



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2021 – 11:00 AM JST

PDB ID : 7CP5
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate of E at 1.76 angstrom resolution
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2020-08-06
Resolution : 1.76 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

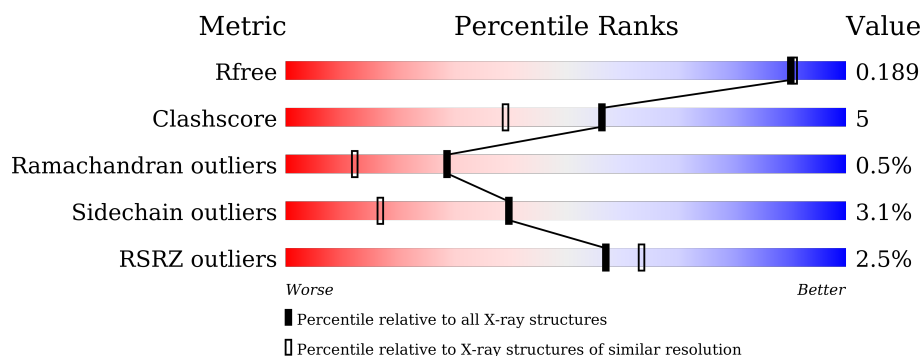
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	N	514	<div> <div>90%</div> <div>10%</div> </div>
2	B	227	<div> <div>83%</div> <div>16%</div> </div>
2	O	227	<div> <div>2%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
3	C	259	<div> <div>92%</div> <div>8%</div> </div>
3	P	259	<div> <div>%</div> <div>88%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	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	602[A]	X	-	-	-
14	HEA	N	602[B]	X	-	-	-
14	HEA	N	602[C]	X	-	-	-
14	HEA	N	603	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34258 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	31	0
			4190	2796	644	711	39			
1	N	514	Total	C	N	O	S	0	35	0
			4213	2816	642	713	42			

- 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	7	0
			1862	1214	281	347	20			
2	O	227	Total	C	N	O	S	0	11	0
			1882	1229	287	345	21			

- 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
			2167	1451	341	360	15			
3	P	259	Total	C	N	O	S	0	12	0
			2161	1448	341	357	15			

- 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	3	0
			1211	790	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1199	781	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	1	0
			860	549	147	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	5	0
			736	458	128	144	6			
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	4	0
			692	448	129	114	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	1	0
			667	420	122	120	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	1	0
			604	391	107	102	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	1	0
			464	299	78	84	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	3	0
			395	260	65	68	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

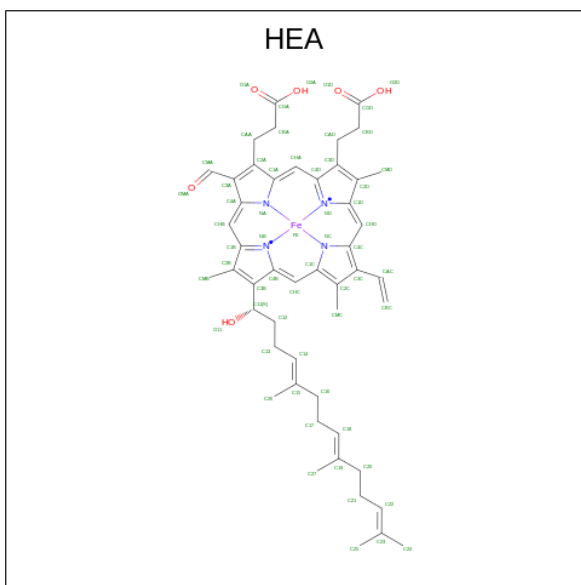
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			384	258	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
			335	223	53	59			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 78	C 66	Fe 1	N 4	O 7	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 78	C 66	Fe 1	N 4	O 7	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

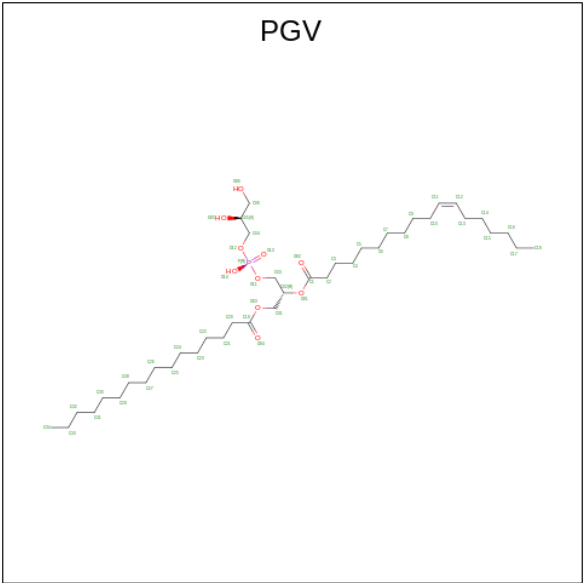
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	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).



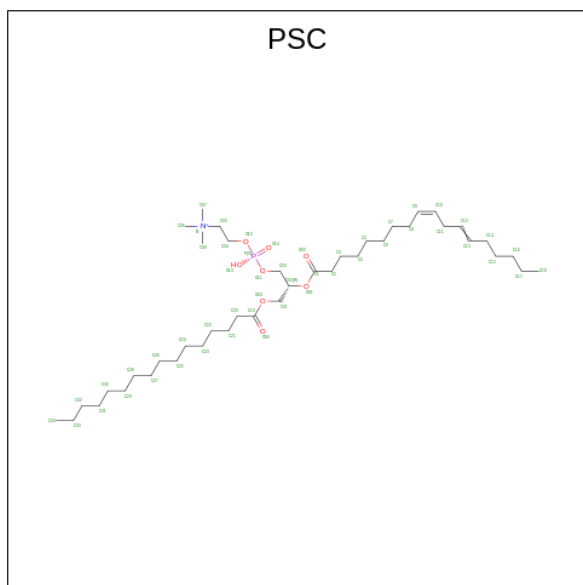
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O		0	0
			22	21	1			
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			48	37	10	1		
18	C	1	Total	C	O		0	0
			28	26	2			
18	G	1	Total	C	O		0	0
			32	30	2			
18	N	1	Total	C			0	0
			24	24				
18	N	1	Total	C	O	P	0	0
			51	40	10	1		

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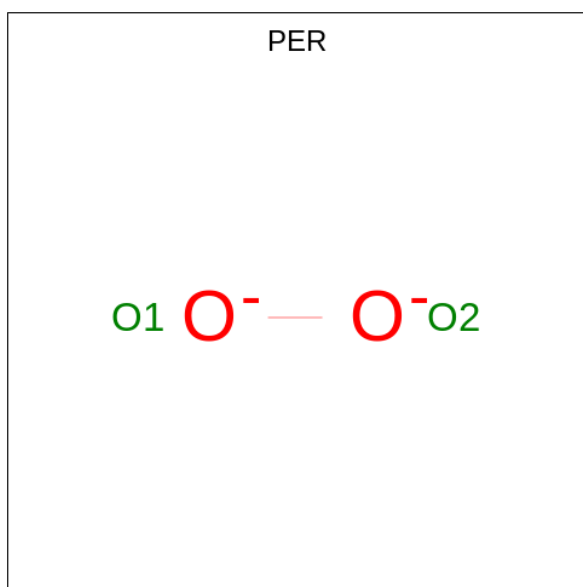
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



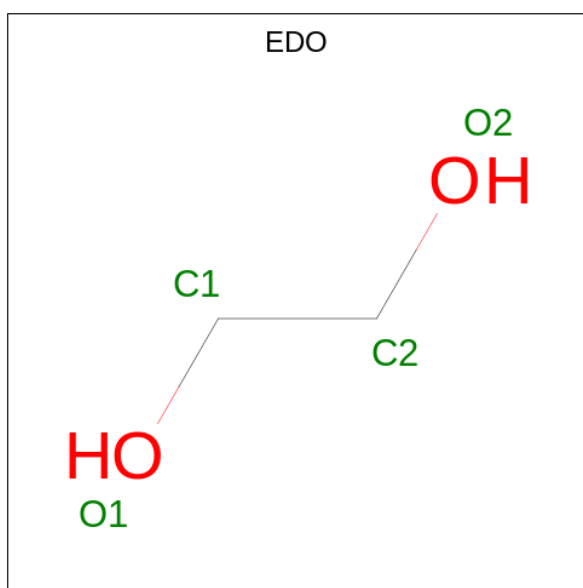
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C	0	0
			27	27		
19	O	1	Total	C	O	0
			30	28	2	

- Molecule 20 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

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



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

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

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

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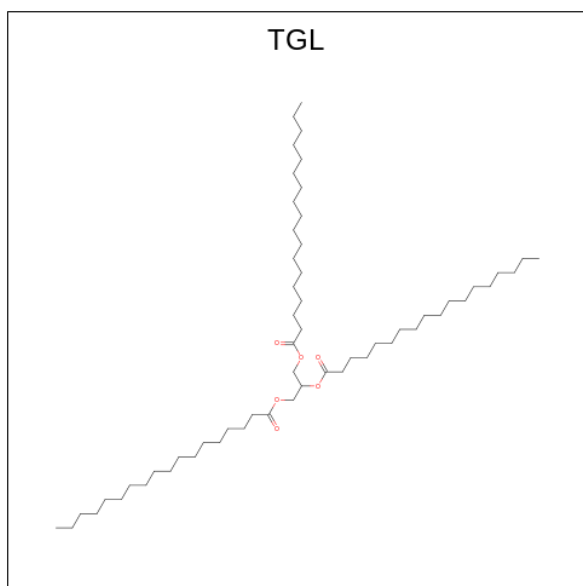
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4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

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

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



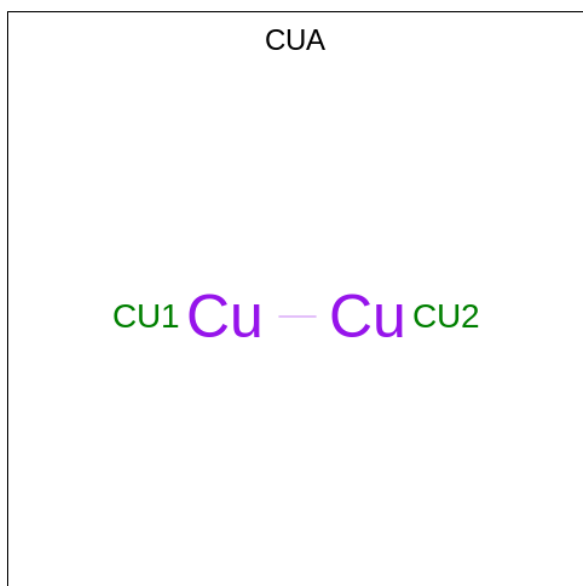
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			49	43	6		
22	D	1	Total	C	O	0	0
			57	51	6		
22	L	1	Total	C	O	0	0
			56	52	4		
22	N	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C		0	0
			48	48			

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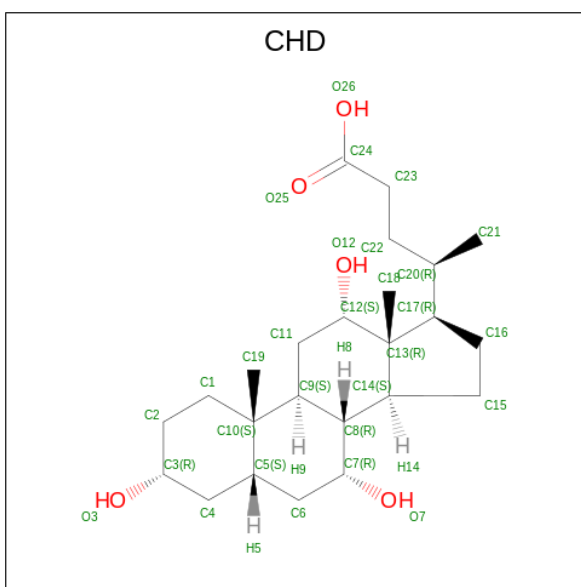
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total	C	O	0	0
			44	39	5		

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



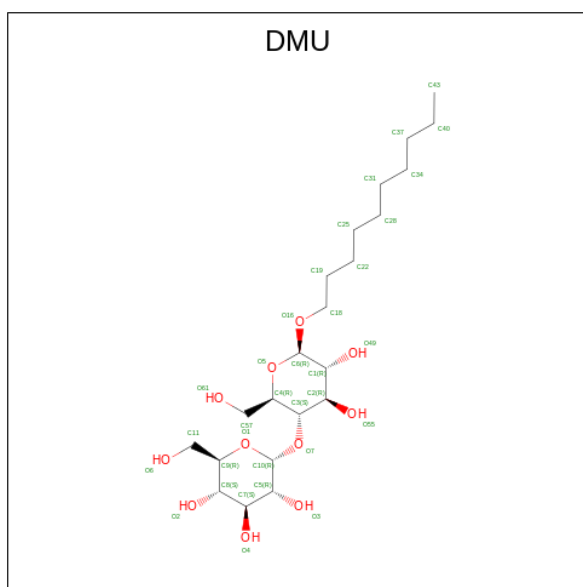
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

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



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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



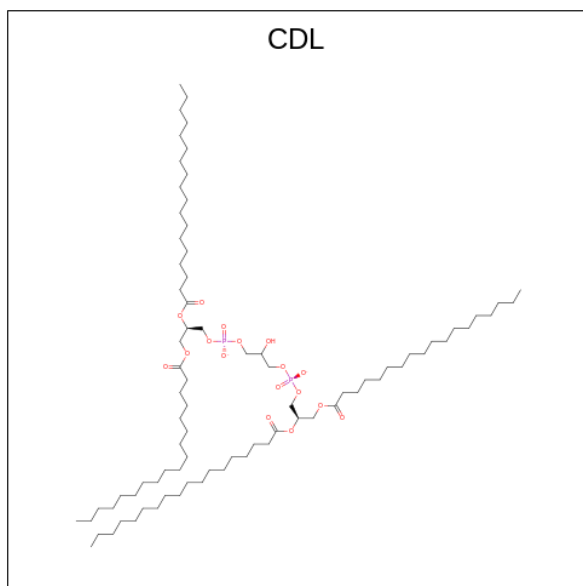
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total 13	C 11	O 2	0	0
25	C	1	Total 21	C 16	O 5	0	0
25	D	1	Total 11	C 10	O 1	0	0
25	D	1	Total 11	C 10	O 1	0	0
25	J	1	Total 11	C 10	O 1	0	0
25	K	1	Total 9	C 9		0	0
25	K	1	Total 10	C 10		0	0
25	K	1	Total 11	C 10	O 1	0	0
25	K	1	Total 9	C 9		0	0
25	K	1	Total 9	C 9		0	0
25	K	1	Total 10	C 10		0	0
25	L	1	Total 21	C 16	O 5	0	0
25	M	1	Total 33	C 22	O 11	0	0
25	O	1	Total 11	C 10	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	P	1	Total C O 13 11 2	0	0
25	P	1	Total C O 11 10 1	0	0
25	Q	1	Total C 10 10	0	0
25	W	1	Total C O 11 10 1	0	0
25	X	1	Total C O 11 10 1	0	0
25	X	1	Total C 10 10	0	0
25	X	1	Total C 9 9	0	0
25	X	1	Total C 10 10	0	0
25	Z	1	Total C O 33 22 11	0	0

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



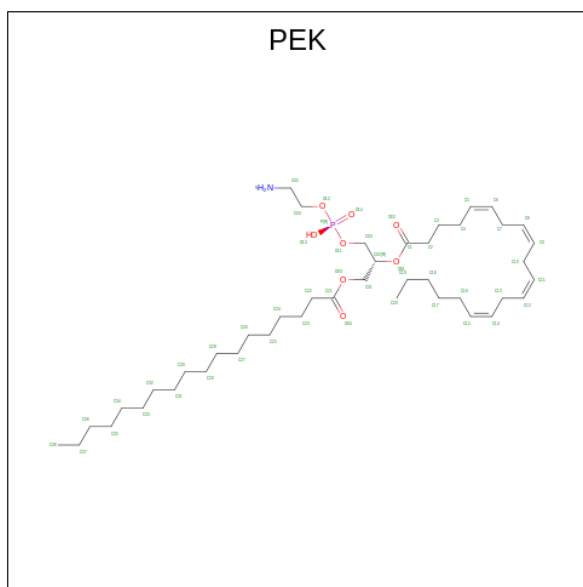
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O 58 56 2	0	0
26	N	1	Total C O 55 54 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	P	1	Total	C	O	0	0
			61	58	3		
26	T	1	Total	C	O	0	0
			57	54	3		

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

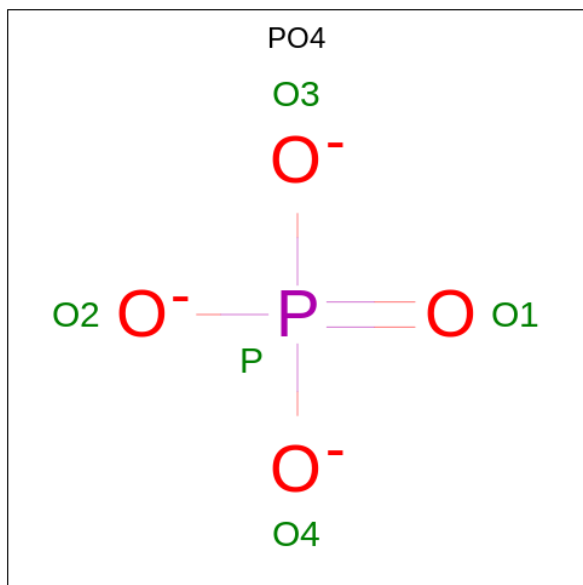


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C				0	0
			25	25					
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	C	1	Total	C				0	0
			36	36					
27	P	1	Total	C				0	0
			20	20					
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C				0	0
			34	34					

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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	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	273	Total	O	0	14
			273	273		
30	B	223	Total	O	0	2
			223	223		
30	C	142	Total	O	0	2
			142	142		
30	D	213	Total	O	0	0
			213	213		
30	E	160	Total	O	0	0
			160	160		
30	F	162	Total	O	0	3
			162	162		

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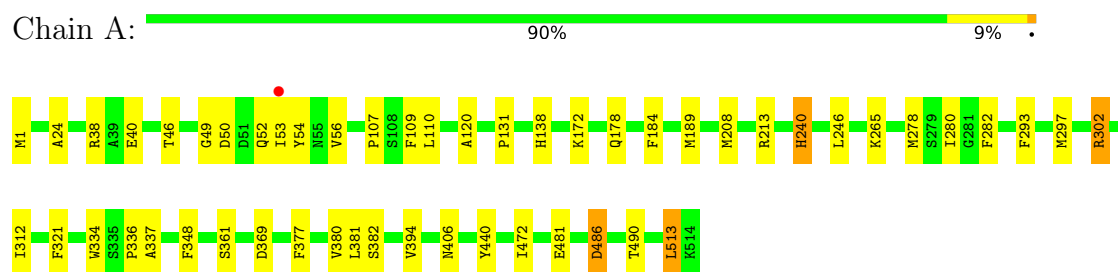
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	G	89	Total 89	O 89	0	0
30	H	94	Total 94	O 94	0	0
30	I	70	Total 70	O 70	0	0
30	J	58	Total 58	O 58	0	0
30	K	44	Total 44	O 44	0	0
30	L	38	Total 38	O 38	0	1
30	M	39	Total 39	O 39	0	0
30	N	273	Total 273	O 273	0	12
30	O	205	Total 205	O 205	0	2
30	P	147	Total 147	O 147	0	0
30	Q	114	Total 114	O 114	0	0
30	R	117	Total 117	O 117	0	0
30	S	141	Total 141	O 141	0	0
30	T	66	Total 66	O 66	0	0
30	U	94	Total 94	O 94	0	0
30	V	72	Total 72	O 72	0	0
30	W	43	Total 43	O 43	0	0
30	X	31	Total 31	O 31	0	0
30	Y	31	Total 31	O 31	0	0
30	Z	29	Total 29	O 29	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

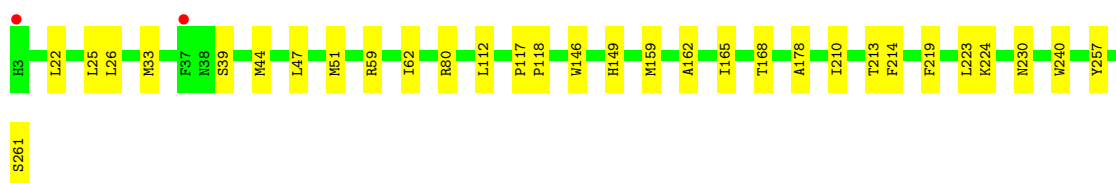
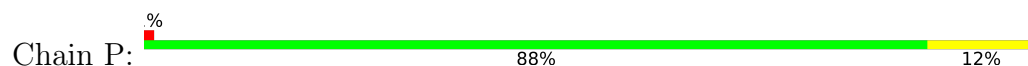




- Molecule 3: Cytochrome c oxidase subunit 3



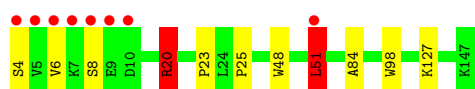
- Molecule 3: Cytochrome c oxidase subunit 3



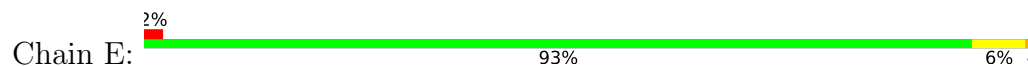
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



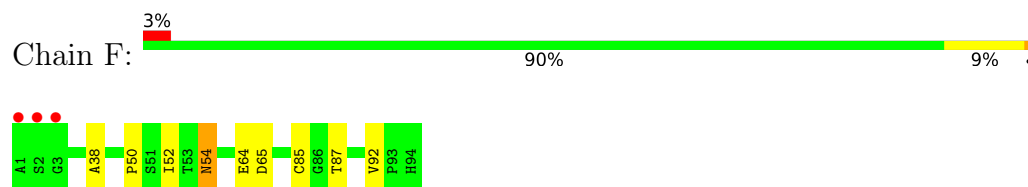
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



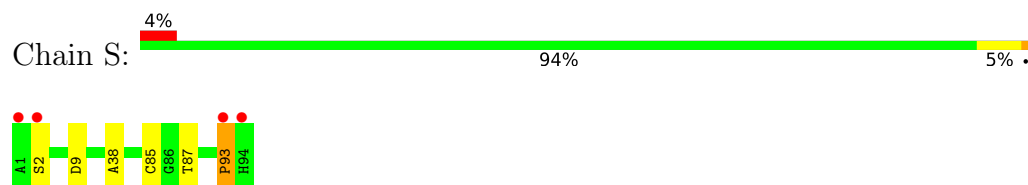
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



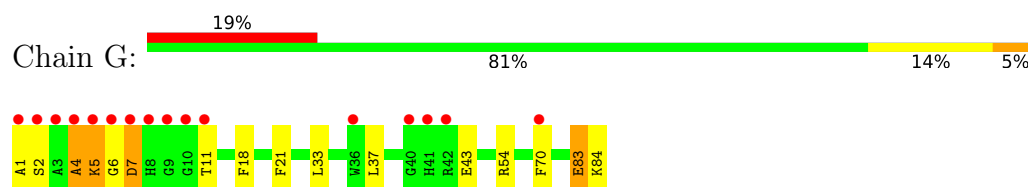
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



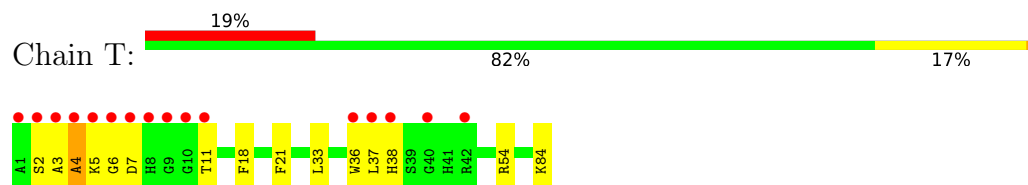
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



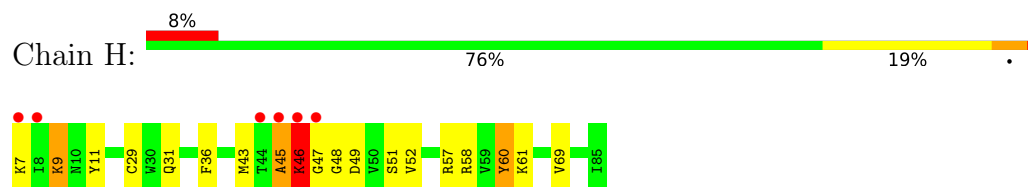
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



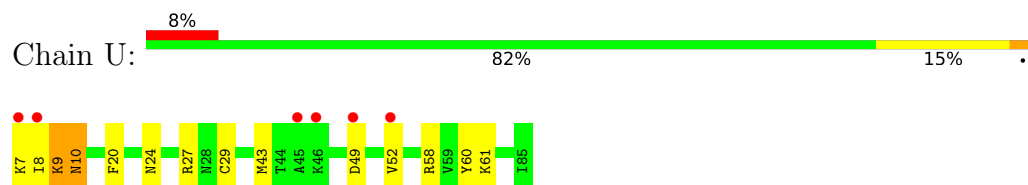
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



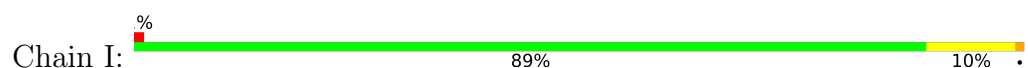
- Molecule 8: Cytochrome c oxidase subunit 6B1

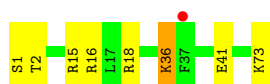


- Molecule 8: Cytochrome c oxidase subunit 6B1

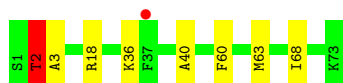
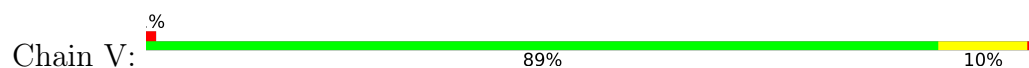


- Molecule 9: Cytochrome c oxidase subunit 6C

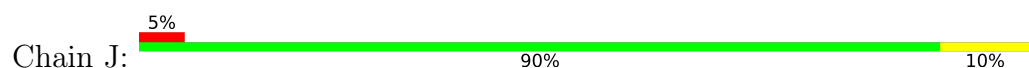




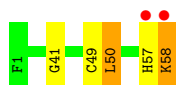
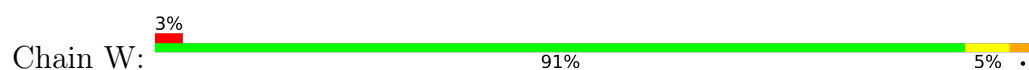
- Molecule 9: Cytochrome c oxidase subunit 6C



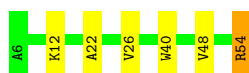
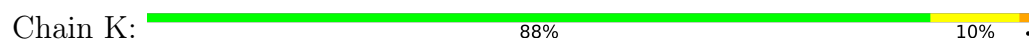
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



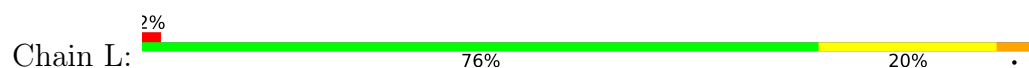
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



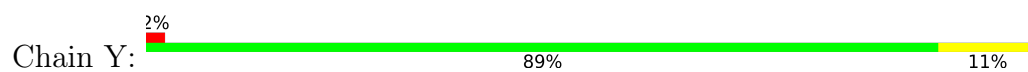
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



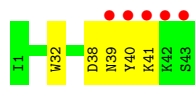
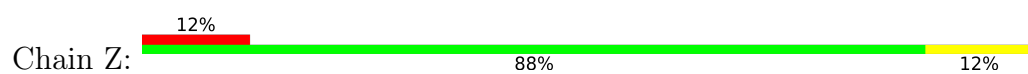
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.59Å 203.22Å 177.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.76 135.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-1.76) 99.8 (135.41-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.76Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.160 , 0.189 0.160 , 0.189	Depositor DCC
R_{free} test set	32242 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34258	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 3.95% 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: FME, PEK, MG, CDL, SAC, TGL, PGV, PO4, PER, DMU, CHD, HEA, ZN, CUA, NA, PSC, EDO, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	2/4411 (0.0%)	0.89	10/6016 (0.2%)
1	N	0.84	0/4434	0.84	5/6051 (0.1%)
2	B	0.84	3/1920 (0.2%)	0.94	3/2613 (0.1%)
2	O	0.75	1/1966 (0.1%)	0.83	2/2675 (0.1%)
3	C	0.84	2/2296 (0.1%)	0.74	0/3136
3	P	0.77	0/2295	0.73	0/3134
4	D	0.82	0/1259	0.81	2/1698 (0.1%)
4	Q	0.60	0/1236	0.68	3/1668 (0.2%)
5	E	0.80	0/871	0.78	2/1182 (0.2%)
5	R	0.64	0/882	0.73	1/1196 (0.1%)
6	F	0.75	0/771	0.76	0/1047
6	S	0.76	0/732	0.80	0/993
7	G	0.74	0/734	0.83	0/997
7	T	0.64	0/699	0.82	0/950
8	H	0.80	1/690 (0.1%)	0.80	1/932 (0.1%)
8	U	0.72	0/682	0.72	0/921
9	I	0.70	0/614	0.77	1/814 (0.1%)
9	V	0.57	0/605	0.71	0/802
10	J	0.61	0/478	0.63	0/644
10	W	0.55	0/472	0.69	0/636
11	K	0.72	0/420	0.68	0/576
11	X	0.63	0/399	0.62	0/546
12	L	0.84	0/401	0.77	0/537
12	Y	0.76	0/393	0.68	0/526
13	M	0.82	0/346	0.77	0/470
13	Z	0.61	0/345	0.69	0/470
All	All	0.79	9/30351 (0.0%)	0.80	30/41230 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	S	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246[A]	ASP	CB-CG	7.83	1.68	1.51
3	C	246[B]	ASP	CB-CG	7.83	1.68	1.51
2	O	193	TYR	CD2-CE2	6.95	1.49	1.39
1	A	278	MET	CG-SD	-5.85	1.66	1.81
2	B	198	GLU	CD-OE2	-5.23	1.19	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	MET	CG-SD-CE	-10.35	83.64	100.20
1	A	189	MET	CG-SD-CE	-8.92	85.93	100.20
2	B	82	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	N	310	MET	CG-SD-CE	-6.83	89.28	100.20
4	D	20	ARG	NE-CZ-NH1	-6.81	116.89	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4190	0	4166	46	0
1	N	4213	0	4222	42	0
2	B	1862	0	1881	21	0
2	O	1882	0	1903	28	0
3	C	2167	0	2104	14	0
3	P	2161	0	2106	26	0
4	D	1211	0	1202	12	0
4	Q	1199	0	1192	8	0
5	E	852	0	845	5	0
5	R	860	0	858	3	0
6	F	736	0	726	11	0
6	S	716	0	697	6	0
7	G	692	0	672	8	0
7	T	672	0	645	4	0
8	H	667	0	629	8	0
8	U	662	0	623	7	0
9	I	604	0	611	3	0
9	V	601	0	613	4	0
10	J	464	0	464	6	0
10	W	461	0	459	4	0
11	K	395	0	389	7	0
11	X	385	0	366	0	0
12	L	384	0	391	14	0
12	Y	380	0	380	1	0
13	M	336	0	352	4	0
13	Z	335	0	352	2	0
14	A	138	0	111	7	0
14	N	138	0	111	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	22	0	33	2	0
18	C	127	0	181	5	0
18	G	32	0	51	2	0
18	N	75	0	114	4	0
18	P	51	0	76	2	0
19	A	27	0	48	4	0
19	O	30	0	47	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	A	40	0	60	2	0
21	B	16	0	24	0	0
21	C	36	0	54	1	0
21	D	12	0	18	0	0
21	E	12	0	18	0	0
21	F	20	0	29	0	0
21	G	8	0	12	0	0
21	J	8	0	12	1	0
21	L	4	0	6	0	0
21	N	36	0	54	0	0
21	O	12	0	18	3	0
21	P	32	0	48	1	0
21	Q	4	0	6	0	0
21	S	20	0	30	1	0
21	T	12	0	18	0	0
21	W	4	0	6	1	0
21	Y	8	0	12	0	0
22	B	49	0	77	1	0
22	D	57	0	95	9	0
22	L	56	0	94	9	0
22	N	155	0	275	14	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	29	0	39	0	0
24	G	29	0	39	1	0
24	L	29	0	39	4	0
24	P	29	0	39	0	0
24	Y	29	0	39	1	0
25	C	34	0	51	5	0
25	D	22	0	40	2	0
25	J	11	0	21	2	0
25	K	58	0	110	4	0
25	L	21	0	30	1	0
25	M	33	0	42	2	0
25	O	11	0	21	0	0
25	P	24	0	42	6	0
25	Q	10	0	19	1	0
25	W	11	0	21	1	0
25	X	40	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Z	33	0	42	1	0
26	C	58	0	100	6	0
26	N	55	0	101	3	0
26	P	61	0	104	4	0
26	T	57	0	88	7	0
27	C	114	0	173	8	0
27	P	107	0	163	9	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	273	0	0	2	0
30	B	223	0	0	1	0
30	C	142	0	0	1	0
30	D	213	0	0	1	0
30	E	160	0	0	2	0
30	F	162	0	0	4	0
30	G	89	0	0	0	0
30	H	94	0	0	1	0
30	I	70	0	0	2	0
30	J	58	0	0	3	0
30	K	44	0	0	2	0
30	L	38	0	0	1	0
30	M	39	0	0	0	0
30	N	273	0	0	4	0
30	O	205	0	0	3	0
30	P	147	0	0	0	0
30	Q	114	0	0	1	0
30	R	117	0	0	0	0
30	S	141	0	0	3	0
30	T	66	0	0	0	0
30	U	94	0	0	0	0
30	V	72	0	0	1	0
30	W	43	0	0	1	0
30	X	31	0	0	0	0
30	Y	31	0	0	0	0
30	Z	29	0	0	2	0
All	All	34258	0	32062	317	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 5.

