



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 12, 2022 – 08:43 PM JST

PDB ID : 7YPY  
Title : Bovine heart cytochrome c oxidase in fully oxidized state at 1.5 angstrom resolution  
Authors : Shimada, A.; Tsukihara, T.  
Deposited on : 2022-08-05  
Resolution : 1.50 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:

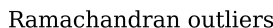
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

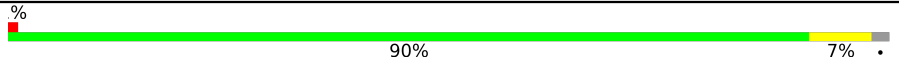
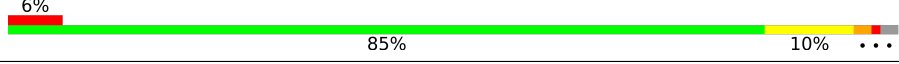

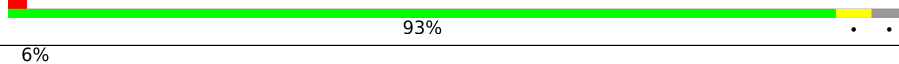

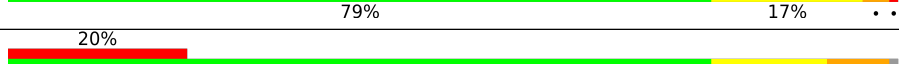
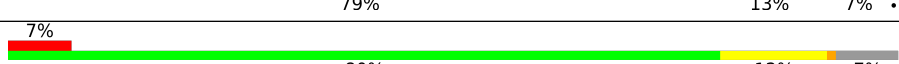
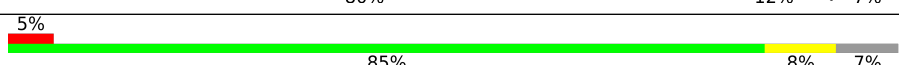
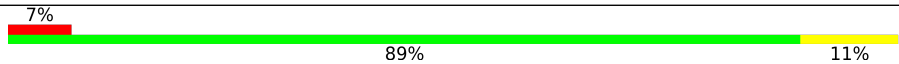
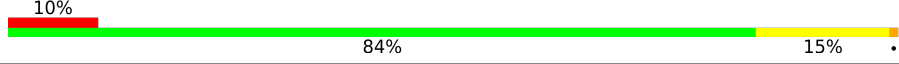
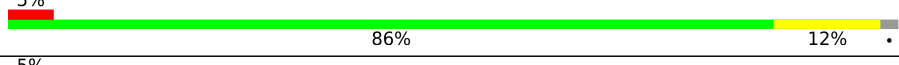
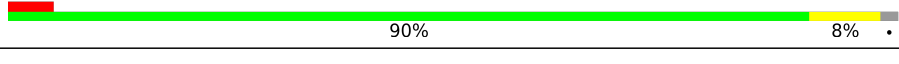
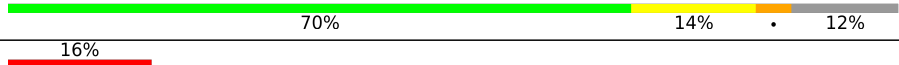

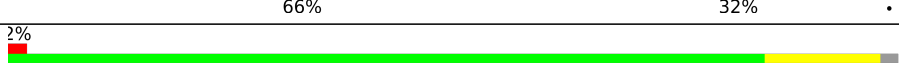




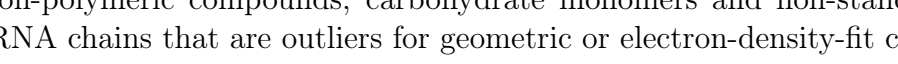
Ramachandran outliers

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.

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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	
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	
14	T	85	

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
15	HEA	A	601[A]	X	-	-	-
15	HEA	A	601[B]	X	-	-	-
15	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	N	601[A]	X	-	-	-
15	HEA	N	601[B]	X	-	-	-
15	HEA	N	602	X	-	-	-
22	EDO	A	610	-	-	X	-
22	EDO	A	621	-	-	X	-
22	EDO	A	622	-	-	-	X
22	EDO	A	625	-	-	X	-
22	EDO	J	103	-	-	-	X
22	EDO	N	622	-	-	X	-
23	DMU	A	628	-	-	-	X
23	DMU	I	101	-	-	-	X
23	DMU	K	101	-	-	-	X
23	DMU	K	102	-	-	-	X
23	DMU	K	104	-	-	-	X
23	DMU	K	105	-	-	-	X
23	DMU	K	106	-	-	-	X
23	DMU	X	102	-	-	-	X
23	DMU	X	103	-	-	-	X
23	DMU	X	105	-	-	-	X
23	DMU	X	106	-	-	-	X
23	DMU	X	107	-	-	-	X
25	CHD	X	101	-	-	-	X
27	CDL	T	102	-	-	X	-
9	SAC	V	1	-	-	-	X



## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 35132 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
1	A	514	Total	C	N	O	S	0	40	0
			4164	2775	638	707	44			
1	N	514	Total	C	N	O	S	0	38	0
			4156	2772	634	706	44			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	11	0
			1854	1207	283	345	19			
2	O	227	Total	C	N	O	S	0	8	0
			1848	1200	284	345	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	10	0
			2138	1428	340	355	15			
3	P	259	Total	C	N	O	S	0	10	0
			2137	1427	340	356	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	4	0
			1208	788	198	218	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1209	788	199	218	4			

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

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
			858	547	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	4	0
			758	469	135	148	6			
6	S	98	Total	C	N	O	S	0	2	0
			753	467	134	146	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total	C	N	O	P	S	0	2	0
			682	437	129	114	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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			
10	W	58	Total	C	N	O	S	0	1	0
			464	299	78	84	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	2	0
			388	253	65	67	3			
11	X	49	Total	C	N	O	S	0	2	0
			388	253	65	67	3			

- 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	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	4	0
			390	260	65	62	3			

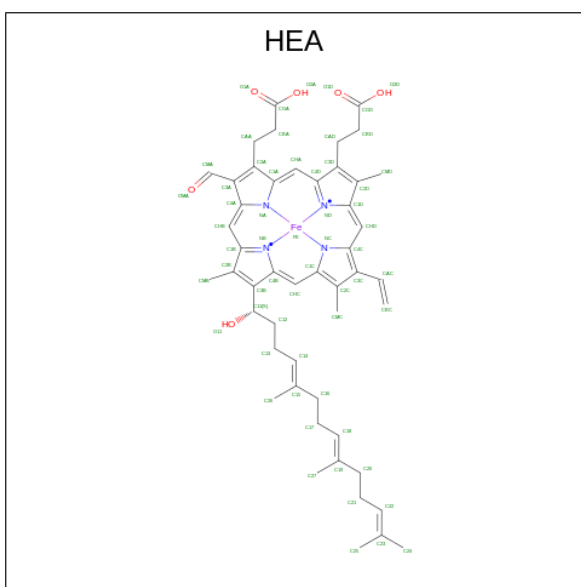
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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 a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	84	Total	C	N	O	S	0	2	0
			678	437	129	111	1			

- Molecule 15 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

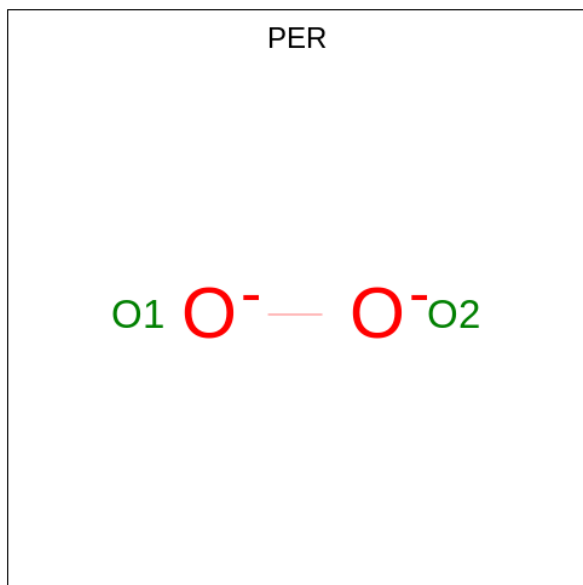
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

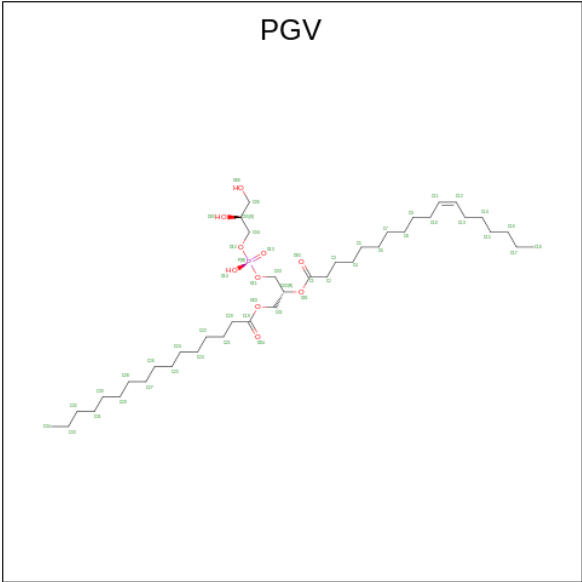
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



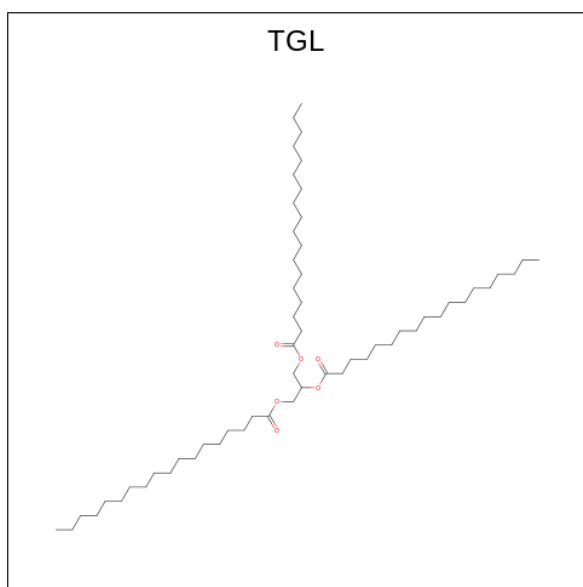
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		
19	N	1	Total	O	0	0
			2	2		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



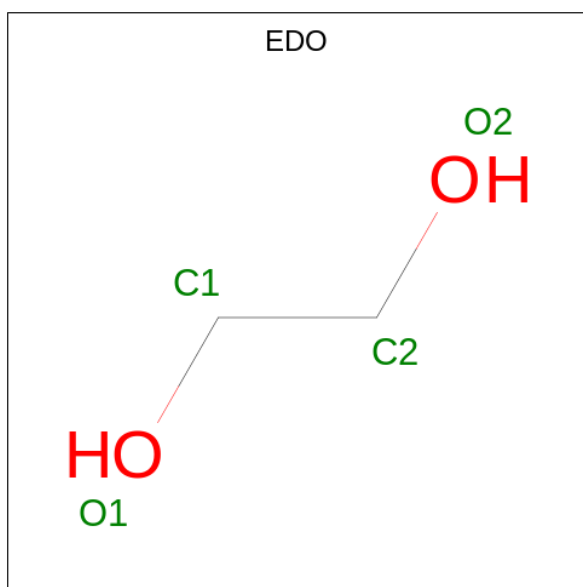
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			48	37	10	1		
20	G	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	Q	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			63	57	6		
21	B	1	Total	C	O	0	0
			62	56	6		
21	D	1	Total	C	O	0	0
			62	56	6		
21	O	1	Total	C	O	0	0
			60	54	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 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
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total 4	C 2	O 2	0	0
22	A	1	Total 4	C 2	O 2	0	0
22	A	1	Total 4	C 2	O 2	0	0
22	A	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	E	1	Total 4	C 2	O 2	0	0
22	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	E	1	Total C O 4 2 2	0	0
22	F	1	Total C O 4 2 2	0	0
22	F	1	Total C O 4 2 2	0	0
22	F	1	Total C O 4 2 2	0	0
22	F	1	Total C O 4 2 2	0	0
22	F	1	Total C O 4 2 2	0	0
22	F	1	Total C O 4 2 2	0	0
22	G	1	Total C O 4 2 2	0	0
22	G	1	Total C O 4 2 2	0	0
22	G	1	Total C O 4 2 2	0	0
22	H	1	Total C O 4 2 2	0	0
22	J	1	Total C O 4 2 2	0	0
22	J	1	Total C O 4 2 2	0	0
22	J	1	Total C O 4 2 2	0	0
22	J	1	Total C O 4 2 2	0	0
22	J	1	Total C O 4 2 2	0	0
22	L	1	Total C O 4 2 2	0	0
22	L	1	Total C O 4 2 2	0	0
22	L	1	Total C O 4 2 2	0	0
22	M	1	Total C O 4 2 2	0	0
22	M	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	O	1	Total	C	O	0	0
			4	2	2		
22	O	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		

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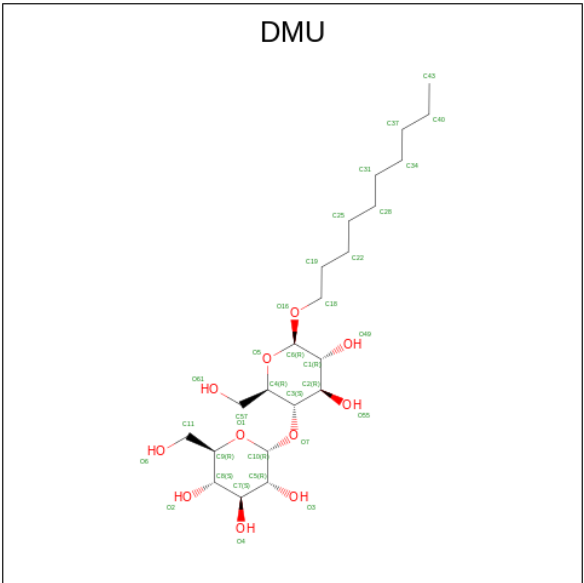
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	P	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		
22	Q	1	Total	C	O	0	0
			4	2	2		
22	Q	1	Total	C	O	0	0
			4	2	2		
22	R	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	V	1	Total	C	O	0	0
			4	2	2		
22	W	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	Y	1	Total	C	O	0	0
			4	2	2		
22	Y	1	Total	C	O	0	0
			4	2	2		
22	Z	1	Total	C	O	0	0
			4	2	2		

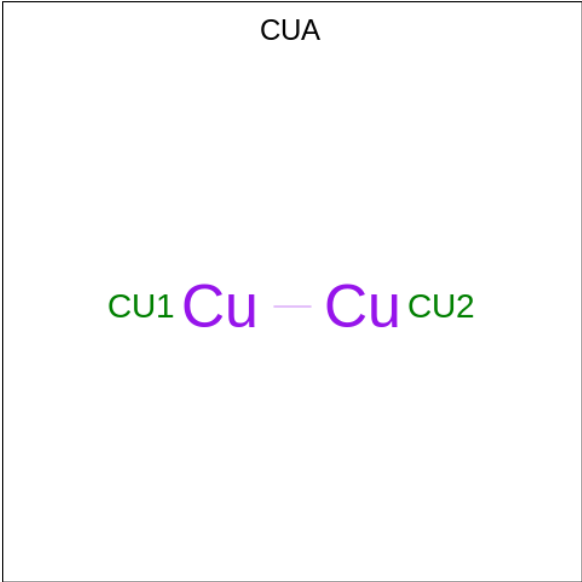
- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



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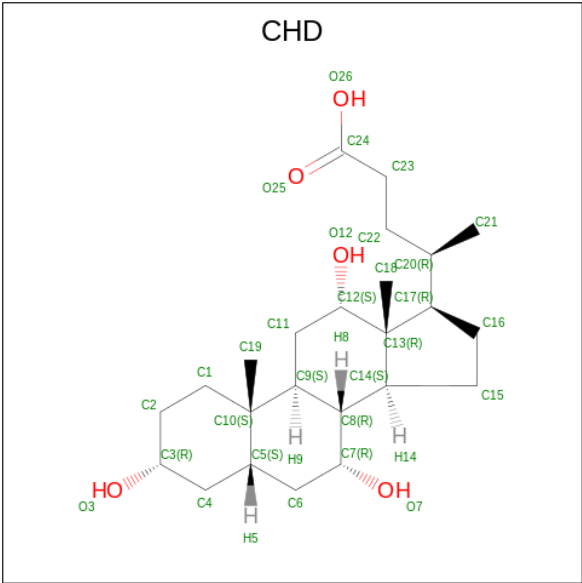
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	K	1	Total	C	O	0	0
			33	22	11		
23	K	1	Total	C	O	0	0
			32	22	10		
23	K	1	Total	C	O	0	0
			33	22	11		
23	K	1	Total	C	O	0	0
			33	22	11		
23	K	1	Total	C	O	0	0
			33	22	11		
23	L	1	Total	C	O	0	0
			33	22	11		
23	M	1	Total	C	O	0	0
			33	22	11		
23	O	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 24 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 25 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



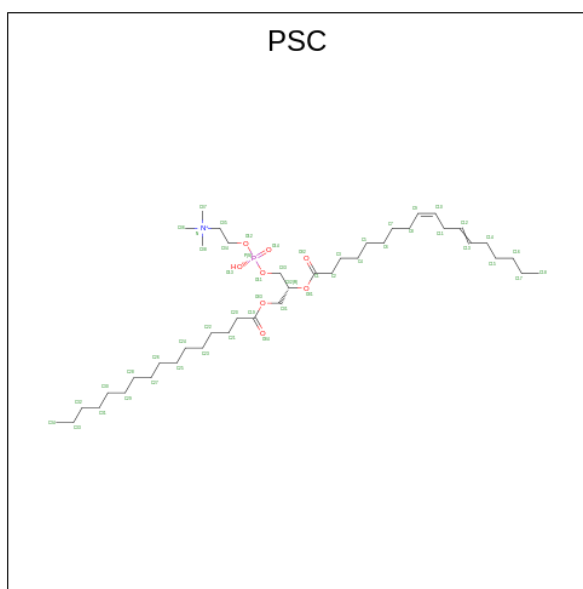
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			29	24	5		
25	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			29	24	5		
25	L	1	Total	C	O	0	0
			29	24	5		
25	O	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		
25	X	1	Total	C	O	0	0
			29	24	5		
25	Y	1	Total	C	O	0	0
			29	24	5		

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)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) (labeled as "Ligand of Interest" by depositor).

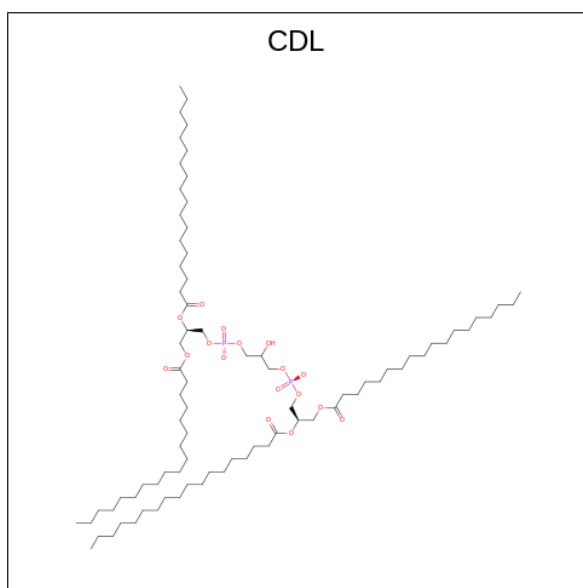


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled

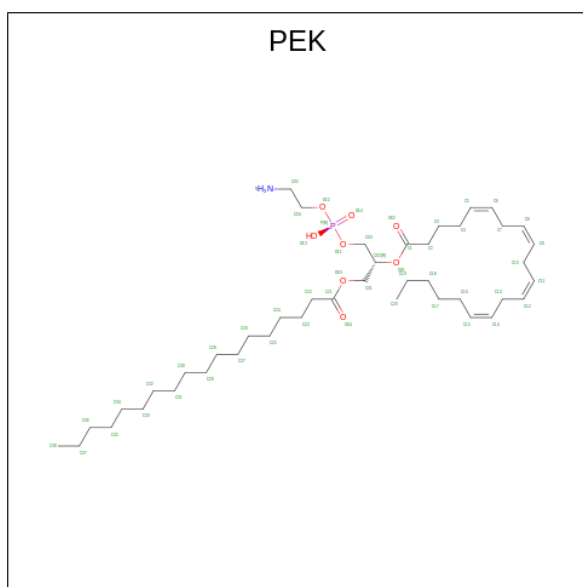


as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	C	1	Total	C	O	P	0	0
			89	71	16	2		
27	G	1	Total	C	O	P	0	0
			100	81	17	2		
27	P	1	Total	C	O	P	0	0
			90	72	16	2		
27	T	1	Total	C	O	P	0	0
			98	79	17	2		

- Molecule 28 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) (labeled as "Ligand of Interest" by depositor).

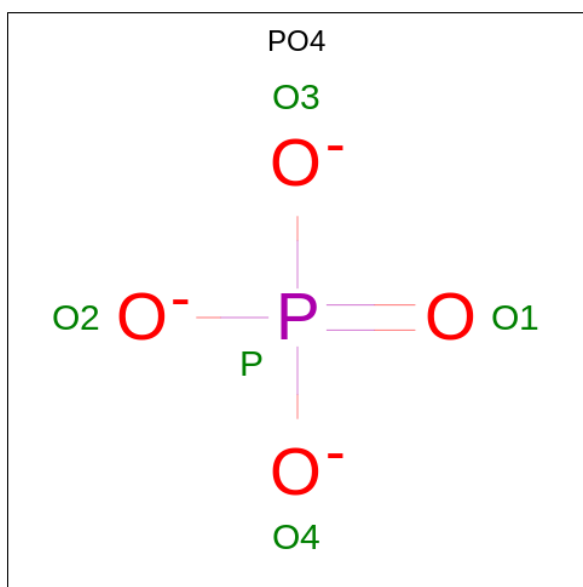


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	C	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	O	P		0	0
			50	41	8	1			

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	1	Total	Zn	0	0
			1	1		
29	S	1	Total	Zn	0	0
			1	1		

- Molecule 30 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 31 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	A	264	Total	O	0	9
			264	264		
31	B	218	Total	O	0	6
			219	219		
31	C	142	Total	O	0	0
			142	142		
31	D	212	Total	O	0	0
			212	212		
31	E	159	Total	O	0	0
			159	159		
31	F	156	Total	O	0	0
			156	156		
31	G	78	Total	O	0	0
			78	78		
31	H	102	Total	O	0	0
			102	102		
31	I	65	Total	O	0	0
			65	65		
31	J	48	Total	O	0	0
			48	48		

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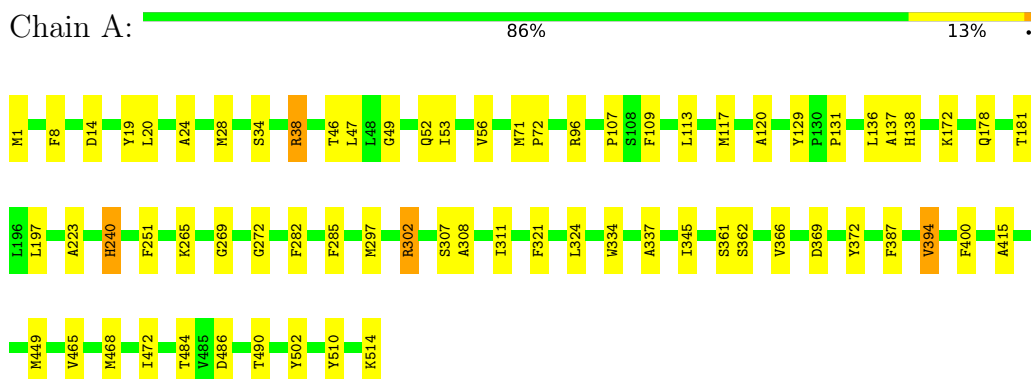
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	K	40	Total 40	O 40	0	0
31	L	36	Total 36	O 36	0	2
31	M	34	Total 34	O 34	0	0
31	N	260	Total 260	O 260	0	13
31	O	184	Total 185	O 185	0	6
31	P	139	Total 139	O 139	0	0
31	Q	97	Total 97	O 97	0	0
31	R	110	Total 110	O 110	0	0
31	S	135	Total 135	O 135	0	0
31	T	60	Total 60	O 60	0	0
31	U	79	Total 79	O 79	0	0
31	V	50	Total 50	O 50	0	0
31	W	40	Total 40	O 40	0	0
31	X	31	Total 31	O 31	0	0
31	Y	30	Total 30	O 30	0	0
31	Z	22	Total 22	O 22	0	0

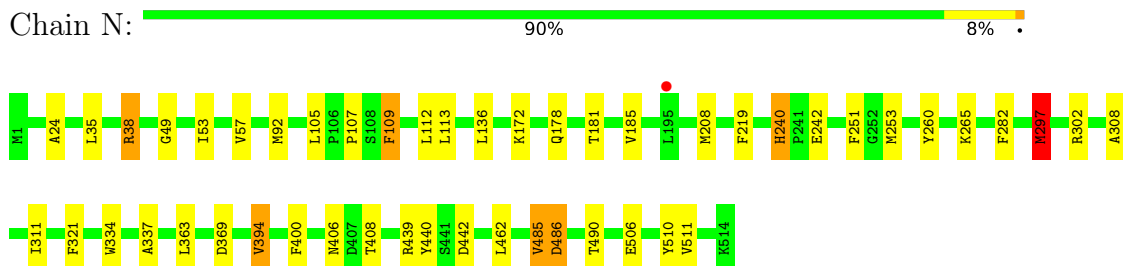
### 3 Residue-property plots

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

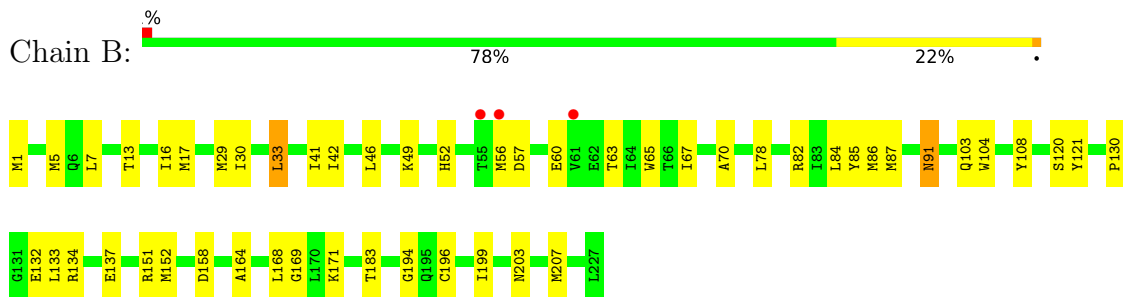
- Molecule 1: Cytochrome c oxidase subunit 1



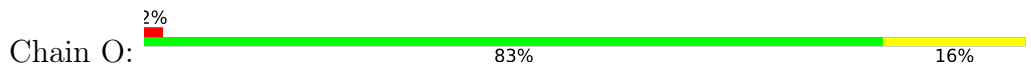
- Molecule 1: Cytochrome c oxidase subunit 1

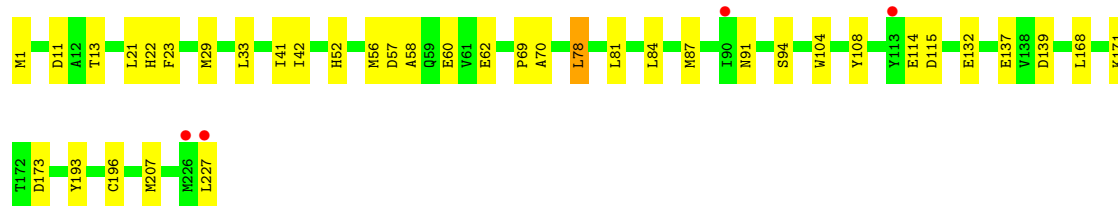


- Molecule 2: Cytochrome c oxidase subunit 2



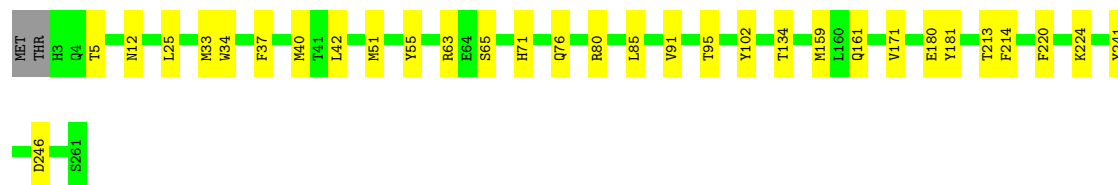
- Molecule 2: Cytochrome c oxidase subunit 2





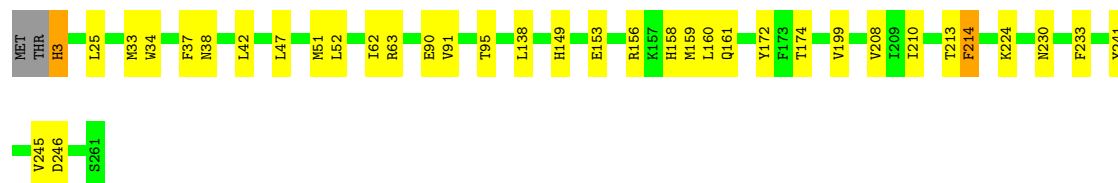
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 12% .



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 85% 13% ..



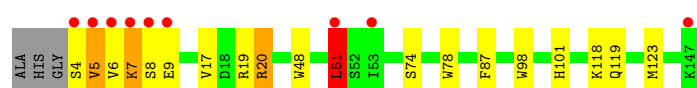
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 90% 7% .



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 85% 10% 6% ...

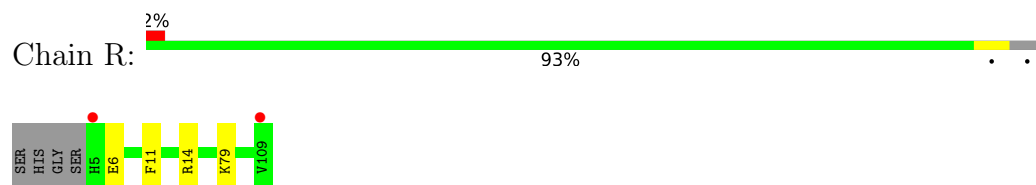


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

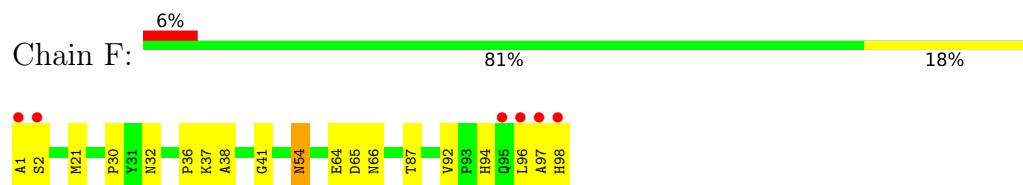
Chain E: 87% 9% .



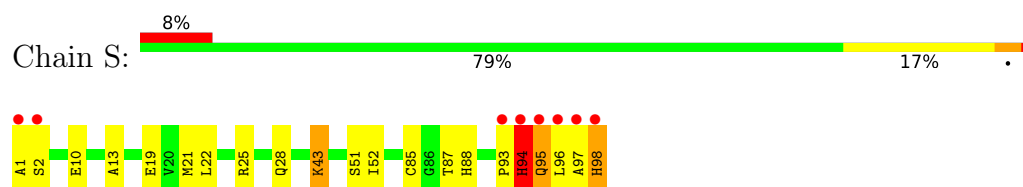
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



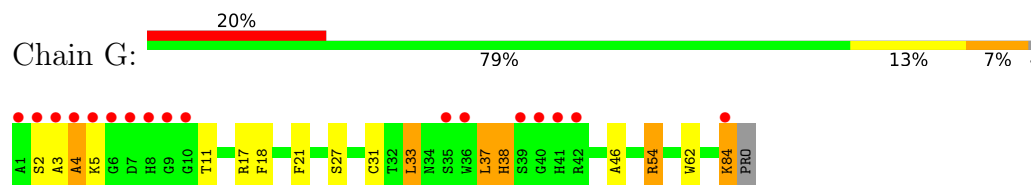
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



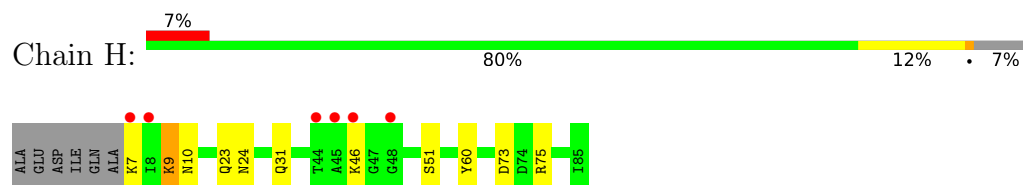
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



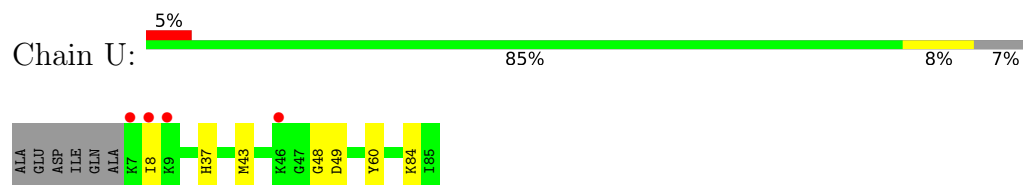
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



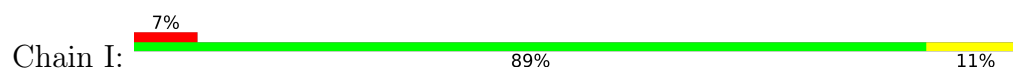
- Molecule 8: Cytochrome c oxidase subunit 6B1

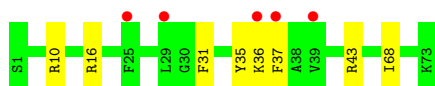


- Molecule 8: Cytochrome c oxidase subunit 6B1

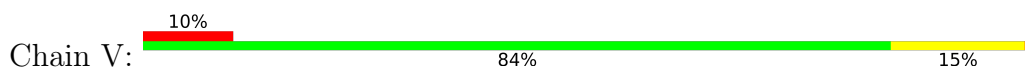


- Molecule 9: Cytochrome c oxidase subunit 6C

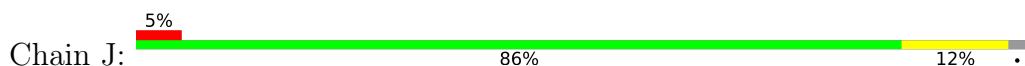




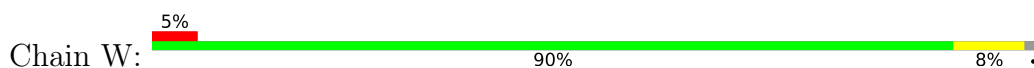
- Molecule 9: Cytochrome c oxidase subunit 6C



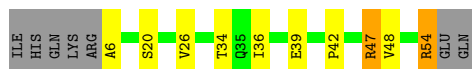
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



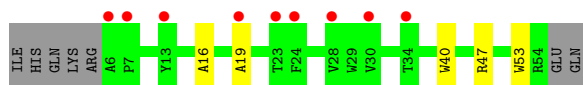
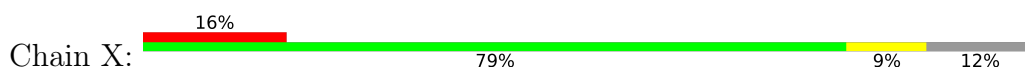
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

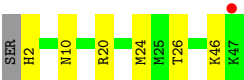
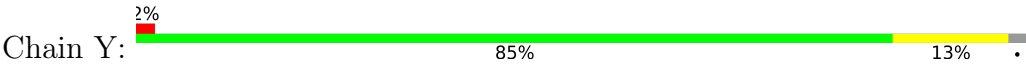


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

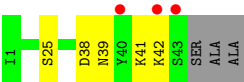
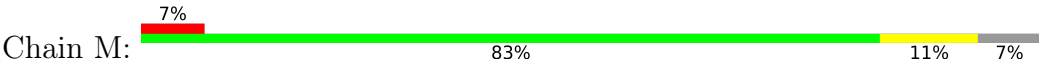


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

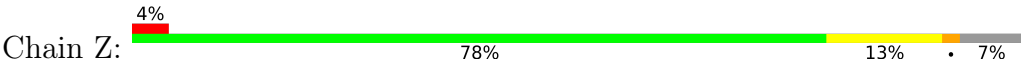




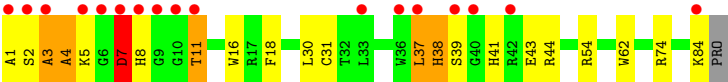
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



• Molecule 14: Cytochrome c oxidase subunit 6A2, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.94Å 204.40Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.95 – 1.50 89.10 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.95-1.50) 98.2 (89.10-1.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.40Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.159 , 0.177 0.160 , 0.177	Depositor DCC
$R_{free}$ test set	63174 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	35132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CHD, PSC, CUA, EDO, FME, DMU, PGV, CU, MG, SAC, ZN, CDL, HEA, TGL, PER, TPO, PEK, NA, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.09	10/4467 (0.2%)	1.14	18/6094 (0.3%)
1	N	0.98	4/4445 (0.1%)	0.99	11/6066 (0.2%)
2	B	0.98	3/1952 (0.2%)	1.08	6/2658 (0.2%)
2	O	0.82	1/1929 (0.1%)	0.94	6/2626 (0.2%)
3	C	0.98	3/2278 (0.1%)	0.95	6/3112 (0.2%)
3	P	0.96	1/2277 (0.0%)	0.90	4/3110 (0.1%)
4	D	0.96	0/1266	0.90	2/1706 (0.1%)
4	Q	0.60	0/1259	0.72	3/1698 (0.2%)
5	E	0.83	1/871 (0.1%)	0.92	4/1182 (0.3%)
5	R	0.69	0/882	0.73	0/1196
6	F	0.88	0/795	0.87	0/1079
6	S	0.77	0/780	0.87	0/1058
7	G	0.79	0/708	0.89	1/961 (0.1%)
8	H	0.89	0/682	0.92	2/921 (0.2%)
8	U	0.71	0/682	0.78	0/921
9	I	0.79	0/605	0.83	2/802 (0.2%)
9	V	0.72	0/605	0.73	1/802 (0.1%)
10	J	0.57	0/471	0.71	1/636 (0.2%)
10	W	0.54	0/480	0.66	1/648 (0.2%)
11	K	0.87	0/413	0.83	1/566 (0.2%)
11	X	0.57	0/413	0.63	0/566
12	L	1.06	1/393 (0.3%)	0.90	0/526
12	Y	0.73	0/427	0.71	0/570
13	M	0.94	0/345	0.89	0/470
13	Z	0.69	0/345	0.69	0/470
14	T	0.75	0/716	0.80	0/974
All	All	0.91	24/30486 (0.1%)	0.94	69/41418 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	S	0	2
All	All	0	4

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	241	TYR	CE1-CZ	-6.16	1.30	1.38
5	E	70	VAL	CB-CG1	-5.91	1.40	1.52
1	A	362[A]	SER	CB-OG	-5.90	1.34	1.42
1	A	362[B]	SER	CB-OG	-5.90	1.34	1.42
3	C	76	GLN	CD-OE1	5.81	1.36	1.24

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	38	ARG	NE-CZ-NH1	11.34	125.97	120.30
4	Q	20	ARG	NE-CZ-NH2	-8.88	115.86	120.30
9	I	16	ARG	NE-CZ-NH2	-8.77	115.92	120.30
3	P	153	GLU	OE1-CD-OE2	8.19	133.13	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4164	0	4140	66	0
1	N	4156	0	4141	46	0
2	B	1854	0	1861	35	0
2	O	1848	0	1847	21	0
3	C	2138	0	2061	27	0
3	P	2137	0	2057	37	0
4	D	1208	0	1199	11	0
4	Q	1209	0	1202	17	0
5	E	852	0	845	2	0
5	R	858	0	854	4	0
6	F	758	0	739	17	0
6	S	753	0	736	16	0
7	G	682	0	650	14	0
8	H	662	0	623	5	0
8	U	662	0	623	2	0
9	I	601	0	613	4	0
9	V	601	0	613	6	0
10	J	460	0	459	5	0
10	W	464	0	461	3	0
11	K	388	0	372	9	0
11	X	388	0	372	5	0
12	L	380	0	380	16	0
12	Y	390	0	390	5	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	T	678	0	651	20	0
15	A	129	0	88	4	0
15	N	129	0	88	4	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	2	0	0	1	0
19	N	2	0	0	1	0
20	A	102	0	152	2	0
20	C	99	0	143	1	0
20	G	51	0	76	2	0
20	N	51	0	76	1	0
20	P	51	0	76	1	0
20	Q	51	0	76	5	0
21	A	63	0	110	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	62	0	105	6	0
21	D	62	0	105	12	0
21	O	60	0	101	4	0
21	Q	63	0	110	8	0
21	Y	63	0	110	8	0
22	A	72	0	107	26	0
22	B	20	0	30	1	0
22	C	24	0	36	1	0
22	D	16	0	24	2	0
22	E	12	0	18	0	0
22	F	24	0	35	0	0
22	G	12	0	18	1	0
22	H	4	0	6	1	0
22	J	20	0	30	1	0
22	L	12	0	18	0	0
22	M	8	0	12	1	0
22	N	68	0	102	12	0
22	O	8	0	12	0	0
22	P	24	0	36	1	0
22	Q	8	0	12	1	0
22	R	4	0	6	0	0
22	S	32	0	48	6	0
22	T	16	0	24	0	0
22	V	4	0	6	2	0
22	W	4	0	6	1	0
22	Y	8	0	12	0	0
22	Z	4	0	6	0	0
23	A	33	0	42	1	0
23	C	132	0	168	6	0
23	D	33	0	42	1	0
23	I	33	0	42	4	0
23	K	197	0	250	8	0
23	L	33	0	42	4	0
23	M	33	0	42	1	0
23	O	33	0	42	0	0
23	P	99	0	126	10	0
23	X	198	0	252	10	0
23	Z	33	0	42	0	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	B	29	0	39	0	0
25	C	58	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	29	0	39	1	0
25	O	29	0	39	1	0
25	P	58	0	78	3	0
25	X	29	0	36	7	0
25	Y	29	0	39	0	0
26	B	52	0	80	11	0
26	O	51	0	75	9	0
27	C	89	0	126	8	0
27	G	100	0	156	18	0
27	P	90	0	133	11	0
27	T	98	0	149	21	0
28	C	158	0	226	20	0
28	P	106	0	154	7	0
28	T	50	0	71	5	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	H	5	0	0	0	0
30	U	5	0	0	0	0
31	A	264	0	0	12	0
31	B	219	0	0	3	0
31	C	142	0	0	3	0
31	D	212	0	0	1	0
31	E	159	0	0	0	0
31	F	156	0	0	1	0
31	G	78	0	0	0	0
31	H	102	0	0	3	0
31	I	65	0	0	1	0
31	J	48	0	0	1	0
31	K	40	0	0	2	0
31	L	36	0	0	2	0
31	M	34	0	0	0	0
31	N	260	0	0	5	0
31	O	185	0	0	0	0
31	P	139	0	0	2	0
31	Q	97	0	0	0	0
31	R	110	0	0	1	0
31	S	135	0	0	2	0
31	T	60	0	0	2	0
31	U	79	0	0	1	0
31	V	50	0	0	0	0
31	W	40	0	0	0	0
31	X	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Y	30	0	0	0	0
31	Z	22	0	0	0	0
All	All	35132	0	33221	471	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 7.

The worst 5 of 471 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)
19:A:606:PER:O2	19:A:606:PER:O1	1.55	1.24
19:N:606:PER:O2	19:N:606:PER:O1	1.55	1.21
4:D:78:TRP:HB3	21:D:201:TGL:HB21	1.38	1.02
12:Y:20:ARG:HH22	21:Y:101:TGL:HC51	1.26	0.96
27:G:101:CDL:H241	27:G:101:CDL:H541	1.52	0.91

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	552/514 (107%)	537 (97%)	15 (3%)	0	100	100
1	N	550/514 (107%)	534 (97%)	16 (3%)	0	100	100
2	B	236/227 (104%)	231 (98%)	5 (2%)	0	100	100
2	O	233/227 (103%)	226 (97%)	7 (3%)	0	100	100
3	C	267/261 (102%)	262 (98%)	5 (2%)	0	100	100
3	P	267/261 (102%)	262 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	143 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	139 (96%)	5 (3%)	1 (1%)	22	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	100/98 (102%)	96 (96%)	3 (3%)	1 (1%)	15	3
6	S	98/98 (100%)	92 (94%)	2 (2%)	4 (4%)	3	0
7	G	83/85 (98%)	70 (84%)	9 (11%)	4 (5%)	2	0
8	H	77/85 (91%)	71 (92%)	6 (8%)	0	100	100
8	U	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	5	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	1 (1%)	1 (1%)	11	1
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
11	X	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	48/47 (102%)	46 (96%)	1 (2%)	1 (2%)	7	1
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
14	T	84/85 (99%)	71 (84%)	7 (8%)	6 (7%)	1	0
All	All	3649/3614 (101%)	3529 (97%)	100 (3%)	20 (0%)	25	9

5 of 20 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/426 (109%)	461 (99%)	4 (1%)	78	61
1	N	463/426 (109%)	454 (98%)	9 (2%)	57	27
2	B	221/210 (105%)	216 (98%)	5 (2%)	50	20
2	O	218/210 (104%)	211 (97%)	7 (3%)	39	10
3	C	234/226 (104%)	232 (99%)	2 (1%)	78	61
3	P	234/226 (104%)	230 (98%)	4 (2%)	60	33
4	D	132/129 (102%)	129 (98%)	3 (2%)	50	20
4	Q	131/129 (102%)	125 (95%)	6 (5%)	27	5
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	22
5	R	93/95 (98%)	93 (100%)	0	100	100
6	F	85/81 (105%)	80 (94%)	5 (6%)	19	2
6	S	83/81 (102%)	81 (98%)	2 (2%)	49	19
7	G	69/68 (102%)	63 (91%)	6 (9%)	10	0
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	1
8	U	71/75 (95%)	69 (97%)	2 (3%)	43	14
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	9
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	3
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	50/50 (100%)	49 (98%)	1 (2%)	55	25
11	K	41/46 (89%)	40 (98%)	1 (2%)	49	19
11	X	41/46 (89%)	40 (98%)	1 (2%)	49	19
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	16
12	Y	43/40 (108%)	42 (98%)	1 (2%)	50	20
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	3
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	1
14	T	70/69 (101%)	62 (89%)	8 (11%)	5	0
All	All	3183/3083 (103%)	3098 (97%)	85 (3%)	46	15

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	230	ASN

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Mol	Chain	Res	Type
14	T	43	GLU
4	Q	7	LYS
6	S	98	HIS
8	U	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
14	T	8	HIS
14	T	34	ASN
9	V	20	HIS
12	L	2	HIS
1	N	178	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	1.36	2 (25%)	7,9,11	1.60	2 (28%)
9	SAC	I	1	9	7,8,9	0.60	0	8,9,11	0.86	0
9	SAC	V	1	9	7,8,9	0.60	0	8,9,11	0.90	1 (12%)
1	FME	N	1	1	8,9,10	0.52	0	7,9,11	1.11	0
2	FME	O	1	2	8,9,10	0.89	0	7,9,11	1.26	2 (28%)
1	FME	A	1	1	8,9,10	0.53	0	7,9,11	1.30	1 (14%)
7	TPO	G	11	7	8,10,11	1.34	1 (12%)	10,14,16	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	0/7/8/10	-
9	SAC	V	1	9	-	2/7/8/10	-
1	FME	N	1	1	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
7	TPO	G	11	7	-	3/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.74	1.59	1.50
2	B	1	FME	CG-SD	-2.38	1.68	1.81
2	B	1	FME	CB-CG	2.33	1.60	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.62	105.66	112.95
2	B	1	FME	O-C-CA	-2.57	118.04	124.78
2	O	1	FME	CG-CB-CA	-2.37	106.37	112.95
1	A	1	FME	O1-CN-N	-2.24	119.36	125.27
9	V	1	SAC	O-C-CA	-2.13	119.19	124.78

