



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 5, 2021 – 10:35 AM JST

PDB ID : 7EV7  
Title : Bovine heart cytochrome c oxidase in the carbon monoxide-bound fully reduced state at a 50 K  
Authors : Shimada, A.; Yoshikawa, S.; Tsukihara, T.  
Deposited on : 2021-05-20  
Resolution : 1.70 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.

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

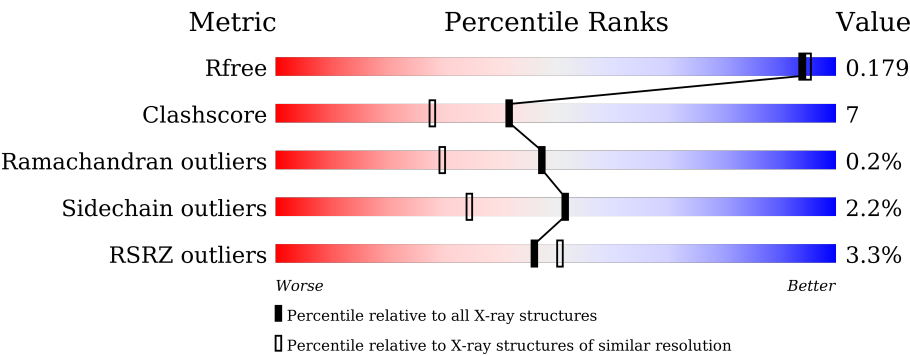
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div><div></div><div></div><div></div><div></div><div></div></div> <div>87%12%.</div>
1	N	514	<div><div></div><div></div><div></div><div></div><div></div></div> <div>87%13%</div>
2	B	227	<div><div></div><div></div><div></div><div></div><div></div></div> <div>3%80%18%.</div>
2	O	227	<div><div></div><div></div><div></div><div></div><div></div></div> <div>2%81%18%.</div>
3	C	261	<div><div></div><div></div><div></div><div></div><div></div></div> <div>91%8%.</div>
3	P	261	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%89%11%.</div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	A	602[A]	X	-	-	-
15	HEA	A	602[B]	X	-	-	-
15	HEA	A	602[C]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	A	603	X	-	-	-
15	HEA	N	602[A]	X	-	-	-
15	HEA	N	602[B]	X	-	-	-
15	HEA	N	602[C]	X	-	-	-
15	HEA	N	603	X	-	-	-
18	NA	C	302	-	-	-	X
20	EDO	A	623	-	-	-	X
20	EDO	B	309	-	-	-	X
20	EDO	B	314	-	-	-	X
20	EDO	D	202	-	-	-	X
20	EDO	D	206	-	-	-	X
20	EDO	G	104	-	-	-	X
20	EDO	H	103	-	-	X	-
20	EDO	N	612	-	-	X	-
20	EDO	N	629	-	-	-	X
20	EDO	N	630	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	I	1	-	-	-	X



## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34489 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	30	0
			4124	2750	635	698	41			
1	N	514	Total	C	N	O	S	0	28	0
			4116	2741	635	699	41			

- 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
			1869	1218	284	348	19			
2	O	227	Total	C	N	O	S	0	10	0
			1865	1216	284	346	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	9	0
			2131	1422	337	357	15			
3	P	259	Total	C	N	O	S	0	11	0
			2141	1428	341	357	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	5	0
			1214	787	202	221	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1206	785	199	218	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	3	0
			723	447	129	142	5			
6	S	94	Total	C	N	O	S	0	3	0
			723	448	128	141	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	1
			678	432	129	115	1	1		

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

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

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

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

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

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

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

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

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

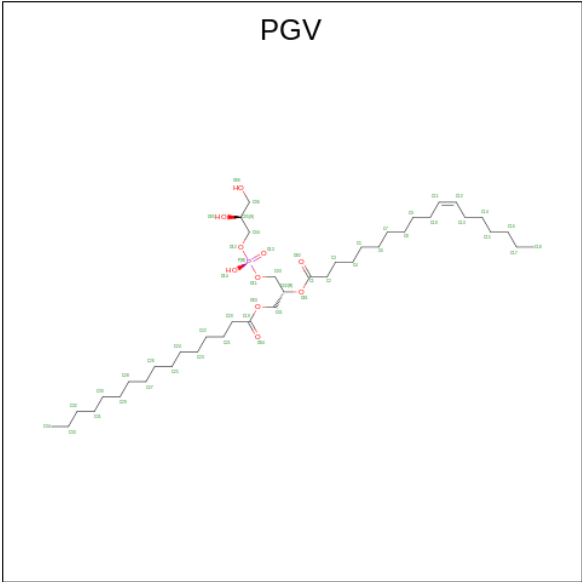
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	2	0
			388	259	66	60	3			
12	Y	46	Total	C	N	O	S	0	4	0
			394	261	66	64	3			

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

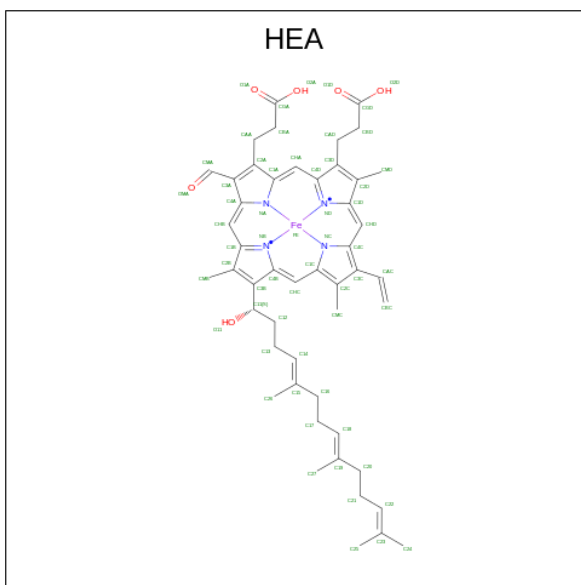
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			51	40	10	1		
14	A	1	Total	C	O	P	0	0
			51	40	10	1		
14	C	1	Total	C	O	P	0	0
			51	40	10	1		
14	C	1	Total	C	O	P	0	0
			51	40	10	1		
14	N	1	Total	C	O	P	0	0
			51	40	10	1		
14	N	1	Total	C	O	P	0	0
			51	40	10	1		
14	P	1	Total	C	O	P	0	0
			51	40	10	1		
14	P	1	Total	C	O	P	0	0
			51	40	10	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	
			79	67	1	4	7	0
15	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
15	N	1	Total	C	Fe	N	O	
			79	67	1	4	7	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

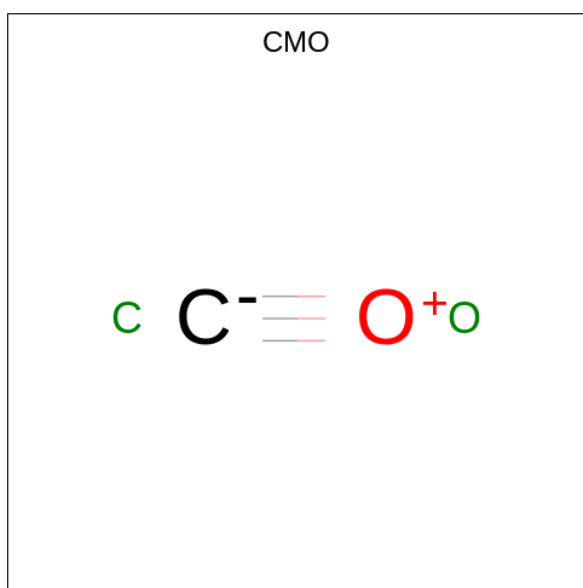
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

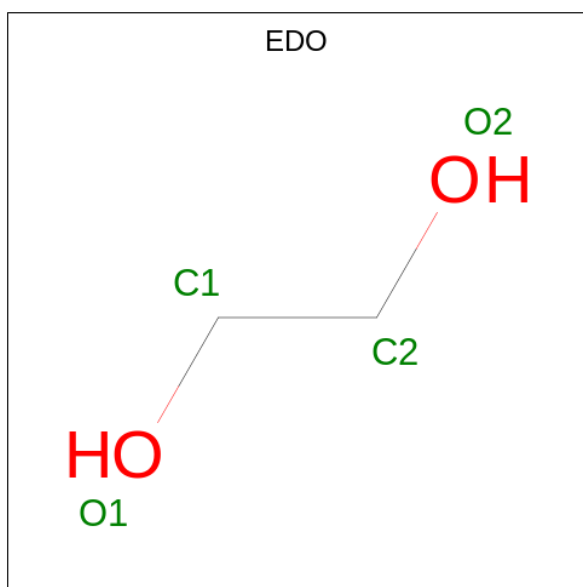
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	C	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		
18	P	1	Total	Na	0	0
			1	1		

- Molecule 19 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	1
			4	2	2		
19	N	1	Total	C	O	0	1
			4	2	2		

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



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	C	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	1
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	H	1	Total	C	O	0	0
			4	2	2		
20	H	1	Total	C	O	0	0
			4	2	2		
20	H	1	Total	C	O	0	0
			4	2	2		
20	J	1	Total	C	O	0	0
			4	2	2		
20	J	1	Total	C	O	0	0
			4	2	2		
20	K	1	Total	C	O	0	0
			4	2	2		
20	K	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		

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

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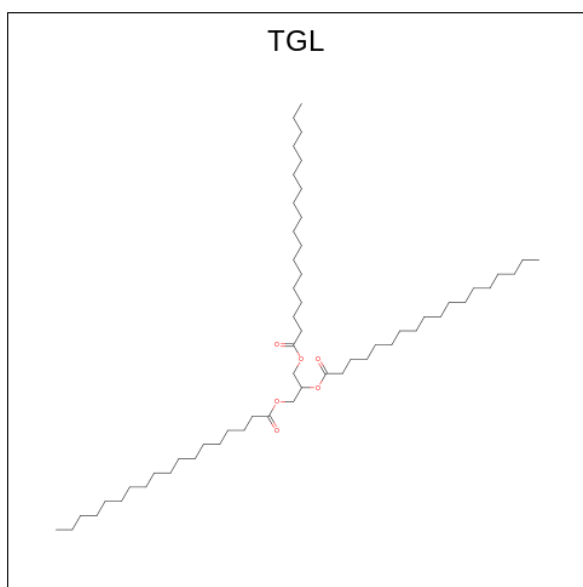
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4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

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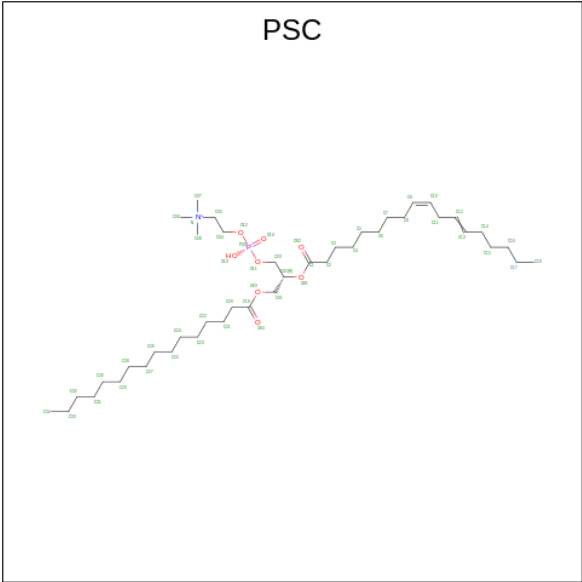
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	U	1	Total	C	O	0	0
			4	2	2		
20	V	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



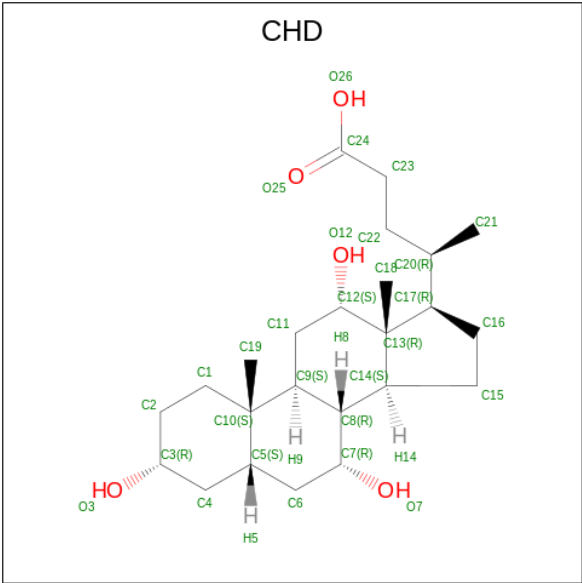
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (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).



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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



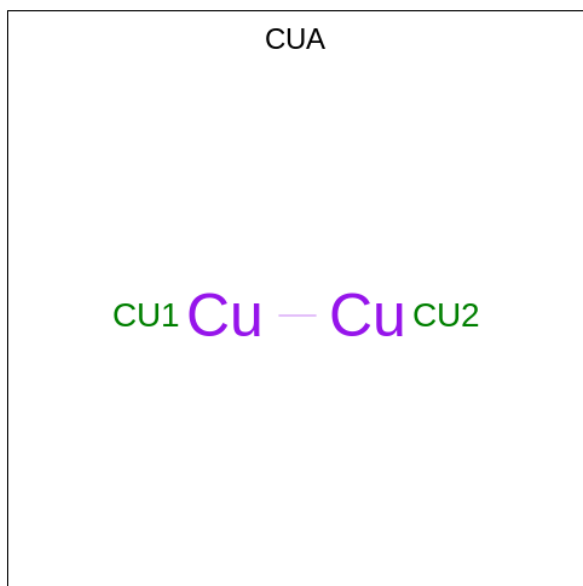
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	G	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0
23	Y	1	Total C O 29 24 5	0	0

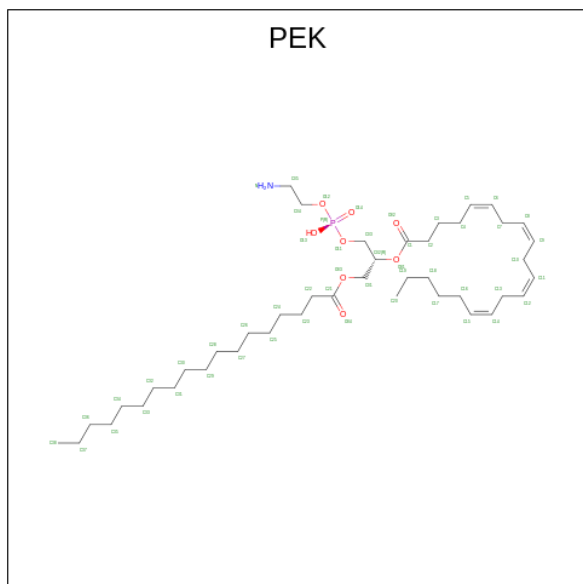
- Molecule 24 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

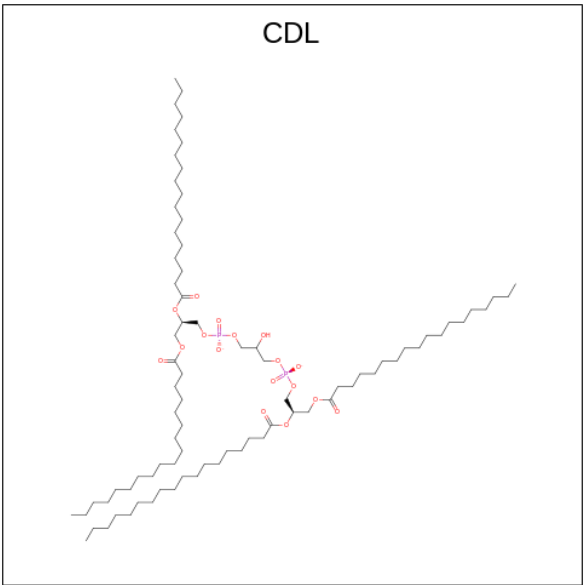


- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



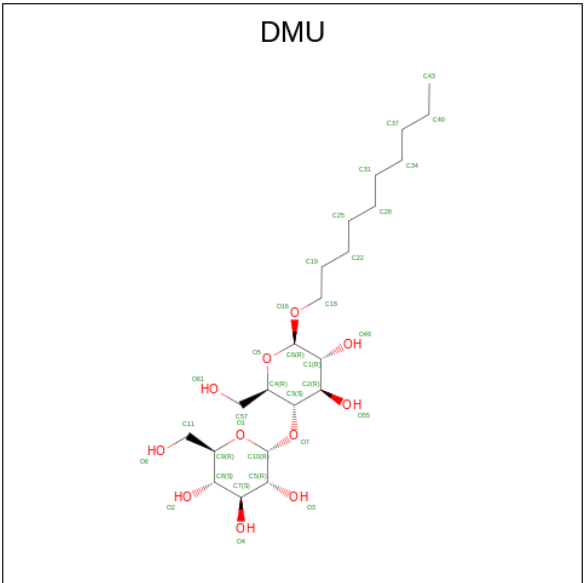
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C<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
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).

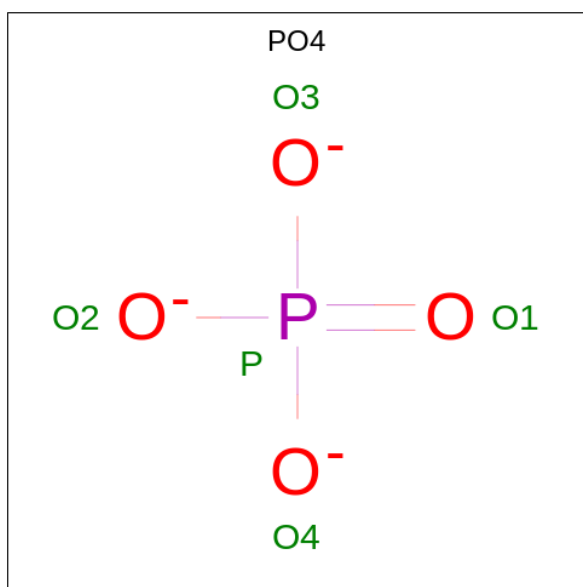


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 33 22 11	0	0
27	C	1	Total C O 33 22 11	0	0
27	G	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	V	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0

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

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

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



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	255	Total	O	0	0
			255	255		
30	B	194	Total	O	0	2
			195	195		
30	C	142	Total	O	0	0
			142	142		
30	D	167	Total	O	0	0
			167	167		
30	E	120	Total	O	0	0
			120	120		
30	F	130	Total	O	0	0
			130	130		
30	G	67	Total	O	0	0
			67	67		
30	H	78	Total	O	0	0
			78	78		
30	I	53	Total	O	0	0
			53	53		
30	J	39	Total	O	0	0
			39	39		

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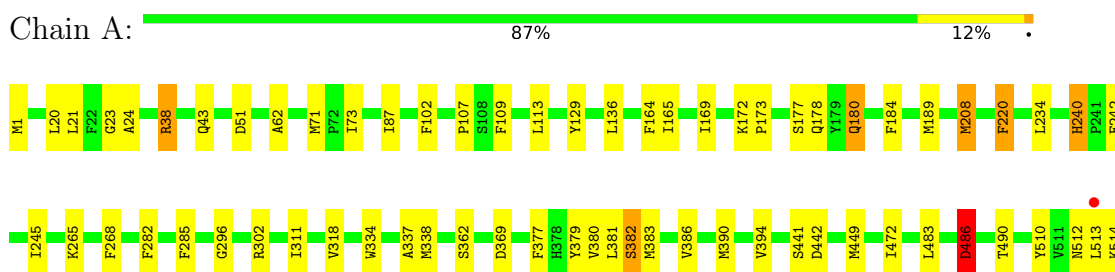
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	43	Total 43	O 43	0	0
30	L	38	Total 38	O 38	0	0
30	M	32	Total 32	O 32	0	0
30	N	240	Total 240	O 240	0	0
30	O	163	Total 164	O 164	0	1
30	P	138	Total 138	O 138	0	0
30	Q	85	Total 85	O 85	0	0
30	R	96	Total 96	O 96	0	0
30	S	129	Total 129	O 129	0	0
30	T	65	Total 65	O 65	0	0
30	U	72	Total 72	O 72	0	0
30	V	40	Total 40	O 40	0	0
30	W	45	Total 45	O 45	0	0
30	X	33	Total 33	O 33	0	0
30	Y	27	Total 27	O 27	0	0
30	Z	21	Total 21	O 21	0	0

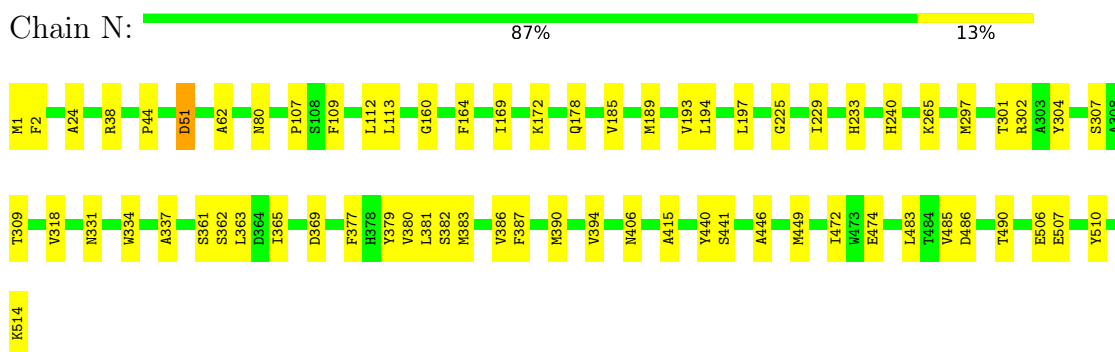
### 3 Residue-property plots

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.

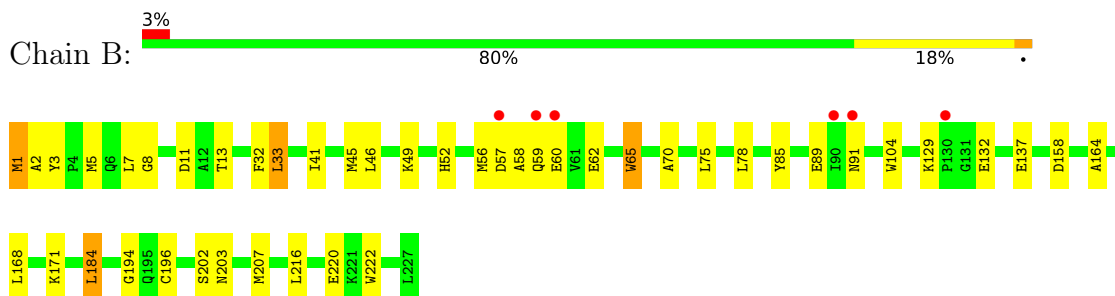
#### • Molecule 1: Cytochrome c oxidase subunit 1



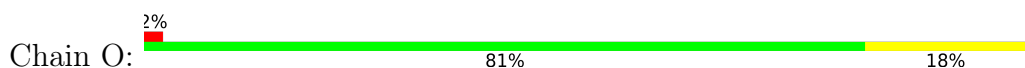
#### • Molecule 1: Cytochrome c oxidase subunit 1

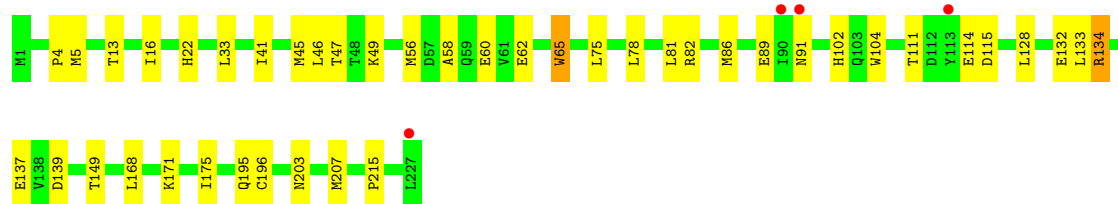


#### • Molecule 2: Cytochrome c oxidase subunit 2



#### • Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 91% 8%



● Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 89% 11%



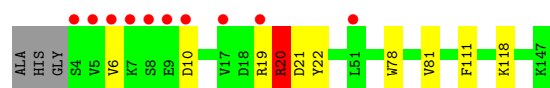
● Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 91% 6%



● Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 91% 6%



● Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 93% 2%

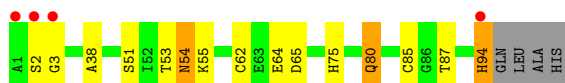
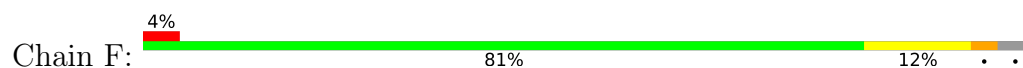


● Molecule 5: Cytochrome c oxidase subunit 5A

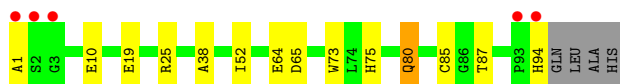
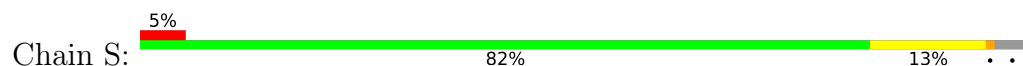
Chain R: 94% 2%



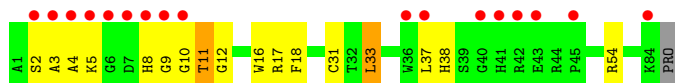
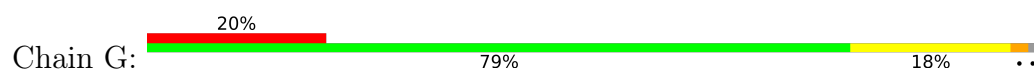
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



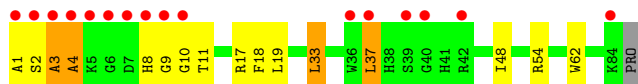
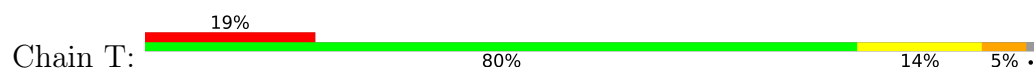
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



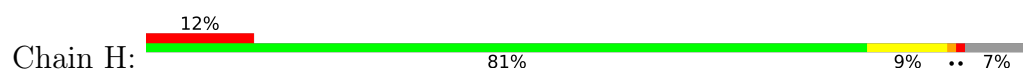
- Molecule 7: Cytochrome c oxidase subunit 6A2



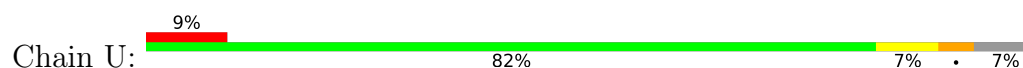
- Molecule 7: Cytochrome c oxidase subunit 6A2



- Molecule 8: Cytochrome c oxidase subunit 6B1

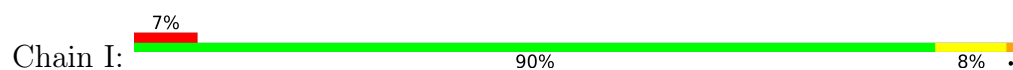


- Molecule 8: Cytochrome c oxidase subunit 6B1

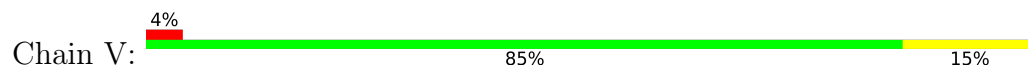


- Molecule 9: Cytochrome c oxidase subunit 6C

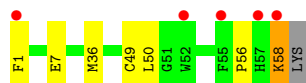
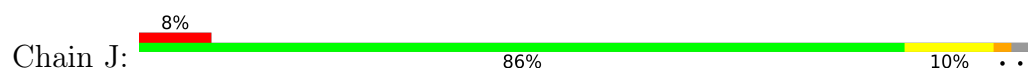




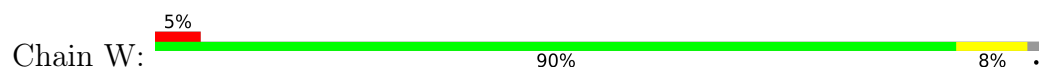
- Molecule 9: Cytochrome c oxidase subunit 6C



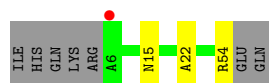
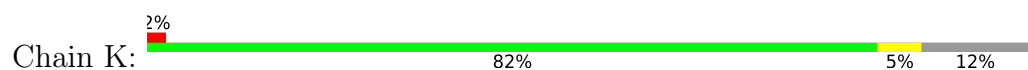
- Molecule 10: Cytochrome c oxidase subunit 7A1



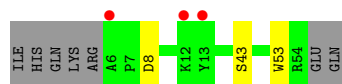
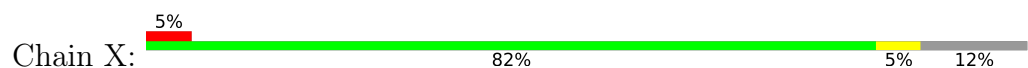
- Molecule 10: Cytochrome c oxidase subunit 7A1



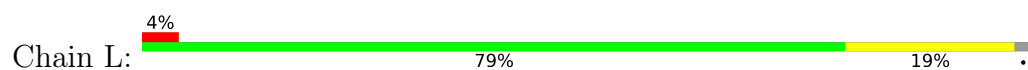
- Molecule 11: Cytochrome c oxidase subunit 7B



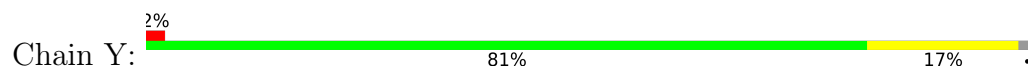
- Molecule 11: Cytochrome c oxidase subunit 7B



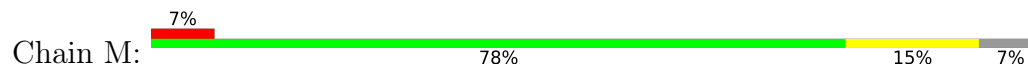
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



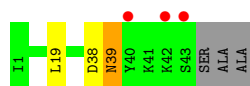
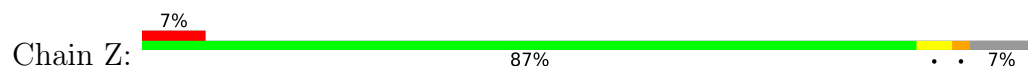
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.54Å 203.66Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 1.70 135.51 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.74-1.70) 99.6 (135.51-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.13-2998-000)	Depositor
R, $R_{free}$	0.159 , 0.178 0.159 , 0.179	Depositor DCC
$R_{free}$ test set	35759 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: CMO, EDO, PGV, CUA, NA, PEK, ZN, PSC, CDL, FME, MG, CHD, DMU, SAC, CU, TPO, TGL, HEA, 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	1.04	6/4390 (0.1%)	0.98	11/5989 (0.2%)
1	N	0.98	3/4371 (0.1%)	0.89	4/5964 (0.1%)
2	B	0.90	0/1961	0.94	6/2672 (0.2%)
2	O	0.81	2/1952 (0.1%)	0.87	4/2660 (0.2%)
3	C	0.94	1/2268 (0.0%)	0.82	0/3099
3	P	0.95	1/2289 (0.0%)	0.83	0/3126
4	D	0.83	0/1273	0.82	2/1716 (0.1%)
4	Q	0.60	0/1258	0.74	4/1696 (0.2%)
5	E	0.80	2/871 (0.2%)	0.76	1/1182 (0.1%)
5	R	0.63	0/871	0.66	0/1182
6	F	0.83	0/755	0.83	0/1026
6	S	0.77	1/755 (0.1%)	0.78	0/1025
7	G	0.81	0/690	0.70	0/937
7	T	0.72	0/698	0.74	0/948
8	H	0.87	0/682	0.80	0/921
8	U	0.74	0/682	0.72	0/921
9	I	0.68	0/605	0.72	1/802 (0.1%)
9	V	0.58	0/605	0.61	0/802
10	J	0.64	0/471	0.69	0/636
10	W	0.57	0/471	0.67	0/636
11	K	0.75	0/398	0.68	0/546
11	X	0.64	0/398	0.59	0/546
12	L	0.87	0/412	0.74	0/551
12	Y	0.80	0/430	0.65	0/575
13	M	0.80	0/345	0.72	0/470
13	Z	0.68	0/345	0.61	0/470
All	All	0.87	16/30246 (0.1%)	0.83	33/41098 (0.1%)

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

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

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

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362[A]	SER	CB-OG	-7.75	1.32	1.42
1	A	362[B]	SER	CB-OG	-7.75	1.32	1.42
1	N	362[A]	SER	CB-OG	-6.02	1.34	1.42
1	N	362[B]	SER	CB-OG	-6.02	1.34	1.42
3	P	94	PHE	CE2-CZ	5.98	1.48	1.37

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-17.52	72.16	100.20
4	Q	20[A]	ARG	NE-CZ-NH2	-8.93	115.83	120.30
4	Q	20[B]	ARG	NE-CZ-NH2	-8.93	115.83	120.30
4	Q	20[A]	ARG	NE-CZ-NH1	8.19	124.40	120.30
4	Q	20[B]	ARG	NE-CZ-NH1	8.19	124.40	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4092	56	0
1	N	4116	0	4070	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1869	0	1872	37	0
2	O	1865	0	1874	36	0
3	C	2131	0	2039	22	0
3	P	2141	0	2056	38	0
4	D	1214	0	1205	15	0
4	Q	1206	0	1196	13	0
5	E	852	0	845	2	0
5	R	852	0	845	1	0
6	F	723	0	702	9	0
6	S	723	0	705	12	0
7	G	675	0	644	18	0
7	T	678	0	644	14	0
8	H	662	0	623	6	0
8	U	662	0	623	7	0
9	I	601	0	613	7	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	3	0
11	K	384	0	366	3	0
11	X	384	0	366	3	0
12	L	388	0	389	12	0
12	Y	394	0	385	8	0
13	M	335	0	352	9	0
13	Z	335	0	352	2	0
14	A	102	0	152	3	0
14	C	102	0	152	4	0
14	N	102	0	152	4	0
14	P	102	0	152	7	0
15	A	139	0	112	6	0
15	N	139	0	112	6	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	C	1	0	0	0	0
18	N	1	0	0	0	0
18	P	1	0	0	1	0
19	A	4	0	0	0	0
19	N	4	0	0	0	0
20	A	76	0	114	9	0
20	B	40	0	60	10	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	28	0	42	3	0
20	D	24	0	33	3	2
20	E	12	0	18	0	0
20	F	24	0	36	1	0
20	G	20	0	30	4	0
20	H	12	0	18	5	0
20	J	8	0	12	2	0
20	K	8	0	12	2	0
20	L	16	0	24	0	0
20	M	16	0	24	3	0
20	N	84	0	126	13	0
20	O	20	0	30	2	0
20	P	44	0	66	5	0
20	Q	8	0	12	0	0
20	R	20	0	30	1	0
20	S	44	0	66	2	0
20	T	8	0	12	0	0
20	U	4	0	6	1	0
20	V	4	0	6	0	0
20	W	12	0	18	2	0
20	Y	8	0	12	0	0
21	B	63	0	110	4	0
21	D	63	0	110	9	0
21	L	63	0	110	11	0
21	N	63	0	110	2	0
21	Q	63	0	110	7	0
21	Y	63	0	110	11	0
22	B	52	0	80	10	0
22	O	52	0	80	5	0
23	B	29	0	39	0	0
23	C	87	0	117	3	0
23	G	29	0	39	1	0
23	J	29	0	39	3	0
23	P	87	0	117	9	0
23	W	29	0	39	3	0
23	Y	29	0	39	4	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	C	159	0	231	8	0
25	P	159	0	231	15	0
26	C	100	0	156	13	0
26	G	100	0	156	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	100	0	156	20	0
26	T	100	0	156	11	0
27	C	66	0	84	3	0
27	G	33	0	42	1	0
27	M	66	0	84	0	0
27	P	99	0	124	6	0
27	V	33	0	42	4	0
27	Z	66	0	84	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	255	0	0	6	0
30	B	195	0	0	3	2
30	C	142	0	0	1	0
30	D	167	0	0	1	2
30	E	120	0	0	1	0
30	F	130	0	0	2	0
30	G	67	0	0	0	0
30	H	78	0	0	1	0
30	I	53	0	0	1	0
30	J	39	0	0	1	0
30	K	43	0	0	0	0
30	L	38	0	0	1	0
30	M	32	0	0	0	0
30	N	240	0	0	3	0
30	O	164	0	0	3	0
30	P	138	0	0	4	0
30	Q	85	0	0	4	0
30	R	96	0	0	1	0
30	S	129	0	0	6	0
30	T	65	0	0	0	0
30	U	72	0	0	2	0
30	V	40	0	0	1	0
30	W	45	0	0	3	0
30	X	33	0	0	1	0
30	Y	27	0	0	1	0
30	Z	21	0	0	0	0
All	All	34489	0	32823	452	4

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 452 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)
8:H:24:ASN:HD21	20:H:103:EDO:H21	1.24	0.98
6:F:75:HIS:H	6:F:80[A]:GLN:HE22	1.12	0.97
1:N:178[B]:GLN:NE2	30:N:701:HOH:O	1.99	0.95
6:S:75:HIS:H	6:S:80[A]:GLN:HE22	1.14	0.93
25:P:305:PEK:H041	7:T:17:ARG:HH22	1.32	0.93

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:314:EDO:C2	20:D:206:EDO:C1[2_584]	1.49	0.71
30:B:479:HOH:O	30:D:306:HOH:O[2_584]	1.96	0.24
20:B:314:EDO:O2	20:D:206:EDO:C1[2_584]	1.97	0.23
30:B:551:HOH:O	30:D:426:HOH:O[2_584]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	543/514 (106%)	532 (98%)	11 (2%)	0	100	100
1	N	541/514 (105%)	532 (98%)	9 (2%)	0	100	100
2	B	236/227 (104%)	231 (98%)	5 (2%)	0	100	100
2	O	235/227 (104%)	228 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	260 (98%)	6 (2%)	0	100	100
3	P	268/261 (103%)	263 (98%)	5 (2%)	0	100	100
4	D	147/147 (100%)	144 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	140 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
6	S	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
7	G	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	13	3
7	T	82/85 (96%)	73 (89%)	6 (7%)	3 (4%)	3	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	12	2
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
12	Y	47/47 (100%)	46 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3616/3614 (100%)	3521 (97%)	87 (2%)	8 (0%)	47	30

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	T	4	ALA
7	G	10	GLY
8	H	8	ILE
8	H	9	LYS
7	T	3	ALA

### 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	455/426 (107%)	445 (98%)	10 (2%)	52	34
1	N	453/426 (106%)	447 (99%)	6 (1%)	69	56
2	B	221/210 (105%)	213 (96%)	8 (4%)	35	16
2	O	220/210 (105%)	212 (96%)	8 (4%)	35	16
3	C	233/226 (103%)	230 (99%)	3 (1%)	69	56
3	P	235/226 (104%)	232 (99%)	3 (1%)	69	56
4	D	133/129 (103%)	131 (98%)	2 (2%)	65	51
4	Q	131/129 (102%)	129 (98%)	2 (2%)	65	51
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	63
5	R	92/95 (97%)	91 (99%)	1 (1%)	73	63
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	3
6	S	81/81 (100%)	79 (98%)	2 (2%)	47	29
7	G	67/68 (98%)	63 (94%)	4 (6%)	19	6
7	T	68/68 (100%)	64 (94%)	4 (6%)	19	6
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	12
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	7
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	43
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	17
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	12
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	12
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	28
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	41/40 (102%)	41 (100%)	0	100	100
12	Y	43/40 (108%)	40 (93%)	3 (7%)	15	3
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	7
All	All	3152/3082 (102%)	3072 (98%)	80 (2%)	52	29

5 of 80 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
9	V	15	ARG
4	Q	20[B]	ARG
7	T	37	LEU
12	Y	2[A]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
8	U	10	ASN
9	V	20	HIS
10	J	57	HIS
13	M	39	ASN
2	O	91	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	TPO	T	11	7	8,10,11	1.32	1 (12%)	10,14,16	0.79	0
9	SAC	I	1	9	7,8,9	0.63	0	8,9,11	0.94	0
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	0.83	0
7	TPO	G	11	7	8,10,11	1.32	1 (12%)	10,14,16	0.85	0
2	FME	O	1	2	8,9,10	0.87	0	7,9,11	0.94	0
2	FME	B	1	2	8,9,10	0.94	0	7,9,11	1.48	1 (14%)
1	FME	A	1	1	8,9,10	0.50	0	7,9,11	1.88	2 (28%)
1	FME	N	1	1	8,9,10	0.42	0	7,9,11	1.29	1 (14%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.81	1.59	1.50
7	G	11	TPO	P-O1P	2.80	1.59	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	3.42	115.91	109.73
1	A	1	FME	CE-SD-CG	2.42	108.71	100.40
2	B	1	FME	O-C-CA	-2.19	119.03	124.78
1	N	1	FME	O-C-CA	-2.02	119.50	124.78

