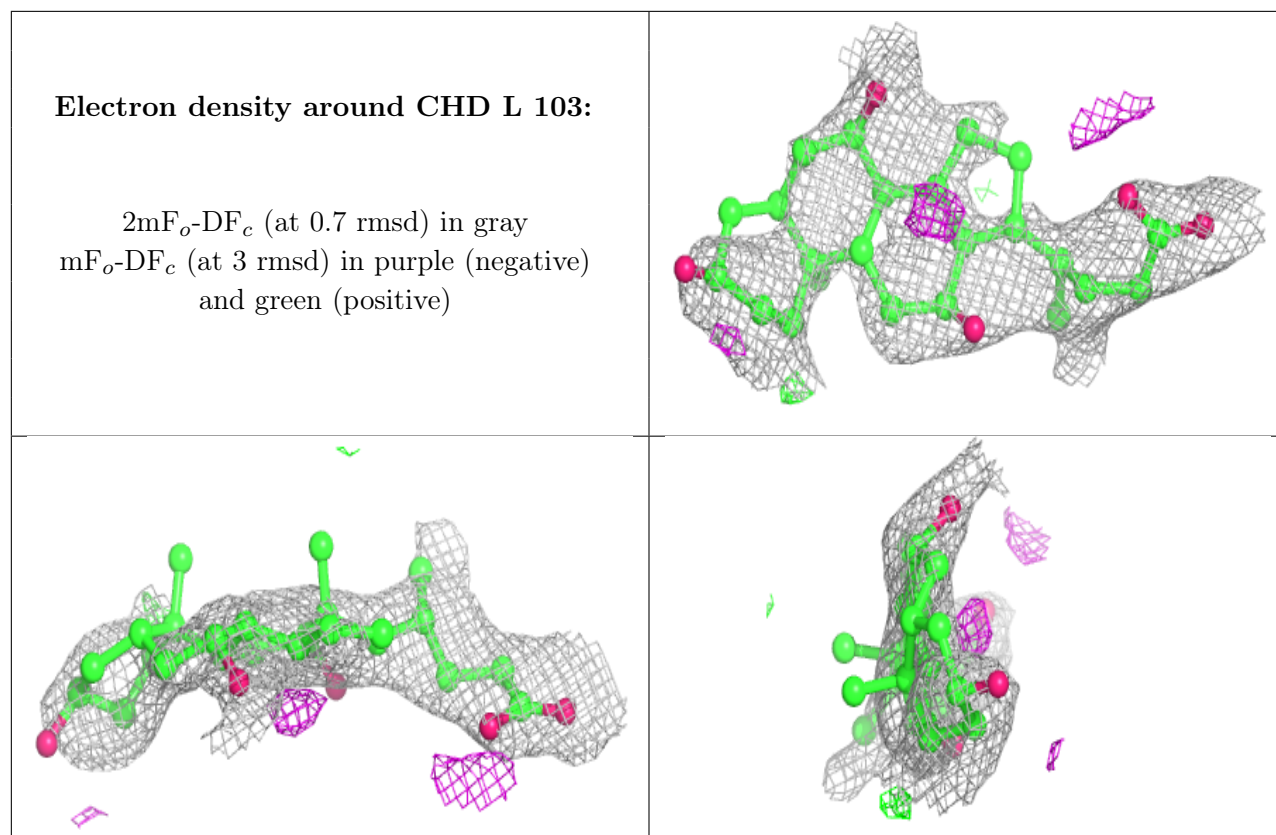
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DMU O 305:**

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

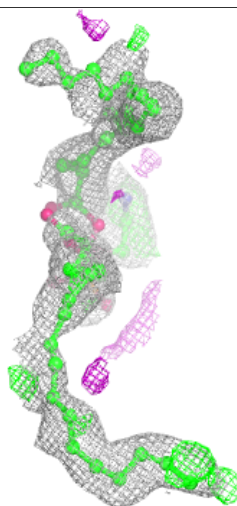
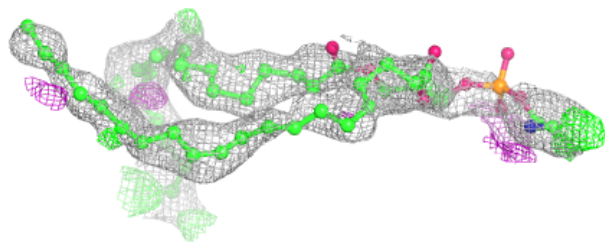
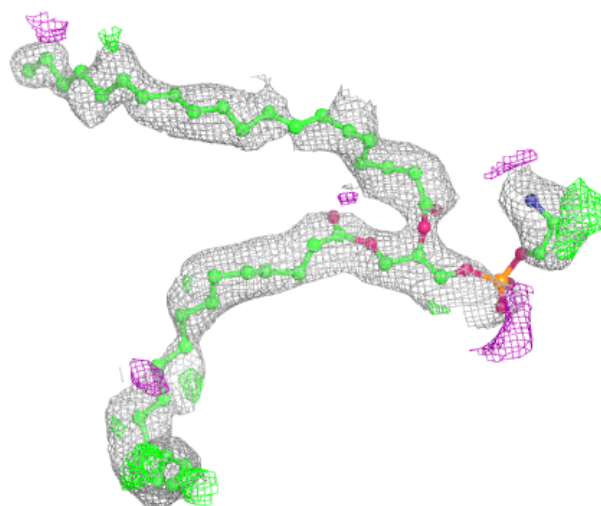


