



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2022 – 06:34 PM JST

PDB ID : 8GVM
Title : The structure of azide-bound cytochrome C oxidase determined using the crystals exposed to 20 mM azide solution for 4 days
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2022-09-15
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

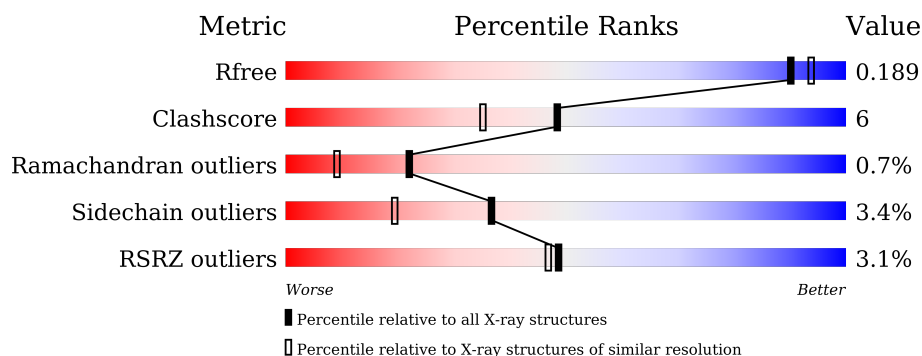
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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>89%</div> <div>11%</div> <div>.</div> </div>
1	N	514	<div> <div>89%</div> <div>11%</div> <div>.</div> </div>
2	B	227	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	O	227	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
3	C	261	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>
3	P	261	<div> <div>90%</div> <div>10%</div> <div>.</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602[A]	X	-	-	-
14	HEA	A	602[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
14	HEA	N	603[A]	X	-	-	-
14	HEA	N	603[B]	X	-	-	-
18	AZI	A	607[A]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	608[A]	-	-	X	-
20	EDO	C	317	-	-	-	X
20	EDO	S	101	-	-	X	-
22	CHD	W	101	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33558 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	20	0
			4125	2753	637	694	41			
1	N	514	Total	C	N	O	S	0	18	0
			4122	2753	634	694	41			

- 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	23	0
			1996	1304	304	368	20			
2	O	227	Total	C	N	O	S	0	20	0
			1975	1289	301	365	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2152	1437	345	356	14			
3	P	259	Total	C	N	O	S	0	9	0
			2173	1449	348	361	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	2	0
			1198	779	197	218	4			
4	Q	144	Total	C	N	O	S	0	2	0
			1213	791	198	220	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			773	478	138	151	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	1
			681	438	129	112	1	1		

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

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

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

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

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

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

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

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

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

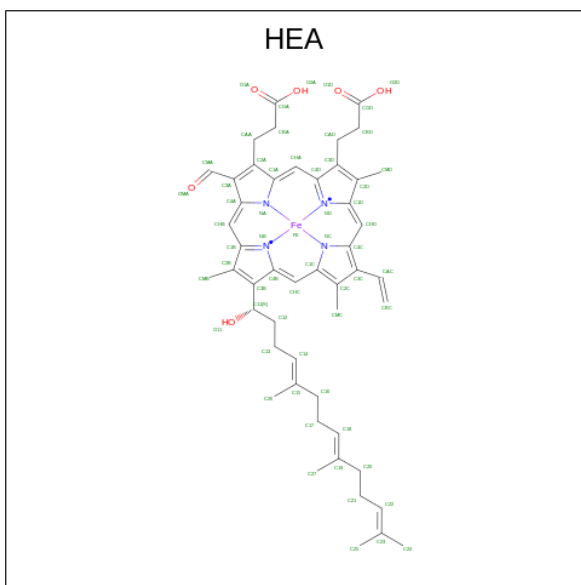
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			383	256	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			383	256	64	60	3			

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

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

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



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

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

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

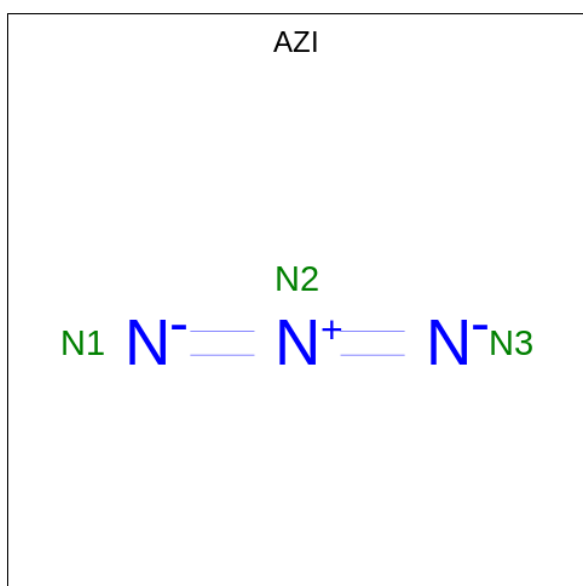
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

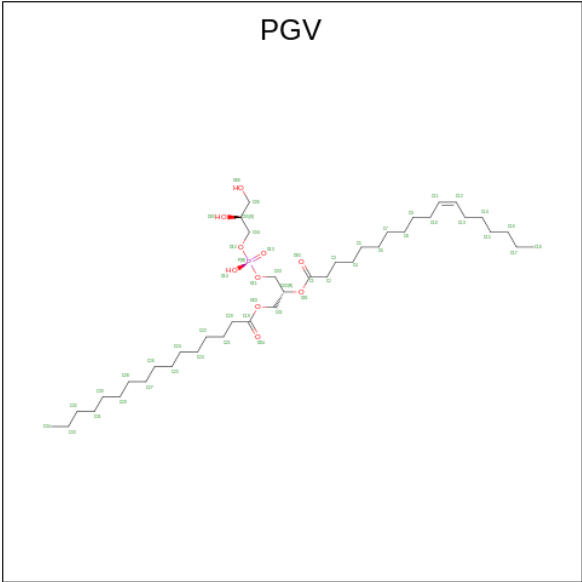
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			49	39	9	1		
19	G	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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

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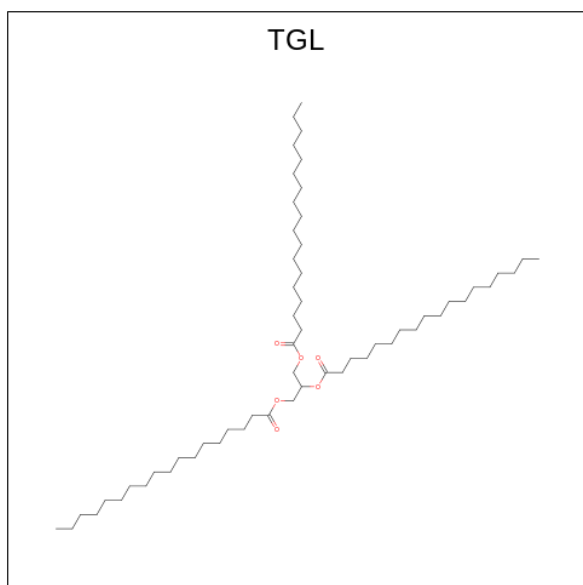
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	G	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0

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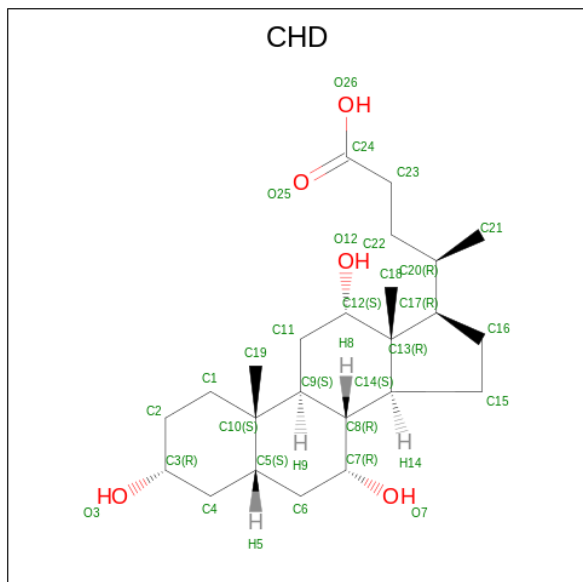
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			61	55	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

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



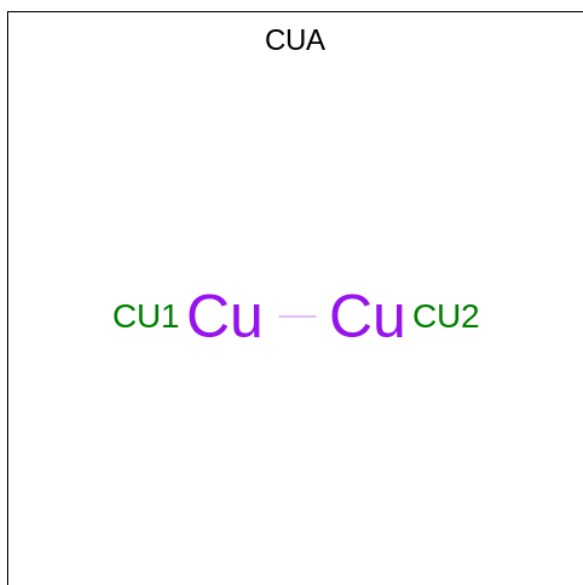
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		

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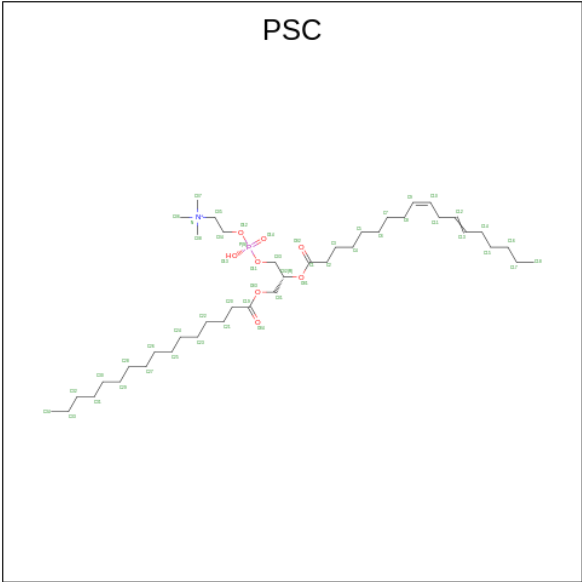
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

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



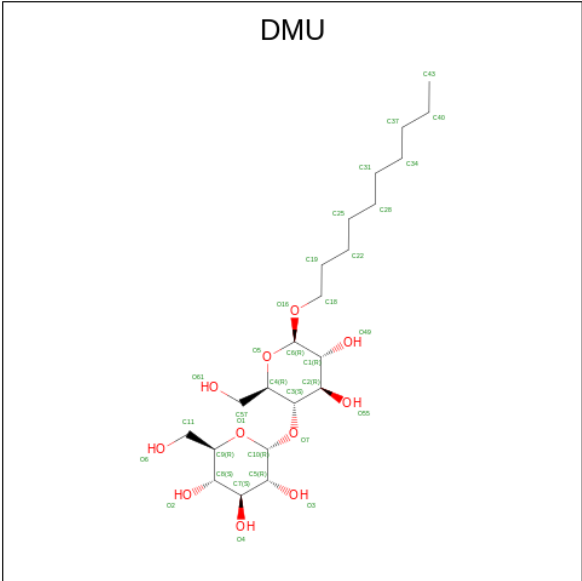
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

- Molecule 24 is (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
24	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
24	O	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



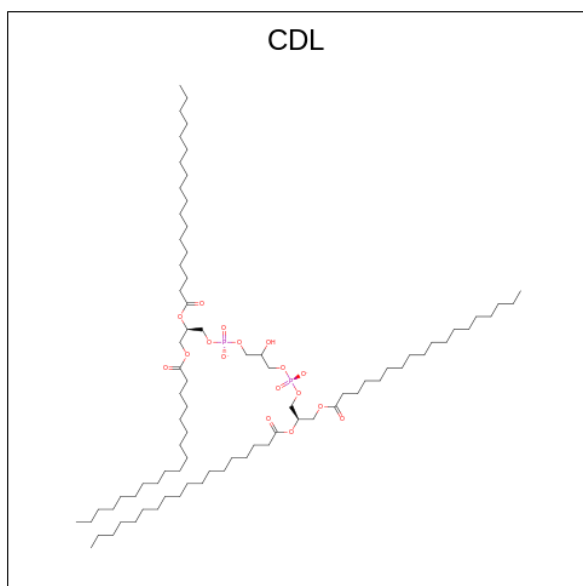
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			22	16	6		
25	L	1	Total	C	O	0	0
			30	19	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	Z	1	Total	C	O	0	0
			33	22	11		

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



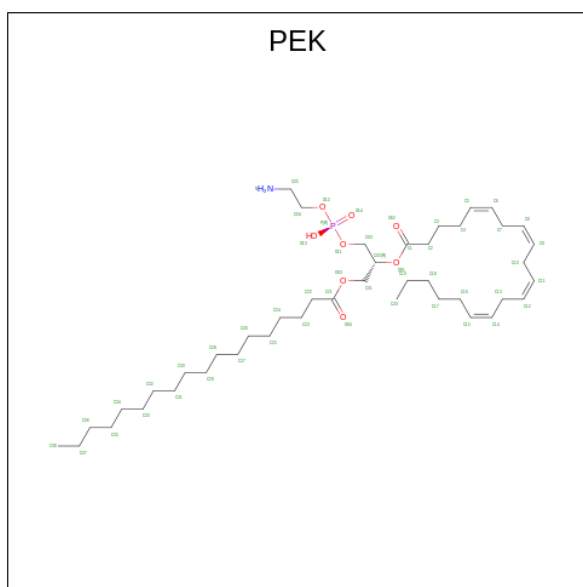
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			89	71	16	2		
26	N	1	Total	C	O	P	0	0
			96	77	17	2		
26	P	1	Total	C	O	P	0	0
			80	62	16	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	T	1	Total	C	O	P	0	0
			97	78	17	2		

- 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	N	O	P	0	0
			53	43	1	8	1		
27	C	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	O	P		0	0
			44	35	8	1			
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	O	P		0	0
			50	41	8	1			

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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	222	Total 222	O 222	0	1
29	B	133	Total 134	O 134	0	2
29	C	99	Total 99	O 99	0	0
29	D	108	Total 108	O 108	0	0
29	E	82	Total 82	O 82	0	0
29	F	79	Total 79	O 79	0	0
29	G	52	Total 52	O 52	0	0
29	H	44	Total 44	O 44	0	0
29	I	27	Total 27	O 27	0	0
29	J	27	Total 27	O 27	0	0
29	K	20	Total 20	O 20	0	0
29	L	26	Total 26	O 26	0	0
29	M	24	Total 24	O 24	0	0
29	N	209	Total 209	O 209	0	1
29	O	111	Total 112	O 112	0	1
29	P	90	Total 90	O 90	0	0
29	Q	38	Total 38	O 38	0	0
29	R	39	Total 39	O 39	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	S	59	Total 59	O 59	0	0
29	T	35	Total 35	O 35	0	0
29	U	33	Total 33	O 33	0	0
29	V	14	Total 14	O 14	0	0
29	W	12	Total 12	O 12	0	0
29	X	11	Total 11	O 11	0	0
29	Y	13	Total 13	O 13	0	0
29	Z	16	Total 16	O 16	0	0

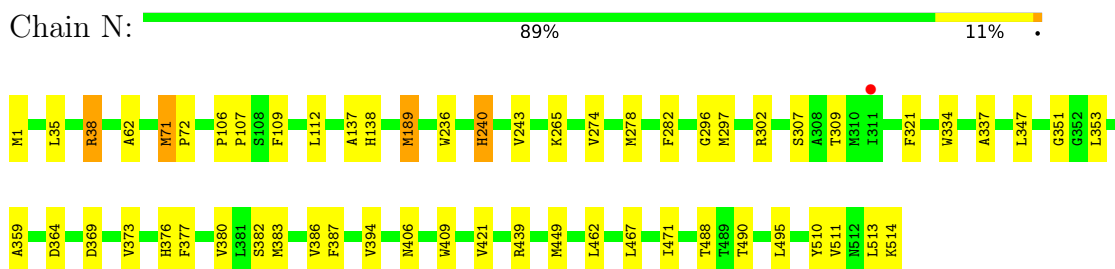
3 Residue-property plots [i](#)

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

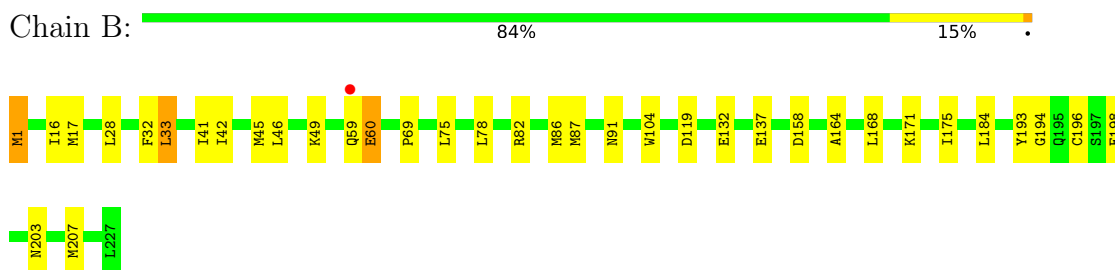
• Molecule 1: Cytochrome c oxidase subunit 1



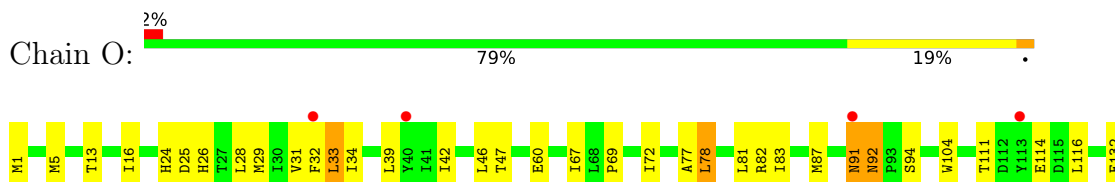
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2

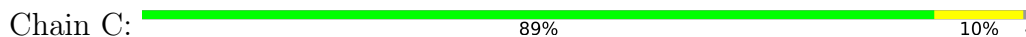


• Molecule 2: Cytochrome c oxidase subunit 2

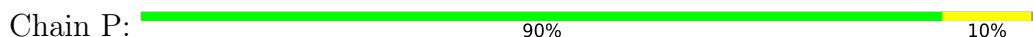




- Molecule 3: Cytochrome c oxidase subunit 3



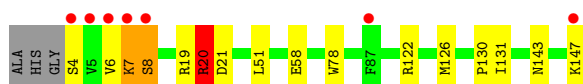
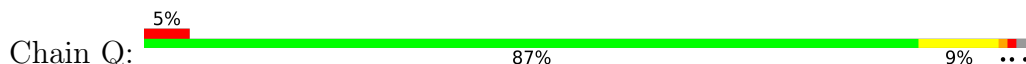
- Molecule 3: Cytochrome c oxidase subunit 3



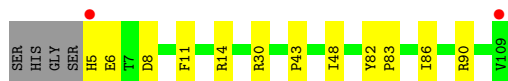
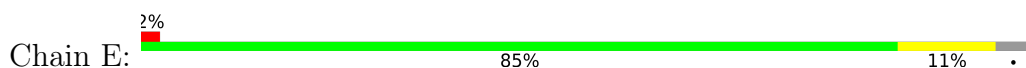
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



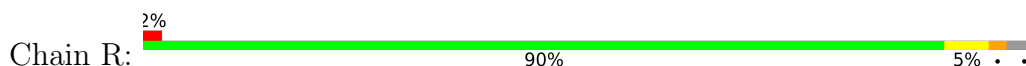
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



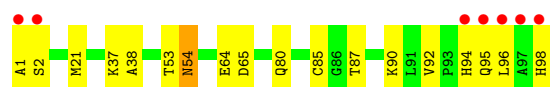
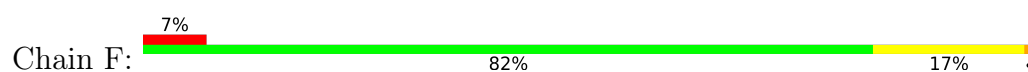
- Molecule 5: Cytochrome c oxidase subunit 5A



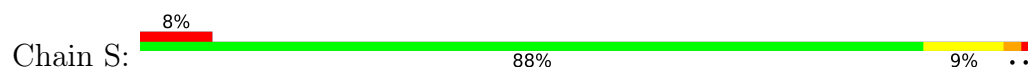
- Molecule 5: Cytochrome c oxidase subunit 5A



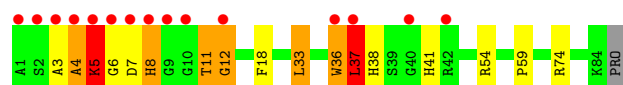
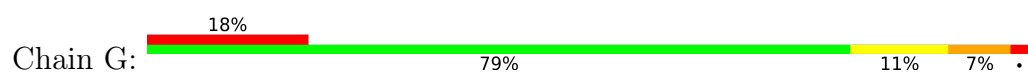
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



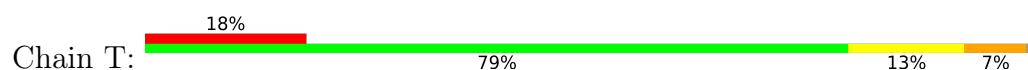
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



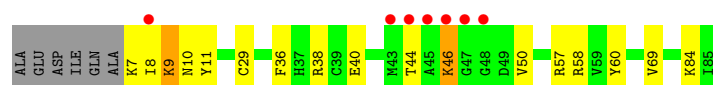
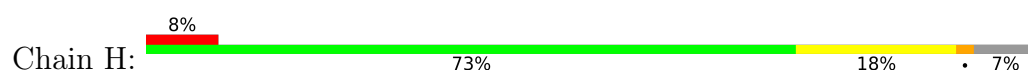
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



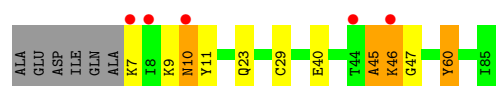
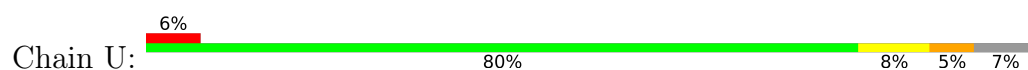
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



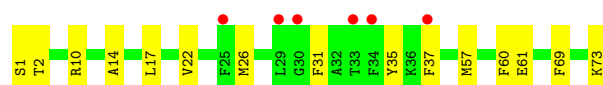
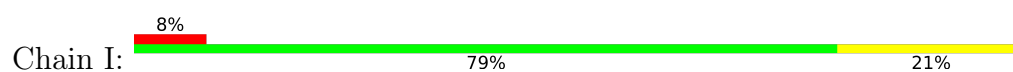
- Molecule 8: Cytochrome c oxidase subunit 6B1



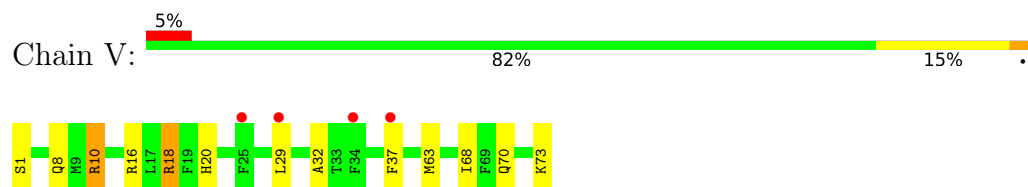
- Molecule 8: Cytochrome c oxidase subunit 6B1



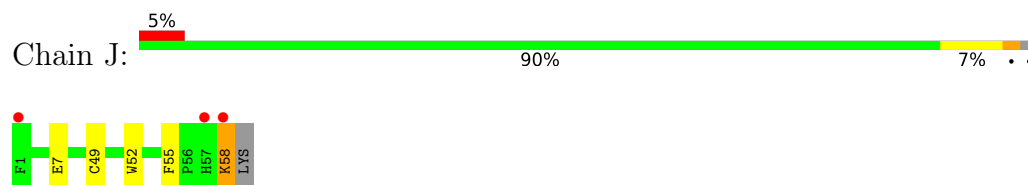
- Molecule 9: Cytochrome c oxidase subunit 6C



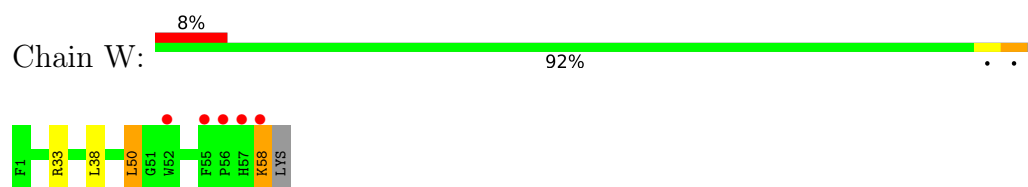
• Molecule 9: Cytochrome c oxidase subunit 6C



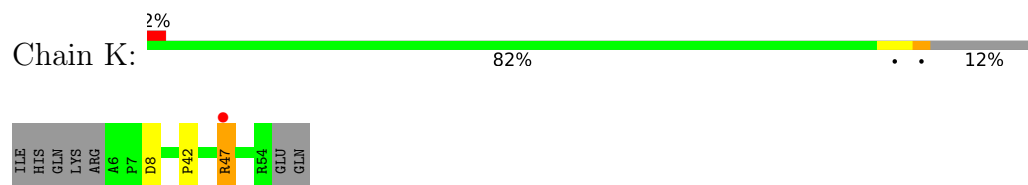
• Molecule 10: Cytochrome c oxidase subunit 7A1



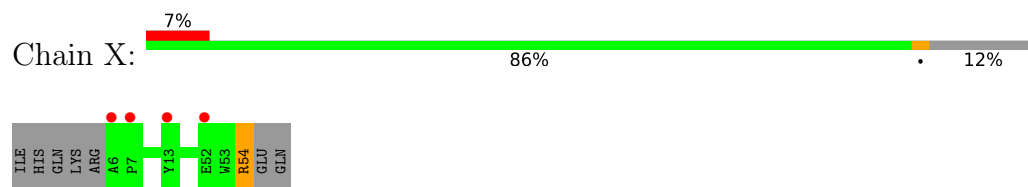
• Molecule 10: Cytochrome c oxidase subunit 7A1



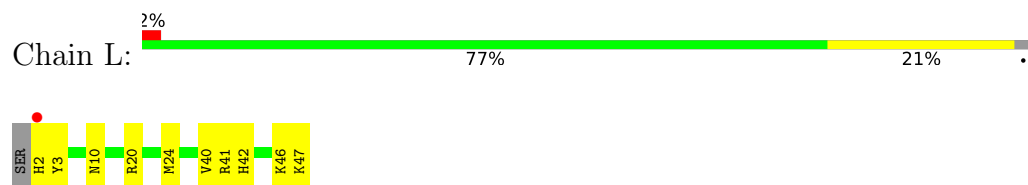
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



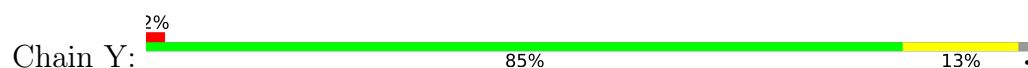
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

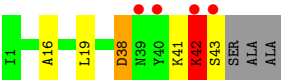
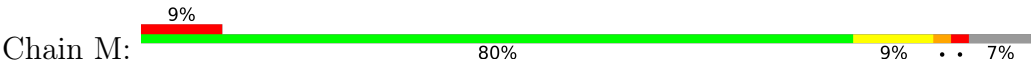


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

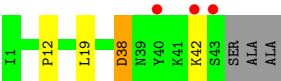
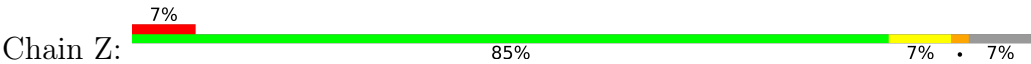




● Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



● 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	183.41Å 206.27Å 177.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 1.85 134.59 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.97-1.85) 99.4 (134.59-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.164 , 0.188 0.164 , 0.189	Depositor DCC
R_{free} test set	28371 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.0	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	33558	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.08	6/4308 (0.1%)	0.93	11/5878 (0.2%)
1	N	0.88	0/4288	0.82	3/5852 (0.1%)
2	B	0.90	2/2047 (0.1%)	0.90	6/2790 (0.2%)
2	O	0.68	0/2024	0.77	2/2757 (0.1%)
3	C	0.90	1/2263 (0.0%)	0.74	0/3090
3	P	0.85	0/2272	0.73	0/3102
4	D	0.90	0/1245	0.79	0/1679
4	Q	0.54	0/1248	0.67	1/1684 (0.1%)
5	E	0.81	0/871	0.76	1/1182 (0.1%)
5	R	0.65	0/871	0.73	0/1182
6	F	0.86	0/795	0.81	0/1079
6	S	0.71	1/780 (0.1%)	0.82	0/1058
7	G	0.85	1/690 (0.1%)	0.86	1/937 (0.1%)
7	T	0.76	1/701 (0.1%)	0.84	1/951 (0.1%)
8	H	0.88	2/682 (0.3%)	0.78	1/921 (0.1%)
8	U	0.66	0/682	0.68	0/921
9	I	0.78	2/605 (0.3%)	0.75	0/802
9	V	0.53	0/605	0.73	1/802 (0.1%)
10	J	0.62	0/471	0.65	0/636
10	W	0.57	0/480	0.63	0/648
11	K	0.79	0/398	0.77	1/546 (0.2%)
11	X	0.47	0/405	0.55	0/556
12	L	0.85	0/401	0.74	0/536
12	Y	0.61	0/401	0.63	0/536
13	M	0.83	0/345	0.75	0/470
13	Z	0.51	0/345	0.58	0/470
All	All	0.84	16/30223 (0.1%)	0.79	29/41065 (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
12	Y	0	1
All	All	0	4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	193	TYR	CD1-CE1	6.55	1.49	1.39
7	T	36	TRP	CB-CG	6.20	1.61	1.50
1	A	346	PHE	CD2-CE2	6.20	1.51	1.39
1	A	74	MET	CB-CG	6.13	1.71	1.51
1	A	220	PHE	CE1-CZ	5.88	1.48	1.37

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-11.24	82.22	100.20
1	N	71	MET	CG-SD-CE	-9.71	84.67	100.20
1	A	96	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	189	MET	CG-SD-CE	-7.65	87.96	100.20
2	B	45	MET	CG-SD-CE	7.17	111.67	100.20

There are no chirality outliers.