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	2	0
2	B	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 209 ligands modelled in this entry, 10 are monoatomic - leaving 199 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	$\# Z  > 2$
20	EDO	F	107	-	3,3,3	0.36	0	2,2,2	0.57	0
20	EDO	A	610	-	3,3,3	0.90	0	2,2,2	1.03	0
20	EDO	W	103	-	3,3,3	0.87	0	2,2,2	0.44	0
20	EDO	R	202	-	3,3,3	0.61	0	2,2,2	0.22	0
20	EDO	A	613	-	3,3,3	0.72	0	2,2,2	0.37	0
20	EDO	C	317	-	3,3,3	0.39	0	2,2,2	0.03	0
20	EDO	B	312	-	3,3,3	0.58	0	2,2,2	0.20	0
20	EDO	M	103	-	3,3,3	0.46	0	2,2,2	0.13	0
21	TGL	L	101	-	62,62,62	1.06	3 (4%)	65,65,65	1.20	8 (12%)
25	PEK	C	305	-	52,52,52	0.94	2 (3%)	55,57,57	1.19	5 (9%)
21	TGL	N	608	-	62,62,62	1.02	3 (4%)	65,65,65	1.20	4 (6%)
20	EDO	S	106	-	3,3,3	0.43	0	2,2,2	0.56	0
29	PO4	H	104	-	4,4,4	0.93	0	6,6,6	0.36	0
27	DMU	P	323	-	34,34,34	0.44	0	45,45,45	0.89	2 (4%)
20	EDO	N	628	-	3,3,3	0.42	0	2,2,2	1.09	0
20	EDO	O	305	-	3,3,3	0.47	0	2,2,2	0.22	0
20	EDO	Y	102	-	3,3,3	0.53	0	2,2,2	0.37	0
20	EDO	G	103	-	3,3,3	0.56	0	2,2,2	0.32	0
20	EDO	R	204	-	3,3,3	0.51	0	2,2,2	0.25	0
24	CUA	O	302	2	0,1,1	0.00	-	-	-	-
20	EDO	A	625	-	3,3,3	0.54	0	2,2,2	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	H	101	-	3,3,3	0.43	0	2,2,2	0.53	0
20	EDO	T	103	-	3,3,3	0.57	0	2,2,2	0.53	0
20	EDO	D	202	-	3,3,3	0.60	0	2,2,2	0.20	0
27	DMU	G	108	-	34,34,34	0.48	0	45,45,45	1.17	3 (6%)
20	EDO	S	109	-	3,3,3	0.47	0	2,2,2	0.44	0
20	EDO	B	305	-	3,3,3	0.48	0	2,2,2	0.68	0
20	EDO	J	102	-	3,3,3	0.40	0	2,2,2	0.35	0
20	EDO	D	203	-	3,3,3	0.50	0	2,2,2	0.14	0
20	EDO	P	315	-	3,3,3	1.06	0	2,2,2	0.56	0
20	EDO	D	207	-	3,3,3	0.48	0	2,2,2	0.77	0
25	PEK	C	304	-	52,52,52	0.86	2 (3%)	55,57,57	1.07	3 (5%)
22	PSC	B	302	-	51,51,51	1.09	3 (5%)	57,59,59	1.34	7 (12%)
20	EDO	A	612	-	3,3,3	0.60	0	2,2,2	0.67	0
20	EDO	S	105	-	3,3,3	0.53	0	2,2,2	0.13	0
20	EDO	C	314	-	3,3,3	0.54	0	2,2,2	0.39	0
15	HEA	N	603	1	44,67,67	1.22	3 (6%)	37,103,103	1.63	9 (24%)
20	EDO	W	102	-	3,3,3	0.30	0	2,2,2	0.67	0
20	EDO	P	317	-	3,3,3	0.66	0	2,2,2	0.17	0
23	CHD	P	301	-	29,32,32	0.86	1 (3%)	48,51,51	1.50	10 (20%)
20	EDO	N	610	-	3,3,3	1.10	0	2,2,2	0.52	0
21	TGL	B	301	-	62,62,62	1.13	4 (6%)	65,65,65	1.29	5 (7%)
20	EDO	G	106	-	3,3,3	0.62	0	2,2,2	0.69	0
23	CHD	C	309	-	29,32,32	0.65	0	48,51,51	1.16	6 (12%)
20	EDO	N	618	-	3,3,3	0.77	0	2,2,2	1.14	0
20	EDO	P	318	-	3,3,3	0.74	0	2,2,2	0.11	0
20	EDO	O	307	-	3,3,3	0.49	0	2,2,2	0.27	0
20	EDO	P	319	-	3,3,3	0.95	0	2,2,2	0.45	0
20	EDO	L	102	-	3,3,3	0.54	0	2,2,2	0.09	0
23	CHD	Y	104	-	29,32,32	0.81	1 (3%)	48,51,51	1.85	14 (29%)
20	EDO	B	310	-	3,3,3	0.45	0	2,2,2	0.24	0
20	EDO	B	313	-	3,3,3	0.56	0	2,2,2	0.37	0
27	DMU	M	101	-	34,34,34	0.50	0	45,45,45	1.09	3 (6%)
20	EDO	B	311	-	3,3,3	0.54	0	2,2,2	0.11	0
20	EDO	M	102	-	3,3,3	0.47	0	2,2,2	0.34	0
20	EDO	N	623	-	3,3,3	0.52	0	2,2,2	0.39	0
20	EDO	P	322	-	3,3,3	0.54	0	2,2,2	0.33	0
20	EDO	A	616	-	3,3,3	0.43	0	2,2,2	0.64	0
23	CHD	W	101	-	29,32,32	0.64	1 (3%)	48,51,51	1.60	7 (14%)
27	DMU	V	102	-	34,34,34	0.55	1 (2%)	45,45,45	1.03	3 (6%)
20	EDO	V	101	-	3,3,3	0.48	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	N	617	-	3,3,3	0.32	0	2,2,2	0.81	0
14	PGV	C	307	-	50,50,50	0.96	2 (4%)	53,56,56	1.58	7 (13%)
20	EDO	B	307	-	3,3,3	0.59	0	2,2,2	0.22	0
20	EDO	B	308	-	3,3,3	0.59	0	2,2,2	0.41	0
20	EDO	Q	203	-	3,3,3	0.42	0	2,2,2	0.40	0
21	TGL	Y	101	-	62,62,62	1.02	3 (4%)	65,65,65	1.14	4 (6%)
20	EDO	G	105	-	3,3,3	0.54	0	2,2,2	0.15	0
20	EDO	A	611	-	3,3,3	0.67	0	2,2,2	0.59	0
20	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.50	0
29	PO4	U	102	-	4,4,4	0.98	0	6,6,6	0.40	0
20	EDO	J	103	-	3,3,3	0.40	0	2,2,2	0.49	0
27	DMU	Z	102	-	34,34,34	0.48	0	45,45,45	1.13	3 (6%)
20	EDO	N	626	-	3,3,3	0.35	0	2,2,2	0.33	0
20	EDO	P	314	-	3,3,3	0.42	0	2,2,2	0.78	0
20	EDO	N	613	-	3,3,3	0.45	0	2,2,2	0.46	0
20	EDO	N	625	-	3,3,3	0.71	0	2,2,2	0.30	0
20	EDO	N	612	-	3,3,3	0.52	0	2,2,2	0.67	0
21	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.00	6 (9%)
27	DMU	C	319	-	34,34,34	0.48	0	45,45,45	1.05	3 (6%)
15	HEA	N	602[A]	-	44,67,67	1.31	4 (9%)	37,103,103	2.33	11 (29%)
14	PGV	N	609	-	50,50,50	1.01	5 (10%)	53,56,56	1.12	3 (5%)
27	DMU	P	324	-	34,34,34	0.55	0	45,45,45	0.73	1 (2%)
26	CDL	T	101	-	99,99,99	1.30	12 (12%)	105,111,111	1.11	6 (5%)
22	PSC	O	301	-	51,51,51	1.10	3 (5%)	57,59,59	1.26	5 (8%)
20	EDO	C	316	-	3,3,3	0.89	0	2,2,2	0.61	0
20	EDO	F	103	-	3,3,3	0.44	0	2,2,2	0.16	0
20	EDO	F	106	-	3,3,3	0.90	0	2,2,2	0.42	0
23	CHD	J	101	-	29,32,32	0.70	1 (3%)	48,51,51	1.76	12 (25%)
19	CMO	N	607[A]	-	0,1,1	0.00	-	-	-	-
20	EDO	P	313	-	3,3,3	0.43	0	2,2,2	0.30	0
20	EDO	N	630	-	3,3,3	0.39	0	2,2,2	0.12	0
23	CHD	P	310	-	29,32,32	0.78	1 (3%)	48,51,51	1.90	12 (25%)
20	EDO	S	108	-	3,3,3	0.72	0	2,2,2	0.42	0
14	PGV	A	608	-	50,50,50	0.88	2 (4%)	53,56,56	0.88	1 (1%)
20	EDO	L	103	-	3,3,3	0.57	0	2,2,2	0.11	0
20	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.21	0
20	EDO	G	104	-	3,3,3	0.44	0	2,2,2	0.52	0
20	EDO	P	316	-	3,3,3	0.67	0	2,2,2	0.36	0
25	PEK	C	303	-	52,52,52	0.93	2 (3%)	55,57,57	1.30	5 (9%)
20	EDO	U	101	-	3,3,3	0.61	0	2,2,2	0.27	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	O	306	-	3,3,3	0.52	0	2,2,2	0.17	0
23	CHD	G	102	-	29,32,32	0.93	0	48,51,51	1.42	7 (14%)
20	EDO	L	104	-	3,3,3	0.82	0	2,2,2	0.15	0
23	CHD	C	311	-	29,32,32	0.80	1 (3%)	48,51,51	1.80	10 (20%)
21	TGL	D	201	-	62,62,62	1.20	4 (6%)	65,65,65	0.94	5 (7%)
15	HEA	N	602[B]	-	44,67,67	1.23	4 (9%)	37,103,103	1.98	9 (24%)
20	EDO	S	110	-	3,3,3	0.66	0	2,2,2	0.66	0
20	EDO	A	622	-	3,3,3	0.33	0	2,2,2	0.57	0
15	HEA	A	603	1	44,67,67	1.17	4 (9%)	37,103,103	1.87	12 (32%)
20	EDO	N	629	-	3,3,3	0.41	0	2,2,2	0.35	0
20	EDO	E	203	-	3,3,3	0.55	0	2,2,2	0.51	0
27	DMU	C	310	-	34,34,34	0.42	0	45,45,45	0.88	0
20	EDO	A	618	-	3,3,3	0.42	0	2,2,2	0.51	0
14	PGV	P	306	-	50,50,50	0.77	1 (2%)	53,56,56	1.23	4 (7%)
19	CMO	N	607[B]	16	0,1,1	0.00	-	-		
19	CMO	A	607[A]	-	0,1,1	0.00	-	-		
20	EDO	K	101	-	3,3,3	0.68	0	2,2,2	0.12	0
20	EDO	N	615	-	3,3,3	0.51	0	2,2,2	0.38	0
20	EDO	R	205	-	3,3,3	0.53	0	2,2,2	0.21	0
20	EDO	D	206	20	3,3,3	0.43	0	2,2,2	0.40	0
20	EDO	A	620	-	3,3,3	0.63	0	2,2,2	1.08	0
23	CHD	C	301	-	29,32,32	1.02	3 (10%)	48,51,51	1.59	8 (16%)
20	EDO	R	203	-	3,3,3	0.55	0	2,2,2	0.25	0
14	PGV	P	307	-	50,50,50	0.97	2 (4%)	53,56,56	1.36	8 (15%)
20	EDO	P	312	-	3,3,3	0.47	0	2,2,2	1.02	0
20	EDO	S	103	-	3,3,3	0.83	0	2,2,2	0.11	0
23	CHD	B	303	-	29,32,32	1.14	2 (6%)	48,51,51	1.79	12 (25%)
14	PGV	N	601	-	50,50,50	0.92	2 (4%)	53,56,56	1.20	5 (9%)
20	EDO	A	627	-	3,3,3	0.83	0	2,2,2	0.56	0
25	PEK	P	305	-	52,52,52	0.96	2 (3%)	55,57,57	1.22	5 (9%)
25	PEK	P	304	-	52,52,52	0.70	2 (3%)	55,57,57	1.12	5 (9%)
20	EDO	M	105	-	3,3,3	1.17	0	2,2,2	0.72	0
20	EDO	O	303	-	3,3,3	0.87	0	2,2,2	0.46	0
20	EDO	Q	202	-	3,3,3	0.42	0	2,2,2	0.33	0
20	EDO	N	621	-	3,3,3	0.59	0	2,2,2	0.26	0
20	EDO	R	201	-	3,3,3	0.60	0	2,2,2	0.52	0
20	EDO	A	619	-	3,3,3	0.39	0	2,2,2	0.86	0
20	EDO	C	315	-	3,3,3	0.61	0	2,2,2	0.47	0
20	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.57	0
20	EDO	S	111	-	3,3,3	0.77	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	O	304	-	3,3,3	0.49	0	2,2,2	0.13	0
20	EDO	F	105	-	3,3,3	0.53	0	2,2,2	0.13	0
27	DMU	P	309	-	34,34,34	0.46	0	45,45,45	0.69	0
20	EDO	A	623	-	3,3,3	0.60	0	2,2,2	0.39	0
26	CDL	C	308	-	99,99,99	1.31	12 (12%)	105,111,111	1.23	9 (8%)
20	EDO	H	102	-	3,3,3	0.54	0	2,2,2	0.16	0
20	EDO	E	201	-	3,3,3	0.41	0	2,2,2	0.46	0
20	EDO	W	104	-	3,3,3	0.52	0	2,2,2	0.30	0
14	PGV	A	601	-	50,50,50	0.96	2 (4%)	53,56,56	1.08	4 (7%)
19	CMO	A	607[B]	16	0,1,1	0.00	-	-		
20	EDO	A	614	-	3,3,3	0.47	0	2,2,2	0.19	0
15	HEA	A	602[A]	-	44,67,67	1.37	6 (13%)	37,103,103	2.20	8 (21%)
20	EDO	T	102	-	3,3,3	0.69	0	2,2,2	0.94	0
20	EDO	P	321	-	3,3,3	0.59	0	2,2,2	0.49	0
20	EDO	Y	103	-	3,3,3	0.44	0	2,2,2	0.24	0
26	CDL	G	101	-	99,99,99	1.32	12 (12%)	105,111,111	1.46	11 (10%)
27	DMU	M	106	-	34,34,34	0.59	1 (2%)	45,45,45	1.19	4 (8%)
20	EDO	S	107	-	3,3,3	0.49	0	2,2,2	0.36	0
20	EDO	A	621	-	3,3,3	0.61	0	2,2,2	0.42	0
20	EDO	N	622	-	3,3,3	0.57	0	2,2,2	0.52	0
20	EDO	S	112	-	3,3,3	0.50	0	2,2,2	1.65	1 (50%)
26	CDL	P	308	-	99,99,99	1.34	12 (12%)	105,111,111	1.32	9 (8%)
20	EDO	A	624	-	3,3,3	0.40	0	2,2,2	0.64	0
20	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.31	0
20	EDO	N	624	-	3,3,3	0.61	0	2,2,2	0.28	0
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.86	2 (4%)
20	EDO	M	104	-	3,3,3	0.63	0	2,2,2	0.50	0
20	EDO	A	617	-	3,3,3	0.66	0	2,2,2	0.17	0
20	EDO	N	619	-	3,3,3	0.55	0	2,2,2	0.28	0
20	EDO	C	318	-	3,3,3	0.70	0	2,2,2	0.09	0
20	EDO	P	320	-	3,3,3	0.47	0	2,2,2	0.29	0
20	EDO	A	626	-	3,3,3	0.68	0	2,2,2	1.03	0
20	EDO	F	104	-	3,3,3	0.88	0	2,2,2	0.07	0
20	EDO	N	620	-	3,3,3	0.59	0	2,2,2	0.43	0
20	EDO	S	104	-	3,3,3	0.82	0	2,2,2	0.74	0
24	CUA	B	304	2	0,1,1	0.00	-	-		
14	PGV	C	306	-	50,50,50	0.80	2 (4%)	53,56,56	0.95	3 (5%)
20	EDO	A	615	-	3,3,3	0.63	0	2,2,2	0.17	0
20	EDO	B	306	-	3,3,3	0.82	0	2,2,2	0.34	0
20	EDO	C	312	-	3,3,3	0.75	0	2,2,2	0.11	0
20	EDO	C	313	-	3,3,3	0.77	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	L	105	-	3,3,3	0.56	0	2,2,2	0.29	0
23	CHD	P	311	-	29,32,32	0.72	0	48,51,51	1.21	7 (14%)
25	PEK	P	303	-	52,52,52	0.94	2 (3%)	55,57,57	1.15	5 (9%)
20	EDO	S	102	-	3,3,3	0.95	0	2,2,2	0.78	0
15	HEA	A	602[B]	-	44,67,67	1.38	6 (13%)	37,103,103	1.91	7 (18%)
20	EDO	H	103	-	3,3,3	0.50	0	2,2,2	0.18	0
20	EDO	D	205	-	3,3,3	0.69	0	2,2,2	0.42	0
20	EDO	N	616	-	3,3,3	0.53	0	2,2,2	0.39	0
20	EDO	E	202	-	3,3,3	0.65	0	2,2,2	0.07	0
20	EDO	B	314	20	3,3,3	0.48	0	2,2,2	0.39	0
20	EDO	B	309	-	3,3,3	0.42	0	2,2,2	0.10	0
20	EDO	G	107	-	3,3,3	0.72	0	2,2,2	0.13	0
20	EDO	N	627	-	3,3,3	0.44	0	2,2,2	0.48	0
20	EDO	N	611	-	3,3,3	0.68	0	2,2,2	0.56	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
20	EDO	F	107	-	-	1/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-
20	EDO	W	103	-	-	1/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	C	317	-	-	0/1/1/1	-
20	EDO	B	312	-	-	0/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-
21	TGL	L	101	-	-	29/65/65/65	-
25	PEK	C	305	-	-	19/56/56/56	-
21	TGL	N	608	-	-	19/65/65/65	-
20	EDO	S	106	-	-	0/1/1/1	-
27	DMU	P	323	-	-	3/19/59/59	0/2/2/2
20	EDO	N	628	-	-	1/1/1/1	-
20	EDO	O	305	-	-	1/1/1/1	-
20	EDO	Y	102	-	-	0/1/1/1	-
20	EDO	G	103	-	-	1/1/1/1	-
20	EDO	R	204	-	-	1/1/1/1	-
15	HEA	A	602[C]	-	3/3/3/16	-	-
20	EDO	A	625	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	H	101	-	-	0/1/1/1	-
20	EDO	T	103	-	-	1/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
27	DMU	G	108	-	-	6/19/59/59	0/2/2/2
20	EDO	S	109	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	J	102	-	-	0/1/1/1	-
20	EDO	D	203	-	-	0/1/1/1	-
20	EDO	P	315	-	-	0/1/1/1	-
20	EDO	D	207	-	-	0/1/1/1	-
25	PEK	C	304	-	-	12/56/56/56	-
22	PSC	B	302	-	-	20/55/55/55	-
20	EDO	A	612	-	-	0/1/1/1	-
20	EDO	S	105	-	-	0/1/1/1	-
20	EDO	C	314	-	-	0/1/1/1	-
15	HEA	N	603	1	3/3/7/16	0/24/76/76	-
20	EDO	W	102	-	-	1/1/1/1	-
20	EDO	P	317	-	-	0/1/1/1	-
23	CHD	P	301	-	-	1/7/74/74	0/4/4/4
20	EDO	N	610	-	-	0/1/1/1	-
21	TGL	B	301	-	-	19/65/65/65	-
20	EDO	G	106	-	-	0/1/1/1	-
23	CHD	C	309	-	-	3/7/74/74	0/4/4/4
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	P	318	-	-	0/1/1/1	-
20	EDO	O	307	-	-	0/1/1/1	-
20	EDO	P	319	-	-	0/1/1/1	-
20	EDO	L	102	-	-	1/1/1/1	-
23	CHD	Y	104	-	-	7/7/74/74	0/4/4/4
20	EDO	B	310	-	-	0/1/1/1	-
20	EDO	B	313	-	-	1/1/1/1	-
27	DMU	M	101	-	-	7/19/59/59	0/2/2/2
20	EDO	B	311	-	-	0/1/1/1	-
20	EDO	M	102	-	-	0/1/1/1	-
20	EDO	N	623	-	-	1/1/1/1	-
20	EDO	P	322	-	-	0/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
23	CHD	W	101	-	-	6/7/74/74	0/4/4/4
27	DMU	V	102	-	-	11/19/59/59	0/2/2/2
20	EDO	V	101	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	617	-	-	0/1/1/1	-
14	PGV	C	307	-	-	12/55/55/55	-
20	EDO	B	307	-	-	1/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	1/1/1/1	-
21	TGL	Y	101	-	-	30/65/65/65	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	J	103	-	-	1/1/1/1	-
27	DMU	Z	102	-	-	9/19/59/59	0/2/2/2
20	EDO	N	626	-	-	0/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	N	625	-	-	1/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	21/65/65/65	-
27	DMU	C	319	-	-	9/19/59/59	0/2/2/2
15	HEA	N	602[A]	-	3/3/7/16	0/24/76/76	-
14	PGV	N	609	-	-	5/55/55/55	-
27	DMU	P	324	-	-	13/19/59/59	0/2/2/2
26	CDL	T	101	-	-	36/110/110/110	-
22	PSC	O	301	-	-	20/55/55/55	-
20	EDO	C	316	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	F	106	-	-	0/1/1/1	-
23	CHD	J	101	-	-	7/7/74/74	0/4/4/4
20	EDO	P	313	-	-	1/1/1/1	-
20	EDO	N	630	-	-	0/1/1/1	-
23	CHD	P	310	-	-	1/7/74/74	0/4/4/4
20	EDO	S	108	-	-	1/1/1/1	-
14	PGV	A	608	-	-	8/55/55/55	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	K	102	-	-	0/1/1/1	-
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	P	316	-	-	1/1/1/1	-
25	PEK	C	303	-	-	21/56/56/56	-
20	EDO	U	101	-	-	0/1/1/1	-
20	EDO	O	306	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	G	102	-	-	0/7/74/74	0/4/4/4
20	EDO	L	104	-	-	1/1/1/1	-
23	CHD	C	311	-	-	1/7/74/74	0/4/4/4
21	TGL	D	201	-	-	19/65/65/65	-
15	HEA	N	602[B]	-	3/3/7/16	1/24/76/76	-
20	EDO	S	110	-	-	0/1/1/1	-
20	EDO	A	622	-	-	0/1/1/1	-
15	HEA	A	603	1	3/3/7/16	0/24/76/76	-
20	EDO	N	629	-	-	1/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
27	DMU	C	310	-	-	4/19/59/59	0/2/2/2
20	EDO	A	618	-	-	0/1/1/1	-
14	PGV	P	306	-	-	8/55/55/55	-
20	EDO	K	101	-	-	0/1/1/1	-
20	EDO	R	205	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	D	206	20	-	0/1/1/1	-
20	EDO	A	620	-	-	1/1/1/1	-
23	CHD	C	301	-	-	0/7/74/74	0/4/4/4
20	EDO	R	203	-	-	0/1/1/1	-
14	PGV	P	307	-	-	10/55/55/55	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
23	CHD	B	303	-	-	0/7/74/74	0/4/4/4
14	PGV	N	601	-	-	20/55/55/55	-
20	EDO	A	627	-	-	0/1/1/1	-
25	PEK	P	305	-	-	21/56/56/56	-
25	PEK	P	304	-	-	9/56/56/56	-
20	EDO	M	105	-	-	1/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	Q	202	-	-	1/1/1/1	-
20	EDO	N	621	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	A	619	-	-	0/1/1/1	-
20	EDO	C	315	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	S	111	-	-	1/1/1/1	-
20	EDO	O	304	-	-	0/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-
15	HEA	N	602[C]	-	3/3/3/16	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	P	309	-	-	6/19/59/59	0/2/2/2
20	EDO	A	623	-	-	0/1/1/1	-
26	CDL	C	308	-	-	38/110/110/110	-
20	EDO	H	102	-	-	0/1/1/1	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	W	104	-	-	1/1/1/1	-
14	PGV	A	601	-	-	11/55/55/55	-
20	EDO	A	614	-	-	0/1/1/1	-
15	HEA	A	602[A]	-	3/3/7/16	1/24/76/76	-
20	EDO	T	102	-	-	0/1/1/1	-
20	EDO	P	321	-	-	1/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-
26	CDL	G	101	-	-	32/110/110/110	-
27	DMU	M	106	-	-	7/19/59/59	0/2/2/2
20	EDO	S	107	-	-	1/1/1/1	-
20	EDO	A	621	-	-	0/1/1/1	-
20	EDO	N	622	-	-	1/1/1/1	-
20	EDO	S	112	-	-	1/1/1/1	-
26	CDL	P	308	-	-	36/110/110/110	-
20	EDO	A	624	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	N	624	-	-	1/1/1/1	-
27	DMU	Z	101	-	-	2/19/59/59	0/2/2/2
20	EDO	M	104	-	-	1/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	N	619	-	-	0/1/1/1	-
20	EDO	C	318	-	-	0/1/1/1	-
20	EDO	P	320	-	-	0/1/1/1	-
20	EDO	A	626	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	N	620	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
14	PGV	C	306	-	-	10/55/55/55	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	C	312	-	-	0/1/1/1	-
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	L	105	-	-	0/1/1/1	-
23	CHD	P	311	-	-	3/7/74/74	0/4/4/4
25	PEK	P	303	-	-	19/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	S	102	-	-	0/1/1/1	-
15	HEA	A	602[B]	-	3/3/7/16	0/24/76/76	-
20	EDO	H	103	-	-	0/1/1/1	-
20	EDO	D	205	-	-	1/1/1/1	-
20	EDO	N	616	-	-	1/1/1/1	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	B	314	20	-	0/1/1/1	-
20	EDO	B	309	-	-	0/1/1/1	-
20	EDO	G	107	-	-	0/1/1/1	-
20	EDO	N	627	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	201	TGL	OG2-CB1	5.06	1.48	1.34
21	B	301	TGL	OG3-CC1	4.91	1.47	1.33
21	B	301	TGL	OG1-CA1	4.83	1.47	1.33
26	G	101	CDL	OA8-CA7	4.62	1.46	1.33
14	A	601	PGV	O03-C19	4.60	1.46	1.33

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[A]	HEA	C13-C12-C11	-8.27	101.93	114.35
15	A	602[A]	HEA	C13-C12-C11	-6.51	104.56	114.35
23	P	310	CHD	C13-C14-C8	-6.48	106.46	114.74
15	N	602[A]	HEA	C1B-C2B-C3B	-6.40	102.54	107.00
15	N	602[B]	HEA	C1B-C2B-C3B	-6.40	102.54	107.00

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	602[A]	HEA	NB
15	A	602[A]	HEA	ND
15	A	602[A]	HEA	NA
15	A	602[B]	HEA	NB
15	A	602[B]	HEA	ND

5 of 652 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
14	A	601	PGV	O04-C19-O03-C01
14	A	601	PGV	C20-C19-O03-C01
14	C	307	PGV	C04-O12-P-O13
14	C	307	PGV	O04-C19-O03-C01
14	C	307	PGV	C20-C19-O03-C01

There are no ring outliers.

89 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	317	EDO	2	0
20	B	312	EDO	3	0
20	M	103	EDO	1	0
21	L	101	TGL	11	0
25	C	305	PEK	4	0
21	N	608	TGL	2	0
27	P	323	DMU	1	0
20	G	103	EDO	1	0
20	D	202	EDO	1	0
27	G	108	DMU	1	0
20	J	102	EDO	1	0
20	P	315	EDO	1	0
20	D	207	EDO	1	0
25	C	304	PEK	1	0
22	B	302	PSC	10	0
15	N	603	HEA	4	0
21	B	301	TGL	4	0
23	C	309	CHD	1	0
20	N	618	EDO	3	0
20	P	319	EDO	2	0
23	Y	104	CHD	4	0
20	B	310	EDO	3	0
20	B	311	EDO	1	0
20	N	623	EDO	1	0
23	W	101	CHD	3	0
27	V	102	DMU	4	0
14	C	307	PGV	2	0
20	B	308	EDO	1	0
21	Y	101	TGL	11	0
20	A	609	EDO	3	0
20	J	103	EDO	1	0
27	Z	102	DMU	1	0
20	P	314	EDO	1	0

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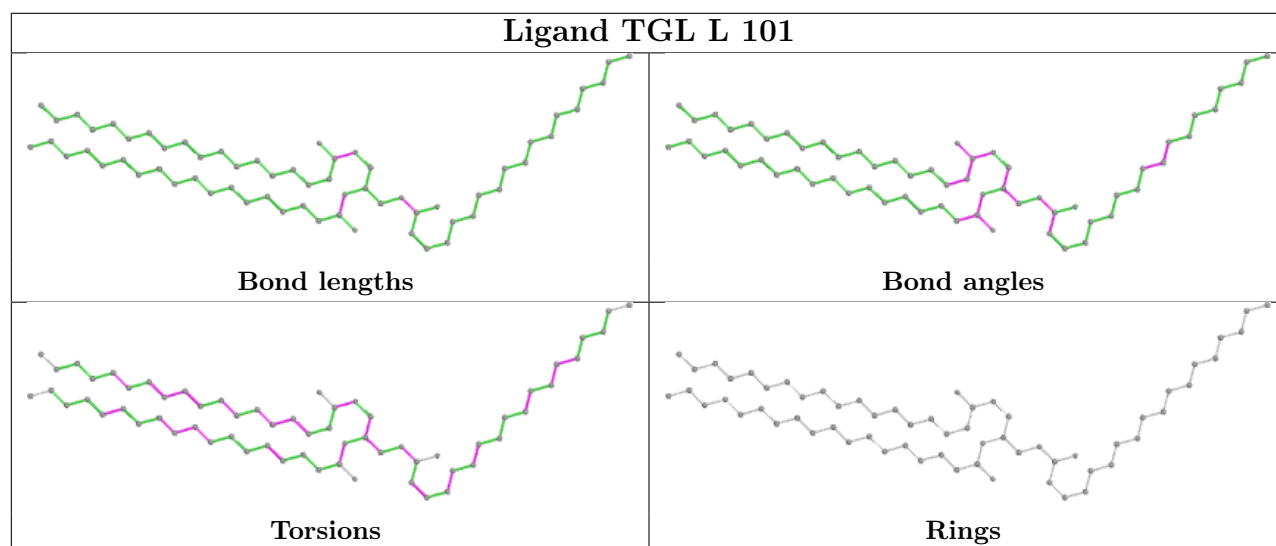
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	612	EDO	5	0
21	Q	201	TGL	7	0
27	C	319	DMU	1	0
15	N	602[A]	HEA	2	0
14	N	609	PGV	1	0
27	P	324	DMU	2	0
26	T	101	CDL	11	0
22	O	301	PSC	5	0
20	C	316	EDO	1	0
20	F	103	EDO	1	0
23	J	101	CHD	3	0
20	N	630	EDO	3	0
23	P	310	CHD	7	0
20	K	102	EDO	2	0
20	G	104	EDO	2	0
25	C	303	PEK	3	0
20	U	101	EDO	1	0
20	O	306	EDO	2	0
23	G	102	CHD	1	0
23	C	311	CHD	2	0
21	D	201	TGL	9	0
15	A	603	HEA	3	0
27	C	310	DMU	2	0
14	P	306	PGV	4	0
20	D	206	EDO	0	2
20	A	620	EDO	1	0
20	R	203	EDO	1	0
14	P	307	PGV	3	0
14	N	601	PGV	3	0
20	A	627	EDO	1	0
25	P	305	PEK	9	0
25	P	304	PEK	3	0
20	A	619	EDO	1	0
27	P	309	DMU	3	0
20	A	623	EDO	1	0
26	C	308	CDL	13	0
20	H	102	EDO	1	0
20	W	104	EDO	2	0
14	A	601	PGV	3	0
20	A	614	EDO	1	0
15	A	602[A]	HEA	3	0
26	G	101	CDL	18	0

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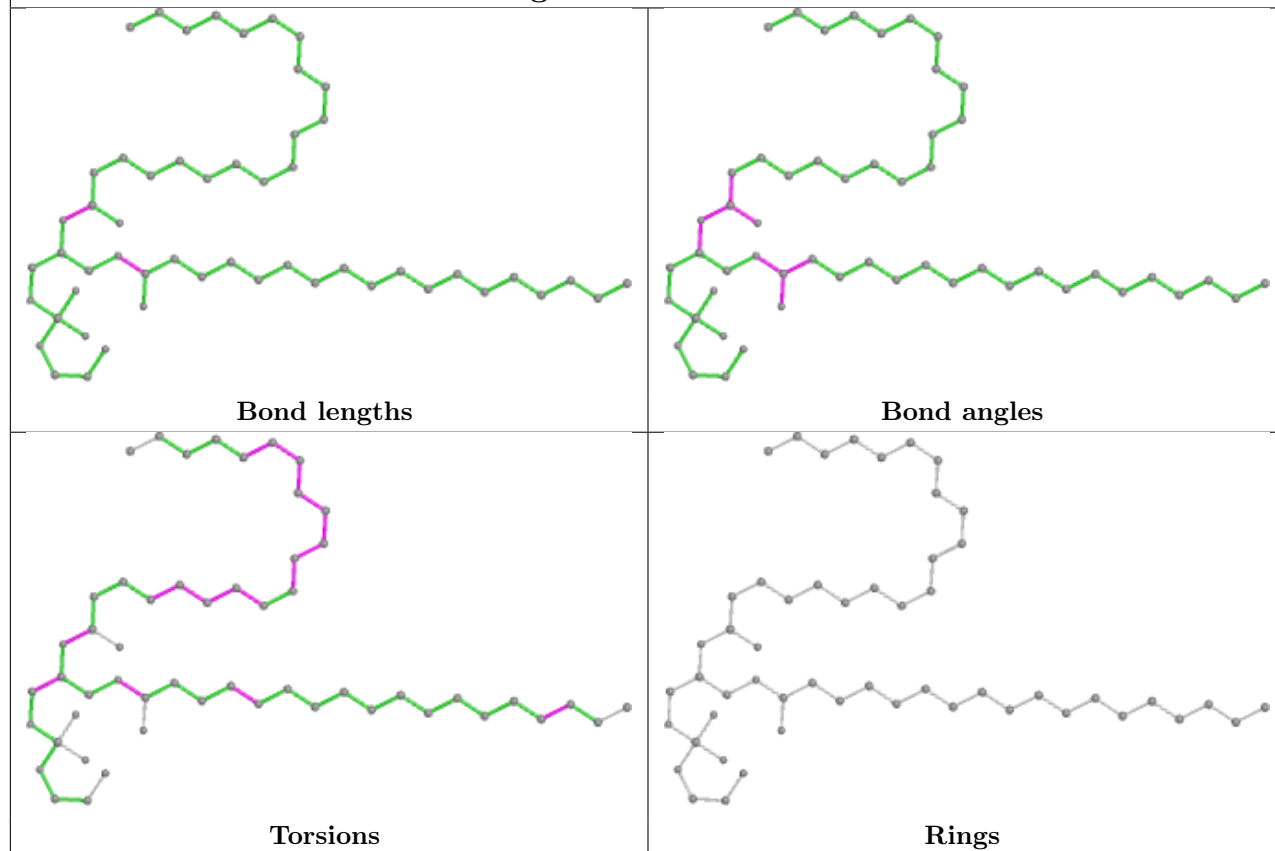
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S	107	EDO	2	0
26	P	308	CDL	20	0
20	A	624	EDO	1	0
20	M	104	EDO	2	0
20	N	619	EDO	1	0
20	P	320	EDO	1	0
14	C	306	PGV	2	0
23	P	311	CHD	2	0
25	P	303	PEK	3	0
20	H	103	EDO	4	0
20	D	205	EDO	1	0
20	B	314	EDO	0	2
20	B	309	EDO	2	0
20	G	107	EDO	1	0

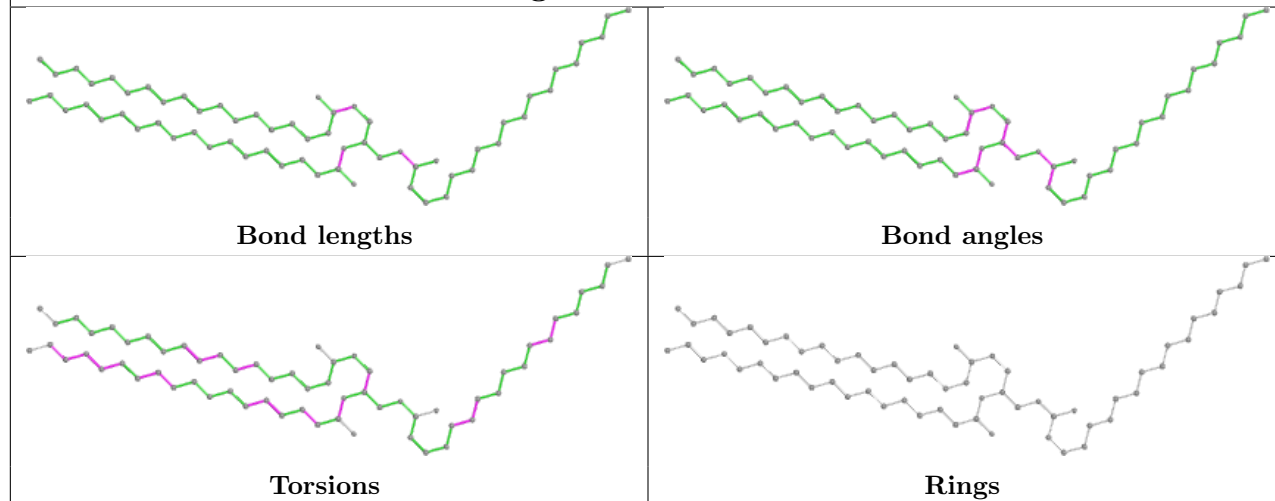
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

