



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 09:17 pm BST

PDB ID : 5Z84  
Title : The structure of azide-bound cytochrome c oxidase determined using the crystals exposed to 20 mM azide solution for 4 days  
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.  
Deposited on : 2018-01-31  
Resolution : 1.85 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 : 2.11  
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) : 2.11

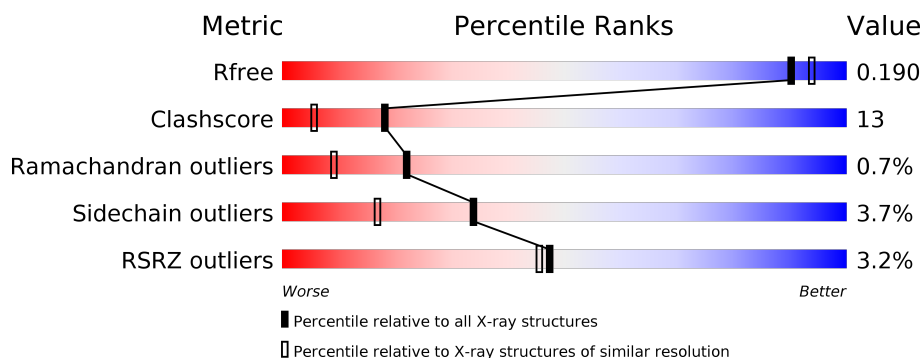
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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>82%</div> <div>16%</div> <div>.</div> </div>
1	N	514	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	227	<div> <div>73%</div> <div>25%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
3	C	261	<div> <div>84%</div> <div>14%</div> <div>..</div> </div>
3	P	261	<div> <div>%</div> <div>81%</div> <div>16%</div> <div>..</div> </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
14	HEA	A	601	X	-	-	-
14	HEA	A	602[A]	X	-	-	-
14	HEA	A	602[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
14	HEA	N	603[A]	X	-	-	-
14	HEA	N	603[B]	X	-	-	-
18	AZI	A	606	-	-	X	-
18	AZI	A	607	-	-	X	-
18	AZI	N	608	-	-	X	-
19	TGL	D	201	-	-	X	-
21	EDO	A	615	-	X	X	-
21	EDO	A	621	-	-	X	-
21	EDO	C	319	-	-	-	X
21	EDO	D	202	-	-	X	-
21	EDO	D	203	-	-	X	X
21	EDO	F	105	-	-	X	-
21	EDO	N	618	-	-	X	-
21	EDO	N	621	-	-	X	-
21	EDO	N	622	-	-	X	-
22	CHD	J	101	-	-	-	X
24	PSC	B	303	-	-	X	-
28	CDL	C	306	-	-	X	-
28	CDL	P	304	-	-	X	-
9	SAC	V	1	-	X	-	-



## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33735 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	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

- 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	10	0
			1904	1239	292	353	20			
2	O	227	Total	C	N	O	S	0	4	0
			1859	1206	287	346	20			

- 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
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	4	0
			1231	800	205	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	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	98	Total	C	N	O	S	0	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	1
			686	440	130	114	1	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			469	302	79	85	3			

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

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	1	0
			391	255	66	68	2			

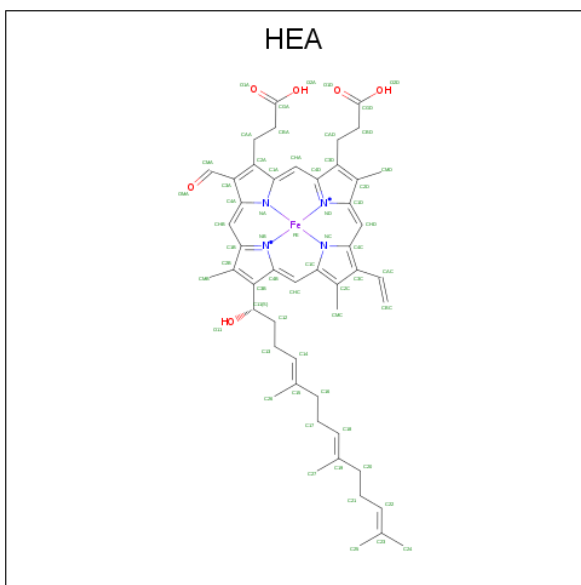
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			385	258	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			388	259	65	61	3			

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 120	C 98	Fe 2	N 8	O 12	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 120	C 98	Fe 2	N 8	O 12	0	1

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

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

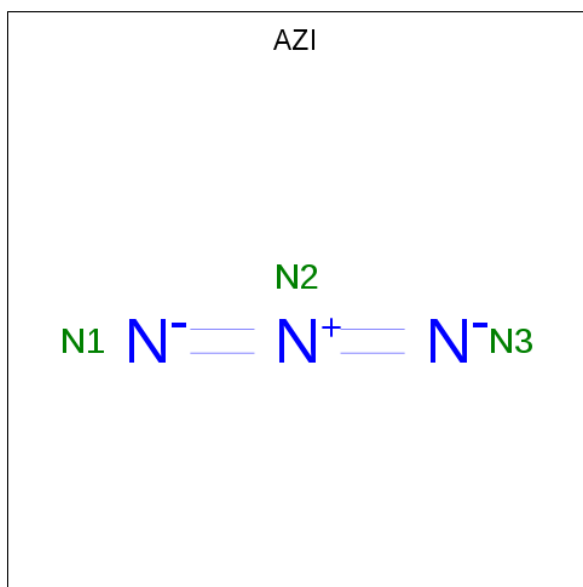
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

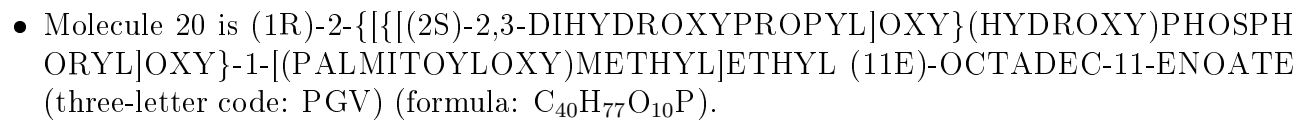
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

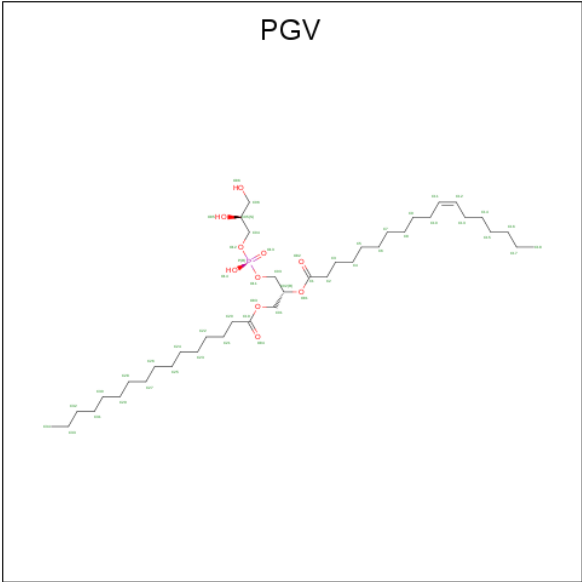
- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	0
18	A	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0

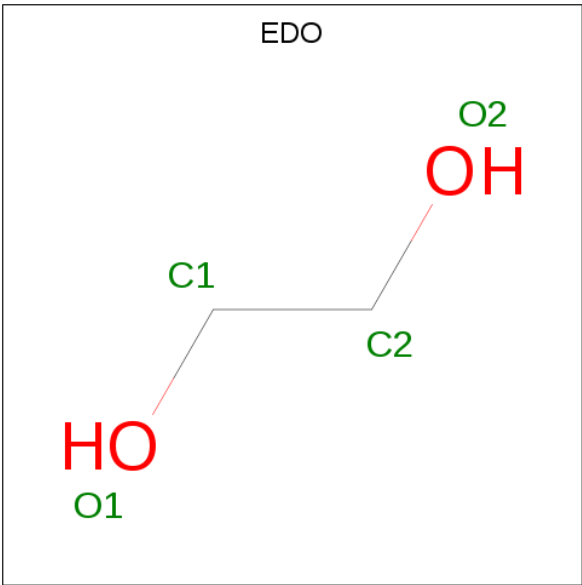
- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).





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

- Molecule 21 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
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		

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

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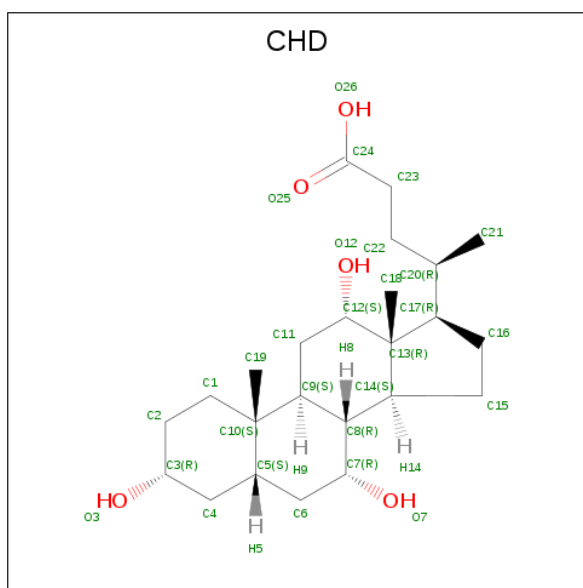
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	H	1	Total 4	C 2	O 2	0	0
21	H	1	Total 4	C 2	O 2	0	0
21	J	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0

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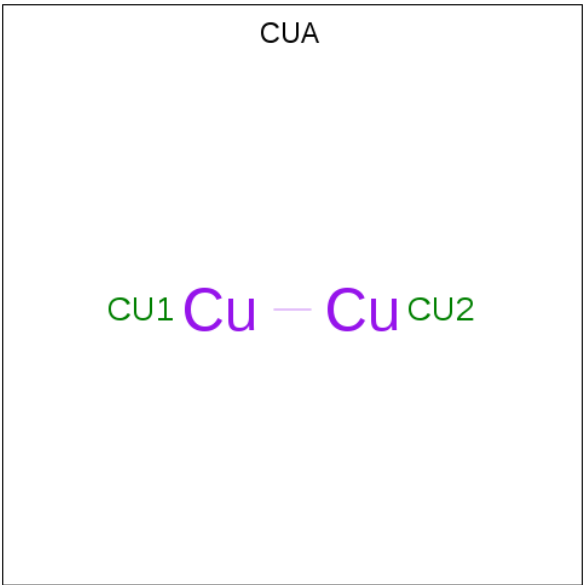
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	U	1	Total 4	C 2	O 2	0	0
21	V	1	Total 4	C 2	O 2	0	0

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



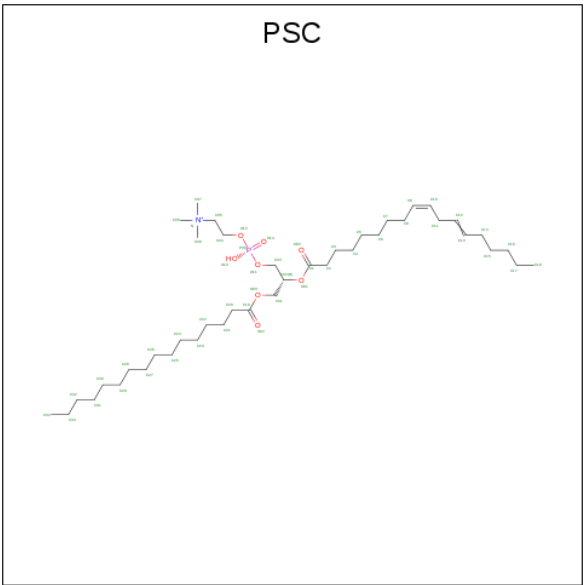
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula:  $Cu_2$ ).



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

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



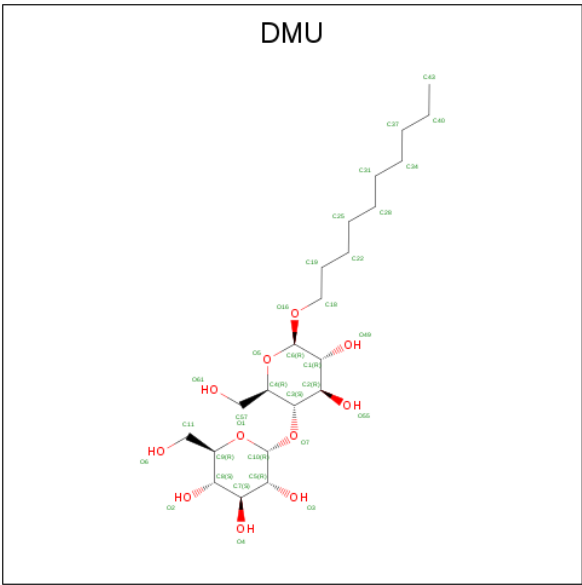
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).

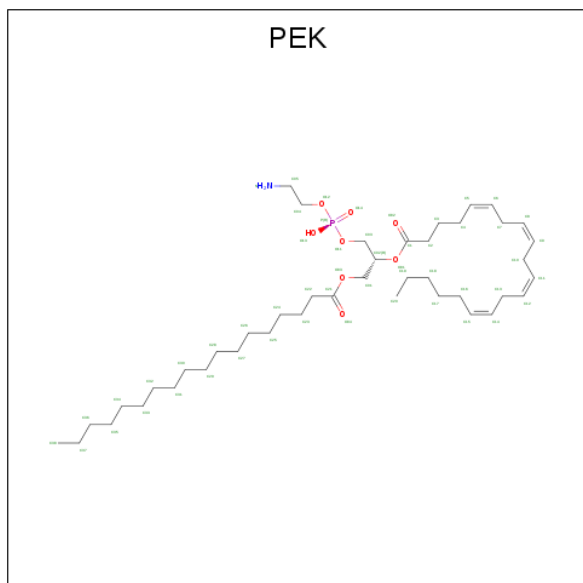


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	L	1	Total	C	O	0	0
			33	22	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 26 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

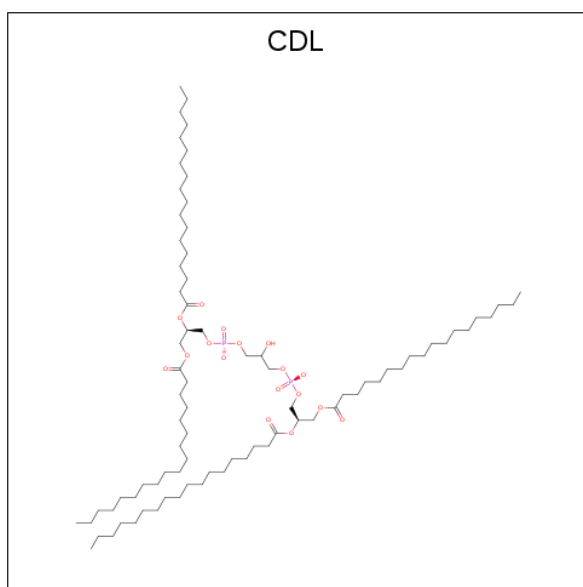
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	P	1	Total X 1 1	0	0
26	C	1	Total X 1 1	0	0

- Molecule 27 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
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	232	Total	O	0	1
			233	233		
30	B	139	Total	O	0	1
			140	140		
30	C	101	Total	O	0	0
			101	101		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	D	110	Total 110	O 110	0	0
30	E	85	Total 85	O 85	0	0
30	F	78	Total 78	O 78	0	0
30	G	51	Total 51	O 51	0	0
30	H	45	Total 45	O 45	0	0
30	I	25	Total 25	O 25	0	0
30	J	28	Total 28	O 28	0	0
30	K	21	Total 21	O 21	0	0
30	L	29	Total 29	O 29	0	0
30	M	27	Total 27	O 27	0	0
30	N	218	Total 219	O 219	0	1
30	O	114	Total 115	O 115	0	1
30	P	90	Total 90	O 90	0	0
30	Q	36	Total 36	O 36	0	0
30	R	39	Total 39	O 39	0	0
30	S	55	Total 55	O 55	0	0
30	T	39	Total 39	O 39	0	0
30	U	33	Total 33	O 33	0	0
30	V	14	Total 14	O 14	0	0
30	W	11	Total 11	O 11	0	0
30	X	11	Total 11	O 11	0	0

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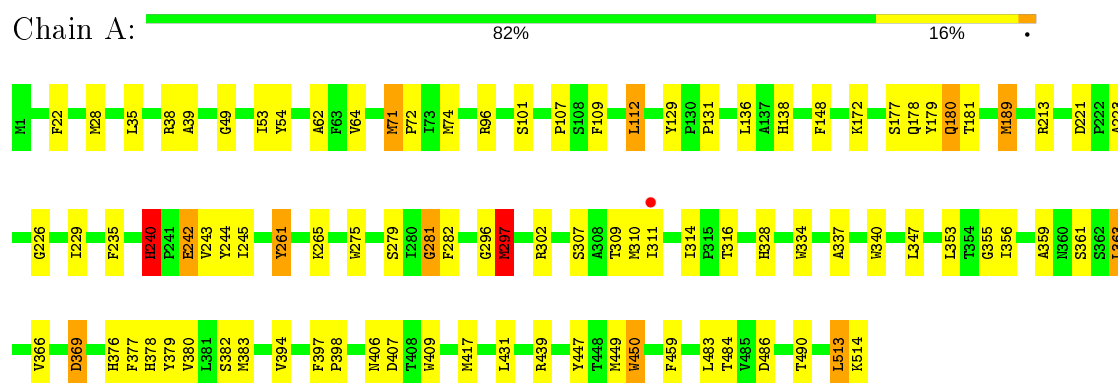
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	Y	14	Total 14	O 14	0	0
30	Z	16	Total 16	O 16	0	0

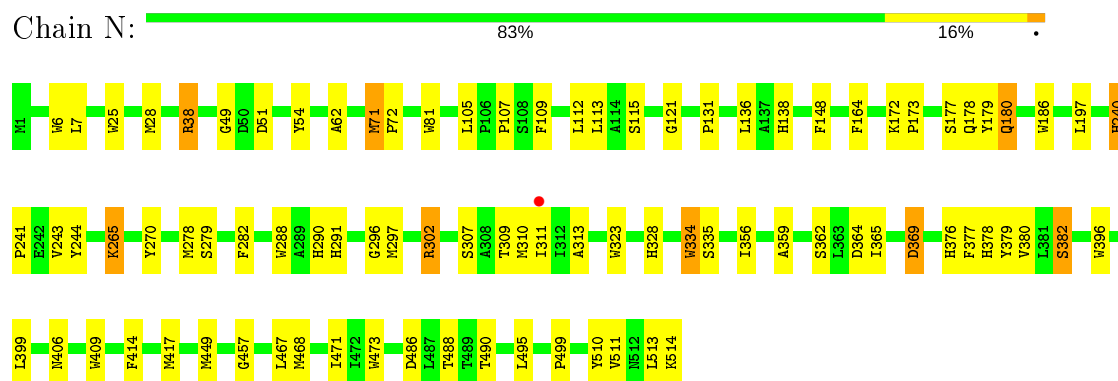
### 3 Residue-property plots

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

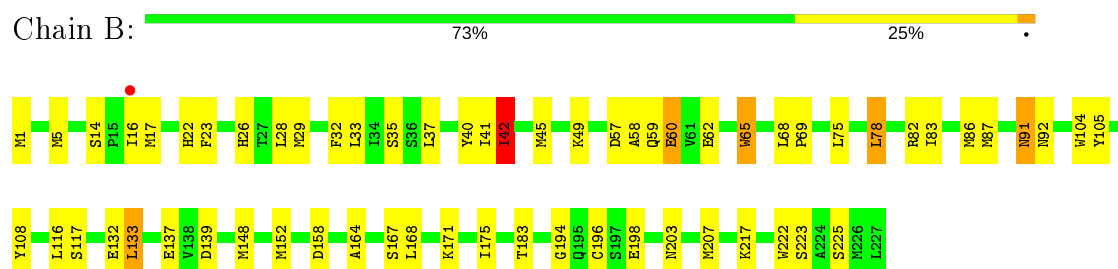
#### • Molecule 1: Cytochrome c oxidase subunit 1



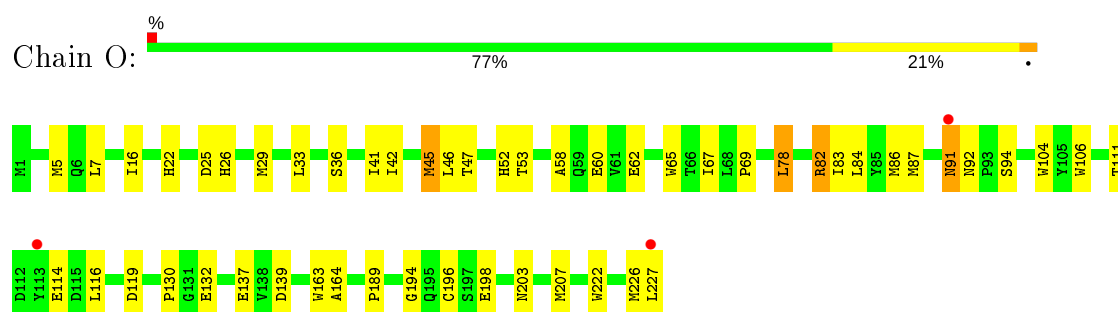
#### • Molecule 1: Cytochrome c oxidase subunit 1



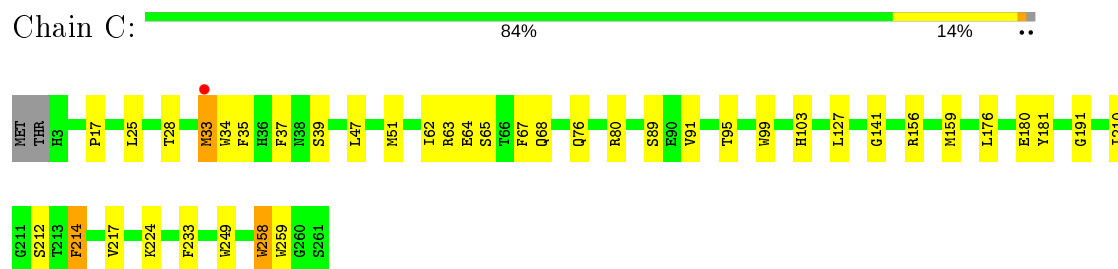
#### • Molecule 2: Cytochrome c oxidase subunit 2



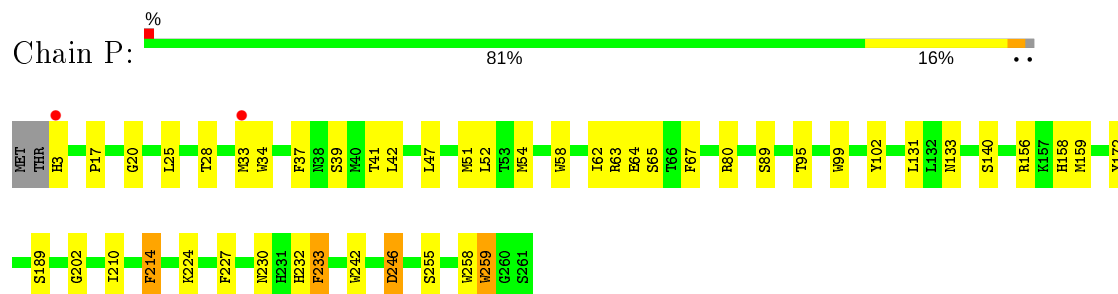
#### • Molecule 2: Cytochrome c oxidase subunit 2



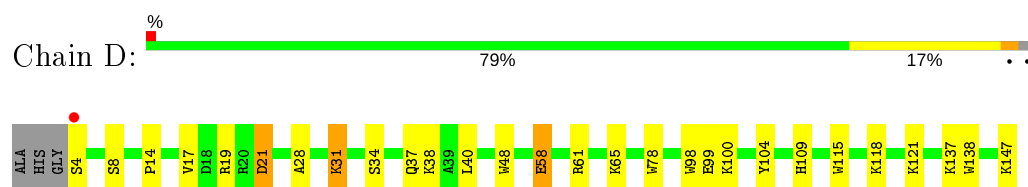
• Molecule 3: Cytochrome c oxidase subunit 3



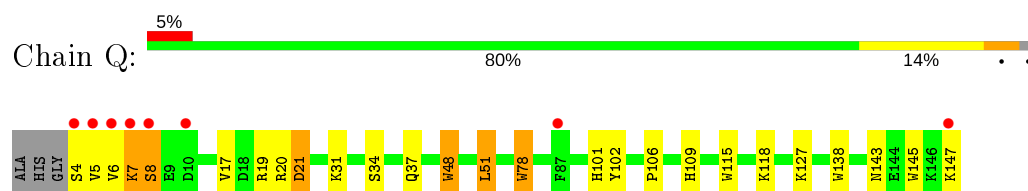
• Molecule 3: Cytochrome c oxidase subunit 3



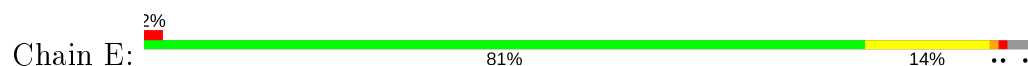
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

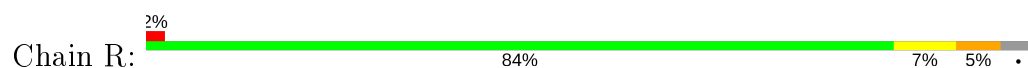


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

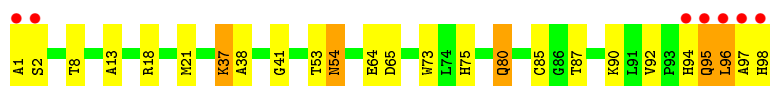
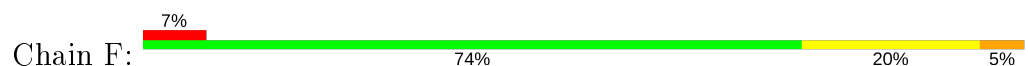




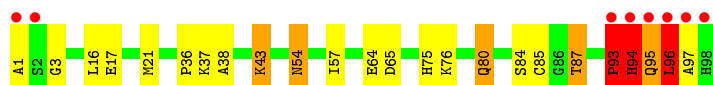
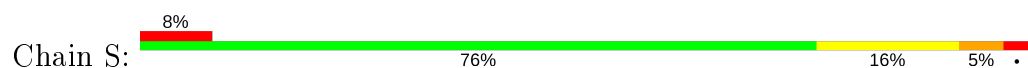
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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



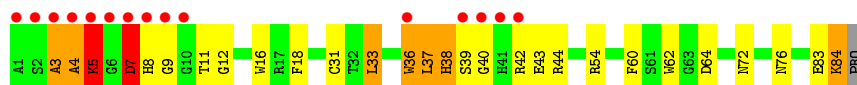
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



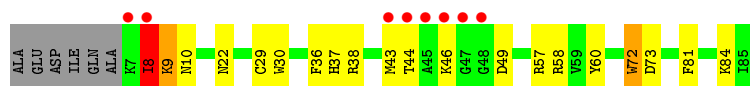
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



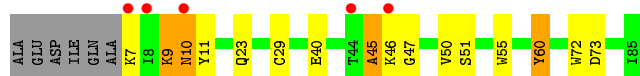
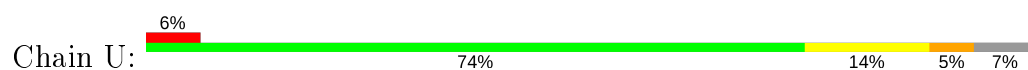
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1



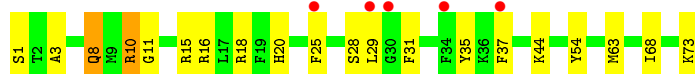
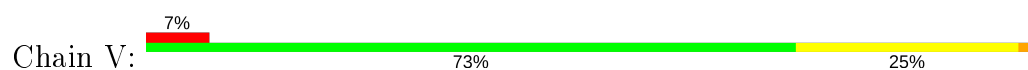
- Molecule 8: Cytochrome c oxidase subunit 6B1



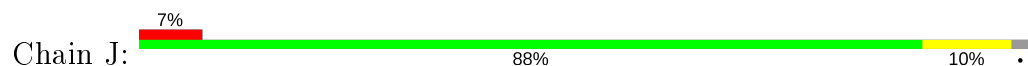
- Molecule 9: Cytochrome c oxidase subunit 6C



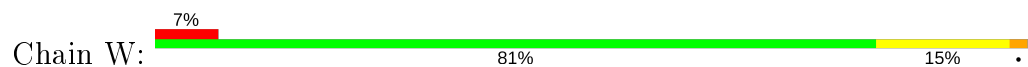
- Molecule 9: Cytochrome c oxidase subunit 6C



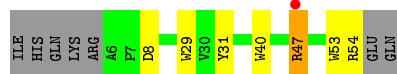
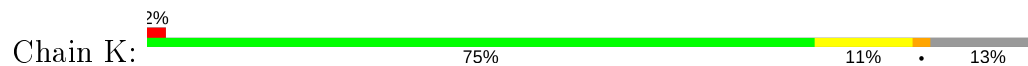
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



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

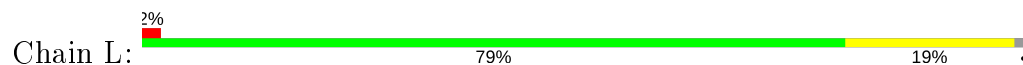


- Molecule 11: cytochrome c oxidase subunit 11, Cytochrome c oxidase subunit 7B, mitochondrial

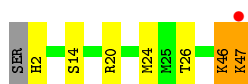
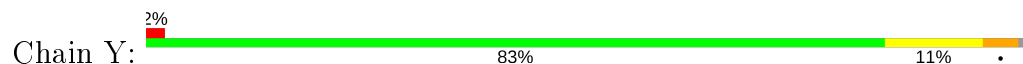




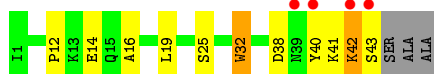
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



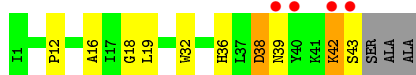
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.41Å 206.27Å 177.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 134.59 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-1.85) 99.4 (134.59-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.163 , 0.189 0.164 , 0.190	Depositor DCC
$R_{free}$ test set	28371 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	33735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: AZI, ZN, CHD, HEA, SAC, TPO, PSC, PEK, MG, TGL, EDO, PGV, CDL, UNX, CUA, NA, FME, CU, DMU

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	1.60	21/4322 (0.5%)	1.28	28/5897 (0.5%)
1	N	1.51	22/4308 (0.5%)	1.19	15/5878 (0.3%)
2	B	1.46	6/1945 (0.3%)	1.25	7/2649 (0.3%)
2	O	1.22	6/1896 (0.3%)	1.08	7/2581 (0.3%)
3	C	1.53	12/2272 (0.5%)	1.09	1/3102 (0.0%)
3	P	1.55	16/2272 (0.7%)	1.14	3/3102 (0.1%)
4	D	1.49	4/1265 (0.3%)	1.22	5/1704 (0.3%)
4	Q	1.11	4/1259 (0.3%)	1.10	5/1698 (0.3%)
5	E	1.45	3/871 (0.3%)	1.27	5/1182 (0.4%)
5	R	1.25	3/871 (0.3%)	1.11	3/1182 (0.3%)
6	F	1.31	3/795 (0.4%)	1.18	3/1079 (0.3%)
6	S	1.25	0/780	1.19	3/1058 (0.3%)
7	G	1.50	3/690 (0.4%)	1.21	7/937 (0.7%)
7	T	1.51	6/702 (0.9%)	1.18	4/953 (0.4%)
8	H	1.29	4/682 (0.6%)	1.02	2/921 (0.2%)
8	U	1.11	2/682 (0.3%)	0.94	1/921 (0.1%)
9	I	1.20	1/605 (0.2%)	1.10	2/802 (0.2%)
9	V	1.04	0/605	1.07	2/802 (0.2%)
10	J	1.21	0/471	1.03	0/636
10	W	1.22	1/480 (0.2%)	1.01	0/648
11	K	1.41	4/398 (1.0%)	1.15	2/546 (0.4%)
11	X	1.15	2/405 (0.5%)	0.85	0/556
12	L	1.36	2/401 (0.5%)	1.12	1/536 (0.2%)
12	Y	1.21	0/401	1.01	0/536
13	M	1.41	2/345 (0.6%)	1.06	0/470
13	Z	1.23	2/345 (0.6%)	0.90	0/470
All	All	1.42	129/30068 (0.4%)	1.16	106/40846 (0.3%)

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	2
1	N	0	1
6	S	0	1
7	T	0	1
12	Y	0	1
All	All	0	6

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	CD-OE2	-9.33	1.15	1.25
11	K	29	TRP	CD2-CE2	8.56	1.51	1.41
4	D	58	GLU	CD-OE1	8.54	1.35	1.25
2	O	65	TRP	CD2-CE2	8.50	1.51	1.41
3	C	89	SER	CB-OG	8.48	1.53	1.42

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-15.54	75.34	100.20
4	Q	20	ARG	NE-CZ-NH2	-15.10	112.75	120.30
1	A	71	MET	CG-SD-CE	-15.09	76.06	100.20
5	E	90	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	A	96	ARG	NE-CZ-NH2	-11.40	114.60	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
7	T	40	GLY	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	95	0
1	N	4179	0	4154	86	0
2	B	1904	0	1909	57	0
2	O	1859	0	1860	38	1
3	C	2185	0	2097	54	0
3	P	2185	0	2097	47	0
4	D	1231	0	1227	47	0
4	Q	1224	0	1211	24	1
5	E	852	0	845	8	0
5	R	852	0	845	7	0
6	F	778	0	754	36	0
6	S	763	0	742	32	0
7	G	675	0	643	37	0
7	T	686	0	651	30	0
8	H	662	0	623	21	0
8	U	662	0	623	8	0
9	I	601	0	613	26	0
9	V	601	0	613	16	0
10	J	460	0	459	5	0
10	W	469	0	464	13	0
11	K	384	0	366	4	0
11	X	391	0	374	5	0
12	L	385	0	389	5	0
12	Y	388	0	388	14	0
13	M	335	0	352	10	0
13	Z	335	0	352	7	0
14	A	180	0	162	27	0
14	N	180	0	162	27	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	6	0	0	7	0
18	N	6	0	0	6	0
19	A	63	0	110	3	0
19	D	63	0	110	21	0
19	L	63	0	110	4	0
19	N	63	0	110	8	0
19	Q	63	0	110	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	63	0	110	13	0
20	A	102	0	152	13	0
20	C	102	0	152	11	0
20	G	51	0	76	4	0
20	N	51	0	76	2	0
20	P	51	0	76	3	0
20	Z	51	0	76	12	0
21	A	52	0	78	20	0
21	B	8	0	12	0	0
21	C	36	0	54	4	0
21	D	24	0	36	15	0
21	E	20	0	30	0	0
21	F	16	0	24	5	0
21	G	8	0	12	1	0
21	H	8	0	12	4	0
21	J	4	0	6	0	0
21	L	4	0	6	0	0
21	N	48	0	72	23	0
21	O	12	0	18	2	0
21	P	16	0	24	1	0
21	Q	8	0	12	0	0
21	R	24	0	36	2	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
21	U	4	0	6	0	0
21	V	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	8	0
22	G	29	0	39	1	0
22	J	29	0	38	2	0
22	P	58	0	78	7	0
22	W	29	0	39	9	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	23	0
24	O	52	0	80	12	0
25	C	99	0	126	18	0
25	L	33	0	42	5	0
25	M	33	0	42	1	0
25	P	99	0	126	18	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	1	0	0	0	0
27	C	106	0	154	19	0
27	G	53	0	77	10	0
27	P	53	0	77	10	0
27	T	106	0	154	8	0
28	C	100	0	156	30	0
28	N	100	0	156	15	0
28	P	100	0	156	25	0
28	T	100	0	156	20	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	233	0	0	15	0
30	B	140	0	0	13	1
30	C	101	0	0	4	0
30	D	110	0	0	19	1
30	E	85	0	0	3	0
30	F	78	0	0	7	0
30	G	51	0	0	4	0
30	H	45	0	0	3	0
30	I	25	0	0	5	0
30	J	28	0	0	2	0
30	K	21	0	0	4	0
30	L	29	0	0	3	0
30	M	27	0	0	3	0
30	N	219	0	0	17	0
30	O	115	0	0	3	0
30	P	90	0	0	2	0
30	Q	36	0	0	3	0
30	R	39	0	0	0	0
30	S	55	0	0	6	0
30	T	39	0	0	3	0
30	U	33	0	0	0	0
30	V	14	0	0	3	0
30	W	11	0	0	2	0
30	X	11	0	0	0	0
30	Y	14	0	0	1	0
30	Z	16	0	0	1	0
All	All	33735	0	32802	872	2

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 13.

