



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 28, 2022 – 06:49 PM JST

PDB ID : 7W3E
Title : Bovine cytochrome c oxidase in CN-bound fully reduced state at 50 K
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2021-11-25
Resolution : 1.45 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 : 2.31.3
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) : 2.31.3

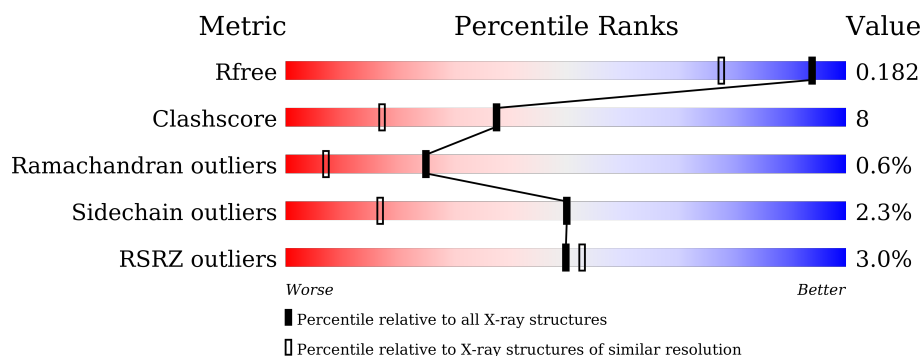
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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.



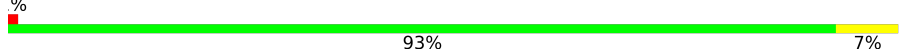

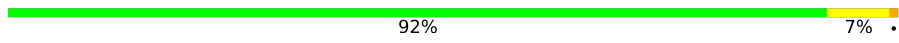
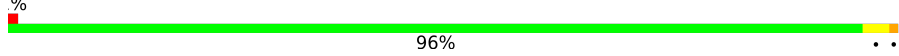
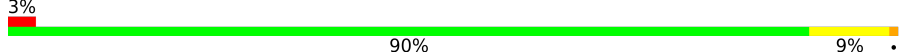


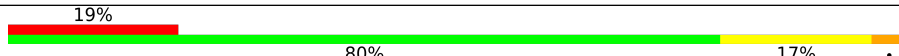
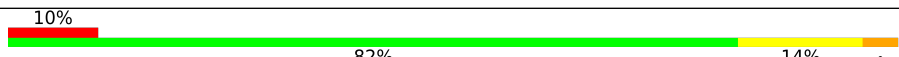
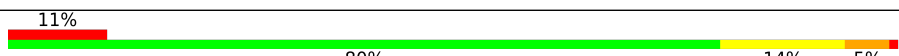
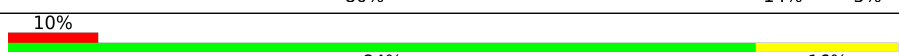
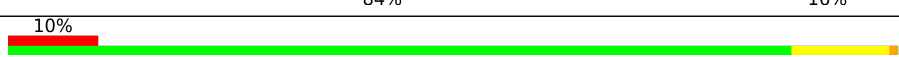

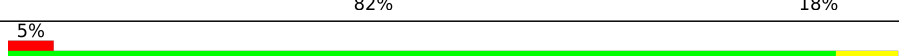
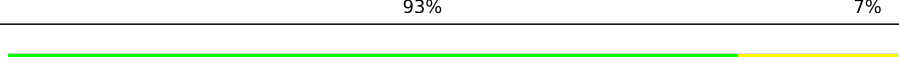

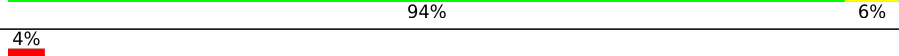
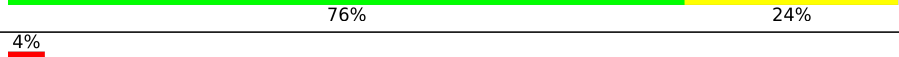
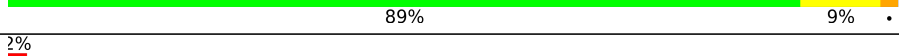
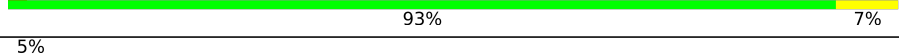
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	
1	N	514	
2	B	227	
2	O	227	
3	C	259	
3	P	259	

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	104	
5	R	104	
6	F	93	
6	S	93	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	57	
10	W	57	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	41	
13	Z	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601[A]	X	-	-	-
14	HEA	A	601[B]	X	-	-	-
14	HEA	A	601[C]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	602[A]	X	-	-	-
14	HEA	A	602[C]	X	-	-	-
14	HEA	N	601[A]	X	-	-	-
14	HEA	N	601[B]	X	-	-	-
14	HEA	N	601[C]	X	-	-	-
14	HEA	N	602[A]	X	-	-	-
14	HEA	N	602[C]	X	-	-	-
21	EDO	B	305	-	-	X	-
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 35109 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	34	0
			4162	2778	639	699	46			
1	N	514	Total	C	N	O	S	1	33	0
			4160	2776	639	698	47			

- 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	26	0
			2000	1306	302	372	20			
2	O	227	Total	C	N	O	S	0	26	0
			1999	1305	303	369	22			

- 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	7	0
			2125	1419	337	355	14			
3	P	259	Total	C	N	O	S	0	6	0
			2121	1417	339	351	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	1	0
			1201	783	196	218	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1209	783	202	220	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	3	0
			720	445	128	142	5			
6	S	93	Total	C	N	O	S	0	4	0
			721	447	127	141	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	S	0	0	0
			642	413	122	106	1			
7	T	84	Total	C	N	O	S	0	2	0
			663	423	126	113	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	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	2	0
			389	253	65	68	3			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

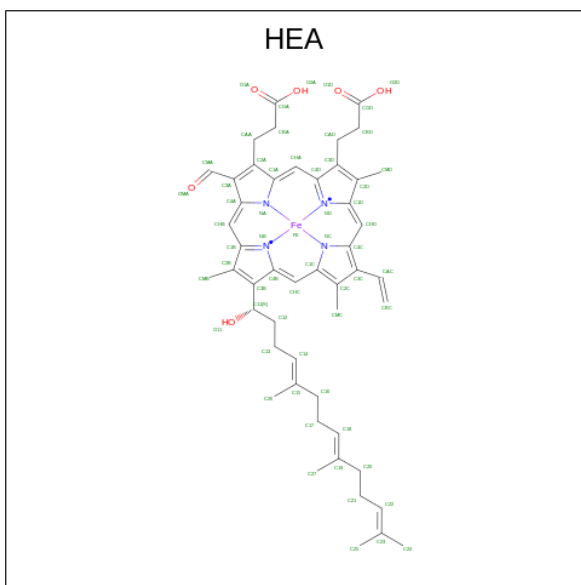
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	61	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	41	Total	C	N	O	0	1	0
			322	216	50	56			
13	Z	41	Total	C	N	O	0	0	0
			320	214	50	56			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	
			79	67	1	4	7	0
14	A	1	Total	C	Fe	N	O	
			111	89	2	8	12	0
14	N	1	Total	C	Fe	N	O	
			79	67	1	4	7	0
14	N	1	Total	C	Fe	N	O	
			111	89	2	8	12	0

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

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

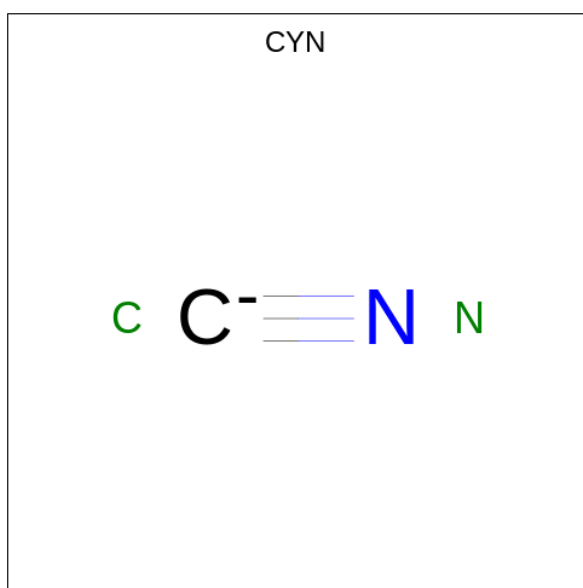
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

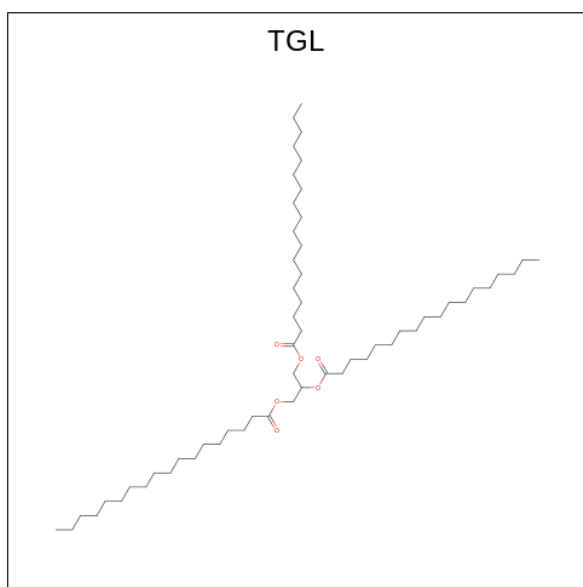
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is CYANIDE ION (three-letter code: CYN) (formula: CN).



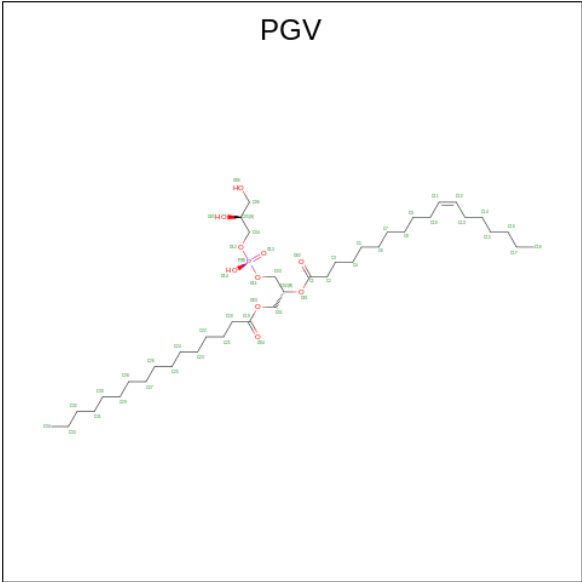
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	N	0	1
			4	2	2		
18	N	1	Total	C	N	0	1
			4	2	2		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



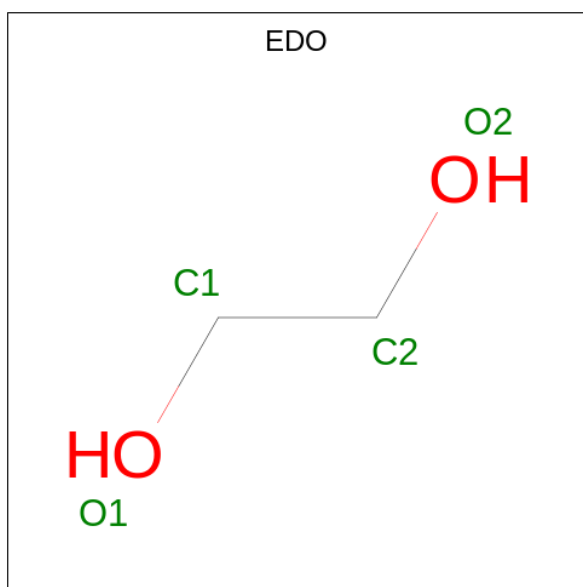
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			62	56	6		
19	D	1	Total	C	O	0	0
			48	42	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 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
20	A	1	Total	C	O	P	0	0
			46	37	8	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			47	36	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			45	34	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	Q	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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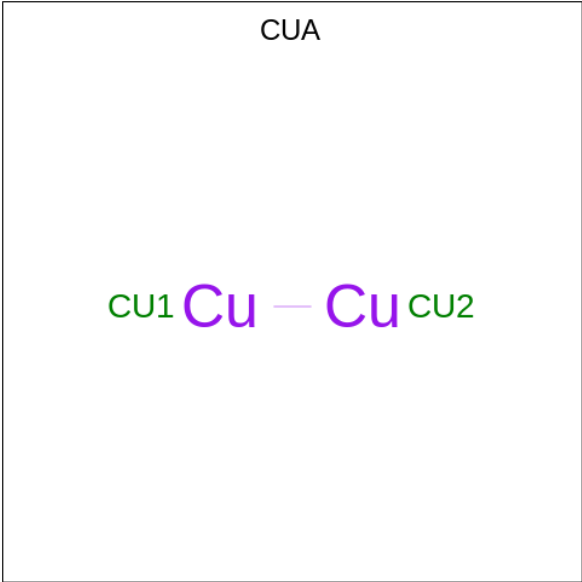
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	C	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4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

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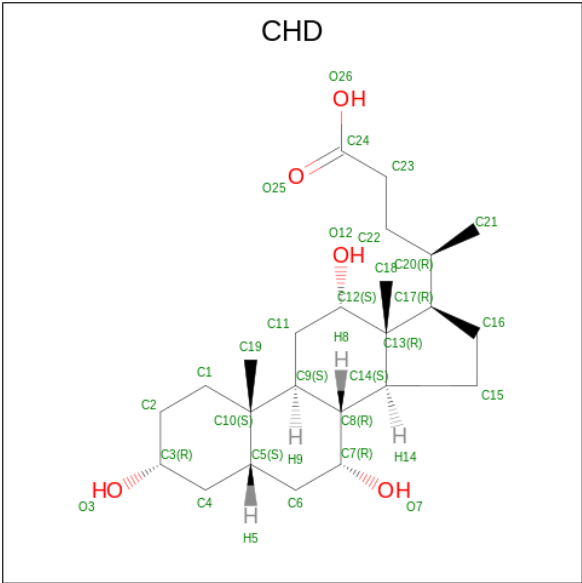
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



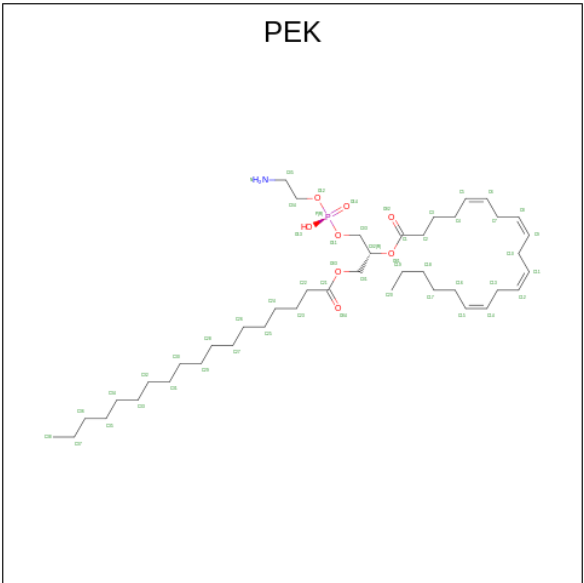
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 24 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).



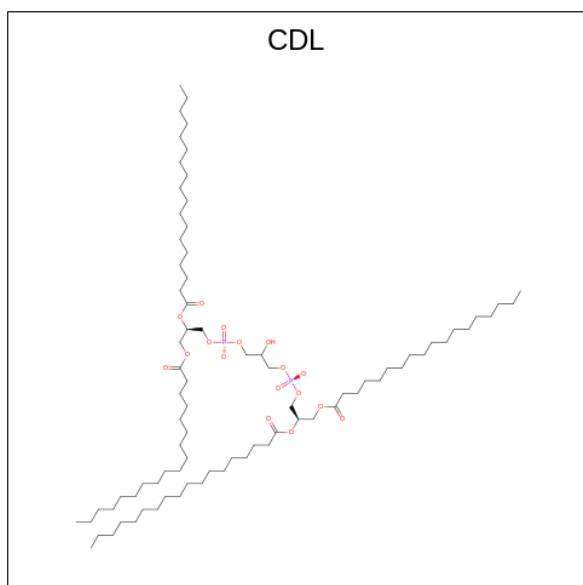
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total 51	C 41	N 1	O 8	P 1	0	0
24	C	1	Total 44	C 40	O 4	0			0
24	P	1	Total 22	C 20	O 2	0			0
24	P	1	Total 53	C 43	N 1	O 8	P 1	0	0

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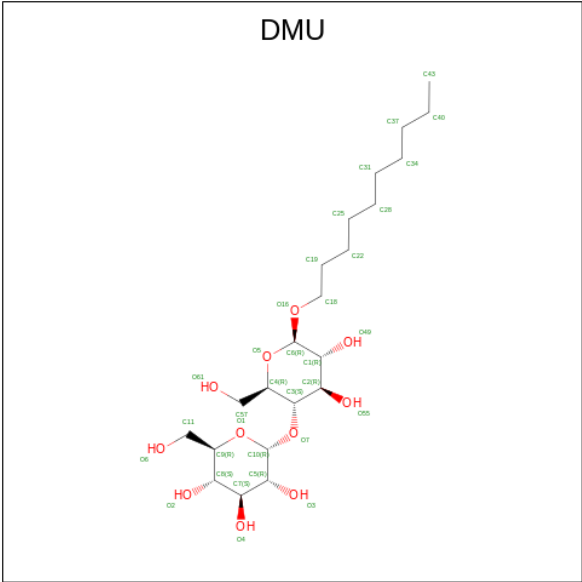
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	P	1	Total	C	O		0	0
			46	41	5			
24	T	1	Total	C	N	O	P	
			49	39	1	8	1	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			86	68	16	2		
25	G	1	Total	C	O	P	0	0
			89	71	16	2		
25	P	1	Total	C	O	P	0	0
			76	64	11	1		
25	T	1	Total	C	O	P	0	0
			80	63	15	2		
25	Y	1	Total	C	O	P	0	0
			87	68	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



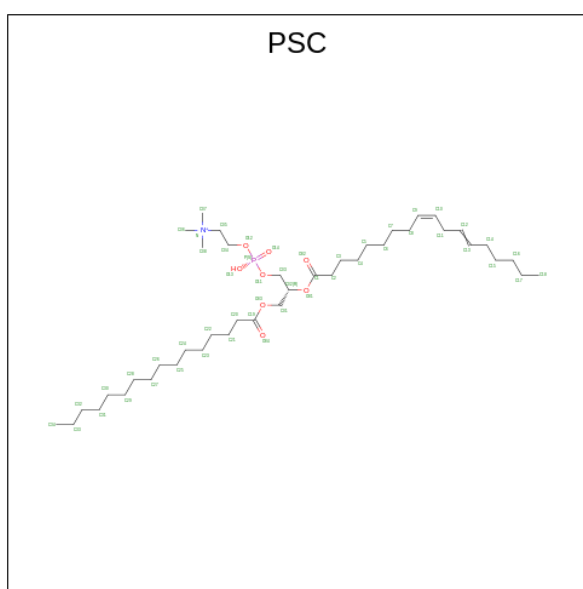
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	G	1	Total	C	O	0	0
			21	16	5		
26	J	1	Total	C	O	0	0
			33	22	11		
26	K	1	Total	C	O	0	0
			22	16	6		
26	K	1	Total	C	O	0	0
			22	16	6		
26	K	1	Total	C	O	0	0
			17	15	2		
26	L	1	Total	C	O	0	0
			18	12	6		
26	M	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			22	16	6		
26	X	1	Total	C	O	0	0
			22	16	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	X	1	Total	C	O	0	0
			22	16	6		
26	X	1	Total	C	O	0	0
			22	16	6		
26	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 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).

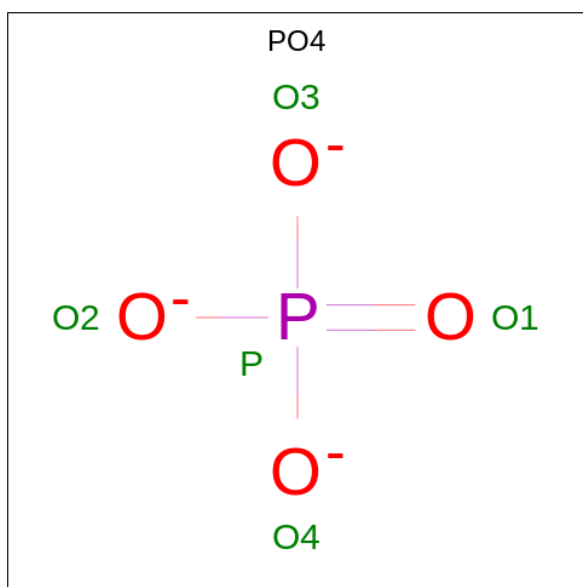


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
27	O	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

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



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

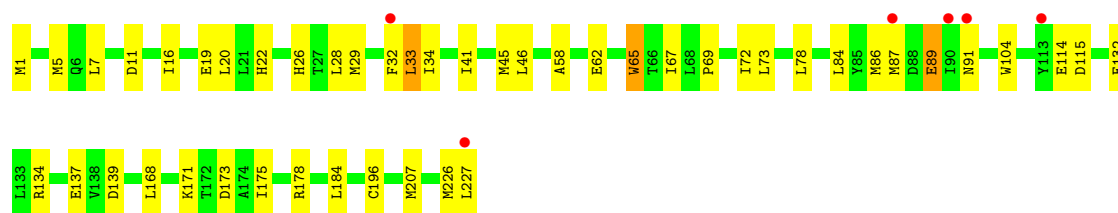
- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	286	Total	O	0	3
			286	286		
30	B	245	Total	O	0	0
			245	245		
30	C	196	Total	O	0	0
			196	196		
30	D	250	Total	O	0	0
			250	250		
30	E	178	Total	O	0	0
			178	178		
30	F	177	Total	O	0	2
			177	177		
30	G	97	Total	O	0	0
			97	97		
30	H	111	Total	O	0	0
			111	111		
30	I	81	Total	O	0	0
			81	81		
30	J	63	Total	O	0	0
			63	63		
30	K	63	Total	O	0	0
			63	63		

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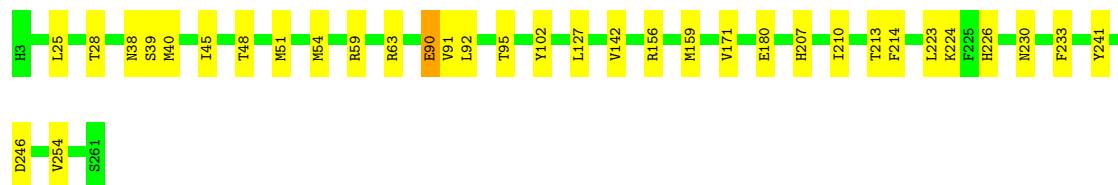
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	L	57	Total 57	O 57	0	0
30	M	46	Total 46	O 46	0	0
30	N	263	Total 263	O 263	0	1
30	O	204	Total 204	O 204	0	0
30	P	179	Total 179	O 179	0	0
30	Q	128	Total 128	O 128	0	0
30	R	131	Total 131	O 131	0	0
30	S	126	Total 126	O 126	0	0
30	T	78	Total 78	O 78	0	0
30	U	121	Total 121	O 121	0	0
30	V	68	Total 68	O 68	0	0
30	W	51	Total 51	O 51	0	0
30	X	50	Total 50	O 50	0	0
30	Y	48	Total 48	O 48	0	0
30	Z	30	Total 30	O 30	0	0



• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 13%



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 92% 8%



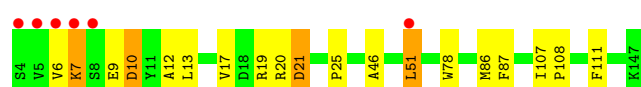
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 93% 7%



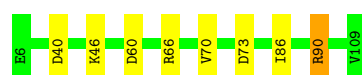
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 87% 10% 4%



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

Chain E: 92% 7%

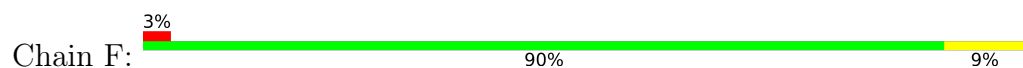


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

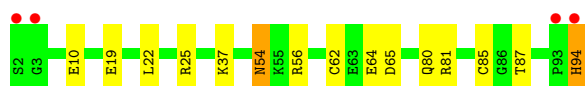
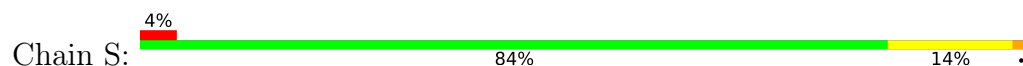
Chain R: 96% 4%



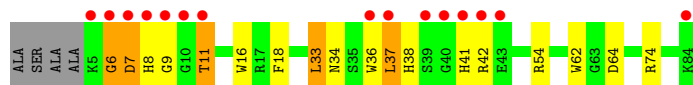
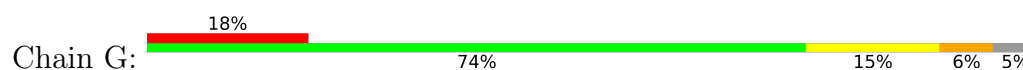
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



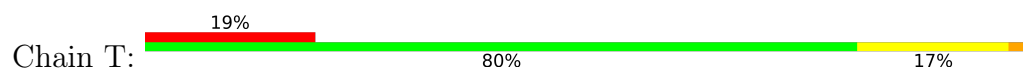
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



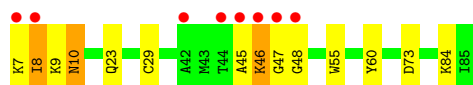
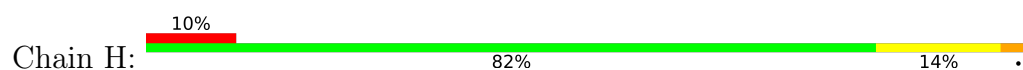
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



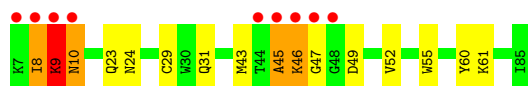
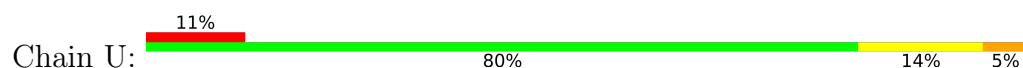
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



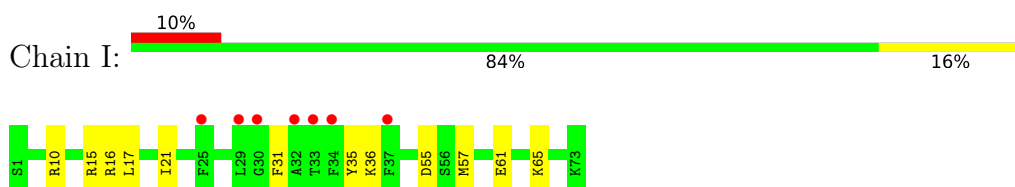
- Molecule 8: Cytochrome c oxidase subunit 6B1



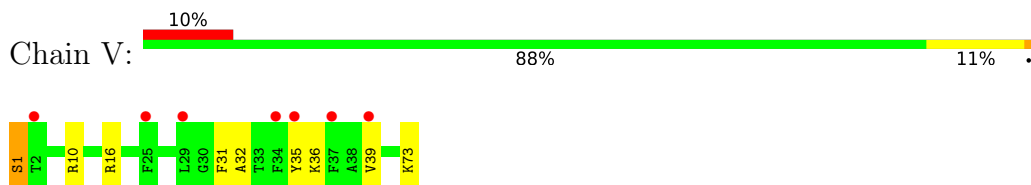
- Molecule 8: Cytochrome c oxidase subunit 6B1



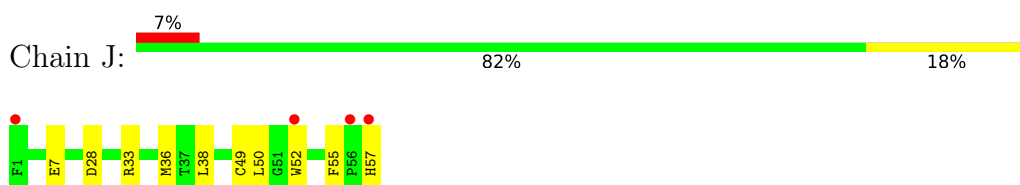
- Molecule 9: Cytochrome c oxidase subunit 6C



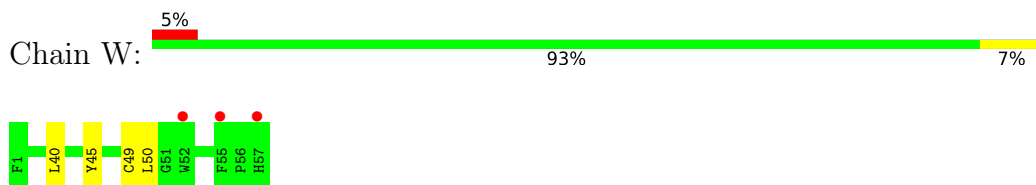
- Molecule 9: Cytochrome c oxidase subunit 6C



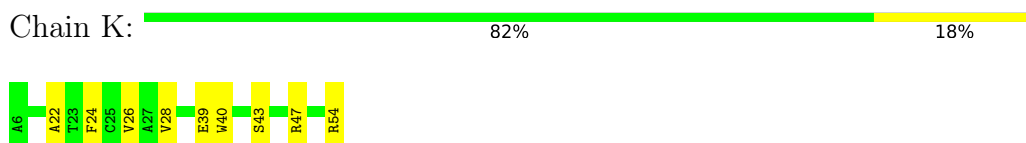
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



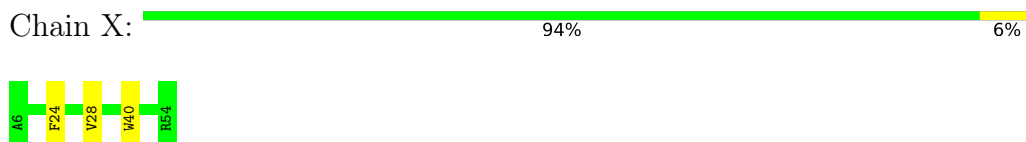
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



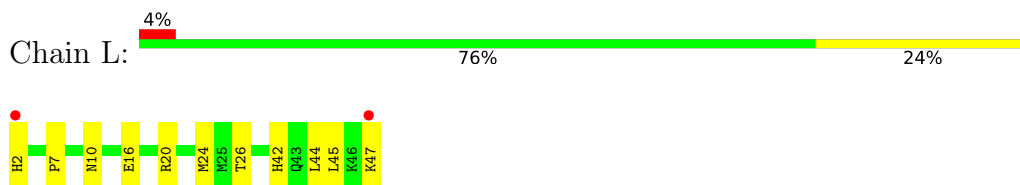
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



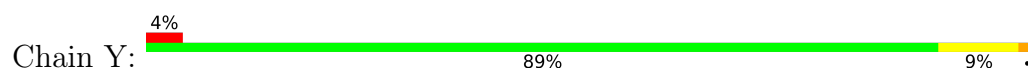
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



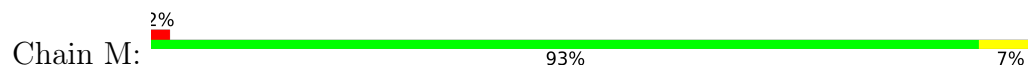
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



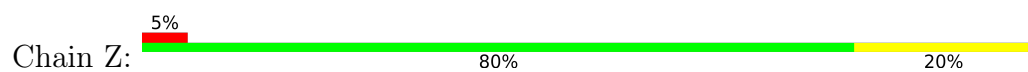
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.67Å 203.75Å 177.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 1.45 135.60 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.76-1.45) 99.9 (135.60-1.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.45Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.162 , 0.182 0.162 , 0.182	Depositor DCC
R_{free} test set	57695 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35109	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.95	3/4449 (0.1%)	1.07	18/6067 (0.3%)
1	N	0.90	2/4447 (0.0%)	0.95	10/6066 (0.2%)
2	B	0.85	1/2067 (0.0%)	1.00	7/2815 (0.2%)
2	O	0.80	0/2065	0.94	6/2811 (0.2%)
3	C	0.89	4/2252 (0.2%)	0.89	2/3077 (0.1%)
3	P	0.88	0/2246	0.89	3/3068 (0.1%)
4	D	0.84	0/1241	0.91	2/1674 (0.1%)
4	Q	0.65	0/1259	0.81	3/1697 (0.2%)
5	E	0.92	1/860 (0.1%)	0.99	4/1167 (0.3%)
5	R	0.76	0/860	0.84	1/1167 (0.1%)
6	F	0.96	1/751 (0.1%)	1.04	0/1019
6	S	0.85	1/758 (0.1%)	0.97	2/1029 (0.2%)
7	G	0.87	1/668 (0.1%)	0.97	2/909 (0.2%)
7	T	0.74	0/699	0.88	0/950
8	H	0.85	0/682	0.96	1/921 (0.1%)
8	U	0.81	0/682	0.85	0/921
9	I	0.71	0/605	0.87	2/802 (0.2%)
9	V	0.71	0/605	0.76	0/802
10	J	0.64	0/462	0.81	2/625 (0.3%)
10	W	0.60	0/462	0.76	0/625
11	K	0.84	1/414 (0.2%)	0.94	1/566 (0.2%)
11	X	0.67	0/399	0.76	0/546
12	L	0.99	1/393 (0.3%)	0.89	0/526
12	Y	0.77	0/400	0.75	0/536
13	M	0.95	0/338	0.94	0/462
13	Z	0.81	1/330 (0.3%)	0.77	0/451
All	All	0.85	17/30394 (0.1%)	0.94	66/41299 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
6	F	0	1
All	All	0	5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	16	GLU	CG-CD	6.54	1.61	1.51
7	G	36	TRP	CB-CG	6.34	1.61	1.50
3	C	102	TYR	CG-CD2	-6.28	1.30	1.39
1	N	514	LYS	CE-NZ	6.24	1.64	1.49
6	F	85	CYS	CB-SG	-6.11	1.71	1.82

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189[A]	MET	CG-SD-CE	-13.95	77.88	100.20
1	A	189[B]	MET	CG-SD-CE	-13.95	77.88	100.20
5	E	60	ASP	CB-CG-OD2	-10.69	108.68	118.30
11	K	47	ARG	NE-CZ-NH1	8.55	124.58	120.30
2	O	134	ARG	NE-CZ-NH2	-8.37	116.12	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	379	TYR	Mainchain
6	F	93	PRO	Peptide
1	N	240	HIS	Sidechain
1	N	379	TYR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4162	0	4144	83	0
1	N	4160	0	4135	66	0
2	B	2000	0	2024	41	0
2	O	1999	0	2031	35	0
3	C	2125	0	2033	32	0
3	P	2121	0	2029	18	0
4	D	1201	0	1188	8	0
4	Q	1209	0	1197	16	0
5	E	842	0	838	2	0
5	R	842	0	838	4	0
6	F	720	0	698	7	0
6	S	721	0	702	12	0
7	G	642	0	606	7	0
7	T	663	0	626	14	0
8	H	662	0	623	12	0
8	U	662	0	623	18	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	451	0	446	8	0
10	W	451	0	446	3	0
11	K	389	0	372	7	0
11	X	385	0	366	3	0
12	L	380	0	380	9	0
12	Y	382	0	383	5	0
13	M	322	0	337	2	0
13	Z	320	0	334	5	0
14	A	190	0	138	28	0
14	N	190	0	138	23	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	0	0
18	N	4	0	0	0	0
19	A	63	0	110	10	0
19	B	62	0	105	6	0
19	D	48	0	77	7	0
19	O	126	0	220	14	0
20	A	46	0	69	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	149	0	217	8	0
20	N	51	0	76	4	0
20	P	96	0	138	1	0
20	Q	51	0	76	6	0
21	A	36	0	54	2	0
21	B	20	0	30	5	0
21	C	4	0	6	0	0
21	D	4	0	6	1	0
21	E	8	0	12	0	0
21	F	12	0	18	0	0
21	G	8	0	12	0	0
21	N	32	0	48	0	0
21	O	16	0	24	1	0
21	P	8	0	12	0	0
21	Q	4	0	6	0	0
21	R	4	0	6	0	0
21	S	28	0	42	3	0
21	T	8	0	12	0	0
21	U	4	0	6	3	0
21	Y	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	0	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	39	4	0
23	P	58	0	78	3	0
23	W	29	0	38	1	0
24	C	95	0	138	4	0
24	P	121	0	179	9	0
24	T	49	0	66	0	0
25	C	86	0	122	14	0
25	G	89	0	133	8	0
25	P	76	0	113	6	0
25	T	80	0	120	15	0
25	Y	87	0	127	4	0
26	C	33	0	42	5	0
26	G	21	0	30	2	0
26	J	33	0	42	3	0
26	K	61	0	84	2	0
26	L	18	0	20	3	0
26	M	33	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	154	0	199	7	0
26	X	66	0	93	5	0
26	Z	33	0	42	1	0
27	E	52	0	80	8	0
27	O	51	0	75	9	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	U	5	0	0	0	0
30	A	286	0	0	13	0
30	B	245	0	0	5	0
30	C	196	0	0	6	0
30	D	250	0	0	3	0
30	E	178	0	0	2	0
30	F	177	0	0	3	0
30	G	97	0	0	0	0
30	H	111	0	0	0	0
30	I	81	0	0	4	0
30	J	63	0	0	3	0
30	K	63	0	0	0	0
30	L	57	0	0	3	0
30	M	46	0	0	0	0
30	N	263	0	0	7	0
30	O	204	0	0	6	0
30	P	179	0	0	4	0
30	Q	128	0	0	3	0
30	R	131	0	0	3	0
30	S	126	0	0	4	0
30	T	78	0	0	1	0
30	U	121	0	0	5	0
30	V	68	0	0	1	0
30	W	51	0	0	0	0
30	X	50	0	0	0	0
30	Y	48	0	0	1	0
30	Z	30	0	0	1	0
All	All	35109	0	32347	493	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 8.