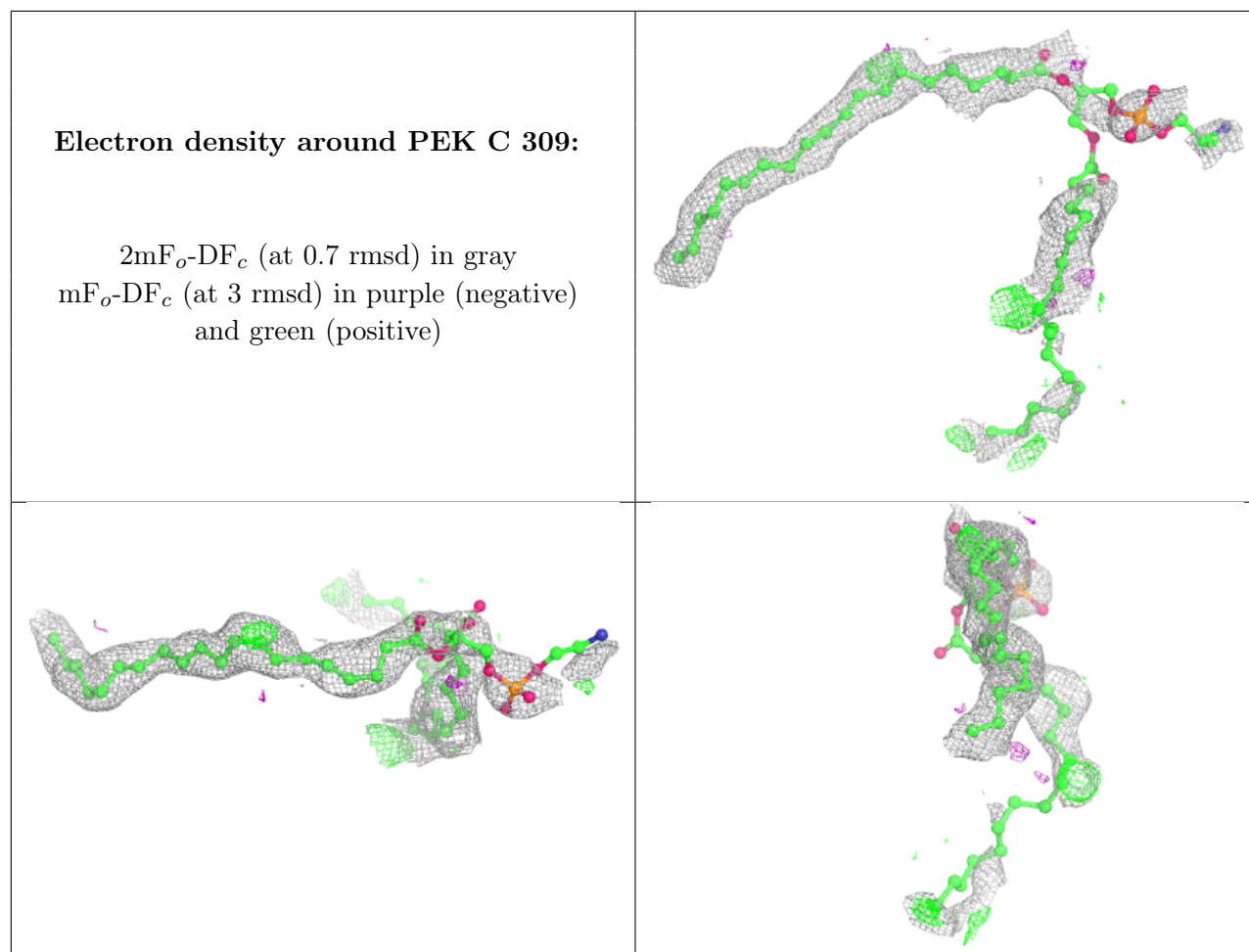




**Electron density around PEK C 307:**

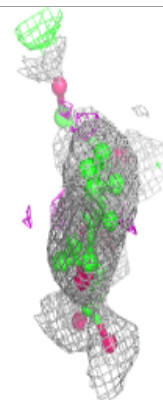
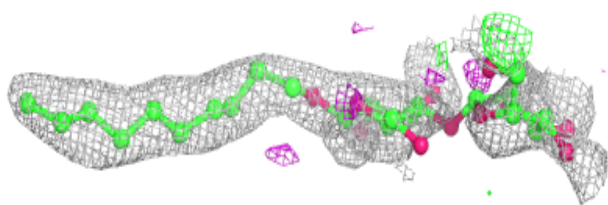
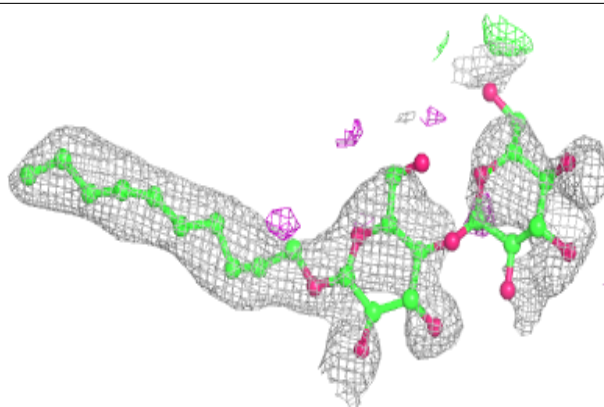
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



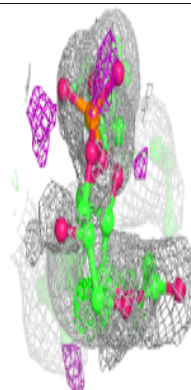
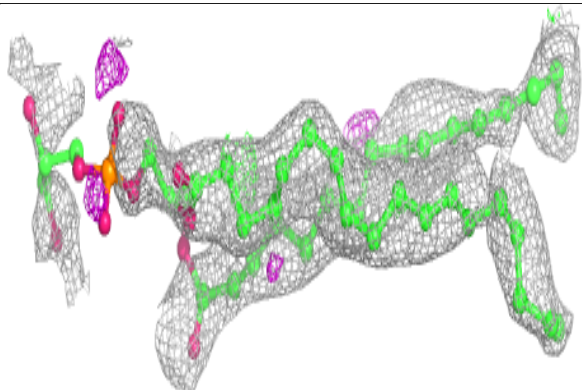
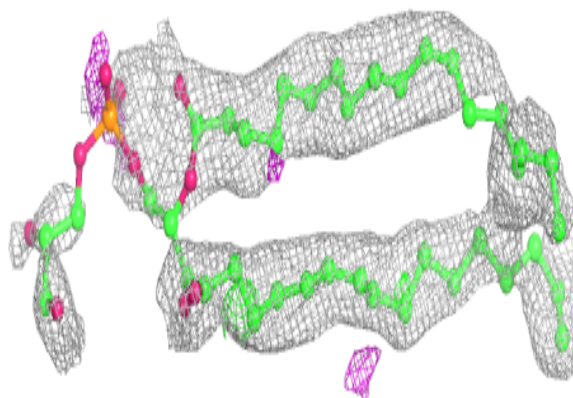


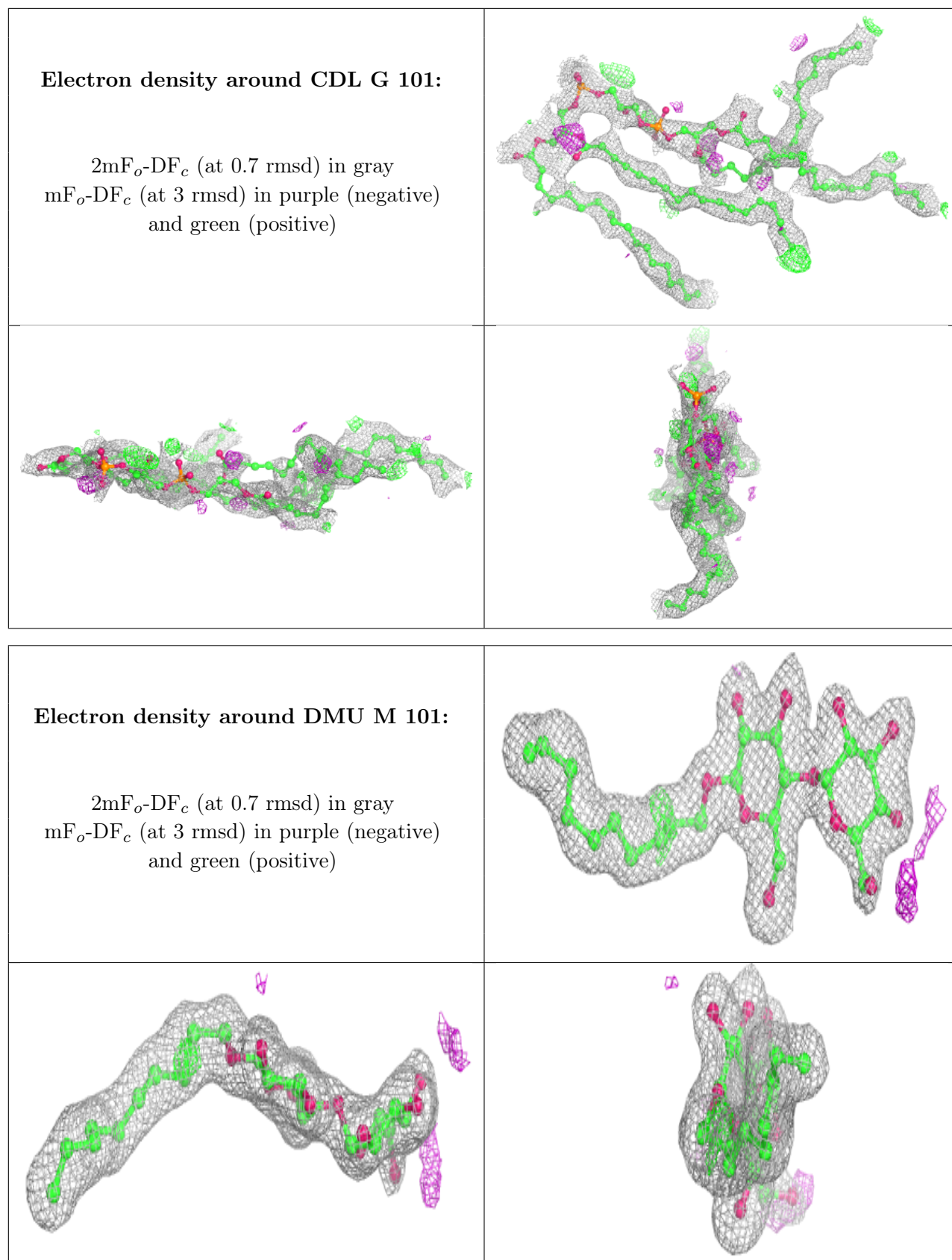
**Electron density around DMU P 314:**

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

**Electron density around PGV N 607:**

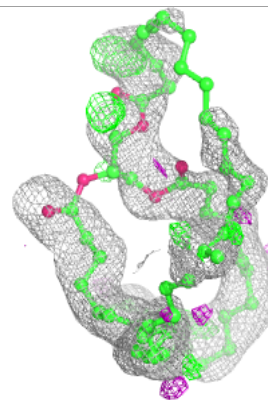
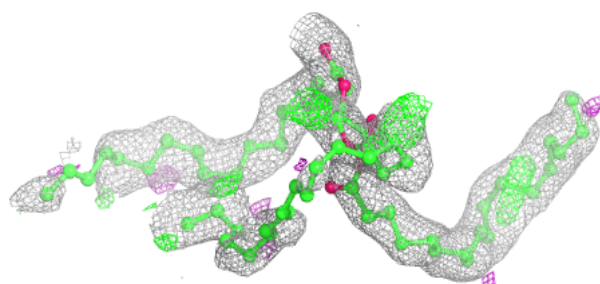
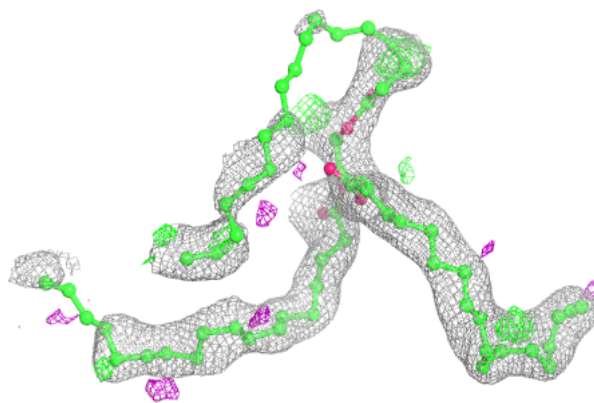
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



