



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 02:08 PM JST

PDB ID : 5ZCO
Title : azide-bound cytochrome c oxidase structure determined using the crystals exposed to 2 mM azide solution for 2 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-02-19
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

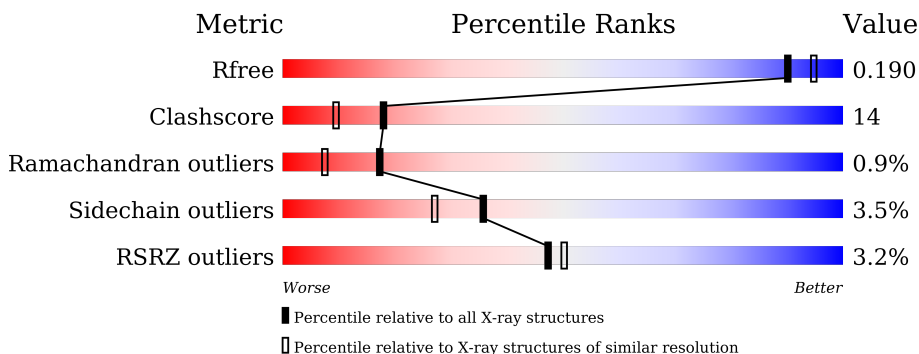
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







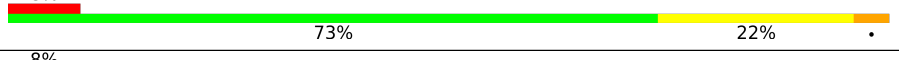
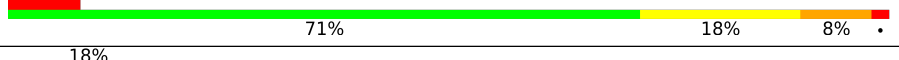

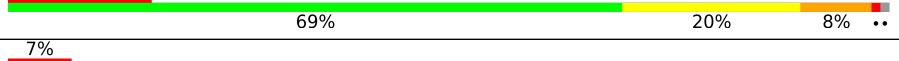

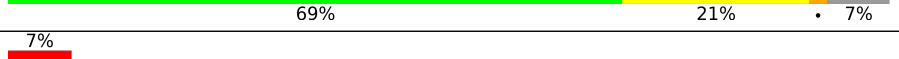
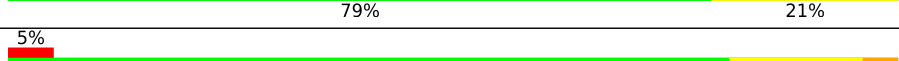
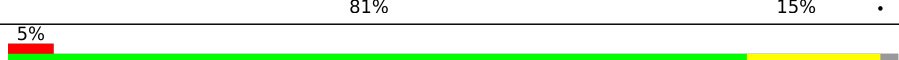

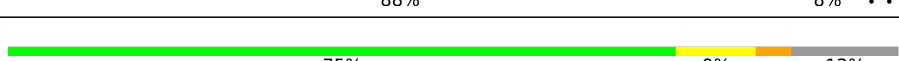
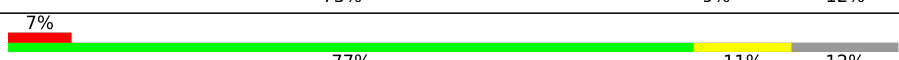
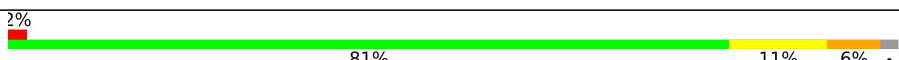
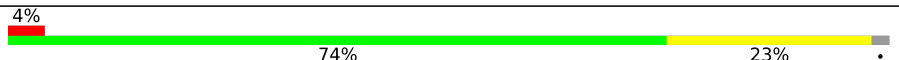
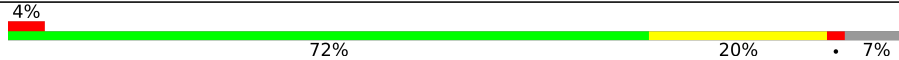


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	 79% 18% .
1	N	514	 79% 18% .
2	B	227	 71% 26% .
2	O	227	 74% 24% .
3	C	261	 80% 18% ..
3	P	261	 79% 18% ..

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	602[B]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	608[B]	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	A	615	-	X	X	-
20	EDO	B	304	-	-	X	-
20	EDO	D	202	-	-	X	-
20	EDO	G	105	-	-	X	-
20	EDO	N	620	-	-	X	-
21	TGL	Y	101	-	-	X	-
26	CDL	C	305	-	-	X	-
26	CDL	N	601	-	-	X	-
26	CDL	P	304	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33609 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
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	Total	C	N	O	S	0	9	0
			1899	1234	292	353	20			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	Total	C	N	O	S	0	4	0
			1233	803	204	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

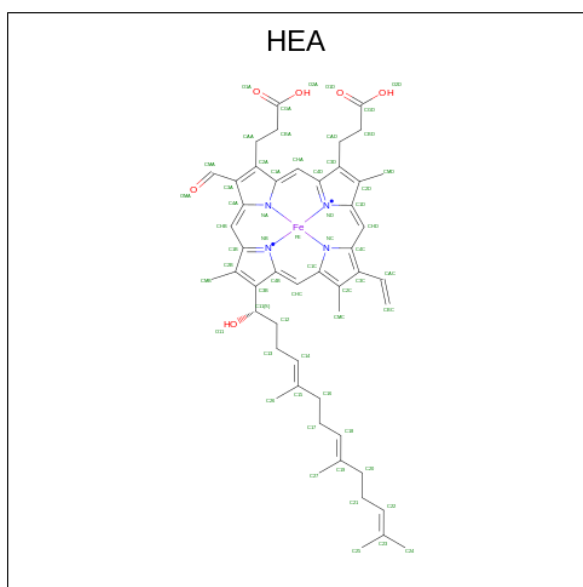
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			388	259	65	61	3			

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

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

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



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

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

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

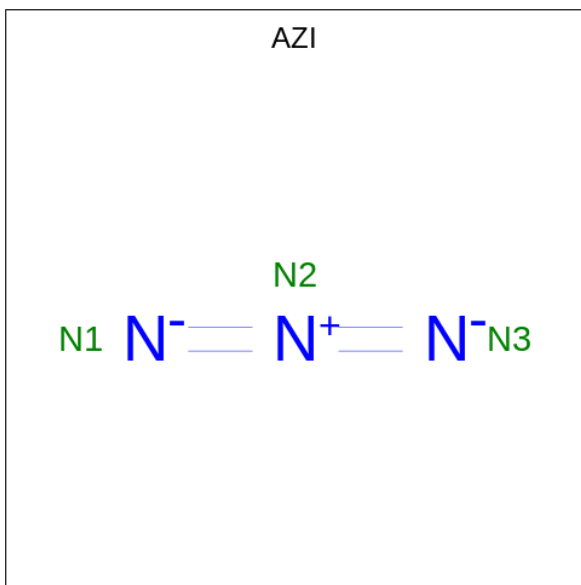
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

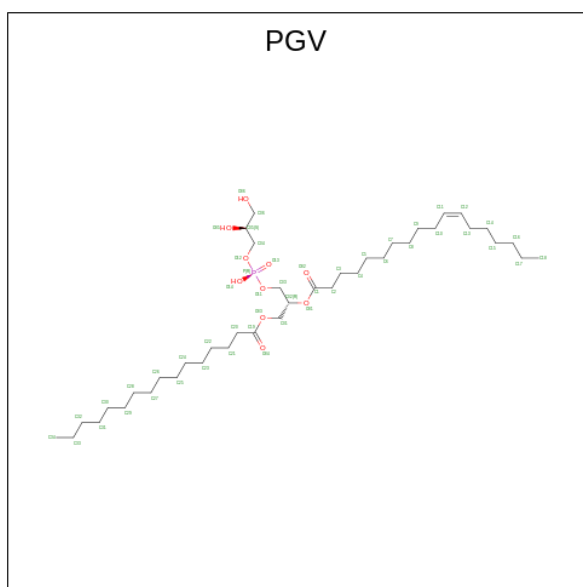
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N₃).



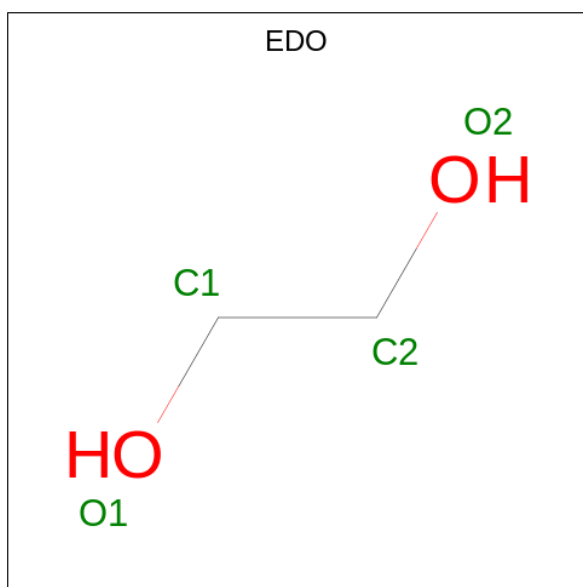
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	1
18	A	1	Total N 6 6	0	1
18	N	1	Total N 3 3	0	1
18	N	1	Total N 6 6	0	1

- Molecule 19 is (1R)-2-{{{(2S)-2,3-DIHYDROXYPROPYL}OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 20 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

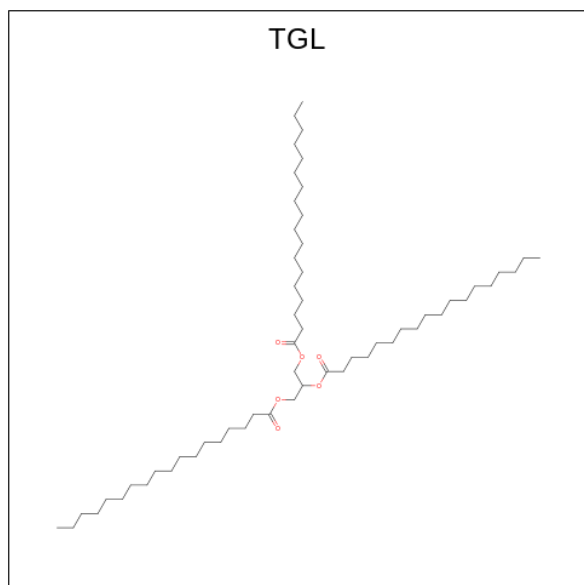
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	D	1	Total 4	C 2	O 2	0	0
20	D	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	N	1	Total	C	O	0	0
			4	2	2		
20	O	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



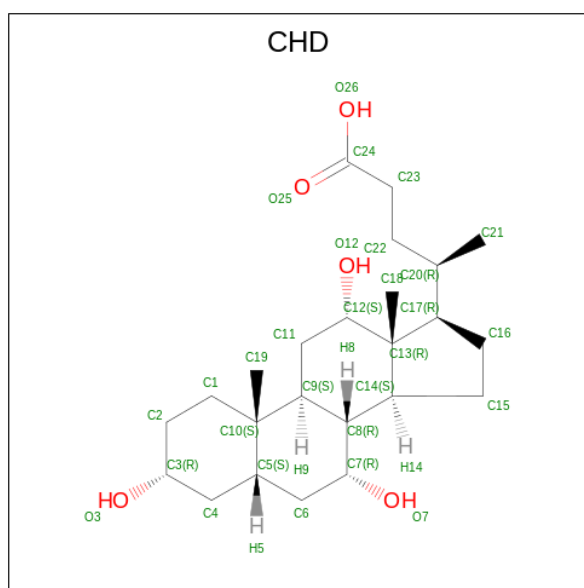
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		

Continued on next page...

Continued from previous page...

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

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



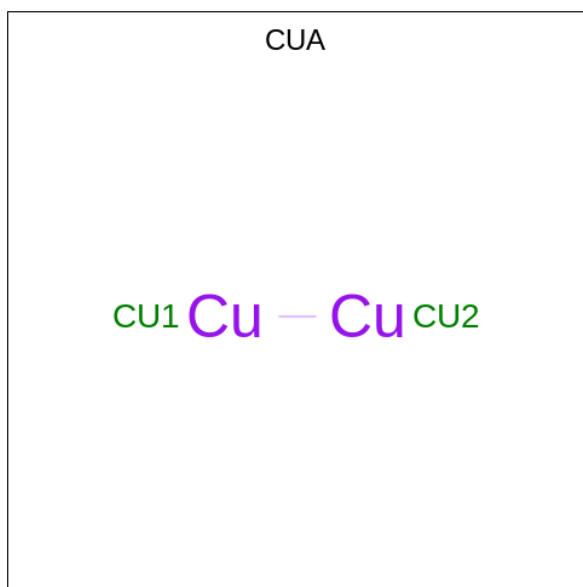
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		

Continued on next page...

Continued from previous page...

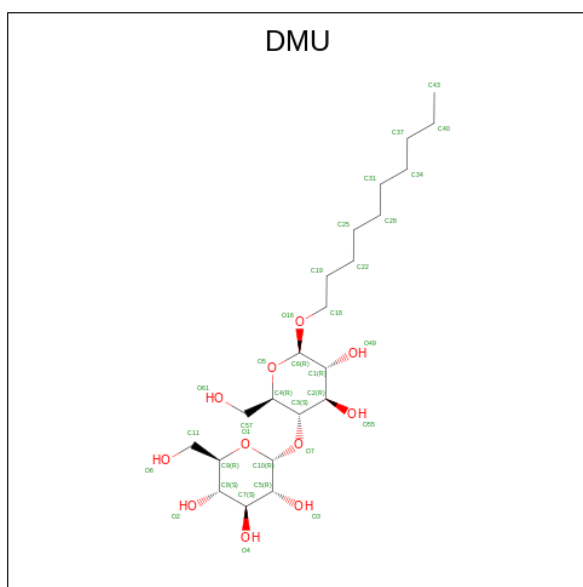
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

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



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

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).

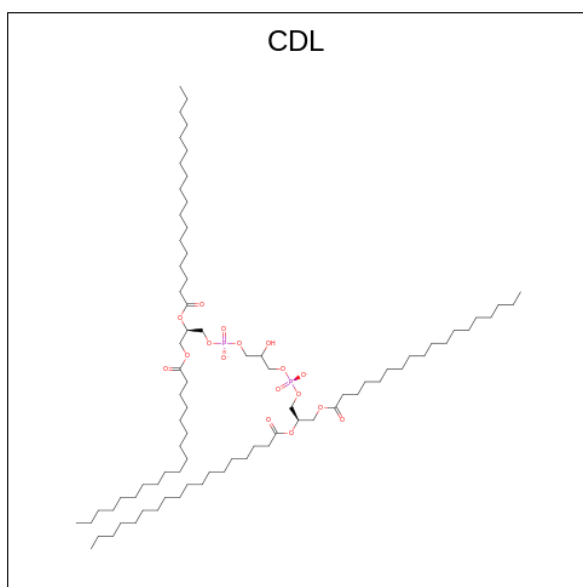


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 33 22 11	0	0
24	C	1	Total C O 33 22 11	0	0
24	C	1	Total C O 33 22 11	0	0
24	M	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	Z	1	Total C O 33 22 11	0	0

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

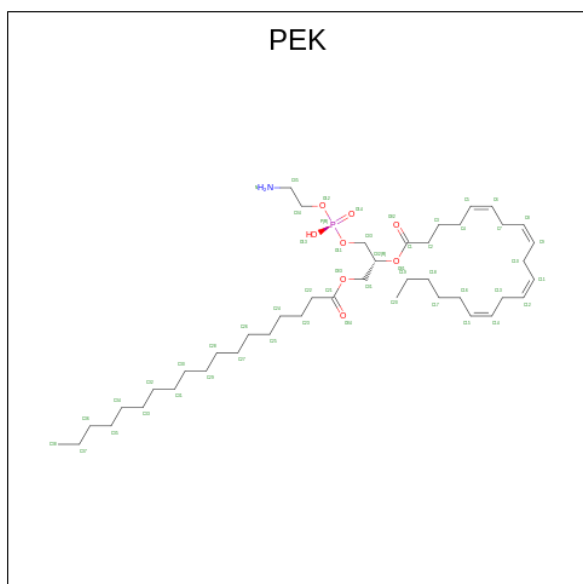
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total X 1 1	0	0
25	P	1	Total X 1 1	0	0

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



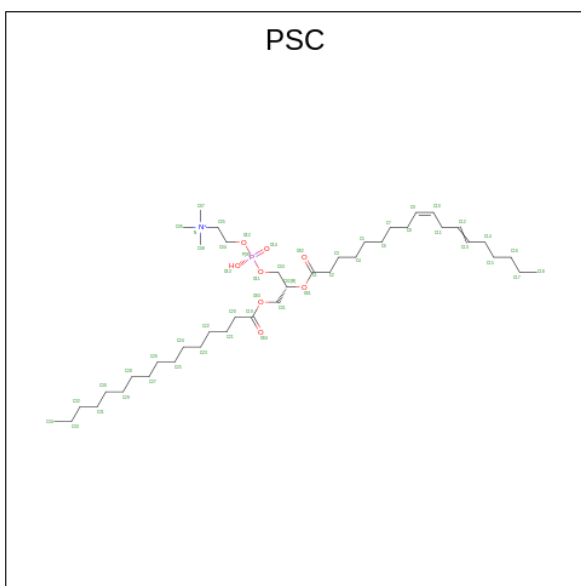
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
26	C	1	100	81	17	2	0	0
26	N	1	100	81	17	2	0	0
26	P	1	100	81	17	2	0	0
26	T	1	100	81	17	2	0	0

- Molecule 27 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



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

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

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	238	Total 238	O 238	0	0
30	B	156	Total 157	O 157	0	1
30	C	102	Total 102	O 102	0	0
30	D	124	Total 124	O 124	0	0
30	E	91	Total 91	O 91	0	0
30	F	97	Total 97	O 97	0	0
30	G	43	Total 43	O 43	0	0
30	H	45	Total 45	O 45	0	0
30	I	28	Total 28	O 28	0	0
30	J	23	Total 23	O 23	0	0
30	K	25	Total 25	O 25	0	0
30	L	38	Total 38	O 38	0	0
30	M	26	Total 26	O 26	0	0
30	N	206	Total 206	O 206	0	0
30	O	100	Total 101	O 101	0	1
30	P	90	Total 90	O 90	0	0
30	Q	29	Total 29	O 29	0	0
30	R	40	Total 40	O 40	0	0

Continued on next page...

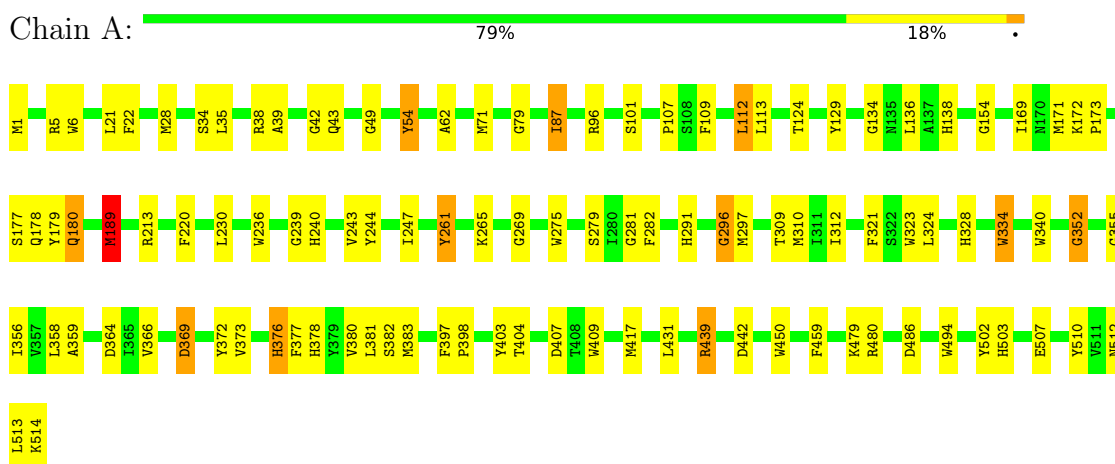
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	S	45	Total O 45 45	0	0
30	T	36	Total O 36 36	0	0
30	U	31	Total O 31 31	0	0
30	V	13	Total O 13 13	0	0
30	W	6	Total O 6 6	0	0
30	X	12	Total O 12 12	0	0
30	Y	12	Total O 12 12	0	0
30	Z	11	Total O 11 11	0	0

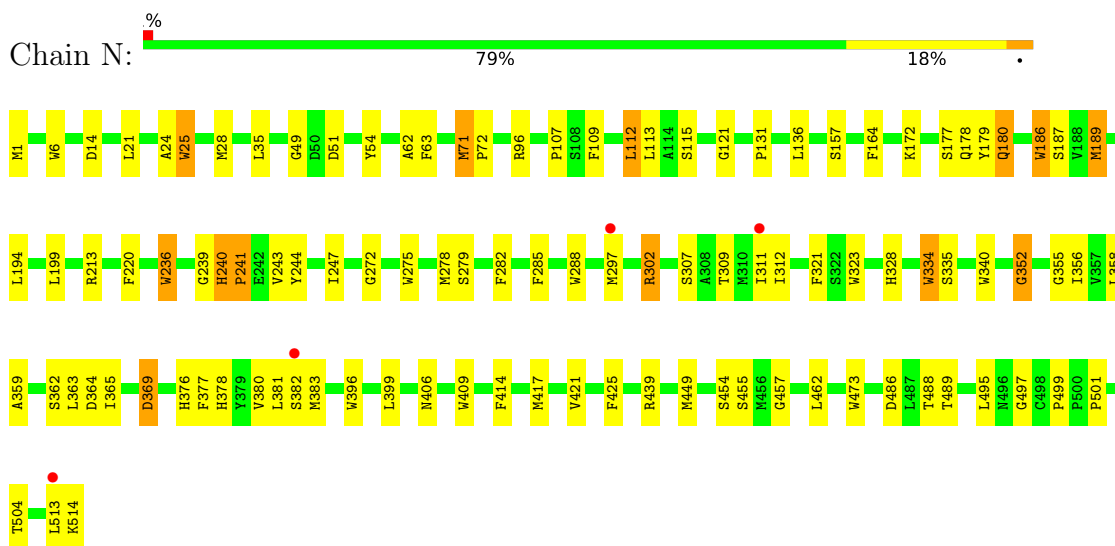
3 Residue-property plots

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

- Molecule 1: Cytochrome c oxidase subunit 1

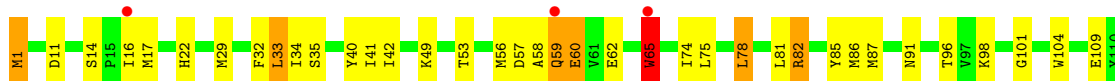


- Molecule 1: Cytochrome c oxidase subunit 1

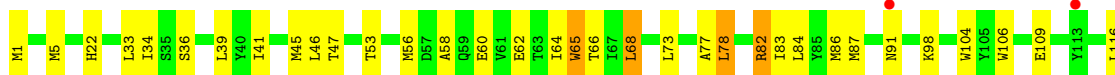
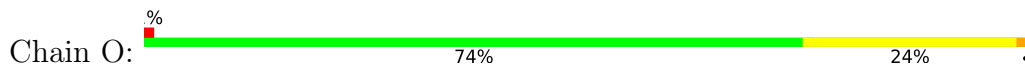


- Molecule 2: Cytochrome c oxidase subunit 2

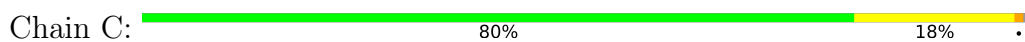




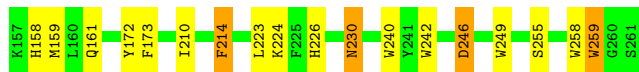
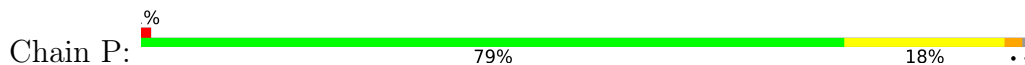
• Molecule 2: Cytochrome c oxidase subunit 2



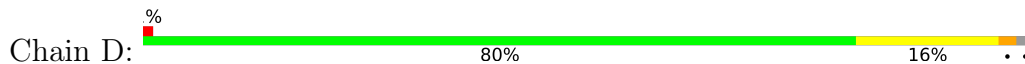
• Molecule 3: Cytochrome c oxidase subunit 3



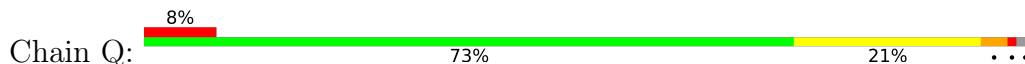
• Molecule 3: Cytochrome c oxidase subunit 3

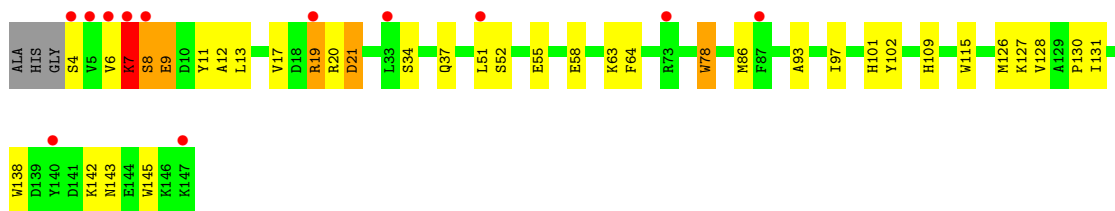


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

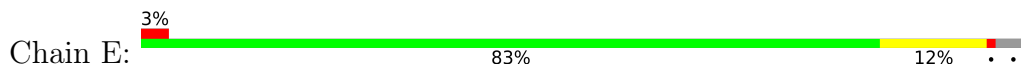


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

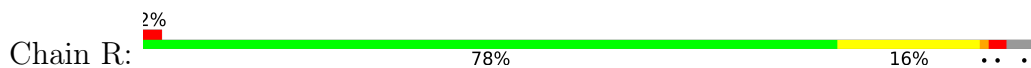




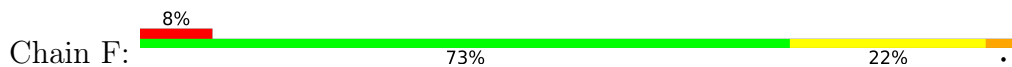
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



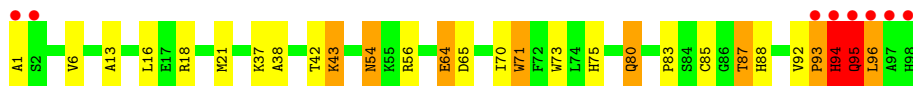
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



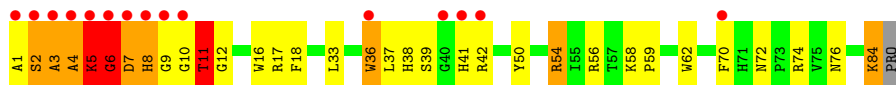
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



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



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

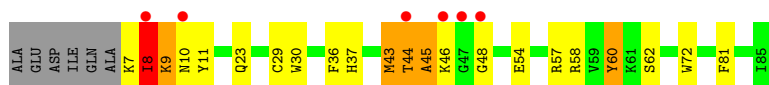


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

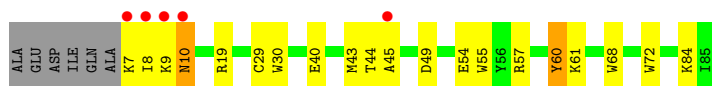




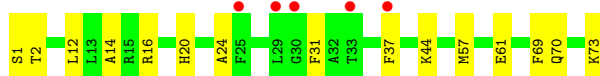
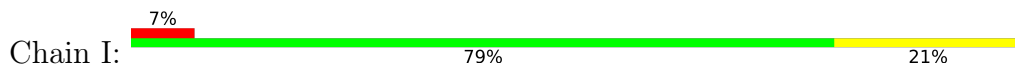
- Molecule 8: Cytochrome c oxidase subunit 6B1



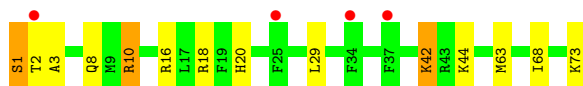
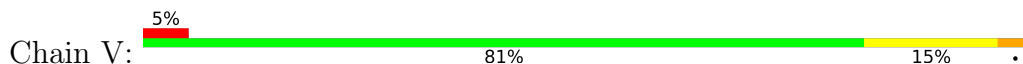
- Molecule 8: Cytochrome c oxidase subunit 6B1



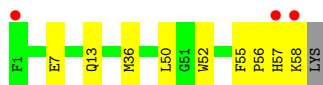
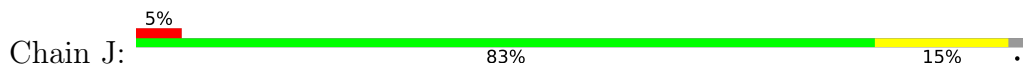
- Molecule 9: Cytochrome c oxidase subunit 6C



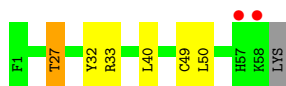
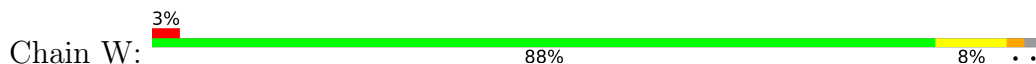
- Molecule 9: Cytochrome c oxidase subunit 6C




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



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




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

Chain K:  75% 9% 12%




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

Chain X:  77% 11% 12% 7%




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

Chain L:  81% 11% 6% 2%



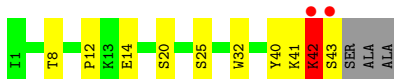
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  74% 23% 7% 4%



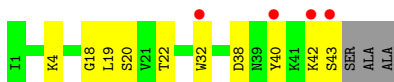
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  72% 20% 7% 4%



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

Chain Z:  72% 22% 7% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.38Å 206.66Å 177.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 137.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.90) 99.7 (137.16-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.24 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.164 , 0.189 0.165 , 0.190	Depositor DCC
R_{free} test set	26414 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtrriage
Anisotropy	0.546	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33609	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.62	35/4322 (0.8%)	1.28	25/5897 (0.4%)
1	N	1.57	33/4308 (0.8%)	1.22	15/5878 (0.3%)
2	B	1.44	12/1937 (0.6%)	1.22	6/2637 (0.2%)
2	O	1.23	5/1908 (0.3%)	1.11	7/2597 (0.3%)
3	C	1.53	16/2272 (0.7%)	1.10	1/3102 (0.0%)
3	P	1.51	18/2272 (0.8%)	1.12	6/3102 (0.2%)
4	D	1.48	7/1268 (0.6%)	1.17	3/1709 (0.2%)
4	Q	1.15	4/1259 (0.3%)	1.09	5/1698 (0.3%)
5	E	1.42	1/871 (0.1%)	1.36	6/1182 (0.5%)
5	R	1.16	1/882 (0.1%)	1.09	5/1196 (0.4%)
6	F	1.42	4/795 (0.5%)	1.21	3/1079 (0.3%)
6	S	1.24	1/780 (0.1%)	1.15	3/1058 (0.3%)
7	G	1.46	5/702 (0.7%)	1.14	4/953 (0.4%)
7	T	1.42	5/702 (0.7%)	1.12	3/953 (0.3%)
8	H	1.34	4/682 (0.6%)	1.00	0/921
8	U	1.24	5/682 (0.7%)	1.00	1/921 (0.1%)
9	I	1.14	1/605 (0.2%)	1.11	0/802
9	V	1.02	0/605	1.09	1/802 (0.1%)
10	J	1.20	0/471	1.00	1/636 (0.2%)
10	W	1.23	0/480	1.08	2/648 (0.3%)
11	K	1.36	3/398 (0.8%)	1.25	4/546 (0.7%)
11	X	1.18	2/405 (0.5%)	0.92	0/556
12	L	1.44	1/393 (0.3%)	1.18	2/526 (0.4%)
12	Y	1.36	2/401 (0.5%)	1.01	0/536
13	M	1.44	3/345 (0.9%)	1.14	0/470
13	Z	1.27	4/345 (1.2%)	1.04	1/470 (0.2%)
All	All	1.43	172/30090 (0.6%)	1.16	104/40875 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
4	Q	0	1
6	F	0	1
6	S	0	2
7	G	0	1
7	T	0	1
All	All	0	9

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	58	GLU	CD-OE1	9.44	1.36	1.25
3	C	181	TYR	CE1-CZ	9.34	1.50	1.38
3	C	89	SER	CB-OG	9.28	1.54	1.42
1	N	179	TYR	CE1-CZ	8.87	1.50	1.38
2	B	65	TRP	CD2-CE2	8.14	1.51	1.41

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH1	18.45	129.53	120.30
5	E	90	ARG	NE-CZ-NH2	-15.05	112.78	120.30
4	Q	20	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	N	71	MET	CG-SD-CE	-14.65	76.76	100.20
1	A	71	MET	CG-SD-CE	-14.45	77.09	100.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
6	F	93	PRO	Peptide
7	G	11	TPO	Peptide
1	N	240	HIS	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	110	0
1	N	4179	0	4154	101	0
2	B	1899	0	1898	70	0
2	O	1870	0	1868	51	0
3	C	2185	0	2097	61	0
3	P	2185	0	2097	51	0
4	D	1233	0	1223	37	0
4	Q	1224	0	1211	33	0
5	E	852	0	845	7	0
5	R	863	0	857	9	0
6	F	778	0	754	23	0
6	S	763	0	742	34	0
7	G	686	0	652	32	0
7	T	686	0	651	26	0
8	H	662	0	623	16	0
8	U	662	0	623	11	0
9	I	601	0	613	17	0
9	V	601	0	613	16	0
10	J	460	0	459	7	0
10	W	469	0	464	3	0
11	K	384	0	366	2	0
11	X	391	0	374	4	0
12	L	380	0	380	15	0
12	Y	388	0	388	17	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0
14	A	180	0	162	36	0
14	N	180	0	162	32	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	9	0	0	4	0
18	N	9	0	0	2	0
19	A	102	0	152	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	102	0	152	8	0
19	N	51	0	76	0	0
19	P	51	0	76	2	0
19	U	51	0	76	1	0
19	Z	51	0	76	11	0
20	A	40	0	60	12	0
20	B	16	0	24	5	0
20	D	8	0	12	12	0
20	E	12	0	18	0	0
20	F	12	0	18	0	0
20	G	8	0	12	6	0
20	L	4	0	6	0	0
20	M	4	0	6	0	0
20	N	40	0	60	7	0
20	O	4	0	6	0	0
20	P	12	0	18	0	0
20	R	4	0	6	0	0
20	S	8	0	12	0	0
20	T	4	0	6	0	0
20	Y	4	0	6	0	0
21	B	63	0	110	4	0
21	D	63	0	110	16	0
21	L	63	0	110	10	0
21	N	63	0	110	6	0
21	Q	63	0	110	13	0
21	Y	63	0	110	23	0
22	B	29	0	39	0	0
22	C	58	0	78	5	0
22	G	29	0	39	1	0
22	J	29	0	38	1	0
22	P	58	0	78	4	0
22	W	29	0	38	2	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	C	99	0	126	20	0
24	M	33	0	42	0	0
24	P	99	0	126	19	0
24	Z	33	0	42	1	0
25	C	1	0	0	0	0
25	P	1	0	0	1	0
26	C	100	0	156	25	0
26	N	100	0	156	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	100	0	156	25	0
26	T	100	0	156	19	0
27	C	106	0	154	27	0
27	G	106	0	154	12	0
27	P	53	0	77	5	0
27	T	53	0	77	1	0
28	E	52	0	80	12	0
28	O	52	0	80	15	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	238	0	0	32	0
30	B	157	0	0	30	2
30	C	102	0	0	6	0
30	D	124	0	0	18	2
30	E	91	0	0	1	0
30	F	97	0	0	4	0
30	G	43	0	0	7	0
30	H	45	0	0	1	0
30	I	28	0	0	4	1
30	J	23	0	0	3	0
30	K	25	0	0	1	0
30	L	38	0	0	3	0
30	M	26	0	0	7	1
30	N	206	0	0	15	0
30	O	101	0	0	3	0
30	P	90	0	0	4	0
30	Q	29	0	0	4	0
30	R	40	0	0	1	0
30	S	45	0	0	2	0
30	T	36	0	0	5	0
30	U	31	0	0	0	0
30	V	13	0	0	2	0
30	W	6	0	0	0	0
30	X	12	0	0	0	0
30	Y	12	0	0	1	0
30	Z	11	0	0	0	0
All	All	33609	0	32572	876	3

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 14.