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 182 ligands modelled in this entry, 8 are monoatomic - leaving 174 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$
22	EDO	P	308	-	3,3,3	0.42	0	2,2,2	0.30	0
23	DMU	L	105	-	34,34,34	0.48	1 (2%)	45,45,45	1.04	1 (2%)
23	DMU	K	104	-	34,34,34	0.53	0	45,45,45	1.19	4 (8%)
23	DMU	D	206	-	34,34,34	0.53	0	45,45,45	1.40	7 (15%)
22	EDO	N	610	-	3,3,3	0.40	0	2,2,2	0.48	0
22	EDO	A	617	-	3,3,3	0.67	0	2,2,2	0.10	0
22	EDO	A	627	-	3,3,3	0.44	0	2,2,2	0.70	0
21	TGL	O	301	-	59,59,62	1.04	3 (5%)	62,62,65	1.02	5 (8%)
28	PEK	C	305	-	52,52,52	1.01	2 (3%)	55,57,57	1.38	8 (14%)
22	EDO	N	621	-	3,3,3	0.70	0	2,2,2	0.25	0
21	TGL	D	201	-	61,61,62	1.20	6 (9%)	64,64,65	1.18	6 (9%)
22	EDO	S	109	-	3,3,3	0.92	0	2,2,2	0.57	0
23	DMU	I	101	-	34,34,34	0.49	0	45,45,45	1.05	3 (6%)
26	PSC	O	304	-	50,50,51	1.15	3 (6%)	56,58,59	1.51	9 (16%)
22	EDO	D	202	-	3,3,3	0.33	0	2,2,2	0.53	0
15	HEA	A	601[B]	-	57,67,67	1.69	12 (21%)	61,103,103	2.16	21 (34%)
22	EDO	C	312	-	3,3,3	0.59	0	2,2,2	0.38	0
22	EDO	P	312	-	3,3,3	0.40	0	2,2,2	0.53	0
22	EDO	O	305	-	3,3,3	0.48	0	2,2,2	0.24	0
22	EDO	N	618	-	3,3,3	0.44	0	2,2,2	0.93	0
22	EDO	Y	103	-	3,3,3	0.45	0	2,2,2	0.37	0
23	DMU	K	101	-	34,34,34	0.59	1 (2%)	45,45,45	1.54	10 (22%)
22	EDO	V	101	-	3,3,3	0.50	0	2,2,2	0.22	0
25	CHD	L	104	-	32,32,32	0.67	0	51,51,51	2.25	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	HEA	A	601[A]	-	57,67,67	1.66	12 (21%)	61,103,103	1.99	20 (32%)
19	PER	A	606	15,16	0,1,1	-	-	-		
22	EDO	O	306	-	3,3,3	0.76	0	2,2,2	0.89	0
22	EDO	A	618	-	3,3,3	1.14	0	2,2,2	0.74	0
25	CHD	P	304	-	32,32,32	0.83	1 (3%)	51,51,51	1.34	8 (15%)
30	PO4	U	101	-	4,4,4	1.08	0	6,6,6	0.37	0
22	EDO	J	101	-	3,3,3	0.56	0	2,2,2	0.09	0
23	DMU	P	314	-	34,34,34	0.57	0	45,45,45	1.39	8 (17%)
22	EDO	N	619	-	3,3,3	0.74	0	2,2,2	0.36	0
15	HEA	A	602	1,19	57,67,67	1.65	11 (19%)	61,103,103	1.92	18 (29%)
20	PGV	C	301	-	50,50,50	0.90	4 (8%)	53,56,56	0.99	4 (7%)
22	EDO	F	105	-	3,3,3	0.79	0	2,2,2	0.44	0
22	EDO	A	622	-	3,3,3	0.56	0	2,2,2	0.40	0
22	EDO	T	106	-	3,3,3	0.49	0	2,2,2	0.36	0
24	CUA	O	302	2	0,1,1	-	-	-		
23	DMU	M	101	-	34,34,34	0.58	0	45,45,45	1.18	3 (6%)
22	EDO	M	102	-	3,3,3	0.46	0	2,2,2	0.13	0
22	EDO	S	103	-	3,3,3	0.34	0	2,2,2	0.56	0
22	EDO	S	107	-	3,3,3	0.47	0	2,2,2	0.31	0
22	EDO	F	103	-	3,3,3	0.60	0	2,2,2	0.65	0
22	EDO	C	310	-	3,3,3	0.94	0	2,2,2	0.09	0
22	EDO	P	310	-	3,3,3	0.78	0	2,2,2	0.31	0
22	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.49	0
23	DMU	X	103	-	34,34,34	0.56	0	45,45,45	1.35	5 (11%)
23	DMU	X	107	-	34,34,34	0.64	1 (2%)	45,45,45	1.29	7 (15%)
28	PEK	C	309	-	52,52,52	1.00	2 (3%)	55,57,57	1.11	4 (7%)
22	EDO	A	619	-	3,3,3	0.57	0	2,2,2	0.50	0
22	EDO	N	614	-	3,3,3	1.23	0	2,2,2	0.24	0
23	DMU	A	628	-	34,34,34	0.59	0	45,45,45	1.12	5 (11%)
28	PEK	P	307	-	52,52,52	0.67	1 (1%)	55,57,57	1.25	4 (7%)
23	DMU	K	105	-	34,34,34	0.53	0	45,45,45	1.19	5 (11%)
22	EDO	N	615	-	3,3,3	0.69	0	2,2,2	0.13	0
22	EDO	A	623	-	3,3,3	0.90	0	2,2,2	0.38	0
22	EDO	C	311	-	3,3,3	0.51	0	2,2,2	0.35	0
22	EDO	P	311	-	3,3,3	0.54	0	2,2,2	0.49	0
20	PGV	Q	201	-	50,50,50	0.96	2 (4%)	53,56,56	1.26	4 (7%)
23	DMU	K	103	-	33,33,34	0.54	0	41,43,45	1.10	3 (7%)
28	PEK	C	307	-	51,51,52	0.76	1 (1%)	54,56,57	1.05	3 (5%)
22	EDO	G	103	-	3,3,3	0.53	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	TGL	Y	101	-	62,62,62	1.09	3 (4%)	65,65,65	1.25	6 (9%)
22	EDO	D	204	-	3,3,3	0.68	0	2,2,2	0.32	0
22	EDO	N	623	-	3,3,3	0.49	0	2,2,2	0.19	0
22	EDO	J	104	-	3,3,3	0.49	0	2,2,2	0.49	0
22	EDO	S	108	-	3,3,3	0.59	0	2,2,2	0.03	0
23	DMU	P	315	-	34,34,34	0.49	0	45,45,45	1.11	2 (4%)
27	CDL	G	101	-	99,99,99	1.32	12 (12%)	105,111,111	1.34	11 (10%)
22	EDO	N	609	-	3,3,3	1.14	0	2,2,2	0.96	0
15	HEA	N	601[B]	-	57,67,67	1.69	14 (24%)	61,103,103	2.00	18 (29%)
21	TGL	A	609	-	62,62,62	1.10	3 (4%)	65,65,65	1.43	10 (15%)
22	EDO	J	103	-	3,3,3	0.48	0	2,2,2	0.29	0
15	HEA	N	602	1,19	57,67,67	1.53	12 (21%)	61,103,103	2.01	18 (29%)
28	PEK	P	301	-	52,52,52	0.96	2 (3%)	55,57,57	1.21	4 (7%)
23	DMU	K	102	-	34,34,34	0.60	1 (2%)	45,45,45	0.97	3 (6%)
22	EDO	R	201	-	3,3,3	0.52	0	2,2,2	0.70	0
22	EDO	P	309	-	3,3,3	0.39	0	2,2,2	0.75	0
22	EDO	T	104	-	3,3,3	0.86	0	2,2,2	0.56	0
22	EDO	A	615	-	3,3,3	0.62	0	2,2,2	0.02	0
22	EDO	A	626	-	3,3,3	0.37	0	2,2,2	0.79	0
15	HEA	N	601[A]	-	57,67,67	1.70	14 (24%)	61,103,103	2.01	19 (31%)
22	EDO	Z	102	-	3,3,3	0.50	0	2,2,2	0.37	0
22	EDO	A	620	-	3,3,3	0.42	0	2,2,2	0.34	0
22	EDO	N	620	-	3,3,3	0.44	0	2,2,2	0.27	0
25	CHD	O	303	-	32,32,32	0.93	1 (3%)	51,51,51	1.37	8 (15%)
22	EDO	B	308	-	3,3,3	0.64	0	2,2,2	0.46	0
22	EDO	N	624	-	3,3,3	0.45	0	2,2,2	0.29	0
22	EDO	E	201	-	3,3,3	0.51	0	2,2,2	0.51	0
22	EDO	E	203	-	3,3,3	0.71	0	2,2,2	0.37	0
24	CUA	B	302	2	0,1,1	-	-	-		
25	CHD	C	304	-	32,32,32	1.20	2 (6%)	51,51,51	1.60	11 (21%)
23	DMU	C	308	-	34,34,34	0.57	0	45,45,45	0.90	2 (4%)
22	EDO	A	610	-	3,3,3	0.22	0	2,2,2	0.27	0
22	EDO	Q	204	-	3,3,3	0.78	0	2,2,2	0.56	0
22	EDO	A	625	-	3,3,3	0.44	0	2,2,2	0.21	0
22	EDO	B	306	-	3,3,3	0.96	0	2,2,2	0.24	0
22	EDO	F	106	-	3,3,3	0.52	0	2,2,2	0.21	0
22	EDO	N	612	-	3,3,3	0.59	0	2,2,2	0.46	0
22	EDO	P	313	-	3,3,3	0.59	0	2,2,2	0.33	0
22	EDO	G	104	-	3,3,3	0.68	0	2,2,2	0.63	0
22	EDO	N	608	-	3,3,3	0.47	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CHD	B	303	-	32,32,32	1.09	2 (6%)	51,51,51	1.48	10 (19%)
22	EDO	B	305	-	3,3,3	0.33	0	2,2,2	0.51	0
22	EDO	S	105	-	3,3,3	0.68	0	2,2,2	0.77	0
19	PER	N	606	15,16	0,1,1	-	-	-	-	-
22	EDO	C	313	-	3,3,3	0.64	0	2,2,2	0.17	0
22	EDO	A	612	-	3,3,3	0.91	0	2,2,2	0.66	0
20	PGV	A	607	-	50,50,50	0.94	2 (4%)	53,56,56	0.96	3 (5%)
22	EDO	W	101	-	3,3,3	0.48	0	2,2,2	0.13	0
22	EDO	A	624	-	3,3,3	1.01	0	2,2,2	0.90	0
22	EDO	F	107	-	3,3,3	0.70	0	2,2,2	1.39	0
28	PEK	T	101	-	49,49,52	1.01	2 (4%)	53,54,57	1.31	6 (11%)
23	DMU	C	318	-	34,34,34	0.64	1 (2%)	45,45,45	1.28	5 (11%)
20	PGV	N	607	-	50,50,50	1.15	5 (10%)	53,56,56	1.22	3 (5%)
22	EDO	C	314	-	3,3,3	0.52	0	2,2,2	0.47	0
22	EDO	N	617	-	3,3,3	0.38	0	2,2,2	0.36	0
22	EDO	S	102	-	3,3,3	0.59	0	2,2,2	0.70	0
22	EDO	A	613	-	3,3,3	0.52	0	2,2,2	0.13	0
23	DMU	X	102	-	34,34,34	0.60	1 (2%)	45,45,45	1.24	5 (11%)
22	EDO	G	105	-	3,3,3	0.48	0	2,2,2	0.34	0
21	TGL	Q	202	-	62,62,62	1.09	4 (6%)	65,65,65	0.89	3 (4%)
23	DMU	O	307	-	34,34,34	0.53	0	45,45,45	1.18	6 (13%)
20	PGV	A	608	-	50,50,50	1.05	4 (8%)	53,56,56	1.19	4 (7%)
22	EDO	D	203	-	3,3,3	0.78	0	2,2,2	0.28	0
22	EDO	H	101	-	3,3,3	0.38	0	2,2,2	0.23	0
22	EDO	T	105	-	3,3,3	0.52	0	2,2,2	0.25	0
22	EDO	Q	203	-	3,3,3	0.64	0	2,2,2	0.70	0
22	EDO	N	622	-	3,3,3	0.78	0	2,2,2	0.29	0
23	DMU	X	104	-	34,34,34	0.53	0	45,45,45	1.16	5 (11%)
22	EDO	J	105	-	3,3,3	0.56	0	2,2,2	0.28	0
23	DMU	P	305	-	34,34,34	0.60	1 (2%)	45,45,45	0.83	0
22	EDO	Y	102	-	3,3,3	0.48	0	2,2,2	0.51	0
25	CHD	Y	104	-	32,32,32	0.71	0	51,51,51	2.24	16 (31%)
22	EDO	T	103	-	3,3,3	0.46	0	2,2,2	0.28	0
22	EDO	A	611	-	3,3,3	0.81	0	2,2,2	0.67	0
22	EDO	A	621	-	3,3,3	0.35	0	2,2,2	0.42	0
22	EDO	A	614	-	3,3,3	0.41	0	2,2,2	0.55	0
23	DMU	Z	101	-	34,34,34	0.53	1 (2%)	45,45,45	0.84	1 (2%)
22	EDO	F	102	-	3,3,3	0.90	0	2,2,2	0.33	0
27	CDL	T	102	-	97,97,99	1.33	12 (12%)	103,109,111	1.32	8 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CHD	X	101	-	32,32,32	0.85	1 (3%)	51,51,51	2.16	19 (37%)
20	PGV	C	306	-	47,47,50	1.03	2 (4%)	50,53,56	1.57	7 (14%)
22	EDO	N	613	-	3,3,3	0.52	0	2,2,2	0.88	0
22	EDO	J	102	-	3,3,3	0.38	0	2,2,2	0.16	0
22	EDO	A	616	-	3,3,3	0.81	0	2,2,2	0.33	0
22	EDO	L	103	-	3,3,3	0.42	0	2,2,2	0.36	0
22	EDO	N	611	-	3,3,3	0.42	0	2,2,2	0.57	0
22	EDO	C	315	-	3,3,3	1.16	0	2,2,2	0.57	0
22	EDO	M	103	-	3,3,3	0.33	0	2,2,2	0.99	0
22	EDO	F	104	-	3,3,3	0.43	0	2,2,2	0.33	0
20	PGV	P	302	-	50,50,50	0.79	2 (4%)	53,56,56	0.99	2 (3%)
22	EDO	S	106	-	3,3,3	0.70	0	2,2,2	0.08	0
22	EDO	B	309	-	3,3,3	0.58	0	2,2,2	0.19	0
30	PO4	H	102	-	4,4,4	0.96	0	6,6,6	0.51	0
25	CHD	C	303	-	32,32,32	0.86	1 (3%)	51,51,51	1.64	11 (21%)
23	DMU	X	106	-	34,34,34	0.60	0	45,45,45	1.81	15 (33%)
27	CDL	C	302	-	86,86,99	1.52	14 (16%)	90,94,111	1.56	13 (14%)
22	EDO	L	102	-	3,3,3	0.40	0	2,2,2	0.80	0
22	EDO	S	104	-	3,3,3	0.61	0	2,2,2	0.69	0
21	TGL	B	301	-	61,61,62	1.06	3 (4%)	64,64,65	1.10	3 (4%)
22	EDO	L	101	-	3,3,3	0.83	0	2,2,2	0.53	0
22	EDO	D	205	-	3,3,3	0.69	0	2,2,2	0.26	0
20	PGV	G	102	-	50,50,50	0.97	2 (4%)	53,56,56	1.15	5 (9%)
22	EDO	B	307	-	3,3,3	0.81	0	2,2,2	0.40	0
23	DMU	C	317	-	34,34,34	0.49	0	45,45,45	1.41	8 (17%)
27	CDL	P	303	-	88,88,99	1.38	11 (12%)	95,98,111	1.59	13 (13%)
23	DMU	K	106	-	34,34,34	0.59	0	45,45,45	1.10	3 (6%)
25	CHD	P	306	-	32,32,32	0.97	1 (3%)	51,51,51	1.40	8 (15%)
22	EDO	E	202	-	3,3,3	0.37	0	2,2,2	0.49	0
23	DMU	X	105	-	34,34,34	0.66	1 (2%)	45,45,45	1.32	7 (15%)
23	DMU	C	316	-	34,34,34	0.60	1 (2%)	45,45,45	1.20	4 (8%)
26	PSC	B	304	-	51,51,51	1.09	3 (5%)	57,59,59	1.36	6 (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
22	EDO	P	308	-	-	0/1/1/1	-
23	DMU	L	105	-	-	11/19/59/59	0/2/2/2
23	DMU	K	104	-	-	10/19/59/59	0/2/2/2
23	DMU	D	206	-	-	9/19/59/59	0/2/2/2
22	EDO	N	610	-	-	1/1/1/1	-
22	EDO	A	617	-	-	1/1/1/1	-
22	EDO	A	627	-	-	1/1/1/1	-
21	TGL	O	301	-	-	24/62/62/65	-
28	PEK	C	305	-	-	27/56/56/56	-
22	EDO	N	621	-	-	1/1/1/1	-
21	TGL	D	201	-	-	26/64/64/65	-
22	EDO	S	109	-	-	0/1/1/1	-
23	DMU	I	101	-	-	9/19/59/59	0/2/2/2
26	PSC	O	304	-	-	29/54/54/55	-
22	EDO	D	202	-	-	1/1/1/1	-
15	HEA	A	601[B]	-	3/3/7/16	6/32/76/76	-
22	EDO	C	312	-	-	0/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
22	EDO	O	305	-	-	0/1/1/1	-
22	EDO	N	618	-	-	1/1/1/1	-
22	EDO	Y	103	-	-	0/1/1/1	-
23	DMU	K	101	-	-	7/19/59/59	0/2/2/2
22	EDO	V	101	-	-	0/1/1/1	-
25	CHD	L	104	-	-	5/9/74/74	1/4/4/4
15	HEA	A	601[A]	-	3/3/7/16	8/32/76/76	-
22	EDO	O	306	-	-	0/1/1/1	-
22	EDO	A	618	-	-	0/1/1/1	-
25	CHD	P	304	-	-	7/9/74/74	0/4/4/4
22	EDO	J	101	-	-	1/1/1/1	-
23	DMU	P	314	-	-	5/19/59/59	0/2/2/2
22	EDO	N	619	-	-	0/1/1/1	-
15	HEA	A	602	1,19	3/3/7/16	4/32/76/76	-
20	PGV	C	301	-	-	9/55/55/55	-
22	EDO	F	105	-	-	0/1/1/1	-
22	EDO	A	622	-	-	0/1/1/1	-
22	EDO	T	106	-	-	0/1/1/1	-
23	DMU	M	101	-	-	4/19/59/59	0/2/2/2
22	EDO	M	102	-	-	0/1/1/1	-
22	EDO	S	103	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	S	107	-	-	1/1/1/1	-
22	EDO	F	103	-	-	0/1/1/1	-
22	EDO	C	310	-	-	0/1/1/1	-
22	EDO	P	310	-	-	0/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
23	DMU	X	103	-	-	9/19/59/59	0/2/2/2
23	DMU	X	107	-	-	9/19/59/59	0/2/2/2
28	PEK	C	309	-	-	17/56/56/56	-
22	EDO	A	619	-	-	1/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
23	DMU	A	628	-	-	4/19/59/59	0/2/2/2
28	PEK	P	307	-	-	11/56/56/56	-
23	DMU	K	105	-	-	9/19/59/59	0/2/2/2
22	EDO	N	615	-	-	1/1/1/1	-
22	EDO	A	623	-	-	1/1/1/1	-
22	EDO	C	311	-	-	0/1/1/1	-
22	EDO	P	311	-	-	0/1/1/1	-
20	PGV	Q	201	-	-	11/55/55/55	-
23	DMU	K	103	-	-	10/19/55/59	0/2/2/2
28	PEK	C	307	-	-	14/55/55/56	-
22	EDO	G	103	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	35/65/65/65	-
22	EDO	D	204	-	-	0/1/1/1	-
22	EDO	N	623	-	-	1/1/1/1	-
22	EDO	J	104	-	-	1/1/1/1	-
22	EDO	S	108	-	-	0/1/1/1	-
23	DMU	P	315	-	-	1/19/59/59	0/2/2/2
27	CDL	G	101	-	-	37/110/110/110	-
22	EDO	N	609	-	-	1/1/1/1	-
15	HEA	N	601[B]	-	3/3/7/16	2/32/76/76	-
21	TGL	A	609	-	-	30/65/65/65	-
22	EDO	J	103	-	-	0/1/1/1	-
15	HEA	N	602	1,19	3/3/7/16	4/32/76/76	-
28	PEK	P	301	-	-	22/56/56/56	-
23	DMU	K	102	-	-	6/19/59/59	0/2/2/2
22	EDO	R	201	-	-	0/1/1/1	-
22	EDO	P	309	-	-	1/1/1/1	-
22	EDO	T	104	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	A	615	-	-	0/1/1/1	-
22	EDO	A	626	-	-	1/1/1/1	-
15	HEA	N	601[A]	-	3/3/7/16	6/32/76/76	-
22	EDO	Z	102	-	-	1/1/1/1	-
22	EDO	A	620	-	-	0/1/1/1	-
22	EDO	N	620	-	-	1/1/1/1	-
25	CHD	O	303	-	-	2/9/74/74	0/4/4/4
22	EDO	B	308	-	-	0/1/1/1	-
22	EDO	N	624	-	-	0/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
22	EDO	E	203	-	-	0/1/1/1	-
25	CHD	C	304	-	-	2/9/74/74	0/4/4/4
23	DMU	C	308	-	-	7/19/59/59	0/2/2/2
22	EDO	A	610	-	-	1/1/1/1	-
22	EDO	Q	204	-	-	0/1/1/1	-
22	EDO	A	625	-	-	1/1/1/1	-
22	EDO	B	306	-	-	0/1/1/1	-
22	EDO	F	106	-	-	0/1/1/1	-
22	EDO	N	612	-	-	0/1/1/1	-
22	EDO	P	313	-	-	0/1/1/1	-
22	EDO	G	104	-	-	0/1/1/1	-
22	EDO	N	608	-	-	1/1/1/1	-
25	CHD	B	303	-	-	2/9/74/74	0/4/4/4
22	EDO	B	305	-	-	0/1/1/1	-
22	EDO	S	105	-	-	0/1/1/1	-
22	EDO	C	313	-	-	1/1/1/1	-
22	EDO	A	612	-	-	0/1/1/1	-
20	PGV	A	607	-	-	5/55/55/55	-
22	EDO	W	101	-	-	0/1/1/1	-
22	EDO	A	624	-	-	0/1/1/1	-
22	EDO	F	107	-	-	0/1/1/1	-
28	PEK	T	101	-	-	24/51/51/56	-
23	DMU	C	318	-	-	9/19/59/59	0/2/2/2
20	PGV	N	607	-	-	7/55/55/55	-
22	EDO	C	314	-	-	0/1/1/1	-
22	EDO	N	617	-	-	1/1/1/1	-
22	EDO	S	102	-	-	0/1/1/1	-
22	EDO	A	613	-	-	1/1/1/1	-
23	DMU	X	102	-	-	8/19/59/59	0/2/2/2
22	EDO	G	105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	Q	202	-	-	21/65/65/65	-
23	DMU	O	307	-	-	5/19/59/59	0/2/2/2
20	PGV	A	608	-	-	14/55/55/55	-
22	EDO	D	203	-	-	0/1/1/1	-
22	EDO	H	101	-	-	0/1/1/1	-
22	EDO	T	105	-	-	0/1/1/1	-
22	EDO	Q	203	-	-	0/1/1/1	-
22	EDO	N	622	-	-	0/1/1/1	-
23	DMU	X	104	-	-	6/19/59/59	0/2/2/2
22	EDO	J	105	-	-	0/1/1/1	-
23	DMU	P	305	-	-	5/19/59/59	0/2/2/2
22	EDO	Y	102	-	-	1/1/1/1	-
25	CHD	Y	104	-	-	4/9/74/74	0/4/4/4
22	EDO	T	103	-	-	0/1/1/1	-
22	EDO	A	611	-	-	1/1/1/1	-
22	EDO	A	621	-	-	0/1/1/1	-
22	EDO	A	614	-	-	0/1/1/1	-
23	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
22	EDO	F	102	-	-	0/1/1/1	-
27	CDL	T	102	-	-	34/108/108/110	-
25	CHD	X	101	-	-	8/9/74/74	0/4/4/4
20	PGV	C	306	-	-	9/52/52/55	-
22	EDO	N	613	-	-	0/1/1/1	-
22	EDO	J	102	-	-	1/1/1/1	-
22	EDO	A	616	-	-	0/1/1/1	-
22	EDO	L	103	-	-	0/1/1/1	-
22	EDO	N	611	-	-	1/1/1/1	-
22	EDO	C	315	-	-	0/1/1/1	-
22	EDO	M	103	-	-	1/1/1/1	-
22	EDO	F	104	-	-	1/1/1/1	-
20	PGV	P	302	-	-	9/55/55/55	-
22	EDO	S	106	-	-	0/1/1/1	-
22	EDO	B	309	-	-	0/1/1/1	-
25	CHD	C	303	-	-	7/9/74/74	0/4/4/4
23	DMU	X	106	-	-	7/19/59/59	0/2/2/2
27	CDL	C	302	-	-	24/89/89/110	-
22	EDO	L	102	-	-	0/1/1/1	-
22	EDO	S	104	-	-	0/1/1/1	-
21	TGL	B	301	-	-	26/64/64/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	L	101	-	-	1/1/1/1	-
22	EDO	D	205	-	-	0/1/1/1	-
20	PGV	G	102	-	-	15/55/55/55	-
22	EDO	B	307	-	-	0/1/1/1	-
23	DMU	C	317	-	-	3/19/59/59	0/2/2/2
27	CDL	P	303	-	-	30/94/94/110	-
23	DMU	K	106	-	-	13/19/59/59	0/2/2/2
25	CHD	P	306	-	-	2/9/74/74	0/4/4/4
22	EDO	E	202	-	-	1/1/1/1	-
23	DMU	X	105	-	-	10/19/59/59	0/2/2/2
23	DMU	C	316	-	-	6/19/59/59	0/2/2/2
26	PSC	B	304	-	-	18/55/55/55	-

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	302	CDL	OA6-CA5	5.77	1.46	1.33
21	A	609	TGL	OG3-CC1	5.06	1.48	1.33
21	Y	101	TGL	OG3-CC1	4.86	1.47	1.33
26	O	304	PSC	O01-C1	4.80	1.47	1.34
28	C	305	PEK	O03-C21	4.76	1.47	1.33

The worst 5 of 501 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	302	CDL	CB4-OB6-CB5	-6.42	101.99	117.79
25	L	104	CHD	C6-C5-C4	-6.23	104.02	111.19
27	G	101	CDL	OB6-CB5-C51	6.16	124.77	111.50
25	Y	104	CHD	C6-C5-C4	-5.99	104.30	111.19
15	N	602	HEA	C3C-C4C-NC	5.87	116.80	109.21

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	601[A]	HEA	ND
15	A	601[A]	HEA	NA
15	A	601[A]	HEA	NB
15	A	601[B]	HEA	ND
15	A	601[B]	HEA	NA

5 of 819 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	601[A]	HEA	C18-C19-C20-C21
15	A	601[A]	HEA	C27-C19-C20-C21
20	A	608	PGV	C2-C1-O01-C02
20	A	608	PGV	O04-C19-O03-C01
20	A	608	PGV	C20-C19-O03-C01

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	L	104	CHD	C1-C10-C2-C3-C4-C5

95 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	105	DMU	4	0
23	K	104	DMU	1	0
23	D	206	DMU	1	0
22	N	610	EDO	1	0
22	A	617	EDO	1	0
22	A	627	EDO	1	0
21	O	301	TGL	4	0
28	C	305	PEK	11	0
21	D	201	TGL	12	0
23	I	101	DMU	4	0
26	O	304	PSC	9	0
22	D	202	EDO	2	0
15	A	601[B]	HEA	1	0
23	K	101	DMU	2	0
22	V	101	EDO	2	0
25	L	104	CHD	1	0
15	A	601[A]	HEA	2	0
19	A	606	PER	1	0
25	P	304	CHD	2	0
23	P	314	DMU	5	0
15	A	602	HEA	1	0
22	A	622	EDO	2	0
23	M	101	DMU	1	0
22	M	102	EDO	1	0
22	S	103	EDO	1	0
22	S	107	EDO	2	0
23	X	103	DMU	3	0
23	X	107	DMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	309	PEK	4	0
22	A	619	EDO	2	0
23	A	628	DMU	1	0
28	P	307	PEK	1	0
23	K	105	DMU	2	0
22	A	623	EDO	1	0
20	Q	201	PGV	5	0
23	K	103	DMU	1	0
28	C	307	PEK	5	0
21	Y	101	TGL	8	0
22	J	104	EDO	1	0
22	S	108	EDO	2	0
23	P	315	DMU	1	0
27	G	101	CDL	18	0
22	N	609	EDO	2	0
15	N	601[B]	HEA	1	0
21	A	609	TGL	12	0
15	N	602	HEA	2	0
28	P	301	PEK	6	0
23	K	102	DMU	2	0
22	A	626	EDO	1	0
15	N	601[A]	HEA	1	0
22	A	620	EDO	2	0
25	O	303	CHD	1	0
22	B	308	EDO	1	0
22	N	624	EDO	1	0
23	C	308	DMU	2	0
22	A	610	EDO	5	0
22	A	625	EDO	4	0
22	P	313	EDO	1	0
19	N	606	PER	1	0
22	C	313	EDO	1	0
22	A	612	EDO	1	0
20	A	607	PGV	1	0
22	W	101	EDO	1	0
28	T	101	PEK	5	0
23	C	318	DMU	1	0
20	N	607	PGV	1	0
22	A	613	EDO	2	0
22	G	105	EDO	1	0
21	Q	202	TGL	8	0
20	A	608	PGV	1	0

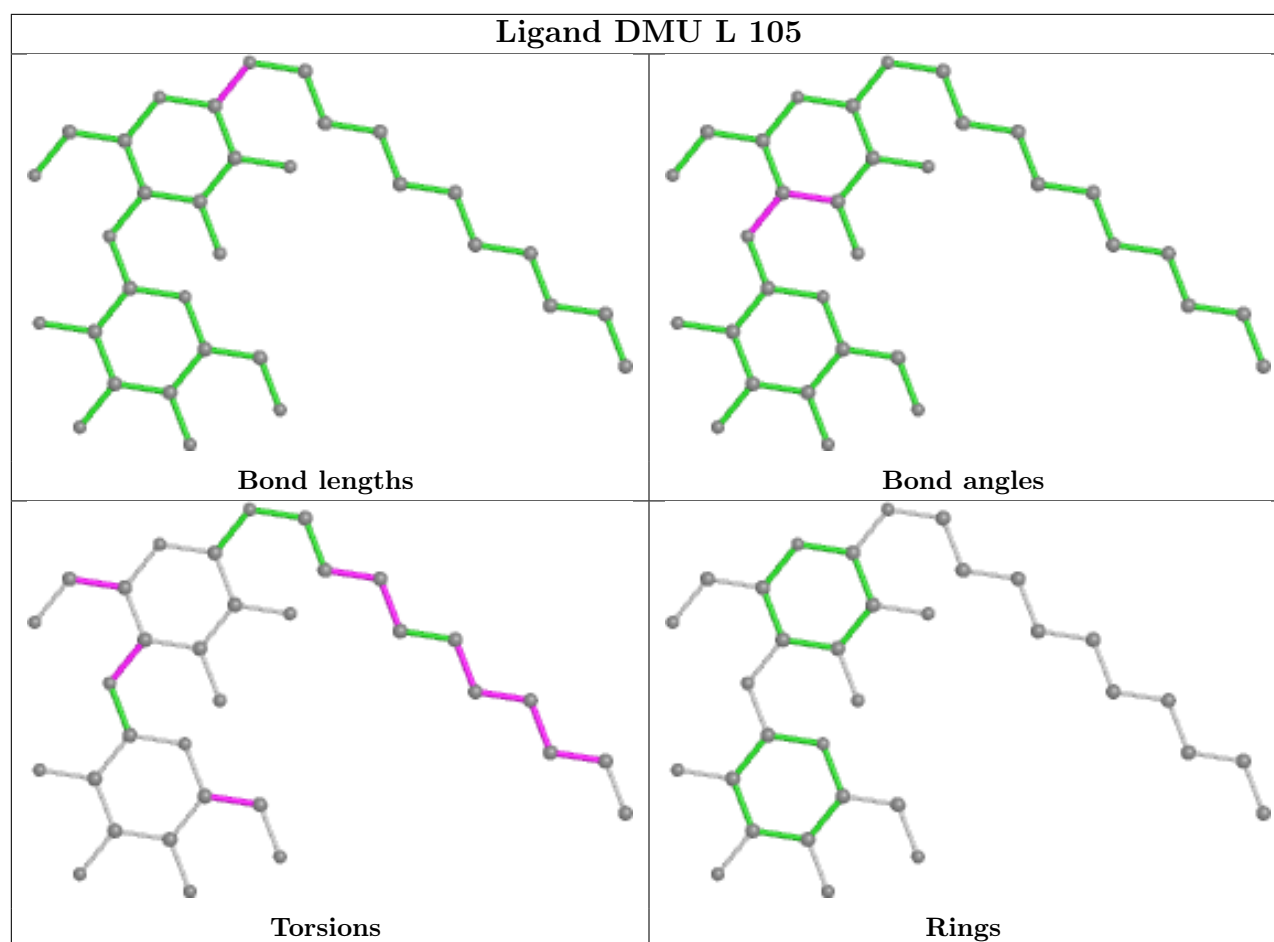
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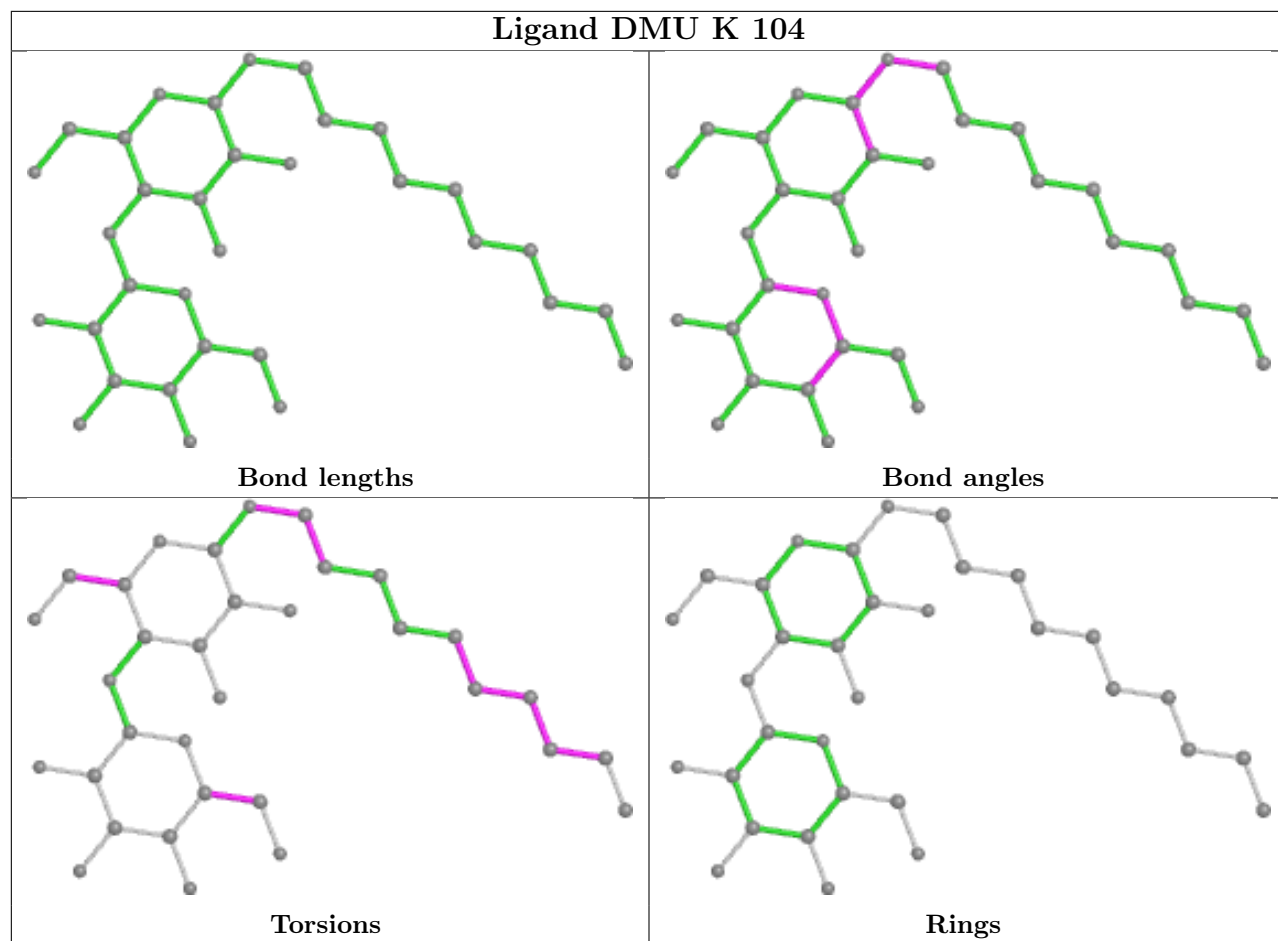


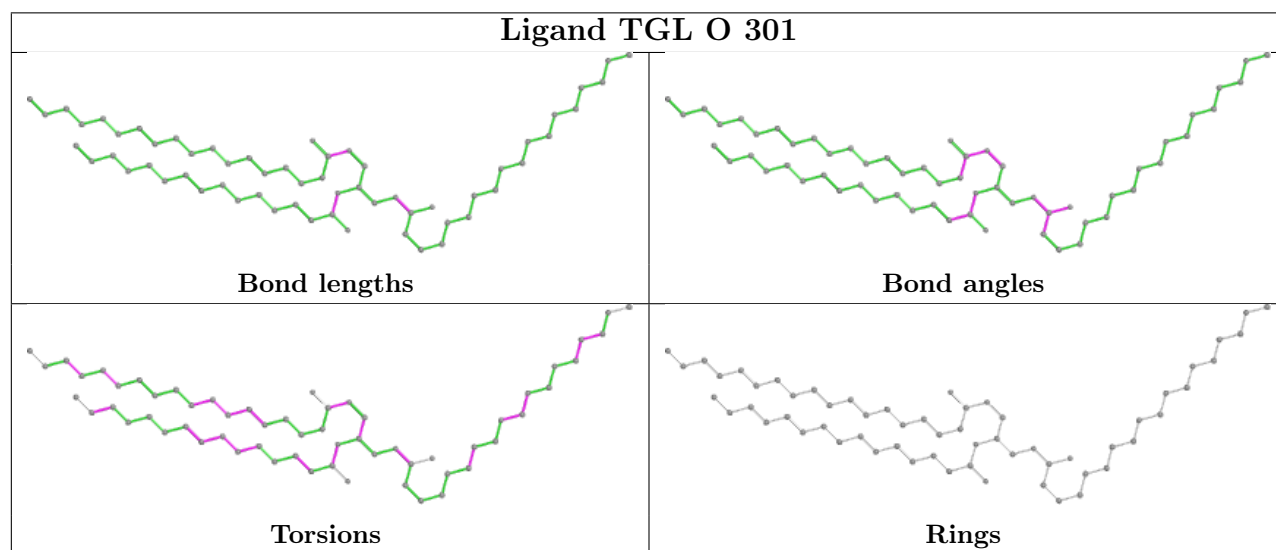
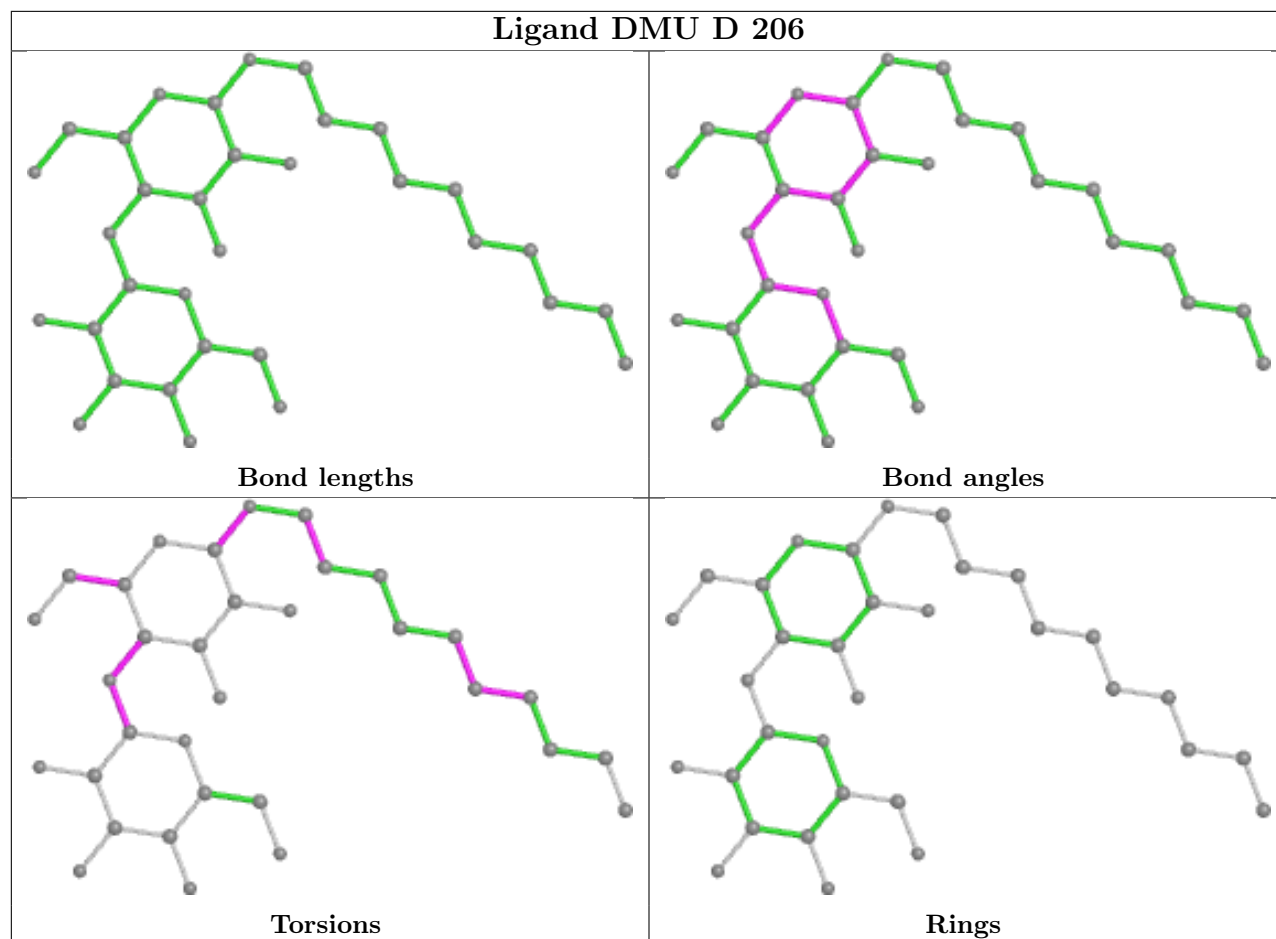
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	101	EDO	1	0
22	Q	203	EDO	1	0
22	N	622	EDO	6	0
23	X	104	DMU	3	0
23	P	305	DMU	4	0
22	A	611	EDO	1	0
22	A	621	EDO	4	0
27	T	102	CDL	21	0
25	X	101	CHD	7	0
20	C	306	PGV	1	0
22	N	613	EDO	2	0
20	P	302	PGV	1	0
25	C	303	CHD	2	0
23	X	106	DMU	2	0
27	C	302	CDL	8	0
22	S	104	EDO	1	0
21	B	301	TGL	6	0
20	G	102	PGV	2	0
23	C	317	DMU	2	0
27	P	303	CDL	11	0
23	K	106	DMU	1	0
25	P	306	CHD	1	0
23	X	105	DMU	2	0
23	C	316	DMU	1	0
26	B	304	PSC	11	0

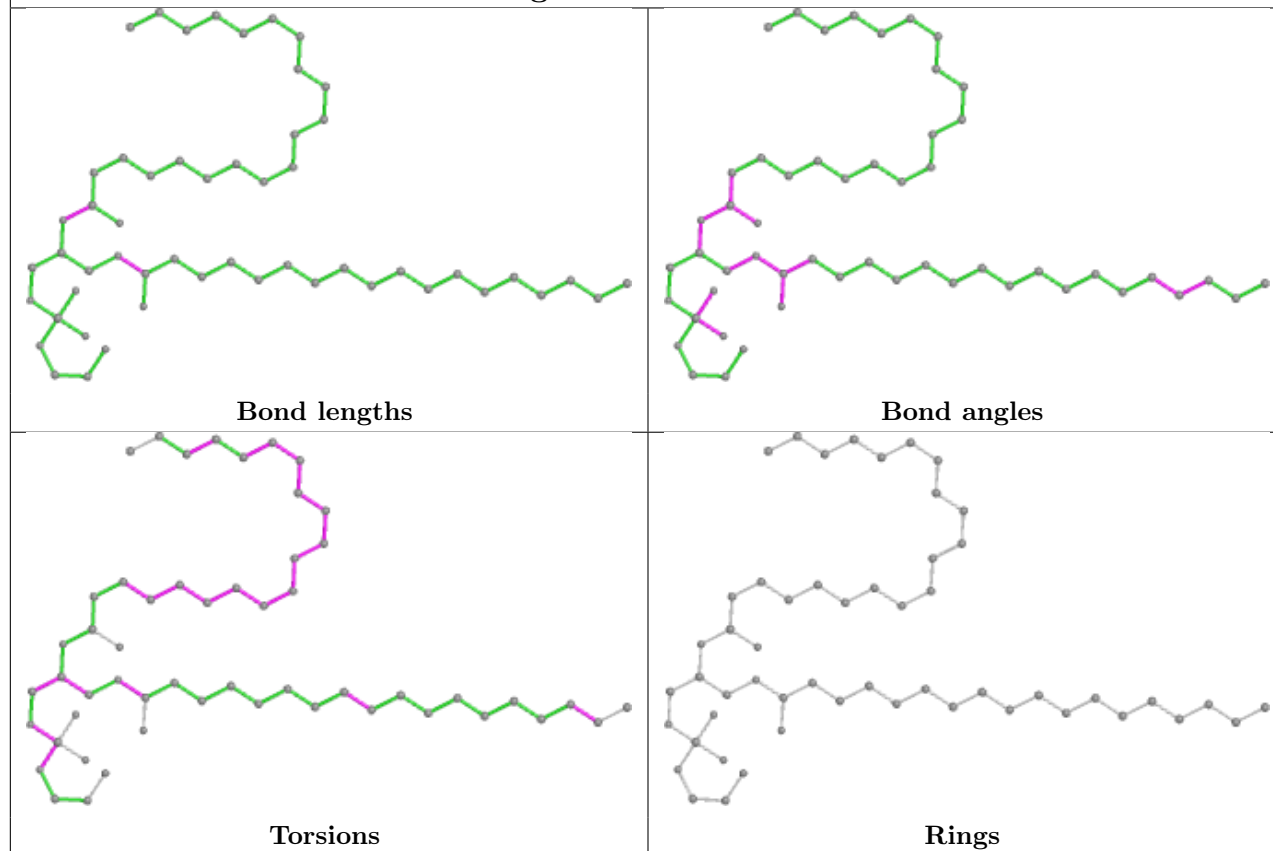
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



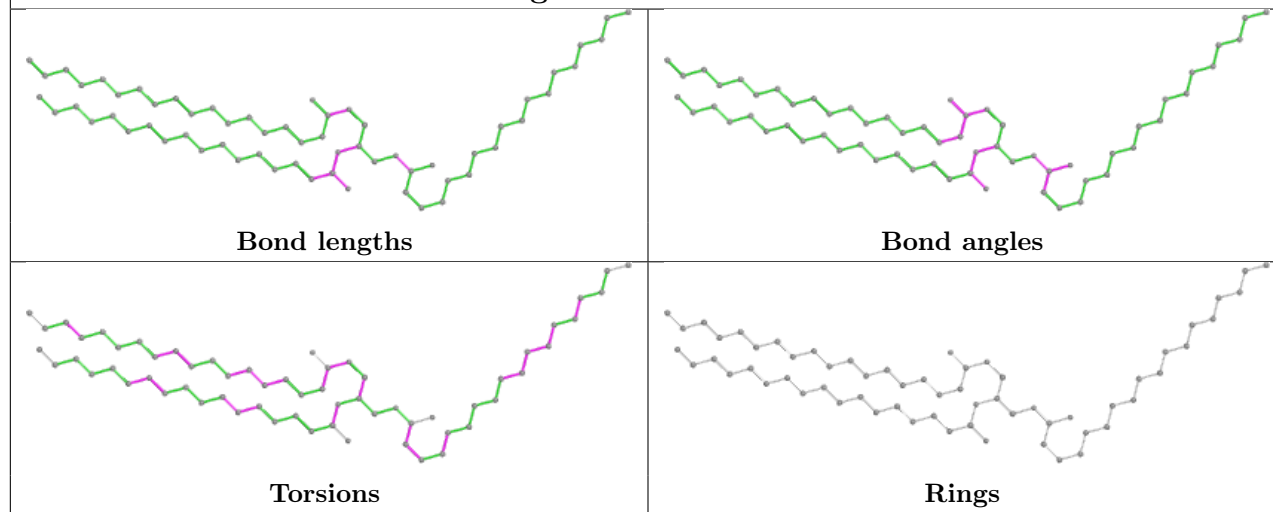


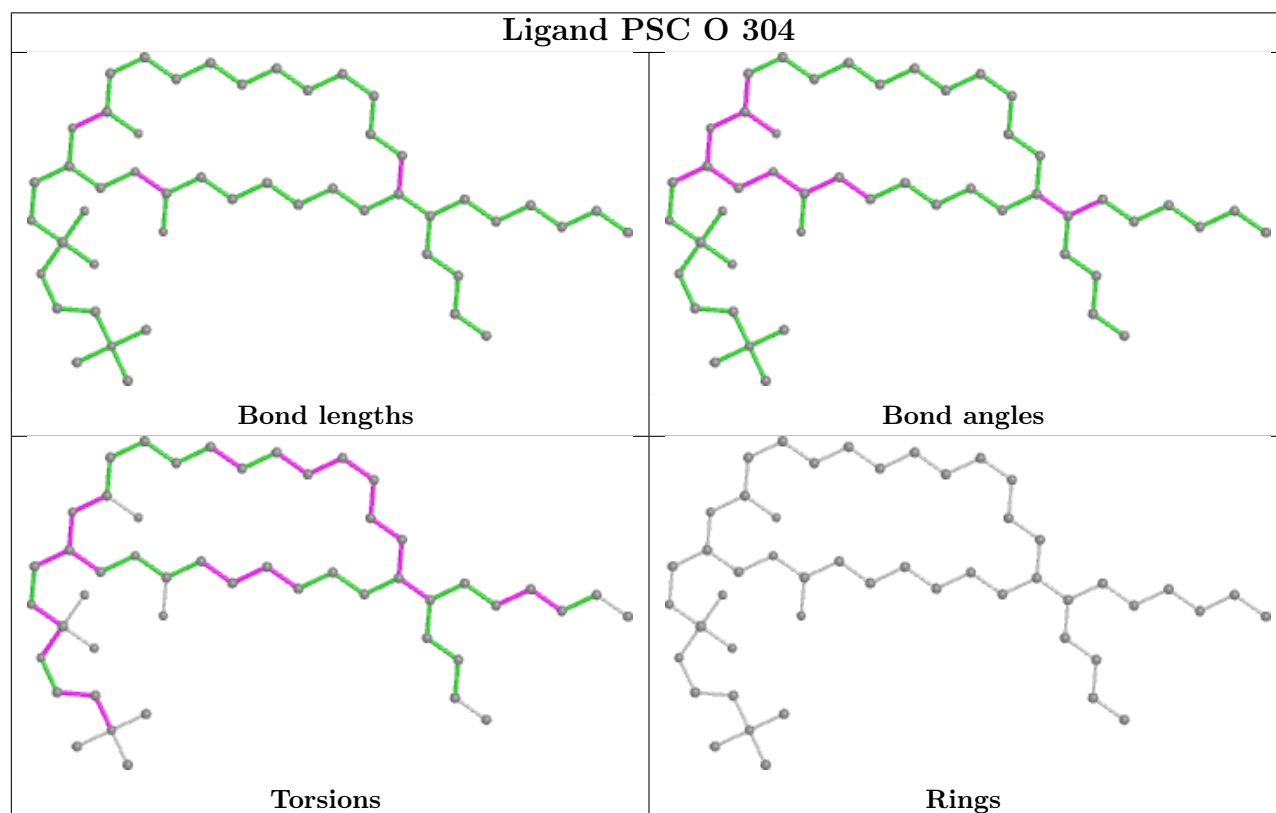
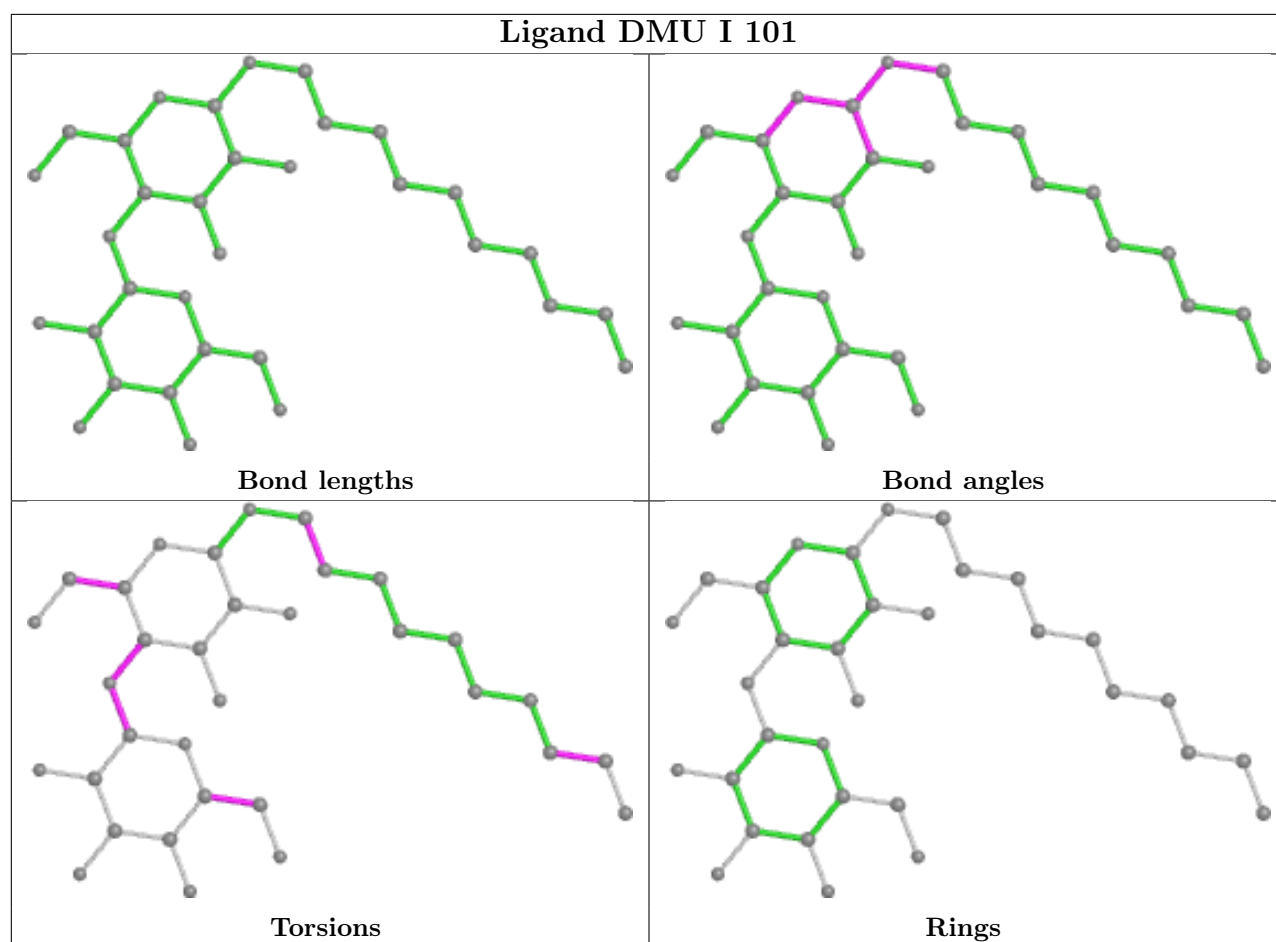