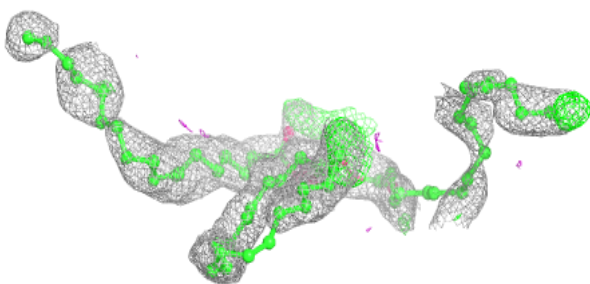
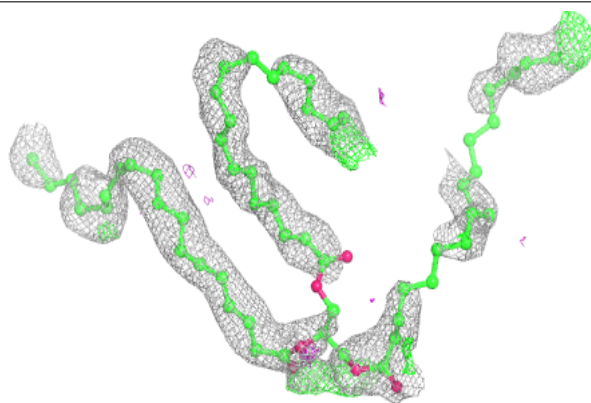


**Electron density around TGL L 101:**

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

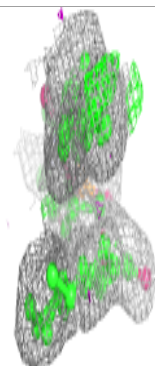
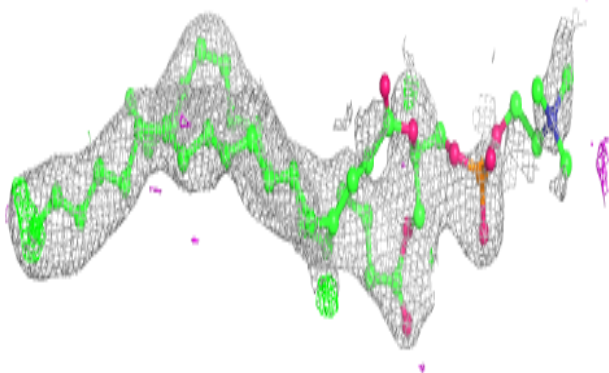
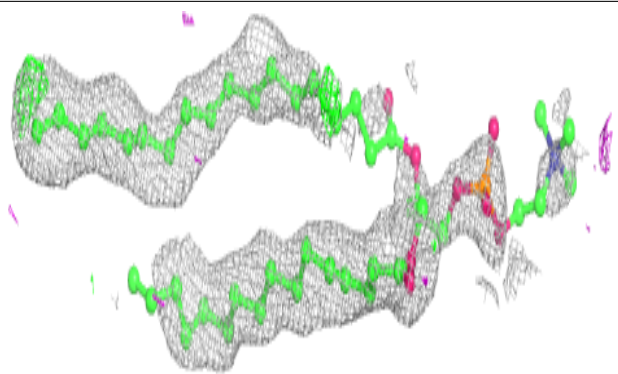
**Electron density around TGL Q 201:**

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

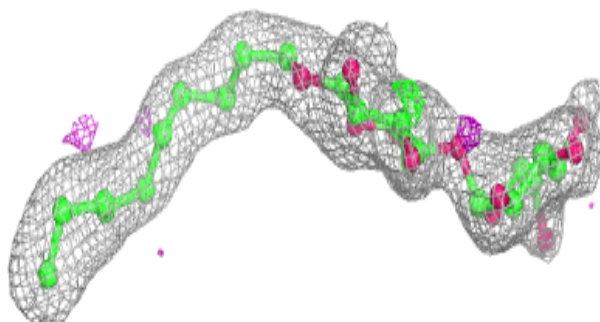
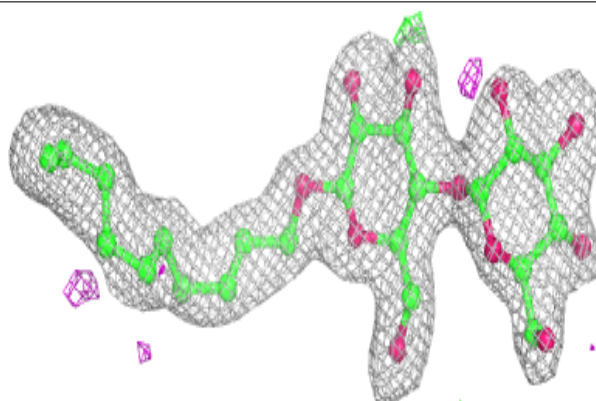


**Electron density around PSC N 608:**

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

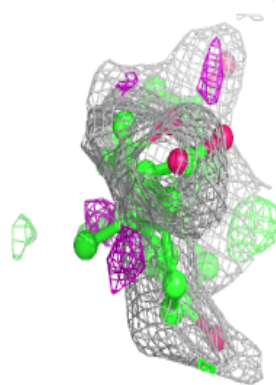
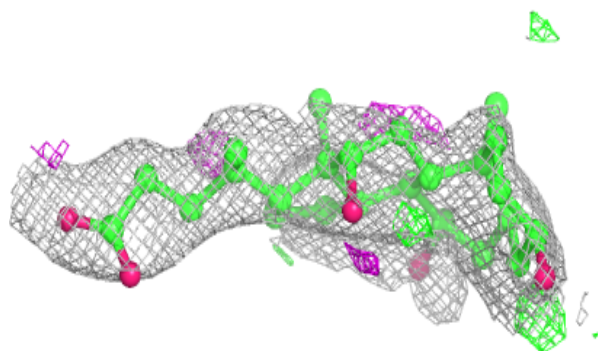
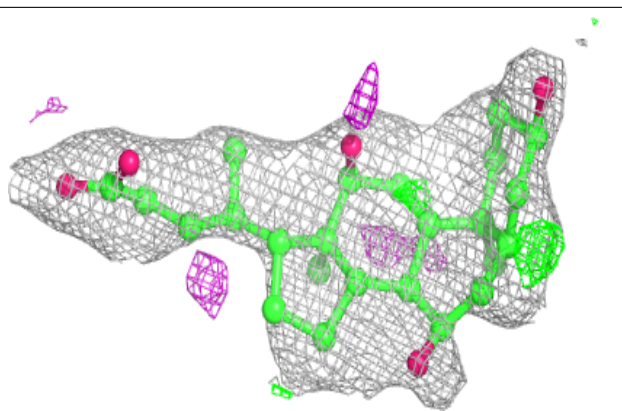
**Electron density around DMU Z 101:**

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

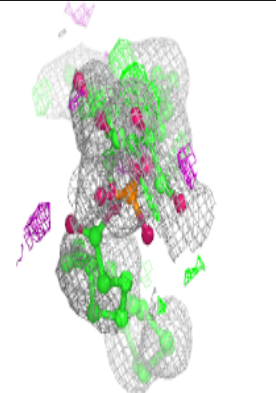
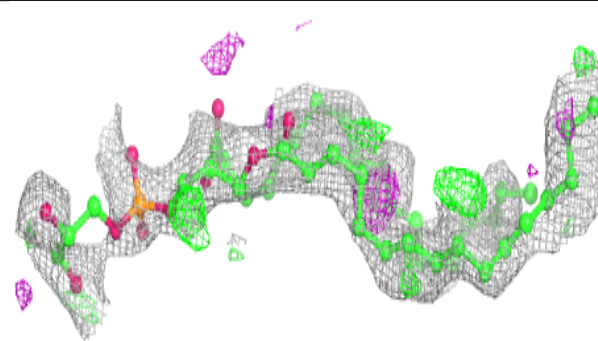
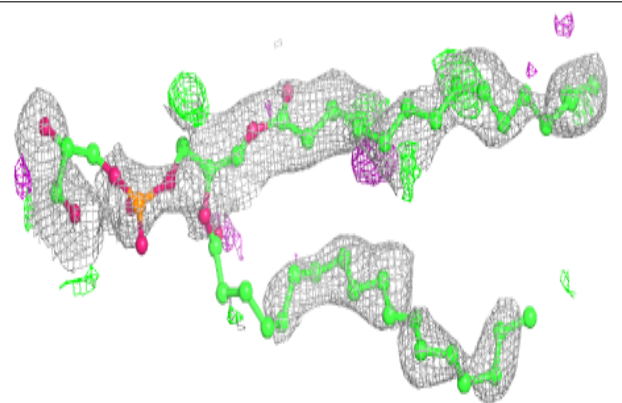


