



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2021 – 10:30 AM JST

PDB ID : 7D5X
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate, IO10, at 1.74 angstrom resolution
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2020-09-28
Resolution : 1.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

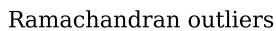
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

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X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
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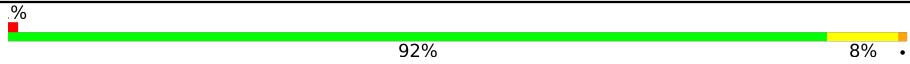
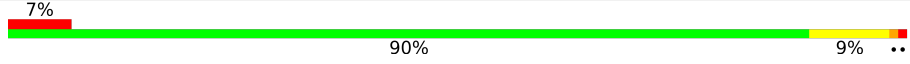
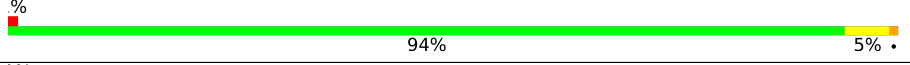
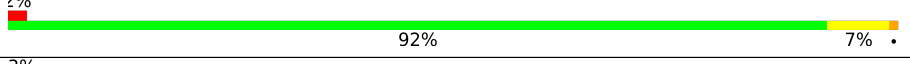


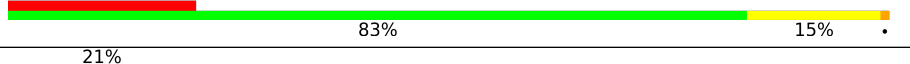

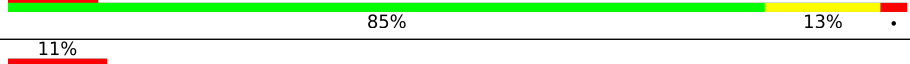

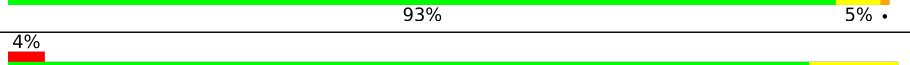
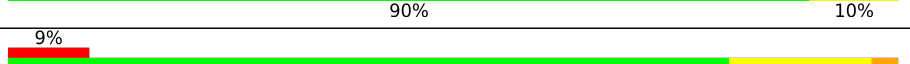

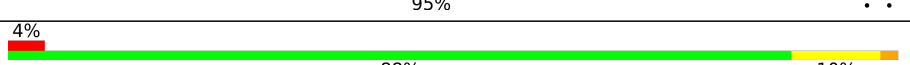

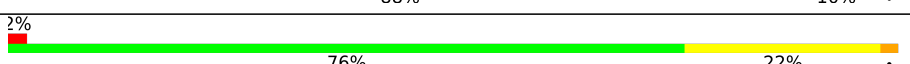
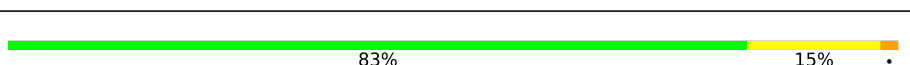
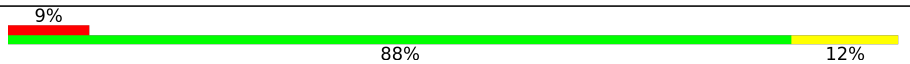
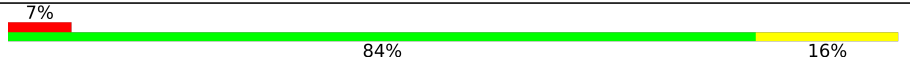

 R_{free}

that have poor fit to the electron density. The numeric value is given above the bar.

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	94	
6	S	94	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	602	X	-	-	-
14	HEA	N	601[A]	X	-	-	-
14	HEA	N	601[B]	X	-	-	-
14	HEA	N	601[C]	X	-	-	-
14	HEA	N	602	X	-	-	-
21	DMU	K	103	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33923 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	34	0
			4183	2789	644	711	39			
1	N	514	Total	C	N	O	S	0	28	0
			4174	2782	645	709	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	14	0
			1867	1214	284	349	20			
2	O	227	Total	C	N	O	S	0	9	0
			1853	1204	283	346	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	12	0
			2143	1430	341	358	14			
3	P	259	Total	C	N	O	S	0	8	0
			2131	1420	340	357	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			
6	S	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			

- 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	S	0	0	0
			672	431	129	111	1			
7	T	84	Total	C	N	O	S	0	0	0
			672	431	129	111	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
			461	297	78	83	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	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
			385	250	65	68	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

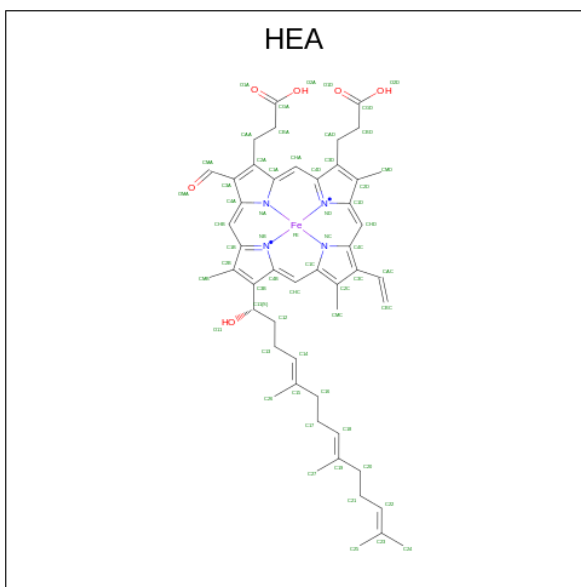
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			336	223	53	60			
13	Z	43	Total	C	N	O	0	0	0
			336	223	53	60			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	
			81	69	1	4	7	0
14	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			81	69	1	4	7	0
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

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

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

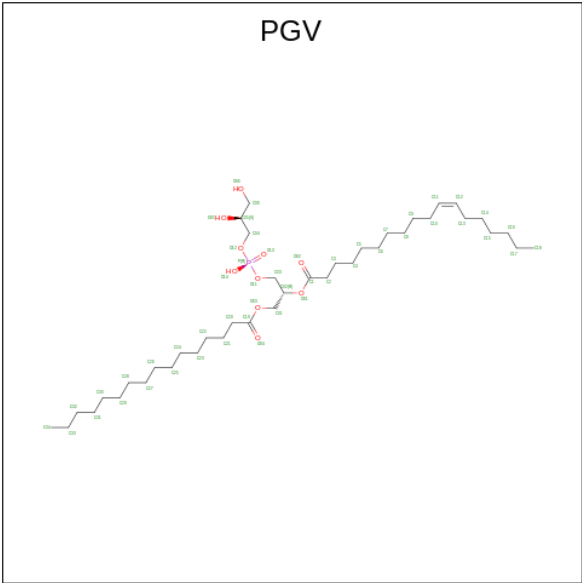
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



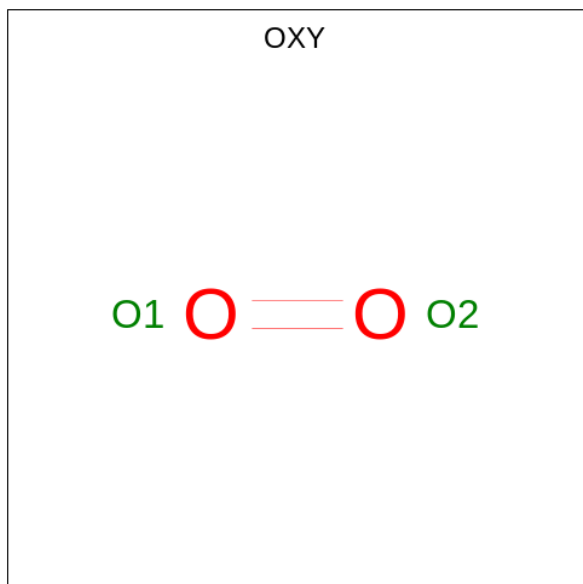
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O		0	0
			33	32	1			
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O		0	0
			37	34	3			
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O		0	0
			38	36	2			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	Q	1	Total	C	O	0	0
			37	35	2		

- Molecule 19 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		
19	N	1	Total	O	0	0
			2	2		

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



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

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

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

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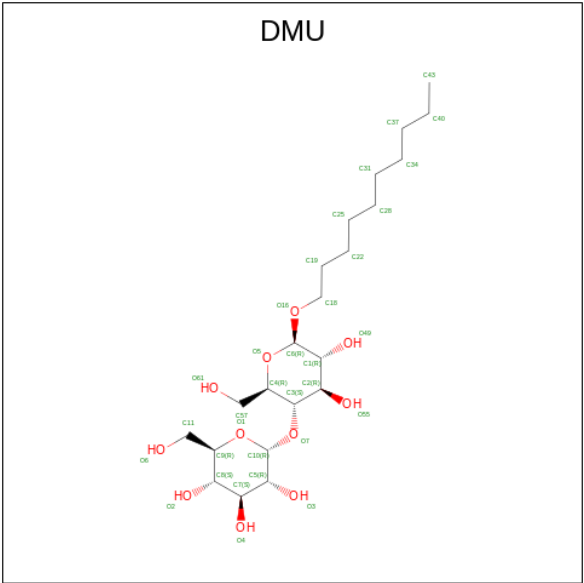
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	O	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20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

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

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



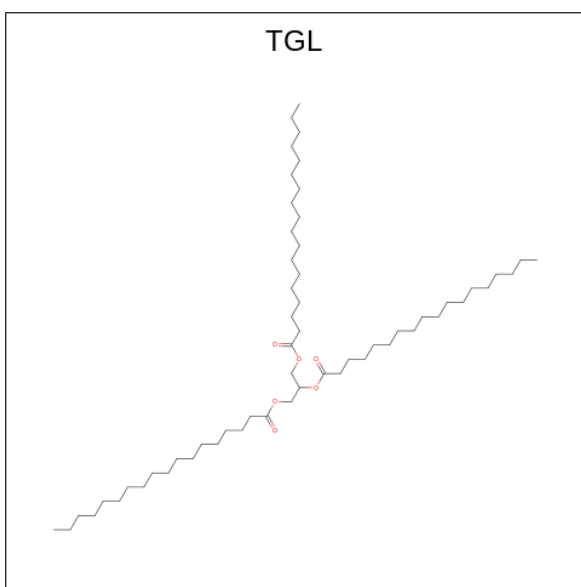
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C		0	0
			9	9			
21	A	1	Total	C		0	0
			8	8			
21	C	1	Total	C	O	0	0
			22	16	6		
21	C	1	Total	C	O	0	0
			12	11	1		
21	D	1	Total	C	O	0	0
			11	10	1		
21	D	1	Total	C		0	0
			8	8			
21	J	1	Total	C	O	0	0
			11	10	1		

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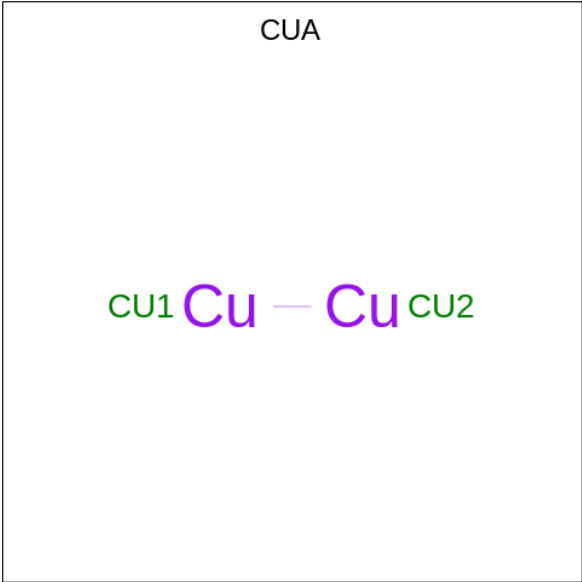
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	1	Total C 9 9	0	0
21	K	1	Total C 9 9	0	0
21	K	1	Total C 9 9	0	0
21	K	1	Total C 10 10	0	0
21	L	1	Total C O 21 16 5	0	0
21	M	1	Total C O 33 22 11	0	0
21	N	1	Total C 9 9	0	0
21	O	1	Total C O 11 10 1	0	0
21	P	1	Total C O 22 16 6	0	0
21	P	1	Total C O 11 10 1	0	0
21	Q	1	Total C 10 10	0	0
21	W	1	Total C O 11 10 1	0	0
21	X	1	Total C 9 9	0	0
21	X	1	Total C 8 8	0	0
21	X	1	Total C 10 10	0	0
21	Z	1	Total C O 33 22 11	0	0

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



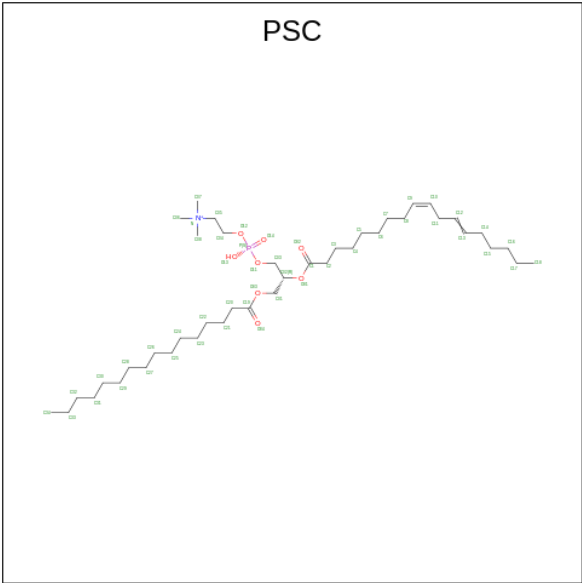
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		
22	D	1	Total	C	O	0	0
			63	57	6		
22	L	1	Total	C	O	0	0
			54	49	5		
22	N	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C		0	0
			43	43			
22	N	1	Total	C	O	0	0
			55	53	2		

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



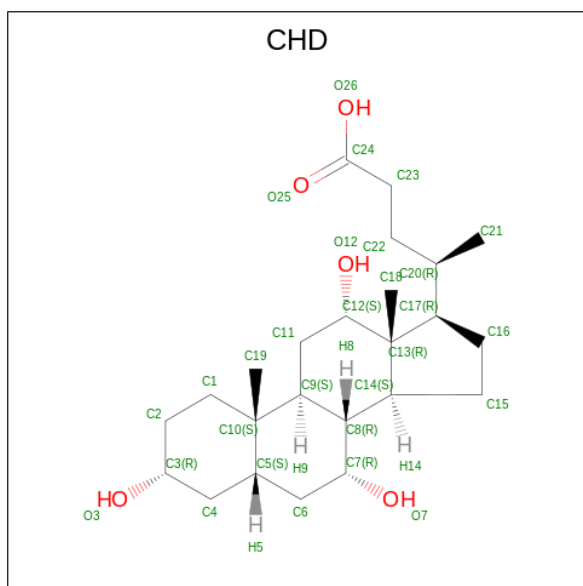
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			41	37	4		

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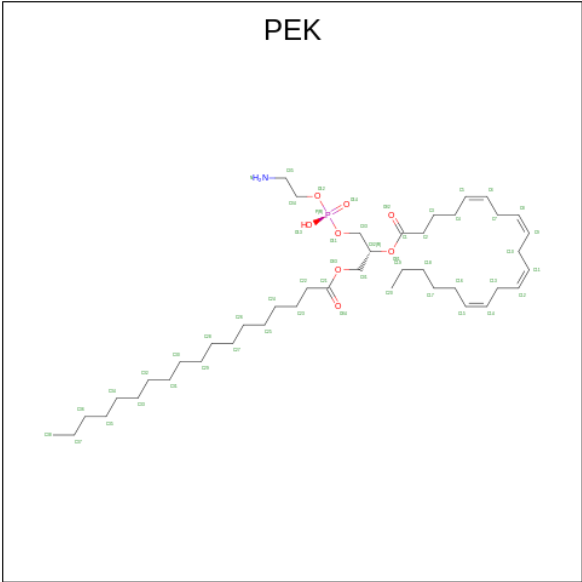
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	O	1	Total	C	O	0	0
			33	32	1		

- Molecule 25 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



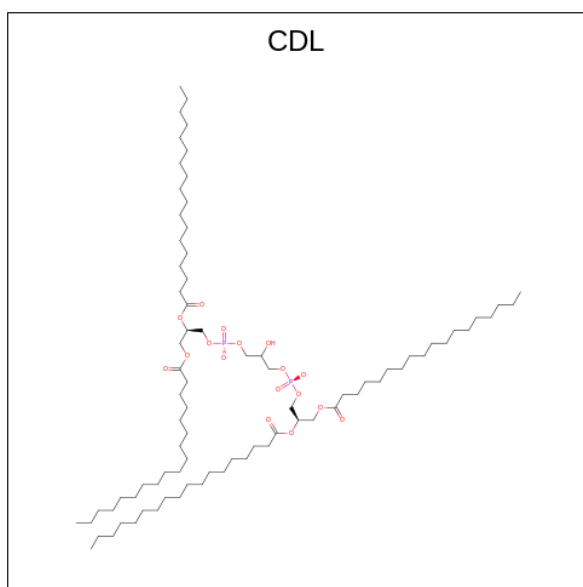
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			29	24	5		
25	C	1	Total	C	O	0	0
			29	24	5		
25	C	1	Total	C	O	0	0
			29	24	5		
25	G	1	Total	C	O	0	0
			29	24	5		
25	L	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C 18 18	0	0
26	C	1	Total C N O P 53 43 1 8 1	0	0
26	C	1	Total C O 40 38 2	0	0
26	P	1	Total C O 28 27 1	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C O 40 38 2	0	0

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

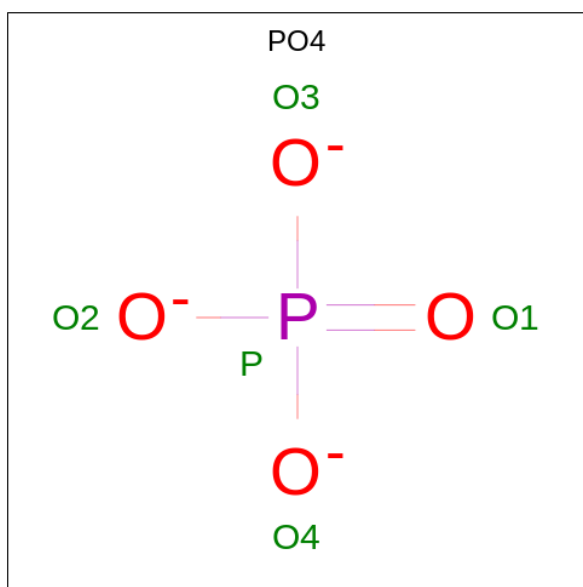


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O P 85 75 9 1	0	0
27	G	1	Total C O 69 67 2	0	0
27	P	1	Total C O 77 72 5	0	0
27	T	1	Total C O 70 66 4	0	0

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

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

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	248	Total	O	0	6
			250	250		
30	B	194	Total	O	0	3
			195	195		
30	C	139	Total	O	0	0
			139	139		
30	D	182	Total	O	0	1
			183	183		
30	E	133	Total	O	0	0
			133	133		
30	F	144	Total	O	0	0
			144	144		
30	G	68	Total	O	0	0
			68	68		
30	H	87	Total	O	0	0
			87	87		
30	I	63	Total	O	0	0
			63	63		
30	J	47	Total	O	0	0
			47	47		

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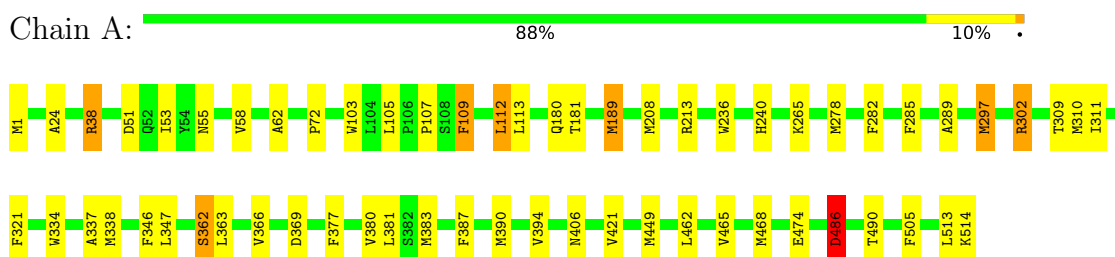
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	38	Total 38	O 38	0	0
30	L	30	Total 30	O 30	0	0
30	M	35	Total 35	O 35	0	0
30	N	247	Total 247	O 247	0	3
30	O	169	Total 169	O 169	0	1
30	P	145	Total 145	O 145	0	0
30	Q	88	Total 88	O 88	0	0
30	R	106	Total 106	O 106	0	0
30	S	133	Total 133	O 133	0	0
30	T	61	Total 61	O 61	0	0
30	U	78	Total 78	O 78	0	0
30	V	48	Total 48	O 48	0	0
30	W	46	Total 46	O 46	0	0
30	X	28	Total 28	O 28	0	0
30	Y	29	Total 29	O 29	0	0
30	Z	22	Total 22	O 22	0	0

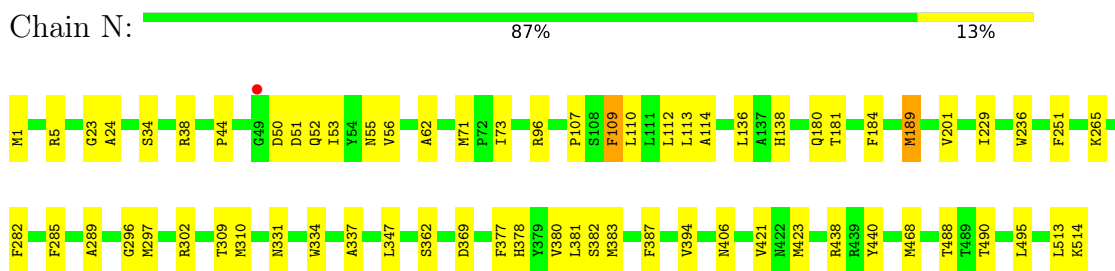
3 Residue-property plots

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

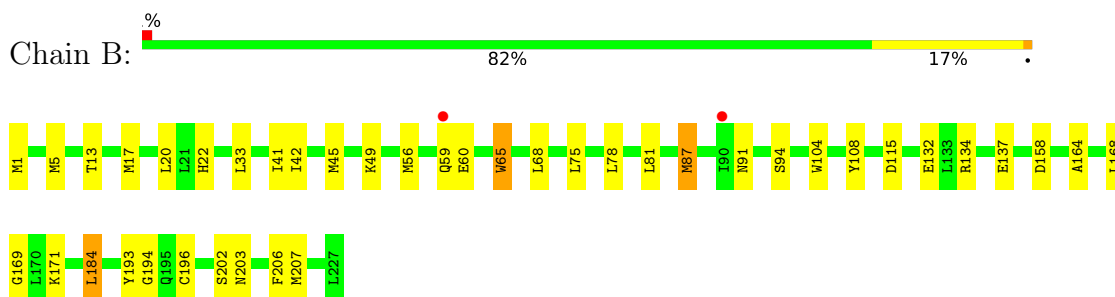
• Molecule 1: Cytochrome c oxidase subunit 1



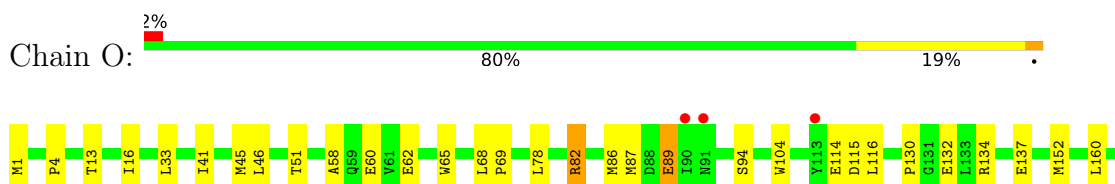
• Molecule 1: Cytochrome c oxidase subunit 1

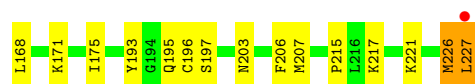


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





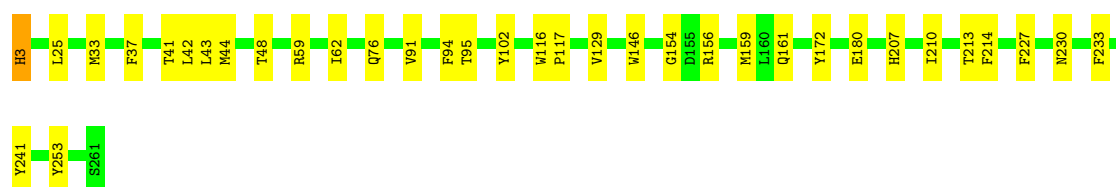
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 89% 11%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 86% 13%



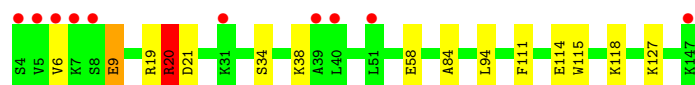
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 92% 8%



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

Chain Q: 90% 7% 9%



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

Chain E: 94% 5% 2%

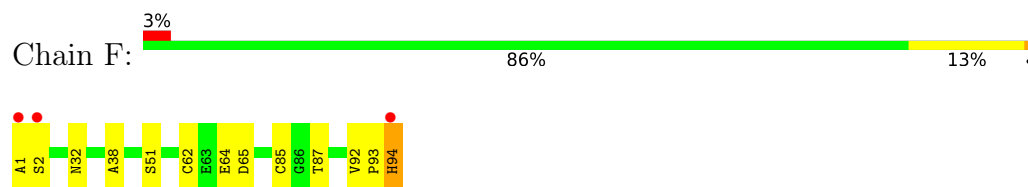


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

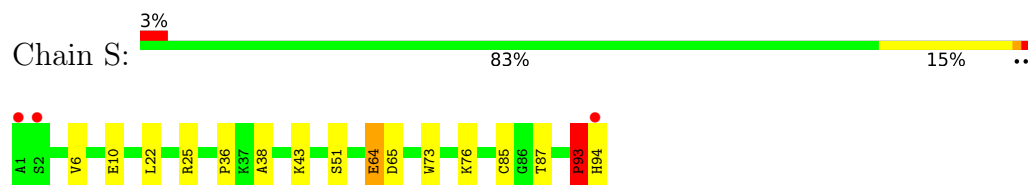
Chain R: 92% 7% 2%



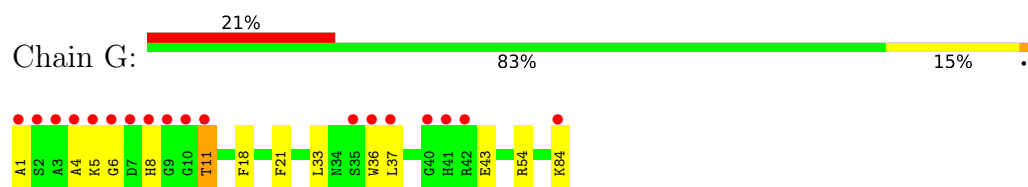
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



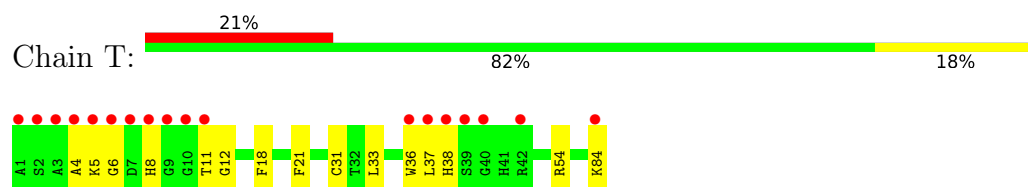
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



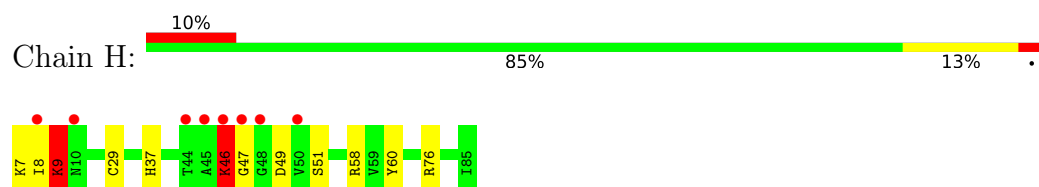
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



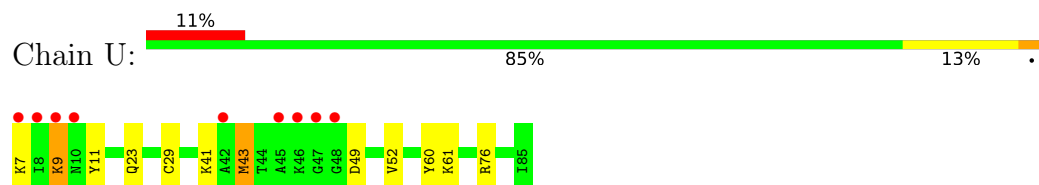
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1

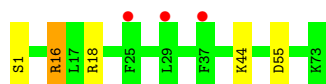


- Molecule 8: Cytochrome c oxidase subunit 6B1

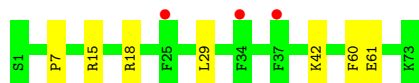
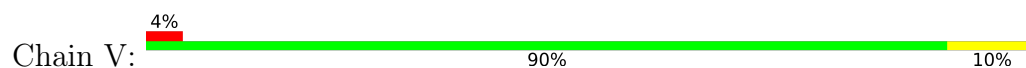


- Molecule 9: Cytochrome c oxidase subunit 6C

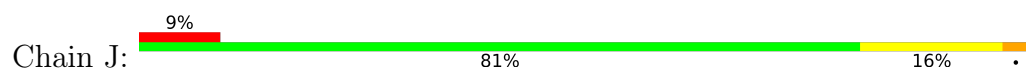




- Molecule 9: Cytochrome c oxidase subunit 6C



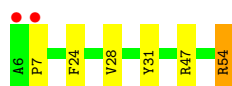
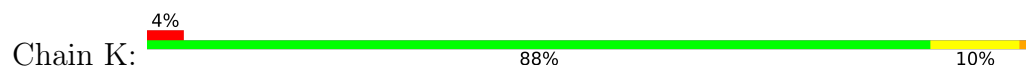
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



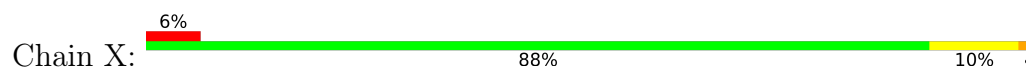
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



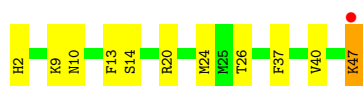
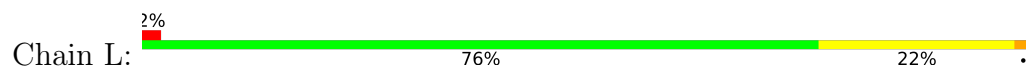
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



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



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

Chain Y:

83%

15%

.



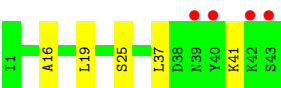
● Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:

9%

88%

12%



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

Chain Z:

7%

84%

16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.77Å 203.30Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 1.74 133.74 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.70-1.74) 99.7 (133.74-1.74)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.156 , 0.184 0.156 , 0.183	Depositor DCC
R_{free} test set	33307 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33923	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.07	4/4419 (0.1%)	1.03	16/6035 (0.3%)
1	N	1.00	3/4370 (0.1%)	0.97	7/5969 (0.1%)
2	B	1.00	4/1975 (0.2%)	1.03	6/2689 (0.2%)
2	O	0.89	2/1937 (0.1%)	0.95	4/2637 (0.2%)
3	C	0.98	1/2295 (0.0%)	0.86	2/3136 (0.1%)
3	P	0.98	4/2263 (0.2%)	0.85	2/3092 (0.1%)
4	D	0.93	0/1229	0.91	2/1658 (0.1%)
4	Q	0.76	0/1229	0.79	2/1658 (0.1%)
5	E	0.91	0/871	0.83	1/1182 (0.1%)
5	R	0.75	0/871	0.82	3/1182 (0.3%)
6	F	0.87	0/732	0.88	0/993
6	S	0.88	0/732	0.86	0/993
7	G	0.91	1/699 (0.1%)	0.89	0/950
7	T	0.86	1/699 (0.1%)	0.86	0/950
8	H	0.94	0/682	0.86	1/921 (0.1%)
8	U	0.82	1/682 (0.1%)	0.81	1/921 (0.1%)
9	I	0.81	0/605	0.85	2/802 (0.2%)
9	V	0.69	0/605	0.76	0/802
10	J	0.79	0/472	0.79	1/636 (0.2%)
10	W	0.73	0/472	0.78	0/636
11	K	0.84	0/399	0.92	1/546 (0.2%)
11	X	0.77	0/399	0.76	1/546 (0.2%)
12	L	1.03	1/393 (0.3%)	0.82	0/526
12	Y	0.86	0/393	0.72	0/526
13	M	0.86	0/346	0.83	0/470
13	Z	0.85	1/346 (0.3%)	0.76	0/470
All	All	0.94	23/30115 (0.1%)	0.91	52/40926 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	F	0	1
6	S	0	1
8	H	0	1
10	J	0	1
All	All	0	5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	227	PHE	CE2-CZ	6.83	1.50	1.37
1	A	346	PHE	CD1-CE1	6.65	1.52	1.39
2	B	193	TYR	CD2-CE2	6.21	1.48	1.39
1	N	438	ARG	CG-CD	6.18	1.67	1.51
2	B	193	TYR	CD1-CE1	6.05	1.48	1.39

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-18.98	69.84	100.20
1	A	278	MET	CG-SD-CE	-15.97	74.65	100.20
1	N	189	MET	CG-SD-CE	-11.01	82.59	100.20
11	K	47	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	189	MET	CG-SD-CE	-10.09	84.06	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	93	PRO	Peptide
8	H	9	LYS	Peptide
10	J	56	PRO	Peptide
6	S	93	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4183	0	4164	58	0
1	N	4174	0	4155	59	0
2	B	1867	0	1886	25	0
2	O	1853	0	1860	29	0
3	C	2143	0	2059	26	0
3	P	2131	0	2036	26	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	15	0
5	E	852	0	845	4	0
5	R	852	0	845	5	0
6	F	716	0	697	11	0
6	S	716	0	697	16	0
7	G	672	0	645	6	0
7	T	672	0	645	9	0
8	H	662	0	623	3	0
8	U	662	0	623	8	0
9	I	601	0	613	2	0
9	V	601	0	613	5	0
10	J	461	0	459	12	0
10	W	461	0	459	3	0
11	K	385	0	366	3	0
11	X	385	0	366	5	0
12	L	380	0	380	11	0
12	Y	380	0	380	6	0
13	M	336	0	352	5	0
13	Z	336	0	352	2	0
14	A	141	0	115	11	0
14	N	141	0	115	10	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	84	0	136	8	0
18	C	88	0	138	2	0
18	N	51	0	76	1	0
18	P	89	0	140	4	0
18	Q	37	0	62	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	2	0	0	0	0
19	N	2	0	0	0	0
20	A	44	0	66	4	0
20	B	24	0	36	0	0
20	C	36	0	54	1	0
20	D	16	0	24	0	0
20	E	12	0	18	0	0
20	F	24	0	36	0	0
20	G	4	0	6	0	0
20	J	8	0	12	1	0
20	L	4	0	6	0	0
20	M	4	0	6	0	0
20	N	44	0	66	1	0
20	O	8	0	12	0	0
20	P	28	0	42	2	0
20	Q	8	0	12	1	0
20	R	8	0	12	2	0
20	S	28	0	41	1	0
20	T	12	0	18	0	0
20	W	8	0	12	2	0
20	Y	4	0	6	0	0
21	A	17	0	32	0	0
21	C	34	0	52	6	0
21	D	19	0	36	0	0
21	J	11	0	21	3	0
21	K	37	0	70	2	0
21	L	21	0	30	1	0
21	M	33	0	42	0	0
21	N	9	0	17	1	0
21	O	11	0	21	0	0
21	P	33	0	52	6	0
21	Q	10	0	19	1	0
21	W	11	0	21	0	0
21	X	27	0	51	0	0
21	Z	33	0	42	0	0
22	B	63	0	110	7	0
22	D	63	0	110	14	0
22	L	54	0	87	9	0
22	N	161	0	294	16	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	41	0	65	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	O	33	0	58	4	0
25	B	29	0	39	0	0
25	C	58	0	78	1	0
25	G	29	0	39	1	0
25	L	29	0	39	1	0
25	P	58	0	78	3	0
26	C	111	0	168	14	0
26	P	121	0	182	13	0
27	C	85	0	143	12	0
27	G	69	0	126	8	0
27	P	77	0	137	10	0
27	T	70	0	125	18	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	250	0	0	7	0
30	B	195	0	0	3	0
30	C	139	0	0	3	0
30	D	183	0	0	4	0
30	E	133	0	0	3	0
30	F	144	0	0	2	0
30	G	68	0	0	2	0
30	H	87	0	0	0	0
30	I	63	0	0	1	0
30	J	47	0	0	3	0
30	K	38	0	0	0	0
30	L	30	0	0	3	0
30	M	35	0	0	0	0
30	N	247	0	0	3	0
30	O	169	0	0	1	0
30	P	145	0	0	2	0
30	Q	88	0	0	2	0
30	R	106	0	0	0	0
30	S	133	0	0	4	0
30	T	61	0	0	3	0
30	U	78	0	0	3	0
30	V	48	0	0	4	0
30	W	46	0	0	1	0
30	X	28	0	0	1	0
30	Y	29	0	0	0	0
30	Z	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33923	0	32137	410	0

