



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 08:03 pm BST

PDB ID : 6JUW
Title : BOVINE HEART CYTOCHROME C OXIDASE IN CATALITIC INTER-MEDIATES AT 1.80 ANGSTROM RESOLUTION
Authors : Shimada, A.; Muramoto, K.; Shinzawa-Itoh, K.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2019-04-15
Resolution : 1.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

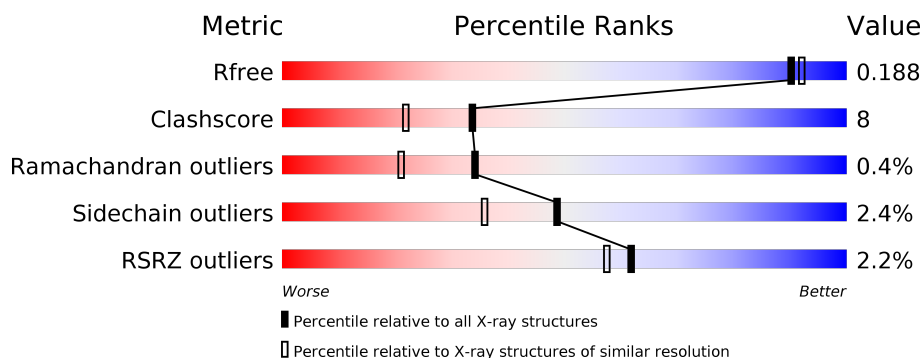
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	N	514	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	B	227	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
3	C	259	<div> <div>88%</div> <div>11%</div> </div>
3	P	259	<div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	

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	602	X	-	-	-
14	HEA	N	602	X	-	-	-
18	DMU	K	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	EDO	N	612	-	-	X	-
22	EDO	N	617	-	-	X	-
22	EDO	U	102	-	-	X	-
25	CDL	G	102	-	-	X	-
25	CDL	T	102	-	-	X	-
7	TPO	G	11	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 34360 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	37	0
			4192	2794	643	710	45			
1	N	514	Total	C	N	O	S	0	21	0
			4152	2770	639	703	40			

- 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	4	0
			1839	1196	281	343	19			
2	O	227	Total	C	N	O	S	0	7	0
			1857	1208	287	343	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	5	0
			2122	1417	336	355	14			
3	P	259	Total	C	N	O	S	0	2	0
			2114	1413	336	353	12			

- 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	1	0
			1198	780	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	1	0
			751	465	135	146	5			
6	S	98	Total	C	N	O	S	0	1	0
			751	465	134	147	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 676	C 431	N 129	O 114	P 1	S 1	0	0	0
7	T	84	Total 685	C 439	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	0	0
			460	297	78	82	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	0	0
			385	250	65	68	2			

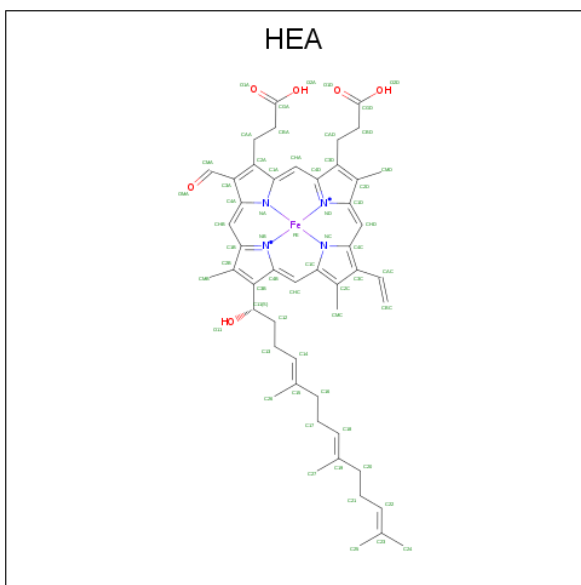
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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	0	0
			380	254	64	60	2			

- 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
			336	223	53	60			
13	Z	43	Total	C	N	O	0	0	0
			336	223	53	60			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 72	C 60	Fe 1	N 4	O 7	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 72	C 60	Fe 1	N 4	O 7	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

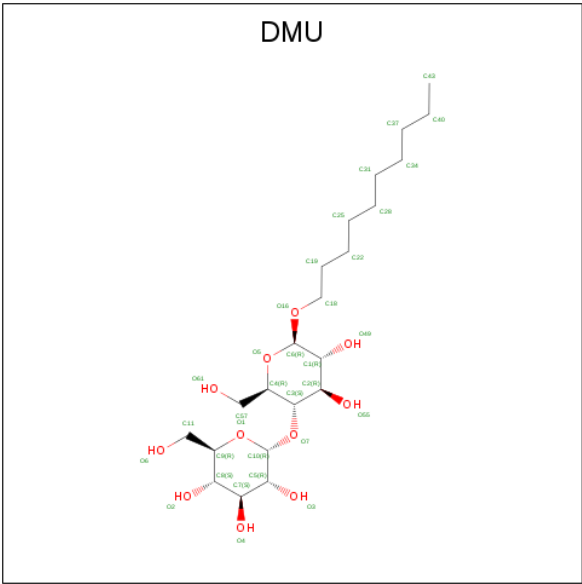
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 18 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



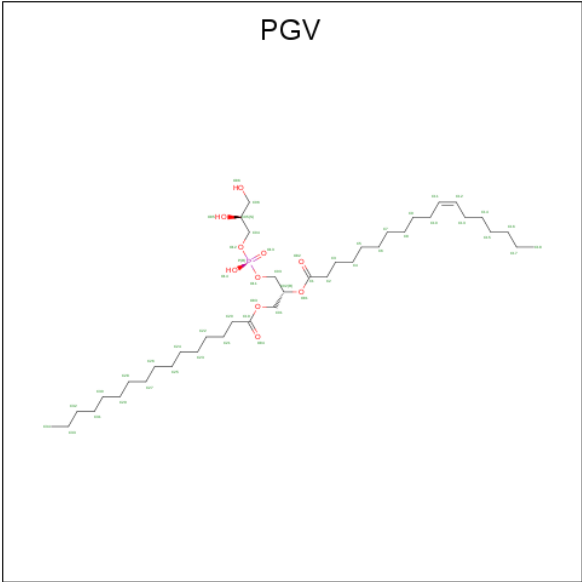
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			13	11	2		
18	B	1	Total	C	O	0	0
			11	10	1		
18	C	1	Total	C	O	0	0
			33	22	11		
18	C	1	Total	C	O	0	0
			22	16	6		
18	C	1	Total	C	O	0	0
			11	10	1		
18	D	1	Total	C	O	0	0
			21	16	5		
18	J	1	Total	C	O	0	0
			21	16	5		

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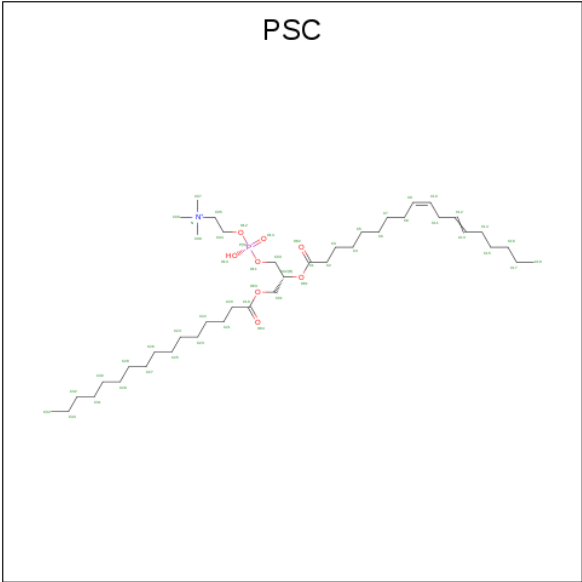
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	K	1	Total	C	O	0	0
			11	10	1		
18	K	1	Total	C	O	0	0
			14	11	3		
18	K	1	Total	C	O	0	0
			22	16	6		
18	K	1	Total	C	O	0	0
			11	10	1		
18	L	1	Total	C	O	0	0
			33	22	11		
18	M	1	Total	C	O	0	0
			33	22	11		
18	O	1	Total	C	O	0	0
			11	10	1		
18	P	1	Total	C	O	0	0
			11	10	1		
18	P	1	Total	C	O	0	0
			33	22	11		
18	Q	1	Total	C	O	0	0
			23	17	6		
18	W	1	Total	C	O	0	0
			21	16	5		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			21	16	5		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			11	10	1		
18	Y	1	Total	C	O	0	0
			33	22	11		
18	Z	1	Total	C	O	0	0
			33	22	11		

- 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: C₄₀H₇₇O₁₀P).



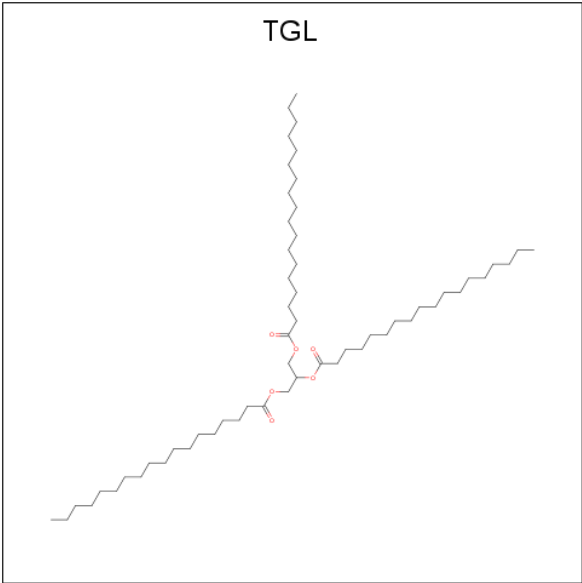
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



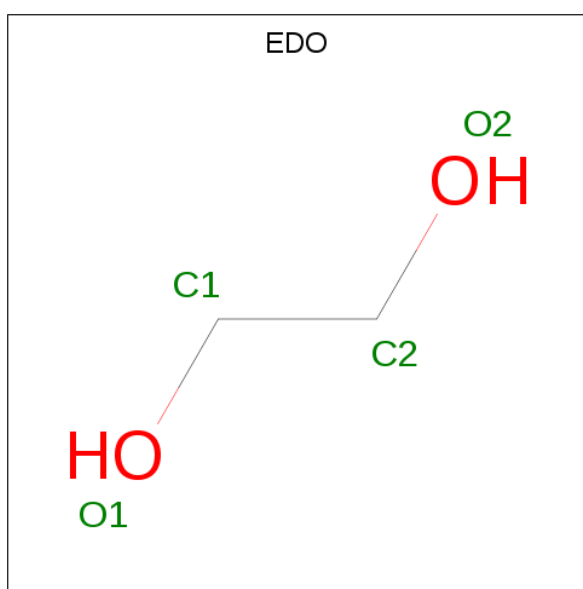
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

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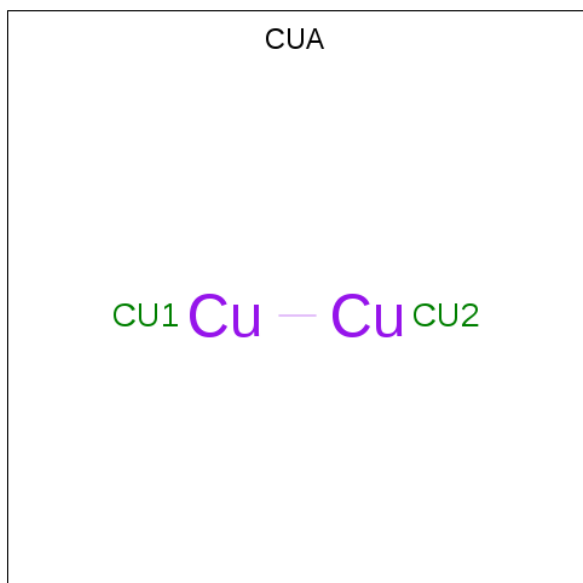
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	O	1	Total 4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

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

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



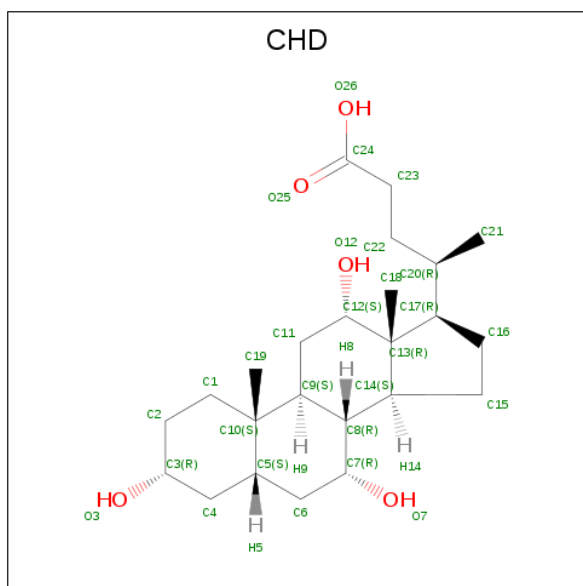
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total Cu 2 2	0	0

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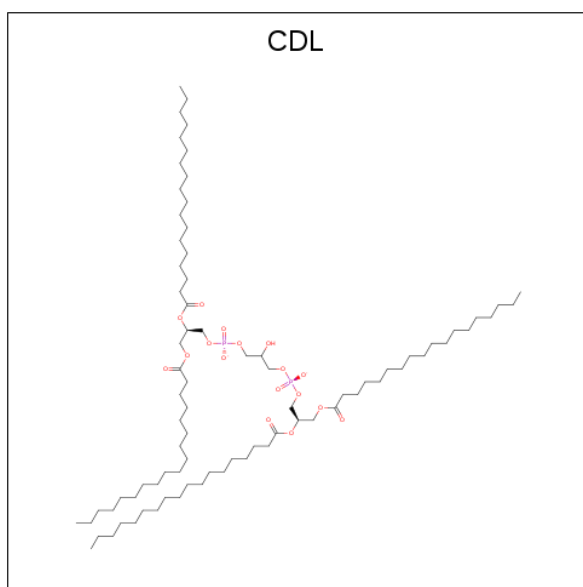
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	O	1	Total	Cu	0	0
			2	2		

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



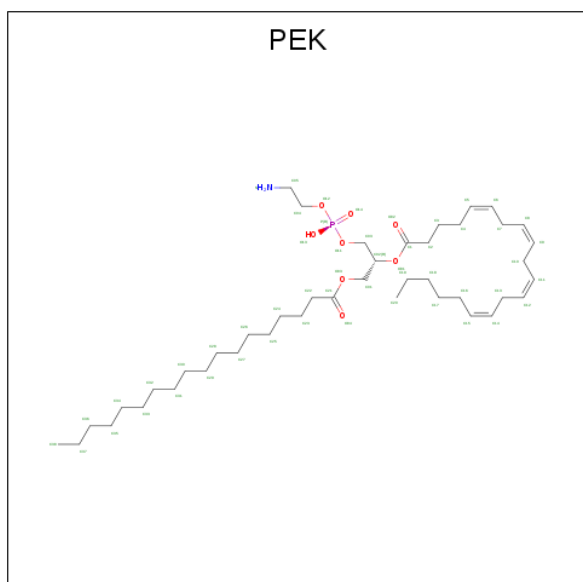
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	J	1	Total	C	O	0	0
			29	24	5		
24	L	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	T	1	Total	C	O	0	0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

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 26 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: C₄₃H₇₈NO₈P).

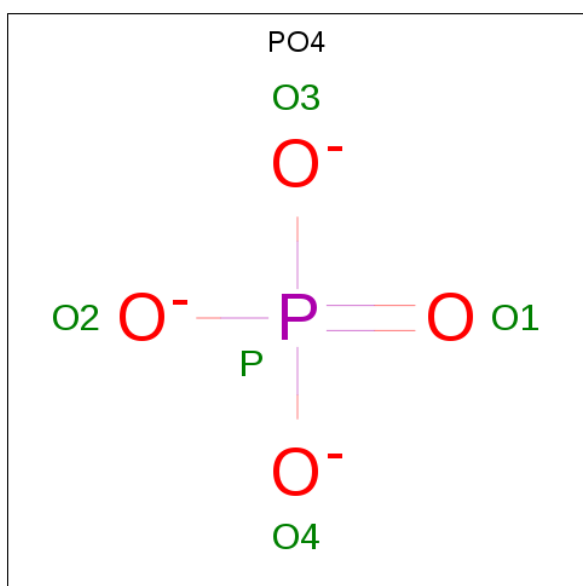


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	F	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	247	Total 250	O 250	0	4
29	B	200	Total 200	O 200	0	0
29	C	136	Total 136	O 136	0	0
29	D	174	Total 174	O 174	0	0
29	E	133	Total 133	O 133	0	0
29	F	117	Total 117	O 117	0	0
29	G	72	Total 72	O 72	0	0
29	H	79	Total 79	O 79	0	0
29	I	56	Total 56	O 56	0	0
29	J	44	Total 44	O 44	0	0
29	K	36	Total 36	O 36	0	0
29	L	42	Total 42	O 42	0	0
29	M	34	Total 34	O 34	0	0
29	N	245	Total 247	O 247	0	3
29	O	166	Total 166	O 166	0	0
29	P	132	Total 132	O 132	0	0
29	Q	99	Total 99	O 99	0	0
29	R	98	Total 98	O 98	0	0
29	S	105	Total 105	O 105	0	0
29	T	75	Total 75	O 75	0	0
29	U	65	Total 65	O 65	0	0

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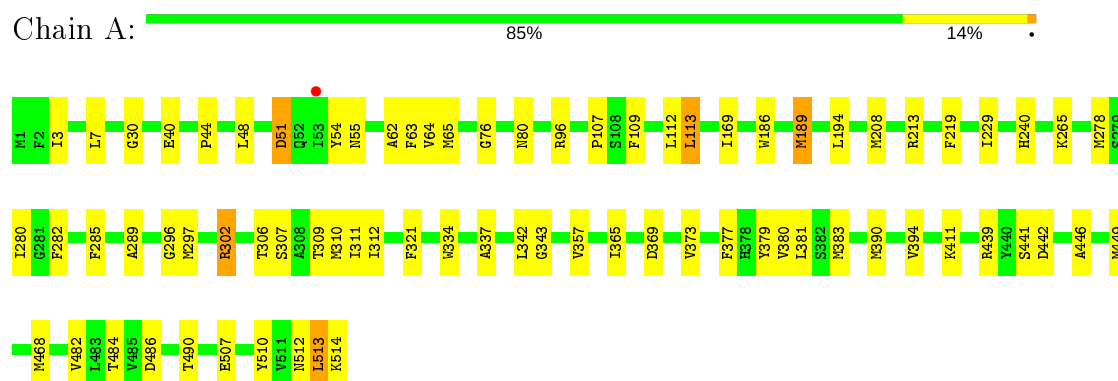
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	V	48	Total 48	O 48	0	0
29	W	27	Total 27	O 27	0	0
29	X	28	Total 28	O 28	0	0
29	Y	31	Total 31	O 31	0	0
29	Z	20	Total 20	O 20	0	0

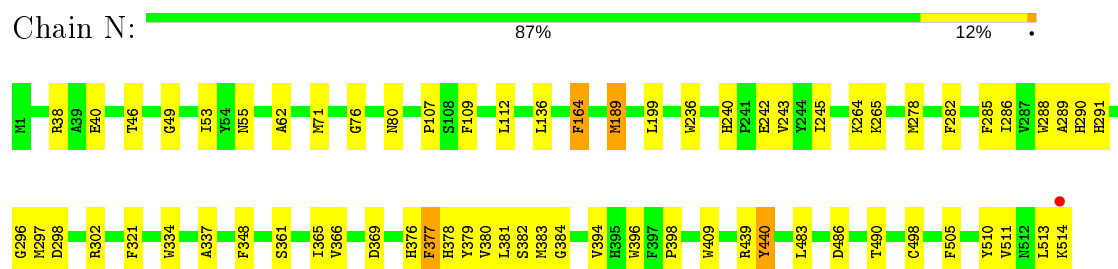
3 Residue-property plots

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

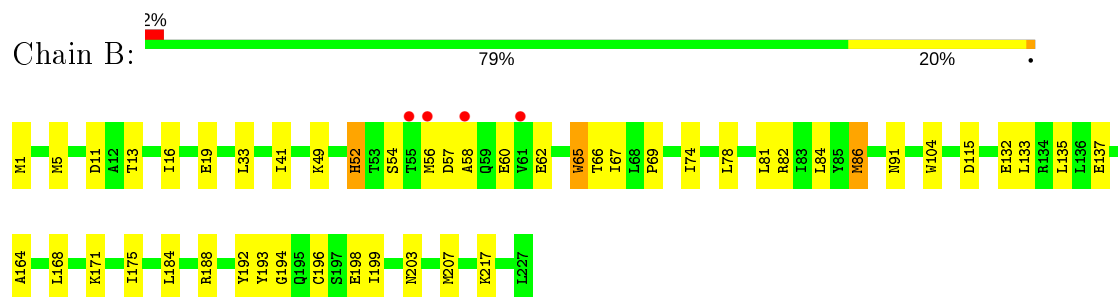
• Molecule 1: Cytochrome c oxidase subunit 1



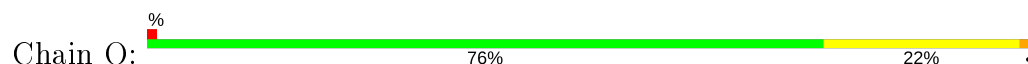
• Molecule 1: Cytochrome c oxidase subunit 1

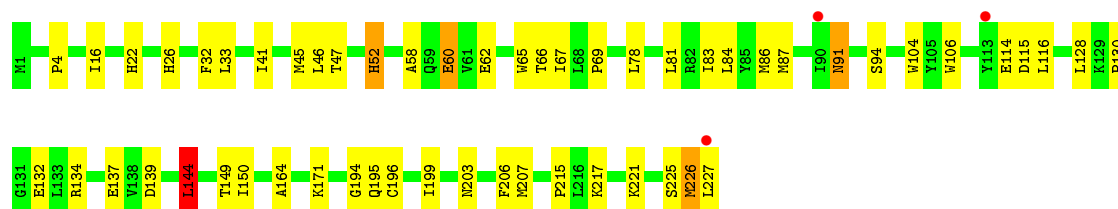


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 88% 11%



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 89% 11%



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

Chain D: 90% 10%



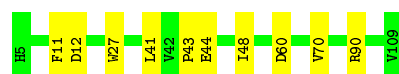
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 4% 87% 9%



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

Chain E: 90% 10%

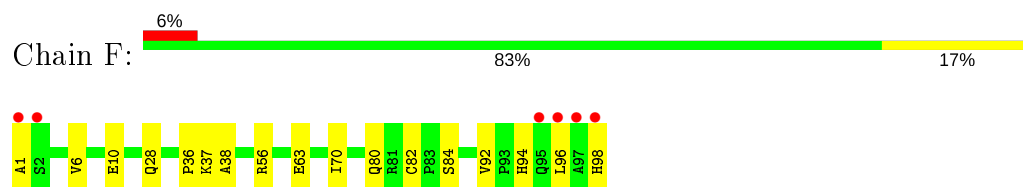


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

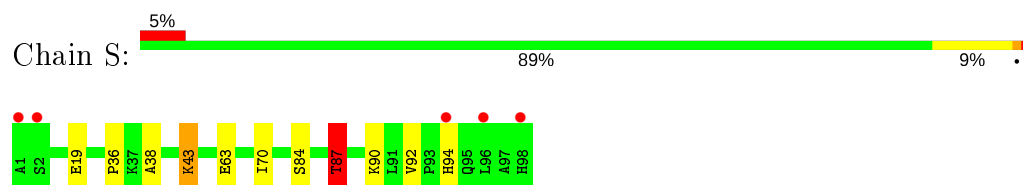
Chain R: 2% 88% 11%



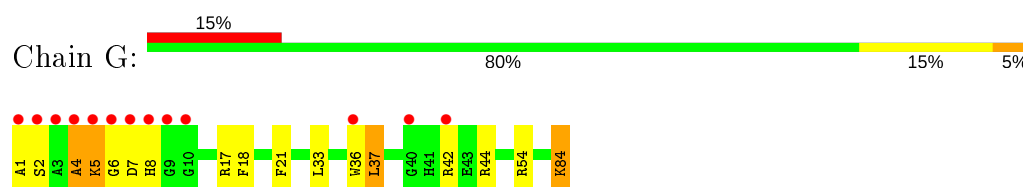
- Molecule 6: Cytochrome c oxidase subunit 5B



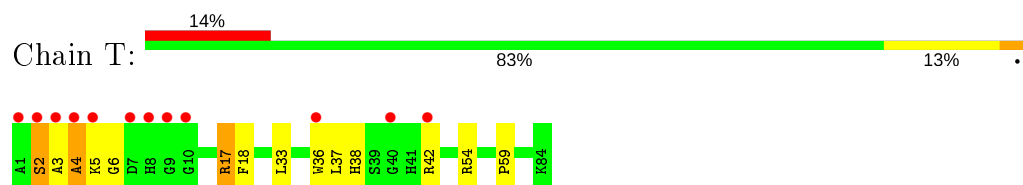
- Molecule 6: Cytochrome c oxidase subunit 5B



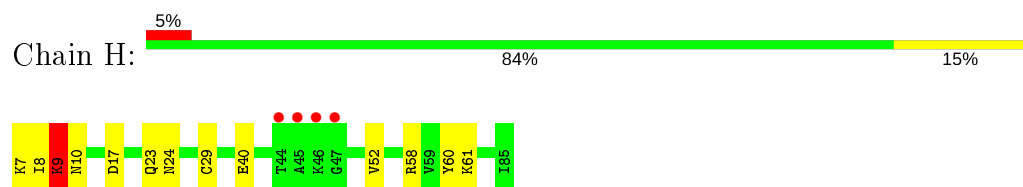
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



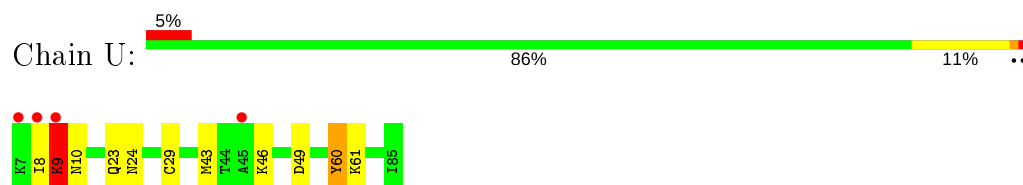
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



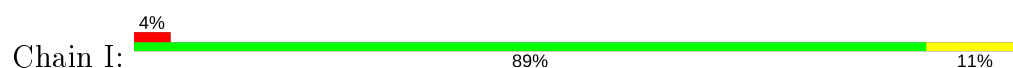
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 8: Cytochrome c oxidase subunit 6B1

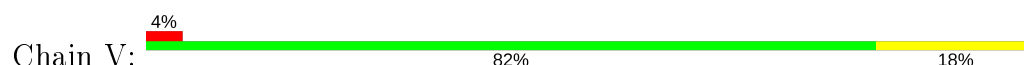


- Molecule 9: Cytochrome c oxidase subunit 6C

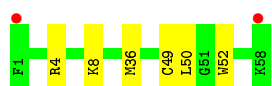
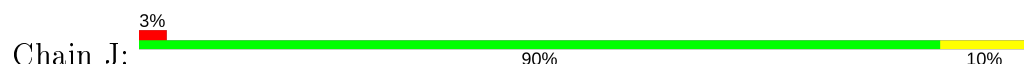




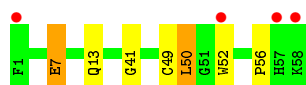
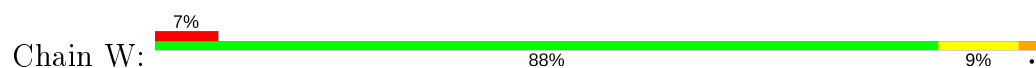
- Molecule 9: Cytochrome c oxidase subunit 6C



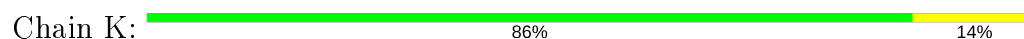
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



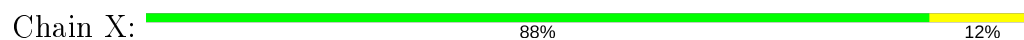
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



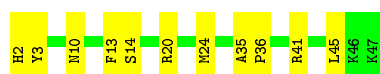
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



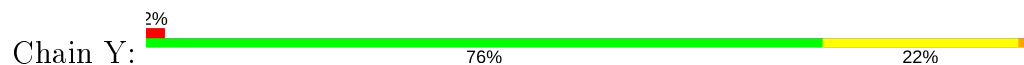
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



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

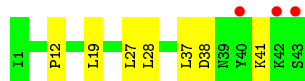
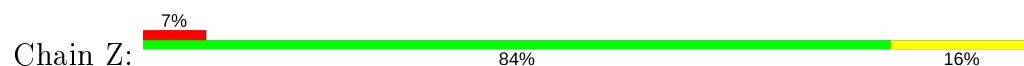




- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- 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, α , β , γ	182.22Å 204.65Å 177.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 1.80 136.09 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.88-1.80) 99.8 (136.09-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.157 , 0.188 0.157 , 0.188	Depositor DCC
R_{free} test set	30366 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34360	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.11	7/4445 (0.2%)	1.00	12/6063 (0.2%)
1	N	1.01	7/4321 (0.2%)	0.94	9/5899 (0.2%)
2	B	0.97	2/1896 (0.1%)	0.97	4/2582 (0.2%)
2	O	0.83	1/1934 (0.1%)	0.89	2/2634 (0.1%)
3	C	0.96	2/2236 (0.1%)	0.83	1/3056 (0.0%)
3	P	0.94	2/2211 (0.1%)	0.80	2/3024 (0.1%)
4	D	0.99	1/1234 (0.1%)	0.87	1/1665 (0.1%)
4	Q	0.69	0/1229	0.72	2/1658 (0.1%)
5	E	0.92	2/871 (0.2%)	0.80	1/1182 (0.1%)
5	R	0.75	0/871	0.82	4/1182 (0.3%)
6	F	0.90	3/774 (0.4%)	0.84	0/1050
6	S	0.81	1/774 (0.1%)	0.80	0/1050
7	G	0.82	0/691	0.87	1/937 (0.1%)
7	T	0.73	0/707	0.81	1/960 (0.1%)
8	H	0.88	0/682	0.90	3/921 (0.3%)
8	U	0.75	0/682	0.74	0/921
9	I	0.74	0/605	0.78	2/802 (0.2%)
9	V	0.59	0/605	0.71	1/802 (0.1%)
10	J	0.65	0/471	0.73	0/636
10	W	0.65	0/471	0.75	0/636
11	K	0.86	0/398	0.77	0/544
11	X	0.61	0/399	0.65	0/546
12	L	1.00	0/393	0.85	0/526
12	Y	0.84	1/393 (0.3%)	0.68	0/526
13	M	0.94	1/346 (0.3%)	0.81	0/470
13	Z	0.71	0/346	0.63	0/470
All	All	0.92	30/29985 (0.1%)	0.87	46/40742 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
8	H	0	1
All	All	0	3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	27	TRP	CE3-CZ3	7.79	1.51	1.38
6	F	82	CYS	CB-SG	7.26	1.94	1.82
2	O	106	TRP	CE3-CZ3	6.62	1.49	1.38
2	B	198	GLU	CD-OE2	-6.60	1.18	1.25
2	B	193	TYR	CD1-CE1	6.54	1.49	1.39

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-15.75	75.00	100.20
8	H	58	ARG	NE-CZ-NH2	-8.40	116.10	120.30
4	Q	20	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	213	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	51[A]	ASP	CB-CG-OD1	6.79	124.41	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4192	0	4181	73	0
1	N	4152	0	4129	61	0
2	B	1839	0	1848	34	0
2	O	1857	0	1858	45	0
3	C	2122	0	2032	33	0
3	P	2114	0	2028	24	0
4	D	1198	0	1189	15	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	8	0
6	F	751	0	726	14	0
6	S	751	0	726	11	0
7	G	676	0	644	16	0
7	T	685	0	648	15	0
8	H	662	0	623	7	0
8	U	662	0	623	9	0
9	I	601	0	613	7	0
9	V	601	0	613	10	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	10	0
11	X	385	0	366	4	0
12	L	380	0	380	13	0
12	Y	380	0	380	11	0
13	M	336	0	352	2	0
13	Z	336	0	352	7	0
14	A	132	0	93	7	0
14	N	132	0	93	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	1	0
18	A	13	0	21	2	0
18	B	11	0	21	0	0
18	C	66	0	94	2	0
18	D	21	0	30	0	0
18	J	21	0	30	4	0
18	K	58	0	94	5	0
18	L	33	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	33	0	42	1	0
18	O	11	0	21	2	0
18	P	44	0	63	3	0
18	Q	23	0	31	2	0
18	W	21	0	30	4	0
18	X	65	0	114	1	0
18	Y	33	0	42	3	0
18	Z	33	0	42	2	0
19	A	102	0	152	6	0
19	C	51	0	76	4	0
19	N	102	0	152	9	0
19	P	102	0	152	12	0
19	T	51	0	74	1	0
20	A	52	0	79	17	0
20	V	52	0	78	7	0
21	A	63	0	110	2	0
21	D	63	0	110	15	0
21	L	63	0	110	16	0
21	N	63	0	110	4	0
21	Q	63	0	110	12	0
21	Y	63	0	110	3	0
22	A	36	0	54	10	0
22	B	20	0	30	3	0
22	C	28	0	42	3	0
22	D	20	0	30	3	0
22	E	12	0	18	2	0
22	F	32	0	48	3	0
22	G	4	0	6	0	0
22	H	4	0	6	2	0
22	J	4	0	6	0	0
22	L	8	0	11	1	0
22	M	4	0	6	0	0
22	N	60	0	90	14	0
22	O	8	0	12	1	0
22	P	28	0	42	3	0
22	Q	12	0	18	4	0
22	S	20	0	30	2	0
22	T	8	0	12	1	0
22	U	4	0	6	4	0
22	W	4	0	6	0	0
22	Y	4	0	6	0	0
23	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	O	2	0	0	0	0
24	C	58	0	78	3	0
24	G	29	0	39	1	0
24	J	29	0	39	1	0
24	L	29	0	39	0	0
24	P	58	0	78	3	0
24	T	29	0	39	1	0
24	Y	29	0	39	1	0
25	C	100	0	156	17	0
25	G	100	0	154	22	0
25	P	100	0	156	11	0
25	T	100	0	154	29	0
26	C	106	0	154	11	0
26	F	53	0	74	6	0
26	P	106	0	154	3	0
26	T	53	0	77	9	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	H	5	0	0	0	0
28	U	5	0	0	0	0
29	A	250	0	0	11	0
29	B	200	0	0	4	2
29	C	136	0	0	8	0
29	D	174	0	0	3	2
29	E	133	0	0	0	0
29	F	117	0	0	2	0
29	G	72	0	0	0	0
29	H	79	0	0	3	0
29	I	56	0	0	5	2
29	J	44	0	0	1	0
29	K	36	0	0	2	0
29	L	42	0	0	2	0
29	M	34	0	0	1	1
29	N	247	0	0	12	0
29	O	166	0	0	4	0
29	P	132	0	0	4	0
29	Q	99	0	0	2	0
29	R	98	0	0	2	0
29	S	105	0	0	4	0
29	T	75	0	0	4	0
29	U	65	0	0	2	0
29	V	48	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	W	27	0	0	1	0
29	X	28	0	0	0	0
29	Y	31	0	0	1	0
29	Z	20	0	0	0	0
All	All	34360	0	32701	548	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 548 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)
25:G:102:CDL:H181	25:G:102:CDL:H512	1.32	1.09
1:A:55[B]:ASN:ND2	29:A:701:HOH:O	1.87	1.05
25:G:102:CDL:H551	25:G:102:CDL:H221	1.37	1.05
12:L:20:ARG:HH21	21:L:103:TGL:HC51	1.23	1.04
1:A:302[B]:ARG:HH12	1:A:365:ILE:HD11	1.25	1.01

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:454:HOH:O	29:D:303:HOH:O[2_584]	2.03	0.17
29:I:129:HOH:O	29:V:201:HOH:O[3_647]	2.03	0.17
29:I:132:HOH:O	29:M:226:HOH:O[2_584]	2.09	0.11
29:B:500:HOH:O	29:D:437:HOH:O[2_584]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/514 (107%)	537 (98%)	13 (2%)	0	100	100
1	N	534/514 (104%)	517 (97%)	15 (3%)	2 (0%)	34	21
2	B	229/227 (101%)	220 (96%)	9 (4%)	0	100	100
2	O	232/227 (102%)	226 (97%)	6 (3%)	0	100	100
3	C	262/259 (101%)	256 (98%)	6 (2%)	0	100	100
3	P	259/259 (100%)	253 (98%)	6 (2%)	0	100	100
4	D	143/144 (99%)	139 (97%)	4 (3%)	0	100	100
4	Q	142/144 (99%)	135 (95%)	4 (3%)	3 (2%)	7	1
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	97/98 (99%)	95 (98%)	2 (2%)	0	100	100
6	S	97/98 (99%)	93 (96%)	4 (4%)	0	100	100
7	G	81/84 (96%)	71 (88%)	7 (9%)	3 (4%)	3	0
7	T	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	2	0
8	H	77/79 (98%)	74 (96%)	2 (3%)	1 (1%)	12	3
8	U	77/79 (98%)	73 (95%)	2 (3%)	2 (3%)	5	1
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	47/49 (96%)	47 (100%)	0	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
All	All	3586/3558 (101%)	3474 (97%)	97 (3%)	15 (0%)	34	21

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	6	GLY
4	Q	9	GLU

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Mol	Chain	Res	Type
4	Q	10	ASP
4	Q	11	TYR

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	461/426 (108%)	459 (100%)	2 (0%)	91	89
1	N	445/426 (104%)	441 (99%)	4 (1%)	78	75
2	B	214/210 (102%)	204 (95%)	10 (5%)	26	12
2	O	217/210 (103%)	206 (95%)	11 (5%)	24	10
3	C	229/224 (102%)	225 (98%)	4 (2%)	60	51
3	P	226/224 (101%)	223 (99%)	3 (1%)	69	62
4	D	129/128 (101%)	128 (99%)	1 (1%)	81	78
4	Q	128/128 (100%)	123 (96%)	5 (4%)	32	17
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	68
5	R	92/92 (100%)	91 (99%)	1 (1%)	73	68
6	F	82/81 (101%)	79 (96%)	3 (4%)	34	19
6	S	82/81 (101%)	78 (95%)	4 (5%)	25	11
7	G	67/67 (100%)	60 (90%)	7 (10%)	7	1
7	T	68/67 (102%)	63 (93%)	5 (7%)	13	4
8	H	71/71 (100%)	67 (94%)	4 (6%)	21	8
8	U	71/71 (100%)	68 (96%)	3 (4%)	30	15
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	48
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	21
10	J	49/49 (100%)	49 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	16
11	K	39/39 (100%)	39 (100%)	0	100	100
11	X	39/39 (100%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/39 (100%)	39 (100%)	0	100	100
12	Y	39/39 (100%)	37 (95%)	2 (5%)	24	10
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	36 (97%)	1 (3%)	44	31
All	All	3116/3040 (102%)	3040 (98%)	76 (2%)	49	36

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	189[A]	MET
2	O	94	SER
9	V	36	LYS
1	N	189[B]	MET
2	O	52	HIS

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

Mol	Chain	Res	Type
6	F	98	HIS
9	V	20	HIS
4	Q	101	HIS
3	C	149	HIS
4	Q	109	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
1	FME	A	1	1	8,9,10	0.65	0	7,9,11	1.62	1 (14%)
9	SAC	I	1	9	7,8,9	0.64	0	8,9,11	0.96	0
9	SAC	V	1	9	7,8,9	0.58	0	8,9,11	0.61	0
7	TPO	G	11	7	8,10,11	1.33	1 (12%)	10,14,16	1.35	1 (10%)
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	1.70	2 (28%)
2	FME	B	1	2	8,9,10	0.96	0	7,9,11	2.08	3 (42%)
1	FME	N	1	1	8,9,10	0.51	0	7,9,11	1.62	1 (14%)
7	TPO	T	11	7	8,10,11	1.34	1 (12%)	10,14,16	1.23	1 (10%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.94	1.60	1.50
7	T	11	TPO	P-O1P	2.73	1.59	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.56	103.07	112.95
2	O	1	FME	CG-CB-CA	-3.51	103.19	112.95
1	N	1	FME	CE-SD-CG	3.25	111.55	100.40
7	G	11	TPO	CG2-CB-CA	3.09	119.27	113.16
1	A	1	FME	CE-SD-CG	2.87	110.25	100.40

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	O-C-CA-CB
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C-CA-N-C1A