**Electron density around CHD Y 102:**

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

**Electron density around PGV C 308:**

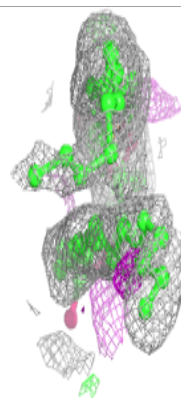
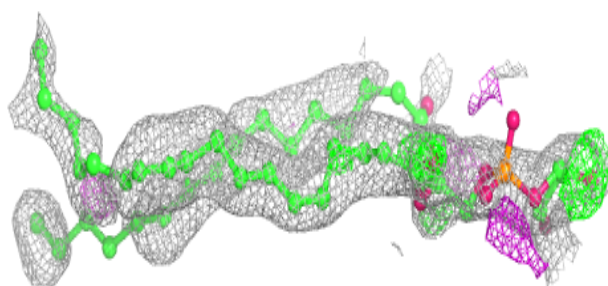
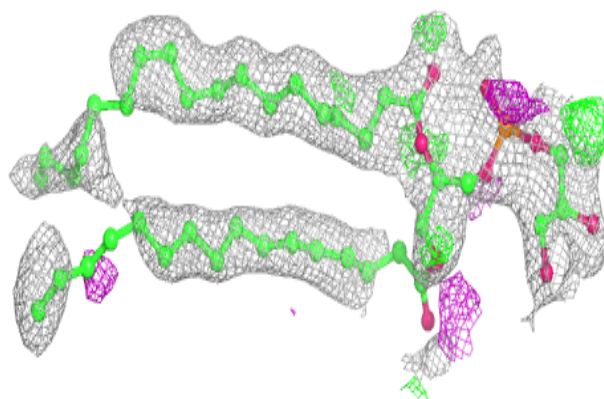
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



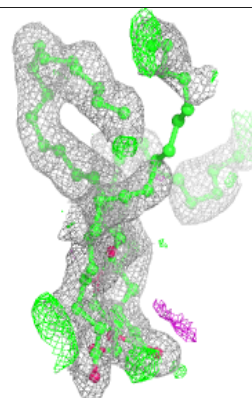
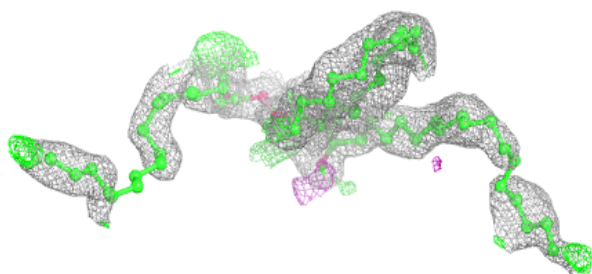
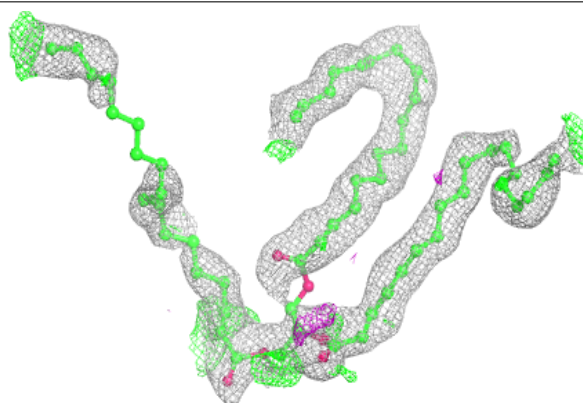


**Electron density around PGV A 608:**

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

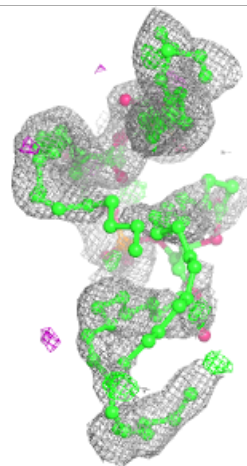
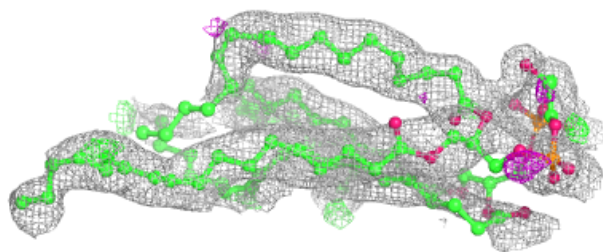
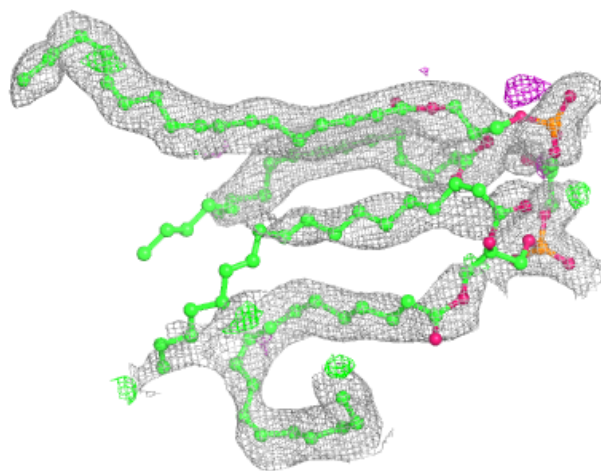
**Electron density around TGL D 201:**

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



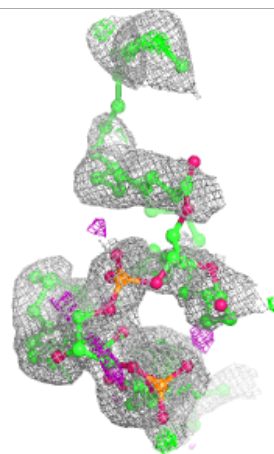
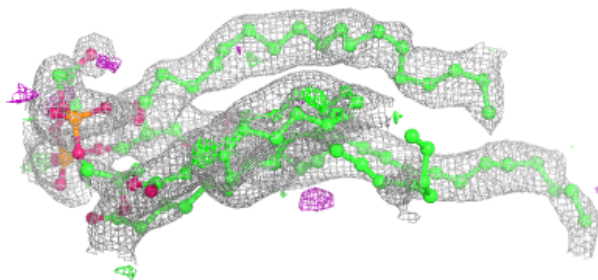
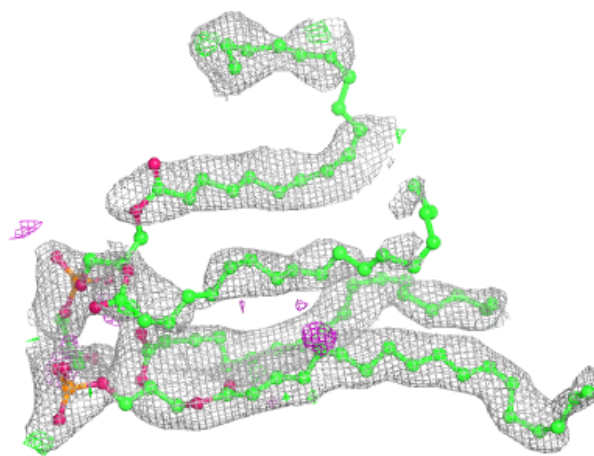
**Electron density around CDL P 306:**

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



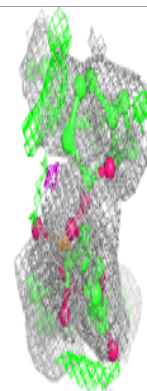
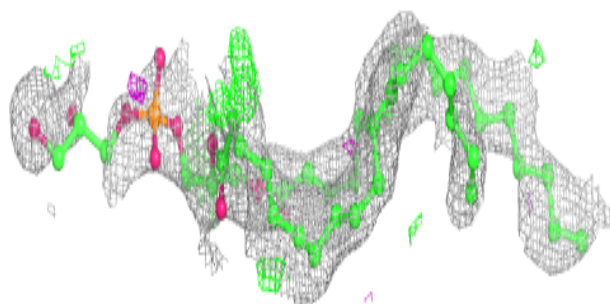
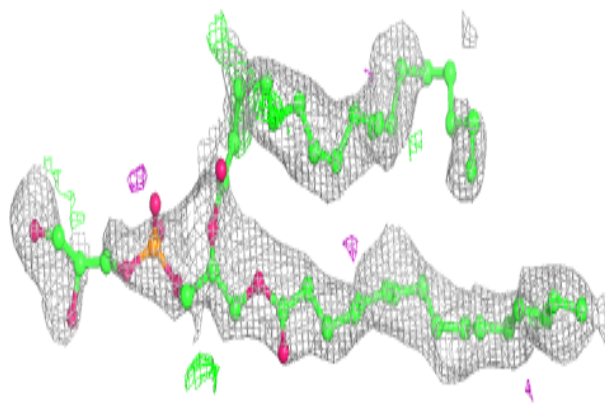
**Electron density around CDL C 304:**