The worst 5 of 872 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)
21:A:615:EDO:C2	21:A:615:EDO:C1	1.78	1.57
20:Z:101:PGV:C2	20:Z:101:PGV:H011	1.50	1.39
21:A:615:EDO:C1	21:A:615:EDO:O2	1.71	1.36
21:C:316:EDO:H11	30:C:486:HOH:O	1.23	1.29
30:A:705:HOH:O	19:D:201:TGL:HG11	1.32	1.26

All (2) 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)
2:O:226:MET:O	4:Q:5:VAL:O[2_684]	2.13	0.07
30:B:466:HOH:O	30:D:302:HOH:O[2_584]	2.18	0.02

## 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	534/514 (104%)	519 (97%)	15 (3%)	0	100	100
1	N	532/514 (104%)	516 (97%)	16 (3%)	0	100	100
2	B	235/227 (104%)	224 (95%)	11 (5%)	0	100	100
2	O	229/227 (101%)	222 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	141 (97%)	5 (3%)	0	100	100
4	Q	145/147 (99%)	139 (96%)	4 (3%)	2 (1%)	11	3
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15	5
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	7	1
6	S	98/98 (100%)	89 (91%)	7 (7%)	2 (2%)	7	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	81/85 (95%)	70 (86%)	5 (6%)	6 (7%)	1	0
7	T	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	12	3
8	U	77/85 (91%)	67 (87%)	7 (9%)	3 (4%)	3	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	6	1
All	All	3596/3614 (100%)	3454 (96%)	119 (3%)	23 (1%)	22	12

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
7	G	4	ALA
7	G	5	LYS
7	G	8	HIS
13	M	42	LYS

### 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	447/426 (105%)	441 (99%)	6 (1%)	69	58
1	N	445/426 (104%)	437 (98%)	8 (2%)	59	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	220/210 (105%)	211 (96%)	9 (4%)	30	13
2	O	214/210 (102%)	209 (98%)	5 (2%)	50	34
3	C	233/226 (103%)	227 (97%)	6 (3%)	46	30
3	P	233/226 (103%)	228 (98%)	5 (2%)	53	38
4	D	132/129 (102%)	128 (97%)	4 (3%)	41	24
4	Q	131/129 (102%)	122 (93%)	9 (7%)	15	4
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	21
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	12
6	F	85/81 (105%)	80 (94%)	5 (6%)	19	6
6	S	83/81 (102%)	71 (86%)	12 (14%)	3	0
7	G	67/68 (98%)	62 (92%)	5 (8%)	13	3
7	T	68/68 (100%)	59 (87%)	9 (13%)	4	0
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	2
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	2
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	8
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	3
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	40
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	14
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	39 (98%)	1 (2%)	47	31
12	L	40/40 (100%)	39 (98%)	1 (2%)	47	31
12	Y	40/40 (100%)	38 (95%)	2 (5%)	24	9
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	2
All	All	3130/3082 (102%)	3011 (96%)	119 (4%)	34	16

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	265	LYS
3	P	230	ASN
9	V	37	PHE
1	N	382[A]	SER
2	O	91	ASN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	22	ASN
2	O	52	HIS
8	U	22	ASN
10	J	29	ASN
1	N	180	GLN

### 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
1	FME	A	1	1	8,9,10	0.87	0	7,9,11	2.27	3 (42%)
1	FME	N	1	1	8,9,10	1.52	1 (12%)	7,9,11	1.61	2 (28%)
7	TPO	T	11	7	8,10,11	1.82	2 (25%)	10,14,16	1.67	2 (20%)
9	SAC	V	1	9	7,8,9	1.64	1 (14%)	8,9,11	1.54	3 (37%)
2	FME	B	1	2	8,9,10	1.97	2 (25%)	7,9,11	2.29	2 (28%)
2	FME	O	1	2	8,9,10	1.21	1 (12%)	7,9,11	1.88	2 (28%)
7	TPO	G	11	7	8,10,11	2.02	2 (25%)	10,14,16	1.39	2 (20%)
9	SAC	I	1	9	7,8,9	1.12	1 (14%)	8,9,11	1.97	2 (25%)

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.17	1.52	1.46
2	B	1	FME	CA-N	3.89	1.51	1.46
1	N	1	FME	CA-N	3.78	1.51	1.46
7	G	11	TPO	P-OG1	3.43	1.65	1.59
7	T	11	TPO	P-O1P	3.08	1.60	1.50

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	C-CA-N	-4.23	102.11	109.73
9	I	1	SAC	OG-CB-CA	-4.10	100.50	110.97
7	T	11	TPO	CG2-CB-CA	3.72	120.51	113.16
2	B	1	FME	CG-CB-CA	-3.71	102.63	112.95
2	O	1	FME	CG-CB-CA	-3.32	103.72	112.95

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 142 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 132 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
14	HEA	N	603[B]	1,18	44,67,67	1.03	1 (2%)	37,103,103	1.92	10 (27%)
21	EDO	D	205	-	3,3,3	0.50	0	2,2,2	0.71	0
21	EDO	T	104	-	3,3,3	1.06	0	2,2,2	0.46	0
21	EDO	N	618	-	3,3,3	0.45	0	2,2,2	1.46	0
19	TGL	Q	201	-	62,62,62	1.49	4 (6%)	65,65,65	1.64	8 (12%)
22	CHD	C	301	-	29,32,32	1.64	5 (17%)	48,51,51	2.65	21 (43%)
27	PEK	C	304	-	52,52,52	1.06	5 (9%)	55,57,57	1.28	8 (14%)
27	PEK	C	308	-	52,52,52	1.27	3 (5%)	55,57,57	1.59	9 (16%)
21	EDO	E	204	-	3,3,3	0.79	0	2,2,2	0.39	0
21	EDO	O	305	-	3,3,3	0.39	0	2,2,2	0.52	0
21	EDO	D	202	-	3,3,3	0.55	0	2,2,2	0.74	0
21	EDO	U	101	-	3,3,3	0.36	0	2,2,2	0.82	0
21	EDO	D	206	-	3,3,3	0.26	0	2,2,2	1.32	0
21	EDO	A	623	-	3,3,3	0.53	0	2,2,2	0.80	0
21	EDO	A	616	-	3,3,3	1.02	0	2,2,2	0.33	0
14	HEA	A	601	1	44,67,67	1.62	7 (15%)	37,103,103	2.63	20 (54%)
21	EDO	A	614	-	3,3,3	0.39	0	2,2,2	1.18	0
21	EDO	P	312	-	3,3,3	0.59	0	2,2,2	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	1.14	0
21	EDO	C	320	-	3,3,3	0.79	0	2,2,2	1.30	0
21	EDO	N	620	-	3,3,3	0.43	0	2,2,2	0.73	0
22	CHD	W	101	-	29,32,32	0.97	0	48,51,51	3.35	20 (41%)
21	EDO	C	319	-	3,3,3	0.68	0	2,2,2	0.26	0
21	EDO	A	621	-	3,3,3	0.80	0	2,2,2	0.23	0
21	EDO	C	315	-	3,3,3	0.68	0	2,2,2	0.51	0
25	DMU	P	309	-	34,34,34	0.89	1 (2%)	45,45,45	1.26	3 (6%)
21	EDO	B	304	-	3,3,3	0.50	0	2,2,2	0.23	0
27	PEK	G	102	-	52,52,52	1.12	2 (3%)	55,57,57	1.49	5 (9%)
21	EDO	C	312	-	3,3,3	1.23	0	2,2,2	0.14	0
27	PEK	P	307	-	52,52,52	1.21	2 (3%)	55,57,57	1.32	6 (10%)
21	EDO	N	615	-	3,3,3	1.57	1 (33%)	2,2,2	0.65	0
20	PGV	A	609	-	50,50,50	1.11	5 (10%)	53,56,56	1.19	5 (9%)
21	EDO	Q	203	-	3,3,3	0.58	0	2,2,2	0.16	0
20	PGV	Z	101	-	50,50,50	1.15	2 (4%)	53,56,56	1.36	7 (13%)
21	EDO	D	204	-	3,3,3	0.61	0	2,2,2	0.98	0
21	EDO	R	202	-	3,3,3	0.18	0	2,2,2	1.29	0
22	CHD	C	307	-	29,32,32	1.12	3 (10%)	48,51,51	3.50	20 (41%)
21	EDO	A	618	-	3,3,3	0.23	0	2,2,2	1.43	0
27	PEK	T	101	-	52,52,52	1.30	2 (3%)	55,57,57	1.43	7 (12%)
18	AZI	A	607	14	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	R	205	-	3,3,3	0.32	0	2,2,2	1.05	0
22	CHD	P	301	-	29,32,32	1.55	7 (24%)	48,51,51	2.16	17 (35%)
19	TGL	A	608	-	62,62,62	1.37	5 (8%)	65,65,65	2.18	11 (16%)
21	EDO	C	316	-	3,3,3	0.52	0	2,2,2	1.52	0
21	EDO	V	101	-	3,3,3	0.39	0	2,2,2	0.90	0
14	HEA	A	602[B]	1,18	44,67,67	1.16	3 (6%)	37,103,103	2.54	15 (40%)
25	DMU	C	311	-	34,34,34	1.43	3 (8%)	45,45,45	2.32	11 (24%)
18	AZI	N	607	15	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	N	616	-	3,3,3	0.56	0	2,2,2	1.11	0
18	AZI	N	608	14	0,2,2	0.00	-	0,1,1	0.00	-
20	PGV	N	609	-	50,50,50	1.13	5 (10%)	53,56,56	1.32	5 (9%)
19	TGL	N	610	-	62,62,62	1.16	4 (6%)	65,65,65	1.77	12 (18%)
23	CUA	B	302	2	0,1,1	0.00	-	-	-	-
21	EDO	C	318	-	3,3,3	0.66	0	2,2,2	0.39	0
24	PSC	O	302	-	51,51,51	1.29	3 (5%)	57,59,59	1.34	4 (7%)
18	AZI	A	606	15	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	N	614	-	3,3,3	0.40	0	2,2,2	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CHD	J	101	-	29,32,32	0.68	0	48,51,51	3.32	29 (60%)
21	EDO	A	622	-	3,3,3	0.30	0	2,2,2	0.48	0
21	EDO	A	617	-	3,3,3	1.21	0	2,2,2	1.28	0
14	HEA	N	603[A]	1,18	44,67,67	1.25	3 (6%)	37,103,103	2.88	14 (37%)
21	EDO	F	104	-	3,3,3	0.33	0	2,2,2	0.47	0
21	EDO	J	102	-	3,3,3	0.39	0	2,2,2	1.78	0
25	DMU	C	302	-	34,34,34	0.94	0	45,45,45	1.73	14 (31%)
21	EDO	H	102	-	3,3,3	0.59	0	2,2,2	1.26	0
21	EDO	R	206	-	3,3,3	1.02	0	2,2,2	0.48	0
21	EDO	P	311	-	3,3,3	0.84	0	2,2,2	0.14	0
21	EDO	R	203	-	3,3,3	0.54	0	2,2,2	0.82	0
21	EDO	E	202	-	3,3,3	0.53	0	2,2,2	0.84	0
21	EDO	O	304	-	3,3,3	0.35	0	2,2,2	0.92	0
21	EDO	D	203	-	3,3,3	0.45	0	2,2,2	0.71	0
21	EDO	R	201	-	3,3,3	1.14	0	2,2,2	1.17	0
21	EDO	O	303	-	3,3,3	0.68	0	2,2,2	0.78	0
14	HEA	N	602	1	44,67,67	1.24	3 (6%)	37,103,103	2.74	15 (40%)
28	CDL	T	103	-	99,99,99	1.51	14 (14%)	105,111,111	1.72	25 (23%)
21	EDO	H	101	-	3,3,3	0.24	0	2,2,2	2.63	2 (100%)
25	DMU	C	310	-	34,34,34	0.87	1 (2%)	45,45,45	2.11	9 (20%)
21	EDO	A	613	-	3,3,3	1.64	1 (33%)	2,2,2	0.92	0
21	EDO	E	203	-	3,3,3	0.31	0	2,2,2	1.26	0
21	EDO	N	611	-	3,3,3	0.36	0	2,2,2	1.12	0
25	DMU	Z	102	-	34,34,34	0.75	1 (2%)	45,45,45	1.33	5 (11%)
19	TGL	Y	101	-	62,62,62	1.45	5 (8%)	65,65,65	1.88	11 (16%)
20	PGV	P	303	-	50,50,50	0.80	1 (2%)	53,56,56	1.25	8 (15%)
21	EDO	E	205	-	3,3,3	0.38	0	2,2,2	0.80	0
21	EDO	P	310	-	3,3,3	0.67	0	2,2,2	2.16	1 (50%)
19	TGL	D	201	-	62,62,62	1.66	5 (8%)	65,65,65	2.26	11 (16%)
21	EDO	Q	202	-	3,3,3	0.36	0	2,2,2	1.09	0
25	DMU	P	306	-	34,34,34	1.02	1 (2%)	45,45,45	1.38	3 (6%)
21	EDO	S	102	-	3,3,3	1.13	0	2,2,2	0.39	0
21	EDO	A	620	-	3,3,3	0.68	0	2,2,2	0.65	0
22	CHD	P	305	-	29,32,32	1.30	4 (13%)	48,51,51	3.64	22 (45%)
21	EDO	C	317	-	3,3,3	0.47	0	2,2,2	0.37	0
21	EDO	G	104	-	3,3,3	0.58	0	2,2,2	0.47	0
25	DMU	P	308	-	34,34,34	0.75	0	45,45,45	2.19	13 (28%)
24	PSC	B	303	-	51,51,51	1.46	4 (7%)	57,59,59	1.46	7 (12%)
21	EDO	G	105	-	3,3,3	0.91	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PGV	C	305	-	50,50,50	1.06	1 (2%)	53,56,56	1.36	7 (13%)
21	EDO	P	313	-	3,3,3	0.60	0	2,2,2	0.70	0
21	EDO	B	305	-	3,3,3	1.73	1 (33%)	2,2,2	0.11	0
20	PGV	G	103	-	50,50,50	1.25	2 (4%)	53,56,56	1.69	6 (11%)
21	EDO	N	612	-	3,3,3	1.36	0	2,2,2	1.62	0
21	EDO	N	617	-	3,3,3	1.05	0	2,2,2	0.14	0
21	EDO	N	619	-	3,3,3	0.55	0	2,2,2	0.04	0
21	EDO	S	103	-	3,3,3	0.68	0	2,2,2	1.76	1 (50%)
21	EDO	F	102	-	3,3,3	1.06	0	2,2,2	0.29	0
21	EDO	L	103	-	3,3,3	0.26	0	2,2,2	1.08	0
21	EDO	A	619	-	3,3,3	1.55	0	2,2,2	1.69	0
21	EDO	R	204	-	3,3,3	0.88	0	2,2,2	0.42	0
21	EDO	E	201	-	3,3,3	0.84	0	2,2,2	0.44	0
21	EDO	D	207	-	3,3,3	0.62	0	2,2,2	0.56	0
20	PGV	A	610	-	50,50,50	1.42	4 (8%)	53,56,56	1.63	8 (15%)
21	EDO	A	612	-	3,3,3	0.51	0	2,2,2	1.15	0
21	EDO	C	313	-	3,3,3	0.36	0	2,2,2	0.80	0
14	HEA	A	602[A]	1,18	44,67,67	1.12	2 (4%)	37,103,103	2.15	11 (29%)
19	TGL	L	101	-	62,62,62	2.03	8 (12%)	65,65,65	2.34	17 (26%)
21	EDO	F	103	-	3,3,3	0.64	0	2,2,2	0.54	0
28	CDL	P	304	-	99,99,99	1.61	18 (18%)	105,111,111	1.60	19 (18%)
22	CHD	B	301	-	29,32,32	2.12	10 (34%)	48,51,51	2.00	15 (31%)
21	EDO	N	621	-	3,3,3	0.33	0	2,2,2	0.89	0
20	PGV	C	309	-	50,50,50	1.41	3 (6%)	53,56,56	1.48	8 (15%)
21	EDO	A	615	-	3,3,3	2.67	1 (33%)	2,2,2	4.78	1 (50%)
22	CHD	G	101	-	29,32,32	1.69	7 (24%)	48,51,51	1.81	10 (20%)
21	EDO	F	105	-	3,3,3	0.66	0	2,2,2	0.42	0
28	CDL	C	306	-	99,99,99	1.58	17 (17%)	105,111,111	1.66	20 (19%)
21	EDO	N	613	-	3,3,3	0.54	0	2,2,2	0.44	0
25	DMU	L	102	-	34,34,34	0.96	1 (2%)	45,45,45	1.73	11 (24%)
27	PEK	T	102	-	52,52,52	1.18	6 (11%)	55,57,57	2.57	7 (12%)
23	CUA	O	301	2	0,1,1	0.00	-	-	-	-
25	DMU	M	101	-	34,34,34	0.71	0	45,45,45	1.41	6 (13%)
21	EDO	N	622	-	3,3,3	0.51	0	2,2,2	0.70	0
21	EDO	C	314	-	3,3,3	0.54	0	2,2,2	0.77	0
28	CDL	N	601	-	99,99,99	1.54	14 (14%)	105,111,111	1.60	20 (19%)

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
14	HEA	N	603[B]	1,18	2/2/7/16	3/24/76/76	-
21	EDO	D	205	-	-	1/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	N	618	-	-	0/1/1/1	-
19	TGL	Q	201	-	-	37/65/65/65	-
22	CHD	C	301	-	-	1/7/74/74	0/4/4/4
27	PEK	C	304	-	-	12/56/56/56	-
27	PEK	C	308	-	-	28/56/56/56	-
21	EDO	E	204	-	-	1/1/1/1	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	D	202	-	-	1/1/1/1	-
21	EDO	U	101	-	-	1/1/1/1	-
21	EDO	D	206	-	-	1/1/1/1	-
21	EDO	A	623	-	-	0/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
14	HEA	A	601	1	3/3/7/16	2/24/76/76	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
22	CHD	W	101	-	-	5/7/74/74	0/4/4/4
21	EDO	C	319	-	-	1/1/1/1	-
21	EDO	A	621	-	-	1/1/1/1	-
21	EDO	C	315	-	-	1/1/1/1	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
21	EDO	B	304	-	-	0/1/1/1	-
27	PEK	G	102	-	-	34/56/56/56	-
21	EDO	C	312	-	-	0/1/1/1	-
27	PEK	P	307	-	-	27/56/56/56	-
21	EDO	N	615	-	-	0/1/1/1	-
20	PGV	A	609	-	-	8/55/55/55	-
21	EDO	Q	203	-	-	1/1/1/1	-
20	PGV	Z	101	-	-	31/55/55/55	-
21	EDO	D	204	-	-	1/1/1/1	-
21	EDO	R	202	-	-	1/1/1/1	-
22	CHD	C	307	-	-	6/7/74/74	0/4/4/4
21	EDO	A	618	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PEK	T	101	-	-	29/56/56/56	-
21	EDO	R	205	-	-	1/1/1/1	-
22	CHD	P	301	-	-	0/7/74/74	0/4/4/4
19	TGL	A	608	-	-	36/65/65/65	-
21	EDO	C	316	-	-	0/1/1/1	-
21	EDO	V	101	-	-	0/1/1/1	-
14	HEA	A	602[B]	1,18	3/3/7/16	2/24/76/76	-
25	DMU	C	311	-	-	8/19/59/59	0/2/2/2
21	EDO	N	616	-	-	1/1/1/1	-
20	PGV	N	609	-	-	13/55/55/55	-
19	TGL	N	610	-	-	39/65/65/65	-
21	EDO	C	318	-	-	1/1/1/1	-
24	PSC	O	302	-	-	33/55/55/55	-
21	EDO	N	614	-	-	1/1/1/1	-
22	CHD	J	101	-	-	6/7/74/74	0/4/4/4
21	EDO	A	622	-	-	1/1/1/1	-
21	EDO	A	617	-	-	1/1/1/1	-
14	HEA	N	603[A]	1,18	3/3/7/16	0/24/76/76	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-
25	DMU	C	302	-	-	7/19/59/59	0/2/2/2
21	EDO	H	102	-	-	1/1/1/1	-
21	EDO	R	206	-	-	1/1/1/1	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	R	203	-	-	1/1/1/1	-
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	O	304	-	-	1/1/1/1	-
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	O	303	-	-	0/1/1/1	-
14	HEA	N	602	1	2/2/7/16	3/24/76/76	-
28	CDL	T	103	-	-	63/110/110/110	-
21	EDO	H	101	-	-	0/1/1/1	-
25	DMU	C	310	-	-	6/19/59/59	0/2/2/2
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	E	203	-	-	1/1/1/1	-
21	EDO	N	611	-	-	1/1/1/1	-
25	DMU	Z	102	-	-	5/19/59/59	0/2/2/2
19	TGL	Y	101	-	-	34/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	303	-	-	11/55/55/55	-
21	EDO	E	205	-	-	0/1/1/1	-
21	EDO	P	310	-	-	1/1/1/1	-
19	TGL	D	201	-	-	40/65/65/65	-
21	EDO	Q	202	-	-	0/1/1/1	-
25	DMU	P	306	-	-	6/19/59/59	0/2/2/2
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	A	620	-	-	0/1/1/1	-
22	CHD	P	305	-	-	4/7/74/74	0/4/4/4
21	EDO	C	317	-	-	1/1/1/1	-
21	EDO	G	104	-	-	1/1/1/1	-
25	DMU	P	308	-	-	7/19/59/59	0/2/2/2
24	PSC	B	303	-	-	28/55/55/55	-
21	EDO	G	105	-	-	1/1/1/1	-
20	PGV	C	305	-	-	14/55/55/55	-
21	EDO	P	313	-	-	1/1/1/1	-
21	EDO	B	305	-	-	1/1/1/1	-
20	PGV	G	103	-	-	33/55/55/55	-
21	EDO	N	612	-	-	1/1/1/1	-
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	L	103	-	-	1/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	R	204	-	-	0/1/1/1	-
21	EDO	E	201	-	-	1/1/1/1	-
21	EDO	D	207	-	-	0/1/1/1	-
20	PGV	A	610	-	-	26/55/55/55	-
21	EDO	A	612	-	-	1/1/1/1	-
21	EDO	C	313	-	-	1/1/1/1	-
14	HEA	A	602[A]	1,18	3/3/7/16	2/24/76/76	-
19	TGL	L	101	-	-	38/65/65/65	-
21	EDO	F	103	-	-	0/1/1/1	-
28	CDL	P	304	-	-	56/110/110/110	-
22	CHD	B	301	-	-	0/7/74/74	0/4/4/4
21	EDO	N	621	-	-	0/1/1/1	-
20	PGV	C	309	-	-	27/55/55/55	-
21	EDO	A	615	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	G	101	-	-	0/7/74/74	0/4/4/4
21	EDO	F	105	-	-	0/1/1/1	-
28	CDL	C	306	-	-	70/110/110/110	-
21	EDO	N	613	-	-	1/1/1/1	-
25	DMU	L	102	-	-	12/19/59/59	0/2/2/2
27	PEK	T	102	-	-	23/56/56/56	-
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	N	622	-	-	1/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
28	CDL	N	601	-	-	53/110/110/110	-

The worst 5 of 211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG3-CC1	9.15	1.60	1.33
19	L	101	TGL	OG2-CB1	9.01	1.59	1.34
19	D	201	TGL	OB1-CB1	7.45	1.44	1.22
19	Y	101	TGL	OG2-CB1	6.77	1.53	1.34
20	C	309	PGV	O01-C1	6.53	1.52	1.34

The worst 5 of 580 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	305	CHD	C23-C22-C20	-17.48	91.17	114.72
22	C	307	CHD	C23-C22-C20	-15.64	93.65	114.72
27	T	102	PEK	C2-C3-C4	14.82	139.64	113.23
19	D	201	TGL	OG2-CB1-CB2	-10.77	88.29	111.50
22	J	101	CHD	C14-C8-C9	-10.23	95.67	109.71

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	603[B]	HEA	ND
14	N	603[B]	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB

5 of 983 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
14	N	603[B]	HEA	C4D-C3D-CAD-CBD
27	C	304	PEK	C10-C11-C12-C13
27	C	308	PEK	C04-O12-P-O14
27	C	308	PEK	O12-C04-C05-N

There are no ring outliers.

79 monomers are involved in 470 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	603[B]	HEA	12	0
21	N	618	EDO	6	0
19	Q	201	TGL	10	0
22	C	301	CHD	2	0
27	C	304	PEK	8	0
27	C	308	PEK	11	0
21	O	305	EDO	1	0
21	D	202	EDO	7	0
21	D	206	EDO	2	0
14	A	601	HEA	6	0
21	P	312	EDO	1	0
22	W	101	CHD	9	0
21	A	621	EDO	5	0
21	C	315	EDO	1	0
25	P	309	DMU	1	0
27	G	102	PEK	10	0
27	P	307	PEK	10	0
20	A	609	PGV	6	0
20	Z	101	PGV	12	0
21	D	204	EDO	2	0
21	R	202	EDO	1	0
22	C	307	CHD	6	0
21	A	618	EDO	3	0
27	T	101	PEK	4	0
18	A	607	AZI	6	0
21	R	205	EDO	1	0
22	P	301	CHD	1	0
19	A	608	TGL	3	0
21	C	316	EDO	2	0
14	A	602[B]	HEA	11	0
25	C	311	DMU	1	0
18	N	607	AZI	1	0
18	N	608	AZI	6	0

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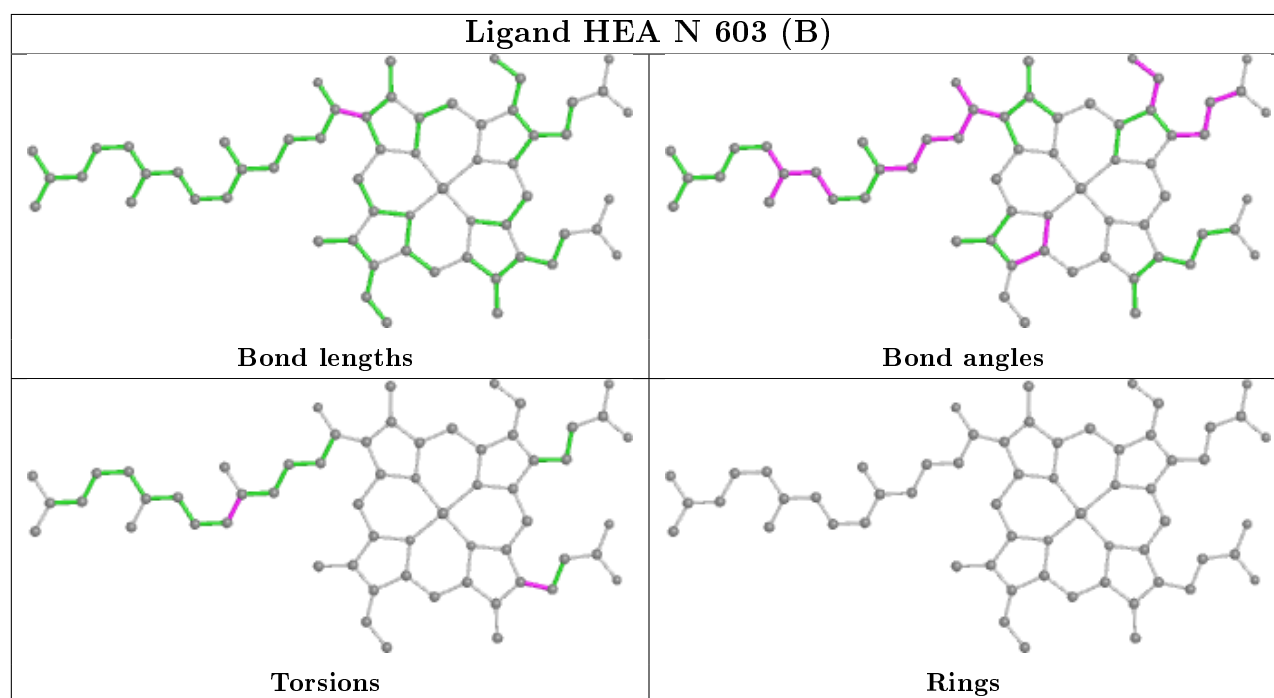
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	609	PGV	2	0
19	N	610	TGL	8	0
24	O	302	PSC	12	0
18	A	606	AZI	2	0
22	J	101	CHD	2	0
21	A	622	EDO	1	0
21	A	617	EDO	1	0
14	N	603[A]	HEA	8	0
25	C	302	DMU	12	0
21	H	102	EDO	1	0
21	O	304	EDO	1	0
21	D	203	EDO	4	0
14	N	602	HEA	7	0
28	T	103	CDL	20	0
21	H	101	EDO	3	0
25	C	310	DMU	5	0
21	A	613	EDO	2	0
19	Y	101	TGL	13	0
20	P	303	PGV	3	0
19	D	201	TGL	21	0
25	P	306	DMU	16	0
22	P	305	CHD	6	0
21	C	317	EDO	1	0
21	G	104	EDO	1	0
25	P	308	DMU	1	0
24	B	303	PSC	23	0
20	C	305	PGV	3	0
20	G	103	PGV	4	0
21	N	612	EDO	3	0
21	A	619	EDO	2	0
20	A	610	PGV	7	0
14	A	602[A]	HEA	10	0
19	L	101	TGL	4	0
28	P	304	CDL	25	0
21	N	621	EDO	6	0
20	C	309	PGV	8	0
21	A	615	EDO	6	0
22	G	101	CHD	1	0
21	F	105	EDO	5	0
28	C	306	CDL	30	0
21	N	613	EDO	1	0
25	L	102	DMU	5	0

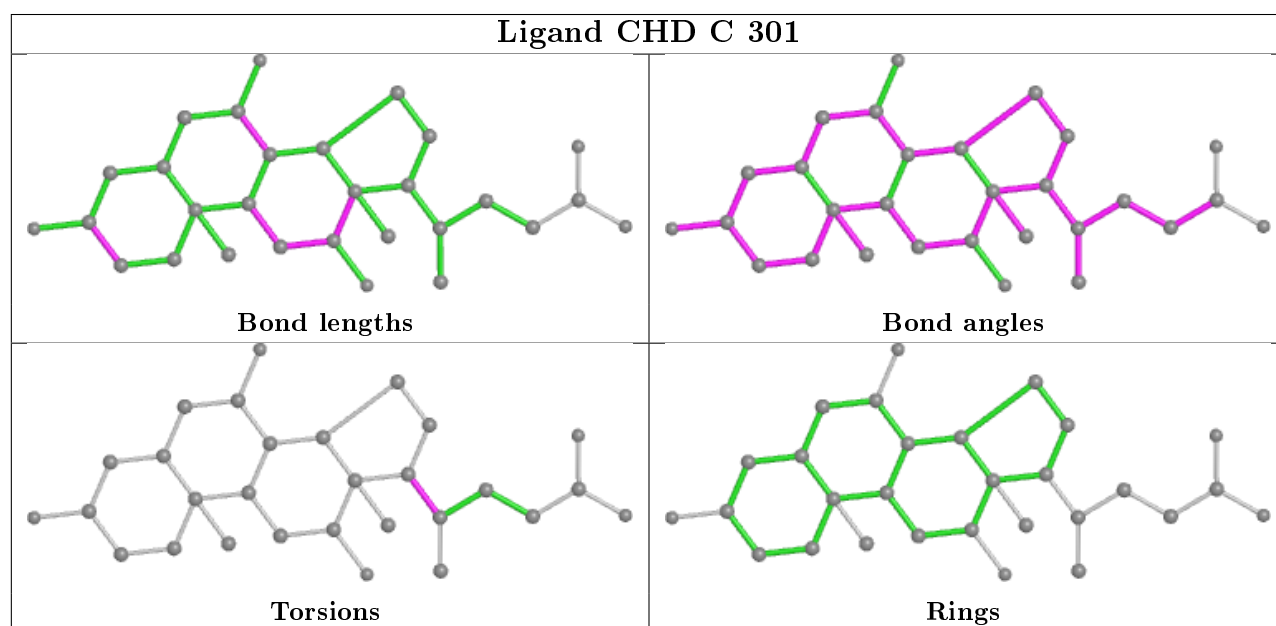
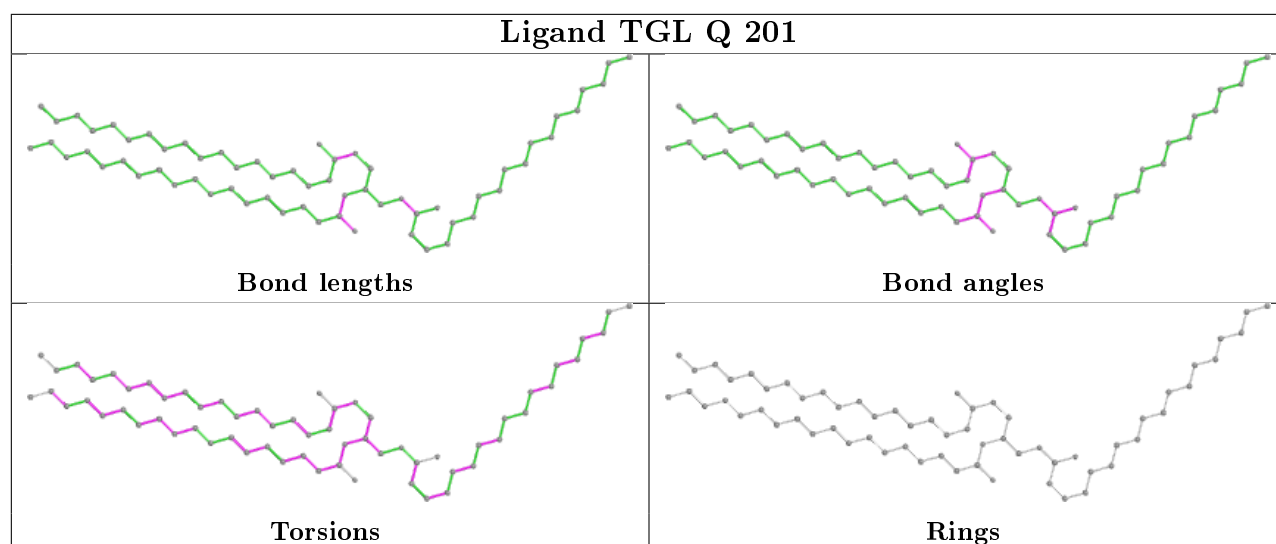
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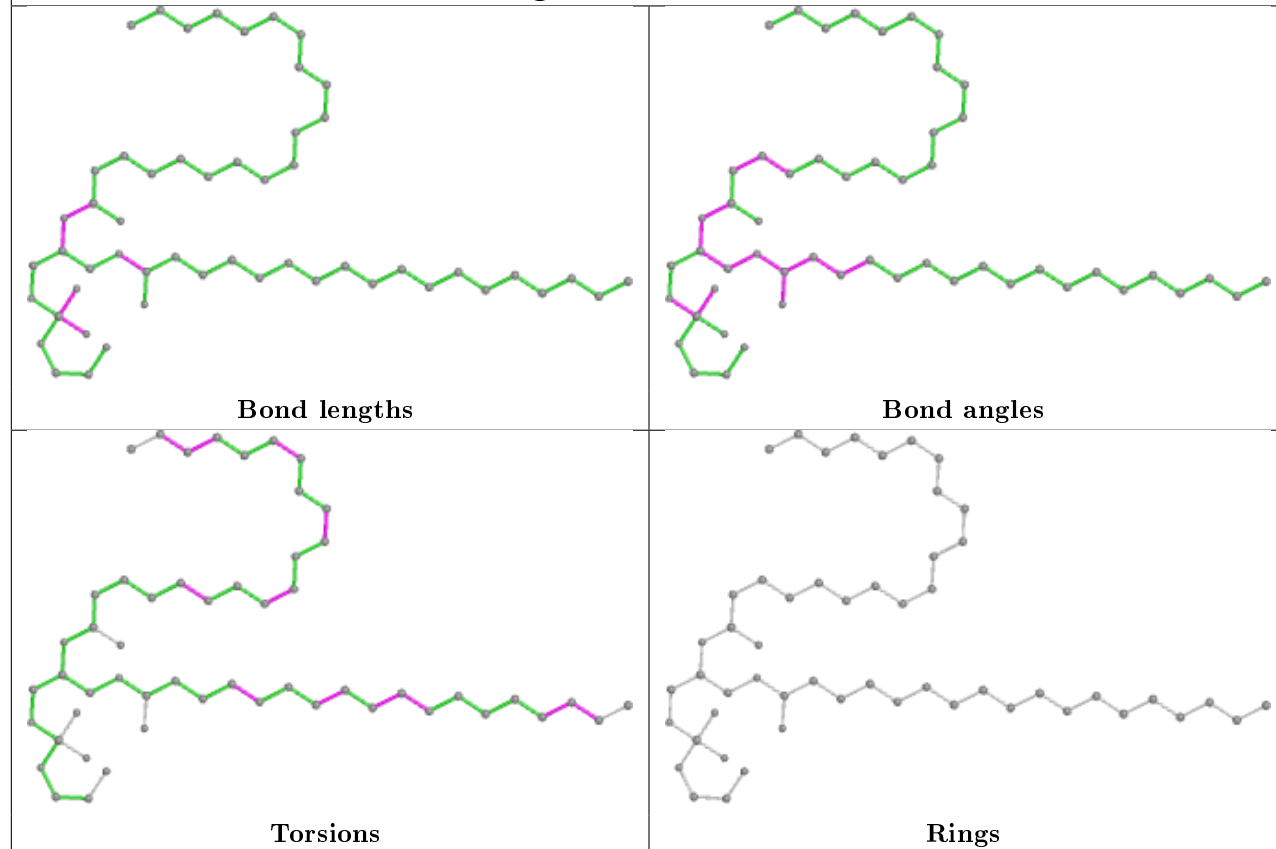
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	T	102	PEK	4	0
25	M	101	DMU	1	0
21	N	622	EDO	7	0
28	N	601	CDL	15	0

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.