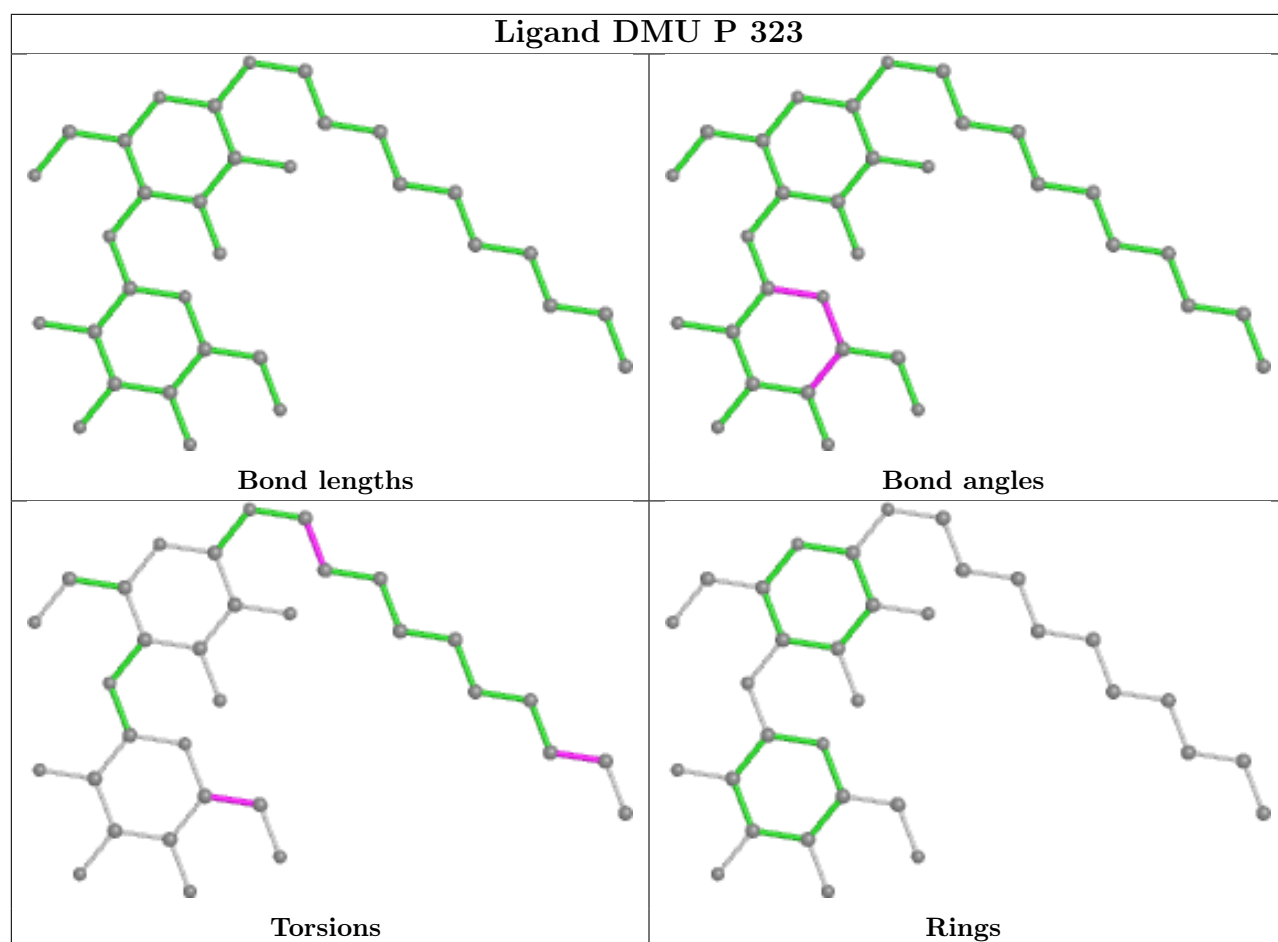


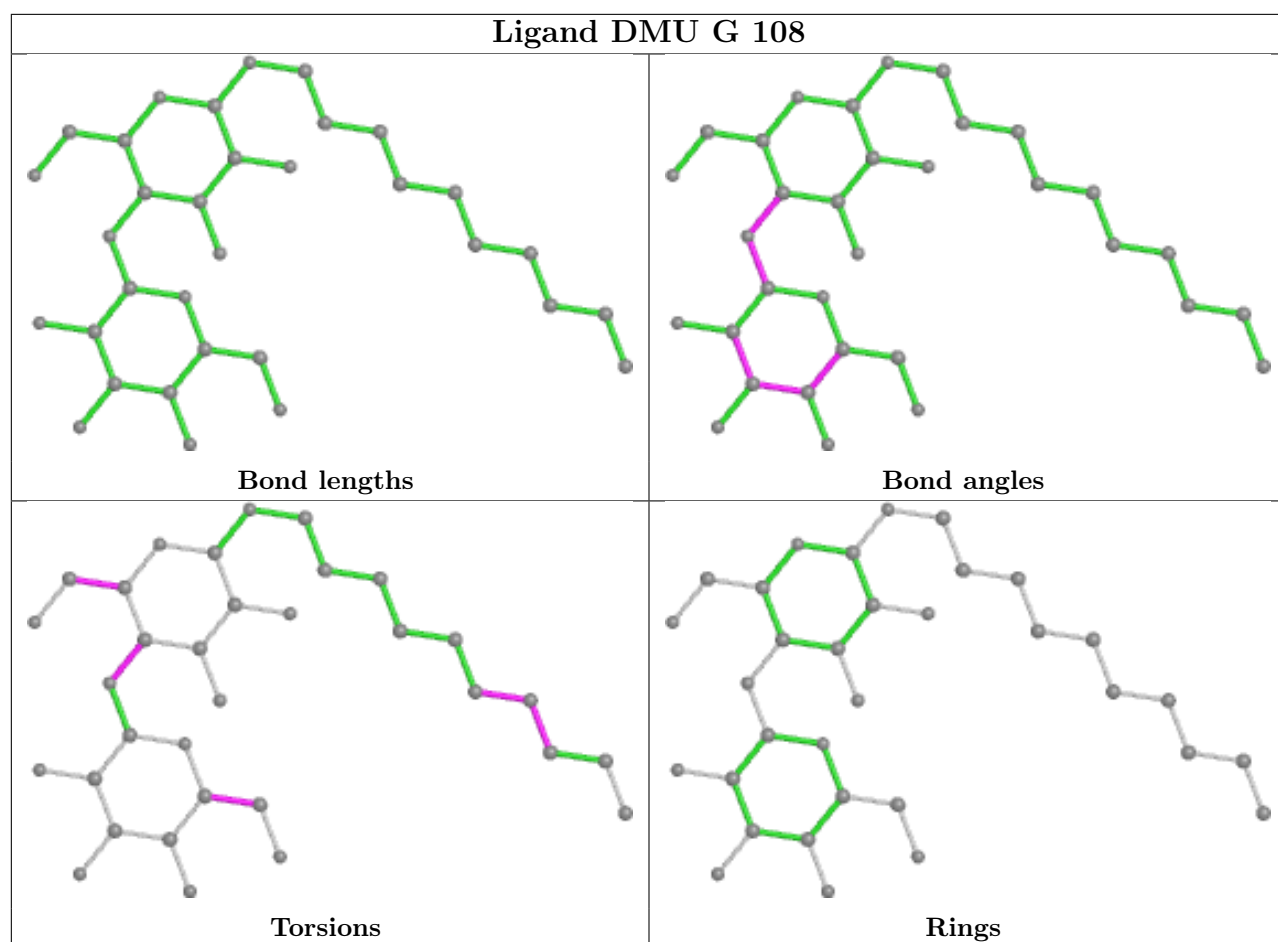
## Ligand PEK C 305

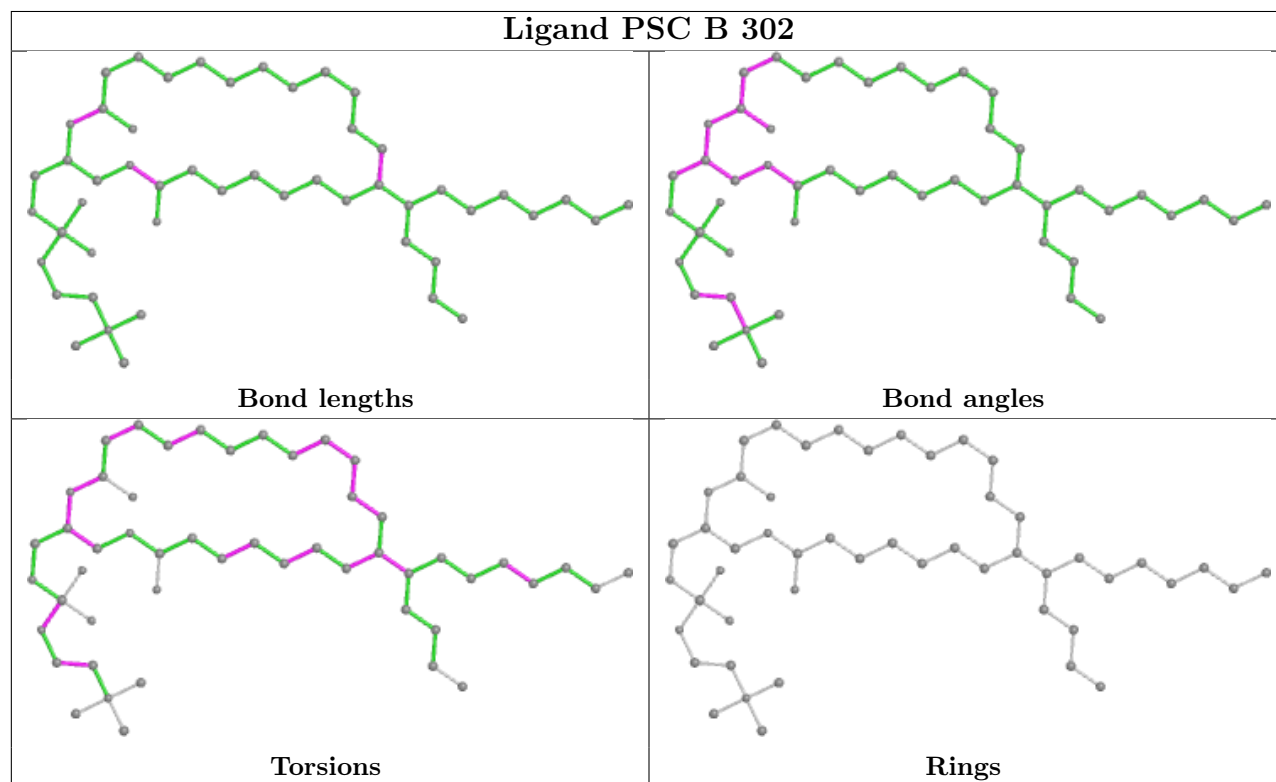
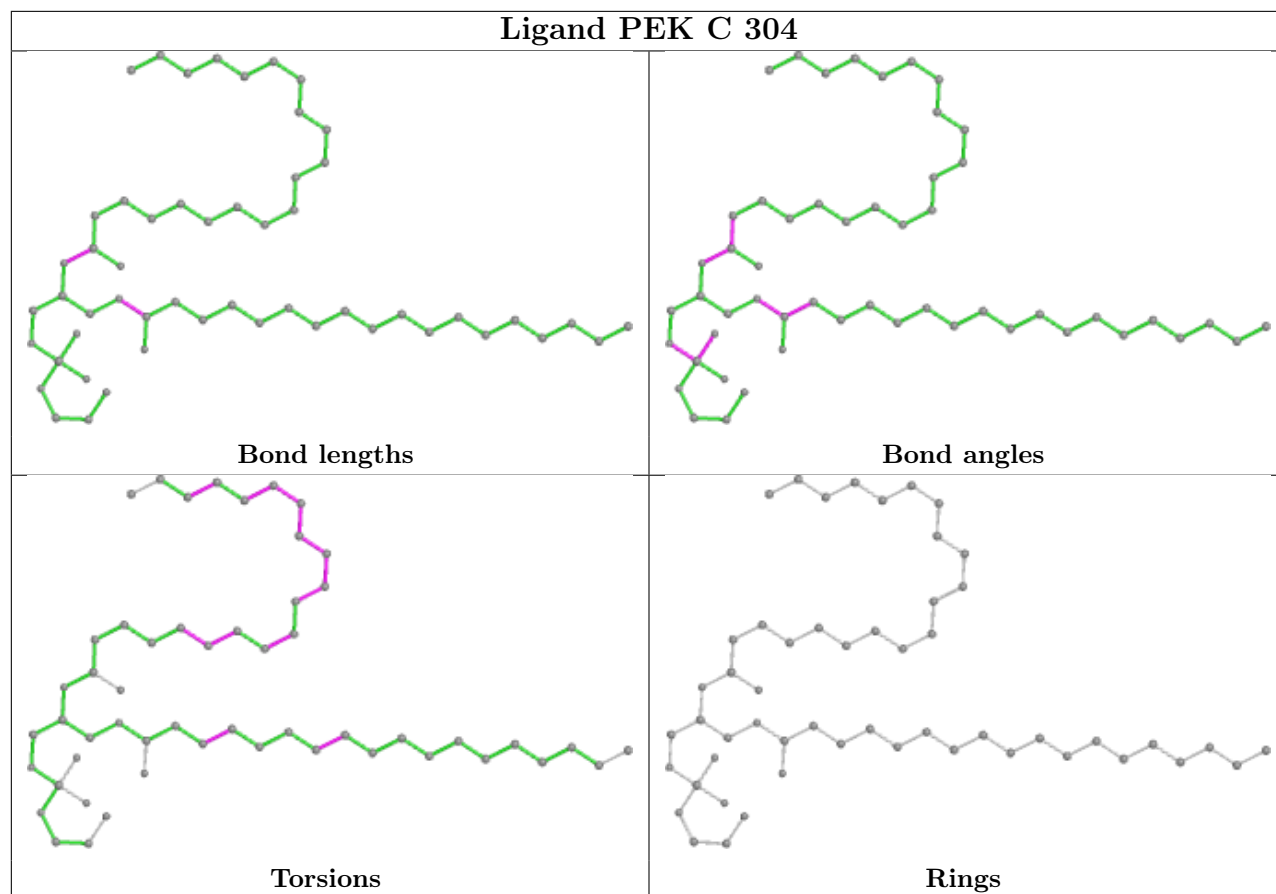


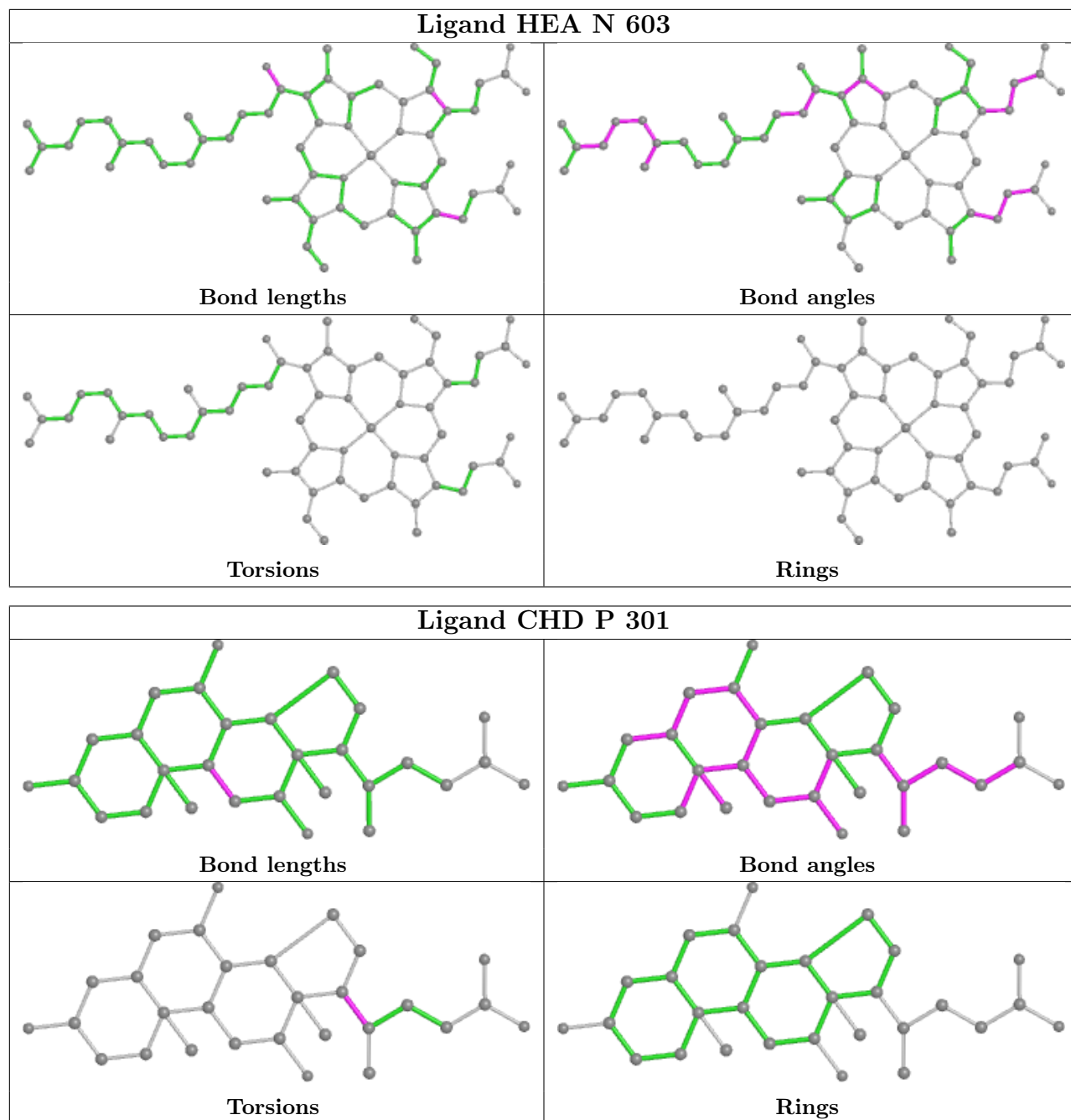
## Ligand TGL N 608



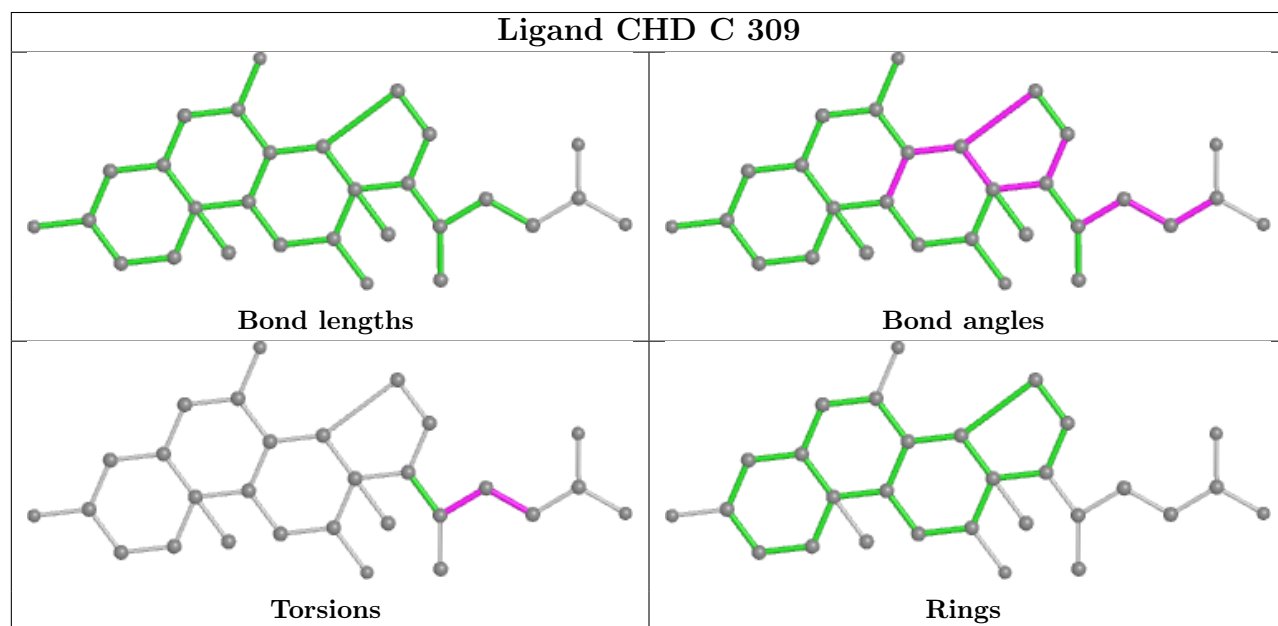
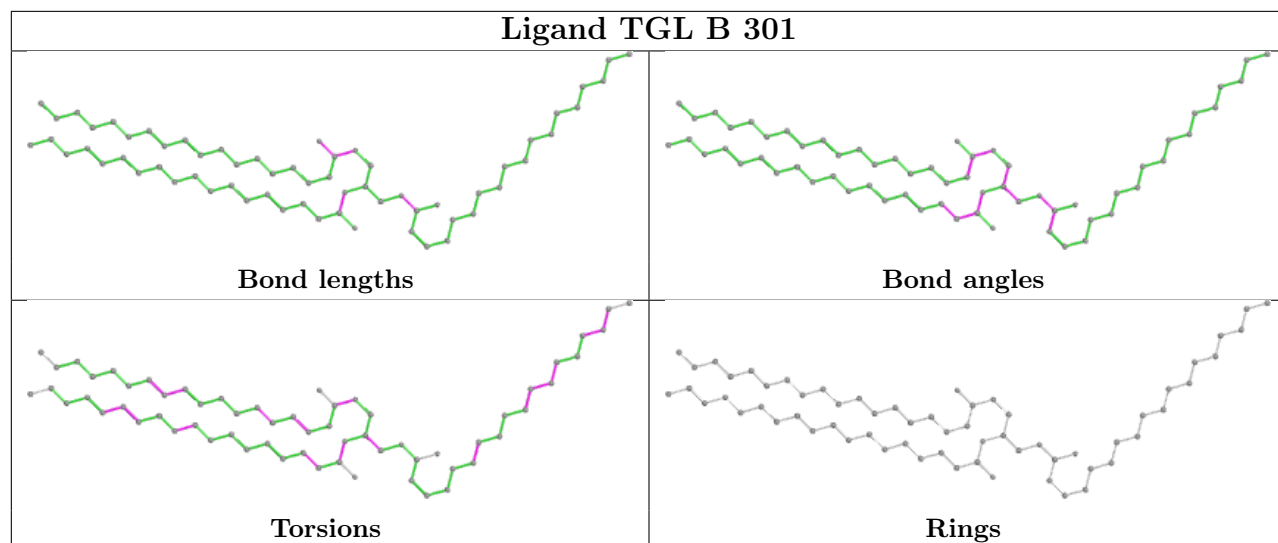


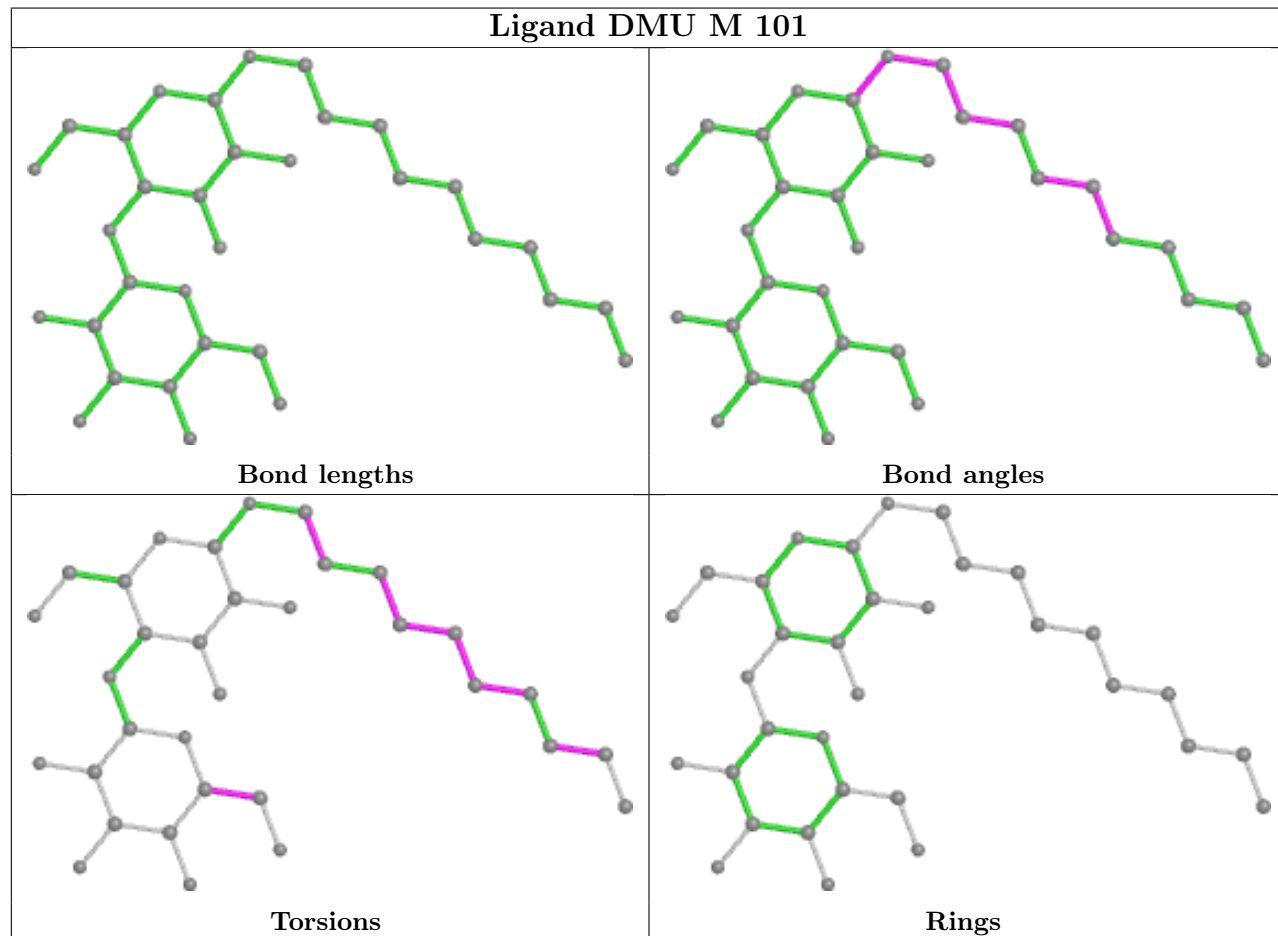
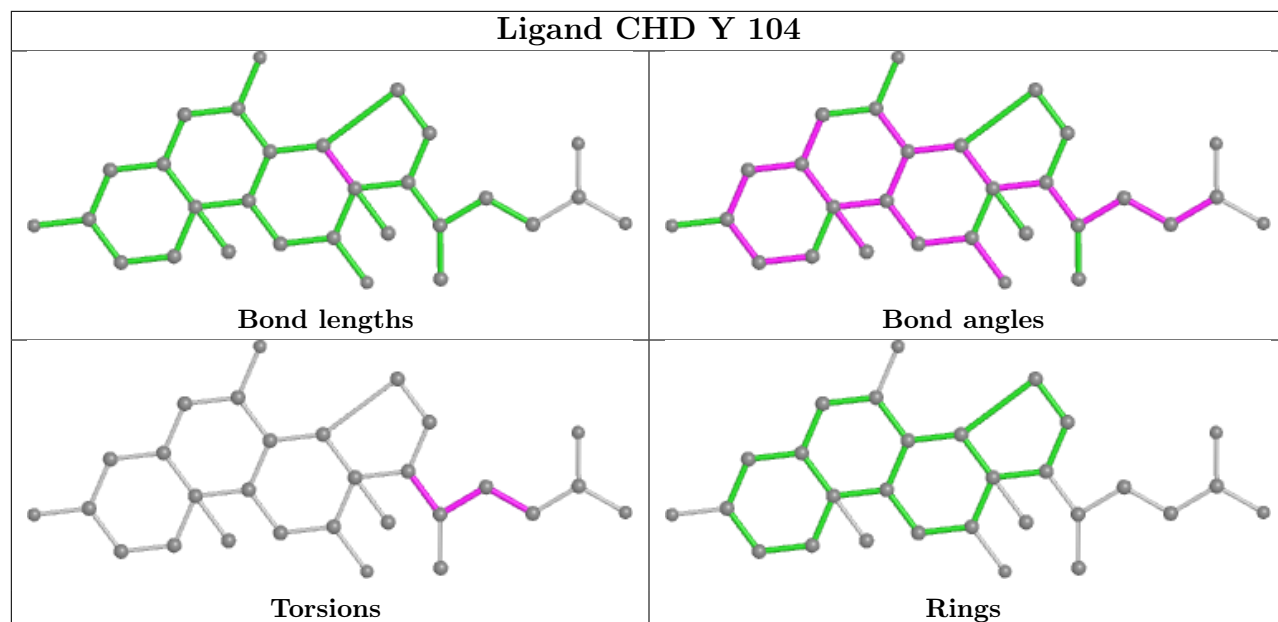




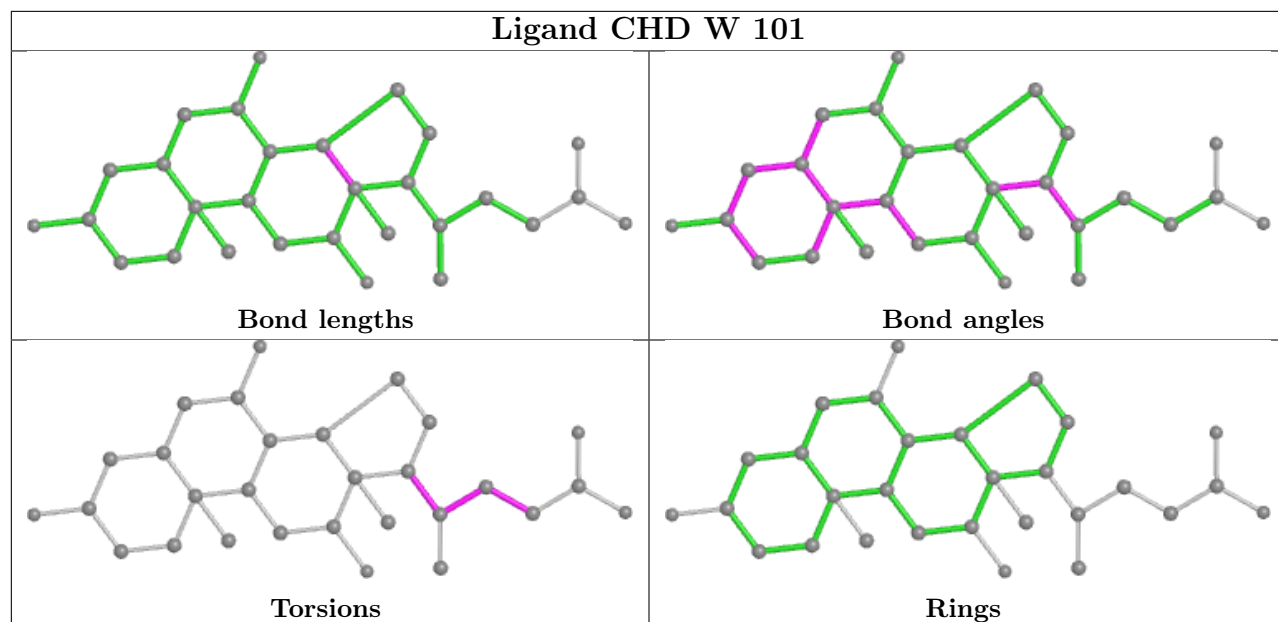




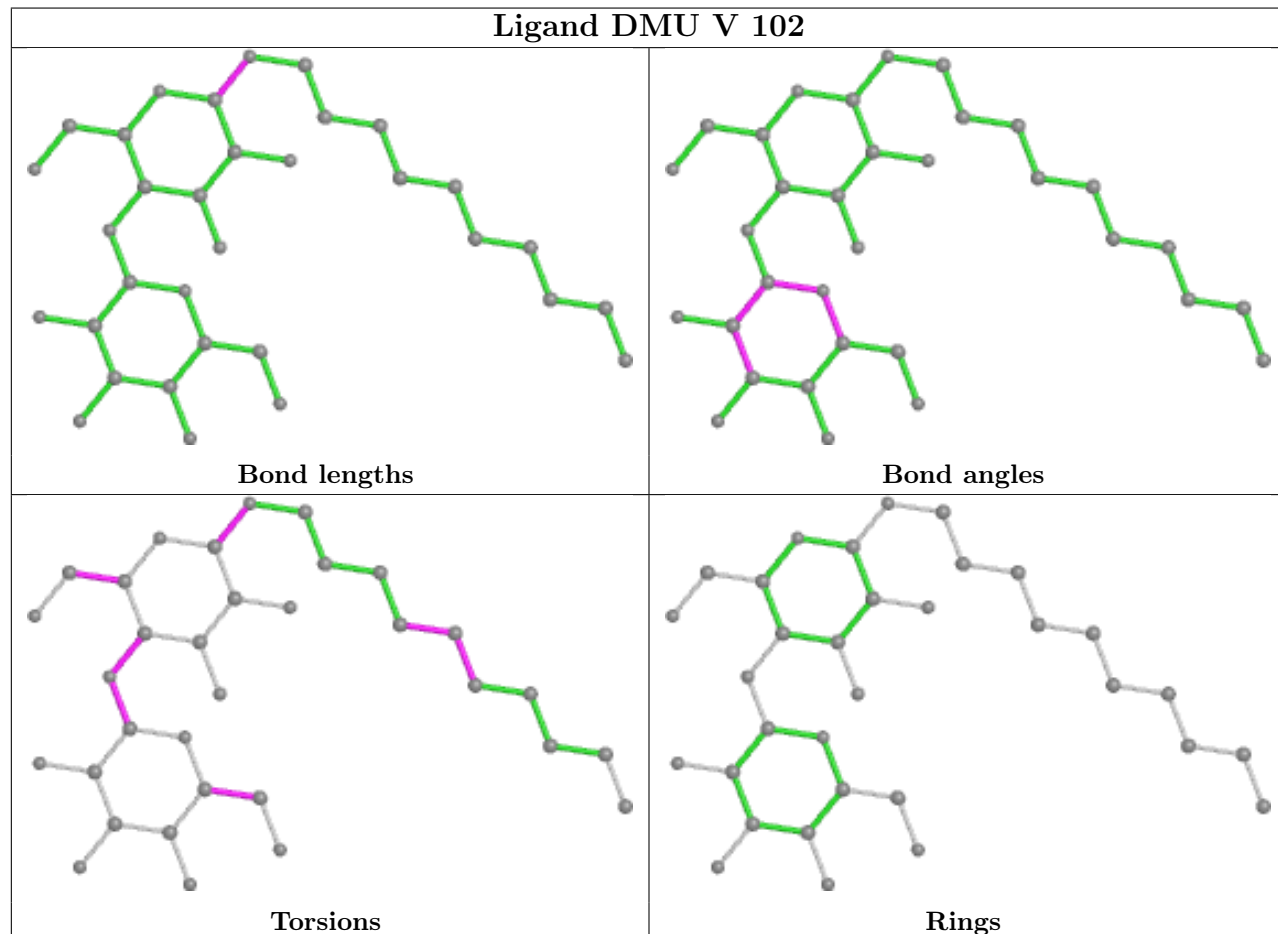


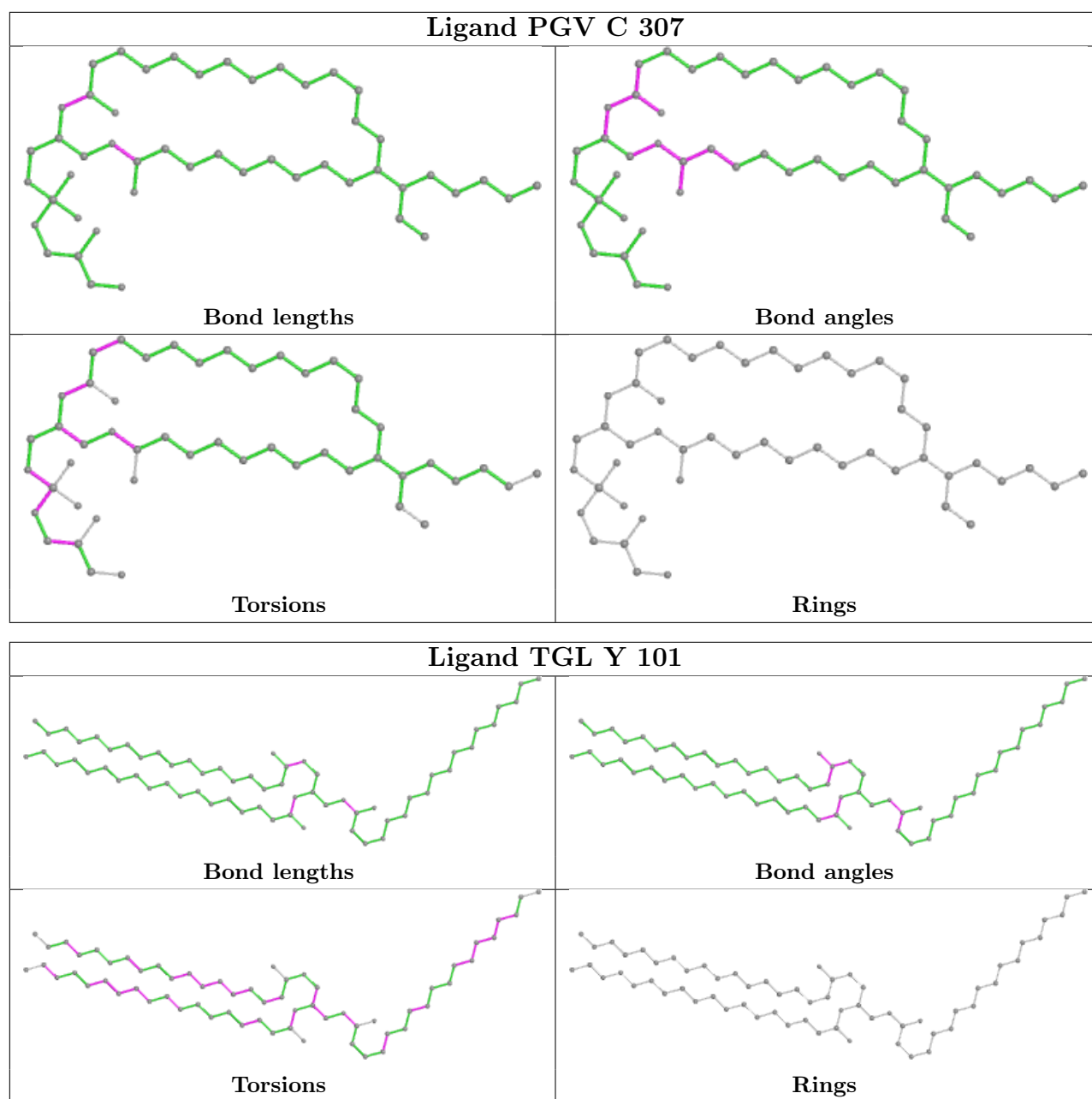


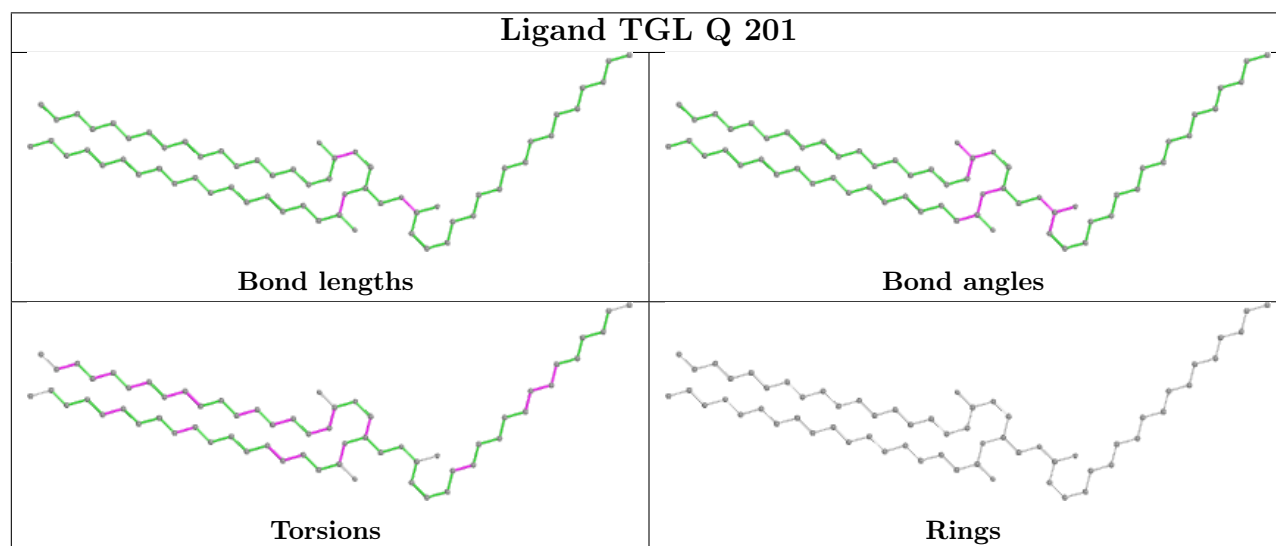
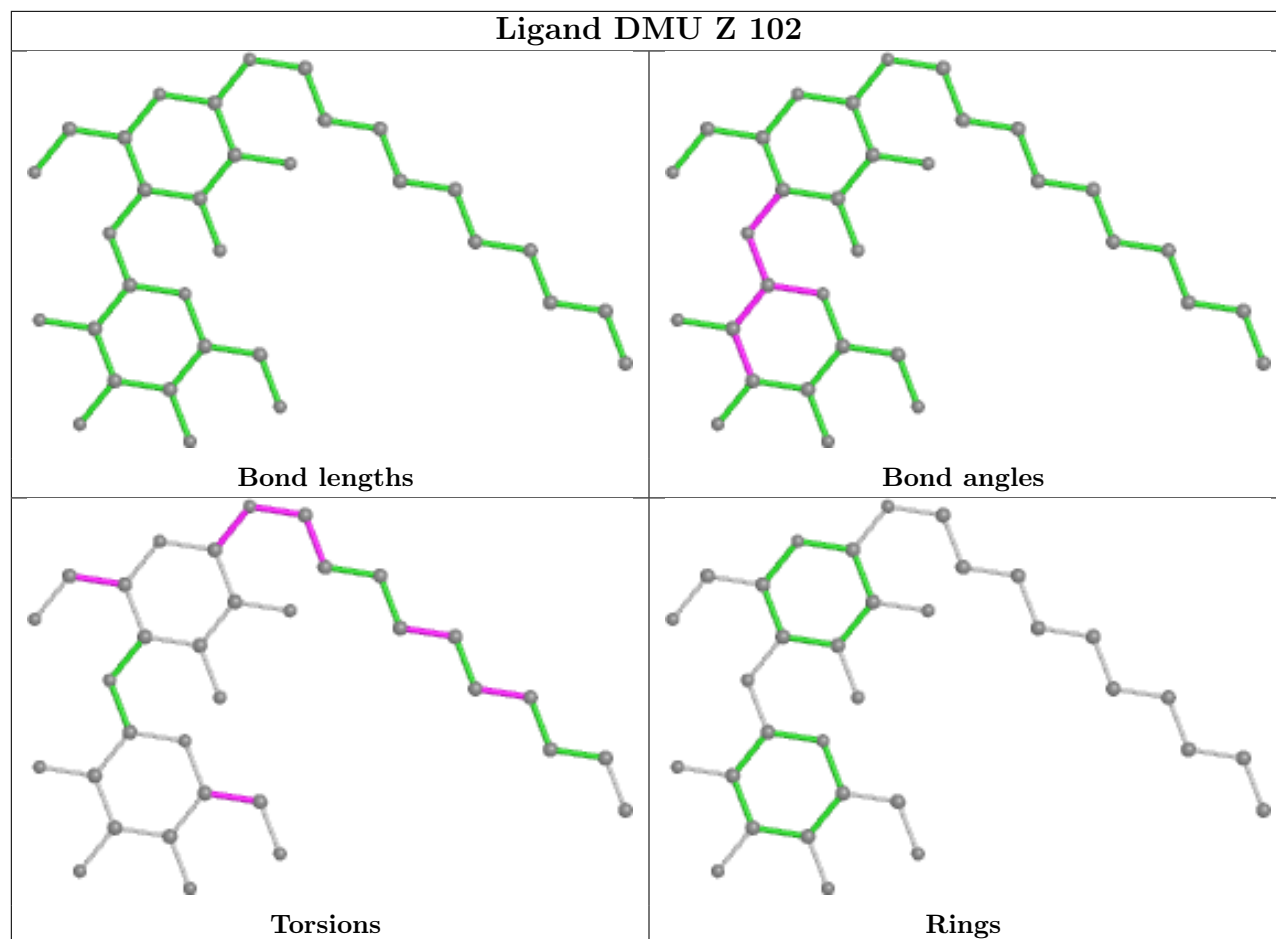
## Ligand CHD W 101