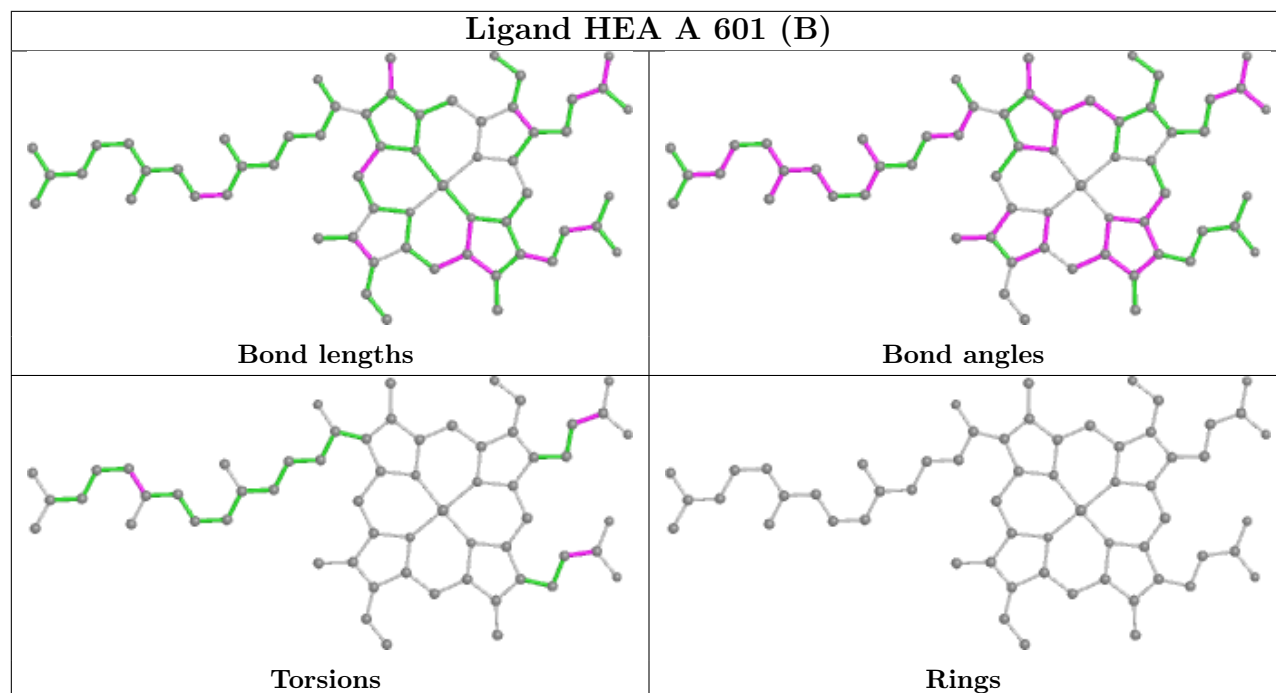
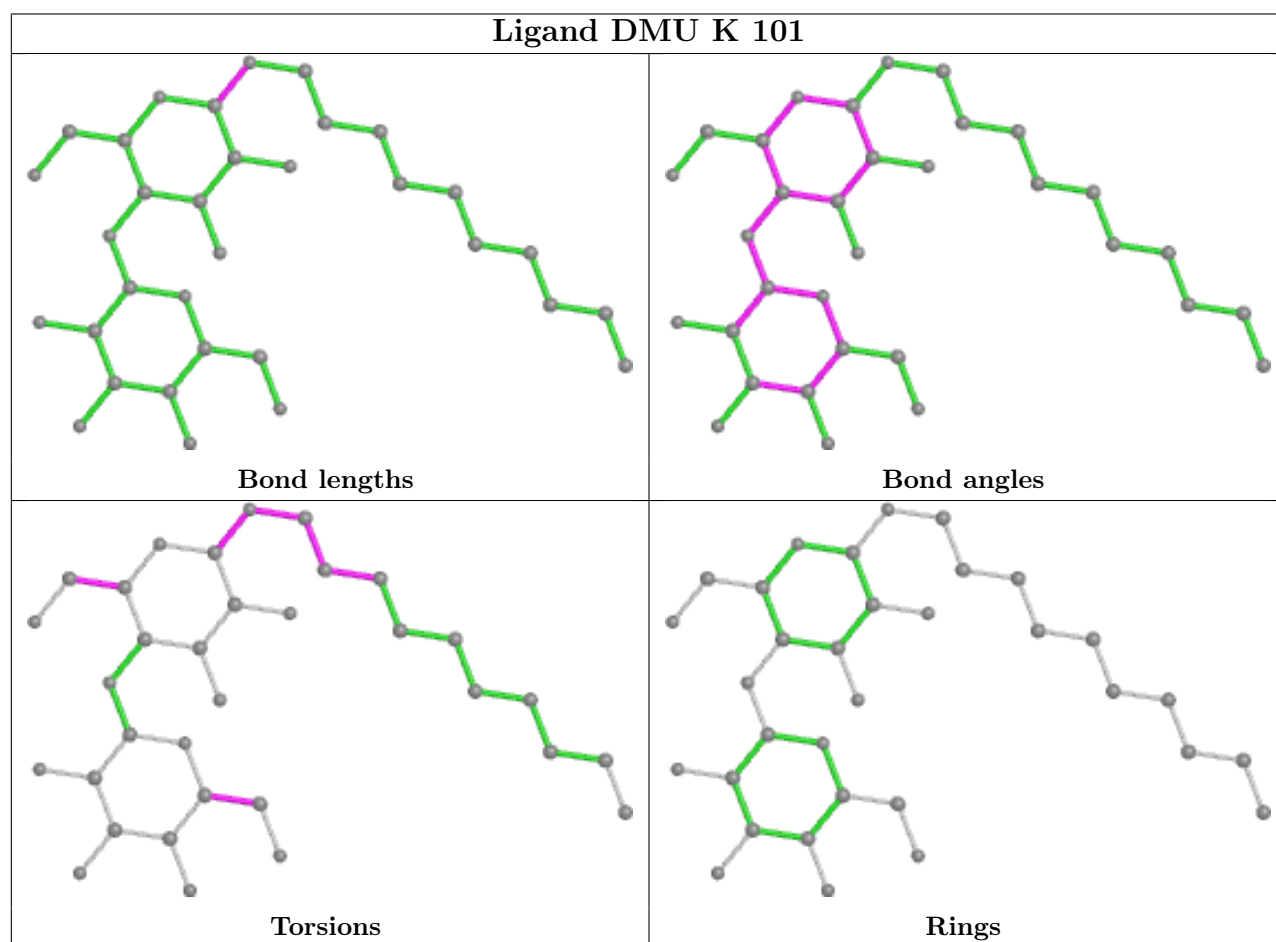
## Ligand PEK C 305

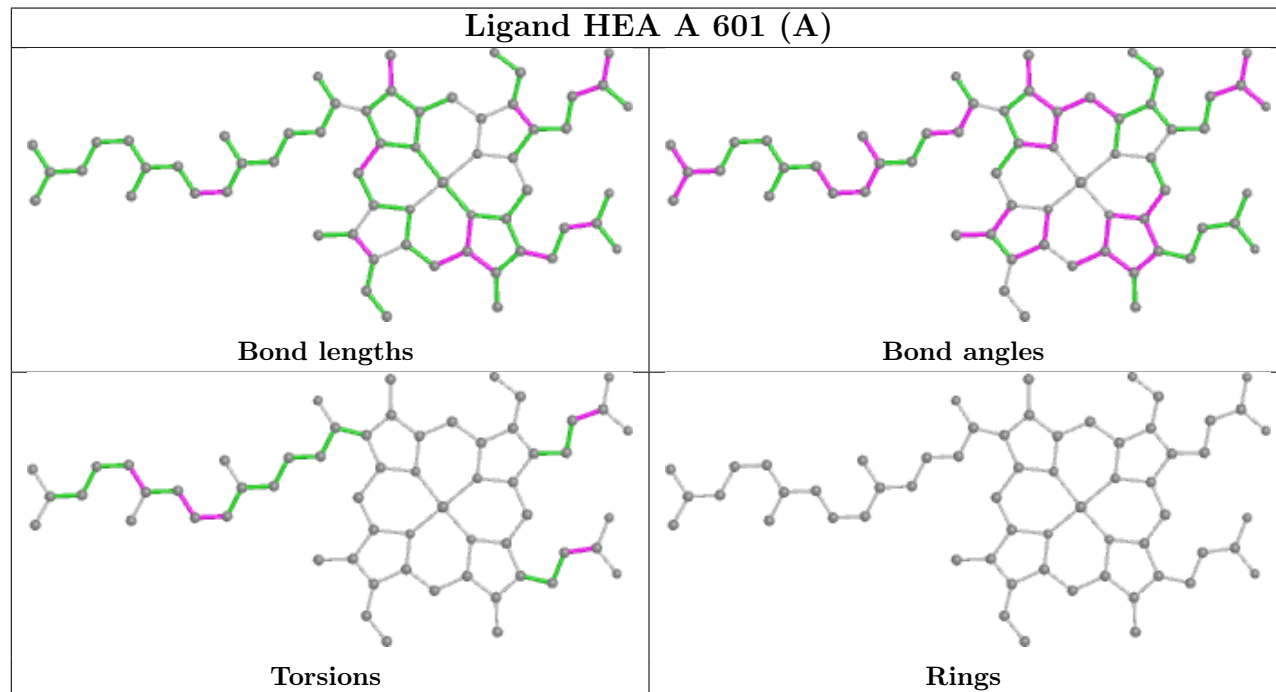
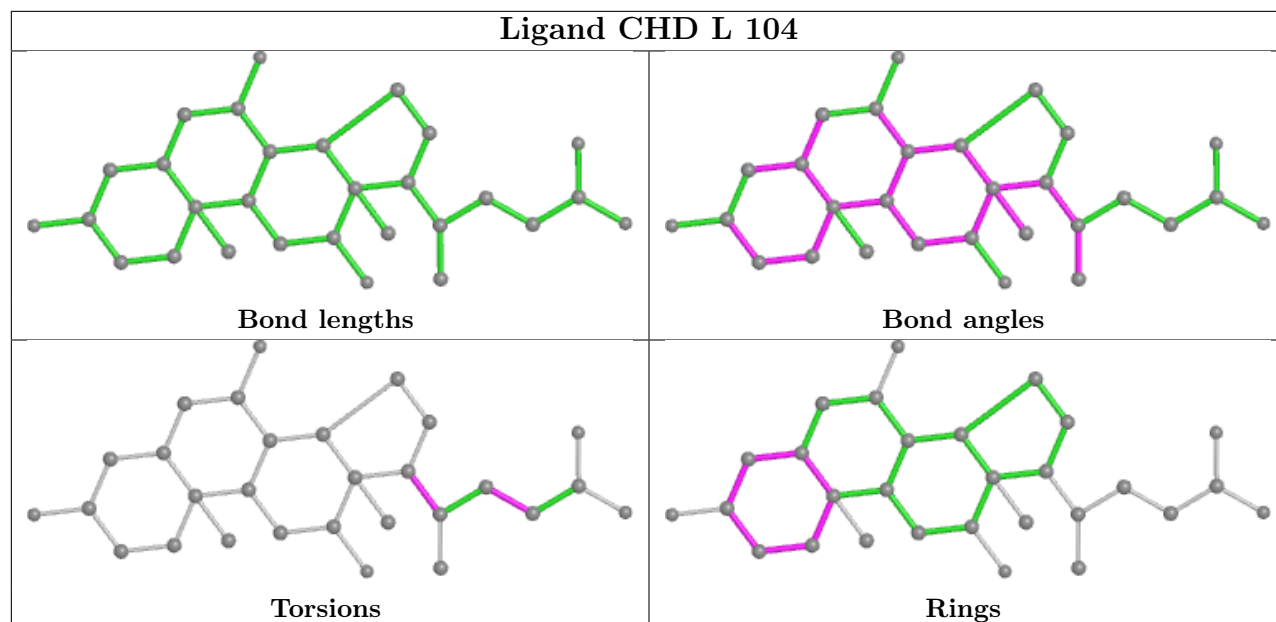


## Ligand TGL D 201

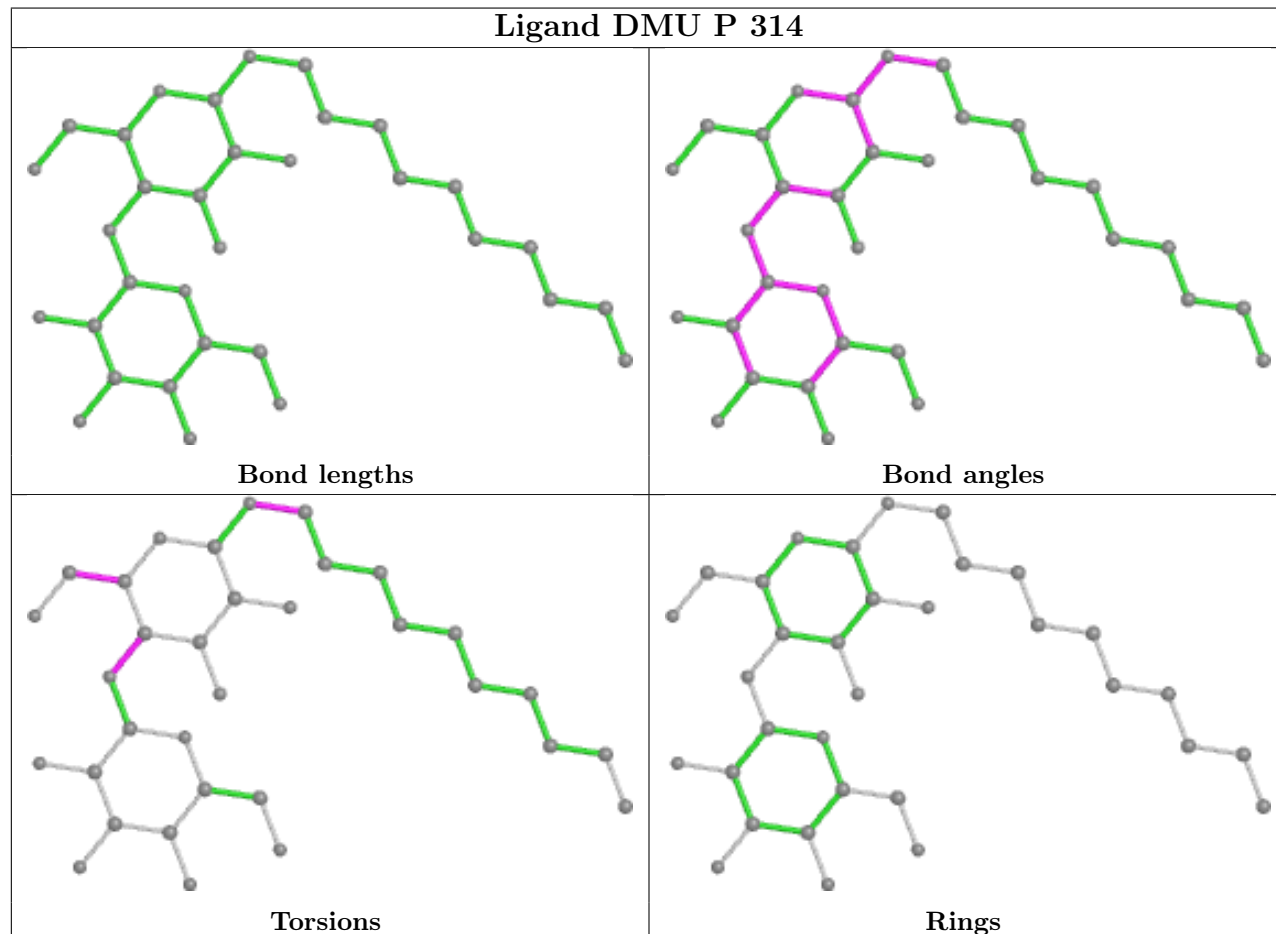
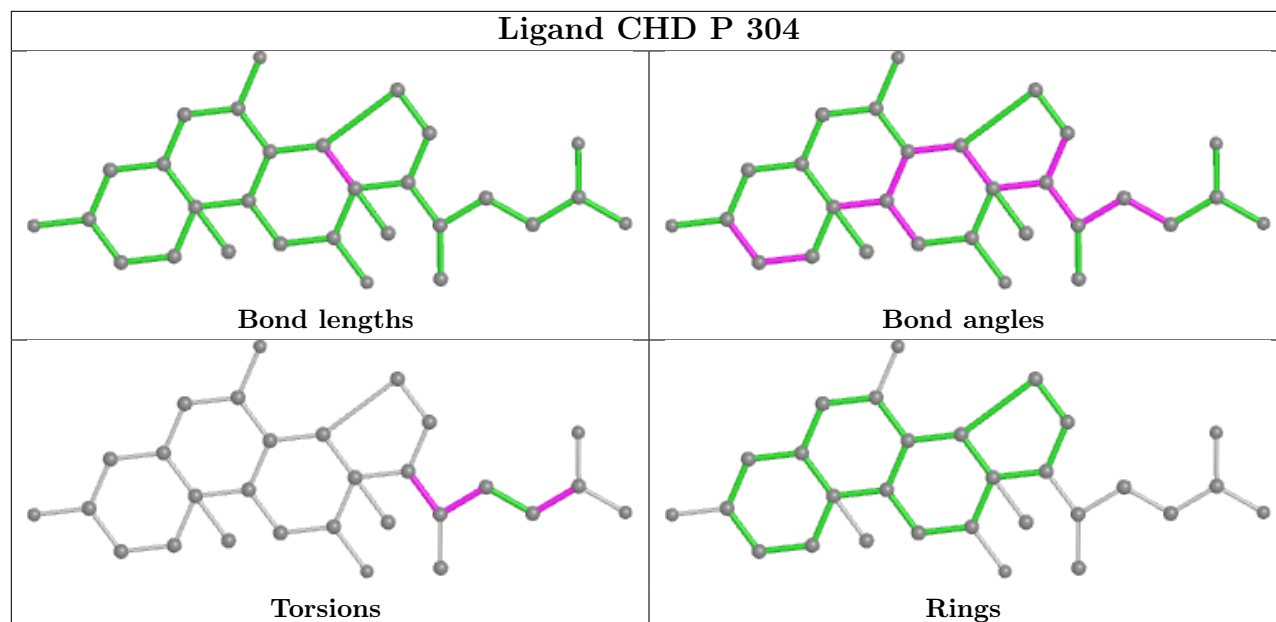


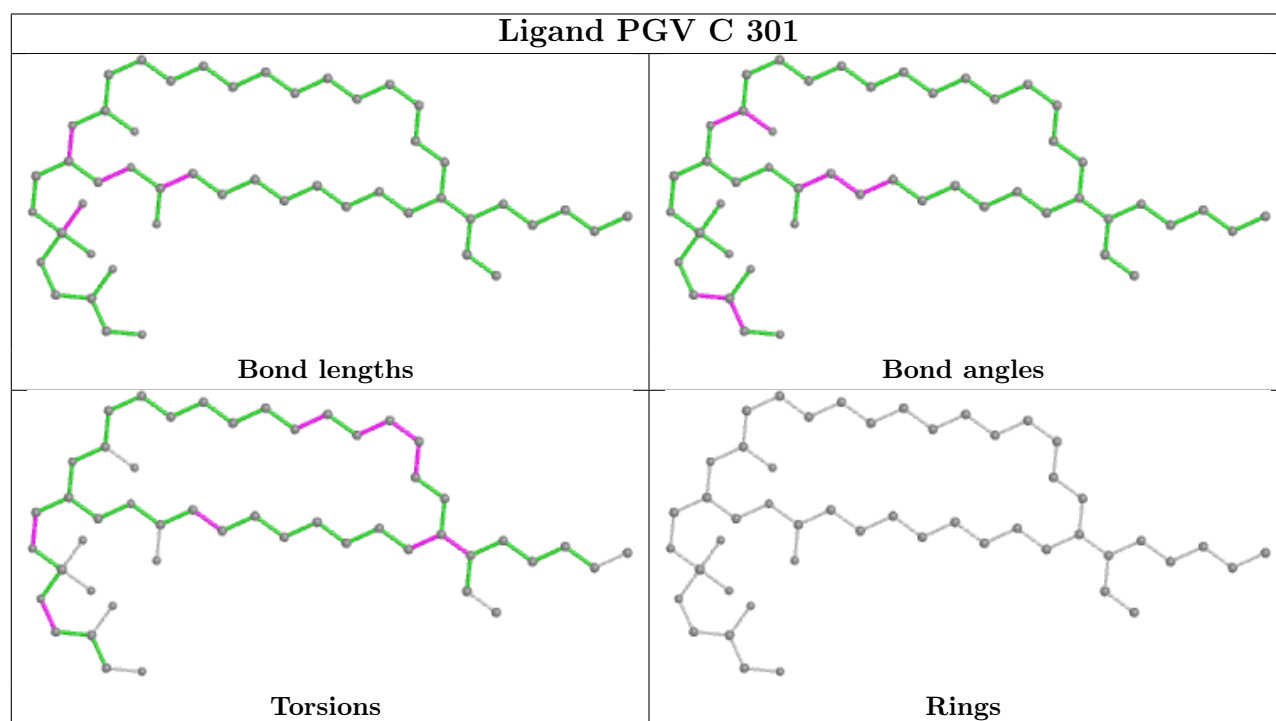
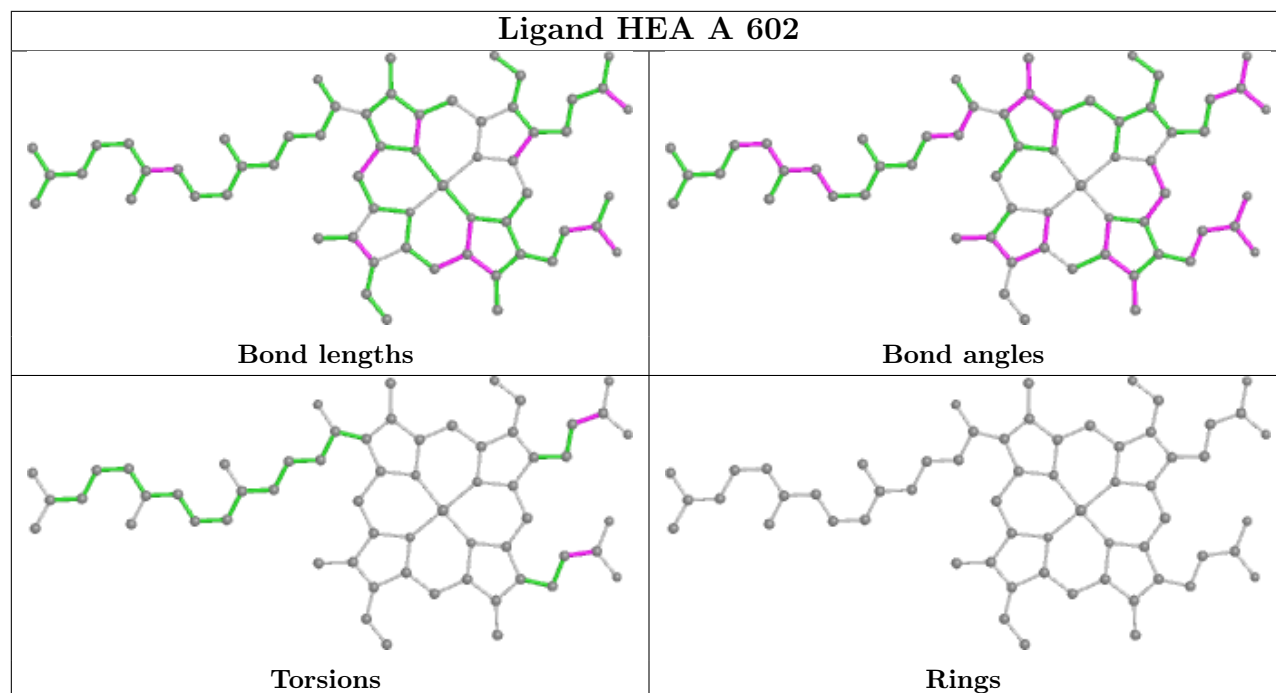


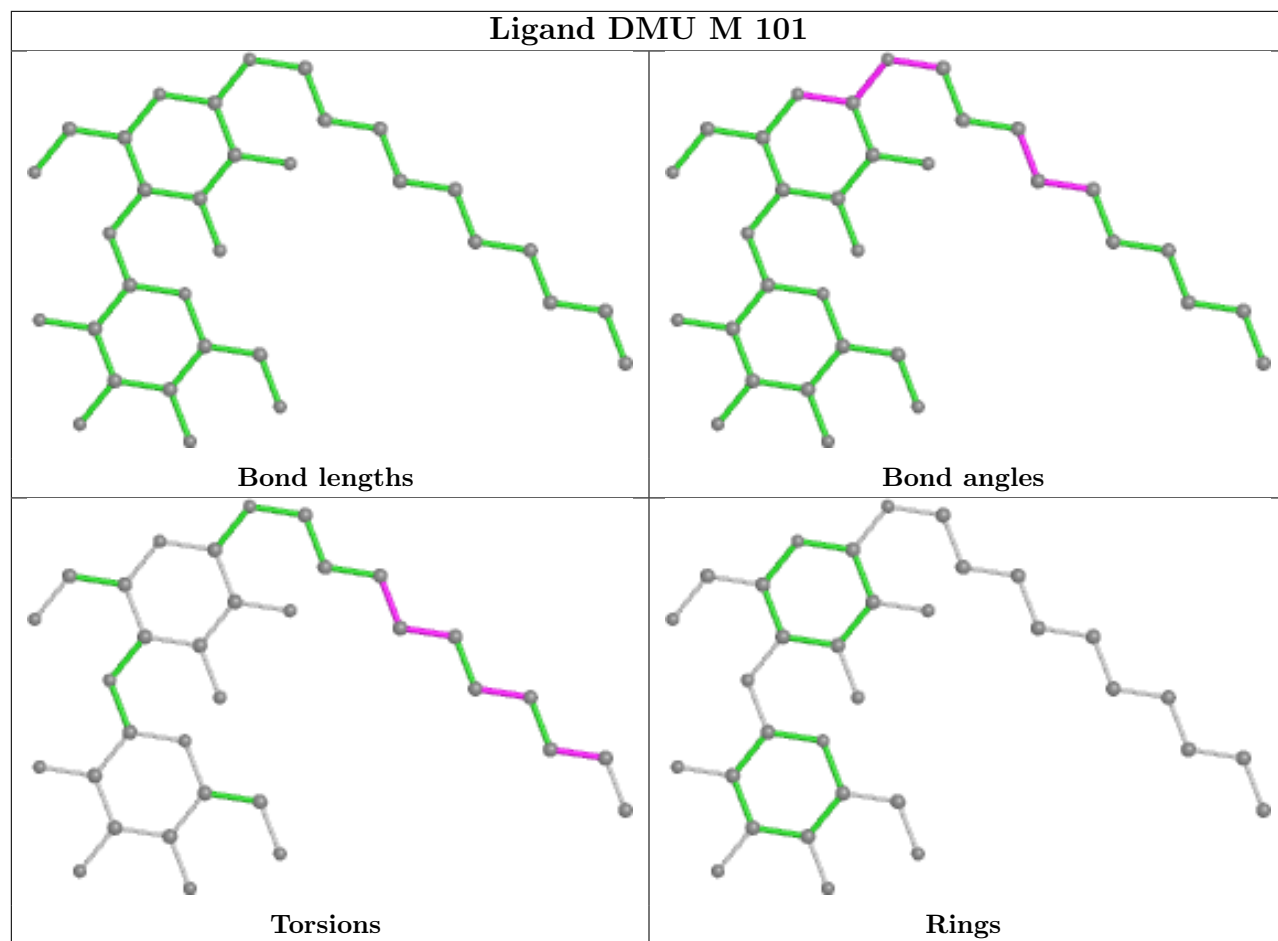
**Ligand HEA A 601 (B)****Ligand DMU K 101**