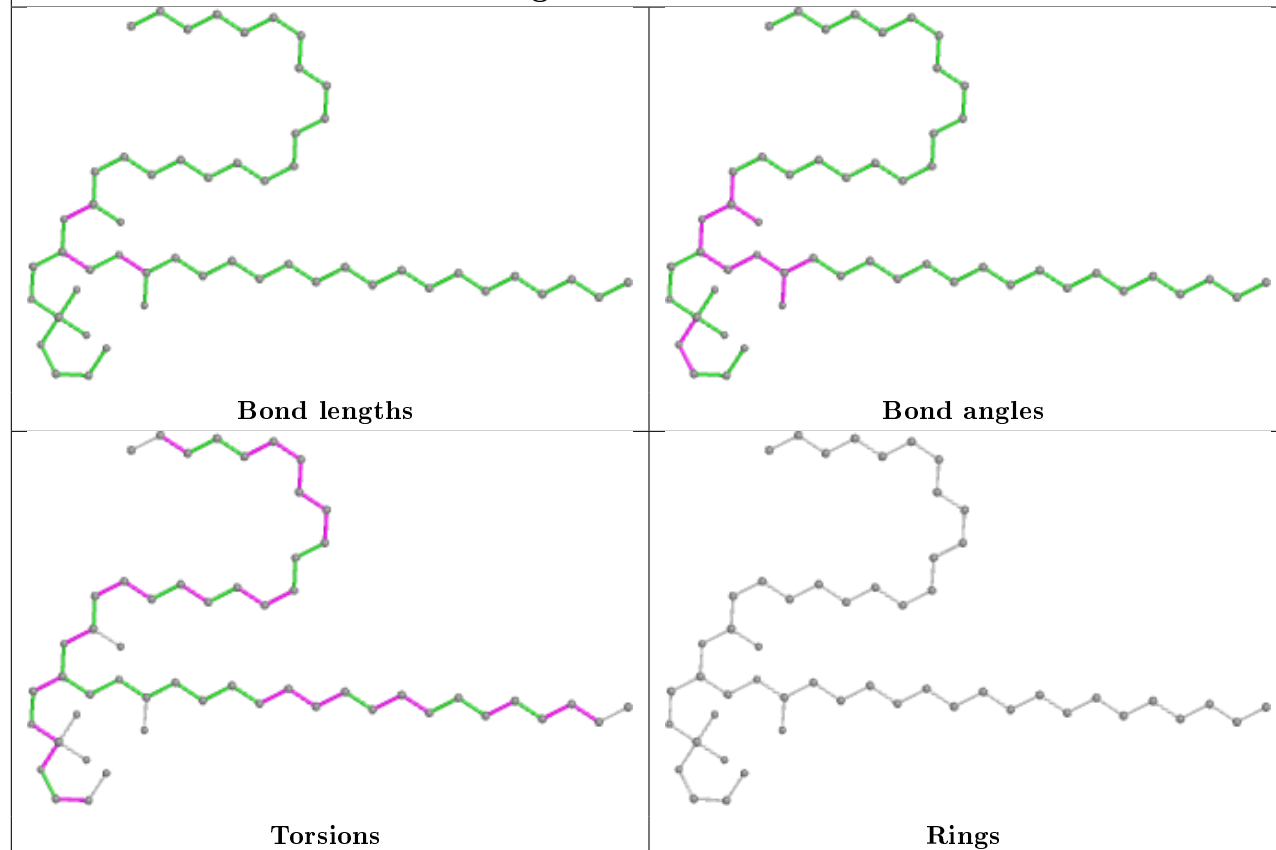


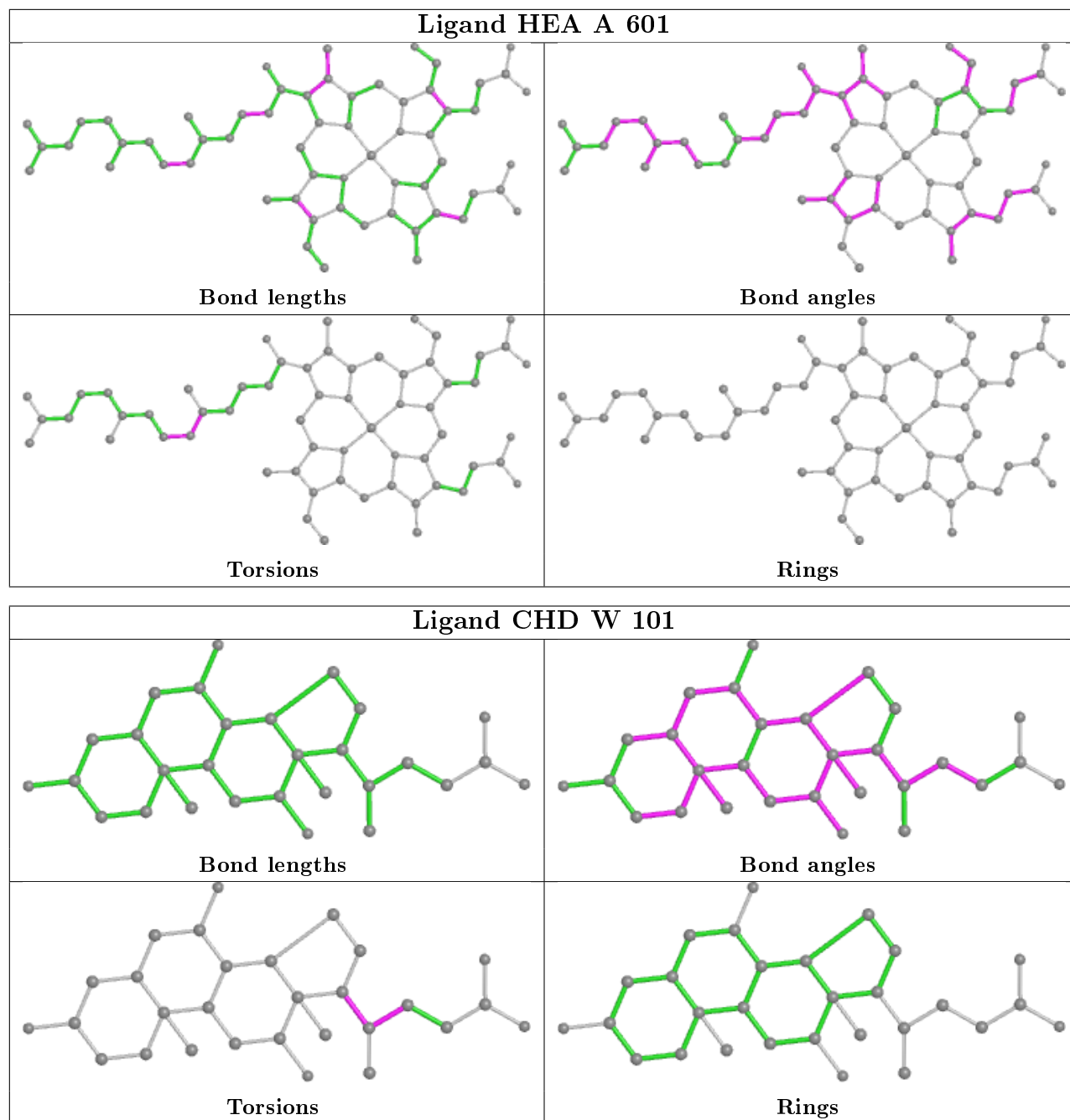


## Ligand PEK C 304

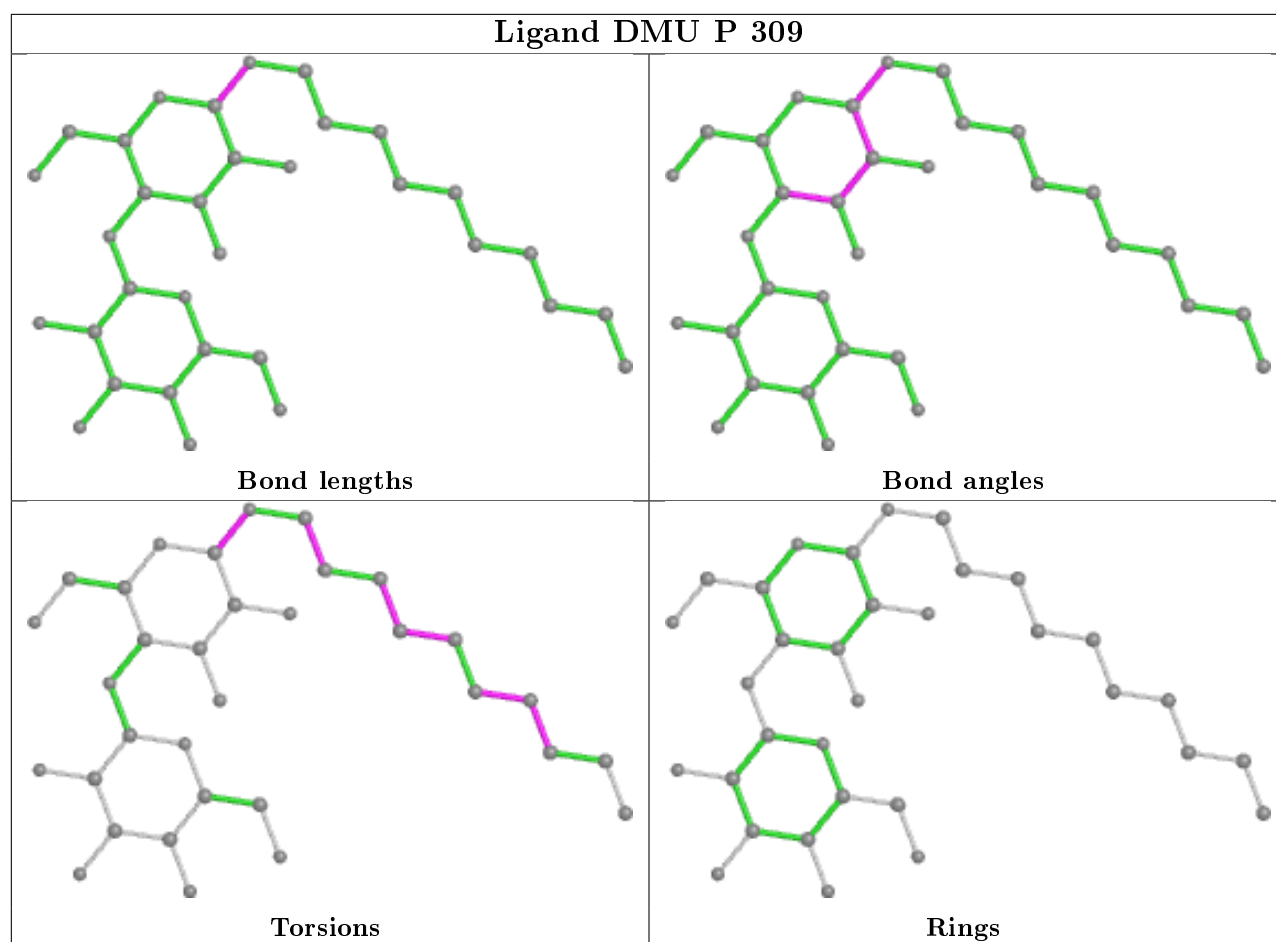


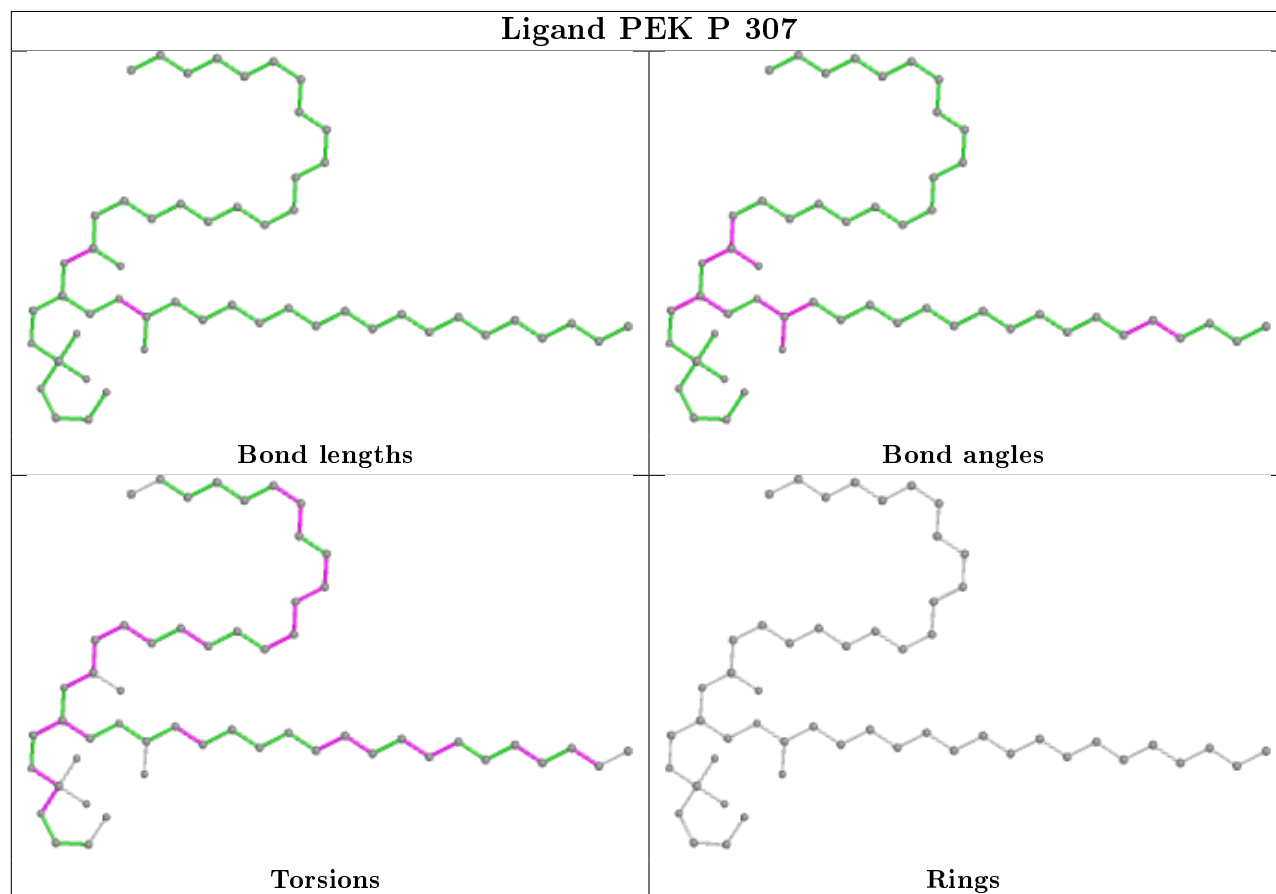
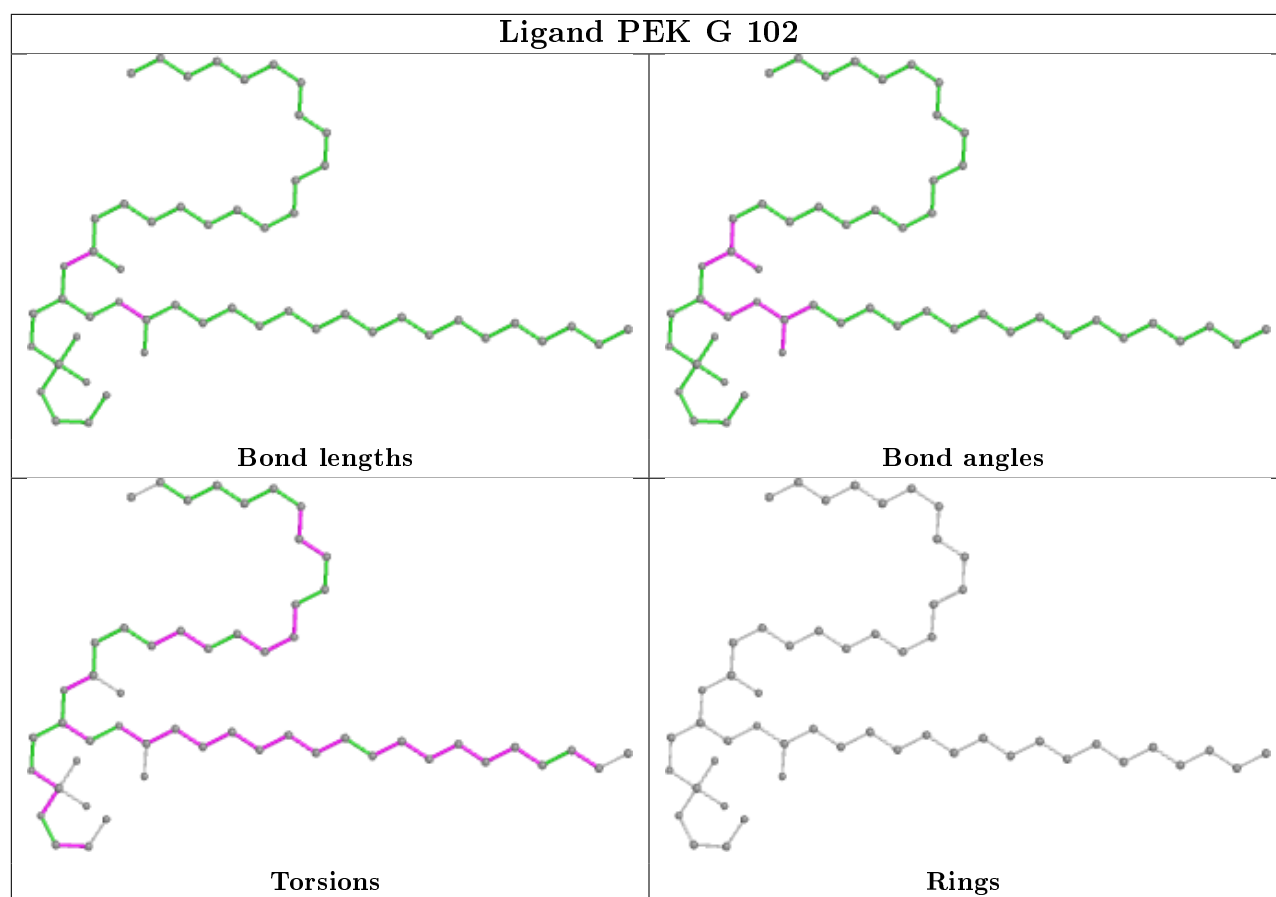
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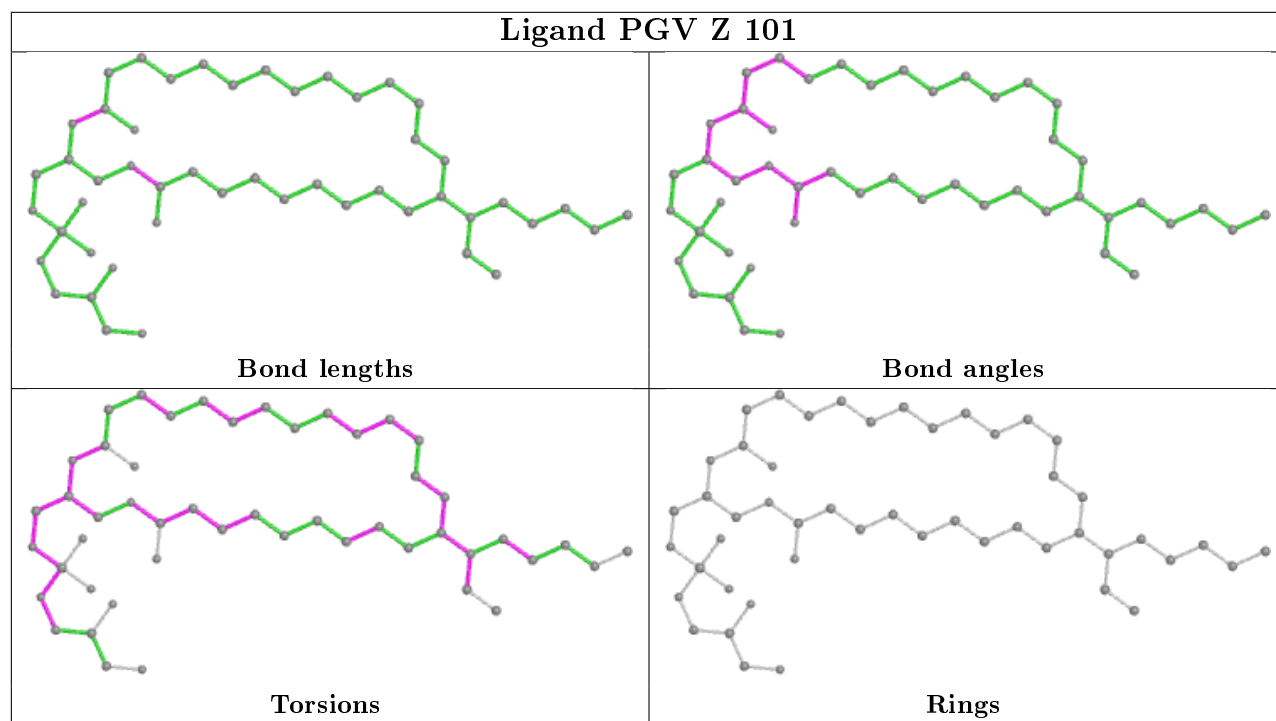
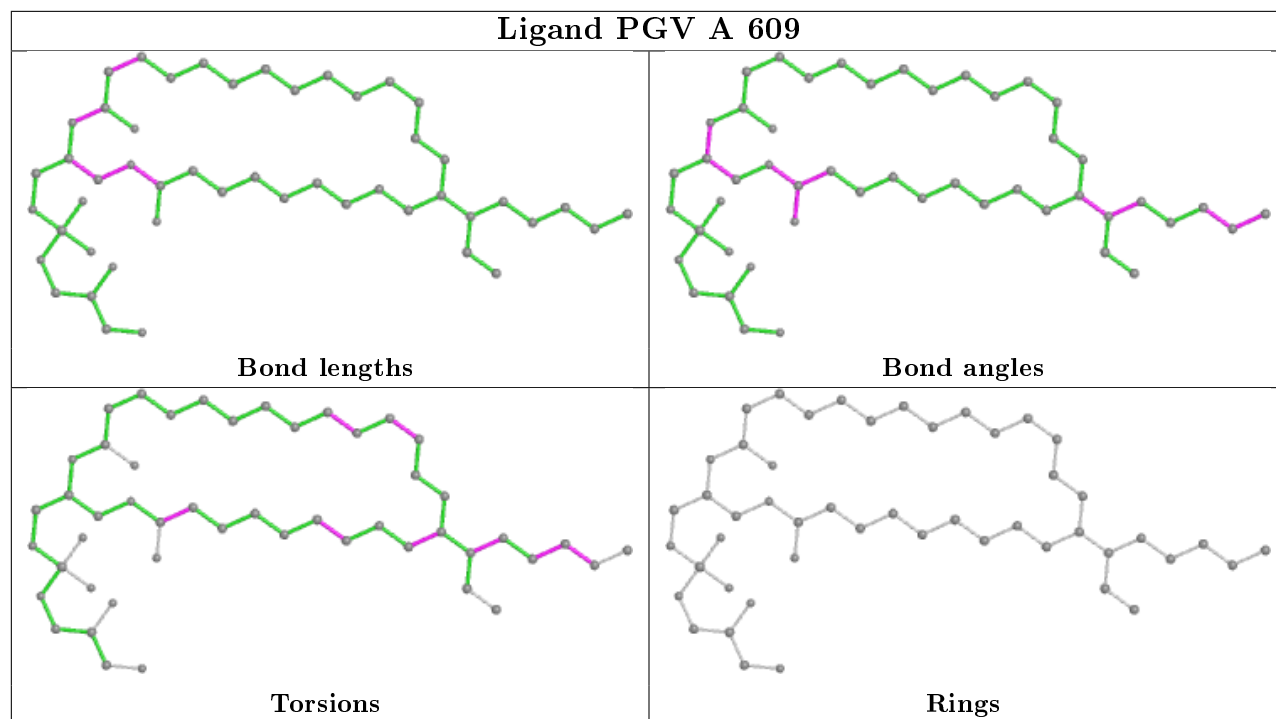


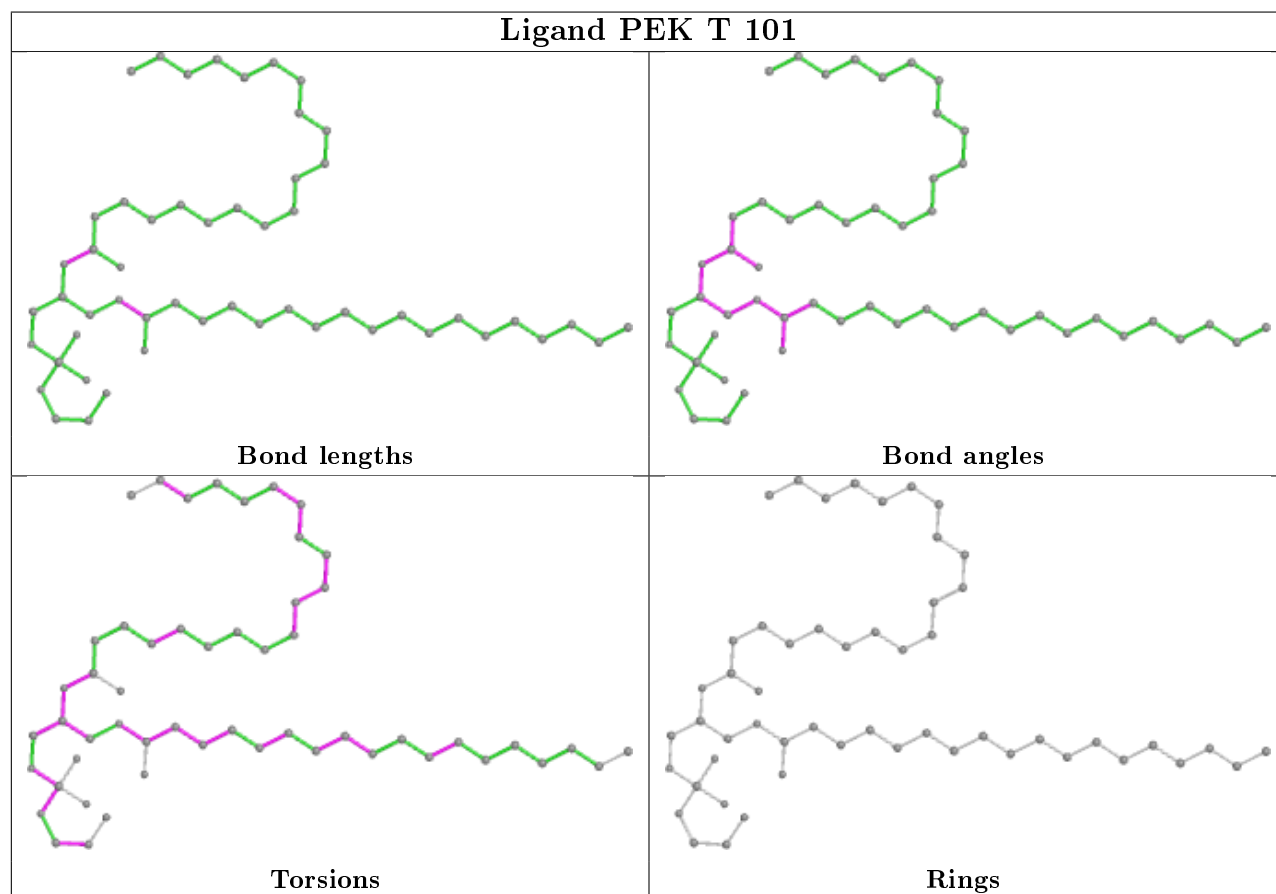
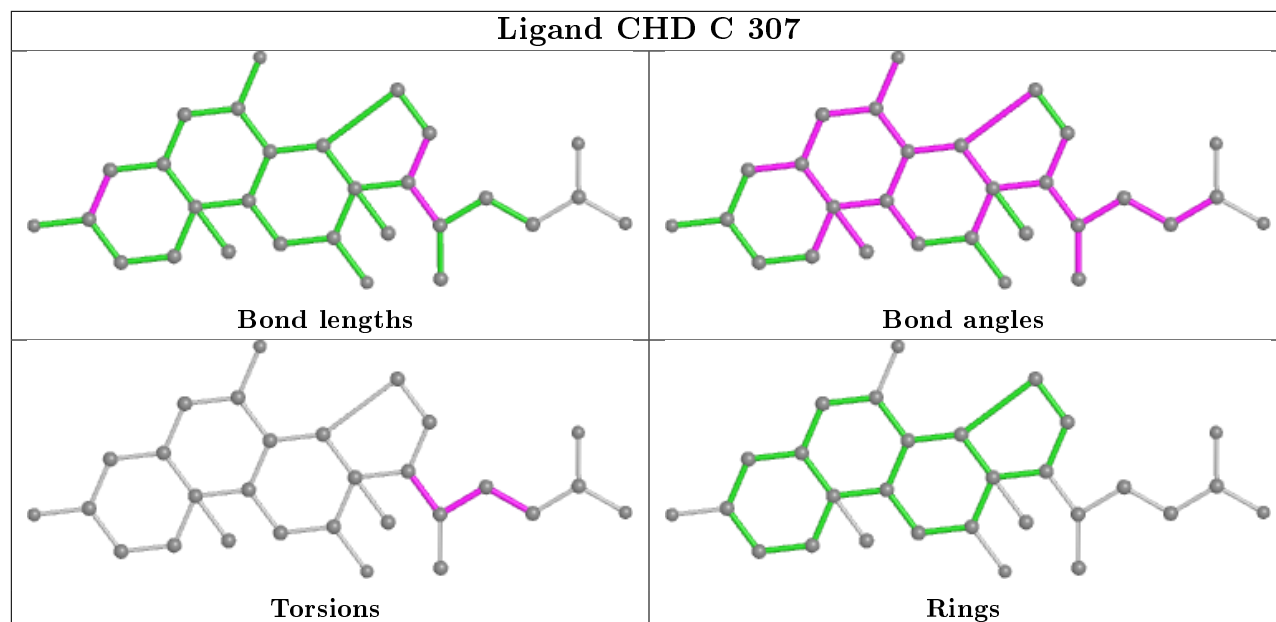


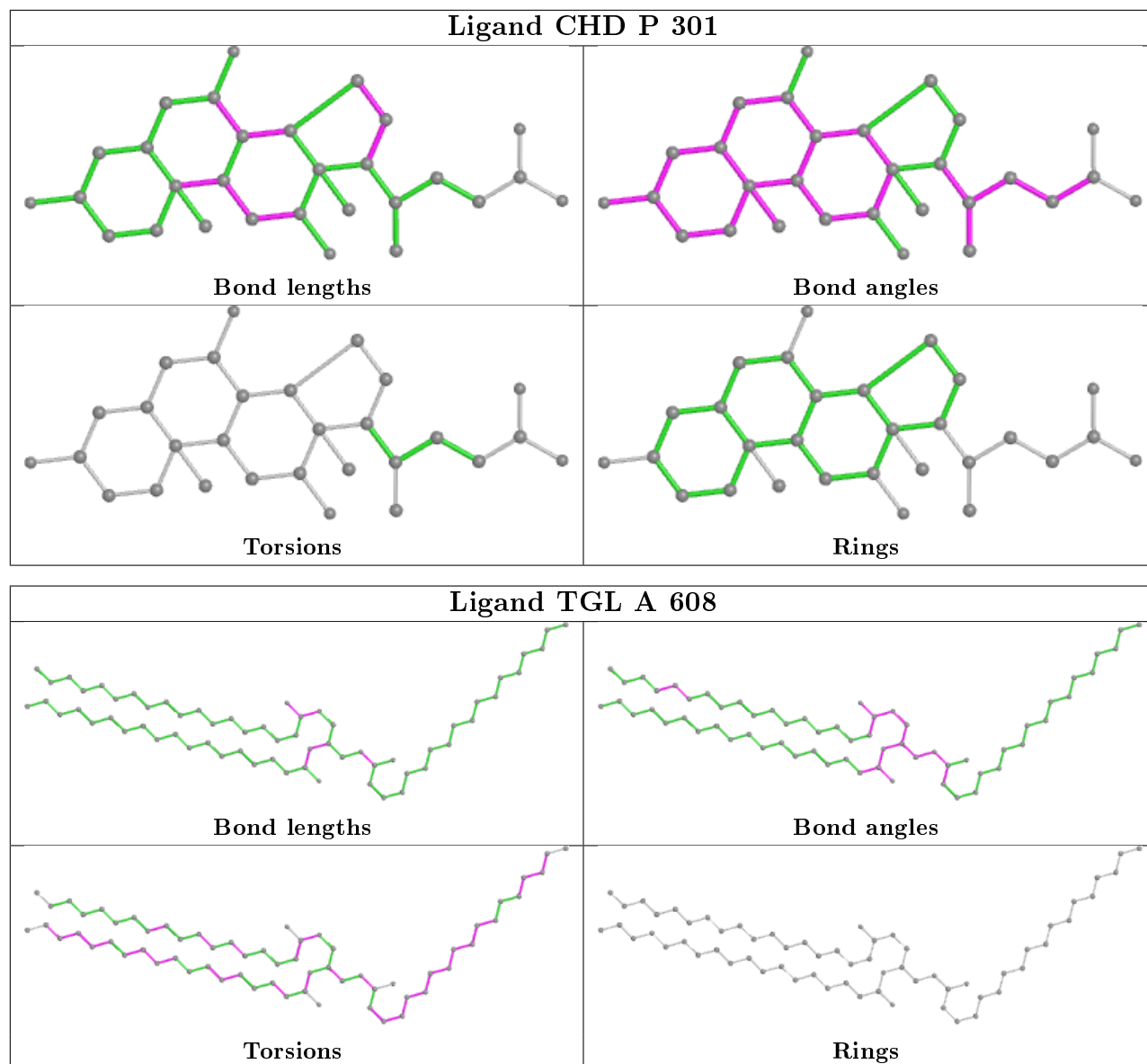


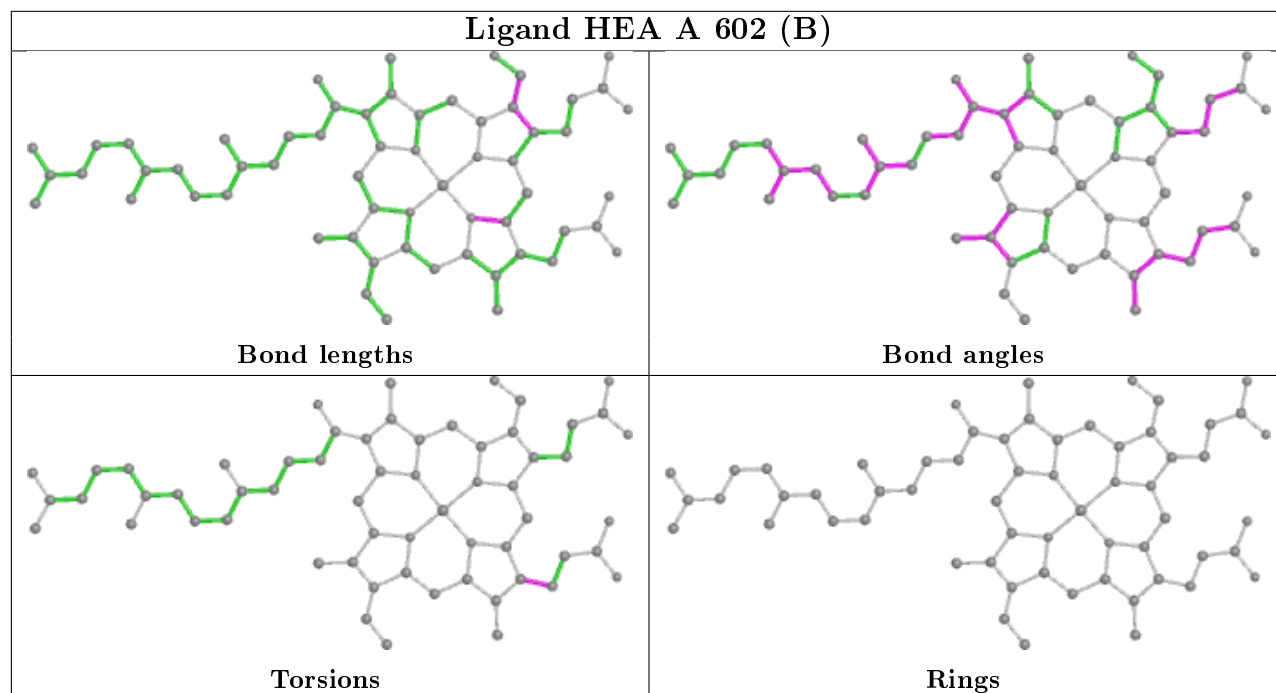
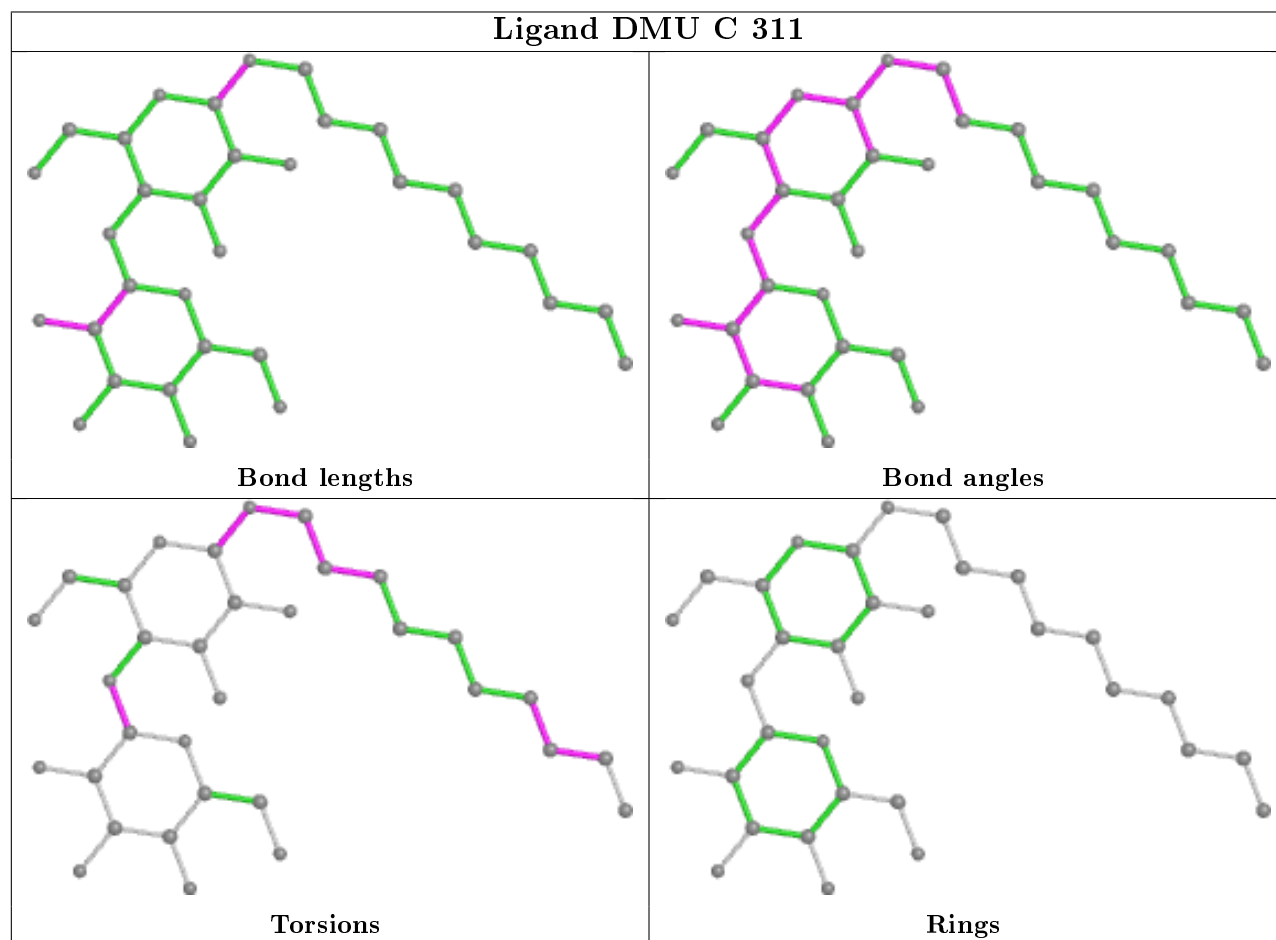