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1	SAC	1	0
9	V	1	SAC	1	0
2	B	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 160 ligands modelled in this entry, 10 are monoatomic - leaving 150 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	EDO	A	619	-	3,3,3	0.43	0	2,2,2	0.65	0
22	EDO	Y	104	-	3,3,3	0.56	0	2,2,2	0.12	0
22	EDO	G	103	-	3,3,3	0.88	0	2,2,2	0.54	0
26	PEK	C	308	-	52,52,52	1.17	2 (3%)	55,57,57	1.40	6 (10%)
22	EDO	C	311	-	3,3,3	0.90	0	2,2,2	0.45	0
22	EDO	T	105	-	3,3,3	0.57	0	2,2,2	0.31	0
19	PGV	T	104	-	50,50,50	1.07	2 (4%)	53,56,56	1.50	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	EDO	C	312	-	3,3,3	0.93	0	2,2,2	0.13	0
24	CHD	P	305	-	29,32,32	0.66	0	48,51,51	1.79	10 (20%)
22	EDO	F	104	-	3,3,3	0.39	0	2,2,2	0.29	0
22	EDO	C	317	-	3,3,3	0.72	0	2,2,2	0.24	0
22	EDO	N	618	-	3,3,3	0.83	0	2,2,2	0.36	0
22	EDO	B	305	-	3,3,3	0.37	0	2,2,2	0.24	0
25	CDL	C	307	-	99,99,99	1.40	14 (14%)	105,111,111	1.66	17 (16%)
14	HEA	A	601[B]	-	44,67,67	1.55	6 (13%)	37,103,103	2.62	16 (43%)
22	EDO	C	315	-	3,3,3	0.50	0	2,2,2	0.57	0
18	DMU	Z	101	-	34,34,34	0.63	1 (2%)	45,45,45	1.06	3 (6%)
22	EDO	F	108	-	3,3,3	0.47	0	2,2,2	0.24	0
19	PGV	A	607	-	50,50,50	1.10	3 (6%)	53,56,56	1.31	7 (13%)
22	EDO	N	613	-	3,3,3	0.61	0	2,2,2	0.25	0
23	CUA	O	301	2	0,1,1	0.00	-	-		
24	CHD	C	306	-	29,32,32	0.80	1 (3%)	48,51,51	2.20	16 (33%)
14	HEA	N	601[B]	-	44,67,67	1.16	3 (6%)	37,103,103	2.66	19 (51%)
22	EDO	N	611	-	3,3,3	1.12	0	2,2,2	0.36	0
24	CHD	T	101	-	29,32,32	1.06	2 (6%)	48,51,51	1.59	9 (18%)
18	DMU	P	302	-	10,10,34	0.44	0	9,9,45	0.38	0
20	PSC	V	101	-	51,51,51	1.19	4 (7%)	57,59,59	1.56	11 (19%)
22	EDO	W	102	-	3,3,3	0.47	0	2,2,2	0.41	0
20	PSC	A	609	-	51,51,51	1.13	3 (5%)	57,59,59	1.53	6 (10%)
22	EDO	E	202	-	3,3,3	0.45	0	2,2,2	0.40	0
22	EDO	D	205	-	3,3,3	0.55	0	2,2,2	0.37	0
18	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.12	4 (8%)
22	EDO	N	620	-	3,3,3	0.64	0	2,2,2	0.19	0
24	CHD	C	305	-	29,32,32	1.03	1 (3%)	48,51,51	1.56	6 (12%)
22	EDO	O	304	-	3,3,3	0.60	0	2,2,2	0.24	0
26	PEK	C	309	-	52,52,52	0.88	2 (3%)	55,57,57	1.23	6 (10%)
22	EDO	N	609	-	3,3,3	0.58	0	2,2,2	0.87	0
22	EDO	N	617	-	3,3,3	0.29	0	2,2,2	0.75	0
22	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.19	0
22	EDO	P	316	-	3,3,3	0.64	0	2,2,2	0.45	0
24	CHD	P	304	-	29,32,32	0.82	0	48,51,51	1.61	8 (16%)
25	CDL	T	102	-	99,99,99	1.36	12 (12%)	105,111,111	1.42	14 (13%)
22	EDO	A	615	-	3,3,3	0.34	0	2,2,2	0.92	0
22	EDO	F	107	-	3,3,3	0.73	0	2,2,2	0.31	0
23	CUA	B	301	2	0,1,1	0.00	-	-		
22	EDO	N	622	-	3,3,3	1.10	0	2,2,2	1.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	P	310	-	50,50,50	1.04	2 (4%)	53,56,56	1.30	5 (9%)
19	PGV	N	607	-	50,50,50	1.01	2 (4%)	53,56,56	1.37	7 (13%)
22	EDO	P	311	-	3,3,3	0.60	0	2,2,2	0.28	0
22	EDO	J	103	-	3,3,3	0.63	0	2,2,2	0.24	0
22	EDO	N	619	-	3,3,3	0.54	0	2,2,2	0.41	0
25	CDL	P	306	-	99,99,99	1.33	12 (12%)	105,111,111	1.58	18 (17%)
22	EDO	D	206	-	3,3,3	0.46	0	2,2,2	0.60	0
18	DMU	X	102	-	21,21,34	0.57	0	24,25,45	1.40	2 (8%)
22	EDO	S	106	-	3,3,3	0.73	0	2,2,2	0.32	0
22	EDO	A	612	-	3,3,3	0.72	0	2,2,2	1.12	0
24	CHD	J	102	-	29,32,32	0.73	0	48,51,51	1.65	13 (27%)
18	DMU	A	606	-	11,11,34	0.36	0	9,9,45	0.71	0
18	DMU	D	201	-	21,21,34	0.89	1 (4%)	24,25,45	1.55	5 (20%)
18	DMU	X	104	-	10,10,34	0.31	0	9,9,45	0.44	0
22	EDO	S	104	-	3,3,3	0.76	0	2,2,2	0.34	0
22	EDO	A	613	-	3,3,3	0.92	0	2,2,2	0.62	0
18	DMU	C	302	-	34,34,34	0.51	0	45,45,45	2.14	15 (33%)
22	EDO	A	617	-	3,3,3	0.39	0	2,2,2	0.65	0
22	EDO	A	618	-	3,3,3	0.66	0	2,2,2	0.24	0
18	DMU	L	101	-	34,34,34	0.68	0	45,45,45	1.64	9 (20%)
22	EDO	N	610	-	3,3,3	0.61	0	2,2,2	0.39	0
22	EDO	A	614	-	3,3,3	0.41	0	2,2,2	0.24	0
26	PEK	P	308	-	52,52,52	0.77	2 (3%)	55,57,57	1.30	5 (9%)
22	EDO	B	306	-	3,3,3	0.76	0	2,2,2	0.39	0
21	TGL	N	608	-	62,62,62	1.15	3 (4%)	65,65,65	1.32	6 (9%)
18	DMU	K	103	-	22,22,34	1.01	1 (4%)	27,27,45	1.33	4 (14%)
22	EDO	N	623	-	3,3,3	0.61	0	2,2,2	0.55	0
26	PEK	F	102	-	52,52,52	1.06	2 (3%)	55,57,57	1.50	5 (9%)
22	EDO	S	102	-	3,3,3	0.74	0	2,2,2	0.65	0
22	EDO	E	201	-	3,3,3	0.49	0	2,2,2	0.26	0
28	PO4	H	101	-	4,4,4	0.99	0	6,6,6	0.39	0
21	TGL	L	103	-	62,62,62	1.32	4 (6%)	65,65,65	2.12	16 (24%)
21	TGL	D	202	-	62,62,62	1.33	5 (8%)	65,65,65	1.16	6 (9%)
18	DMU	Q	201	-	22,22,34	0.86	1 (4%)	27,27,45	1.74	7 (25%)
18	DMU	X	101	-	10,10,34	0.44	0	9,9,45	0.45	0
22	EDO	B	304	-	3,3,3	0.41	0	2,2,2	0.49	0
22	EDO	N	614	-	3,3,3	0.54	0	2,2,2	0.22	0
22	EDO	M	102	-	3,3,3	0.40	0	2,2,2	0.19	0
26	PEK	P	307	-	52,52,52	1.09	2 (3%)	55,57,57	1.38	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	601[A]	-	44,67,67	1.41	6 (13%)	37,103,103	2.50	13 (35%)
22	EDO	F	105	-	3,3,3	0.65	0	2,2,2	0.64	0
22	EDO	L	104	-	3,3,3	0.68	0	2,2,2	0.54	0
22	EDO	B	303	-	3,3,3	0.67	0	2,2,2	0.65	0
22	EDO	Q	204	-	3,3,3	0.40	0	2,2,2	0.54	0
22	EDO	A	616	-	3,3,3	0.61	0	2,2,2	0.27	0
18	DMU	B	302	-	10,10,34	0.42	0	9,9,45	0.44	0
18	DMU	J	101	-	21,21,34	0.93	1 (4%)	24,25,45	1.36	4 (16%)
22	EDO	Q	205	-	3,3,3	0.75	0	2,2,2	0.28	0
22	EDO	N	616	-	3,3,3	0.68	0	2,2,2	0.26	0
19	PGV	N	606	-	50,50,50	1.02	2 (4%)	53,56,56	1.28	6 (11%)
21	TGL	Y	103	-	62,62,62	1.33	3 (4%)	65,65,65	1.57	9 (13%)
22	EDO	F	110	-	3,3,3	0.70	0	2,2,2	0.18	0
14	HEA	N	601[A]	-	44,67,67	1.10	2 (4%)	37,103,103	2.30	13 (35%)
18	DMU	O	302	-	10,10,34	0.40	0	9,9,45	0.40	0
22	EDO	E	203	-	3,3,3	0.42	0	2,2,2	0.55	0
22	EDO	A	611	-	3,3,3	0.69	0	2,2,2	0.50	0
22	EDO	S	105	-	3,3,3	0.36	0	2,2,2	0.28	0
22	EDO	P	314	-	3,3,3	0.92	0	2,2,2	0.07	0
22	EDO	F	109	-	3,3,3	0.59	0	2,2,2	0.30	0
18	DMU	Y	101	-	34,34,34	0.73	0	45,45,45	1.13	3 (6%)
19	PGV	C	310	-	50,50,50	0.76	1 (2%)	53,56,56	1.16	5 (9%)
28	PO4	U	101	-	4,4,4	0.91	0	6,6,6	0.58	0
21	TGL	A	610	-	62,62,62	1.18	3 (4%)	65,65,65	1.34	6 (9%)
22	EDO	H	102	-	3,3,3	0.27	0	2,2,2	0.79	0
19	PGV	A	608	-	50,50,50	0.89	4 (8%)	53,56,56	1.28	2 (3%)
18	DMU	P	303	-	34,34,34	0.64	0	45,45,45	2.08	15 (33%)
22	EDO	P	313	-	3,3,3	0.95	0	2,2,2	0.34	0
22	EDO	N	615	-	3,3,3	0.68	0	2,2,2	0.39	0
22	EDO	Q	203	-	3,3,3	0.48	0	2,2,2	0.27	0
22	EDO	T	106	-	3,3,3	0.86	0	2,2,2	1.06	0
22	EDO	O	303	-	3,3,3	0.71	0	2,2,2	0.62	0
19	PGV	P	309	-	50,50,50	0.82	4 (8%)	53,56,56	1.08	4 (7%)
18	DMU	K	102	-	12,12,34	0.49	0	10,11,45	0.47	0
18	DMU	W	101	-	21,21,34	0.92	1 (4%)	24,25,45	1.54	5 (20%)
22	EDO	F	106	-	3,3,3	0.96	0	2,2,2	0.29	0
22	EDO	D	207	-	3,3,3	0.58	0	2,2,2	0.31	0
22	EDO	P	317	-	3,3,3	0.69	0	2,2,2	0.60	0
18	DMU	K	104	-	10,10,34	0.31	0	9,9,45	0.50	0
18	DMU	X	105	-	10,10,34	0.38	0	9,9,45	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	EDO	S	103	-	3,3,3	0.65	0	2,2,2	0.57	0
22	EDO	D	203	-	3,3,3	0.75	0	2,2,2	0.28	0
22	EDO	B	307	-	3,3,3	0.77	0	2,2,2	0.69	0
14	HEA	N	602	1,29	44,67,67	1.20	5 (11%)	37,103,103	2.38	20 (54%)
18	DMU	C	304	-	10,10,34	0.40	0	9,9,45	0.29	0
18	DMU	X	103	-	10,10,34	0.38	0	9,9,45	0.27	0
22	EDO	C	314	-	3,3,3	0.75	0	2,2,2	1.02	0
22	EDO	P	312	-	3,3,3	0.39	0	2,2,2	0.78	0
18	DMU	C	303	-	22,22,34	0.80	1 (4%)	27,27,45	1.56	3 (11%)
24	CHD	Y	102	-	29,32,32	0.58	0	48,51,51	2.22	15 (31%)
22	EDO	L	105	-	3,3,3	0.49	0	2,2,2	0.27	0
21	TGL	Q	202	-	62,62,62	1.12	3 (4%)	65,65,65	0.95	5 (7%)
22	EDO	C	313	-	3,3,3	0.38	0	2,2,2	0.68	0
22	EDO	C	316	-	3,3,3	0.89	0	2,2,2	0.53	0
22	EDO	N	621	-	3,3,3	0.53	0	2,2,2	0.81	0
24	CHD	G	101	-	29,32,32	0.86	0	48,51,51	1.41	8 (16%)
22	EDO	P	315	-	3,3,3	1.08	0	2,2,2	0.66	0
22	EDO	U	102	-	3,3,3	0.53	0	2,2,2	0.13	0
18	DMU	K	101	-	10,10,34	0.27	0	9,9,45	0.78	0
25	CDL	G	102	-	99,99,99	1.41	12 (12%)	105,111,111	1.25	9 (8%)
24	CHD	L	102	-	29,32,32	0.57	0	48,51,51	2.52	18 (37%)
22	EDO	D	204	-	3,3,3	0.41	0	2,2,2	0.50	0
26	PEK	T	103	-	52,52,52	1.09	2 (3%)	55,57,57	1.48	6 (10%)
22	EDO	F	103	-	3,3,3	0.72	0	2,2,2	0.55	0
14	HEA	A	602	1,29	44,67,67	1.27	5 (11%)	37,103,103	2.28	13 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	A	619	-	-	1/1/1/1	-
22	EDO	Y	104	-	-	1/1/1/1	-
22	EDO	G	103	-	-	0/1/1/1	-
26	PEK	C	308	-	-	17/56/56/56	-
22	EDO	C	311	-	-	1/1/1/1	-
22	EDO	T	105	-	-	1/1/1/1	-
19	PGV	T	104	-	-	19/55/55/55	-
22	EDO	C	312	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	P	305	-	-	3/7/74/74	0/4/4/4
22	EDO	F	104	-	-	0/1/1/1	-
22	EDO	C	317	-	-	1/1/1/1	-
22	EDO	N	618	-	-	1/1/1/1	-
22	EDO	B	305	-	-	1/1/1/1	-
25	CDL	C	307	-	-	43/110/110/110	-
14	HEA	A	601[B]	-	-	0/24/76/76	-
22	EDO	C	315	-	-	0/1/1/1	-
18	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
22	EDO	F	108	-	-	0/1/1/1	-
19	PGV	A	607	-	-	18/55/55/55	-
22	EDO	N	613	-	-	0/1/1/1	-
24	CHD	C	306	-	-	7/7/74/74	0/4/4/4
14	HEA	N	601[B]	-	-	0/24/76/76	-
22	EDO	N	611	-	-	0/1/1/1	-
24	CHD	T	101	-	-	0/7/74/74	0/4/4/4
18	DMU	P	302	-	-	0/8/8/59	-
20	PSC	V	101	-	-	20/55/55/55	-
22	EDO	W	102	-	-	1/1/1/1	-
20	PSC	A	609	-	-	15/55/55/55	-
22	EDO	E	202	-	-	1/1/1/1	-
22	EDO	D	205	-	-	0/1/1/1	-
22	EDO	A	615	-	-	1/1/1/1	-
22	EDO	N	620	-	-	0/1/1/1	-
24	CHD	C	305	-	-	0/7/74/74	0/4/4/4
22	EDO	O	304	-	-	0/1/1/1	-
26	PEK	C	309	-	-	16/56/56/56	-
22	EDO	N	609	-	-	0/1/1/1	-
22	EDO	N	617	-	-	1/1/1/1	-
22	EDO	N	612	-	-	1/1/1/1	-
22	EDO	P	316	-	-	0/1/1/1	-
24	CHD	P	304	-	-	0/7/74/74	0/4/4/4
25	CDL	T	102	-	-	43/110/110/110	-
22	EDO	F	105	-	-	0/1/1/1	-
22	EDO	F	107	-	-	0/1/1/1	-
22	EDO	N	622	-	-	1/1/1/1	-
19	PGV	P	310	-	-	16/55/55/55	-
19	PGV	N	607	-	-	7/55/55/55	-
22	EDO	P	311	-	-	0/1/1/1	-
22	EDO	J	103	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	N	619	-	-	1/1/1/1	-
25	CDL	P	306	-	-	42/110/110/110	-
22	EDO	D	206	-	-	0/1/1/1	-
18	DMU	X	102	-	-	8/13/29/59	0/1/1/2
22	EDO	S	106	-	-	0/1/1/1	-
22	EDO	A	612	-	-	0/1/1/1	-
24	CHD	J	102	-	-	3/7/74/74	0/4/4/4
18	DMU	A	606	-	-	2/8/8/59	-
18	DMU	D	201	-	-	4/13/29/59	0/1/1/2
18	DMU	X	104	-	-	3/8/8/59	-
22	EDO	S	104	-	-	0/1/1/1	-
22	EDO	A	613	-	-	0/1/1/1	-
18	DMU	C	302	-	-	10/19/59/59	0/2/2/2
22	EDO	A	617	-	-	0/1/1/1	-
22	EDO	A	618	-	-	1/1/1/1	-
18	DMU	L	101	-	-	8/19/59/59	0/2/2/2
22	EDO	N	610	-	-	0/1/1/1	-
18	DMU	M	101	-	-	7/19/59/59	0/2/2/2
22	EDO	A	614	-	-	0/1/1/1	-
26	PEK	P	308	-	-	11/56/56/56	-
22	EDO	B	306	-	-	1/1/1/1	-
21	TGL	N	608	-	-	33/65/65/65	-
18	DMU	K	103	-	-	6/13/33/59	0/1/1/2
22	EDO	N	623	-	-	1/1/1/1	-
26	PEK	F	102	-	-	24/56/56/56	-
22	EDO	S	102	-	-	0/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
21	TGL	L	103	-	-	32/65/65/65	-
21	TGL	D	202	-	-	21/65/65/65	-
18	DMU	Q	201	-	-	5/13/33/59	0/1/1/2
18	DMU	X	101	-	-	1/8/8/59	-
22	EDO	B	304	-	-	1/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
22	EDO	M	102	-	-	0/1/1/1	-
26	PEK	P	307	-	-	22/56/56/56	-
14	HEA	A	601[A]	-	-	2/24/76/76	-
22	EDO	L	104	-	-	0/1/1/1	-
22	EDO	B	303	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	Q	204	-	-	0/1/1/1	-
22	EDO	A	616	-	-	0/1/1/1	-
18	DMU	B	302	-	-	3/8/8/59	-
18	DMU	J	101	-	-	4/13/29/59	0/1/1/2
22	EDO	Q	205	-	-	1/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
19	PGV	N	606	-	-	15/55/55/55	-
21	TGL	Y	103	-	-	32/65/65/65	-
22	EDO	F	110	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	5/24/76/76	-
18	DMU	O	302	-	-	0/8/8/59	-
22	EDO	E	203	-	-	0/1/1/1	-
22	EDO	A	611	-	-	1/1/1/1	-
22	EDO	S	105	-	-	0/1/1/1	-
22	EDO	P	314	-	-	1/1/1/1	-
22	EDO	F	109	-	-	1/1/1/1	-
18	DMU	Y	101	-	-	5/19/59/59	0/2/2/2
19	PGV	C	310	-	-	8/55/55/55	-
21	TGL	A	610	-	-	36/65/65/65	-
22	EDO	H	102	-	-	0/1/1/1	-
19	PGV	A	608	-	-	4/55/55/55	-
18	DMU	P	303	-	-	6/19/59/59	0/2/2/2
22	EDO	P	313	-	-	1/1/1/1	-
22	EDO	N	615	-	-	0/1/1/1	-
22	EDO	Q	203	-	-	1/1/1/1	-
22	EDO	T	106	-	-	0/1/1/1	-
22	EDO	O	303	-	-	0/1/1/1	-
19	PGV	P	309	-	-	10/55/55/55	-
18	DMU	K	102	-	-	4/9/10/59	-
18	DMU	W	101	-	-	4/13/29/59	0/1/1/2
22	EDO	F	106	-	-	0/1/1/1	-
22	EDO	D	207	-	-	0/1/1/1	-
22	EDO	P	317	-	-	1/1/1/1	-
18	DMU	K	104	-	-	4/8/8/59	-
18	DMU	X	105	-	-	4/8/8/59	-
22	EDO	S	103	-	-	1/1/1/1	-
22	EDO	D	203	-	-	1/1/1/1	-
22	EDO	B	307	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	602	1,29	3/3/7/16	0/24/76/76	-
18	DMU	C	304	-	-	5/8/8/59	-
18	DMU	X	103	-	-	4/8/8/59	-
22	EDO	C	314	-	-	0/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
18	DMU	C	303	-	-	7/13/33/59	0/1/1/2
24	CHD	Y	102	-	-	1/7/74/74	0/4/4/4
22	EDO	L	105	-	-	0/1/1/1	-
21	TGL	Q	202	-	-	28/65/65/65	-
22	EDO	C	313	-	-	0/1/1/1	-
22	EDO	C	316	-	-	1/1/1/1	-
22	EDO	N	621	-	-	0/1/1/1	-
24	CHD	G	101	-	-	0/7/74/74	0/4/4/4
22	EDO	P	315	-	-	1/1/1/1	-
22	EDO	U	102	-	-	1/1/1/1	-
18	DMU	K	101	-	-	3/8/8/59	-
25	CDL	G	102	-	-	40/110/110/110	-
24	CHD	L	102	-	-	5/7/74/74	0/4/4/4
22	EDO	D	204	-	-	0/1/1/1	-
26	PEK	T	103	-	-	24/56/56/56	-
22	EDO	F	103	-	-	0/1/1/1	-
14	HEA	A	602	1,29	3/3/7/16	1/24/76/76	-

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	103	TGL	OG2-CB1	6.24	1.51	1.34
21	Y	103	TGL	OG2-CB1	6.12	1.51	1.34
21	Y	103	TGL	OG3-CC1	5.88	1.50	1.33
25	G	102	CDL	OA6-CA5	5.48	1.49	1.34
21	N	608	TGL	OG2-CB1	5.38	1.49	1.34

The worst 5 of 477 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	102	CHD	C10-C9-C8	7.39	119.75	111.82
21	L	103	TGL	OG2-CB1-CB2	7.35	127.34	111.50
20	A	609	PSC	C03-C02-C01	-7.04	95.14	111.79
14	N	601[B]	HEA	C1B-C2B-C3B	-6.78	102.28	107.00
14	N	601[A]	HEA	C1B-C2B-C3B	-6.78	102.28	107.00

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NA

5 of 769 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	C	308	PEK	C03-O11-P-O12
26	C	308	PEK	C03-O11-P-O13
26	C	308	PEK	C03-O11-P-O14
26	C	308	PEK	O04-C21-O03-C01
26	C	308	PEK	C22-C21-O03-C01

There are no ring outliers.

89 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	308	PEK	5	0
22	C	311	EDO	1	0
22	T	105	EDO	1	0
19	T	104	PGV	1	0
24	P	305	CHD	2	0
22	N	618	EDO	1	0
22	B	305	EDO	2	0
25	C	307	CDL	17	0
14	A	601[B]	HEA	1	0
18	Z	101	DMU	2	0
22	F	108	EDO	1	0
19	A	607	PGV	5	0
22	N	613	EDO	1	0
24	C	306	CHD	3	0
14	N	601[B]	HEA	1	0
24	T	101	CHD	1	0
20	V	101	PSC	7	0
20	A	609	PSC	17	0
22	D	205	EDO	1	0
18	M	101	DMU	1	0
22	O	304	EDO	1	0
26	C	309	PEK	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	617	EDO	4	0
22	N	612	EDO	4	0
22	P	316	EDO	2	0
24	P	304	CHD	1	0
25	T	102	CDL	29	0
22	A	615	EDO	3	0
22	N	622	EDO	2	0
19	P	310	PGV	9	0
19	N	607	PGV	2	0
25	P	306	CDL	11	0
22	D	206	EDO	1	0
18	X	102	DMU	1	0
24	J	102	CHD	1	0
18	A	606	DMU	2	0
18	C	302	DMU	1	0
22	A	617	EDO	3	0
22	A	618	EDO	1	0
18	L	101	DMU	2	0
22	A	614	EDO	1	0
26	P	308	PEK	2	0
21	N	608	TGL	4	0
18	K	103	DMU	5	0
22	N	623	EDO	1	0
26	F	102	PEK	6	0
21	L	103	TGL	16	0
21	D	202	TGL	15	0
18	Q	201	DMU	2	0
26	P	307	PEK	1	0
14	A	601[A]	HEA	1	0
22	L	104	EDO	1	0
22	Q	204	EDO	2	0
22	A	616	EDO	1	0
18	J	101	DMU	4	0
22	Q	205	EDO	1	0
19	N	606	PGV	7	0
21	Y	103	TGL	3	0
22	F	110	EDO	1	0
14	N	601[A]	HEA	1	0
18	O	302	DMU	2	0
22	E	203	EDO	2	0
22	A	611	EDO	1	0
22	S	105	EDO	2	0

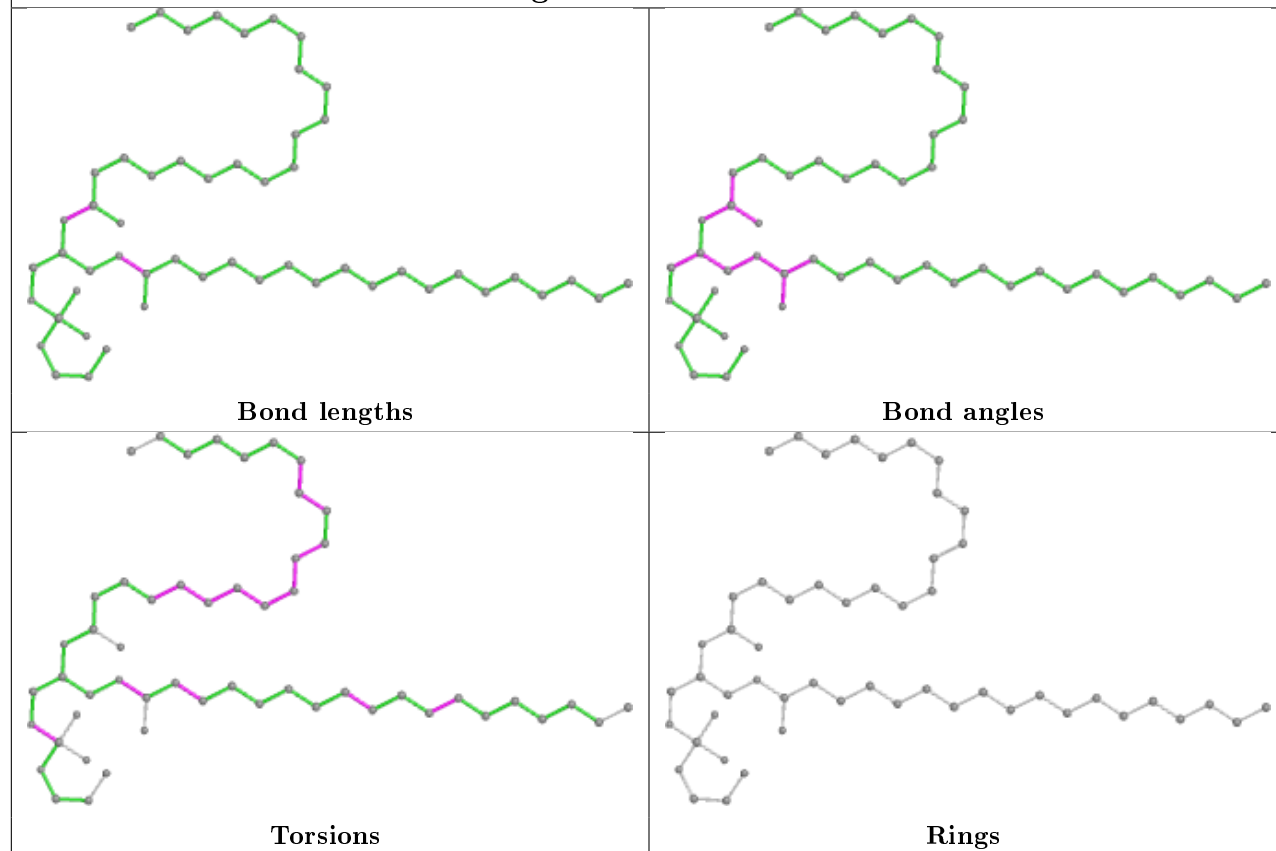
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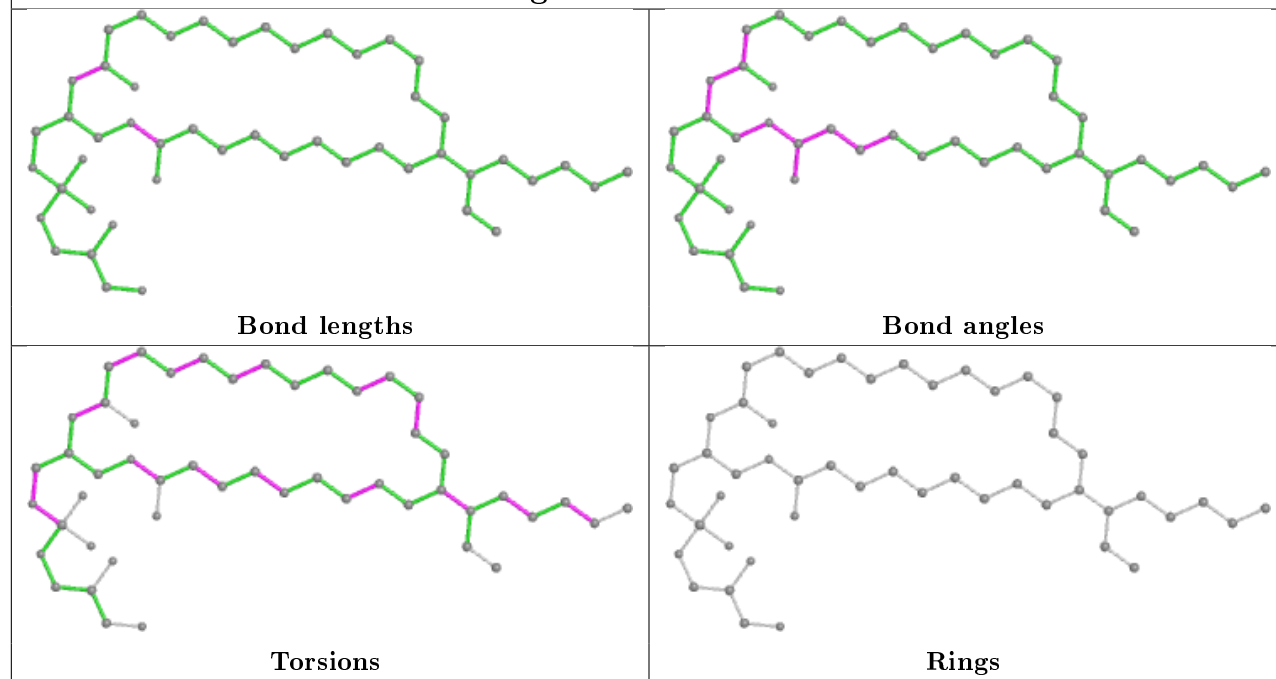
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	109	EDO	1	0
18	Y	101	DMU	3	0
19	C	310	PGV	4	0
21	A	610	TGL	2	0
22	H	102	EDO	2	0
19	A	608	PGV	1	0
18	P	303	DMU	3	0
22	P	313	EDO	1	0
22	N	615	EDO	1	0
22	Q	203	EDO	1	0
19	P	309	PGV	3	0
18	W	101	DMU	4	0
22	D	203	EDO	1	0
22	B	307	EDO	1	0
14	N	602	HEA	6	0
18	C	303	DMU	1	0
24	Y	102	CHD	1	0
21	Q	202	TGL	12	0
22	C	313	EDO	1	0
22	C	316	EDO	1	0
24	G	101	CHD	1	0
22	U	102	EDO	4	0
25	G	102	CDL	22	0
26	T	103	PEK	9	0
14	A	602	HEA	5	0

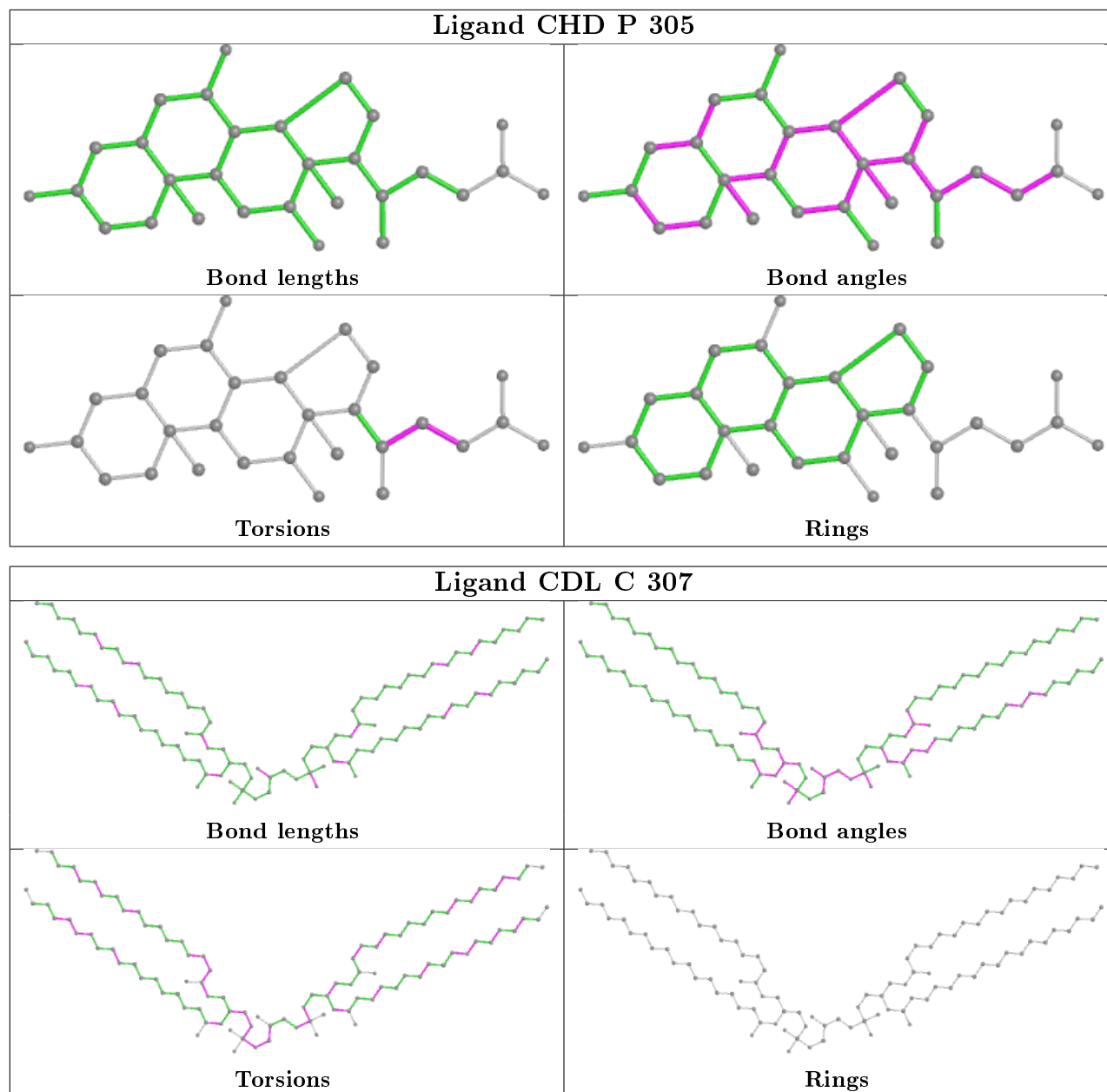
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

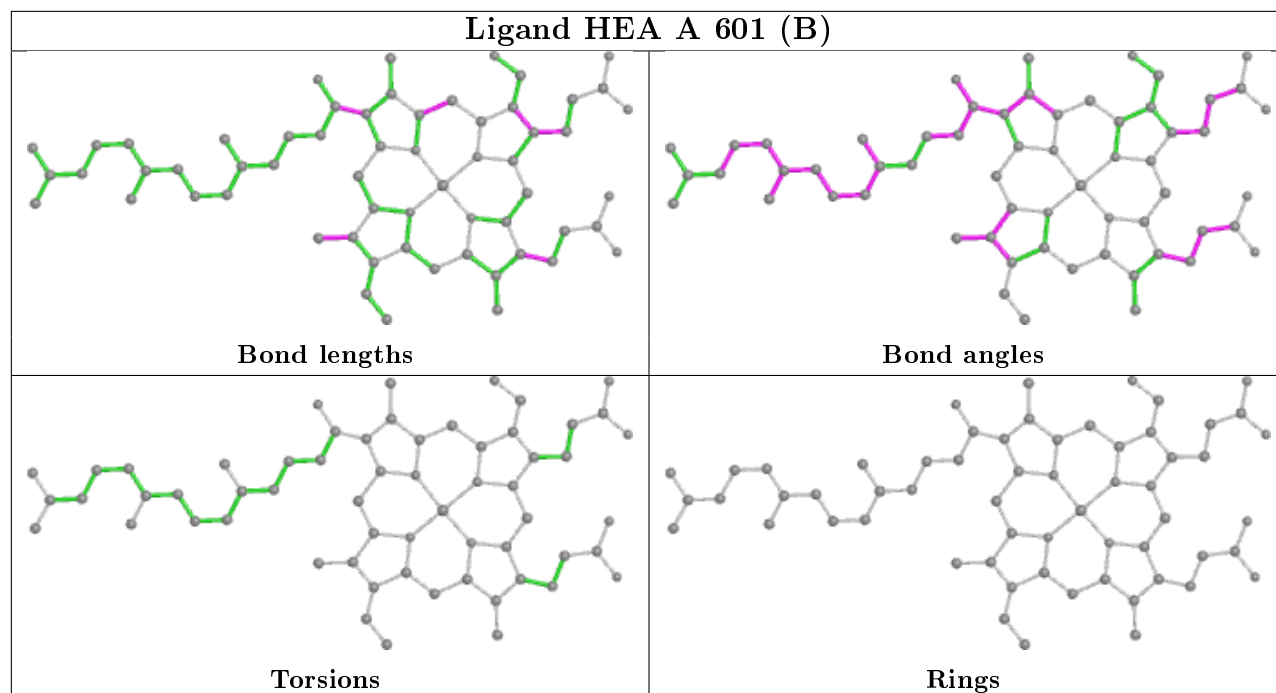
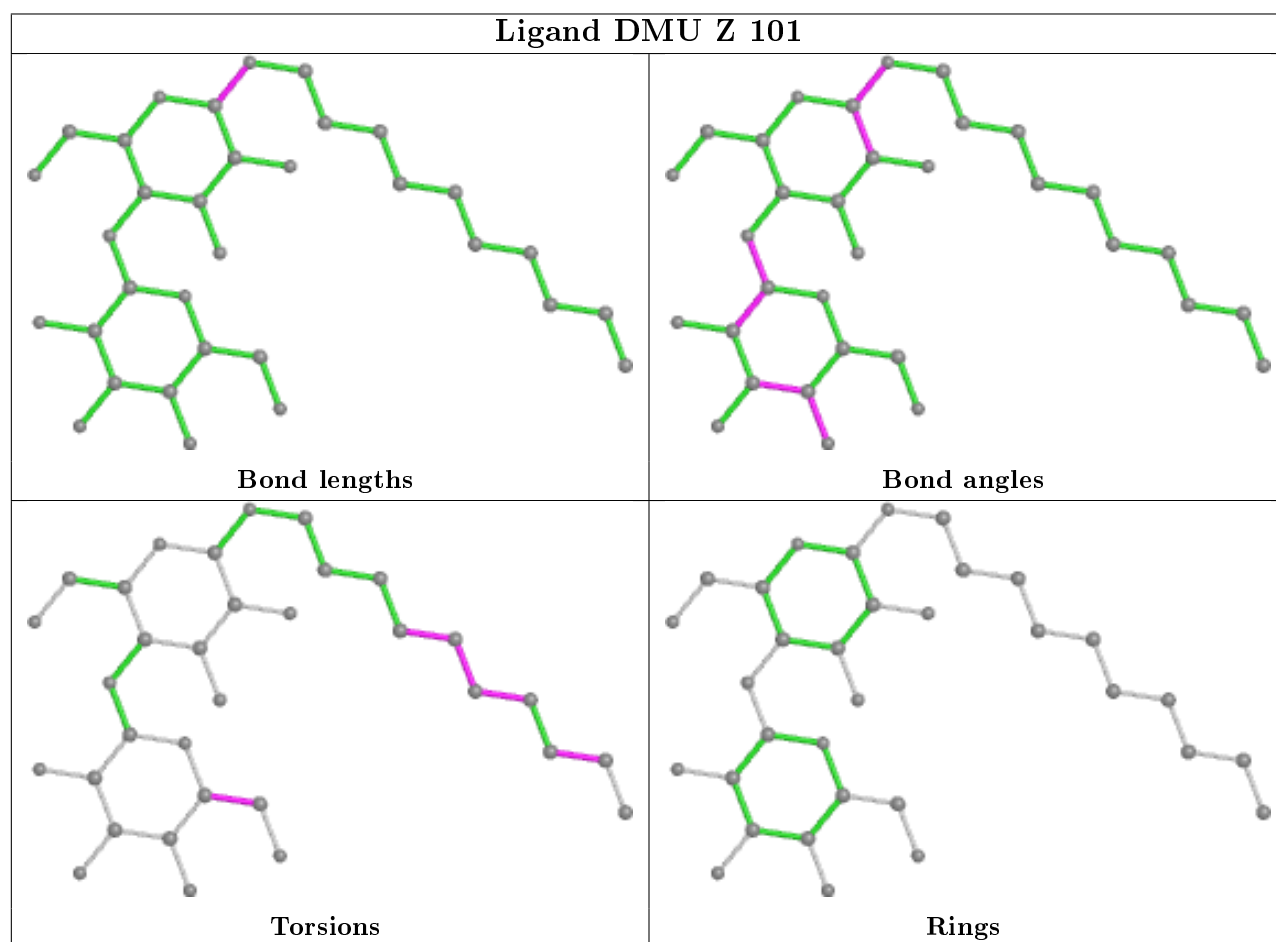
Ligand PEK C 308