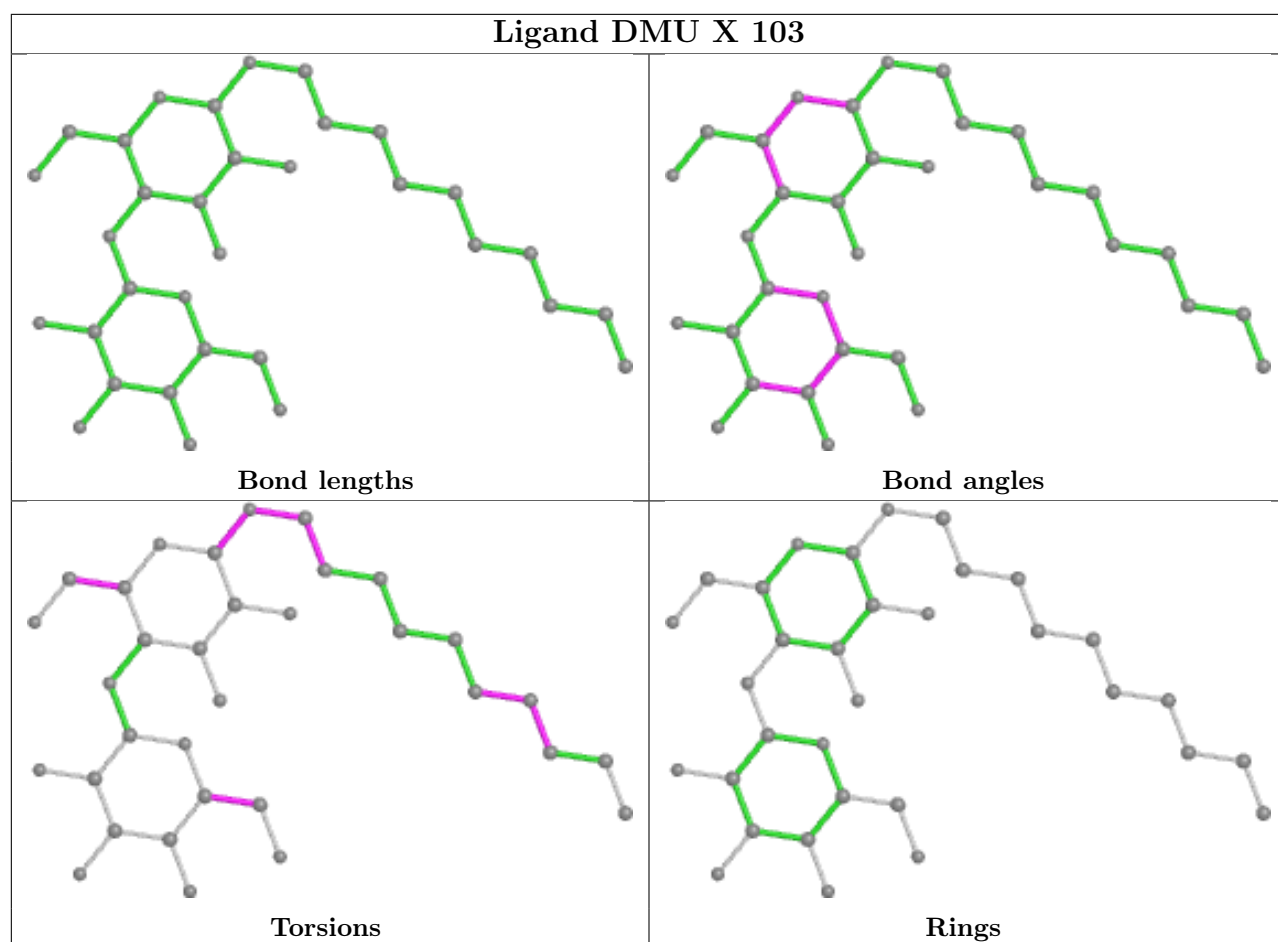


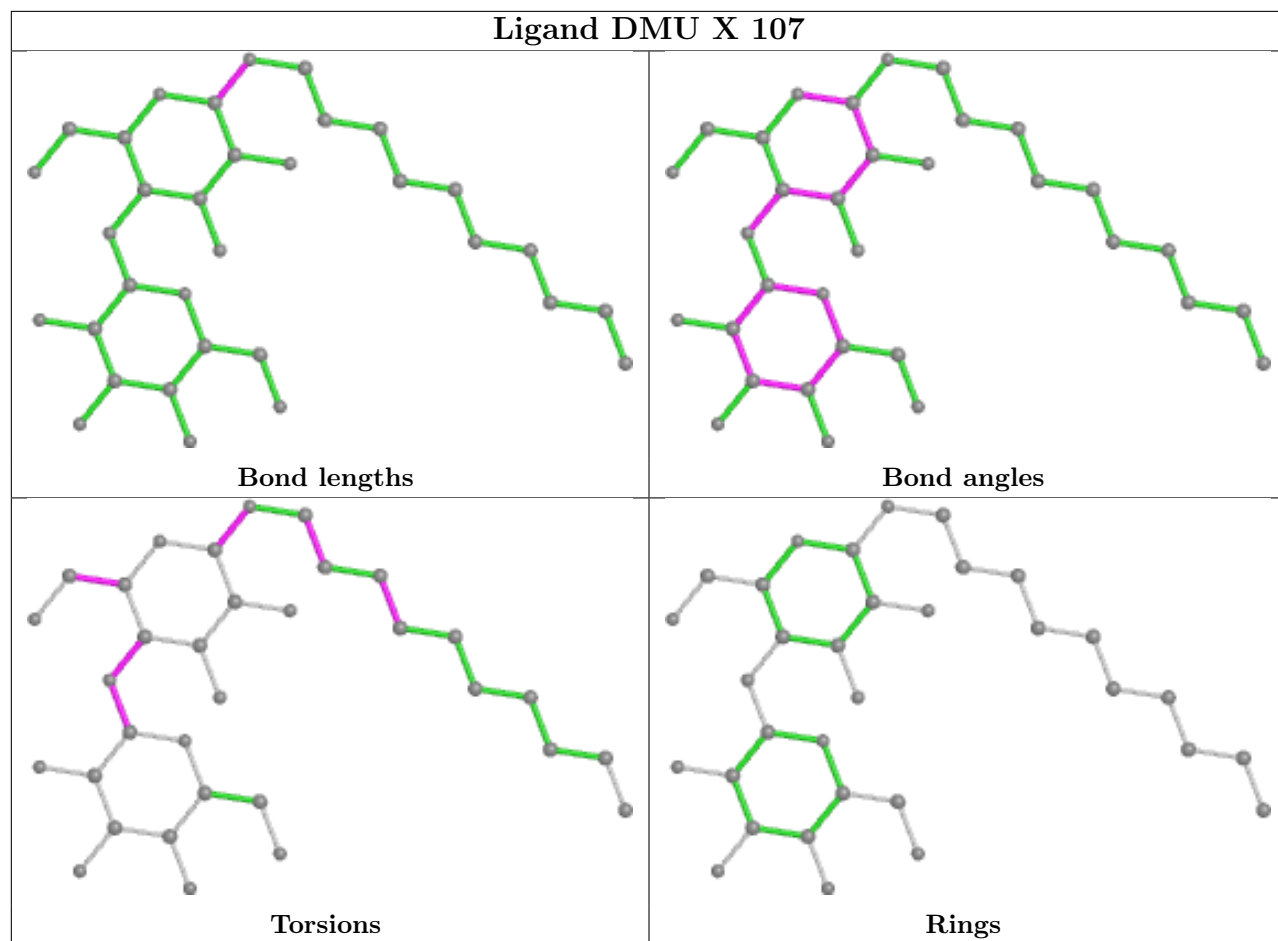


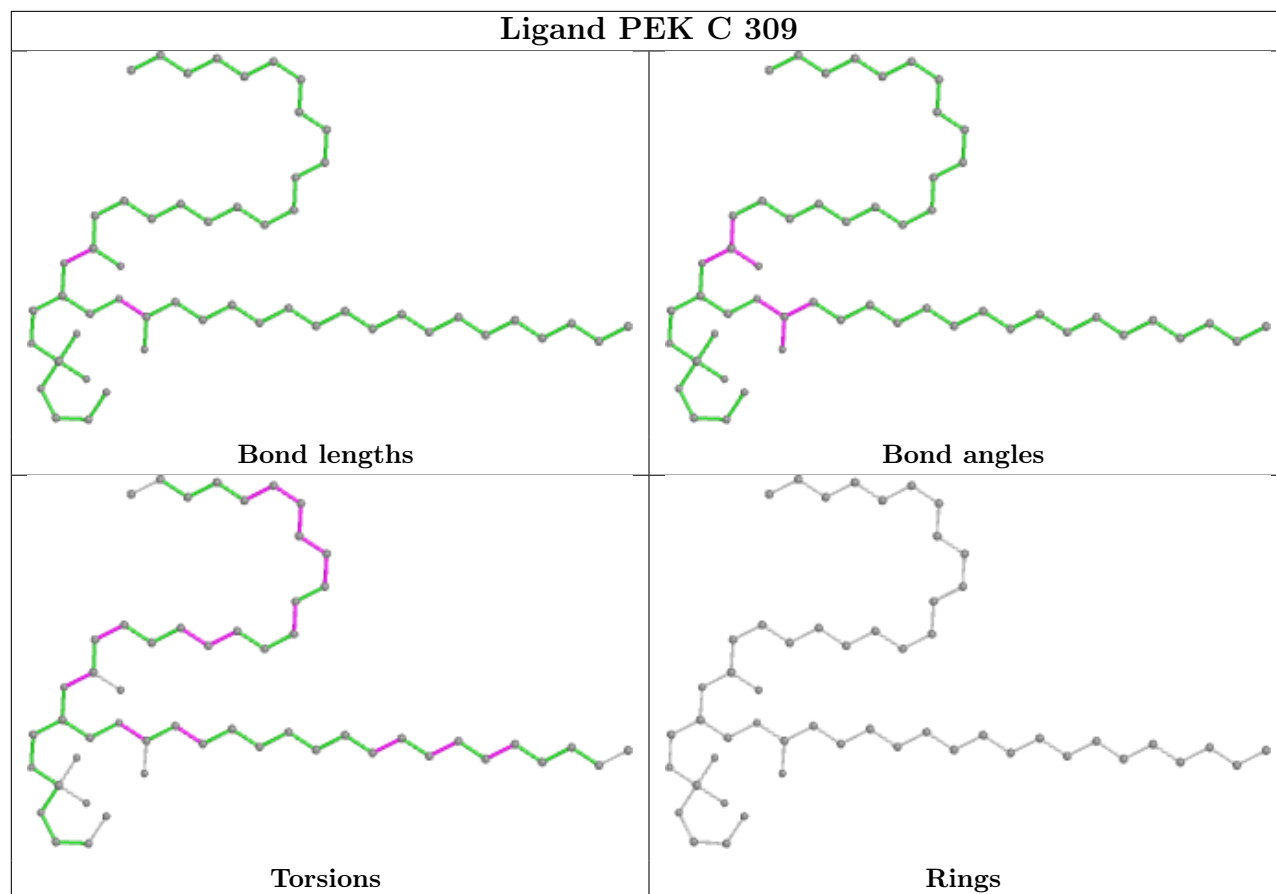


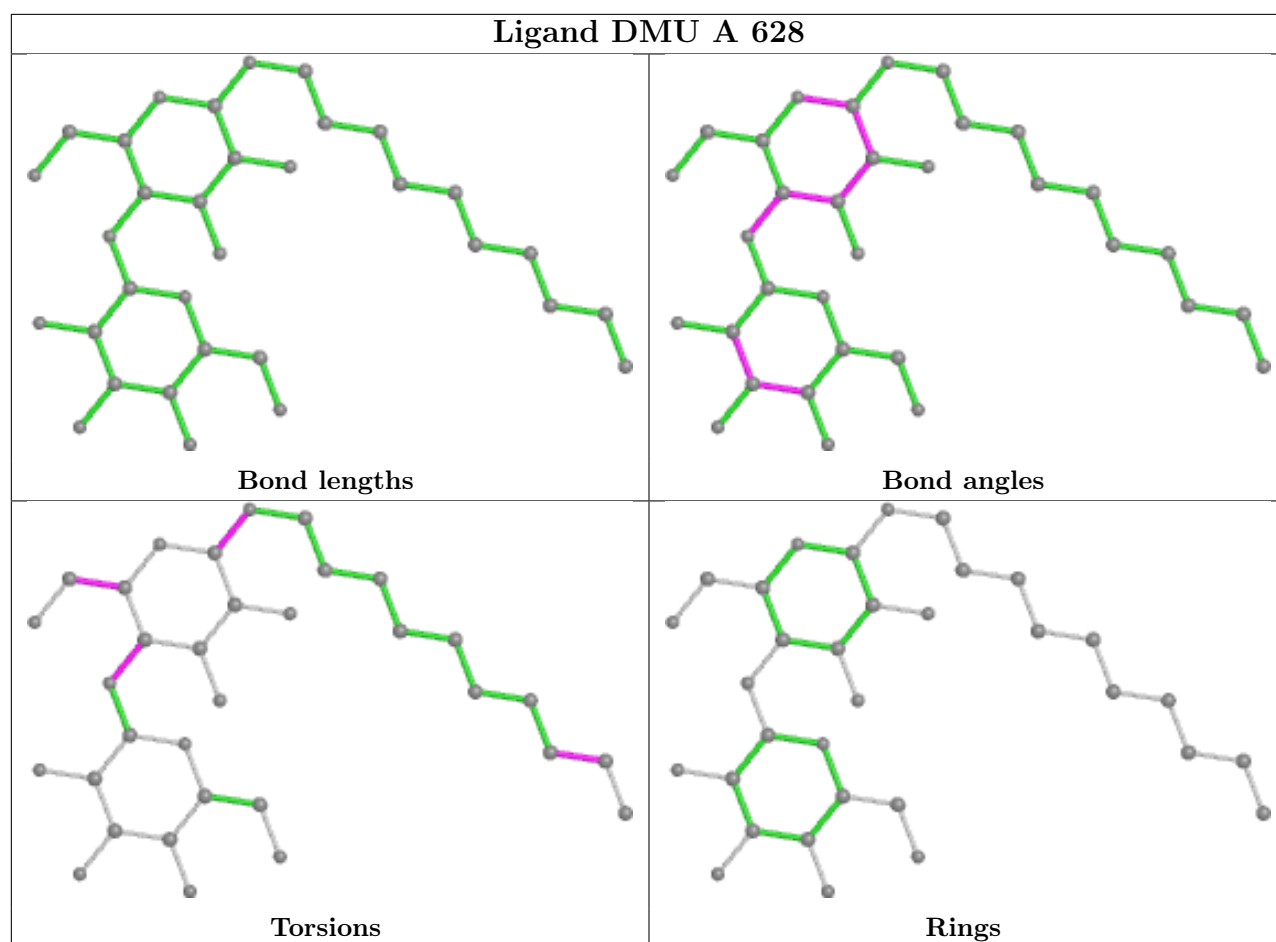


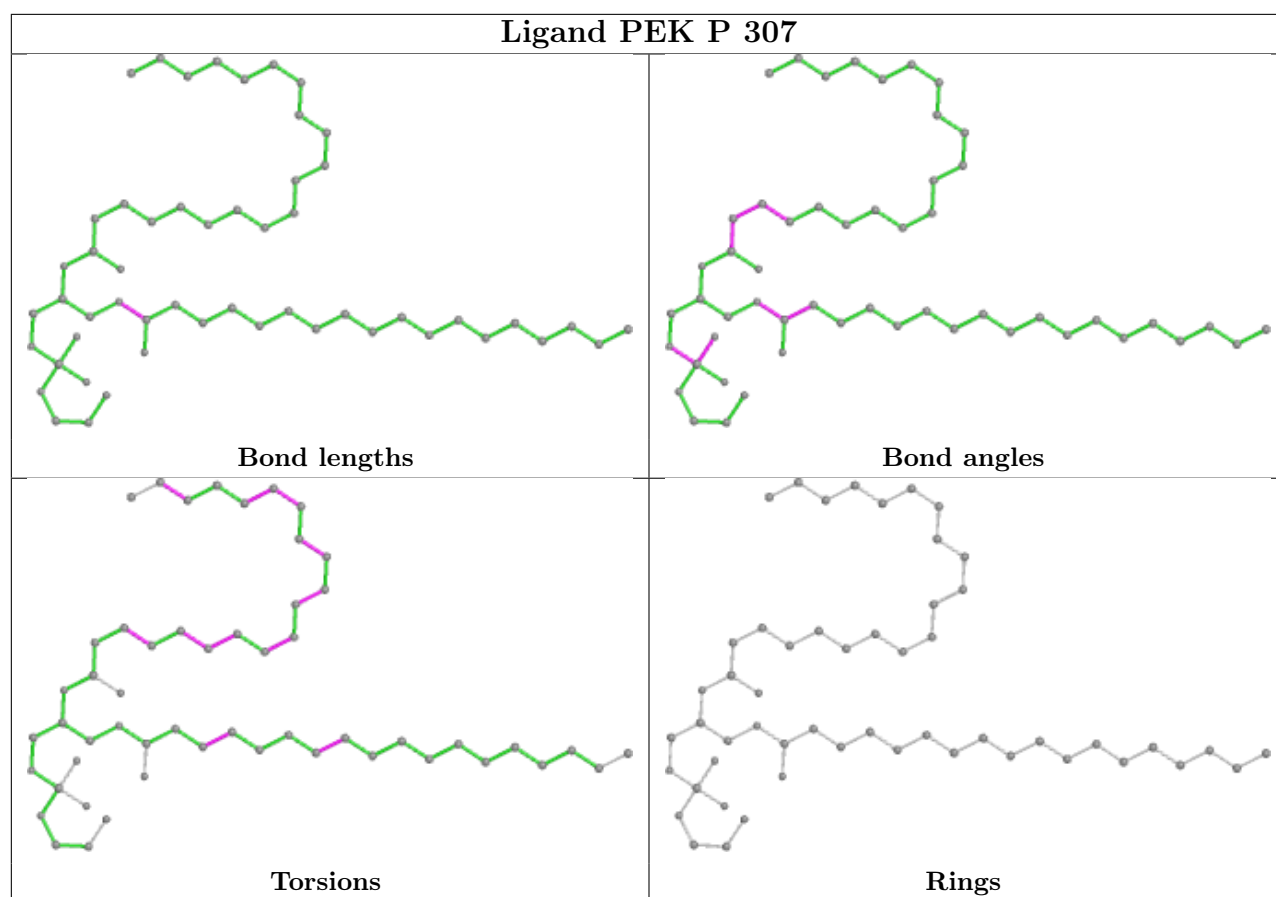






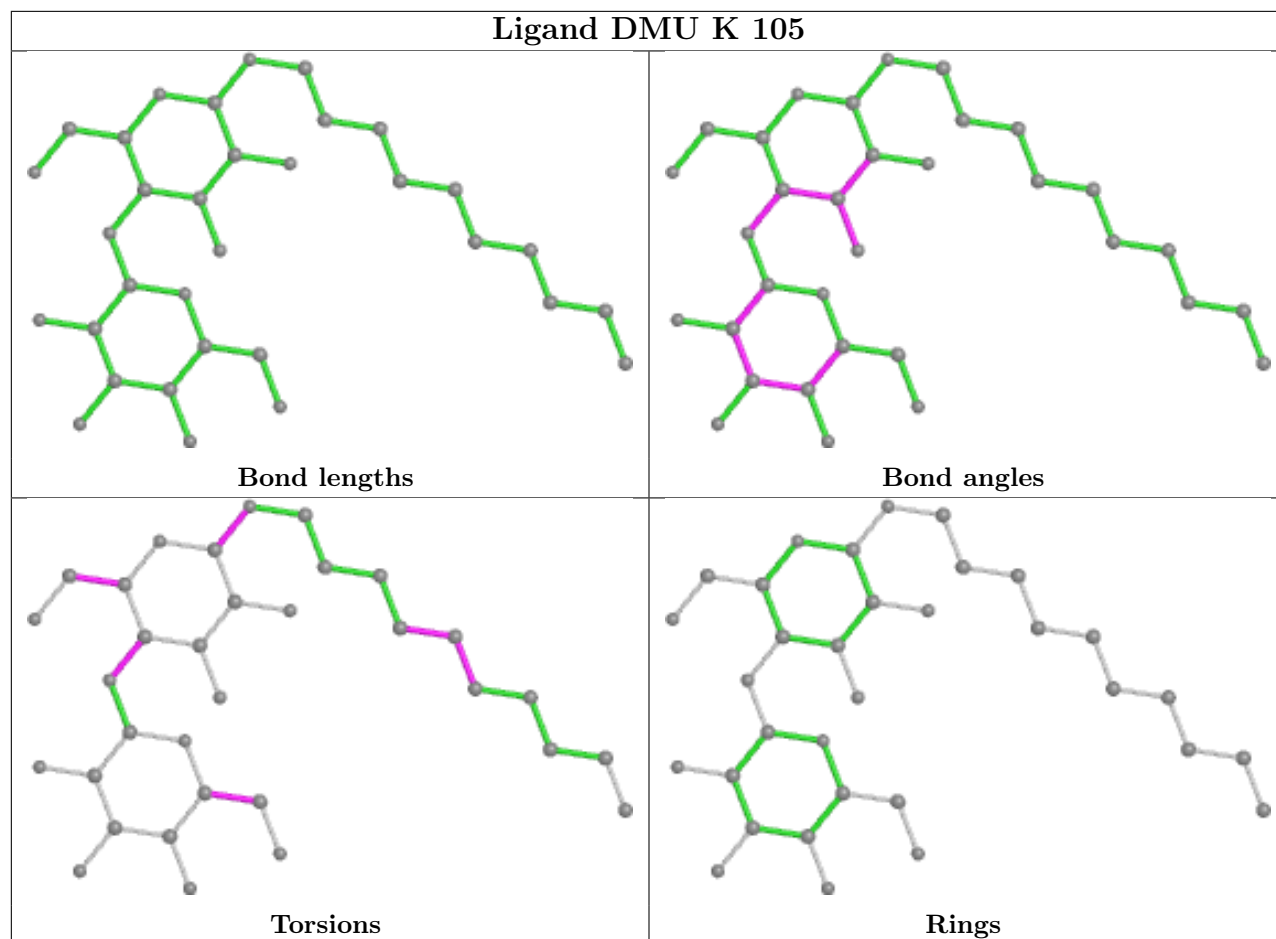




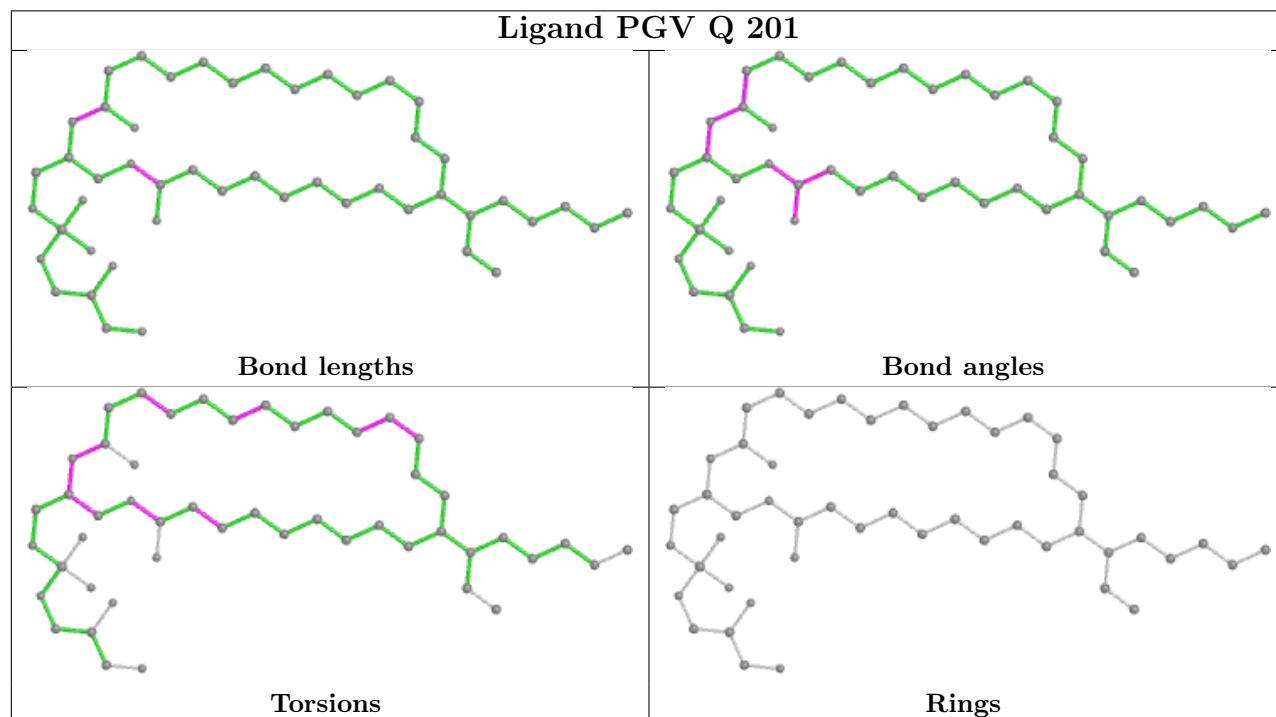


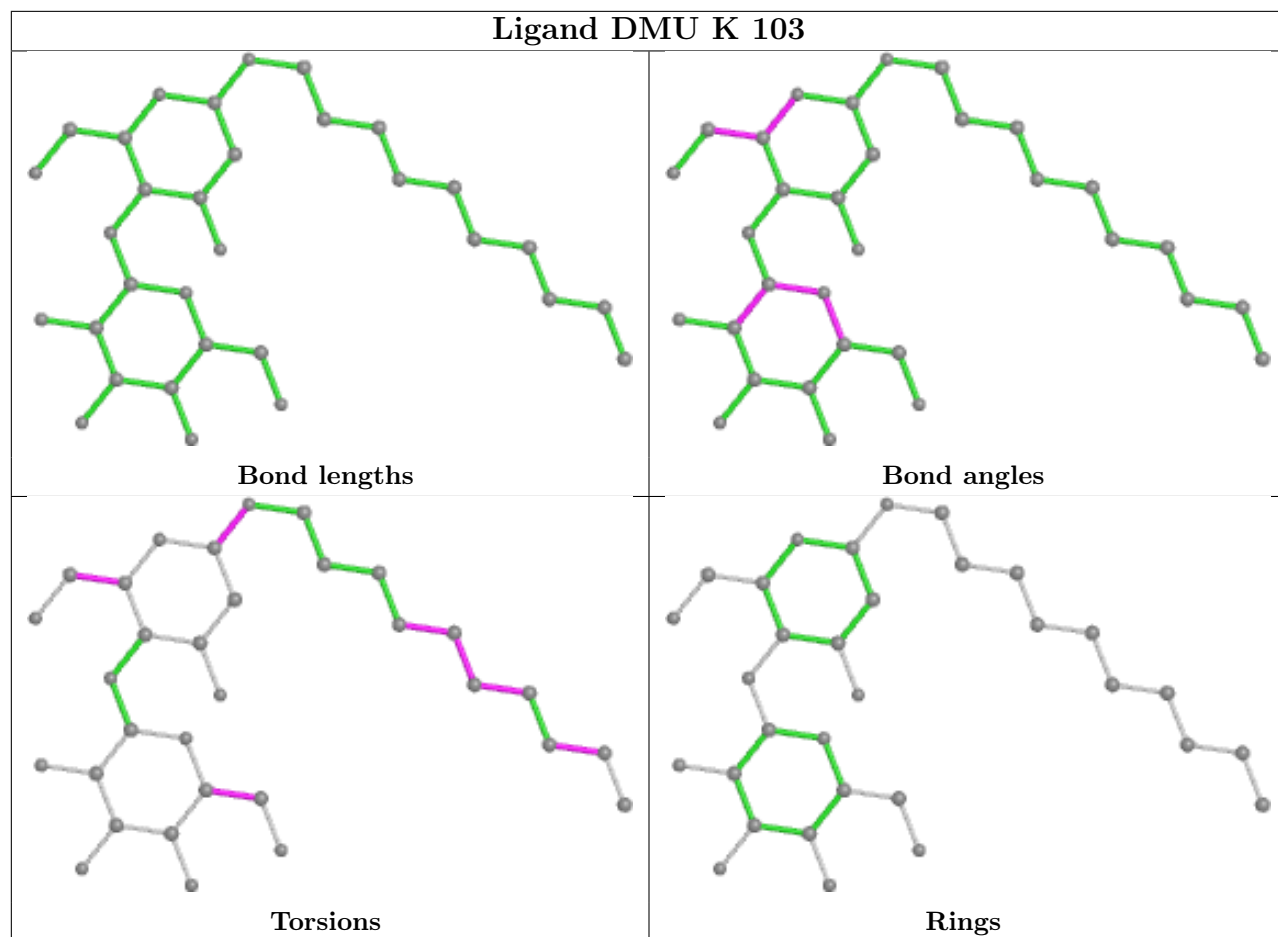


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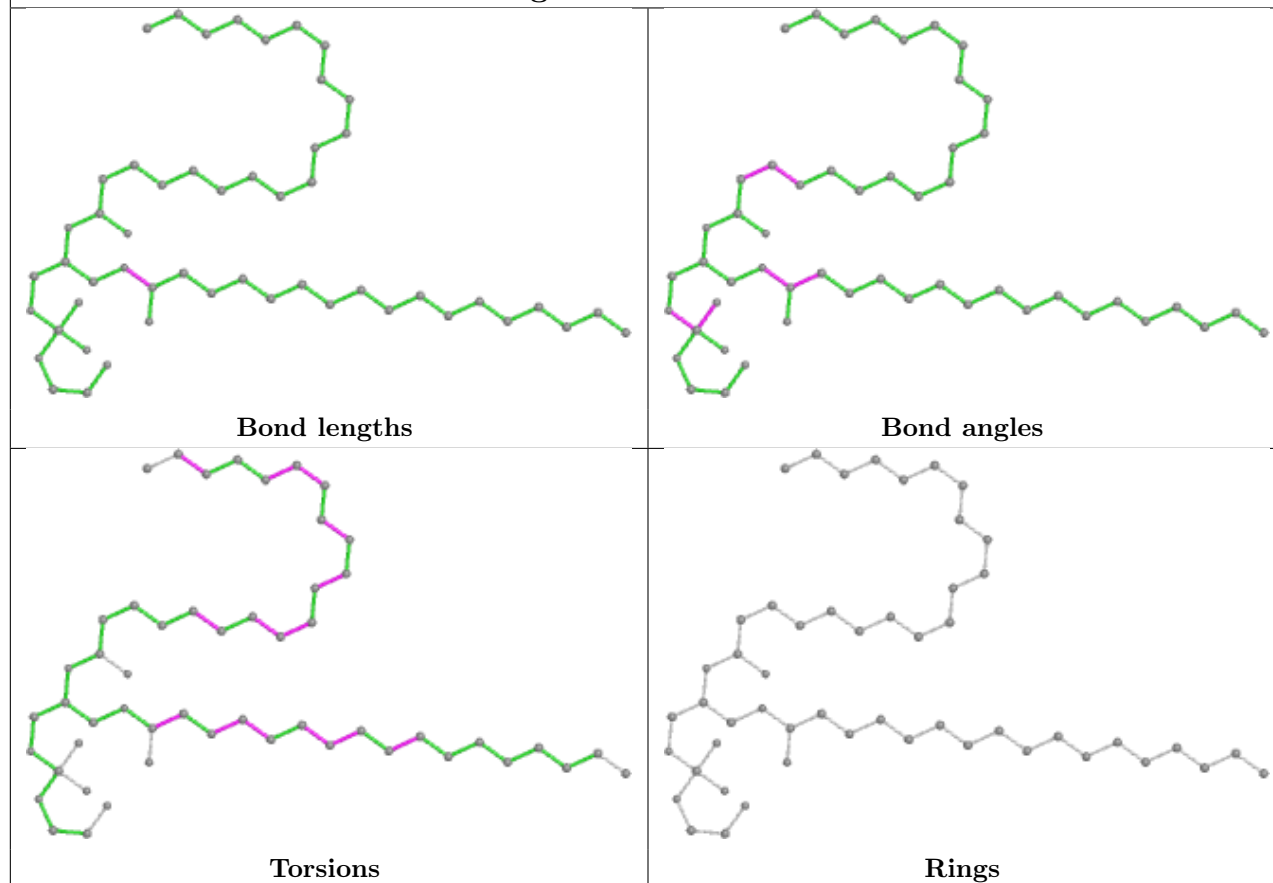


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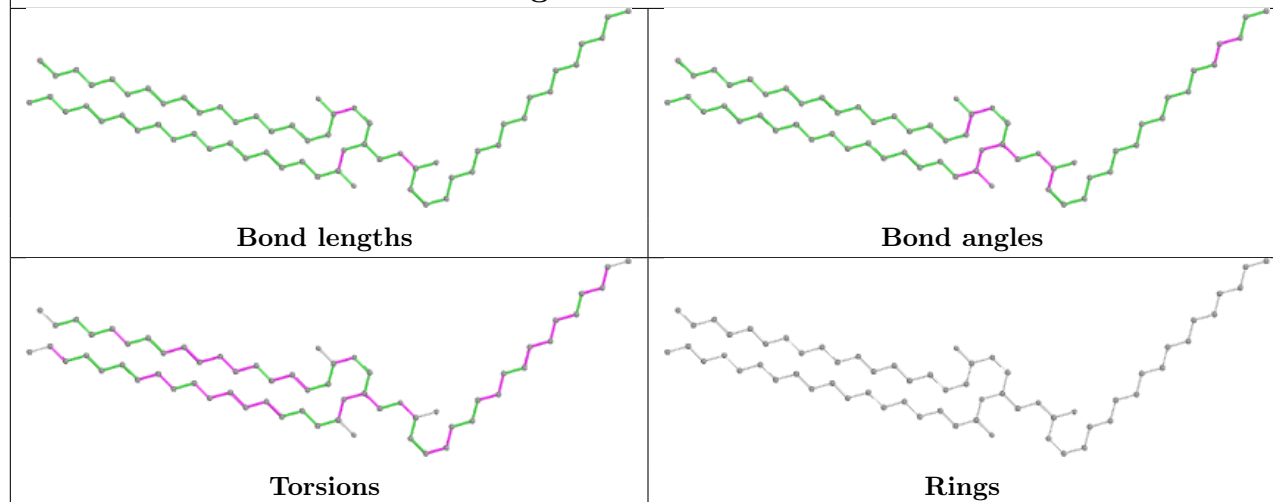


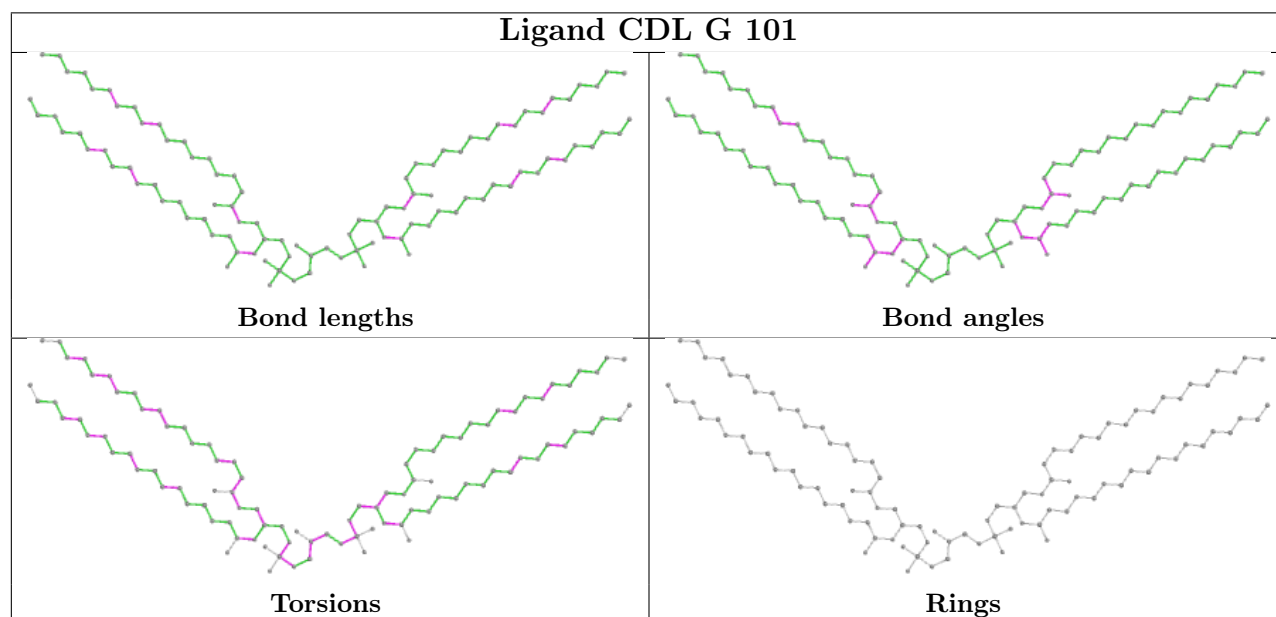
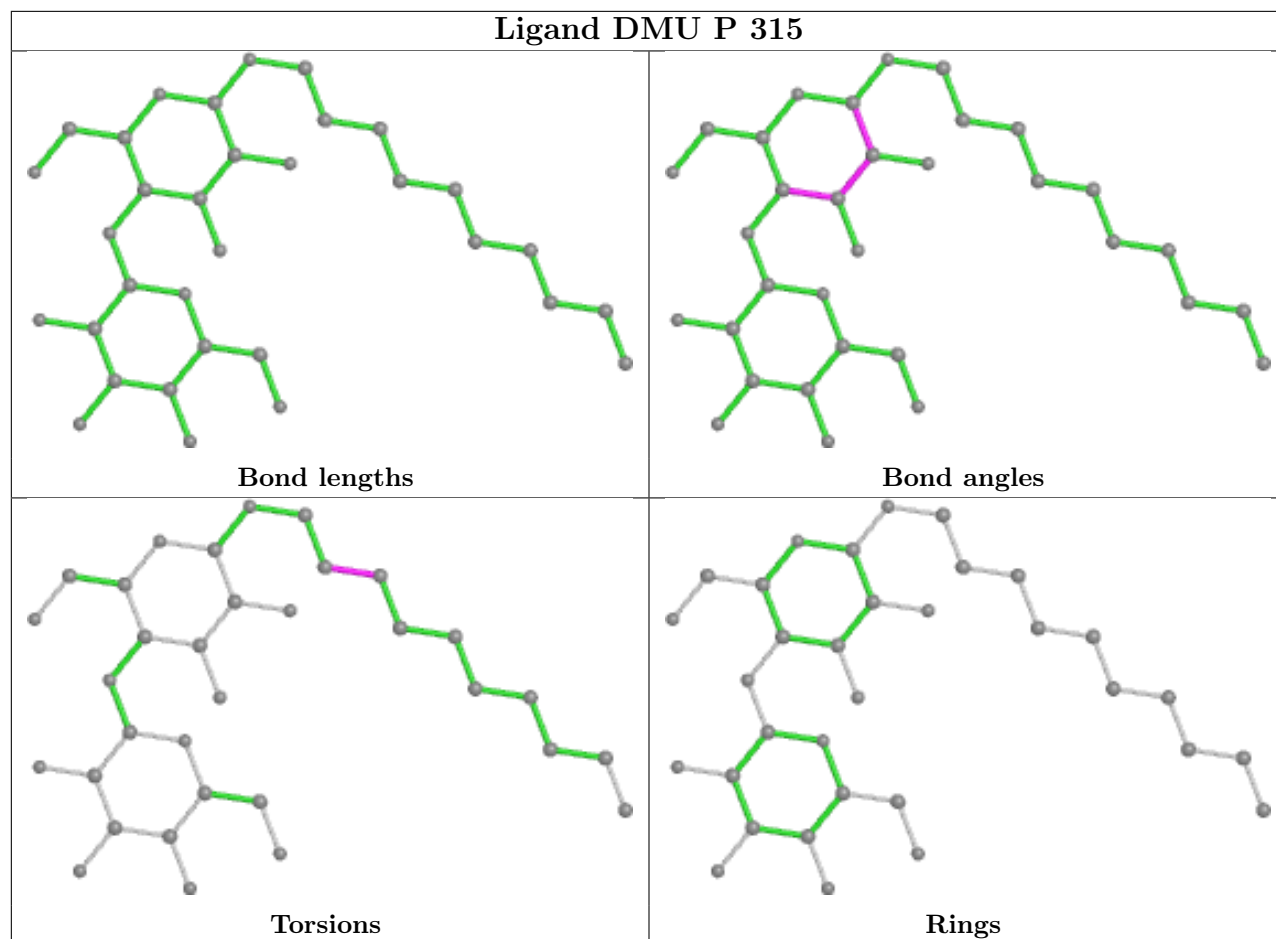


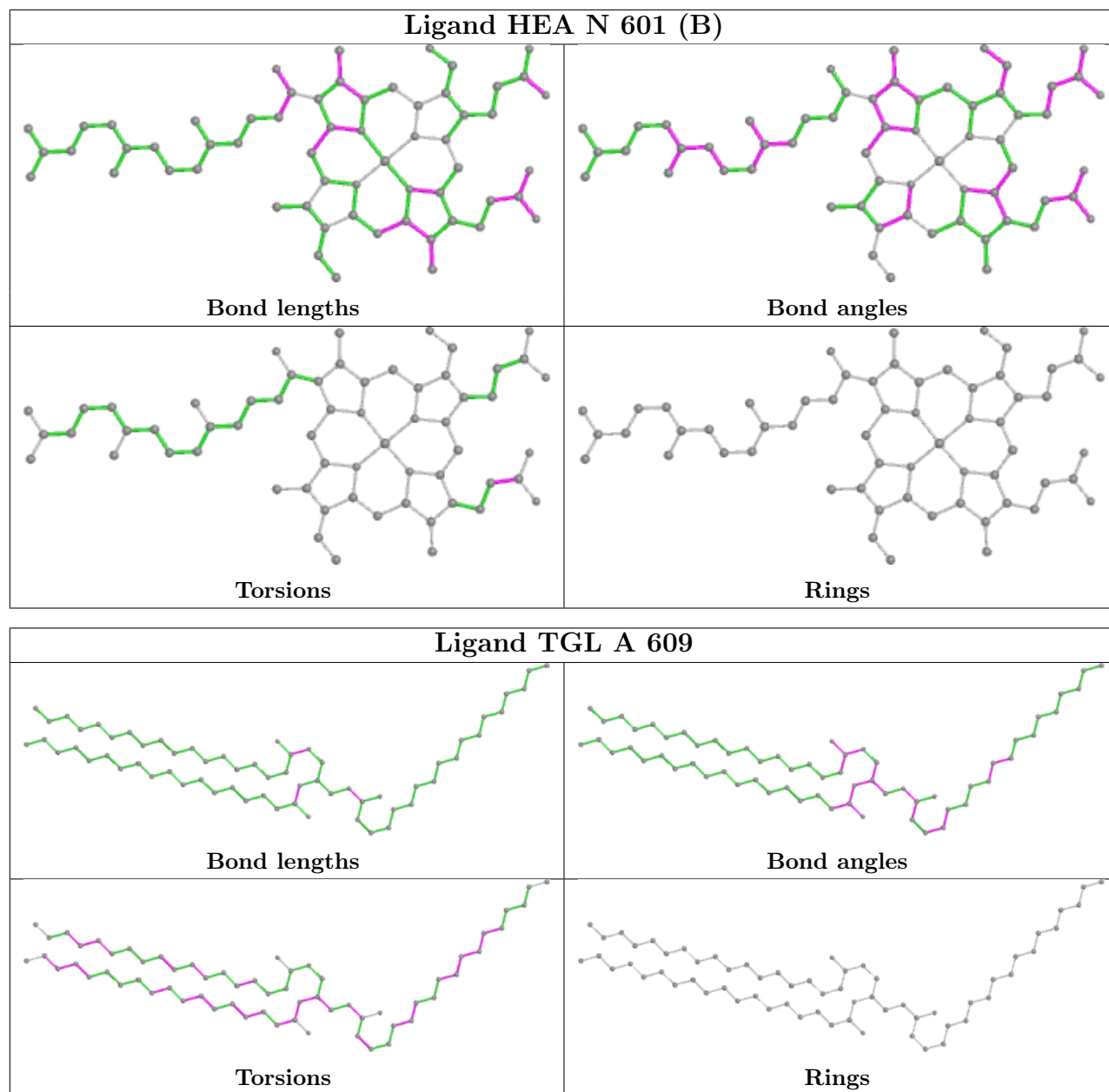
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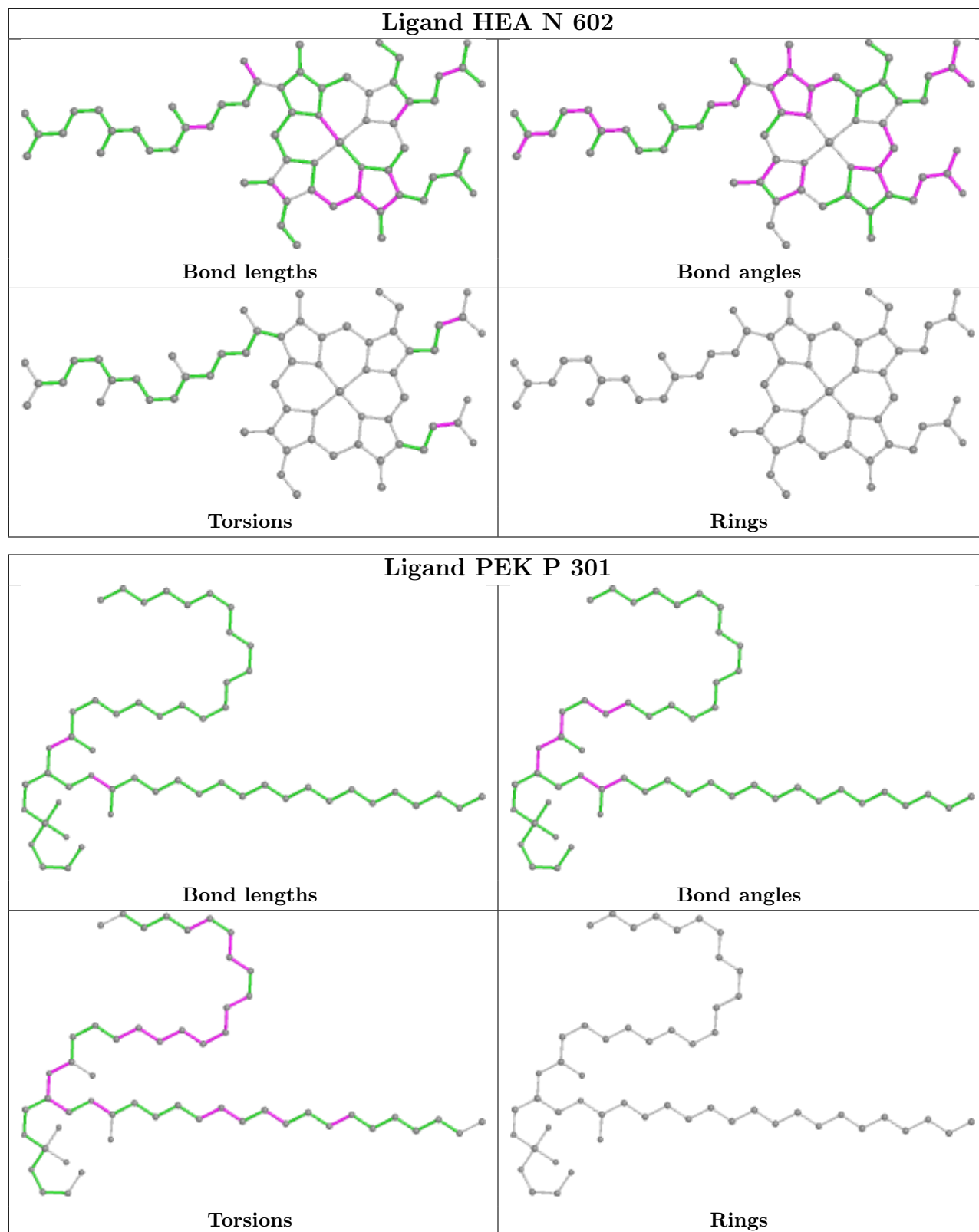


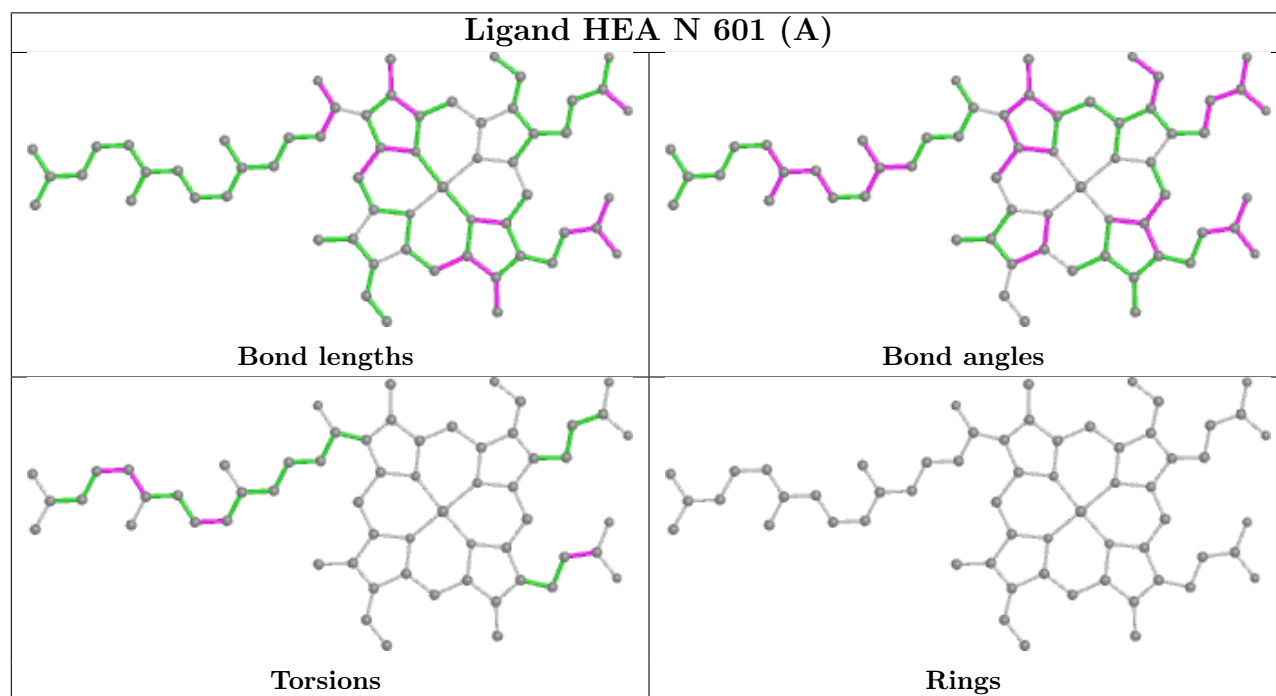
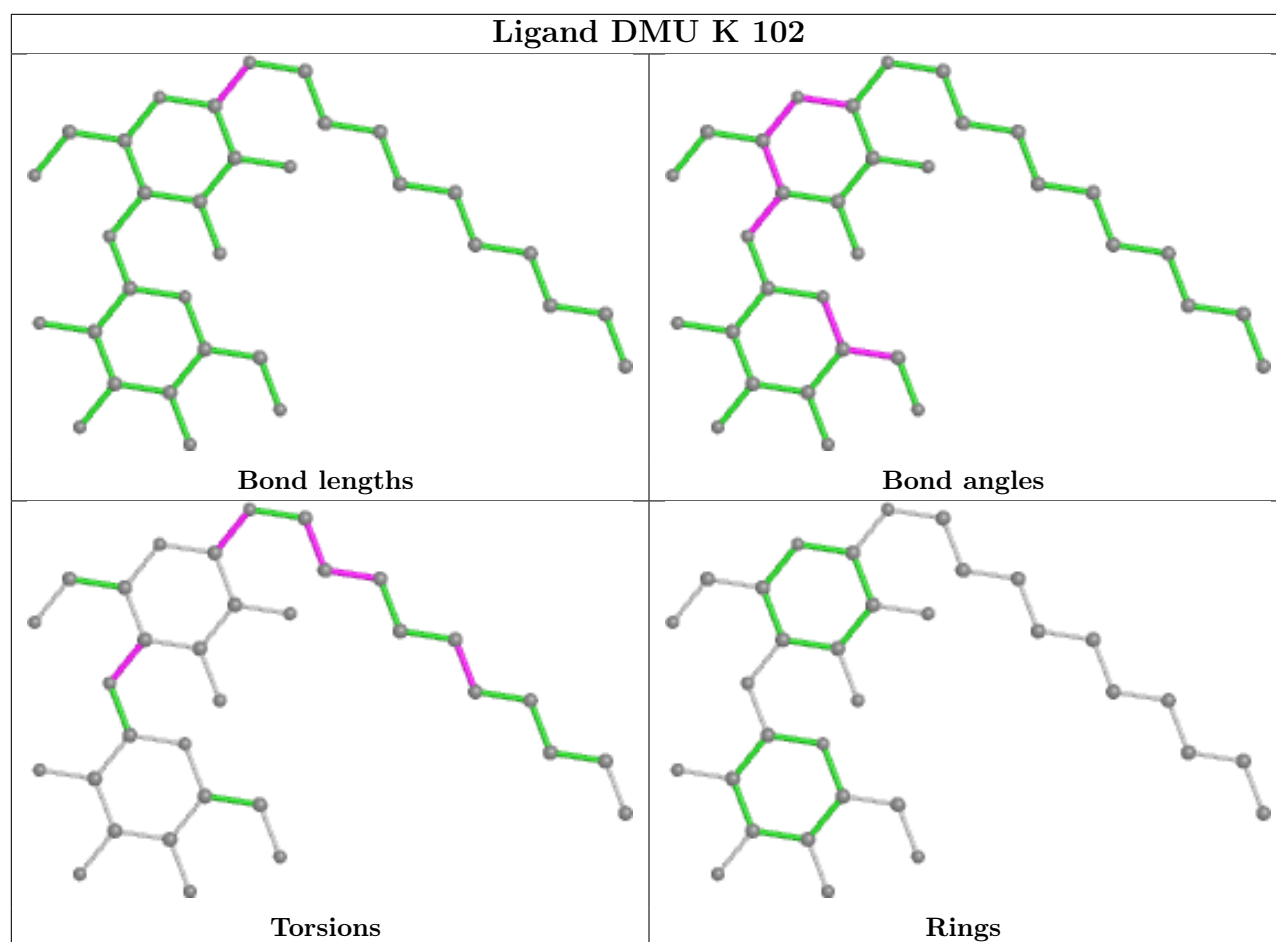
## Ligand TGL Y 101

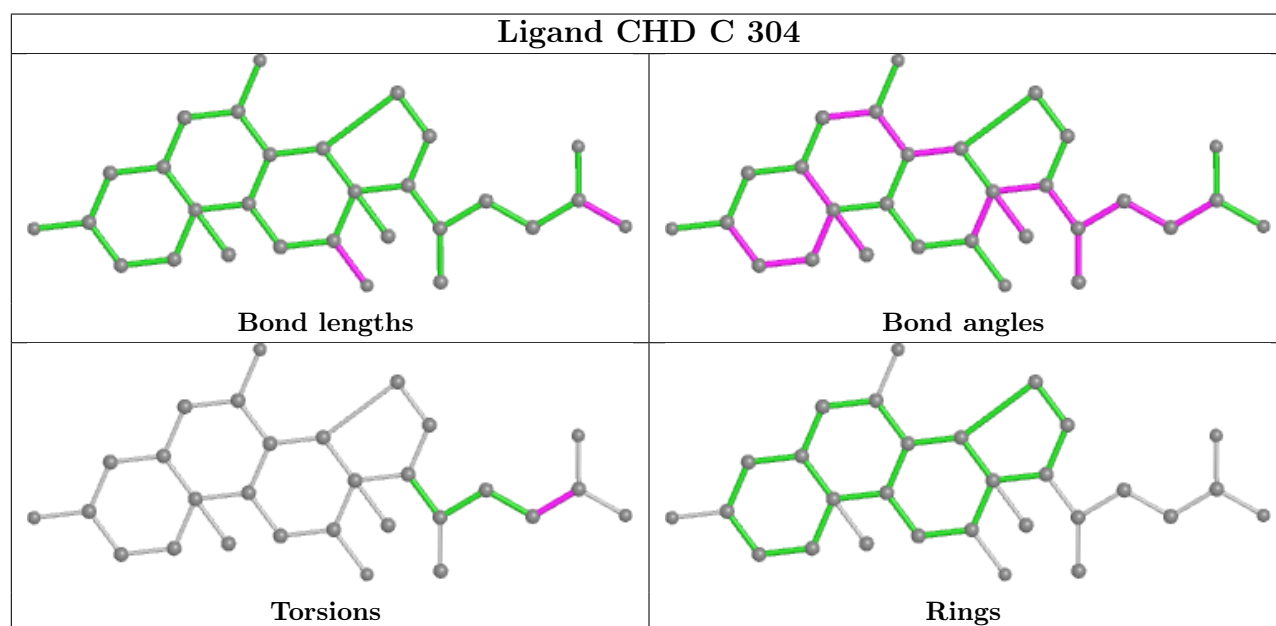
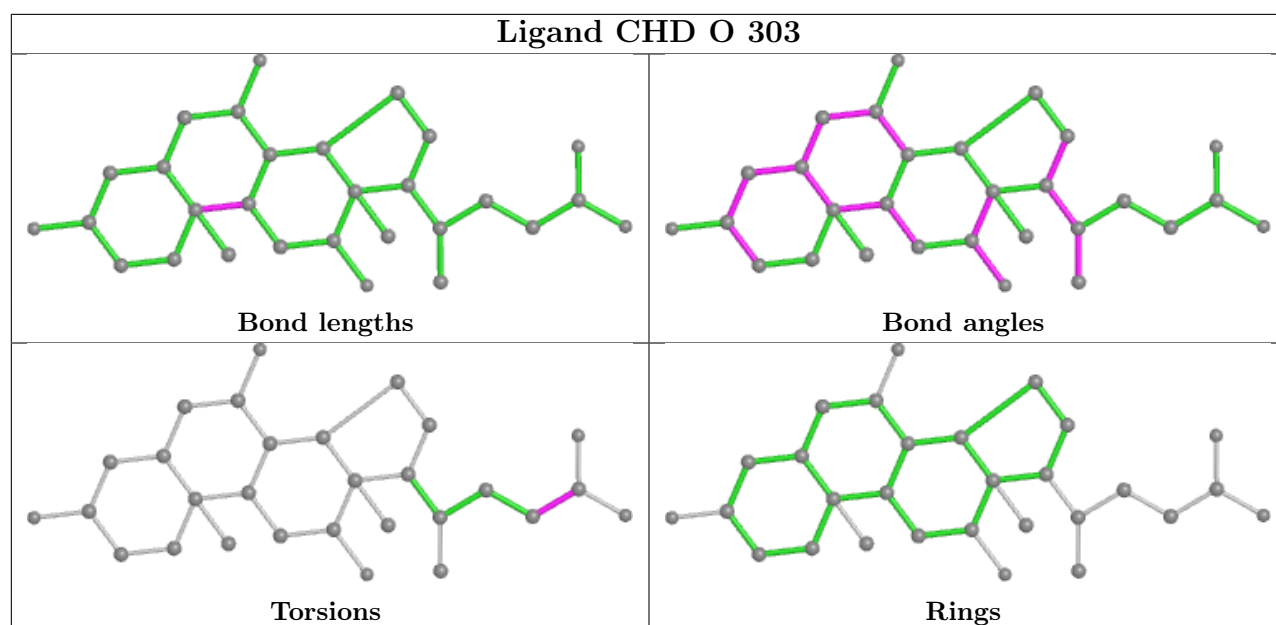




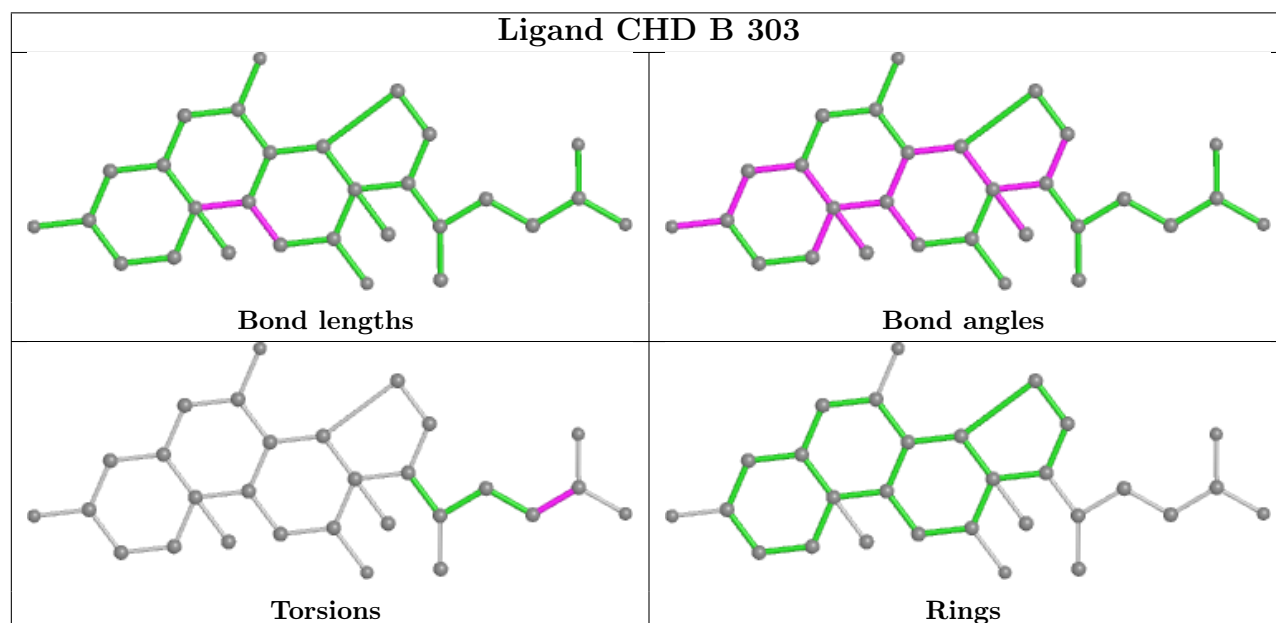
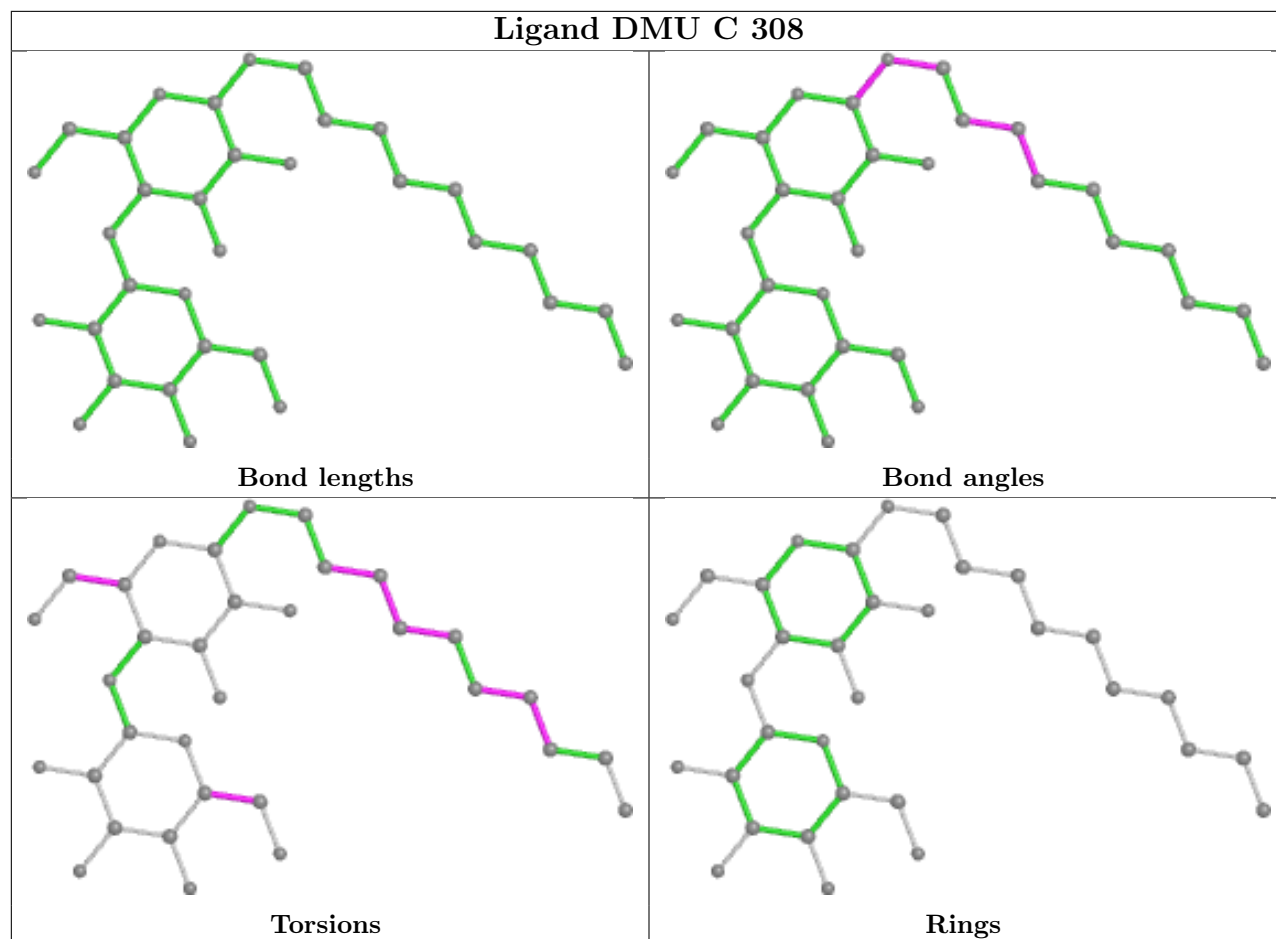


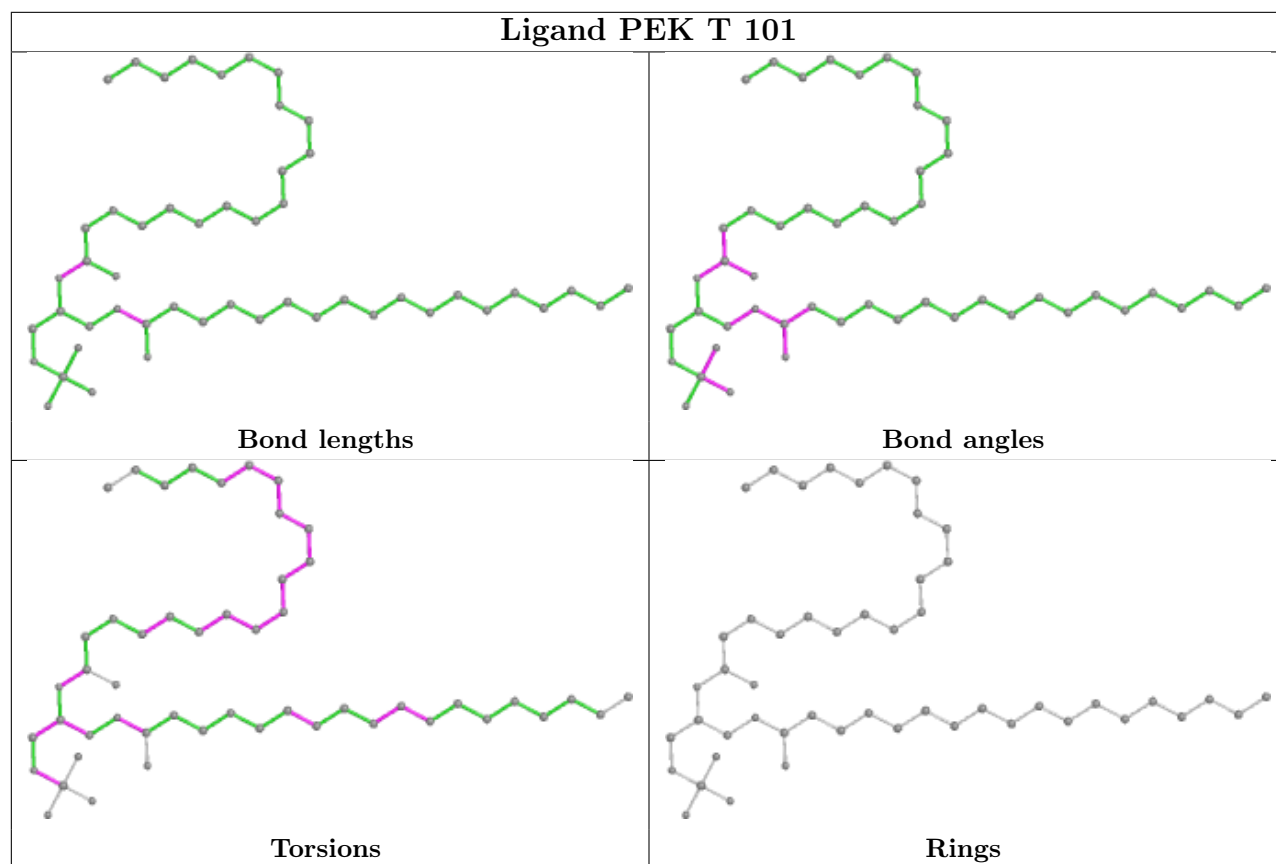
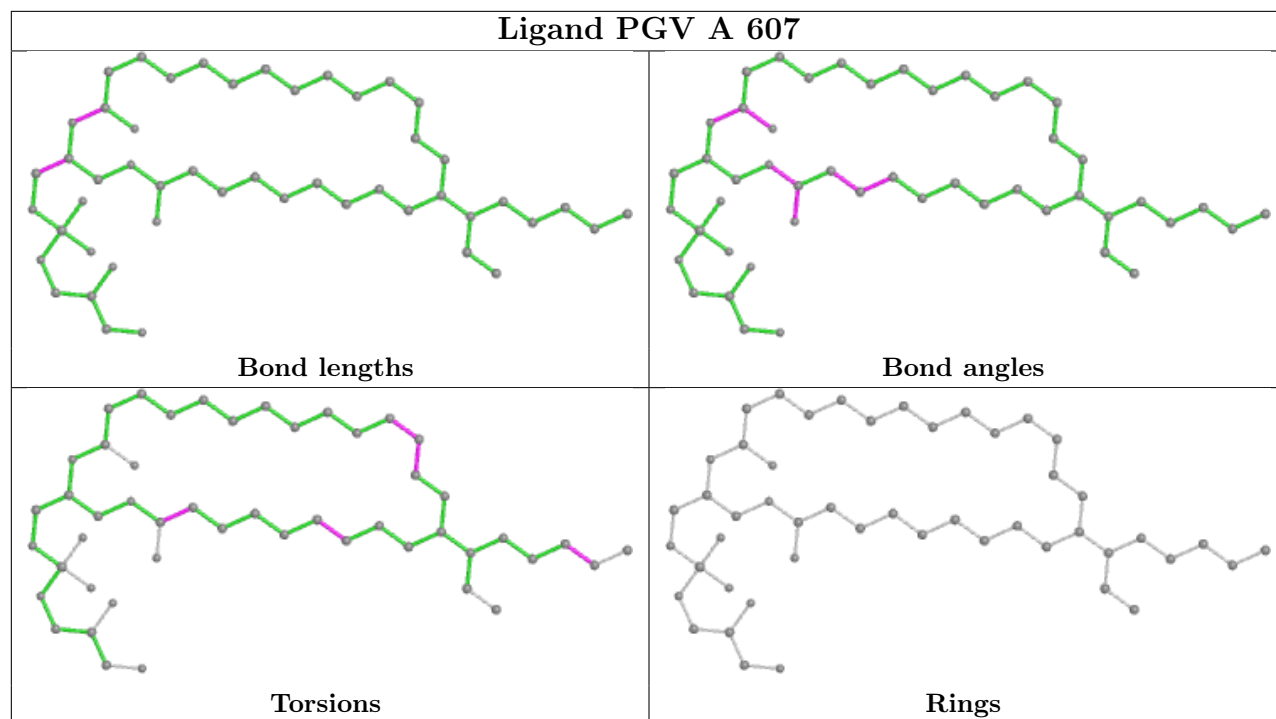


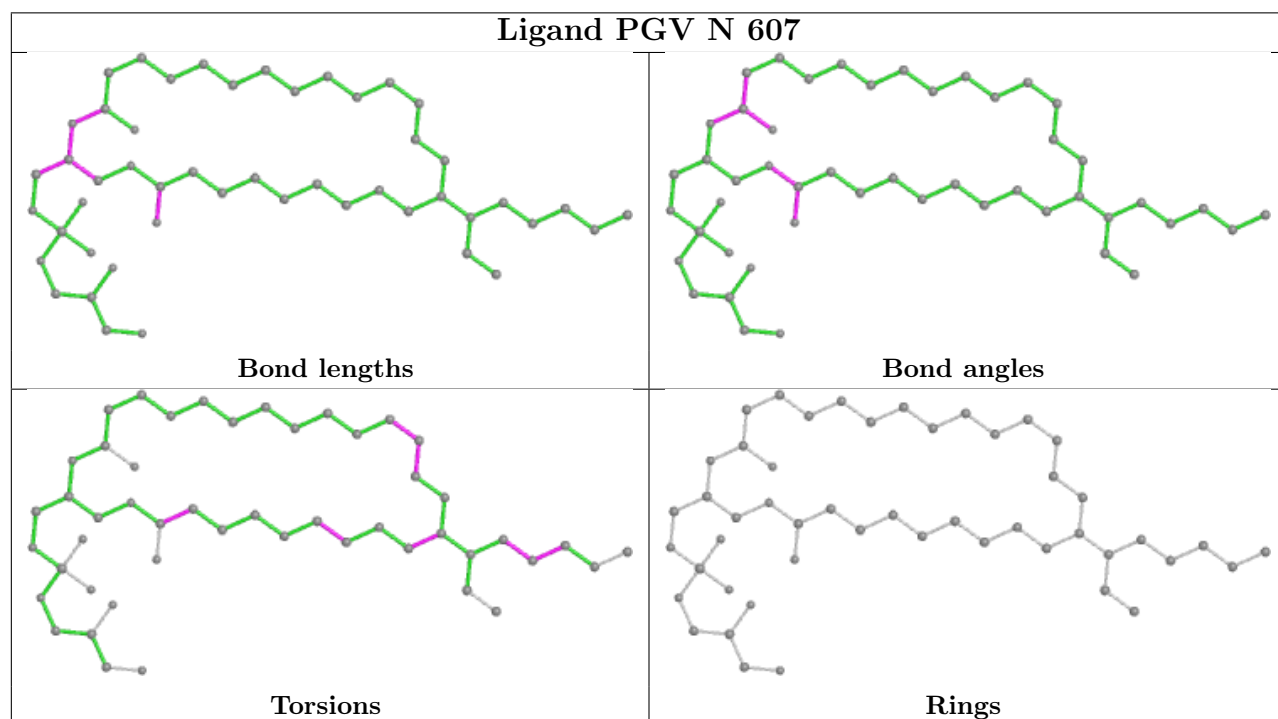
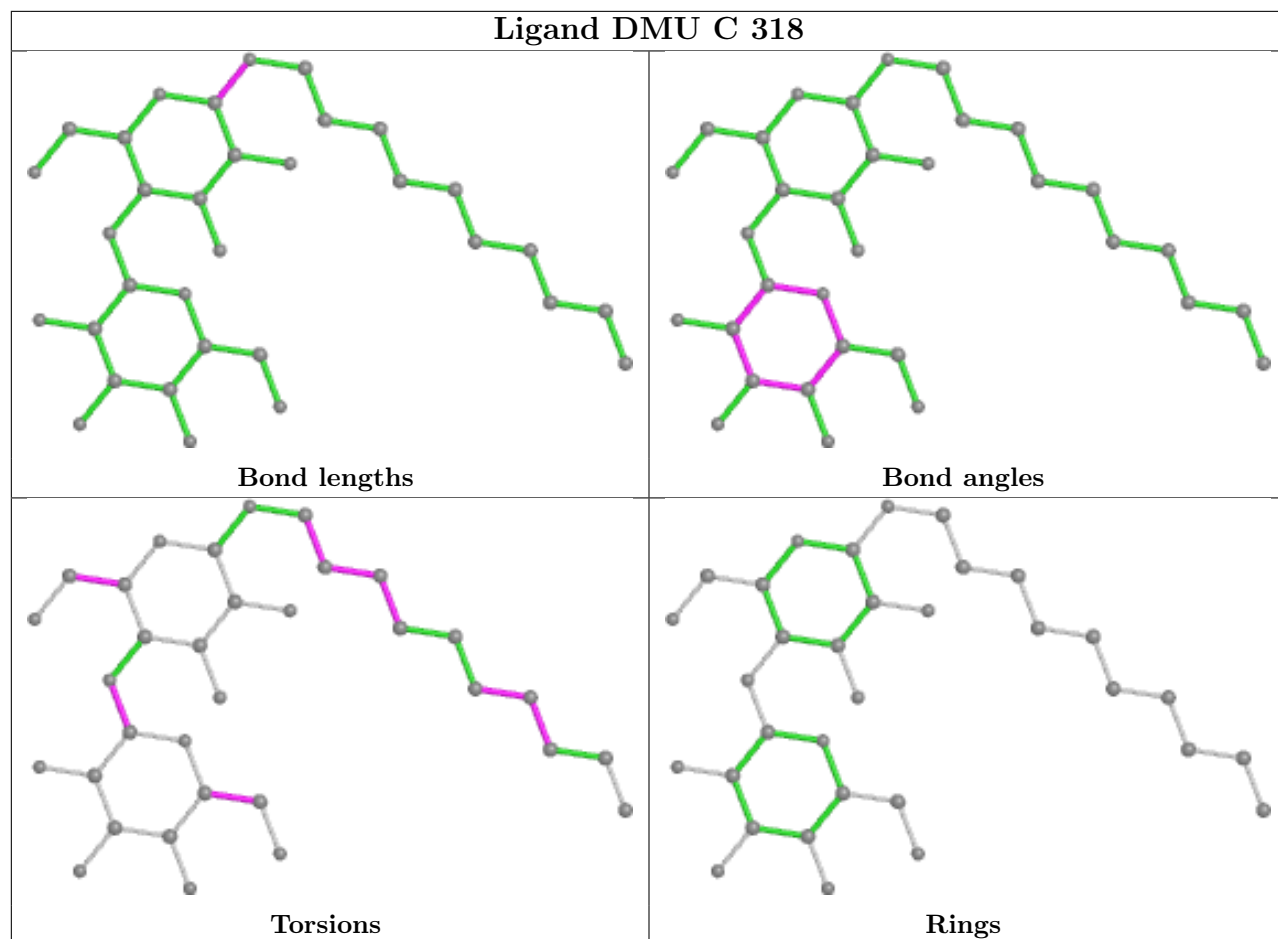