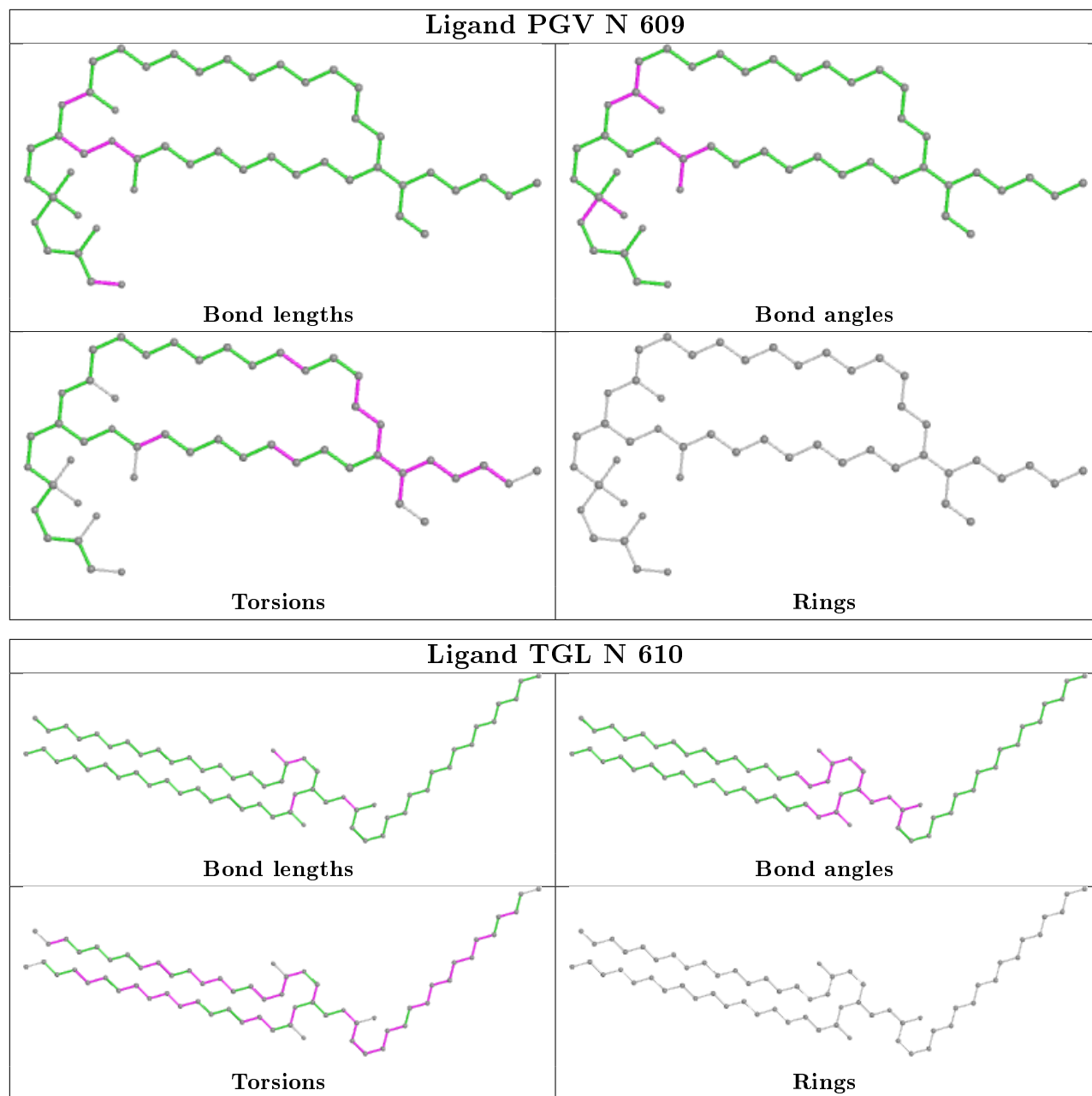




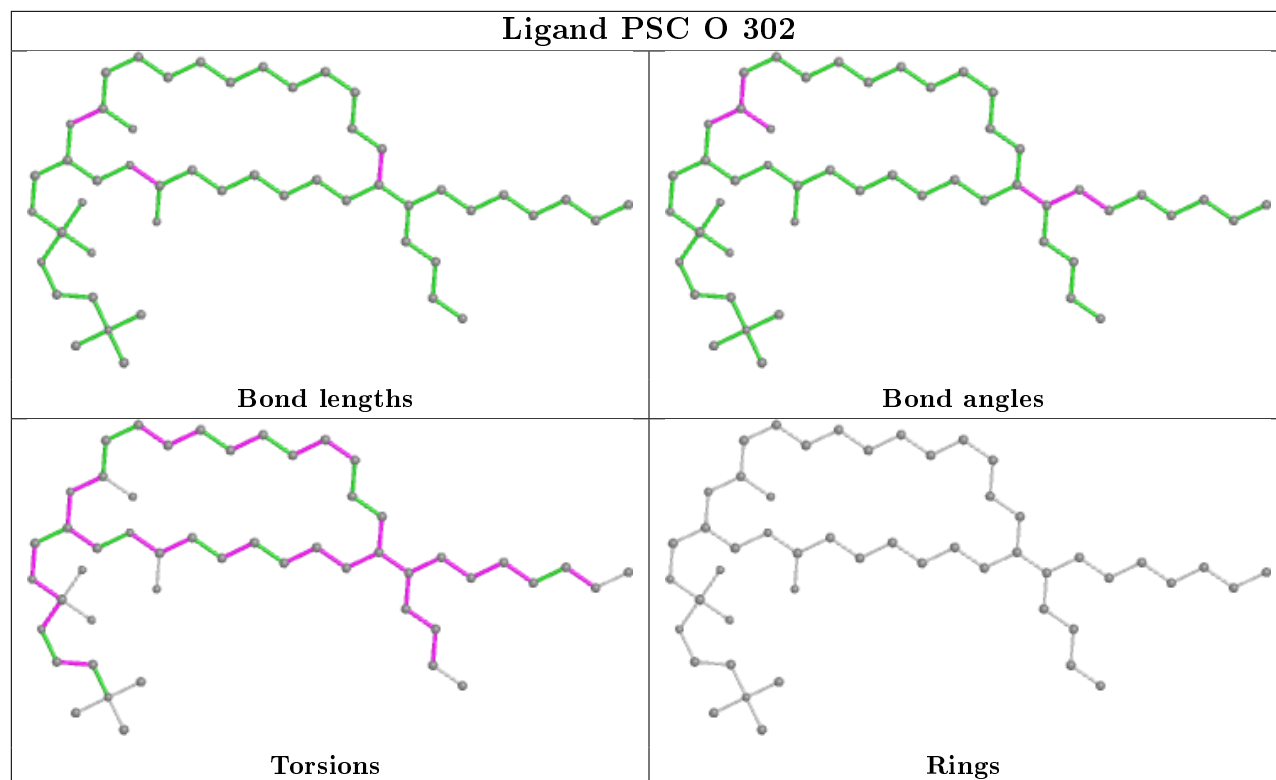




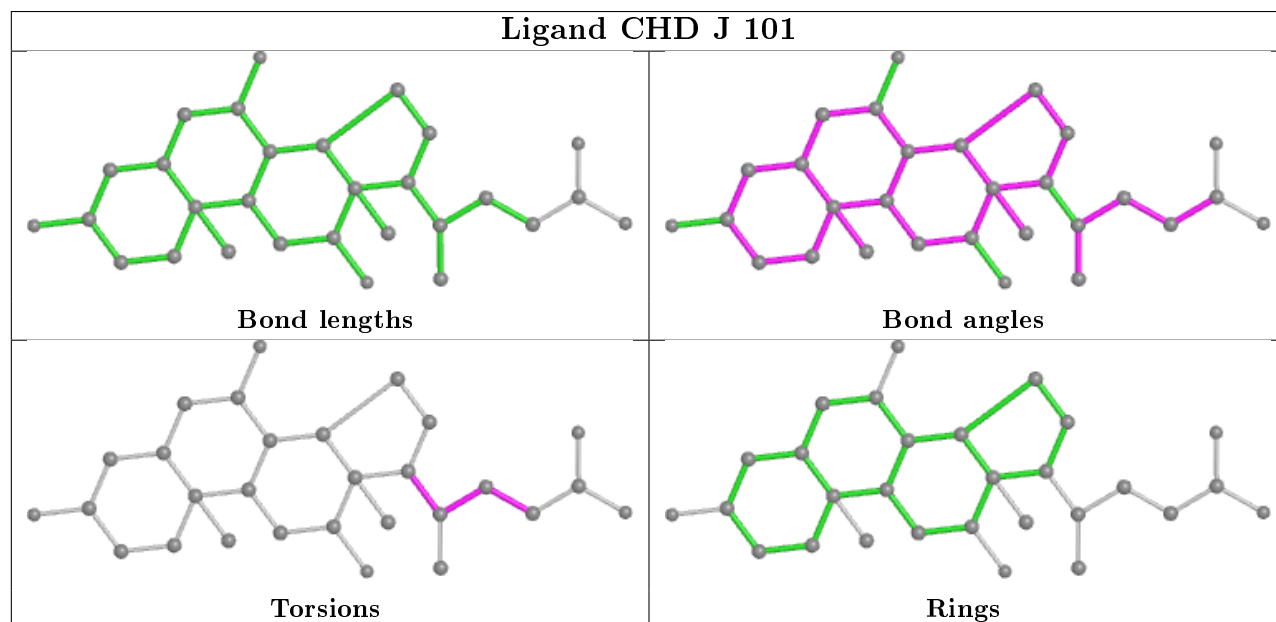
**Ligand HEA A 602 (B)****Ligand DMU C 311**



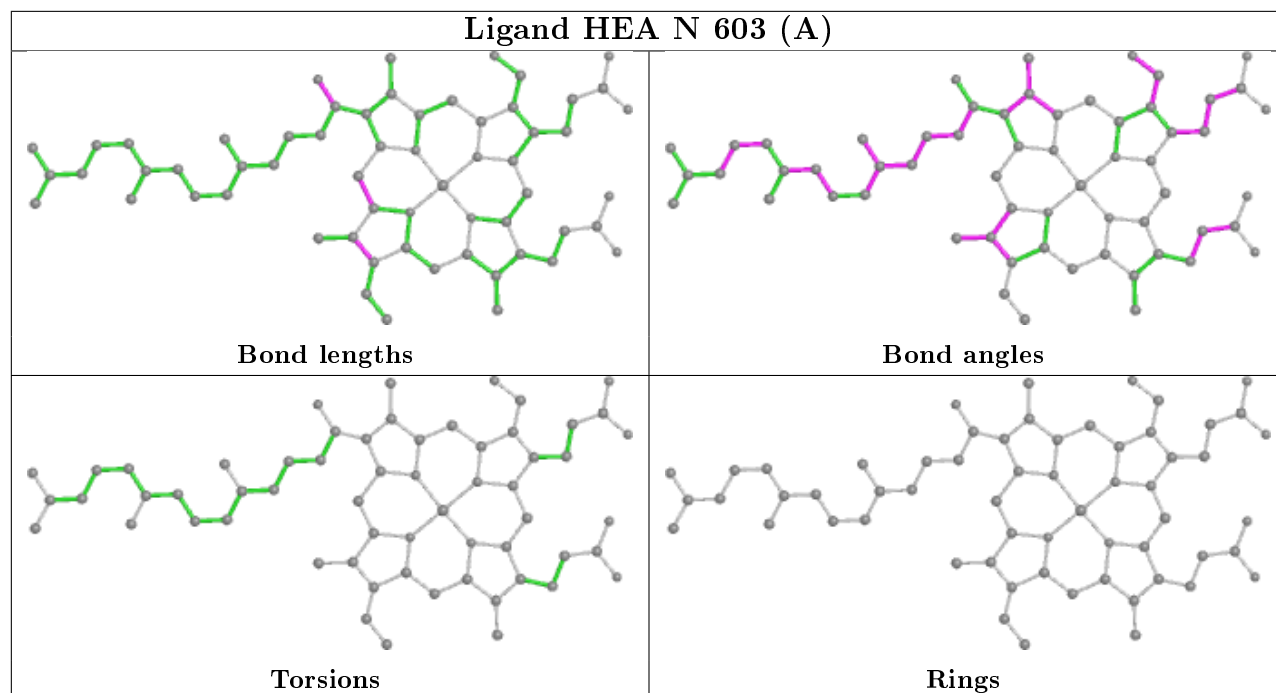
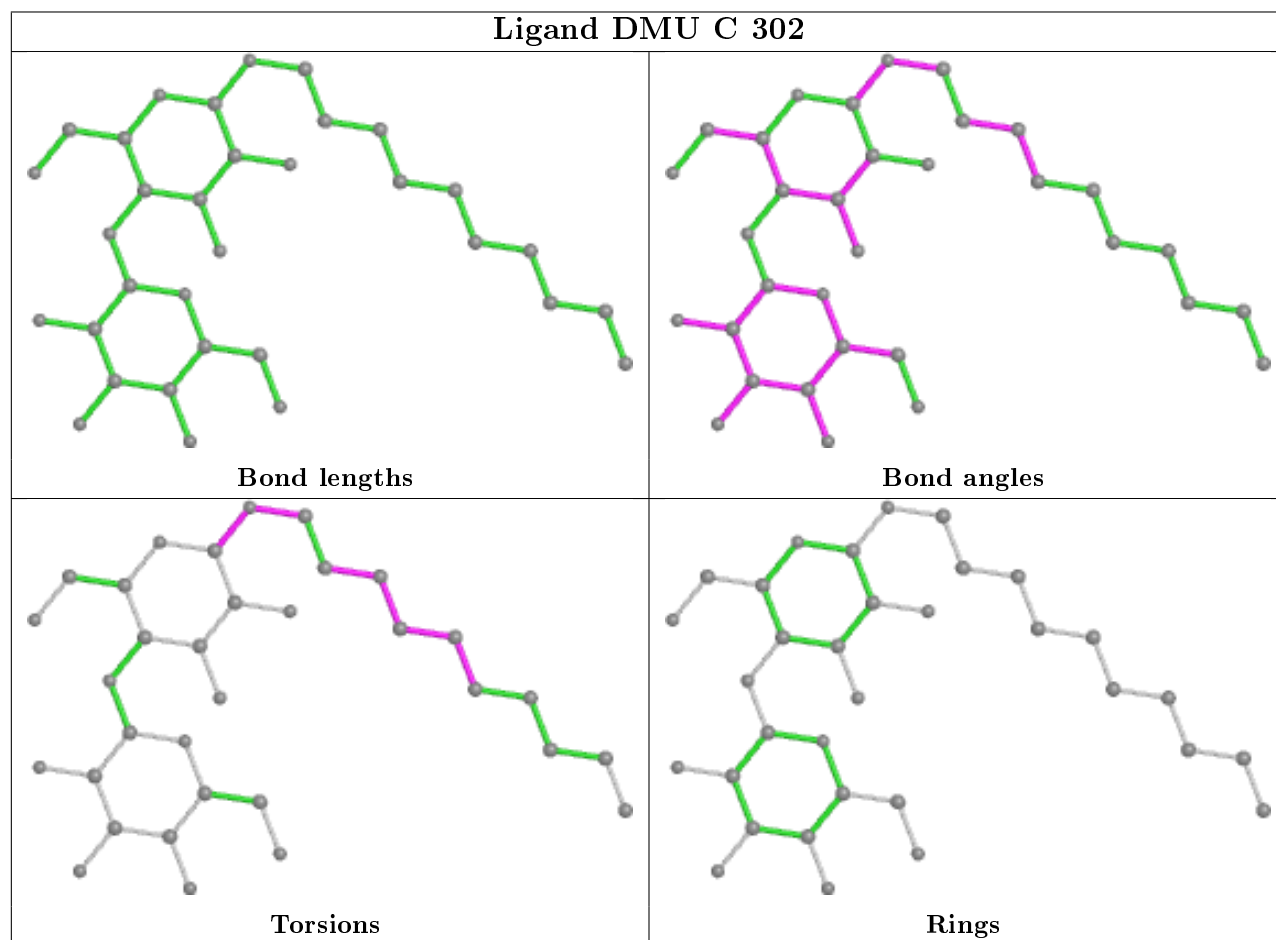
## Ligand PSC O 302

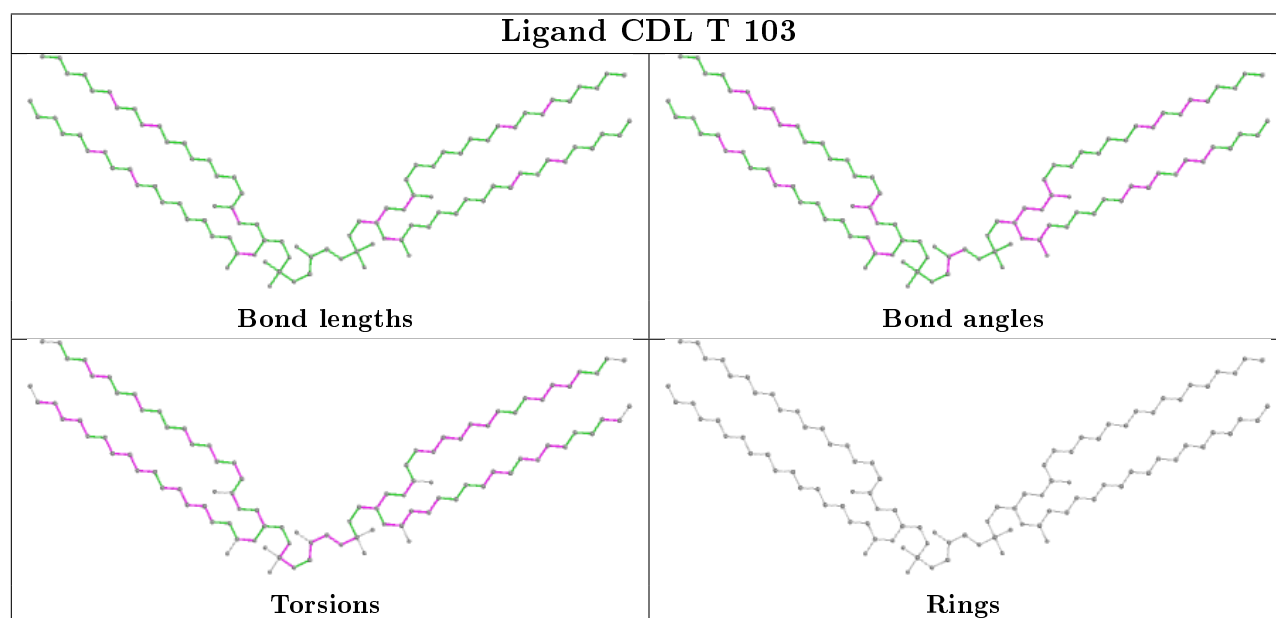
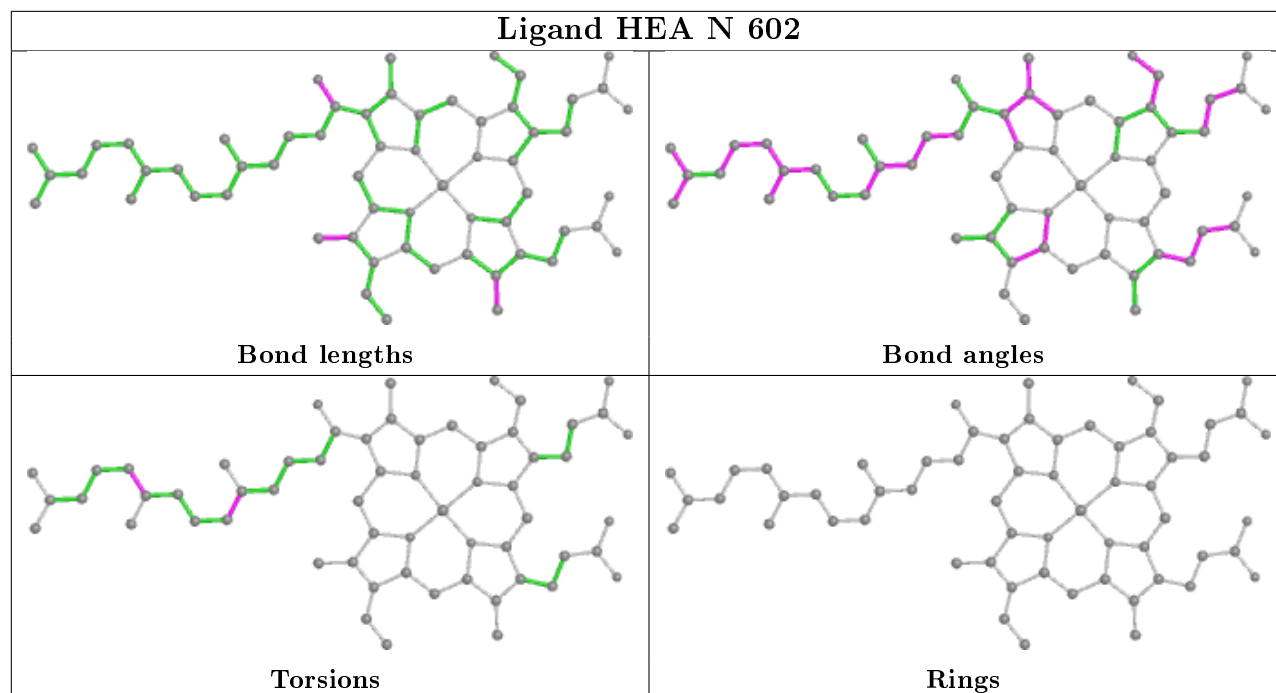


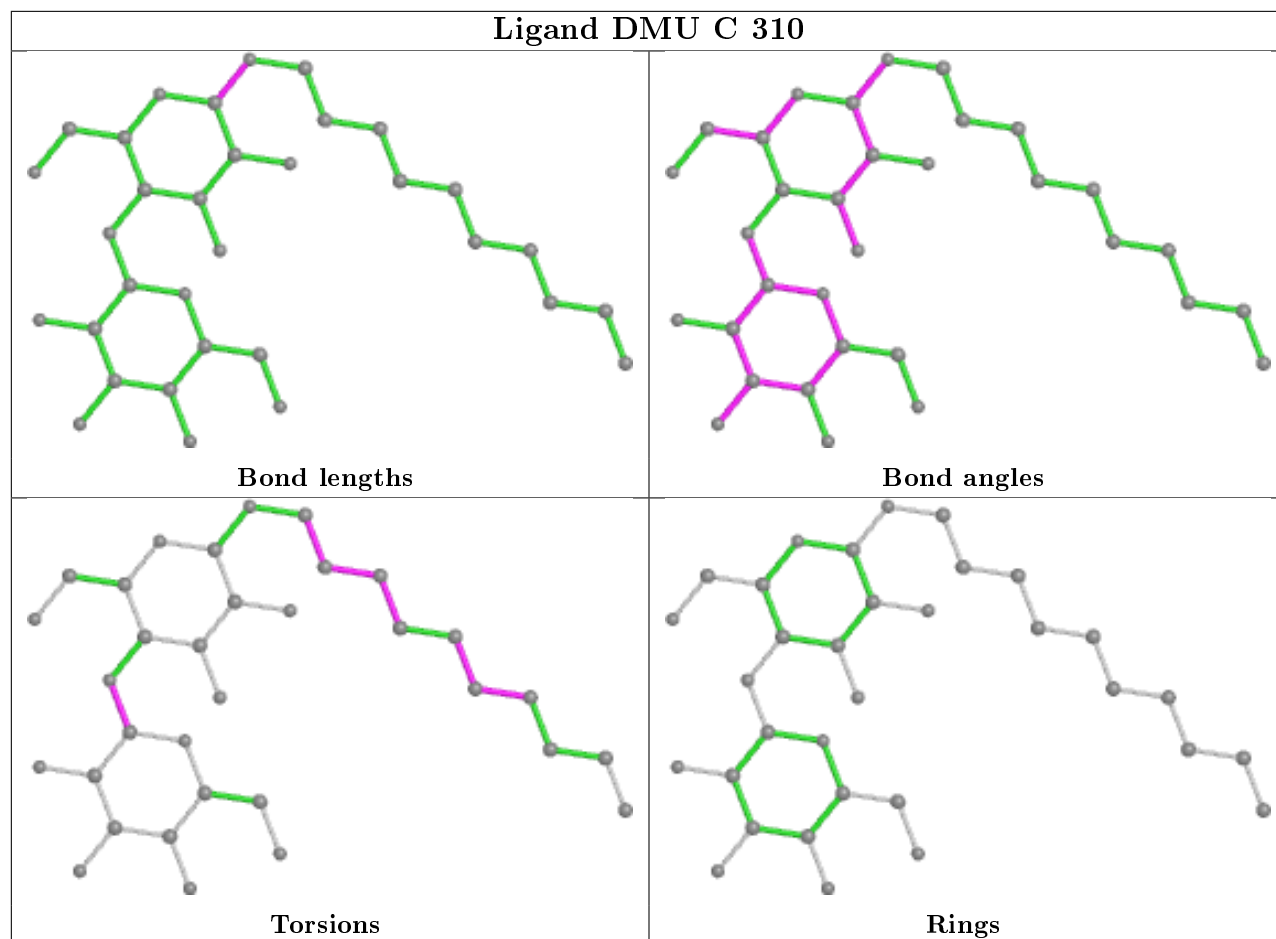
## Ligand CHD J 101

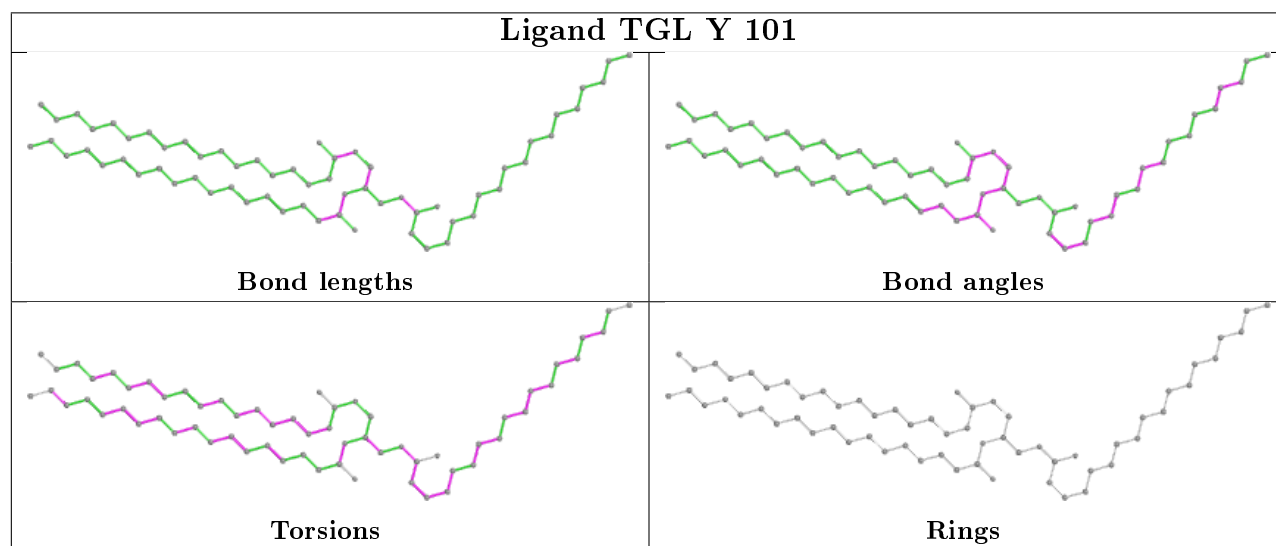
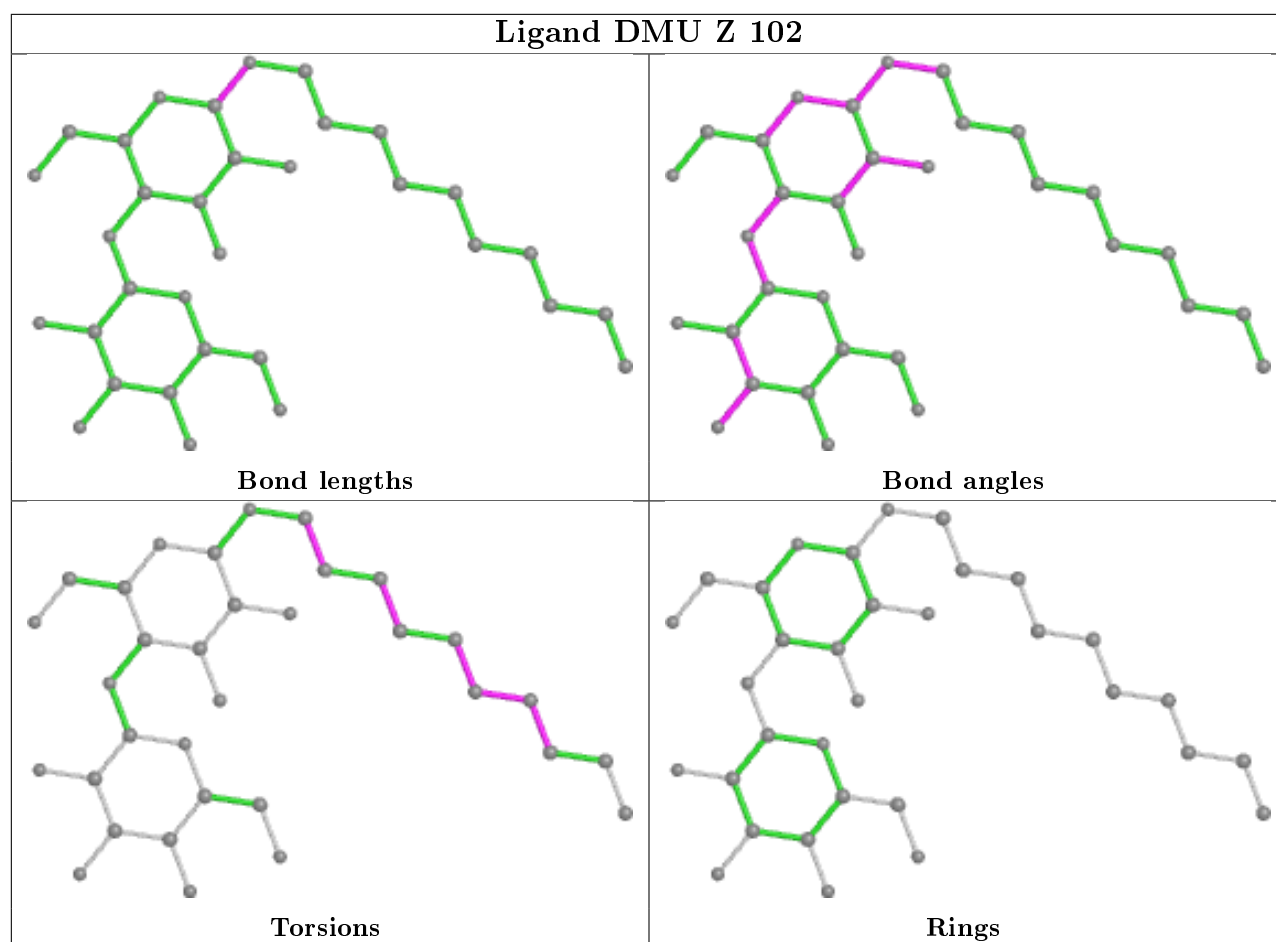


