



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 2, 2022 – 04:27 PM EDT

PDB ID : 7TIE
Title : Structure of oxidized bovine cytochrome c oxidase at 1.90 Angstrom resolution
obtained by synchrotron X-rays
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.
Deposited on : 2022-01-13
Resolution : 1.90 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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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	:	2.29
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)	:	2.29

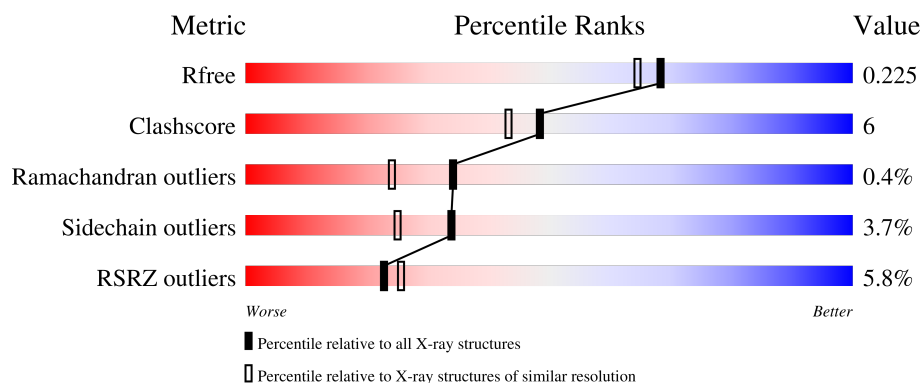
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.

















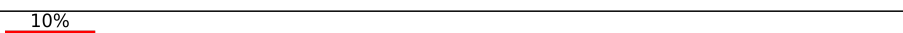
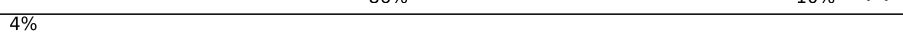





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
2	O	227	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>.</div> </div> </div>
3	C	261	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	605	X	-	-	-
18	HEA	A	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	607	X	-	-	-
18	HEA	N	608	X	-	-	-
19	EDO	A	618	-	-	-	X
19	EDO	W	303	-	-	-	X
27	DMU	G	101	-	-	-	X
29	SAC	V	101	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32913 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- 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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	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	0	0
			1195	777	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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	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	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	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
			384	250	65	67	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	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
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

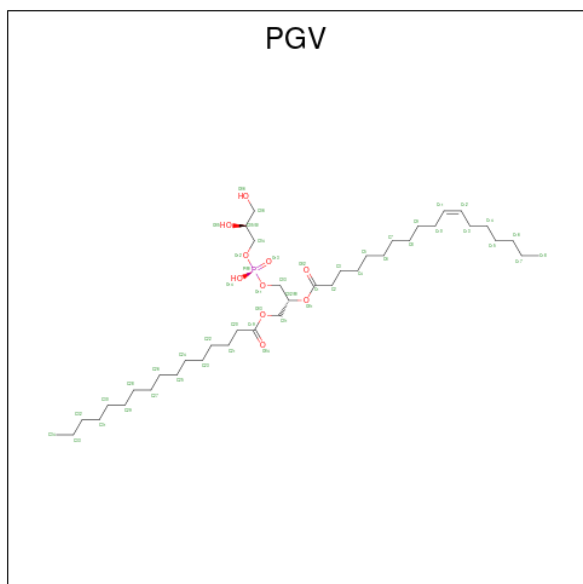
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

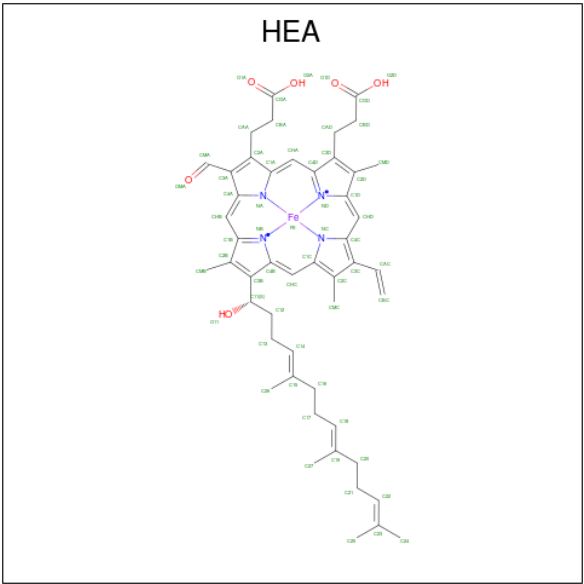
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 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).



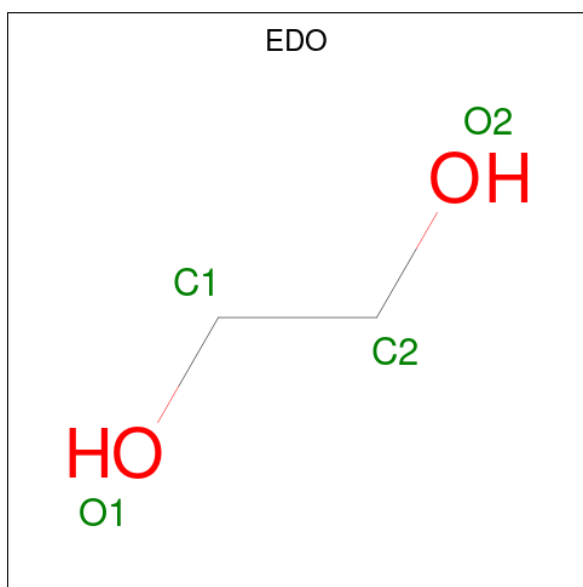
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	M	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0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

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

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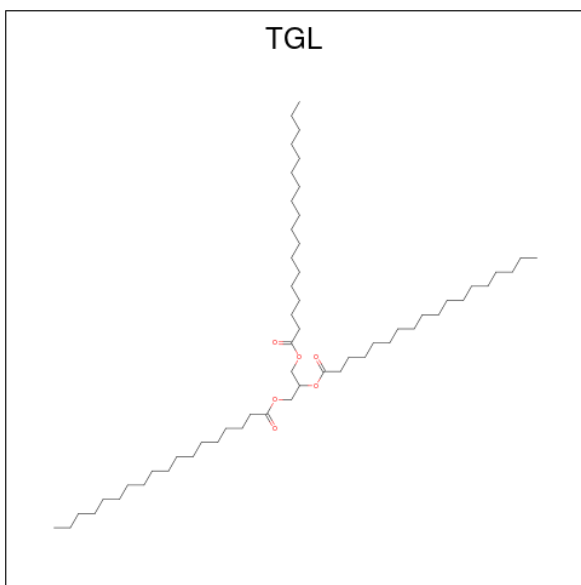
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	O	1	Total 4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

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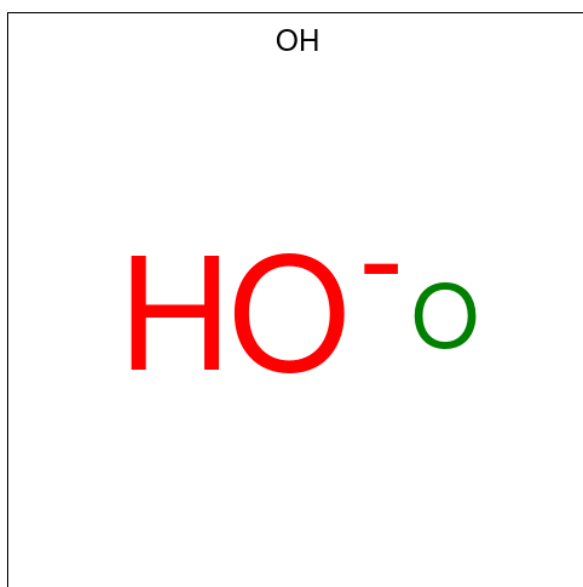
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	U	1	Total	C	O	0	0
			4	2	2		
19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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆) (labeled as "Ligand of Interest" by depositor).



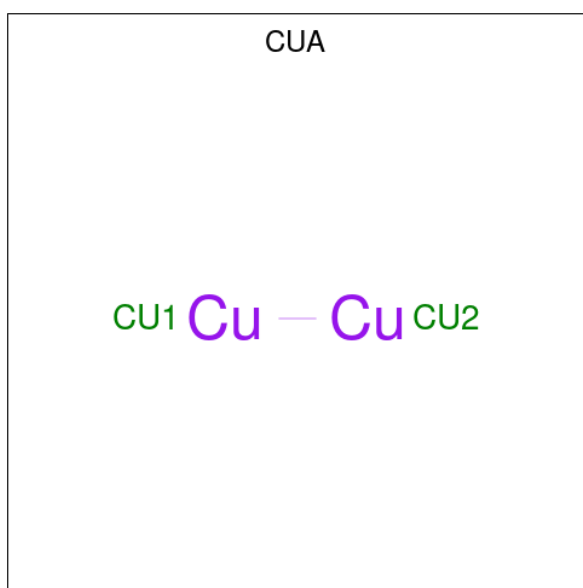
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



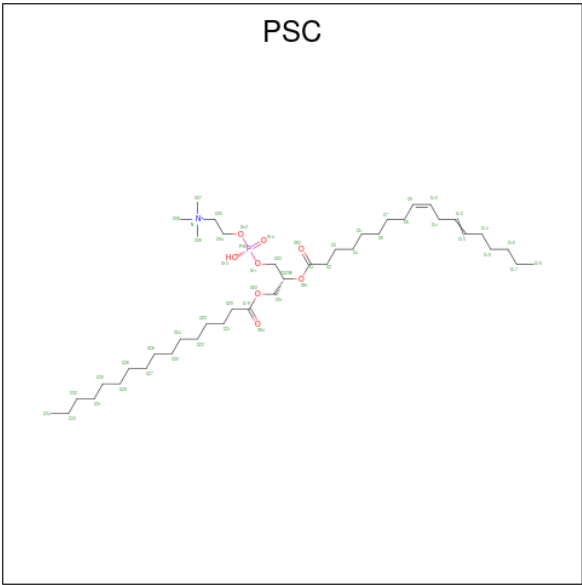
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total O 1 1	0	0
21	N	1	Total O 1 1	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



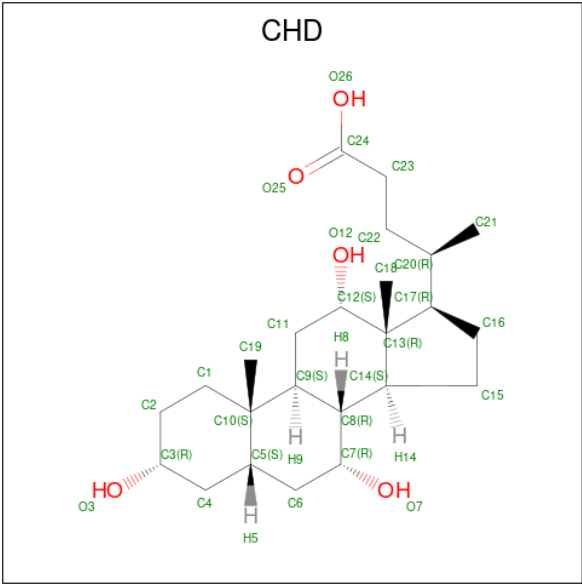
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 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).



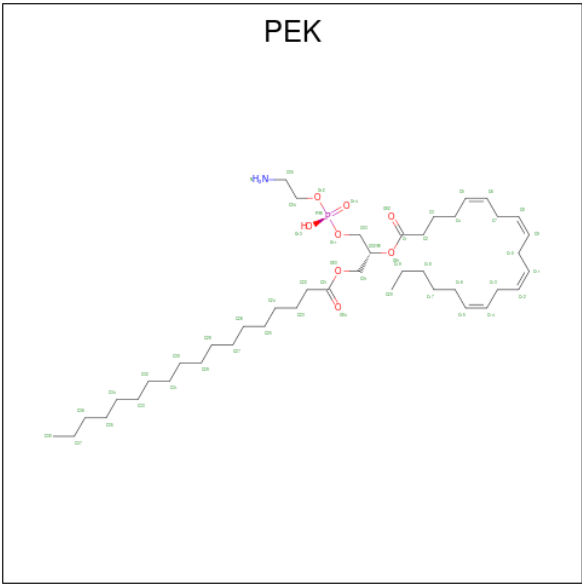
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



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

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



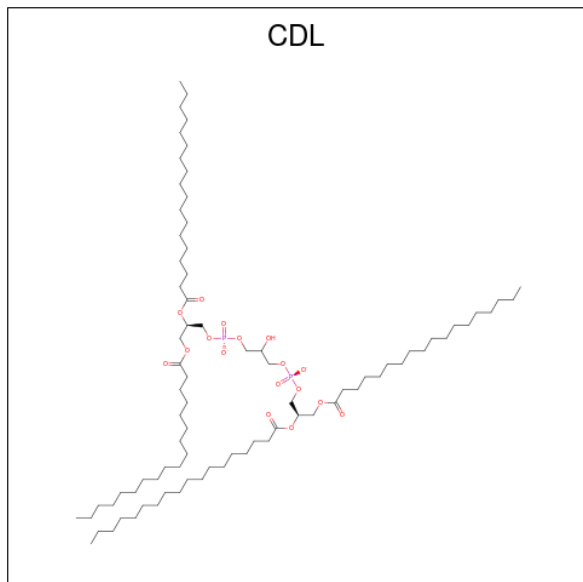
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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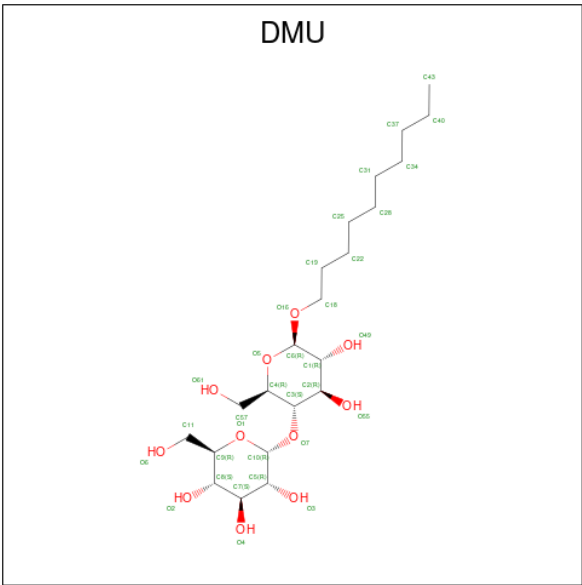
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

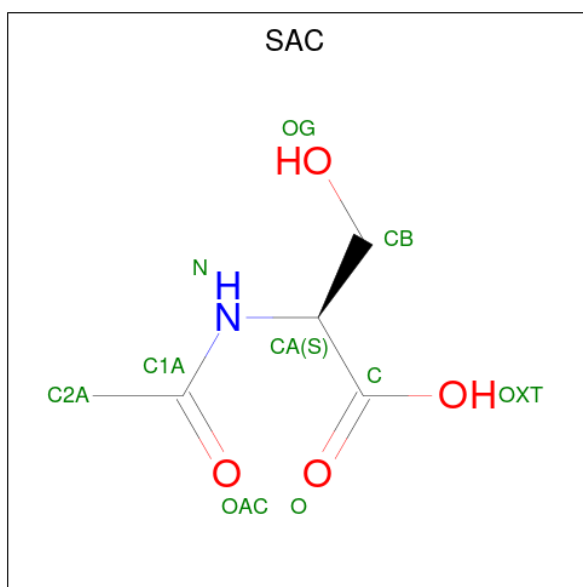


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	Z	1	Total	C	O	0	0
			33	22	11		

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

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

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	I	1	Total	C	N	O	0	0
			9	5	1	3		
29	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	215	Total	O	0	0
			215	215		
30	B	149	Total	O	0	0
			149	149		
30	C	111	Total	O	0	0
			111	111		
30	D	98	Total	O	0	0
			98	98		
30	E	81	Total	O	0	0
			81	81		
30	F	85	Total	O	0	0
			85	85		
30	G	45	Total	O	0	0
			45	45		
30	H	50	Total	O	0	0
			50	50		
30	I	31	Total	O	0	0
			31	31		
30	J	32	Total	O	0	0
			32	32		

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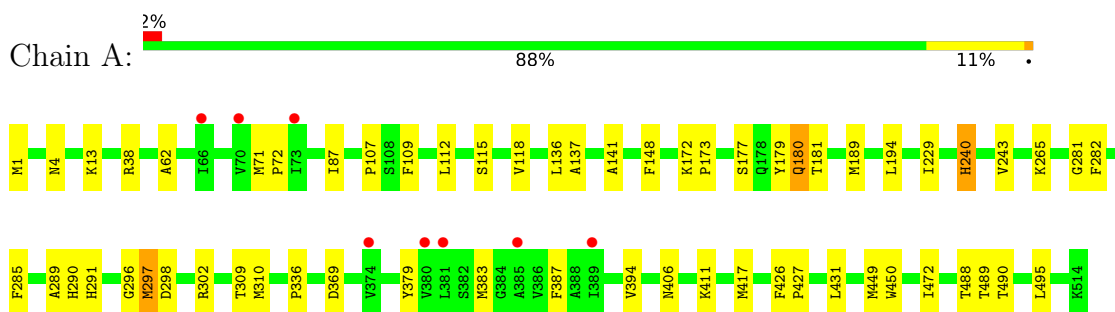
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	24	Total 24	O 24	0	0
30	L	24	Total 24	O 24	0	0
30	M	23	Total 23	O 23	0	0
30	N	184	Total 184	O 184	0	0
30	O	111	Total 111	O 111	0	0
30	P	96	Total 96	O 96	0	0
30	Q	59	Total 59	O 59	0	0
30	R	58	Total 58	O 58	0	0
30	S	73	Total 73	O 73	0	0
30	T	35	Total 35	O 35	0	0
30	U	47	Total 47	O 47	0	0
30	V	18	Total 18	O 18	0	0
30	W	18	Total 18	O 18	0	0
30	X	14	Total 14	O 14	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	6	Total 6	O 6	0	0

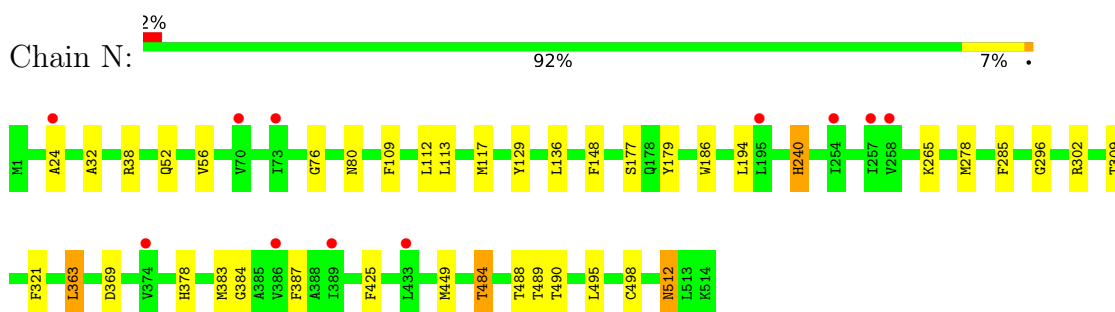
3 Residue-property plots

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

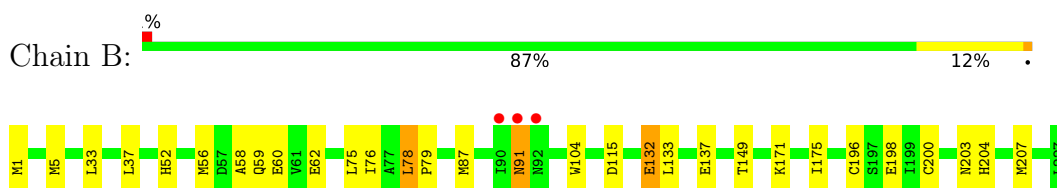
• Molecule 1: Cytochrome c oxidase subunit 1



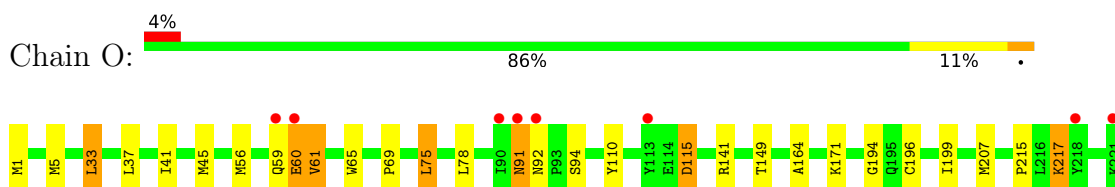
• Molecule 1: Cytochrome c oxidase subunit 1

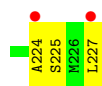


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 92% 7% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 89% 10% .



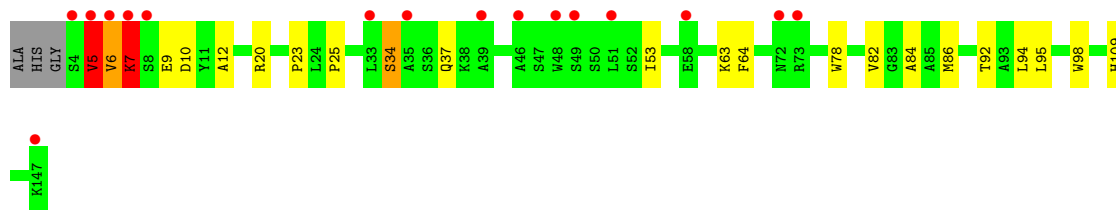
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 89% 7% ..



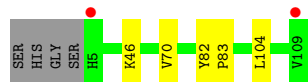
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 11% 82% 13% ...



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

Chain E: 2% 92% 5% .

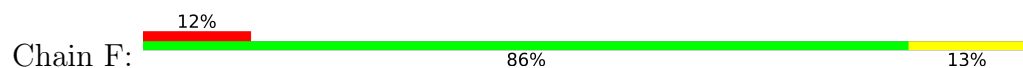


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

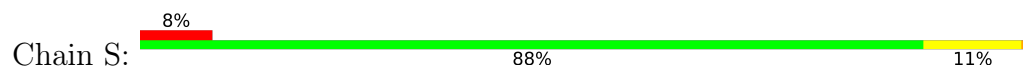
Chain R: 4% 90% 6% .



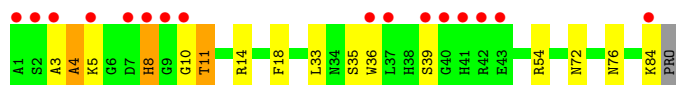
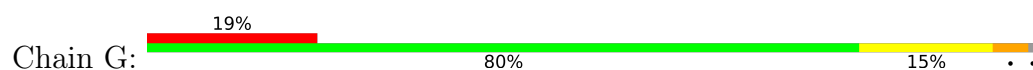
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



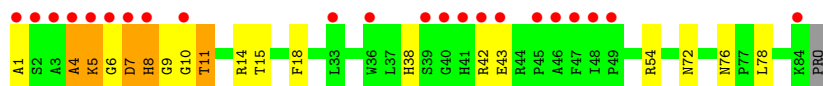
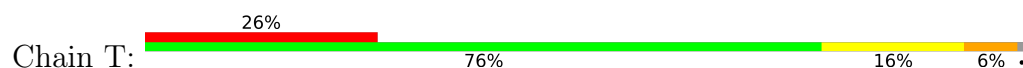
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



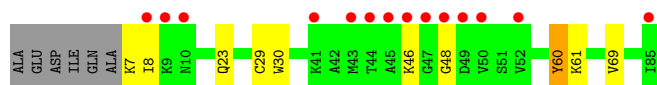
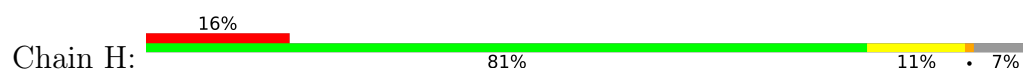
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



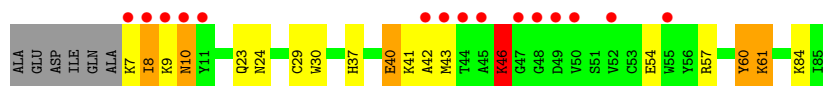
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



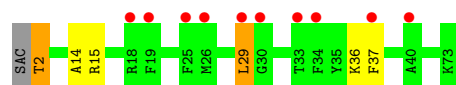
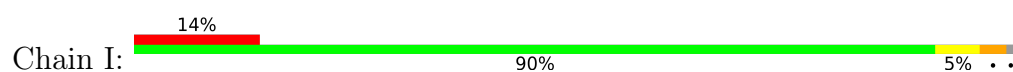
- Molecule 8: Cytochrome c oxidase subunit 6B1



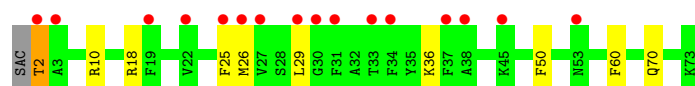
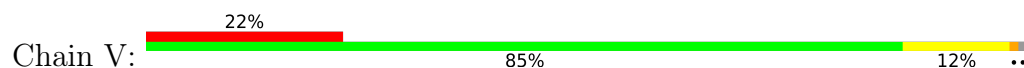
- Molecule 8: Cytochrome c oxidase subunit 6B1



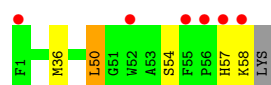
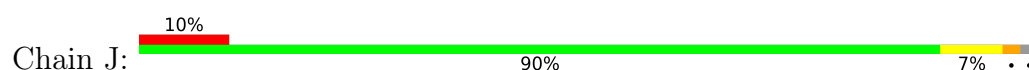
- Molecule 9: Cytochrome c oxidase subunit 6C



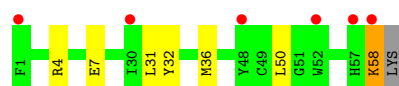
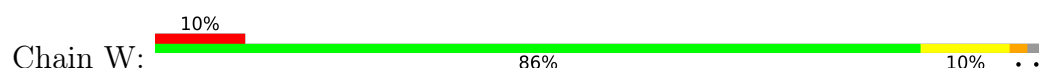
- Molecule 9: Cytochrome c oxidase subunit 6C



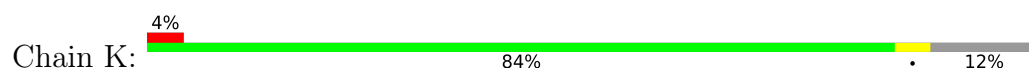
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



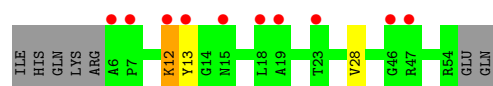
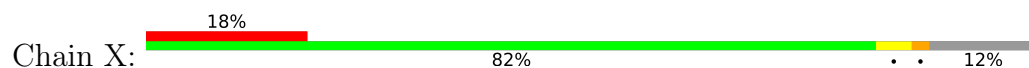
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



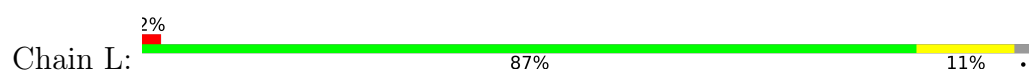
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial




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

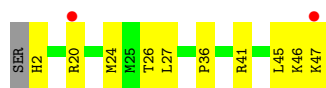


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial




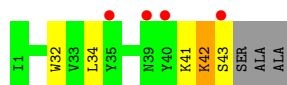
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  4% 77% 21% .




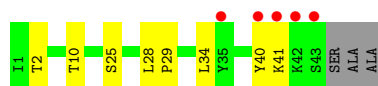
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  9% 83% 9% . 7%



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

Chain Z:  11% 76% 17% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.12Å 182.41Å 208.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 1.90 39.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.99-1.90) 99.8 (39.96-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.215 0.196 , 0.225	Depositor DCC
R_{free} test set	26755 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32913	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/4156	0.84	1/5678 (0.0%)
1	N	0.77	0/4156	0.81	2/5678 (0.0%)
2	B	0.82	2/1860 (0.1%)	0.93	0/2534
2	O	0.74	0/1860	0.88	1/2534 (0.0%)
3	C	0.74	0/2197	0.79	2/3005 (0.1%)
3	P	0.79	0/2197	0.78	0/3005
4	D	0.76	0/1229	0.85	3/1658 (0.2%)
4	Q	0.73	0/1229	0.78	1/1658 (0.1%)
5	E	0.74	0/871	0.81	0/1182
5	R	0.70	0/871	0.80	0/1182
6	F	0.78	0/765	0.92	0/1038
6	S	0.76	0/765	0.85	0/1038
7	G	0.71	0/690	0.89	0/937
7	T	0.71	0/690	0.85	1/937 (0.1%)
8	H	0.74	0/682	0.85	0/921
8	U	0.68	0/682	0.86	0/921
9	I	0.74	0/605	0.87	0/802
9	V	0.69	0/605	0.86	0/802
10	J	0.66	0/471	0.81	1/636 (0.2%)
10	W	0.78	0/471	0.77	0/636
11	K	0.73	0/398	0.84	0/546
11	X	0.69	0/398	0.71	0/546
12	L	0.68	0/393	0.83	0/526
12	Y	0.73	0/393	0.80	0/526
13	M	0.76	0/345	0.85	0/470
13	Z	0.67	0/345	0.79	0/470
All	All	0.75	2/29324 (0.0%)	0.83	12/39866 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	GLU	CD-OE2	5.34	1.31	1.25
2	B	198	GLU	CD-OE2	-5.27	1.19	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH1	-7.77	116.41	120.30
4	Q	20	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	N	240	HIS	CA-CB-CG	-6.09	103.24	113.60
10	J	36	MET	CG-SD-CE	-6.04	90.53	100.20
2	O	92	ASN	CB-CA-C	5.45	121.31	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	49	0
1	N	4027	0	4001	39	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	22	0
3	C	2110	0	2027	16	0
3	P	2110	0	2027	16	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	16	0
5	E	852	0	845	3	0
5	R	852	0	845	5	0
6	F	748	0	728	7	0
6	S	748	0	728	7	0
7	G	675	0	644	20	0
7	T	675	0	643	21	0
8	H	662	0	623	8	0
8	U	662	0	623	17	0
9	I	592	0	604	8	0
9	V	592	0	604	10	0
10	J	460	0	459	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	460	0	459	5	0
11	K	384	0	366	4	0
11	X	384	0	366	3	0
12	L	380	0	380	4	0
12	Y	380	0	380	13	0
13	M	335	0	352	5	0
13	Z	335	0	352	10	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	51	0	76	4	0
17	C	102	0	152	7	0
17	M	51	0	76	6	0
17	N	102	0	152	16	0
17	P	102	0	152	1	0
18	A	120	0	108	7	0
18	N	120	0	108	8	0
19	A	44	0	66	6	0
19	B	32	0	48	2	0
19	C	20	0	30	1	0
19	D	16	0	24	0	0
19	E	20	0	30	0	0
19	F	24	0	36	0	0
19	G	16	0	24	0	0
19	H	4	0	6	1	0
19	I	8	0	12	0	0
19	J	8	0	12	0	0
19	K	4	0	6	0	0
19	L	12	0	18	0	0
19	M	4	0	6	0	0
19	N	48	0	72	4	0
19	O	8	0	12	0	0
19	P	16	0	24	0	0
19	Q	16	0	24	0	0
19	R	8	0	12	1	0
19	S	24	0	36	1	0
19	T	8	0	12	0	0
19	U	4	0	6	3	0
19	V	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	W	8	0	12	0	0
20	A	63	0	110	0	0
20	D	63	0	110	10	0
20	L	63	0	110	3	0
20	N	189	0	330	11	0
21	A	1	0	0	1	0
21	N	1	0	0	1	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	8	0
23	R	52	0	80	6	0
24	B	29	0	39	1	0
24	C	58	0	78	1	0
24	G	29	0	39	0	0
24	J	29	0	39	2	0
24	P	58	0	78	1	0
24	T	29	0	39	4	0
24	W	29	0	39	1	0
24	Y	29	0	39	4	0
25	C	106	0	154	4	0
25	G	53	0	77	7	0
25	P	159	0	231	10	0
26	C	200	0	312	4	0
26	P	200	0	312	13	0
27	C	33	0	42	0	0
27	G	66	0	84	0	0
27	M	33	0	42	0	0
27	P	33	0	42	0	0
27	Z	33	0	42	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	2	0
29	V	9	0	8	3	0
30	A	215	0	0	7	0
30	B	149	0	0	6	0
30	C	111	0	0	1	0
30	D	98	0	0	2	0
30	E	81	0	0	0	0
30	F	85	0	0	0	0
30	G	45	0	0	0	0
30	H	50	0	0	2	0
30	I	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	J	32	0	0	1	0
30	K	24	0	0	2	0
30	L	24	0	0	3	0
30	M	23	0	0	3	0
30	N	184	0	0	7	0
30	O	111	0	0	1	0
30	P	96	0	0	2	0
30	Q	59	0	0	3	0
30	R	58	0	0	4	0
30	S	73	0	0	1	0
30	T	35	0	0	1	0
30	U	47	0	0	5	0
30	V	18	0	0	0	0
30	W	18	0	0	0	0
30	X	14	0	0	1	0
30	Y	6	0	0	1	0
30	Z	6	0	0	0	0
All	All	32913	0	32023	381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 381 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)
3:P:44:MET:HG3	30:P:495:HOH:O	1.49	1.11
7:G:11:TPO:HA	7:G:11:TPO:O3P	1.51	1.05
1:N:484:THR:HG23	30:N:870:HOH:O	1.58	1.03
23:B:302:PSC:H42	9:I:14:ALA:HB2	1.35	1.01
1:A:177:SER:HB2	7:T:10:GLY:HA2	1.46	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	499 (98%)	12 (2%)	1 (0%)	47	38
2	B	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
2	O	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	4 (3%)	4 (3%)	5	1
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
6	S	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
7	G	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	4
7	T	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	3	0
8	H	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	12	4
8	U	77/85 (91%)	68 (88%)	6 (8%)	3 (4%)	3	0
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3502/3614 (97%)	3393 (97%)	96 (3%)	13 (0%)	34	24

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
4	Q	6	VAL
4	Q	7	LYS
7	T	7	ASP
8	U	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	419 (98%)	7 (2%)	62	60
1	N	426/426 (100%)	419 (98%)	7 (2%)	62	60
2	B	210/210 (100%)	202 (96%)	8 (4%)	33	24
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	9
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	55
3	P	224/226 (99%)	220 (98%)	4 (2%)	59	55
4	D	128/129 (99%)	125 (98%)	3 (2%)	50	45
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	32
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	47
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	19
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	15
6	S	81/81 (100%)	77 (95%)	4 (5%)	25	15
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	3
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	20
8	U	71/75 (95%)	62 (87%)	9 (13%)	4	1
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	7
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	7
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	21
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	39
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	2
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	13
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	13
All	All	3040/3082 (99%)	2929 (96%)	111 (4%)	34	25

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	75	LEU
13	Z	41	LYS
4	Q	7	LYS
13	Z	34	LEU
9	V	18	ARG