All (4) 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
12	Y	46	LYS	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	4125	0	4107	38	0
1	N	4122	0	4101	52	0
2	B	1996	0	2031	24	0
2	O	1975	0	2000	33	0
3	C	2152	0	2068	26	0
3	P	2173	0	2081	20	0
4	D	1198	0	1179	7	0
4	Q	1213	0	1199	7	0
5	E	852	0	845	7	0
5	R	852	0	845	3	0
6	F	773	0	751	12	0
6	S	763	0	742	8	0
7	G	675	0	643	12	0
7	T	681	0	648	10	0
8	H	662	0	623	7	0
8	U	662	0	623	5	0
9	I	601	0	613	9	0
9	V	601	0	613	11	0
10	J	460	0	459	7	0
10	W	469	0	463	7	0
11	K	384	0	366	2	0
11	X	391	0	374	1	0
12	L	383	0	385	7	0
12	Y	383	0	385	5	0
13	M	335	0	352	4	0
13	Z	335	0	352	3	0
14	A	180	0	162	17	0
14	N	180	0	162	20	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	9	0	0	7	0
18	N	9	0	0	6	0
19	A	102	0	152	6	0
19	C	100	0	148	3	0
19	G	51	0	76	4	0
19	N	102	0	152	9	0
19	P	51	0	76	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	40	0	60	3	0
20	B	8	0	12	0	0
20	C	32	0	48	2	0
20	D	16	0	24	1	0
20	E	20	0	30	0	0
20	F	20	0	30	0	0
20	G	8	0	12	1	0
20	H	8	0	12	2	0
20	L	4	0	6	0	0
20	N	32	0	48	1	0
20	O	12	0	18	1	0
20	P	12	0	18	0	0
20	Q	8	0	12	0	0
20	R	24	0	36	2	0
20	S	12	0	18	5	0
20	T	4	0	6	0	0
20	U	4	0	6	0	0
20	V	4	0	6	0	0
21	B	63	0	110	7	0
21	D	63	0	110	11	0
21	L	63	0	110	4	0
21	N	61	0	102	0	0
21	Q	63	0	110	7	0
21	Y	63	0	110	7	0
22	B	29	0	39	0	0
22	C	58	0	78	4	0
22	G	29	0	39	1	0
22	J	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	37	4	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	50	0	72	10	0
24	O	51	0	75	6	0
25	C	88	0	115	10	0
25	L	30	0	33	4	0
25	M	33	0	42	1	0
25	P	99	0	126	9	0
25	Z	33	0	42	1	0
26	C	89	0	133	13	0
26	N	96	0	140	10	0
26	P	80	0	106	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	T	97	0	146	11	0
27	C	97	0	133	4	0
27	G	97	0	131	3	0
27	P	53	0	77	1	0
27	T	50	0	71	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	222	0	0	1	0
29	B	134	0	0	2	0
29	C	99	0	0	0	0
29	D	108	0	0	2	0
29	E	82	0	0	1	0
29	F	79	0	0	2	0
29	G	52	0	0	1	0
29	H	44	0	0	0	0
29	I	27	0	0	2	0
29	J	27	0	0	1	0
29	K	20	0	0	1	0
29	L	26	0	0	0	0
29	M	24	0	0	0	0
29	N	209	0	0	0	0
29	O	112	0	0	0	0
29	P	90	0	0	1	0
29	Q	38	0	0	1	0
29	R	39	0	0	0	0
29	S	59	0	0	1	0
29	T	35	0	0	0	0
29	U	33	0	0	0	0
29	V	14	0	0	0	0
29	W	12	0	0	0	0
29	X	11	0	0	0	0
29	Y	13	0	0	0	0
29	Z	16	0	0	1	0
All	All	33558	0	32582	387	0

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

The worst 5 of 387 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:CYS:SG	6:F:87[B]:THR:HG23	2.09	0.93
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.61	0.82
26:N:601:CDL:H371	2:O:78:LEU:HD12	1.63	0.79
1:N:309:THR:HG22	14:N:603[B]:HEA:HMB2	1.66	0.78
7:T:7:ASP:O	7:T:9:GLY:N	2.17	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/514 (104%)	514 (97%)	18 (3%)	0	100	100
1	N	530/514 (103%)	517 (98%)	13 (2%)	0	100	100
2	B	248/227 (109%)	242 (98%)	6 (2%)	0	100	100
2	O	245/227 (108%)	239 (98%)	5 (2%)	1 (0%)	34	19
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
4	Q	144/147 (98%)	138 (96%)	4 (3%)	2 (1%)	11	3
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15	5
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	7	1
6	S	98/98 (100%)	92 (94%)	3 (3%)	3 (3%)	4	0
7	G	81/85 (95%)	70 (86%)	5 (6%)	6 (7%)	1	0
7	T	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	0
8	H	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
8	U	77/85 (91%)	72 (94%)	2 (3%)	3 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	45/47 (96%)	42 (93%)	2 (4%)	1 (2%)	6	1
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3617/3614 (100%)	3494 (97%)	99 (3%)	24 (1%)	22	9

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	8	HIS
13	M	42	LYS
4	Q	7	LYS
4	Q	8	SER

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	445/426 (104%)	440 (99%)	5 (1%)	73	65
1	N	443/426 (104%)	436 (98%)	7 (2%)	62	49
2	B	233/210 (111%)	224 (96%)	9 (4%)	32	15
2	O	230/210 (110%)	222 (96%)	8 (4%)	36	18
3	C	232/226 (103%)	229 (99%)	3 (1%)	69	58
3	P	233/226 (103%)	228 (98%)	5 (2%)	53	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	130/129 (101%)	129 (99%)	1 (1%)	81	76
4	Q	130/129 (101%)	121 (93%)	9 (7%)	15	4
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	65
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	12
6	F	85/81 (105%)	80 (94%)	5 (6%)	19	6
6	S	83/81 (102%)	78 (94%)	5 (6%)	19	5
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	1
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	0
8	H	71/75 (95%)	64 (90%)	7 (10%)	8	1
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	2
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	8
9	V	57/57 (100%)	51 (90%)	6 (10%)	7	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	40
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	14
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	39 (98%)	1 (2%)	47	31
12	L	40/40 (100%)	39 (98%)	1 (2%)	47	31
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47	31
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	8
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	8
All	All	3151/3082 (102%)	3043 (97%)	108 (3%)	37	19

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	171	LYS
4	Q	143	ASN
9	V	37	PHE
3	P	40	MET
4	Q	6	VAL

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

Mol	Chain	Res	Type
8	H	37	HIS
2	O	24	HIS
8	U	22	ASN
3	P	133	ASN
4	Q	101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	G	11	7	8,10,11	1.62	2 (25%)	10,14,16	1.13	1 (10%)
7	TPO	T	11	7	8,10,11	1.47	1 (12%)	10,14,16	1.35	1 (10%)
2	FME	O	1	2	8,9,10	0.59	0	7,9,11	1.44	2 (28%)
1	FME	N	1	1	8,9,10	0.43	0	7,9,11	1.42	1 (14%)
1	FME	A	1	1	8,9,10	0.56	0	7,9,11	1.79	1 (14%)
9	SAC	V	1	9	7,8,9	0.55	0	8,9,11	1.05	1 (12%)
9	SAC	I	1	9	7,8,9	0.59	0	8,9,11	1.15	1 (12%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	1.97	2 (28%)

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
7	TPO	G	11	7	-	5/9/11/13	-
7	TPO	T	11	7	-	5/9/11/13	-

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.88	1.59	1.50
7	G	11	TPO	P-O1P	2.84	1.59	1.50
7	G	11	TPO	P-OG1	2.61	1.64	1.59

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.15	101.42	112.95
7	T	11	TPO	CG2-CB-CA	3.02	119.12	113.16
1	A	1	FME	C-CA-N	2.91	114.99	109.73
2	O	1	FME	CG-CB-CA	-2.70	105.45	112.95
1	N	1	FME	O-C-CA	-2.61	117.94	124.78

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 134 ligands modelled in this entry, 10 are monoatomic - leaving 124 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	DMU	M	101	-	34,34,34	0.45	0	45,45,45	1.35	4 (8%)
20	EDO	A	615	-	3,3,3	0.80	0	2,2,2	0.71	0
18	AZI	A	606[A]	15	0,2,2	-	-	0,1,1	-	-
20	EDO	C	312	-	3,3,3	0.48	0	2,2,2	0.42	0
20	EDO	R	202	-	3,3,3	0.36	0	2,2,2	0.51	0
22	CHD	G	102	-	32,32,32	0.83	0	51,51,51	1.29	7 (13%)
20	EDO	D	203	-	3,3,3	0.39	0	2,2,2	0.30	0
18	AZI	N	608[B]	15,14	0,2,2	-	-	0,1,1	-	-
20	EDO	N	612	-	3,3,3	0.49	0	2,2,2	0.24	0
14	HEA	A	602[A]	18,1	57,67,67	1.62	11 (19%)	61,103,103	2.08	16 (26%)
22	CHD	J	101	-	32,32,32	0.79	1 (3%)	51,51,51	1.27	5 (9%)
25	DMU	C	310	-	22,22,34	0.46	0	27,27,45	0.97	1 (3%)
20	EDO	C	315	-	3,3,3	0.53	0	2,2,2	0.18	0
22	CHD	W	101	10	32,32,32	0.82	1 (3%)	51,51,51	2.51	19 (37%)
20	EDO	T	103	-	3,3,3	0.93	0	2,2,2	0.59	0
22	CHD	C	306	-	32,32,32	0.93	0	51,51,51	2.14	16 (31%)
20	EDO	F	106	-	3,3,3	0.42	0	2,2,2	0.71	0
25	DMU	P	307	-	34,34,34	0.63	0	45,45,45	1.94	10 (22%)
20	EDO	S	104	-	3,3,3	0.70	0	2,2,2	0.54	0
20	EDO	H	102	-	3,3,3	0.45	0	2,2,2	0.58	0
20	EDO	R	201	-	3,3,3	0.69	0	2,2,2	0.52	0
20	EDO	O	304	-	3,3,3	0.49	0	2,2,2	0.48	0
27	PEK	C	307	-	52,52,52	1.08	2 (3%)	55,57,57	1.57	10 (18%)
20	EDO	A	610	-	3,3,3	0.36	0	2,2,2	0.77	0
19	PGV	A	608	-	50,50,50	1.03	3 (6%)	53,56,56	0.93	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	N	603[A]	18,1	57,67,67	1.53	10 (17%)	61,103,103	2.04	23 (37%)
25	DMU	P	308	-	34,34,34	0.65	1 (2%)	45,45,45	0.98	1 (2%)
20	EDO	E	201	-	3,3,3	0.73	0	2,2,2	0.24	0
20	EDO	Q	202	-	3,3,3	0.45	0	2,2,2	0.60	0
22	CHD	P	301	-	32,32,32	0.83	0	51,51,51	1.45	7 (13%)
20	EDO	O	303	-	3,3,3	0.59	0	2,2,2	0.94	0
20	EDO	A	614	-	3,3,3	0.92	0	2,2,2	0.27	0
27	PEK	P	312	-	52,52,52	0.86	3 (5%)	55,57,57	2.31	9 (16%)
20	EDO	A	618	-	3,3,3	0.35	0	2,2,2	0.46	0
19	PGV	C	304	-	50,50,50	0.87	3 (6%)	53,56,56	1.13	7 (13%)
20	EDO	N	618	-	3,3,3	0.44	0	2,2,2	0.39	0
22	CHD	B	302	-	32,32,32	1.15	2 (6%)	51,51,51	1.46	9 (17%)
19	PGV	P	303	-	50,50,50	0.70	2 (4%)	53,56,56	1.08	5 (9%)
20	EDO	D	202	-	3,3,3	0.45	0	2,2,2	0.79	0
24	PSC	B	304	-	48,48,51	1.31	4 (8%)	53,55,59	1.28	4 (7%)
20	EDO	S	103	-	3,3,3	0.96	0	2,2,2	0.48	0
19	PGV	C	308	-	48,48,50	1.22	3 (6%)	51,53,56	1.33	4 (7%)
20	EDO	E	204	-	3,3,3	0.74	0	2,2,2	0.11	0
20	EDO	C	311	-	3,3,3	0.76	0	2,2,2	0.33	0
20	EDO	G	106	-	3,3,3	0.67	0	2,2,2	0.38	0
20	EDO	B	305	-	3,3,3	0.61	0	2,2,2	0.14	0
20	EDO	O	305	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	P	309	-	3,3,3	0.51	0	2,2,2	0.70	0
20	EDO	A	612	-	3,3,3	1.13	0	2,2,2	0.87	0
26	CDL	N	601	-	93,93,99	1.43	12 (12%)	97,103,111	1.19	11 (11%)
20	EDO	A	616	-	3,3,3	0.99	0	2,2,2	0.89	0
18	AZI	N	608[A]	14	0,2,2	-	-	0,1,1	-	-
26	CDL	P	304	-	77,77,99	1.48	10 (12%)	84,85,111	1.68	13 (15%)
27	PEK	G	101	-	52,52,52	0.85	4 (7%)	55,57,57	1.13	5 (9%)
20	EDO	F	104	-	3,3,3	0.38	0	2,2,2	0.48	0
20	EDO	Q	203	-	3,3,3	0.55	0	2,2,2	0.18	0
19	PGV	G	104	-	50,50,50	1.08	2 (4%)	53,56,56	1.54	10 (18%)
20	EDO	P	311	-	3,3,3	0.58	0	2,2,2	0.46	0
20	EDO	R	203	-	3,3,3	0.49	0	2,2,2	0.41	0
20	EDO	C	314	-	3,3,3	0.48	0	2,2,2	0.56	0
21	TGL	B	301	-	62,62,62	1.20	3 (4%)	65,65,65	1.38	6 (9%)
14	HEA	A	602[B]	18,1	57,67,67	1.51	9 (15%)	61,103,103	2.09	18 (29%)
20	EDO	N	614	-	3,3,3	1.22	0	2,2,2	0.59	0
21	TGL	Q	201	-	62,62,62	1.06	4 (6%)	65,65,65	0.90	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	E	202	-	3,3,3	0.49	0	2,2,2	0.57	0
20	EDO	L	103	-	3,3,3	0.41	0	2,2,2	0.49	0
18	AZI	N	607[A]	15	0,2,2	-	-	0,1,1	-	-
20	EDO	C	318	-	3,3,3	0.67	0	2,2,2	0.79	0
27	PEK	T	101	-	49,49,52	1.13	3 (6%)	53,54,57	1.58	9 (16%)
14	HEA	A	601	1	57,67,67	1.77	13 (22%)	61,103,103	2.33	24 (39%)
20	EDO	H	101	-	3,3,3	0.32	0	2,2,2	0.86	0
25	DMU	P	306	-	34,34,34	0.67	1 (2%)	45,45,45	0.88	2 (4%)
14	HEA	N	603[B]	18,1	57,67,67	1.55	10 (17%)	61,103,103	2.04	20 (32%)
21	TGL	D	201	-	62,62,62	1.24	4 (6%)	65,65,65	1.21	5 (7%)
20	EDO	N	613	-	3,3,3	0.61	0	2,2,2	0.44	0
25	DMU	C	302	-	34,34,34	0.69	0	45,45,45	1.66	8 (17%)
21	TGL	N	610	-	59,59,62	1.14	3 (5%)	61,61,65	1.39	7 (11%)
20	EDO	N	611	-	3,3,3	0.38	0	2,2,2	0.54	0
20	EDO	E	203	-	3,3,3	0.42	0	2,2,2	0.46	0
18	AZI	A	607[B]	15,14	0,2,2	-	-	0,1,1	-	-
25	DMU	L	102	-	31,31,34	0.91	0	42,42,45	1.83	12 (28%)
20	EDO	R	206	-	3,3,3	0.63	0	2,2,2	0.25	0
20	EDO	A	613	-	3,3,3	0.95	0	2,2,2	0.59	0
19	PGV	N	609	-	50,50,50	0.94	3 (6%)	53,56,56	1.38	7 (13%)
20	EDO	C	316	-	3,3,3	0.55	0	2,2,2	0.32	0
23	CUA	O	301	2	0,1,1	-	-	-	-	-
21	TGL	L	101	-	62,62,62	1.60	5 (8%)	65,65,65	1.99	15 (23%)
20	EDO	P	310	-	3,3,3	0.58	0	2,2,2	0.32	0
20	EDO	F	103	-	3,3,3	0.59	0	2,2,2	0.49	0
20	EDO	F	102	-	3,3,3	0.83	0	2,2,2	0.66	0
20	EDO	N	617	-	3,3,3	0.57	0	2,2,2	0.22	0
20	EDO	V	101	-	3,3,3	0.46	0	2,2,2	0.54	0
25	DMU	Z	101	-	34,34,34	0.44	0	45,45,45	0.86	1 (2%)
23	CUA	B	303	2	0,1,1	-	-	-	-	-
24	PSC	O	302	-	50,50,51	1.16	3 (6%)	56,58,59	1.31	5 (8%)
20	EDO	N	616	-	3,3,3	0.77	0	2,2,2	0.09	0
20	EDO	R	204	-	3,3,3	0.68	0	2,2,2	0.41	0
20	EDO	E	205	-	3,3,3	0.48	0	2,2,2	0.44	0
20	EDO	R	205	-	3,3,3	0.45	0	2,2,2	0.59	0
22	CHD	C	301	-	32,32,32	1.01	2 (6%)	51,51,51	1.77	12 (23%)
20	EDO	U	101	-	3,3,3	0.49	0	2,2,2	0.22	0
20	EDO	A	619	-	3,3,3	0.47	0	2,2,2	0.40	0
20	EDO	A	617	-	3,3,3	0.68	0	2,2,2	0.47	0
21	TGL	Y	101	-	62,62,62	1.18	3 (4%)	65,65,65	1.45	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	B	306	-	3,3,3	1.03	0	2,2,2	0.27	0
20	EDO	C	317	-	3,3,3	0.57	0	2,2,2	0.34	0
27	PEK	C	319	-	43,43,52	1.15	2 (4%)	46,48,57	1.67	8 (17%)
20	EDO	F	105	-	3,3,3	0.36	0	2,2,2	0.77	0
20	EDO	A	611	-	3,3,3	0.57	0	2,2,2	0.64	0
14	HEA	N	602	1	57,67,67	1.45	8 (14%)	61,103,103	2.20	24 (39%)
22	CHD	P	305	-	32,32,32	0.77	0	51,51,51	1.89	11 (21%)
26	CDL	C	305	-	87,87,99	1.48	14 (16%)	95,97,111	1.73	22 (23%)
20	EDO	D	204	-	3,3,3	0.36	0	2,2,2	0.64	0
25	DMU	C	309	-	34,34,34	0.69	1 (2%)	45,45,45	1.66	8 (17%)
27	PEK	G	103	-	43,43,52	1.09	2 (4%)	46,48,57	1.59	9 (19%)
20	EDO	D	205	-	3,3,3	0.58	0	2,2,2	0.36	0
20	EDO	G	105	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	C	313	-	3,3,3	0.53	0	2,2,2	0.36	0
20	EDO	S	101	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	N	615	-	3,3,3	0.51	0	2,2,2	0.66	0
19	PGV	N	619	-	50,50,50	1.04	2 (4%)	53,56,56	1.22	6 (11%)
18	AZI	A	607[A]	14	0,2,2	-	-	0,1,1	-	-
26	CDL	T	102	-	95,95,99	1.40	12 (12%)	100,106,111	1.48	13 (13%)
19	PGV	A	609	-	50,50,50	1.25	4 (8%)	53,56,56	1.64	10 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
20	EDO	A	615	-	-	1/1/1/1	-
20	EDO	C	312	-	-	1/1/1/1	-
20	EDO	R	202	-	-	1/1/1/1	-
22	CHD	G	102	-	-	3/9/74/74	0/4/4/4
20	EDO	D	203	-	-	1/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
14	HEA	A	602[A]	18,1	3/3/7/16	6/32/76/76	-
22	CHD	J	101	-	-	4/9/74/74	0/4/4/4
25	DMU	C	310	-	-	4/13/33/59	0/1/1/2
20	EDO	C	315	-	-	1/1/1/1	-
22	CHD	W	101	10	-	8/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	T	103	-	-	0/1/1/1	-
22	CHD	C	306	-	-	6/9/74/74	0/4/4/4
20	EDO	F	106	-	-	0/1/1/1	-
25	DMU	P	307	-	-	8/19/59/59	0/2/2/2
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	H	102	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	O	304	-	-	1/1/1/1	-
27	PEK	C	307	-	-	27/56/56/56	-
20	EDO	A	610	-	-	1/1/1/1	-
19	PGV	A	608	-	-	7/55/55/55	-
14	HEA	N	603[A]	18,1	3/3/7/16	6/32/76/76	-
25	DMU	P	308	-	-	6/19/59/59	0/2/2/2
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	Q	202	-	-	0/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
27	PEK	P	312	-	-	19/56/56/56	-
20	EDO	A	618	-	-	1/1/1/1	-
19	PGV	C	304	-	-	12/55/55/55	-
20	EDO	N	618	-	-	0/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
19	PGV	P	303	-	-	7/55/55/55	-
20	EDO	D	202	-	-	1/1/1/1	-
24	PSC	B	304	-	-	21/50/50/55	-
20	EDO	S	103	-	-	0/1/1/1	-
19	PGV	C	308	-	-	21/52/52/55	-
20	EDO	E	204	-	-	1/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	G	106	-	-	1/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	O	305	-	-	0/1/1/1	-
20	EDO	P	309	-	-	1/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
26	CDL	N	601	-	-	47/100/100/110	-
20	EDO	A	616	-	-	0/1/1/1	-
26	CDL	P	304	-	-	25/75/77/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PEK	G	101	-	-	10/56/56/56	-
20	EDO	F	104	-	-	1/1/1/1	-
20	EDO	Q	203	-	-	0/1/1/1	-
19	PGV	G	104	-	-	28/55/55/55	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	R	203	-	-	0/1/1/1	-
20	EDO	C	314	-	-	0/1/1/1	-
21	TGL	B	301	-	-	30/65/65/65	-
14	HEA	A	602[B]	18,1	3/3/7/16	5/32/76/76	-
20	EDO	N	614	-	-	0/1/1/1	-
21	TGL	Q	201	-	-	30/65/65/65	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	C	318	-	-	1/1/1/1	-
27	PEK	T	101	-	-	21/51/51/56	-
14	HEA	A	601	1	3/3/7/16	4/32/76/76	-
20	EDO	H	101	-	-	1/1/1/1	-
25	DMU	P	306	-	-	7/19/59/59	0/2/2/2
14	HEA	N	603[B]	18,1	3/3/7/16	5/32/76/76	-
21	TGL	D	201	-	-	36/65/65/65	-
20	EDO	N	613	-	-	1/1/1/1	-
25	DMU	C	302	-	-	5/19/59/59	0/2/2/2
21	TGL	N	610	-	-	29/60/60/65	-
20	EDO	N	611	-	-	1/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
25	DMU	L	102	-	-	10/16/56/59	0/2/2/2
20	EDO	R	206	-	-	1/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
19	PGV	N	609	-	-	9/55/55/55	-
20	EDO	C	316	-	-	1/1/1/1	-
21	TGL	L	101	-	-	37/65/65/65	-
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
20	EDO	V	101	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
24	PSC	O	302	-	-	30/54/54/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	616	-	-	0/1/1/1	-
20	EDO	E	205	-	-	0/1/1/1	-
20	EDO	R	205	-	-	0/1/1/1	-
22	CHD	C	301	-	-	3/9/74/74	0/4/4/4
20	EDO	U	101	-	-	1/1/1/1	-
20	EDO	A	619	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	30/65/65/65	-
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	C	317	-	-	1/1/1/1	-
27	PEK	C	319	-	-	28/47/47/56	-
20	EDO	F	105	-	-	1/1/1/1	-
20	EDO	A	611	-	-	1/1/1/1	-
14	HEA	N	602	1	3/3/7/16	7/32/76/76	-
22	CHD	P	305	-	-	5/9/74/74	0/4/4/4
26	CDL	C	305	-	-	51/91/91/110	-
20	EDO	D	204	-	-	1/1/1/1	-
25	DMU	C	309	-	-	8/19/59/59	0/2/2/2
27	PEK	G	103	-	-	23/47/47/56	-
20	EDO	D	205	-	-	0/1/1/1	-
20	EDO	G	105	-	-	1/1/1/1	-
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	S	101	-	-	1/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
19	PGV	N	619	-	-	23/55/55/55	-
20	EDO	R	204	-	-	0/1/1/1	-
26	CDL	T	102	-	-	52/104/104/110	-
19	PGV	A	609	-	-	21/55/55/55	-

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	101	TGL	OG3-CC1	7.63	1.55	1.33
21	L	101	TGL	OG2-CB1	7.07	1.54	1.34
21	B	301	TGL	OG2-CB1	5.54	1.49	1.34
19	C	308	PGV	O03-C19	5.51	1.49	1.33
21	Y	101	TGL	OG2-CB1	5.34	1.49	1.34

The worst 5 of 477 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	312	PEK	C2-C3-C4	11.86	134.37	113.23
21	L	101	TGL	OG2-CB1-CB2	8.28	129.34	111.50
22	C	306	CHD	C23-C22-C20	-7.67	100.50	114.52
27	P	312	PEK	O01-C1-O02	-7.62	105.29	123.70
21	B	301	TGL	OG2-CB1-CB2	7.06	126.72	111.50

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	A	602[A]	HEA	ND
14	A	602[A]	HEA	NA

5 of 824 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	603[B]	HEA	C4D-C3D-CAD-CBD
19	A	609	PGV	C04-C05-C06-O06
19	A	609	PGV	O05-C05-C06-O06
19	A	609	PGV	C2-C1-O01-C02

There are no ring outliers.