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

The worst 5 of 410 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:161[A]:GLN:HE22	26:P:305:PEK:H41	1.27	0.97
1:N:113:LEU:HB2	22:N:607:TGL:H312	1.44	0.95
1:A:486[B]:ASP:OD2	4:D:19:ARG:HD2	1.67	0.93
12:L:20:ARG:HH21	22:L:101:TGL:HC32	1.36	0.88
1:A:113:LEU:HB2	22:L:101:TGL:H302	1.54	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/514 (106%)	531 (97%)	16 (3%)	0	100	100
1	N	540/514 (105%)	529 (98%)	11 (2%)	0	100	100
2	B	239/227 (105%)	232 (97%)	7 (3%)	0	100	100
2	O	234/227 (103%)	227 (97%)	7 (3%)	0	100	100
3	C	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
3	P	265/259 (102%)	259 (98%)	6 (2%)	0	100	100
4	D	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
5	E	103/105 (98%)	103 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	103/105 (98%)	103 (100%)	0	0	100	100
6	F	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
6	S	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
7	G	82/84 (98%)	70 (85%)	8 (10%)	4 (5%)	2	0
7	T	82/84 (98%)	69 (84%)	11 (13%)	2 (2%)	6	1
8	H	77/79 (98%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	12	2
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	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	41 (100%)	0	0	100	100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3604/3550 (102%)	3492 (97%)	102 (3%)	10 (0%)	41	23

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	37	LEU
8	H	46	LYS
8	H	47	GLY
7	G	5	LYS
7	T	5	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/426 (108%)	446 (97%)	12 (3%)	46	22
1	N	451/426 (106%)	446 (99%)	5 (1%)	73	59
2	B	224/210 (107%)	211 (94%)	13 (6%)	20	4
2	O	219/210 (104%)	208 (95%)	11 (5%)	24	6
3	C	236/224 (105%)	233 (99%)	3 (1%)	69	52
3	P	232/224 (104%)	227 (98%)	5 (2%)	52	29
4	D	128/128 (100%)	127 (99%)	1 (1%)	81	72
4	Q	128/128 (100%)	124 (97%)	4 (3%)	40	16
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	59
5	R	92/92 (100%)	92 (100%)	0	100	100
6	F	78/78 (100%)	76 (97%)	2 (3%)	46	22
6	S	78/78 (100%)	76 (97%)	2 (3%)	46	22
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	1
7	T	68/68 (100%)	62 (91%)	6 (9%)	10	1
8	H	71/71 (100%)	64 (90%)	7 (10%)	8	1
8	U	71/71 (100%)	67 (94%)	4 (6%)	21	4
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	38
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	12
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	33
10	W	49/49 (100%)	48 (98%)	1 (2%)	55	33
11	K	39/39 (100%)	37 (95%)	2 (5%)	24	5
11	X	39/39 (100%)	38 (97%)	1 (3%)	46	22
12	L	39/39 (100%)	37 (95%)	2 (5%)	24	5
12	Y	39/39 (100%)	37 (95%)	2 (5%)	24	5
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	34 (92%)	3 (8%)	11	1
All	All	3136/3036 (103%)	3038 (97%)	98 (3%)	41	16

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	33	LEU
3	P	214	PHE
2	O	60[B]	GLU

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Mol	Chain	Res	Type
2	O	171	LYS
4	Q	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	35	GLN
2	O	195	GLN
11	X	35	GLN
6	S	94	HIS
9	V	8	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SAC	I	1	9	7,8,9	0.62	0	8,9,11	1.25	2 (25%)
9	SAC	V	1	9	7,8,9	0.60	0	8,9,11	0.97	0
2	FME	B	1	2	8,9,10	1.19	0	7,9,11	2.13	4 (57%)
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.78	2 (28%)
1	FME	A	1	1	8,9,10	0.67	0	7,9,11	1.74	2 (28%)
2	FME	O	1	2	8,9,10	1.09	0	7,9,11	1.37	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	I	1	9	-	2/7/8/10	-
9	SAC	V	1	9	-	3/7/8/10	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.54	103.10	112.95
1	N	1	FME	O-C-CA	-3.18	116.45	124.78
1	A	1	FME	CE-SD-CG	3.11	111.10	100.40
1	N	1	FME	CE-SD-CG	3.10	111.04	100.40
2	B	1	FME	C-CA-N	-2.71	104.84	109.73

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 10 are monoatomic - leaving 151 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	$\# Z > 2$
25	CHD	C	301	-	29,32,32	1.03	2 (6%)	48,51,51	1.78	14 (29%)
20	EDO	P	315	-	3,3,3	0.48	0	2,2,2	0.99	0
20	EDO	S	105	-	3,3,3	3.33	1 (33%)	2,2,2	2.01	1 (50%)
20	EDO	N	618	-	3,3,3	0.48	0	2,2,2	0.39	0
20	EDO	E	201	-	3,3,3	0.52	0	2,2,2	0.35	0
20	EDO	C	315	-	3,3,3	0.56	0	2,2,2	0.18	0
21	DMU	W	103	-	10,10,34	0.31	0	9,9,45	0.88	0
20	EDO	P	313	-	3,3,3	0.44	0	2,2,2	0.23	0
20	EDO	C	318	-	3,3,3	0.51	0	2,2,2	0.61	0
14	HEA	N	602	19,1	44,67,67	1.33	6 (13%)	37,103,103	2.13	9 (24%)
20	EDO	J	101	-	3,3,3	0.50	0	2,2,2	0.25	0
20	EDO	N	612	-	3,3,3	1.04	0	2,2,2	0.61	0
21	DMU	O	305	-	10,10,34	0.32	0	9,9,45	0.43	0
21	DMU	K	104	-	9,9,34	0.35	0	8,8,45	0.53	0
20	EDO	E	202	-	3,3,3	0.63	0	2,2,2	0.24	0
26	PEK	C	304	-	52,52,52	0.85	2 (3%)	55,57,57	1.13	2 (3%)
20	EDO	R	202	-	3,3,3	0.29	0	2,2,2	0.72	0
26	PEK	P	305	-	38,38,52	0.91	1 (2%)	37,37,57	1.04	3 (8%)
20	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.68	0
20	EDO	A	610	-	3,3,3	0.94	0	2,2,2	0.59	0
22	TGL	N	608	-	52,52,62	0.72	1 (1%)	50,50,65	0.80	1 (2%)
20	EDO	P	314	-	3,3,3	0.82	0	2,2,2	0.24	0
20	EDO	B	310	-	3,3,3	0.48	0	2,2,2	0.72	0
18	PGV	P	306	-	50,50,50	0.79	2 (4%)	53,56,56	1.27	4 (7%)
20	EDO	W	102	-	3,3,3	0.22	0	2,2,2	0.77	0
29	PO4	U	101	-	4,4,4	1.18	0	6,6,6	1.04	0
26	PEK	P	303	-	26,26,52	0.35	0	24,24,57	0.88	1 (4%)
19	OXY	A	607	14,15	1,1,1	0.09	0	-	-	-
20	EDO	N	614	-	3,3,3	0.66	0	2,2,2	0.37	0
27	CDL	P	308	-	73,73,99	1.34	11 (15%)	73,73,111	2.28	9 (12%)
20	EDO	G	103	-	3,3,3	0.70	0	2,2,2	0.84	0
20	EDO	A	611	-	3,3,3	0.70	0	2,2,2	0.17	0
21	DMU	K	102	-	8,8,34	0.35	0	7,7,45	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	C	316	-	3,3,3	0.57	0	2,2,2	0.90	0
21	DMU	X	101	-	8,8,34	0.38	0	7,7,45	0.42	0
21	DMU	Z	101	-	34,34,34	0.61	1 (2%)	45,45,45	1.08	3 (6%)
25	CHD	P	301	-	29,32,32	0.72	0	48,51,51	1.60	9 (18%)
20	EDO	F	105	-	3,3,3	0.76	0	2,2,2	0.63	0
20	EDO	W	101	-	3,3,3	0.48	0	2,2,2	0.50	0
21	DMU	A	621	-	7,7,34	0.25	0	6,6,45	0.44	0
20	EDO	A	609	-	3,3,3	0.52	0	2,2,2	0.85	0
20	EDO	N	615	-	3,3,3	0.55	0	2,2,2	0.35	0
21	DMU	L	104	-	21,21,34	0.70	0	24,25,45	1.65	4 (16%)
20	EDO	A	619	-	3,3,3	0.45	0	2,2,2	0.55	0
20	EDO	B	307	-	3,3,3	0.35	0	2,2,2	0.83	0
20	EDO	N	620	-	3,3,3	0.80	0	2,2,2	0.22	0
21	DMU	C	320	-	11,11,34	0.46	0	10,10,45	0.85	0
18	PGV	A	606	-	31,31,50	0.52	0	29,29,56	0.70	1 (3%)
20	EDO	A	618	-	3,3,3	0.47	0	2,2,2	0.52	0
24	PSC	O	302	-	31,31,51	0.78	1 (3%)	29,29,59	1.36	3 (10%)
26	PEK	P	304	-	52,52,52	0.75	2 (3%)	55,57,57	1.11	2 (3%)
20	EDO	P	316	-	3,3,3	0.30	0	2,2,2	1.46	0
20	EDO	A	616	-	3,3,3	0.16	0	2,2,2	0.29	0
20	EDO	O	303	-	3,3,3	0.79	0	2,2,2	0.67	0
21	DMU	X	103	-	9,9,34	0.51	0	8,8,45	0.35	0
20	EDO	C	312	-	3,3,3	0.79	0	2,2,2	0.23	0
23	CUA	O	301	2	0,1,1	0.00	-	-	-	-
21	DMU	N	622	-	8,8,34	0.25	0	7,7,45	0.64	0
27	CDL	G	101	-	65,65,99	1.28	9 (13%)	62,62,111	1.12	3 (4%)
20	EDO	C	314	-	3,3,3	0.34	0	2,2,2	0.46	0
20	EDO	A	613	-	3,3,3	0.59	0	2,2,2	0.16	0
21	DMU	D	206	-	10,10,34	0.36	0	9,9,45	0.46	0
18	PGV	Q	201	-	35,35,50	0.86	1 (2%)	34,34,56	1.37	3 (8%)
20	EDO	E	203	-	3,3,3	0.48	0	2,2,2	0.59	0
20	EDO	D	202	-	3,3,3	0.40	0	2,2,2	0.36	0
14	HEA	N	601[A]	-	44,67,67	1.22	4 (9%)	37,103,103	2.30	13 (35%)
20	EDO	F	103	-	3,3,3	0.86	0	2,2,2	0.49	0
20	EDO	P	312	-	3,3,3	0.86	0	2,2,2	0.23	0
20	EDO	B	308	-	3,3,3	0.54	0	2,2,2	0.54	0
21	DMU	K	103	-	8,8,34	0.47	0	7,7,45	0.29	0
20	EDO	A	614	-	3,3,3	0.78	0	2,2,2	0.27	0
18	PGV	C	306	-	50,50,50	0.84	2 (4%)	53,56,56	1.02	5 (9%)
20	EDO	T	104	-	3,3,3	0.67	0	2,2,2	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CDL	T	101	-	67,67,99	1.44	10 (14%)	67,67,111	1.64	12 (17%)
23	CUA	B	302	2	0,1,1	0.00	-	-		
20	EDO	C	311	-	3,3,3	1.10	0	2,2,2	0.46	0
20	EDO	B	305	-	3,3,3	0.68	0	2,2,2	0.19	0
20	EDO	M	102	-	3,3,3	0.45	0	2,2,2	0.31	0
25	CHD	L	102	-	29,32,32	0.71	0	48,51,51	2.85	21 (43%)
20	EDO	C	319	-	3,3,3	0.46	0	2,2,2	0.43	0
20	EDO	P	317	-	3,3,3	0.37	0	2,2,2	0.51	0
20	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.12	0
20	EDO	S	106	-	3,3,3	0.67	0	2,2,2	0.87	0
20	EDO	L	103	-	3,3,3	0.56	0	2,2,2	0.63	0
20	EDO	D	205	-	3,3,3	0.41	0	2,2,2	0.67	0
18	PGV	N	610	-	50,50,50	1.04	3 (6%)	53,56,56	1.27	6 (11%)
20	EDO	A	615	-	3,3,3	0.42	0	2,2,2	0.45	0
21	DMU	K	101	-	8,8,34	0.22	0	7,7,45	0.58	0
21	DMU	Q	202	-	9,9,34	0.54	0	8,8,45	0.33	0
14	HEA	A	602	19,1	44,67,67	1.36	7 (15%)	37,103,103	1.89	8 (21%)
20	EDO	P	311	-	3,3,3	0.27	0	2,2,2	0.80	0
14	HEA	A	601[A]	-	44,67,67	1.35	4 (9%)	37,103,103	2.15	9 (24%)
20	EDO	T	103	-	3,3,3	0.62	0	2,2,2	0.29	0
22	TGL	B	301	-	62,62,62	1.07	3 (4%)	65,65,65	1.51	5 (7%)
29	PO4	H	101	-	4,4,4	0.70	0	6,6,6	0.81	0
21	DMU	A	620	-	8,8,34	0.34	0	7,7,45	0.53	0
20	EDO	F	107	-	3,3,3	0.62	0	2,2,2	0.08	0
20	EDO	Q	204	-	3,3,3	0.30	0	2,2,2	0.56	0
20	EDO	F	104	-	3,3,3	0.39	0	2,2,2	0.58	0
21	DMU	X	102	-	7,7,34	0.41	0	6,6,45	0.34	0
20	EDO	N	619	-	3,3,3	0.57	0	2,2,2	0.61	0
22	TGL	L	101	-	50,50,62	1.00	2 (4%)	48,48,65	1.33	5 (10%)
19	OXY	N	609	14,15	1,1,1	0.11	0	-		
20	EDO	J	102	-	3,3,3	0.34	0	2,2,2	0.62	0
21	DMU	M	101	-	34,34,34	0.51	0	45,45,45	1.20	6 (13%)
22	TGL	D	201	-	62,62,62	1.17	3 (4%)	65,65,65	1.58	10 (15%)
25	CHD	B	304	-	29,32,32	0.94	0	48,51,51	1.71	13 (27%)
25	CHD	C	309	-	29,32,32	0.75	0	48,51,51	1.36	7 (14%)
20	EDO	O	304	-	3,3,3	0.32	0	2,2,2	0.17	0
20	EDO	B	306	-	3,3,3	0.51	0	2,2,2	0.49	0
20	EDO	F	106	-	3,3,3	0.55	0	2,2,2	0.60	0
20	EDO	B	309	-	3,3,3	0.77	0	2,2,2	0.22	0
20	EDO	D	204	-	3,3,3	0.43	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	PGV	A	608	-	50,50,50	1.08	4 (8%)	53,56,56	1.14	6 (11%)
20	EDO	S	107	-	3,3,3	0.94	0	2,2,2	0.66	0
26	PEK	C	303	-	17,17,52	0.47	0	15,16,57	0.97	1 (6%)
18	PGV	P	307	-	36,36,50	1.00	1 (2%)	35,35,56	1.32	4 (11%)
20	EDO	N	616	-	3,3,3	0.67	0	2,2,2	0.51	0
26	PEK	C	305	-	38,38,52	0.93	1 (2%)	37,37,57	1.43	4 (10%)
18	PGV	C	307	-	35,35,50	0.95	1 (2%)	34,34,56	1.49	5 (14%)
20	EDO	R	201	-	3,3,3	0.65	0	2,2,2	0.51	0
20	EDO	S	104	-	3,3,3	0.68	0	2,2,2	0.18	0
27	CDL	C	308	-	79,82,99	1.27	10 (12%)	78,83,111	1.57	12 (15%)
24	PSC	B	303	-	40,40,51	1.31	3 (7%)	42,42,59	1.91	5 (11%)
25	CHD	P	309	-	29,32,32	0.94	0	48,51,51	2.00	14 (29%)
21	DMU	J	103	-	10,10,34	0.48	0	9,9,45	0.62	0
21	DMU	C	310	-	22,22,34	1.03	1 (4%)	27,27,45	1.58	6 (22%)
21	DMU	P	318	-	10,10,34	0.33	0	9,9,45	0.47	0
20	EDO	C	313	-	3,3,3	0.69	0	2,2,2	0.42	0
20	EDO	T	102	-	3,3,3	0.52	0	2,2,2	0.31	0
25	CHD	G	102	-	29,32,32	1.14	2 (6%)	48,51,51	1.63	12 (25%)
20	EDO	Y	101	-	3,3,3	0.38	0	2,2,2	0.22	0
22	TGL	N	606	-	62,62,62	1.09	3 (4%)	65,65,65	1.17	4 (6%)
20	EDO	N	617	-	3,3,3	0.45	0	2,2,2	0.57	0
20	EDO	A	617	-	3,3,3	1.06	0	2,2,2	0.74	0
22	TGL	N	607	-	40,40,62	0.42	0	37,37,65	0.87	1 (2%)
20	EDO	C	317	-	3,3,3	0.29	0	2,2,2	0.16	0
20	EDO	N	611	-	3,3,3	0.43	0	2,2,2	0.66	0
20	EDO	N	621	-	3,3,3	0.22	0	2,2,2	0.96	0
20	EDO	A	612	-	3,3,3	0.37	0	2,2,2	0.43	0
20	EDO	S	108	-	3,3,3	0.30	0	2,2,2	1.01	0
21	DMU	P	310	-	22,22,34	1.07	1 (4%)	27,27,45	1.55	4 (14%)
20	EDO	S	102	-	3,3,3	1.04	0	2,2,2	0.74	0
21	DMU	D	207	-	7,7,34	0.44	0	6,6,45	0.40	0
20	EDO	D	203	-	3,3,3	0.56	0	2,2,2	0.26	0
20	EDO	N	613	-	3,3,3	0.89	0	2,2,2	0.32	0
20	EDO	Q	203	-	3,3,3	0.40	0	2,2,2	0.18	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
25	CHD	C	301	-	-	0/7/74/74	0/4/4/4
20	EDO	P	315	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	3/3/5/16	-	-
14	HEA	A	601[C]	-	3/3/5/16	-	-
20	EDO	S	105	-	-	0/1/1/1	-
20	EDO	N	618	-	-	0/1/1/1	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	C	315	-	-	0/1/1/1	-
21	DMU	W	103	-	-	4/8/8/59	-
20	EDO	P	313	-	-	1/1/1/1	-
20	EDO	C	318	-	-	1/1/1/1	-
14	HEA	N	602	19,1	3/3/7/16	1/24/76/76	-
20	EDO	J	101	-	-	0/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-
21	DMU	O	305	-	-	6/8/8/59	-
21	DMU	K	104	-	-	2/7/7/59	-
20	EDO	E	202	-	-	1/1/1/1	-
26	PEK	C	304	-	-	15/56/56/56	-
20	EDO	R	202	-	-	0/1/1/1	-
26	PEK	P	305	-	-	15/35/35/56	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-
22	TGL	N	608	-	-	25/47/47/65	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	B	310	-	-	0/1/1/1	-
18	PGV	P	306	-	-	12/55/55/55	-
20	EDO	W	102	-	-	1/1/1/1	-
26	PEK	P	303	-	-	10/21/22/56	-
20	EDO	N	614	-	-	1/1/1/1	-
27	CDL	P	308	-	-	30/70/70/110	-
20	EDO	G	103	-	-	0/1/1/1	-
20	EDO	A	611	-	-	1/1/1/1	-
21	DMU	K	102	-	-	3/6/6/59	-
20	EDO	C	316	-	-	1/1/1/1	-
21	DMU	X	101	-	-	2/6/6/59	-
21	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
25	CHD	P	301	-	-	0/7/74/74	0/4/4/4
20	EDO	F	105	-	-	0/1/1/1	-
20	EDO	W	101	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	A	621	-	-	2/5/5/59	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
21	DMU	L	104	-	-	6/13/29/59	0/1/1/2
20	EDO	A	619	-	-	1/1/1/1	-
20	EDO	B	307	-	-	1/1/1/1	-
20	EDO	N	620	-	-	1/1/1/1	-
21	DMU	C	320	-	-	2/9/9/59	-
18	PGV	A	606	-	-	10/26/27/55	-
20	EDO	A	618	-	-	0/1/1/1	-
24	PSC	O	302	-	-	12/26/27/55	-
26	PEK	P	304	-	-	10/56/56/56	-
20	EDO	P	316	-	-	1/1/1/1	-
20	EDO	A	616	-	-	1/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-
21	DMU	X	103	-	-	0/7/7/59	-
20	EDO	C	312	-	-	0/1/1/1	-
21	DMU	N	622	-	-	4/6/6/59	-
27	CDL	G	101	-	-	17/58/58/110	-
20	EDO	C	314	-	-	1/1/1/1	-
20	EDO	A	613	-	-	1/1/1/1	-
21	DMU	D	206	-	-	4/8/8/59	-
18	PGV	Q	201	-	-	10/32/32/55	-
20	EDO	E	203	-	-	0/1/1/1	-
20	EDO	D	202	-	-	0/1/1/1	-
14	HEA	N	601[A]	-	3/3/7/16	2/24/76/76	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
21	DMU	K	103	-	-	4/6/6/59	-
20	EDO	A	614	-	-	0/1/1/1	-
18	PGV	C	306	-	-	13/55/55/55	-
20	EDO	T	104	-	-	0/1/1/1	-
27	CDL	T	101	-	-	30/64/64/110	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	M	102	-	-	1/1/1/1	-
25	CHD	L	102	-	-	5/7/74/74	0/4/4/4
20	EDO	C	319	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	P	317	-	-	1/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
14	HEA	N	601[B]	-	3/3/5/16	-	-
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	D	205	-	-	0/1/1/1	-
18	PGV	N	610	-	-	6/55/55/55	-
20	EDO	A	615	-	-	1/1/1/1	-
21	DMU	K	101	-	-	2/6/6/59	-
21	DMU	Q	202	-	-	3/7/7/59	-
14	HEA	A	602	19,1	3/3/7/16	2/24/76/76	-
20	EDO	P	311	-	-	1/1/1/1	-
14	HEA	A	601[A]	-	3/3/7/16	4/24/76/76	-
20	EDO	T	103	-	-	1/1/1/1	-
22	TGL	B	301	-	-	34/65/65/65	-
21	DMU	A	620	-	-	2/6/6/59	-
20	EDO	F	107	-	-	1/1/1/1	-
20	EDO	Q	204	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
21	DMU	X	102	-	-	1/5/5/59	-
20	EDO	N	619	-	-	0/1/1/1	-
22	TGL	L	101	-	-	25/43/44/65	-
20	EDO	J	102	-	-	1/1/1/1	-
21	DMU	M	101	-	-	6/19/59/59	0/2/2/2
22	TGL	D	201	-	-	35/65/65/65	-
25	CHD	B	304	-	-	0/7/74/74	0/4/4/4
25	CHD	C	309	-	-	3/7/74/74	0/4/4/4
20	EDO	O	304	-	-	0/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	F	106	-	-	0/1/1/1	-
20	EDO	B	309	-	-	1/1/1/1	-
20	EDO	D	204	-	-	0/1/1/1	-
18	PGV	A	608	-	-	7/55/55/55	-
20	EDO	S	107	-	-	0/1/1/1	-
26	PEK	C	303	-	-	9/15/15/56	-
14	HEA	N	601[C]	-	3/3/5/16	-	-
18	PGV	P	307	-	-	13/33/33/55	-
20	EDO	N	616	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEK	C	305	-	-	17/35/35/56	-
18	PGV	C	307	-	-	8/32/32/55	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
27	CDL	C	308	-	-	33/76/80/110	-
24	PSC	B	303	-	-	16/41/41/55	-
25	CHD	P	309	-	-	3/7/74/74	0/4/4/4
21	DMU	J	103	-	-	1/8/8/59	-
21	DMU	C	310	-	-	7/13/33/59	0/1/1/2
21	DMU	P	318	-	-	2/8/8/59	-
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	T	102	-	-	0/1/1/1	-
25	CHD	G	102	-	-	0/7/74/74	0/4/4/4
20	EDO	Y	101	-	-	0/1/1/1	-
22	TGL	N	606	-	-	33/65/65/65	-
20	EDO	N	617	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
22	TGL	N	607	-	-	19/34/34/65	-
20	EDO	C	317	-	-	1/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	N	621	-	-	1/1/1/1	-
20	EDO	A	612	-	-	1/1/1/1	-
20	EDO	S	108	-	-	0/1/1/1	-
21	DMU	P	310	-	-	3/13/33/59	0/1/1/2
20	EDO	S	102	-	-	0/1/1/1	-
21	DMU	D	207	-	-	1/5/5/59	-
20	EDO	D	203	-	-	0/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	1/1/1/1	-

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	105	EDO	O1-C1	-5.61	1.13	1.42
18	P	307	PGV	O03-C19	5.38	1.49	1.33
22	D	201	TGL	OG2-CB1	5.32	1.49	1.34
27	G	101	CDL	OB8-CB7	5.24	1.48	1.33
27	T	101	CDL	OB8-CB7	5.21	1.48	1.33

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	308	CDL	CB4-OB6-CB5	-14.96	98.63	117.88
22	B	301	TGL	OG2-CB1-CB2	8.53	129.88	111.50
14	N	601[A]	HEA	C13-C12-C11	-8.01	102.32	114.35
27	T	101	CDL	OB6-CB5-C51	7.54	127.76	111.50
24	B	303	PSC	C02-O01-C1	6.74	126.55	117.88

5 of 24 chirality outliers are listed below:

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

5 of 586 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602	HEA	C2D-C3D-CAD-CBD
14	A	602	HEA	C4D-C3D-CAD-CBD
18	A	606	PGV	C1-C2-C3-C4
20	A	615	EDO	O1-C1-C2-O2
21	L	104	DMU	O5-C6-O16-C18

There are no ring outliers.

55 monomers are involved in 204 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S	105	EDO	1	0
14	N	602	HEA	6	0
21	K	104	DMU	1	0
26	C	304	PEK	9	0
20	R	202	EDO	2	0
26	P	305	PEK	7	0
22	N	608	TGL	2	0
18	P	306	PGV	1	0
20	W	102	EDO	2	0
26	P	303	PEK	1	0
27	P	308	CDL	10	0
20	A	609	EDO	2	0
21	L	104	DMU	1	0
18	A	606	PGV	3	0
24	O	302	PSC	4	0

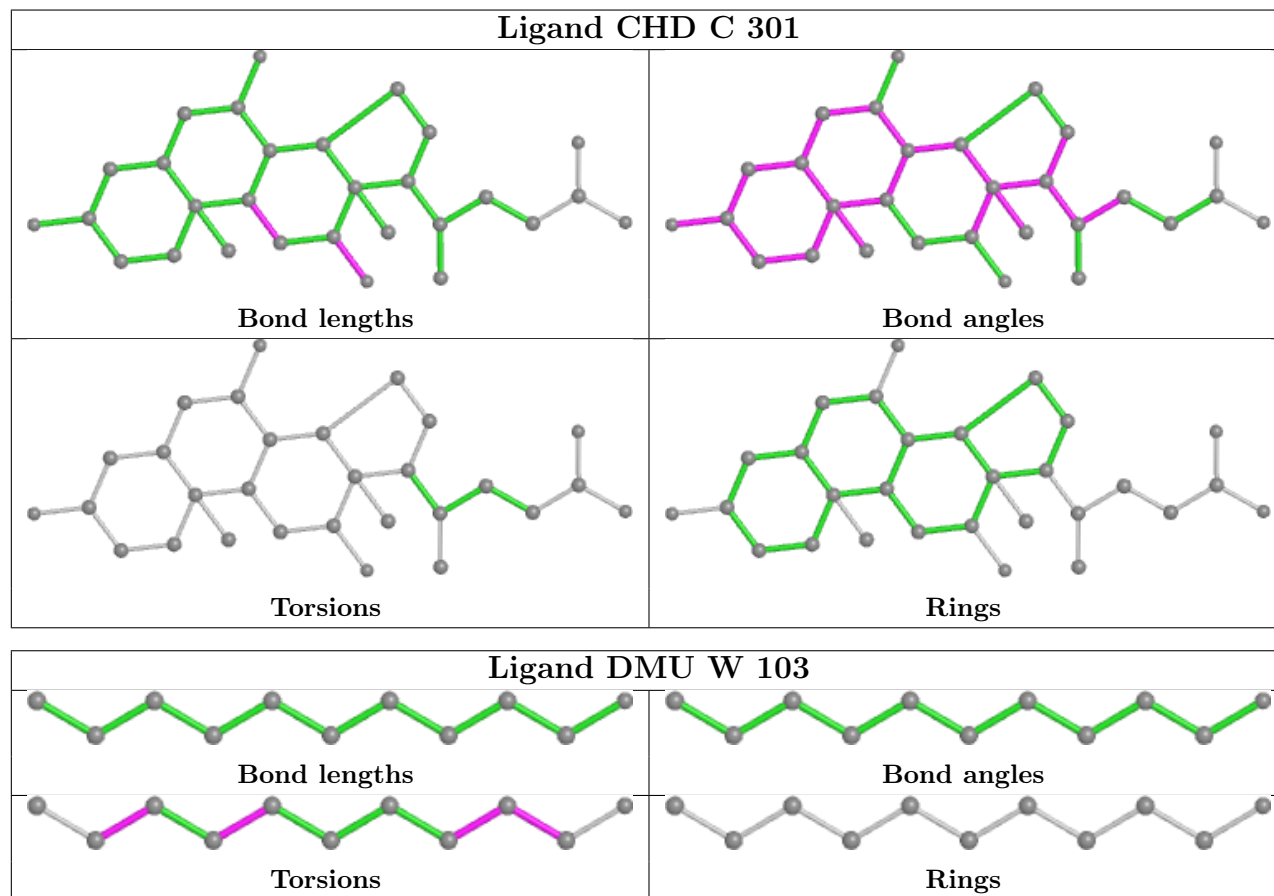
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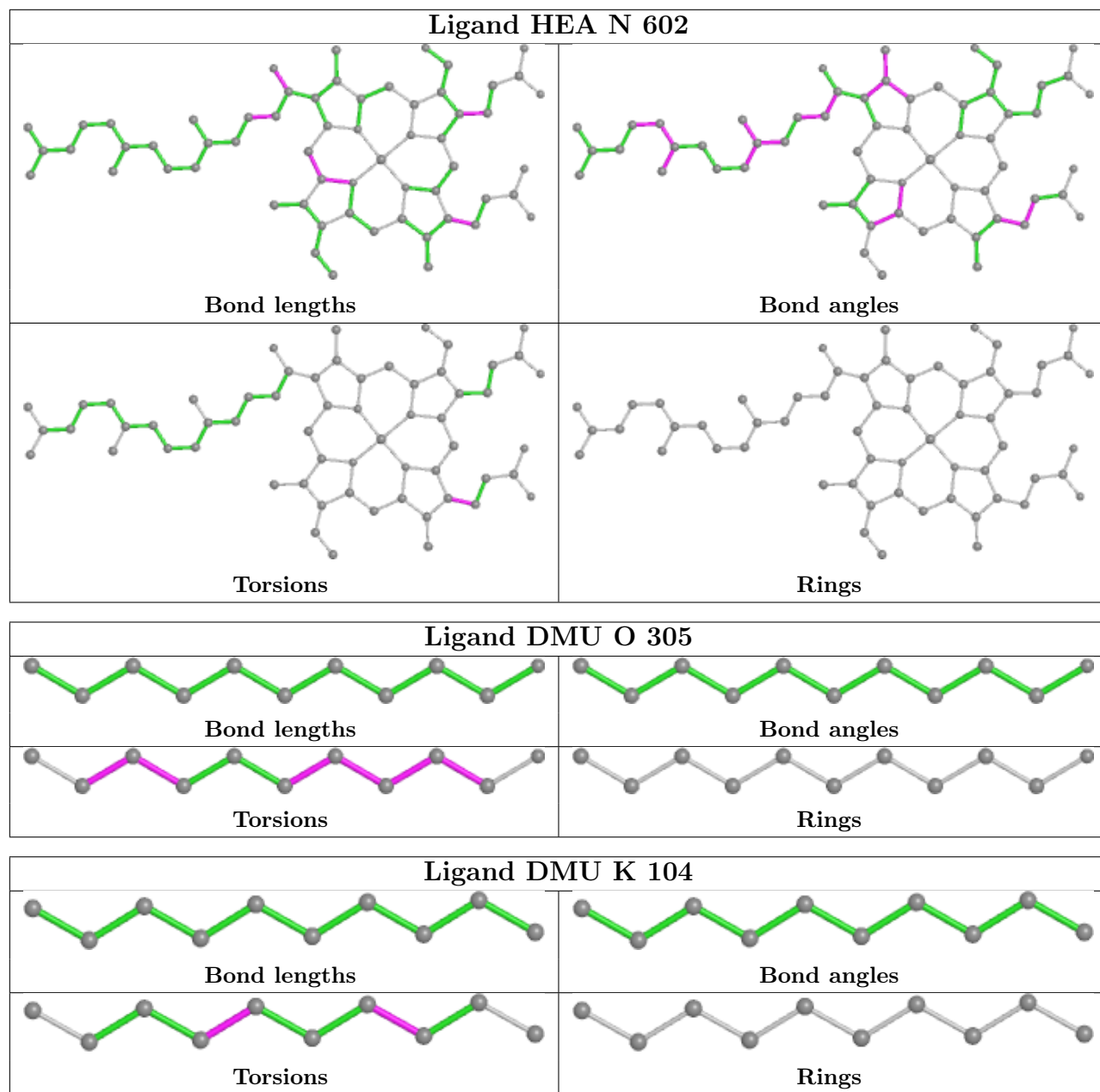
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	304	PEK	5	0
20	P	316	EDO	1	0
20	A	616	EDO	1	0
21	N	622	DMU	1	0
27	G	101	CDL	8	0
20	C	314	EDO	1	0
18	Q	201	PGV	6	0
14	N	601[A]	HEA	3	0
21	K	103	DMU	1	0
18	C	306	PGV	1	0
27	T	101	CDL	18	0
25	L	102	CHD	1	0
18	N	610	PGV	1	0
20	A	615	EDO	1	0
21	Q	202	DMU	1	0
14	A	602	HEA	8	0
20	P	311	EDO	1	0
14	A	601[A]	HEA	3	0
22	B	301	TGL	7	0
22	L	101	TGL	9	0
20	J	102	EDO	1	0
22	D	201	TGL	14	0
25	C	309	CHD	1	0
18	A	608	PGV	5	0
14	N	601[C]	HEA	1	0
18	P	307	PGV	3	0
26	C	305	PEK	5	0
18	C	307	PGV	1	0
27	C	308	CDL	12	0
24	B	303	PSC	7	0
25	P	309	CHD	3	0
21	J	103	DMU	3	0
21	C	310	DMU	6	0
21	P	318	DMU	1	0
25	G	102	CHD	1	0
22	N	606	TGL	8	0
22	N	607	TGL	6	0
20	N	621	EDO	1	0
21	P	310	DMU	5	0
20	Q	203	EDO	1	0

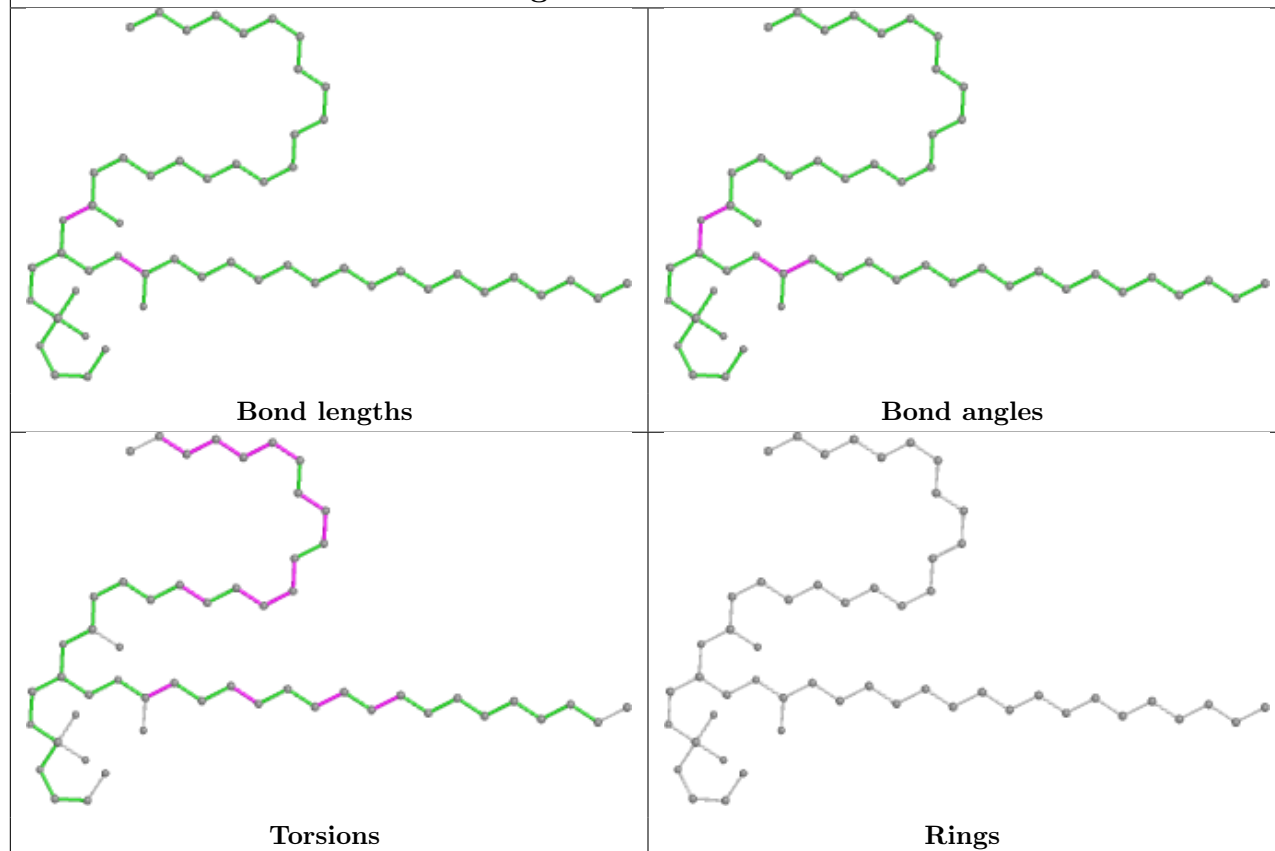
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