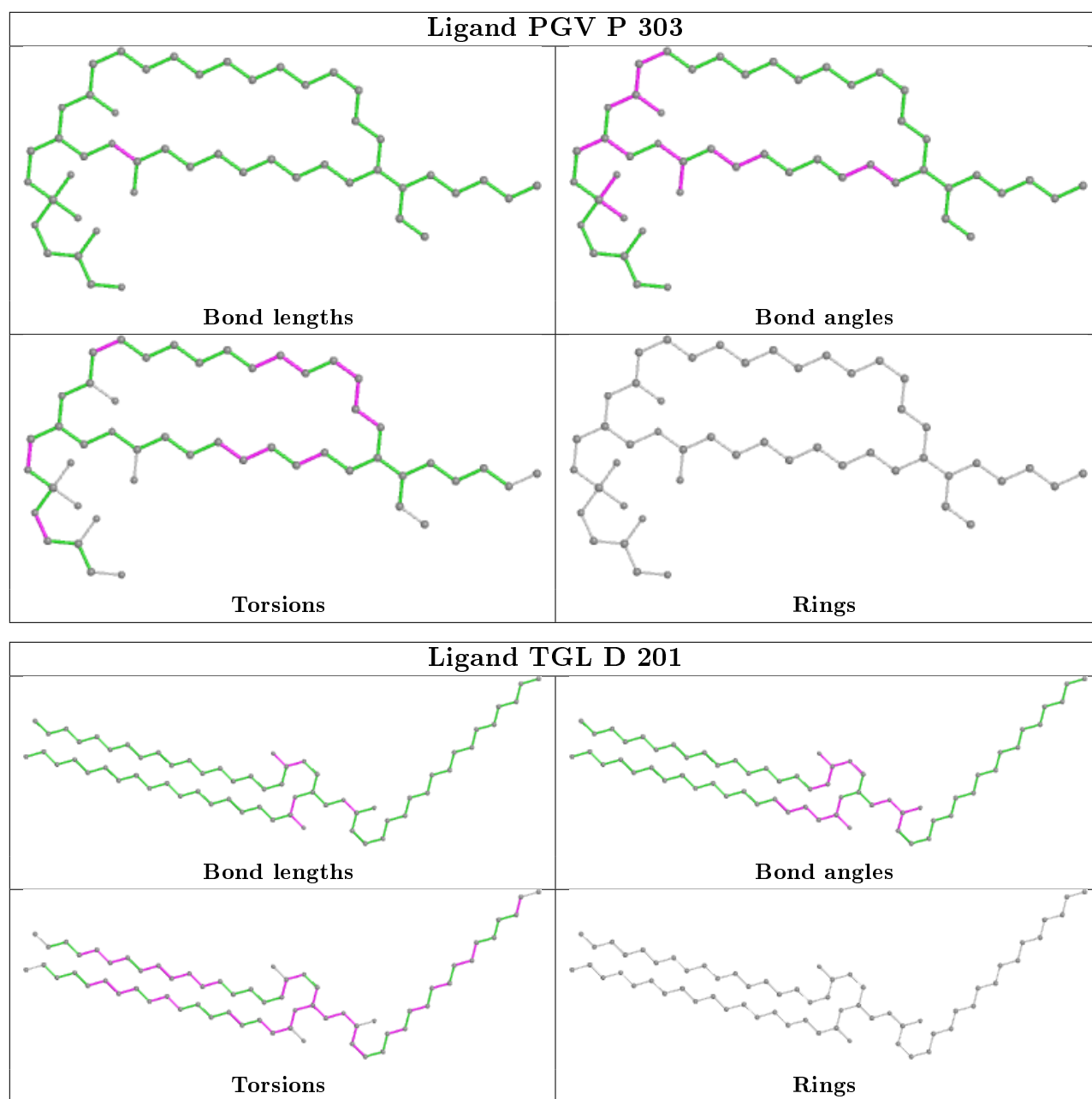


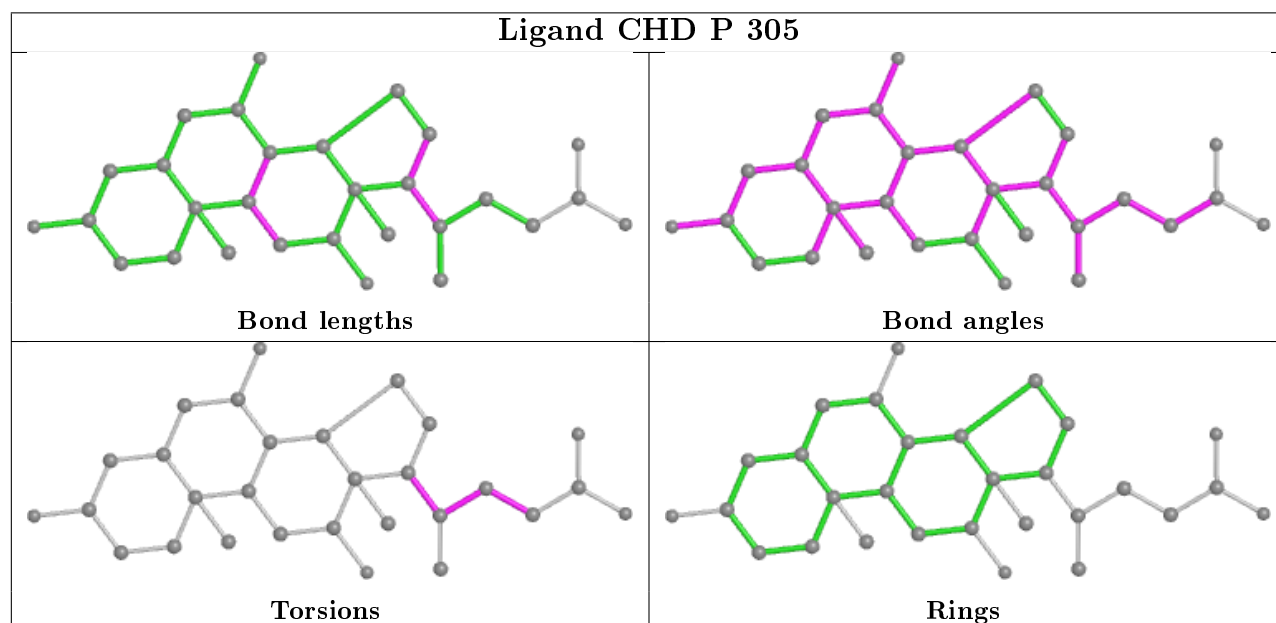
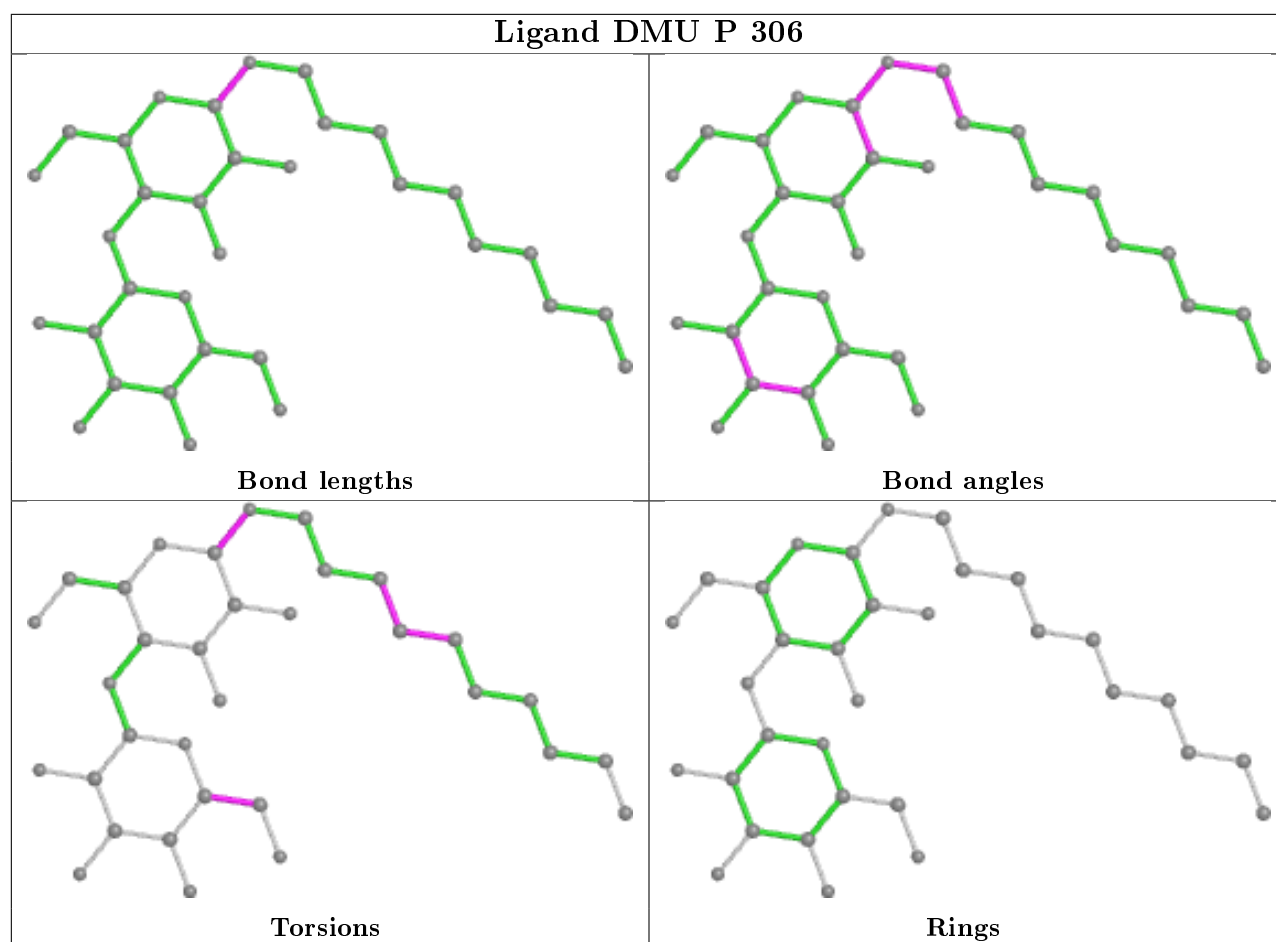
**Ligand HEA N 603 (A)****Ligand DMU C 302**

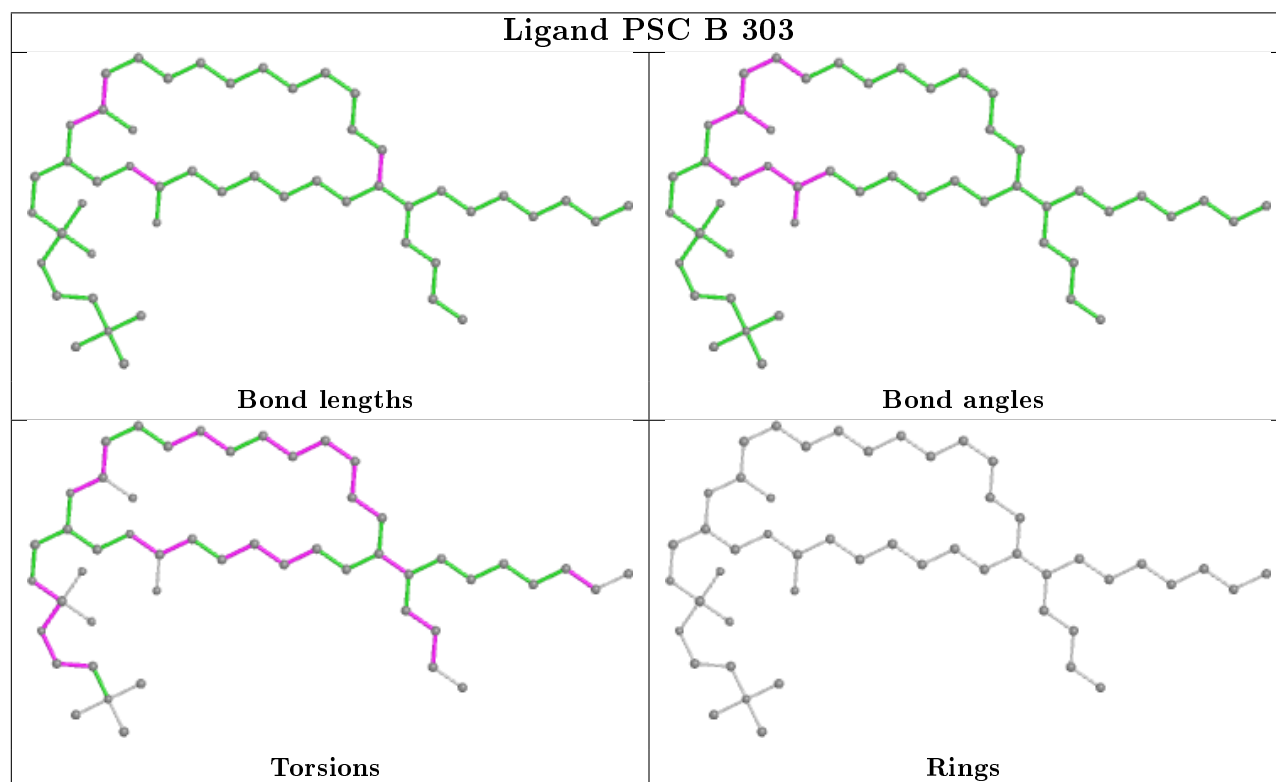
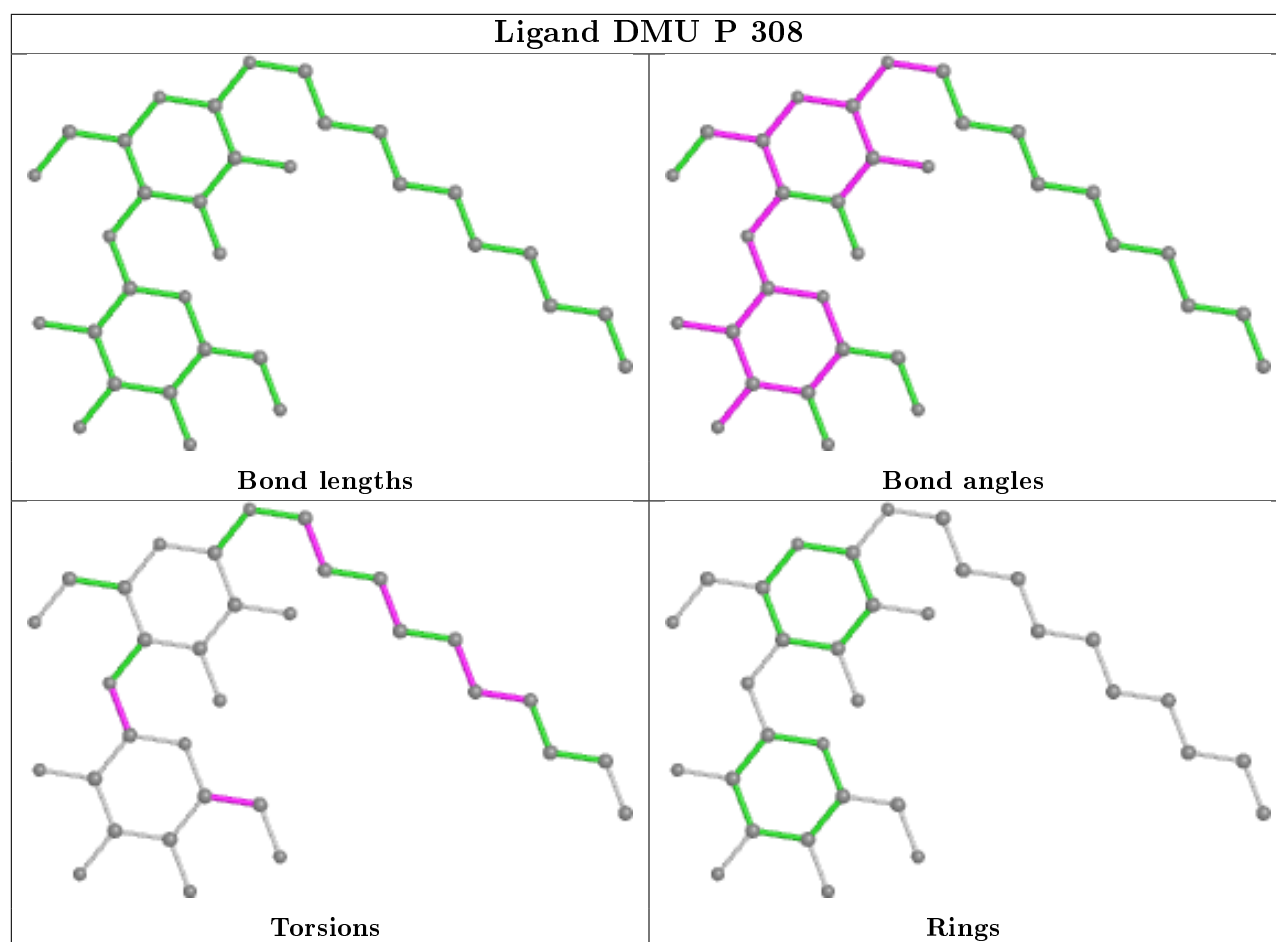


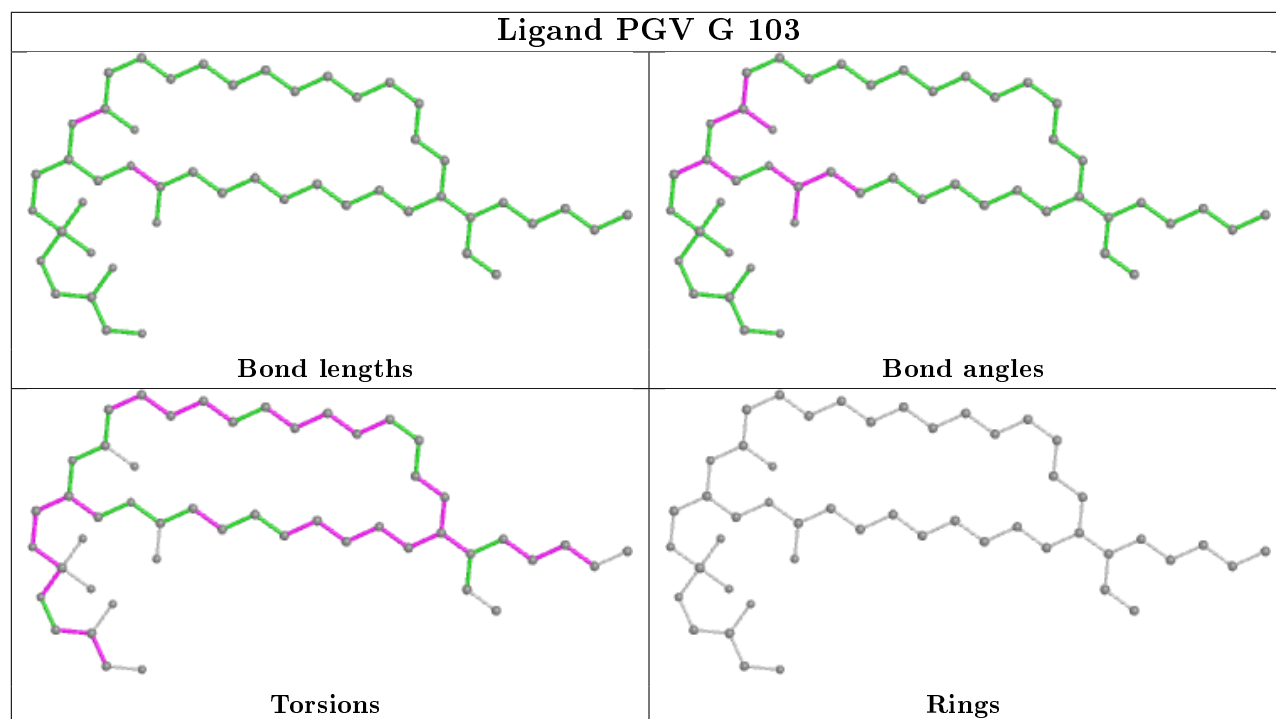
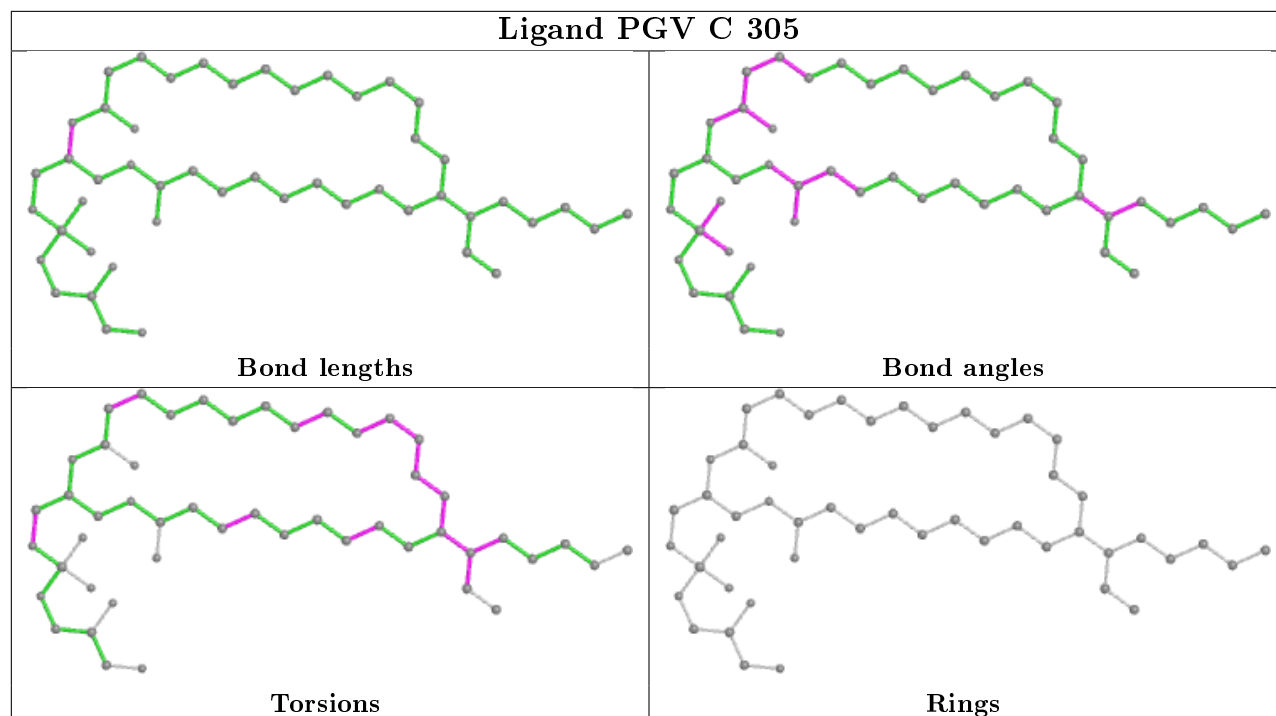




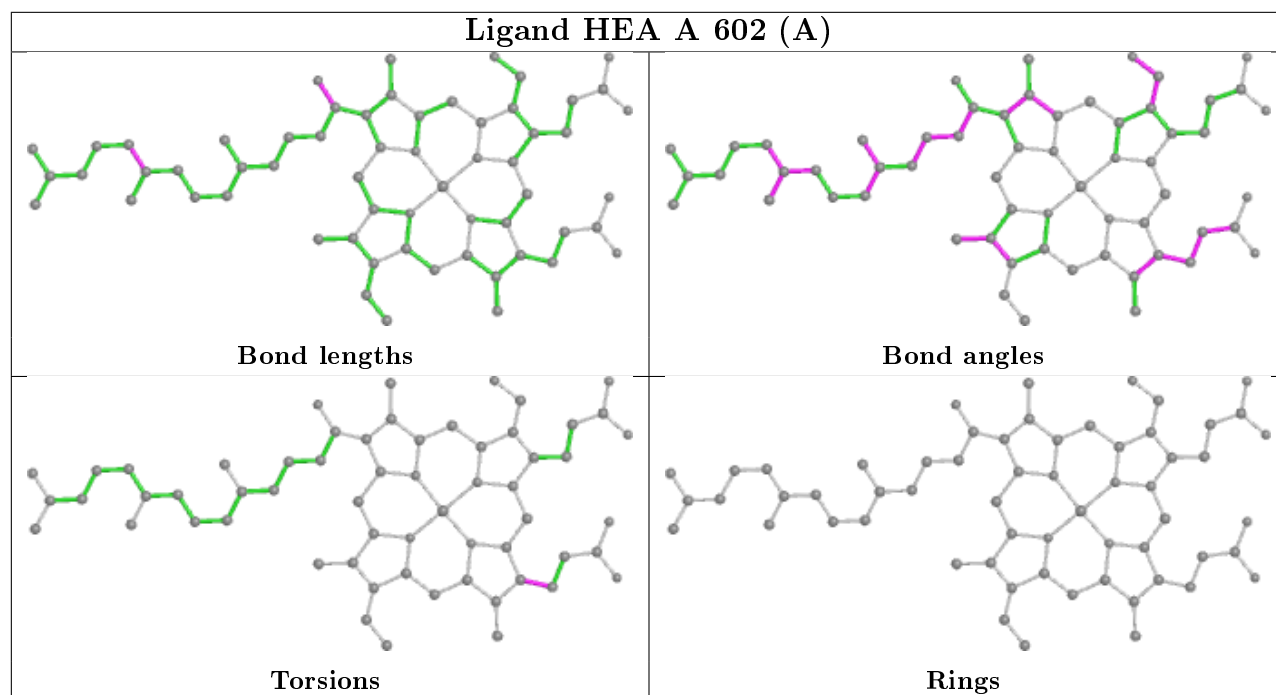
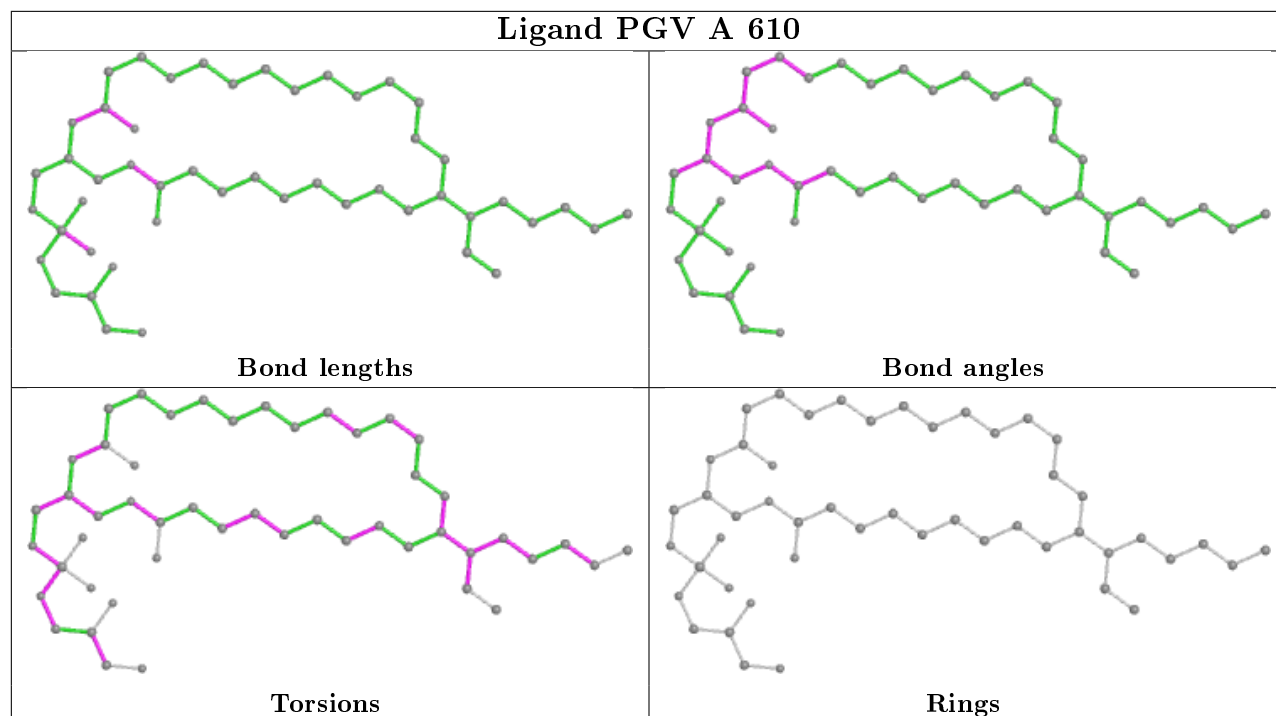


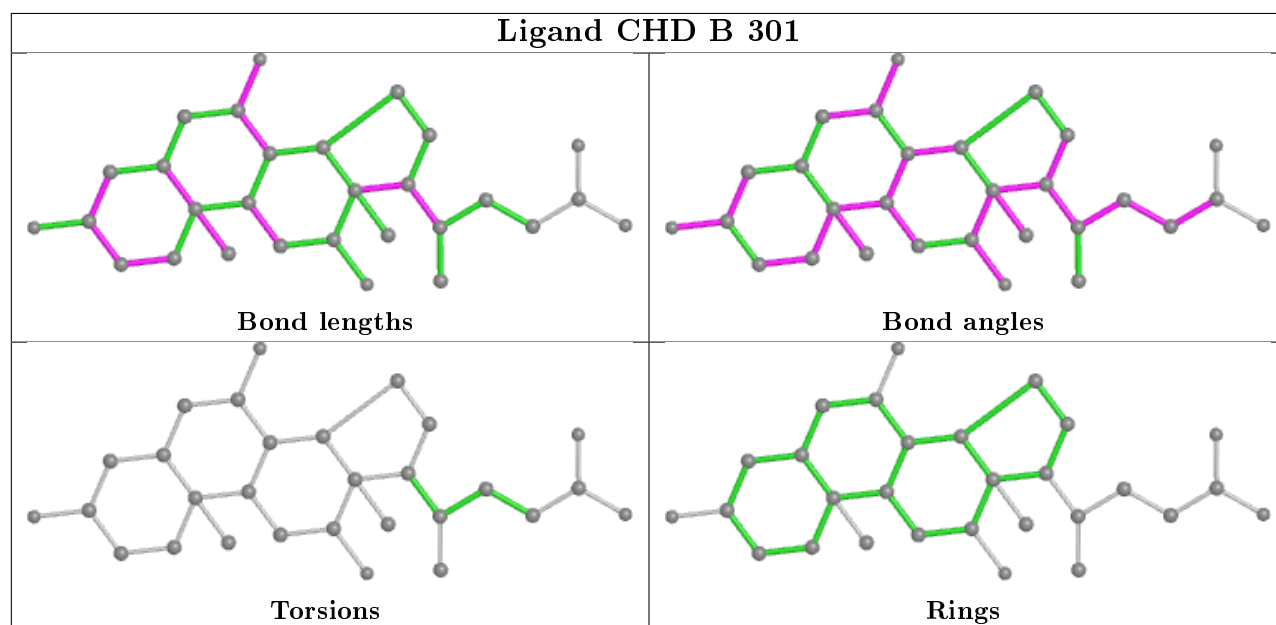
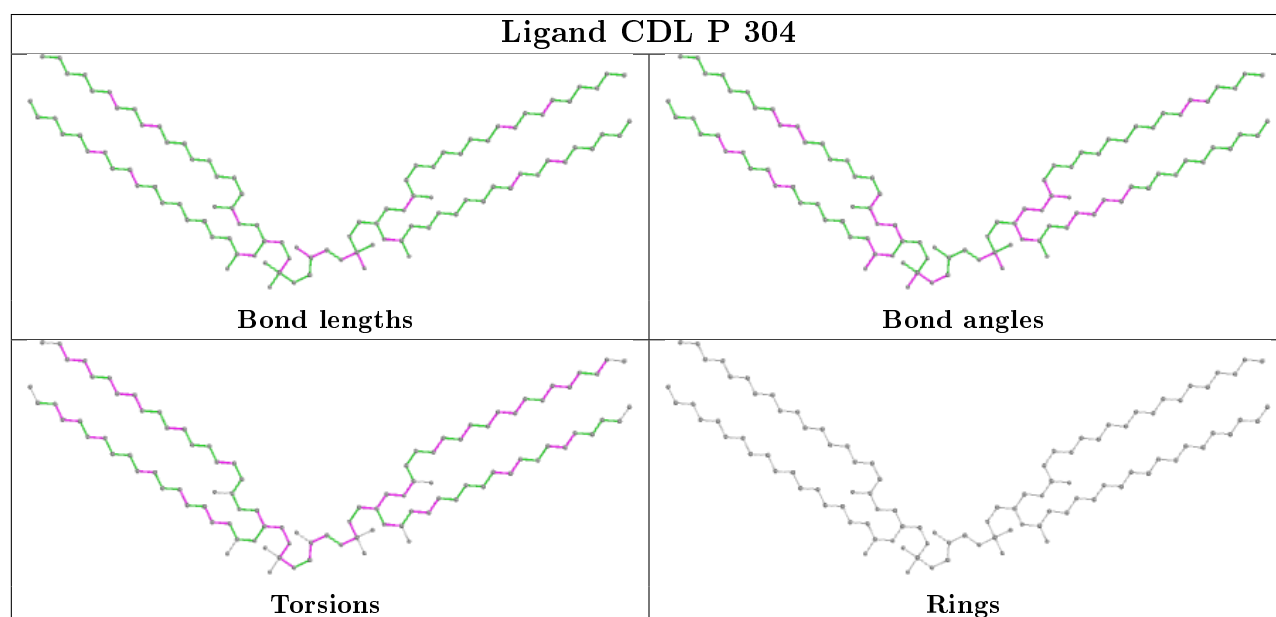
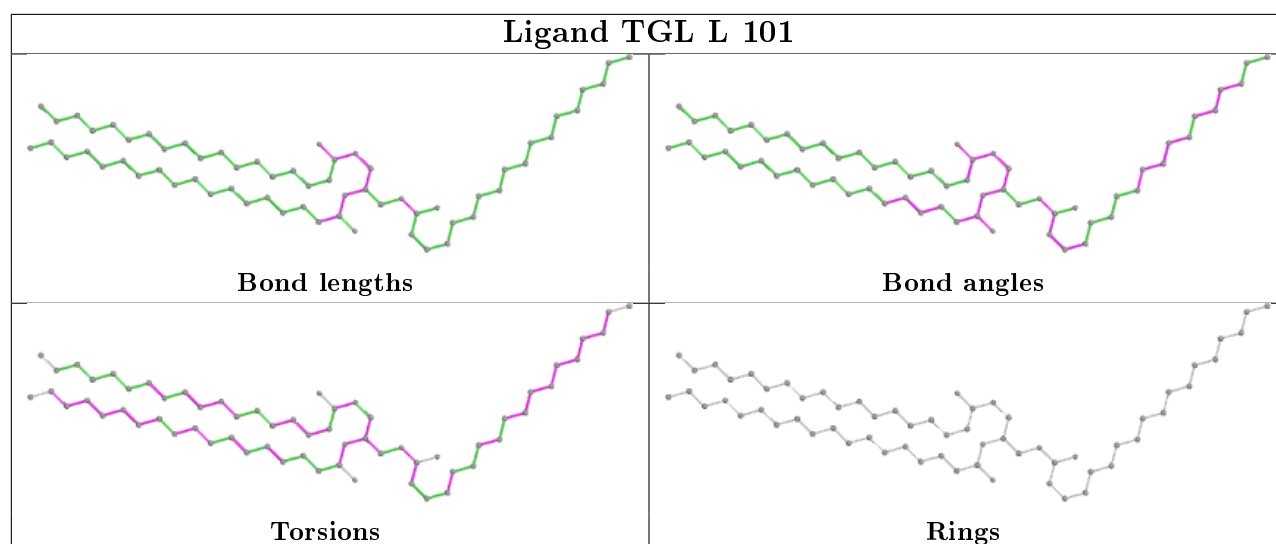


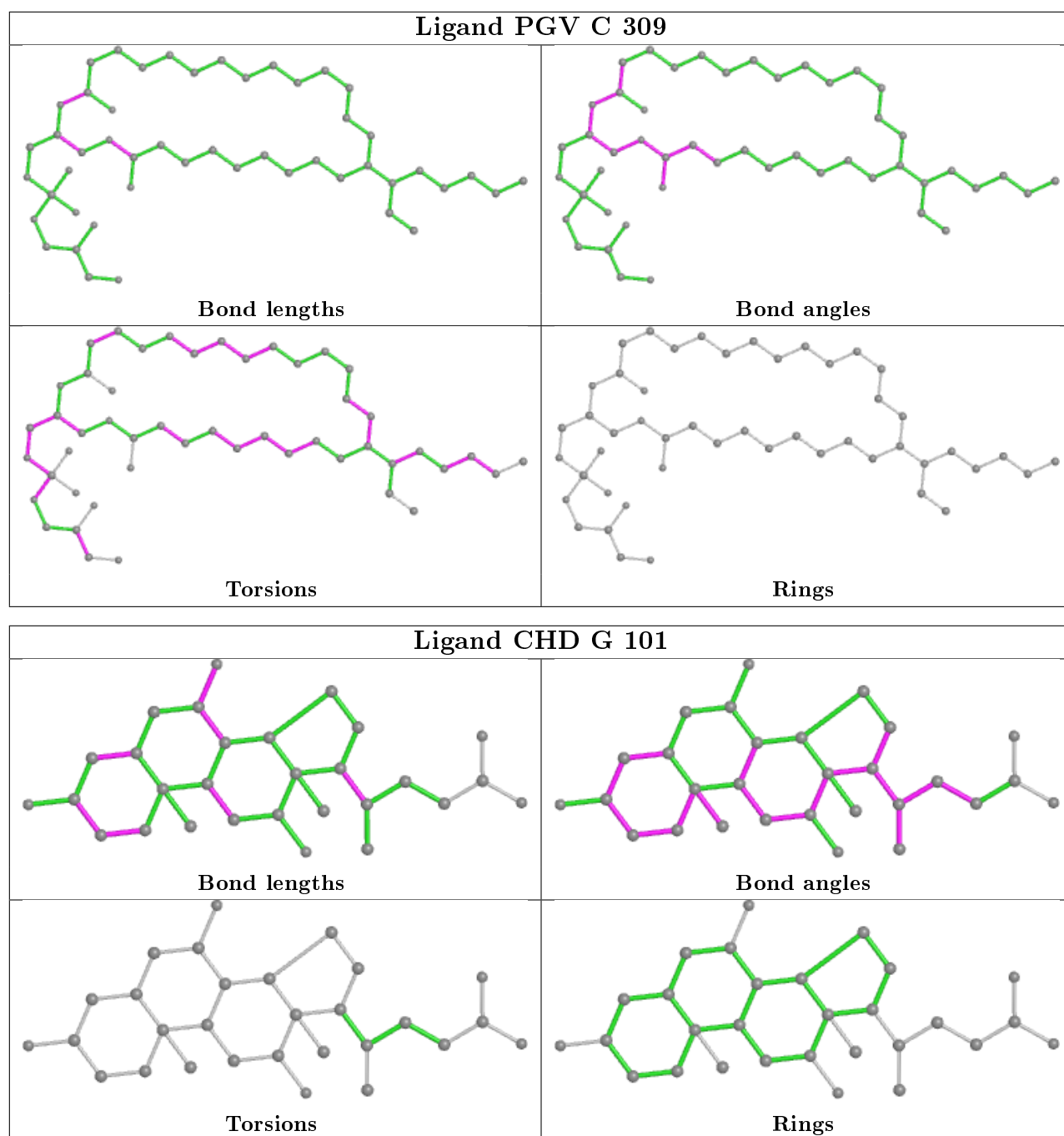


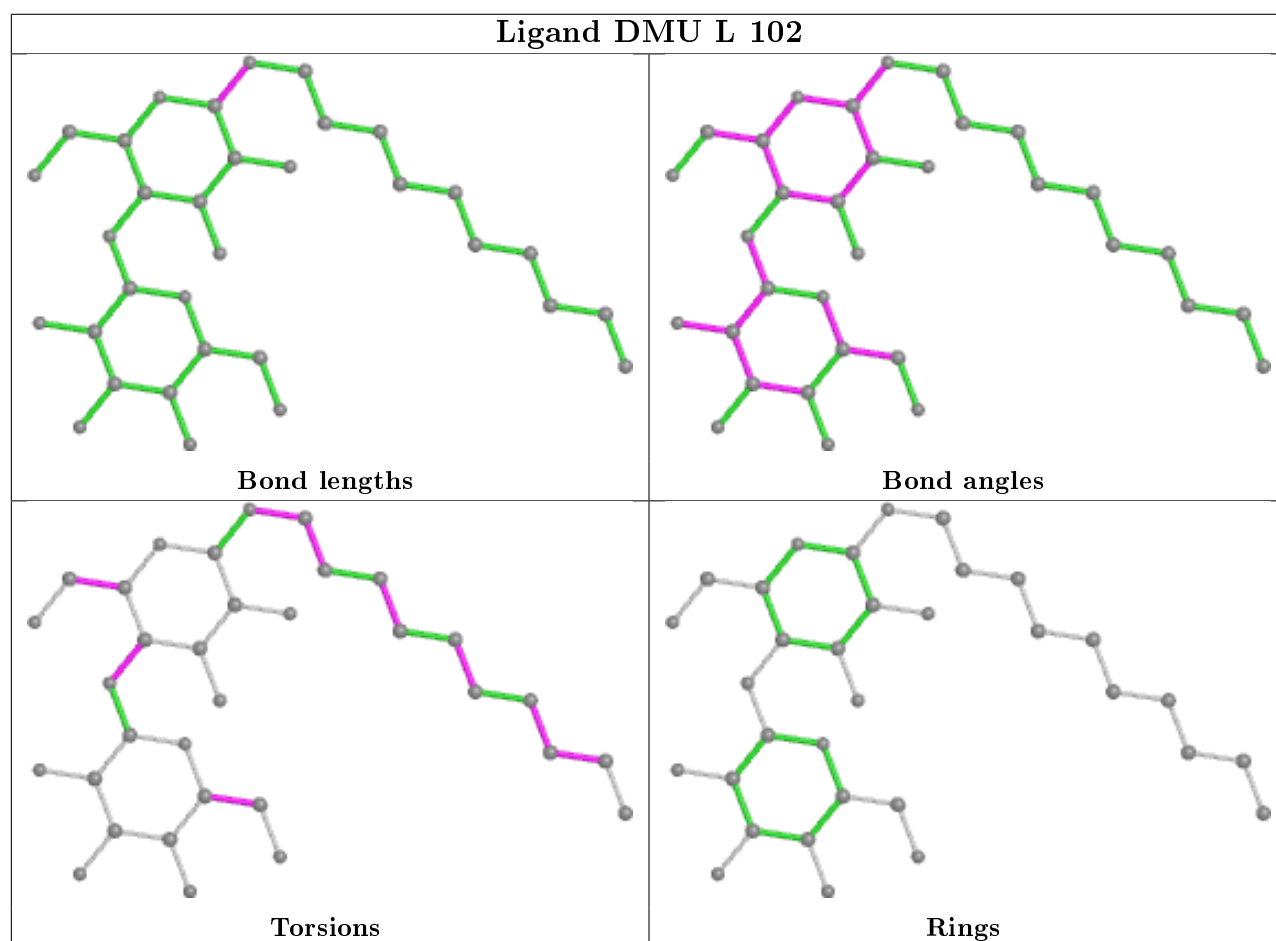
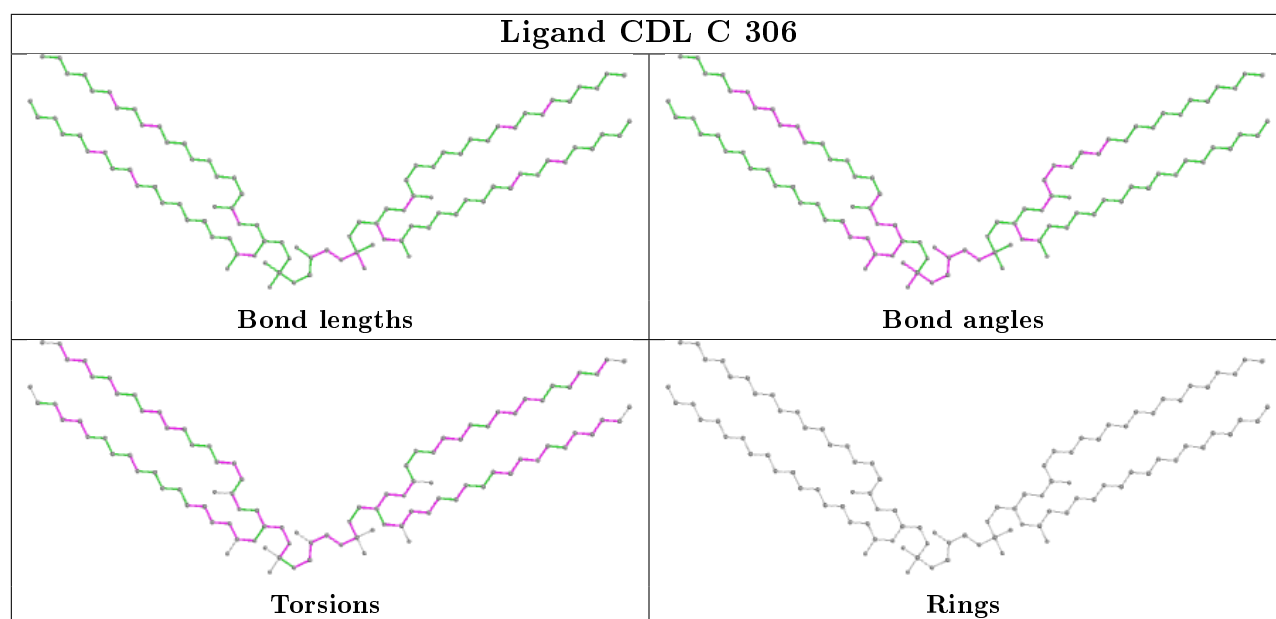