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

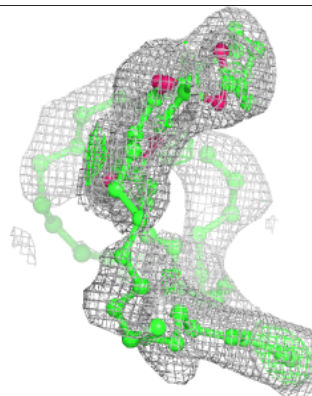
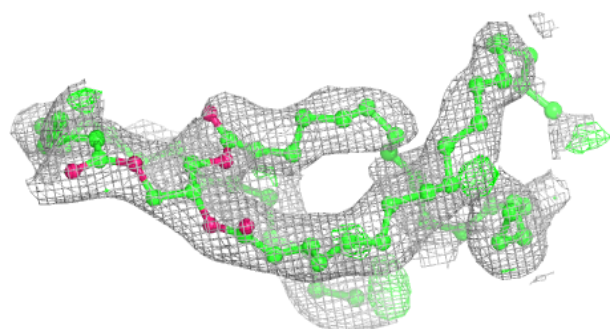
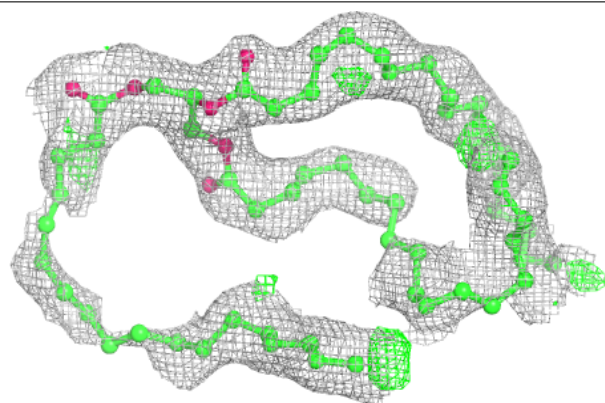


**Electron density around PGV P 302:**

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

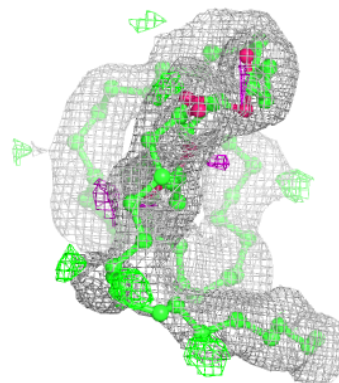
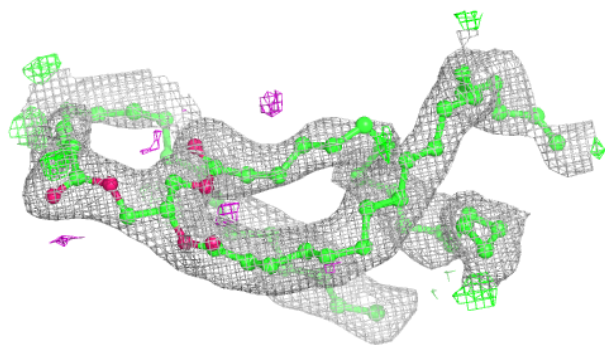
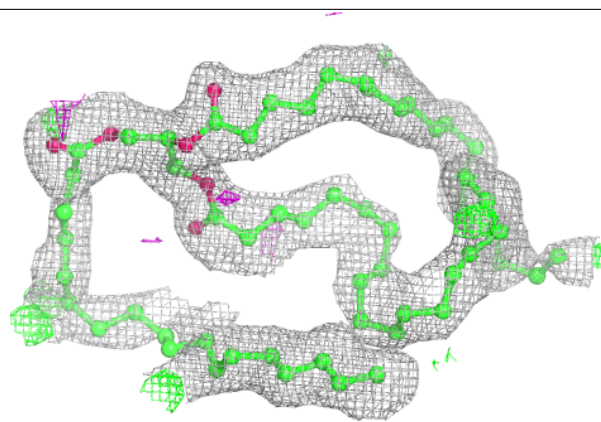
**Electron density around TGL O 301:**

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

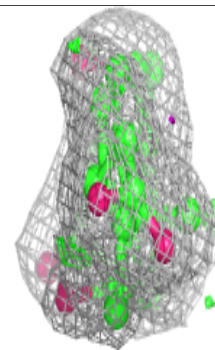
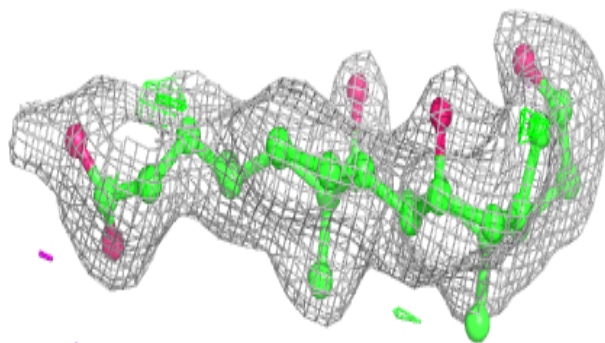
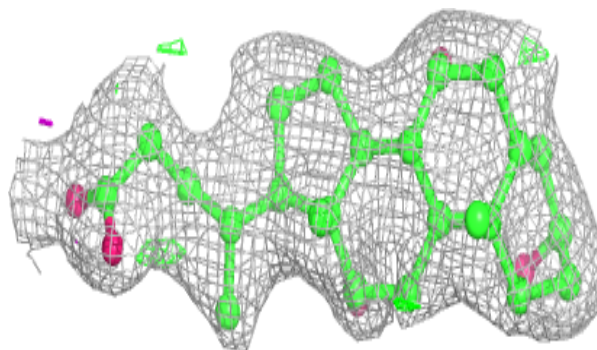


**Electron density around TGL B 301:**

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

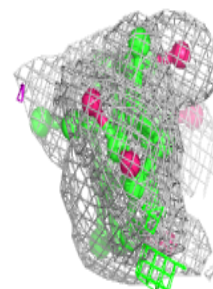
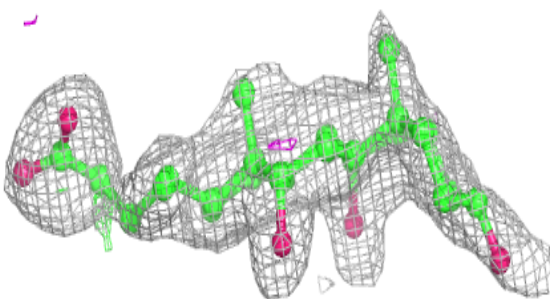
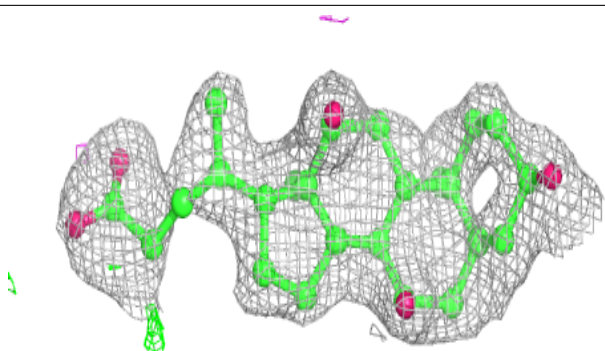
**Electron density around CHD P 307:**

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

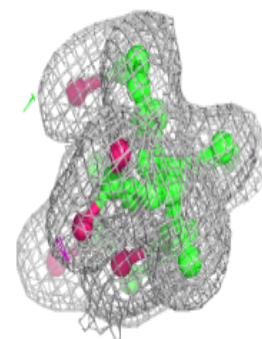
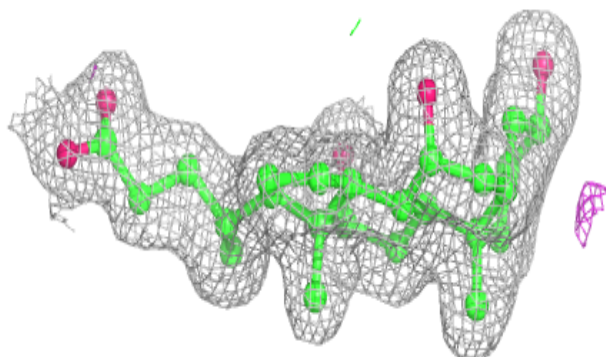
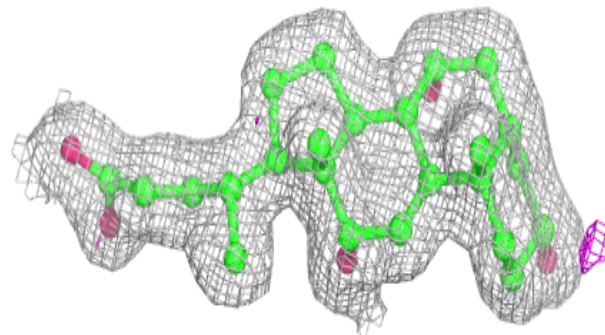


**Electron density around CHD C 305:**

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

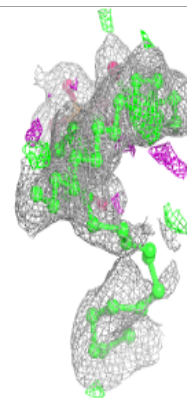
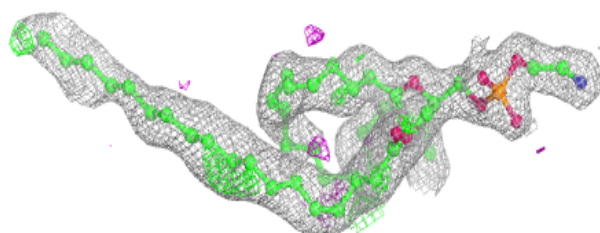
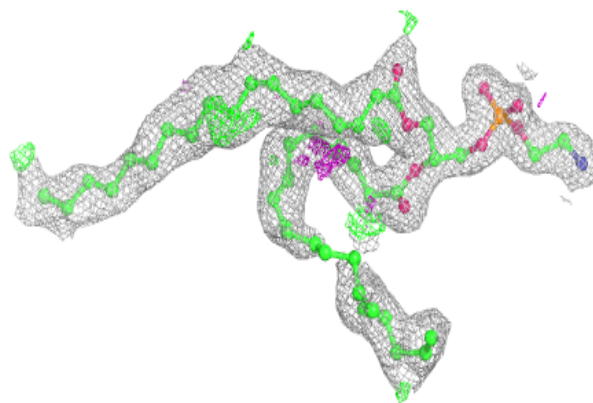
**Electron density around CHD P 308:**