The worst 5 of 876 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)
20:A:615:EDO:C2	20:A:615:EDO:C1	1.76	1.55
6:S:43:LYS:H	6:S:43:LYS:CD	1.19	1.45
19:Z:101:PGV:C2	19:Z:101:PGV:H011	1.50	1.38
20:A:615:EDO:C2	20:A:615:EDO:O1	1.70	1.33
9:I:73:LYS:HE2	30:I:118:HOH:O	1.16	1.32

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:I:126:HOH:O	30:M:211:HOH:O[2_584]	1.94	0.26
30:B:540:HOH:O	30:D:394:HOH:O[2_584]	1.95	0.25
30:B:459:HOH:O	30:D:385:HOH:O[2_584]	2.07	0.13

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	534/514 (104%)	520 (97%)	14 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100
2	B	234/227 (103%)	223 (95%)	11 (5%)	0	100	100
2	O	230/227 (101%)	222 (96%)	8 (4%)	0	100	100
3	C	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	142 (97%)	4 (3%)	0	100	100
4	Q	145/147 (99%)	137 (94%)	6 (4%)	2 (1%)	11	3
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	104/109 (95%)	103 (99%)	0	1 (1%)	15	6
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	98/98 (100%)	91 (93%)	3 (3%)	4 (4%)	3	0
7	G	82/85 (96%)	69 (84%)	6 (7%)	7 (8%)	1	0
7	T	82/85 (96%)	73 (89%)	5 (6%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	1 (1%)	6 (8%)	1	0
8	U	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	5	1
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	6	1
12	Y	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3597/3614 (100%)	3456 (96%)	111 (3%)	30 (1%)	17	9

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	2	SER
7	G	4	ALA
8	H	44	THR
4	Q	7	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/426 (105%)	442 (99%)	5 (1%)	73	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	445/426 (104%)	439 (99%)	6 (1%)	69	68
2	B	219/210 (104%)	210 (96%)	9 (4%)	30	21
2	O	215/210 (102%)	207 (96%)	8 (4%)	34	25
3	C	233/226 (103%)	227 (97%)	6 (3%)	46	39
3	P	233/226 (103%)	229 (98%)	4 (2%)	60	57
4	D	132/129 (102%)	129 (98%)	3 (2%)	50	45
4	Q	131/129 (102%)	123 (94%)	8 (6%)	18	9
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	47
5	R	93/95 (98%)	89 (96%)	4 (4%)	29	19
6	F	85/81 (105%)	83 (98%)	2 (2%)	49	43
6	S	83/81 (102%)	73 (88%)	10 (12%)	5	1
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	2
7	T	68/68 (100%)	62 (91%)	6 (9%)	10	4
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	7
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	4
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	27
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	7
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	51
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	22
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	39
11	X	40/46 (87%)	39 (98%)	1 (2%)	47	41
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	40/40 (100%)	38 (95%)	2 (5%)	24	15
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	38
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	4
All	All	3131/3082 (102%)	3022 (96%)	109 (4%)	36	27

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	171	LYS
5	R	6	GLU
9	V	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	17	PRO
4	Q	19[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	68	GLN
6	S	94	HIS
3	P	76	GLN
5	R	94	ASN
7	T	8	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	V	1	9	7,8,9	1.59	1 (14%)	8,9,11	1.58	2 (25%)
2	FME	O	1	2	8,9,10	1.12	0	7,9,11	1.95	3 (42%)
7	TPO	G	11	7	8,10,11	2.13	2 (25%)	10,14,16	1.22	1 (10%)
9	SAC	I	1	9	7,8,9	1.26	1 (14%)	8,9,11	2.07	2 (25%)
1	FME	N	1	1	8,9,10	1.42	1 (12%)	7,9,11	1.63	2 (28%)
1	FME	A	1	1	8,9,10	0.96	0	7,9,11	2.29	4 (57%)
2	FME	B	1	2	8,9,10	1.67	2 (25%)	7,9,11	2.32	3 (42%)
7	TPO	T	11	7	8,10,11	1.69	1 (12%)	10,14,16	1.49	2 (20%)

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
9	SAC	V	1	9	-	6/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	N	1	1	-	3/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.05	1.52	1.46
7	G	11	TPO	P-O1P	3.54	1.62	1.50
1	N	1	FME	CA-N	3.45	1.51	1.46
7	T	11	TPO	P-O1P	3.21	1.60	1.50
9	I	1	SAC	CA-N	3.03	1.50	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.55	100.30	112.95
9	I	1	SAC	OG-CB-CA	-4.39	99.77	110.97
1	A	1	FME	CE-SD-CG	3.96	114.02	100.40
2	O	1	FME	CG-CB-CA	-3.05	104.47	112.95
2	B	1	FME	C-CA-N	-2.99	104.34	109.73

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 101 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	EDO	A	611	-	3,3,3	0.61	0	2,2,2	0.97	0
18	AZI	N	608[B]	15	0,2,2	-	-	0,1,1	-	-
20	EDO	E	203	-	3,3,3	0.70	0	2,2,2	0.11	0
20	EDO	L	102	-	3,3,3	0.70	0	2,2,2	0.77	0
18	AZI	A	607[A]	15,14	0,2,2	-	-	0,1,1	-	-
23	CUA	O	301	2	0,1,1	-	-	-	-	-
27	PEK	T	101	-	52,52,52	1.37	7 (13%)	55,57,57	2.19	9 (16%)
20	EDO	A	619	-	3,3,3	0.57	0	2,2,2	0.70	0
24	DMU	P	309	-	34,34,34	1.09	2 (5%)	45,45,45	1.89	11 (24%)
26	CDL	T	102	-	99,99,99	1.43	13 (13%)	105,111,111	1.41	14 (13%)
24	DMU	P	306	-	34,34,34	1.12	1 (2%)	45,45,45	1.67	8 (17%)
20	EDO	N	611	-	3,3,3	1.56	1 (33%)	2,2,2	1.01	0
22	CHD	P	305	-	32,32,32	1.22	4 (12%)	51,51,51	3.48	22 (43%)
14	HEA	A	602[A]	18,1	57,67,67	1.61	12 (21%)	61,103,103	2.19	21 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	M	102	-	3,3,3	0.33	0	2,2,2	0.78	0
22	CHD	B	302	-	32,32,32	2.07	14 (43%)	51,51,51	2.11	20 (39%)
20	EDO	B	304	-	3,3,3	0.54	0	2,2,2	1.05	0
20	EDO	O	303	-	3,3,3	0.82	0	2,2,2	1.03	0
20	EDO	F	104	-	3,3,3	0.67	0	2,2,2	0.59	0
20	EDO	G	105	-	3,3,3	0.52	0	2,2,2	0.53	0
20	EDO	D	203	-	3,3,3	0.71	0	2,2,2	0.39	0
24	DMU	C	302	-	34,34,34	0.72	0	45,45,45	1.42	7 (15%)
19	PGV	P	303	-	50,50,50	0.90	2 (4%)	53,56,56	1.26	5 (9%)
19	PGV	Z	101	-	50,50,50	1.14	2 (4%)	53,56,56	1.33	7 (13%)
20	EDO	N	619	-	3,3,3	0.37	0	2,2,2	0.52	0
18	AZI	N	608[A]	15,14	0,2,2	-	-	0,1,1	-	-
14	HEA	N	603[A]	18,1	57,67,67	1.66	14 (24%)	61,103,103	2.47	28 (45%)
18	AZI	N	607[B]	14	0,2,2	-	-	0,1,1	-	-
20	EDO	N	620	-	3,3,3	0.87	0	2,2,2	1.25	0
20	EDO	A	618	-	3,3,3	0.29	0	2,2,2	1.56	0
21	TGL	D	201	-	62,62,62	1.77	4 (6%)	65,65,65	2.27	10 (15%)
24	DMU	Z	102	-	34,34,34	0.70	1 (2%)	45,45,45	1.28	6 (13%)
27	PEK	G	103	-	52,52,52	1.14	2 (3%)	55,57,57	1.26	3 (5%)
24	DMU	P	308	-	34,34,34	0.75	0	45,45,45	2.21	14 (31%)
28	PSC	O	302	-	51,51,51	1.27	3 (5%)	57,59,59	1.26	4 (7%)
20	EDO	P	312	-	3,3,3	0.44	0	2,2,2	0.66	0
20	EDO	N	613	-	3,3,3	0.64	0	2,2,2	0.83	0
20	EDO	Y	102	-	3,3,3	0.50	0	2,2,2	0.67	0
26	CDL	C	305	-	99,99,99	1.50	16 (16%)	105,111,111	1.44	17 (16%)
20	EDO	A	616	-	3,3,3	1.13	0	2,2,2	0.43	0
28	PSC	E	201	-	51,51,51	1.38	4 (7%)	57,59,59	1.47	6 (10%)
19	PGV	A	609	-	50,50,50	1.22	4 (8%)	53,56,56	1.46	8 (15%)
22	CHD	W	101	-	32,32,32	1.34	5 (15%)	51,51,51	2.84	24 (47%)
26	CDL	N	601	-	99,99,99	1.49	13 (13%)	105,111,111	1.50	15 (14%)
24	DMU	C	310	-	34,34,34	0.87	1 (2%)	45,45,45	2.36	13 (28%)
20	EDO	A	613	-	3,3,3	1.59	1 (33%)	2,2,2	1.17	0
20	EDO	A	617	-	3,3,3	0.34	0	2,2,2	1.30	0
22	CHD	C	306	-	32,32,32	1.19	3 (9%)	51,51,51	3.23	19 (37%)
20	EDO	N	616	-	3,3,3	0.61	0	2,2,2	0.56	0
20	EDO	S	103	-	3,3,3	0.64	0	2,2,2	1.67	1 (50%)
19	PGV	A	608	-	50,50,50	1.13	4 (8%)	53,56,56	1.42	8 (15%)
24	DMU	M	101	-	34,34,34	0.82	1 (2%)	45,45,45	1.43	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	G	102	-	32,32,32	1.72	8 (25%)	51,51,51	1.98	18 (35%)
20	EDO	A	610	-	3,3,3	0.38	0	2,2,2	1.09	0
22	CHD	J	101	-	32,32,32	0.89	0	51,51,51	2.84	22 (43%)
20	EDO	N	618	-	3,3,3	1.19	0	2,2,2	0.25	0
18	AZI	A	607[B]	15	0,2,2	-	-	0,1,1	-	-
14	HEA	N	602	1	57,67,67	1.77	15 (26%)	61,103,103	2.41	28 (45%)
20	EDO	T	103	-	3,3,3	1.05	0	2,2,2	0.70	0
20	EDO	A	615	-	3,3,3	2.46	1 (33%)	2,2,2	4.78	1 (50%)
22	CHD	P	301	-	32,32,32	1.47	6 (18%)	51,51,51	2.33	14 (27%)
19	PGV	N	609	-	50,50,50	1.11	5 (10%)	53,56,56	1.45	7 (13%)
20	EDO	E	204	-	3,3,3	0.77	0	2,2,2	0.42	0
21	TGL	B	301	-	62,62,62	1.23	4 (6%)	65,65,65	1.81	10 (15%)
26	CDL	P	304	-	99,99,99	1.56	17 (17%)	105,111,111	1.56	20 (19%)
23	CUA	B	303	2	0,1,1	-	-	-	-	-
21	TGL	Y	101	-	62,62,62	1.44	5 (8%)	65,65,65	1.60	13 (20%)
20	EDO	B	305	-	3,3,3	0.43	0	2,2,2	0.52	0
21	TGL	Q	201	-	62,62,62	1.49	4 (6%)	65,65,65	1.39	6 (9%)
20	EDO	F	103	-	3,3,3	1.21	0	2,2,2	0.35	0
27	PEK	C	307	-	52,52,52	1.55	6 (11%)	55,57,57	1.59	9 (16%)
24	DMU	C	311	-	34,34,34	1.04	1 (2%)	45,45,45	2.42	11 (24%)
21	TGL	L	101	-	62,62,62	1.32	3 (4%)	65,65,65	1.91	17 (26%)
20	EDO	A	612	-	3,3,3	0.57	0	2,2,2	0.40	0
27	PEK	G	101	-	52,52,52	0.96	5 (9%)	55,57,57	1.17	4 (7%)
14	HEA	N	603[B]	18,1	57,67,67	1.60	10 (17%)	61,103,103	2.15	19 (31%)
19	PGV	C	308	-	50,50,50	1.40	2 (4%)	53,56,56	1.68	11 (20%)
20	EDO	A	614	-	3,3,3	0.58	0	2,2,2	1.92	1 (50%)
18	AZI	A	606[B]	14	0,2,2	-	-	0,1,1	-	-
20	EDO	N	615	-	3,3,3	0.91	0	2,2,2	0.14	0
20	EDO	G	104	-	3,3,3	0.88	0	2,2,2	0.63	0
20	EDO	N	617	-	3,3,3	0.80	0	2,2,2	0.53	0
20	EDO	F	102	-	3,3,3	1.11	0	2,2,2	0.60	0
22	CHD	C	301	-	32,32,32	1.96	13 (40%)	51,51,51	2.10	16 (31%)
20	EDO	B	306	-	3,3,3	1.79	1 (33%)	2,2,2	0.35	0
20	EDO	E	202	-	3,3,3	0.62	0	2,2,2	0.92	0
14	HEA	A	601	1	57,67,67	1.70	14 (24%)	61,103,103	2.26	21 (34%)
19	PGV	C	304	-	50,50,50	0.93	2 (4%)	53,56,56	1.13	5 (9%)
21	TGL	N	610	-	62,62,62	1.16	3 (4%)	65,65,65	1.68	9 (13%)
27	PEK	P	307	-	52,52,52	1.26	2 (3%)	55,57,57	1.37	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	614	-	3,3,3	1.29	0	2,2,2	0.28	0
19	PGV	U	101	-	50,50,50	1.19	2 (4%)	53,56,56	1.53	8 (15%)
20	EDO	D	202	-	3,3,3	0.66	0	2,2,2	0.77	0
27	PEK	C	309	-	52,52,52	1.26	2 (3%)	55,57,57	1.40	6 (10%)
14	HEA	A	602[B]	18,1	57,67,67	1.64	12 (21%)	61,103,103	2.00	15 (24%)
20	EDO	R	201	-	3,3,3	0.82	0	2,2,2	0.35	0
20	EDO	P	310	-	3,3,3	1.03	0	2,2,2	0.32	0
20	EDO	B	307	-	3,3,3	0.80	0	2,2,2	0.71	0
20	EDO	S	102	-	3,3,3	1.27	0	2,2,2	0.76	0
20	EDO	P	311	-	3,3,3	0.70	0	2,2,2	1.87	1 (50%)
20	EDO	N	612	-	3,3,3	0.56	0	2,2,2	1.41	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	EDO	A	611	-	-	0/1/1/1	-
20	EDO	E	203	-	-	1/1/1/1	-
20	EDO	L	102	-	-	1/1/1/1	-
27	PEK	T	101	-	-	25/56/56/56	-
20	EDO	A	619	-	-	0/1/1/1	-
24	DMU	P	309	-	-	12/19/59/59	0/2/2/2
26	CDL	T	102	-	-	59/110/110/110	-
24	DMU	P	306	-	-	3/19/59/59	0/2/2/2
20	EDO	N	611	-	-	0/1/1/1	-
22	CHD	P	305	-	-	5/9/74/74	0/4/4/4
14	HEA	A	602[A]	18,1	-	5/32/76/76	-
20	EDO	M	102	-	-	0/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
20	EDO	B	304	-	-	0/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	D	203	-	-	0/1/1/1	-
24	DMU	C	302	-	-	9/19/59/59	0/2/2/2
19	PGV	P	303	-	-	14/55/55/55	-
19	PGV	Z	101	-	-	29/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	619	-	-	0/1/1/1	-
14	HEA	N	603[A]	18,1	-	4/32/76/76	-
20	EDO	N	620	-	-	1/1/1/1	-
20	EDO	A	618	-	-	1/1/1/1	-
21	TGL	D	201	-	-	41/65/65/65	-
24	DMU	Z	102	-	-	4/19/59/59	0/2/2/2
27	PEK	G	103	-	-	31/56/56/56	-
24	DMU	P	308	-	-	6/19/59/59	0/2/2/2
28	PSC	O	302	-	-	24/55/55/55	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	Y	102	-	-	0/1/1/1	-
26	CDL	C	305	-	-	62/110/110/110	-
20	EDO	A	616	-	-	0/1/1/1	-
28	PSC	E	201	-	-	38/55/55/55	-
19	PGV	A	609	-	-	22/55/55/55	-
22	CHD	W	101	-	-	6/9/74/74	0/4/4/4
26	CDL	N	601	-	-	57/110/110/110	-
24	DMU	C	310	-	-	6/19/59/59	0/2/2/2
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
22	CHD	C	306	-	-	7/9/74/74	0/4/4/4
20	EDO	N	616	-	-	0/1/1/1	-
20	EDO	S	103	-	-	1/1/1/1	-
19	PGV	A	608	-	-	8/55/55/55	-
24	DMU	M	101	-	-	5/19/59/59	0/2/2/2
22	CHD	G	102	-	-	2/9/74/74	0/4/4/4
20	EDO	A	610	-	-	1/1/1/1	-
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
20	EDO	N	618	-	-	0/1/1/1	-
14	HEA	N	602	1	-	6/32/76/76	-
20	EDO	T	103	-	-	0/1/1/1	-
20	EDO	A	615	-	-	1/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
19	PGV	N	609	-	-	6/55/55/55	-
20	EDO	E	204	-	-	0/1/1/1	-
21	TGL	B	301	-	-	33/65/65/65	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	P	304	-	-	57/110/110/110	-
21	TGL	Y	101	-	-	41/65/65/65	-
20	EDO	B	305	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	29/65/65/65	-
20	EDO	F	103	-	-	0/1/1/1	-
27	PEK	C	307	-	-	32/56/56/56	-
24	DMU	C	311	-	-	9/19/59/59	0/2/2/2
21	TGL	L	101	-	-	41/65/65/65	-
20	EDO	A	612	-	-	0/1/1/1	-
27	PEK	G	101	-	-	17/56/56/56	-
14	HEA	N	603[B]	18,1	-	5/32/76/76	-
19	PGV	C	308	-	-	27/55/55/55	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	N	617	-	-	1/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	E	202	-	-	0/1/1/1	-
14	HEA	A	601	1	-	7/32/76/76	-
19	PGV	C	304	-	-	17/55/55/55	-
21	TGL	N	610	-	-	35/65/65/65	-
27	PEK	P	307	-	-	24/56/56/56	-
20	EDO	N	614	-	-	0/1/1/1	-
19	PGV	U	101	-	-	25/55/55/55	-
20	EDO	D	202	-	-	1/1/1/1	-
27	PEK	C	309	-	-	25/56/56/56	-
14	HEA	A	602[B]	18,1	-	4/32/76/76	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-

The worst 5 of 277 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	201	TGL	OB1-CB1	8.22	1.46	1.22
21	Y	101	TGL	OG2-CB1	6.50	1.52	1.34
19	C	308	PGV	O01-C1	6.36	1.52	1.34
27	C	307	PEK	O01-C1	6.35	1.52	1.34
21	L	101	TGL	OG2-CB1	6.30	1.52	1.34

The worst 5 of 607 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	305	CHD	C23-C22-C20	-16.38	84.59	114.52
22	C	306	CHD	C23-C22-C20	-14.41	88.20	114.52
24	C	311	DMU	O16-C6-C1	11.51	126.27	108.30
21	D	201	TGL	OG2-CB1-CB2	-10.50	88.87	111.50
27	T	101	PEK	C2-C3-C4	9.42	130.02	113.23

There are no chirality outliers.

5 of 949 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
19	A	609	PGV	C02-C03-O11-P
19	A	609	PGV	C04-C05-C06-O06
19	A	609	PGV	O02-C1-O01-C02

There are no ring outliers.

58 monomers are involved in 428 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	608[B]	AZI	2	0
27	T	101	PEK	1	0
20	A	619	EDO	1	0
24	P	309	DMU	2	0
26	T	102	CDL	19	0
24	P	306	DMU	16	0
22	P	305	CHD	4	0
14	A	602[A]	HEA	2	0
20	B	304	EDO	4	0
20	G	105	EDO	6	0
24	C	302	DMU	16	0
19	P	303	PGV	2	0
19	Z	101	PGV	11	0

Continued on next page...

Continued from previous page...

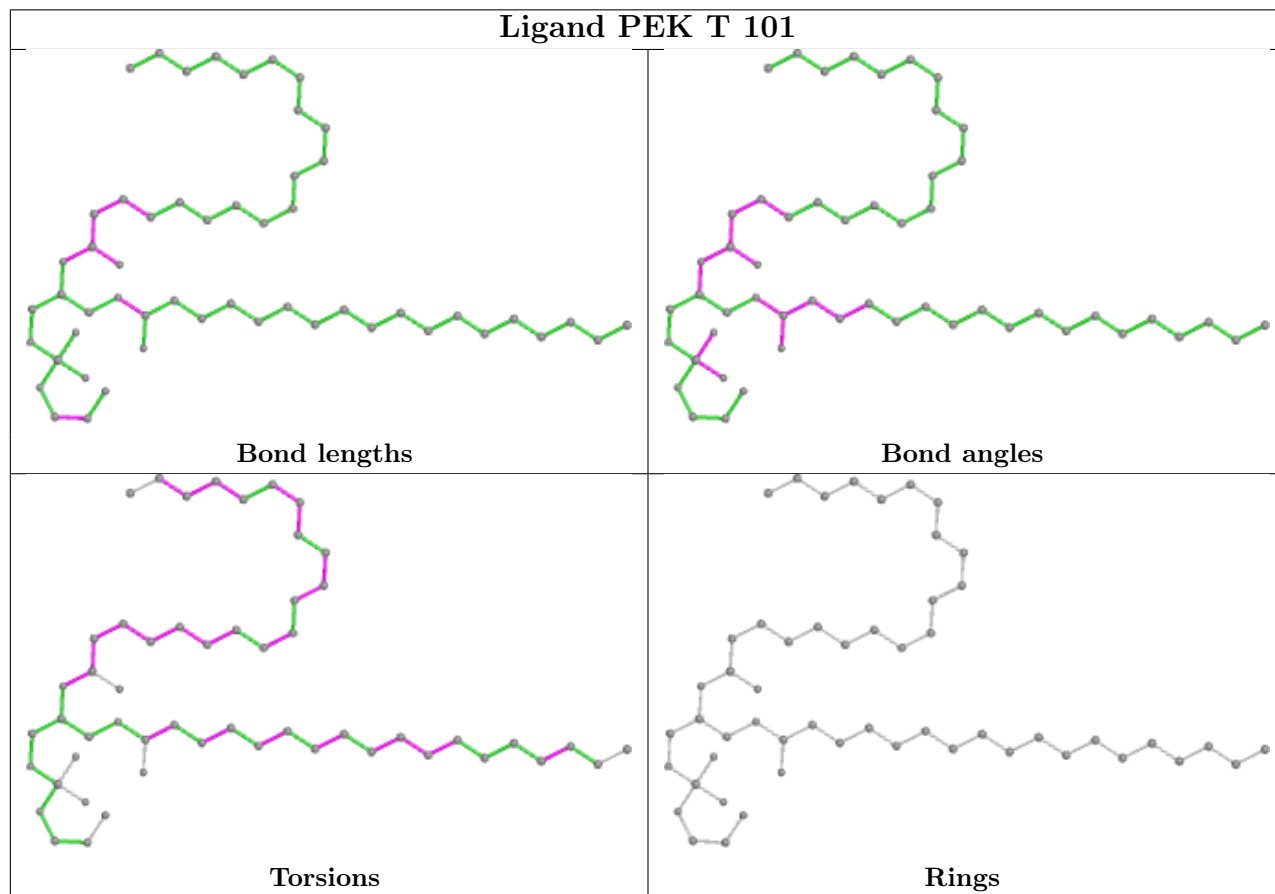
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	619	EDO	1	0
14	N	603[A]	HEA	2	0
20	N	620	EDO	5	0
20	A	618	EDO	3	0
21	D	201	TGL	16	0
24	Z	102	DMU	1	0
27	G	103	PEK	4	0
24	P	308	DMU	2	0
28	O	302	PSC	15	0
26	C	305	CDL	25	0
28	E	201	PSC	12	0
19	A	609	PGV	9	0
22	W	101	CHD	2	0
26	N	601	CDL	26	0
24	C	310	DMU	4	0
20	A	617	EDO	2	0
22	C	306	CHD	4	0
19	A	608	PGV	3	0
22	G	102	CHD	1	0
22	J	101	CHD	1	0
18	A	607[B]	AZI	4	0
14	N	602	HEA	10	0
20	A	615	EDO	6	0
21	B	301	TGL	4	0
26	P	304	CDL	25	0
21	Y	101	TGL	23	0
20	B	305	EDO	1	0
21	Q	201	TGL	13	0
27	C	307	PEK	16	0
24	C	311	DMU	2	0
21	L	101	TGL	10	0
27	G	101	PEK	8	0
14	N	603[B]	HEA	20	0
19	C	308	PGV	2	0
18	A	606[B]	AZI	1	0
20	N	617	EDO	1	0
22	C	301	CHD	1	0
14	A	601	HEA	11	0
19	C	304	PGV	6	0
21	N	610	TGL	6	0
27	P	307	PEK	5	0
19	U	101	PGV	1	0

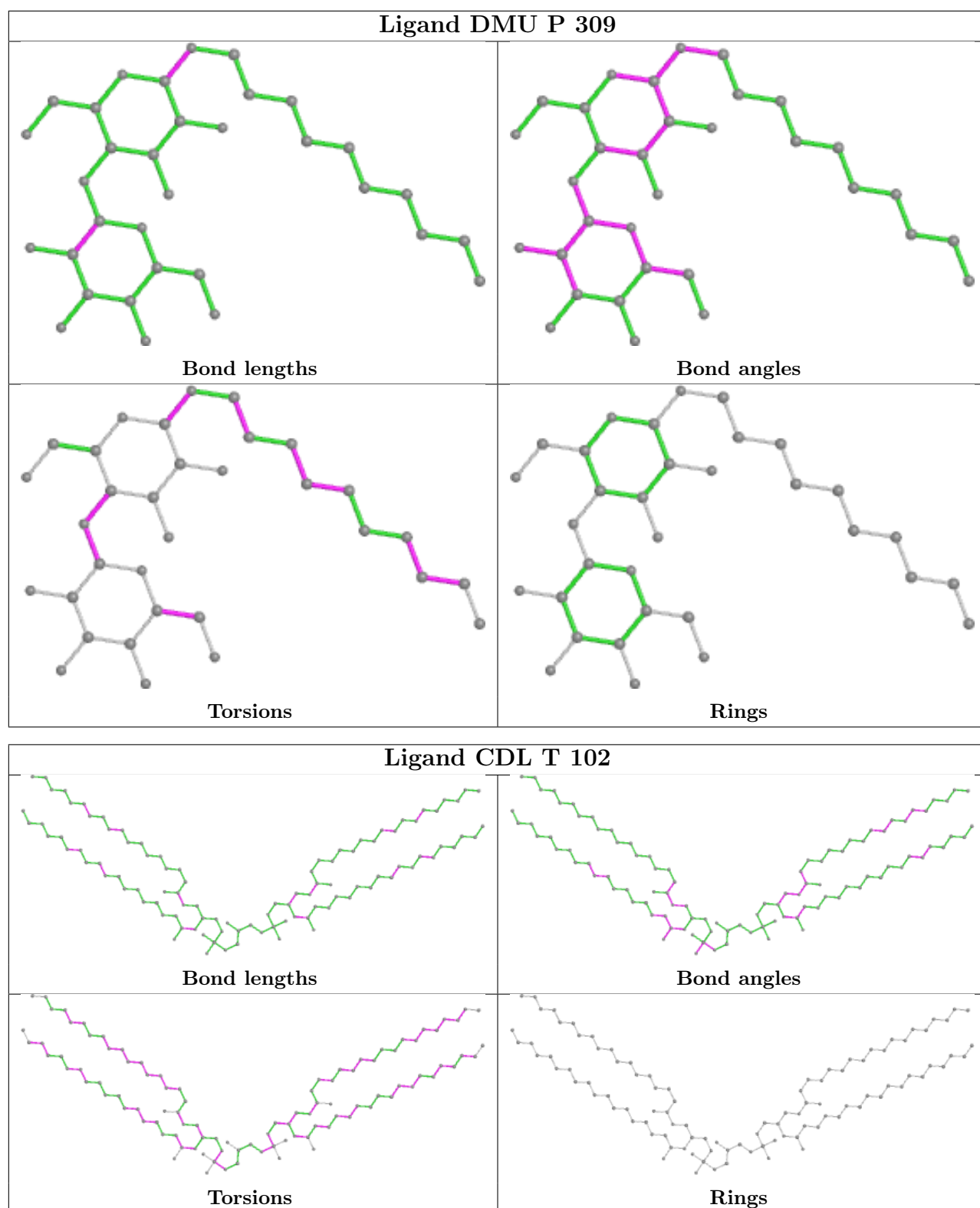
Continued on next page...

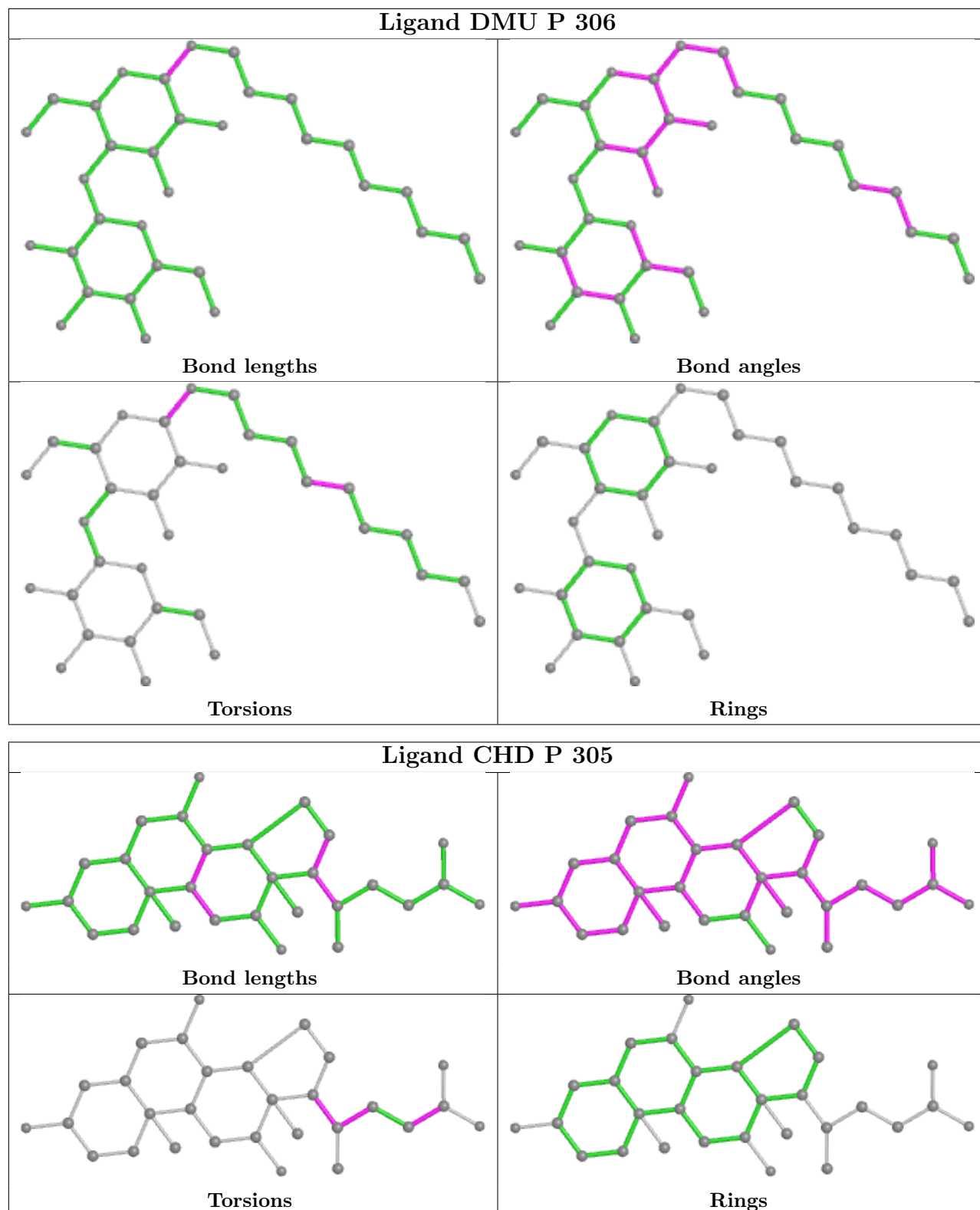
Continued from previous page...

