



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2020 – 03:32 PM BST

PDB ID : 5Z86  
Title : azide-bound cytochrome c oxidase structure determined using the crystals exposed to 20 mM azide solution for 3 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	:	2.14.3.dev2
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)	:	2.14.3.dev2

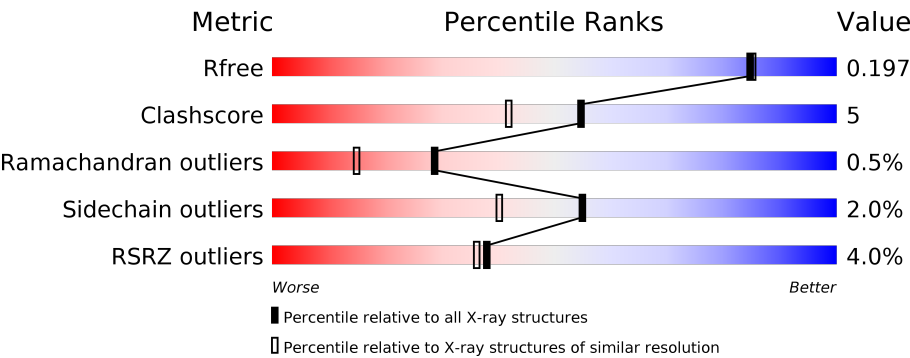
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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.



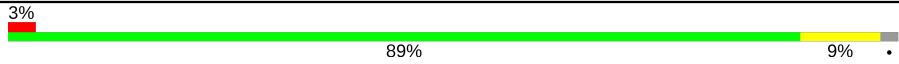
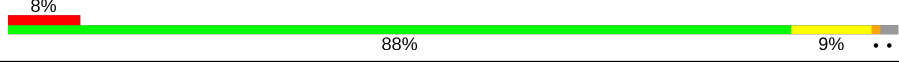
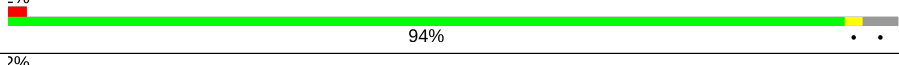
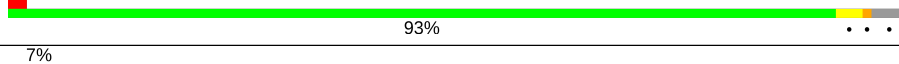

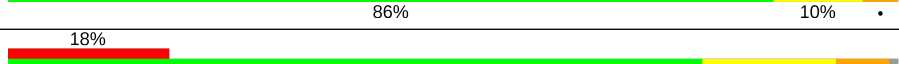
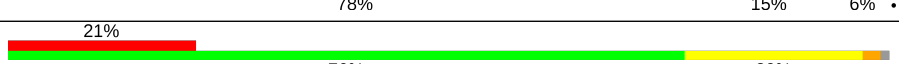
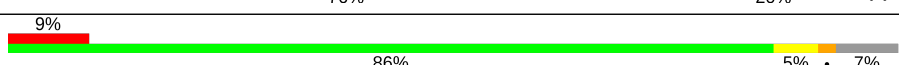
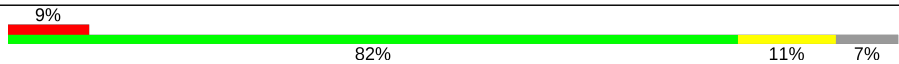
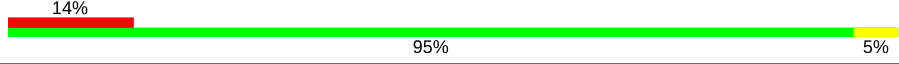
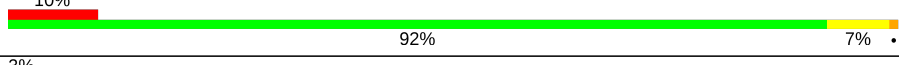
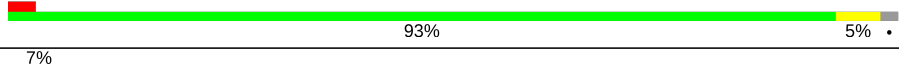
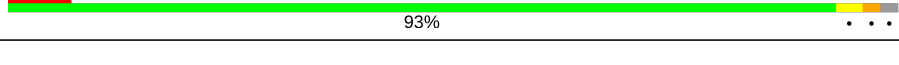
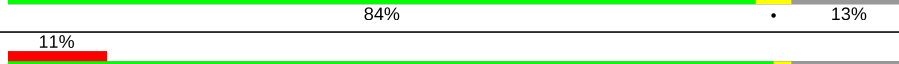
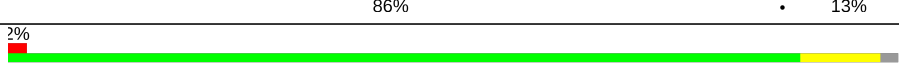
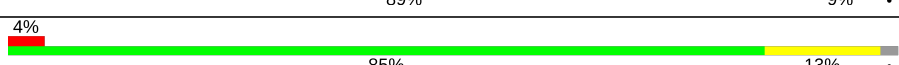

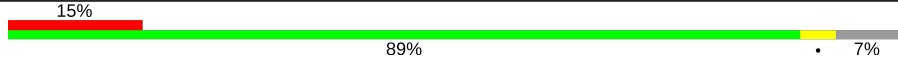

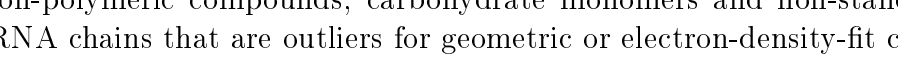
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	601	X	-	-	-
14	HEA	N	602[A]	X	-	-	-
14	HEA	N	602[B]	X	-	-	-
18	AZI	A	607	-	-	X	-
18	AZI	N	607	-	-	X	-
20	EDO	A	617	-	-	-	X
20	EDO	A	618	-	-	-	X
20	EDO	C	318	-	-	-	X
20	EDO	D	202	-	-	X	-
22	CHD	W	101	-	-	-	X
9	SAC	V	1	-	-	-	X



## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33590 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	21	0
			4185	2789	648	706	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	8	0
			1891	1229	291	352	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	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	8	0
			2176	1452	348	360	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	3	0
			1224	797	202	221	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 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0

- 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 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			

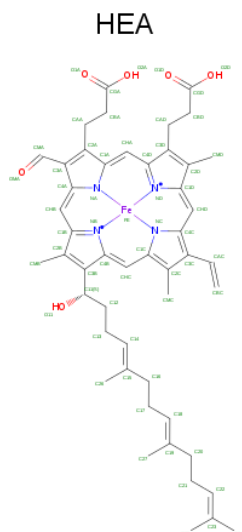
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
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 1 1	0	0
15	N	1	Total Cu 1 1	0	0

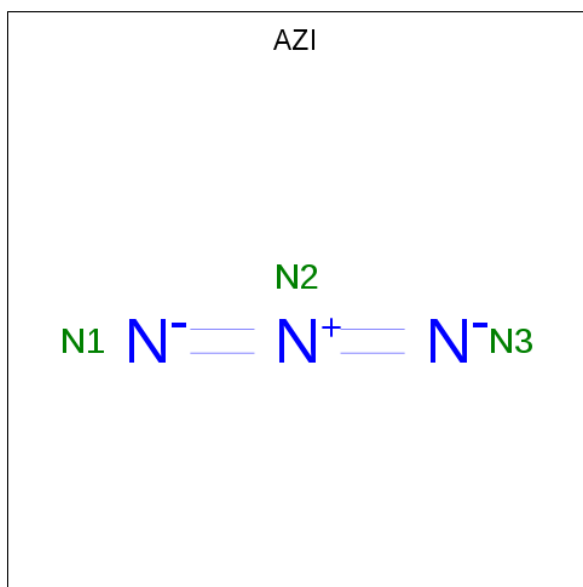
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

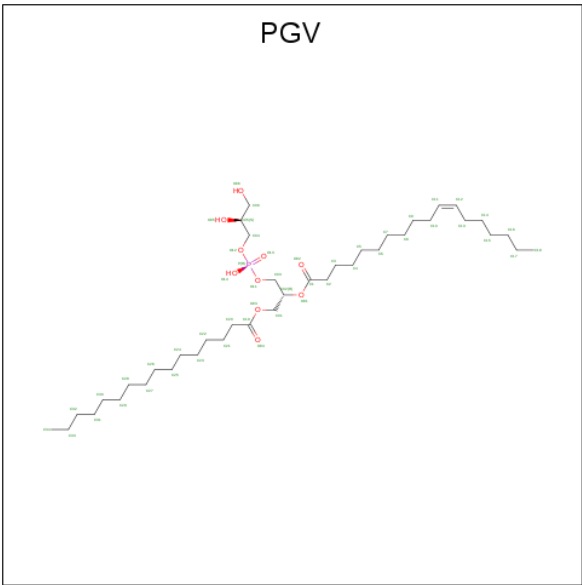
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



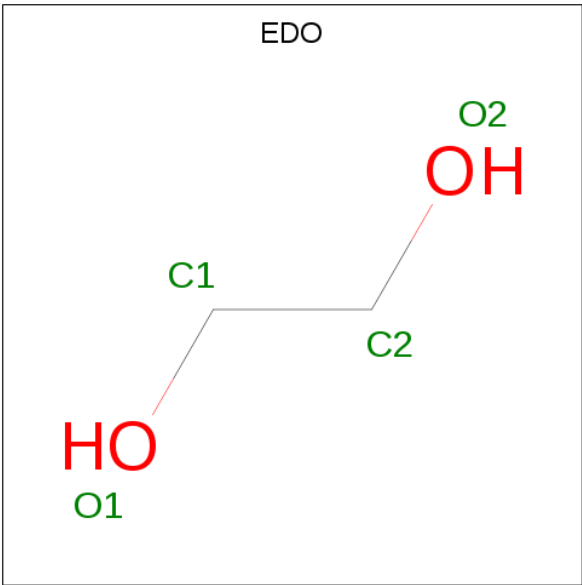
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	0
18	A	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0

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



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

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



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

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

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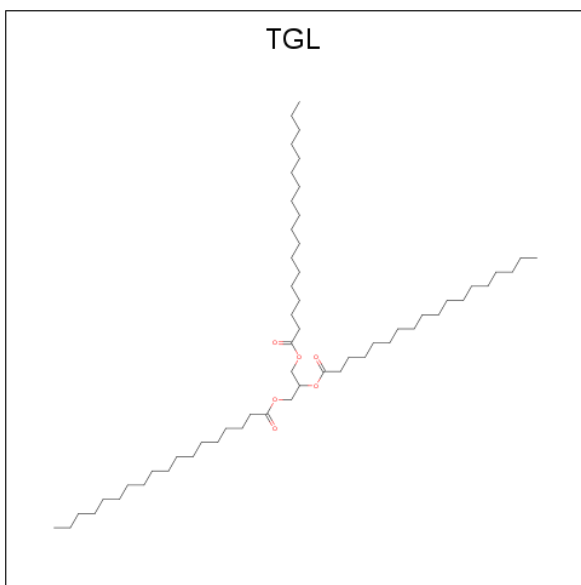
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	G	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4	C 2	O 2	0	0
20	J	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4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

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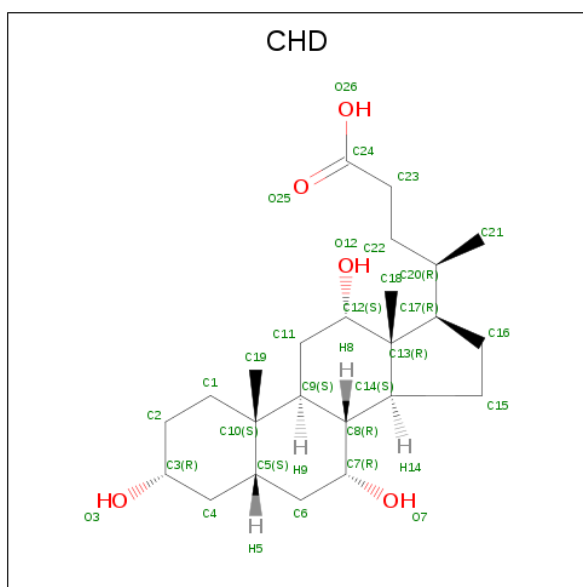
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	Q	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4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

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



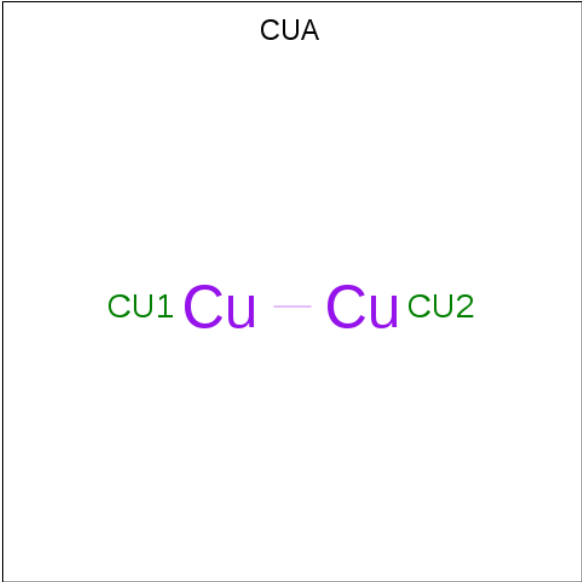
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



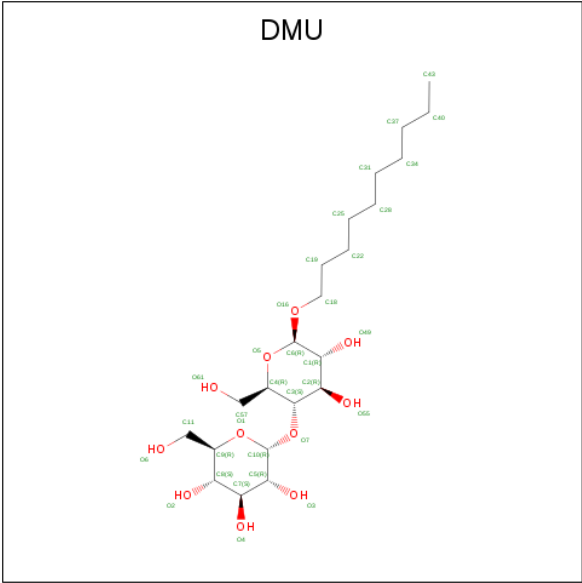
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

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



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

- Molecule 24 is 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
24	C	1	Total	C	O	0	0
			33	22	11		

Continued on next page...

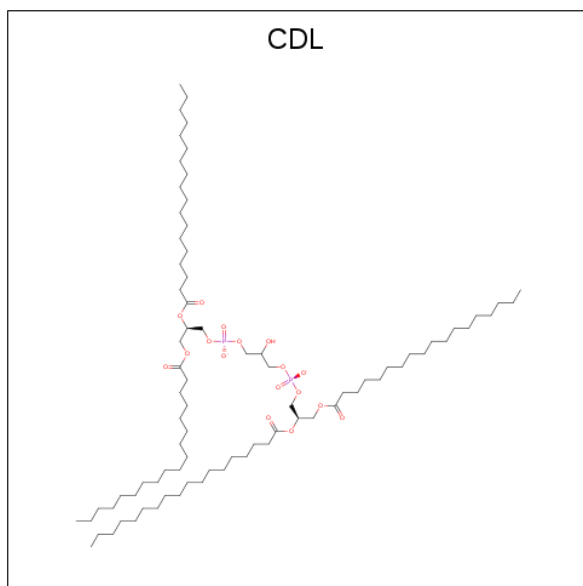
*Continued from previous page...*

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

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

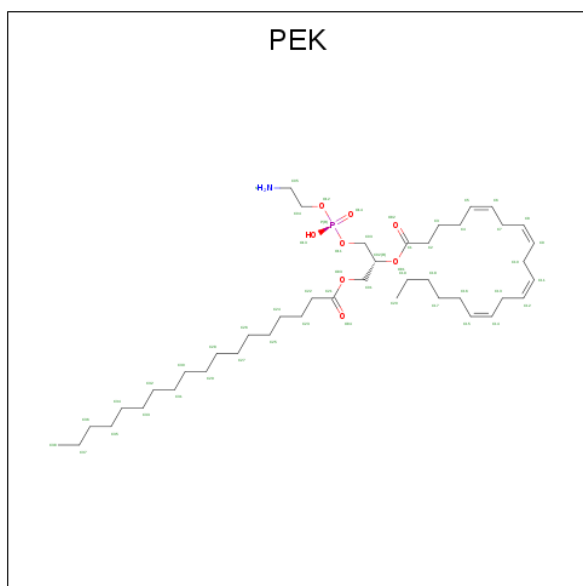
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	X	0	0
			1	1		
25	C	1	Total	X	0	0
			1	1		

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



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

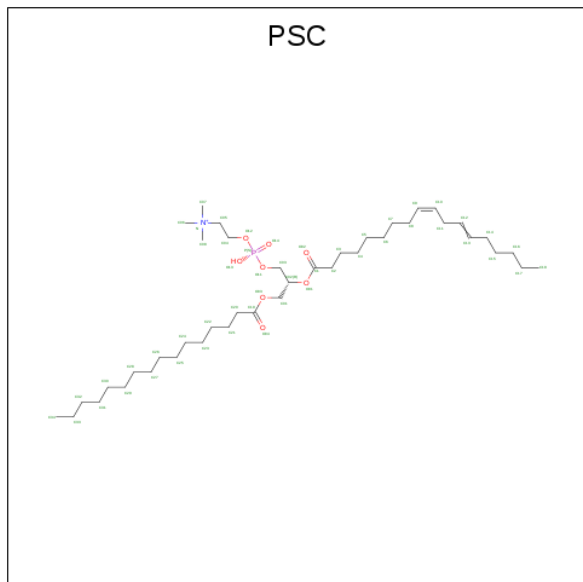
- Molecule 27 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



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	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		

- Molecule 28 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
28	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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	223	Total	O	0	0
			223	223		
30	B	140	Total	O	0	1
			141	141		
30	C	100	Total	O	0	0
			100	100		
30	D	97	Total	O	0	0
			97	97		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	E	78	Total 78	O 78	0	0
30	F	86	Total 86	O 86	0	0
30	G	42	Total 42	O 42	0	0
30	H	35	Total 35	O 35	0	0
30	I	21	Total 21	O 21	0	0
30	J	21	Total 21	O 21	0	0
30	K	26	Total 26	O 26	0	0
30	L	29	Total 29	O 29	0	0
30	M	25	Total 25	O 25	0	0
30	N	204	Total 204	O 204	0	0
30	O	101	Total 102	O 102	0	1
30	P	102	Total 102	O 102	0	0
30	Q	36	Total 36	O 36	0	0
30	R	37	Total 37	O 37	0	0
30	S	53	Total 53	O 53	0	0
30	T	44	Total 44	O 44	0	0
30	U	39	Total 39	O 39	0	0
30	V	12	Total 12	O 12	0	0
30	W	8	Total 8	O 8	0	0
30	X	11	Total 11	O 11	0	0
30	Y	14	Total 14	O 14	0	0

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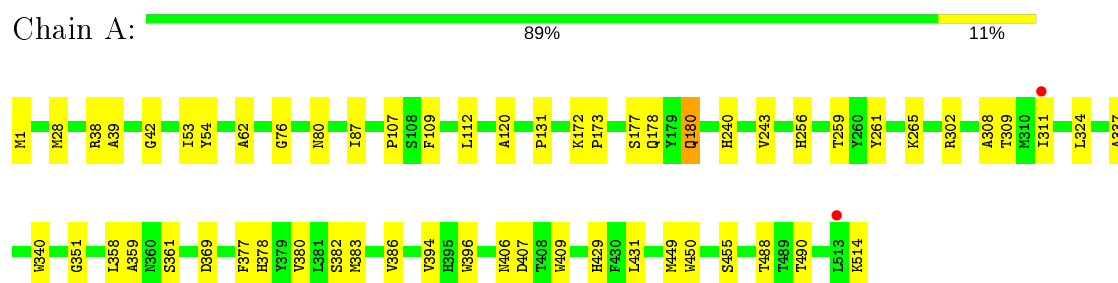
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	Z	11	Total	O	0	0
			11	11		

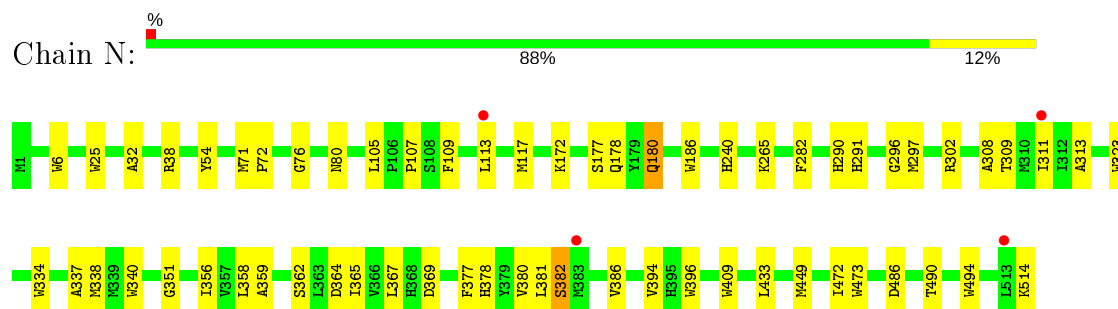
### 3 Residue-property plots

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

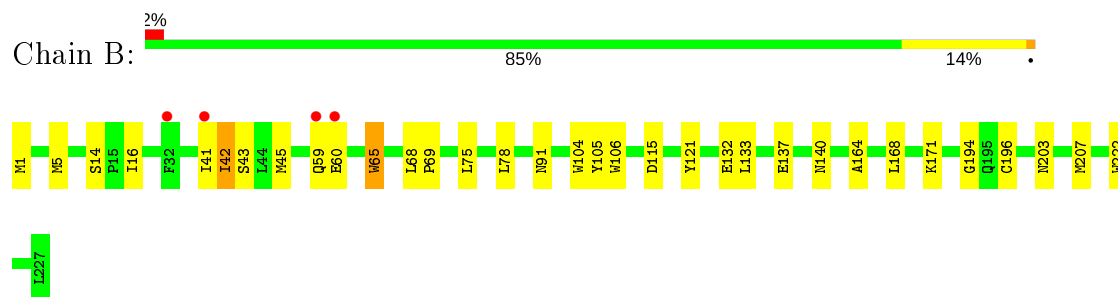
#### • Molecule 1: Cytochrome c oxidase subunit 1



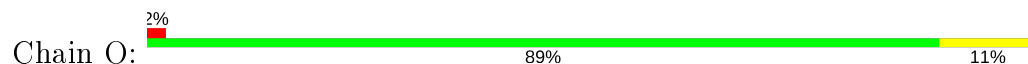
#### • Molecule 1: Cytochrome c oxidase subunit 1



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



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





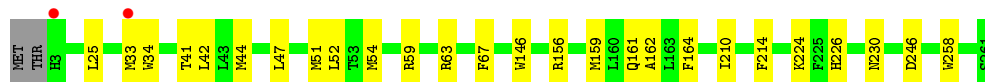
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 11% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 89% 10% .



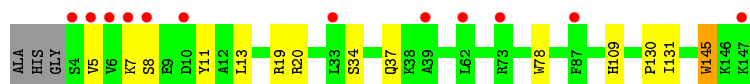
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 89% 9% .



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

Chain Q: 88% 9% ..



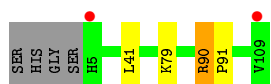
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E: 94% ..

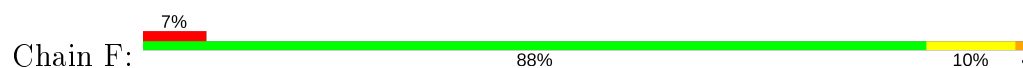


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

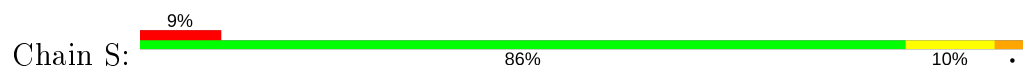
Chain R: 93% ...



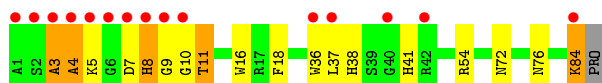
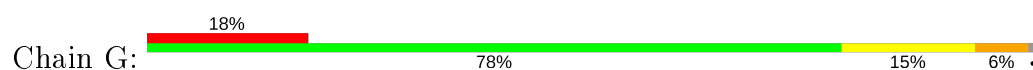
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



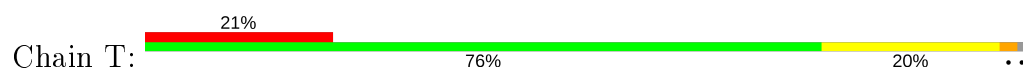
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



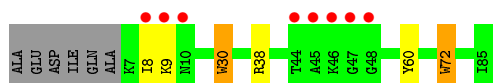
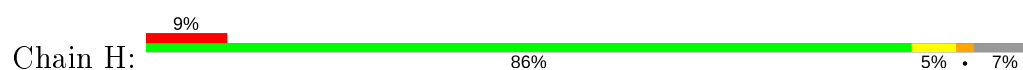
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



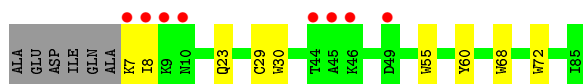
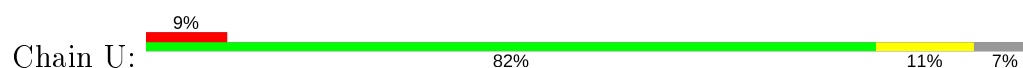
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



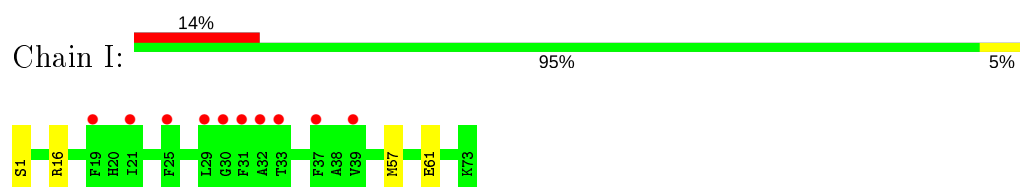
- Molecule 8: Cytochrome c oxidase subunit 6B1



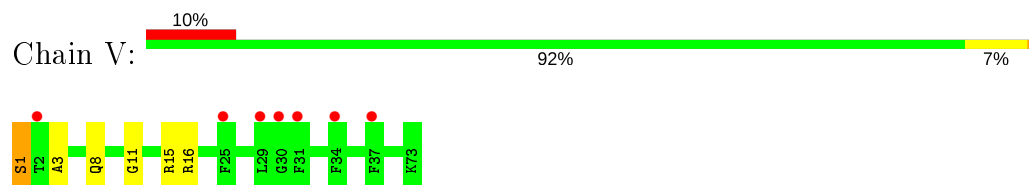
- Molecule 8: Cytochrome c oxidase subunit 6B1



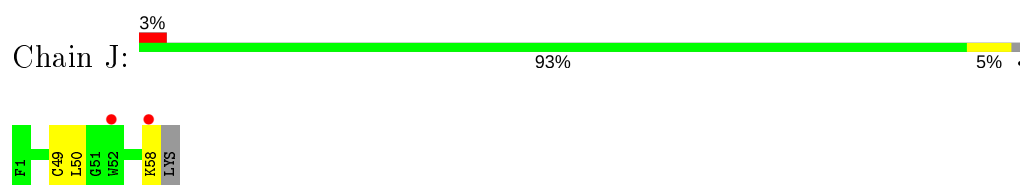
- Molecule 9: Cytochrome c oxidase subunit 6C



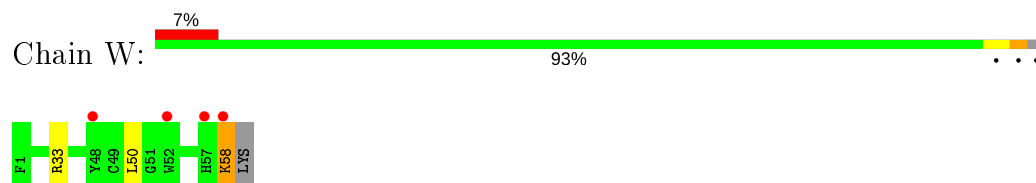
- Molecule 9: Cytochrome c oxidase subunit 6C



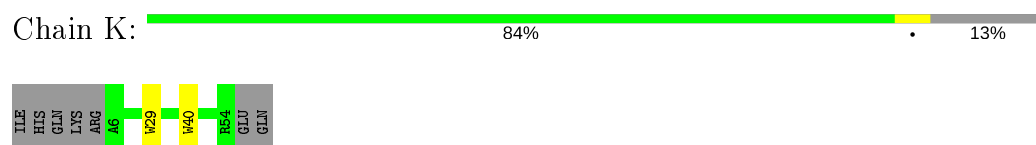
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



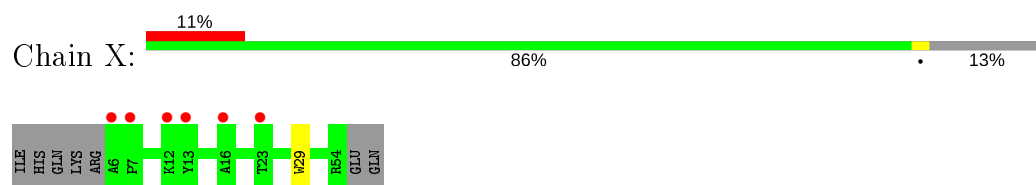
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



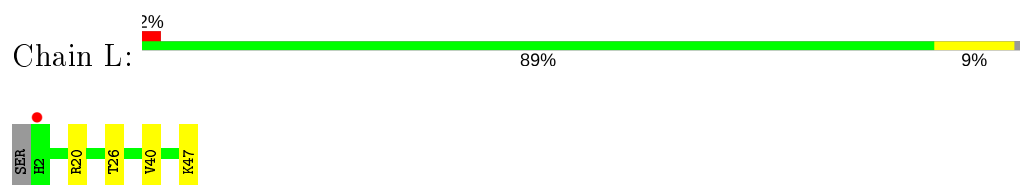
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



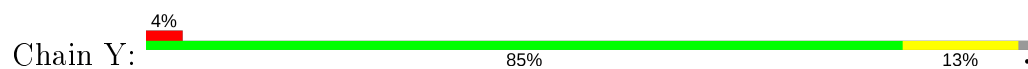
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



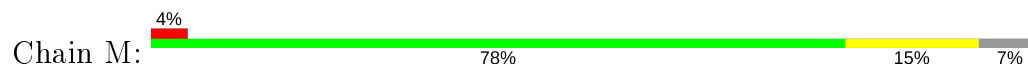
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



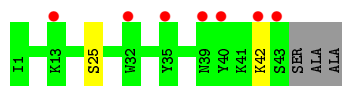
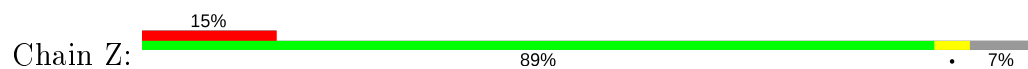
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.49Å 206.29Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 108.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-1.85) 99.5 (108.53-1.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.06 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.181 , 0.196 0.181 , 0.197	Depositor DCC
$R_{free}$ test set	28473 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.3	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	0.96	EDS
Total number of atoms	33590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.62	3/4314 (0.1%)	0.58	0/5886
1	N	0.61	8/4308 (0.2%)	0.56	0/5878
2	B	0.54	3/1929 (0.2%)	0.62	0/2627
2	O	0.51	0/1908	0.57	0/2597
3	C	0.67	5/2263 (0.2%)	0.51	0/3090
3	P	0.66	2/2272 (0.1%)	0.52	0/3102
4	D	0.60	3/1259 (0.2%)	0.52	0/1698
4	Q	0.57	2/1259 (0.2%)	0.50	0/1698
5	E	0.50	1/871 (0.1%)	0.50	0/1182
5	R	0.47	0/871	0.52	0/1182
6	F	0.53	2/795 (0.3%)	0.57	0/1079
6	S	0.51	0/780	0.55	0/1058
7	G	0.65	2/702 (0.3%)	0.58	0/953
7	T	0.65	2/702 (0.3%)	0.57	0/953
8	H	0.61	2/682 (0.3%)	0.52	0/921
8	U	0.61	4/682 (0.6%)	0.51	0/921
9	I	0.38	0/605	0.48	0/802
9	V	0.37	0/605	0.47	0/802
10	J	0.50	0/471	0.45	0/636
10	W	0.50	0/480	0.49	0/648
11	K	0.68	2/398 (0.5%)	0.52	0/546
11	X	0.66	1/405 (0.2%)	0.49	0/556
12	L	0.57	0/393	0.51	0/526
12	Y	0.53	0/401	0.47	0/536
13	M	0.55	1/345 (0.3%)	0.52	0/470
13	Z	0.52	0/345	0.46	0/470
All	All	0.59	43/30045 (0.1%)	0.54	0/40817

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
6	S	0	1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	115	TRP	CD2-CE2	5.31	1.47	1.41
3	C	57	TRP	CD2-CE2	5.30	1.47	1.41
1	N	323	TRP	CD2-CE2	5.28	1.47	1.41
4	D	48	TRP	CD2-CE2	5.26	1.47	1.41
1	N	409	TRP	CD2-CE2	5.26	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4185	0	4159	59	0
1	N	4179	0	4154	50	0
2	B	1891	0	1890	18	0
2	O	1870	0	1868	17	0
3	C	2176	0	2092	26	0
3	P	2185	0	2097	23	0
4	D	1224	0	1211	10	0
4	Q	1224	0	1211	9	0
5	E	852	0	845	1	0
5	R	852	0	845	2	0
6	F	778	0	754	9	0
6	S	763	0	742	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	686	0	652	16	0
7	T	686	0	652	9	0
8	H	662	0	623	4	0
8	U	662	0	623	1	0
9	I	601	0	613	2	0
9	V	601	0	613	3	0
10	J	460	0	459	2	0
10	W	469	0	464	2	0
11	K	384	0	366	0	0
11	X	391	0	374	0	0
12	L	380	0	380	6	0
12	Y	388	0	388	6	0
13	M	335	0	352	6	0
13	Z	335	0	352	1	0
14	A	180	0	162	23	0
14	N	180	0	162	19	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	4	0
18	N	6	0	0	6	0
19	A	102	0	152	6	0
19	C	102	0	152	5	0
19	N	51	0	76	0	0
19	P	102	0	152	3	0
19	Z	51	0	76	3	0
20	A	48	0	72	9	0
20	B	4	0	6	0	0
20	C	32	0	48	2	0
20	D	20	0	30	8	0
20	E	20	0	30	0	0
20	F	12	0	18	0	0
20	G	12	0	18	0	0
20	H	4	0	6	1	0
20	J	4	0	6	0	0
20	N	44	0	66	3	0
20	O	12	0	18	0	0
20	P	12	0	18	1	0
20	Q	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	R	20	0	30	0	0
20	S	12	0	18	1	0
20	T	4	0	6	0	0
20	U	4	0	6	0	0
20	V	4	0	6	0	0
20	W	4	0	6	0	0
21	B	63	0	110	1	0
21	D	63	0	110	7	0
21	L	63	0	110	5	0
21	N	63	0	110	2	0
21	Q	63	0	110	2	0
21	Y	63	0	110	6	0
22	B	29	0	39	0	0
22	C	58	0	78	2	0
22	G	29	0	39	1	0
22	J	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	39	4	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	C	99	0	126	5	0
24	M	33	0	42	0	0
24	P	99	0	126	0	0
24	Z	33	0	42	0	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	14	0
26	G	100	0	156	7	0
26	P	100	0	156	8	0
26	T	100	0	156	4	0
27	C	106	0	154	2	0
27	G	53	0	77	4	0
27	P	106	0	154	1	0
27	T	53	0	77	3	0
28	E	52	0	80	5	0
28	O	52	0	80	5	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	223	0	0	2	0
30	B	141	0	0	4	1
30	C	100	0	0	4	0
30	D	97	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	E	78	0	0	1	0
30	F	86	0	0	3	0
30	G	42	0	0	0	0
30	H	35	0	0	0	0
30	I	21	0	0	1	0
30	J	21	0	0	0	0
30	K	26	0	0	0	0
30	L	29	0	0	0	0
30	M	25	0	0	1	0
30	N	204	0	0	2	0
30	O	102	0	0	0	0
30	P	102	0	0	1	0
30	Q	36	0	0	1	0
30	R	37	0	0	0	0
30	S	53	0	0	3	0
30	T	44	0	0	0	0
30	U	39	0	0	0	0
30	V	12	0	0	1	0
30	W	8	0	0	0	0
30	X	11	0	0	0	0
30	Y	14	0	0	0	0
30	Z	11	0	0	0	0
All	All	33590	0	32691	336	1

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 5.