The worst 5 of 317 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:610[A]:PER:O2	20:N:610[A]:PER:O1	1.54	1.25
20:A:608[A]:PER:O2	20:A:608[A]:PER:O1	1.55	1.25
1:N:311[A]:ILE:HG22	26:N:601:CDL:H441	1.58	0.85
3:P:224[B]:LYS:HE2	26:P:304:CDL:H131	1.62	0.82
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.47	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/514 (106%)	530 (97%)	15 (3%)	0	100	100
1	N	550/514 (107%)	538 (98%)	12 (2%)	0	100	100
2	B	232/227 (102%)	227 (98%)	5 (2%)	0	100	100
2	O	236/227 (104%)	229 (97%)	6 (2%)	1 (0%)	34	17
3	C	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
3	P	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
4	D	145/144 (101%)	142 (98%)	3 (2%)	0	100	100
4	Q	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	104/105 (99%)	103 (99%)	1 (1%)	0	100	100
6	F	97/94 (103%)	95 (98%)	2 (2%)	0	100	100
6	S	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
7	G	86/84 (102%)	77 (90%)	4 (5%)	5 (6%)	1	0
7	T	82/84 (98%)	72 (88%)	5 (6%)	5 (6%)	1	0
8	H	78/79 (99%)	70 (90%)	5 (6%)	3 (4%)	3	0
8	U	77/79 (98%)	72 (94%)	4 (5%)	1 (1%)	12	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	11	2
10	J	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	50/49 (102%)	48 (96%)	2 (4%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	43 (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	3632/3550 (102%)	3525 (97%)	91 (2%)	16 (0%)	29	17

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	37	LEU
7	T	4	ALA
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	456/426 (107%)	447 (98%)	9 (2%)	55	34
1	N	460/426 (108%)	454 (99%)	6 (1%)	69	54
2	B	217/210 (103%)	206 (95%)	11 (5%)	24	6
2	O	221/210 (105%)	206 (93%)	15 (7%)	16	3
3	C	236/224 (105%)	232 (98%)	4 (2%)	60	42
3	P	236/224 (105%)	233 (99%)	3 (1%)	69	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	131/128 (102%)	129 (98%)	2 (2%)	65	49
4	Q	129/128 (101%)	126 (98%)	3 (2%)	50	28
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	60
5	R	93/92 (101%)	93 (100%)	0	100	100
6	F	83/78 (106%)	81 (98%)	2 (2%)	49	26
6	S	78/78 (100%)	76 (97%)	2 (3%)	46	23
7	G	72/68 (106%)	62 (86%)	10 (14%)	3	0
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	0
8	H	72/71 (101%)	65 (90%)	7 (10%)	8	1
8	U	71/71 (100%)	66 (93%)	5 (7%)	15	2
9	I	58/57 (102%)	54 (93%)	4 (7%)	15	2
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	13
10	J	50/49 (102%)	50 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	10
11	K	42/39 (108%)	41 (98%)	1 (2%)	49	26
11	X	39/39 (100%)	39 (100%)	0	100	100
12	L	40/39 (103%)	38 (95%)	2 (5%)	24	6
12	Y	39/39 (100%)	35 (90%)	4 (10%)	7	1
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	35 (95%)	2 (5%)	22	5
All	All	3163/3036 (104%)	3058 (97%)	105 (3%)	40	15

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	417[A]	MET
2	O	225	SER
12	Y	2	HIS
2	O	33	LEU
2	O	91	ASN

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

Mol	Chain	Res	Type
6	F	94	HIS
2	O	195	GLN
4	Q	109	HIS
4	Q	101	HIS
4	D	109	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	O	1	2	8,9,10	0.80	0	7,9,11	1.54	2 (28%)
1	FME	A	1	1	8,9,10	0.47	0	7,9,11	1.26	1 (14%)
2	FME	B	1	2	8,9,10	1.01	1 (12%)	7,9,11	1.86	2 (28%)
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	0.90	0
9	SAC	I	1	9	7,8,9	0.68	0	8,9,11	1.42	1 (12%)
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.47	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.03	1.70	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.36	103.62	112.95
2	O	1	FME	CG-CB-CA	-2.67	105.52	112.95
1	N	1	FME	O-C-CA	-2.67	117.79	124.78
9	I	1	SAC	CA-N-C1A	-2.58	118.38	123.15
2	B	1	FME	C-CA-N	-2.46	105.29	109.73

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	C2A-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 150 ligands modelled in this entry, 10 are monoatomic - leaving 140 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	$\# Z > 2$
27	PEK	C	306	-	23,23,52	0.39	0	21,21,57	0.42	0
21	EDO	D	205	-	3,3,3	0.67	0	2,2,2	0.24	0
25	DMU	X	101	-	9,9,34	0.41	0	8,8,45	0.44	0
21	EDO	T	103	-	3,3,3	0.49	0	2,2,2	0.34	0
21	EDO	A	616	-	3,3,3	0.47	0	2,2,2	0.42	0
21	EDO	B	305	-	3,3,3	0.41	0	2,2,2	0.78	0
21	EDO	A	615	-	3,3,3	0.76	0	2,2,2	0.25	0
27	PEK	P	306	-	52,52,52	0.75	2 (3%)	55,57,57	1.09	4 (7%)
21	EDO	J	103	-	3,3,3	0.34	0	2,2,2	0.58	0
21	EDO	C	312	-	3,3,3	0.47	0	2,2,2	0.14	0
21	EDO	S	105	-	3,3,3	0.78	0	2,2,2	0.53	0
21	EDO	F	104	-	3,3,3	0.58	0	2,2,2	0.68	0
25	DMU	X	103	-	8,8,34	0.40	0	7,7,45	0.53	0
18	PGV	C	311	-	26,26,50	1.17	1 (3%)	25,25,56	2.06	5 (20%)
21	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.50	0
21	EDO	P	314	-	3,3,3	0.44	0	2,2,2	0.87	0
22	TGL	N	612	-	43,43,62	1.18	2 (4%)	45,45,65	1.60	8 (17%)
27	PEK	C	309	-	34,34,52	0.35	0	32,32,57	0.62	0
25	DMU	X	102	-	9,9,34	0.39	0	8,8,45	0.37	0
25	DMU	P	303	-	11,11,34	0.43	0	10,10,45	0.37	0
25	DMU	L	101	-	21,21,34	0.66	1 (4%)	24,25,45	2.46	6 (25%)
21	EDO	P	316	-	3,3,3	0.58	0	2,2,2	0.42	0
22	TGL	D	202	-	56,56,62	1.17	3 (5%)	59,59,65	1.13	5 (8%)
21	EDO	P	310	-	3,3,3	0.61	0	2,2,2	0.15	0
21	EDO	P	313	-	3,3,3	0.80	0	2,2,2	0.15	0
20	PER	A	608[A]	15,14	0,1,1	0.00	-	-		
20	PER	N	610[A]	15,14	0,1,1	0.00	-	-		
21	EDO	P	315	-	3,3,3	0.40	0	2,2,2	1.15	0
18	PGV	P	307	-	50,50,50	0.69	2 (4%)	53,56,56	1.09	5 (9%)
25	DMU	X	104	-	9,9,34	0.46	0	8,8,45	0.18	0
22	TGL	B	301	-	47,47,62	1.16	3 (6%)	50,50,65	1.47	5 (10%)
26	CDL	N	601	-	51,51,99	1.20	8 (15%)	47,47,111	0.88	1 (2%)
25	DMU	J	101	-	10,10,34	0.36	0	9,9,45	0.39	0
21	EDO	A	613	-	3,3,3	0.51	0	2,2,2	0.26	0
18	PGV	C	301	-	50,50,50	0.94	4 (8%)	53,56,56	1.21	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	B	307	-	3,3,3	0.64	0	2,2,2	0.25	0
14	HEA	A	601[C]	-	44,58,67	1.28	3 (6%)	37,91,103	3.97	15 (40%)
18	PGV	N	608	-	50,50,50	0.90	4 (8%)	53,56,56	1.24	5 (9%)
25	DMU	K	101	-	8,8,34	0.28	0	7,7,45	0.59	0
21	EDO	O	305	-	3,3,3	0.56	0	2,2,2	0.13	0
21	EDO	A	618	-	3,3,3	0.70	0	2,2,2	0.78	0
22	TGL	L	103	-	53,53,62	0.74	1 (1%)	51,51,65	1.08	3 (5%)
24	CHD	B	303	-	29,32,32	0.92	1 (3%)	48,51,51	1.64	10 (20%)
21	EDO	P	311	-	3,3,3	0.46	0	2,2,2	0.31	0
24	CHD	Y	101	-	29,32,32	0.73	0	48,51,51	2.40	18 (37%)
21	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.06	0
21	EDO	C	320	-	3,3,3	0.68	0	2,2,2	0.53	0
14	HEA	A	601[A]	-	44,67,67	1.17	2 (4%)	37,103,103	2.39	15 (40%)
21	EDO	T	104	-	3,3,3	0.72	0	2,2,2	0.41	0
27	PEK	P	308	-	32,32,52	0.43	0	29,30,57	0.57	0
27	PEK	C	307	-	52,52,52	0.84	2 (3%)	55,57,57	1.07	3 (5%)
21	EDO	F	103	-	3,3,3	0.63	0	2,2,2	0.17	0
21	EDO	B	304	-	3,3,3	0.63	0	2,2,2	0.34	0
25	DMU	Q	201	-	9,9,34	0.45	0	8,8,45	0.22	0
29	PO4	U	101	-	4,4,4	1.14	0	6,6,6	0.76	0
21	EDO	Y	102	-	3,3,3	0.46	0	2,2,2	0.21	0
27	PEK	P	305	-	19,19,52	0.30	0	18,18,57	0.57	0
25	DMU	K	104	-	8,8,34	0.53	0	7,7,45	0.25	0
21	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.54	0
24	CHD	G	101	-	29,32,32	0.84	0	48,51,51	1.34	7 (14%)
25	DMU	D	201	-	10,10,34	0.33	0	9,9,45	0.41	0
21	EDO	N	618	-	3,3,3	0.50	0	2,2,2	0.36	0
21	EDO	B	306	-	3,3,3	0.82	0	2,2,2	0.33	0
25	DMU	P	309	-	10,10,34	0.33	0	9,9,45	0.55	0
21	EDO	G	103	-	3,3,3	0.62	0	2,2,2	0.55	0
14	HEA	N	603	20,1,30	44,67,67	1.13	3 (6%)	37,103,103	1.81	9 (24%)
25	DMU	K	106	-	9,9,34	0.28	0	8,8,45	0.32	0
26	CDL	C	305	-	54,54,99	1.04	5 (9%)	50,50,111	1.12	5 (10%)
21	EDO	W	102	-	3,3,3	0.34	0	2,2,2	0.24	0
21	EDO	A	609	-	3,3,3	0.57	0	2,2,2	0.60	0
25	DMU	O	302	-	10,10,34	0.20	0	9,9,45	0.72	0
25	DMU	D	203	-	9,9,34	0.36	0	8,8,45	0.55	0
21	EDO	N	619	-	3,3,3	0.74	0	2,2,2	0.18	0
21	EDO	E	201	-	3,3,3	0.54	0	2,2,2	0.38	0
26	CDL	P	304	-	57,57,99	1.22	7 (12%)	54,54,111	1.05	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	D	206	-	3,3,3	0.56	0	2,2,2	0.13	0
24	CHD	P	301	-	29,32,32	0.68	0	48,51,51	1.58	9 (18%)
21	EDO	E	202	-	3,3,3	0.43	0	2,2,2	0.32	0
14	HEA	A	602	20,1,30	44,67,67	1.17	4 (9%)	37,103,103	2.00	10 (27%)
21	EDO	N	617	-	3,3,3	0.51	0	2,2,2	0.36	0
21	EDO	S	106	-	3,3,3	0.43	0	2,2,2	0.79	0
26	CDL	T	101	-	52,53,99	1.34	8 (15%)	49,51,111	1.21	4 (8%)
22	TGL	N	609	-	62,62,62	1.13	3 (4%)	65,65,65	1.07	4 (6%)
21	EDO	O	306	-	3,3,3	0.49	0	2,2,2	0.09	0
21	EDO	Y	103	-	3,3,3	0.50	0	2,2,2	0.71	0
18	PGV	N	607	-	22,22,50	0.36	0	20,20,56	0.52	0
14	HEA	N	602[A]	-	44,67,67	0.83	1 (2%)	37,103,103	1.90	13 (35%)
21	EDO	C	317	-	3,3,3	0.62	0	2,2,2	0.18	0
25	DMU	K	105	-	8,8,34	0.24	0	7,7,45	0.61	0
21	EDO	P	312	-	3,3,3	0.58	0	2,2,2	0.28	0
18	PGV	C	308	-	47,47,50	0.84	1 (2%)	50,53,56	0.93	3 (6%)
18	PGV	A	606	-	20,20,50	0.51	0	18,18,56	0.78	0
25	DMU	K	102	-	9,9,34	0.27	0	8,8,45	0.46	0
25	DMU	M	101	-	34,34,34	0.57	0	45,45,45	1.28	4 (8%)
21	EDO	N	615	-	3,3,3	0.58	0	2,2,2	0.12	0
21	EDO	C	316	-	3,3,3	0.40	0	2,2,2	0.36	0
21	EDO	S	104	-	3,3,3	0.50	0	2,2,2	0.23	0
22	TGL	N	611	-	45,45,62	0.36	0	42,42,65	0.44	0
21	EDO	F	106	-	3,3,3	0.68	0	2,2,2	0.76	0
18	PGV	G	102	-	30,30,50	0.98	1 (3%)	28,29,56	1.48	3 (10%)
23	CUA	O	301	2	0,1,1	0.00	-	-	-	-
21	EDO	L	104	-	3,3,3	0.53	0	2,2,2	0.76	0
21	EDO	T	102	-	3,3,3	0.65	0	2,2,2	0.77	0
21	EDO	N	613	-	3,3,3	0.81	0	2,2,2	0.75	0
25	DMU	Z	101	-	34,34,34	0.51	0	45,45,45	1.03	2 (4%)
21	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.28	0
21	EDO	F	105	-	3,3,3	0.58	0	2,2,2	0.36	0
21	EDO	G	104	-	3,3,3	0.62	0	2,2,2	0.16	0
25	DMU	C	310	-	21,21,34	0.88	1 (4%)	24,25,45	1.35	3 (12%)
21	EDO	P	317	-	3,3,3	0.55	0	2,2,2	0.17	0
21	EDO	Q	202	-	3,3,3	0.46	0	2,2,2	0.64	0
21	EDO	A	614	-	3,3,3	0.48	0	2,2,2	0.48	0
24	CHD	C	304	-	29,32,32	0.78	0	48,51,51	1.57	7 (14%)
14	HEA	N	602[C]	-	44,58,67	3.53	1 (2%)	37,91,103	4.75	16 (43%)
21	EDO	A	611	-	3,3,3	0.81	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DMU	W	101	-	10,10,34	0.38	0	9,9,45	0.54	0
21	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.35	0
21	EDO	J	102	-	3,3,3	0.53	0	2,2,2	0.37	0
25	DMU	C	303	-	12,12,34	0.54	0	10,11,45	0.35	0
25	DMU	K	103	-	10,10,34	0.40	0	9,9,45	0.48	0
21	EDO	C	319	-	3,3,3	0.60	0	2,2,2	0.16	0
21	EDO	N	621	-	3,3,3	0.56	0	2,2,2	0.09	0
23	CUA	B	302	2	0,1,1	0.00	-	-		
21	EDO	S	102	-	3,3,3	0.80	0	2,2,2	0.74	0
21	EDO	A	617	-	3,3,3	0.62	0	2,2,2	0.13	0
21	EDO	D	204	-	3,3,3	0.57	0	2,2,2	0.13	0
21	EDO	C	315	-	3,3,3	0.39	0	2,2,2	1.06	0
21	EDO	N	620	-	3,3,3	0.76	0	2,2,2	0.34	0
19	PSC	A	607	-	25,25,51	0.81	1 (4%)	22,23,59	0.93	0
21	EDO	C	313	-	3,3,3	0.70	0	2,2,2	0.61	0
21	EDO	C	314	-	3,3,3	0.84	0	2,2,2	0.40	0
21	EDO	A	612	-	3,3,3	0.79	0	2,2,2	0.67	0
21	EDO	C	318	-	3,3,3	0.56	0	2,2,2	0.49	0
24	CHD	L	102	-	29,32,32	0.72	0	48,51,51	2.87	20 (41%)
29	PO4	H	101	-	4,4,4	0.77	0	6,6,6	0.66	0
21	EDO	E	203	-	3,3,3	0.57	0	2,2,2	0.27	0
19	PSC	O	303	-	25,28,51	0.79	1 (4%)	23,27,59	0.95	1 (4%)
21	EDO	O	304	-	3,3,3	0.66	0	2,2,2	0.30	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
27	PEK	C	306	-	-	9/19/19/56	-
21	EDO	D	205	-	-	1/1/1/1	-
25	DMU	X	101	-	-	0/7/7/59	-
21	EDO	T	103	-	-	0/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
27	PEK	P	306	-	-	14/56/56/56	-
21	EDO	J	103	-	-	1/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	F	104	-	-	0/1/1/1	-
25	DMU	X	103	-	-	1/6/6/59	-
18	PGV	C	311	-	-	10/23/23/55	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	P	314	-	-	0/1/1/1	-
22	TGL	N	612	-	-	26/45/45/65	-
27	PEK	C	309	-	-	15/30/30/56	-
25	DMU	X	102	-	-	2/7/7/59	-
25	DMU	P	303	-	-	4/9/9/59	-
25	DMU	L	101	-	-	4/13/29/59	0/1/1/2
21	EDO	P	316	-	-	0/1/1/1	-
22	TGL	D	202	-	-	32/59/59/65	-
21	EDO	P	310	-	-	1/1/1/1	-
21	EDO	P	313	-	-	0/1/1/1	-
21	EDO	P	315	-	-	1/1/1/1	-
18	PGV	P	307	-	-	6/55/55/55	-
25	DMU	X	104	-	-	0/7/7/59	-
22	TGL	B	301	-	-	29/50/50/65	-
26	CDL	N	601	-	-	17/42/43/110	-
25	DMU	J	101	-	-	6/8/8/59	-
21	EDO	A	613	-	-	1/1/1/1	-
18	PGV	C	301	-	-	8/55/55/55	-
21	EDO	B	307	-	-	0/1/1/1	-
14	HEA	A	601[C]	-	3/3/5/16	4/24/60/76	-
18	PGV	N	608	-	-	9/55/55/55	-
25	DMU	K	101	-	-	0/6/6/59	-
21	EDO	O	305	-	-	1/1/1/1	-
21	EDO	A	618	-	-	0/1/1/1	-
22	TGL	L	103	-	-	24/47/48/65	-
24	CHD	B	303	-	-	0/7/74/74	0/4/4/4
14	HEA	A	601[B]	-	3/3/5/16	-	-
21	EDO	P	311	-	-	1/1/1/1	-
24	CHD	Y	101	-	-	4/7/74/74	0/4/4/4
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
14	HEA	A	601[A]	-	3/3/7/16	2/24/76/76	-
21	EDO	T	104	-	-	1/1/1/1	-
27	PEK	P	308	-	-	12/28/28/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PEK	C	307	-	-	15/56/56/56	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
25	DMU	Q	201	-	-	4/7/7/59	-
21	EDO	Y	102	-	-	0/1/1/1	-
27	PEK	P	305	-	-	10/17/17/56	-
25	DMU	K	104	-	-	2/6/6/59	-
21	EDO	F	102	-	-	0/1/1/1	-
24	CHD	G	101	-	-	0/7/74/74	0/4/4/4
25	DMU	D	201	-	-	3/8/8/59	-
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
25	DMU	P	309	-	-	2/8/8/59	-
21	EDO	G	103	-	-	0/1/1/1	-
14	HEA	N	603	20,1,30	3/3/7/16	0/24/76/76	-
25	DMU	K	106	-	-	3/7/7/59	-
26	CDL	C	305	-	-	14/45/46/110	-
21	EDO	W	102	-	-	1/1/1/1	-
21	EDO	A	609	-	-	0/1/1/1	-
25	DMU	O	302	-	-	3/8/8/59	-
25	DMU	D	203	-	-	2/7/7/59	-
21	EDO	N	619	-	-	1/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
26	CDL	P	304	-	-	17/49/50/110	-
21	EDO	D	206	-	-	0/1/1/1	-
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
21	EDO	E	202	-	-	1/1/1/1	-
14	HEA	A	602	20,1,30	3/3/7/16	0/24/76/76	-
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	S	106	-	-	0/1/1/1	-
26	CDL	T	101	-	-	21/47/47/110	-
22	TGL	N	609	-	-	34/65/65/65	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	Y	103	-	-	1/1/1/1	-
18	PGV	N	607	-	-	5/18/18/55	-
14	HEA	N	602[A]	-	3/3/7/16	0/24/76/76	-
21	EDO	C	317	-	-	0/1/1/1	-
25	DMU	K	105	-	-	4/6/6/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	P	312	-	-	0/1/1/1	-
18	PGV	C	308	-	-	10/52/52/55	-
18	PGV	A	606	-	-	3/15/16/55	-
25	DMU	K	102	-	-	3/7/7/59	-
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	C	316	-	-	0/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
22	TGL	N	611	-	-	20/39/39/65	-
21	EDO	F	106	-	-	0/1/1/1	-
18	PGV	G	102	-	-	7/27/27/55	-
21	EDO	L	104	-	-	1/1/1/1	-
21	EDO	T	102	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
21	EDO	G	104	-	-	1/1/1/1	-
25	DMU	C	310	-	-	5/13/29/59	0/1/1/2
21	EDO	P	317	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
24	CHD	C	304	-	-	0/7/74/74	0/4/4/4
14	HEA	N	602[C]	-	3/3/5/16	7/24/60/76	-
21	EDO	A	611	-	-	0/1/1/1	-
25	DMU	W	101	-	-	1/8/8/59	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-
25	DMU	C	303	-	-	2/9/10/59	-
25	DMU	K	103	-	-	6/8/8/59	-
21	EDO	C	319	-	-	0/1/1/1	-
14	HEA	N	602[B]	-	3/3/5/16	-	-
21	EDO	N	621	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	D	204	-	-	0/1/1/1	-
21	EDO	C	315	-	-	0/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
19	PSC	A	607	-	-	10/21/21/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	C	313	-	-	0/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	C	318	-	-	0/1/1/1	-
24	CHD	L	102	-	-	6/7/74/74	0/4/4/4
21	EDO	E	203	-	-	1/1/1/1	-
19	PSC	O	303	-	-	7/22/24/55	-
21	EDO	O	304	-	-	0/1/1/1	-

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[C]	HEA	C18-C19	22.89	1.87	1.33
22	N	612	TGL	OG2-CB1	5.58	1.50	1.34
18	C	311	PGV	O03-C19	5.52	1.49	1.33
22	N	609	TGL	OG2-CB1	5.12	1.48	1.34
22	D	202	TGL	OG1-CA1	4.92	1.47	1.33

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[C]	HEA	C20-C19-C18	18.57	158.70	121.12
14	N	602[C]	HEA	C27-C19-C18	-17.43	78.95	123.68
14	A	601[C]	HEA	C20-C19-C18	13.27	147.98	121.12
14	A	601[C]	HEA	C27-C19-C18	-12.76	90.94	123.68
14	A	601[C]	HEA	C13-C12-C11	-9.41	100.21	114.35

5 of 24 chirality outliers are listed below:

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

5 of 493 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[C]	HEA	C11-C12-C13-C14
14	N	602[C]	HEA	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	N	602[C]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C17-C18-C19-C20
18	A	606	PGV	C1-C2-C3-C4

There are no ring outliers.

62 monomers are involved in 144 short contacts:

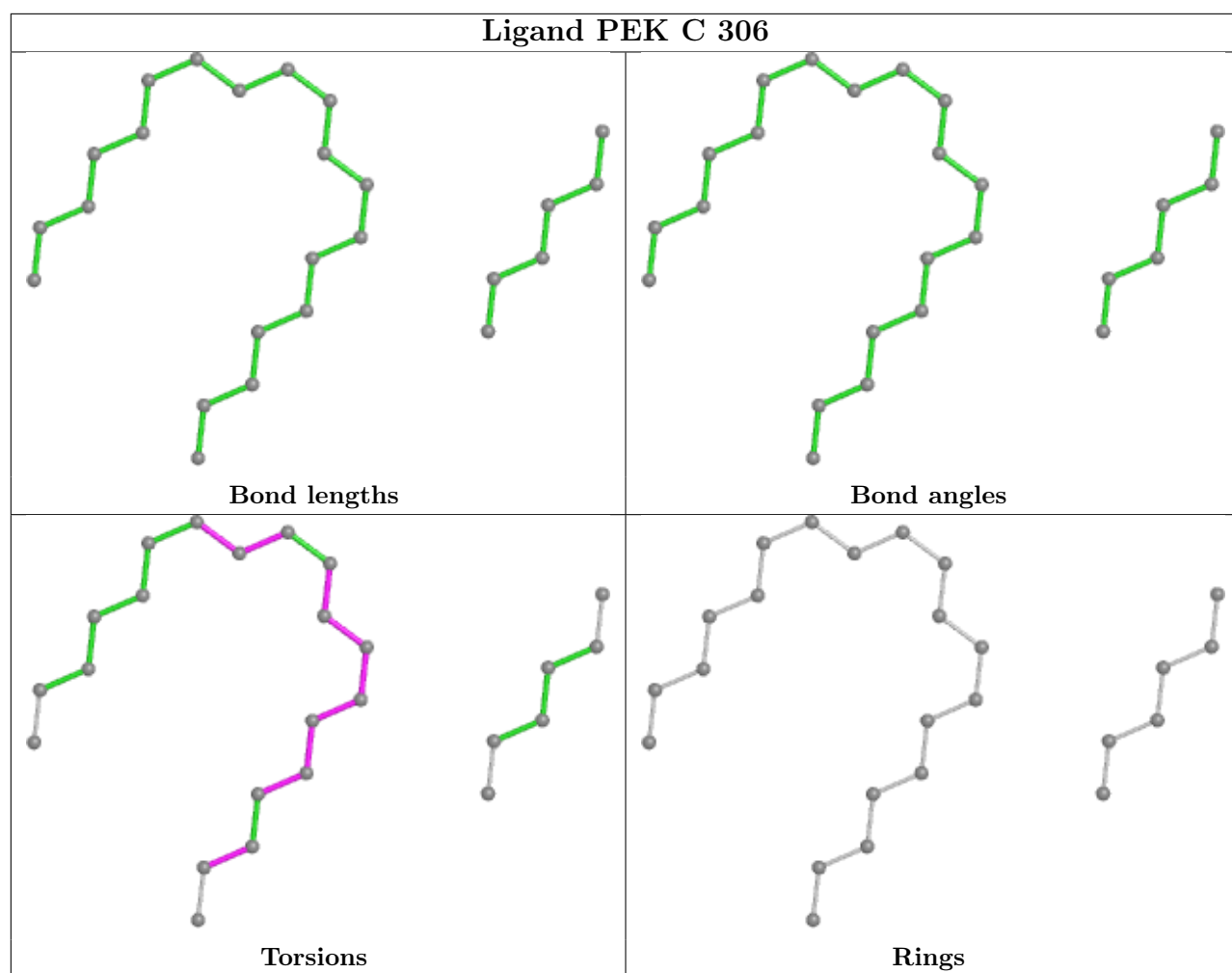
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	615	EDO	1	0
27	P	306	PEK	5	0
21	J	103	EDO	1	0
18	C	311	PGV	2	0
22	N	612	TGL	3	0
27	C	309	PEK	4	0
25	P	303	DMU	1	0
25	L	101	DMU	1	0
22	D	202	TGL	9	0
21	P	310	EDO	1	0
20	A	608[A]	PER	1	0
20	N	610[A]	PER	1	0
18	P	307	PGV	2	0
22	B	301	TGL	1	0
26	N	601	CDL	3	0
25	J	101	DMU	2	0
21	A	613	EDO	1	0
18	C	301	PGV	1	0
14	A	601[C]	HEA	1	0
18	N	608	PGV	3	0
25	K	101	DMU	1	0
21	O	305	EDO	2	0
22	L	103	TGL	9	0
14	A	601[B]	HEA	1	0
24	Y	101	CHD	1	0
21	C	320	EDO	1	0
14	A	601[A]	HEA	2	0
27	P	308	PEK	4	0
27	C	307	PEK	4	0
25	Q	201	DMU	1	0
25	K	104	DMU	1	0
24	G	101	CHD	1	0
25	D	201	DMU	2	0
25	P	309	DMU	5	0

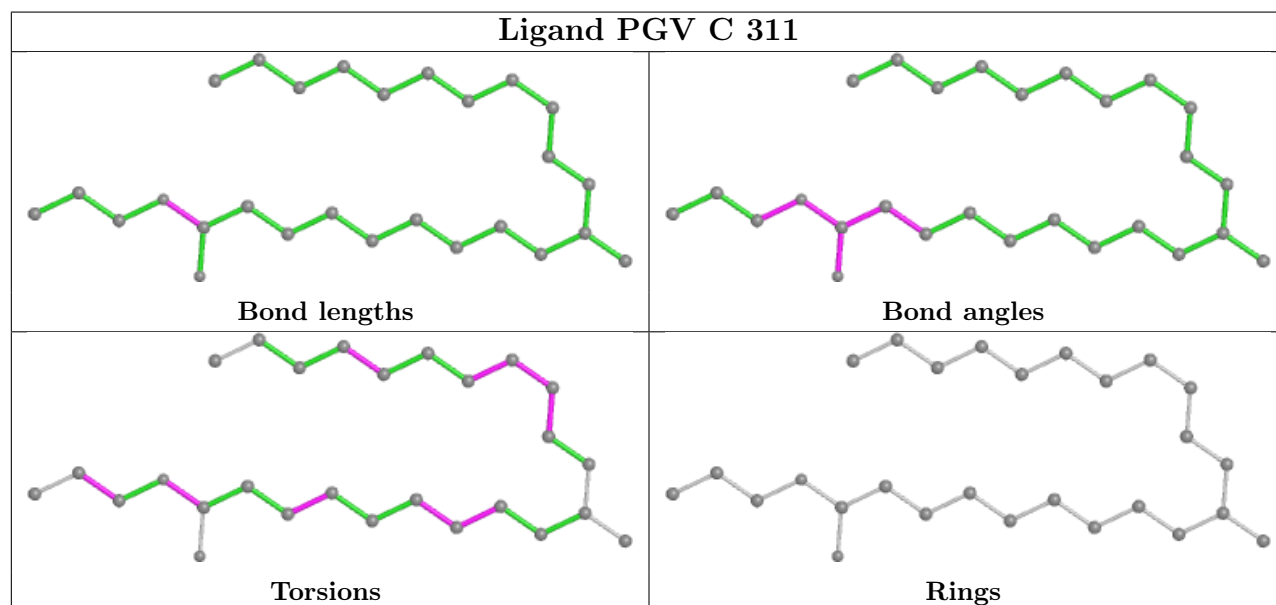
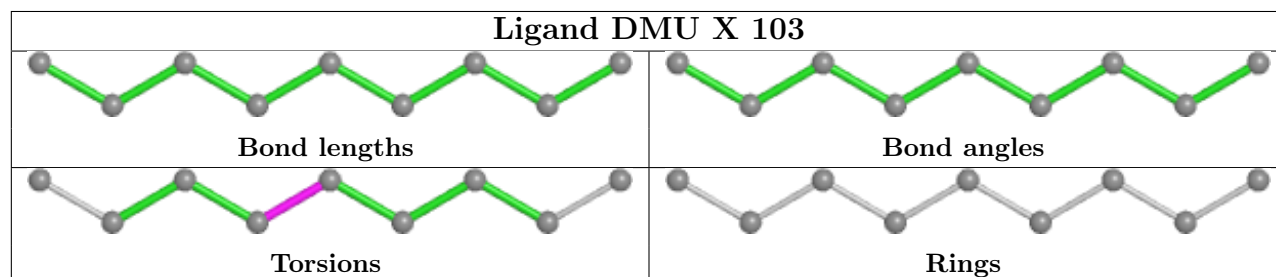
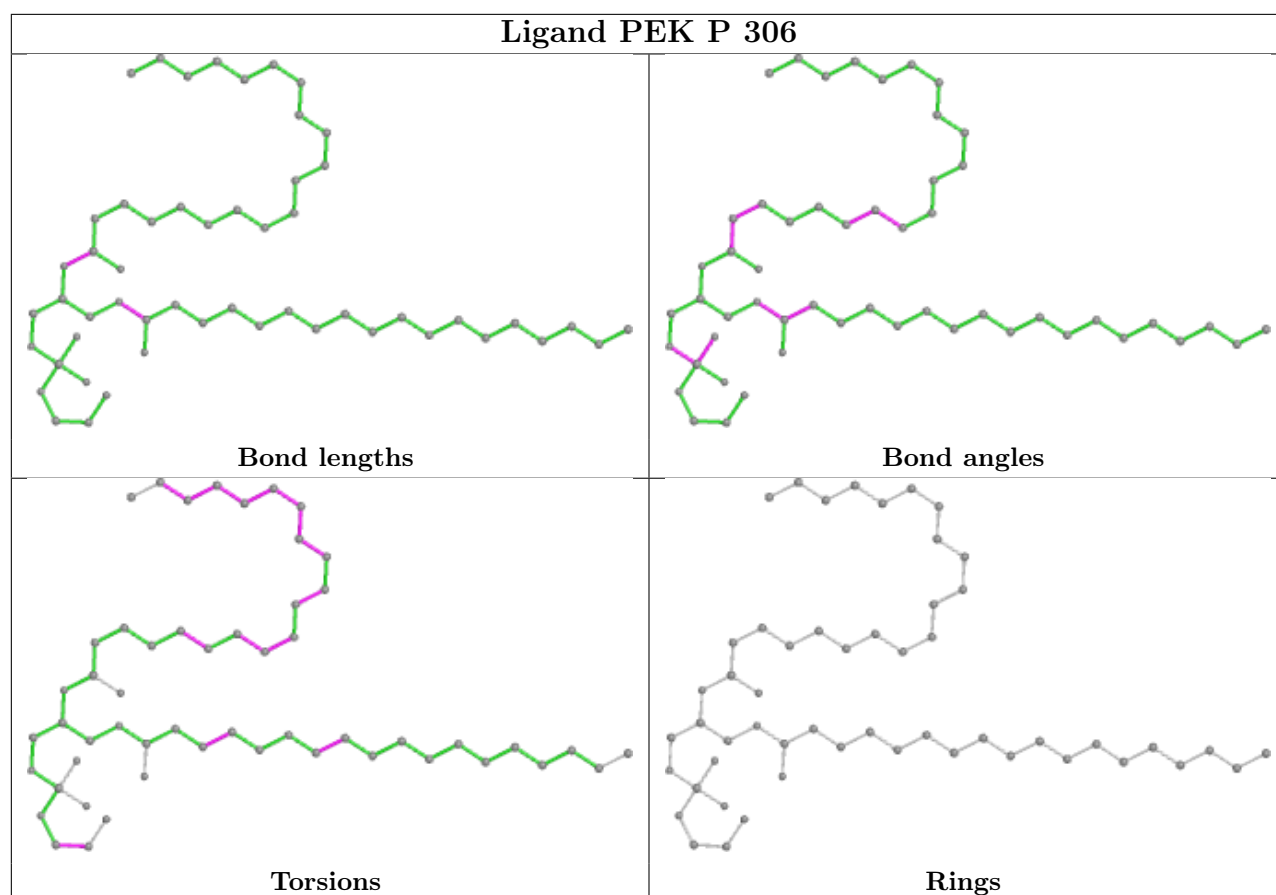
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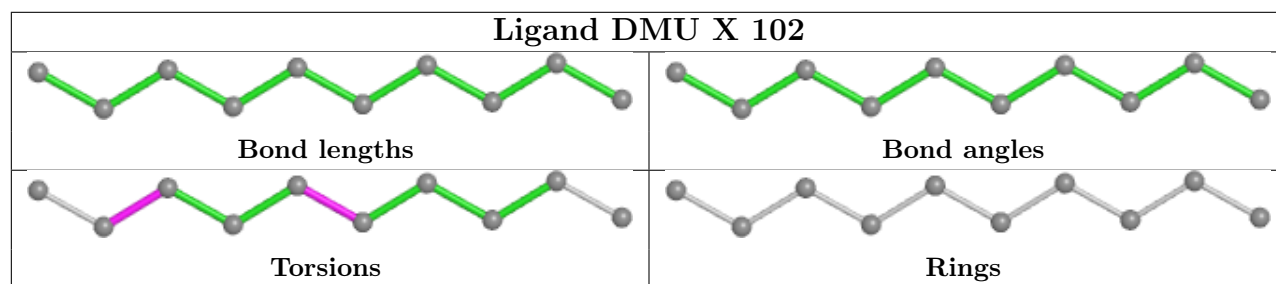
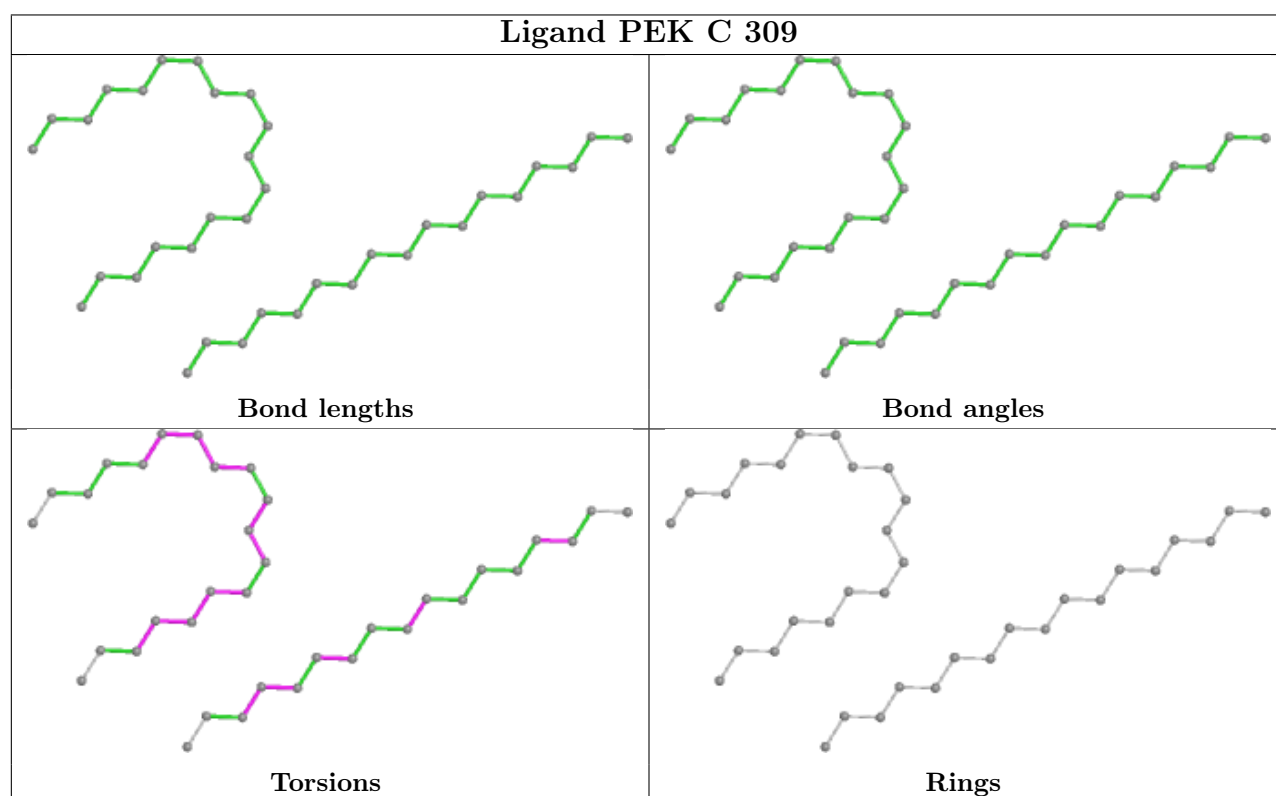
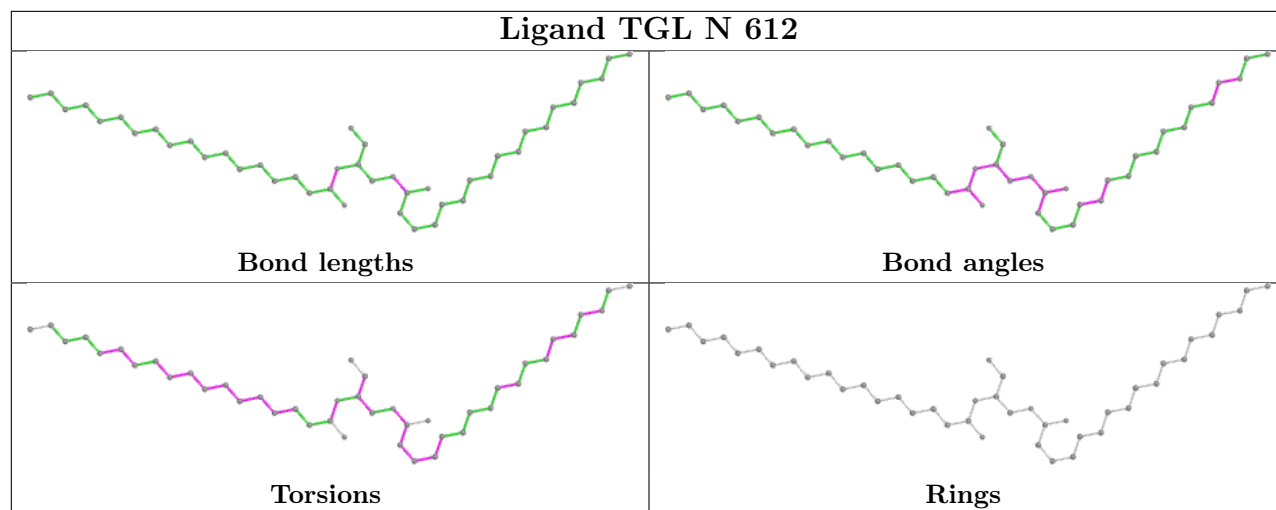
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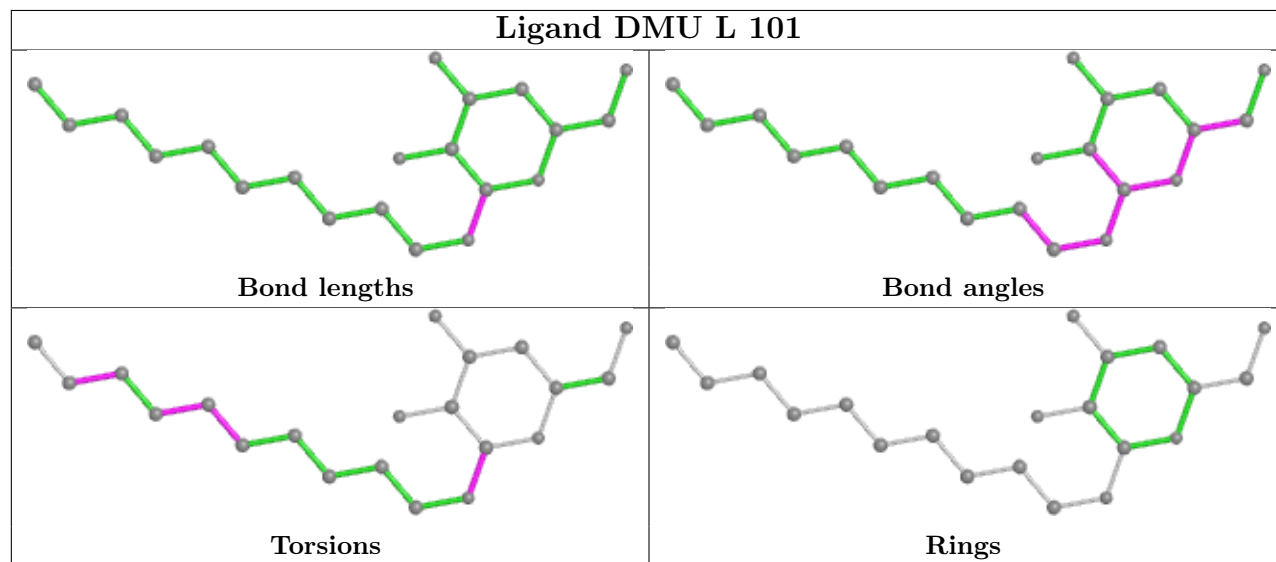
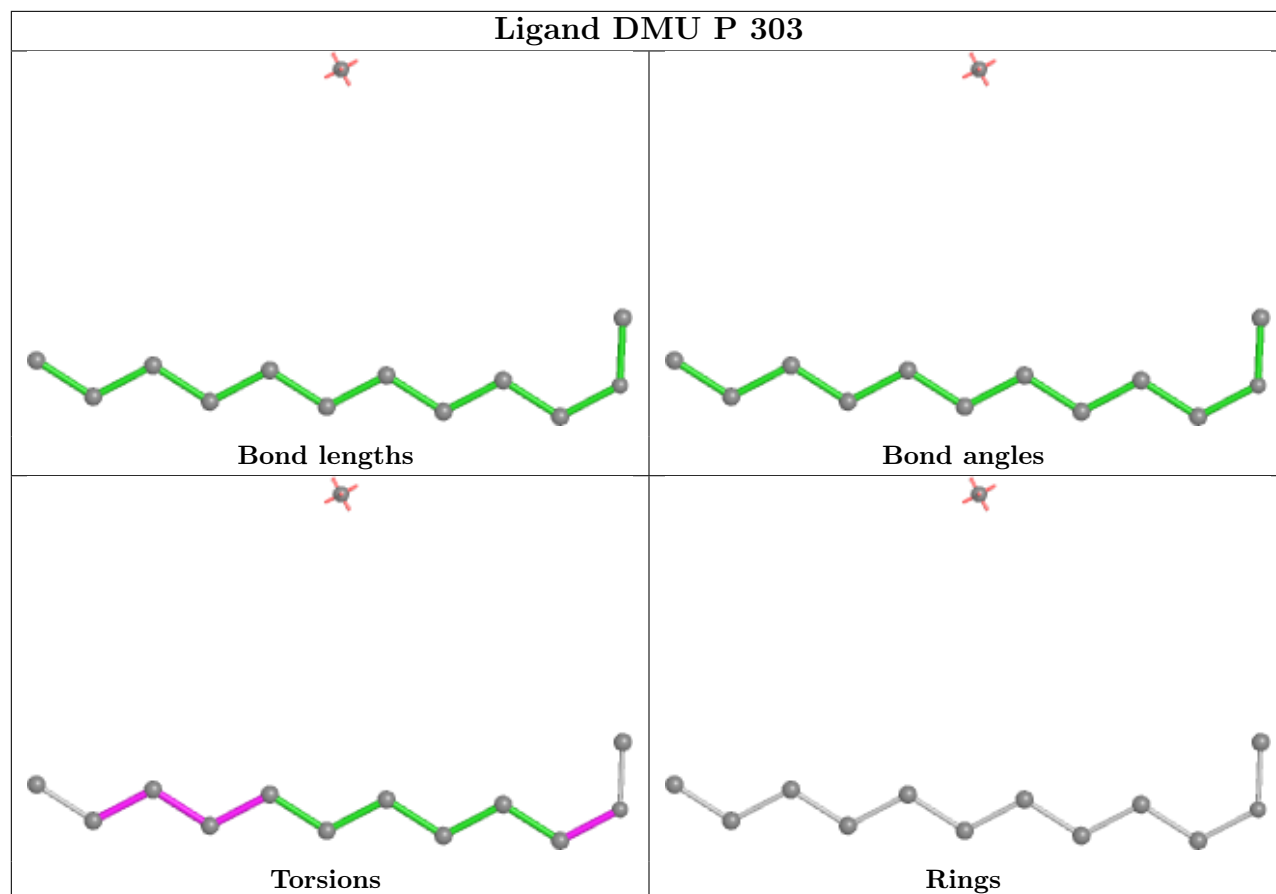
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	603	HEA	5	0
25	K	106	DMU	1	0
26	C	305	CDL	6	0
21	W	102	EDO	1	0
26	P	304	CDL	4	0
14	A	602	HEA	3	0
21	S	106	EDO	1	0
26	T	101	CDL	7	0
22	N	609	TGL	6	0
21	O	306	EDO	1	0
18	N	607	PGV	1	0
14	N	602[A]	HEA	2	0
25	K	105	DMU	1	0
18	C	308	PGV	2	0
18	A	606	PGV	2	0
25	K	102	DMU	1	0
25	M	101	DMU	2	0
22	N	611	TGL	5	0
18	G	102	PGV	2	0
25	Z	101	DMU	1	0
25	C	310	DMU	4	0
14	N	602[C]	HEA	1	0
25	W	101	DMU	1	0
25	C	303	DMU	1	0
25	K	103	DMU	1	0
19	A	607	PSC	4	0
24	L	102	CHD	4	0
19	O	303	PSC	4	0