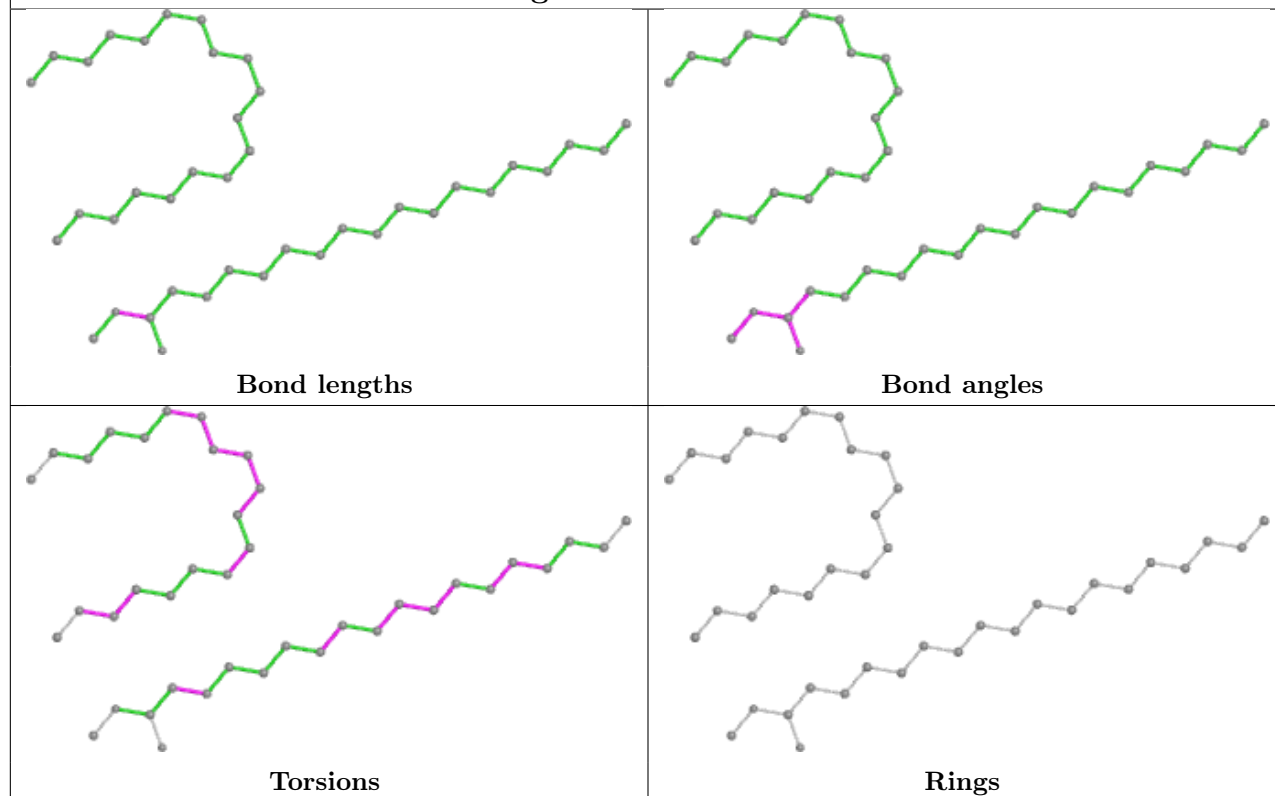


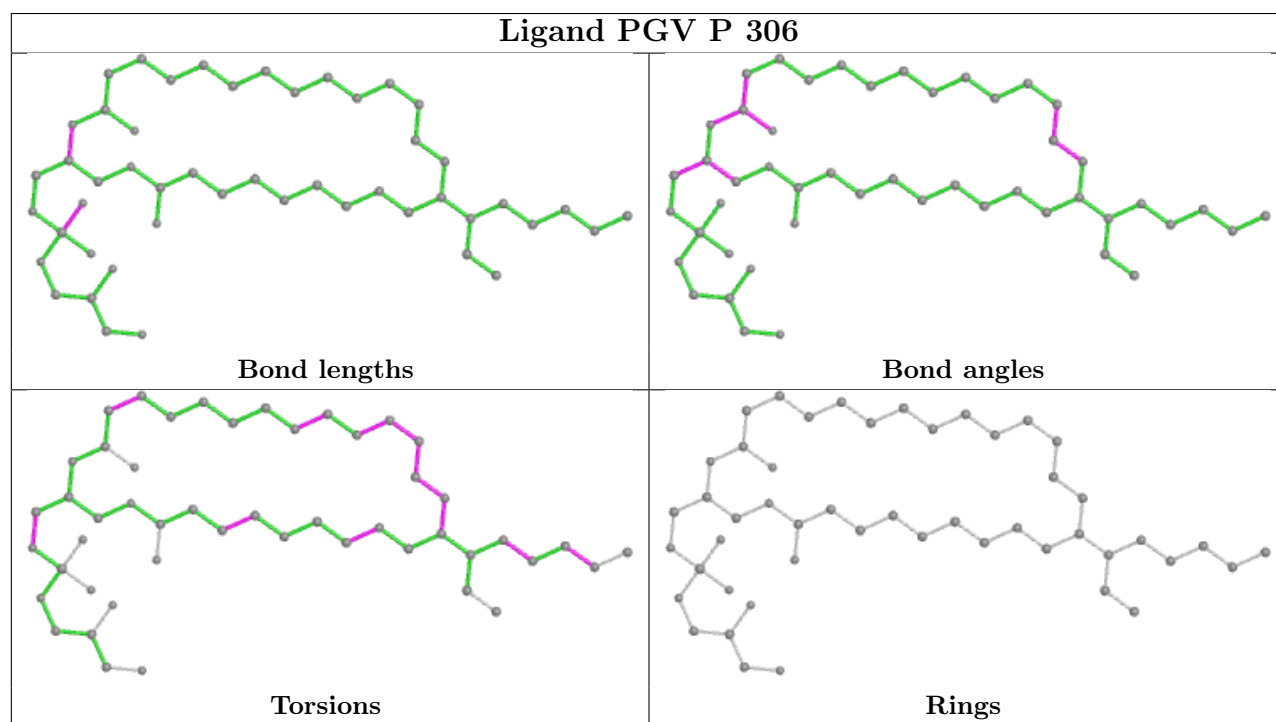
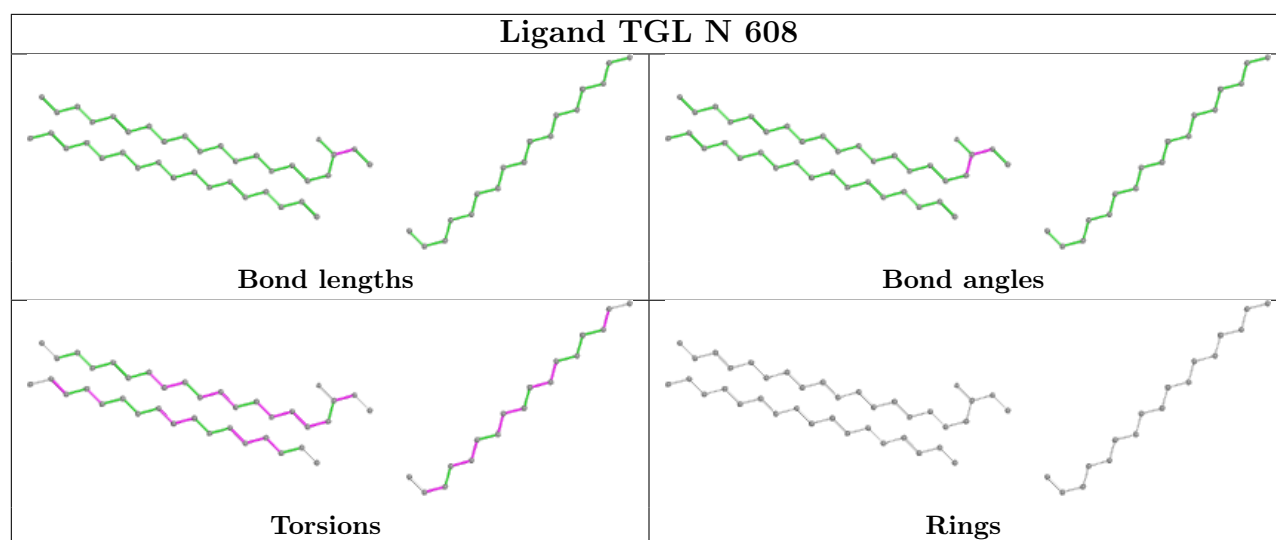


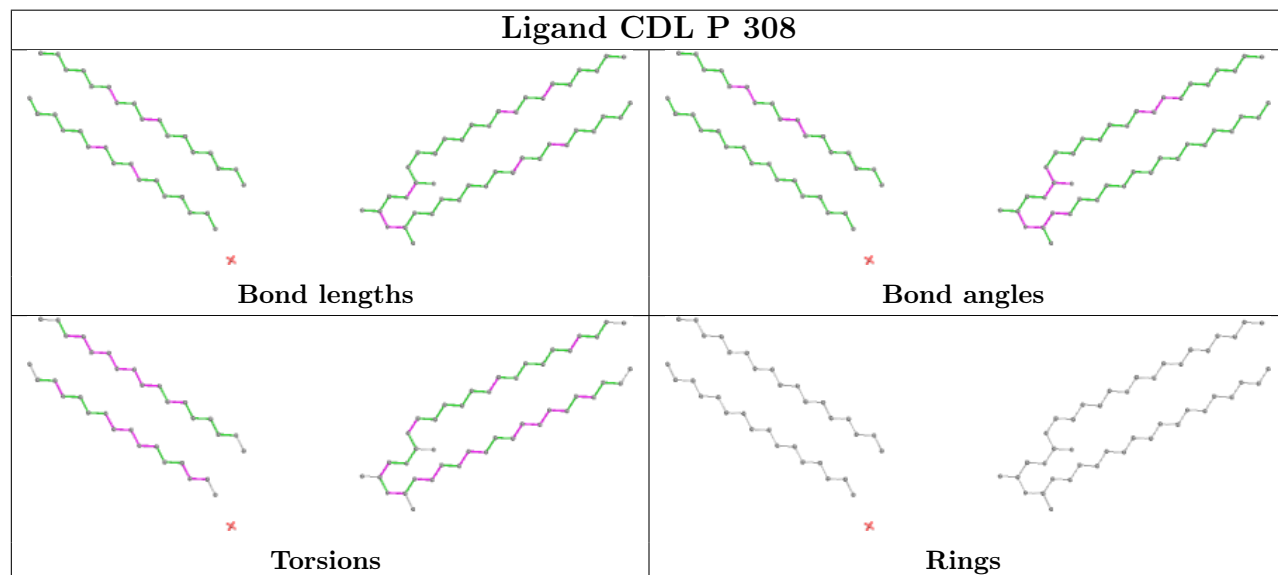
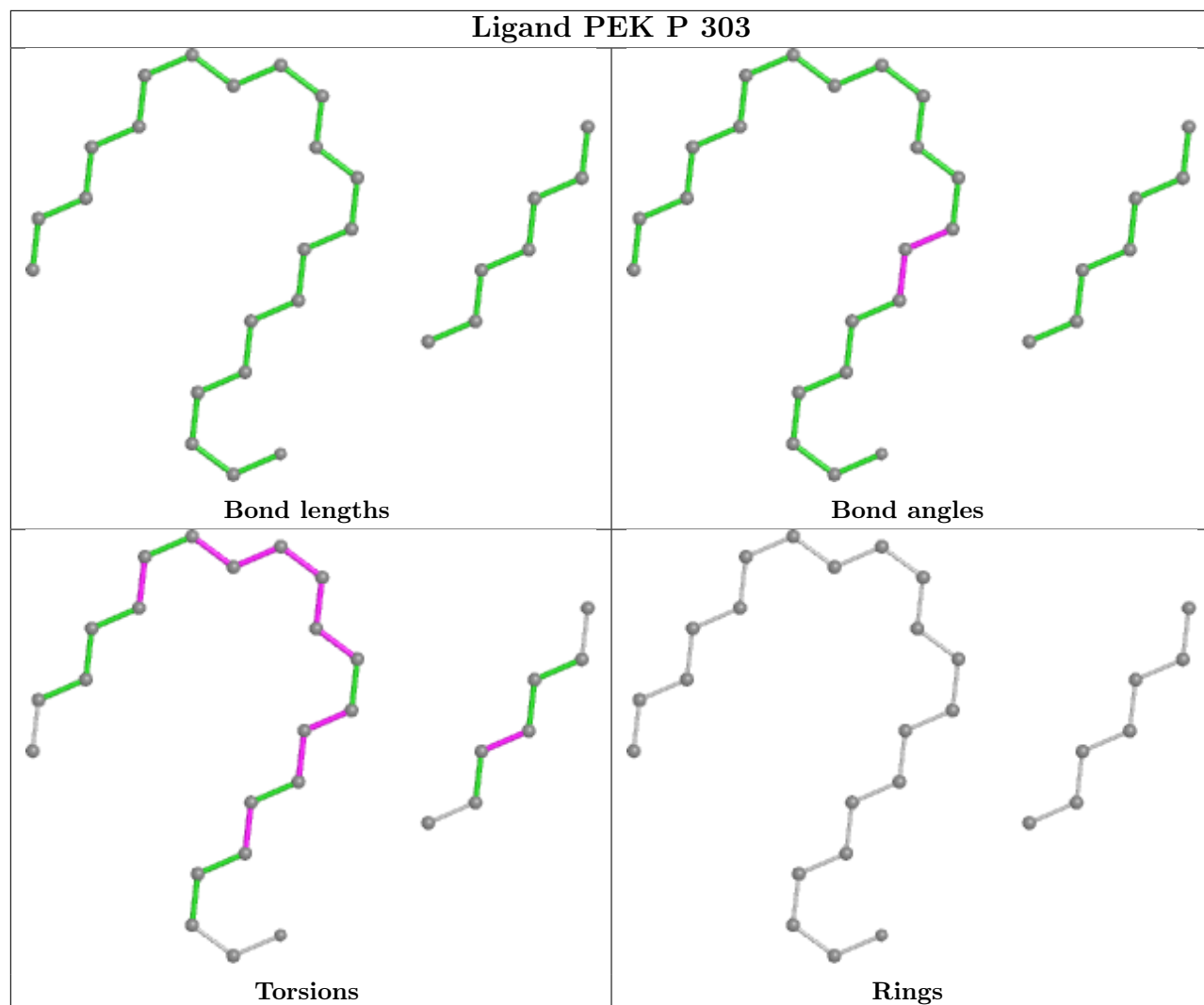
Ligand PEK C 304

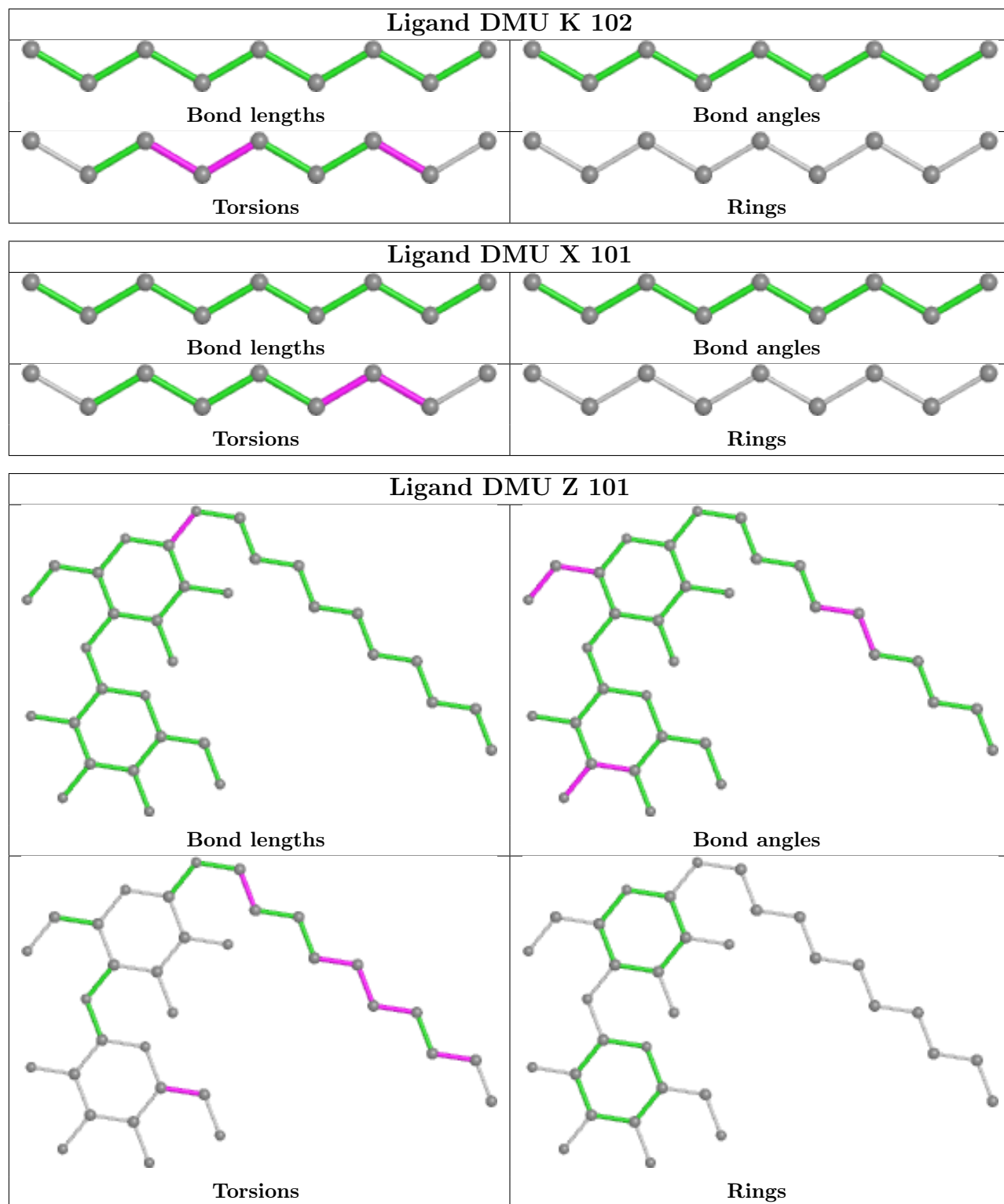


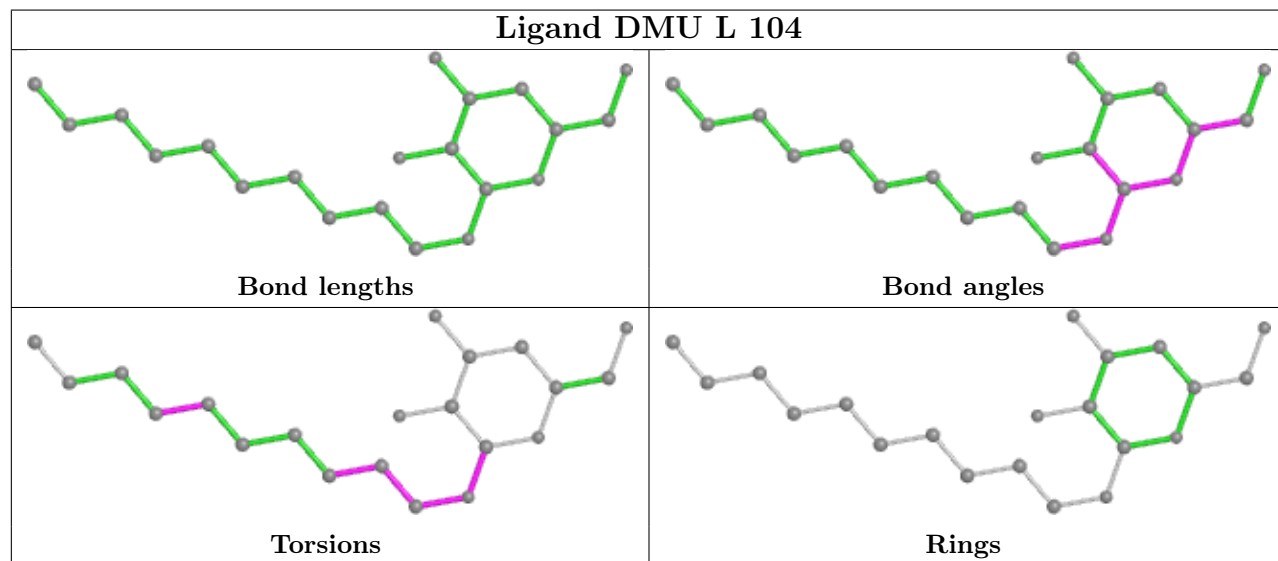
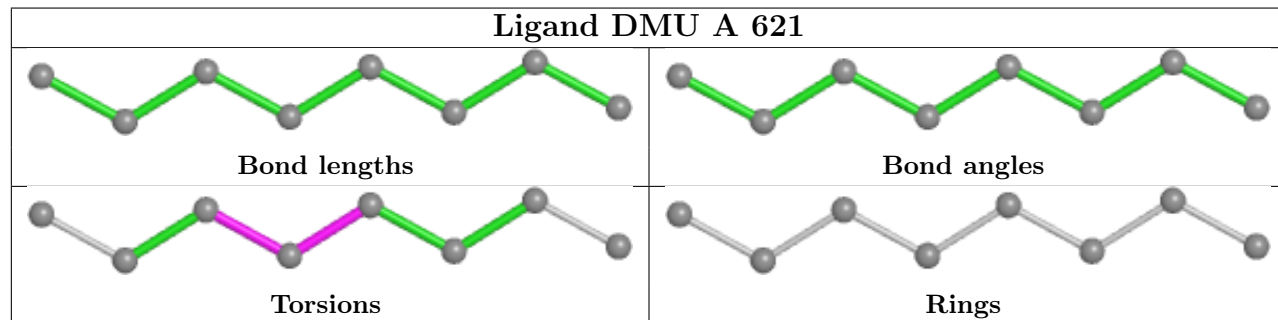
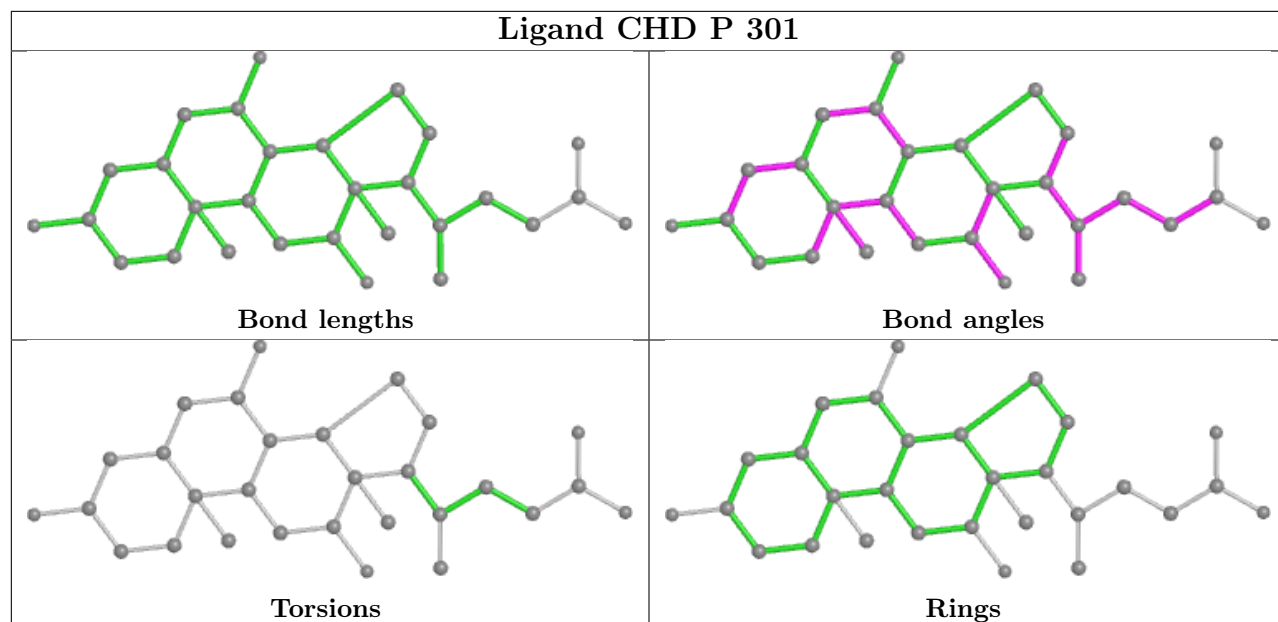
Ligand PEK P 305

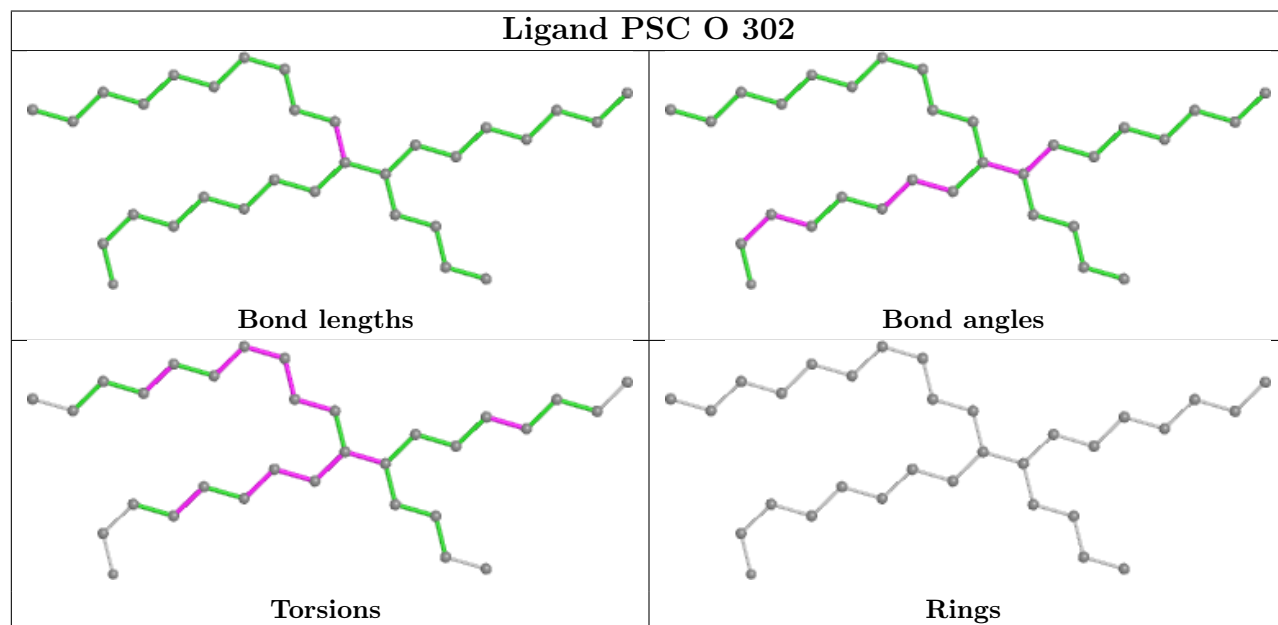
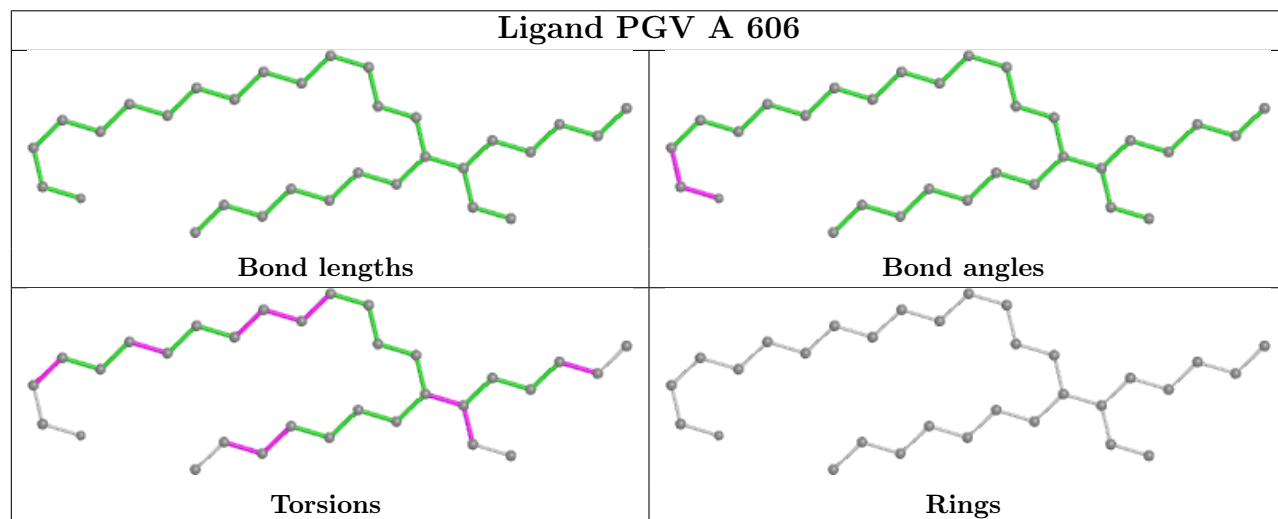
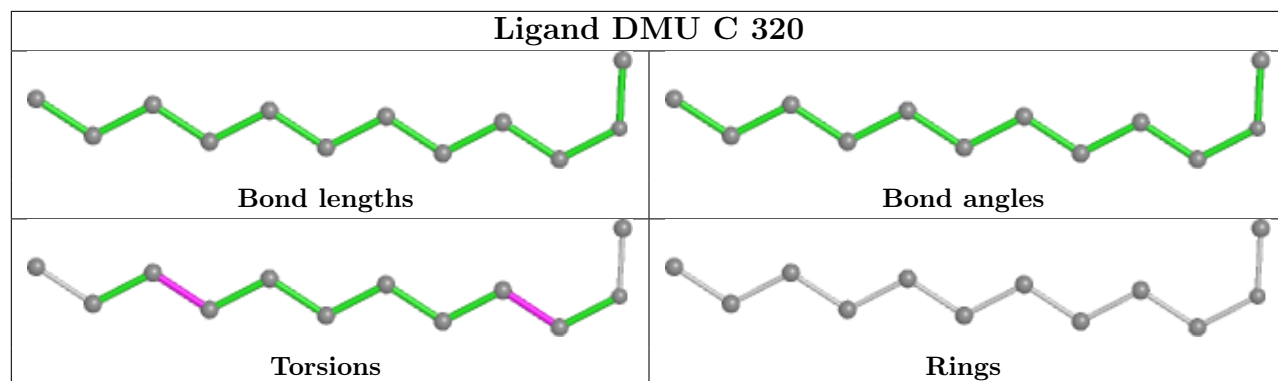


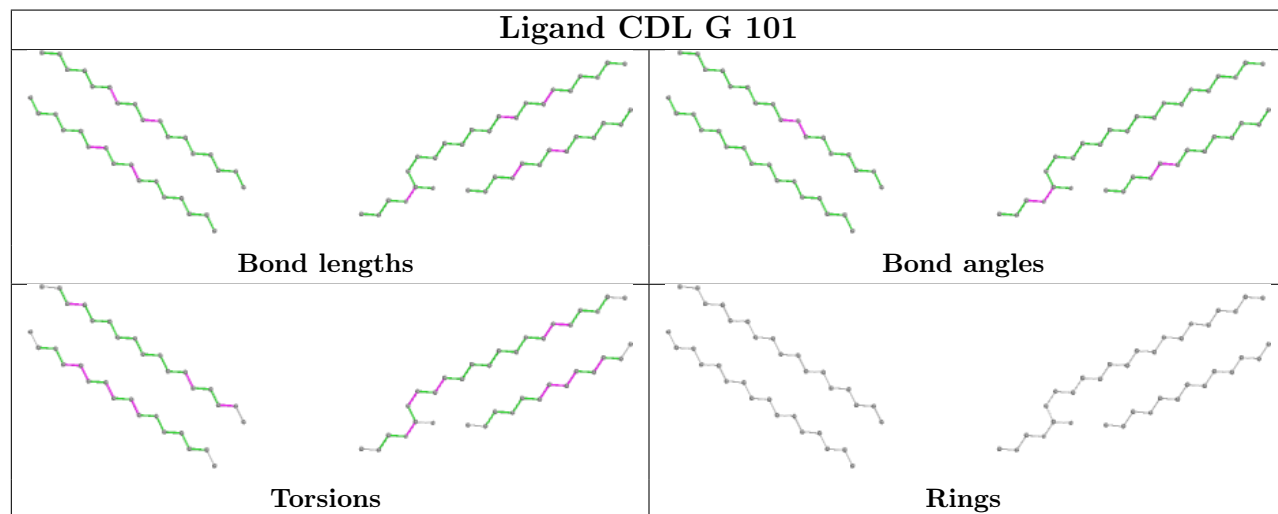
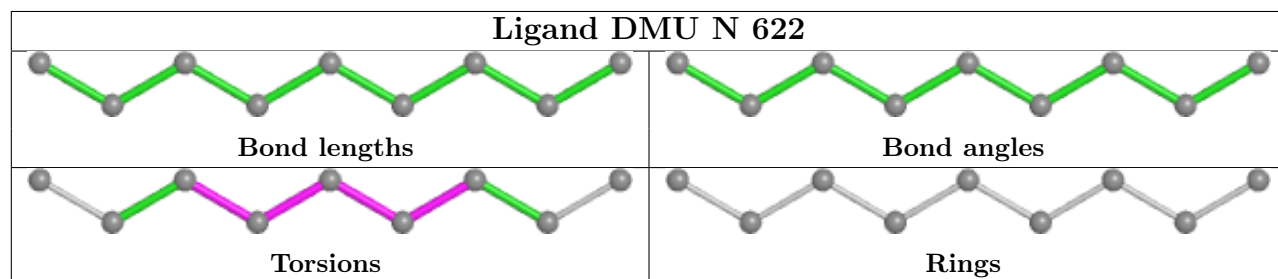
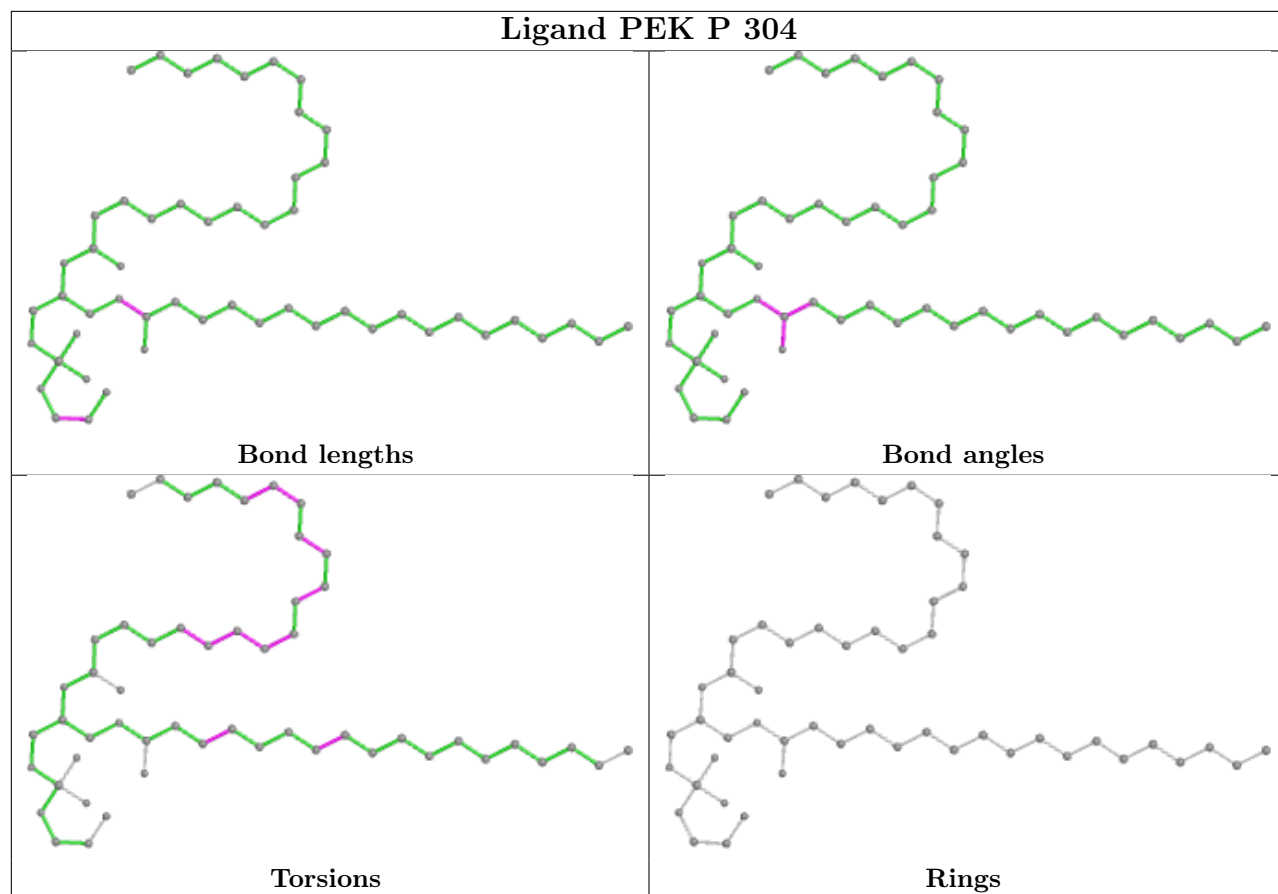