The worst 5 of 336 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)
6:S:43:LYS:HE2	6:S:43:LYS:H	1.14	1.12
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.53	1.08
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:HBC1	1.38	1.02
21:D:201:TGL:HG31	30:D:343:HOH:O	1.62	0.98
14:N:602[B]:HEA:HMC1	14:N:602[B]:HEA:HBC1	1.44	0.97

All (1) 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)
30:B:437:HOH:O	30:D:335:HOH:O[2_584]	1.87	0.33

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/514 (104%)	517 (97%)	16 (3%)	0	100	100
1	N	532/514 (104%)	520 (98%)	12 (2%)	0	100	100
2	B	233/227 (103%)	229 (98%)	4 (2%)	0	100	100
2	O	230/227 (101%)	225 (98%)	4 (2%)	1 (0%)	34	19
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	22	9
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	100/98 (102%)	95 (95%)	3 (3%)	2 (2%)	7	1
6	S	98/98 (100%)	93 (95%)	3 (3%)	2 (2%)	7	1
7	G	82/85 (96%)	69 (84%)	7 (8%)	6 (7%)	1	0
7	T	82/85 (96%)	72 (88%)	7 (8%)	3 (4%)	3	0
8	H	77/85 (91%)	75 (97%)	1 (1%)	1 (1%)	12	3
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	12	3
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	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%)	46 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	1
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3592/3614 (99%)	3487 (97%)	87 (2%)	18 (0%)	29	15

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	T	8	HIS
6	F	95	GLN
12	Y	46	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	446/426 (105%)	442 (99%)	4 (1%)	78	72
1	N	445/426 (104%)	438 (98%)	7 (2%)	62	49
2	B	218/210 (104%)	209 (96%)	9 (4%)	30	13
2	O	215/210 (102%)	210 (98%)	5 (2%)	50	34
3	C	232/226 (103%)	228 (98%)	4 (2%)	60	47
3	P	233/226 (103%)	230 (99%)	3 (1%)	69	58
4	D	131/129 (102%)	129 (98%)	2 (2%)	65	53
4	Q	131/129 (102%)	130 (99%)	1 (1%)	81	76
5	E	92/95 (97%)	92 (100%)	0	100	100
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	36
6	F	85/81 (105%)	83 (98%)	2 (2%)	49	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S	83/81 (102%)	79 (95%)	4 (5%)	25	10
7	G	68/68 (100%)	65 (96%)	3 (4%)	28	12
7	T	68/68 (100%)	63 (93%)	5 (7%)	13	3
8	H	71/75 (95%)	69 (97%)	2 (3%)	43	27
8	U	71/75 (95%)	68 (96%)	3 (4%)	30	13
9	I	57/57 (100%)	57 (100%)	0	100	100
9	V	57/57 (100%)	56 (98%)	1 (2%)	59	45
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%)	40 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	30
12	Y	40/40 (100%)	40 (100%)	0	100	100
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	29
13	Z	37/38 (97%)	36 (97%)	1 (3%)	44	29
All	All	3126/3082 (101%)	3063 (98%)	63 (2%)	55	40

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	42	LYS
1	N	382[B]	SER
8	U	60	TYR
1	N	38	ARG
1	N	180	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
10	J	29	ASN
7	T	76	ASN
7	G	34	ASN
7	G	38	HIS



### 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	$\# Z  > 2$
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	1.15	0
1	FME	A	1	1	8,9,10	0.53	0	7,9,11	1.45	1 (14%)
2	FME	B	1	2	8,9,10	0.64	0	7,9,11	1.08	0
9	SAC	I	1	9	7,8,9	1.00	1 (14%)	8,9,11	0.76	0
7	TPO	G	11	7	8,10,11	1.38	1 (12%)	10,14,16	0.68	0
1	FME	N	1	1	8,9,10	0.58	0	7,9,11	1.17	0
9	SAC	V	1	9	7,8,9	1.25	1 (14%)	8,9,11	0.94	0
7	TPO	T	11	7	8,10,11	1.41	1 (12%)	10,14,16	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
9	SAC	I	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	3/9/11/13	-
1	FME	N	1	1	-	2/7/9/11	-
9	SAC	V	1	9	-	6/7/8/10	-
7	TPO	T	11	7	-	5/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	3.14	1.50	1.46
7	G	11	TPO	P-O1P	2.83	1.59	1.50
7	T	11	TPO	P-O1P	2.78	1.59	1.50
9	I	1	SAC	CA-N	2.40	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	2.53	114.30	109.73

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 125 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
20	EDO	N	620	-	3,3,3	0.47	0	2,2,2	0.37	0
21	TGL	Y	101	-	62,62,62	1.06	3 (4%)	65,65,65	1.10	4 (6%)
20	EDO	A	614	-	3,3,3	0.52	0	2,2,2	1.03	0
19	PGV	N	608	-	50,50,50	0.86	2 (4%)	53,56,56	0.88	2 (3%)
26	CDL	G	102	-	99,99,99	1.32	12 (12%)	105,111,111	1.07	4 (3%)
20	EDO	C	319	-	3,3,3	0.51	0	2,2,2	0.19	0
20	EDO	C	317	-	3,3,3	0.48	0	2,2,2	0.31	0
19	PGV	A	609	-	50,50,50	0.97	2 (4%)	53,56,56	1.03	2 (3%)
24	DMU	M	101	-	34,34,34	0.45	0	45,45,45	0.67	1 (2%)
23	CUA	O	301	2	0,1,1	0.00	-	-	-	-
18	AZI	N	607	14	0,2,2	0.00	-	0,1,1	0.00	-
20	EDO	G	106	-	3,3,3	0.48	0	2,2,2	0.24	0
20	EDO	P	314	-	3,3,3	0.43	0	2,2,2	0.39	0
20	EDO	R	203	-	3,3,3	0.47	0	2,2,2	0.36	0
20	EDO	O	304	-	3,3,3	0.43	0	2,2,2	0.44	0
20	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.24	0
20	EDO	C	313	-	3,3,3	0.46	0	2,2,2	0.36	0
19	PGV	C	304	-	50,50,50	0.89	2 (4%)	53,56,56	0.78	3 (5%)
20	EDO	O	303	-	3,3,3	0.46	0	2,2,2	0.42	0
20	EDO	C	312	-	3,3,3	0.51	0	2,2,2	0.32	0
20	EDO	S	104	-	3,3,3	0.39	0	2,2,2	0.51	0
20	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.54	0
19	PGV	A	608	-	50,50,50	0.91	2 (4%)	53,56,56	0.89	3 (5%)
20	EDO	D	206	-	3,3,3	0.41	0	2,2,2	0.45	0
20	EDO	G	104	-	3,3,3	0.42	0	2,2,2	0.40	0
20	EDO	A	619	-	3,3,3	0.49	0	2,2,2	0.29	0
20	EDO	F	103	-	3,3,3	0.47	0	2,2,2	0.33	0
27	PEK	C	309	-	52,52,52	0.95	2 (3%)	55,57,57	1.00	3 (5%)
20	EDO	E	205	-	3,3,3	0.46	0	2,2,2	0.28	0
14	HEA	N	601	1	44,67,67	0.86	2 (4%)	37,103,103	1.53	7 (18%)
24	DMU	C	310	-	34,34,34	0.52	0	45,45,45	1.06	3 (6%)
14	HEA	A	601	1	44,67,67	0.85	1 (2%)	37,103,103	1.60	8 (21%)
14	HEA	N	602[A]	1,18	44,67,67	0.95	1 (2%)	37,103,103	1.97	9 (24%)
20	EDO	A	618	-	3,3,3	0.46	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	PEK	G	101	-	52,52,52	0.86	2 (3%)	55,57,57	0.81	1 (1%)
20	EDO	F	104	-	3,3,3	0.43	0	2,2,2	0.33	0
20	EDO	A	617	-	3,3,3	0.40	0	2,2,2	0.44	0
20	EDO	C	316	-	3,3,3	0.47	0	2,2,2	0.32	0
20	EDO	R	201	-	3,3,3	0.42	0	2,2,2	0.41	0
24	DMU	P	311	-	34,34,34	0.49	0	45,45,45	0.76	0
20	EDO	C	314	-	3,3,3	0.46	0	2,2,2	0.37	0
20	EDO	Q	202	-	3,3,3	0.43	0	2,2,2	0.42	0
27	PEK	T	101	-	52,52,52	0.86	2 (3%)	55,57,57	0.86	3 (5%)
26	CDL	C	305	-	99,99,99	1.31	12 (12%)	105,111,111	1.11	6 (5%)
20	EDO	N	614	-	3,3,3	0.58	0	2,2,2	0.28	0
20	EDO	D	203	-	3,3,3	0.47	0	2,2,2	0.12	0
21	TGL	D	201	-	62,62,62	1.03	3 (4%)	65,65,65	0.90	3 (4%)
27	PEK	P	302	-	52,52,52	0.95	2 (3%)	55,57,57	0.98	3 (5%)
24	DMU	P	308	-	34,34,34	0.50	0	45,45,45	0.74	0
20	EDO	A	613	-	3,3,3	0.42	0	2,2,2	0.47	0
20	EDO	N	610	-	3,3,3	0.45	0	2,2,2	0.31	0
21	TGL	B	301	-	62,62,62	1.03	3 (4%)	65,65,65	1.07	4 (6%)
20	EDO	R	205	-	3,3,3	0.52	0	2,2,2	0.25	0
20	EDO	N	618	-	3,3,3	0.47	0	2,2,2	0.30	0
20	EDO	P	312	-	3,3,3	0.48	0	2,2,2	0.28	0
20	EDO	E	203	-	3,3,3	0.45	0	2,2,2	0.39	0
18	AZI	A	606	15	0,2,2	0.00	-	0,1,1	0.00	-
20	EDO	O	305	-	3,3,3	0.45	0	2,2,2	0.35	0
19	PGV	P	303	-	50,50,50	0.96	2 (4%)	53,56,56	0.92	2 (3%)
27	PEK	C	307	-	52,52,52	0.95	2 (3%)	55,57,57	1.00	2 (3%)
18	AZI	A	607	14	0,2,2	0.00	-	0,1,1	0.00	-
20	EDO	E	204	-	3,3,3	0.39	0	2,2,2	0.51	0
21	TGL	N	609	-	62,62,62	1.02	3 (4%)	65,65,65	1.03	3 (4%)
21	TGL	L	101	-	62,62,62	1.03	3 (4%)	65,65,65	1.08	5 (7%)
26	CDL	P	306	-	99,99,99	1.32	12 (12%)	105,111,111	1.08	5 (4%)
20	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.45	0
18	AZI	N	606	15	0,2,2	0.00	-	0,1,1	0.00	-
20	EDO	V	101	-	3,3,3	0.44	0	2,2,2	0.39	0
22	CHD	P	301	-	29,32,32	0.55	0	48,51,51	0.93	1 (2%)
24	DMU	P	310	-	34,34,34	0.52	0	45,45,45	1.09	2 (4%)
20	EDO	H	101	-	3,3,3	0.41	0	2,2,2	0.54	0
20	EDO	D	205	-	3,3,3	0.44	0	2,2,2	0.29	0
20	EDO	W	102	-	3,3,3	0.42	0	2,2,2	0.42	0
20	EDO	A	616	-	3,3,3	0.44	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	E	202	-	3,3,3	0.49	0	2,2,2	0.30	0
22	CHD	J	101	-	29,32,32	0.49	0	48,51,51	1.25	6 (12%)
20	EDO	Q	203	-	3,3,3	0.49	0	2,2,2	0.44	0
22	CHD	C	301	-	29,32,32	0.54	0	48,51,51	0.87	1 (2%)
20	EDO	A	610	-	3,3,3	0.41	0	2,2,2	0.47	0
22	CHD	B	302	-	29,32,32	0.64	0	48,51,51	0.85	1 (2%)
14	HEA	A	602[A]	1,18	44,67,67	0.97	1 (2%)	37,103,103	1.77	7 (18%)
27	PEK	P	309	-	52,52,52	0.95	2 (3%)	55,57,57	0.89	2 (3%)
20	EDO	E	206	-	3,3,3	0.45	0	2,2,2	0.39	0
20	EDO	N	619	-	3,3,3	0.44	0	2,2,2	0.41	0
23	CUA	B	303	2	0,1,1	0.00	-	-		
20	EDO	N	613	-	3,3,3	0.40	0	2,2,2	0.47	0
20	EDO	D	204	-	3,3,3	0.50	0	2,2,2	0.25	0
19	PGV	C	308	-	50,50,50	0.97	2 (4%)	53,56,56	0.97	3 (5%)
20	EDO	R	204	-	3,3,3	0.46	0	2,2,2	0.39	0
20	EDO	C	318	-	3,3,3	0.48	0	2,2,2	0.29	0
20	EDO	N	611	-	3,3,3	0.52	0	2,2,2	0.37	0
20	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.27	0
20	EDO	S	102	-	3,3,3	0.52	0	2,2,2	0.29	0
20	EDO	G	105	-	3,3,3	0.53	0	2,2,2	0.21	0
14	HEA	A	602[B]	1,18	44,67,67	0.90	1 (2%)	37,103,103	1.57	7 (18%)
20	EDO	N	617	-	3,3,3	0.49	0	2,2,2	0.14	0
14	HEA	N	602[B]	1,18	44,67,67	0.93	1 (2%)	37,103,103	1.63	5 (13%)
20	EDO	A	615	-	3,3,3	0.54	0	2,2,2	0.33	0
24	DMU	C	302	-	34,34,34	0.45	0	45,45,45	0.70	1 (2%)
26	CDL	T	102	-	99,99,99	1.32	12 (12%)	105,111,111	1.10	5 (4%)
22	CHD	G	103	-	29,32,32	0.60	0	48,51,51	0.91	1 (2%)
19	PGV	Z	101	-	50,50,50	0.96	2 (4%)	53,56,56	1.10	3 (5%)
20	EDO	N	615	-	3,3,3	0.43	0	2,2,2	0.35	0
20	EDO	A	620	-	3,3,3	0.37	0	2,2,2	0.71	0
20	EDO	C	315	-	3,3,3	0.42	0	2,2,2	0.63	0
20	EDO	N	612	-	3,3,3	0.47	0	2,2,2	0.36	0
20	EDO	A	621	-	3,3,3	0.44	0	2,2,2	0.37	0
20	EDO	Q	204	-	3,3,3	0.48	0	2,2,2	0.20	0
20	EDO	D	202	-	3,3,3	0.34	0	2,2,2	0.53	0
24	DMU	Z	102	-	34,34,34	0.46	0	45,45,45	0.68	1 (2%)
22	CHD	C	306	-	29,32,32	0.49	0	48,51,51	1.25	5 (10%)
22	CHD	W	101	-	29,32,32	0.47	0	48,51,51	2.18	15 (31%)
24	DMU	C	311	-	34,34,34	0.61	1 (2%)	45,45,45	1.31	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	J	102	-	3,3,3	0.45	0	2,2,2	0.38	0
20	EDO	P	313	-	3,3,3	0.53	0	2,2,2	0.23	0
22	CHD	P	307	-	29,32,32	0.52	0	48,51,51	1.45	10 (20%)
20	EDO	T	103	-	3,3,3	0.54	0	2,2,2	0.28	0
20	EDO	U	101	-	3,3,3	0.45	0	2,2,2	0.35	0
21	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.02	3 (4%)
28	PSC	E	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.00	2 (3%)
20	EDO	S	103	-	3,3,3	0.44	0	2,2,2	0.46	0
19	PGV	P	305	-	50,50,50	0.87	2 (4%)	53,56,56	0.76	0
20	EDO	F	102	-	3,3,3	0.51	0	2,2,2	0.30	0
20	EDO	R	202	-	3,3,3	0.46	0	2,2,2	0.39	0
28	PSC	O	302	-	51,51,51	1.10	3 (5%)	57,59,59	1.01	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	620	-	-	1/1/1/1	-
21	TGL	Y	101	-	-	38/65/65/65	-
20	EDO	A	614	-	-	1/1/1/1	-
19	PGV	N	608	-	-	10/55/55/55	-
26	CDL	G	102	-	-	66/110/110/110	-
20	EDO	C	319	-	-	1/1/1/1	-
20	EDO	C	317	-	-	0/1/1/1	-
19	PGV	A	609	-	-	26/55/55/55	-
24	DMU	M	101	-	-	3/19/59/59	0/2/2/2
20	EDO	G	106	-	-	1/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	R	203	-	-	0/1/1/1	-
20	EDO	O	304	-	-	1/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
20	EDO	C	313	-	-	0/1/1/1	-
19	PGV	C	304	-	-	20/55/55/55	-
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	C	312	-	-	0/1/1/1	-
20	EDO	S	104	-	-	1/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
19	PGV	A	608	-	-	9/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	D	206	-	-	1/1/1/1	-
20	EDO	G	104	-	-	1/1/1/1	-
20	EDO	A	619	-	-	1/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
27	PEK	C	309	-	-	33/56/56/56	-
20	EDO	E	205	-	-	1/1/1/1	-
14	HEA	N	601	1	3/3/7/16	6/24/76/76	-
24	DMU	C	310	-	-	6/19/59/59	0/2/2/2
14	HEA	A	601	1	3/3/7/16	5/24/76/76	-
14	HEA	N	602[A]	1,18	3/3/7/16	0/24/76/76	-
20	EDO	A	618	-	-	1/1/1/1	-
27	PEK	G	101	-	-	15/56/56/56	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
20	EDO	C	316	-	-	1/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
24	DMU	P	311	-	-	13/19/59/59	0/2/2/2
20	EDO	C	314	-	-	1/1/1/1	-
20	EDO	Q	202	-	-	0/1/1/1	-
27	PEK	T	101	-	-	18/56/56/56	-
26	CDL	C	305	-	-	63/110/110/110	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	D	203	-	-	1/1/1/1	-
21	TGL	D	201	-	-	38/65/65/65	-
27	PEK	P	302	-	-	31/56/56/56	-
24	DMU	P	308	-	-	8/19/59/59	0/2/2/2
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	N	610	-	-	1/1/1/1	-
21	TGL	B	301	-	-	43/65/65/65	-
20	EDO	R	205	-	-	1/1/1/1	-
20	EDO	N	618	-	-	0/1/1/1	-
20	EDO	P	312	-	-	1/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
20	EDO	O	305	-	-	0/1/1/1	-
19	PGV	P	303	-	-	30/55/55/55	-
27	PEK	C	307	-	-	34/56/56/56	-
20	EDO	E	204	-	-	1/1/1/1	-
21	TGL	N	609	-	-	41/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	L	101	-	-	39/65/65/65	-
26	CDL	P	306	-	-	53/110/110/110	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	V	101	-	-	0/1/1/1	-
22	CHD	P	301	-	-	0/7/74/74	0/4/4/4
24	DMU	P	310	-	-	9/19/59/59	0/2/2/2
20	EDO	H	101	-	-	0/1/1/1	-
20	EDO	D	205	-	-	1/1/1/1	-
20	EDO	W	102	-	-	1/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	E	202	-	-	0/1/1/1	-
22	CHD	J	101	-	-	7/7/74/74	0/4/4/4
20	EDO	Q	203	-	-	0/1/1/1	-
22	CHD	C	301	-	-	0/7/74/74	0/4/4/4
20	EDO	A	610	-	-	1/1/1/1	-
22	CHD	B	302	-	-	0/7/74/74	0/4/4/4
14	HEA	A	602[A]	1,18	3/3/7/16	2/24/76/76	-
27	PEK	P	309	-	-	30/56/56/56	-
20	EDO	E	206	-	-	0/1/1/1	-
20	EDO	N	619	-	-	1/1/1/1	-
20	EDO	N	613	-	-	1/1/1/1	-
20	EDO	D	204	-	-	1/1/1/1	-
19	PGV	C	308	-	-	31/55/55/55	-
20	EDO	R	204	-	-	1/1/1/1	-
20	EDO	C	318	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	B	304	-	-	0/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	G	105	-	-	0/1/1/1	-
14	HEA	A	602[B]	1,18	3/3/7/16	2/24/76/76	-
20	EDO	N	617	-	-	0/1/1/1	-
14	HEA	N	602[B]	1,18	3/3/7/16	3/24/76/76	-
20	EDO	A	615	-	-	0/1/1/1	-
24	DMU	C	302	-	-	11/19/59/59	0/2/2/2
26	CDL	T	102	-	-	70/110/110/110	-
22	CHD	G	103	-	-	0/7/74/74	0/4/4/4
19	PGV	Z	101	-	-	30/55/55/55	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	A	620	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	C	315	-	-	0/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
20	EDO	A	621	-	-	1/1/1/1	-
20	EDO	Q	204	-	-	0/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
24	DMU	Z	102	-	-	7/19/59/59	0/2/2/2
22	CHD	C	306	-	-	4/7/74/74	0/4/4/4
22	CHD	W	101	-	-	5/7/74/74	0/4/4/4
24	DMU	C	311	-	-	8/19/59/59	0/2/2/2
20	EDO	J	102	-	-	1/1/1/1	-
20	EDO	P	313	-	-	0/1/1/1	-
22	CHD	P	307	-	-	7/7/74/74	0/4/4/4
20	EDO	T	103	-	-	0/1/1/1	-
20	EDO	U	101	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	35/65/65/65	-
28	PSC	E	201	-	-	27/55/55/55	-
20	EDO	S	103	-	-	0/1/1/1	-
19	PGV	P	305	-	-	15/55/55/55	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	R	202	-	-	1/1/1/1	-
28	PSC	O	302	-	-	35/55/55/55	-

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	101	TGL	OG2-CB1	4.64	1.47	1.34
26	P	306	CDL	OB8-CB7	4.64	1.46	1.33
26	C	305	CDL	OB8-CB7	4.62	1.46	1.33
19	Z	101	PGV	O03-C19	4.60	1.46	1.33
21	Y	101	TGL	OG3-CC1	4.56	1.46	1.33

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	CAD-CBD-CGD	-5.92	102.74	112.67
22	W	101	CHD	C14-C8-C7	5.82	119.52	111.81
22	W	101	CHD	C6-C5-C4	-5.27	105.12	111.19
14	N	602[A]	HEA	OMA-CMA-C3A	-5.02	113.98	124.91
21	Y	101	TGL	OG2-CB1-CB2	4.79	121.83	111.50

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	601	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA

5 of 1018 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	Y	101	TGL	CB2-CB1-OG2-CG2
21	Y	101	TGL	OB1-CB1-OG2-CG2
26	G	102	CDL	CA3-OA5-PA1-OA2
26	G	102	CDL	C11-CA5-OA6-CA4
26	G	102	CDL	CB2-OB2-PB2-OB3

There are no ring outliers.

57 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	Y	101	TGL	6	0
20	A	614	EDO	1	0
26	G	102	CDL	7	0
19	A	609	PGV	4	0
18	N	607	AZI	6	0
20	N	616	EDO	1	0
19	C	304	PGV	1	0
20	S	104	EDO	1	0
20	A	612	EDO	3	0
19	A	608	PGV	2	0
27	C	309	PEK	2	0
14	N	601	HEA	3	0
24	C	310	DMU	1	0
14	A	601	HEA	8	0
14	N	602[A]	HEA	9	0
20	A	618	EDO	1	0
27	G	101	PEK	4	0
20	A	617	EDO	2	0
27	T	101	PEK	3	0
26	C	305	CDL	14	0
20	D	203	EDO	3	0
21	D	201	TGL	7	0

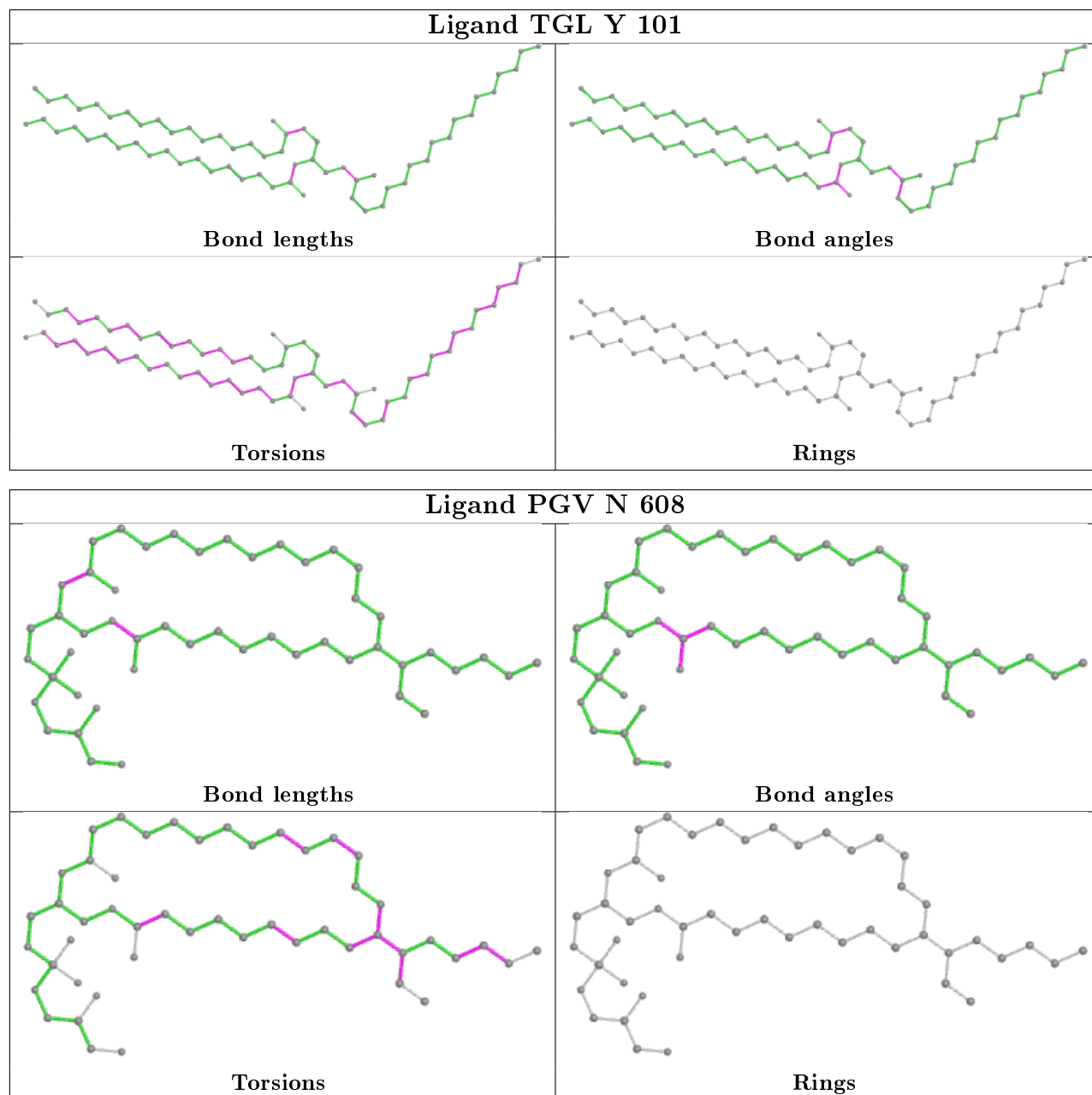
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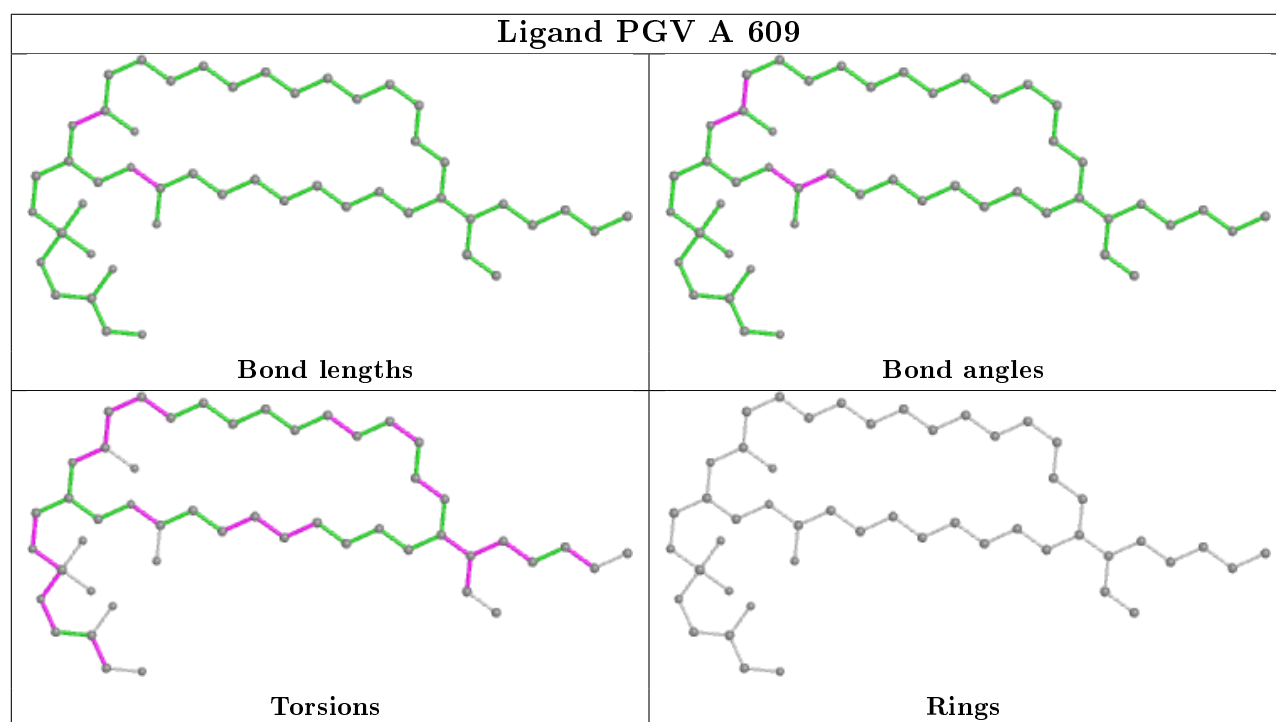
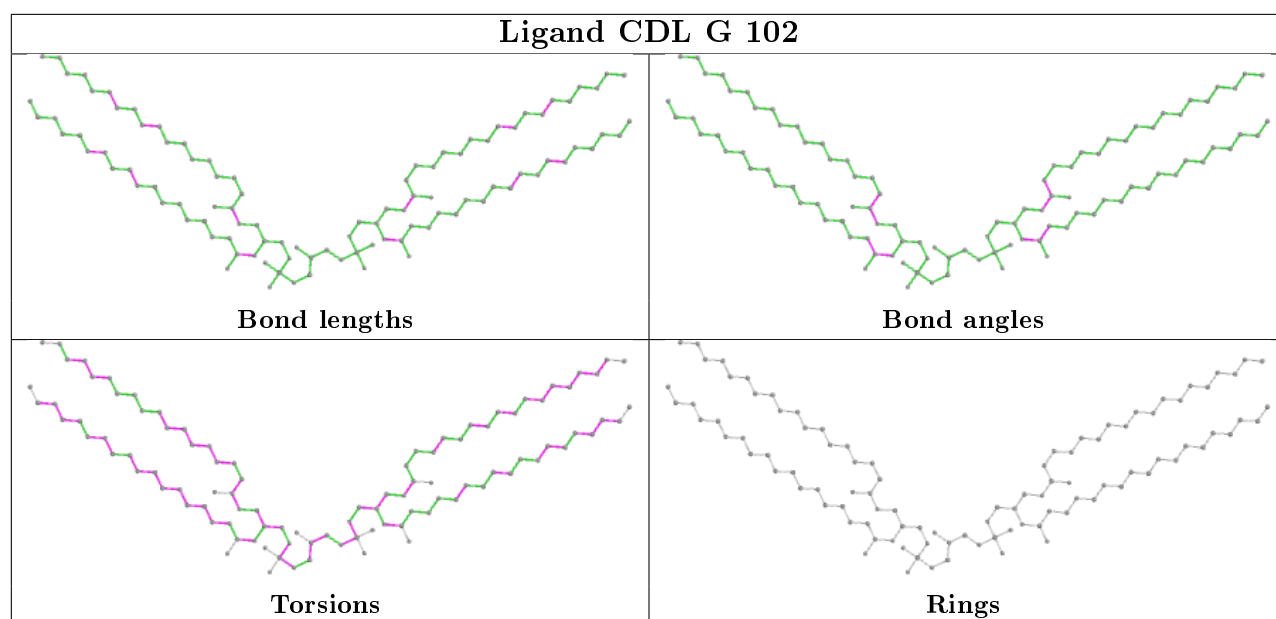
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	301	TGL	1	0
20	P	312	EDO	1	0
18	A	606	AZI	1	0
19	P	303	PGV	1	0
18	A	607	AZI	4	0
21	N	609	TGL	2	0
21	L	101	TGL	5	0
26	P	306	CDL	8	0
20	A	611	EDO	1	0
18	N	606	AZI	1	0
20	H	101	EDO	1	0
22	J	101	CHD	1	0
22	C	301	CHD	1	0
14	A	602[A]	HEA	6	0
27	P	309	PEK	1	0
19	C	308	PGV	4	0
20	N	611	EDO	1	0
14	A	602[B]	HEA	9	0
20	N	617	EDO	1	0
14	N	602[B]	HEA	7	0
24	C	302	DMU	4	0
26	T	102	CDL	4	0
22	G	103	CHD	1	0
19	Z	101	PGV	3	0
20	C	315	EDO	2	0
20	A	621	EDO	1	0
20	Q	204	EDO	1	0
20	D	202	EDO	5	0
22	C	306	CHD	1	0
22	W	101	CHD	4	0
22	P	307	CHD	3	0
21	Q	201	TGL	2	0
28	E	201	PSC	5	0
19	P	305	PGV	2	0
28	O	302	PSC	5	0

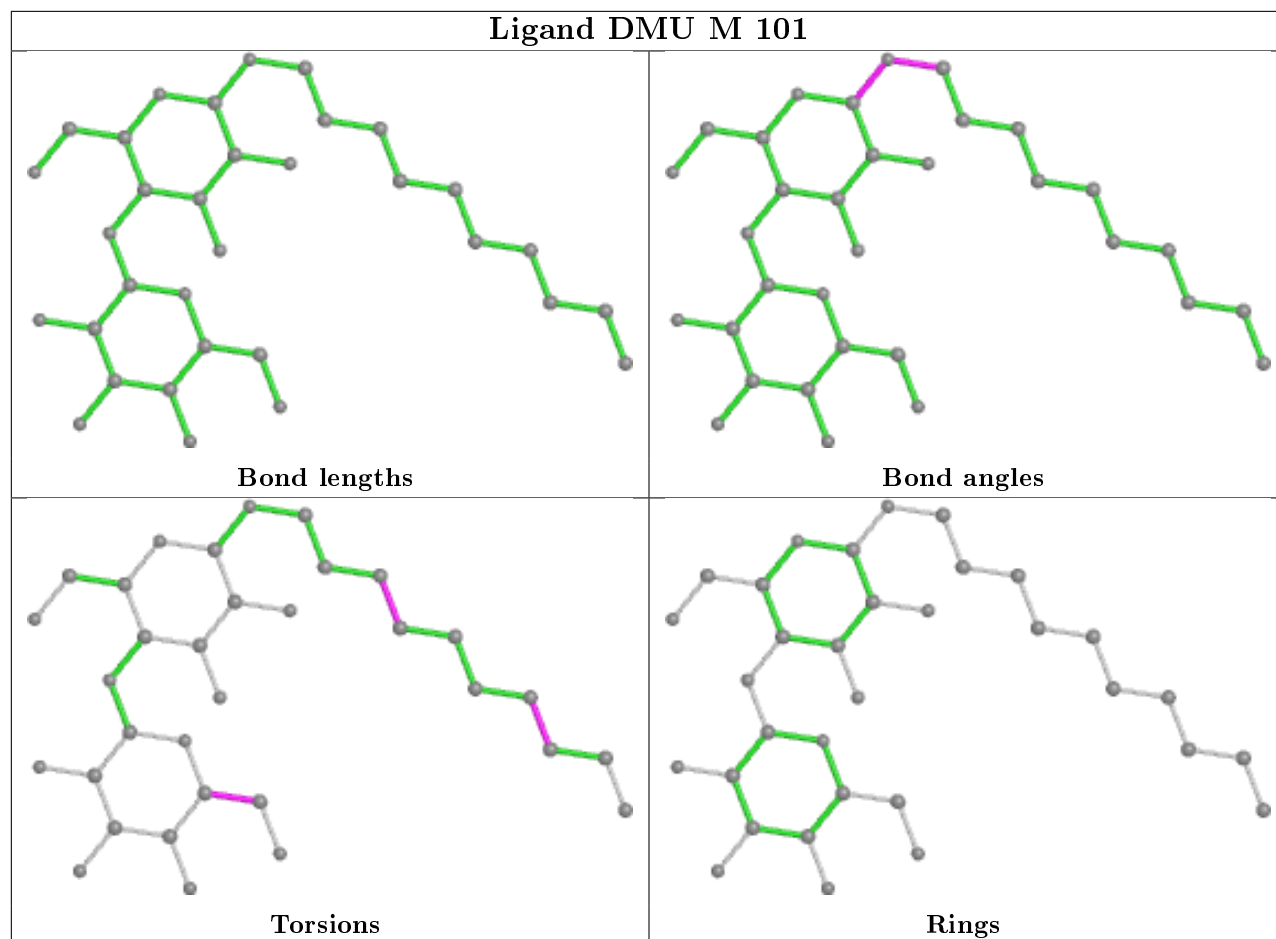
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