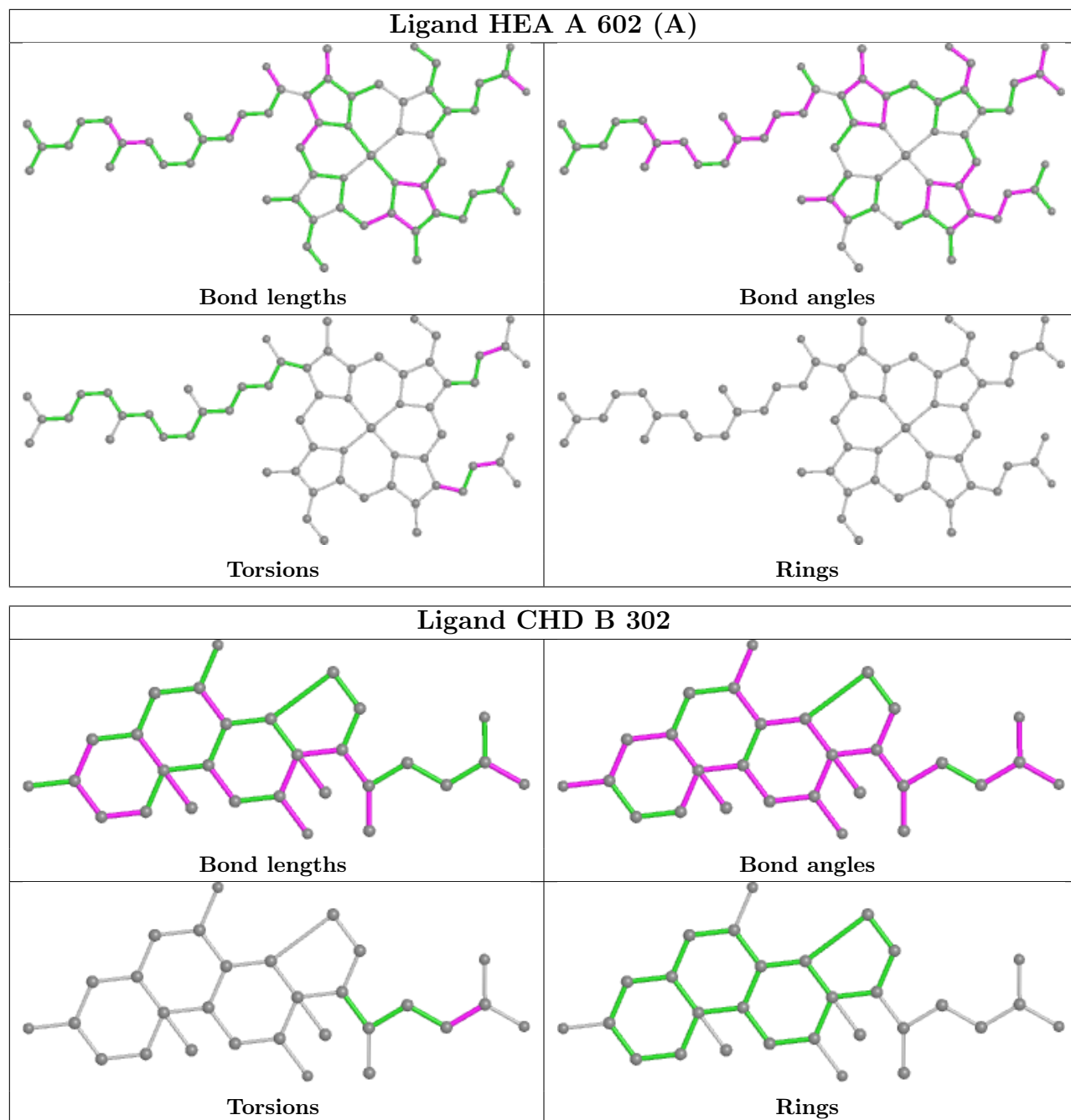
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	202	EDO	12	0
27	C	309	PEK	11	0
14	A	602[B]	HEA	23	0

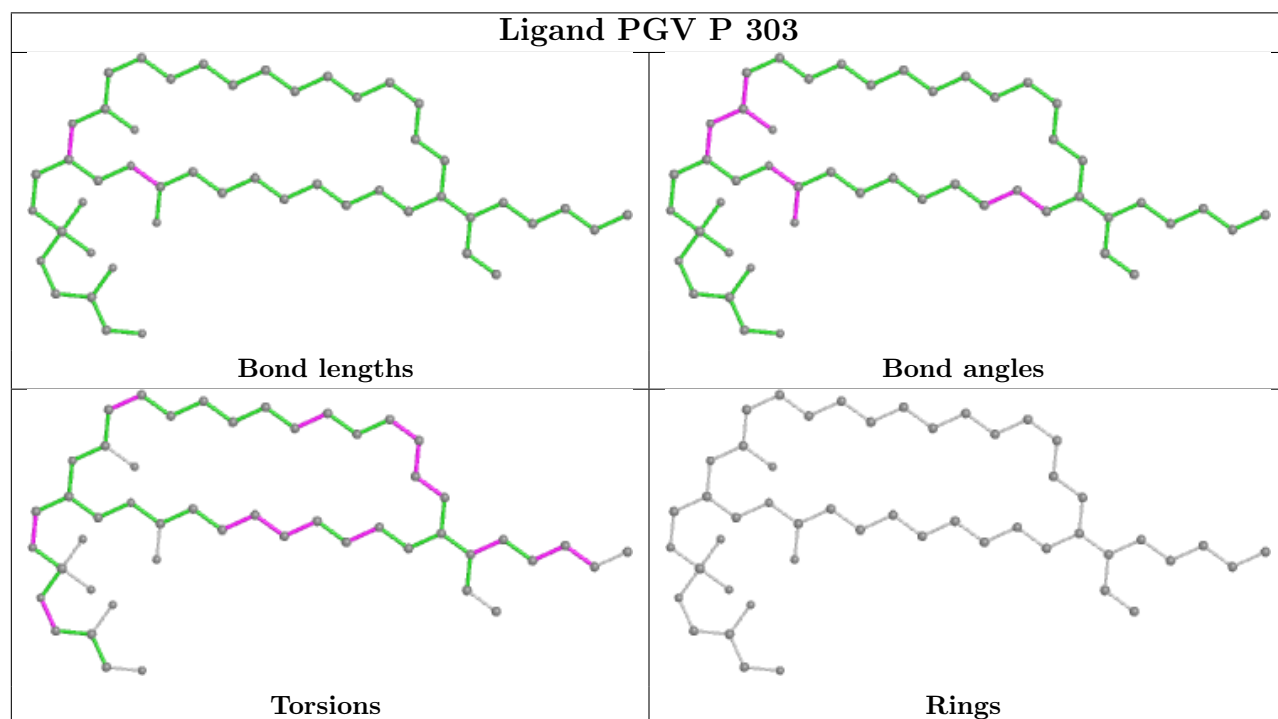
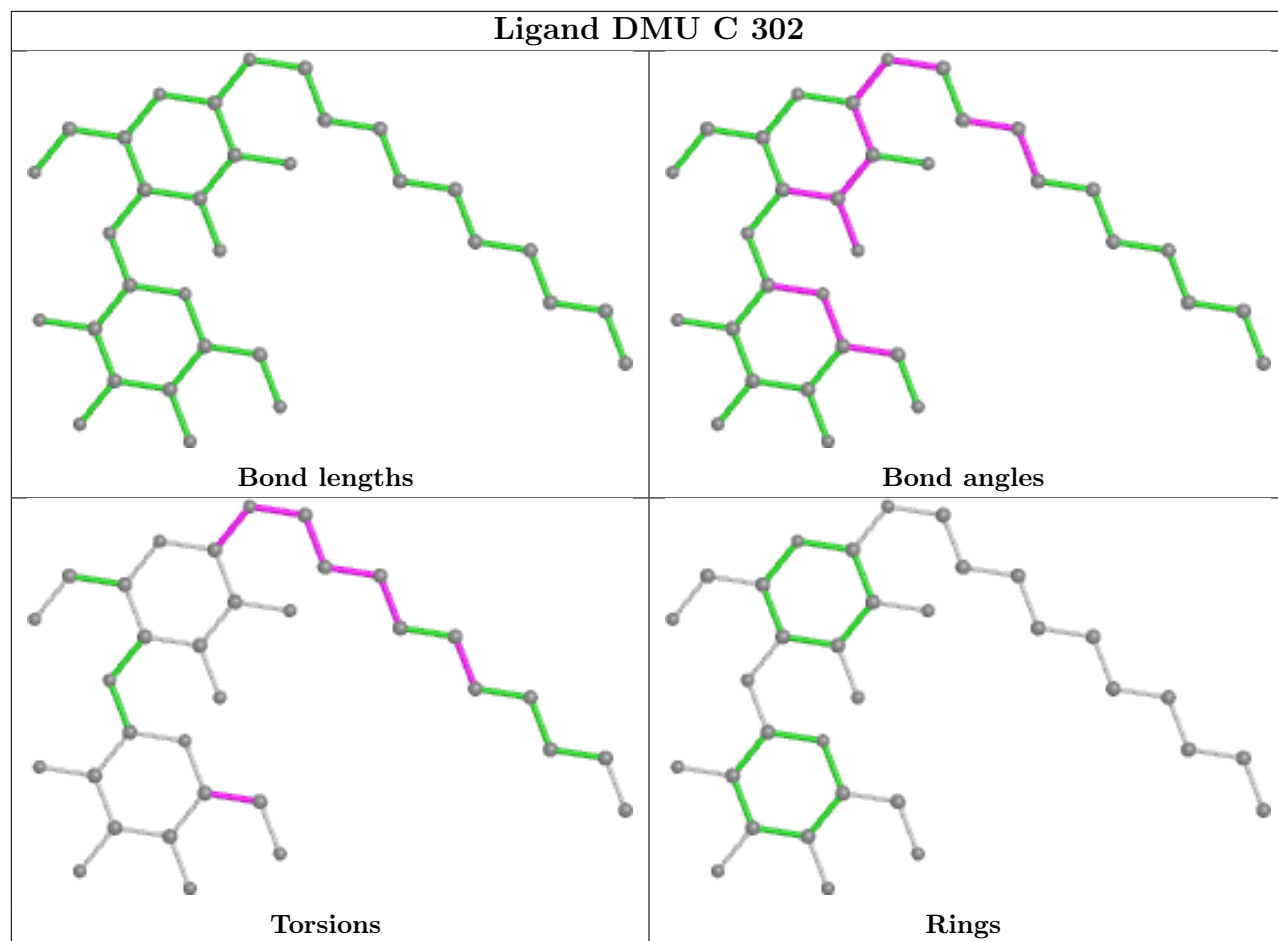
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

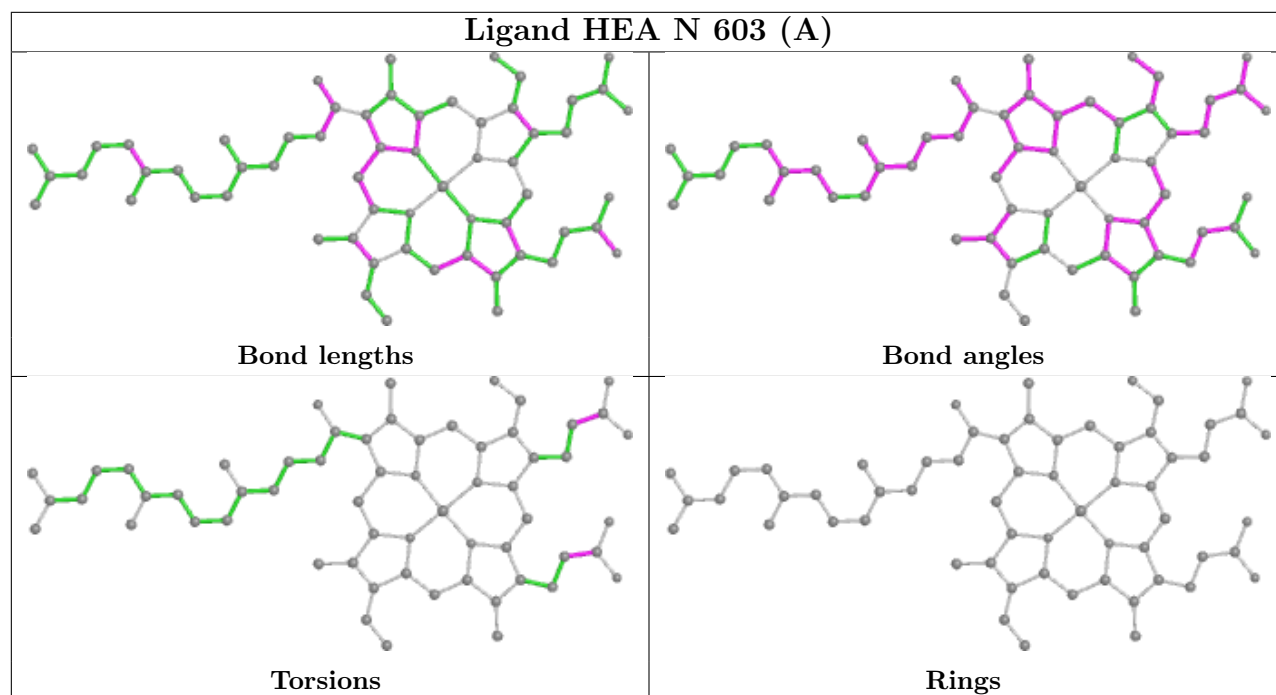
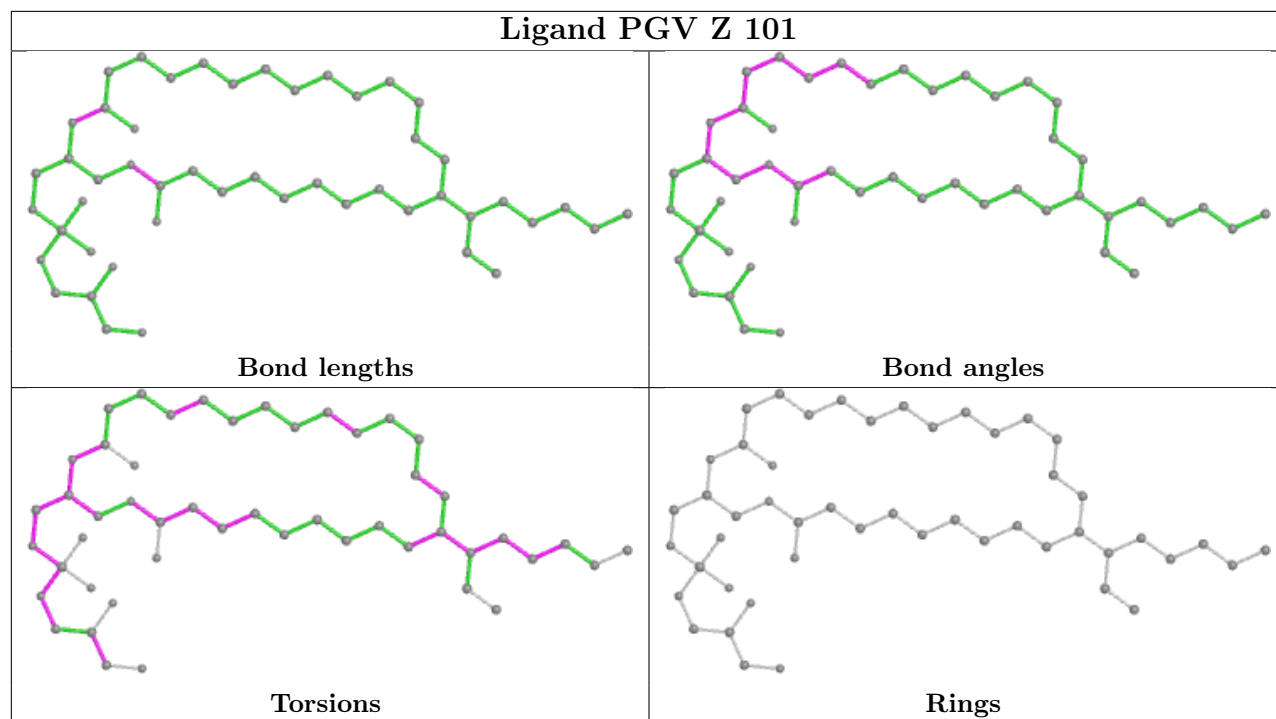


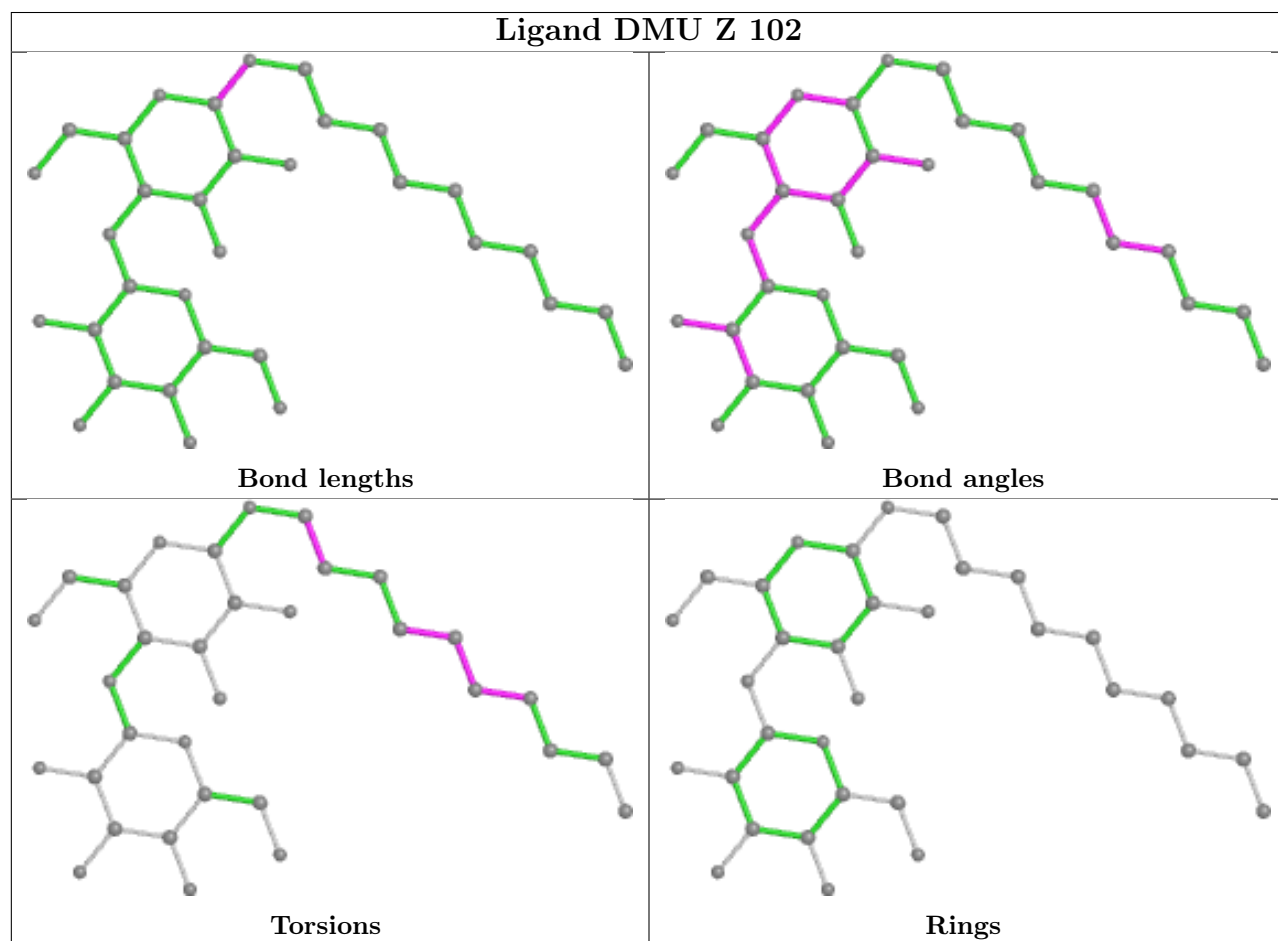
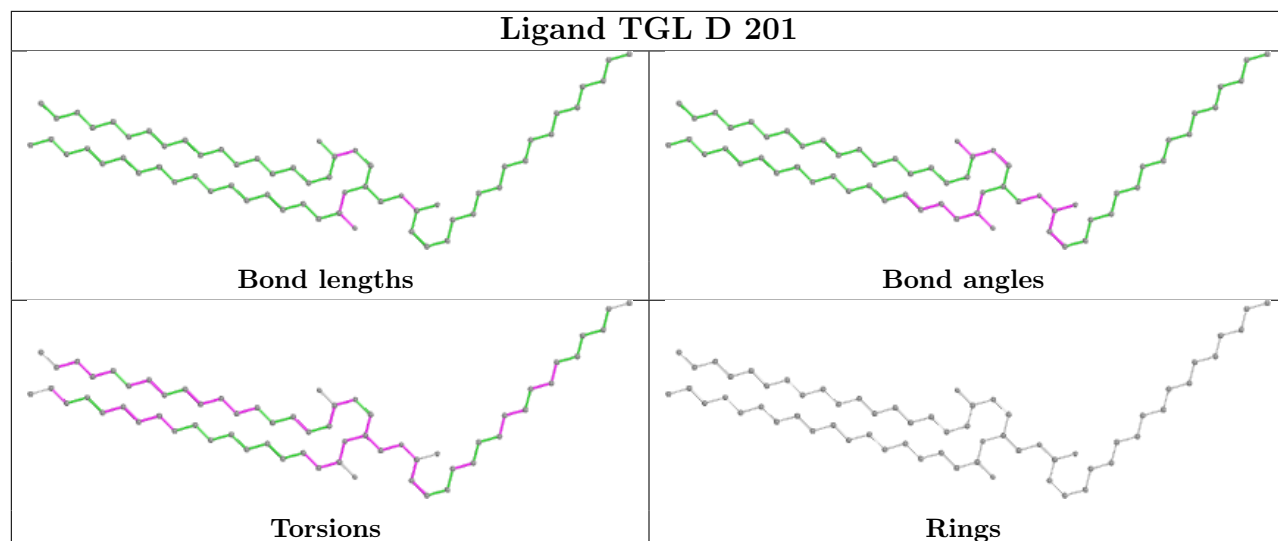


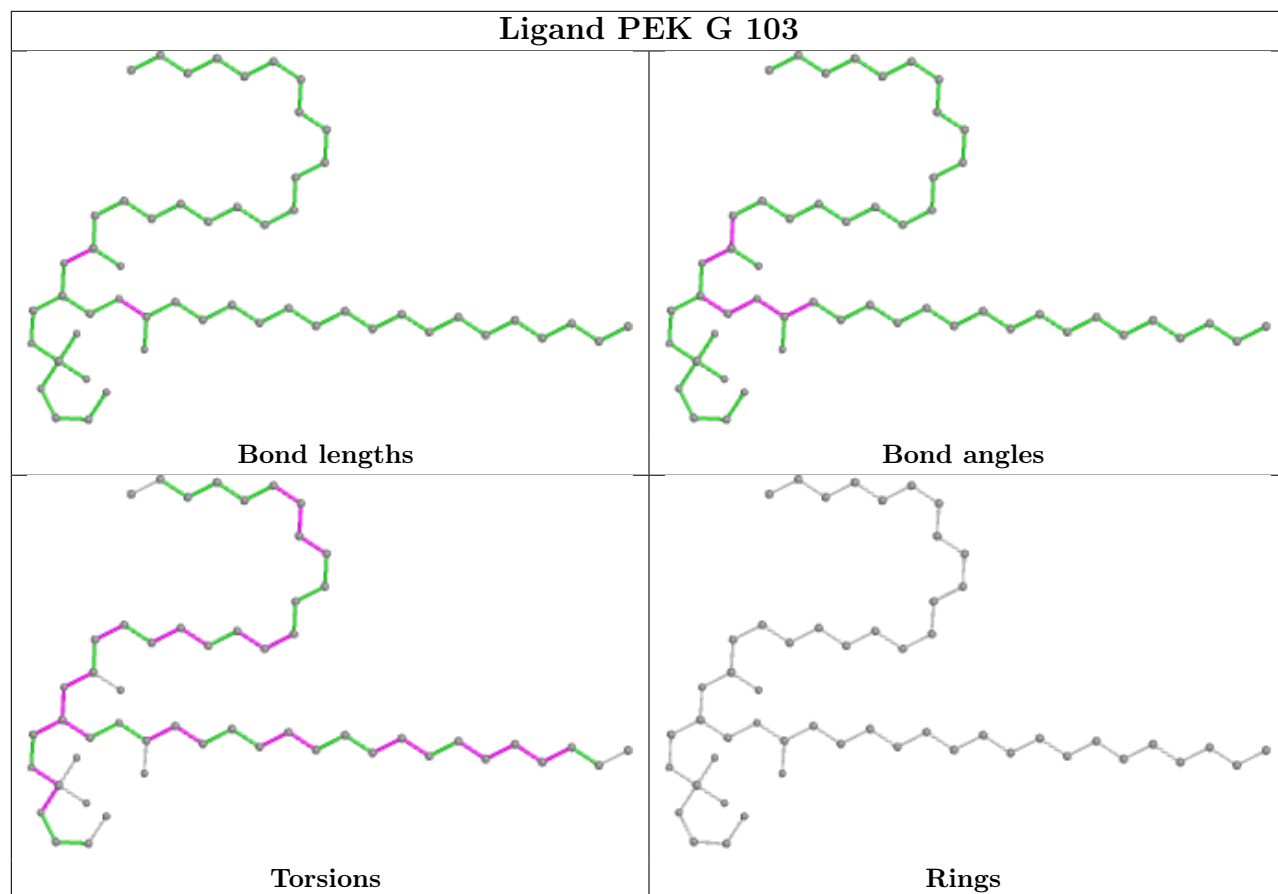


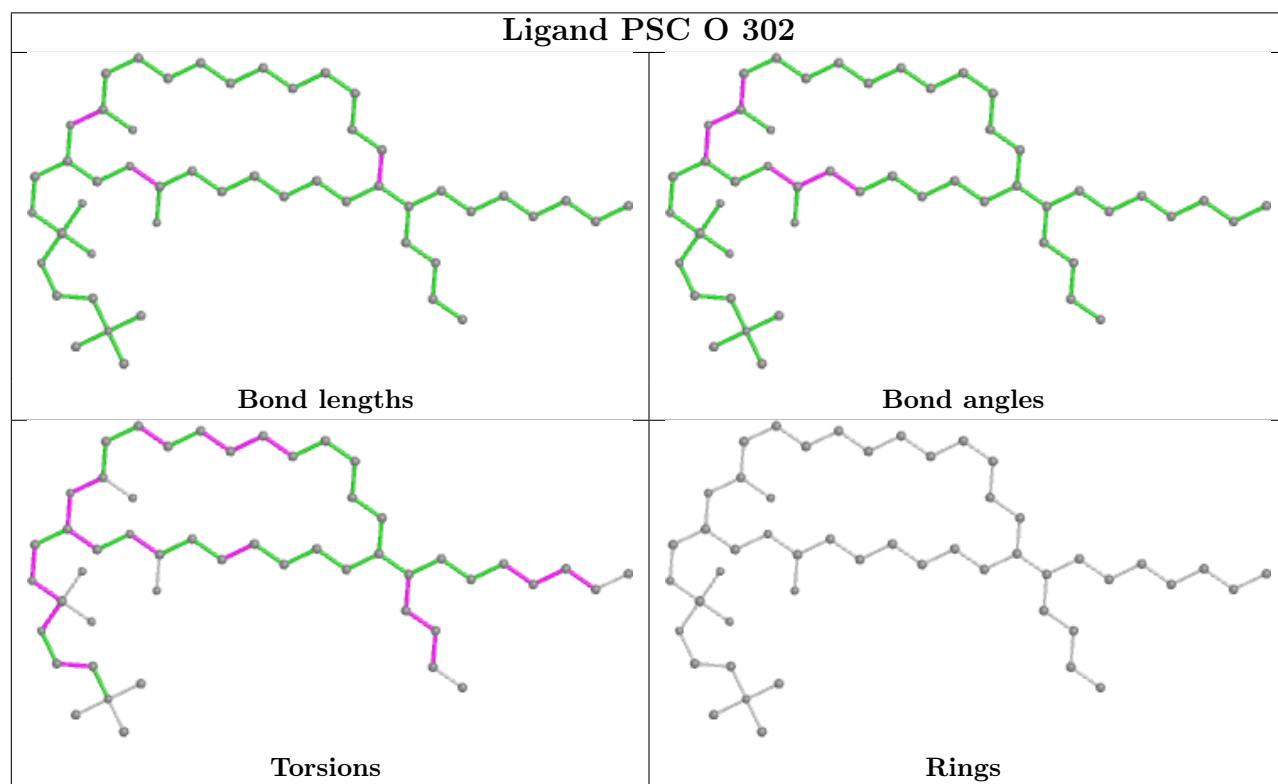
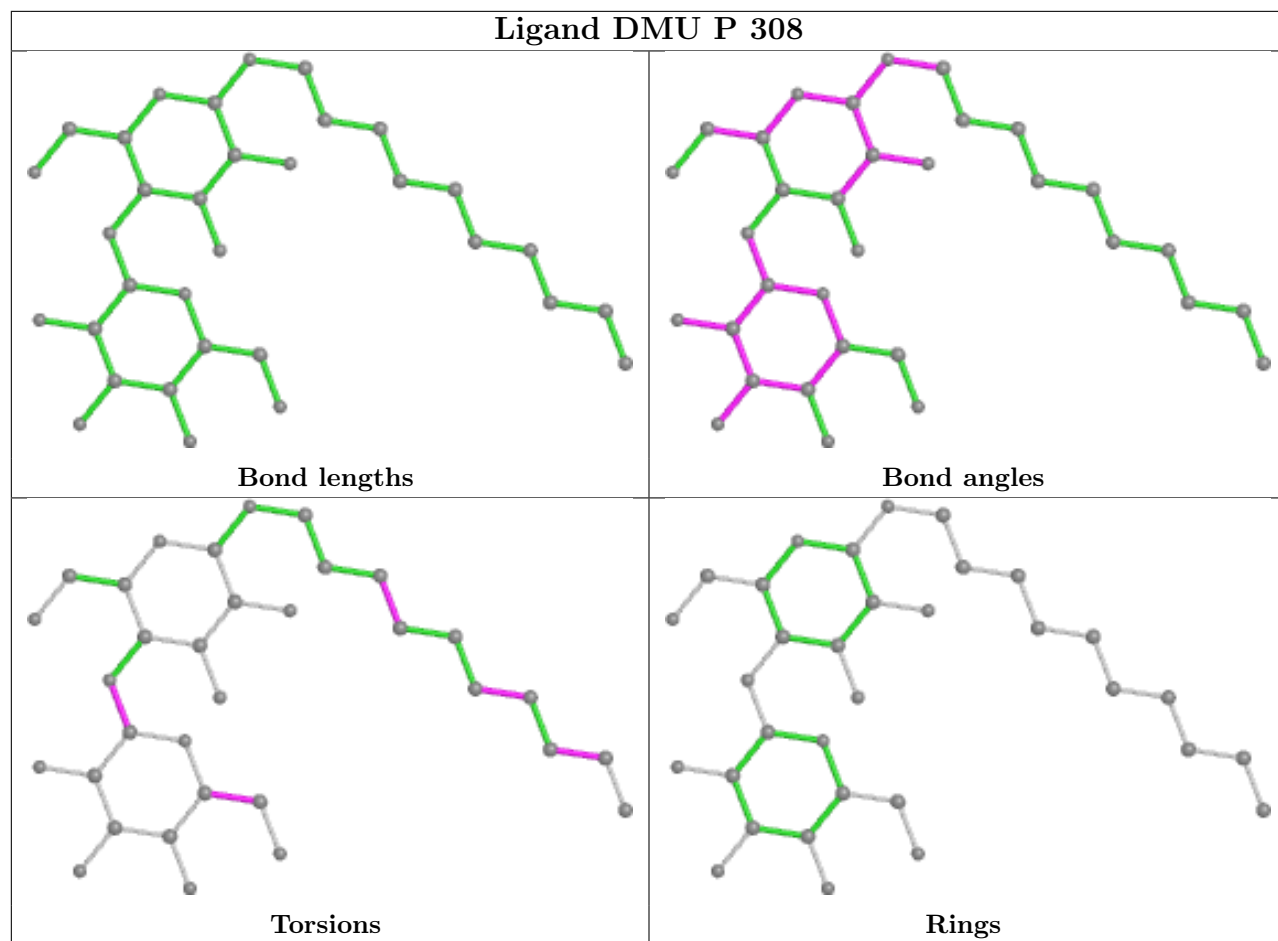


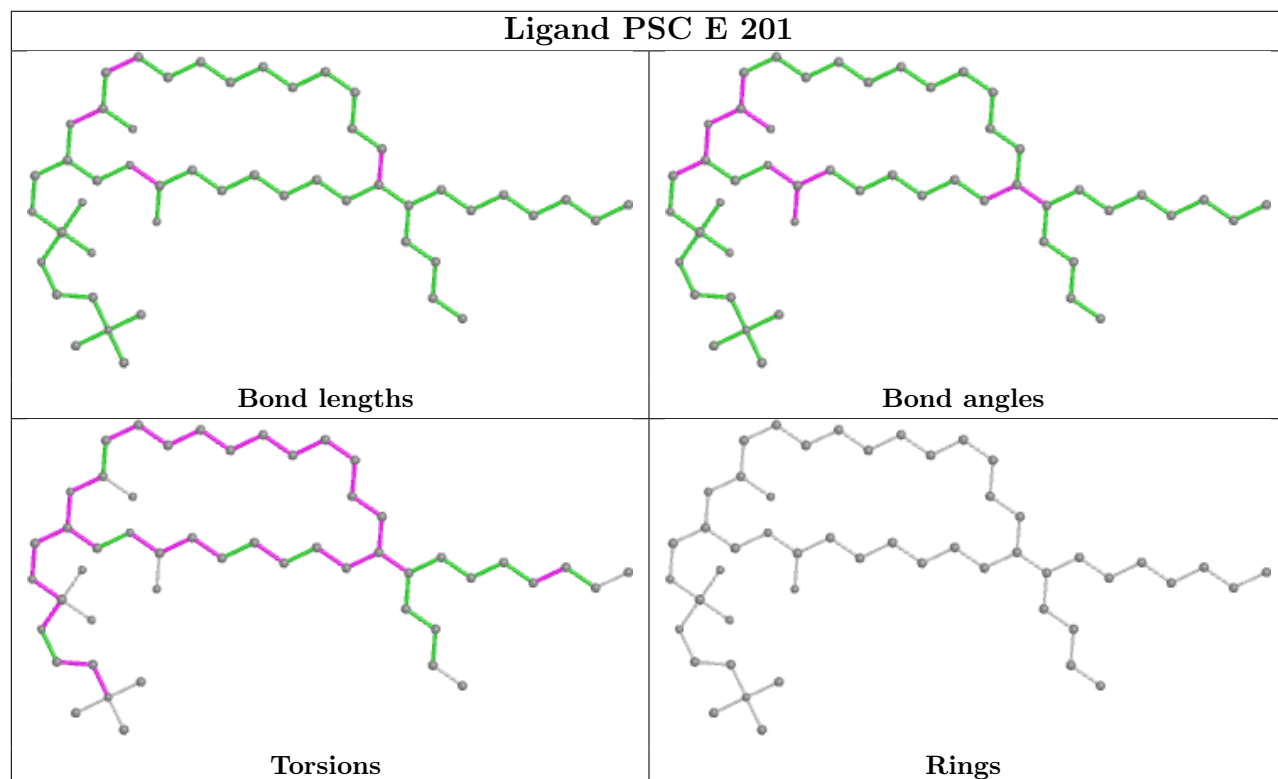
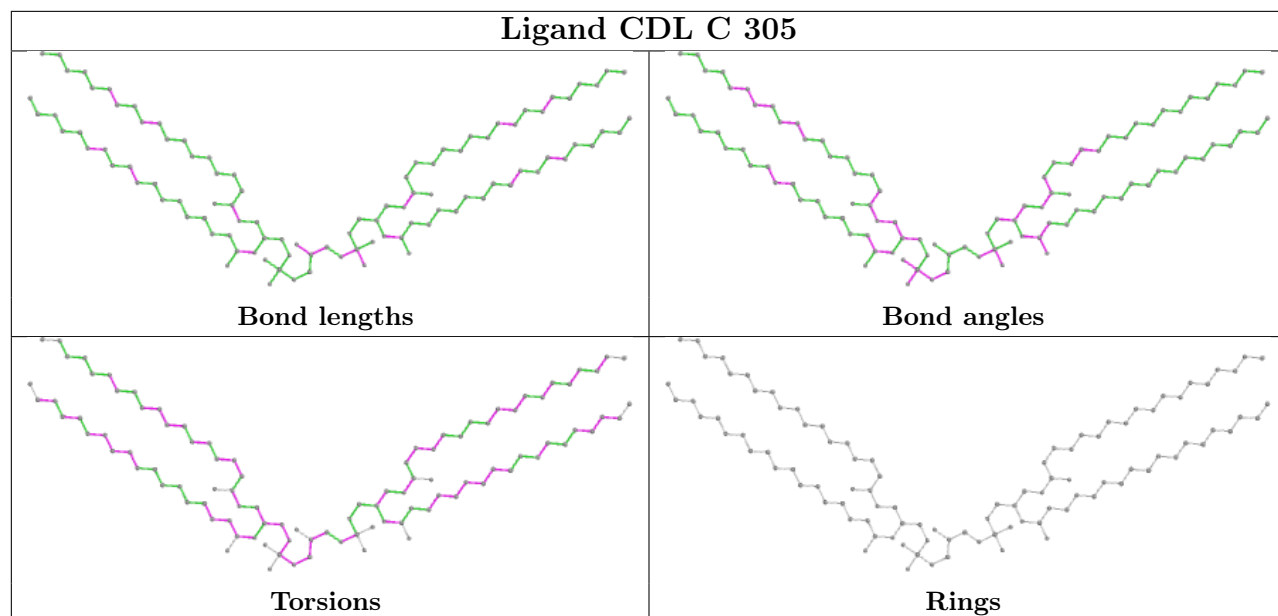