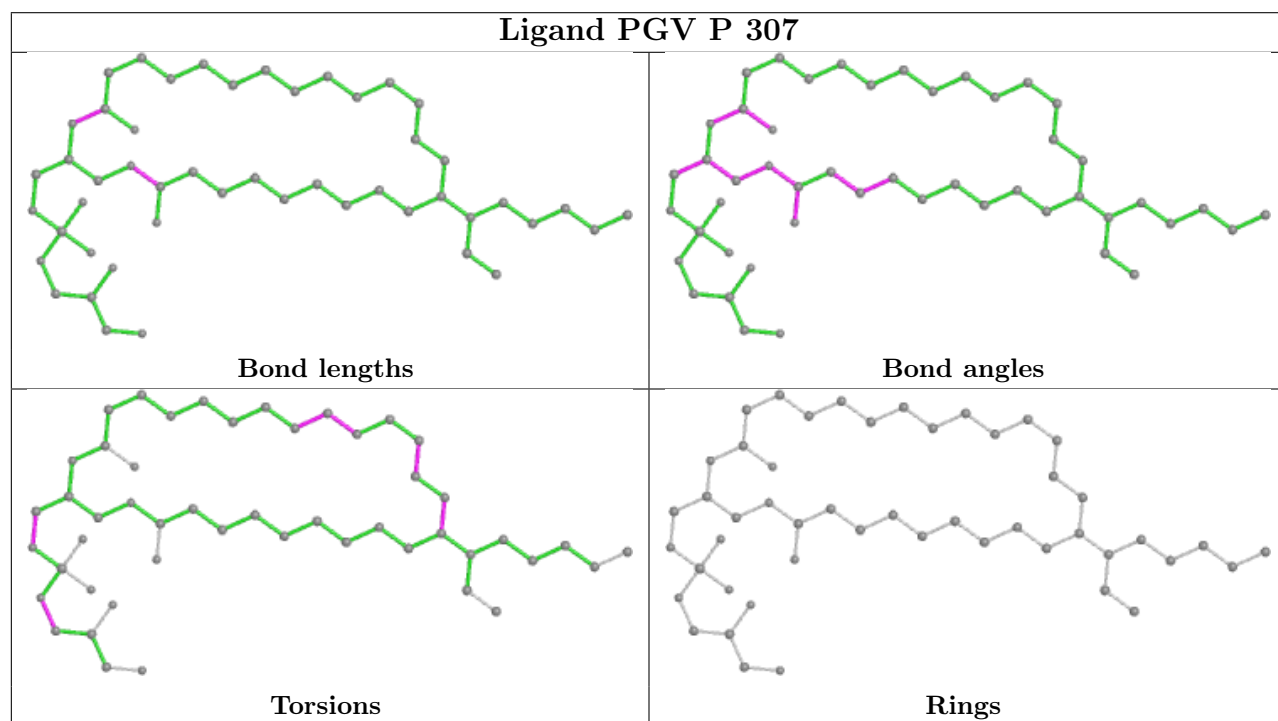
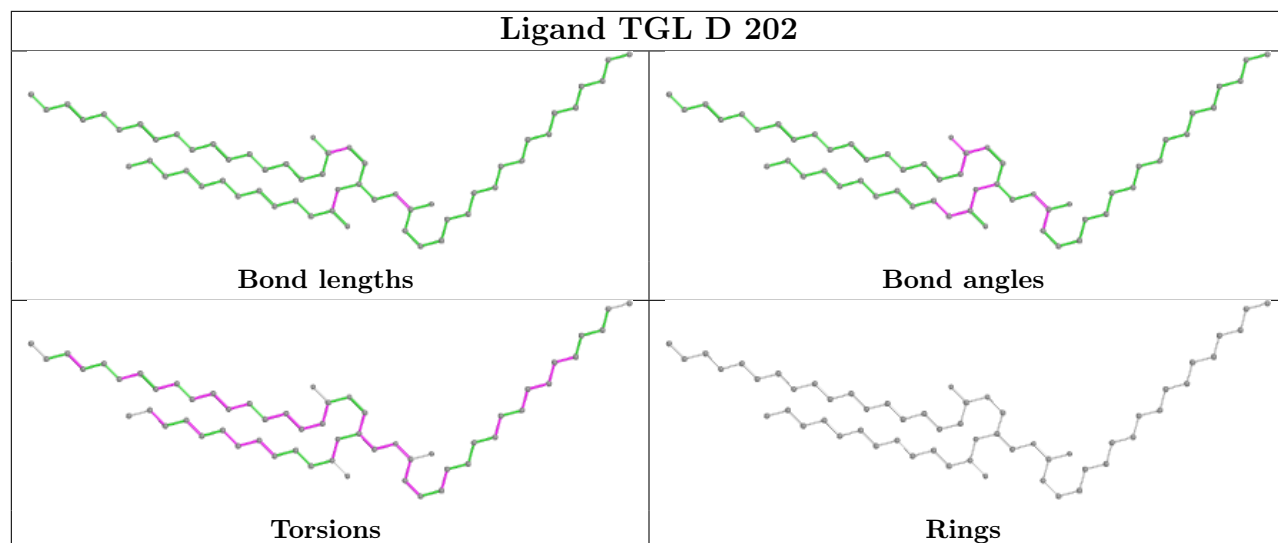
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

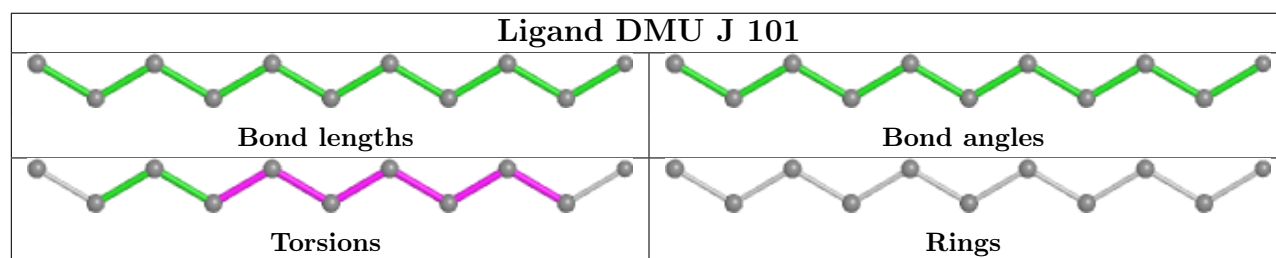
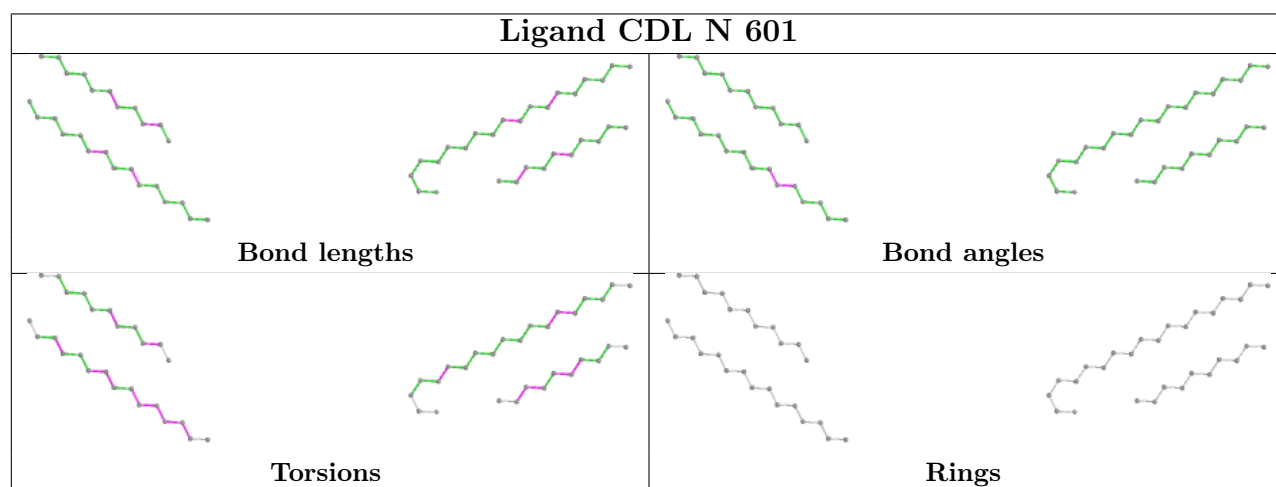
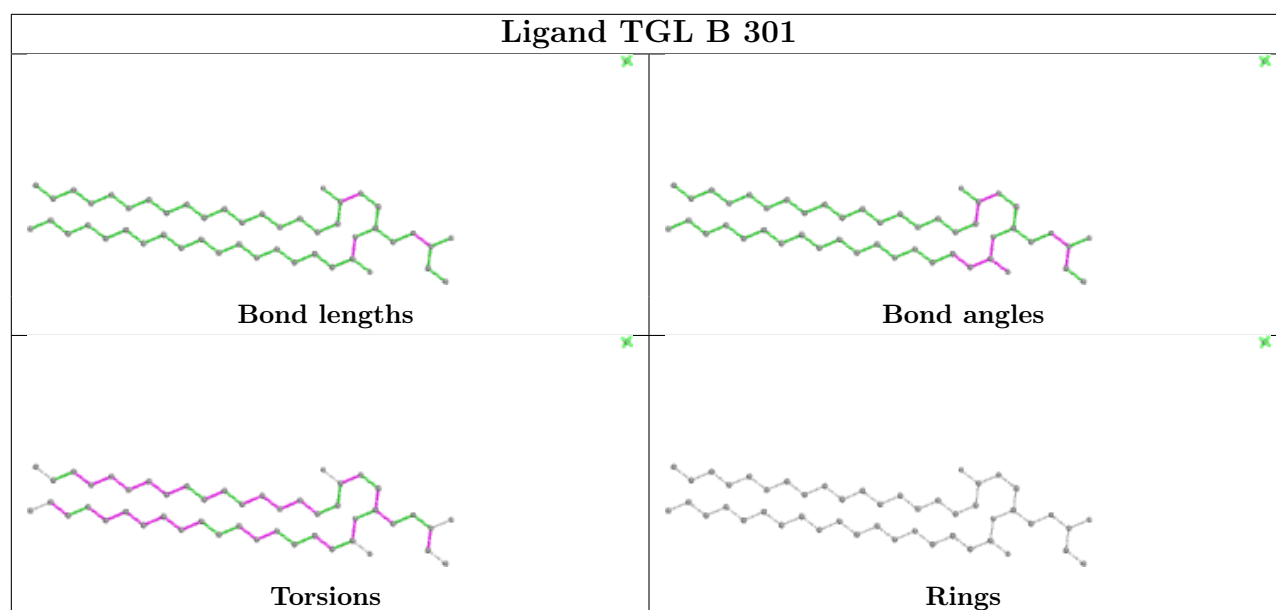


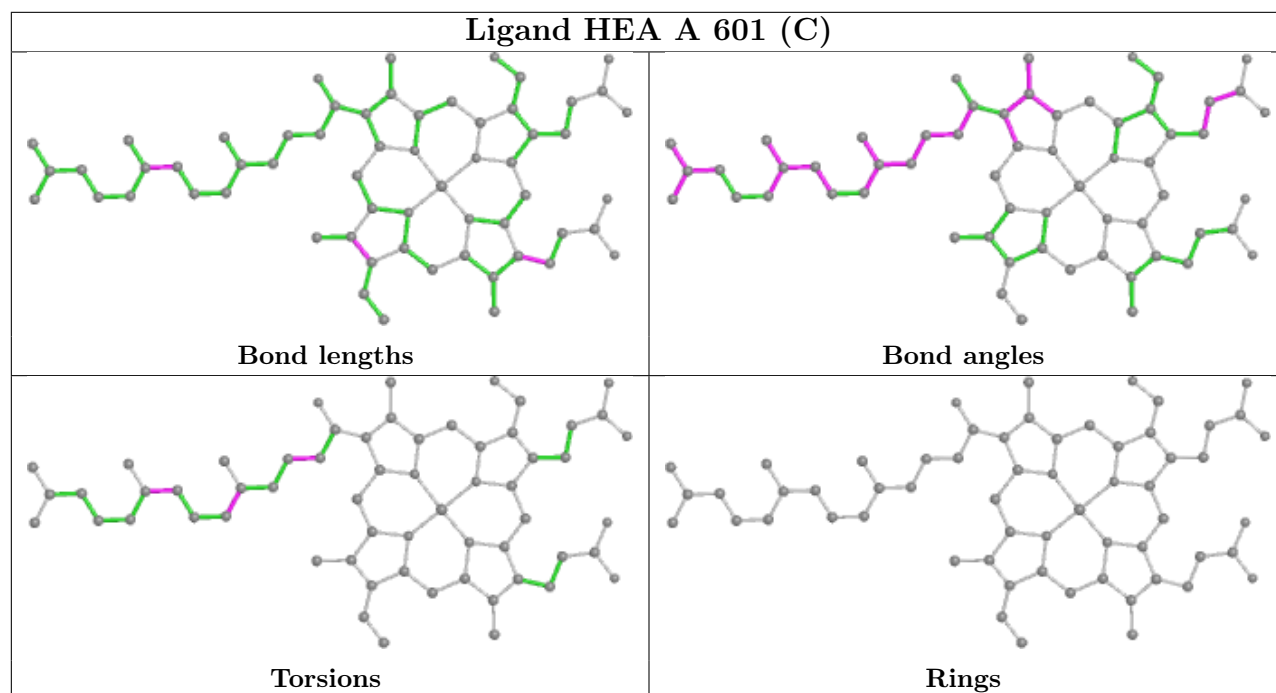
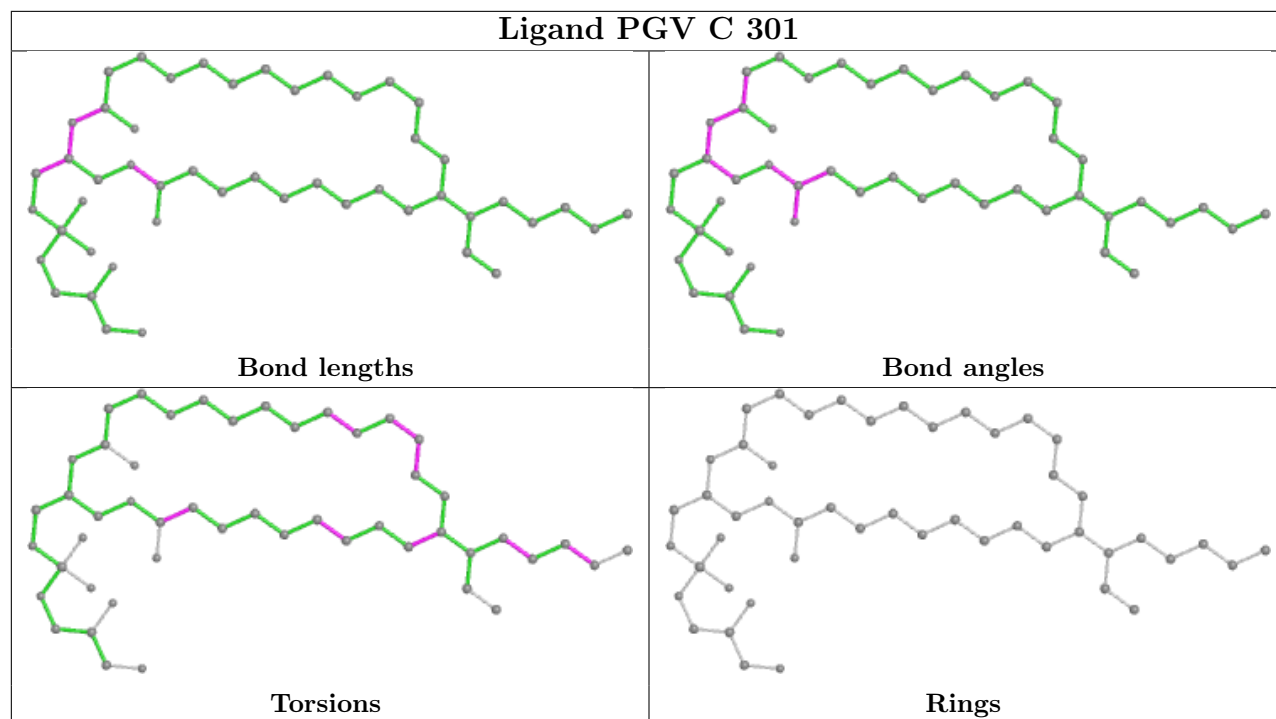


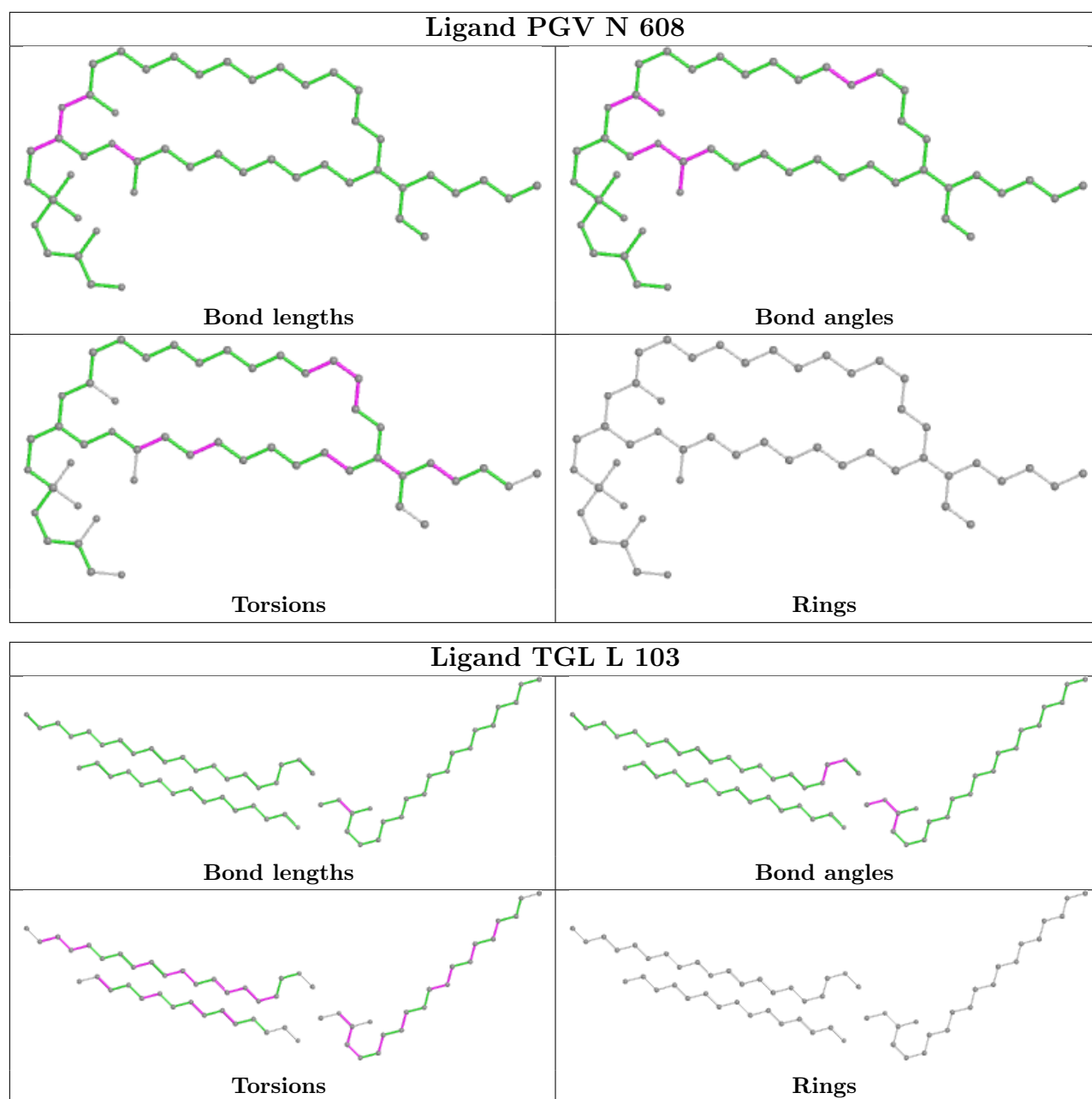


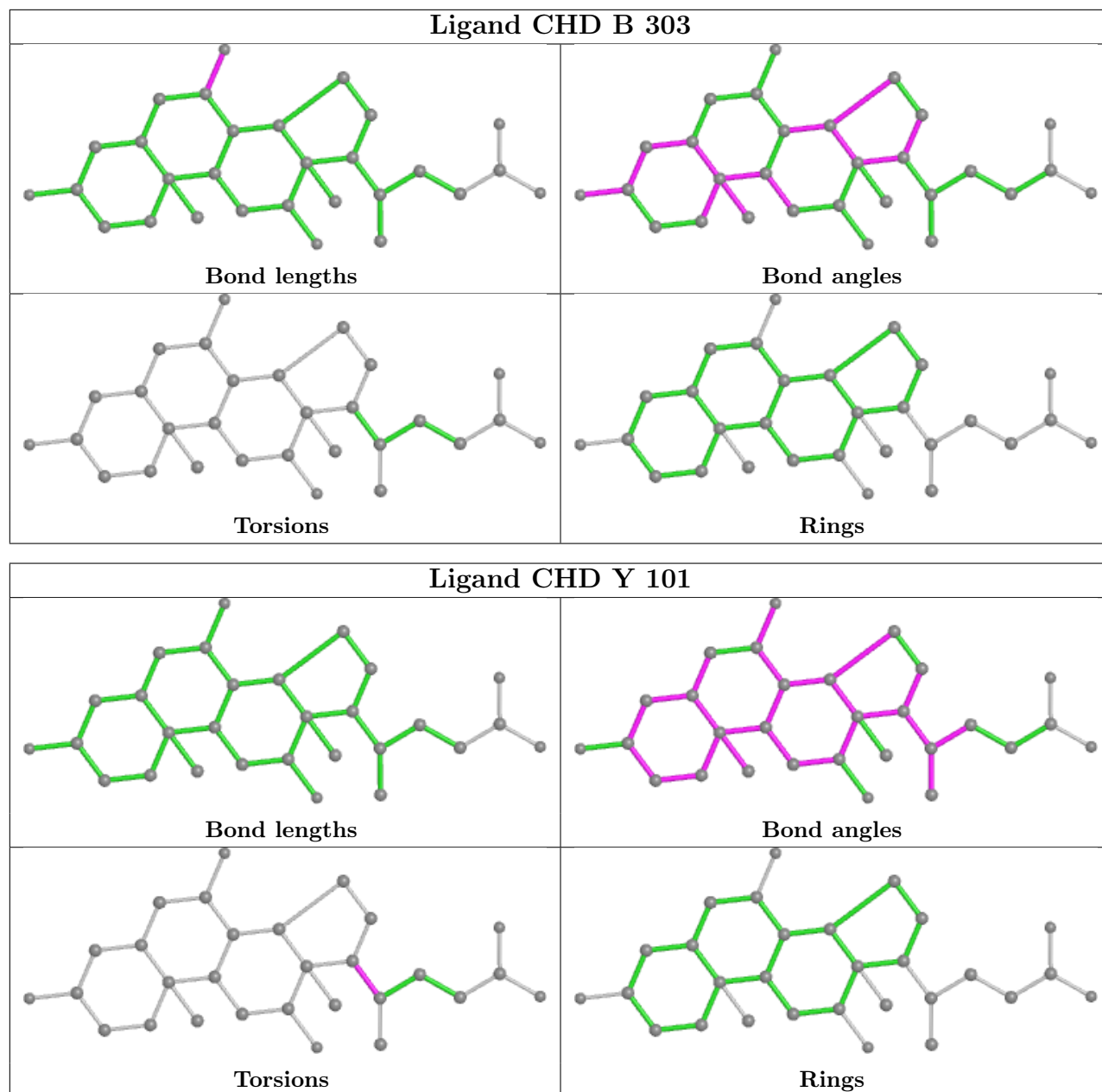


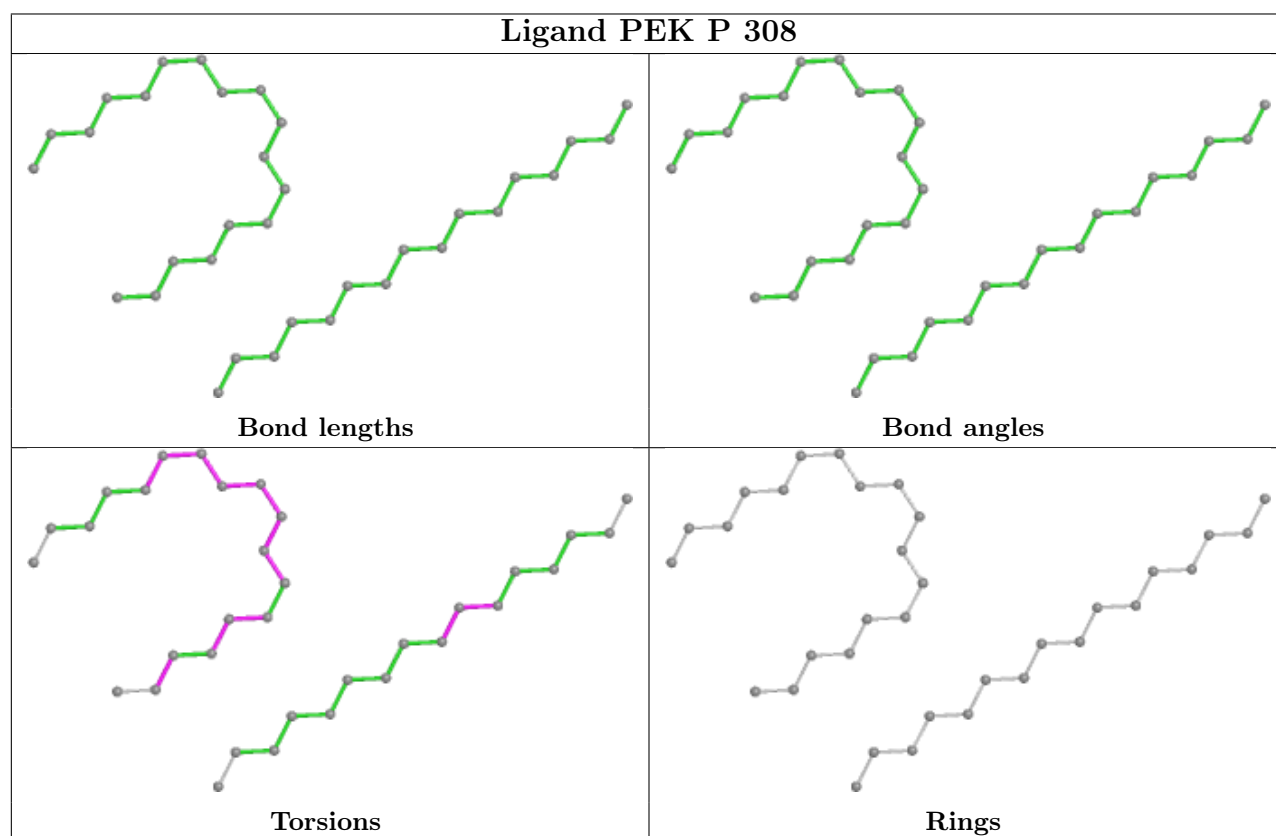
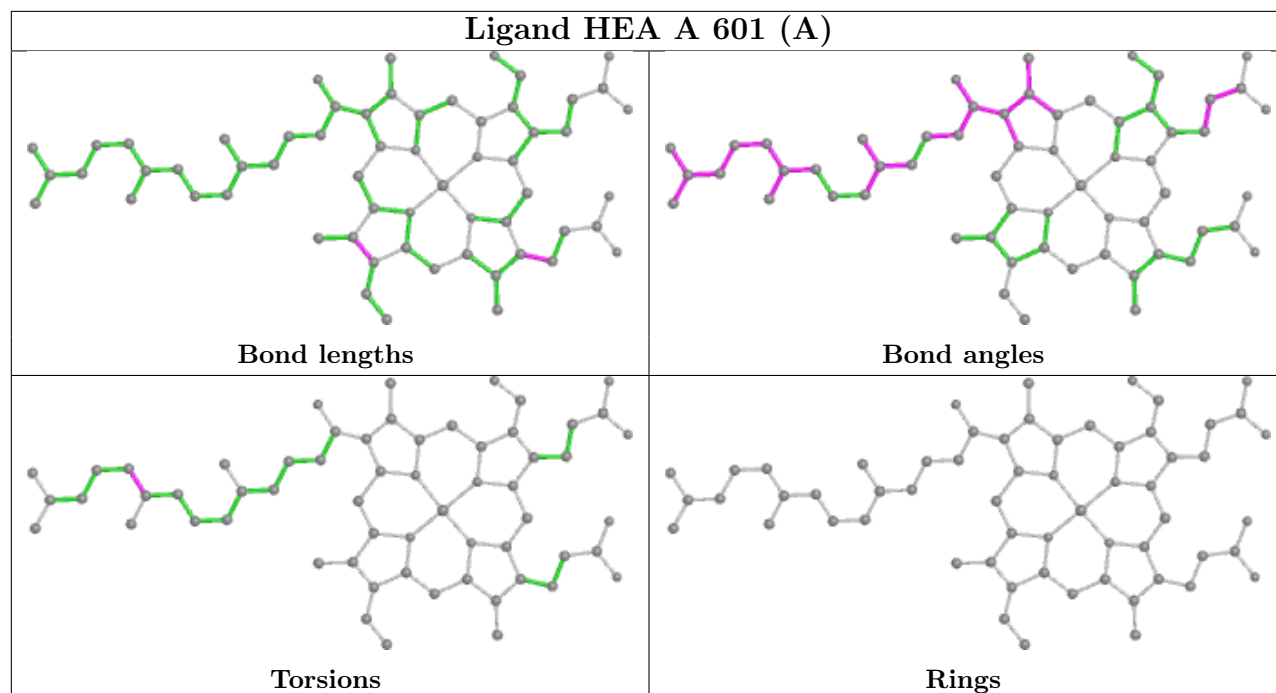