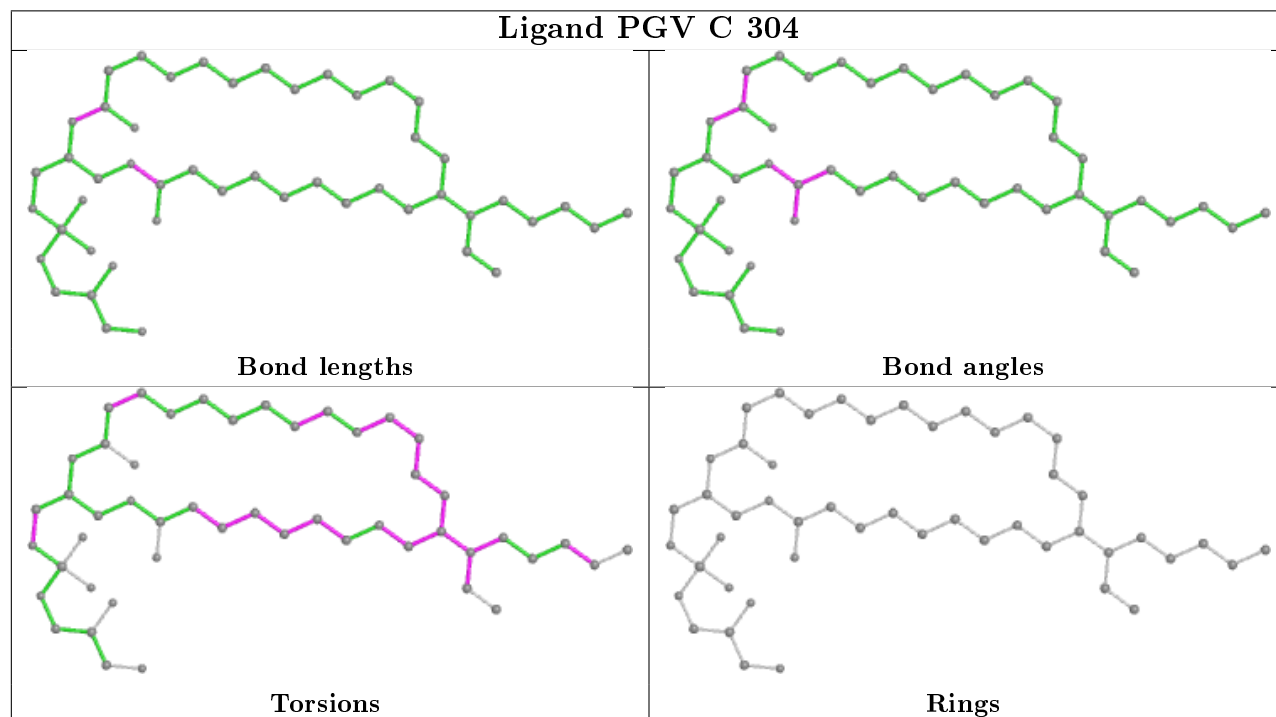


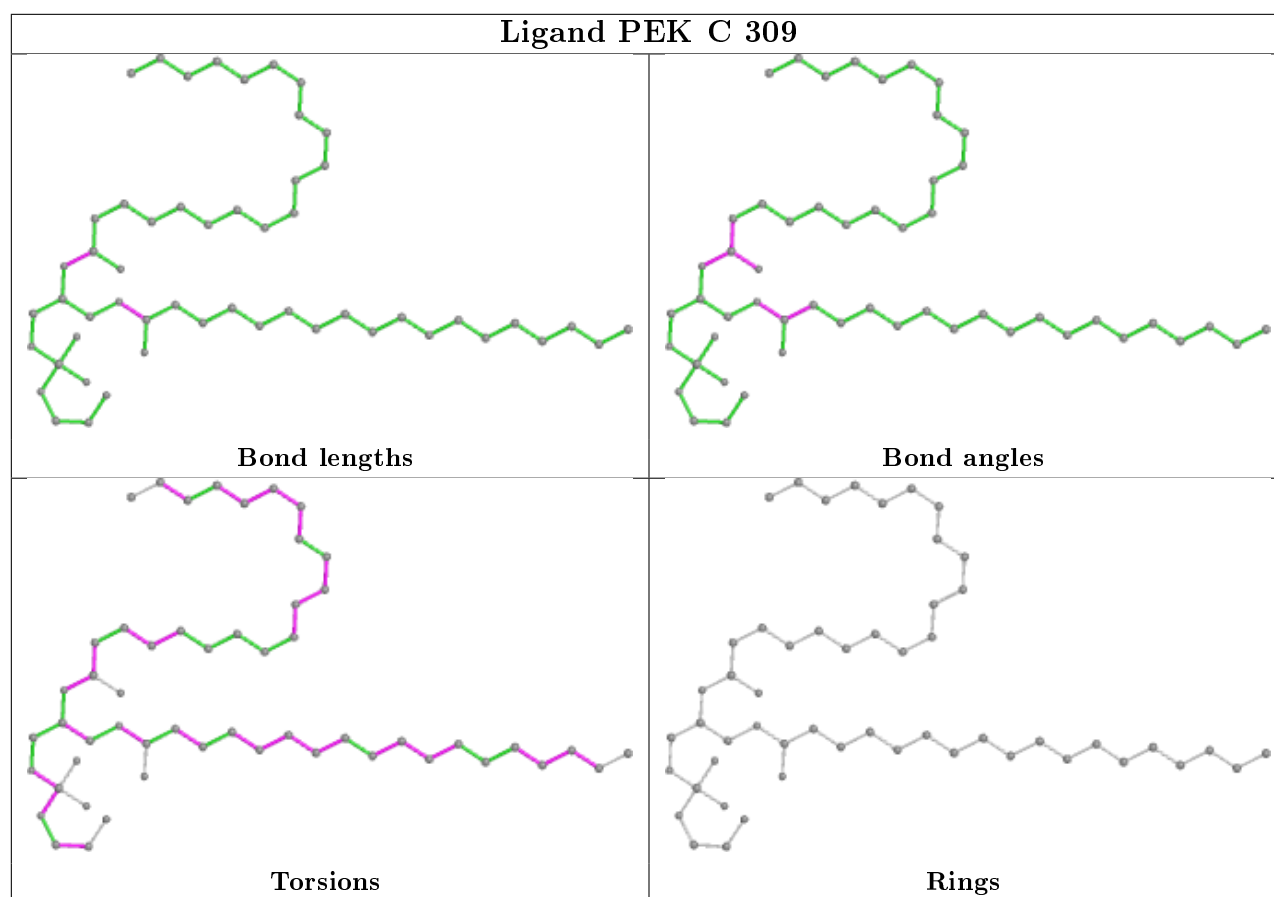
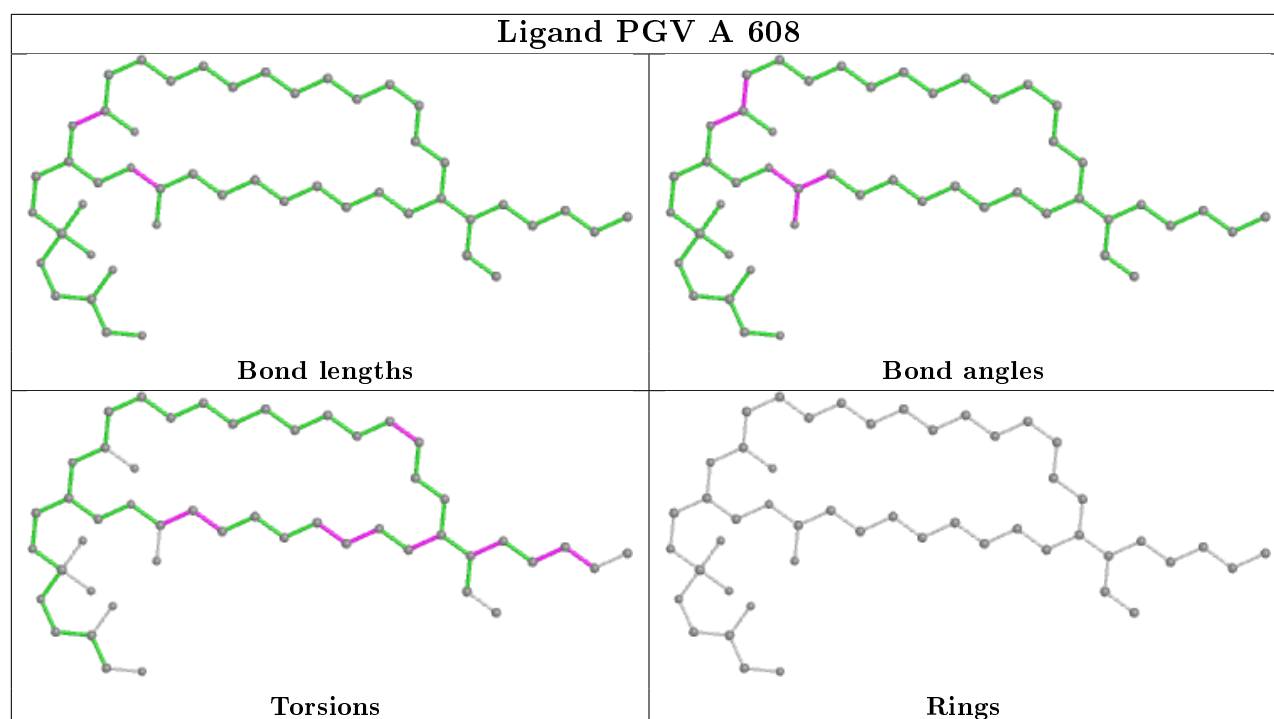


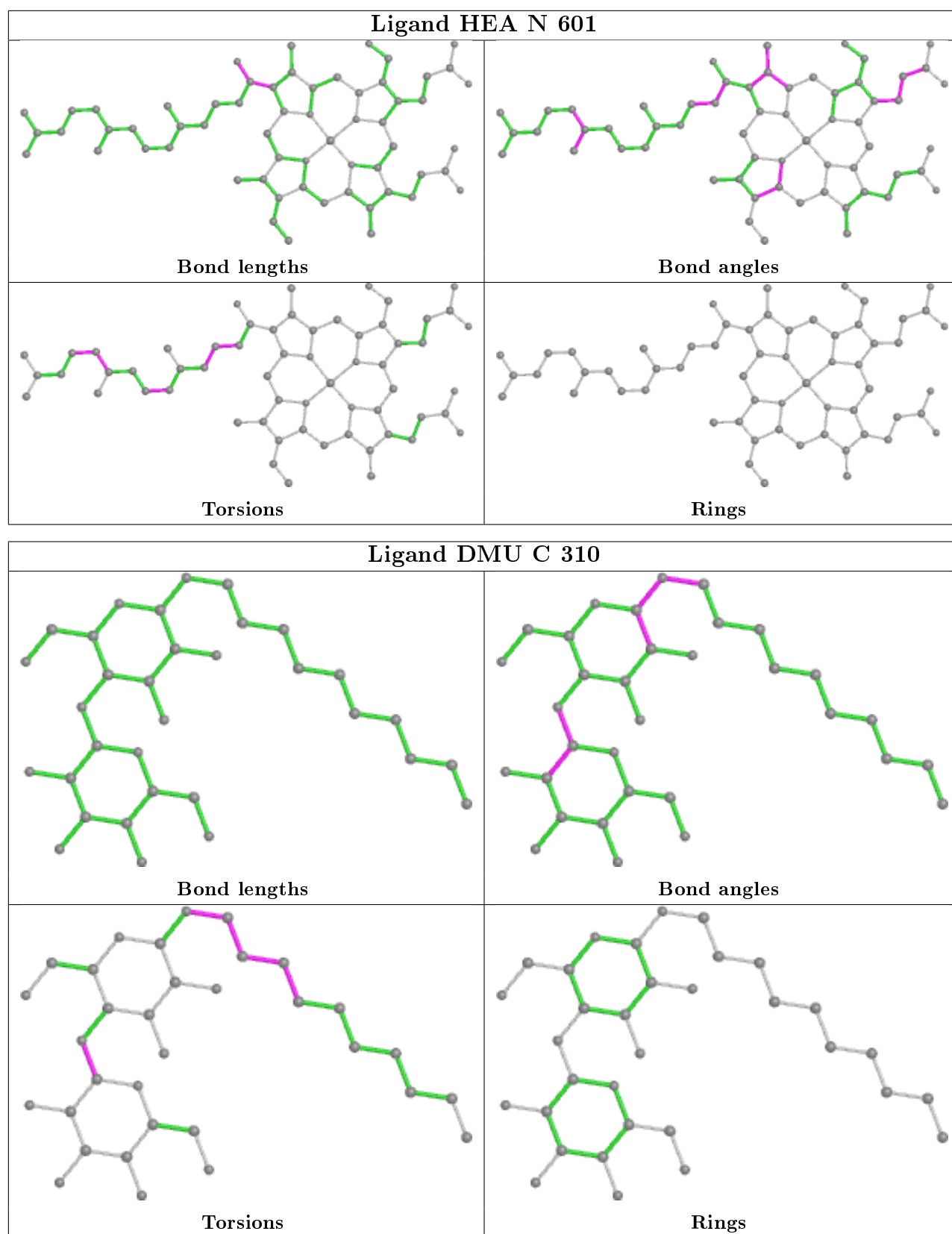
## Ligand DMU M 101



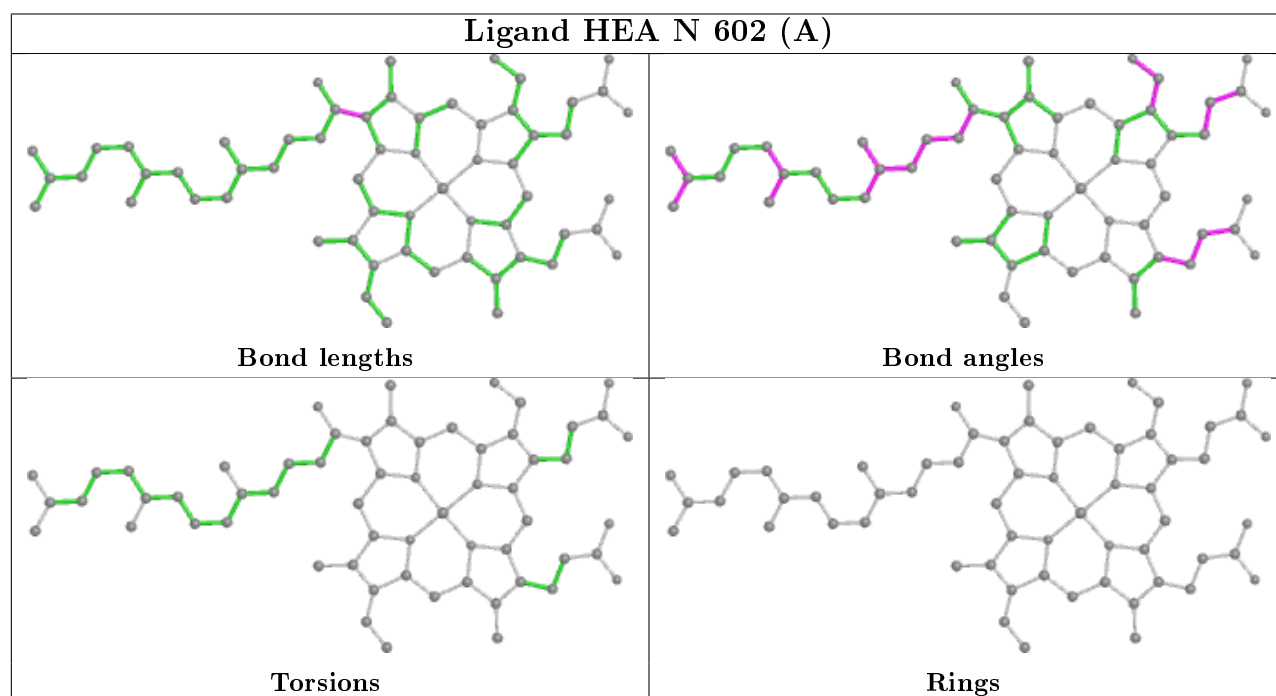
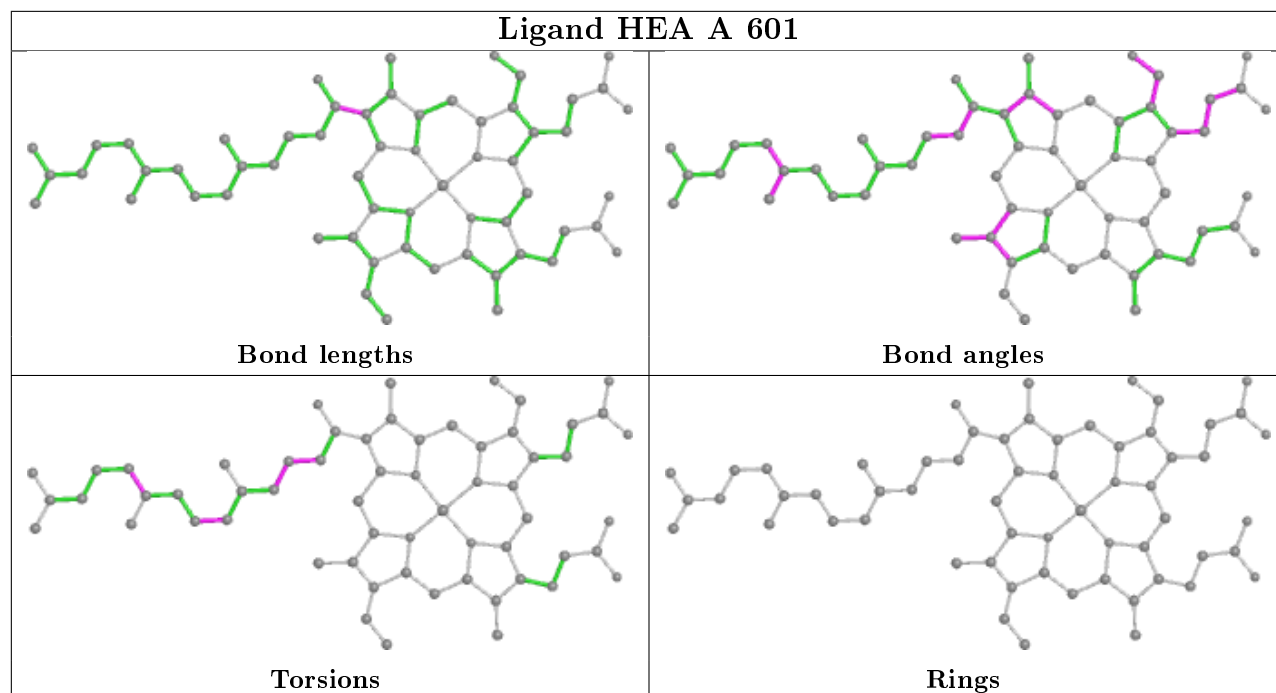
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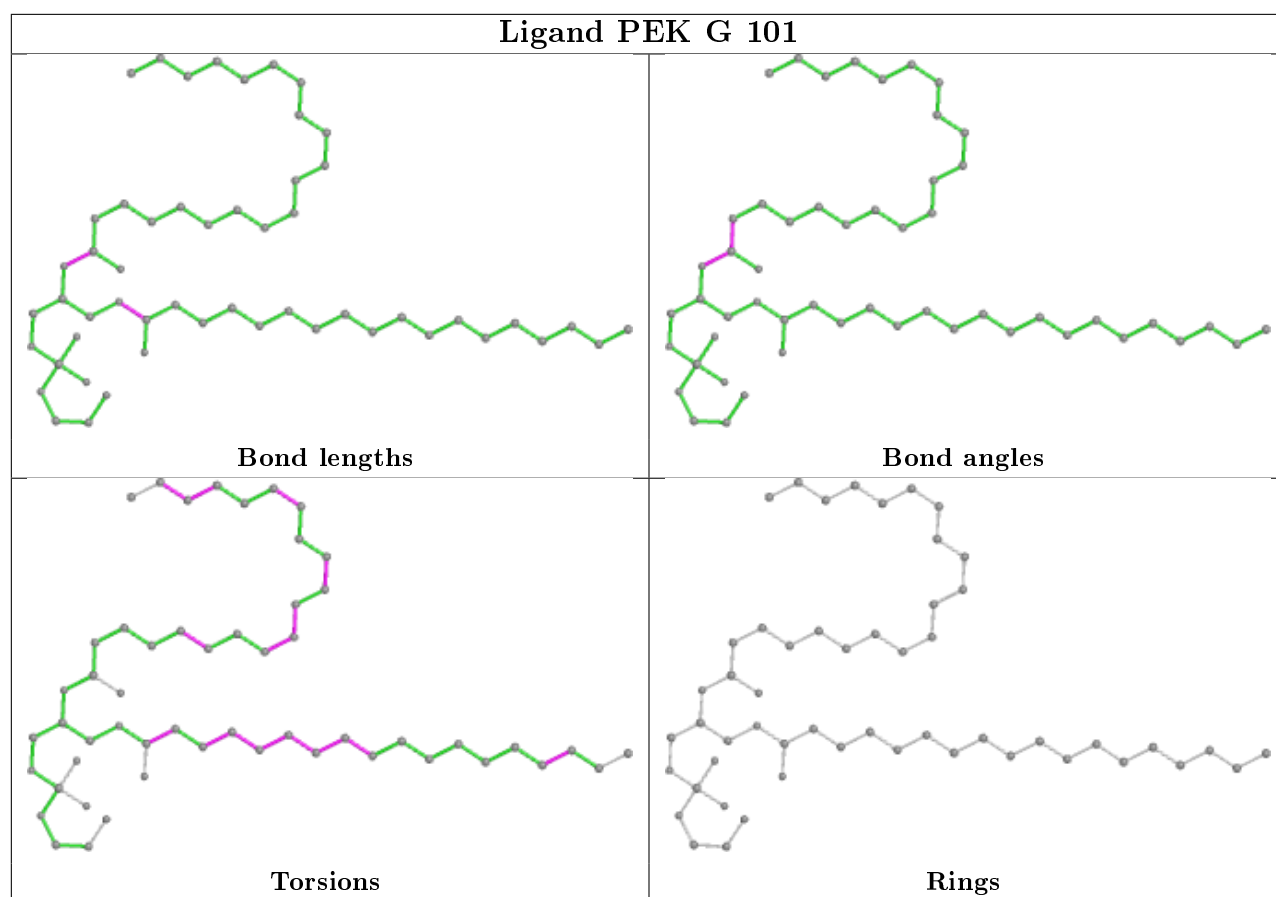


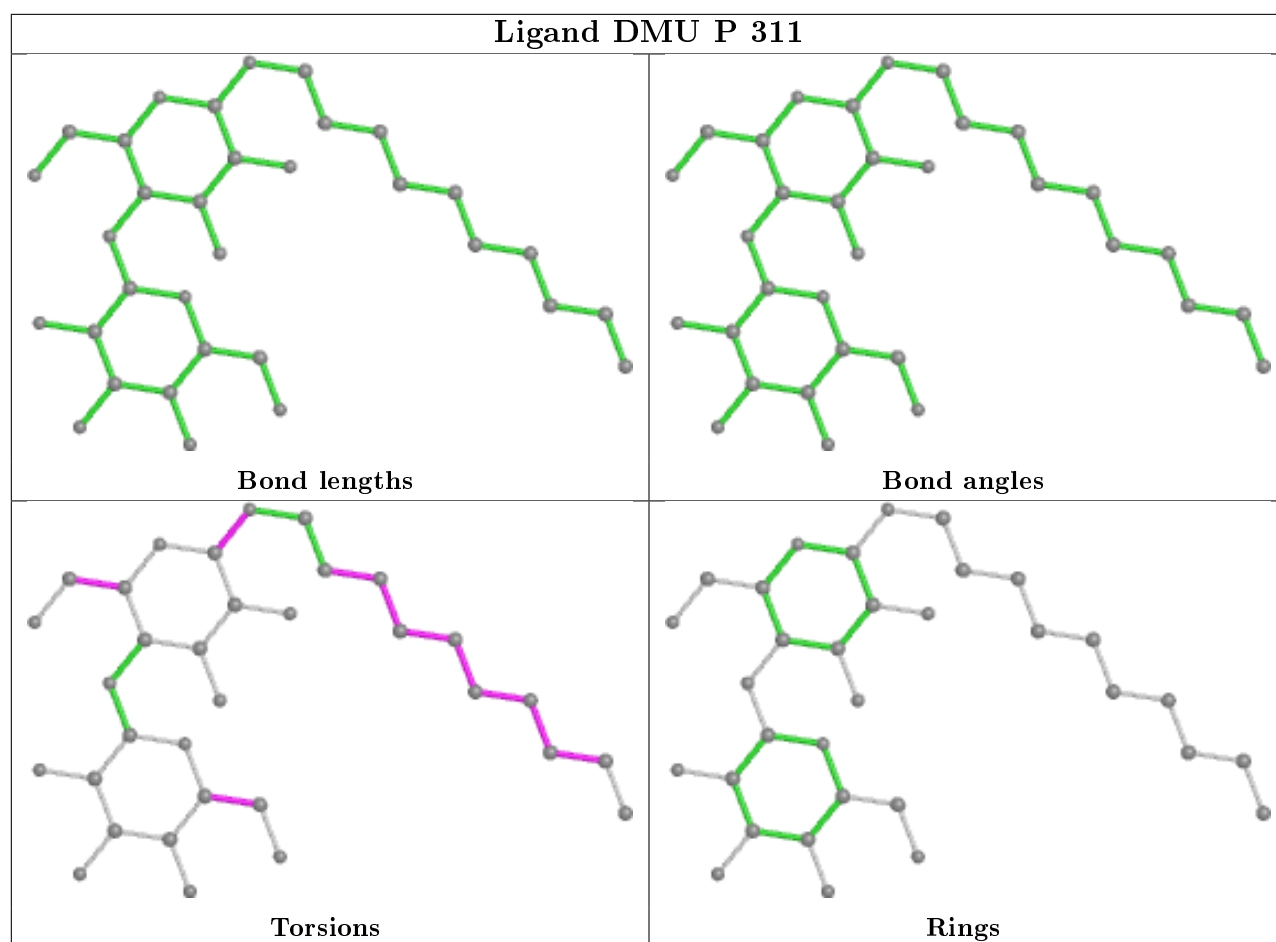


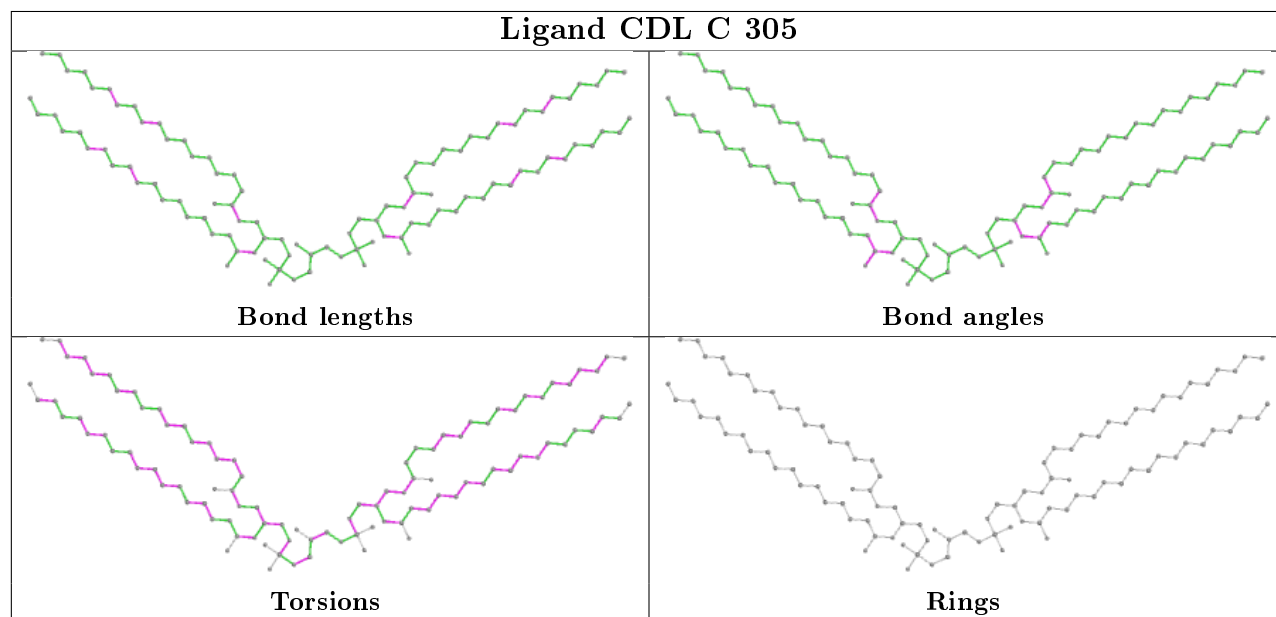
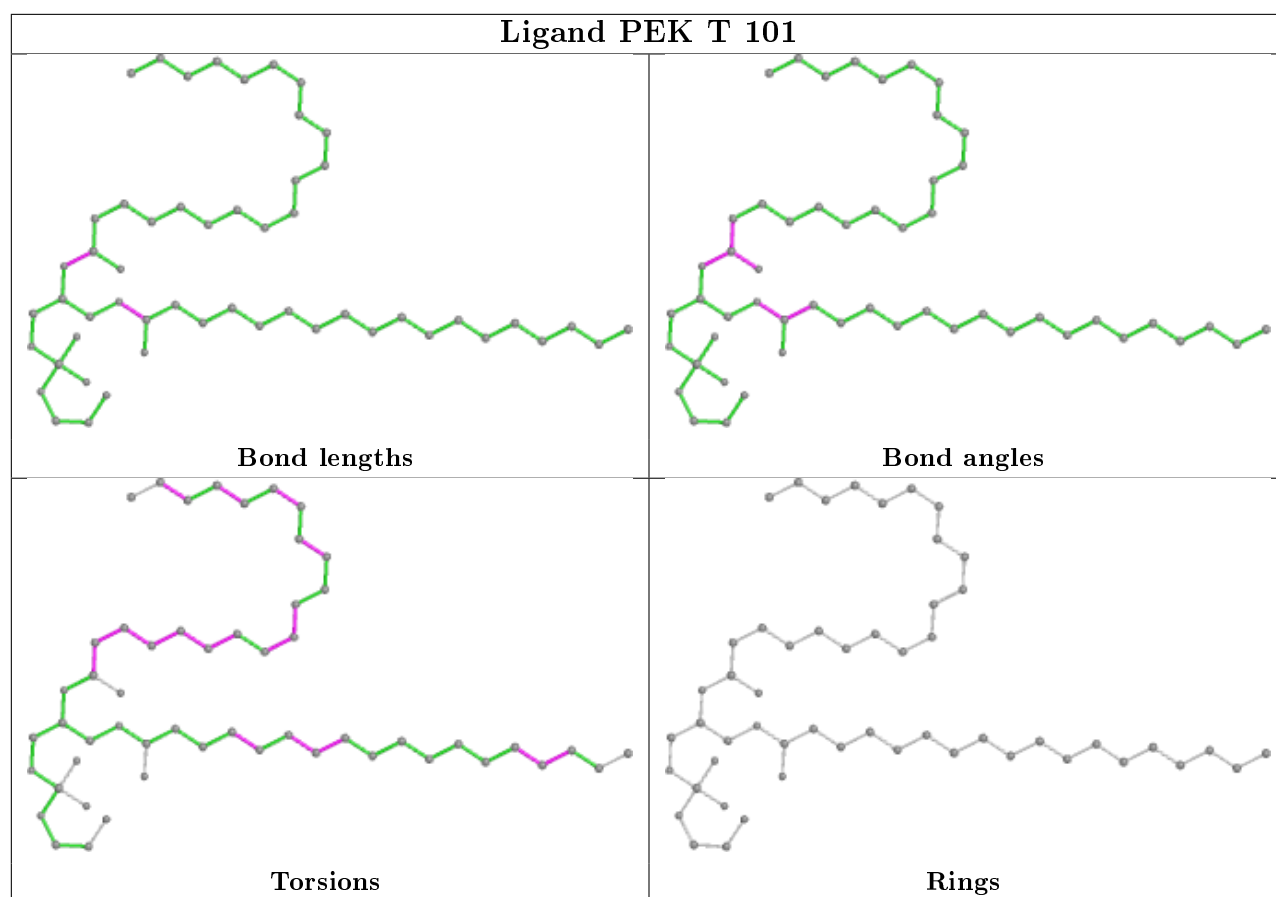


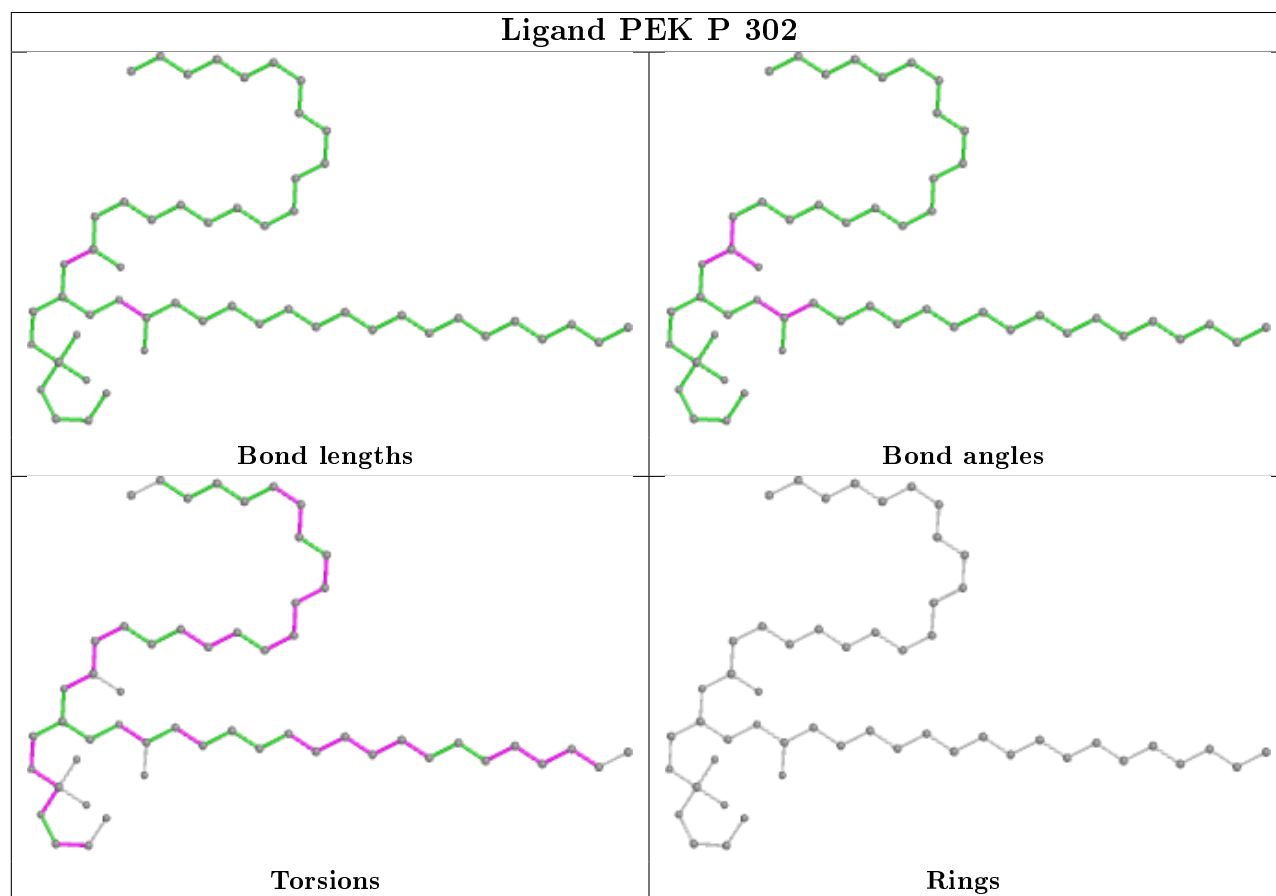
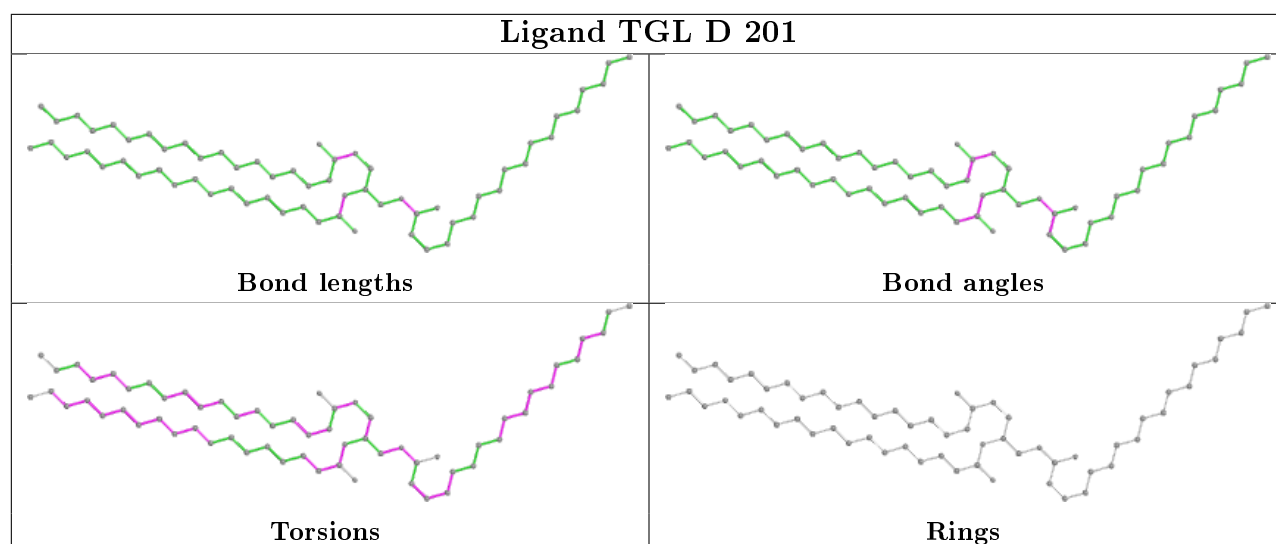