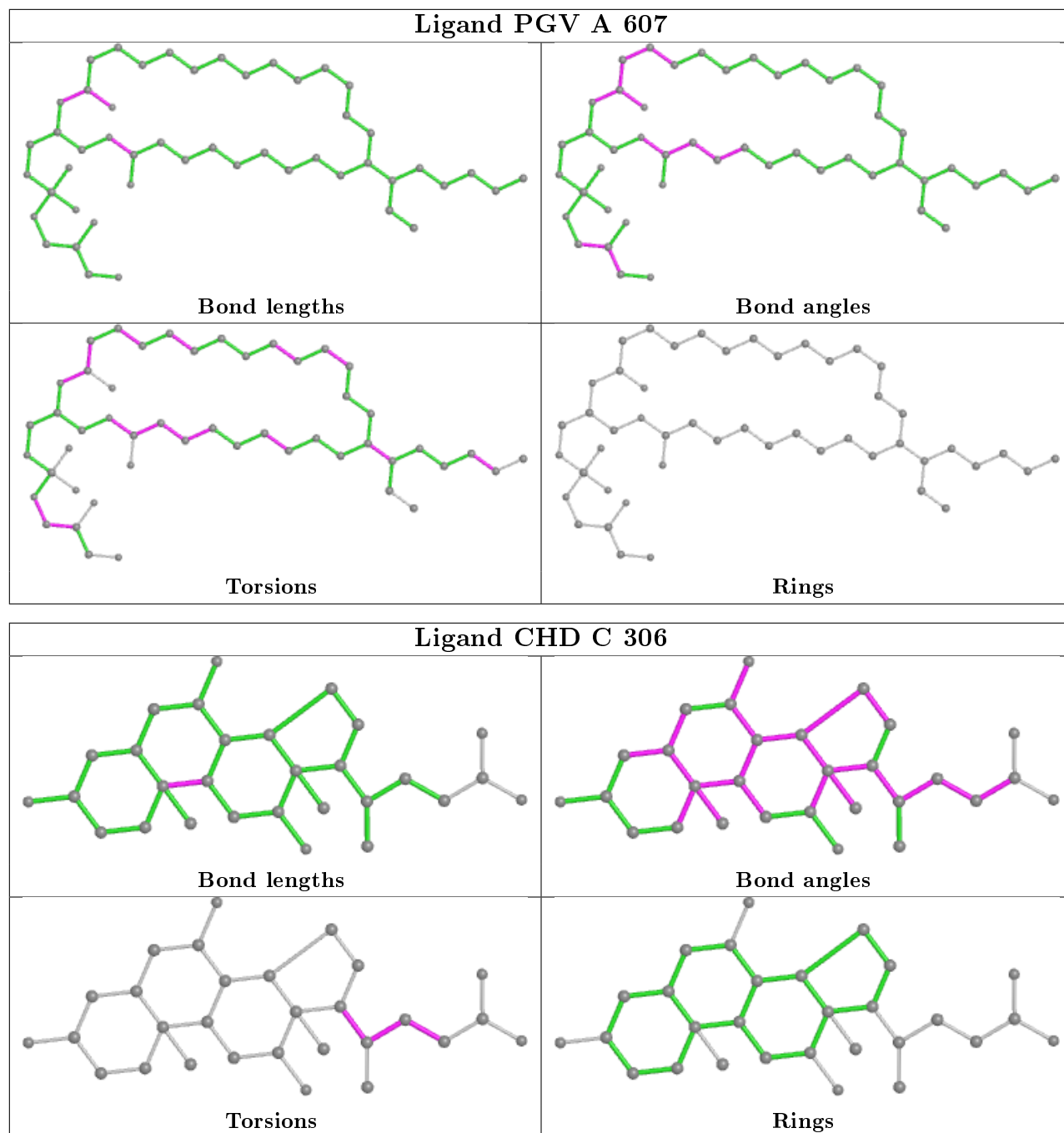


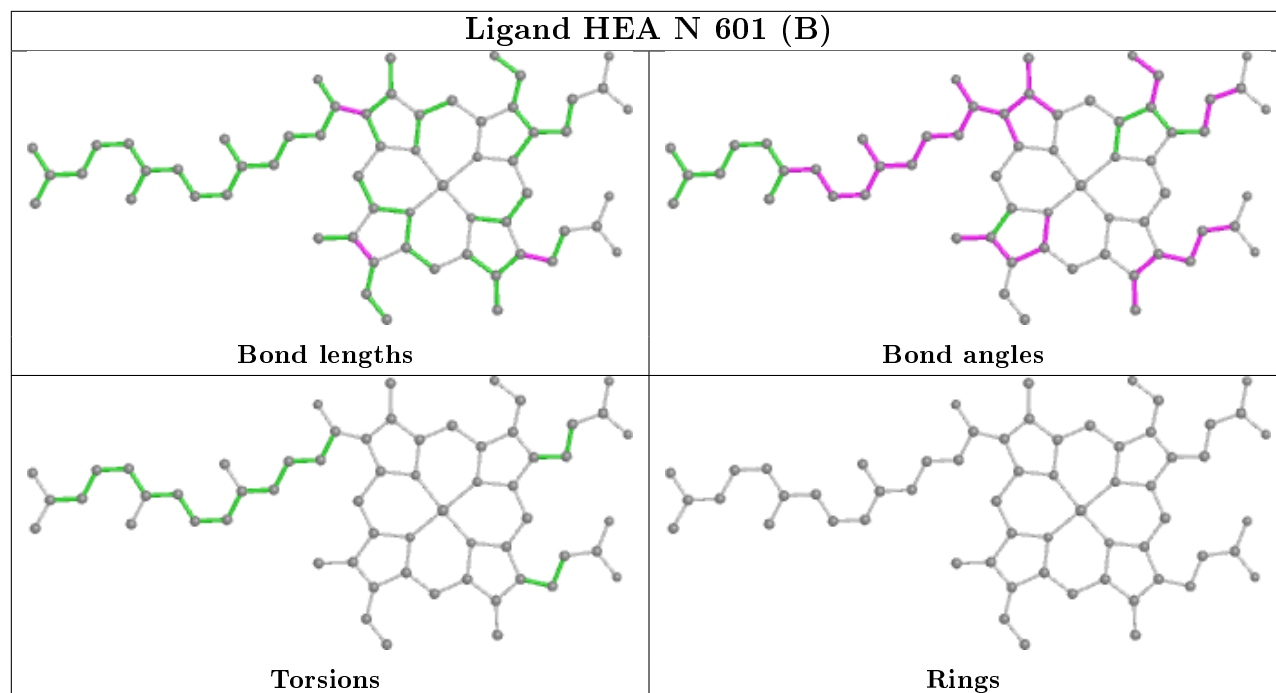
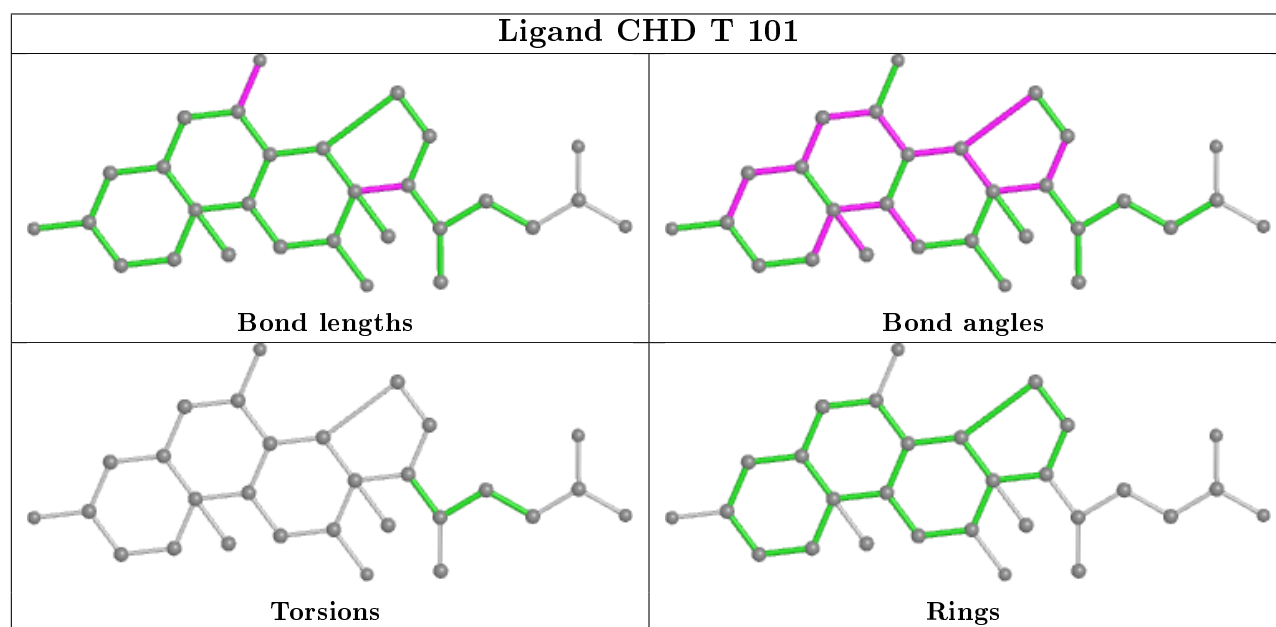
Ligand PGV T 104



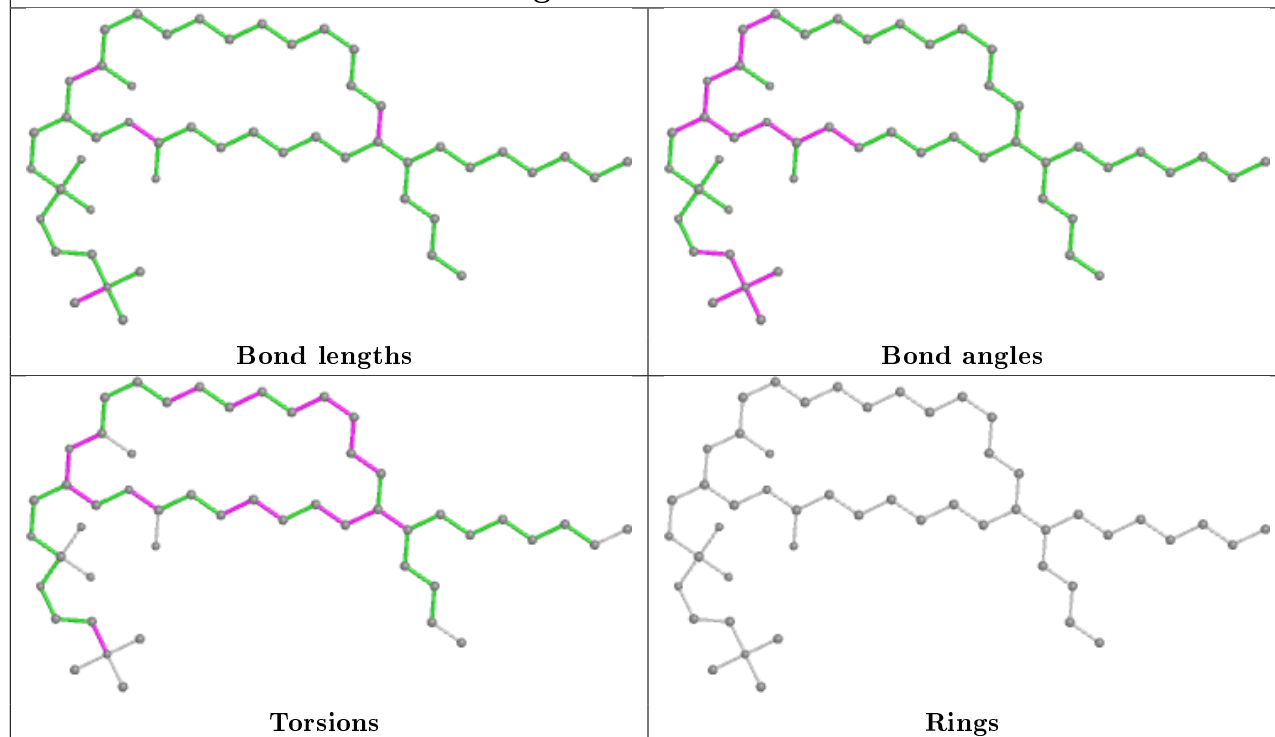


Ligand HEA A 601 (B)**Ligand DMU Z 101**

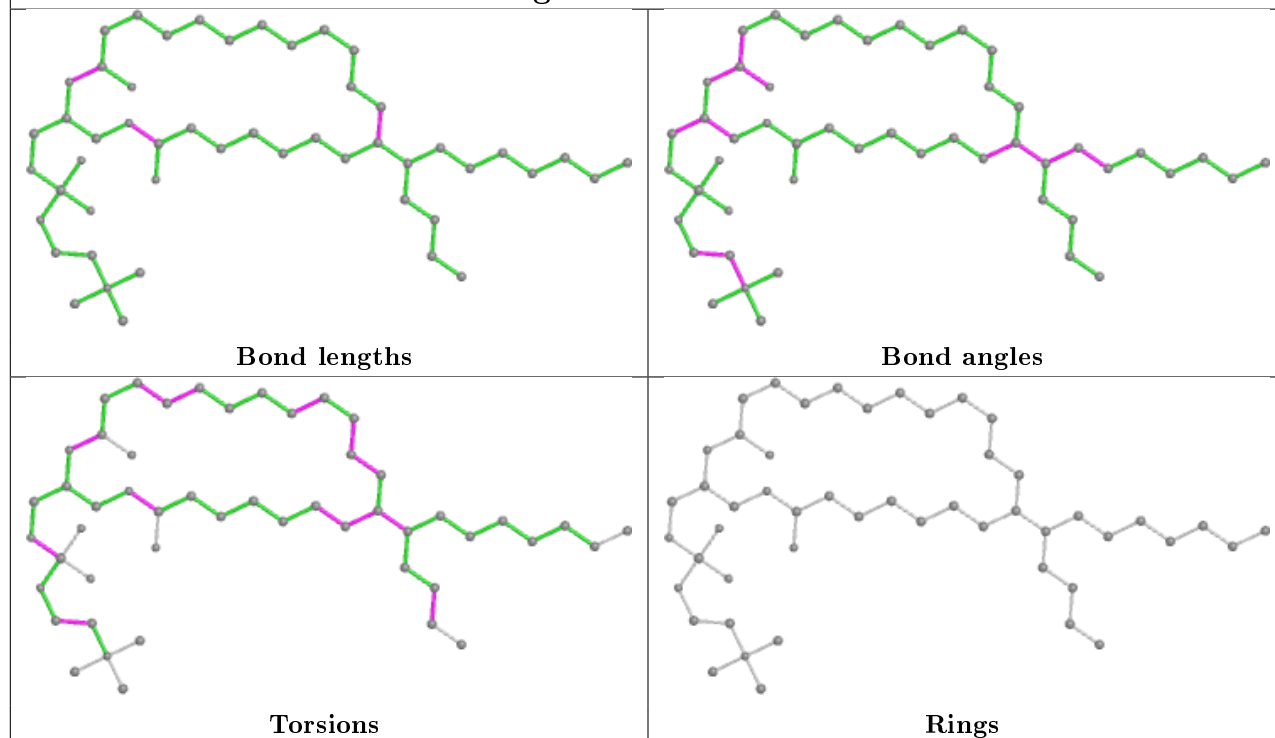


Ligand HEA N 601 (B)**Ligand CHD T 101**

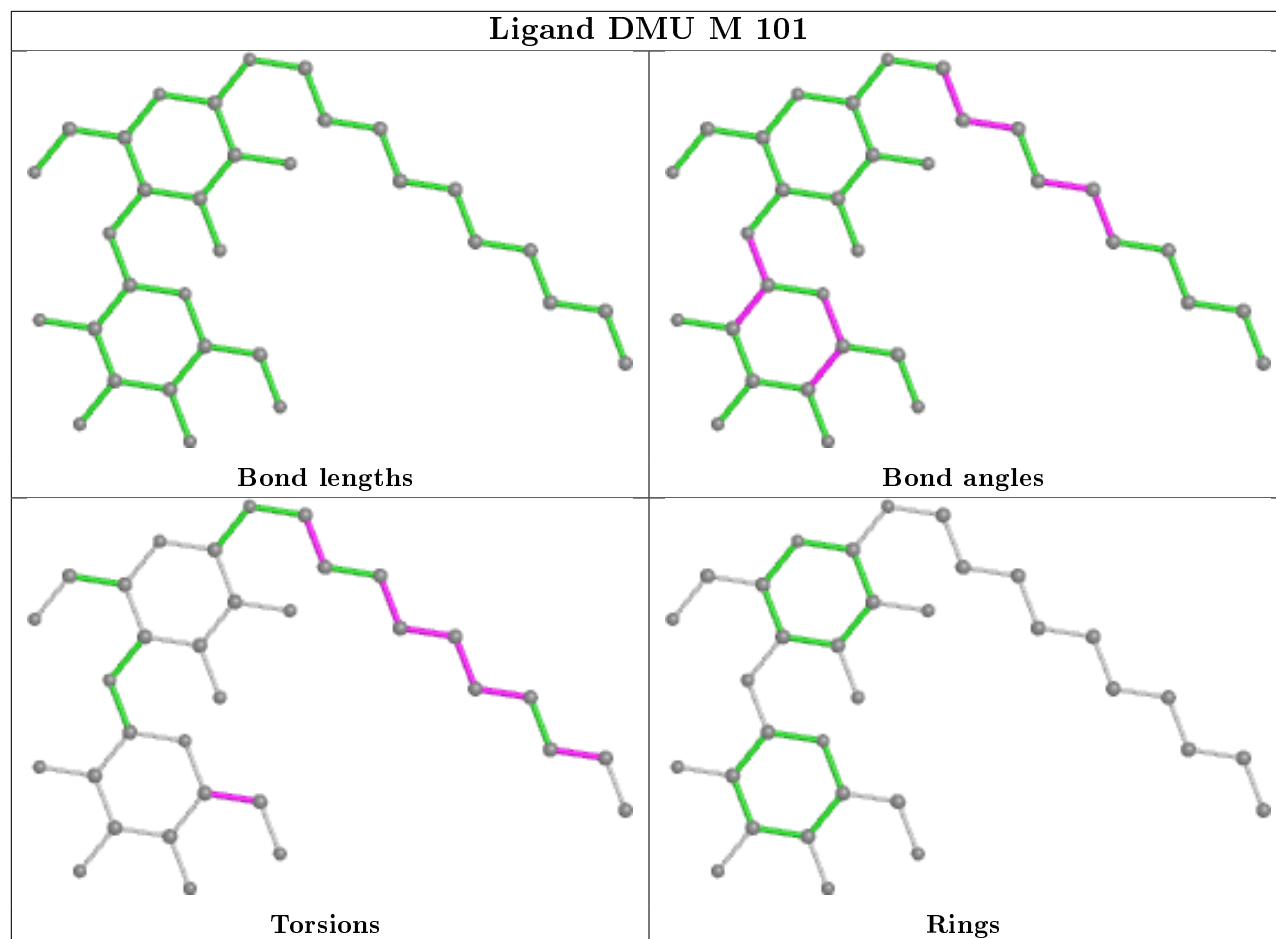
Ligand PSC V 101



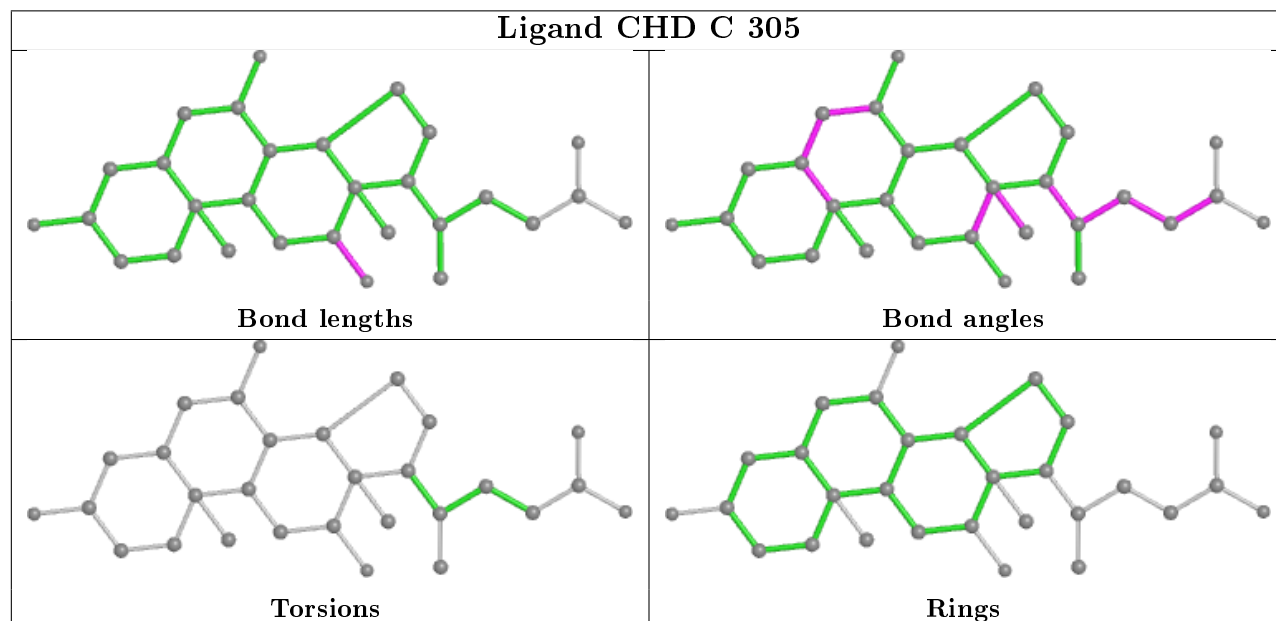
Ligand PSC A 609



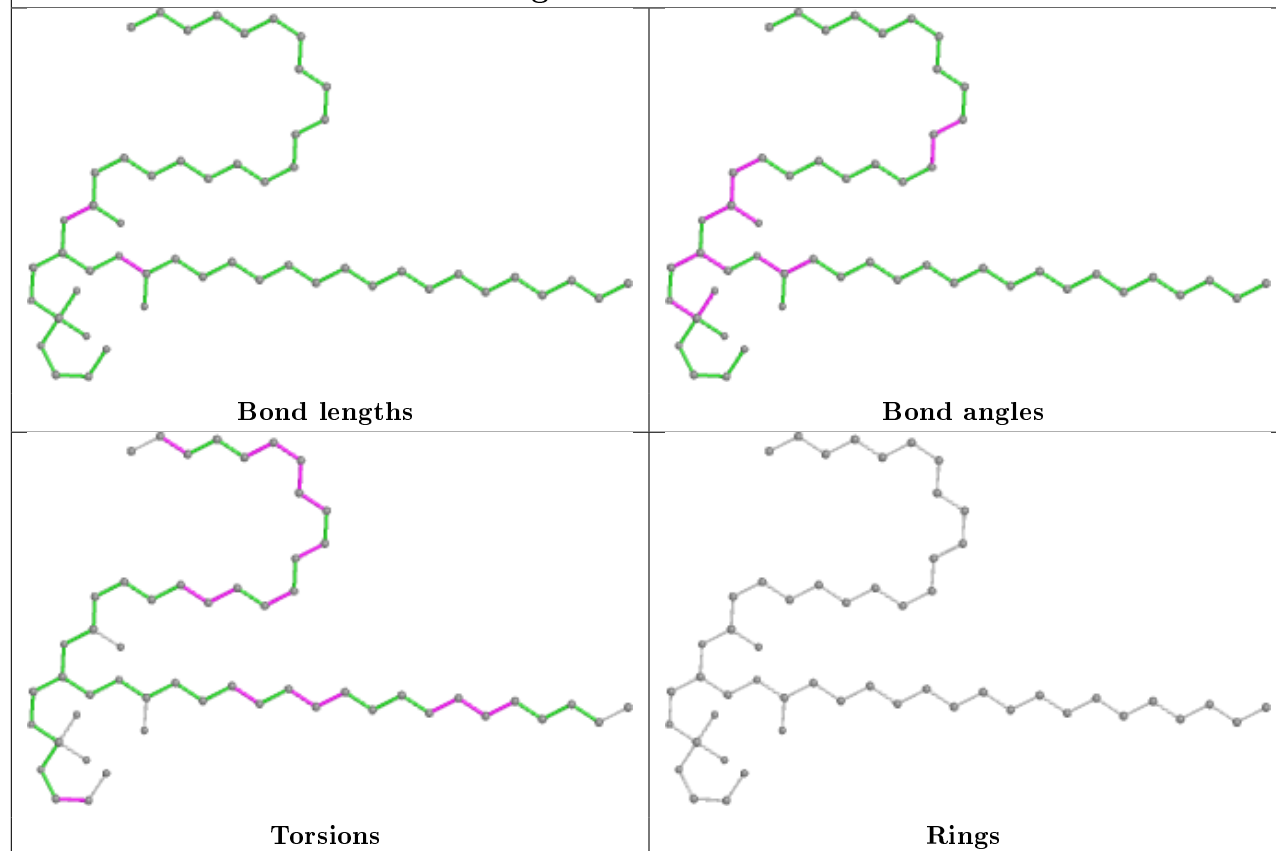
Ligand DMU M 101



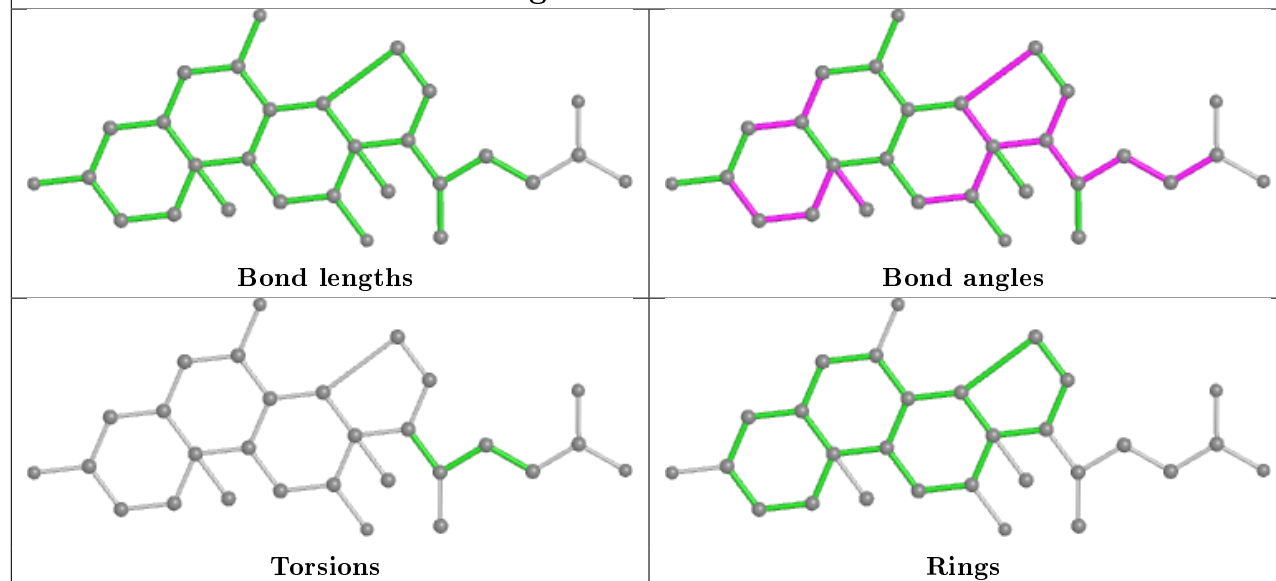
Ligand CHD C 305

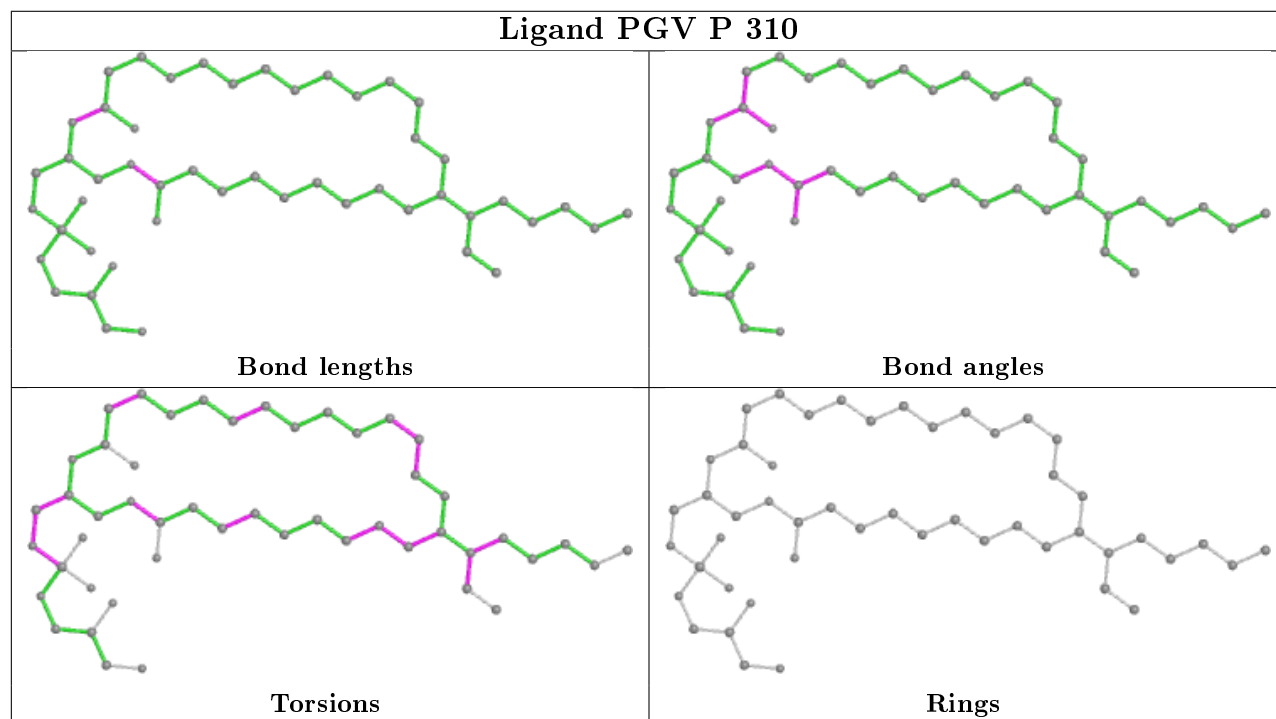
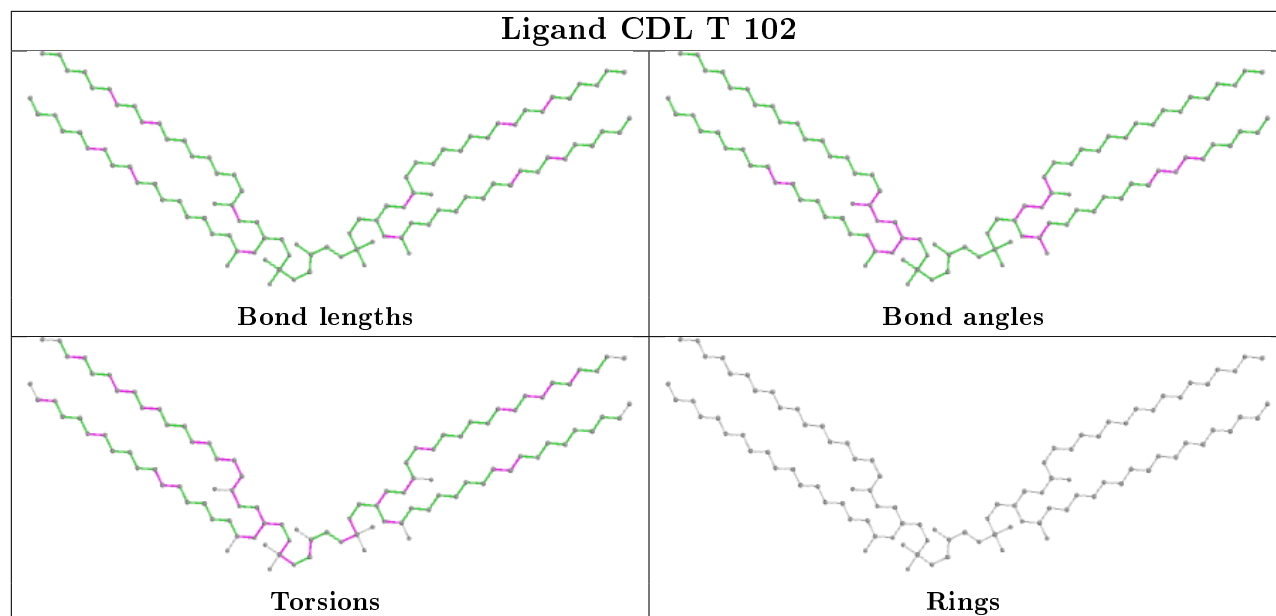


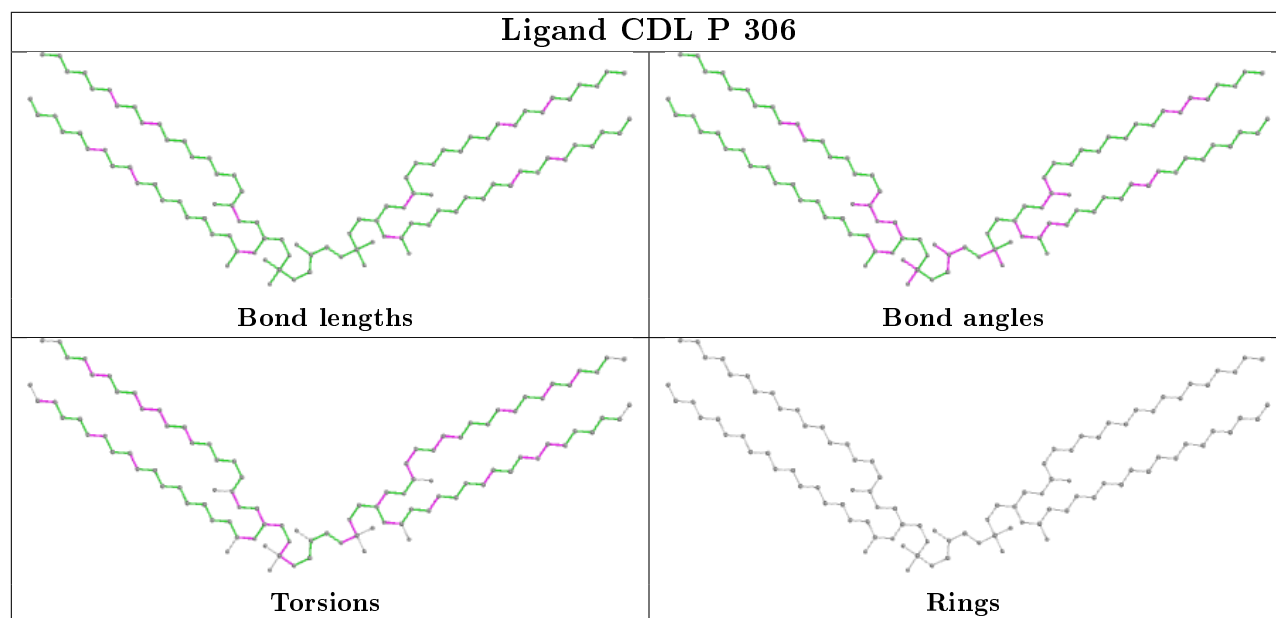
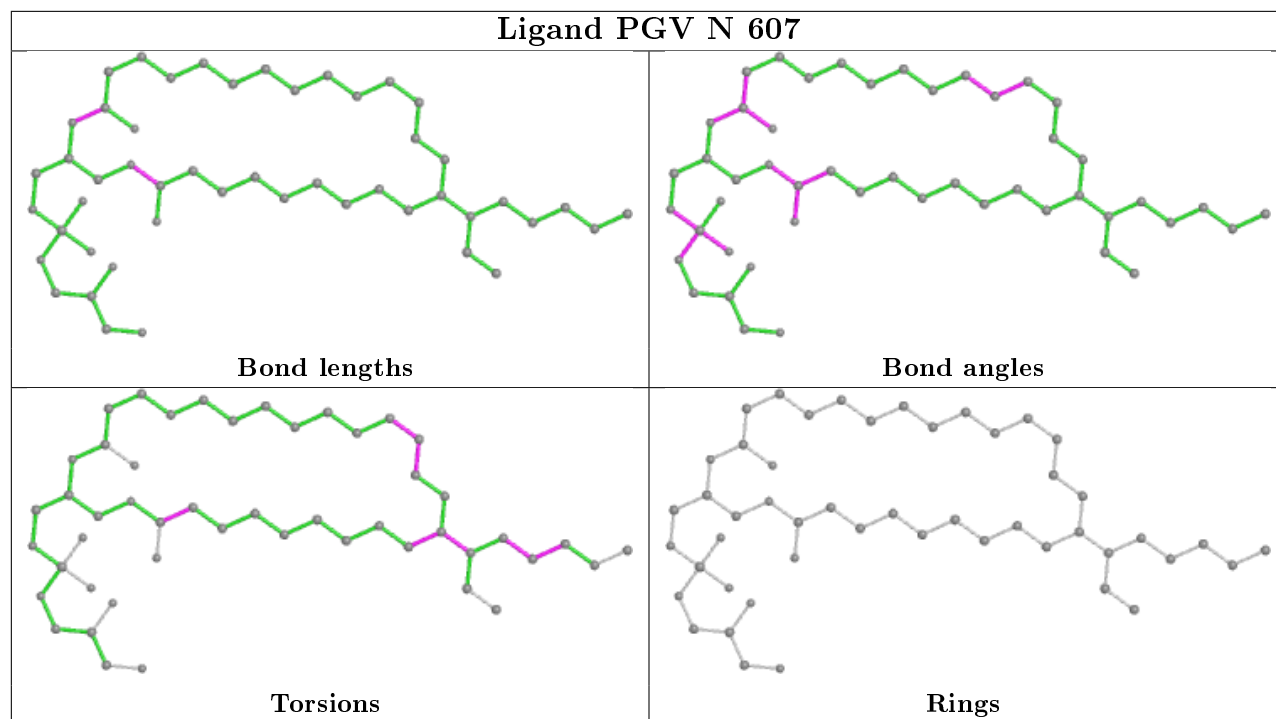
Ligand PEK C 309

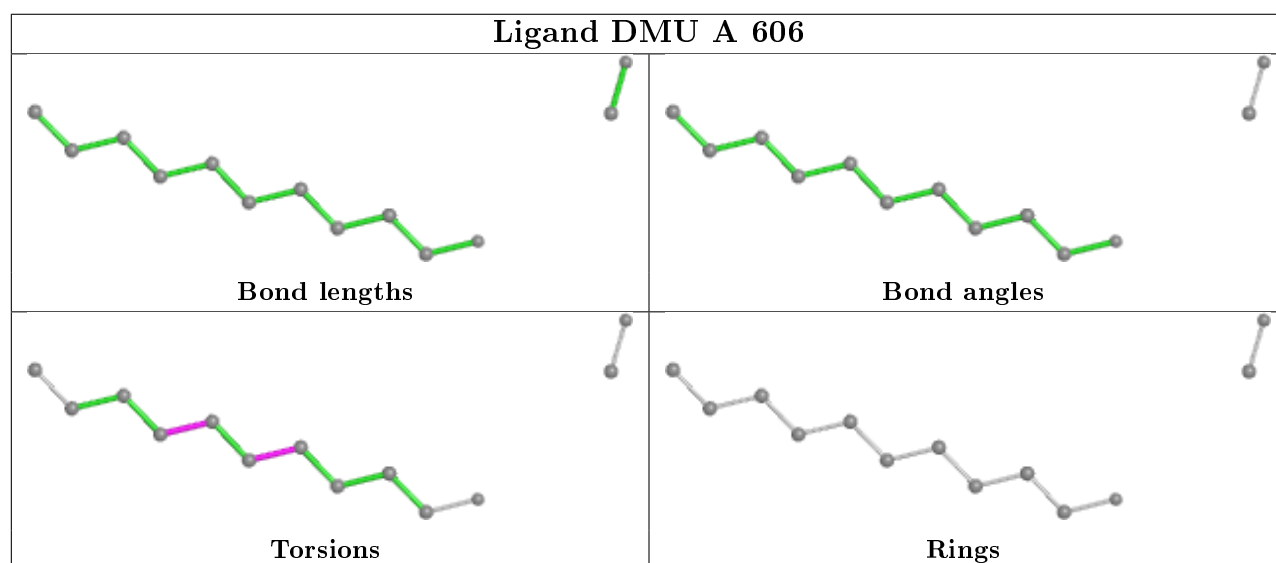
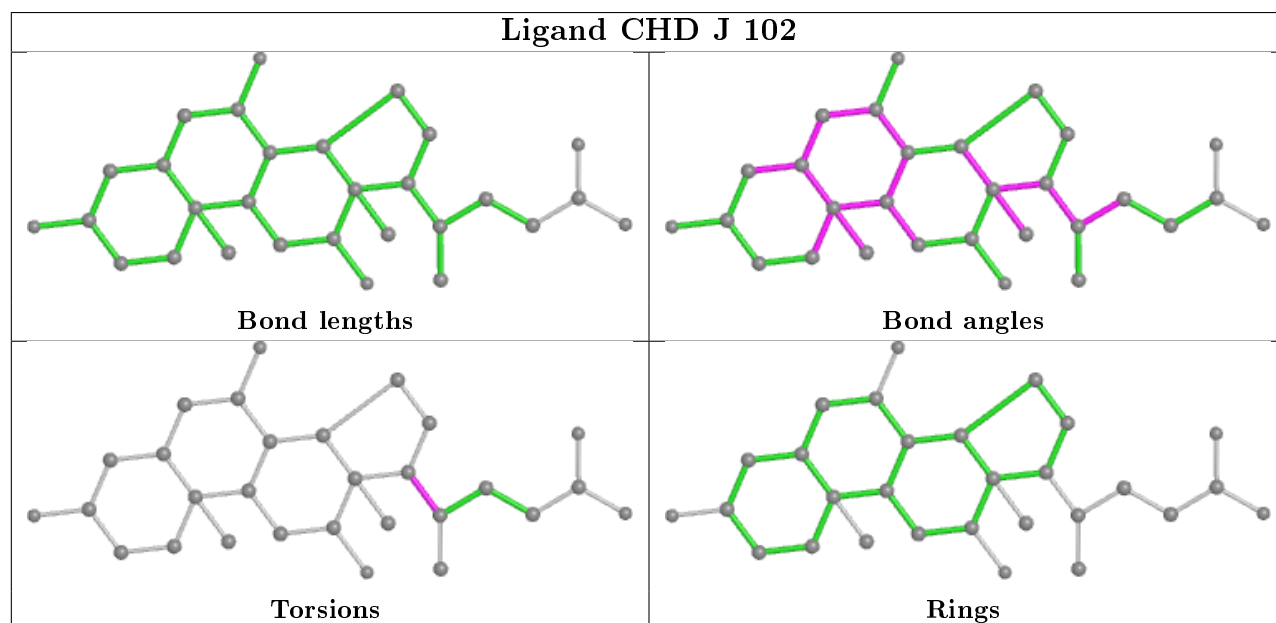
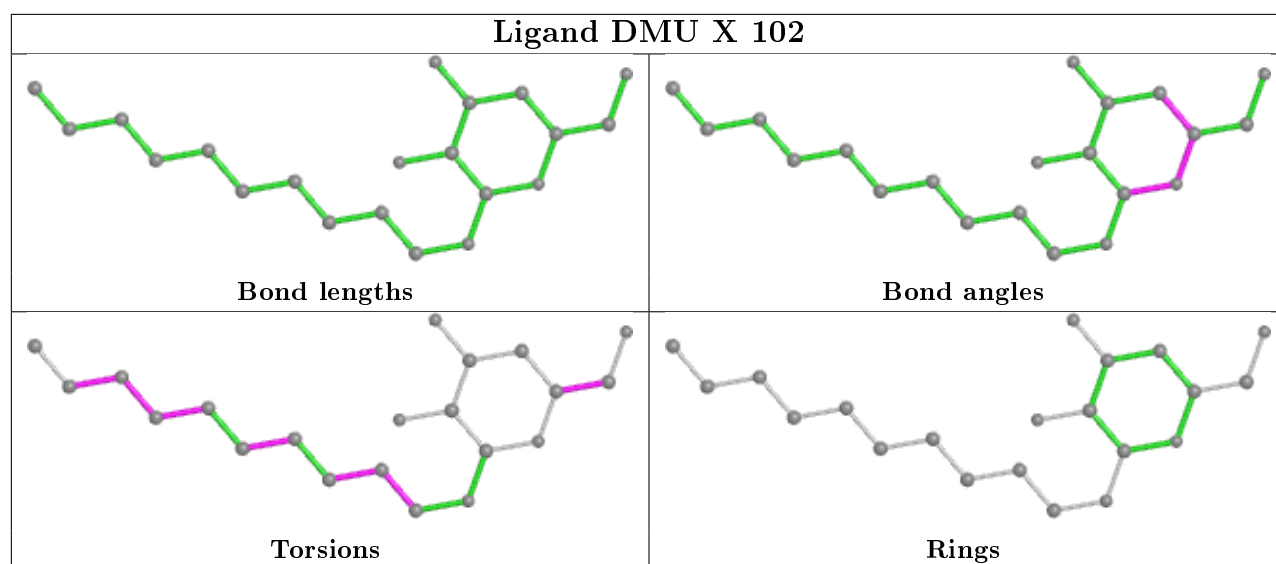