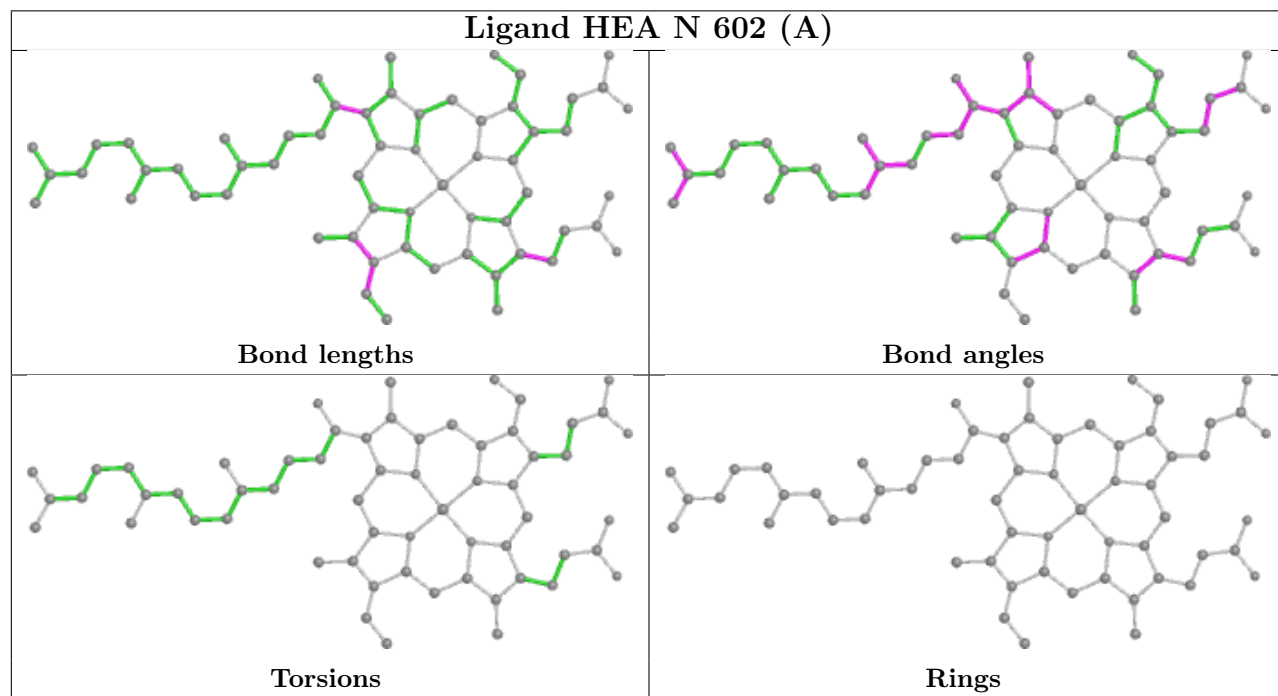
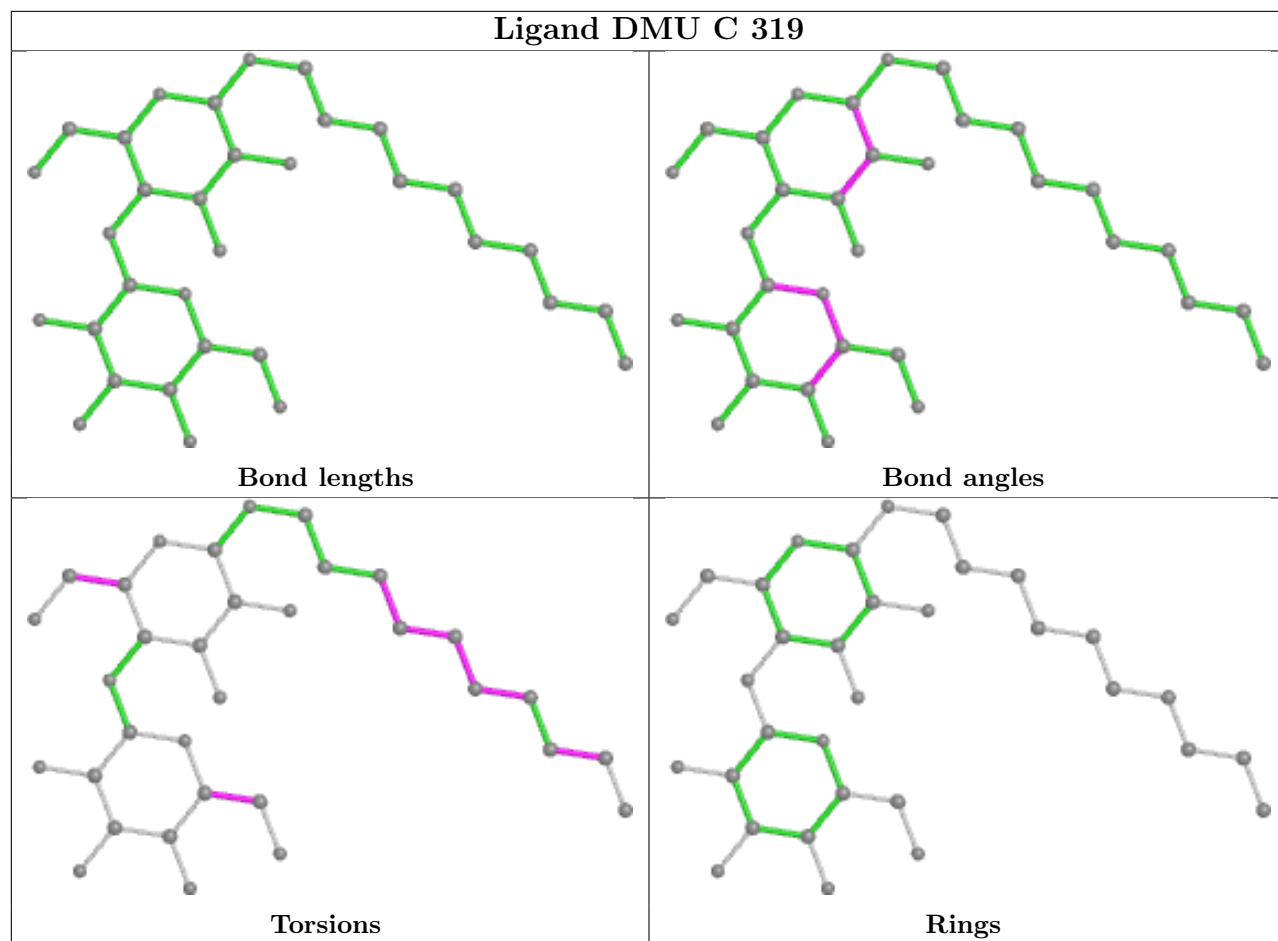


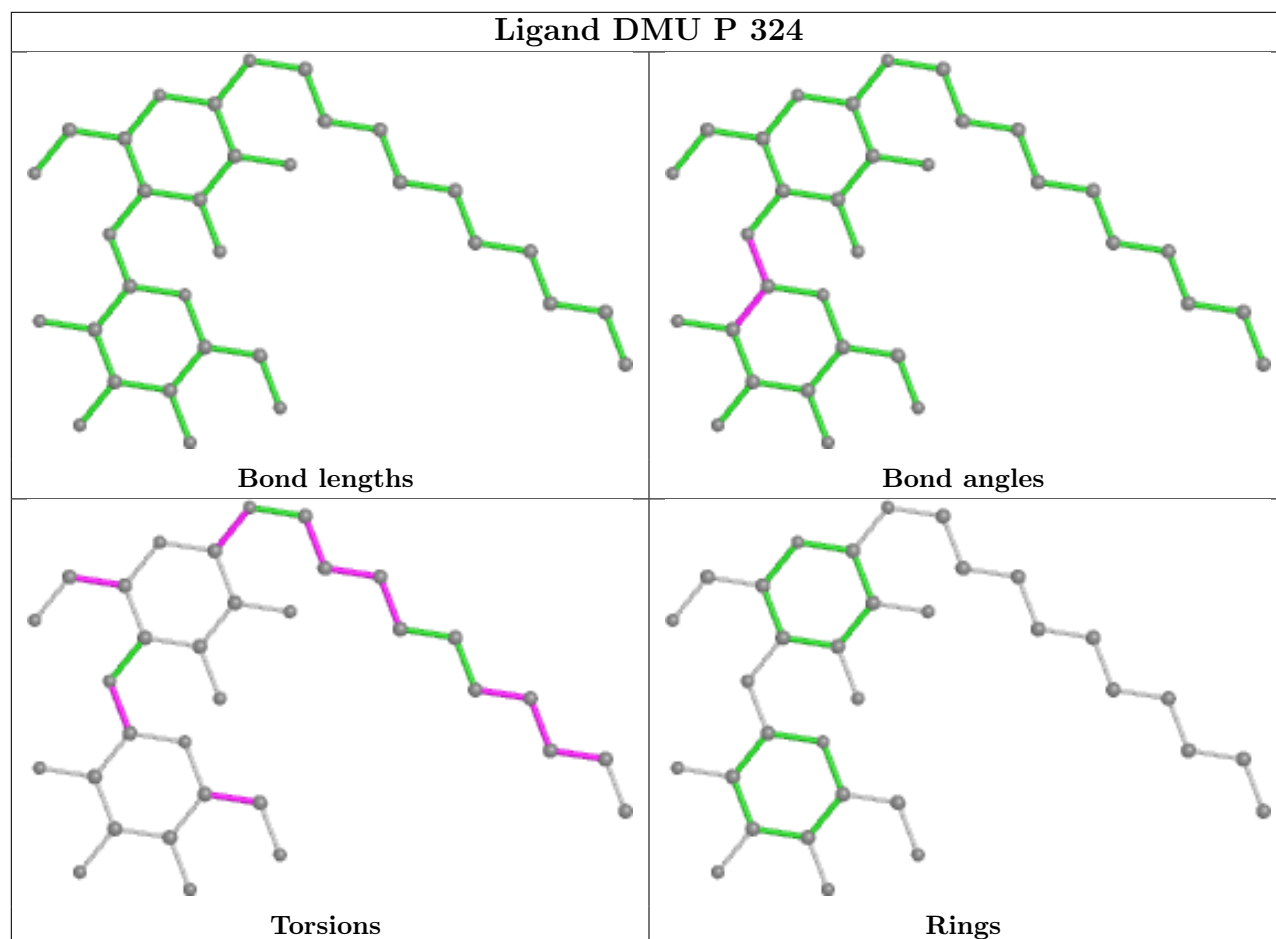
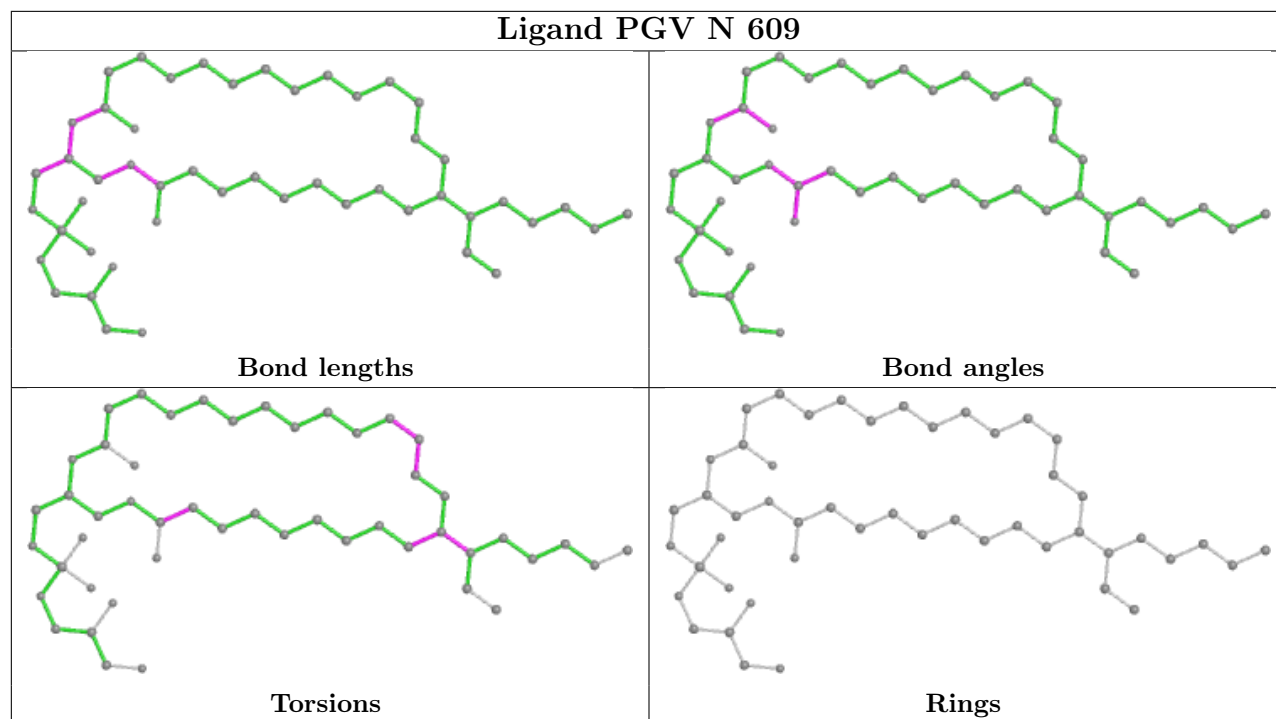
## Ligand DMU V 102

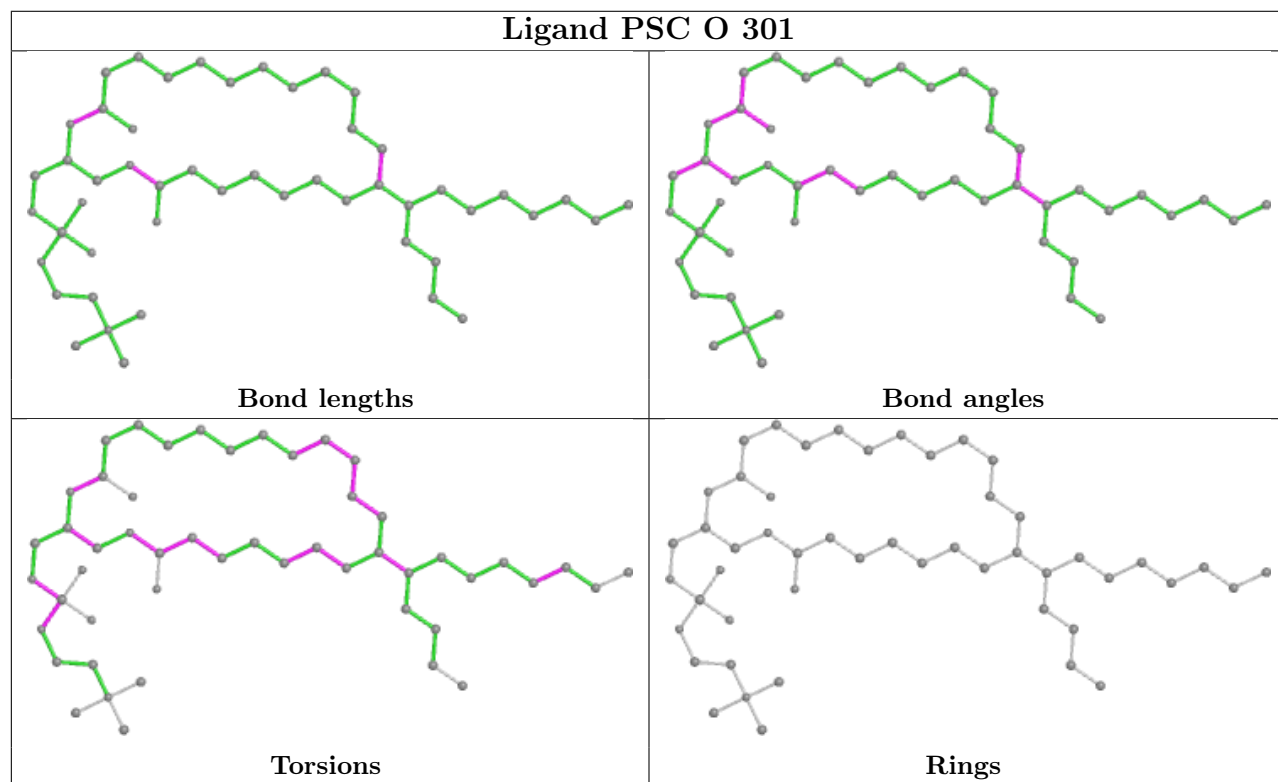
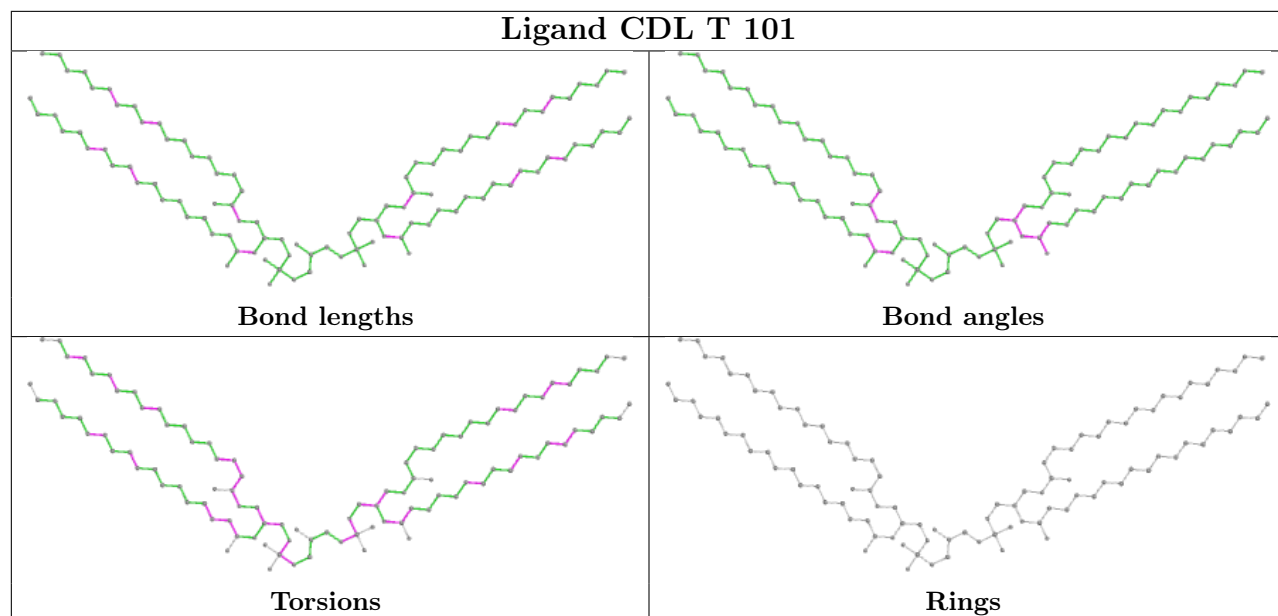






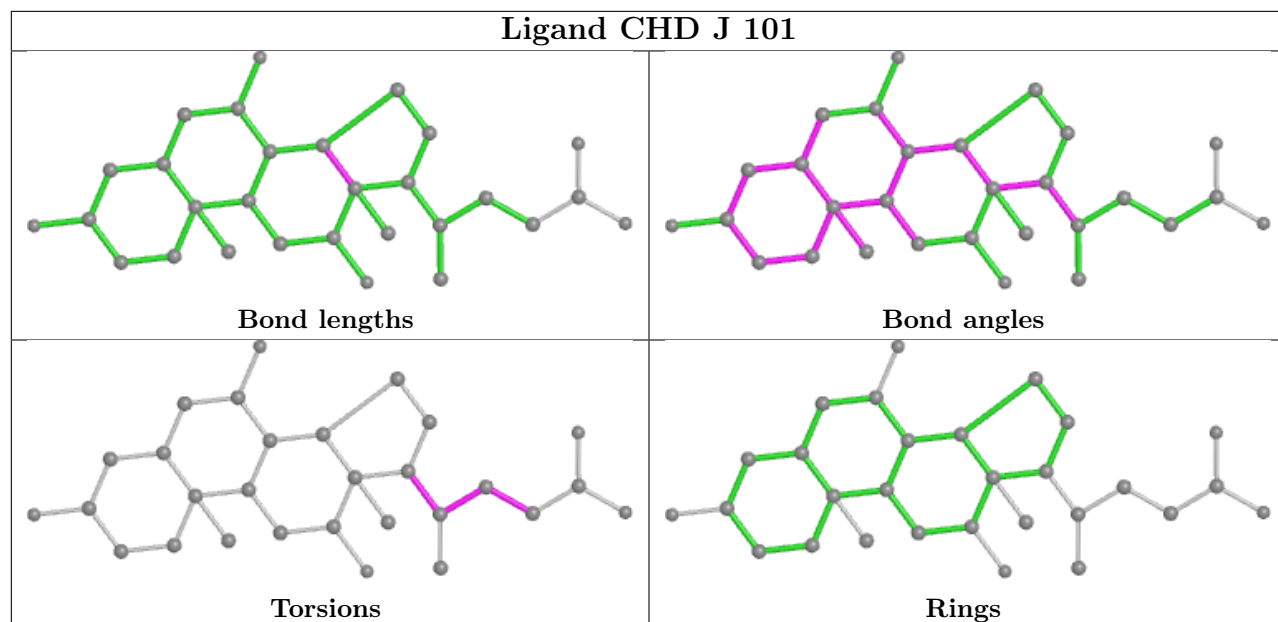




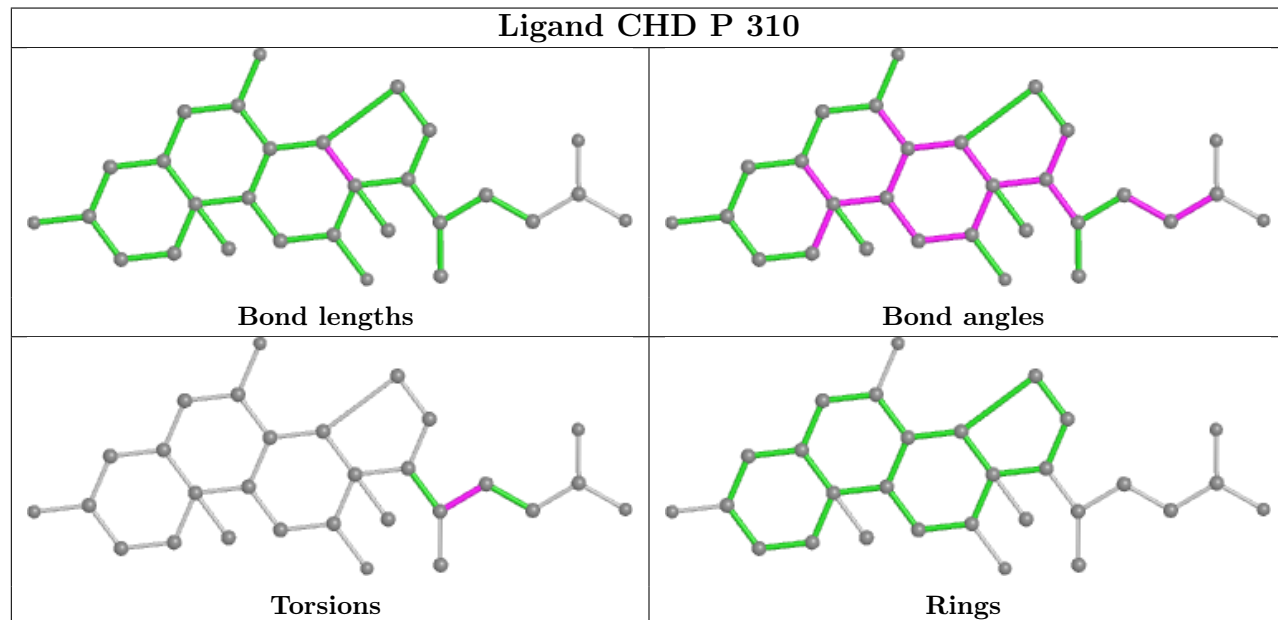


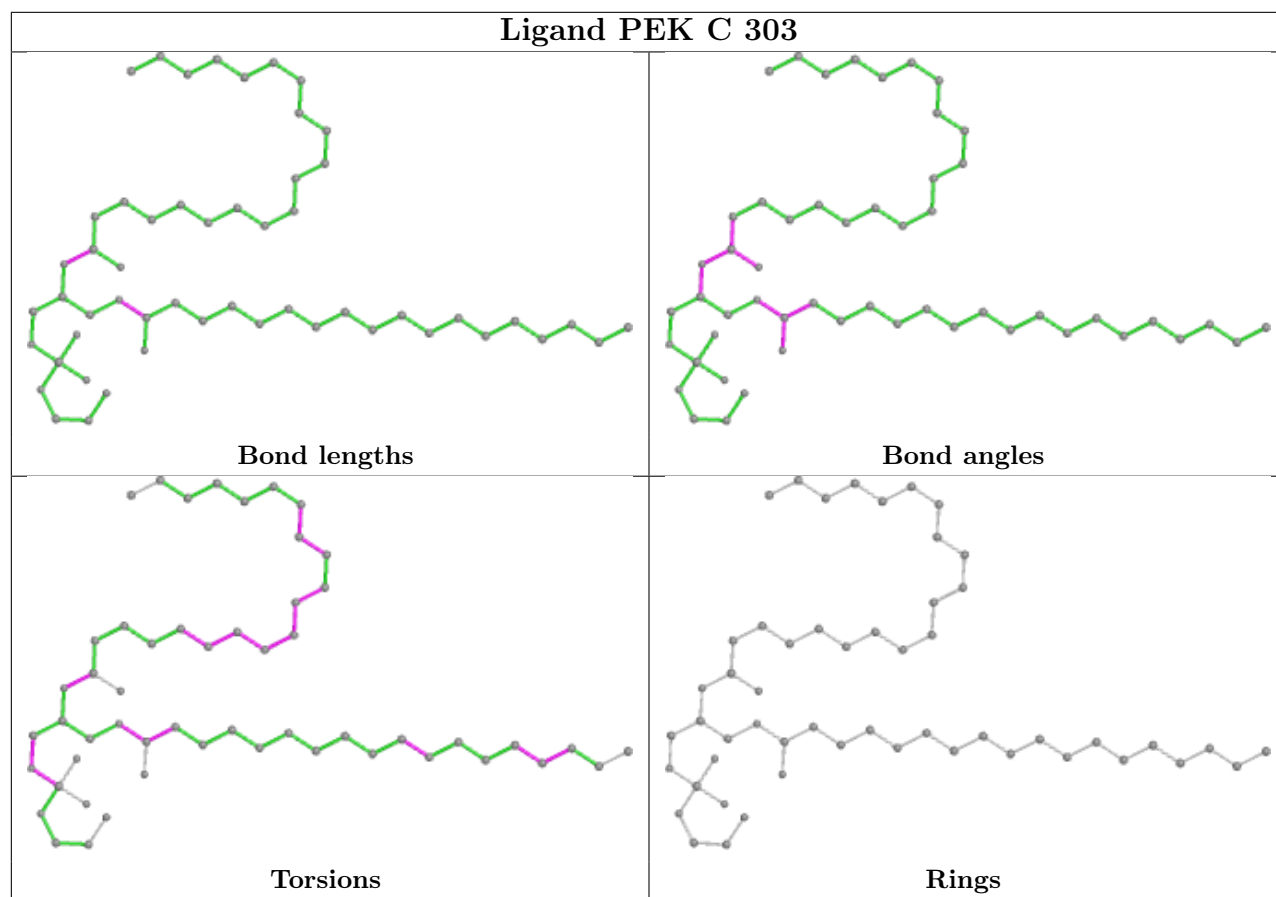
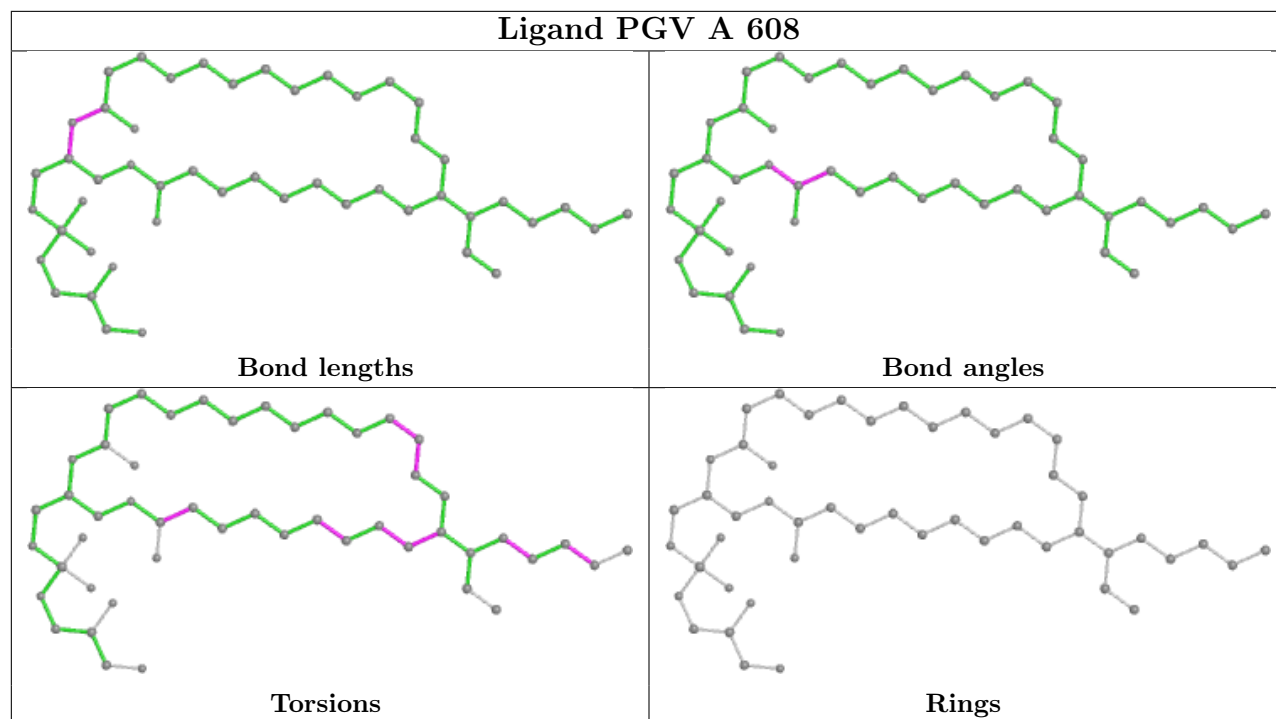


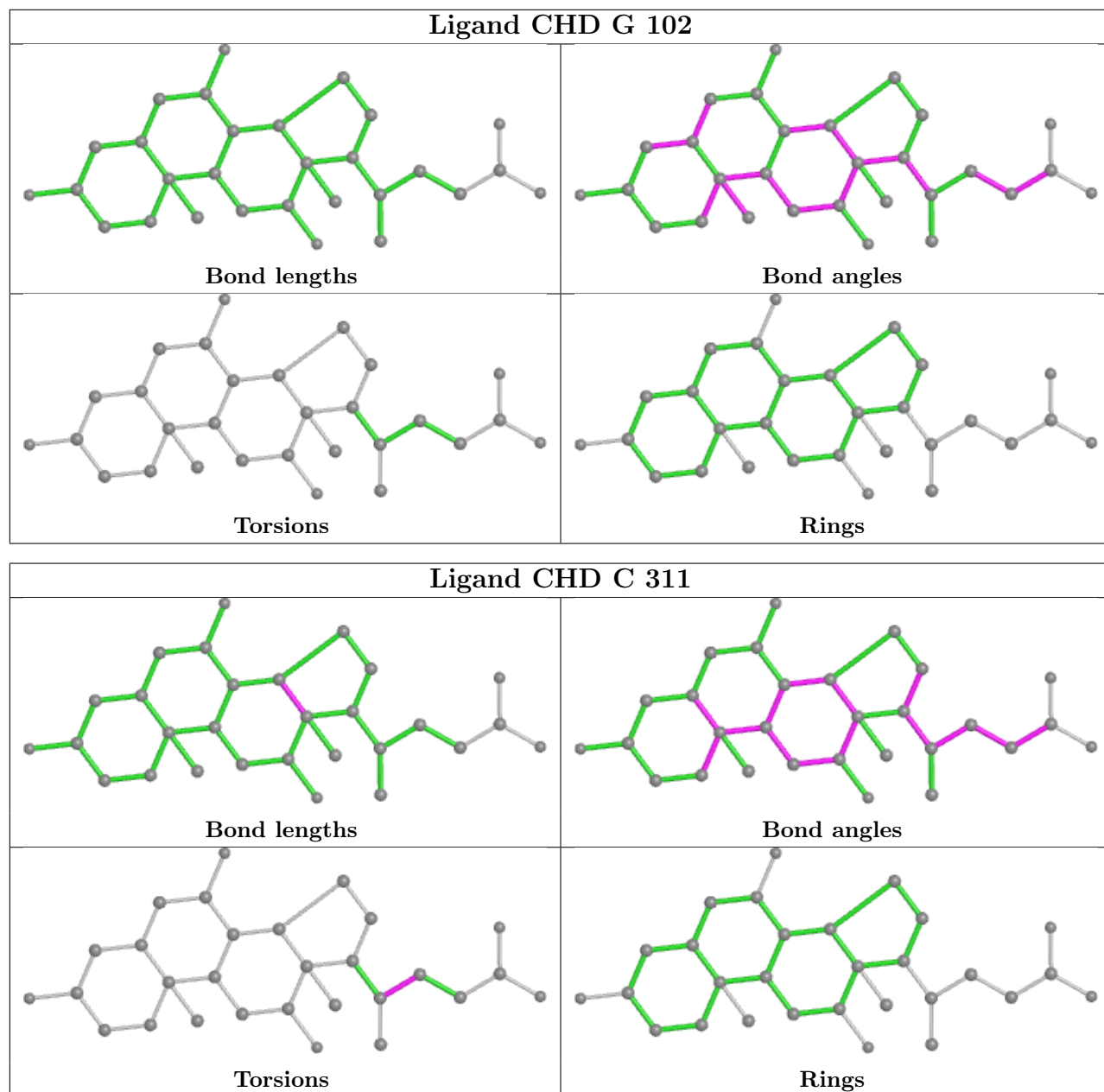
## Ligand CHD J 101

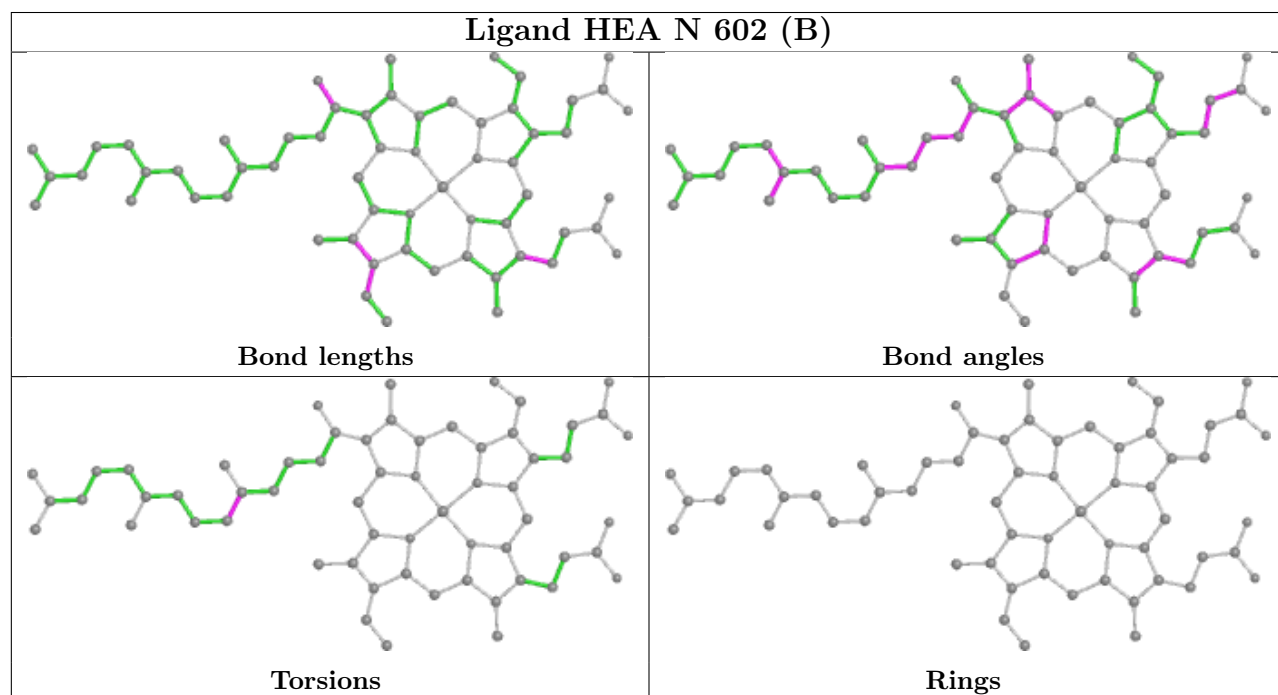
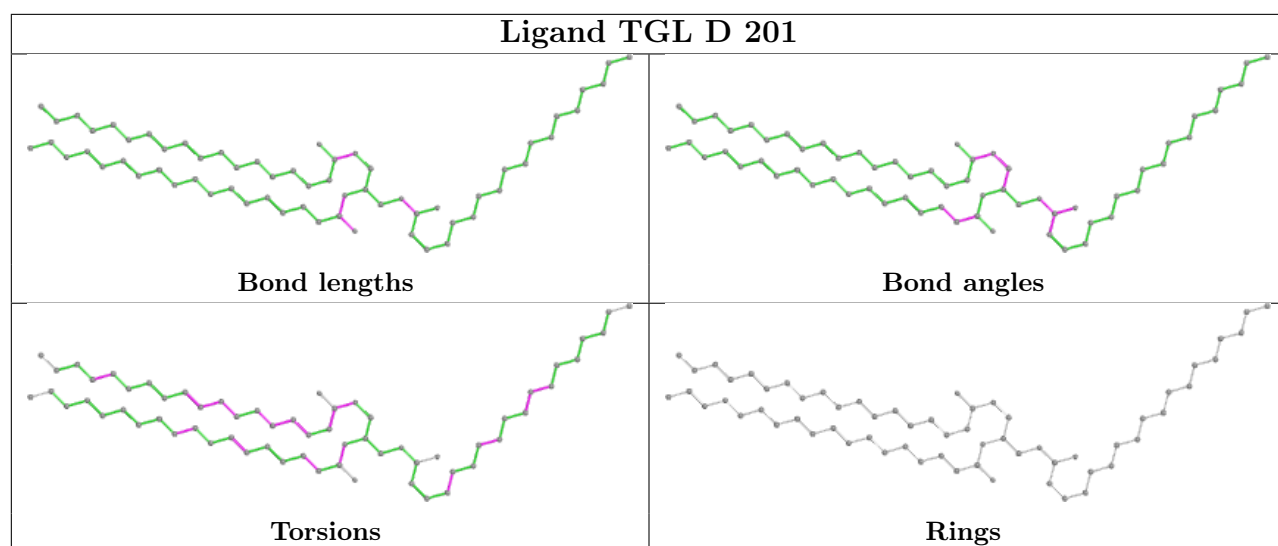