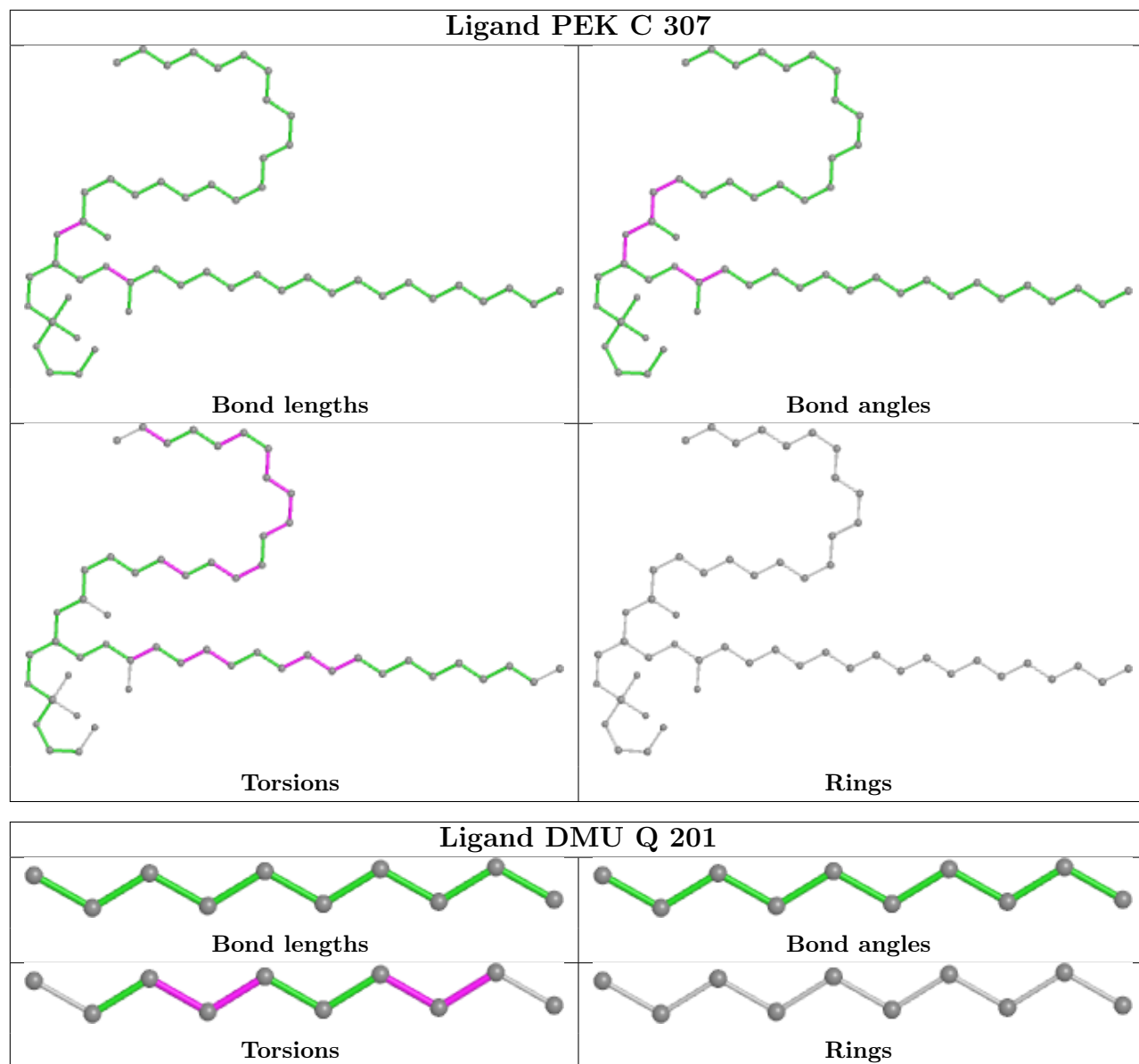


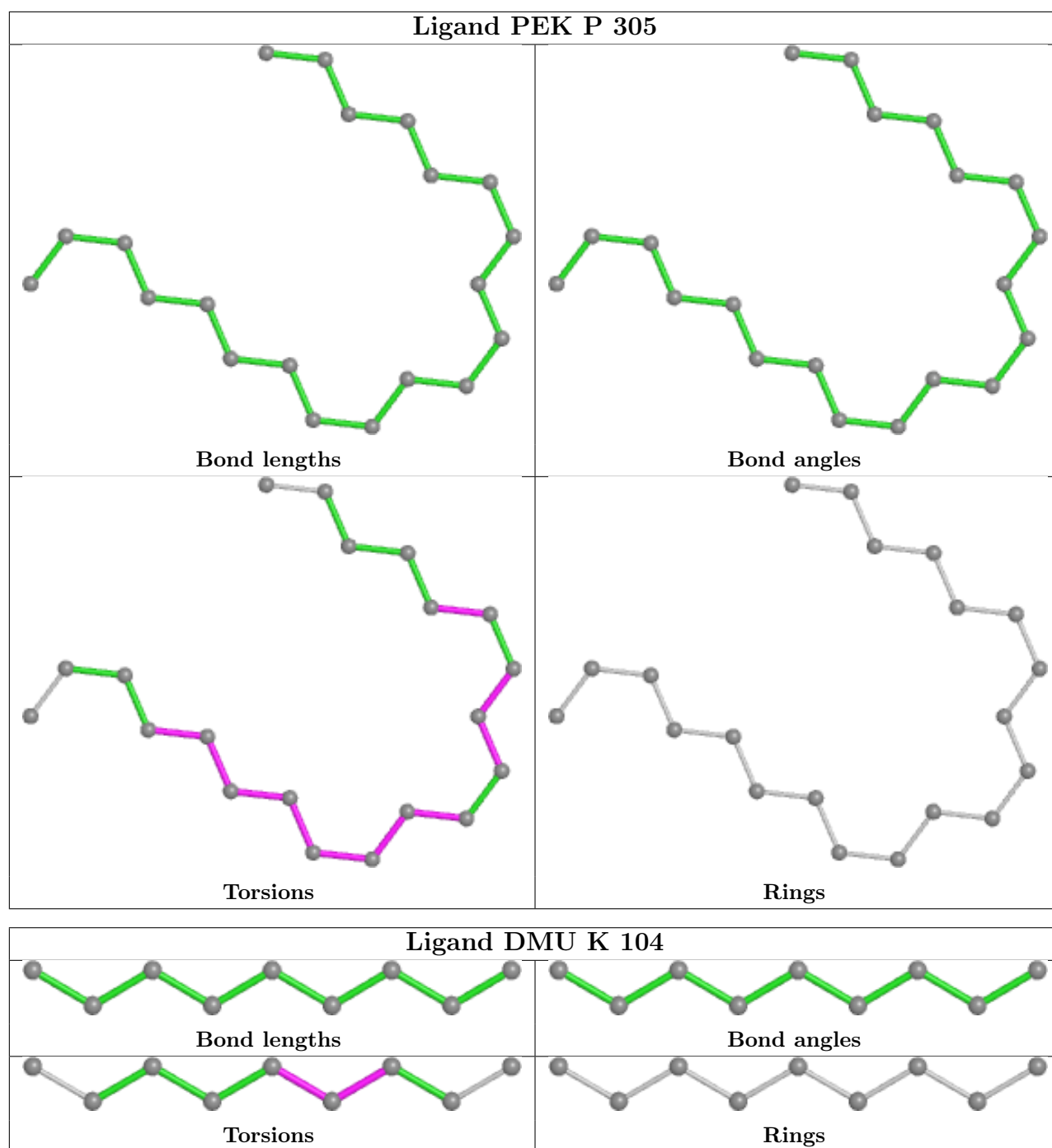


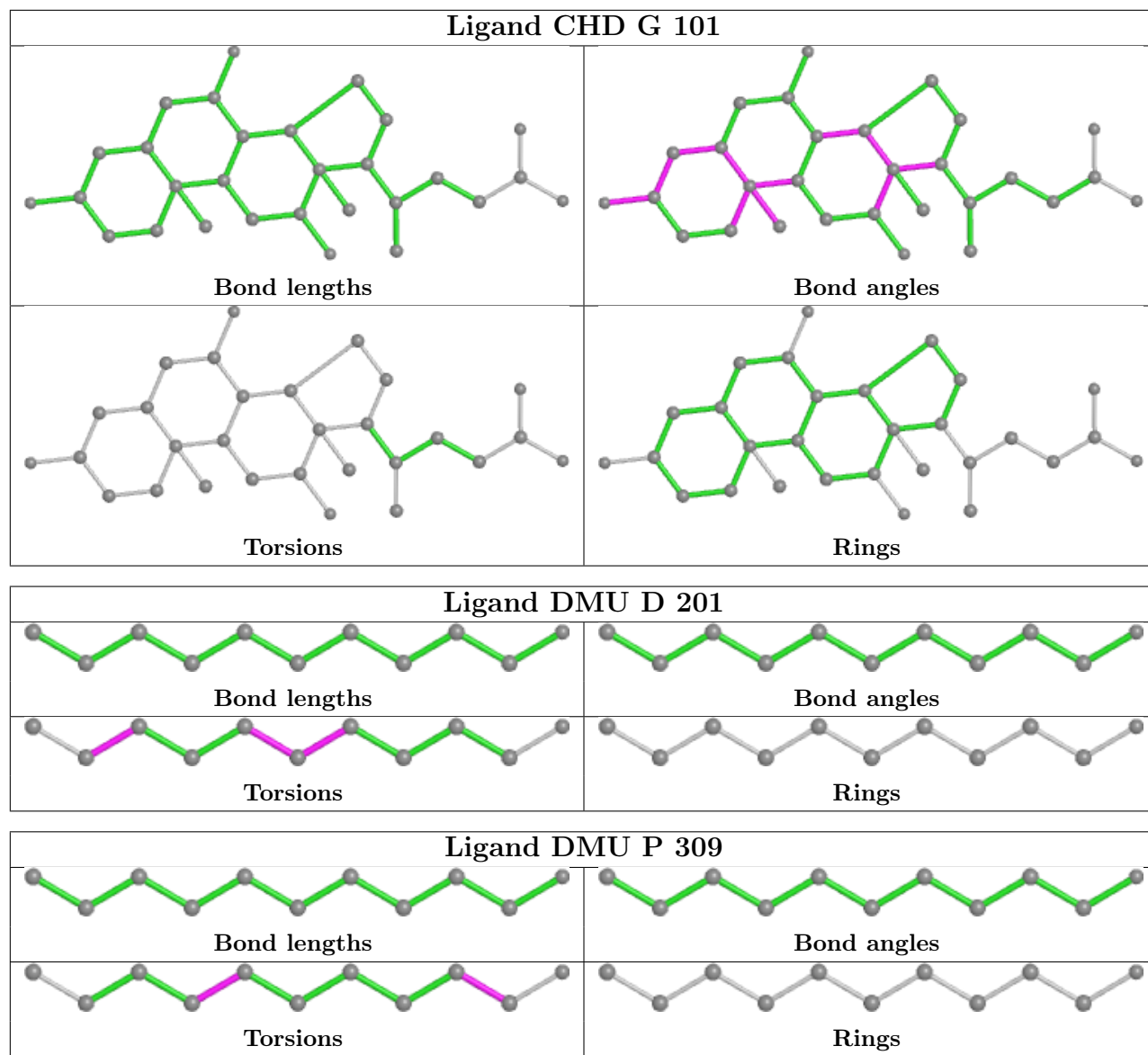


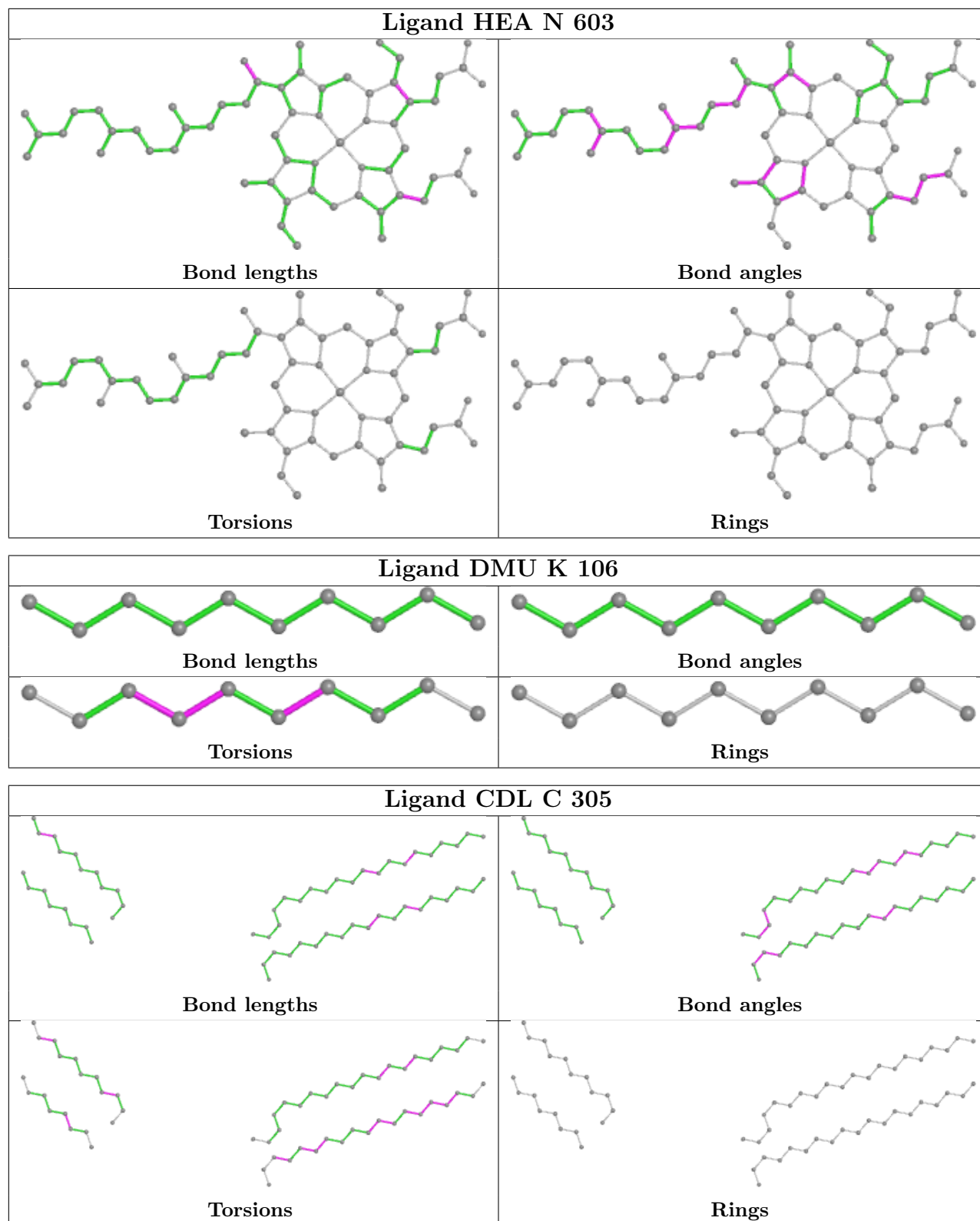


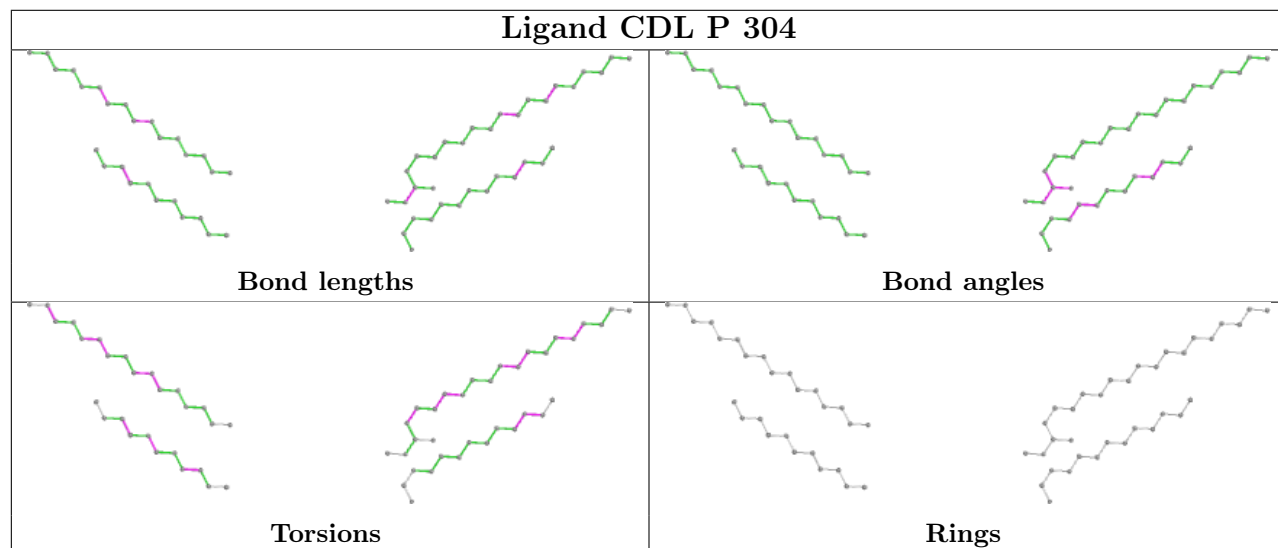
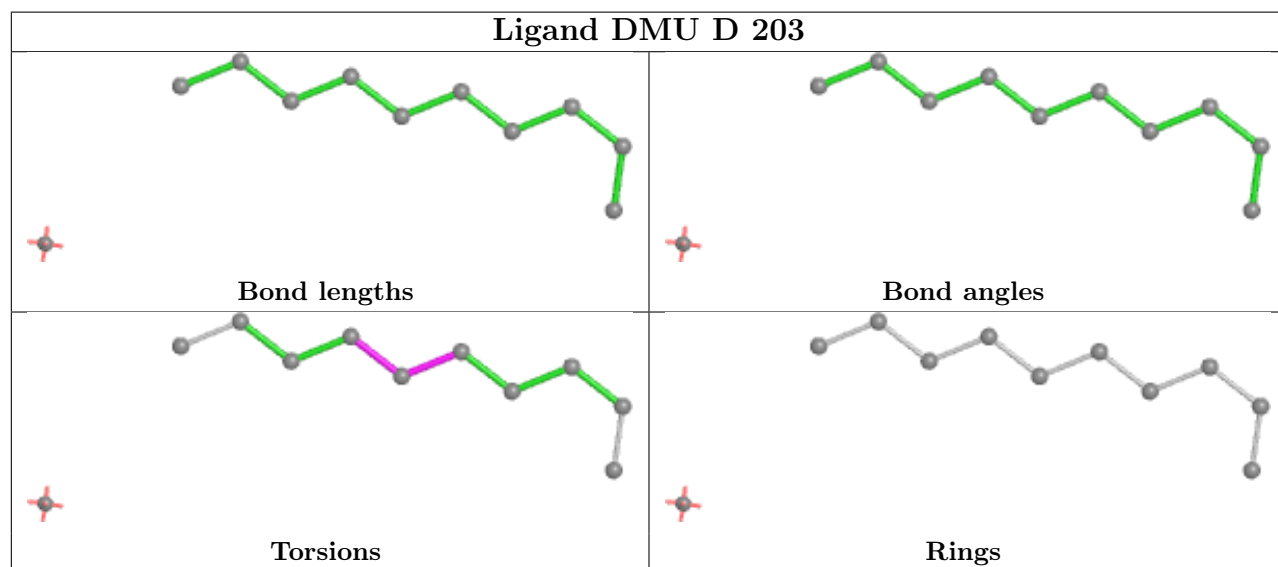
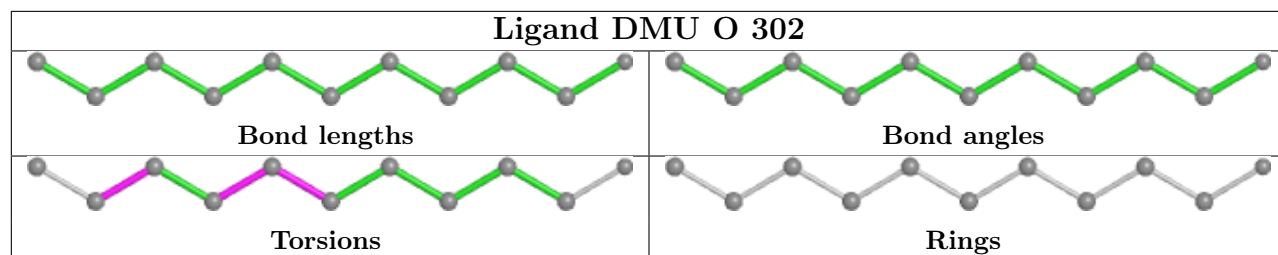


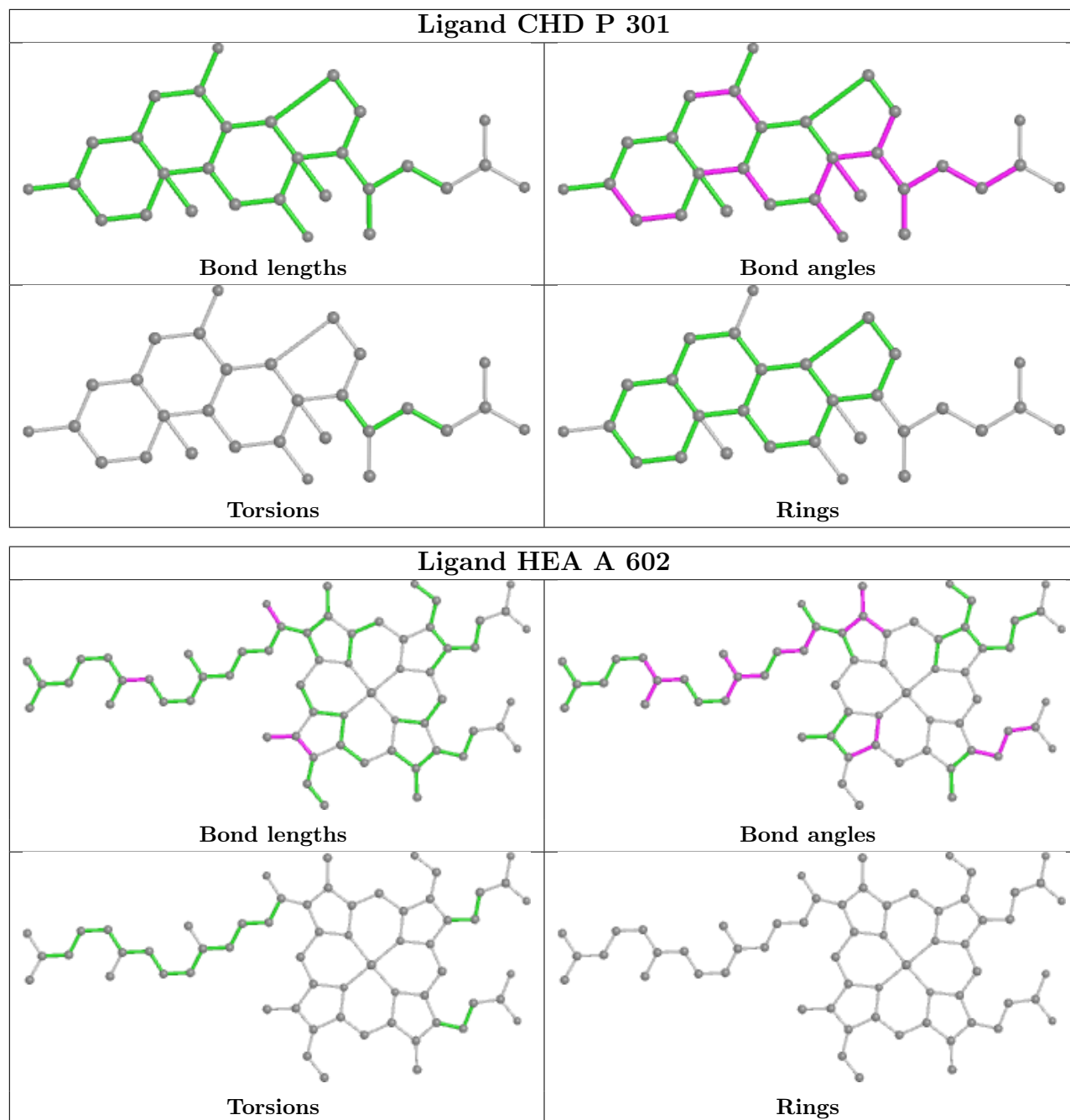


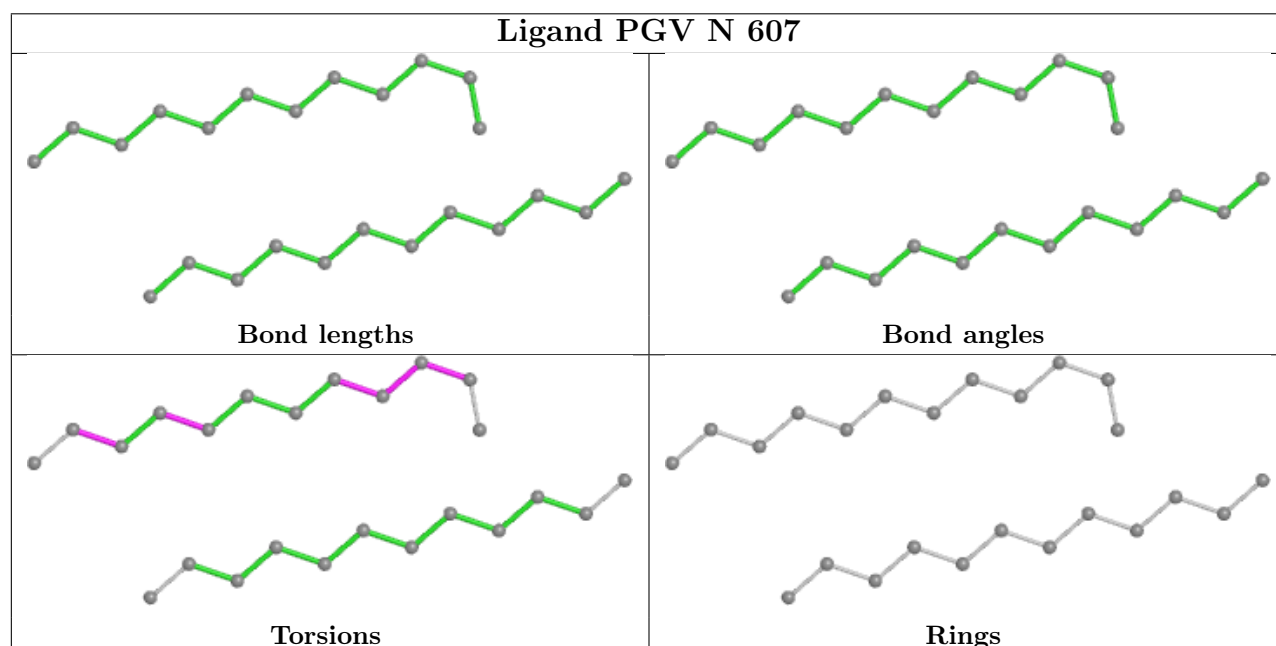
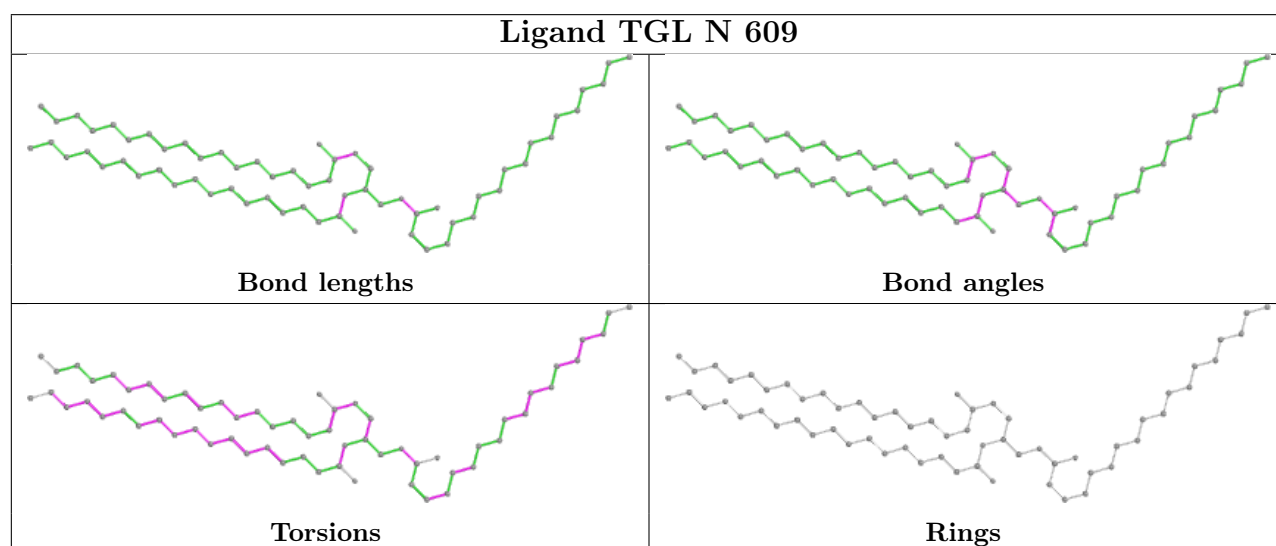
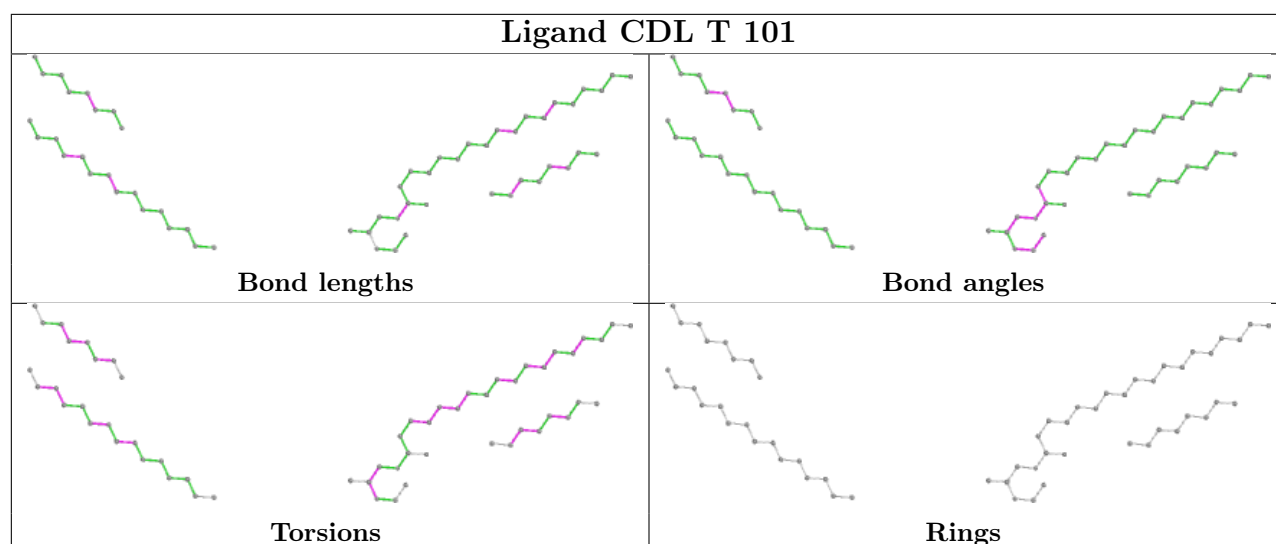