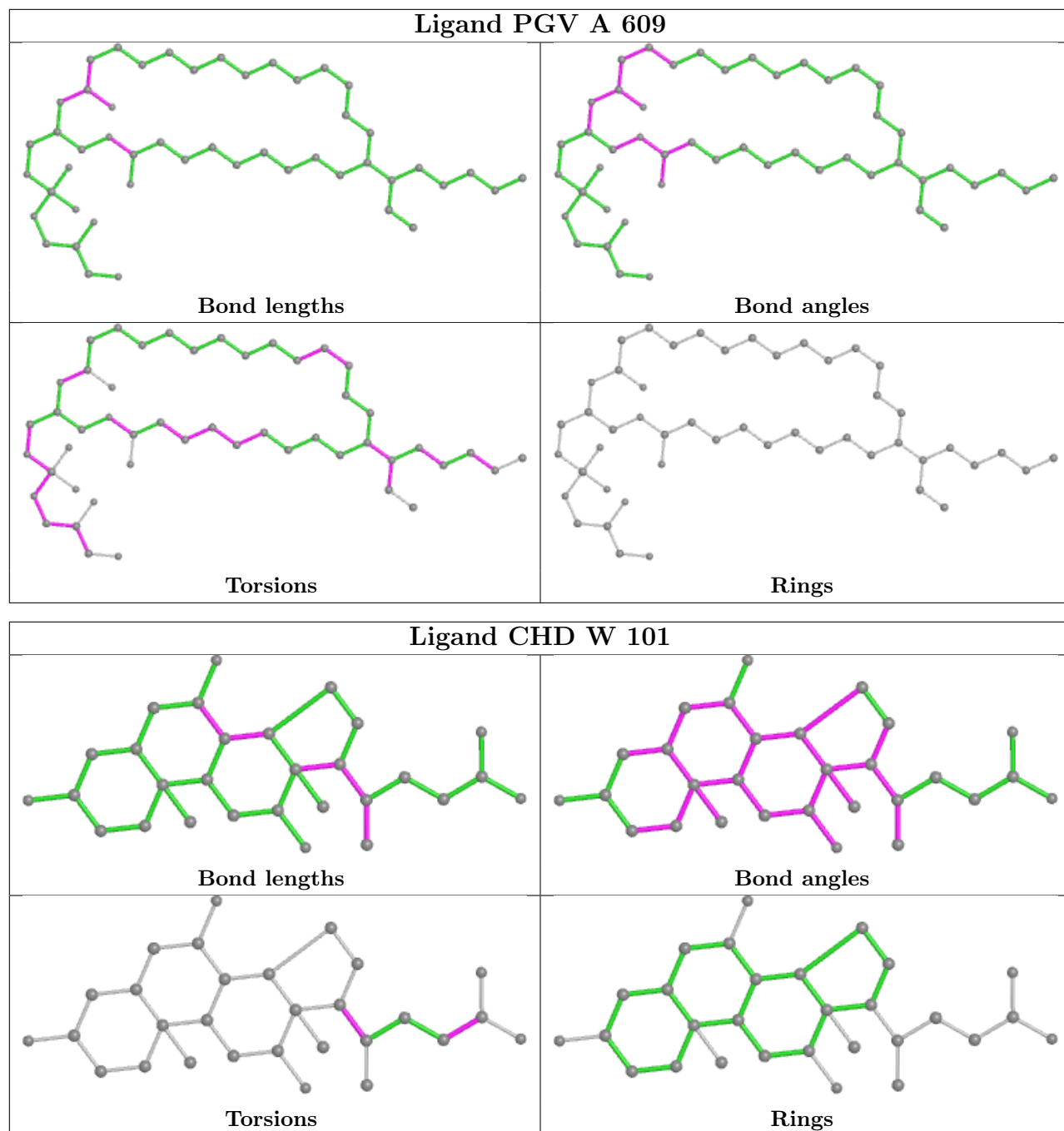


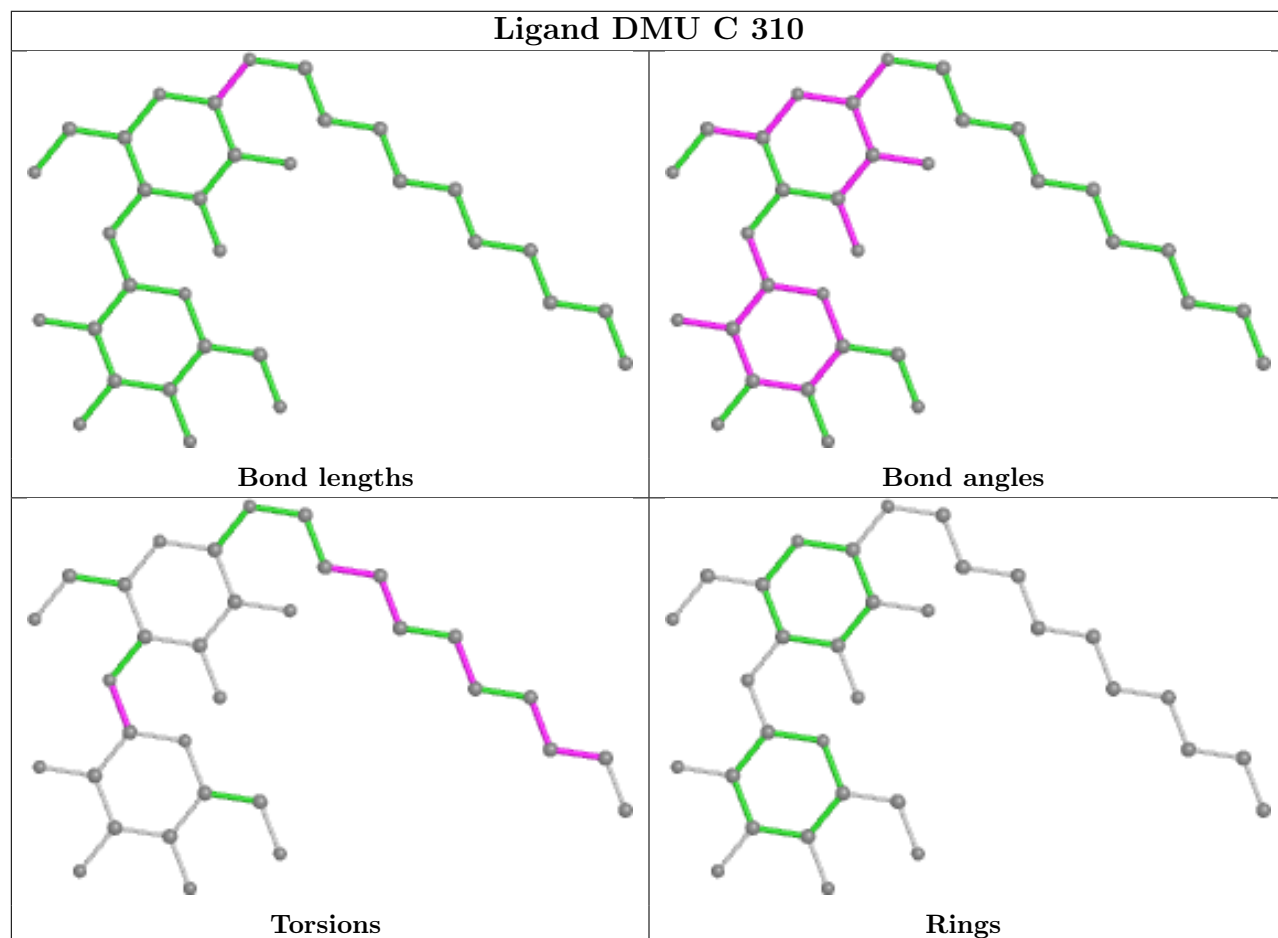
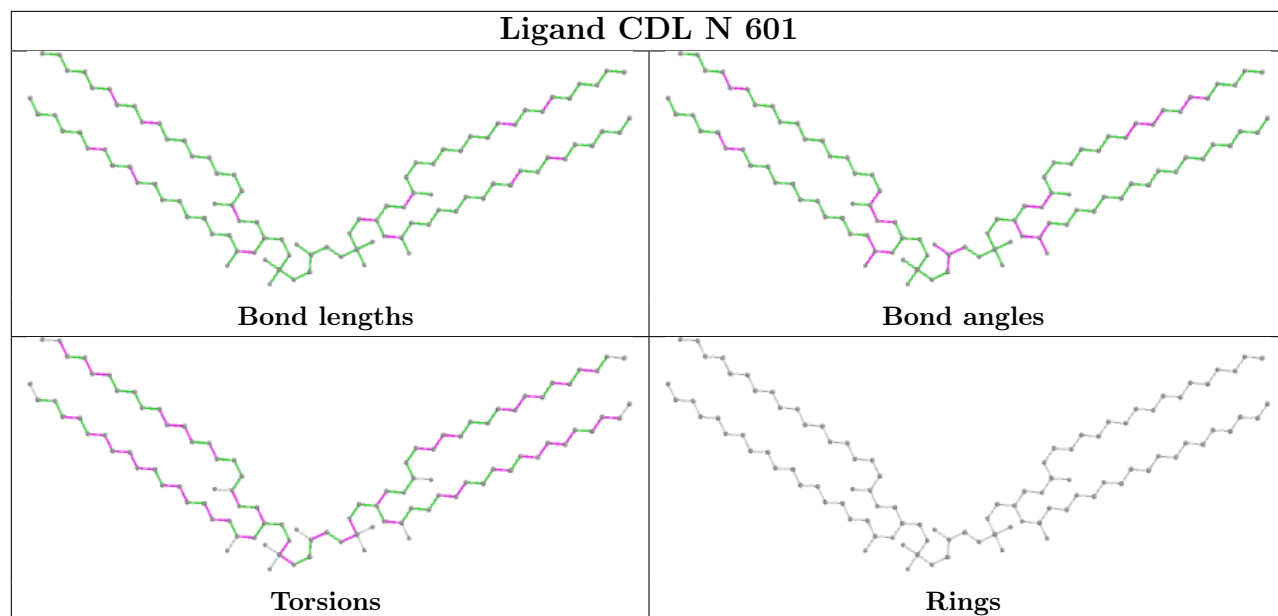


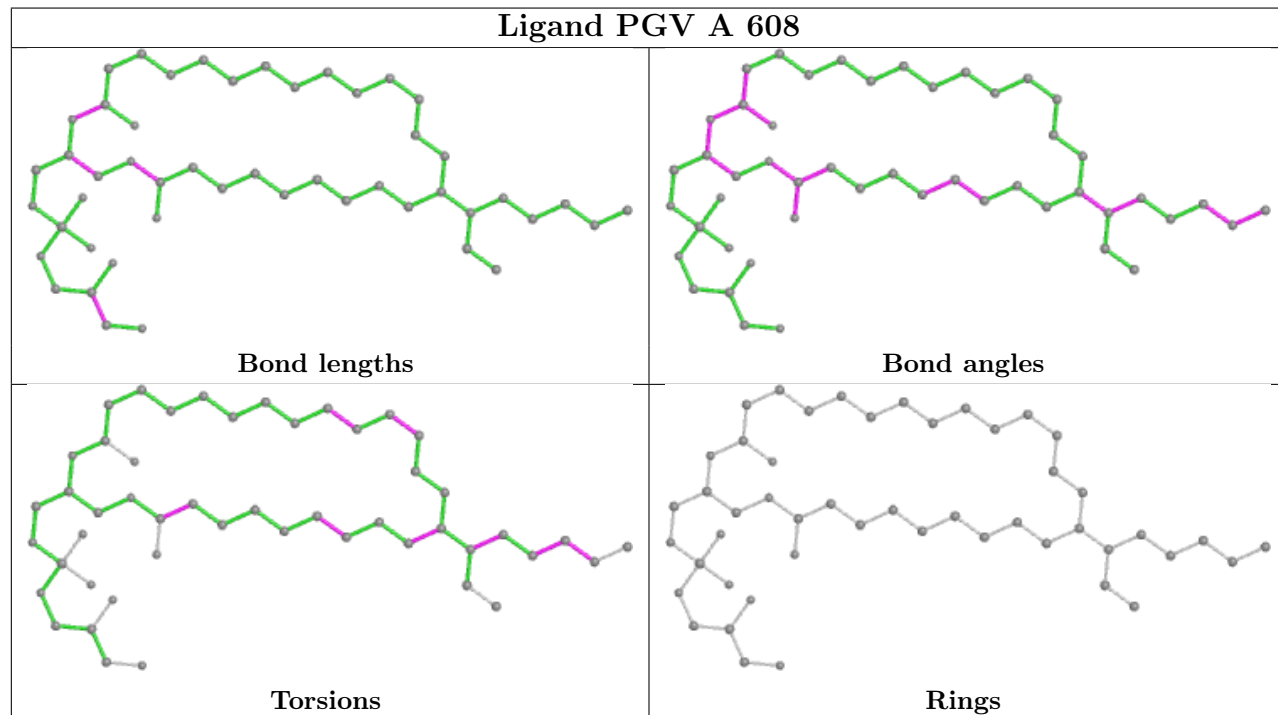
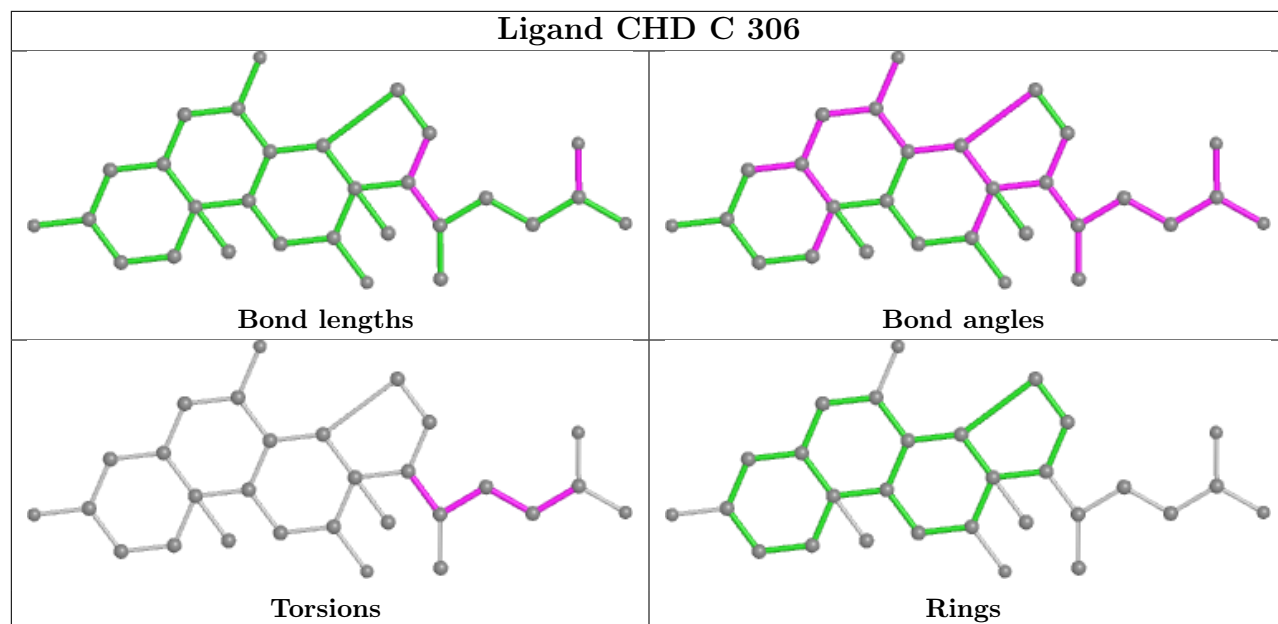


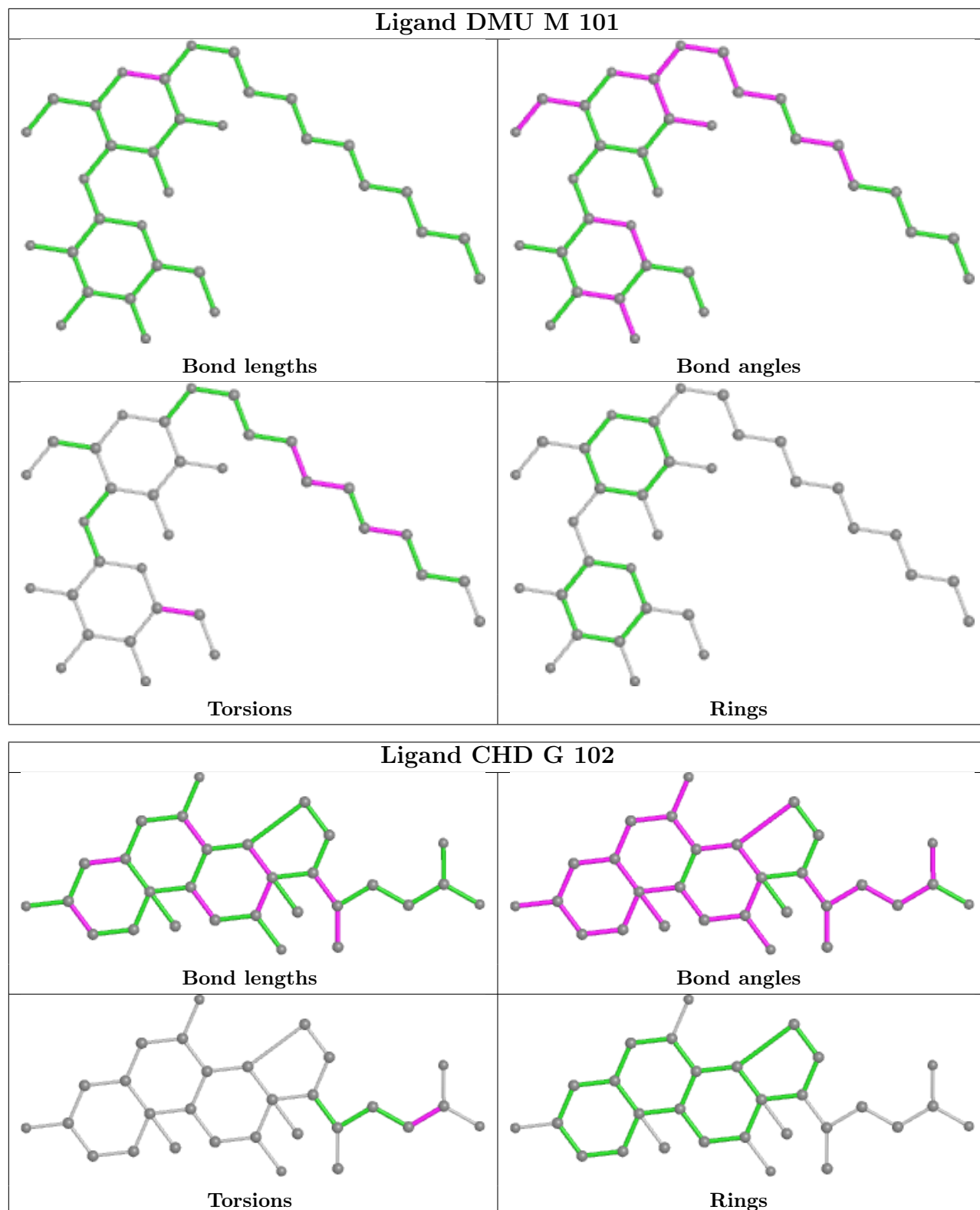


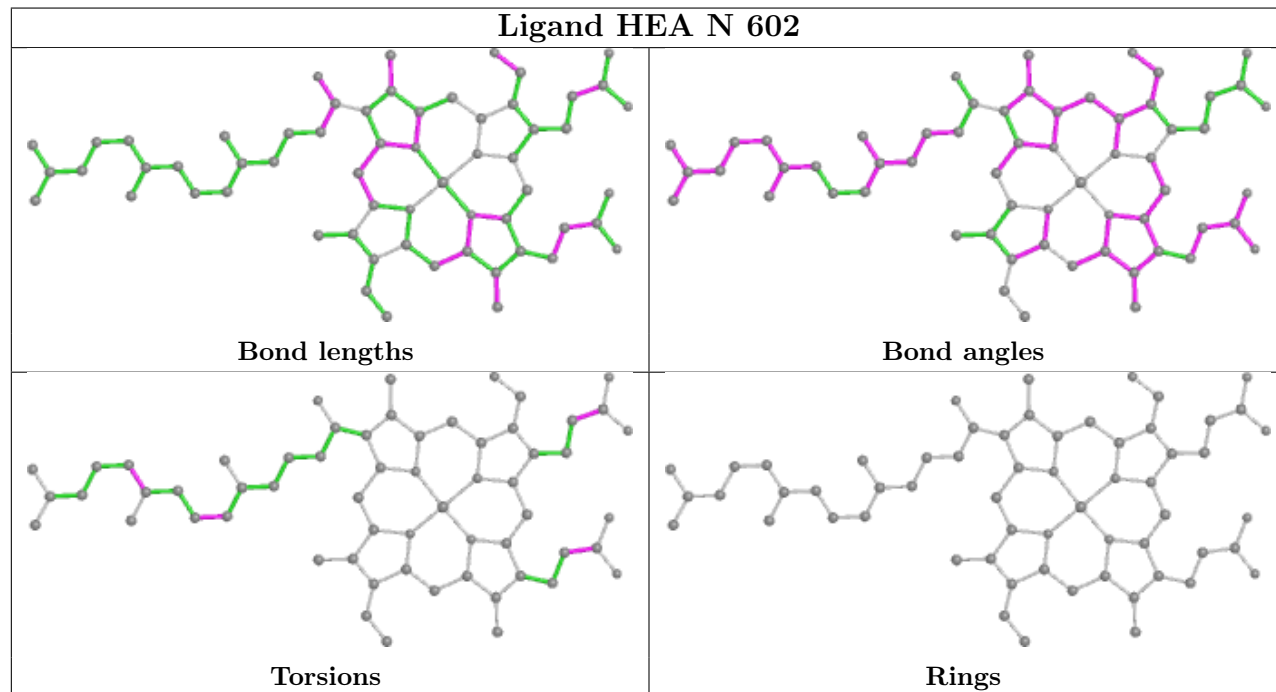
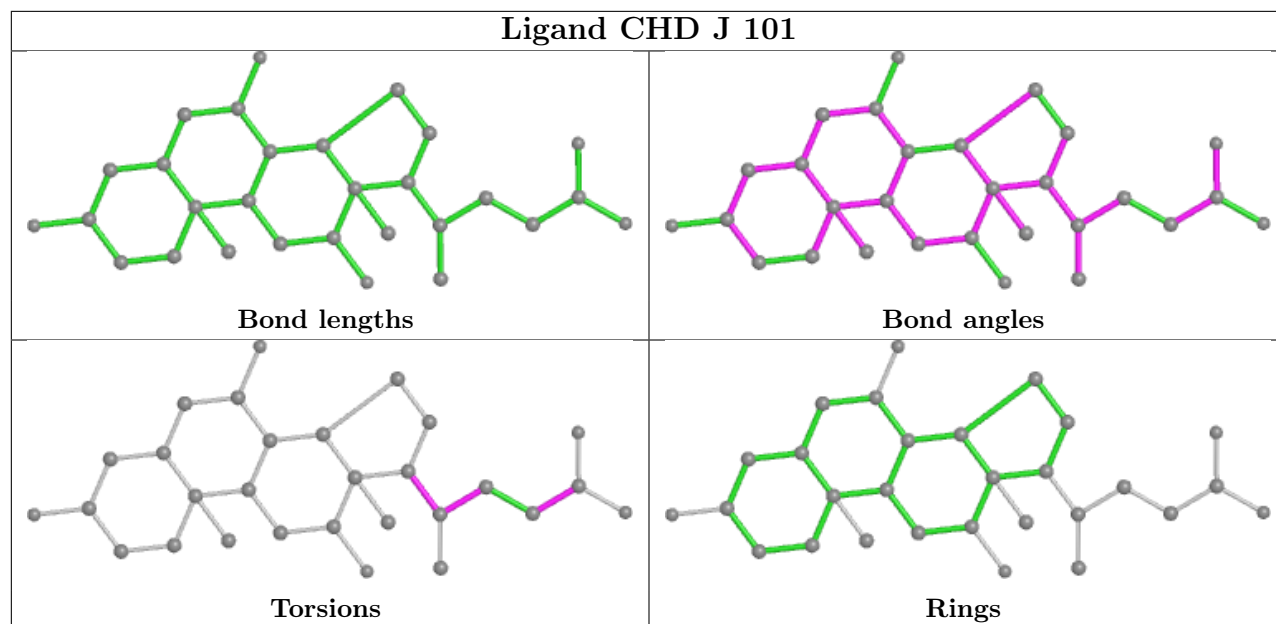


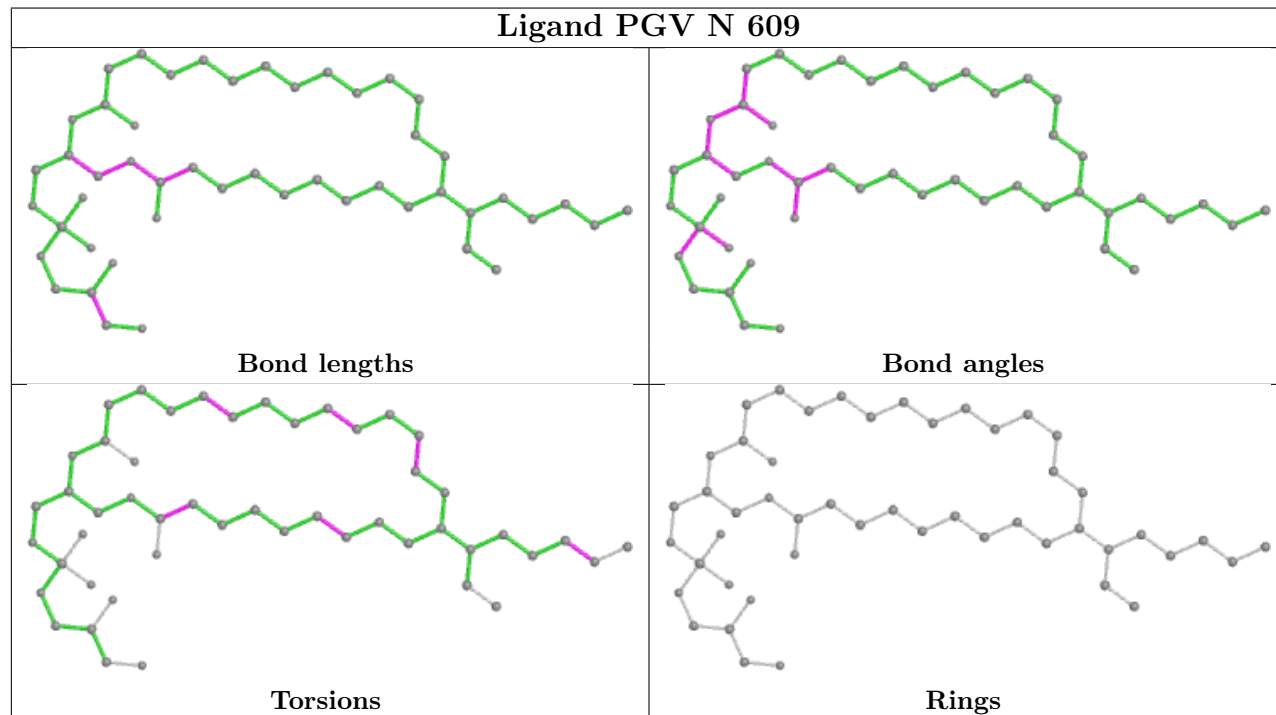
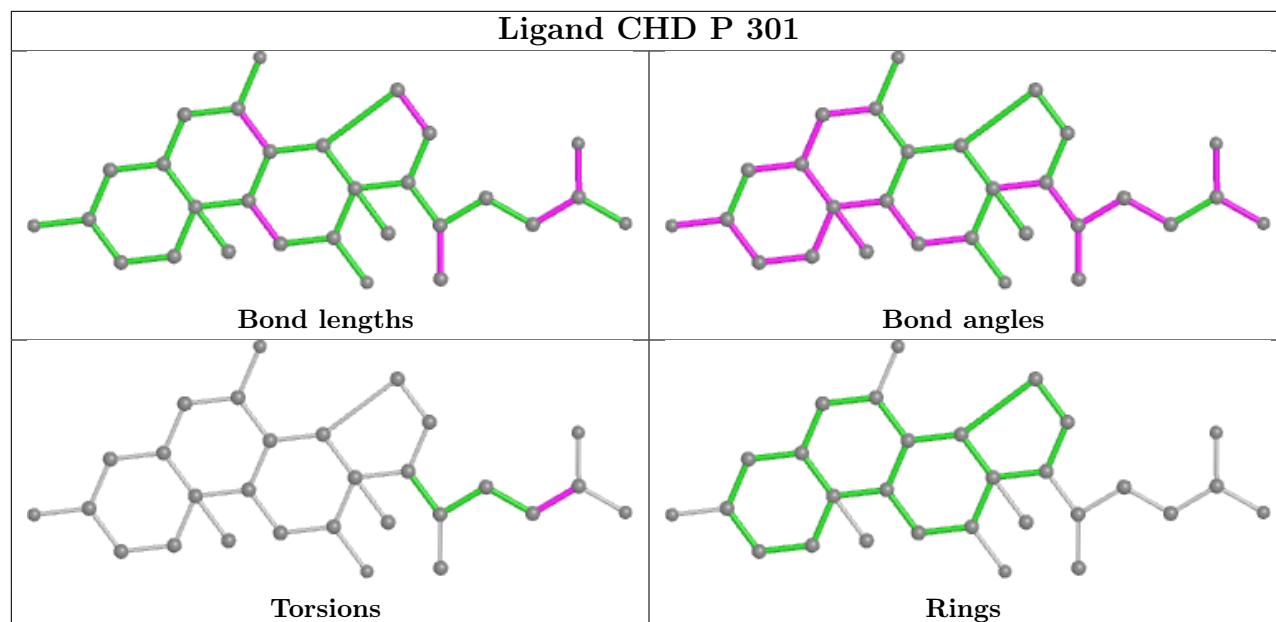


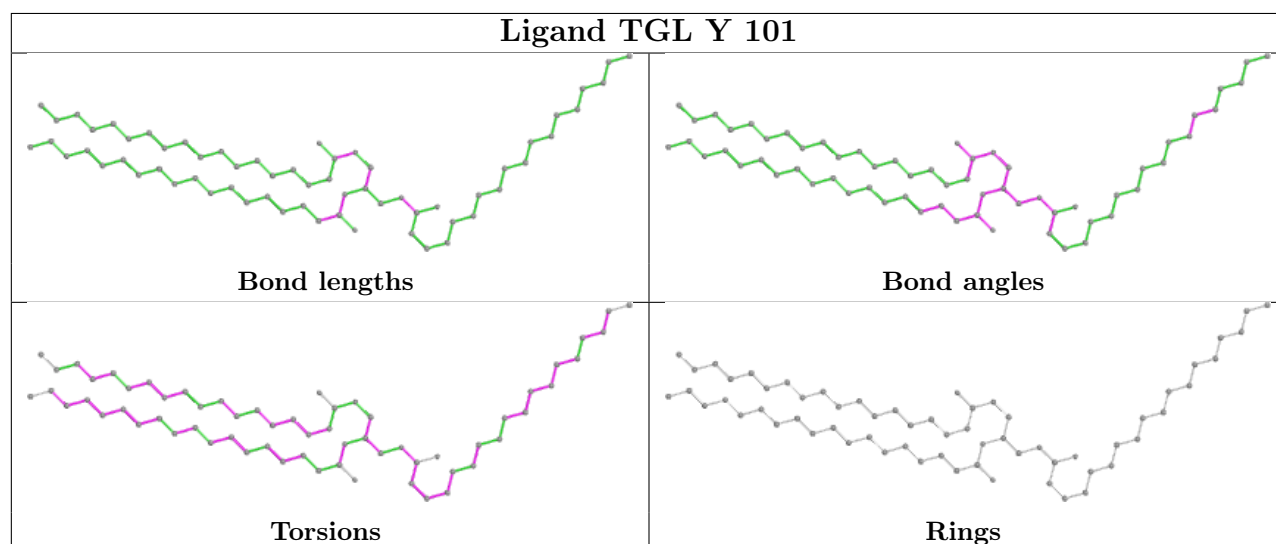
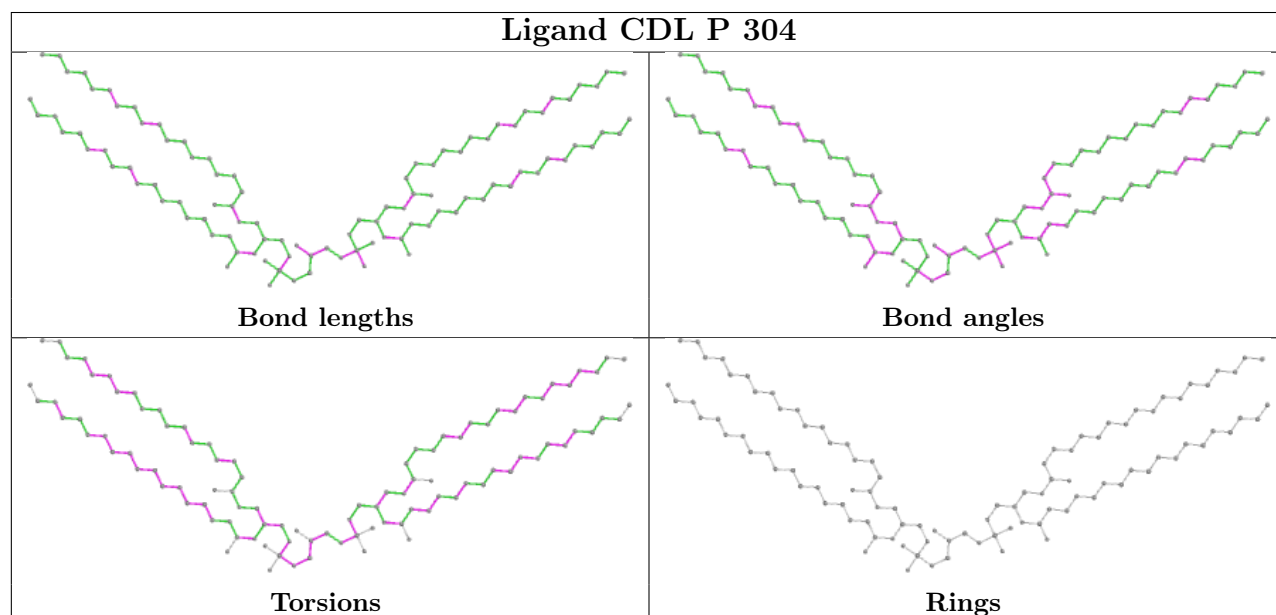
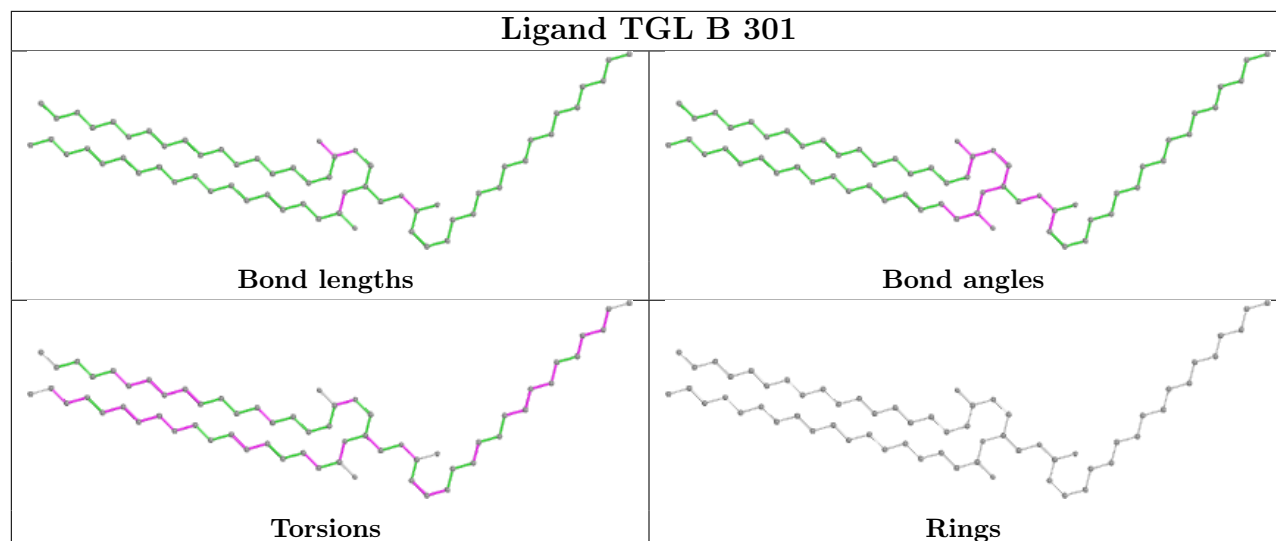