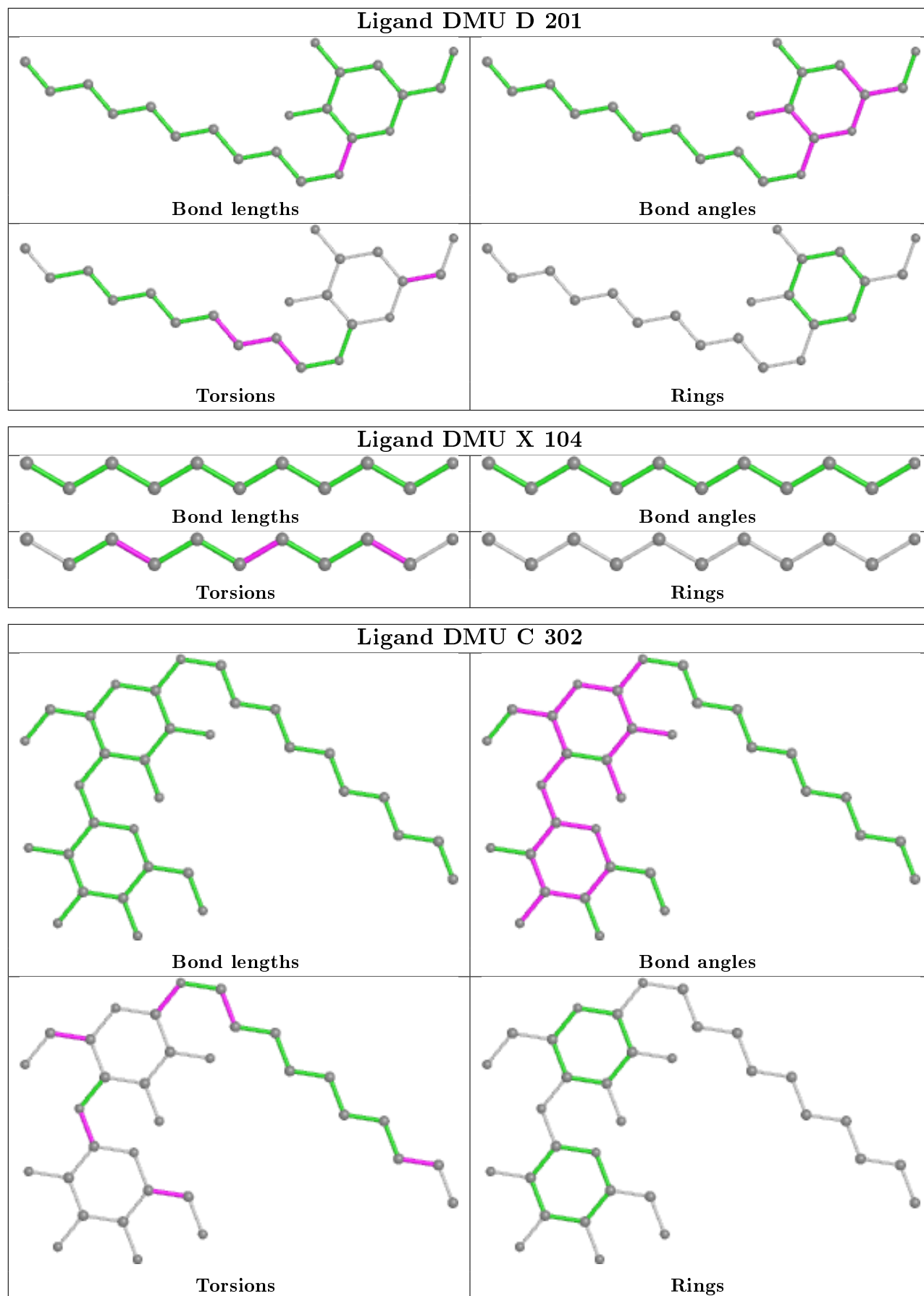
Ligand CHD P 304

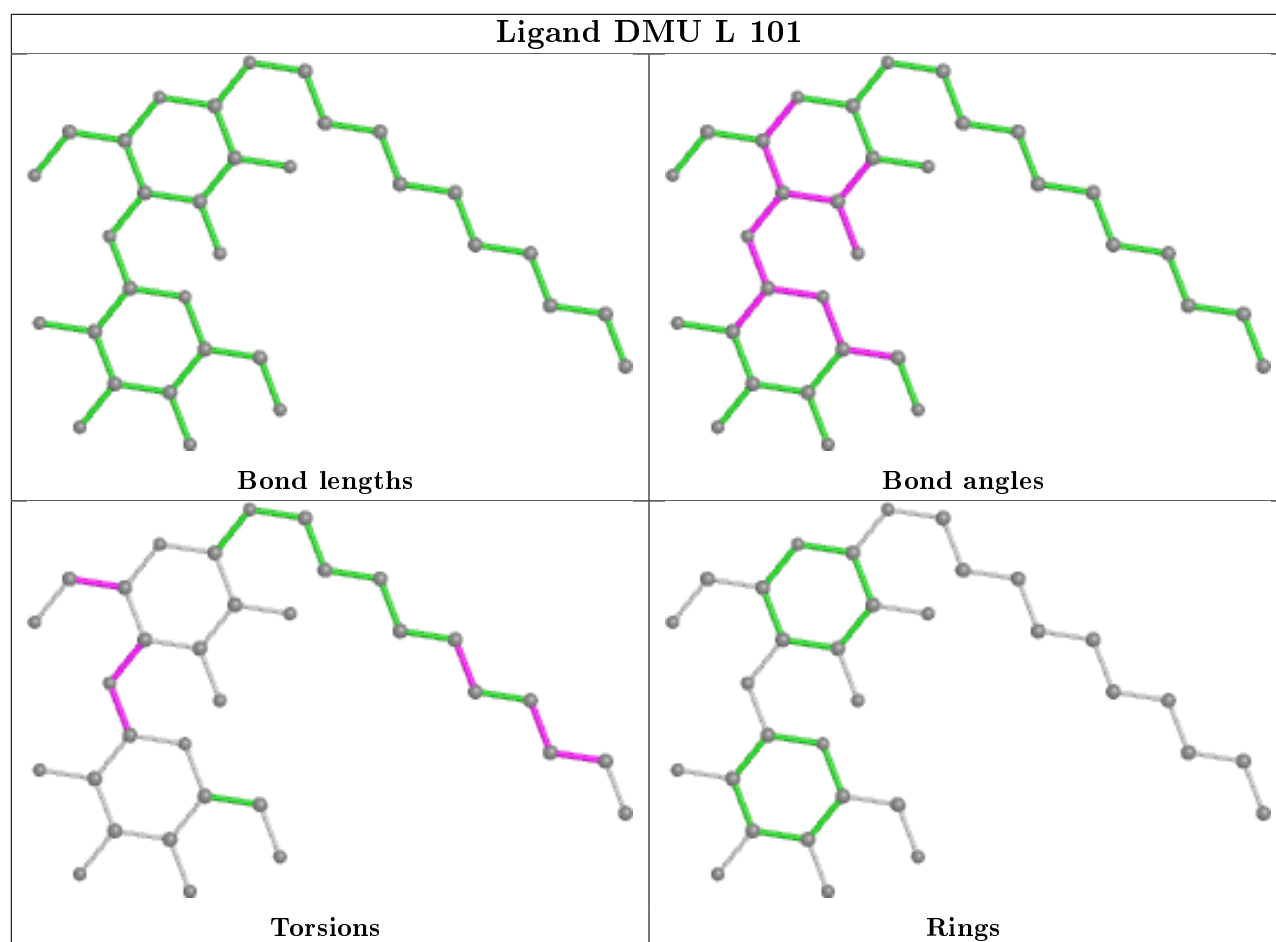




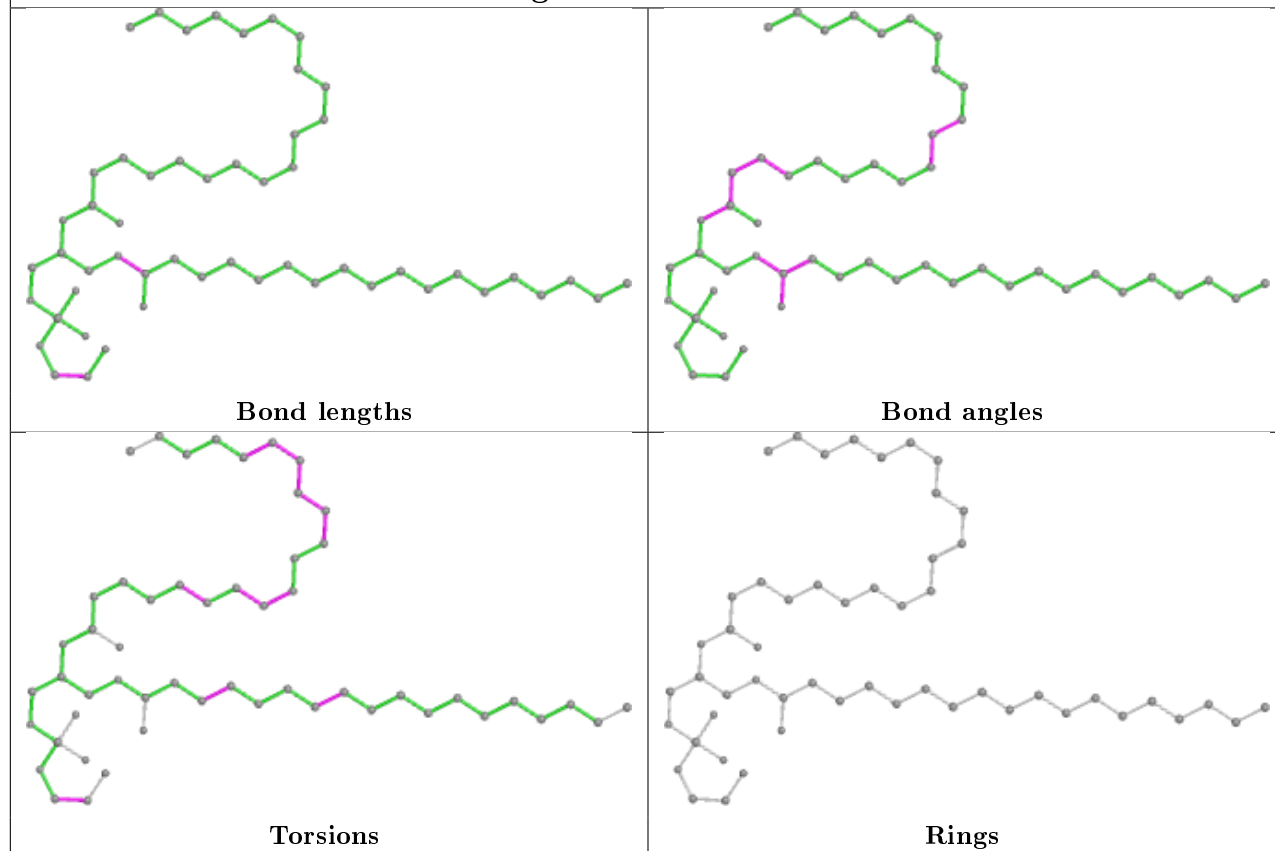




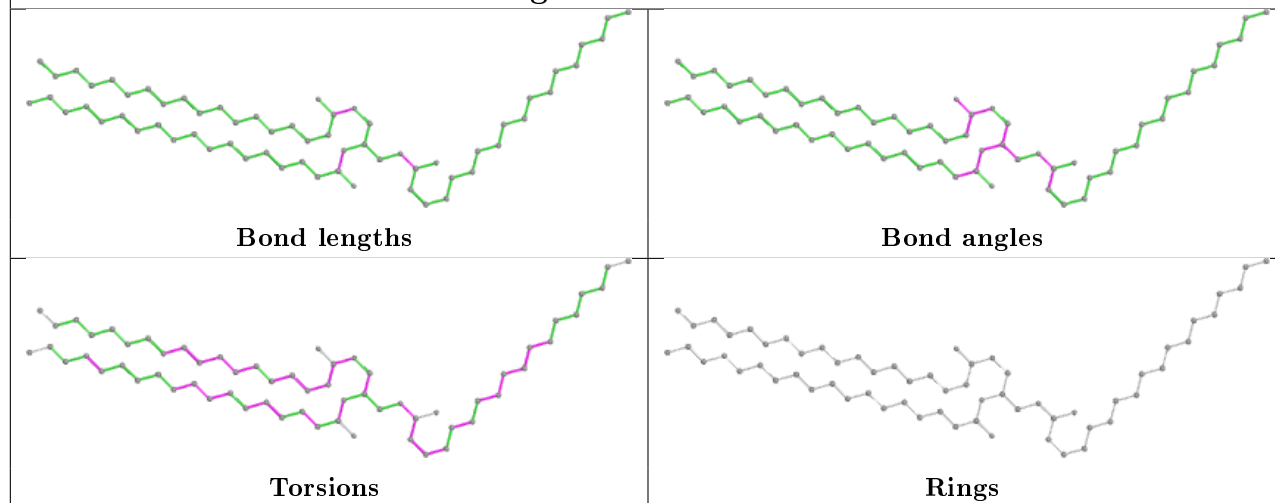


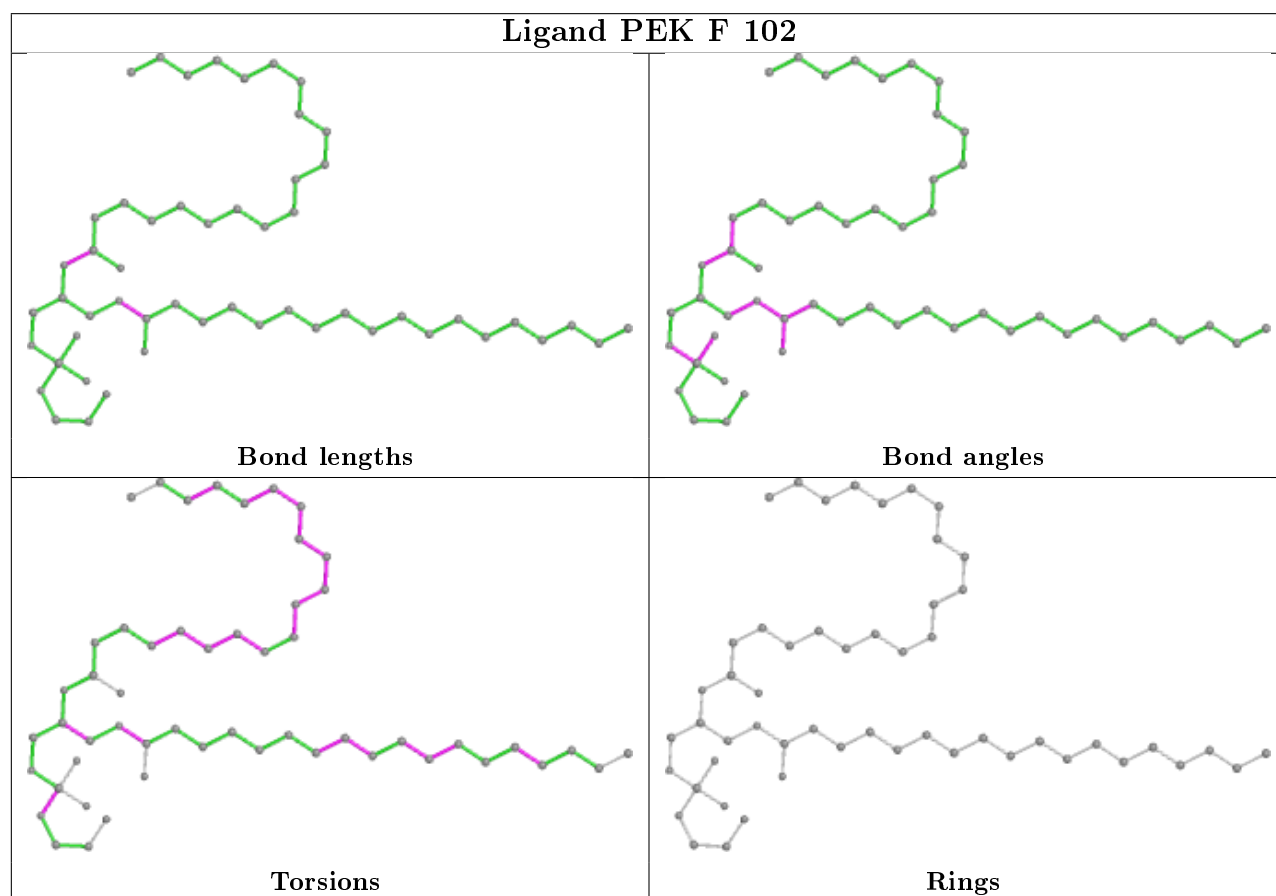
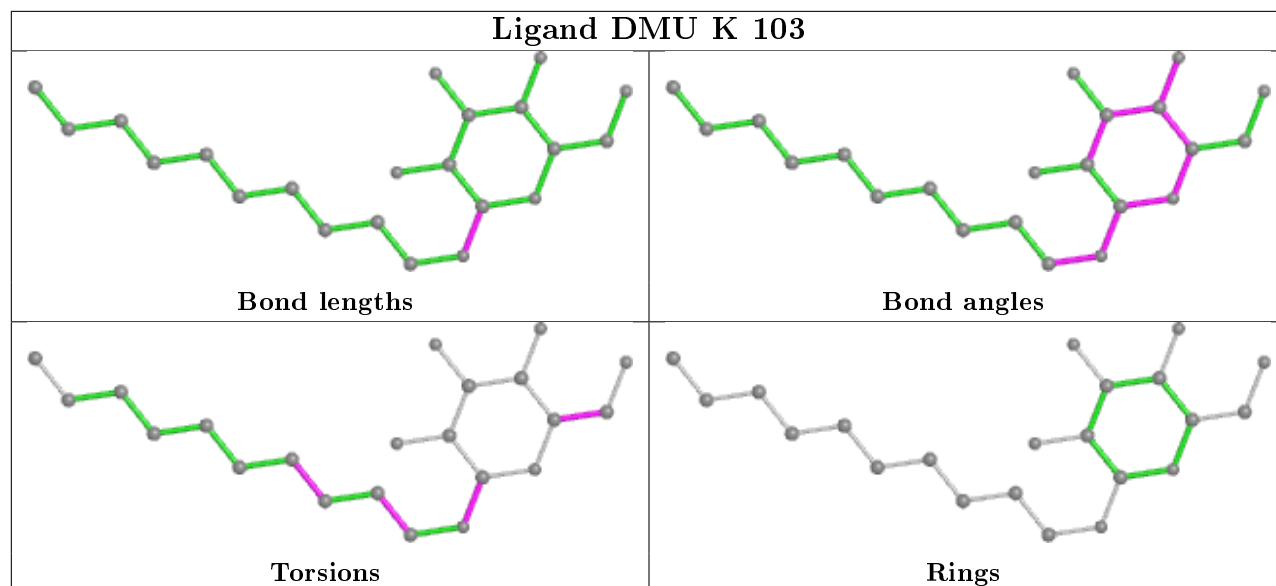


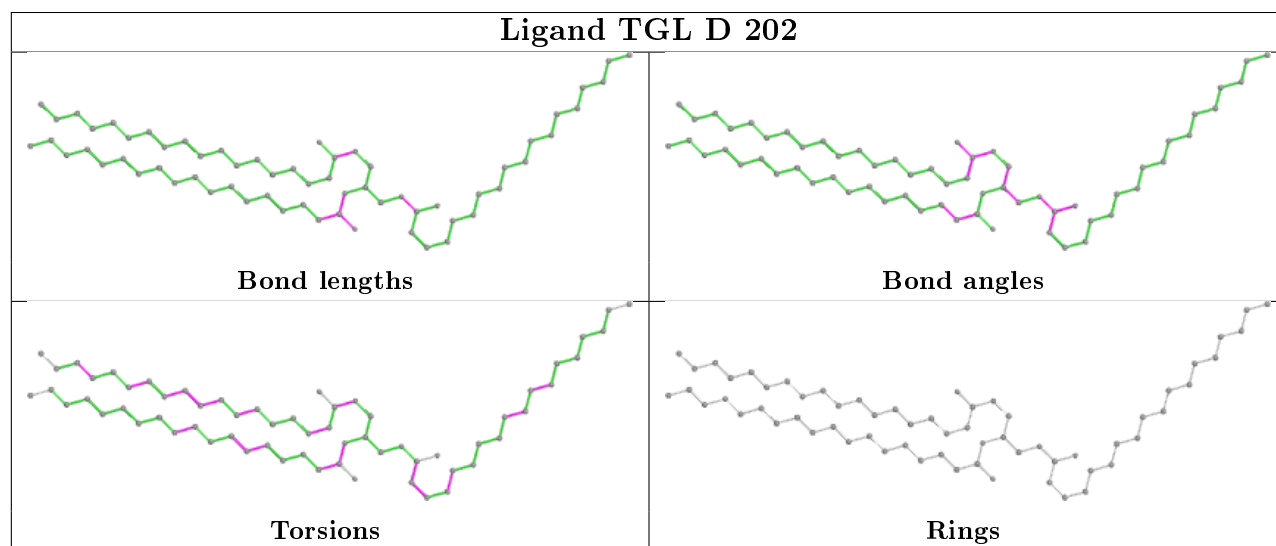
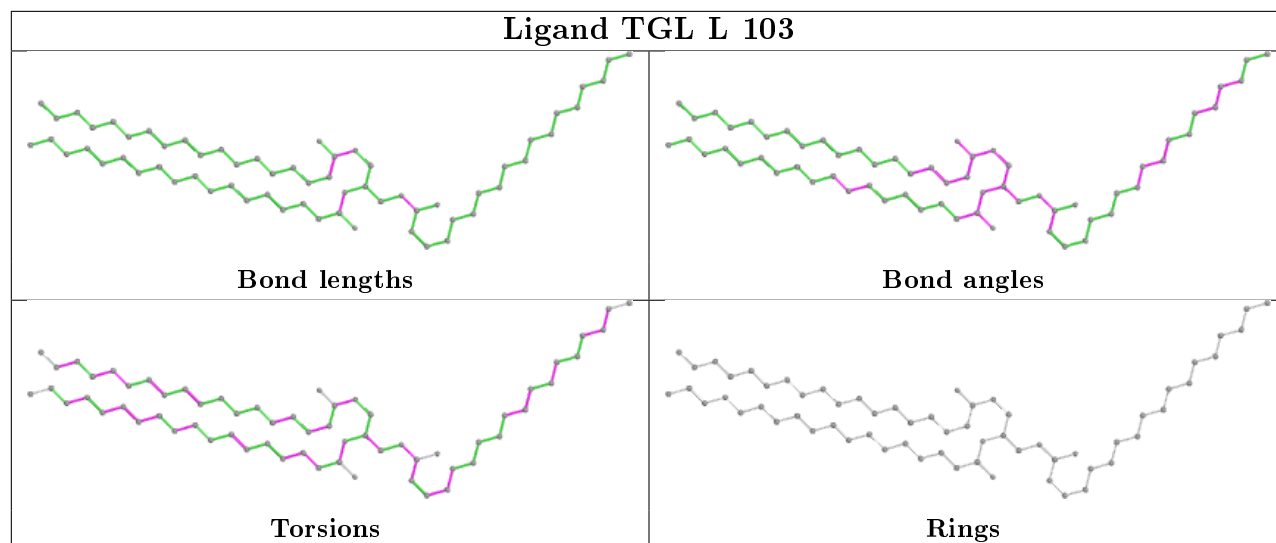
Ligand PEK P 308

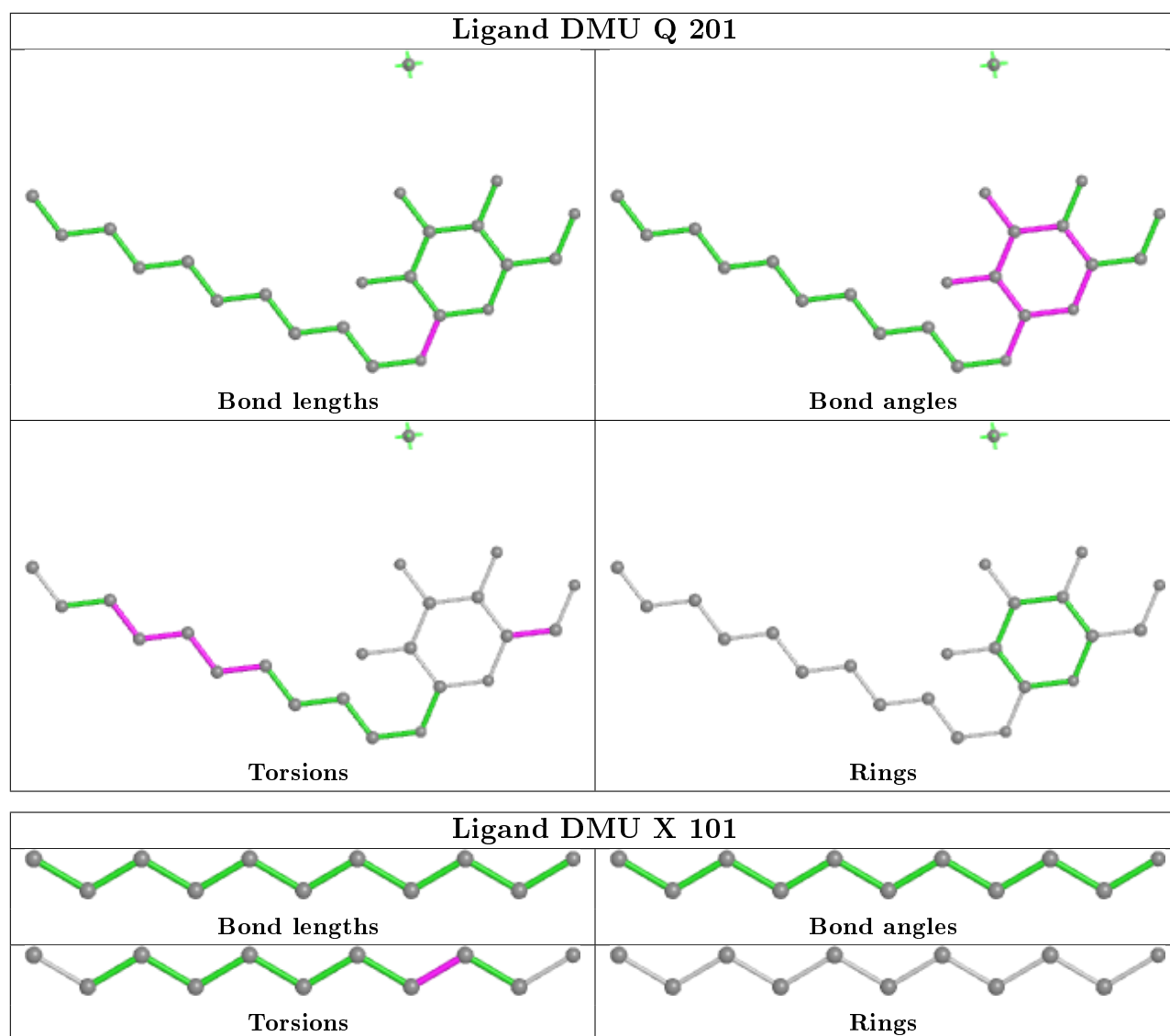


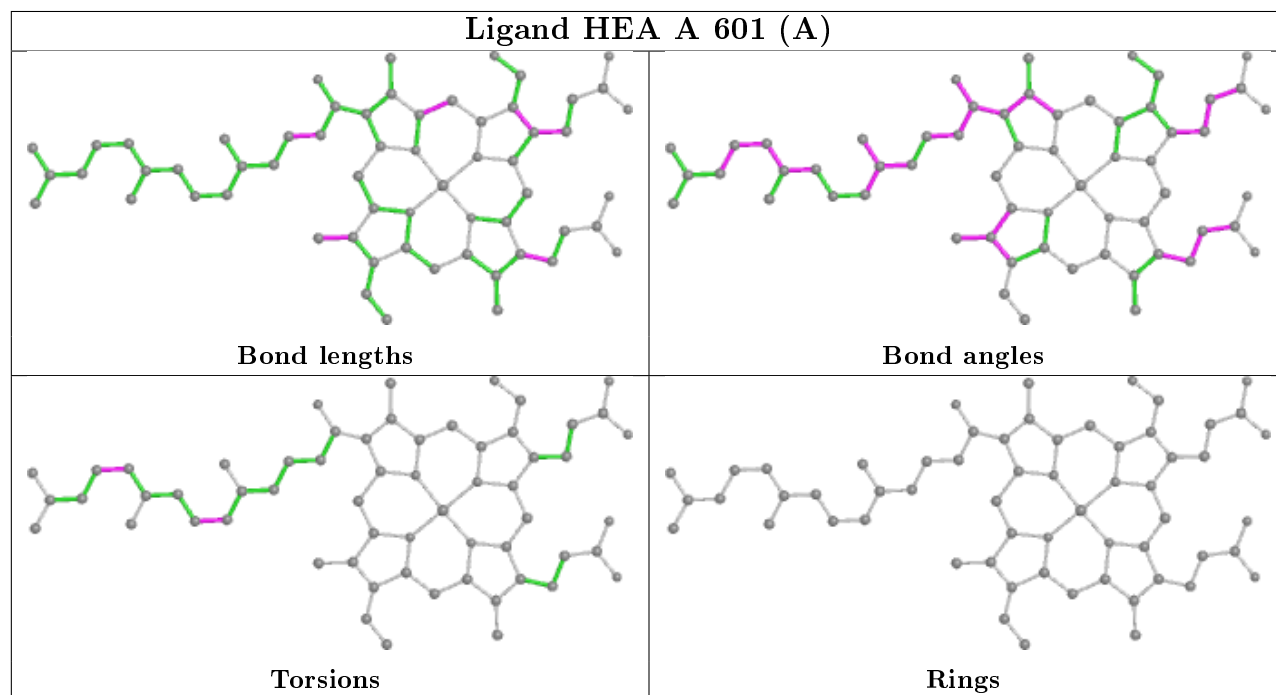
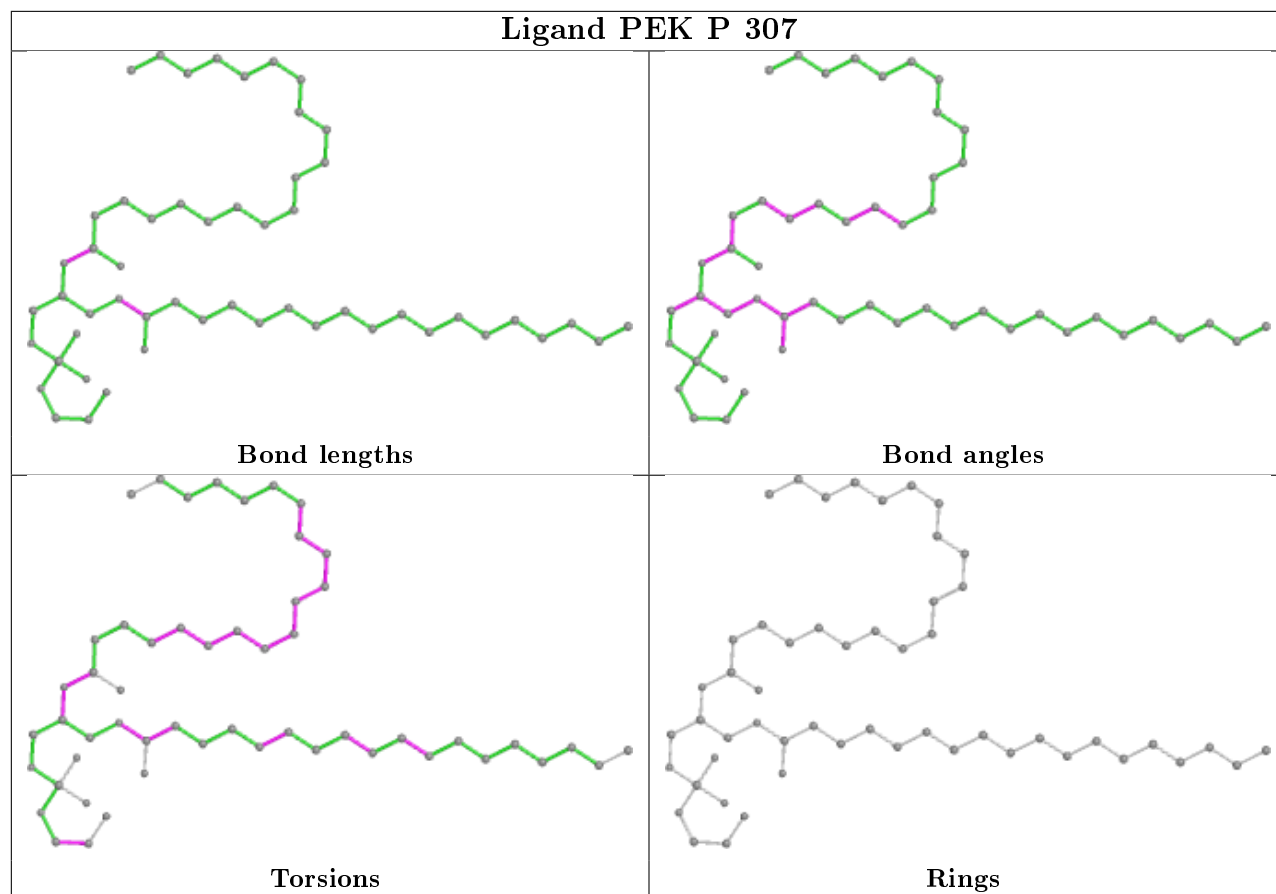
Ligand TGL N 608

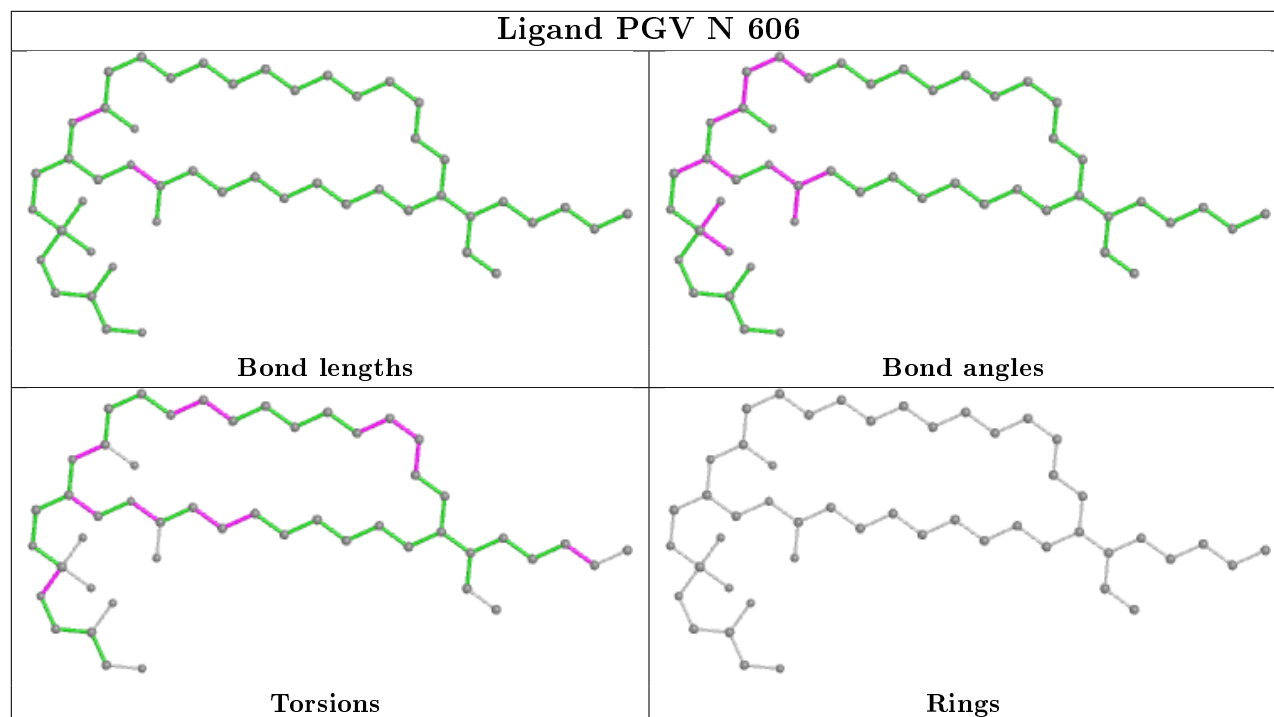
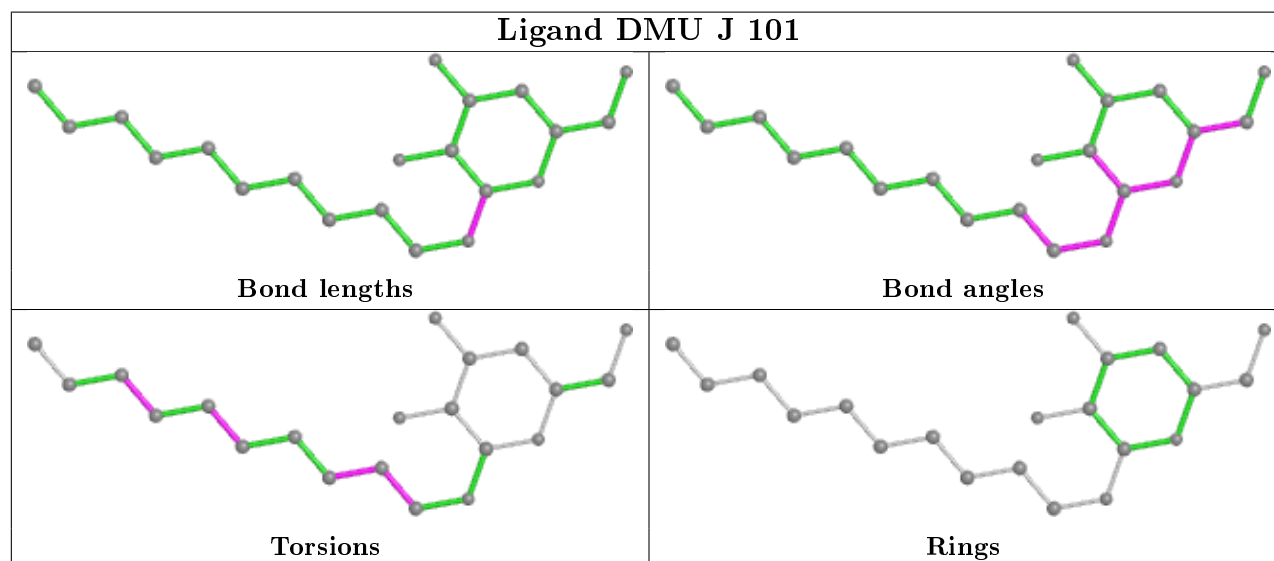
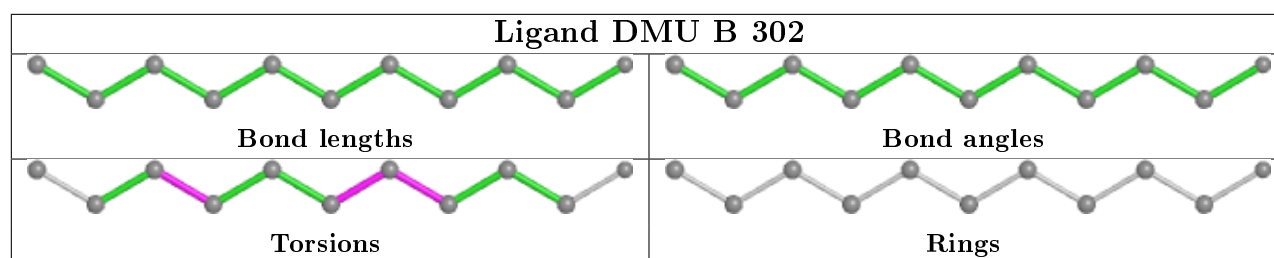


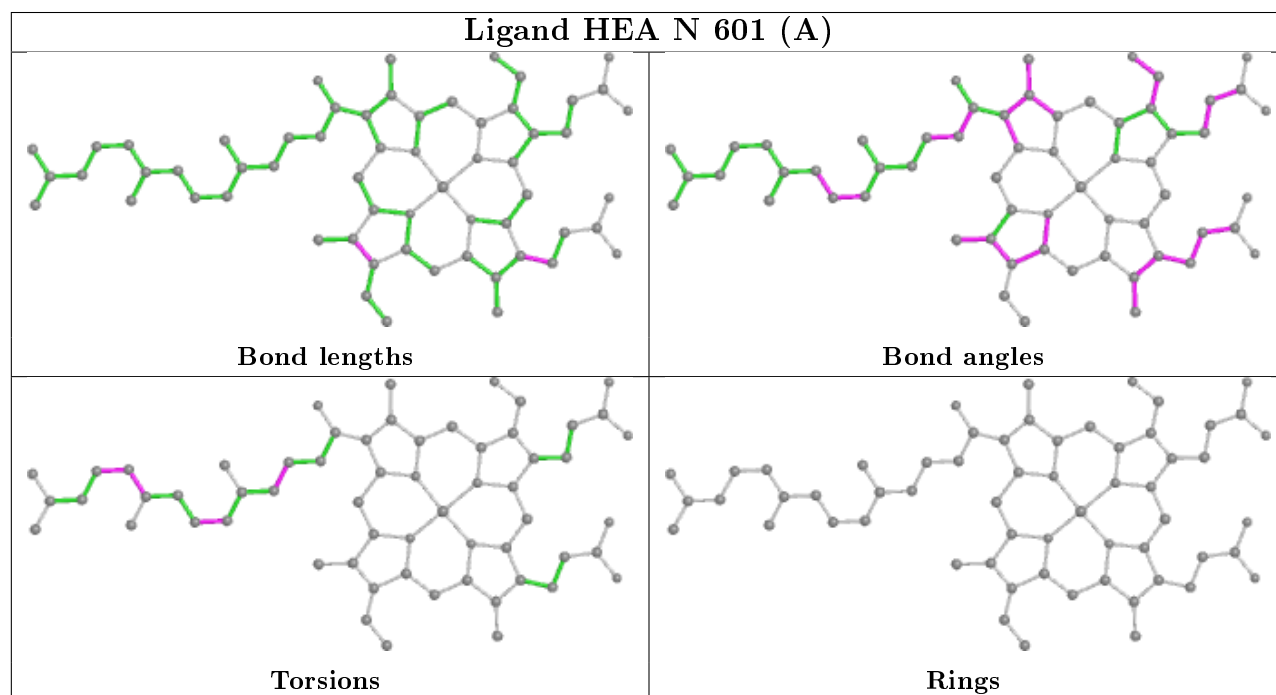
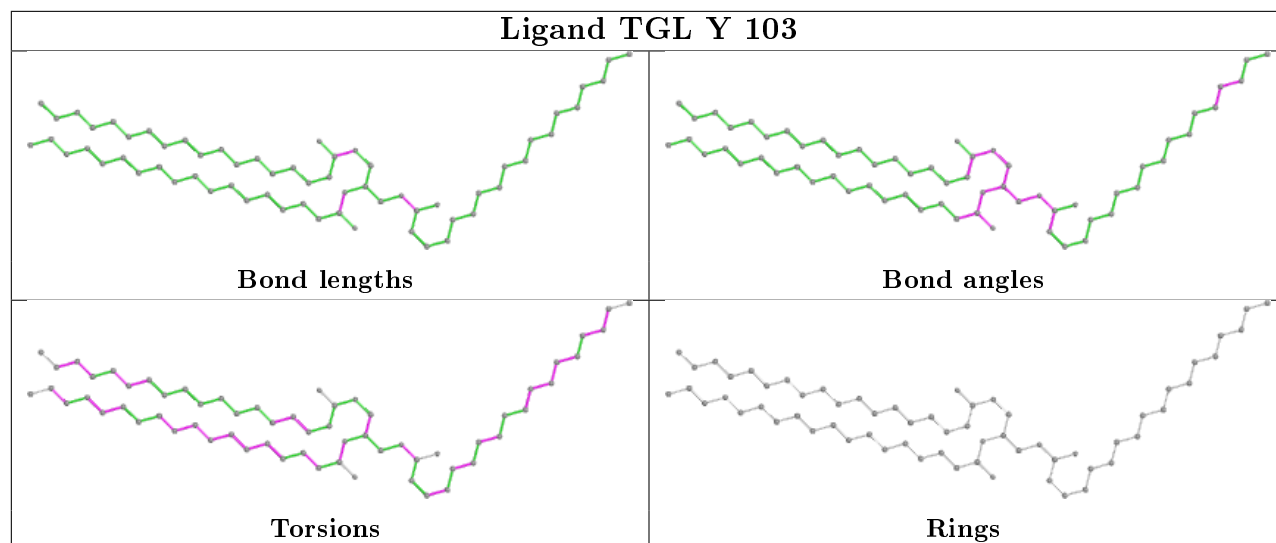