62 monomers are involved in 225 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	M	101	DMU	1	0
18	A	606[A]	AZI	1	0
20	R	202	EDO	1	0
22	G	102	CHD	1	0
14	A	602[A]	HEA	6	0
22	J	101	CHD	1	0
22	W	101	CHD	4	0
22	C	306	CHD	4	0
25	P	307	DMU	3	0
20	H	102	EDO	1	0
27	C	307	PEK	3	0
20	A	610	EDO	1	0
19	A	608	PGV	2	0
14	N	603[A]	HEA	8	0
25	P	308	DMU	1	0

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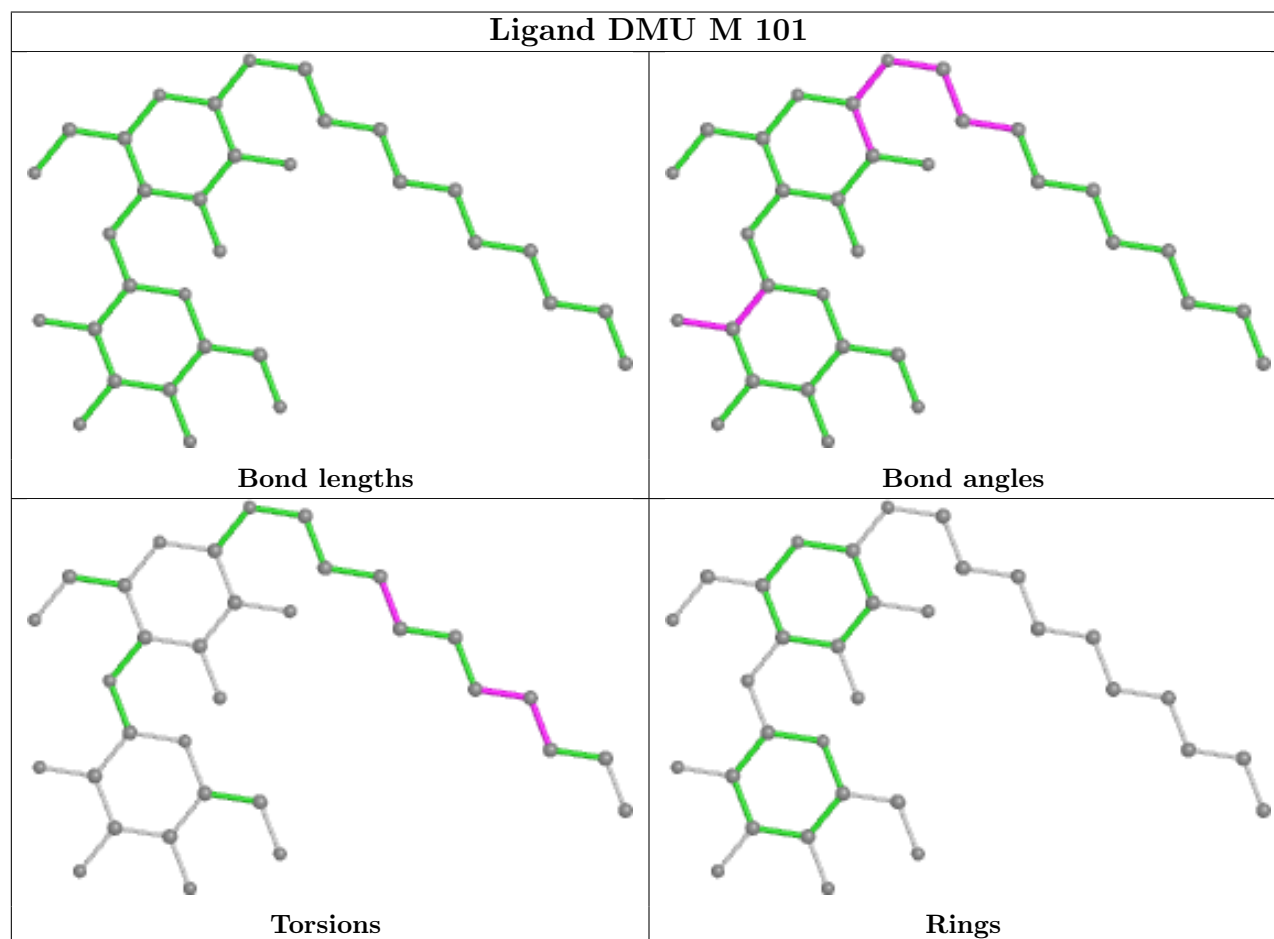
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	P	312	PEK	1	0
19	C	304	PGV	1	0
19	P	303	PGV	1	0
24	B	304	PSC	10	0
19	C	308	PGV	2	0
20	O	305	EDO	1	0
26	N	601	CDL	10	0
20	A	616	EDO	2	0
18	N	608[A]	AZI	6	0
26	P	304	CDL	8	0
27	G	101	PEK	2	0
19	G	104	PGV	4	0
20	C	314	EDO	1	0
21	B	301	TGL	7	0
14	A	602[B]	HEA	8	0
21	Q	201	TGL	7	0
18	N	607[A]	AZI	1	0
20	C	318	EDO	1	0
27	T	101	PEK	4	0
14	A	601	HEA	3	0
20	H	101	EDO	1	0
25	P	306	DMU	5	0
14	N	603[B]	HEA	8	0
21	D	201	TGL	11	0
20	N	613	EDO	1	0
25	C	302	DMU	8	0
18	A	607[B]	AZI	2	0
25	L	102	DMU	4	0
19	N	609	PGV	2	0
21	L	101	TGL	4	0
25	Z	101	DMU	1	0
24	O	302	PSC	6	0
20	R	205	EDO	1	0
21	Y	101	TGL	7	0
27	C	319	PEK	1	0
14	N	602	HEA	4	0
22	P	305	CHD	3	0
26	C	305	CDL	13	0
20	D	204	EDO	1	0
25	C	309	DMU	2	0
27	G	103	PEK	1	0
20	G	105	EDO	1	0

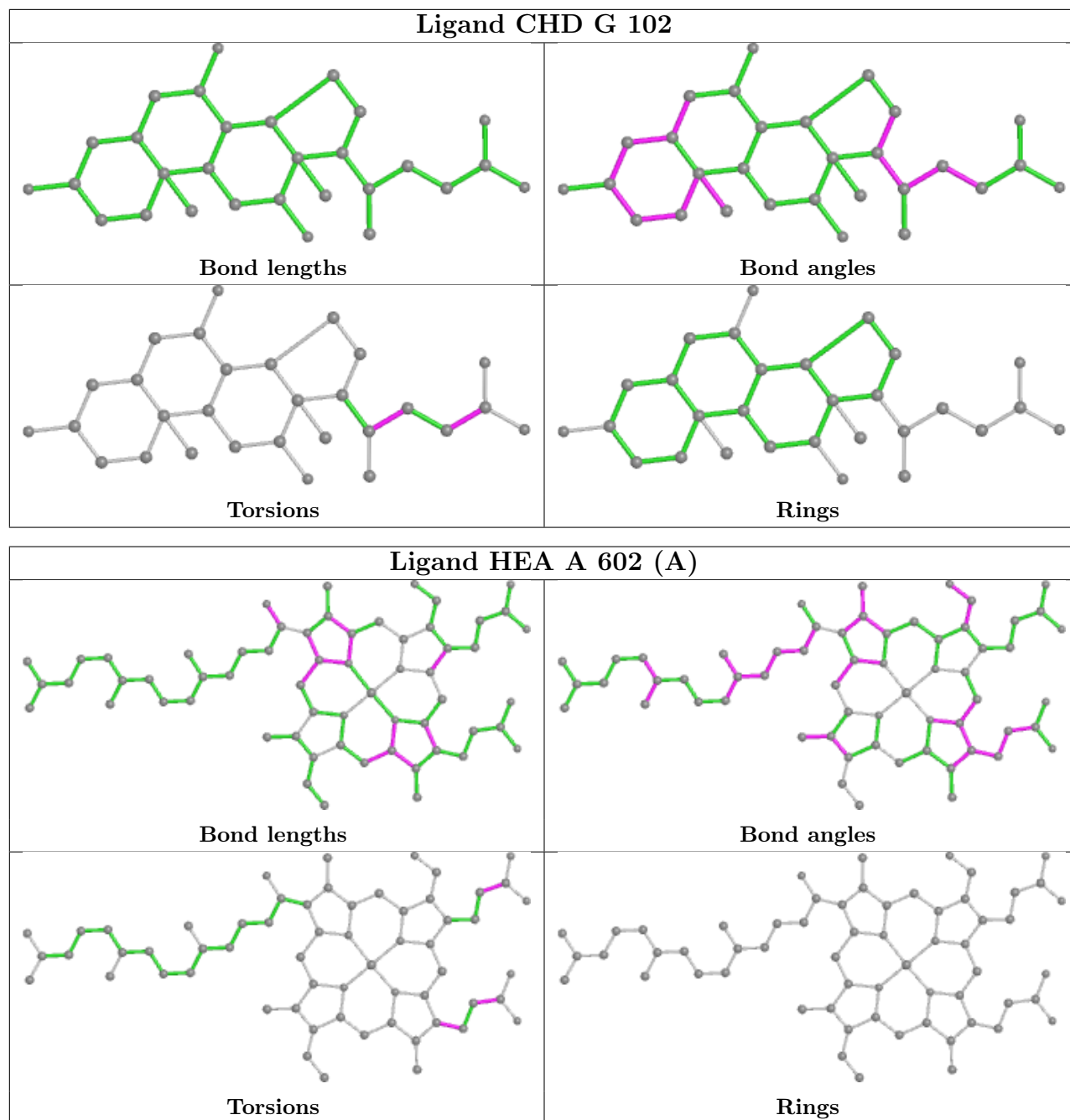
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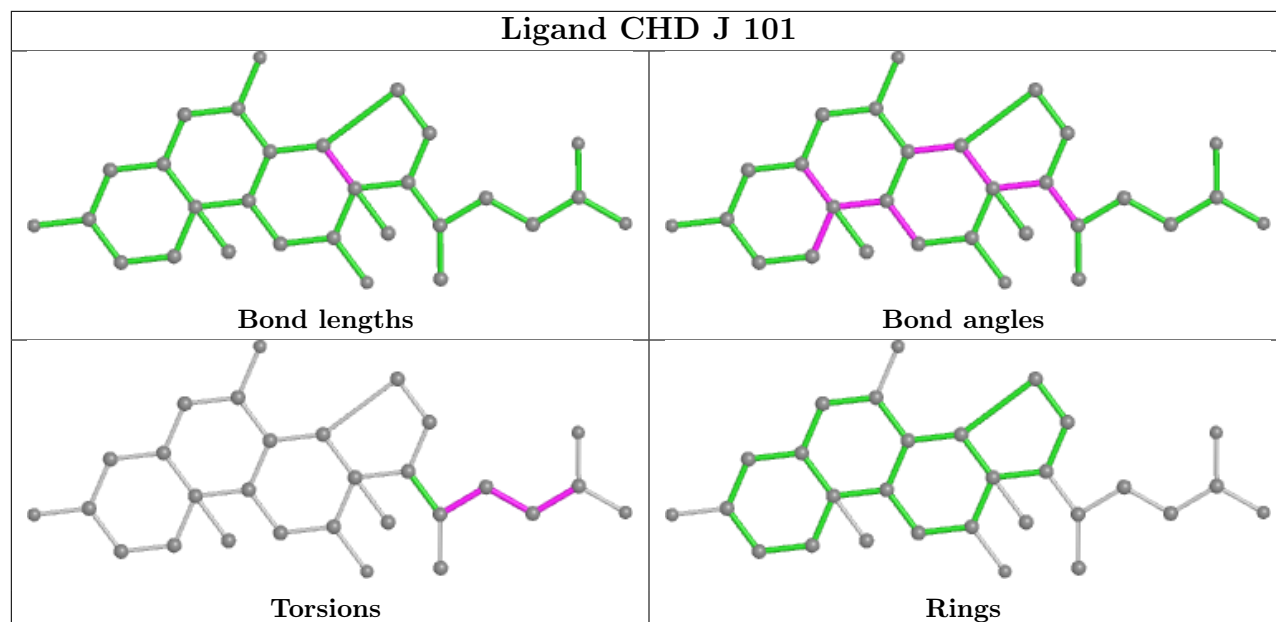
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S	101	EDO	5	0
19	N	619	PGV	7	0
18	A	607[A]	AZI	5	0
26	T	102	CDL	11	0
19	A	609	PGV	4	0

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.

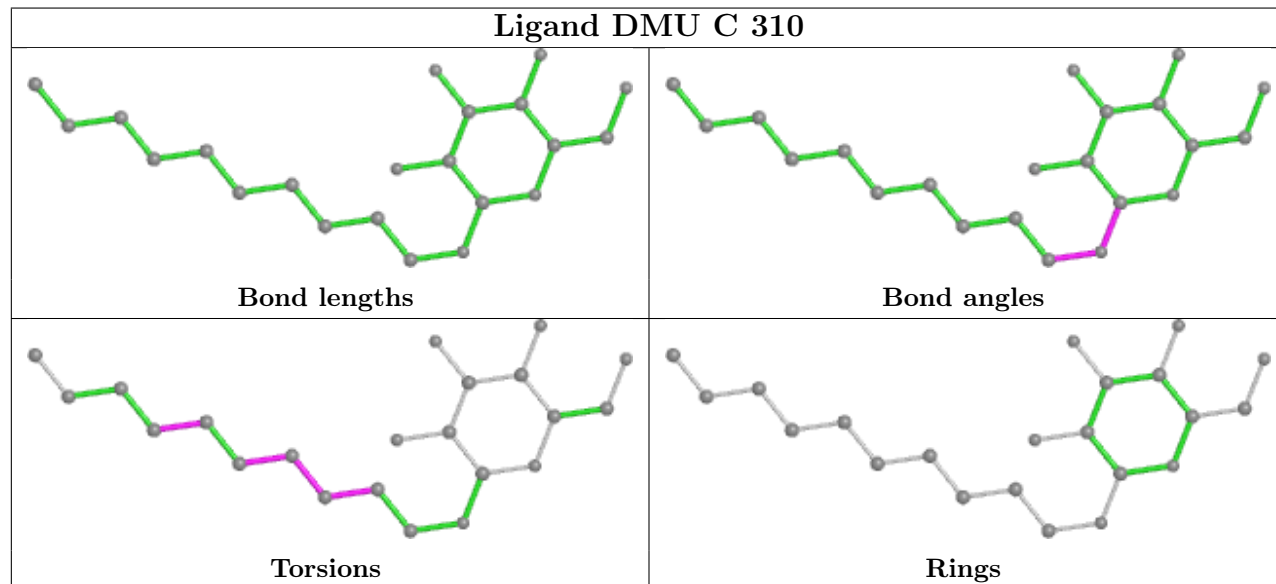


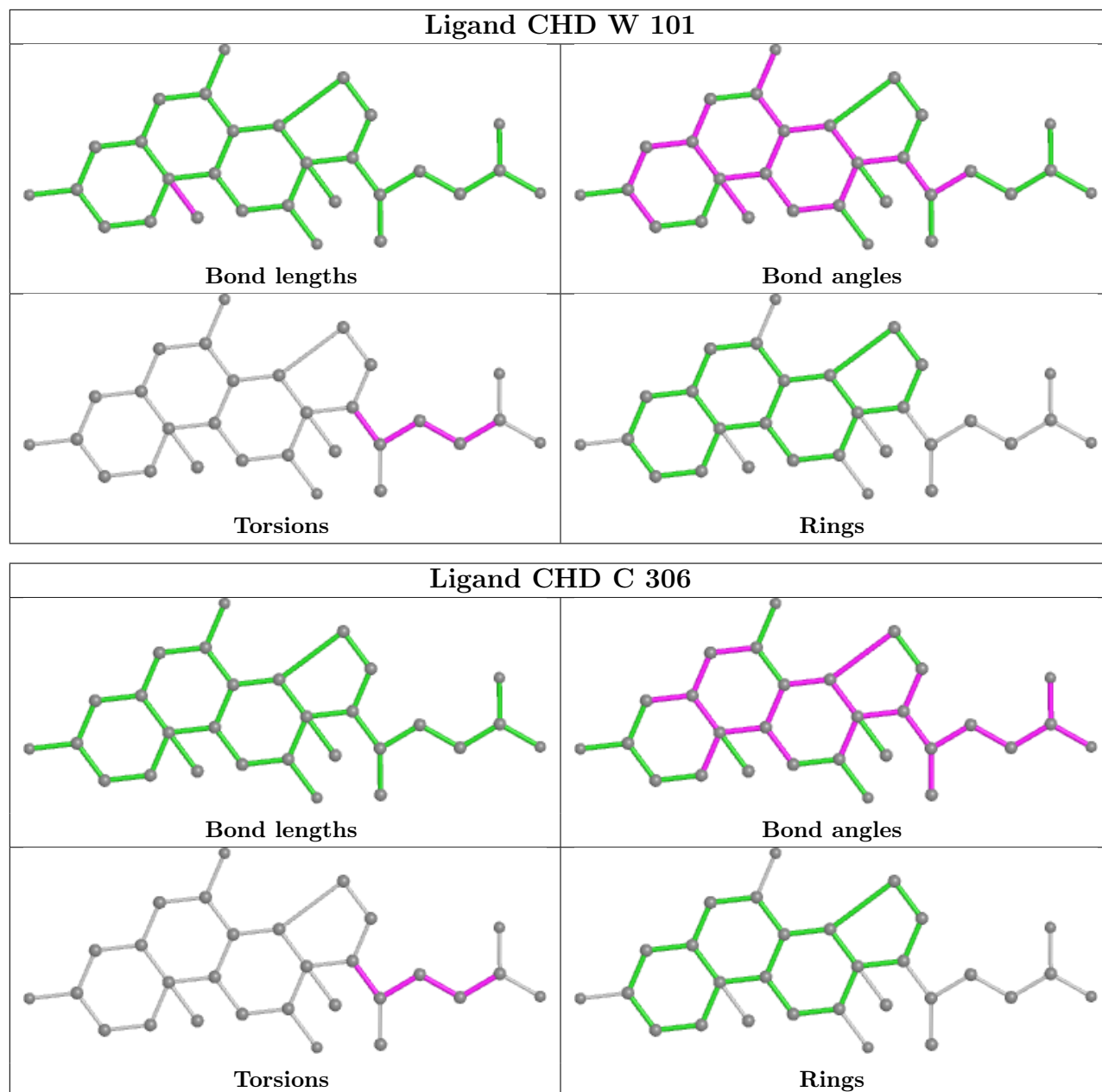


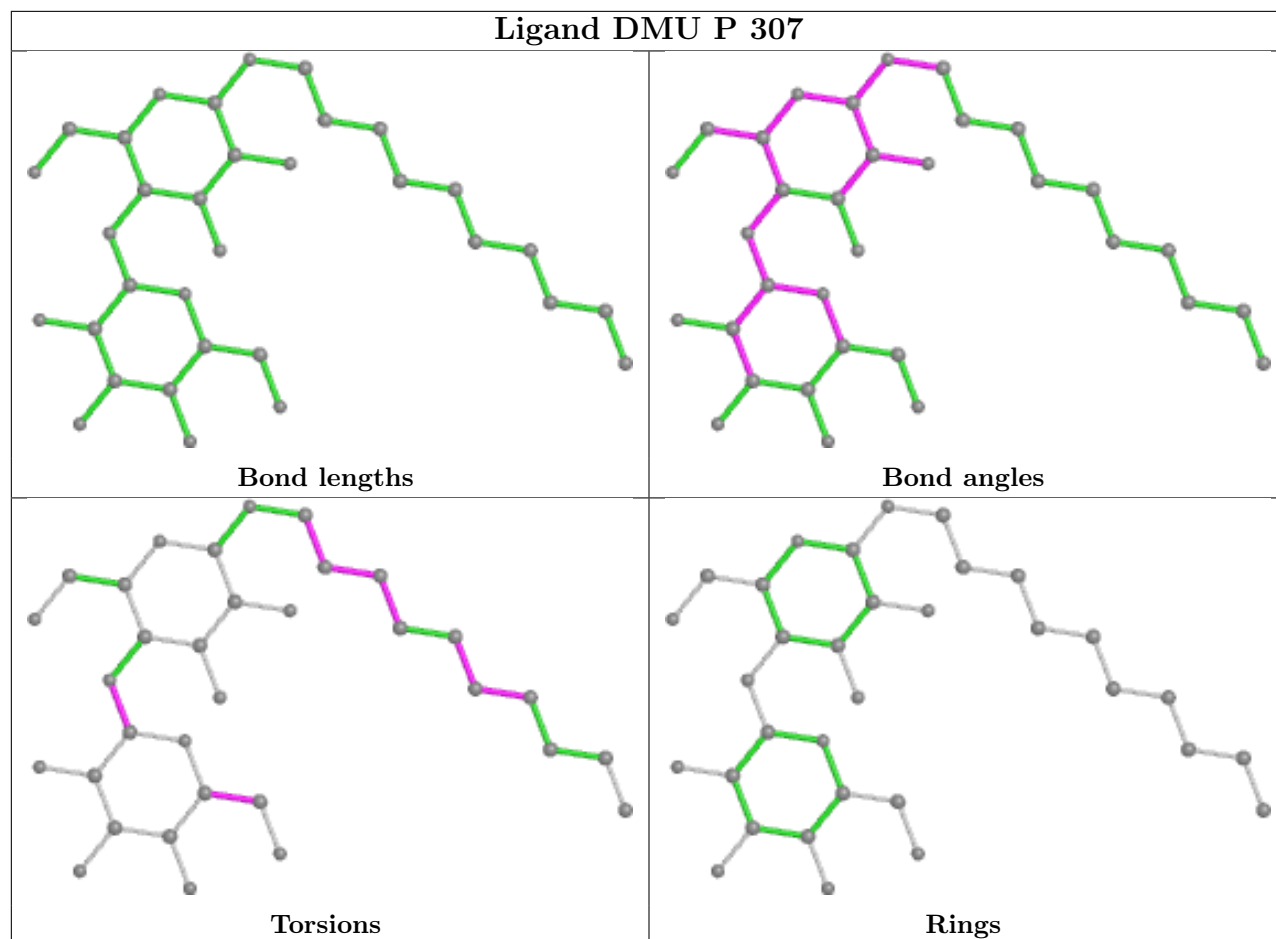
Ligand CHD J 101

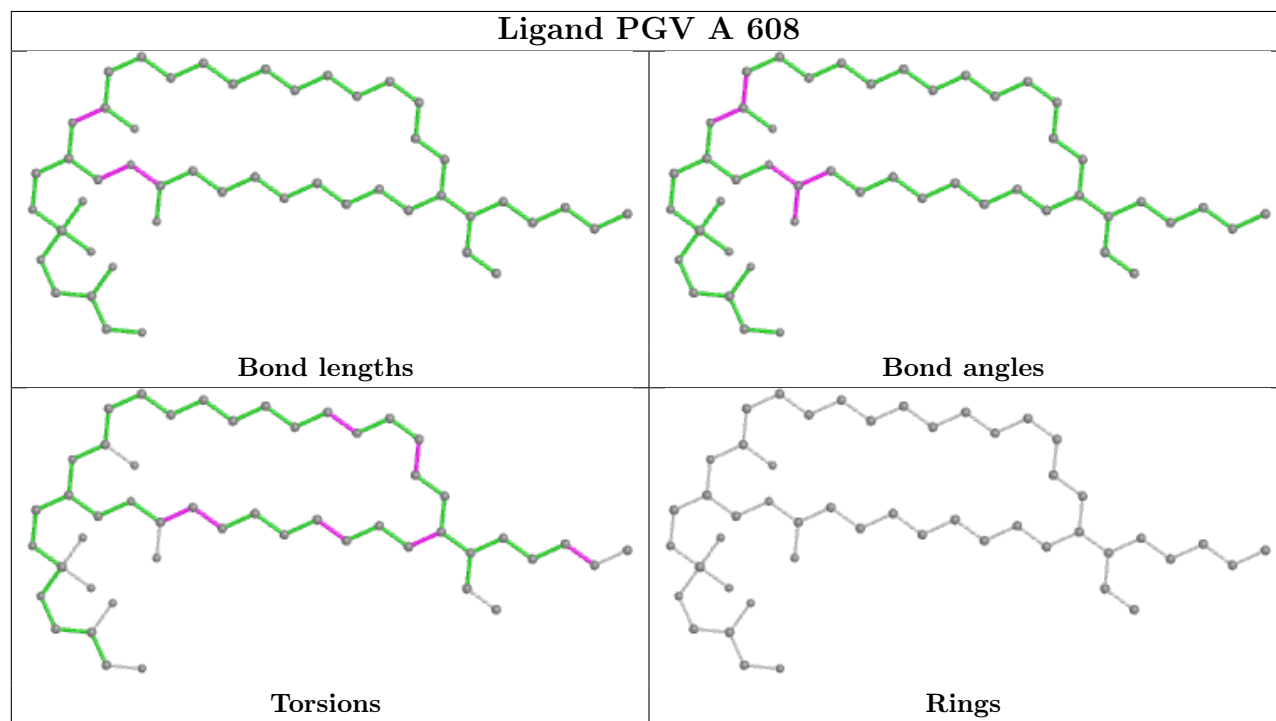
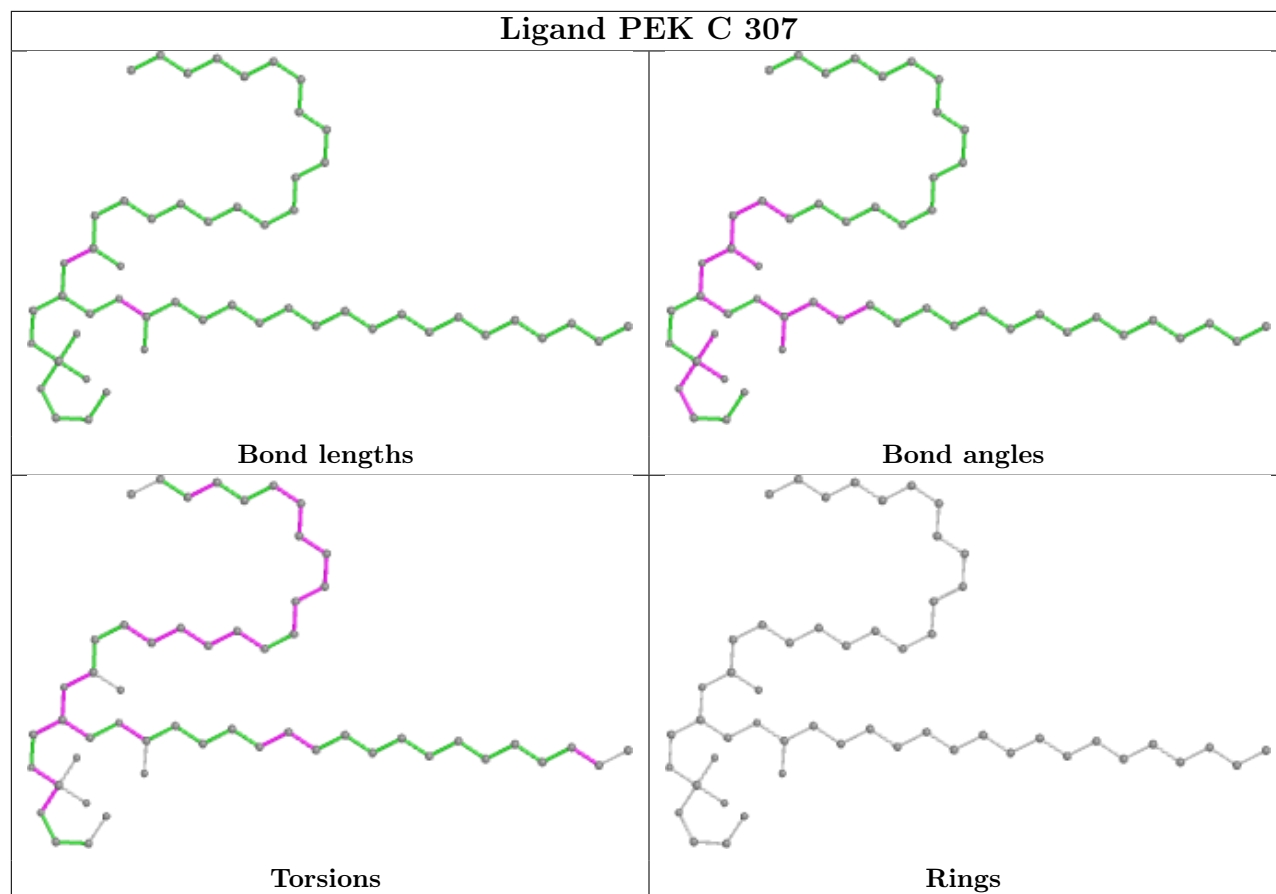