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

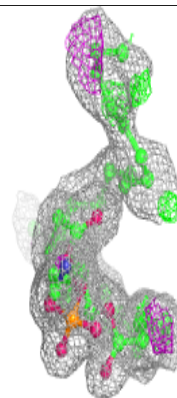
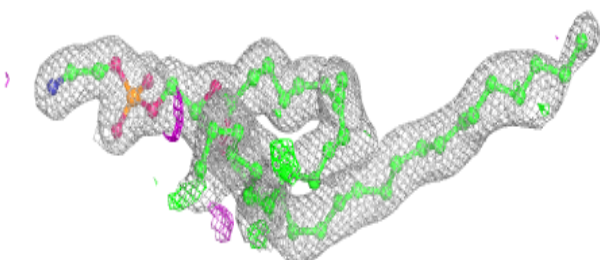
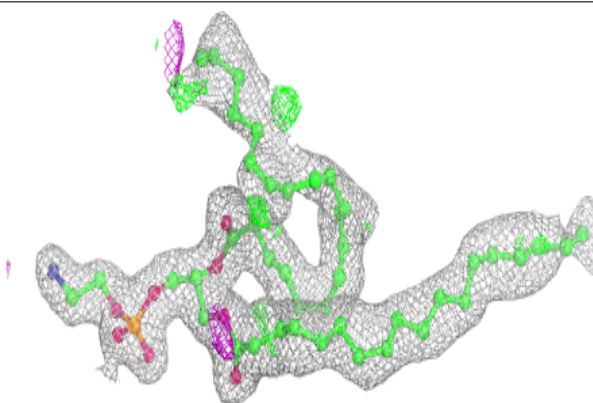


**Electron density around PEK P 304:**

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

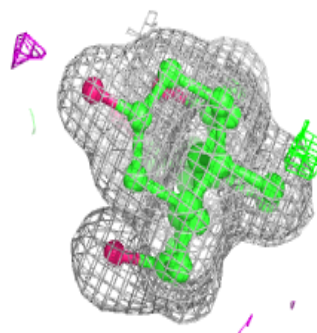
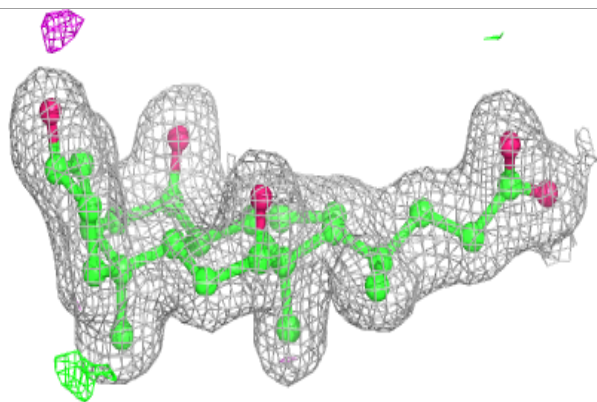
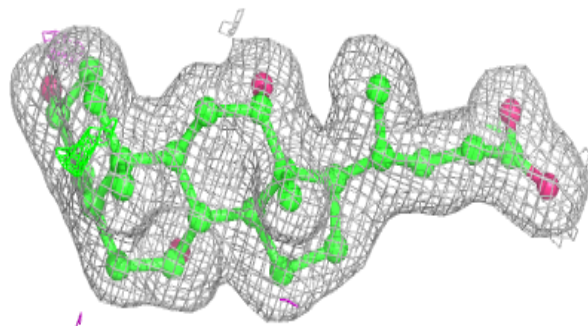
**Electron density around PEK C 302:**

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

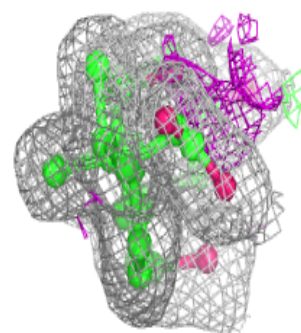
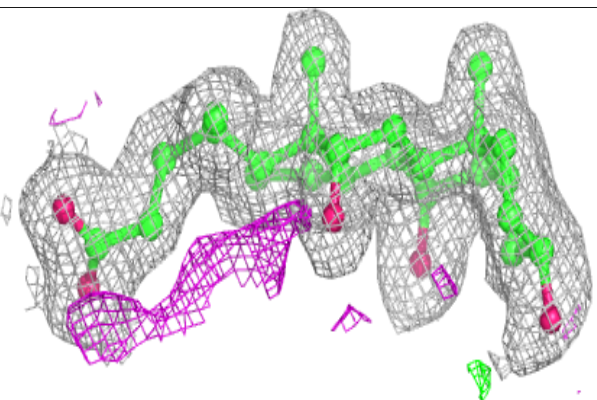
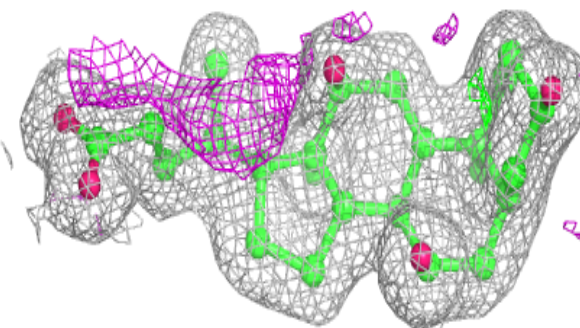


**Electron density around CHD C 306:**

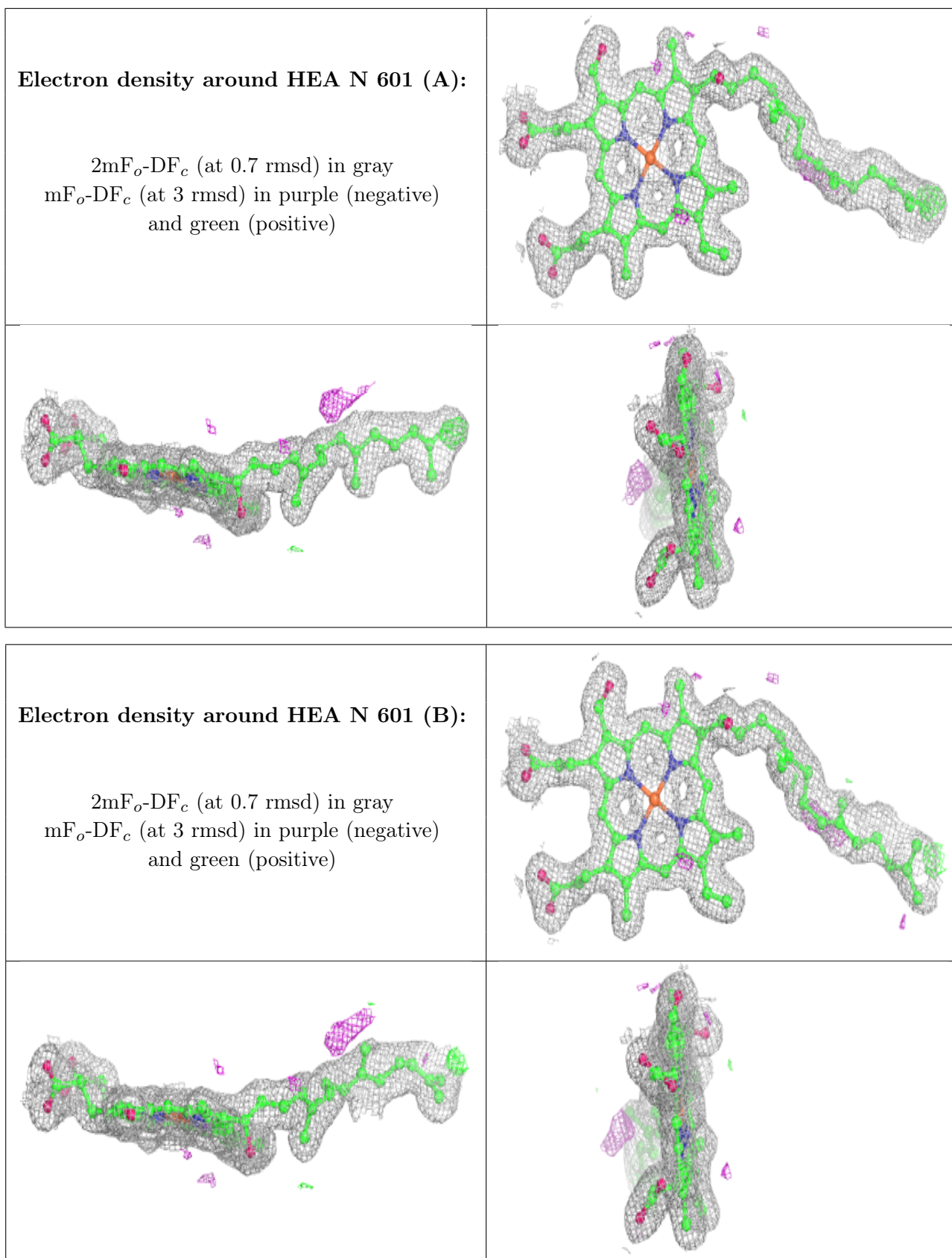
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