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

Mol	Chain	Res	Type
6	S	54	ASN
6	S	80	GLN
9	V	70	GLN
4	D	109	HIS
4	D	101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	O	1	2	8,9,10	0.82	1 (12%)	7,9,11	1.25	1 (14%)
7	TPO	G	11	7	8,10,11	1.50	1 (12%)	10,14,16	1.03	1 (10%)
1	FME	N	1	1	8,9,10	0.41	0	7,9,11	0.97	0
2	FME	B	1	2	8,9,10	0.67	0	7,9,11	1.16	0
1	FME	A	1	1	8,9,10	0.52	0	7,9,11	0.94	0
7	TPO	T	11	7	8,10,11	1.52	1 (12%)	10,14,16	1.19	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
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	4/7/9/11	-
1	FME	A	1	1	-	0/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	3.81	1.66	1.59
7	G	11	TPO	P-OG1	3.62	1.66	1.59
2	O	1	FME	CG-SD	-2.11	1.70	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	11	TPO	P-OG1-CB	2.83	131.76	123.21
2	O	1	FME	CG-CB-CA	-2.44	106.18	112.95
7	G	11	TPO	O-C-CA	-2.26	118.87	124.78

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	3	0
2	B	1	FME	5	0
1	A	1	FME	1	0
7	T	11	TPO	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 151 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 141 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	$\# Z > 2$
19	EDO	A	612	-	3,3,3	0.28	0	2,2,2	0.21	0
19	EDO	V	104	-	3,3,3	0.57	0	2,2,2	0.83	0
19	EDO	B	308	-	3,3,3	0.29	0	2,2,2	0.20	0
17	PGV	N	606	-	50,50,50	0.50	0	53,56,56	0.68	1 (1%)
26	CDL	C	310	-	99,99,99	0.38	0	105,111,111	0.43	0
26	CDL	P	312	-	99,99,99	0.35	0	105,111,111	0.41	0
19	EDO	S	106	-	3,3,3	0.20	0	2,2,2	0.31	0
19	EDO	A	615	-	3,3,3	0.10	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	D	203	-	3,3,3	0.12	0	2,2,2	0.05	0
19	EDO	P	311	-	3,3,3	0.09	0	2,2,2	0.24	0
19	EDO	R	202	-	3,3,3	0.16	0	2,2,2	0.14	0
20	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.37	0
24	CHD	C	306	-	32,32,32	0.60	0	51,51,51	0.75	1 (1%)
29	SAC	V	101	-	7,8,9	0.53	0	8,9,11	1.38	1 (12%)
27	DMU	G	104	-	34,34,34	1.70	7 (20%)	45,45,45	1.77	15 (33%)
19	EDO	S	105	-	3,3,3	0.16	0	2,2,2	0.20	0
19	EDO	S	103	-	3,3,3	0.39	0	2,2,2	0.37	0
18	HEA	N	608	1	57,67,67	2.10	15 (26%)	61,103,103	2.48	25 (40%)
24	CHD	B	303	-	32,32,32	0.56	0	51,51,51	0.90	2 (3%)
19	EDO	W	303	-	3,3,3	0.10	0	2,2,2	0.17	0
19	EDO	R	203	-	3,3,3	0.01	0	2,2,2	0.10	0
18	HEA	N	607	1	57,67,67	1.85	15 (26%)	61,103,103	2.35	20 (32%)
24	CHD	Y	101	-	32,32,32	0.69	0	51,51,51	1.22	6 (11%)
19	EDO	N	617	-	3,3,3	0.23	0	2,2,2	0.34	0
19	EDO	C	309	-	3,3,3	0.12	0	2,2,2	0.28	0
19	EDO	N	613	-	3,3,3	0.21	0	2,2,2	0.09	0
19	EDO	B	306	-	3,3,3	0.35	0	2,2,2	0.28	0
29	SAC	I	101	-	7,8,9	0.62	0	8,9,11	0.89	0
19	EDO	G	103	-	3,3,3	0.39	0	2,2,2	0.57	0
19	EDO	M	103	-	3,3,3	0.11	0	2,2,2	0.33	0
19	EDO	S	104	-	3,3,3	0.22	0	2,2,2	0.15	0
20	TGL	N	618	-	62,62,62	0.31	0	65,65,65	0.39	0
19	EDO	A	616	-	3,3,3	0.12	0	2,2,2	0.47	0
19	EDO	I	102	-	3,3,3	0.07	0	2,2,2	0.11	0
20	TGL	N	605	-	62,62,62	0.37	0	65,65,65	0.49	1 (1%)
20	TGL	L	502	-	62,62,62	0.40	0	65,65,65	0.38	0
19	EDO	N	612	-	3,3,3	0.38	0	2,2,2	0.70	0
19	EDO	V	103	-	3,3,3	0.10	0	2,2,2	0.18	0
19	EDO	E	205	-	3,3,3	0.04	0	2,2,2	0.42	0
25	PEK	P	304	-	52,52,52	0.41	0	55,57,57	0.91	5 (9%)
19	EDO	A	607	-	3,3,3	0.40	0	2,2,2	0.63	0
17	PGV	P	306	-	50,50,50	0.49	0	53,56,56	0.55	1 (1%)
19	EDO	P	314	-	3,3,3	0.05	0	2,2,2	0.25	0
19	EDO	Q	1604	-	3,3,3	0.30	0	2,2,2	0.43	0
17	PGV	N	622	-	50,50,50	0.44	0	53,56,56	0.53	0
19	EDO	N	614	-	3,3,3	0.13	0	2,2,2	0.47	0
19	EDO	D	202	-	3,3,3	0.17	0	2,2,2	0.21	0
24	CHD	C	301	-	32,32,32	0.68	0	51,51,51	0.82	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	H	101	-	3,3,3	0.39	0	2,2,2	0.16	0
19	EDO	N	620	-	3,3,3	0.27	0	2,2,2	0.29	0
24	CHD	P	303	-	32,32,32	0.65	1 (3%)	51,51,51	0.70	0
19	EDO	A	610	-	3,3,3	0.11	0	2,2,2	0.08	0
19	EDO	B	310	-	3,3,3	0.08	0	2,2,2	0.18	0
19	EDO	A	611	-	3,3,3	0.35	0	2,2,2	0.31	0
23	PSC	R	201	-	51,51,51	0.39	0	57,59,59	0.50	0
19	EDO	L	501	-	3,3,3	0.16	0	2,2,2	0.15	0
17	PGV	A	604	-	50,50,50	0.57	0	53,56,56	0.70	1 (1%)
19	EDO	A	618	-	3,3,3	0.28	0	2,2,2	0.52	0
25	PEK	P	305	-	52,52,52	0.41	0	55,57,57	0.48	0
19	EDO	B	311	-	3,3,3	0.08	0	2,2,2	0.20	0
19	EDO	A	609	-	3,3,3	0.36	0	2,2,2	0.20	0
19	EDO	B	305	-	3,3,3	0.32	0	2,2,2	0.10	0
19	EDO	J	102	-	3,3,3	0.15	0	2,2,2	0.20	0
19	EDO	B	309	-	3,3,3	0.15	0	2,2,2	0.34	0
19	EDO	G	105	-	3,3,3	0.09	0	2,2,2	0.24	0
19	EDO	A	614	-	3,3,3	0.04	0	2,2,2	0.18	0
19	EDO	S	102	-	3,3,3	0.48	0	2,2,2	0.35	0
19	EDO	J	103	-	3,3,3	0.42	0	2,2,2	0.20	0
27	DMU	C	311	-	34,34,34	1.89	8 (23%)	45,45,45	2.16	12 (26%)
27	DMU	G	101	-	34,34,34	2.13	7 (20%)	45,45,45	2.00	11 (24%)
17	PGV	P	307	-	50,50,50	0.34	0	53,56,56	0.43	0
27	DMU	M	102	-	34,34,34	1.62	5 (14%)	45,45,45	1.69	9 (20%)
19	EDO	O	302	-	3,3,3	0.03	0	2,2,2	0.23	0
19	EDO	D	204	-	3,3,3	0.21	0	2,2,2	0.17	0
19	EDO	I	103	-	3,3,3	0.46	0	2,2,2	0.28	0
19	EDO	V	102	-	3,3,3	0.12	0	2,2,2	0.38	0
19	EDO	S	107	-	3,3,3	0.09	0	2,2,2	0.72	0
24	CHD	W	302	-	32,32,32	0.58	0	51,51,51	0.70	1 (1%)
19	EDO	G	108	-	3,3,3	0.07	0	2,2,2	0.23	0
23	PSC	B	302	-	51,51,51	0.50	0	57,59,59	0.58	0
19	EDO	F	702	-	3,3,3	0.27	0	2,2,2	0.10	0
19	EDO	D	205	-	3,3,3	0.10	0	2,2,2	0.31	0
19	EDO	U	1501	-	3,3,3	0.31	0	2,2,2	0.40	0
19	EDO	B	307	-	3,3,3	0.27	0	2,2,2	0.29	0
25	PEK	C	302	-	52,52,52	0.43	0	55,57,57	0.55	1 (1%)
19	EDO	C	312	-	3,3,3	0.67	0	2,2,2	0.92	0
19	EDO	P	313	-	3,3,3	0.57	0	2,2,2	0.50	0
27	DMU	P	302	-	34,34,34	0.91	3 (8%)	45,45,45	1.65	8 (17%)
22	CUA	O	301	2	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PGV	C	303	-	50,50,50	0.42	0	53,56,56	0.54	0
20	TGL	A	613	-	62,62,62	0.43	0	65,65,65	0.79	1 (1%)
19	EDO	E	203	-	3,3,3	0.15	0	2,2,2	0.08	0
19	EDO	W	301	-	3,3,3	0.09	0	2,2,2	0.04	0
26	CDL	C	305	-	99,99,99	0.38	0	105,111,111	0.69	4 (3%)
19	EDO	F	706	-	3,3,3	0.32	0	2,2,2	0.19	0
19	EDO	T	1301	-	3,3,3	0.36	0	2,2,2	0.18	0
19	EDO	F	707	-	3,3,3	0.13	0	2,2,2	0.13	0
19	EDO	L	504	-	3,3,3	0.12	0	2,2,2	0.23	0
24	CHD	P	309	-	32,32,32	0.65	0	51,51,51	1.09	3 (5%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-
19	EDO	C	313	-	3,3,3	0.35	0	2,2,2	0.09	0
19	EDO	T	1303	-	3,3,3	0.31	0	2,2,2	0.15	0
19	EDO	N	611	-	3,3,3	0.23	0	2,2,2	0.31	0
19	EDO	Q	1603	-	3,3,3	0.15	0	2,2,2	0.23	0
19	EDO	F	704	-	3,3,3	0.10	0	2,2,2	0.27	0
19	EDO	B	304	-	3,3,3	0.27	0	2,2,2	0.32	0
19	EDO	F	701	-	3,3,3	0.23	0	2,2,2	0.52	0
19	EDO	P	310	-	3,3,3	0.07	0	2,2,2	0.19	0
27	DMU	Z	101	-	34,34,34	0.99	2 (5%)	45,45,45	1.46	9 (20%)
17	PGV	M	101	-	50,50,50	0.48	0	53,56,56	0.79	2 (3%)
19	EDO	C	307	-	3,3,3	0.46	0	2,2,2	0.39	0
19	EDO	E	204	-	3,3,3	0.10	0	2,2,2	0.07	0
26	CDL	P	308	-	99,99,99	0.37	0	105,111,111	0.49	1 (0%)
19	EDO	A	608	-	3,3,3	0.34	0	2,2,2	0.07	0
18	HEA	A	606	1	57,67,67	1.74	10 (17%)	61,103,103	2.68	27 (44%)
25	PEK	P	301	-	52,52,52	0.36	0	55,57,57	0.60	1 (1%)
19	EDO	N	609	-	3,3,3	0.15	0	2,2,2	0.51	0
19	EDO	Q	1601	-	3,3,3	0.11	0	2,2,2	0.07	0
24	CHD	G	107	-	32,32,32	0.64	0	51,51,51	0.75	0
19	EDO	E	202	-	3,3,3	0.18	0	2,2,2	0.35	0
17	PGV	C	304	-	50,50,50	0.50	0	53,56,56	0.65	0
19	EDO	N	619	-	3,3,3	0.12	0	2,2,2	0.12	0
19	EDO	C	308	-	3,3,3	0.13	0	2,2,2	0.22	0
19	EDO	O	303	-	3,3,3	0.39	0	2,2,2	0.05	0
19	EDO	N	616	-	3,3,3	0.16	0	2,2,2	0.31	0
25	PEK	C	314	-	52,52,52	0.41	0	55,57,57	0.59	0
19	EDO	A	617	-	3,3,3	0.30	0	2,2,2	0.58	0
19	EDO	E	201	-	3,3,3	0.08	0	2,2,2	0.11	0
19	EDO	N	621	-	3,3,3	0.31	0	2,2,2	0.52	0
24	CHD	J	101	-	32,32,32	0.62	1 (3%)	51,51,51	0.96	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	G	102	-	52,52,52	0.47	0	55,57,57	0.66	0
19	EDO	K	201	-	3,3,3	0.10	0	2,2,2	0.15	0
18	HEA	A	605	1	57,67,67	1.64	10 (17%)	61,103,103	2.38	25 (40%)
19	EDO	F	705	-	3,3,3	0.35	0	2,2,2	0.36	0
19	EDO	N	615	-	3,3,3	0.63	0	2,2,2	0.66	0
19	EDO	N	610	-	3,3,3	0.43	0	2,2,2	0.09	0
19	EDO	Q	1602	-	3,3,3	0.17	0	2,2,2	0.21	0
19	EDO	L	503	-	3,3,3	0.09	0	2,2,2	0.10	0
20	TGL	N	604	-	62,62,62	0.34	0	65,65,65	0.59	1 (1%)
24	CHD	T	1302	-	32,32,32	0.63	0	51,51,51	0.99	1 (1%)
19	EDO	G	106	-	3,3,3	0.23	0	2,2,2	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	A	612	-	-	0/1/1/1	-
19	EDO	V	104	-	-	0/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
17	PGV	N	606	-	-	9/55/55/55	-
26	CDL	C	310	-	-	53/110/110/110	-
26	CDL	P	312	-	-	53/110/110/110	-
19	EDO	S	106	-	-	1/1/1/1	-
19	EDO	A	615	-	-	0/1/1/1	-
19	EDO	D	203	-	-	0/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
19	EDO	R	202	-	-	0/1/1/1	-
20	TGL	D	201	-	-	30/65/65/65	-
24	CHD	C	306	-	-	2/9/74/74	0/4/4/4
29	SAC	V	101	-	-	2/7/8/10	-
27	DMU	G	104	-	-	11/19/59/59	0/2/2/2
19	EDO	S	105	-	-	1/1/1/1	-
19	EDO	S	103	-	-	1/1/1/1	-
18	HEA	N	608	1	3/3/7/16	4/32/76/76	-
24	CHD	B	303	-	-	2/9/74/74	0/4/4/4
19	EDO	W	303	-	-	1/1/1/1	-
19	EDO	R	203	-	-	1/1/1/1	-
18	HEA	N	607	1	3/3/7/16	4/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	Y	101	-	-	9/9/74/74	1/4/4/4
19	EDO	N	617	-	-	1/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	613	-	-	0/1/1/1	-
19	EDO	B	306	-	-	0/1/1/1	-
29	SAC	I	101	-	-	5/7/8/10	-
19	EDO	G	103	-	-	0/1/1/1	-
19	EDO	M	103	-	-	1/1/1/1	-
19	EDO	S	104	-	-	0/1/1/1	-
20	TGL	N	618	-	-	38/65/65/65	-
19	EDO	A	616	-	-	1/1/1/1	-
19	EDO	I	102	-	-	1/1/1/1	-
20	TGL	N	605	-	-	34/65/65/65	-
20	TGL	L	502	-	-	39/65/65/65	-
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	V	103	-	-	1/1/1/1	-
19	EDO	E	205	-	-	1/1/1/1	-
25	PEK	P	304	-	-	19/56/56/56	-
19	EDO	A	607	-	-	0/1/1/1	-
17	PGV	P	306	-	-	15/55/55/55	-
19	EDO	P	314	-	-	0/1/1/1	-
19	EDO	Q	1604	-	-	1/1/1/1	-
17	PGV	N	622	-	-	25/55/55/55	-
19	EDO	N	614	-	-	1/1/1/1	-
19	EDO	D	202	-	-	1/1/1/1	-
24	CHD	C	301	-	-	1/9/74/74	0/4/4/4
19	EDO	H	101	-	-	1/1/1/1	-
19	EDO	N	620	-	-	1/1/1/1	-
24	CHD	P	303	-	-	2/9/74/74	0/4/4/4
19	EDO	A	610	-	-	1/1/1/1	-
19	EDO	B	310	-	-	1/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-
23	PSC	R	201	-	-	35/55/55/55	-
19	EDO	L	501	-	-	1/1/1/1	-
17	PGV	A	604	-	-	14/55/55/55	-
19	EDO	A	618	-	-	0/1/1/1	-
25	PEK	P	305	-	-	30/56/56/56	-
19	EDO	B	311	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	B	305	-	-	0/1/1/1	-
19	EDO	J	102	-	-	0/1/1/1	-
19	EDO	B	309	-	-	1/1/1/1	-
19	EDO	G	105	-	-	1/1/1/1	-
19	EDO	A	614	-	-	0/1/1/1	-
19	EDO	S	102	-	-	1/1/1/1	-
19	EDO	J	103	-	-	0/1/1/1	-
27	DMU	C	311	-	-	7/19/59/59	0/2/2/2
27	DMU	G	101	-	-	14/19/59/59	0/2/2/2
17	PGV	P	307	-	-	30/55/55/55	-
27	DMU	M	102	-	-	7/19/59/59	0/2/2/2
19	EDO	O	302	-	-	1/1/1/1	-
19	EDO	D	204	-	-	0/1/1/1	-
19	EDO	I	103	-	-	0/1/1/1	-
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	S	107	-	-	0/1/1/1	-
24	CHD	W	302	-	-	1/9/74/74	0/4/4/4
19	EDO	G	108	-	-	1/1/1/1	-
23	PSC	B	302	-	-	28/55/55/55	-
19	EDO	F	702	-	-	1/1/1/1	-
19	EDO	D	205	-	-	0/1/1/1	-
19	EDO	U	1501	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-
25	PEK	C	302	-	-	28/56/56/56	-
19	EDO	C	312	-	-	0/1/1/1	-
19	EDO	P	313	-	-	0/1/1/1	-
27	DMU	P	302	-	-	9/19/59/59	0/2/2/2
17	PGV	C	303	-	-	15/55/55/55	-
20	TGL	A	613	-	-	37/65/65/65	-
19	EDO	E	203	-	-	1/1/1/1	-
19	EDO	W	301	-	-	0/1/1/1	-
26	CDL	C	305	-	-	66/110/110/110	-
19	EDO	F	706	-	-	0/1/1/1	-
19	EDO	T	1301	-	-	1/1/1/1	-
19	EDO	F	707	-	-	0/1/1/1	-
19	EDO	L	504	-	-	0/1/1/1	-
24	CHD	P	309	-	-	2/9/74/74	0/4/4/4
19	EDO	C	313	-	-	1/1/1/1	-
19	EDO	T	1303	-	-	1/1/1/1	-
19	EDO	N	611	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	Q	1603	-	-	1/1/1/1	-
19	EDO	F	704	-	-	0/1/1/1	-
19	EDO	B	304	-	-	0/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-
19	EDO	P	310	-	-	1/1/1/1	-
27	DMU	Z	101	-	-	8/19/59/59	0/2/2/2
17	PGV	M	101	-	-	40/55/55/55	-
19	EDO	C	307	-	-	1/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
26	CDL	P	308	-	-	58/110/110/110	-
19	EDO	A	608	-	-	0/1/1/1	-
18	HEA	A	606	1	2/2/7/16	1/32/76/76	-
25	PEK	P	301	-	-	34/56/56/56	-
19	EDO	N	609	-	-	1/1/1/1	-
19	EDO	Q	1601	-	-	1/1/1/1	-
24	CHD	G	107	-	-	3/9/74/74	0/4/4/4
19	EDO	E	202	-	-	1/1/1/1	-
17	PGV	C	304	-	-	29/55/55/55	-
19	EDO	N	619	-	-	1/1/1/1	-
19	EDO	C	308	-	-	0/1/1/1	-
19	EDO	O	303	-	-	0/1/1/1	-
19	EDO	N	616	-	-	1/1/1/1	-
25	PEK	C	314	-	-	30/56/56/56	-
19	EDO	A	617	-	-	0/1/1/1	-
19	EDO	E	201	-	-	1/1/1/1	-
19	EDO	N	621	-	-	1/1/1/1	-
24	CHD	J	101	-	-	3/9/74/74	0/4/4/4
25	PEK	G	102	-	-	21/56/56/56	-
19	EDO	K	201	-	-	1/1/1/1	-
18	HEA	A	605	1	3/3/7/16	4/32/76/76	-
19	EDO	F	705	-	-	0/1/1/1	-
19	EDO	N	615	-	-	0/1/1/1	-
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	Q	1602	-	-	0/1/1/1	-
19	EDO	L	503	-	-	1/1/1/1	-
20	TGL	N	604	-	-	29/65/65/65	-
24	CHD	T	1302	-	-	6/9/74/74	1/4/4/4
19	EDO	G	106	-	-	1/1/1/1	-

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	101	DMU	O16-C6	8.88	1.55	1.40
27	C	311	DMU	O16-C6	6.77	1.51	1.40
27	M	102	DMU	O16-C6	6.43	1.51	1.40
18	N	608	HEA	C1D-ND	-5.43	1.31	1.40
18	N	608	HEA	C3C-C2C	4.90	1.47	1.40

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	311	DMU	C18-O16-C6	8.17	127.38	113.84
27	G	101	DMU	C18-O16-C6	7.56	126.37	113.84
18	A	606	HEA	C3D-C4D-ND	7.45	117.58	110.36
18	N	607	HEA	CAD-CBD-CGD	-6.92	98.70	113.60
27	P	302	DMU	C6-O5-C4	6.21	125.87	113.69

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	605	HEA	NA
18	A	605	HEA	NB
18	A	605	HEA	ND
18	A	606	HEA	NB
18	A	606	HEA	ND

5 of 999 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	304	PGV	C03-O11-P-O12
17	C	304	PGV	C03-O11-P-O14
17	C	304	PGV	C04-O12-P-O13
17	C	304	PGV	C04-O12-P-O14
17	M	101	PGV	O03-C01-C02-O01

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	Y	101	CHD	C1-C10-C2-C3-C4-C5
24	T	1302	CHD	C1-C10-C2-C3-C4-C5

52 monomers are involved in 160 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	612	EDO	1	0

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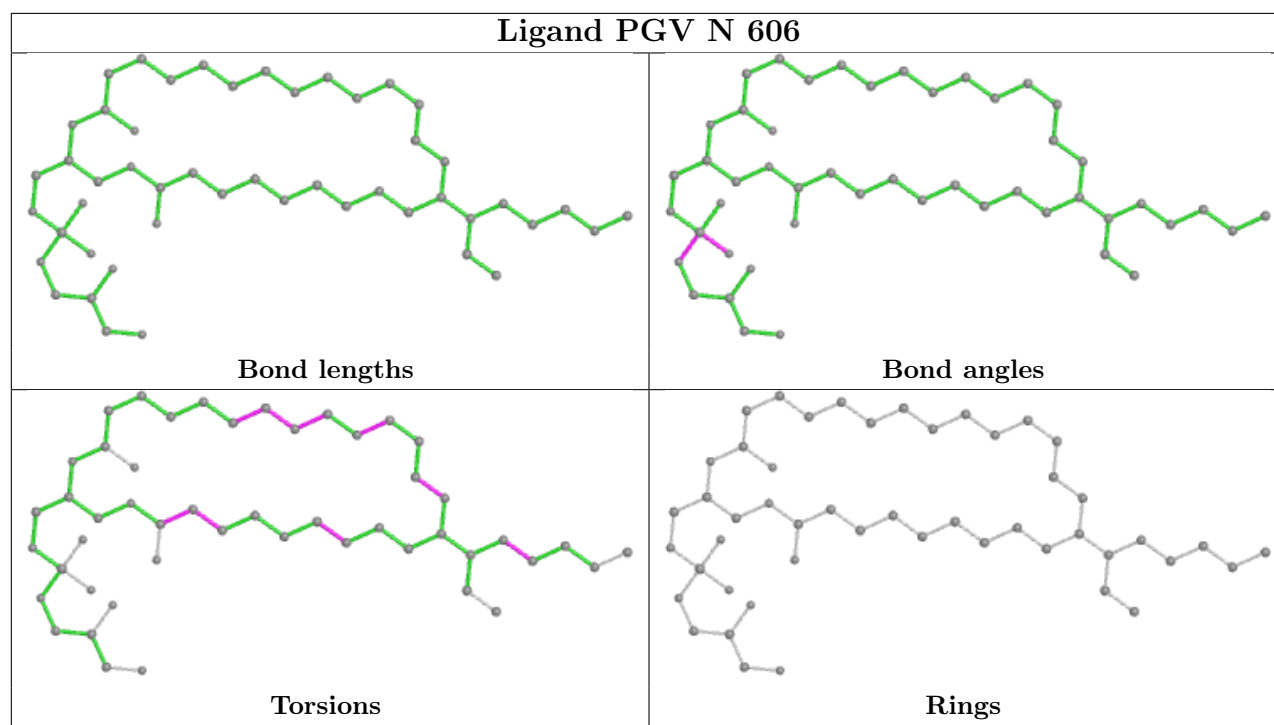
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	310	CDL	2	0
26	P	312	CDL	10	0
19	S	106	EDO	1	0
19	A	615	EDO	1	0
20	D	201	TGL	10	0
29	V	101	SAC	3	0
18	N	608	HEA	4	0
24	B	303	CHD	1	0
19	R	203	EDO	1	0
18	N	607	HEA	4	0
24	Y	101	CHD	4	0
29	I	101	SAC	2	0
20	N	618	TGL	5	0
20	N	605	TGL	6	0
20	L	502	TGL	3	0
19	N	612	EDO	2	0
19	V	103	EDO	1	0
25	P	304	PEK	4	0
17	N	622	PGV	16	0
24	C	301	CHD	1	0
19	H	101	EDO	1	0
24	P	303	CHD	1	0
19	A	611	EDO	1	0
23	R	201	PSC	6	0
17	A	604	PGV	4	0
19	A	618	EDO	2	0
25	P	305	PEK	5	0
19	B	311	EDO	1	0
19	B	305	EDO	1	0
19	A	614	EDO	1	0
17	P	307	PGV	1	0
24	W	302	CHD	1	0
23	B	302	PSC	8	0
19	U	1501	EDO	3	0
25	C	302	PEK	3	0
19	C	312	EDO	1	0
17	C	303	PGV	1	0
26	C	305	CDL	2	0
19	N	611	EDO	1	0
27	Z	101	DMU	4	0
17	M	101	PGV	6	0
26	P	308	CDL	3	0