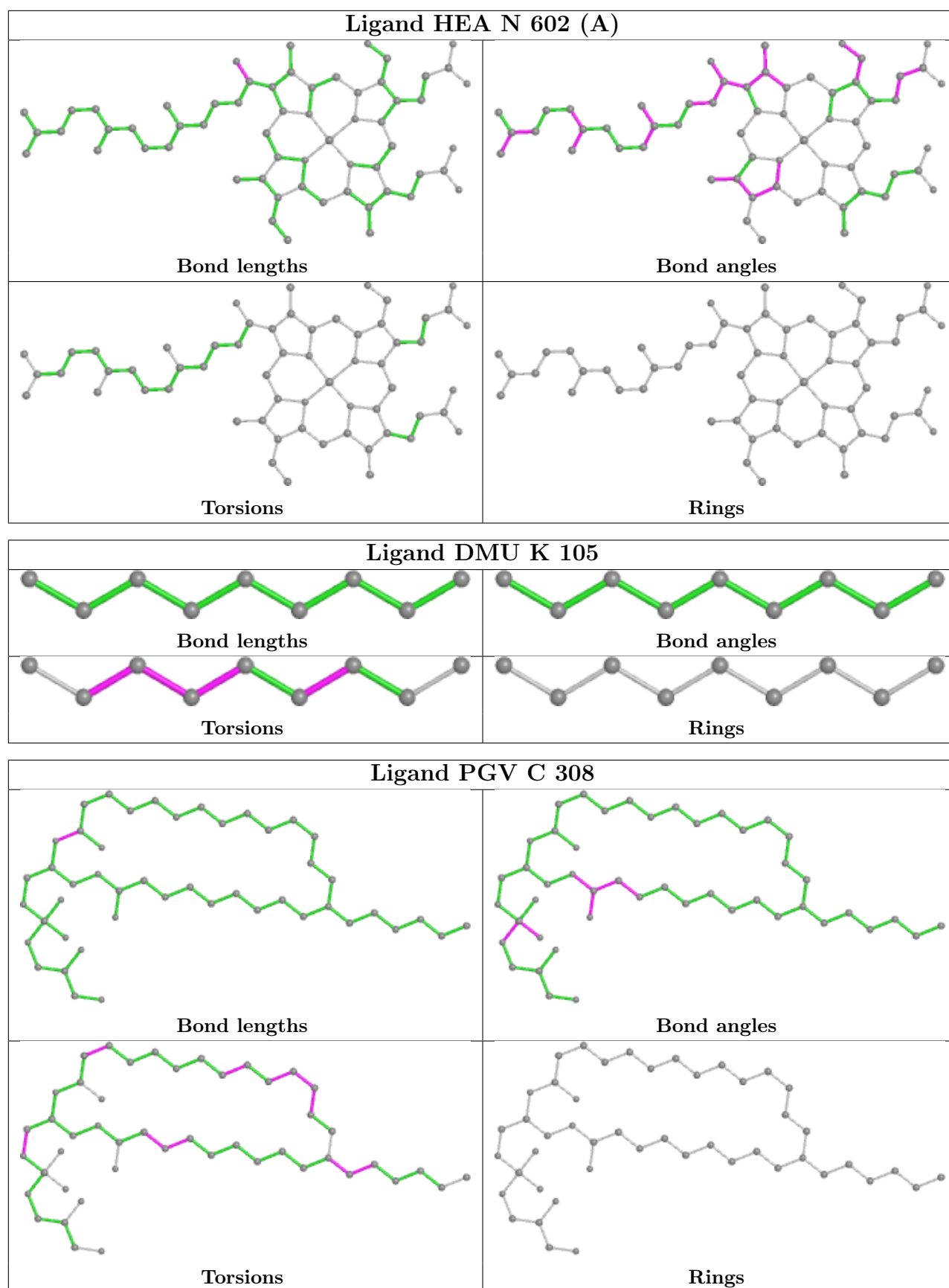


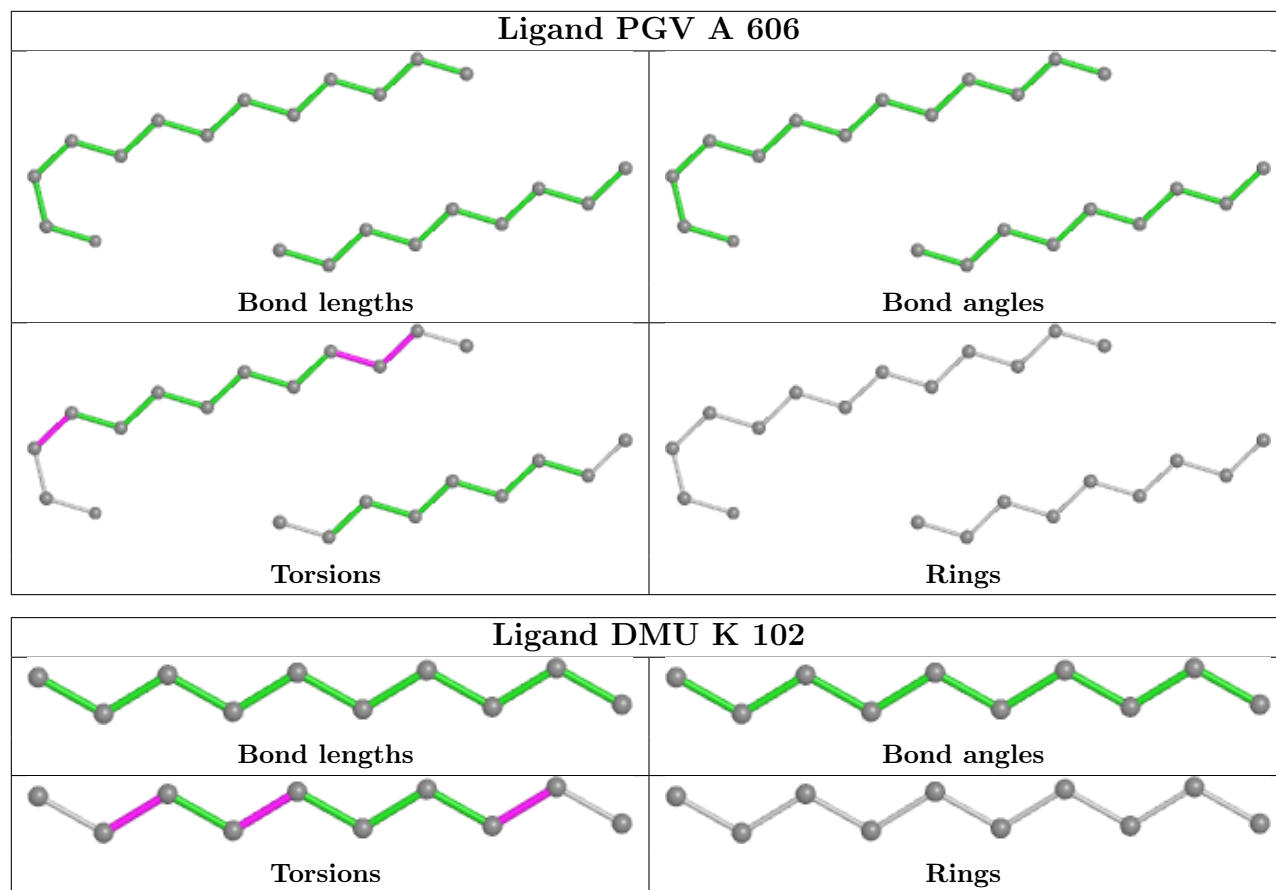


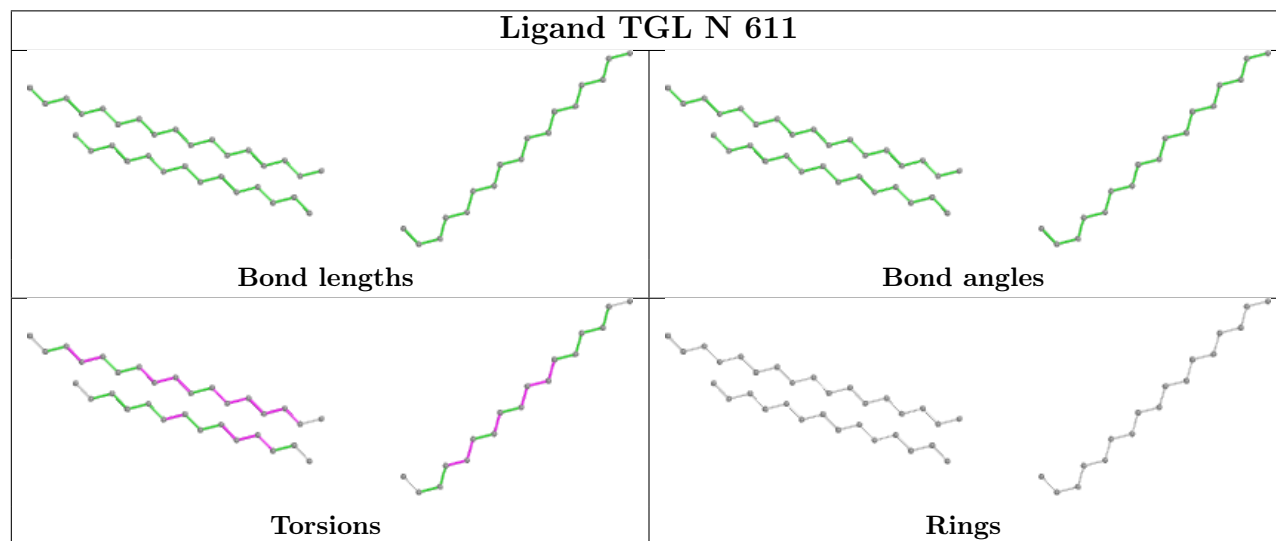
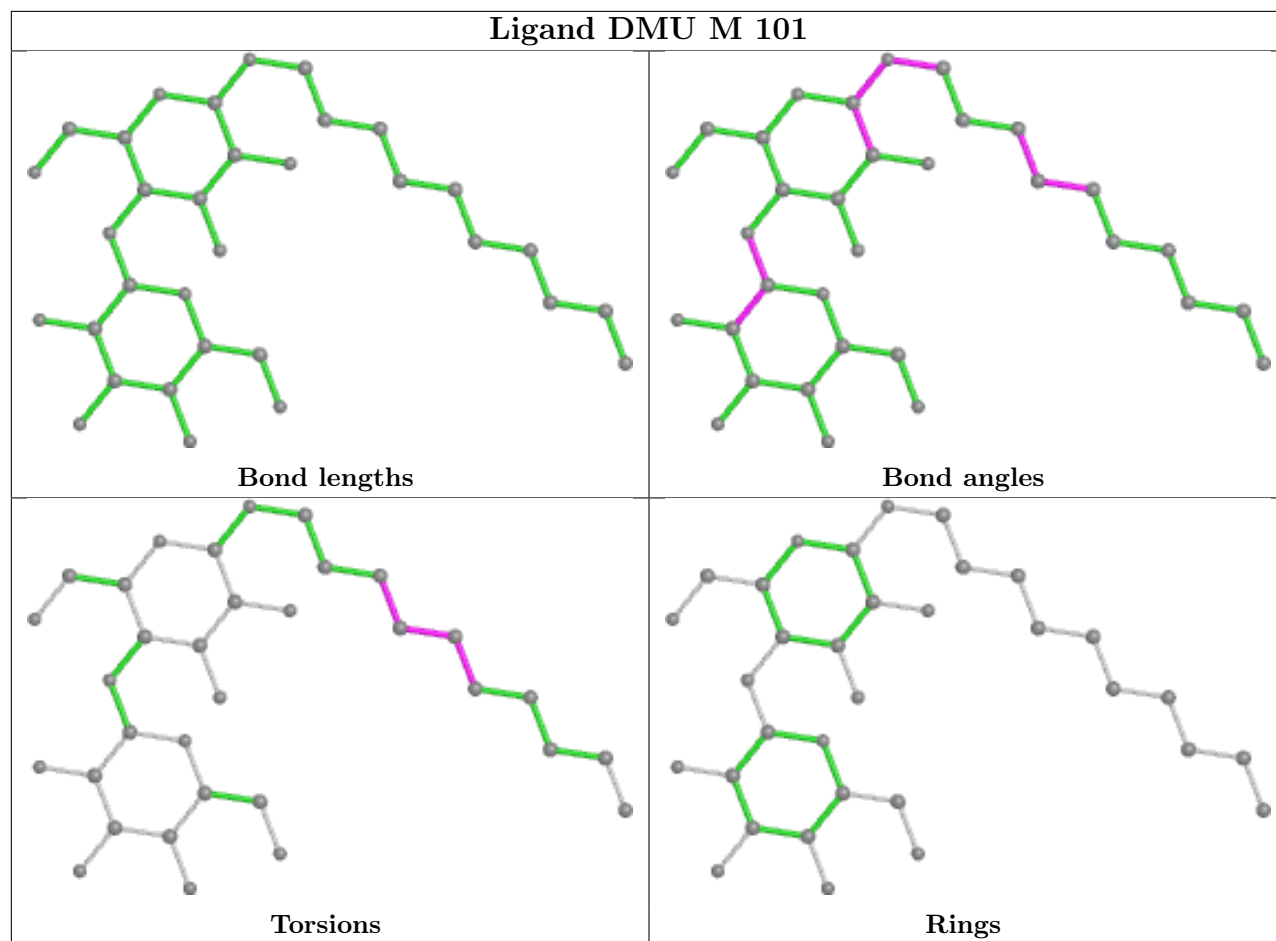


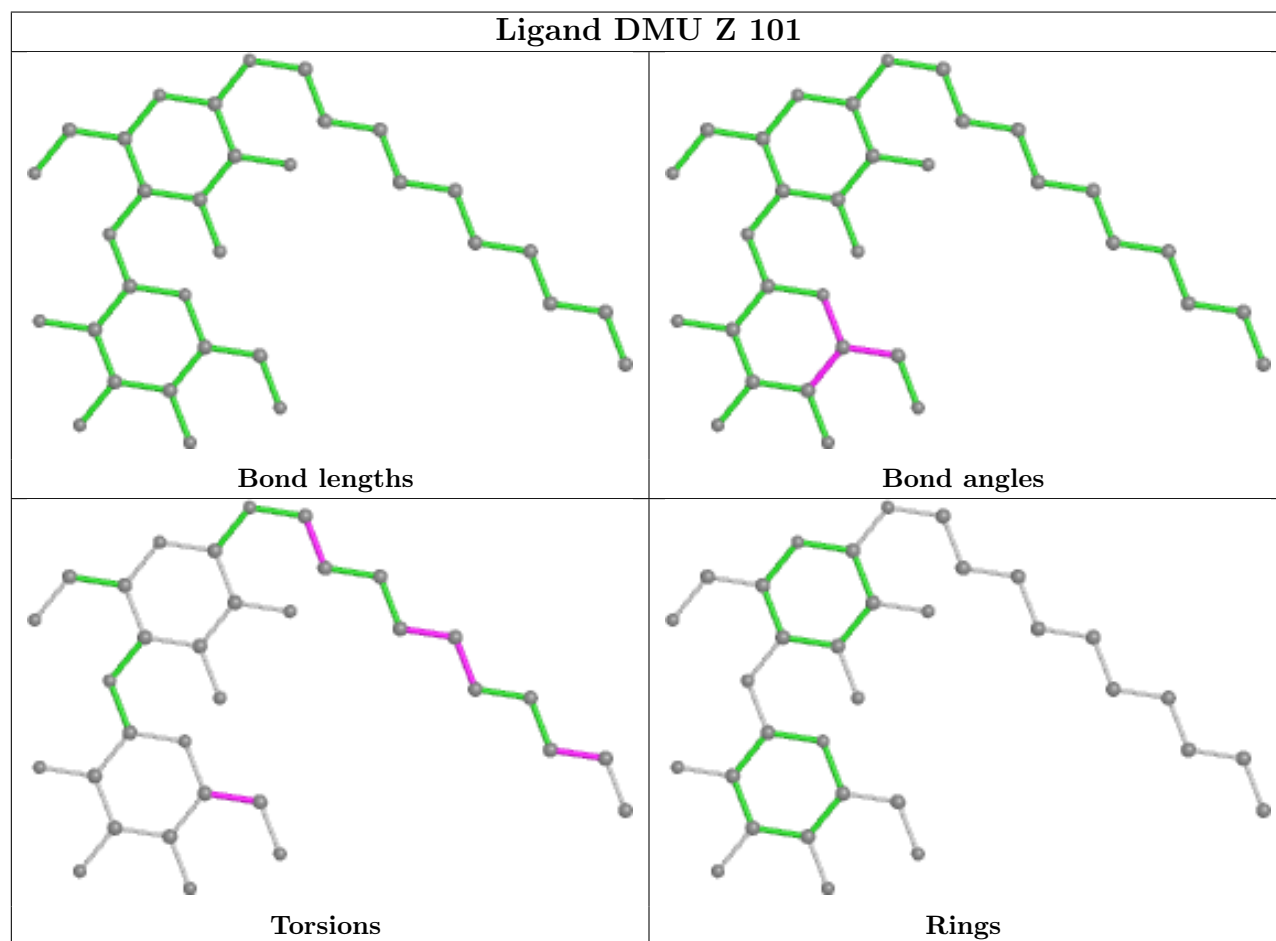
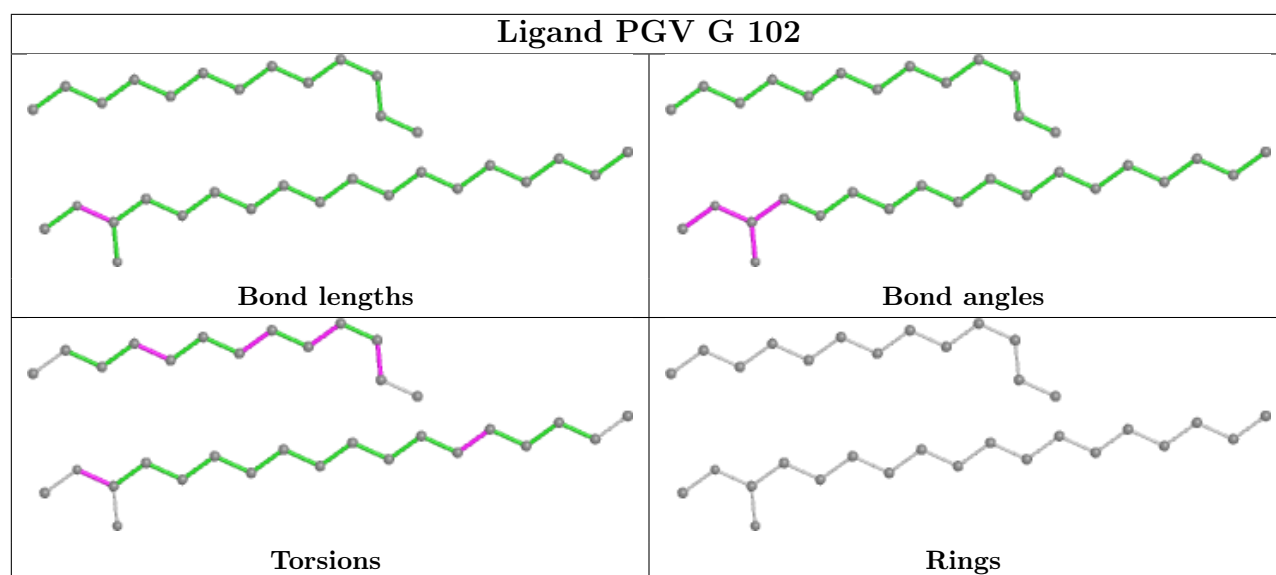


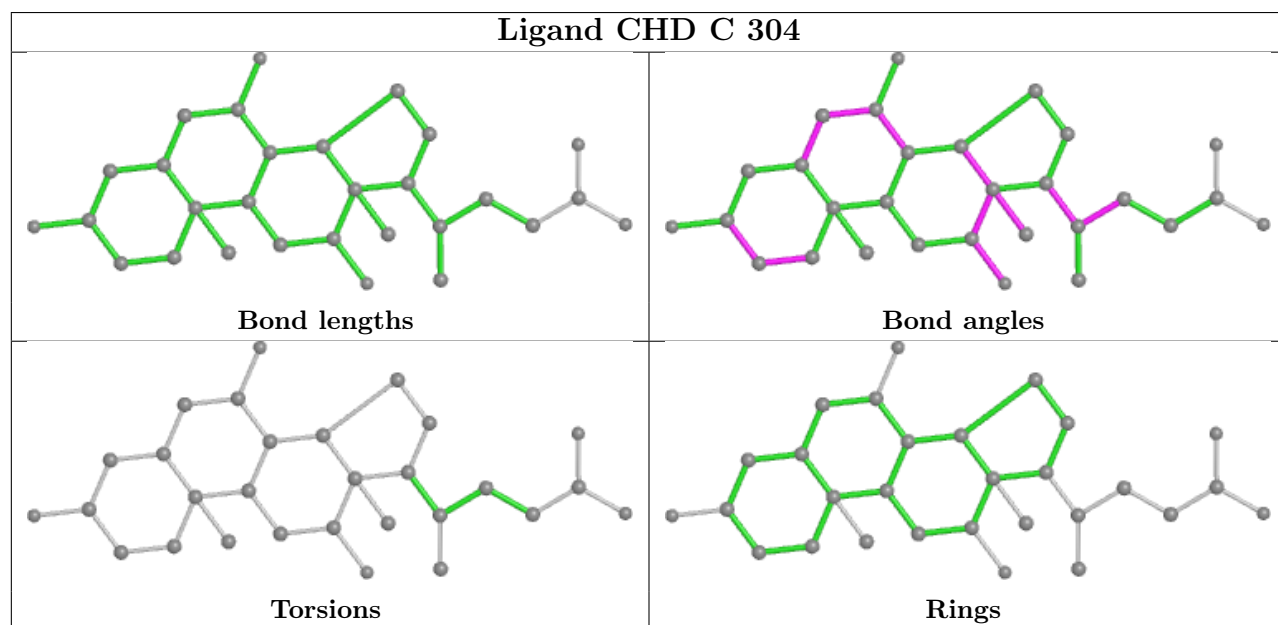
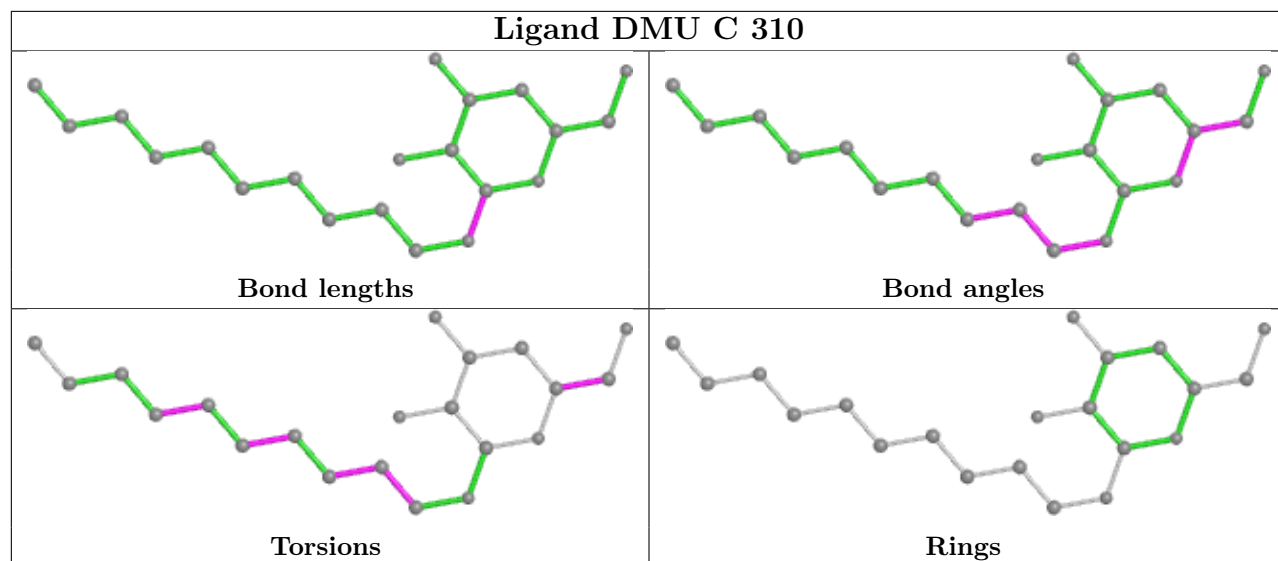