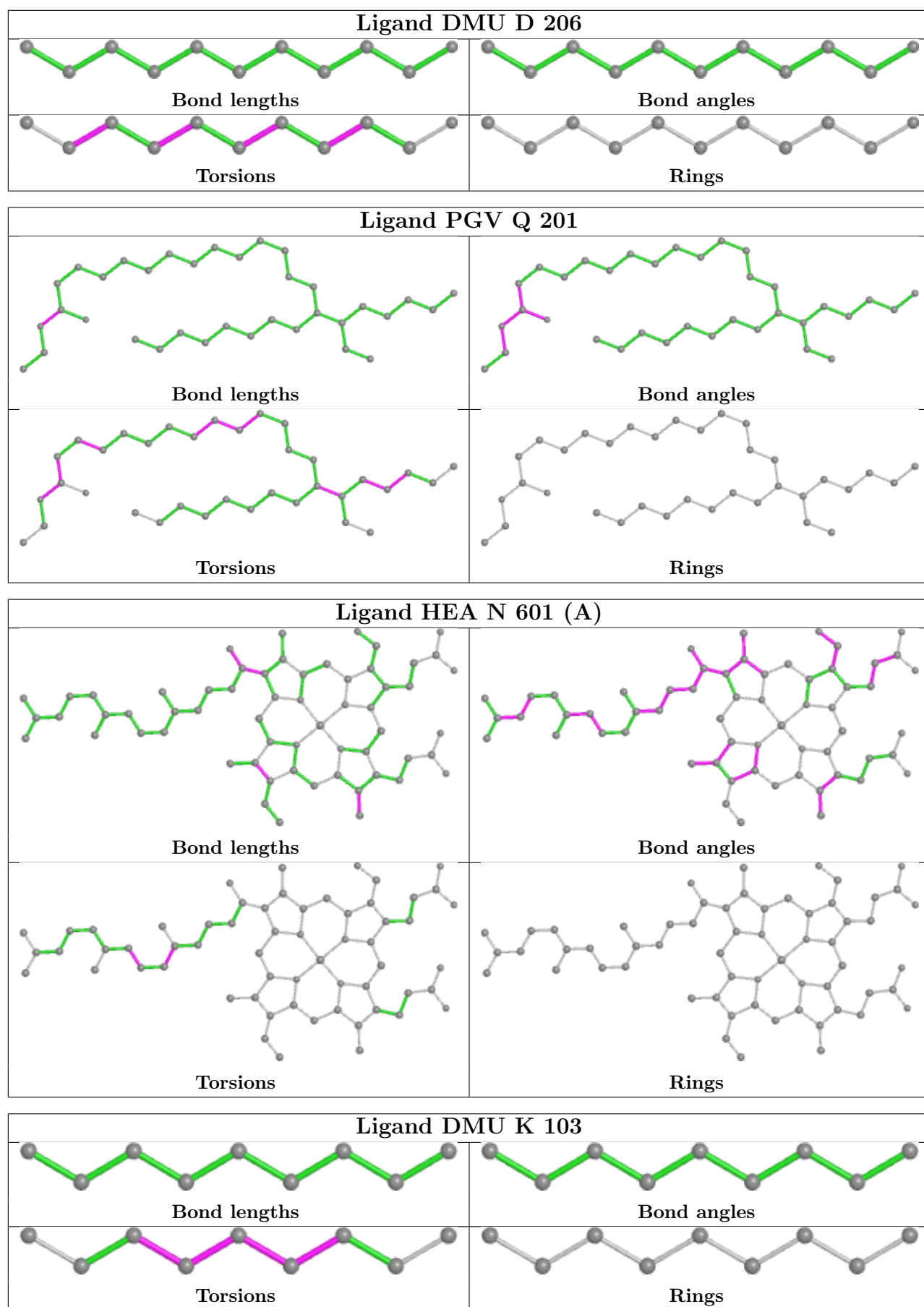


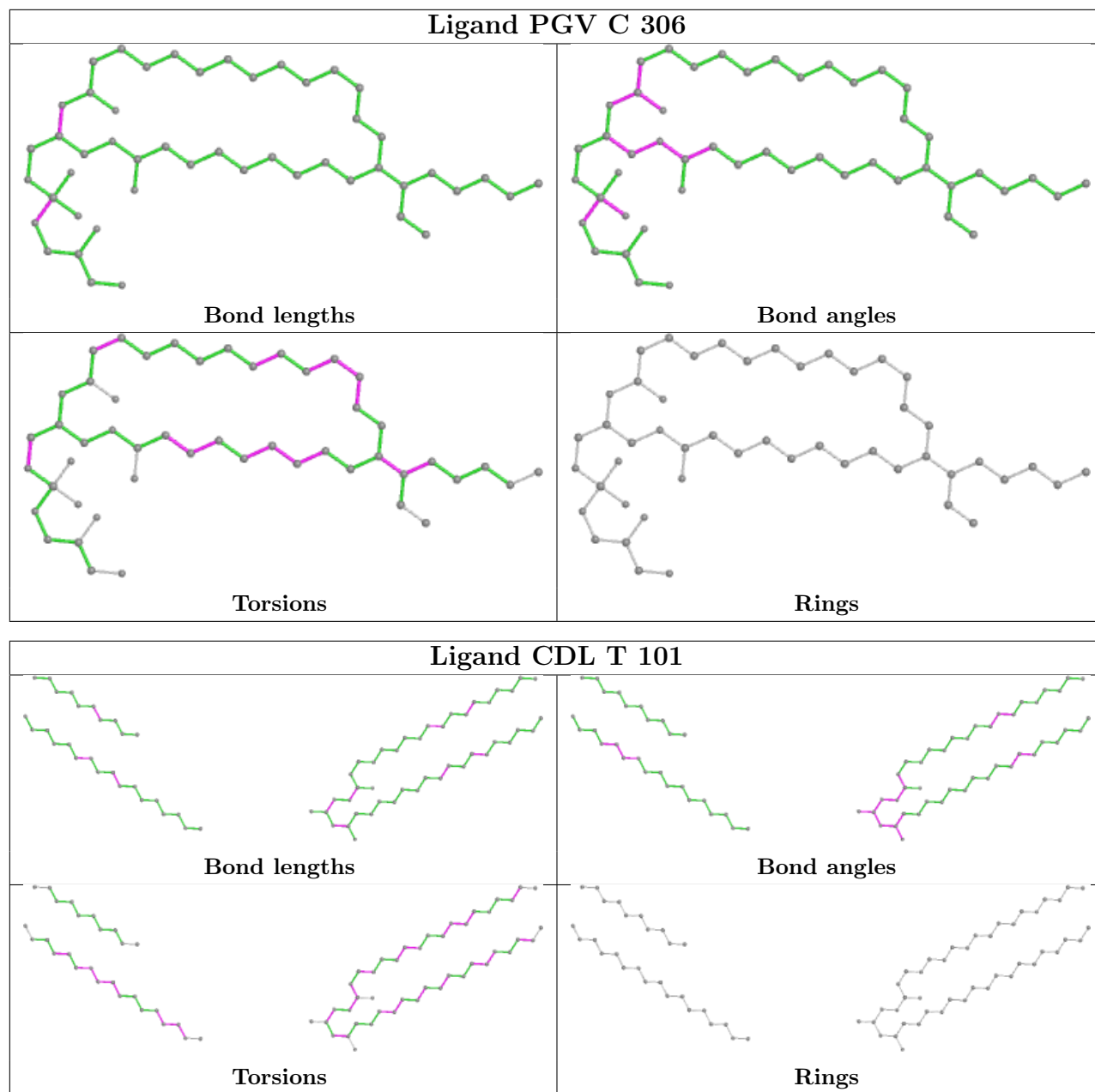


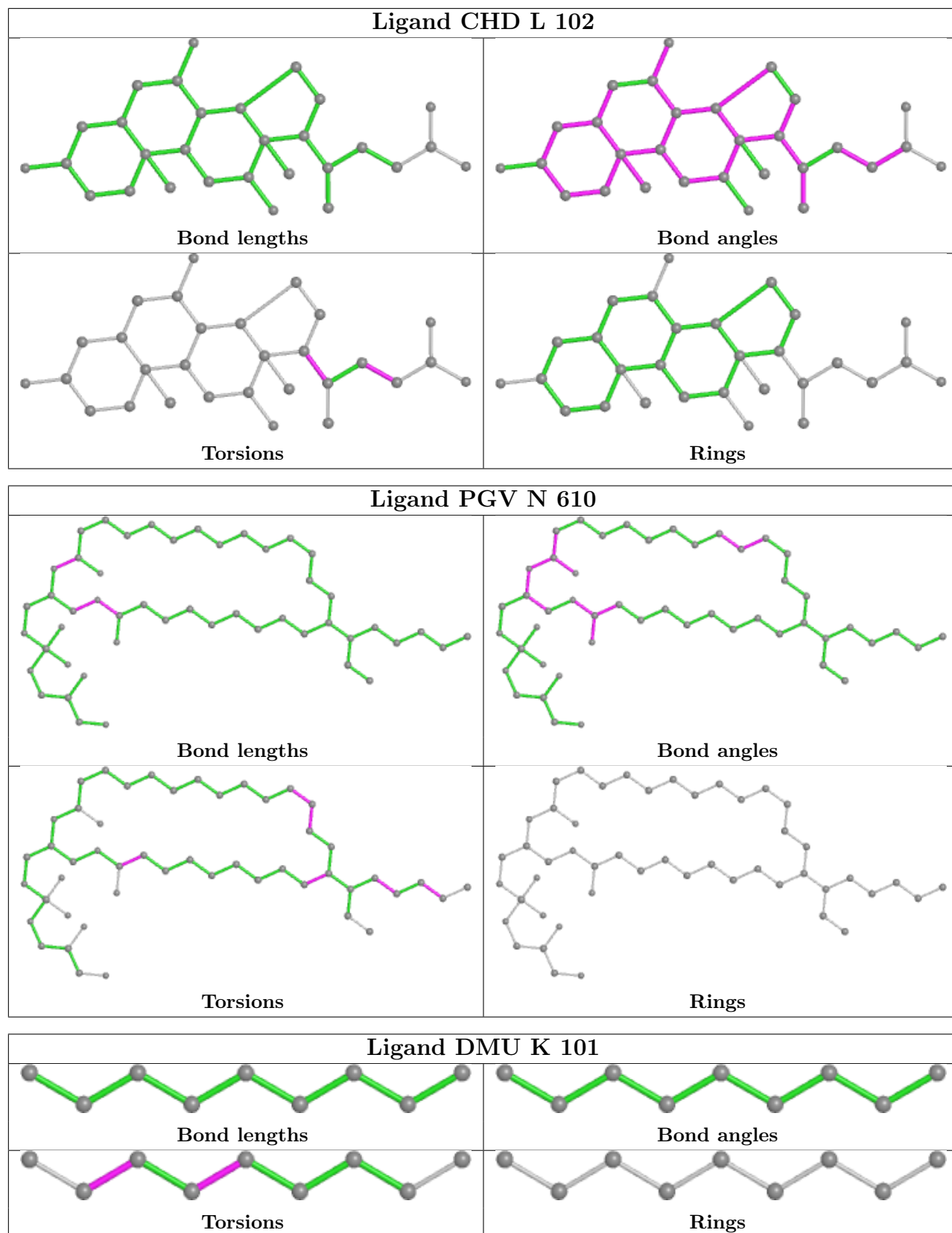


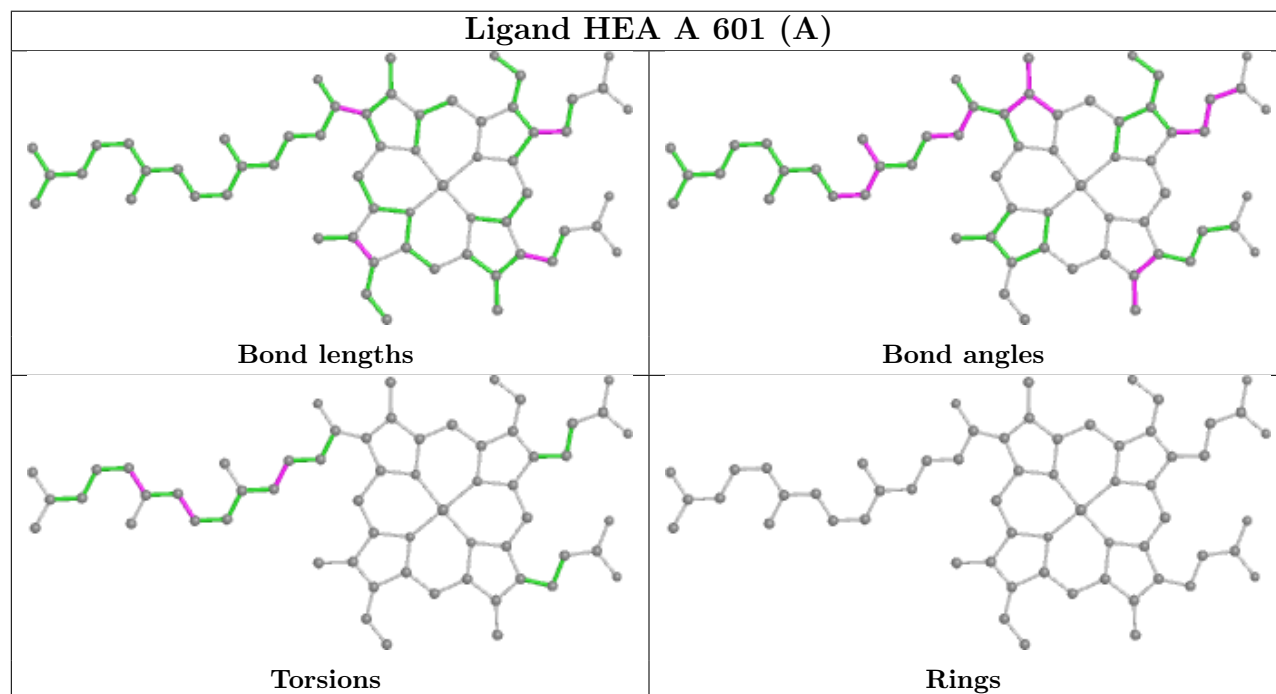
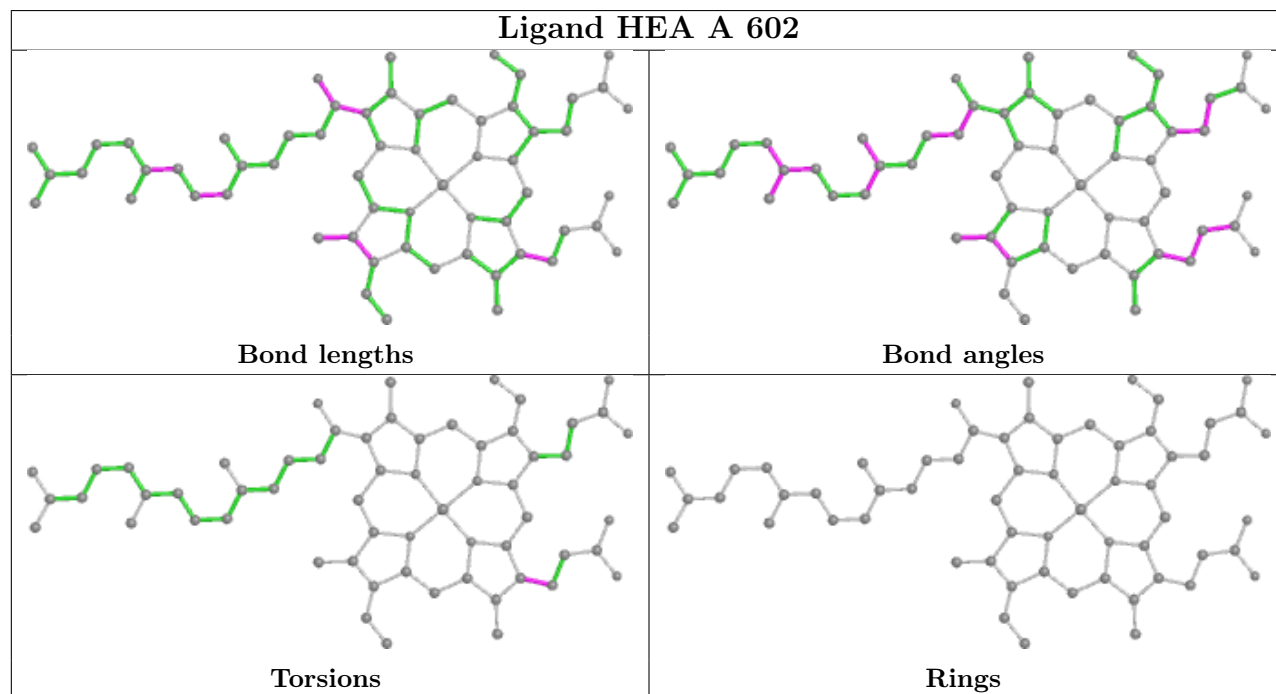
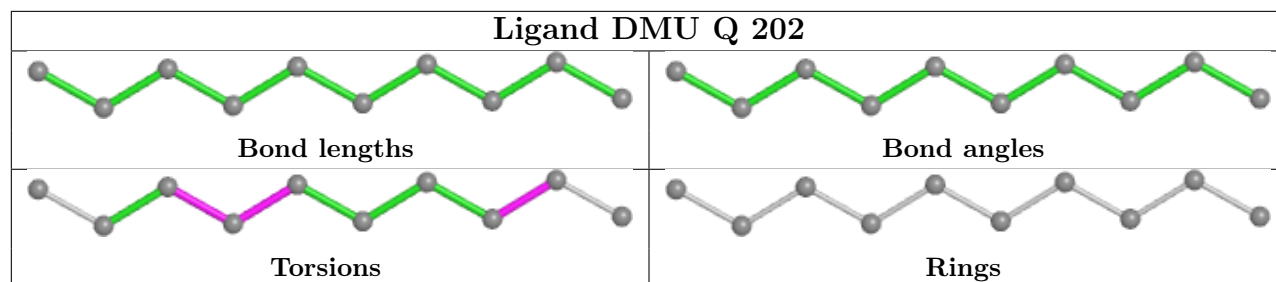


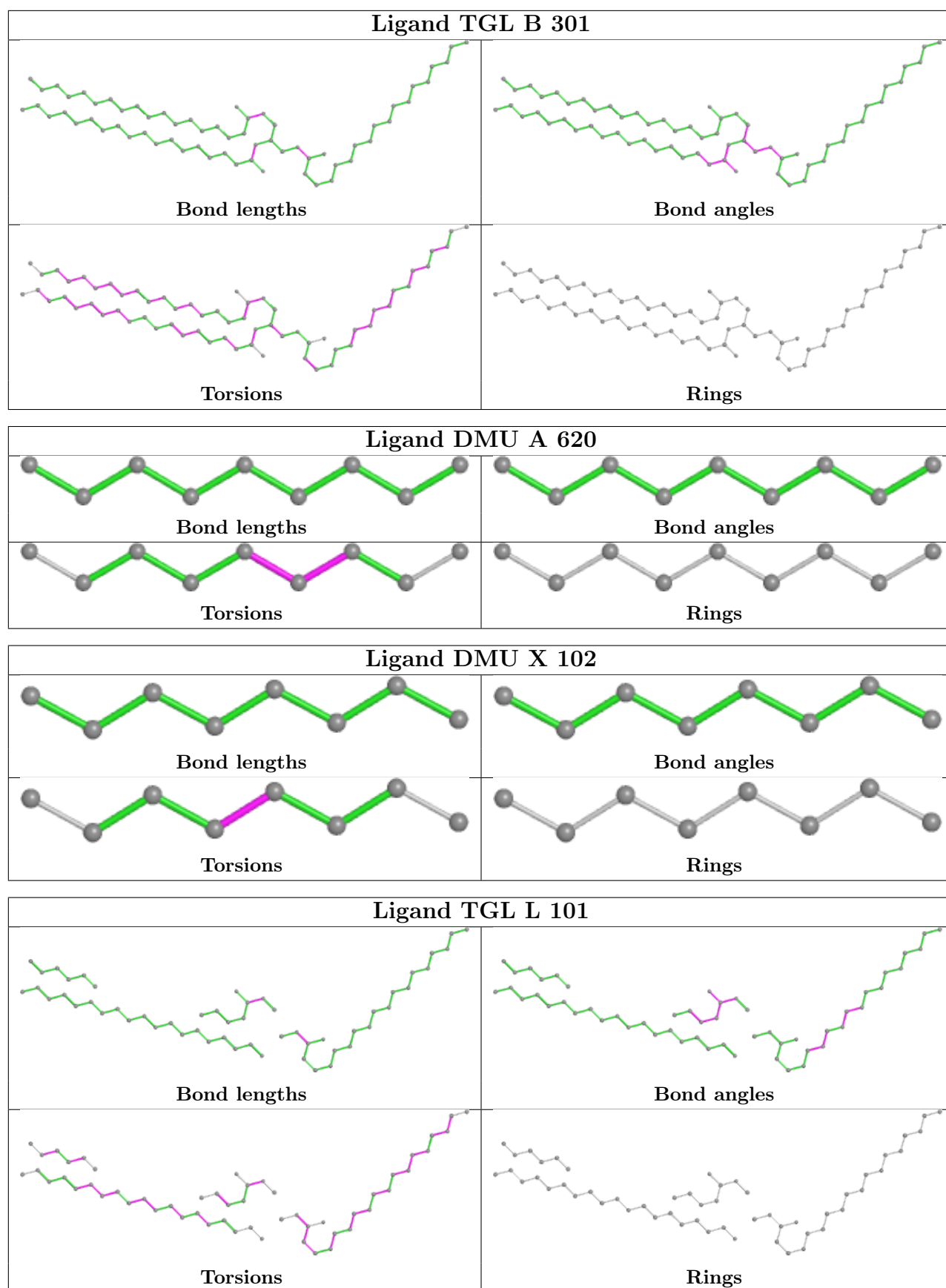


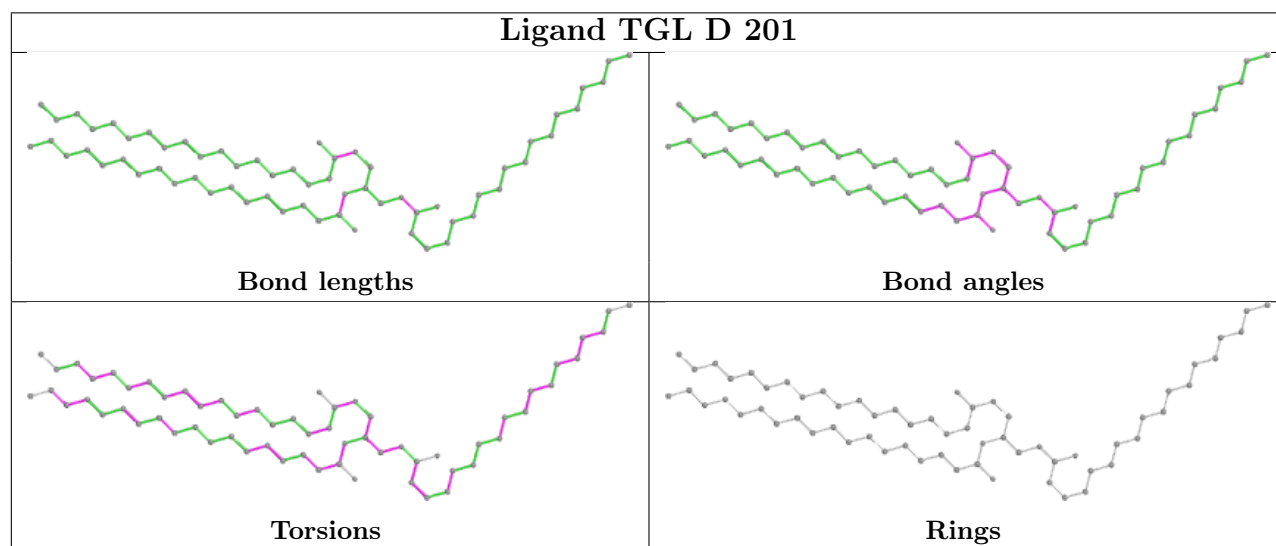
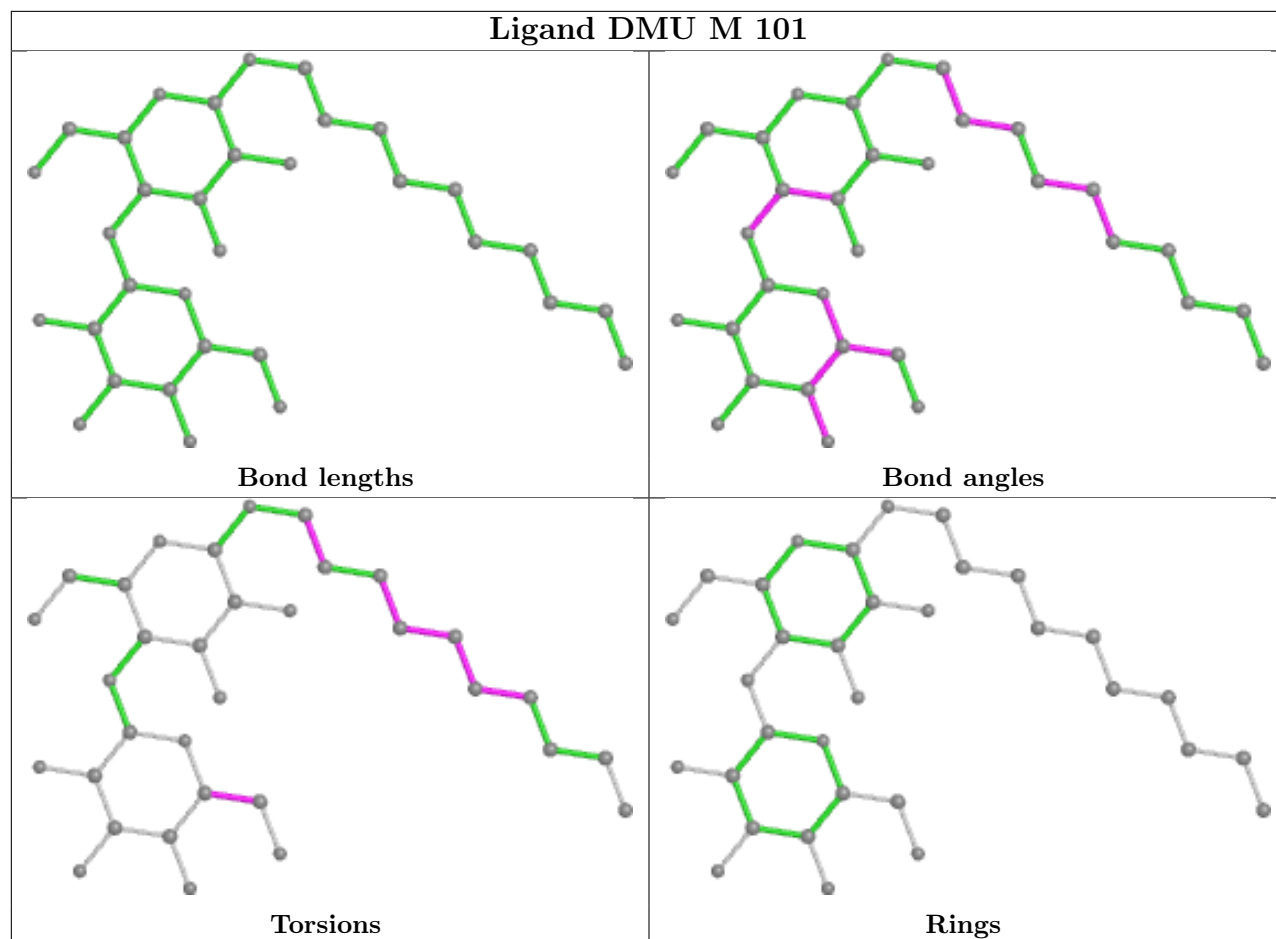