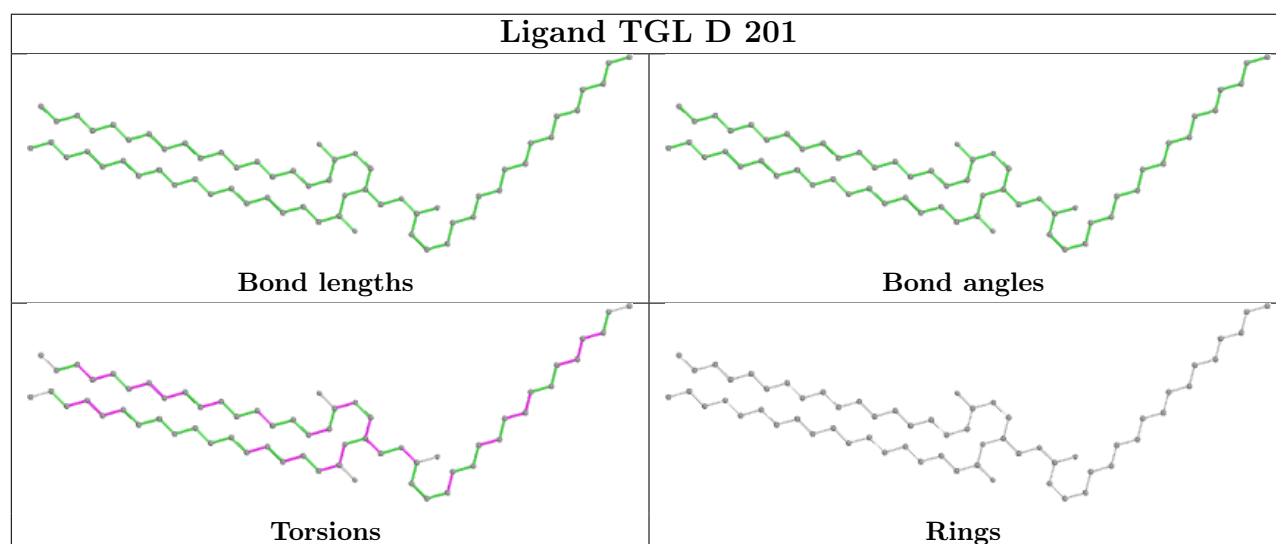
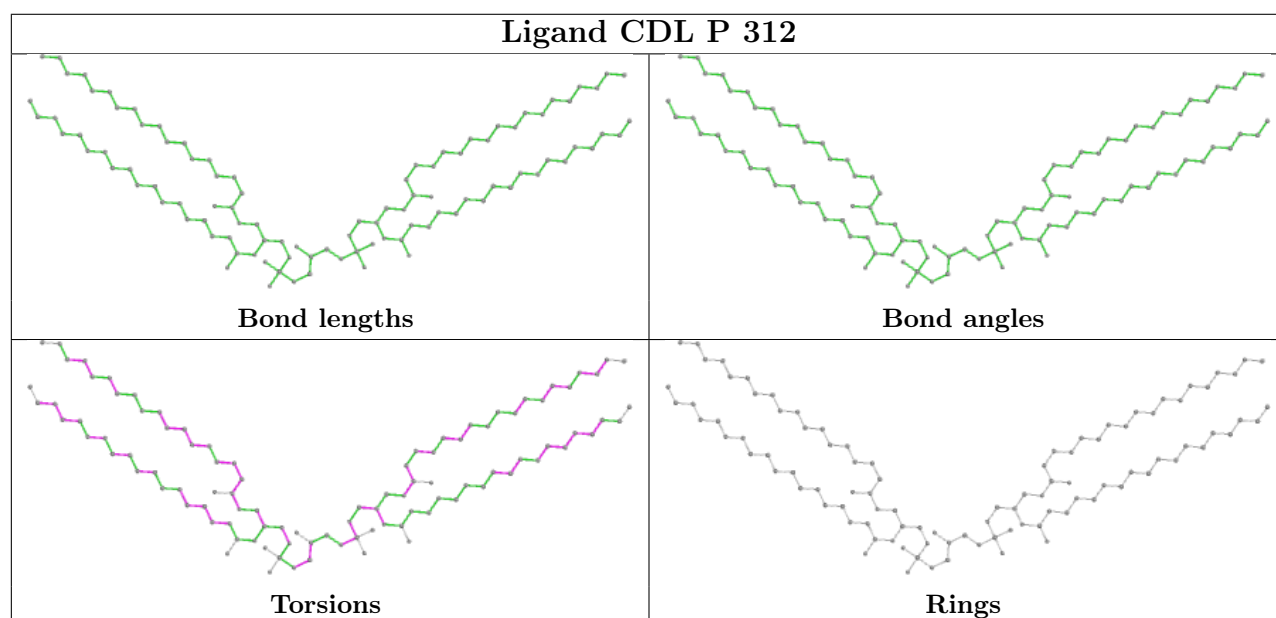
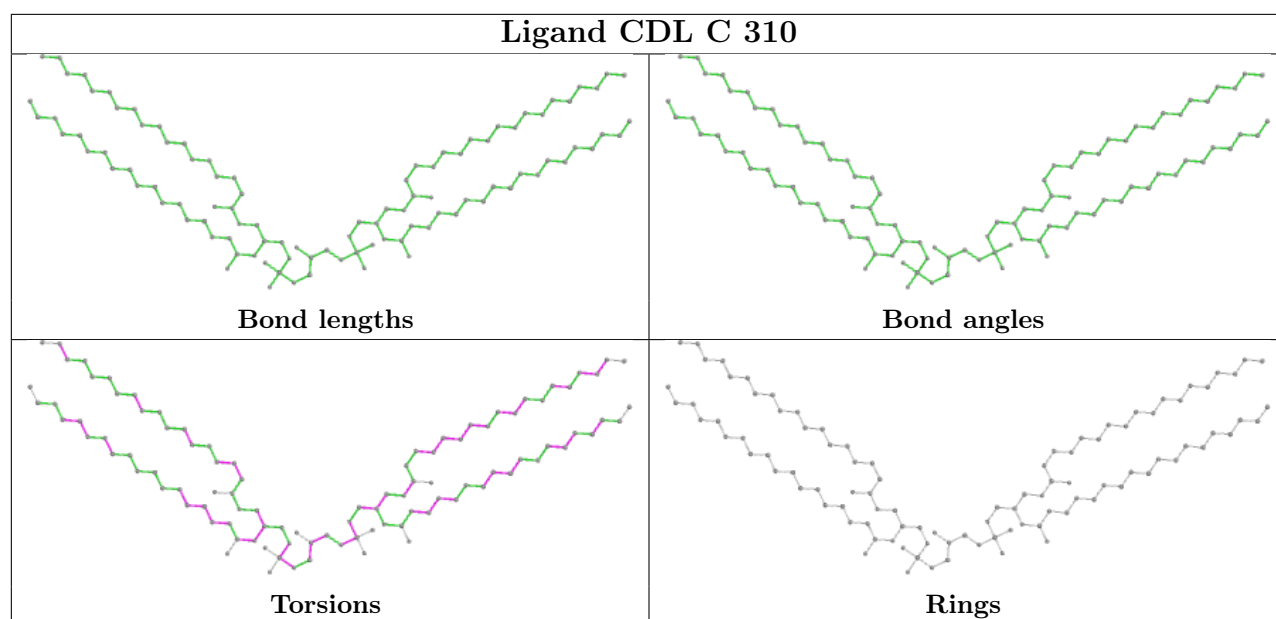
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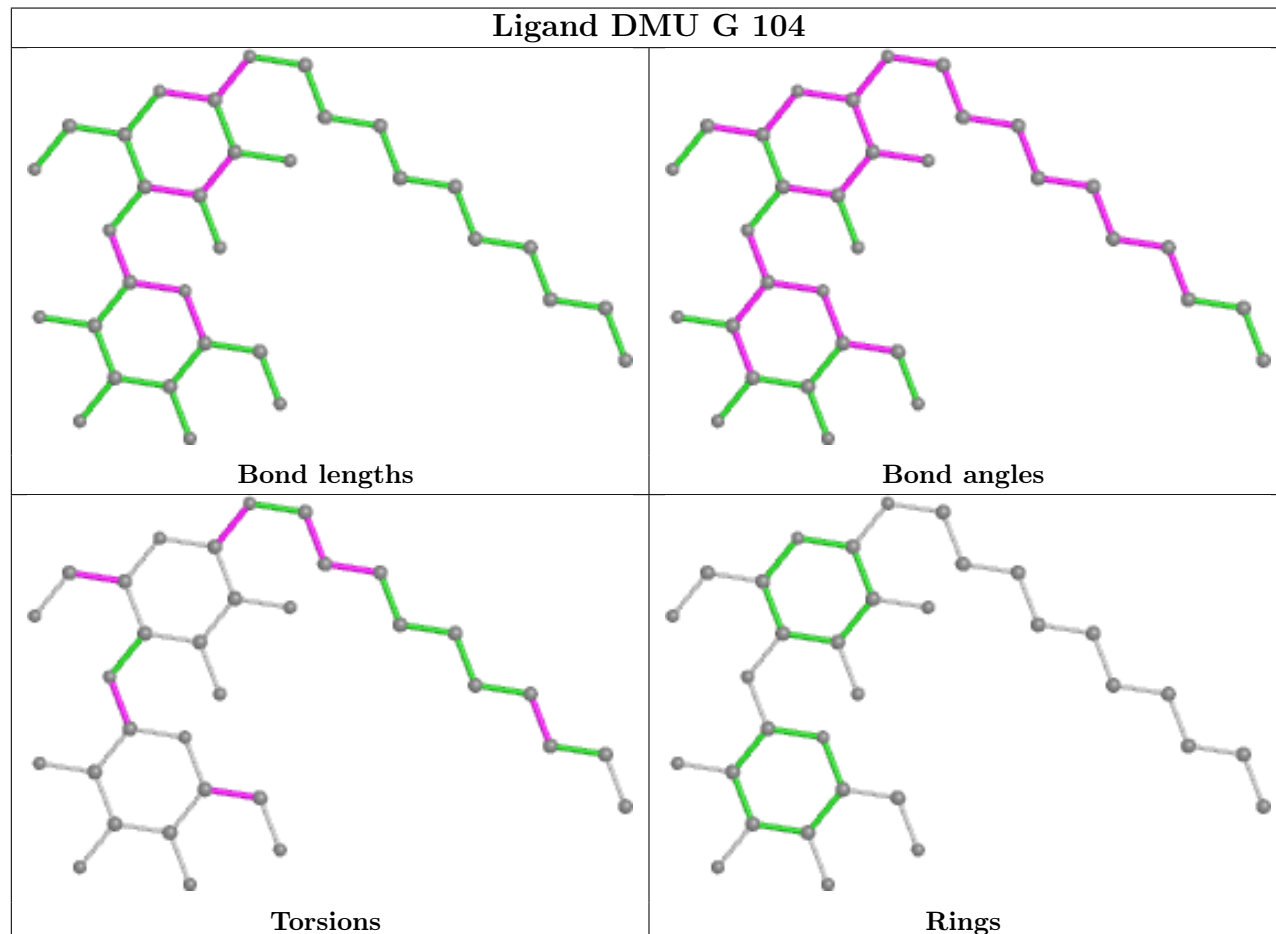
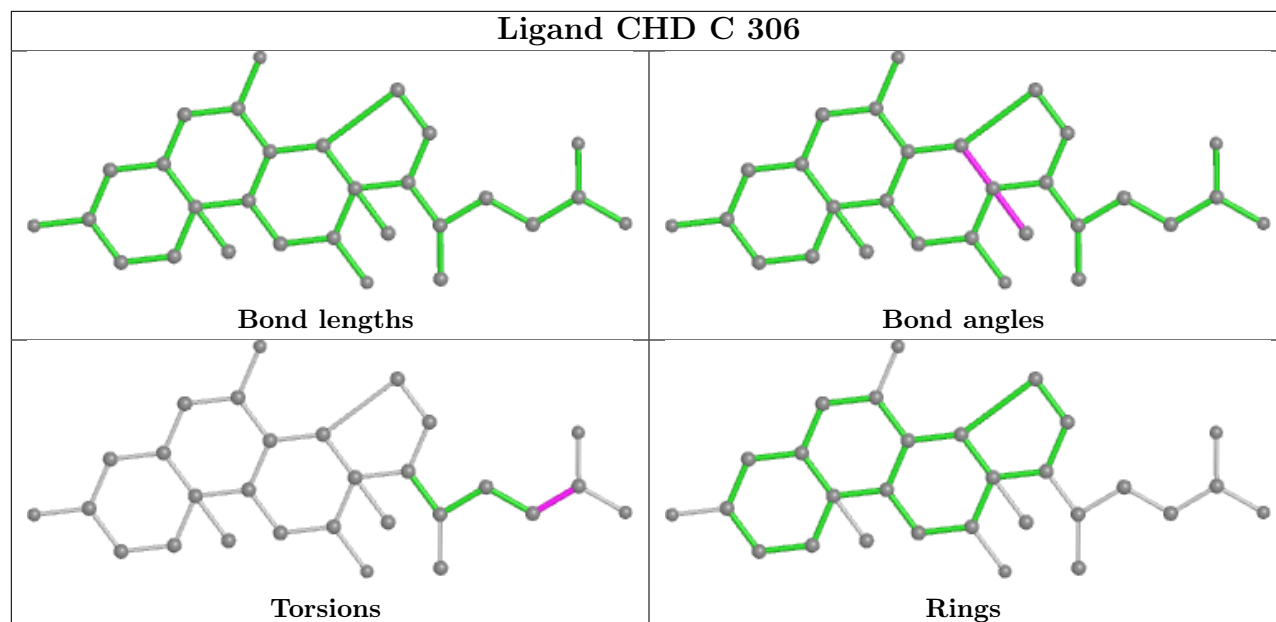
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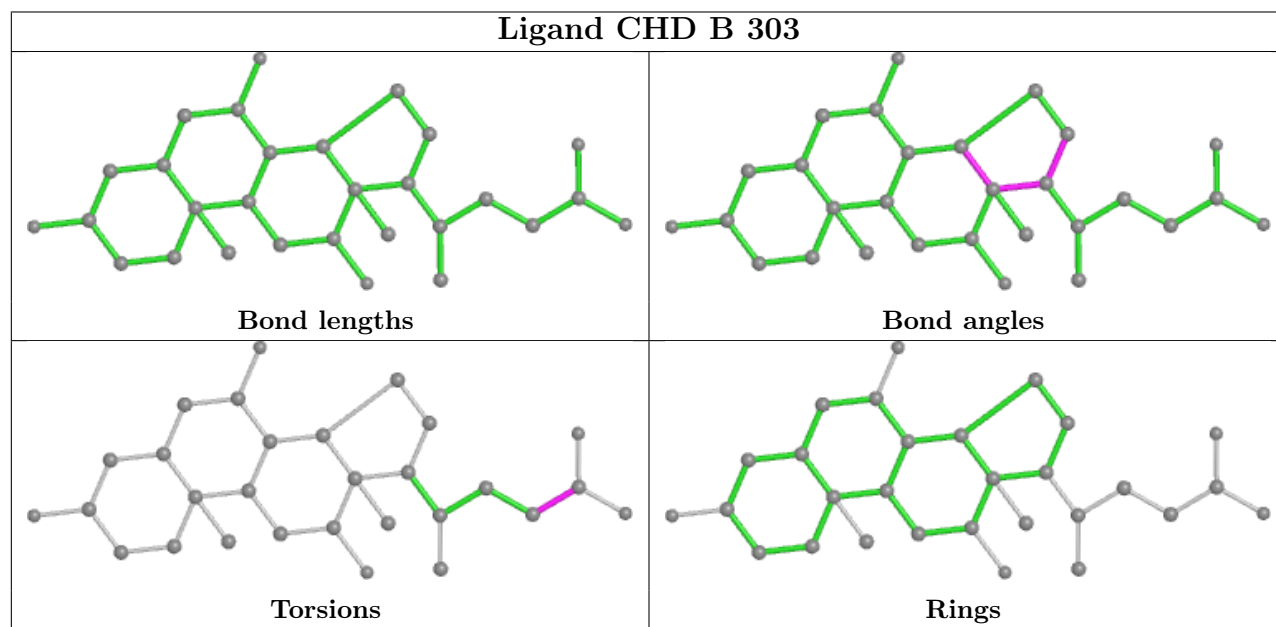
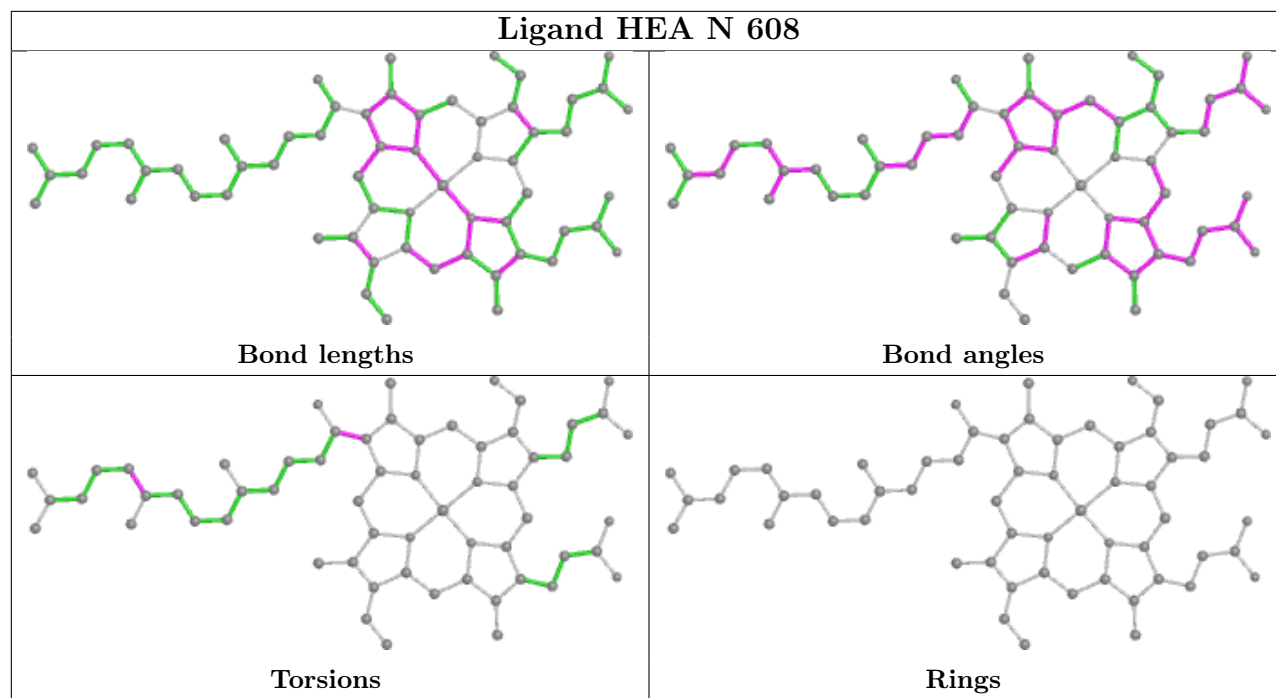
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	606	HEA	3	0
25	P	301	PEK	1	0
17	C	304	PGV	6	0
25	C	314	PEK	1	0
24	J	101	CHD	2	0
25	G	102	PEK	7	0
18	A	605	HEA	4	0
19	N	615	EDO	1	0
24	T	1302	CHD	4	0

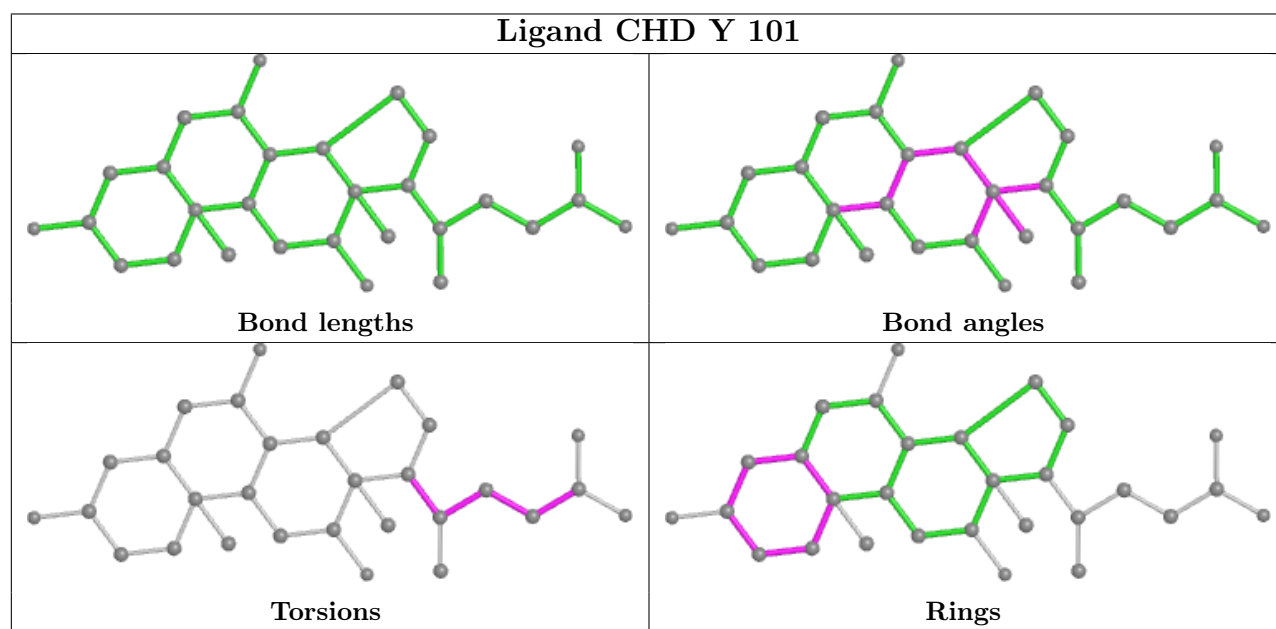
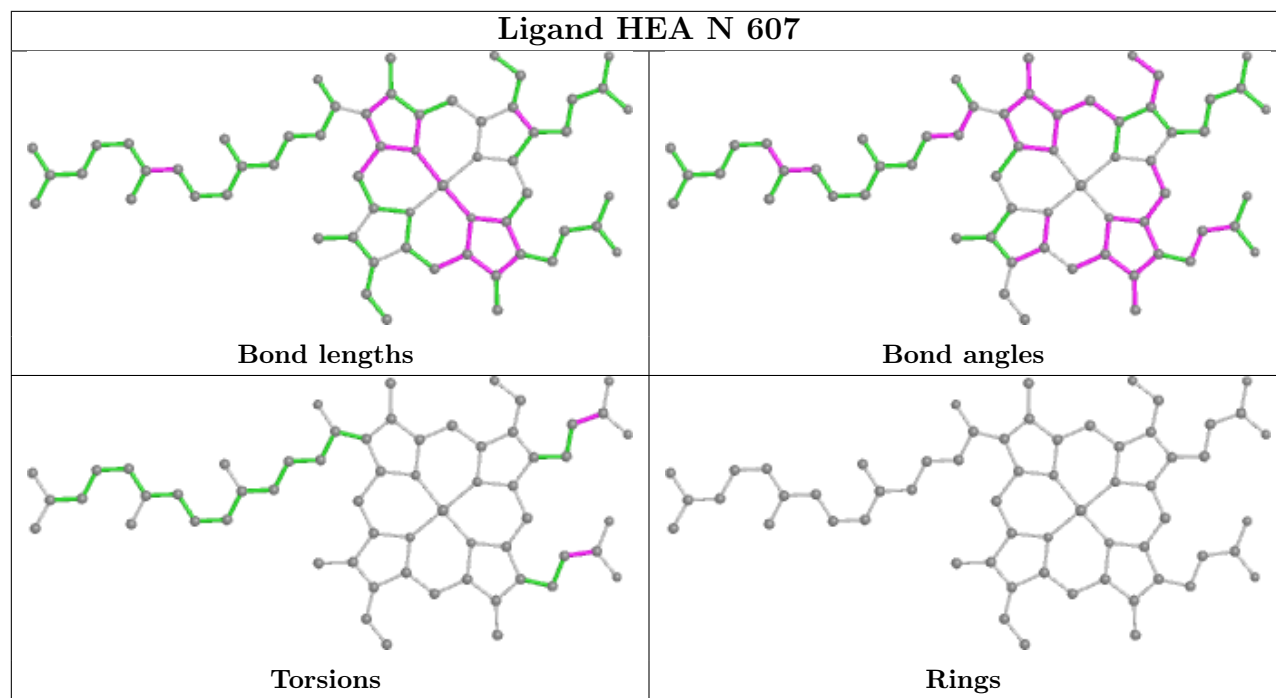
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

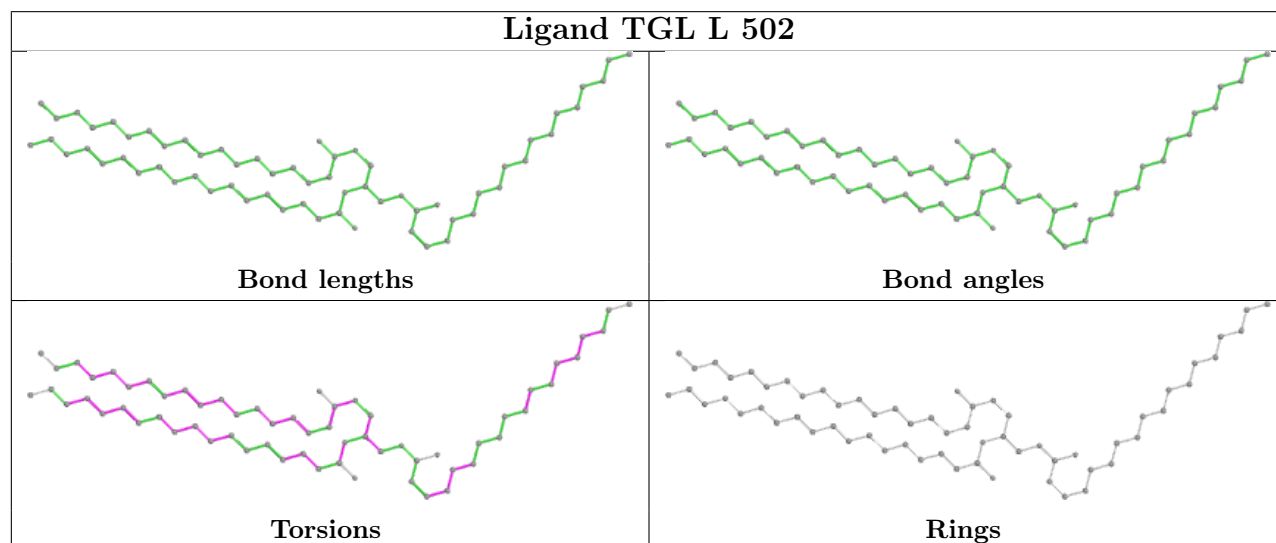
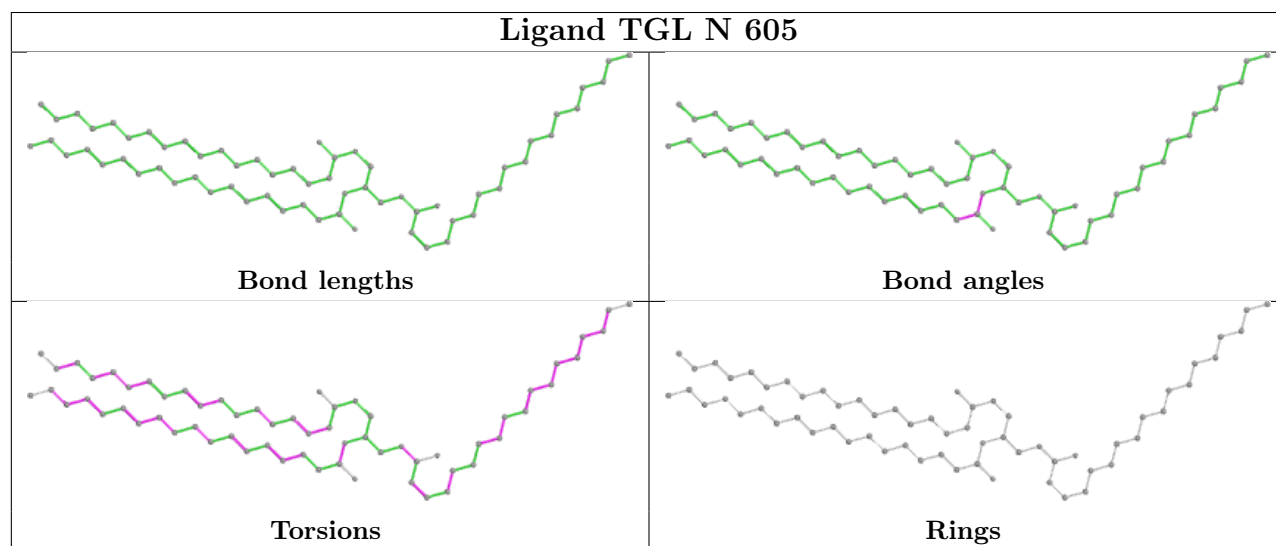
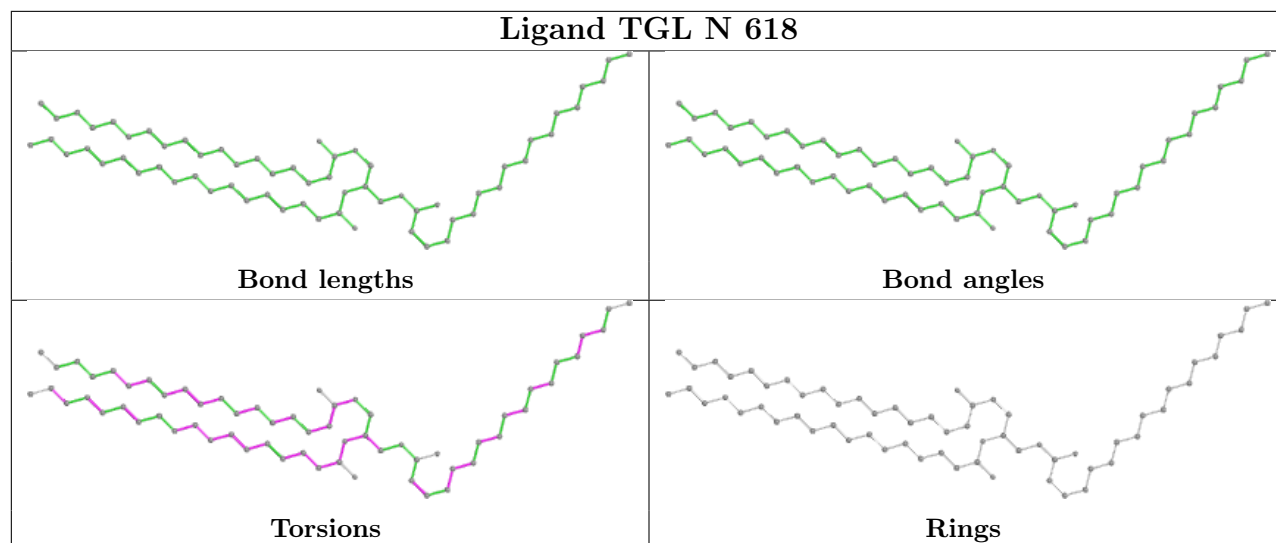


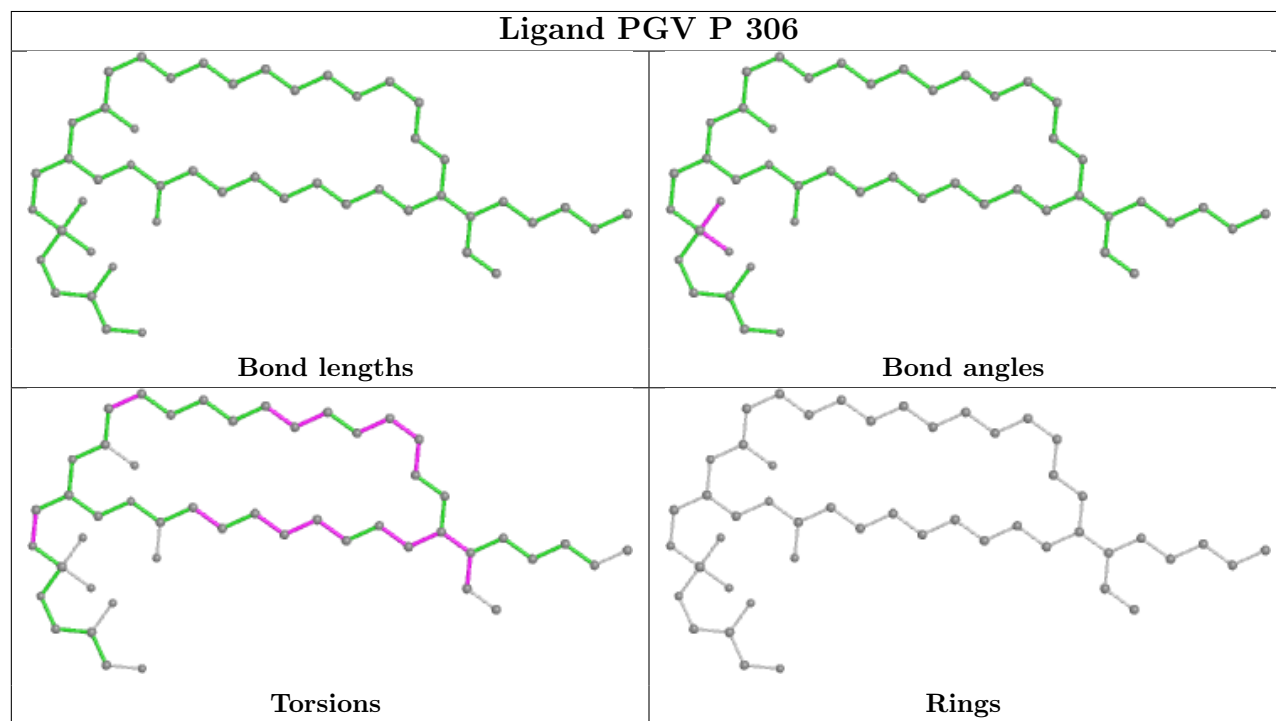
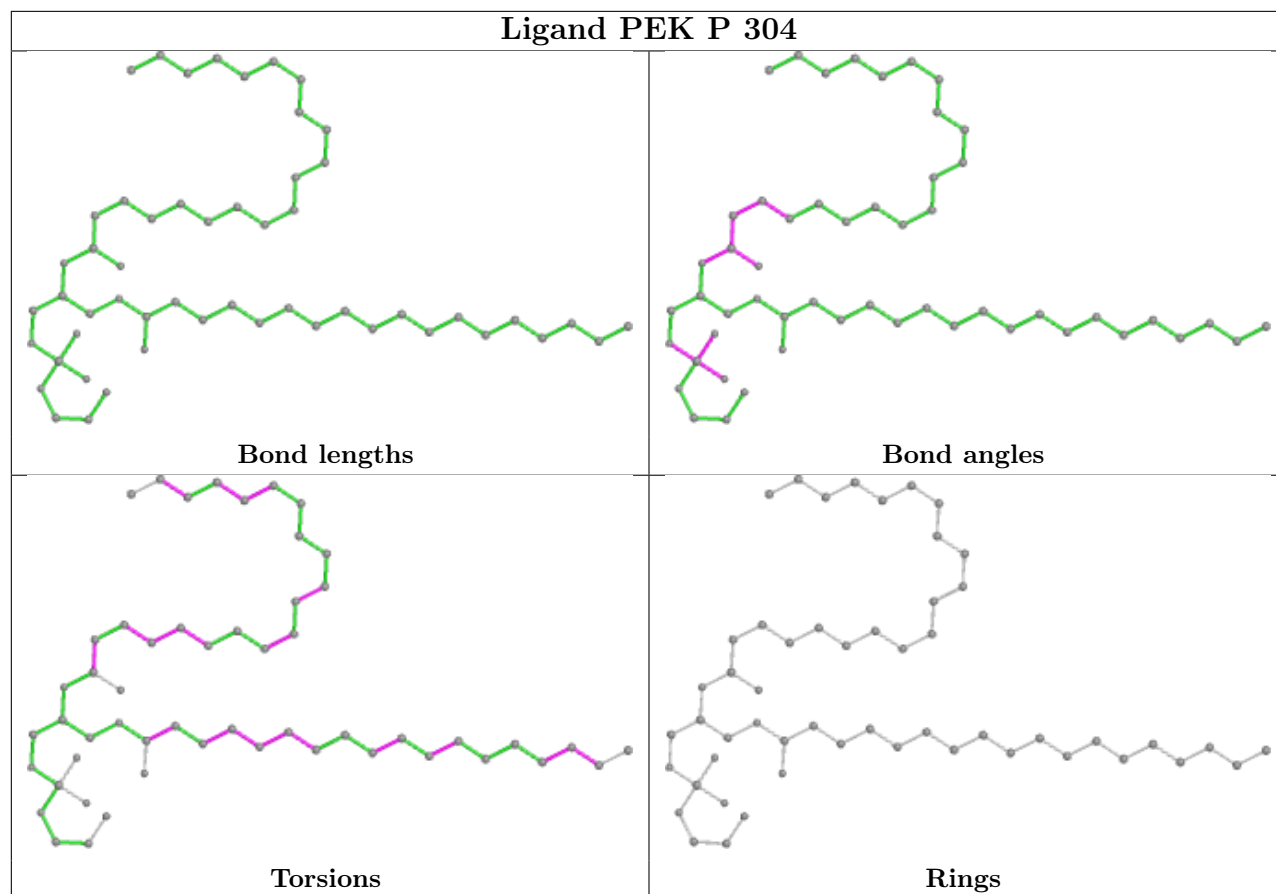


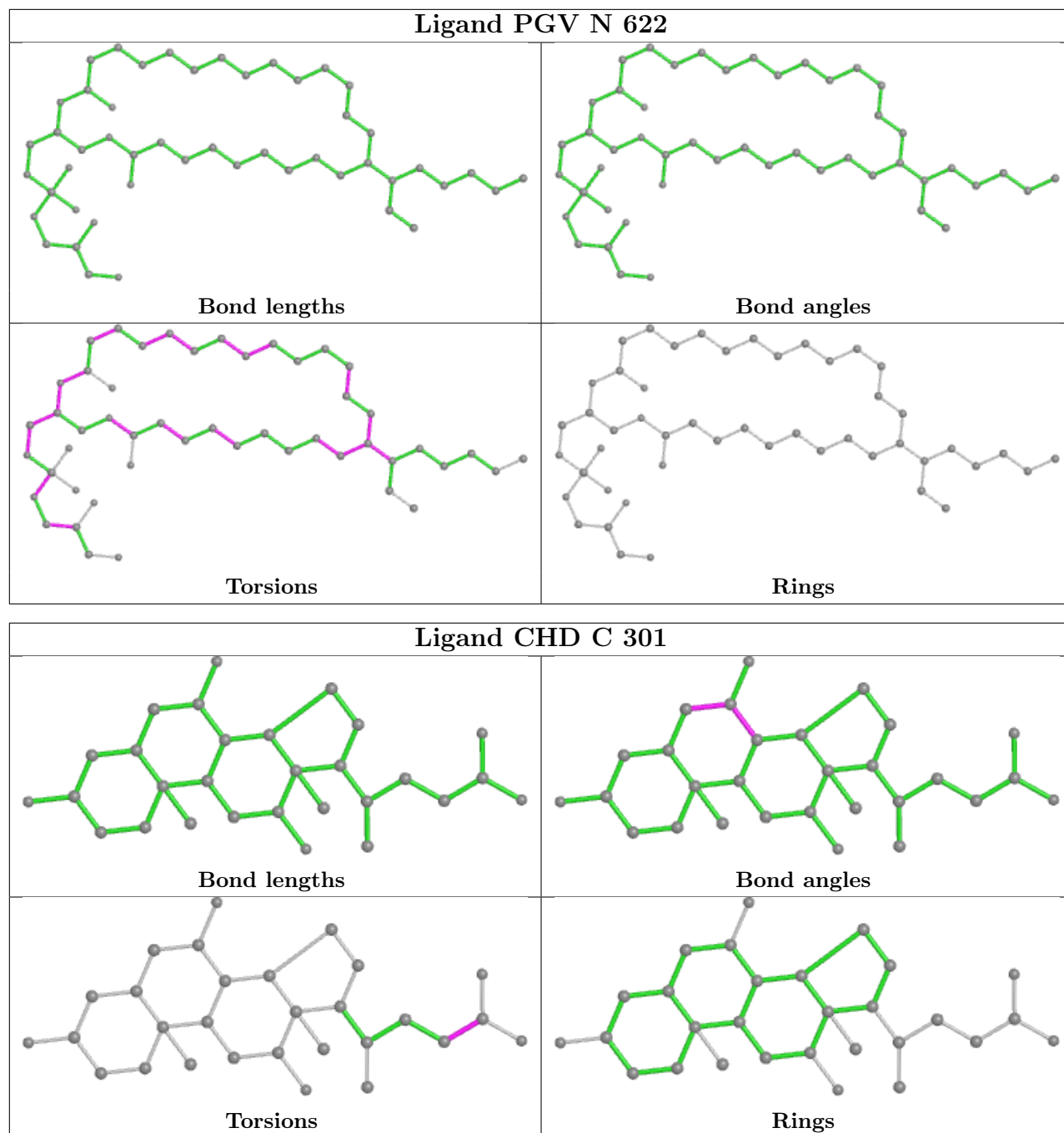


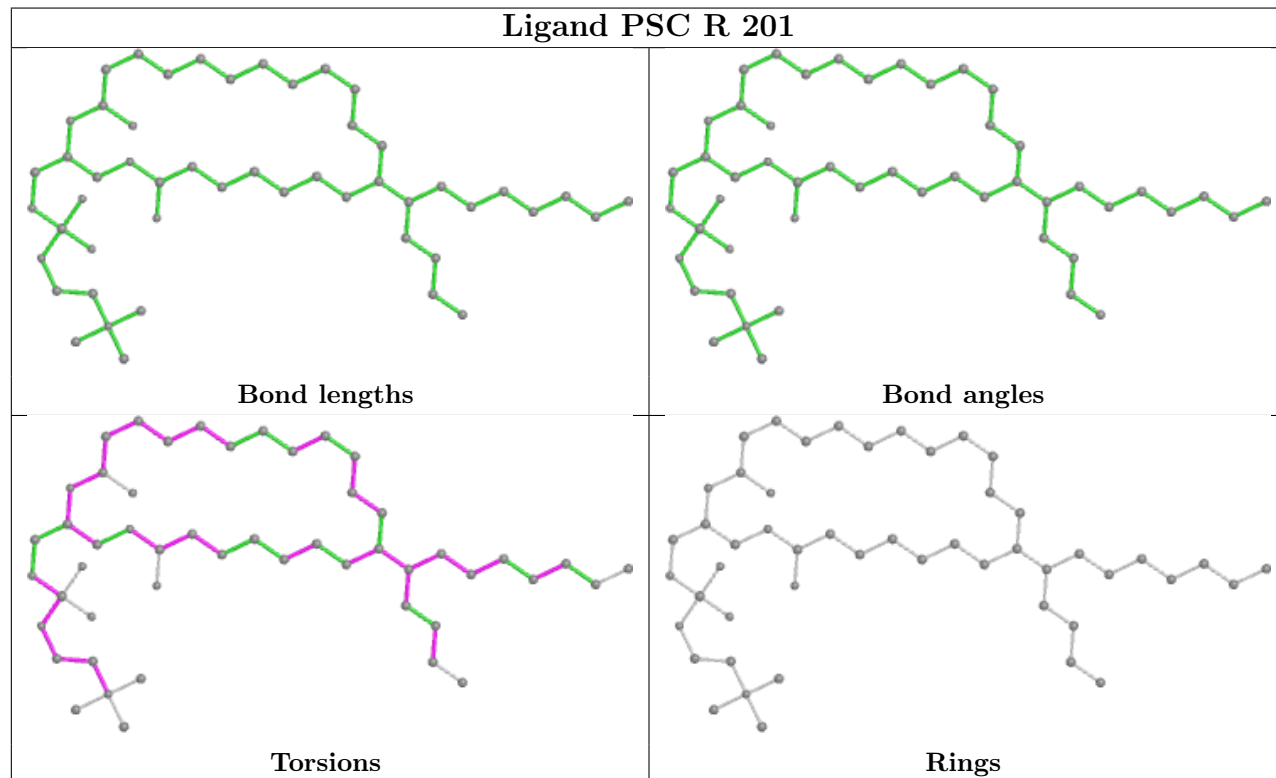
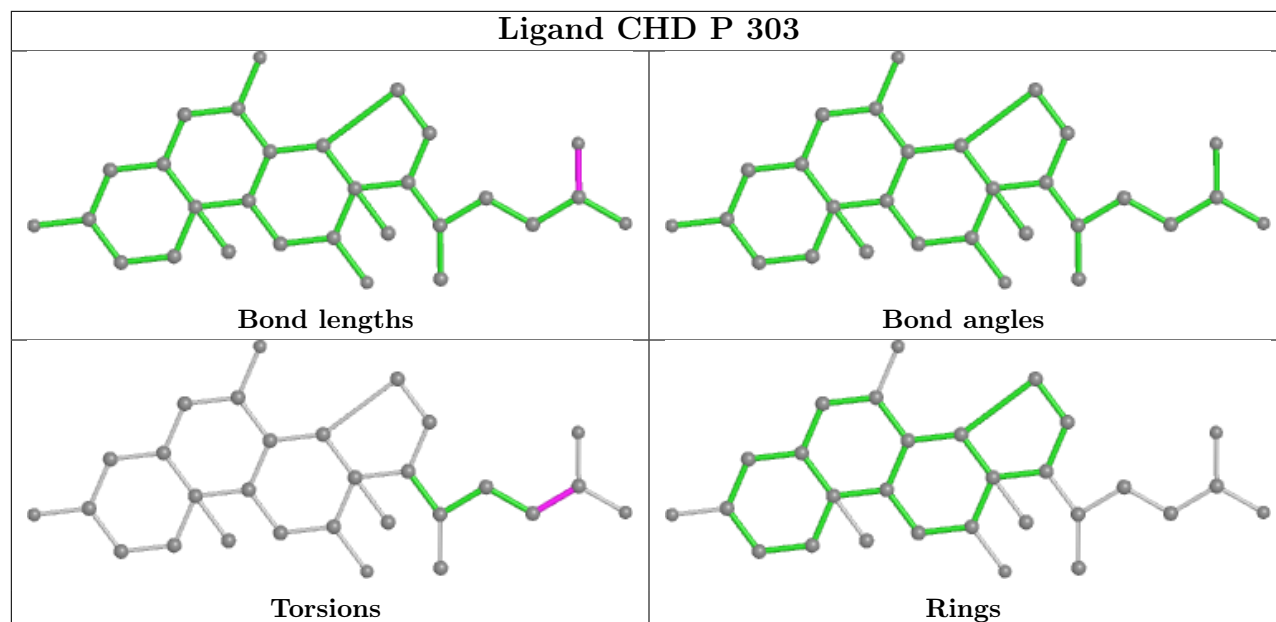