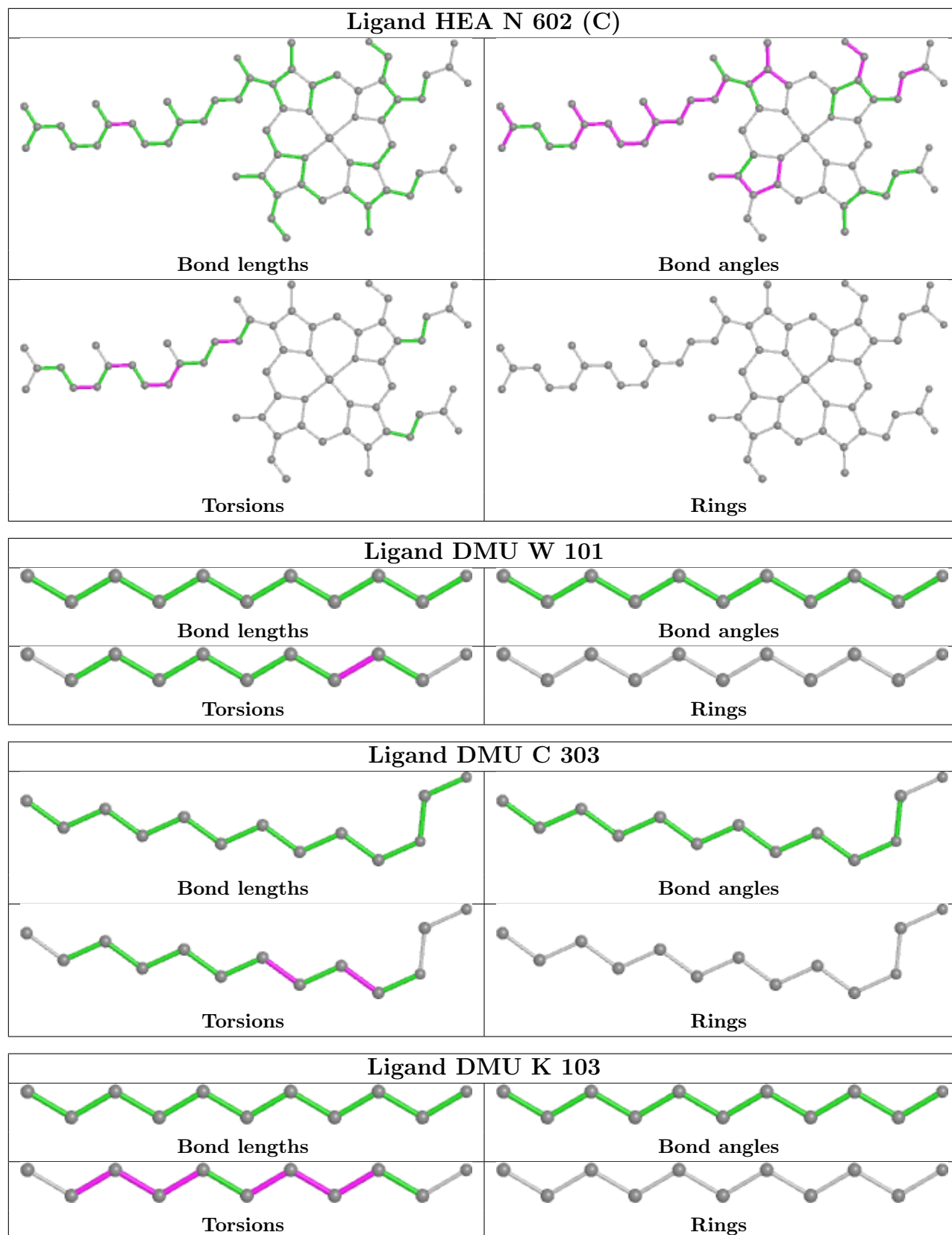




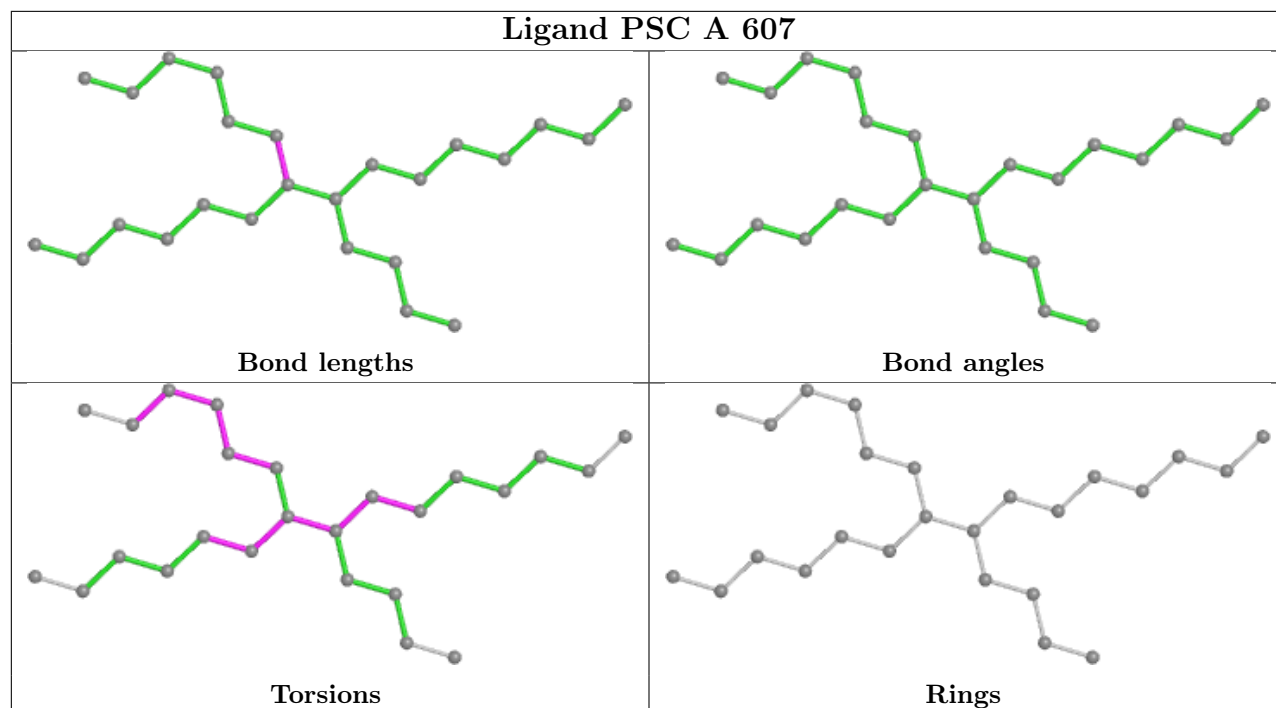




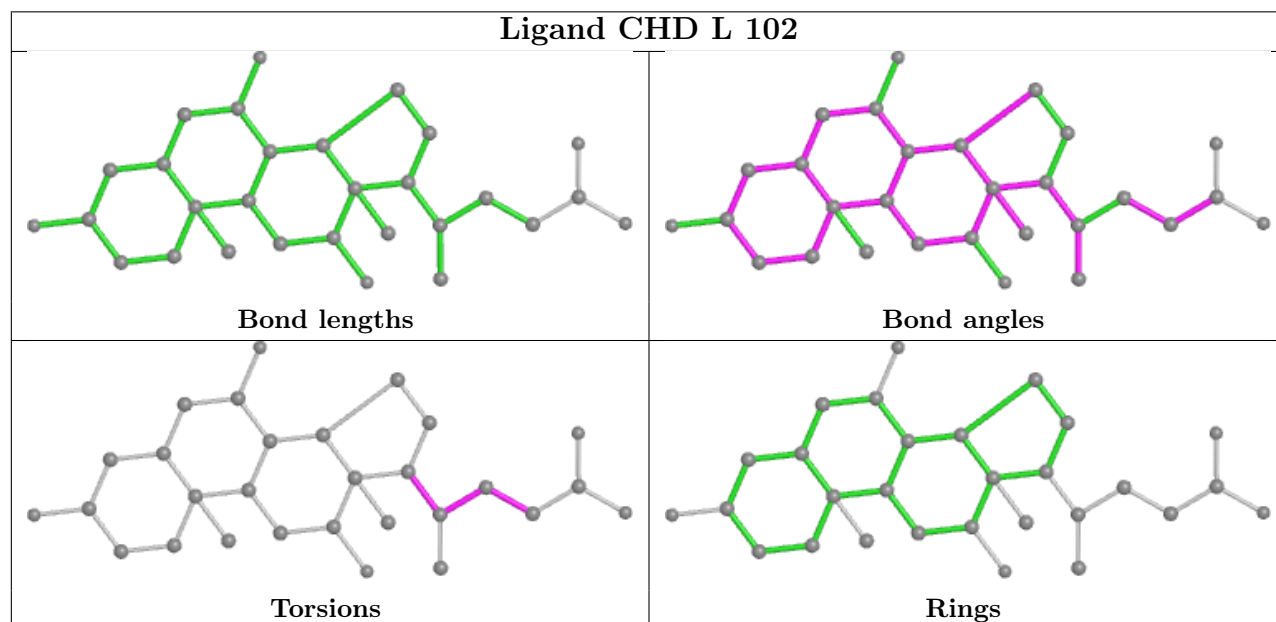


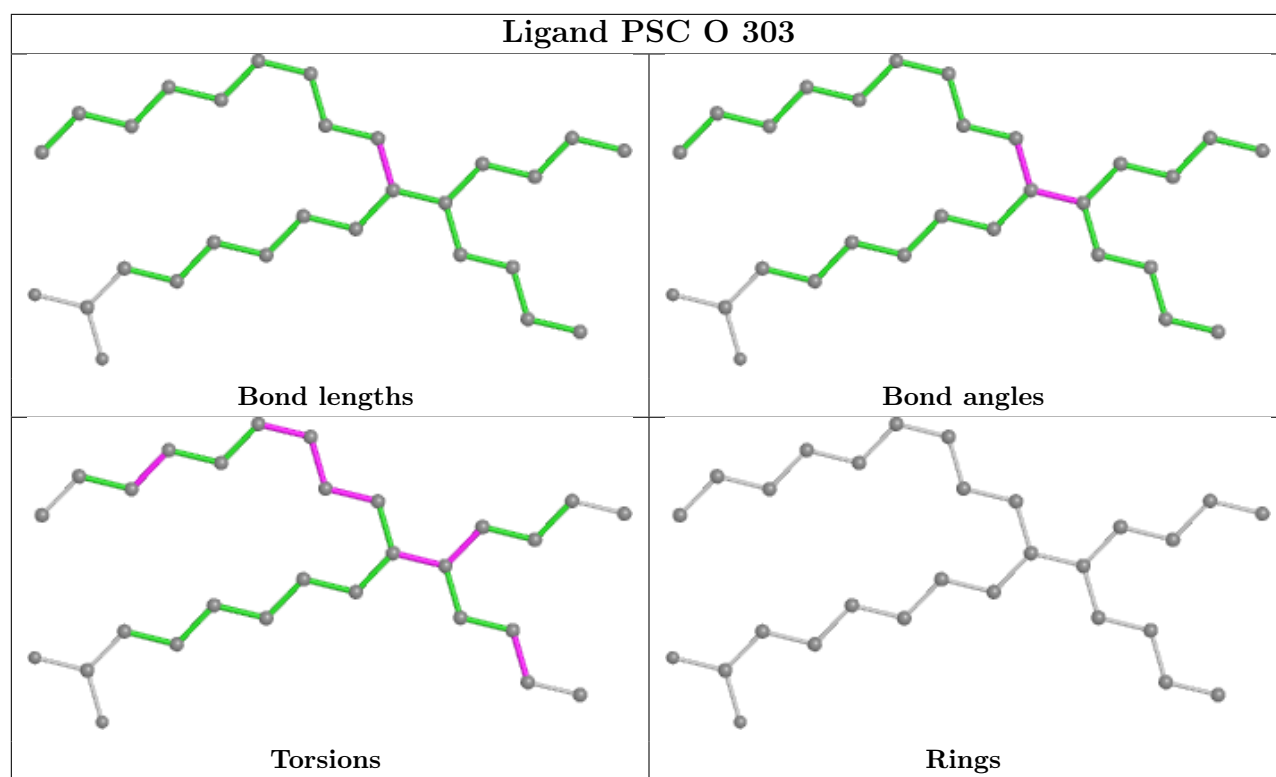


Ligand PSC A 607



Ligand CHD L 102





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.01	1 (0%) 95 96	20, 24, 32, 88	0
1	N	513/514 (99%)	-0.04	0 100 100	21, 27, 36, 89	0
2	B	226/227 (99%)	-0.10	1 (0%) 92 94	21, 30, 60, 105	0
2	O	226/227 (99%)	-0.03	4 (1%) 68 76	24, 34, 75, 148	0
3	C	259/259 (100%)	-0.05	0 100 100	21, 27, 41, 105	0
3	P	259/259 (100%)	-0.02	2 (0%) 86 90	22, 28, 46, 111	0
4	D	144/144 (100%)	-0.22	0 100 100	25, 31, 57, 97	0
4	Q	144/144 (100%)	0.99	8 (5%) 24 30	30, 46, 101, 215	0
5	E	105/105 (100%)	-0.16	2 (1%) 66 74	25, 32, 66, 157	0
5	R	105/105 (100%)	-0.01	2 (1%) 66 74	29, 41, 78, 155	0
6	F	94/94 (100%)	0.02	3 (3%) 47 54	23, 33, 66, 148	0
6	S	94/94 (100%)	0.07	4 (4%) 35 41	23, 32, 73, 159	0
7	G	84/84 (100%)	0.74	16 (19%) 1 1	25, 36, 137, 156	0
7	T	84/84 (100%)	1.00	16 (19%) 1 1	25, 38, 137, 184	0
8	H	79/79 (100%)	0.30	6 (7%) 13 18	26, 36, 116, 171	0
8	U	79/79 (100%)	0.24	6 (7%) 13 18	30, 40, 117, 216	0
9	I	72/73 (98%)	0.14	1 (1%) 75 82	29, 45, 77, 103	0
9	V	72/73 (98%)	0.22	1 (1%) 75 82	30, 52, 96, 146	0
10	J	58/58 (100%)	0.26	3 (5%) 27 33	27, 38, 93, 172	0
10	W	58/58 (100%)	0.22	2 (3%) 45 51	29, 42, 92, 152	0
11	K	49/49 (100%)	-0.04	0 100 100	29, 37, 59, 79	0
11	X	49/49 (100%)	0.33	2 (4%) 37 44	36, 48, 98, 113	0
12	L	46/46 (100%)	-0.11	1 (2%) 62 69	25, 29, 57, 111	0
12	Y	46/46 (100%)	0.05	1 (2%) 62 69	29, 36, 85, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.06	2 (4%) 31 37	25, 29, 95, 126	0
13	Z	43/43 (100%)	0.32	5 (11%) 4 6	32, 37, 110, 225	0
All	All	3544/3550 (99%)	0.08	89 (2%) 57 63	20, 31, 78, 225	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	37.3
4	Q	4	SER	35.1
4	Q	6	VAL	23.4
4	Q	8	SER	15.8
7	T	3	ALA	14.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.25	0.34	113,156,190,197	0
9	SAC	I	1	9/10	0.82	0.23	112,134,180,200	0
1	FME	N	1	10/11	0.94	0.14	38,42,98,131	0
2	FME	B	1	10/11	0.97	0.12	27,28,38,142	0
1	FME	A	1	10/11	0.97	0.09	35,49,83,103	0
2	FME	O	1	10/11	0.98	0.09	31,34,42,112	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	DMU	X	102	10/33	0.38	0.33	62,71,99,116	0
25	DMU	D	203	11/33	0.60	0.32	52,74,124,137	0
21	EDO	C	312	4/4	0.63	0.19	48,71,72,75	0
26	CDL	T	101	57/100	0.66	0.25	42,72,104,149	0
21	EDO	N	619	4/4	0.68	0.24	51,52,54,67	0
21	EDO	A	615	4/4	0.68	0.18	49,58,60,64	0
21	EDO	P	312	4/4	0.69	0.15	67,72,73,77	0
25	DMU	K	104	9/33	0.69	0.27	49,70,113,125	0
25	DMU	X	104	10/33	0.74	0.27	62,84,90,92	0
25	DMU	Q	201	10/33	0.74	0.16	52,62,68,111	0
21	EDO	F	103	4/4	0.75	0.16	50,61,64,82	0
25	DMU	P	309	11/33	0.76	0.30	42,58,101,104	0
21	EDO	P	316	4/4	0.77	0.15	39,56,66,82	0
22	TGL	N	611	48/63	0.77	0.18	48,68,120,134	0
24	CHD	Y	101	29/29	0.77	0.27	56,95,143,158	0
21	EDO	P	310	4/4	0.77	0.10	46,60,67,75	0
21	EDO	C	317	4/4	0.77	0.13	55,56,72,75	0
26	CDL	N	601	55/100	0.78	0.28	51,69,104,118	0
25	DMU	X	103	9/33	0.78	0.30	55,62,94,101	0
21	EDO	P	311	4/4	0.80	0.14	62,62,65,73	0
27	PEK	C	309	36/53	0.80	0.23	42,75,110,130	0
27	PEK	P	308	34/53	0.80	0.25	37,70,117,134	0
18	PGV	C	311	28/51	0.81	0.19	41,66,117,126	0
21	EDO	P	317	4/4	0.81	0.11	57,90,97,106	0
25	DMU	L	101	21/33	0.81	0.17	42,81,114,129	0
18	PGV	G	102	32/51	0.81	0.20	39,72,108,130	0
22	TGL	N	612	44/63	0.81	0.23	41,59,127,197	0
27	PEK	P	305	20/53	0.81	0.17	47,56,95,96	0
21	EDO	C	313	4/4	0.81	0.12	30,32,33,94	0
25	DMU	X	101	11/33	0.82	0.16	43,59,104,225	0
21	EDO	C	320	4/4	0.82	0.24	32,56,75,112	0
25	DMU	K	102	10/33	0.82	0.21	46,69,87,103	0
18	PGV	N	607	24/51	0.83	0.19	41,53,106,166	0
27	PEK	C	306	25/53	0.83	0.22	41,57,96,119	0
21	EDO	L	104	4/4	0.83	0.20	50,51,77,148	0
22	TGL	D	202	57/63	0.83	0.16	32,65,134,156	0
25	DMU	K	105	9/33	0.83	0.34	72,75,92,107	0
22	TGL	B	301	49/63	0.84	0.15	38,61,98,147	0
24	CHD	L	102	29/29	0.84	0.30	51,100,145,177	0
21	EDO	G	104	4/4	0.84	0.14	33,77,87,92	0
21	EDO	A	609	4/4	0.84	0.14	34,38,47,146	0
25	DMU	O	302	11/33	0.84	0.20	54,58,104,111	0
25	DMU	P	303	13/33	0.84	0.14	53,62,94,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	DMU	C	303	13/33	0.85	0.11	53,63,88,92	0
26	CDL	C	305	58/100	0.85	0.18	44,65,131,156	0
21	EDO	Q	202	4/4	0.85	0.14	43,50,52,56	0
25	DMU	W	101	11/33	0.85	0.20	51,59,82,111	0
22	TGL	L	103	56/63	0.86	0.17	28,56,121,139	0
25	DMU	K	103	11/33	0.86	0.23	50,70,100,120	0
25	DMU	J	101	11/33	0.86	0.17	49,58,81,102	0
25	DMU	C	310	21/33	0.87	0.18	29,58,111,142	0
22	TGL	N	609	63/63	0.87	0.18	40,72,117,154	0
21	EDO	D	204	4/4	0.87	0.22	37,47,79,85	0
21	EDO	A	614	4/4	0.87	0.21	55,66,70,75	0
26	CDL	P	304	61/100	0.88	0.18	37,69,128,196	0
21	EDO	C	314	4/4	0.88	0.14	32,39,42,44	0
19	PSC	O	303	30/52	0.89	0.16	37,59,103,106	0
21	EDO	O	306	4/4	0.89	0.15	48,63,79,92	0
25	DMU	D	201	11/33	0.89	0.14	44,69,79,88	0
21	EDO	B	306	4/4	0.90	0.12	29,35,41,55	0
25	DMU	K	106	10/33	0.90	0.19	52,65,91,120	0
21	EDO	T	103	4/4	0.90	0.23	43,65,78,97	0
21	EDO	N	621	4/4	0.90	0.10	46,52,52,62	0
21	EDO	J	102	4/4	0.91	0.30	52,52,100,116	0
25	DMU	K	101	9/33	0.91	0.14	41,52,77,94	0
19	PSC	A	607	27/52	0.91	0.18	36,66,100,129	0
18	PGV	A	606	22/51	0.91	0.14	31,45,70,94	0
21	EDO	T	104	4/4	0.91	0.22	39,49,54,71	0
29	PO4	U	101	5/5	0.91	0.17	47,54,128,200	0
25	DMU	Z	101	33/33	0.92	0.10	38,46,79,84	0
21	EDO	O	305	4/4	0.92	0.31	42,46,51,95	0
21	EDO	N	620	4/4	0.92	0.17	33,34,66,104	0
21	EDO	W	102	4/4	0.92	0.19	47,57,68,111	0
21	EDO	S	104	4/4	0.92	0.20	40,56,58,88	0
21	EDO	S	106	4/4	0.93	0.17	39,47,67,81	0
21	EDO	A	610	4/4	0.93	0.13	39,48,53,70	0
21	EDO	C	316	4/4	0.93	0.11	53,56,61,69	0
21	EDO	J	103	4/4	0.93	0.20	51,52,72,74	0
25	DMU	M	101	33/33	0.93	0.10	31,40,53,69	0
21	EDO	B	307	4/4	0.93	0.16	34,45,46,48	0
21	EDO	A	617	4/4	0.94	0.25	37,39,46,63	0
21	EDO	C	318	4/4	0.94	0.20	40,60,63,111	0
21	EDO	P	315	4/4	0.94	0.15	53,58,63,73	0
21	EDO	F	106	4/4	0.94	0.19	35,38,76,104	0
21	EDO	N	616	4/4	0.94	0.21	33,41,44,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CHD	C	304	29/29	0.94	0.09	26,29,35,41	0
21	EDO	Y	103	4/4	0.94	0.31	46,59,90,134	0
21	EDO	A	618	4/4	0.94	0.16	33,34,39,87	0
21	EDO	N	614	4/4	0.95	0.10	37,38,39,44	0
21	EDO	C	319	4/4	0.95	0.29	43,53,61,115	0
17	NA	P	302	1/1	0.95	0.10	30,30,30,30	0
21	EDO	A	612	4/4	0.95	0.15	28,31,32,38	0
21	EDO	T	102	4/4	0.95	0.13	31,32,37,40	0
21	EDO	P	313	4/4	0.95	0.18	34,37,39,39	0
21	EDO	E	203	4/4	0.95	0.12	42,45,54,117	0
21	EDO	A	613	4/4	0.95	0.15	28,39,46,48	0
24	CHD	G	101	29/29	0.95	0.09	21,26,35,42	0
21	EDO	Y	102	4/4	0.95	0.20	48,57,57,83	0
24	CHD	P	301	29/29	0.95	0.08	24,29,35,40	0
21	EDO	D	205	4/4	0.96	0.13	44,45,46,101	0
18	PGV	N	608	51/51	0.96	0.13	23,34,69,80	0
21	EDO	P	314	4/4	0.96	0.10	30,35,40,62	0
21	EDO	S	105	4/4	0.96	0.10	31,31,31,33	0
27	PEK	P	306	53/53	0.96	0.11	28,41,84,122	0
21	EDO	N	617	4/4	0.96	0.10	22,29,30,32	0
21	EDO	O	304	4/4	0.96	0.08	30,31,32,32	0
21	EDO	C	315	4/4	0.97	0.15	28,35,50,72	0
21	EDO	G	103	4/4	0.97	0.08	30,31,35,35	0
21	EDO	A	616	4/4	0.97	0.11	30,42,68,94	0
24	CHD	B	303	29/29	0.97	0.08	21,26,31,46	0
18	PGV	C	301	51/51	0.97	0.11	22,32,67,80	0
21	EDO	D	206	4/4	0.97	0.11	36,38,58,71	0
21	EDO	E	201	4/4	0.97	0.09	37,38,38,39	0
21	EDO	N	613	4/4	0.97	0.11	28,29,29,32	0
21	EDO	E	202	4/4	0.97	0.09	31,38,43,45	0
27	PEK	C	307	53/53	0.97	0.12	26,42,102,136	0
21	EDO	N	615	4/4	0.97	0.16	37,40,41,67	0
20	PER	A	608[A]	2/2	0.97	0.12	23,23,23,23	2
20	PER	N	610[A]	2/2	0.97	0.09	28,28,28,28	2
21	EDO	N	618	4/4	0.97	0.15	31,41,43,47	0
29	PO4	H	101	5/5	0.97	0.18	56,61,94,161	0
21	EDO	F	105	4/4	0.97	0.14	39,44,64,96	0
14	HEA	N	602[A]	60/60	0.98	0.11	20,25,38,46	17
14	HEA	N	602[B]	52/60	0.98	0.11	16,24,33,47	9
14	HEA	N	602[C]	52/60	0.98	0.11	20,24,40,52	9
18	PGV	P	307	51/51	0.98	0.12	23,32,97,138	0
14	HEA	N	603	60/60	0.98	0.09	19,23,29,38	0

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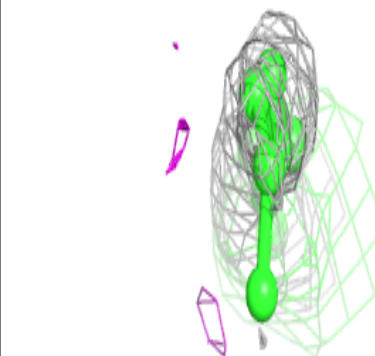
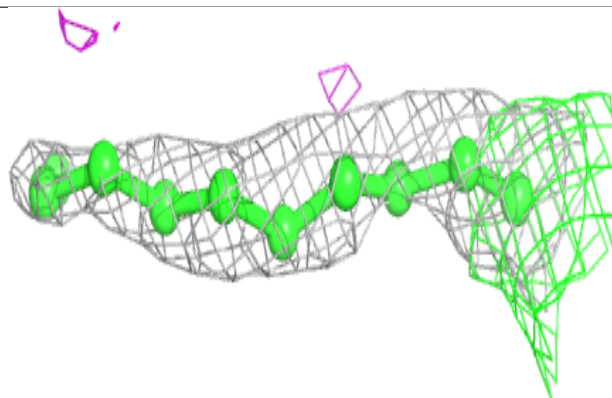
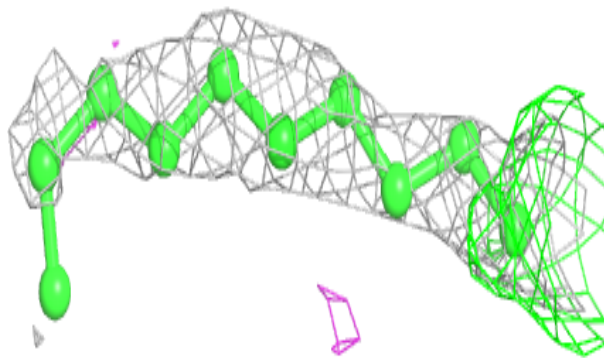
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	B	304	4/4	0.98	0.10	24,25,27,29	0
21	EDO	B	305	4/4	0.98	0.13	32,34,45,103	0
16	MG	A	604	1/1	0.98	0.04	19,19,19,19	0
17	NA	C	302	1/1	0.98	0.08	31,31,31,31	0
14	HEA	A	601[A]	60/60	0.98	0.11	17,21,33,63	17
21	EDO	S	102	4/4	0.98	0.15	23,25,25,25	0
21	EDO	S	103	4/4	0.98	0.07	32,33,38,41	0
14	HEA	A	601[B]	52/60	0.98	0.11	10,20,27,55	9
21	EDO	F	104	4/4	0.98	0.15	30,30,31,32	0
14	HEA	A	601[C]	52/60	0.98	0.11	17,21,31,57	9
18	PGV	C	308	48/51	0.98	0.11	22,29,71,88	0
14	HEA	A	602	60/60	0.98	0.09	18,22,28,38	0
16	MG	N	605	1/1	0.99	0.04	21,21,21,21	0
21	EDO	F	102	4/4	0.99	0.10	24,25,26,27	0
17	NA	N	606	1/1	0.99	0.07	28,28,28,28	0
21	EDO	A	611	4/4	0.99	0.10	22,24,27,28	0
17	NA	A	605	1/1	0.99	0.06	24,24,24,24	0
15	CU	A	603	1/1	1.00	0.13	22,22,22,22	0
23	CUA	B	302	2/2	1.00	0.13	22,22,22,22	0
28	ZN	F	101	1/1	1.00	0.09	25,25,25,25	0
28	ZN	S	101	1/1	1.00	0.10	26,26,26,26	0
23	CUA	O	301	2/2	1.00	0.10	26,26,26,26	0
15	CU	N	604	1/1	1.00	0.12	24,24,24,24	0

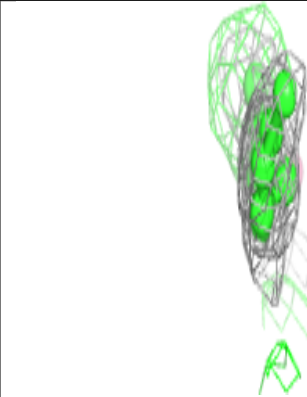
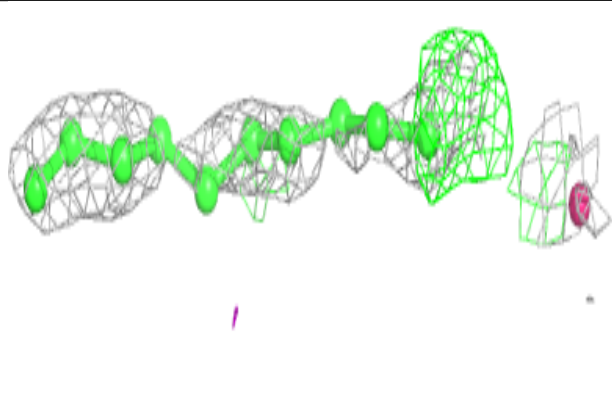
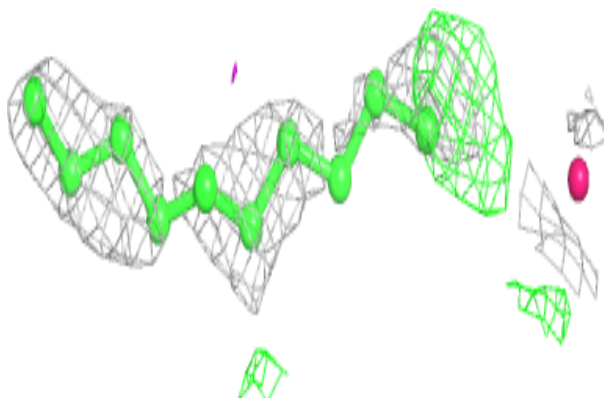
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU X 102:

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

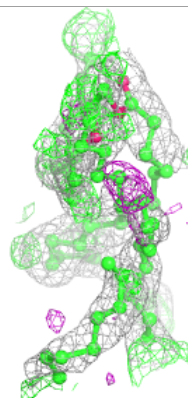
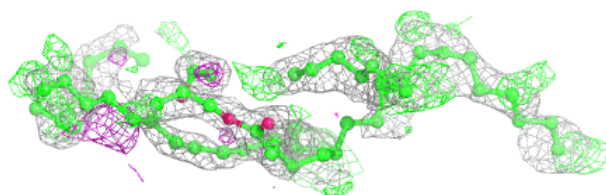
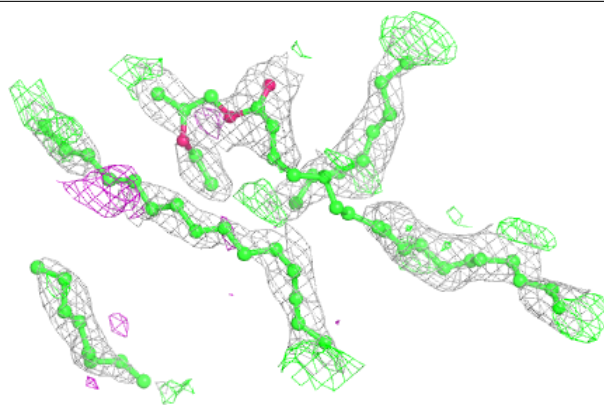
**Electron density around DMU D 203:**

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

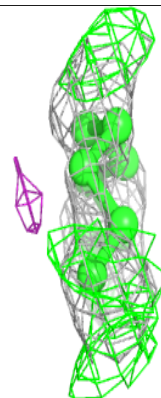
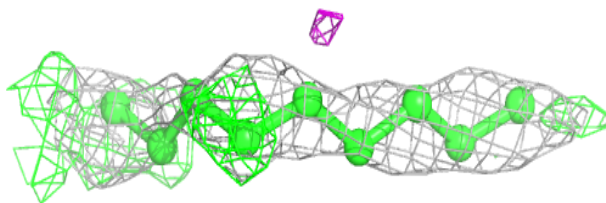
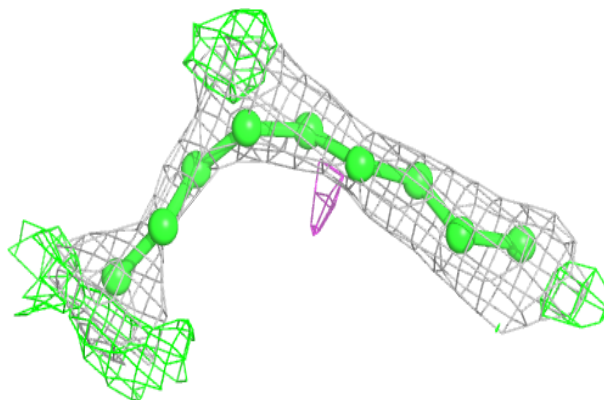


Electron density around CDL T 101:

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

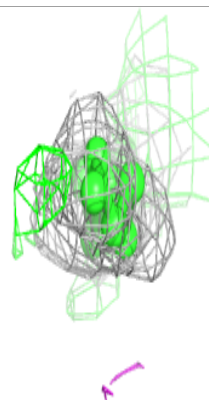
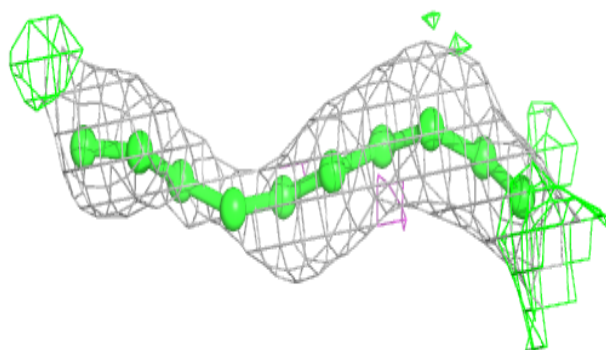
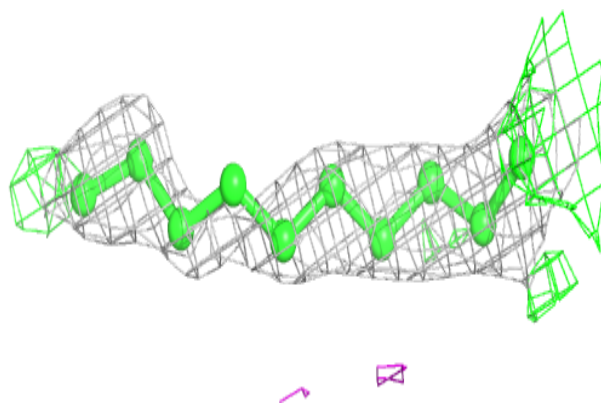
**Electron density around DMU K 104:**

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

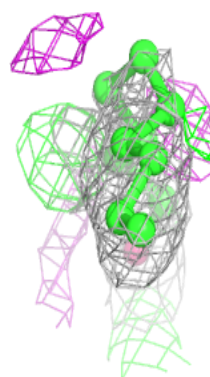
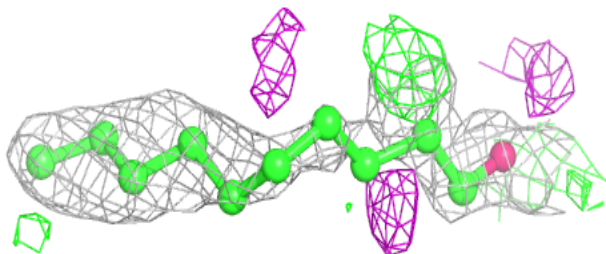
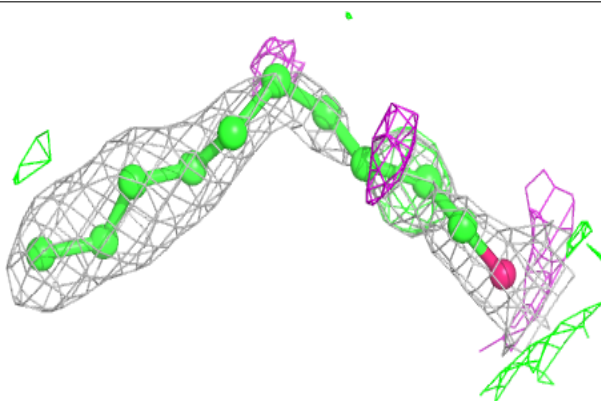


Electron density around DMU Q 201:

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

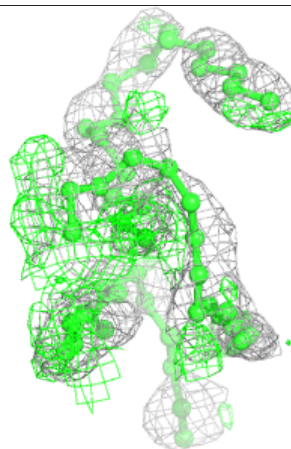
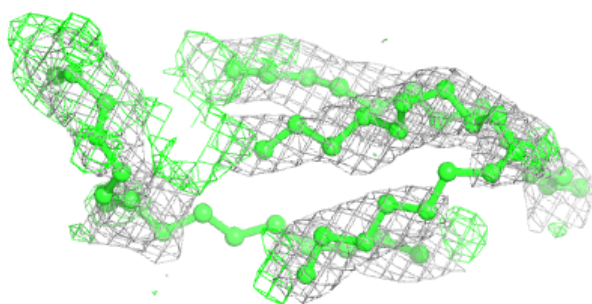
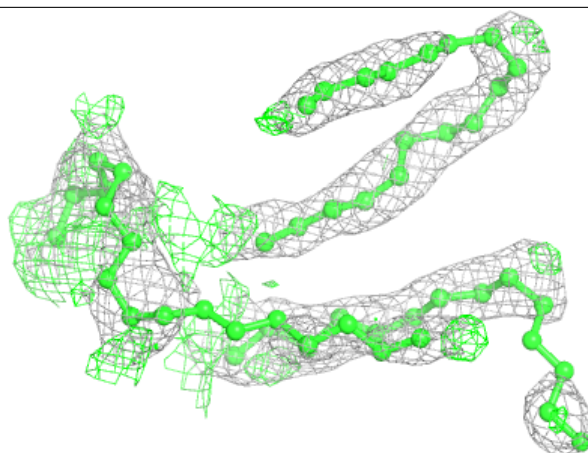
**Electron density around DMU P 309:**

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

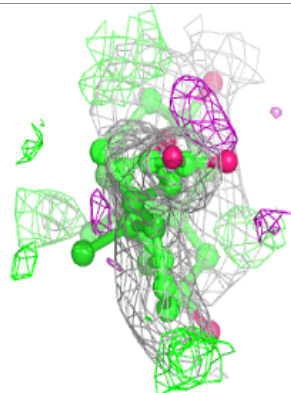
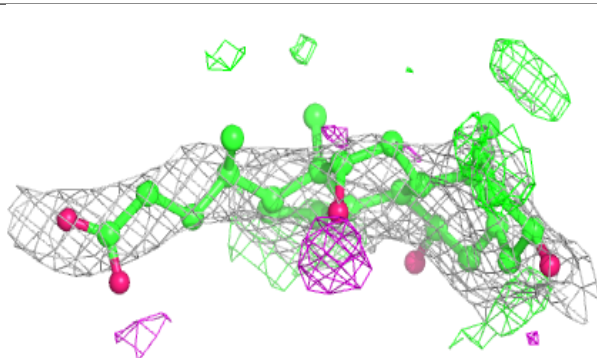
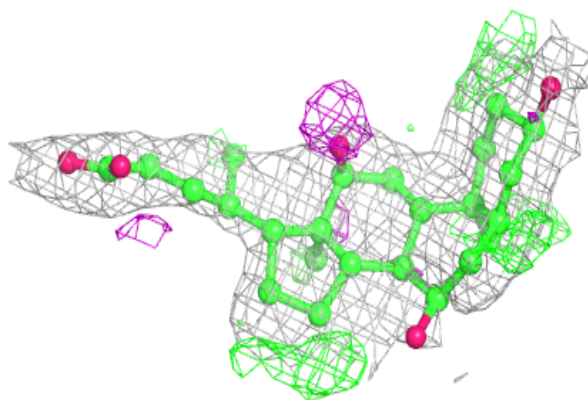


Electron density around TGL N 611:

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

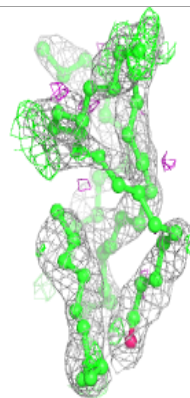
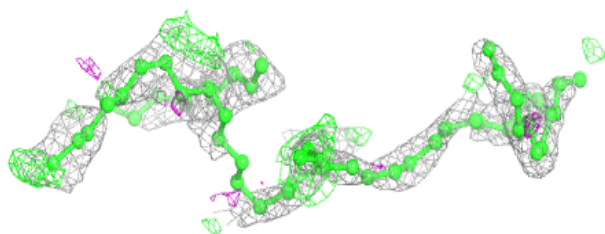
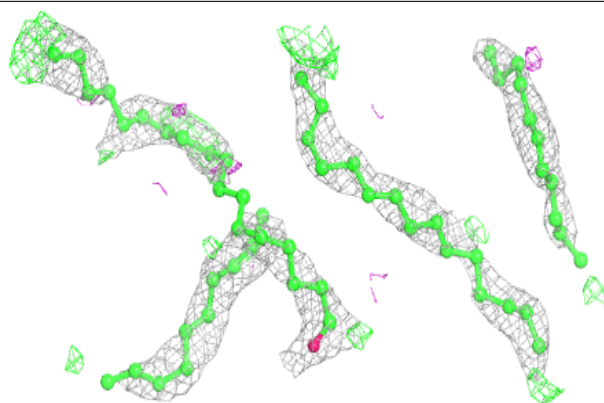
**Electron density around CHD Y 101:**

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

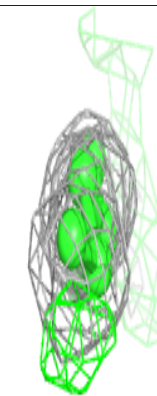
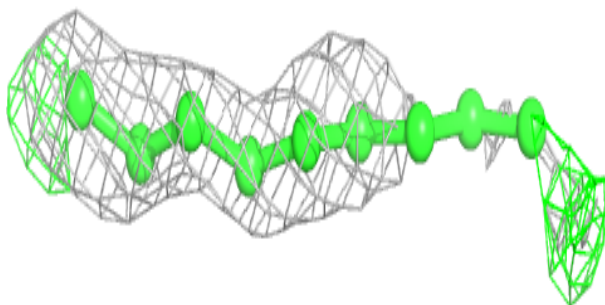
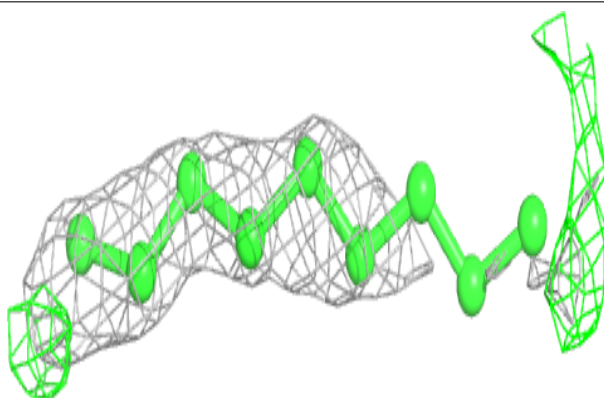


Electron density around CDL N 601:

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

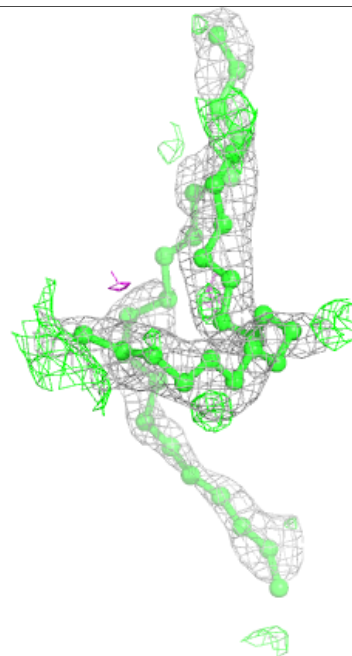
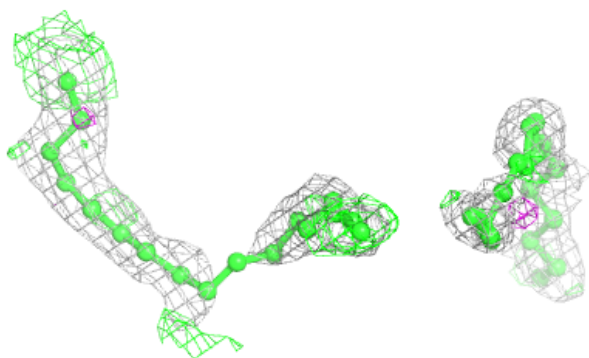
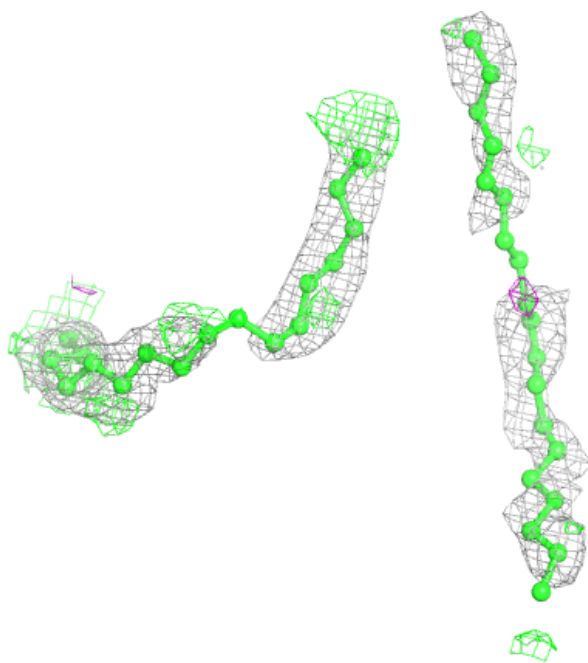
**Electron density around DMU X 103:**

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



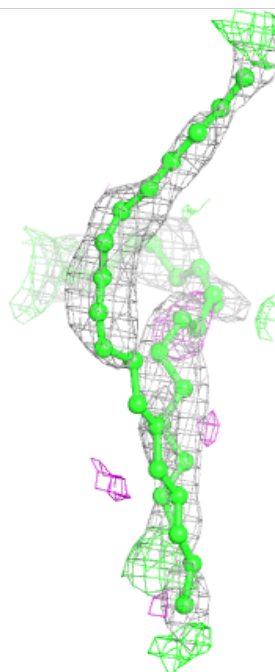
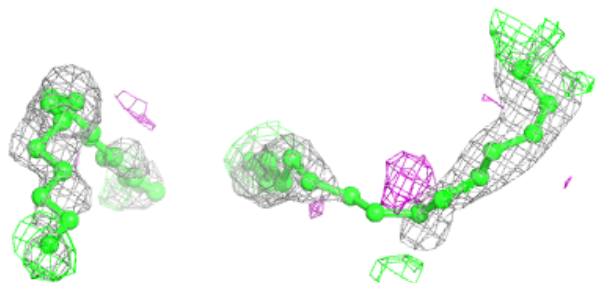
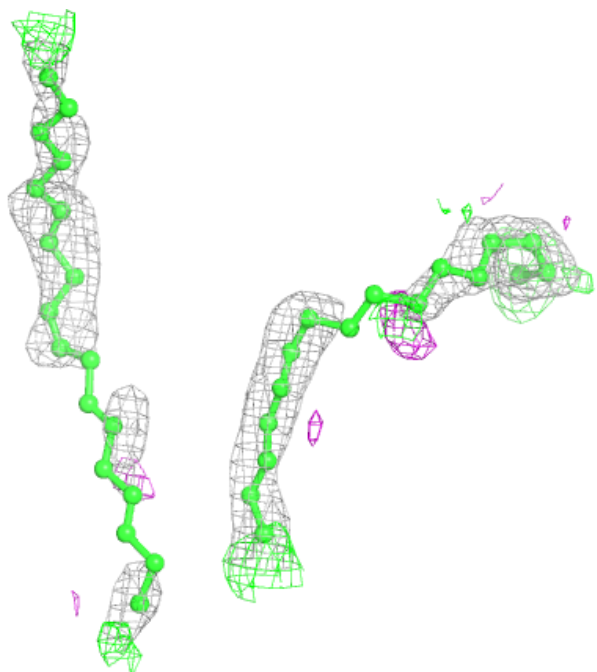
Electron density around PEK C 309:

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



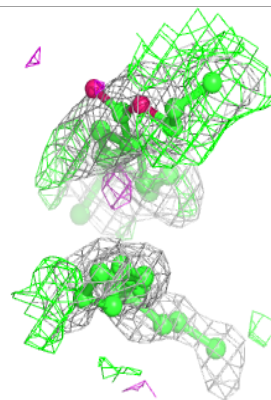
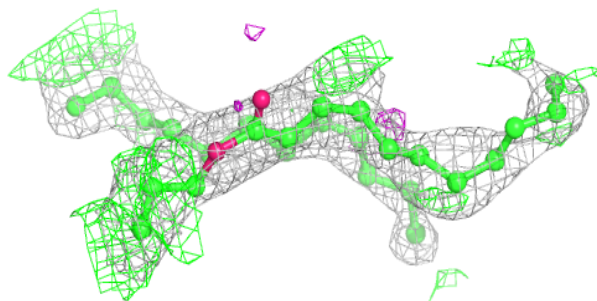
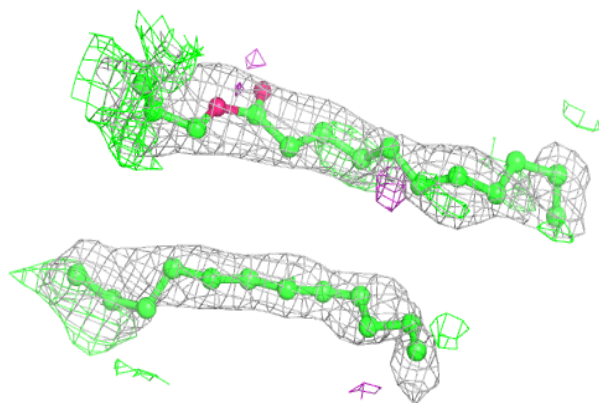
Electron density around PEK P 308:

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

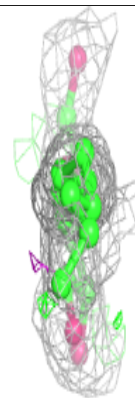
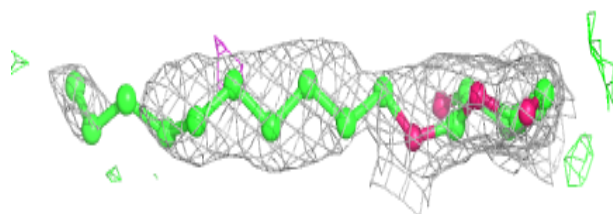
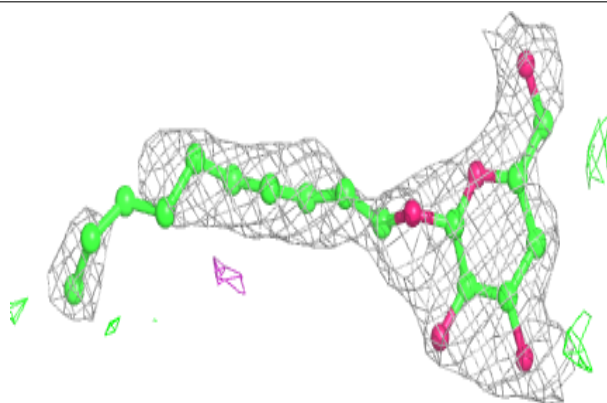


Electron density around PGV C 311:

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

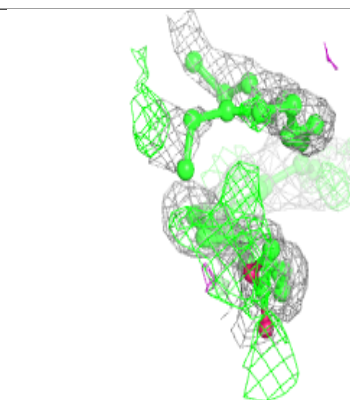
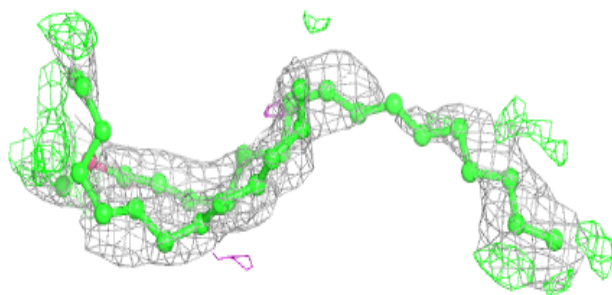
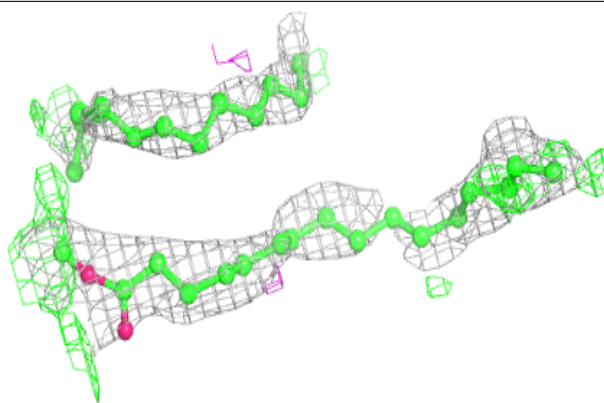
**Electron density around DMU L 101:**