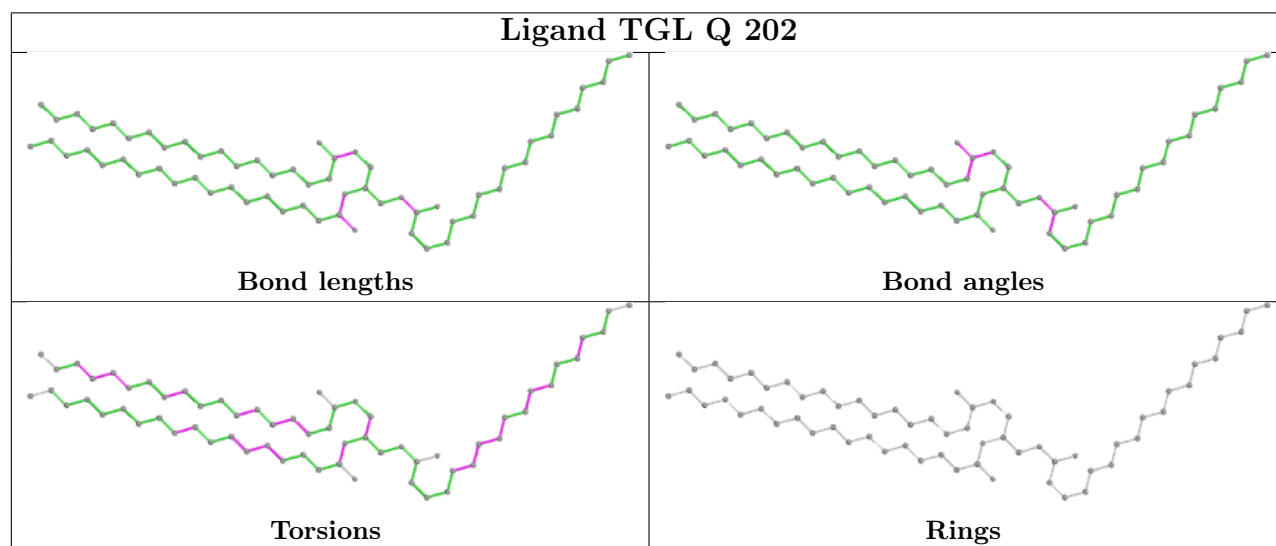
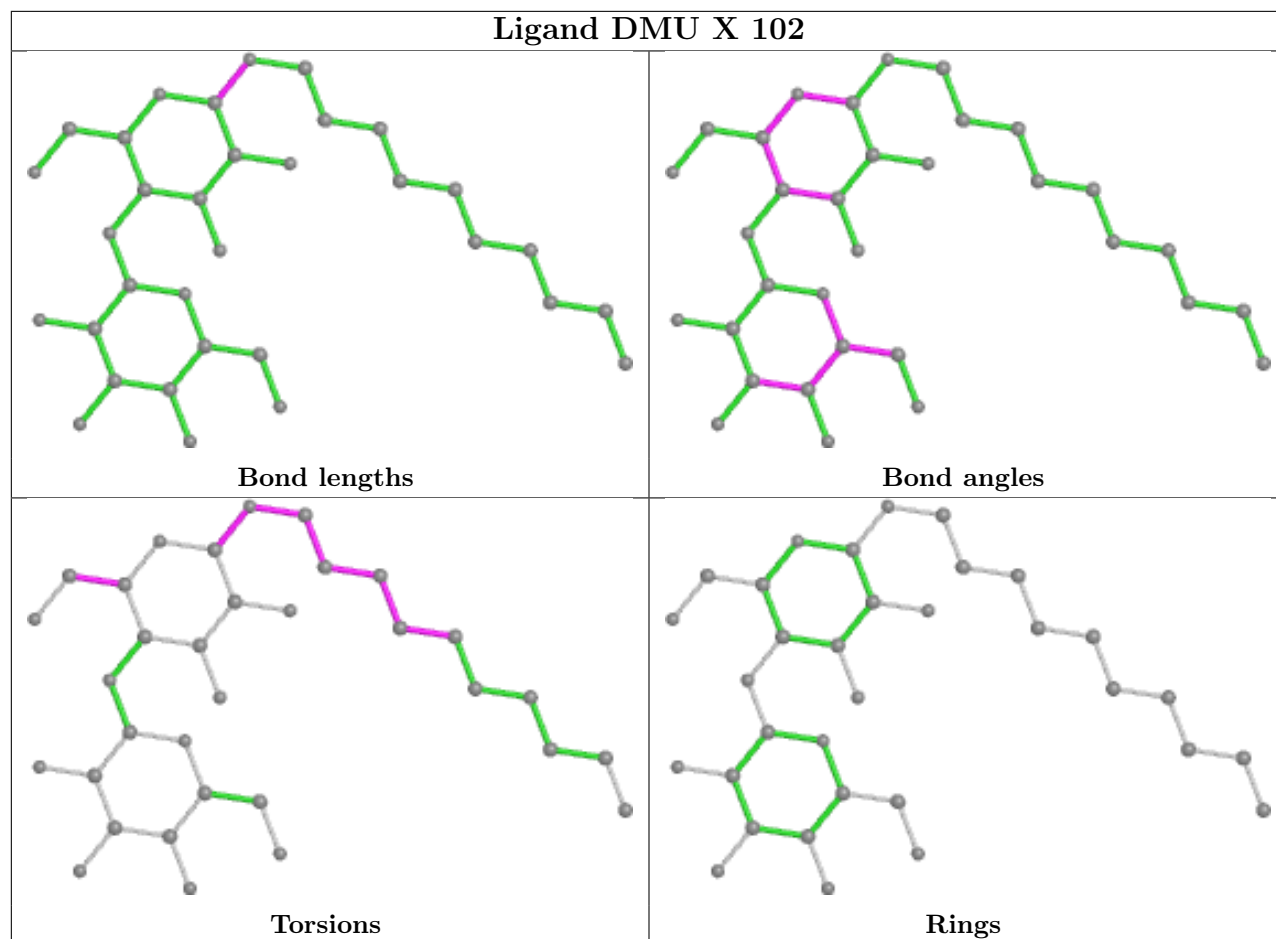


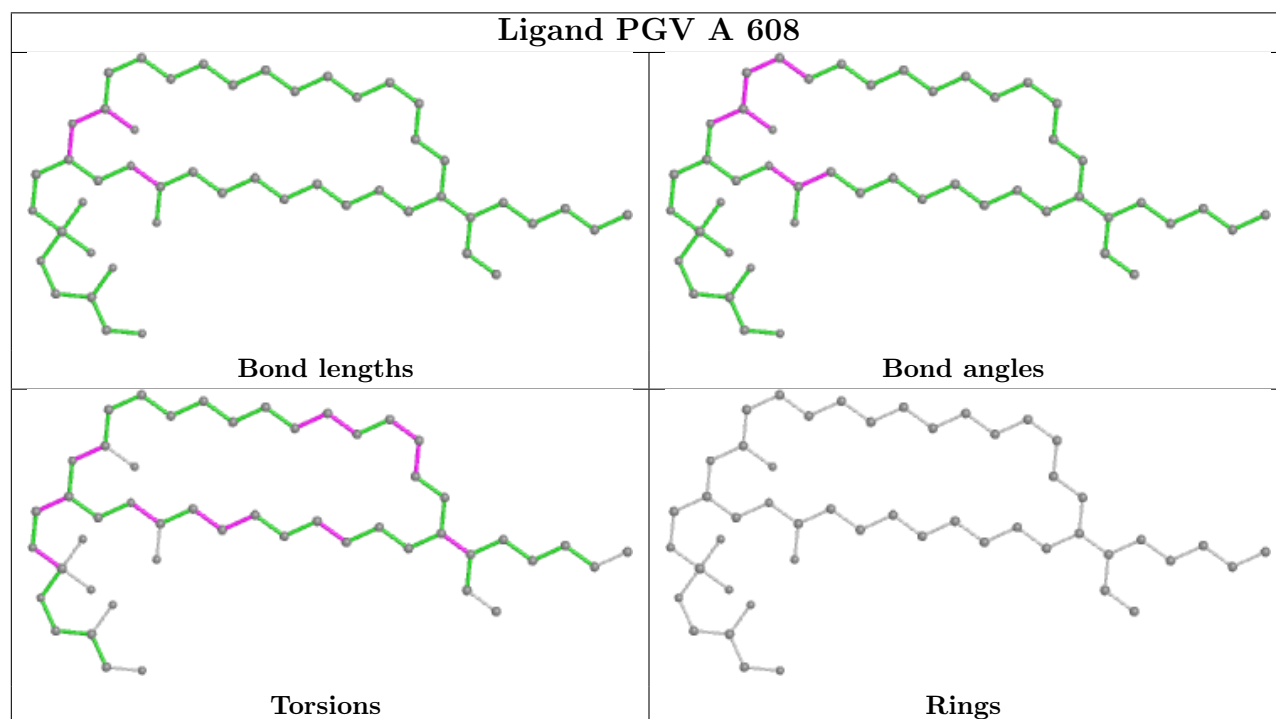
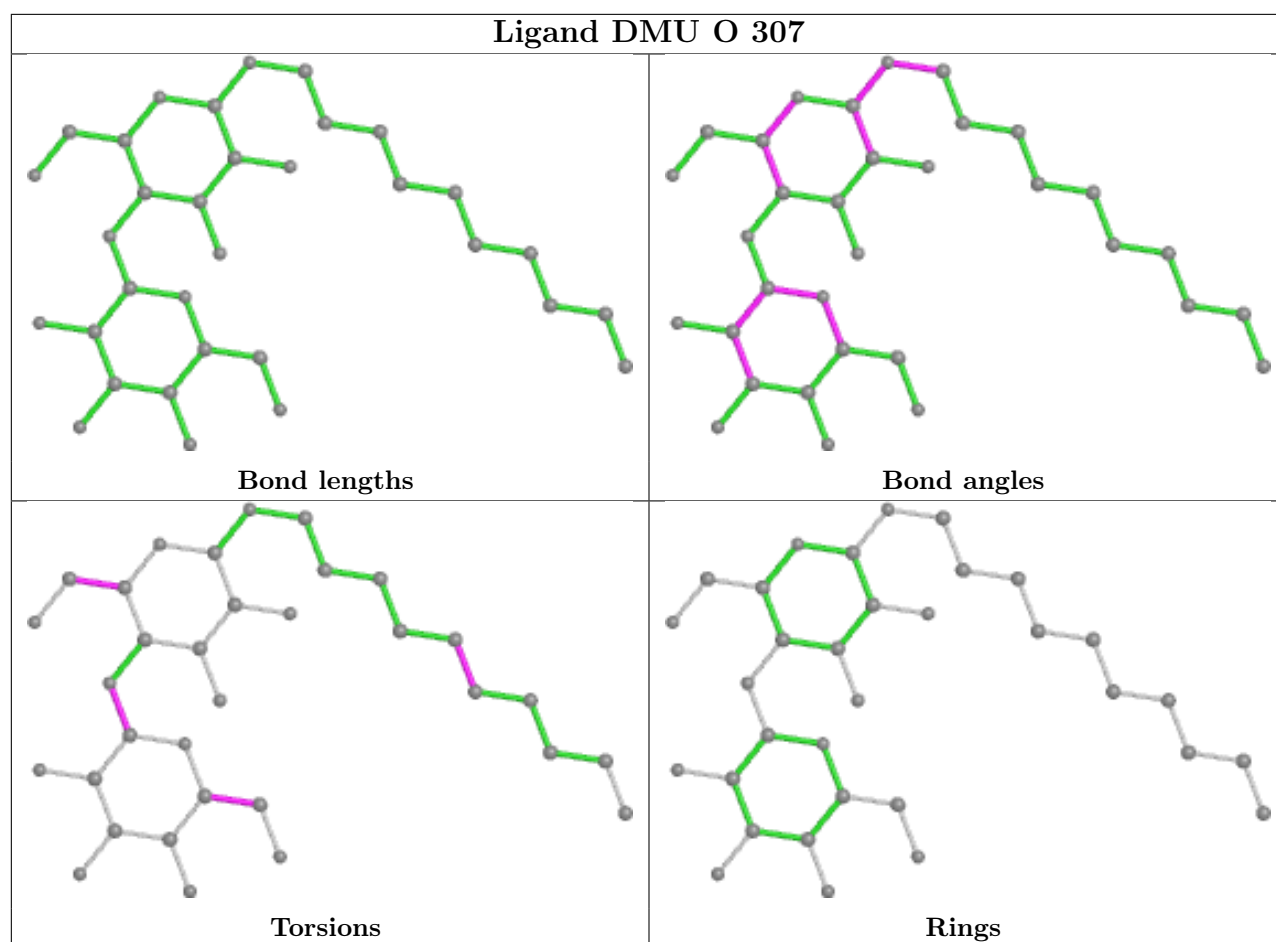


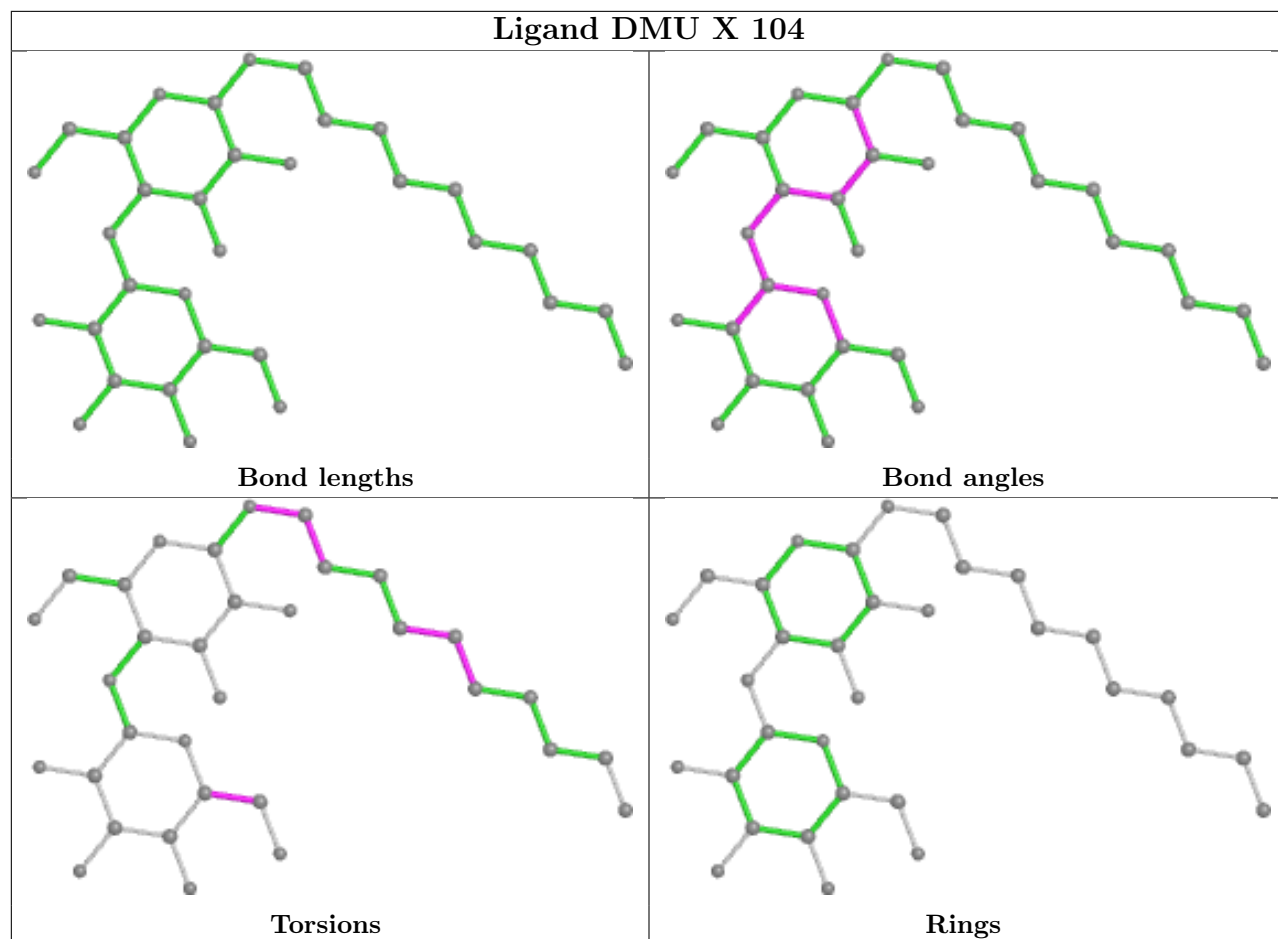


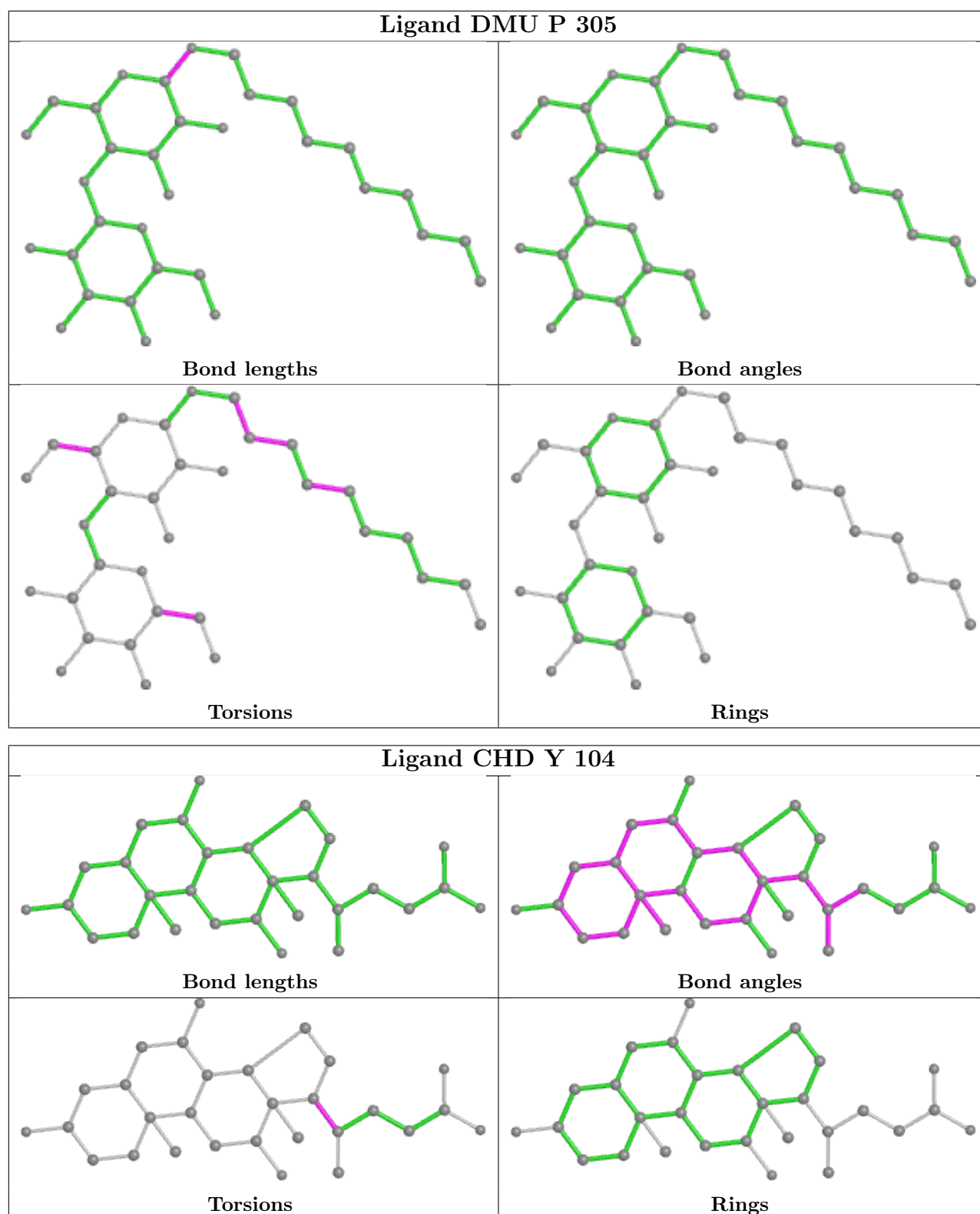


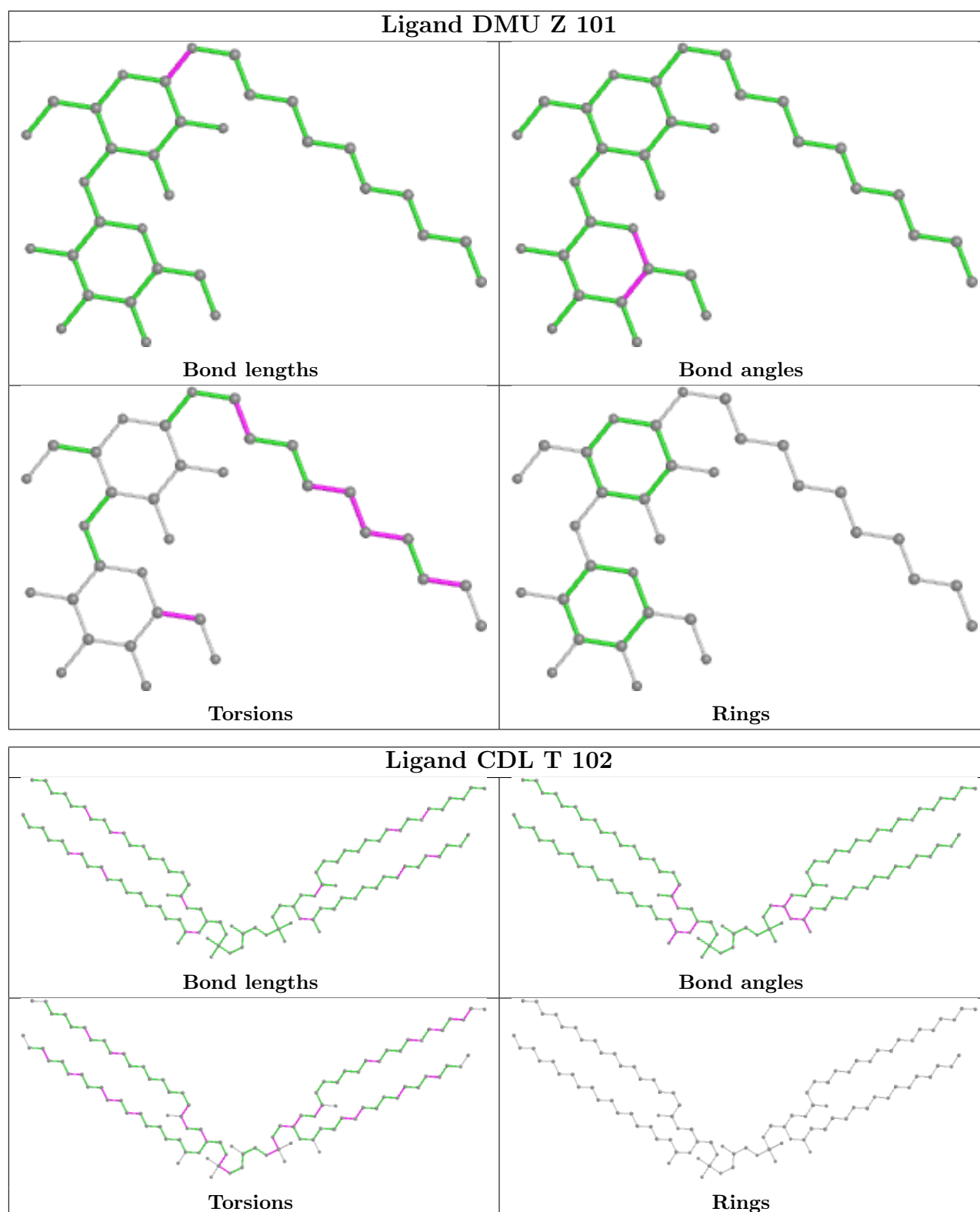




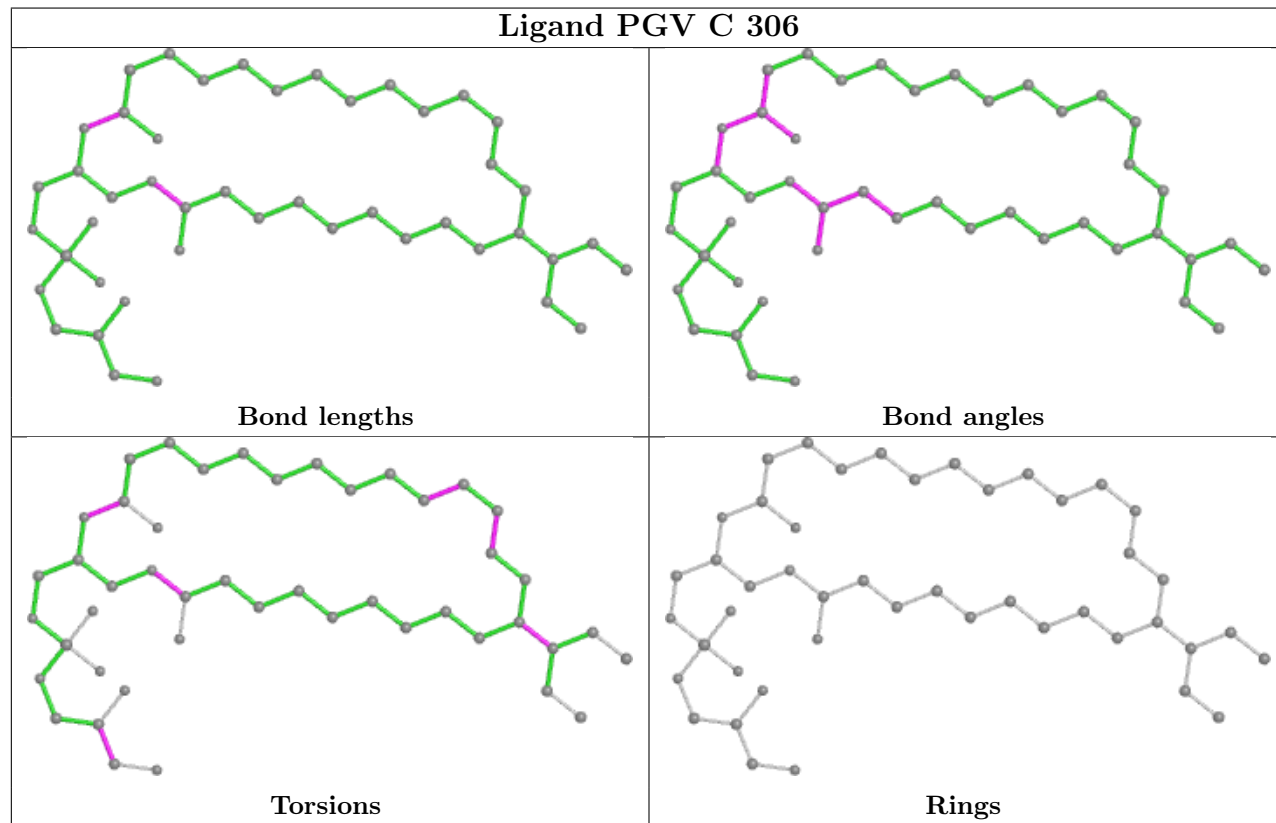
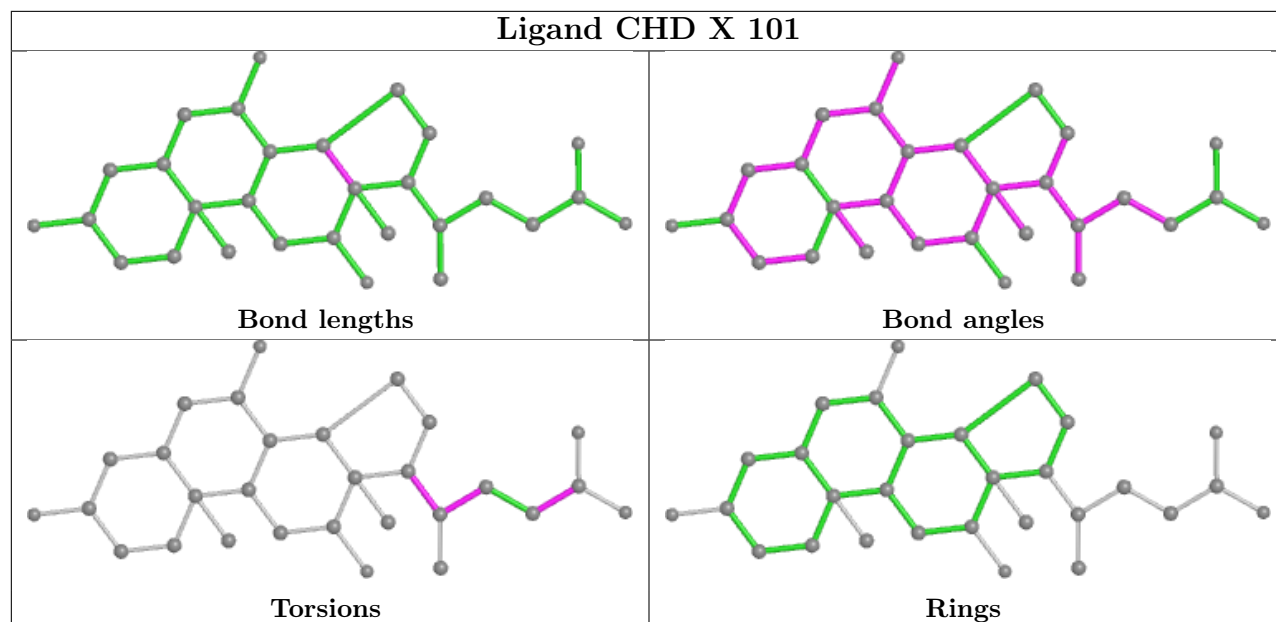




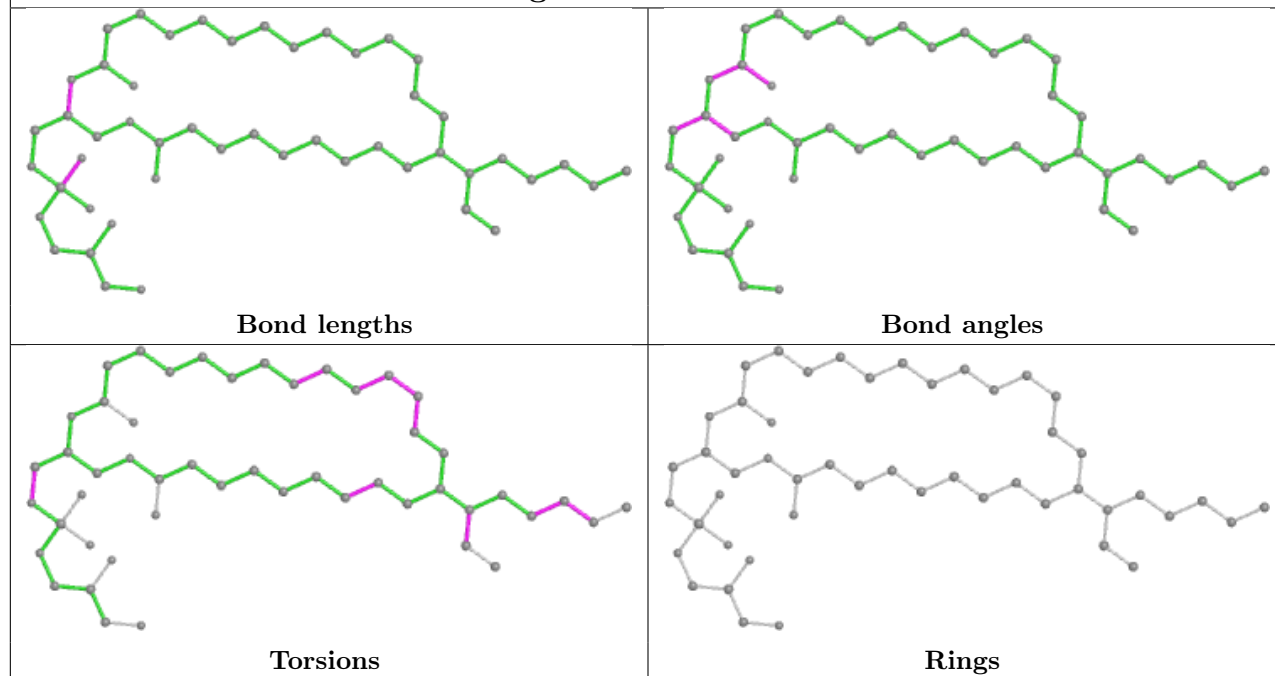




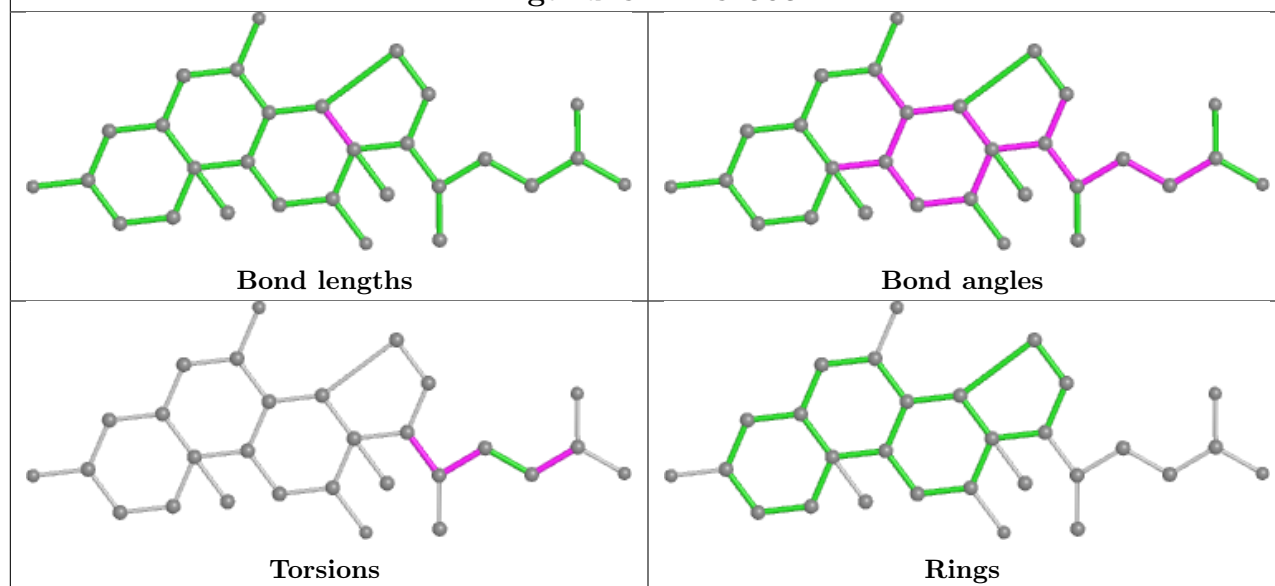


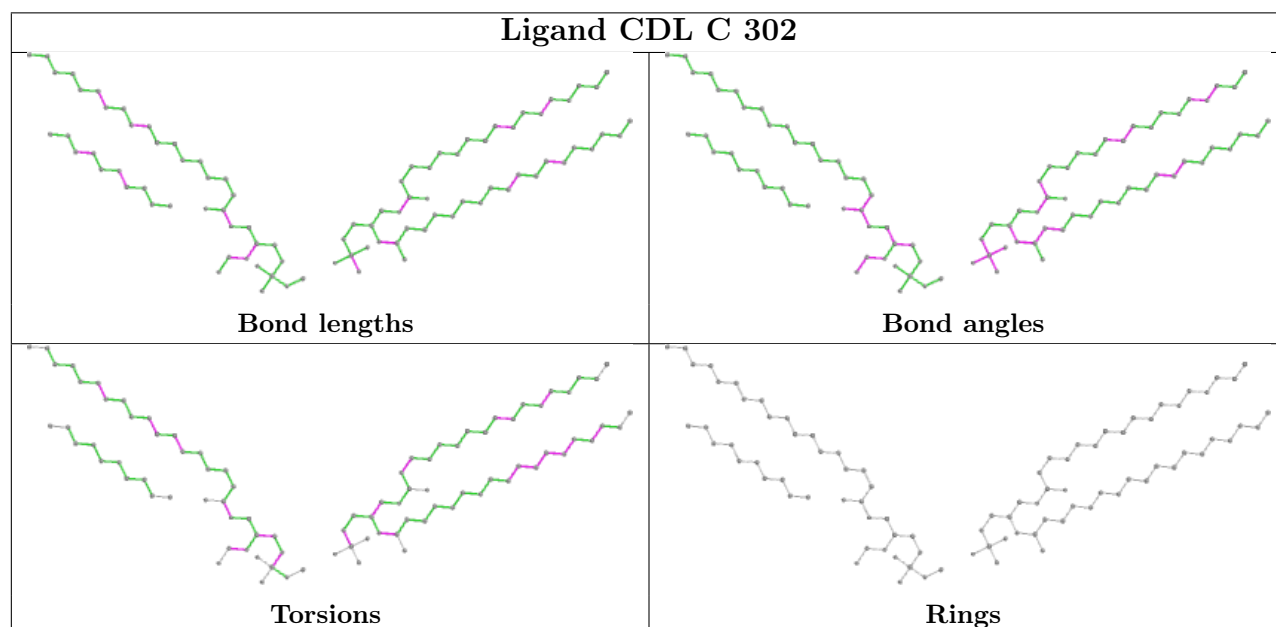
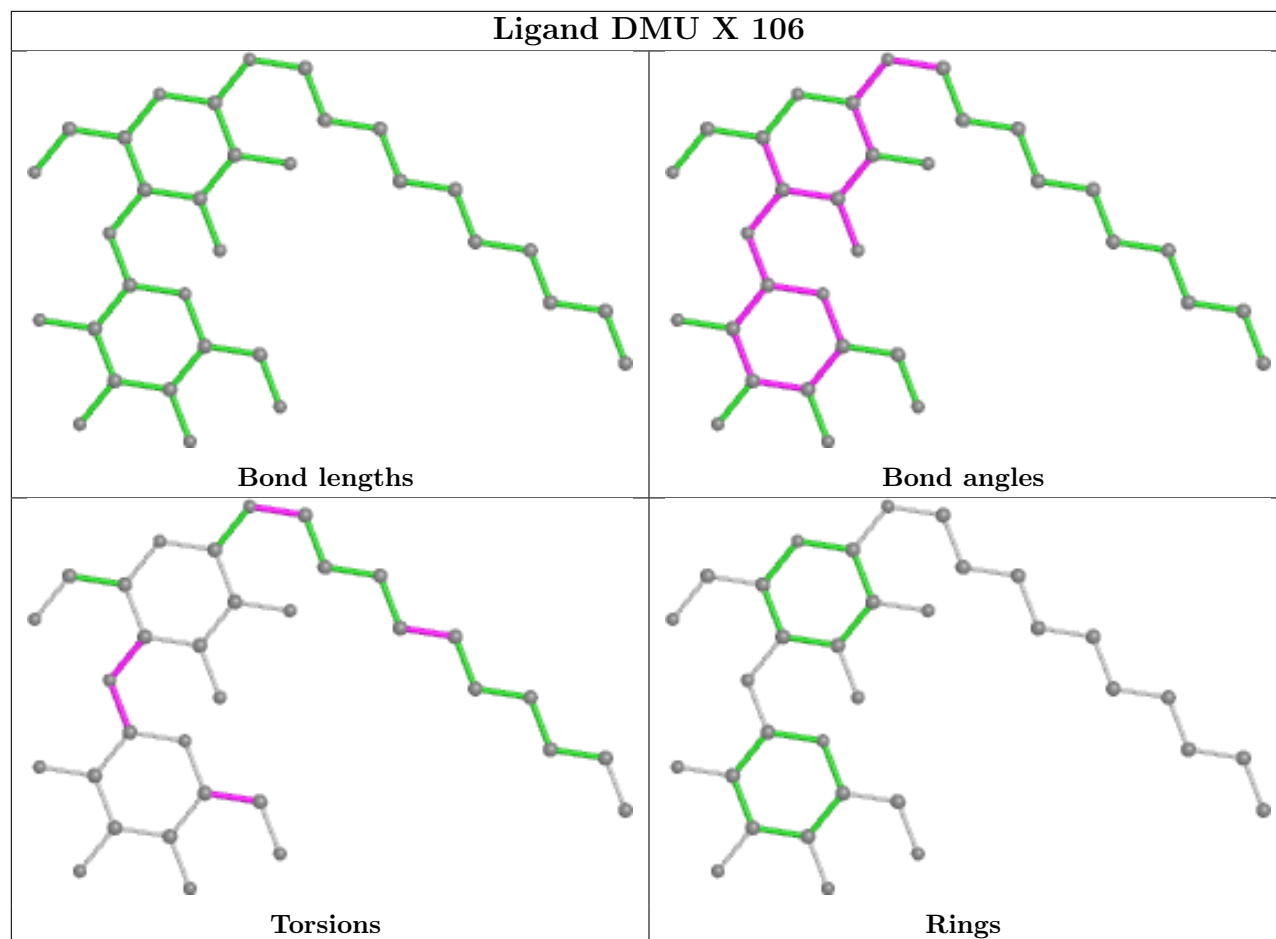


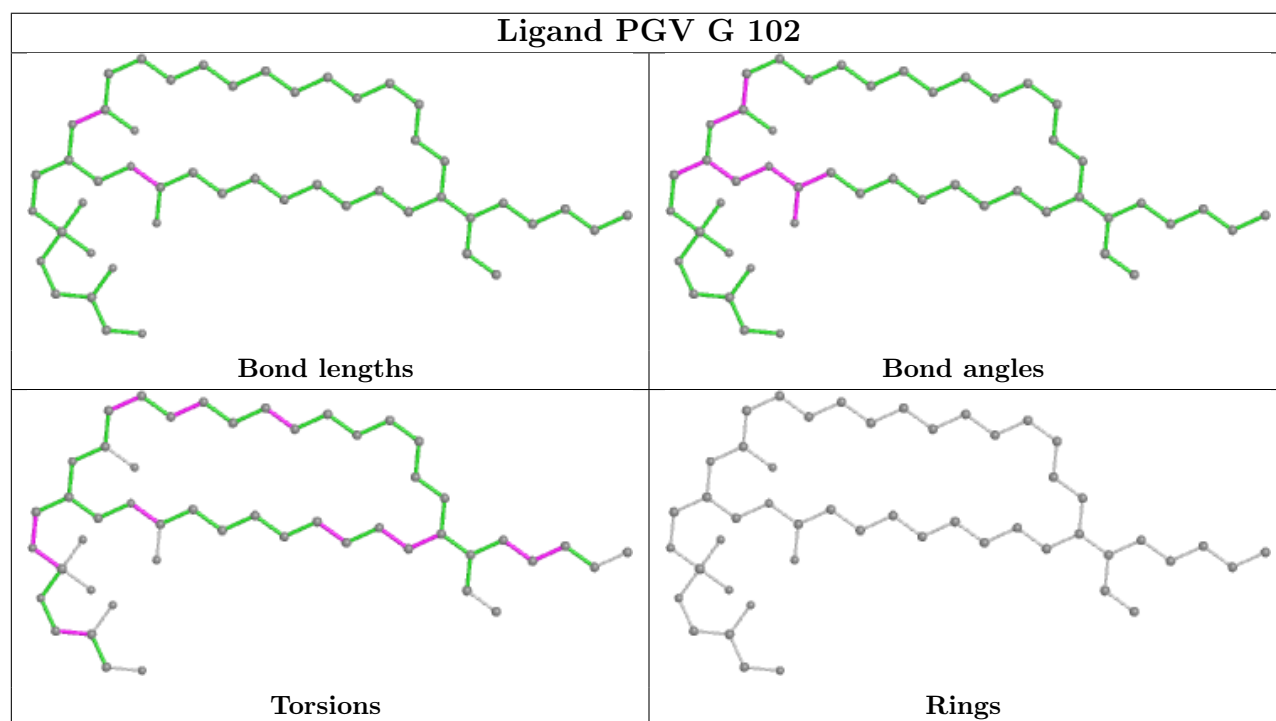
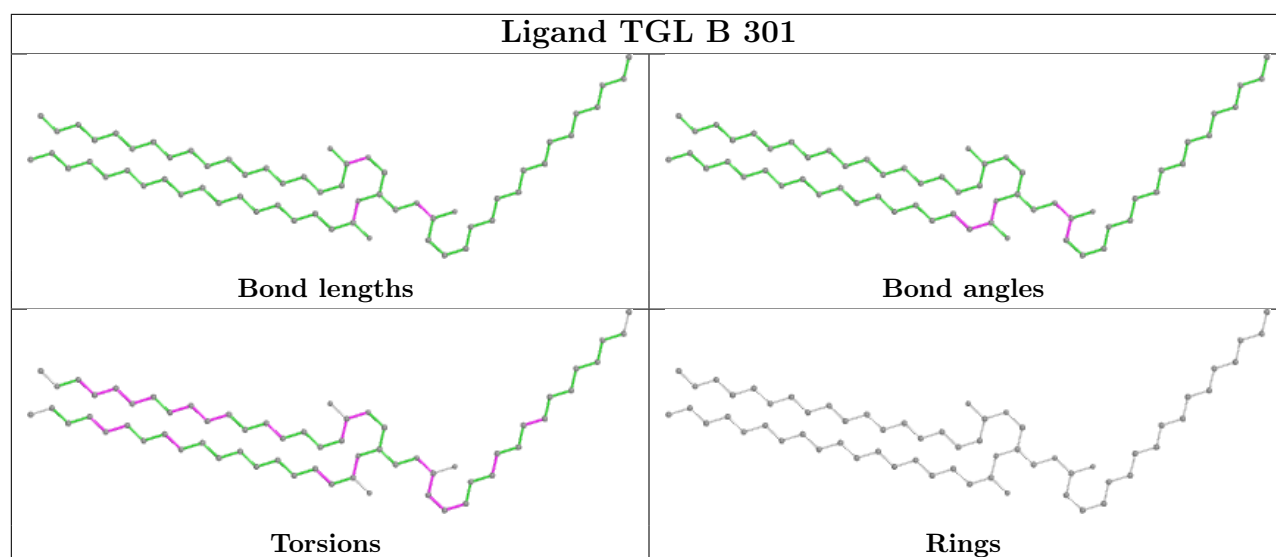
## Ligand PGV P 302

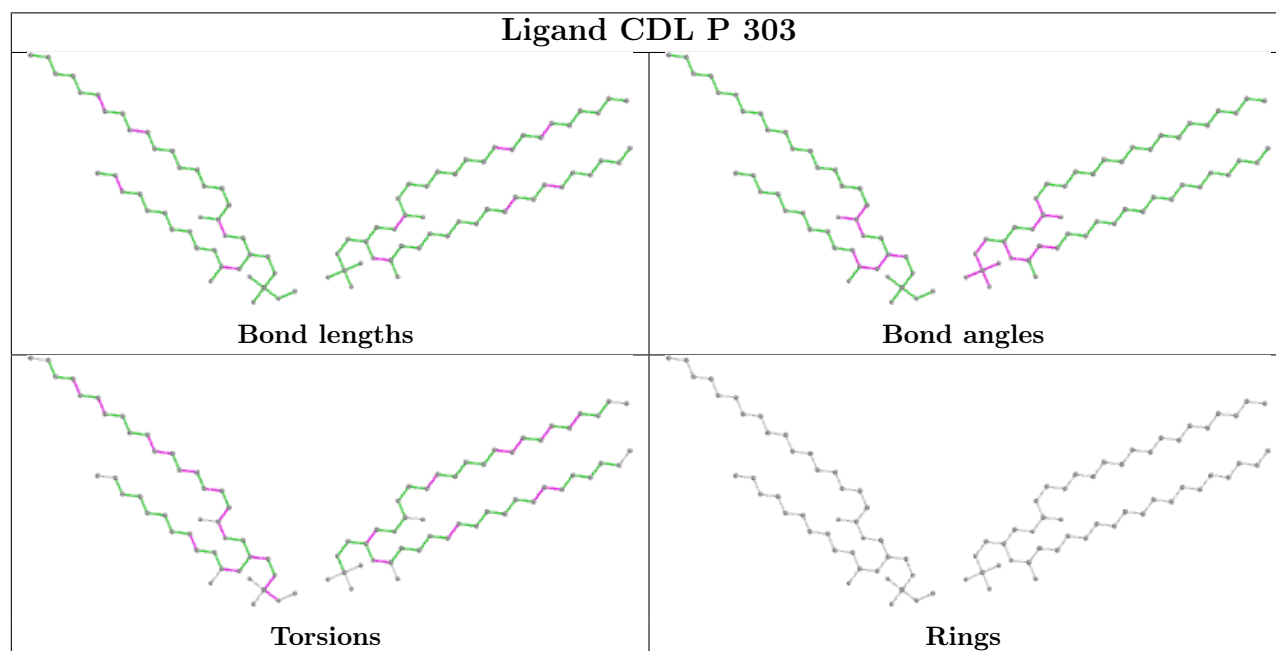
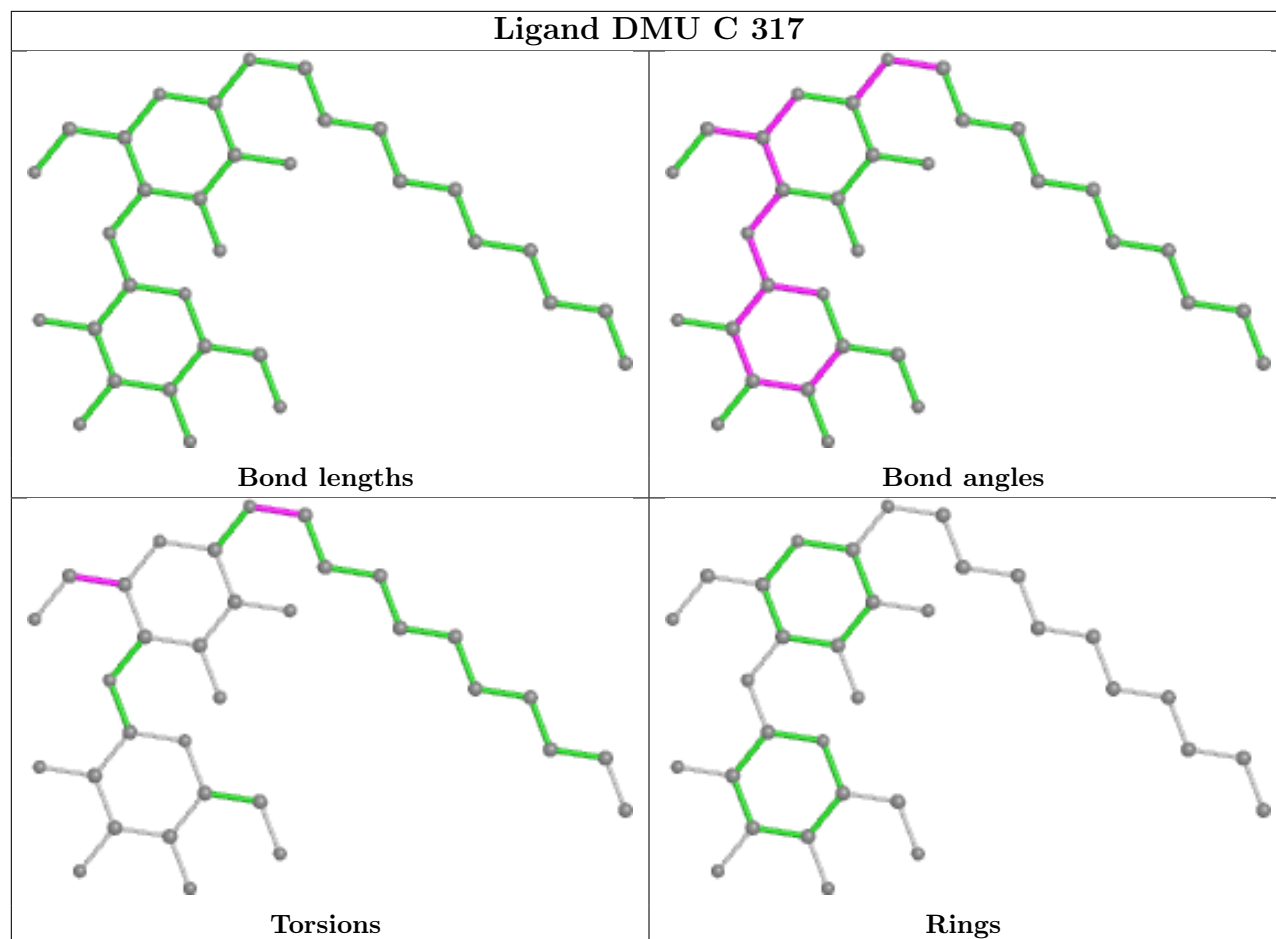