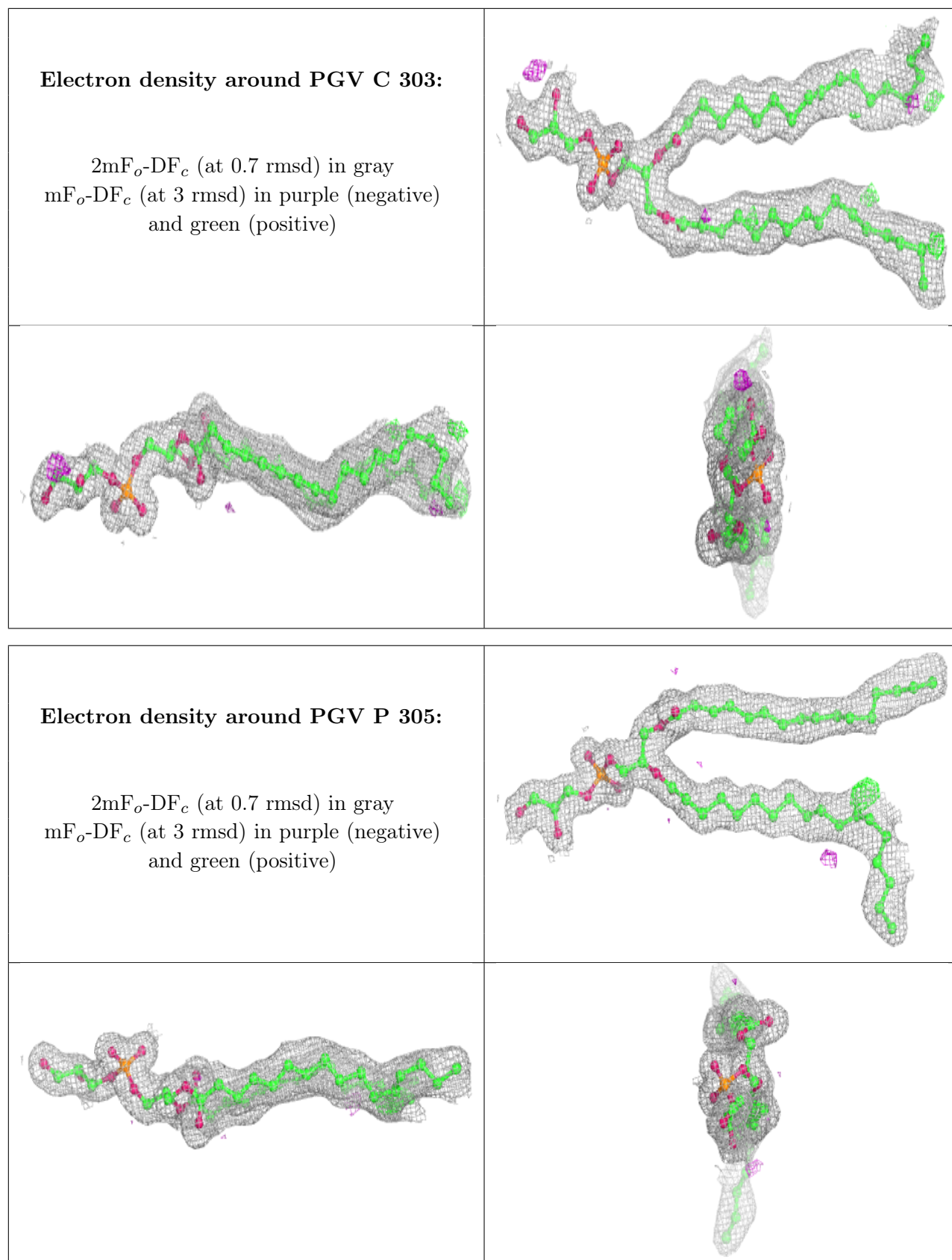
**Electron density around CHD G 103:**

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



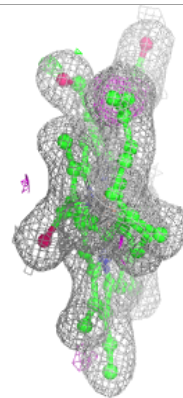
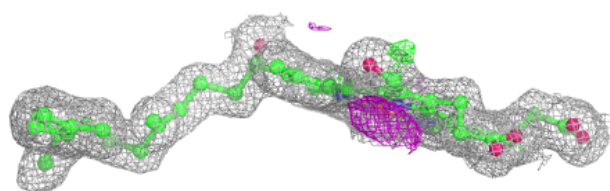
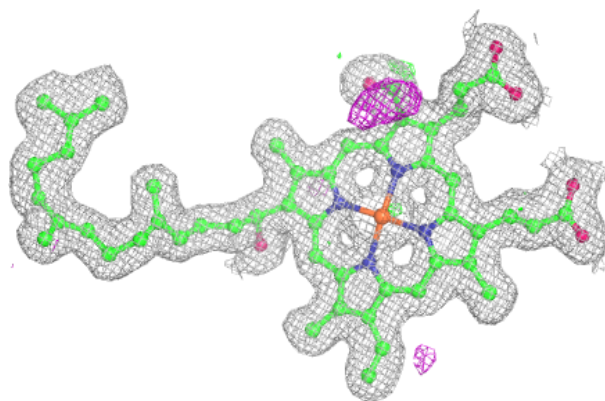




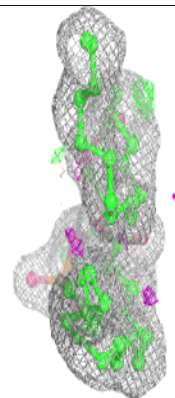
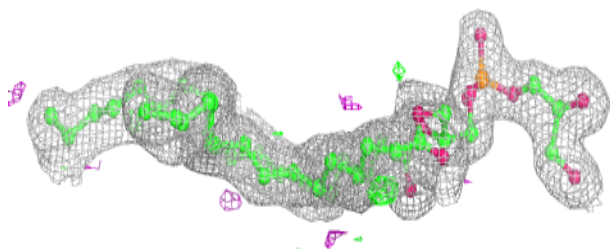
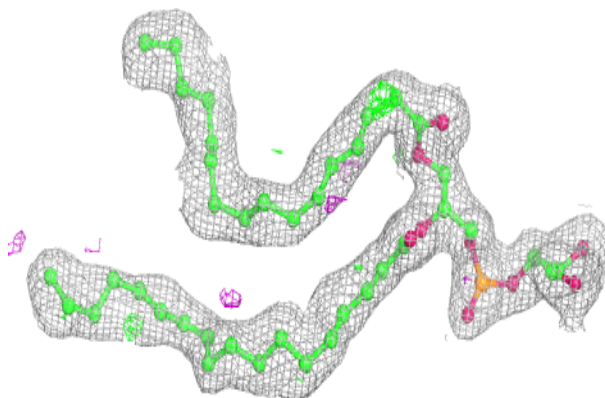


**Electron density around HEA A 602:**

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

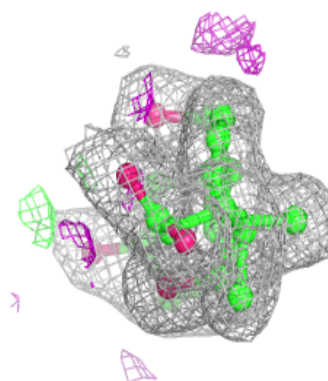
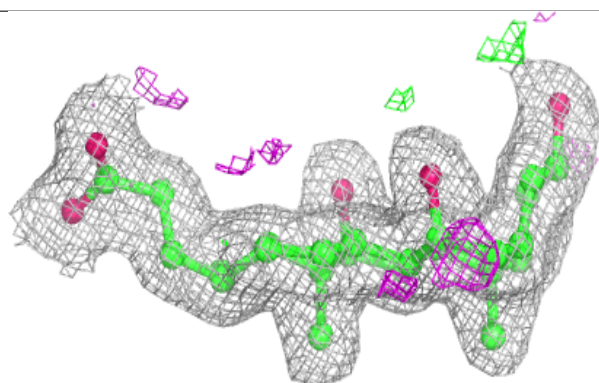
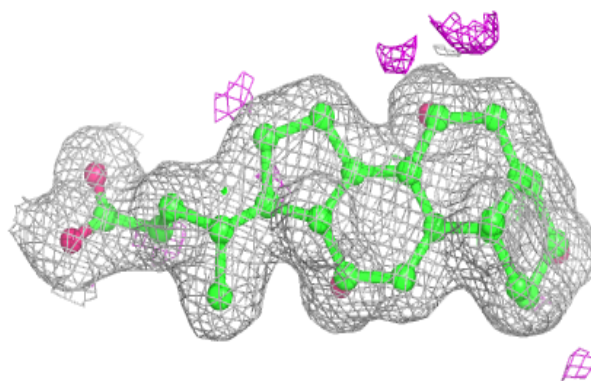
**Electron density around PGV P 301:**