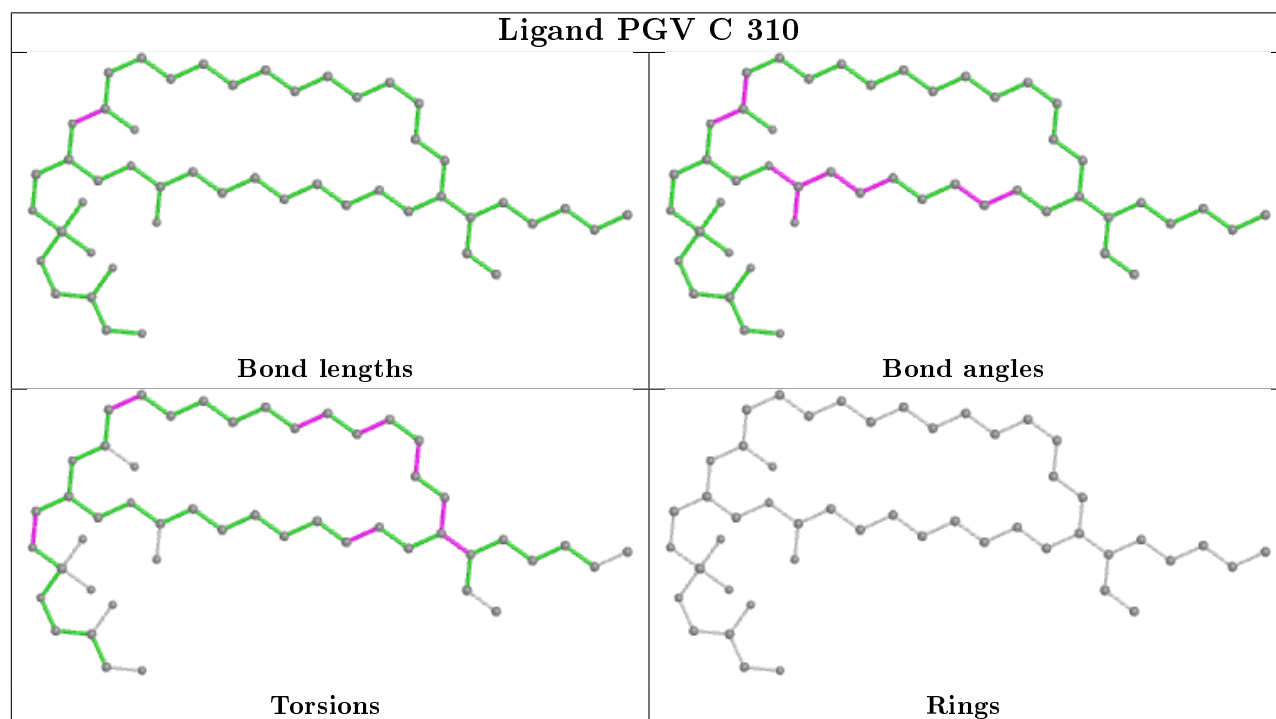
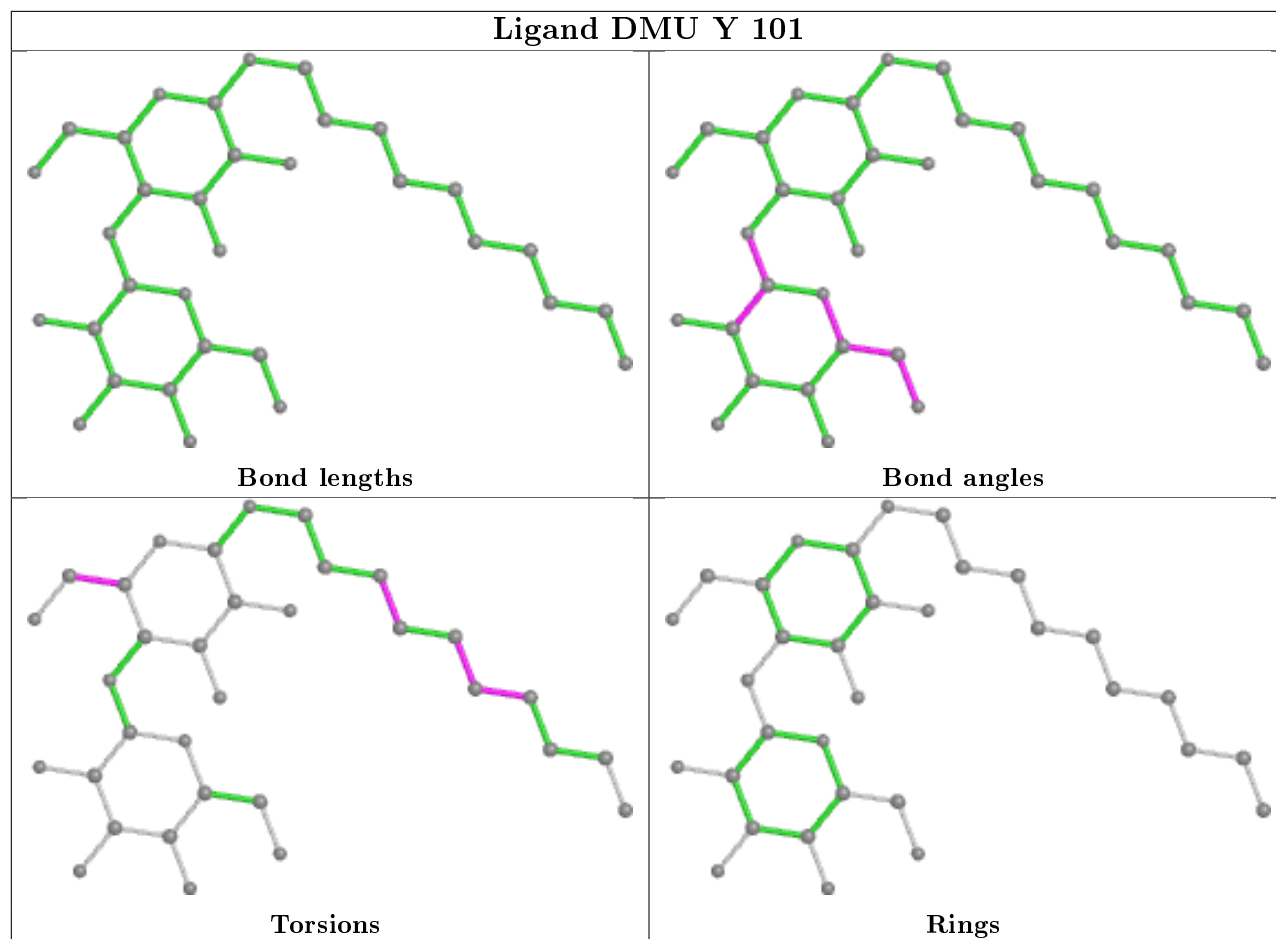


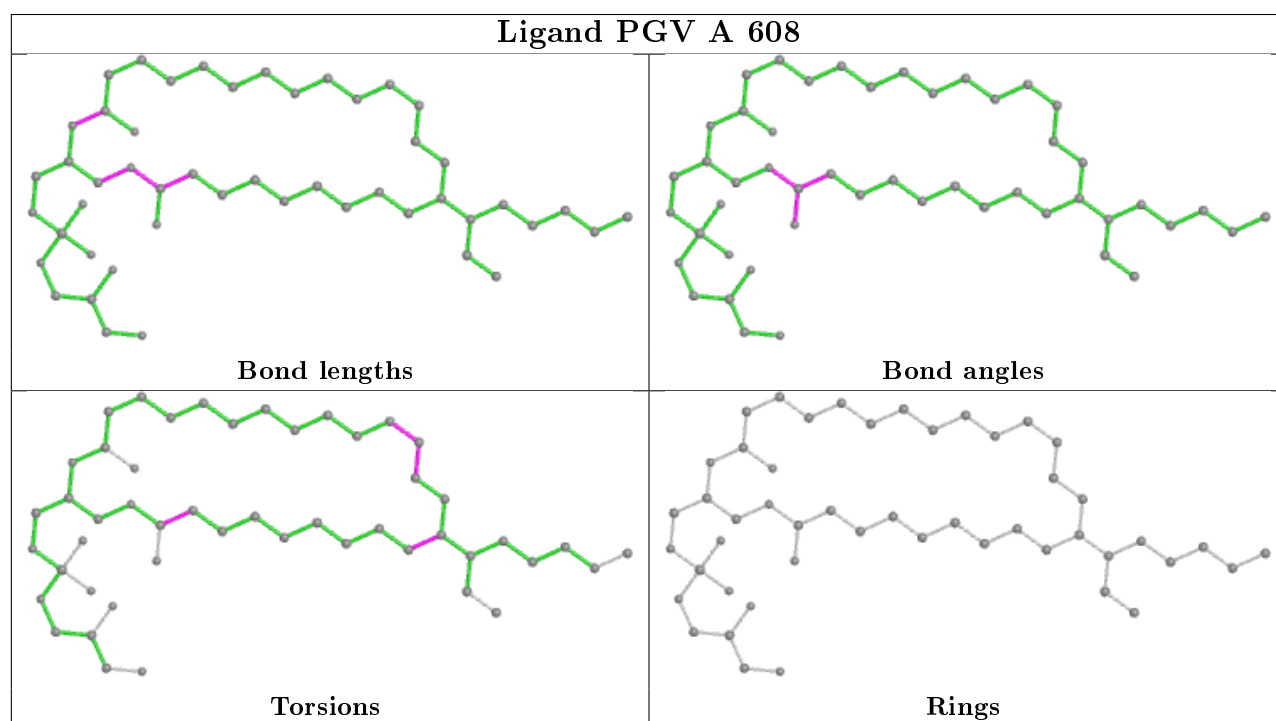
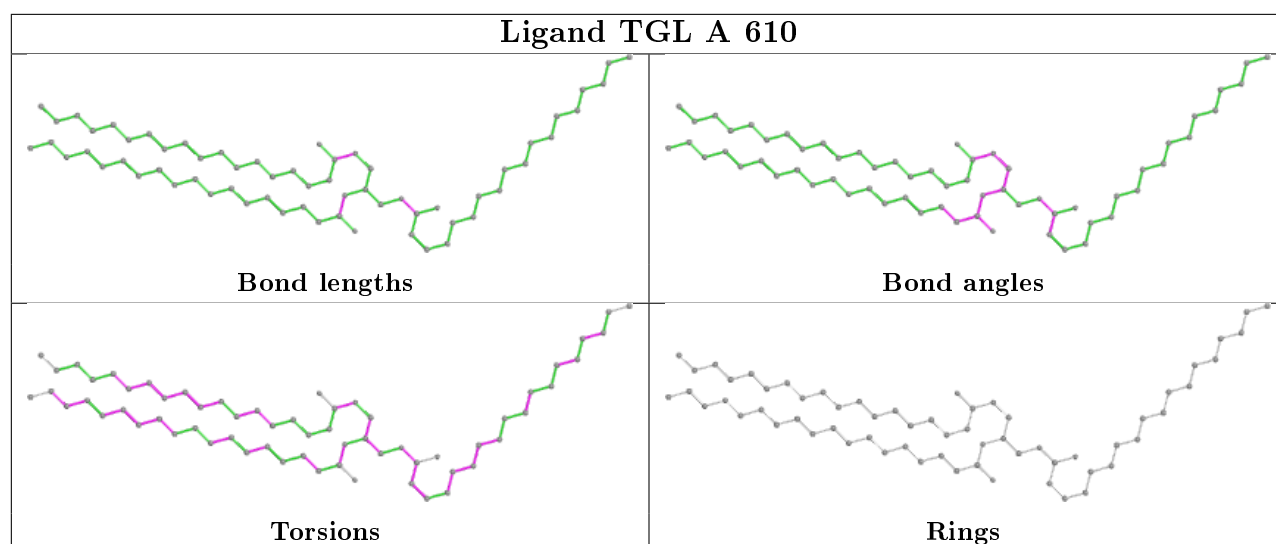


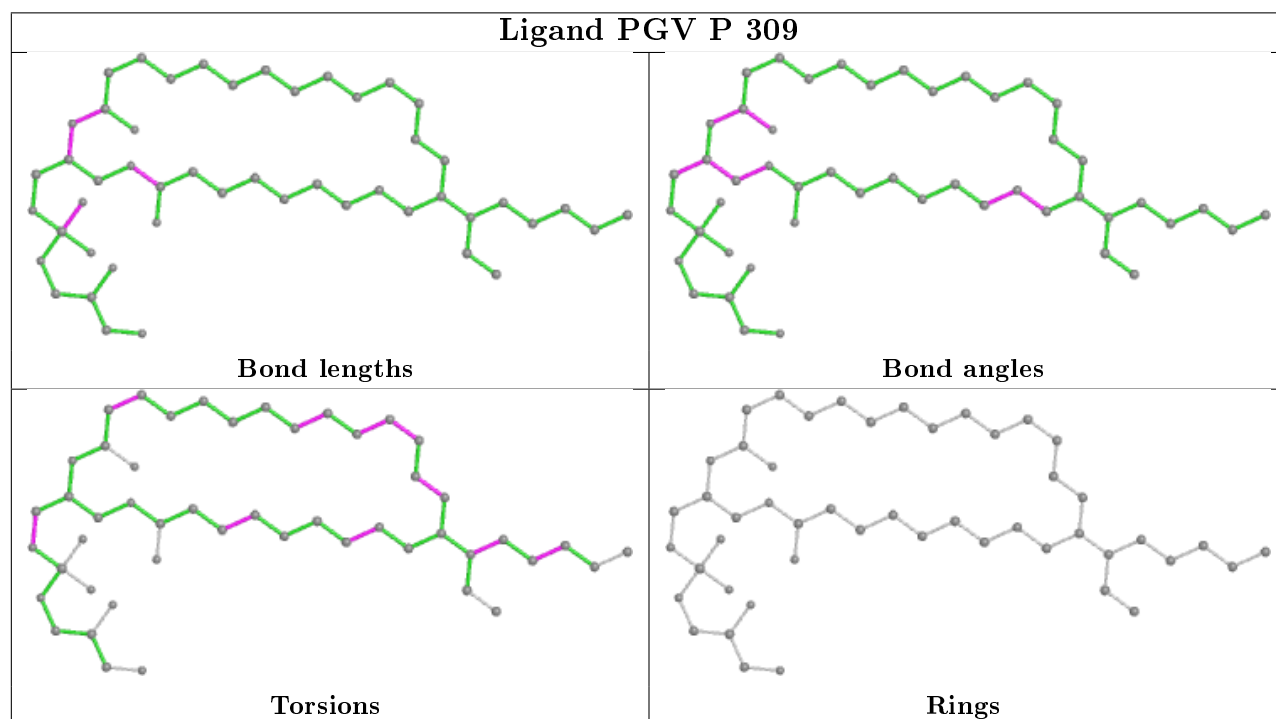
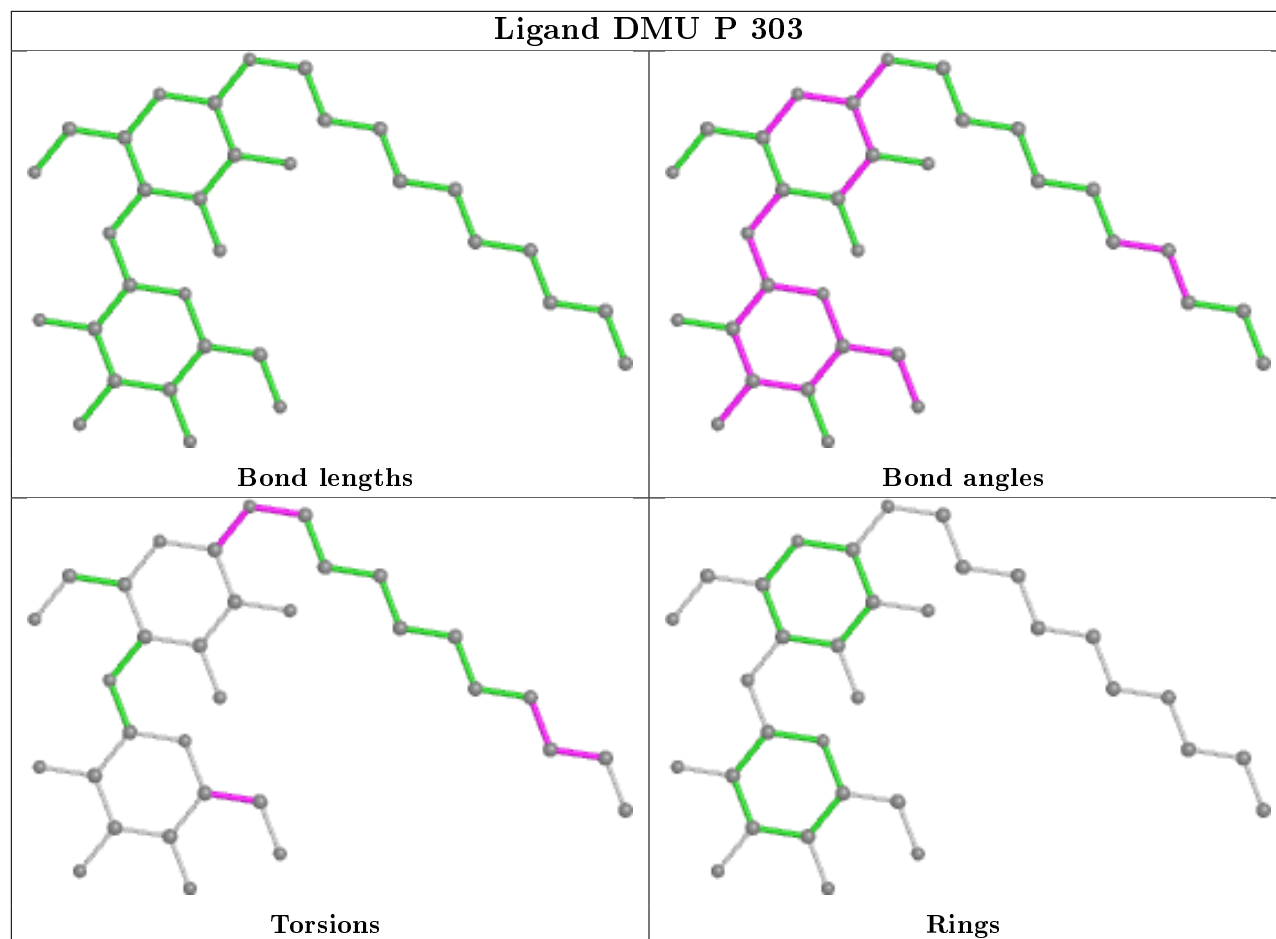


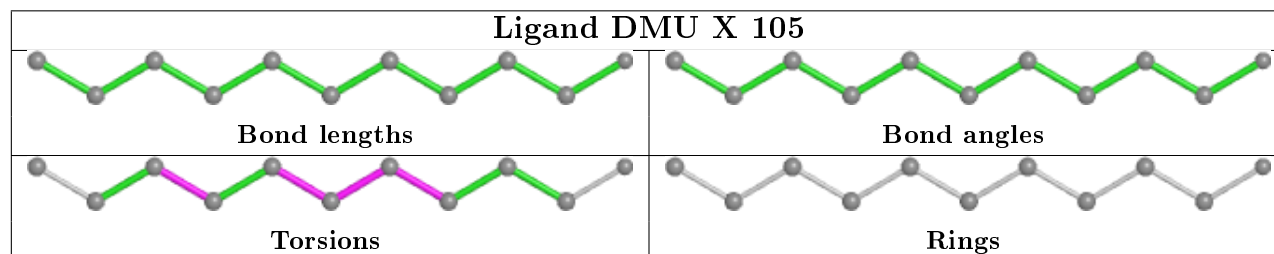
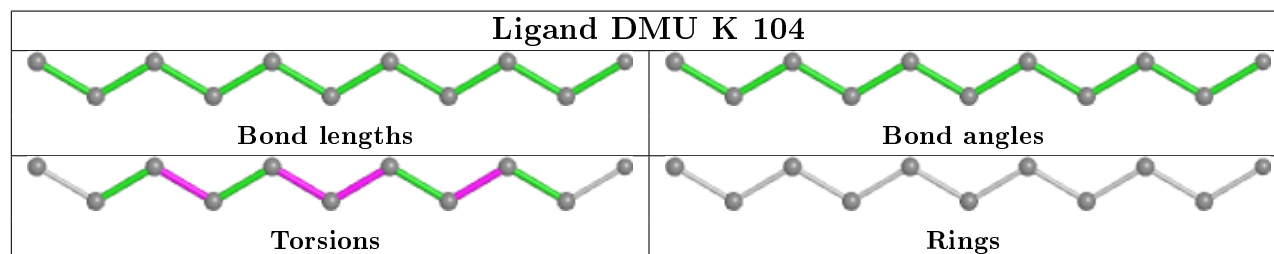
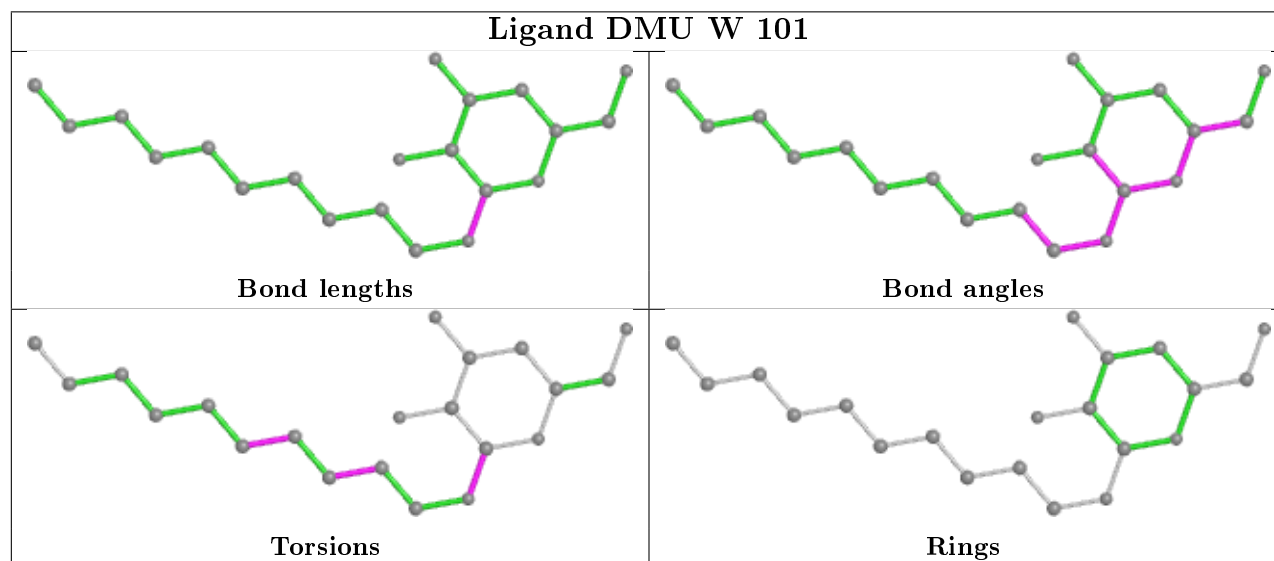
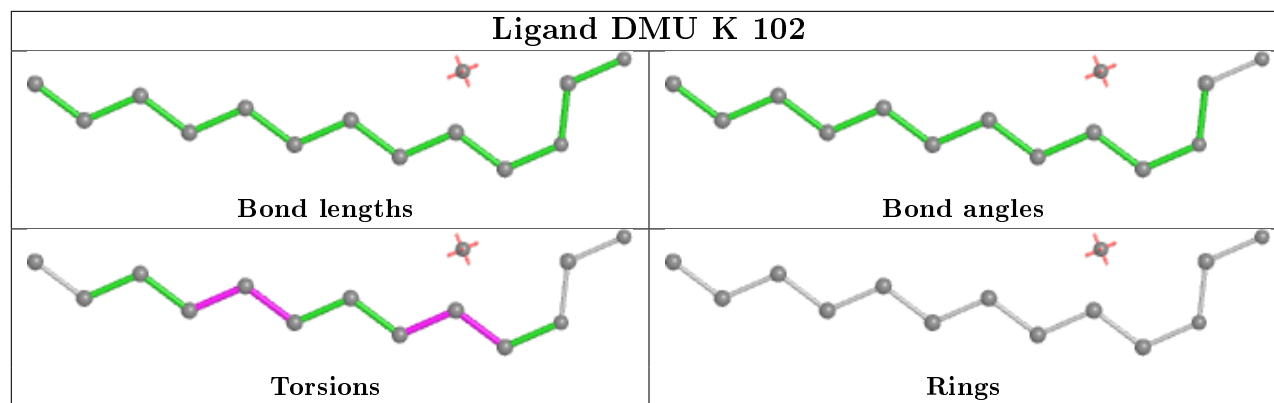


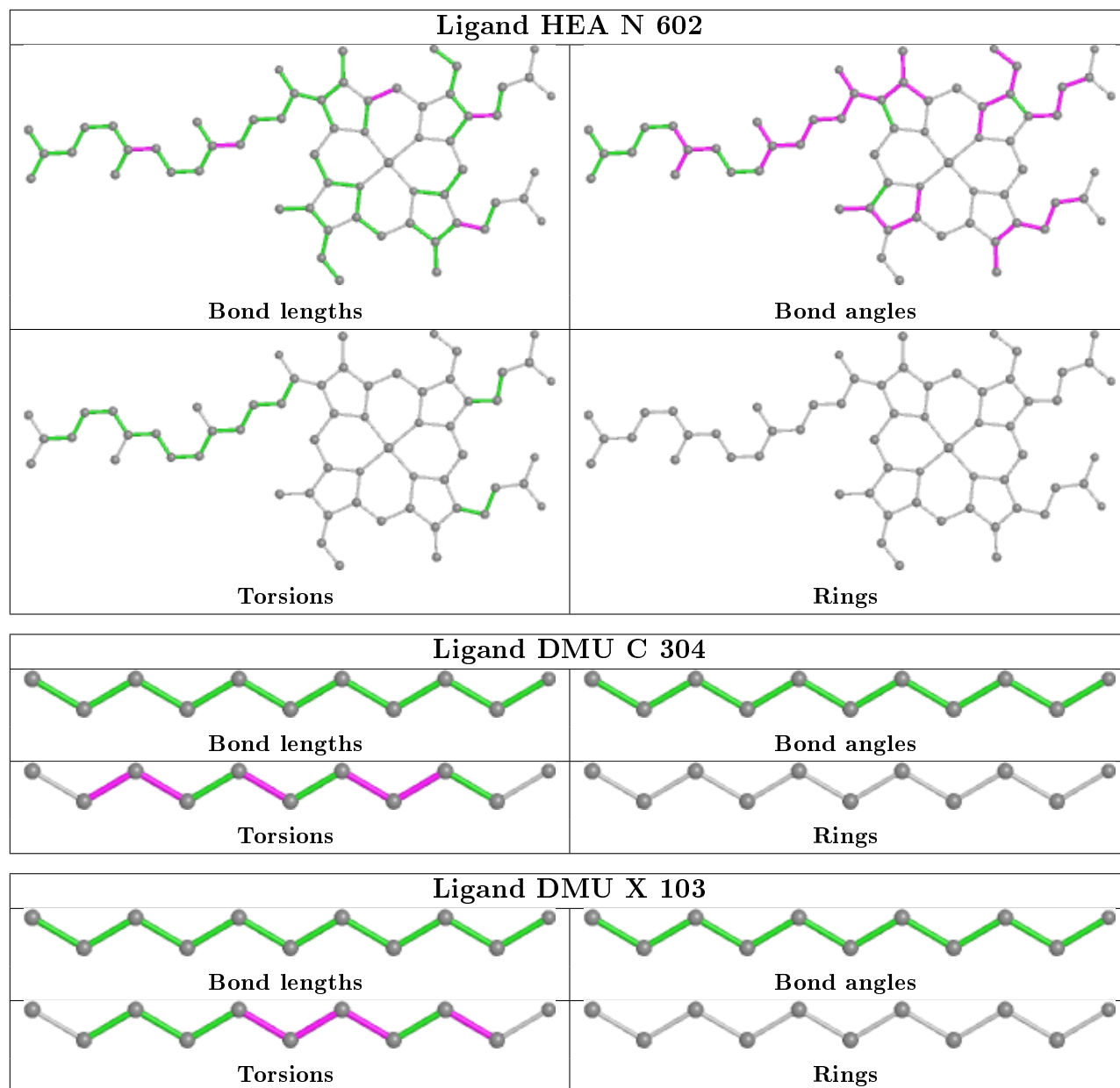


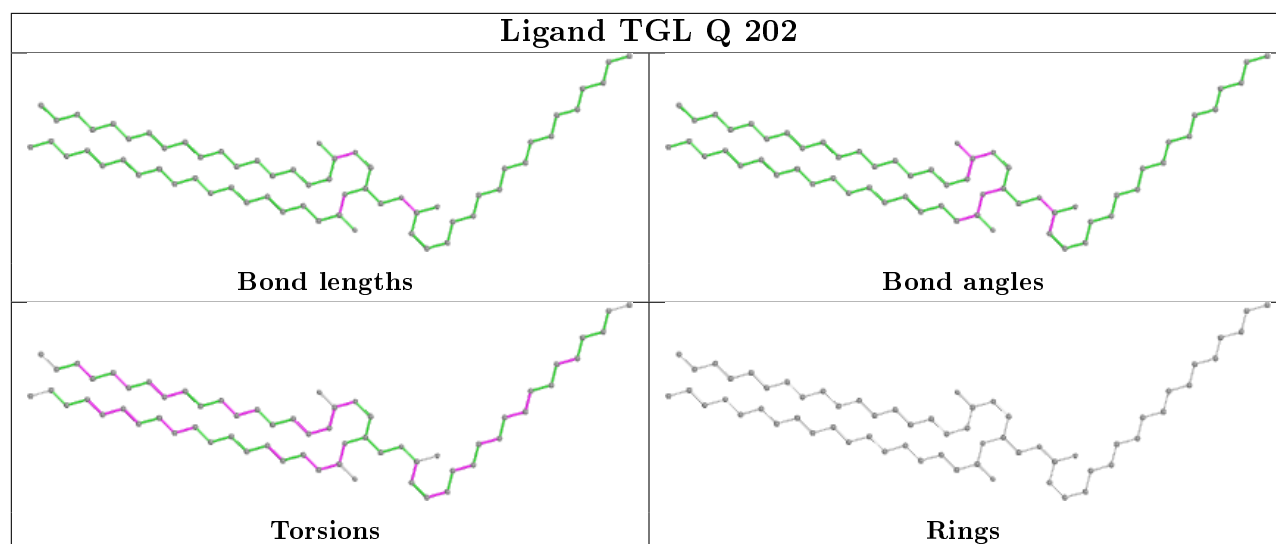
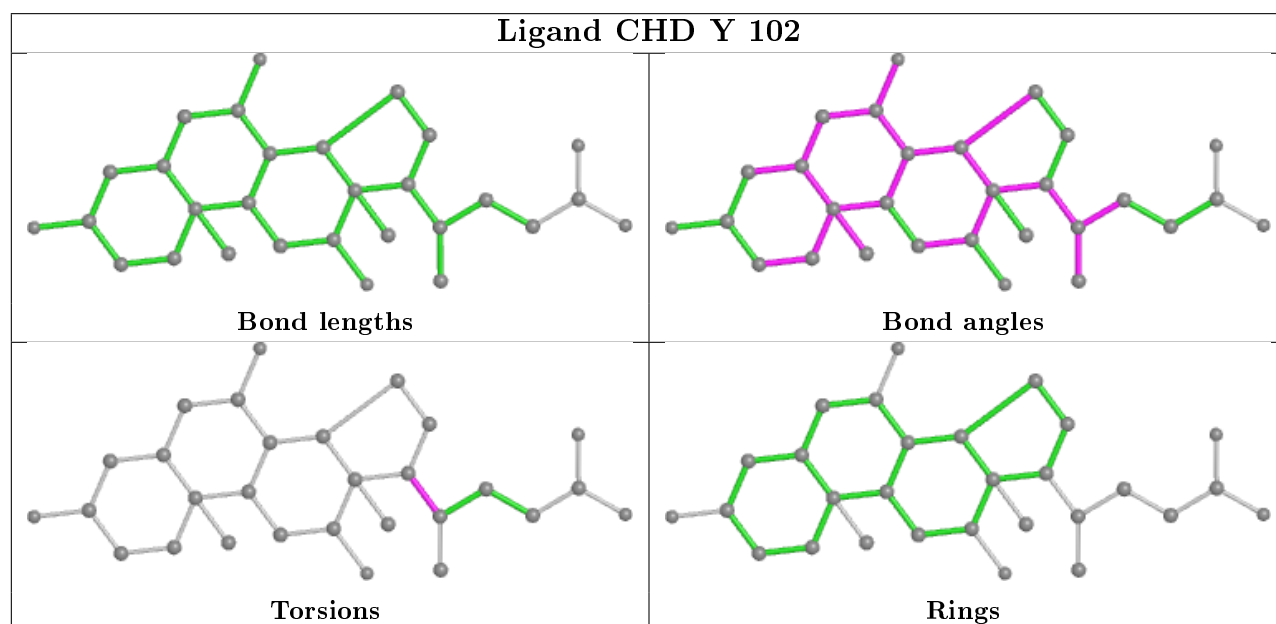
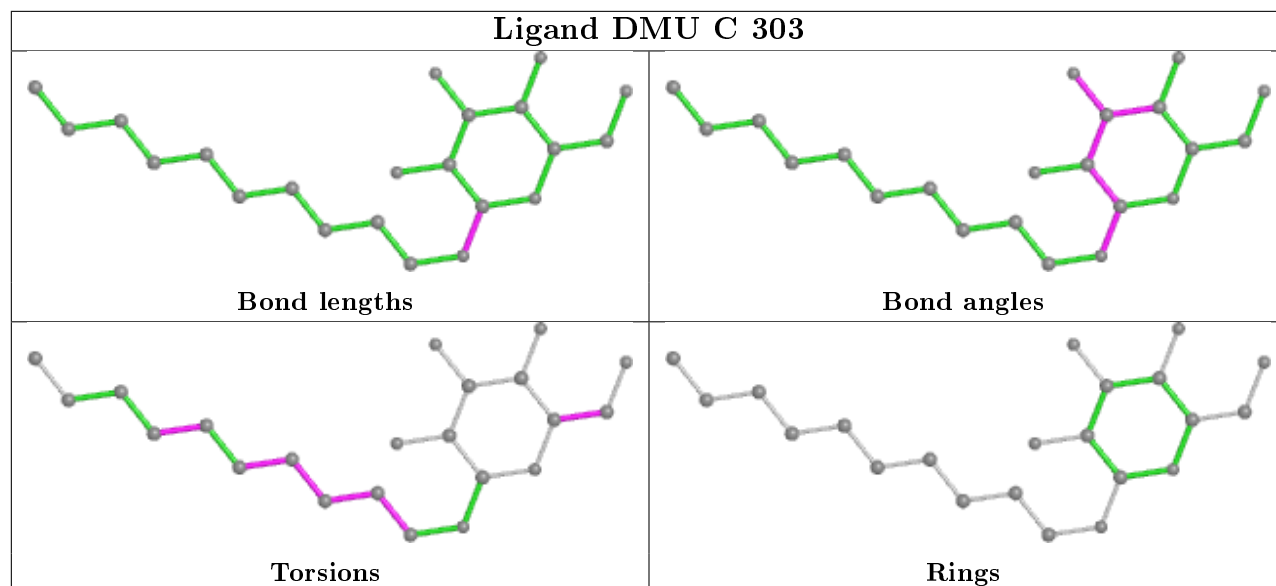