The worst 5 of 493 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:HE1	21:S:108:EDO:H22	1.28	0.96
8:U:24:ASN:HD21	21:U:101:EDO:H21	1.31	0.93
10:J:50:LEU:HB2	26:J:101:DMU:H20	1.51	0.93
1:N:356:ILE:HD13	14:N:602[C]:HEA:HMB1	1.51	0.91
1:A:347:LEU:HD22	1:A:383[A]:MET:SD	2.10	0.91

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	550/514 (107%)	531 (96%)	17 (3%)	2 (0%)	34	13
1	N	549/514 (107%)	532 (97%)	15 (3%)	2 (0%)	34	13
2	B	251/227 (111%)	246 (98%)	5 (2%)	0	100	100
2	O	251/227 (111%)	245 (98%)	6 (2%)	0	100	100
3	C	264/259 (102%)	260 (98%)	4 (2%)	0	100	100
3	P	263/259 (102%)	257 (98%)	6 (2%)	0	100	100
4	D	143/144 (99%)	140 (98%)	3 (2%)	0	100	100
4	Q	145/144 (101%)	141 (97%)	2 (1%)	2 (1%)	11	2
5	E	102/104 (98%)	102 (100%)	0	0	100	100
5	R	102/104 (98%)	102 (100%)	0	0	100	100
6	F	94/93 (101%)	92 (98%)	2 (2%)	0	100	100
6	S	95/93 (102%)	93 (98%)	2 (2%)	0	100	100
7	G	78/84 (93%)	71 (91%)	2 (3%)	5 (6%)	1	0
7	T	84/84 (100%)	73 (87%)	7 (8%)	4 (5%)	2	0
8	H	77/79 (98%)	70 (91%)	4 (5%)	3 (4%)	3	0
8	U	77/79 (98%)	69 (90%)	4 (5%)	4 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	55/57 (96%)	55 (100%)	0	0	100	100
10	W	55/57 (96%)	55 (100%)	0	0	100	100
11	K	49/49 (100%)	48 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
12	Y	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
13	M	40/41 (98%)	39 (98%)	1 (2%)	0	100	100
13	Z	39/41 (95%)	39 (100%)	0	0	100	100
All	All	3641/3540 (103%)	3533 (97%)	86 (2%)	22 (1%)	25	7

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384[A]	GLY
1	A	384[B]	GLY
7	G	7	ASP
7	G	8	HIS
8	H	10	ASN

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	463/426 (109%)	459 (99%)	4 (1%)	78	57
1	N	462/426 (108%)	455 (98%)	7 (2%)	65	35
2	B	236/210 (112%)	227 (96%)	9 (4%)	33	5
2	O	236/210 (112%)	229 (97%)	7 (3%)	41	9
3	C	231/224 (103%)	227 (98%)	4 (2%)	60	28
3	P	230/224 (103%)	226 (98%)	4 (2%)	60	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	129/128 (101%)	128 (99%)	1 (1%)	81	62
4	Q	131/128 (102%)	129 (98%)	2 (2%)	65	35
5	E	91/91 (100%)	90 (99%)	1 (1%)	73	48
5	R	91/91 (100%)	90 (99%)	1 (1%)	73	48
6	F	81/78 (104%)	79 (98%)	2 (2%)	47	14
6	S	82/78 (105%)	80 (98%)	2 (2%)	49	16
7	G	65/68 (96%)	59 (91%)	6 (9%)	9	0
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	0
8	H	71/71 (100%)	67 (94%)	4 (6%)	21	1
8	U	71/71 (100%)	66 (93%)	5 (7%)	15	1
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	26
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	6
10	J	48/48 (100%)	48 (100%)	0	100	100
10	W	48/48 (100%)	47 (98%)	1 (2%)	53	19
11	K	41/39 (105%)	41 (100%)	0	100	100
11	X	39/39 (100%)	39 (100%)	0	100	100
12	L	39/39 (100%)	38 (97%)	1 (3%)	46	13
12	Y	40/39 (103%)	38 (95%)	2 (5%)	24	2
13	M	36/35 (103%)	35 (97%)	1 (3%)	43	11
13	Z	35/35 (100%)	34 (97%)	1 (3%)	42	10
All	All	3178/3028 (105%)	3102 (98%)	76 (2%)	50	16

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

Mol	Chain	Res	Type
7	T	2	SER
9	V	73	LYS
7	T	18	PHE
8	U	8	ILE
13	Z	39	ASN

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	94	HIS
7	T	34	ASN
11	X	35	GLN
8	H	37	HIS
8	H	23	GLN

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	B	1	2	8,9,10	1.34	1 (12%)	7,9,11	1.12	0
9	SAC	I	1	9	7,8,9	0.72	0	8,9,11	1.04	0
1	FME	N	1	1	8,9,10	0.46	0	7,9,11	1.83	2 (28%)
9	SAC	V	1	9	7,8,9	0.65	0	8,9,11	0.94	1 (12%)
1	FME	A	1	1	8,9,10	1.09	0	7,9,11	2.41	5 (71%)
2	FME	O	1	2	8,9,10	0.78	0	7,9,11	1.09	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	5/7/8/10	-
1	FME	N	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	5/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CB-CG	2.48	1.61	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CE-SD-CG	3.66	112.98	100.40
1	A	1	FME	CE-SD-CG	3.50	112.42	100.40
1	A	1	FME	CA-N-CN	-3.37	117.64	122.82
1	N	1	FME	O-C-CA	-2.44	118.37	124.78
1	A	1	FME	CG-CB-CA	-2.33	106.47	112.95

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	SAC	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 128 ligands modelled in this entry, 10 are monoatomic - leaving 118 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	P	306	-	44,44,50	0.82	2 (4%)	47,50,56	1.12	3 (6%)
26	DMU	J	101	-	34,34,34	0.95	1 (2%)	45,45,45	1.47	8 (17%)
26	DMU	K	101	-	22,22,34	1.27	1 (4%)	27,27,45	1.61	7 (25%)
14	HEA	N	601[B]	-	57,67,67	1.56	13 (22%)	61,103,103	1.74	15 (24%)
18	CYN	A	606[C]	15	0,1,1	-	-	-	-	-
23	CHD	C	309	-	32,32,32	0.91	0	51,51,51	2.52	13 (25%)
21	EDO	O	305	-	3,3,3	0.79	0	2,2,2	0.75	0
20	PGV	Q	201	-	50,50,50	1.02	2 (4%)	53,56,56	1.53	8 (15%)
26	DMU	X	102	-	22,22,34	1.35	3 (13%)	27,27,45	1.39	5 (18%)
21	EDO	O	306	-	3,3,3	0.81	0	2,2,2	0.20	0
26	DMU	P	312	-	34,34,34	0.80	1 (2%)	45,45,45	1.25	4 (8%)
26	DMU	X	101	-	22,22,34	1.56	2 (9%)	27,27,45	1.99	9 (33%)
23	CHD	G	102	-	32,32,32	0.80	1 (3%)	51,51,51	1.51	7 (13%)
19	TGL	A	607	-	62,62,62	1.22	3 (4%)	65,65,65	2.02	18 (27%)
19	TGL	O	301	-	62,62,62	1.11	3 (4%)	65,65,65	1.40	7 (10%)
21	EDO	S	103	-	3,3,3	0.65	0	2,2,2	0.18	0
29	PO4	U	102	-	4,4,4	0.58	0	6,6,6	0.70	0
20	PGV	C	306	-	50,50,50	0.85	2 (4%)	53,56,56	0.90	2 (3%)
22	CUA	O	303	2	0,1,1	-	-	-	-	-
23	CHD	C	301	-	32,32,32	1.10	2 (6%)	51,51,51	1.67	10 (19%)
21	EDO	U	101	-	3,3,3	0.65	0	2,2,2	0.38	0
21	EDO	O	307	-	3,3,3	0.58	0	2,2,2	0.51	0
21	EDO	A	617	-	3,3,3	0.70	0	2,2,2	0.71	0
21	EDO	N	608	-	3,3,3	0.79	0	2,2,2	0.65	0
21	EDO	N	612	-	3,3,3	0.49	0	2,2,2	0.35	0
21	EDO	A	610	-	3,3,3	1.08	0	2,2,2	1.03	0
20	PGV	N	607	-	50,50,50	1.10	6 (12%)	53,56,56	1.26	5 (9%)
21	EDO	F	102	-	3,3,3	0.89	0	2,2,2	0.55	0
21	EDO	A	612	-	3,3,3	0.33	0	2,2,2	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PEK	P	303	-	21,21,52	1.11	1 (4%)	21,21,57	1.26	3 (14%)
21	EDO	E	202	-	3,3,3	0.65	0	2,2,2	0.40	0
18	CYN	N	606[A]	15	0,1,1	-	-	-	-	-
23	CHD	P	309	-	32,32,32	0.78	0	51,51,51	1.87	12 (23%)
26	DMU	K	102	-	22,22,34	1.45	5 (22%)	27,27,45	1.78	6 (22%)
21	EDO	Y	102	-	3,3,3	0.48	0	2,2,2	0.06	0
25	CDL	T	102	-	79,79,99	1.36	9 (11%)	84,89,111	1.57	18 (21%)
21	EDO	A	615	-	3,3,3	0.35	0	2,2,2	0.67	0
14	HEA	N	602[A]	1	57,67,67	1.48	9 (15%)	61,103,103	2.15	21 (34%)
25	CDL	Y	101	-	86,86,99	1.35	10 (11%)	92,98,111	1.23	8 (8%)
21	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.44	0
21	EDO	S	108	-	3,3,3	0.68	0	2,2,2	0.57	0
21	EDO	N	615	-	3,3,3	0.62	0	2,2,2	0.50	0
21	EDO	G	104	-	3,3,3	0.63	0	2,2,2	0.60	0
25	CDL	C	308	-	84,84,99	1.41	13 (15%)	91,94,111	1.59	17 (18%)
21	EDO	N	611	-	3,3,3	0.65	0	2,2,2	0.86	0
21	EDO	S	106	-	3,3,3	0.68	0	2,2,2	0.52	0
21	EDO	T	104	-	3,3,3	0.56	0	2,2,2	0.28	0
20	PGV	P	307	-	50,50,50	1.06	2 (4%)	53,56,56	1.60	7 (13%)
21	EDO	A	609	-	3,3,3	0.42	0	2,2,2	0.32	0
25	CDL	P	308	-	71,74,99	1.60	10 (14%)	72,78,111	1.63	10 (13%)
18	CYN	N	606[C]	15	0,1,1	-	-	-	-	-
24	PEK	T	101	-	48,48,52	1.20	2 (4%)	51,53,57	1.56	9 (17%)
21	EDO	E	203	-	3,3,3	0.48	0	2,2,2	0.59	0
14	HEA	N	602[C]	1	57,67,67	1.49	7 (12%)	61,103,103	2.04	19 (31%)
20	PGV	C	305	-	50,50,50	0.79	0	53,56,56	0.87	0
21	EDO	F	103	-	3,3,3	0.88	0	2,2,2	0.28	0
21	EDO	S	105	-	3,3,3	0.98	0	2,2,2	0.88	0
21	EDO	N	613	-	3,3,3	0.64	0	2,2,2	0.54	0
21	EDO	P	313	-	3,3,3	0.84	0	2,2,2	0.48	0
21	EDO	A	613	-	3,3,3	0.78	0	2,2,2	0.28	0
21	EDO	Q	202	-	3,3,3	0.60	0	2,2,2	0.14	0
20	PGV	A	608	-	45,45,50	1.18	4 (8%)	49,50,56	1.44	6 (12%)
25	CDL	G	101	-	87,87,99	1.43	13 (14%)	91,97,111	1.52	10 (10%)
26	DMU	X	103	-	22,22,34	1.18	1 (4%)	27,27,45	1.69	7 (25%)
21	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.53	0
21	EDO	B	306	-	3,3,3	0.79	0	2,2,2	0.51	0
21	EDO	P	314	-	3,3,3	0.39	0	2,2,2	1.36	0
21	EDO	S	107	-	3,3,3	0.66	0	2,2,2	0.68	0
21	EDO	A	614	-	3,3,3	0.73	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	S	104	-	3,3,3	0.65	0	2,2,2	0.98	0
21	EDO	B	308	-	3,3,3	1.24	0	2,2,2	0.73	0
14	HEA	N	601[A]	-	57,67,67	1.53	13 (22%)	61,103,103	1.80	13 (21%)
14	HEA	A	601[A]	-	57,67,67	1.62	14 (24%)	61,103,103	1.96	16 (26%)
21	EDO	A	616	-	3,3,3	0.81	0	2,2,2	0.55	0
21	EDO	C	310	-	3,3,3	0.90	0	2,2,2	0.25	0
21	EDO	N	609	-	3,3,3	0.28	0	2,2,2	0.55	0
23	CHD	J	102	-	32,32,32	0.89	1 (3%)	51,51,51	2.70	22 (43%)
21	EDO	G	103	-	3,3,3	0.72	0	2,2,2	0.56	0
23	CHD	B	303	-	32,32,32	0.82	1 (3%)	51,51,51	1.91	17 (33%)
26	DMU	P	315	-	34,34,34	1.05	3 (8%)	45,45,45	1.92	12 (26%)
23	CHD	W	101	-	32,32,32	0.87	0	51,51,51	2.36	18 (35%)
21	EDO	F	104	-	3,3,3	0.76	0	2,2,2	0.64	0
23	CHD	P	301	-	32,32,32	0.93	2 (6%)	51,51,51	1.47	8 (15%)
27	PSC	O	304	-	50,50,51	1.24	3 (6%)	56,58,59	1.98	11 (19%)
24	PEK	P	305	-	45,45,52	1.21	2 (4%)	47,47,57	1.57	4 (8%)
20	PGV	C	307	-	46,46,50	1.27	2 (4%)	49,52,56	1.83	9 (18%)
27	PSC	E	201	-	51,51,51	1.21	3 (5%)	57,59,59	1.83	7 (12%)
14	HEA	A	601[B]	-	57,67,67	1.65	13 (22%)	61,103,103	1.88	14 (22%)
21	EDO	T	103	-	3,3,3	0.83	0	2,2,2	0.83	0
26	DMU	L	101	-	18,18,34	1.21	1 (5%)	23,23,45	1.56	3 (13%)
26	DMU	M	101	-	34,34,34	0.65	1 (2%)	45,45,45	1.38	9 (20%)
14	HEA	A	602[C]	1	57,67,67	1.42	10 (17%)	61,103,103	2.24	25 (40%)
21	EDO	S	102	-	3,3,3	0.72	0	2,2,2	0.52	0
26	DMU	C	311	-	34,34,34	0.86	0	45,45,45	1.83	12 (26%)
26	DMU	Z	101	-	34,34,34	0.51	0	45,45,45	1.18	4 (8%)
21	EDO	B	304	-	3,3,3	0.71	0	2,2,2	0.47	0
19	TGL	O	302	-	62,62,62	1.12	4 (6%)	65,65,65	1.10	4 (6%)
24	PEK	P	304	-	52,52,52	0.56	0	55,57,57	1.17	3 (5%)
21	EDO	B	305	-	3,3,3	0.91	0	2,2,2	1.48	1 (50%)
21	EDO	B	307	-	3,3,3	0.49	0	2,2,2	0.42	0
24	PEK	C	304	-	43,43,52	1.16	2 (4%)	44,44,57	1.41	5 (11%)
26	DMU	P	311	-	34,34,34	0.80	1 (2%)	45,45,45	1.23	6 (13%)
26	DMU	P	310	-	34,34,34	0.53	0	45,45,45	1.31	5 (11%)
26	DMU	G	105	-	21,21,34	1.24	2 (9%)	24,25,45	2.11	7 (29%)
18	CYN	A	606[A]	15	0,1,1	-	-	-	-	-
19	TGL	B	301	-	61,61,62	1.18	3 (4%)	64,64,65	1.61	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	602[A]	1	57,67,67	1.50	9 (15%)	61,103,103	2.25	26 (42%)
19	TGL	D	201	-	47,47,62	1.71	5 (10%)	50,50,65	1.27	8 (16%)
21	EDO	O	308	-	3,3,3	0.56	0	2,2,2	0.56	0
26	DMU	P	316	-	22,22,34	1.20	2 (9%)	27,27,45	2.22	9 (33%)
24	PEK	C	303	-	50,50,52	0.75	2 (4%)	53,55,57	1.05	4 (7%)
22	CUA	B	302	2	0,1,1	-	-	-	-	-
21	EDO	R	201	-	3,3,3	0.61	0	2,2,2	0.60	0
21	EDO	N	610	-	3,3,3	0.34	0	2,2,2	1.04	0
26	DMU	K	103	-	17,17,34	0.65	0	17,18,45	1.20	1 (5%)
21	EDO	A	611	-	3,3,3	0.29	0	2,2,2	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	306	-	-	8/49/49/55	-
26	DMU	J	101	-	-	5/19/59/59	0/2/2/2
26	DMU	K	101	-	-	4/13/33/59	0/1/1/2
14	HEA	N	601[B]	-	3/3/7/16	5/32/76/76	-
23	CHD	C	309	-	-	6/9/74/74	0/4/4/4
21	EDO	O	305	-	-	0/1/1/1	-
20	PGV	Q	201	-	-	14/55/55/55	-
26	DMU	X	102	-	-	9/13/33/59	0/1/1/2
21	EDO	O	306	-	-	0/1/1/1	-
26	DMU	P	312	-	-	5/19/59/59	0/2/2/2
26	DMU	X	101	-	-	5/13/33/59	0/1/1/2
23	CHD	G	102	-	-	2/9/74/74	0/4/4/4
19	TGL	A	607	-	-	31/65/65/65	-
19	TGL	O	301	-	-	33/65/65/65	-
21	EDO	S	103	-	-	0/1/1/1	-
20	PGV	C	306	-	-	12/55/55/55	-
23	CHD	C	301	-	-	2/9/74/74	0/4/4/4
21	EDO	U	101	-	-	1/1/1/1	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	A	617	-	-	1/1/1/1	-
21	EDO	N	608	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	A	610	-	-	0/1/1/1	-
20	PGV	N	607	-	-	4/55/55/55	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
24	PEK	P	303	-	-	7/19/19/56	-
21	EDO	E	202	-	-	0/1/1/1	-
23	CHD	P	309	-	-	5/9/74/74	0/4/4/4
26	DMU	K	102	-	-	8/13/33/59	0/1/1/2
21	EDO	Y	102	-	-	0/1/1/1	-
25	CDL	T	102	-	-	30/87/87/110	-
21	EDO	A	615	-	-	0/1/1/1	-
14	HEA	N	602[A]	1	3/3/7/16	7/32/76/76	-
25	CDL	Y	101	-	-	39/97/97/110	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	S	108	-	-	1/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	G	104	-	-	0/1/1/1	-
25	CDL	C	308	-	-	35/90/90/110	-
21	EDO	N	611	-	-	0/1/1/1	-
21	EDO	S	106	-	-	1/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
20	PGV	P	307	-	-	14/55/55/55	-
21	EDO	A	609	-	-	0/1/1/1	-
25	CDL	P	308	-	-	23/73/77/110	-
24	PEK	T	101	-	-	18/52/52/56	-
21	EDO	E	203	-	-	0/1/1/1	-
14	HEA	N	602[C]	1	3/3/7/16	6/32/76/76	-
20	PGV	C	305	-	-	7/55/55/55	-
21	EDO	F	103	-	-	0/1/1/1	-
14	HEA	A	601[C]	-	3/3/3/16	-	-
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	P	313	-	-	0/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	1/1/1/1	-
20	PGV	A	608	-	-	18/47/47/55	-
25	CDL	G	101	-	-	31/94/94/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DMU	X	103	-	-	7/13/33/59	0/1/1/2
21	EDO	D	202	-	-	1/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	P	314	-	-	1/1/1/1	-
21	EDO	S	107	-	-	1/1/1/1	-
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	B	308	-	-	0/1/1/1	-
14	HEA	N	601[A]	-	3/3/7/16	4/32/76/76	-
14	HEA	A	601[A]	-	3/3/7/16	8/32/76/76	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	N	609	-	-	0/1/1/1	-
23	CHD	J	102	-	-	7/9/74/74	0/4/4/4
21	EDO	G	103	-	-	0/1/1/1	-
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
26	DMU	P	315	-	-	10/19/59/59	0/2/2/2
23	CHD	W	101	-	-	5/9/74/74	0/4/4/4
21	EDO	F	104	-	-	0/1/1/1	-
23	CHD	P	301	-	-	1/9/74/74	0/4/4/4
14	HEA	N	601[C]	-	3/3/3/16	-	-
27	PSC	O	304	-	-	24/54/54/55	-
24	PEK	P	305	-	-	22/47/47/56	-
20	PGV	C	307	-	-	18/51/51/55	-
27	PSC	E	201	-	-	28/55/55/55	-
14	HEA	A	601[B]	-	3/3/7/16	5/32/76/76	-
21	EDO	T	103	-	-	0/1/1/1	-
26	DMU	L	101	-	-	2/9/29/59	0/1/1/2
26	DMU	M	101	-	-	5/19/59/59	0/2/2/2
14	HEA	A	602[C]	1	3/3/7/16	5/32/76/76	-
21	EDO	S	102	-	-	0/1/1/1	-
26	DMU	C	311	-	-	7/19/59/59	0/2/2/2
26	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
21	EDO	B	304	-	-	0/1/1/1	-
19	TGL	O	302	-	-	26/65/65/65	-
24	PEK	P	304	-	-	8/56/56/56	-
21	EDO	B	305	-	-	1/1/1/1	-
21	EDO	B	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	C	304	-	-	22/43/43/56	-
26	DMU	P	311	-	-	7/19/59/59	0/2/2/2
26	DMU	P	310	-	-	9/19/59/59	0/2/2/2
26	DMU	G	105	-	-	6/13/29/59	0/1/1/2
19	TGL	B	301	-	-	33/64/64/65	-
14	HEA	A	602[A]	1	3/3/7/16	7/32/76/76	-
19	TGL	D	201	-	-	19/50/50/65	-
21	EDO	O	308	-	-	0/1/1/1	-
26	DMU	P	316	-	-	7/13/33/59	0/1/1/2
24	PEK	C	303	-	-	14/54/54/56	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
26	DMU	K	103	-	-	4/11/19/59	0/1/1/2
21	EDO	A	611	-	-	0/1/1/1	-

The worst 5 of 227 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	7.11	1.43	1.22
19	A	607	TGL	OG2-CB1	5.83	1.50	1.34
20	C	307	PGV	O03-C19	5.83	1.50	1.33
25	P	308	CDL	OA8-CA7	5.78	1.50	1.33
19	D	201	TGL	OG2-CB1	5.70	1.50	1.34

The worst 5 of 566 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	309	CHD	C23-C22-C20	-10.67	95.03	114.52
27	E	201	PSC	C03-C02-C01	-9.39	89.58	111.79
25	G	101	CDL	OA6-CA5-C11	8.69	130.24	111.50
23	W	101	CHD	C13-C17-C20	8.16	129.24	119.50
19	O	301	TGL	OG2-CB1-CB2	7.52	127.70	111.50

5 of 30 chirality outliers are listed below:

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

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

5 of 730 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C12-C11-C3B-C2B
14	A	601[B]	HEA	C14-C15-C16-C17
14	A	601[B]	HEA	C26-C15-C16-C17
14	A	602[C]	HEA	C4D-C3D-CAD-CBD
14	N	601[A]	HEA	C12-C11-C3B-C2B

There are no ring outliers.

55 monomers are involved in 239 short contacts:

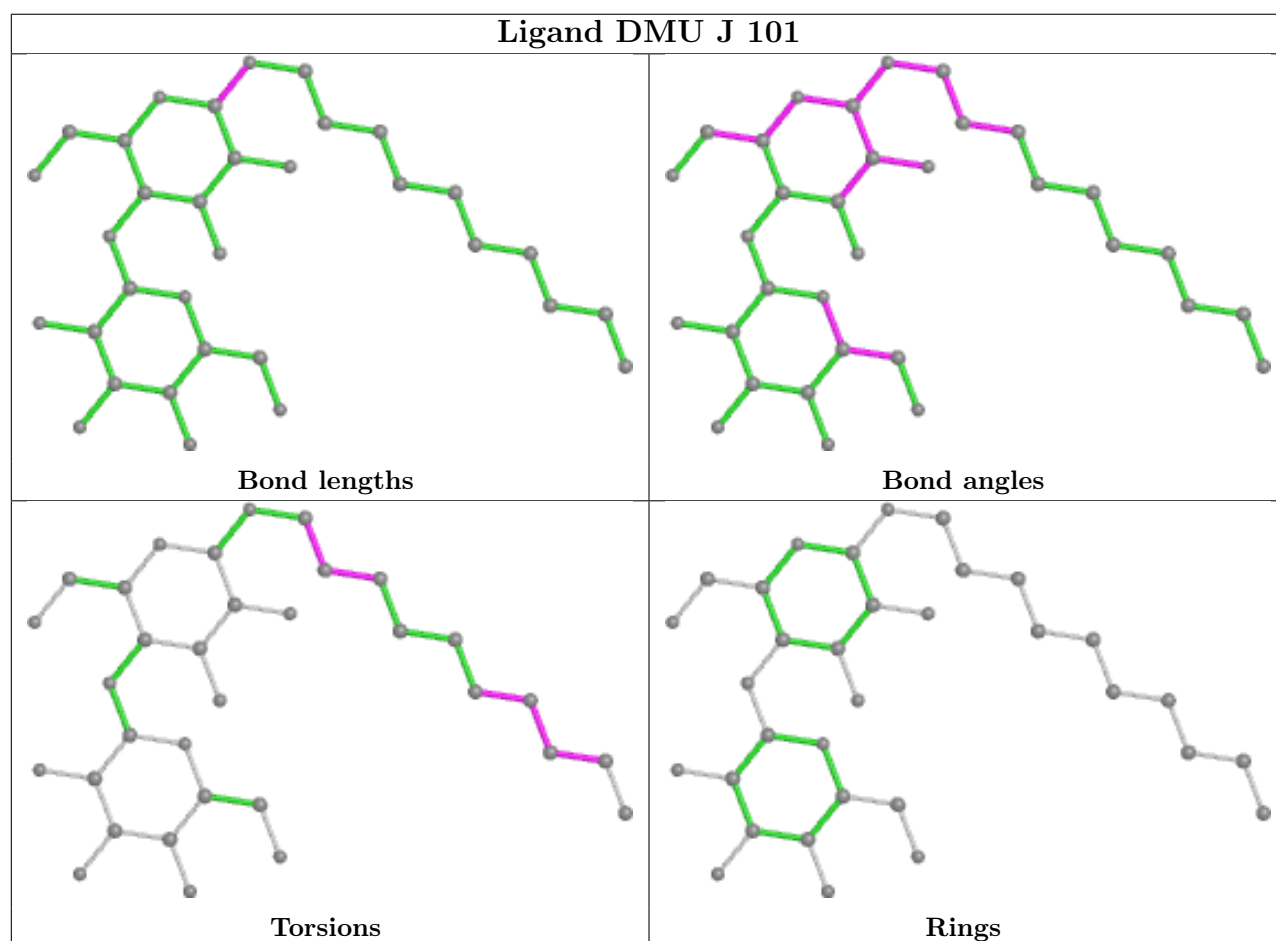
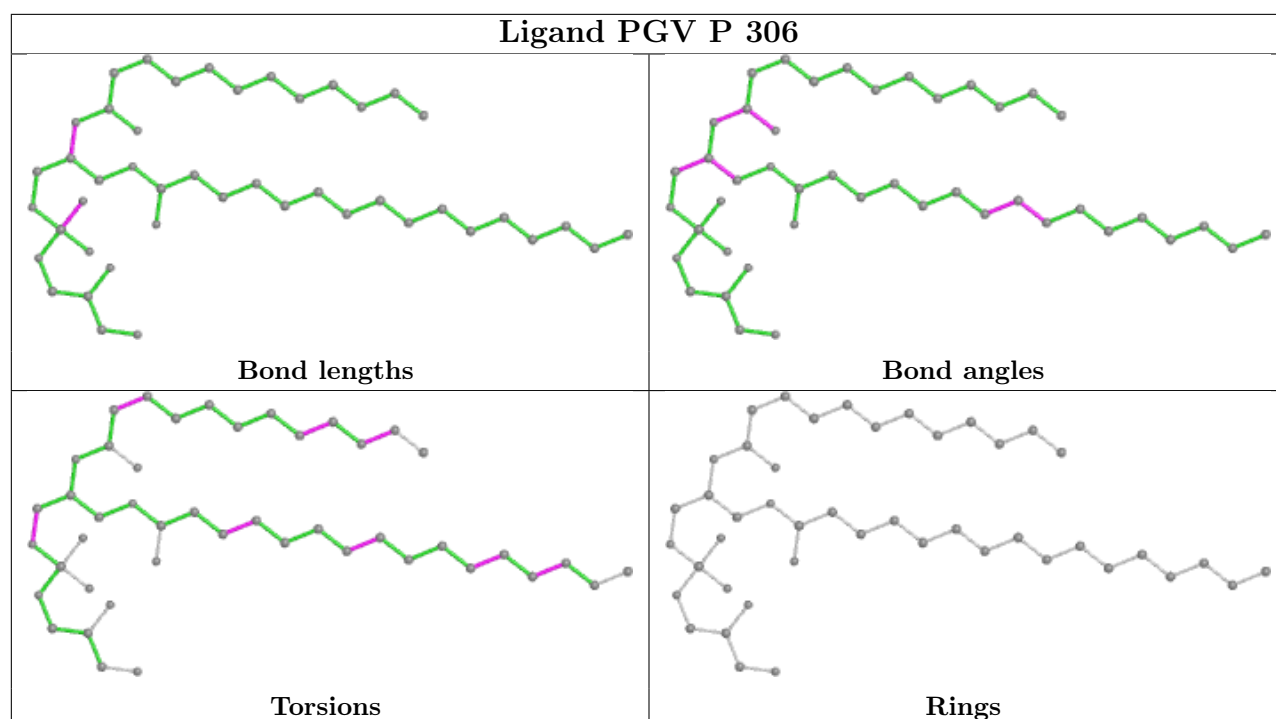
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	J	101	DMU	3	0
26	K	101	DMU	1	0
23	C	309	CHD	5	0
20	Q	201	PGV	6	0
26	X	102	DMU	1	0
26	P	312	DMU	2	0
26	X	101	DMU	1	0
23	G	102	CHD	1	0
19	A	607	TGL	10	0
19	O	301	TGL	3	0
20	C	306	PGV	4	0
21	U	101	EDO	3	0
21	O	307	EDO	1	0
21	A	617	EDO	1	0
20	N	607	PGV	4	0
23	P	309	CHD	3	0
25	T	102	CDL	15	0
21	A	615	EDO	1	0
14	N	602[A]	HEA	4	0
25	Y	101	CDL	4	0
21	S	108	EDO	3	0
25	C	308	CDL	14	0
20	P	307	PGV	1	0
25	P	308	CDL	6	0
14	N	602[C]	HEA	15	0
20	C	305	PGV	3	0

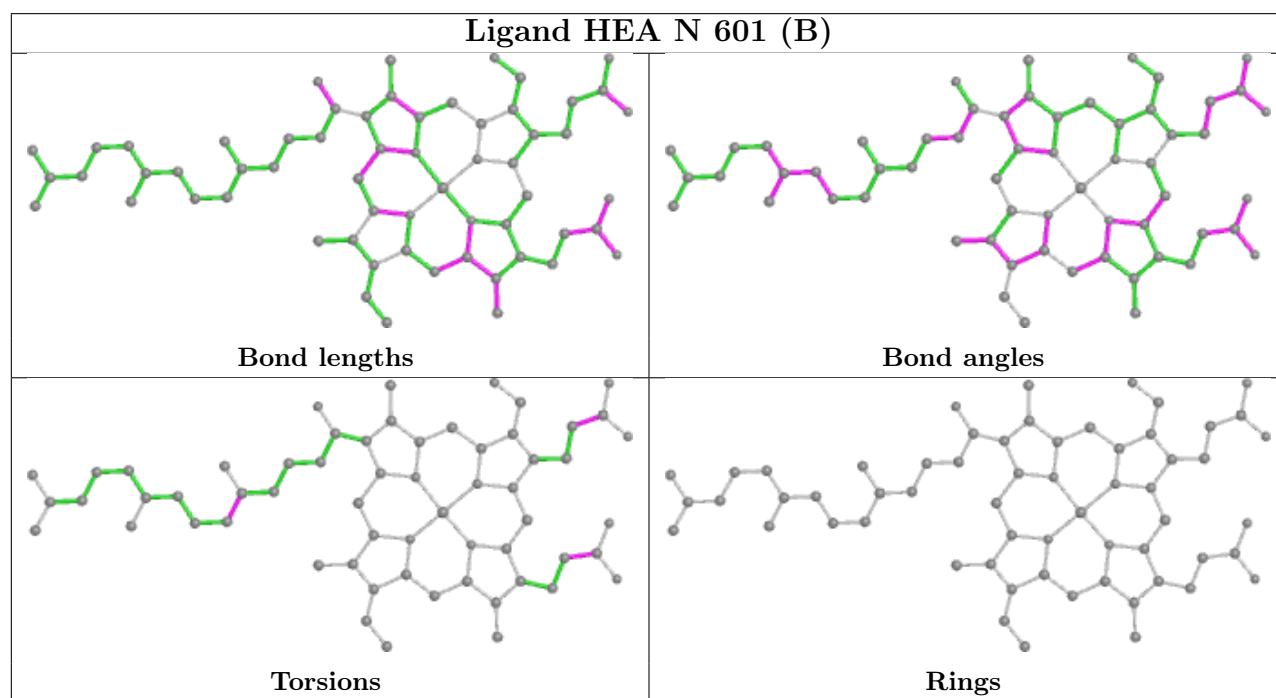
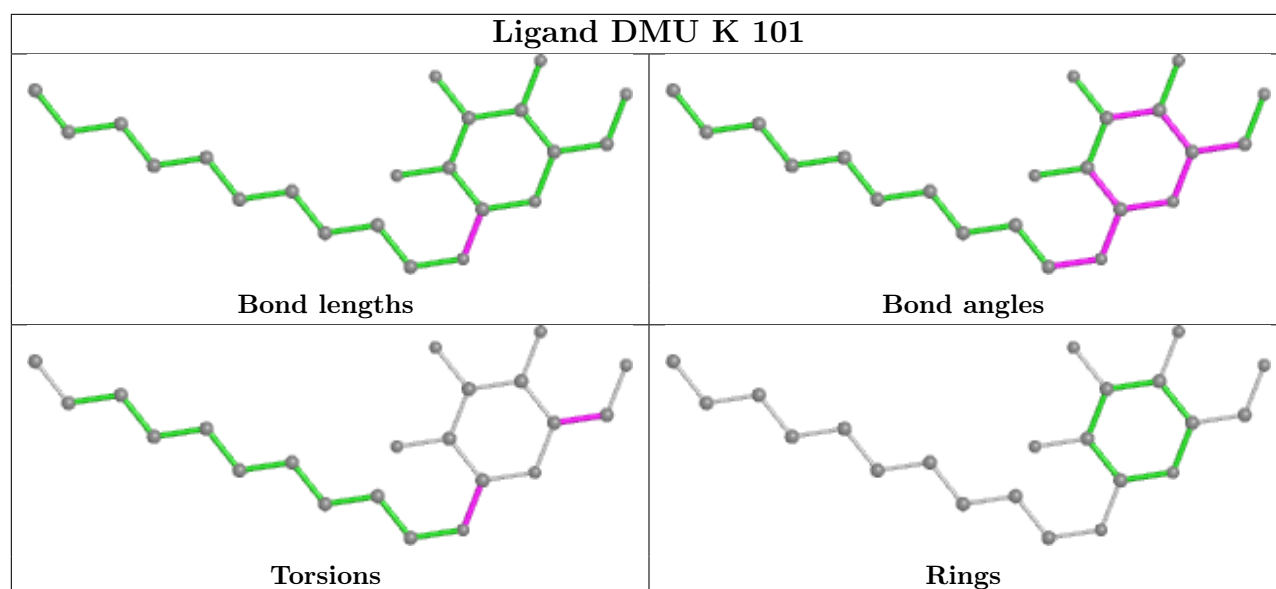
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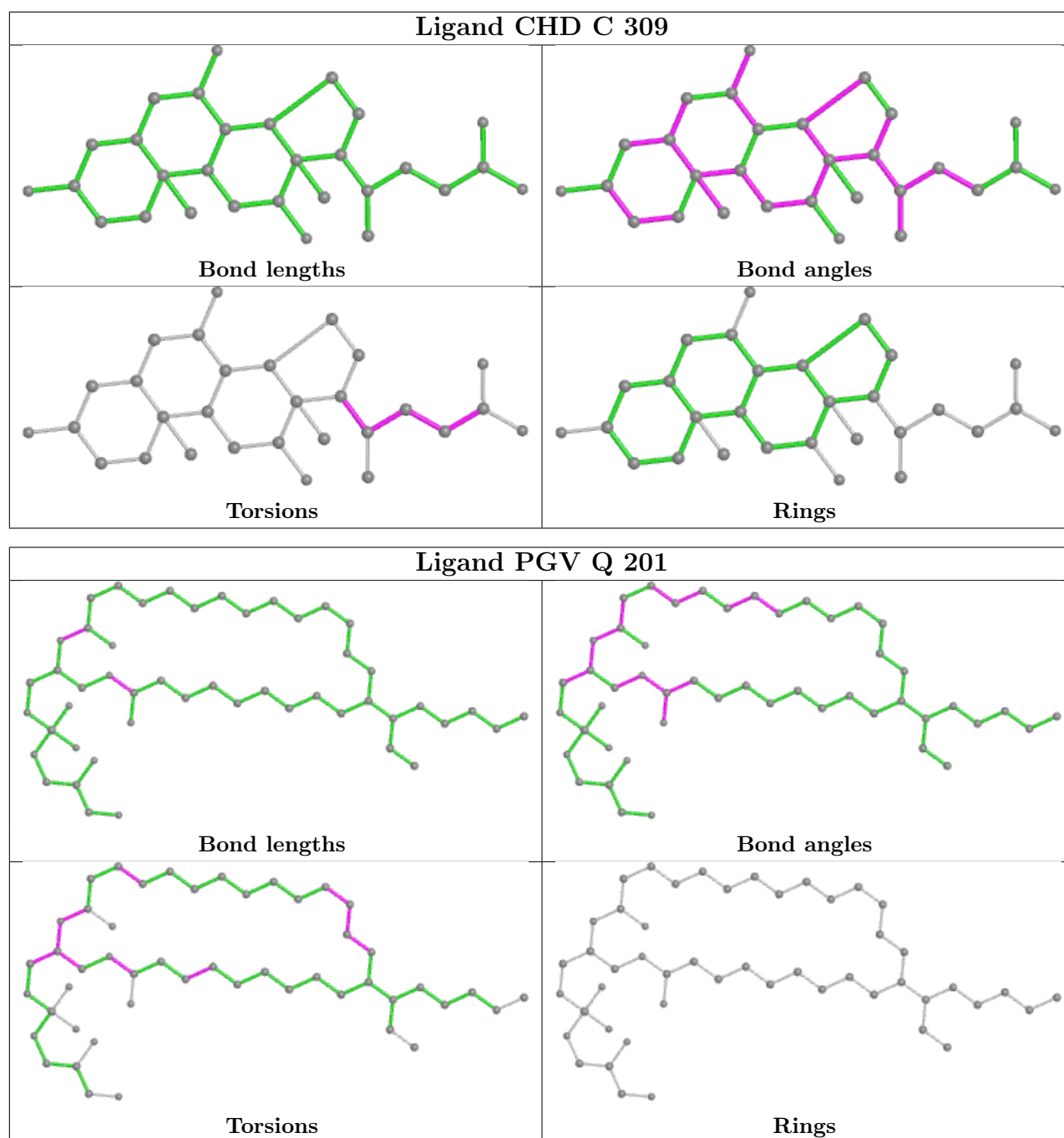
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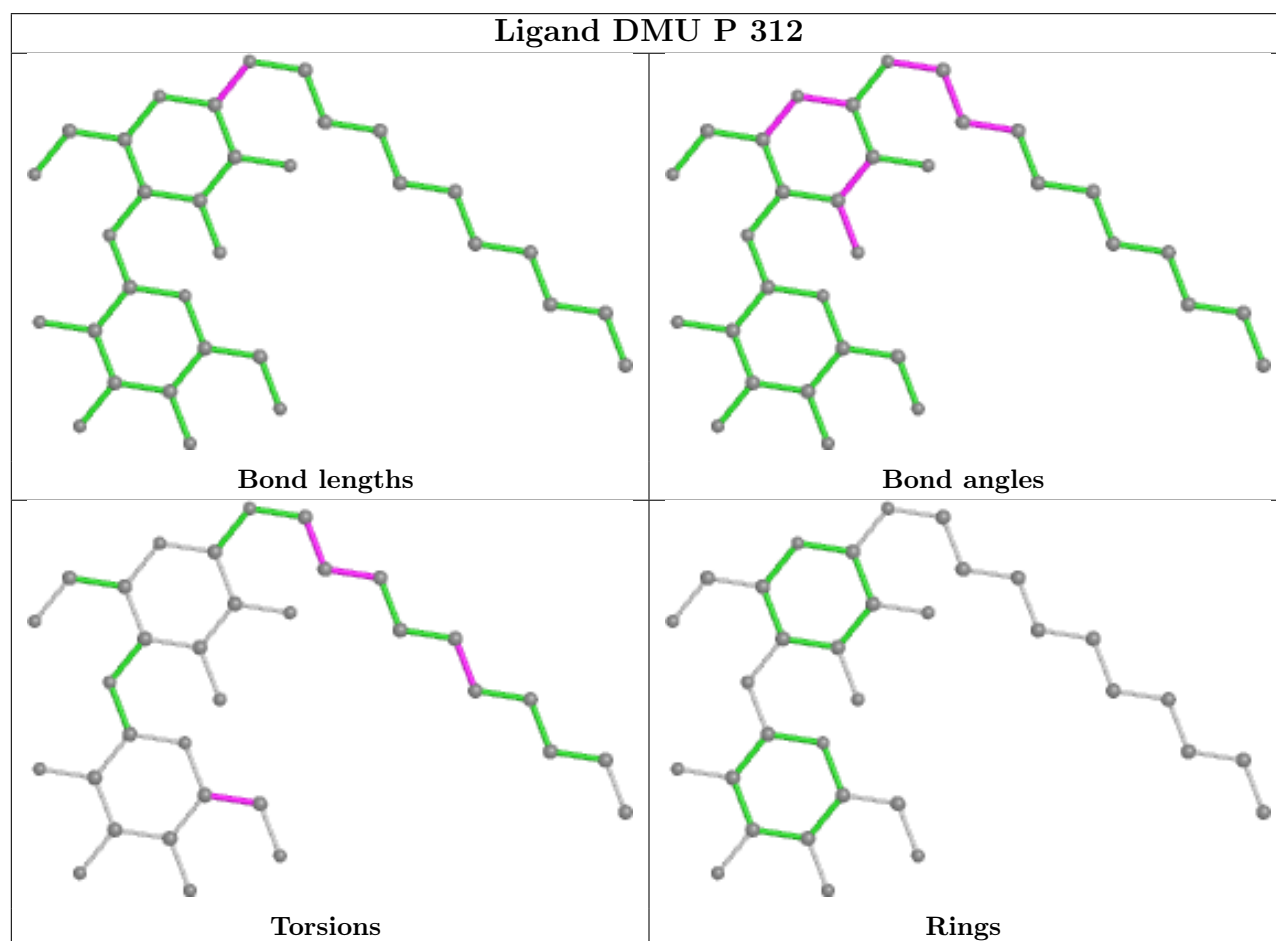
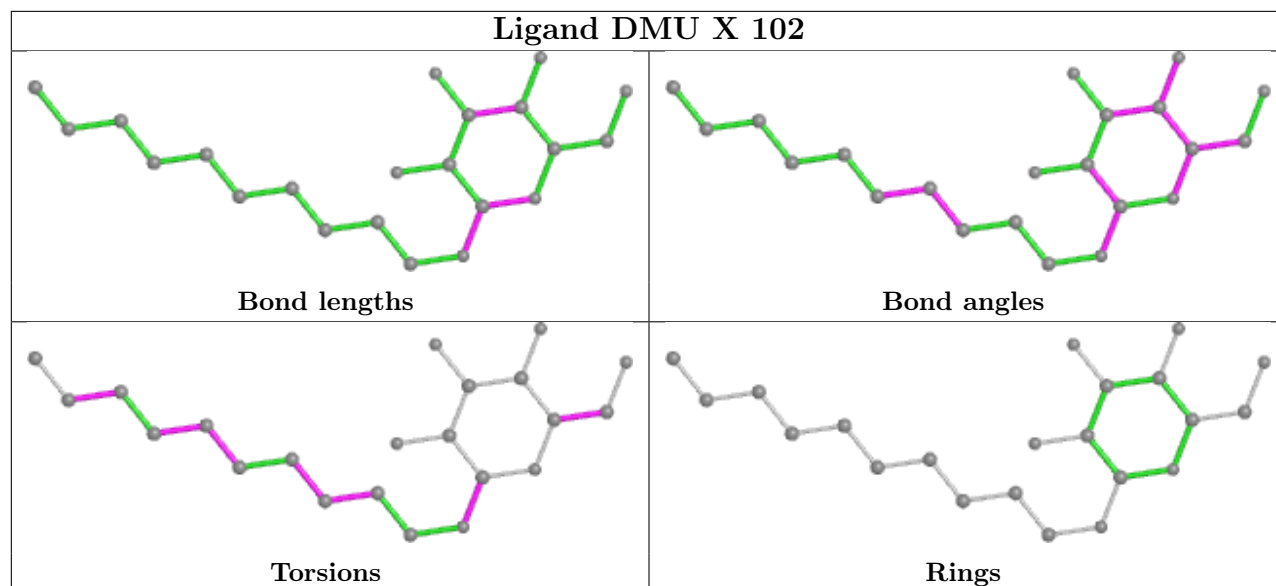
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	608	PGV	7	0
25	G	101	CDL	8	0
26	X	103	DMU	4	0
21	D	202	EDO	1	0
14	N	601[A]	HEA	4	0
14	A	601[A]	HEA	4	0
23	J	102	CHD	4	0
26	P	315	DMU	1	0
23	W	101	CHD	1	0
27	O	304	PSC	9	0
24	P	305	PEK	2	0
20	C	307	PGV	1	0
27	E	201	PSC	8	0
14	A	601[B]	HEA	3	0
26	L	101	DMU	3	0
14	A	602[C]	HEA	14	0
26	C	311	DMU	5	0
26	Z	101	DMU	1	0
19	O	302	TGL	11	0
24	P	304	PEK	7	0
21	B	305	EDO	5	0
26	P	311	DMU	2	0
26	P	310	DMU	4	0
26	G	105	DMU	2	0
19	B	301	TGL	6	0
14	A	602[A]	HEA	7	0
19	D	201	TGL	7	0
24	C	303	PEK	4	0
26	K	103	DMU	1	0