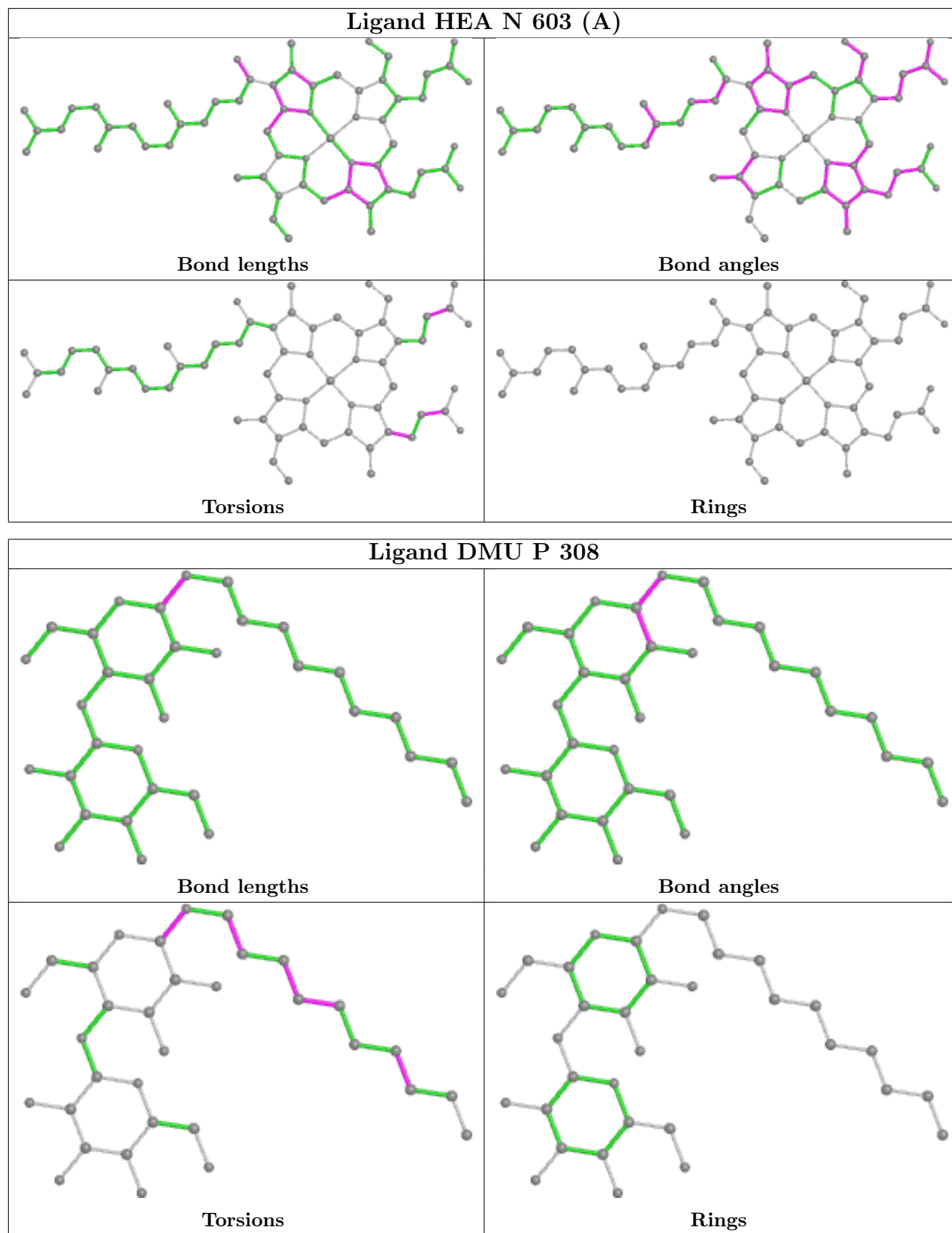
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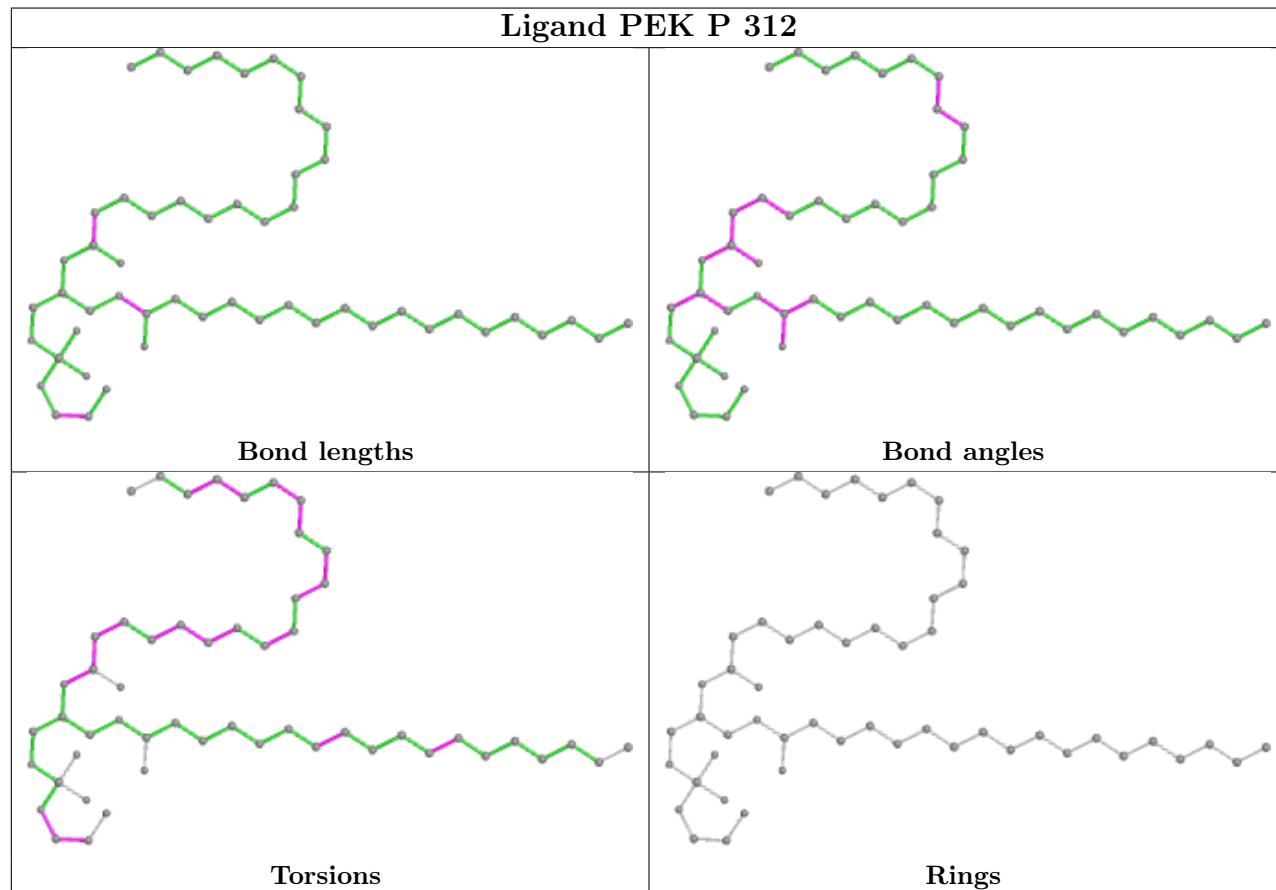
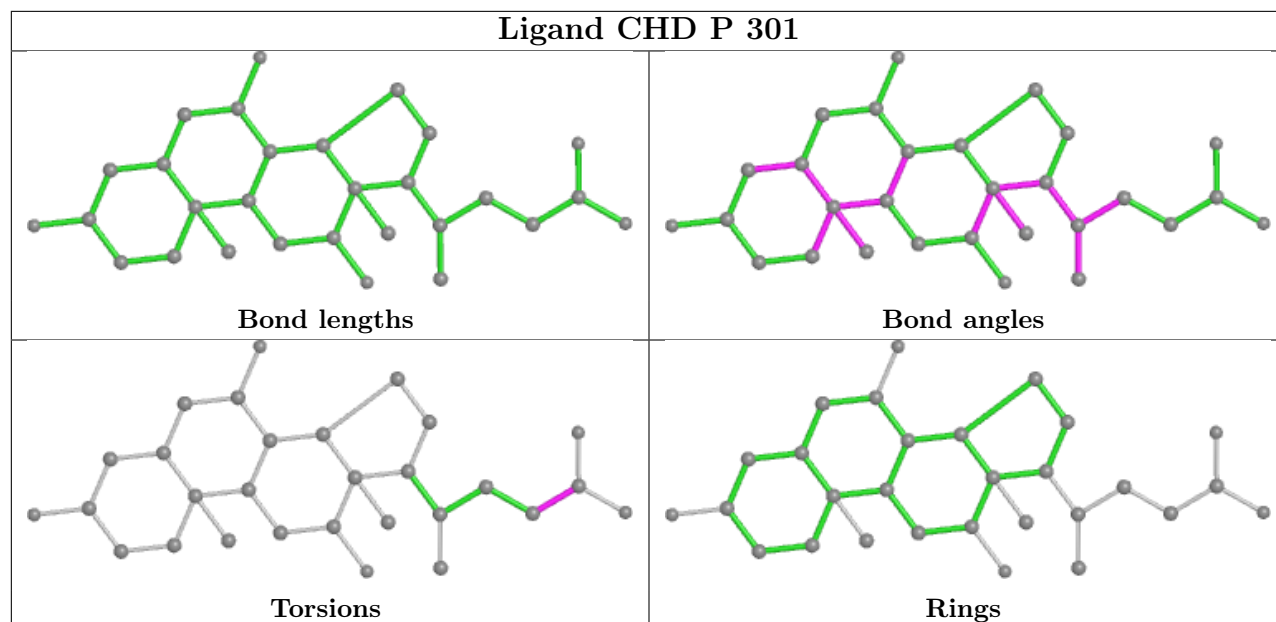


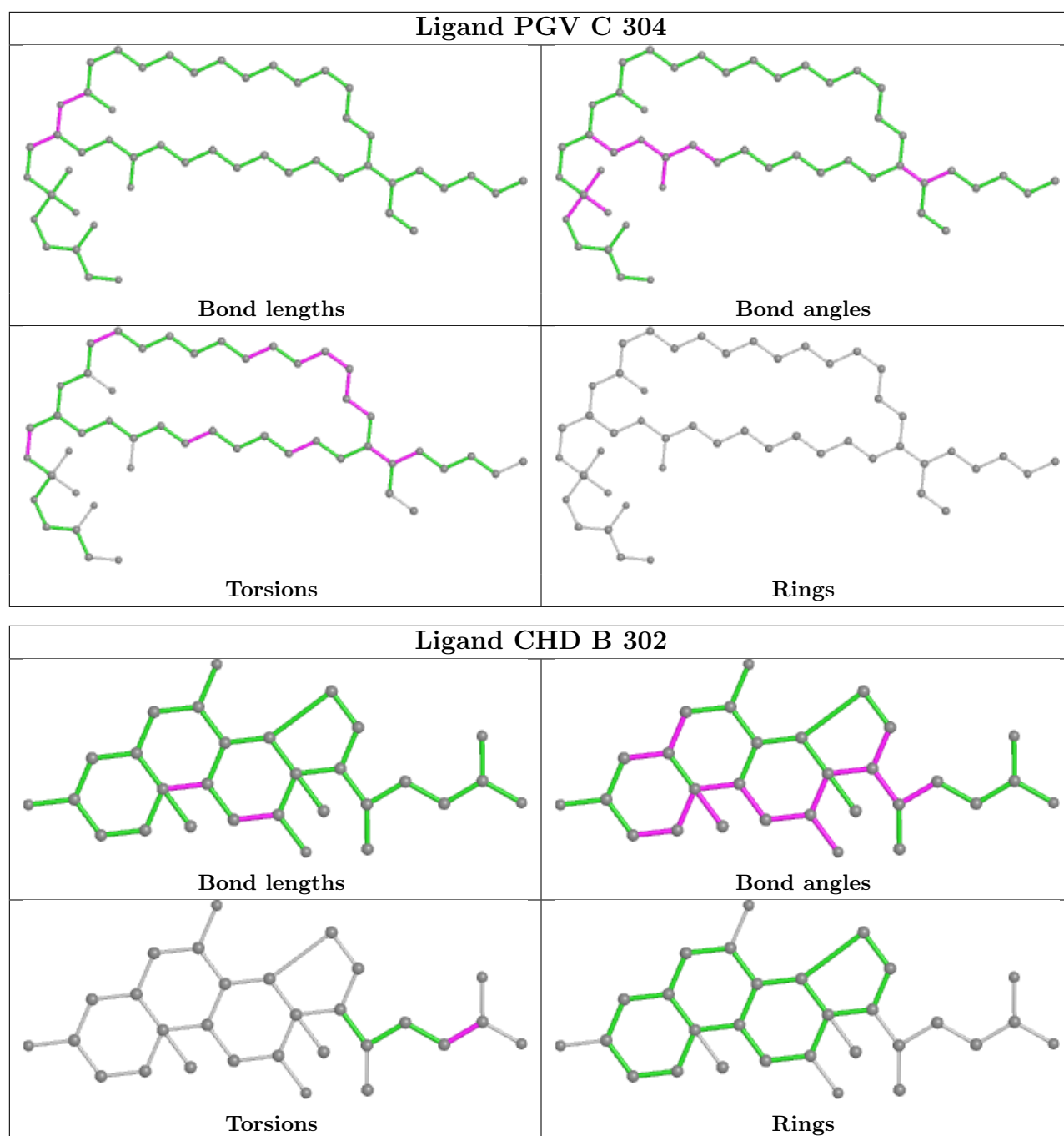




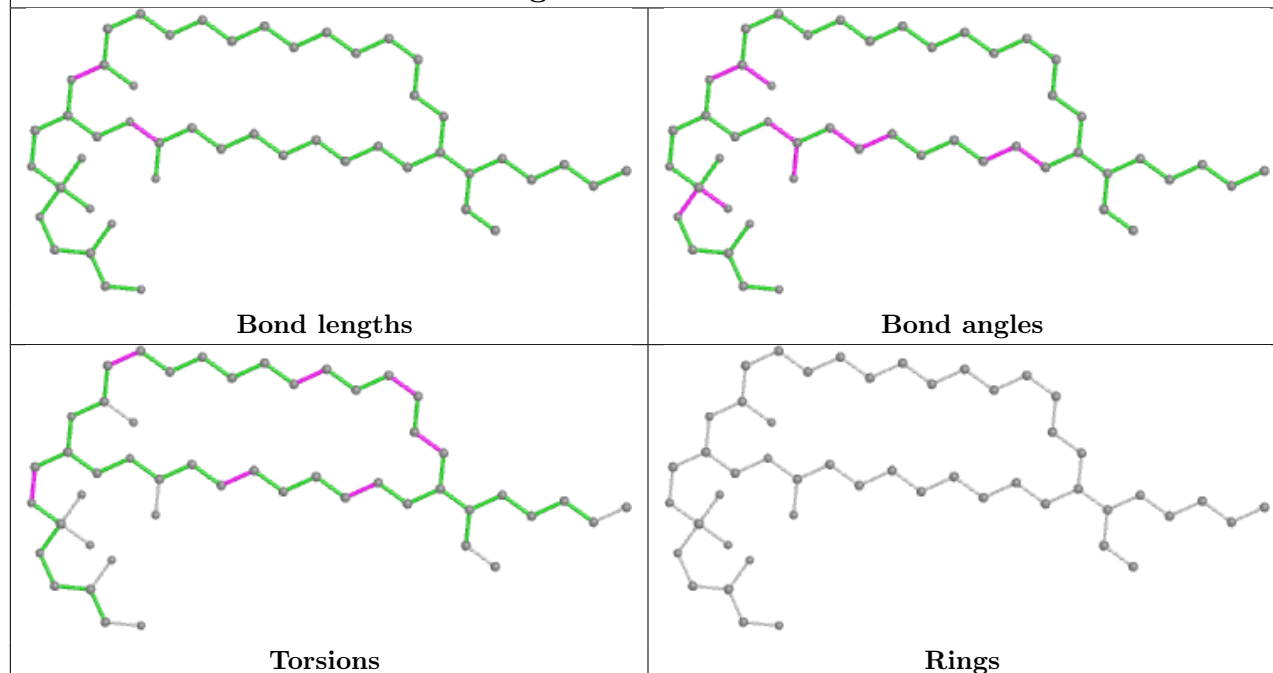




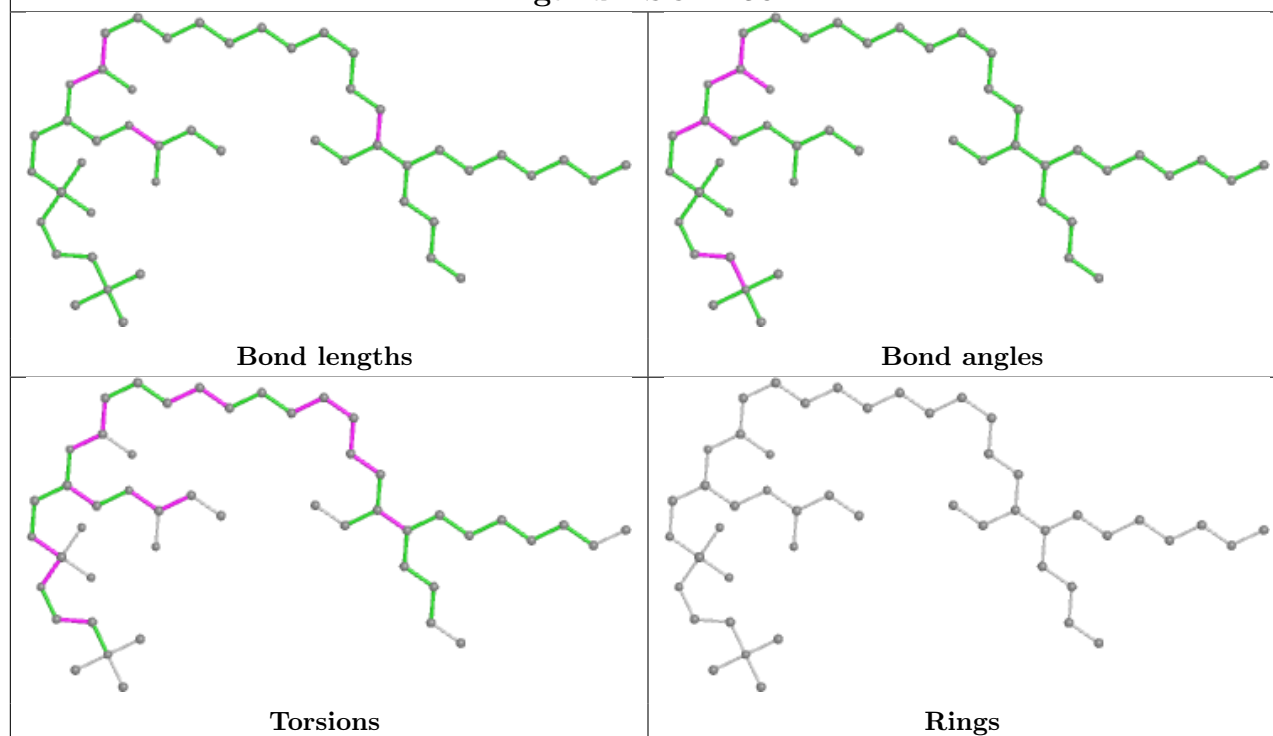


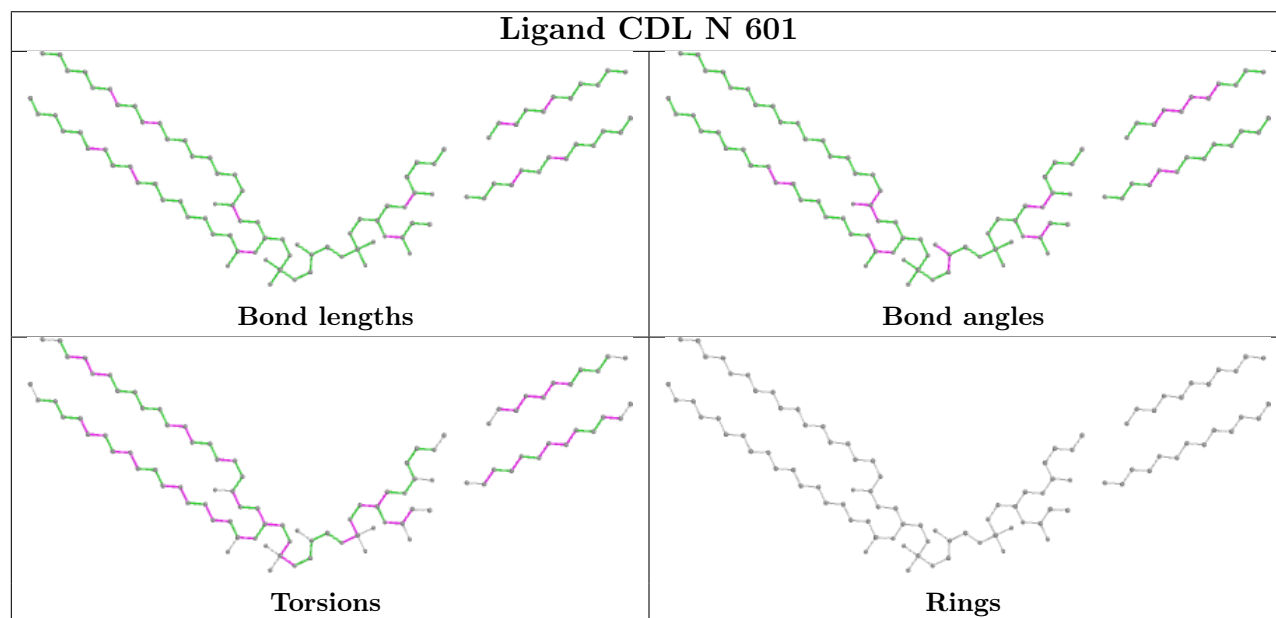
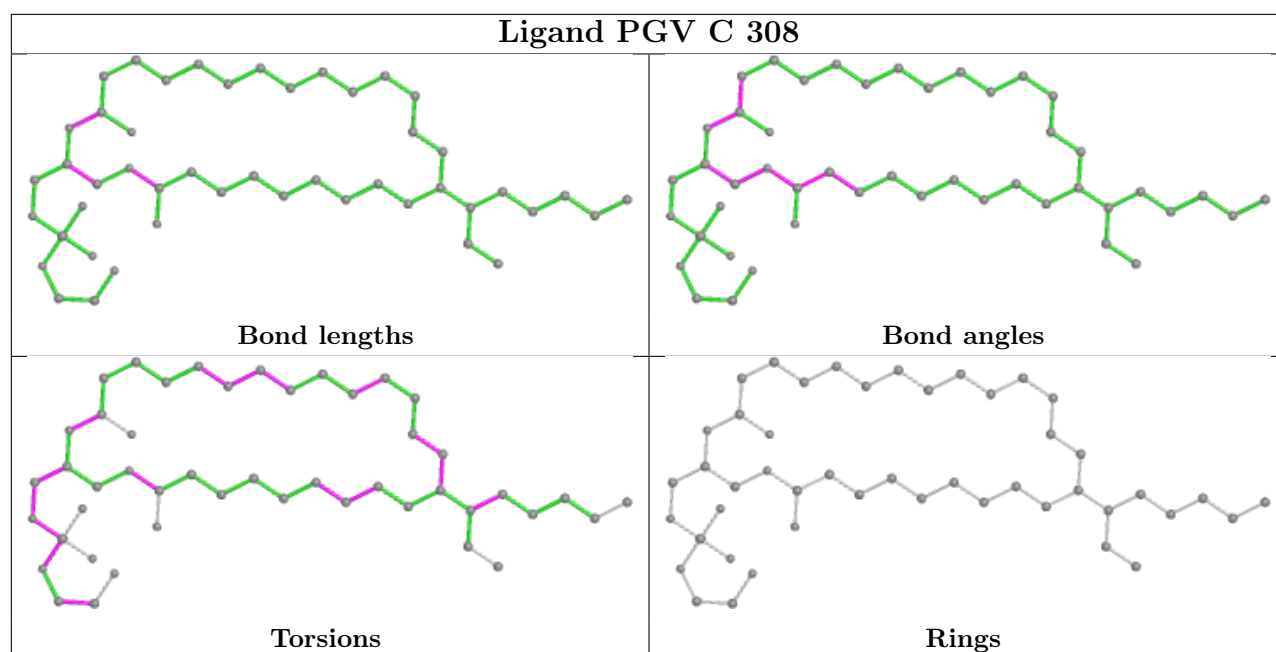