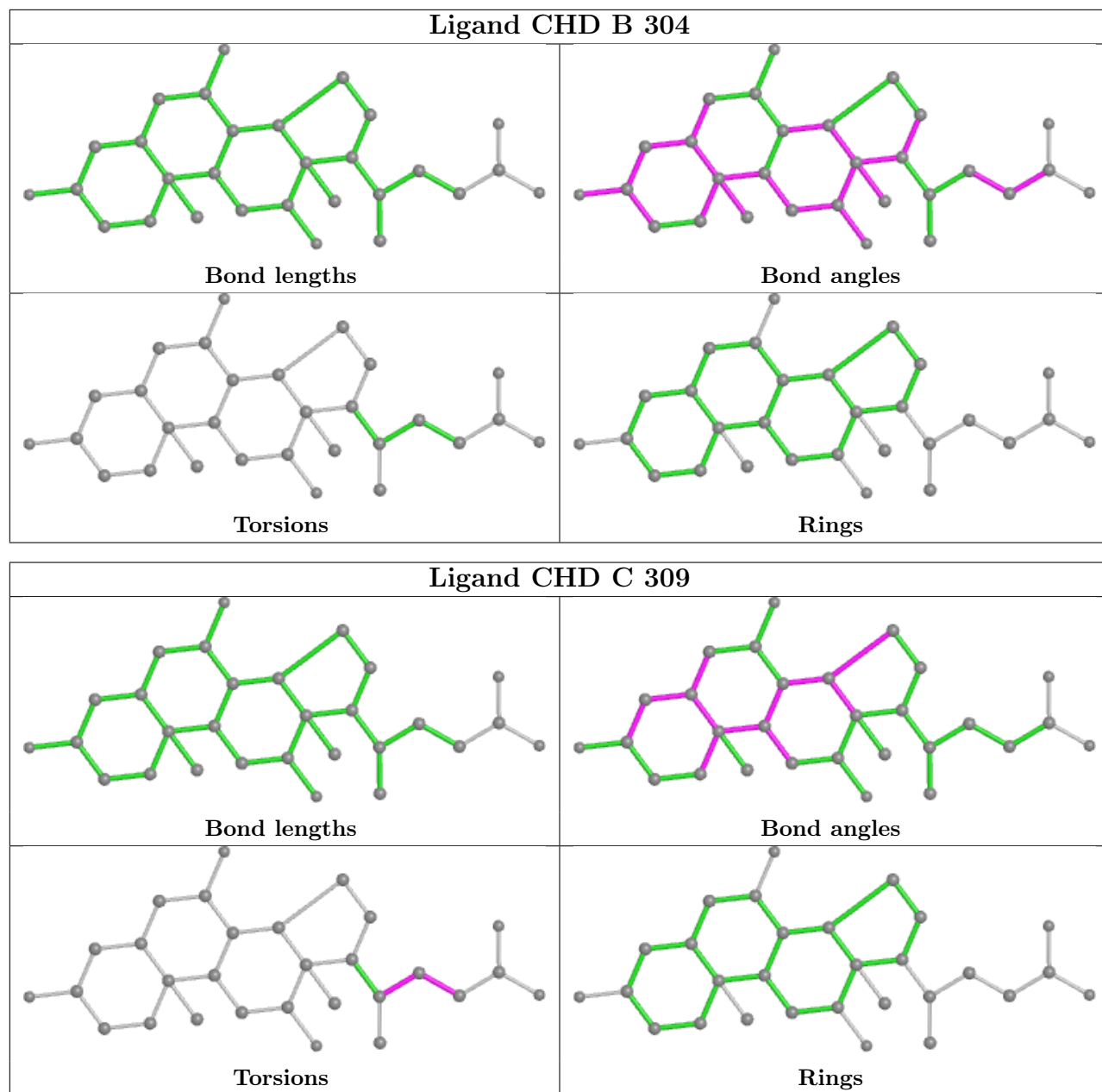


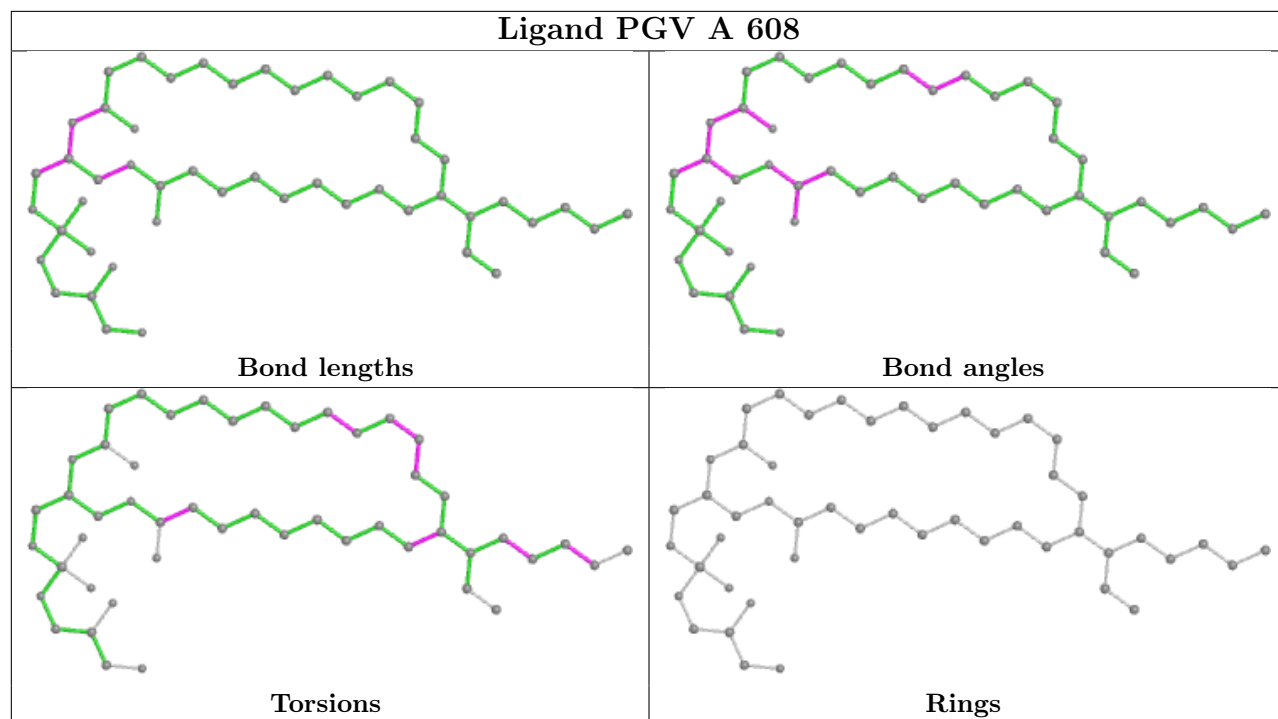


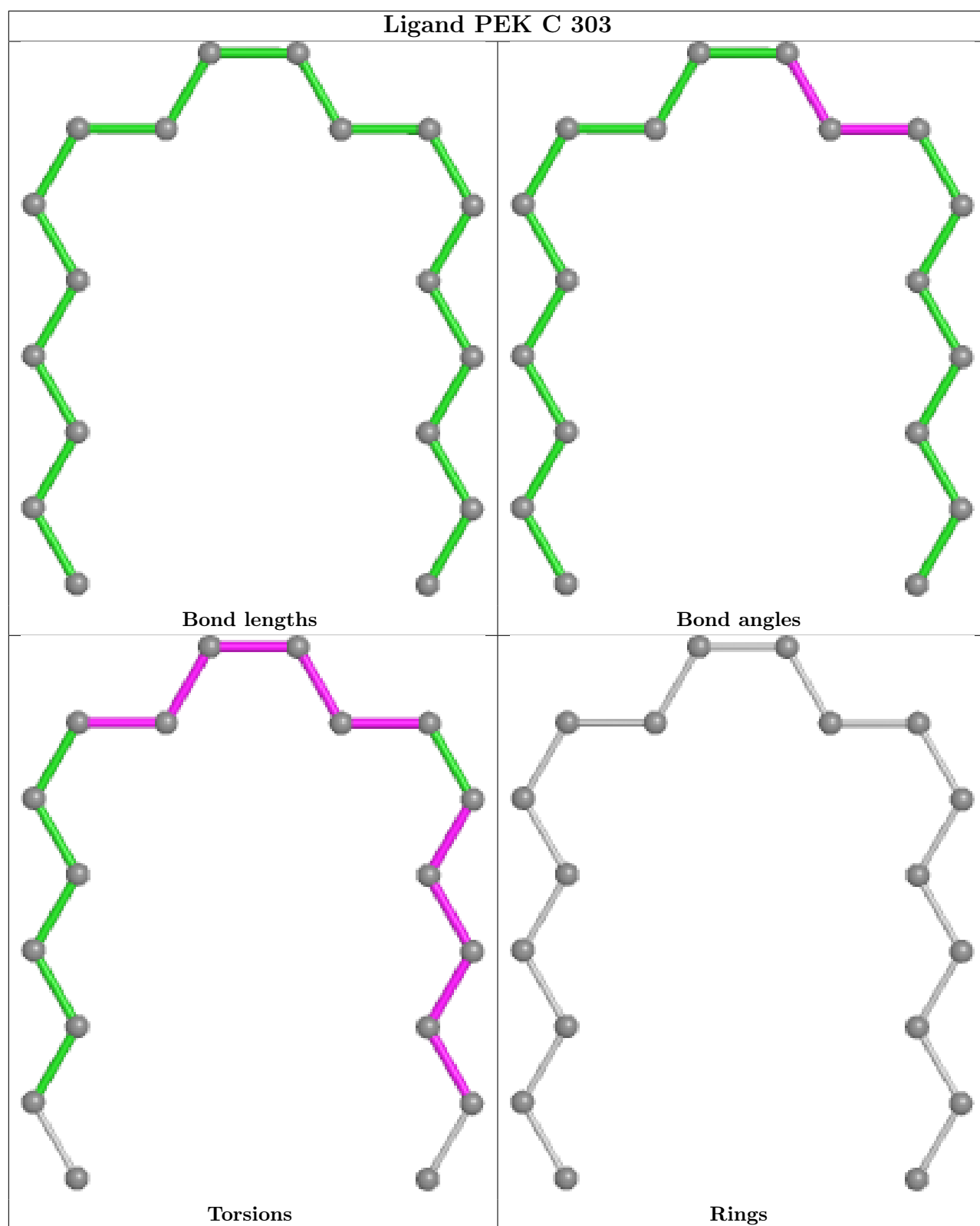


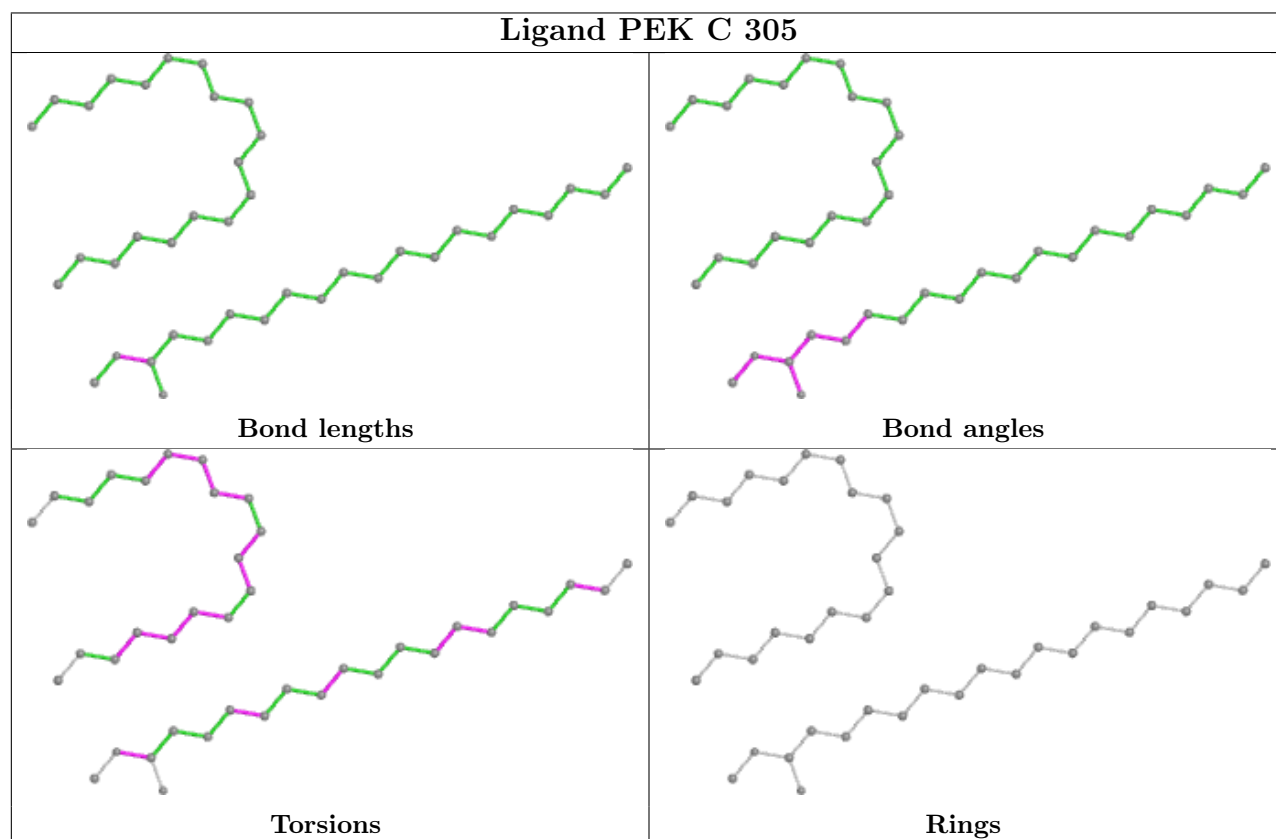
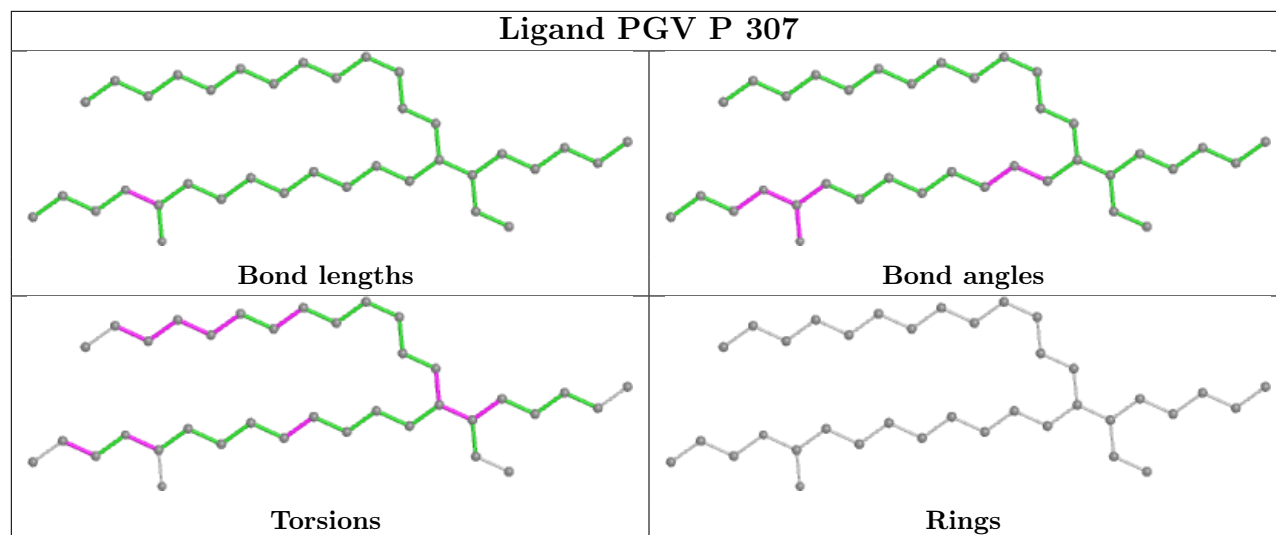


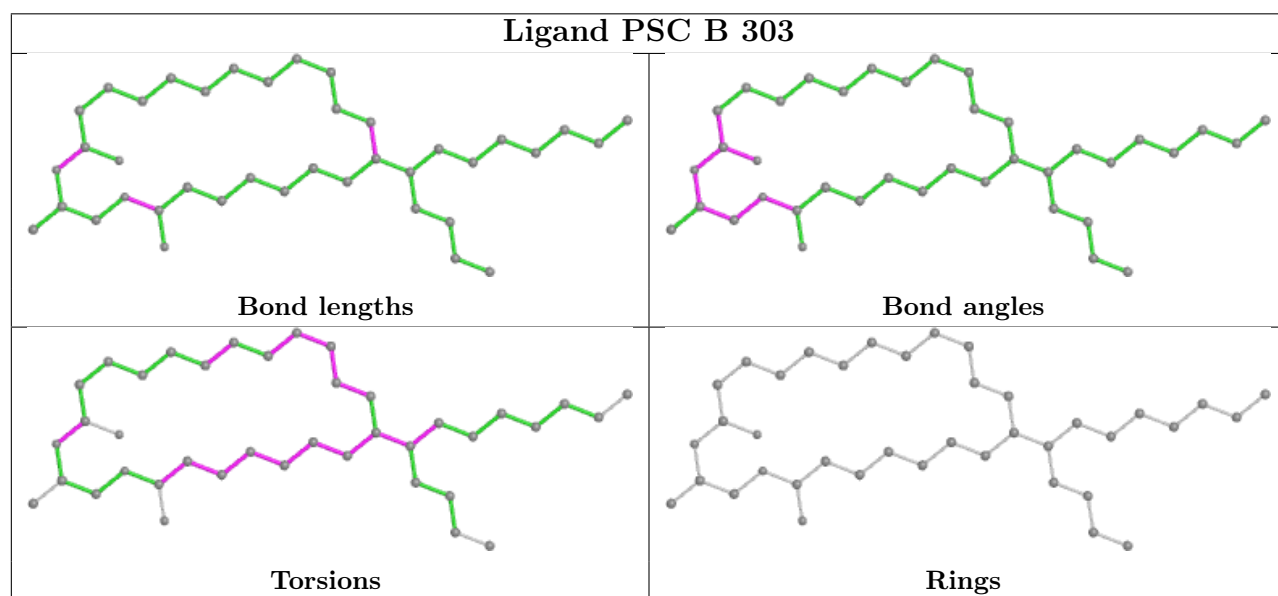
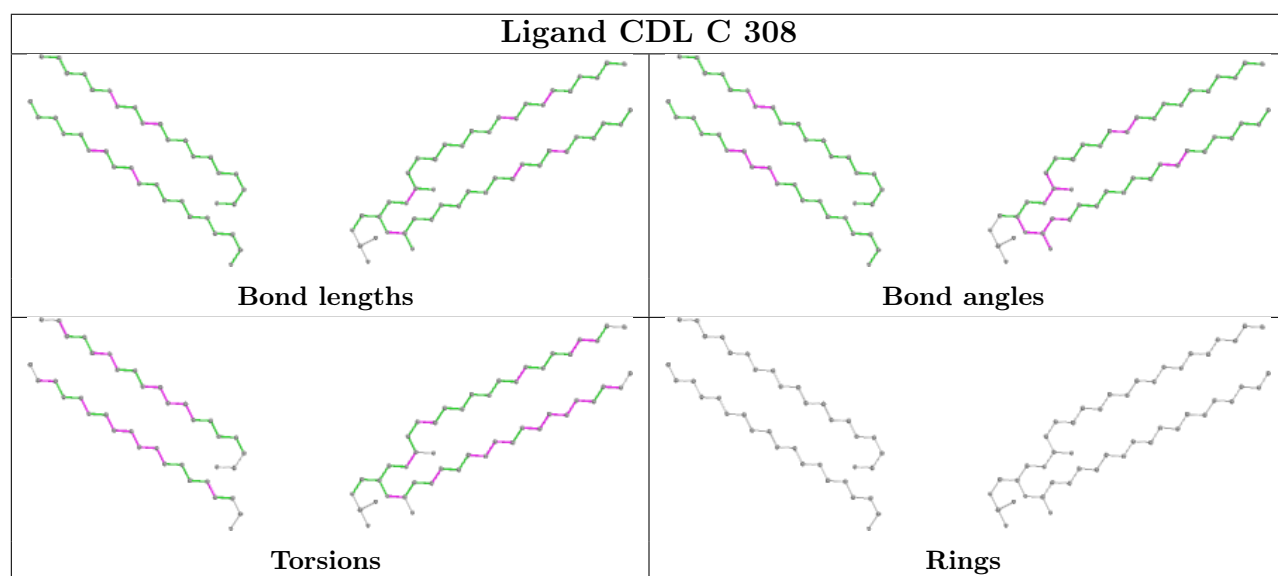
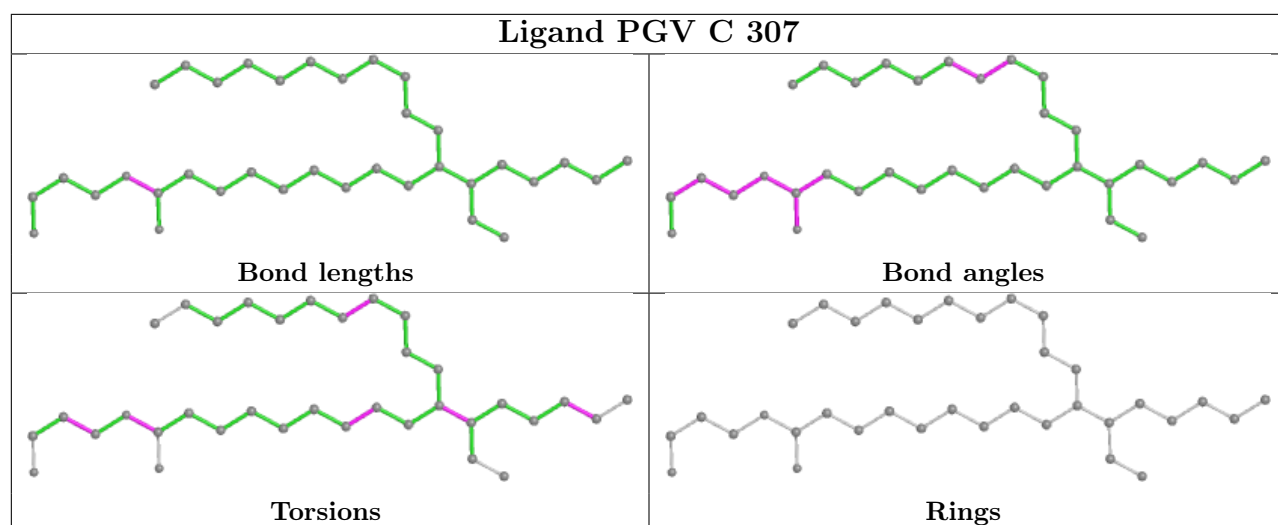


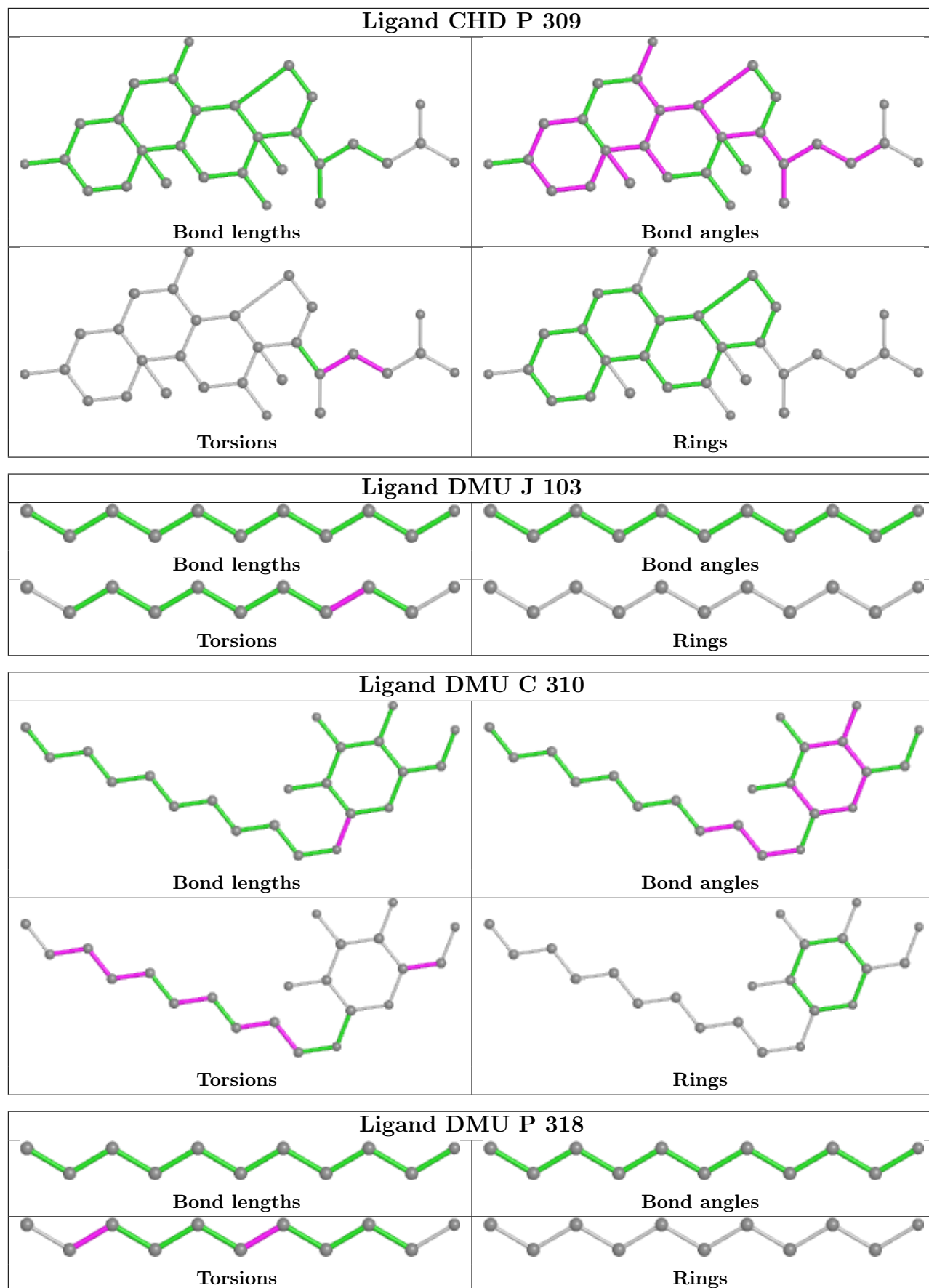


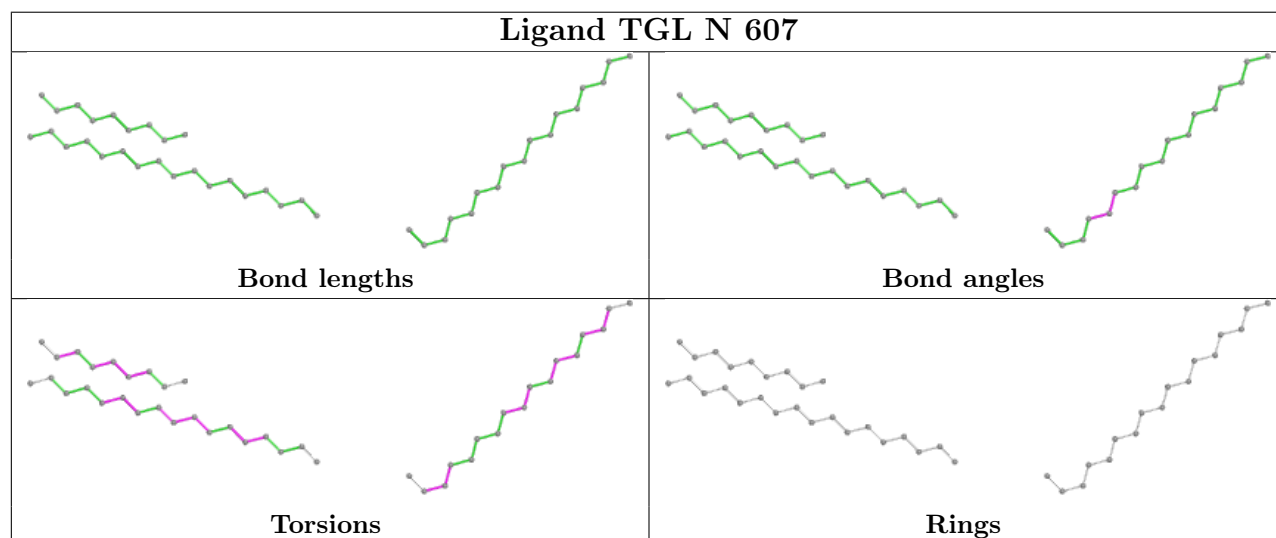
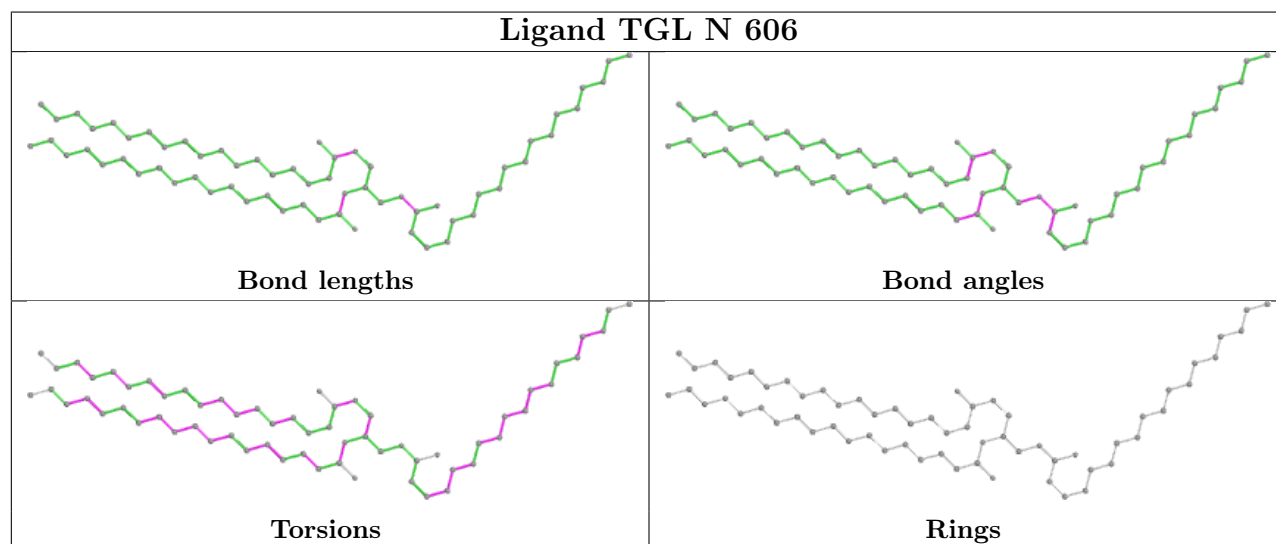
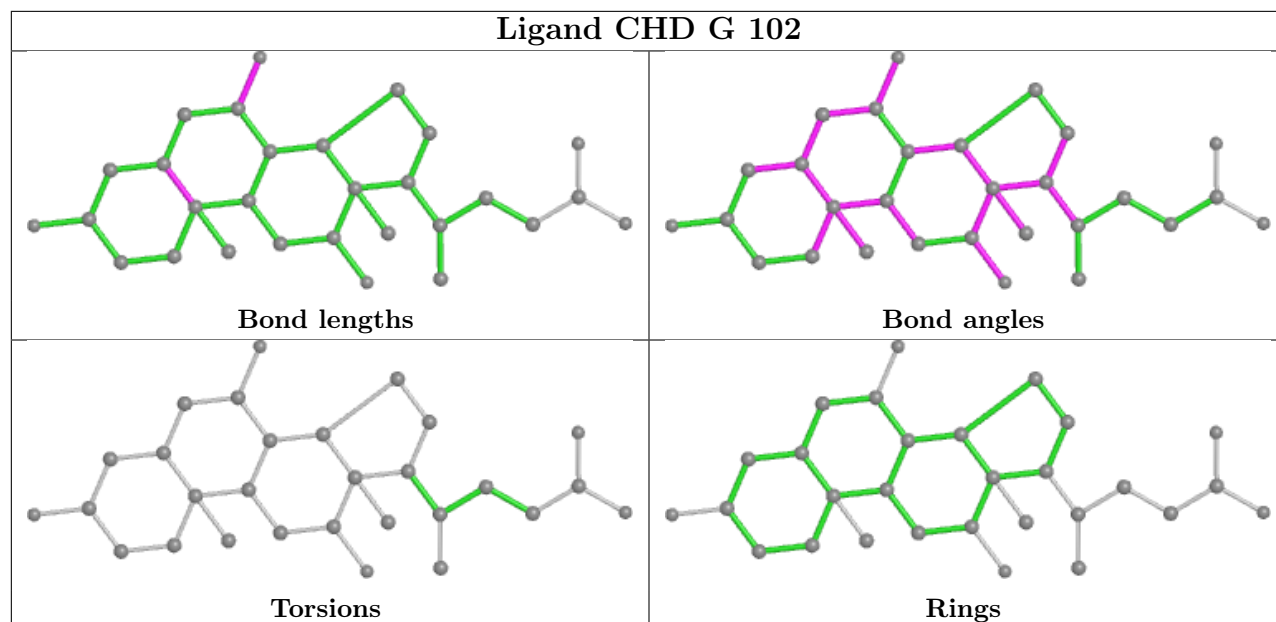


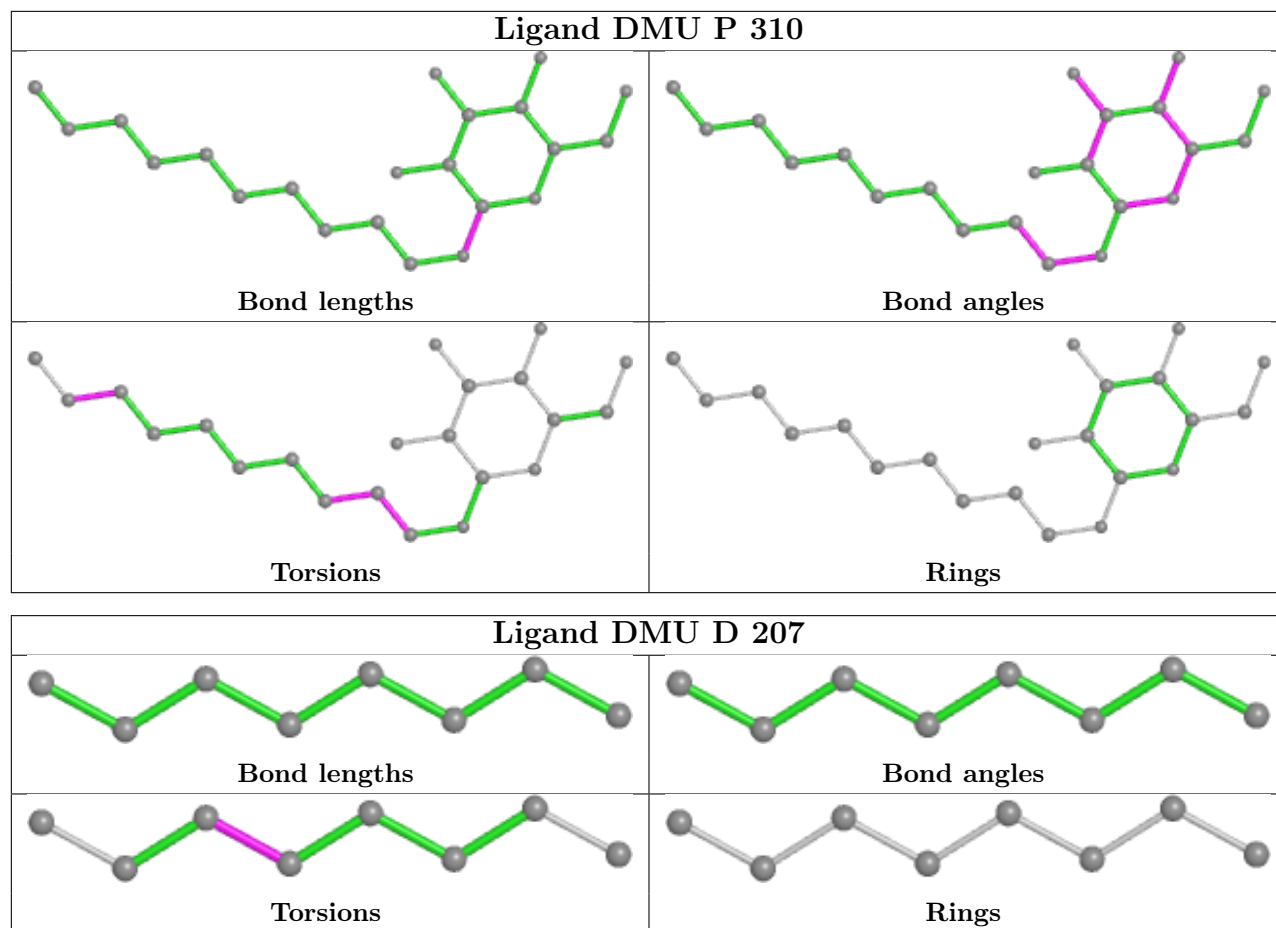












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.01	0 100 100	19, 25, 33, 89	0
1	N	513/514 (99%)	0.01	1 (0%) 95 96	20, 27, 36, 76	0
2	B	226/227 (99%)	0.01	2 (0%) 84 88	23, 33, 61, 112	0
2	O	226/227 (99%)	0.05	4 (1%) 68 74	27, 36, 68, 130	0
3	C	259/259 (100%)	-0.05	0 100 100	22, 28, 41, 91	0
3	P	259/259 (100%)	-0.04	0 100 100	21, 28, 41, 91	0
4	D	144/144 (100%)	-0.19	1 (0%) 87 91	26, 34, 62, 94	0
4	Q	144/144 (100%)	0.40	10 (6%) 16 21	32, 48, 89, 218	0
5	E	105/105 (100%)	-0.16	1 (0%) 82 87	26, 33, 62, 155	0
5	R	105/105 (100%)	-0.09	2 (1%) 66 73	28, 40, 75, 159	0
6	F	94/94 (100%)	0.05	3 (3%) 47 53	23, 35, 61, 166	0
6	S	94/94 (100%)	0.09	3 (3%) 47 53	23, 32, 64, 131	0
7	G	84/84 (100%)	1.16	18 (21%) 0 1	26, 37, 140, 219	0
7	T	84/84 (100%)	1.63	18 (21%) 0 1	25, 39, 146, 232	0
8	H	79/79 (100%)	0.49	8 (10%) 7 8	29, 39, 117, 155	0
8	U	79/79 (100%)	0.47	9 (11%) 5 6	32, 43, 133, 164	0
9	I	72/73 (98%)	0.35	3 (4%) 36 41	28, 46, 78, 102	0
9	V	72/73 (98%)	0.39	3 (4%) 36 41	29, 53, 91, 134	0
10	J	58/58 (100%)	0.30	5 (8%) 10 13	27, 38, 86, 149	0
10	W	58/58 (100%)	0.15	5 (8%) 10 13	28, 40, 79, 154	0
11	K	49/49 (100%)	0.03	2 (4%) 37 42	31, 40, 58, 69	0
11	X	49/49 (100%)	0.37	3 (6%) 21 25	38, 47, 84, 101	0
12	L	46/46 (100%)	-0.06	1 (2%) 62 68	26, 30, 53, 113	0
12	Y	46/46 (100%)	-0.04	0 100 100	29, 36, 71, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.14	4 (9%) 8 10	26, 31, 87, 146	0
13	Z	43/43 (100%)	0.19	3 (6%) 16 21	34, 39, 103, 174	0
All	All	3544/3550 (99%)	0.12	109 (3%) 49 55	19, 32, 74, 232	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	3	ALA	25.9
4	Q	6	VAL	15.0
7	T	8	HIS	14.1
7	T	1	ALA	13.1
6	F	1	ALA	11.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.62	0.34	180,189,197,198	0
9	SAC	I	1	9/10	0.84	0.15	99,114,130,131	0
1	FME	N	1	10/11	0.95	0.12	34,43,83,105	0
2	FME	B	1	10/11	0.97	0.12	27,31,39,120	0
2	FME	O	1	10/11	0.98	0.10	35,36,43,78	0
1	FME	A	1	10/11	0.98	0.08	35,49,83,99	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	DMU	K	103	9/33	0.59	0.40	61,87,107,112	0
21	DMU	A	620	9/33	0.63	0.30	69,78,97,104	0
21	DMU	P	310	22/33	0.66	0.30	40,68,94,112	0
20	EDO	C	317	4/4	0.67	0.15	43,69,73,74	0
21	DMU	X	103	10/33	0.68	0.20	63,81,89,91	0
21	DMU	X	101	9/33	0.72	0.31	60,74,88,88	0
27	CDL	G	101	69/100	0.72	0.21	43,74,103,114	0
21	DMU	L	104	21/33	0.74	0.20	51,77,98,107	0
20	EDO	S	104	4/4	0.75	0.15	55,60,61,83	0
20	EDO	N	620	4/4	0.75	0.21	49,53,55,64	0
27	CDL	T	101	70/100	0.75	0.22	46,72,109,137	0
20	EDO	P	311	4/4	0.76	0.14	55,58,66,107	0
18	PGV	P	307	38/51	0.78	0.20	41,74,97,111	0
26	PEK	P	303	28/53	0.78	0.17	45,58,92,106	0
20	EDO	L	103	4/4	0.79	0.19	38,75,81,126	0
20	EDO	C	314	4/4	0.79	0.21	57,60,86,89	0
24	PSC	B	303	41/52	0.79	0.24	46,78,116,162	0
26	PEK	C	303	18/53	0.80	0.18	44,52,87,92	0
26	PEK	C	305	40/53	0.80	0.24	42,70,103,122	0
20	EDO	C	318	4/4	0.80	0.17	57,74,80,83	0
22	TGL	N	608	55/63	0.80	0.15	49,72,120,127	0
21	DMU	X	102	8/33	0.80	0.17	65,71,83,84	0
20	EDO	M	102	4/4	0.81	0.17	58,60,82,86	0
26	PEK	P	305	40/53	0.81	0.24	38,75,101,126	0
25	CHD	L	102	29/29	0.82	0.30	52,97,132,158	0
20	EDO	T	102	4/4	0.82	0.25	40,74,80,92	0
20	EDO	C	315	4/4	0.82	0.14	49,58,68,72	0
22	TGL	D	201	63/63	0.82	0.16	33,67,134,153	0
22	TGL	N	607	43/63	0.82	0.19	41,60,99,125	0
21	DMU	W	103	11/33	0.82	0.14	52,63,72,91	0
20	EDO	S	105	4/4	0.82	0.31	60,74,77,87	0
21	DMU	D	207	8/33	0.83	0.31	59,75,89,97	0
20	EDO	F	107	4/4	0.83	0.10	46,49,61,109	0
21	DMU	K	104	10/33	0.83	0.15	52,65,87,94	0
20	EDO	P	312	4/4	0.83	0.13	39,40,47,54	0
21	DMU	O	305	11/33	0.83	0.11	60,66,96,97	0
20	EDO	C	319	4/4	0.83	0.11	70,70,71,94	0
21	DMU	C	310	22/33	0.83	0.26	29,59,107,121	0
18	PGV	C	307	37/51	0.84	0.19	41,72,107,115	0
21	DMU	P	318	11/33	0.84	0.12	45,62,80,85	0
21	DMU	Q	202	10/33	0.84	0.22	58,61,87,98	0
20	EDO	B	310	4/4	0.84	0.19	41,47,48,52	0
20	EDO	W	101	4/4	0.84	0.33	49,73,83,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	DMU	J	103	11/33	0.84	0.16	49,59,88,96	0
20	EDO	D	203	4/4	0.85	0.17	37,47,73,80	0
25	CHD	P	309	29/29	0.85	0.16	40,77,135,146	0
21	DMU	K	102	9/33	0.85	0.25	61,71,95,102	0
22	TGL	L	101	54/63	0.85	0.17	30,56,125,171	0
20	EDO	B	309	4/4	0.86	0.18	31,46,47,64	0
27	CDL	C	308	85/100	0.86	0.18	42,72,133,153	0
20	EDO	A	613	4/4	0.86	0.25	43,53,63,82	0
21	DMU	D	206	11/33	0.86	0.17	46,70,82,83	0
22	TGL	N	606	63/63	0.87	0.17	45,77,110,145	0
20	EDO	A	611	4/4	0.87	0.28	47,55,63,109	0
17	NA	P	302	1/1	0.87	0.12	39,39,39,39	0
22	TGL	B	301	63/63	0.87	0.15	33,71,116,127	0
25	CHD	C	309	29/29	0.87	0.17	46,58,110,165	0
20	EDO	A	619	4/4	0.87	0.20	53,62,70,73	0
27	CDL	P	308	77/100	0.87	0.20	41,75,129,151	0
18	PGV	Q	201	37/51	0.87	0.18	43,65,110,121	0
18	PGV	A	606	33/51	0.88	0.19	32,56,99,123	0
20	EDO	P	317	4/4	0.88	0.15	54,59,60,67	0
21	DMU	C	320	12/33	0.88	0.12	60,63,88,92	0
20	EDO	J	102	4/4	0.88	0.15	53,56,56,70	0
20	EDO	O	304	4/4	0.89	0.14	42,47,54,57	0
20	EDO	N	621	4/4	0.89	0.18	43,55,64,70	0
20	EDO	D	205	4/4	0.90	0.15	56,60,62,71	0
20	EDO	F	106	4/4	0.90	0.09	37,38,45,101	0
20	EDO	A	616	4/4	0.90	0.19	42,49,58,67	0
20	EDO	C	311	4/4	0.90	0.16	33,39,42,42	0
20	EDO	Q	204	4/4	0.90	0.14	47,50,53,61	0
21	DMU	N	622	9/33	0.91	0.12	48,68,78,80	0
20	EDO	S	106	4/4	0.91	0.17	37,42,58,59	0
20	EDO	N	614	4/4	0.91	0.19	33,36,50,107	0
21	DMU	Z	101	33/33	0.91	0.12	37,47,69,80	0
24	PSC	O	302	33/52	0.91	0.16	29,62,99,125	0
20	EDO	P	313	4/4	0.91	0.14	55,57,62,74	0
21	DMU	K	101	9/33	0.91	0.19	54,62,82,91	0
21	DMU	M	101	33/33	0.91	0.10	34,43,60,77	0
20	EDO	E	203	4/4	0.92	0.10	44,44,48,70	0
20	EDO	J	101	4/4	0.92	0.26	50,51,84,98	0
20	EDO	C	313	4/4	0.92	0.17	35,56,64,109	0
20	EDO	F	105	4/4	0.93	0.20	33,39,68,69	0
20	EDO	A	617	4/4	0.93	0.09	28,29,31,34	0
20	EDO	W	102	4/4	0.93	0.12	50,64,72,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	R	202	4/4	0.93	0.14	47,62,63,78	0
29	PO4	U	101	5/5	0.93	0.20	53,54,120,187	0
20	EDO	P	315	4/4	0.94	0.12	28,39,40,52	0
20	EDO	S	107	4/4	0.94	0.11	28,30,33,33	0
20	EDO	B	307	4/4	0.94	0.12	41,50,54,81	0
20	EDO	T	103	4/4	0.94	0.20	39,45,60,65	0
20	EDO	A	615	4/4	0.94	0.13	32,39,39,119	0
19	OXY	A	607	2/2	0.94	1.21	14,14,14,29	2
20	EDO	Y	101	4/4	0.94	0.12	46,54,58,61	0
20	EDO	D	204	4/4	0.94	0.15	45,49,58,58	0
21	DMU	A	621	8/33	0.94	0.09	46,50,67,77	0
20	EDO	B	305	4/4	0.94	0.15	37,44,49,54	0
20	EDO	R	201	4/4	0.95	0.14	41,41,42,44	0
20	EDO	N	617	4/4	0.95	0.20	32,42,45,66	0
20	EDO	F	104	4/4	0.95	0.14	39,40,59,88	0
20	EDO	P	314	4/4	0.95	0.17	35,36,37,44	0
26	PEK	P	304	53/53	0.95	0.12	27,44,94,113	0
20	EDO	A	614	4/4	0.95	0.17	39,40,43,47	0
20	EDO	P	316	4/4	0.95	0.10	49,57,59,62	0
20	EDO	S	108	4/4	0.95	0.13	38,50,60,72	0
20	EDO	N	611	4/4	0.95	0.12	22,27,29,32	0
17	NA	C	302	1/1	0.95	0.08	40,40,40,40	0
25	CHD	P	301	29/29	0.95	0.09	25,29,37,39	0
20	EDO	B	306	4/4	0.96	0.11	25,27,30,33	0
20	EDO	N	613	4/4	0.96	0.09	38,39,42,47	0
25	CHD	C	301	29/29	0.96	0.09	25,28,35,38	0
20	EDO	T	104	4/4	0.96	0.10	29,32,38,43	0
25	CHD	G	102	29/29	0.96	0.09	22,26,30,39	0
18	PGV	N	610	51/51	0.96	0.12	24,31,69,80	0
20	EDO	N	615	4/4	0.96	0.07	41,41,42,50	0
20	EDO	C	316	4/4	0.96	0.14	29,34,40,52	0
20	EDO	N	618	4/4	0.96	0.18	29,45,62,64	0
20	EDO	G	103	4/4	0.97	0.09	29,32,37,37	0
20	EDO	N	616	4/4	0.97	0.17	36,41,42,47	0
20	EDO	E	202	4/4	0.97	0.09	36,38,40,45	0
26	PEK	C	304	53/53	0.97	0.12	25,43,94,114	0
20	EDO	B	308	4/4	0.97	0.15	34,38,47,113	0
20	EDO	N	619	4/4	0.97	0.12	30,38,39,43	0
20	EDO	F	103	4/4	0.97	0.16	31,31,31,33	0
18	PGV	C	306	51/51	0.97	0.12	23,29,83,100	0
25	CHD	B	304	29/29	0.97	0.09	23,27,32,43	0
18	PGV	P	306	51/51	0.97	0.12	22,30,82,104	0