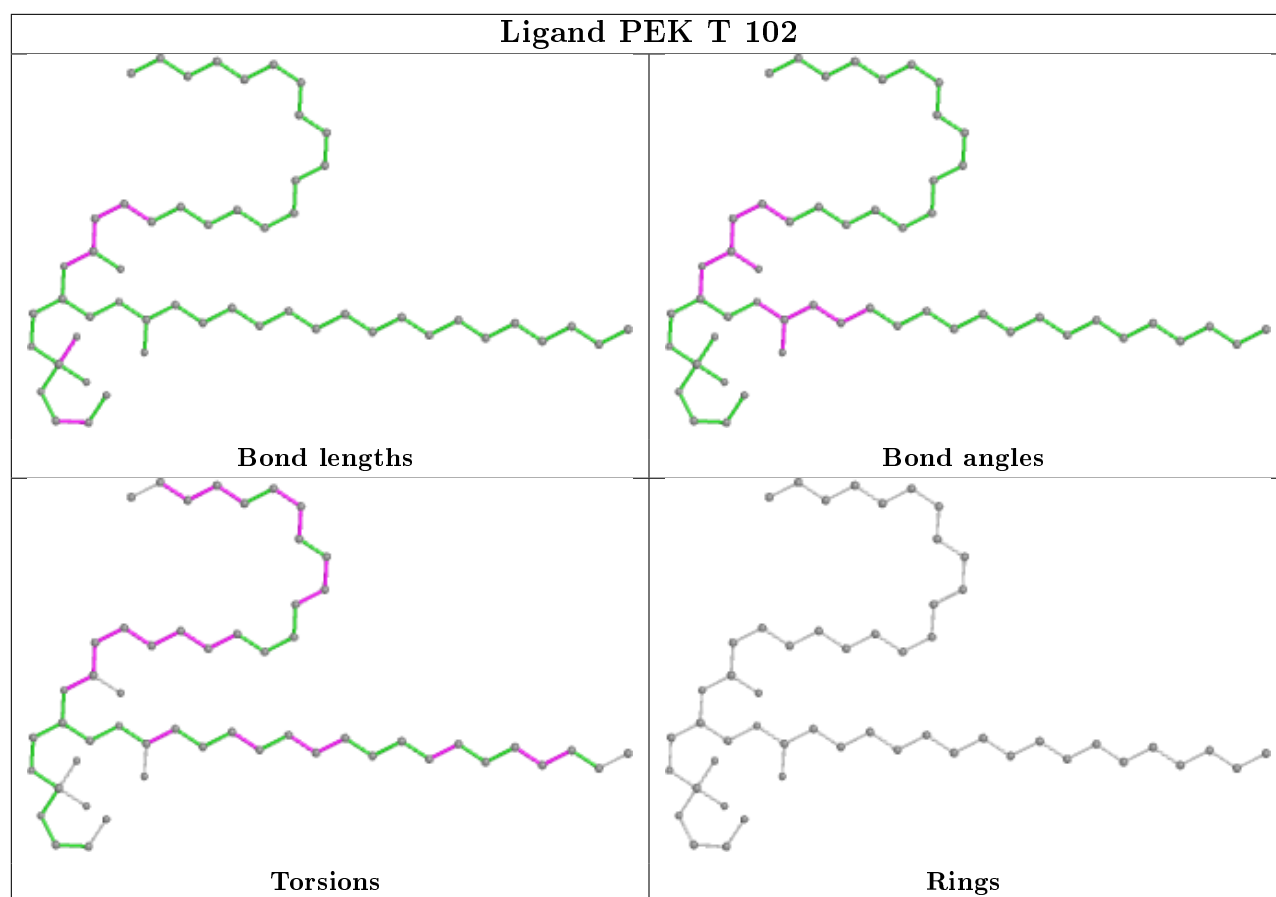


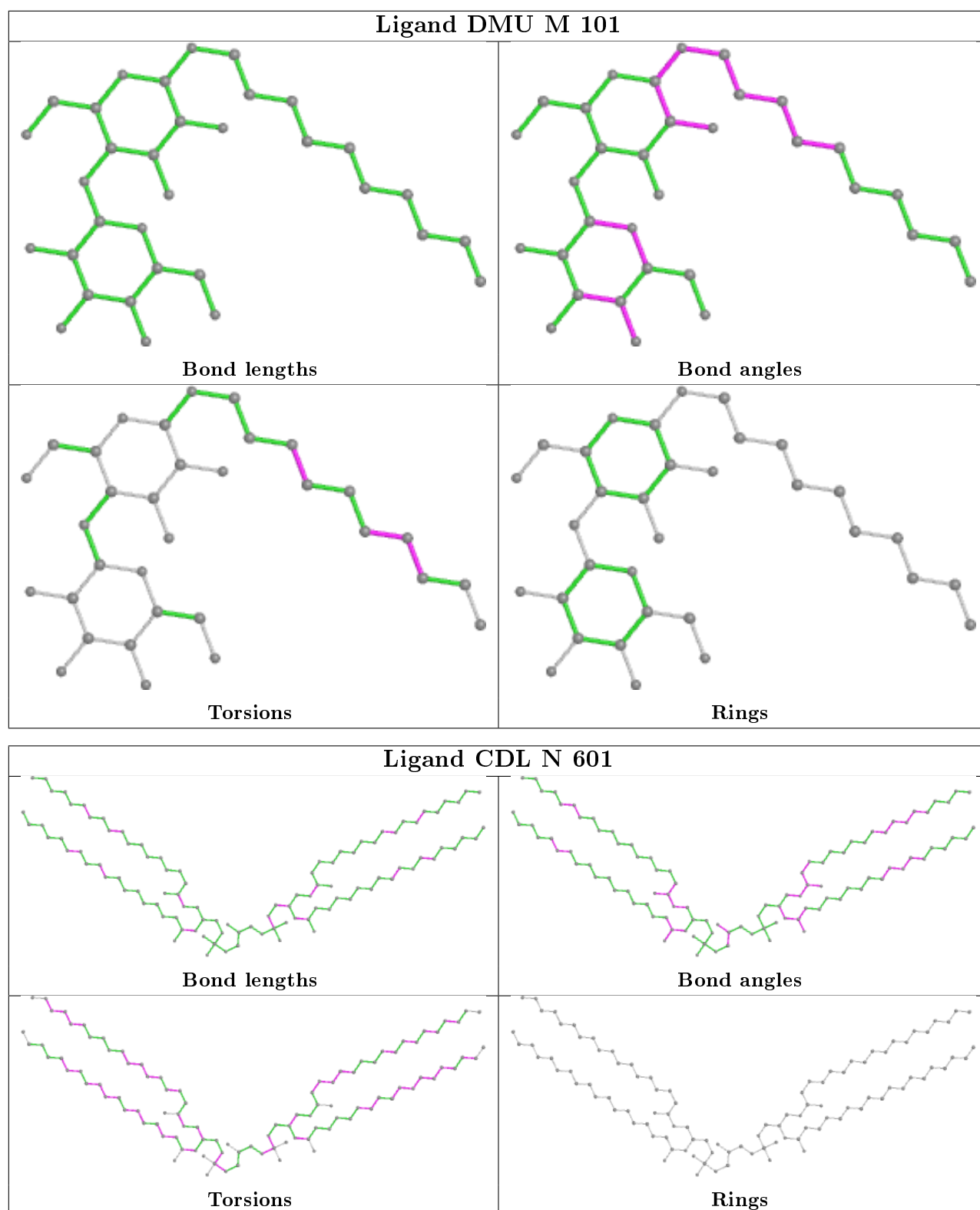












## 5.7 Other polymers ⓘ

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 94	25, 30, 38, 76	0
1	N	513/514 (99%)	-0.02	1 (0%) 95 94	27, 35, 44, 77	0
2	B	226/227 (99%)	0.10	1 (0%) 92 92	28, 38, 57, 78	0
2	O	226/227 (99%)	0.08	3 (1%) 77 78	34, 45, 69, 89	0
3	C	259/261 (99%)	0.06	1 (0%) 92 92	26, 33, 45, 84	0
3	P	259/261 (99%)	0.02	2 (0%) 86 86	28, 35, 46, 72	0
4	D	144/147 (97%)	-0.09	1 (0%) 87 88	30, 39, 60, 82	0
4	Q	144/147 (97%)	0.51	8 (5%) 24 23	39, 53, 78, 152	0
5	E	105/109 (96%)	-0.07	2 (1%) 66 66	31, 38, 63, 113	0
5	R	105/109 (96%)	-0.04	2 (1%) 66 66	38, 46, 65, 120	0
6	F	98/98 (100%)	0.54	7 (7%) 16 15	30, 41, 95, 147	0
6	S	98/98 (100%)	0.73	8 (8%) 11 11	31, 42, 104, 148	0
7	G	83/85 (97%)	0.90	15 (18%) 1 1	32, 43, 113, 127	0
7	T	83/85 (97%)	0.84	15 (18%) 1 1	31, 43, 101, 133	0
8	H	79/85 (92%)	0.30	8 (10%) 7 6	35, 45, 91, 104	0
8	U	79/85 (92%)	0.30	5 (6%) 20 19	39, 50, 102, 116	0
9	I	72/73 (98%)	0.43	5 (6%) 16 16	35, 49, 85, 92	0
9	V	72/73 (98%)	0.41	5 (6%) 16 16	36, 58, 83, 102	0
10	J	58/59 (98%)	0.37	4 (6%) 16 16	34, 44, 70, 107	0
10	W	58/59 (98%)	0.40	4 (6%) 16 16	37, 48, 72, 125	0
11	K	49/56 (87%)	0.01	1 (2%) 65 64	38, 45, 59, 65	0
11	X	49/56 (87%)	0.34	4 (8%) 11 11	48, 55, 77, 82	0
12	L	46/47 (97%)	0.07	1 (2%) 62 61	31, 37, 56, 86	0
12	Y	46/47 (97%)	0.12	1 (2%) 62 61	38, 45, 68, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.28	4 (9%) 8 8	32, 36, 71, 103	0
13	Z	43/46 (93%)	0.34	4 (9%) 8 8	43, 50, 83, 142	0
All	All	3550/3614 (98%)	0.18	113 (3%) 47 45	25, 38, 71, 152	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	22.1
6	F	98	HIS	13.5
4	Q	6	VAL	12.8
4	Q	4	SER	12.6
6	F	97	ALA	12.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	TPO	G	11	11/12	0.45	0.38	92,121,130,132	0
7	TPO	T	11	11/12	0.51	0.31	109,118,139,142	0
9	SAC	V	1	9/10	0.68	0.22	101,116,124,132	0
9	SAC	I	1	9/10	0.85	0.24	70,80,87,89	0
1	FME	N	1	10/11	0.96	0.13	47,56,74,79	0
1	FME	A	1	10/11	0.97	0.14	41,50,81,95	0
2	FME	B	1	10/11	0.98	0.13	33,35,45,66	0
2	FME	O	1	10/11	0.98	0.13	41,42,54,65	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	EDO	C	319	4/4	0.20	0.85	81,98,105,107	0
21	EDO	Q	203	4/4	0.47	0.23	81,81,88,91	0
22	CHD	W	101	29/29	0.53	0.37	69,124,145,148	0
22	CHD	J	101	29/29	0.55	0.42	99,135,149,150	0
21	EDO	D	207	4/4	0.60	0.17	62,66,70,75	0
25	DMU	C	311	33/33	0.61	0.22	56,82,119,129	0
25	DMU	L	102	33/33	0.63	0.25	54,93,139,139	0
21	EDO	A	619	4/4	0.65	0.37	50,57,58,83	0
28	CDL	T	103	100/100	0.66	0.32	54,88,145,159	0
27	PEK	T	101	53/53	0.66	0.35	51,87,154,155	0
25	DMU	C	302	33/33	0.67	0.34	35,79,111,124	0
24	PSC	B	303	52/52	0.71	0.33	42,85,156,156	0
21	EDO	A	620	4/4	0.71	0.24	64,64,67,70	0
28	CDL	N	601	100/100	0.72	0.32	57,90,140,159	0
27	PEK	G	102	53/53	0.74	0.29	52,95,154,154	0
28	CDL	P	304	100/100	0.74	0.31	43,87,119,134	0
19	TGL	Q	201	63/63	0.74	0.21	52,76,98,109	0
21	EDO	C	318	4/4	0.74	0.35	58,86,90,94	0
27	PEK	P	307	53/53	0.75	0.25	45,78,128,145	0
21	EDO	O	305	4/4	0.76	0.12	67,74,79,79	0
27	PEK	C	308	53/53	0.76	0.24	49,80,136,148	0
25	DMU	P	306	33/33	0.77	0.29	47,79,120,123	0
21	EDO	F	105	4/4	0.77	0.22	69,74,77,78	0
21	EDO	C	313	4/4	0.78	0.14	77,84,85,95	0
24	PSC	O	302	52/52	0.78	0.33	48,84,160,160	0
20	PGV	C	309	51/51	0.78	0.20	45,78,121,151	0
20	PGV	G	103	51/51	0.79	0.25	53,83,119,139	0
21	EDO	D	203	4/4	0.80	0.44	55,61,73,93	0
21	EDO	N	611	4/4	0.81	0.17	72,73,74,76	0
21	EDO	H	102	4/4	0.81	0.14	68,73,79,94	0
28	CDL	C	306	100/100	0.81	0.28	40,80,115,128	0
25	DMU	C	310	33/33	0.81	0.26	56,82,112,121	0
19	TGL	Y	101	63/63	0.81	0.28	48,78,110,148	0
21	EDO	A	617	4/4	0.82	0.26	49,53,56,62	0
20	PGV	Z	101	51/51	0.82	0.31	51,83,138,144	0
21	EDO	G	104	4/4	0.83	0.27	56,67,71,89	0
21	EDO	R	201	4/4	0.83	0.29	57,61,66,72	0
19	TGL	L	101	63/63	0.83	0.20	36,64,99,119	0
25	DMU	P	309	33/33	0.84	0.23	65,87,106,112	0
19	TGL	N	610	63/63	0.84	0.24	52,82,110,122	0
21	EDO	D	204	4/4	0.84	0.32	65,69,81,85	0
20	PGV	A	610	51/51	0.84	0.26	36,72,112,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	DMU	P	308	33/33	0.84	0.20	55,78,101,105	0
21	EDO	C	315	4/4	0.84	0.32	60,75,77,79	0
26	UNX	C	303	1/1	0.85	0.16	28,28,28,28	0
19	TGL	D	201	63/63	0.85	0.21	37,67,90,97	0
21	EDO	L	103	4/4	0.85	0.16	71,75,76,99	0
21	EDO	P	313	4/4	0.86	0.24	54,62,70,73	0
21	EDO	U	101	4/4	0.86	0.14	66,70,70,84	0
22	CHD	P	305	29/29	0.86	0.22	53,65,71,76	0
21	EDO	C	317	4/4	0.86	0.15	68,69,71,84	0
21	EDO	E	203	4/4	0.86	0.27	50,59,66,70	0
21	EDO	A	612	4/4	0.86	0.18	52,61,65,67	0
21	EDO	C	314	4/4	0.86	0.13	60,64,67,85	0
21	EDO	A	616	4/4	0.86	0.18	46,47,50,50	0
19	TGL	A	608	63/63	0.87	0.19	43,79,109,121	0
21	EDO	A	623	4/4	0.87	0.26	55,57,62,63	0
25	DMU	Z	102	33/33	0.88	0.15	50,60,75,78	0
21	EDO	N	622	4/4	0.88	0.32	55,58,81,101	0
21	EDO	R	205	4/4	0.89	0.45	57,58,61,75	0
22	CHD	C	307	29/29	0.89	0.21	52,65,72,75	0
21	EDO	B	305	4/4	0.89	0.19	35,45,53,55	0
21	EDO	A	614	4/4	0.90	0.16	59,69,74,83	0
26	UNX	P	302	1/1	0.90	0.21	28,28,28,28	0
21	EDO	J	102	4/4	0.90	0.27	52,75,78,81	0
21	EDO	H	101	4/4	0.91	0.11	54,57,67,73	0
21	EDO	R	202	4/4	0.91	0.12	61,67,72,78	0
21	EDO	E	201	4/4	0.92	0.12	43,46,56,58	0
21	EDO	A	615	4/4	0.92	0.15	25,30,31,46	0
21	EDO	E	205	4/4	0.92	0.23	60,63,68,78	0
21	EDO	N	618	4/4	0.92	0.55	60,63,67,70	0
21	EDO	V	101	4/4	0.92	0.18	62,68,74,75	0
21	EDO	N	617	4/4	0.92	0.12	50,53,53,57	0
21	EDO	S	103	4/4	0.92	0.24	44,56,72,72	0
21	EDO	P	312	4/4	0.92	0.33	52,60,72,75	0
16	MG	N	605	1/1	0.93	0.08	35,35,35,35	0
21	EDO	P	310	4/4	0.93	0.15	36,42,48,59	0
21	EDO	A	613	4/4	0.93	0.14	35,37,39,41	0
21	EDO	O	304	4/4	0.93	0.15	63,67,67,83	0
21	EDO	A	618	4/4	0.93	0.40	43,68,78,83	0
21	EDO	N	612	4/4	0.93	0.25	36,41,53,64	0
21	EDO	D	202	4/4	0.93	0.57	44,51,52,68	0
25	DMU	M	101	33/33	0.94	0.12	43,50,62,73	0
21	EDO	R	203	4/4	0.94	0.23	53,63,69,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	EDO	R	206	4/4	0.94	0.20	47,52,58,63	0
21	EDO	N	621	4/4	0.94	0.20	48,51,51,71	0
21	EDO	N	614	4/4	0.95	0.14	56,59,66,69	0
21	EDO	D	206	4/4	0.95	0.19	54,62,67,73	0
21	EDO	F	104	4/4	0.95	0.23	50,52,62,64	0
21	EDO	F	103	4/4	0.95	0.13	40,41,42,45	0
21	EDO	A	621	4/4	0.96	0.45	38,52,62,68	0
21	EDO	E	204	4/4	0.96	0.10	43,44,47,50	0
22	CHD	C	301	29/29	0.96	0.10	30,33,37,40	0
27	PEK	T	102	53/53	0.96	0.15	34,51,84,97	0
21	EDO	N	615	4/4	0.96	0.12	38,39,43,47	0
21	EDO	T	104	4/4	0.96	0.16	39,41,42,49	0
21	EDO	N	619	4/4	0.96	0.18	50,53,59,62	0
21	EDO	Q	202	4/4	0.96	0.14	62,66,69,69	0
21	EDO	C	320	4/4	0.97	0.16	37,45,48,63	0
21	EDO	A	622	4/4	0.97	0.24	37,45,60,64	0
21	EDO	N	613	4/4	0.97	0.17	42,49,49,54	0
27	PEK	C	304	53/53	0.97	0.15	32,49,84,106	0
21	EDO	R	204	4/4	0.97	0.17	45,49,49,50	0
21	EDO	D	205	4/4	0.97	0.15	40,41,58,58	0
22	CHD	P	301	29/29	0.97	0.08	31,36,39,46	0
21	EDO	A	611	4/4	0.97	0.18	39,44,46,56	0
21	EDO	C	316	4/4	0.97	0.23	41,61,67,70	0
20	PGV	C	305	51/51	0.98	0.13	29,38,92,108	0
21	EDO	P	311	4/4	0.98	0.21	44,44,47,48	0
22	CHD	G	101	29/29	0.98	0.11	32,34,38,43	0
22	CHD	B	301	29/29	0.98	0.12	29,33,36,44	0
21	EDO	E	202	4/4	0.98	0.13	44,46,46,48	0
18	AZI	A	607	3/3	0.98	0.18	34,34,37,37	0
20	PGV	A	609	51/51	0.98	0.14	27,38,69,73	0
21	EDO	N	616	4/4	0.98	0.12	34,37,38,39	0
18	AZI	N	608	3/3	0.98	0.12	39,39,39,41	0
21	EDO	O	303	4/4	0.98	0.20	41,41,42,44	0
21	EDO	S	102	4/4	0.98	0.14	33,34,36,36	0
14	HEA	N	602	60/60	0.98	0.12	28,34,56,65	0
20	PGV	N	609	51/51	0.98	0.13	30,40,71,77	0
21	EDO	B	304	4/4	0.98	0.14	32,33,38,40	0
21	EDO	N	620	4/4	0.98	0.15	49,59,67,73	0
21	EDO	C	312	4/4	0.98	0.10	42,42,45,45	0
21	EDO	G	105	4/4	0.98	0.09	35,38,42,44	0
14	HEA	A	602[B]	60/60	0.99	0.15	21,26,35,39	60
17	NA	A	605	1/1	0.99	0.09	32,32,32,32	0

*Continued on next page...*

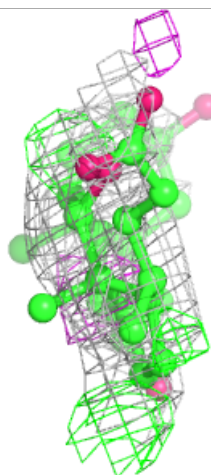
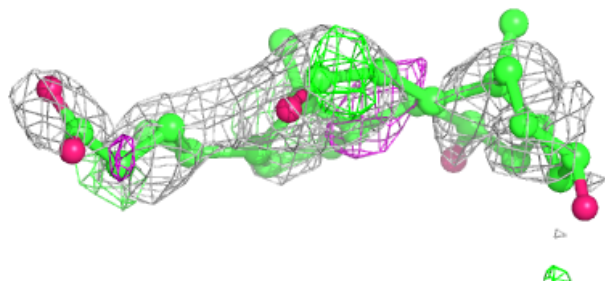
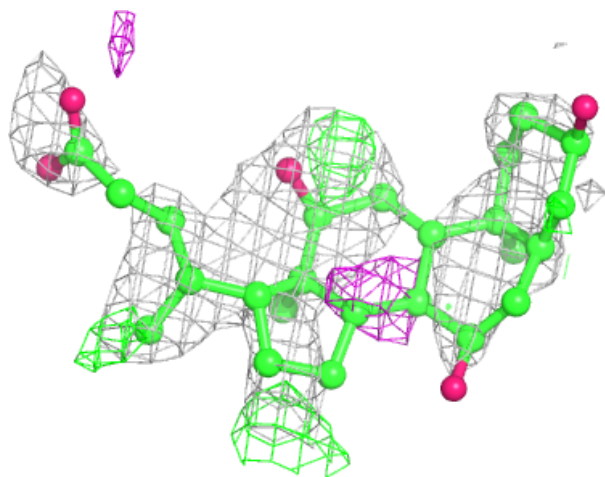
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	HEA	A	601	60/60	0.99	0.12	23,28,49,51	0
14	HEA	N	603[A]	60/60	0.99	0.14	24,27,33,35	60
18	AZI	N	607	3/3	0.99	0.12	39,39,40,42	0
18	AZI	A	606	3/3	0.99	0.16	33,33,36,36	0
16	MG	A	604	1/1	0.99	0.09	28,28,28,28	0
14	HEA	N	603[B]	60/60	0.99	0.14	26,33,45,47	60
14	HEA	A	602[A]	60/60	0.99	0.15	21,27,31,36	60
17	NA	N	606	1/1	0.99	0.06	39,39,39,39	0
20	PGV	P	303	51/51	0.99	0.14	31,40,77,86	0
23	CUA	O	301	2/2	0.99	0.16	36,36,36,36	0
21	EDO	F	102	4/4	0.99	0.10	29,31,31,33	0
29	ZN	S	101	1/1	1.00	0.14	38,38,38,38	0
15	CU	A	603	1/1	1.00	0.17	30,30,30,30	0
23	CUA	B	302	2/2	1.00	0.18	30,30,30,31	0
29	ZN	F	101	1/1	1.00	0.15	36,36,36,36	0
15	CU	N	604	1/1	1.00	0.18	33,33,33,33	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.

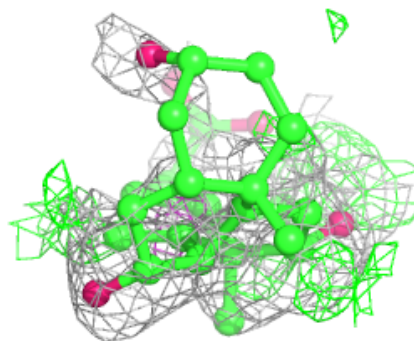
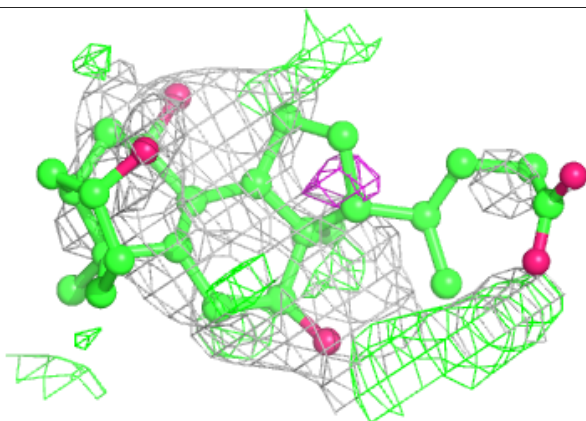
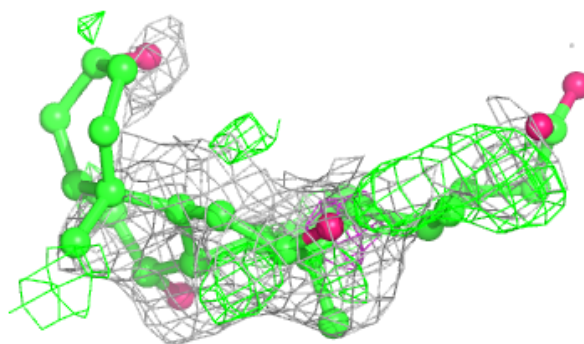
**Electron density around CHD W 101:**

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

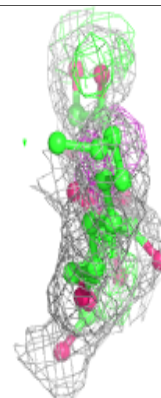
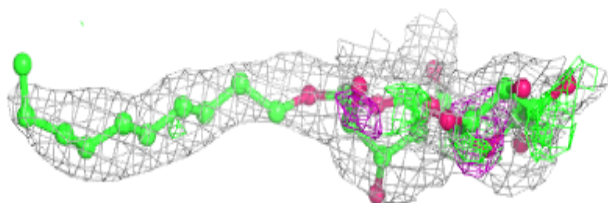
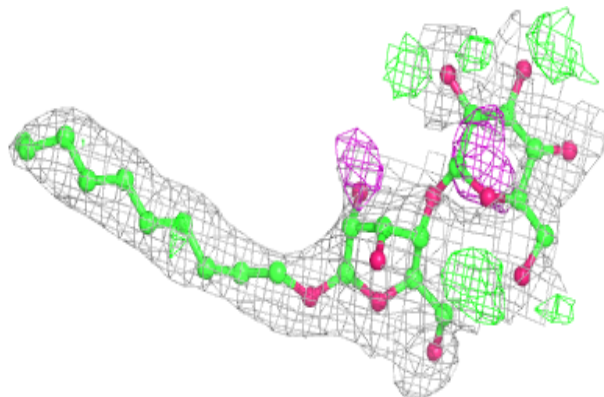


**Electron density around CHD J 101:**

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

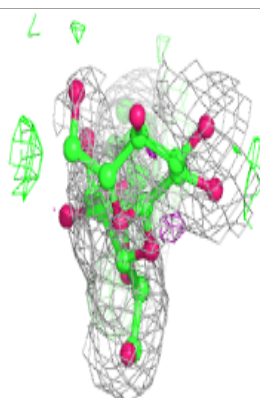
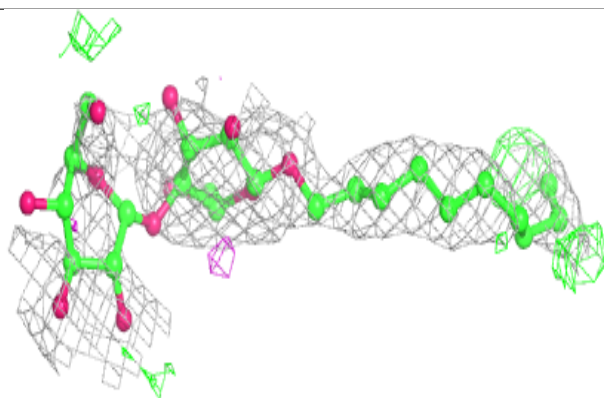
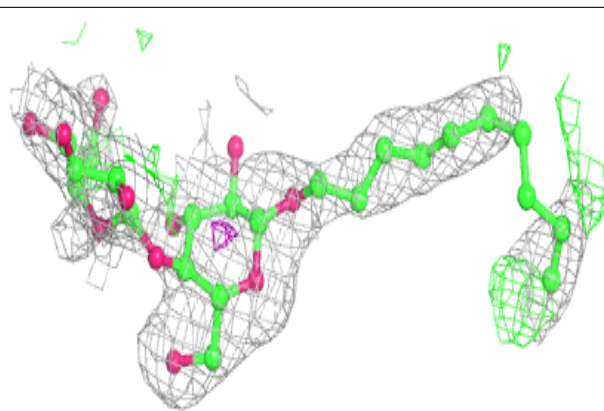
**Electron density around DMU C 311:**

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

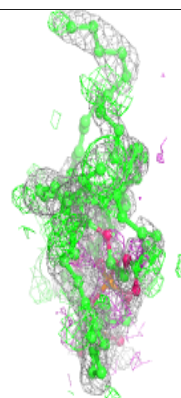
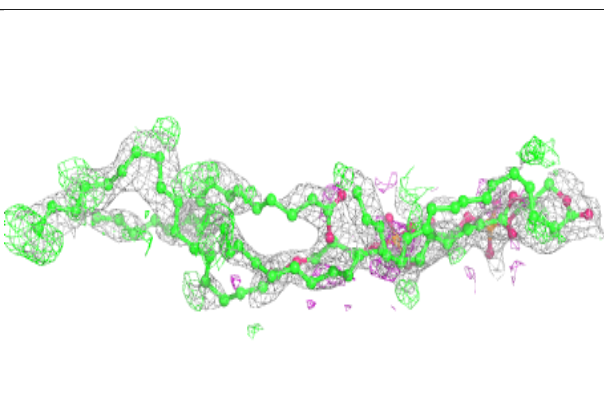
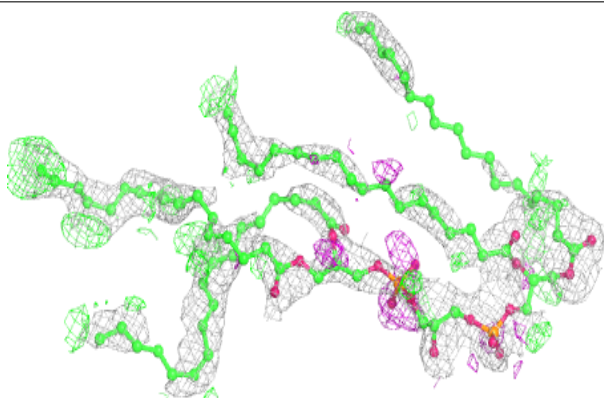


**Electron density around DMU L 102:**

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

**Electron density around CDL T 103:**

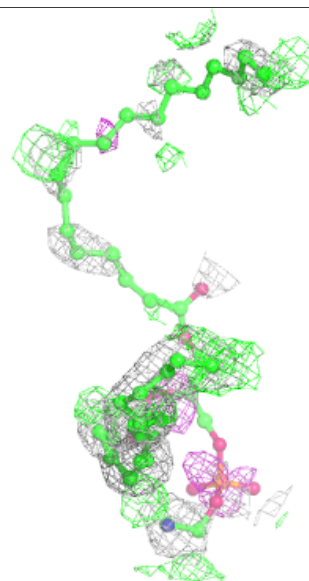
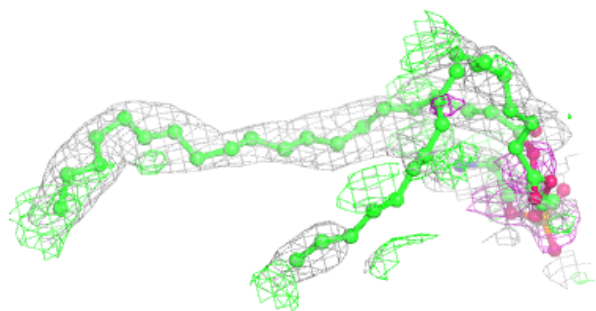
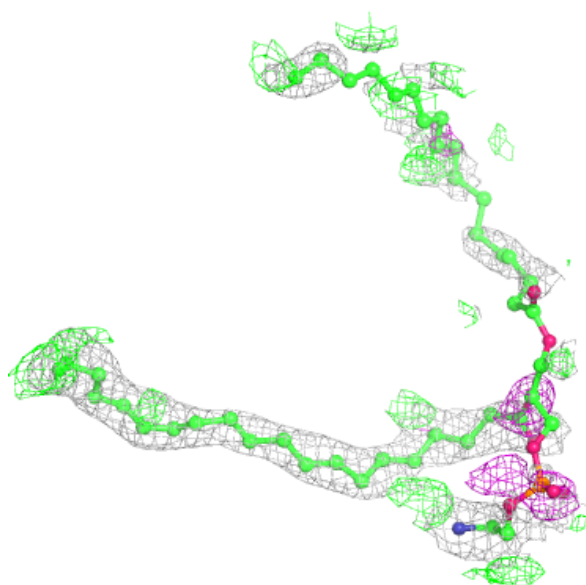
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