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

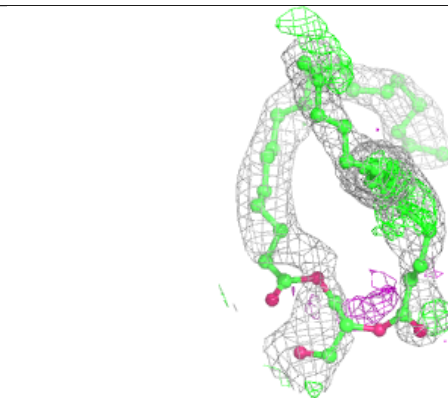
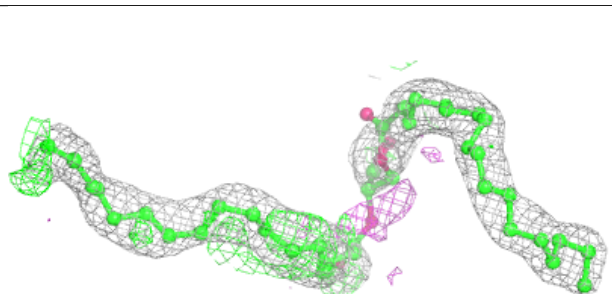
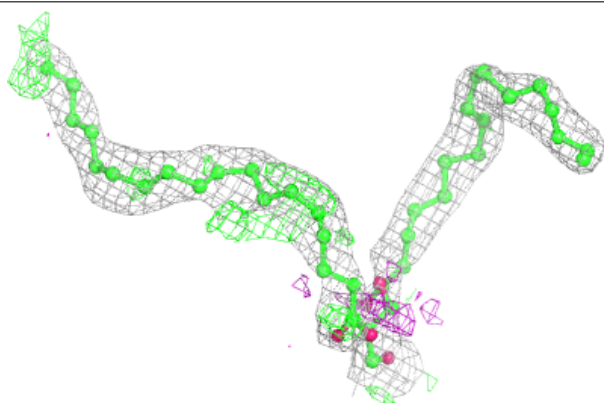


Electron density around PGV G 102:

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

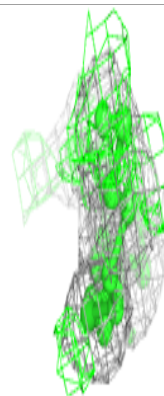
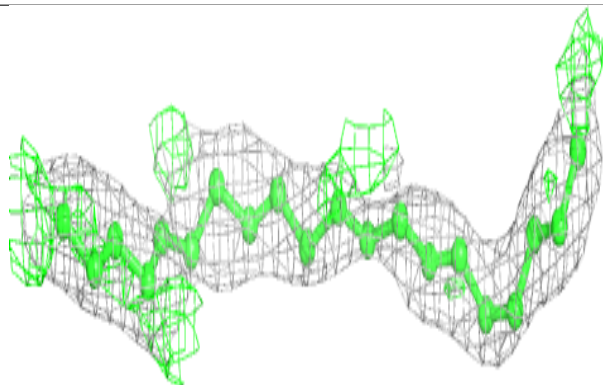
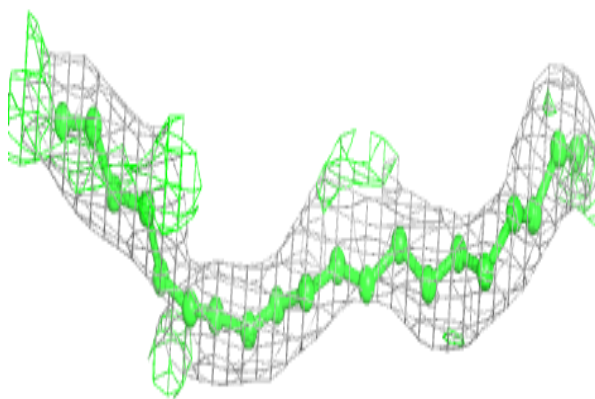
**Electron density around TGL N 612:**

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

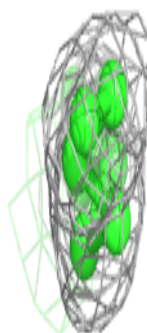
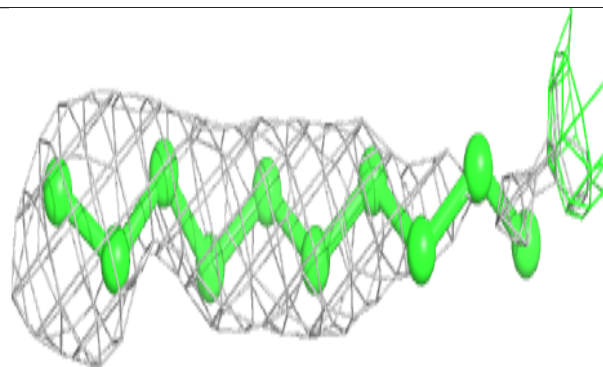
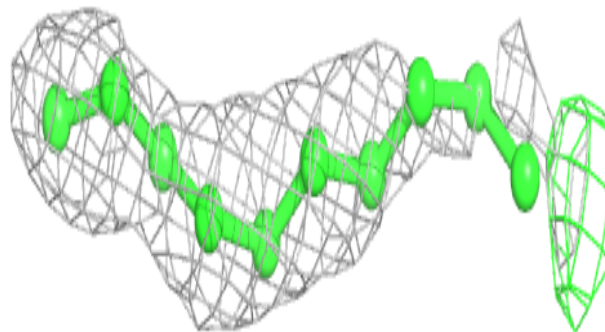


Electron density around PEK P 305:

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

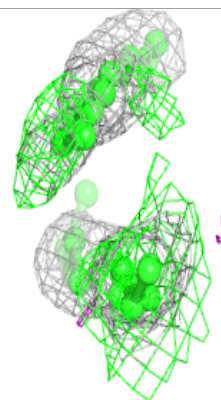
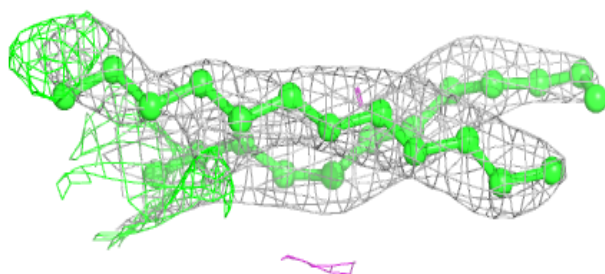
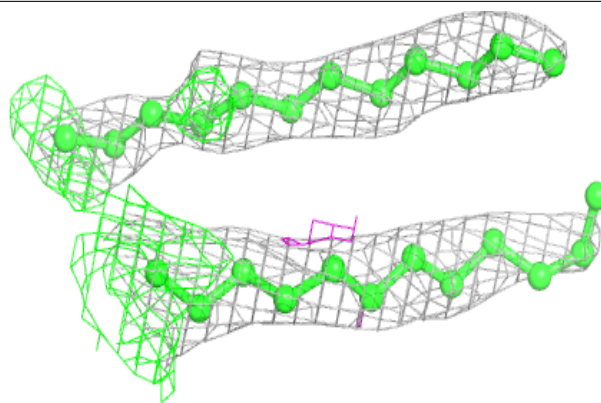
**Electron density around DMU K 102:**

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

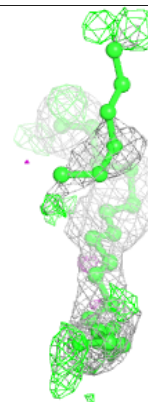
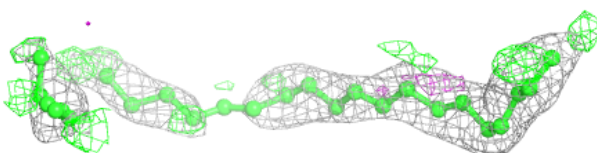
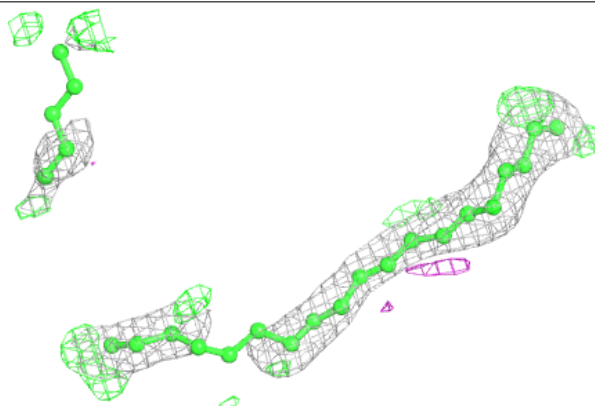


Electron density around PGV N 607:

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

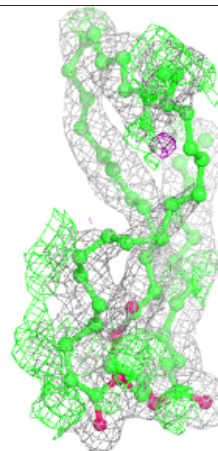
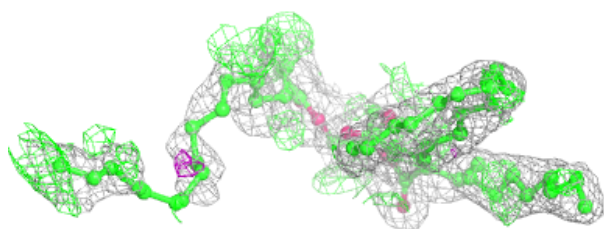
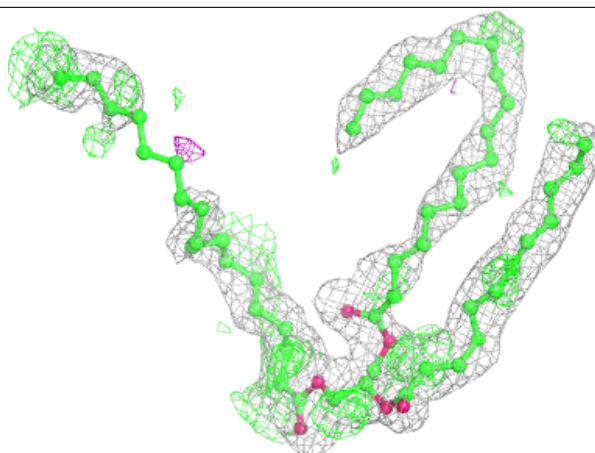
**Electron density around PEK C 306:**

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

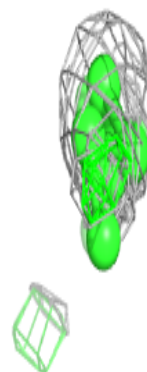
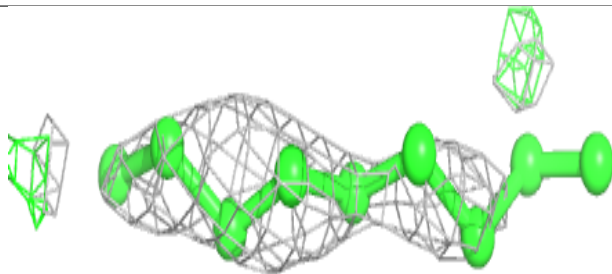
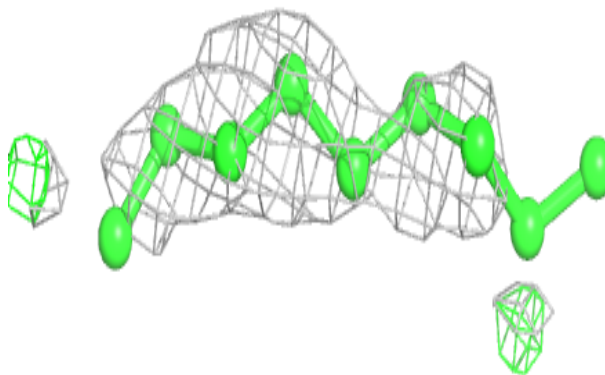


Electron density around TGL D 202:

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

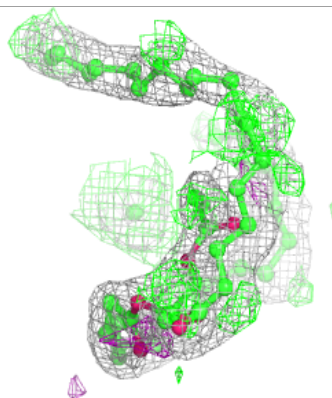
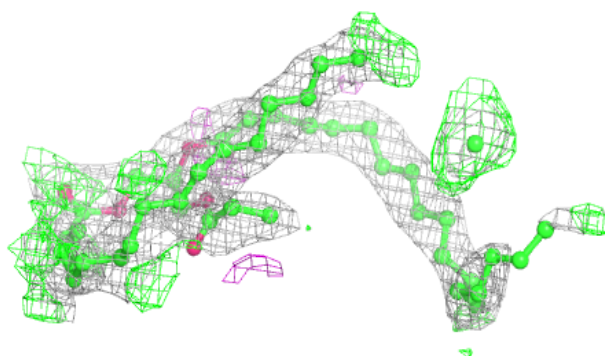
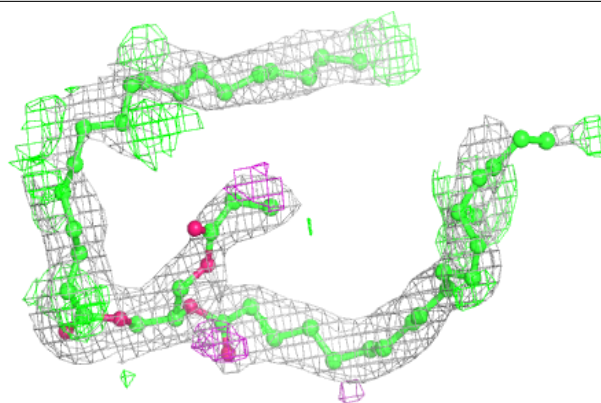
**Electron density around DMU K 105:**

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

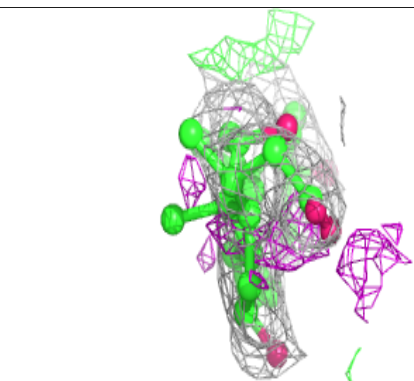
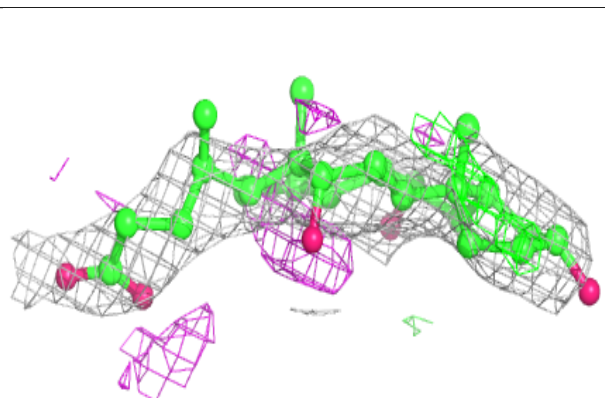
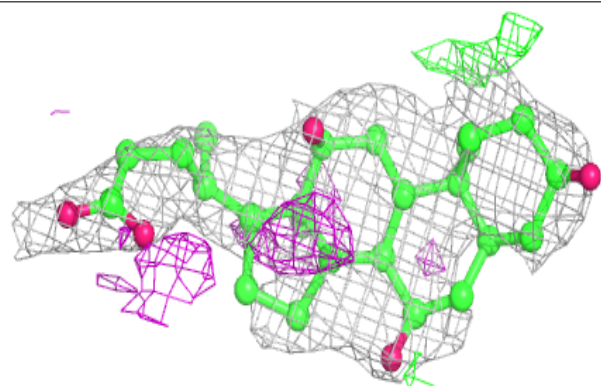


Electron density around TGL B 301:

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

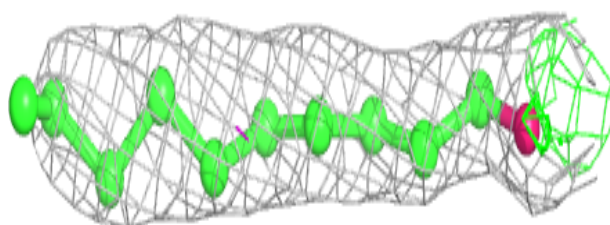
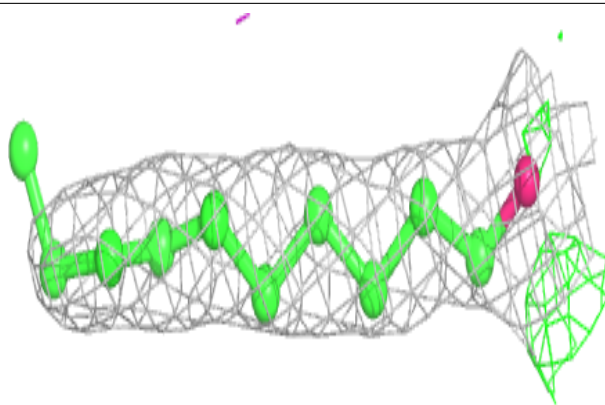
**Electron density around CHD L 102:**

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

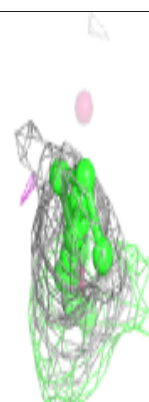
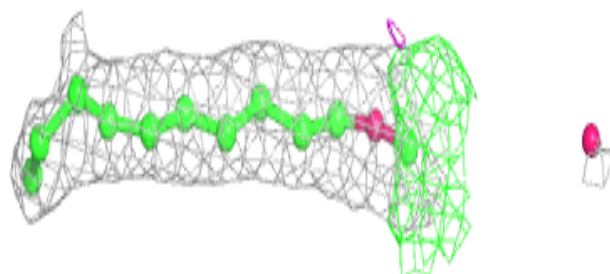
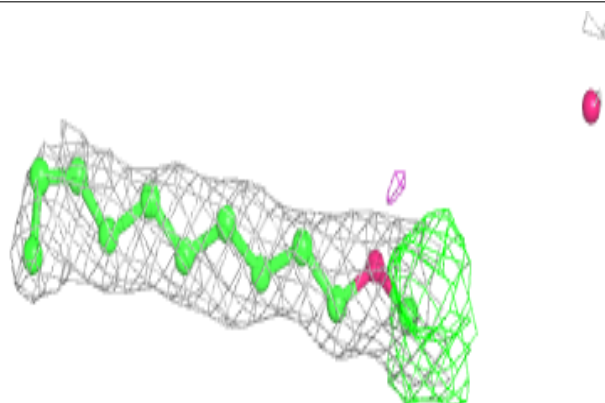


Electron density around DMU O 302:

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

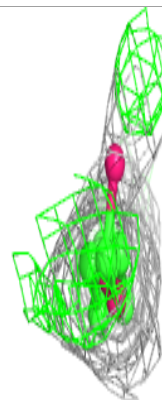
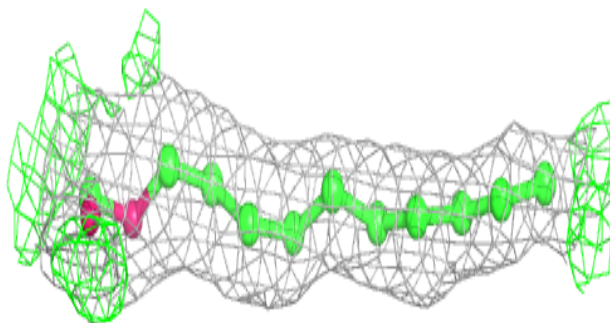
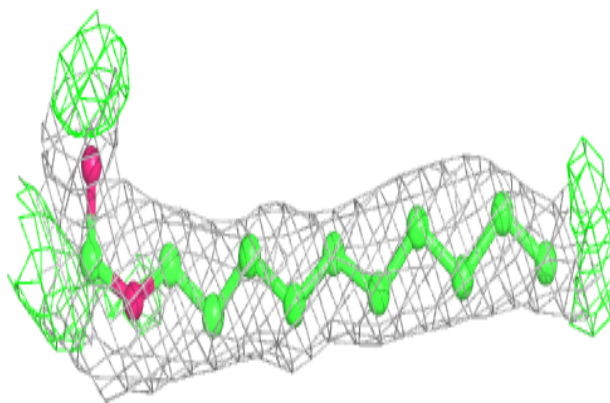
**Electron density around DMU P 303:**

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

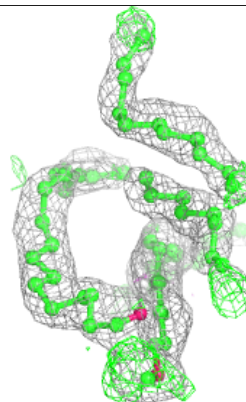
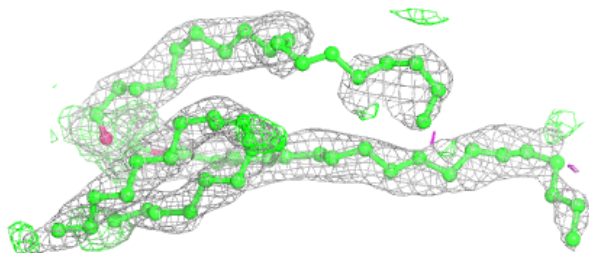
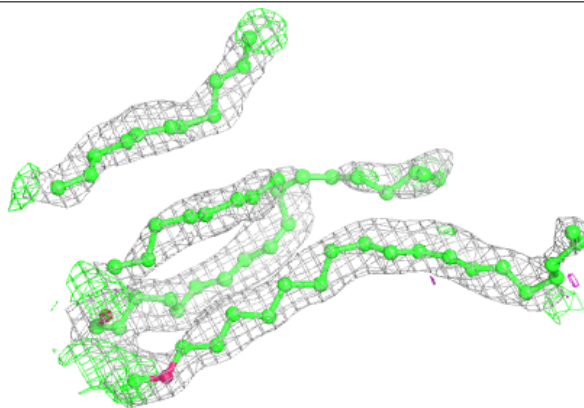


Electron density around DMU C 303:

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

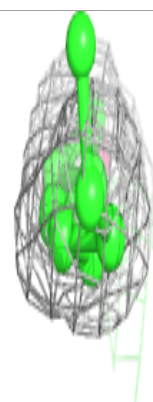
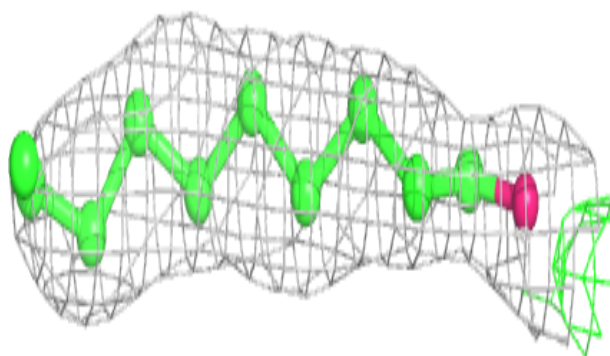
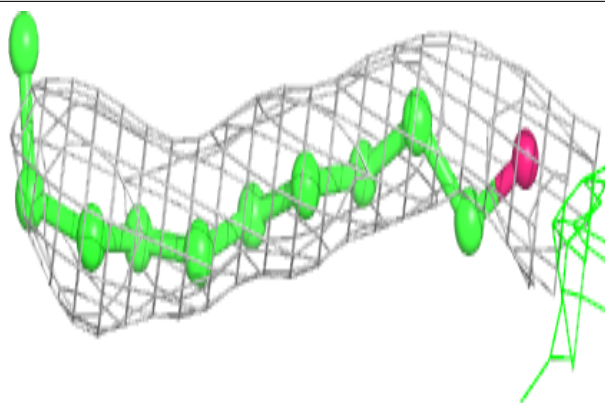
**Electron density around CDL C 305:**

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



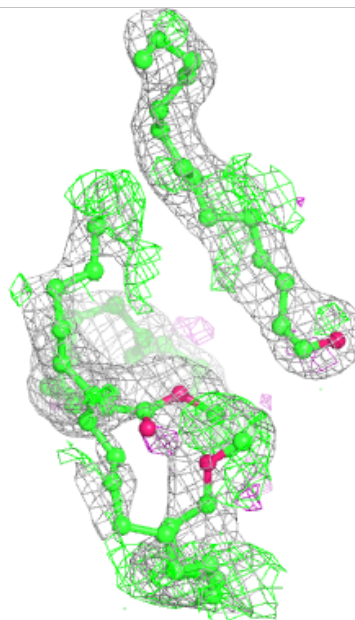
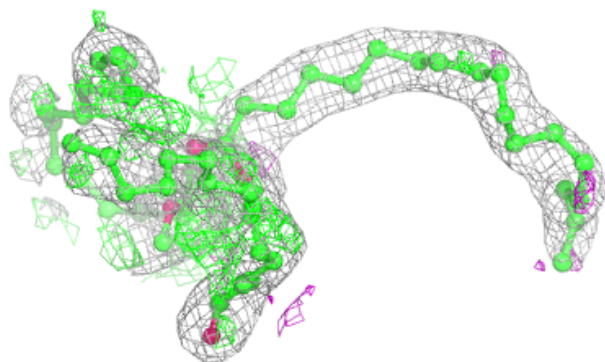
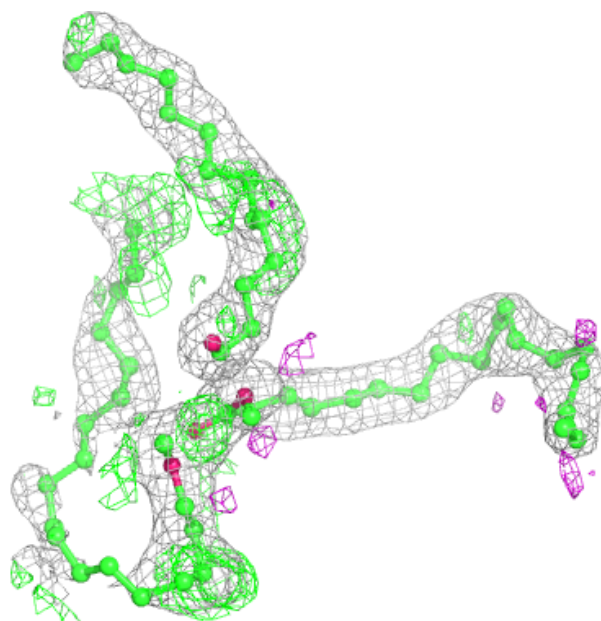
Electron density around DMU W 101:

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



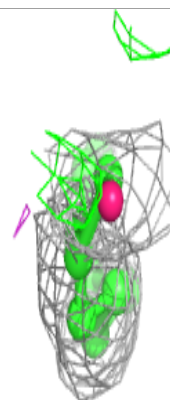
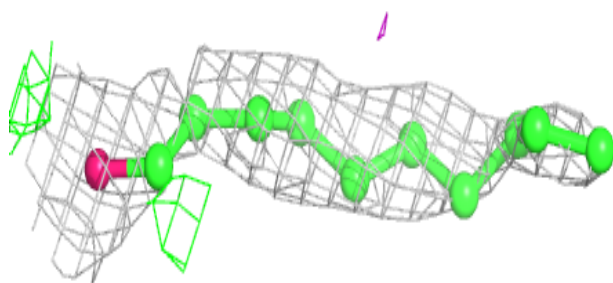
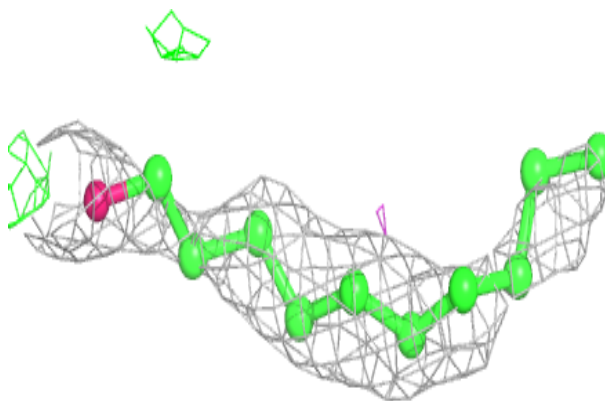
Electron density around TGL L 103:

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

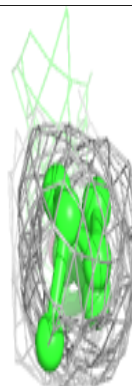
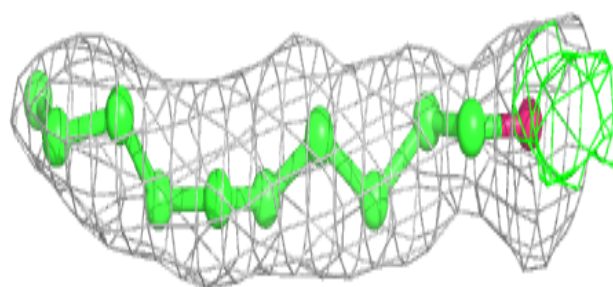
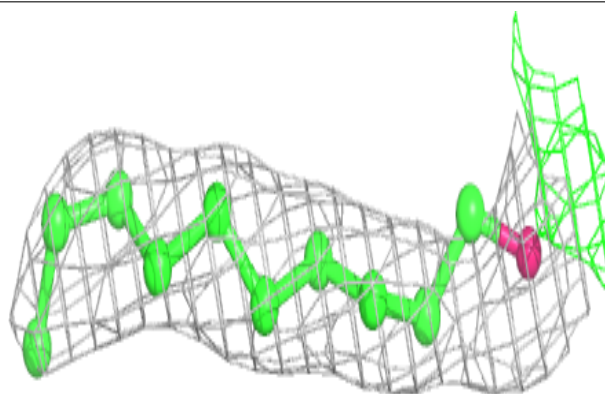


Electron density around DMU K 103:

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

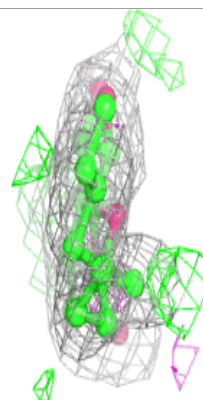
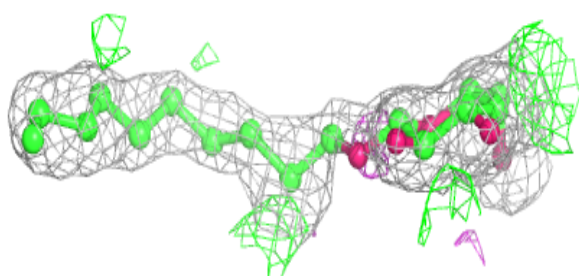
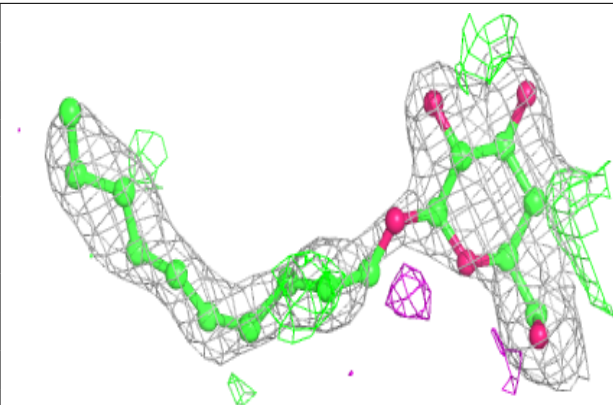
**Electron density around DMU J 101:**

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

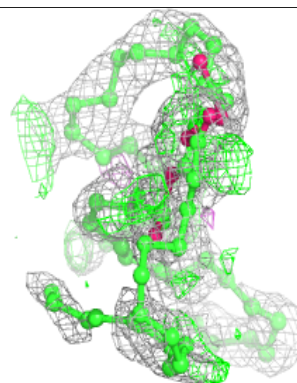
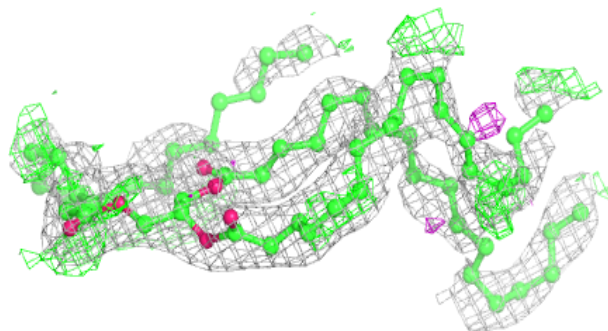
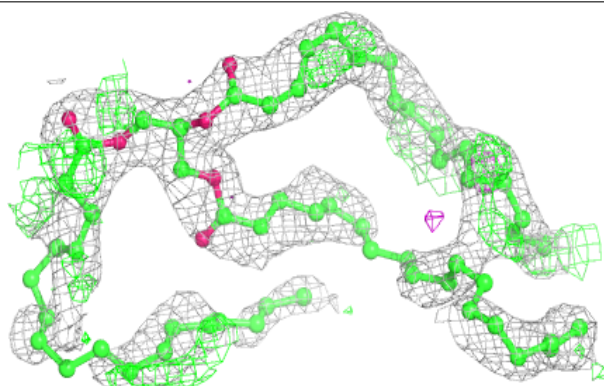


Electron density around DMU C 310:

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

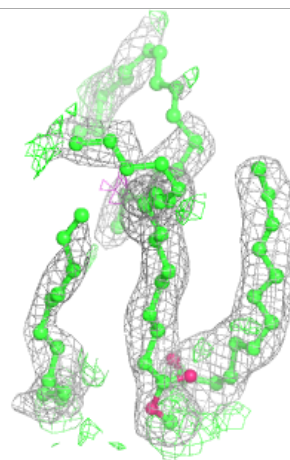
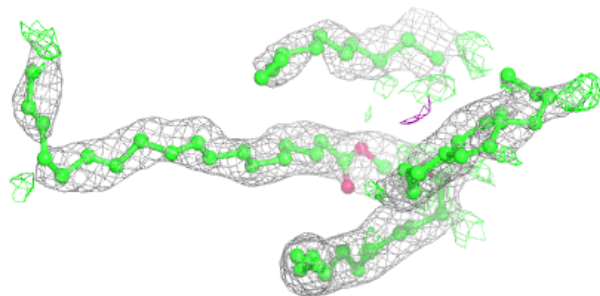
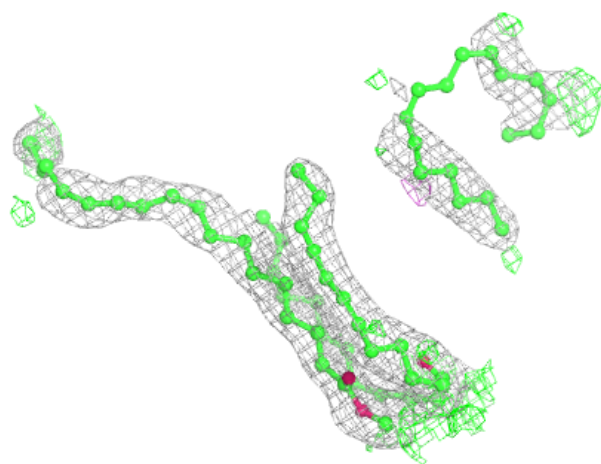
**Electron density around TGL N 609:**

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



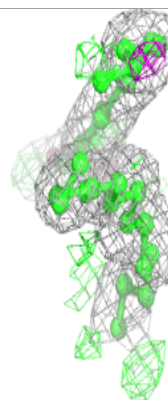
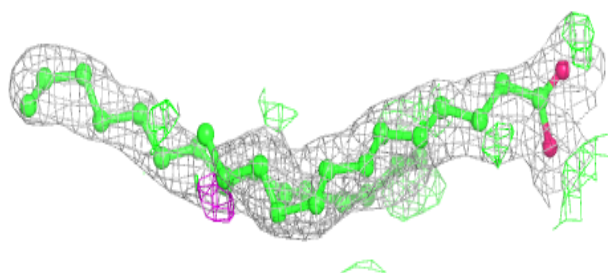
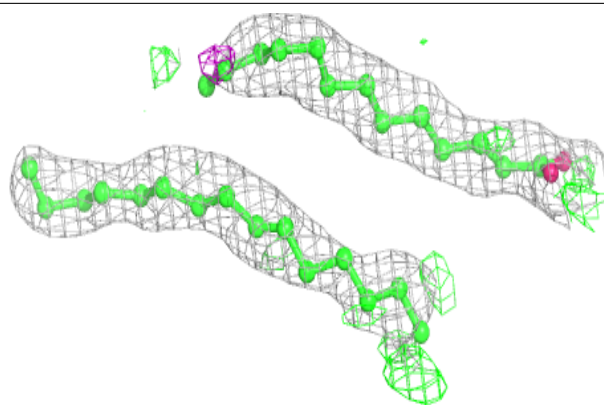
Electron density around CDL P 304:

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

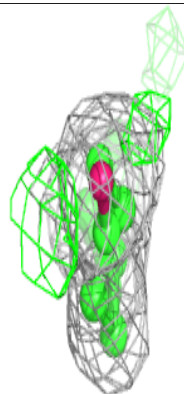
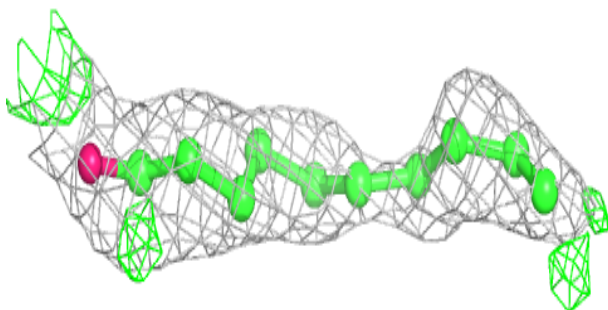
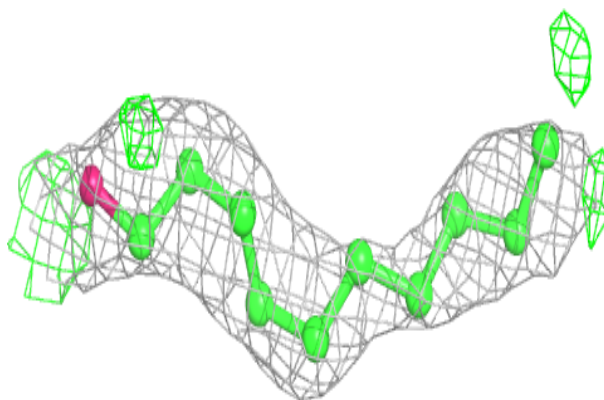