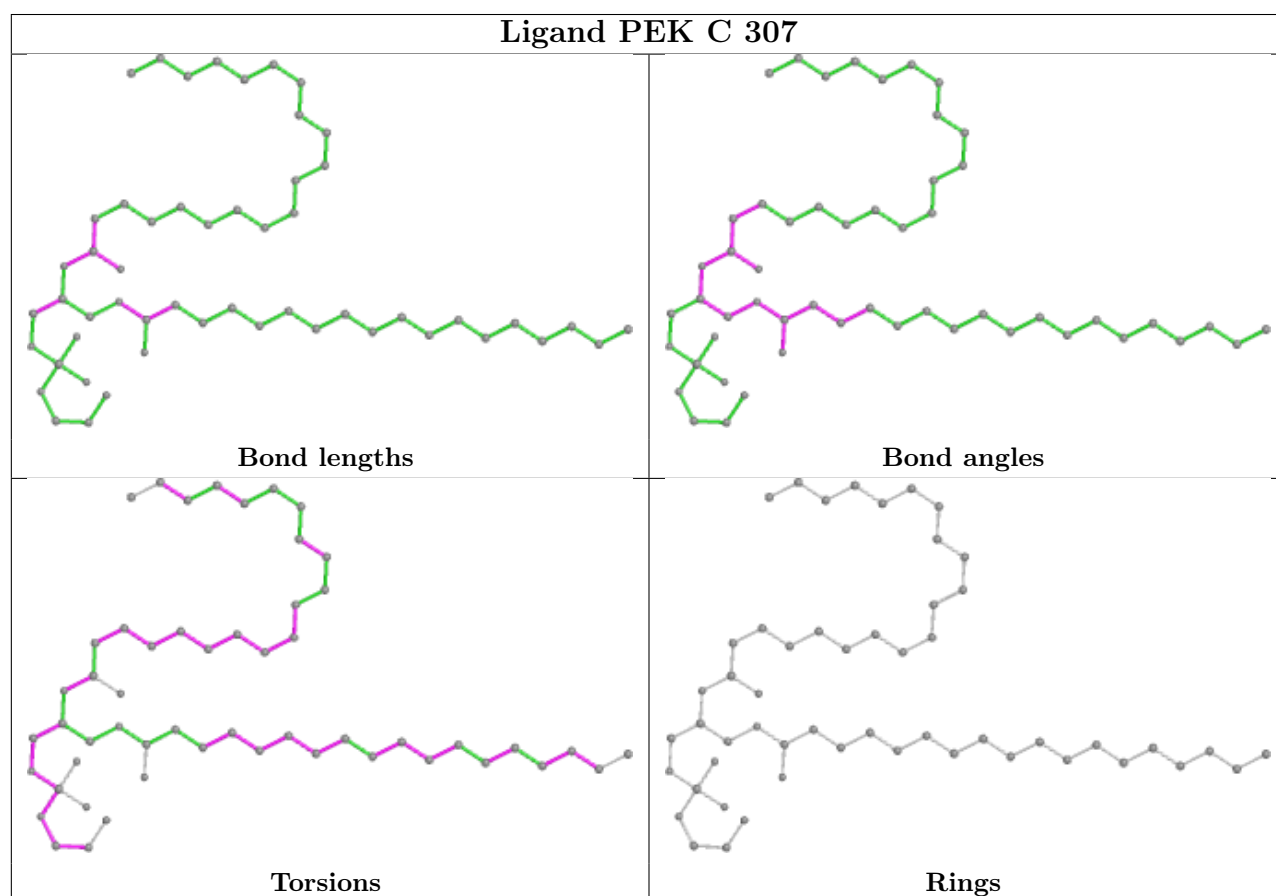
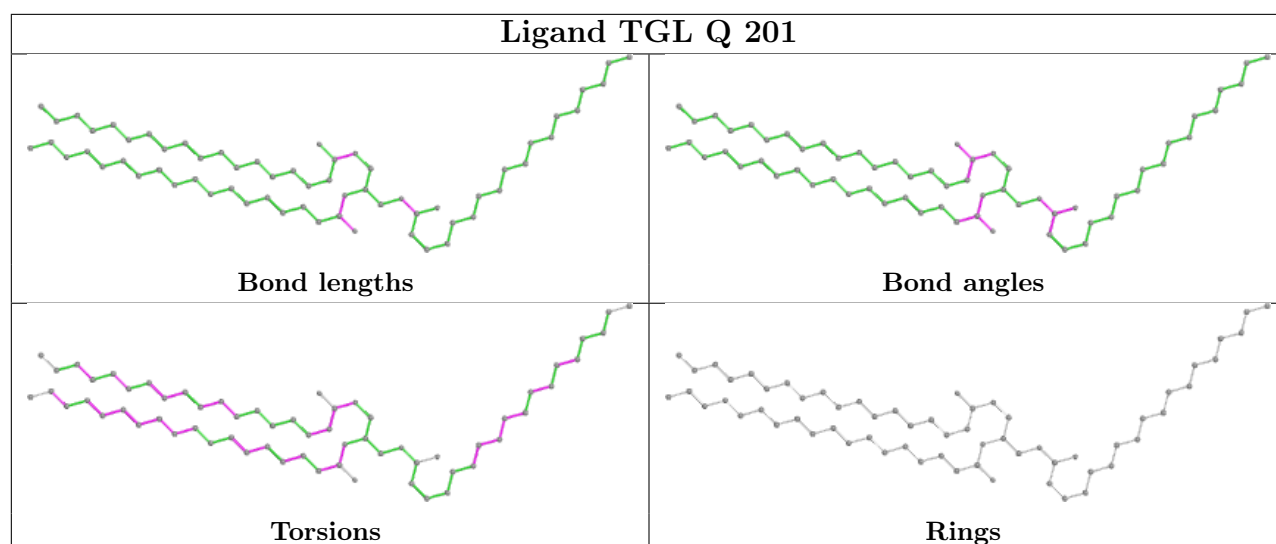


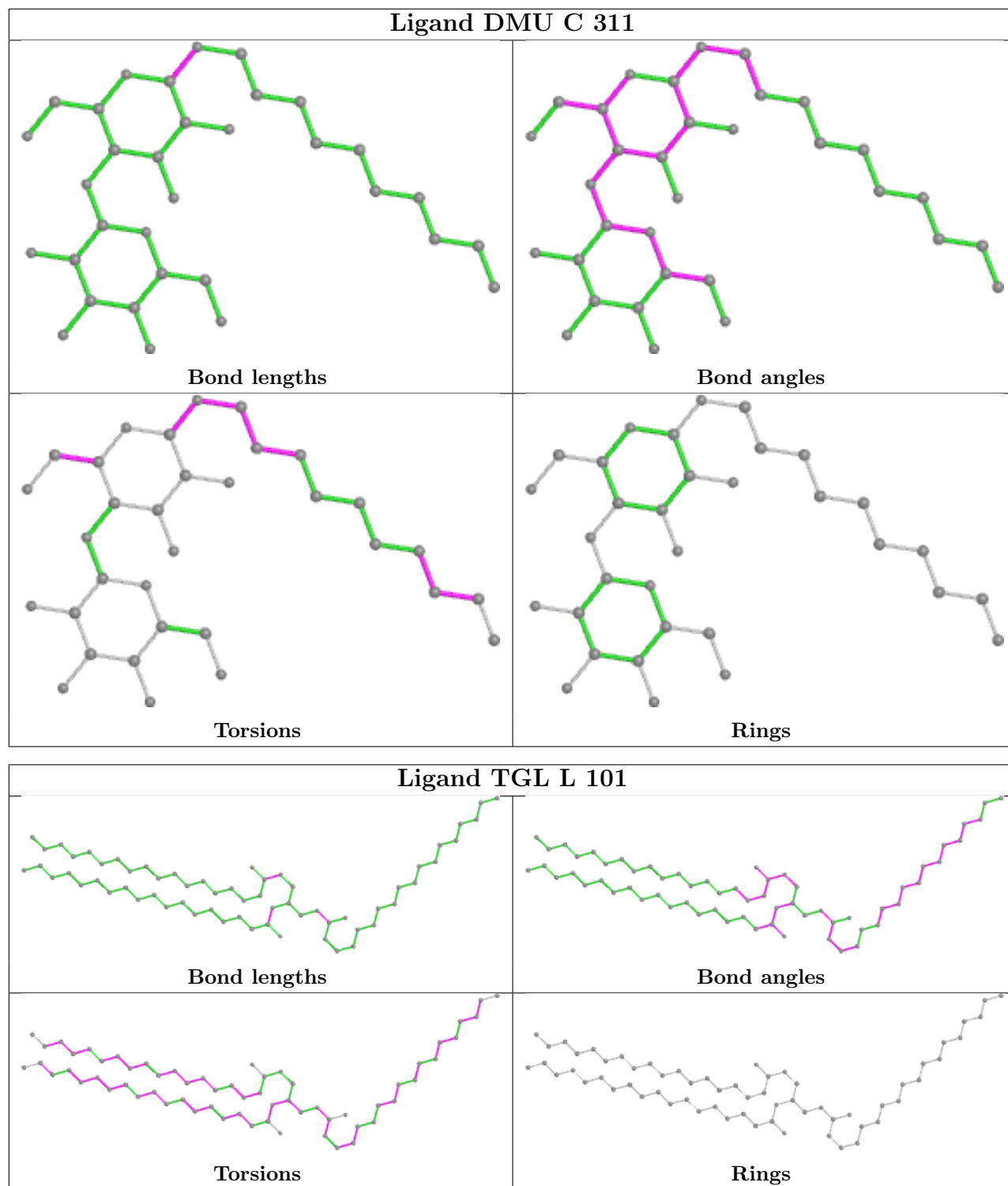


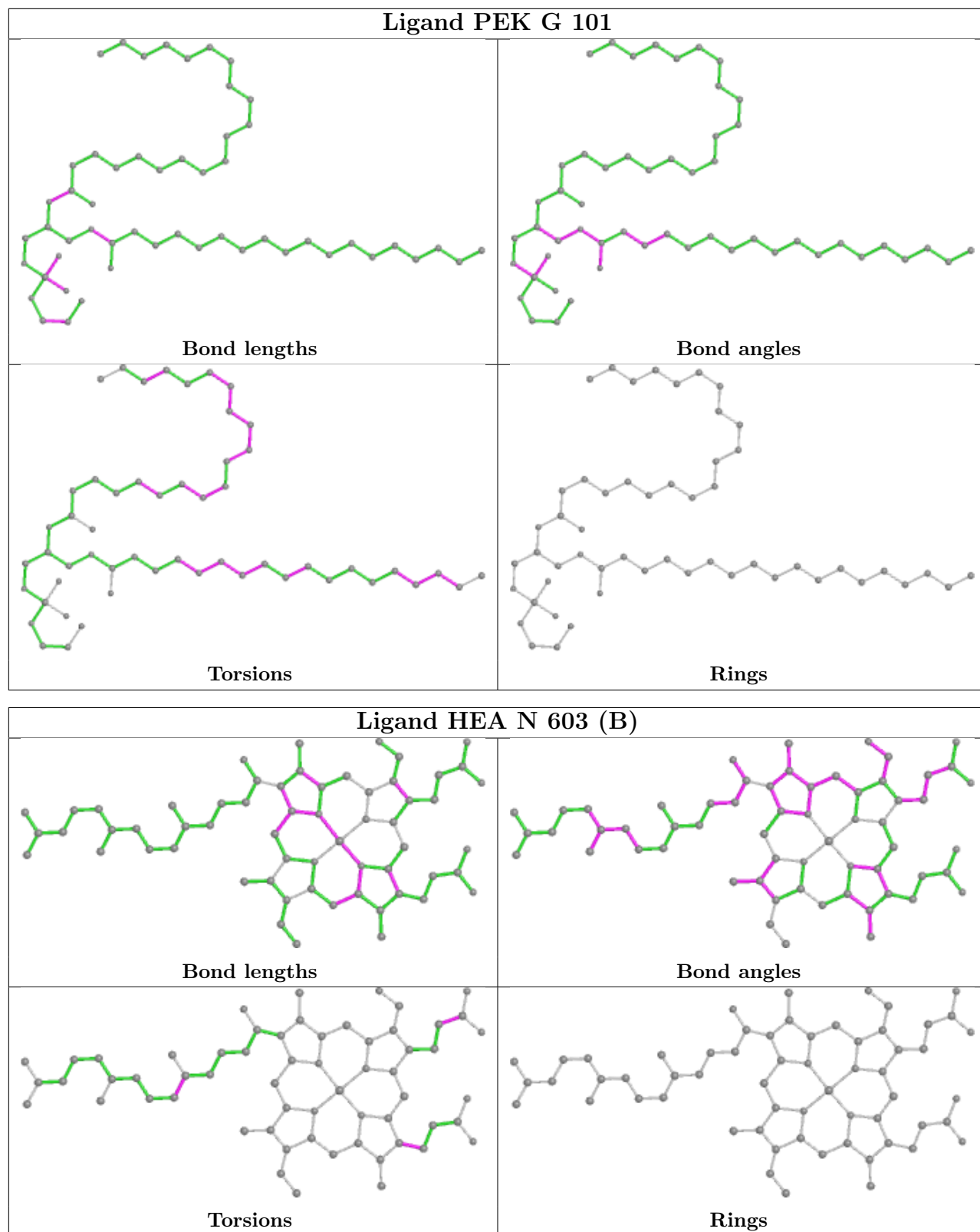


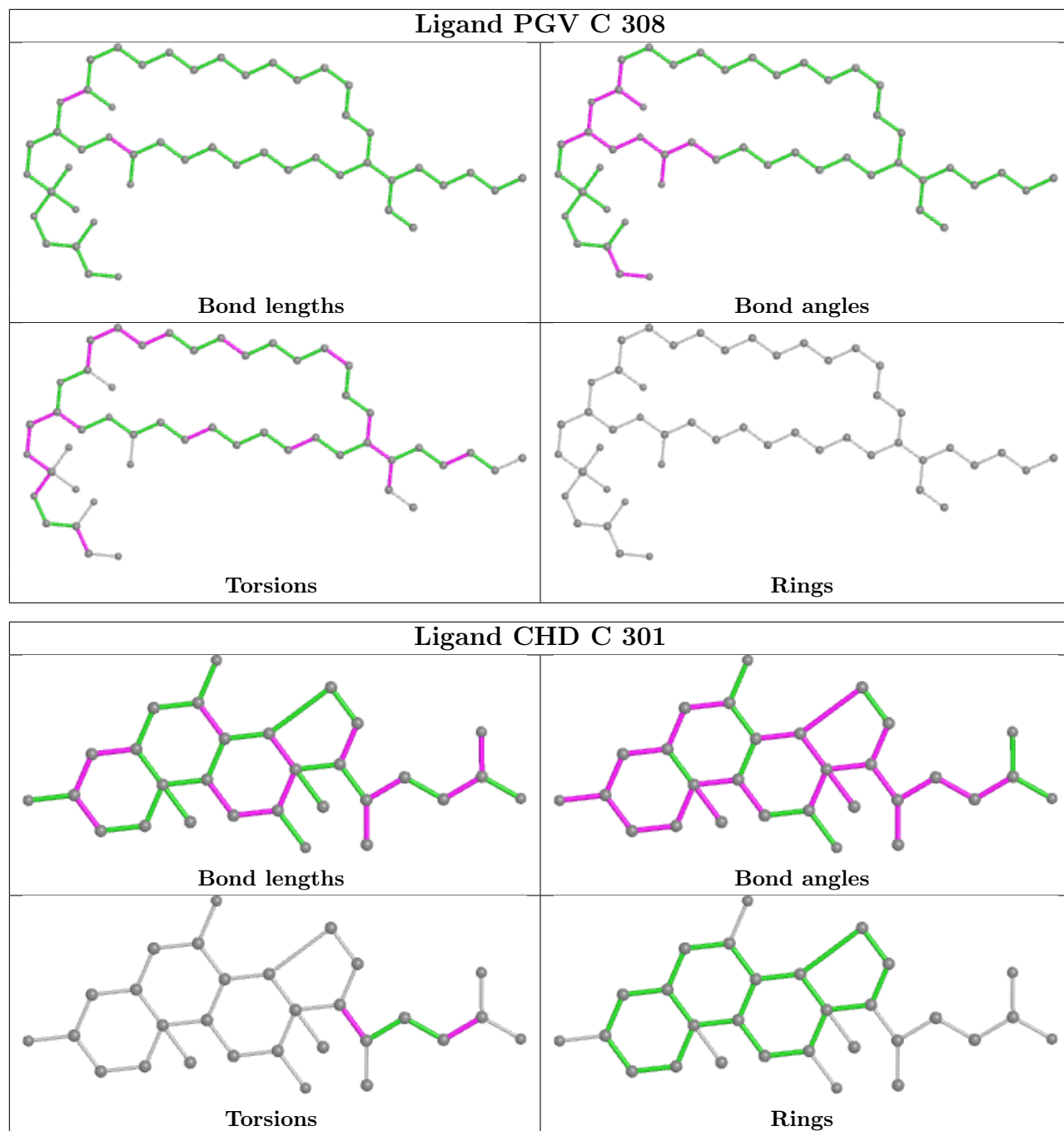


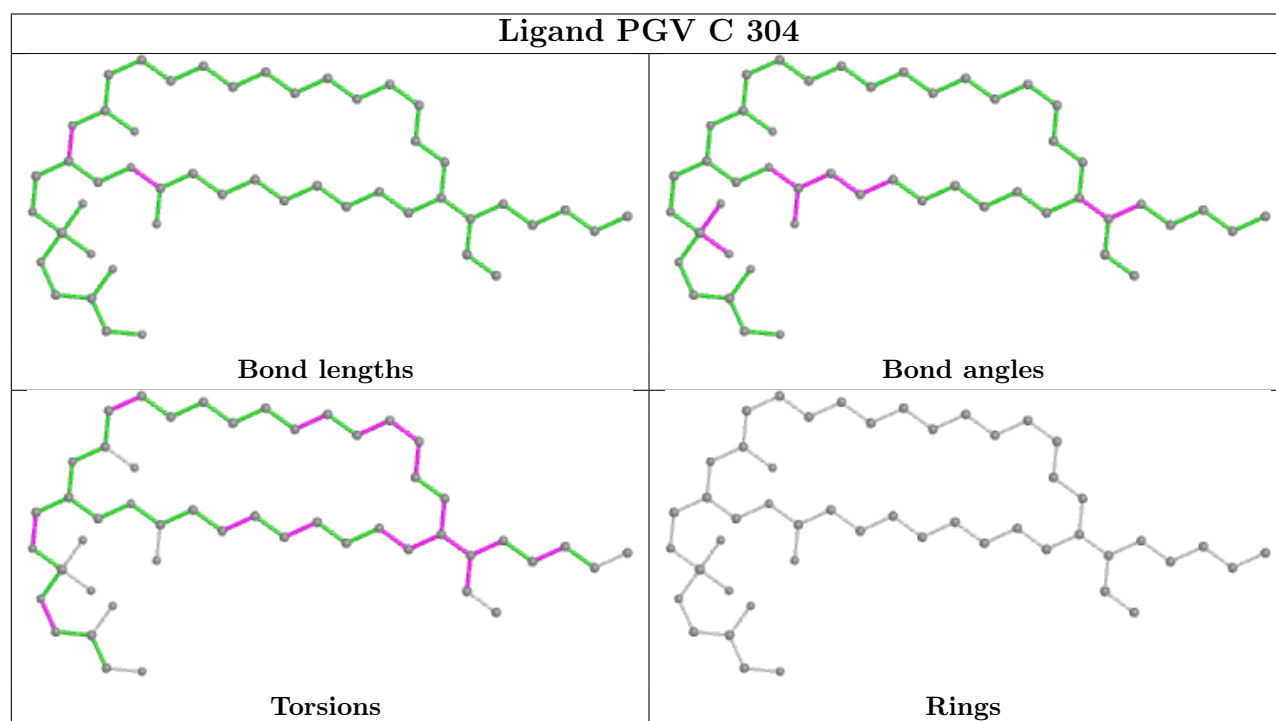
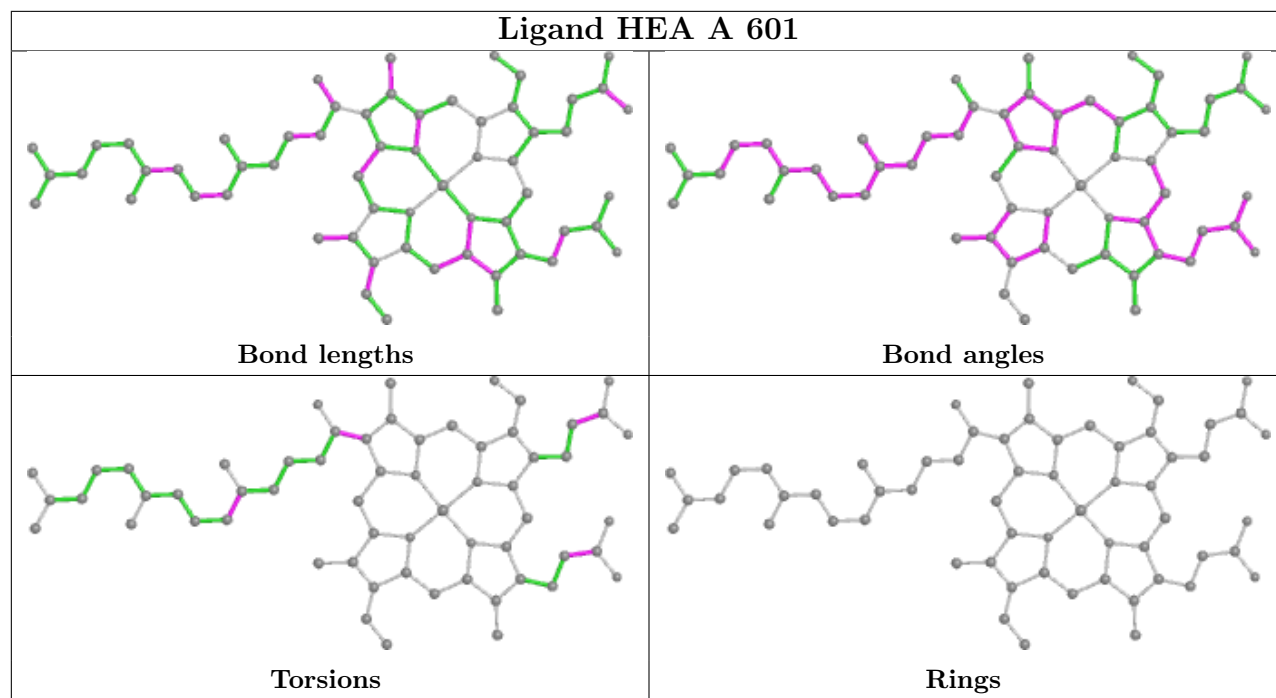


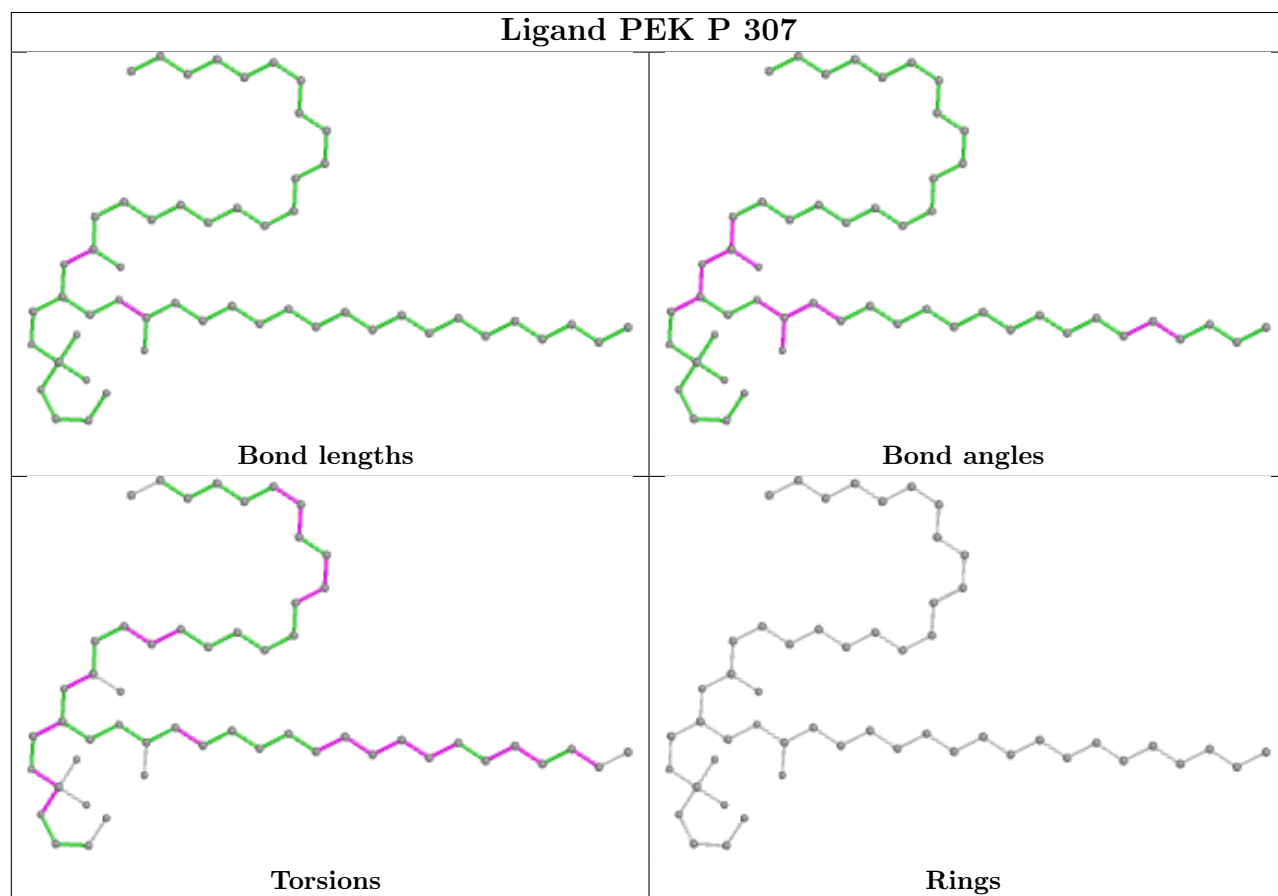
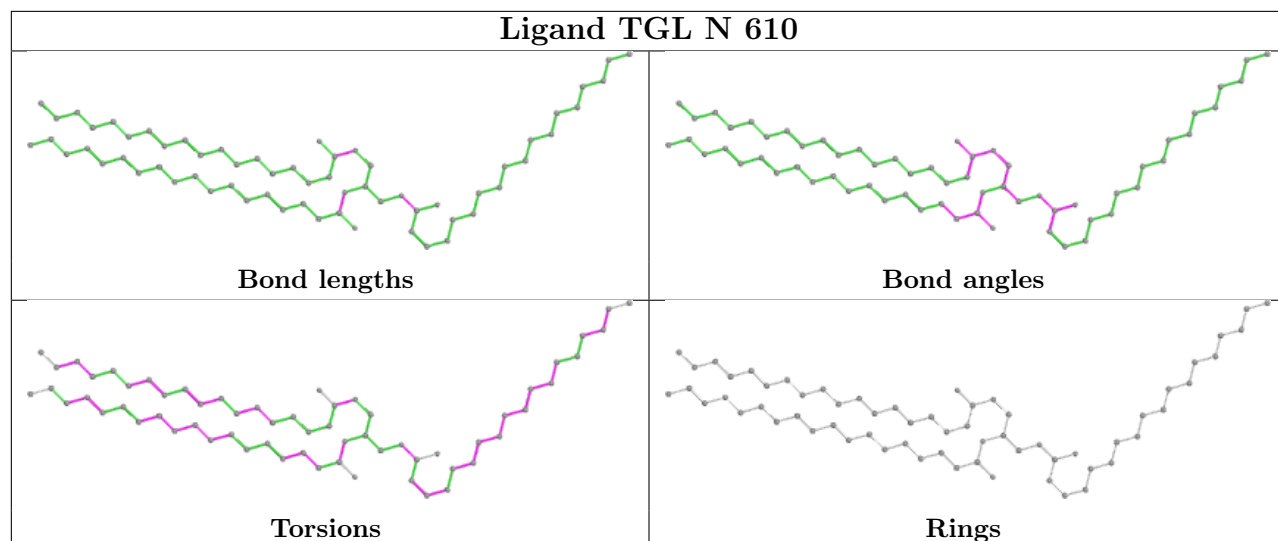


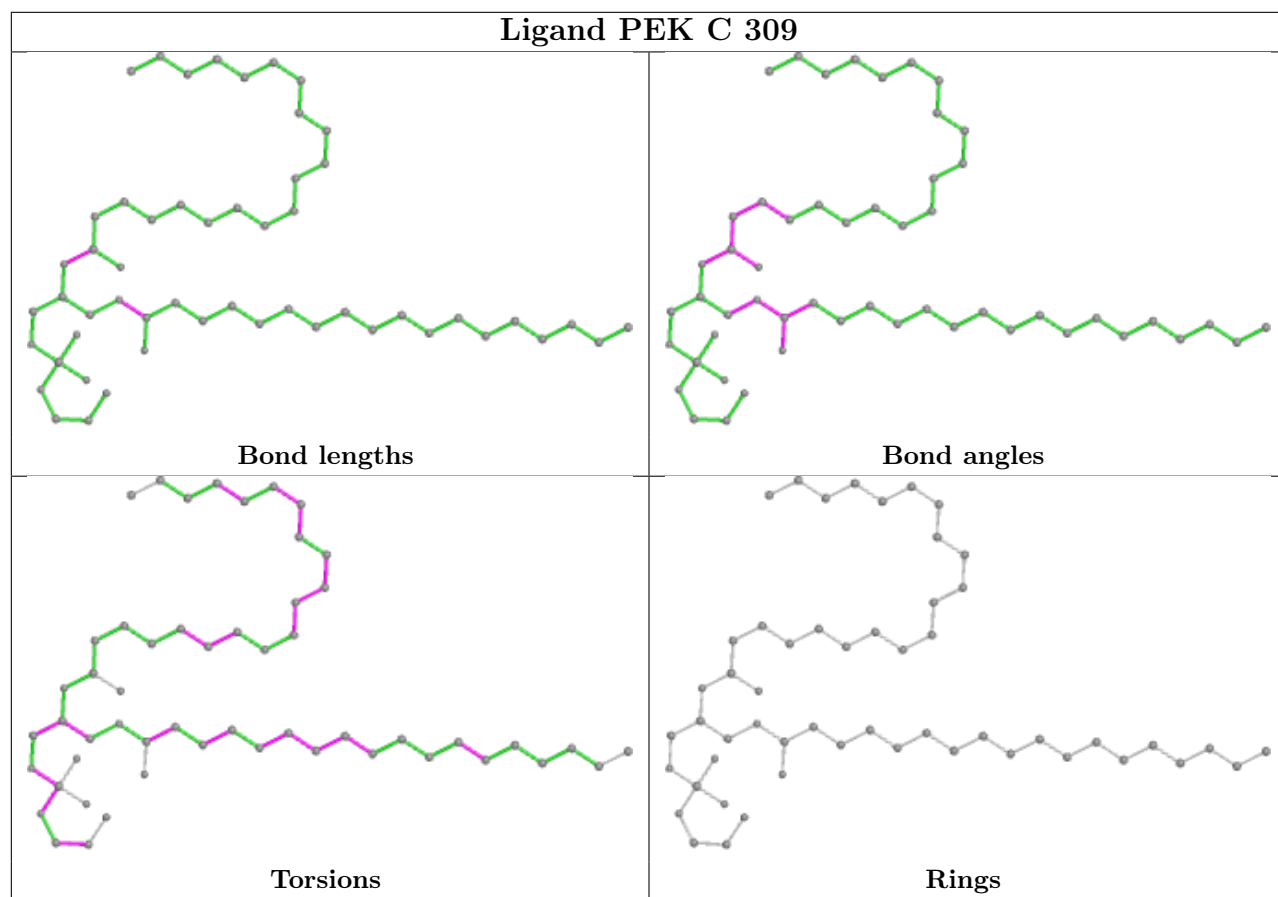
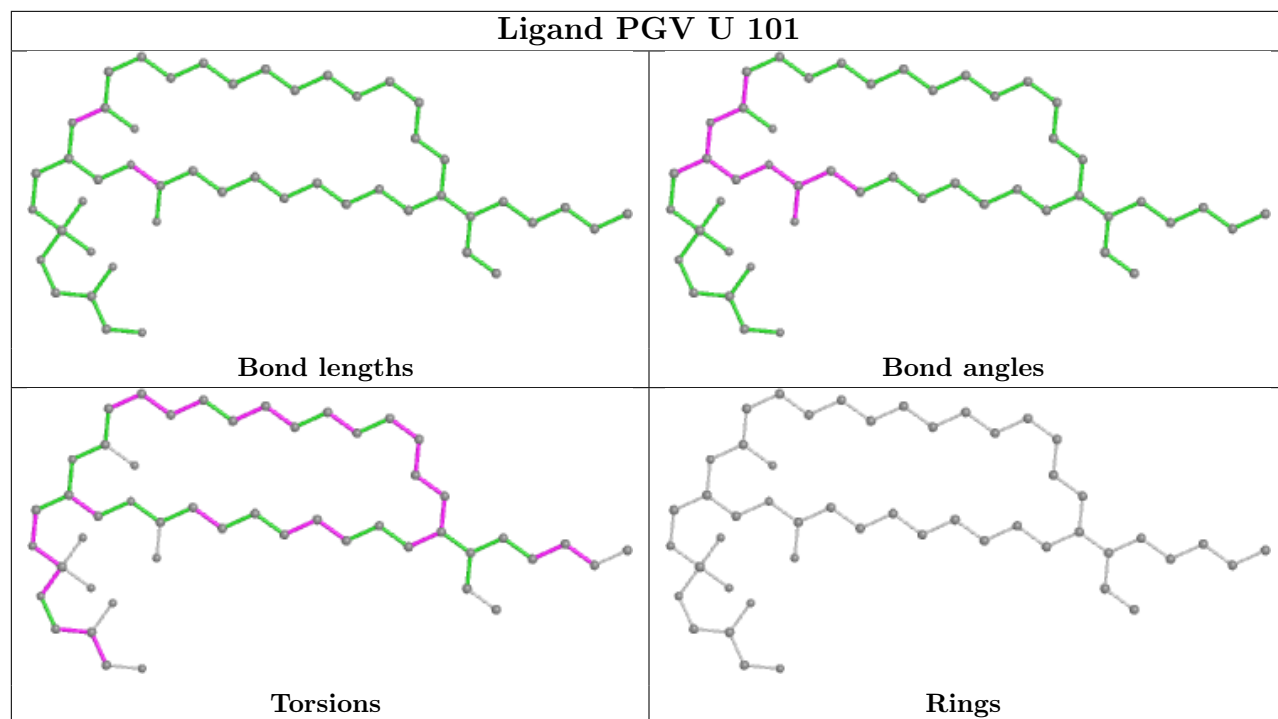