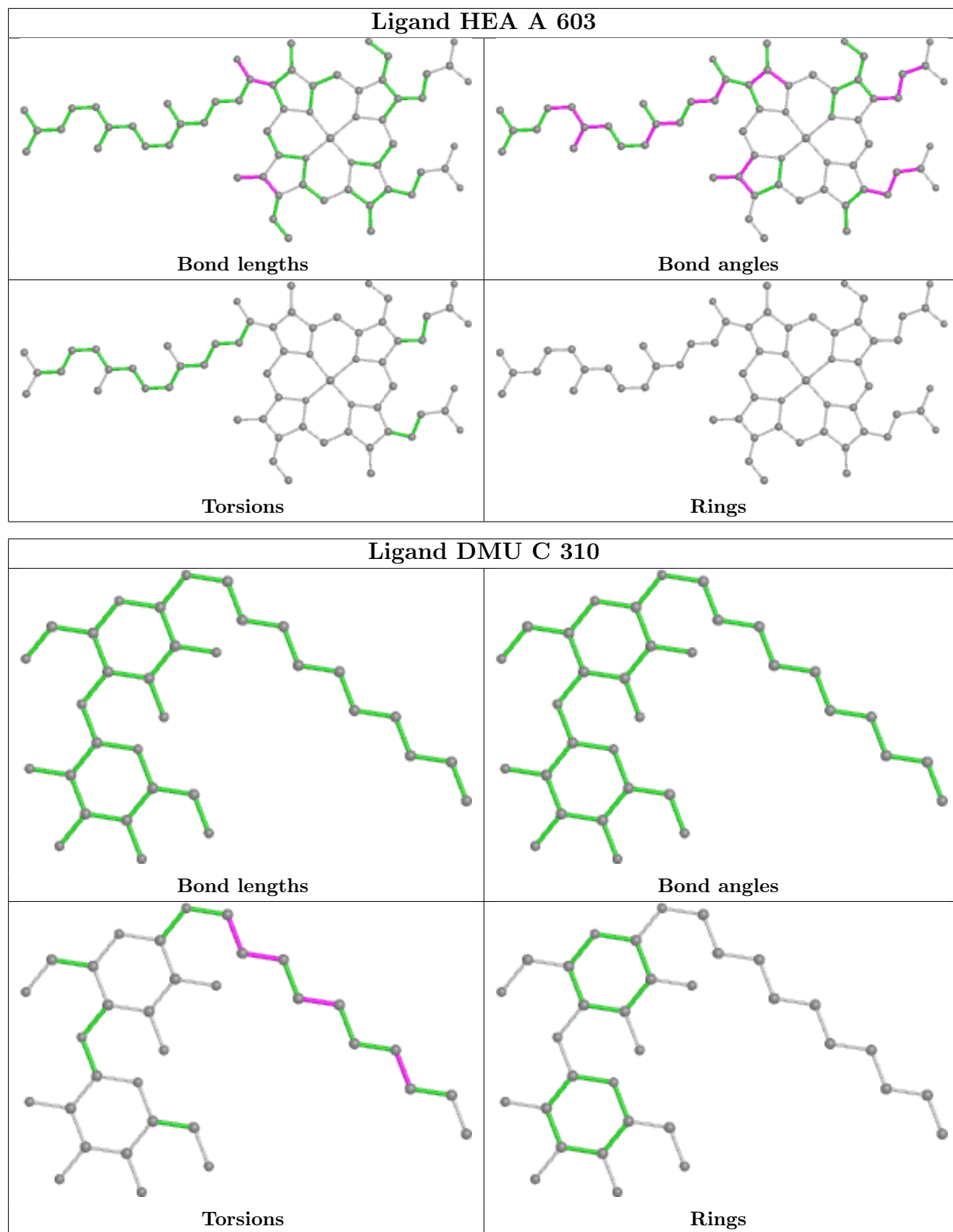
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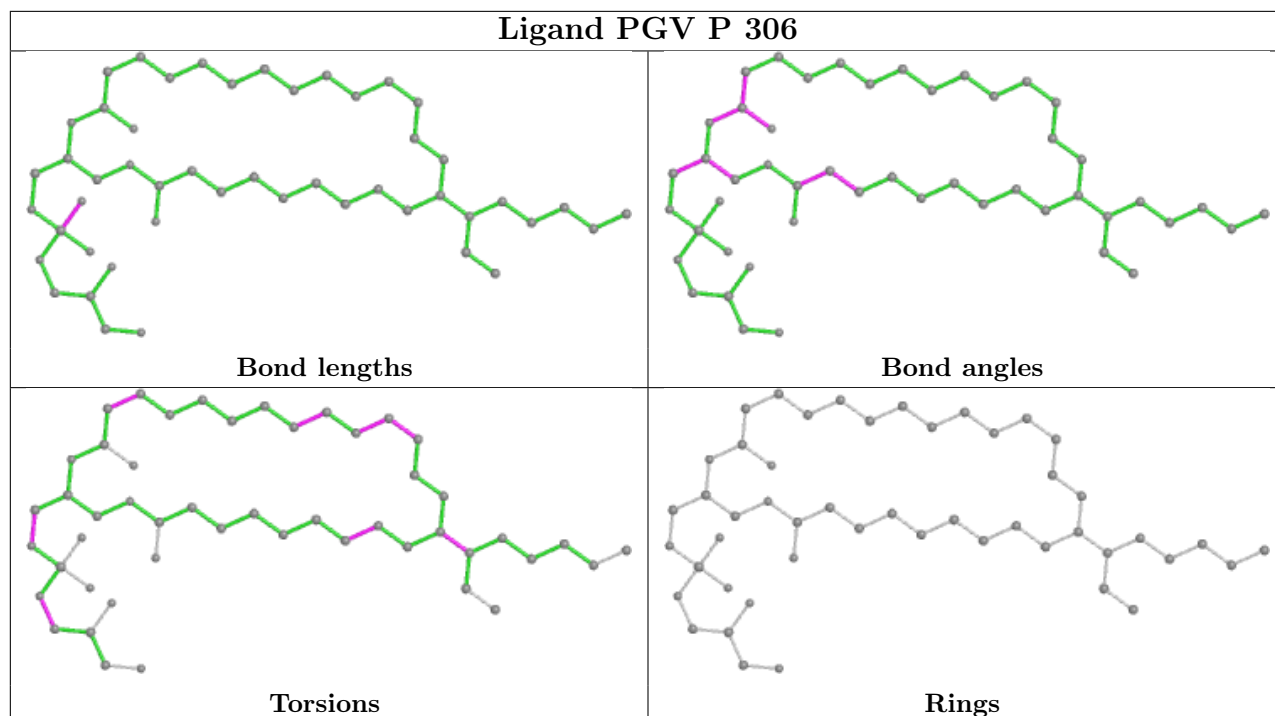




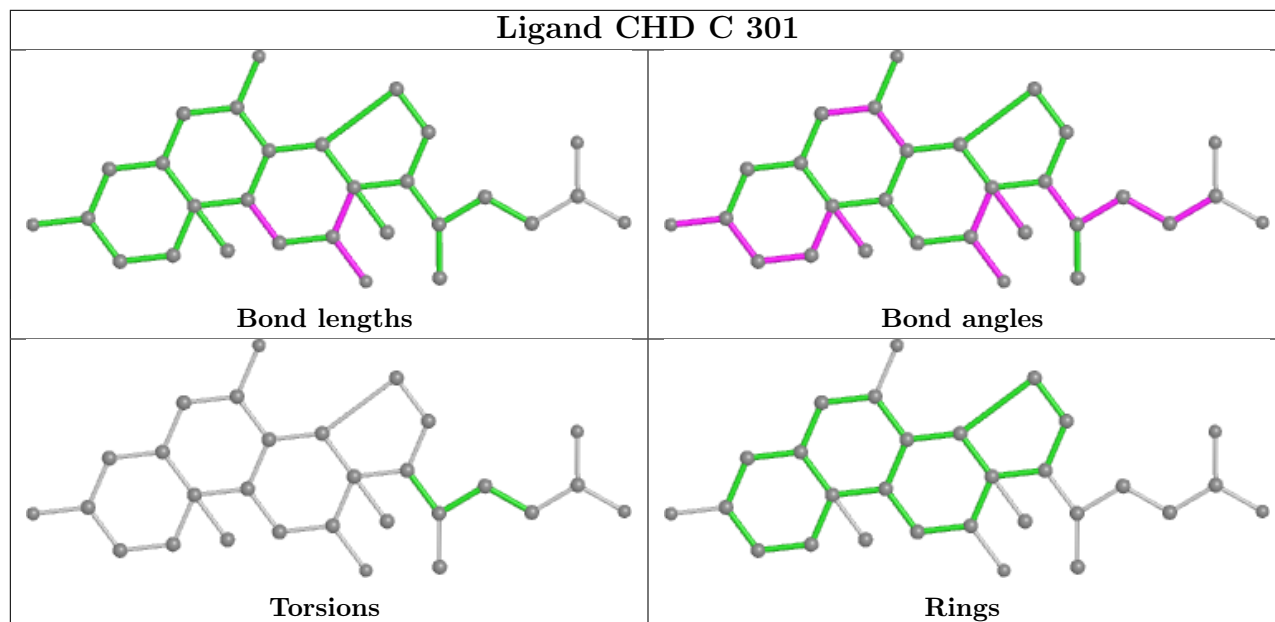




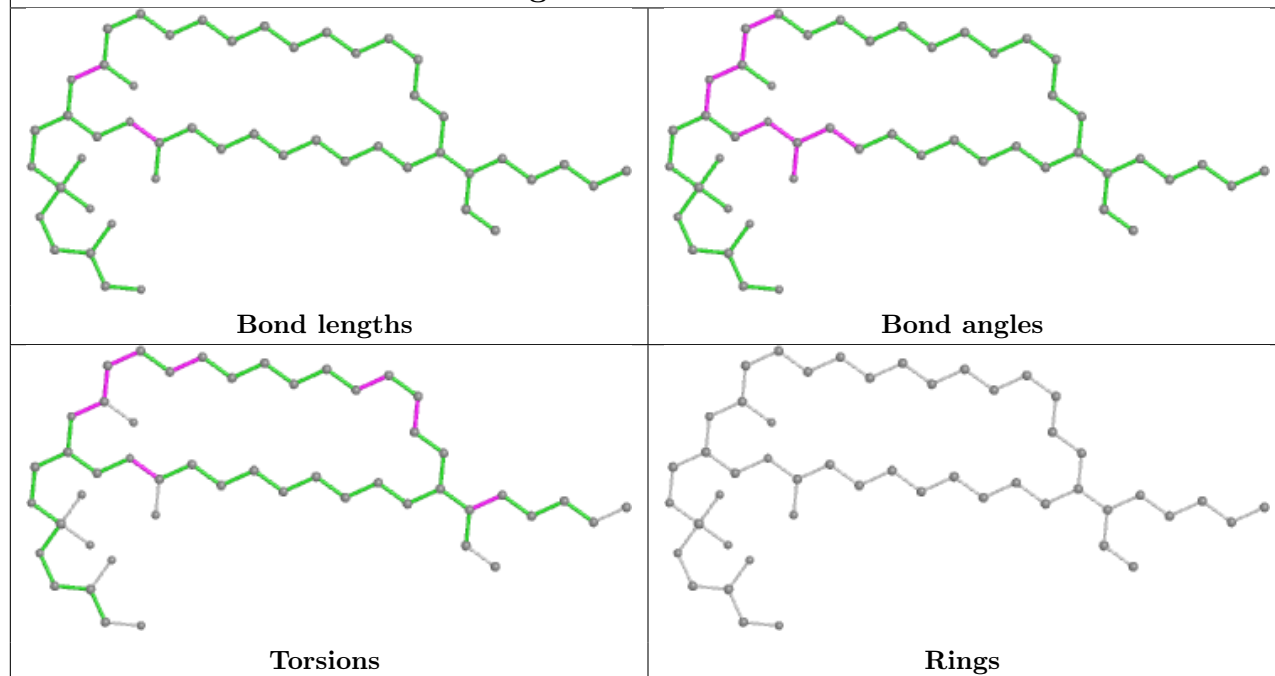
## Ligand PGV P 306



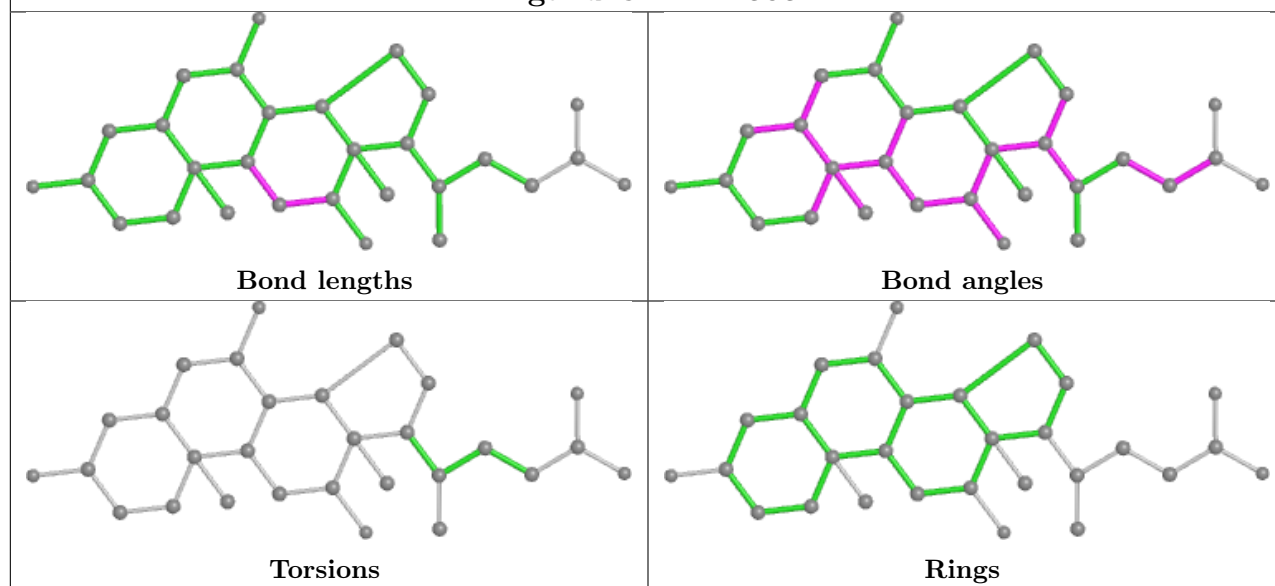
## Ligand CHD C 301

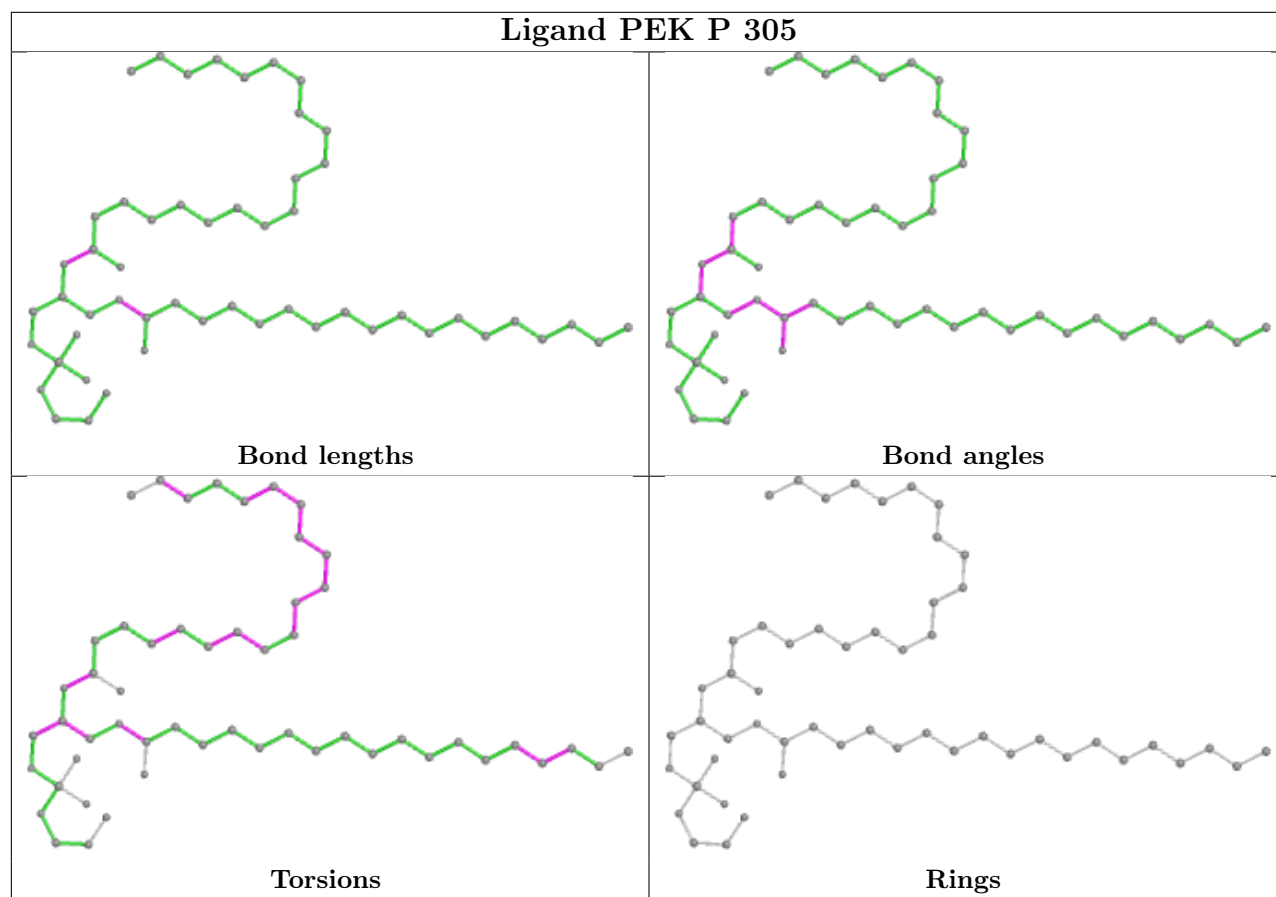
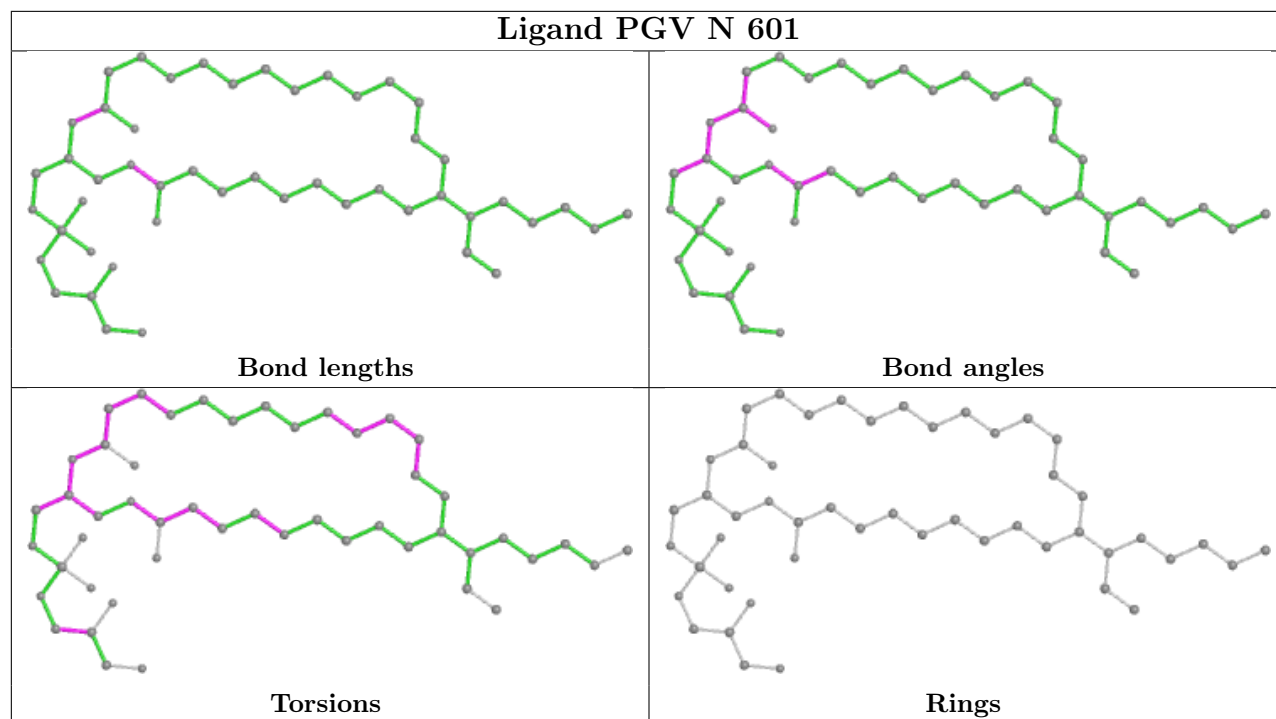


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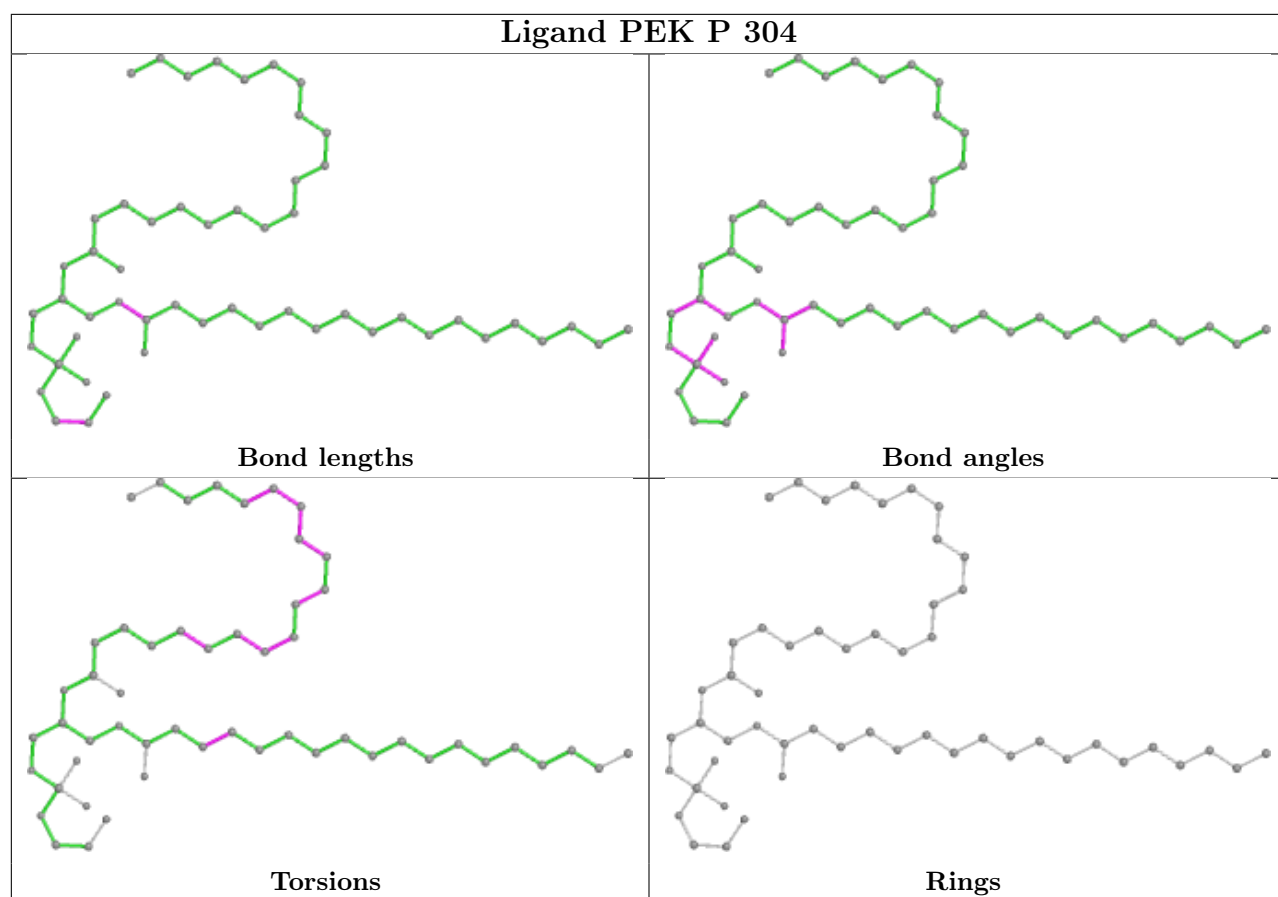


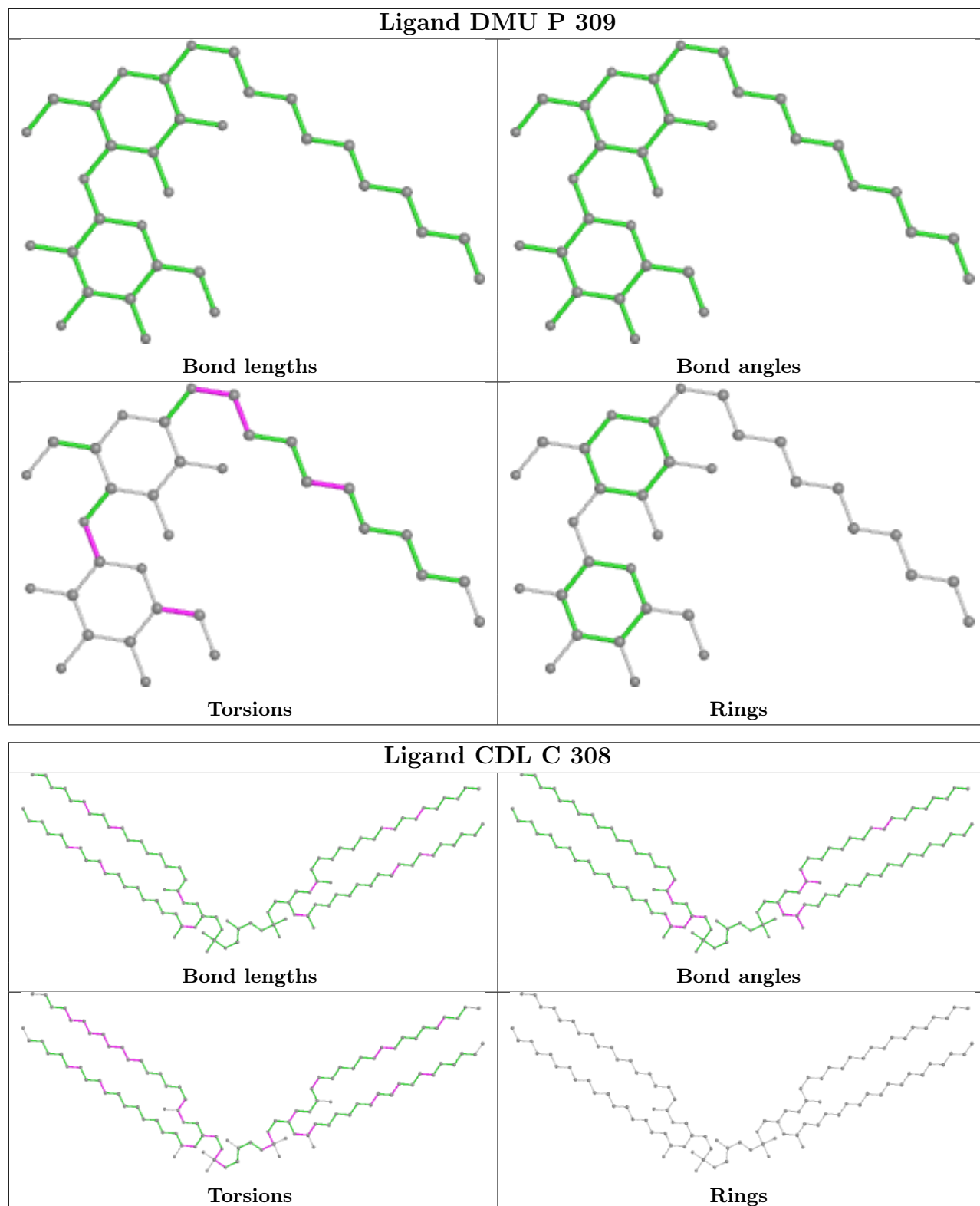
## Ligand CHD B 303

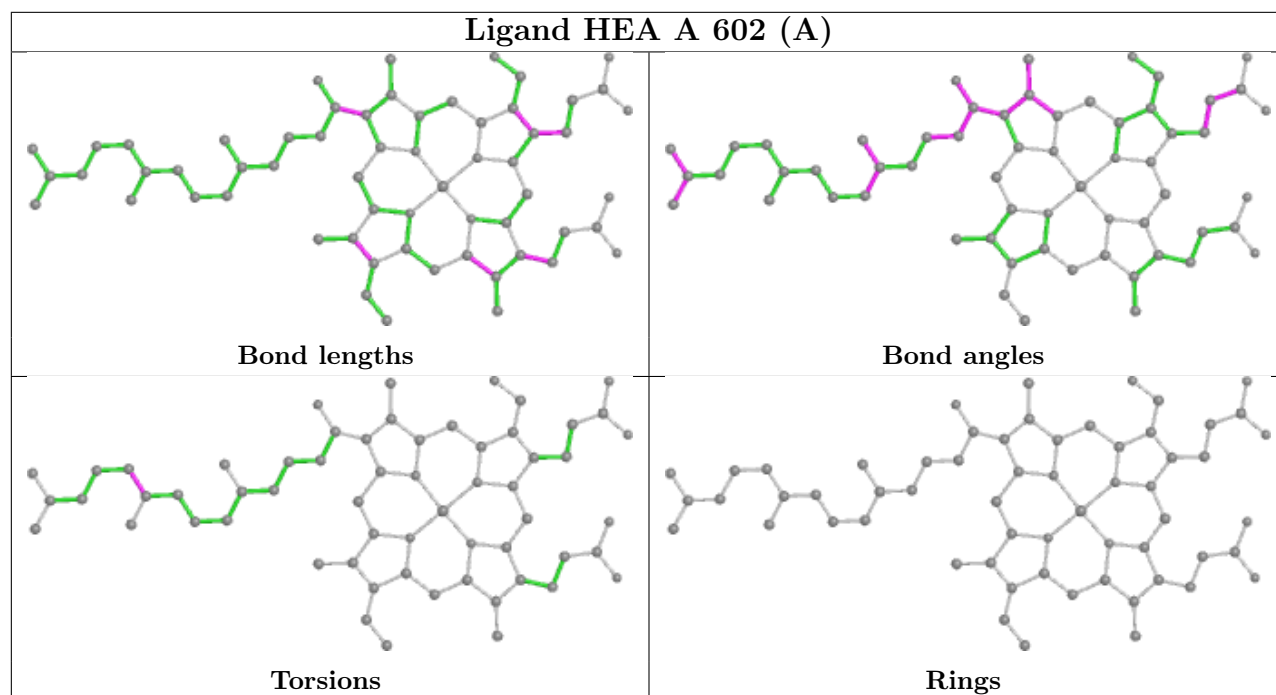
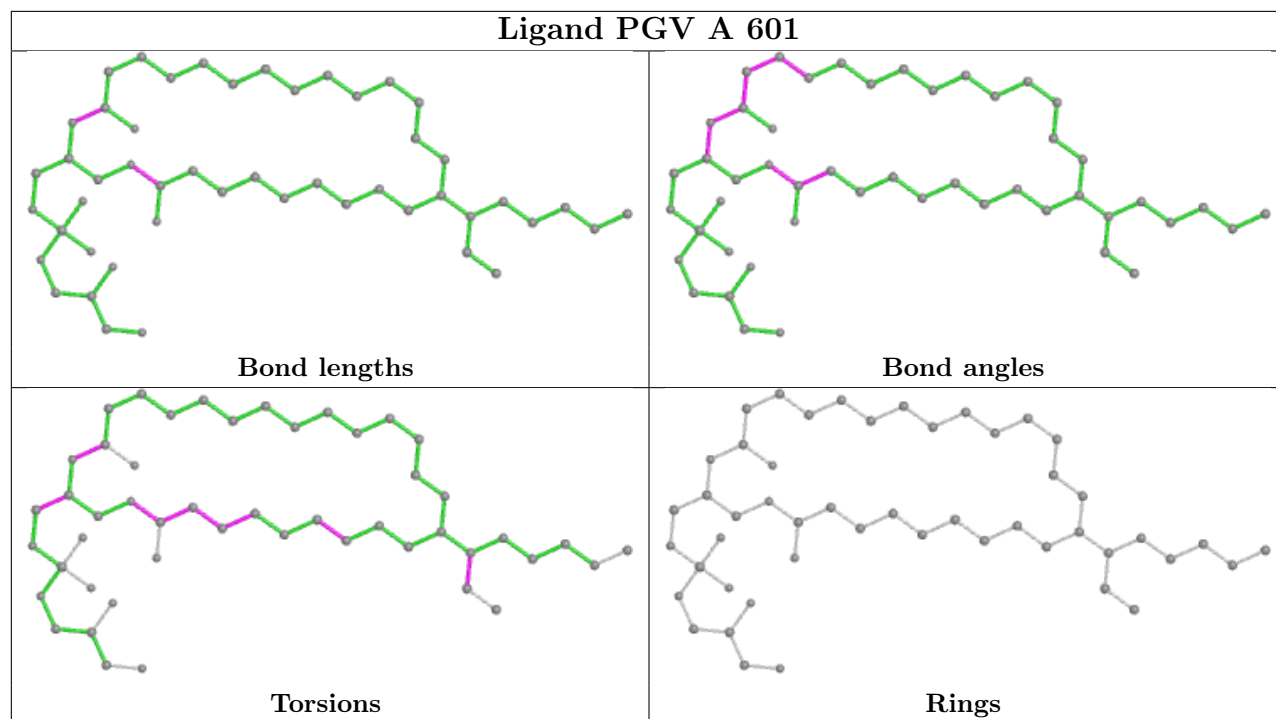


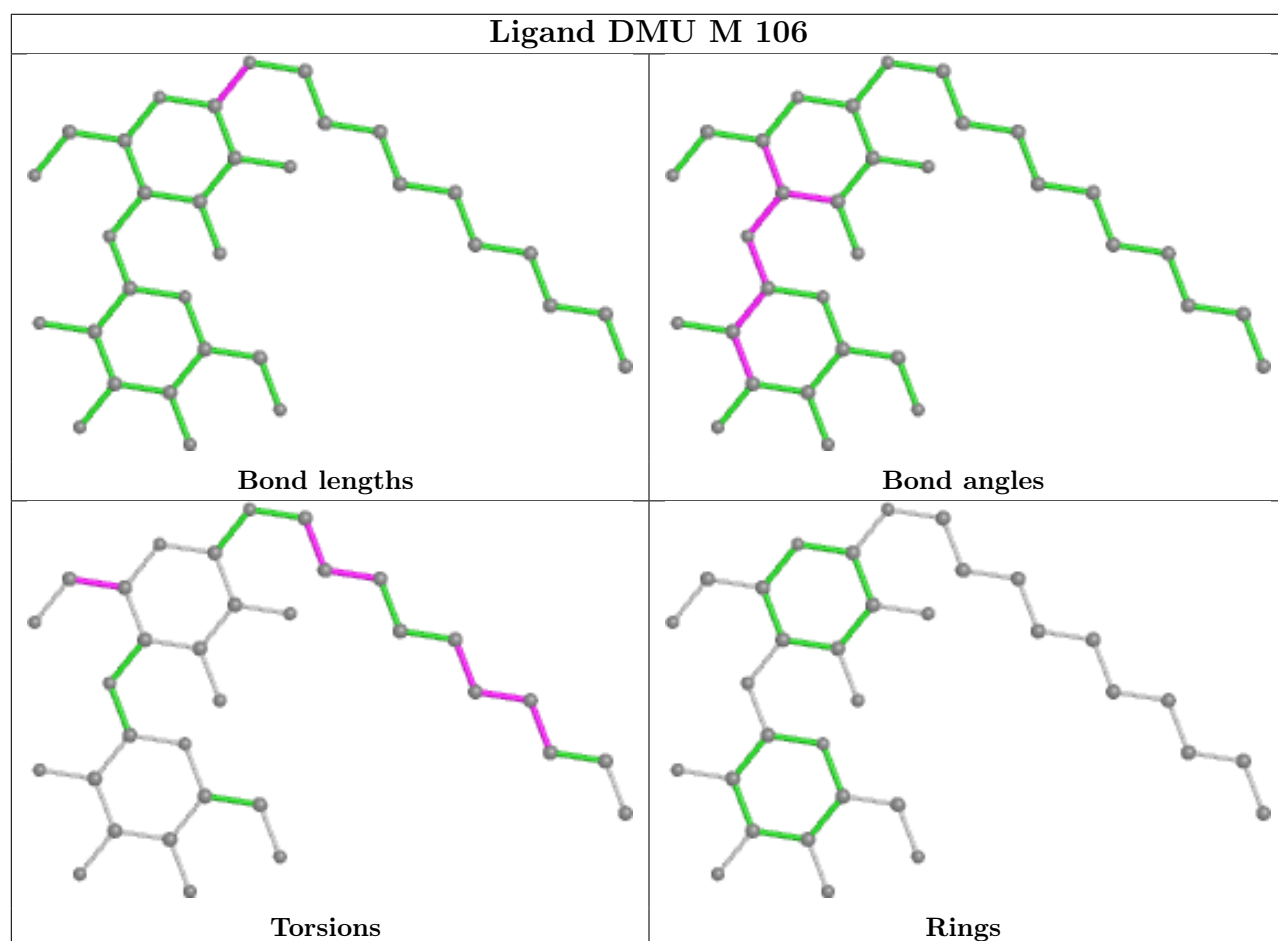
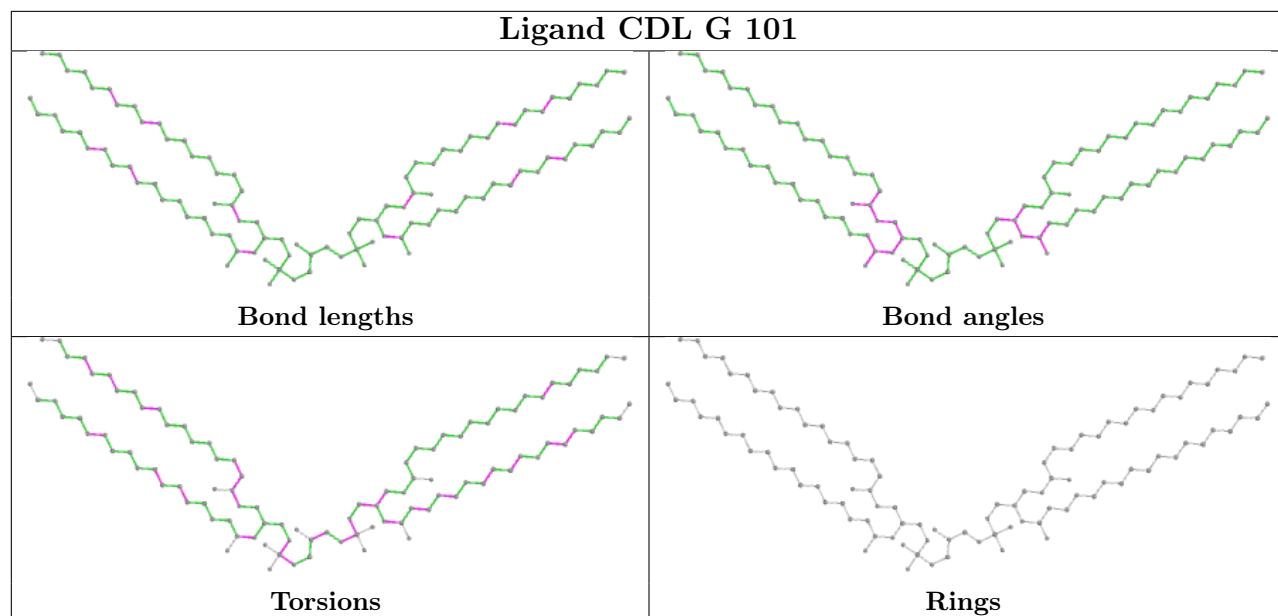