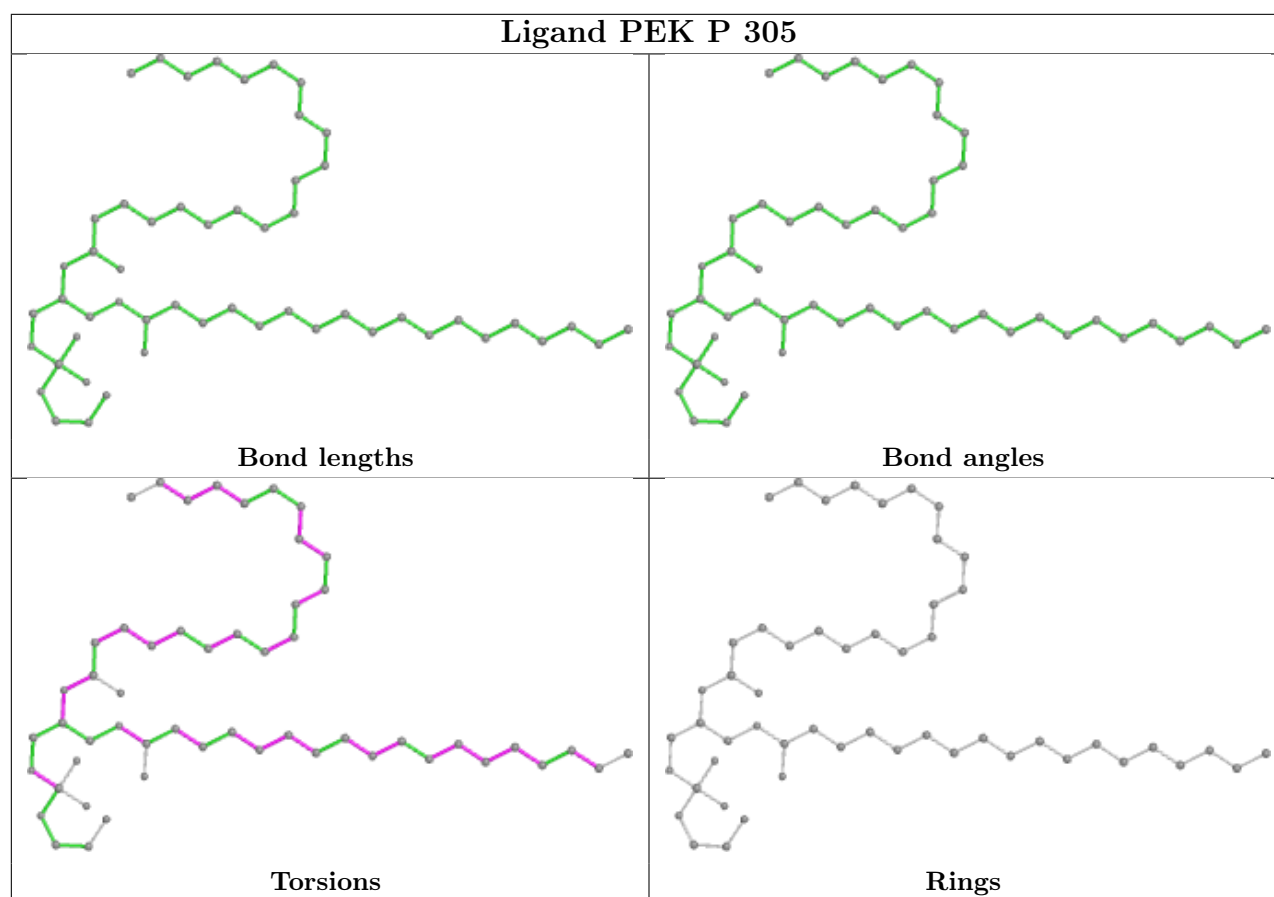
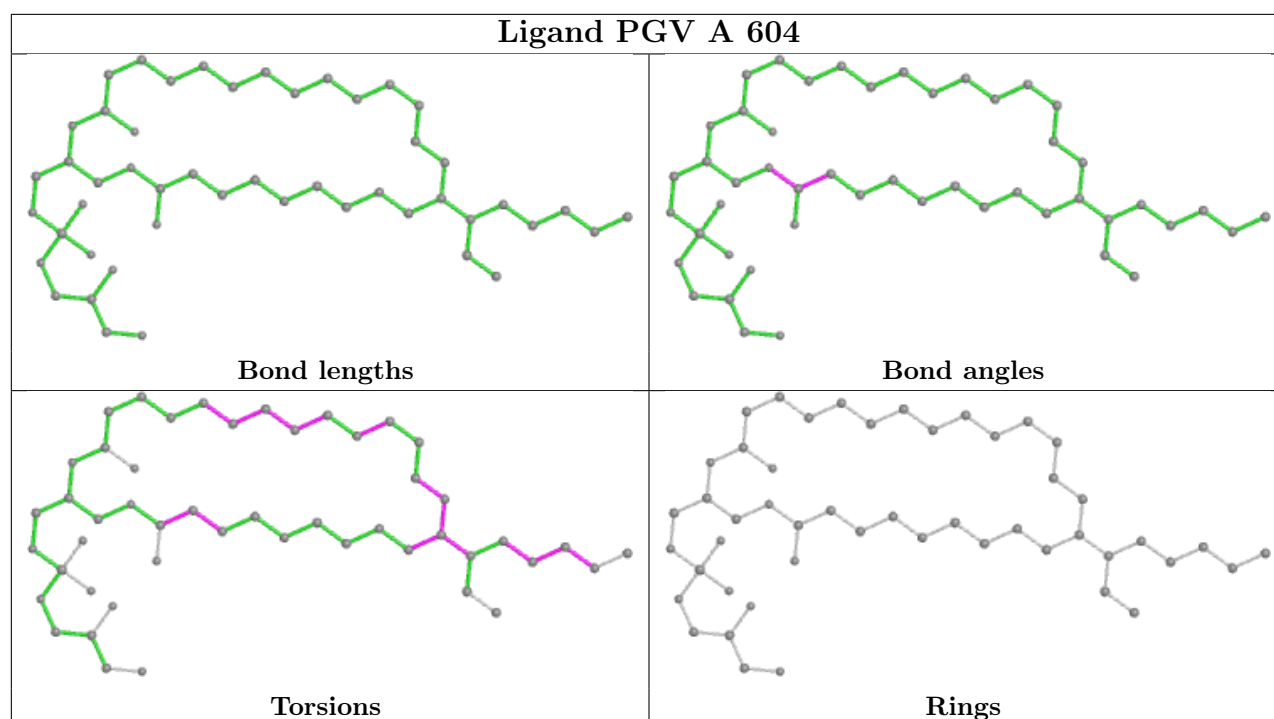


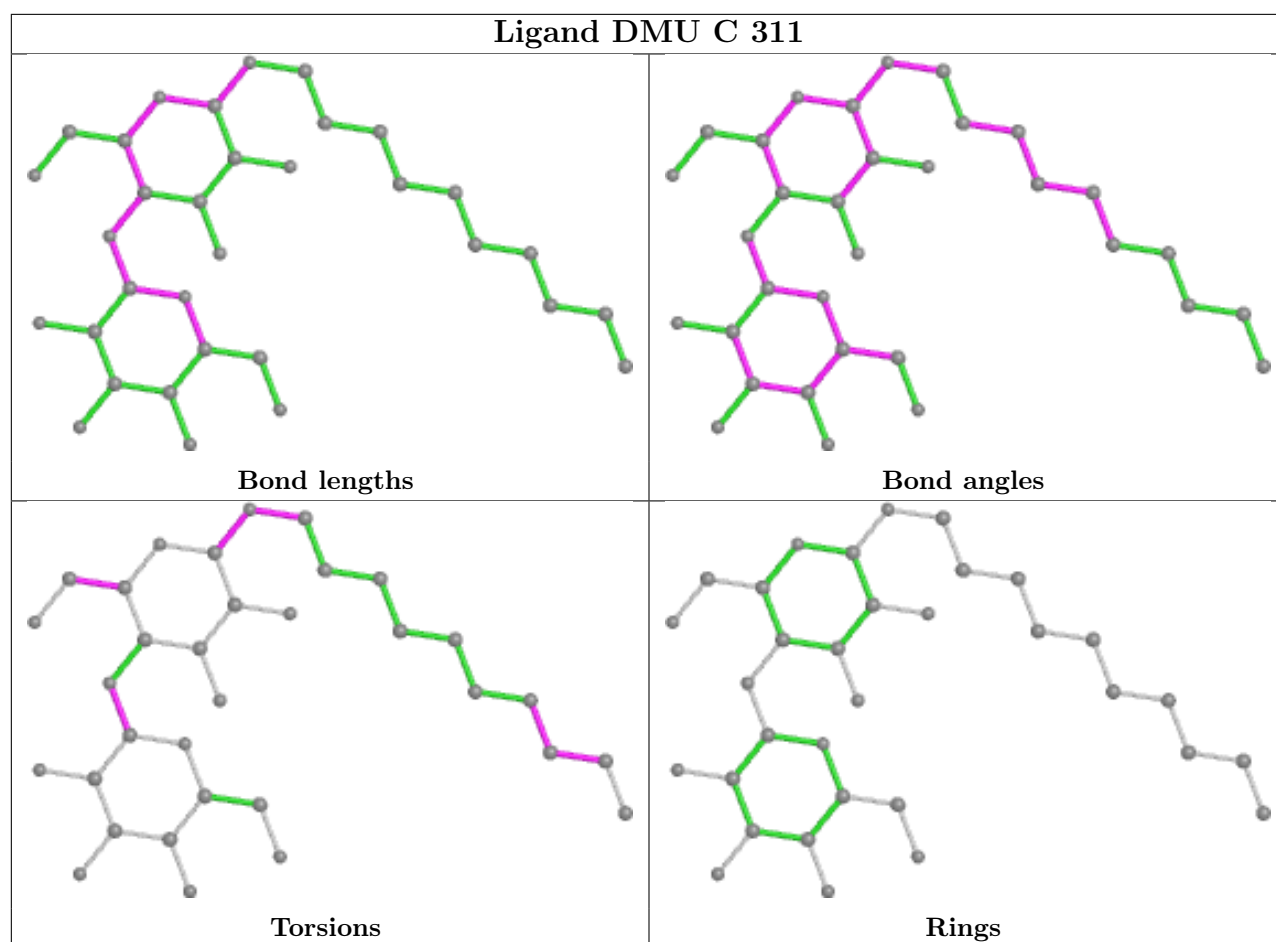




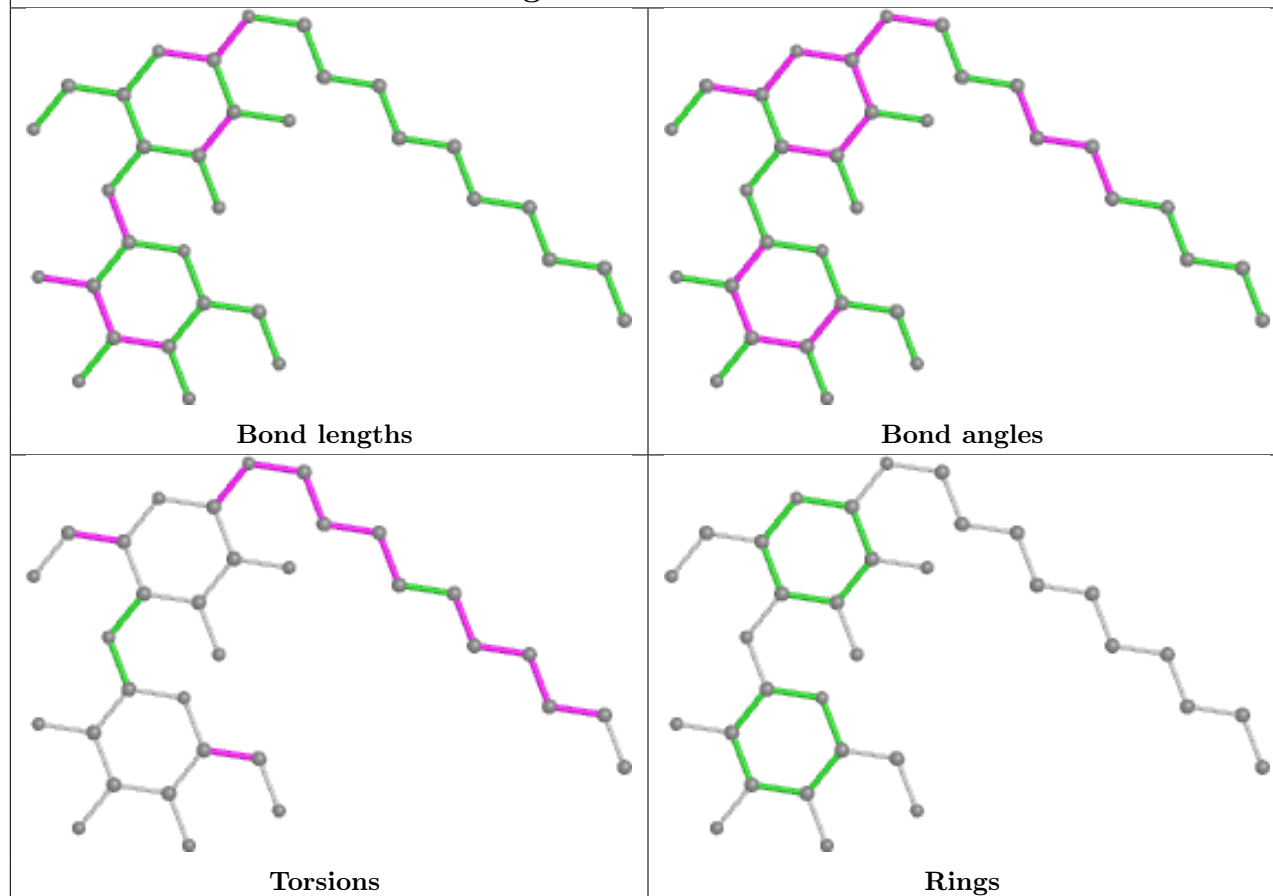




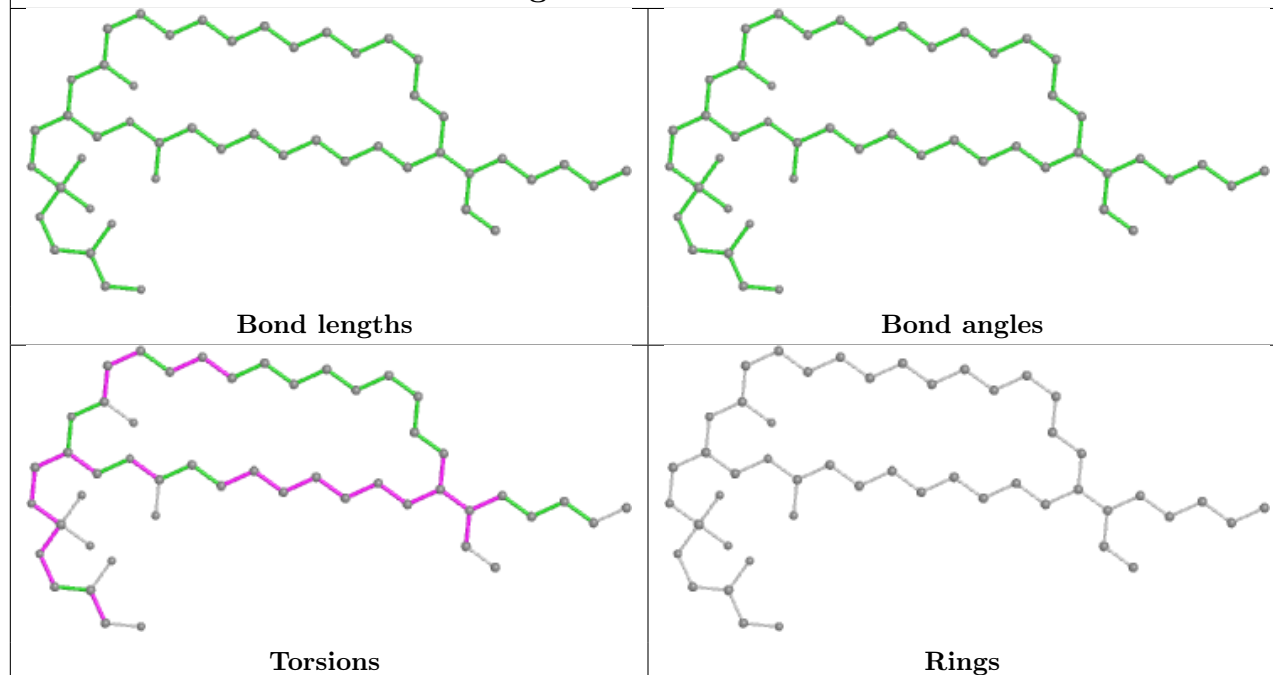




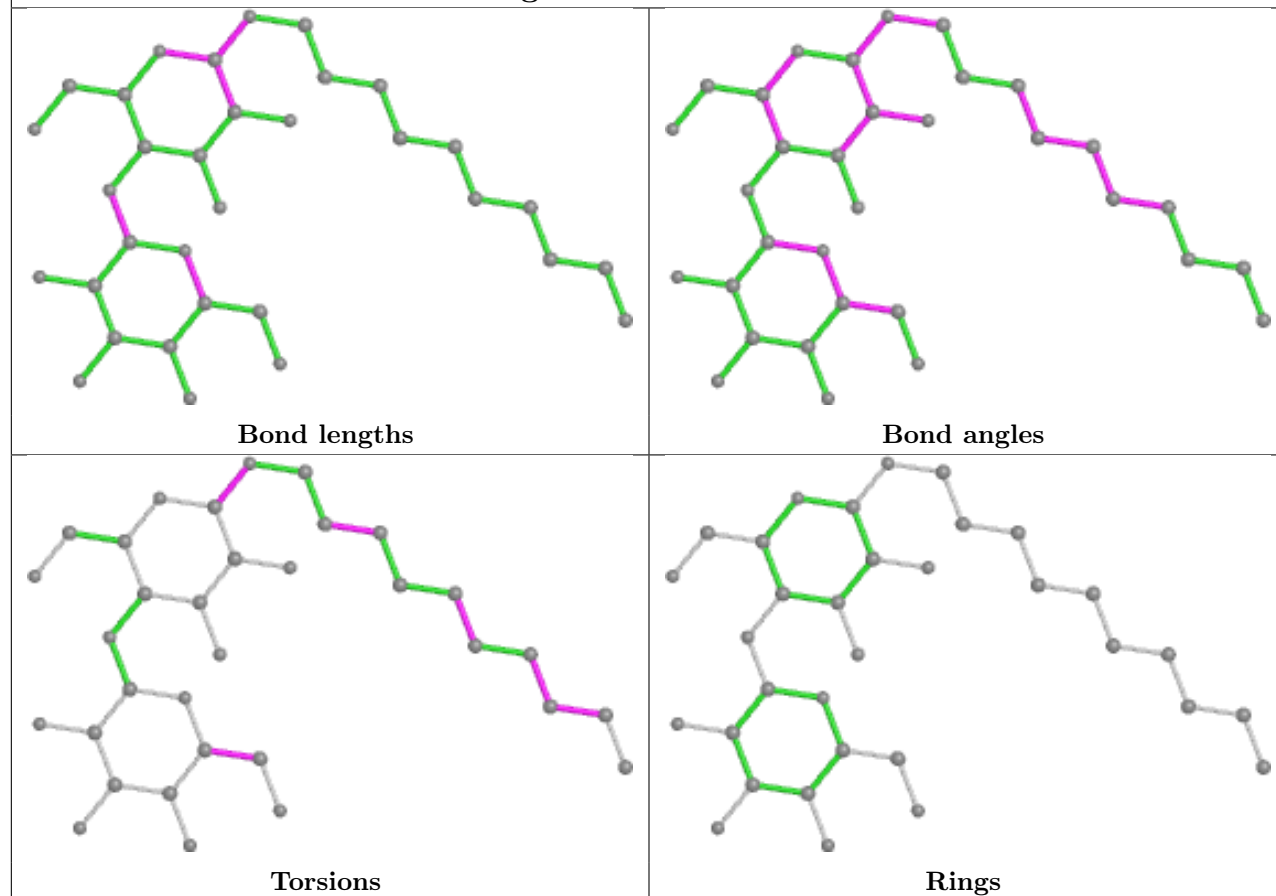
Ligand DMU G 101



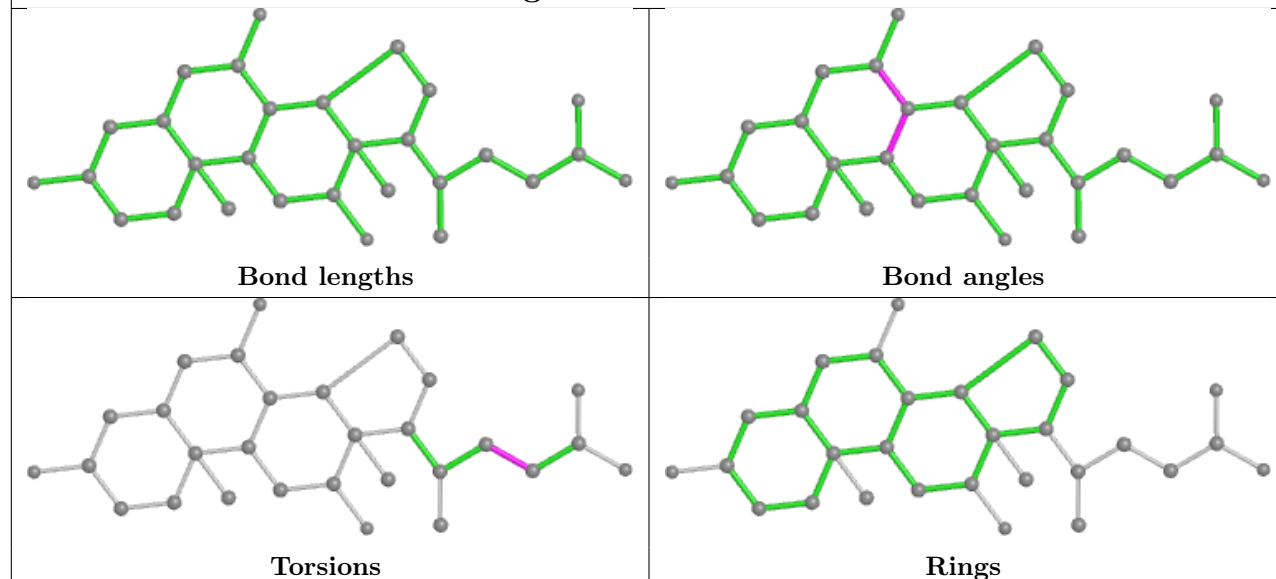
Ligand PGV P 307

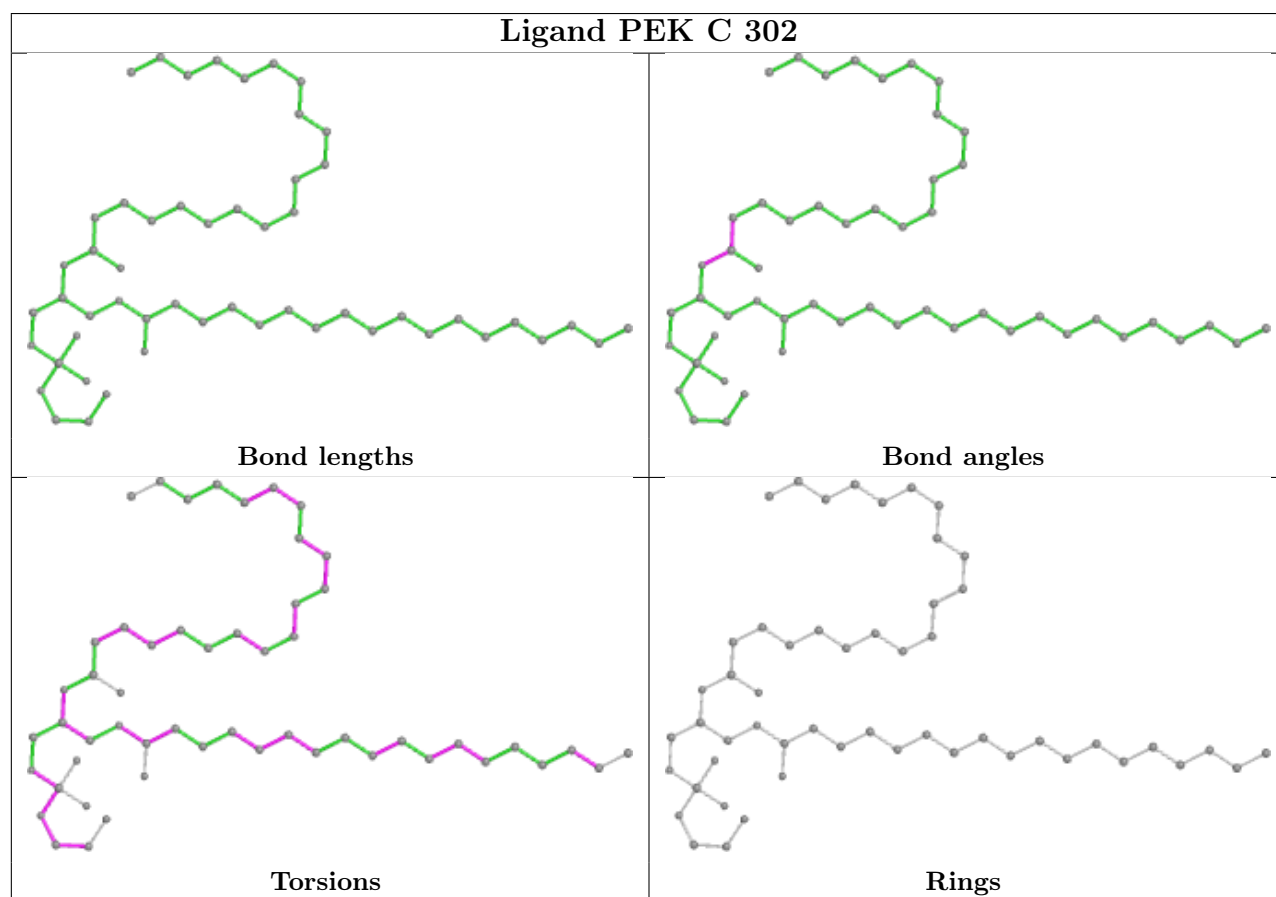
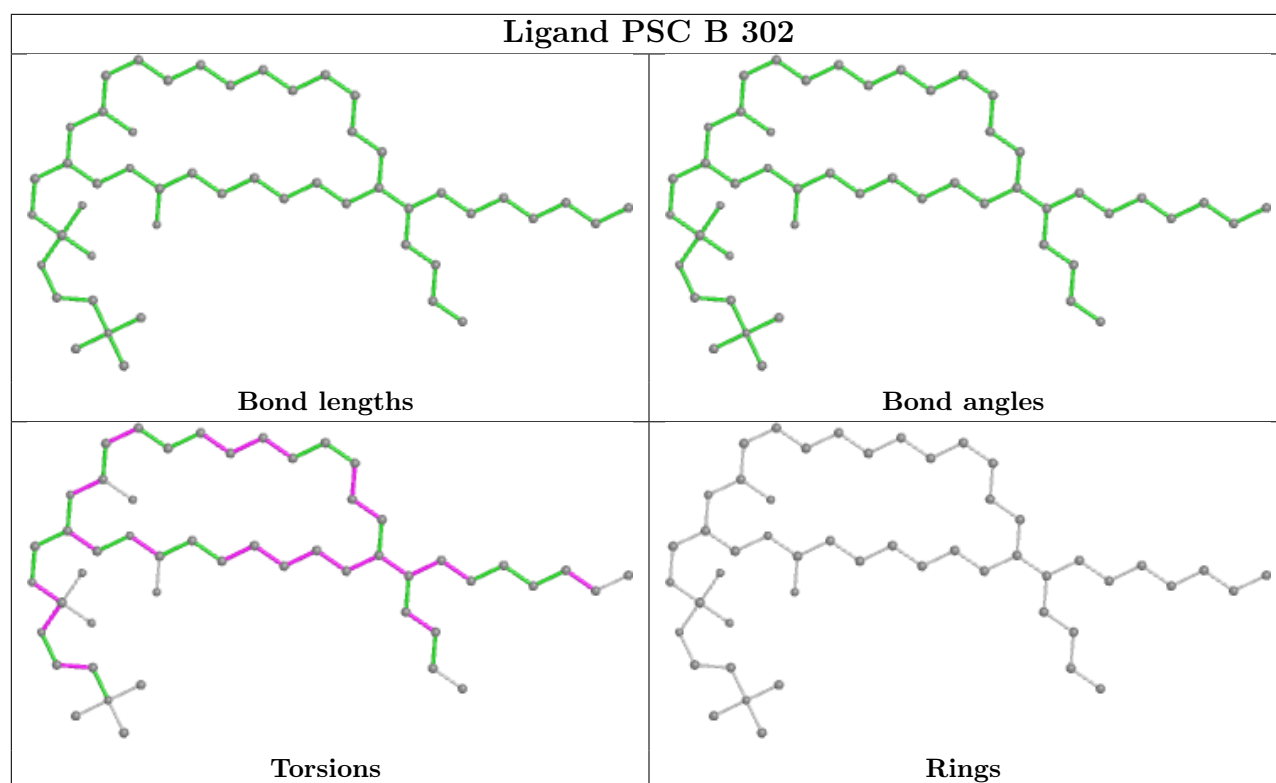