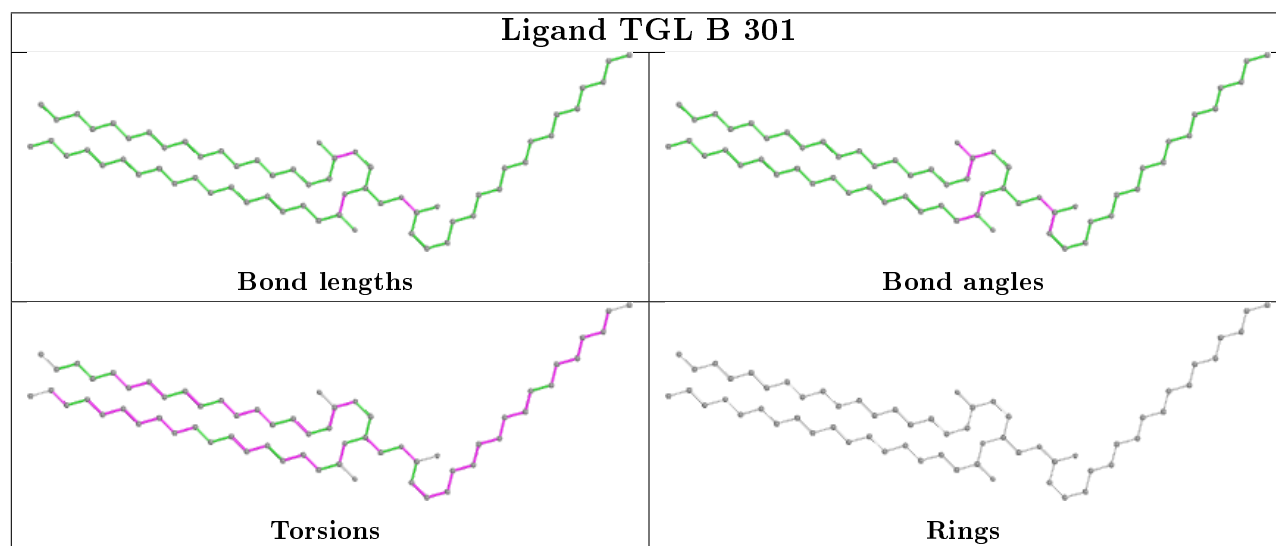
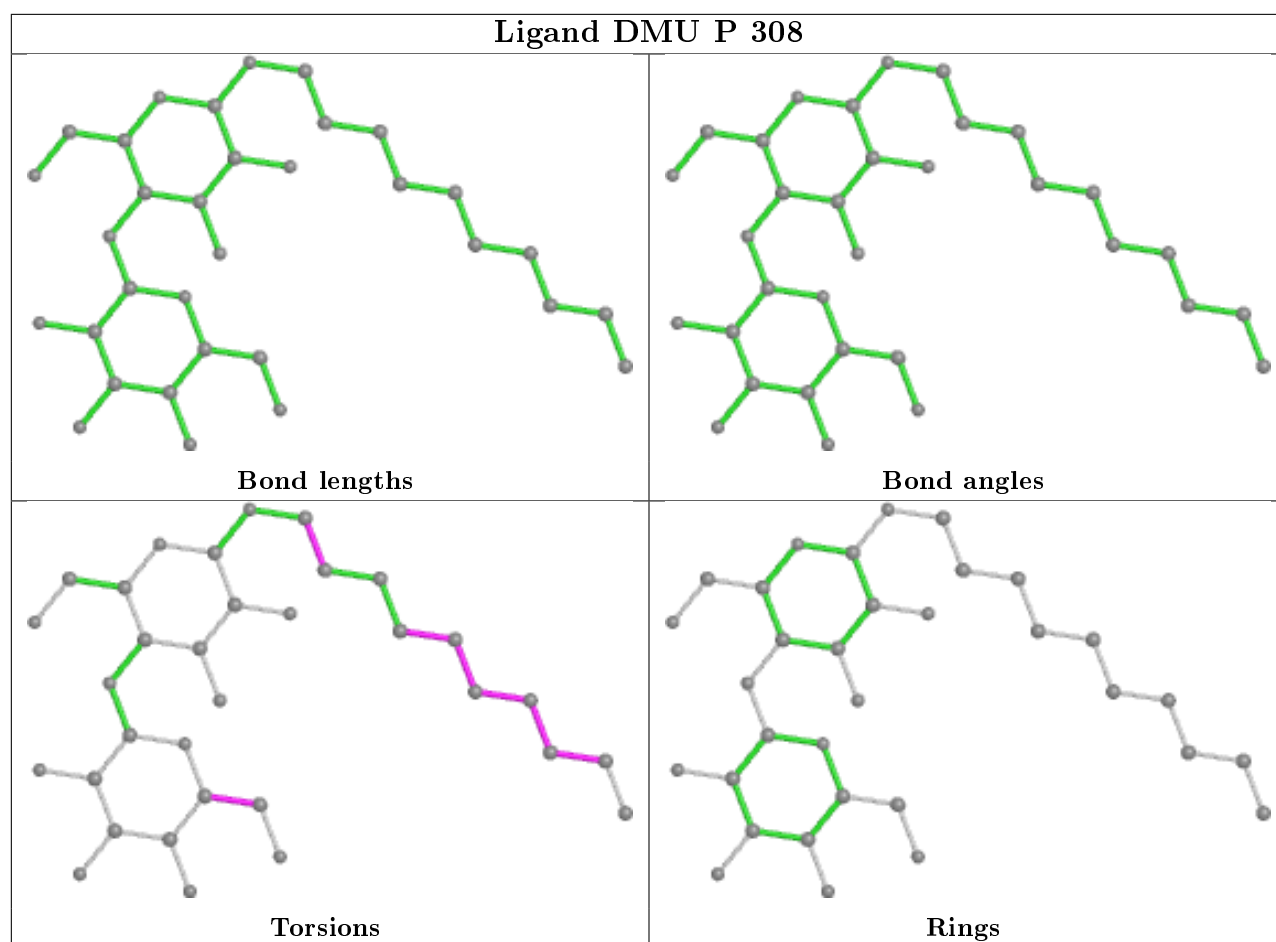


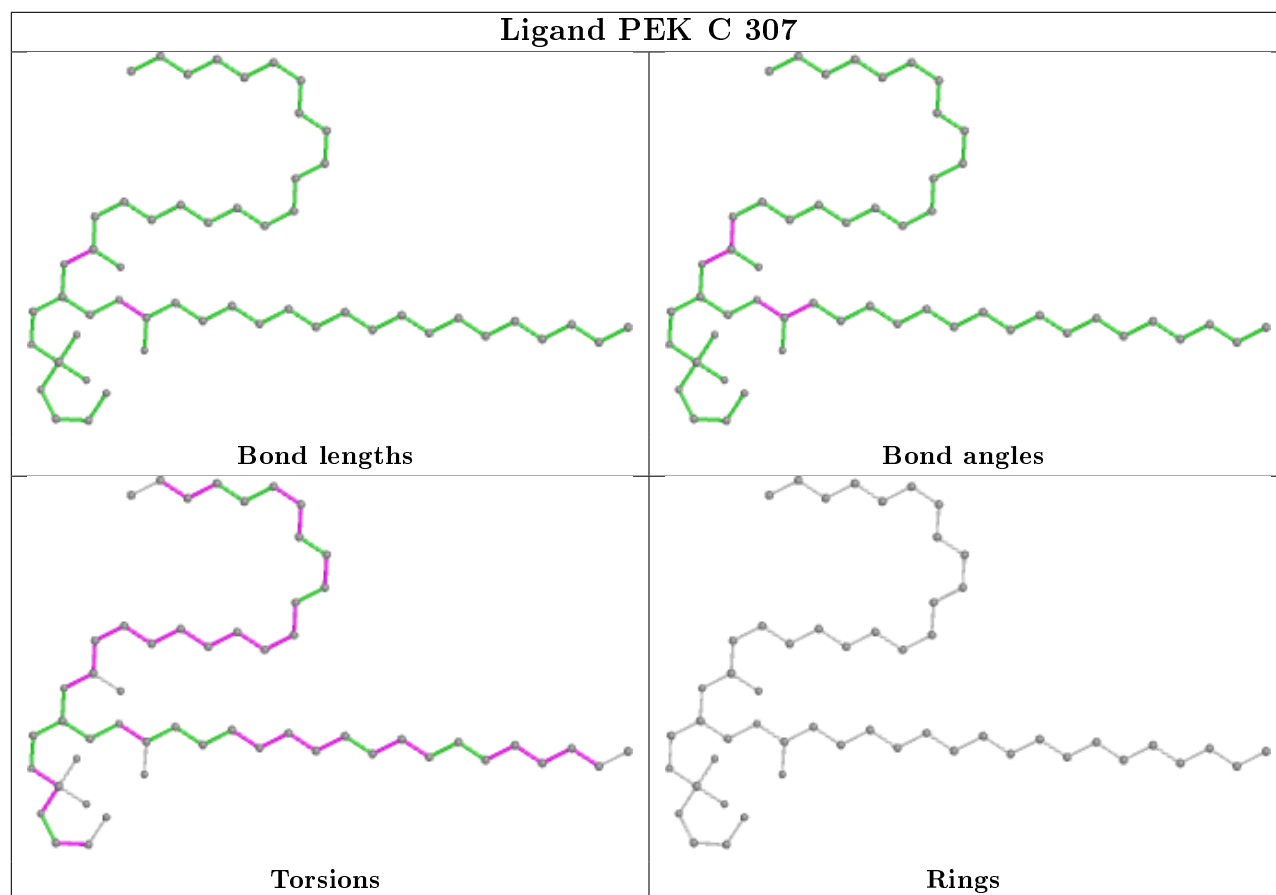
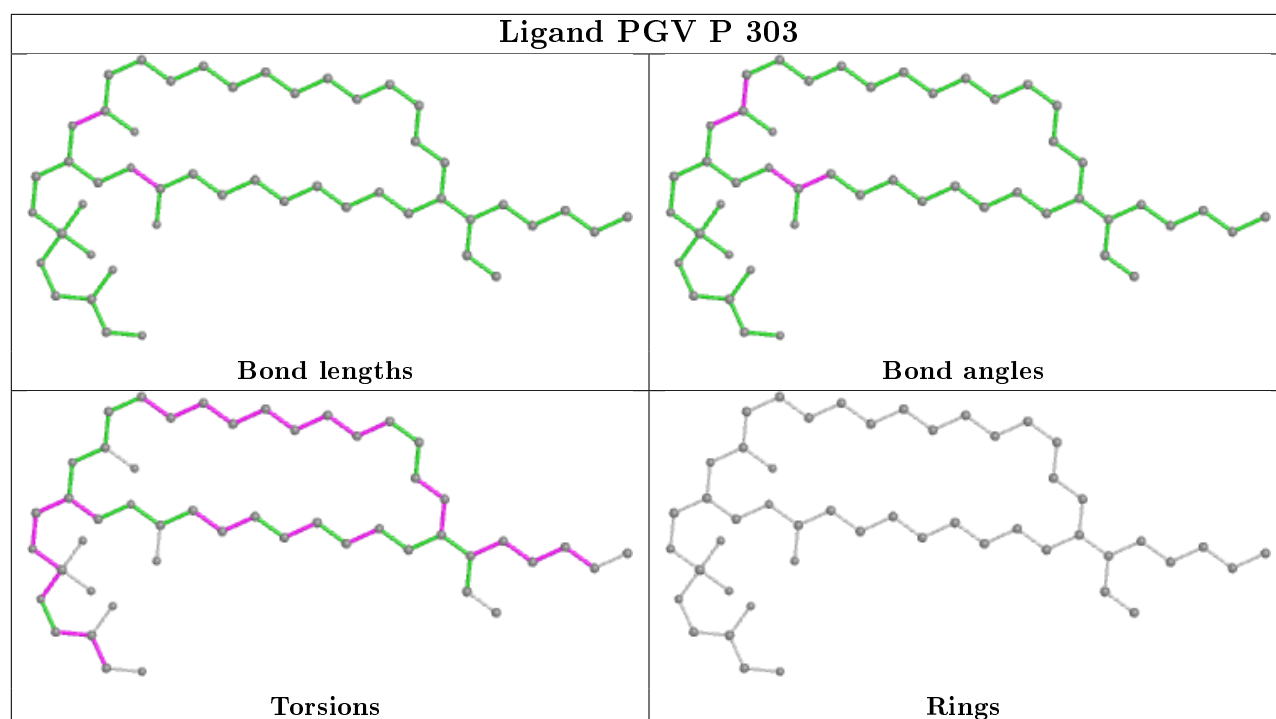


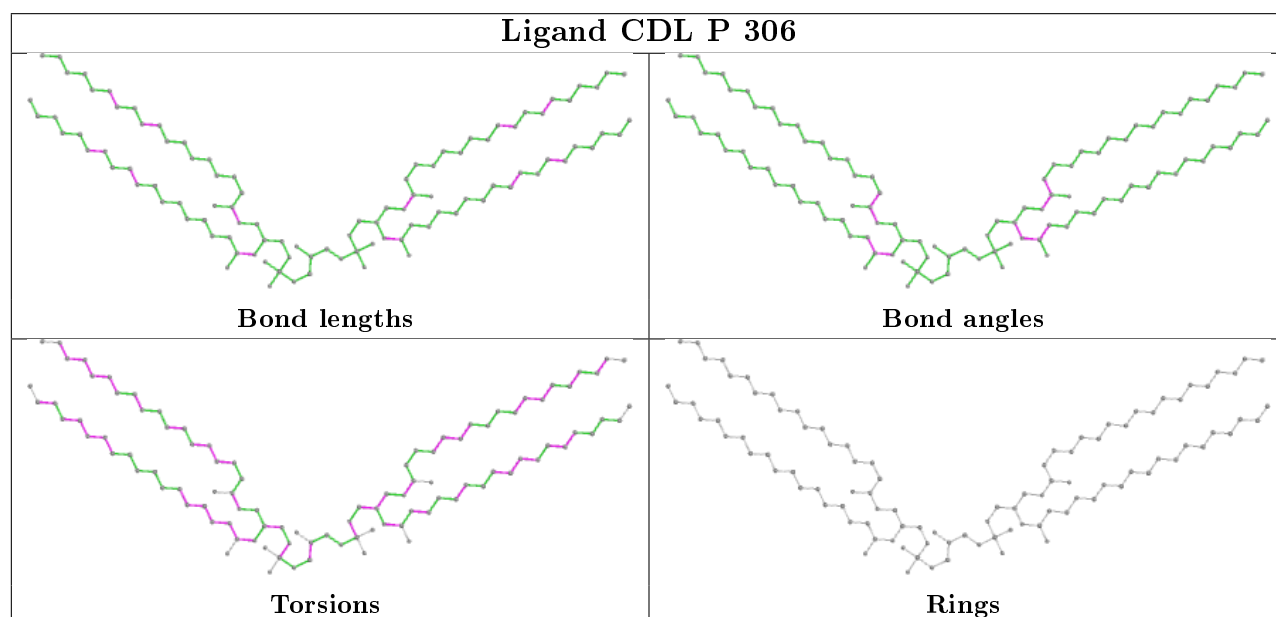
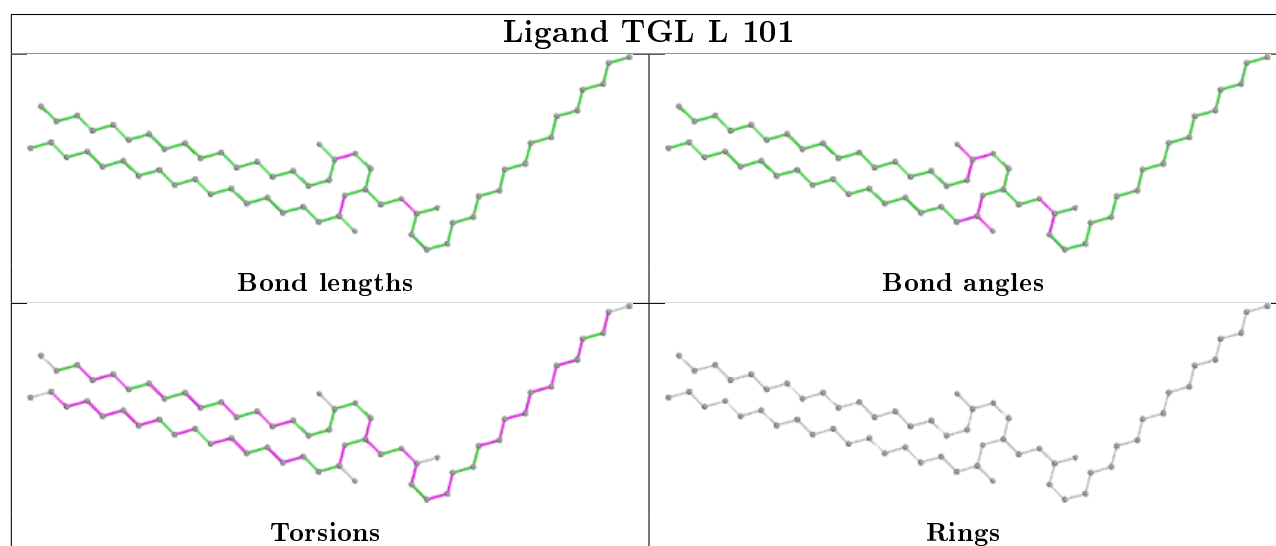
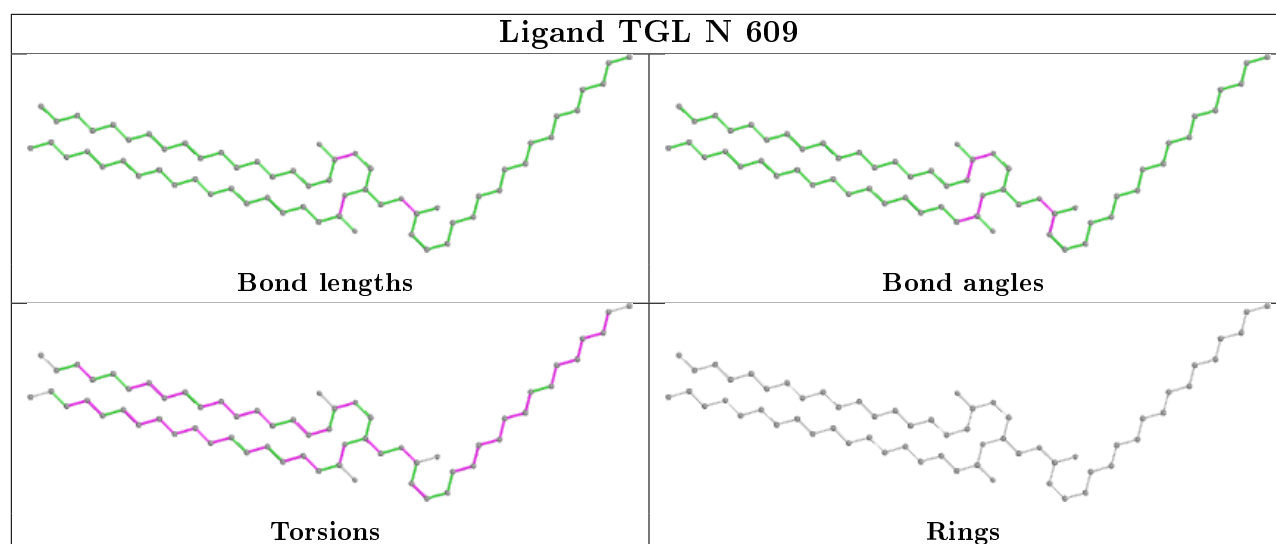




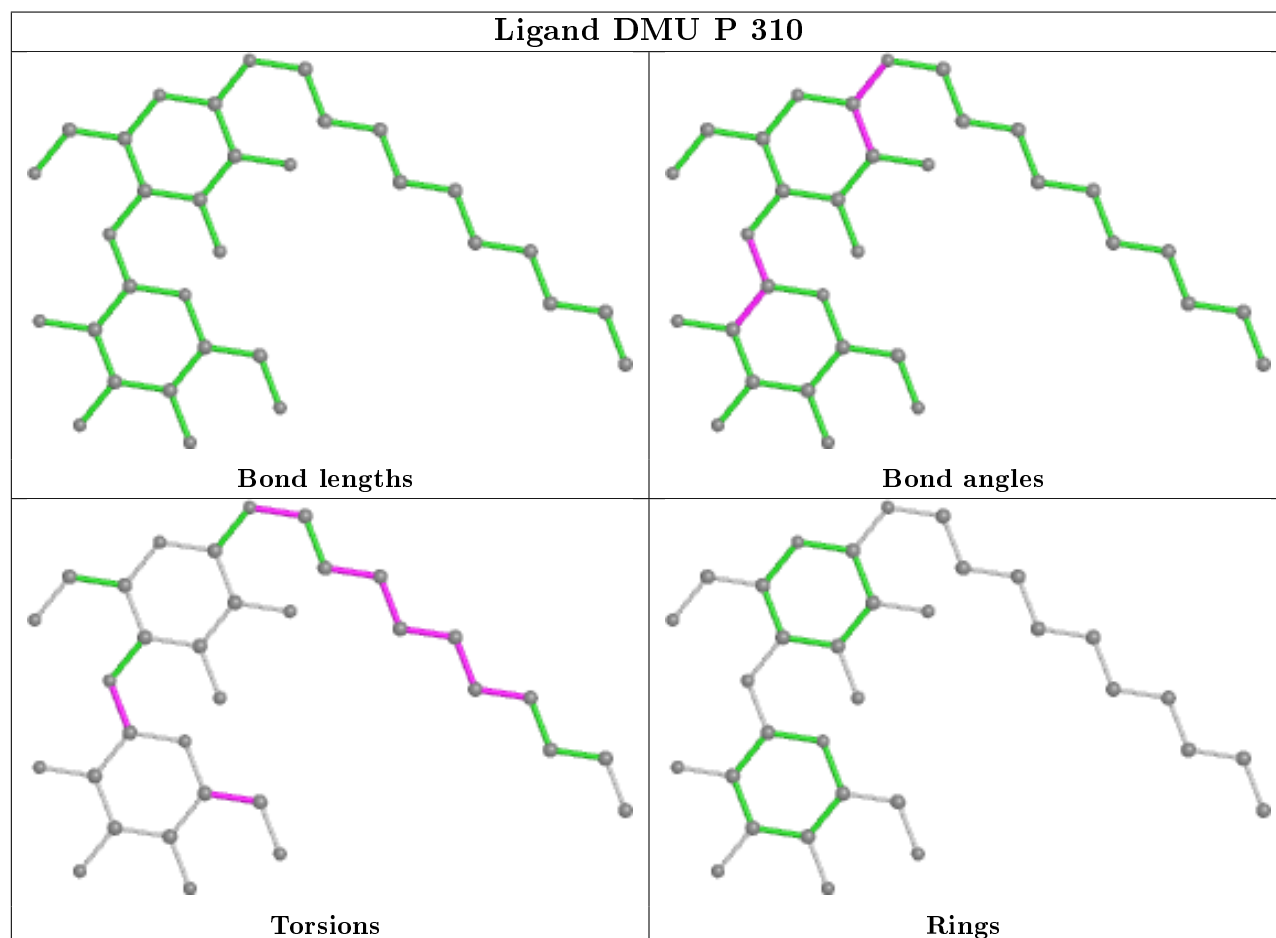
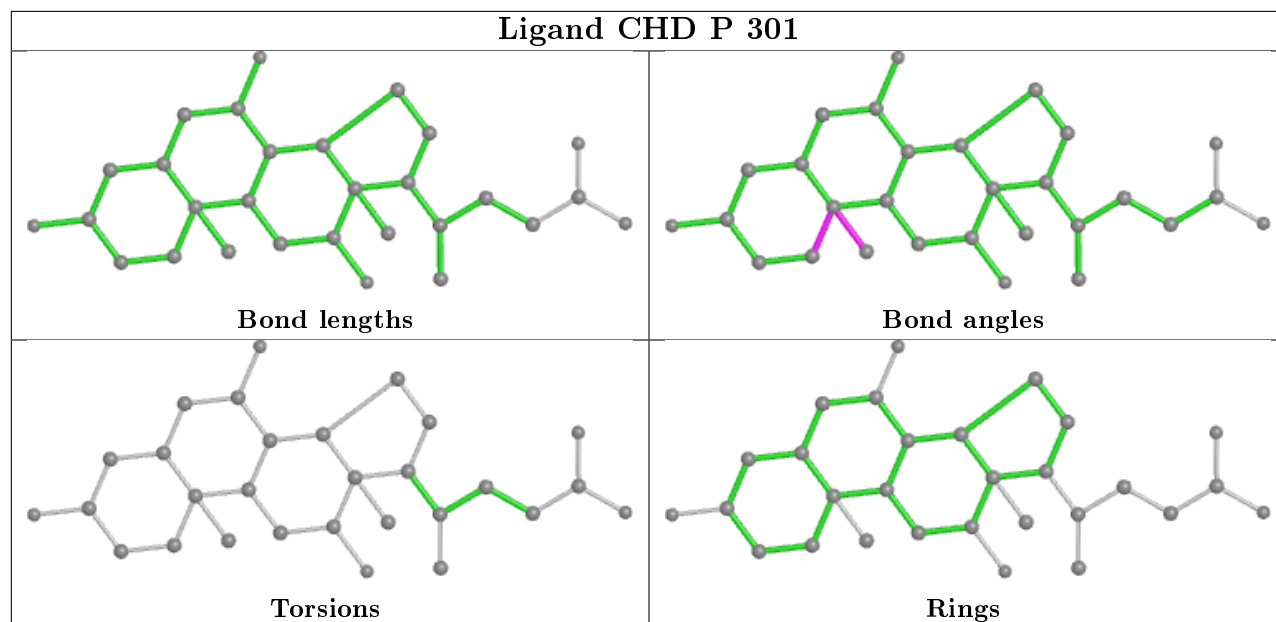




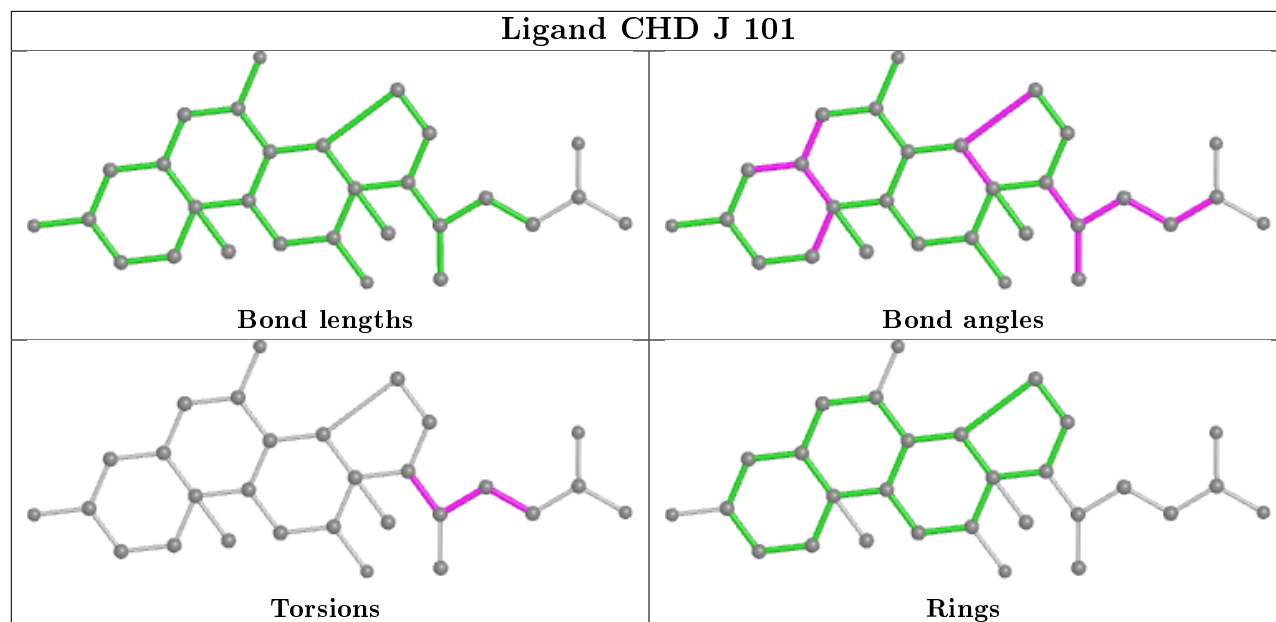




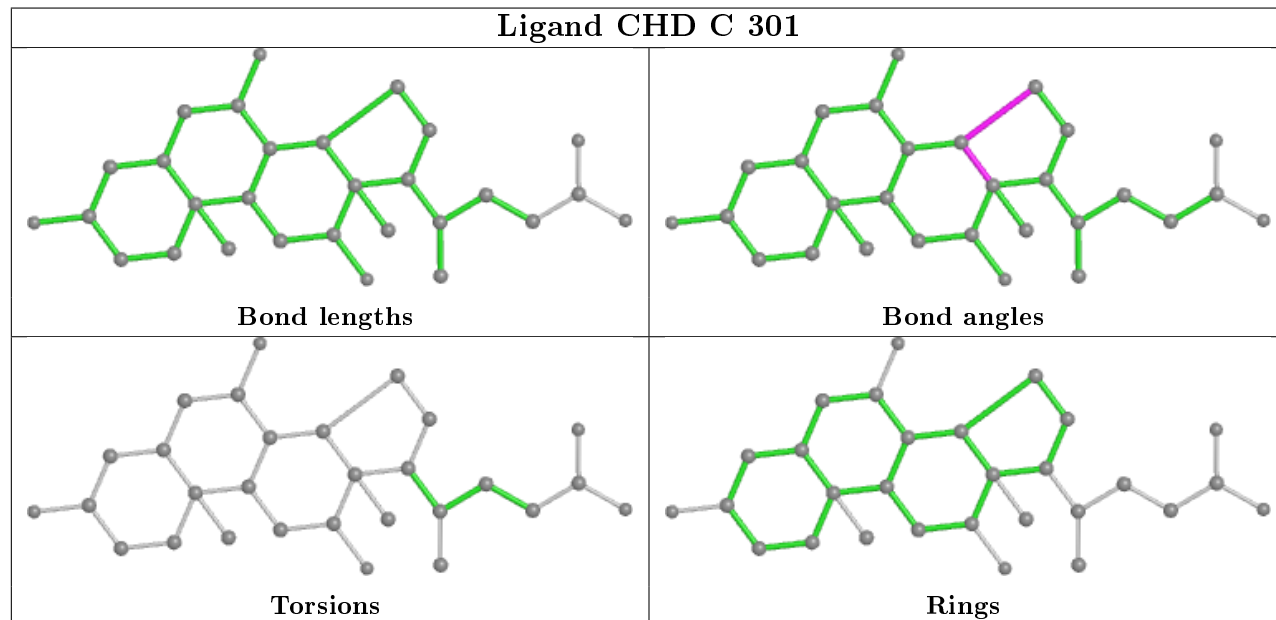


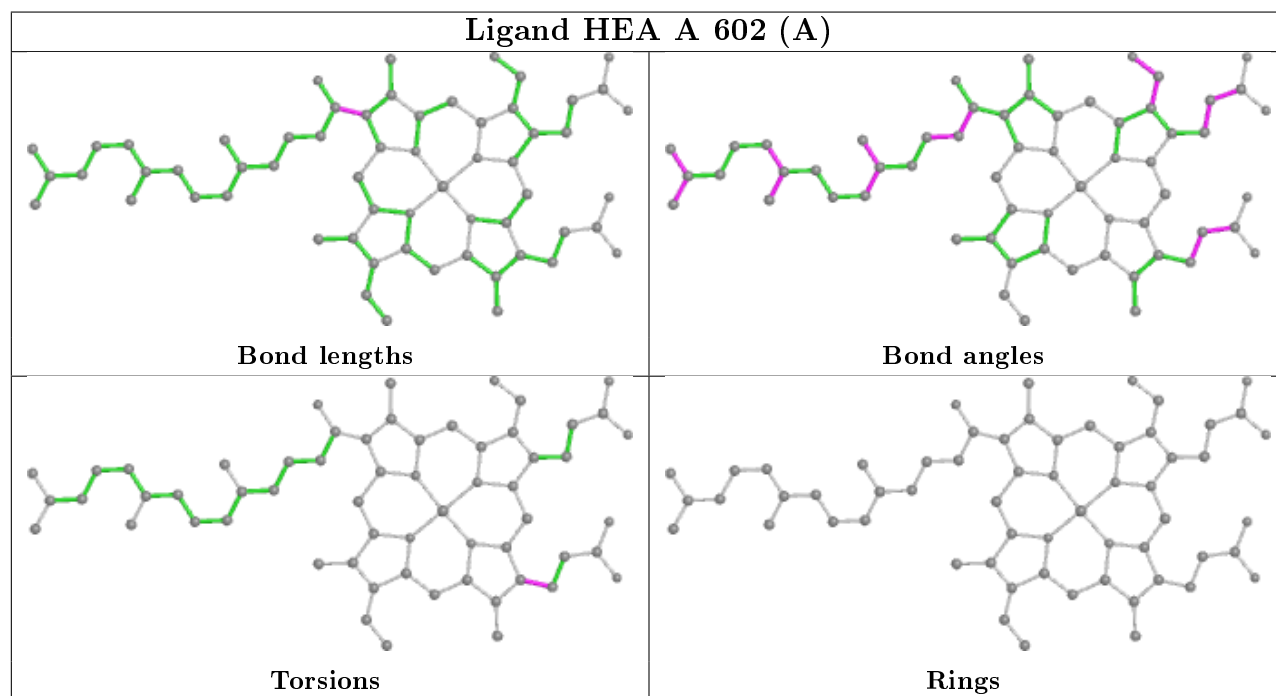
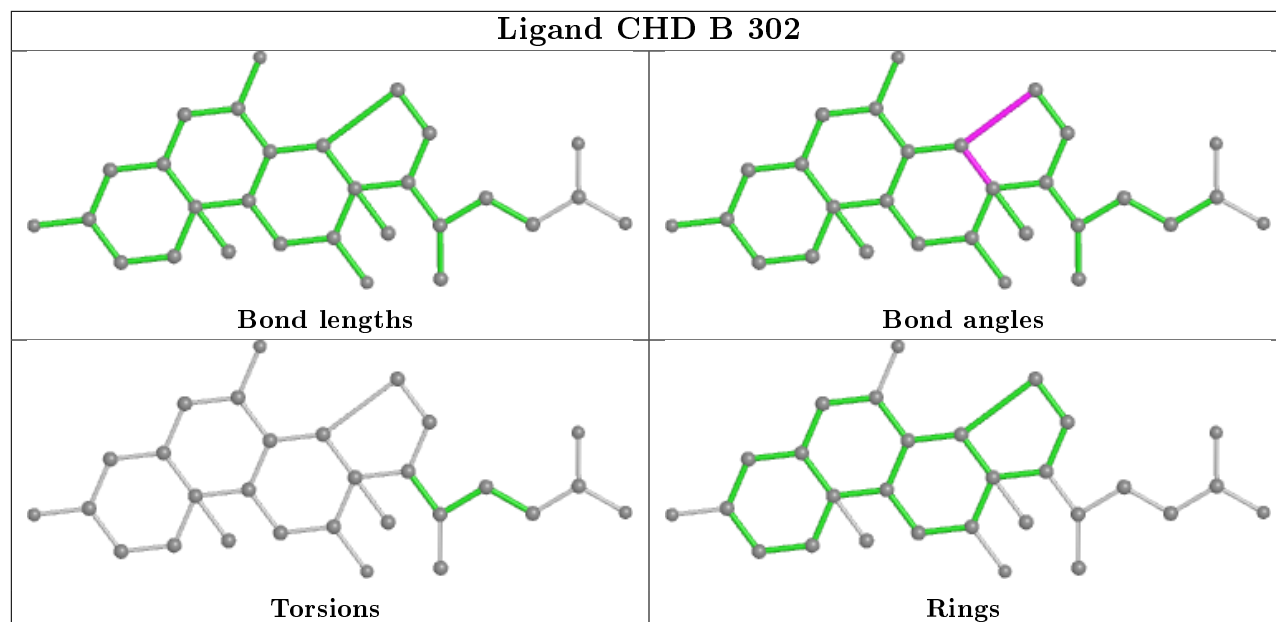