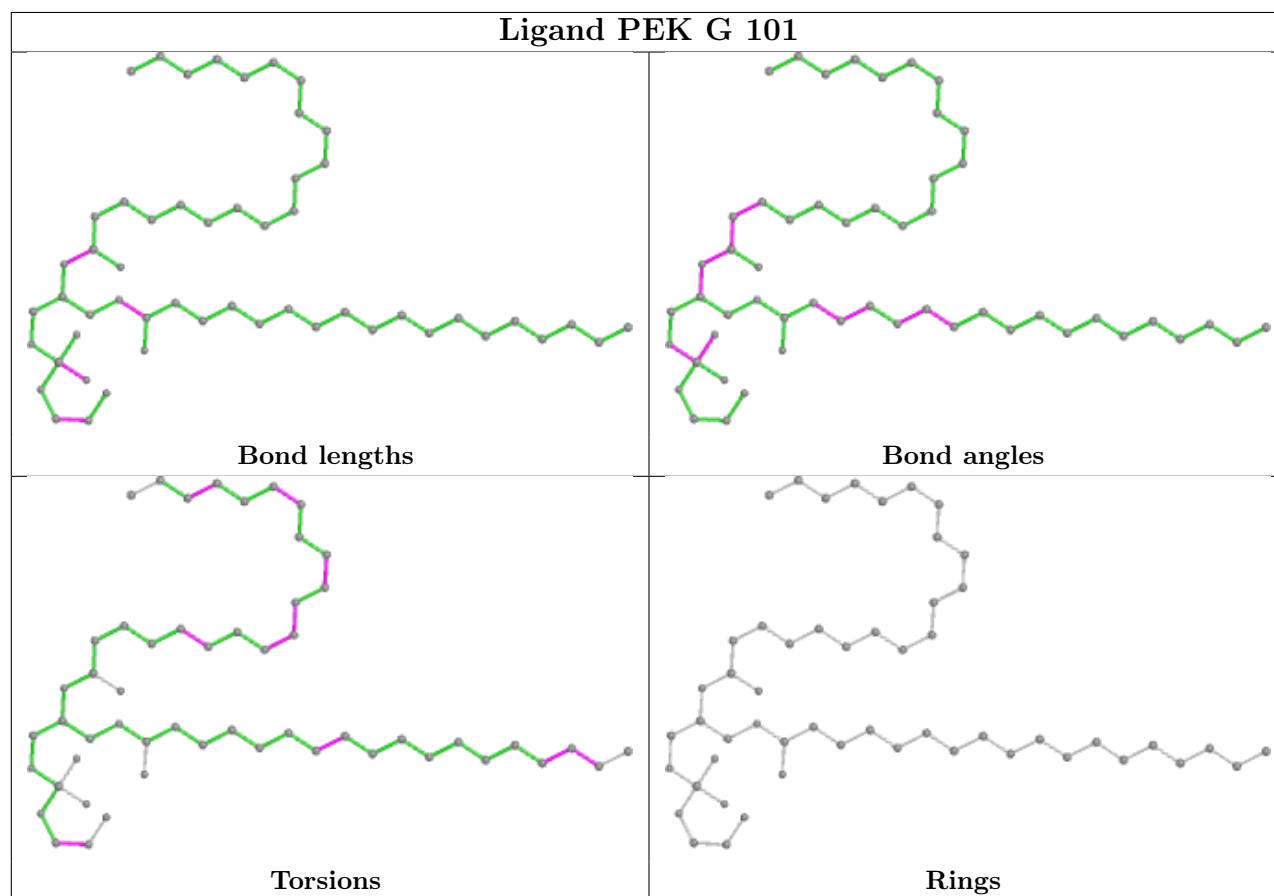
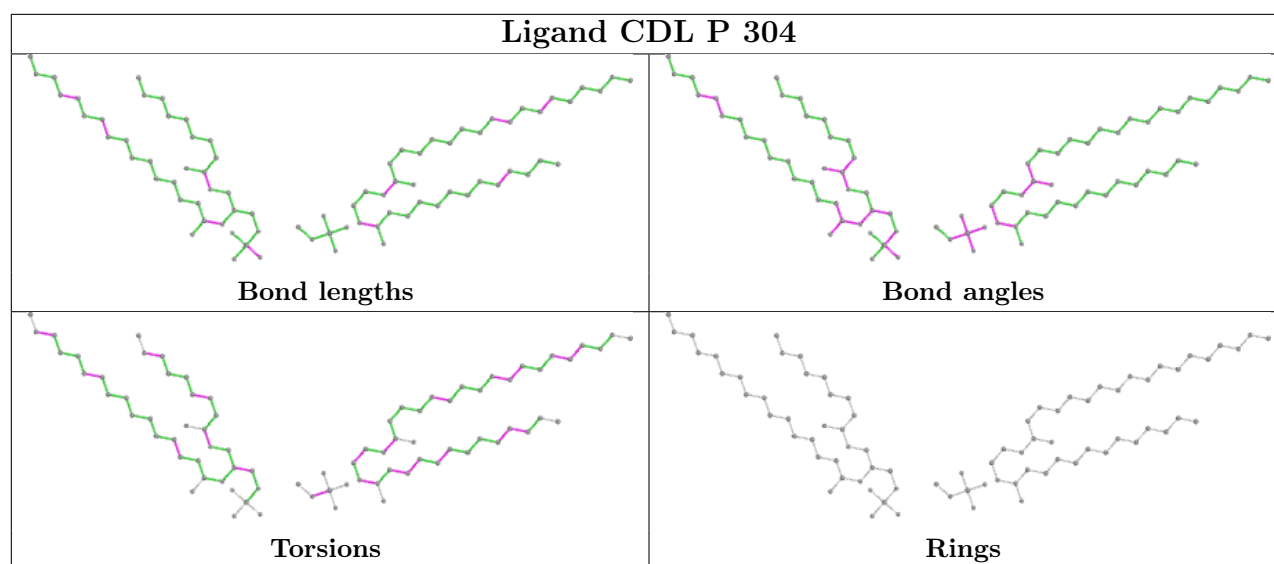
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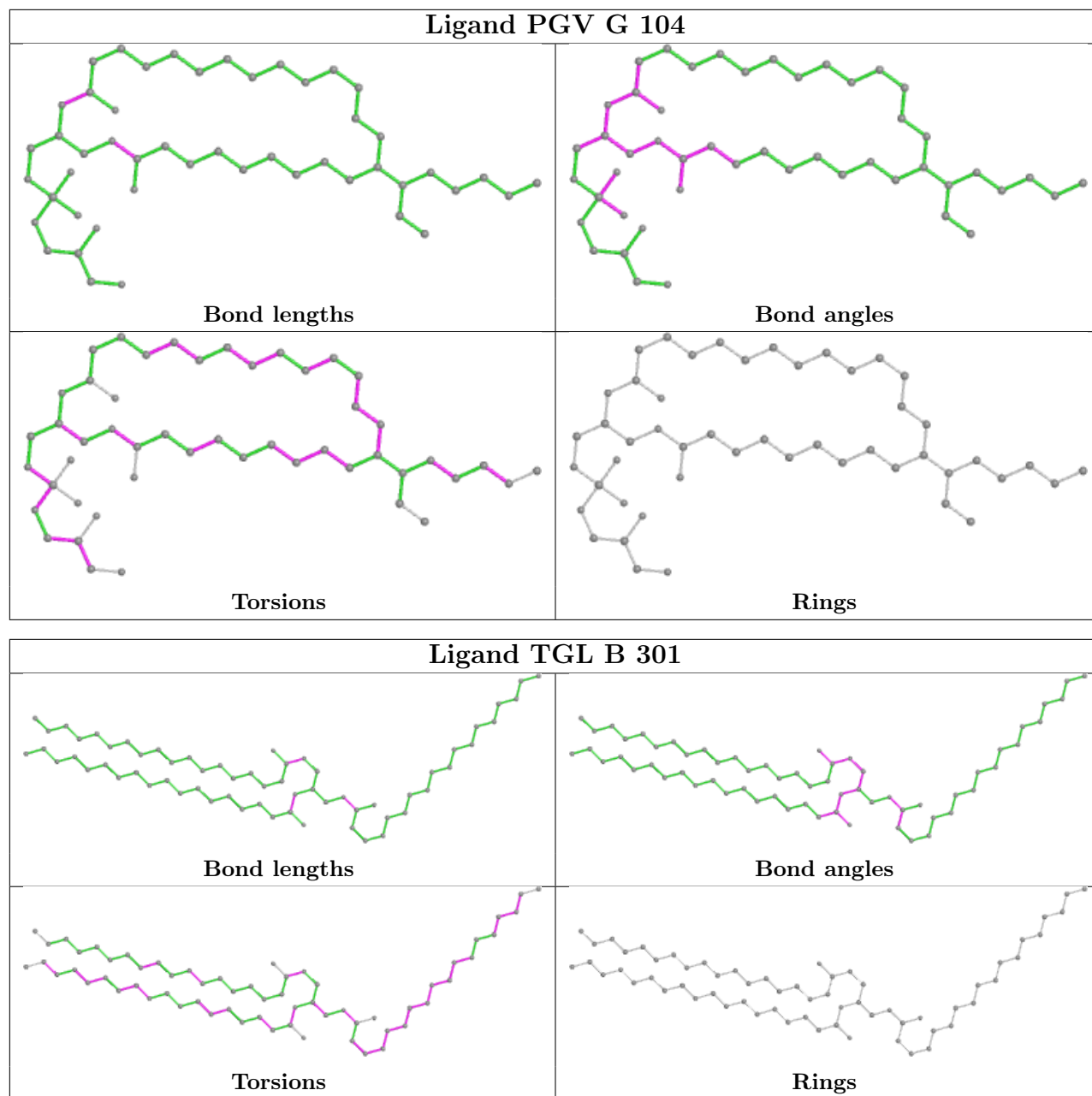


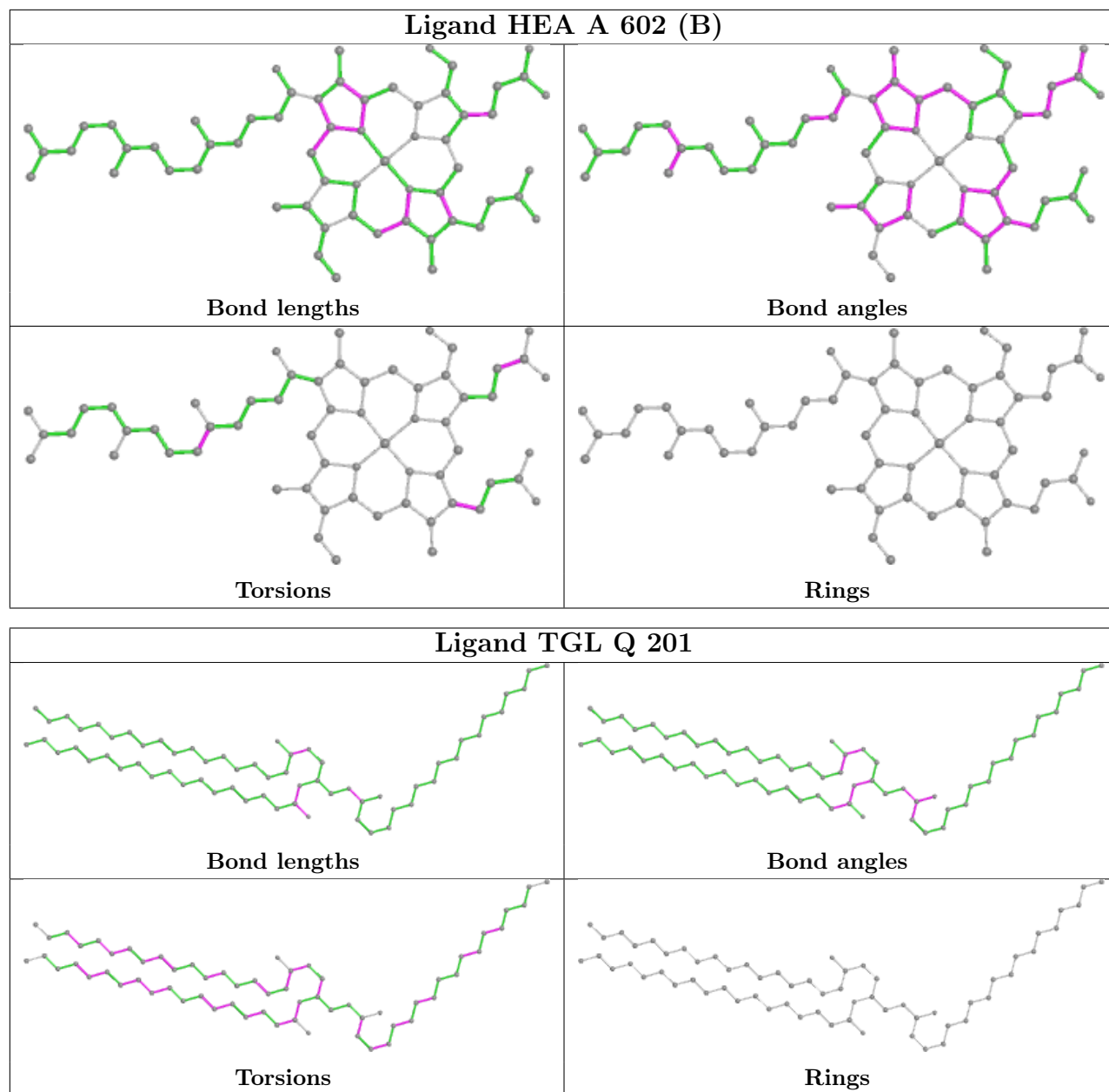
Ligand PSC B 304



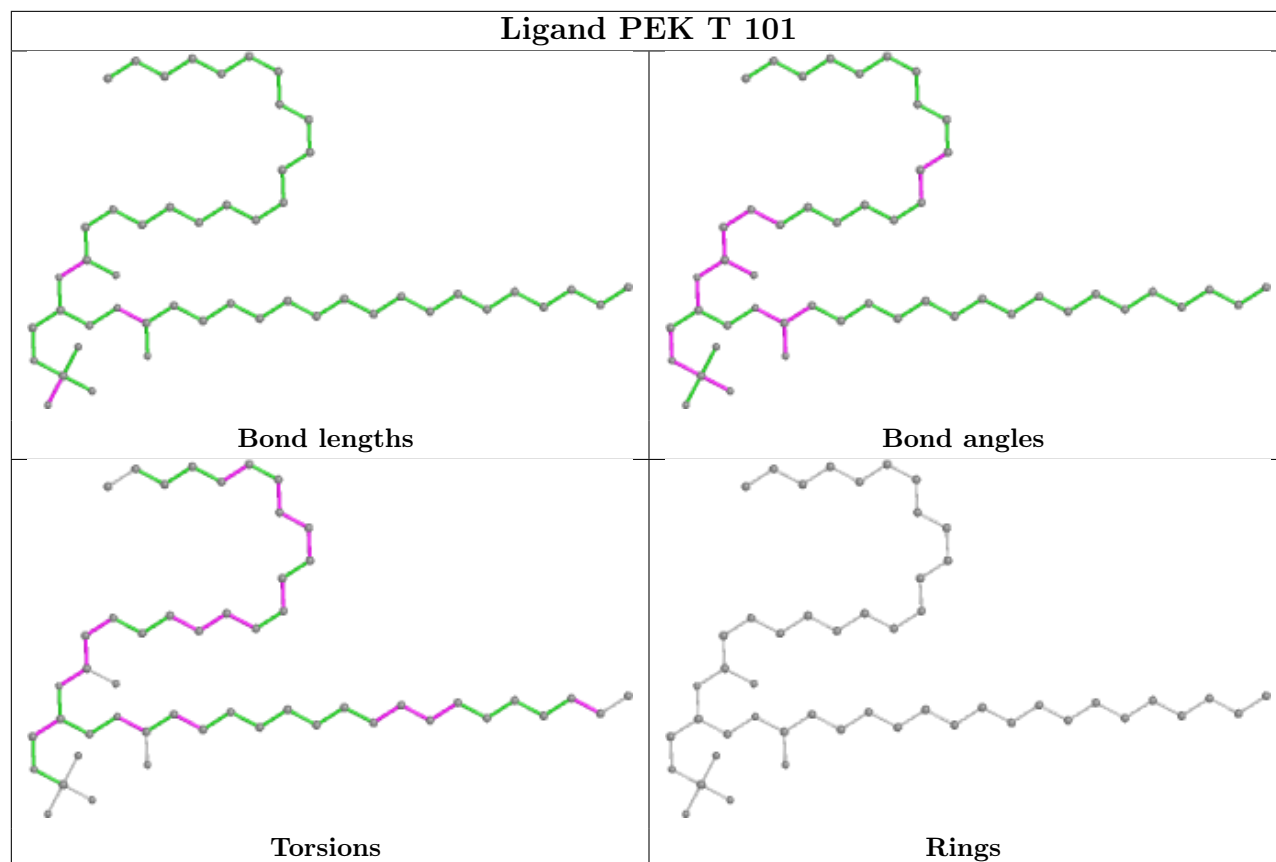




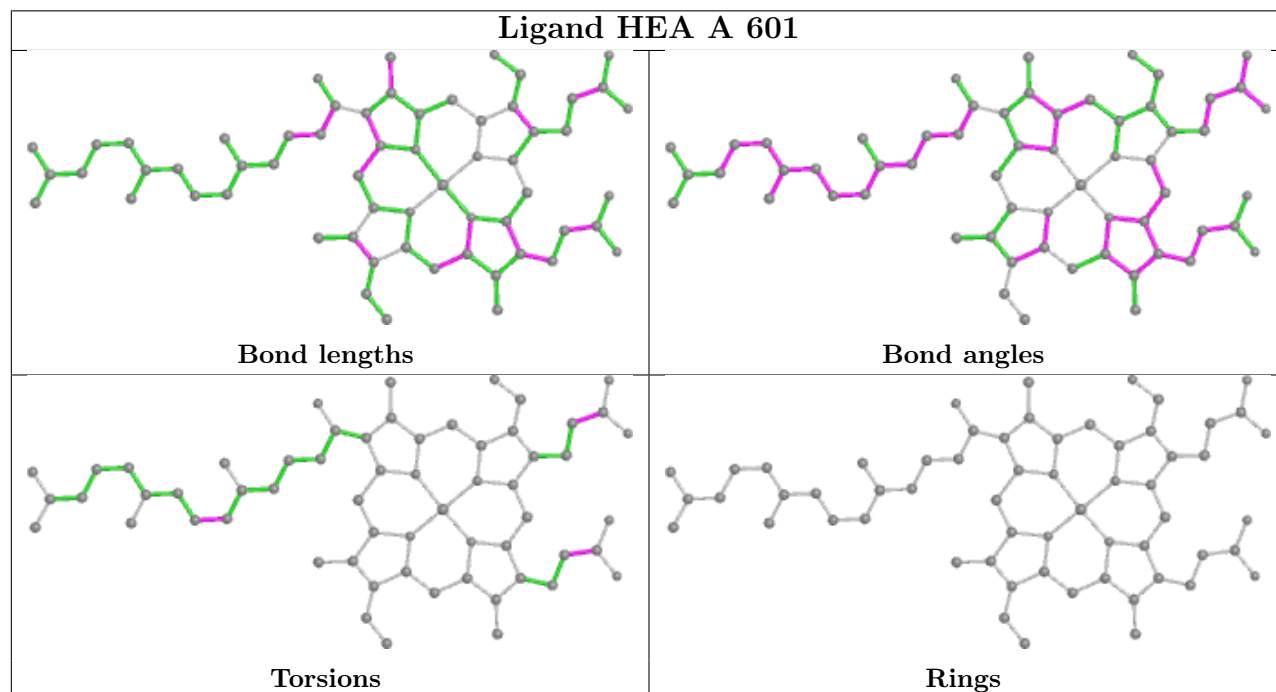


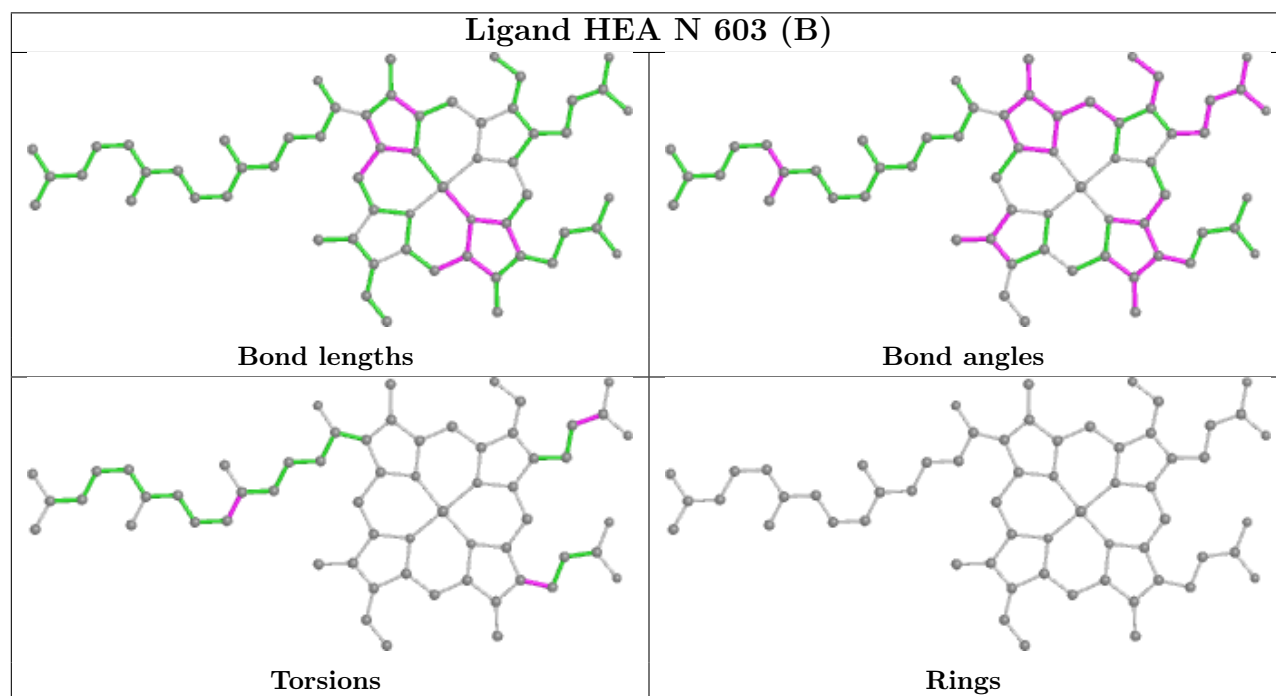
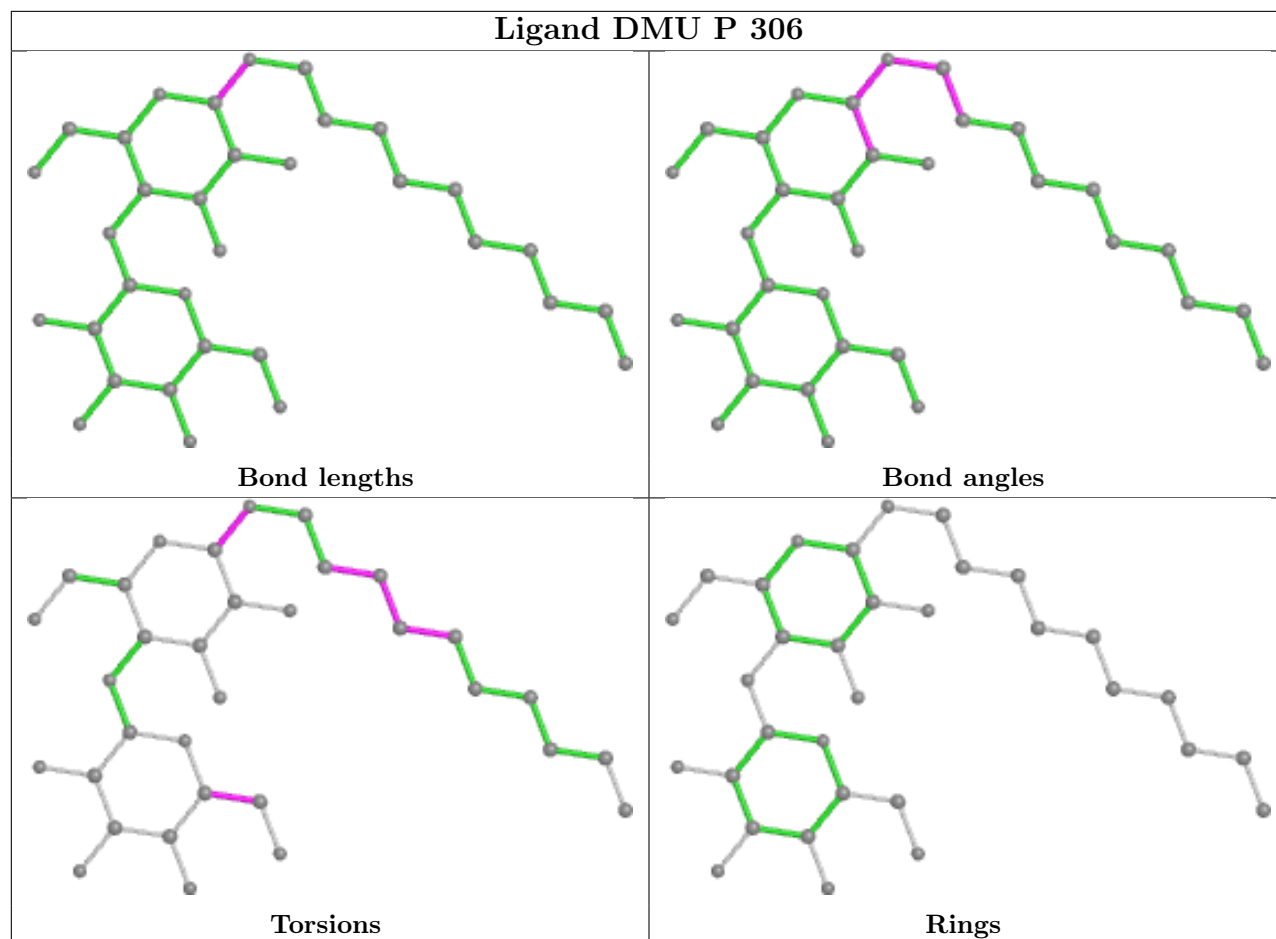