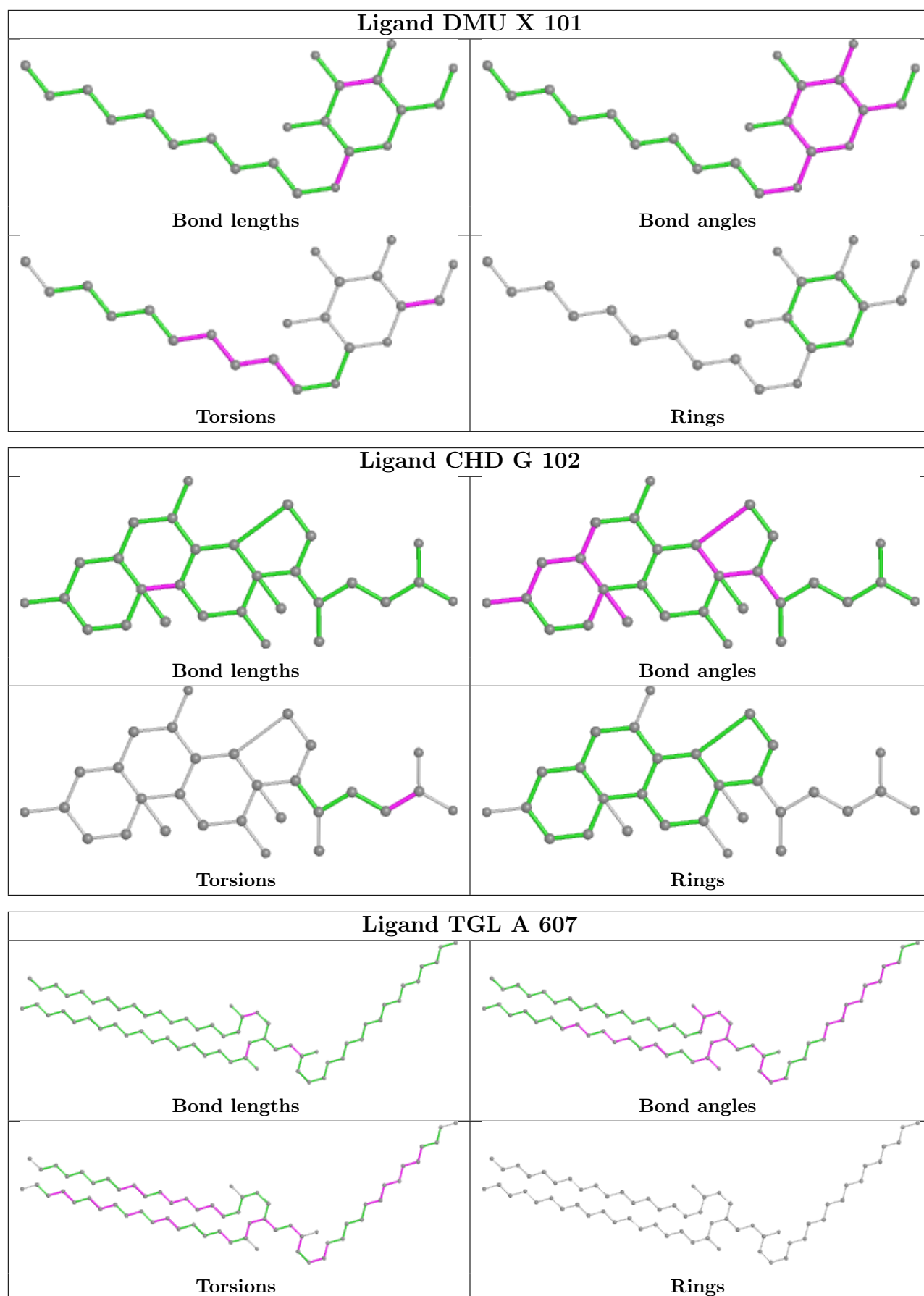
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

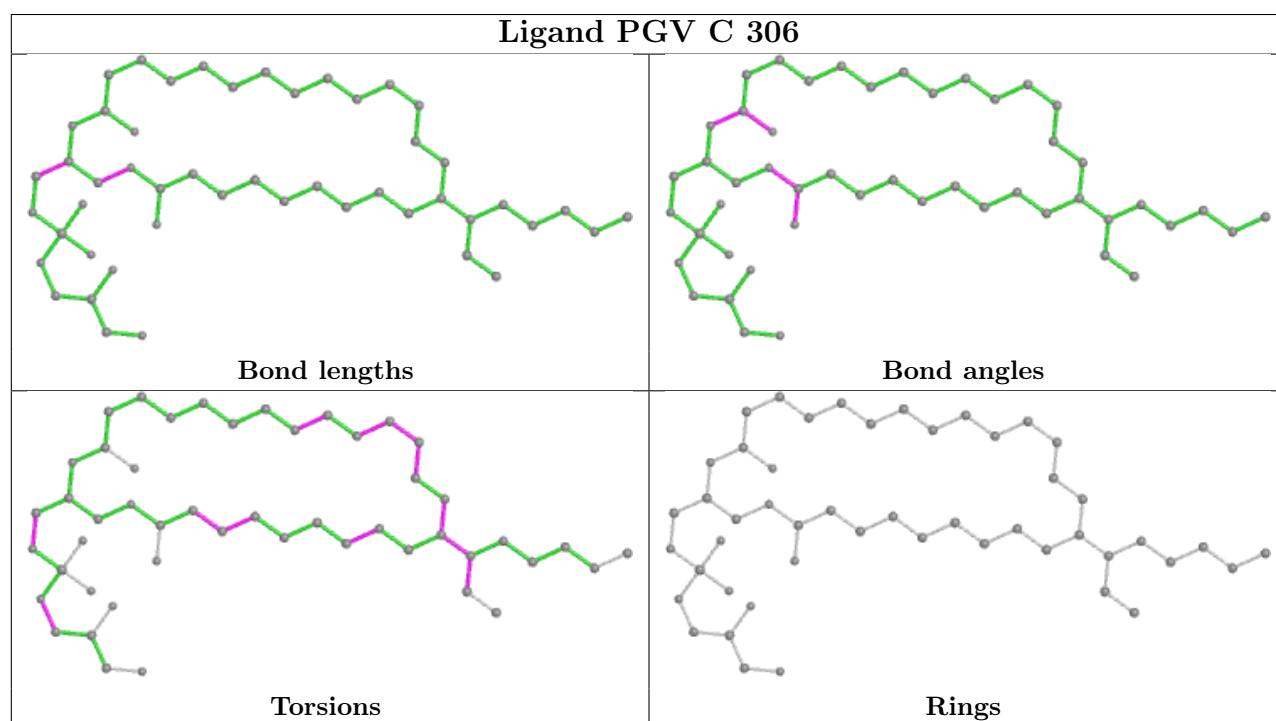
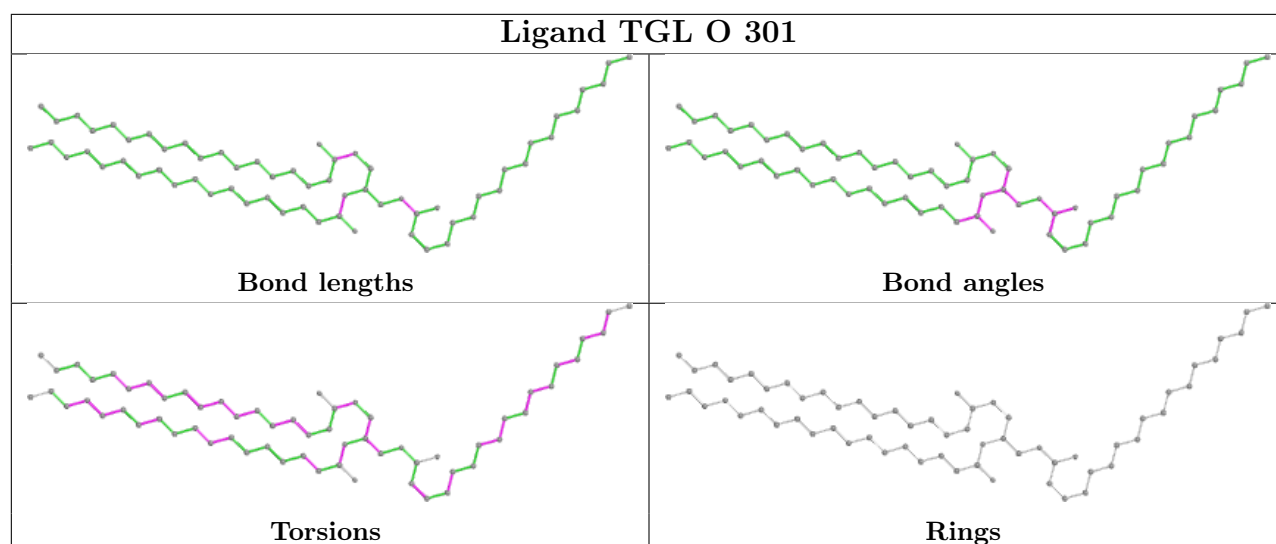


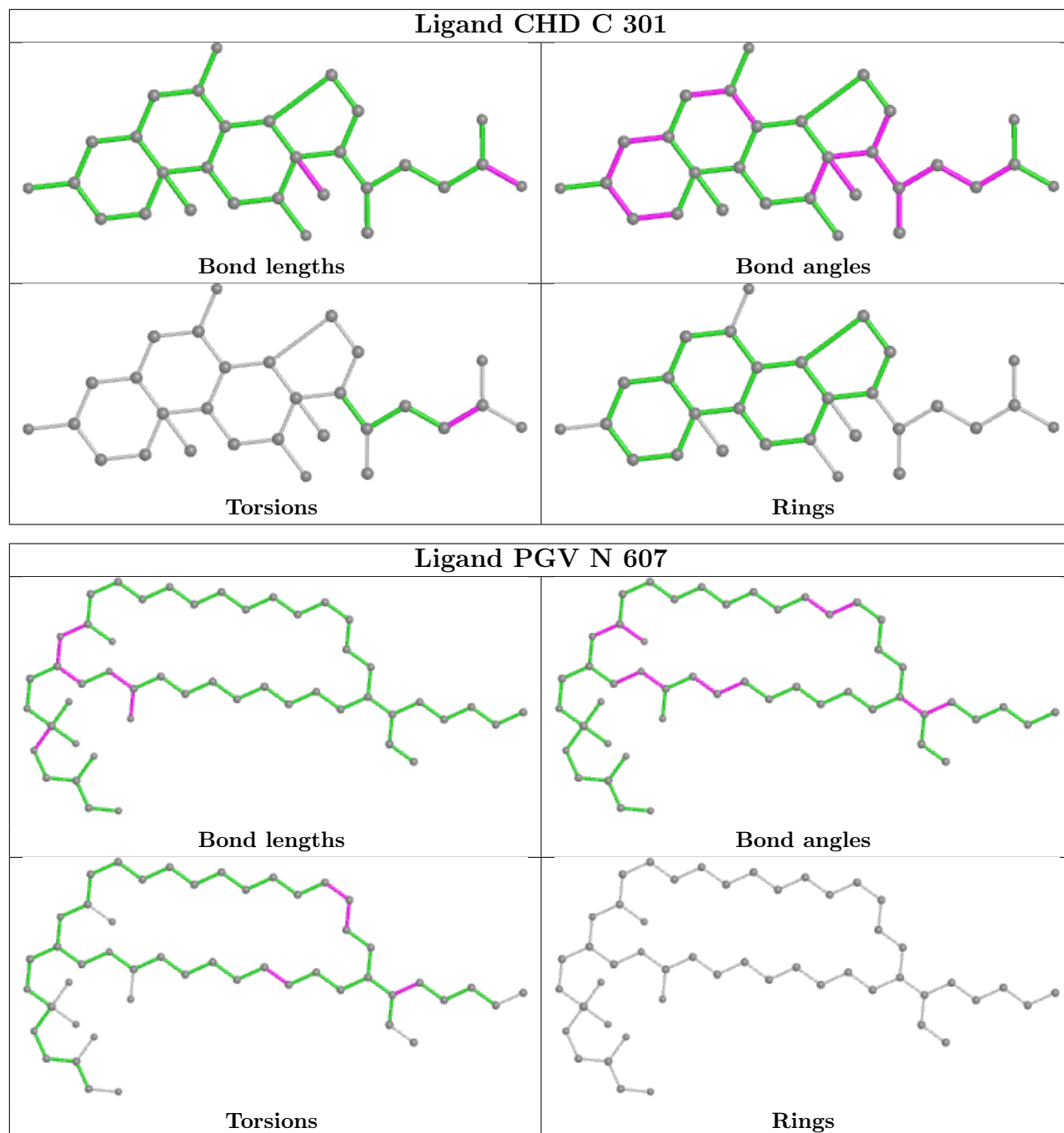


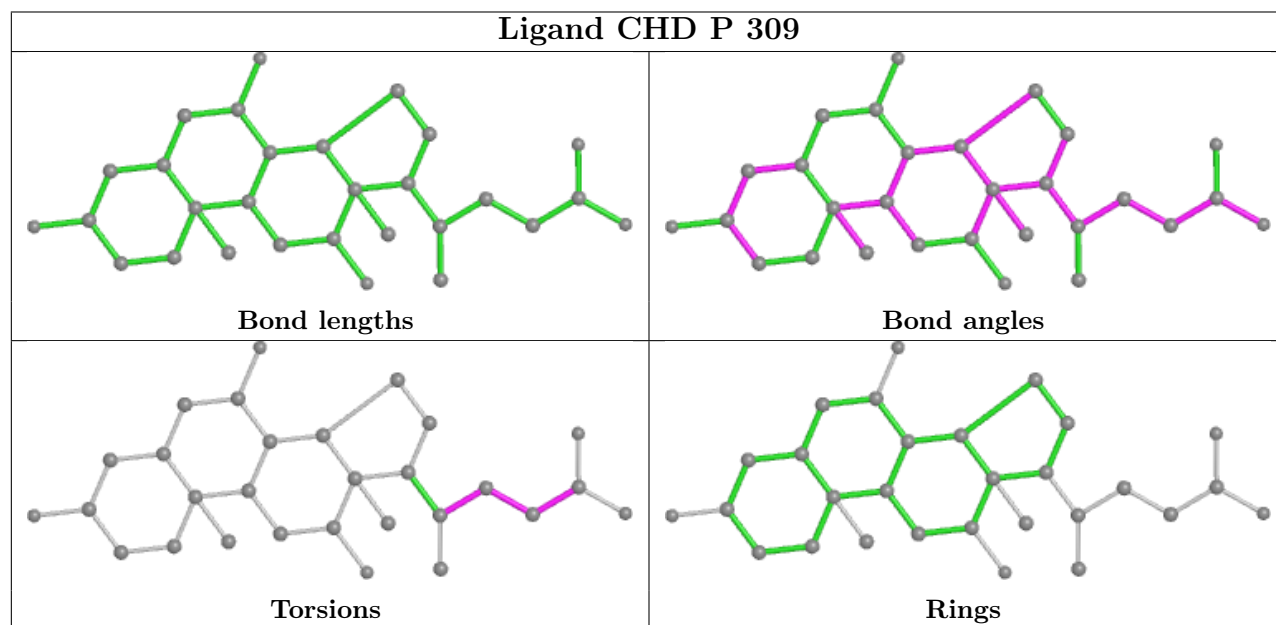
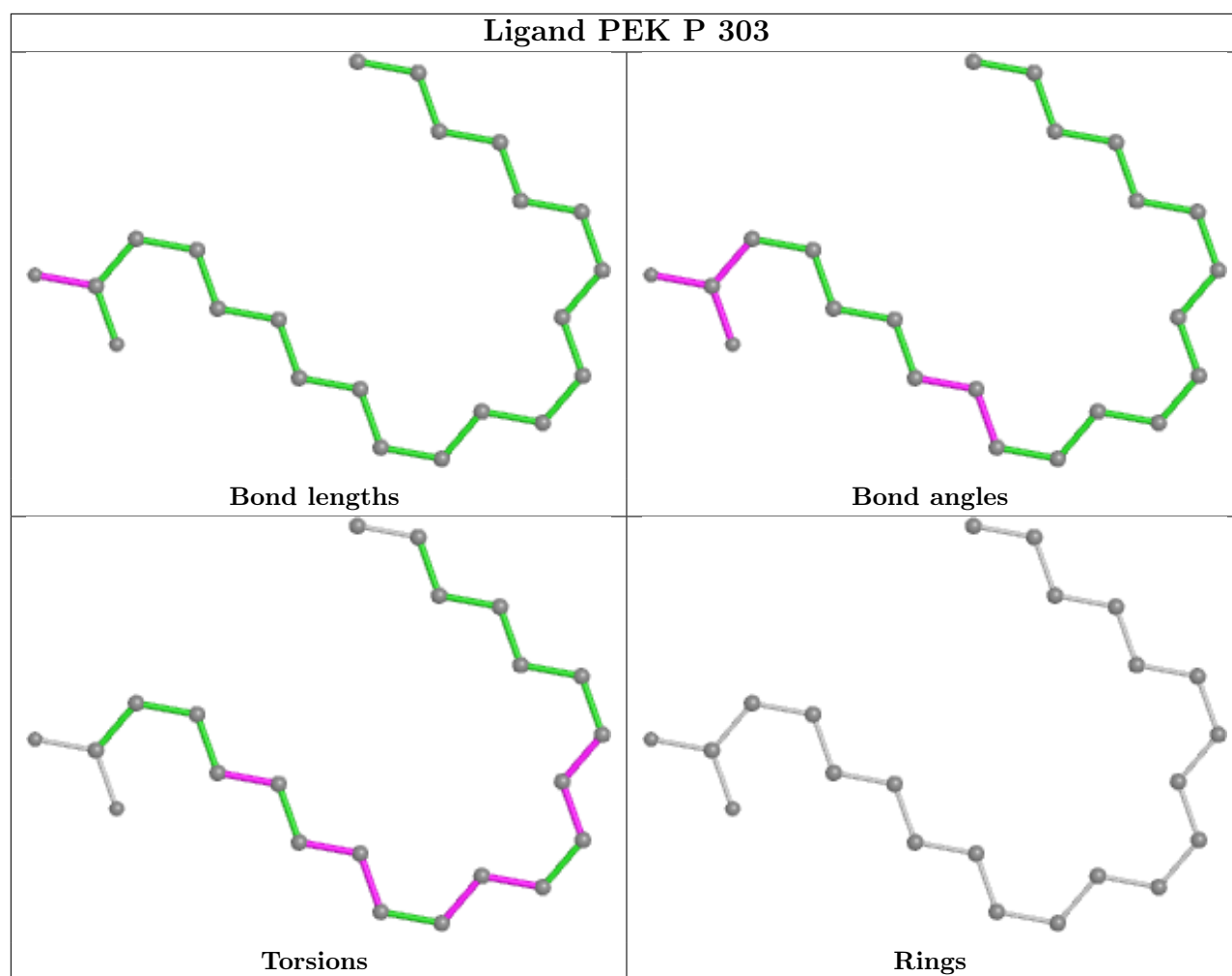


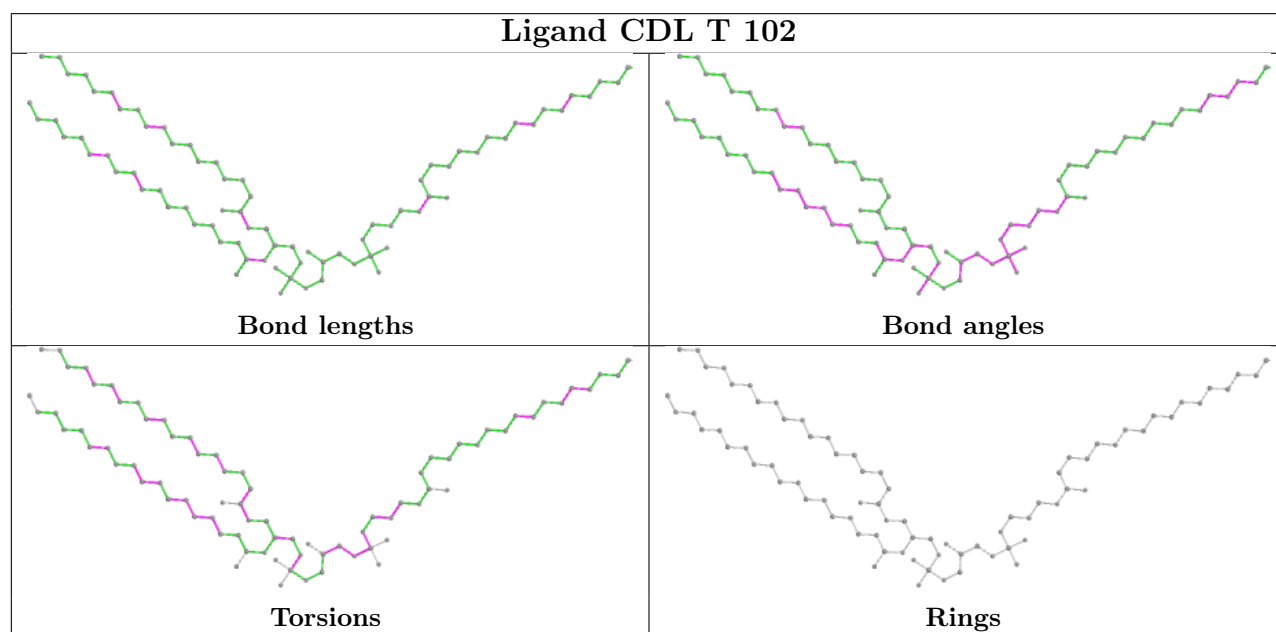
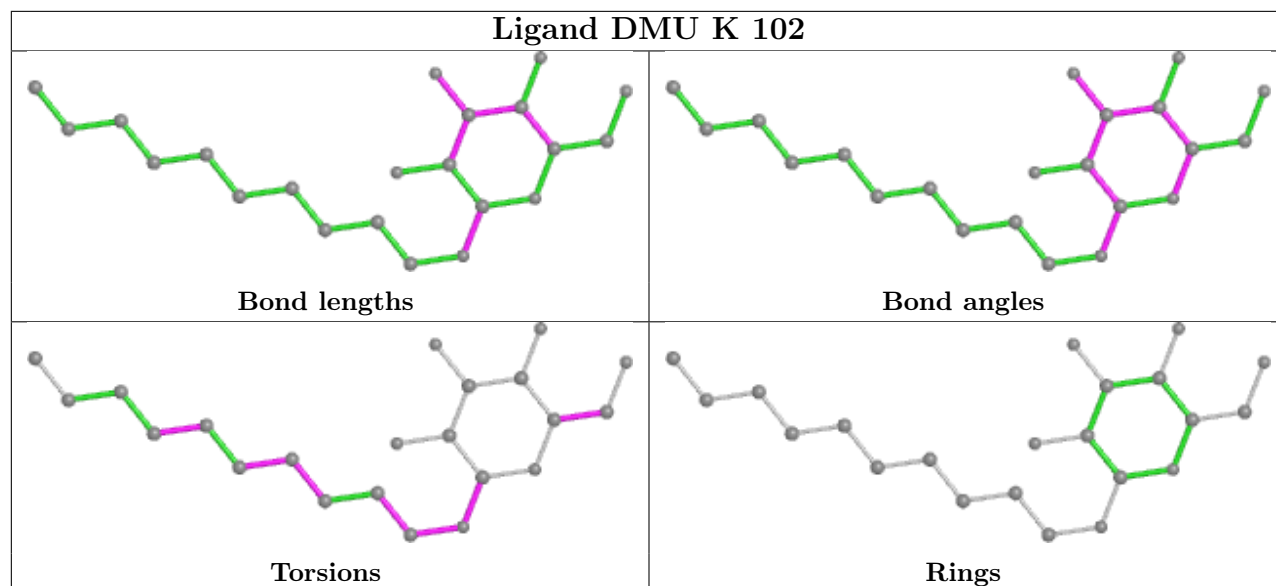


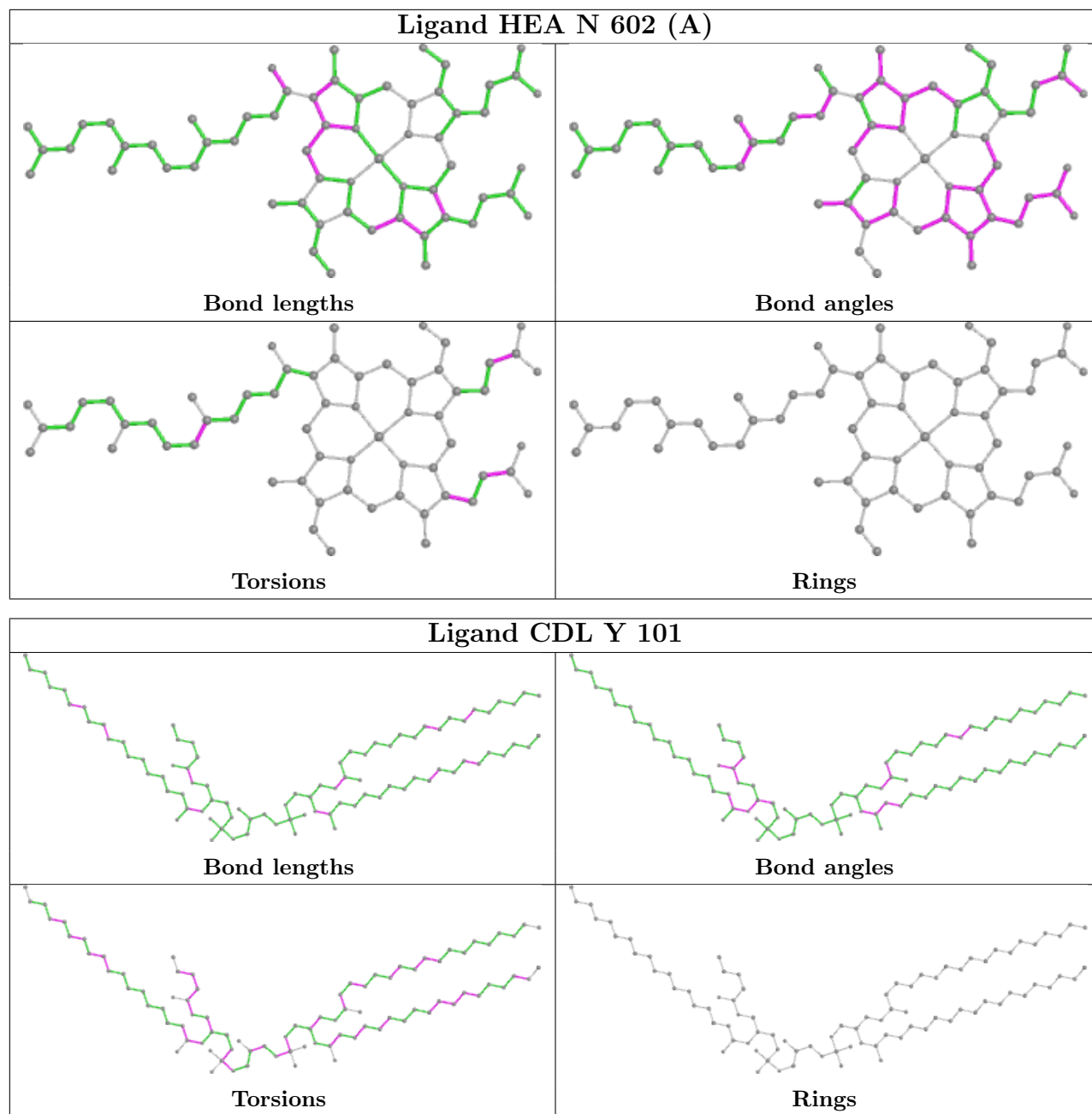


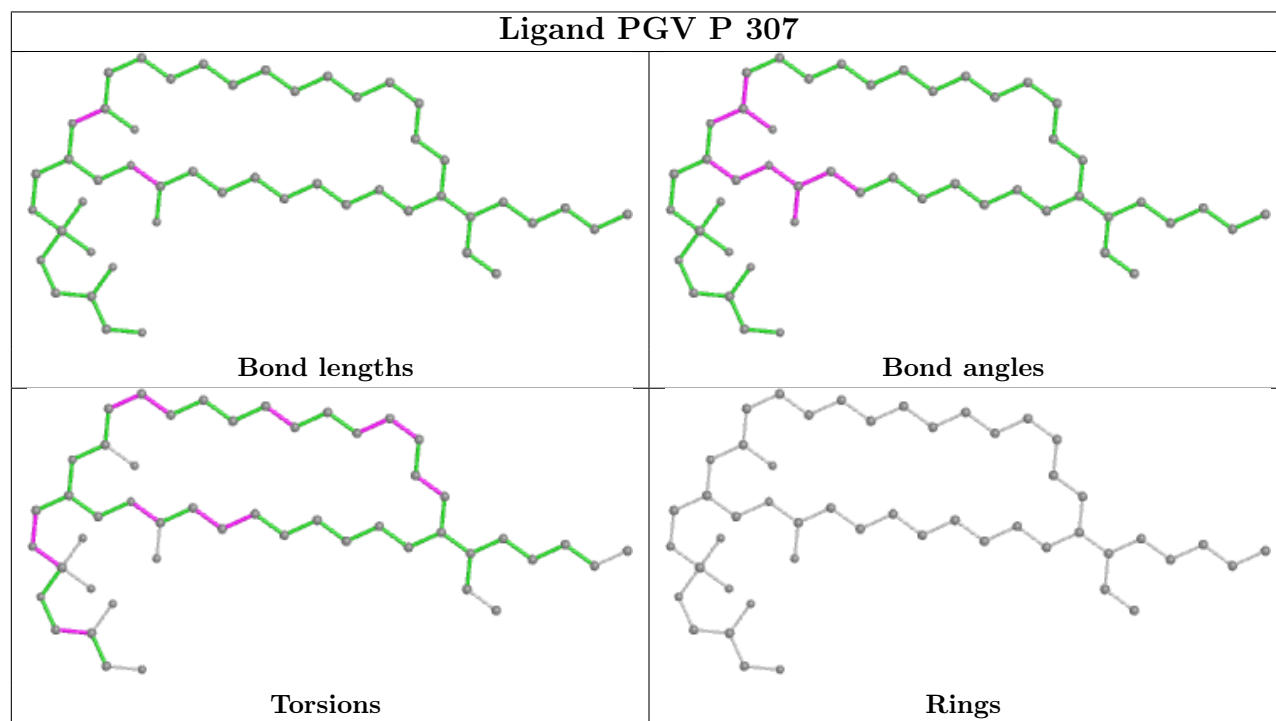
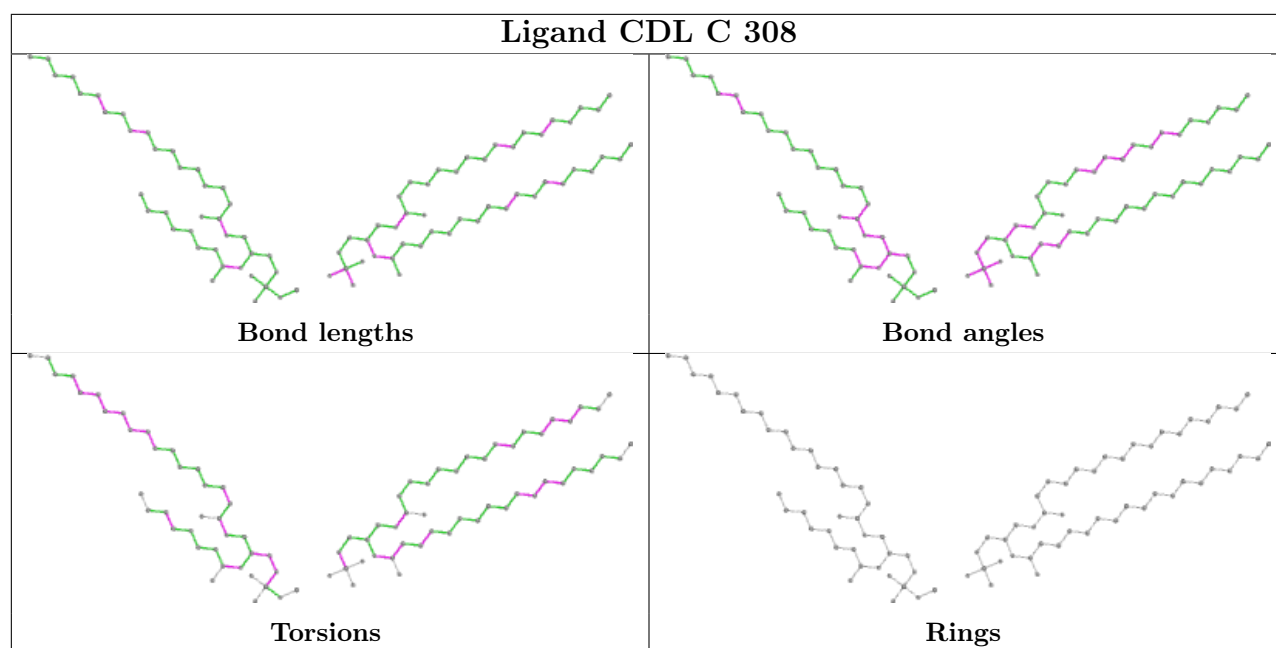


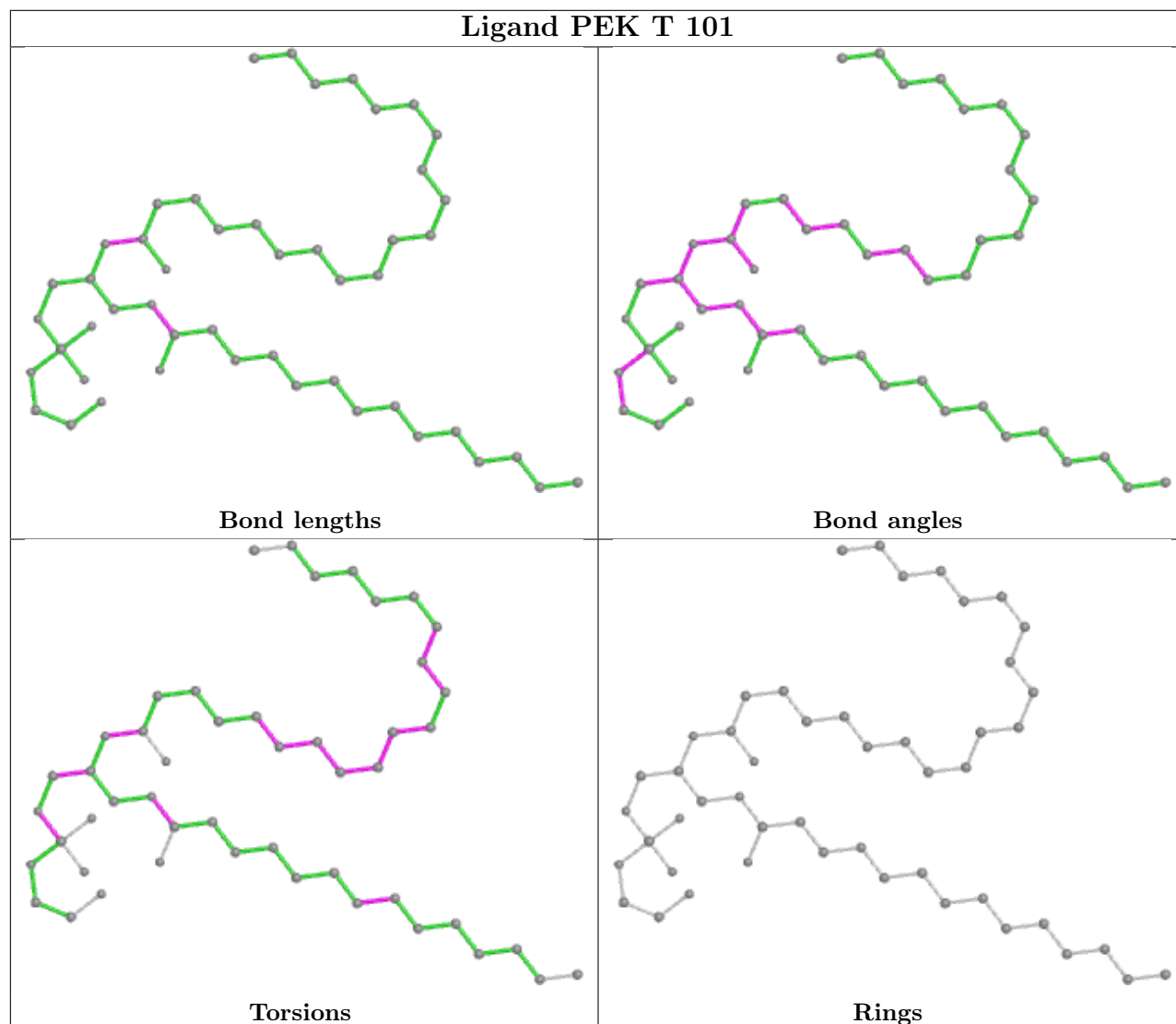
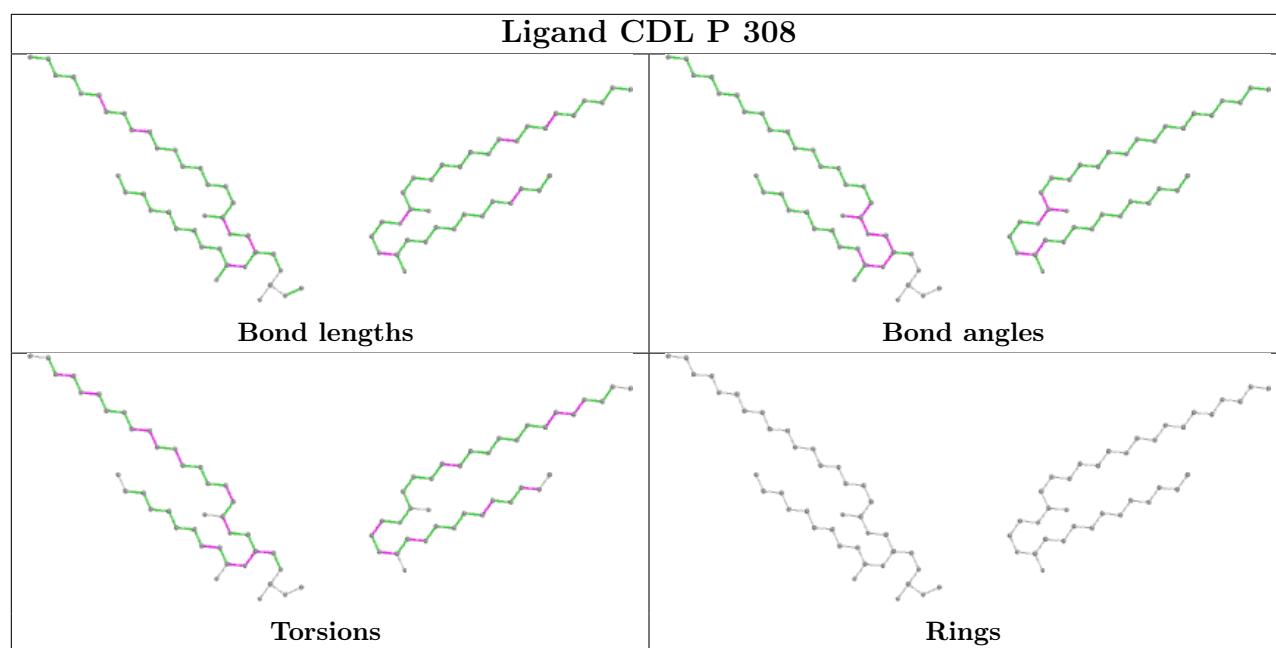