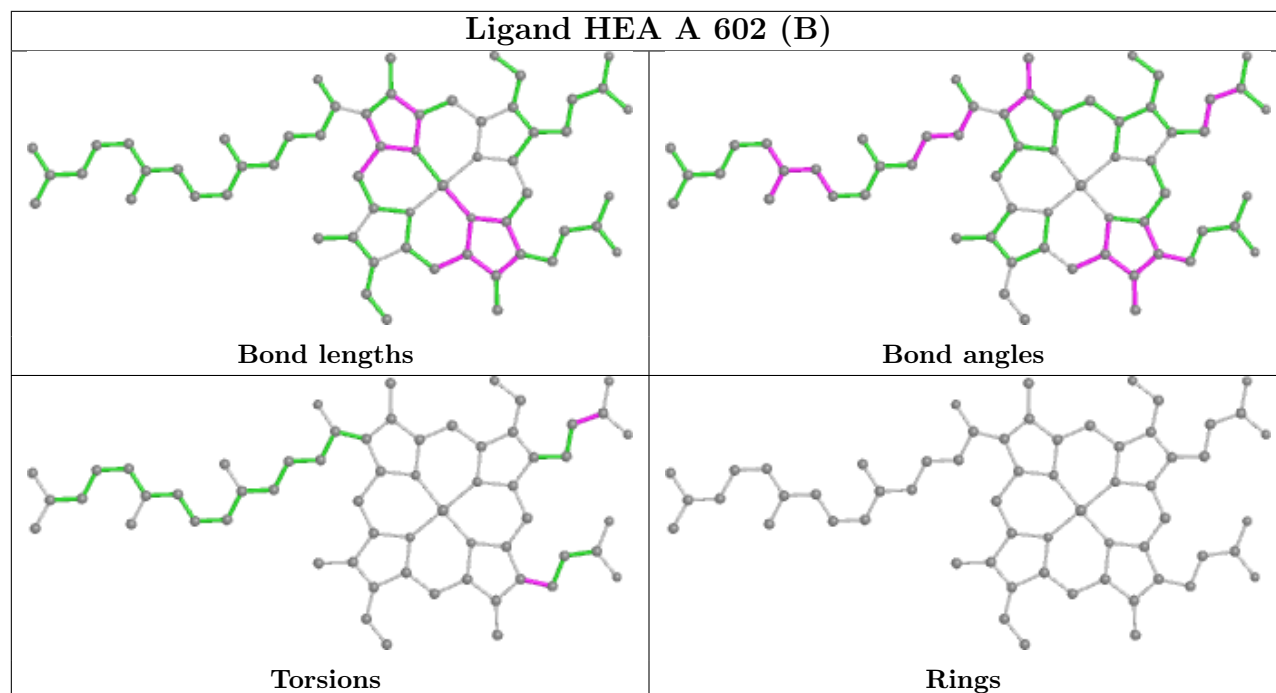












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.19	0 100 100	22, 28, 36, 73	0
1	N	513/514 (99%)	0.09	4 (0%) 86 87	25, 32, 41, 73	0
2	B	226/227 (99%)	0.13	3 (1%) 77 79	26, 35, 52, 74	0
2	O	226/227 (99%)	0.13	3 (1%) 77 79	32, 42, 66, 91	0
3	C	259/261 (99%)	0.16	1 (0%) 92 93	25, 32, 42, 79	0
3	P	259/261 (99%)	0.11	2 (0%) 86 87	26, 33, 45, 76	0
4	D	144/147 (97%)	0.00	1 (0%) 87 88	29, 37, 58, 79	0
4	Q	144/147 (97%)	0.78	12 (8%) 11 13	37, 51, 81, 145	0
5	E	105/109 (96%)	0.02	3 (2%) 51 54	29, 36, 59, 115	0
5	R	105/109 (96%)	0.05	2 (1%) 66 69	36, 44, 64, 121	0
6	F	98/98 (100%)	0.62	8 (8%) 11 13	29, 39, 92, 150	0
6	S	98/98 (100%)	0.69	8 (8%) 11 13	29, 40, 96, 144	0
7	G	83/85 (97%)	1.03	15 (18%) 1 1	30, 40, 110, 146	0
7	T	83/85 (97%)	0.92	14 (16%) 1 1	29, 41, 101, 137	0
8	H	79/85 (92%)	0.26	6 (7%) 13 15	32, 43, 92, 104	0
8	U	79/85 (92%)	0.31	5 (6%) 20 22	37, 47, 105, 121	0
9	I	72/73 (98%)	0.45	5 (6%) 16 19	34, 47, 78, 91	0
9	V	72/73 (98%)	0.38	4 (5%) 24 27	33, 56, 76, 104	0
10	J	58/59 (98%)	0.36	3 (5%) 27 30	32, 42, 65, 112	0
10	W	58/59 (98%)	0.33	2 (3%) 45 48	36, 47, 73, 117	0
11	K	49/56 (87%)	0.03	0 100 100	35, 42, 57, 66	0
11	X	49/56 (87%)	0.40	4 (8%) 11 13	45, 52, 77, 83	0
12	L	46/47 (97%)	0.22	1 (2%) 62 64	29, 35, 56, 94	0
12	Y	46/47 (97%)	0.29	2 (4%) 35 38	36, 42, 63, 122	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.39	2 (4%) 31 34	30, 34, 70, 121	0
13	Z	43/46 (93%)	0.44	4 (9%) 8 10	40, 46, 84, 127	0
All	All	3550/3614 (98%)	0.26	114 (3%) 47 50	22, 36, 68, 150	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	27.1
4	Q	5	VAL	16.9
6	S	97	ALA	16.6
6	F	97	ALA	13.9
6	F	2	SER	11.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.44	0.36	82,111,131,134	0
7	TPO	T	11	11/12	0.60	0.29	97,108,122,128	0
9	SAC	V	1	9/10	0.84	0.33	103,119,127,139	0
9	SAC	I	1	9/10	0.87	0.18	67,77,80,86	0
2	FME	O	1	10/11	0.97	0.12	37,40,50,63	0
1	FME	A	1	10/11	0.97	0.14	42,48,75,93	0
1	FME	N	1	10/11	0.97	0.14	45,54,74,87	0
2	FME	B	1	10/11	0.98	0.13	31,33,43,58	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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
20	EDO	D	203	4/4	0.68	0.21	61,64,65,67	0
22	CHD	W	101	29/29	0.68	0.34	59,93,115,119	0
28	PSC	E	201	52/52	0.69	0.30	38,84,156,157	0
27	PEK	C	307	53/53	0.71	0.23	42,81,145,153	0
27	PEK	C	309	53/53	0.72	0.34	52,97,147,150	0
24	DMU	C	302	33/33	0.73	0.38	32,83,118,129	0
27	PEK	G	103	53/53	0.74	0.27	50,84,152,154	0
26	CDL	T	102	100/100	0.74	0.24	53,88,128,152	0
26	CDL	N	601	100/100	0.76	0.27	58,91,133,158	0
19	PGV	C	308	51/51	0.76	0.22	46,76,120,137	0
21	TGL	Q	201	63/63	0.76	0.22	49,76,96,110	0
27	PEK	P	307	53/53	0.78	0.26	42,75,124,141	0
24	DMU	P	306	33/33	0.78	0.32	47,78,120,125	0
28	PSC	O	302	52/52	0.78	0.28	44,86,158,160	0
26	CDL	P	304	100/100	0.79	0.26	38,82,120,130	0
20	EDO	G	105	4/4	0.79	0.31	55,63,64,79	0
24	DMU	C	311	33/33	0.80	0.21	56,79,102,119	0
21	TGL	Y	101	63/63	0.81	0.28	45,79,114,142	0
19	PGV	U	101	51/51	0.82	0.23	48,78,115,140	0
24	DMU	C	310	33/33	0.82	0.27	58,79,103,110	0
24	DMU	P	309	33/33	0.82	0.18	66,87,99,103	0
24	DMU	P	308	33/33	0.83	0.23	53,79,102,105	0
20	EDO	A	611	4/4	0.83	0.25	52,62,67,69	0
26	CDL	C	305	100/100	0.83	0.26	39,77,116,124	0
19	PGV	Z	101	51/51	0.83	0.25	50,75,113,131	0
20	EDO	L	102	4/4	0.84	0.32	59,72,89,95	0
20	EDO	A	616	4/4	0.85	0.27	46,48,49,51	0
20	EDO	N	620	4/4	0.85	0.32	43,52,54,68	0
22	CHD	J	101	29/29	0.85	0.23	54,79,113,116	0
21	TGL	D	201	63/63	0.85	0.21	35,64,87,100	0
21	TGL	L	101	63/63	0.85	0.20	34,59,94,111	0
21	TGL	N	610	63/63	0.86	0.20	53,78,101,119	0
24	DMU	Z	102	33/33	0.86	0.17	47,58,71,78	0
20	EDO	N	615	4/4	0.86	0.17	56,56,62,63	0
19	PGV	A	609	51/51	0.87	0.26	36,75,108,126	0
21	TGL	B	301	63/63	0.89	0.16	41,73,97,103	0
20	EDO	N	619	4/4	0.90	0.28	49,54,65,67	0
25	UNX	C	303	1/1	0.90	0.17	34,34,34,34	0
20	EDO	M	102	4/4	0.90	0.14	63,64,71,73	0
20	EDO	D	202	4/4	0.91	0.68	37,52,55,65	0
22	CHD	P	305	29/29	0.91	0.13	49,55,62,73	0
22	CHD	C	306	29/29	0.91	0.17	47,55,65,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	P	312	4/4	0.92	0.36	51,56,62,82	0
20	EDO	Y	102	4/4	0.92	0.26	64,67,70,77	0
20	EDO	B	306	4/4	0.92	0.21	33,46,51,53	0
20	EDO	N	616	4/4	0.92	0.21	53,59,64,68	0
20	EDO	A	612	4/4	0.92	0.24	53,55,58,59	0
20	EDO	B	305	4/4	0.92	0.48	54,58,72,89	0
16	MG	N	605	1/1	0.93	0.09	32,32,32,32	0
20	EDO	A	617	4/4	0.93	0.35	54,60,60,63	0
24	DMU	M	101	33/33	0.93	0.11	40,47,56,68	0
20	EDO	S	103	4/4	0.93	0.25	43,57,66,74	0
20	EDO	A	614	4/4	0.93	0.17	51,63,63,73	0
20	EDO	A	615	4/4	0.93	0.15	23,26,28,43	0
20	EDO	A	618	4/4	0.94	0.38	45,66,70,79	0
20	EDO	A	613	4/4	0.94	0.12	33,33,36,36	0
20	EDO	P	311	4/4	0.95	0.17	35,36,42,49	0
20	EDO	A	619	4/4	0.95	0.20	55,58,59,63	0
20	EDO	R	201	4/4	0.95	0.14	43,45,47,48	0
20	EDO	N	618	4/4	0.95	0.13	45,47,49,50	0
20	EDO	T	103	4/4	0.95	0.12	39,41,43,46	0
27	PEK	T	101	53/53	0.95	0.15	31,49,83,91	0
20	EDO	N	614	4/4	0.95	0.15	44,45,50,52	0
20	EDO	E	204	4/4	0.95	0.11	45,46,51,59	0
27	PEK	G	101	53/53	0.96	0.14	30,48,79,102	0
22	CHD	C	301	29/29	0.96	0.11	28,31,36,38	0
20	EDO	N	617	4/4	0.96	0.17	41,47,48,53	0
20	EDO	E	203	4/4	0.96	0.10	41,44,45,50	0
20	EDO	F	103	4/4	0.96	0.15	37,44,47,58	0
20	EDO	F	104	4/4	0.96	0.13	39,39,39,41	0
20	EDO	N	613	4/4	0.97	0.20	44,54,61,66	0
22	CHD	P	301	29/29	0.97	0.09	27,32,36,40	0
20	EDO	B	304	4/4	0.97	0.42	49,50,84,90	0
20	EDO	A	610	4/4	0.97	0.18	38,43,46,55	0
20	EDO	O	303	4/4	0.97	0.13	38,39,41,42	0
25	UNX	P	302	1/1	0.97	0.08	32,32,32,32	0
22	CHD	B	302	29/29	0.97	0.12	27,31,35,45	0
19	PGV	A	608	51/51	0.97	0.14	27,37,63,66	0
20	EDO	N	611	4/4	0.97	0.15	34,38,40,42	0
20	EDO	P	310	4/4	0.98	0.17	44,45,46,48	0
20	EDO	B	307	4/4	0.98	0.14	30,31,37,37	0
19	PGV	P	303	51/51	0.98	0.14	29,39,80,94	0
22	CHD	G	102	29/29	0.98	0.10	28,31,39,40	0
20	EDO	N	612	4/4	0.98	0.11	29,34,35,36	0

Continued on next page...

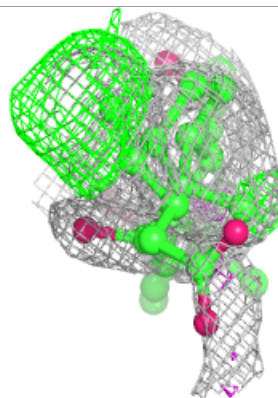
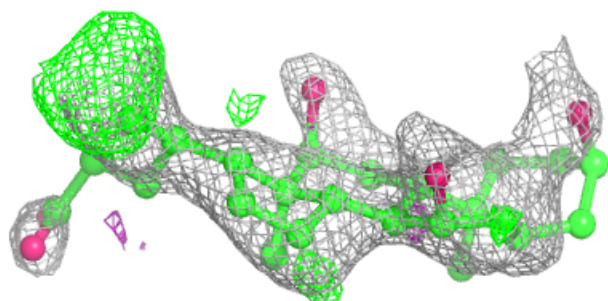
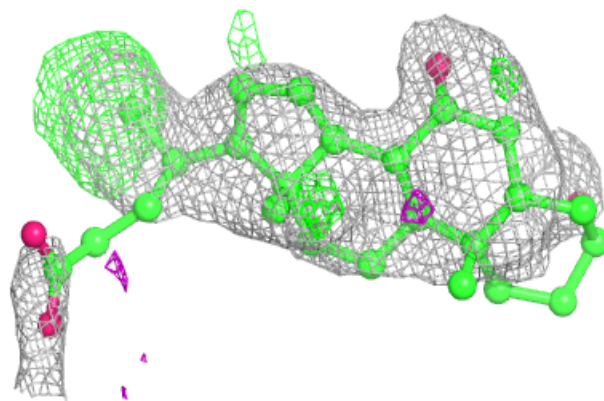
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	S	102	4/4	0.98	0.10	31,32,33,33	0
14	HEA	A	602[A]	60/60	0.98	0.16	20,24,29,35	60
20	EDO	E	202	4/4	0.98	0.12	40,45,45,46	0
18	AZI	N	607[B]	3/3	0.98	0.27	22,22,23,23	3
14	HEA	A	602[B]	60/60	0.98	0.16	17,25,28,30	60
14	HEA	N	603[A]	60/60	0.98	0.16	22,27,33,37	60
19	PGV	C	304	51/51	0.98	0.14	27,36,83,91	0
20	EDO	G	104	4/4	0.98	0.11	33,39,41,43	0
14	HEA	N	603[B]	60/60	0.98	0.16	24,30,41,44	60
19	PGV	N	609	51/51	0.98	0.12	30,41,66,76	0
14	HEA	N	602	60/60	0.99	0.12	25,31,56,65	0
18	AZI	N	608[A]	3/3	0.99	0.19	25,25,30,33	3
20	EDO	F	102	4/4	0.99	0.11	29,31,31,32	0
18	AZI	N	608[B]	3/3	0.99	0.19	22,22,22,23	3
16	MG	A	604	1/1	0.99	0.09	27,27,27,27	0
14	HEA	A	601	60/60	0.99	0.13	21,26,47,50	0
17	NA	N	606	1/1	0.99	0.06	35,35,35,35	0
18	AZI	A	606[B]	3/3	0.99	0.51	21,21,25,26	3
15	CU	A	603	1/1	1.00	0.18	28,28,28,28	0
15	CU	N	604	1/1	1.00	0.18	31,31,31,31	0
18	AZI	A	607[A]	3/3	1.00	0.19	25,25,27,29	3
18	AZI	A	607[B]	3/3	1.00	0.19	21,21,26,30	3
23	CUA	B	303	2/2	1.00	0.16	28,28,28,29	0
23	CUA	O	301	2/2	1.00	0.14	33,33,33,34	0
17	NA	A	605	1/1	1.00	0.09	29,29,29,29	0
29	ZN	F	101	1/1	1.00	0.15	34,34,34,34	0
29	ZN	S	101	1/1	1.00	0.15	36,36,36,36	0

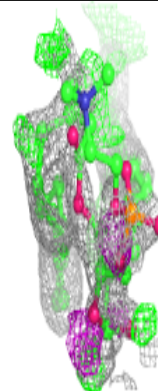
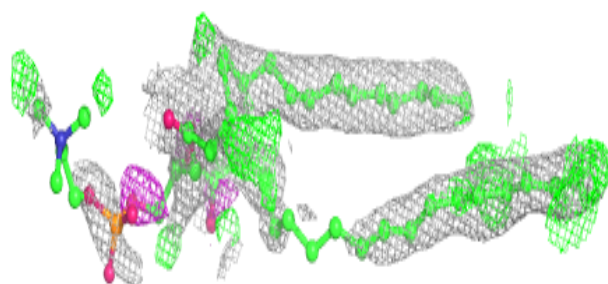
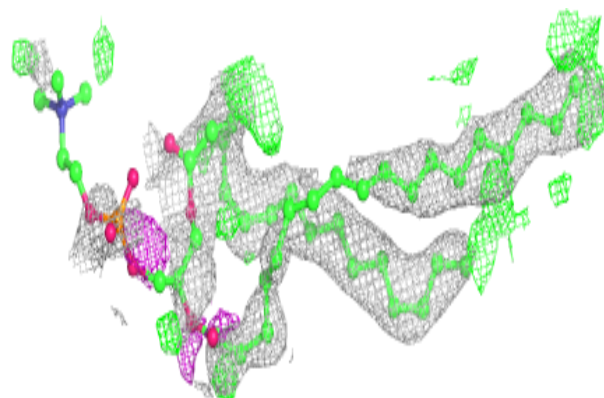
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

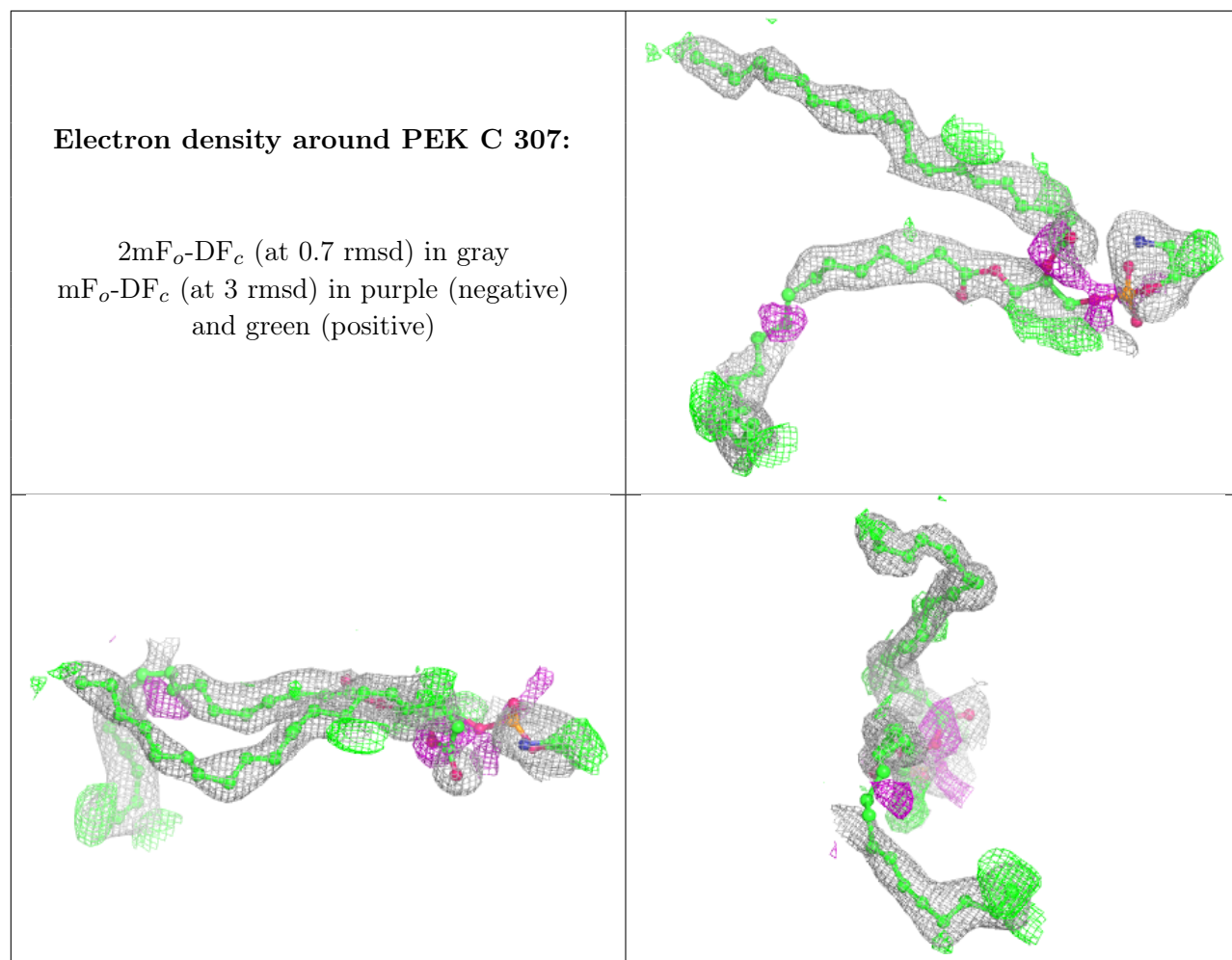
Electron density around CHD W 101:

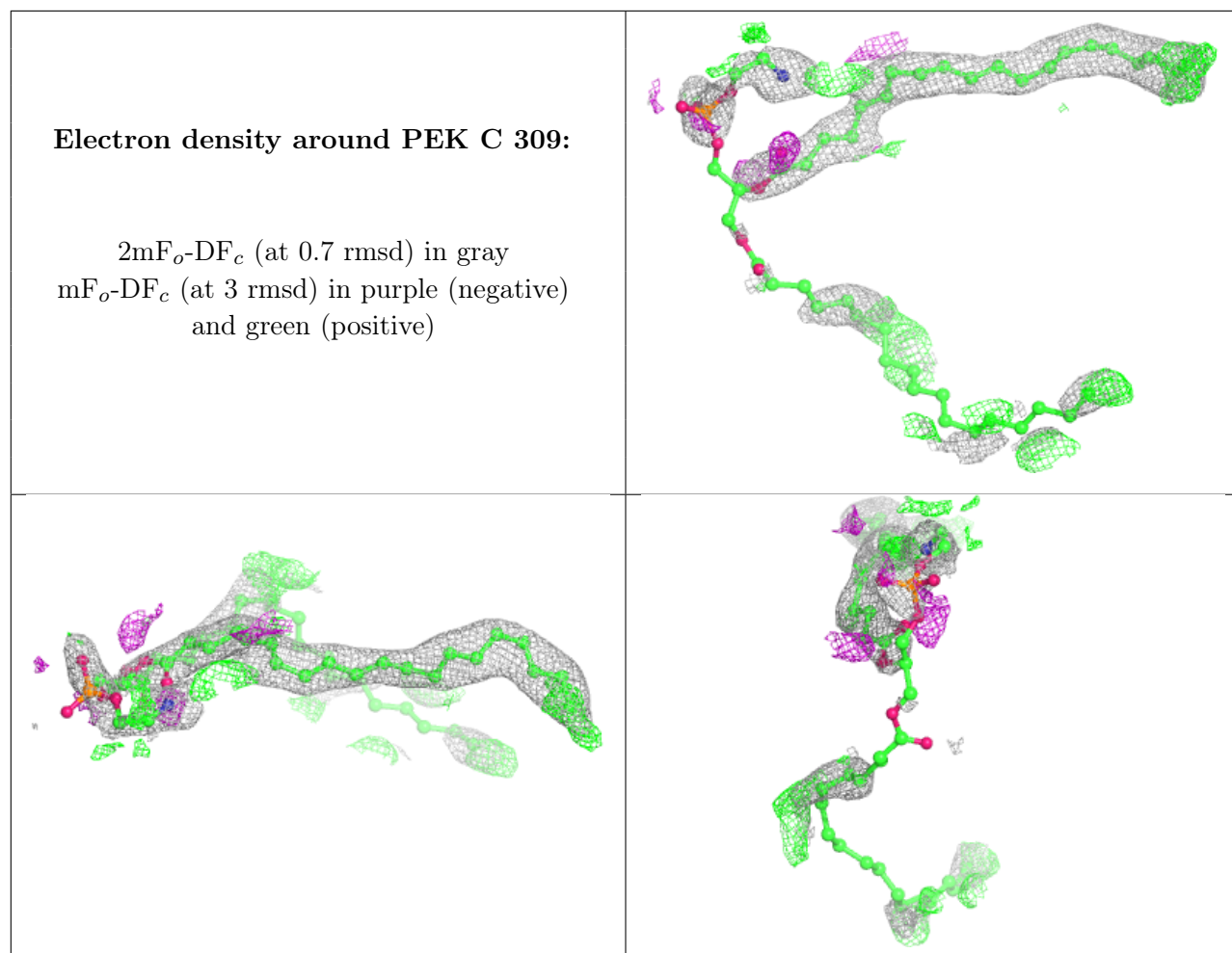
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 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)

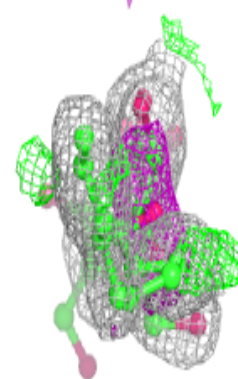
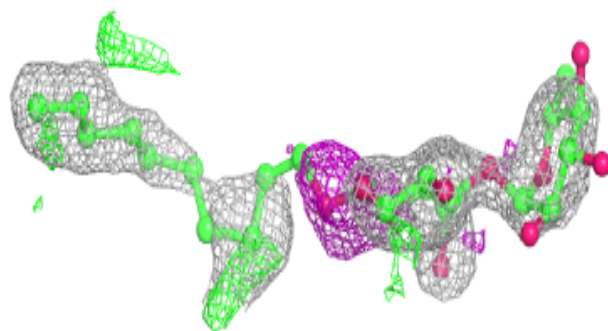
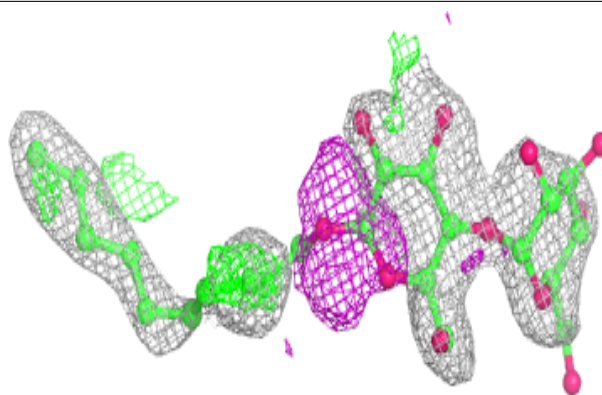




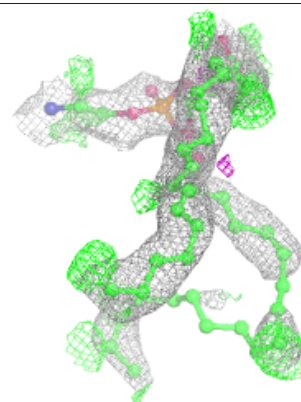
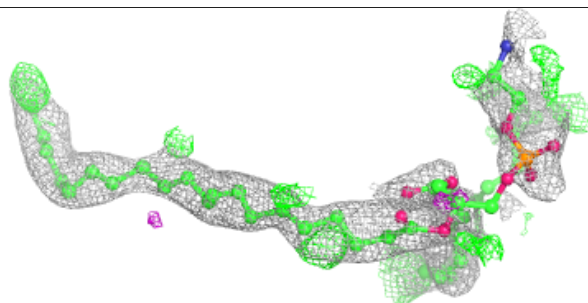
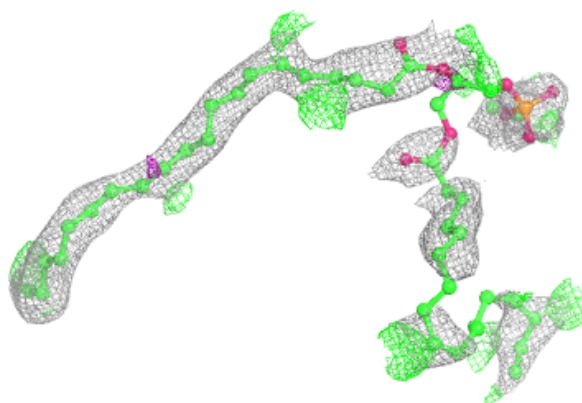


Electron density around DMU C 302:

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

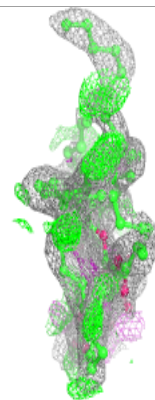
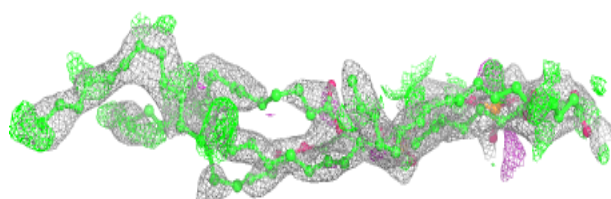
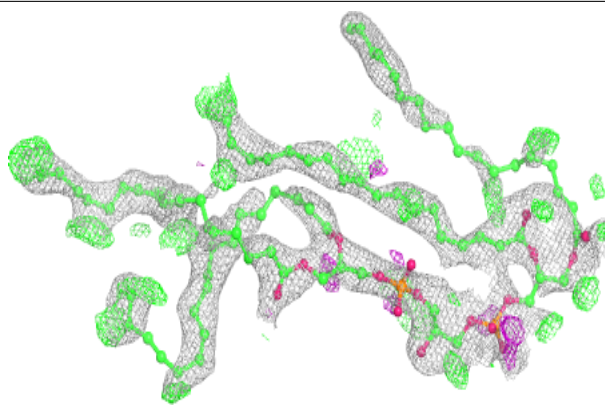
**Electron density around PEK G 103:**

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

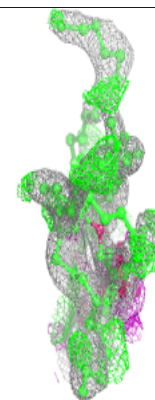
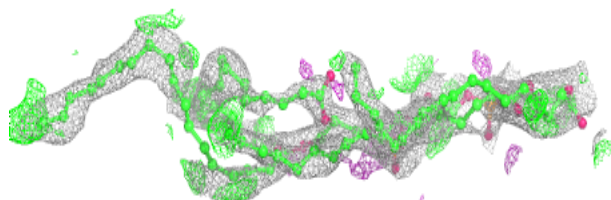
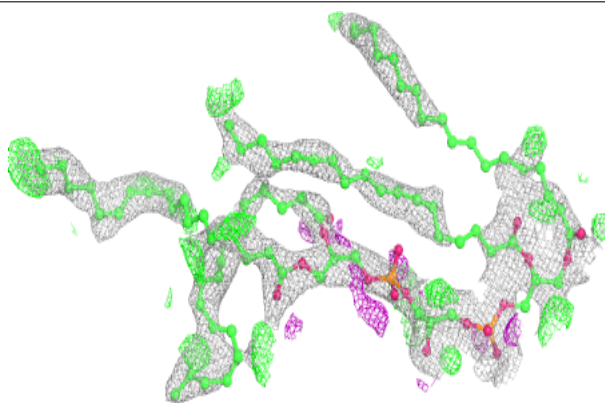


Electron density around CDL T 102:

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

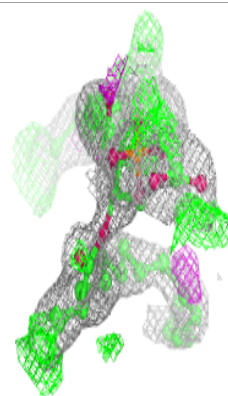
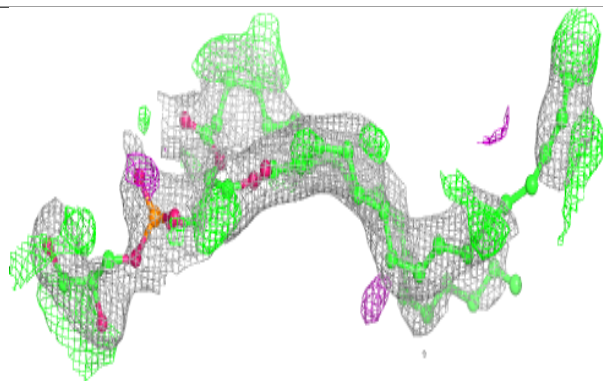
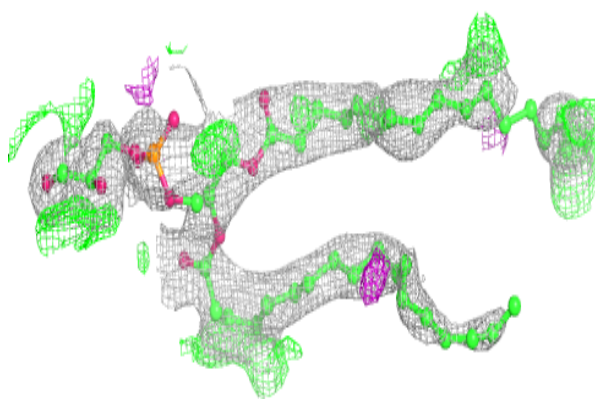
**Electron density around CDL N 601:**

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

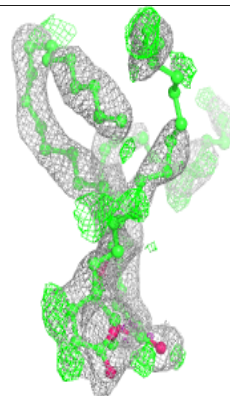
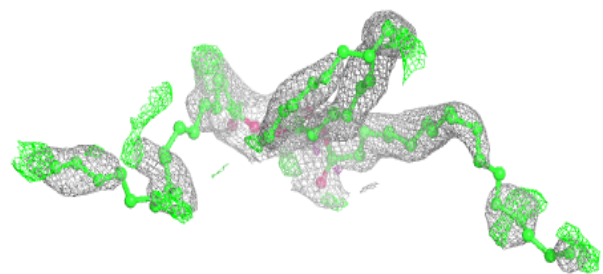
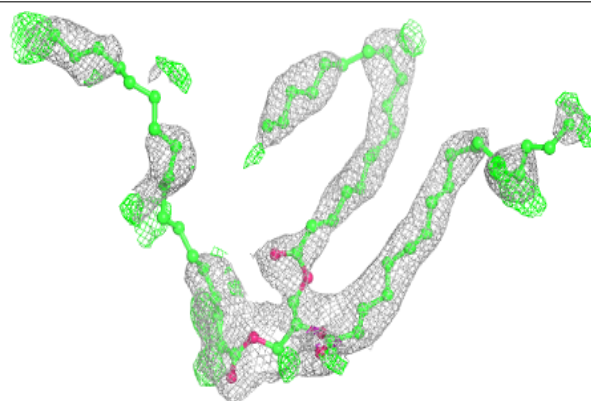


Electron density around PGV C 308:

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

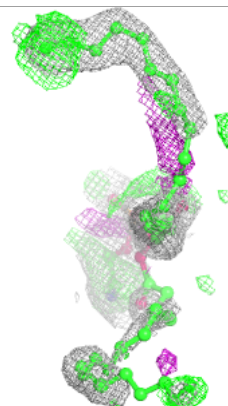
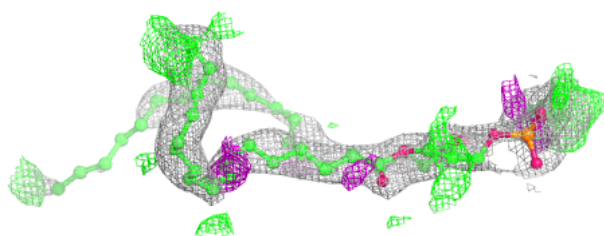
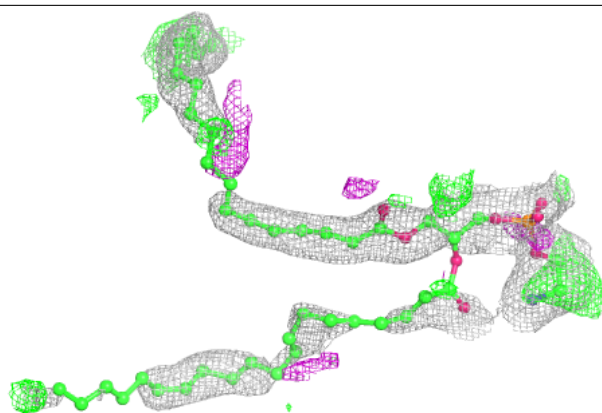
**Electron density around TGL Q 201:**

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

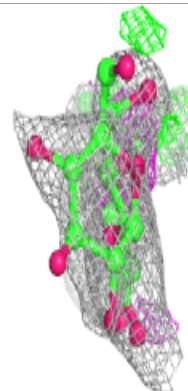
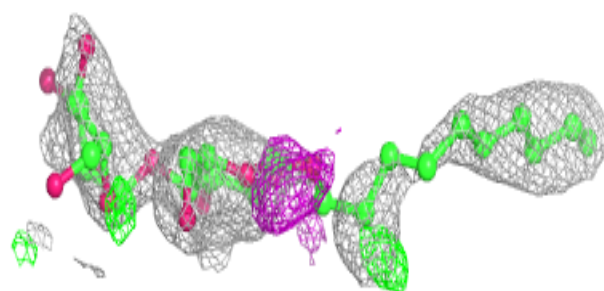
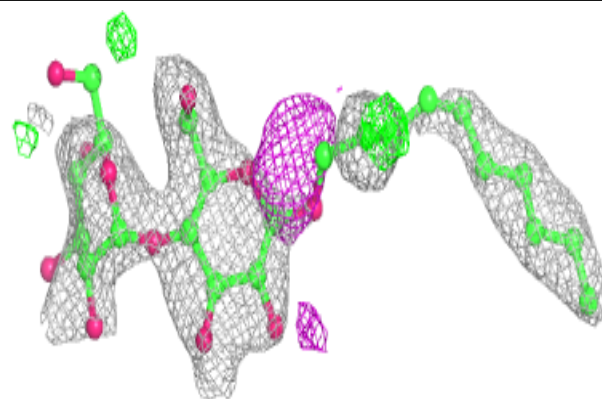