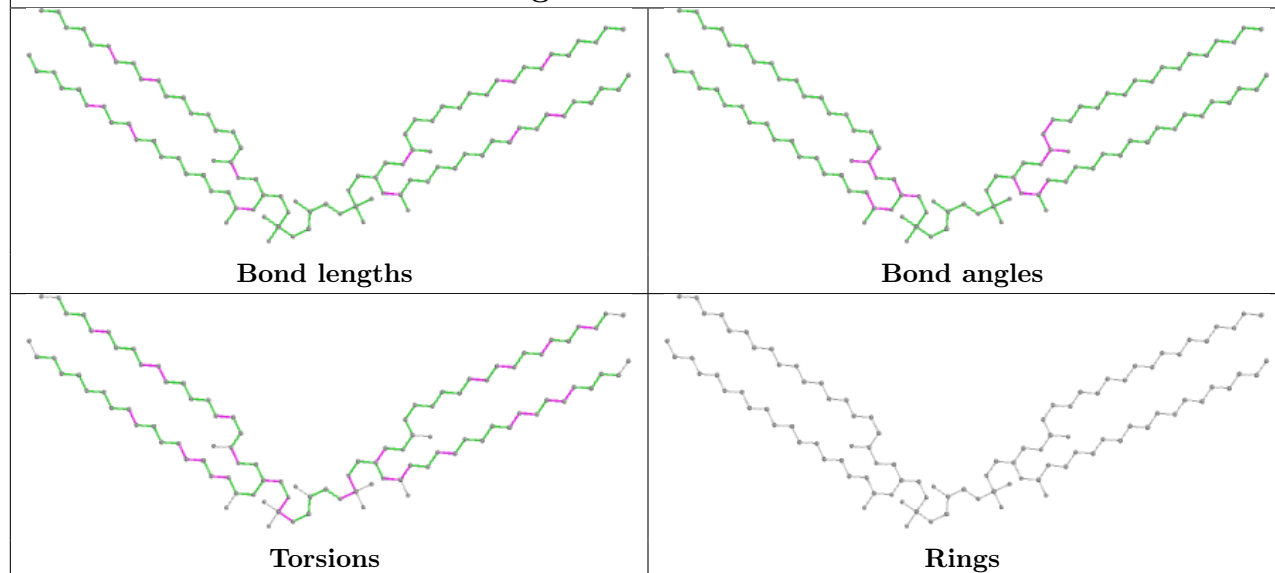




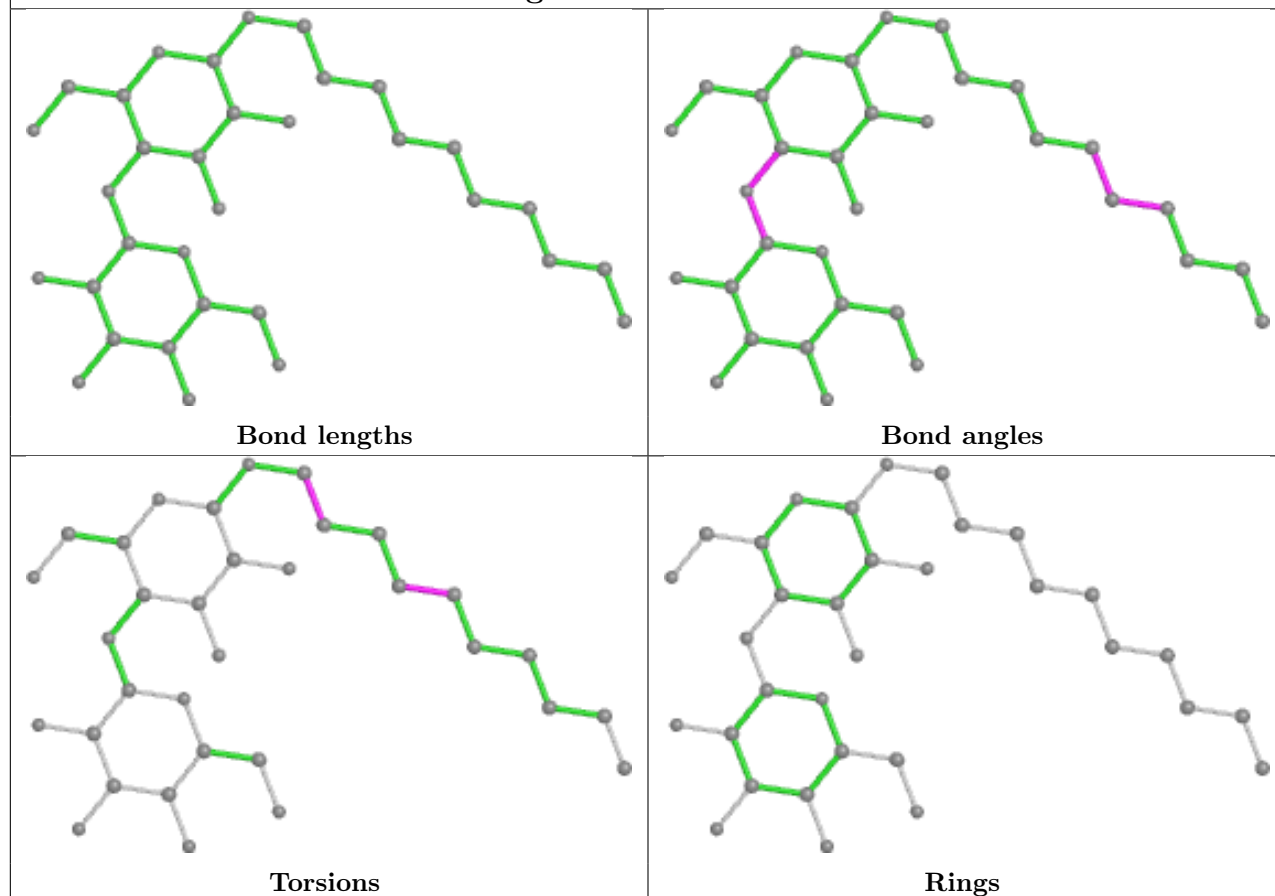


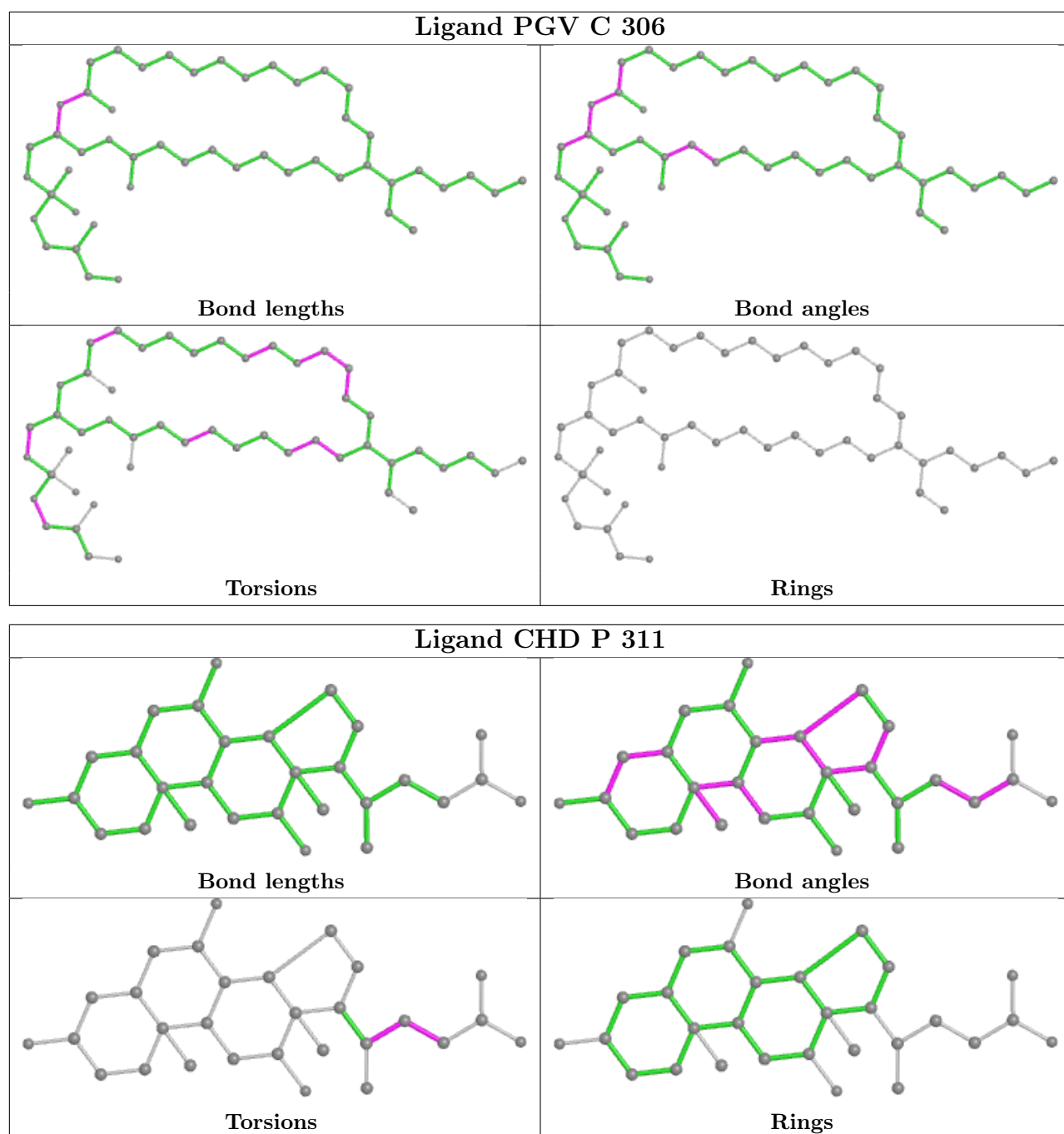


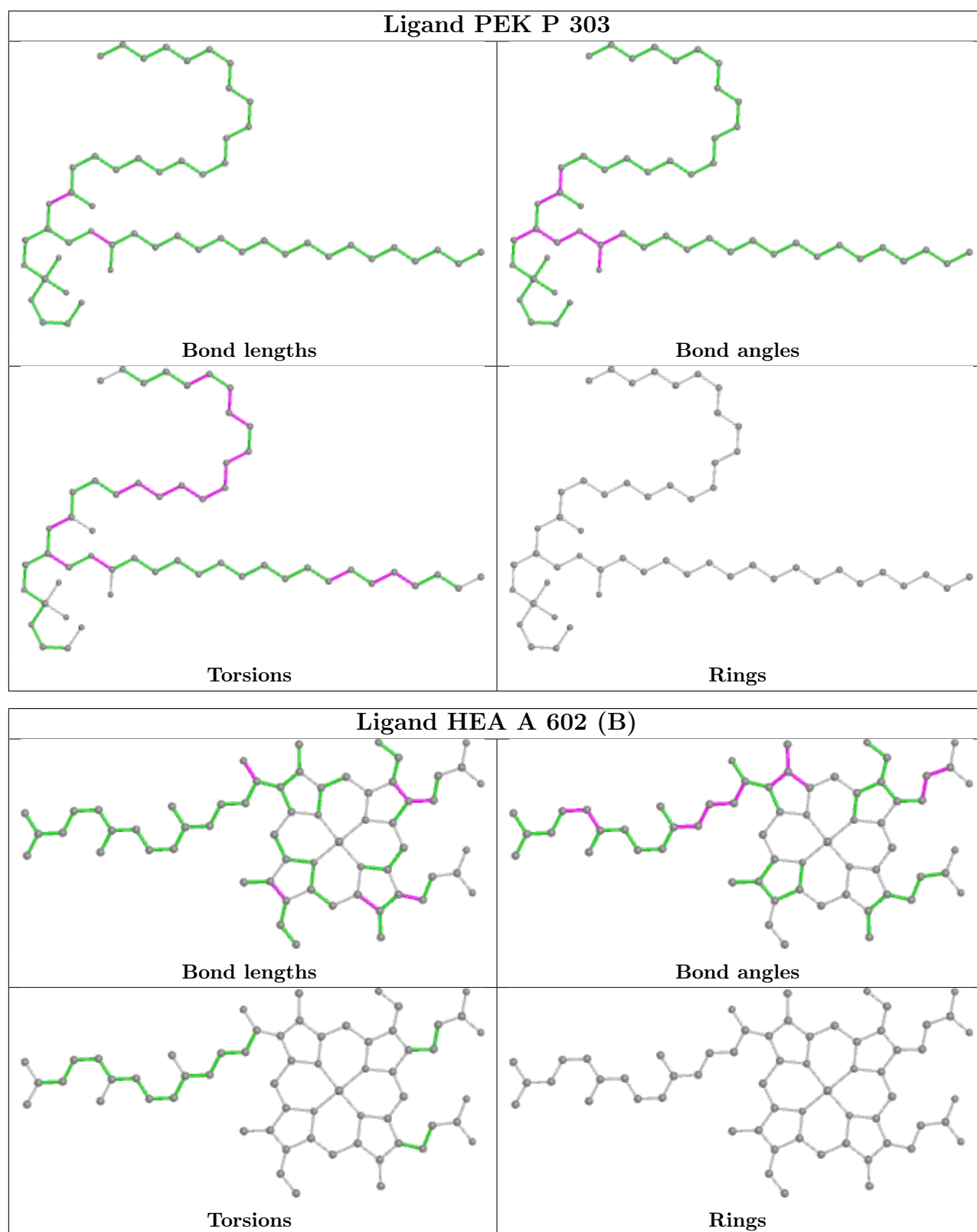
## Ligand CDL P 308



## Ligand DMU Z 101







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	-0.12	1 (0%) 95 95	18, 23, 30, 74	0
1	N	513/514 (99%)	-0.16	0 100 100	19, 25, 33, 69	0
2	B	226/227 (99%)	-0.08	6 (2%) 54 58	21, 29, 53, 108	0
2	O	226/227 (99%)	-0.13	4 (1%) 68 72	25, 34, 62, 118	0
3	C	259/261 (99%)	-0.14	0 100 100	20, 26, 39, 84	0
3	P	259/261 (99%)	-0.04	2 (0%) 86 88	20, 27, 40, 108	0
4	D	144/147 (97%)	-0.28	1 (0%) 87 90	25, 32, 50, 86	0
4	Q	144/147 (97%)	0.90	10 (6%) 16 19	30, 44, 89, 254	0
5	E	105/109 (96%)	-0.24	2 (1%) 66 70	26, 31, 57, 134	0
5	R	105/109 (96%)	-0.20	2 (1%) 66 70	26, 38, 64, 127	0
6	F	94/98 (95%)	0.04	4 (4%) 35 39	22, 32, 61, 160	0
6	S	94/98 (95%)	0.08	5 (5%) 26 29	22, 31, 58, 169	0
7	G	83/85 (97%)	1.01	17 (20%) 1 0	25, 33, 142, 185	0
7	T	83/85 (97%)	1.02	16 (19%) 1 1	24, 36, 141, 185	0
8	H	79/85 (92%)	0.44	10 (12%) 3 4	26, 35, 117, 150	0
8	U	79/85 (92%)	0.40	8 (10%) 7 8	30, 40, 135, 187	0
9	I	72/73 (98%)	0.18	5 (6%) 16 19	28, 42, 71, 85	0
9	V	72/73 (98%)	0.35	3 (4%) 36 40	28, 49, 81, 147	0
10	J	58/59 (98%)	0.30	5 (8%) 10 12	26, 36, 78, 150	0
10	W	58/59 (98%)	0.10	3 (5%) 27 30	27, 37, 80, 213	0
11	K	49/56 (87%)	-0.09	1 (2%) 65 69	28, 36, 50, 82	0
11	X	49/56 (87%)	0.17	3 (6%) 21 23	35, 44, 76, 96	0
12	L	46/47 (97%)	-0.02	2 (4%) 35 39	24, 29, 44, 108	0
12	Y	46/47 (97%)	-0.00	1 (2%) 62 66	28, 34, 63, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.16	3 (6%) 16 18	24, 29, 69, 120	0
13	Z	43/46 (93%)	0.39	3 (6%) 16 18	31, 37, 96, 250	0
All	All	3542/3614 (98%)	0.04	117 (3%) 46 51	18, 30, 66, 254	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	42.6
4	Q	6	VAL	26.1
4	Q	4	SER	22.7
6	F	1	ALA	15.3
7	T	3	ALA	12.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	TPO	T	11	11/12	0.13	0.55	140,173,213,214	0
7	TPO	G	11	11/12	0.47	0.46	130,158,180,180	0
9	SAC	V	1	9/10	0.58	0.39	179,194,204,205	0
9	SAC	I	1	9/10	0.66	0.41	124,152,158,159	0
1	FME	A	1	10/11	0.94	0.11	35,41,68,72	0
2	FME	B	1	10/11	0.97	0.11	27,29,34,51	0
1	FME	N	1	10/11	0.97	0.09	35,41,68,69	0
2	FME	O	1	10/11	0.98	0.10	34,36,41,51	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
18	NA	C	302	1/1	-0.24	1.00	809,809,809,809	0
20	EDO	N	619	4/4	0.20	0.38	85,86,89,89	0
20	EDO	A	614	4/4	0.25	0.36	108,110,111,113	0
20	EDO	D	206	4/4	0.28	0.52	167,169,170,172	0
20	EDO	D	202	4/4	0.29	0.48	83,91,98,99	0
27	DMU	P	324	33/33	0.29	0.27	56,122,149,154	0
20	EDO	N	629	4/4	0.33	0.42	110,114,115,115	0
20	EDO	N	623	4/4	0.33	0.36	90,91,93,94	0
20	EDO	K	102	4/4	0.35	0.34	97,97,98,99	0
20	EDO	B	309	4/4	0.36	0.42	98,99,99,100	0
20	EDO	S	105	4/4	0.38	0.30	84,88,90,91	0
20	EDO	L	104	4/4	0.43	0.17	58,59,60,60	0
20	EDO	P	319	4/4	0.43	0.30	47,54,56,58	0
27	DMU	V	102	33/33	0.43	0.38	71,155,170,171	0
20	EDO	D	203	4/4	0.48	0.24	85,87,90,91	0
20	EDO	B	314	4/4	0.50	0.52	167,168,169,169	0
23	CHD	C	311	29/29	0.51	0.36	104,140,160,162	0
20	EDO	C	313	4/4	0.53	0.32	56,66,73,73	0
20	EDO	O	305	4/4	0.54	0.35	89,94,97,99	0
20	EDO	P	316	4/4	0.55	0.26	53,58,65,66	0
20	EDO	M	103	4/4	0.55	0.36	91,92,94,96	0
20	EDO	B	310	4/4	0.56	0.33	89,94,97,99	0
25	PEK	P	305	53/53	0.56	0.33	39,89,206,231	0
20	EDO	W	104	4/4	0.57	0.25	80,83,86,86	0
20	EDO	O	307	4/4	0.57	0.27	85,87,88,89	0
20	EDO	D	205	4/4	0.57	0.29	60,62,71,74	0
20	EDO	B	311	4/4	0.57	0.28	79,80,81,82	0
20	EDO	B	312	4/4	0.57	0.39	59,63,64,66	0
20	EDO	W	103	4/4	0.58	0.16	47,49,56,57	0
20	EDO	U	101	4/4	0.59	0.34	67,70,71,72	0
26	CDL	G	101	100/100	0.59	0.34	55,112,187,207	0
21	TGL	Q	201	63/63	0.60	0.20	53,80,101,104	0
27	DMU	C	310	33/33	0.61	0.33	48,101,111,113	0
27	DMU	P	309	33/33	0.61	0.29	46,101,136,137	0
20	EDO	M	105	4/4	0.61	0.22	35,47,53,56	0
26	CDL	T	101	100/100	0.61	0.32	58,102,162,185	0
14	PGV	P	307	51/51	0.62	0.30	65,96,161,165	0
23	CHD	P	310	29/29	0.62	0.30	92,136,146,150	0
20	EDO	G	105	4/4	0.62	0.17	74,75,75,77	0
20	EDO	N	618	4/4	0.63	0.19	41,41,44,47	0
20	EDO	N	630	4/4	0.63	0.53	94,94,94,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	PGV	C	307	51/51	0.63	0.28	51,91,167,179	0
20	EDO	N	612	4/4	0.63	0.37	42,50,50,54	0
23	CHD	Y	104	29/29	0.64	0.32	94,123,130,131	0
25	PEK	P	303	53/53	0.64	0.29	47,94,170,176	0
23	CHD	W	101	29/29	0.64	0.28	97,102,131,133	0
20	EDO	P	320	4/4	0.65	0.22	85,85,87,88	0
27	DMU	C	319	33/33	0.65	0.24	50,98,119,120	0
23	CHD	J	101	29/29	0.65	0.25	101,111,135,139	0
26	CDL	P	308	100/100	0.65	0.33	43,112,160,168	0
20	EDO	P	315	4/4	0.65	0.28	32,50,59,60	0
20	EDO	S	111	4/4	0.66	0.36	49,52,60,60	0
27	DMU	M	106	33/33	0.67	0.28	59,101,127,131	0
20	EDO	M	104	4/4	0.67	0.15	57,58,58,66	0
25	PEK	C	305	53/53	0.68	0.27	47,79,141,144	0
27	DMU	G	108	33/33	0.68	0.27	61,124,156,158	0
27	DMU	Z	102	33/33	0.68	0.28	75,102,117,127	0
20	EDO	R	205	4/4	0.69	0.20	68,73,75,76	0
21	TGL	L	101	63/63	0.69	0.28	30,76,115,139	0
29	PO4	U	102	5/5	0.69	0.24	157,157,158,159	0
25	PEK	C	303	53/53	0.71	0.35	46,134,181,186	0
23	CHD	P	311	29/29	0.71	0.18	80,96,107,109	0
20	EDO	R	202	4/4	0.71	0.16	60,61,61,67	0
20	EDO	O	306	4/4	0.71	0.35	73,80,80,82	0
14	PGV	N	601	51/51	0.74	0.28	45,87,144,151	0
20	EDO	B	305	4/4	0.74	0.18	50,52,54,54	0
20	EDO	B	307	4/4	0.74	0.19	60,61,66,67	0
20	EDO	R	203	4/4	0.74	0.15	60,64,66,68	0
21	TGL	Y	101	63/63	0.74	0.25	42,68,122,141	0
26	CDL	C	308	100/100	0.74	0.29	41,94,151,153	0
22	PSC	B	302	52/52	0.76	0.32	44,121,206,217	0
20	EDO	A	623	4/4	0.76	0.49	51,66,75,81	0
20	EDO	C	317	4/4	0.76	0.25	75,78,78,79	0
20	EDO	G	104	4/4	0.76	0.56	107,109,111,112	0
23	CHD	C	309	29/29	0.77	0.17	68,78,95,97	0
21	TGL	D	201	63/63	0.77	0.20	36,71,99,104	0
20	EDO	R	204	4/4	0.78	0.18	68,68,69,70	0
20	EDO	P	321	4/4	0.78	0.26	53,61,65,68	0
20	EDO	A	617	4/4	0.78	0.22	52,56,61,62	0
20	EDO	H	101	4/4	0.78	0.14	56,57,62,63	0
20	EDO	N	625	4/4	0.80	0.24	54,56,58,59	0
20	EDO	P	313	4/4	0.80	0.11	60,62,63,63	0
20	EDO	S	108	4/4	0.80	0.16	43,53,63,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	PGV	A	601	51/51	0.81	0.28	32,79,182,190	0
20	EDO	F	105	4/4	0.81	0.21	65,68,73,75	0
21	TGL	N	608	63/63	0.81	0.20	52,73,109,113	0
20	EDO	P	322	4/4	0.81	0.12	57,58,58,60	0
20	EDO	S	110	4/4	0.81	0.14	51,53,58,58	0
20	EDO	N	616	4/4	0.83	0.10	61,62,63,65	0
20	EDO	J	102	4/4	0.83	0.34	111,111,113,114	0
21	TGL	B	301	63/63	0.83	0.17	45,67,109,115	0
20	EDO	L	102	4/4	0.84	0.12	68,70,71,73	0
27	DMU	P	323	33/33	0.85	0.14	51,88,98,100	0
20	EDO	C	314	4/4	0.85	0.22	54,57,62,63	0
20	EDO	P	314	4/4	0.85	0.14	49,50,55,55	0
20	EDO	V	101	4/4	0.85	0.20	60,65,68,71	0
20	EDO	L	105	4/4	0.85	0.09	53,55,57,59	0
20	EDO	A	624	4/4	0.86	0.15	58,59,60,64	0
22	PSC	O	301	52/52	0.86	0.30	35,100,221,227	0
20	EDO	Q	202	4/4	0.86	0.15	65,67,71,77	0
20	EDO	E	202	4/4	0.87	0.12	53,54,56,60	0
20	EDO	N	617	4/4	0.88	0.18	61,65,70,71	0
20	EDO	Y	102	4/4	0.88	0.08	59,59,61,65	0
20	EDO	G	103	4/4	0.88	0.14	45,49,51,54	0
20	EDO	D	207	4/4	0.88	0.15	44,44,49,54	0
20	EDO	M	102	4/4	0.88	0.14	61,67,68,69	0
20	EDO	N	615	4/4	0.88	0.11	55,57,57,61	0
20	EDO	H	103	4/4	0.88	0.20	34,38,43,45	0
20	EDO	A	621	4/4	0.89	0.14	40,47,52,55	0
20	EDO	H	102	4/4	0.89	0.24	50,50,54,55	0
20	EDO	N	621	4/4	0.89	0.16	47,49,49,50	0
27	DMU	Z	101	33/33	0.89	0.13	37,45,63,69	0
20	EDO	A	622	4/4	0.89	0.15	63,65,67,67	0
20	EDO	G	107	4/4	0.89	0.11	35,50,57,58	0
20	EDO	N	627	4/4	0.90	0.19	64,65,67,70	0
20	EDO	N	628	4/4	0.90	0.15	33,42,47,50	0
20	EDO	S	107	4/4	0.90	0.36	56,62,64,66	0
20	EDO	A	609	4/4	0.90	0.41	32,46,54,57	0
20	EDO	C	318	4/4	0.90	0.20	39,53,59,60	0
20	EDO	Q	203	4/4	0.90	0.19	47,58,58,61	0
20	EDO	J	103	4/4	0.90	0.18	57,61,65,72	0
20	EDO	P	318	4/4	0.90	0.17	38,42,46,46	0
20	EDO	C	316	4/4	0.90	0.18	31,39,40,41	0
20	EDO	S	106	4/4	0.91	0.15	40,51,51,56	0
20	EDO	S	112	4/4	0.91	0.25	39,43,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	L	103	4/4	0.91	0.11	56,58,59,64	0
27	DMU	M	101	33/33	0.91	0.10	34,40,57,62	0
20	EDO	A	612	4/4	0.91	0.16	39,41,42,42	0
20	EDO	B	308	4/4	0.91	0.28	46,50,51,52	0
20	EDO	A	620	4/4	0.92	0.17	37,40,42,47	0
20	EDO	D	204[A]	4/4	0.92	0.23	46,55,59,64	1
20	EDO	A	625	4/4	0.92	0.10	50,54,60,61	0
20	EDO	B	313	4/4	0.92	0.16	39,44,47,48	0
20	EDO	W	102	4/4	0.92	0.19	58,59,62,67	0
20	EDO	A	626	4/4	0.92	0.23	30,36,48,52	0
20	EDO	A	613	4/4	0.92	0.15	37,40,48,50	0
20	EDO	N	624	4/4	0.92	0.19	29,40,56,67	0
20	EDO	Y	103	4/4	0.92	0.22	57,57,61,63	0
20	EDO	F	103	4/4	0.92	0.26	38,52,57,58	0
20	EDO	N	626	4/4	0.92	0.19	59,60,63,65	0
20	EDO	A	615	4/4	0.93	0.19	36,41,50,51	0
20	EDO	A	627	4/4	0.93	0.17	27,31,37,41	0
20	EDO	F	104	4/4	0.93	0.09	32,37,37,42	0
29	PO4	H	104	5/5	0.93	0.15	90,91,95,96	0
20	EDO	E	201	4/4	0.93	0.10	59,62,66,68	0
20	EDO	T	103	4/4	0.94	0.19	40,46,48,51	0
20	EDO	S	103	4/4	0.94	0.08	33,34,38,38	0
20	EDO	A	618	4/4	0.94	0.15	30,42,54,61	0
20	EDO	N	614	4/4	0.94	0.11	36,37,41,44	0
23	CHD	P	301	29/29	0.94	0.08	24,27,32,34	0
20	EDO	O	304	4/4	0.94	0.16	40,40,44,46	0
20	EDO	S	104	4/4	0.95	0.11	28,29,31,32	0
20	EDO	A	610	4/4	0.95	0.11	27,27,31,32	0
20	EDO	F	107	4/4	0.95	0.16	43,45,57,66	0
20	EDO	C	315	4/4	0.95	0.16	29,34,42,48	0
23	CHD	C	301	29/29	0.95	0.08	23,27,31,33	0
25	PEK	P	304	53/53	0.95	0.12	25,44,95,99	0
20	EDO	R	201	4/4	0.95	0.09	40,40,41,41	0
20	EDO	O	303	4/4	0.95	0.09	29,29,30,30	0
20	EDO	A	616	4/4	0.95	0.21	28,36,38,38	0
20	EDO	C	312	4/4	0.95	0.07	31,34,34,35	0
20	EDO	K	101	4/4	0.95	0.07	49,49,50,53	0
20	EDO	A	619	4/4	0.95	0.28	33,35,47,48	0
20	EDO	N	610	4/4	0.96	0.11	26,26,26,31	0
23	CHD	G	102	29/29	0.96	0.08	22,24,28,36	0
25	PEK	C	304	53/53	0.96	0.13	26,43,87,91	0
20	EDO	T	102	4/4	0.96	0.12	31,31,36,38	0

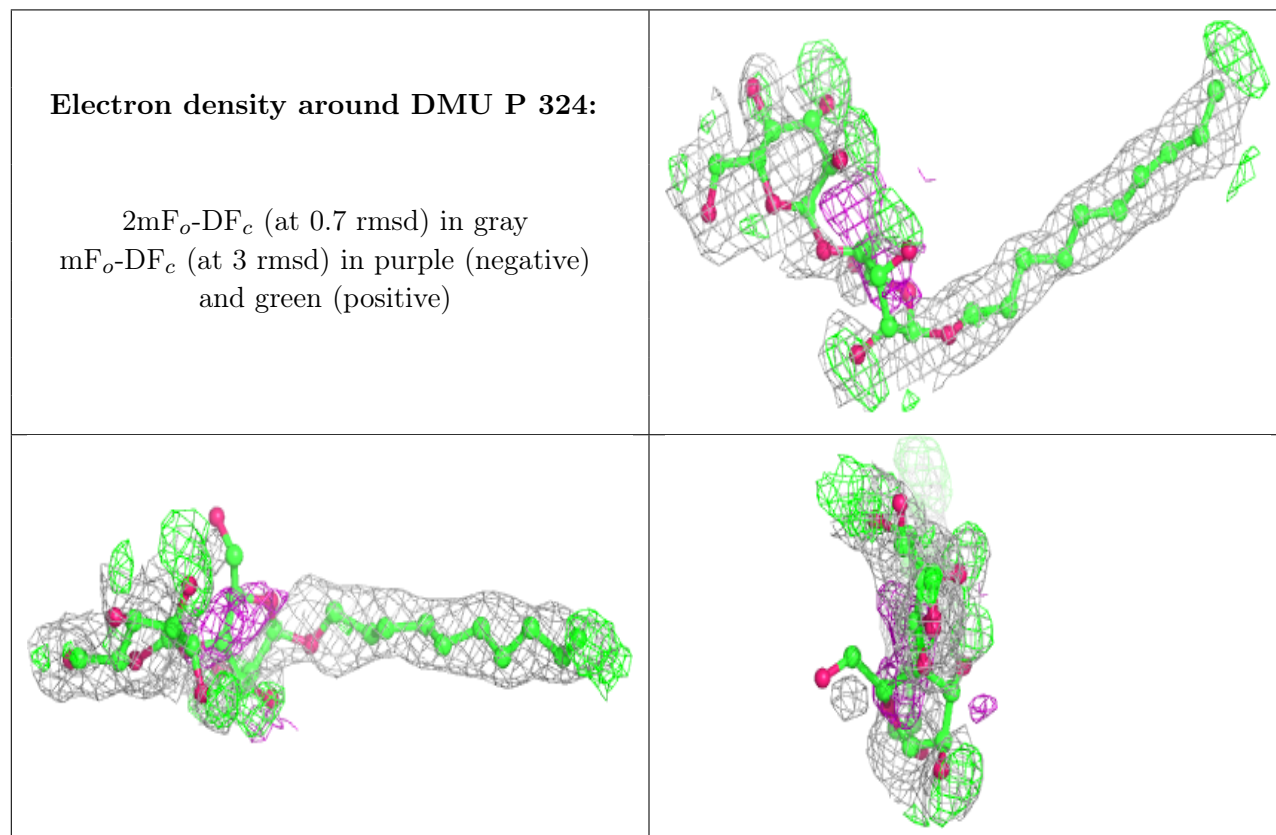
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	PGV	C	306	51/51	0.96	0.12	21,28,77,81	0
23	CHD	B	303	29/29	0.96	0.08	22,25,33,38	0
20	EDO	N	620	4/4	0.96	0.10	37,38,41,42	0
20	EDO	P	317	4/4	0.96	0.17	36,39,40,42	0
18	NA	P	302	1/1	0.97	0.31	17,17,17,17	1
19	CMO	N	607[A]	2/2	0.97	0.22	19,19,19,19	2
19	CMO	N	607[B]	2/2	0.97	0.22	18,18,18,19	2
14	PGV	P	306	51/51	0.97	0.12	21,30,78,81	0
20	EDO	G	106	4/4	0.97	0.09	28,30,34,36	0
14	PGV	A	608	51/51	0.97	0.11	21,26,56,58	0
20	EDO	N	611	4/4	0.97	0.12	36,39,40,41	0
20	EDO	N	622	4/4	0.97	0.17	30,36,38,39	0
14	PGV	N	609	51/51	0.97	0.11	22,27,56,61	0
20	EDO	N	613	4/4	0.97	0.11	22,26,27,30	0
20	EDO	S	109	4/4	0.97	0.18	28,39,46,47	0
20	EDO	P	312	4/4	0.97	0.12	28,34,39,47	0
20	EDO	F	106	4/4	0.97	0.12	29,31,32,35	0
15	HEA	A	602[B]	60/60	0.98	0.10	18,21,28,30	18
19	CMO	A	607[A]	2/2	0.98	0.23	16,16,16,16	2
19	CMO	A	607[B]	2/2	0.98	0.23	16,16,16,16	2
15	HEA	A	602[C]	43/60	0.98	0.10	18,20,22,25	1
24	CUA	O	302	2/2	0.98	0.11	25,25,25,25	0
20	EDO	S	102	4/4	0.98	0.08	22,23,23,23	0
20	EDO	B	306	4/4	0.98	0.10	23,23,26,30	0
15	HEA	A	603	60/60	0.98	0.09	18,20,27,30	0
20	EDO	E	203	4/4	0.98	0.08	36,39,40,41	0
15	HEA	N	602[A]	60/60	0.98	0.10	21,25,30,32	18
15	HEA	N	602[B]	60/60	0.98	0.10	21,25,30,32	18
15	HEA	N	602[C]	43/60	0.98	0.10	21,24,26,27	1
15	HEA	N	603	60/60	0.98	0.09	19,23,28,30	0
15	HEA	A	602[A]	60/60	0.98	0.10	18,21,28,29	18
18	NA	N	606	1/1	0.99	0.07	31,31,31,31	0
17	MG	A	605	1/1	0.99	0.09	22,22,22,22	0
20	EDO	F	102	4/4	0.99	0.09	22,23,23,25	0
24	CUA	B	304	2/2	0.99	0.12	21,21,21,21	0
17	MG	N	605	1/1	0.99	0.12	26,26,26,26	0
28	ZN	F	101	1/1	0.99	0.12	27,27,27,27	0
16	CU	N	604	1/1	0.99	0.15	23,23,23,23	0
20	EDO	A	611	4/4	0.99	0.12	21,23,24,27	0
28	ZN	S	101	1/1	1.00	0.13	27,27,27,27	0
18	NA	A	606	1/1	1.00	0.08	26,26,26,26	0
16	CU	A	604	1/1	1.00	0.14	20,20,20,20	0



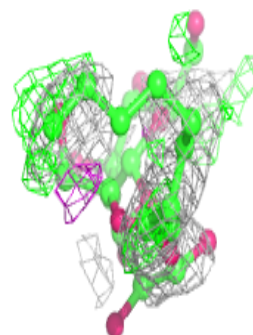
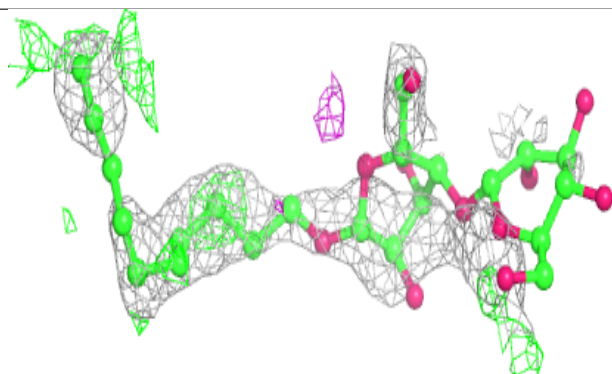
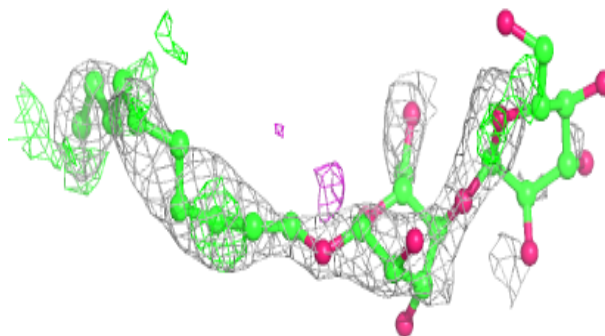
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



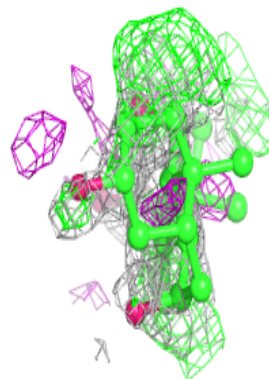
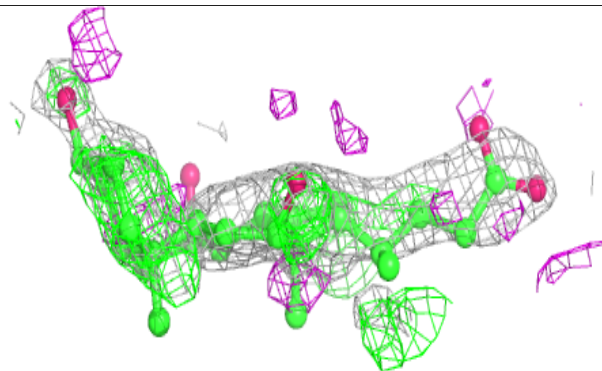
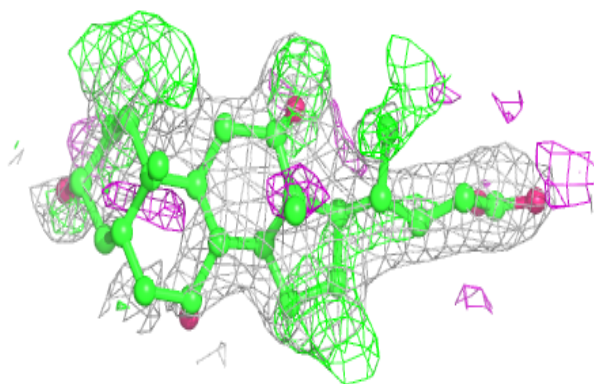


**Electron density around DMU V 102:**

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

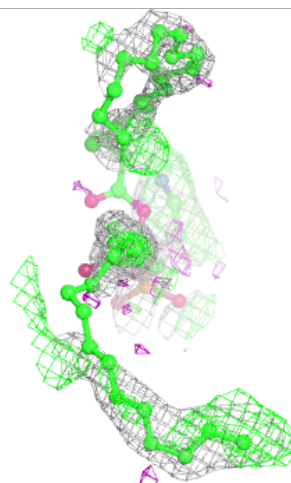
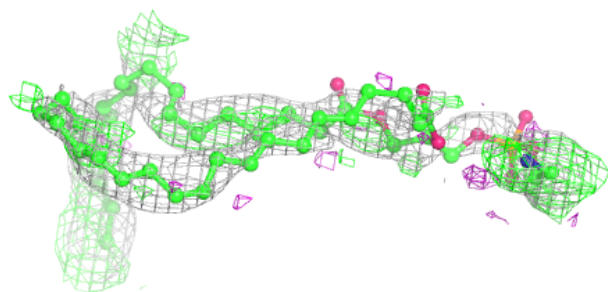
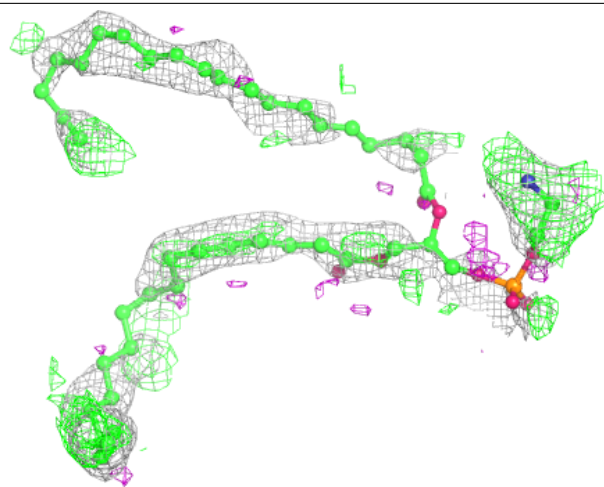
**Electron density around CHD C 311:**

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



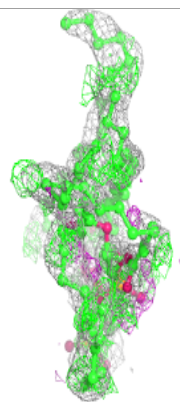
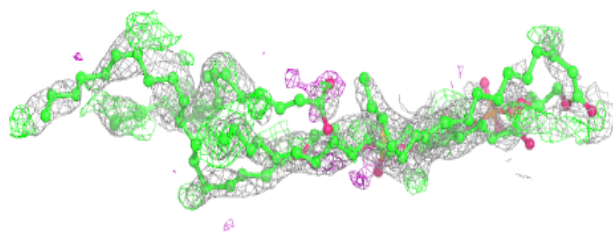
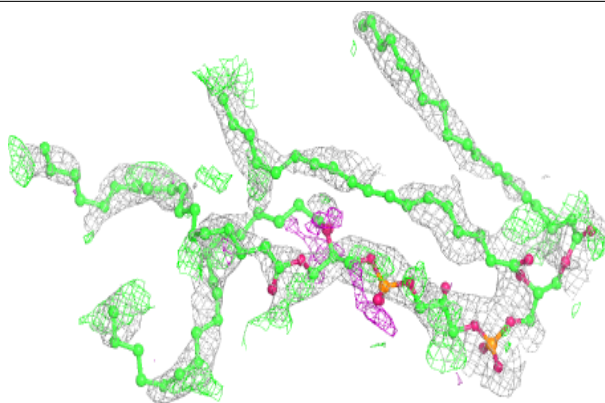
**Electron density around PEK P 305:**

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

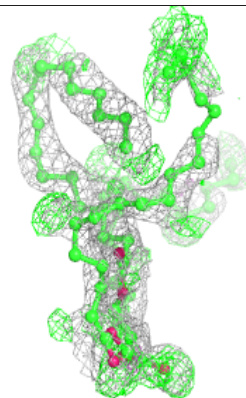
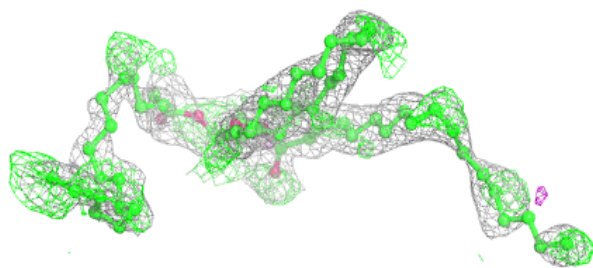
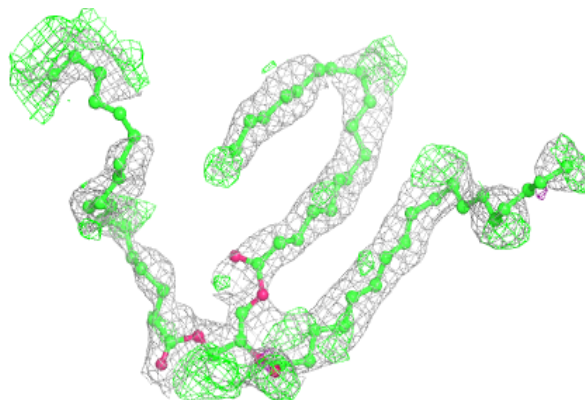


**Electron density around CDL G 101:**

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

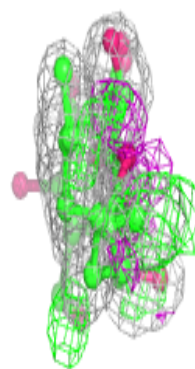
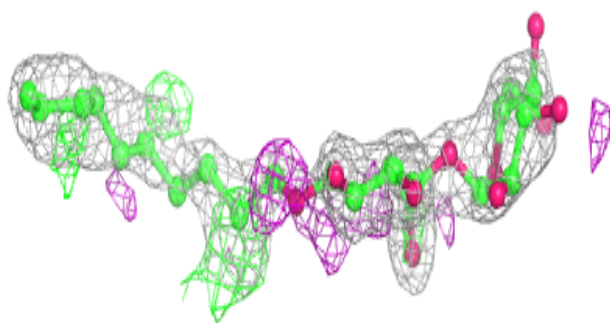
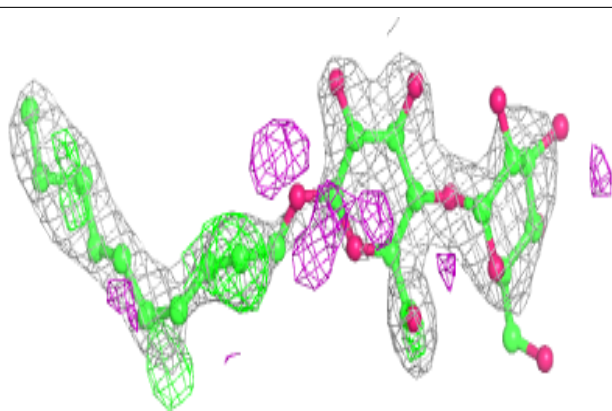
**Electron density around TGL Q 201:**