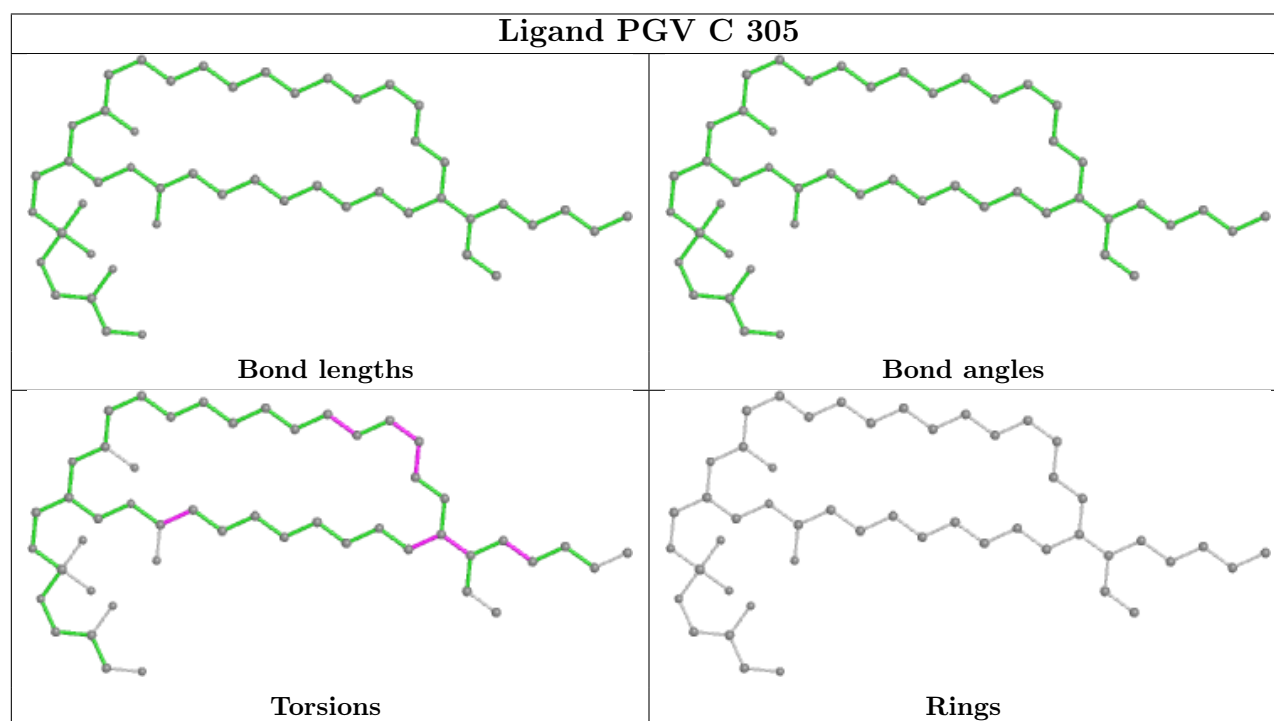
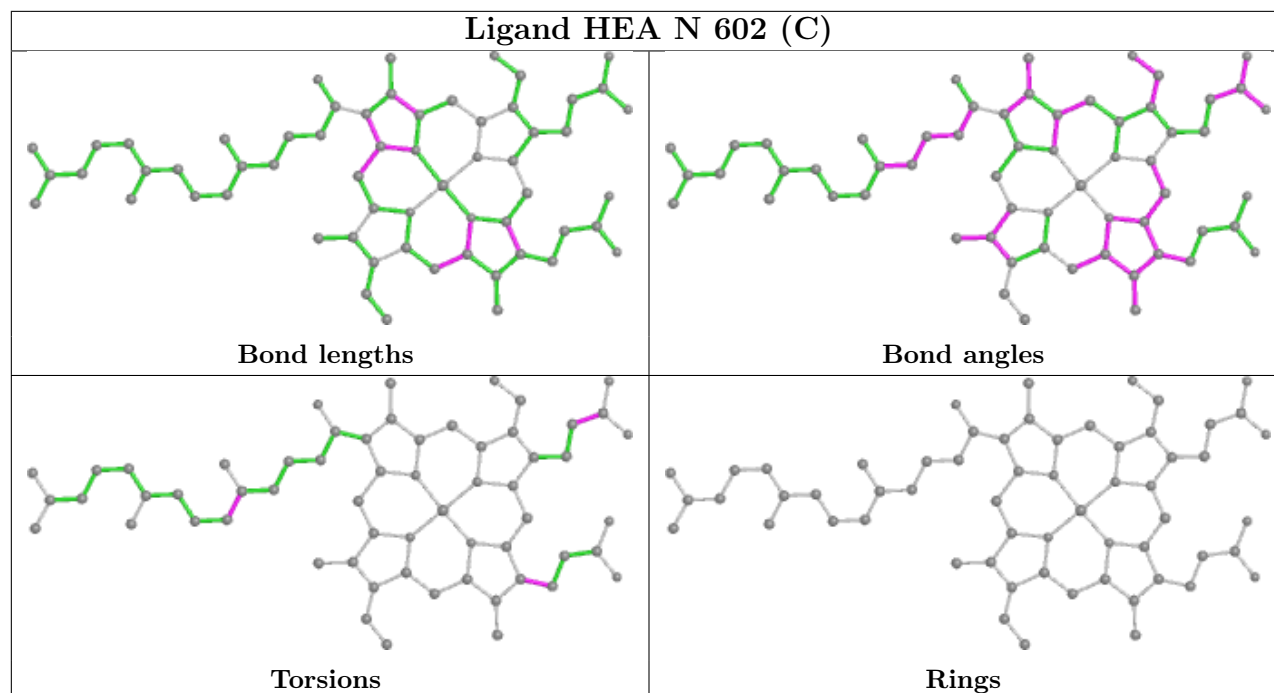


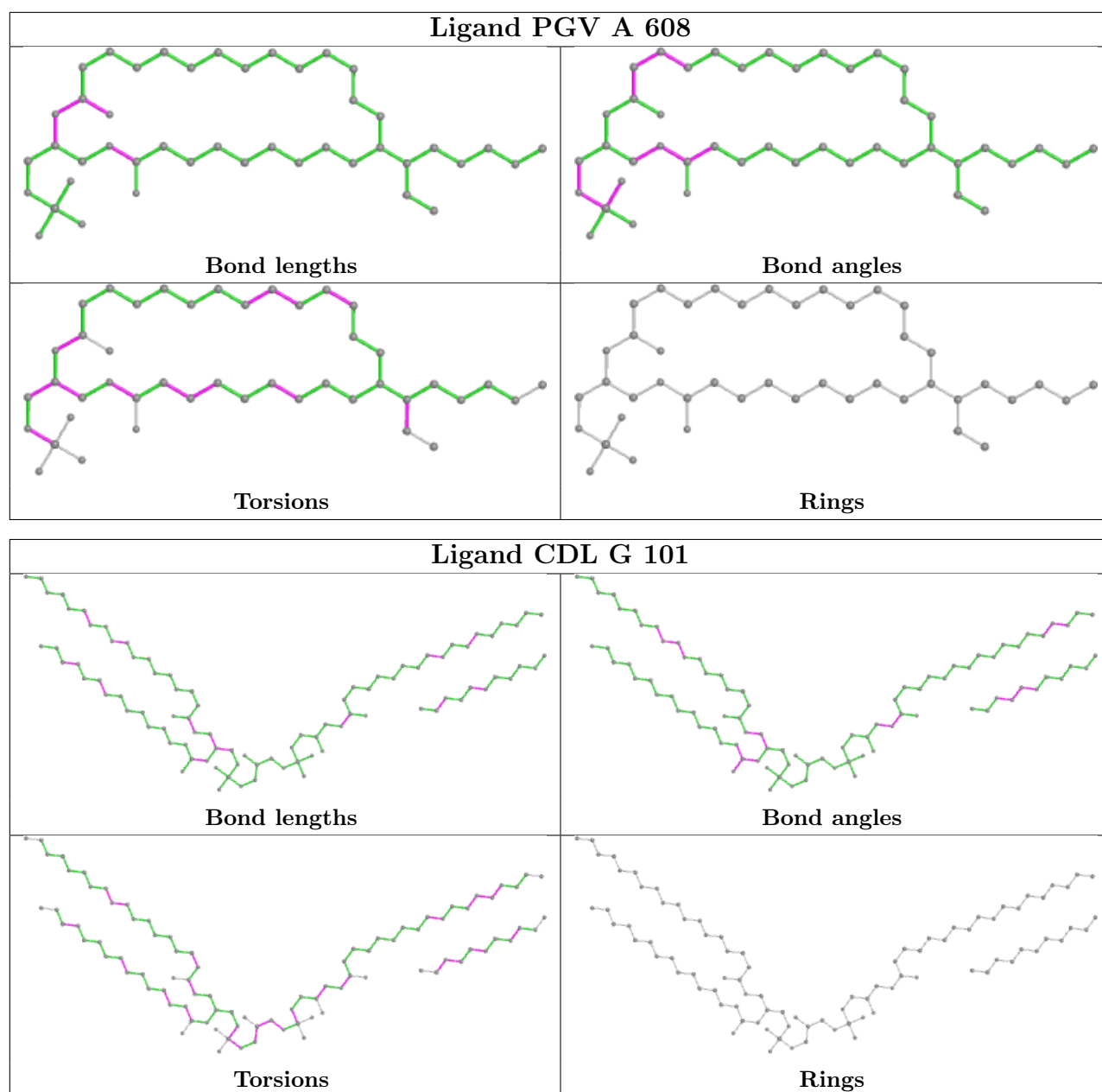


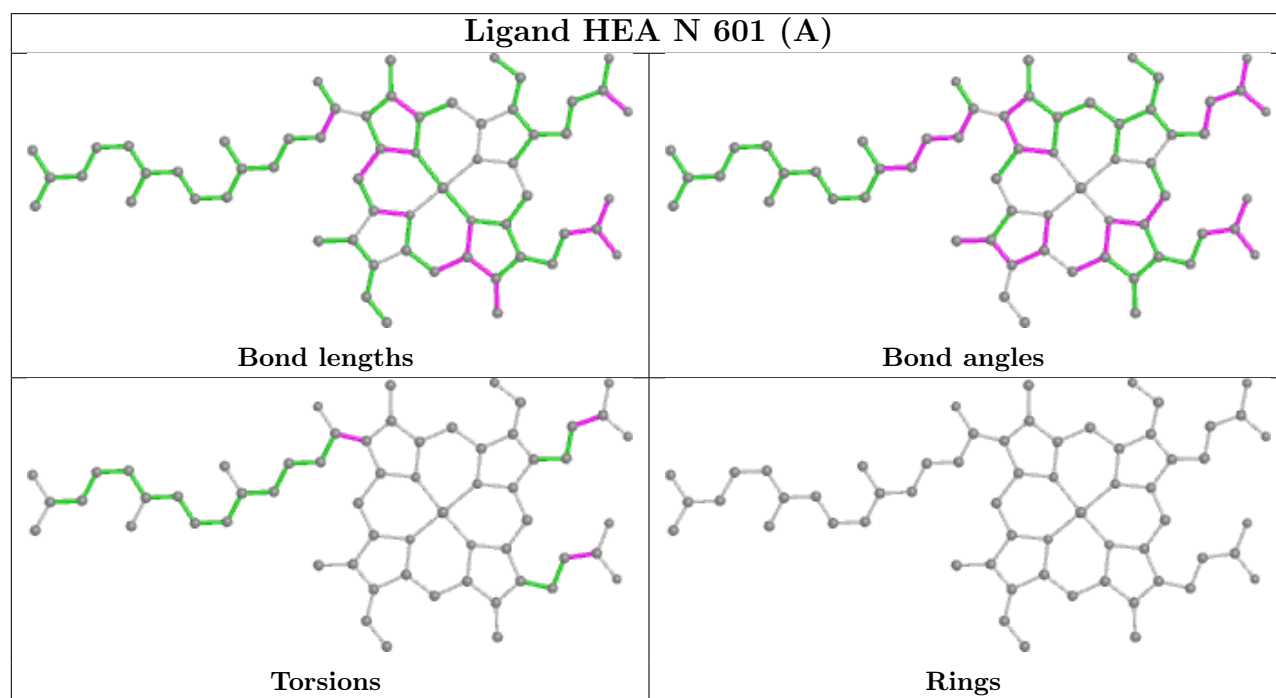
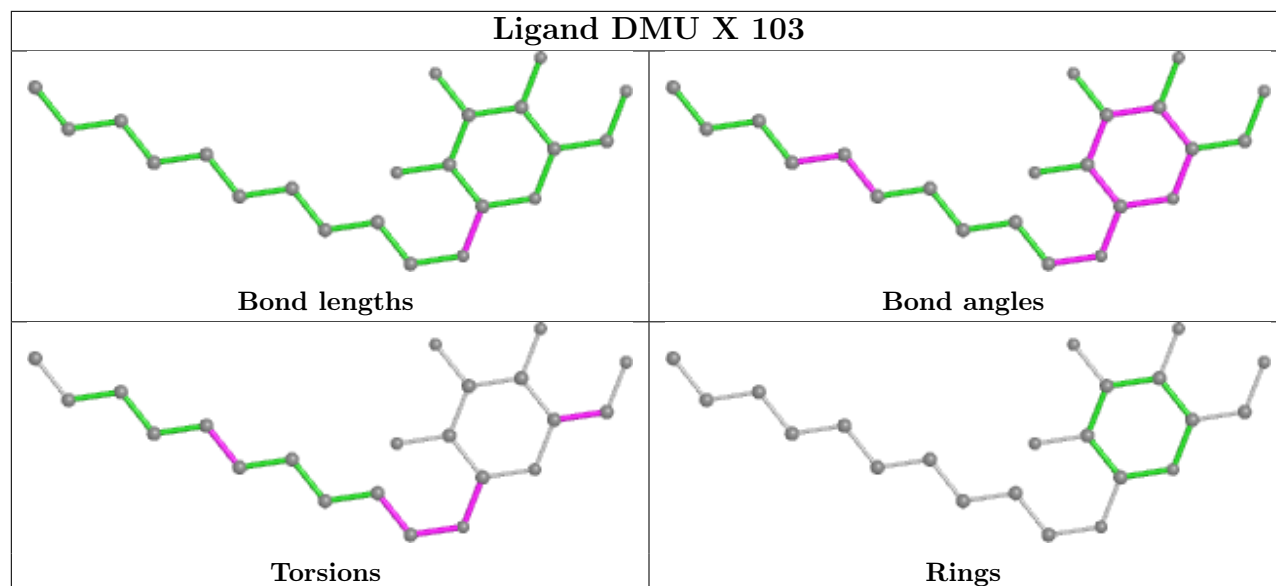




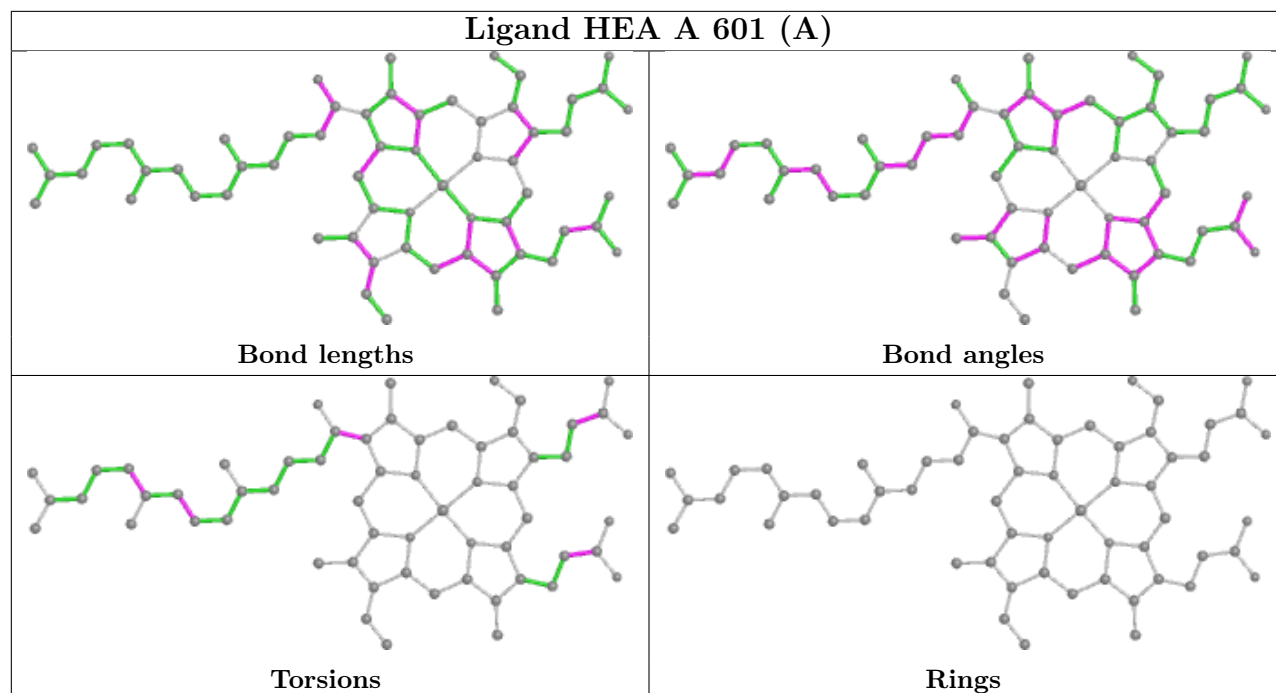




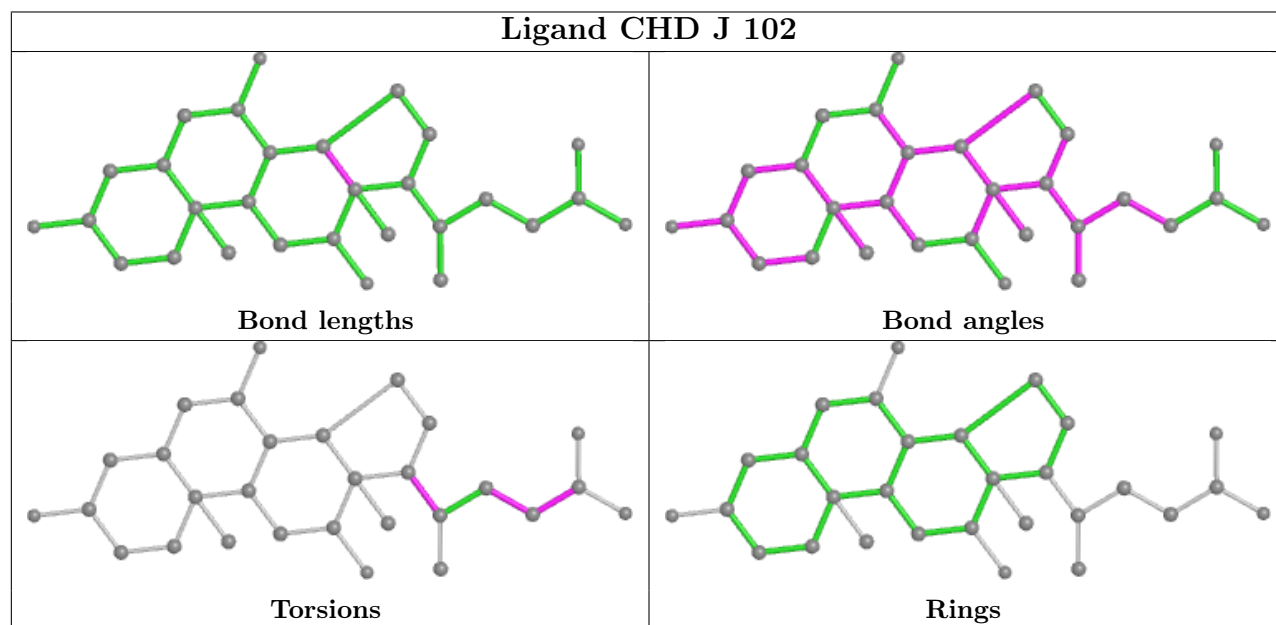


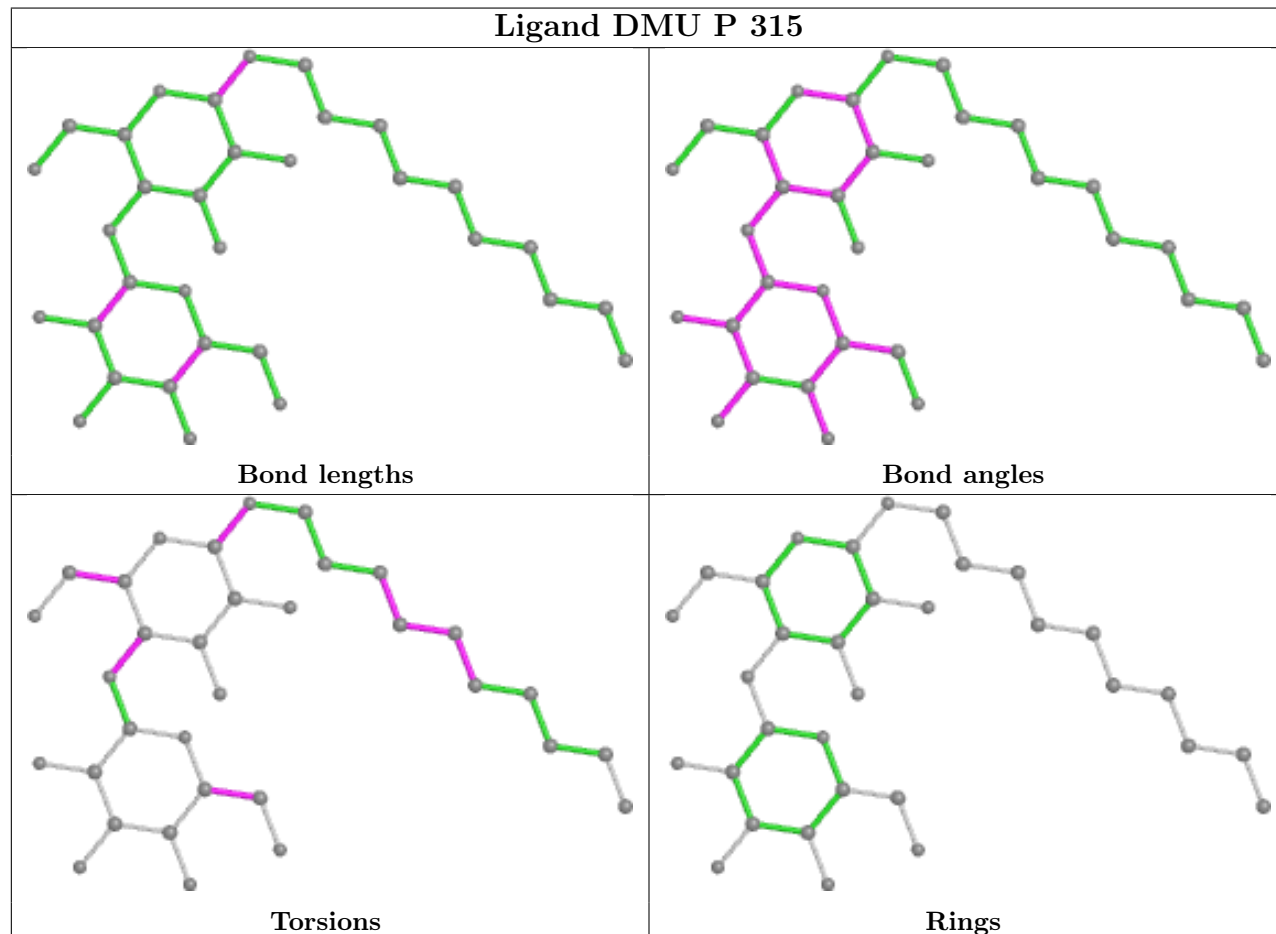
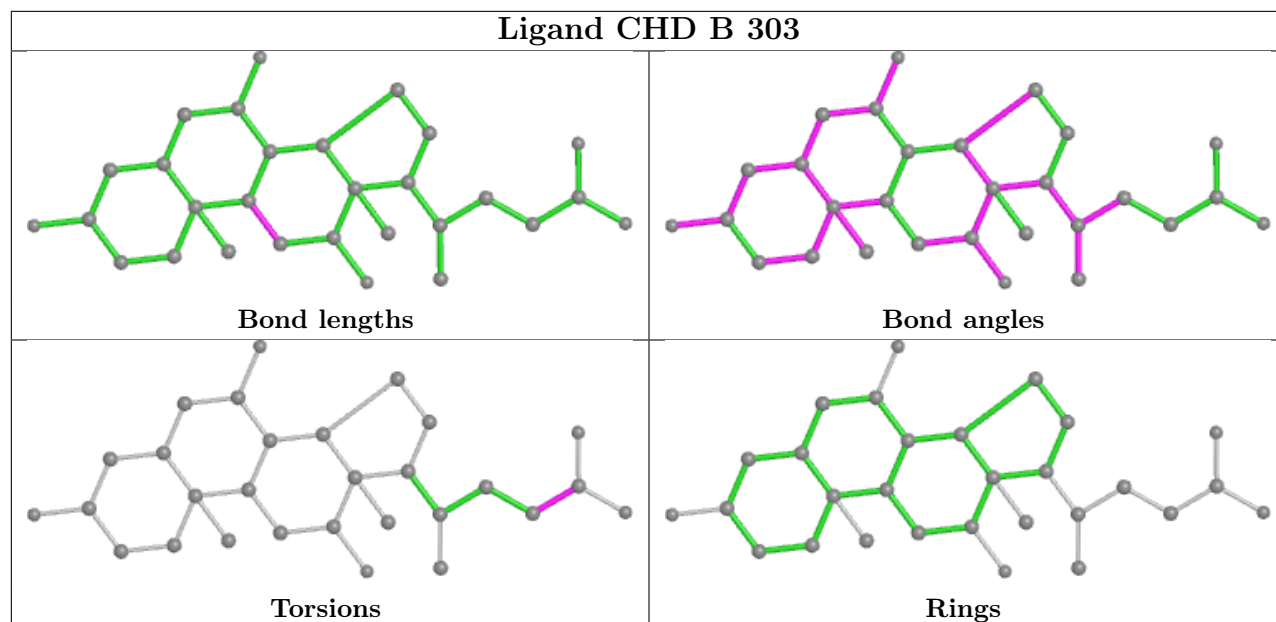


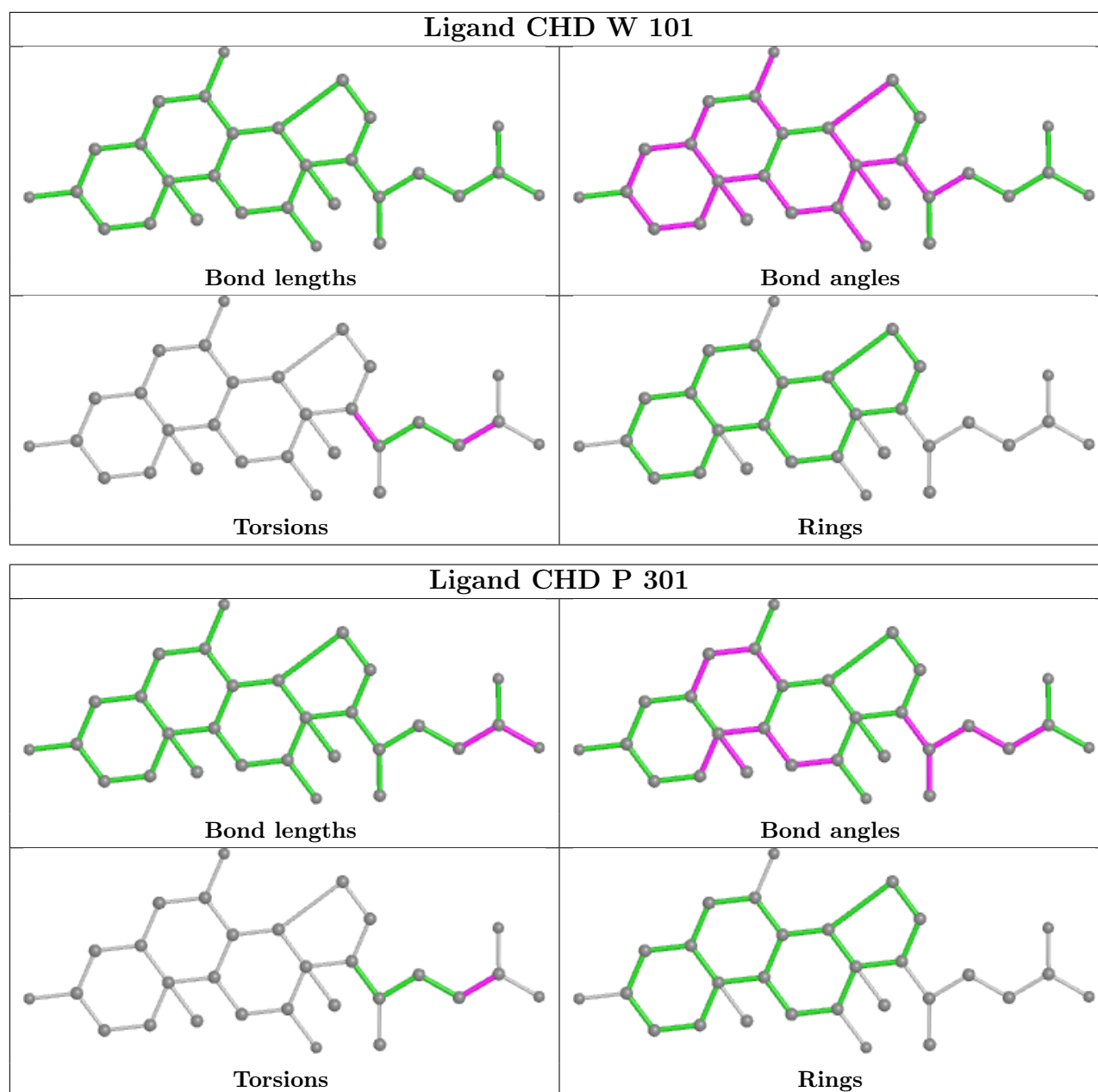
Ligand HEA A 601 (A)

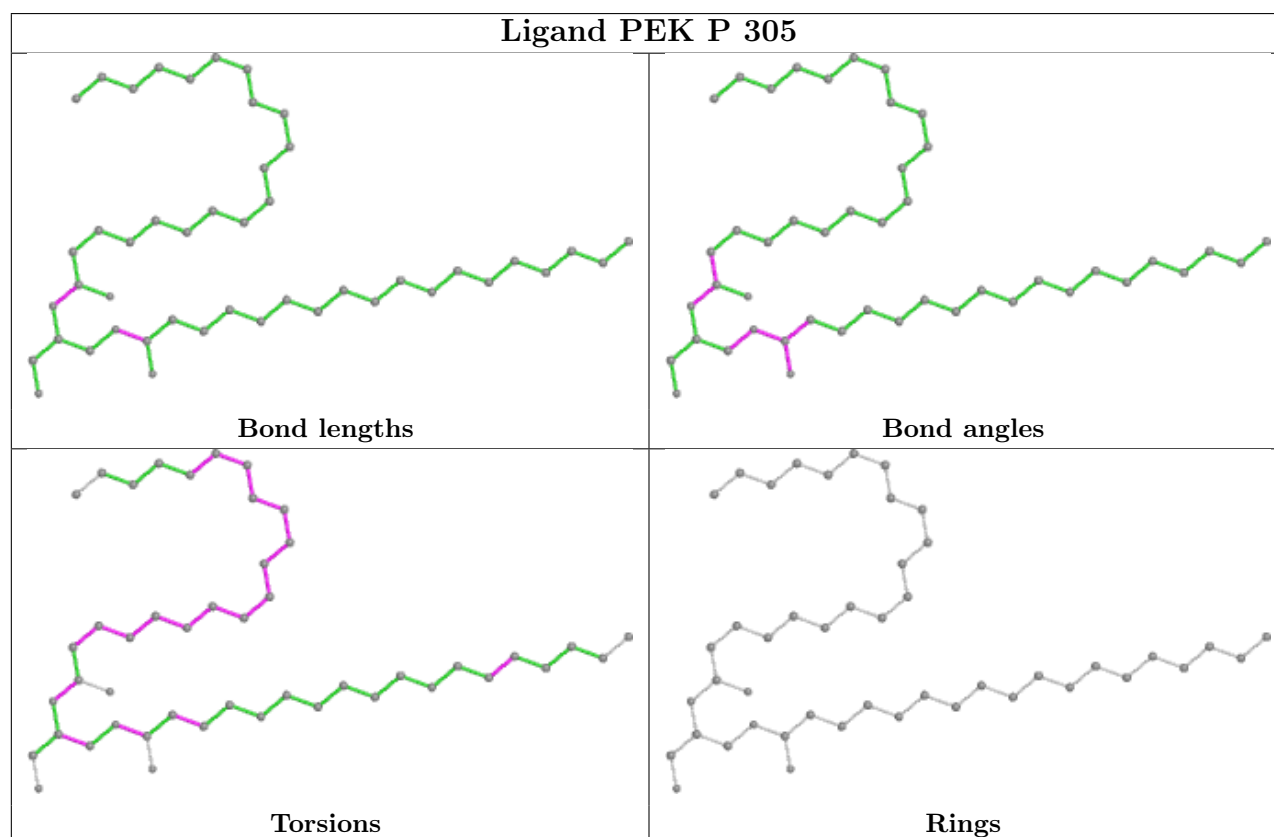
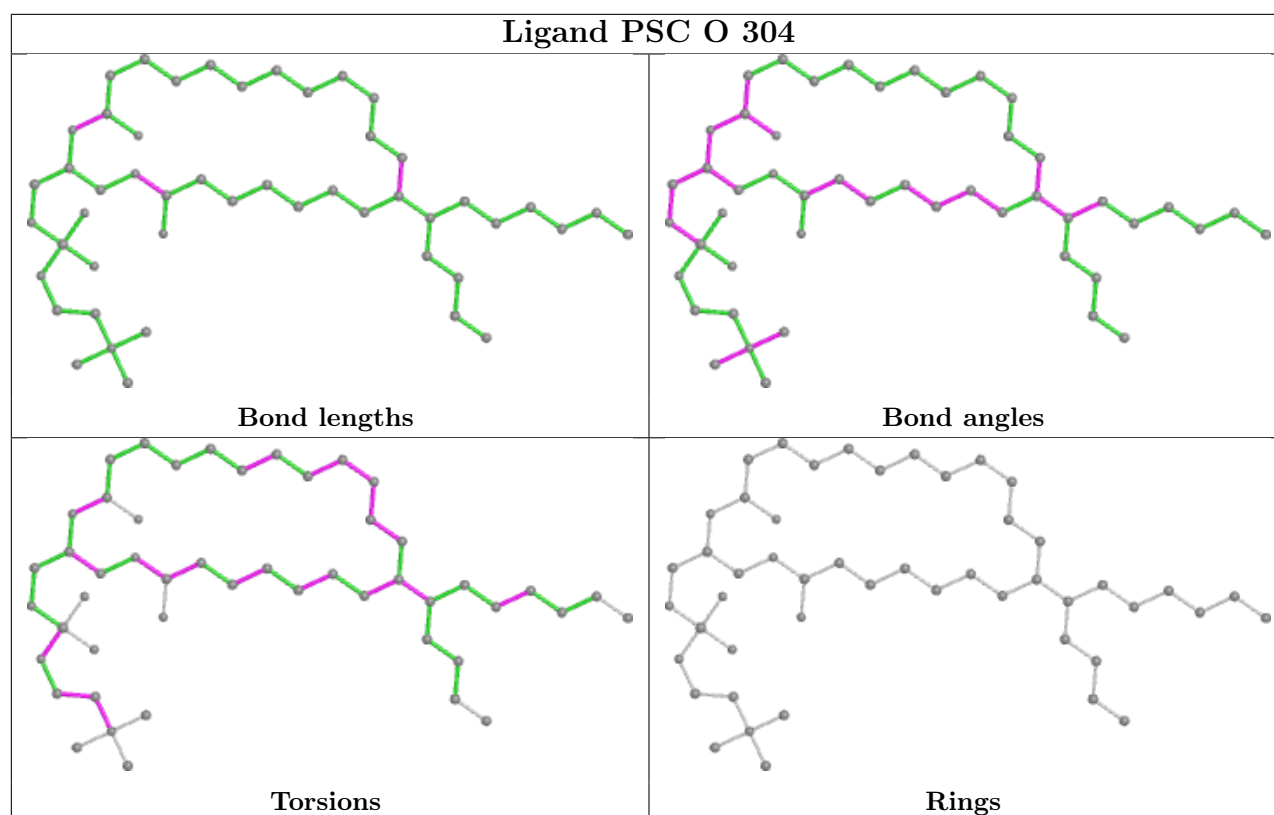


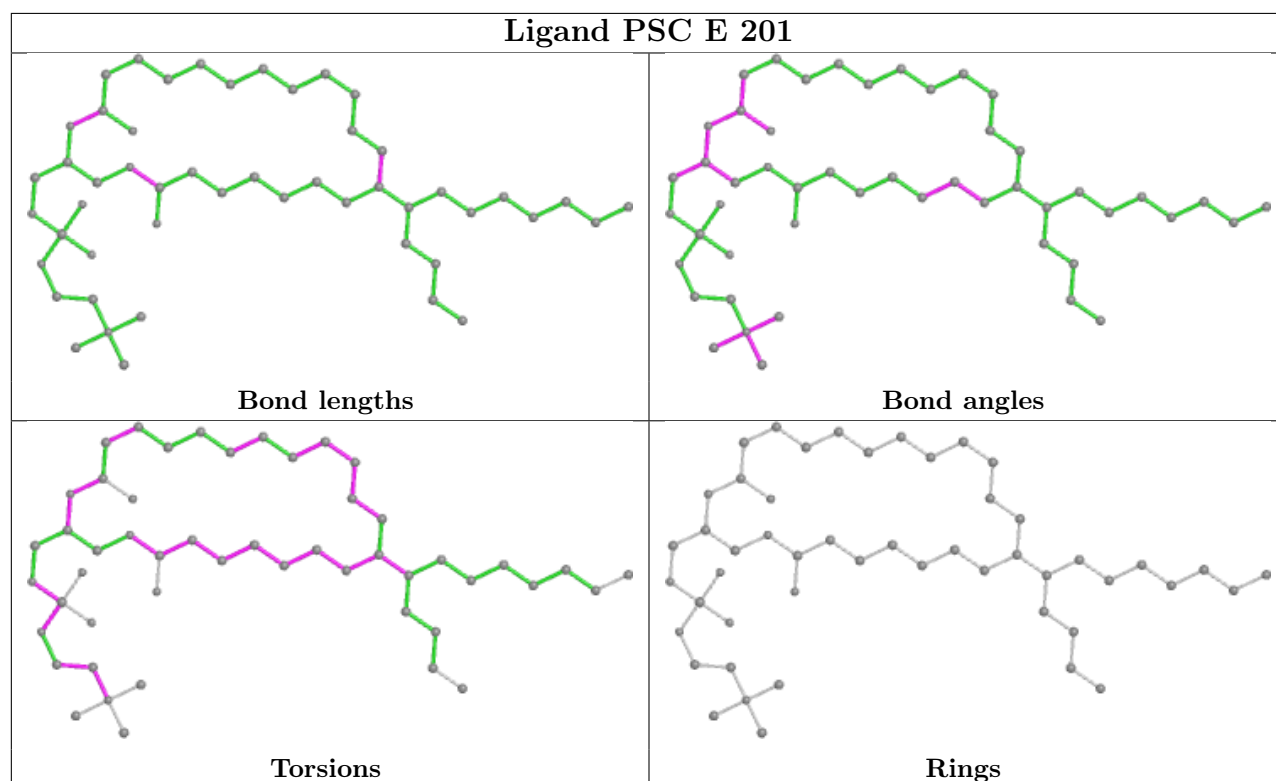
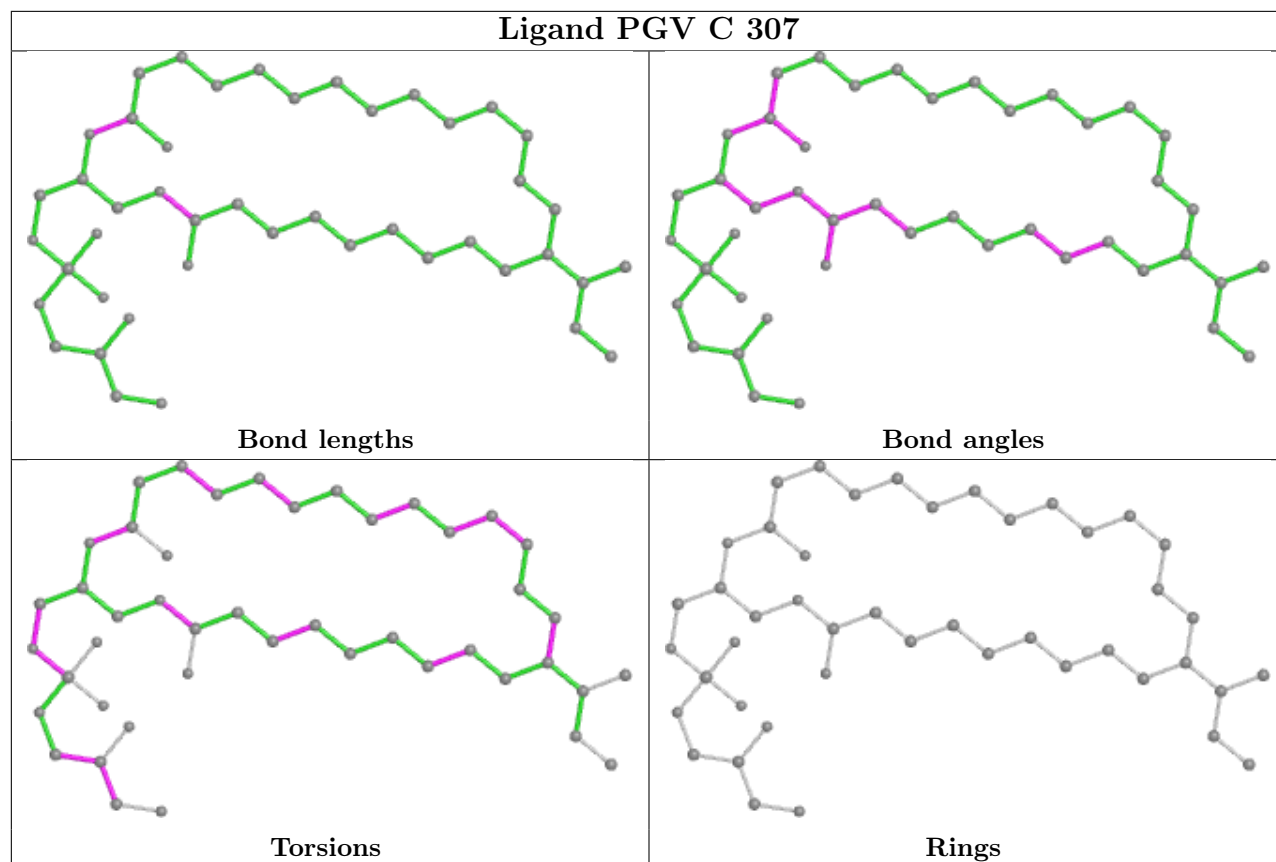
Ligand CHD J 102