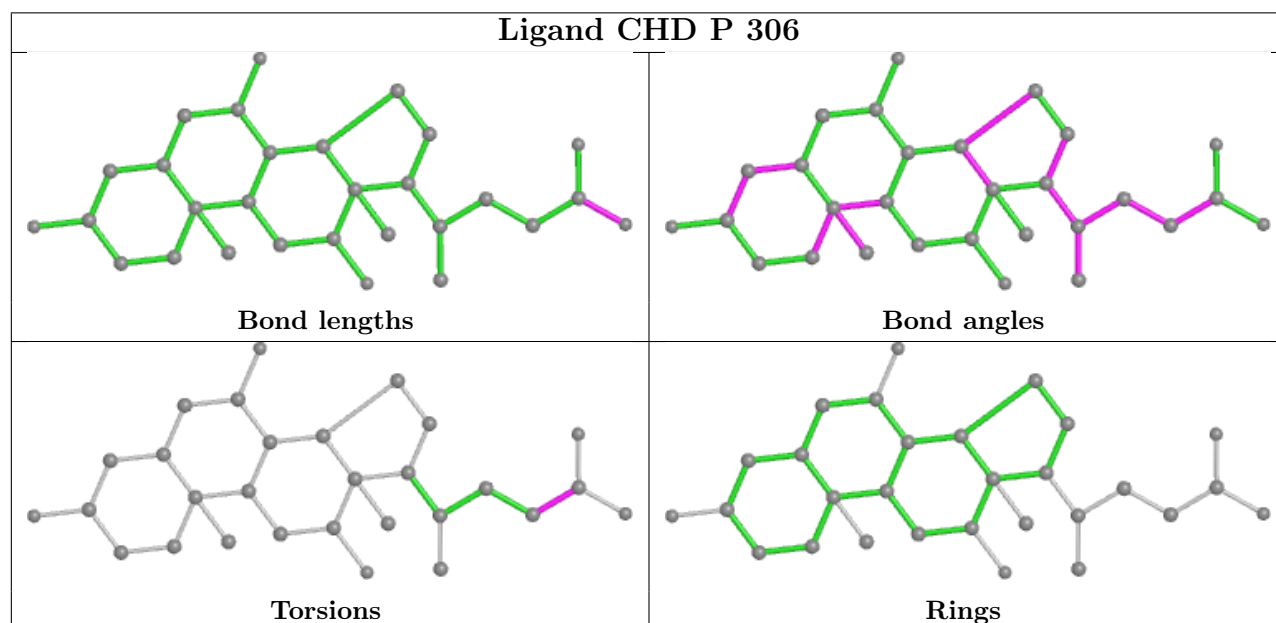
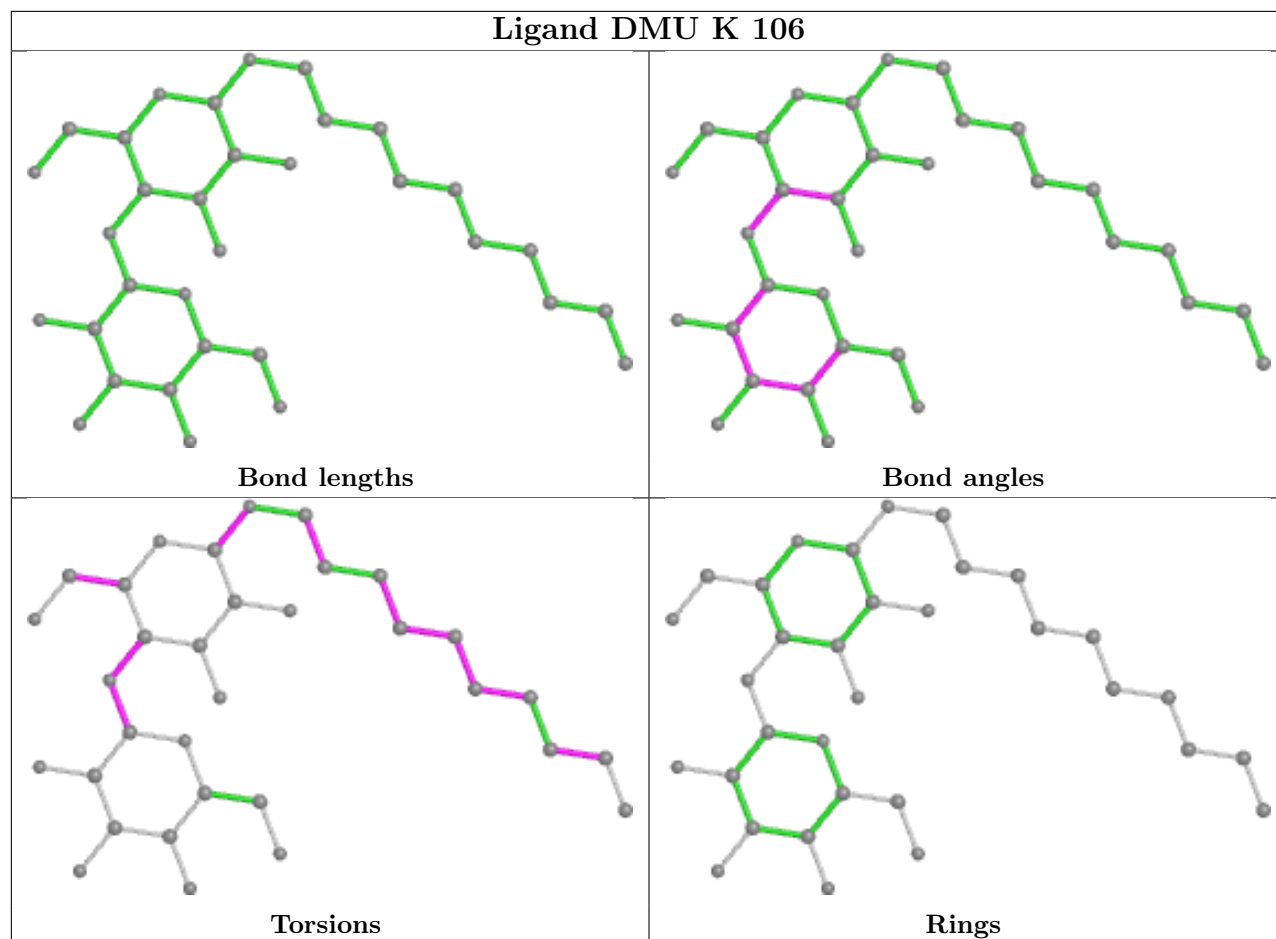
## Ligand CHD C 303

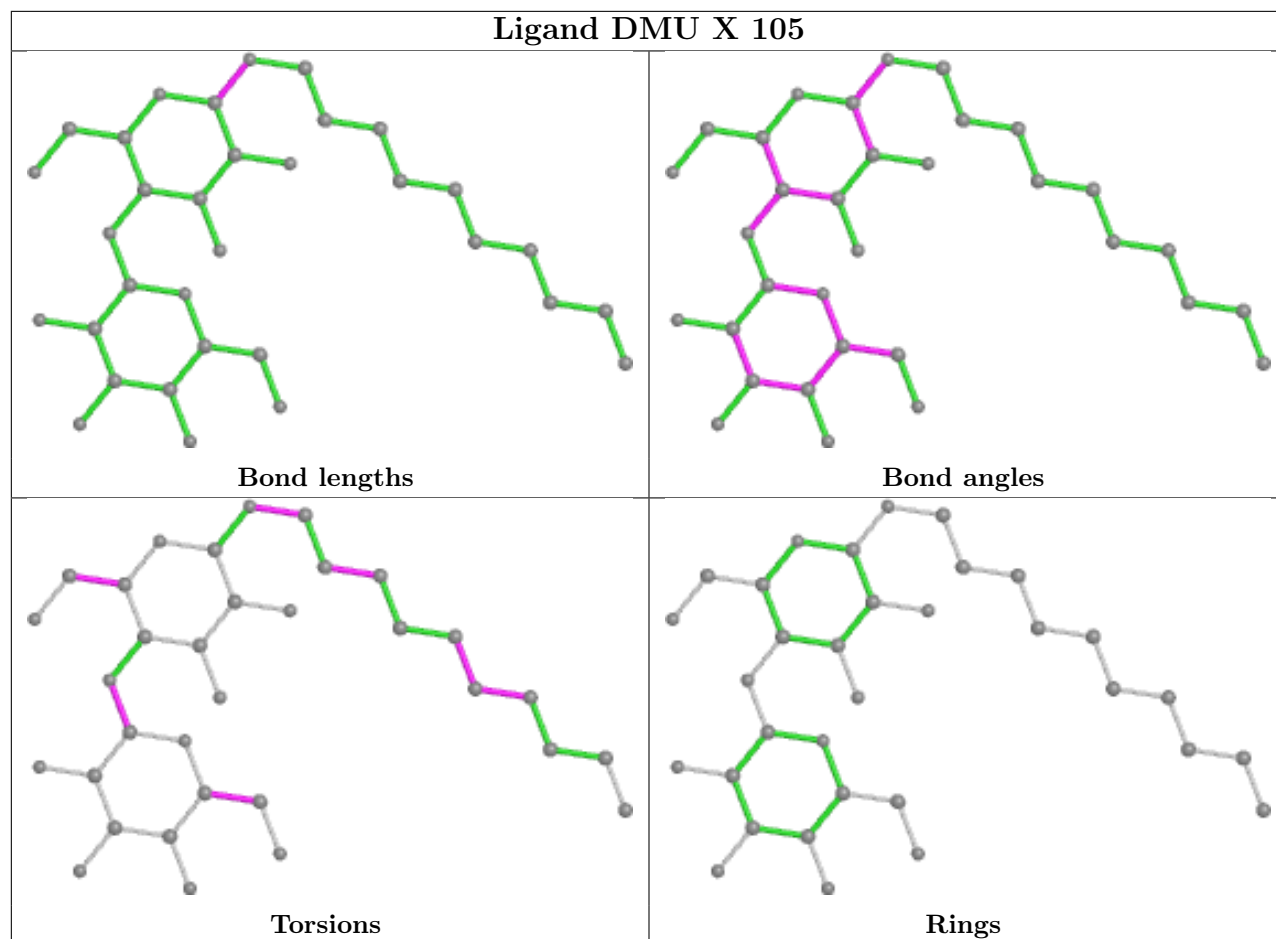


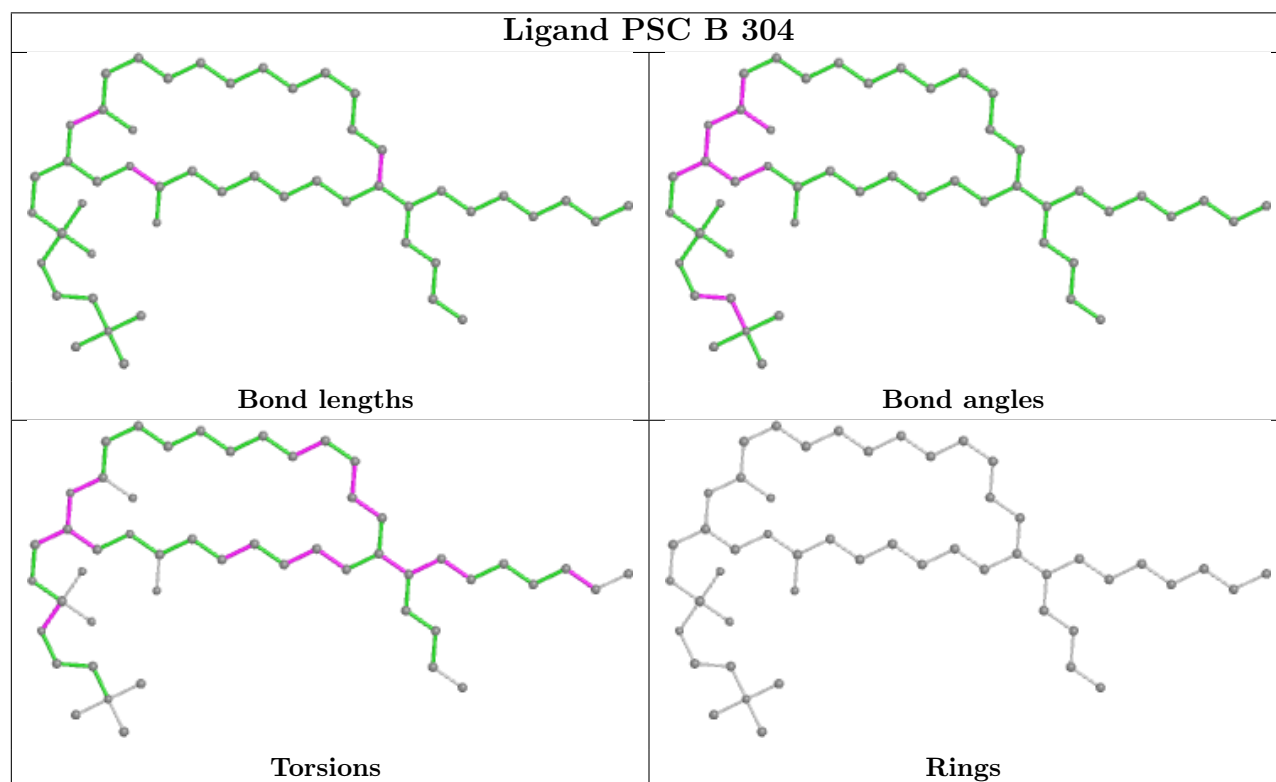
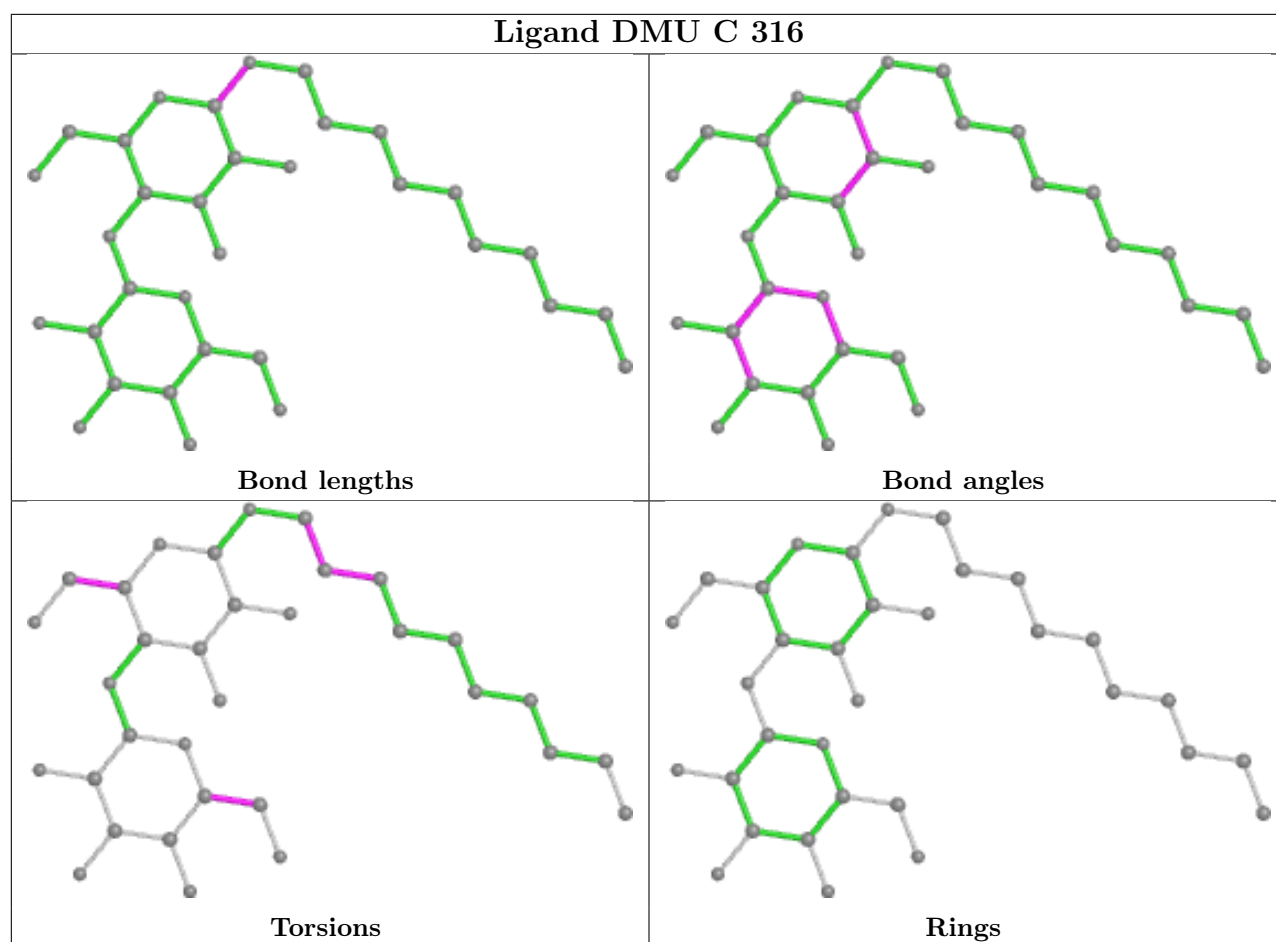














## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-0.33	1 (0%) 95 95	17, 21, 28, 84	0
1	N	513/514 (99%)	-0.32	1 (0%) 95 95	18, 25, 34, 70	0
2	B	226/227 (99%)	-0.34	3 (1%) 77 81	20, 28, 62, 117	0
2	O	226/227 (99%)	-0.33	4 (1%) 68 73	25, 33, 76, 138	0
3	C	259/261 (99%)	-0.68	0 100 100	19, 25, 40, 80	0
3	P	259/261 (99%)	-0.59	0 100 100	20, 26, 43, 111	0
4	D	144/147 (97%)	-0.67	1 (0%) 87 90	24, 30, 63, 106	0
4	Q	144/147 (97%)	0.41	9 (6%) 20 21	30, 46, 115, 259	0
5	E	105/109 (96%)	-0.63	1 (0%) 82 85	23, 30, 72, 157	0
5	R	105/109 (96%)	-0.19	2 (1%) 66 71	26, 38, 81, 173	0
6	F	98/98 (100%)	-0.06	6 (6%) 21 23	21, 31, 118, 176	0
6	S	98/98 (100%)	-0.25	8 (8%) 11 12	22, 31, 114, 172	0
7	G	83/85 (97%)	0.75	17 (20%) 1 1	24, 32, 135, 176	0
8	H	79/85 (92%)	-0.24	6 (7%) 13 14	24, 35, 133, 157	0
8	U	79/85 (92%)	-0.27	4 (5%) 28 30	31, 41, 166, 191	0
9	I	72/73 (98%)	0.24	5 (6%) 16 17	27, 42, 93, 119	0
9	V	72/73 (98%)	0.48	7 (9%) 7 8	27, 54, 130, 251	0
10	J	58/59 (98%)	0.27	3 (5%) 27 30	25, 35, 95, 145	0
10	W	58/59 (98%)	-0.12	3 (5%) 27 30	27, 37, 100, 186	0
11	K	49/56 (87%)	-0.32	0 100 100	27, 34, 65, 92	0
11	X	49/56 (87%)	0.98	9 (18%) 1 1	35, 46, 126, 135	0
12	L	46/47 (97%)	-0.66	0 100 100	22, 26, 58, 119	0
12	Y	46/47 (97%)	-0.60	1 (2%) 62 67	28, 34, 88, 160	0
13	M	43/46 (93%)	-0.28	3 (6%) 16 17	23, 27, 91, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	Z	43/46 (93%)	-0.05	2 (4%) 31 34	31, 37, 118, 255	0
14	T	84/85 (98%)	0.70	17 (20%) 1 1	23, 36, 145, 257	0
All	All	3551/3614 (98%)	-0.24	113 (3%) 47 52	17, 29, 86, 259	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	18.8
4	Q	5	VAL	15.7
14	T	8	HIS	14.4
4	Q	4	SER	13.2
7	G	3	ALA	10.9

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	0.66	0.63	336,360,399,412	0
7	TPO	G	11	11/12	0.73	0.25	82,115,176,188	0
9	SAC	I	1	9/10	0.81	0.19	111,135,185,189	0
1	FME	N	1	10/11	0.94	0.11	34,39,109,122	0
1	FME	A	1	10/11	0.96	0.09	32,41,86,119	0
2	FME	B	1	10/11	0.96	0.06	25,26,35,139	0
2	FME	O	1	10/11	0.97	0.06	33,34,48,155	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
23	DMU	X	106	33/33	0.11	0.69	70,86,93,94	0
23	DMU	C	318	33/33	0.20	0.35	54,98,133,144	0
23	DMU	X	102	33/33	0.28	0.49	43,111,135,146	0
23	DMU	K	106	33/33	0.31	0.62	45,112,131,135	0
23	DMU	K	104	33/33	0.33	0.54	39,109,133,136	0
23	DMU	X	105	33/33	0.37	0.66	54,113,130,144	0
22	EDO	P	311	4/4	0.40	0.26	70,73,76,82	0
23	DMU	K	102	33/33	0.44	0.49	54,109,126,129	0
23	DMU	A	628	33/33	0.46	0.61	66,104,128,132	0
23	DMU	K	101	33/33	0.46	0.42	37,115,128,133	0
23	DMU	X	107	33/33	0.47	0.73	68,119,135,145	0
23	DMU	P	314	33/33	0.54	0.28	48,96,128,144	0
23	DMU	X	103	33/33	0.55	0.48	63,102,135,139	0
22	EDO	J	103	4/4	0.58	0.53	63,82,84,128	0
23	DMU	C	316	33/33	0.59	0.37	51,103,124,128	0
23	DMU	D	206	33/33	0.60	0.37	56,126,197,214	0
23	DMU	O	307	33/33	0.60	0.33	44,104,142,148	0
23	DMU	C	317	33/33	0.62	0.37	47,96,125,129	0
22	EDO	A	623	4/4	0.62	0.20	44,48,56,69	0
22	EDO	B	309	4/4	0.63	0.16	49,62,73,76	0
23	DMU	K	105	33/33	0.63	0.40	56,93,126,128	0
22	EDO	G	105	4/4	0.64	0.26	56,81,84,93	0
23	DMU	I	101	33/33	0.64	0.40	49,114,130,139	0
25	CHD	X	101	29/29	0.64	0.55	50,92,112,115	0
23	DMU	K	103	32/33	0.65	0.30	48,98,121,134	0
28	PEK	T	101	50/53	0.65	0.28	40,82,148,188	0
22	EDO	V	101	4/4	0.66	0.12	71,76,82,83	0
26	PSC	B	304	52/52	0.67	0.32	39,97,184,225	0
23	DMU	P	315	33/33	0.68	0.31	52,102,118,126	0
22	EDO	A	610	4/4	0.69	0.24	49,66,66,70	0
22	EDO	A	627	4/4	0.69	0.14	64,66,68,74	0
22	EDO	A	622	4/4	0.69	0.43	35,67,74,77	0
22	EDO	S	107	4/4	0.69	0.27	49,64,69,79	0
23	DMU	L	105	33/33	0.70	0.34	51,103,129,133	0
23	DMU	X	104	33/33	0.70	0.36	50,95,122,127	0
22	EDO	A	619	4/4	0.71	0.18	47,51,53,59	0
27	CDL	T	102	98/100	0.72	0.28	42,92,166,203	0
27	CDL	G	101	100/100	0.73	0.33	47,95,178,197	0
22	EDO	D	203	4/4	0.73	0.15	38,53,58,65	0
20	PGV	G	102	51/51	0.73	0.26	42,82,161,206	0
28	PEK	C	309	53/53	0.74	0.27	45,85,184,201	0
22	EDO	G	103	4/4	0.75	0.12	44,61,76,77	0
25	CHD	P	304	29/29	0.75	0.36	56,105,138,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	N	615	4/4	0.76	0.17	46,50,57,62	0
28	PEK	C	305	53/53	0.77	0.23	36,78,161,193	0
25	CHD	Y	104	29/29	0.77	0.35	62,82,119,131	0
22	EDO	P	313	4/4	0.77	0.17	45,52,65,81	0
23	DMU	P	305	33/33	0.78	0.23	36,92,151,168	0
21	TGL	Y	101	63/63	0.79	0.22	38,64,124,183	0
23	DMU	C	308	33/33	0.79	0.26	30,79,126,143	0
28	PEK	P	301	53/53	0.79	0.26	46,85,150,179	0
22	EDO	D	205	4/4	0.79	0.17	37,40,64,65	0
22	EDO	F	106	4/4	0.80	0.09	64,66,70,74	0
25	CHD	C	303	29/29	0.80	0.36	51,96,140,144	0
21	TGL	Q	202	63/63	0.80	0.18	43,73,114,139	0
20	PGV	A	608	51/51	0.81	0.23	29,85,159,205	0
22	EDO	N	622	4/4	0.81	0.16	29,44,59,66	0
22	EDO	O	305	4/4	0.81	0.16	70,74,76,81	0
21	TGL	D	201	62/63	0.81	0.17	30,64,107,130	0
25	CHD	L	104	29/29	0.81	0.32	53,80,105,110	0
22	EDO	C	315	4/4	0.82	0.12	30,37,45,49	0
22	EDO	C	313	4/4	0.83	0.24	30,75,75,75	0
22	EDO	Q	204	4/4	0.83	0.12	46,46,50,51	0
22	EDO	A	617	4/4	0.83	0.15	43,49,54,71	0
22	EDO	D	202	4/4	0.83	0.26	49,51,56,63	0
22	EDO	N	611	4/4	0.83	0.19	68,74,75,75	0
20	PGV	C	306	48/51	0.84	0.21	40,80,142,210	0
21	TGL	B	301	62/63	0.84	0.17	34,64,100,116	0
26	PSC	O	304	51/52	0.84	0.25	37,81,202,224	0
27	CDL	P	303	90/100	0.85	0.24	29,74,149,171	0
22	EDO	L	101	4/4	0.85	0.12	38,47,54,86	0
23	DMU	M	101	33/33	0.85	0.15	33,39,51,57	0
22	EDO	N	609	4/4	0.85	0.16	30,34,65,68	0
20	PGV	Q	201	51/51	0.85	0.28	43,84,152,180	0
21	TGL	A	609	63/63	0.85	0.20	29,58,121,168	0
22	EDO	P	309	4/4	0.86	0.12	53,53,68,78	0
23	DMU	Z	101	33/33	0.86	0.16	40,48,69,88	0
22	EDO	N	623	4/4	0.86	0.12	42,45,77,80	0
22	EDO	T	105	4/4	0.86	0.18	46,53,71,82	0
27	CDL	C	302	89/100	0.86	0.29	26,75,138,150	0
22	EDO	M	103	4/4	0.86	0.08	60,63,64,69	0
21	TGL	O	301	60/63	0.87	0.24	39,76,110,133	0
22	EDO	S	105	4/4	0.88	0.09	37,39,45,49	0
22	EDO	J	101	4/4	0.89	0.18	47,48,64,103	0
22	EDO	N	610	4/4	0.89	0.20	31,43,72,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	C	312	4/4	0.89	0.27	37,55,60,90	0
22	EDO	N	608	4/4	0.89	0.15	39,49,72,73	0
22	EDO	N	618	4/4	0.90	0.12	29,38,46,52	0
25	CHD	P	306	29/29	0.90	0.07	25,28,33,33	0
22	EDO	Z	102	4/4	0.90	0.14	56,70,88,122	0
22	EDO	N	620	4/4	0.90	0.25	69,70,73,82	0
22	EDO	A	611	4/4	0.90	0.11	31,35,41,74	0
22	EDO	E	203	4/4	0.90	0.08	41,44,47,49	0
22	EDO	T	106	4/4	0.90	0.19	49,59,61,88	0
22	EDO	D	204	4/4	0.91	0.09	40,40,52,55	0
22	EDO	F	107	4/4	0.91	0.11	31,33,47,51	0
22	EDO	H	101	4/4	0.91	0.17	35,36,66,67	0
22	EDO	L	103	4/4	0.91	0.09	51,55,61,62	0
22	EDO	Q	203	4/4	0.91	0.12	34,39,41,41	0
22	EDO	Y	102	4/4	0.91	0.12	46,57,75,94	0
22	EDO	M	102	4/4	0.91	0.15	52,63,72,77	0
25	CHD	C	304	29/29	0.92	0.07	25,27,33,35	0
22	EDO	S	108	4/4	0.92	0.17	38,42,52,77	0
22	EDO	A	615	4/4	0.92	0.16	31,32,72,74	0
22	EDO	S	104	4/4	0.92	0.12	29,35,37,39	0
22	EDO	A	612	4/4	0.93	0.12	29,29,65,67	0
22	EDO	W	101	4/4	0.93	0.15	47,52,83,100	0
22	EDO	A	625	4/4	0.93	0.21	29,38,43,93	0
22	EDO	Y	103	4/4	0.93	0.06	50,51,52,64	0
22	EDO	N	619	4/4	0.93	0.08	34,37,41,42	0
22	EDO	C	314	4/4	0.93	0.23	36,58,63,109	0
22	EDO	G	104	4/4	0.93	0.06	29,31,34,34	0
22	EDO	N	614	4/4	0.93	0.07	33,33,34,35	0
22	EDO	B	308	4/4	0.94	0.09	35,39,49,69	0
22	EDO	J	105	4/4	0.94	0.23	36,48,53,55	0
22	EDO	A	613	4/4	0.94	0.15	32,42,71,78	0
22	EDO	P	308	4/4	0.94	0.08	28,34,37,44	0
22	EDO	T	103	4/4	0.94	0.09	36,39,41,55	0
22	EDO	L	102	4/4	0.94	0.14	40,69,74,95	0
22	EDO	A	624	4/4	0.94	0.16	26,28,36,46	0
22	EDO	P	312	4/4	0.94	0.09	47,48,62,84	0
19	PER	A	606	2/2	0.94	0.17	16,16,16,23	0
22	EDO	A	616	4/4	0.94	0.10	36,38,40,42	0
22	EDO	B	306	4/4	0.94	0.07	27,34,37,45	0
30	PO4	U	101	5/5	0.94	0.11	52,54,131,144	0
22	EDO	S	103	4/4	0.95	0.11	36,49,74,79	0
22	EDO	A	618	4/4	0.95	0.07	23,25,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	A	626	4/4	0.95	0.14	30,34,48,89	0
22	EDO	C	310	4/4	0.95	0.06	28,28,31,32	0
22	EDO	C	311	4/4	0.95	0.10	28,30,37,50	0
19	PER	N	606	2/2	0.95	0.19	19,19,19,26	0
22	EDO	B	305	4/4	0.95	0.10	36,44,62,83	0
22	EDO	J	102	4/4	0.95	0.26	43,57,69,78	0
22	EDO	F	102	4/4	0.95	0.11	32,34,35,40	0
22	EDO	J	104	4/4	0.95	0.19	35,48,75,79	0
22	EDO	F	104	4/4	0.95	0.21	38,41,64,89	0
22	EDO	N	617	4/4	0.95	0.08	33,40,41,53	0
22	EDO	A	620	4/4	0.95	0.10	28,37,38,46	0
22	EDO	R	201	4/4	0.95	0.08	34,36,38,43	0
30	PO4	H	102	5/5	0.95	0.17	56,58,101,148	0
25	CHD	O	303	29/29	0.95	0.06	22,25,29,37	0
18	NA	N	605	1/1	0.96	0.05	28,28,28,28	0
22	EDO	N	616	4/4	0.96	0.06	27,34,59,72	0
22	EDO	N	621	4/4	0.96	0.10	29,32,39,77	0
28	PEK	C	307	52/53	0.96	0.10	25,41,93,123	0
25	CHD	B	303	29/29	0.96	0.06	22,25,31,39	0
22	EDO	P	310	4/4	0.96	0.07	32,36,38,40	0
28	PEK	P	307	53/53	0.96	0.11	26,46,96,119	0
22	EDO	T	104	4/4	0.96	0.06	31,32,36,39	0
22	EDO	N	612	4/4	0.96	0.07	25,26,26,26	0
22	EDO	A	621	4/4	0.96	0.14	22,38,78,106	0
22	EDO	E	202	4/4	0.97	0.07	32,35,38,40	0
22	EDO	S	109	4/4	0.97	0.09	28,29,29,32	0
22	EDO	O	306	4/4	0.97	0.04	28,30,31,31	0
22	EDO	N	613	4/4	0.97	0.07	23,26,26,29	0
20	PGV	C	301	51/51	0.97	0.08	20,29,88,95	0
22	EDO	E	201	4/4	0.97	0.07	32,34,35,36	0
20	PGV	N	607	51/51	0.98	0.08	21,29,61,93	0
20	PGV	P	302	51/51	0.98	0.08	21,29,85,110	0
20	PGV	A	607	51/51	0.98	0.08	20,28,72,88	0
15	HEA	N	602	60/60	0.98	0.09	18,21,27,33	0
22	EDO	N	624	4/4	0.98	0.09	29,30,63,75	0
15	HEA	A	601[A]	60/60	0.98	0.08	16,19,32,41	9
22	EDO	S	102	4/4	0.98	0.06	22,22,22,23	0
15	HEA	A	601[B]	60/60	0.98	0.08	16,19,32,41	9
22	EDO	F	103	4/4	0.98	0.13	27,28,29,30	0
22	EDO	A	614	4/4	0.98	0.10	20,21,22,25	0
22	EDO	S	106	4/4	0.98	0.04	31,32,35,36	0
15	HEA	A	602	60/60	0.98	0.07	16,18,25,31	0

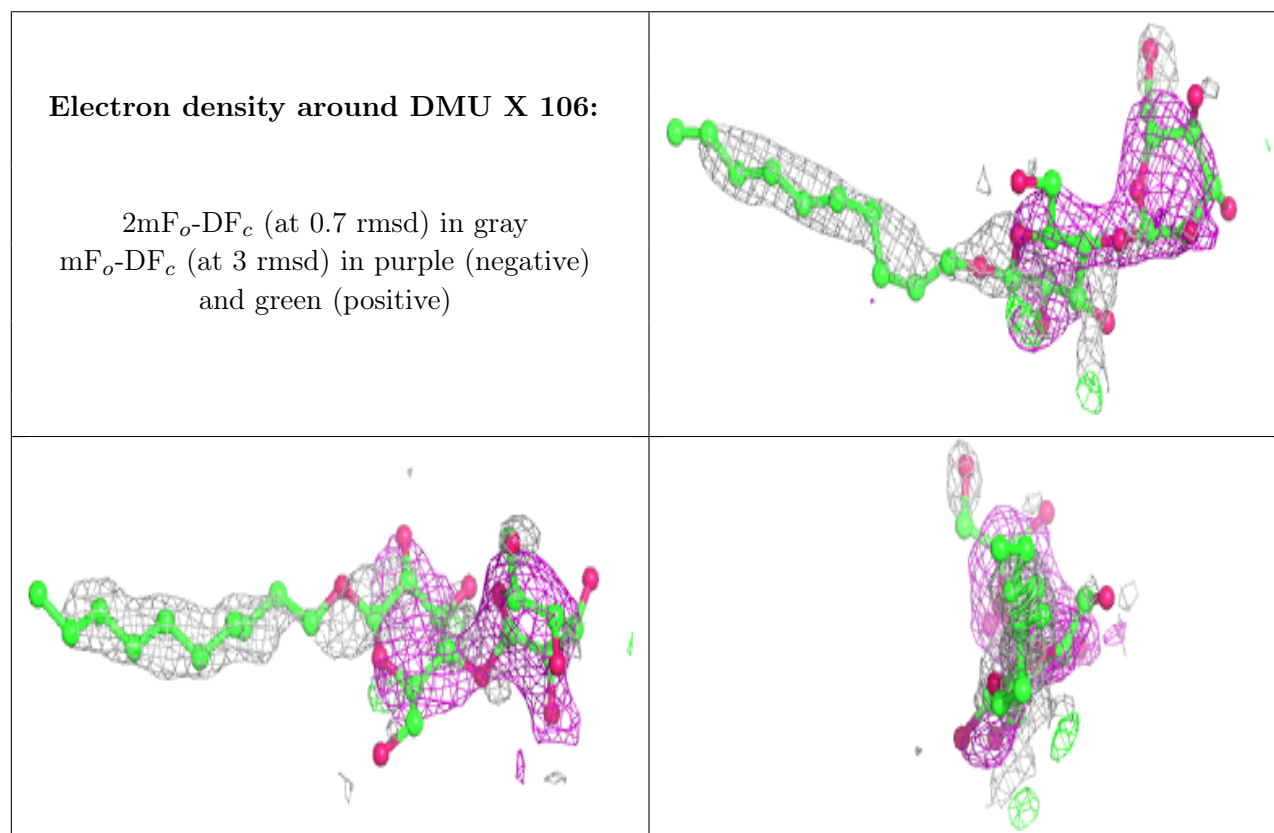
*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	CU	N	603	1/1	0.99	0.08	21,21,21,21	0
17	MG	A	604	1/1	0.99	0.03	19,19,19,19	0
17	MG	N	604	1/1	0.99	0.02	22,22,22,22	0
24	CUA	O	302	2/2	0.99	0.07	26,26,26,26	0
22	EDO	F	105	4/4	0.99	0.06	21,21,22,22	0
18	NA	A	605	1/1	0.99	0.03	22,22,22,22	0
15	HEA	N	601[B]	60/60	0.99	0.08	20,23,32,35	9
22	EDO	B	307	4/4	0.99	0.05	23,23,23,27	0
15	HEA	N	601[A]	60/60	0.99	0.08	20,23,38,41	9
29	ZN	F	101	1/1	1.00	0.03	25,25,25,25	0
29	ZN	S	101	1/1	1.00	0.04	25,25,25,25	0
16	CU	A	603	1/1	1.00	0.08	19,19,19,19	0
24	CUA	B	302	2/2	1.00	0.08	20,20,20,21	0

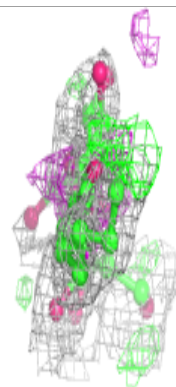
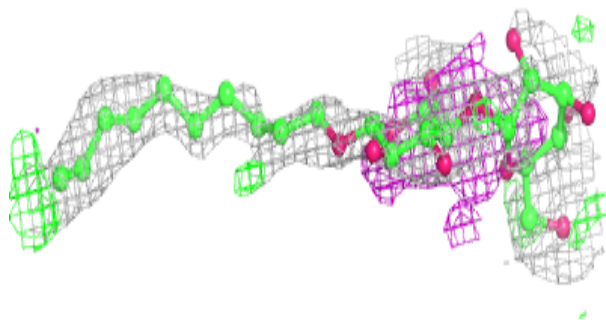
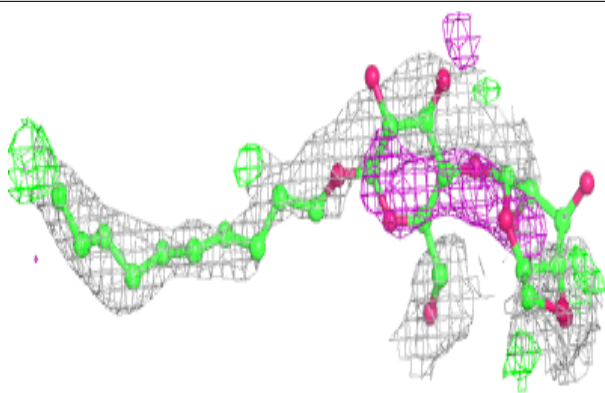
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



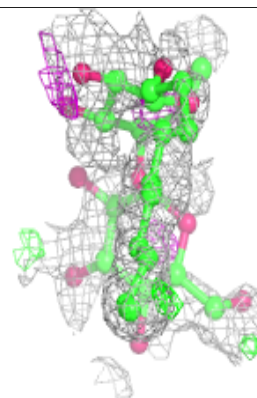
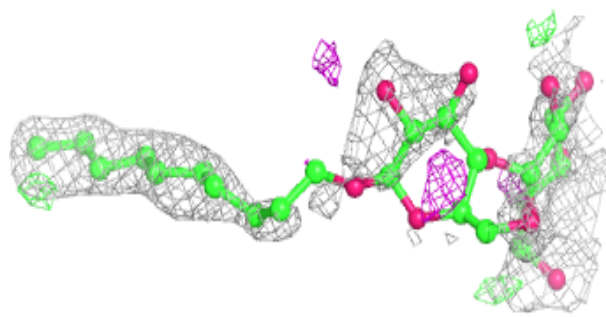
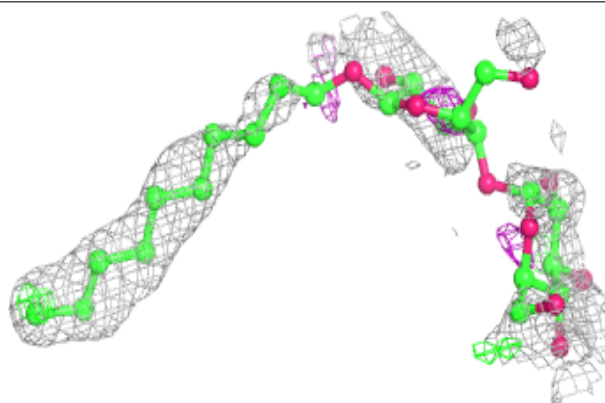


**Electron density around DMU C 318:**

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

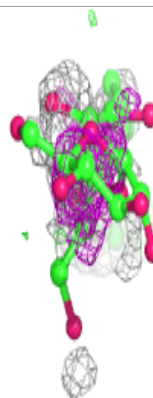
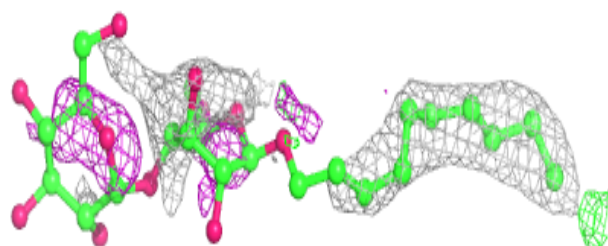
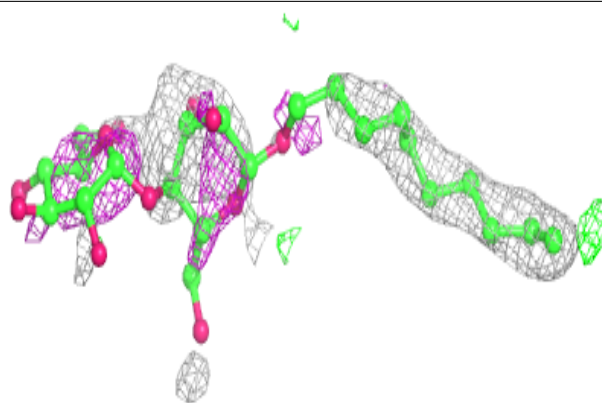
**Electron density around DMU X 102:**

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

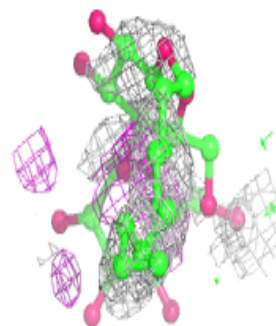
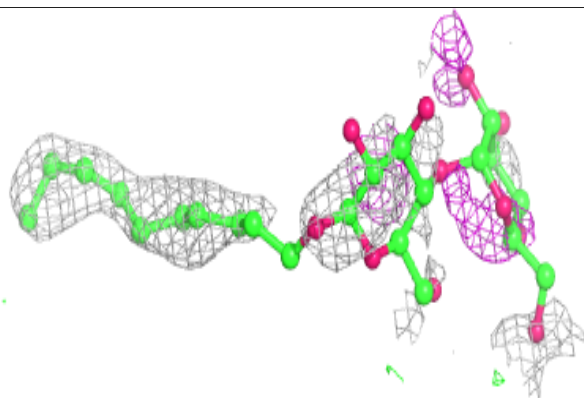
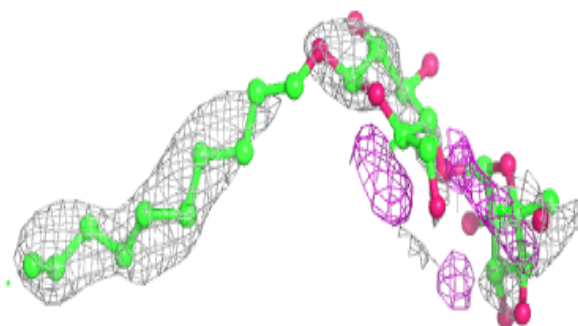


**Electron density around DMU K 106:**

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

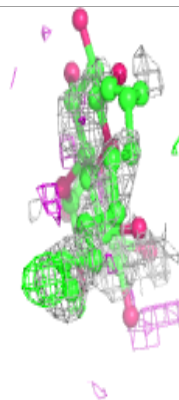
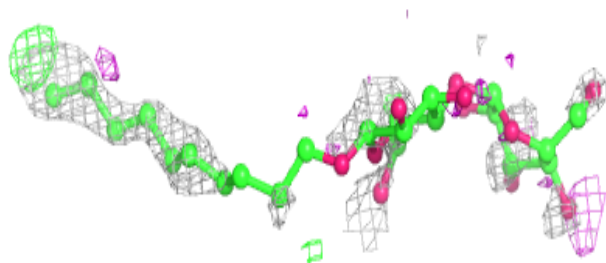
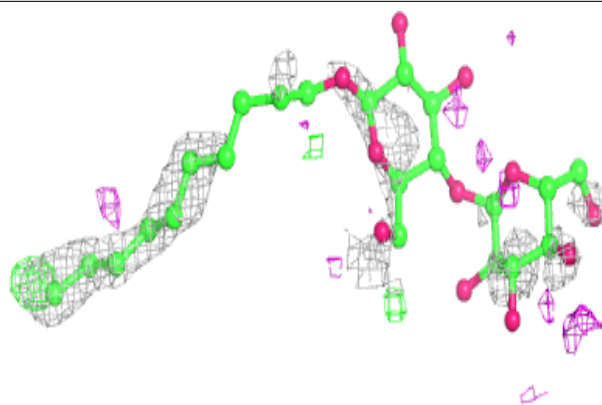
**Electron density around DMU K 104:**

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

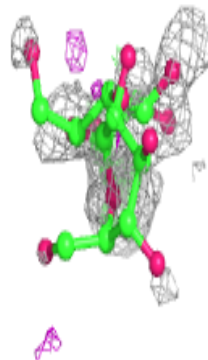
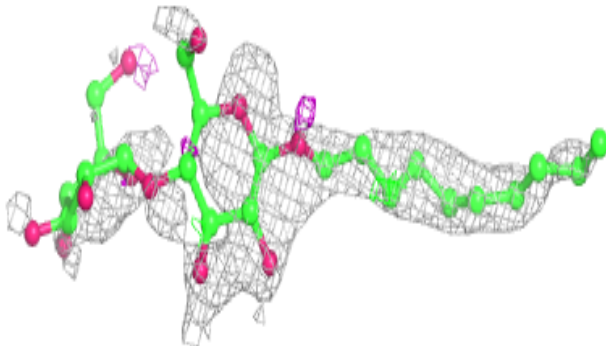
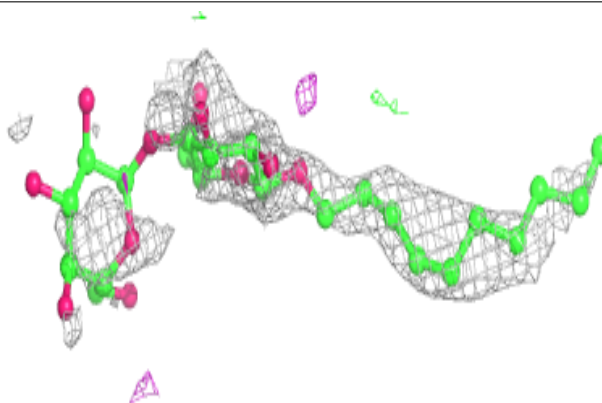


**Electron density around DMU X 105:**

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

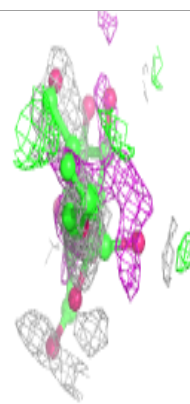
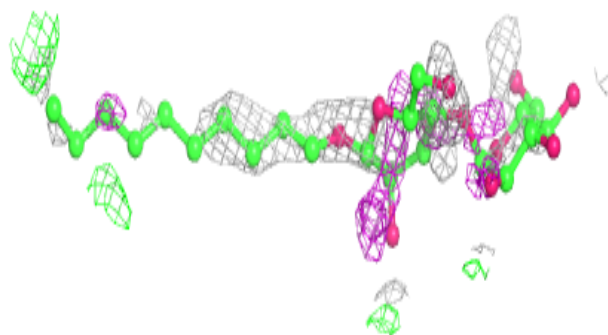
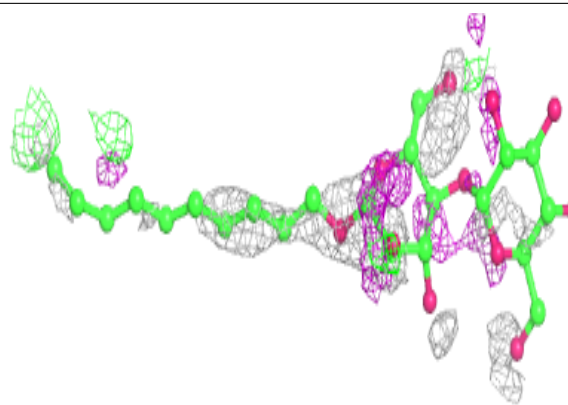
**Electron density around DMU K 102:**