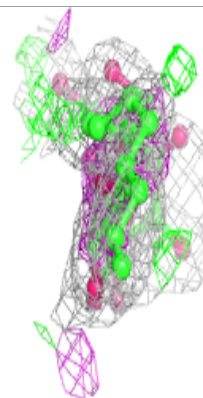
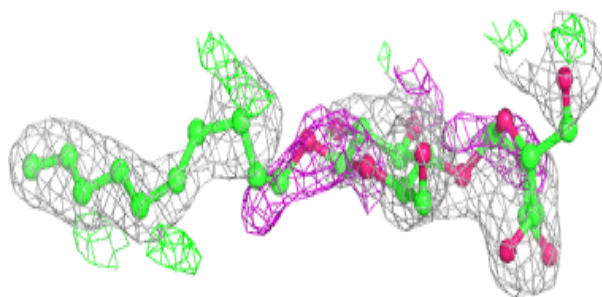
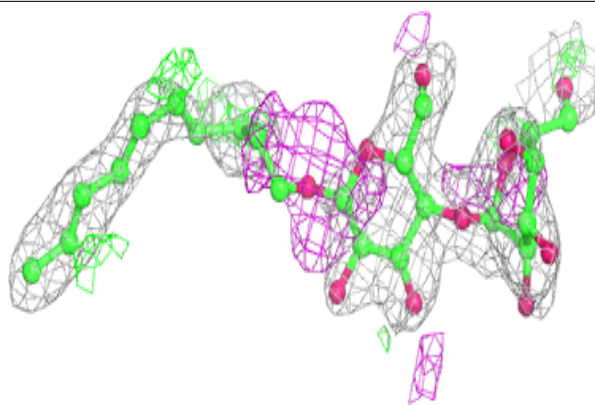
**Electron density around PEK T 101:**

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

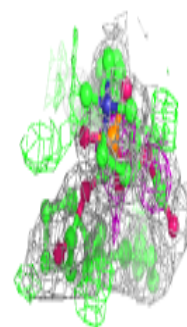
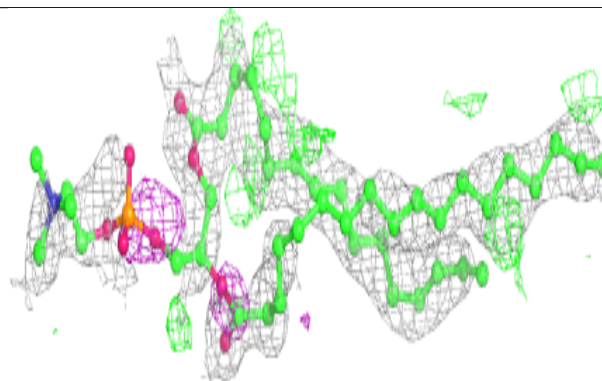
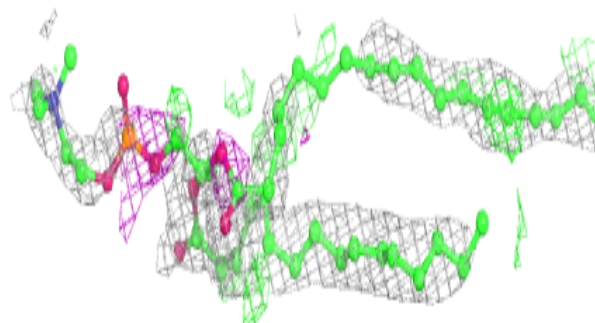


**Electron density around DMU C 302:**

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

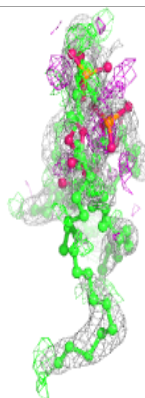
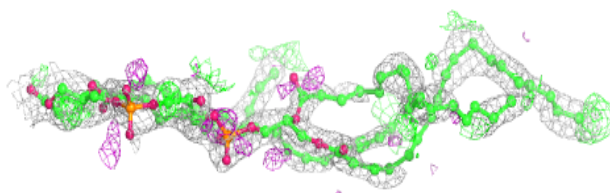
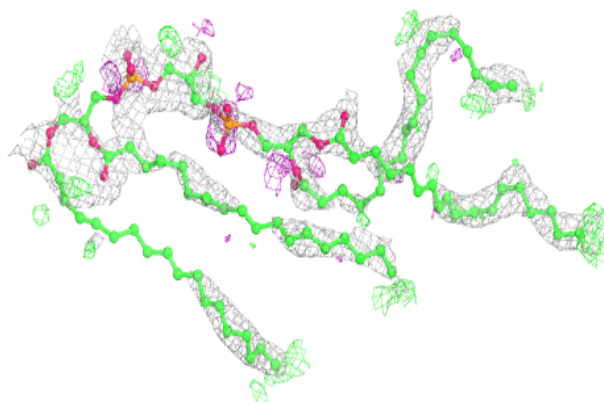
**Electron density around PSC B 303:**

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



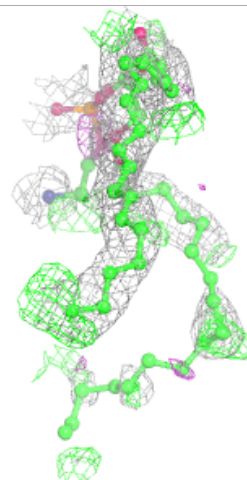
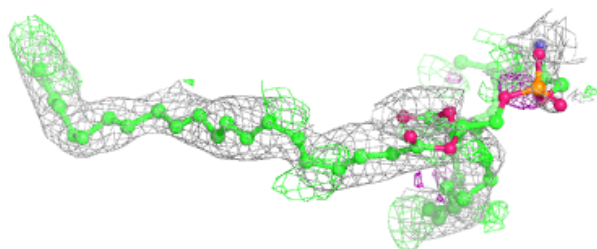
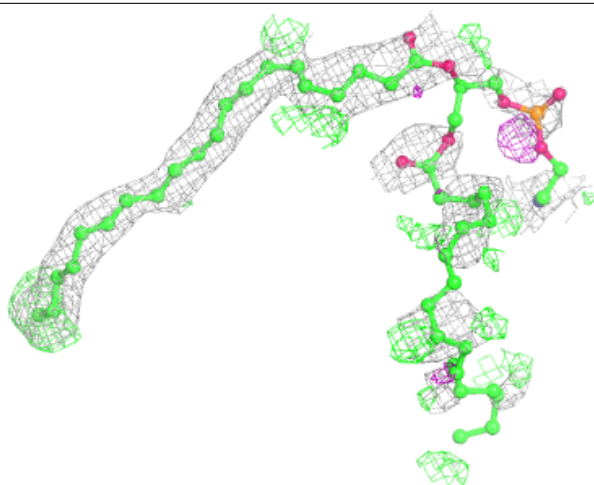
**Electron density around CDL N 601:**

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



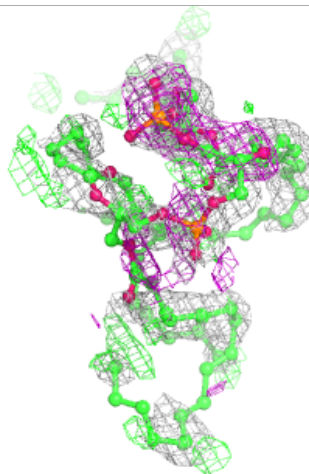
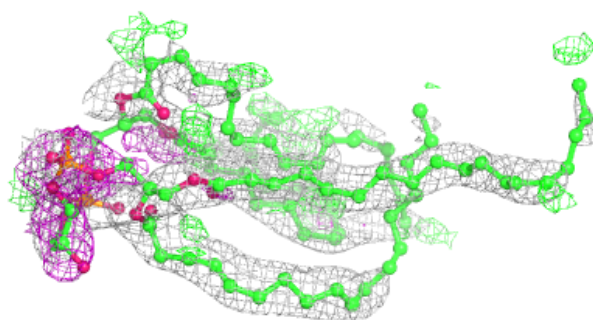
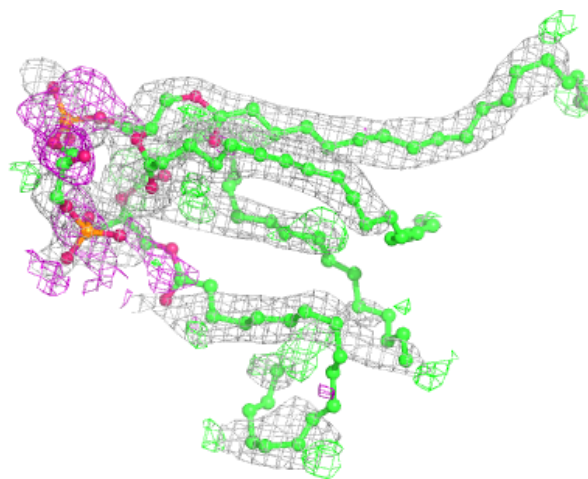
**Electron density around PEK G 102:**

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



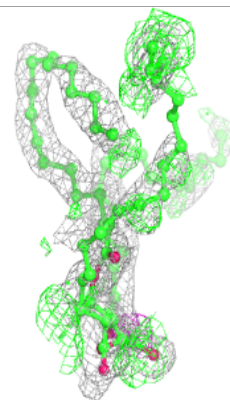
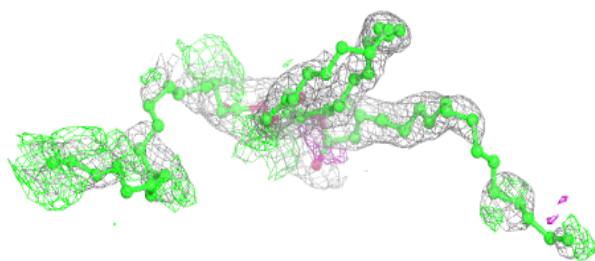
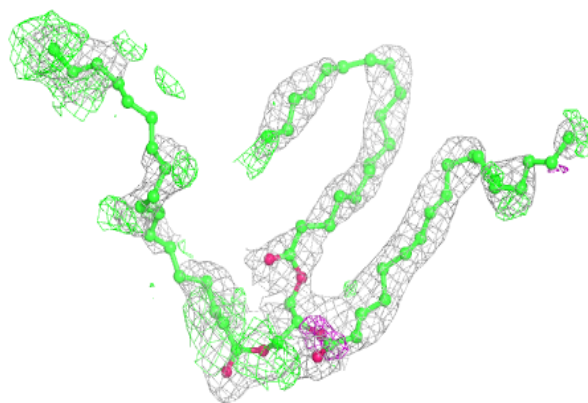
**Electron density around CDL P 304:**

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

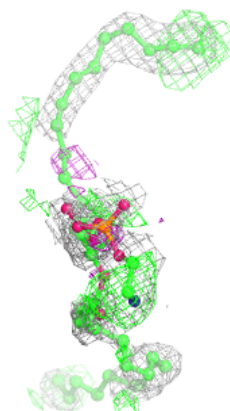
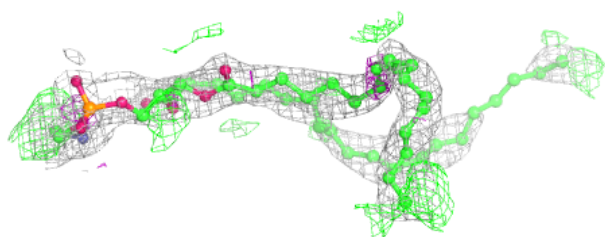
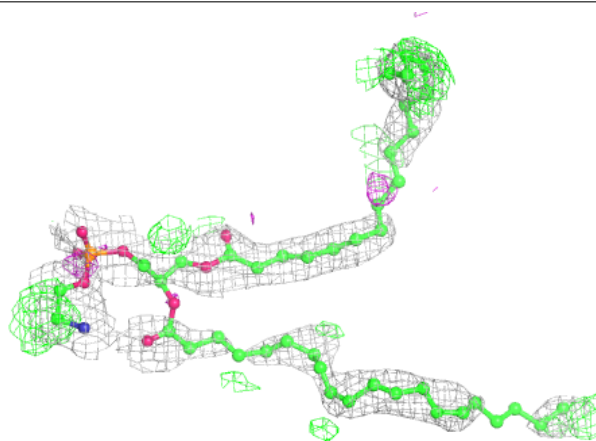


**Electron density around TGL Q 201:**

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

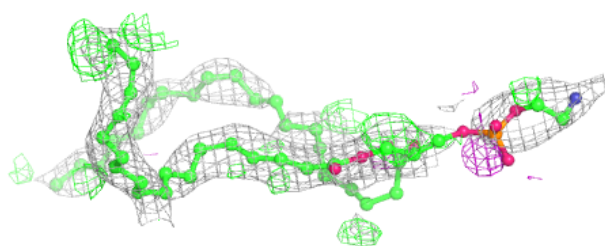
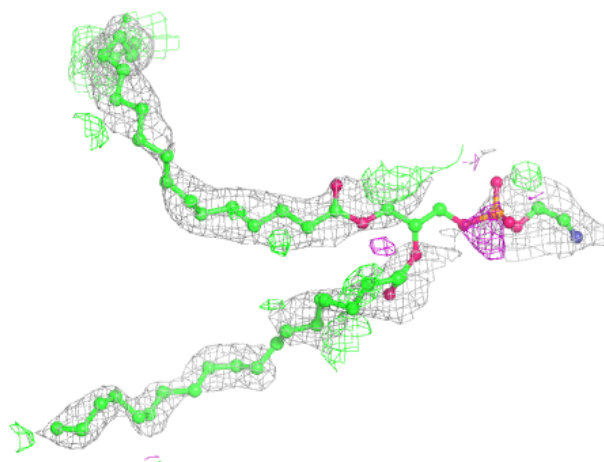
**Electron density around PEK P 307:**

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



**Electron density around PEK C 308:**

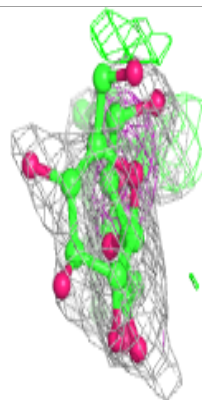
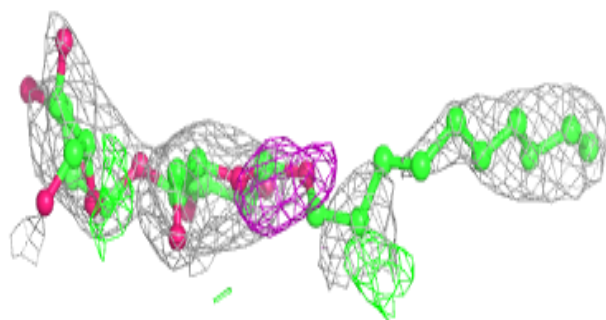
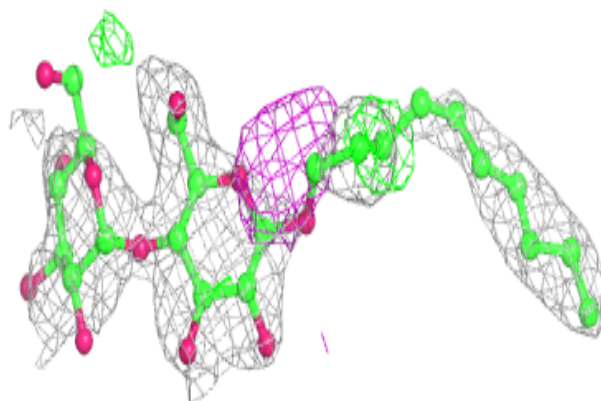
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



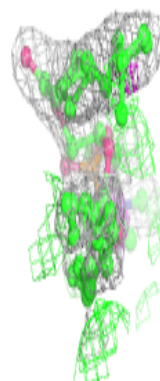
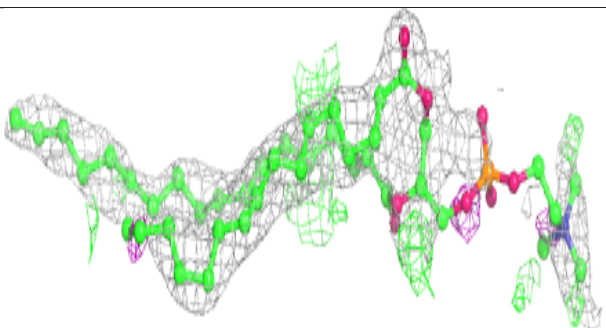
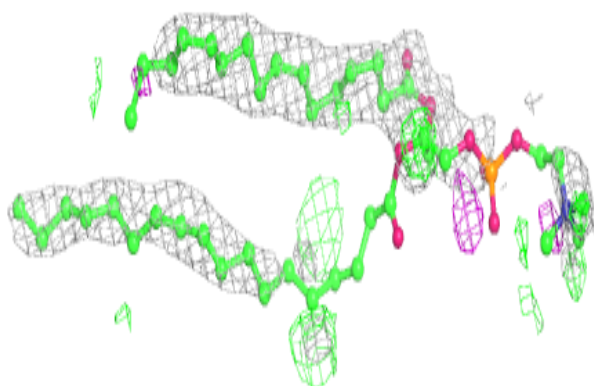


**Electron density around DMU P 306:**

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

**Electron density around PSC O 302:**

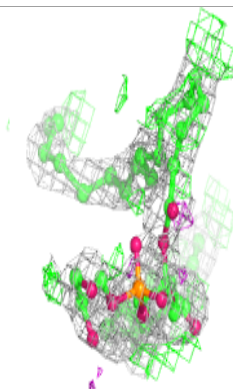
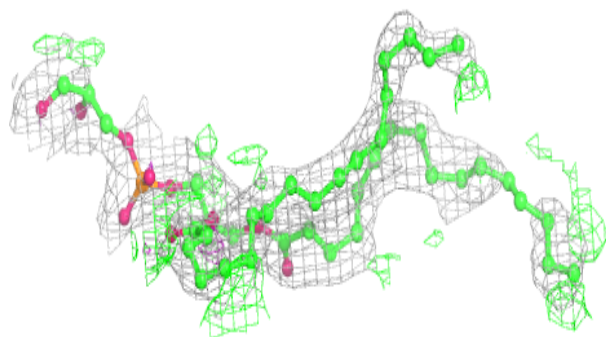
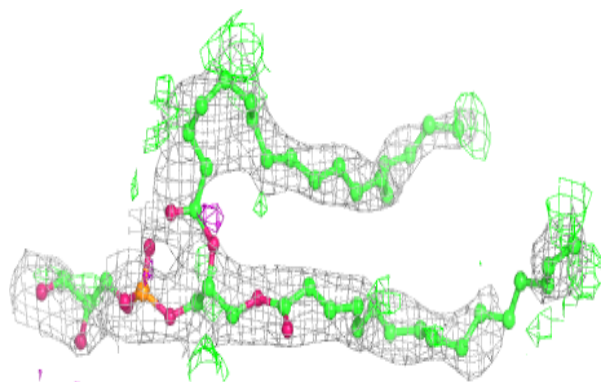
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



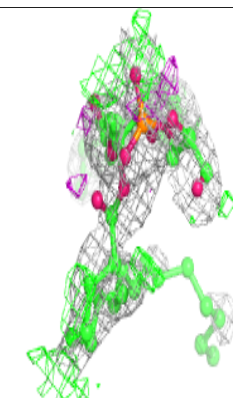
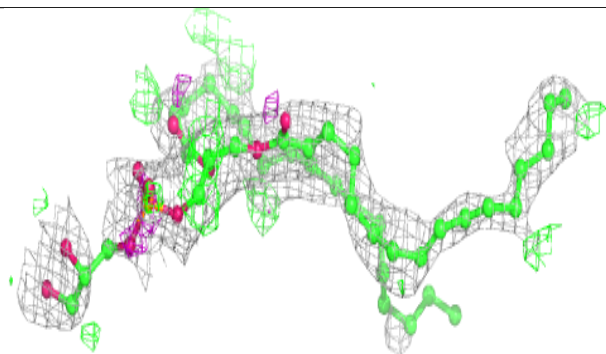
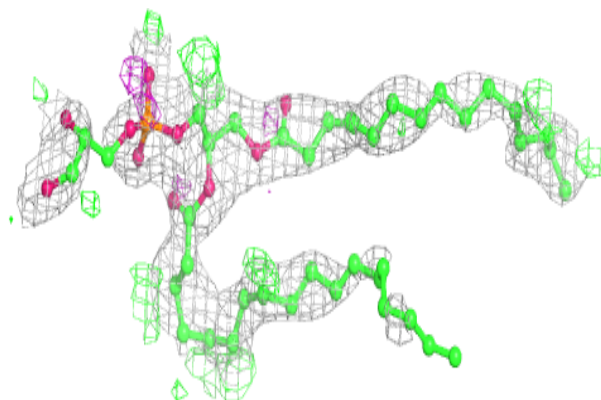


**Electron density around PGV C 309:**

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

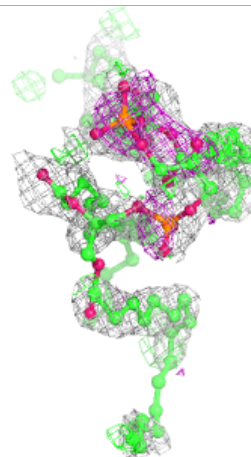
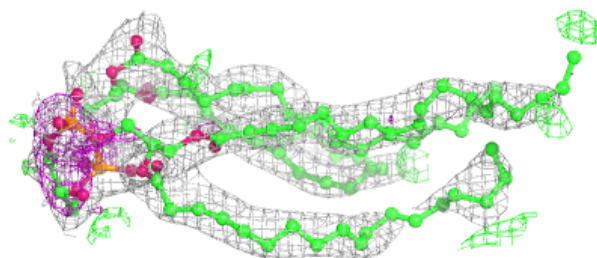
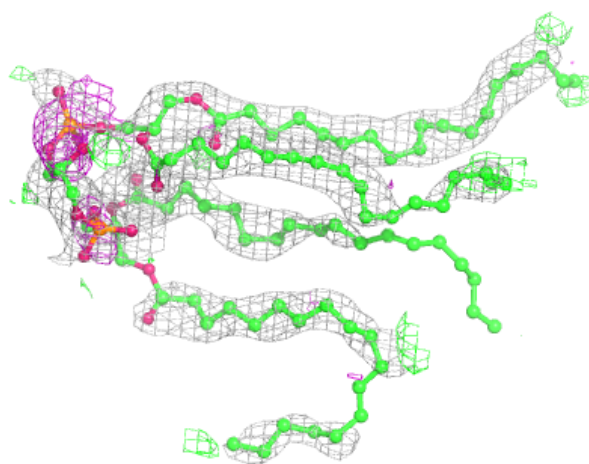
**Electron density around PGV G 103:**

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



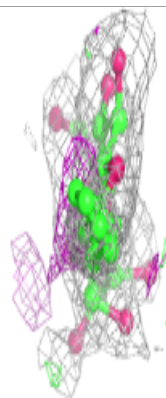
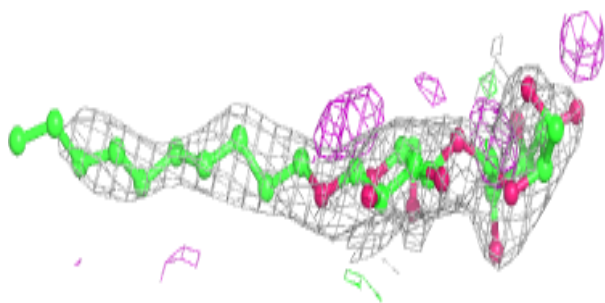
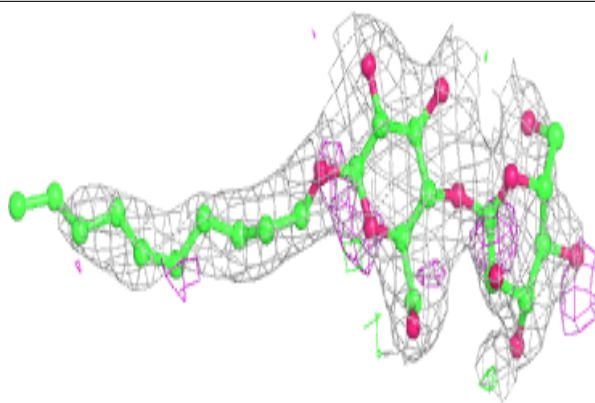
**Electron density around CDL C 306:**

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

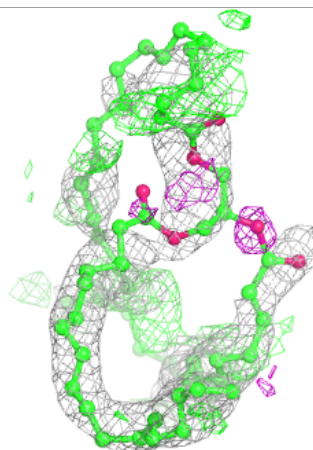
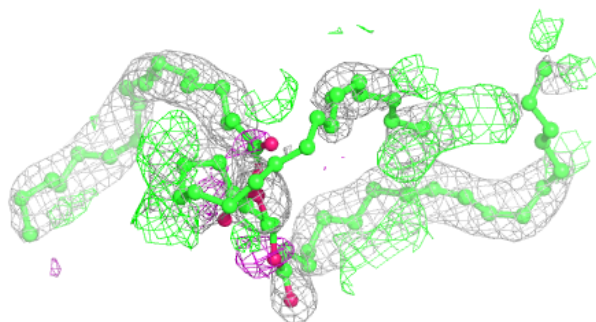
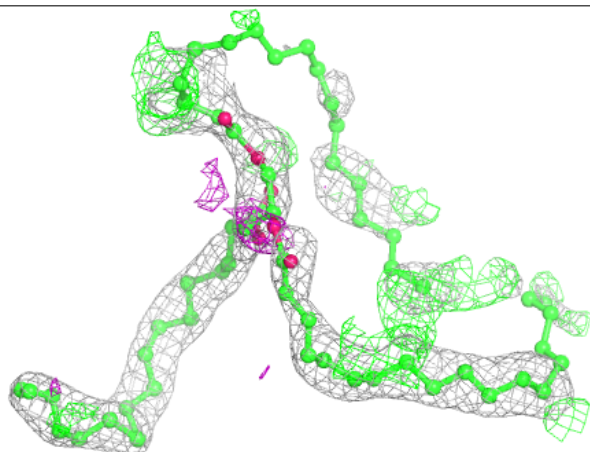


**Electron density around DMU C 310:**

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

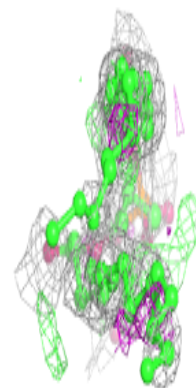
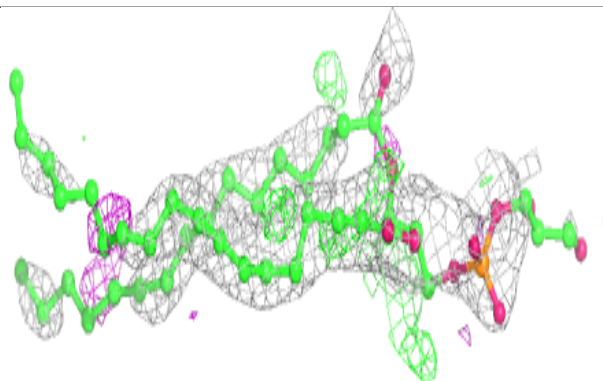
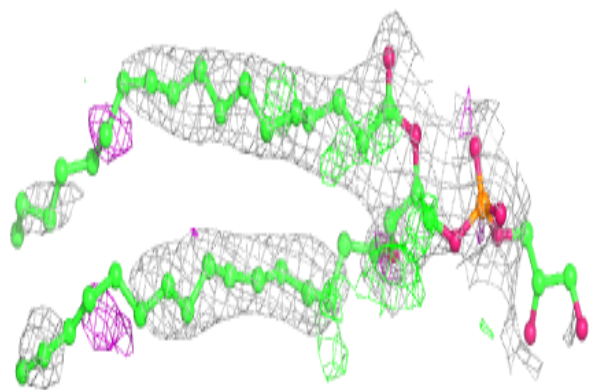
**Electron density around TGL Y 101:**

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



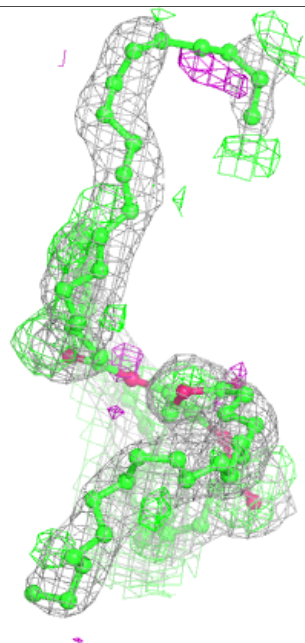
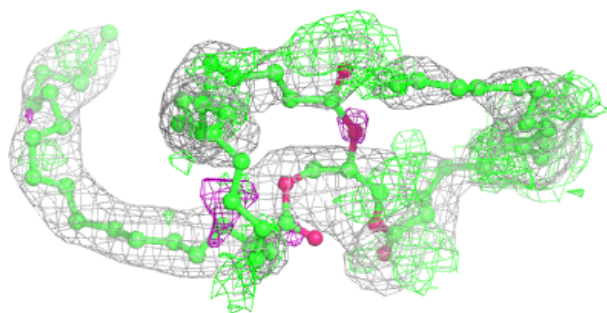
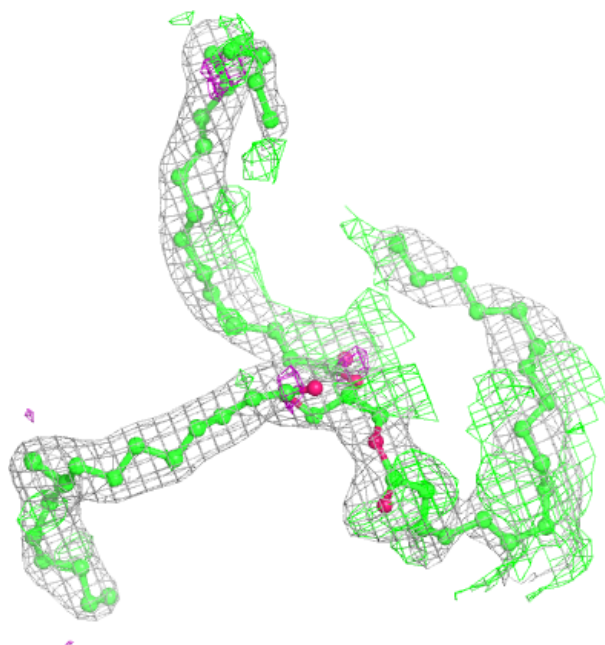
**Electron density around PGV Z 101:**

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



**Electron density around TGL L 101:**

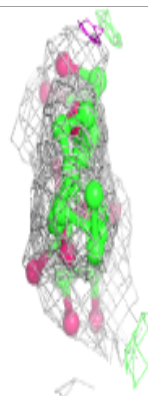
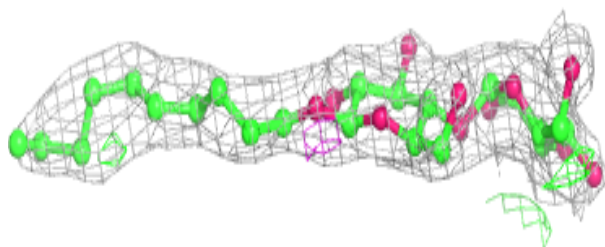
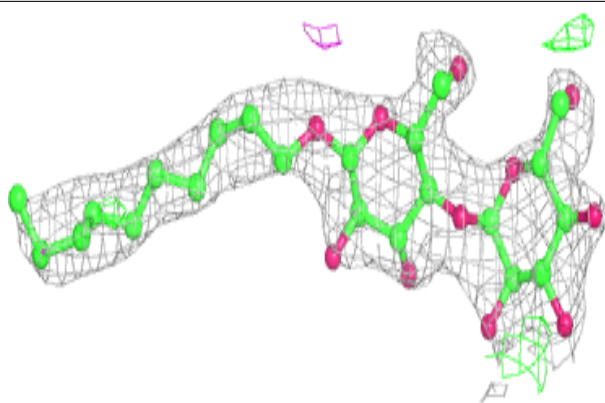
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



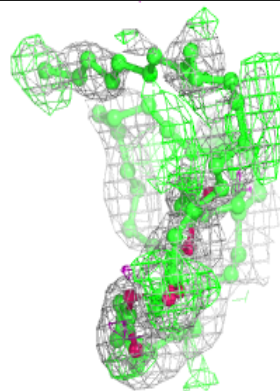
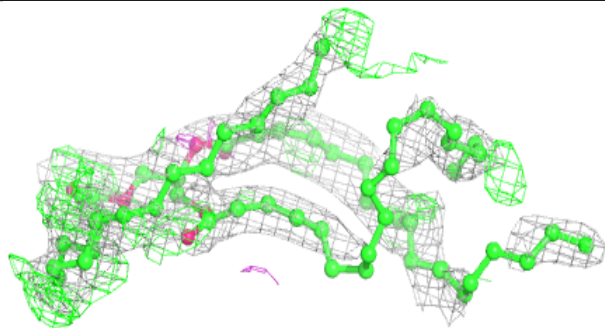
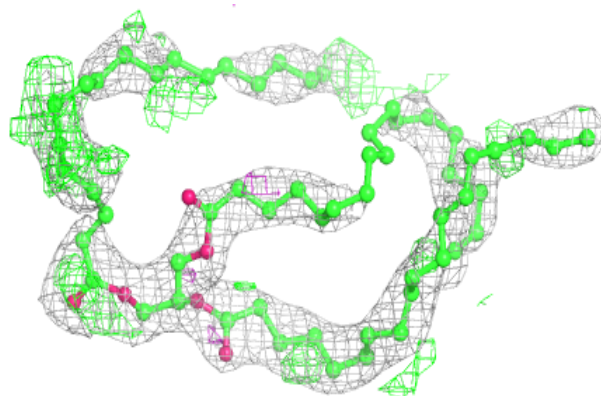


**Electron density around DMU P 309:**

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

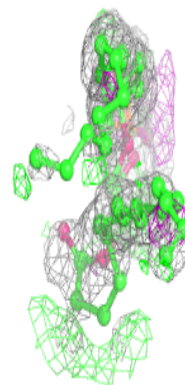
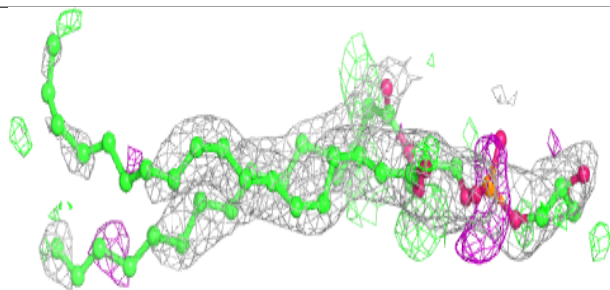
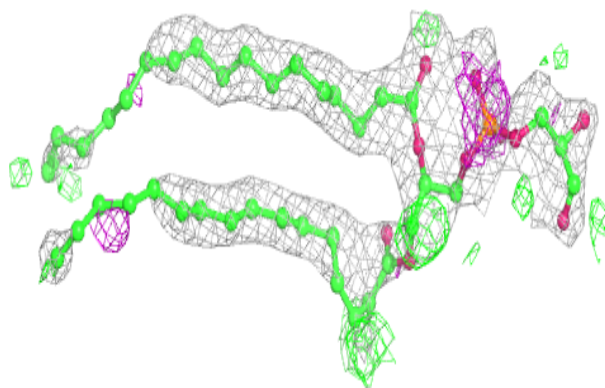
**Electron density around TGL N 610:**

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

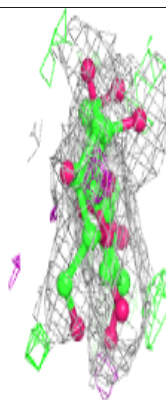
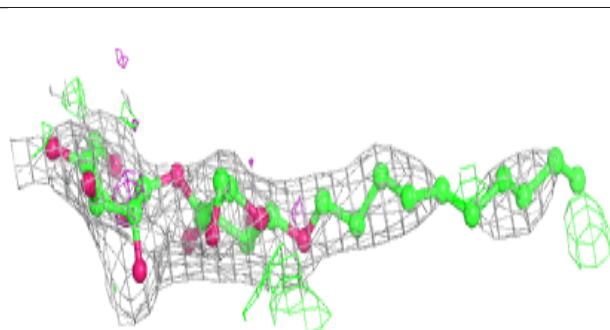
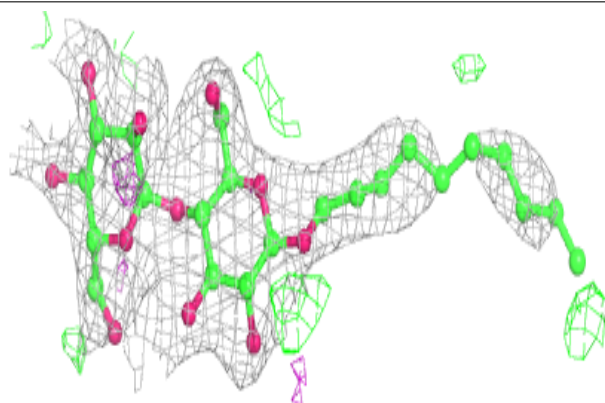