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

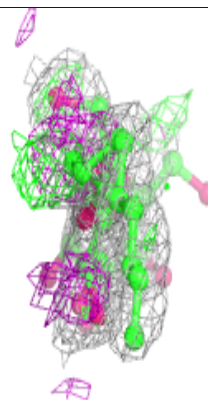
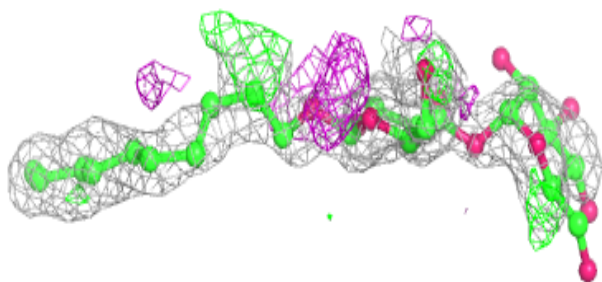
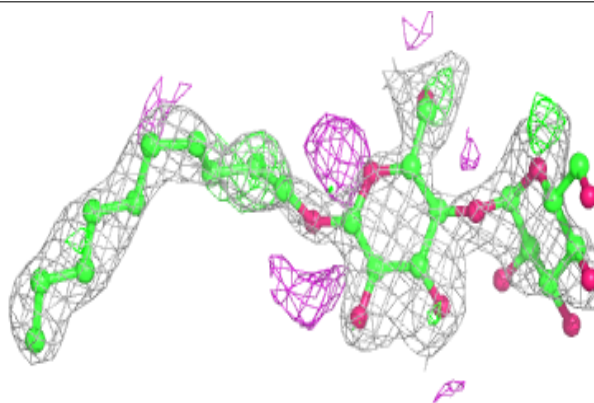


**Electron density around DMU C 310:**

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

**Electron density around DMU P 309:**

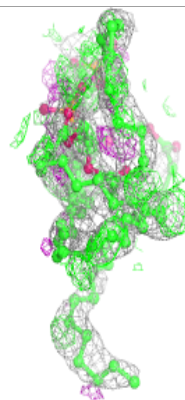
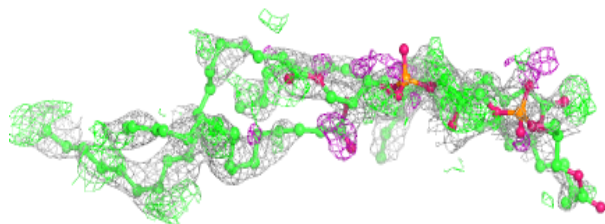
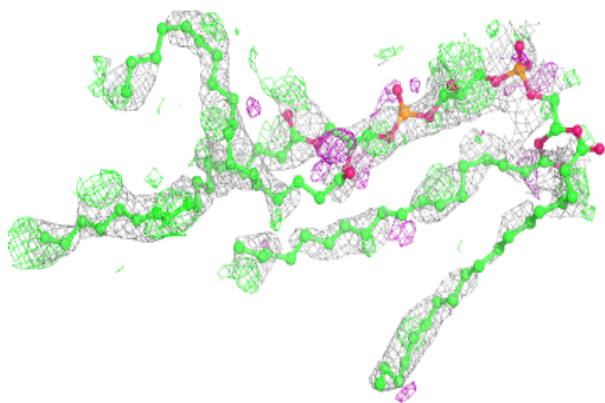
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



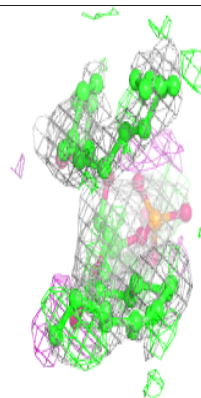
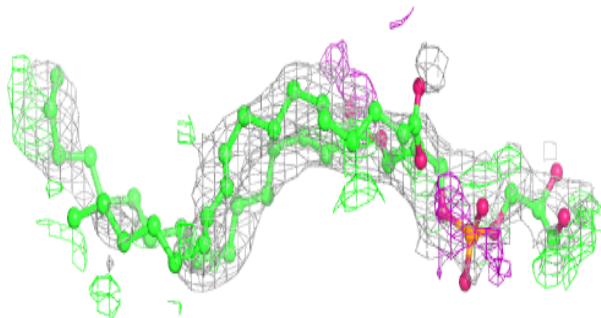
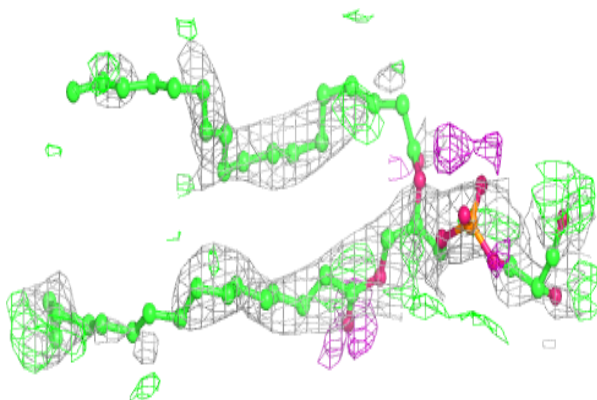


**Electron density around CDL T 101:**

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

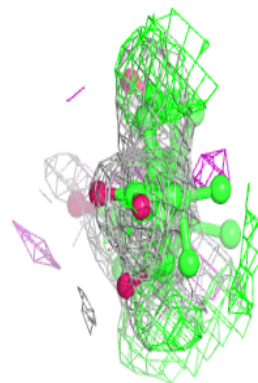
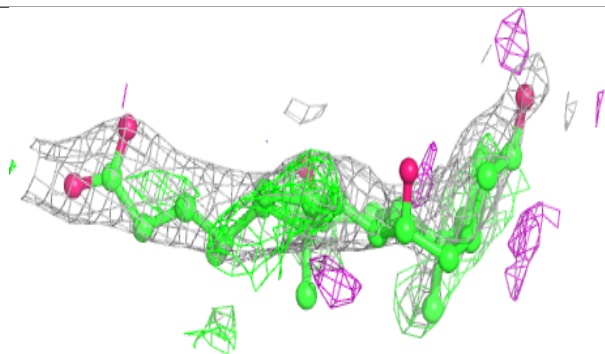
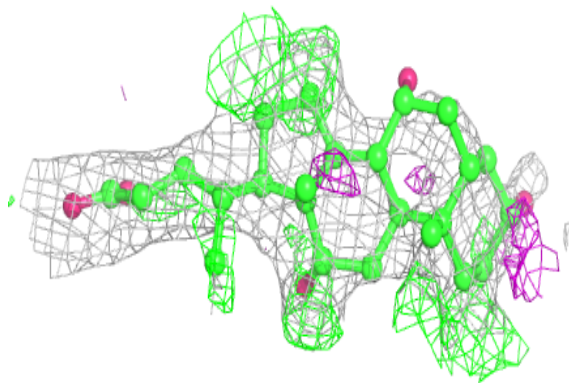
**Electron density around PGV P 307:**

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

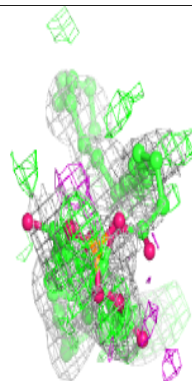
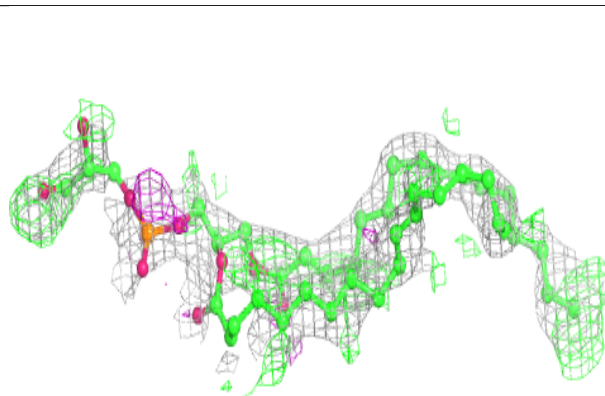
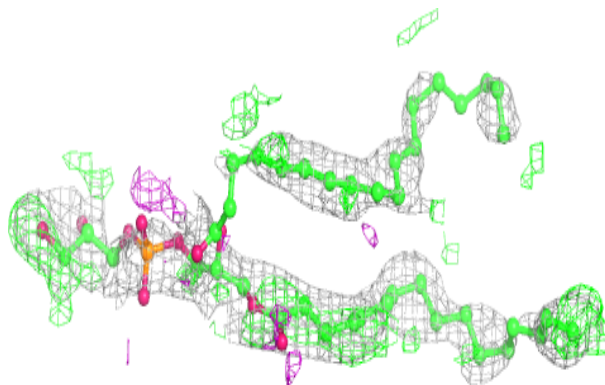


**Electron density around CHD P 310:**

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

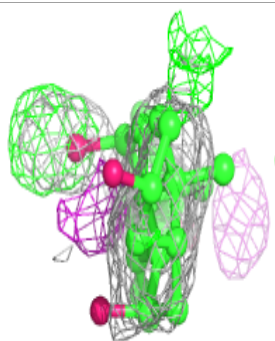
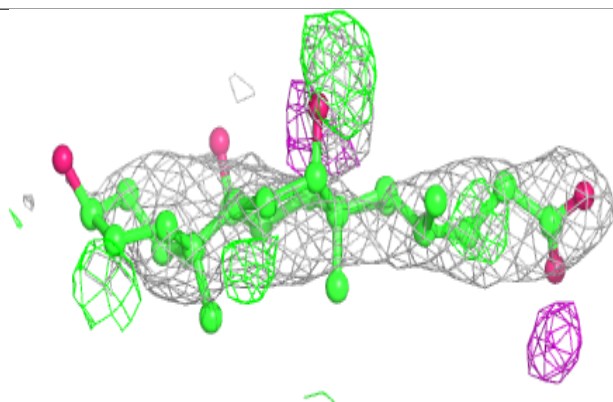
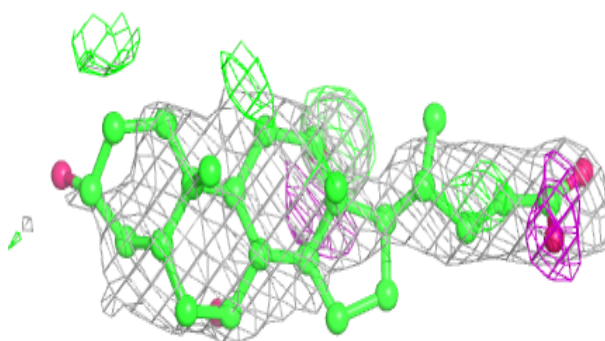
**Electron density around PGV C 307:**

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

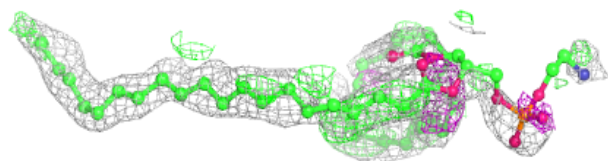
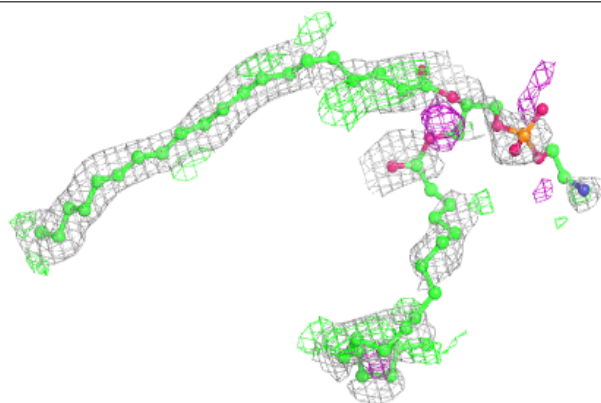


**Electron density around CHD Y 104:**

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

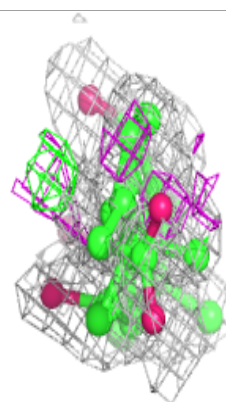
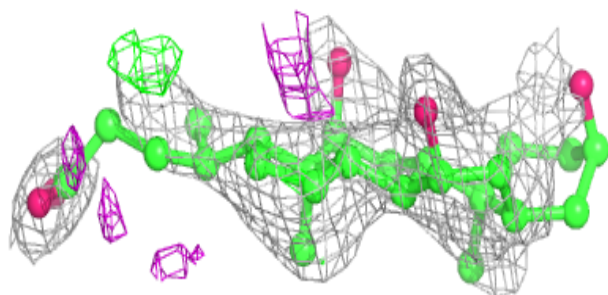
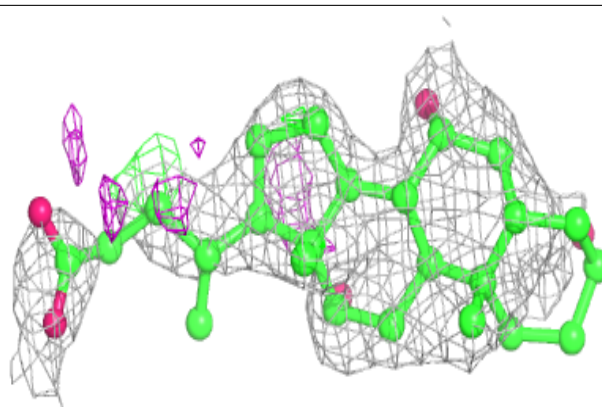
**Electron density around PEK P 303:**

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

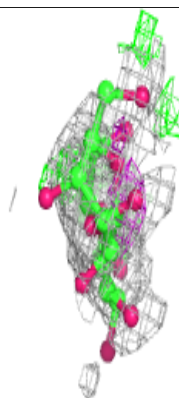
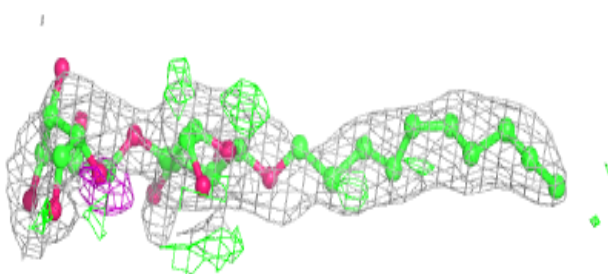
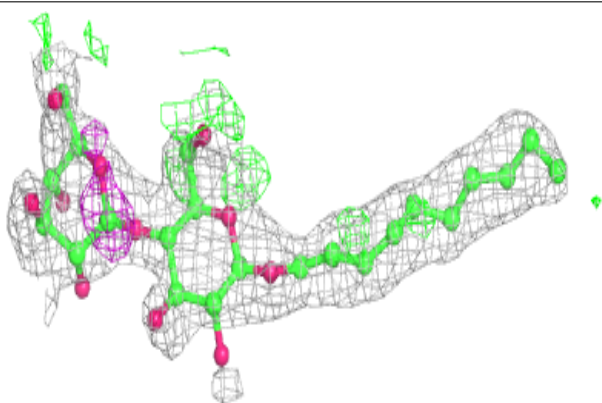


**Electron density around CHD W 101:**

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

**Electron density around DMU C 319:**

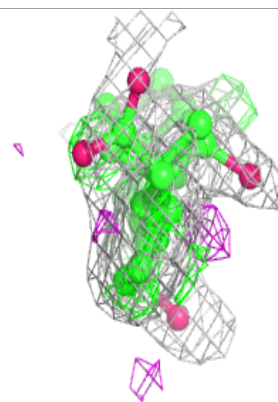
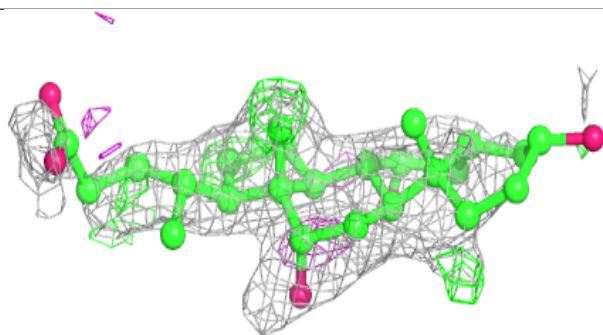
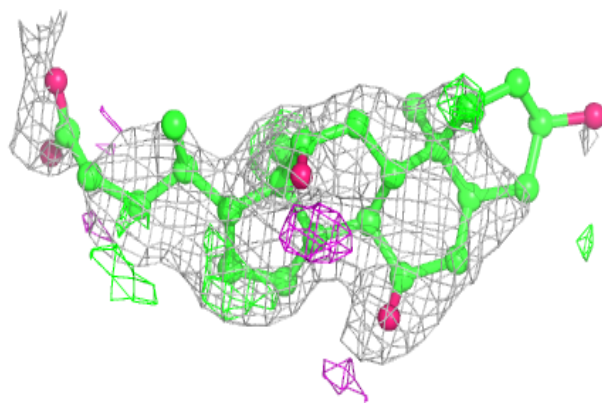
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





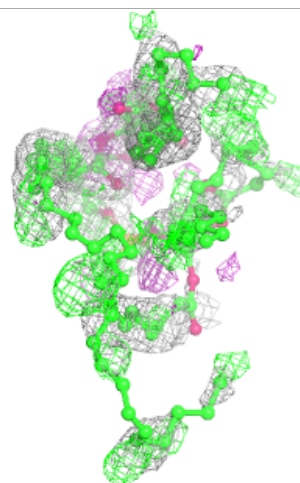
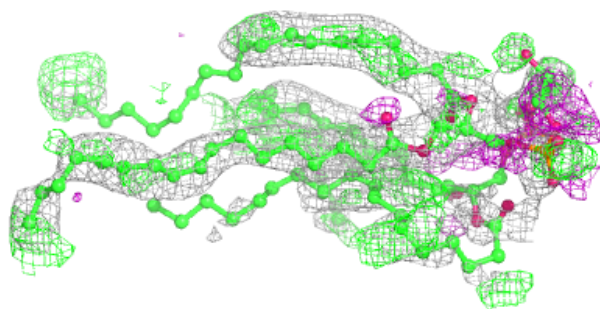
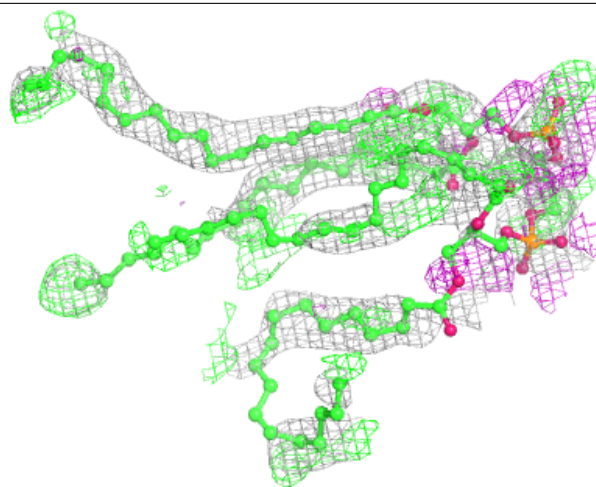
**Electron density around CHD J 101:**

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



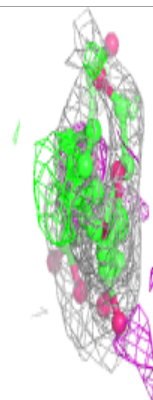
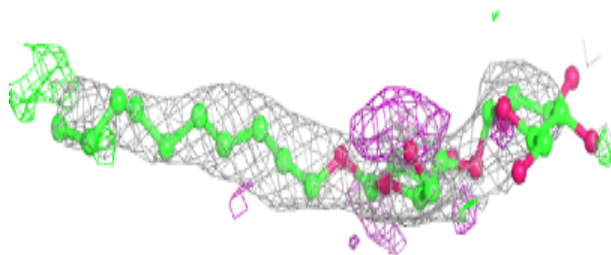
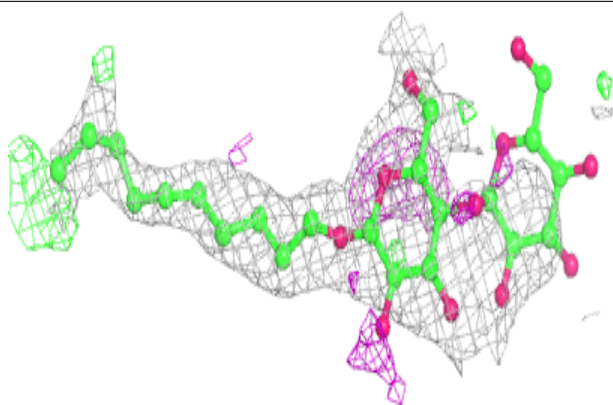
**Electron density around CDL P 308:**

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



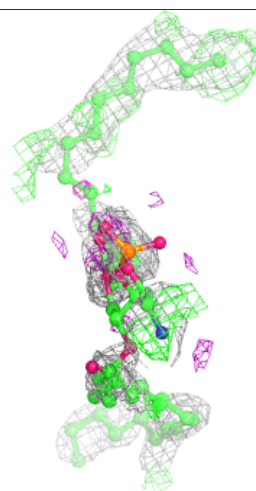
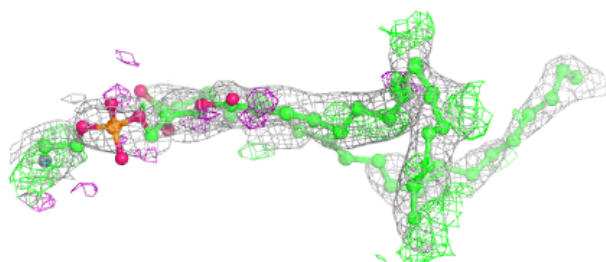
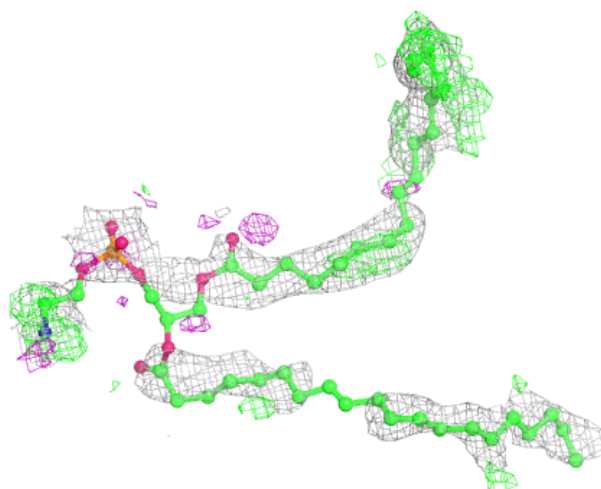
**Electron density around DMU M 106:**

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



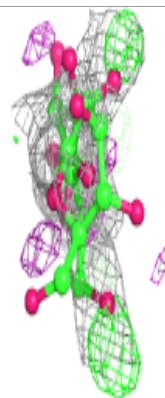
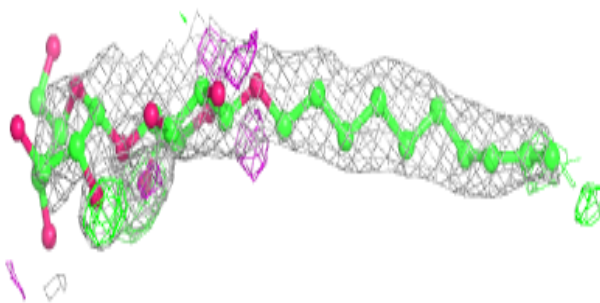
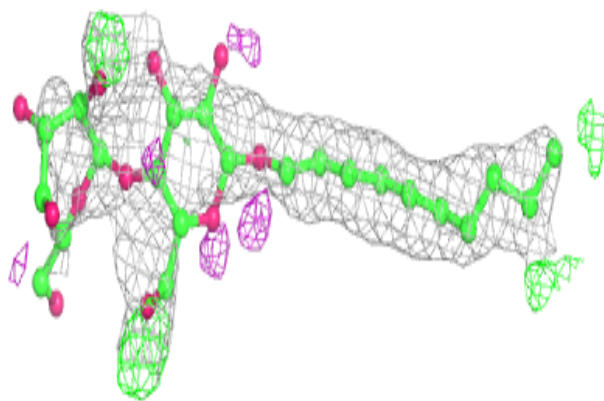
**Electron density around PEK C 305:**

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

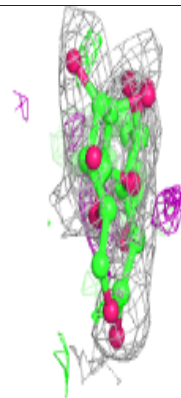
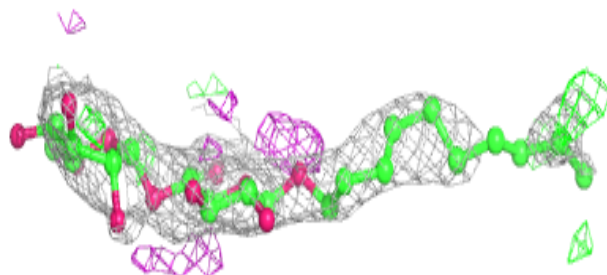
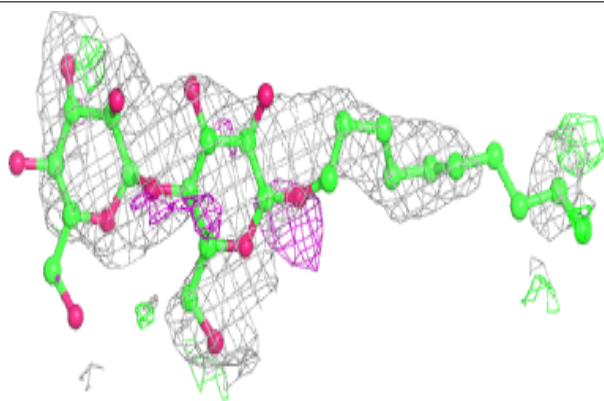


**Electron density around DMU G 108:**

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

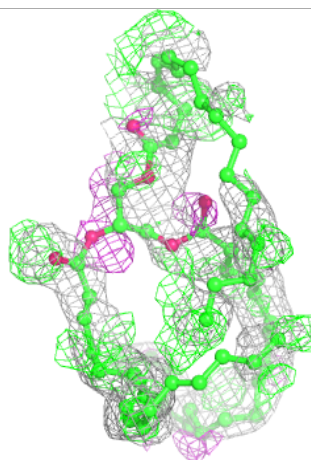
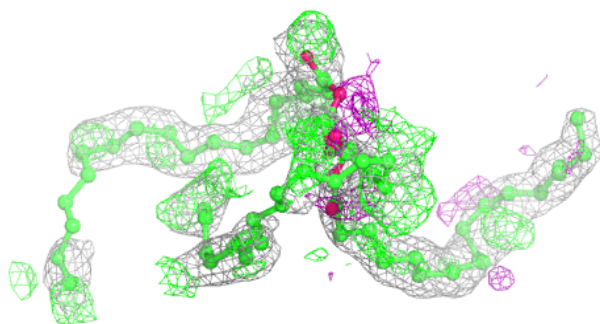
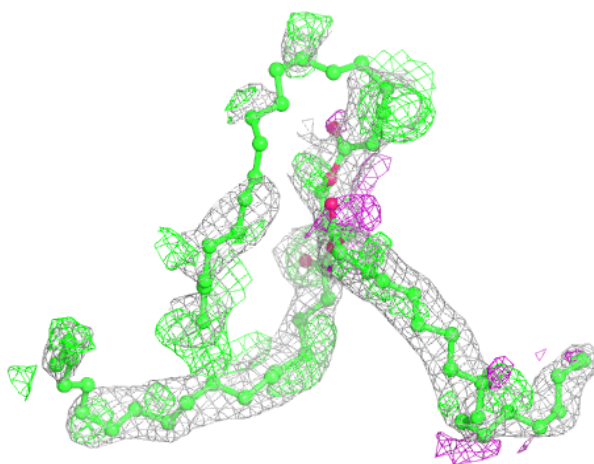
**Electron density around DMU Z 102:**

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



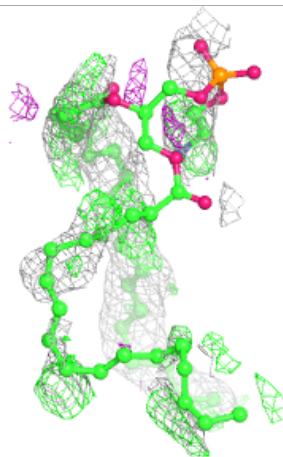
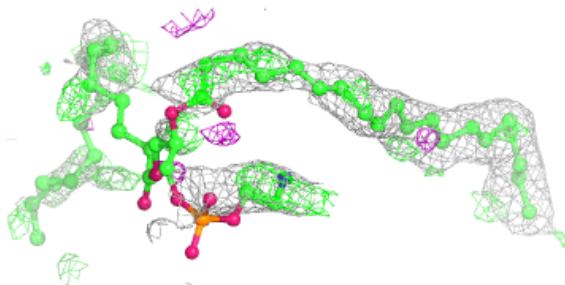
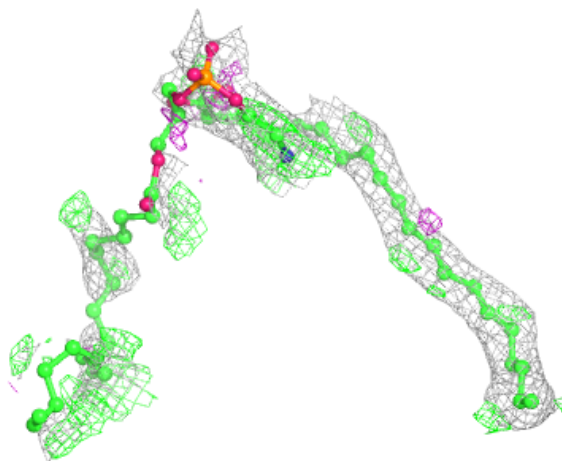
**Electron density around TGL L 101:**

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



**Electron density around PEK C 303:**

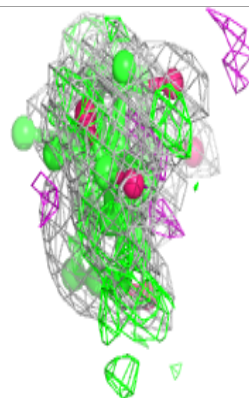
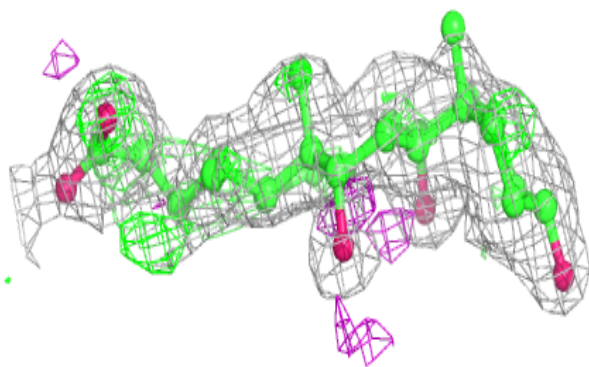
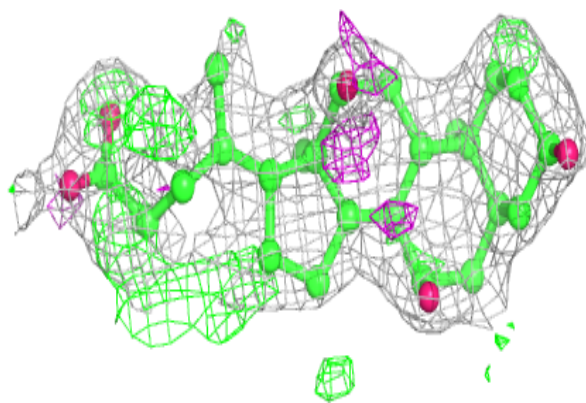
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



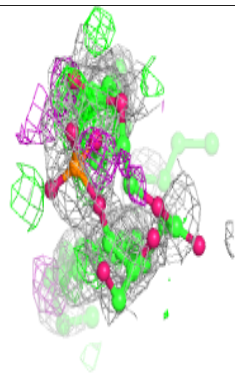
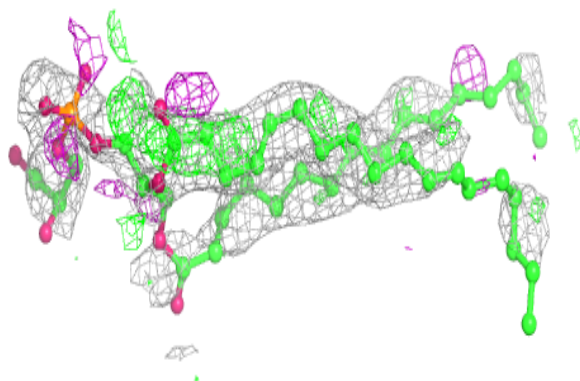
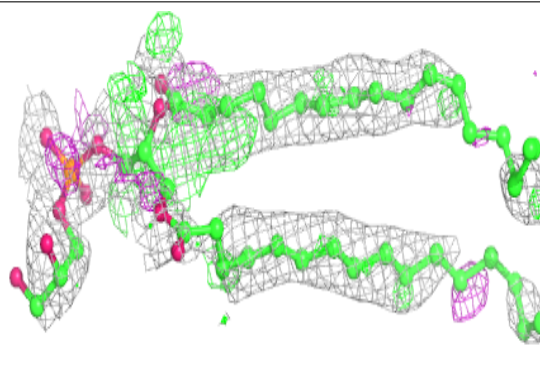


**Electron density around CHD P 311:**

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

**Electron density around PGV N 601:**

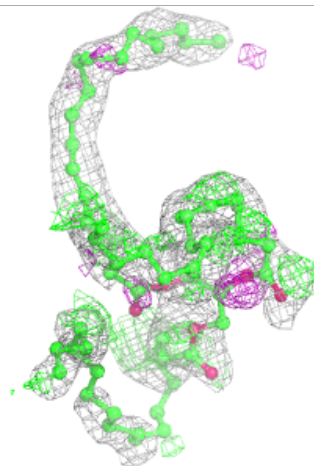
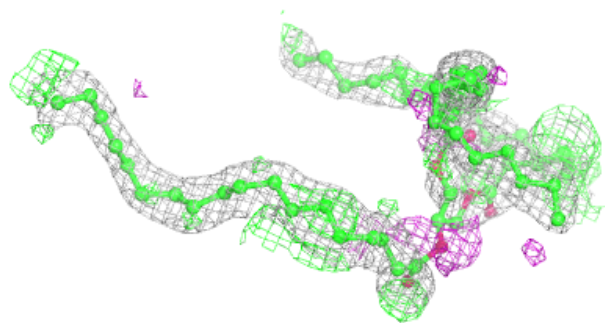
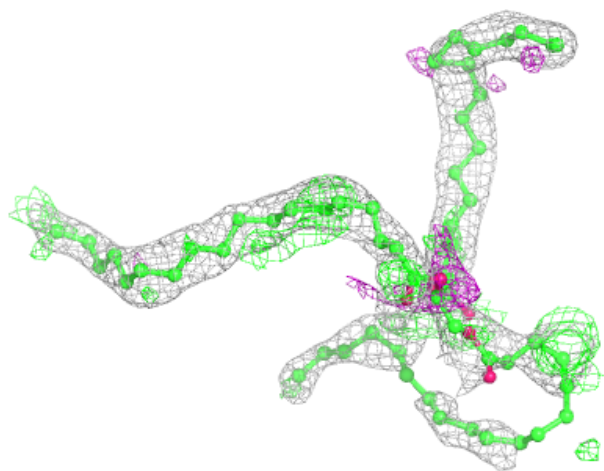
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





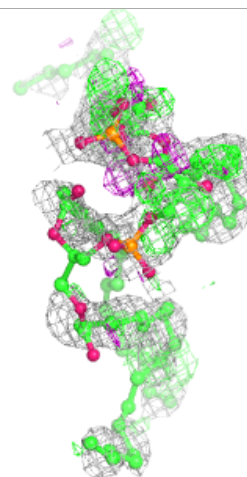
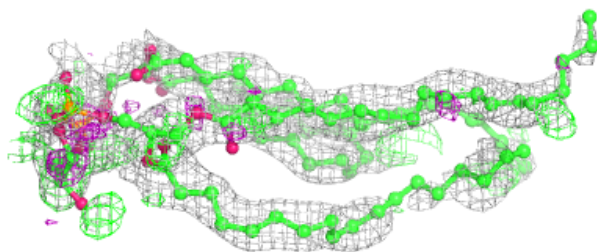
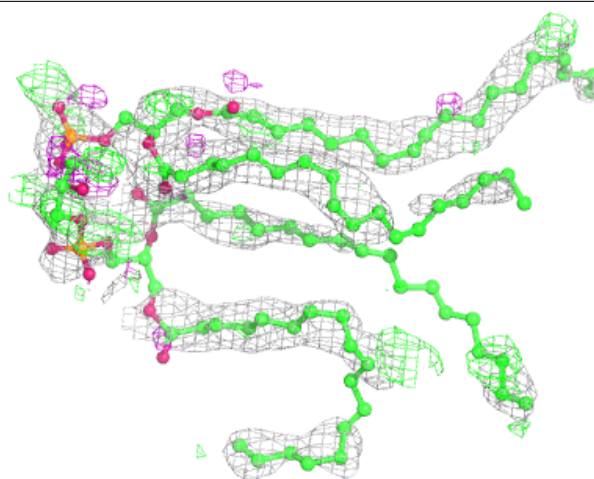
**Electron density around TGL Y 101:**

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



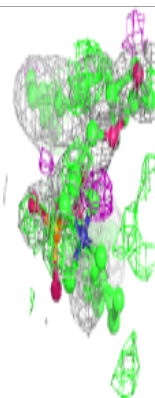
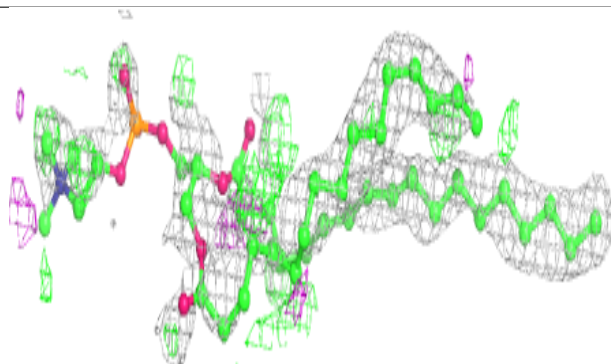
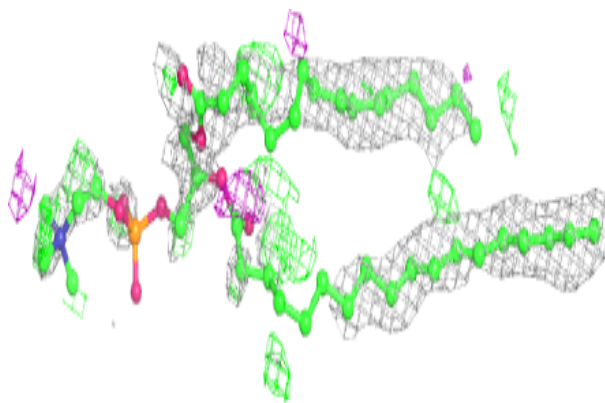
**Electron density around CDL C 308:**

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

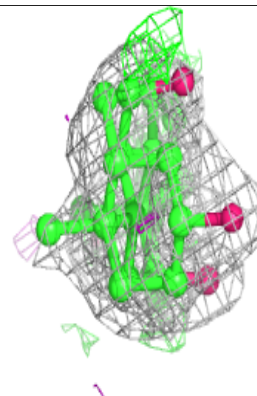
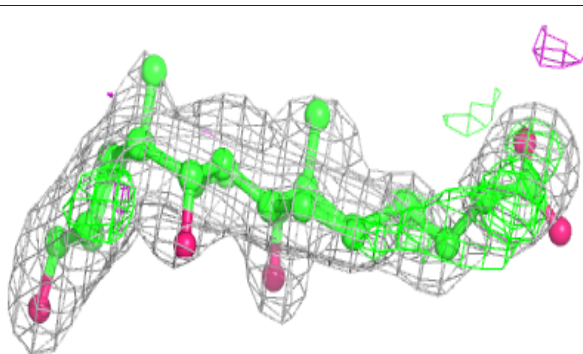
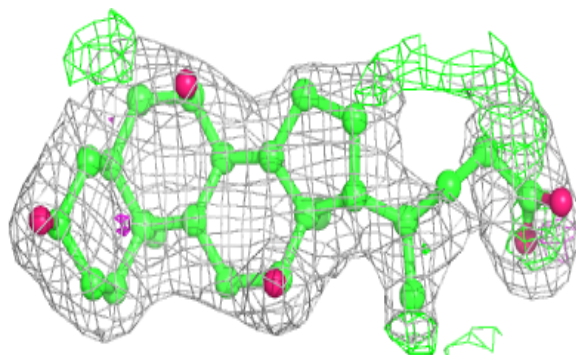