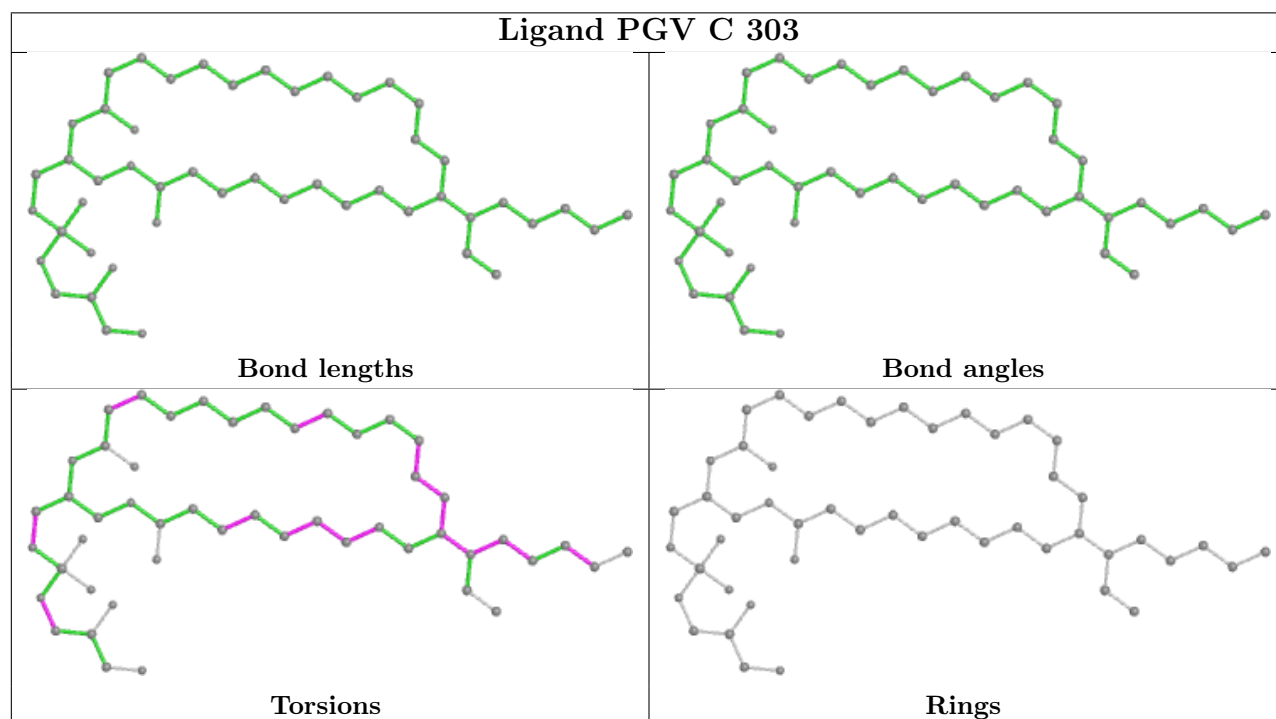
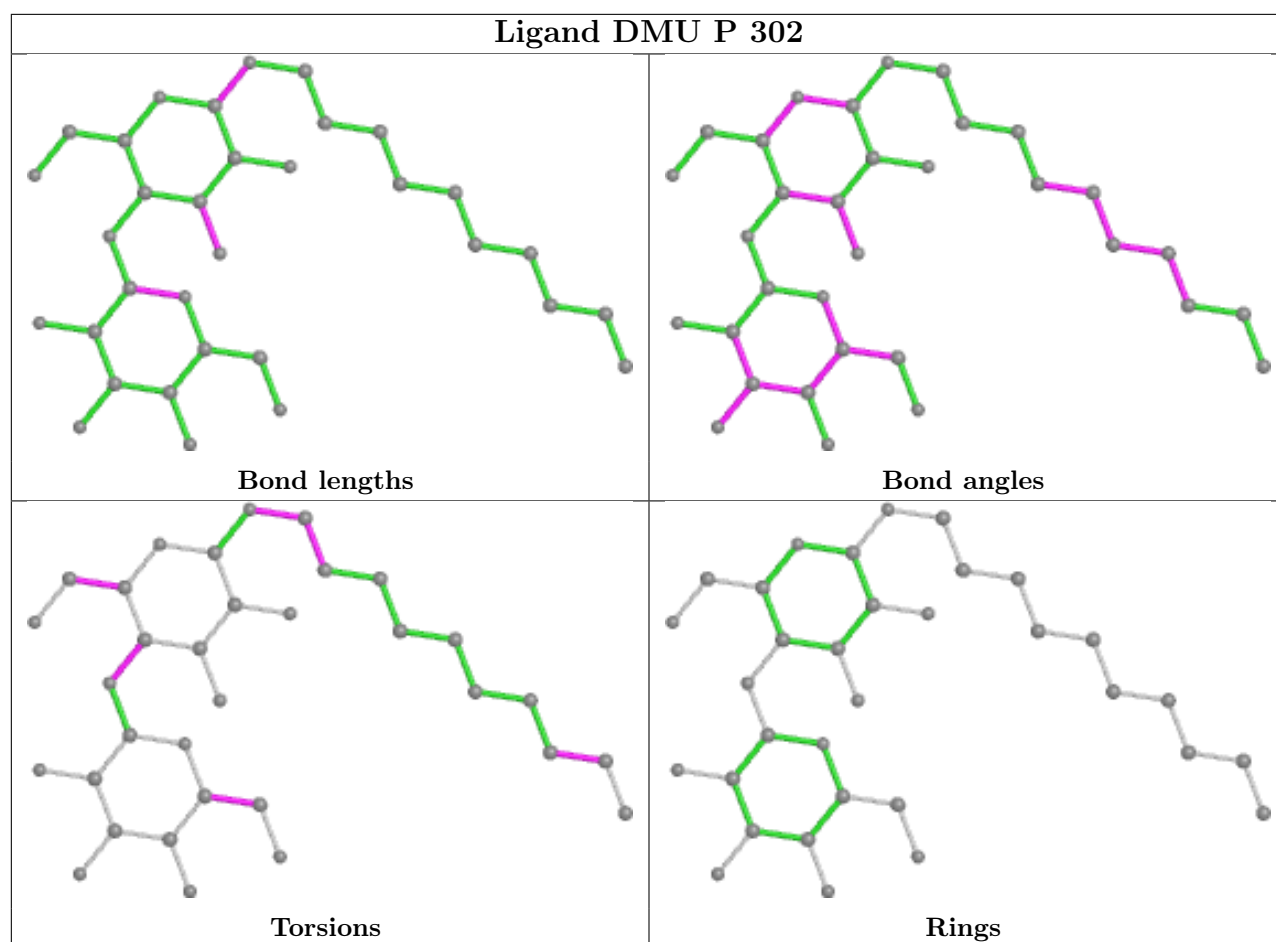
Ligand DMU M 102

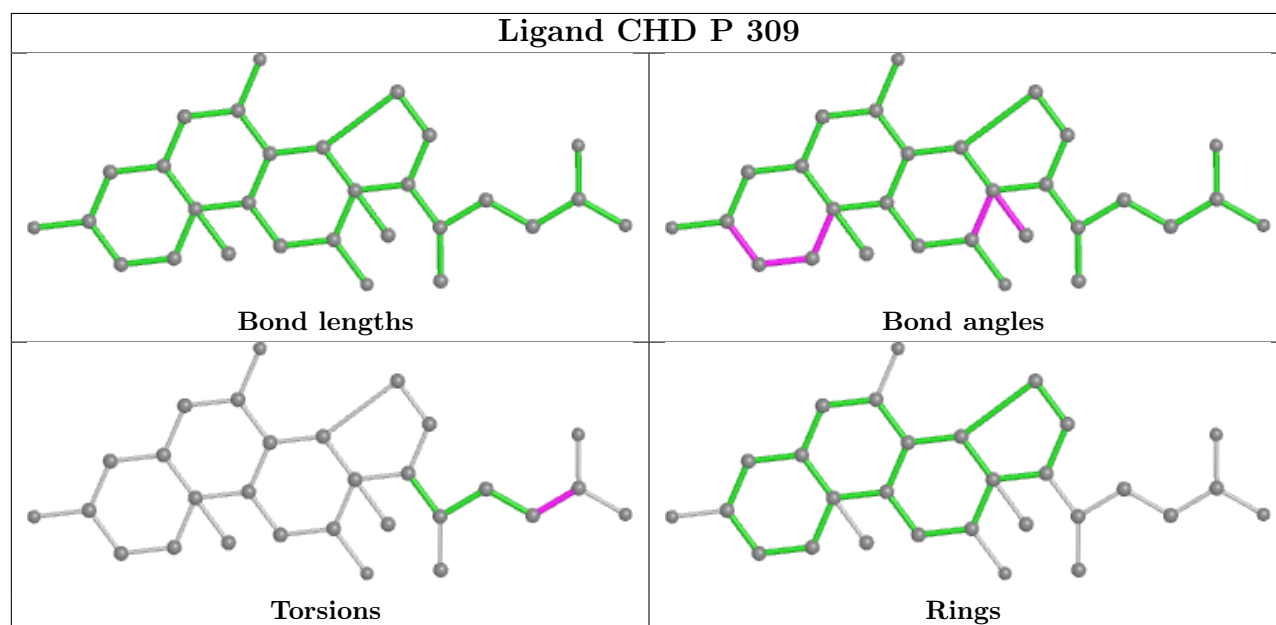
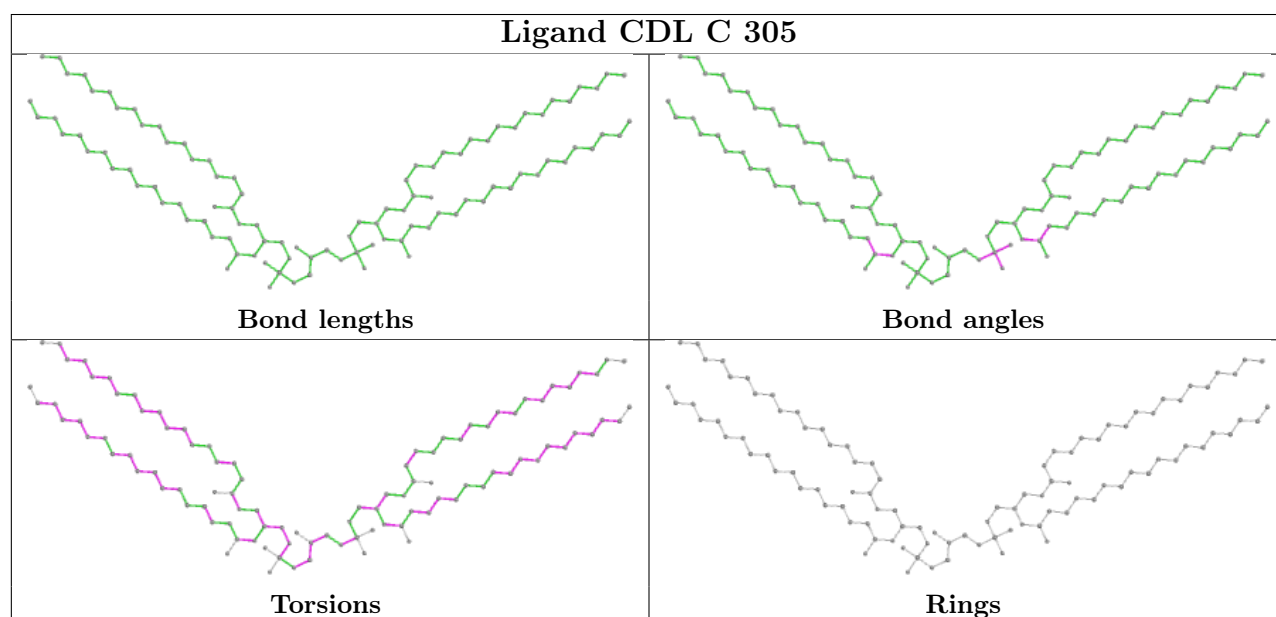
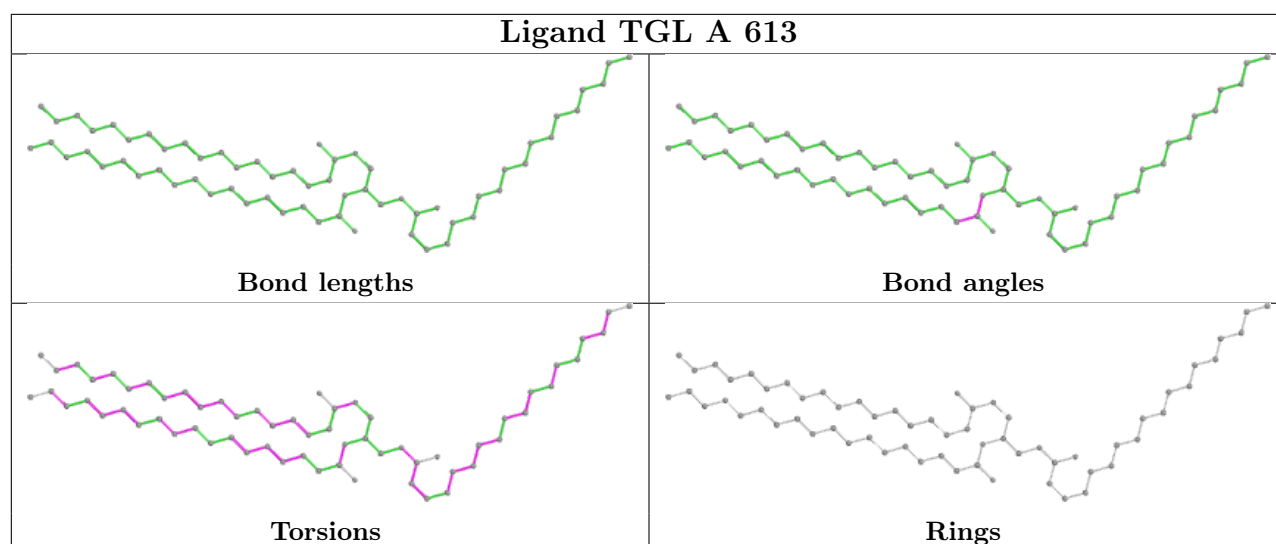


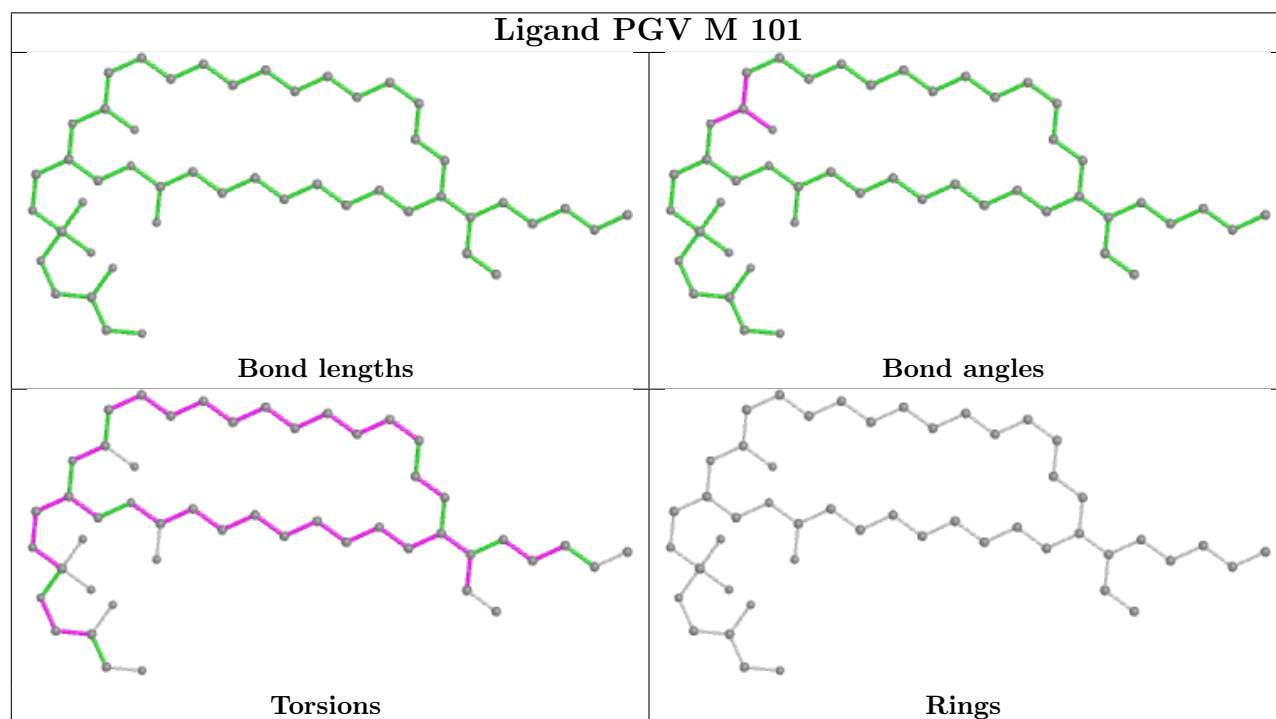
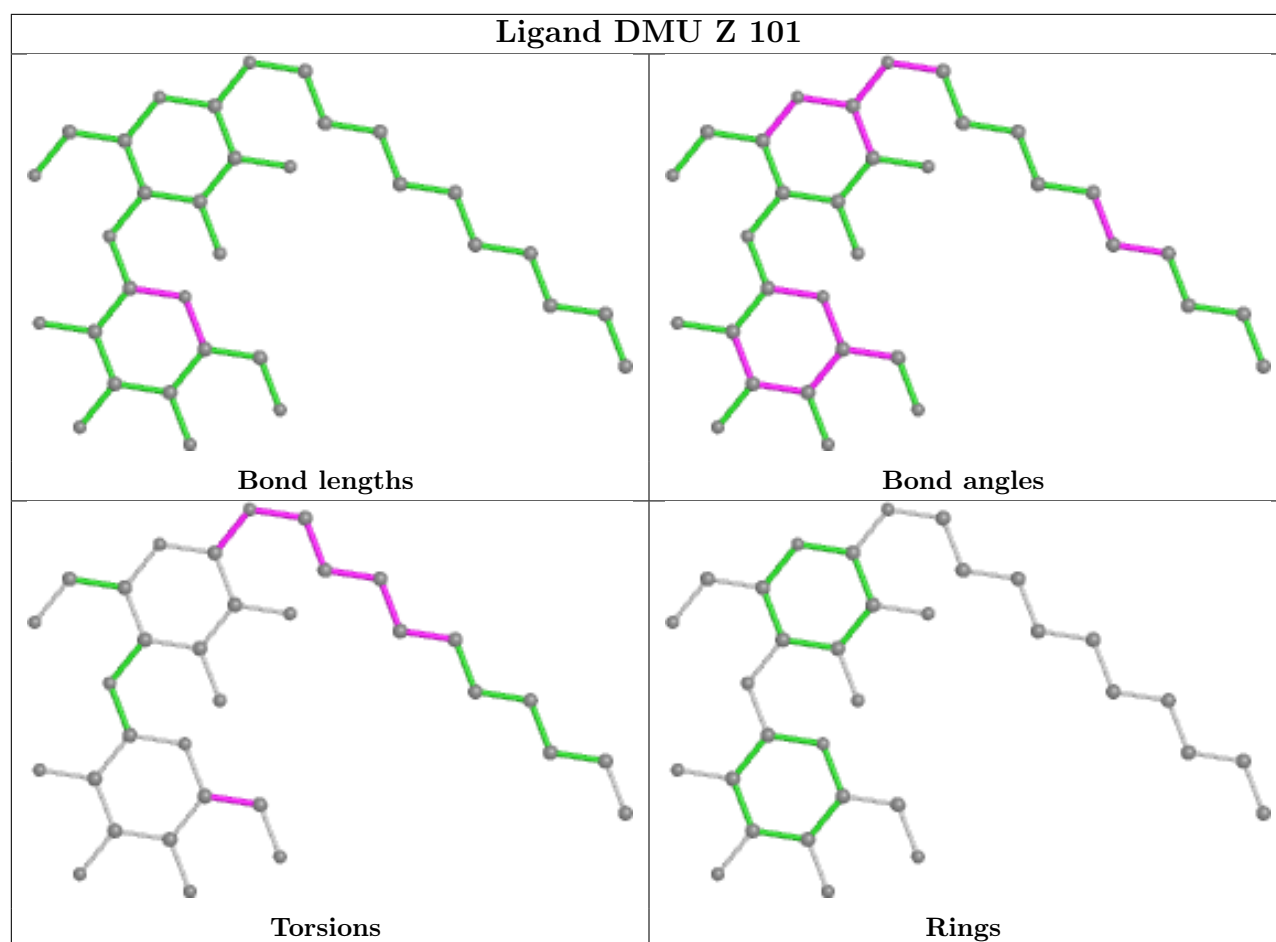
Ligand CHD W 302

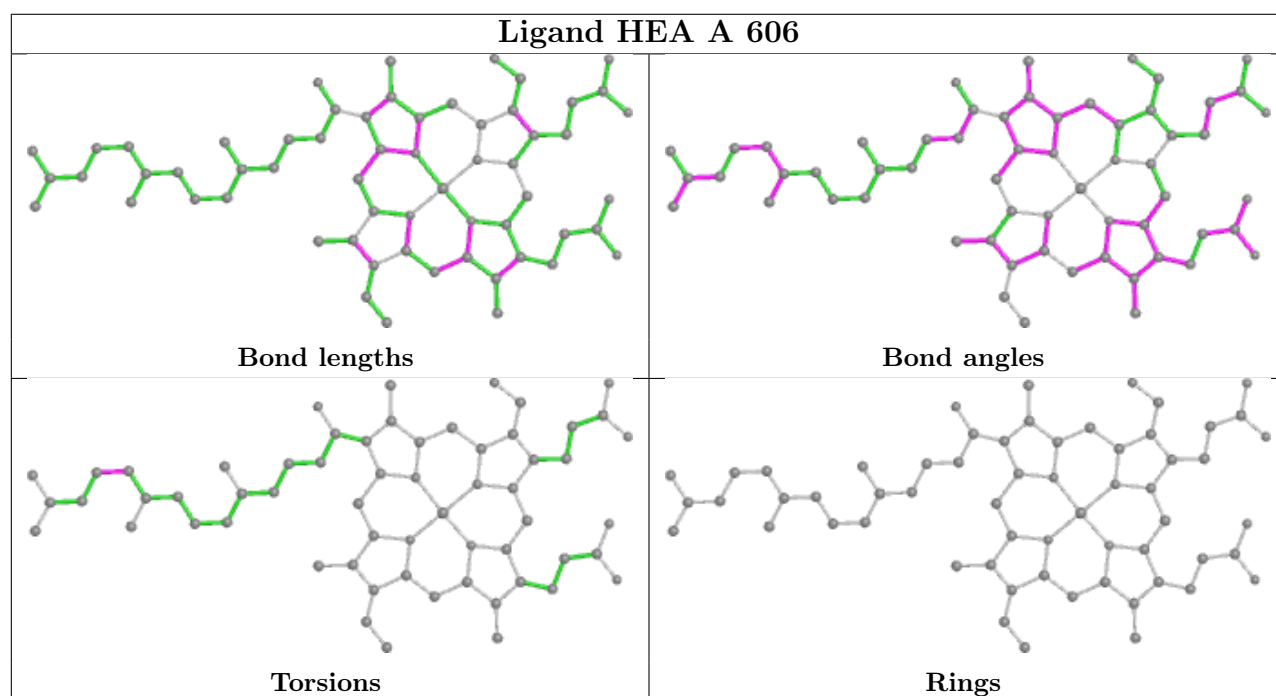
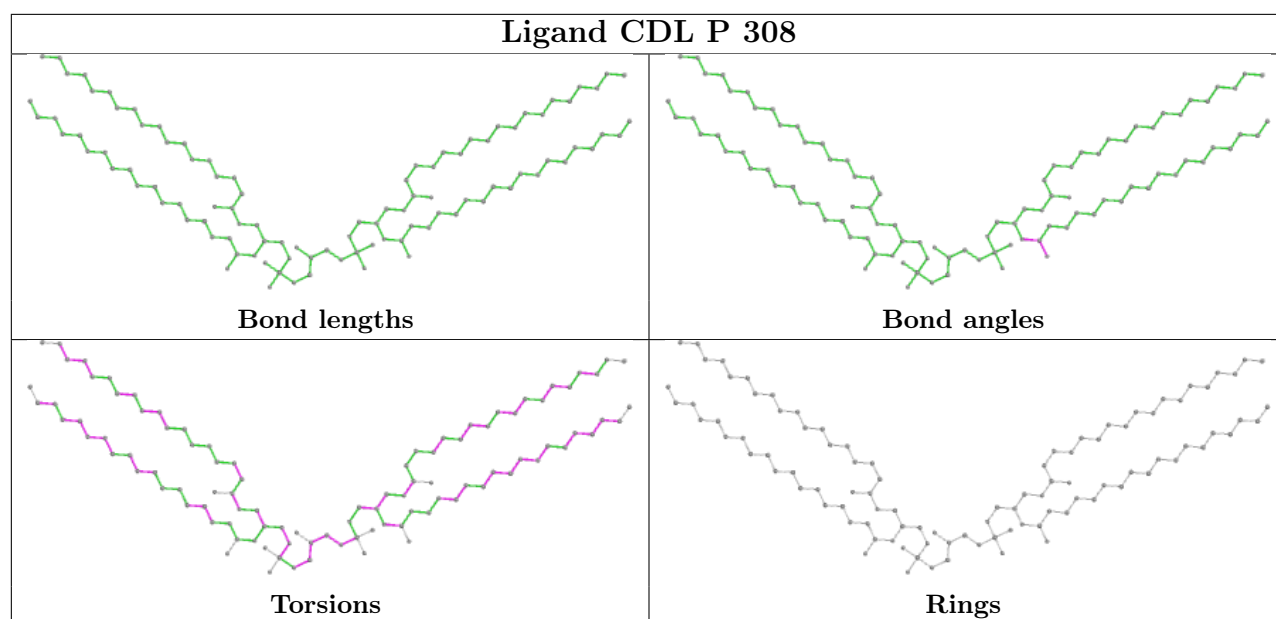




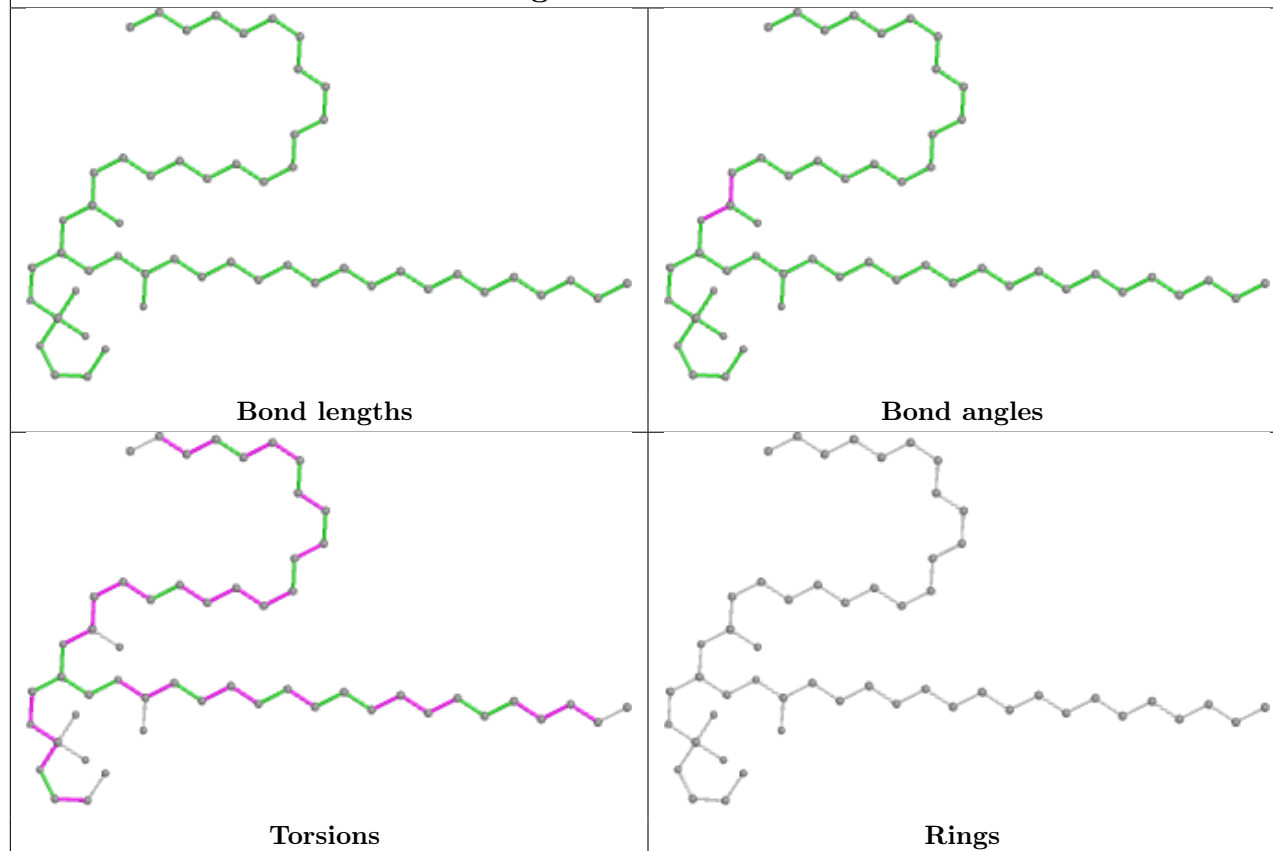




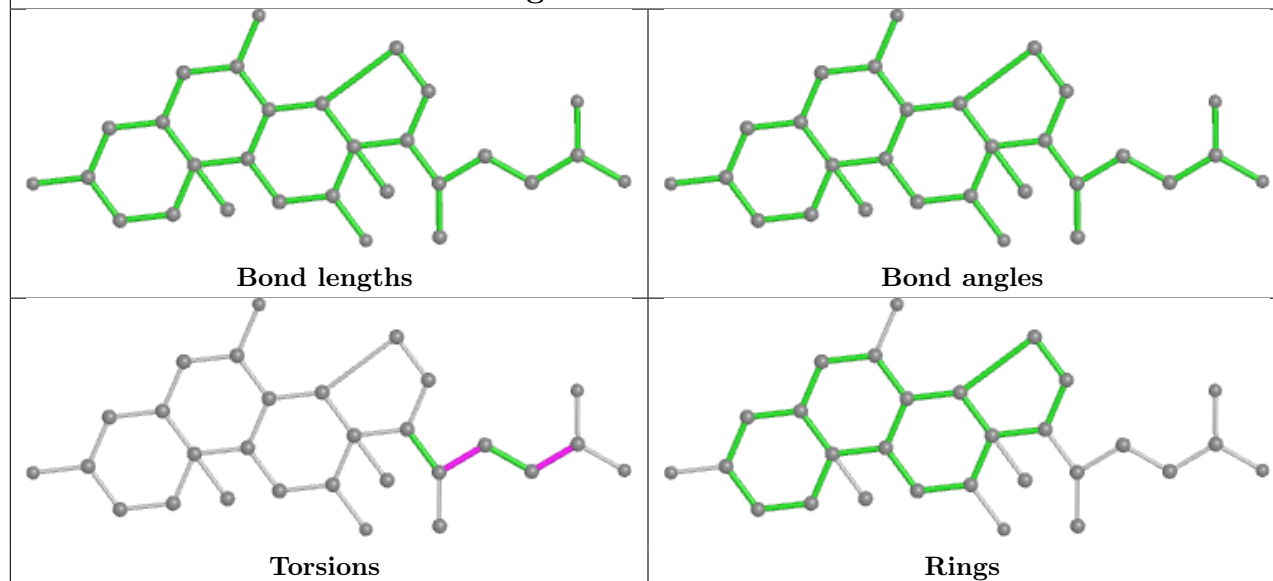


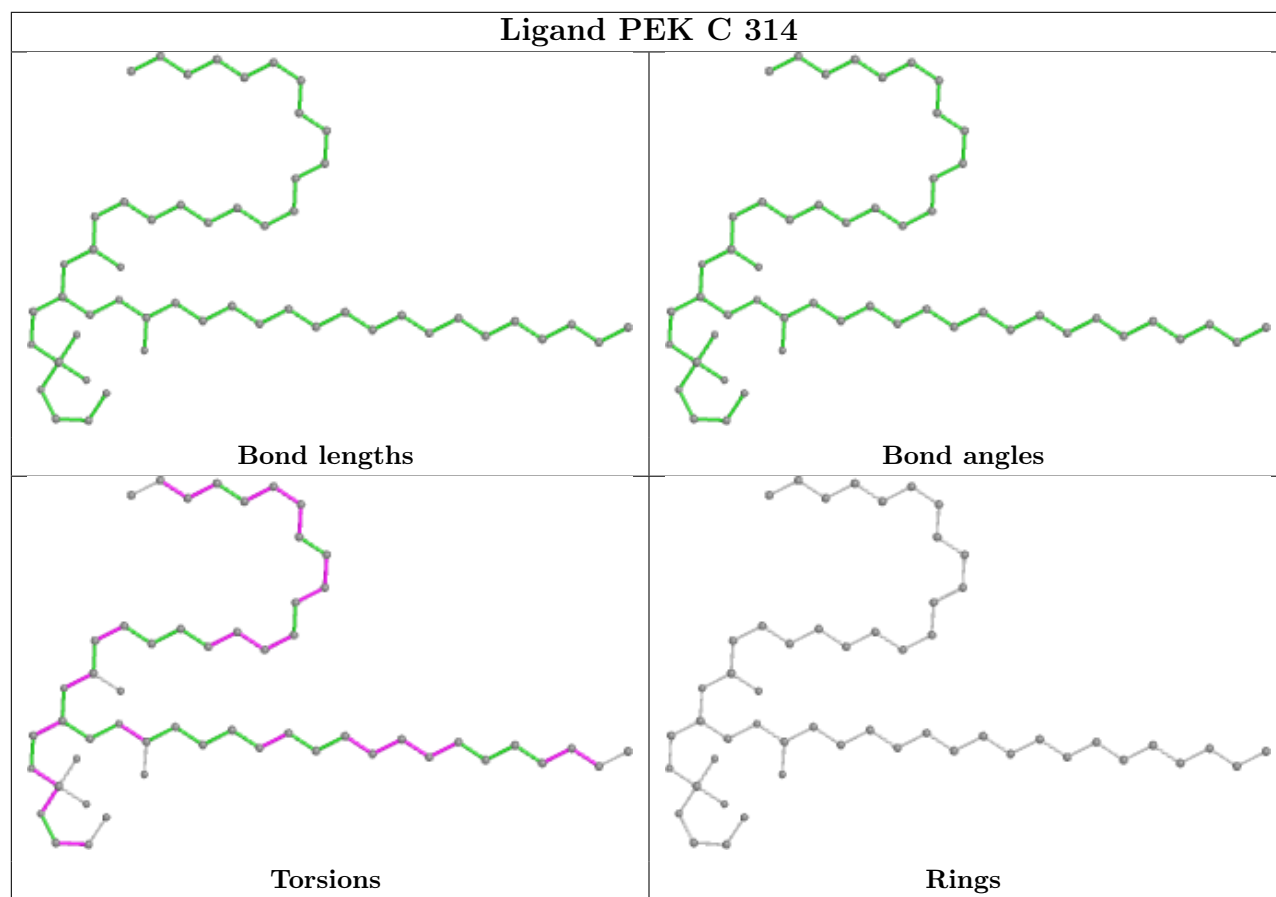
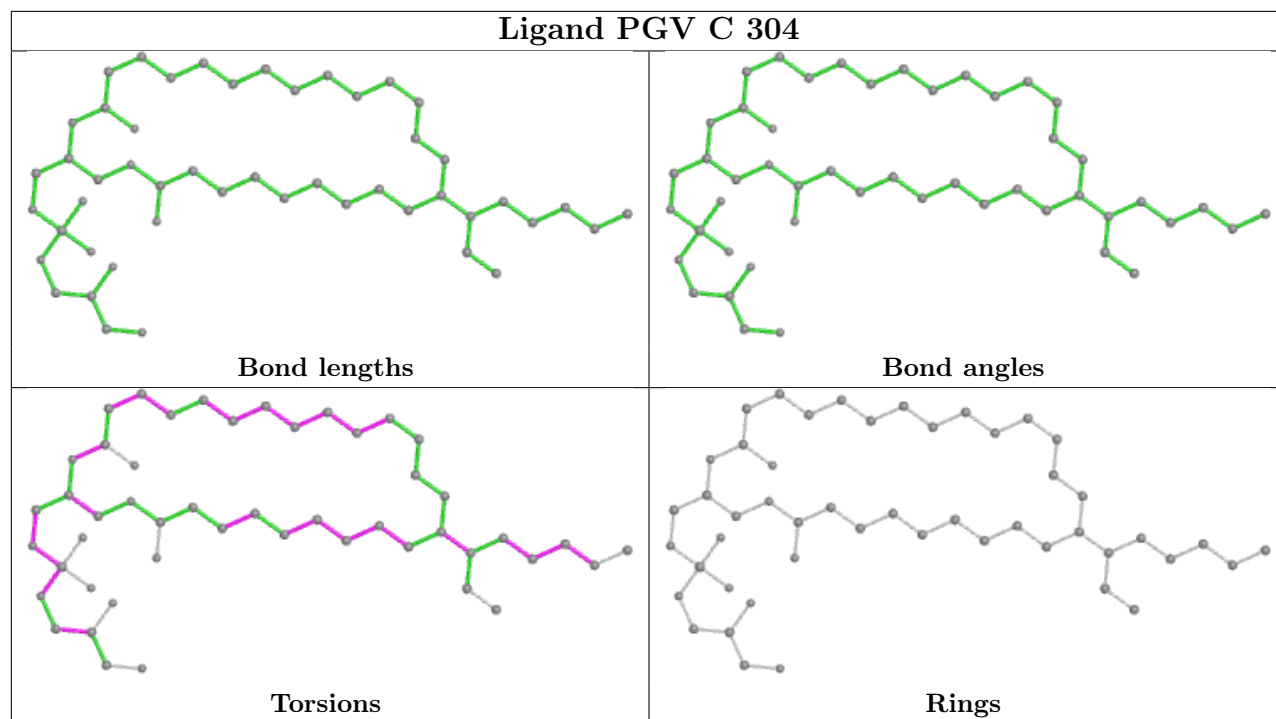