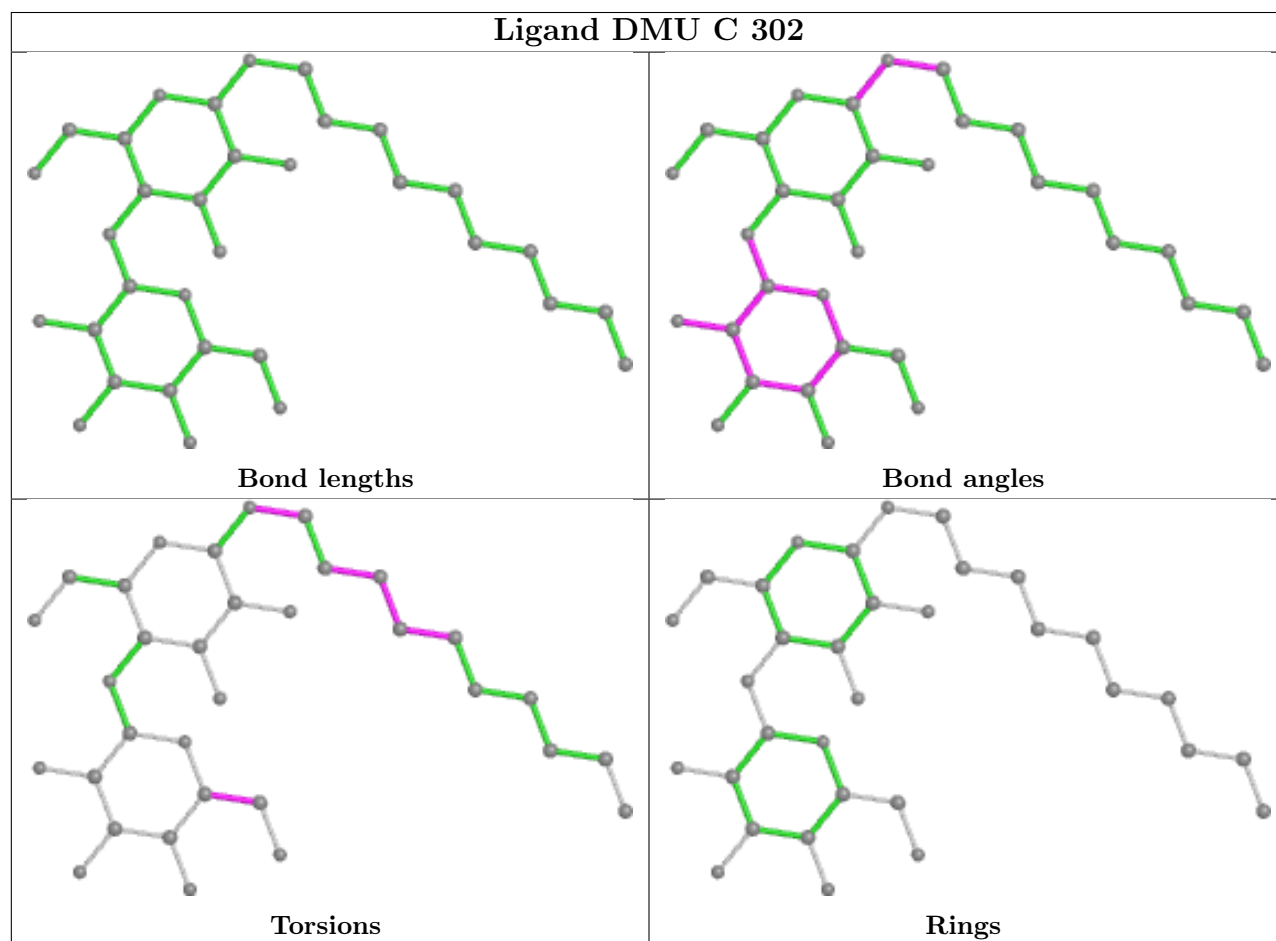
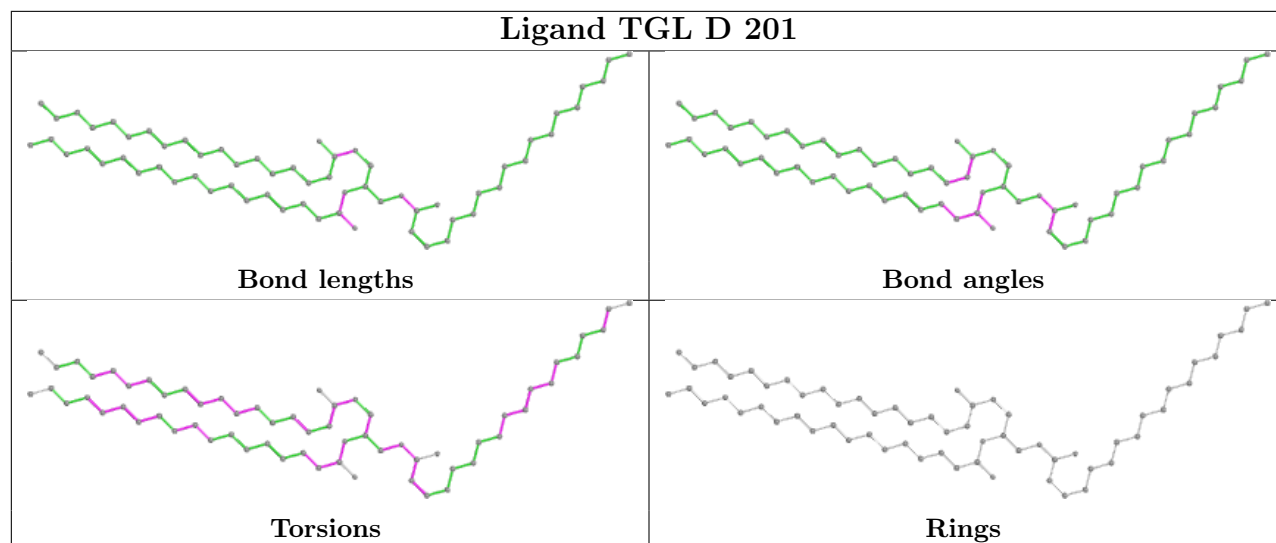
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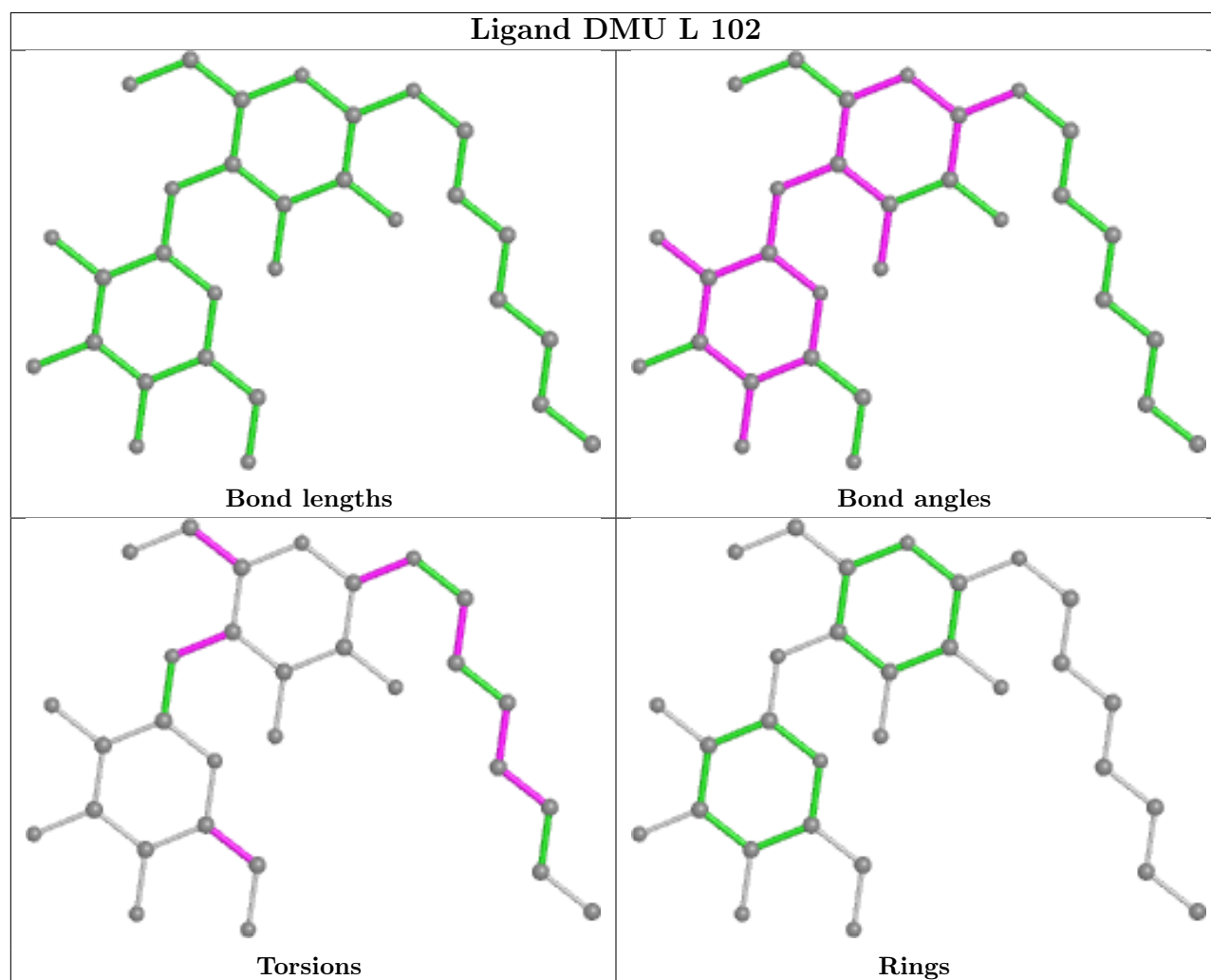
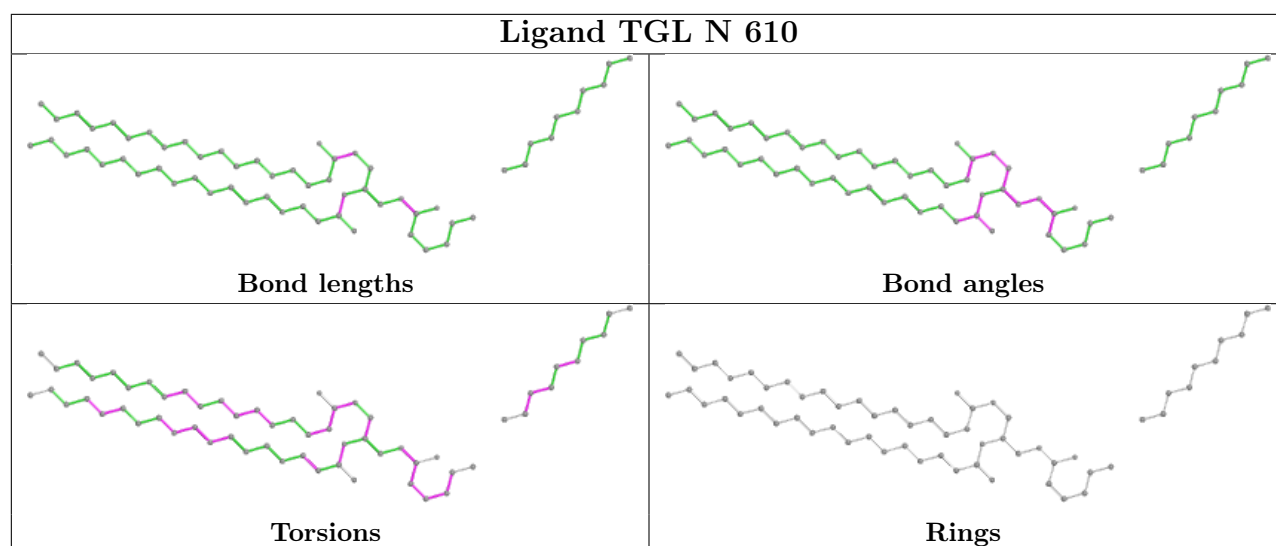


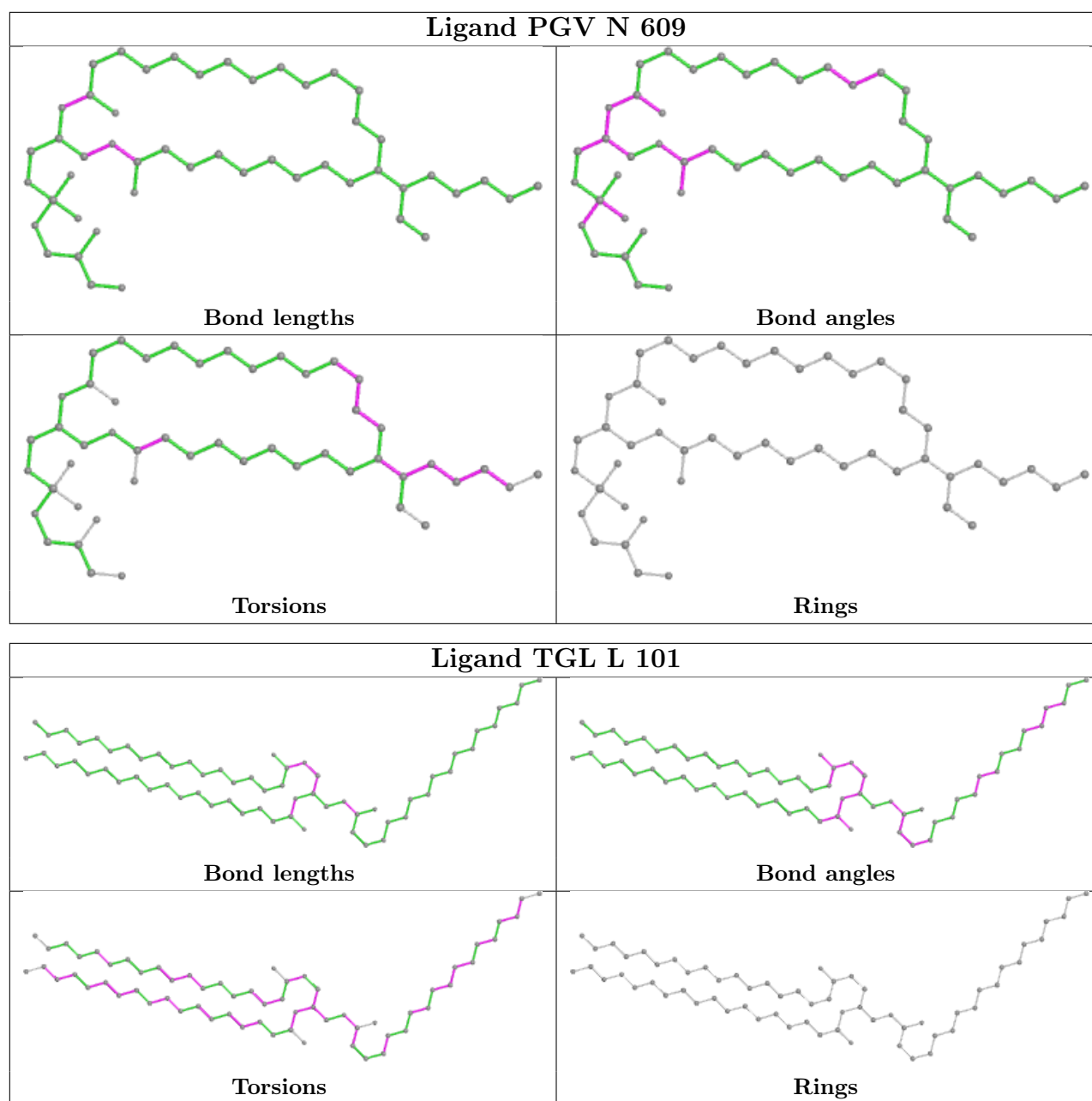
Ligand HEA A 601

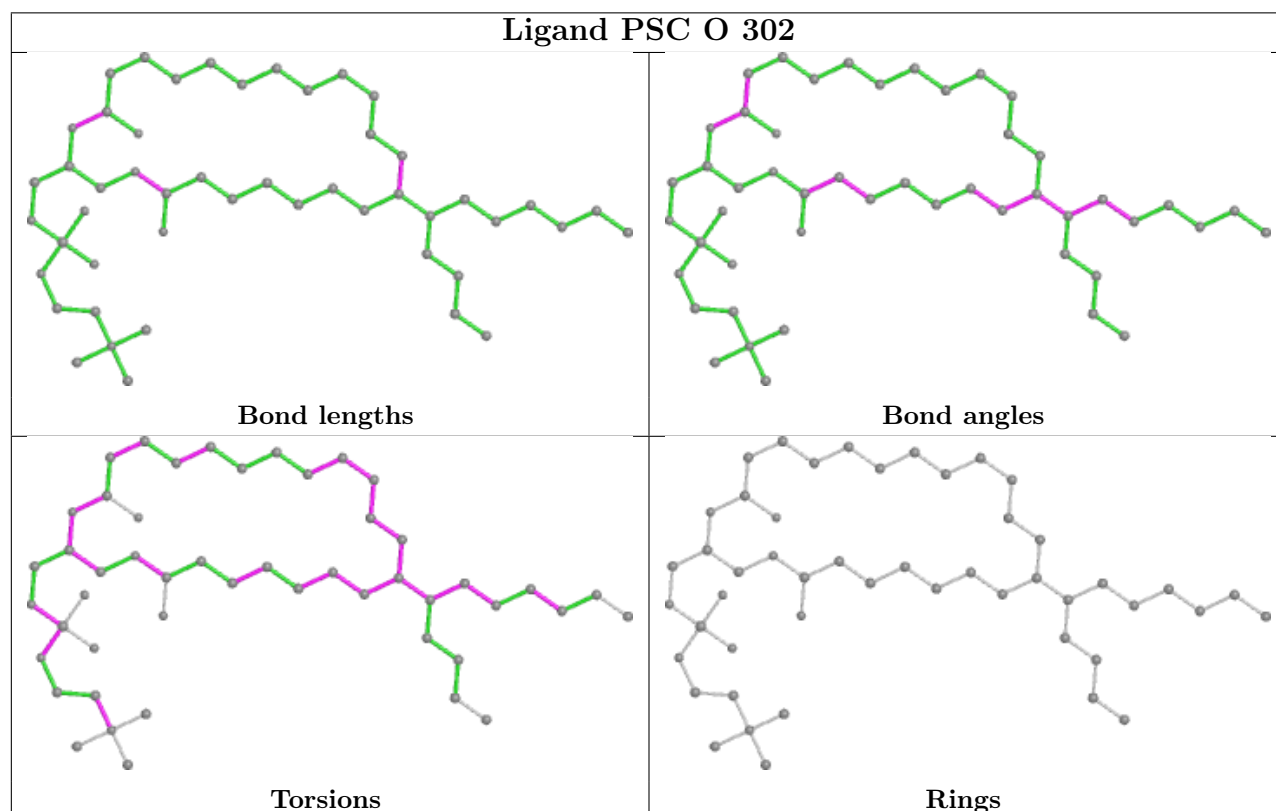
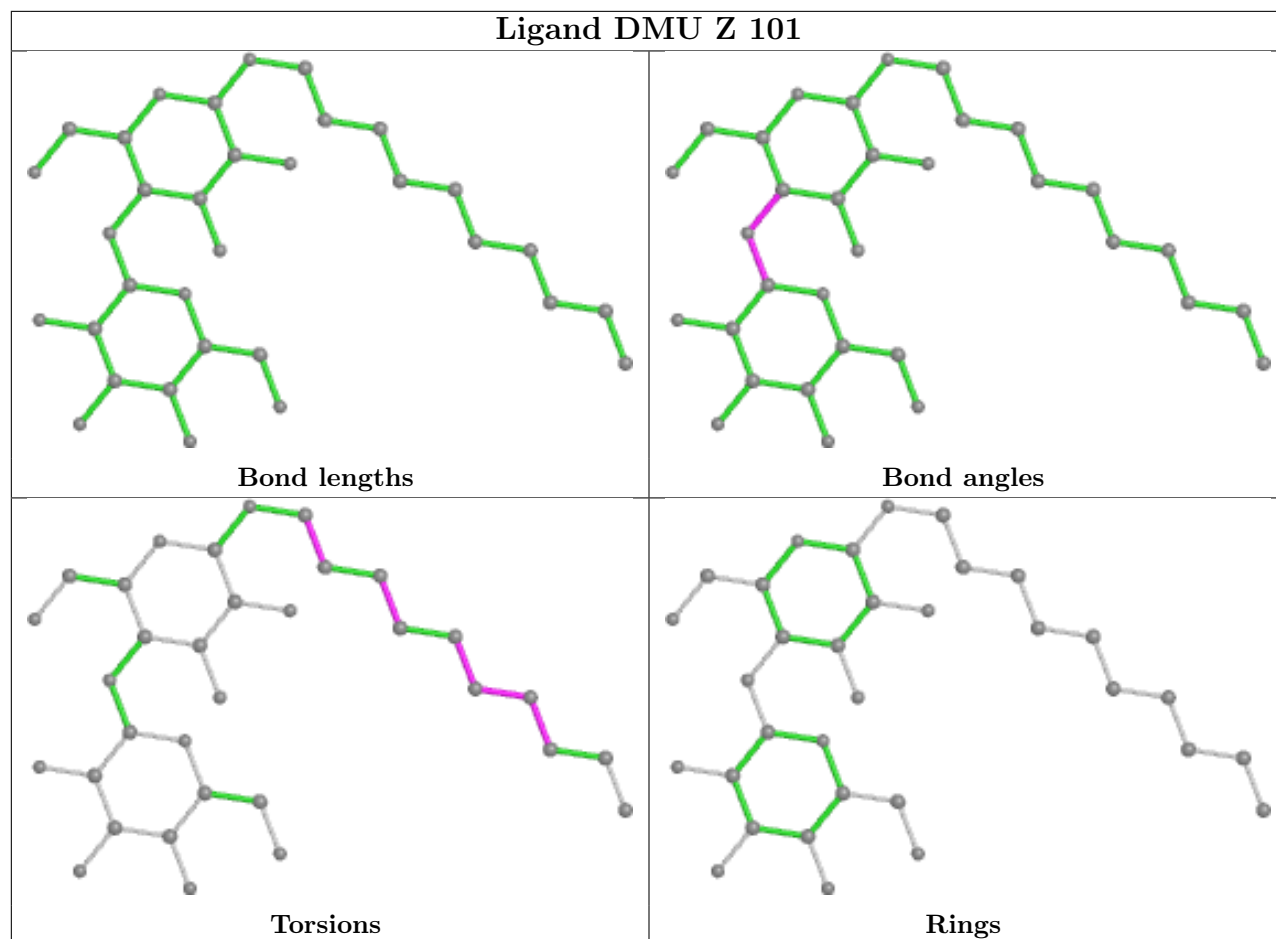