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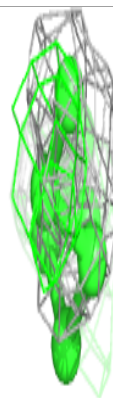
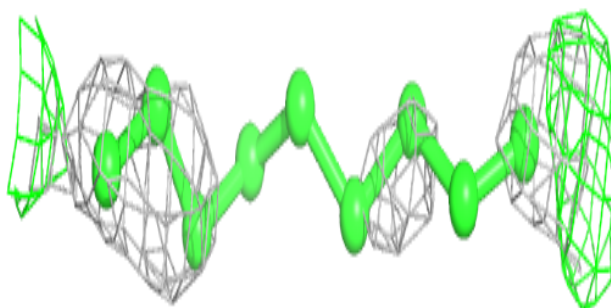
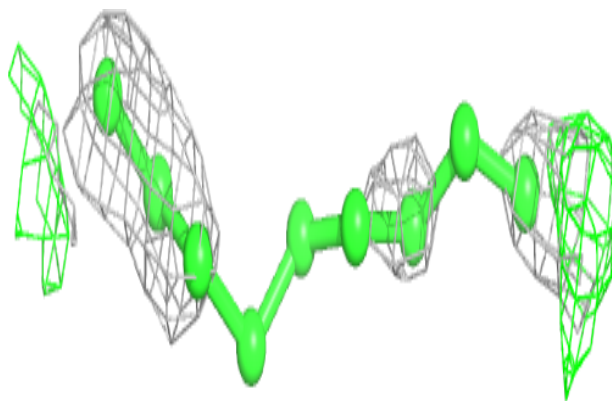
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	S	103	4/4	0.97	0.10	35,37,40,45	0
20	EDO	A	612	4/4	0.97	0.12	28,40,76,100	0
29	PO4	H	101	5/5	0.97	0.23	59,71,91,156	0
20	EDO	C	312	4/4	0.97	0.08	32,34,35,36	0
18	PGV	A	608	51/51	0.98	0.11	22,28,70,89	0
14	HEA	A	602	60/60	0.98	0.09	19,23,29,36	0
20	EDO	N	612	4/4	0.98	0.08	26,27,28,29	0
20	EDO	E	201	4/4	0.98	0.11	38,40,43,43	0
14	HEA	N	601[A]	60/60	0.98	0.10	17,26,42,50	18
20	EDO	Q	203	4/4	0.98	0.17	29,47,51,73	0
14	HEA	N	601[B]	54/60	0.98	0.10	20,25,38,41	12
14	HEA	N	601[C]	51/60	0.98	0.10	20,25,36,42	9
14	HEA	N	602	60/60	0.98	0.10	20,24,30,35	0
20	EDO	S	102	4/4	0.98	0.14	23,24,25,25	0
20	EDO	A	618	4/4	0.98	0.14	30,37,45,51	0
14	HEA	A	601[A]	60/60	0.98	0.11	15,21,41,52	18
14	HEA	A	601[B]	54/60	0.98	0.11	17,21,31,38	12
20	EDO	A	609	4/4	0.98	0.18	29,33,44,92	0
20	EDO	O	303	4/4	0.98	0.12	30,32,32,33	0
20	EDO	A	610	4/4	0.98	0.10	21,23,26,29	0
20	EDO	D	202	4/4	0.98	0.10	33,35,56,63	0
14	HEA	A	601[C]	51/60	0.98	0.11	17,21,28,36	9
16	MG	N	604	1/1	0.99	0.06	23,23,23,23	0
20	EDO	F	102	4/4	0.99	0.09	24,24,24,26	0
17	NA	A	605	1/1	0.99	0.07	27,27,27,27	0
19	OXY	N	609	2/2	0.99	0.78	16,16,16,25	2
16	MG	A	604	1/1	0.99	0.06	20,20,20,20	0
28	ZN	S	101	1/1	0.99	0.11	27,27,27,27	0
17	NA	N	605	1/1	0.99	0.08	31,31,31,31	0
23	CUA	O	301	2/2	0.99	0.11	27,27,27,27	0
28	ZN	F	101	1/1	1.00	0.11	26,26,26,26	0
23	CUA	B	302	2/2	1.00	0.13	24,24,24,24	0
15	CU	A	603	1/1	1.00	0.14	22,22,22,22	0
15	CU	N	603	1/1	1.00	0.13	24,24,24,24	0

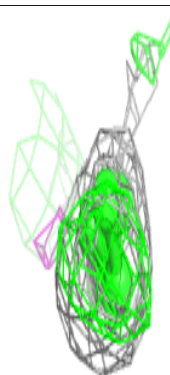
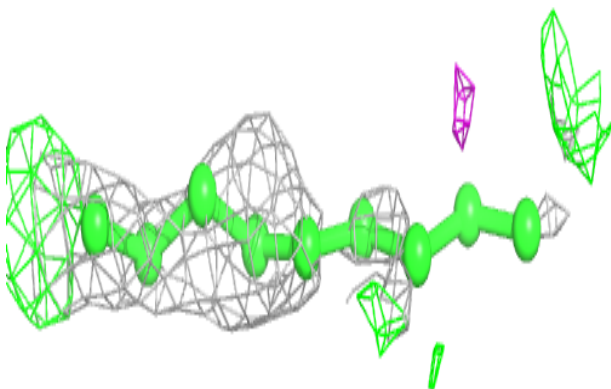
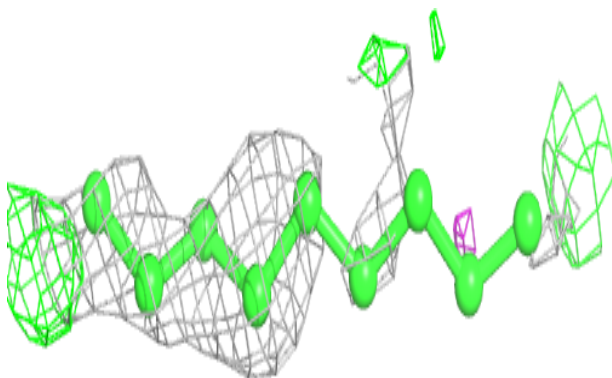
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU K 103:

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

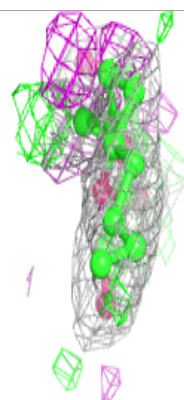
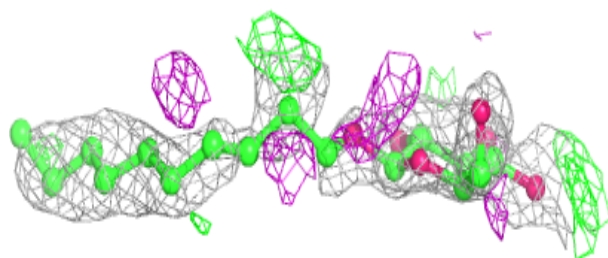
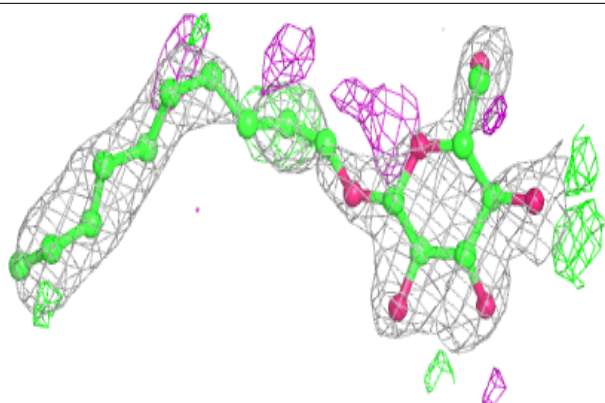
**Electron density around DMU A 620:**

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

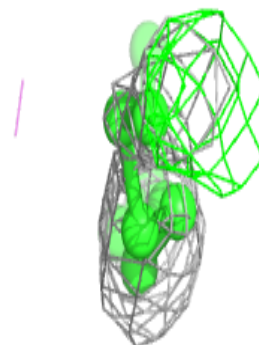
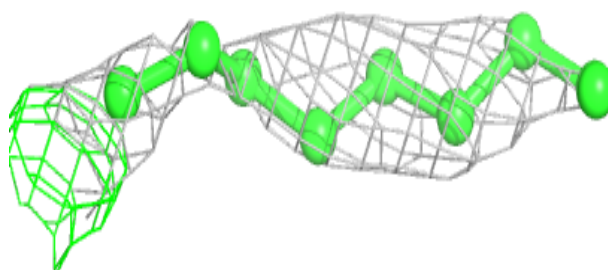
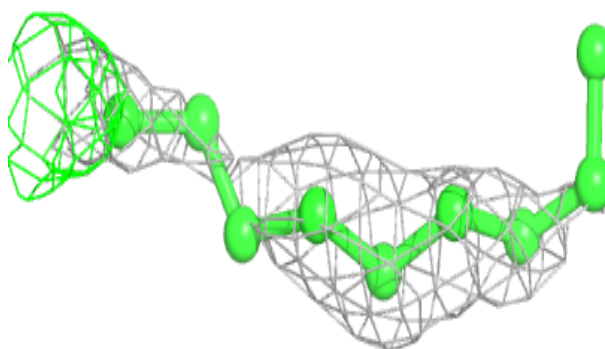


Electron density around DMU P 310:

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

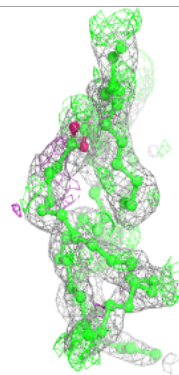
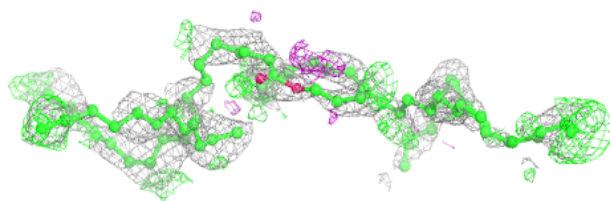
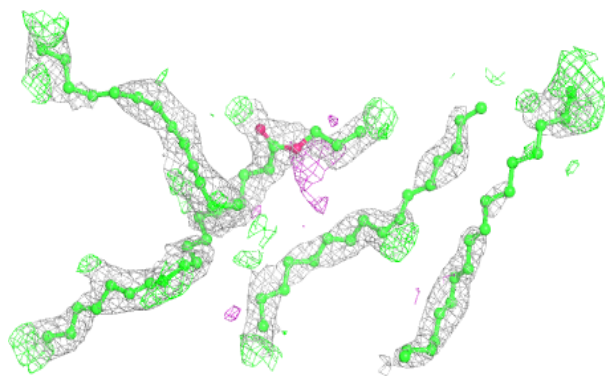
**Electron density around DMU X 101:**

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

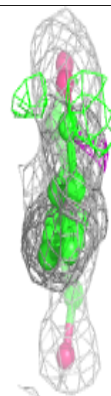
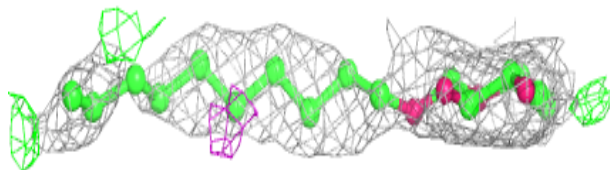
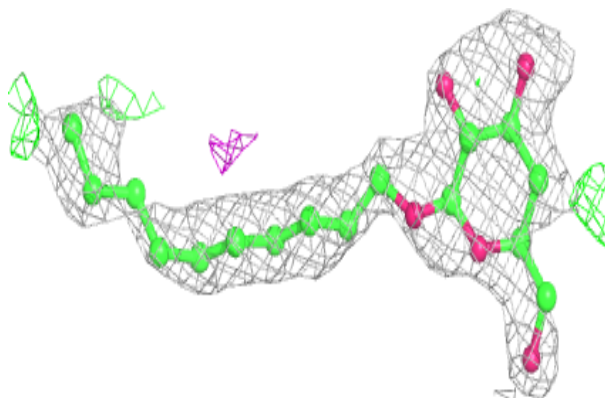


Electron density around CDL G 101:

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

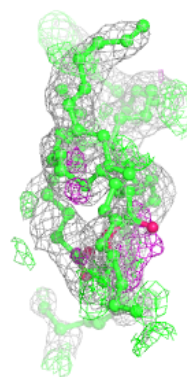
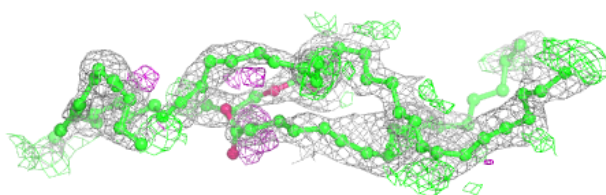
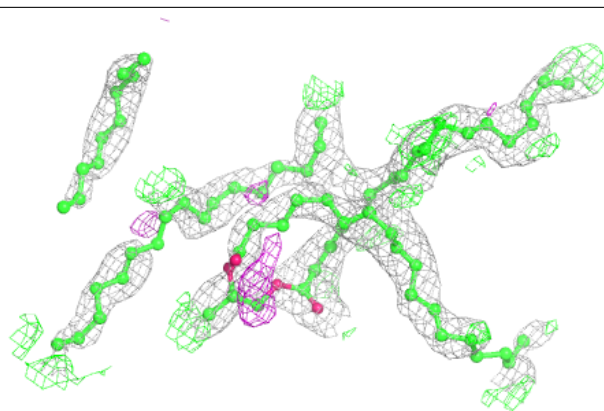
**Electron density around DMU L 104:**

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

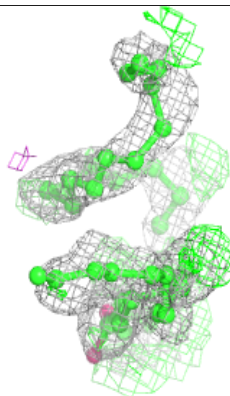
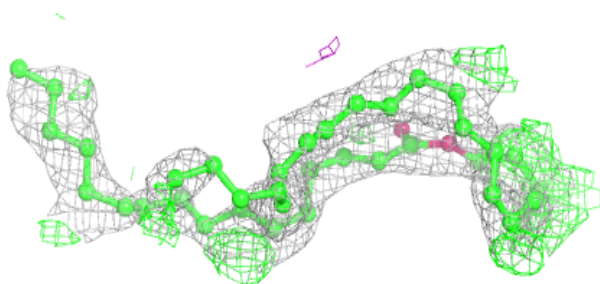
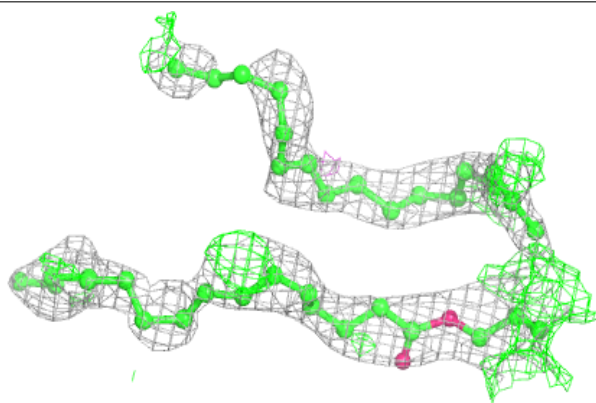


Electron density around CDL T 101:

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

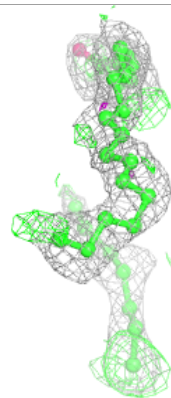
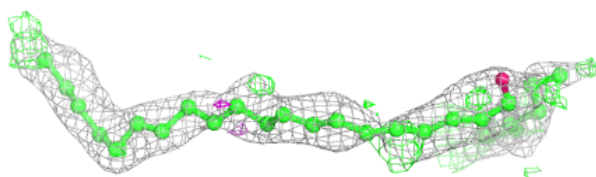
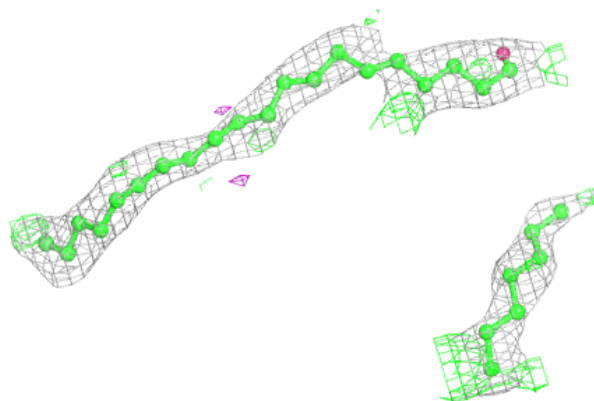
**Electron density around PGV P 307:**

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

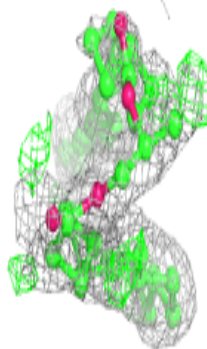
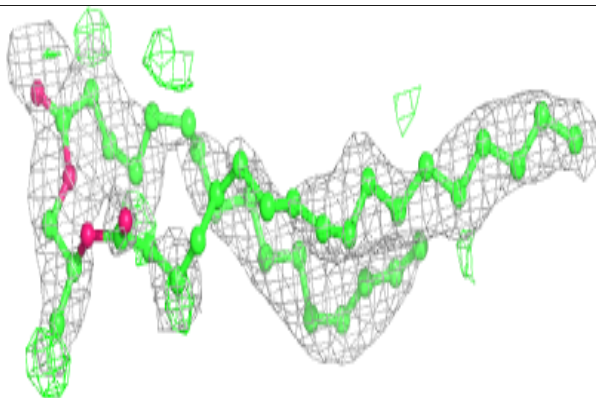
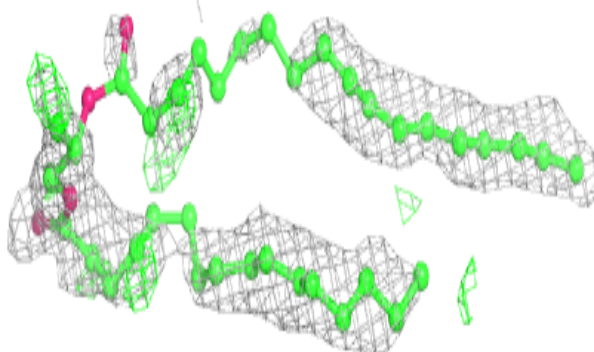


Electron density around PEK P 303:

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

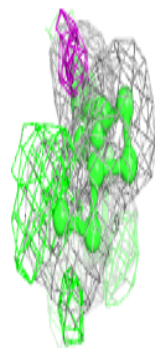
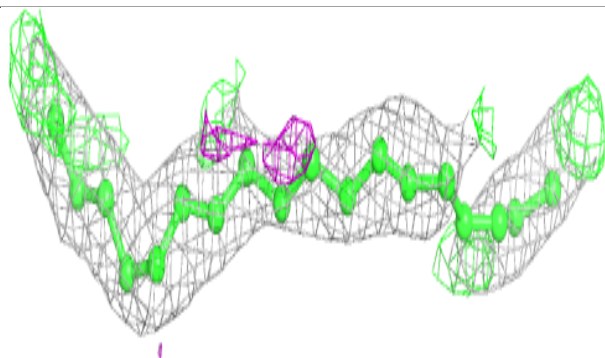
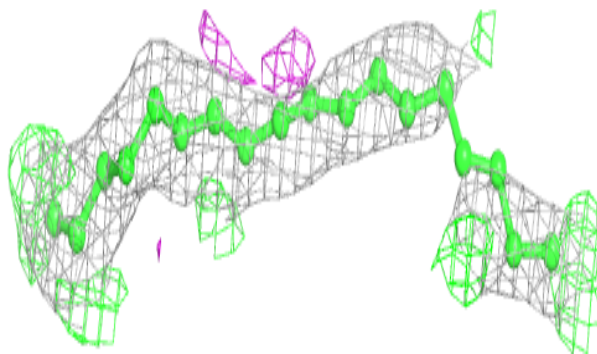
**Electron density around PSC B 303:**

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



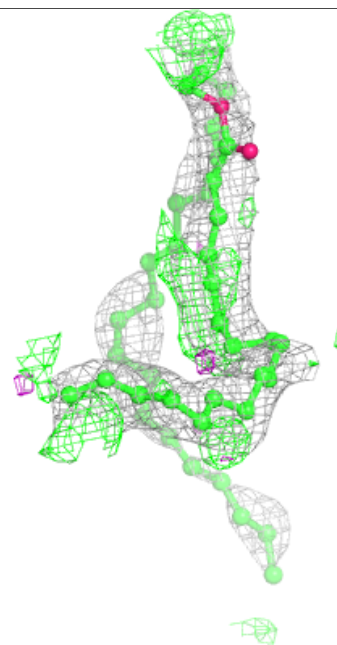
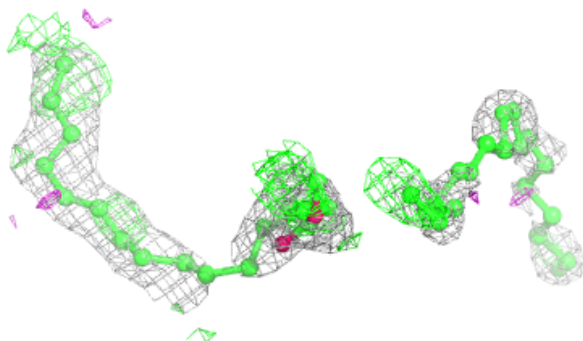
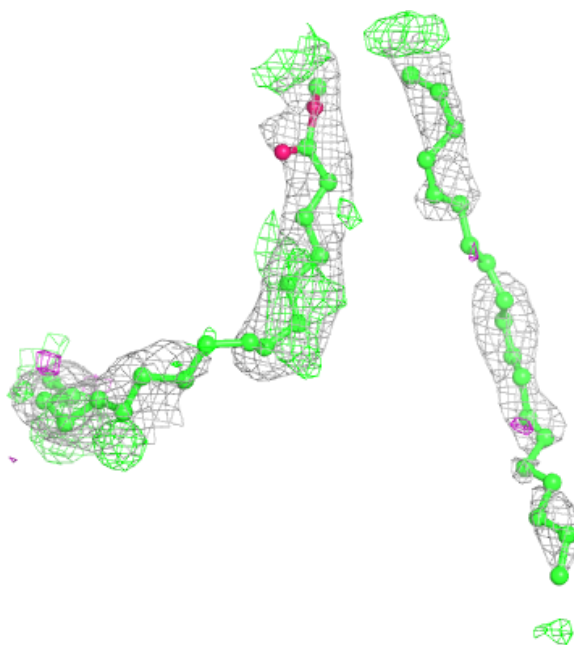
Electron density around PEK C 303:

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



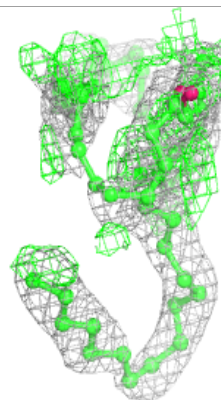
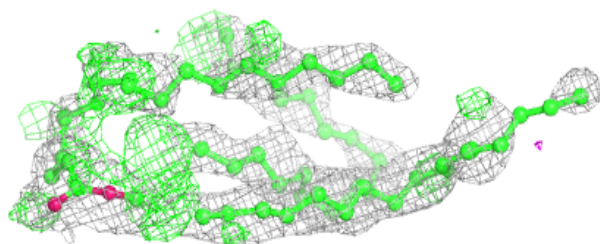
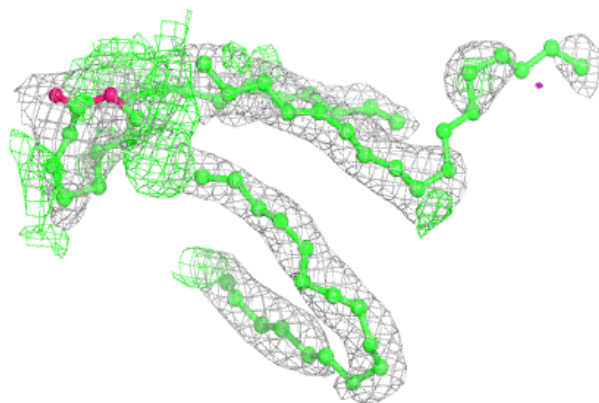
Electron density around PEK C 305:

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

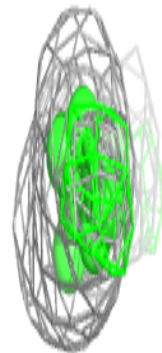
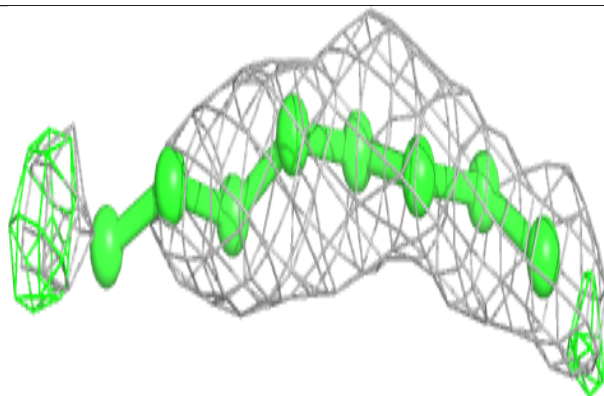
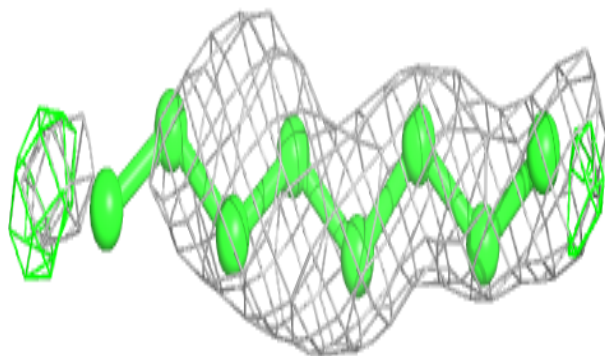


Electron density around TGL N 608:

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

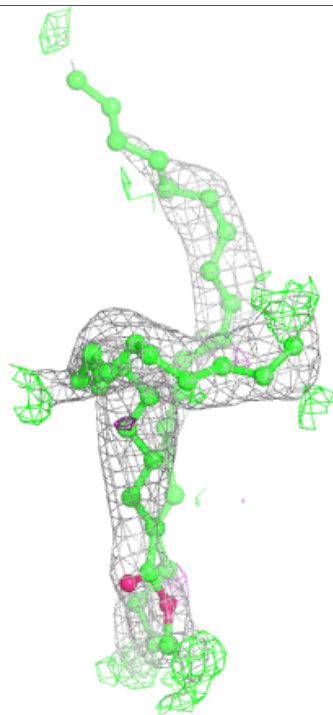
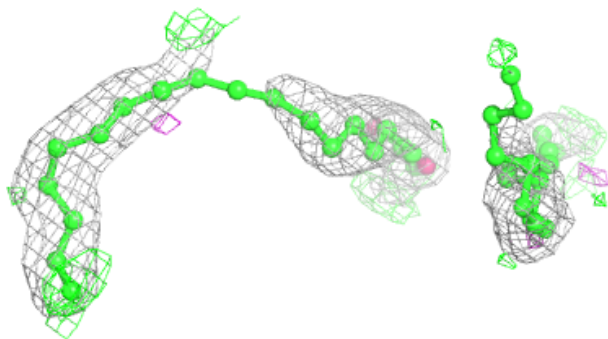
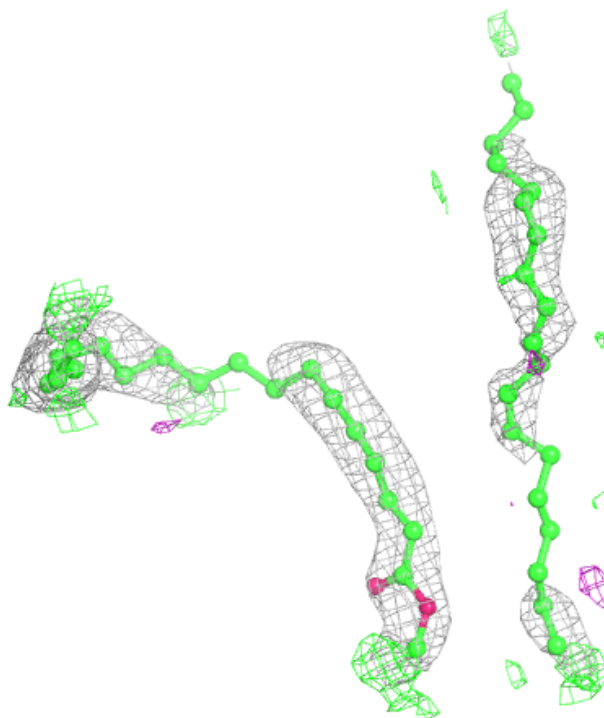
**Electron density around DMU X 102:**

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



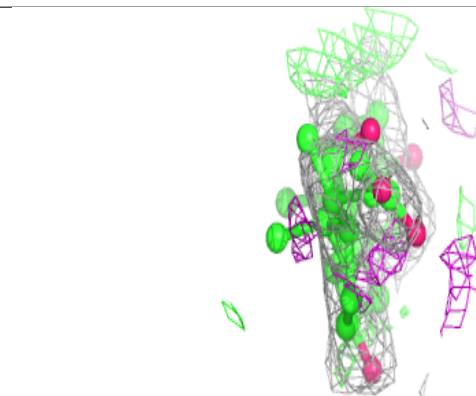
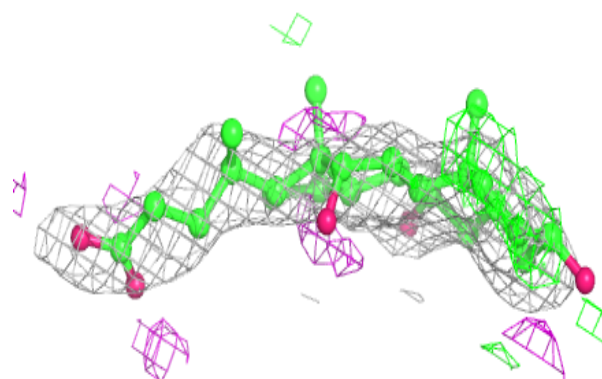
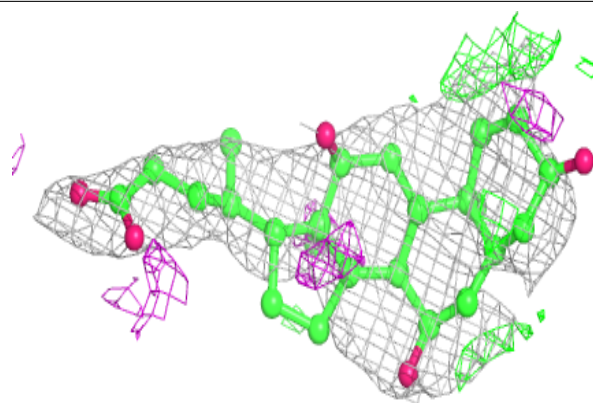
Electron density around PEK P 305:

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

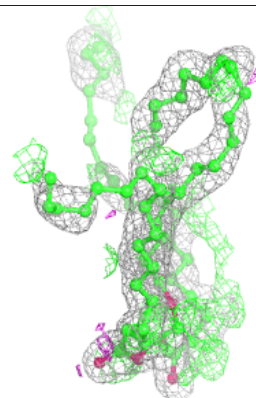
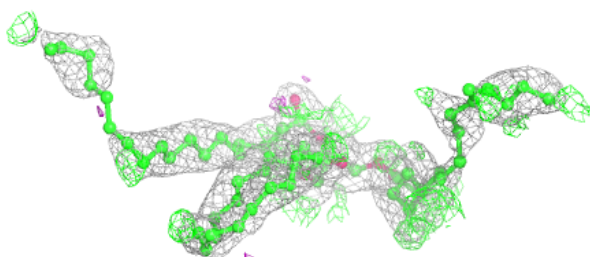
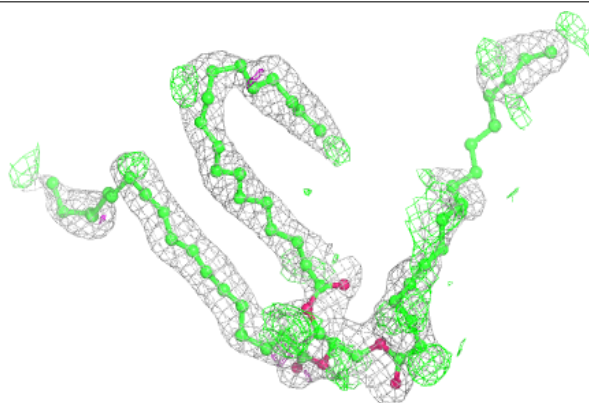


Electron density around CHD L 102:

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

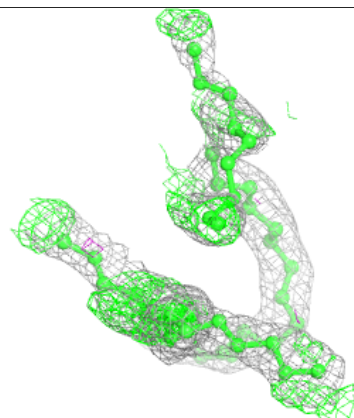
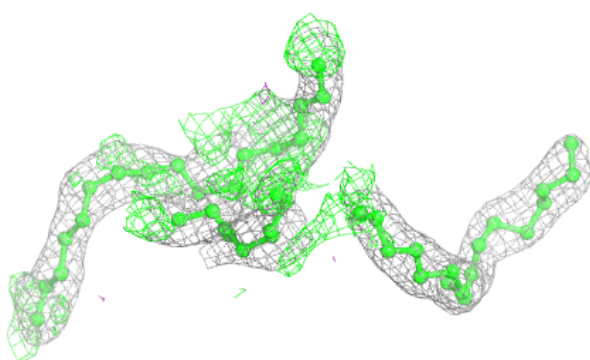
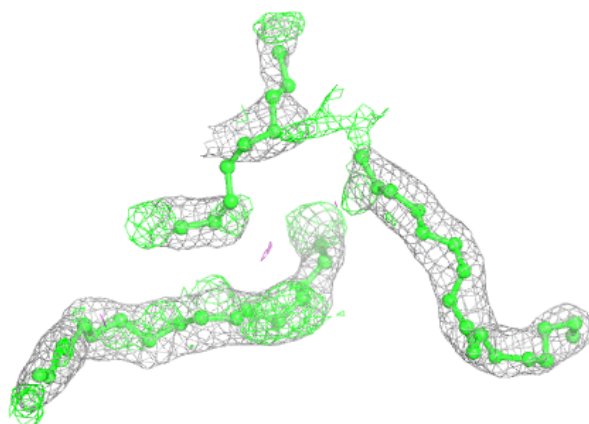
**Electron density around TGL D 201:**

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

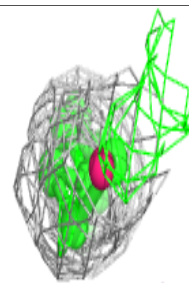
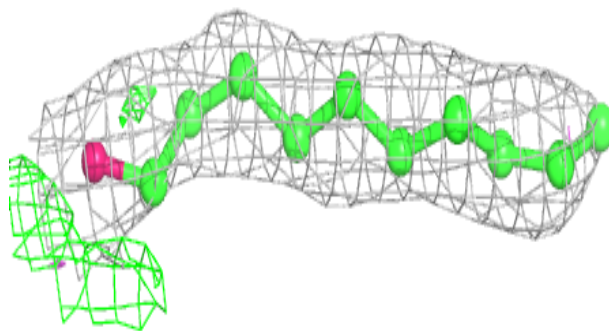
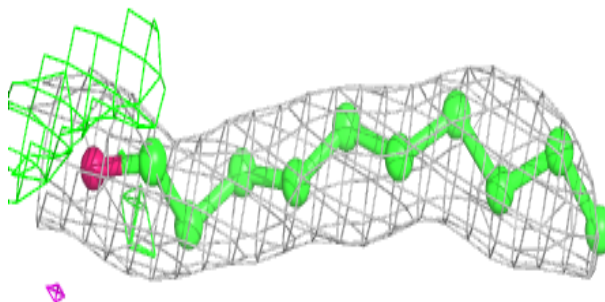


Electron density around TGL N 607:

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

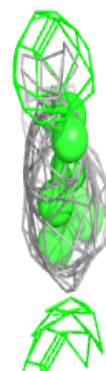
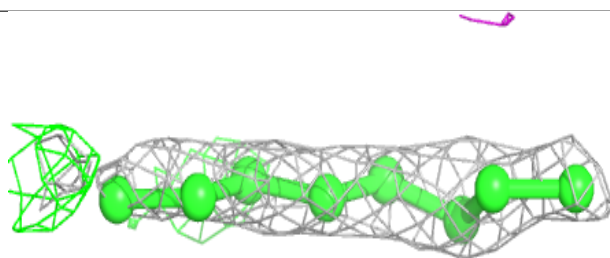
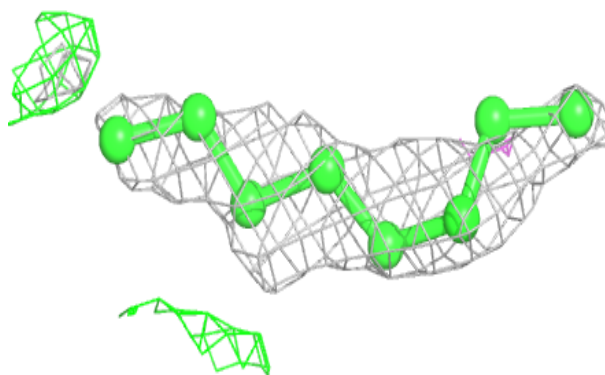
**Electron density around DMU W 103:**

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

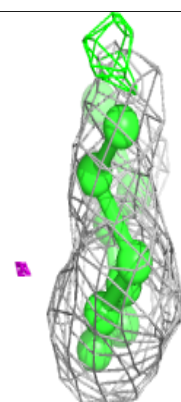
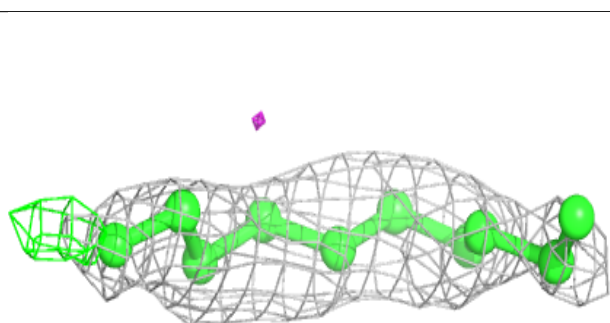
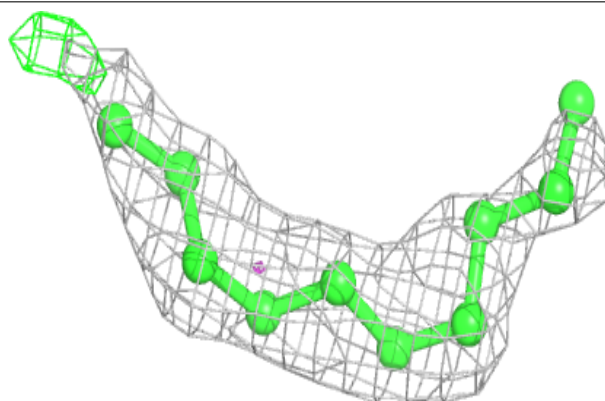


Electron density around DMU D 207:

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

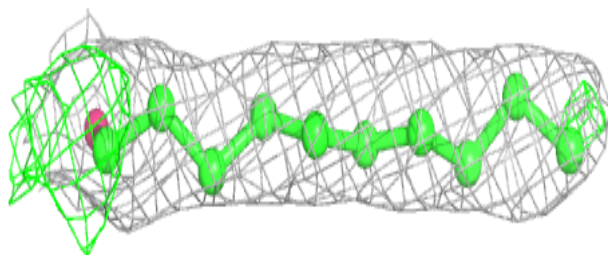
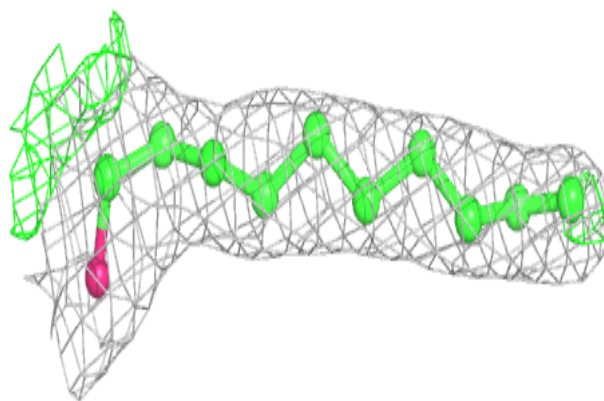
**Electron density around DMU K 104:**

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

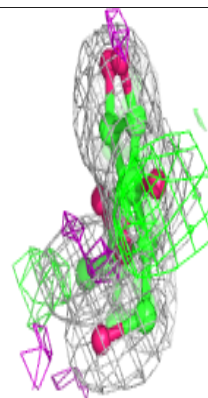
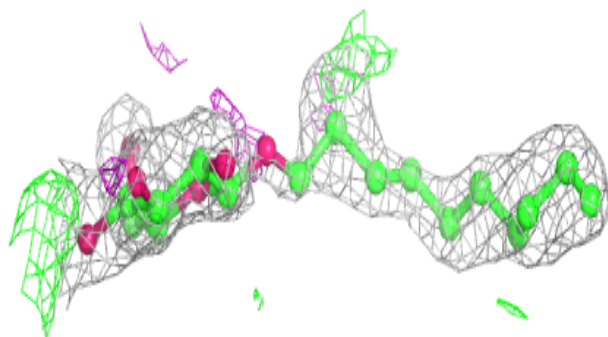
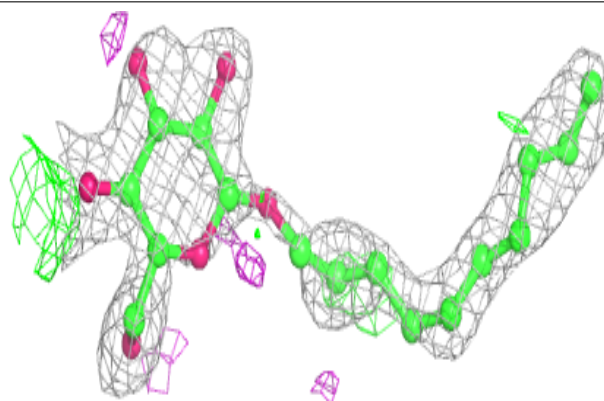


Electron density around DMU O 305:

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

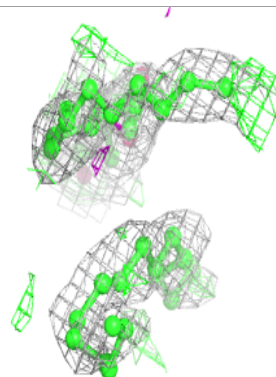
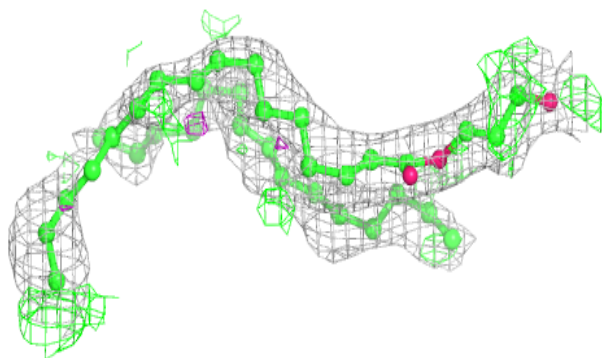
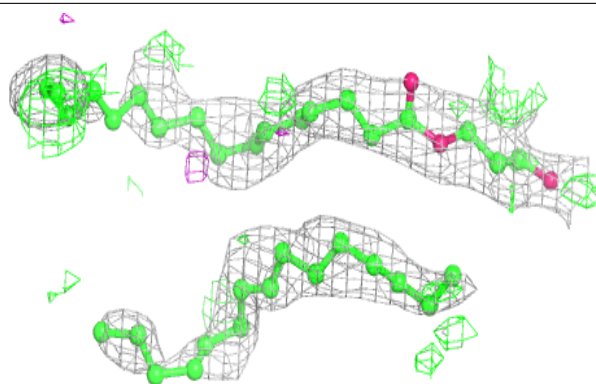
**Electron density around DMU C 310:**

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

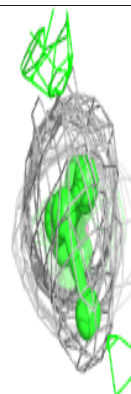
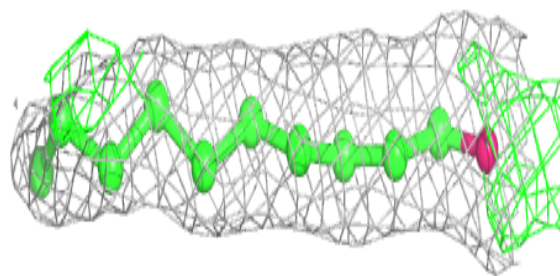
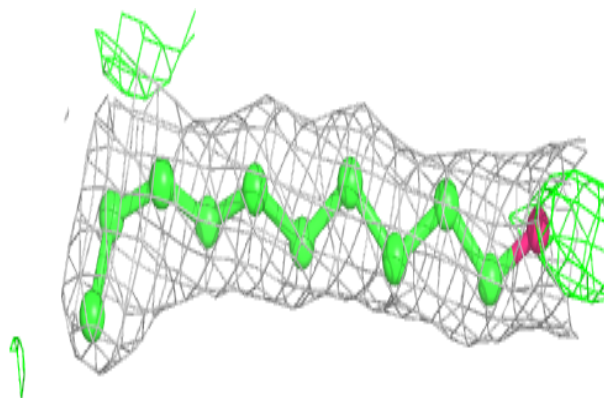


Electron density around PGV C 307:

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

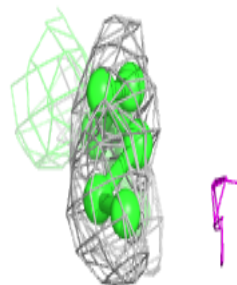
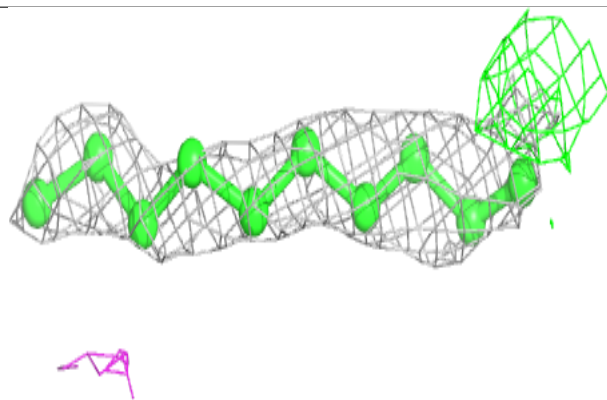
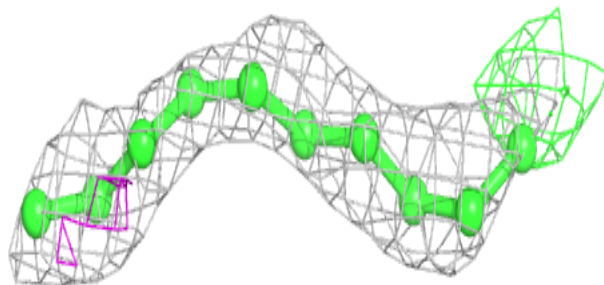
**Electron density around DMU P 318:**

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

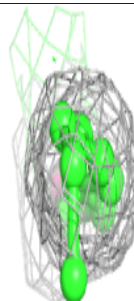
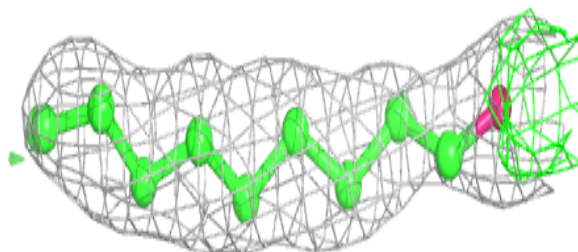
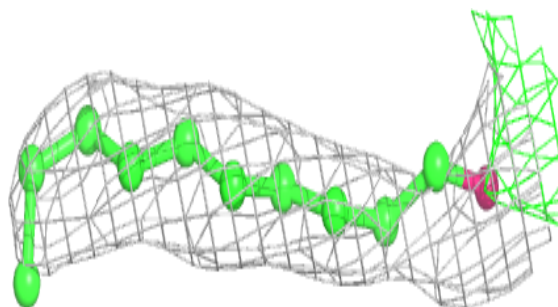


Electron density around DMU Q 202:

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

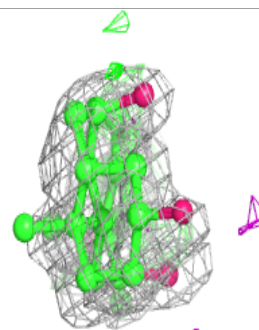
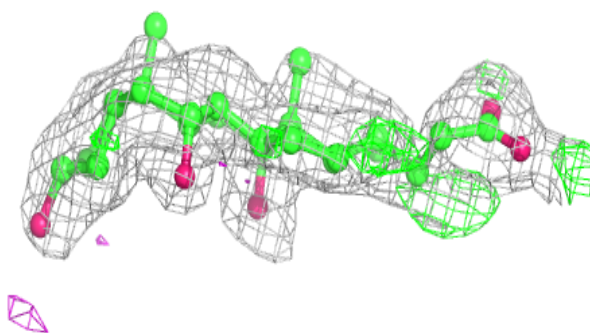
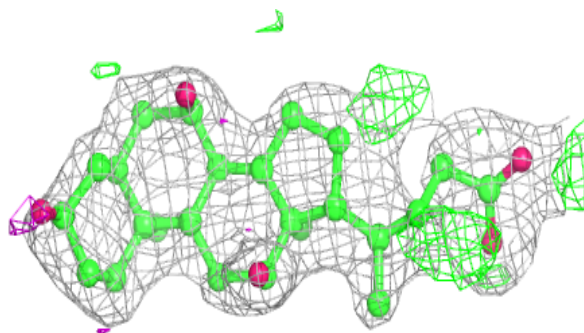
**Electron density around DMU J 103:**

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

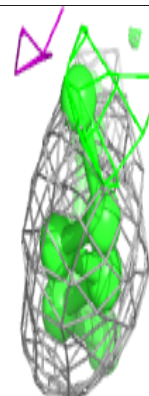
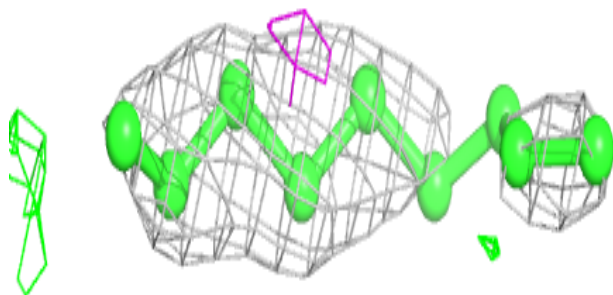
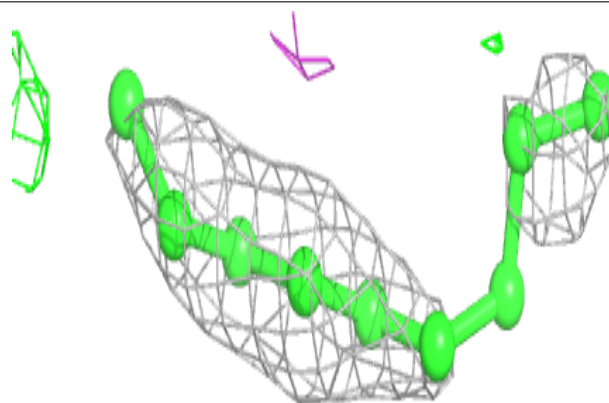


Electron density around CHD P 309:

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

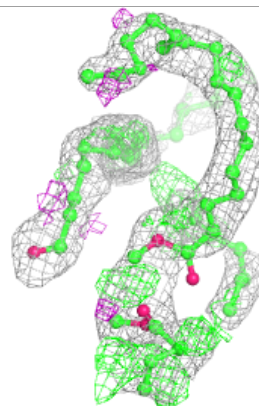
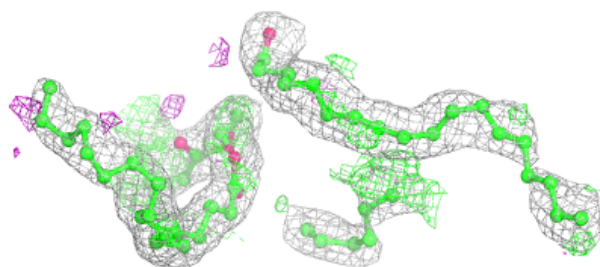
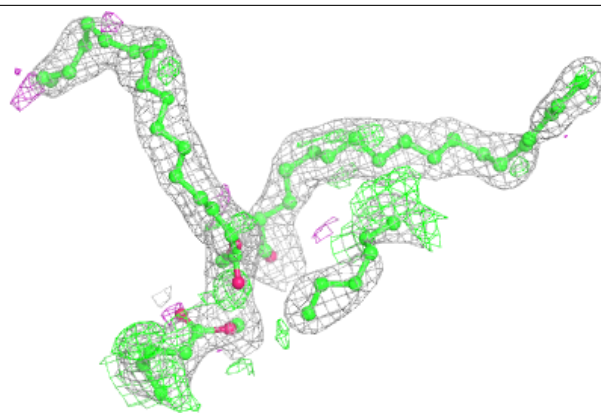
**Electron density around DMU K 102:**

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



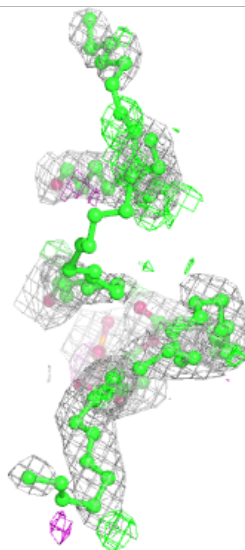
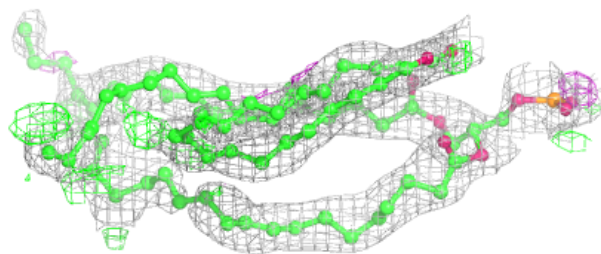
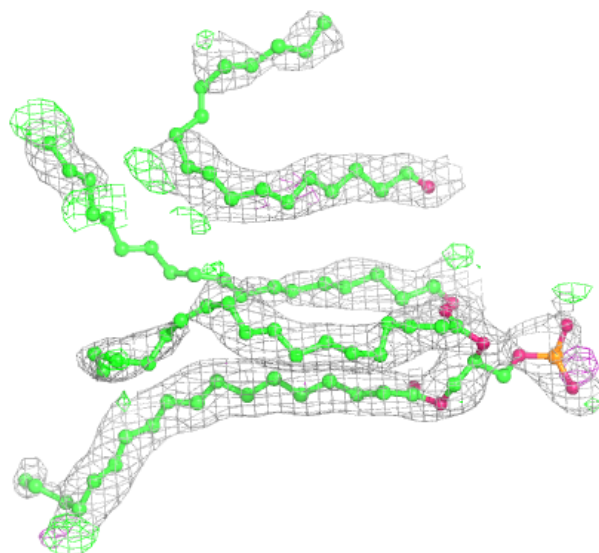
Electron density around TGL L 101:

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



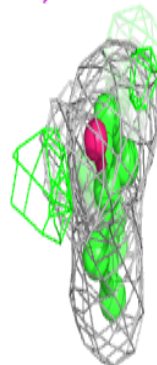
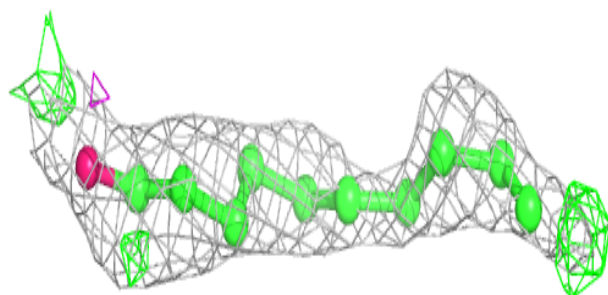
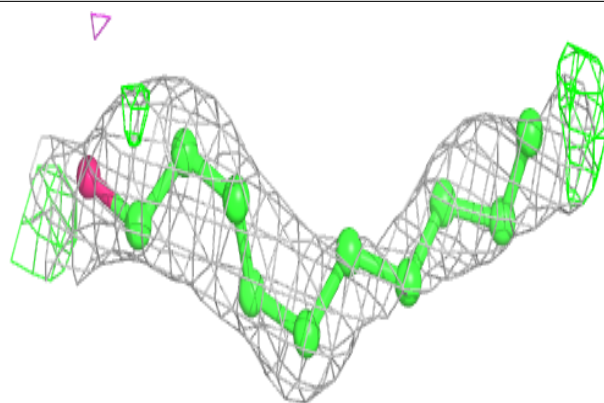
Electron density around CDL C 308:

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

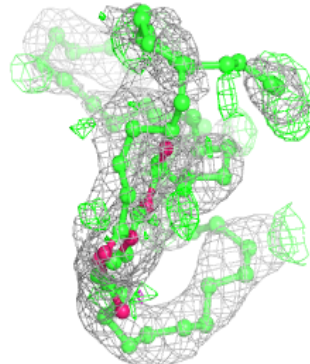
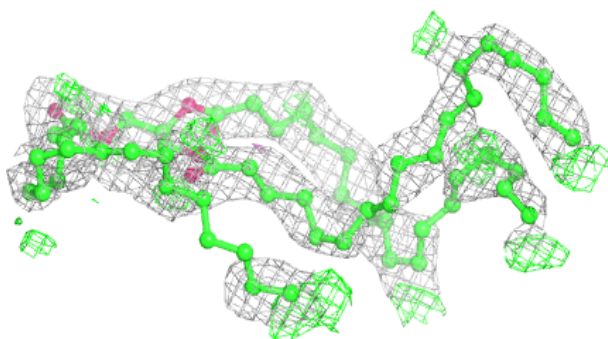
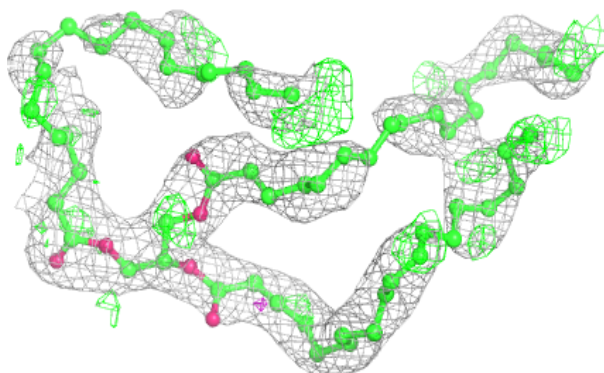


Electron density around DMU D 206:

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

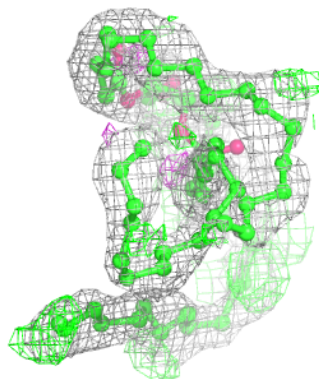
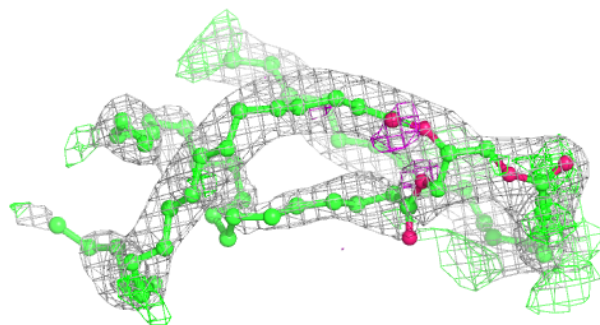
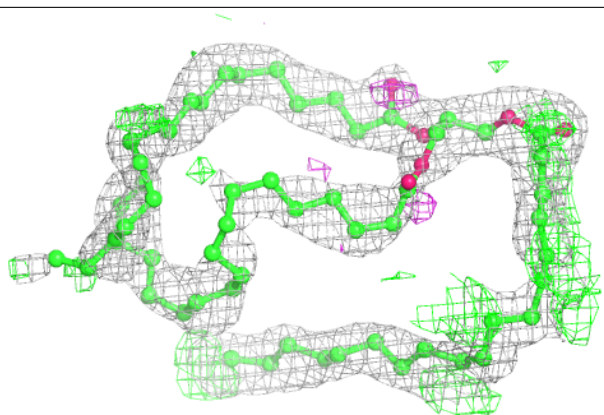
**Electron density around TGL N 606:**

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

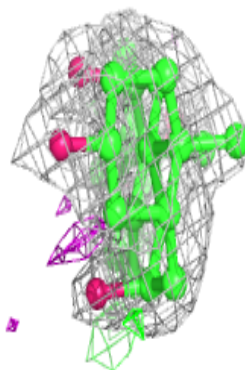
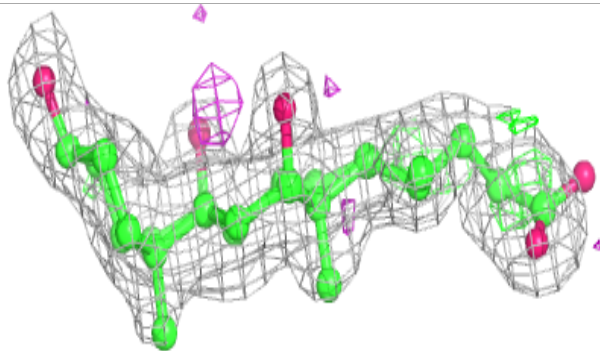
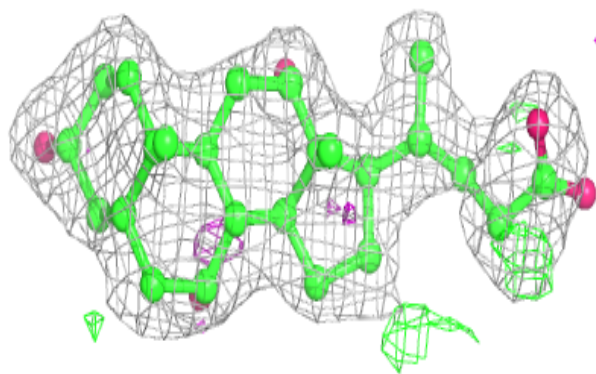


Electron density around TGL B 301:

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

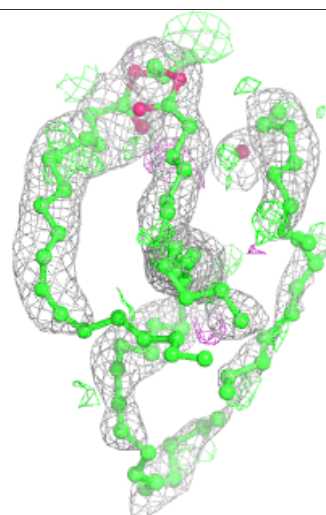
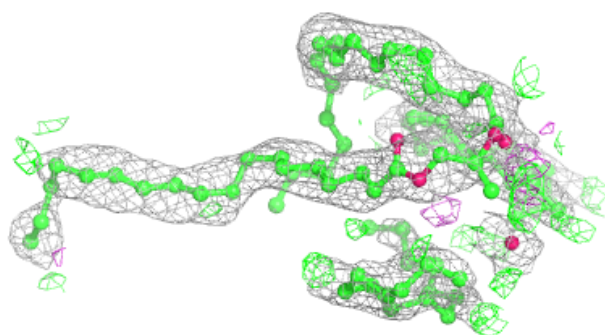
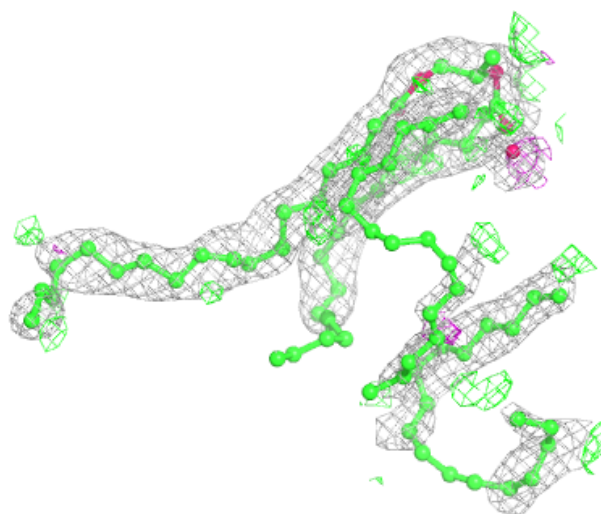
**Electron density around CHD C 309:**

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



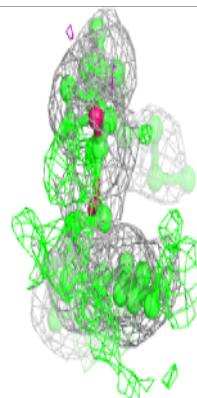
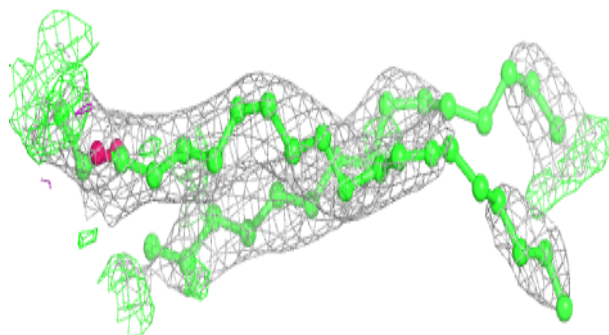
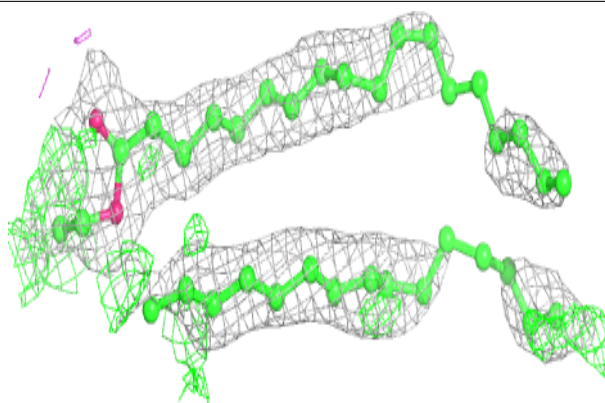
Electron density around CDL P 308:

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

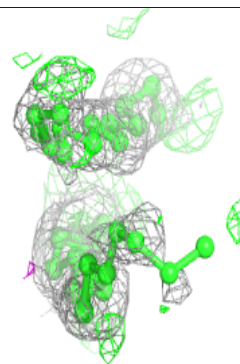
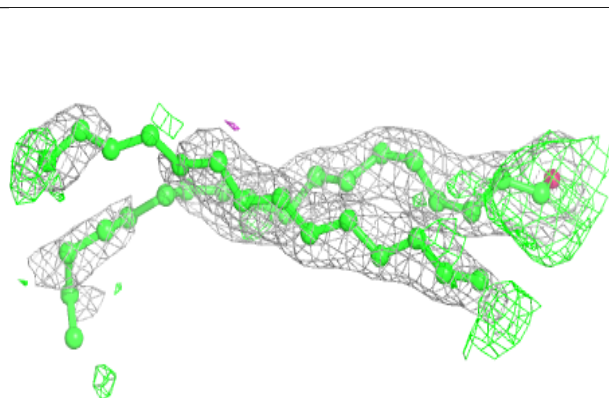
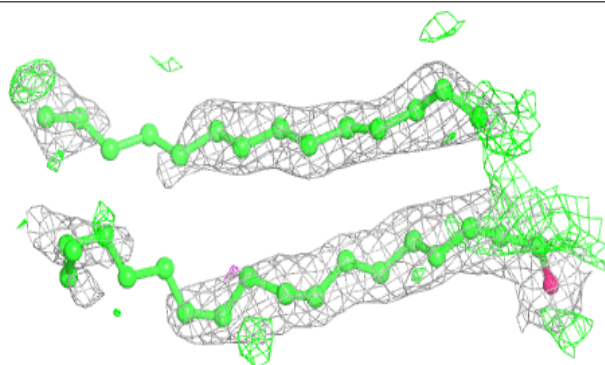