## Ligand CHD J 101

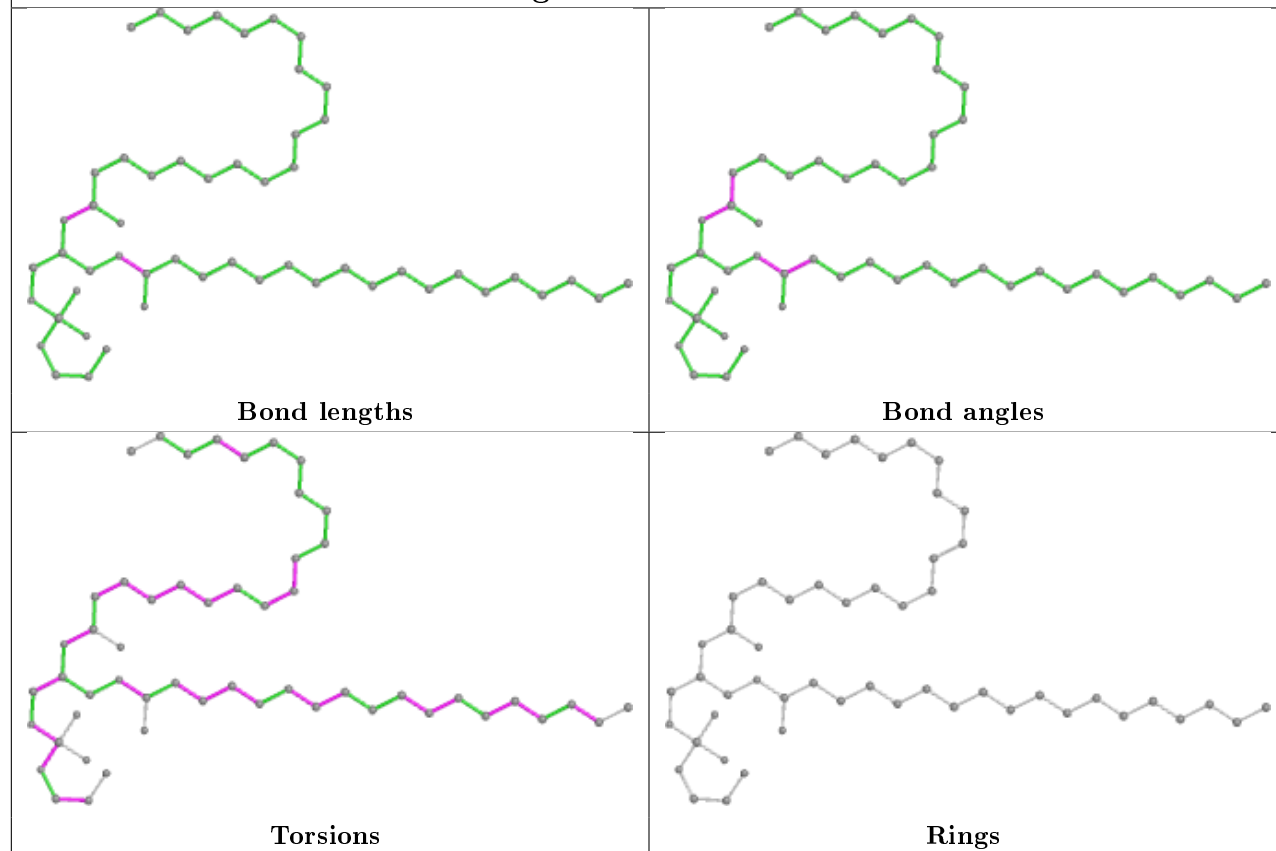


## Ligand CHD C 301

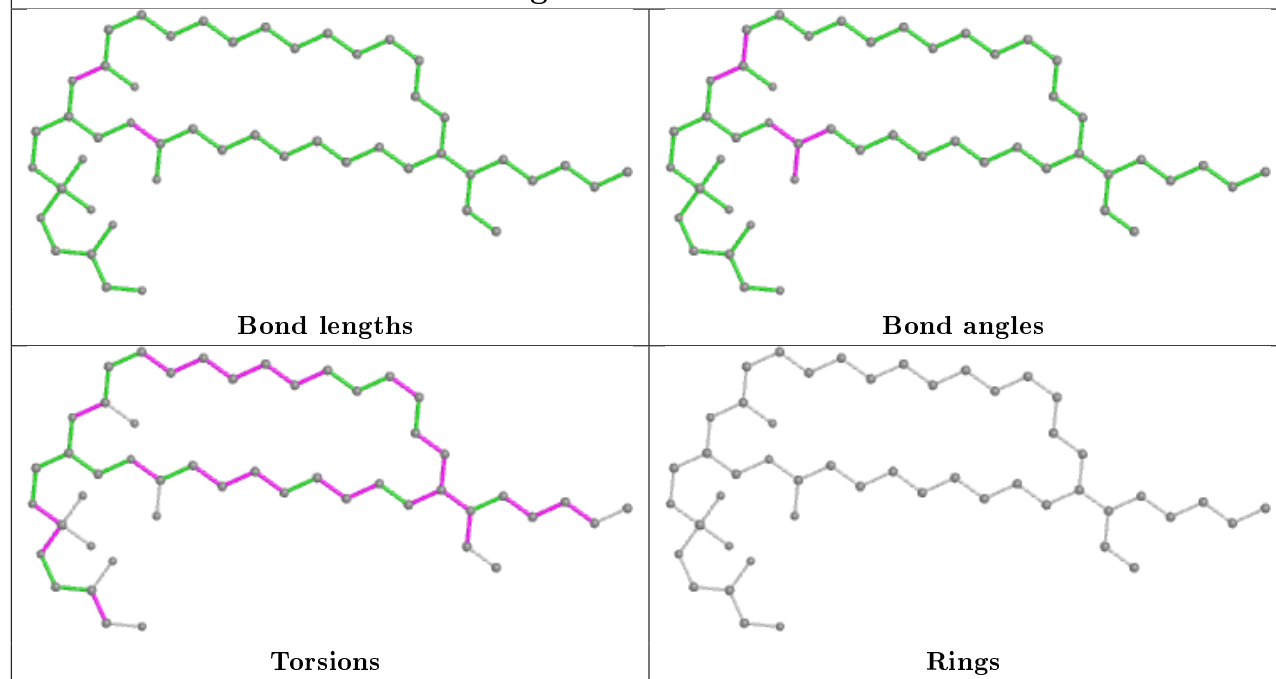


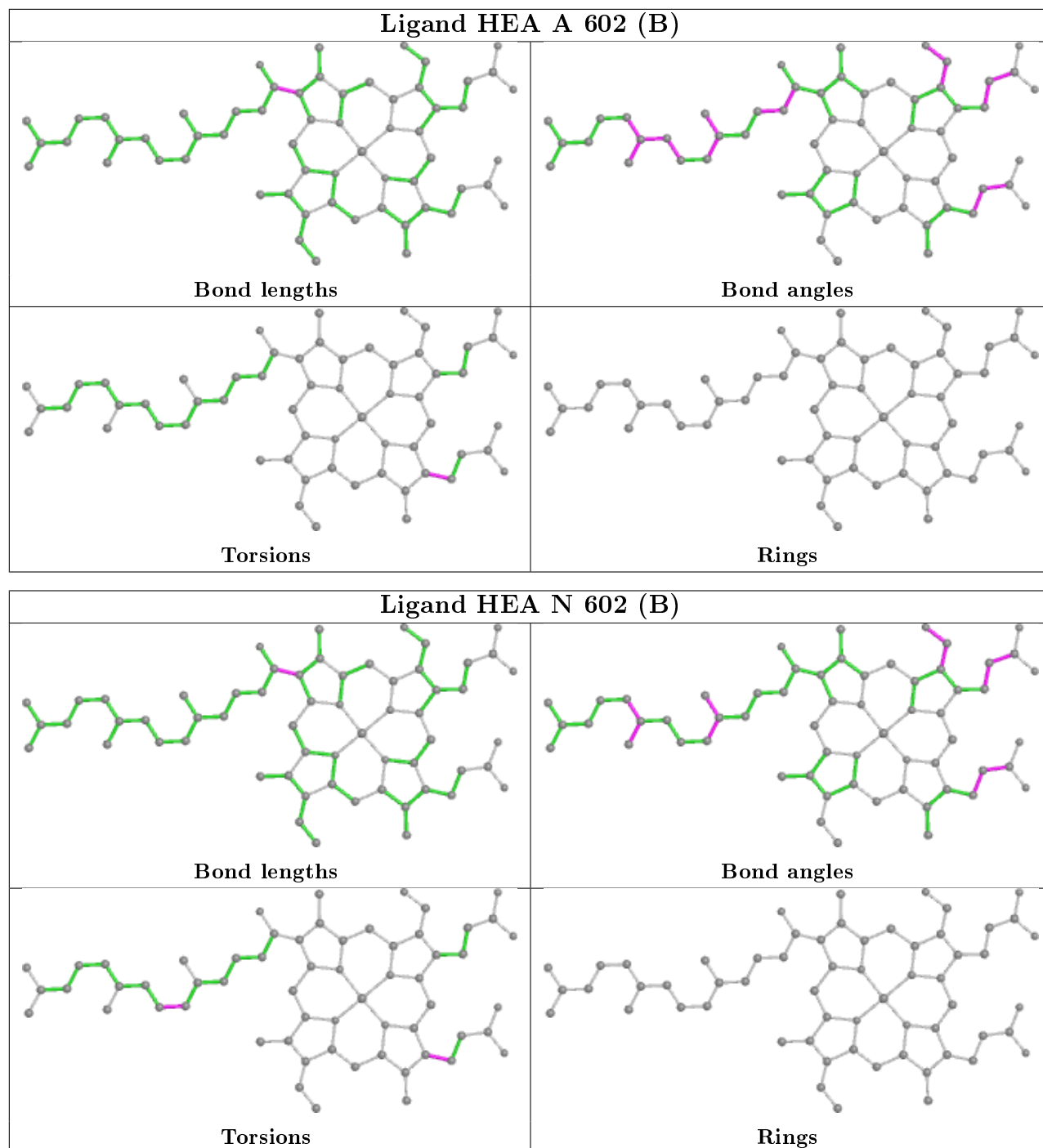


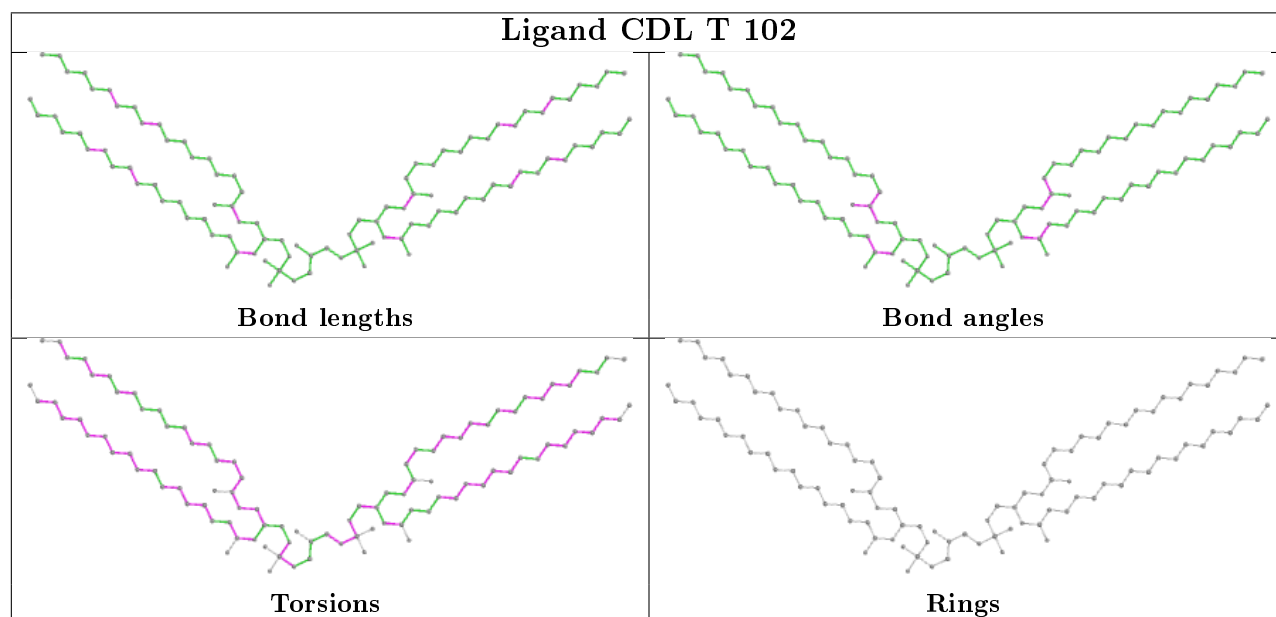
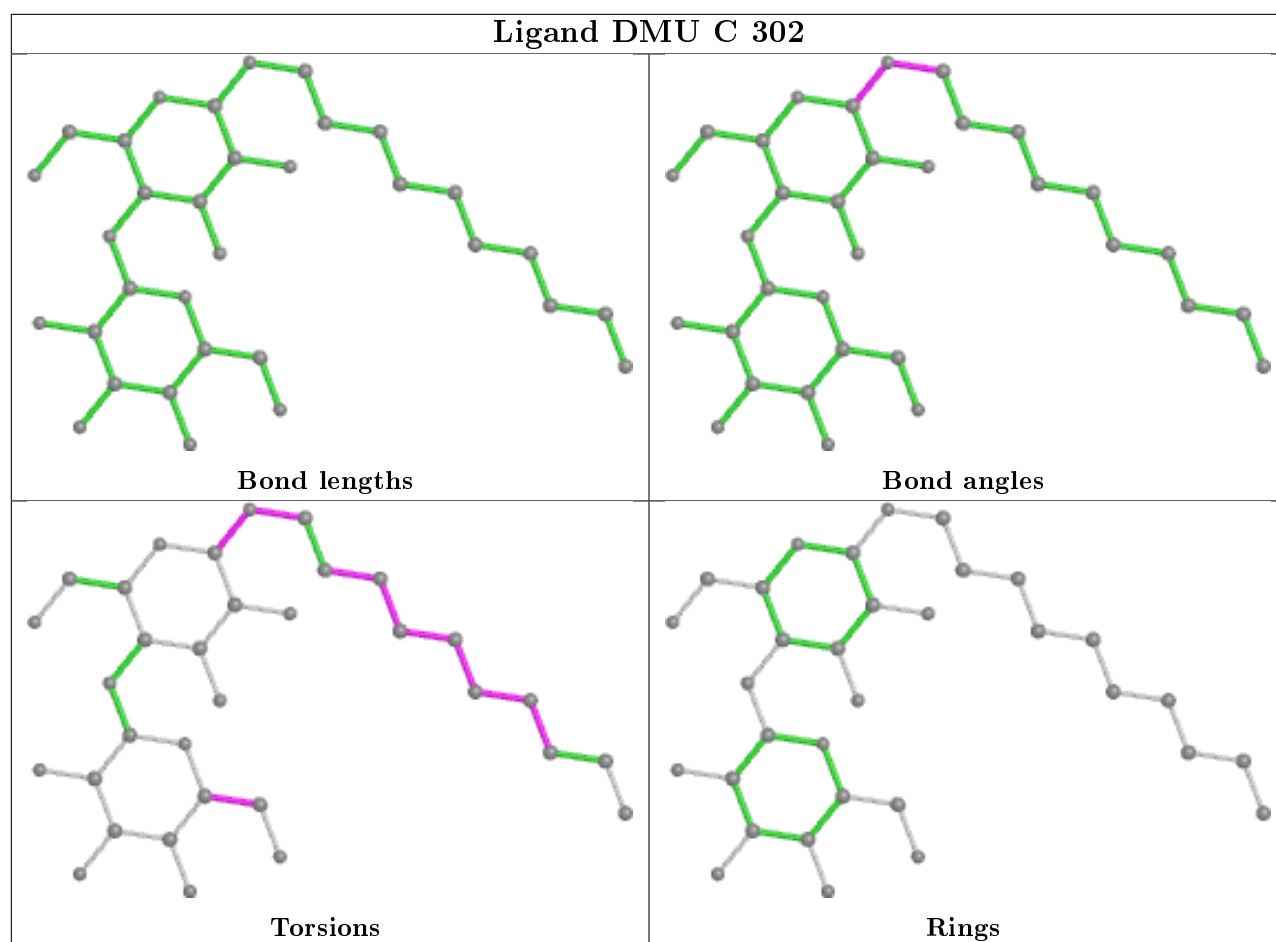
## Ligand PEK P 309

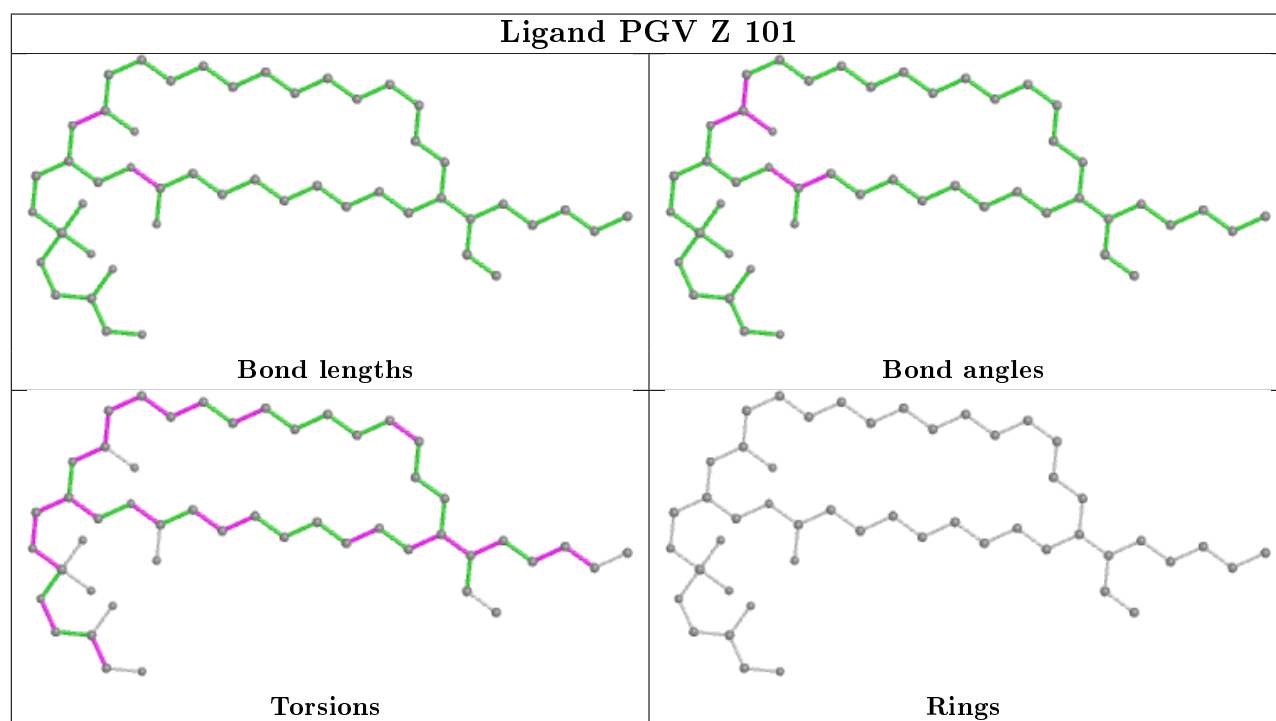
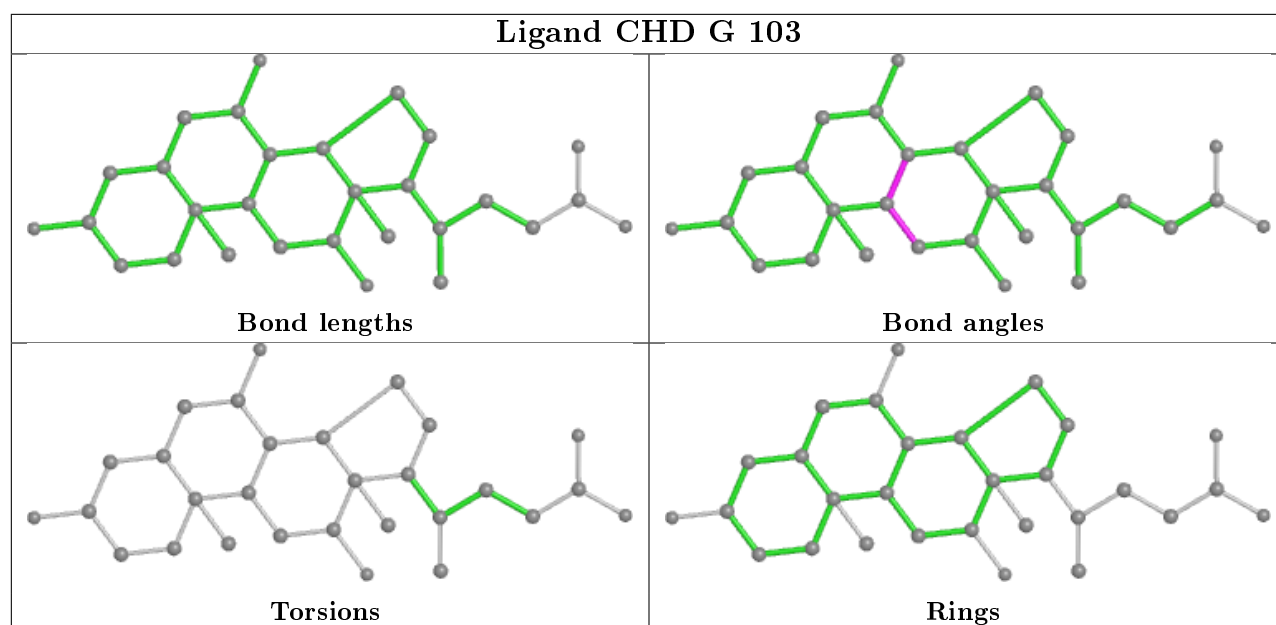


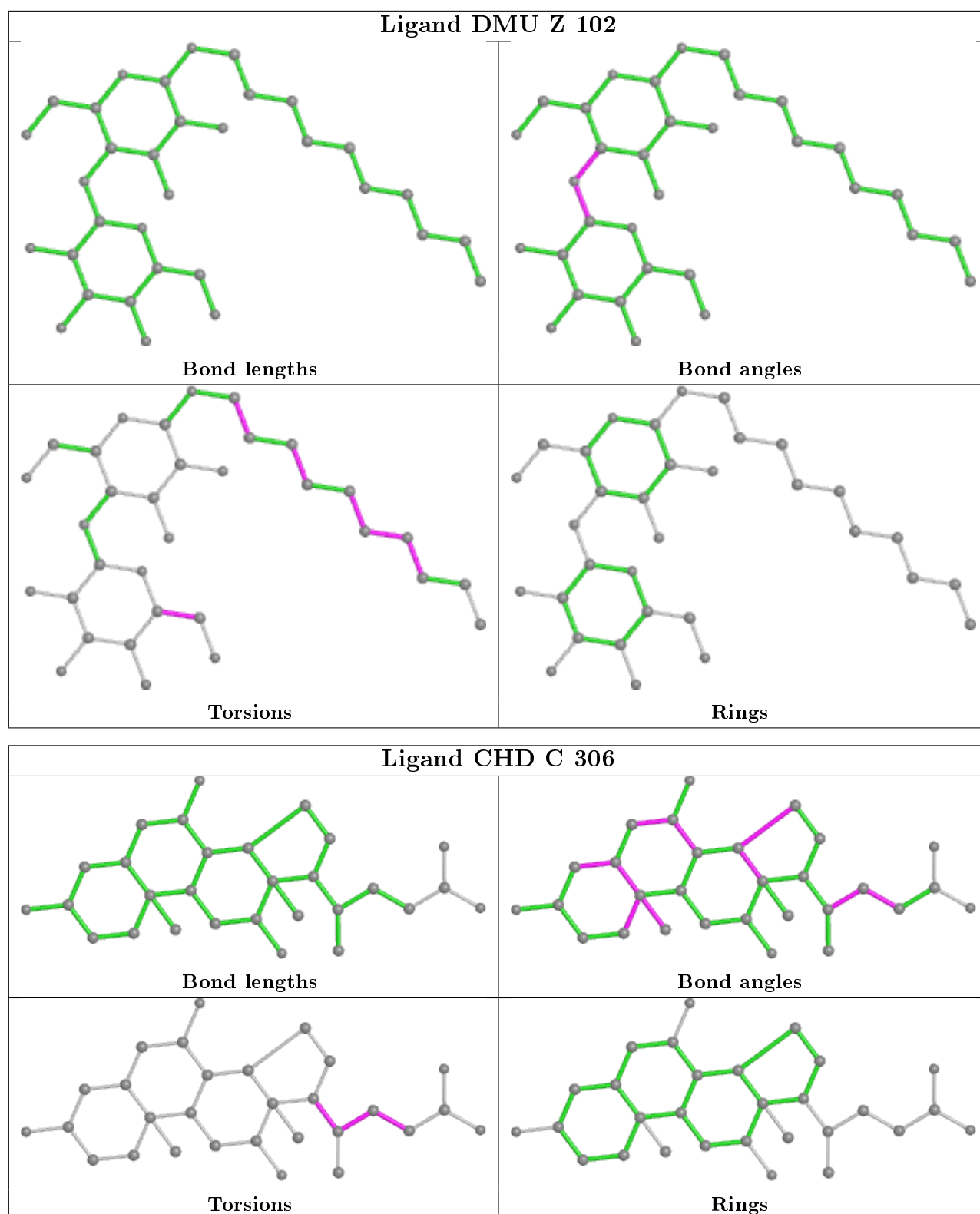
## Ligand PGV C 308



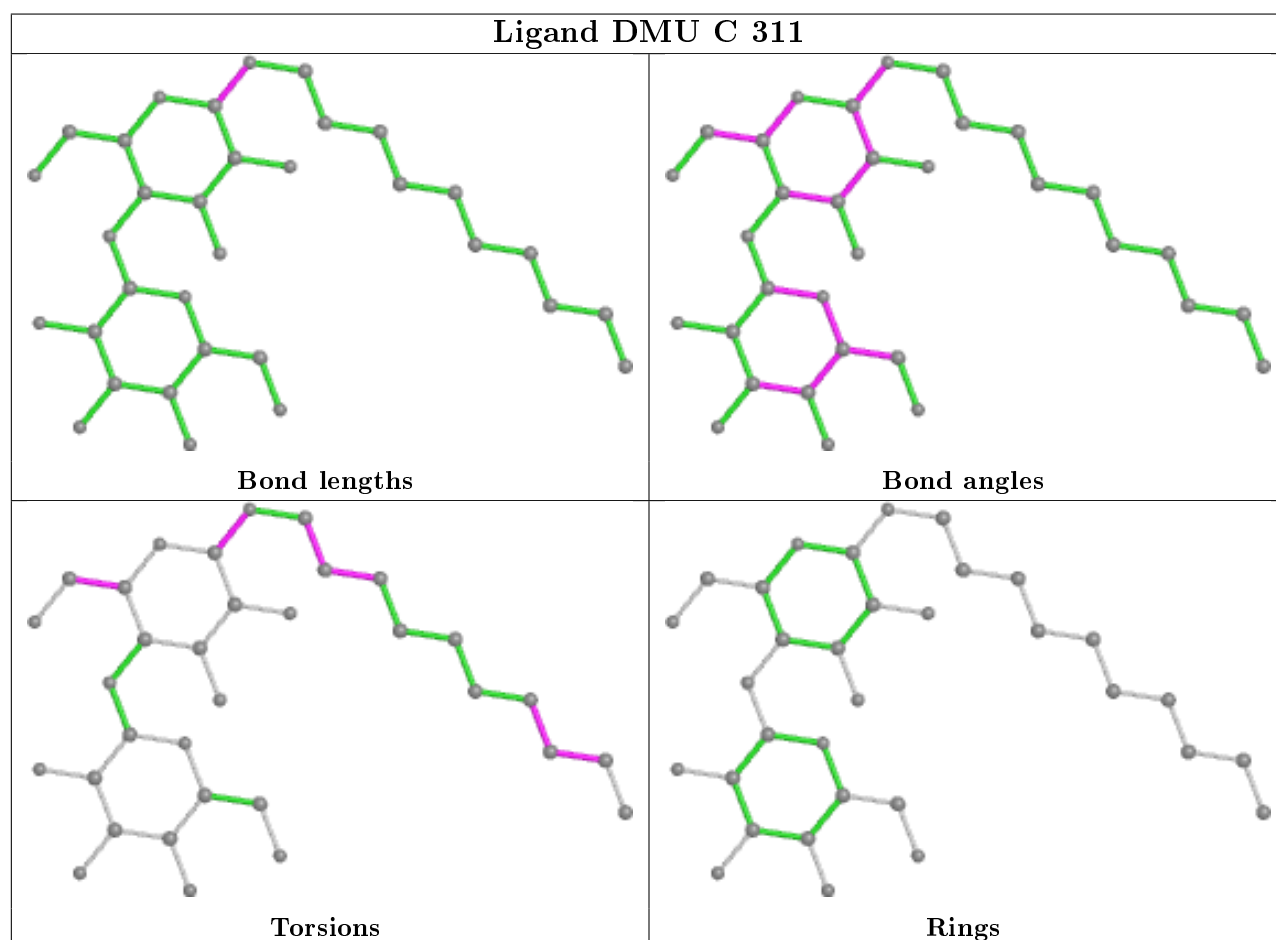
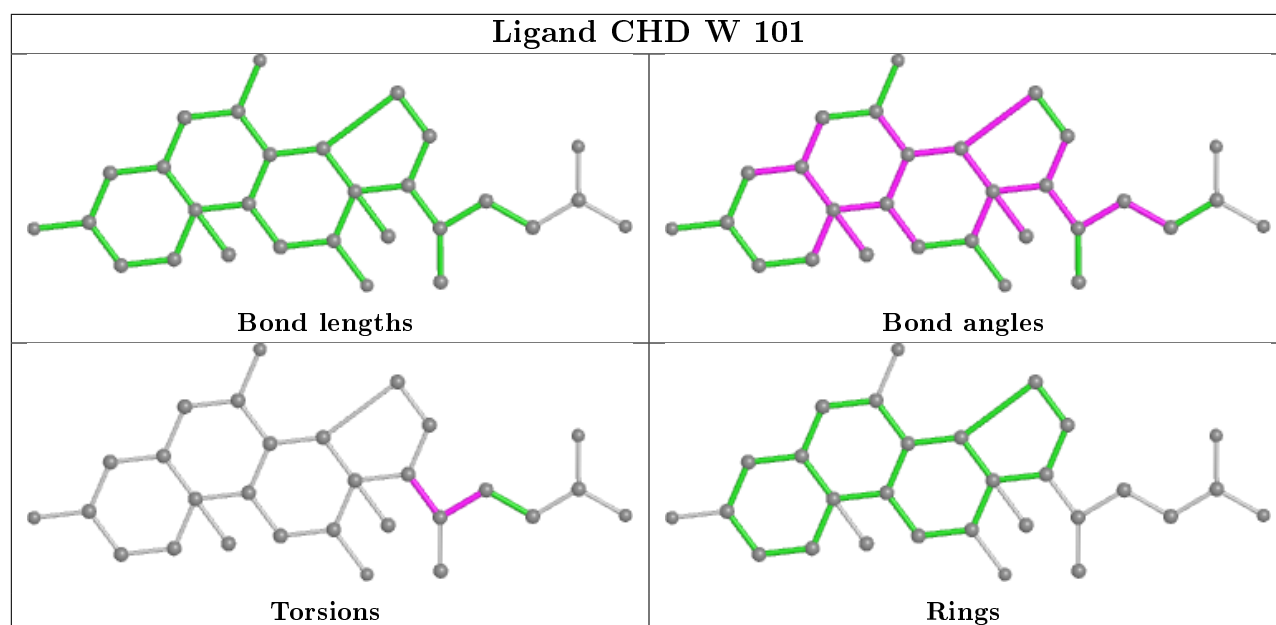