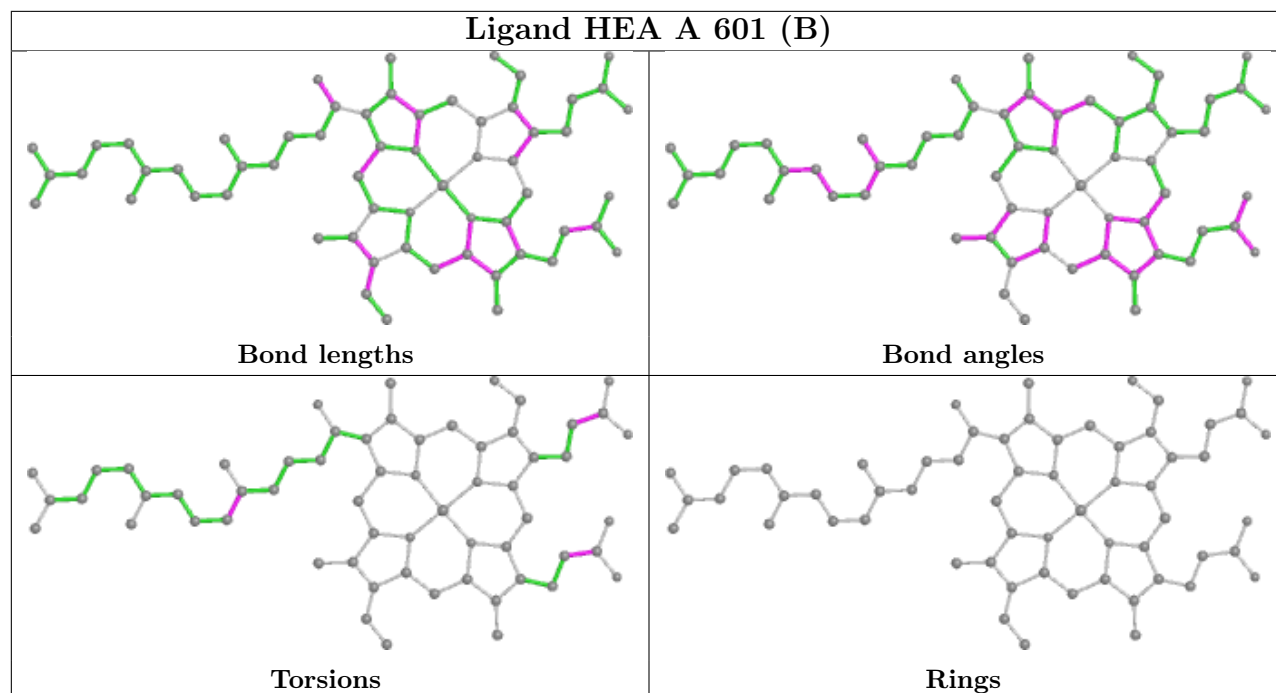




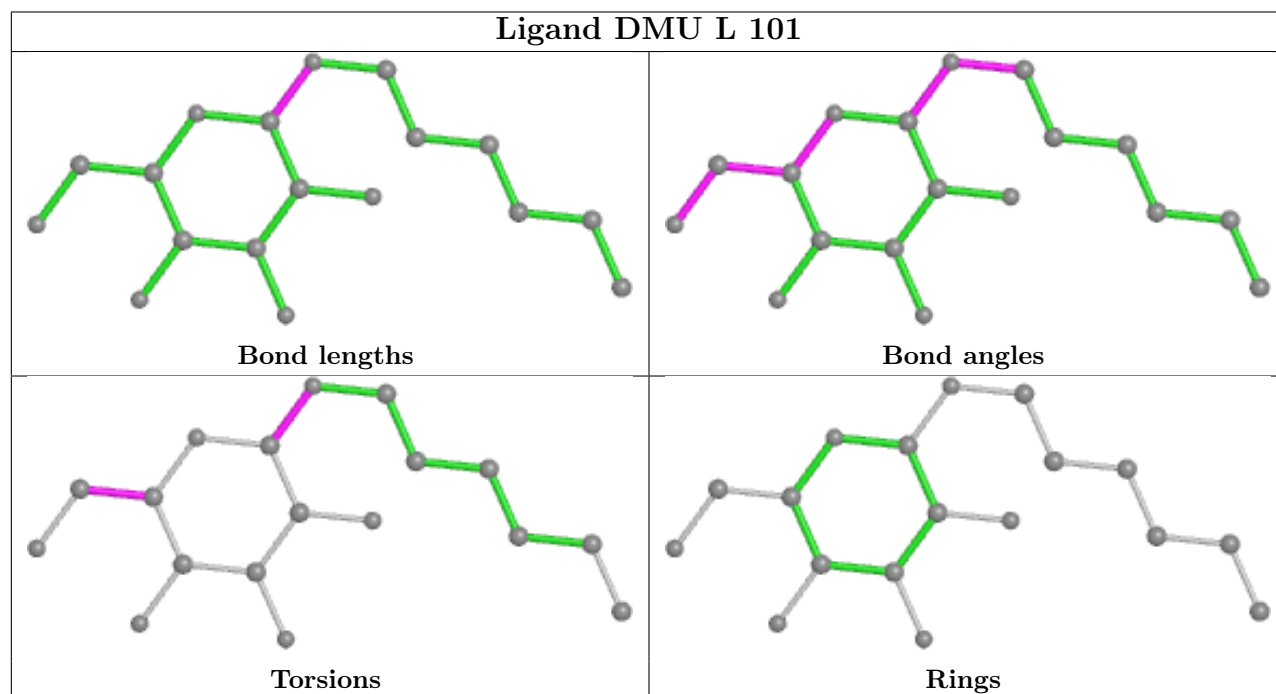




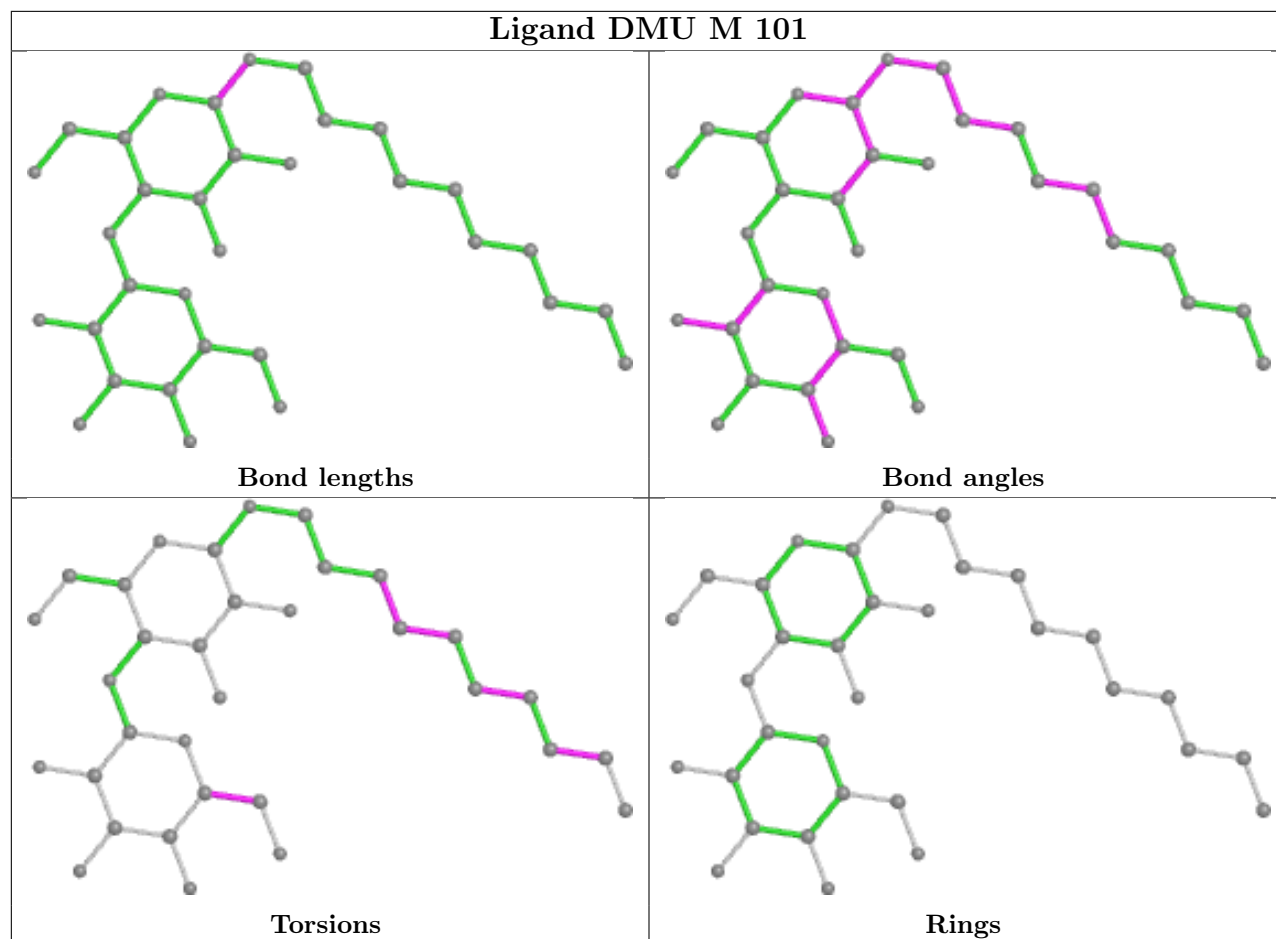
Ligand HEA A 601 (B)



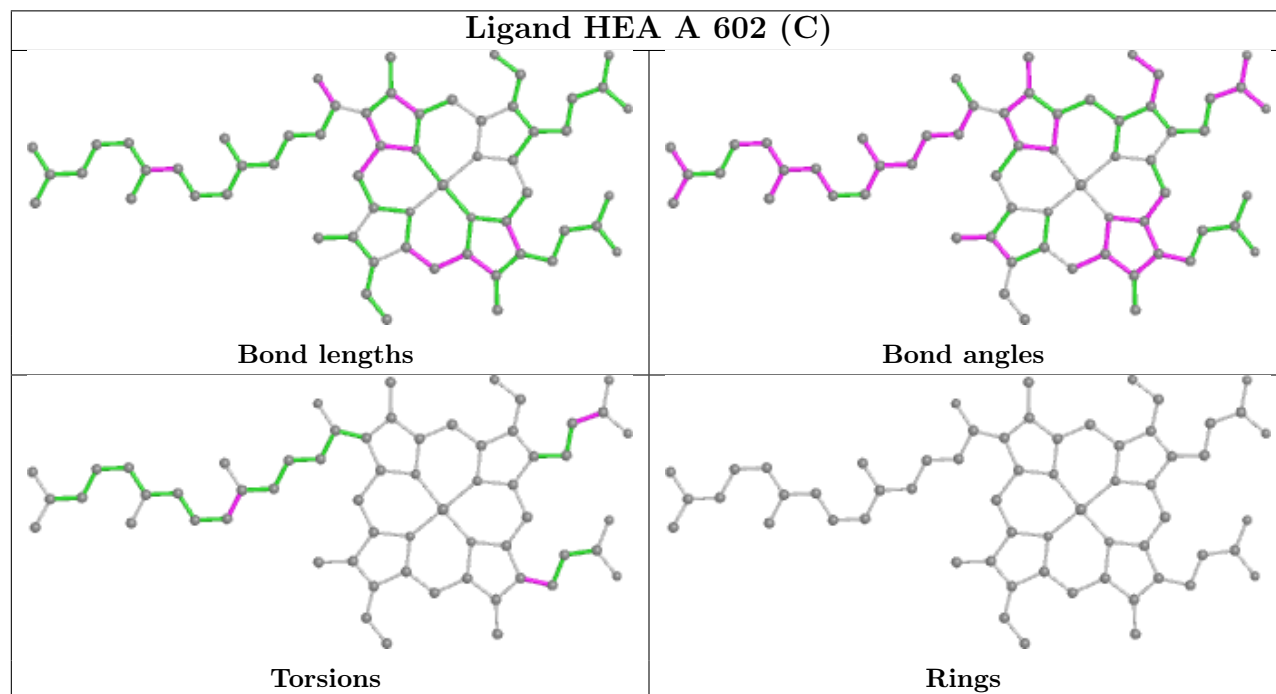
Ligand DMU L 101

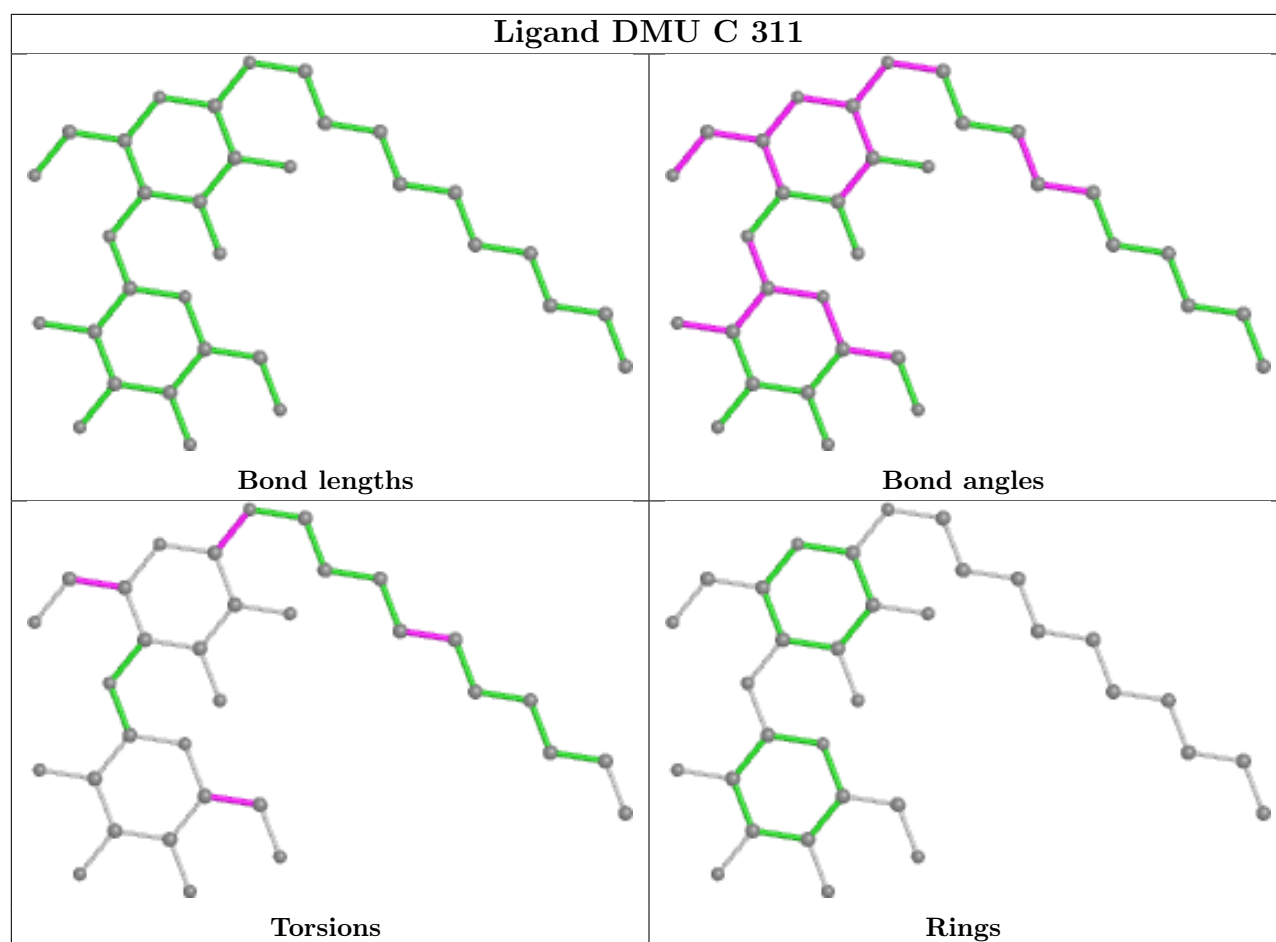


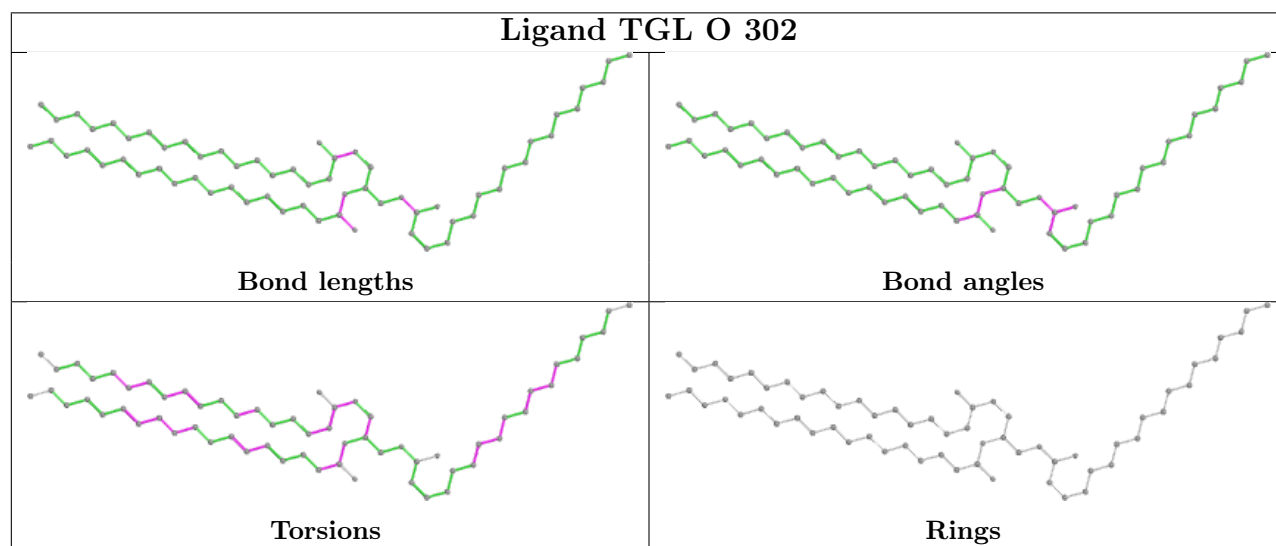
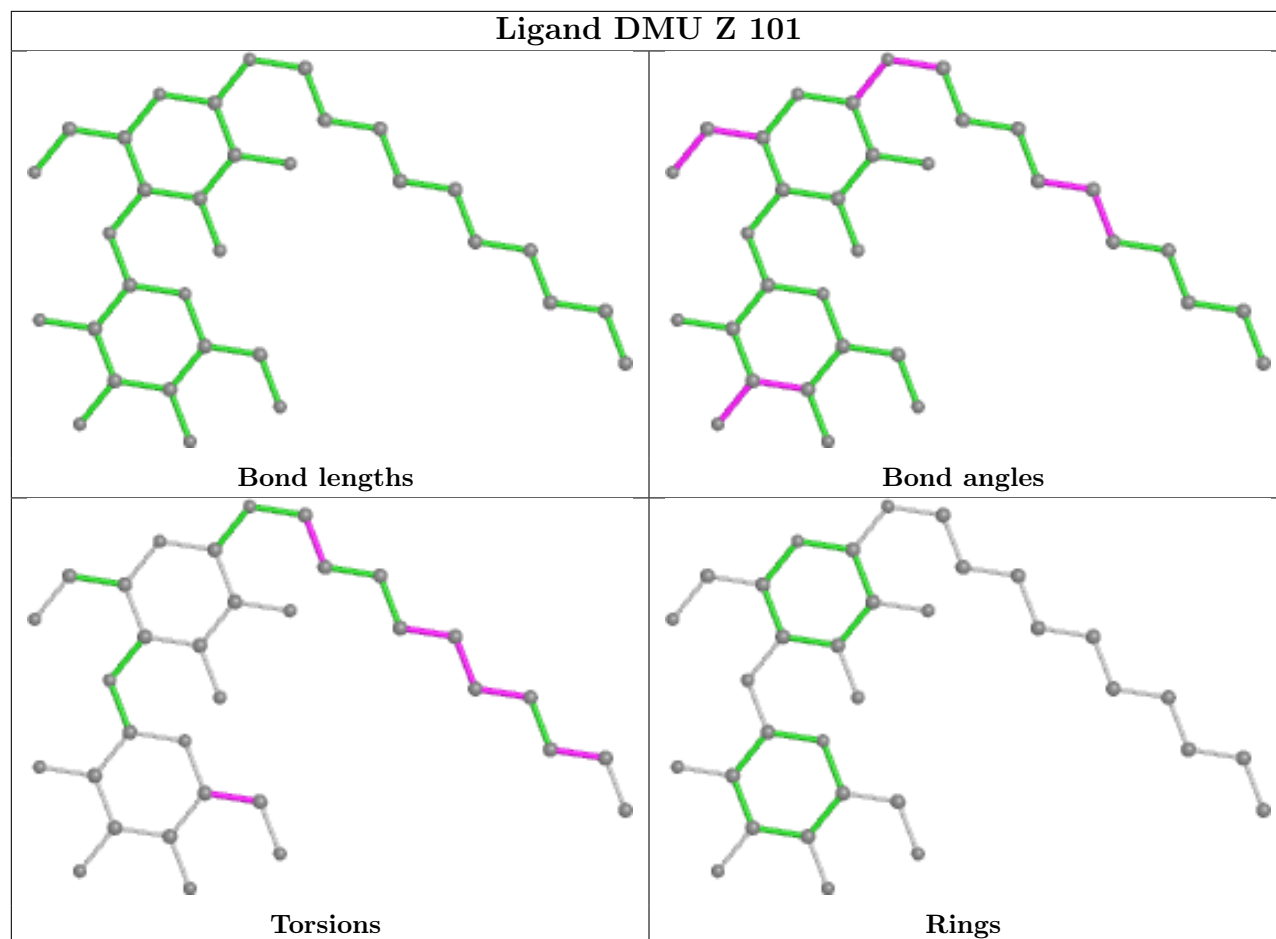
Ligand DMU M 101

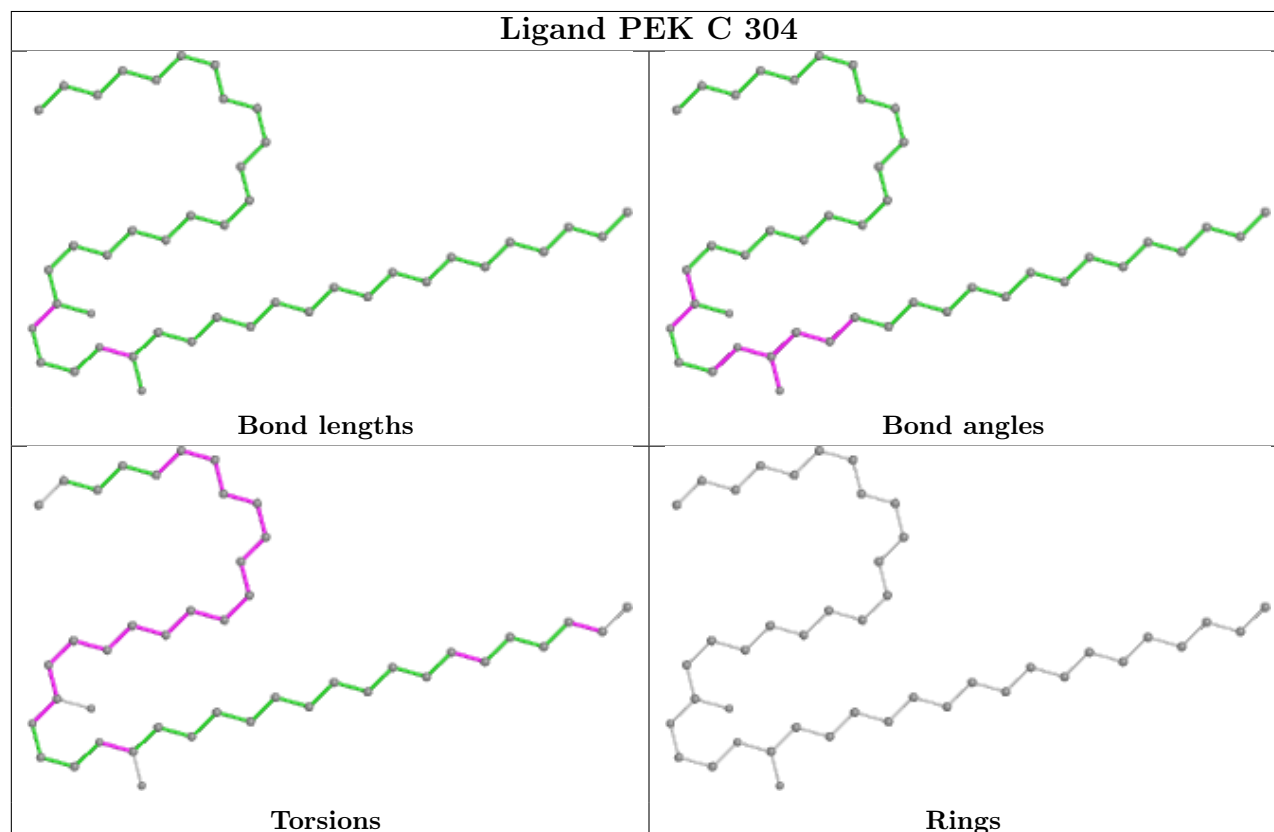
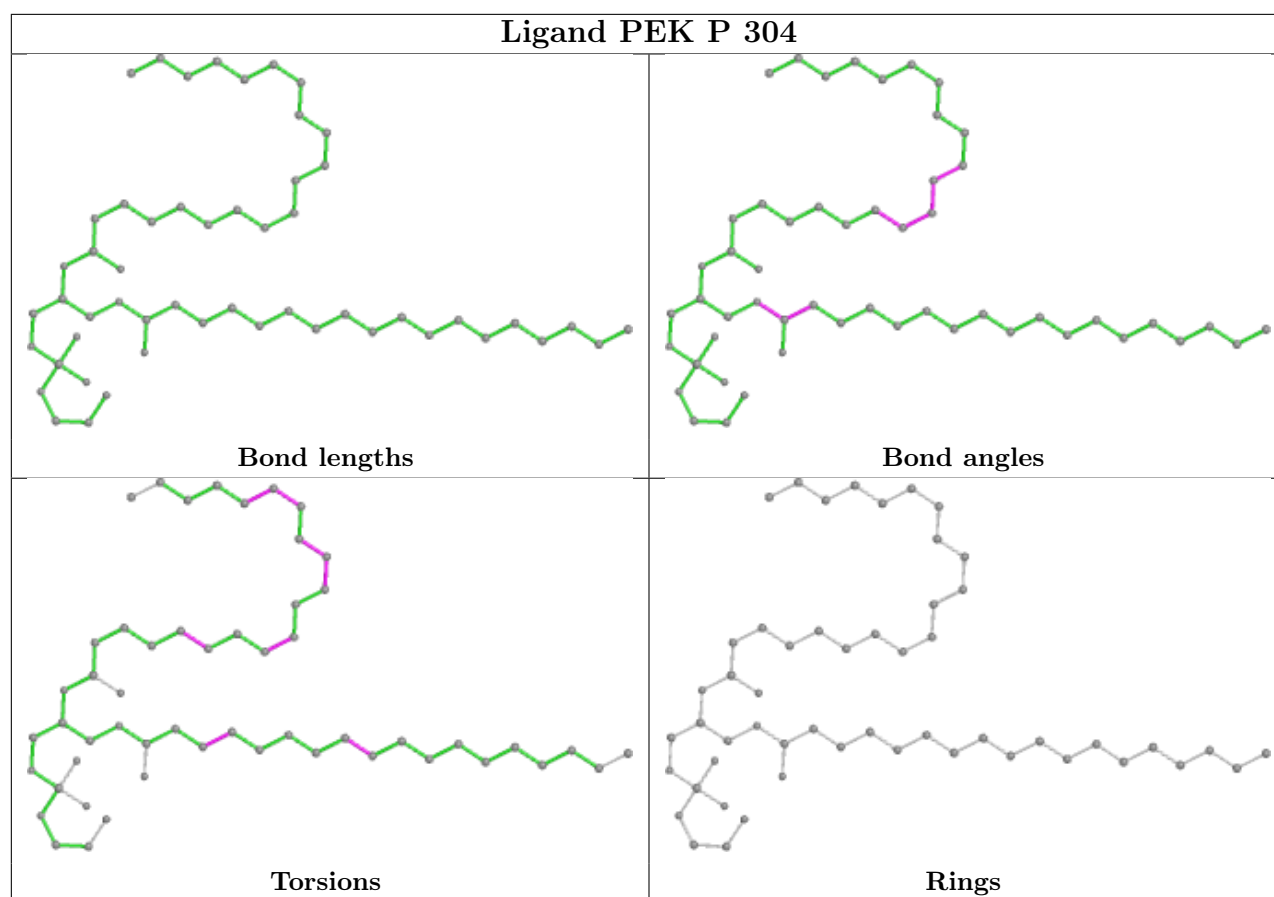


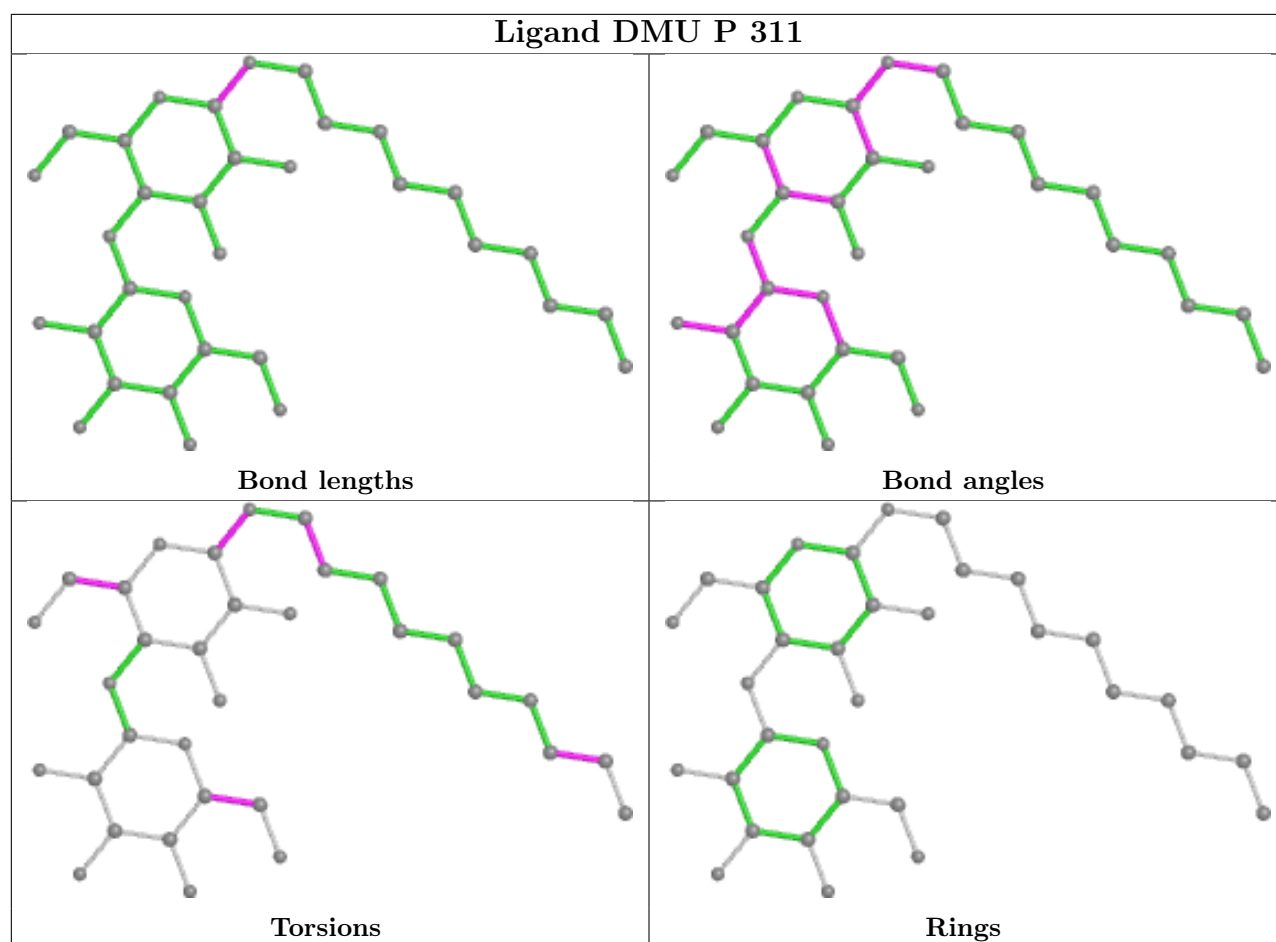
Ligand HEA A 602 (C)

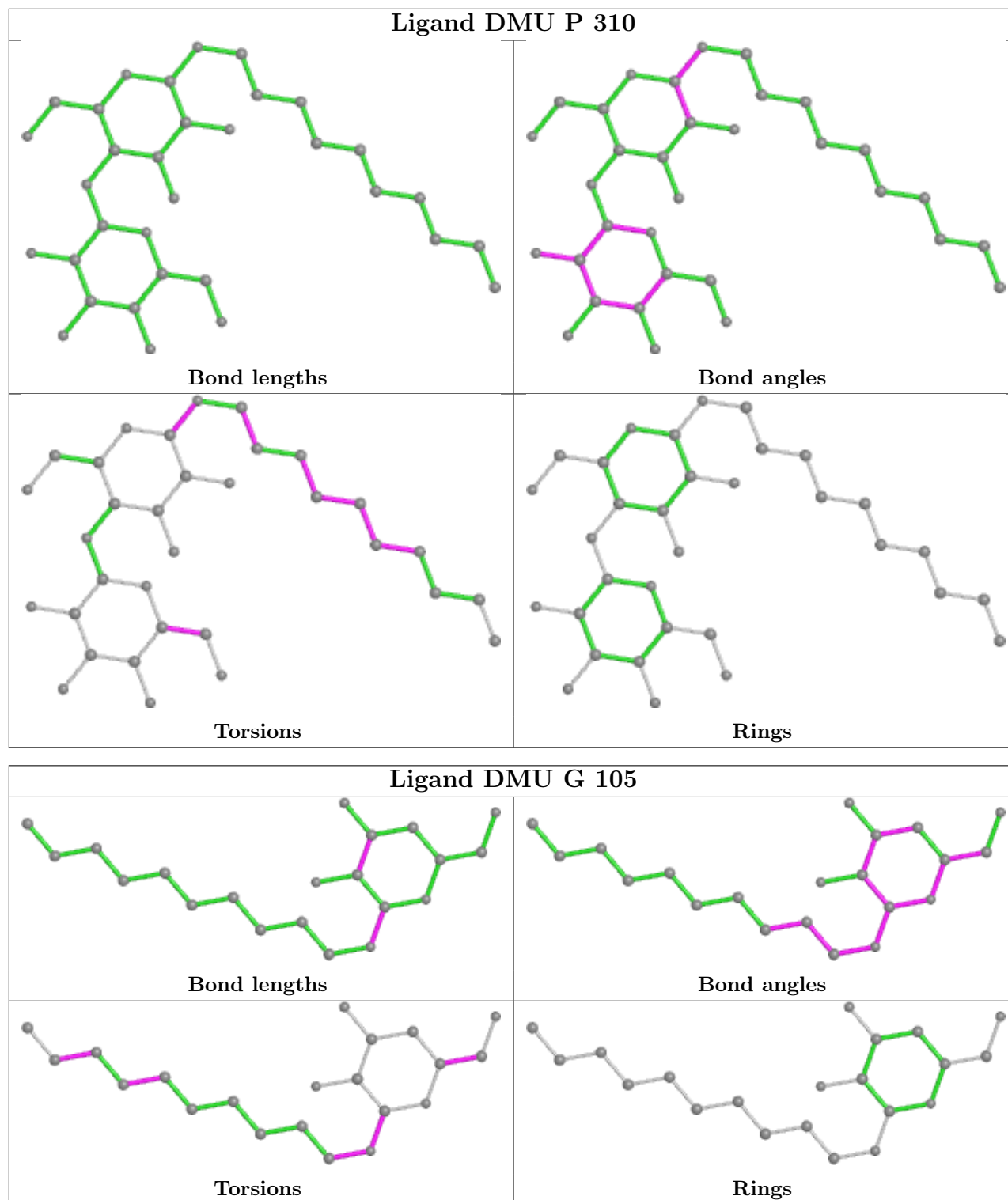


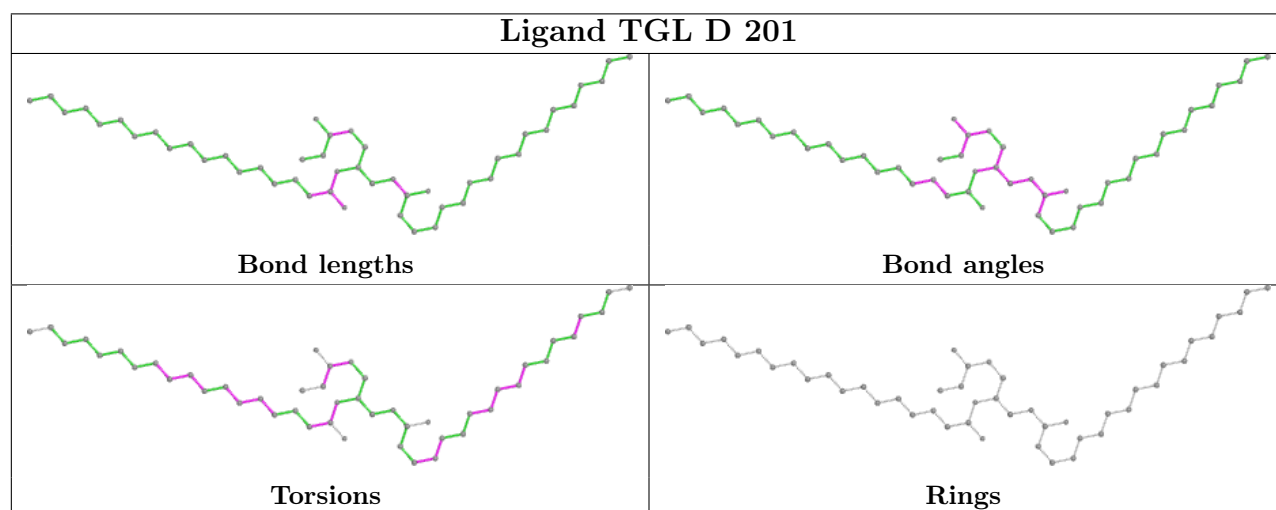
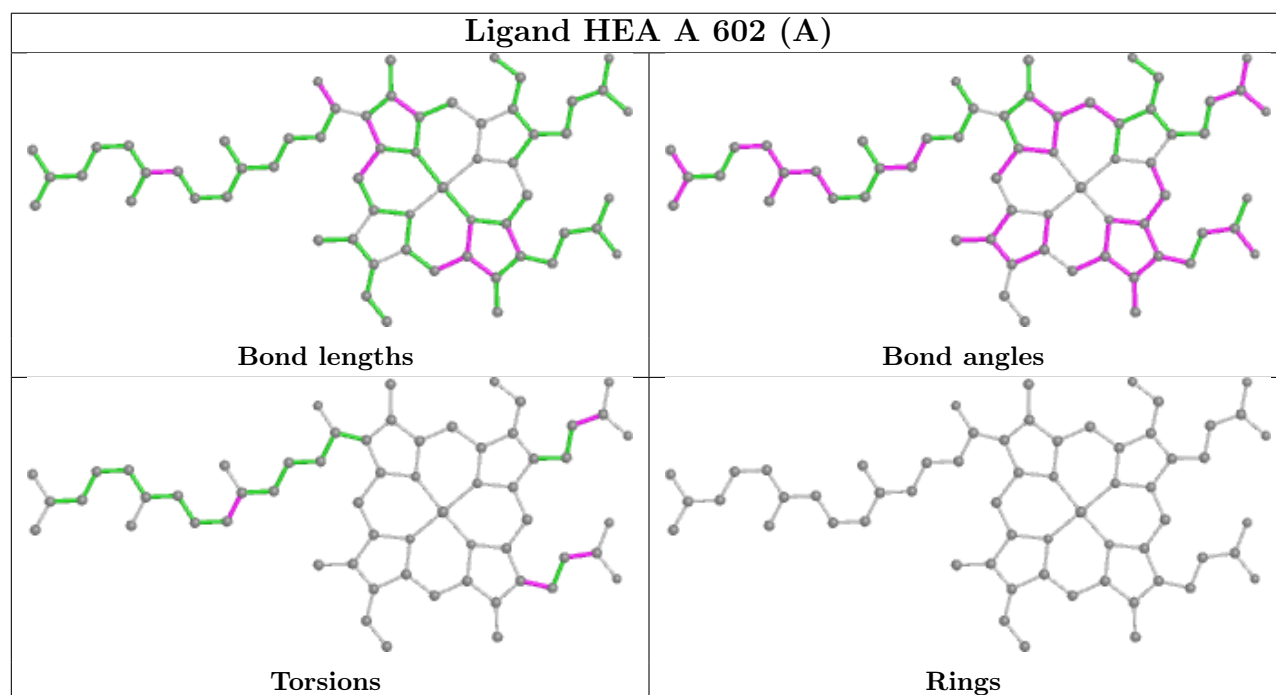
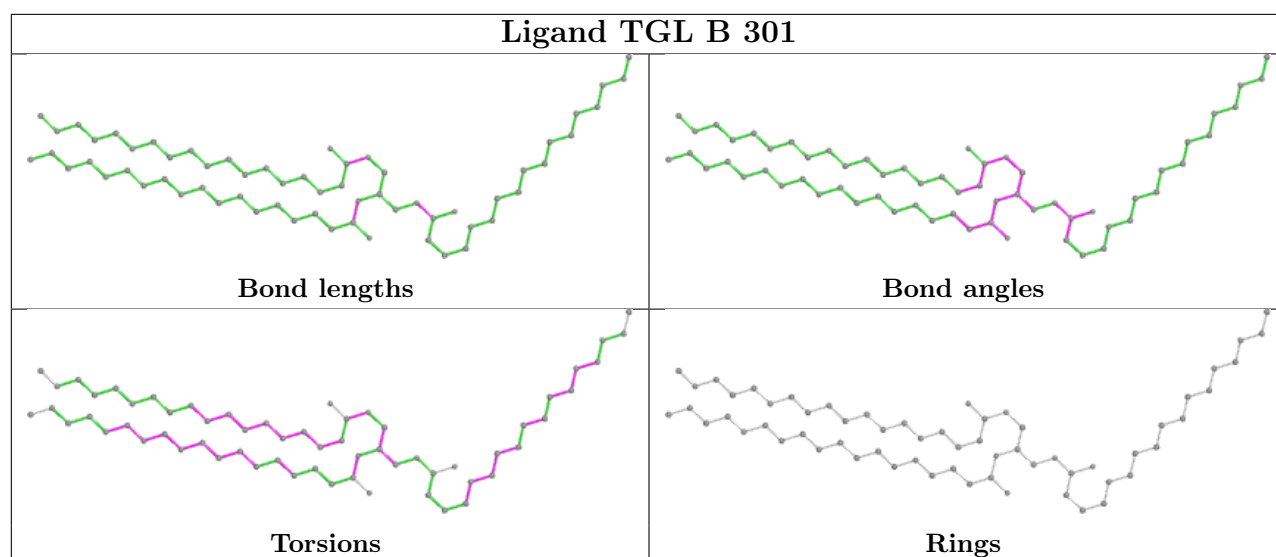