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

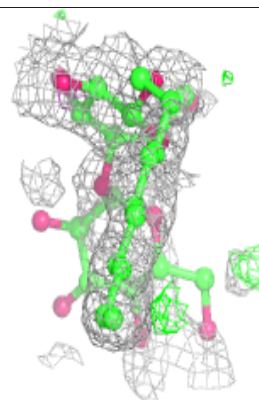
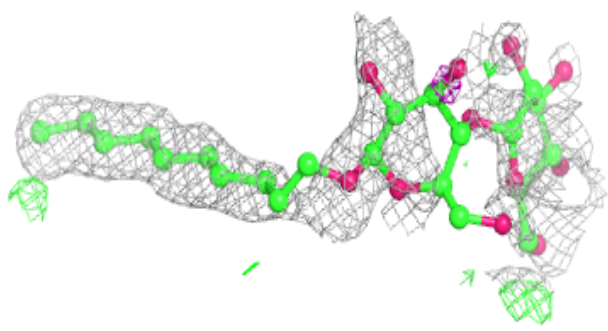
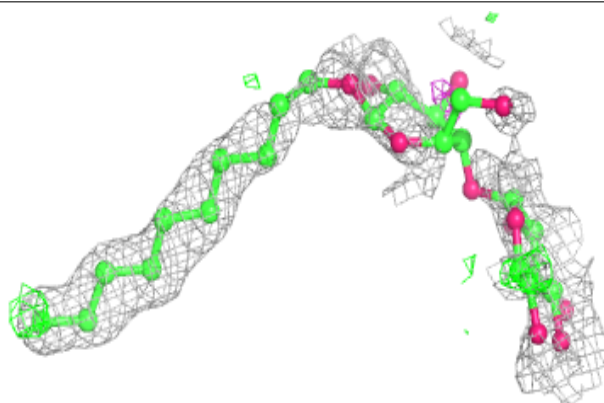


**Electron density around DMU A 628:**

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

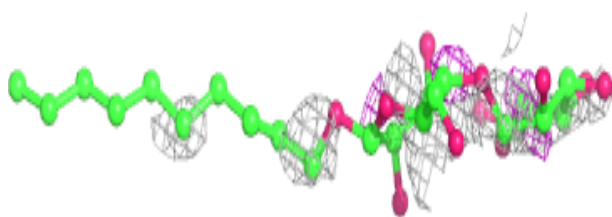
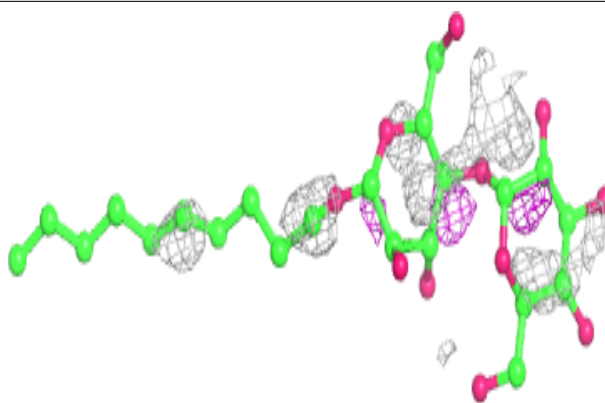
**Electron density around DMU K 101:**

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

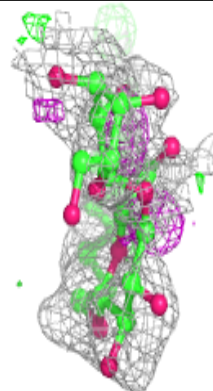
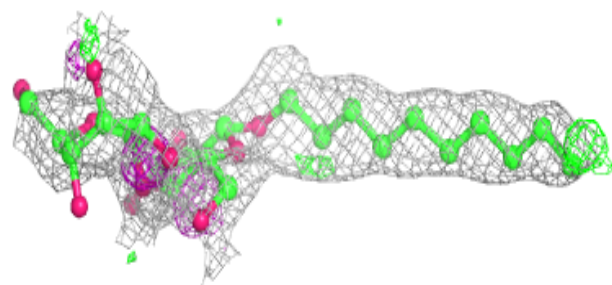
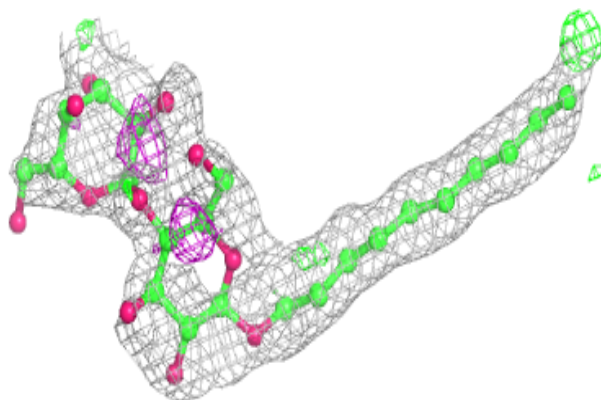


**Electron density around DMU X 107:**

$2mF_o-DF_c$  (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:**

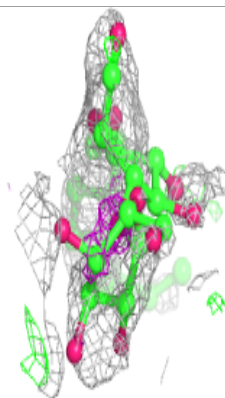
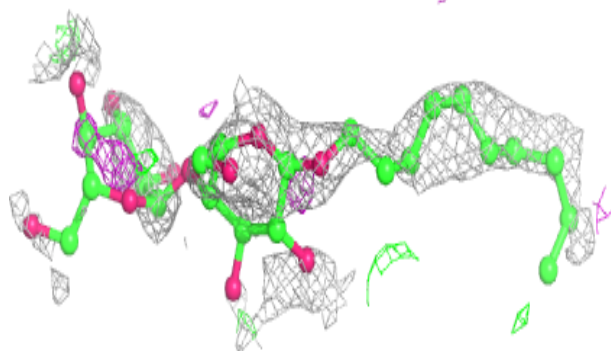
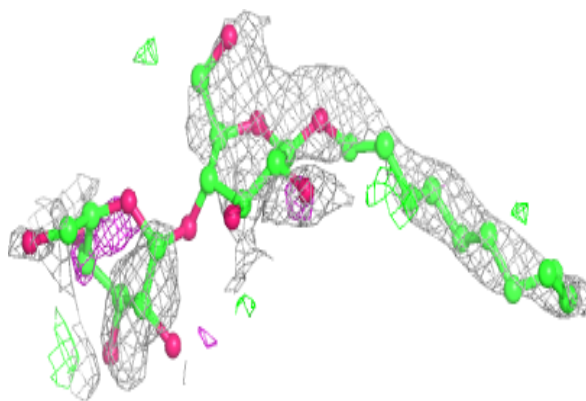
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



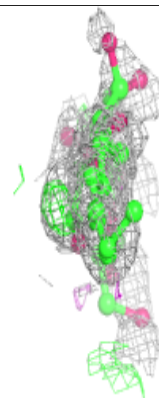
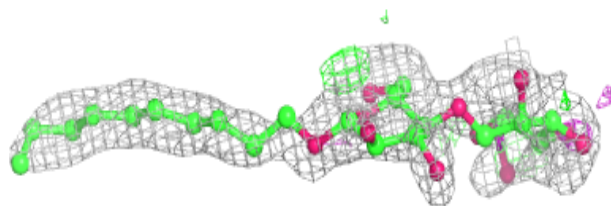
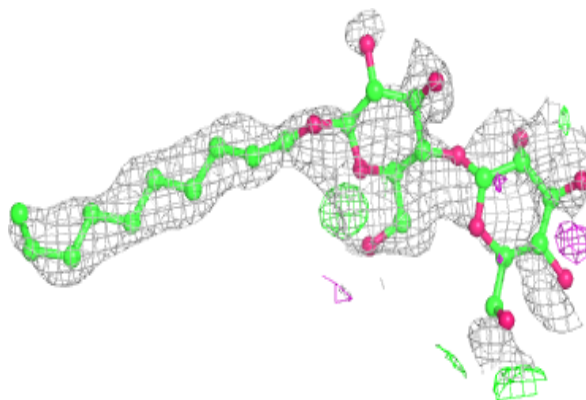


**Electron density around DMU X 103:**

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

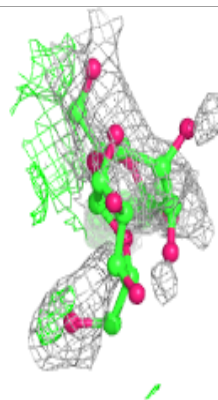
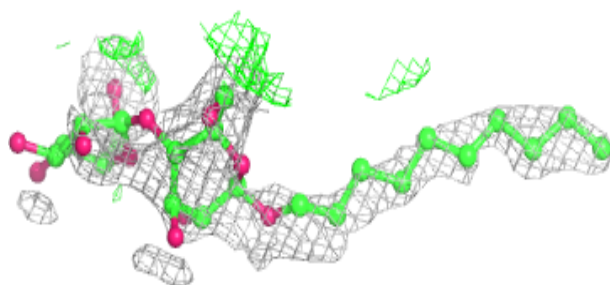
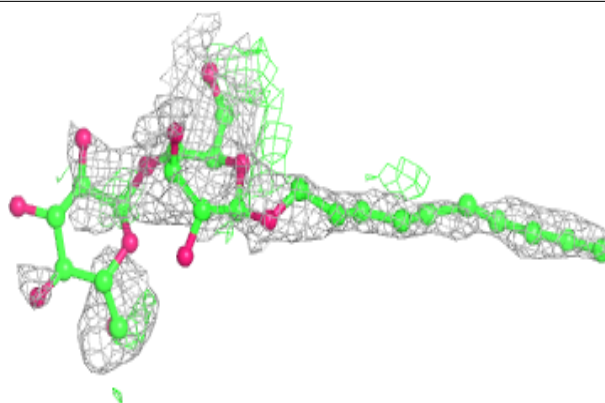
**Electron density around DMU C 316:**

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

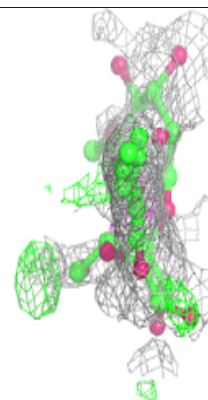
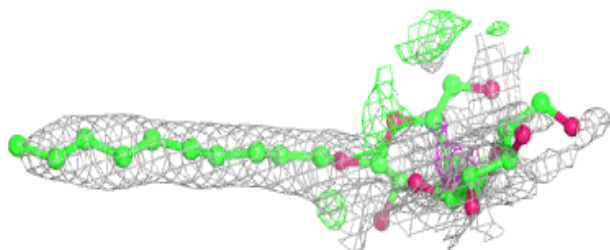
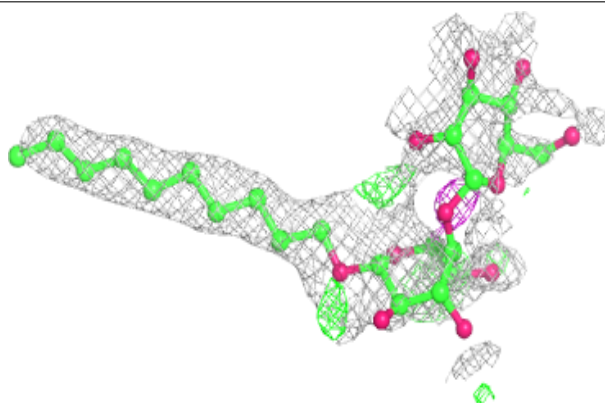


**Electron density around DMU D 206:**

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

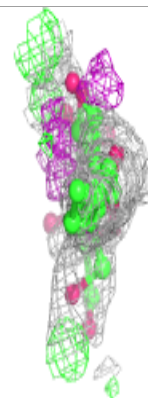
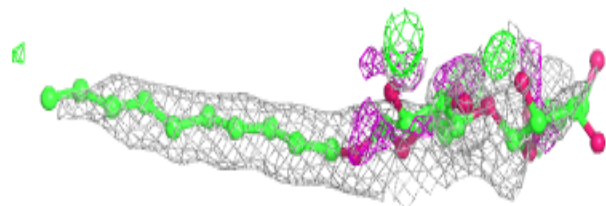
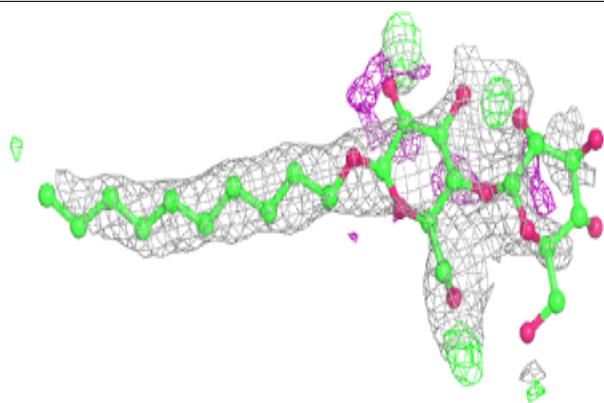
**Electron density around DMU O 307:**

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

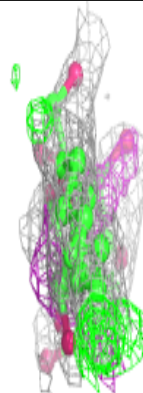
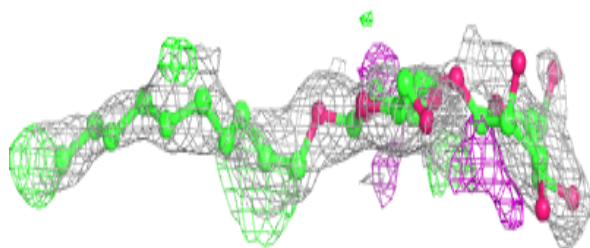
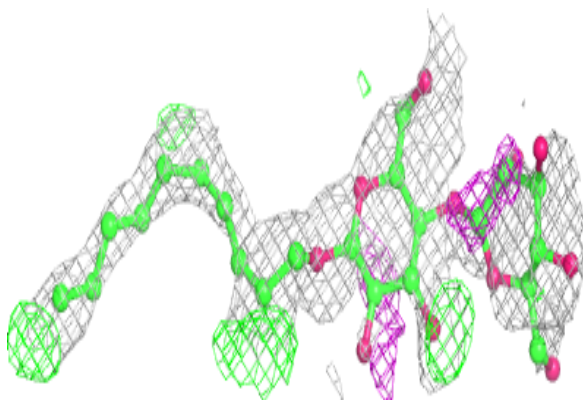


**Electron density around DMU C 317:**

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

**Electron density around DMU K 105:**

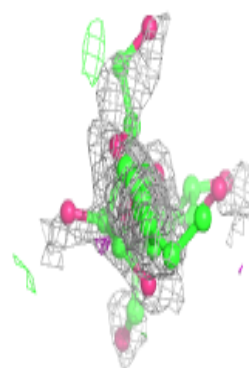
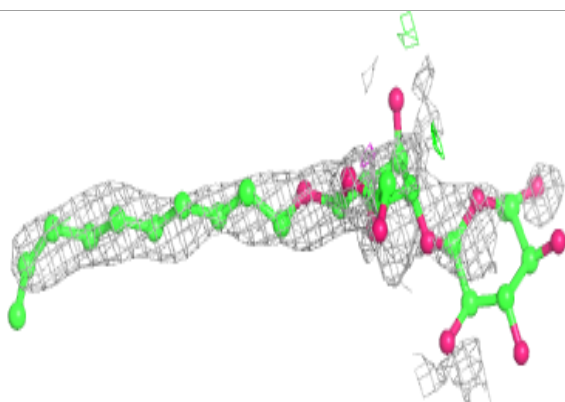
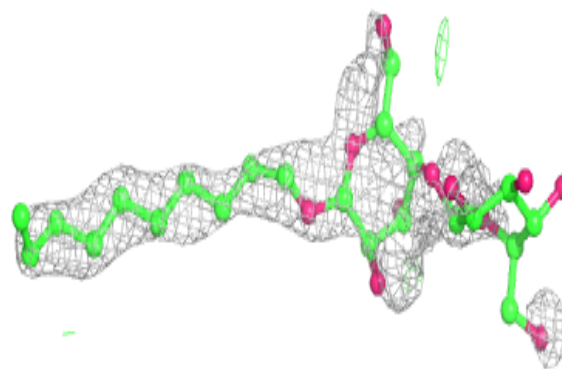
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



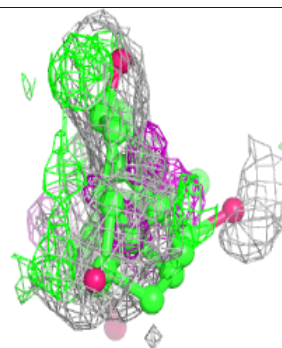
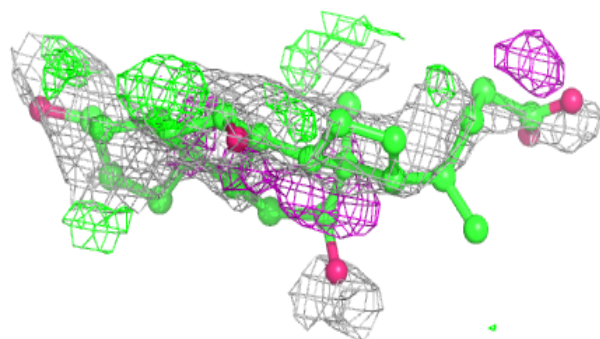
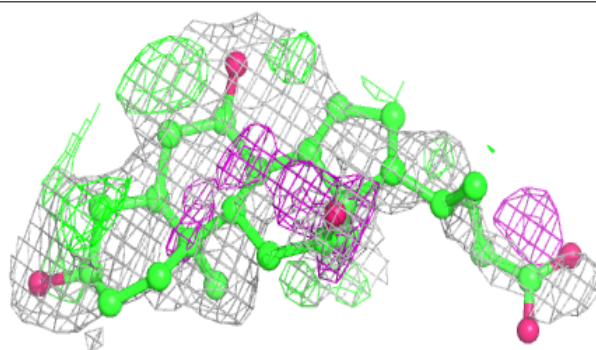


**Electron density around DMU I 101:**

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

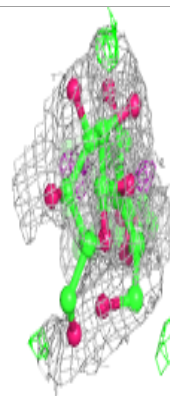
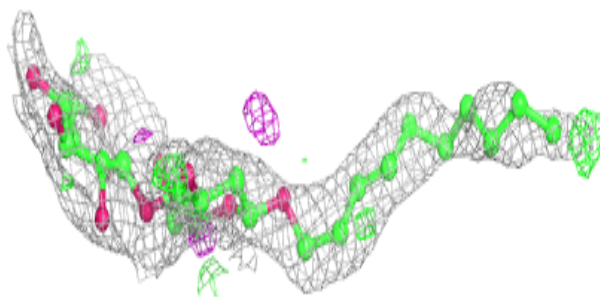
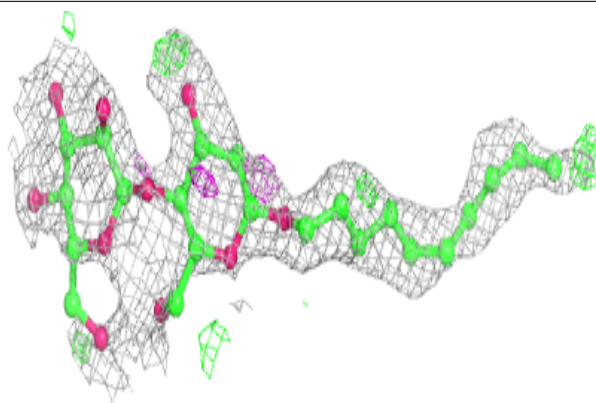
**Electron density around CHD X 101:**

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



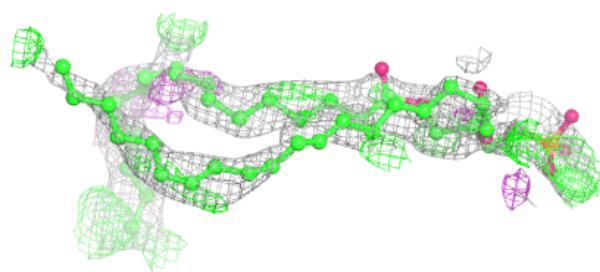
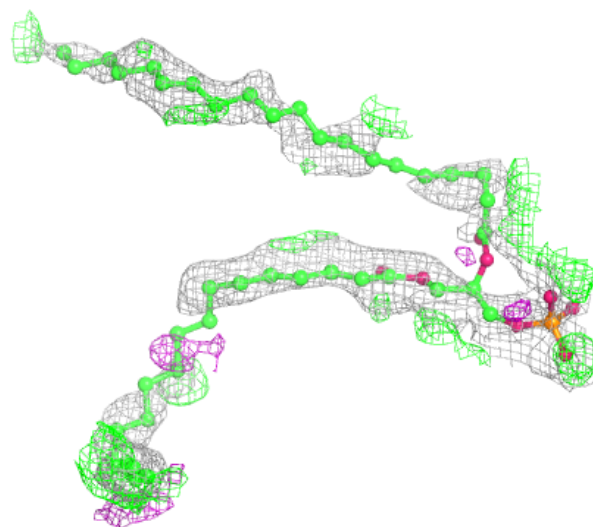
**Electron density around DMU K 103:**

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



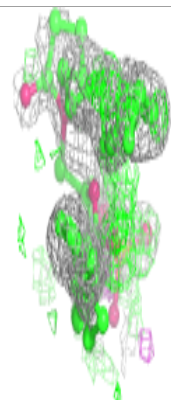
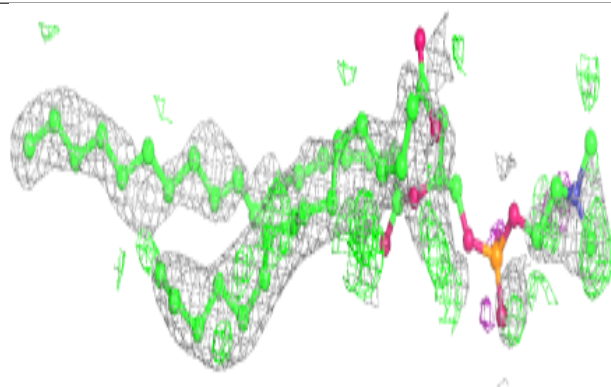
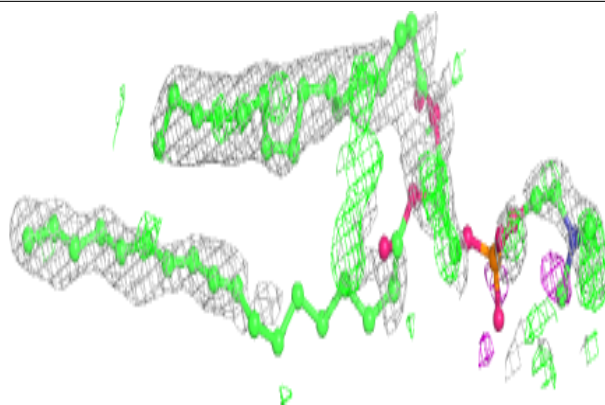
**Electron density around PEK T 101:**

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

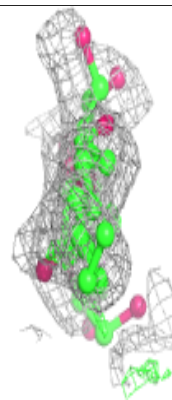
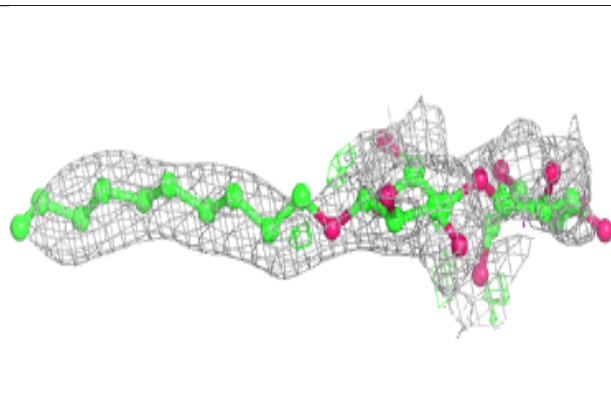
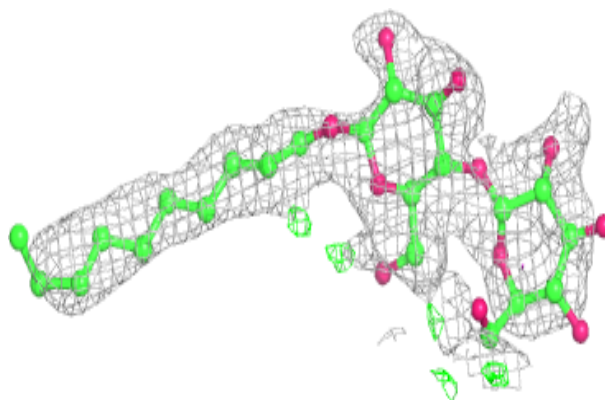


**Electron density around PSC B 304:**

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

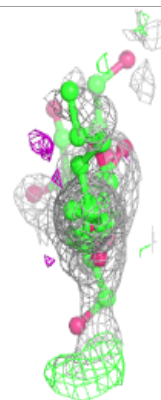
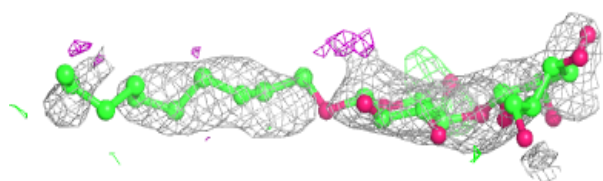
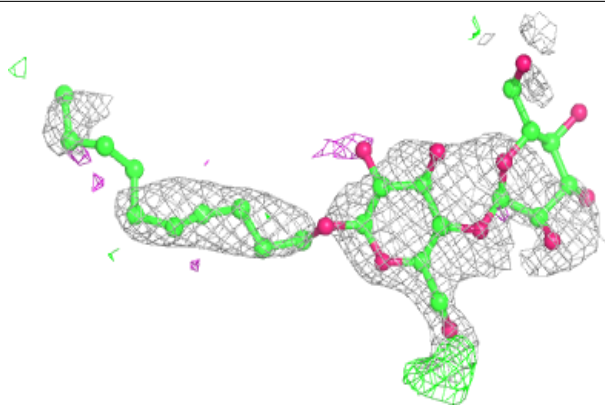
**Electron density around DMU P 315:**

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

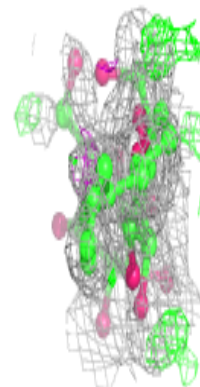
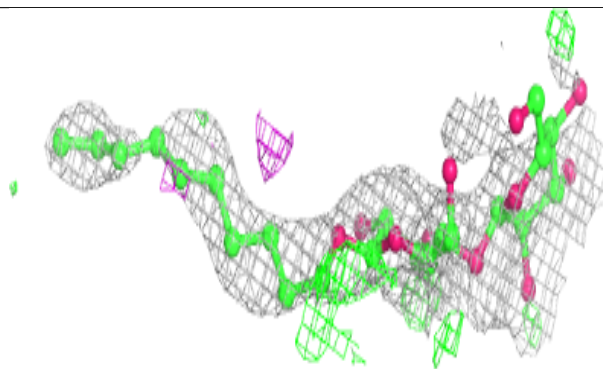
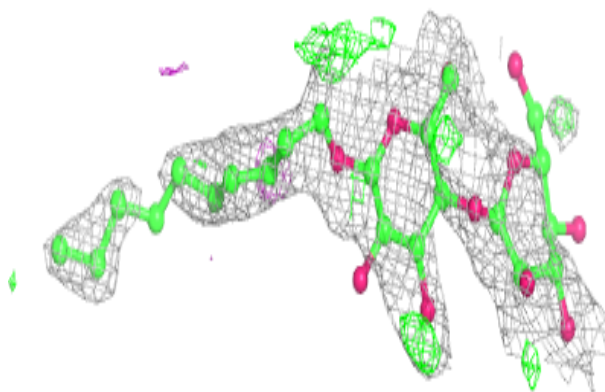


**Electron density around DMU L 105:**

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

**Electron density around DMU X 104:**

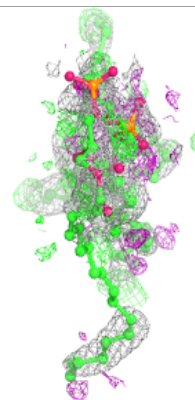
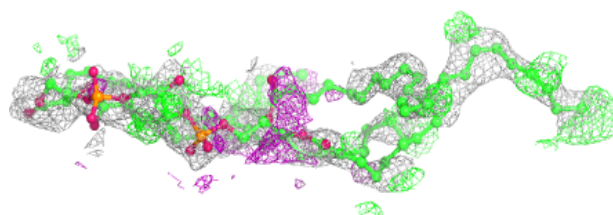
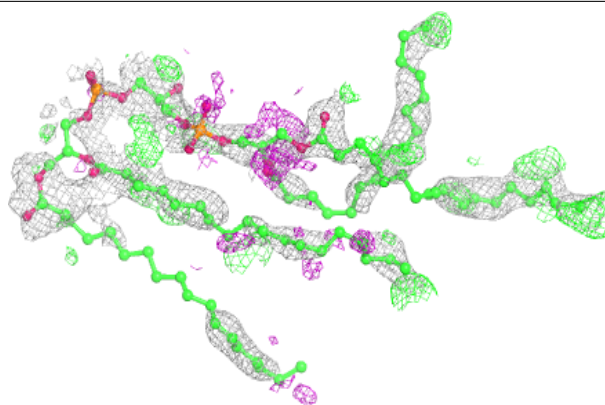
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



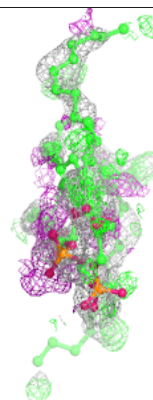
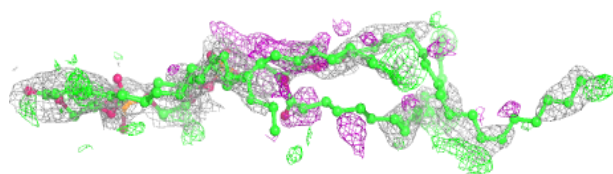
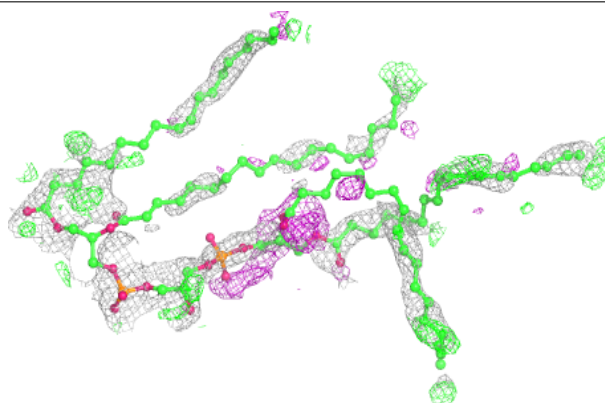


**Electron density around CDL T 102:**

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

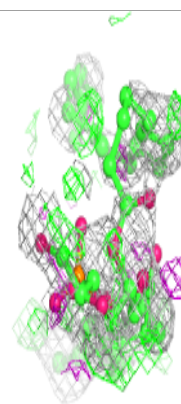
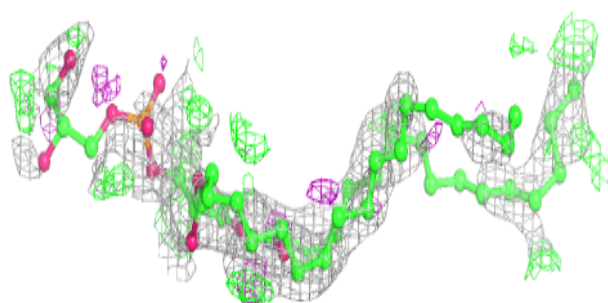
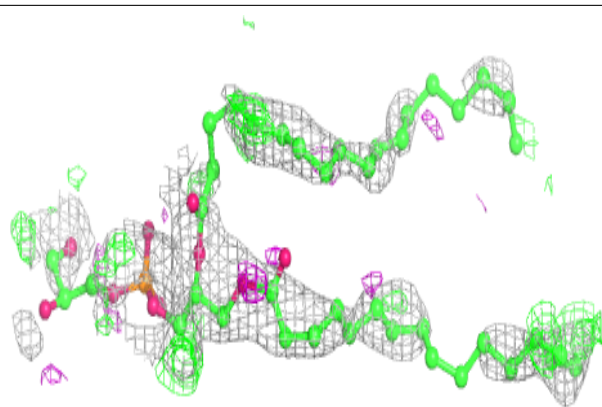
**Electron density around CDL G 101:**

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

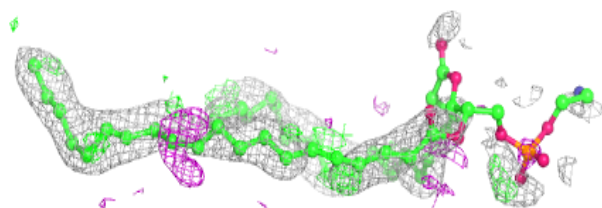
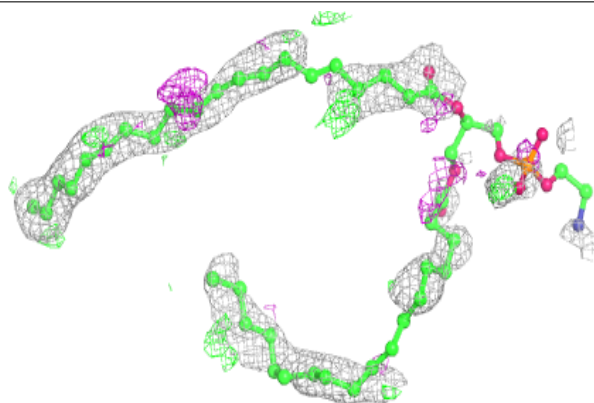


**Electron density around PGV G 102:**

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

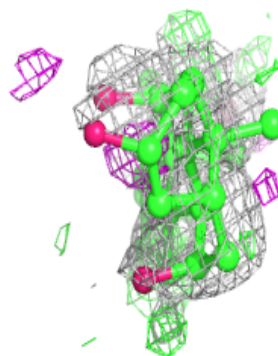
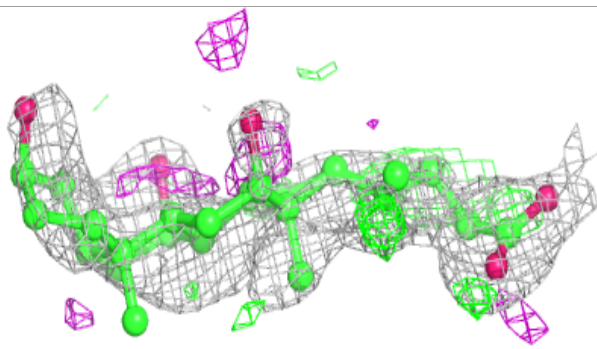
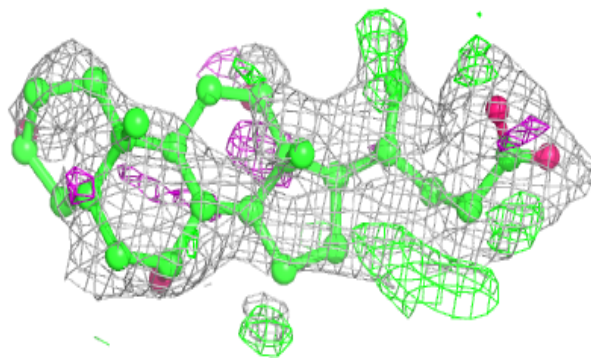
**Electron density around PEK C 309:**

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



**Electron density around CHD P 304:**

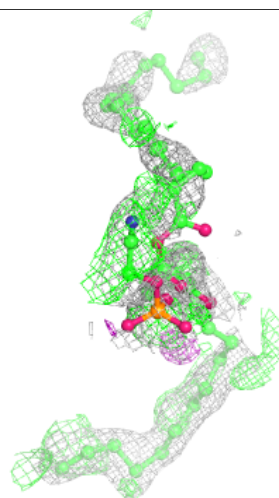
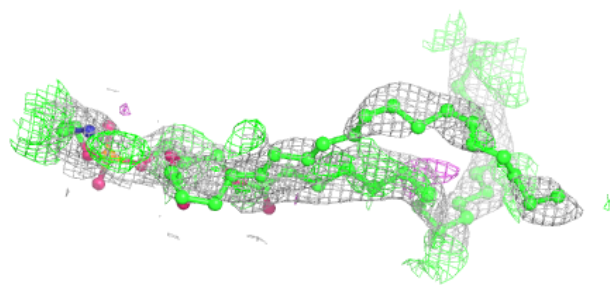
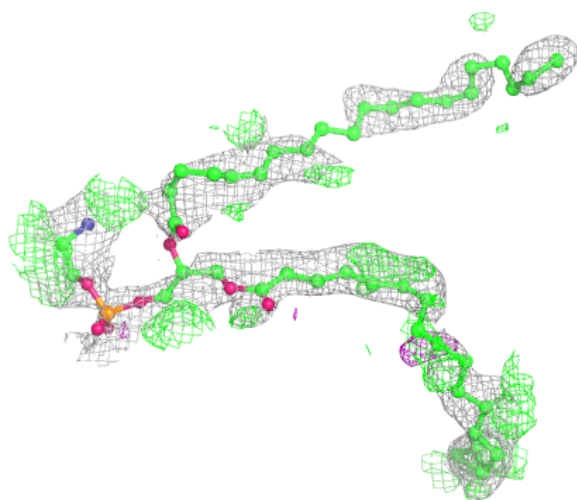
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





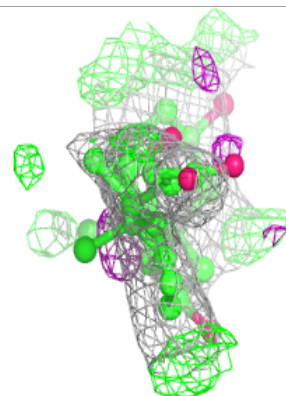
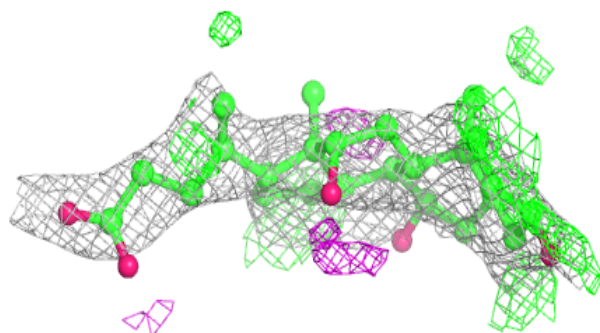
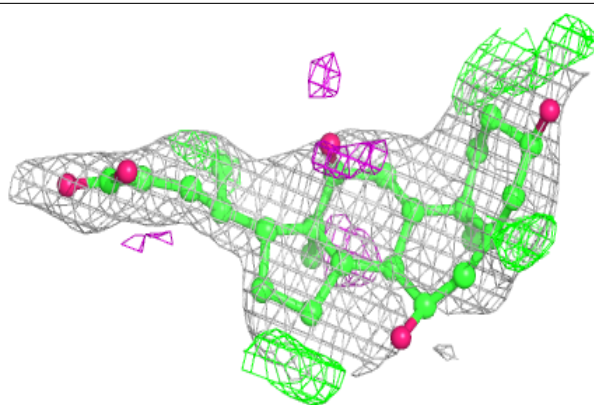
**Electron density around PEK C 305:**

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

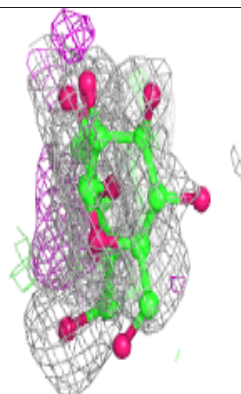
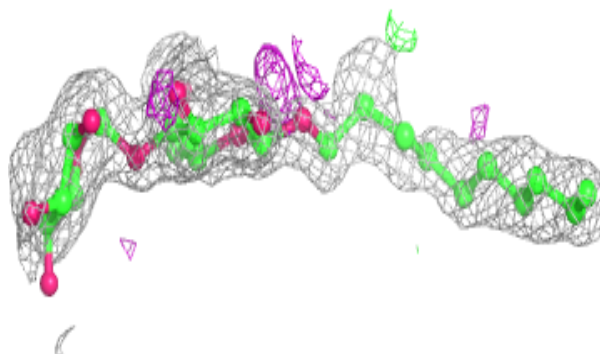
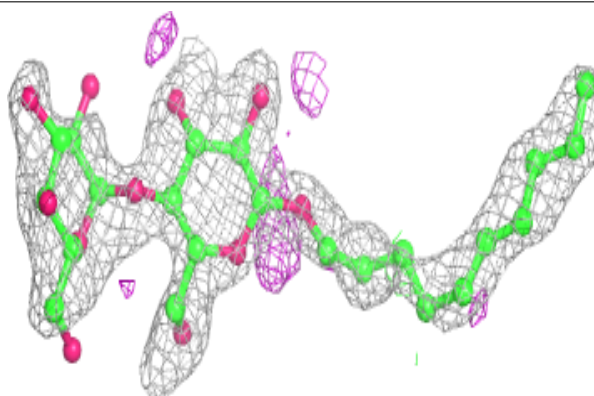


**Electron density around CHD Y 104:**

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

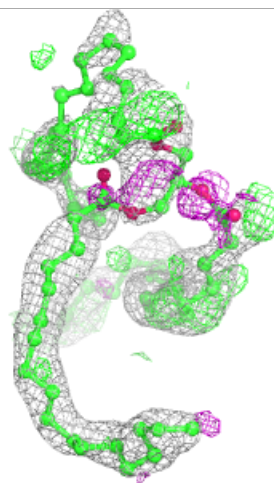
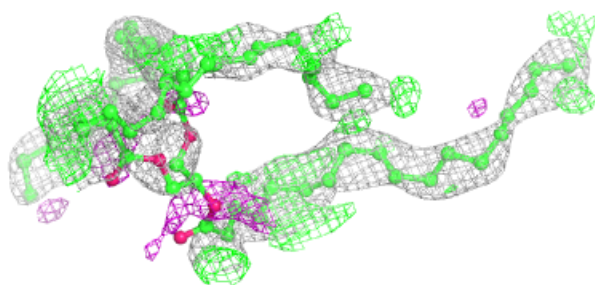
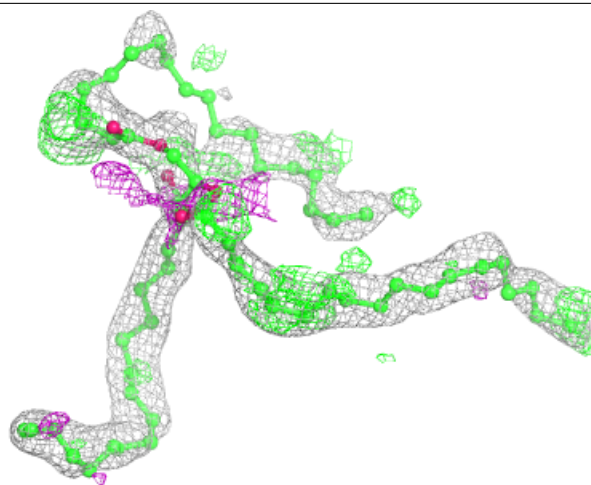
**Electron density around DMU P 305:**

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



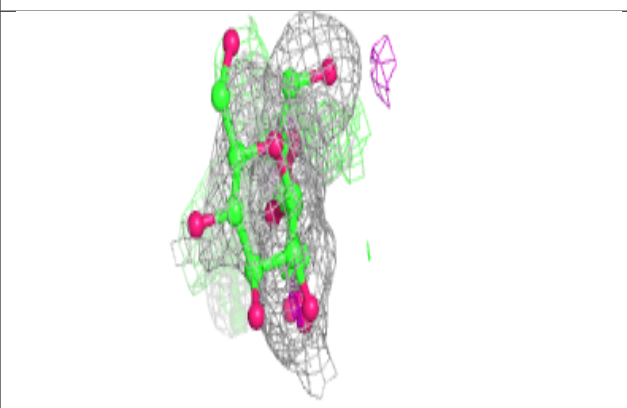
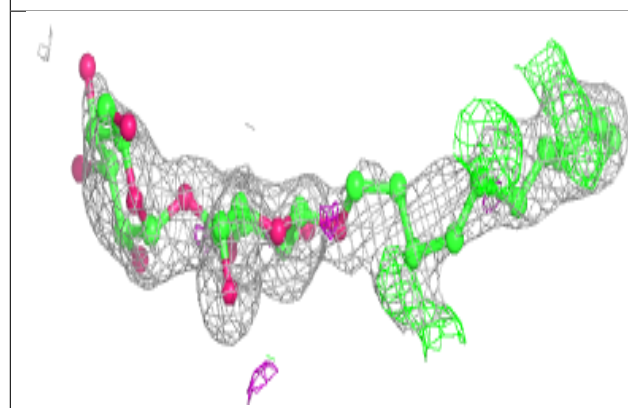
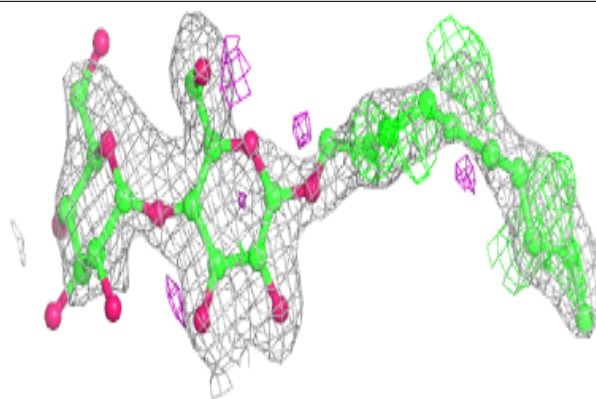
**Electron density around TGL Y 101:**

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

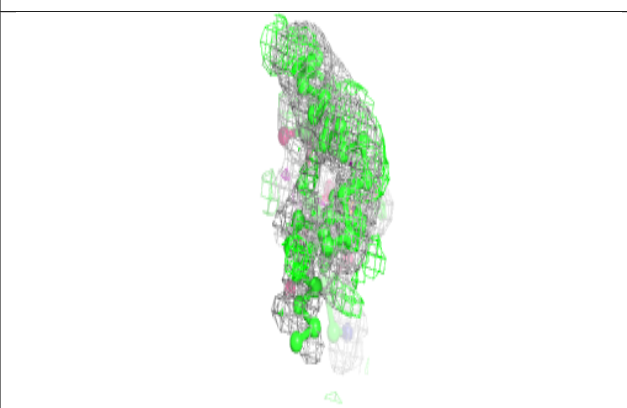
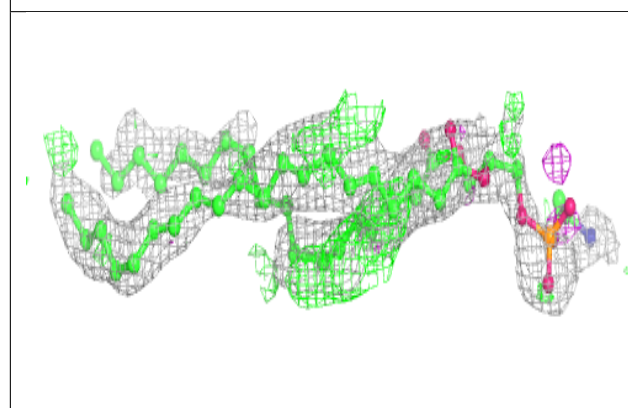
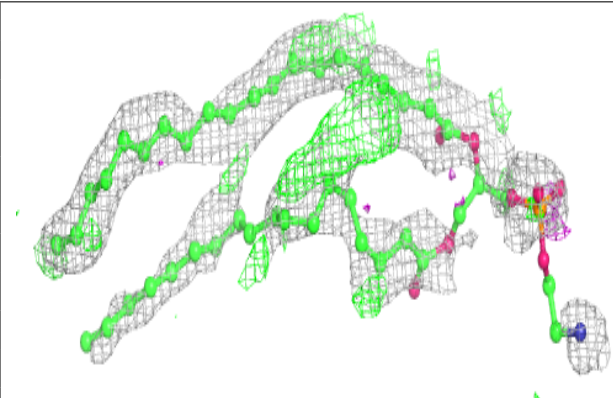


**Electron density around DMU C 308:**

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

**Electron density around PEK P 301:**

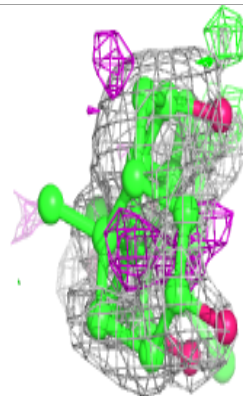
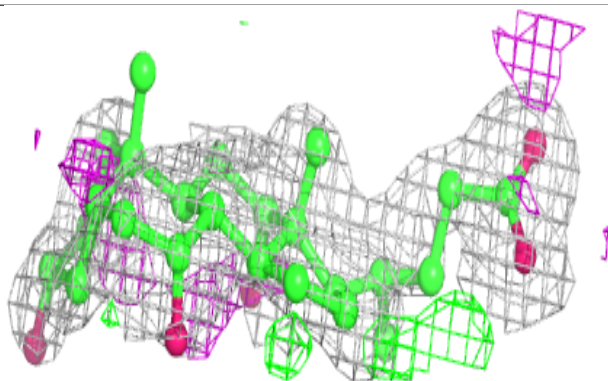
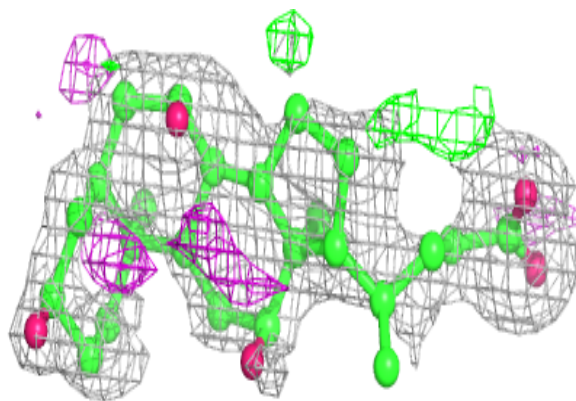
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



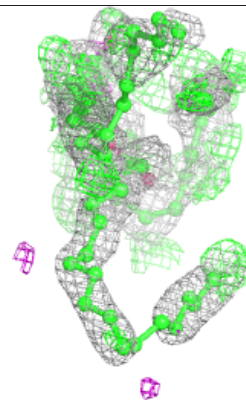
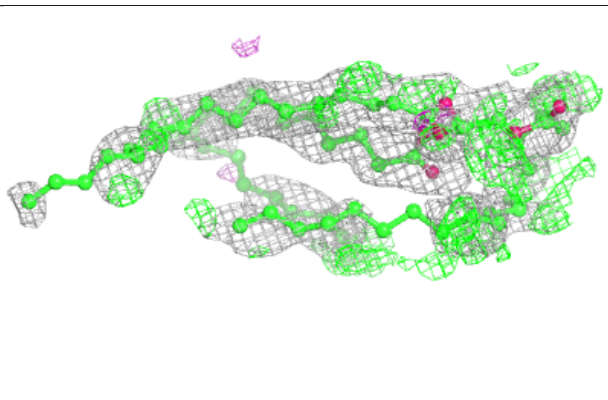
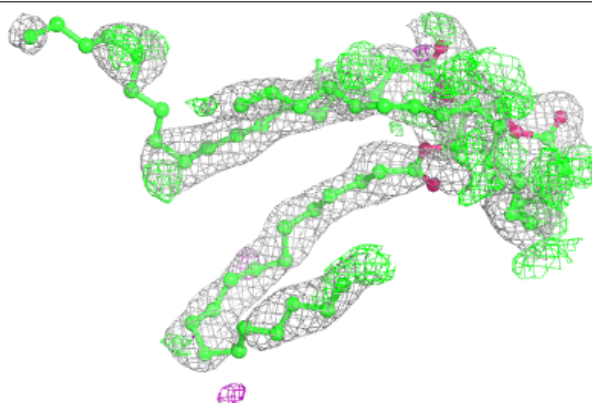