Ligand PEK P 301

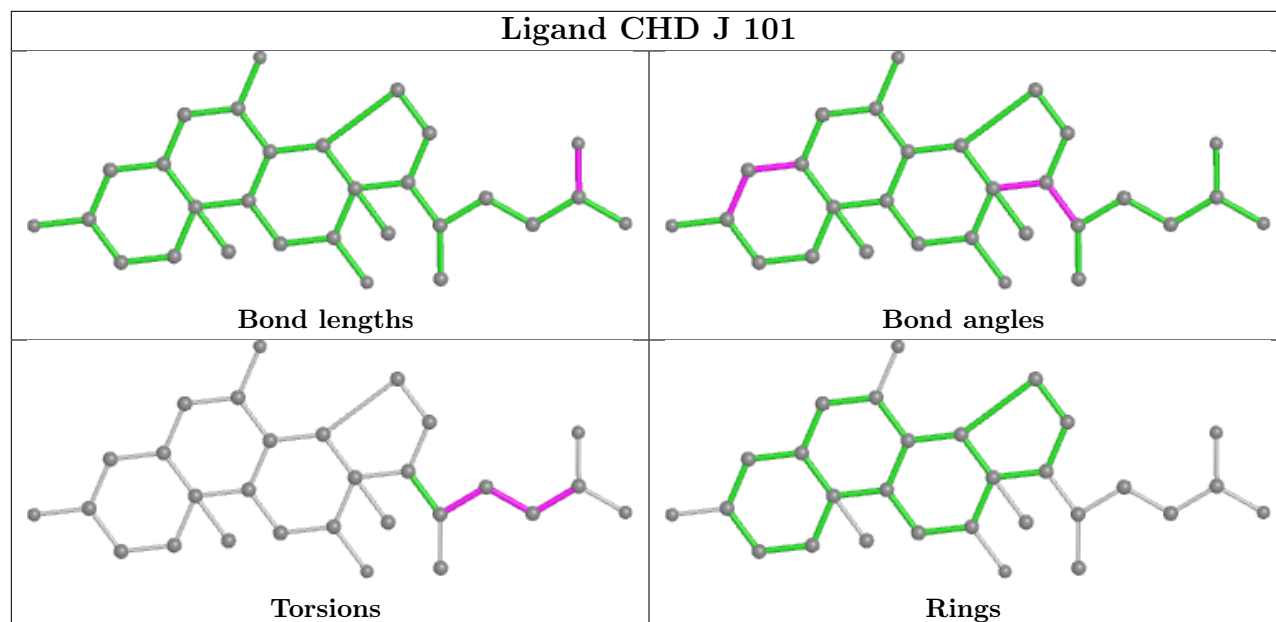


Ligand CHD G 107

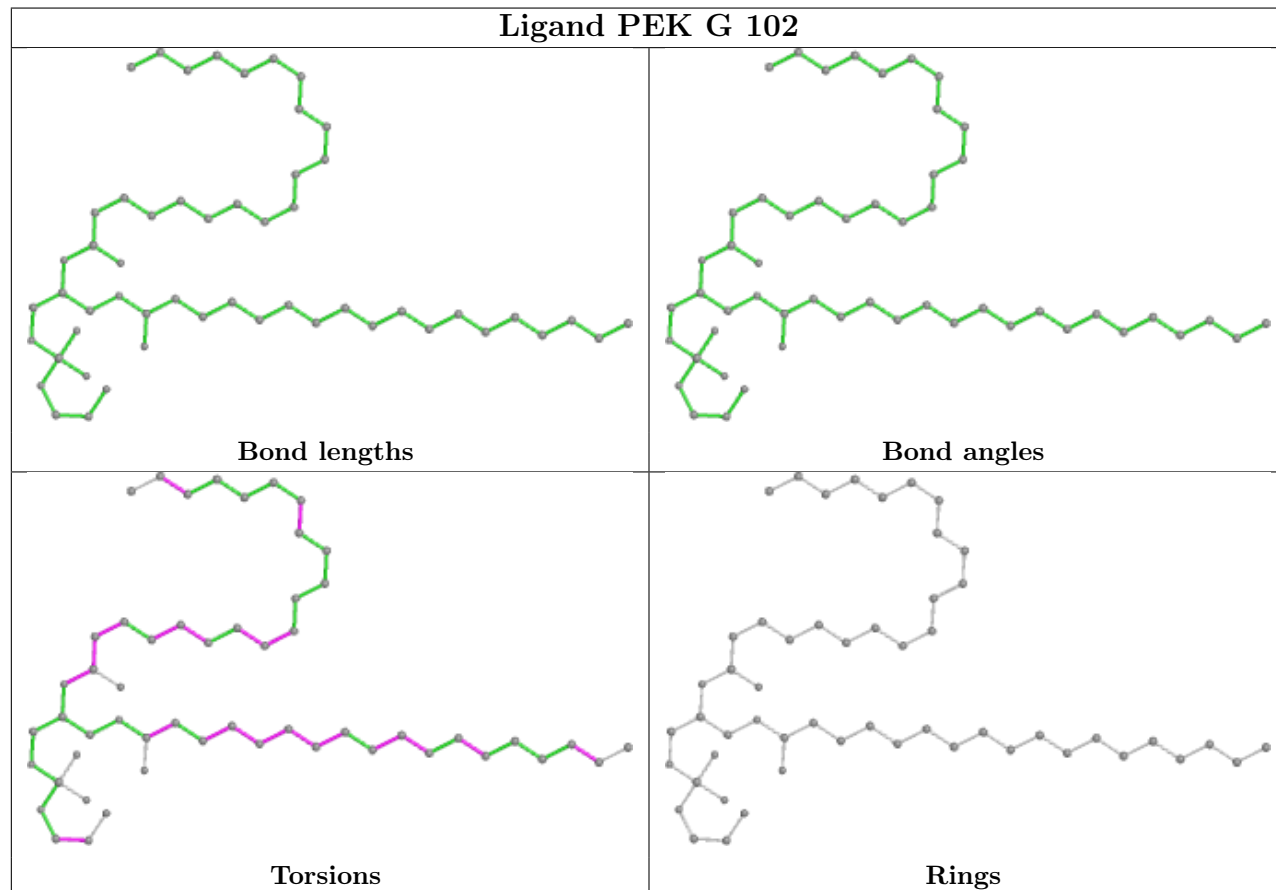


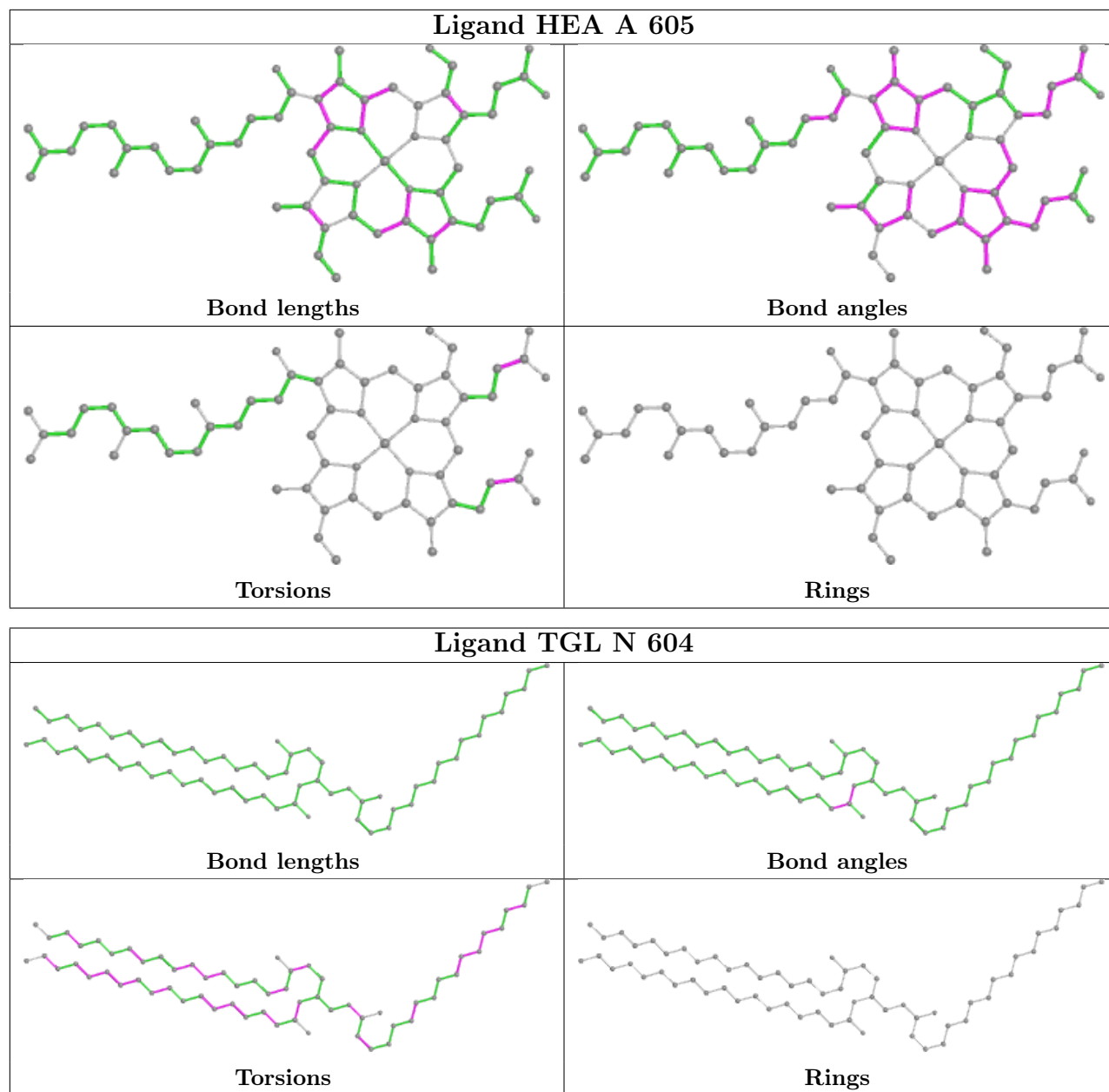


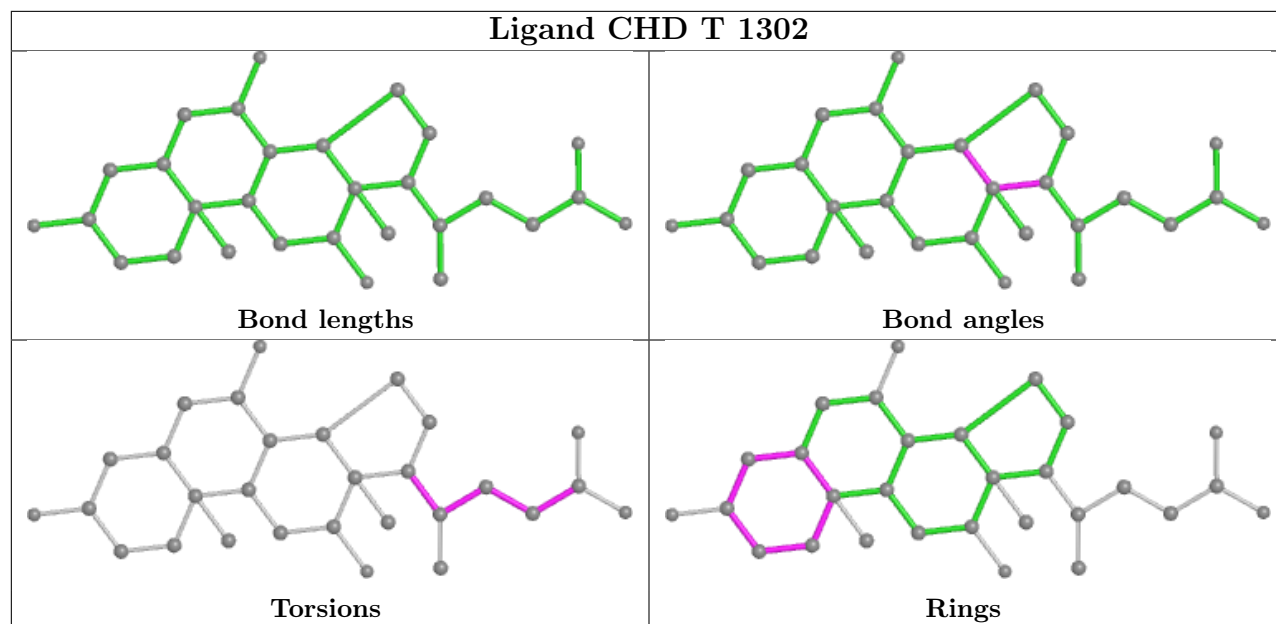
Ligand CHD J 101



Ligand PEK G 102







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%)	0.09	8 (1%) 72 74	23, 29, 37, 72	0
1	N	513/514 (99%)	0.10	11 (2%) 63 66	28, 35, 46, 77	0
2	B	226/227 (99%)	-0.24	3 (1%) 77 79	25, 35, 57, 78	0
2	O	226/227 (99%)	-0.06	10 (4%) 34 37	33, 43, 70, 90	0
3	C	259/261 (99%)	-0.41	1 (0%) 92 93	27, 33, 45, 81	0
3	P	259/261 (99%)	-0.46	1 (0%) 92 93	29, 37, 51, 84	0
4	D	144/147 (97%)	-0.35	2 (1%) 75 77	32, 39, 54, 80	0
4	Q	144/147 (97%)	0.73	16 (11%) 5 6	41, 55, 81, 164	0
5	E	105/109 (96%)	-0.18	2 (1%) 66 69	34, 42, 67, 120	0
5	R	105/109 (96%)	0.23	4 (3%) 40 43	39, 51, 69, 119	0
6	F	98/98 (100%)	0.58	12 (12%) 4 4	30, 40, 82, 140	0
6	S	98/98 (100%)	0.26	8 (8%) 11 13	32, 44, 81, 118	0
7	G	83/85 (97%)	0.75	16 (19%) 1 1	31, 40, 110, 119	0
7	T	83/85 (97%)	1.02	22 (26%) 0 0	32, 46, 108, 117	0
8	H	79/85 (92%)	0.51	14 (17%) 1 1	31, 43, 92, 105	0
8	U	79/85 (92%)	0.84	15 (18%) 1 1	40, 49, 104, 130	0
9	I	72/73 (98%)	0.61	10 (13%) 2 3	32, 48, 69, 83	0
9	V	72/73 (98%)	0.82	16 (22%) 0 0	38, 54, 77, 100	0
10	J	58/59 (98%)	0.21	6 (10%) 6 7	33, 44, 71, 119	0
10	W	58/59 (98%)	0.39	6 (10%) 6 7	39, 50, 77, 122	0
11	K	49/56 (87%)	0.29	2 (4%) 37 40	32, 42, 59, 81	0
11	X	49/56 (87%)	1.06	10 (20%) 1 1	47, 54, 74, 111	0
12	L	46/47 (97%)	-0.37	1 (2%) 62 64	30, 36, 57, 99	0
12	Y	46/47 (97%)	-0.08	2 (4%) 35 38	39, 47, 75, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.05	4 (9%) 8 10	33, 36, 64, 99	0
13	Z	43/46 (93%)	0.55	5 (11%) 4 5	43, 50, 76, 112	0
All	All	3550/3614 (98%)	0.11	207 (5%) 23 25	23, 39, 71, 164	0

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	18.1
4	Q	6	VAL	15.4
6	F	97	ALA	14.0
6	F	98	HIS	12.2
4	Q	4	SER	10.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	TPO	T	11	11/12	0.63	0.33	42,81,138,146	0
7	TPO	G	11	11/12	0.77	0.24	45,80,126,126	0
1	FME	A	1	10/11	0.95	0.15	43,47,72,89	0
2	FME	O	1	10/11	0.97	0.13	37,42,53,65	0
1	FME	N	1	10/11	0.97	0.20	51,56,89,89	0
2	FME	B	1	10/11	0.98	0.11	31,34,50,51	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
27	DMU	G	101	33/33	0.21	0.50	79,121,140,147	0
29	SAC	V	101	9/10	0.26	0.55	95,103,113,114	0
29	SAC	I	101	9/10	0.32	0.37	81,96,103,109	0
19	EDO	W	303	4/4	0.45	0.50	90,96,96,99	0
19	EDO	G	108	4/4	0.56	0.20	90,90,94,98	0
19	EDO	J	102	4/4	0.62	0.14	73,74,74,78	0
25	PEK	C	302	53/53	0.63	0.24	65,84,142,176	0
25	PEK	P	301	53/53	0.65	0.24	55,83,136,152	0
23	PSC	B	302	52/52	0.65	0.33	47,82,154,167	0
26	CDL	C	310	100/100	0.66	0.30	65,91,146,163	0
24	CHD	Y	101	29/29	0.66	0.33	91,127,145,177	0
19	EDO	P	310	4/4	0.67	0.29	73,73,73,75	0
20	TGL	N	605	63/63	0.67	0.24	52,72,118,136	0
17	PGV	C	304	51/51	0.68	0.26	43,82,124,144	0
25	PEK	P	305	53/53	0.68	0.25	52,87,152,165	0
26	CDL	P	312	100/100	0.69	0.24	68,96,141,163	0
25	PEK	C	314	53/53	0.70	0.27	59,83,139,159	0
26	CDL	P	308	100/100	0.70	0.23	48,88,121,129	0
20	TGL	N	618	63/63	0.71	0.21	64,82,103,110	0
23	PSC	R	201	52/52	0.72	0.32	44,100,157,168	0
20	TGL	A	613	63/63	0.72	0.26	51,74,117,120	0
17	PGV	N	622	51/51	0.73	0.33	54,89,159,169	0
17	PGV	P	307	51/51	0.73	0.27	64,96,123,143	0
20	TGL	N	604	63/63	0.75	0.27	58,83,114,119	0
27	DMU	G	104	33/33	0.75	0.23	64,106,127,137	0
27	DMU	Z	101	33/33	0.76	0.28	58,69,87,94	0
19	EDO	A	618	4/4	0.76	0.46	58,69,77,79	0
24	CHD	T	1302	29/29	0.76	0.36	97,136,151,152	0
19	EDO	V	103	4/4	0.77	0.23	75,79,82,83	0
20	TGL	D	201	63/63	0.77	0.20	49,79,97,114	0
19	EDO	P	311	4/4	0.77	0.27	55,68,74,84	0
19	EDO	N	621	4/4	0.78	0.21	57,60,61,70	0
26	CDL	C	305	100/100	0.78	0.25	45,82,118,125	0
20	TGL	L	502	63/63	0.79	0.19	45,65,91,99	0
27	DMU	P	302	33/33	0.80	0.33	59,101,117,119	0
17	PGV	M	101	51/51	0.80	0.25	48,92,149,181	0
19	EDO	B	307	4/4	0.81	0.19	58,67,71,76	0
19	EDO	P	314	4/4	0.81	0.23	70,71,74,81	0
19	EDO	A	610	4/4	0.83	0.18	56,65,66,69	0
19	EDO	N	615	4/4	0.83	0.15	55,59,61,74	0
19	EDO	B	308	4/4	0.84	0.25	50,57,66,69	0
27	DMU	C	311	33/33	0.84	0.24	60,85,105,107	0
19	EDO	D	202	4/4	0.84	0.14	60,61,70,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	K	201	4/4	0.84	0.16	61,64,65,71	0
19	EDO	L	503	4/4	0.84	0.21	58,63,64,71	0
19	EDO	M	103	4/4	0.84	0.19	65,68,69,69	0
24	CHD	W	302	29/29	0.84	0.30	61,76,89,94	0
19	EDO	V	102	4/4	0.84	0.13	69,70,71,77	0
19	EDO	H	101	4/4	0.85	0.35	66,68,68,77	0
19	EDO	O	302	4/4	0.85	0.22	62,71,72,86	0
19	EDO	Q	1603	4/4	0.85	0.23	72,72,77,81	0
19	EDO	A	611	4/4	0.85	0.17	49,55,61,69	0
19	EDO	N	614	4/4	0.87	0.21	55,67,68,76	0
27	DMU	M	102	33/33	0.87	0.22	43,52,65,81	0
19	EDO	C	308	4/4	0.87	0.10	71,72,73,76	0
19	EDO	G	105	4/4	0.88	0.18	75,75,80,101	0
19	EDO	I	102	4/4	0.88	0.10	74,76,76,80	0
19	EDO	B	311	4/4	0.88	0.27	65,71,77,89	0
19	EDO	N	612	4/4	0.88	0.24	59,63,65,74	0
19	EDO	S	103	4/4	0.88	0.13	53,66,68,69	0
19	EDO	U	1501	4/4	0.88	0.25	57,60,62,68	0
19	EDO	T	1301	4/4	0.89	0.23	56,59,64,66	0
19	EDO	R	203	4/4	0.89	0.32	64,68,71,77	0
19	EDO	B	309	4/4	0.89	0.11	62,68,69,74	0
19	EDO	S	104	4/4	0.89	0.13	52,55,59,61	0
24	CHD	J	101	29/29	0.89	0.28	56,70,84,95	0
19	EDO	V	104	4/4	0.89	0.15	51,65,68,72	0
19	EDO	C	313	4/4	0.90	0.22	58,60,62,71	0
19	EDO	S	105	4/4	0.90	0.21	44,58,64,69	0
19	EDO	G	106	4/4	0.90	0.10	65,65,65,69	0
19	EDO	Q	1604	4/4	0.90	0.15	59,70,72,89	0
19	EDO	B	305	4/4	0.90	0.15	50,57,64,68	0
19	EDO	F	702	4/4	0.90	0.22	57,69,73,86	0
19	EDO	I	103	4/4	0.91	0.12	58,60,62,67	0
19	EDO	Q	1602	4/4	0.91	0.18	70,73,76,83	0
19	EDO	N	613	4/4	0.91	0.18	65,67,75,77	0
19	EDO	A	617	4/4	0.92	0.17	56,59,61,63	0
19	EDO	S	106	4/4	0.92	0.14	65,68,69,75	0
19	EDO	E	203	4/4	0.92	0.25	63,70,73,77	0
19	EDO	E	204	4/4	0.92	0.18	72,74,78,81	0
19	EDO	A	612	4/4	0.92	0.20	55,56,59,61	0
19	EDO	N	616	4/4	0.92	0.11	47,55,60,62	0
19	EDO	C	309	4/4	0.92	0.12	73,74,77,78	0
19	EDO	C	312	4/4	0.92	0.15	52,55,57,62	0
19	EDO	B	310	4/4	0.92	0.17	55,64,65,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CHD	P	309	29/29	0.93	0.18	51,60,67,72	0
19	EDO	S	107	4/4	0.93	0.11	49,54,60,61	0
19	EDO	D	205	4/4	0.93	0.33	60,70,70,78	0
19	EDO	N	620	4/4	0.93	0.14	45,56,59,69	0
19	EDO	A	609	4/4	0.93	0.22	34,36,42,43	0
19	EDO	N	617	4/4	0.94	0.15	44,61,71,80	0
19	EDO	N	619	4/4	0.94	0.18	48,52,56,61	0
19	EDO	A	607	4/4	0.94	0.14	42,48,54,55	0
19	EDO	J	103	4/4	0.94	0.25	57,60,62,63	0
19	EDO	R	202	4/4	0.94	0.14	49,50,51,51	0
19	EDO	A	614	4/4	0.94	0.12	42,59,61,65	0
19	EDO	E	201	4/4	0.94	0.11	47,48,49,50	0
19	EDO	A	615	4/4	0.94	0.26	50,56,58,64	0
25	PEK	P	304	53/53	0.94	0.18	36,57,87,100	0
19	EDO	W	301	4/4	0.94	0.30	55,71,76,82	0
24	CHD	C	306	29/29	0.94	0.20	46,55,60,61	0
19	EDO	L	504	4/4	0.95	0.11	55,63,64,66	0
19	EDO	E	205	4/4	0.95	0.12	56,62,65,65	0
19	EDO	N	611	4/4	0.95	0.11	51,52,53,54	0
15	MG	N	602	1/1	0.95	0.12	35,35,35,35	0
25	PEK	G	102	53/53	0.95	0.20	31,53,79,97	0
19	EDO	B	306	4/4	0.95	0.09	37,42,49,51	0
19	EDO	E	202	4/4	0.95	0.16	43,47,52,53	0
19	EDO	A	616	4/4	0.95	0.14	53,61,63,72	0
19	EDO	L	501	4/4	0.95	0.26	49,62,63,65	0
19	EDO	D	203	4/4	0.95	0.29	53,62,67,70	0
19	EDO	C	307	4/4	0.96	0.07	39,42,46,47	0
17	PGV	P	306	51/51	0.96	0.15	29,45,86,96	0
19	EDO	Q	1601	4/4	0.96	0.12	44,57,57,59	0
17	PGV	N	606	51/51	0.96	0.19	31,50,77,82	0
17	PGV	A	604	51/51	0.96	0.18	26,42,71,76	0
19	EDO	F	704	4/4	0.96	0.12	56,56,59,63	0
19	EDO	F	706	4/4	0.96	0.12	39,43,48,49	0
19	EDO	F	707	4/4	0.96	0.15	49,61,64,65	0
24	CHD	C	301	29/29	0.96	0.07	29,33,39,42	0
19	EDO	O	303	4/4	0.96	0.10	39,40,42,43	0
19	EDO	A	608	4/4	0.96	0.16	28,28,28,29	0
24	CHD	B	303	29/29	0.97	0.07	30,34,41,46	0
19	EDO	D	204	4/4	0.97	0.20	63,65,71,78	0
18	HEA	N	608	60/60	0.97	0.16	27,33,49,63	0
19	EDO	P	313	4/4	0.97	0.09	37,46,48,53	0
24	CHD	P	303	29/29	0.97	0.07	33,36,42,43	0

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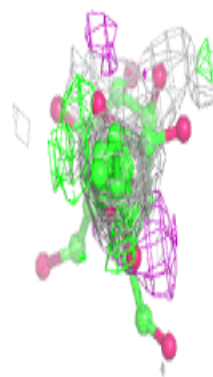
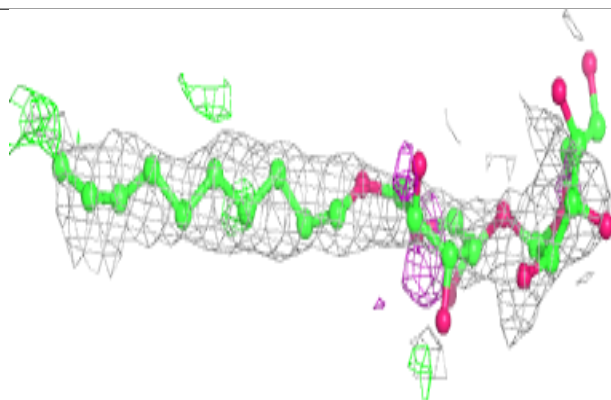
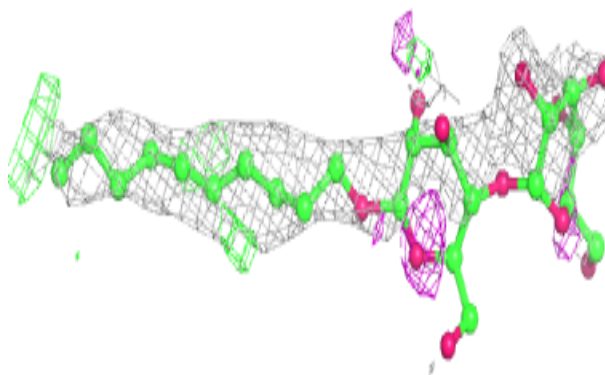
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	G	103	4/4	0.97	0.10	33,34,41,43	0
17	PGV	C	303	51/51	0.97	0.20	26,39,103,112	0
19	EDO	S	102	4/4	0.97	0.11	31,32,33,36	0
19	EDO	T	1303	4/4	0.97	0.19	36,40,43,44	0
18	HEA	A	606	60/60	0.98	0.14	20,26,54,64	0
19	EDO	N	609	4/4	0.98	0.11	36,37,38,41	0
24	CHD	G	107	29/29	0.98	0.05	31,35,39,42	0
19	EDO	N	610	4/4	0.98	0.23	36,40,43,43	0
18	HEA	N	607	60/60	0.98	0.13	25,29,36,43	0
19	EDO	F	705	4/4	0.98	0.20	28,30,30,31	0
19	EDO	B	304	4/4	0.98	0.13	27,29,30,34	0
16	NA	N	603	1/1	0.98	0.05	40,40,40,40	0
19	EDO	F	701	4/4	0.98	0.14	38,39,41,42	0
15	MG	A	602	1/1	0.99	0.10	28,28,28,28	0
18	HEA	A	605	60/60	0.99	0.13	21,26,32,37	0
16	NA	A	603	1/1	0.99	0.04	25,25,25,25	0
21	OH	A	619	1/1	0.99	0.20	24,24,24,24	0
28	ZN	F	703	1/1	0.99	0.05	34,34,34,34	0
28	ZN	S	101	1/1	0.99	0.06	38,38,38,38	0
21	OH	N	623	1/1	0.99	0.18	31,31,31,31	0
22	CUA	O	301	2/2	0.99	0.06	34,34,34,35	0
14	CU	N	601	1/1	1.00	0.11	34,34,34,34	0
14	CU	A	601	1/1	1.00	0.10	28,28,28,28	0
22	CUA	B	301	2/2	1.00	0.07	26,26,26,26	0

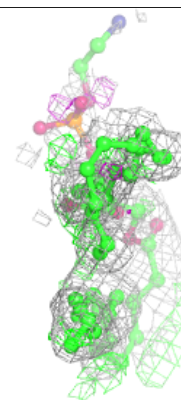
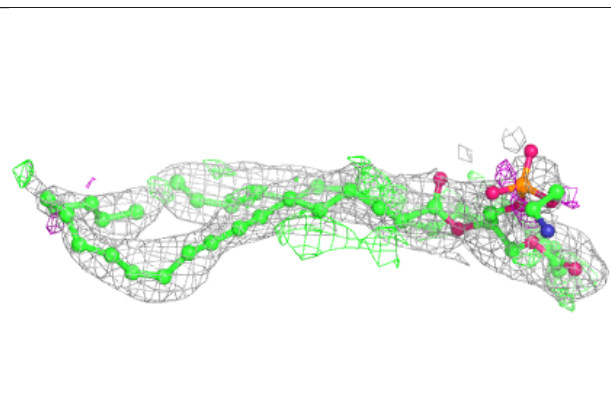
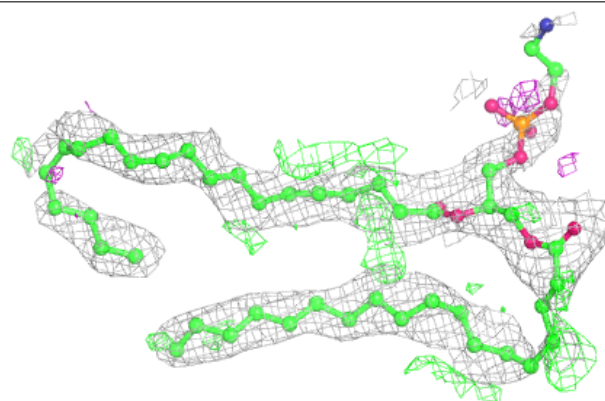
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU 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)

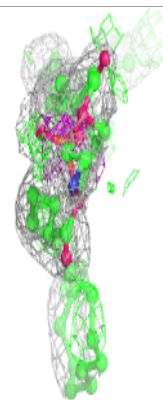
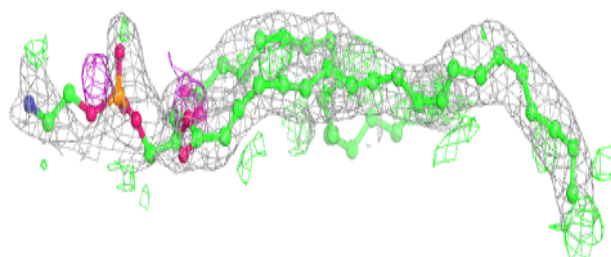
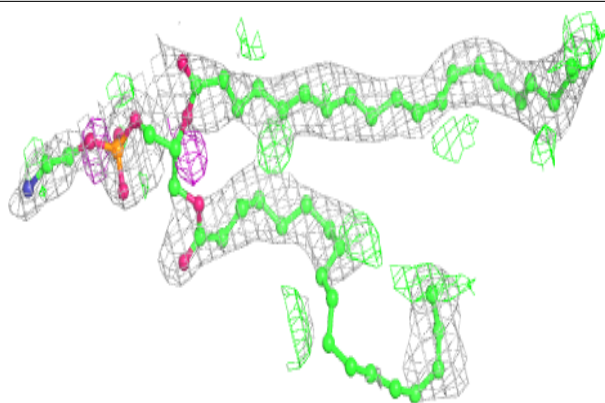
**Electron density around PEK C 302:**

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

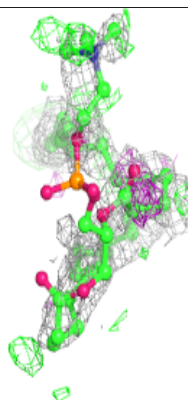
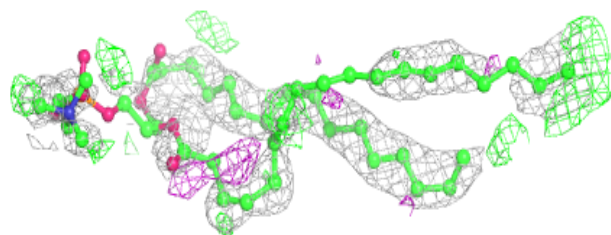
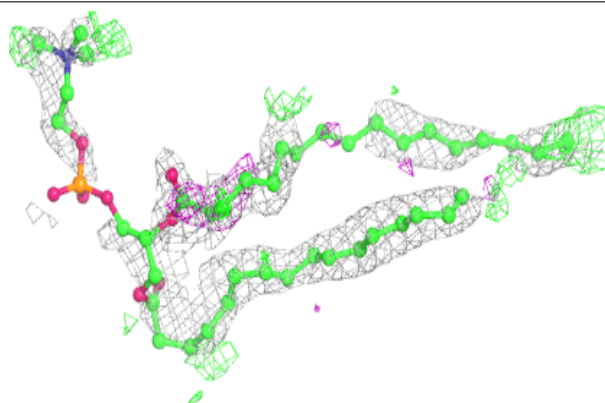


Electron density around PEK P 301:

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

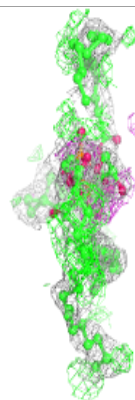
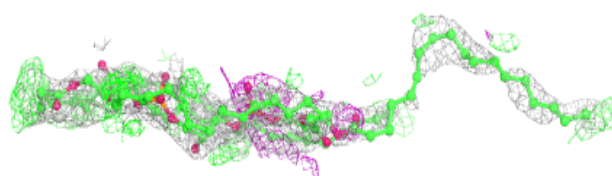
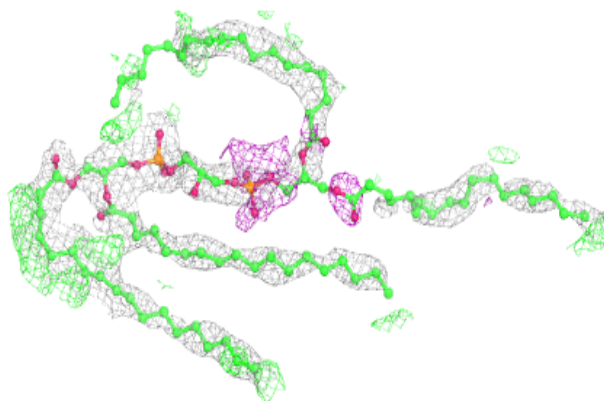
**Electron density around PSC B 302:**