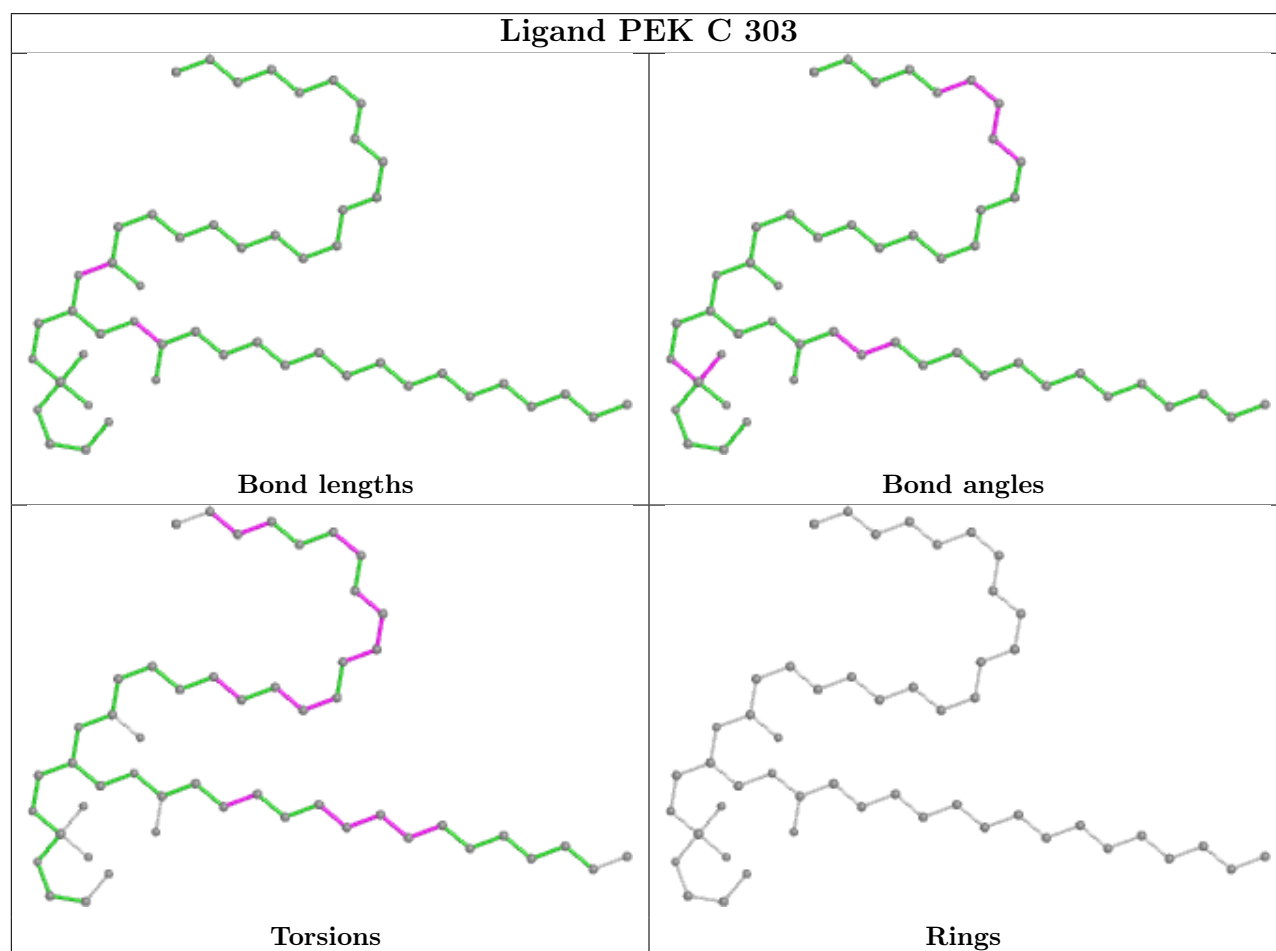
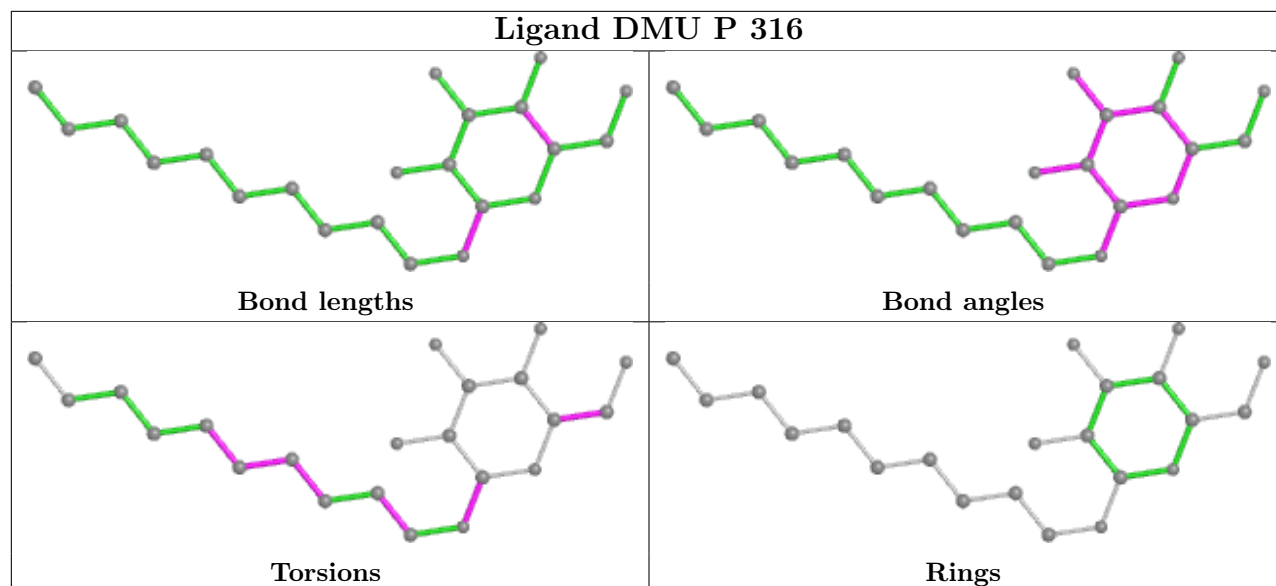


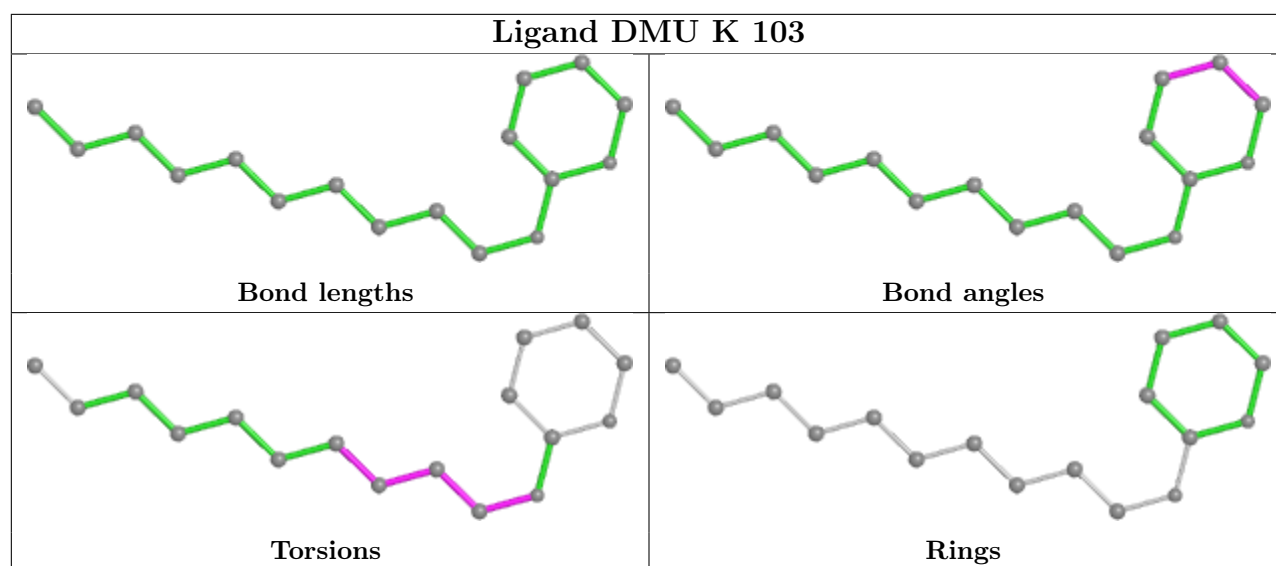












5.7 Other polymers [i](#)

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%)	-0.24	0	100	100	20, 24, 33, 97	0
1	N	513/514 (99%)	-0.31	0	100	100	21, 27, 36, 81	0
2	B	226/227 (99%)	-0.19	7 (3%)	49	52	23, 32, 65, 117	0
2	O	226/227 (99%)	-0.21	6 (2%)	54	56	26, 36, 72, 110	0
3	C	259/259 (100%)	-0.25	0	100	100	22, 28, 42, 81	0
3	P	259/259 (100%)	-0.27	2 (0%)	86	87	22, 28, 45, 110	0
4	D	144/144 (100%)	-0.38	1 (0%)	87	89	26, 33, 63, 101	0
4	Q	144/144 (100%)	0.30	6 (4%)	36	39	32, 47, 97, 205	0
5	E	104/104 (100%)	-0.36	0	100	100	26, 33, 61, 88	0
5	R	104/104 (100%)	-0.22	1 (0%)	82	84	30, 39, 67, 97	0
6	F	93/93 (100%)	-0.27	3 (3%)	47	50	23, 32, 63, 111	0
6	S	93/93 (100%)	-0.20	4 (4%)	35	38	24, 32, 63, 108	0
7	G	80/84 (95%)	0.71	15 (18%)	1	1	26, 37, 97, 117	0
7	T	84/84 (100%)	0.76	16 (19%)	1	1	25, 38, 125, 148	0
8	H	79/79 (100%)	0.18	8 (10%)	7	8	27, 37, 112, 130	0
8	U	79/79 (100%)	0.08	9 (11%)	5	5	31, 43, 132, 178	0
9	I	72/73 (98%)	0.44	7 (9%)	7	9	30, 46, 114, 194	0
9	V	72/73 (98%)	0.41	7 (9%)	7	9	30, 56, 98, 182	0
10	J	57/57 (100%)	-0.05	4 (7%)	16	18	28, 37, 78, 102	0
10	W	57/57 (100%)	-0.07	3 (5%)	26	29	28, 39, 80, 144	0
11	K	49/49 (100%)	-0.34	0	100	100	30, 37, 59, 72	0
11	X	49/49 (100%)	-0.08	0	100	100	36, 47, 84, 104	0
12	L	46/46 (100%)	-0.16	2 (4%)	35	38	24, 29, 50, 115	0
12	Y	46/46 (100%)	-0.13	2 (4%)	35	38	29, 34, 69, 209	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	41/41 (100%)	-0.21	1 (2%) 59 61	26, 29, 58, 81	0
13	Z	41/41 (100%)	-0.03	2 (4%) 29 32	33, 38, 77, 122	0
All	All	3530/3540 (99%)	-0.13	106 (3%) 50 53	20, 31, 76, 209	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	17.4
4	Q	5	VAL	14.0
4	Q	6	VAL	13.9
7	T	8	HIS	11.6
12	Y	47	LYS	9.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.45	0.42	261,280,298,300	0
9	SAC	I	1	9/10	0.83	0.18	123,141,157,179	0
1	FME	A	1	10/11	0.96	0.10	34,45,69,100	0
2	FME	O	1	10/11	0.97	0.07	34,36,42,117	0
1	FME	N	1	10/11	0.97	0.09	35,42,79,80	0
2	FME	B	1	10/11	0.98	0.08	27,30,35,81	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
26	DMU	X	101	22/33	0.25	0.33	49,75,84,89	0
26	DMU	G	105	21/33	0.29	0.23	53,70,81,87	0
26	DMU	K	101	22/33	0.32	0.32	40,67,83,84	0
26	DMU	K	102	22/33	0.36	0.34	46,73,82,87	0
26	DMU	X	102	22/33	0.43	0.30	62,71,84,89	0
26	DMU	P	316	22/33	0.46	0.21	50,68,84,87	0
26	DMU	X	103	22/33	0.47	0.35	61,72,82,86	0
26	DMU	C	311	33/33	0.54	0.26	53,68,90,99	0
24	PEK	P	305	46/53	0.67	0.26	48,75,102,117	0
25	CDL	G	101	89/100	0.67	0.28	51,77,107,188	0
21	EDO	S	107	4/4	0.67	0.28	52,58,59,63	0
26	DMU	L	101	18/33	0.67	0.18	46,65,84,84	0
27	PSC	E	201	52/52	0.67	0.34	45,77,123,221	0
24	PEK	T	101	49/53	0.69	0.33	47,76,117,205	0
20	PGV	P	307	51/51	0.69	0.25	42,75,109,197	0
19	TGL	O	302	63/63	0.70	0.19	49,71,97,104	0
25	CDL	T	102	80/100	0.71	0.29	42,78,116,206	0
23	CHD	W	101	29/29	0.72	0.33	60,74,91,109	0
24	PEK	C	304	44/53	0.72	0.26	47,74,99,130	0
27	PSC	O	304	51/52	0.72	0.26	43,74,116,204	0
25	CDL	Y	101	87/100	0.73	0.26	38,78,116,159	0
26	DMU	P	310	33/33	0.74	0.21	61,75,97,110	0
26	DMU	P	311	33/33	0.74	0.28	57,85,99,101	0
26	DMU	P	312	33/33	0.74	0.26	38,75,97,106	0
20	PGV	Q	201	51/51	0.75	0.27	47,72,111,195	0
20	PGV	C	307	47/51	0.75	0.23	39,73,103,206	0
26	DMU	K	103	17/33	0.75	0.27	55,70,77,89	0
26	DMU	P	315	33/33	0.75	0.26	41,67,84,90	0
21	EDO	S	108	4/4	0.75	0.11	49,55,62,64	0
25	CDL	P	308	76/100	0.76	0.22	31,74,108,157	0
25	CDL	C	308	86/100	0.77	0.21	29,73,103,171	0
17	NA	P	302	1/1	0.79	0.08	38,38,38,38	0
26	DMU	J	101	33/33	0.79	0.25	31,70,97,106	0
19	TGL	D	201	48/63	0.81	0.14	30,59,91,127	0
24	PEK	P	303	22/53	0.81	0.11	51,60,86,98	0
23	CHD	P	309	29/29	0.82	0.18	47,59,82,103	0
21	EDO	S	104	4/4	0.83	0.15	43,45,55,57	0
19	TGL	O	301	63/63	0.84	0.18	37,74,90,106	0
23	CHD	J	102	29/29	0.84	0.24	50,74,103,112	0
23	CHD	C	309	29/29	0.86	0.18	45,58,84,85	0
19	TGL	A	607	63/63	0.86	0.20	32,62,96,123	0
20	PGV	A	608	46/51	0.86	0.21	33,67,110,193	0
21	EDO	B	308	4/4	0.87	0.18	31,34,38,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	DMU	Z	101	33/33	0.87	0.10	38,46,63,74	0
29	PO4	U	102	5/5	0.87	0.26	53,58,65,65	0
19	TGL	B	301	62/63	0.88	0.14	28,65,88,98	0
21	EDO	A	614	4/4	0.88	0.14	37,39,42,46	0
21	EDO	G	104	4/4	0.89	0.14	42,62,72,77	0
21	EDO	B	306	4/4	0.89	0.14	29,45,56,75	0
26	DMU	M	101	33/33	0.89	0.09	33,39,56,71	0
21	EDO	A	610	4/4	0.90	0.10	29,29,30,31	0
21	EDO	A	613	4/4	0.90	0.12	39,39,41,56	0
21	EDO	O	308	4/4	0.91	0.17	38,46,48,51	0
21	EDO	N	614	4/4	0.92	0.08	38,41,41,41	0
21	EDO	A	616	4/4	0.92	0.11	38,38,40,41	0
21	EDO	P	314	4/4	0.92	0.15	47,58,60,61	0
21	EDO	N	610	4/4	0.93	0.13	31,50,52,52	0
21	EDO	U	101	4/4	0.93	0.34	35,37,62,63	0
21	EDO	Y	102	4/4	0.93	0.20	53,55,61,65	0
21	EDO	N	612	4/4	0.93	0.09	42,42,45,46	0
21	EDO	A	617	4/4	0.93	0.12	31,37,41,65	0
21	EDO	O	306	4/4	0.93	0.12	34,36,42,46	0
18	CYN	N	606[A]	2/2	0.94	0.22	26,26,26,28	2
18	CYN	N	606[C]	2/2	0.94	0.22	20,20,20,24	2
17	NA	C	302	1/1	0.94	0.09	38,38,38,38	0
21	EDO	D	202	4/4	0.94	0.11	42,45,53,61	0
23	CHD	P	301	29/29	0.94	0.07	27,30,34,35	0
21	EDO	E	203	4/4	0.94	0.08	49,50,54,58	0
21	EDO	B	304	4/4	0.95	0.20	35,39,40,43	0
21	EDO	B	305	4/4	0.95	0.26	30,31,38,43	0
21	EDO	S	105	4/4	0.95	0.09	28,30,31,33	0
17	NA	N	605	1/1	0.95	0.06	29,29,29,29	0
21	EDO	N	615	4/4	0.95	0.08	38,39,40,43	0
21	EDO	T	104	4/4	0.95	0.16	37,44,47,59	0
21	EDO	F	103	4/4	0.95	0.08	36,36,40,55	0
21	EDO	O	307	4/4	0.95	0.08	35,42,48,60	0
23	CHD	C	301	29/29	0.95	0.07	25,30,35,36	0
21	EDO	B	307	4/4	0.95	0.10	25,25,26,28	0
23	CHD	G	102	29/29	0.95	0.07	26,29,33,41	0
21	EDO	O	305	4/4	0.96	0.08	29,30,31,31	0
21	EDO	T	103	4/4	0.96	0.07	31,31,36,37	0
21	EDO	Q	202	4/4	0.96	0.14	30,49,53,65	0
21	EDO	C	310	4/4	0.96	0.06	29,30,30,31	0
21	EDO	A	612	4/4	0.96	0.19	41,53,56,68	0
24	PEK	C	303	51/53	0.96	0.12	27,43,85,92	0

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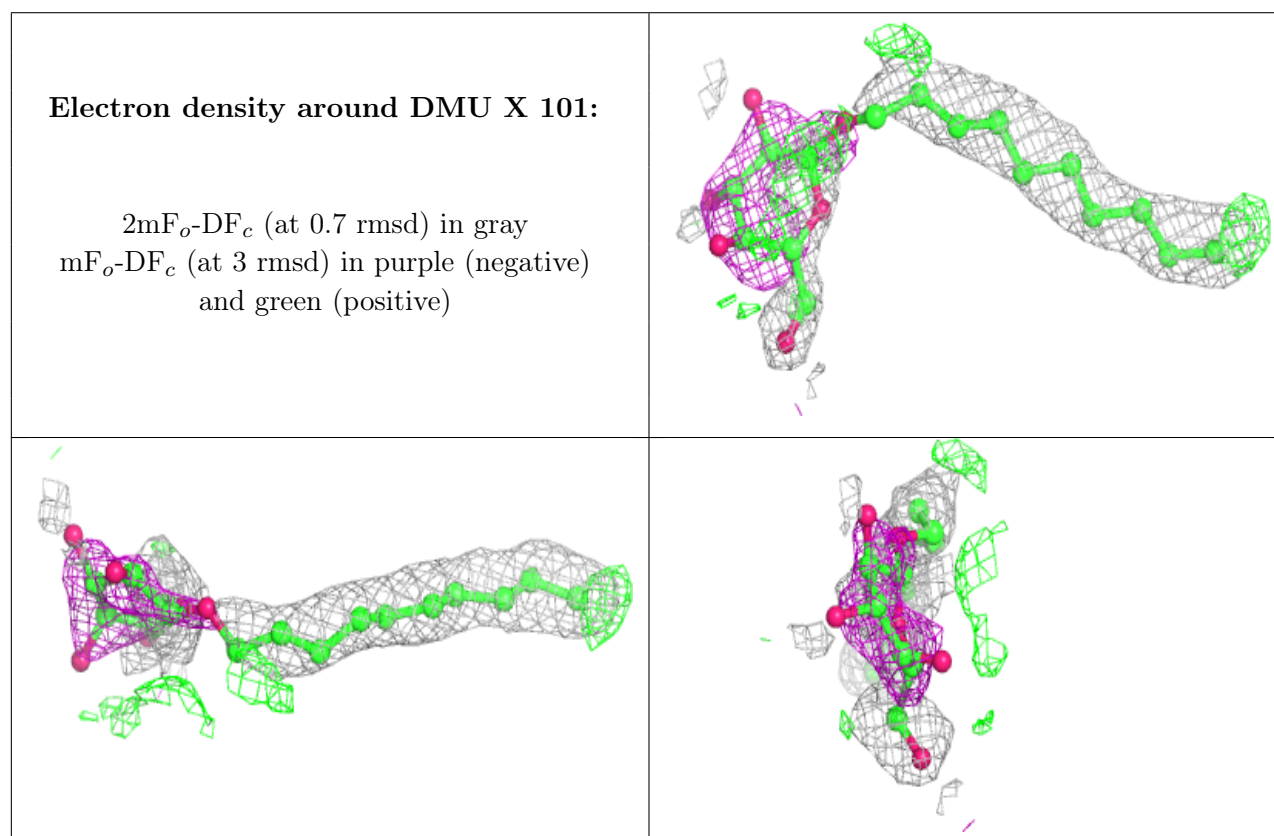
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	S	106	4/4	0.96	0.35	40,49,50,52	0
21	EDO	N	611	4/4	0.96	0.08	37,38,41,44	0
24	PEK	P	304	53/53	0.96	0.11	28,46,85,94	0
20	PGV	N	607	51/51	0.97	0.10	22,29,75,83	0
21	EDO	F	104	4/4	0.97	0.07	31,31,31,32	0
20	PGV	P	306	45/51	0.97	0.09	24,29,58,76	0
21	EDO	N	608	4/4	0.97	0.10	28,29,30,31	0
21	EDO	N	609	4/4	0.97	0.07	26,27,29,30	0
20	PGV	C	306	51/51	0.97	0.09	23,29,83,91	0
21	EDO	P	313	4/4	0.97	0.11	33,35,38,38	0
20	PGV	C	305	51/51	0.97	0.10	22,28,72,81	0
21	EDO	A	615	4/4	0.97	0.18	32,48,68,71	0
23	CHD	B	303	29/29	0.97	0.07	26,29,38,54	0
21	EDO	R	201	4/4	0.97	0.08	38,40,41,43	0
21	EDO	S	103	4/4	0.97	0.07	33,34,37,38	0
14	HEA	A	601[C]	43/60	0.98	0.09	19,21,23,28	1
18	CYN	A	606[A]	2/2	0.98	0.25	24,24,24,25	2
18	CYN	A	606[C]	2/2	0.98	0.25	17,17,17,18	2
14	HEA	A	602[A]	60/60	0.98	0.10	17,22,37,43	51
21	EDO	N	613	4/4	0.98	0.14	32,34,35,39	0
14	HEA	A	602[C]	60/60	0.98	0.10	16,21,37,43	51
14	HEA	N	601[A]	60/60	0.98	0.08	21,25,32,35	18
21	EDO	A	609	4/4	0.98	0.14	29,33,34,38	0
14	HEA	N	601[B]	60/60	0.98	0.08	23,25,34,44	18
21	EDO	E	202	4/4	0.98	0.07	36,37,39,40	0
14	HEA	N	601[C]	43/60	0.98	0.08	23,25,27,28	1
14	HEA	N	602[A]	60/60	0.98	0.09	19,23,35,39	51
14	HEA	N	602[C]	60/60	0.98	0.09	19,24,35,39	51
21	EDO	G	103	4/4	0.98	0.06	30,32,33,36	0
14	HEA	A	601[A]	60/60	0.98	0.09	12,22,31,33	18
14	HEA	A	601[B]	60/60	0.98	0.09	19,22,30,46	18
21	EDO	S	102	4/4	0.99	0.08	24,24,24,26	0
16	MG	N	604	1/1	0.99	0.04	23,23,23,23	0
17	NA	A	605	1/1	0.99	0.05	25,25,25,25	0
21	EDO	A	611	4/4	0.99	0.09	23,24,24,27	0
28	ZN	F	101	1/1	0.99	0.13	29,29,29,29	0
21	EDO	F	102	4/4	0.99	0.07	23,24,24,25	0
15	CU	A	603	1/1	1.00	0.13	23,23,23,23	0
15	CU	N	603	1/1	1.00	0.12	25,25,25,25	0
16	MG	A	604	1/1	1.00	0.07	22,22,22,22	0
22	CUA	B	302	2/2	1.00	0.12	24,24,24,24	0
28	ZN	S	101	1/1	1.00	0.13	28,28,28,28	0

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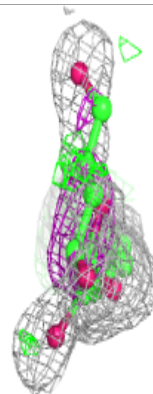
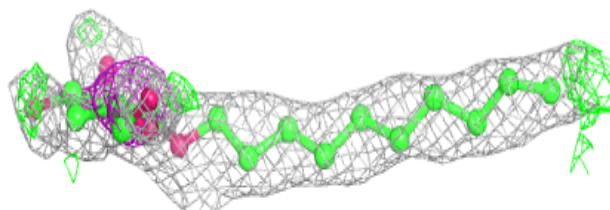
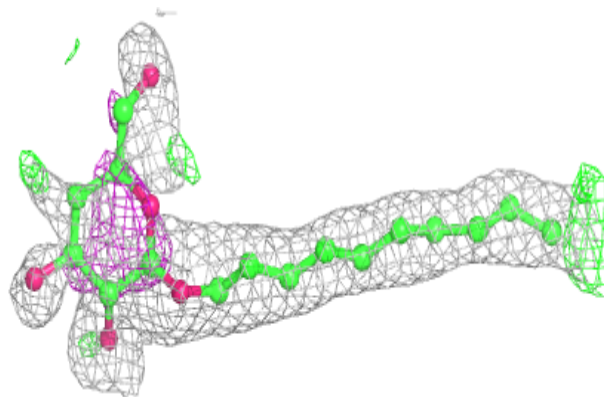
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CUA	O	303	2/2	1.00	0.10	27,27,27,28	0

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.

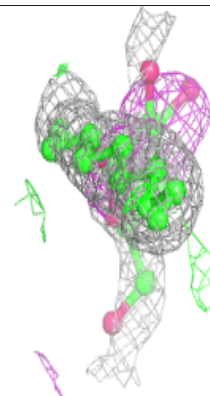
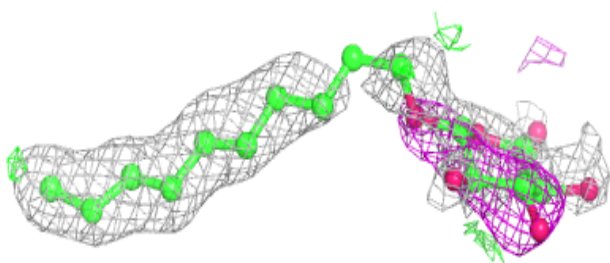
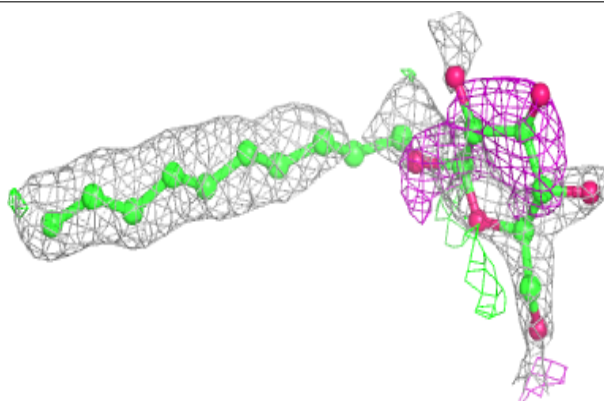


Electron density around DMU G 105:

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

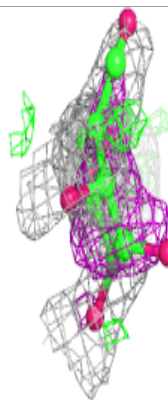
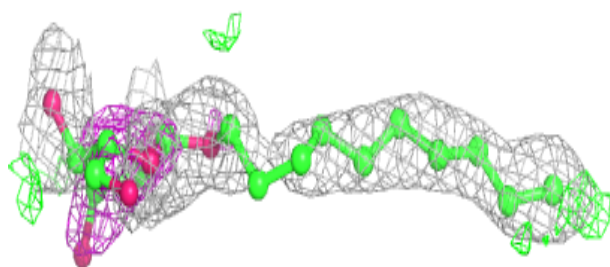
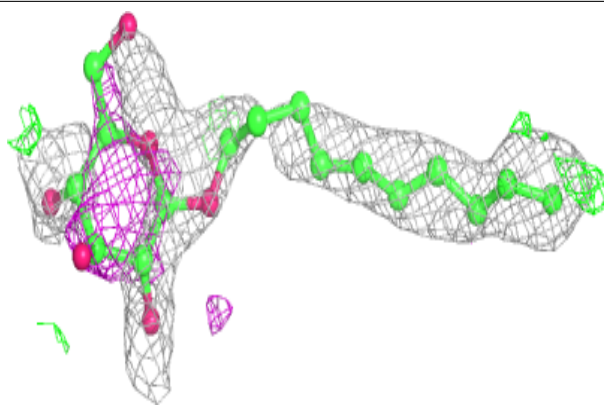
**Electron density around DMU K 101:**

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

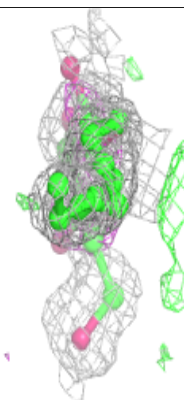
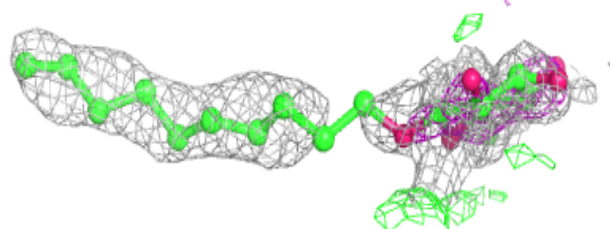
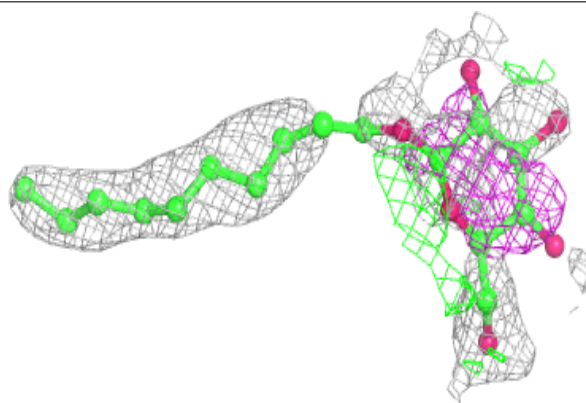


Electron density around DMU K 102:

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

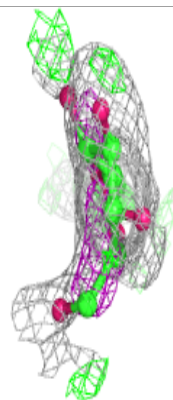
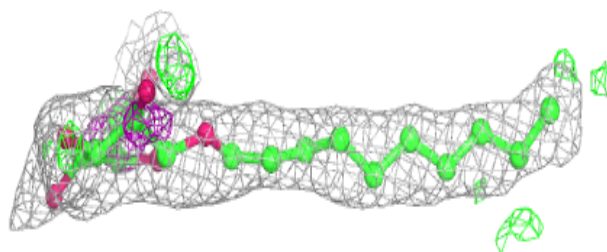
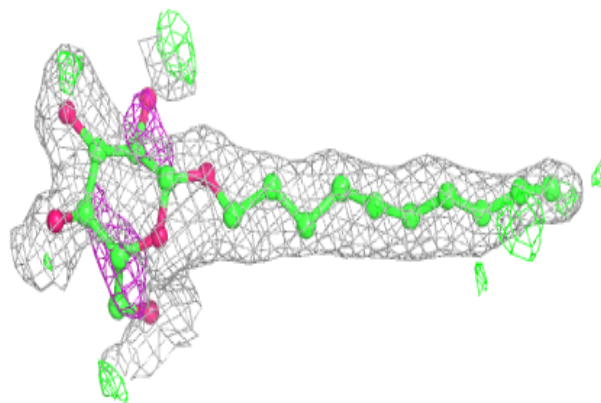
**Electron density around DMU X 102:**

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

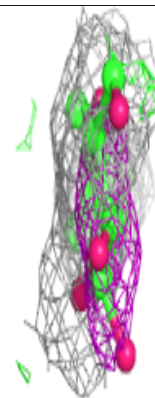
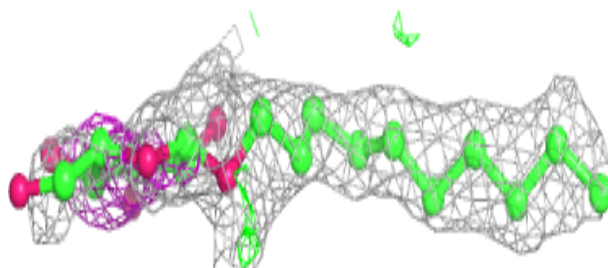
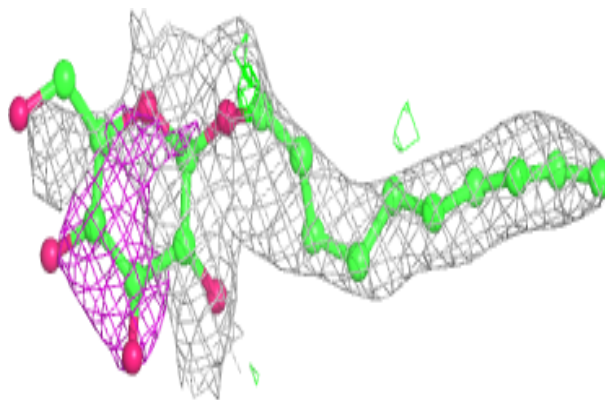


Electron density around DMU P 316:

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

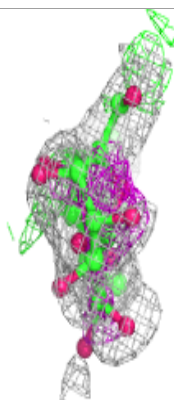
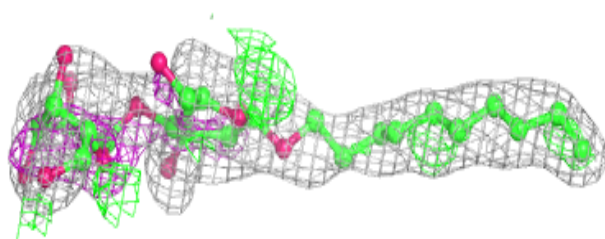
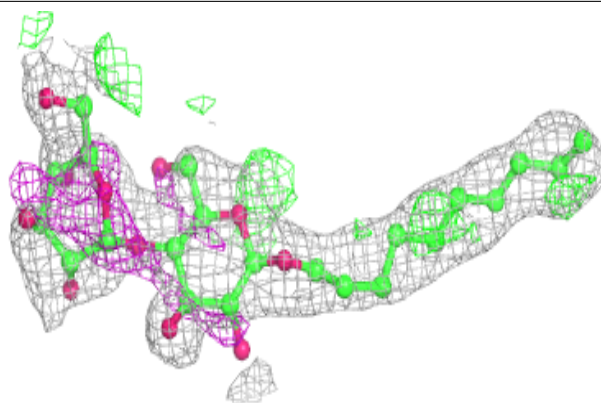
**Electron density around DMU X 103:**

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



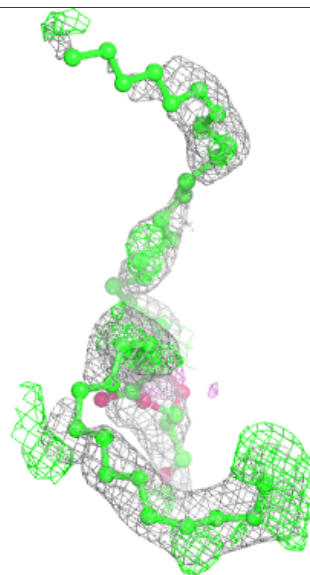
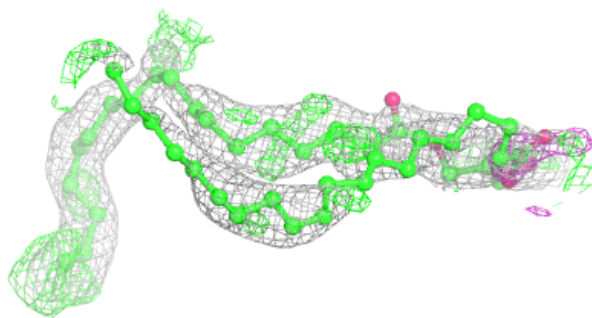
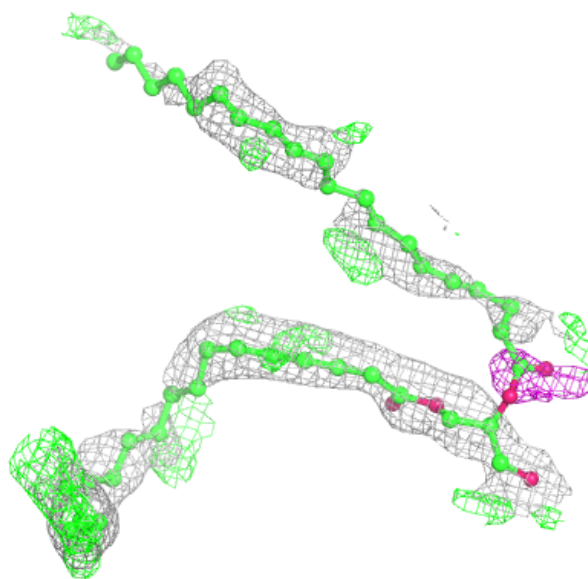
Electron density around DMU C 311:

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



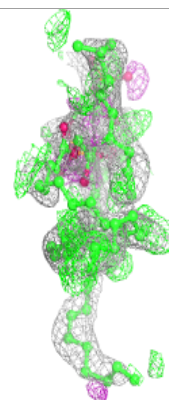
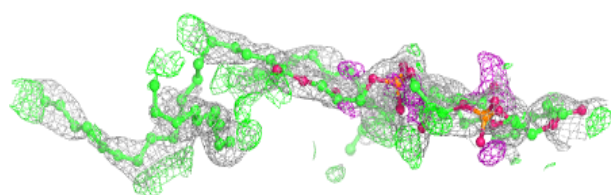
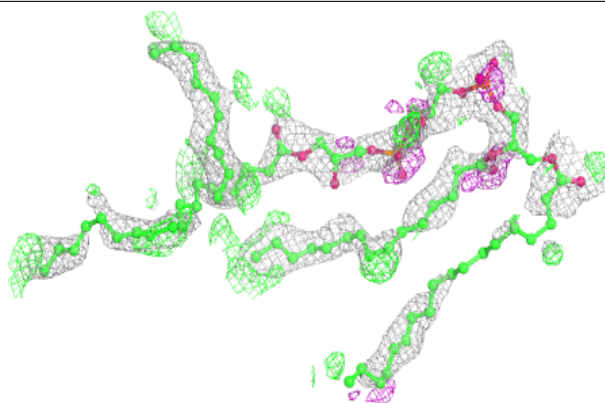
Electron density around PEK P 305:

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

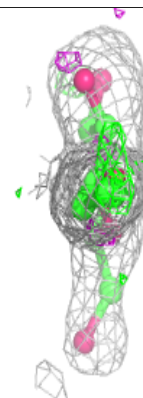
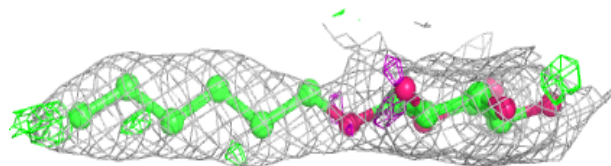
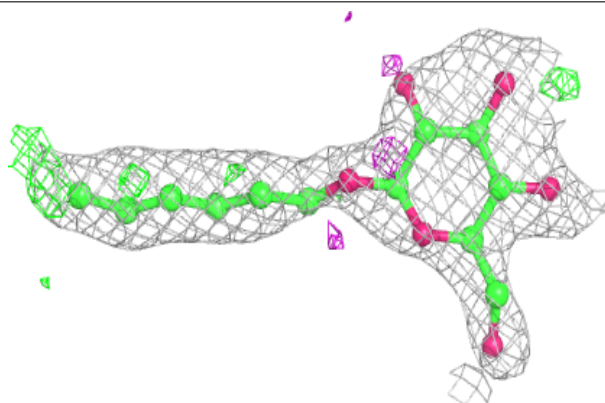


Electron density around CDL G 101:

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

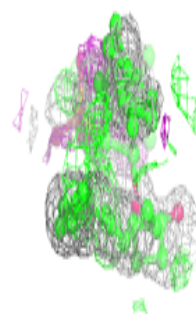
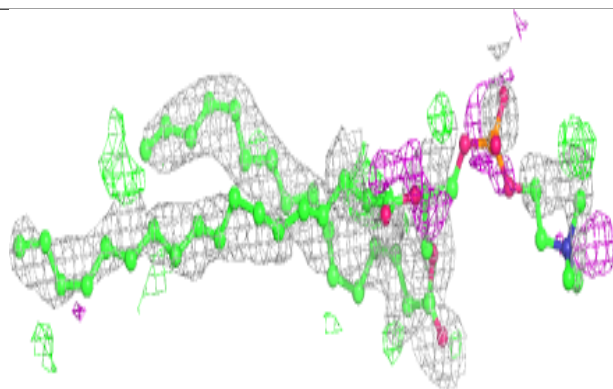
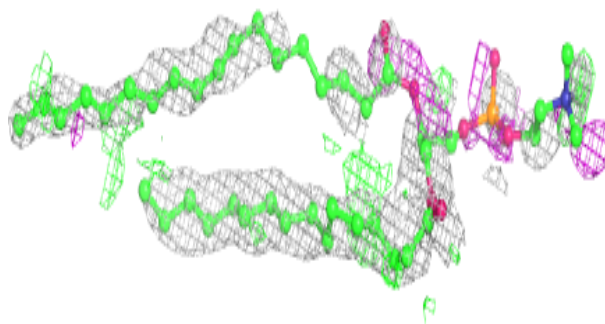
**Electron density around DMU L 101:**

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



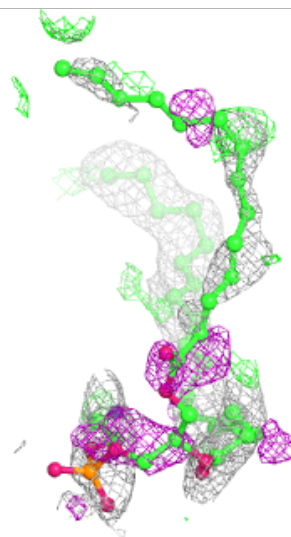
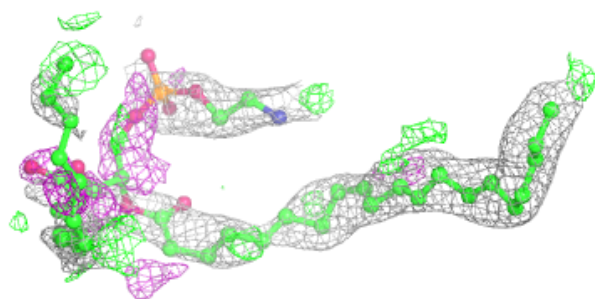
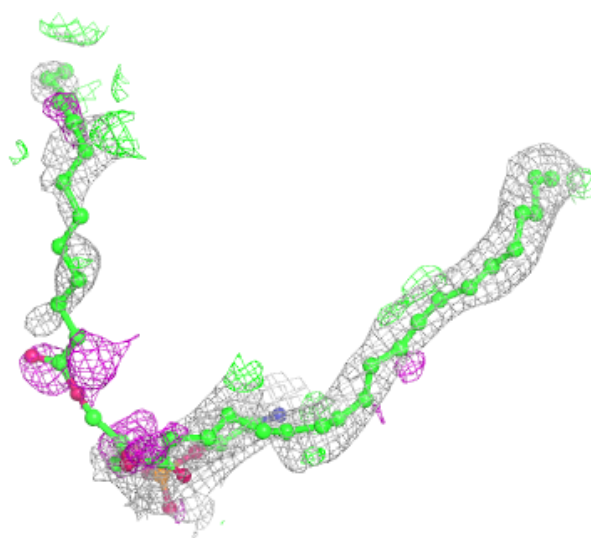
Electron density around PSC E 201:

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



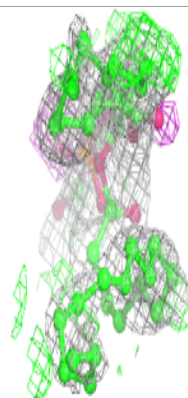
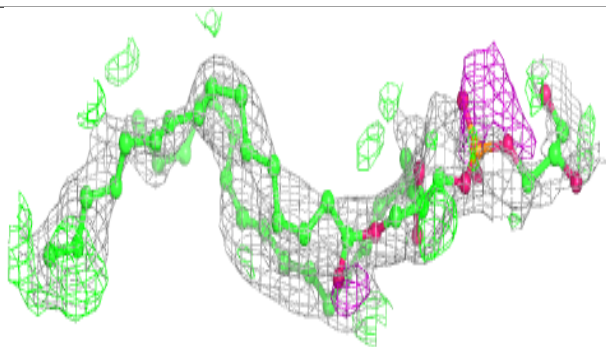
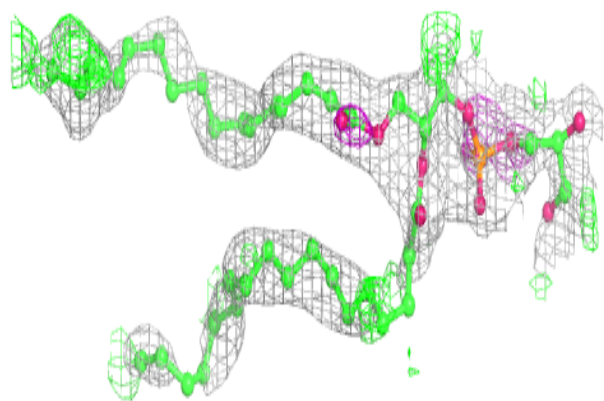
Electron density around PEK T 101:

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

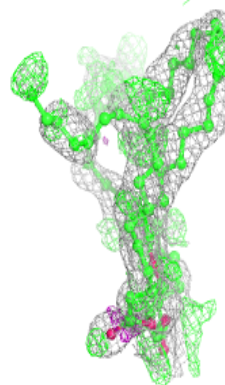
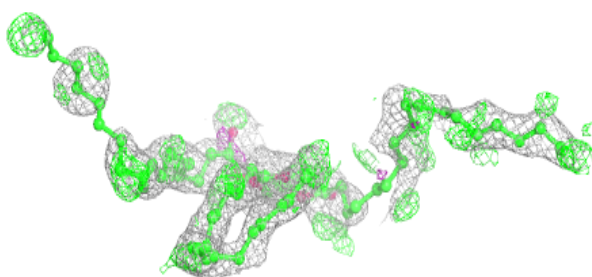
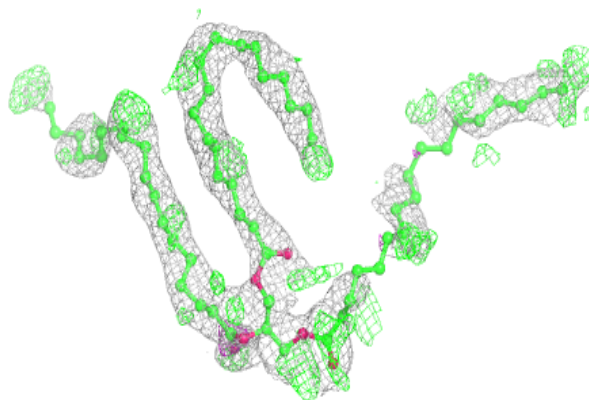


Electron density around PGV P 307:

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

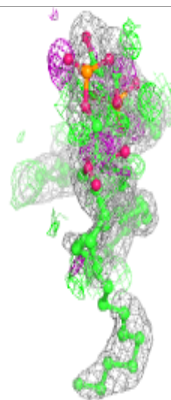
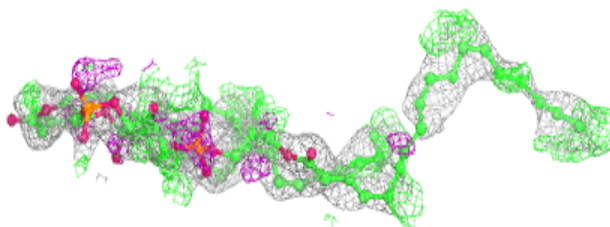
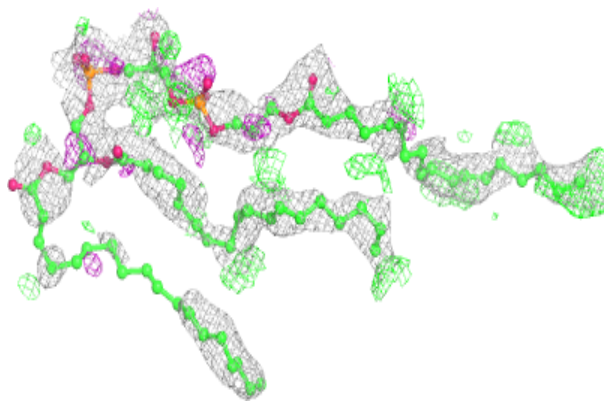
**Electron density around TGL O 302:**

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

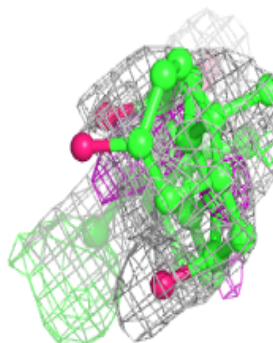
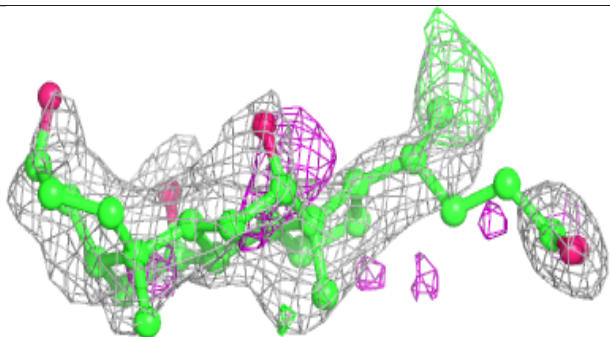
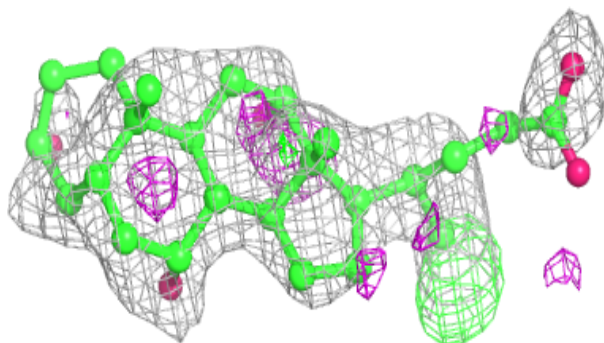


Electron density around CDL T 102:

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

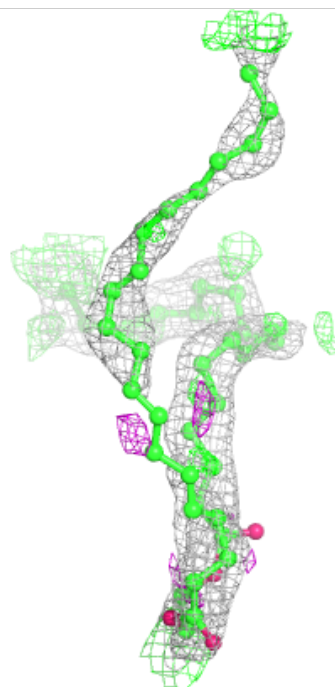
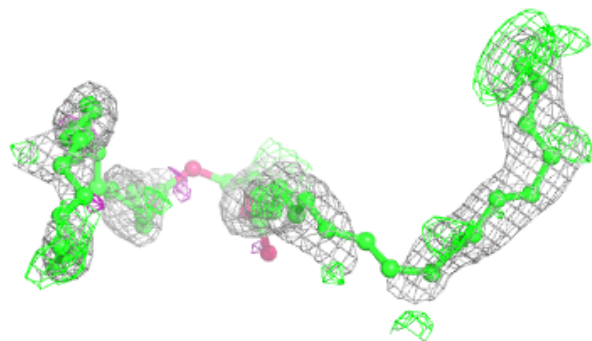
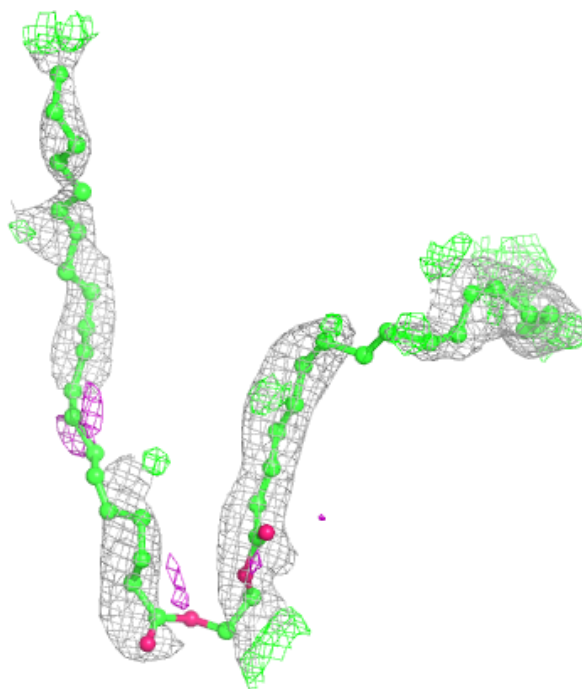
**Electron density around CHD W 101:**

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



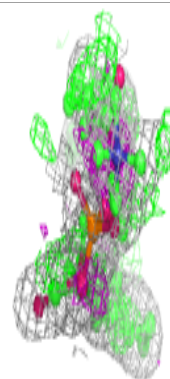
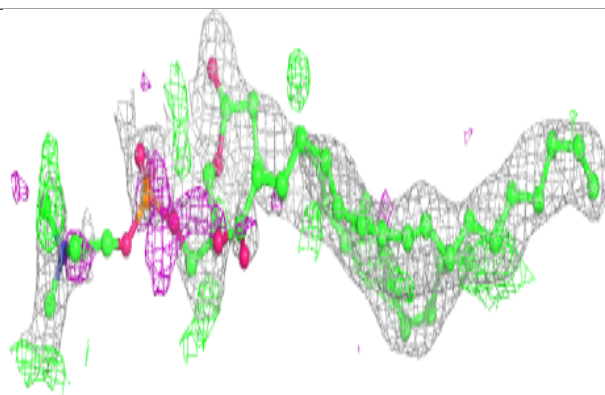
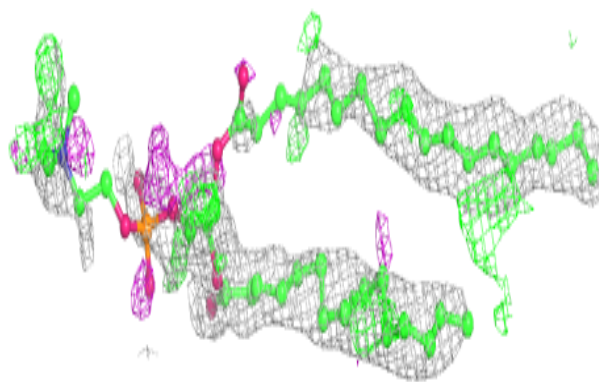
Electron density around PEK C 304:

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



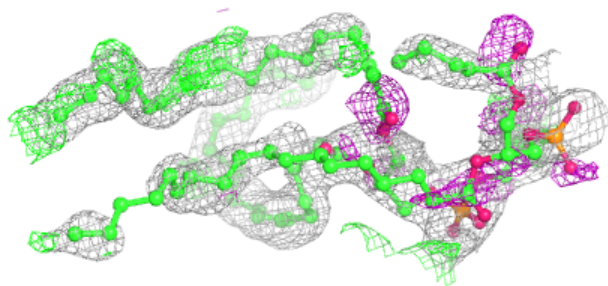
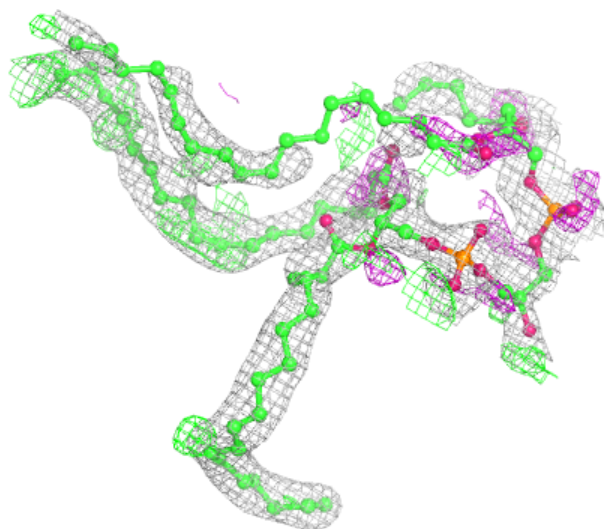
Electron density around PSC O 304:

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



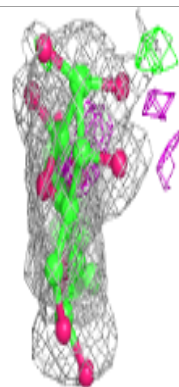
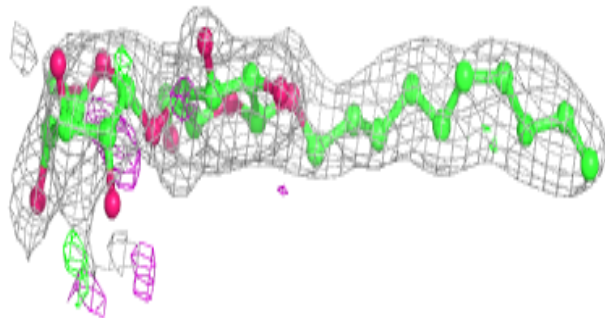
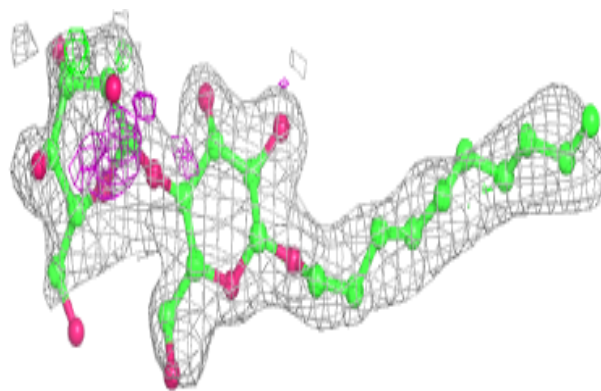
Electron density around CDL Y 101:

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

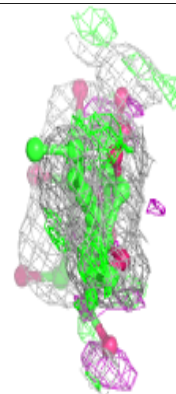
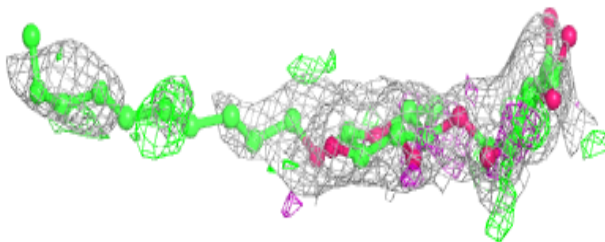
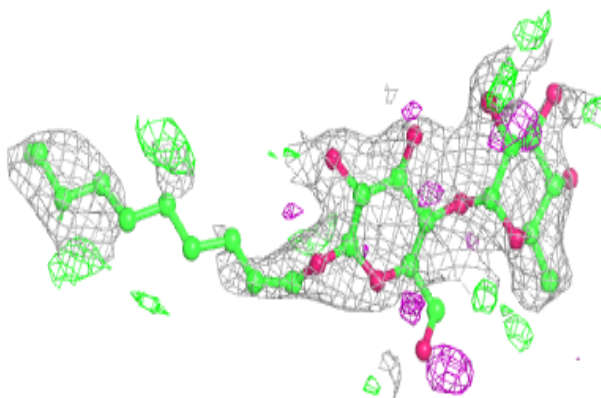


Electron density around DMU P 310:

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

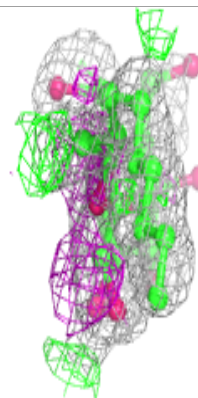
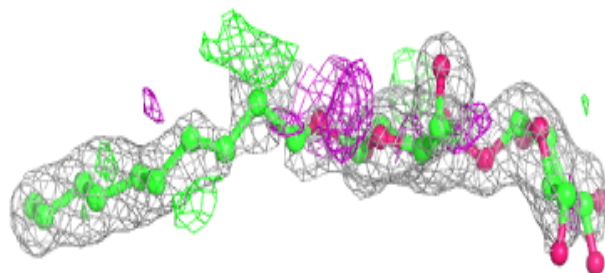
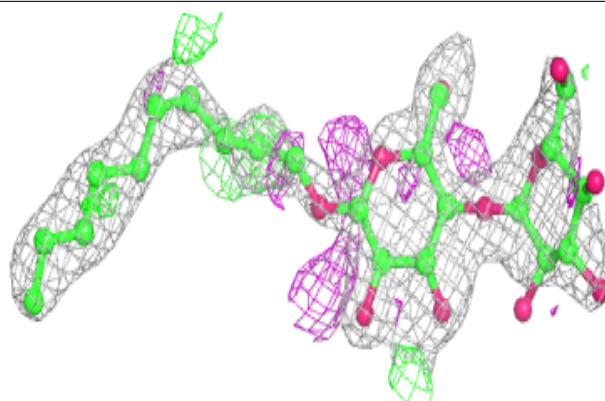
**Electron density around DMU P 311:**

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

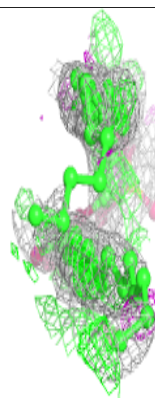
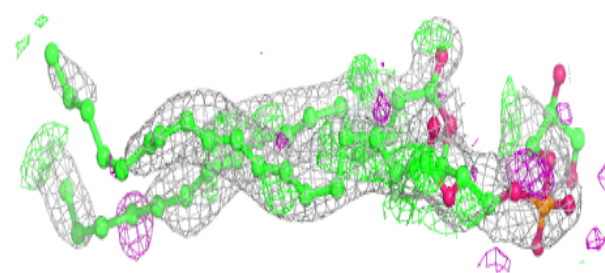
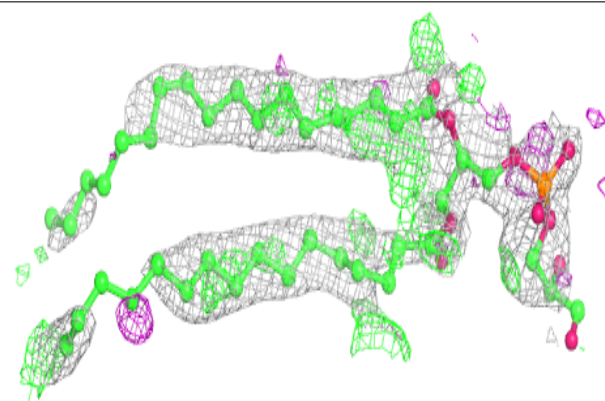


Electron density around DMU P 312:

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

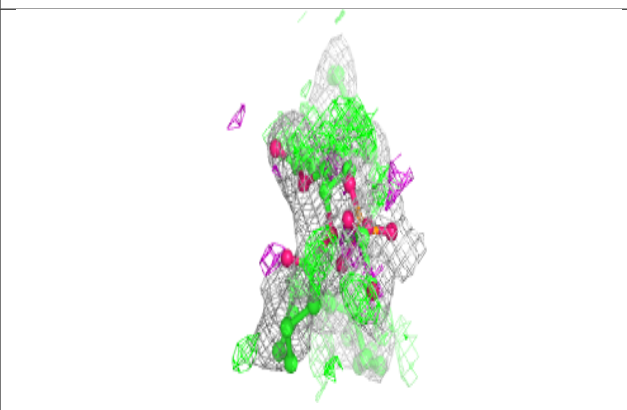
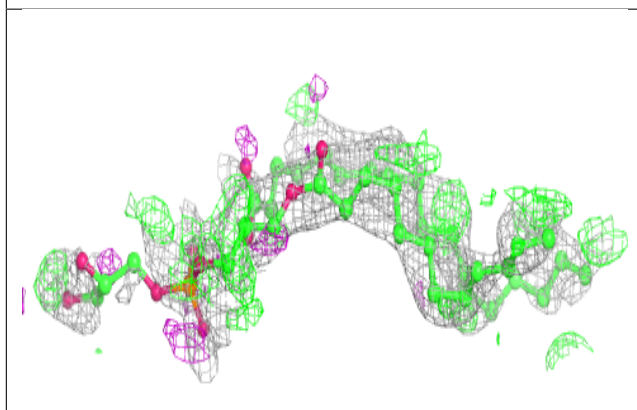
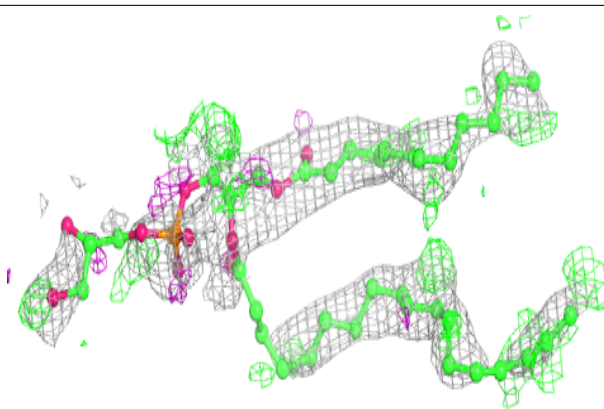
**Electron density around PGV Q 201:**

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

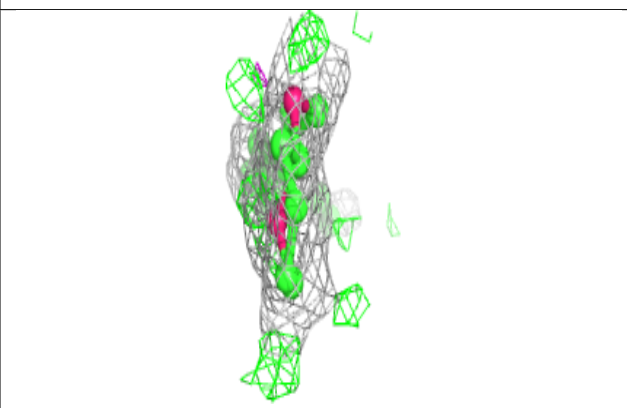
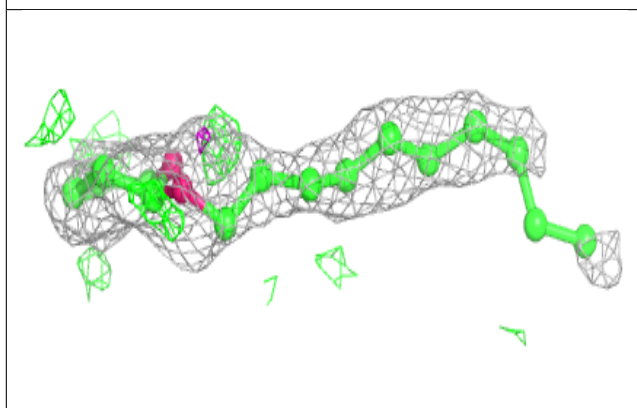
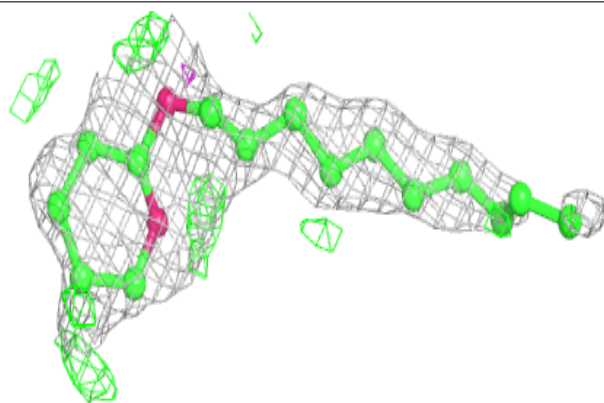


Electron density around PGV C 307:

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

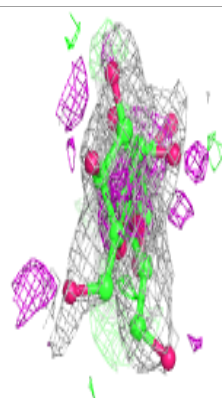
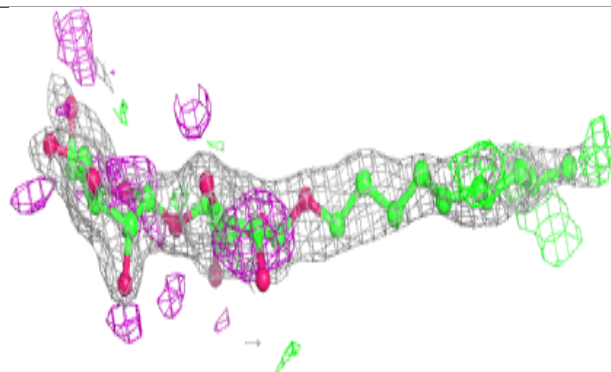
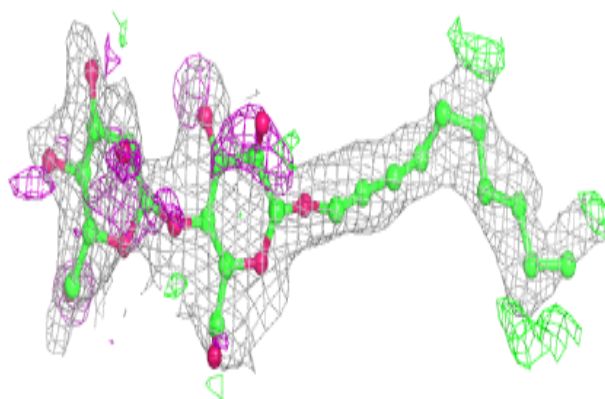
**Electron density around DMU K 103:**

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

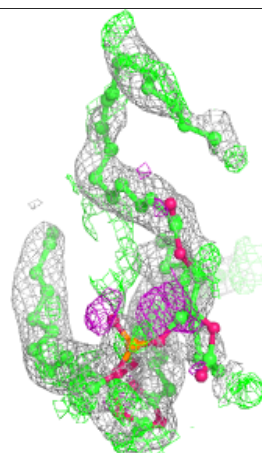
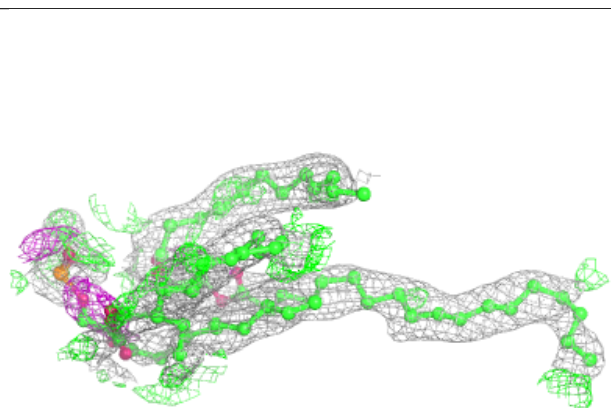
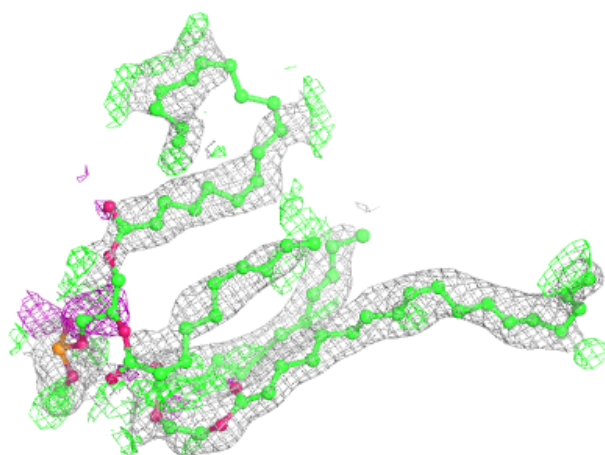


Electron density around DMU P 315:

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

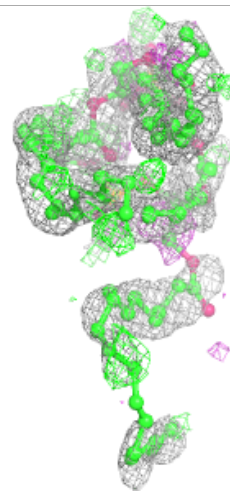
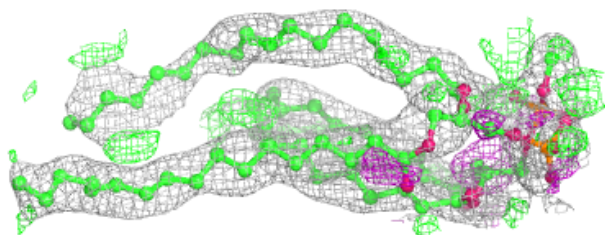
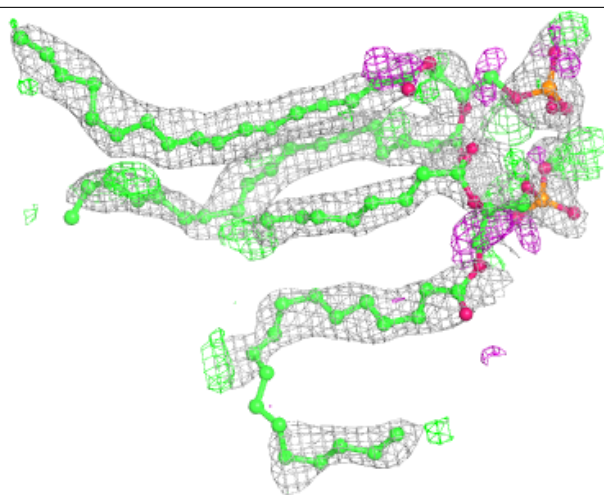
**Electron density around CDL P 308:**

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



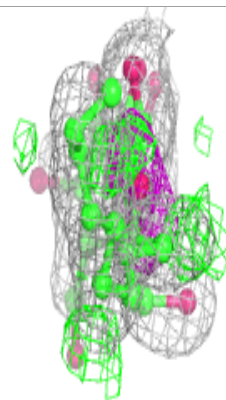
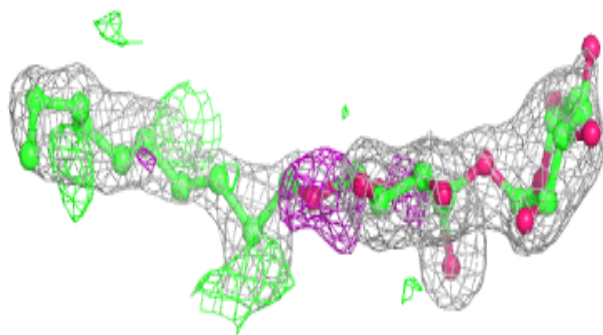
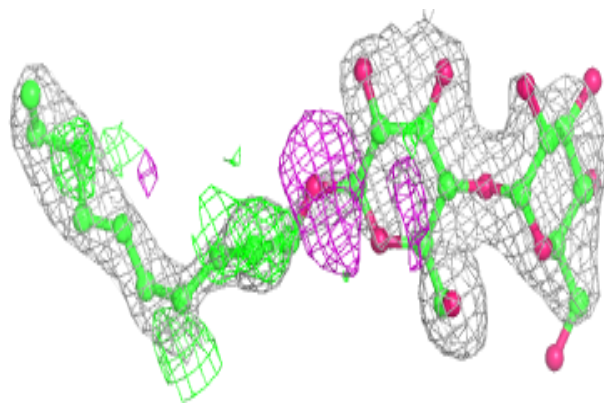
Electron density around CDL C 308:

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



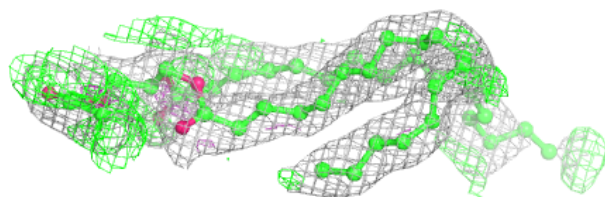
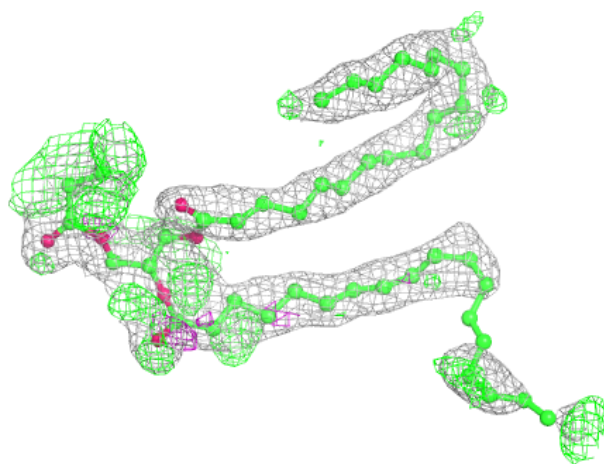
Electron density around DMU J 101:

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



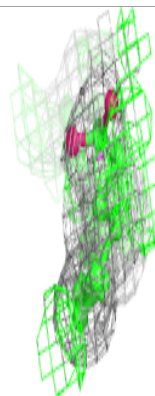
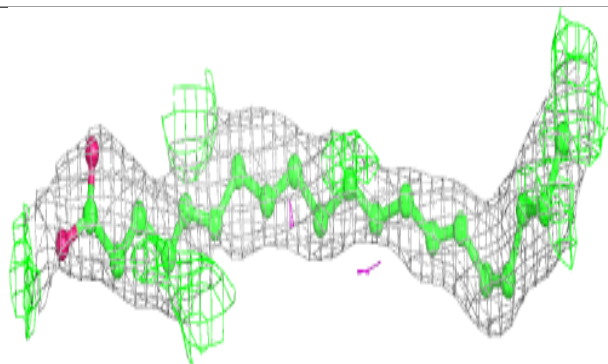
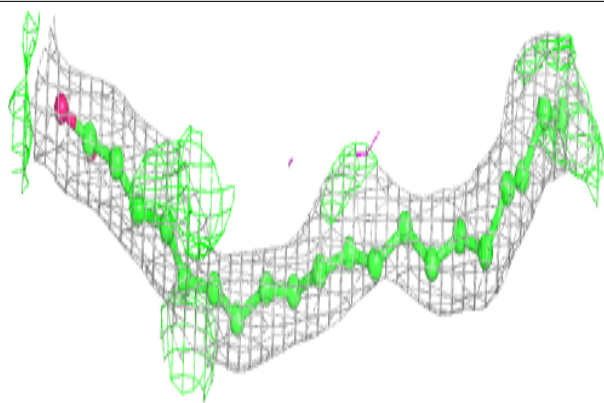
Electron density around TGL D 201:

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

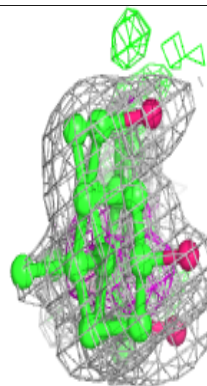
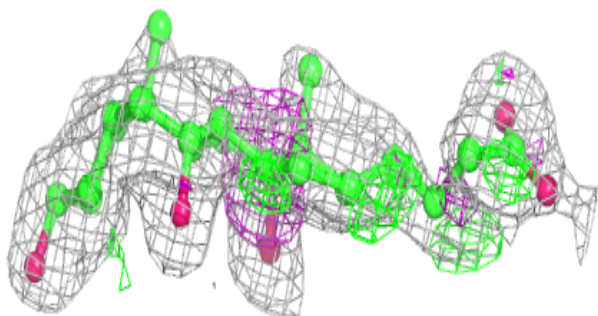
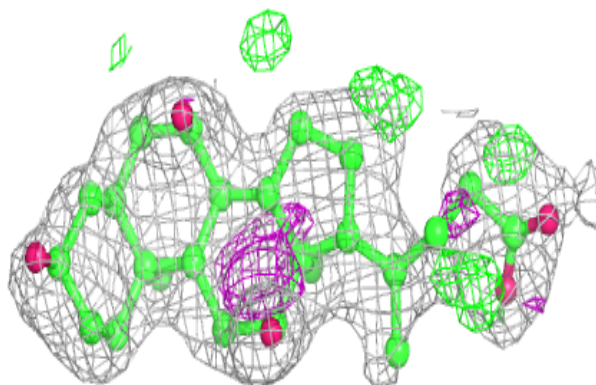


Electron density around PEK P 303:

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

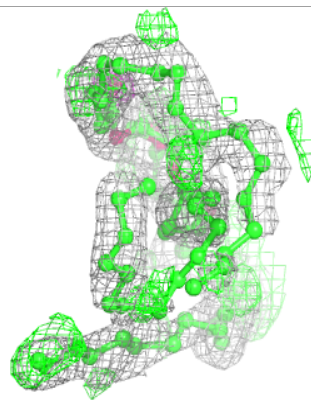
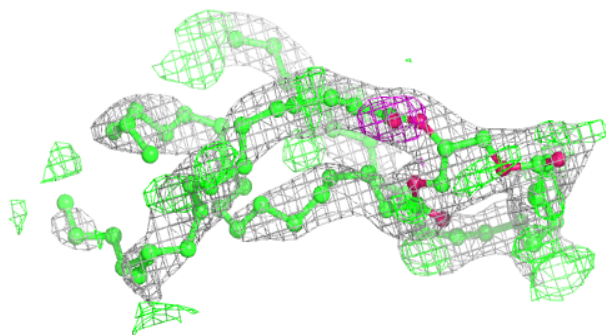
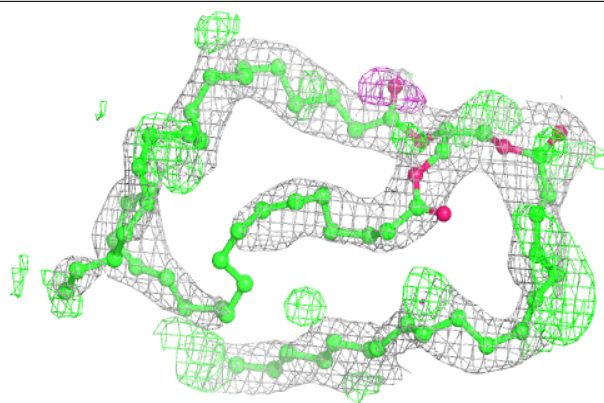
**Electron density around CHD P 309:**