**Electron density around PGV A 610:**

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

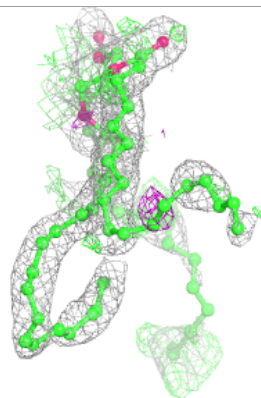
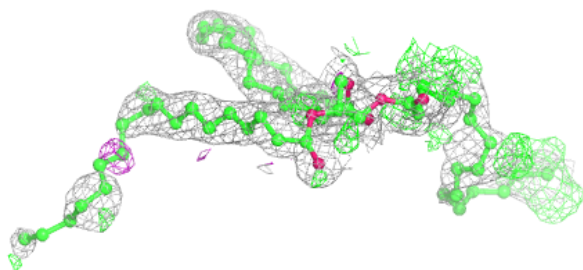
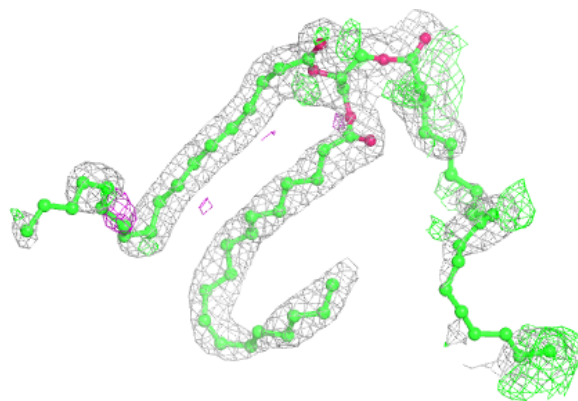
**Electron density around DMU P 308:**

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

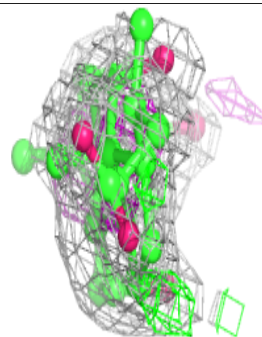
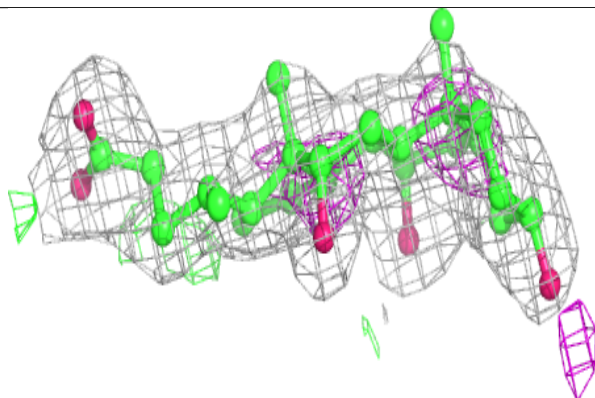
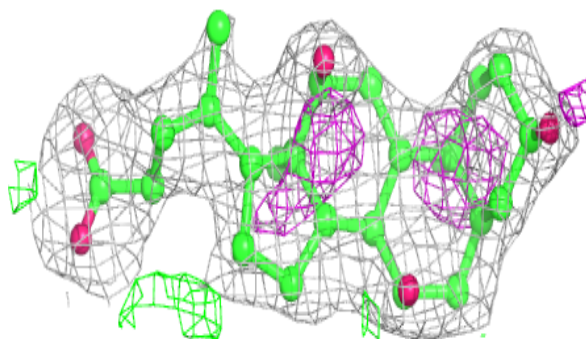


**Electron density around TGL D 201:**

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

**Electron density around CHD P 305:**

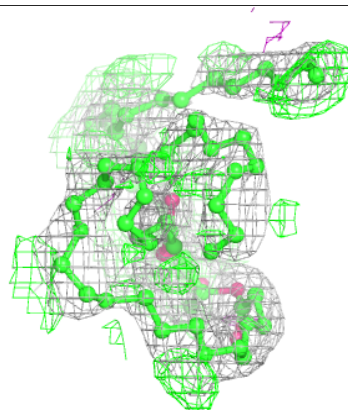
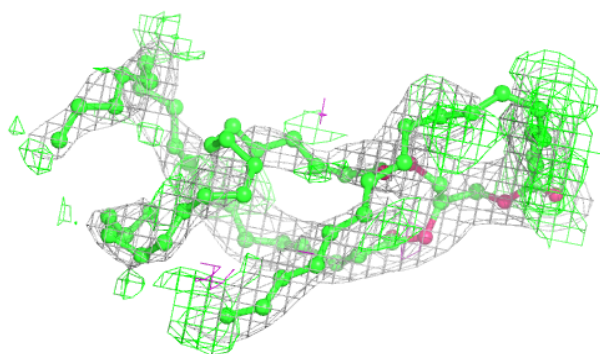
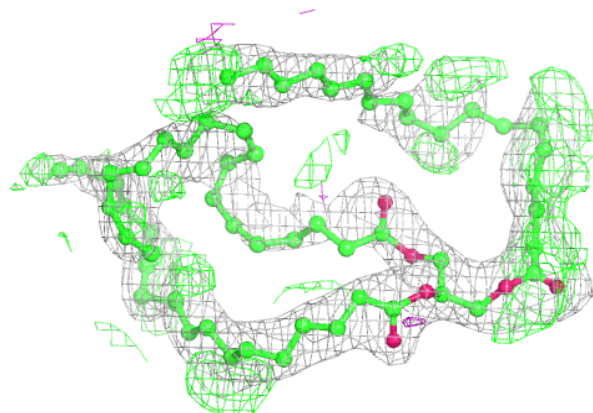
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



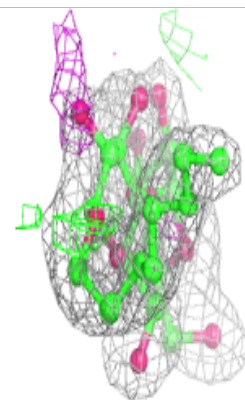
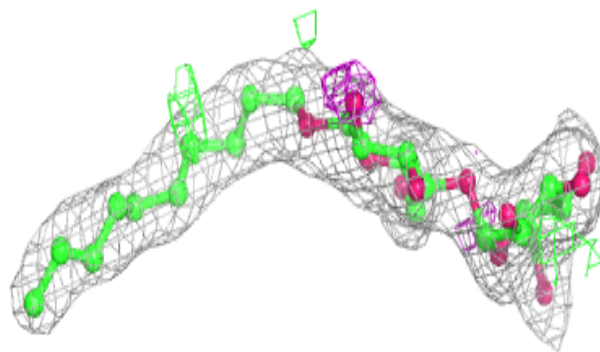
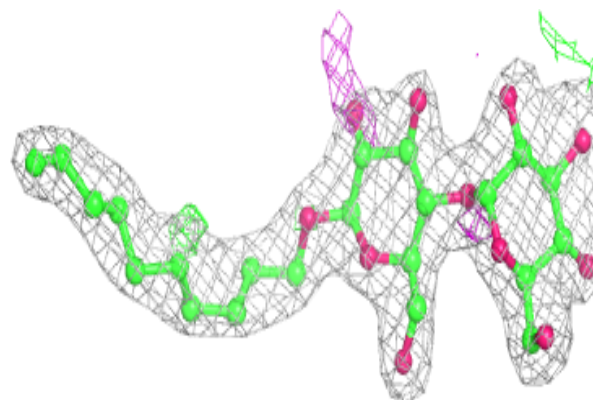


**Electron density around TGL A 608:**

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

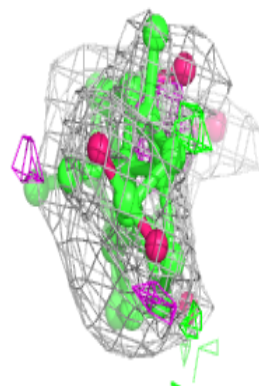
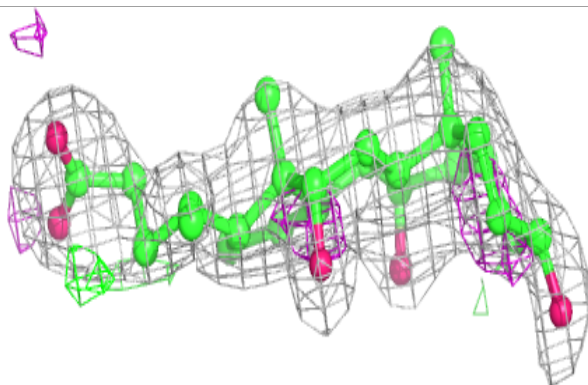
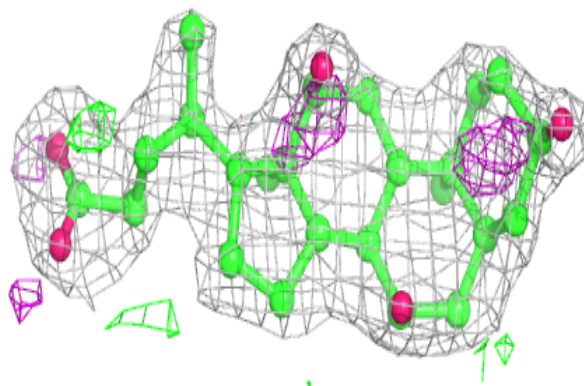
**Electron density around DMU Z 102:**

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

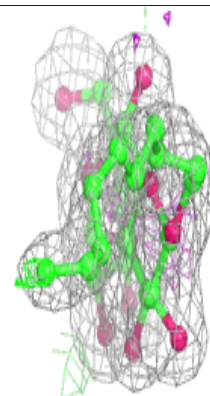
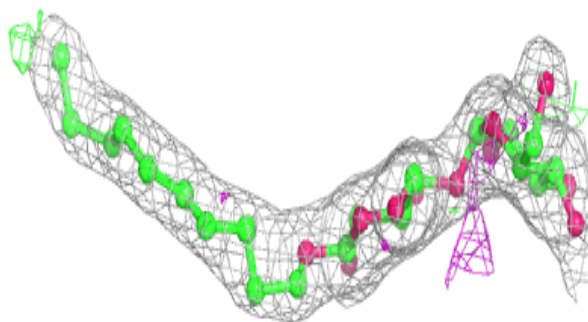
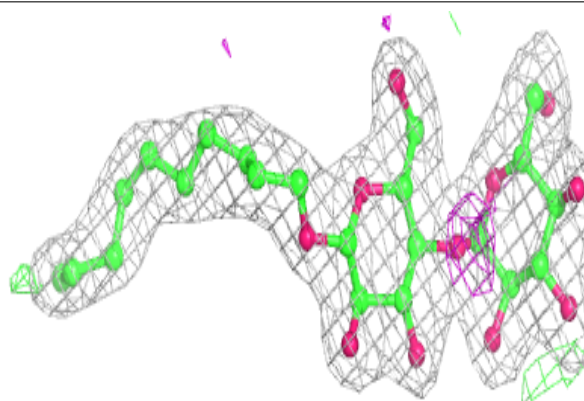


**Electron density around CHD C 307:**

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

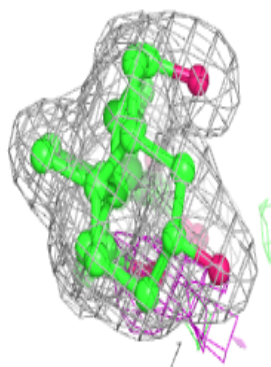
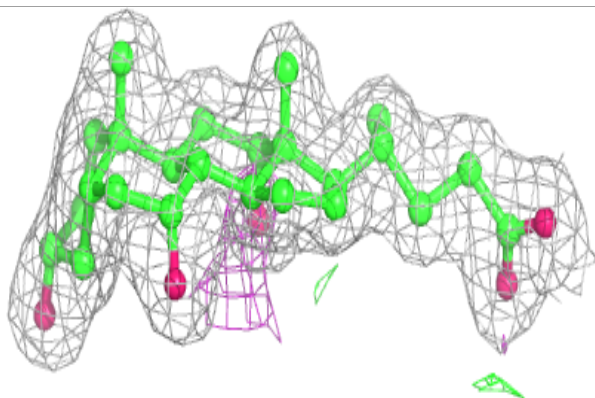
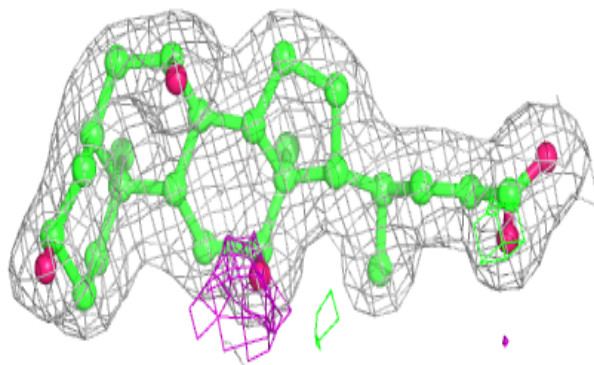
**Electron density around DMU M 101:**

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

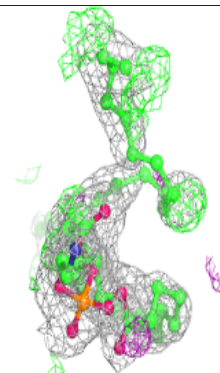
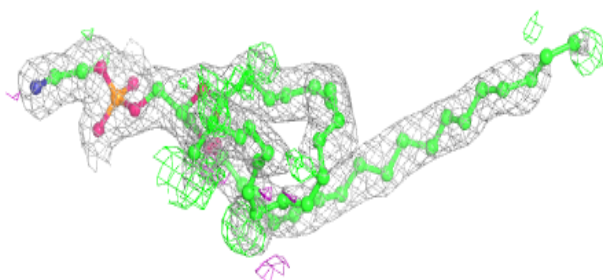
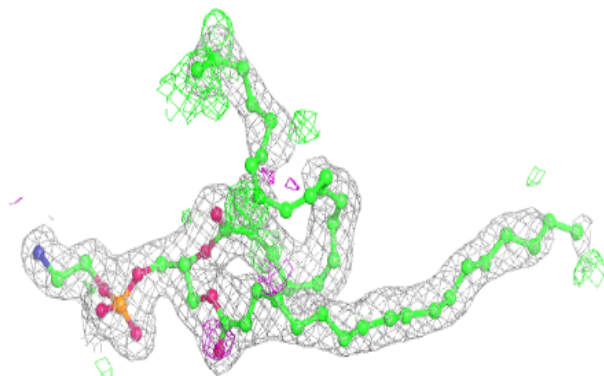


**Electron density around CHD C 301:**

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

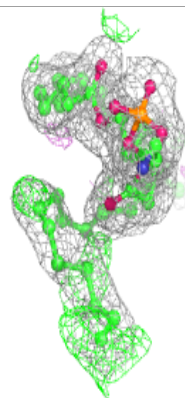
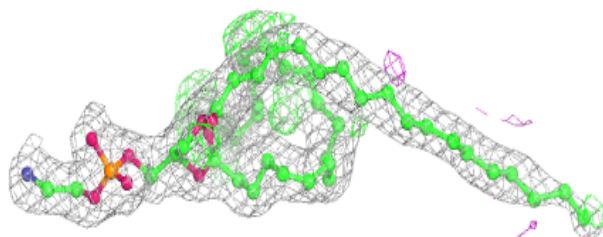
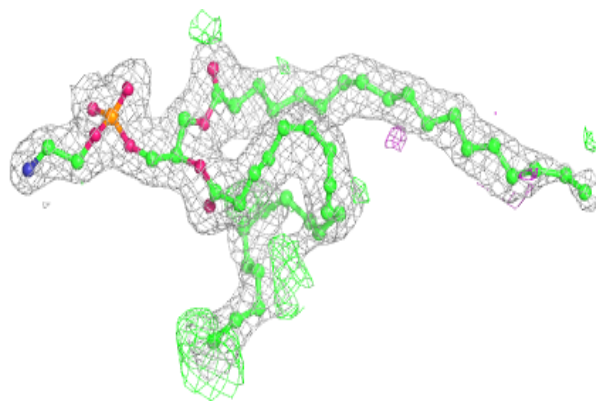
**Electron density around PEK T 102:**

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

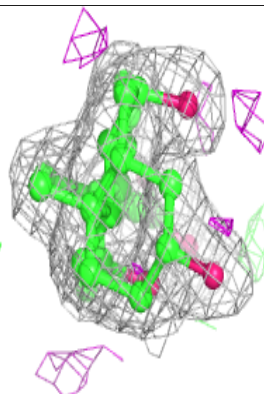
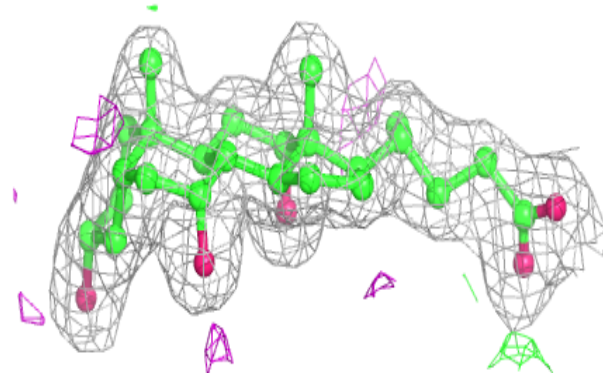
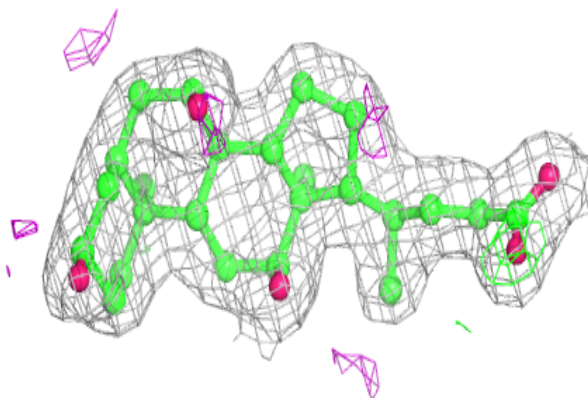


**Electron density around PEK C 304:**

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

**Electron density around CHD P 301:**

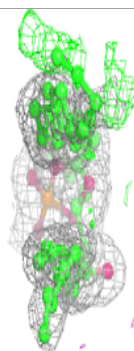
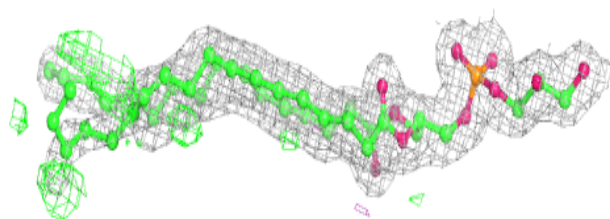
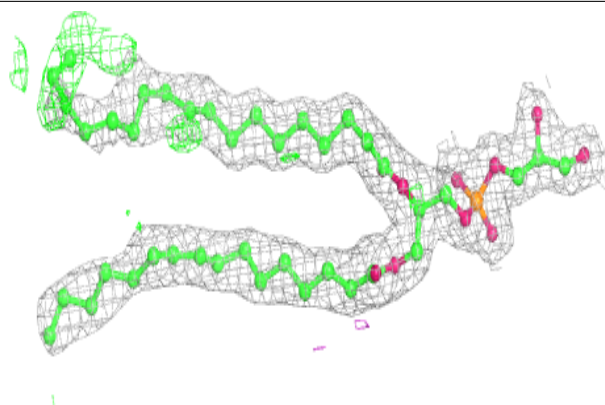
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



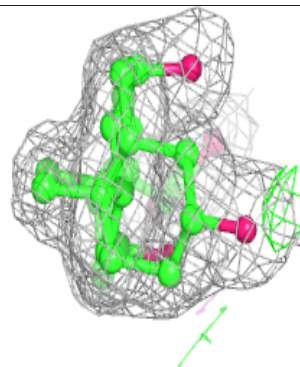
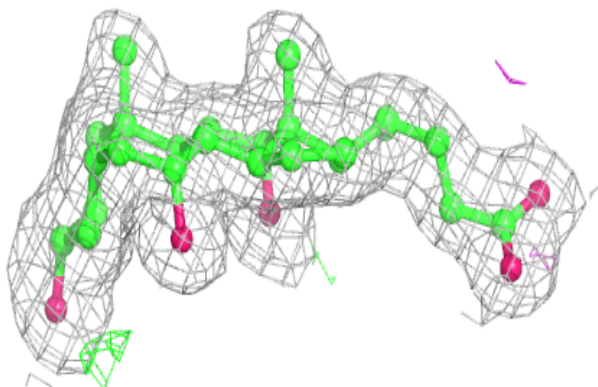
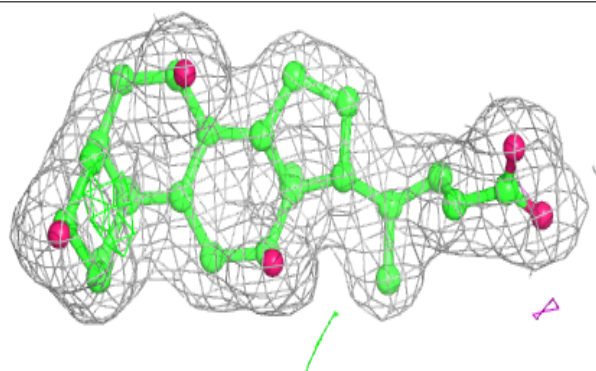


**Electron density around PGV C 305:**

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

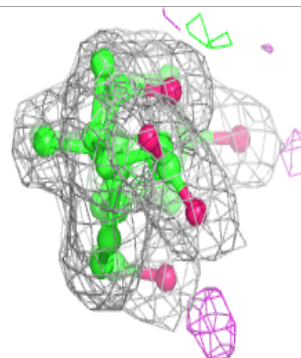
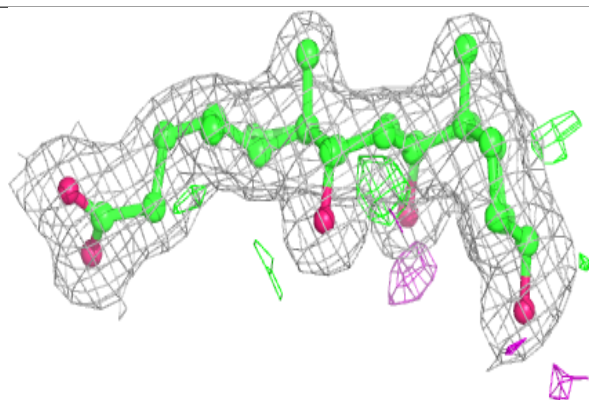
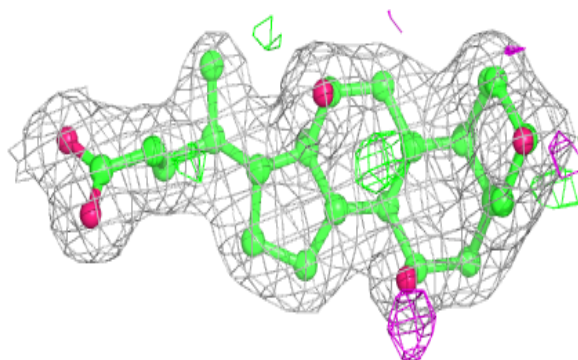
**Electron density around CHD G 101:**

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

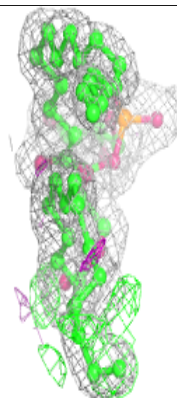
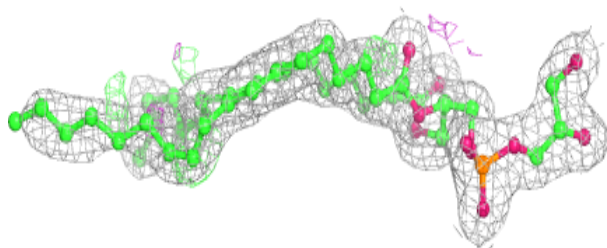
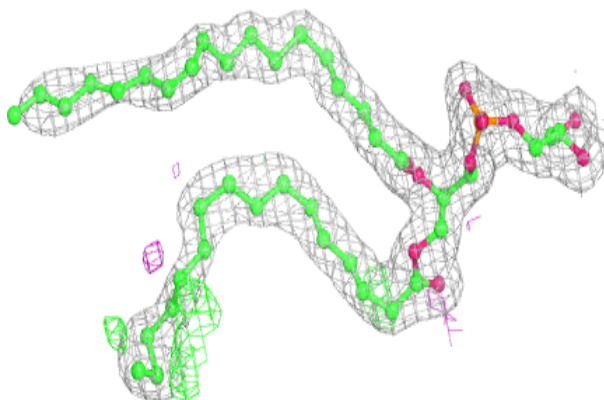


**Electron density around CHD B 301:**

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

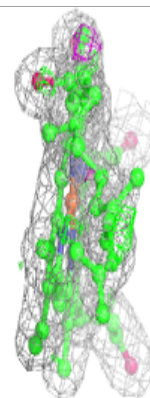
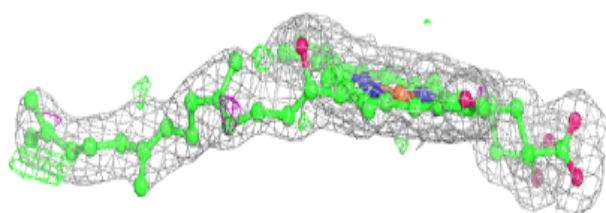
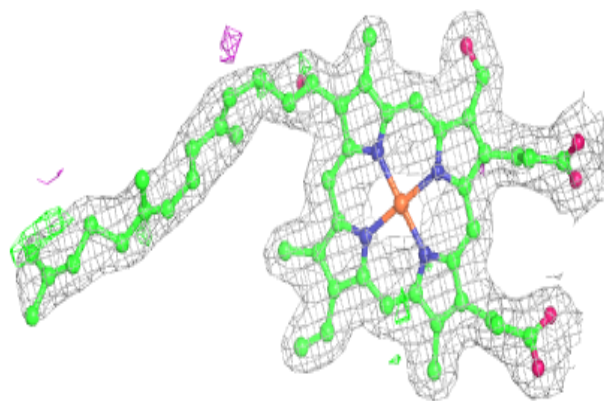
**Electron density around PGV A 609:**

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

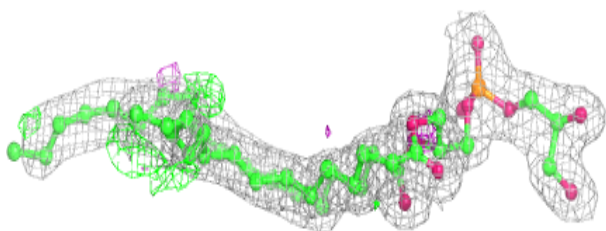
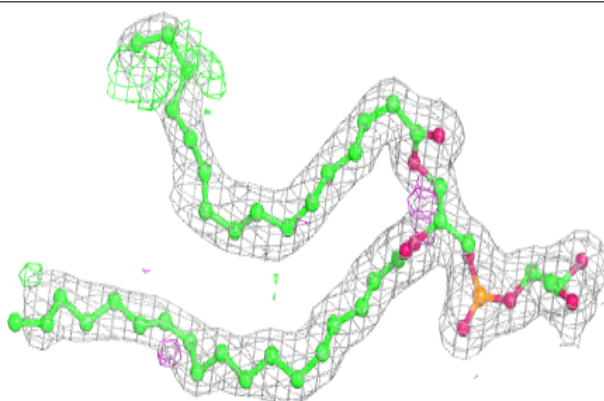


**Electron density around HEA N 602:**

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

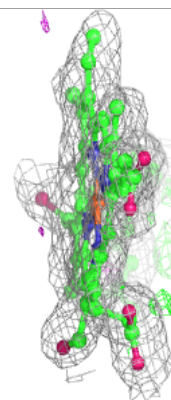
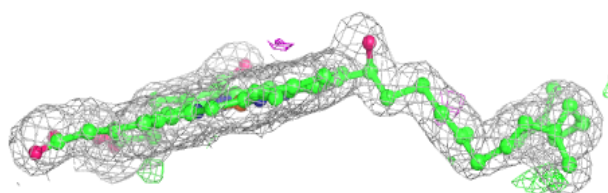
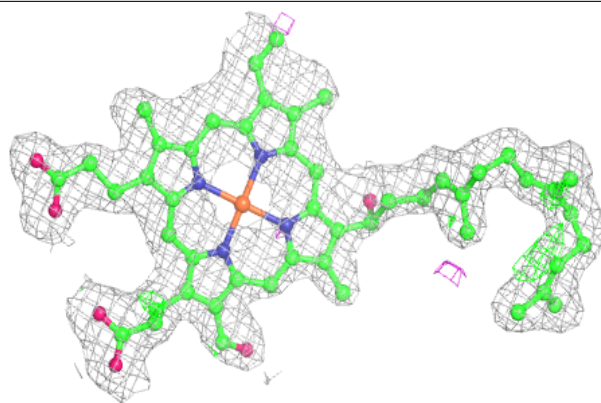
**Electron density around PGV N 609:**

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

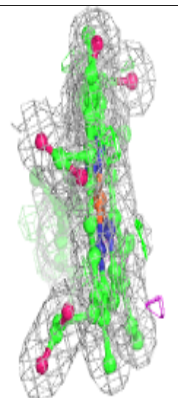
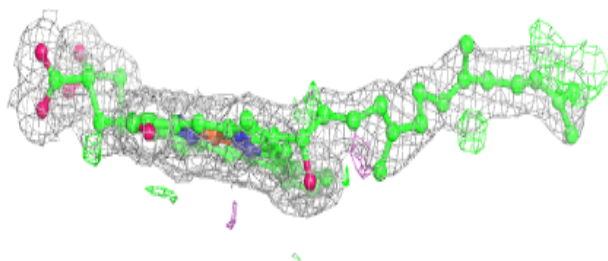
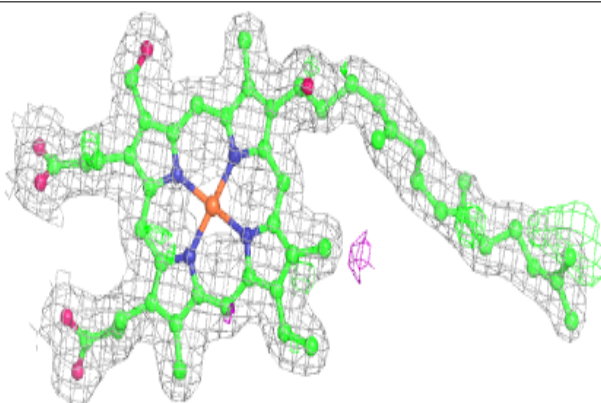


**Electron density around HEA A 602 (B):**

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

**Electron density around HEA A 601:**

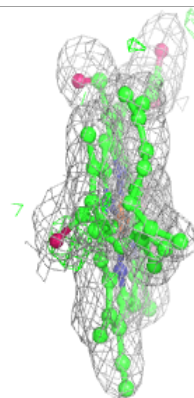
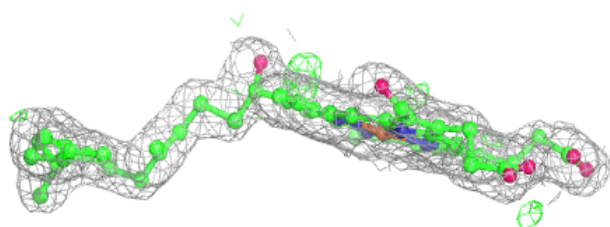
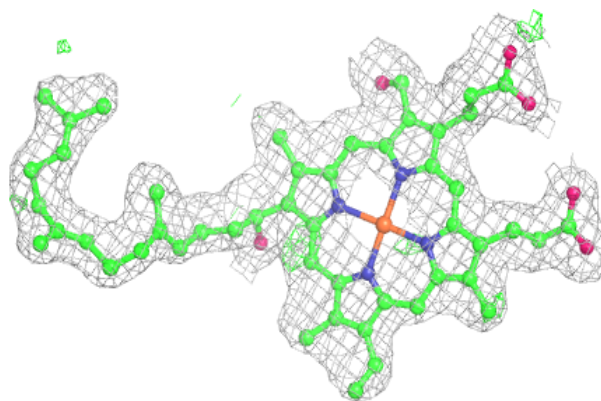
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



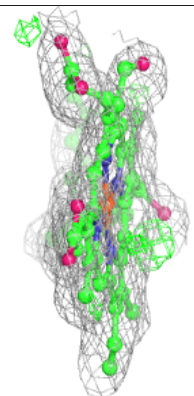
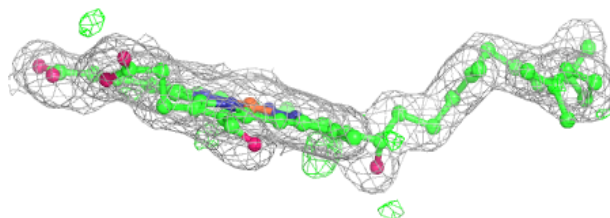
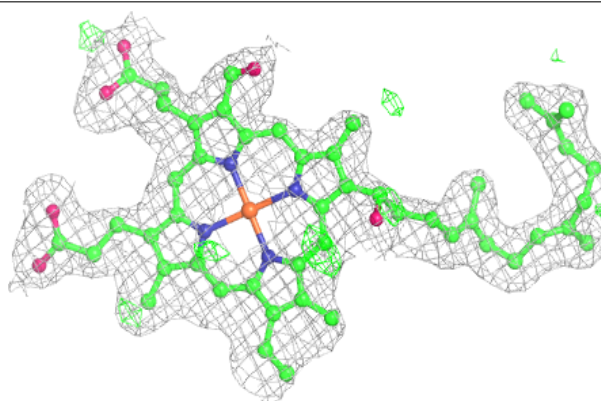


**Electron density around HEA N 603 (A):**

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

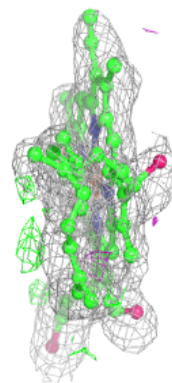
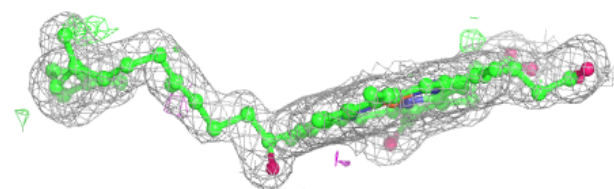
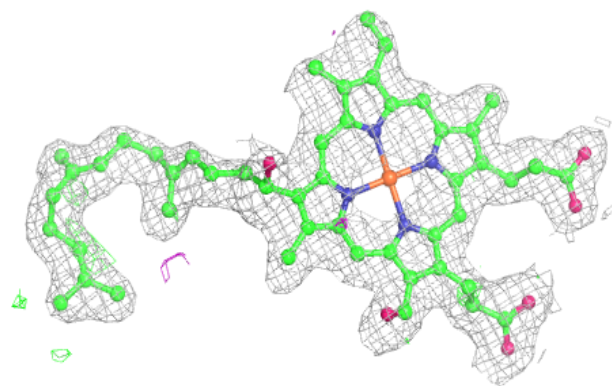
**Electron density around HEA N 603 (B):**

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

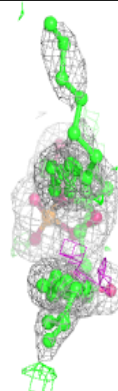
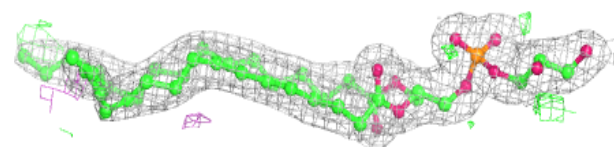
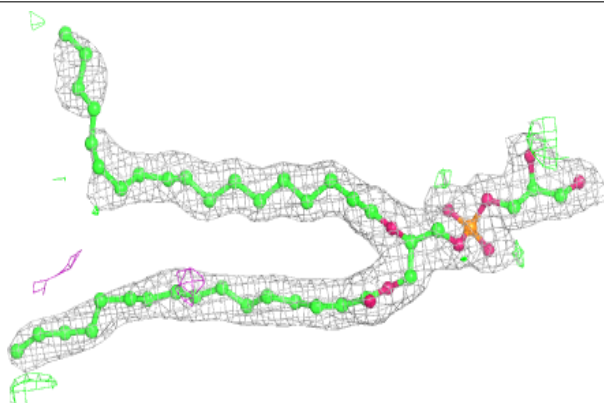


**Electron density around HEA A 602 (A):**

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

**Electron density around PGV 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.