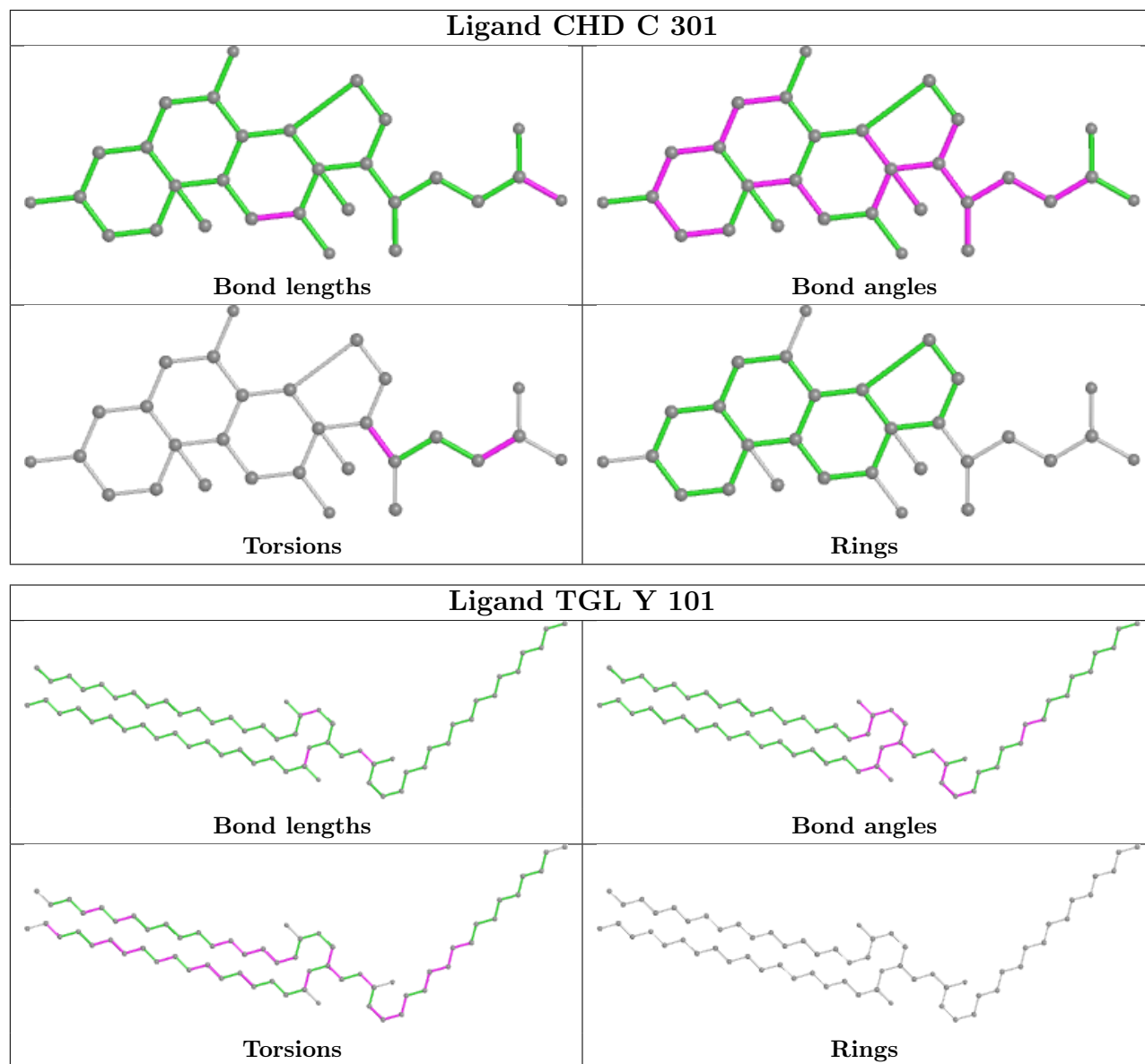


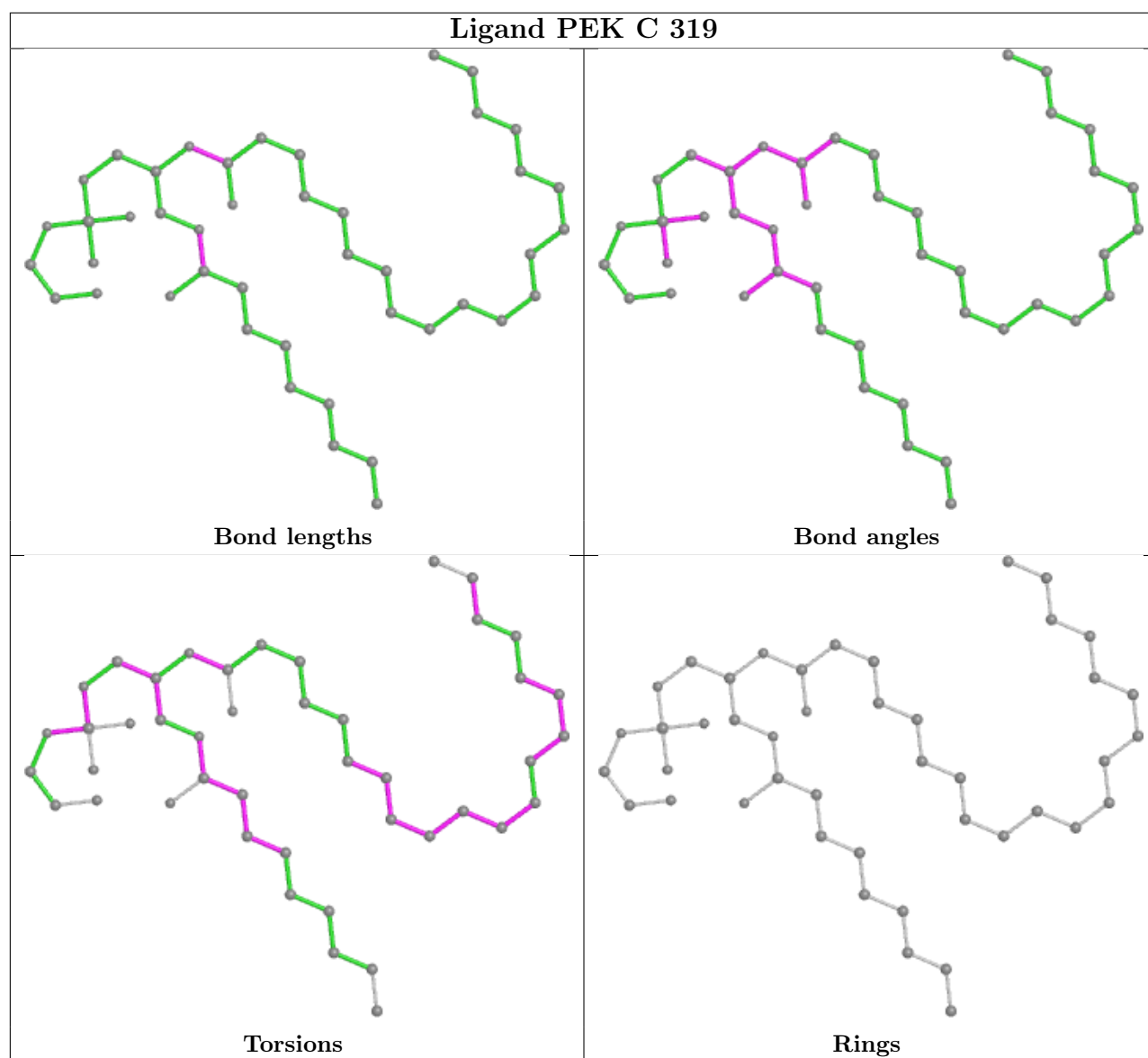


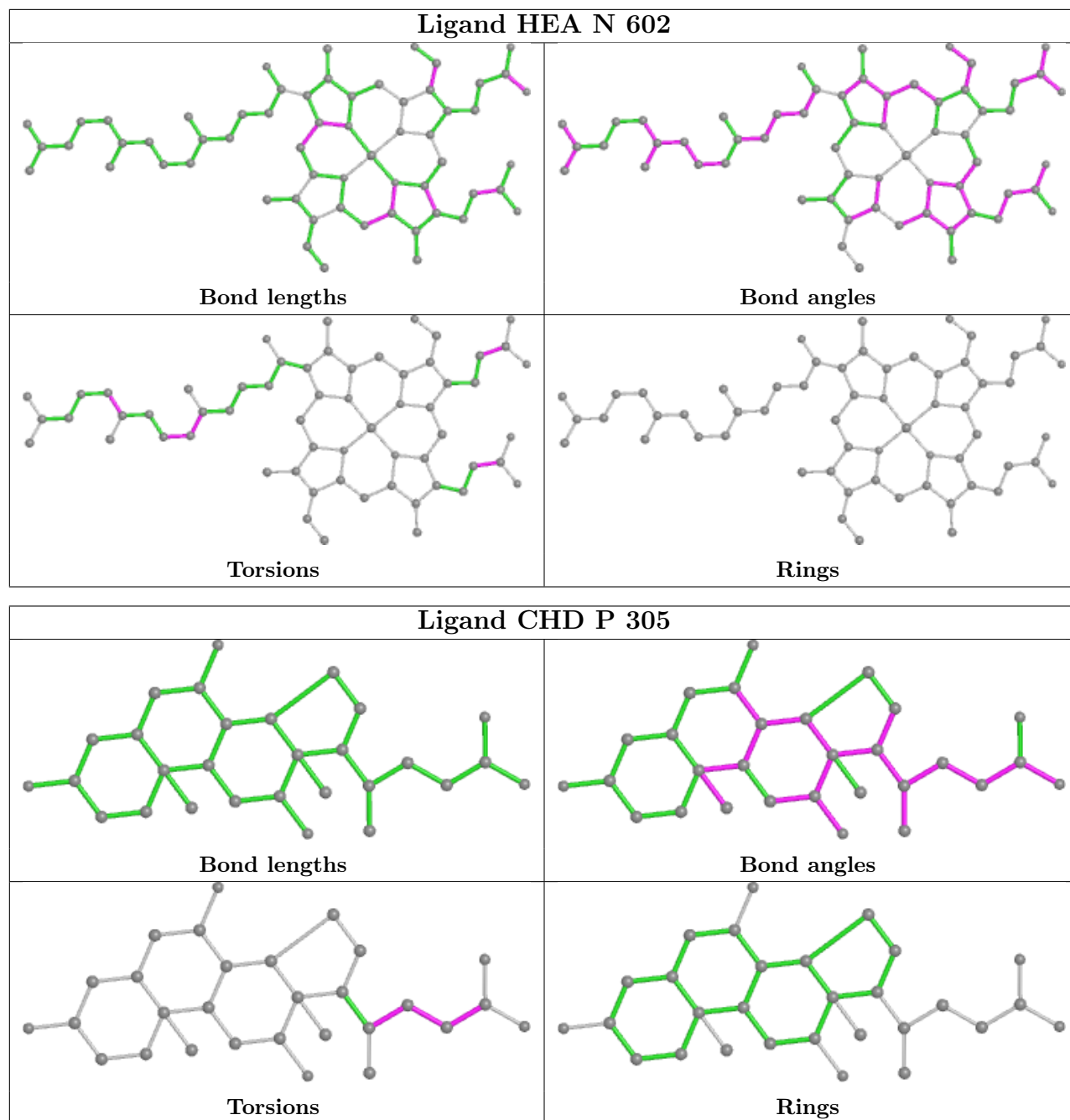


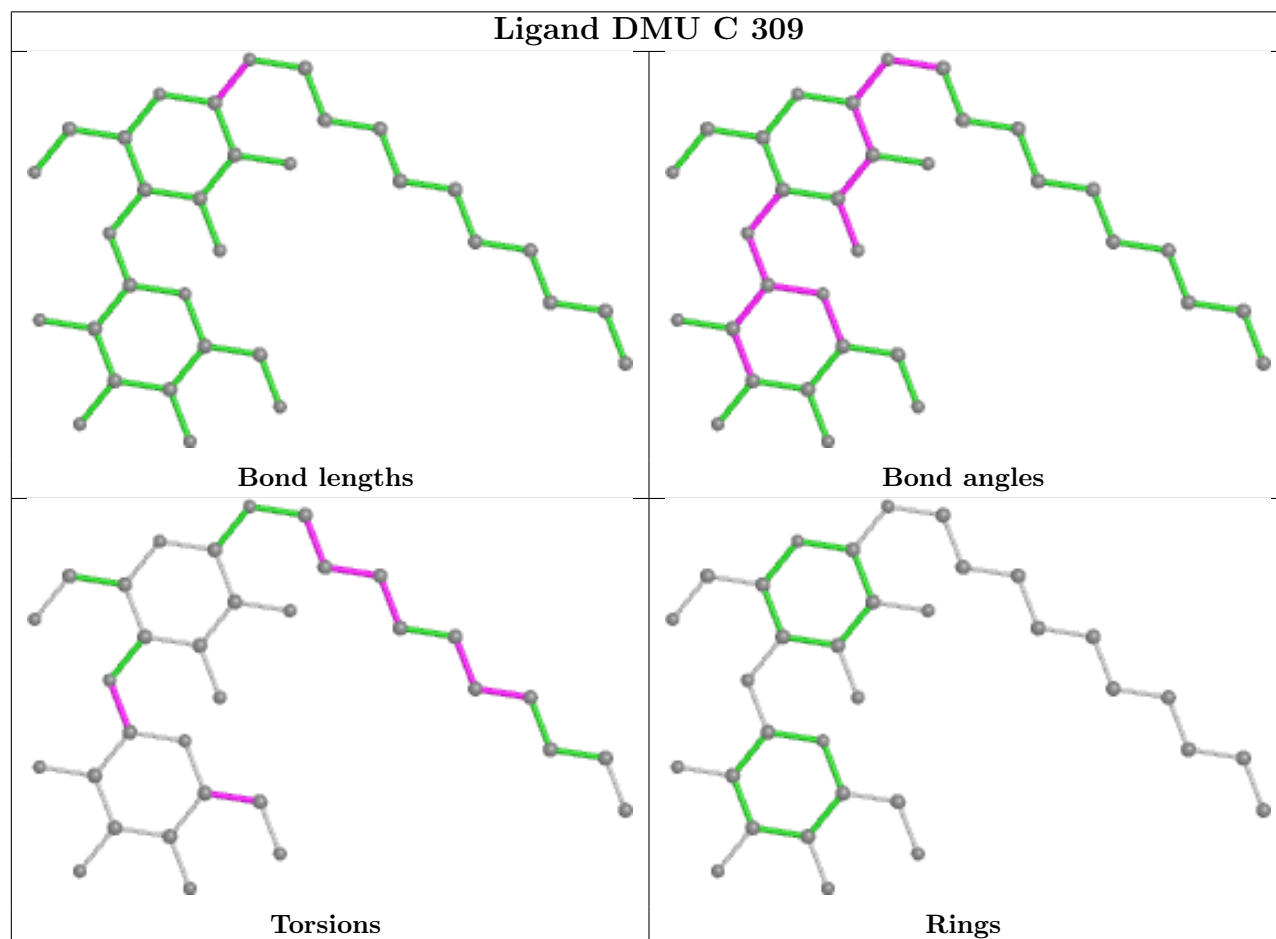
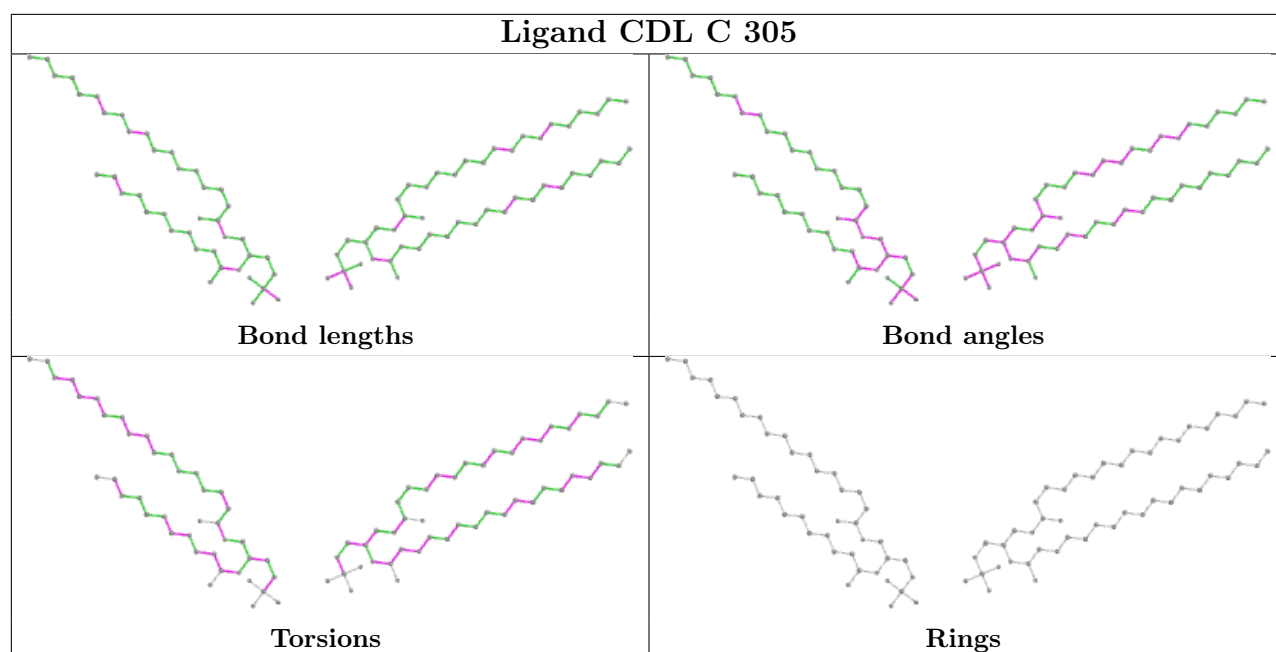


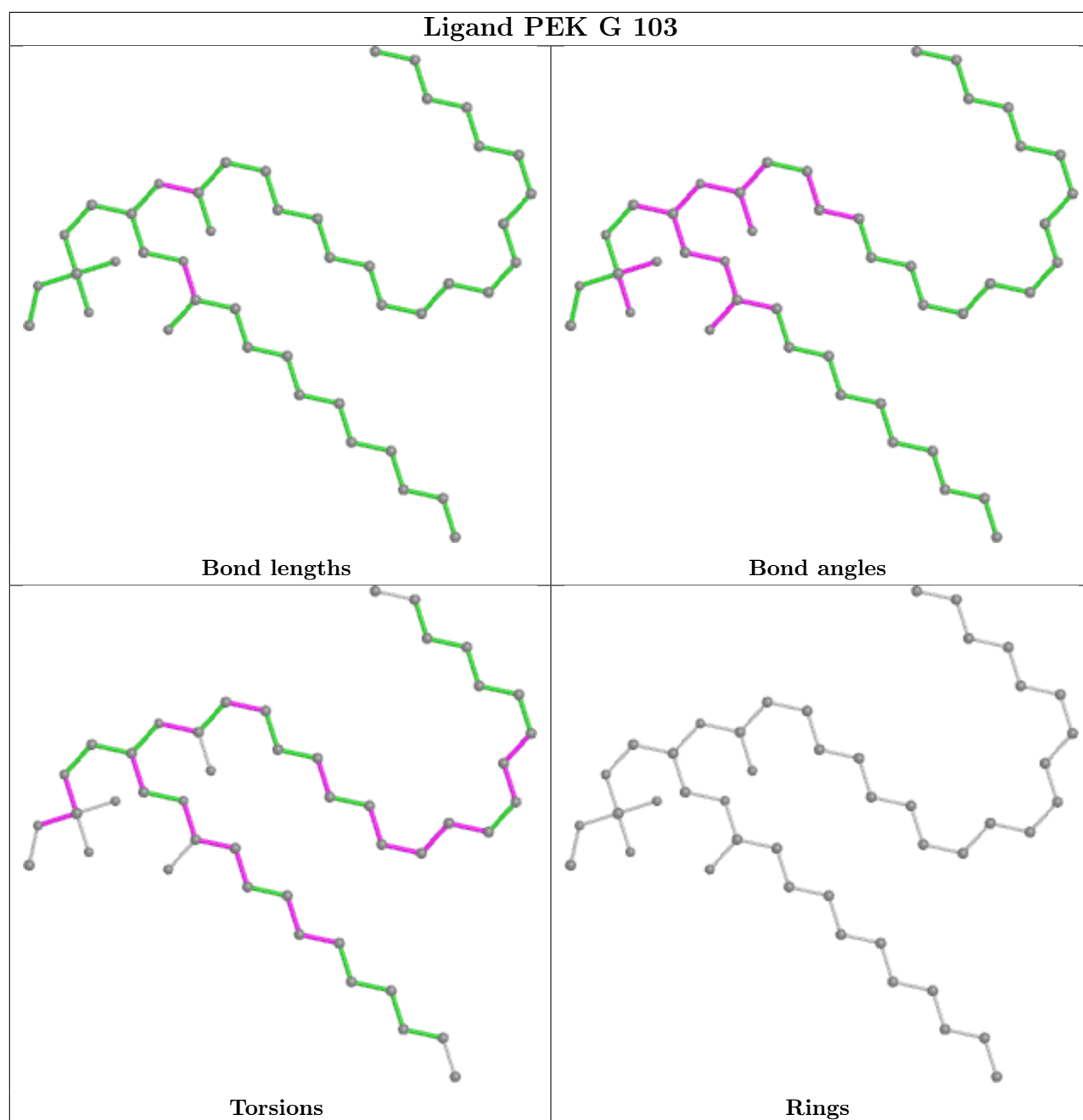


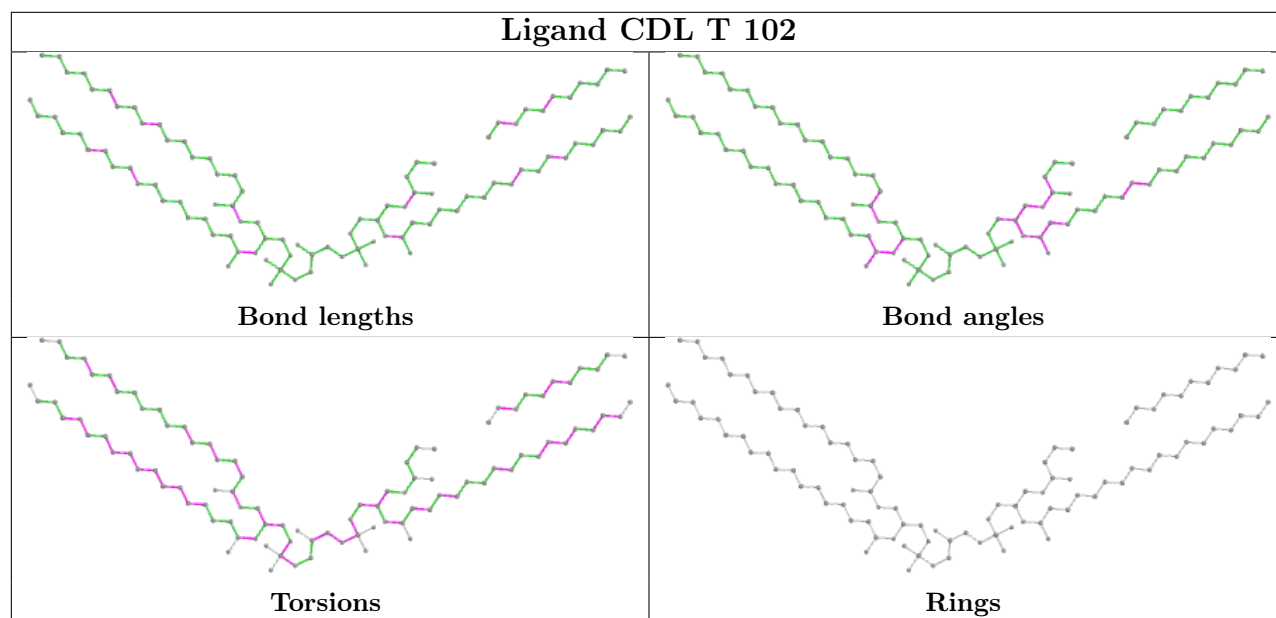
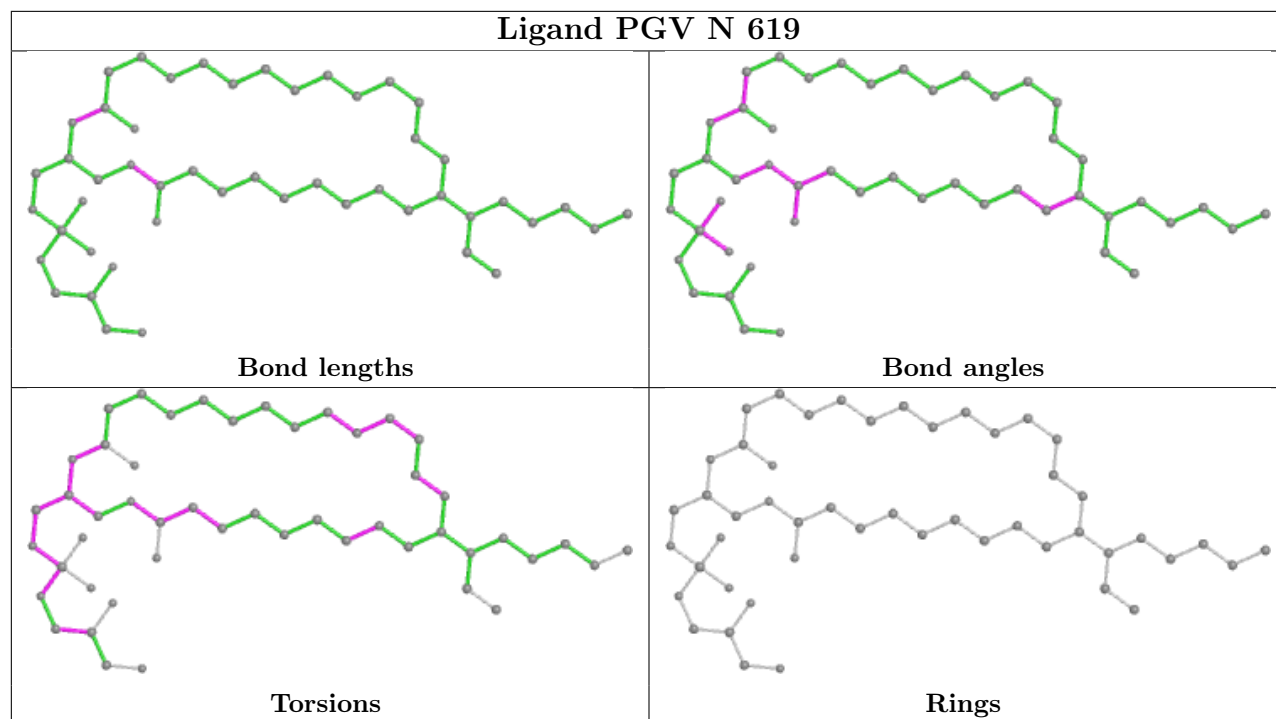


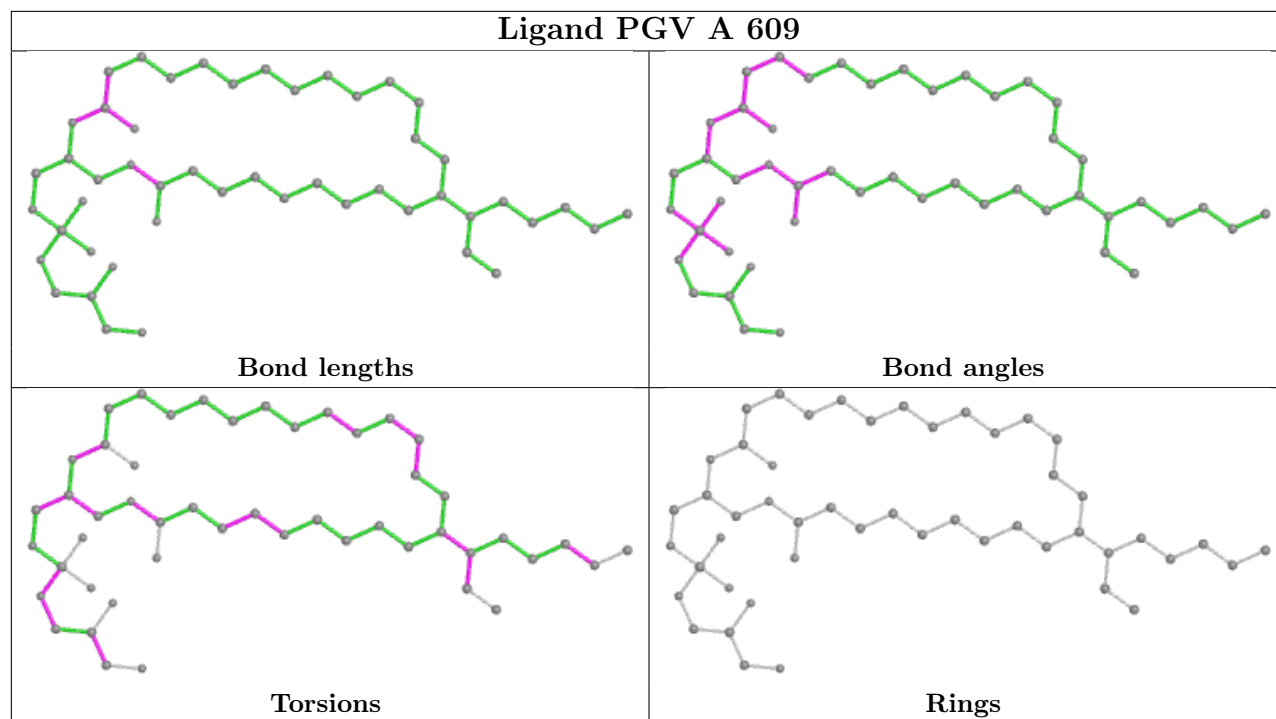












5.7 Other polymers [i](#)

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%)	0.05	0 100 100	23, 29, 38, 83	0
1	N	513/514 (99%)	-0.01	1 (0%) 95 94	27, 35, 46, 84	0
2	B	226/227 (99%)	0.09	1 (0%) 92 92	27, 38, 59, 83	0
2	O	226/227 (99%)	0.13	4 (1%) 68 68	33, 45, 75, 104	0
3	C	259/261 (99%)	0.06	0 100 100	26, 33, 47, 97	0
3	P	259/261 (99%)	0.01	1 (0%) 92 92	28, 35, 48, 84	0
4	D	144/147 (97%)	-0.07	2 (1%) 75 76	31, 41, 67, 89	0
4	Q	144/147 (97%)	0.51	7 (4%) 29 28	43, 57, 90, 177	0
5	E	105/109 (96%)	-0.02	2 (1%) 66 66	33, 40, 66, 127	0
5	R	105/109 (96%)	-0.01	2 (1%) 66 66	38, 49, 73, 133	0
6	F	98/98 (100%)	0.46	7 (7%) 16 15	30, 41, 114, 163	0
6	S	98/98 (100%)	0.74	8 (8%) 11 11	32, 44, 117, 165	0
7	G	83/85 (97%)	0.92	15 (18%) 1 1	32, 42, 124, 144	0
7	T	83/85 (97%)	0.84	15 (18%) 1 1	30, 44, 113, 143	0
8	H	79/85 (92%)	0.29	7 (8%) 9 9	34, 46, 103, 121	0
8	U	79/85 (92%)	0.30	5 (6%) 20 19	39, 51, 118, 143	0
9	I	72/73 (98%)	0.43	6 (8%) 11 11	35, 51, 88, 99	0
9	V	72/73 (98%)	0.36	4 (5%) 24 23	38, 64, 88, 140	0
10	J	58/59 (98%)	0.31	3 (5%) 27 26	34, 44, 77, 122	0
10	W	58/59 (98%)	0.36	5 (8%) 10 10	37, 51, 80, 148	0
11	K	49/56 (87%)	0.03	1 (2%) 65 64	35, 44, 60, 69	0
11	X	49/56 (87%)	0.31	4 (8%) 11 11	49, 59, 87, 96	0
12	L	46/47 (97%)	0.02	1 (2%) 62 61	30, 35, 59, 93	0
12	Y	46/47 (97%)	0.11	1 (2%) 62 61	39, 47, 78, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.23	4 (9%) 8 8	32, 37, 74, 118	0
13	Z	43/46 (93%)	0.29	3 (6%) 16 15	45, 53, 95, 174	0
All	All	3550/3614 (98%)	0.17	109 (3%) 49 47	23, 39, 78, 177	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	26.1
4	Q	6	VAL	14.2
4	Q	4	SER	13.5
4	Q	5	VAL	12.3
6	F	98	HIS	12.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.52	0.38	98,137,157,162	0
7	TPO	T	11	11/12	0.62	0.29	115,127,158,161	0
9	SAC	V	1	9/10	0.69	0.19	128,153,165,171	0
9	SAC	I	1	9/10	0.87	0.17	79,99,108,120	0
1	FME	N	1	10/11	0.97	0.12	44,59,81,83	0
1	FME	A	1	10/11	0.98	0.13	40,51,92,92	0
2	FME	O	1	10/11	0.98	0.13	38,44,54,89	0
2	FME	B	1	10/11	0.99	0.12	29,34,46,89	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	Q	203	4/4	0.40	0.20	78,79,90,92	0
20	EDO	C	317	4/4	0.53	0.71	75,93,107,109	0
22	CHD	W	101	29/29	0.55	0.41	54,125,146,153	0
20	EDO	D	205	4/4	0.57	0.16	61,62,70,72	0
26	CDL	T	102	97/100	0.63	0.33	41,86,149,173	0
25	DMU	C	302	33/33	0.65	0.37	32,85,116,134	0
27	PEK	C	319	44/53	0.67	0.35	50,80,155,168	0
20	EDO	A	616	4/4	0.68	0.39	45,53,54,102	0
25	DMU	L	102	30/33	0.68	0.25	45,95,141,147	0
27	PEK	T	101	50/53	0.68	0.28	40,82,132,162	0
24	PSC	B	304	50/52	0.69	0.33	35,80,154,170	0
26	CDL	N	601	96/100	0.70	0.35	50,90,144,168	0
20	EDO	C	316	4/4	0.71	0.36	56,80,96,103	0
22	CHD	J	101	29/29	0.71	0.24	88,129,148,149	0
27	PEK	G	103	44/53	0.73	0.26	45,84,153,164	0
25	DMU	P	306	33/33	0.74	0.30	45,83,118,130	0
21	TGL	Q	201	63/63	0.74	0.22	46,77,102,118	0
26	CDL	P	304	80/100	0.77	0.29	44,84,125,140	0
19	PGV	C	308	49/51	0.77	0.21	42,76,127,157	0
27	PEK	C	307	53/53	0.77	0.25	43,78,143,155	0
20	EDO	O	305	4/4	0.78	0.12	71,75,78,79	0
20	EDO	A	617	4/4	0.78	0.23	59,62,68,72	0
21	TGL	Y	101	63/63	0.79	0.29	45,74,117,149	0
20	EDO	C	312	4/4	0.79	0.14	68,81,88,93	0
19	PGV	G	104	51/51	0.80	0.27	47,82,123,155	0
24	PSC	O	302	51/52	0.80	0.34	46,87,162,170	0
21	TGL	N	610	61/63	0.81	0.25	52,82,106,121	0
20	EDO	A	619	4/4	0.81	0.23	52,52,61,67	0
20	EDO	G	105	4/4	0.81	0.26	55,66,73,94	0
25	DMU	C	309	33/33	0.81	0.27	53,79,115,123	0
21	TGL	D	201	63/63	0.81	0.22	36,68,97,114	0
21	TGL	L	101	63/63	0.81	0.21	29,65,102,125	0
26	CDL	C	305	89/100	0.81	0.25	46,79,109,126	0
20	EDO	D	202	4/4	0.82	0.34	66,77,81,95	0
25	DMU	C	310	22/33	0.82	0.17	59,73,96,117	0
20	EDO	R	201	4/4	0.82	0.27	64,66,69,82	0
19	PGV	N	619	51/51	0.82	0.33	45,84,139,154	0
20	EDO	R	205	4/4	0.83	0.42	54,57,60,80	0
22	CHD	P	305	29/29	0.83	0.24	54,67,81,93	0
20	EDO	C	314	4/4	0.83	0.29	58,79,79,82	0
20	EDO	H	101	4/4	0.84	0.19	53,54,73,76	0
25	DMU	P	307	33/33	0.84	0.21	50,76,108,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	DMU	P	308	33/33	0.85	0.24	57,85,106,118	0
20	EDO	A	615	4/4	0.85	0.31	48,58,59,63	0
20	EDO	L	103	4/4	0.85	0.17	67,72,75,104	0
21	TGL	B	301	63/63	0.86	0.19	35,76,108,120	0
25	DMU	Z	101	33/33	0.87	0.16	51,63,80,84	0
19	PGV	A	609	51/51	0.87	0.25	34,68,120,156	0
20	EDO	N	616	4/4	0.87	0.14	48,50,53,60	0
20	EDO	E	203	4/4	0.88	0.28	46,49,59,75	0
20	EDO	A	614	4/4	0.88	0.17	39,45,47,50	0
20	EDO	C	315	4/4	0.88	0.17	62,74,76,83	0
17	NA	P	302	1/1	0.88	0.14	43,43,43,43	0
20	EDO	B	306	4/4	0.89	0.19	32,40,50,61	0
20	EDO	N	613	4/4	0.89	0.14	54,58,68,70	0
22	CHD	C	306	29/29	0.89	0.24	48,66,79,86	0
20	EDO	U	101	4/4	0.89	0.14	67,68,73,85	0
20	EDO	A	611	4/4	0.89	0.18	51,54,64,72	0
20	EDO	C	313	4/4	0.89	0.12	57,64,65,88	0
20	EDO	P	311	4/4	0.89	0.29	45,61,76,77	0
17	NA	C	303	1/1	0.89	0.11	41,41,41,41	0
20	EDO	R	202	4/4	0.90	0.13	56,67,69,85	0
20	EDO	V	101	4/4	0.90	0.20	56,66,74,78	0
20	EDO	S	101	4/4	0.90	0.22	44,52,59,64	0
20	EDO	A	612	4/4	0.91	0.12	32,33,35,39	0
20	EDO	H	102	4/4	0.91	0.10	66,67,78,83	0
20	EDO	P	309	4/4	0.91	0.23	34,43,47,60	0
25	DMU	M	101	33/33	0.91	0.12	38,50,65,78	0
20	EDO	E	205	4/4	0.92	0.21	58,58,71,77	0
20	EDO	E	201	4/4	0.92	0.11	43,49,54,66	0
20	EDO	Q	202	4/4	0.92	0.15	62,64,67,73	0
20	EDO	N	612	4/4	0.93	0.22	40,50,54,55	0
20	EDO	D	204	4/4	0.93	0.22	50,62,68,74	0
20	EDO	N	614	4/4	0.93	0.14	36,37,37,46	0
20	EDO	F	103	4/4	0.93	0.14	36,37,41,41	0
20	EDO	N	617	4/4	0.93	0.21	48,49,54,58	0
20	EDO	O	304	4/4	0.93	0.13	55,67,68,82	0
20	EDO	R	206	4/4	0.93	0.25	47,50,60,71	0
20	EDO	F	105	4/4	0.93	0.18	49,57,71,82	0
20	EDO	S	104	4/4	0.93	0.29	42,47,81,88	0
20	EDO	F	106	4/4	0.93	0.14	42,54,65,68	0
16	MG	N	605	1/1	0.94	0.05	29,29,29,29	0
20	EDO	E	204	4/4	0.94	0.07	39,41,41,49	0
27	PEK	P	312	53/53	0.94	0.16	32,52,90,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	F	104	4/4	0.94	0.21	45,51,62,72	0
20	EDO	N	611	4/4	0.95	0.20	65,65,72,81	0
20	EDO	N	615	4/4	0.95	0.12	30,36,39,41	0
20	EDO	R	203	4/4	0.95	0.19	48,64,68,73	0
22	CHD	C	301	29/29	0.95	0.10	30,33,39,43	0
20	EDO	C	318	4/4	0.96	0.26	38,40,47,70	0
18	AZI	A	607[B]	3/3	0.96	0.14	21,21,29,42	3
20	EDO	A	618	4/4	0.96	0.24	35,42,67,70	0
18	AZI	N	608[A]	3/3	0.96	0.12	38,38,40,42	0
27	PEK	G	101	53/53	0.96	0.15	31,48,87,113	0
18	AZI	N	608[B]	3/3	0.96	0.12	29,29,38,39	3
22	CHD	P	301	29/29	0.96	0.09	31,37,46,47	0
18	AZI	A	607[A]	3/3	0.96	0.14	30,30,32,34	3
20	EDO	A	610	4/4	0.97	0.26	34,41,45,77	0
20	EDO	P	310	4/4	0.97	0.20	44,44,45,51	0
20	EDO	T	103	4/4	0.97	0.16	39,39,40,42	0
20	EDO	E	202	4/4	0.97	0.14	44,45,46,47	0
20	EDO	C	311	4/4	0.97	0.09	40,42,44,46	0
20	EDO	G	106	4/4	0.97	0.11	33,36,41,45	0
19	PGV	C	304	51/51	0.97	0.13	26,35,94,112	0
19	PGV	N	609	51/51	0.97	0.14	26,38,74,82	0
20	EDO	O	303	4/4	0.97	0.16	36,39,40,41	0
20	EDO	R	204	4/4	0.97	0.15	41,48,49,52	0
20	EDO	A	613	4/4	0.97	0.11	28,29,32,37	0
22	CHD	B	302	29/29	0.97	0.11	28,33,37,48	0
19	PGV	A	608	51/51	0.97	0.14	25,34,74,81	0
22	CHD	G	102	29/29	0.98	0.11	30,35,41,47	0
20	EDO	D	203	4/4	0.98	0.16	40,43,57,69	0
17	NA	N	606	1/1	0.98	0.07	38,38,38,38	0
19	PGV	P	303	51/51	0.98	0.14	29,39,75,93	0
14	HEA	N	602	60/60	0.98	0.12	27,34,58,61	0
14	HEA	N	603[A]	60/60	0.98	0.14	16,27,36,40	60
20	EDO	N	618	4/4	0.98	0.18	44,57,61,71	0
14	HEA	N	603[B]	60/60	0.98	0.14	19,31,50,59	60
20	EDO	B	305	4/4	0.98	0.15	29,30,34,38	0
14	HEA	A	602[A]	60/60	0.98	0.14	16,26,35,51	60
20	EDO	F	102	4/4	0.98	0.09	27,30,31,32	0
20	EDO	S	103	4/4	0.98	0.14	33,33,35,37	0
14	HEA	A	602[B]	60/60	0.98	0.14	15,26,36,40	60
16	MG	A	604	1/1	0.99	0.07	25,25,25,25	0
14	HEA	A	601	60/60	0.99	0.12	21,27,49,67	0
18	AZI	N	607[A]	3/3	0.99	0.13	34,34,34,39	0