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

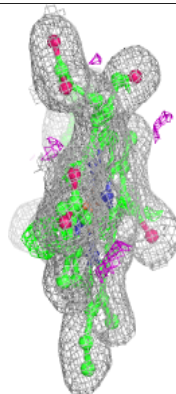
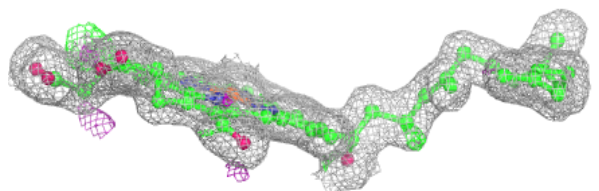
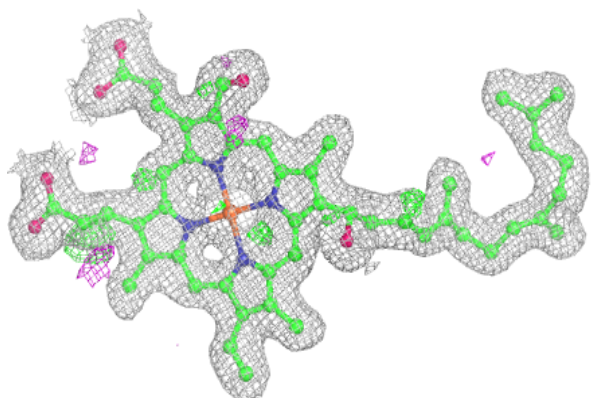


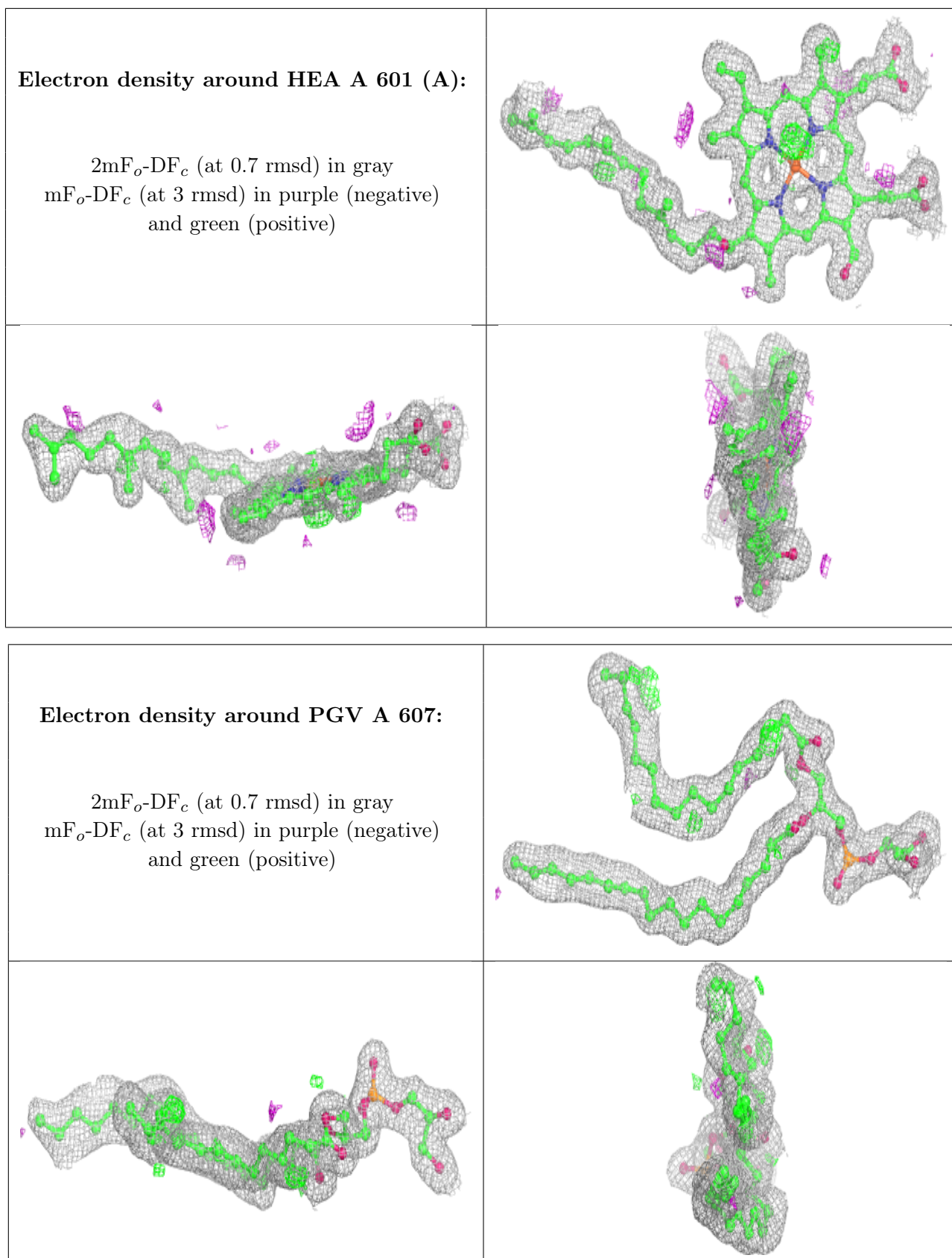
**Electron density around CHD T 101:**

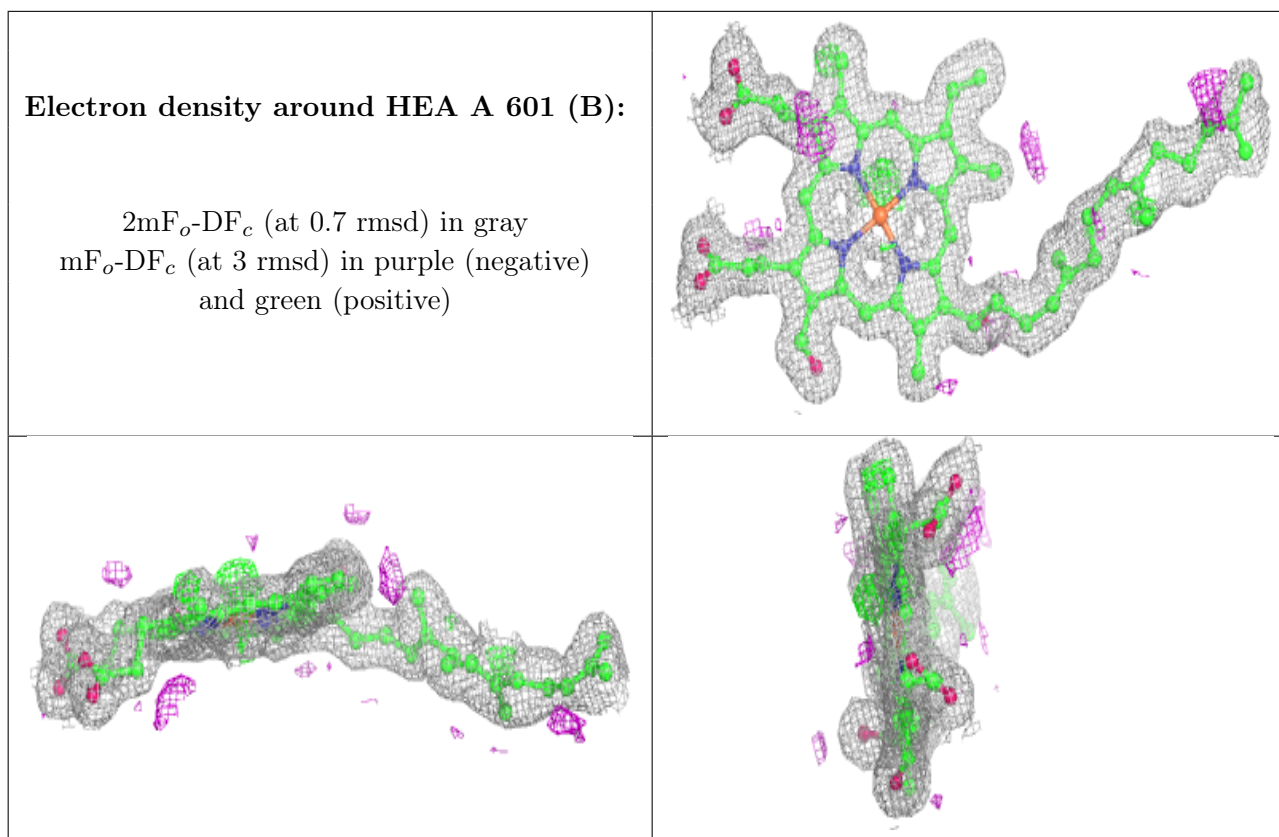
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HEA N 602:**

$2mF_o-DF_c$  (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.