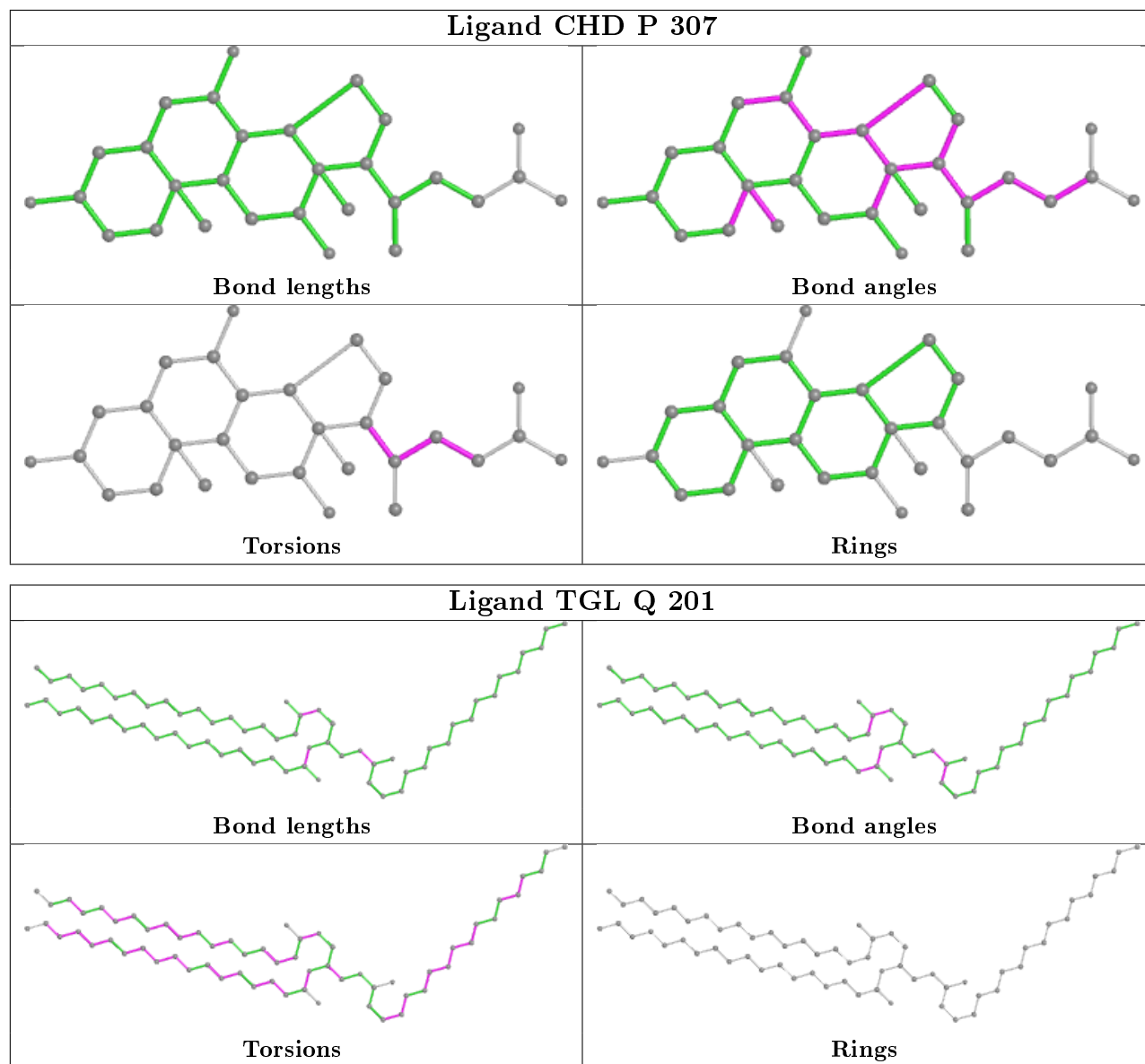


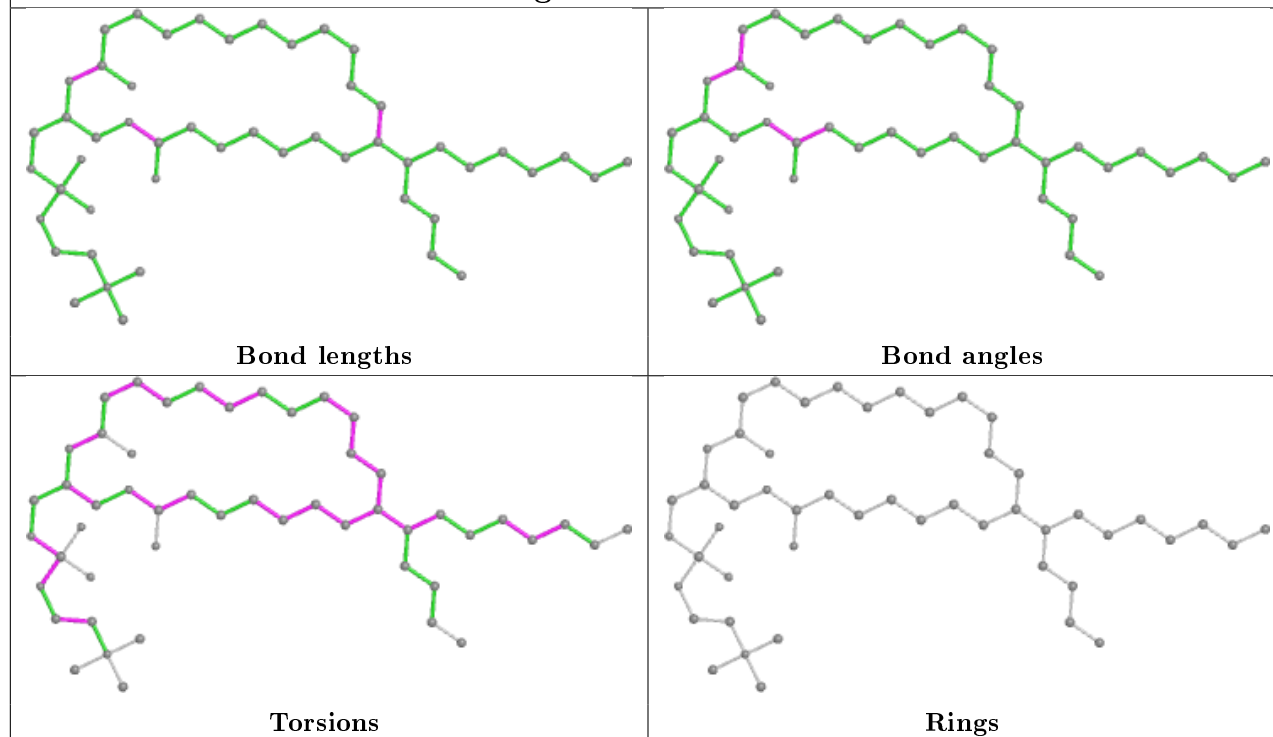
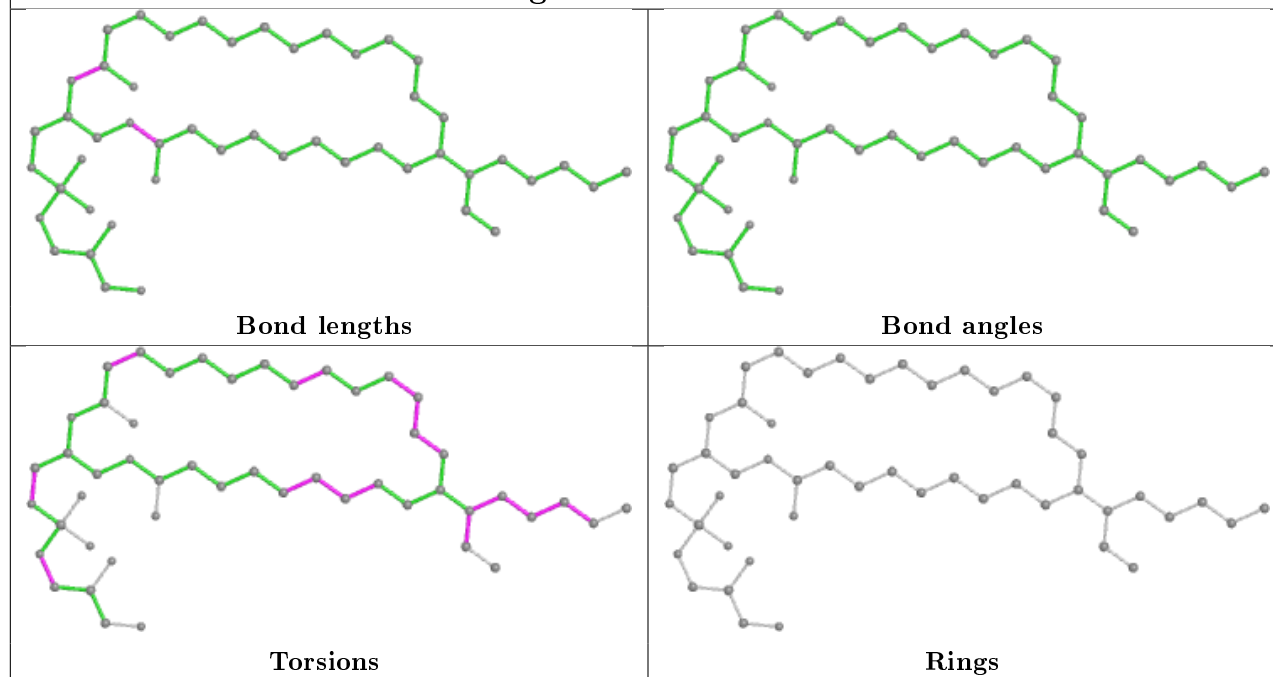


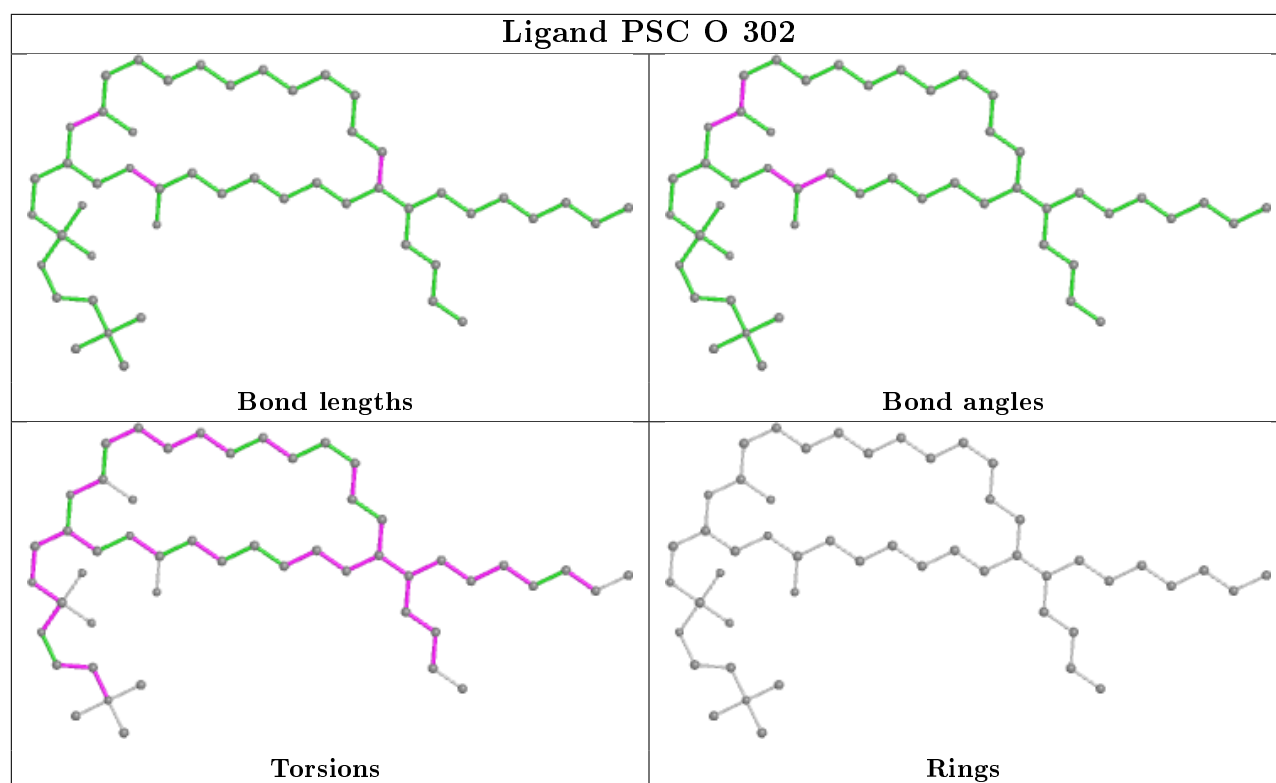








**Ligand PSC E 201****Ligand PGV P 305**



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	0.05	2 (0%) 92 92	23, 28, 36, 71	0
1	N	513/514 (99%)	-0.01	4 (0%) 86 86	26, 33, 42, 72	0
2	B	226/227 (99%)	0.06	4 (1%) 68 68	27, 36, 55, 71	0
2	O	226/227 (99%)	0.15	4 (1%) 68 68	32, 43, 65, 84	0
3	C	259/261 (99%)	0.19	1 (0%) 92 92	25, 32, 42, 71	0
3	P	259/261 (99%)	0.03	2 (0%) 86 86	27, 33, 43, 65	0
4	D	144/147 (97%)	-0.07	4 (2%) 53 52	29, 38, 59, 74	0
4	Q	144/147 (97%)	0.79	12 (8%) 11 11	40, 51, 74, 130	0
5	E	105/109 (96%)	-0.10	2 (1%) 66 66	30, 37, 57, 108	0
5	R	105/109 (96%)	0.06	2 (1%) 66 66	36, 45, 64, 117	0
6	F	98/98 (100%)	0.63	7 (7%) 16 15	29, 39, 96, 147	0
6	S	98/98 (100%)	1.04	9 (9%) 9 8	30, 42, 104, 130	0
7	G	83/85 (97%)	1.27	15 (18%) 1 1	31, 40, 102, 145	0
7	T	83/85 (97%)	1.15	18 (21%) 0 0	30, 42, 96, 133	0
8	H	79/85 (92%)	0.38	8 (10%) 7 6	34, 43, 90, 100	0
8	U	79/85 (92%)	0.43	8 (10%) 7 6	38, 48, 95, 119	0
9	I	72/73 (98%)	0.72	10 (13%) 2 3	35, 48, 81, 93	0
9	V	72/73 (98%)	0.61	7 (9%) 7 7	34, 58, 79, 93	0
10	J	58/59 (98%)	0.47	2 (3%) 45 42	33, 42, 64, 110	0
10	W	58/59 (98%)	0.52	4 (6%) 16 16	37, 47, 68, 123	0
11	K	49/56 (87%)	0.03	0 100 100	35, 42, 56, 62	0
11	X	49/56 (87%)	0.62	6 (12%) 4 4	45, 53, 68, 77	0
12	L	46/47 (97%)	0.09	1 (2%) 62 61	30, 34, 53, 88	0
12	Y	46/47 (97%)	0.32	2 (4%) 35 33	37, 44, 64, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.20	2 (4%) 31 30	31, 35, 68, 107	0
13	Z	43/46 (93%)	0.72	7 (16%) 1 2	41, 48, 78, 130	0
All	All	3550/3614 (98%)	0.25	143 (4%) 38 36	23, 37, 68, 147	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	30.4
4	Q	5	VAL	17.7
4	Q	6	VAL	17.1
6	F	1	ALA	15.9
4	Q	7	LYS	14.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.07	0.56	110,113,117,121	0
7	TPO	G	11	11/12	0.31	0.39	93,113,122,123	0
7	TPO	T	11	11/12	0.50	0.29	95,116,126,126	0
9	SAC	I	1	9/10	0.81	0.25	67,72,74,75	0
1	FME	A	1	10/11	0.91	0.13	42,46,67,74	0
1	FME	N	1	10/11	0.93	0.14	48,52,70,72	0
2	FME	O	1	10/11	0.95	0.14	41,42,50,52	0
2	FME	B	1	10/11	0.96	0.14	34,35,42,47	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CHD	W	101	29/29	0.19	0.52	101,119,127,128	0
20	EDO	C	318	4/4	0.24	0.92	92,94,95,96	0
20	EDO	C	317	4/4	0.50	0.39	72,80,80,81	0
26	CDL	T	102	100/100	0.52	0.34	63,89,130,135	0
20	EDO	Q	204	4/4	0.53	0.22	76,76,78,79	0
27	PEK	C	309	53/53	0.54	0.40	56,100,141,149	0
20	EDO	D	203	4/4	0.54	0.38	68,72,72,77	0
27	PEK	C	307	53/53	0.55	0.29	56,84,135,140	0
21	TGL	Y	101	63/63	0.56	0.37	55,85,115,134	0
20	EDO	A	619	4/4	0.58	0.22	66,67,67,70	0
27	PEK	P	309	53/53	0.59	0.31	50,75,113,116	0
28	PSC	E	201	52/52	0.59	0.35	55,80,147,151	0
20	EDO	D	204	4/4	0.61	0.33	75,77,80,80	0
27	PEK	P	302	53/53	0.61	0.28	53,90,138,147	0
26	CDL	G	102	100/100	0.63	0.37	62,94,124,132	0
20	EDO	C	316	4/4	0.65	0.20	73,75,77,80	0
26	CDL	P	306	100/100	0.65	0.32	51,84,110,116	0
28	PSC	O	302	52/52	0.65	0.32	53,91,144,152	0
21	TGL	Q	201	63/63	0.66	0.26	66,80,94,97	0
19	PGV	C	308	51/51	0.66	0.24	60,78,106,113	0
21	TGL	L	101	63/63	0.67	0.30	43,74,92,95	0
24	DMU	C	302	33/33	0.68	0.38	51,80,99,103	0
19	PGV	P	303	51/51	0.68	0.31	62,85,114,123	0
20	EDO	O	305	4/4	0.70	0.17	76,77,78,78	0
20	EDO	G	106	4/4	0.71	0.23	72,73,74,74	0
19	PGV	Z	101	51/51	0.71	0.36	58,80,101,104	0
24	DMU	P	308	33/33	0.71	0.36	53,81,112,114	0
20	EDO	J	102	4/4	0.72	0.15	85,86,86,88	0
24	DMU	P	310	33/33	0.73	0.23	70,78,88,92	0
21	TGL	D	201	63/63	0.74	0.24	51,67,90,94	0
24	DMU	C	310	33/33	0.74	0.27	65,78,99,100	0
19	PGV	A	609	51/51	0.74	0.32	43,78,96,102	0
20	EDO	C	314	4/4	0.75	0.26	67,70,71,73	0
26	CDL	C	305	100/100	0.75	0.28	55,78,108,113	0
24	DMU	C	311	33/33	0.76	0.19	61,82,101,103	0
20	EDO	A	618	4/4	0.76	0.53	55,59,61,62	0
20	EDO	H	101	4/4	0.77	0.17	62,65,66,69	0
22	CHD	J	101	29/29	0.77	0.26	82,86,100,102	0
20	EDO	N	611	4/4	0.77	0.37	41,42,46,53	0
20	EDO	Q	203	4/4	0.77	0.35	63,64,66,67	0
21	TGL	N	609	63/63	0.77	0.27	60,82,100,104	0
20	EDO	C	313	4/4	0.77	0.19	67,67,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	G	104	4/4	0.78	0.20	70,70,72,74	0
20	EDO	A	617	4/4	0.80	0.42	64,67,69,72	0
20	EDO	U	101	4/4	0.80	0.17	70,70,70,73	0
21	TGL	B	301	63/63	0.81	0.26	50,78,104,107	0
20	EDO	A	614	4/4	0.81	0.19	28,30,32,45	0
20	EDO	D	202	4/4	0.81	0.70	51,54,55,56	0
20	EDO	R	204	4/4	0.82	0.42	62,63,66,67	0
20	EDO	N	620	4/4	0.83	0.34	46,55,55,56	0
22	CHD	P	307	29/29	0.84	0.19	57,59,62,64	0
22	CHD	C	306	29/29	0.84	0.17	59,61,63,67	0
24	DMU	P	311	33/33	0.85	0.23	72,89,98,99	0
20	EDO	N	610	4/4	0.85	0.15	74,74,74,75	0
20	EDO	A	616	4/4	0.85	0.23	53,54,54,61	0
20	EDO	E	204	4/4	0.85	0.25	55,58,59,60	0
20	EDO	N	617	4/4	0.86	0.32	47,50,52,53	0
20	EDO	C	315	4/4	0.86	0.26	44,54,56,60	0
24	DMU	Z	102	33/33	0.86	0.20	52,58,70,70	0
20	EDO	A	615	4/4	0.87	0.19	45,46,46,47	0
20	EDO	S	103	4/4	0.87	0.31	61,63,67,69	0
20	EDO	N	616	4/4	0.87	0.15	50,50,51,53	0
20	EDO	R	201	4/4	0.88	0.21	67,68,68,71	0
20	EDO	F	104	4/4	0.88	0.28	53,53,55,57	0
20	EDO	P	312	4/4	0.89	0.21	37,42,43,49	0
20	EDO	R	205	4/4	0.89	0.25	49,52,54,55	0
20	EDO	A	613	4/4	0.90	0.22	67,70,71,73	0
20	EDO	V	101	4/4	0.90	0.18	63,64,64,64	0
20	EDO	N	619	4/4	0.90	0.25	54,60,62,72	0
20	EDO	W	102	4/4	0.91	0.31	55,60,60,67	0
20	EDO	A	620	4/4	0.91	0.47	49,50,52,53	0
20	EDO	A	611	4/4	0.91	0.21	52,56,58,61	0
20	EDO	A	612	4/4	0.91	0.20	39,45,47,53	0
20	EDO	C	319	4/4	0.91	0.22	39,45,46,53	0
20	EDO	D	206	4/4	0.91	0.19	59,60,61,64	0
16	MG	N	604	1/1	0.92	0.12	33,33,33,33	0
20	EDO	O	304	4/4	0.92	0.16	66,67,67,70	0
20	EDO	E	206	4/4	0.92	0.26	65,65,66,68	0
18	AZI	N	607	3/3	0.92	0.13	35,35,36,36	0
20	EDO	R	202	4/4	0.92	0.21	58,61,62,64	0
20	EDO	N	613	4/4	0.92	0.20	60,62,65,68	0
24	DMU	M	101	33/33	0.93	0.14	43,49,55,58	0
20	EDO	N	618	4/4	0.93	0.25	53,56,58,58	0
20	EDO	F	103	4/4	0.94	0.12	38,39,39,41	0

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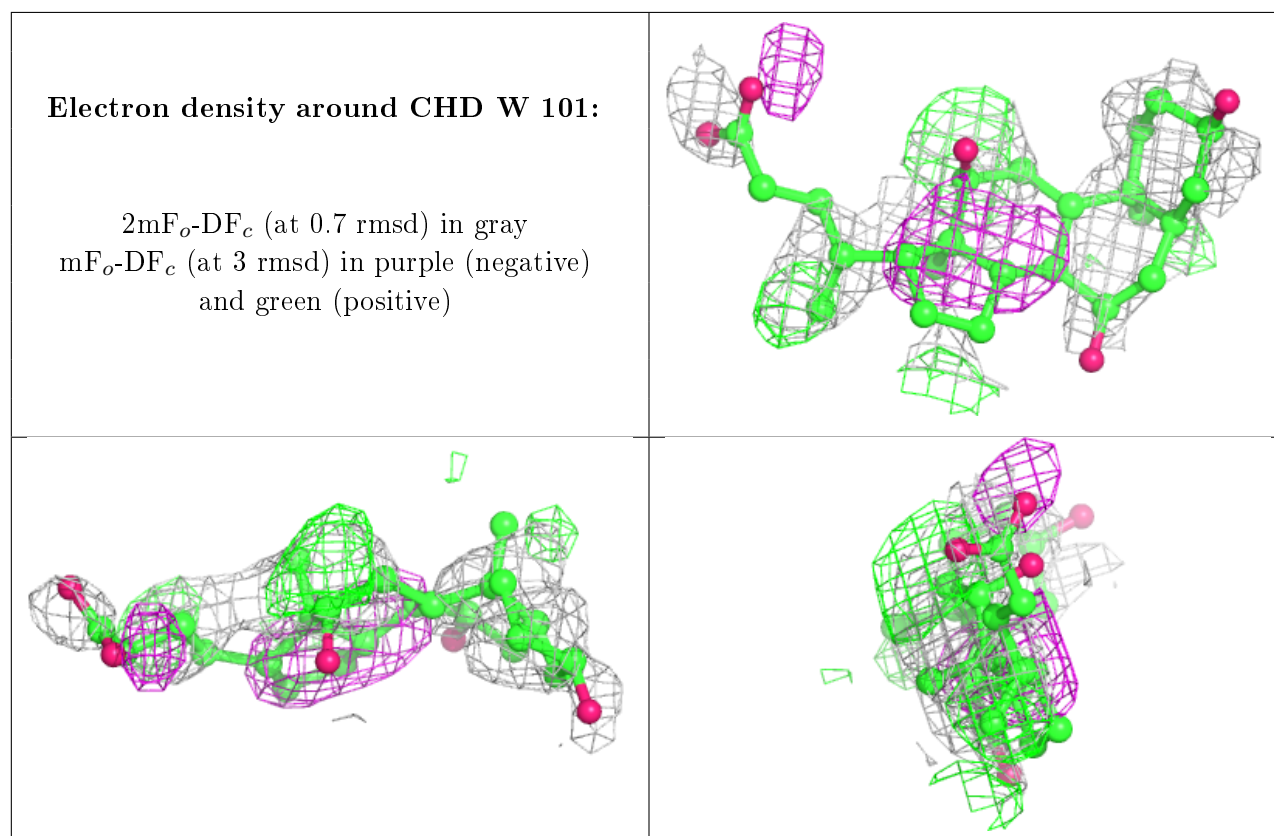
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	A	604	1/1	0.94	0.10	27,27,27,27	0
20	EDO	Q	202	4/4	0.94	0.22	69,69,70,71	0
27	PEK	T	101	53/53	0.94	0.17	34,52,79,81	0
20	EDO	S	104	4/4	0.94	0.21	49,50,50,52	0
20	EDO	R	203	4/4	0.94	0.12	45,46,46,46	0
18	AZI	A	607	3/3	0.94	0.17	32,32,33,33	0
20	EDO	N	614	4/4	0.95	0.11	37,38,40,40	0
20	EDO	D	205	4/4	0.95	0.20	43,45,49,53	0
27	PEK	G	101	53/53	0.95	0.17	33,50,79,81	0
20	EDO	N	612	4/4	0.95	0.19	42,45,46,47	0
20	EDO	P	314	4/4	0.95	0.29	61,62,65,66	0
20	EDO	E	202	4/4	0.95	0.13	45,46,50,52	0
22	CHD	C	301	29/29	0.96	0.09	30,32,34,35	0
22	CHD	B	302	29/29	0.96	0.12	30,31,34,39	0
20	EDO	T	103	4/4	0.96	0.18	40,42,43,44	0
20	EDO	E	205	4/4	0.96	0.12	41,41,43,45	0
25	UNX	C	303	1/1	0.96	0.24	32,32,32,32	0
14	HEA	N	602[B]	60/60	0.97	0.15	26,28,39,40	60
23	CUA	O	301	2/2	0.97	0.15	34,34,34,35	0
19	PGV	C	304	51/51	0.97	0.16	30,38,76,84	0
19	PGV	A	608	51/51	0.97	0.16	28,37,58,63	0
22	CHD	G	103	29/29	0.97	0.13	31,33,36,40	0
22	CHD	P	301	29/29	0.97	0.08	31,34,36,39	0
20	EDO	O	303	4/4	0.97	0.22	40,40,41,41	0
20	EDO	A	610	4/4	0.97	0.21	40,43,44,44	0
20	EDO	A	621	4/4	0.97	0.20	37,43,43,44	0
19	PGV	N	608	51/51	0.97	0.14	31,39,63,67	0
19	PGV	P	305	51/51	0.97	0.15	31,39,73,77	0
14	HEA	N	602[A]	60/60	0.97	0.15	28,30,33,33	60
25	UNX	P	304	1/1	0.97	0.20	28,28,28,28	0
14	HEA	A	602[B]	60/60	0.98	0.14	24,26,30,31	60
14	HEA	A	601	60/60	0.98	0.12	23,26,45,47	0
14	HEA	N	601	60/60	0.98	0.13	29,32,51,53	0
23	CUA	B	303	2/2	0.98	0.17	28,28,28,29	0
14	HEA	A	602[A]	60/60	0.98	0.14	22,25,29,31	60
20	EDO	E	203	4/4	0.98	0.11	43,43,45,46	0
20	EDO	B	304	4/4	0.98	0.14	31,33,36,36	0
20	EDO	G	105	4/4	0.98	0.10	34,36,39,40	0
20	EDO	N	615	4/4	0.98	0.12	33,36,37,37	0
20	EDO	P	313	4/4	0.98	0.24	43,43,43,45	0
17	NA	A	605	1/1	0.99	0.07	30,30,30,30	0
18	AZI	A	606	3/3	0.99	0.15	30,30,31,32	0

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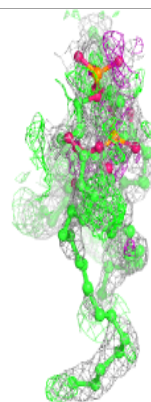
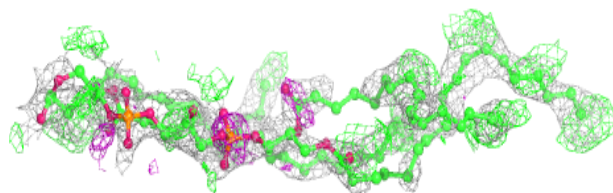
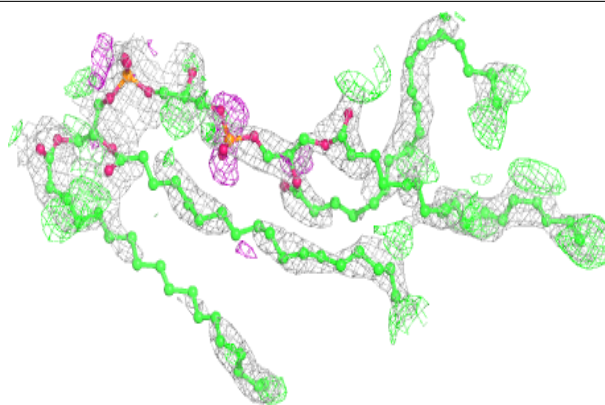
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	S	102	4/4	0.99	0.10	32,33,33,33	0
17	NA	N	605	1/1	0.99	0.05	38,38,38,38	0
20	EDO	F	102	4/4	0.99	0.12	28,28,29,30	0
20	EDO	C	312	4/4	0.99	0.09	40,41,41,42	0
18	AZI	N	606	3/3	0.99	0.12	36,36,36,37	0
15	CU	A	603	1/1	1.00	0.16	28,28,28,28	0
29	ZN	S	101	1/1	1.00	0.14	37,37,37,37	0
29	ZN	F	101	1/1	1.00	0.15	34,34,34,34	0
15	CU	N	603	1/1	1.00	0.18	32,32,32,32	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.



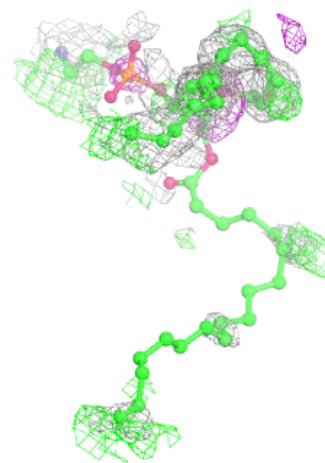
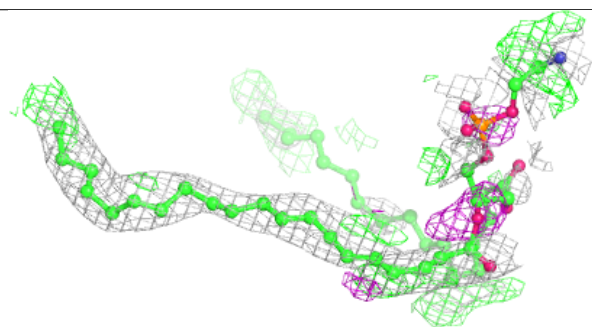
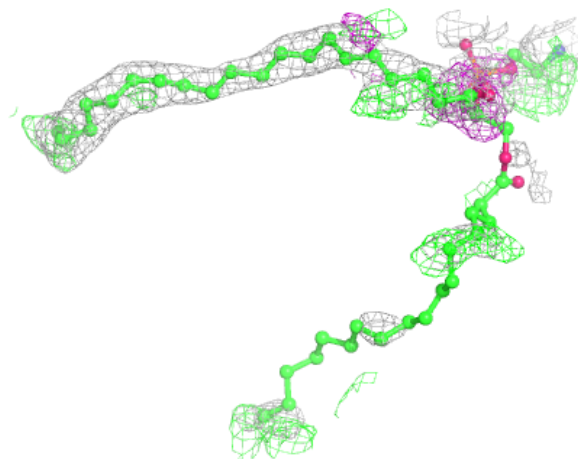
**Electron density around CDL T 102:**

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



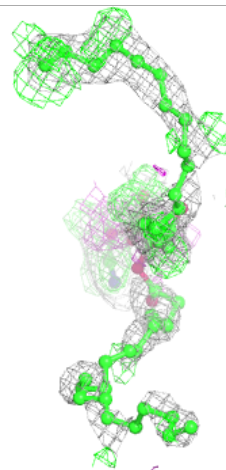
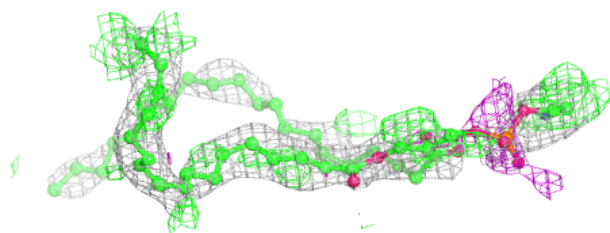
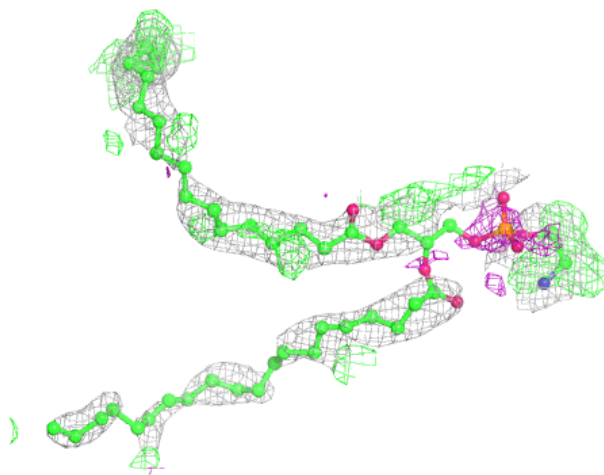
**Electron density around PEK C 309:**

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



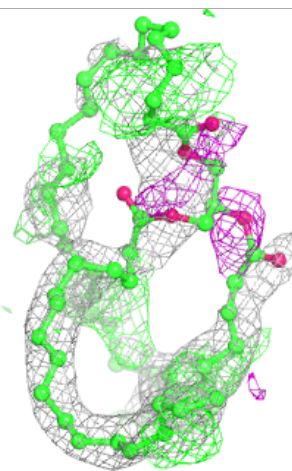
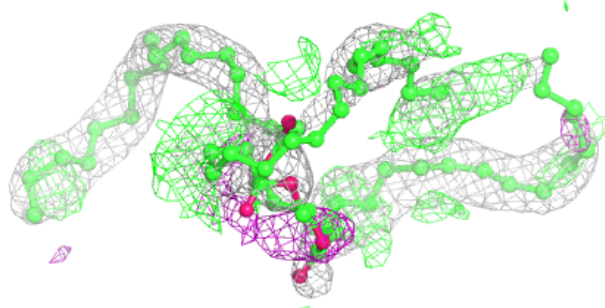
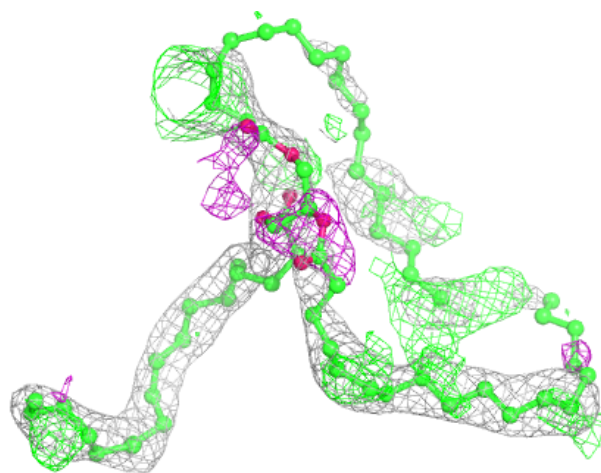
**Electron density around PEK C 307:**

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



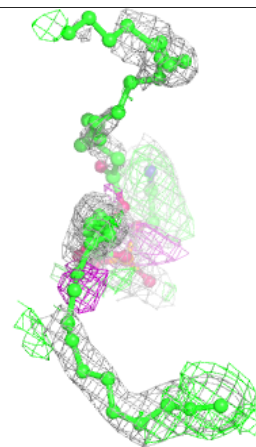
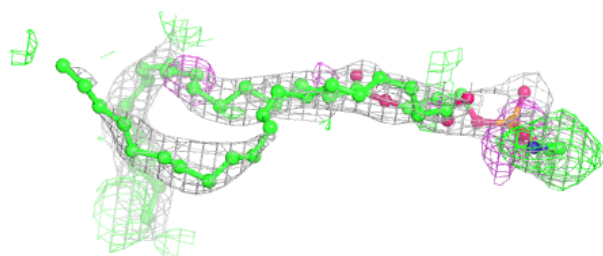
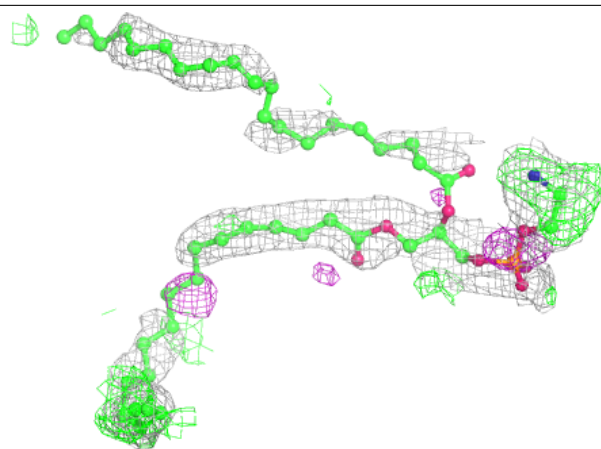
**Electron density around TGL Y 101:**

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

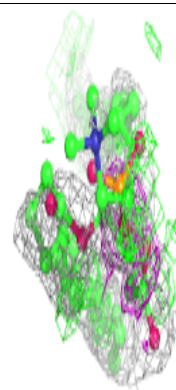
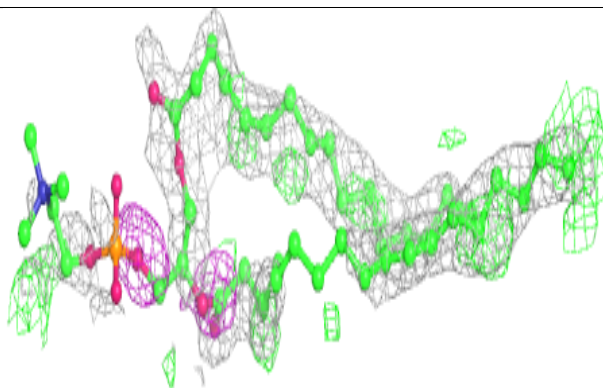
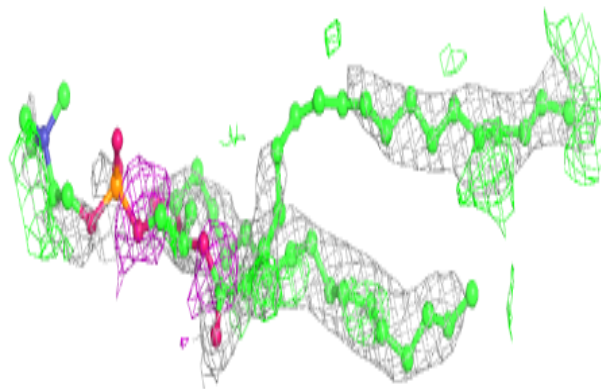