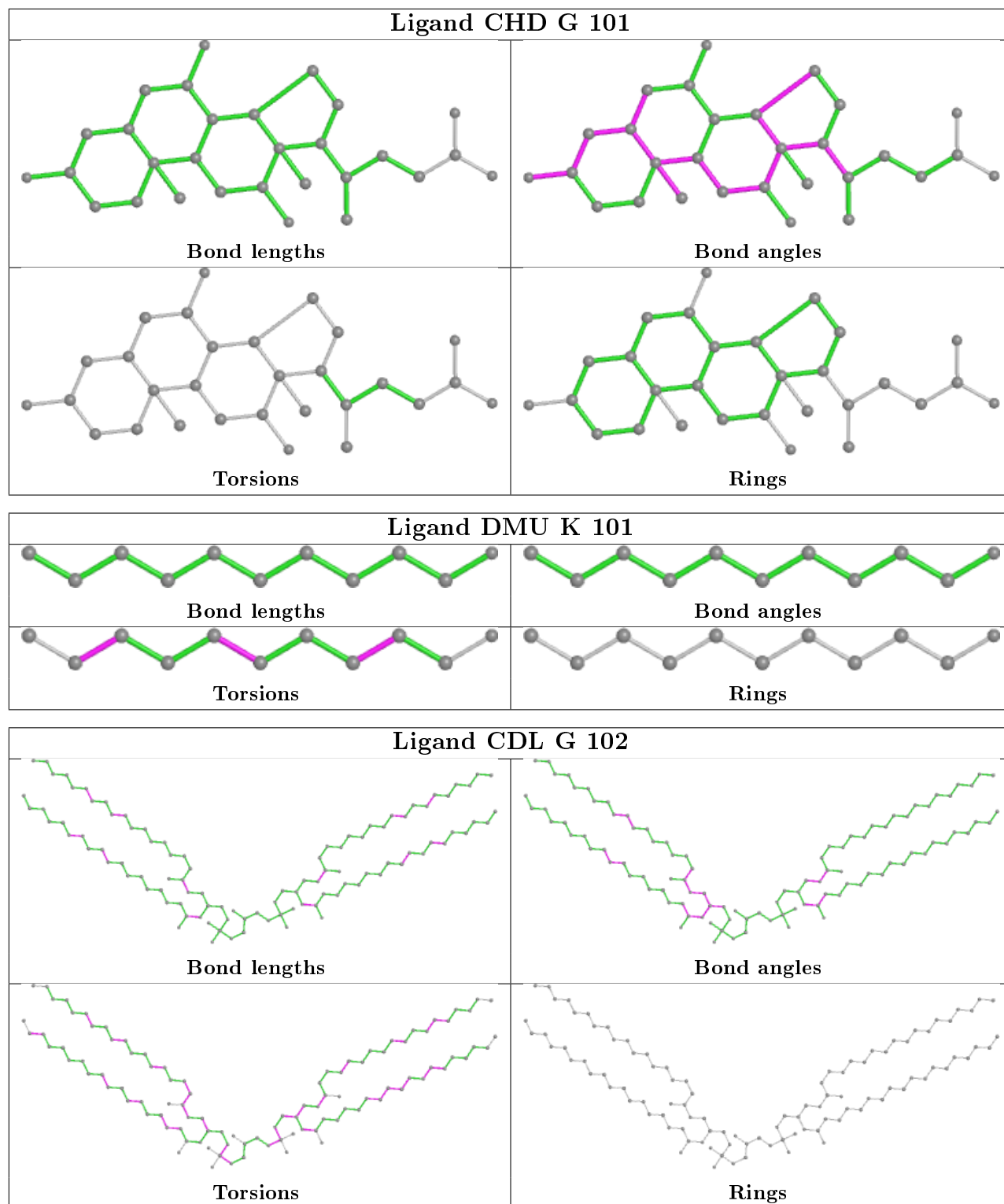


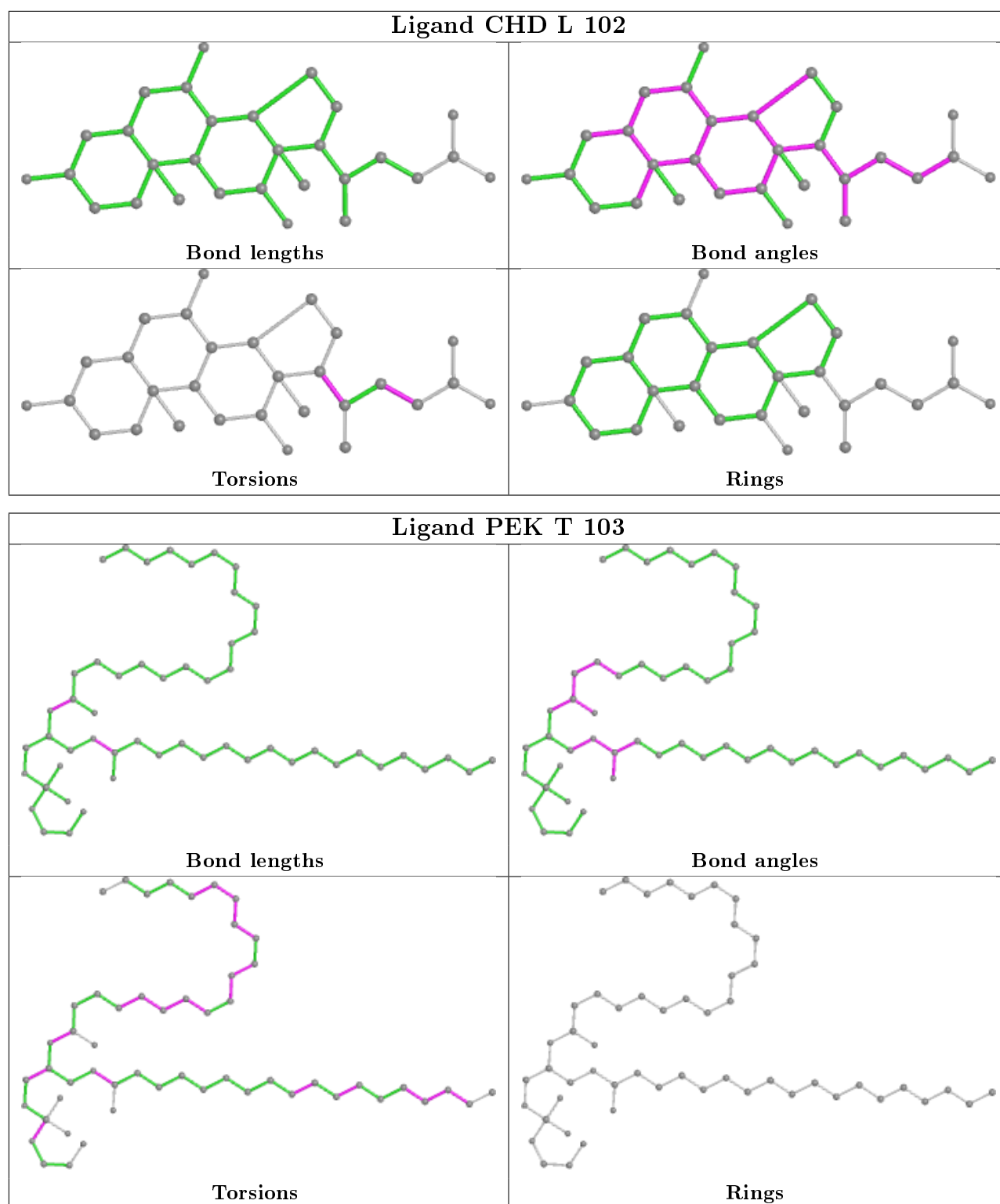


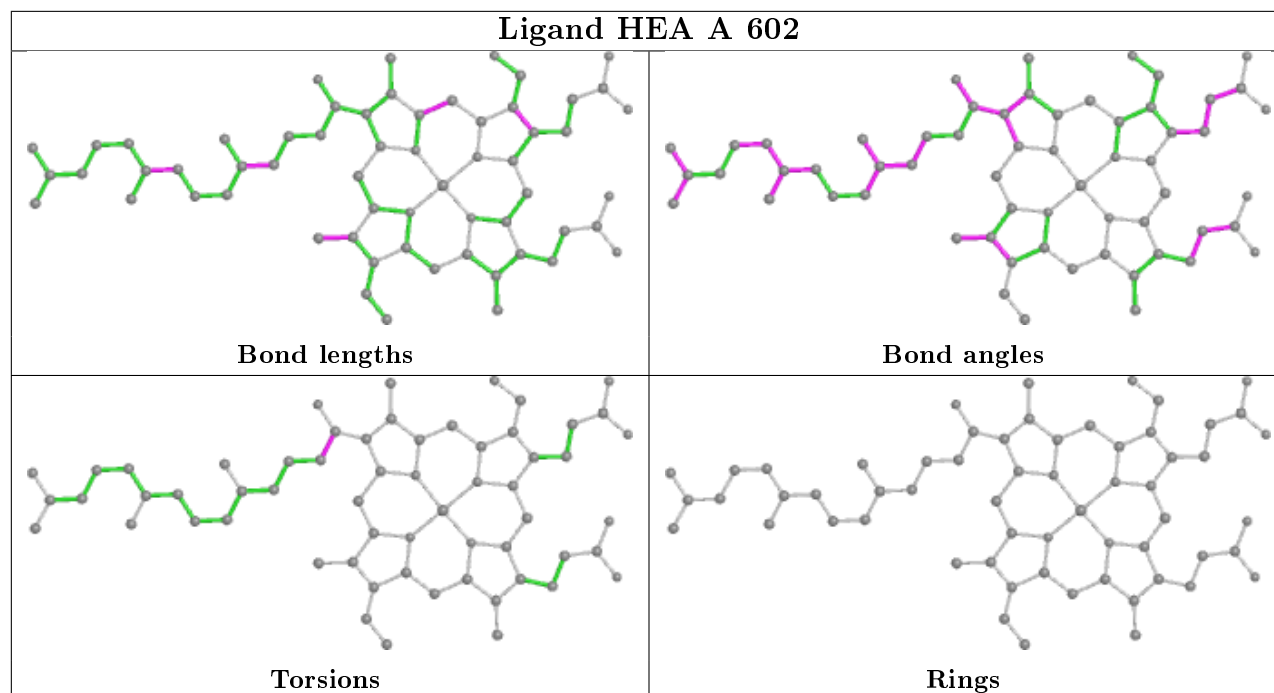












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	513/514 (99%)	-0.04	1 (0%) 95 93	22, 28, 38, 103	0
1	N	513/514 (99%)	-0.16	1 (0%) 95 93	23, 31, 43, 111	0
2	B	226/227 (99%)	-0.13	4 (1%) 68 64	26, 37, 73, 143	0
2	O	226/227 (99%)	-0.15	3 (1%) 77 74	30, 42, 81, 124	0
3	C	259/259 (100%)	-0.09	0 100 100	25, 32, 50, 99	0
3	P	259/259 (100%)	-0.13	0 100 100	26, 33, 55, 94	0
4	D	144/144 (100%)	-0.25	0 100 100	28, 39, 64, 120	0
4	Q	144/144 (100%)	0.47	6 (4%) 36 30	36, 52, 106, 286	0
5	E	105/105 (100%)	-0.27	0 100 100	29, 37, 72, 132	0
5	R	105/105 (100%)	-0.20	2 (1%) 66 63	33, 47, 83, 161	0
6	F	98/98 (100%)	0.28	6 (6%) 21 16	28, 41, 147, 232	0
6	S	98/98 (100%)	0.15	5 (5%) 28 22	29, 42, 130, 198	0
7	G	83/84 (98%)	0.63	13 (15%) 2 1	29, 41, 129, 212	0
7	T	83/84 (98%)	0.72	12 (14%) 2 1	28, 45, 138, 226	0
8	H	79/79 (100%)	0.18	4 (5%) 28 22	33, 45, 118, 155	0
8	U	79/79 (100%)	0.26	4 (5%) 28 22	36, 48, 144, 220	0
9	I	72/73 (98%)	0.07	3 (4%) 36 30	34, 54, 87, 116	0
9	V	72/73 (98%)	0.14	3 (4%) 36 30	34, 61, 104, 191	0
10	J	58/58 (100%)	0.03	2 (3%) 45 39	31, 43, 94, 131	0
10	W	58/58 (100%)	0.09	4 (6%) 16 13	33, 47, 94, 161	0
11	K	49/49 (100%)	-0.18	0 100 100	35, 43, 67, 78	0
11	X	49/49 (100%)	-0.12	0 100 100	43, 54, 93, 113	0
12	L	46/46 (100%)	-0.09	0 100 100	29, 33, 62, 118	0
12	Y	46/46 (100%)	-0.16	1 (2%) 62 57	34, 42, 87, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.05	2 (4%) 31 25	29, 34, 83, 143	0
13	Z	43/43 (100%)	0.11	3 (6%) 16 13	40, 46, 123, 185	0
All	All	3550/3558 (99%)	-0.01	79 (2%) 62 57	22, 37, 85, 286	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	21.7
4	Q	6	VAL	19.2
4	Q	4	SER	16.8
4	Q	8	SER	15.6
7	T	8	HIS	14.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
9	SAC	V	1	9/10	0.45	0.62	210,249,270,285	0
7	TPO	G	11	11/12	0.63	0.41	137,171,213,223	0
7	TPO	T	11	11/12	0.81	0.31	124,161,188,220	0
9	SAC	I	1	9/10	0.82	0.20	131,136,147,157	0
1	FME	N	1	10/11	0.96	0.11	38,54,95,119	0
1	FME	A	1	10/11	0.96	0.13	39,52,94,106	0
2	FME	O	1	10/11	0.98	0.10	35,40,46,125	0
2	FME	B	1	10/11	0.98	0.10	32,35,43,114	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
22	EDO	Q	205	4/4	0.48	0.27	67,78,84,107	0
18	DMU	X	105	11/33	0.58	0.38	80,95,123,124	0
18	DMU	K	104	11/33	0.62	0.39	73,94,107,107	0
18	DMU	Q	201	23/33	0.67	0.35	52,92,138,154	0
22	EDO	C	316	4/4	0.67	0.22	52,60,77,128	0
18	DMU	K	103	22/33	0.68	0.54	66,110,139,152	0
22	EDO	S	103	4/4	0.71	0.19	61,71,80,83	0
22	EDO	P	313	4/4	0.71	0.21	50,57,70,84	0
24	CHD	J	102	29/29	0.73	0.32	61,109,143,153	0
18	DMU	X	103	11/33	0.73	0.25	67,83,110,113	0
22	EDO	P	317	4/4	0.73	0.10	61,66,67,80	0
18	DMU	C	303	22/33	0.74	0.26	53,89,148,160	0
22	EDO	F	110	4/4	0.75	0.22	66,70,80,81	0
25	CDL	T	102	100/100	0.76	0.30	42,103,168,206	0
22	EDO	P	315	4/4	0.76	0.33	41,52,78,113	0
26	PEK	C	308	53/53	0.77	0.31	48,101,182,205	0
24	CHD	Y	102	29/29	0.77	0.35	68,98,143,174	0
18	DMU	C	304	11/33	0.77	0.15	56,65,86,100	0
18	DMU	P	303	33/33	0.77	0.23	49,107,135,152	0
18	DMU	O	302	11/33	0.79	0.15	57,67,89,89	0
18	DMU	Y	101	33/33	0.79	0.26	52,105,145,149	0
22	EDO	D	203	4/4	0.79	0.17	45,66,83,84	0
26	PEK	T	103	53/53	0.79	0.31	49,78,169,233	0
18	DMU	C	302	33/33	0.80	0.25	53,103,152,162	0
20	PSC	A	609	52/52	0.80	0.35	42,101,181,243	0
25	CDL	G	102	100/100	0.80	0.28	51,99,177,197	0
18	DMU	D	201	21/33	0.80	0.21	51,85,132,140	0
26	PEK	P	307	53/53	0.81	0.22	50,74,159,190	0
18	DMU	X	102	21/33	0.81	0.21	68,102,136,151	0
19	PGV	T	104	51/51	0.81	0.26	50,97,182,229	0
19	PGV	P	310	51/51	0.81	0.28	51,97,153,200	0
18	DMU	X	101	11/33	0.81	0.16	48,75,115,125	0
22	EDO	L	104	4/4	0.82	0.34	41,94,96,97	0
24	CHD	L	102	29/29	0.82	0.27	51,91,123,145	0
21	TGL	Q	202	63/63	0.82	0.21	37,73,125,139	0
22	EDO	S	105	4/4	0.83	0.49	73,85,94,103	0
18	DMU	P	302	11/33	0.83	0.14	52,60,93,94	0
26	PEK	F	102	53/53	0.83	0.27	46,79,162,232	0
22	EDO	N	618	4/4	0.83	0.24	41,54,66,72	0
18	DMU	W	101	21/33	0.83	0.33	42,75,111,128	0
25	CDL	P	306	100/100	0.84	0.25	40,100,173,211	0
18	DMU	J	101	21/33	0.84	0.27	32,68,123,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	EDO	M	102	4/4	0.84	0.14	71,76,76,93	0
22	EDO	C	314	4/4	0.84	0.16	41,45,49,59	0
21	TGL	Y	103	63/63	0.84	0.23	39,73,128,179	0
22	EDO	C	311	4/4	0.84	0.35	35,61,78,103	0
20	PSC	V	101	52/52	0.85	0.29	43,92,191,241	0
21	TGL	D	202	63/63	0.85	0.18	34,68,120,140	0
24	CHD	P	305	29/29	0.85	0.17	59,75,113,132	0
22	EDO	T	105	4/4	0.86	0.23	58,81,89,108	0
22	EDO	E	203	4/4	0.86	0.47	67,79,81,82	0
22	EDO	A	613	4/4	0.86	0.19	39,40,46,80	0
18	DMU	K	101	11/33	0.86	0.15	47,70,93,99	0
22	EDO	P	314	4/4	0.86	0.21	46,48,65,82	0
25	CDL	C	307	100/100	0.86	0.20	39,85,148,175	0
21	TGL	N	608	63/63	0.86	0.15	48,70,116,129	0
18	DMU	X	104	11/33	0.87	0.30	56,71,105,109	0
22	EDO	N	616	4/4	0.87	0.11	49,54,55,66	0
22	EDO	Q	203	4/4	0.87	0.27	78,86,87,105	0
18	DMU	K	102	14/33	0.87	0.19	60,80,119,123	0
22	EDO	N	611	4/4	0.87	0.17	37,37,43,56	0
22	EDO	A	619	4/4	0.87	0.25	59,67,69,89	0
18	DMU	L	101	33/33	0.87	0.22	49,102,136,160	0
22	EDO	C	317	4/4	0.87	0.28	45,73,80,84	0
18	DMU	Z	101	33/33	0.87	0.12	44,58,89,96	0
18	DMU	B	302	11/33	0.87	0.24	61,78,97,105	0
19	PGV	A	607	51/51	0.87	0.22	31,70,159,167	0
24	CHD	C	306	29/29	0.88	0.16	51,80,118,135	0
21	TGL	A	610	63/63	0.88	0.14	36,73,112,133	0
19	PGV	N	606	51/51	0.88	0.27	41,94,148,194	0
22	EDO	N	623	4/4	0.88	0.19	67,76,79,96	0
22	EDO	D	206	4/4	0.88	0.41	46,59,99,113	0
22	EDO	F	109	4/4	0.88	0.18	53,57,67,98	0
24	CHD	C	305	29/29	0.89	0.12	35,42,60,67	0
21	TGL	L	103	63/63	0.89	0.18	29,63,125,169	0
22	EDO	A	618	4/4	0.89	0.13	38,57,68,73	0
22	EDO	N	620	4/4	0.89	0.21	45,56,92,96	0
22	EDO	N	615	4/4	0.90	0.26	40,56,59,88	0
18	DMU	A	606	13/33	0.90	0.19	43,67,113,117	0
22	EDO	U	102	4/4	0.90	0.25	42,53,67,72	0
22	EDO	L	105	4/4	0.90	0.11	56,59,64,85	0
22	EDO	C	312	4/4	0.90	0.09	38,46,49,49	0
22	EDO	F	107	4/4	0.90	0.25	54,60,63,83	0
22	EDO	O	304	4/4	0.90	0.18	56,64,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	EDO	B	307	4/4	0.91	0.14	36,57,74,101	0
22	EDO	D	204	4/4	0.91	0.13	54,55,56,95	0
22	EDO	B	306	4/4	0.91	0.12	35,46,51,94	0
22	EDO	W	102	4/4	0.92	0.20	53,80,80,128	0
24	CHD	P	304	29/29	0.92	0.11	34,44,64,70	0
22	EDO	F	106	4/4	0.92	0.10	43,43,53,54	0
22	EDO	T	106	4/4	0.92	0.16	38,40,45,52	0
18	DMU	M	101	33/33	0.93	0.12	36,46,68,80	0
22	EDO	F	108	4/4	0.93	0.31	74,76,86,88	0
22	EDO	A	611	4/4	0.93	0.18	37,41,41,94	0
22	EDO	N	619	4/4	0.93	0.30	49,65,71,83	0
22	EDO	N	612	4/4	0.93	0.21	40,55,59,61	0
22	EDO	B	304	4/4	0.93	0.15	59,73,85,88	0
22	EDO	Y	104	4/4	0.93	0.29	56,71,73,83	0
22	EDO	N	613	4/4	0.93	0.24	52,55,73,74	0
22	EDO	N	617	4/4	0.93	0.19	48,48,58,79	0
22	EDO	P	316	4/4	0.94	0.17	32,52,92,94	0
22	EDO	A	617	4/4	0.94	0.66	49,69,96,141	0
22	EDO	N	622	4/4	0.94	0.24	29,50,67,70	0
22	EDO	D	207	4/4	0.94	0.20	42,70,72,108	0
28	PO4	U	101	5/5	0.94	0.16	59,65,141,151	0
22	EDO	J	103	4/4	0.94	0.19	44,70,75,83	0
22	EDO	H	102	4/4	0.94	0.23	41,41,57,84	0
22	EDO	A	615	4/4	0.95	0.23	30,61,69,139	0
22	EDO	S	106	4/4	0.95	0.16	38,45,59,63	0
22	EDO	Q	204	4/4	0.95	0.20	35,64,73,77	0
22	EDO	A	612	4/4	0.95	0.12	24,28,31,31	0
22	EDO	F	104	4/4	0.95	0.28	60,66,79,83	0
22	EDO	G	103	4/4	0.95	0.08	31,37,40,44	0
22	EDO	D	205	4/4	0.95	0.18	53,58,60,87	0
28	PO4	H	101	5/5	0.95	0.19	63,70,118,149	0
22	EDO	P	312	4/4	0.96	0.13	37,43,47,68	0
22	EDO	S	102	4/4	0.96	0.11	33,33,35,39	0
22	EDO	B	305	4/4	0.96	0.16	44,56,58,76	0
26	PEK	P	308	53/53	0.96	0.12	31,50,93,125	0
22	EDO	F	105	4/4	0.96	0.20	36,39,40,42	0
22	EDO	N	621	4/4	0.96	0.17	37,47,53,79	0
24	CHD	G	101	29/29	0.96	0.09	27,32,38,49	0
22	EDO	P	311	4/4	0.96	0.22	40,46,48,56	0
22	EDO	S	104	4/4	0.96	0.10	32,35,38,42	0
22	EDO	A	616	4/4	0.96	0.17	48,53,72,112	0
22	EDO	C	315	4/4	0.96	0.25	51,65,79,108	0

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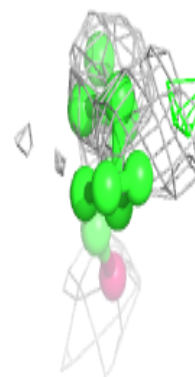
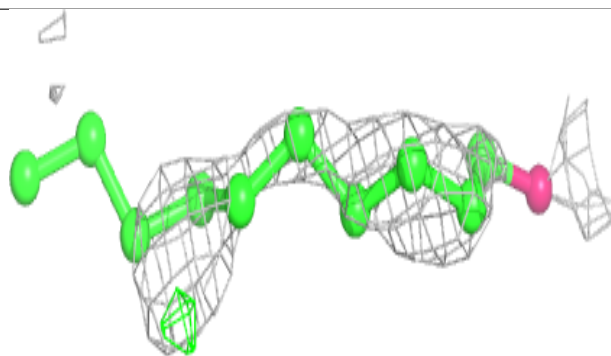
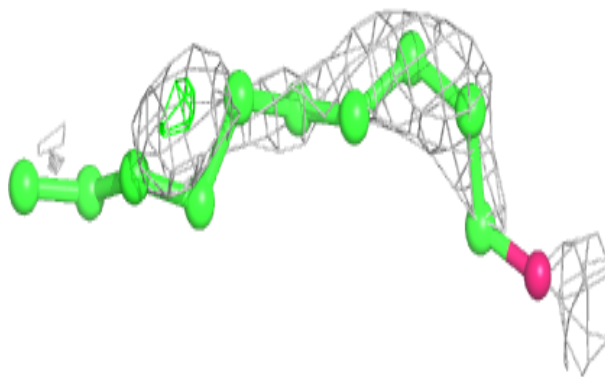
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	EDO	O	303	4/4	0.96	0.10	33,35,37,38	0
24	CHD	T	101	29/29	0.96	0.09	28,33,41,65	0
26	PEK	C	309	53/53	0.96	0.13	31,48,111,119	0
19	PGV	P	309	51/51	0.97	0.12	26,37,83,126	0
19	PGV	N	607	51/51	0.97	0.12	26,38,64,78	0
27	ZN	S	101	1/1	0.97	0.19	55,55,55,55	0
19	PGV	A	608	51/51	0.97	0.12	26,33,69,92	0
22	EDO	N	610	4/4	0.97	0.25	33,57,77,86	0
22	EDO	E	202	4/4	0.97	0.08	37,40,47,53	0
27	ZN	F	101	1/1	0.97	0.17	55,55,55,55	0
19	PGV	C	310	51/51	0.97	0.12	26,33,93,120	0
22	EDO	N	609	4/4	0.97	0.15	29,32,35,37	0
22	EDO	C	313	4/4	0.97	0.17	34,41,56,57	0
14	HEA	A	602	60/60	0.97	0.11	22,27,38,47	0
14	HEA	N	601[B]	60/60	0.98	0.12	24,30,48,56	12
16	MG	A	604	1/1	0.98	0.07	29,29,29,29	0
17	NA	N	605	1/1	0.98	0.07	34,34,34,34	0
14	HEA	A	601[A]	60/60	0.98	0.11	20,24,41,51	12
22	EDO	E	201	4/4	0.98	0.10	44,47,50,56	0
17	NA	P	301	1/1	0.98	0.26	22,22,22,22	0
14	HEA	N	602	60/60	0.98	0.10	24,28,33,47	0
22	EDO	B	303	4/4	0.98	0.11	30,31,32,40	0
15	CU	N	603	1/1	0.98	0.15	30,30,30,30	0
14	HEA	A	601[B]	60/60	0.98	0.11	20,24,41,51	12
14	HEA	N	601[A]	60/60	0.98	0.12	23,30,48,53	12
22	EDO	N	614	4/4	0.98	0.23	38,45,67,71	0
22	EDO	F	103	4/4	0.98	0.12	31,35,37,40	0
22	EDO	A	614	4/4	0.98	0.12	36,57,62,82	0
17	NA	A	605	1/1	0.99	0.08	29,29,29,29	0
17	NA	C	301	1/1	0.99	0.24	22,22,22,22	0
16	MG	N	604	1/1	0.99	0.05	31,31,31,31	0
23	CUA	O	301	2/2	0.99	0.14	32,32,32,33	0
15	CU	A	603	1/1	1.00	0.13	29,29,29,29	0
23	CUA	B	301	2/2	1.00	0.16	28,28,28,29	0

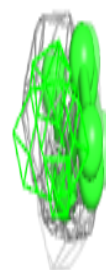
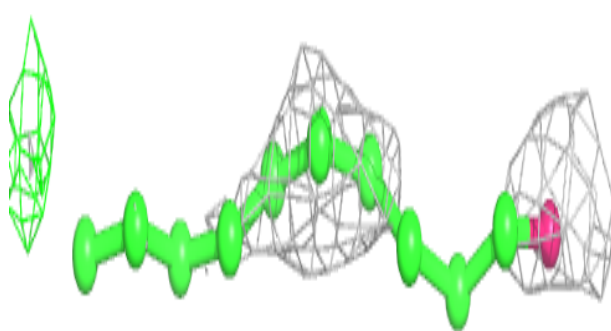
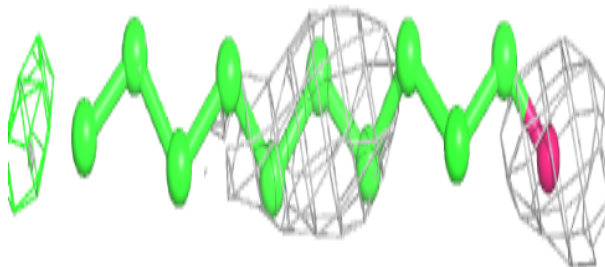
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU X 105:

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

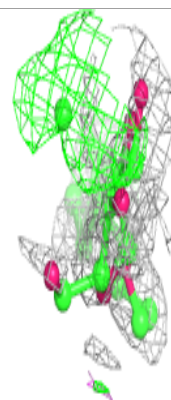
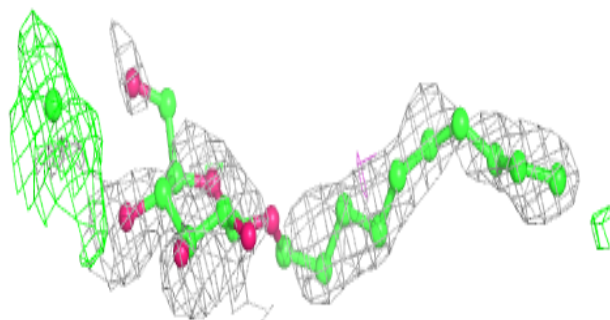
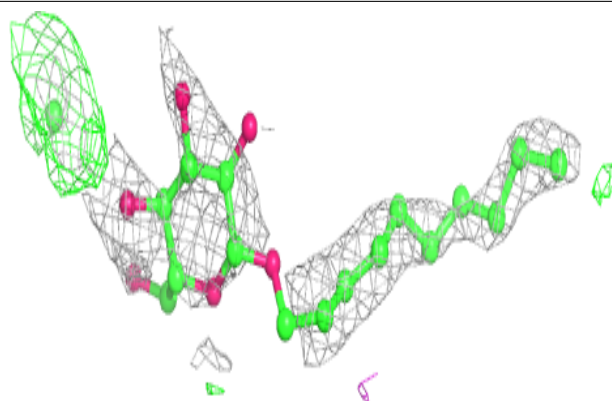
**Electron density around DMU K 104:**

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

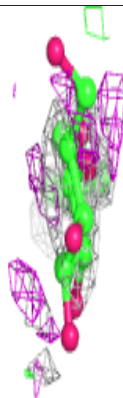
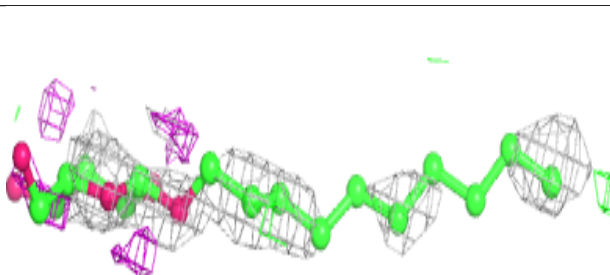
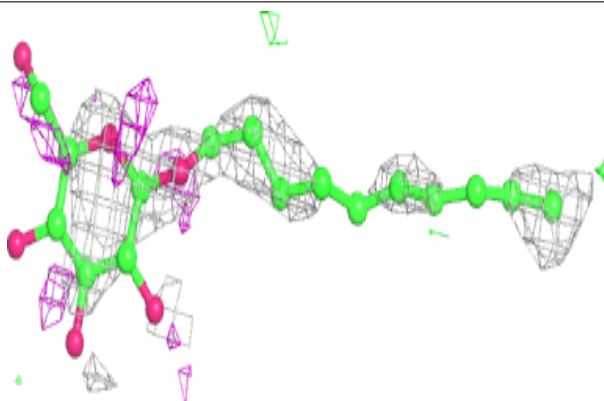


Electron density around DMU Q 201:

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

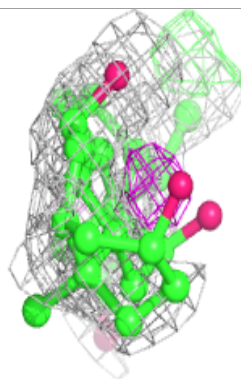
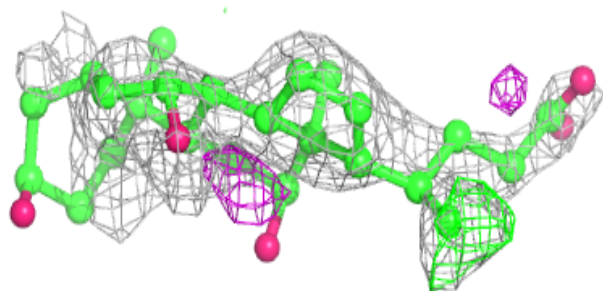
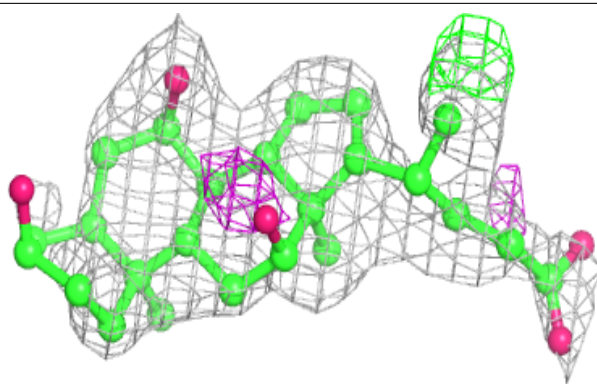
**Electron density around DMU K 103:**

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

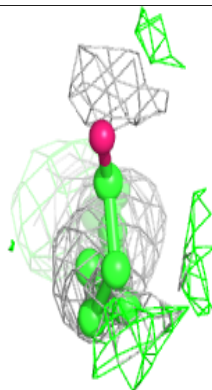
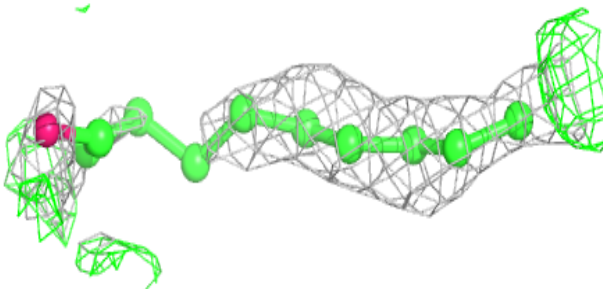
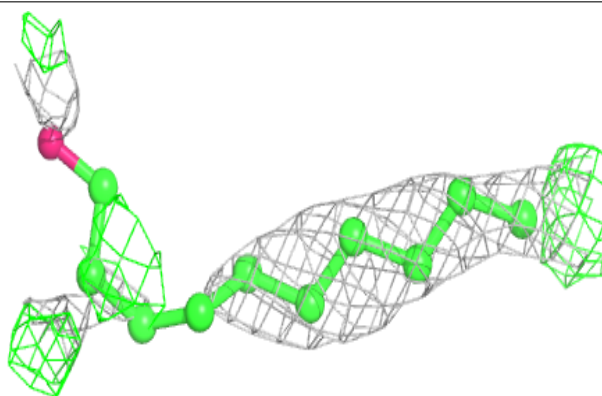


Electron density around CHD J 102:

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

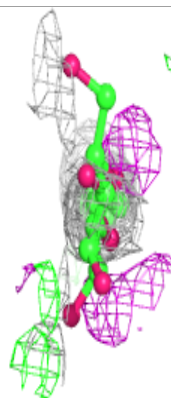
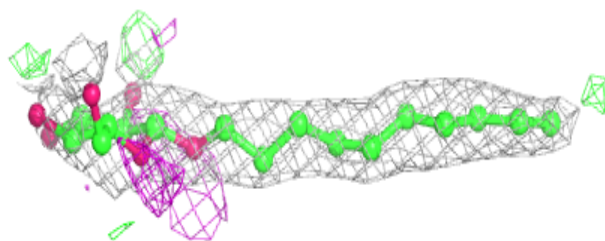
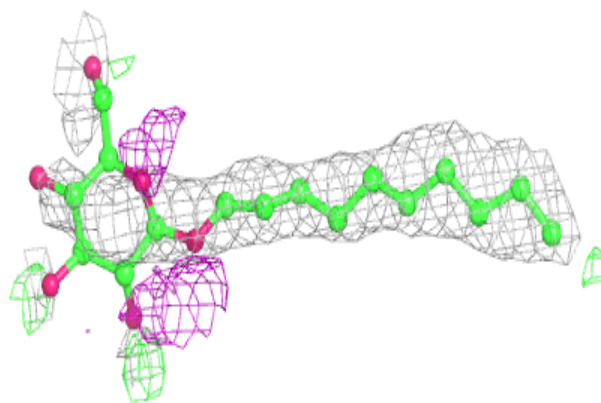
**Electron density around DMU X 103:**

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

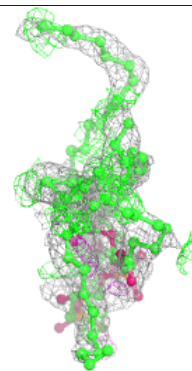
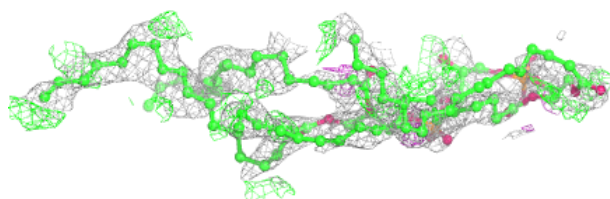
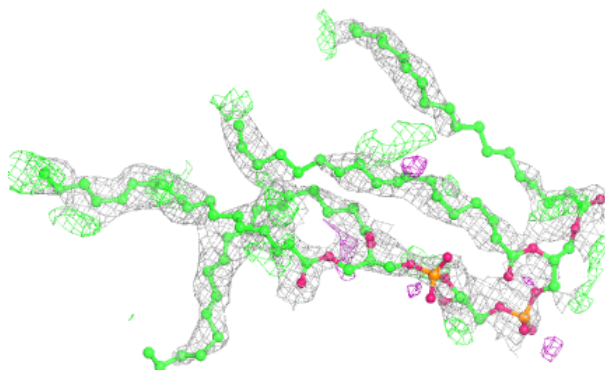


Electron density around DMU C 303:

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

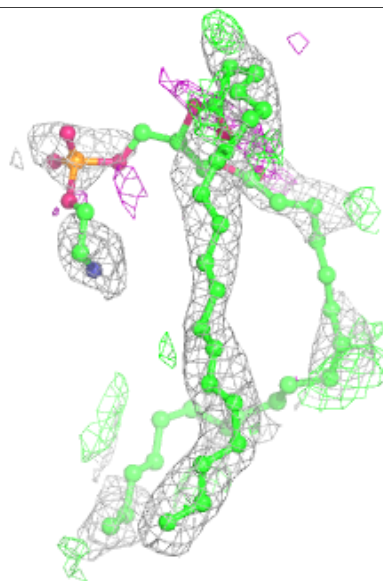
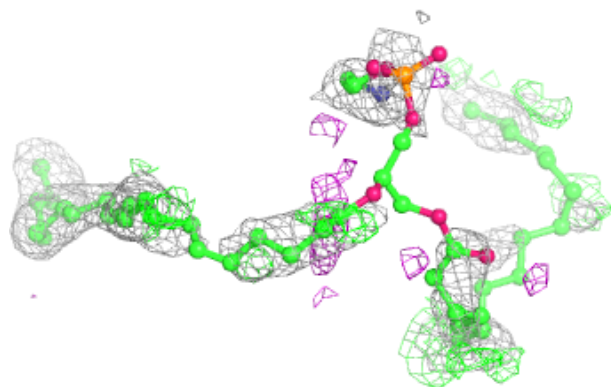
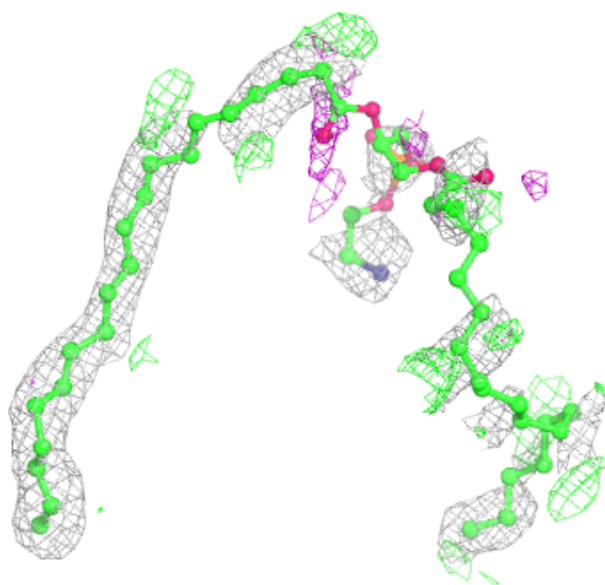
**Electron density around CDL T 102:**

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



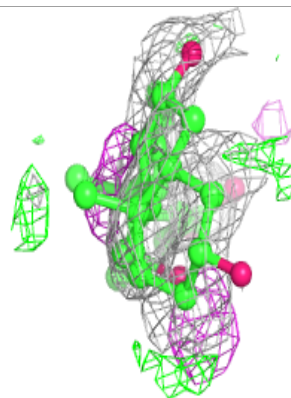
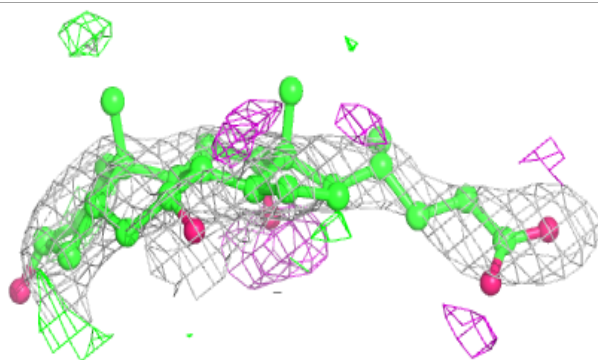
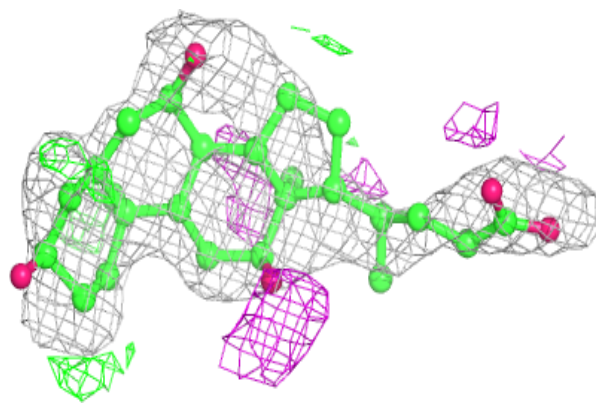
Electron density around PEK C 308:

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

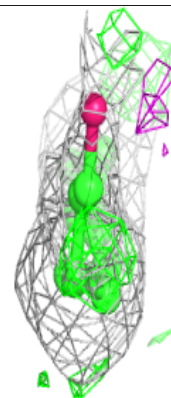
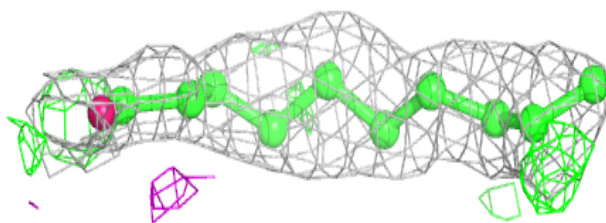
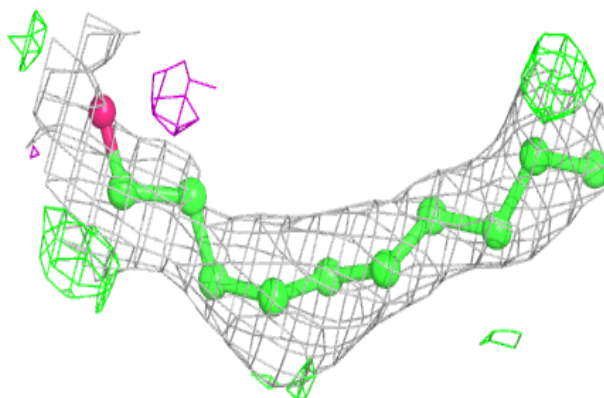


Electron density around CHD Y 102:

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

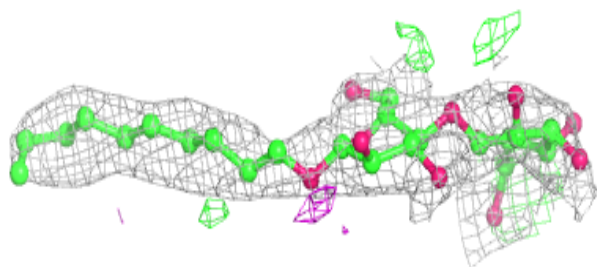
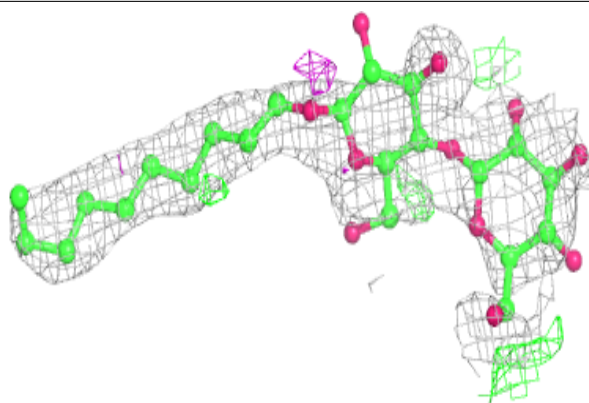
**Electron density around DMU C 304:**

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

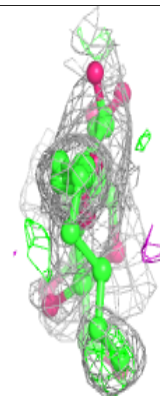
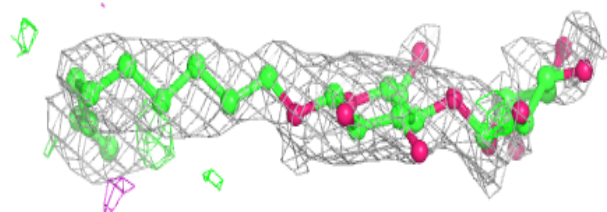
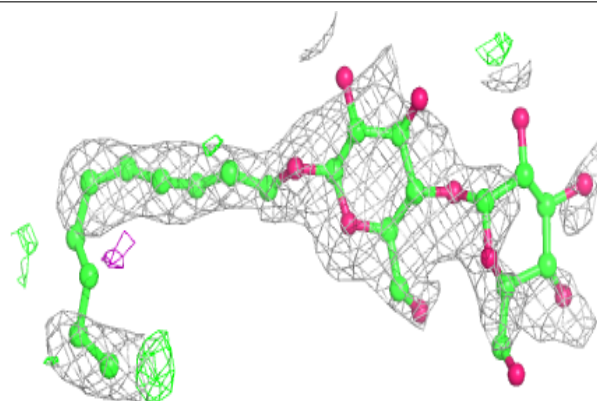


Electron density around DMU P 303:

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

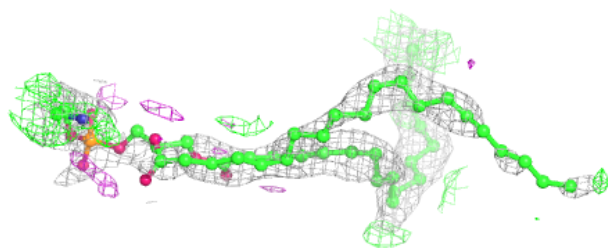
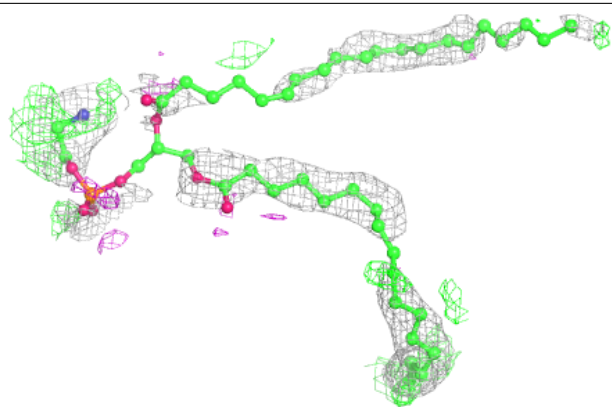
**Electron density around DMU Y 101:**

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

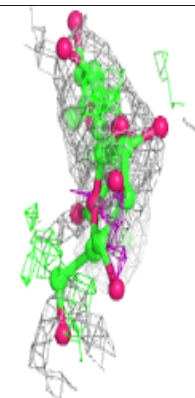
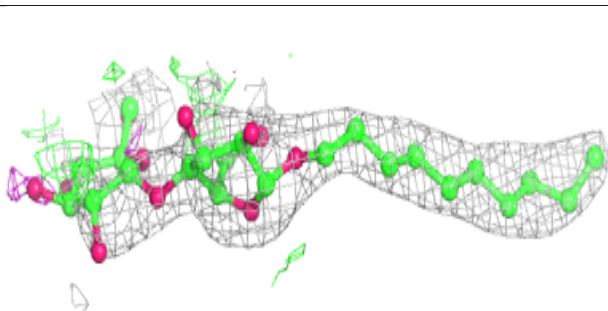
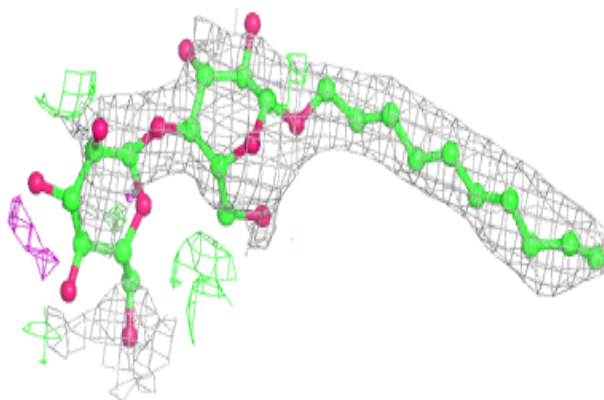


Electron density around PEK T 103:

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

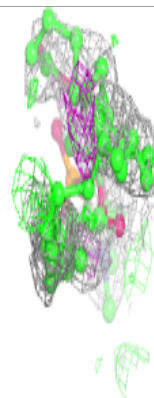
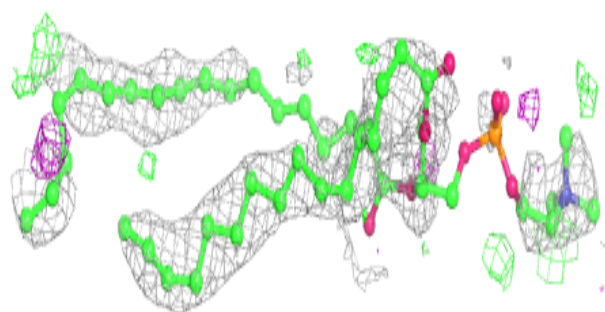
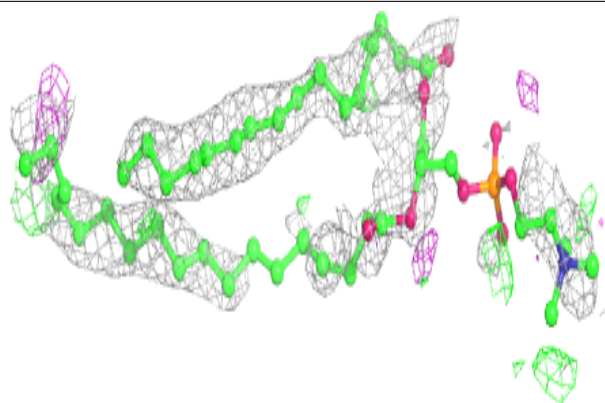
**Electron density around DMU C 302:**

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

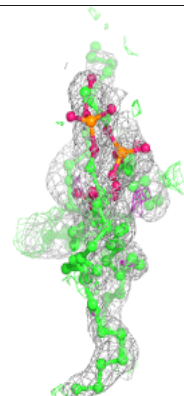
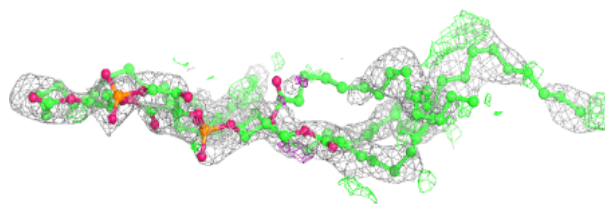
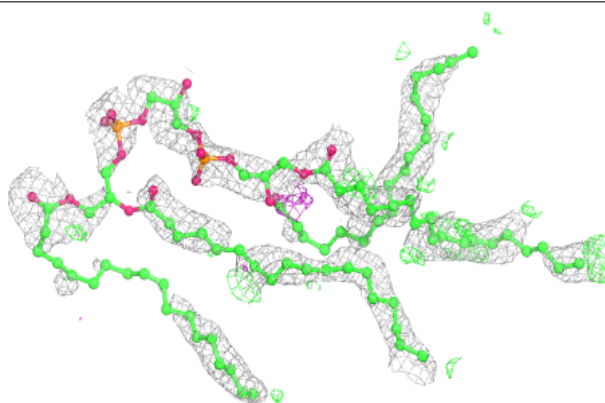


Electron density around PSC A 609:

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

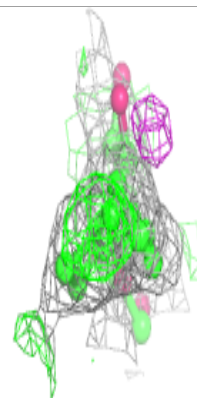
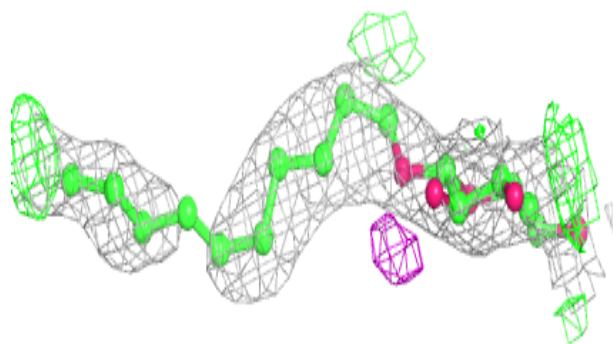
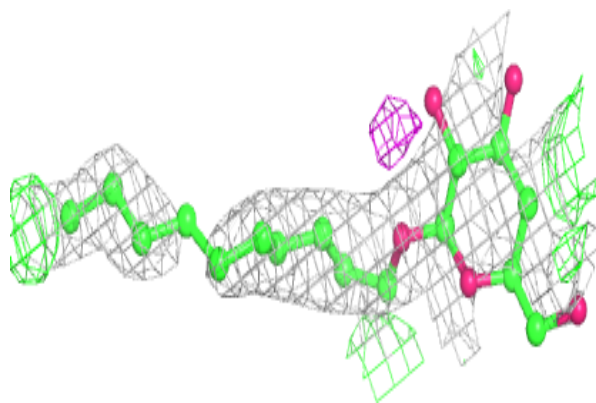
**Electron density around CDL G 102:**

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

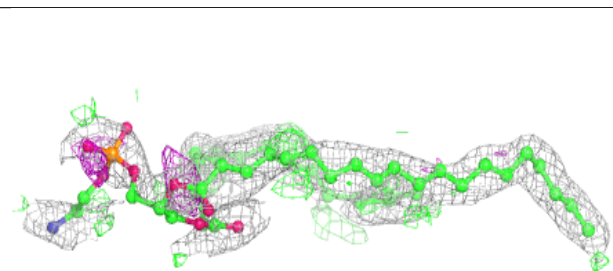
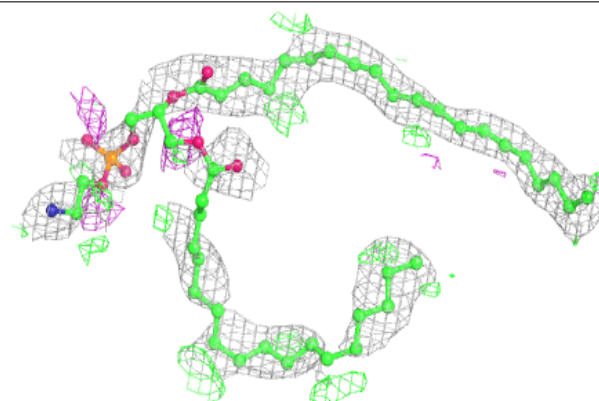


Electron density around DMU D 201:

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

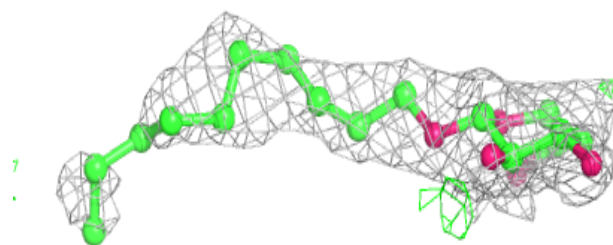
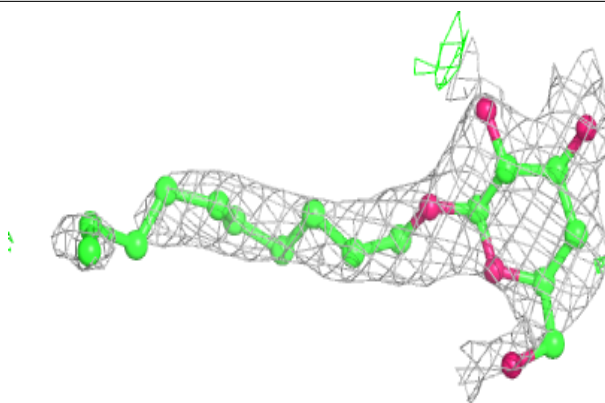
**Electron density around PEK P 307:**

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

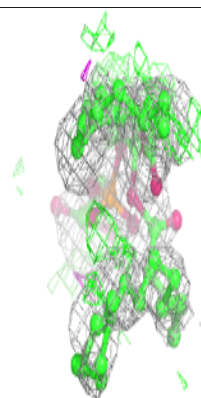
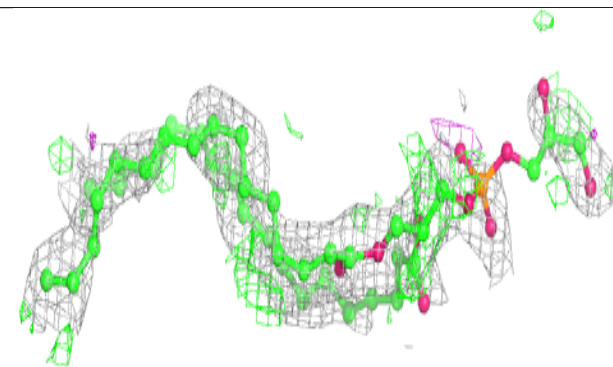
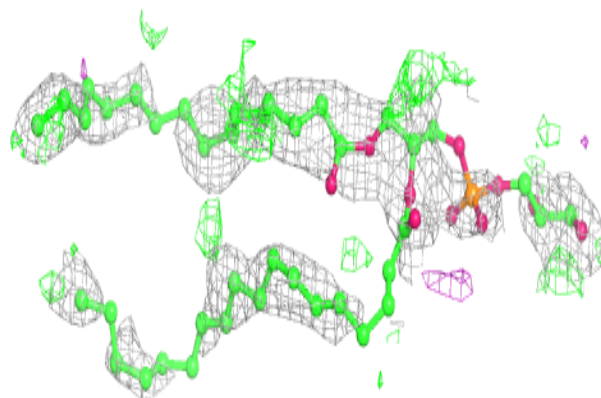


Electron density around DMU X 102:

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

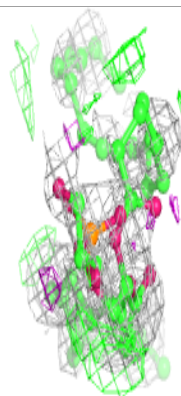
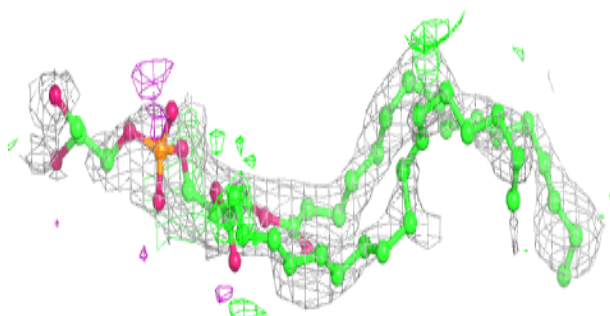
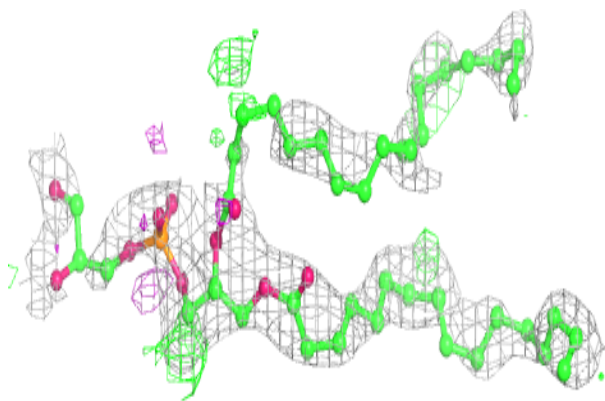
**Electron density around PGV T 104:**

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

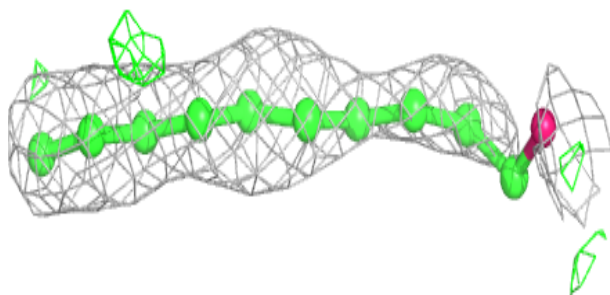
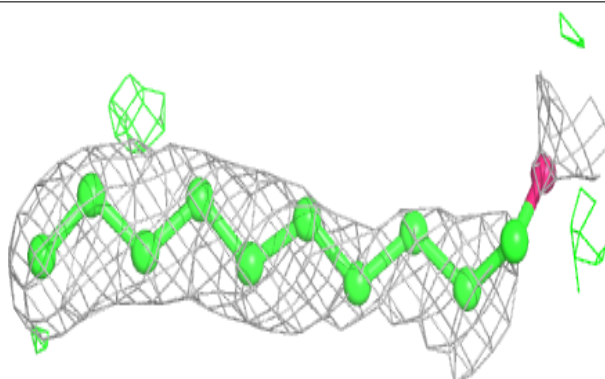


Electron density around PGV P 310:

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

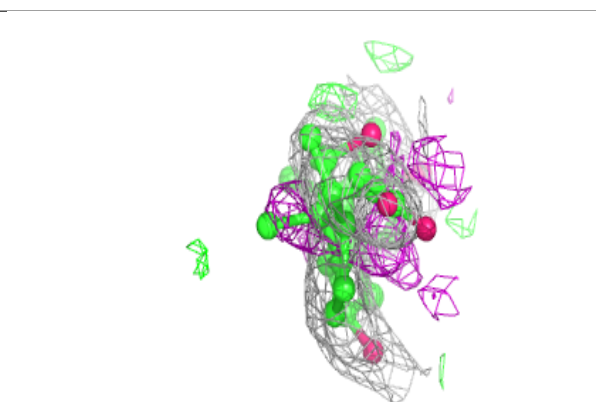
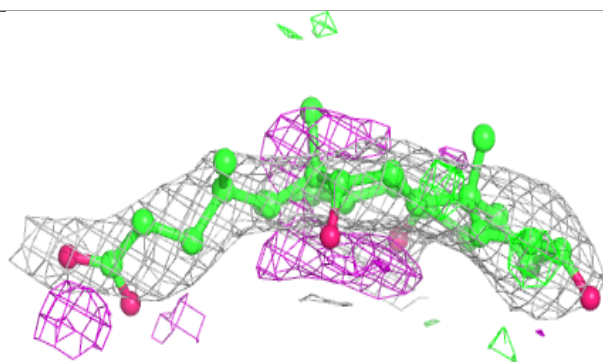
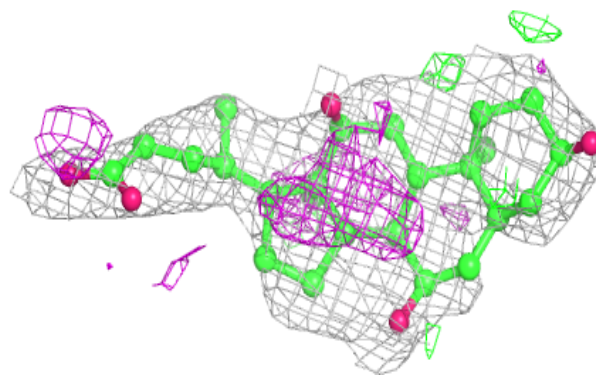
**Electron density around DMU X 101:**

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

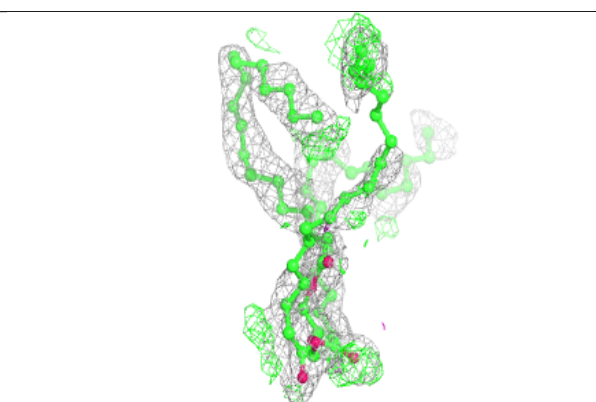
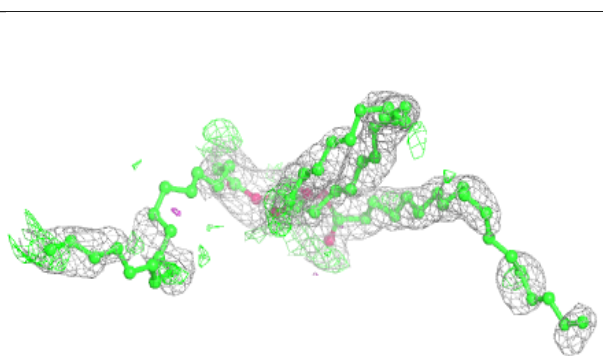
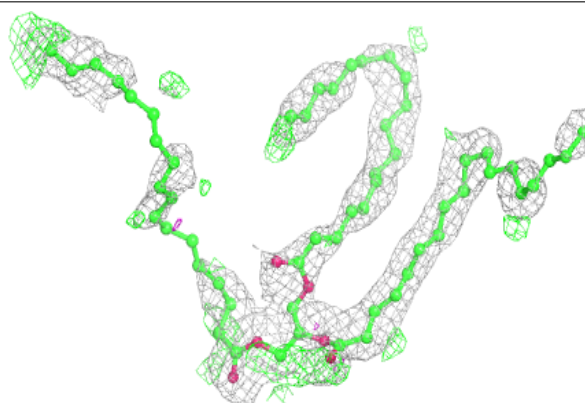


Electron density around CHD L 102:

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

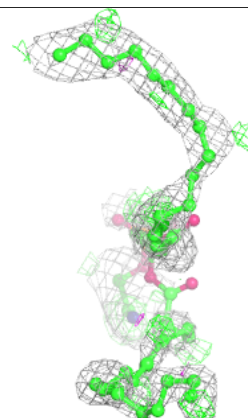
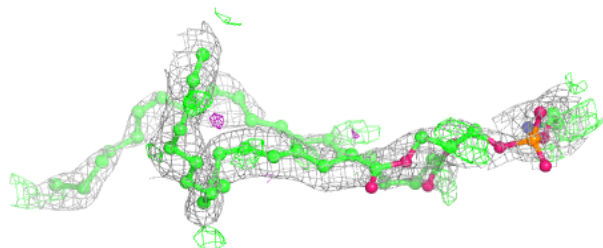
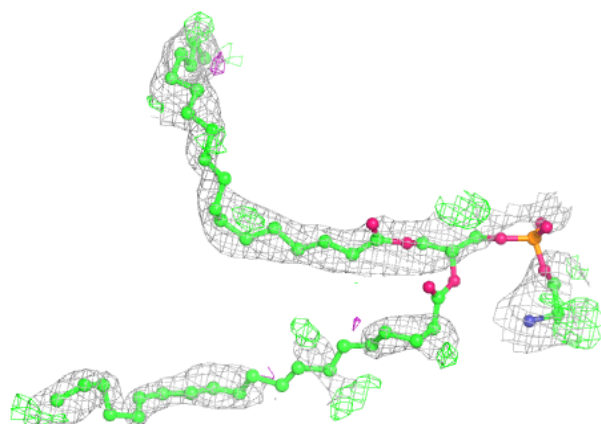
**Electron density around TGL Q 202:**

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

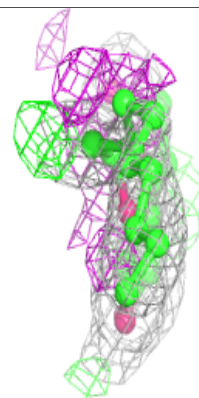
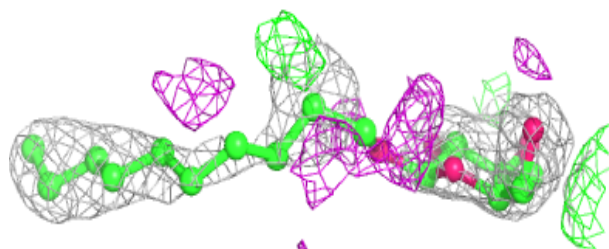
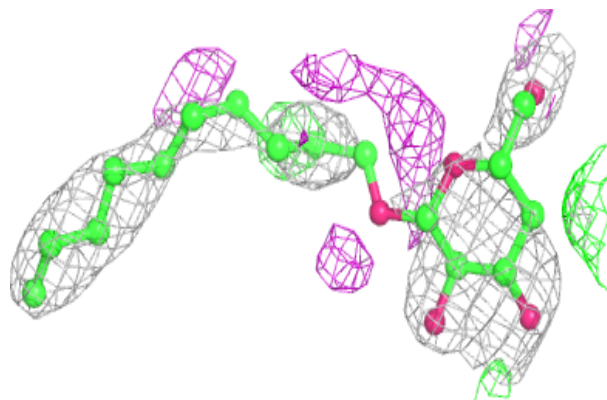


Electron density around PEK F 102:

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

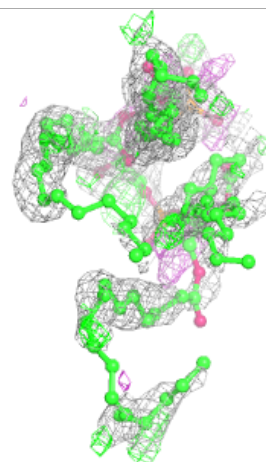
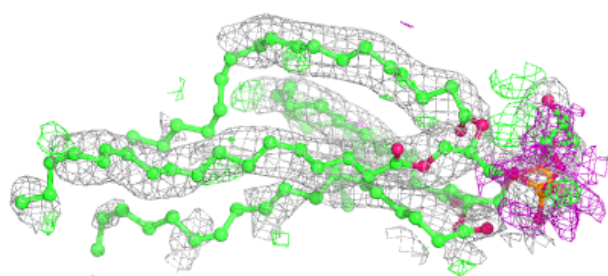
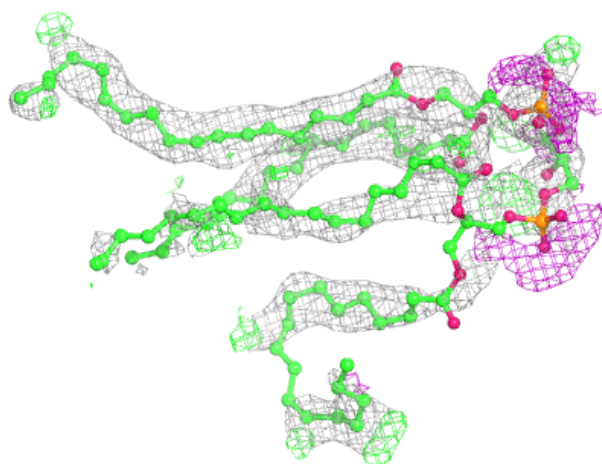
**Electron density around DMU W 101:**

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



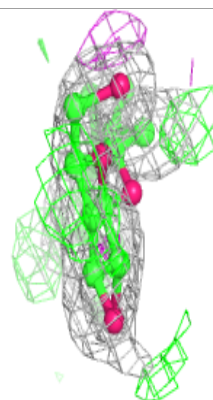
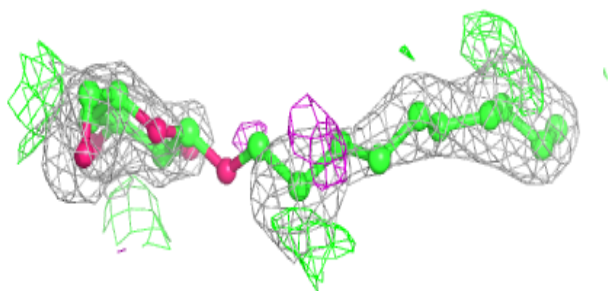
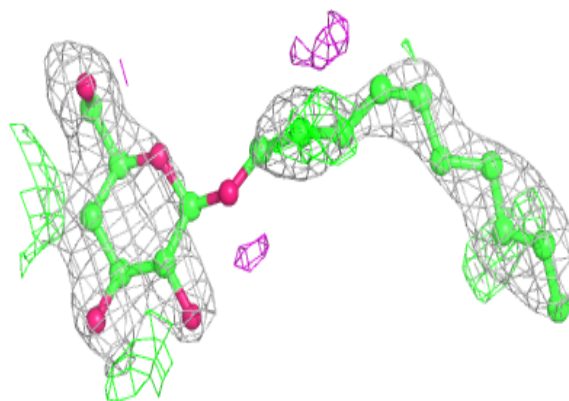
Electron density around CDL P 306:

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

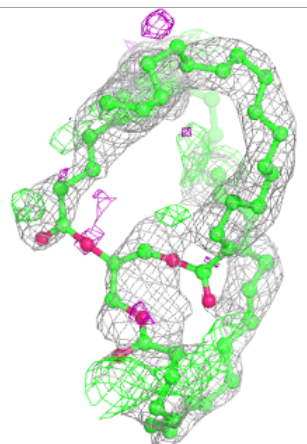
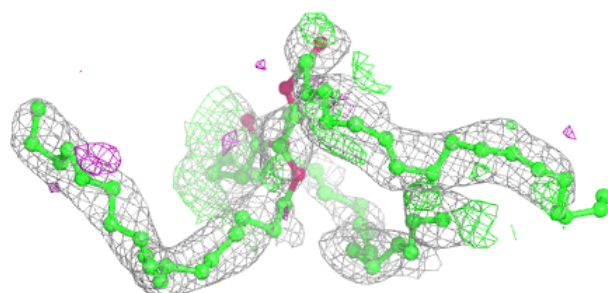
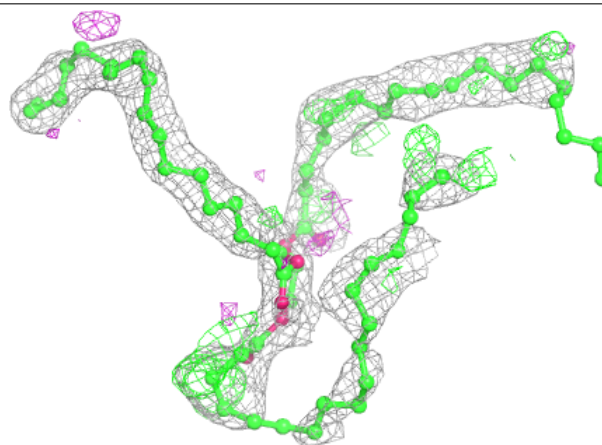


Electron density around DMU J 101:

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

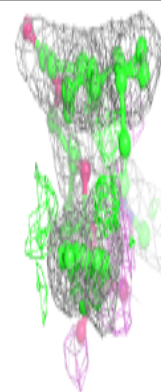
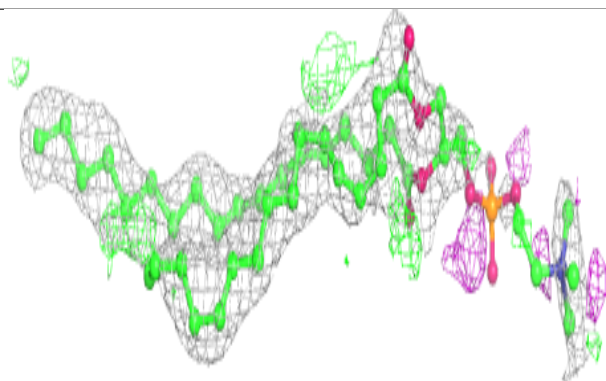
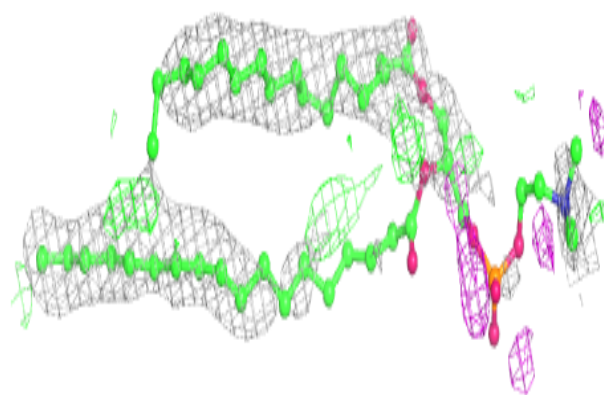
**Electron density around TGL Y 103:**

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

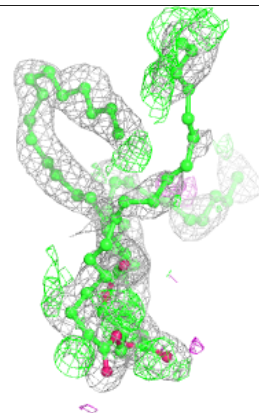
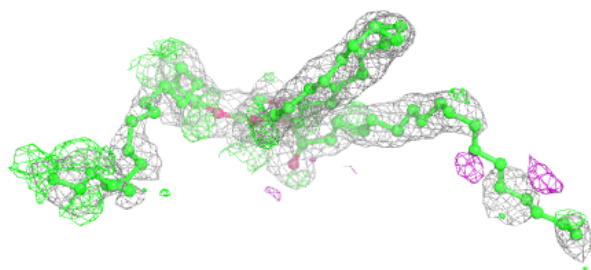
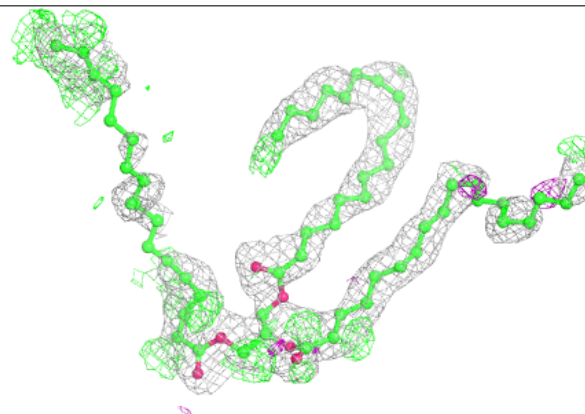


Electron density around PSC V 101:

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

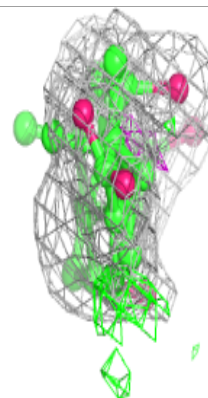
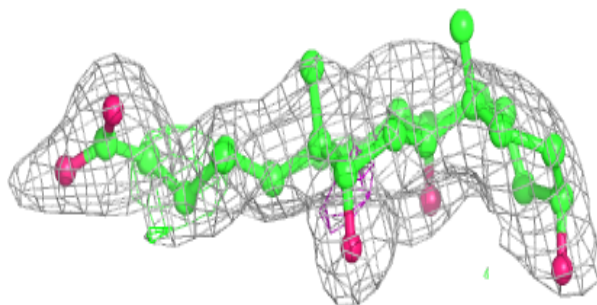
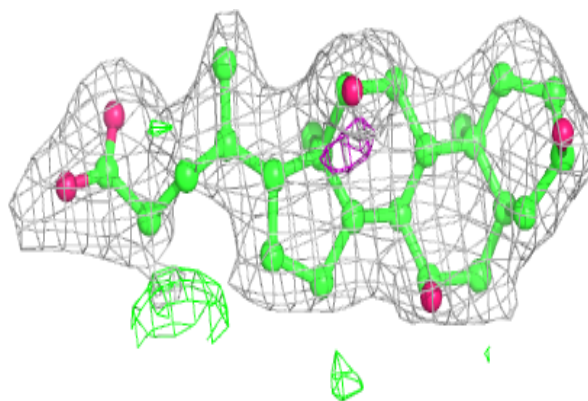
**Electron density around TGL D 202:**

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

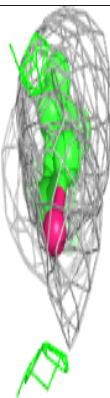
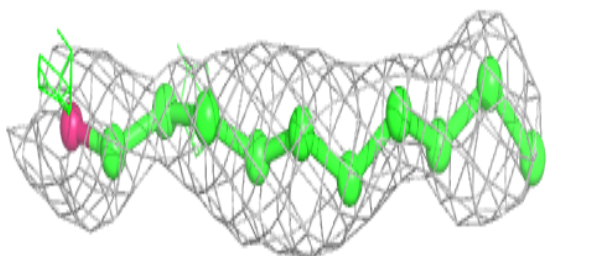
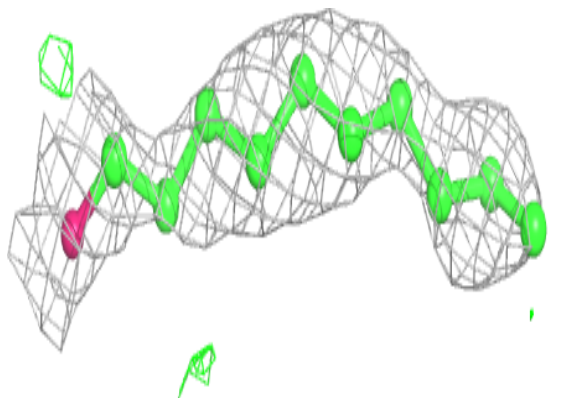


Electron density around CHD P 305:

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

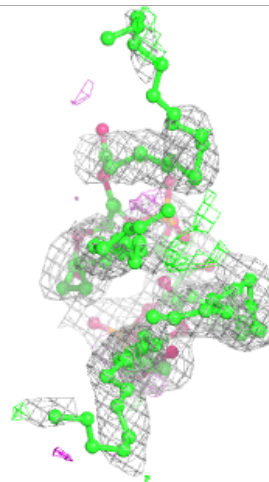
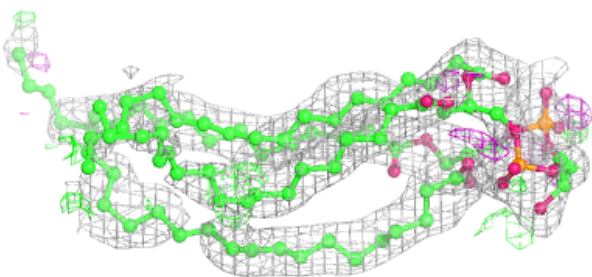
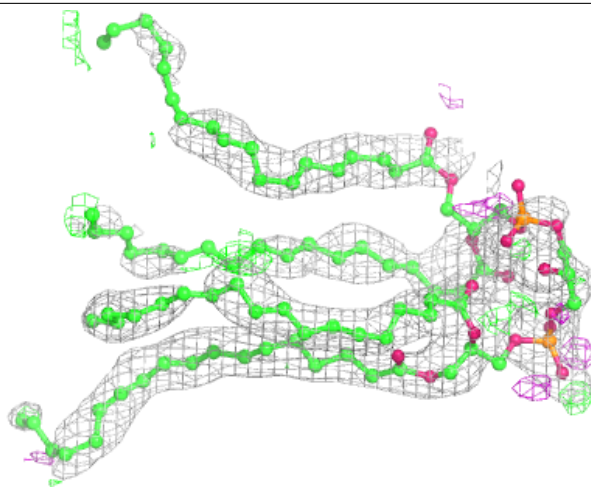
**Electron density around DMU K 101:**

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



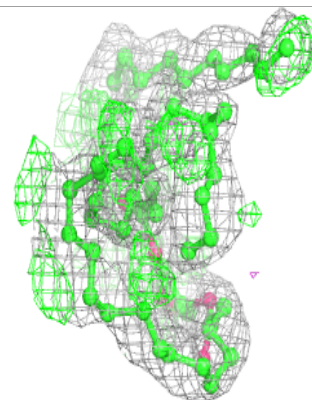
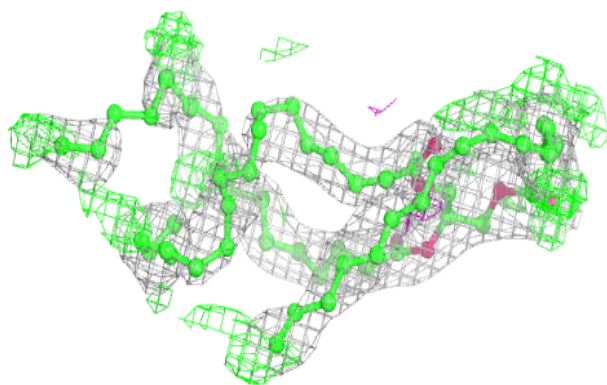
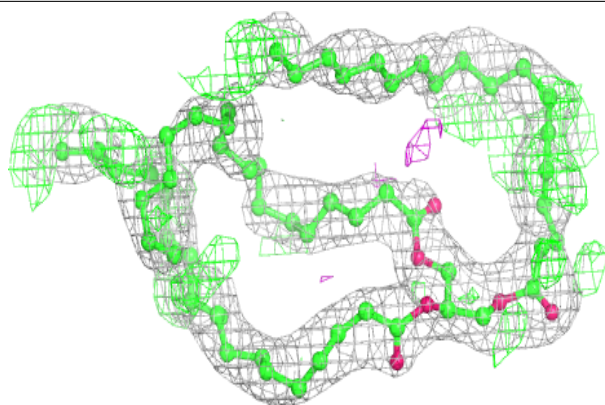
Electron density around CDL C 307:

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

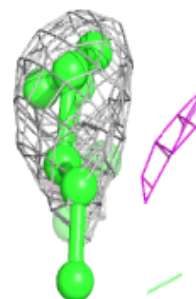
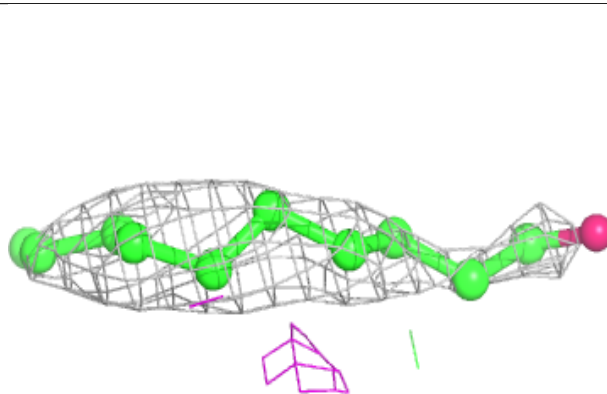
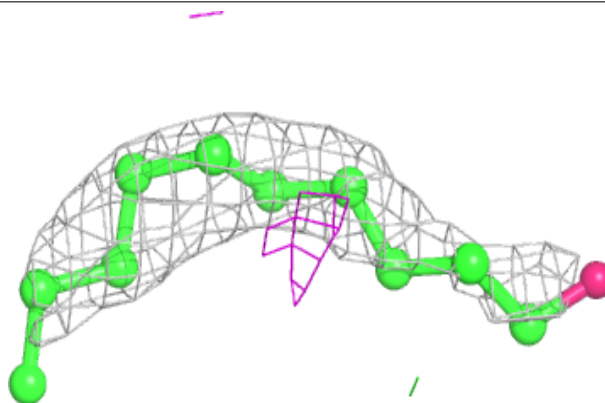


Electron density around TGL N 608:

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

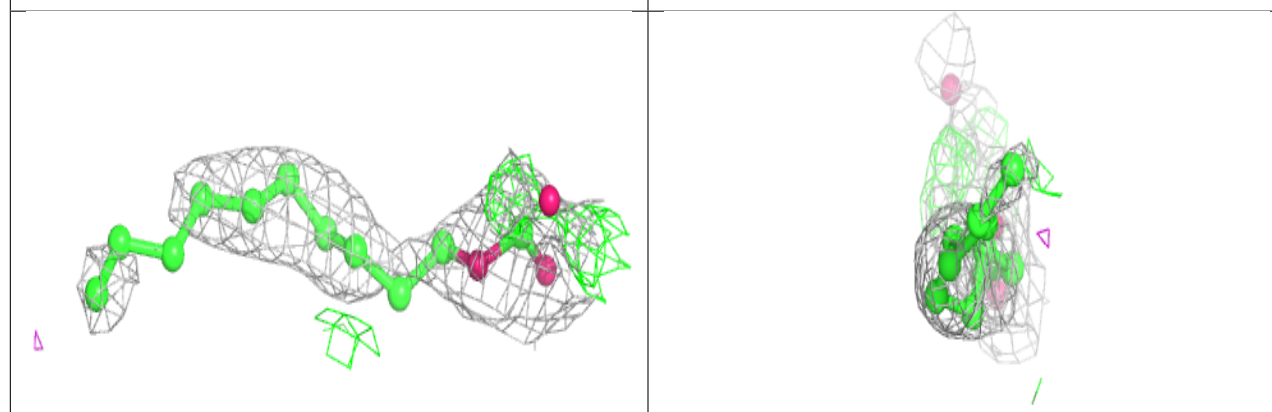
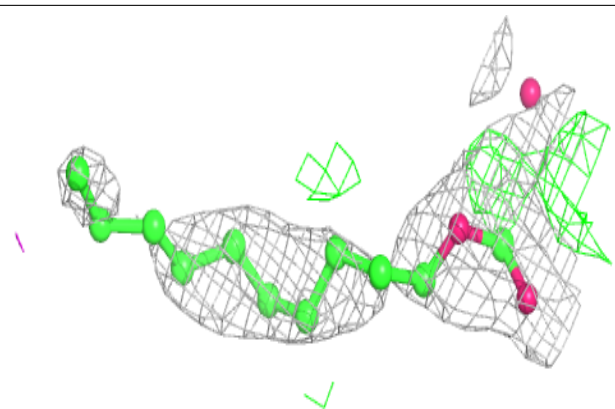
**Electron density around DMU X 104:**

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

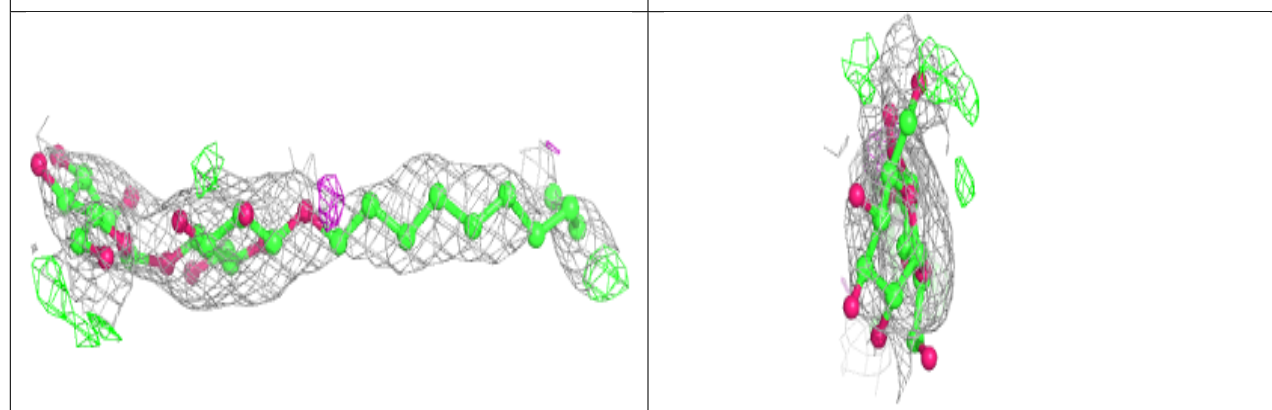
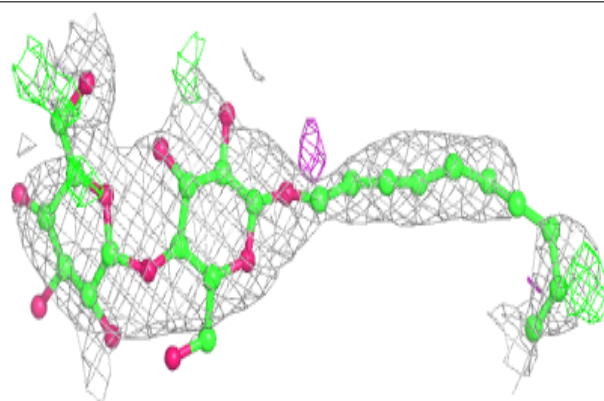