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

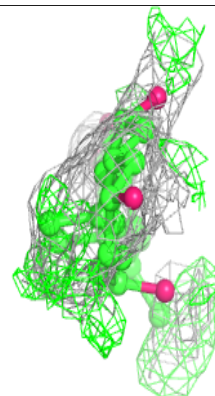
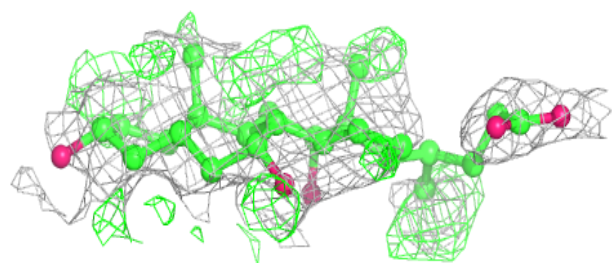
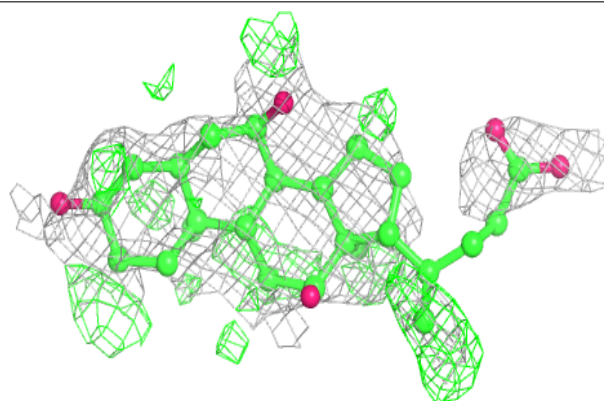


Electron density around CDL C 310:

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

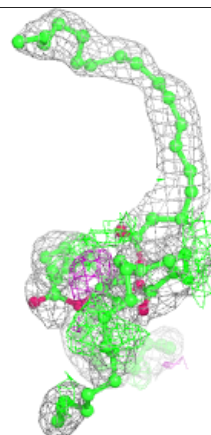
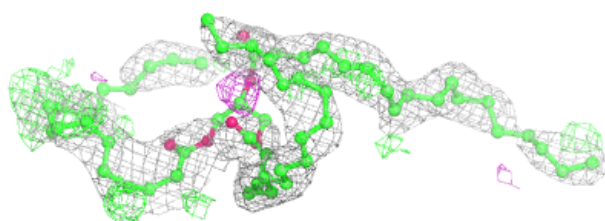
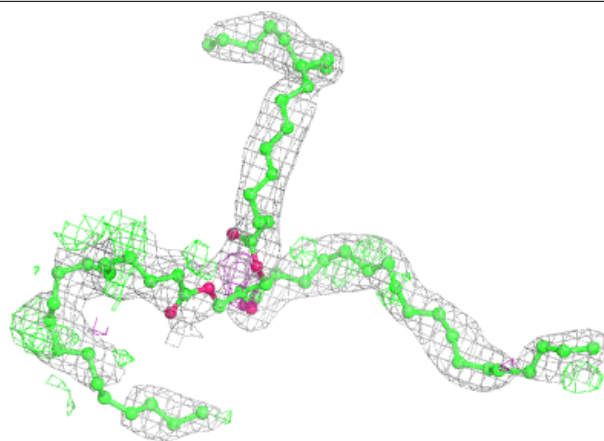
**Electron density around CHD Y 101:**

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

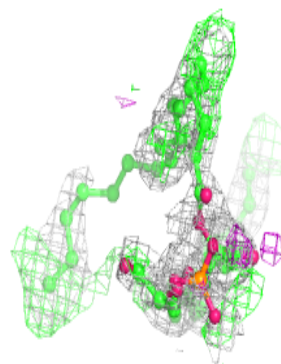
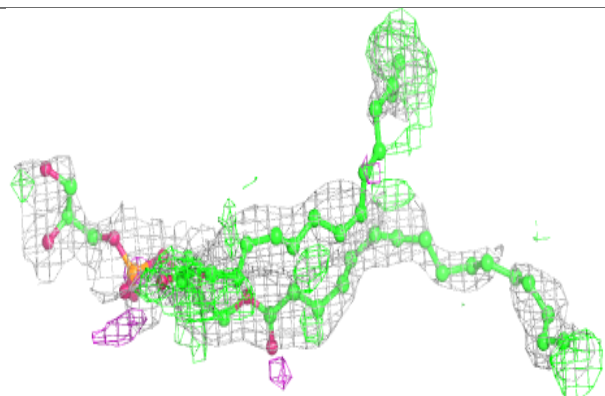
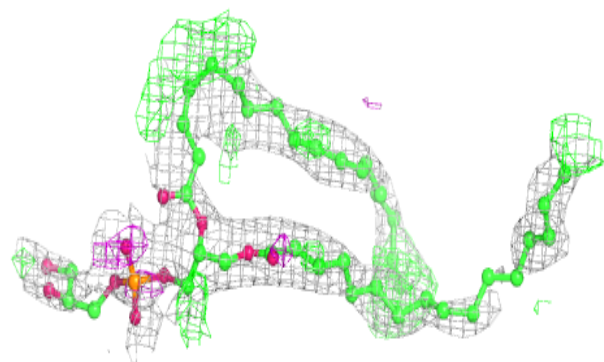


Electron density around TGL N 605:

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

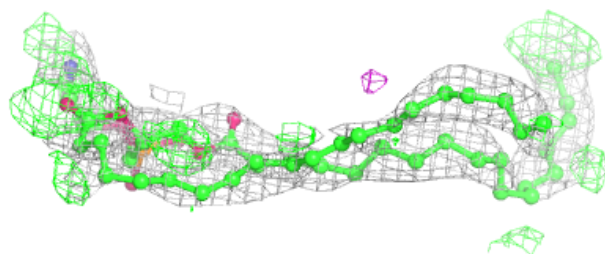
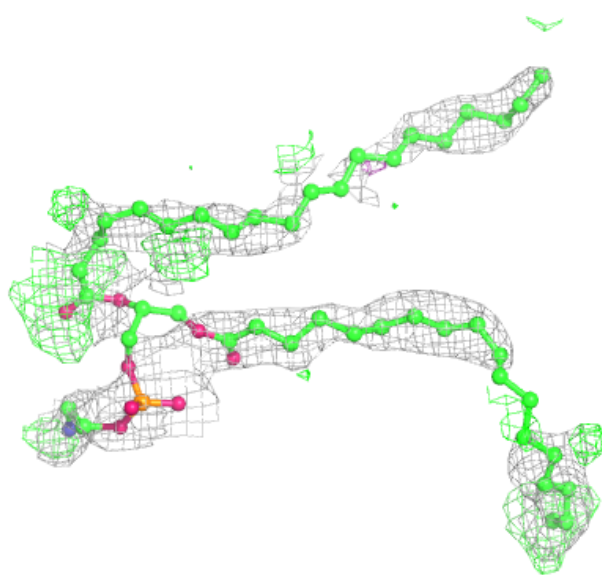
**Electron density around PGV C 304:**

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



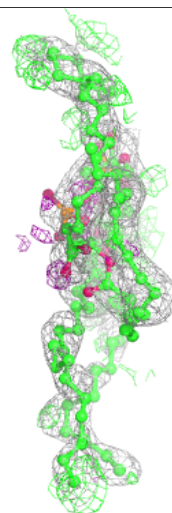
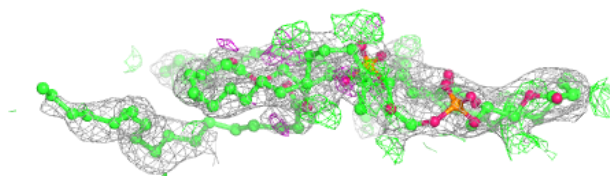
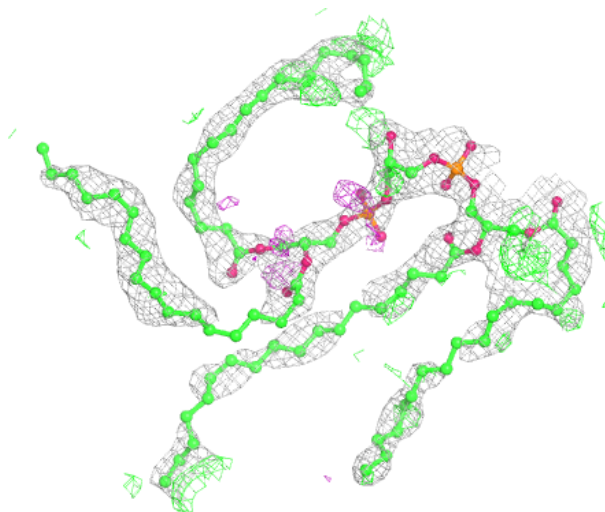
Electron density around PEK P 305:

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



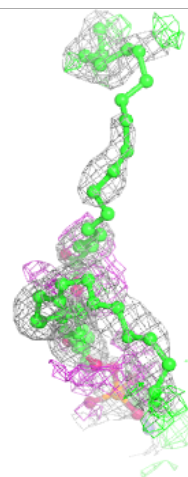
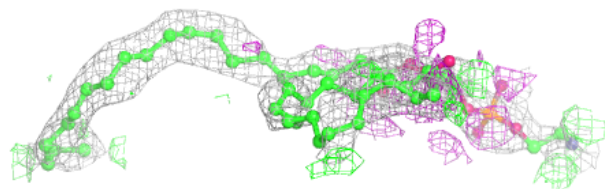
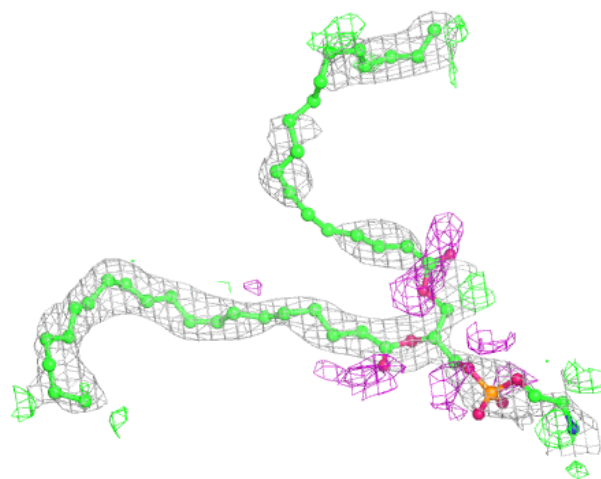
Electron density around CDL P 312:

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



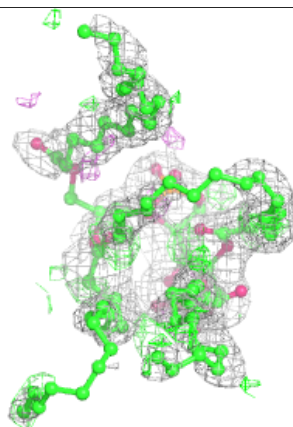
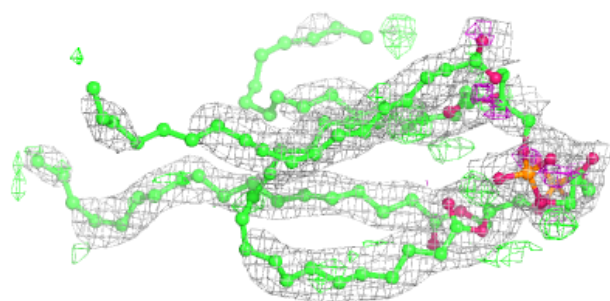
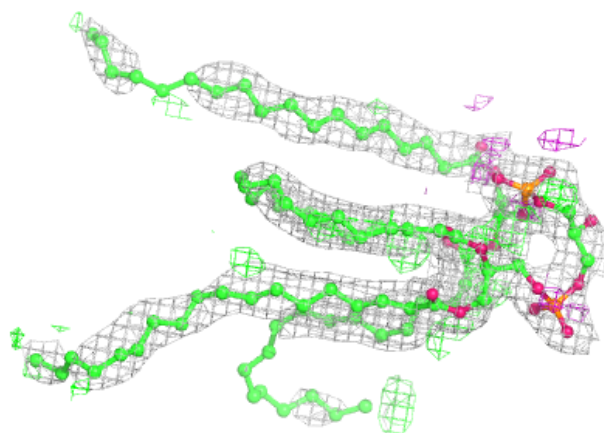
Electron density around PEK C 314:

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

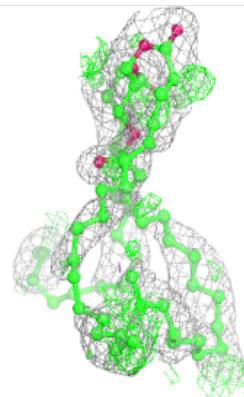
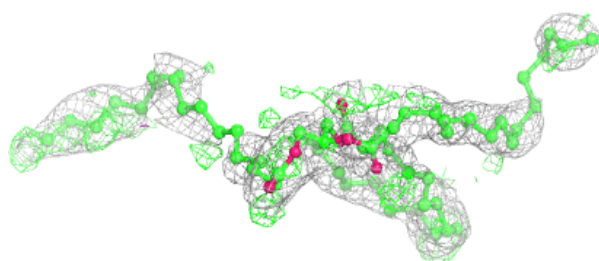
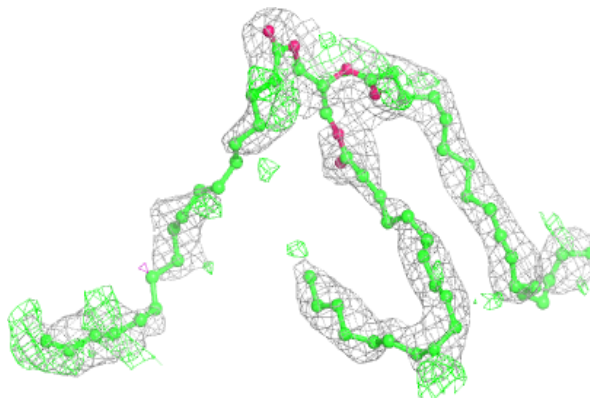


Electron density around CDL P 308:

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

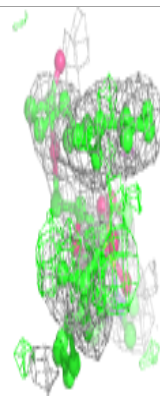
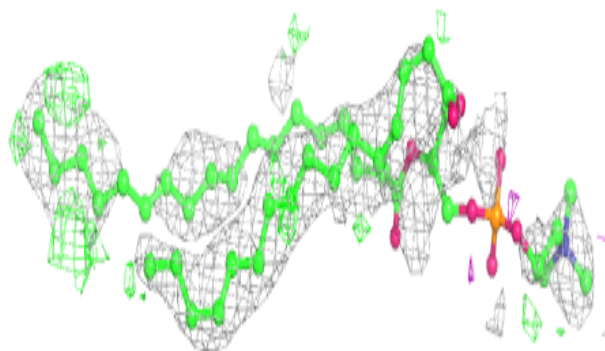
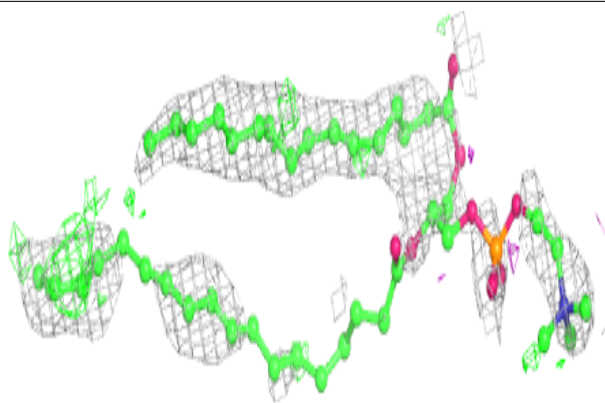
**Electron density around TGL N 618:**

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

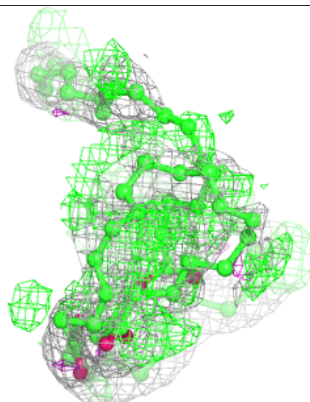
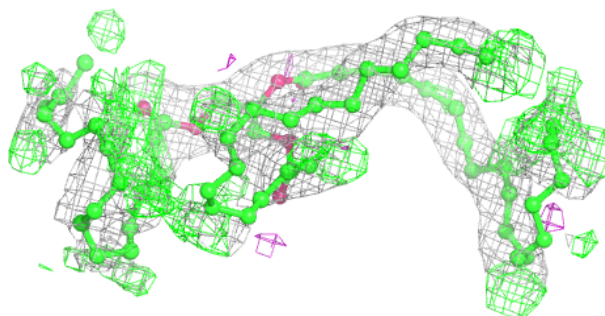
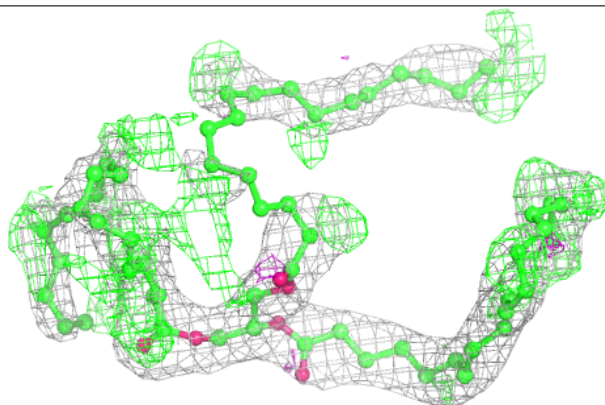


Electron density around PSC R 201:

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

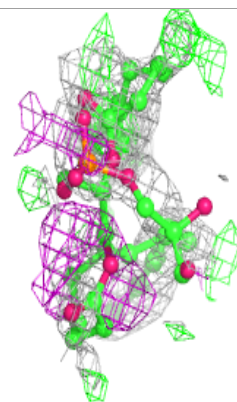
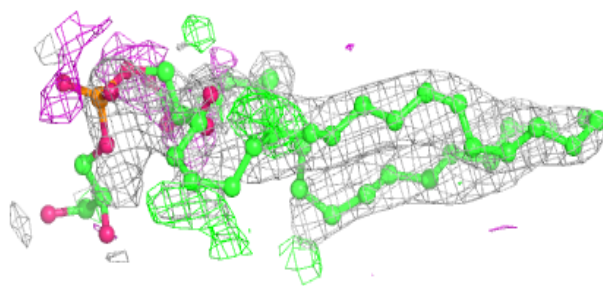
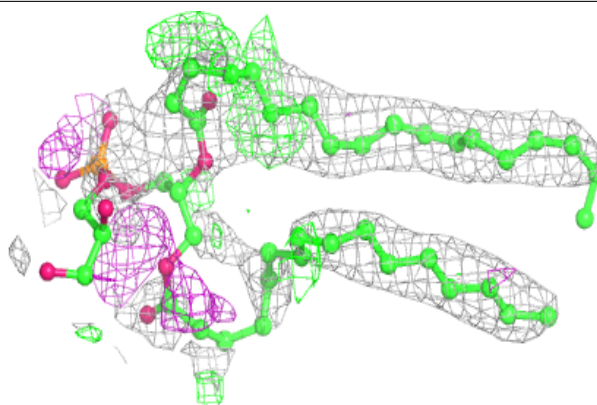
**Electron density around TGL A 613:**

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

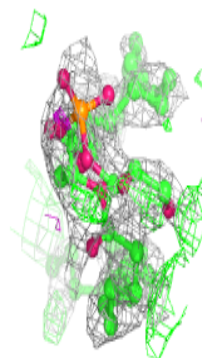
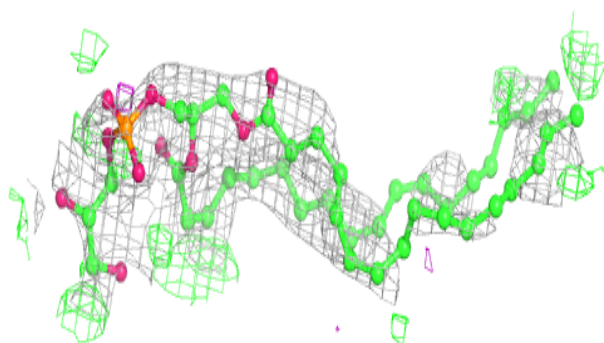
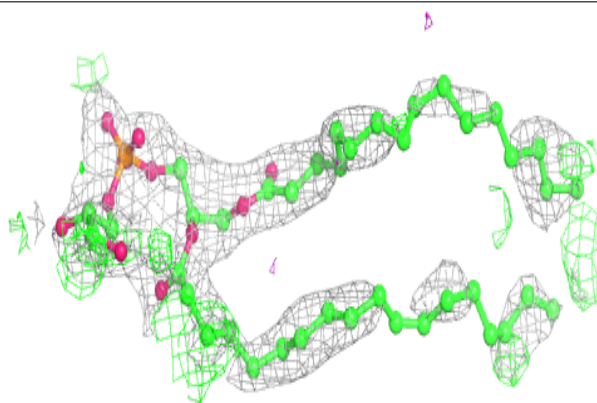


Electron density around PGV N 622:

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

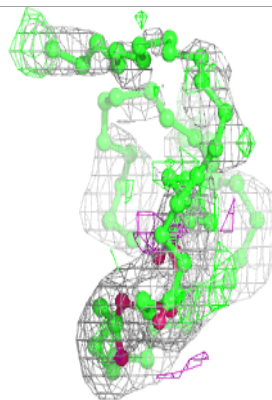
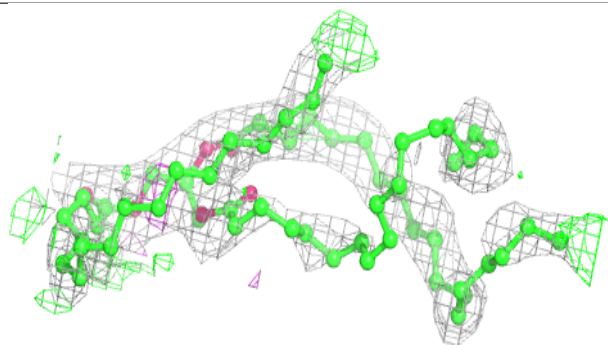
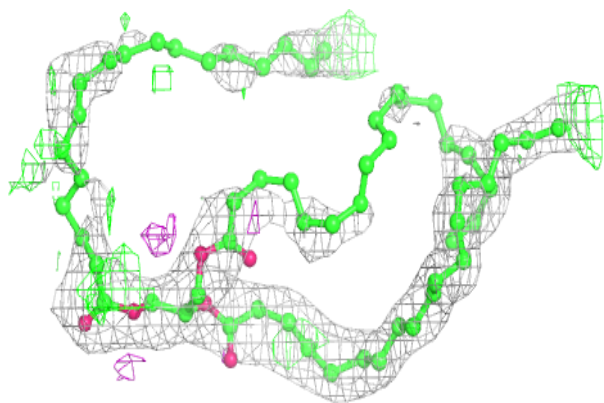
**Electron density around PGV P 307:**

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

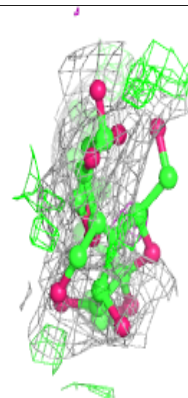
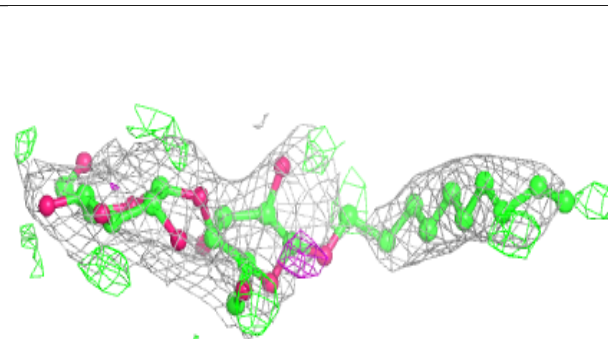
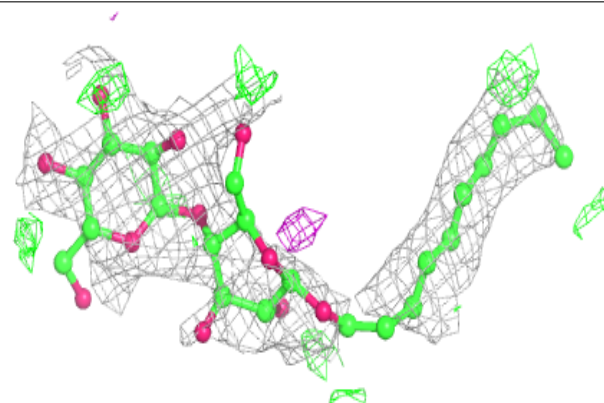


Electron density around TGL N 604:

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

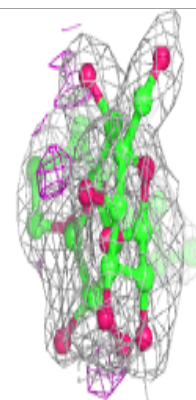
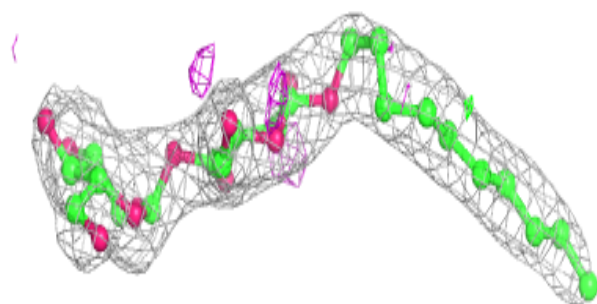
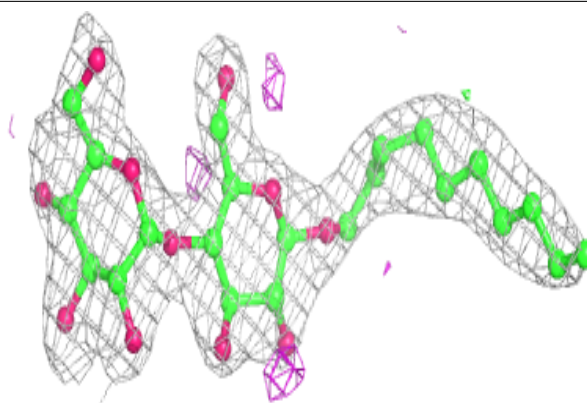
**Electron density around DMU G 104:**

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

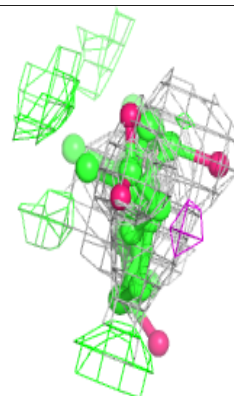
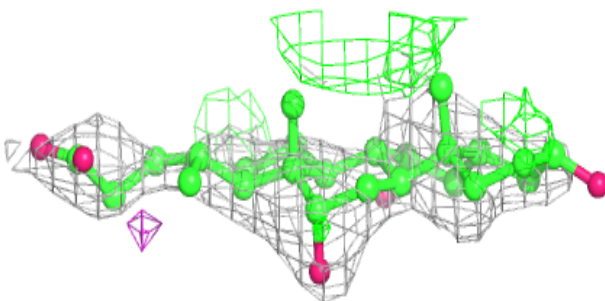
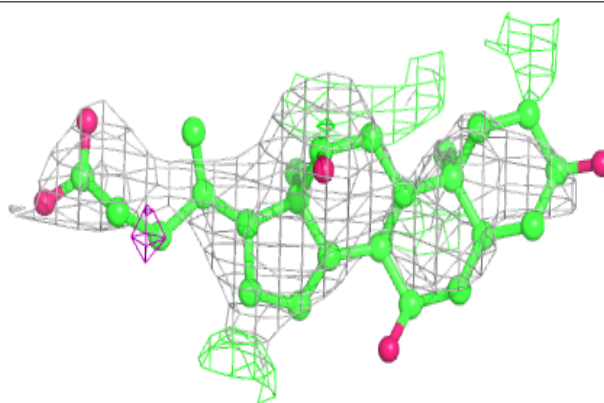


Electron density around DMU Z 101:

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

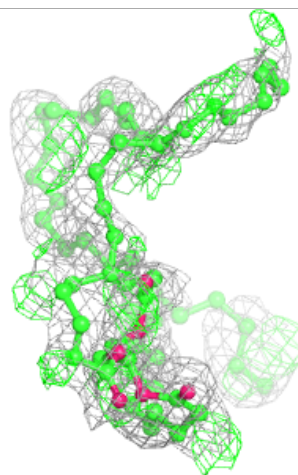
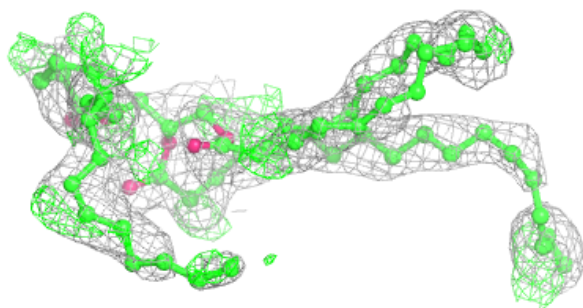
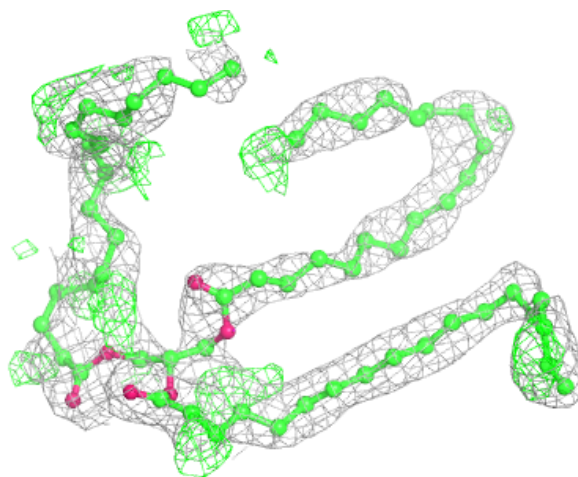
**Electron density around CHD T 1302:**

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



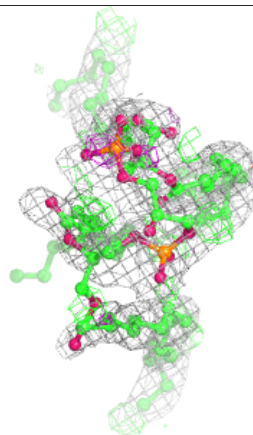
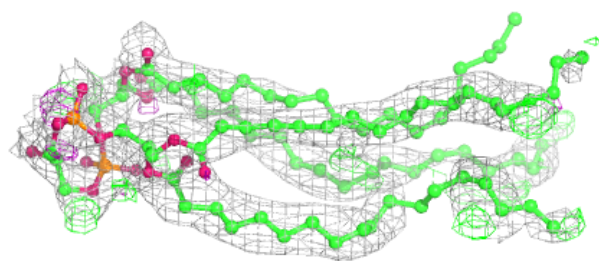
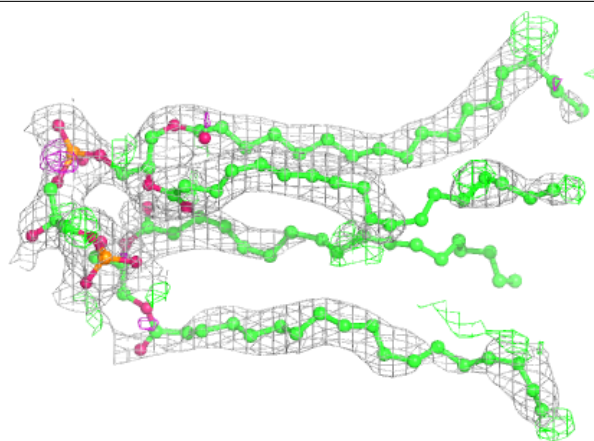
Electron density around TGL D 201:

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



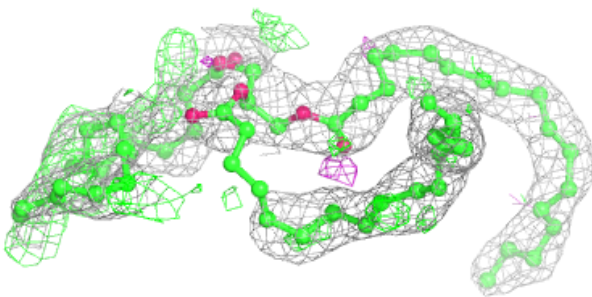
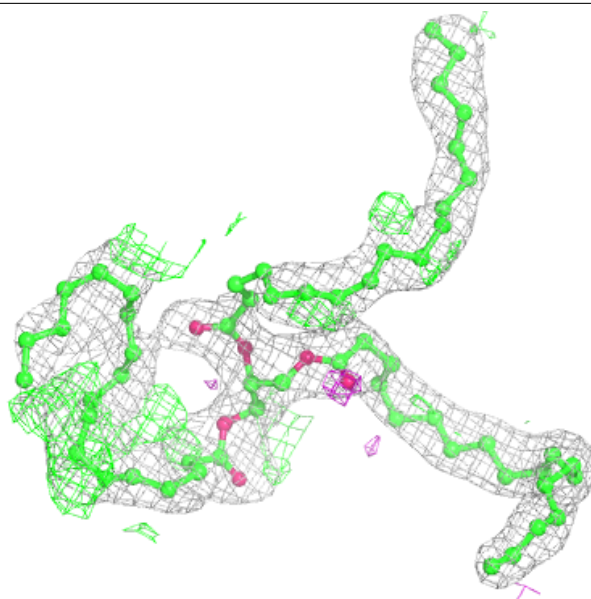
Electron density around CDL C 305:

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



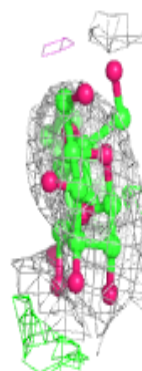
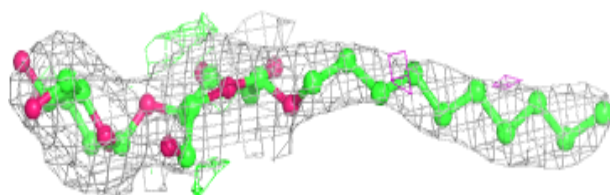
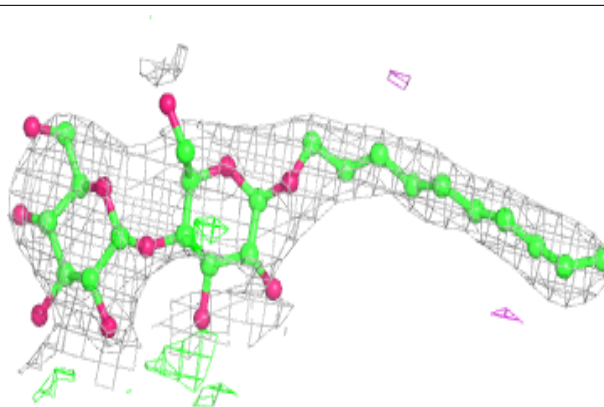
Electron density around TGL L 502:

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

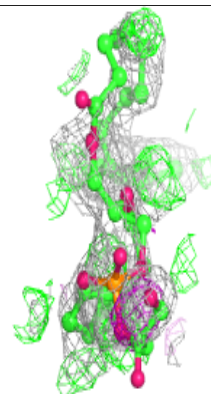
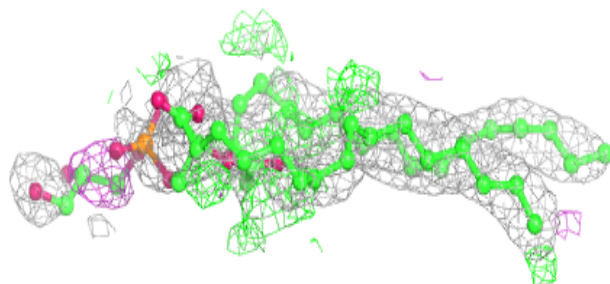
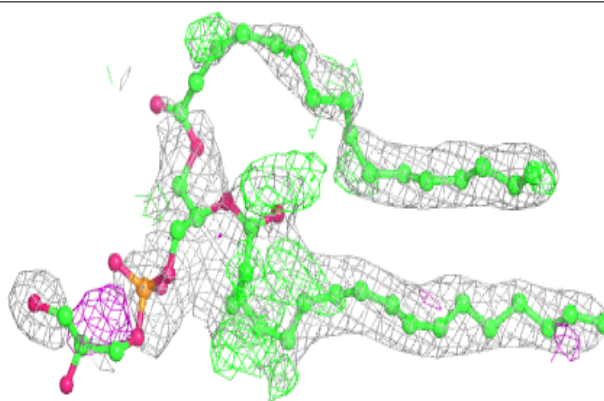


Electron density around DMU P 302:

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

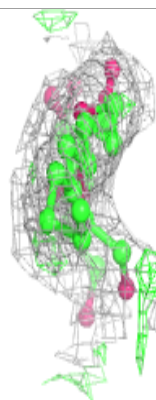
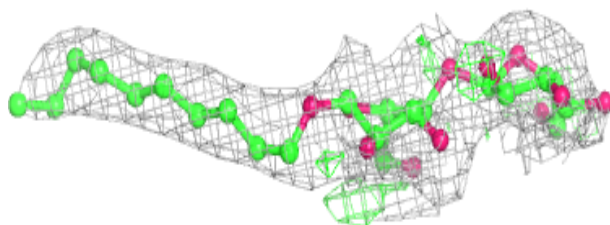
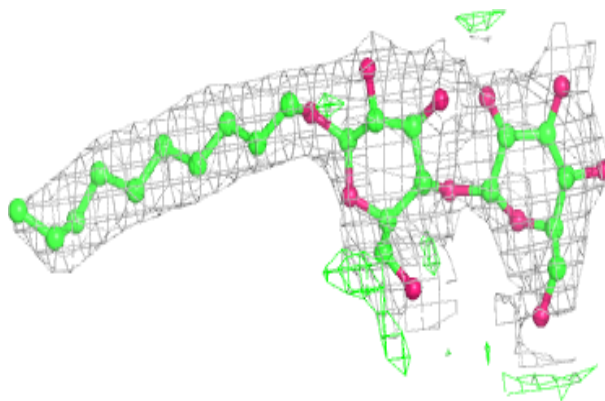
**Electron density around PGV M 101:**

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

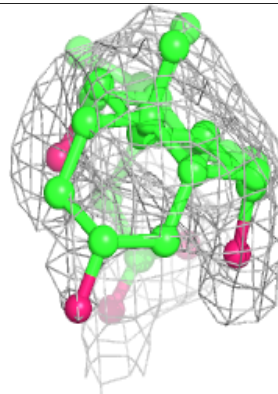
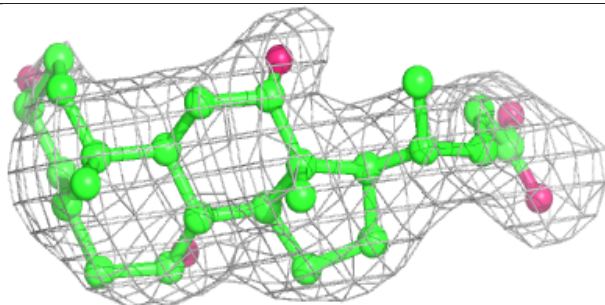
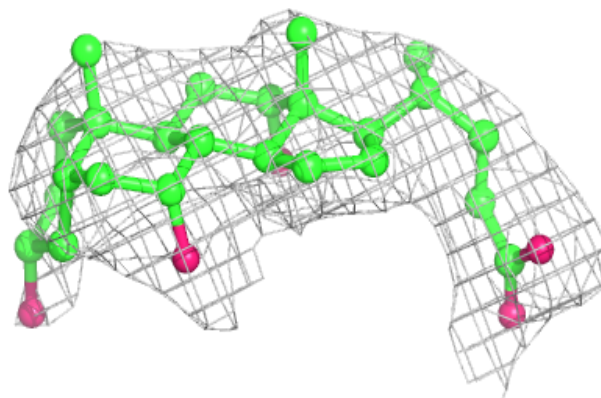


Electron density around DMU C 311:

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

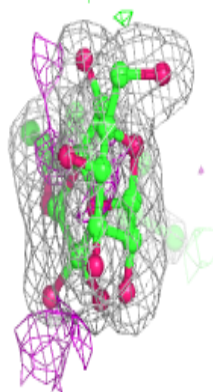
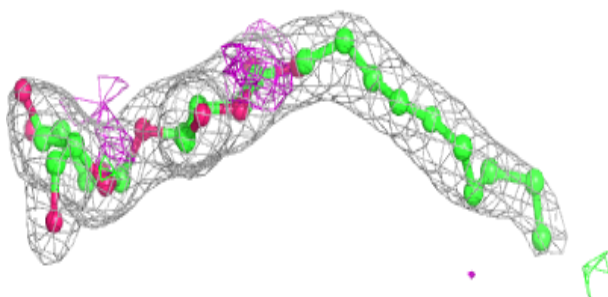
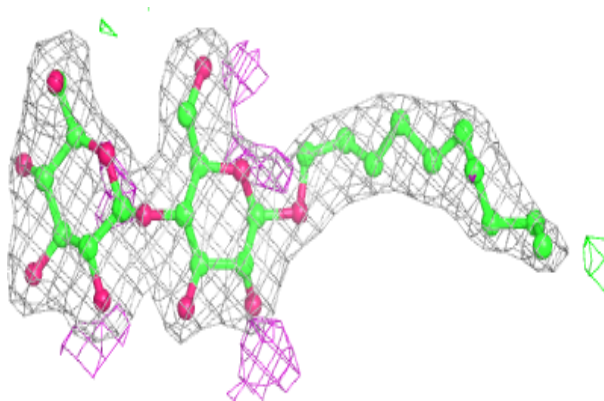
**Electron density around CHD W 302:**

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

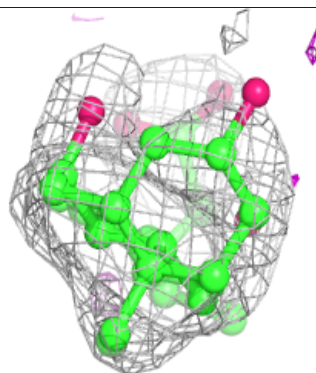
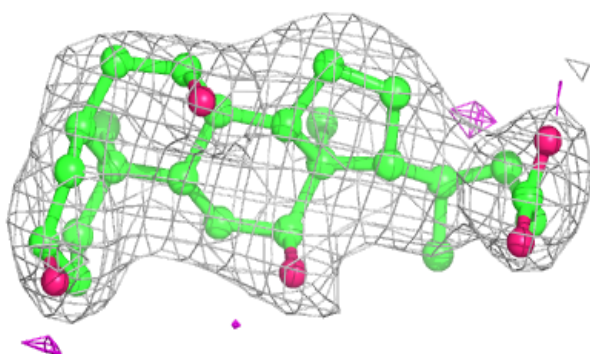
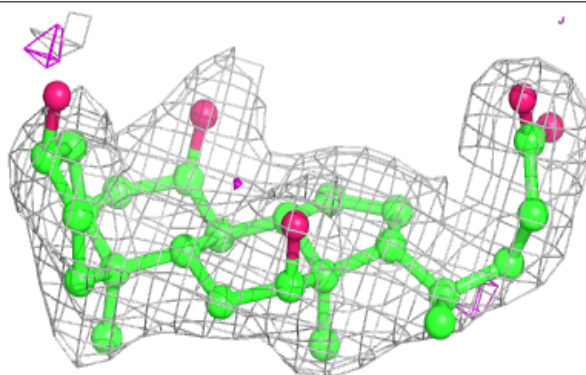


Electron density around DMU M 102:

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

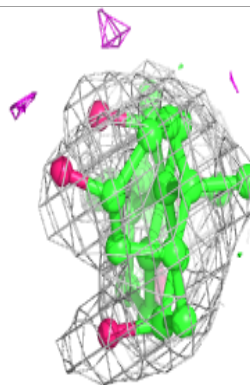
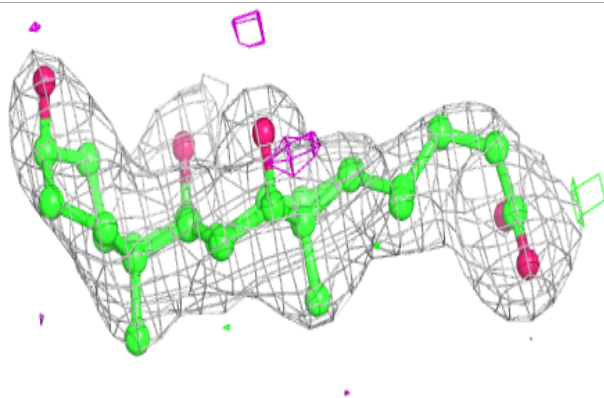
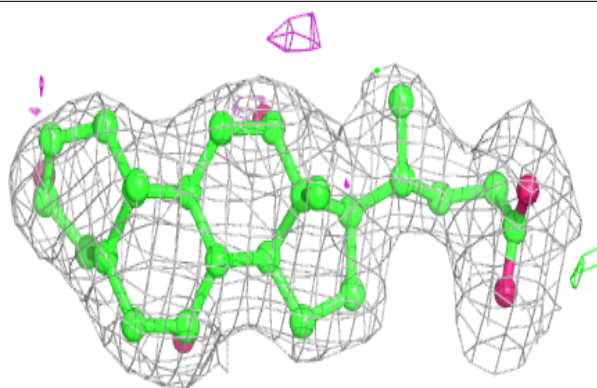
**Electron density around CHD J 101:**

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

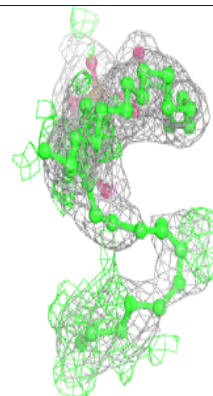
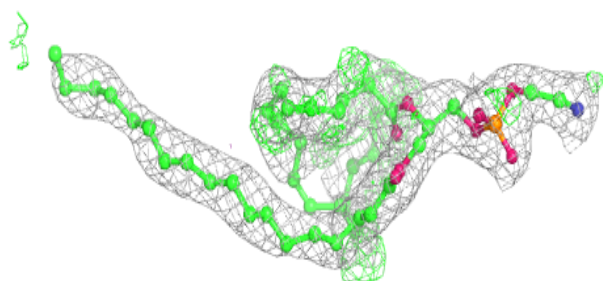
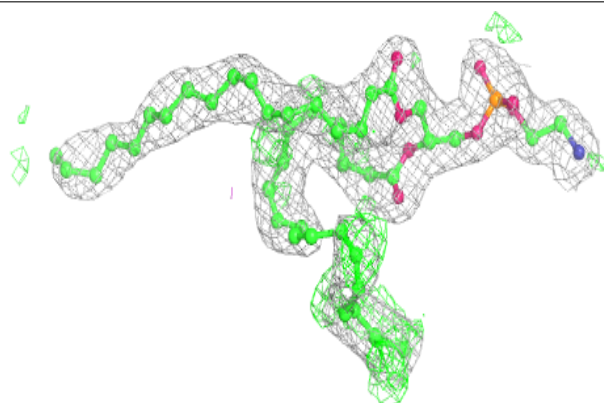


Electron density around CHD P 309:

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

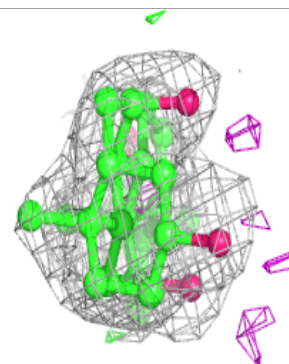
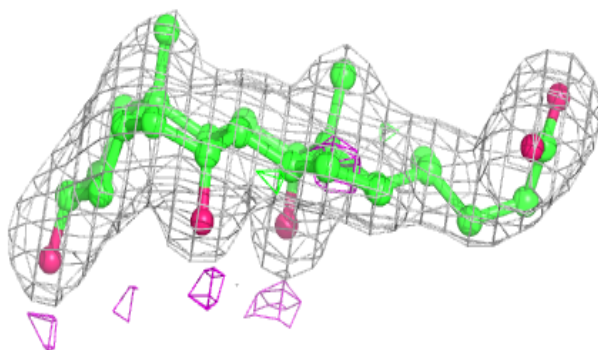
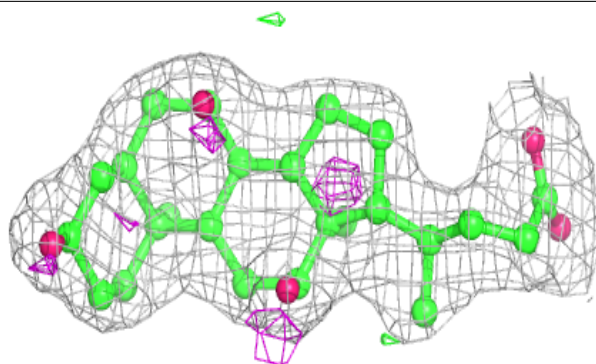
**Electron density around PEK P 304:**

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

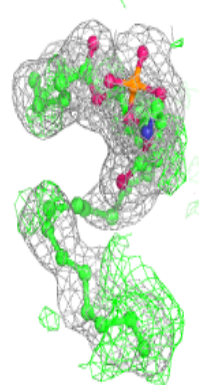
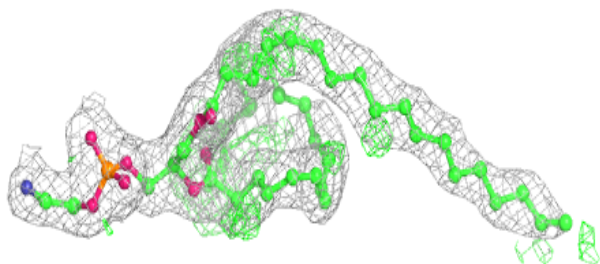
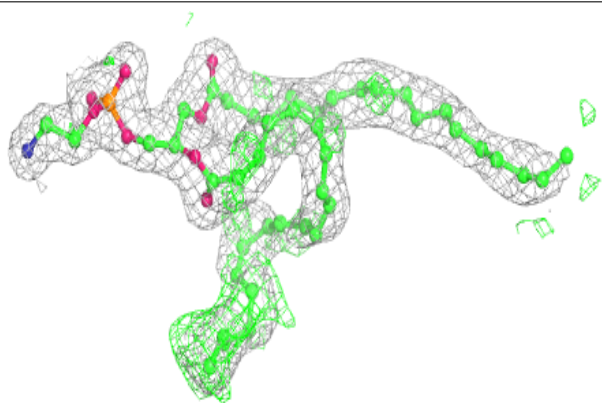


Electron density around CHD C 306:

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

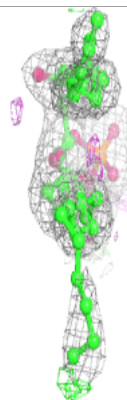
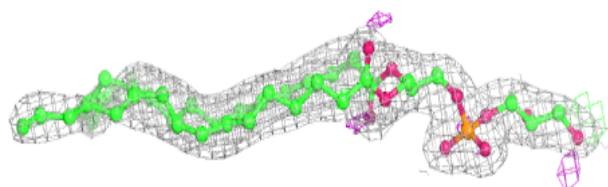
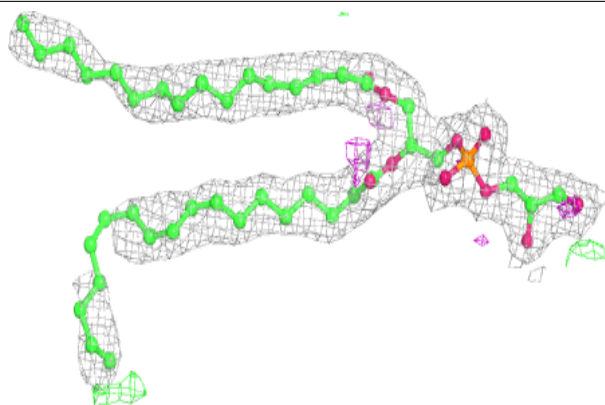
**Electron density around PEK G 102:**

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

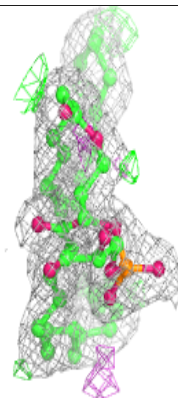
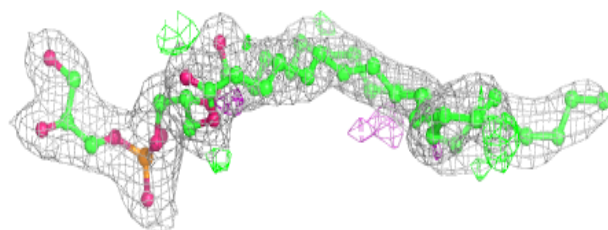
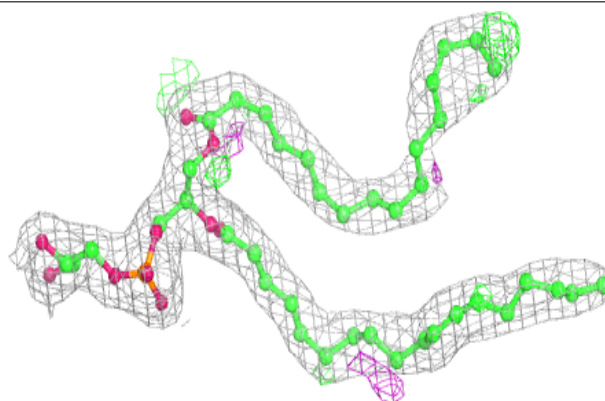


Electron density around PGV P 306:

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

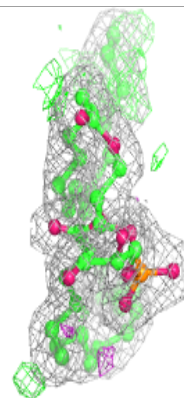
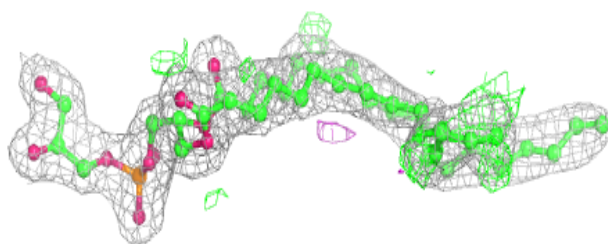
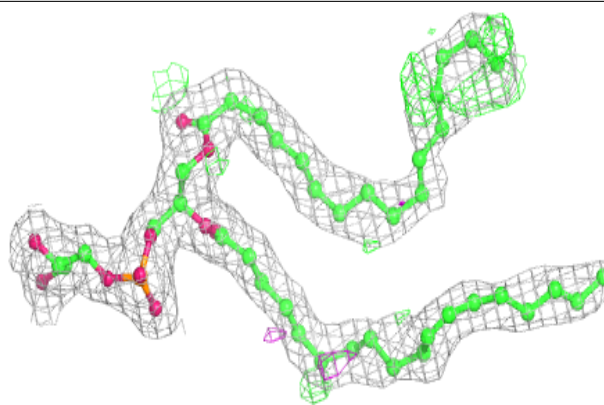
**Electron density around PGV N 606:**

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

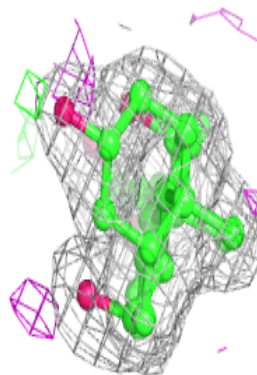
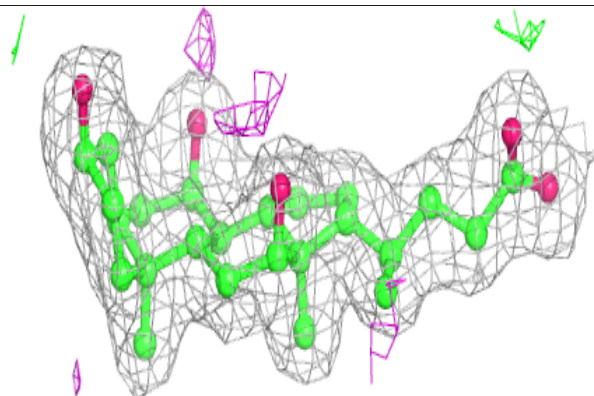
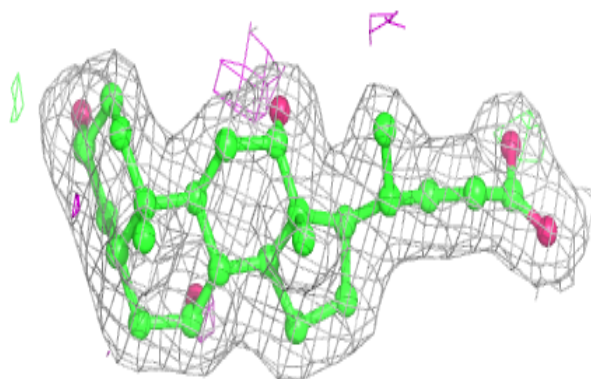


Electron density around PGV A 604:

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

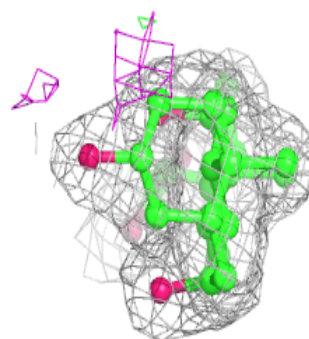
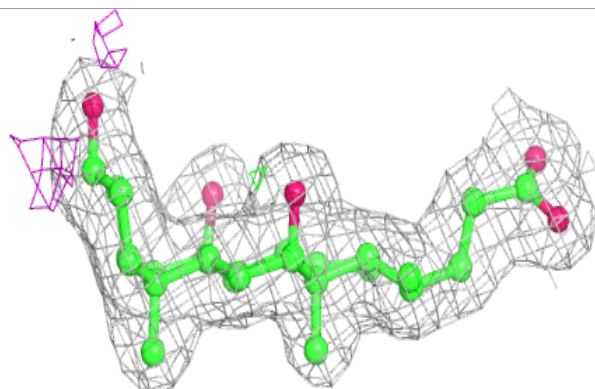
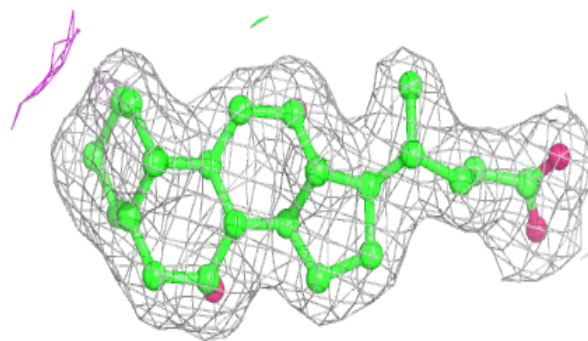
**Electron density around CHD C 301:**

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

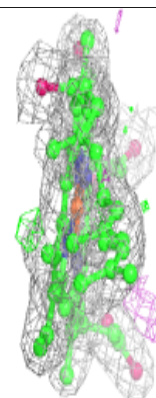
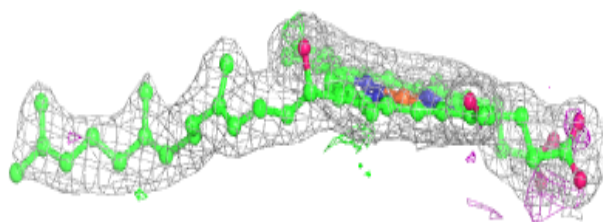
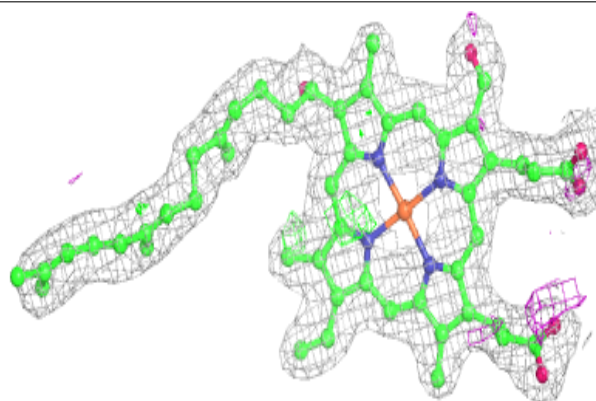


Electron density around CHD B 303:

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

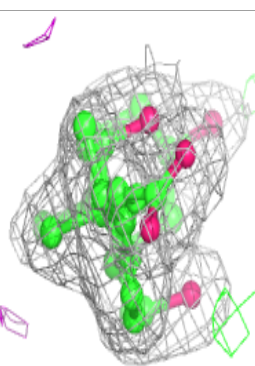
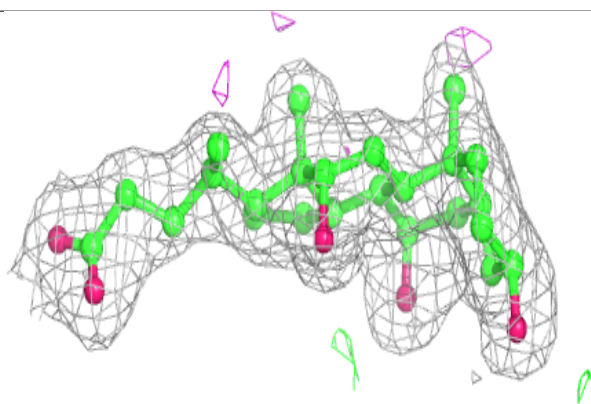
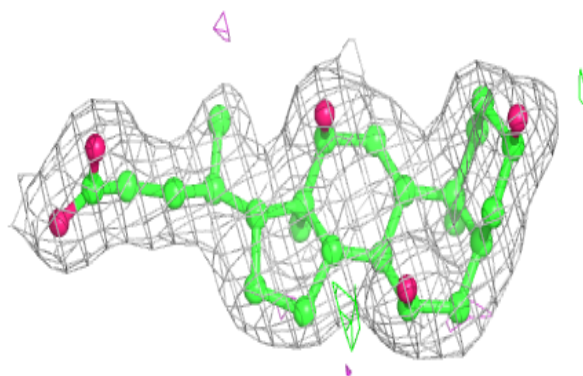
**Electron density around HEA N 608:**

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

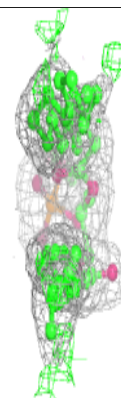
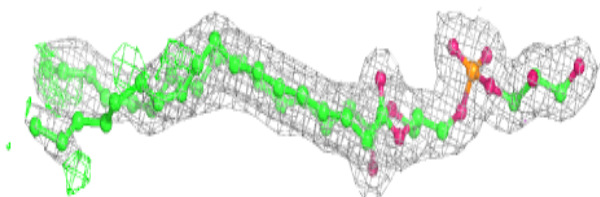
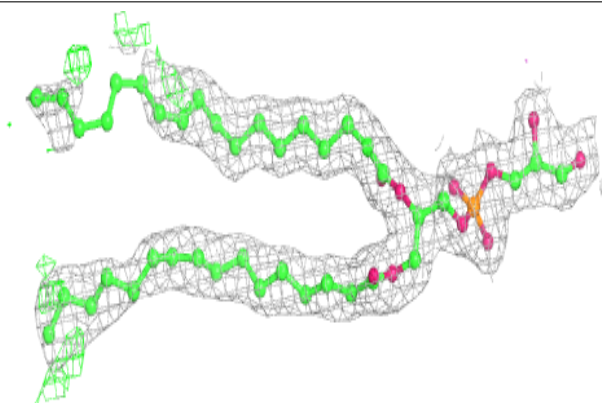


Electron density around CHD P 303:

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

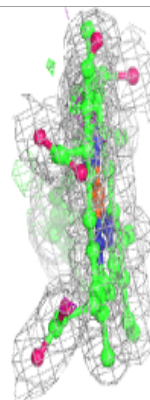
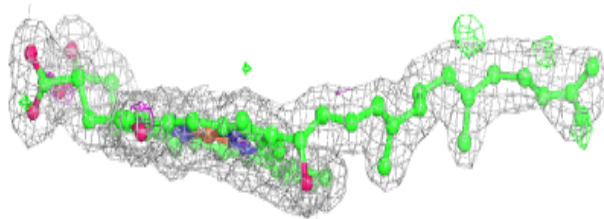
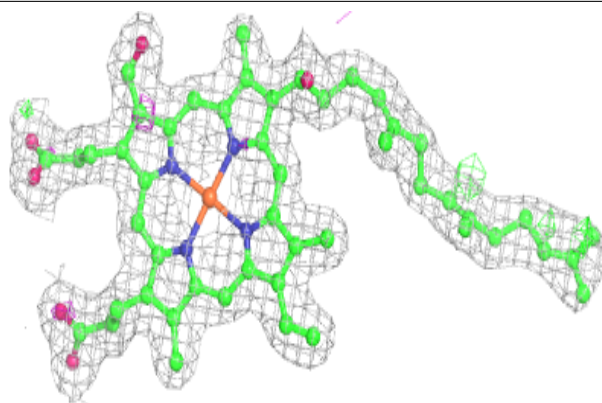
**Electron density around PGV C 303:**

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

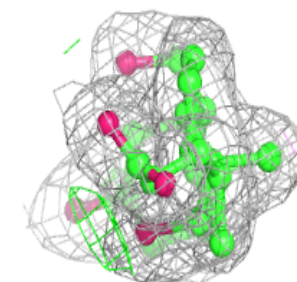
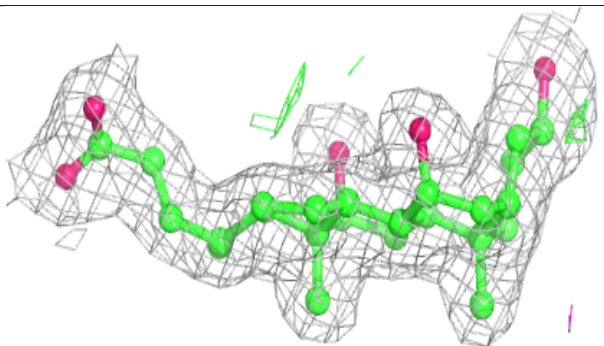
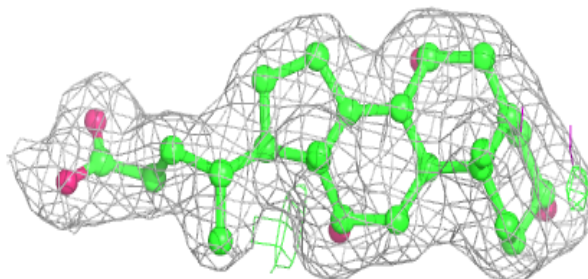


Electron density around HEA A 606:

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

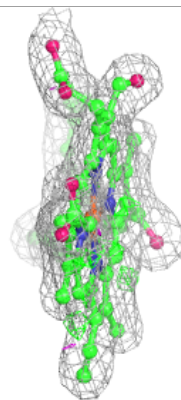
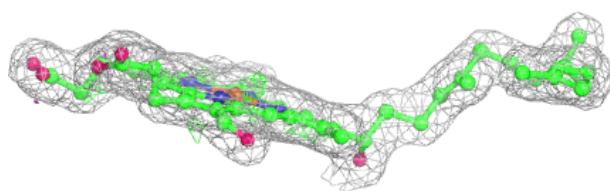
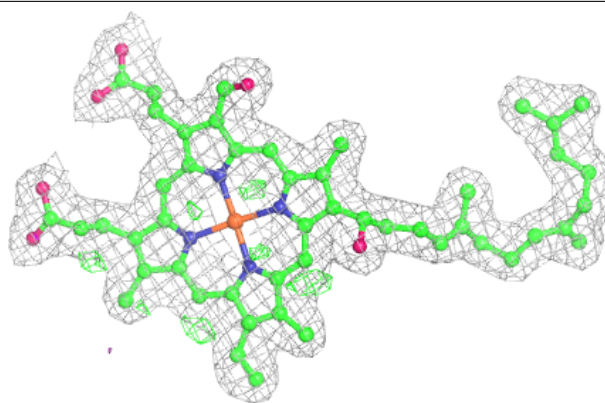
**Electron density around CHD G 107:**

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

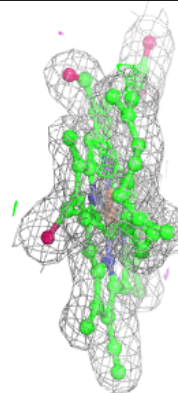
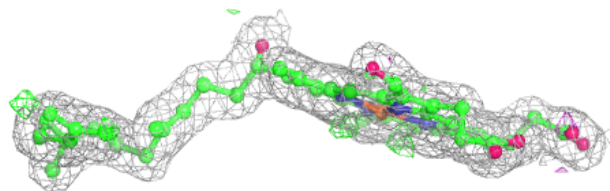
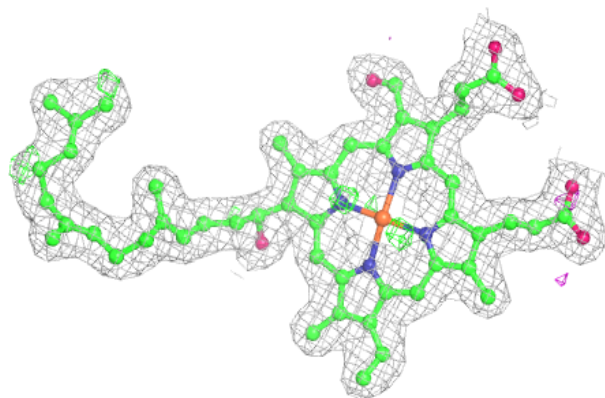


Electron density around HEA N 607:

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

**Electron density around HEA A 605:**

$2mF_o-DF_c$ (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.