**Electron density around PSC B 302:**

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

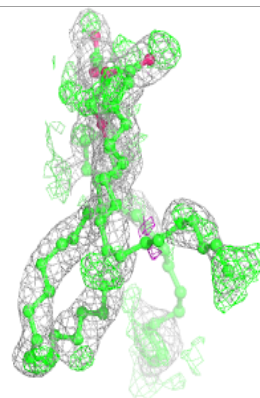
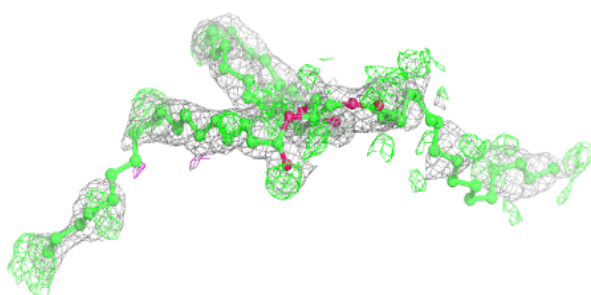
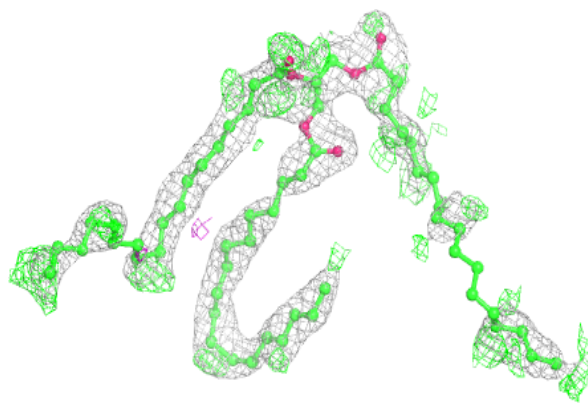
**Electron density around CHD C 309:**

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

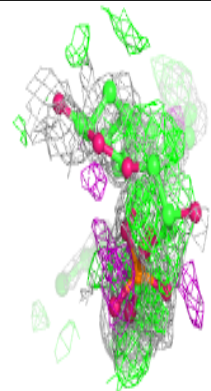
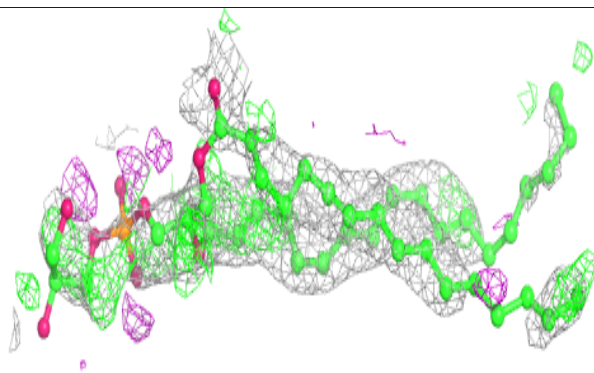
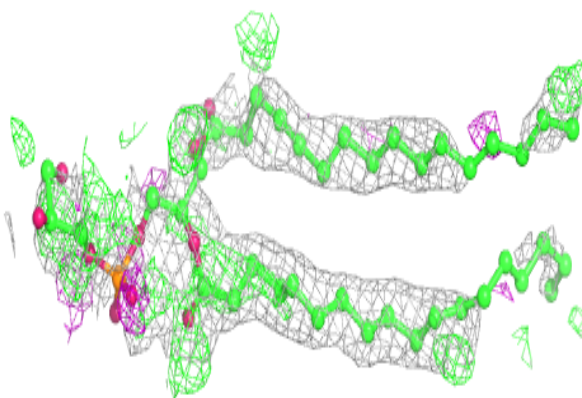


**Electron density around TGL D 201:**

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

**Electron density around PGV A 601:**

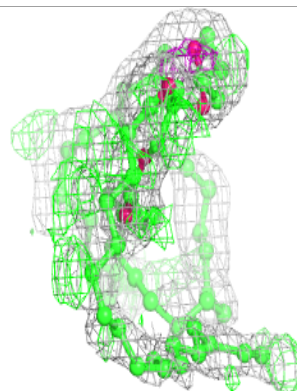
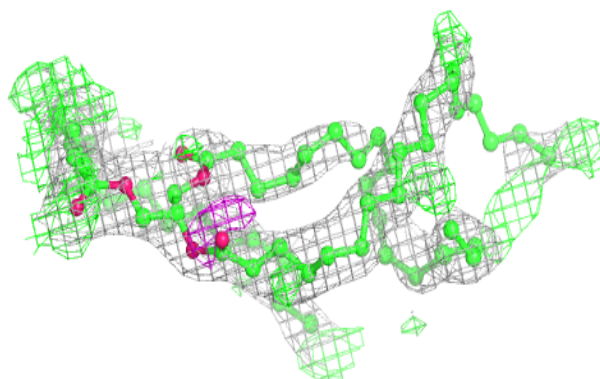
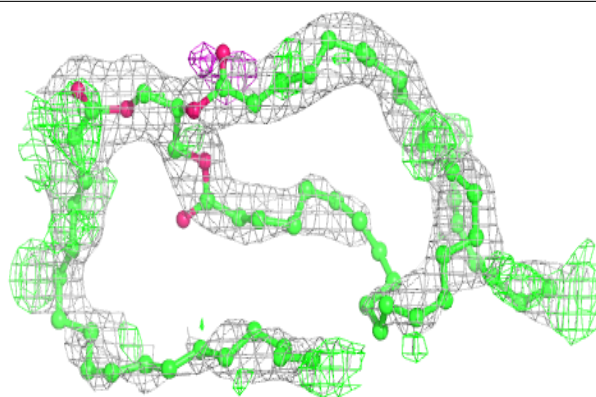
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



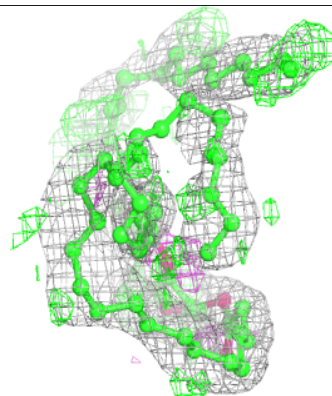
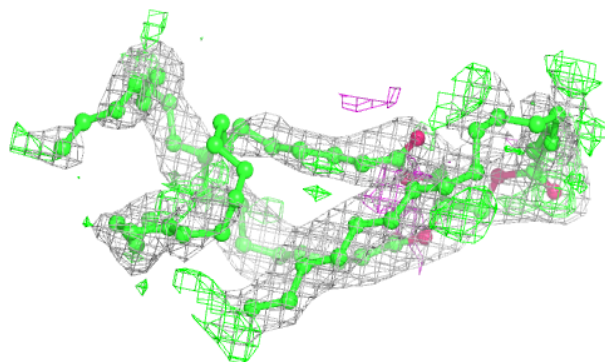
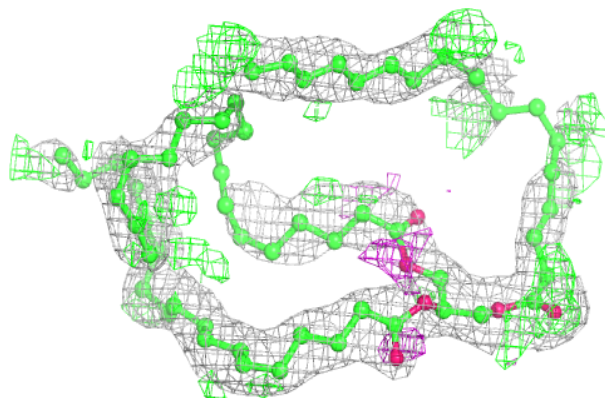


**Electron density around TGL N 608:**

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

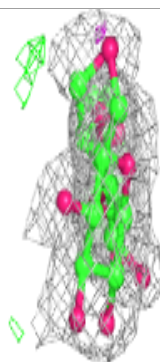
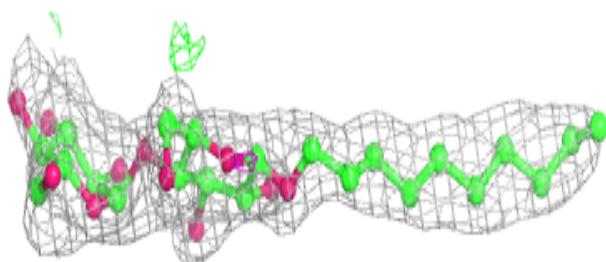
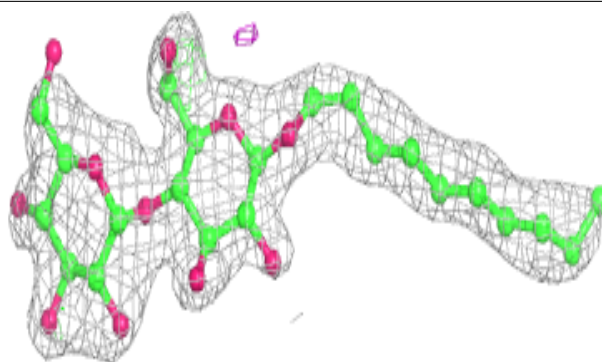
**Electron density around TGL B 301:**

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

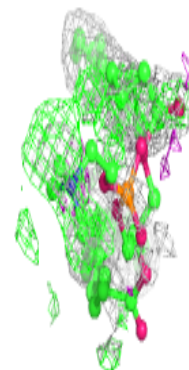
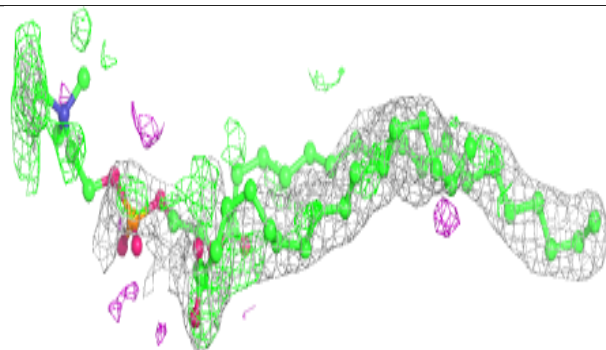
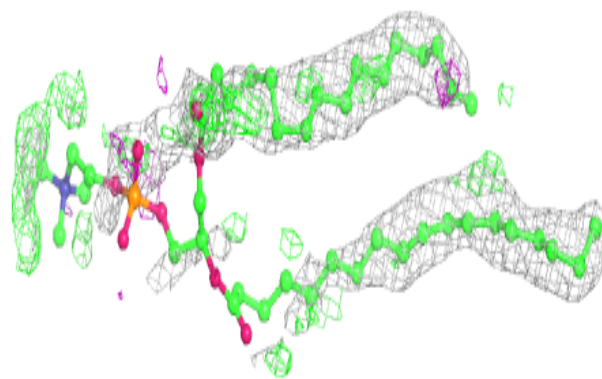


**Electron density around DMU P 323:**

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

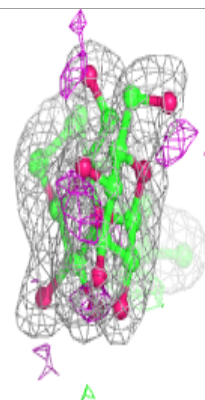
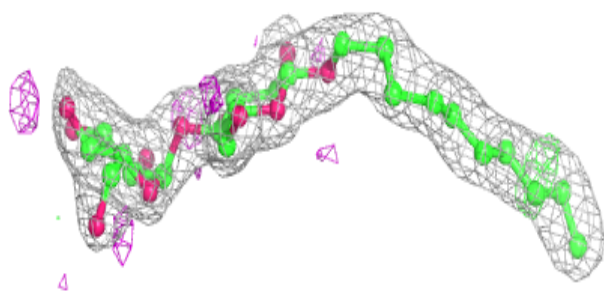
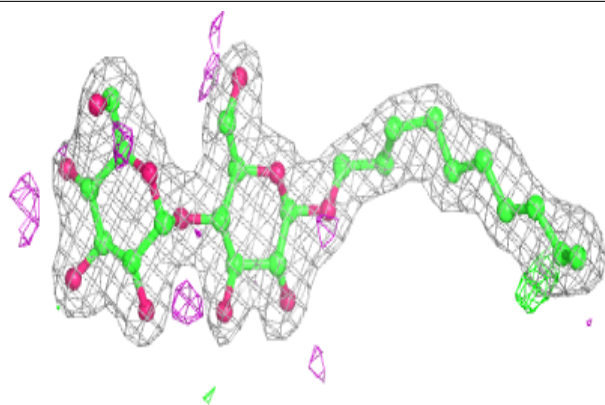
**Electron density around PSC O 301:**

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

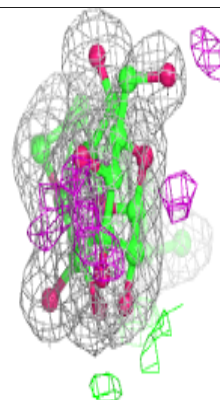
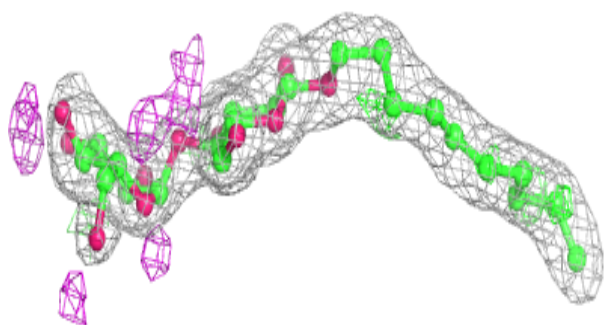
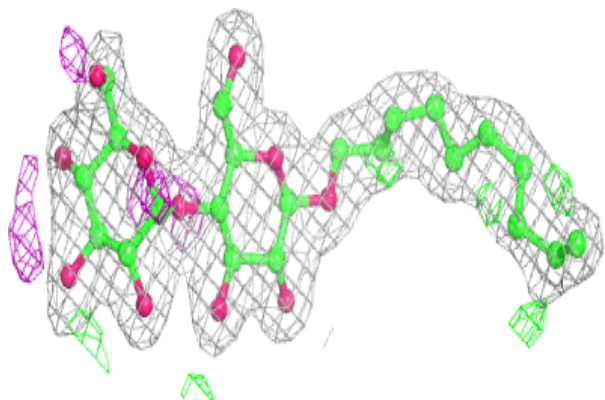


**Electron density around DMU Z 101:**

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

**Electron density around DMU M 101:**

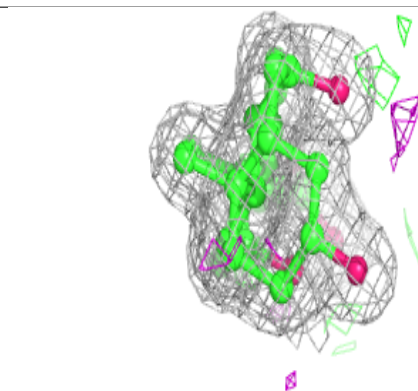
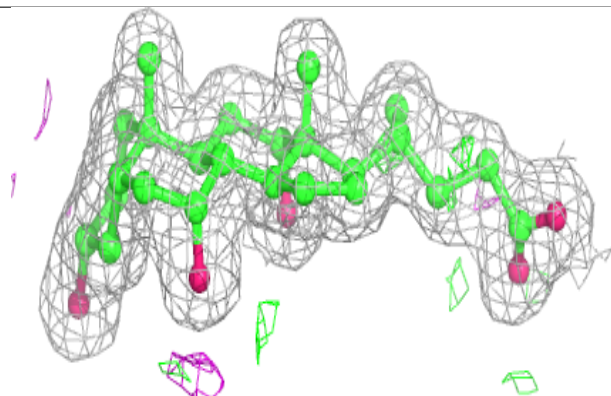
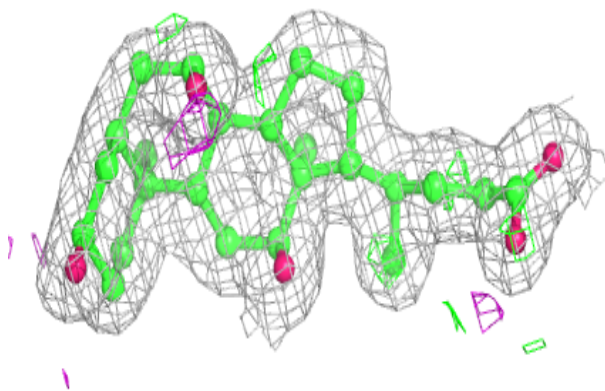
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



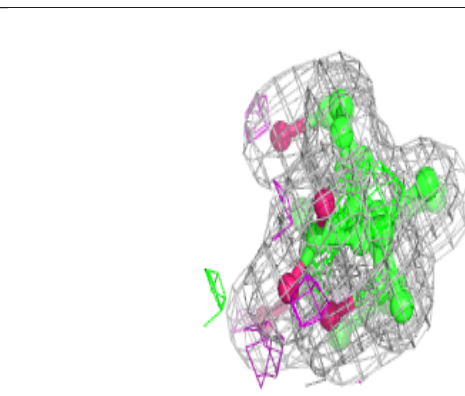
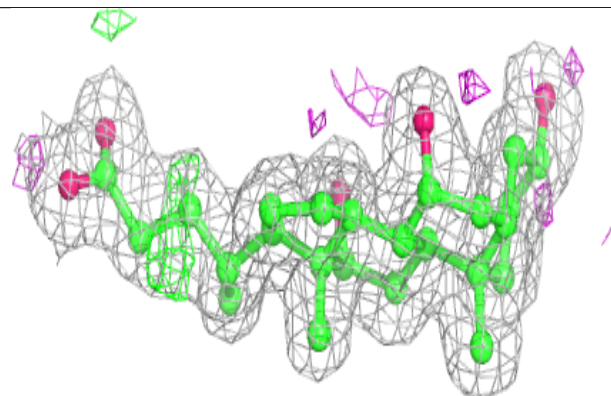
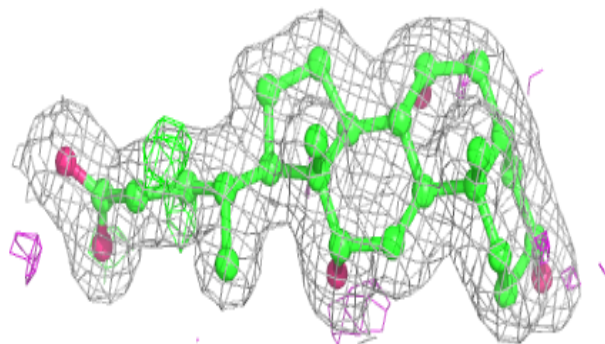


**Electron density around CHD P 301:**

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

**Electron density around CHD C 301:**

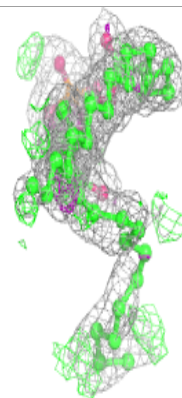
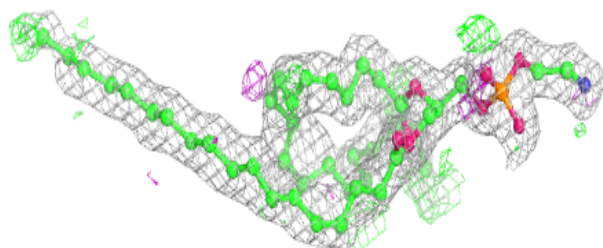
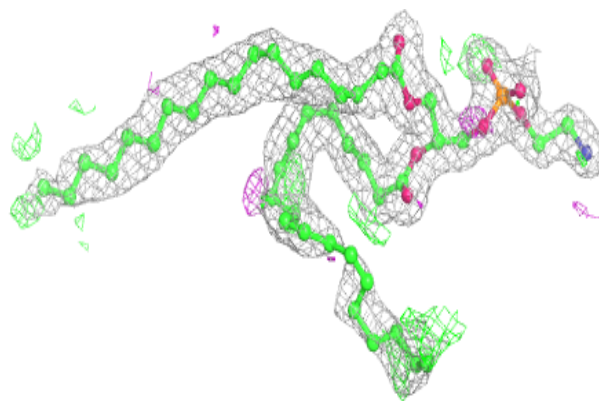
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



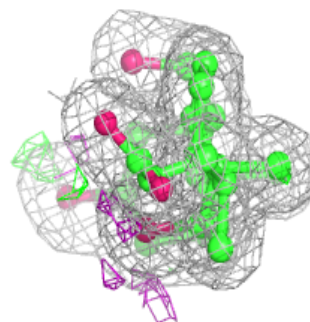
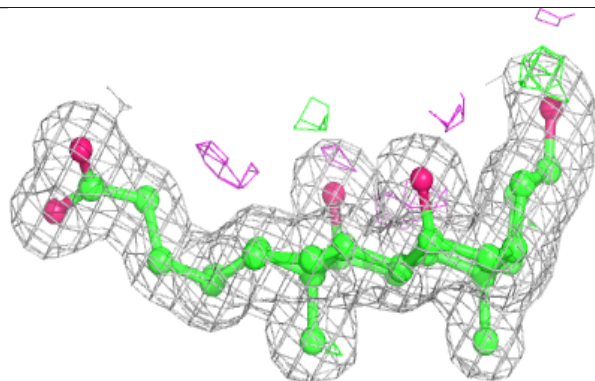
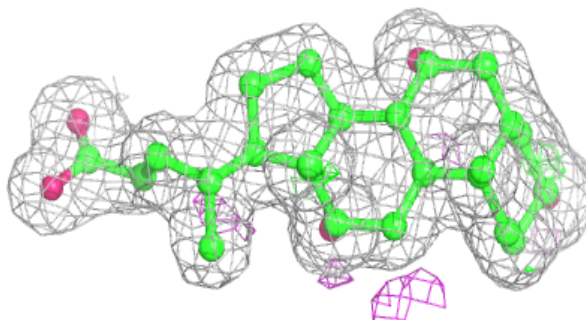


**Electron density around PEK P 304:**

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

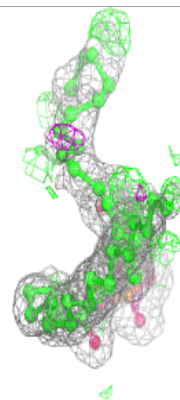
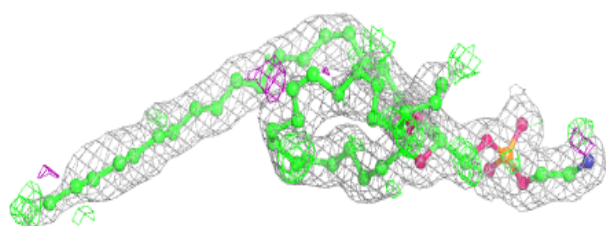
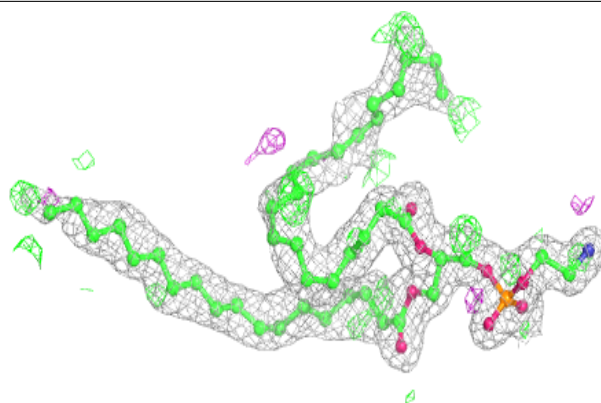
**Electron density around CHD G 102:**

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

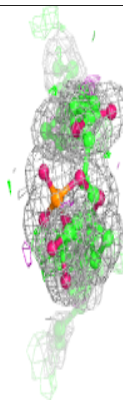
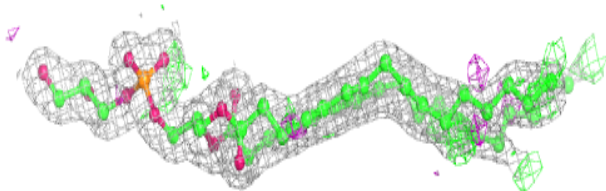
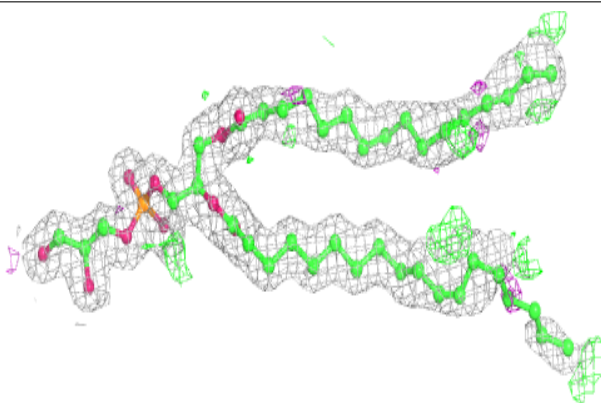


**Electron density around PEK C 304:**

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

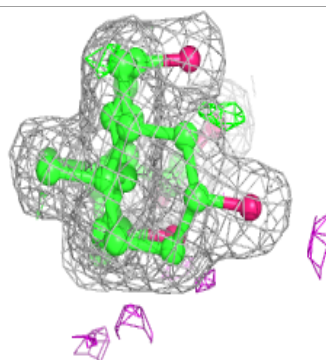
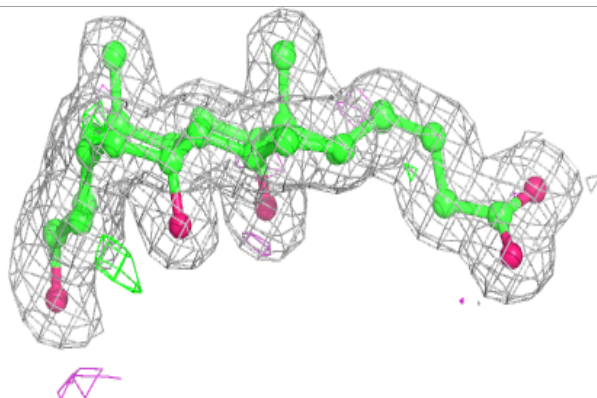
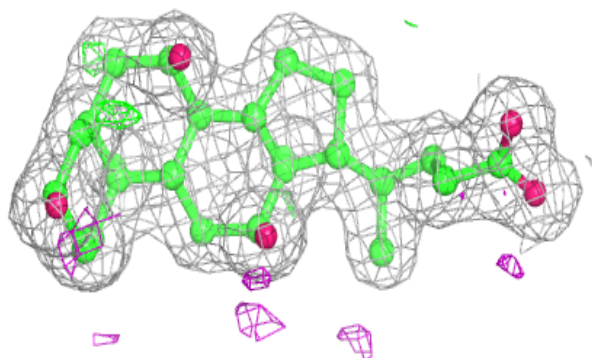
**Electron density around PGV C 306:**

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

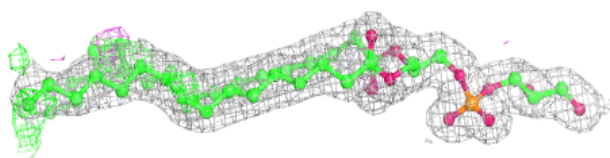
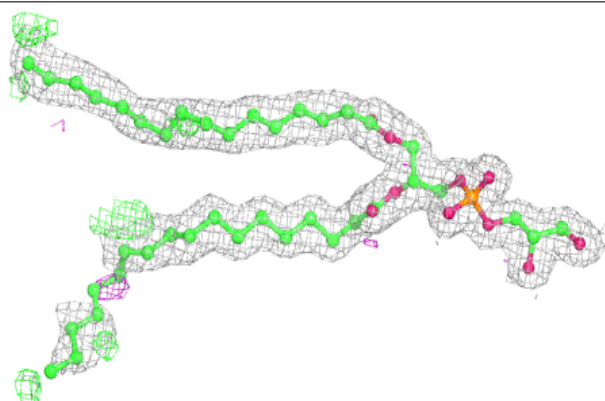


**Electron density around CHD B 303:**

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

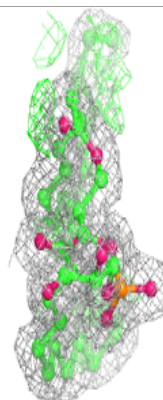
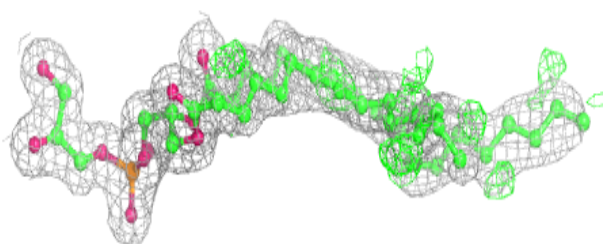
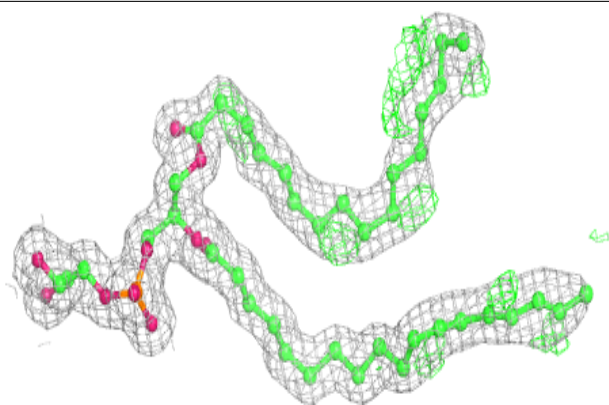
**Electron density around PGV P 306:**

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

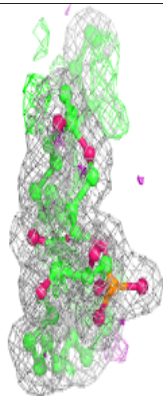
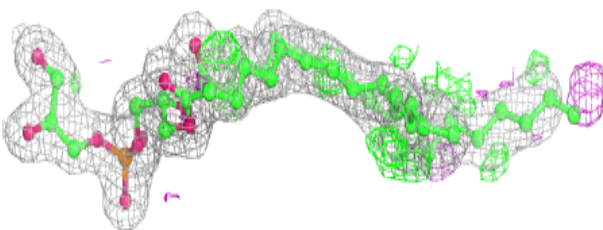
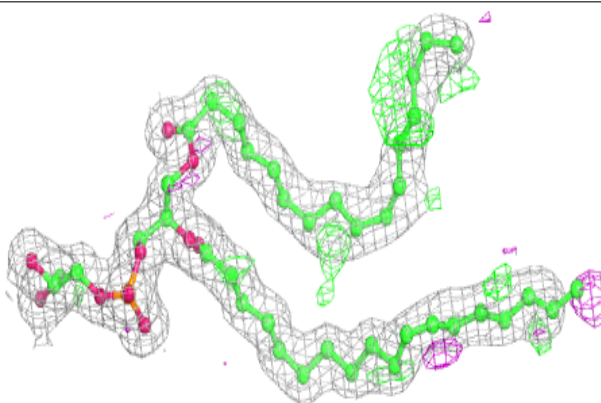


**Electron density around PGV A 608:**

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

**Electron density around PGV N 609:**

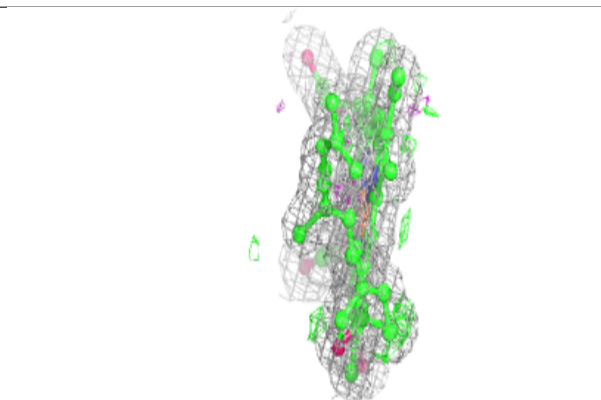
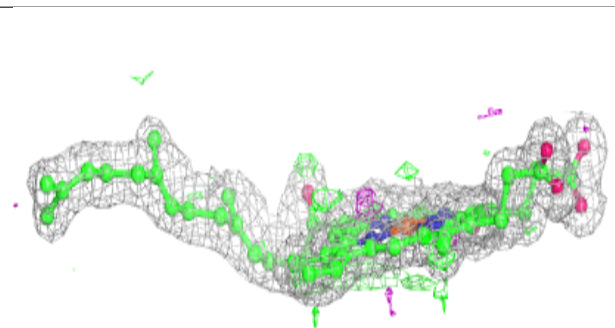
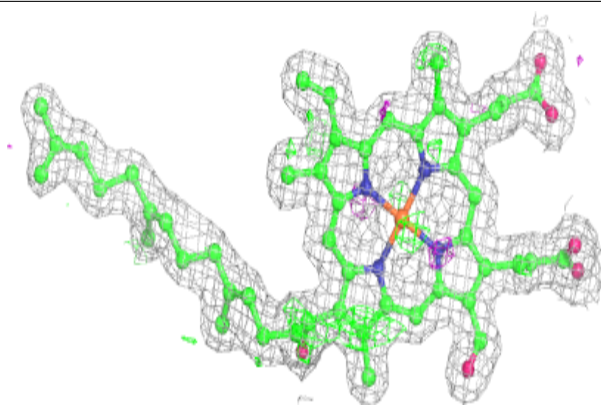
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



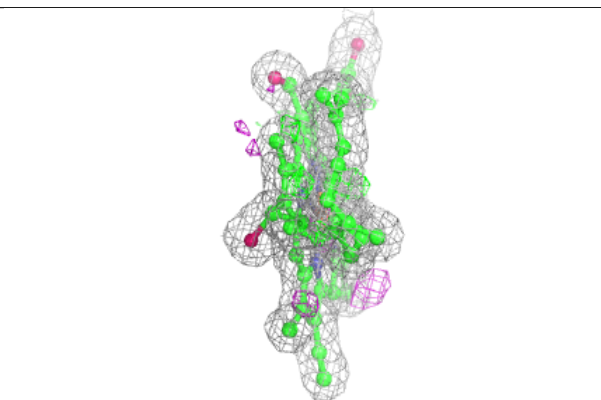
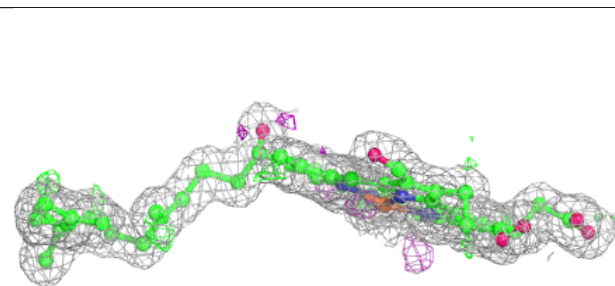
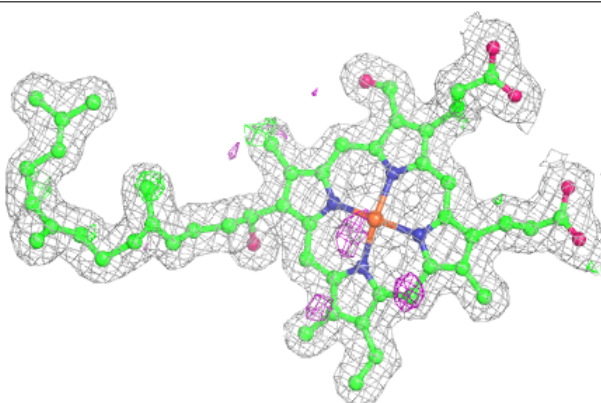


**Electron density around HEA A 602 (B):**

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

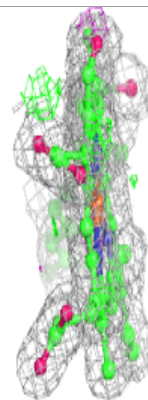
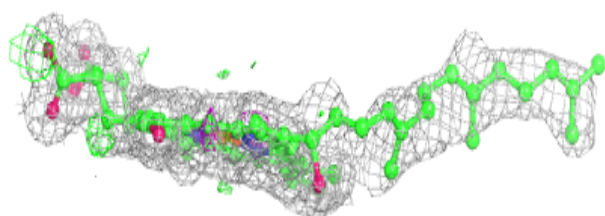
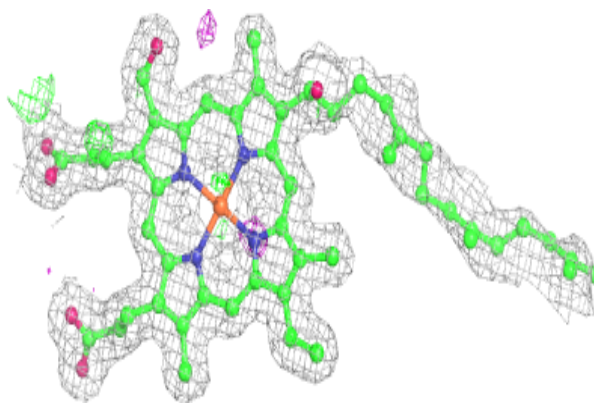
**Electron density around HEA A 603:**

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

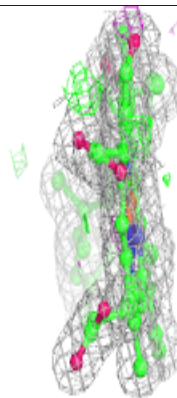
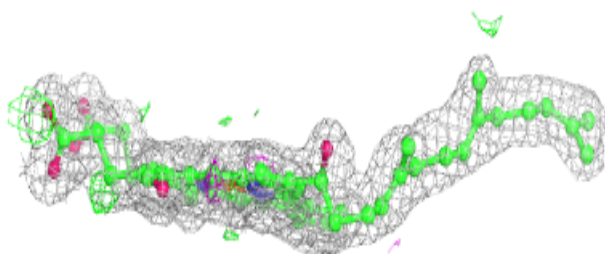
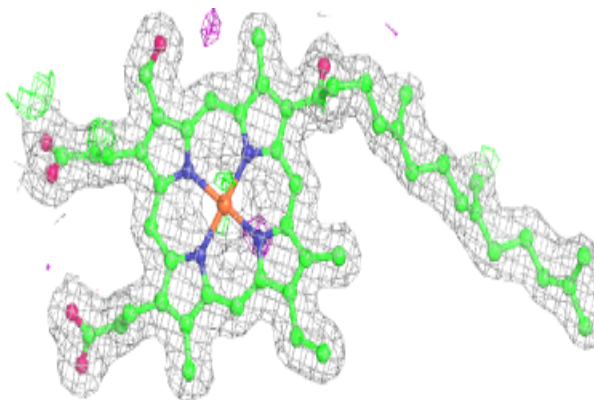


**Electron density around HEA N 602 (A):**

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

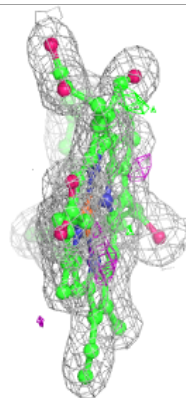
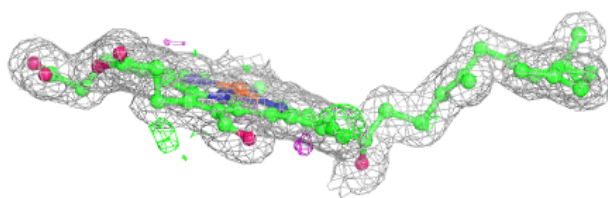
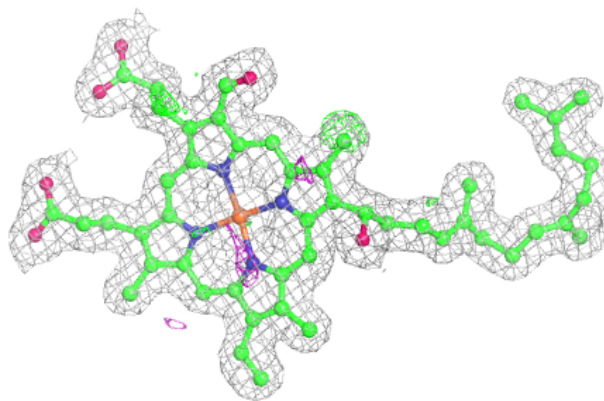
**Electron density around HEA N 602 (B):**

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

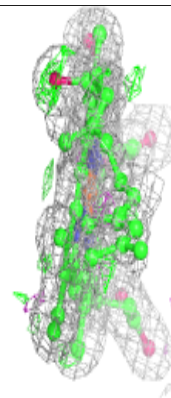
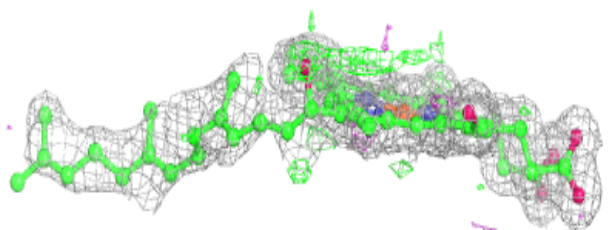
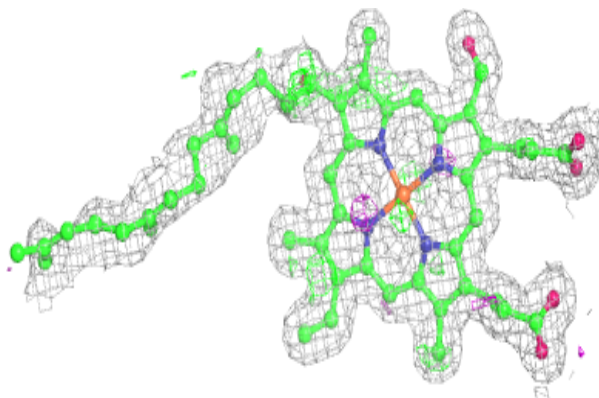


**Electron density around HEA N 603:**

$2mF_o-DF_c$  (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 (A):**

$2mF_o-DF_c$  (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.