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

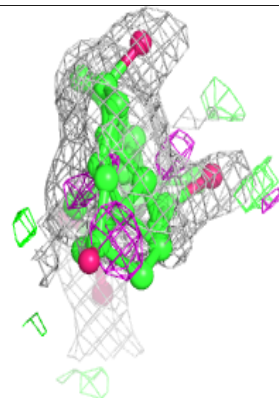
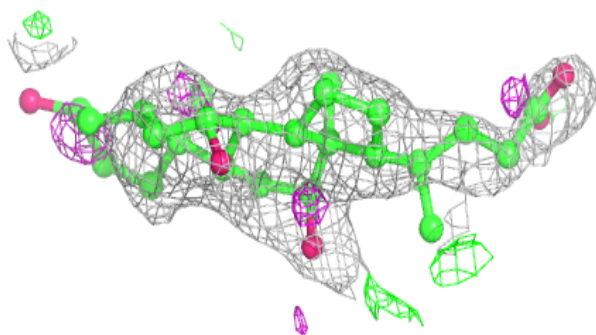
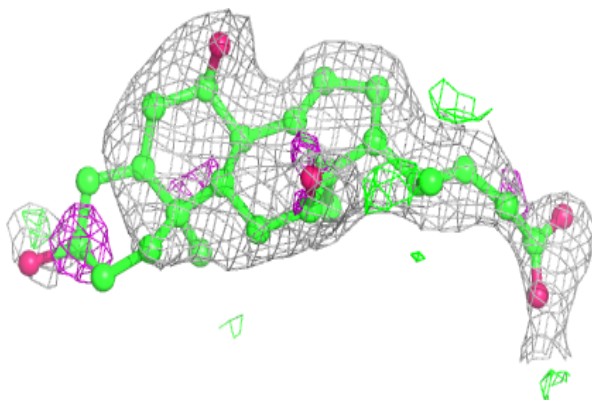


Electron density around TGL O 301:

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

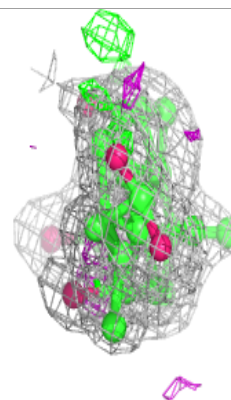
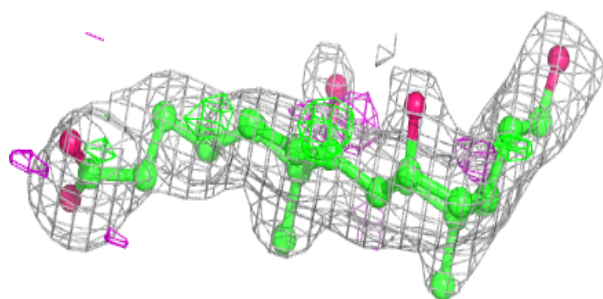
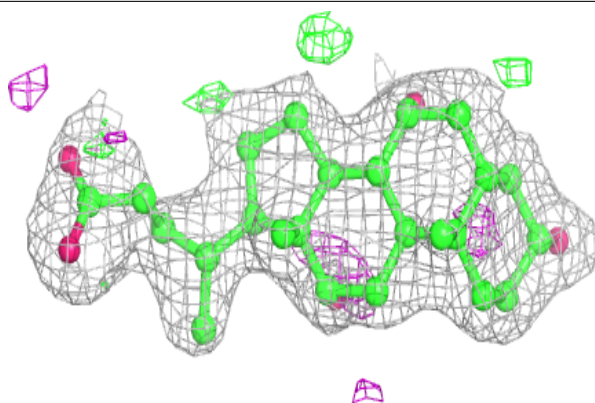
**Electron density around CHD J 102:**

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

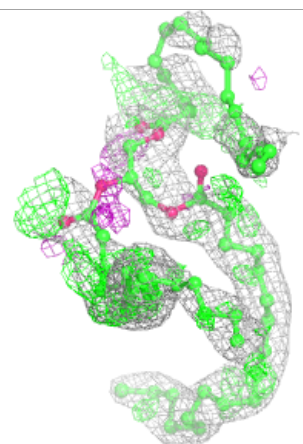
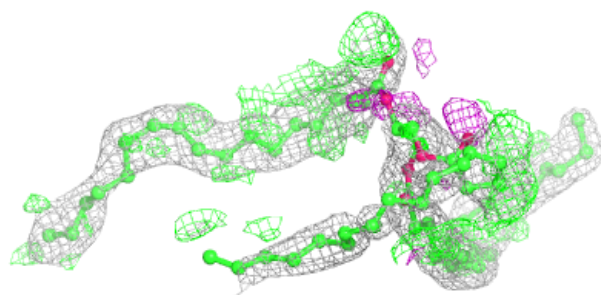
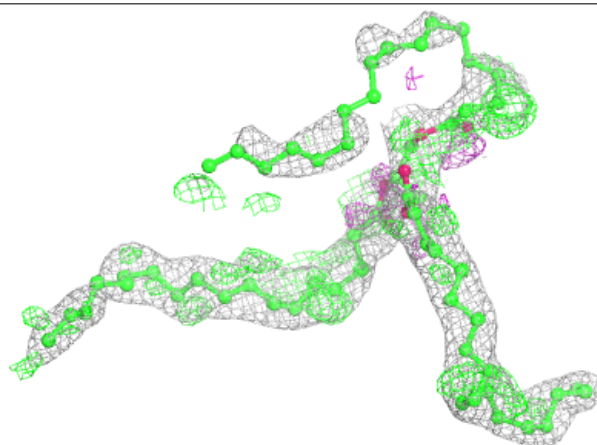


Electron density around CHD C 309:

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

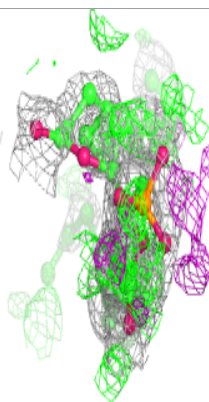
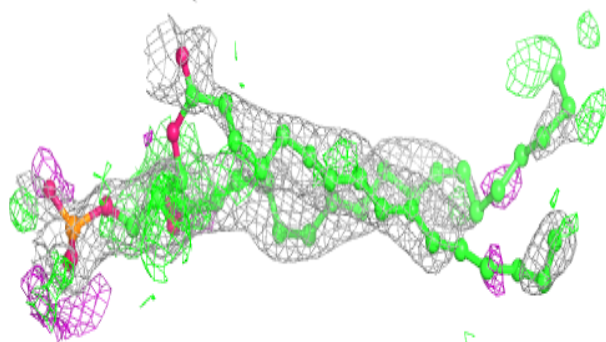
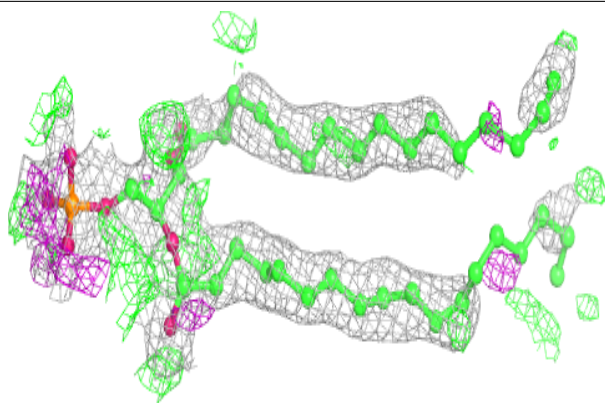
**Electron density around TGL A 607:**

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

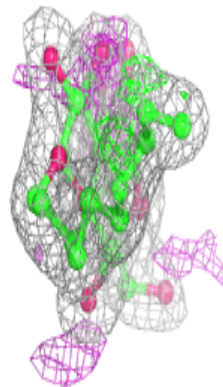
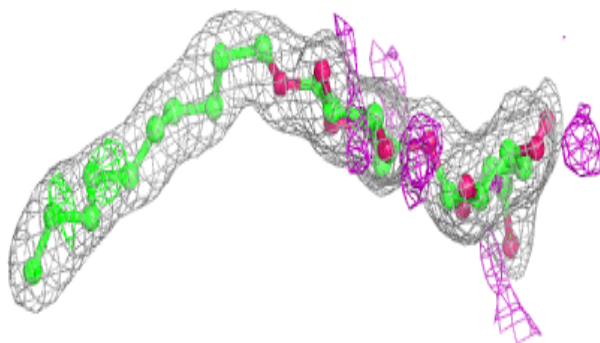
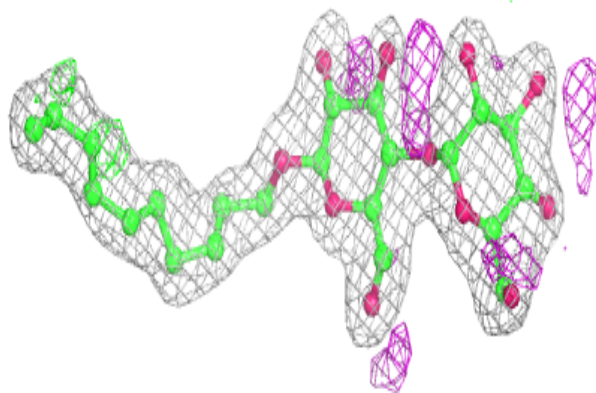


Electron density around PGV A 608:

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

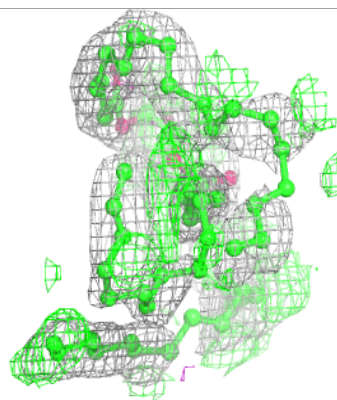
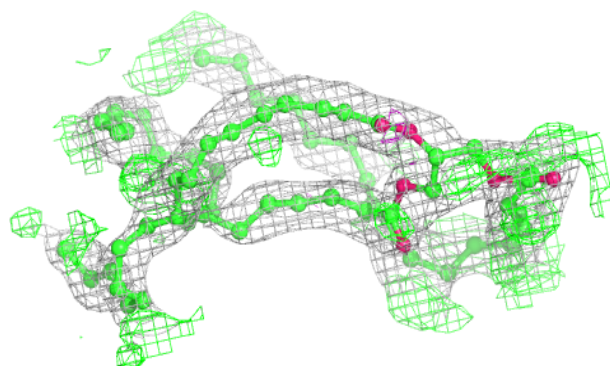
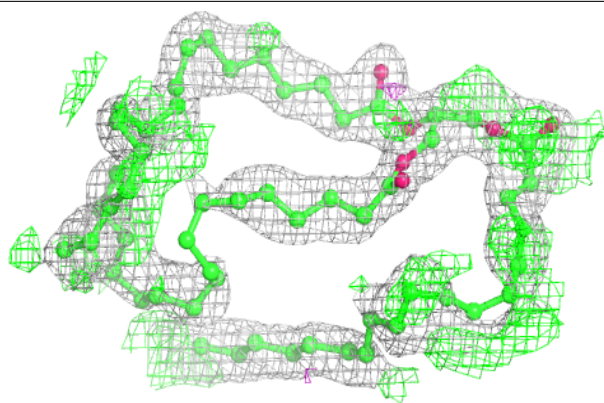
**Electron density around DMU Z 101:**

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

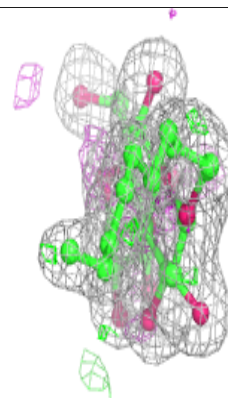
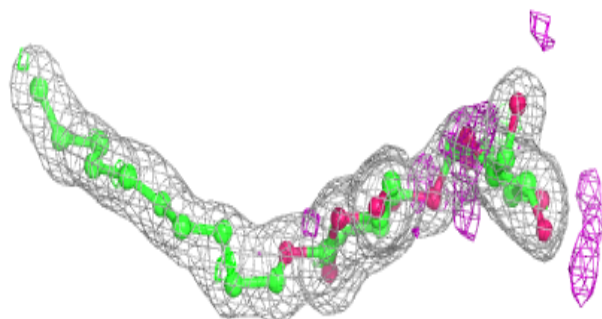
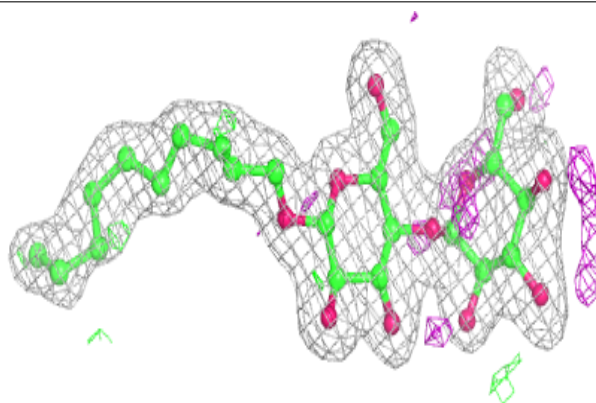


Electron density around TGL B 301:

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

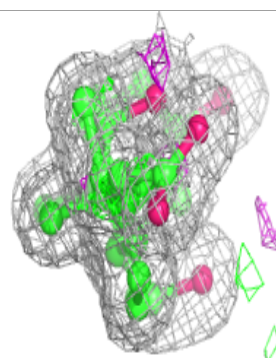
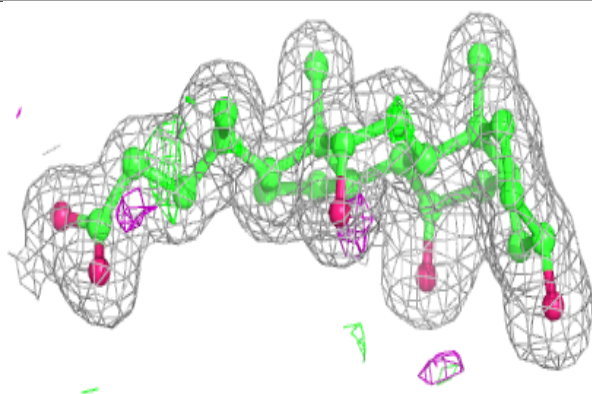
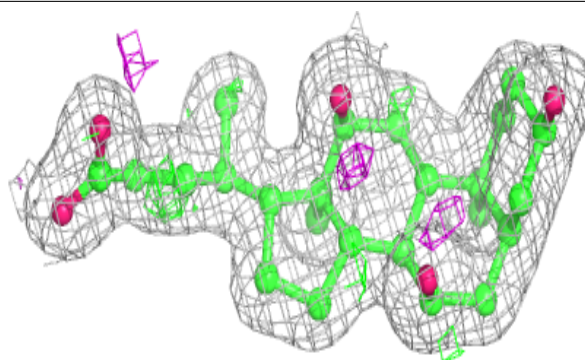
**Electron density around DMU M 101:**

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

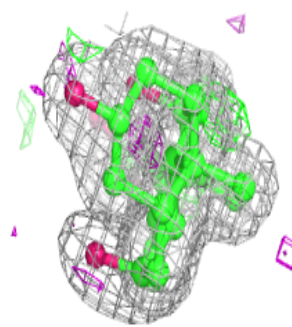
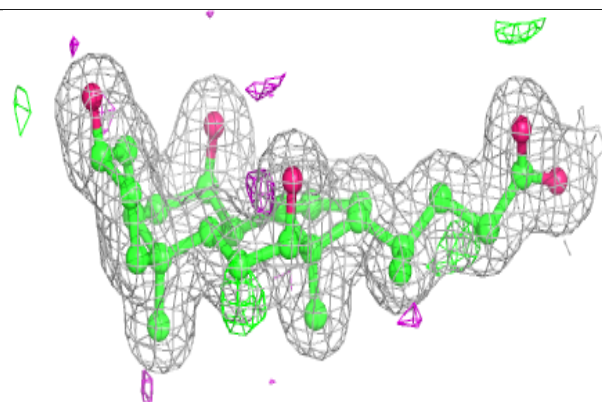
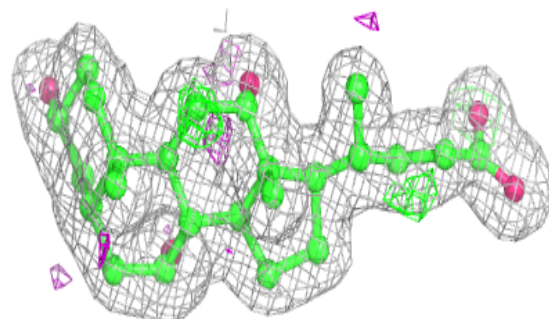


Electron density around CHD P 301:

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

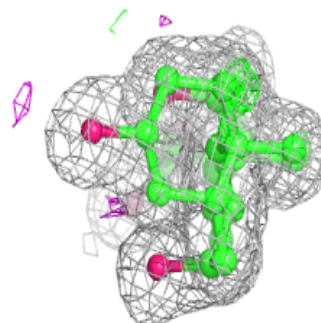
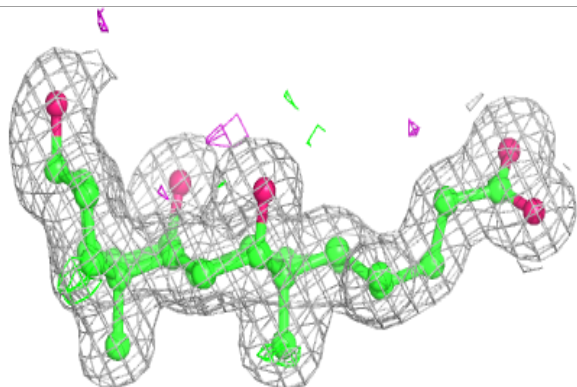
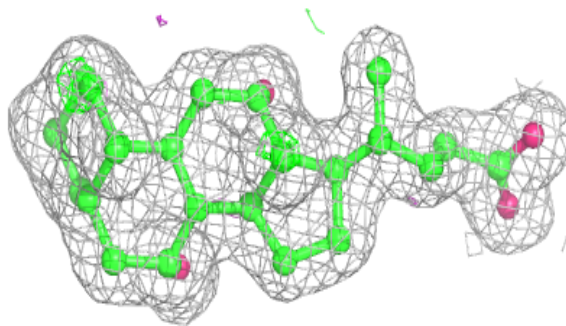
**Electron density around CHD C 301:**

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

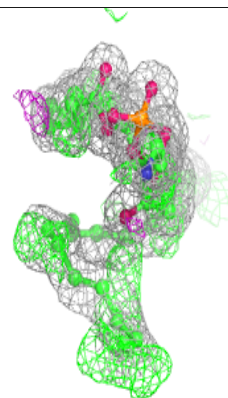
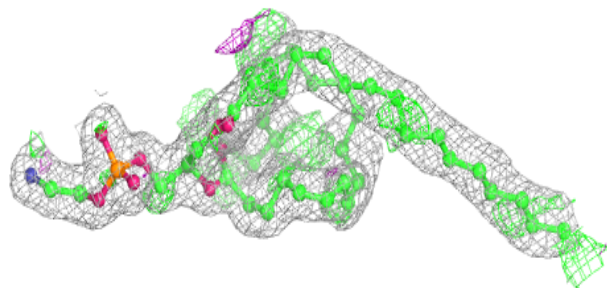
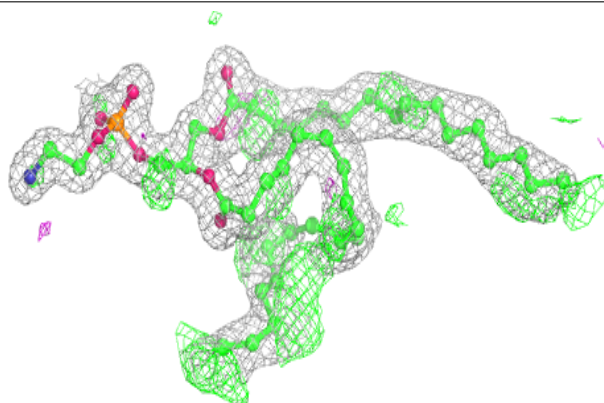


Electron density around CHD G 102:

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

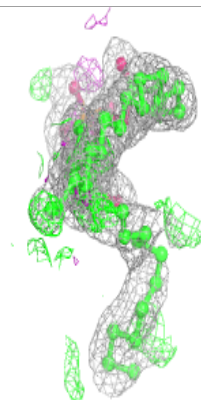
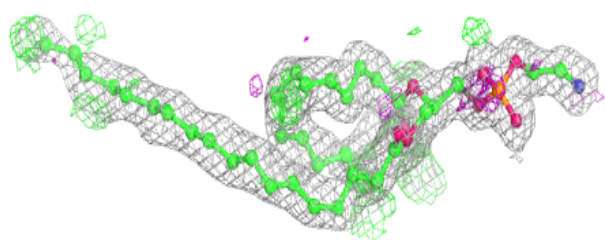
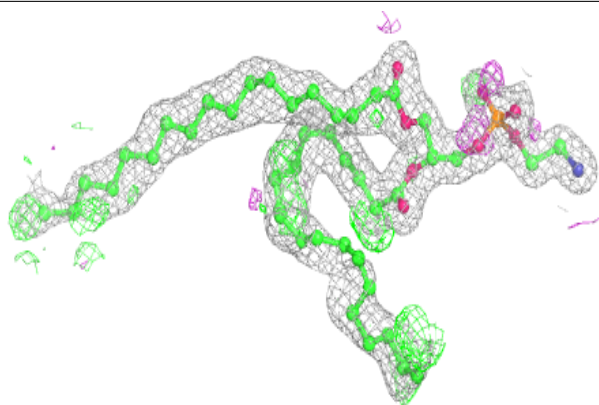
**Electron density around PEK C 303:**

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

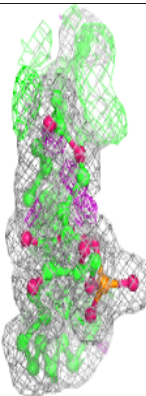
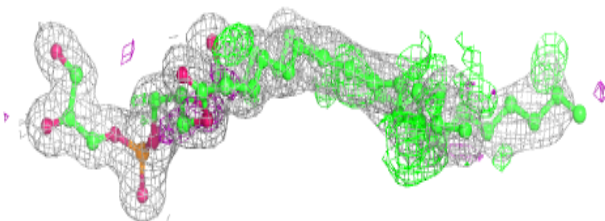
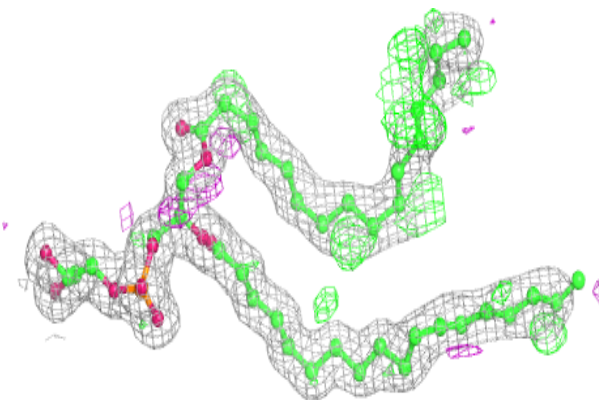


Electron density around PEK P 304:

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

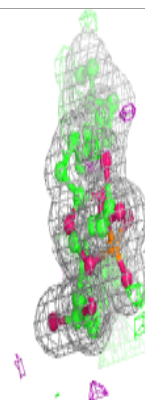
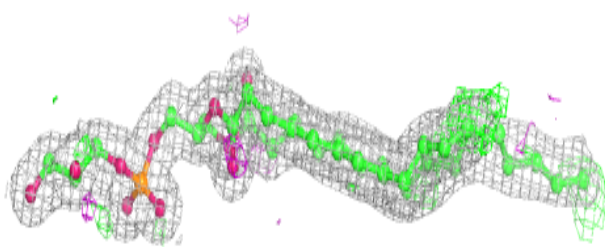
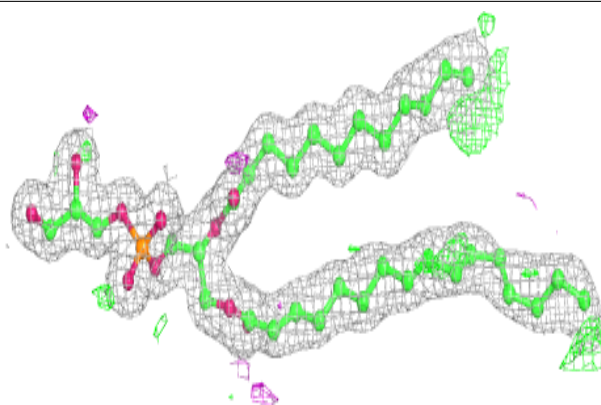
**Electron density around PGV N 607:**

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

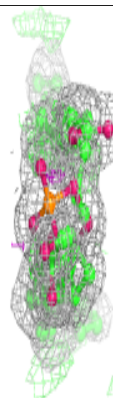
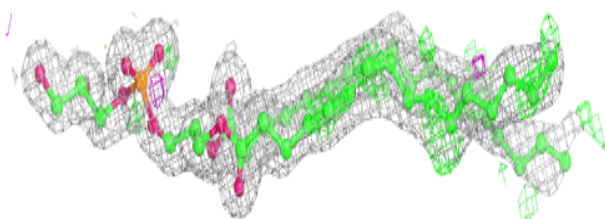
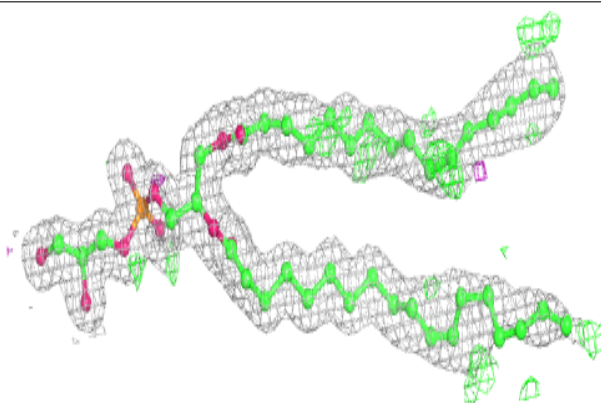


Electron density around PGV P 306:

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

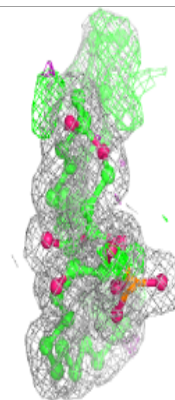
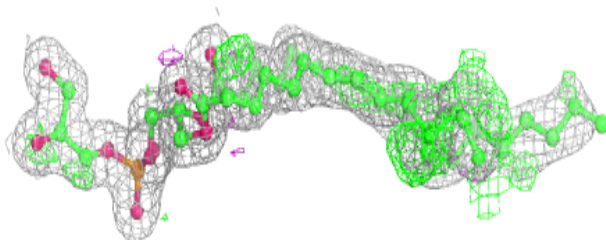
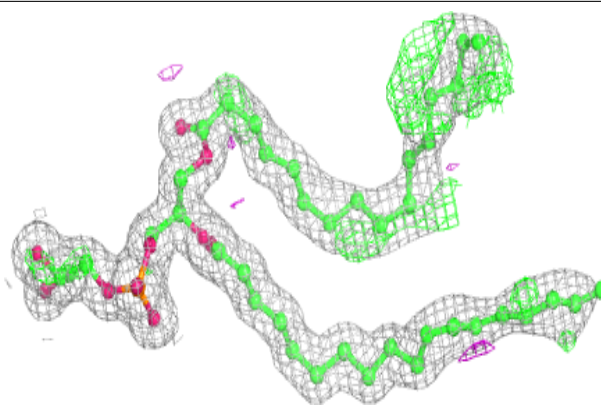
**Electron density around PGV C 306:**

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

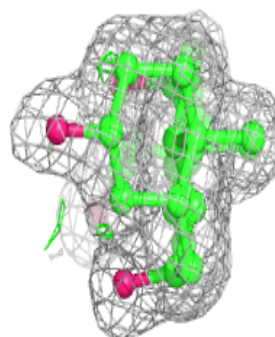
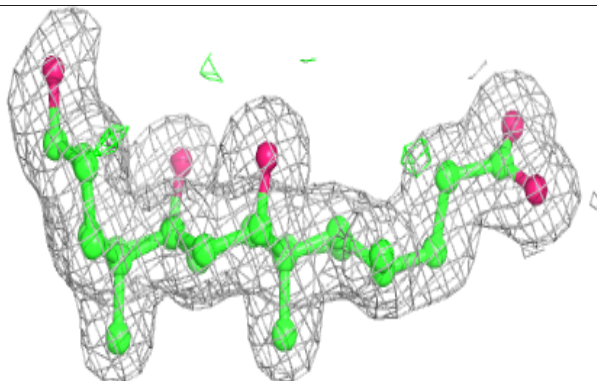
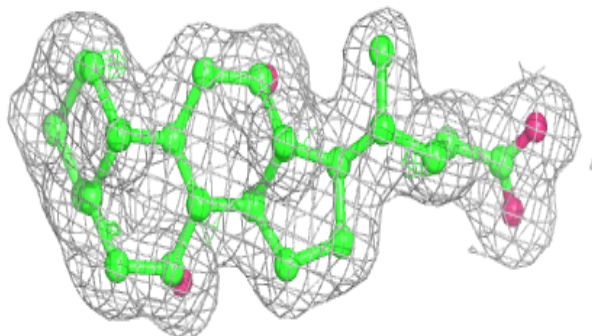


Electron density around PGV C 305:

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

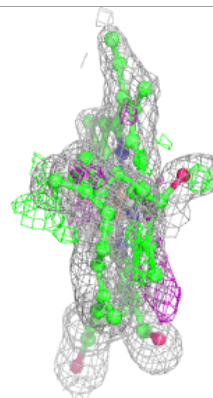
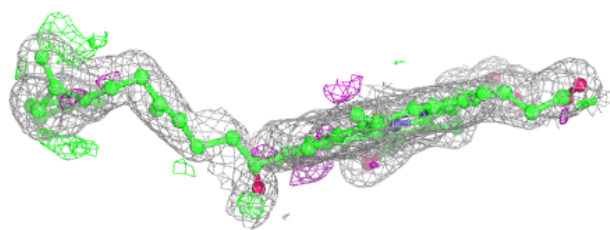
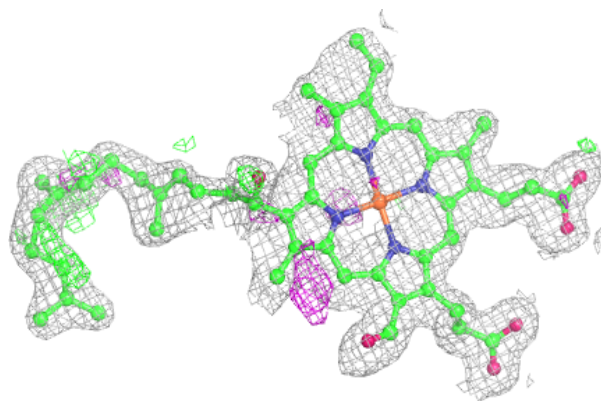
**Electron density around CHD B 303:**

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

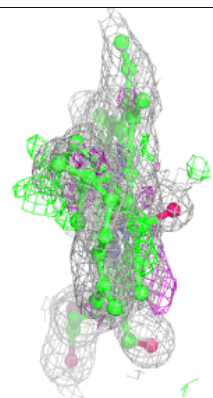
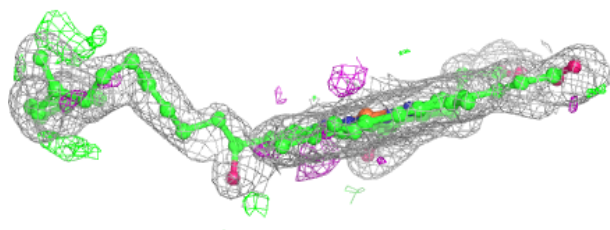
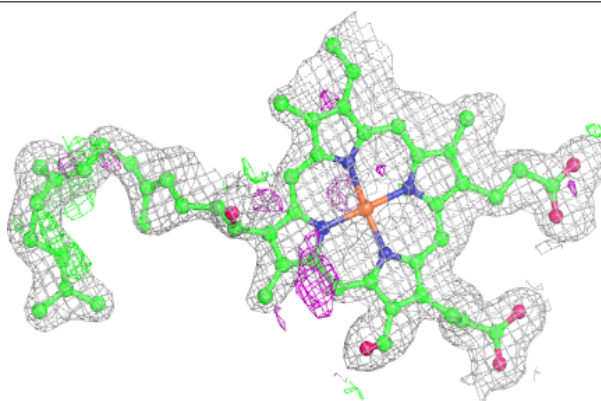


Electron density around HEA A 602 (A):

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

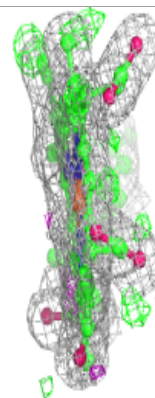
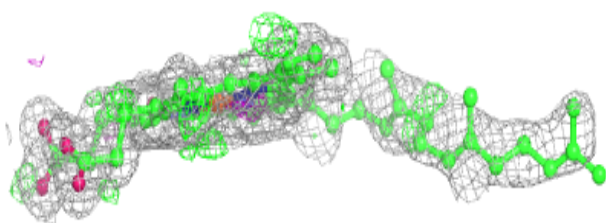
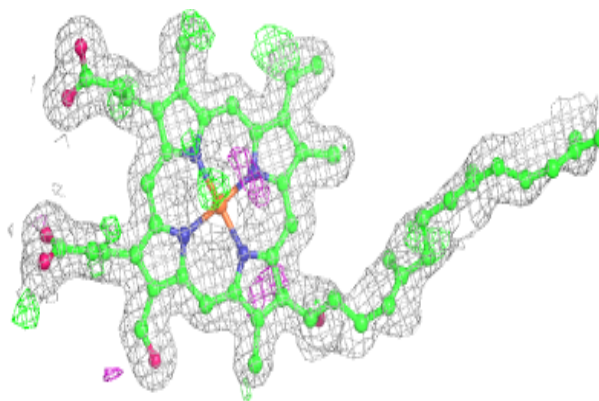
**Electron density around HEA A 602 (C):**

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

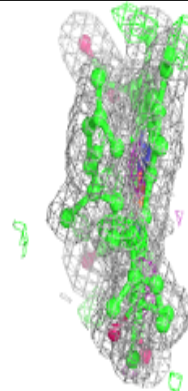
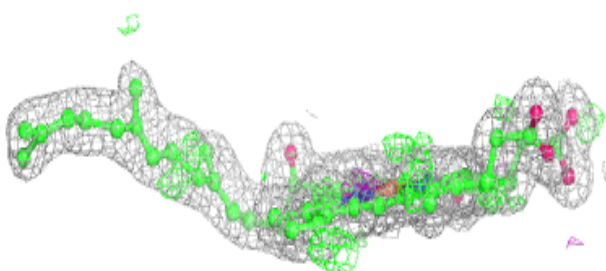
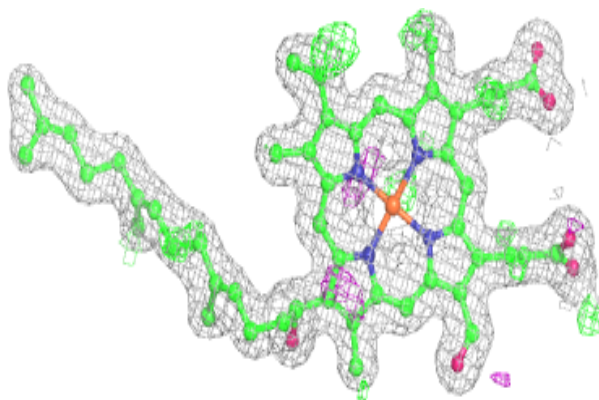


Electron density around HEA N 601 (A):

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

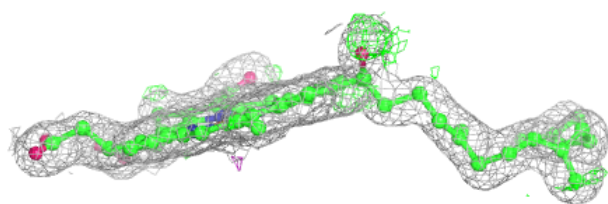
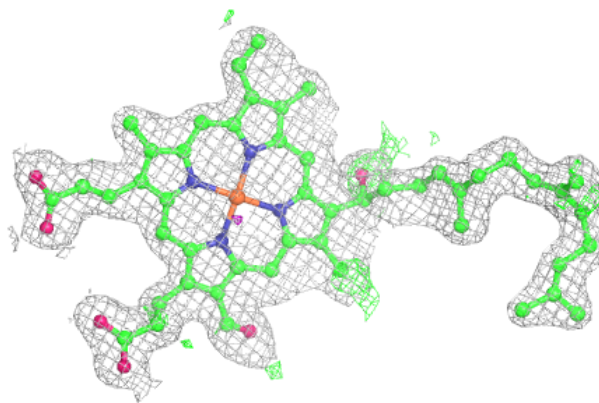
**Electron density around HEA N 601 (B):**

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

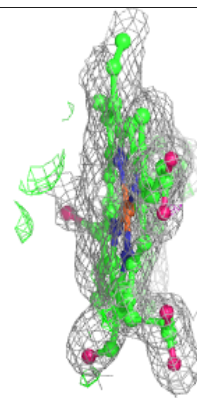
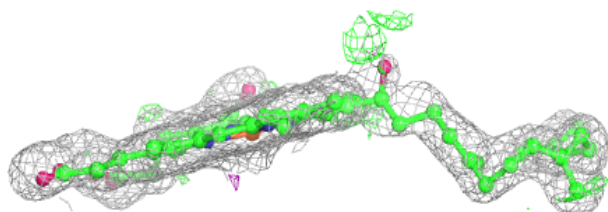
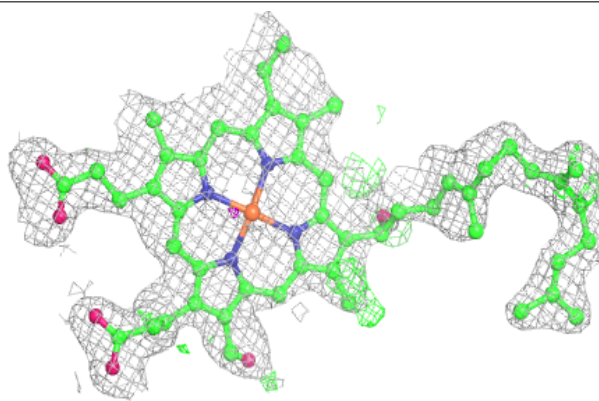


Electron density around HEA N 602 (A):

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

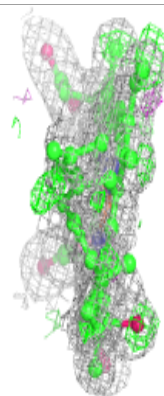
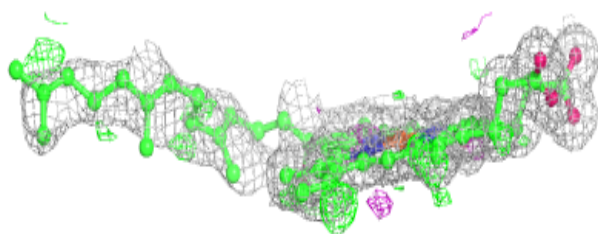
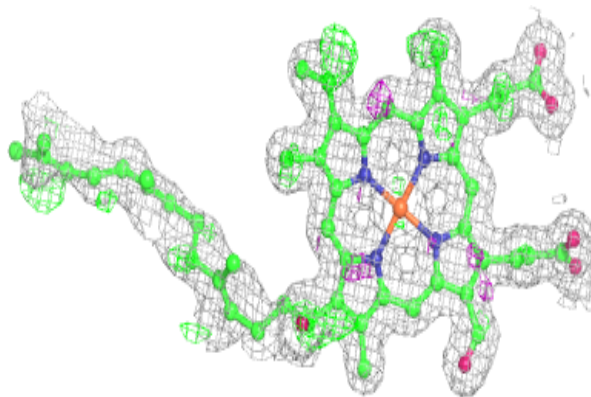
**Electron density around HEA N 602 (C):**

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

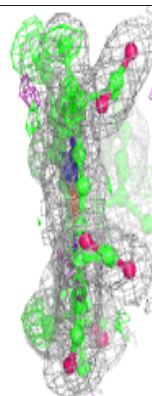
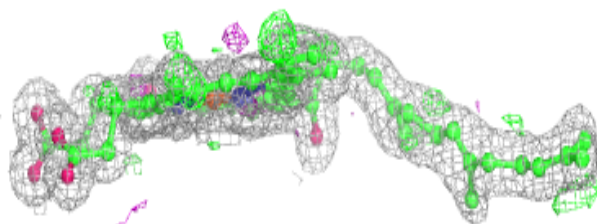
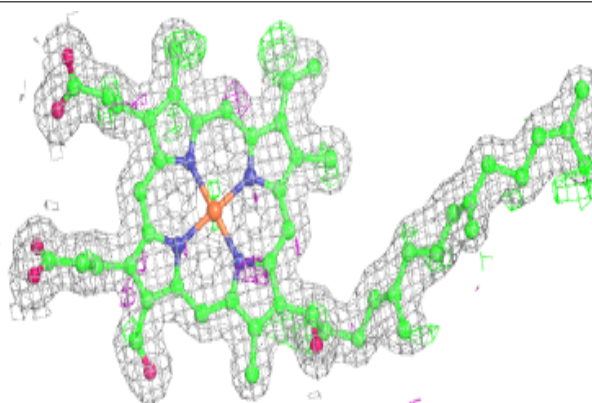


Electron density around HEA A 601 (A):

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

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

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



6.5 Other polymers [i](#)

There are no such residues in this entry.