Electron density around PGV Q 201:

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

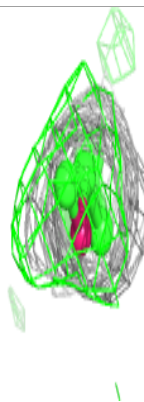
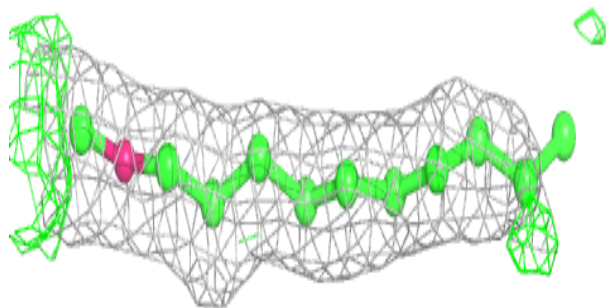
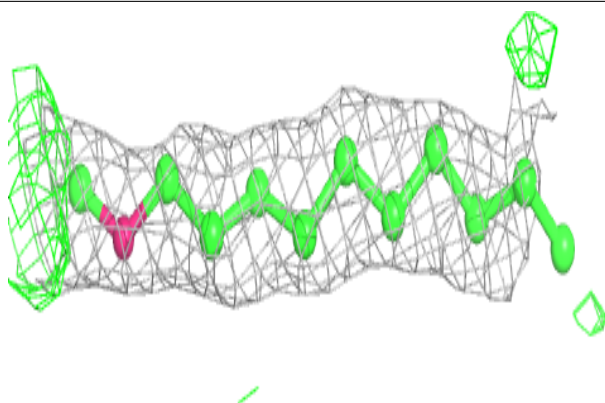
**Electron density around PGV A 606:**

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

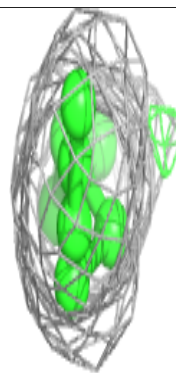
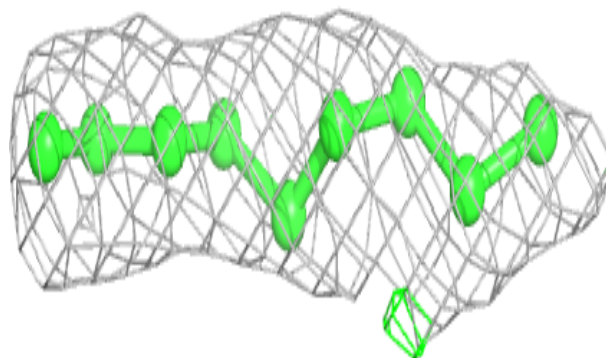
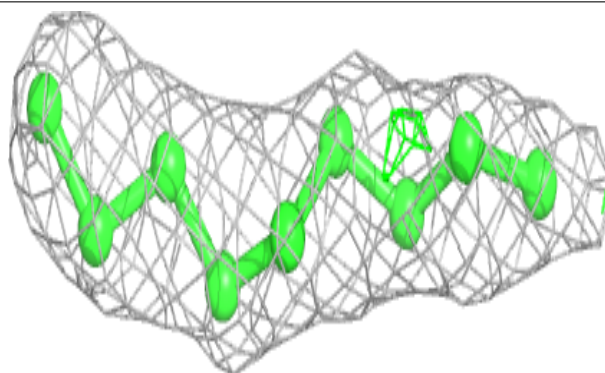


Electron density around DMU C 320:

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

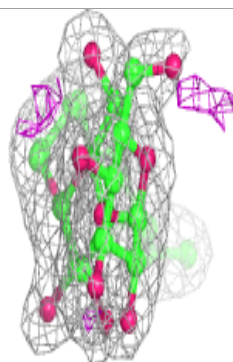
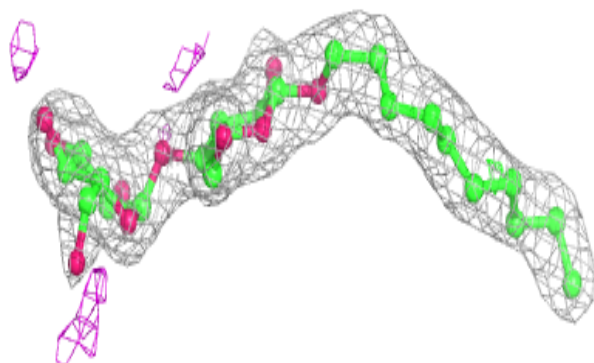
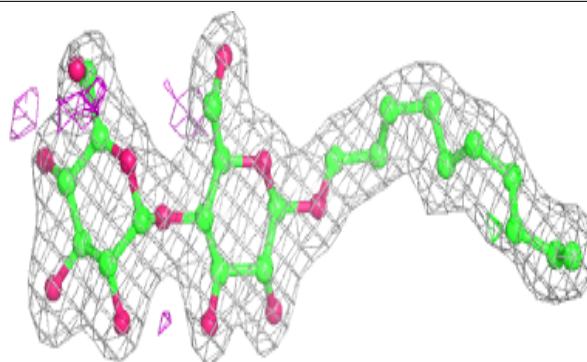
**Electron density around DMU N 622:**

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

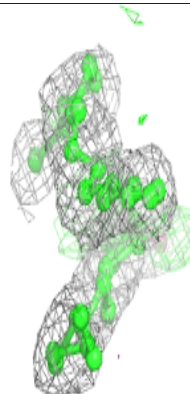
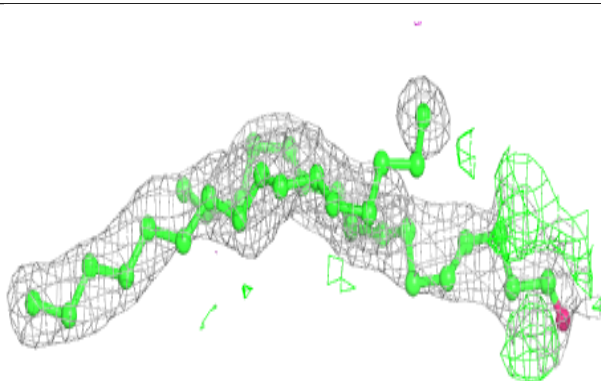
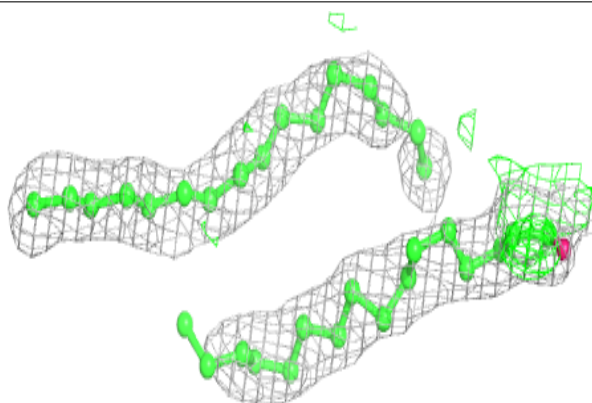


Electron density around DMU Z 101:

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

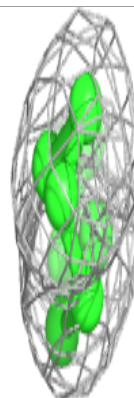
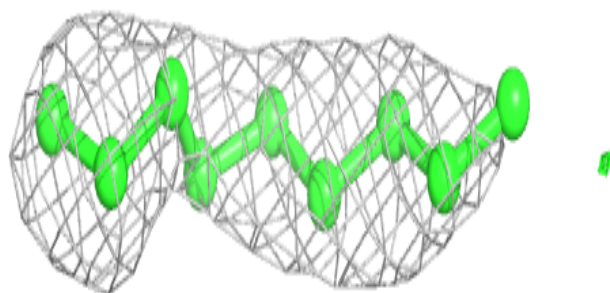
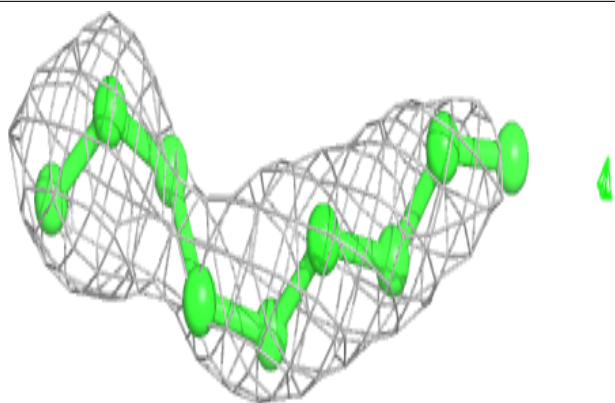
**Electron density around PSC O 302:**

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

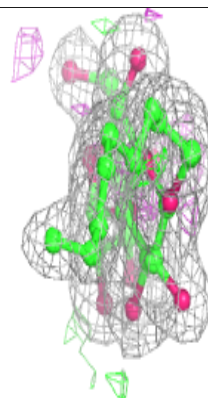
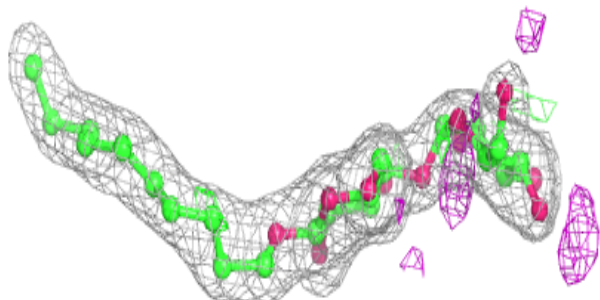
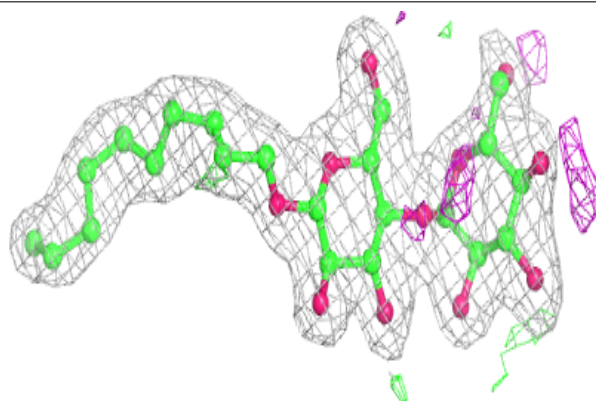


Electron density around DMU K 101:

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

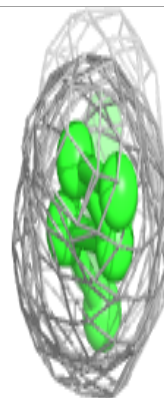
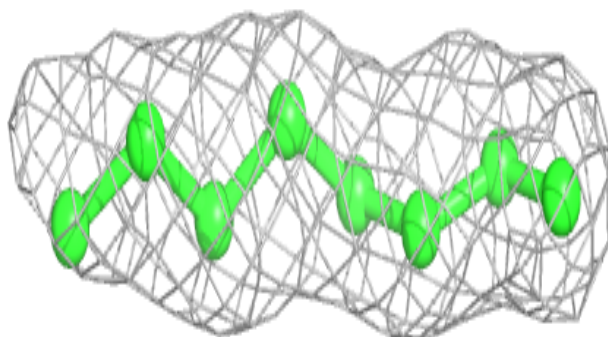
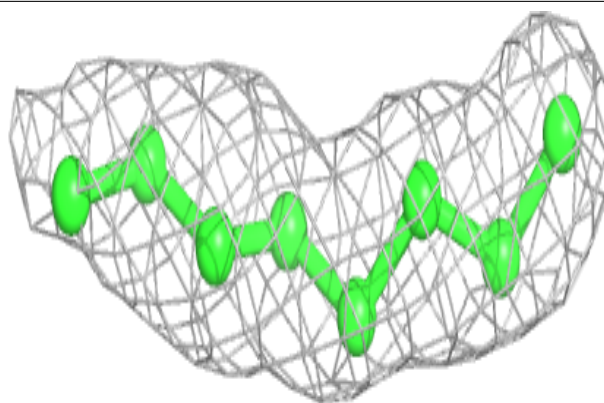
**Electron density around DMU M 101:**

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

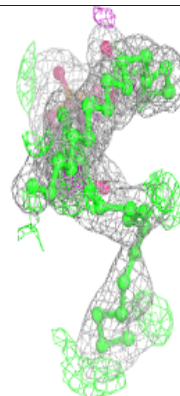
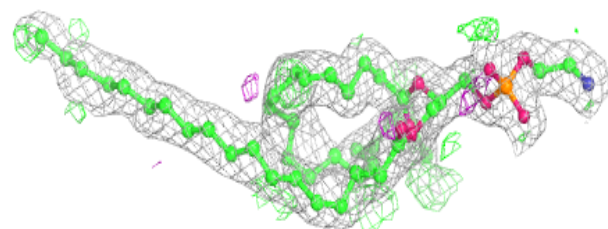
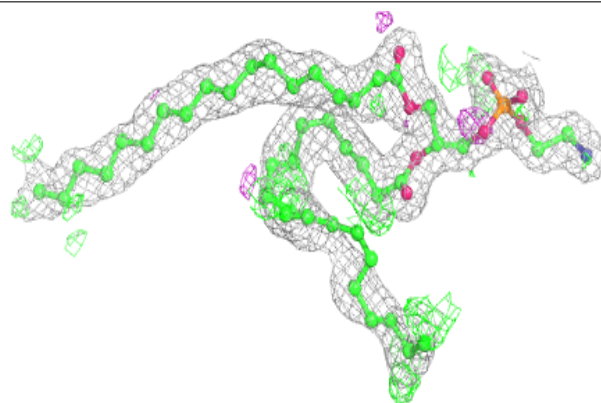


Electron density around DMU A 621:

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

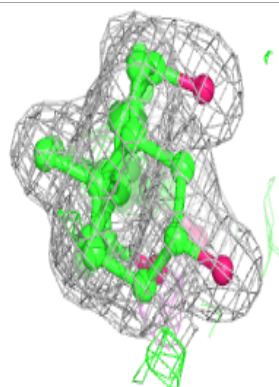
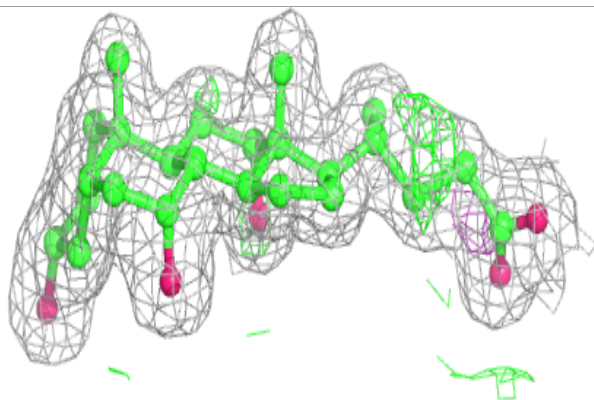
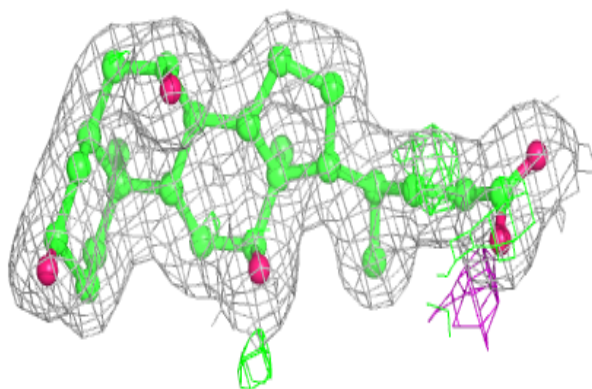
**Electron density around PEK P 304:**

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

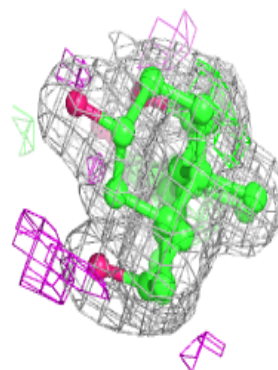
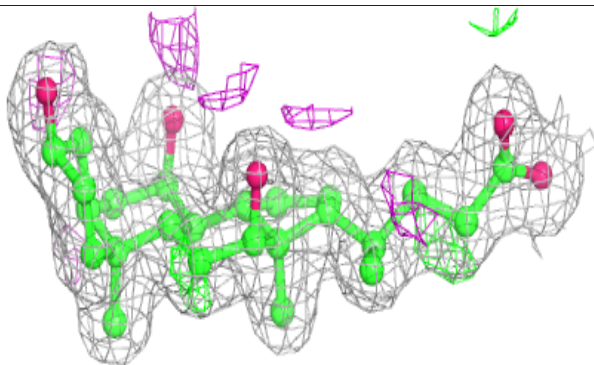
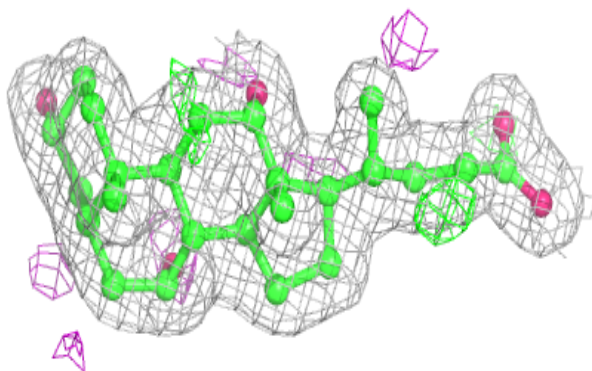


Electron density around CHD P 301:

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

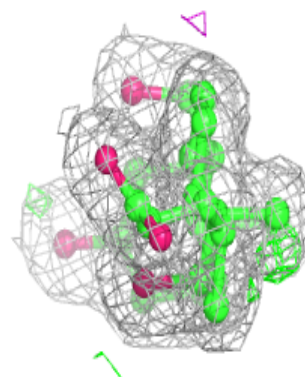
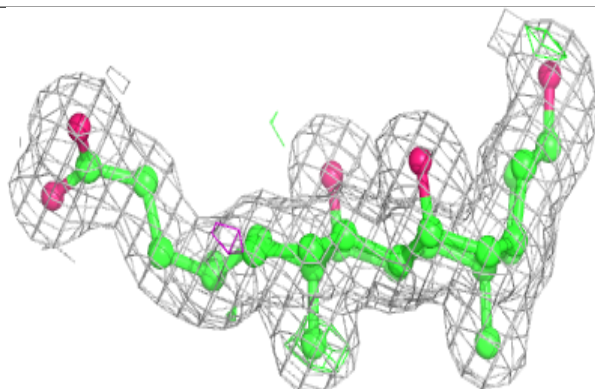
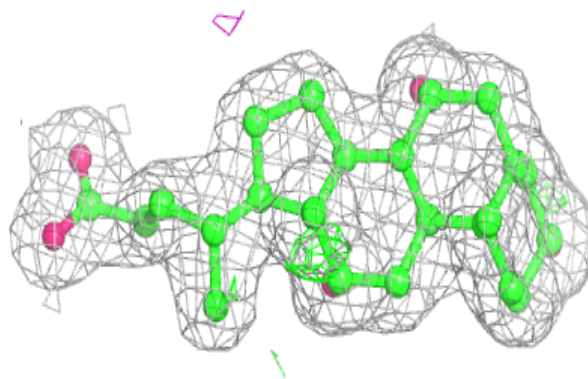
**Electron density around CHD C 301:**

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

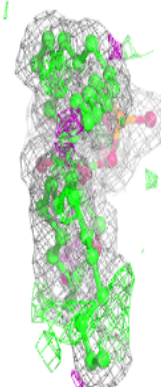
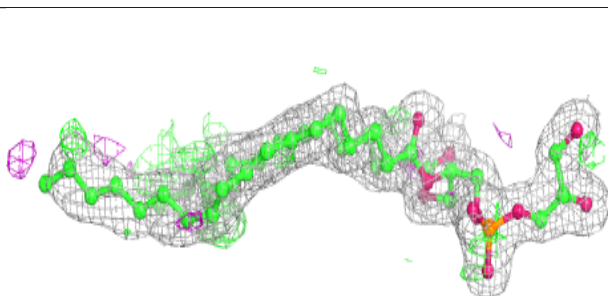
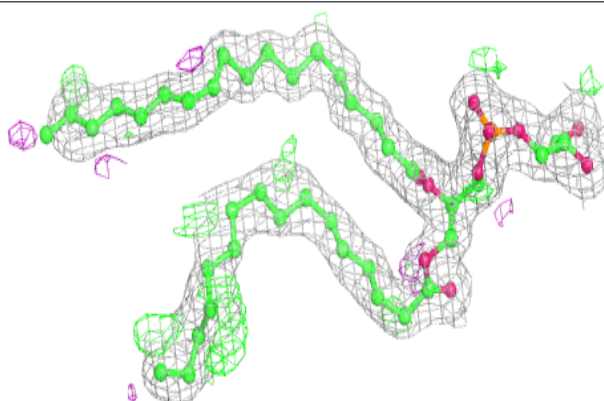


Electron density around CHD G 102:

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

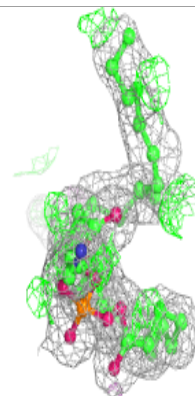
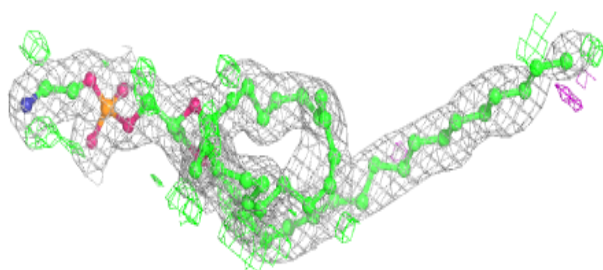
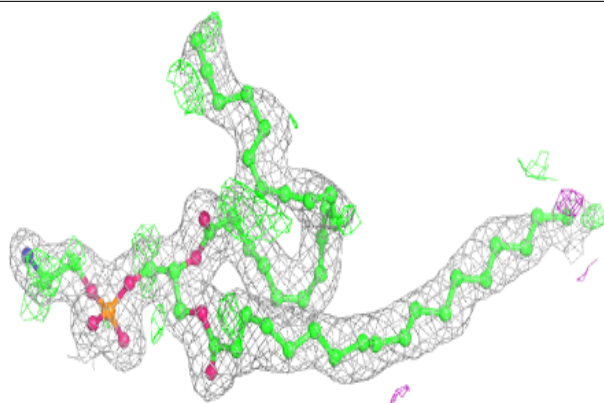
**Electron density around PGV N 610:**

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

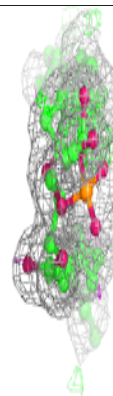
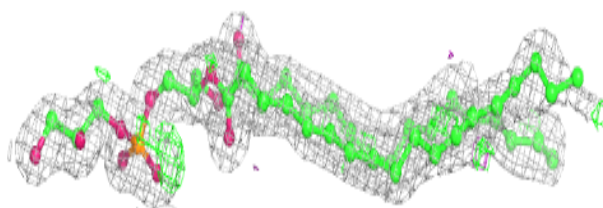
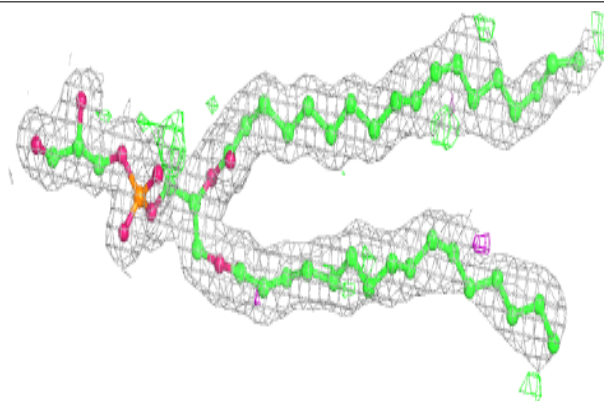


Electron density around PEK C 304:

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

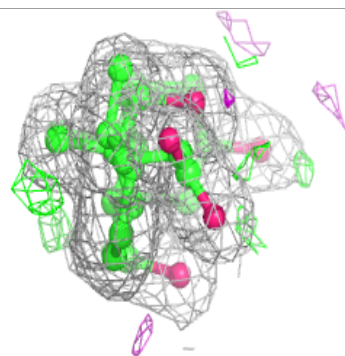
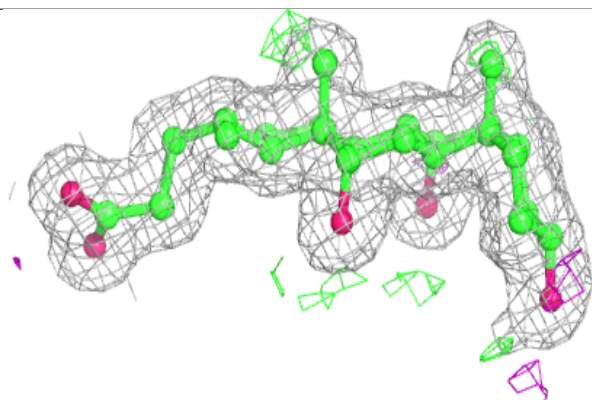
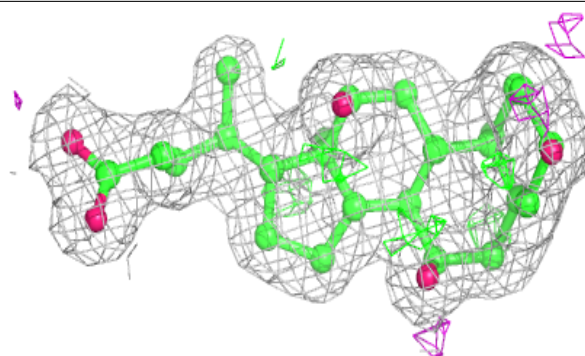
**Electron density around PGV C 306:**

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

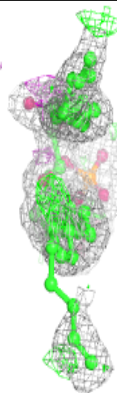
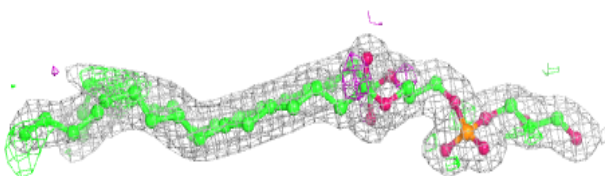
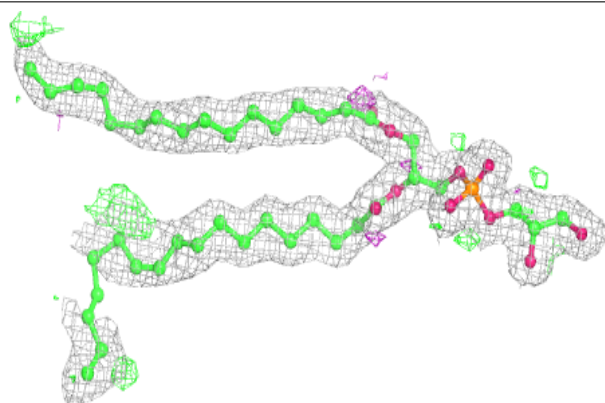


Electron density around CHD B 304:

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

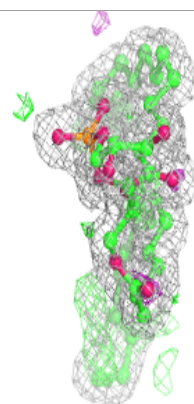
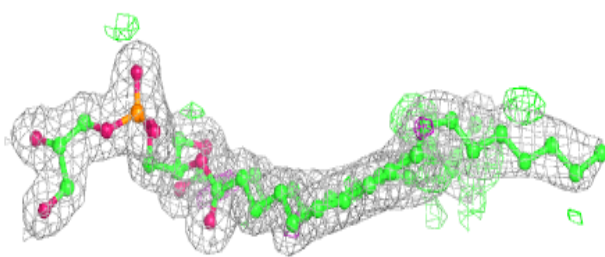
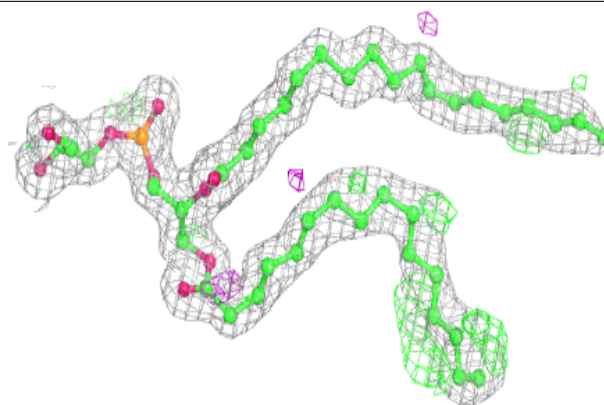
**Electron density around PGV P 306:**

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

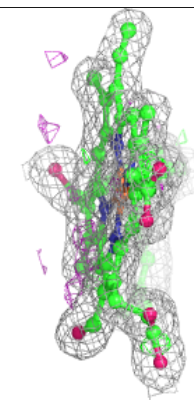
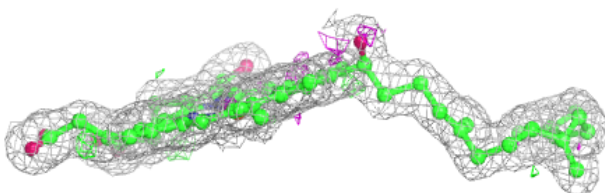
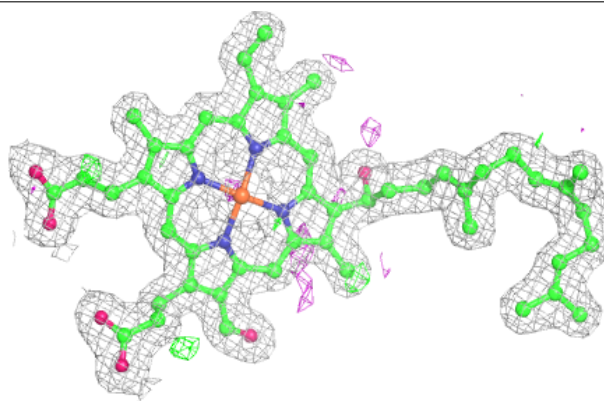


Electron density around PGV A 608:

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

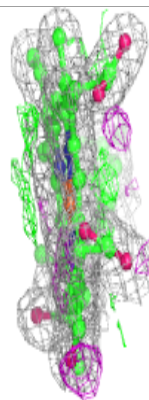
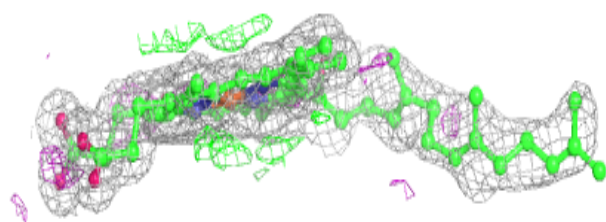
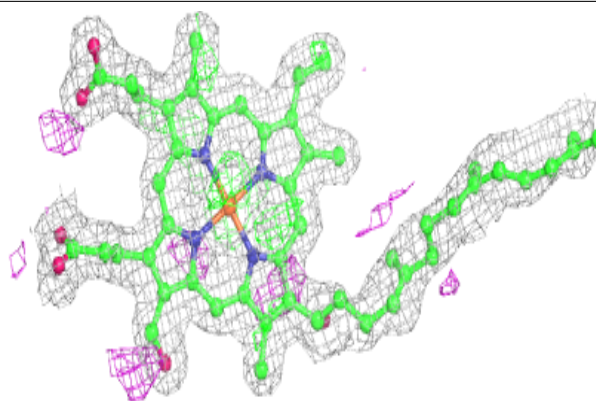
**Electron density around HEA A 602:**

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

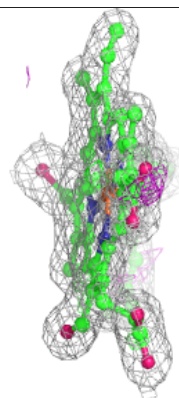
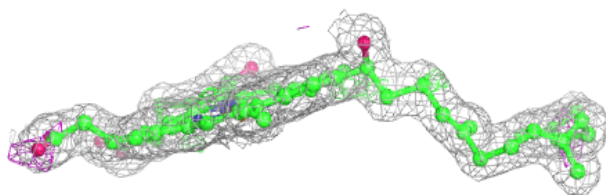
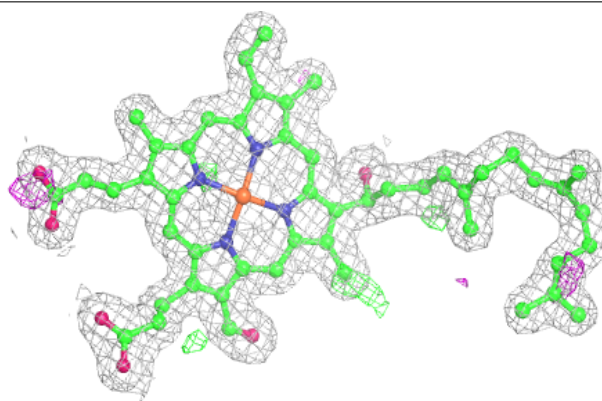


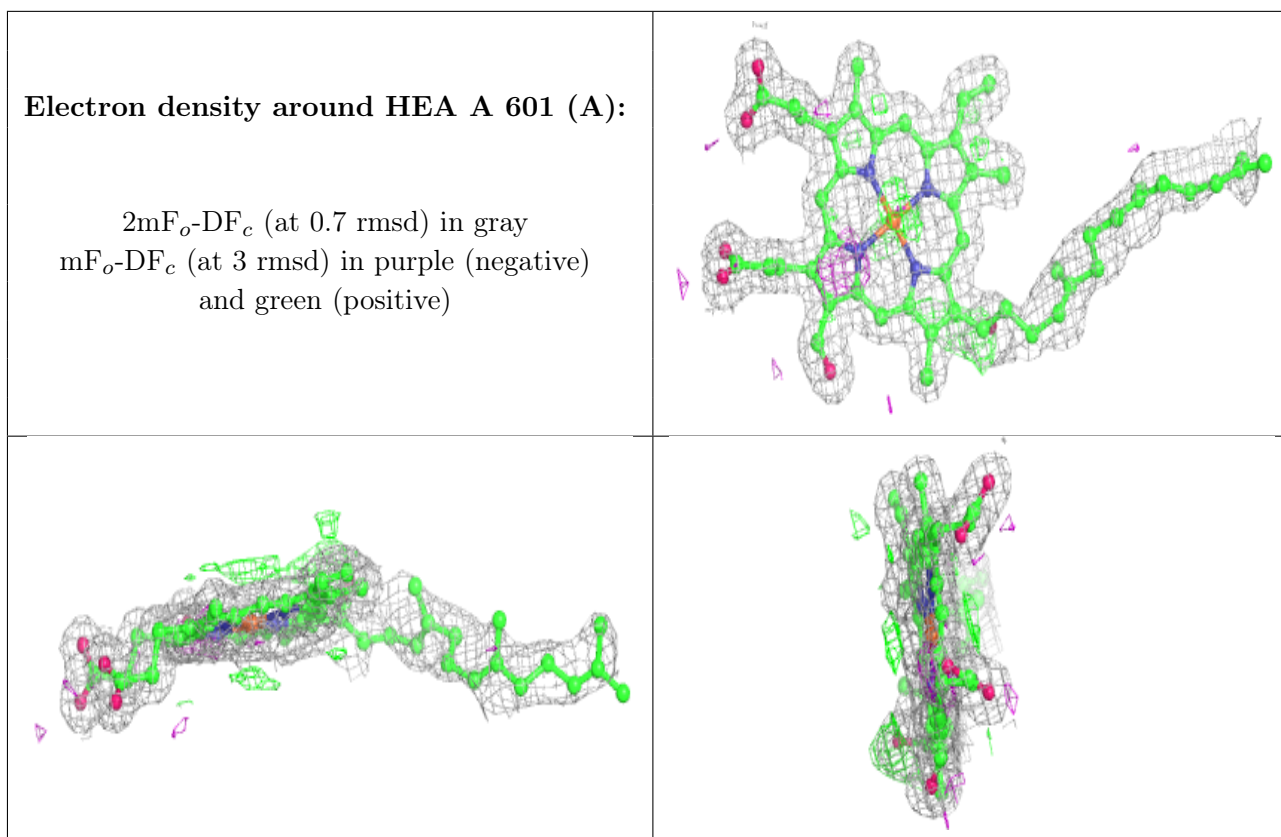
Electron density around HEA N 601 (A):

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

**Electron density around HEA N 602:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.