**Electron density around CHD C 303:**

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

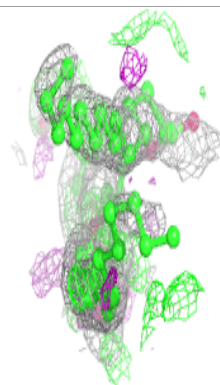
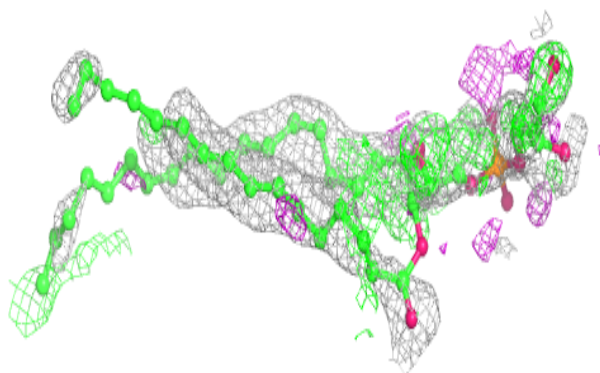
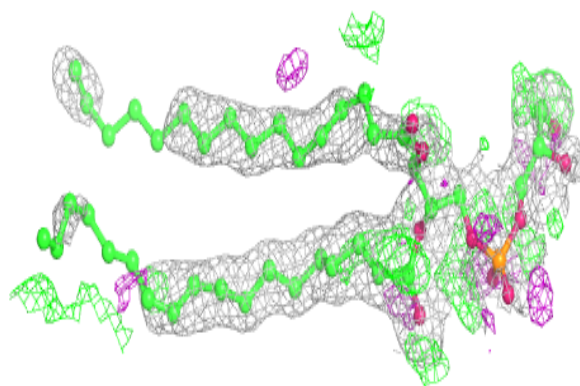
**Electron density around TGL Q 202:**

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

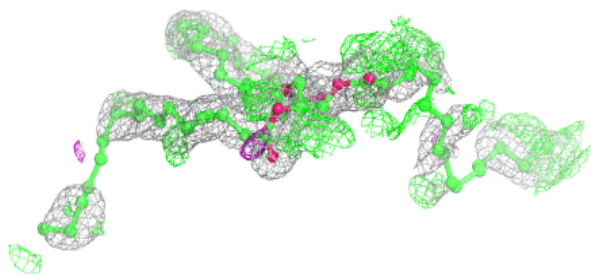
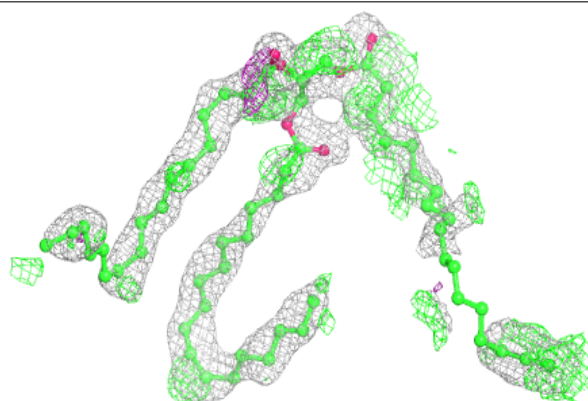


**Electron density around PGV A 608:**

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

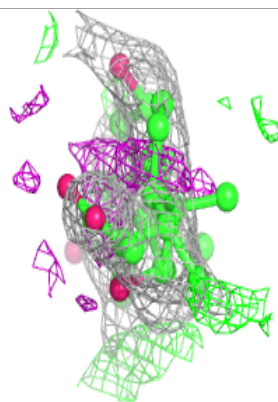
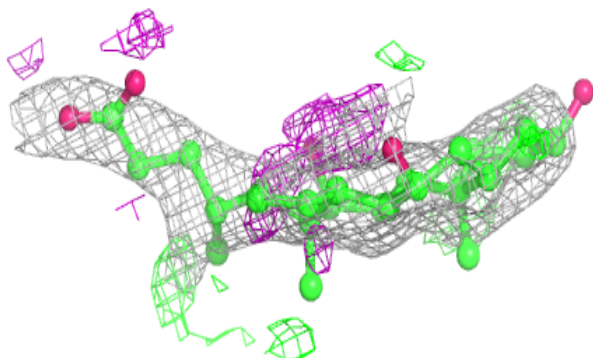
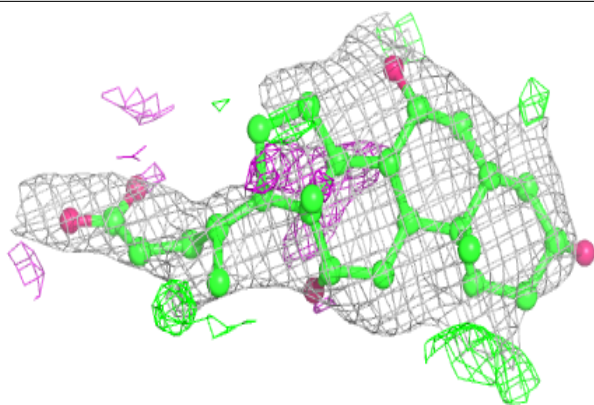
**Electron density around TGL D 201:**

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

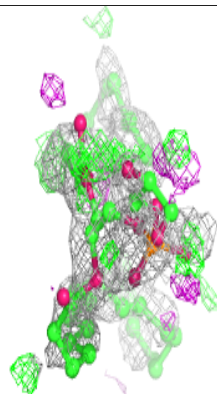
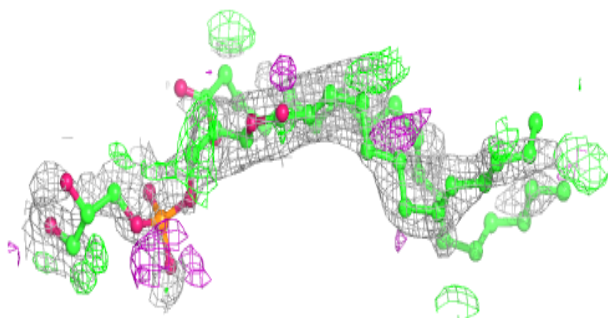
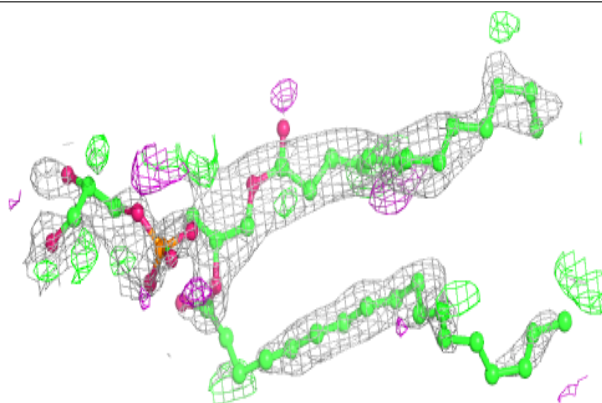


**Electron density around CHD L 104:**

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

**Electron density around PGV C 306:**

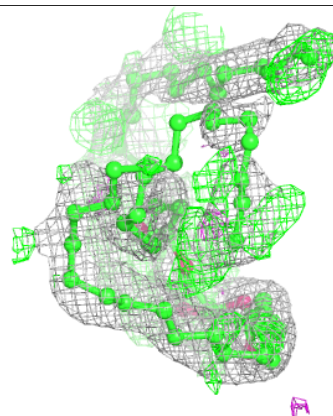
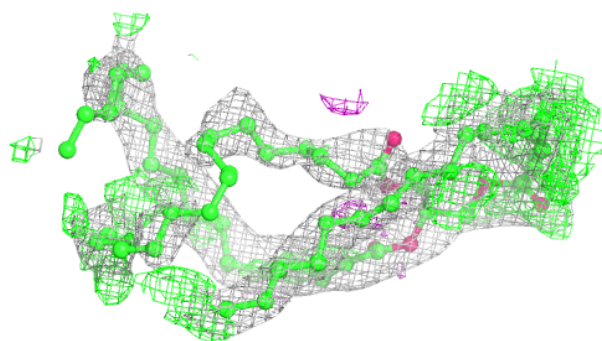
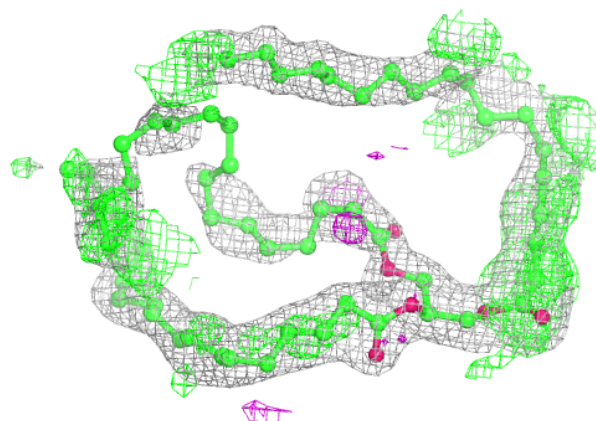
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



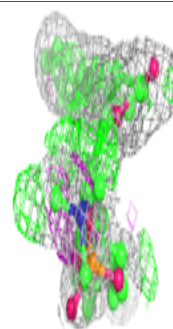
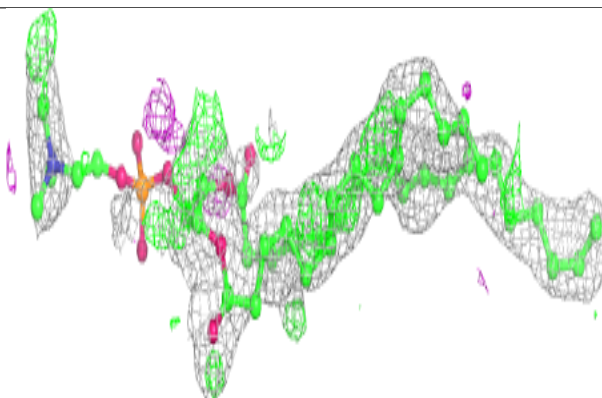
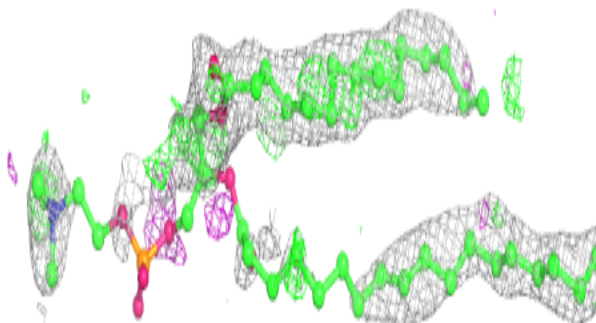


**Electron density around TGL B 301:**

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

**Electron density around PSC O 304:**

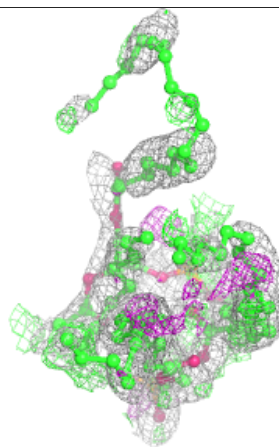
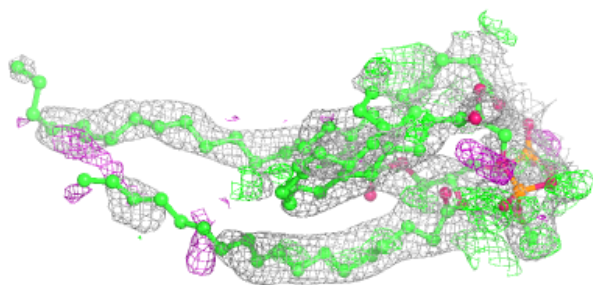
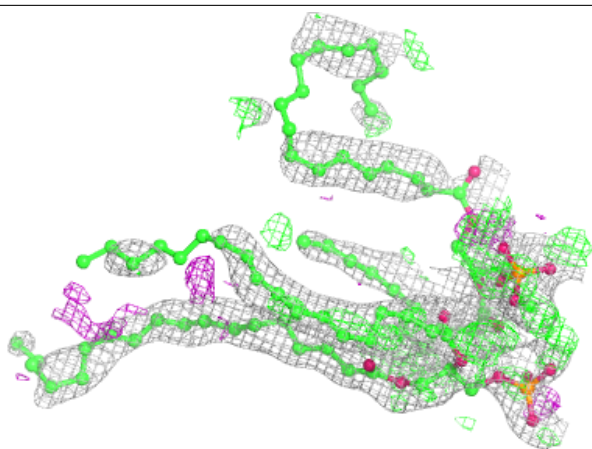
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



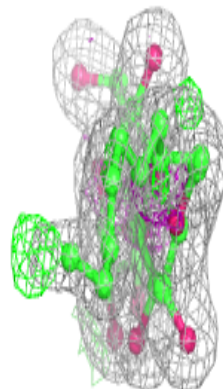
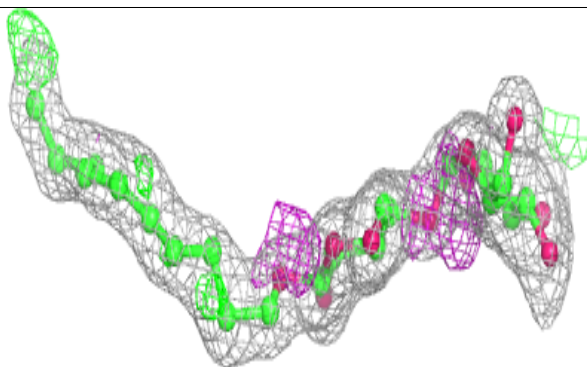
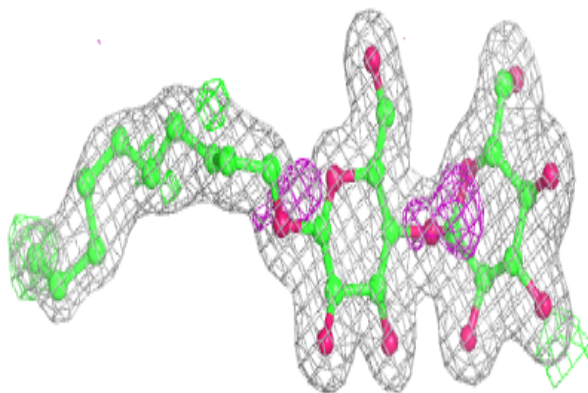


**Electron density around CDL P 303:**

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

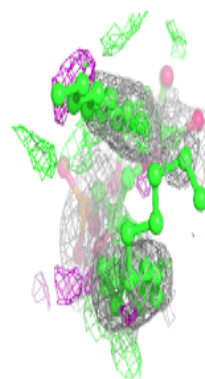
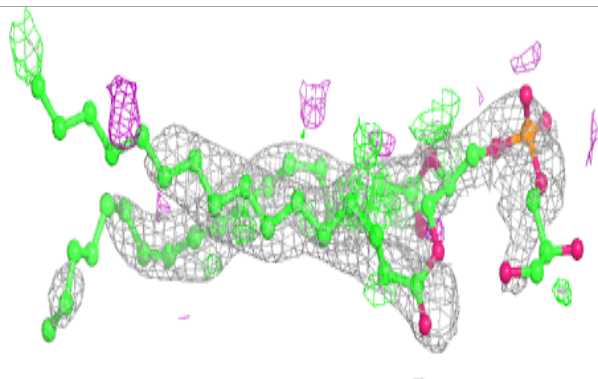
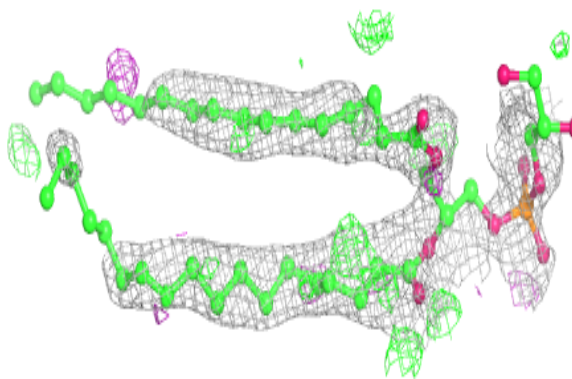
**Electron density around DMU M 101:**

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



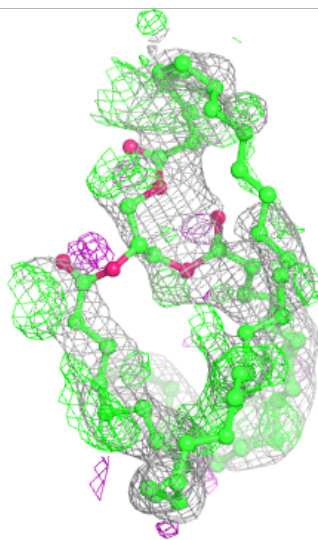
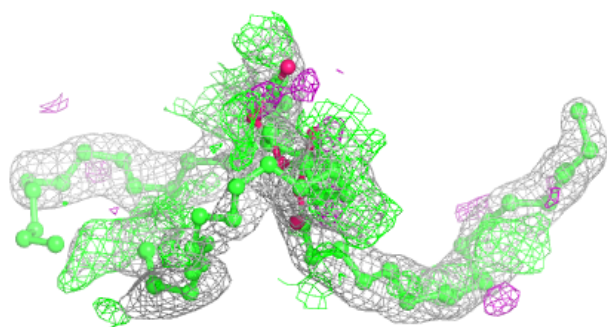
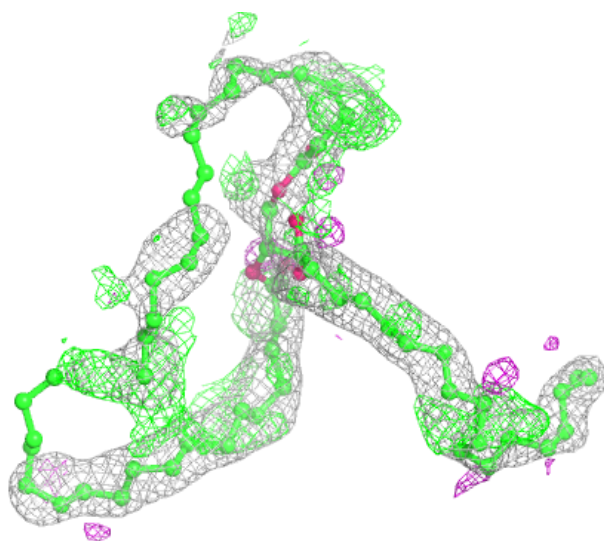
**Electron density around PGV Q 201:**

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



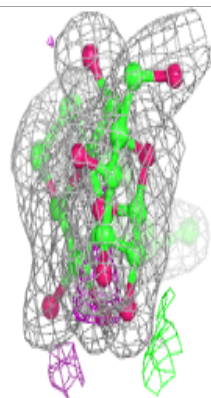
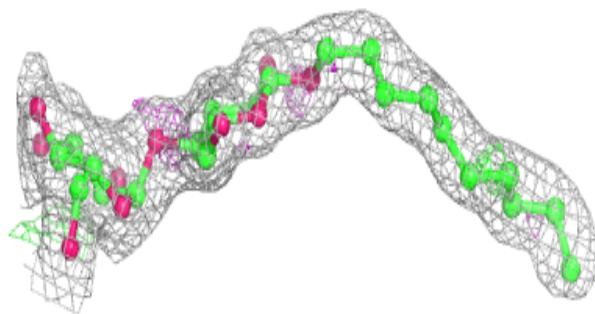
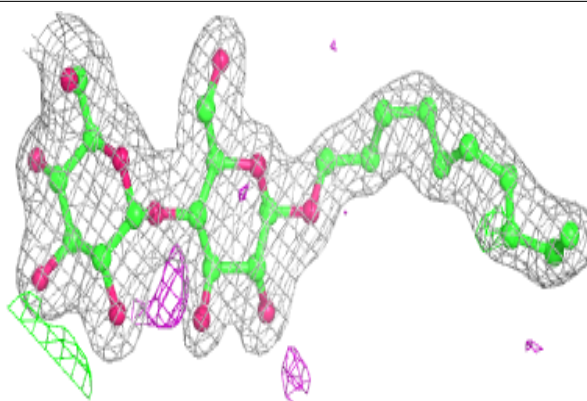
**Electron density around TGL A 609:**

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



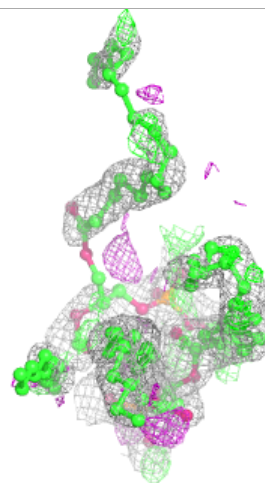
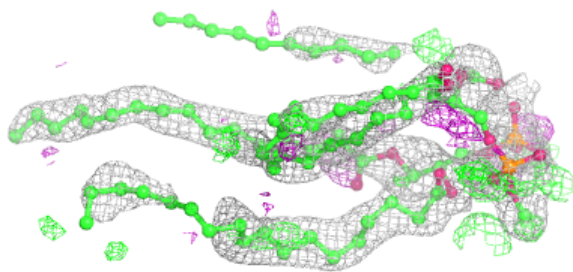
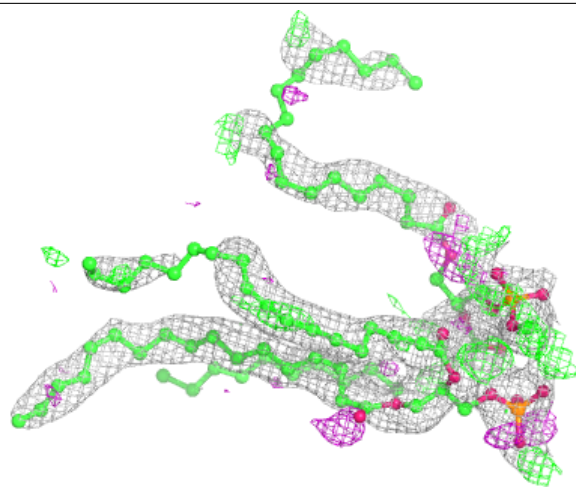
**Electron density around DMU Z 101:**

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



**Electron density around CDL C 302:**

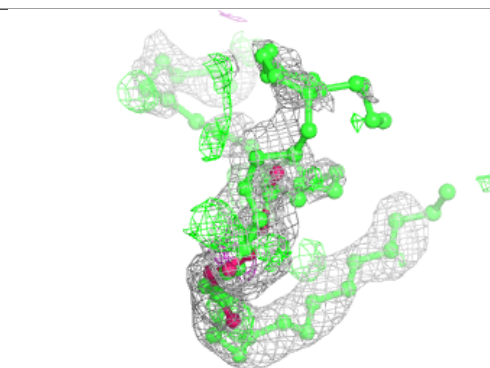
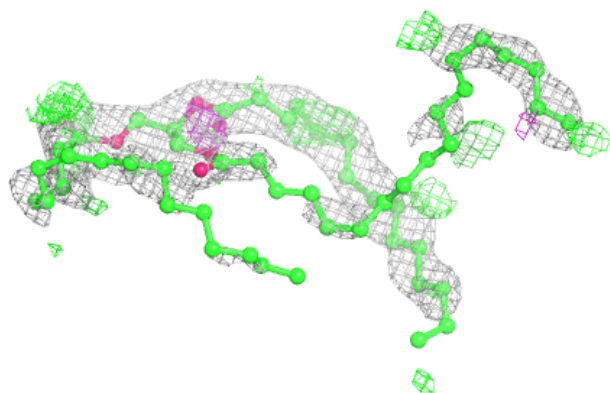
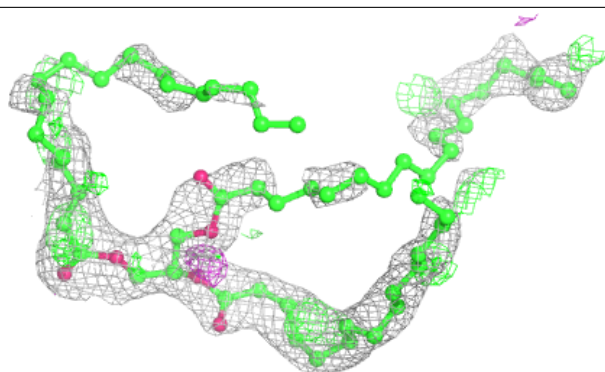
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



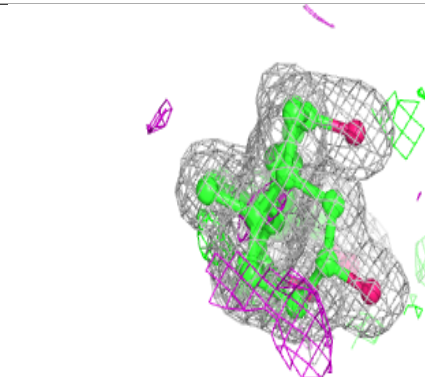
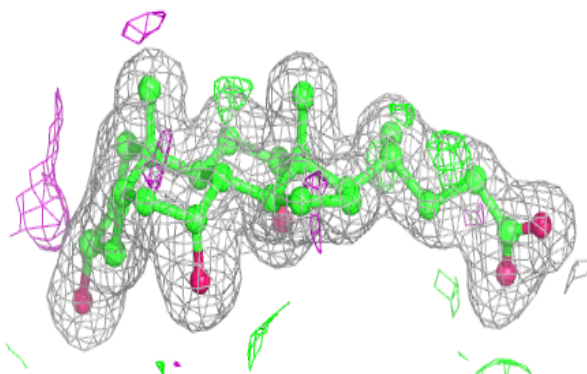
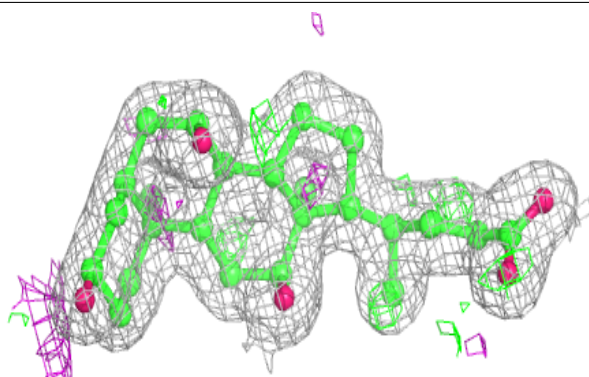


**Electron density around TGL O 301:**

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

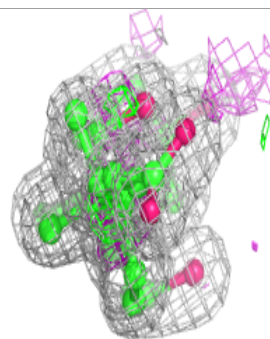
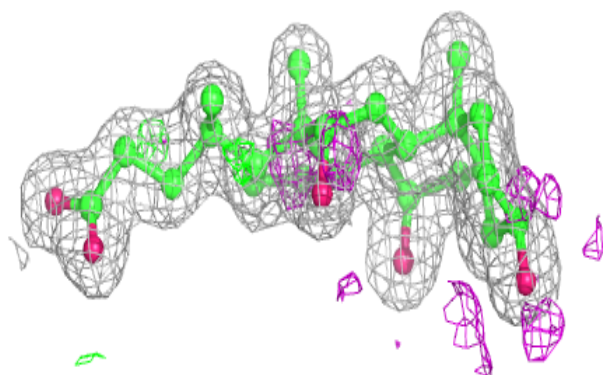
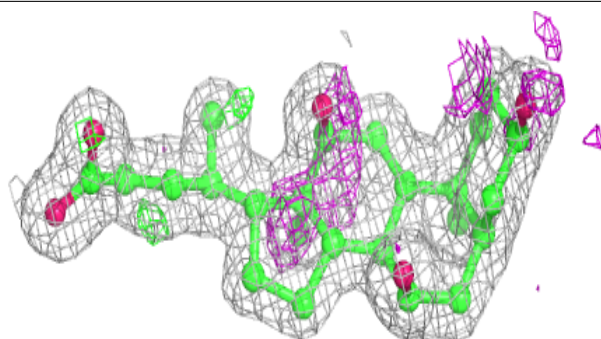
**Electron density around CHD P 306:**

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

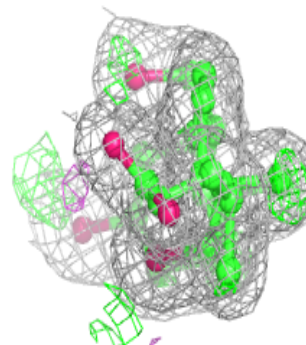
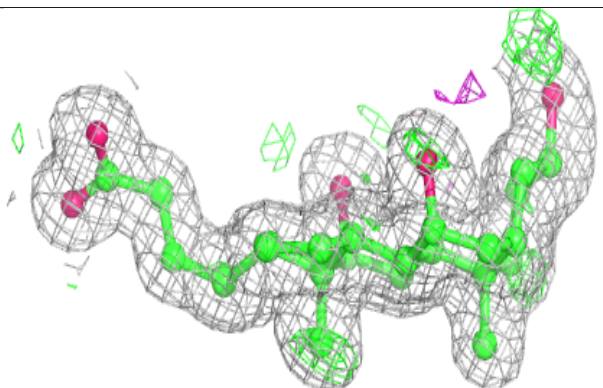
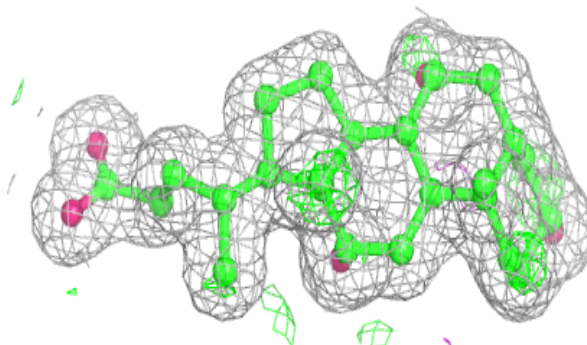


**Electron density around CHD C 304:**

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

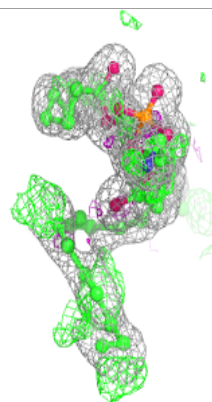
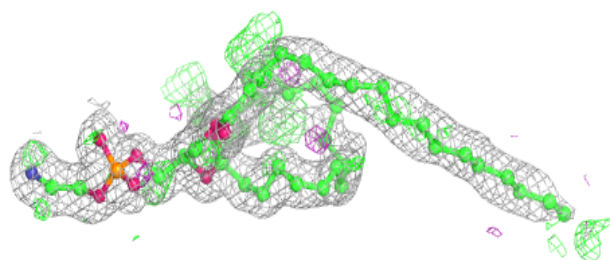
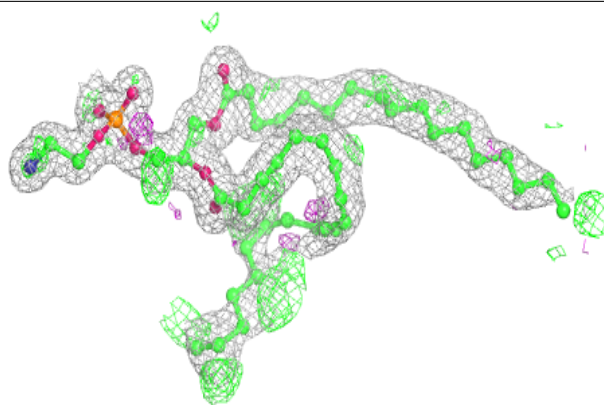
**Electron density around CHD O 303:**

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

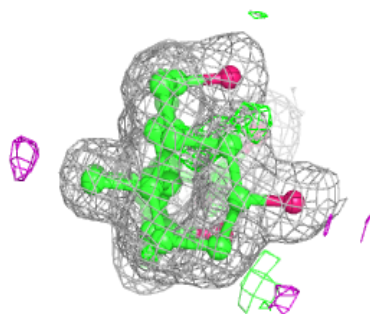
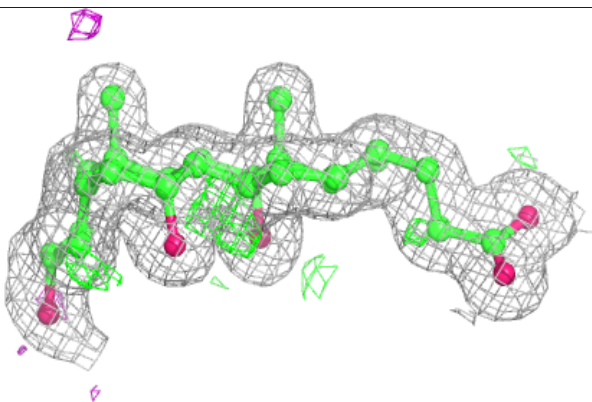
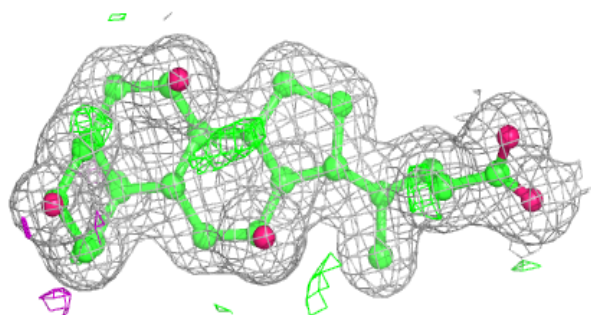


**Electron density around PEK C 307:**

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

**Electron density around CHD B 303:**

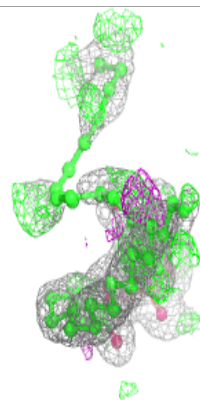
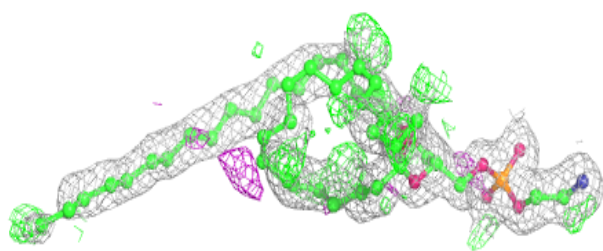
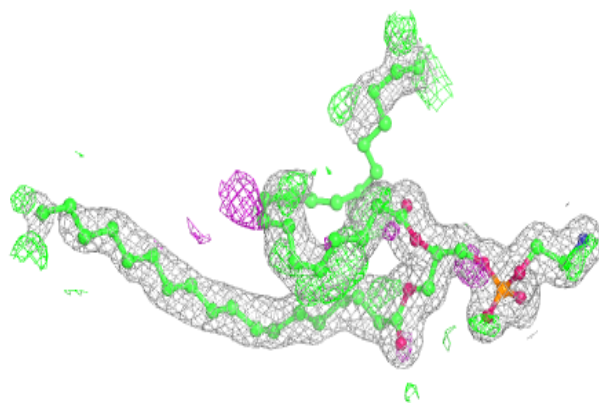
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



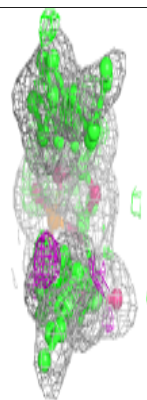
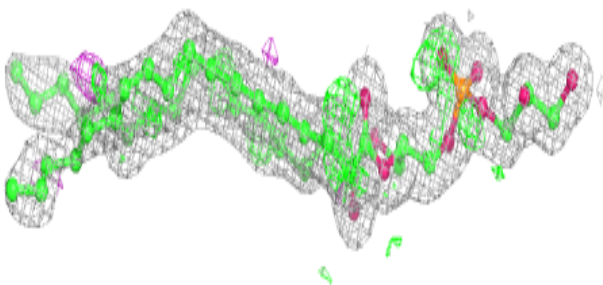
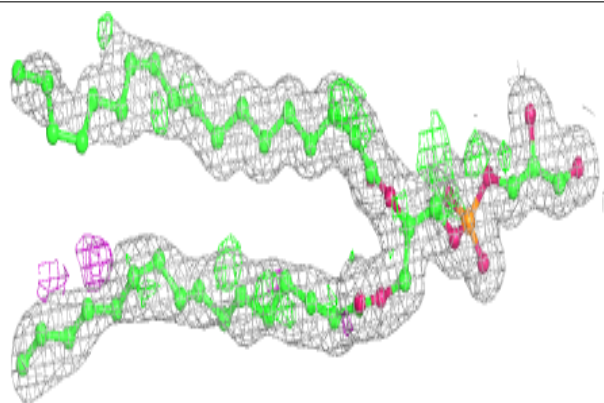


**Electron density around PEK P 307:**

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

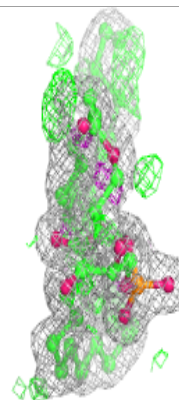
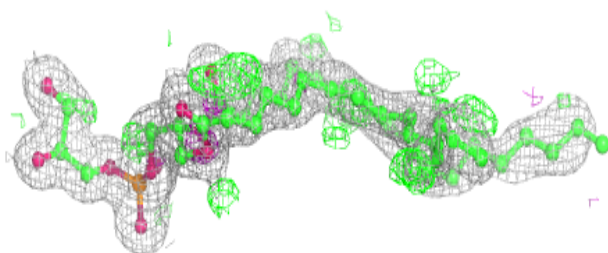
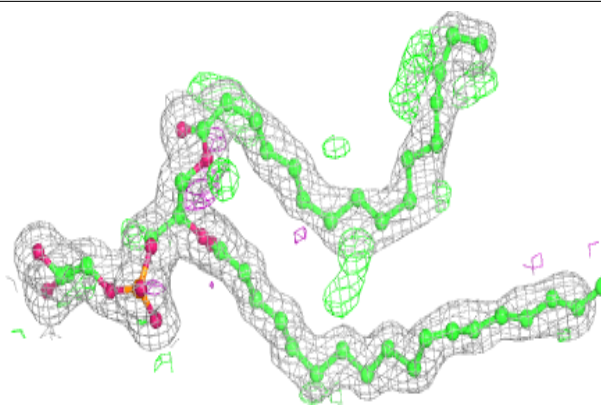
**Electron density around PGV C 301:**

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

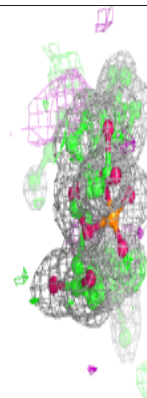
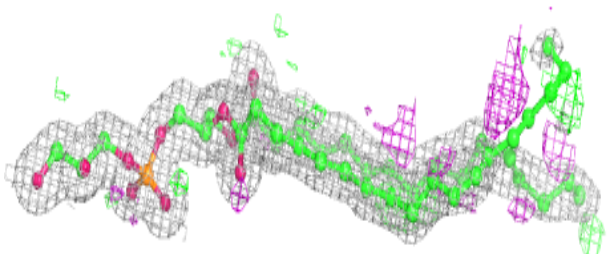
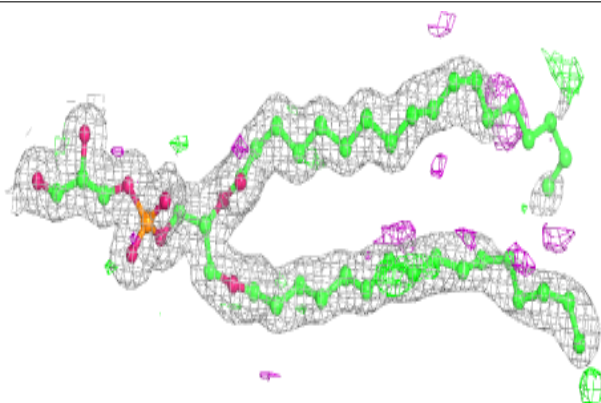


**Electron density around PGV N 607:**

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

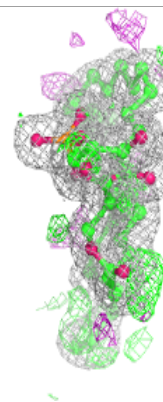
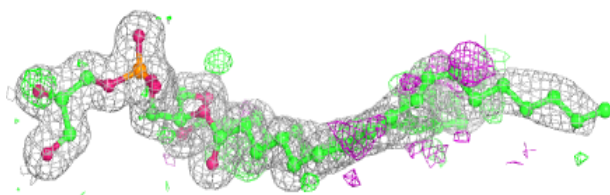
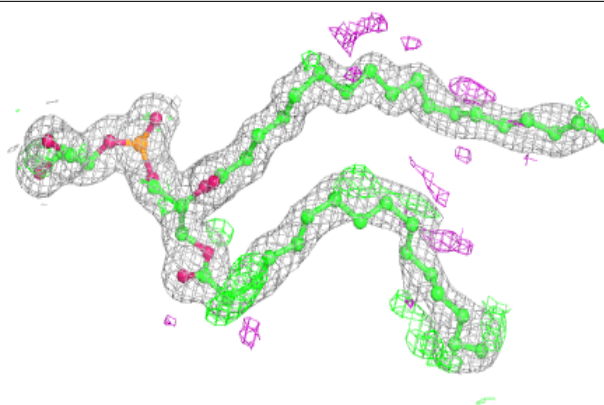
**Electron density around PGV P 302:**

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

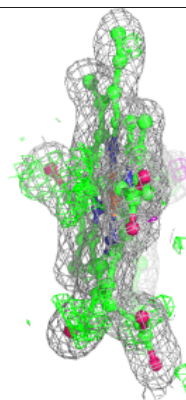
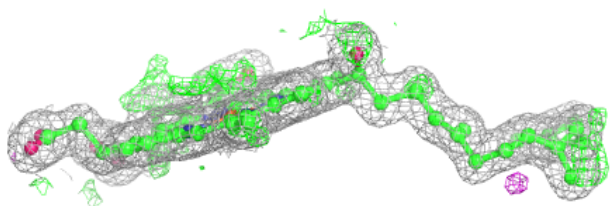
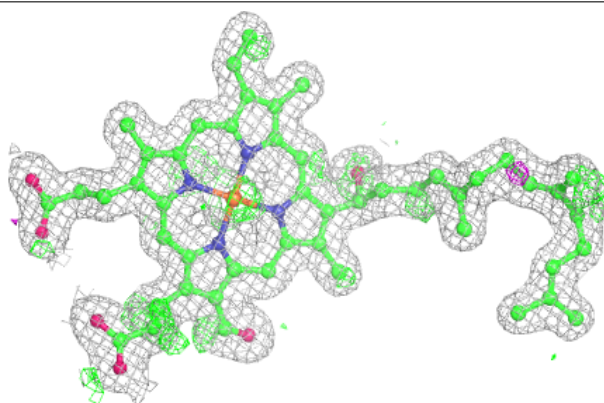


**Electron density around PGV A 607:**

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

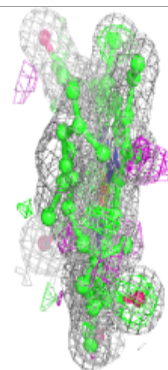
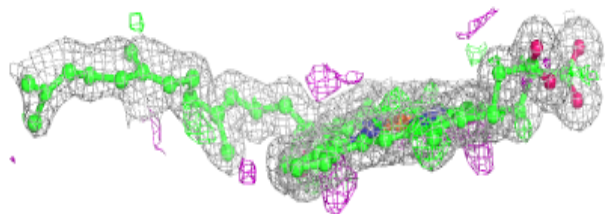
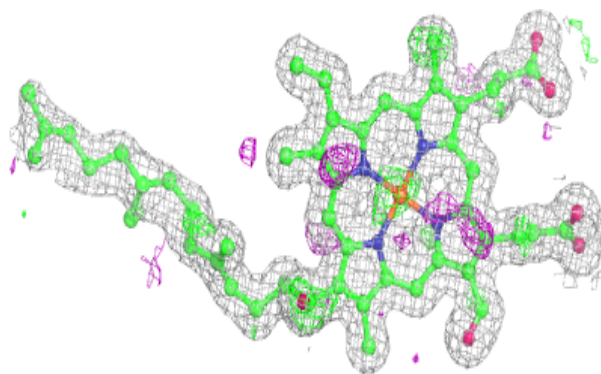
**Electron density around HEA N 602:**

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

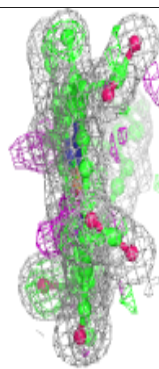
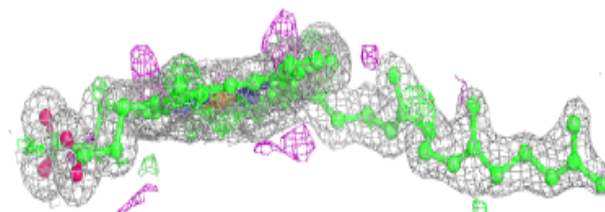
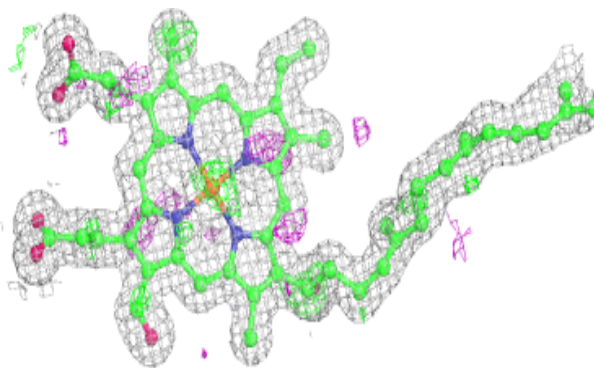


**Electron density around HEA A 601 (A):**

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

**Electron density around HEA A 601 (B):**

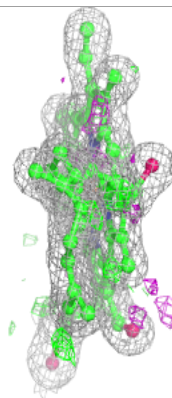
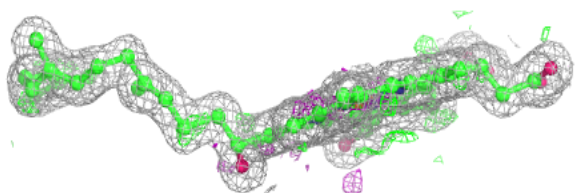
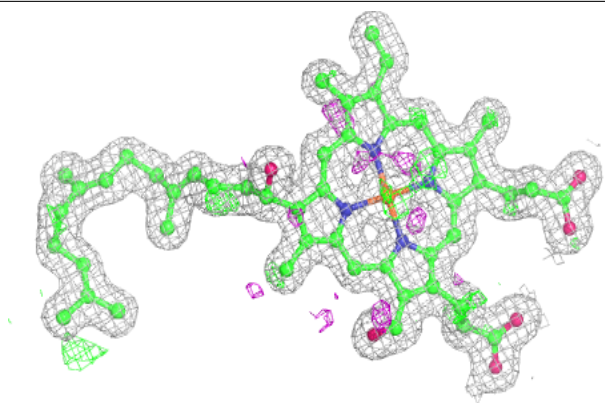
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



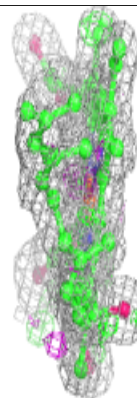
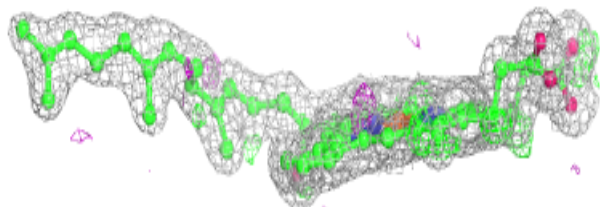
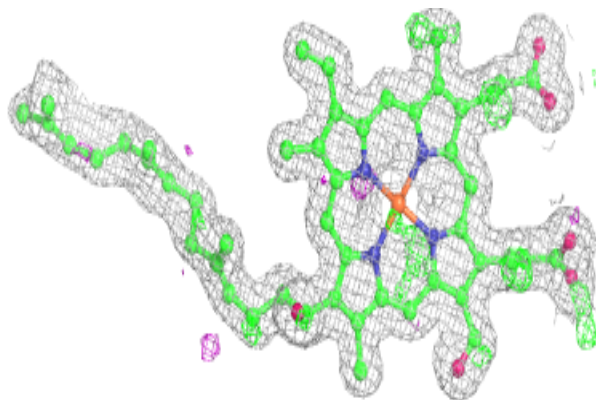


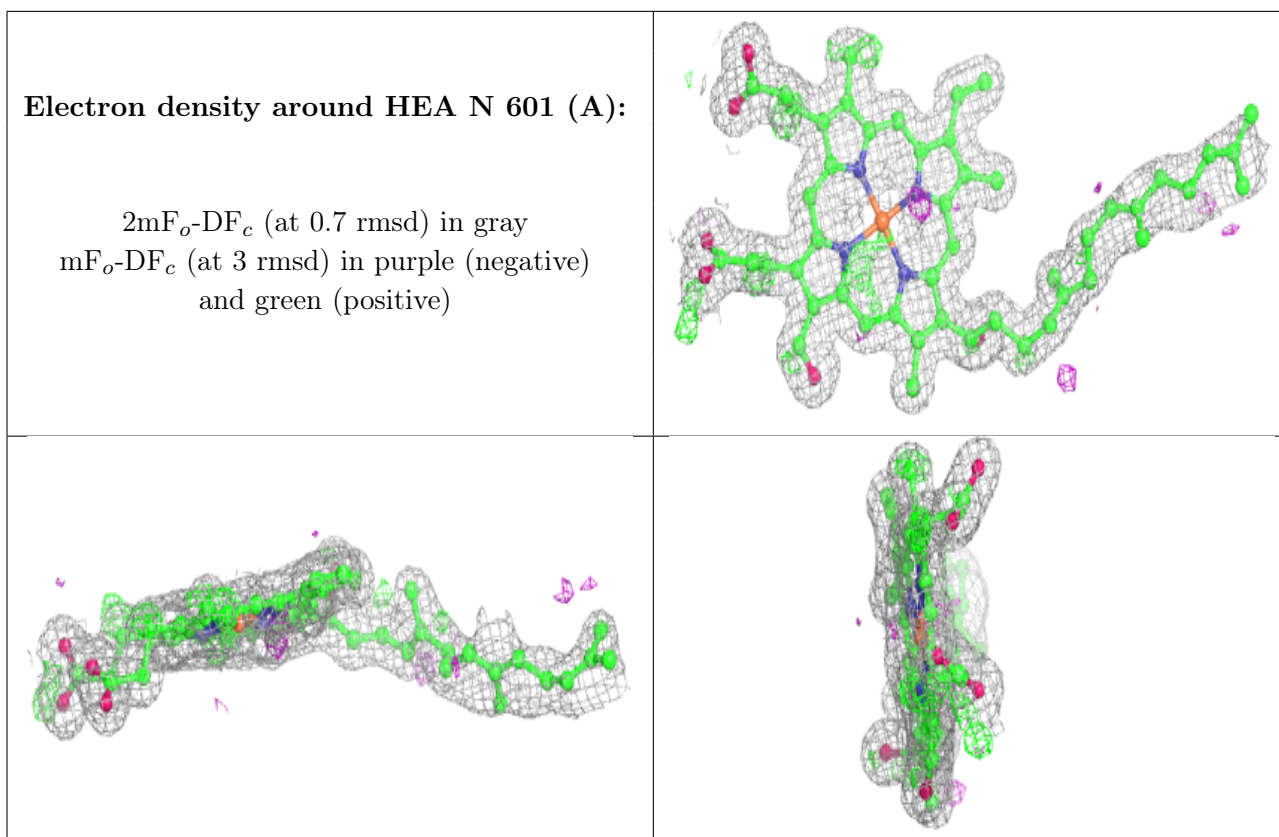
**Electron density around HEA A 602:**

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

**Electron density around HEA N 601 (B):**

$2mF_o-DF_c$  (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.