**Electron density around PEK P 309:**

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

**Electron density around PSC E 201:**

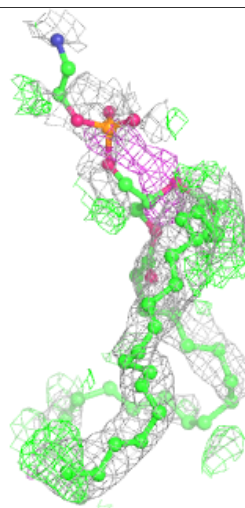
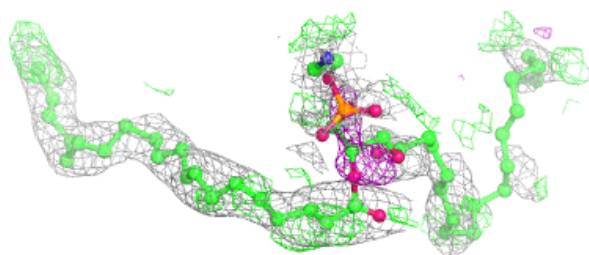
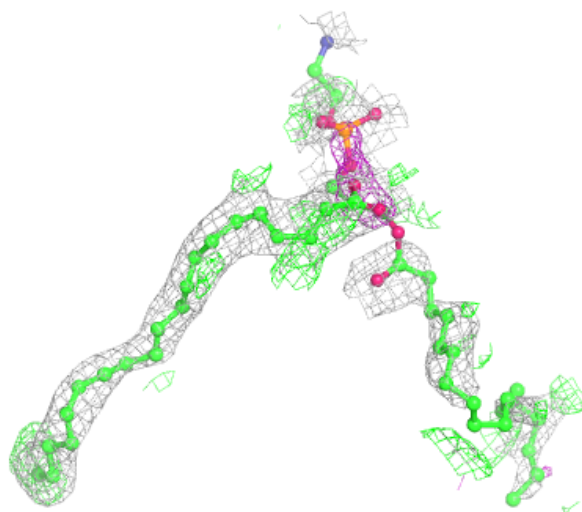
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PEK P 302:**

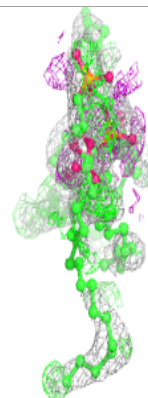
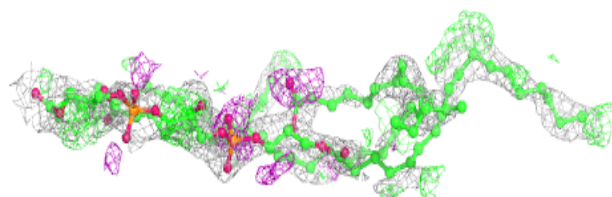
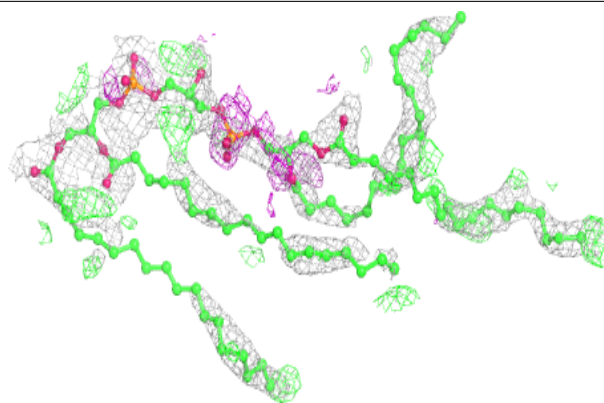
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



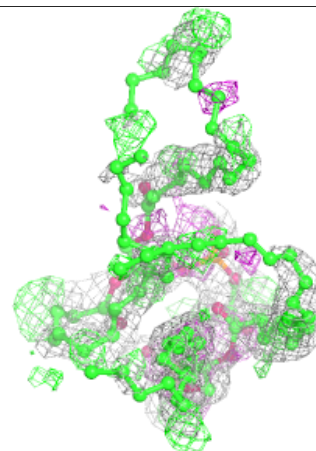
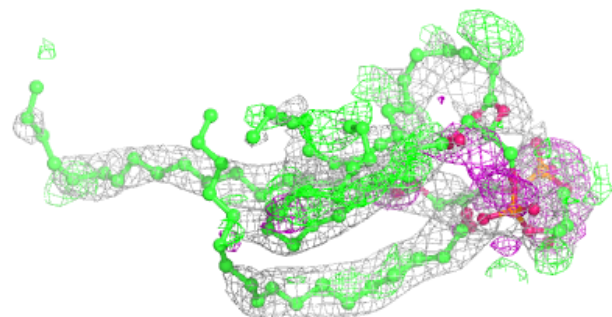
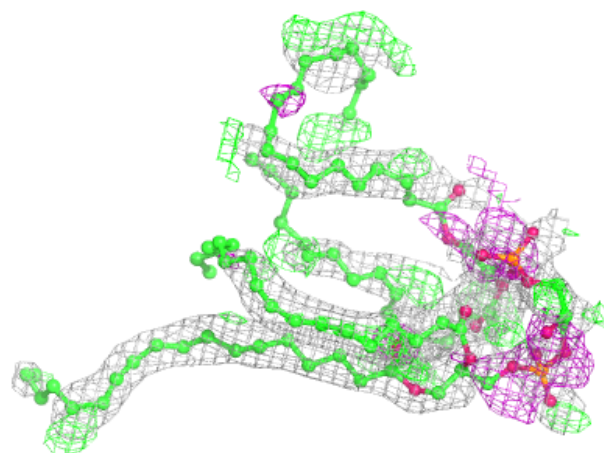


**Electron density around CDL G 102:**

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

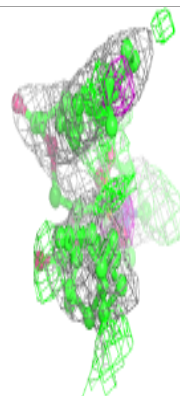
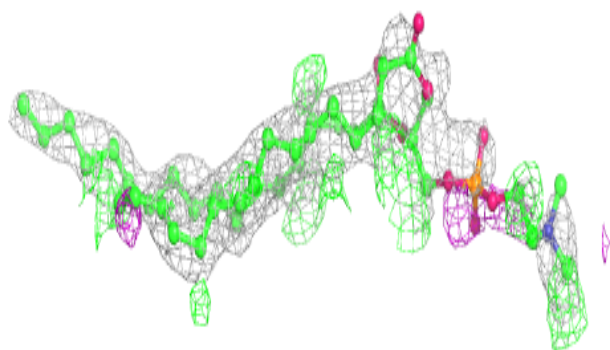
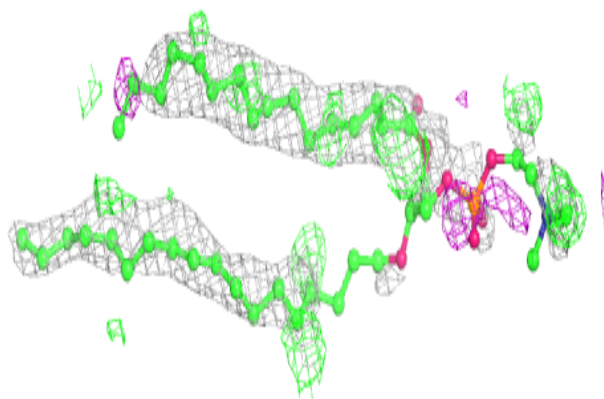
**Electron density around CDL P 306:**

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

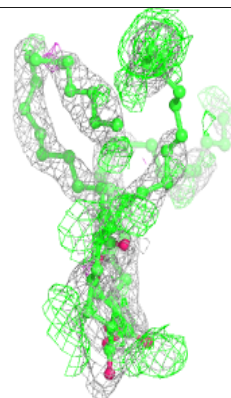
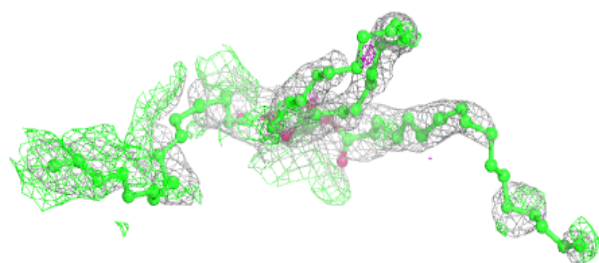
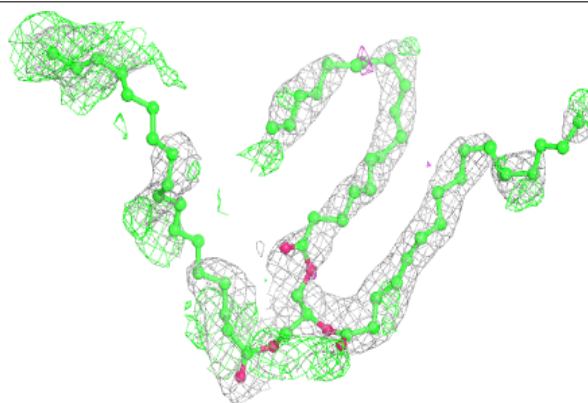


**Electron density around PSC O 302:**

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

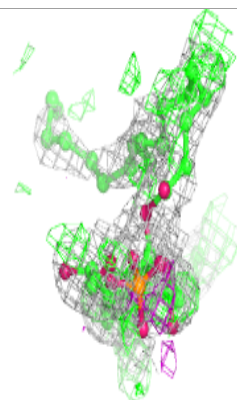
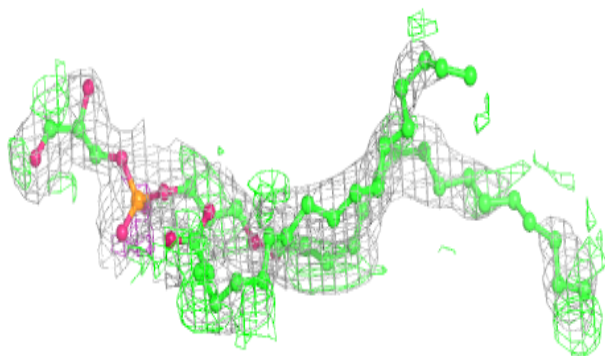
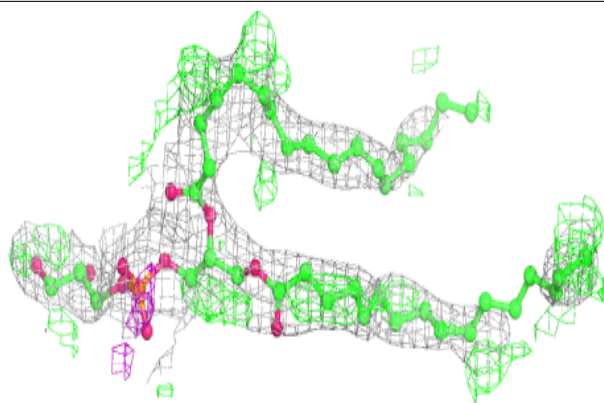
**Electron density around TGL Q 201:**

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



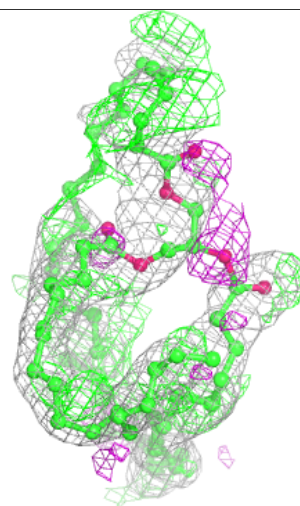
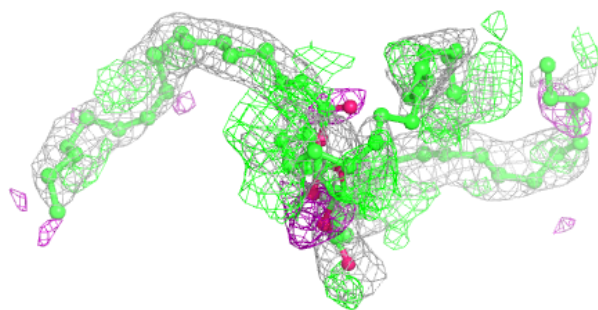
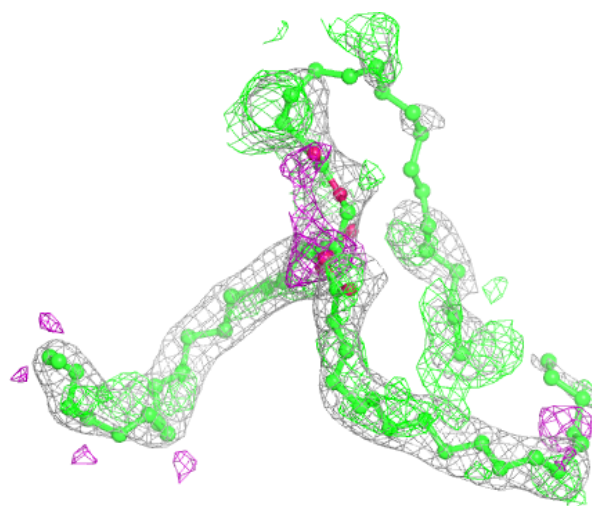
**Electron density around PGV C 308:**

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



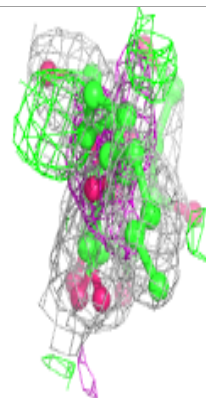
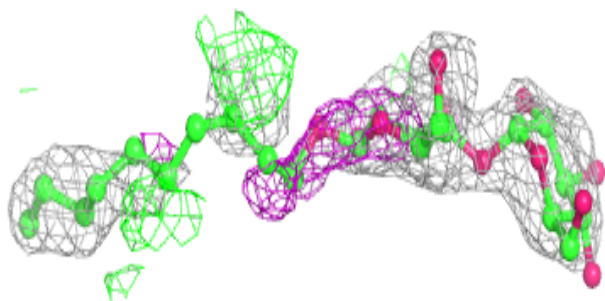
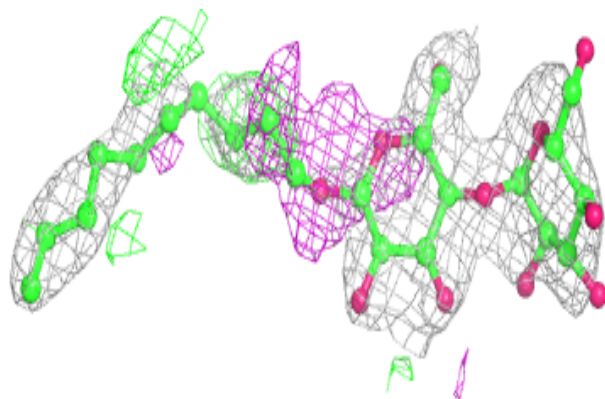
**Electron density around TGL L 101:**

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

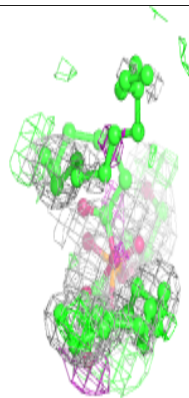
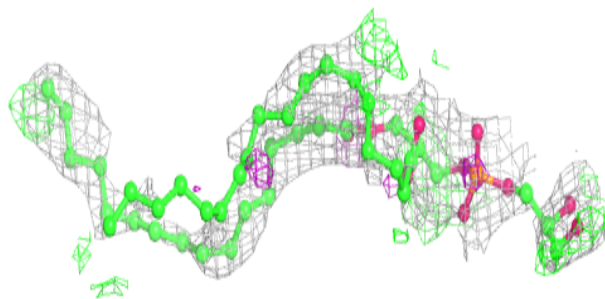
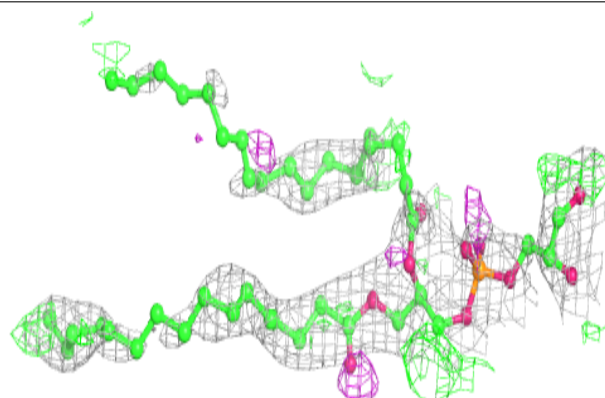


**Electron density around DMU C 302:**

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

**Electron density around PGV P 303:**

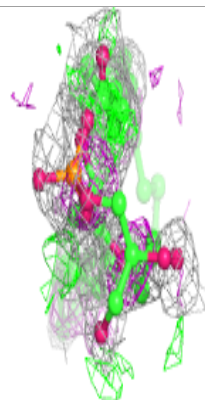
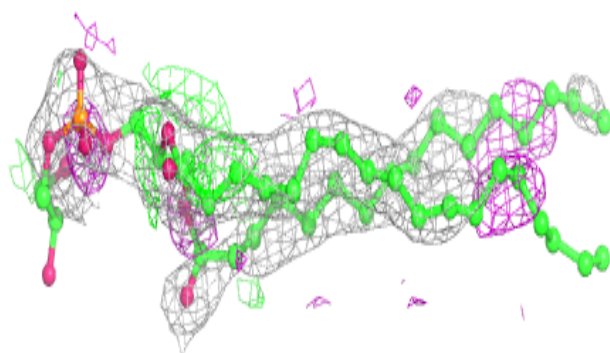
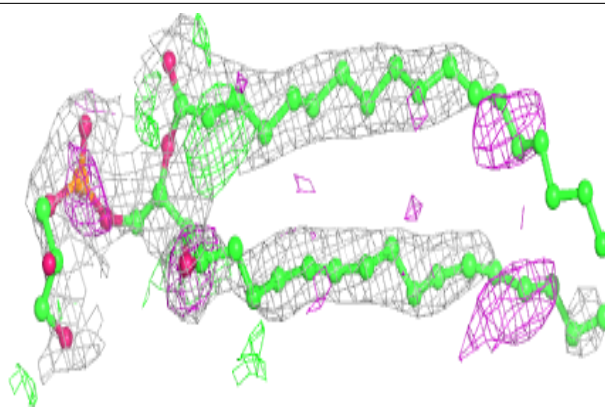
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



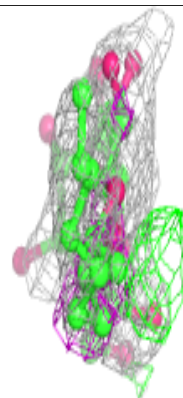
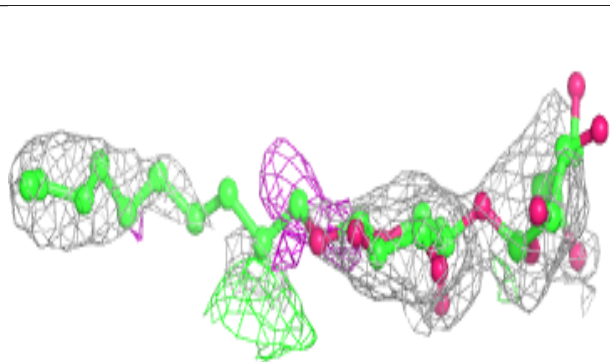
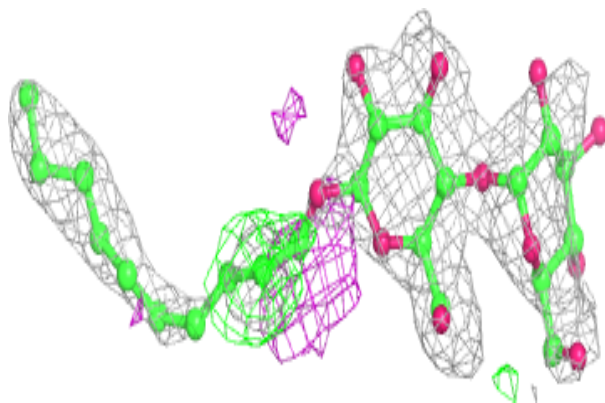


**Electron density around PGV Z 101:**

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

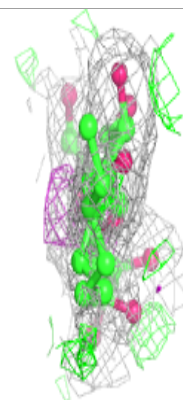
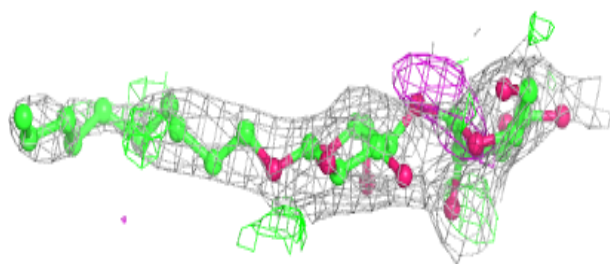
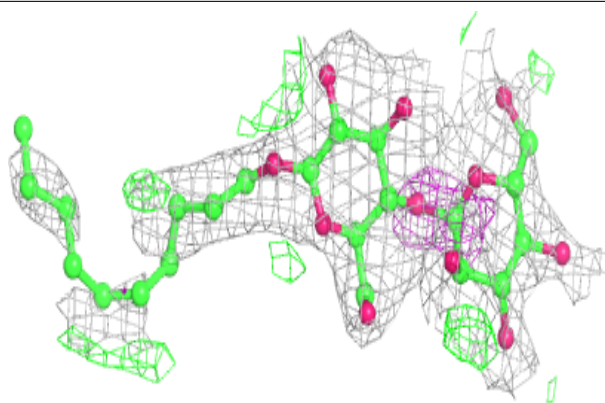
**Electron density around DMU P 308:**

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

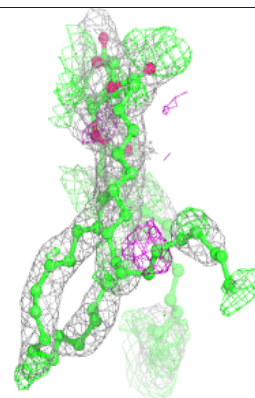
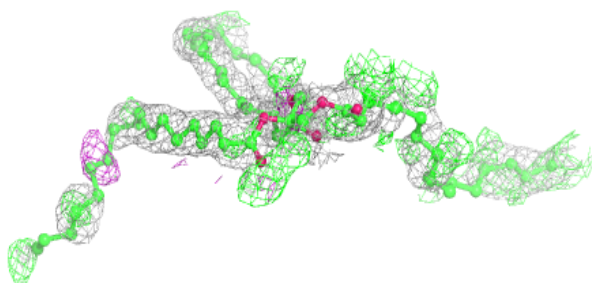
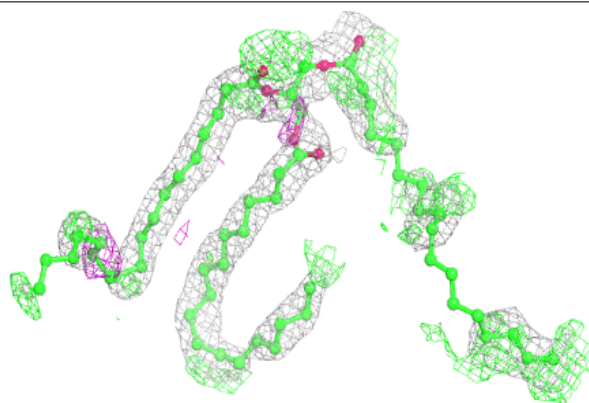


**Electron density around DMU P 310:**

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

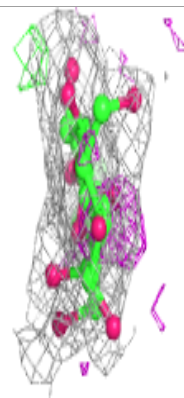
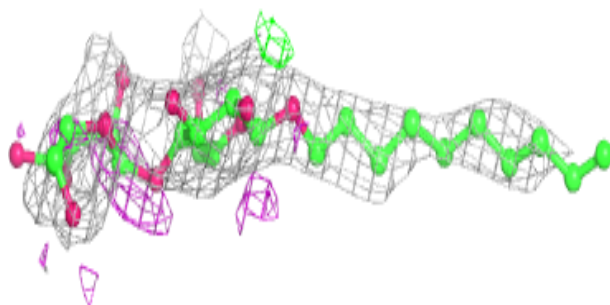
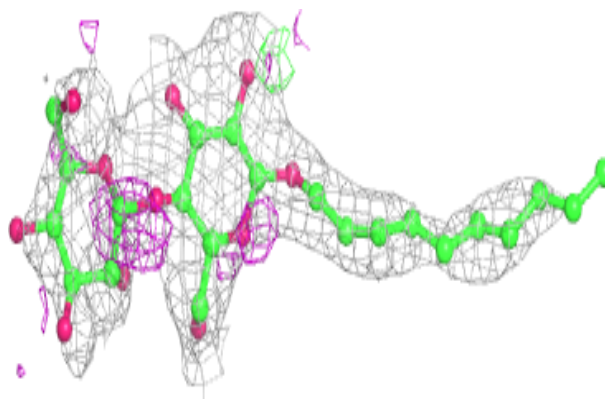
**Electron density around TGL D 201:**

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

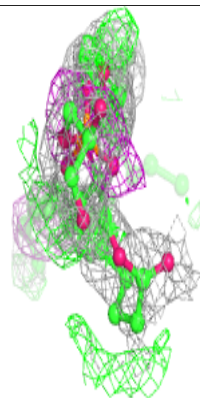
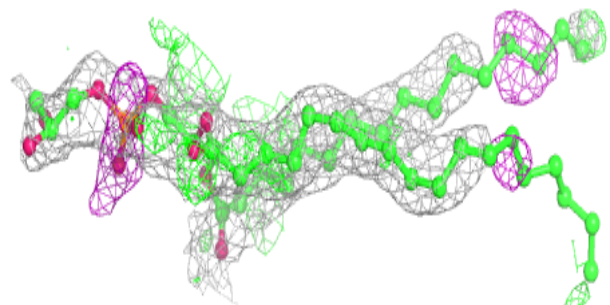
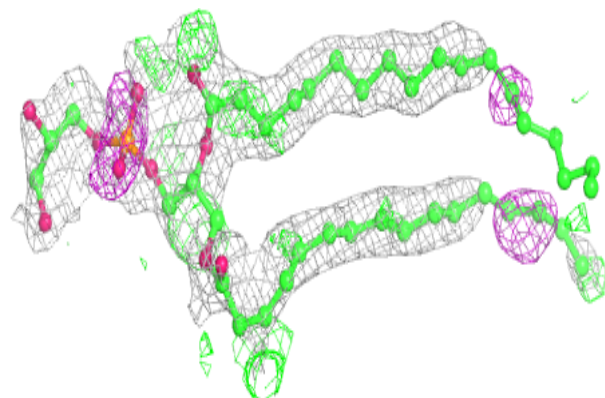


**Electron density around DMU C 310:**

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

**Electron density around PGV A 609:**

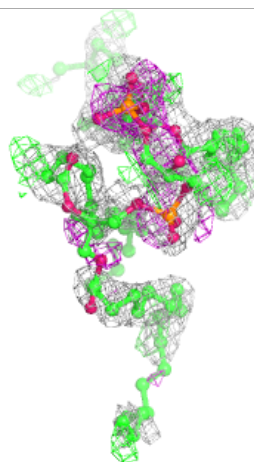
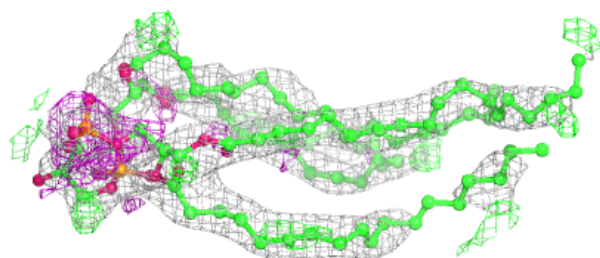
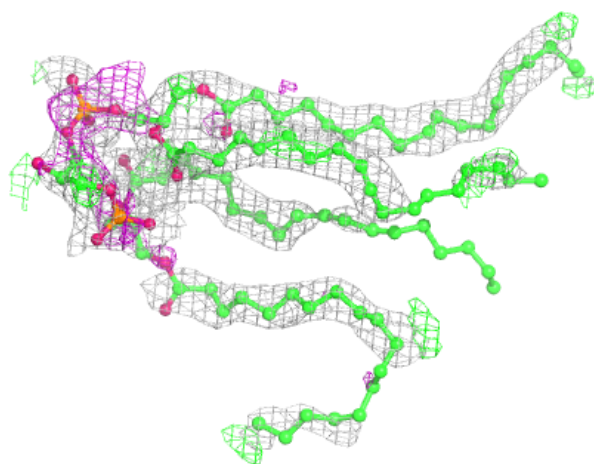
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





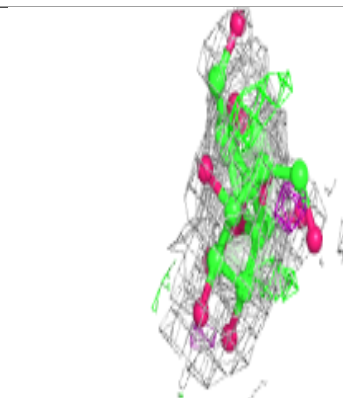
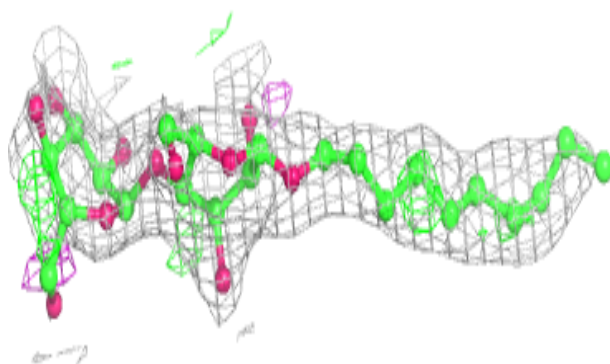
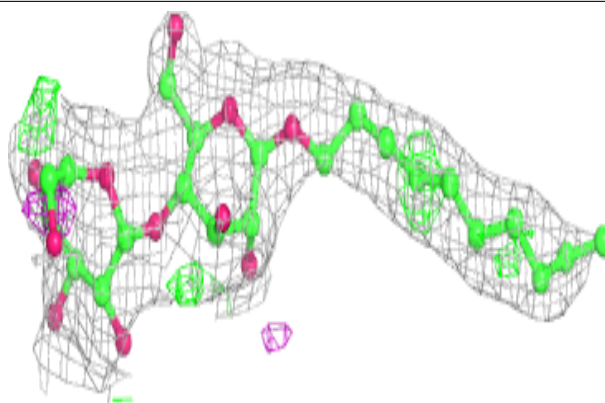
**Electron density around CDL C 305:**

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

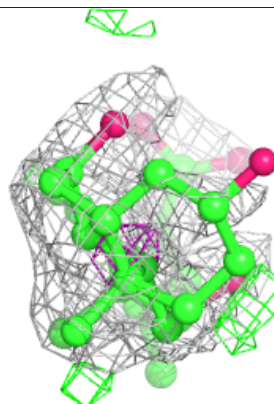
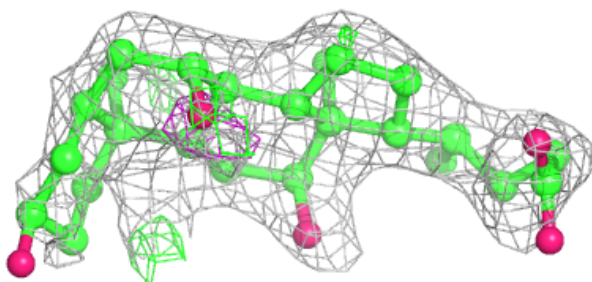
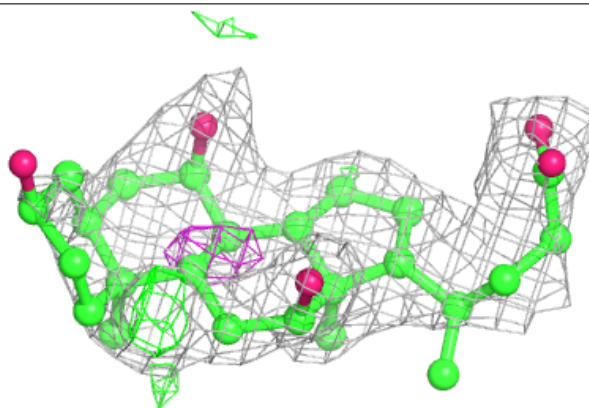


**Electron density around DMU C 311:**

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

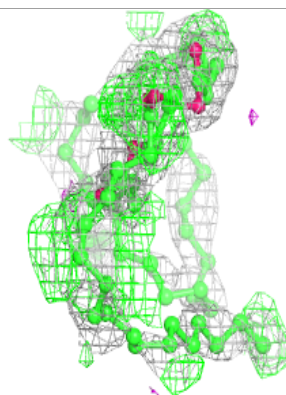
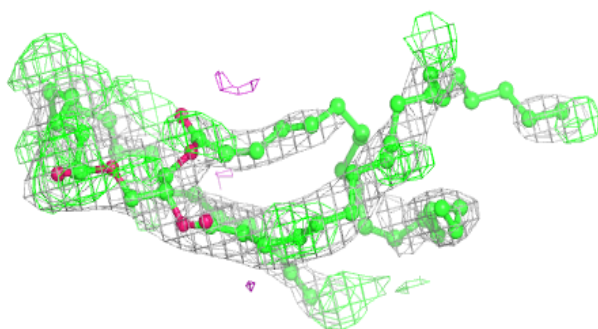
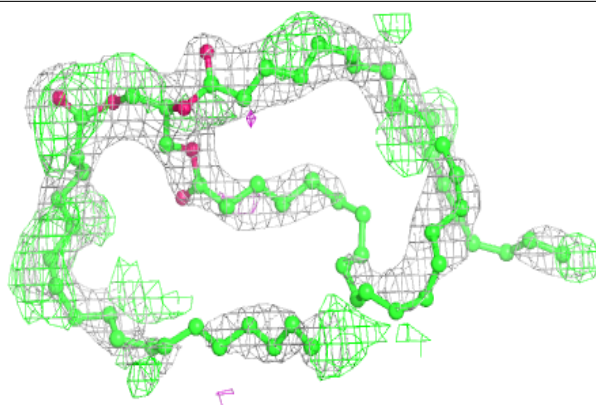
**Electron density around CHD J 101:**

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

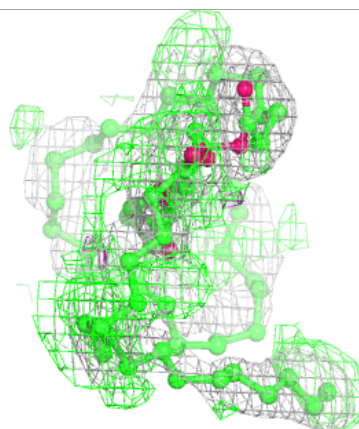
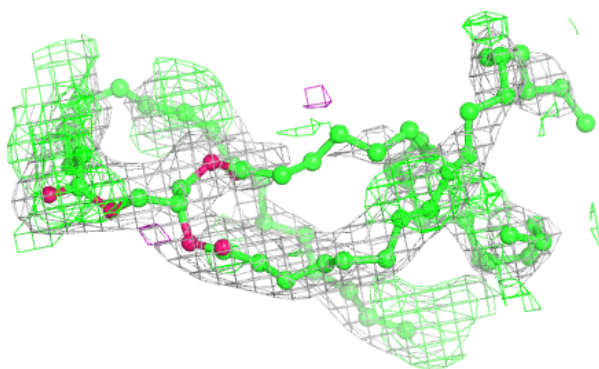
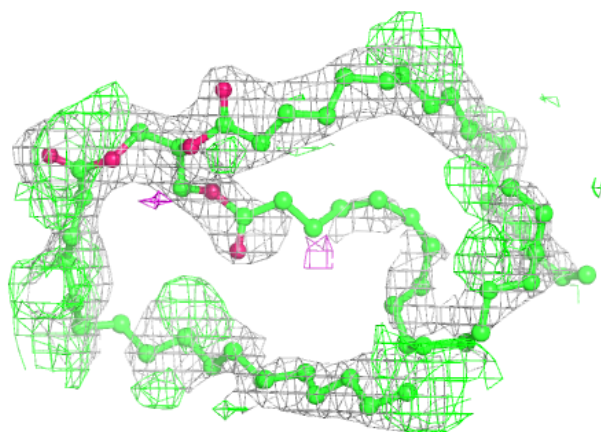