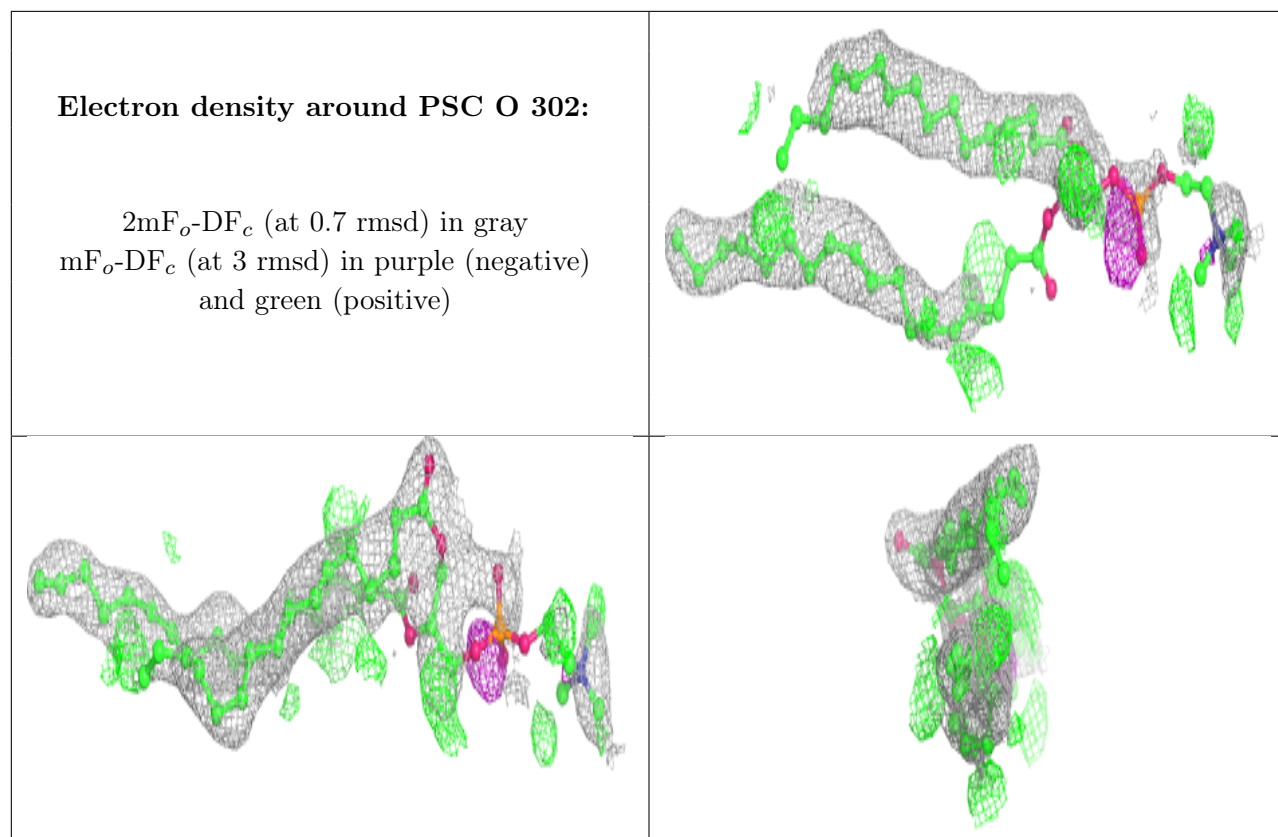
Electron density around PEK P 307:

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

**Electron density around DMU P 306:**

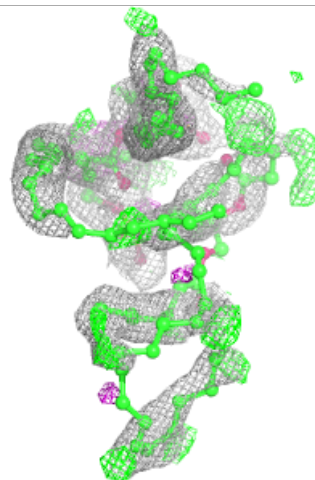
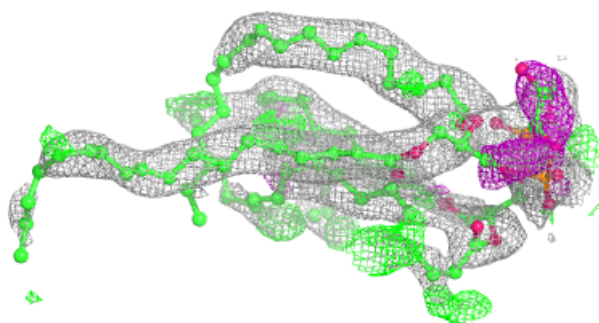
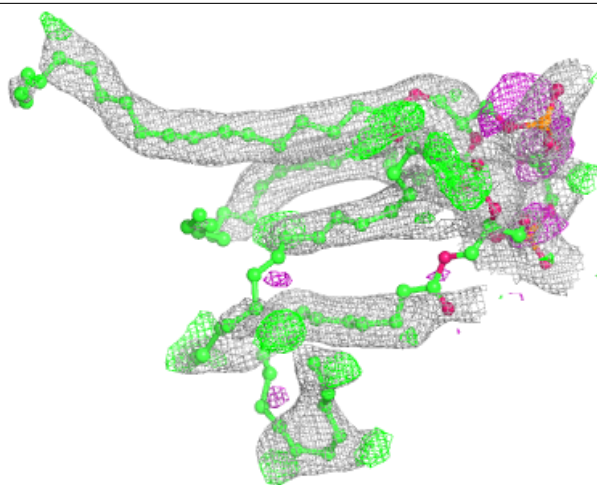
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

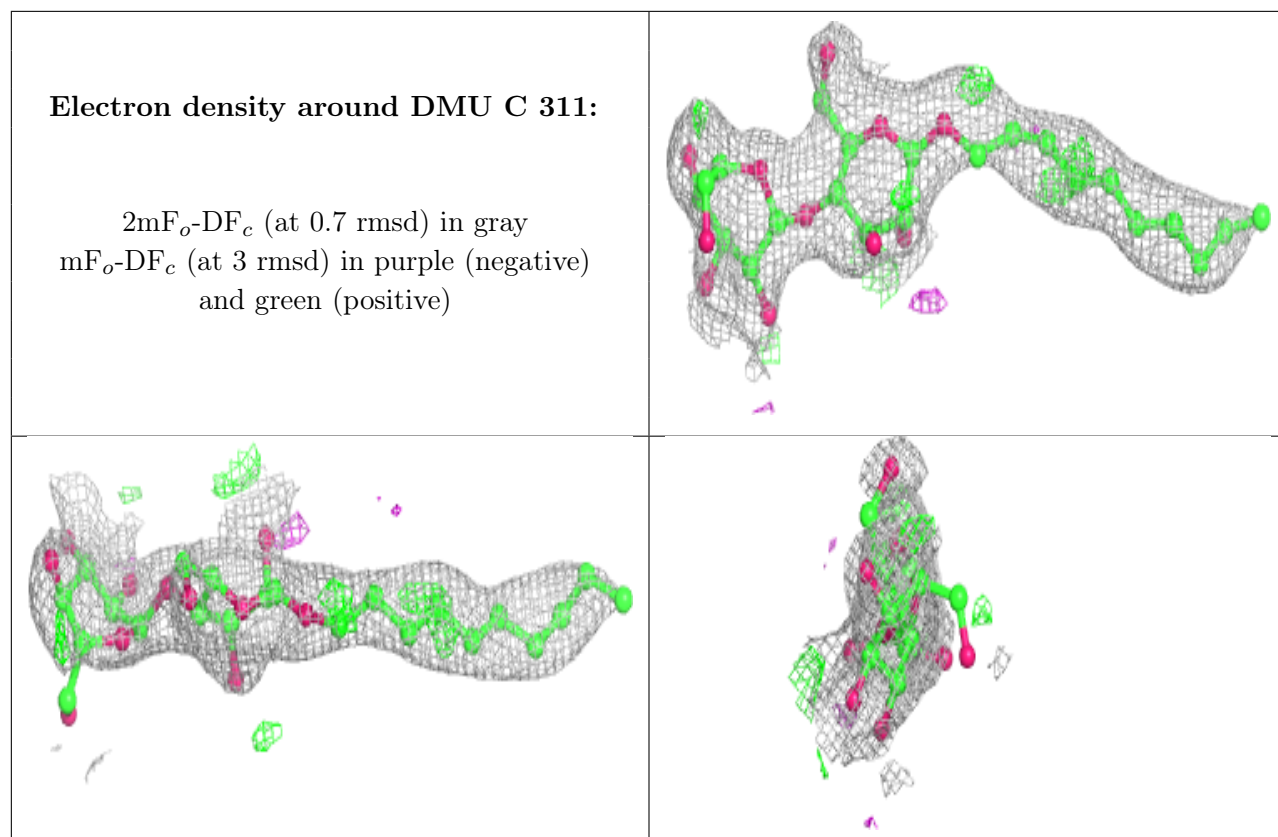


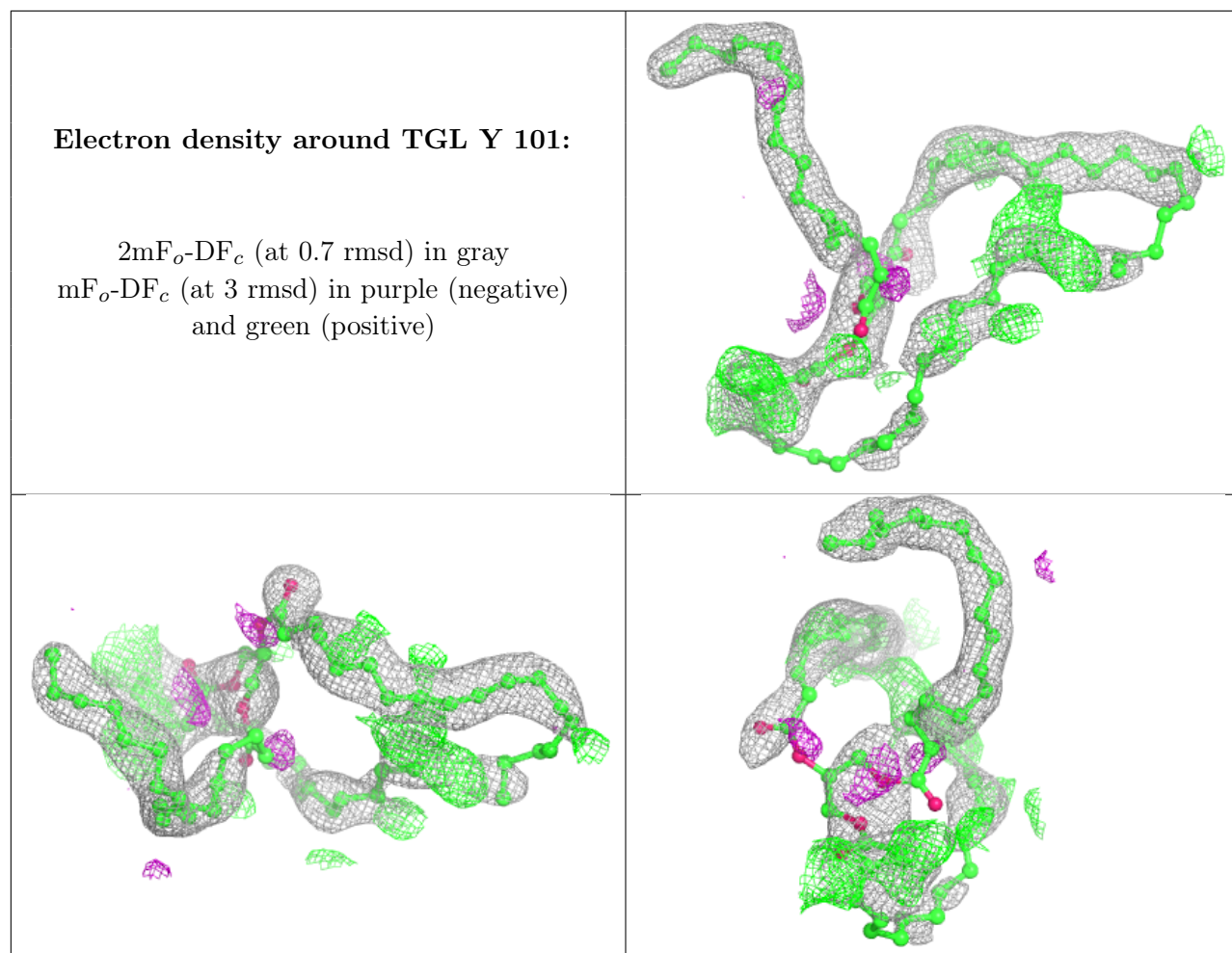


Electron density around CDL P 304:

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

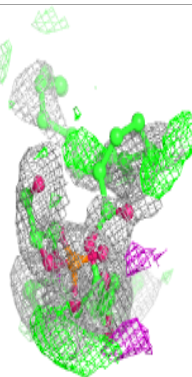
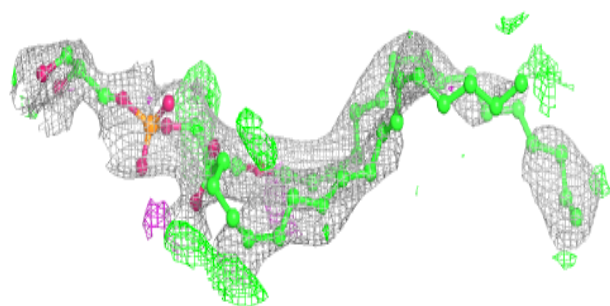
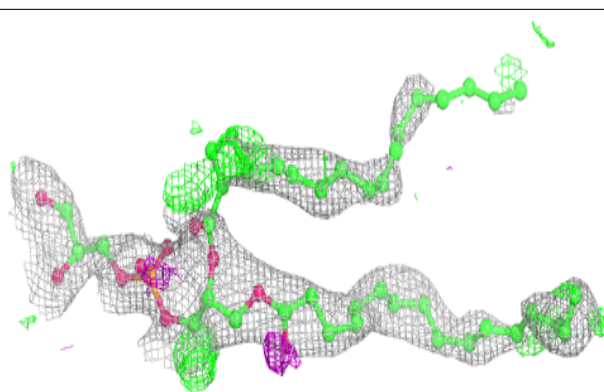




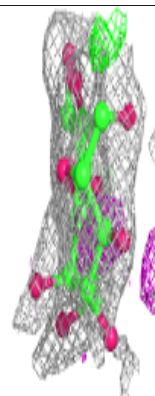
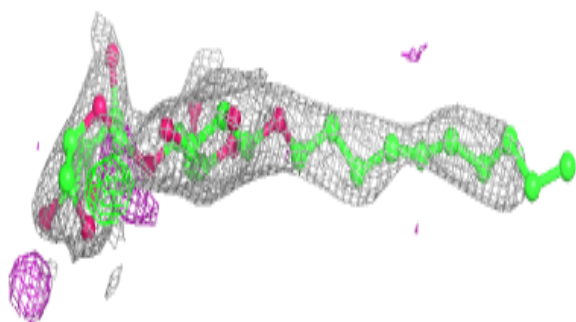
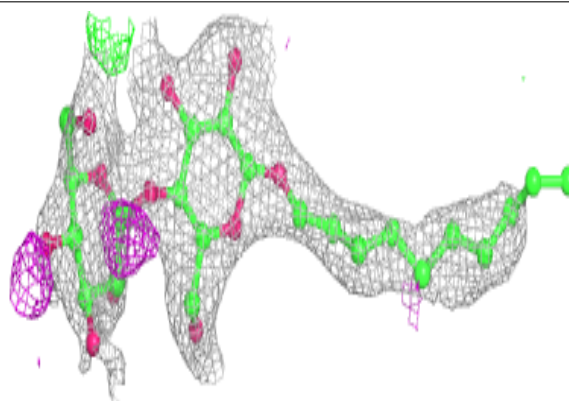


Electron density around PGV U 101:

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

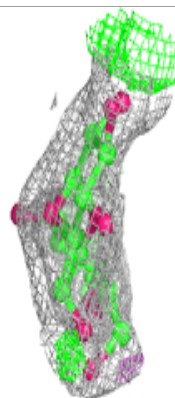
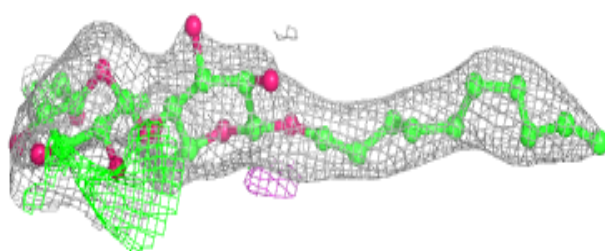
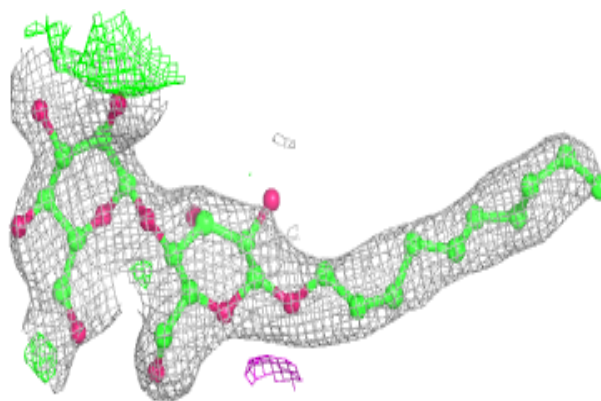
**Electron density around DMU C 310:**

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

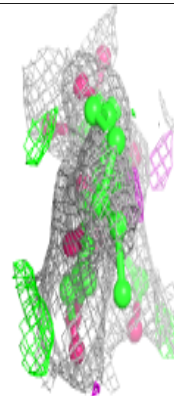
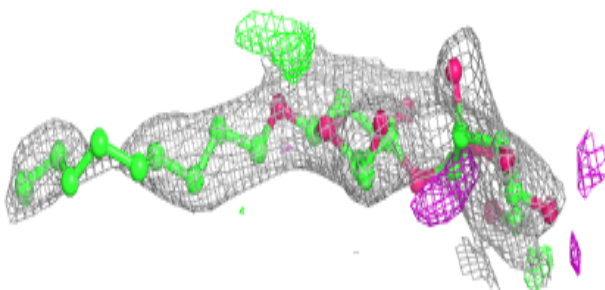
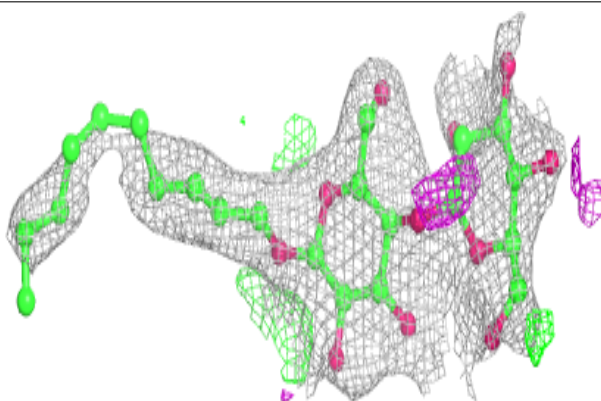


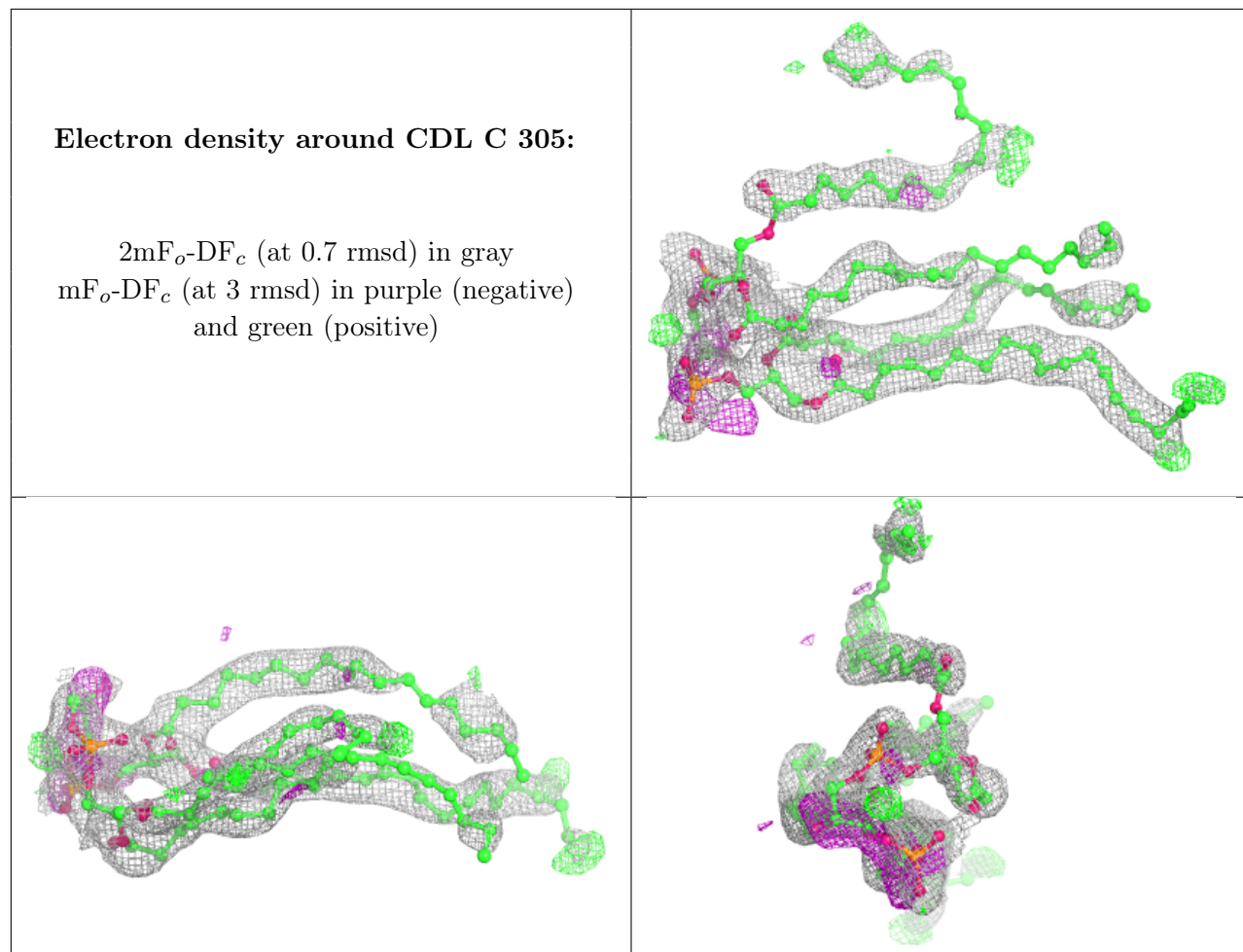
Electron density around DMU P 309:

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

**Electron density around DMU P 308:**

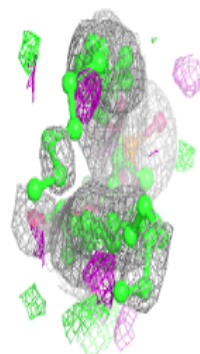
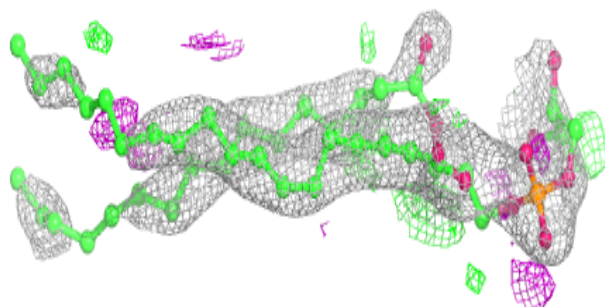
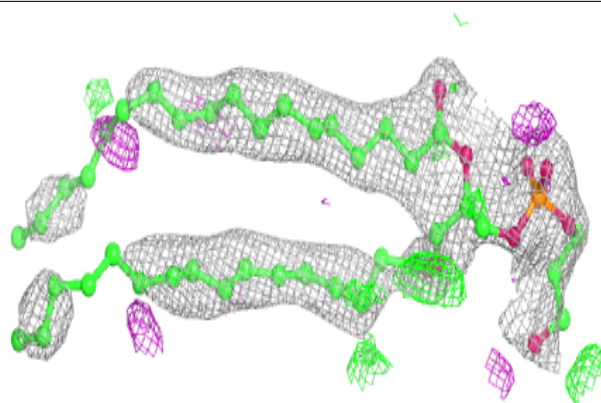
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



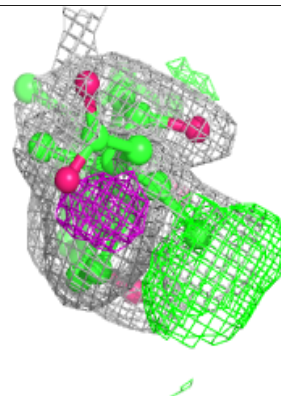
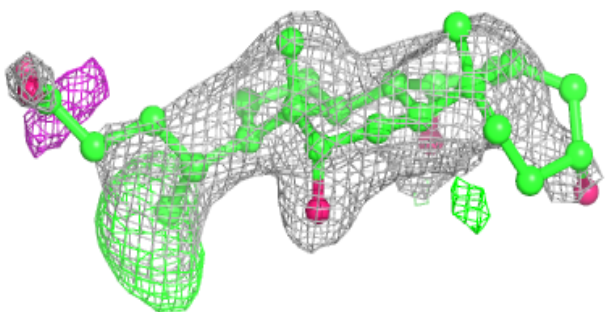
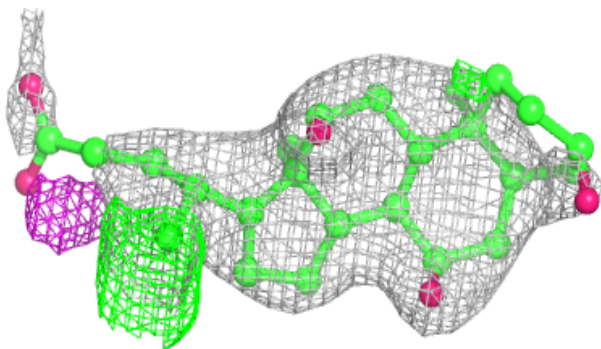


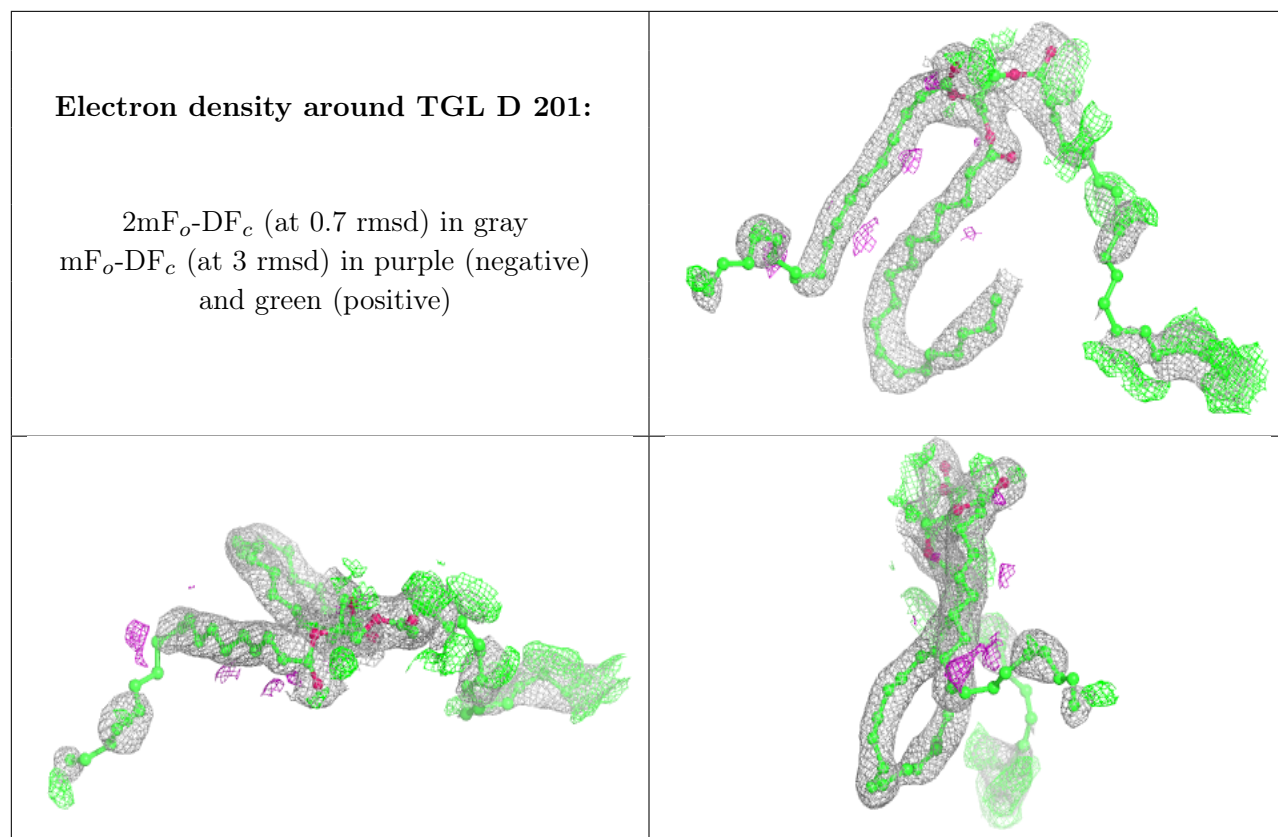
Electron density around PGV Z 101:

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

**Electron density around CHD J 101:**

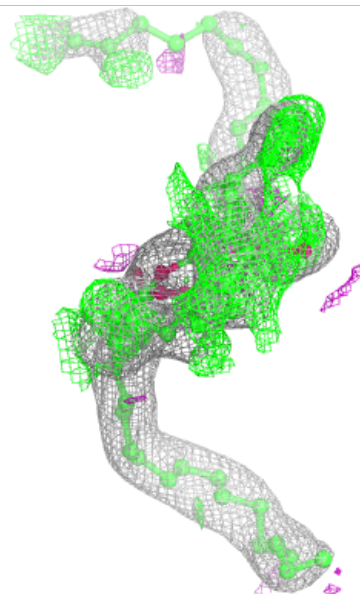
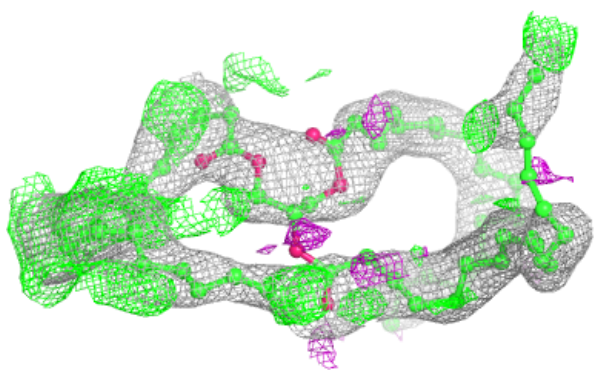
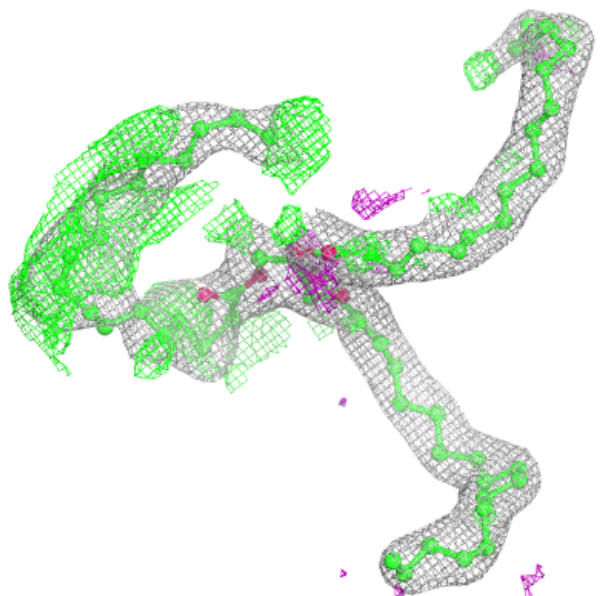
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

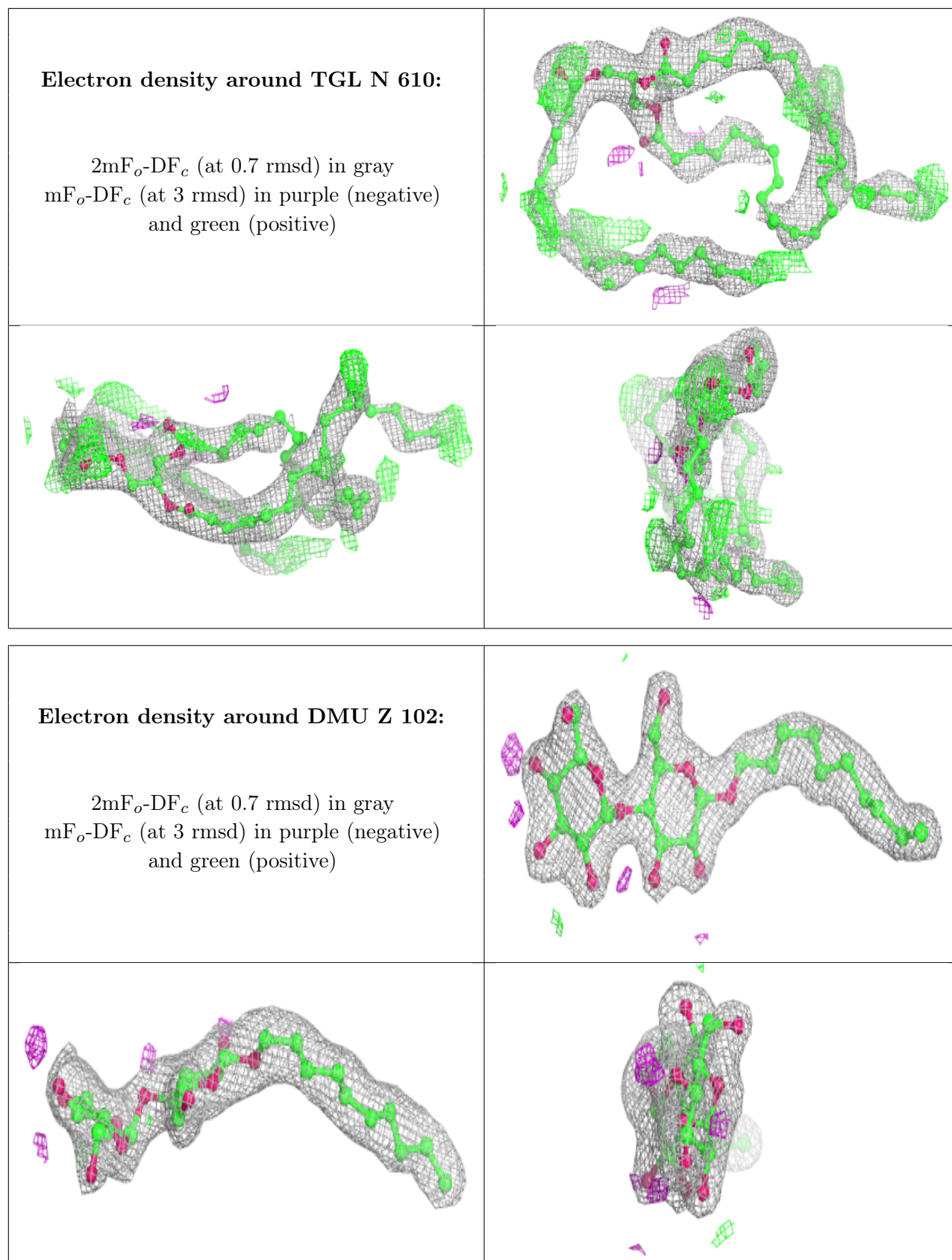




Electron density around TGL L 101:

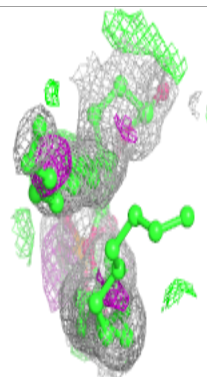
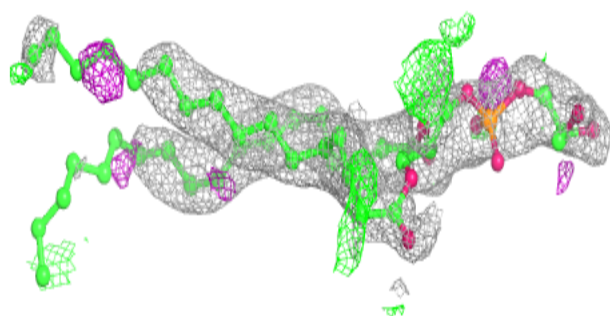
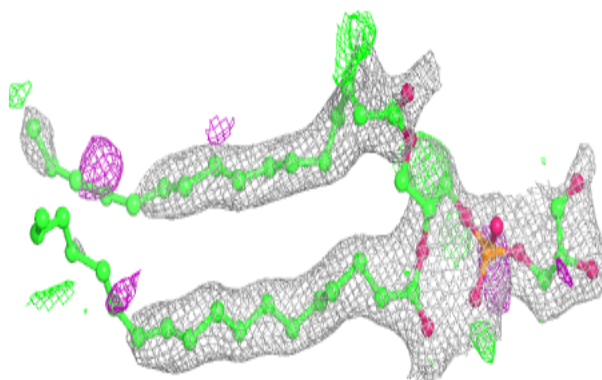
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



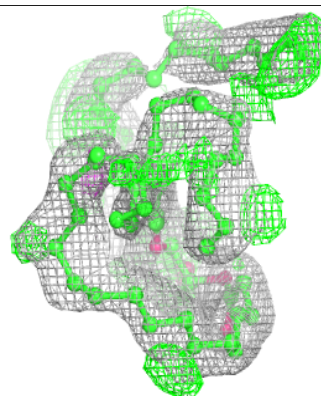
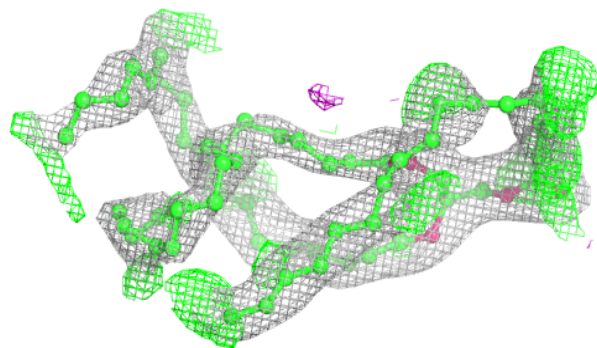
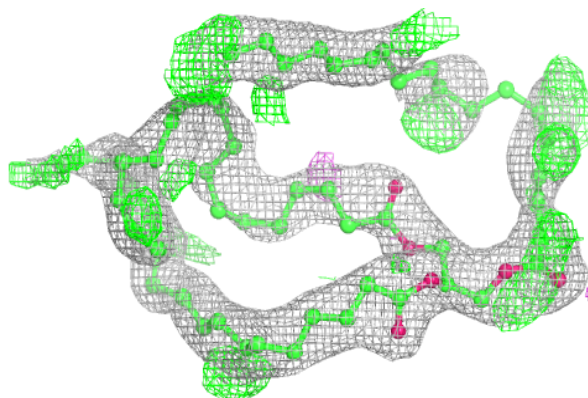


Electron density around PGV A 609:

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

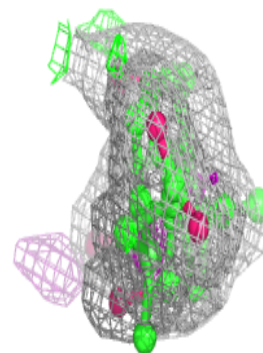
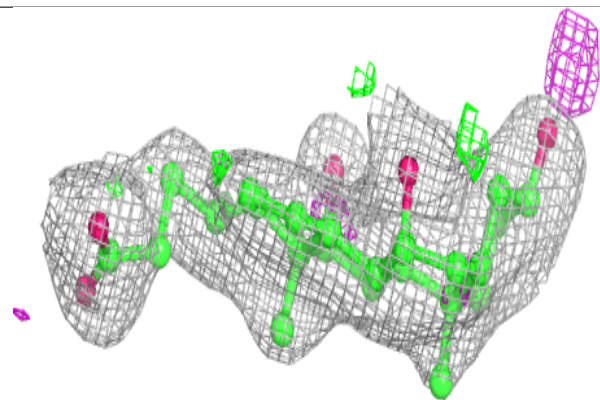
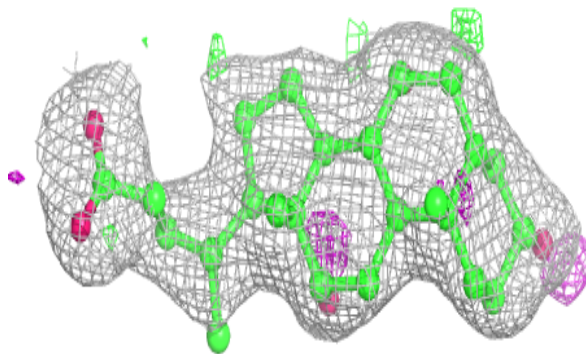
**Electron density around TGL B 301:**

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

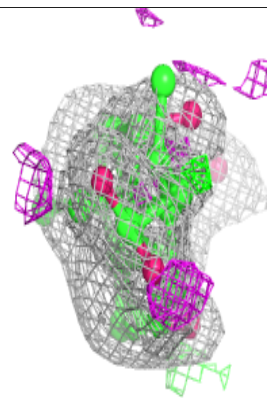
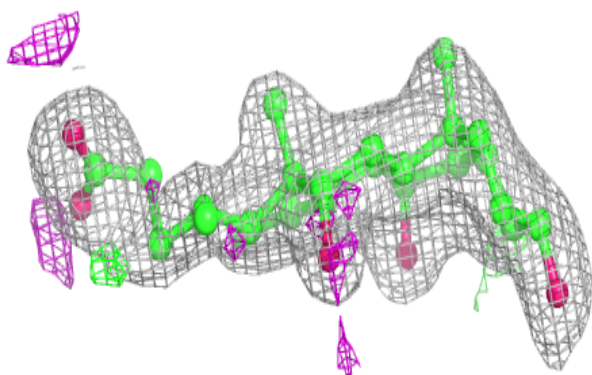
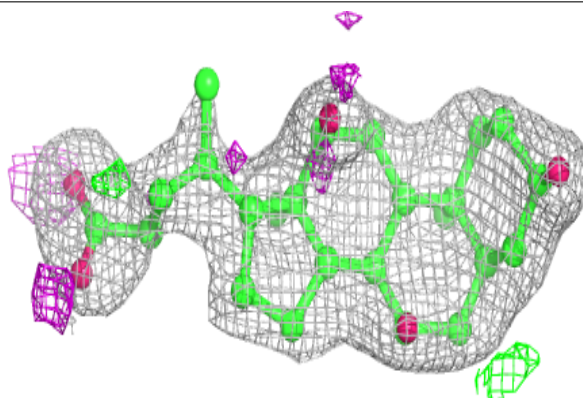


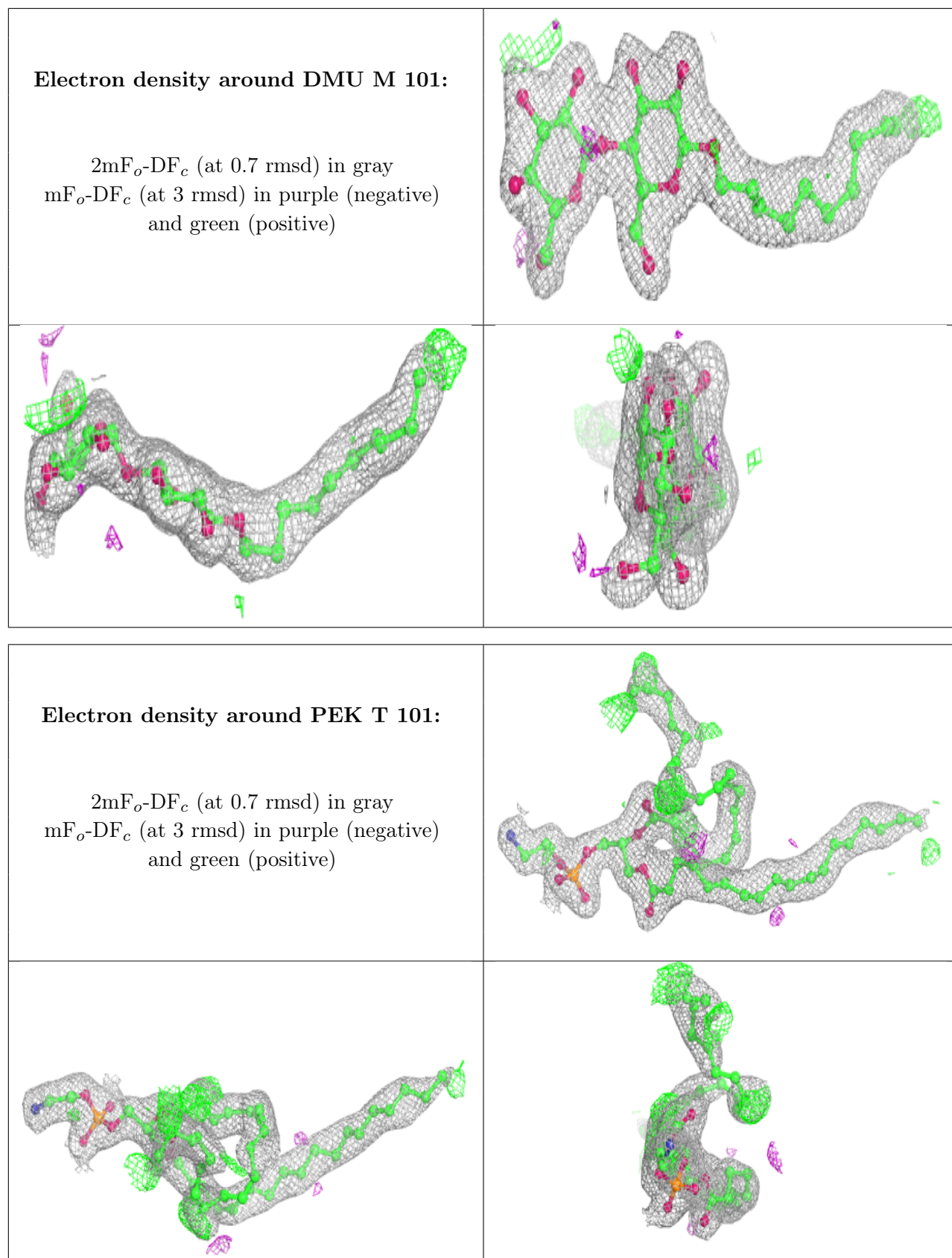
Electron density around CHD P 305:

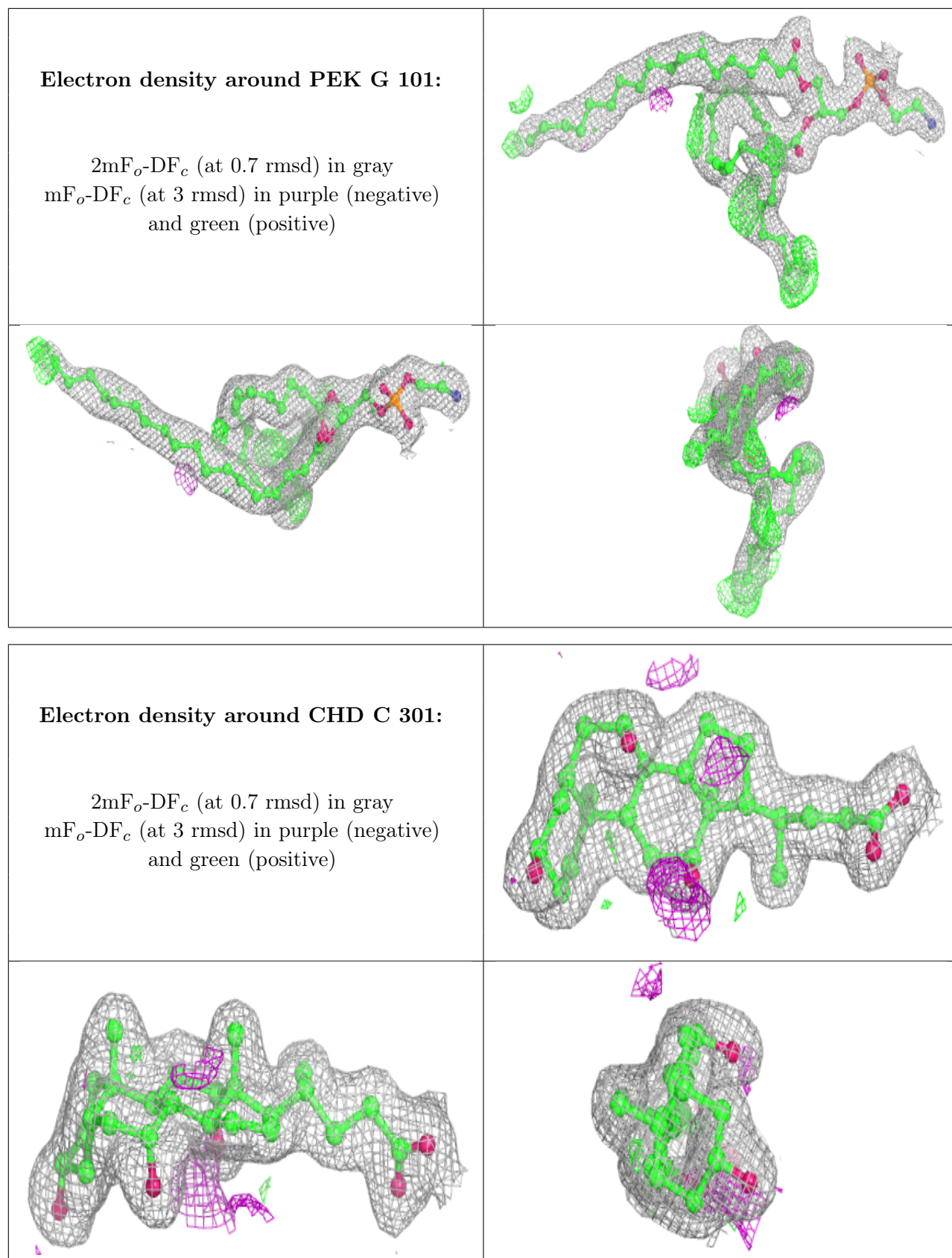
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CHD 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)

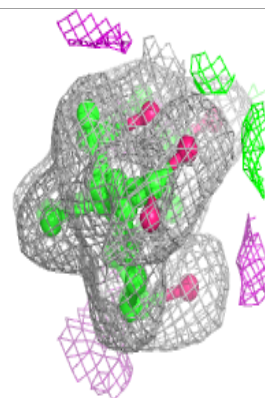
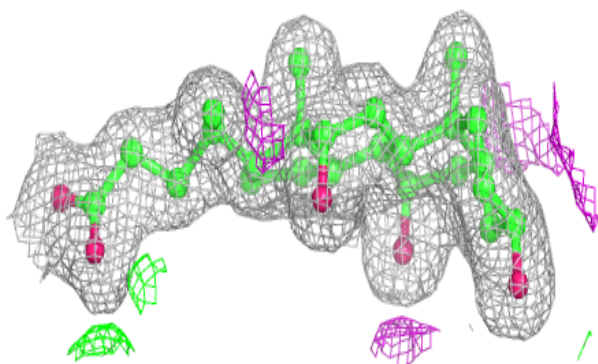
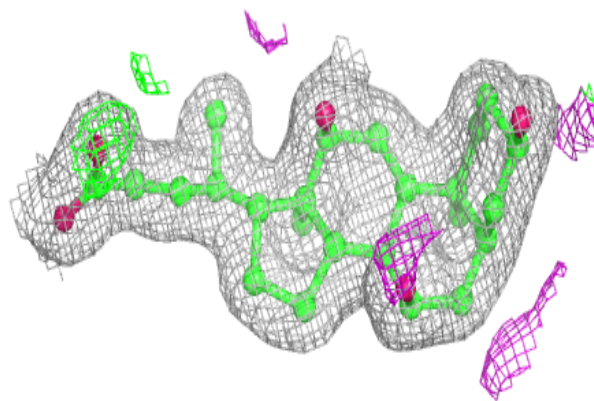




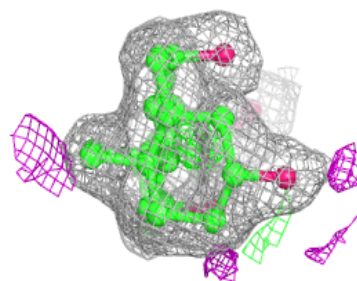
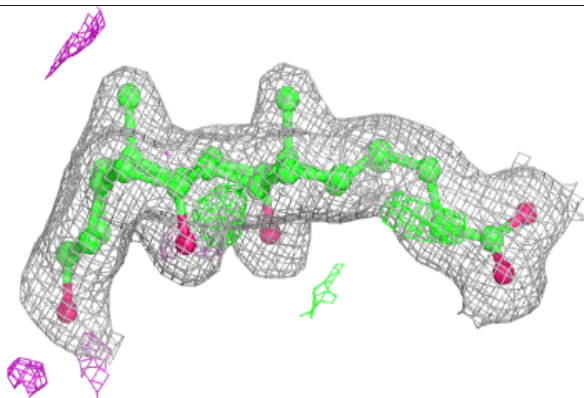
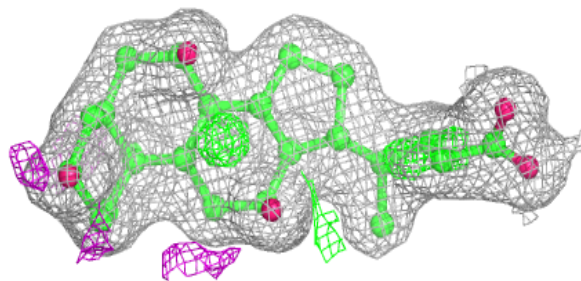


Electron density around CHD P 301:

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

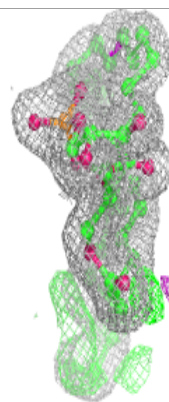
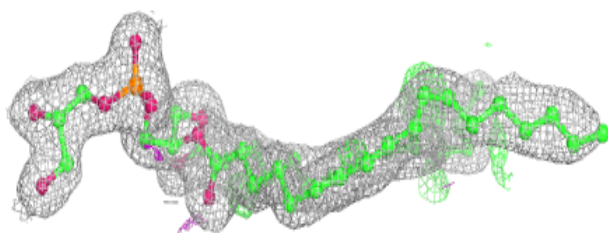
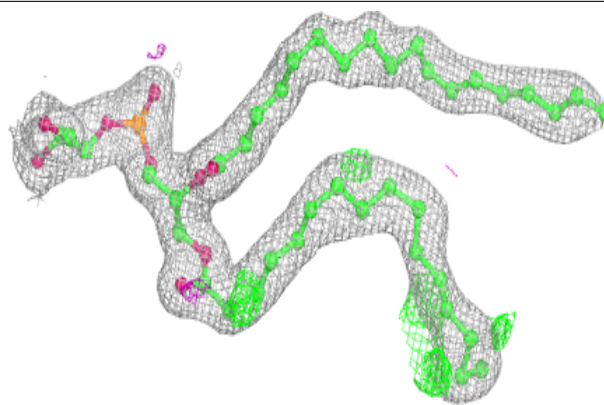
**Electron density around CHD B 302:**

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

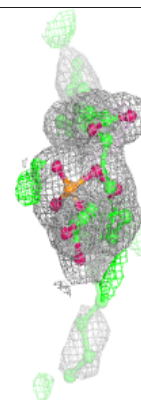
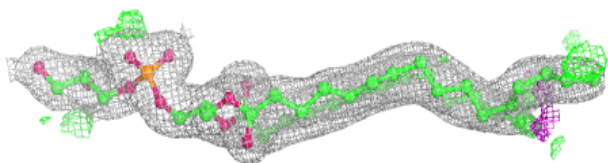
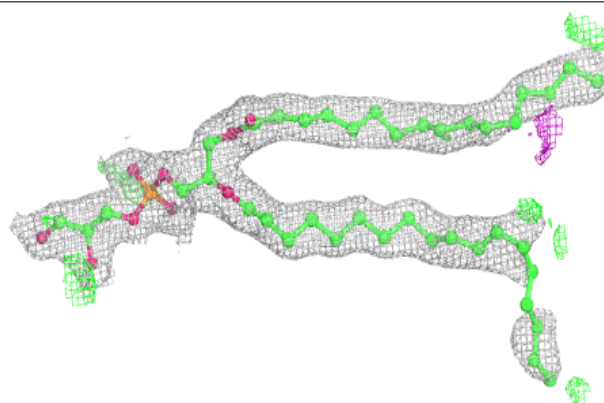


Electron density around PGV A 608:

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

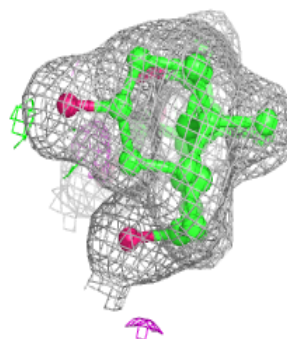
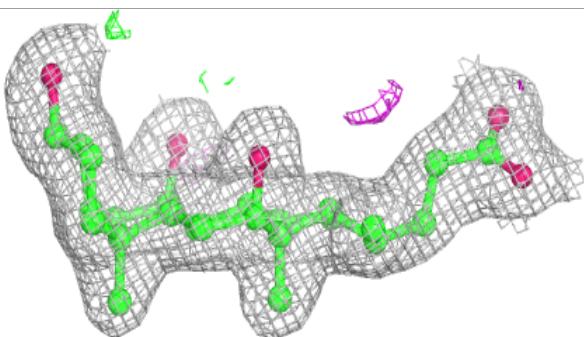
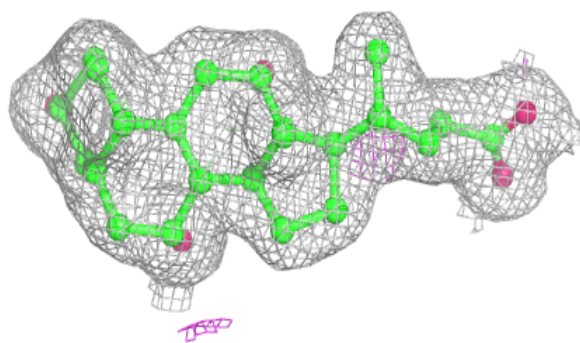
**Electron density around PGV P 303:**

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

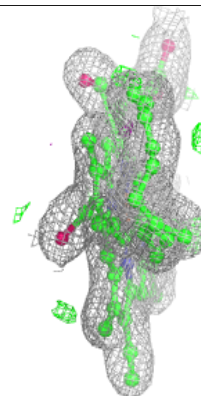
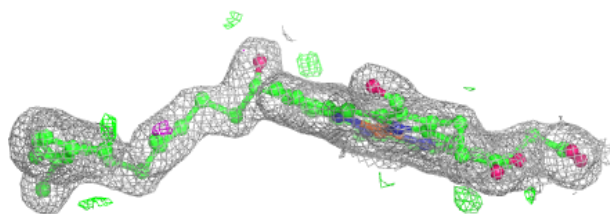
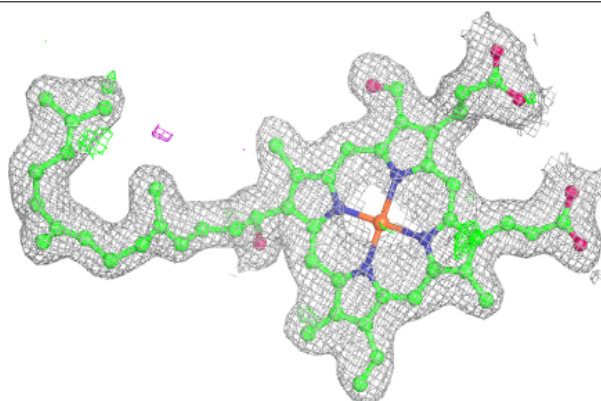


Electron density around CHD G 102:

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

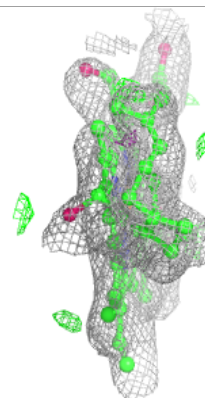
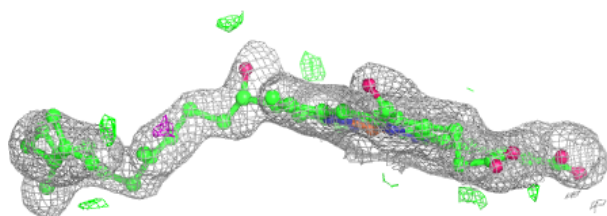
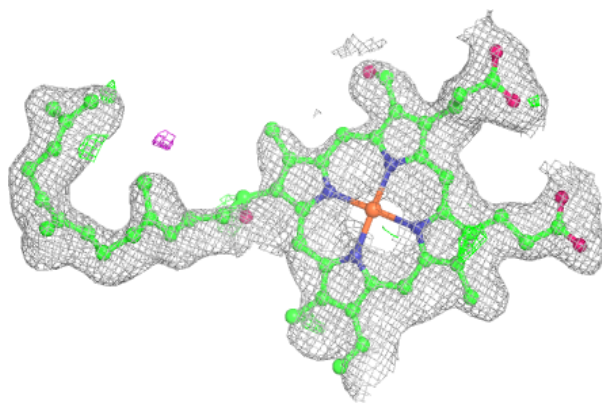
**Electron density around HEA A 602 (A):**

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

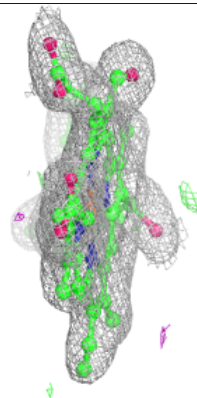
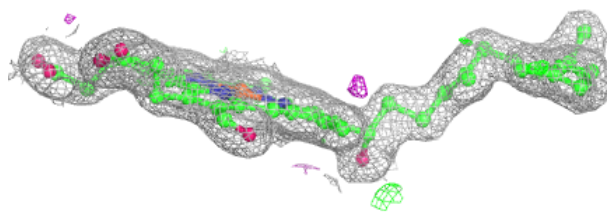
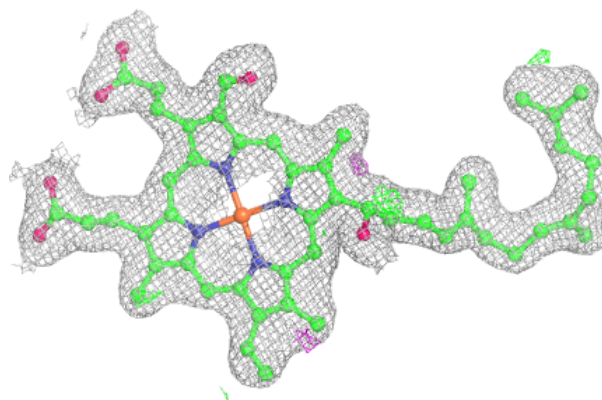


Electron density around HEA A 602 (B):

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

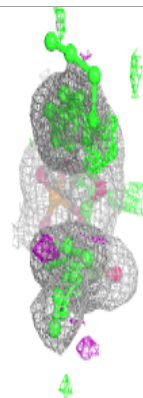
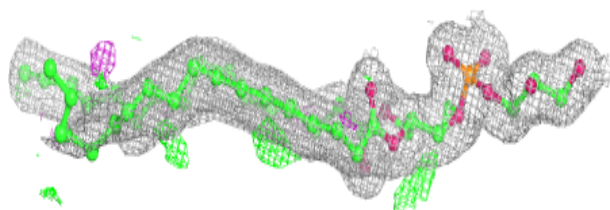
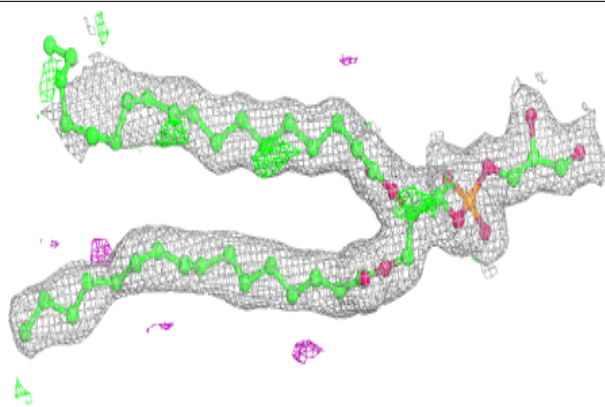
**Electron density around HEA N 603 (A):**

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

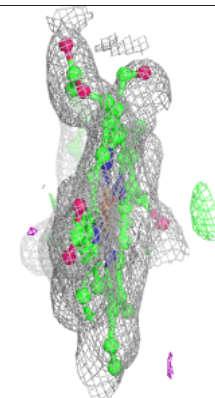
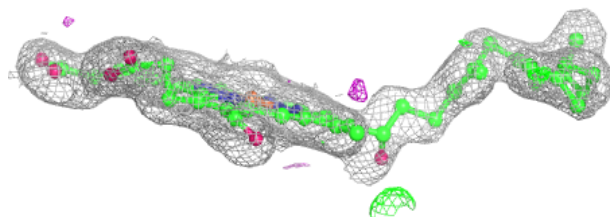
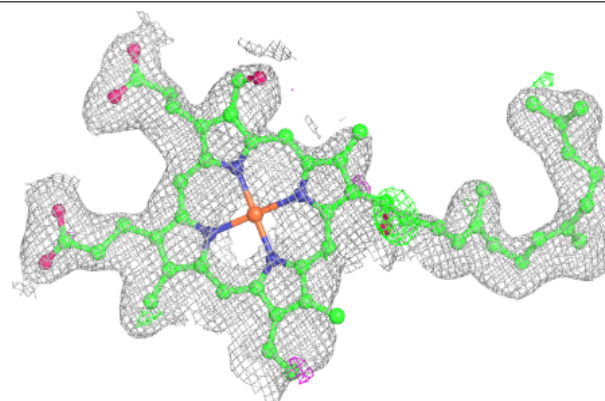


Electron density around PGV C 304:

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

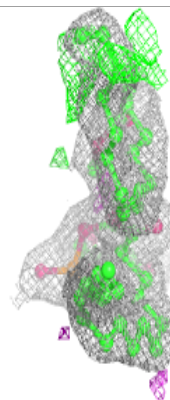
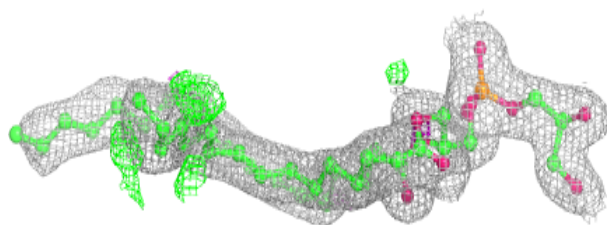
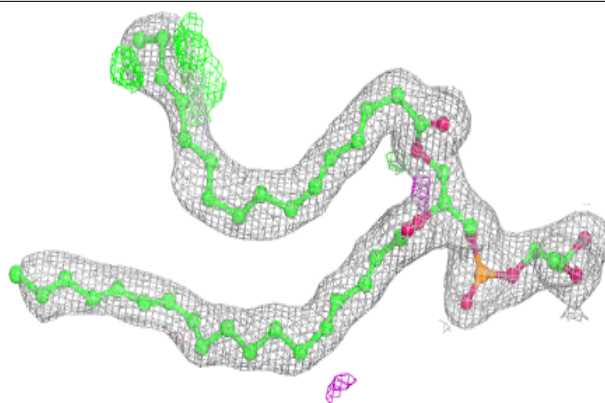
**Electron density around HEA N 603 (B):**

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

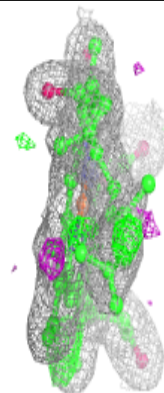
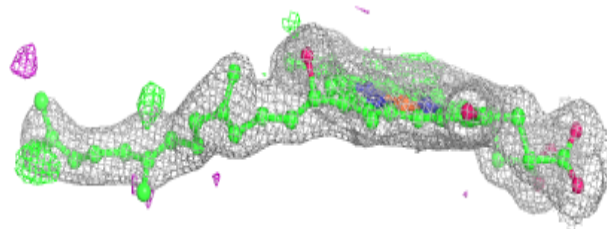
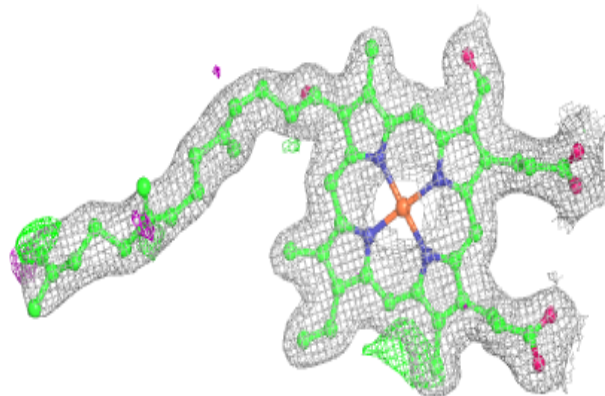


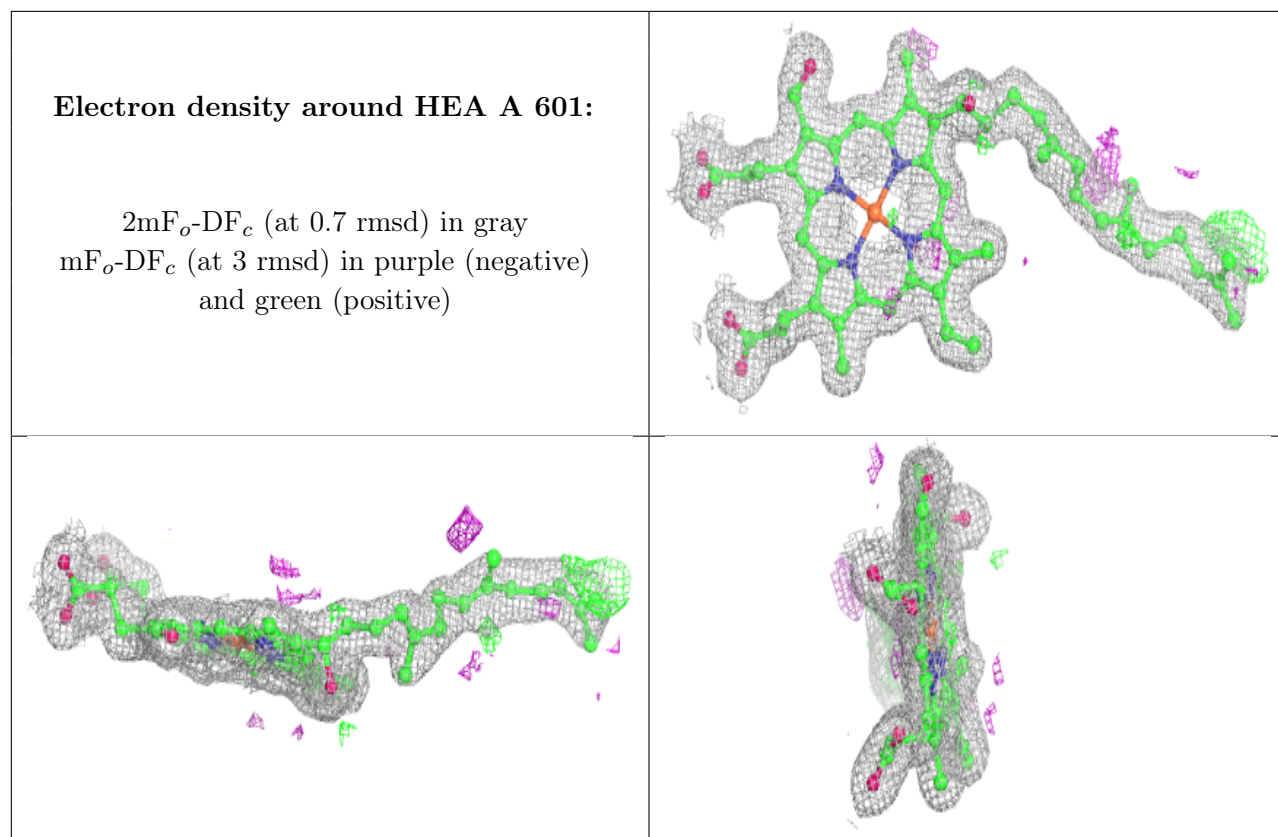
Electron density around PGV N 609:

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

**Electron density around HEA N 602:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.