Electron density around DMU K 102:

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

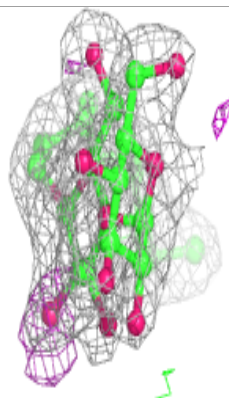
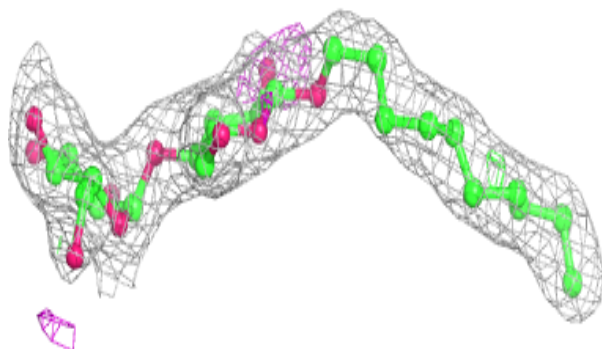
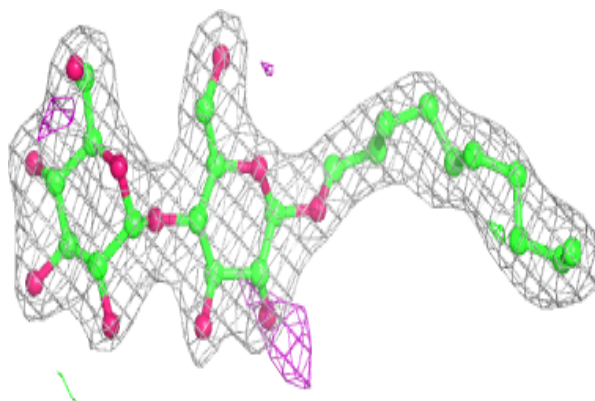
**Electron density around DMU L 101:**

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

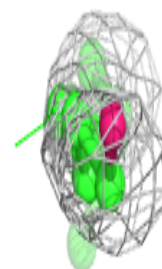
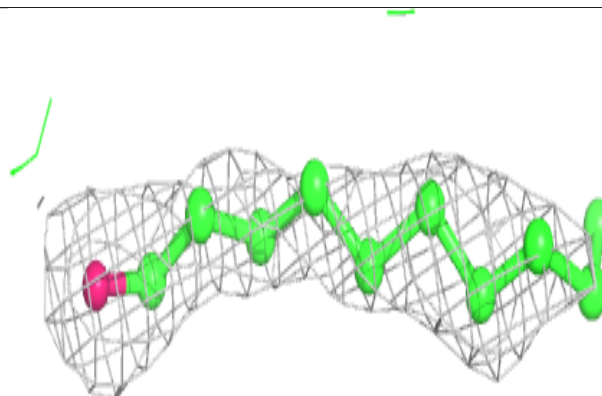
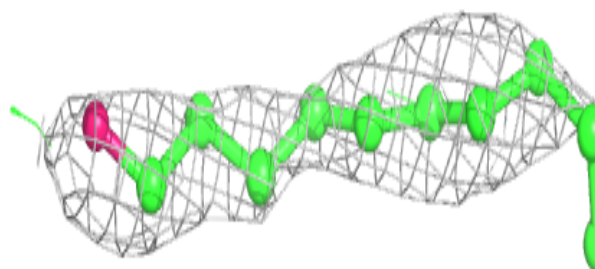


Electron density around DMU Z 101:

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

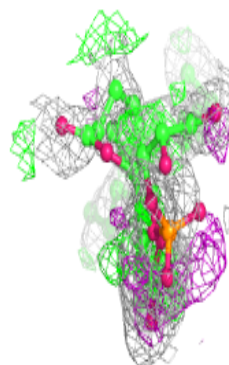
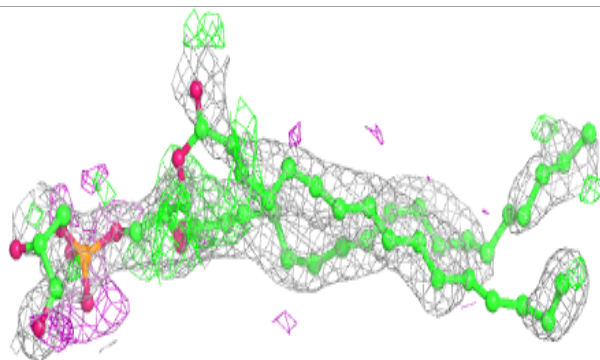
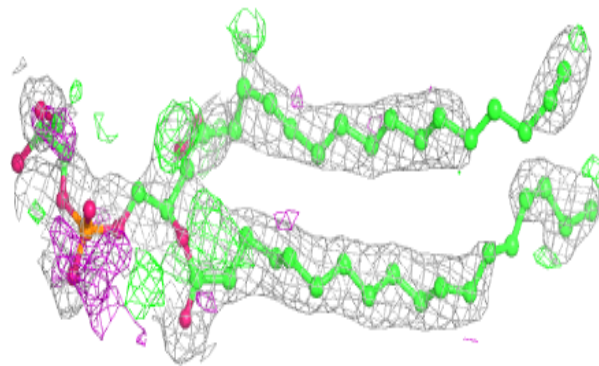
**Electron density around DMU B 302:**

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

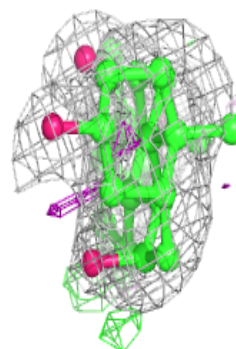
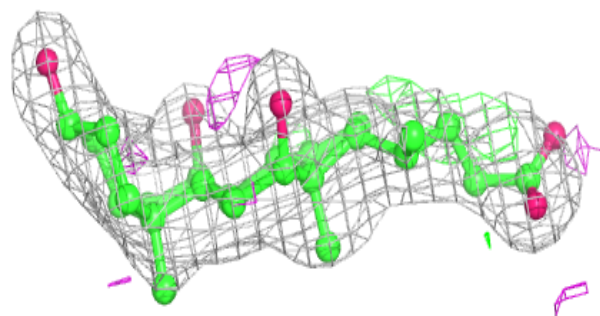
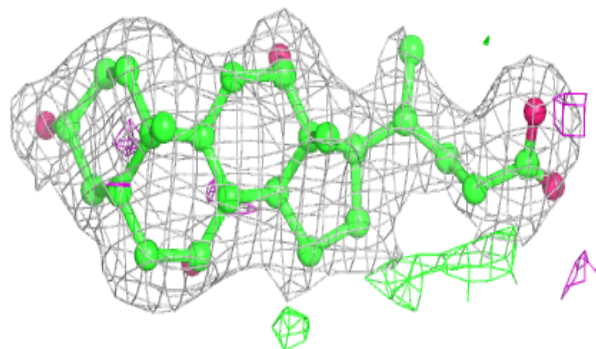


Electron density around PGV A 607:

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

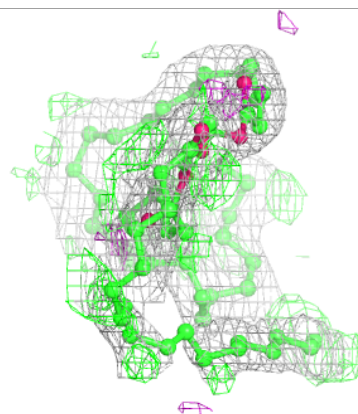
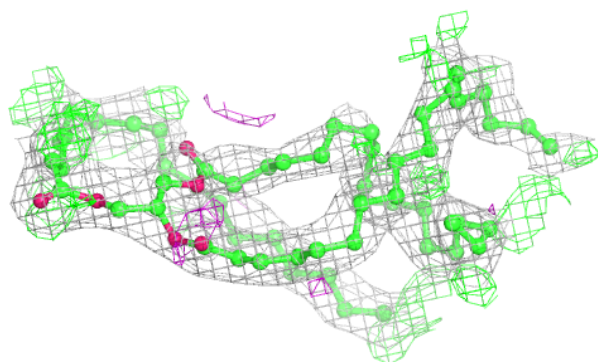
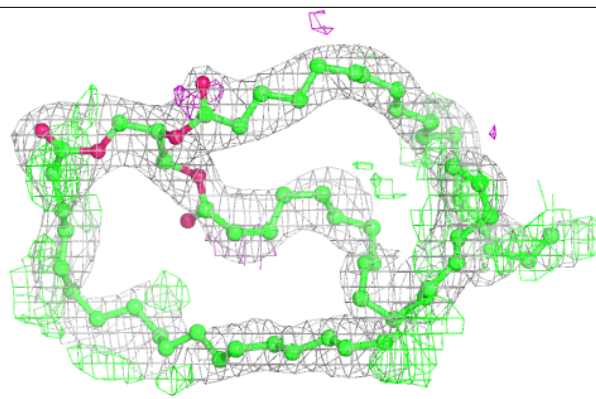
**Electron density around CHD C 306:**

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

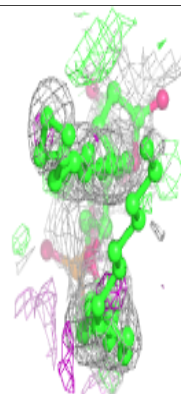
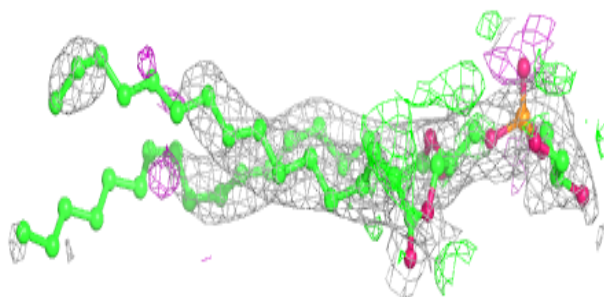
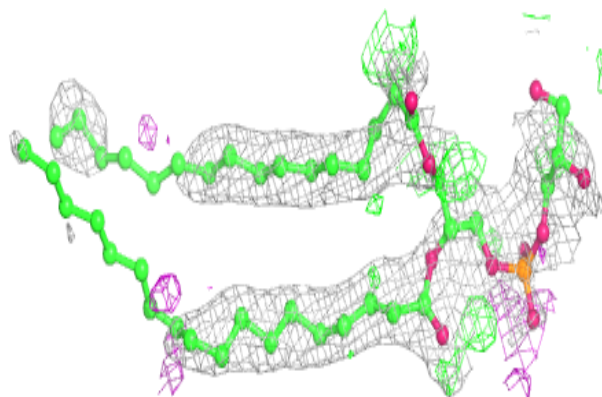


Electron density around TGL A 610:

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

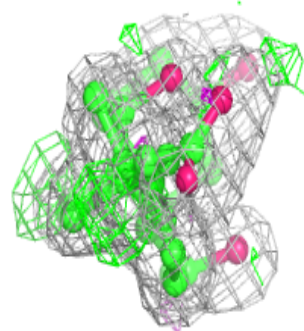
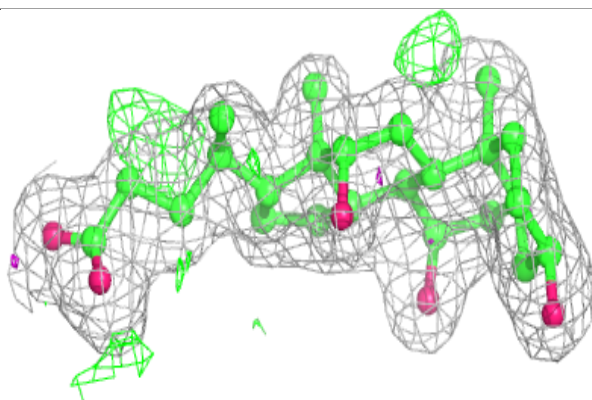
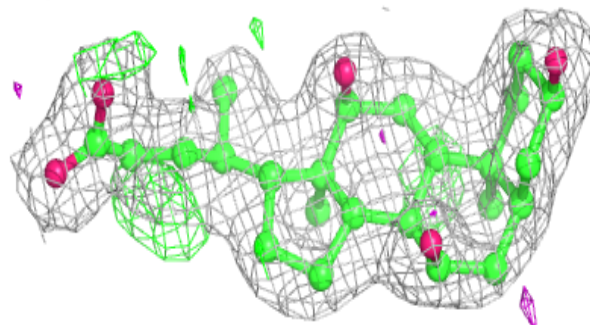
**Electron density around PGV N 606:**

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



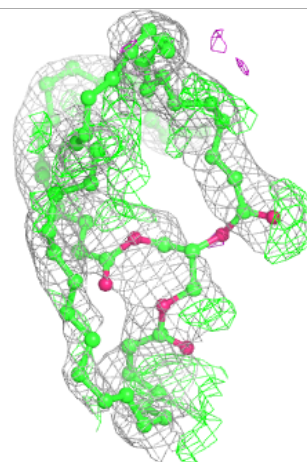
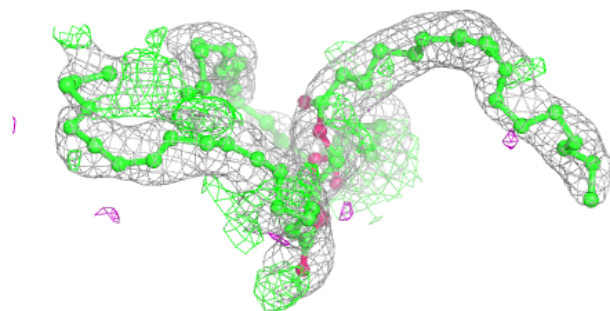
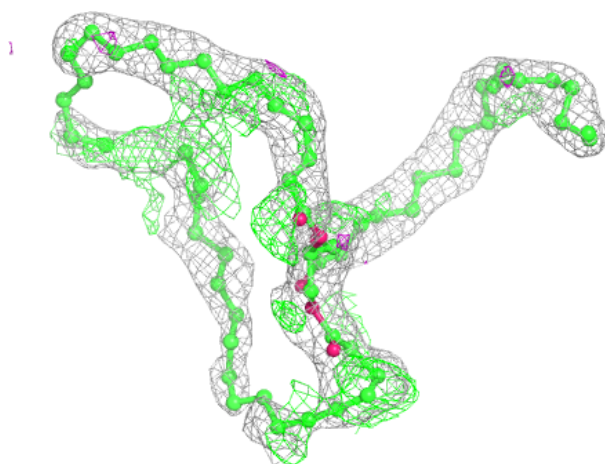
Electron density around CHD C 305:

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



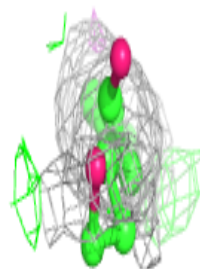
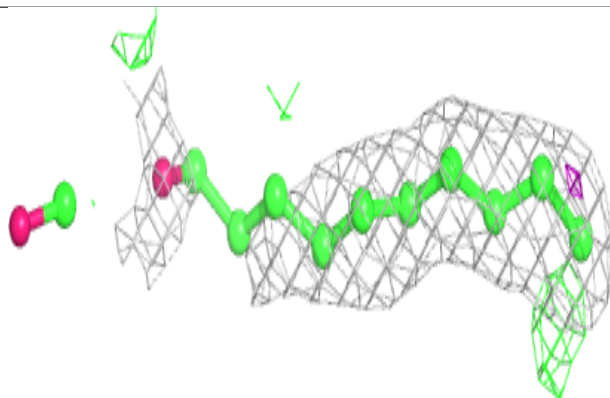
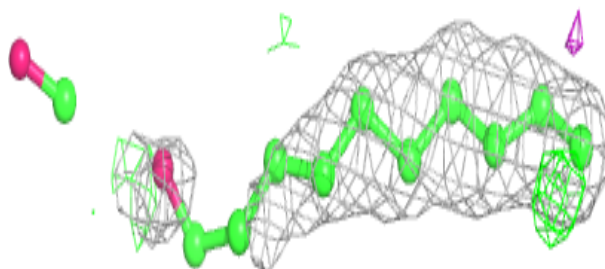
Electron density around TGL L 103:

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

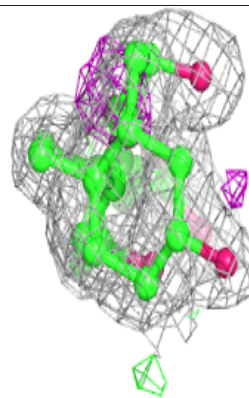
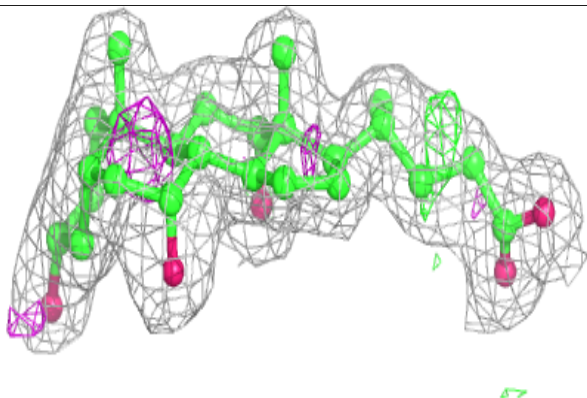
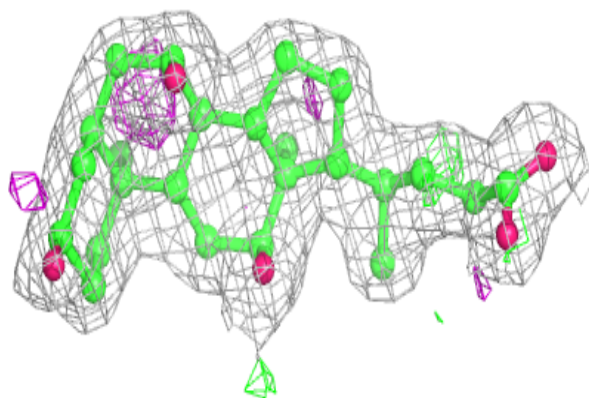


Electron density around DMU A 606:

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

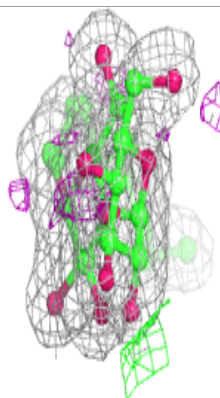
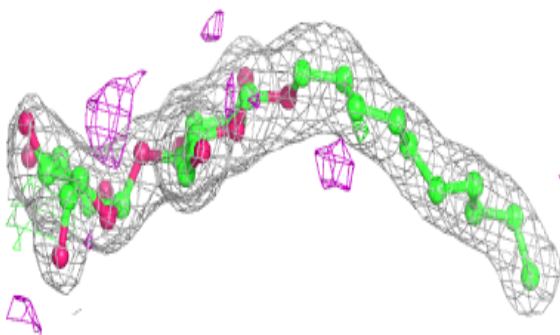
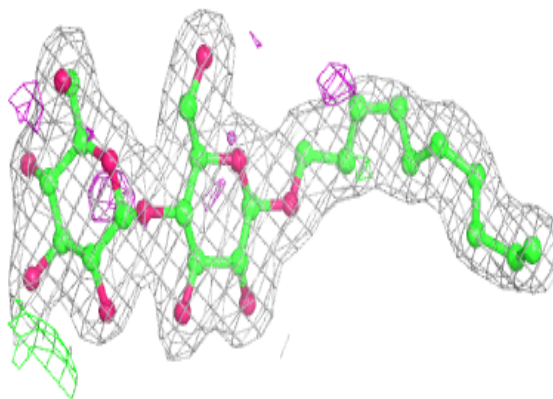
**Electron density around CHD P 304:**

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

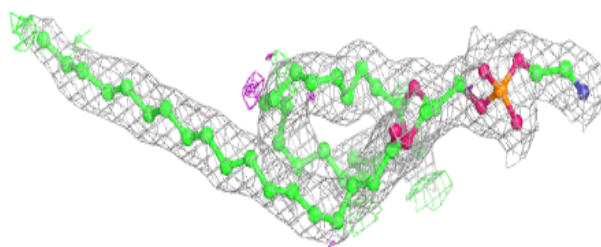
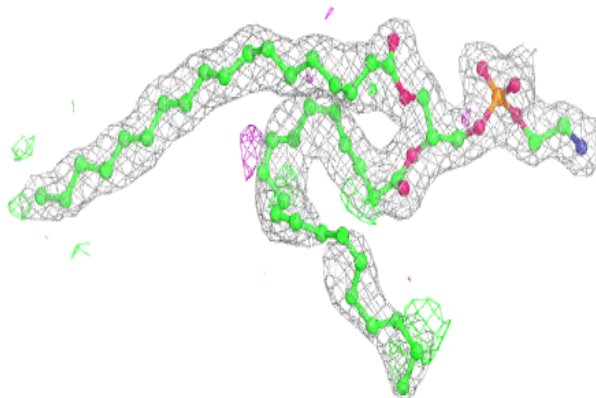


Electron density around DMU M 101:

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

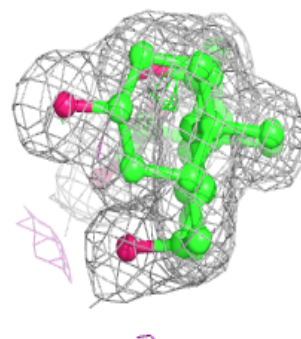
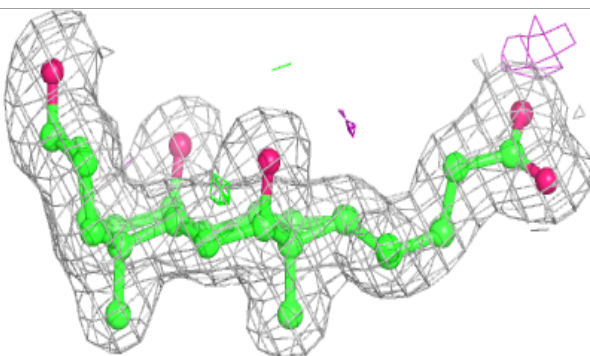
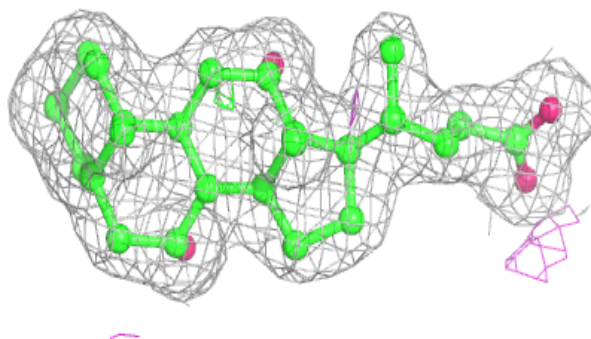
**Electron density around PEK P 308:**

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

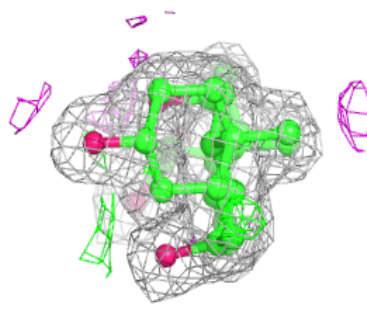
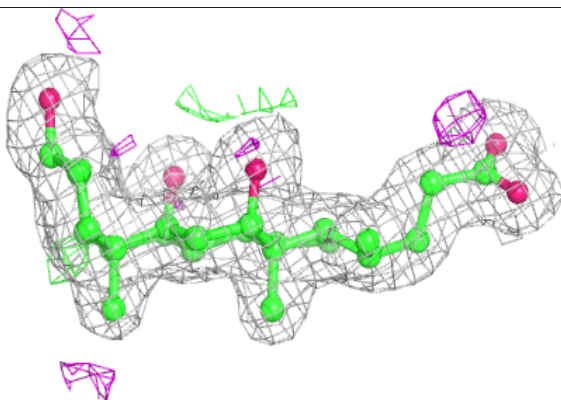
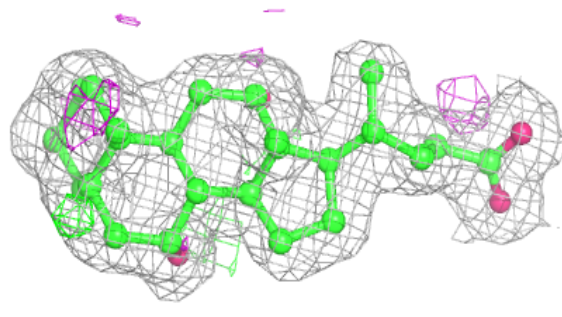


Electron density around CHD G 101:

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

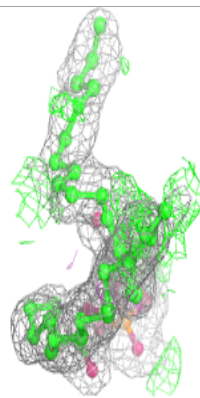
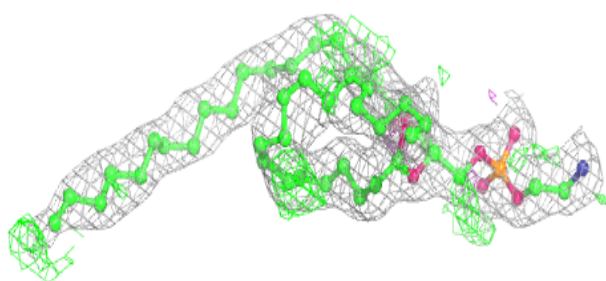
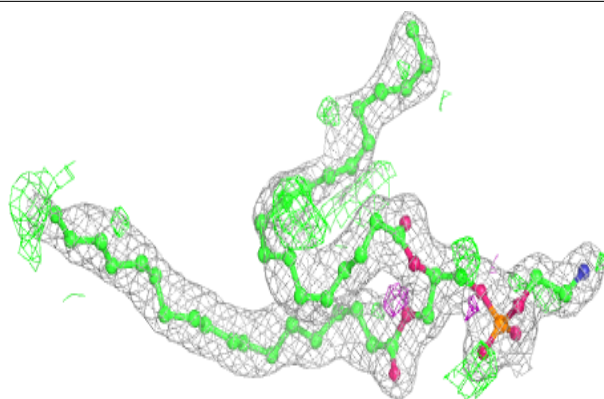
**Electron density around CHD T 101:**

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

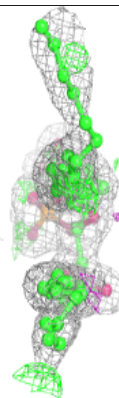
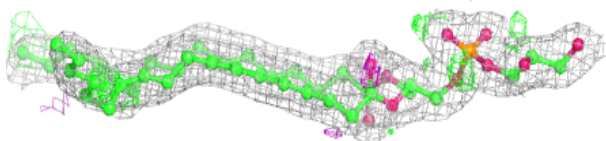
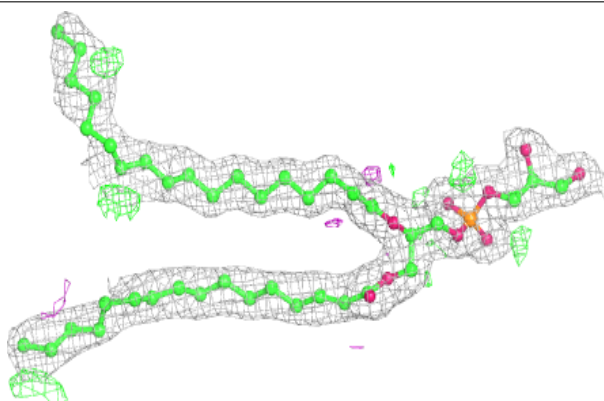


Electron density around PEK C 309:

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

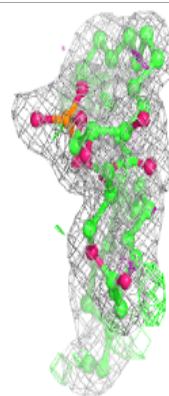
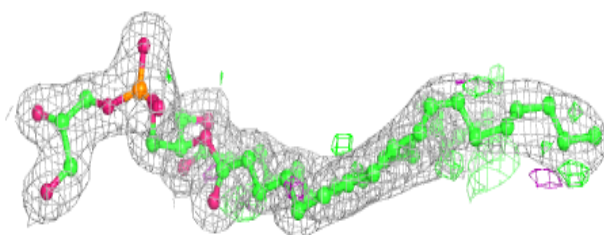
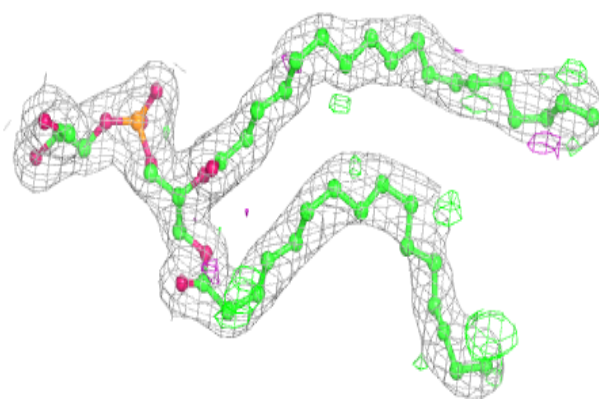
**Electron density around PGV P 309:**

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

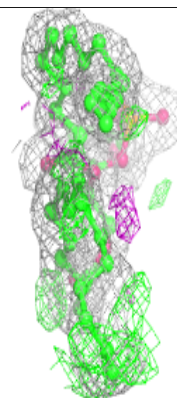
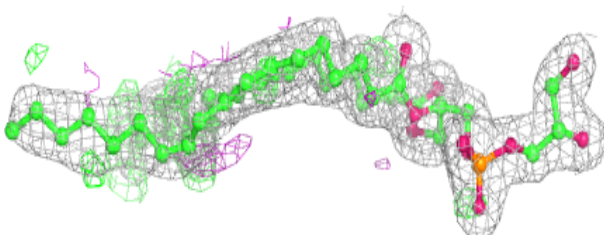
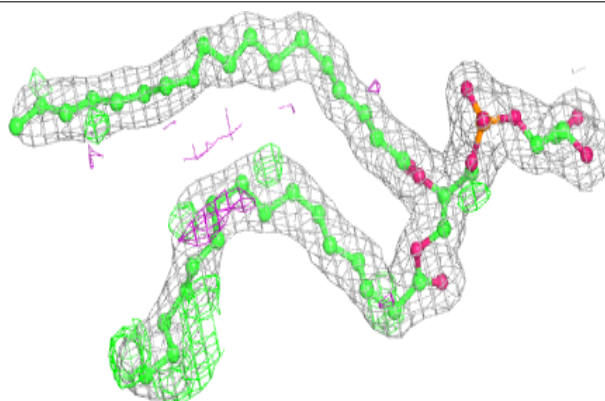


Electron density around PGV N 607:

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

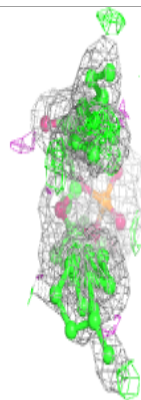
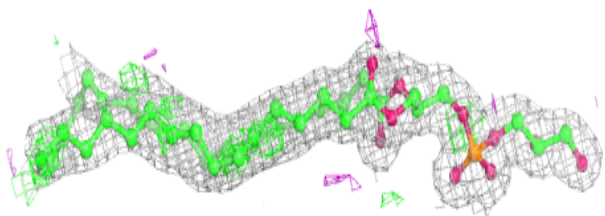
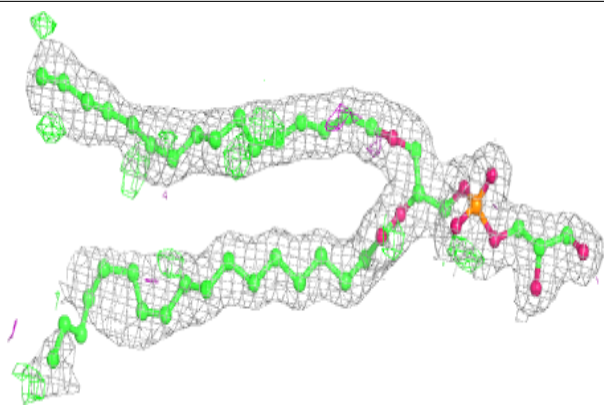
**Electron density around PGV A 608:**

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

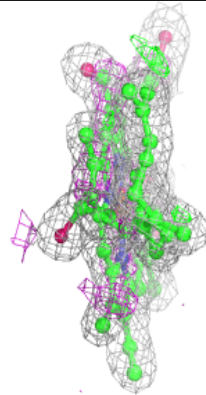
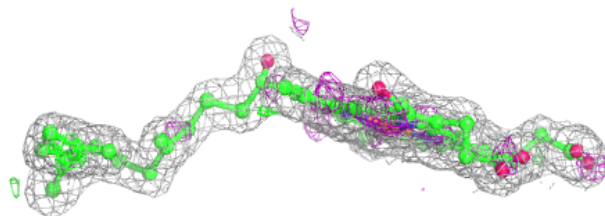
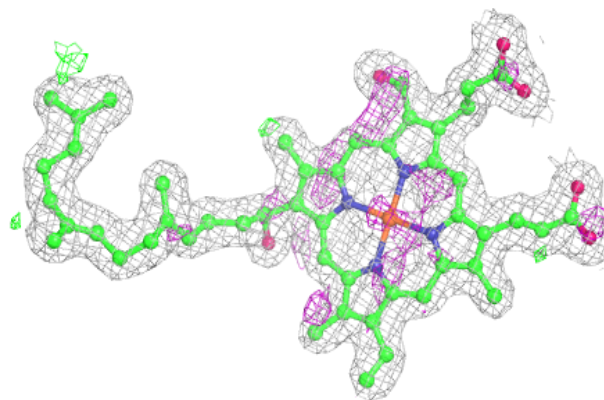


Electron density around PGV C 310:

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

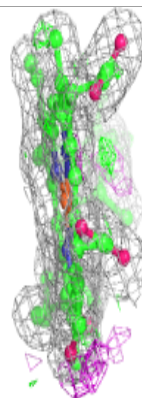
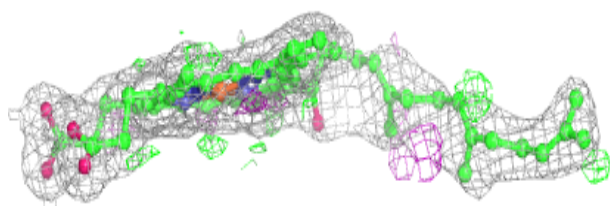
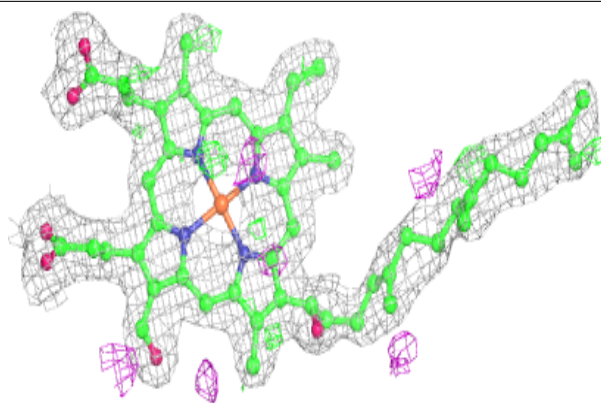
**Electron density around HEA A 602:**

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

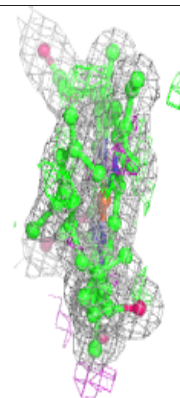
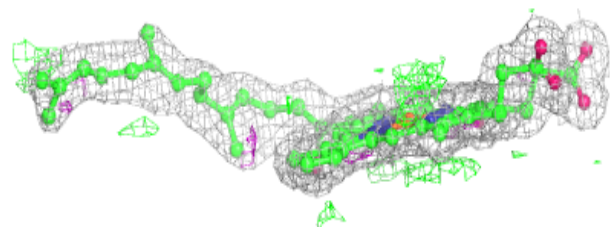
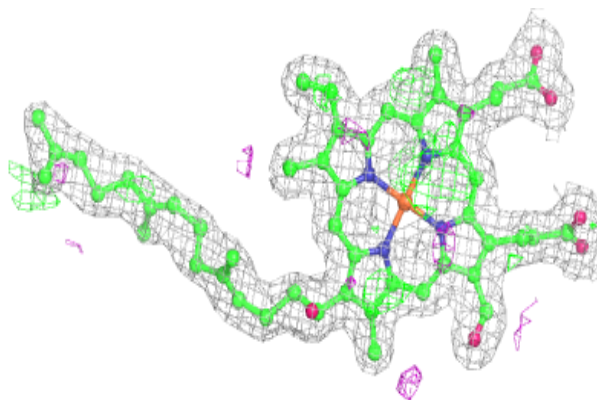


Electron density around HEA N 601 (B):

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

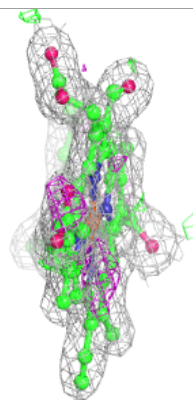
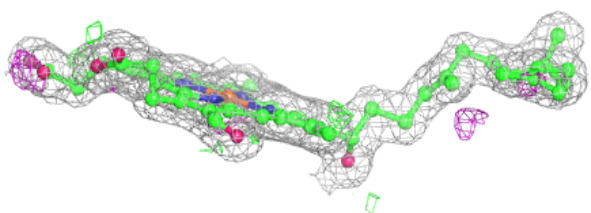
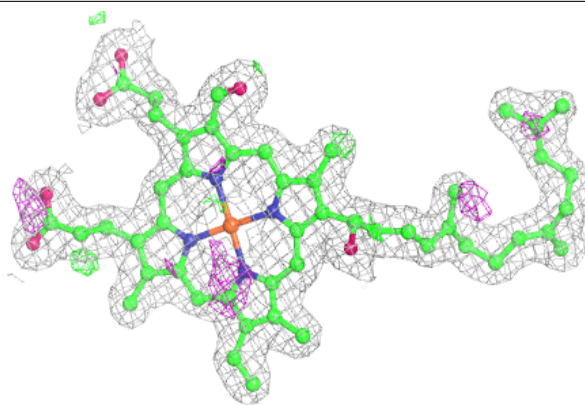
**Electron density around HEA A 601 (A):**

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

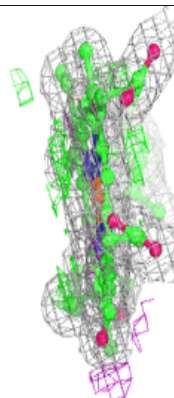
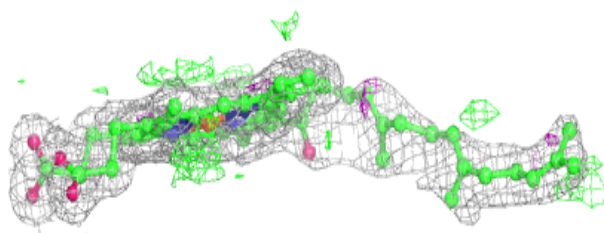
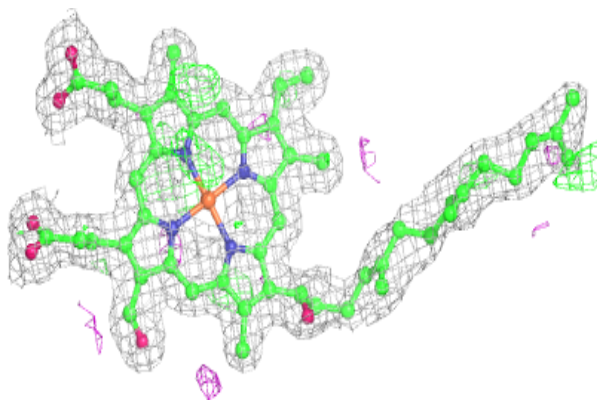


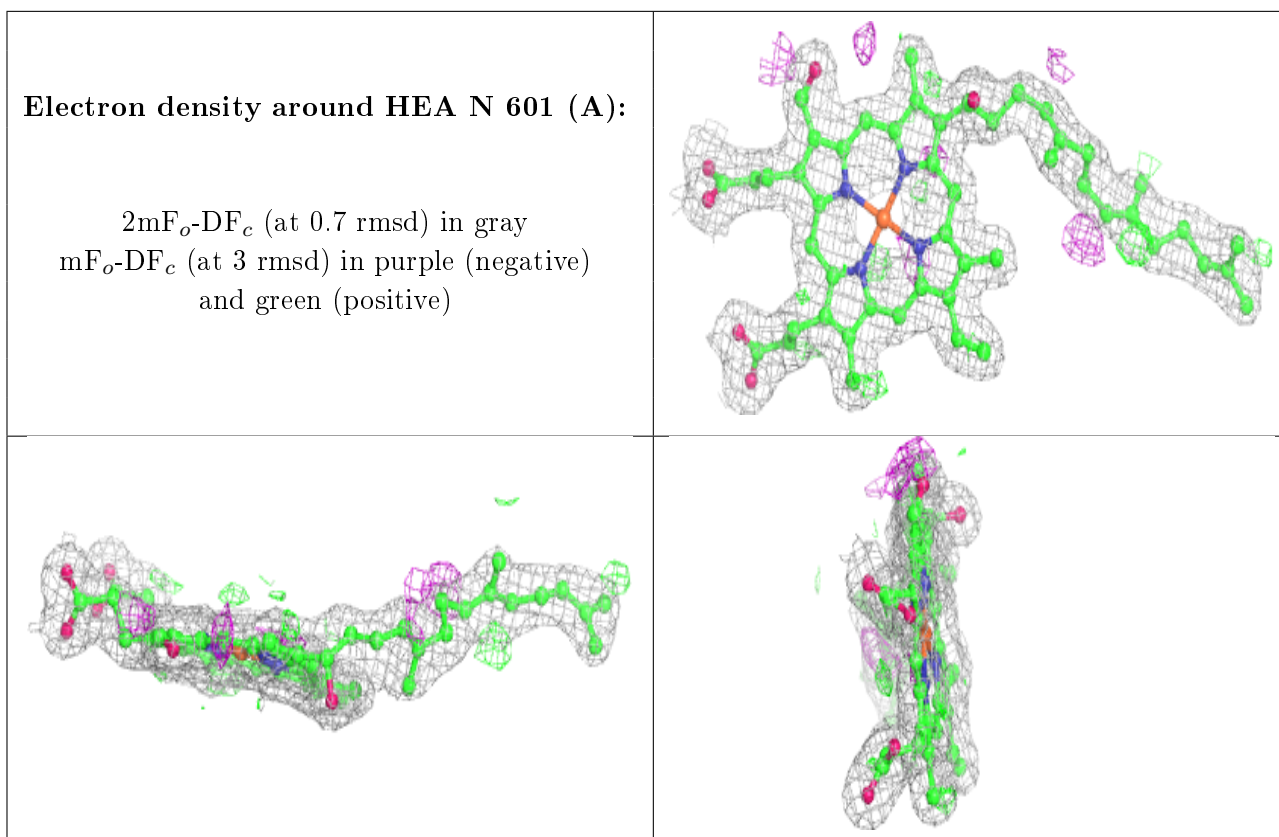
Electron density around HEA N 602:

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

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

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





6.5 Other polymers [i](#)

There are no such residues in this entry.