**Electron density around TGL N 609:**

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

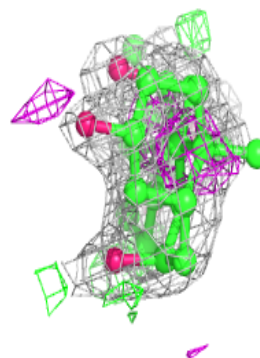
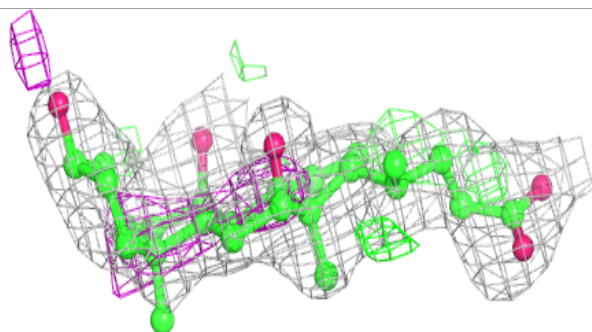
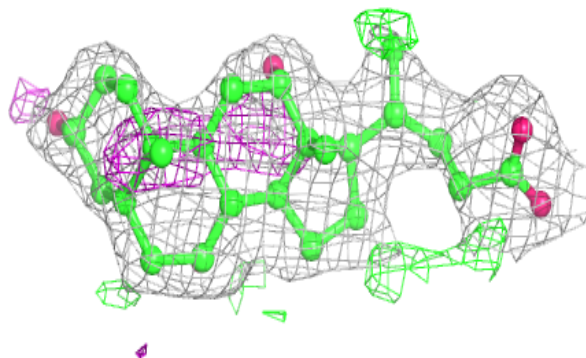
**Electron density around TGL B 301:**

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

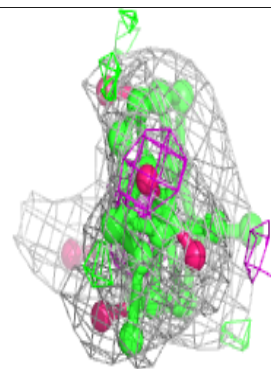
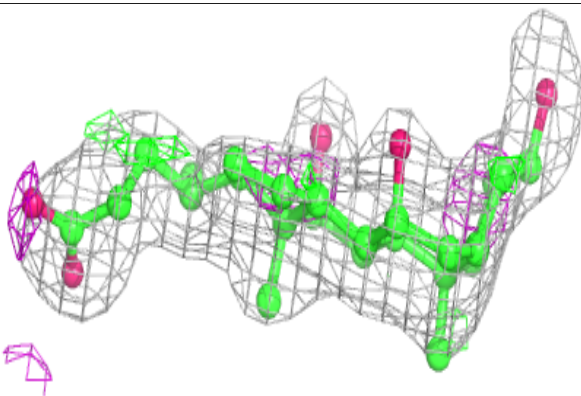
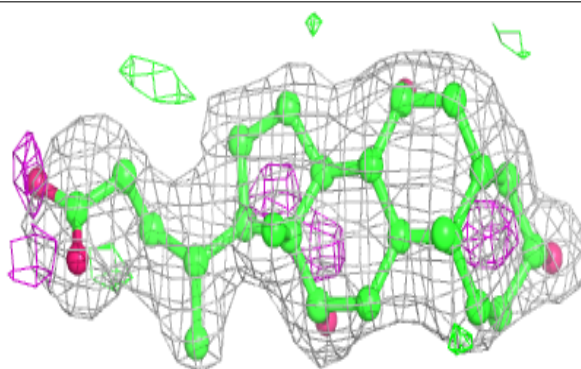


**Electron density around CHD P 307:**

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

**Electron density around CHD C 306:**

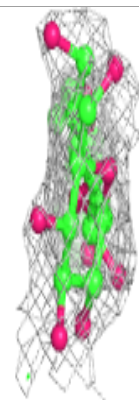
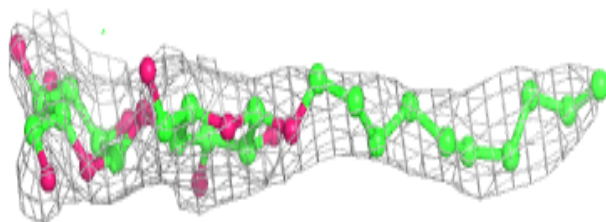
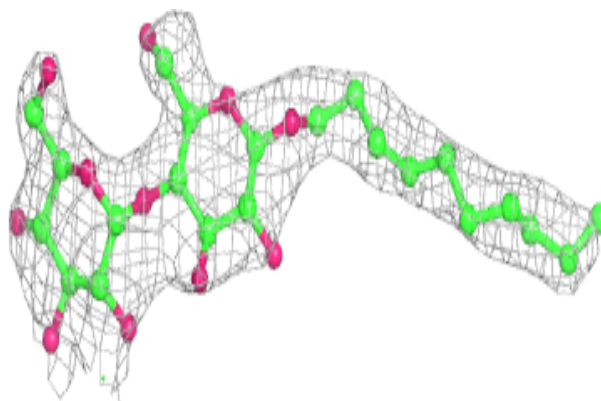
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



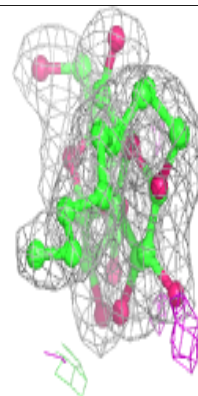
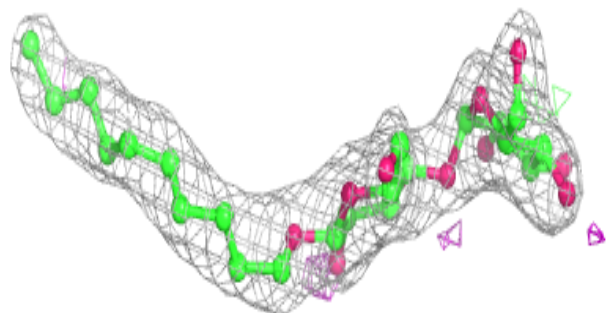
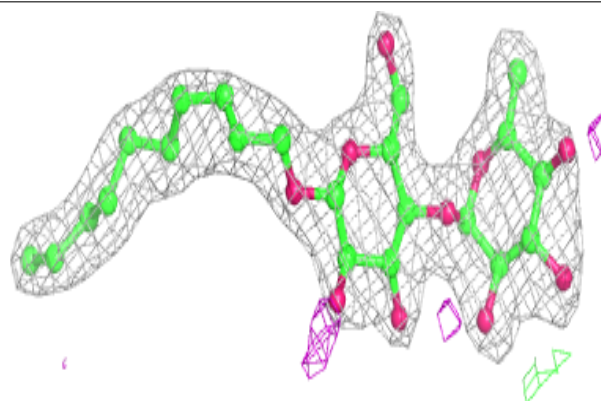


**Electron density around DMU P 311:**

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

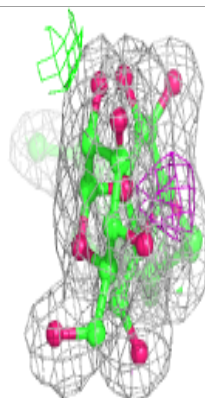
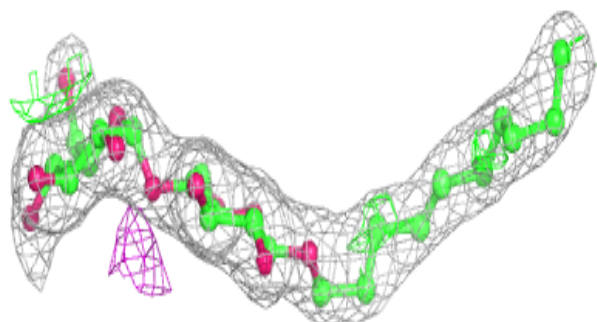
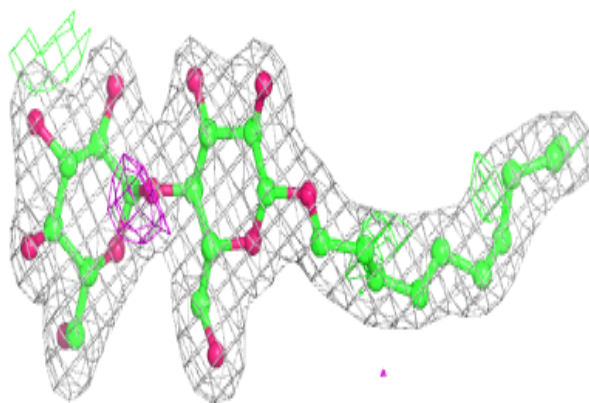
**Electron density around DMU Z 102:**

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

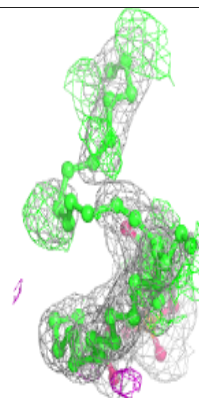
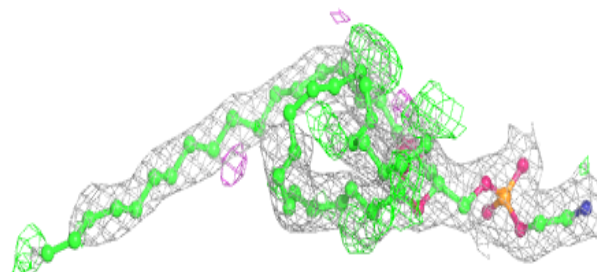
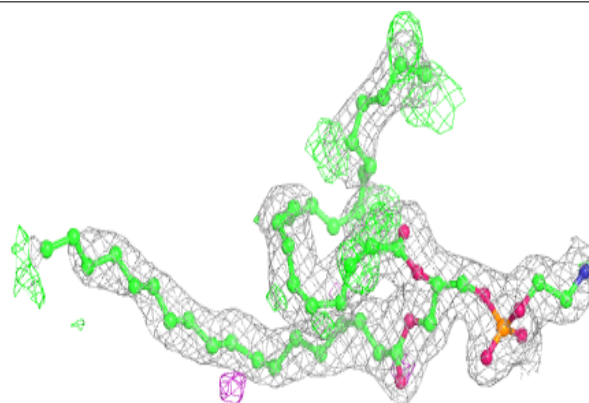


**Electron density around DMU M 101:**

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

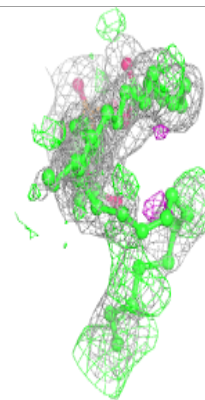
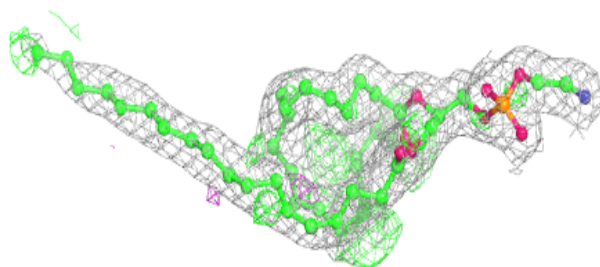
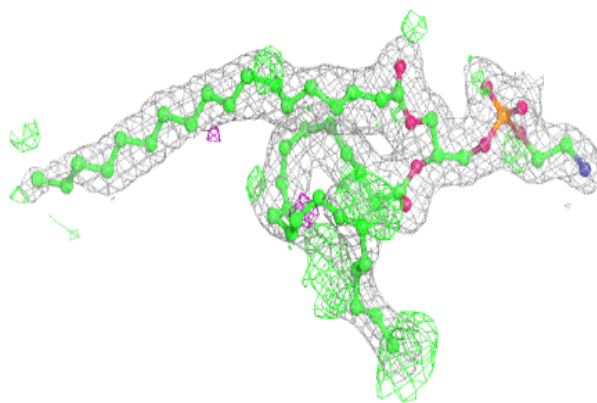
**Electron density around PEK T 101:**

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

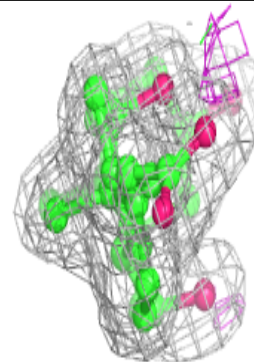
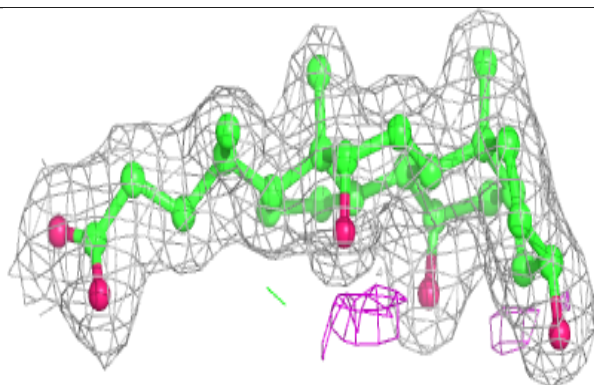
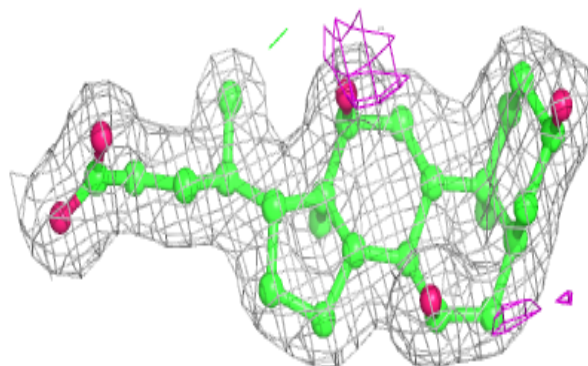


**Electron density around PEK G 101:**

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

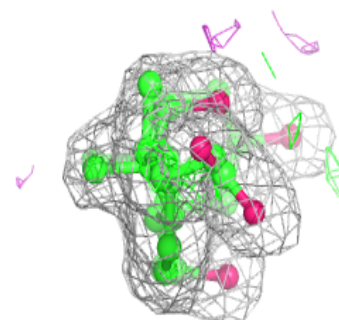
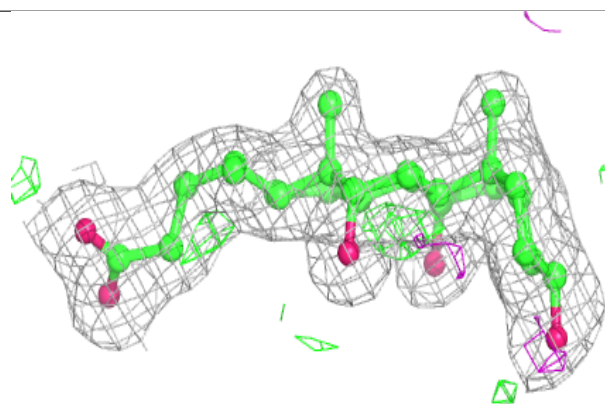
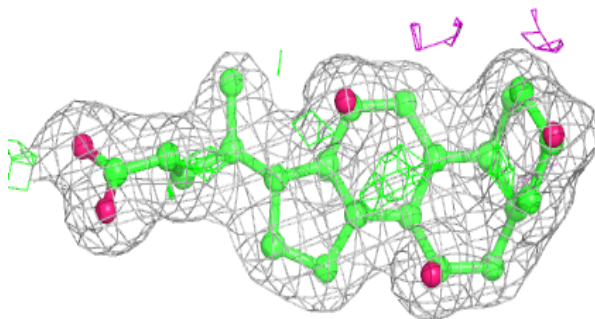
**Electron density around CHD C 301:**

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

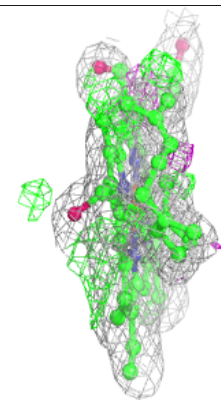
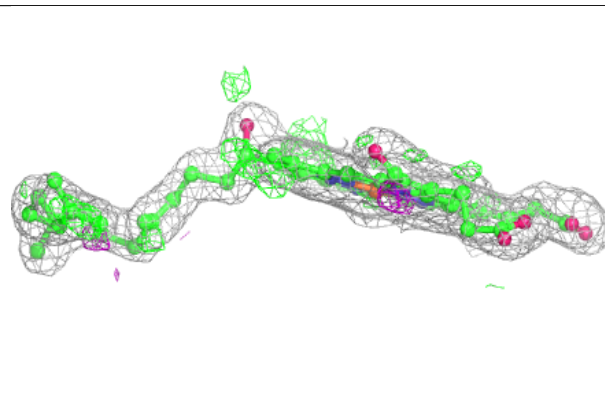
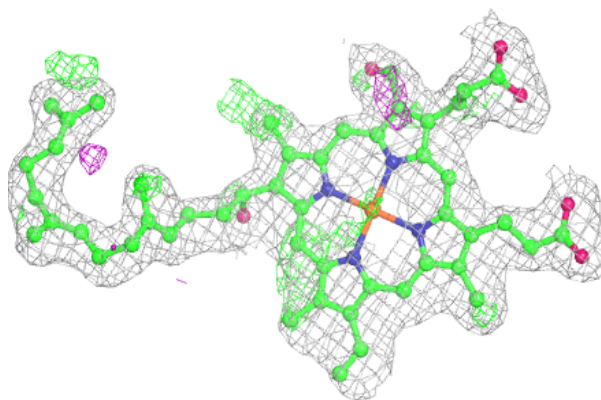


**Electron density around CHD B 302:**

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

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

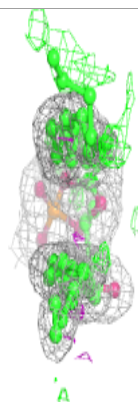
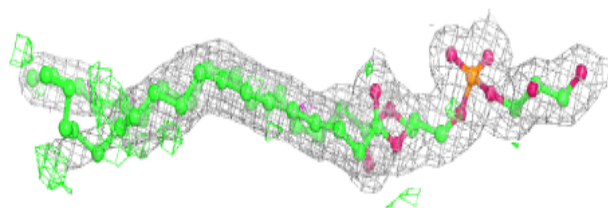
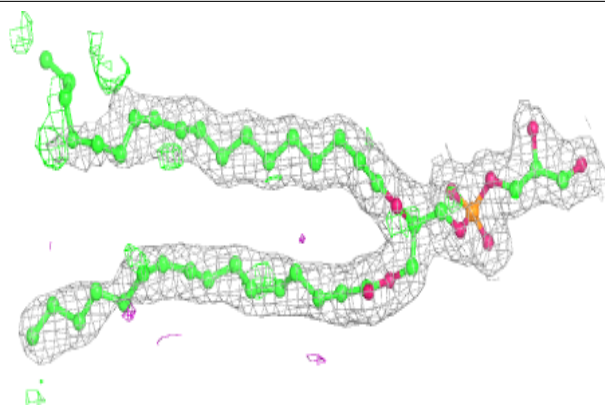
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



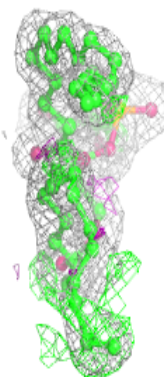
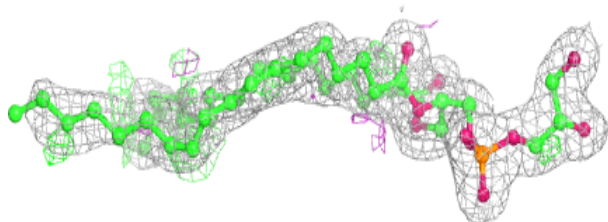
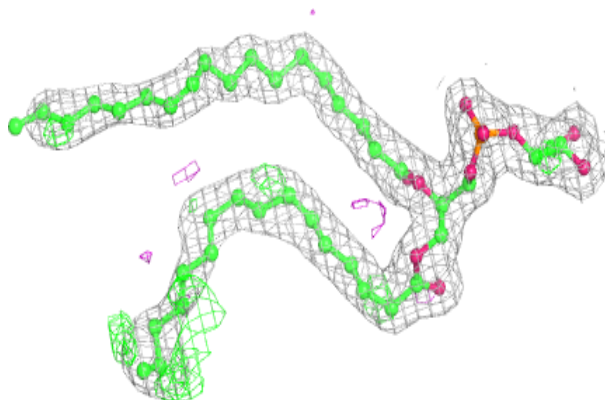


**Electron density around PGV C 304:**

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

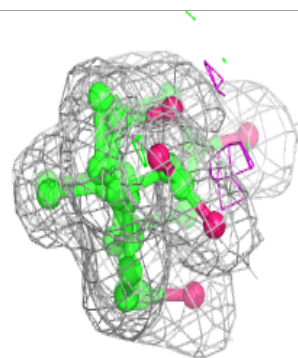
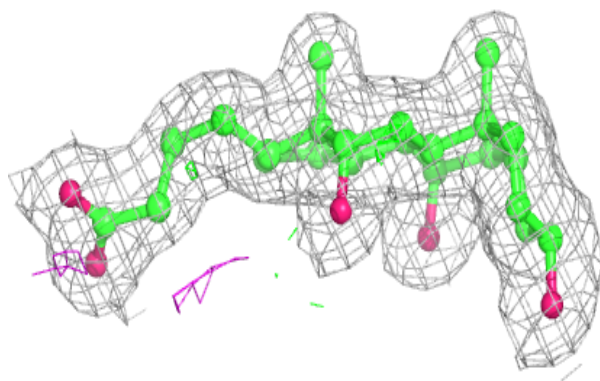
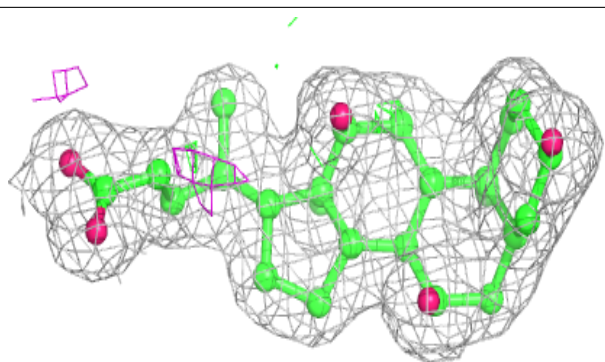
**Electron density around PGV A 608:**

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

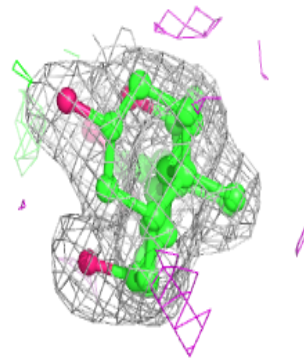
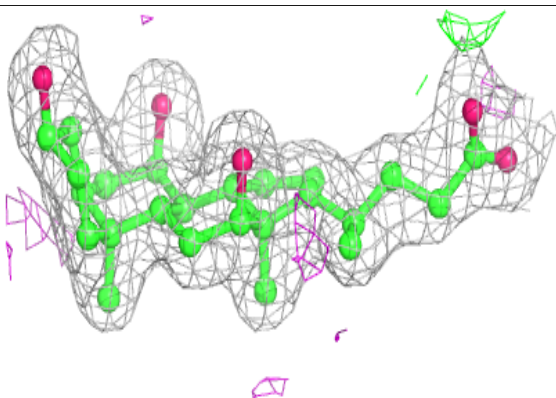
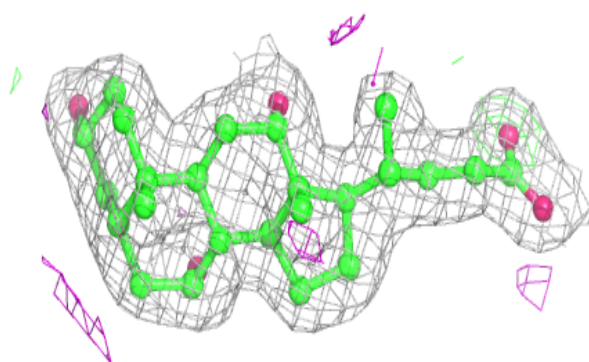


**Electron density around CHD G 103:**

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

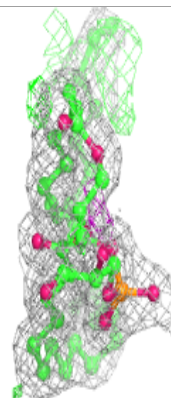
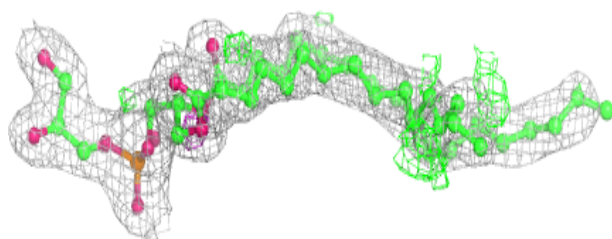
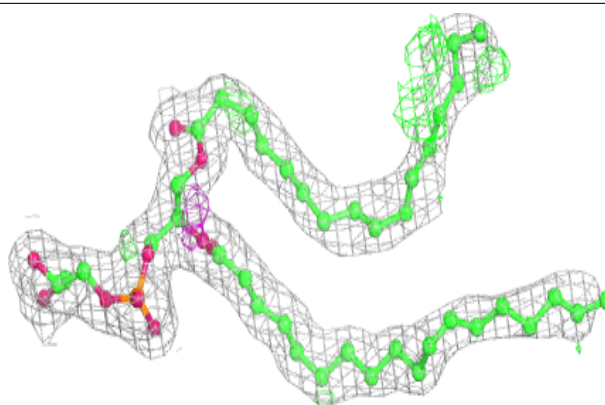
**Electron density around CHD P 301:**

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

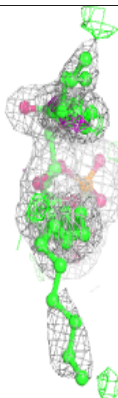
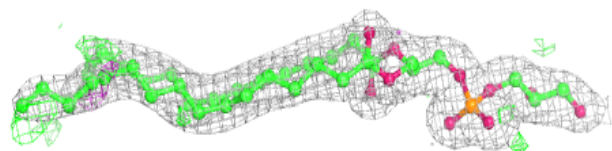
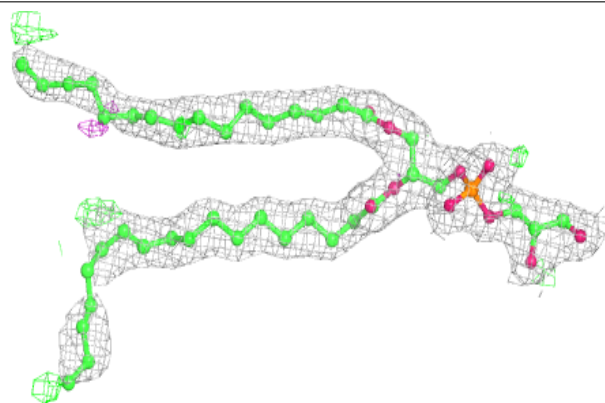


**Electron density around PGV N 608:**

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

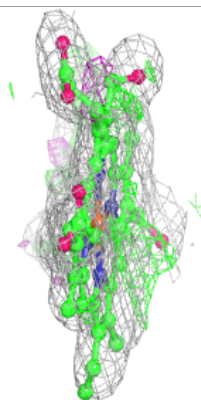
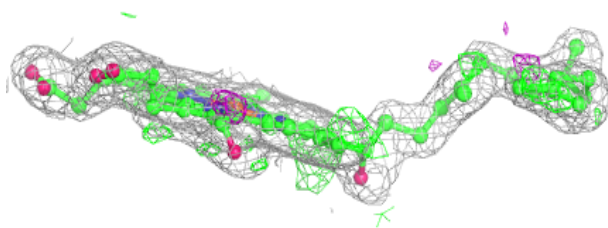
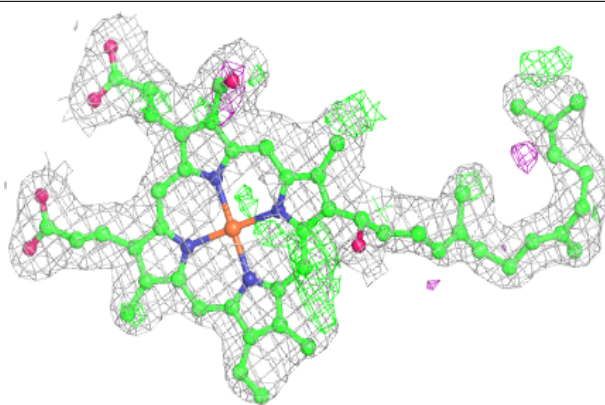
**Electron density around PGV P 305:**

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

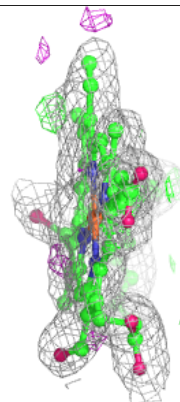
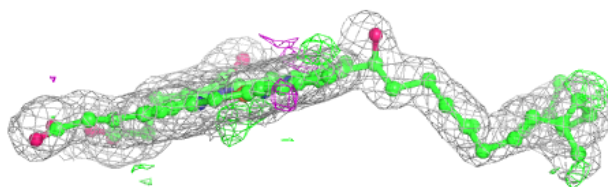
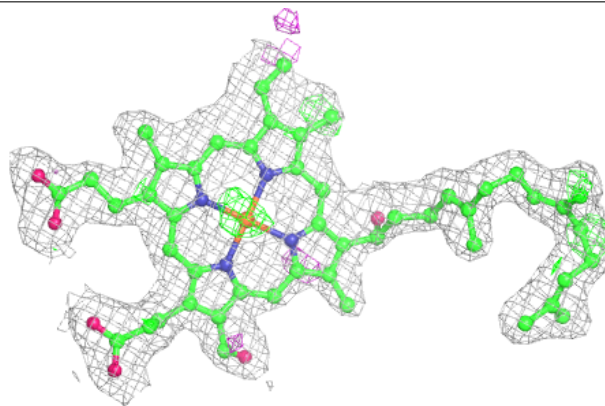


**Electron density around HEA N 602 (A):**

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

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

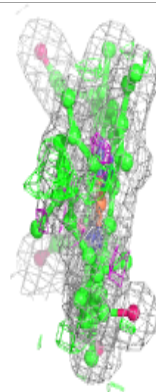
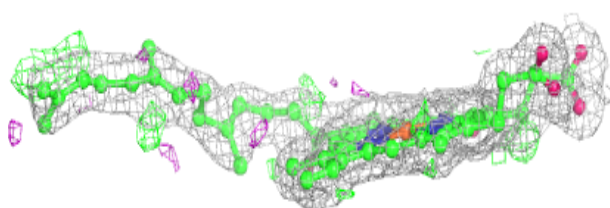
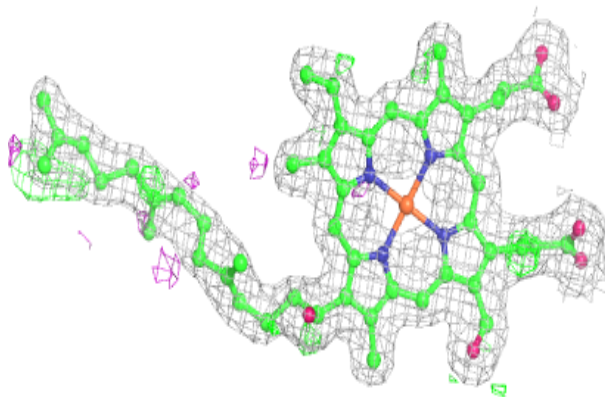
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



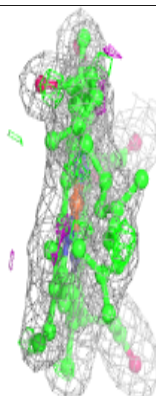
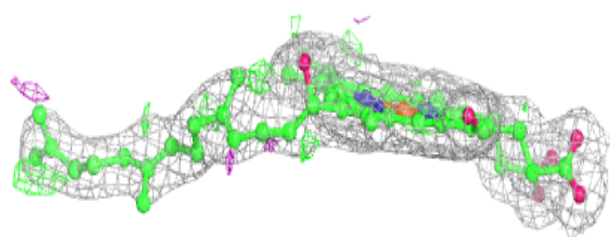
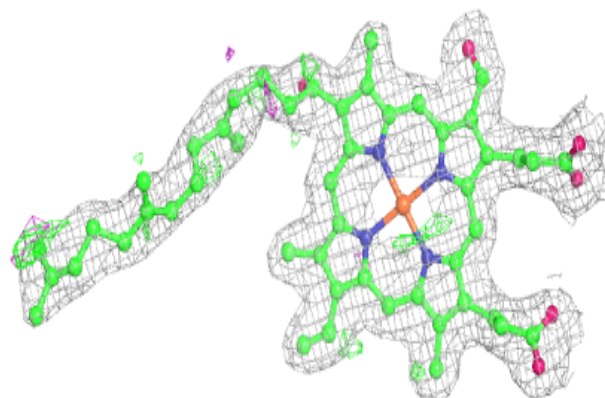


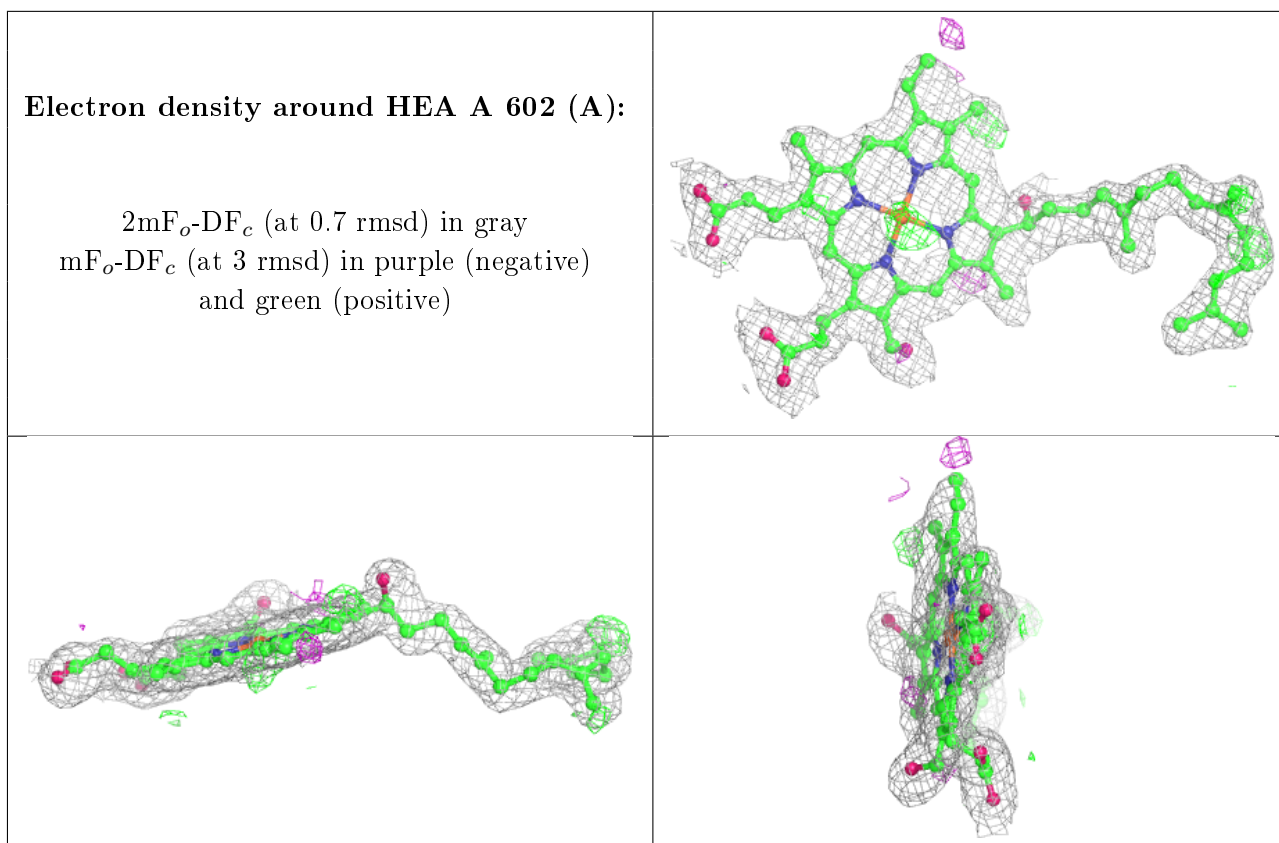
**Electron density around HEA A 601:**

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

**Electron density around HEA N 601:**

$2mF_o-DF_c$  (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.