Electron density around PSC O 303:

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

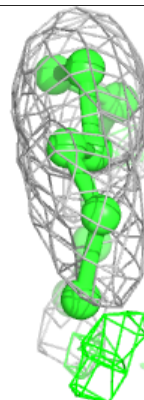
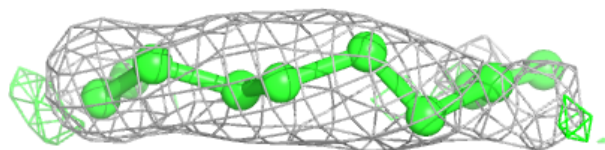
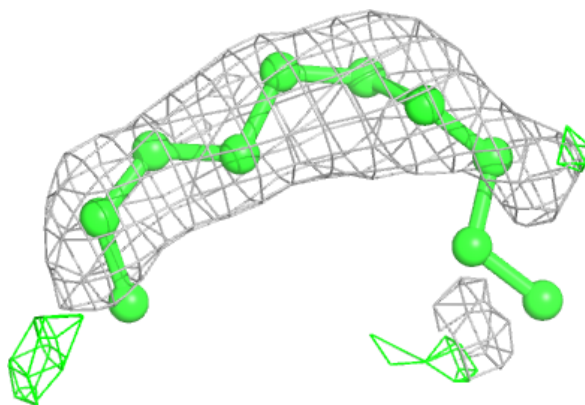
**Electron density around DMU D 201:**

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

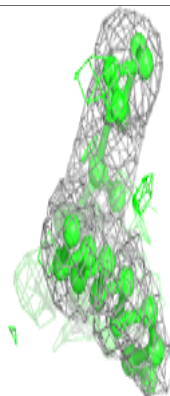
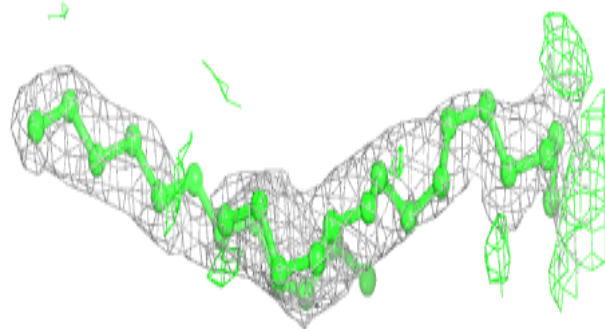
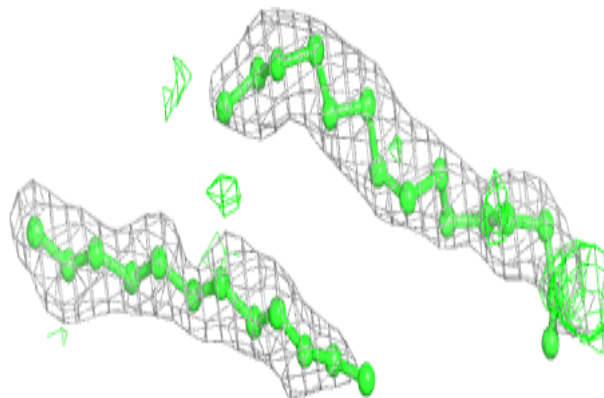


Electron density around DMU K 106:

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

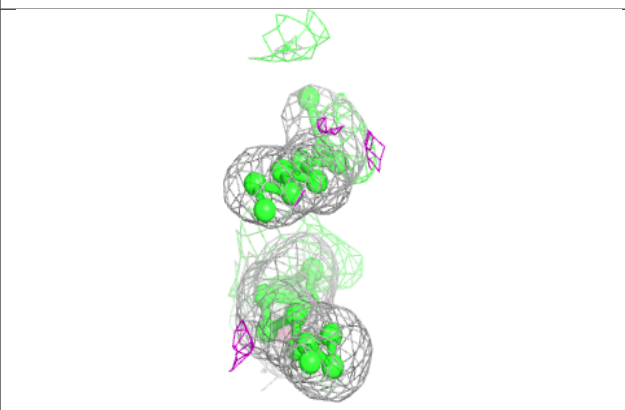
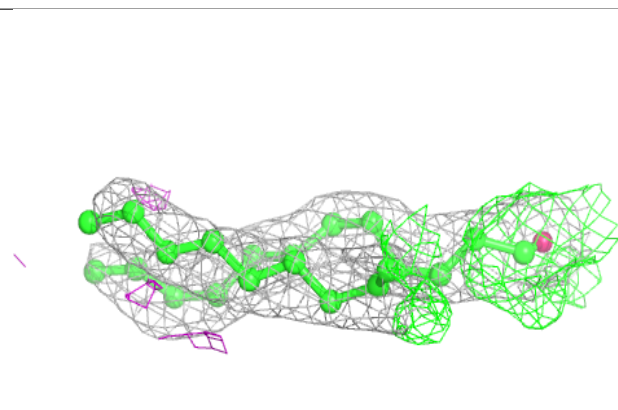
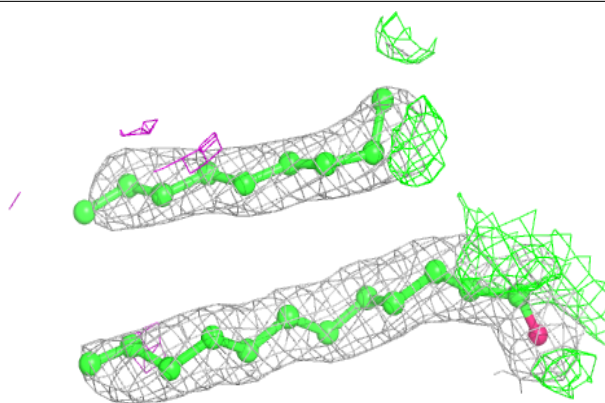
**Electron density around PSC A 607:**

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

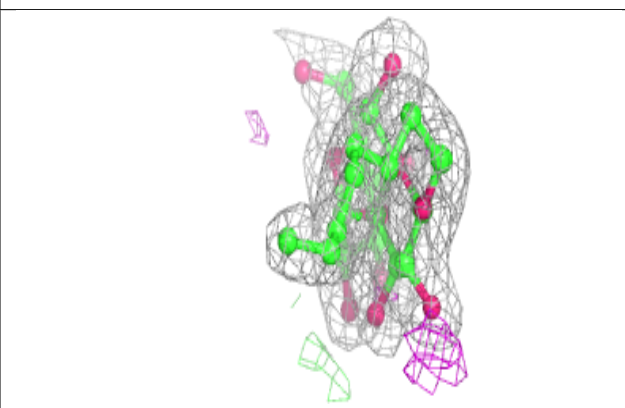
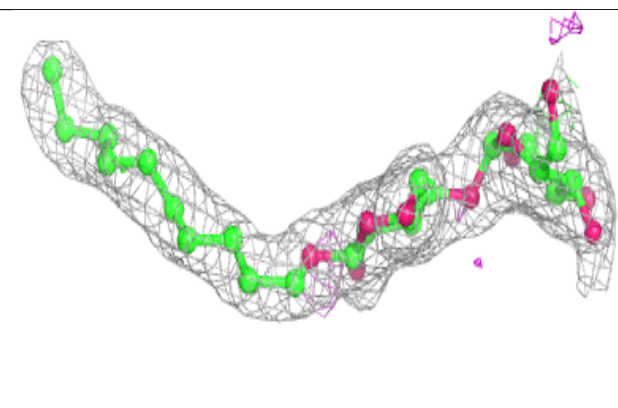
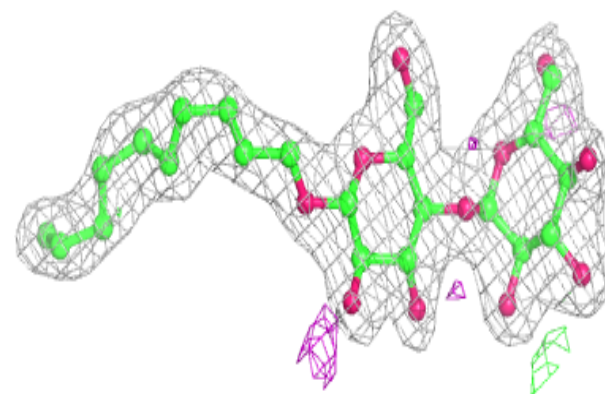


Electron density around PGV A 606:

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

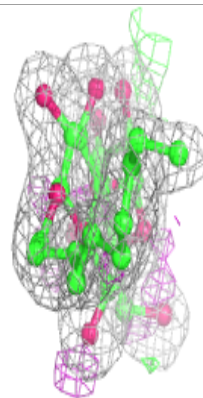
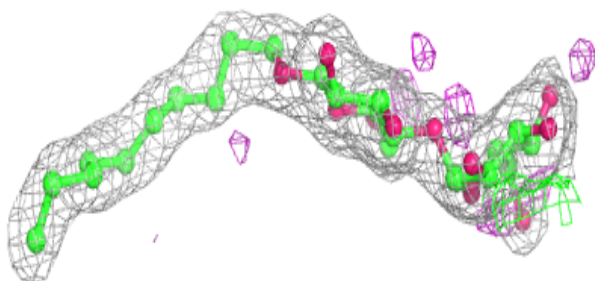
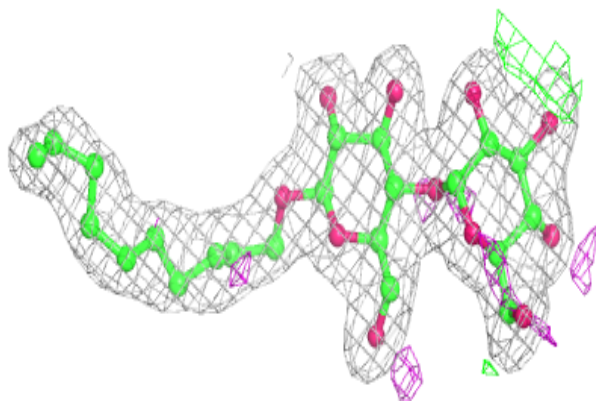
**Electron density around DMU Z 101:**

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

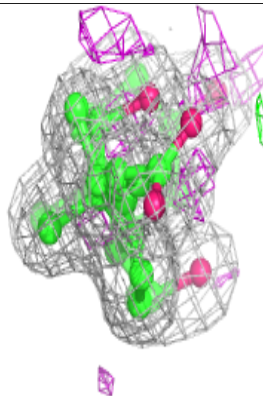
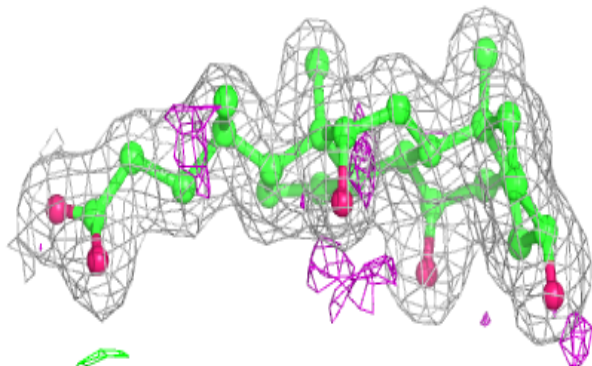
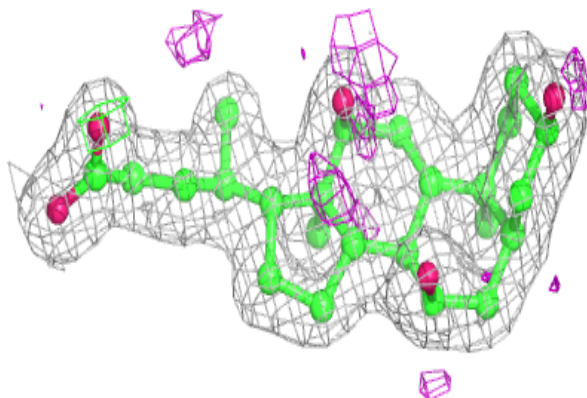


Electron density around DMU M 101:

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

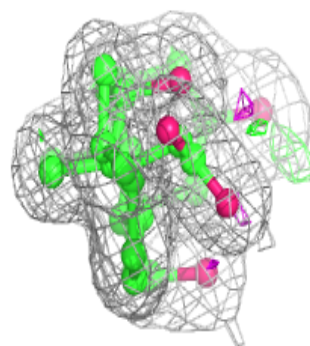
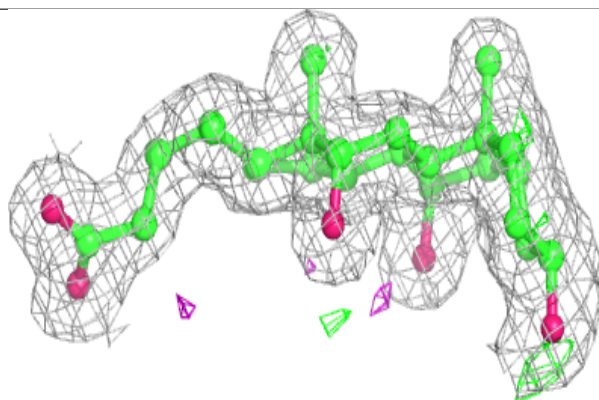
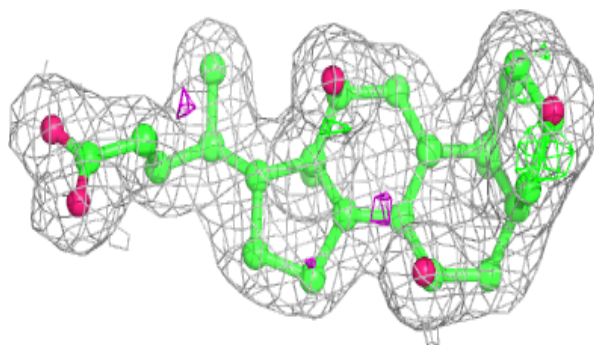
**Electron density around CHD C 304:**

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

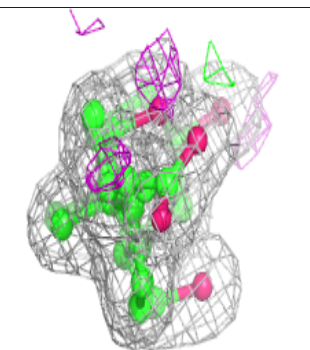
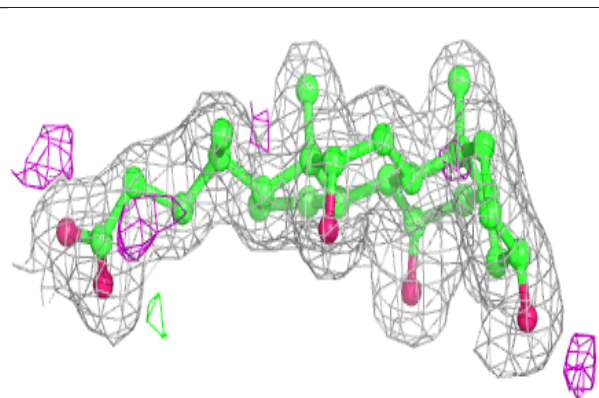
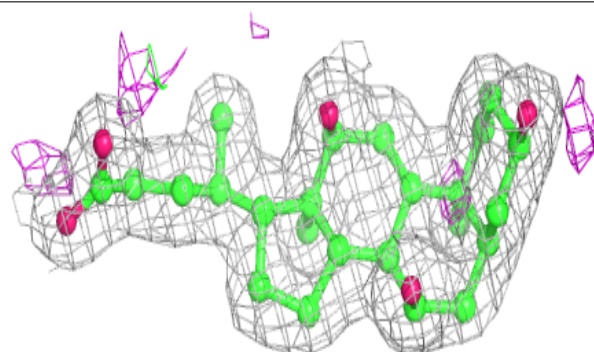


Electron density around CHD G 101:

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

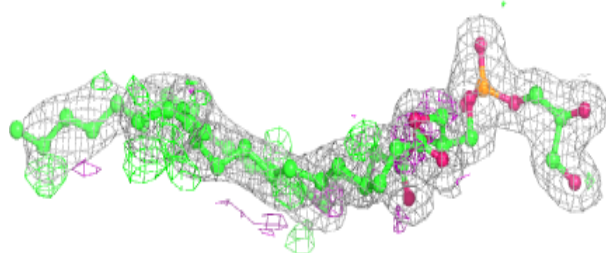
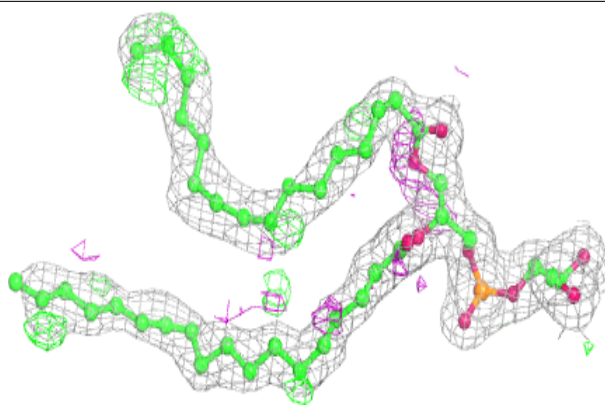
**Electron density around CHD P 301:**

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

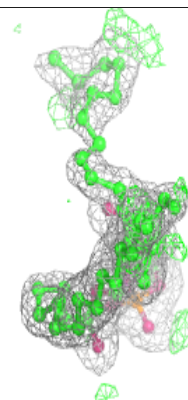
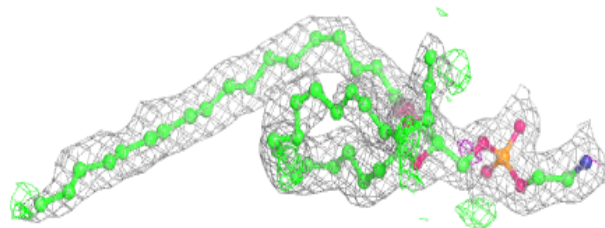
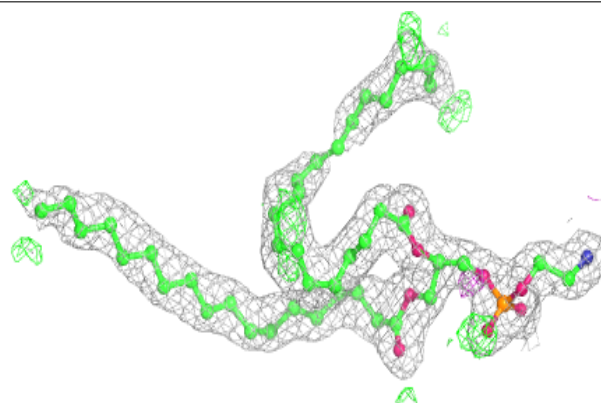


Electron density around PGV N 608:

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

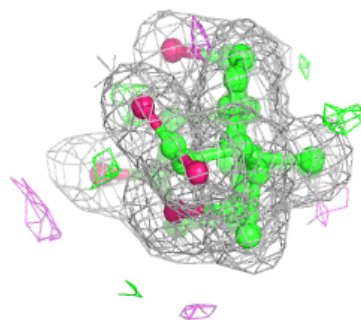
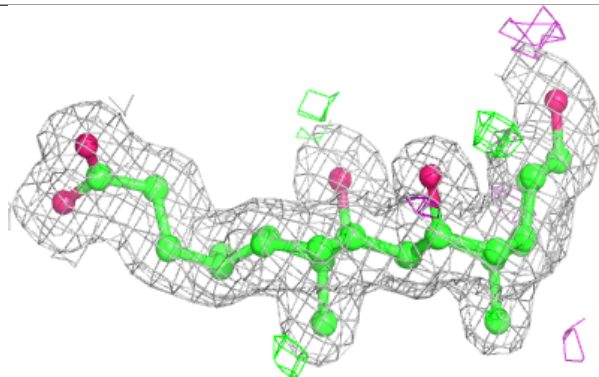
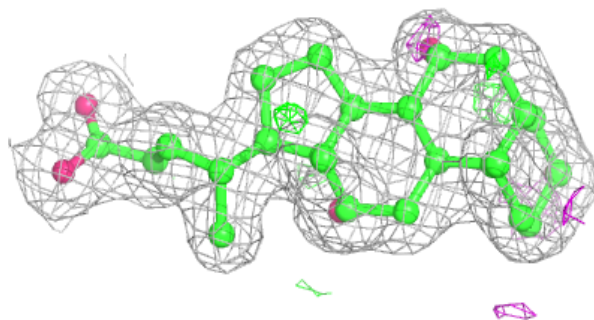
**Electron density around PEK P 306:**

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

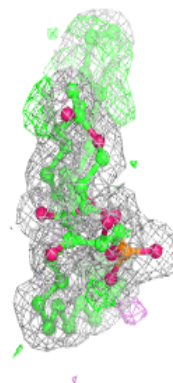
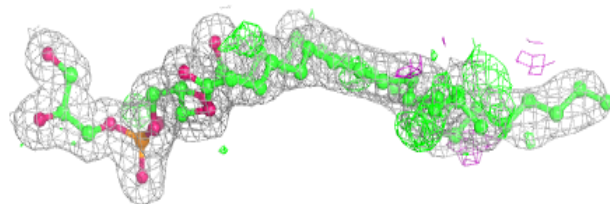
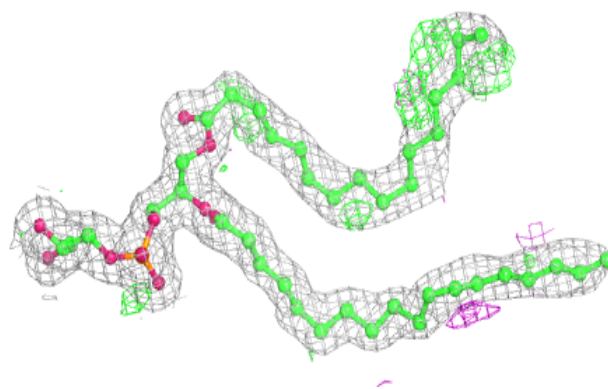


Electron density around CHD B 303:

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

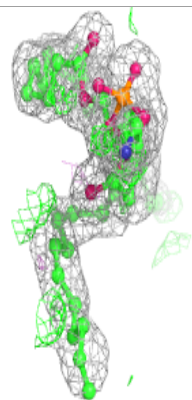
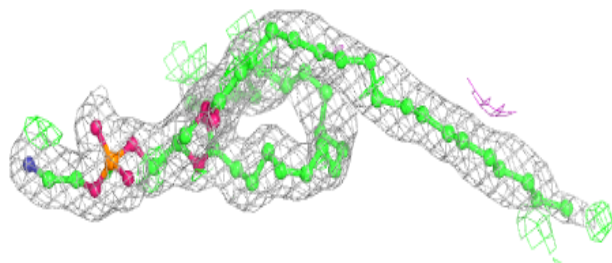
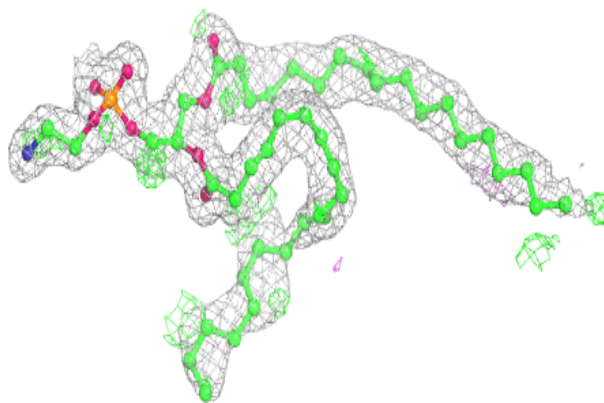
**Electron density around PGV C 301:**

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

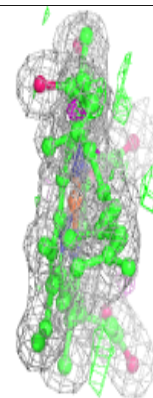
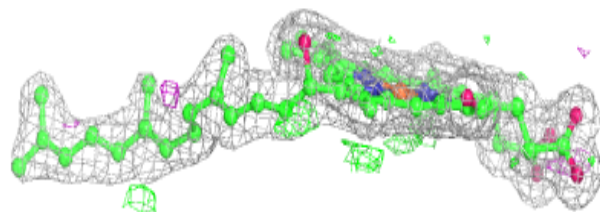
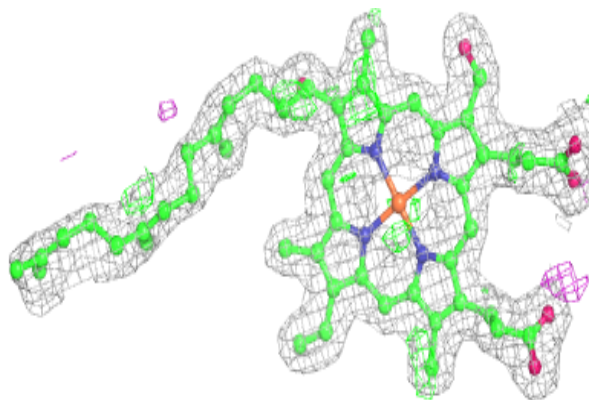


Electron density around PEK C 307:

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

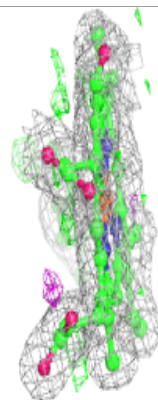
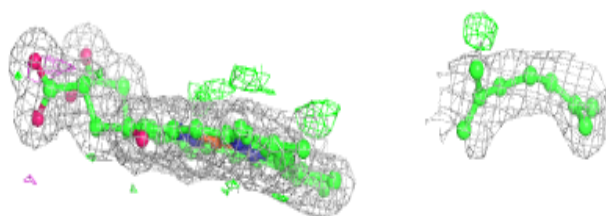
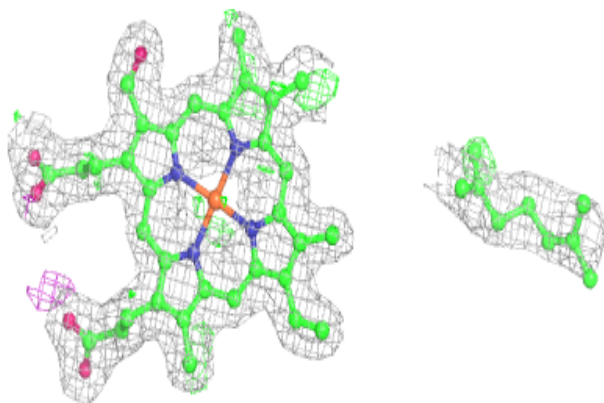
**Electron density around HEA N 602 (A):**

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

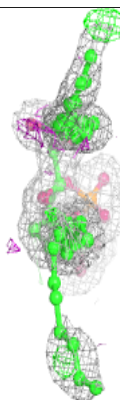
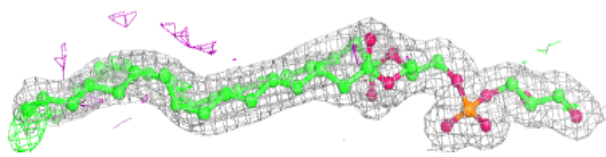
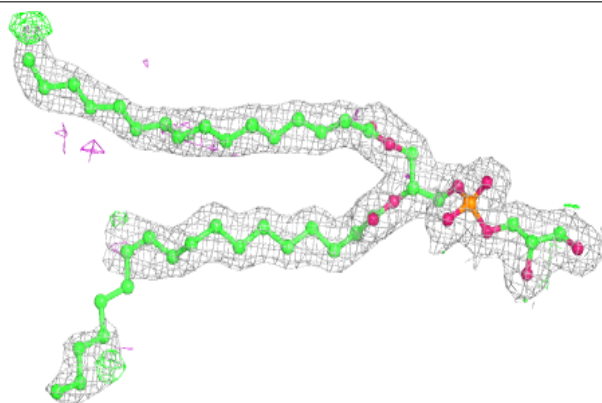


Electron density around HEA N 602 (C):

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

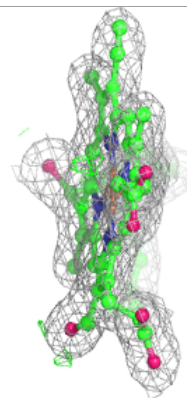
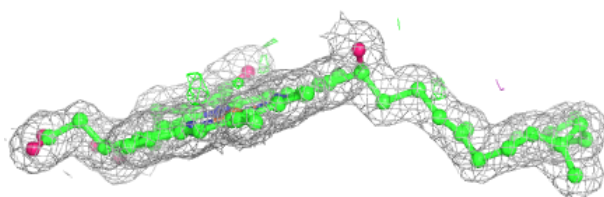
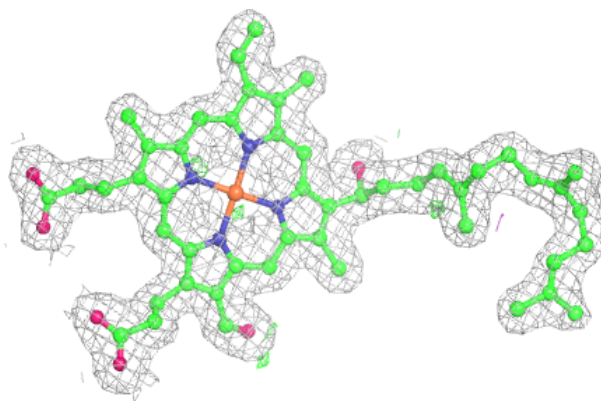
**Electron density around PGV P 307:**

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

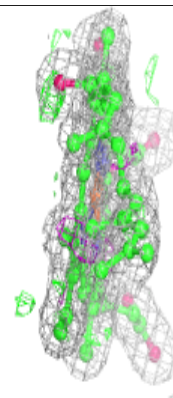
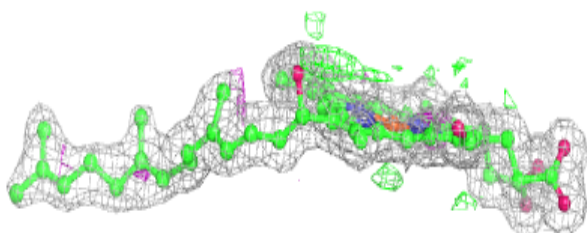
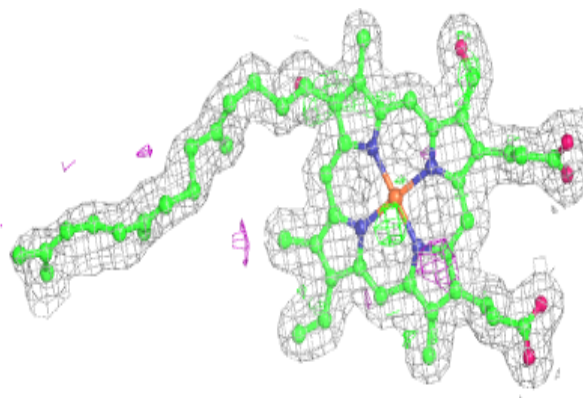


Electron density around HEA N 603:

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

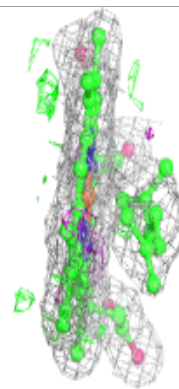
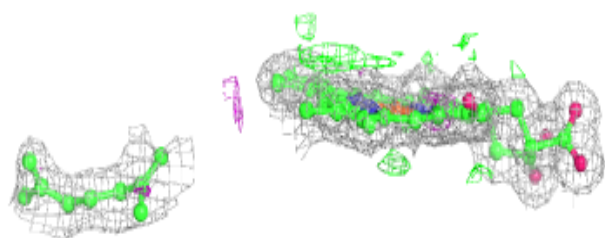
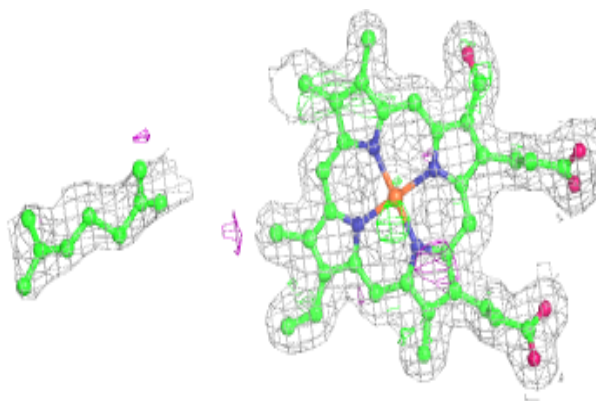
**Electron density around HEA A 601 (A):**

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

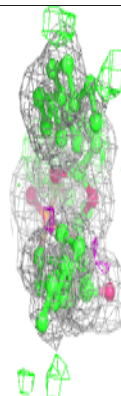
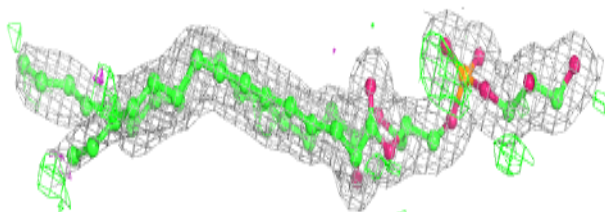
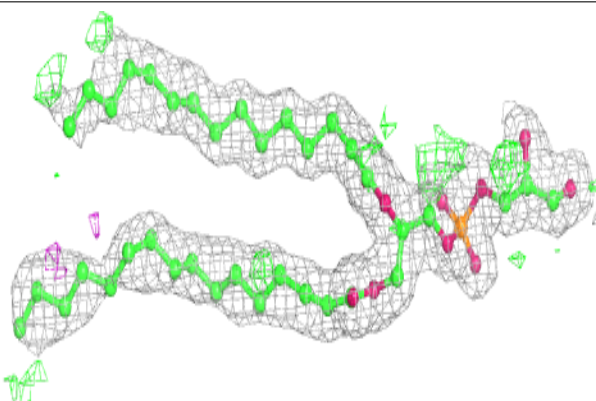


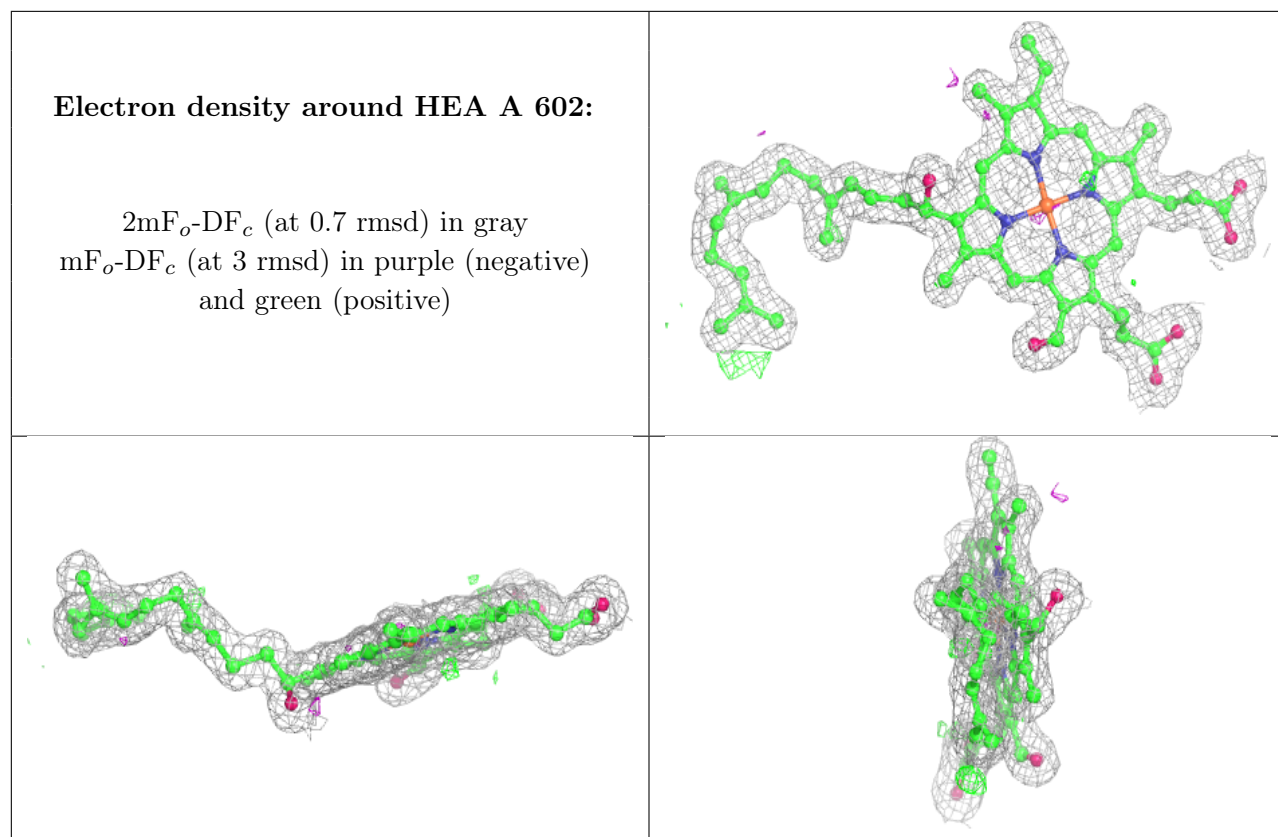
Electron density around HEA A 601 (C):

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

**Electron density around PGV C 308:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.