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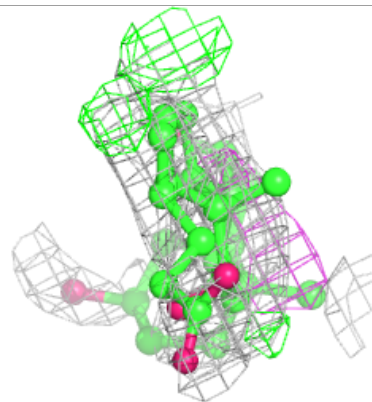
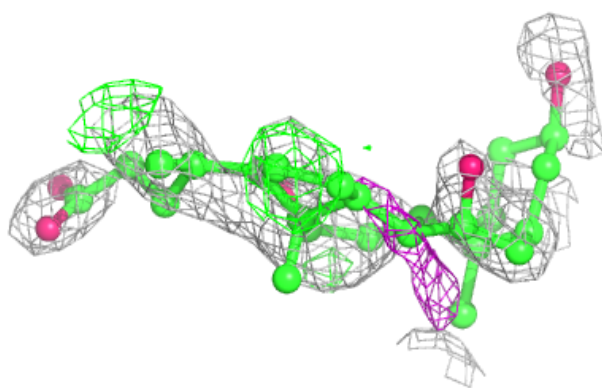
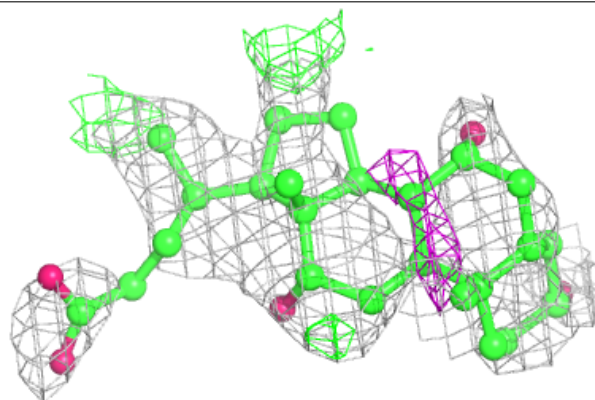
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	NA	A	605	1/1	0.99	0.09	30,30,30,30	0
18	AZI	A	606[A]	3/3	0.99	0.18	27,27,30,33	3
15	CU	A	603	1/1	1.00	0.16	28,28,28,28	0
23	CUA	B	303	2/2	1.00	0.17	28,28,28,29	0
23	CUA	O	301	2/2	1.00	0.14	34,34,34,34	0
15	CU	N	604	1/1	1.00	0.17	31,31,31,31	0
28	ZN	F	101	1/1	1.00	0.13	33,33,33,33	0
28	ZN	S	102	1/1	1.00	0.12	35,35,35,35	0

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

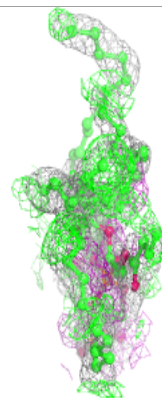
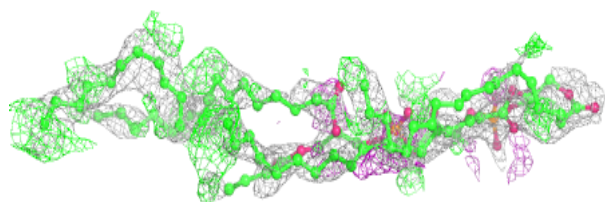
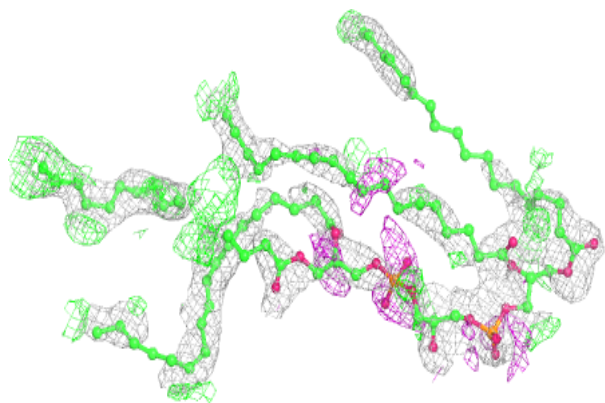
Electron density around CHD W 101:

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

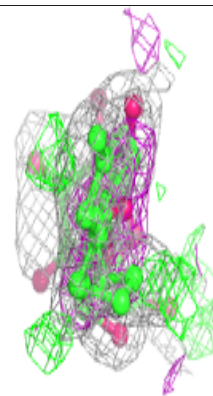
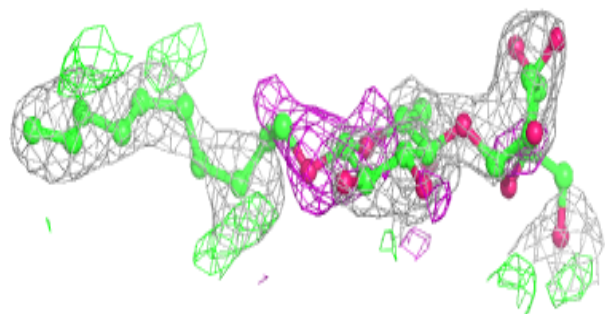
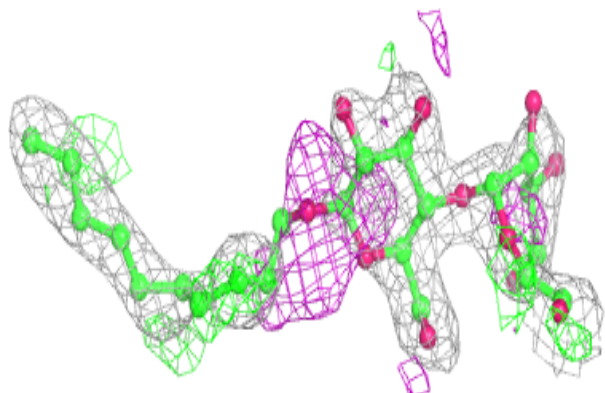


Electron density around CDL T 102:

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

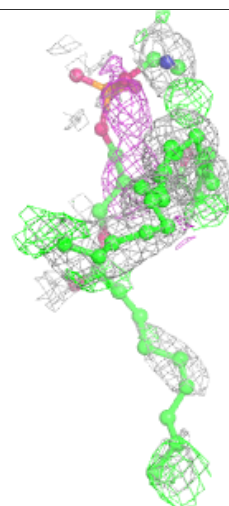
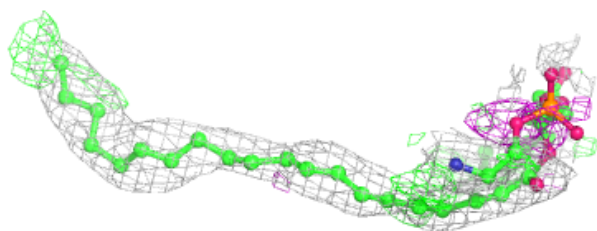
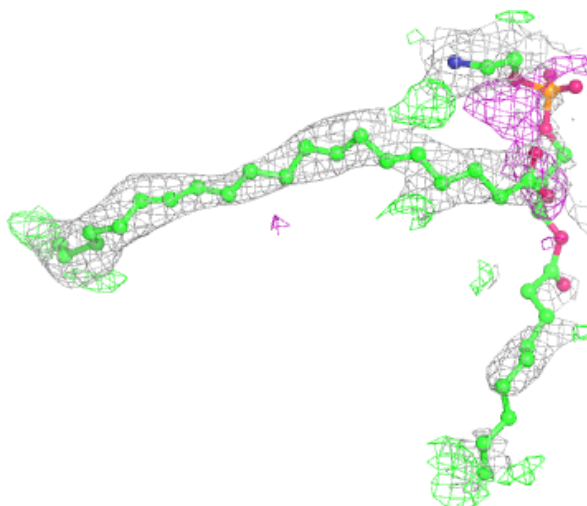
**Electron density around DMU C 302:**

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



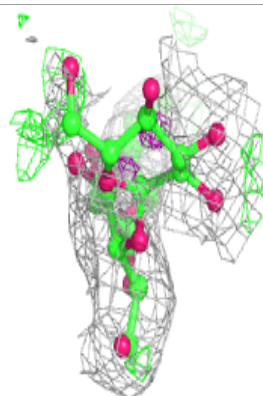
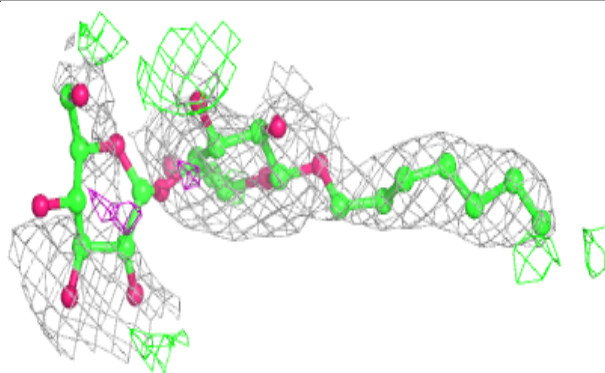
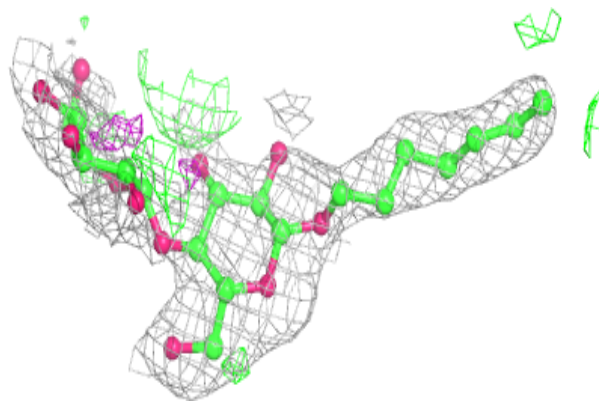
Electron density around PEK C 319:

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

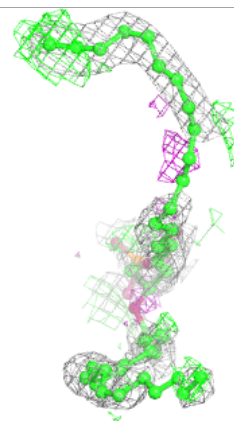
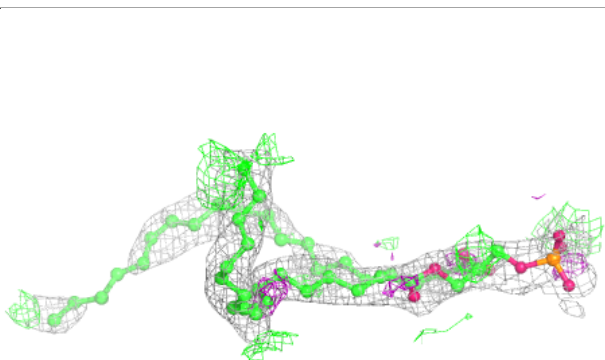
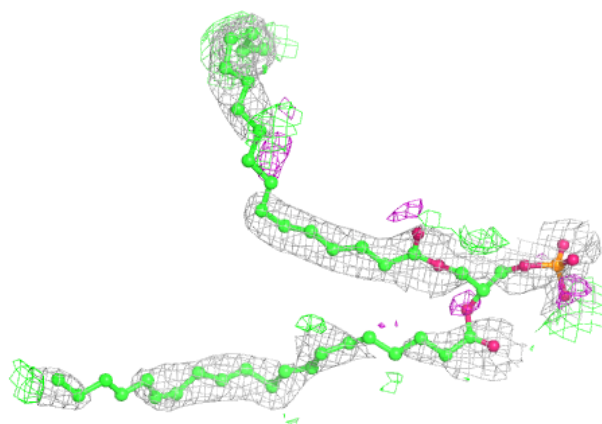


Electron density around DMU L 102:

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

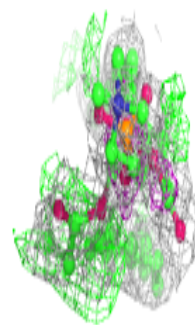
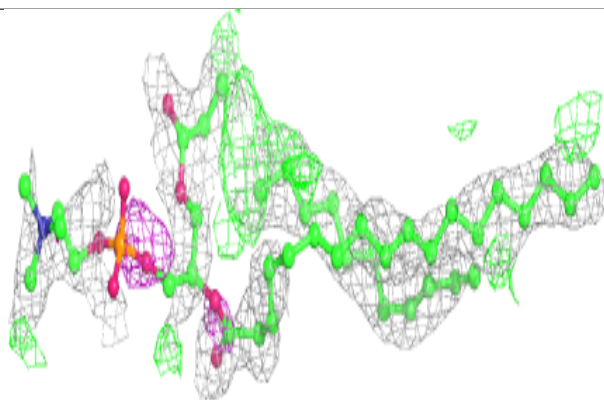
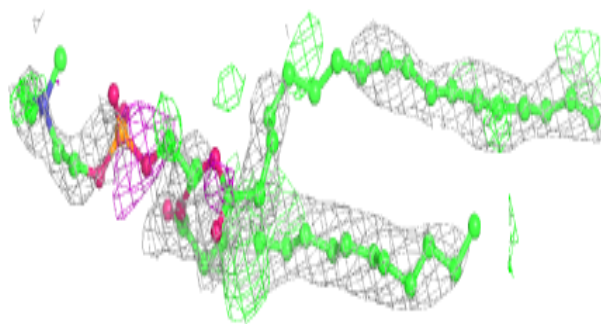
**Electron density around PEK T 101:**

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

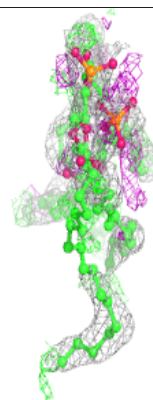
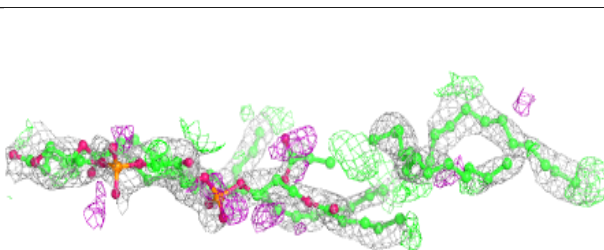
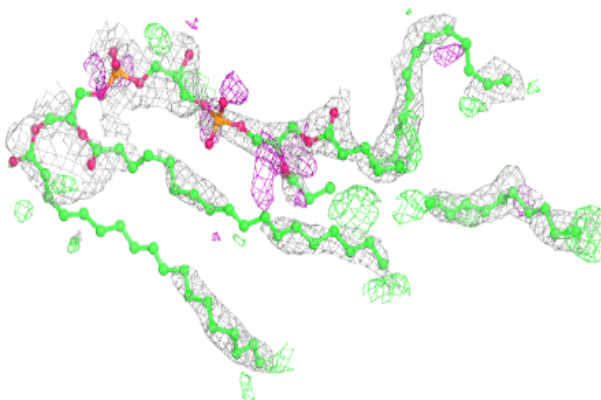


Electron density around PSC B 304:

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

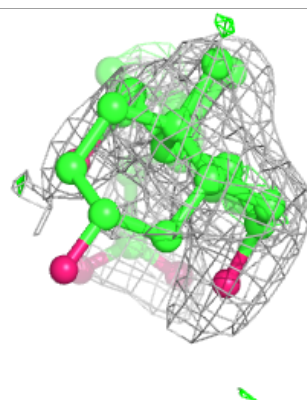
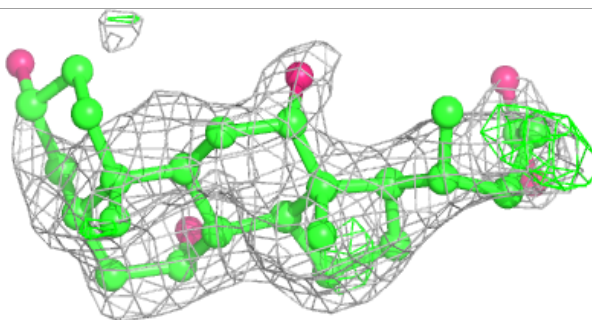
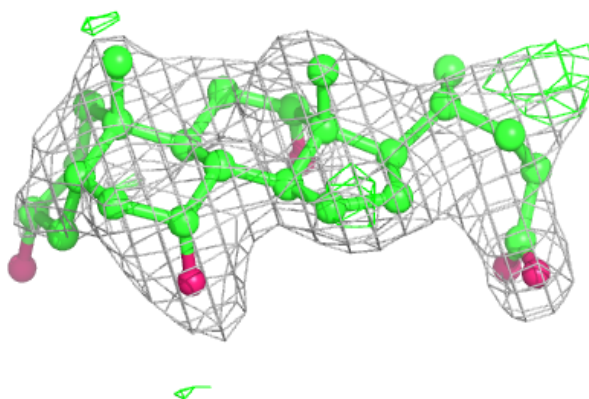
**Electron density around CDL N 601:**

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

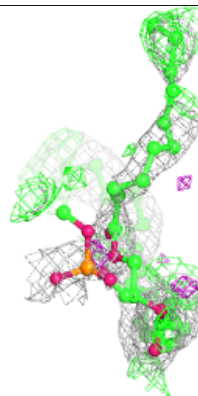
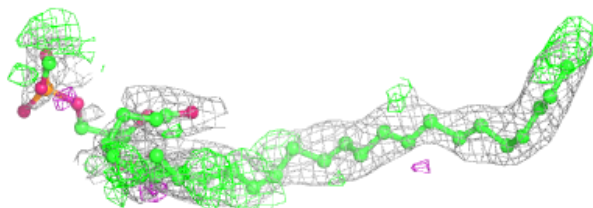
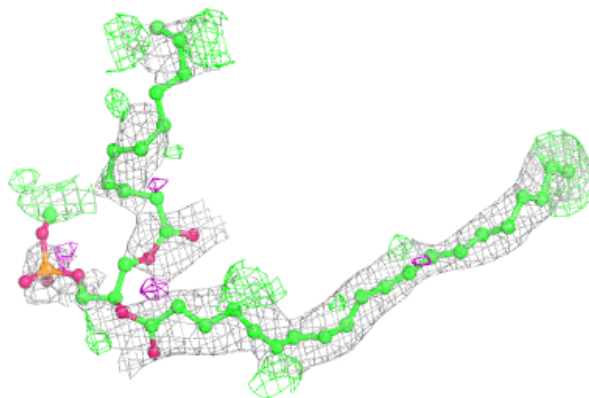


Electron density around CHD J 101:

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

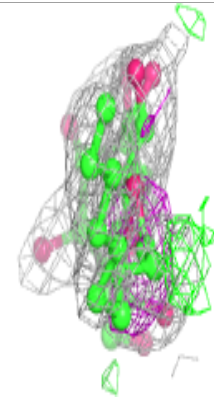
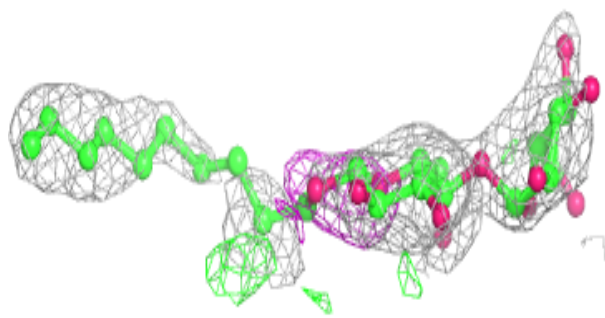
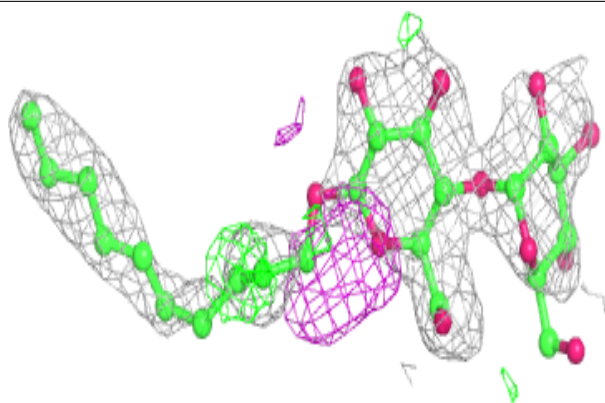
**Electron density around PEK G 103:**

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

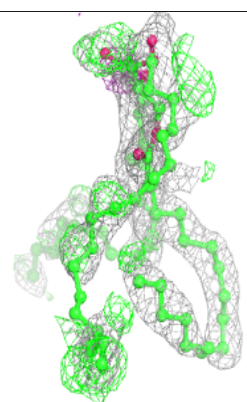
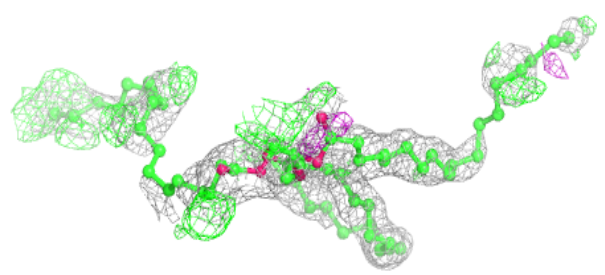
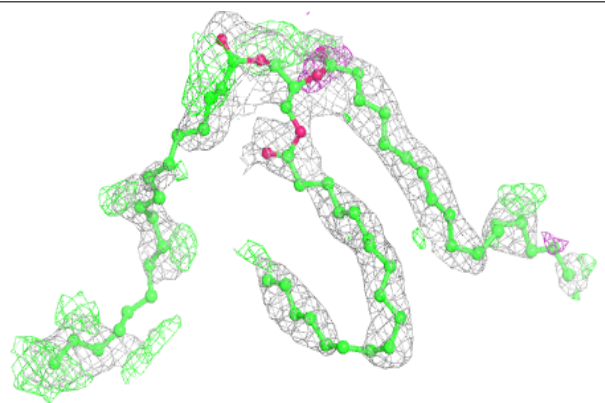


Electron density around DMU P 306:

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

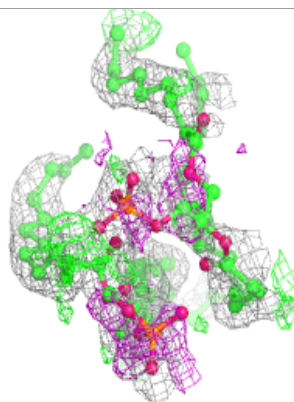
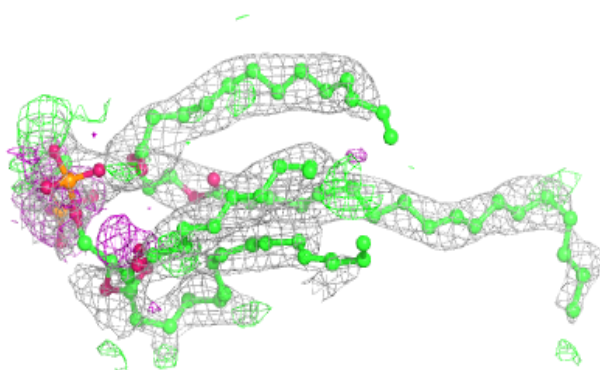
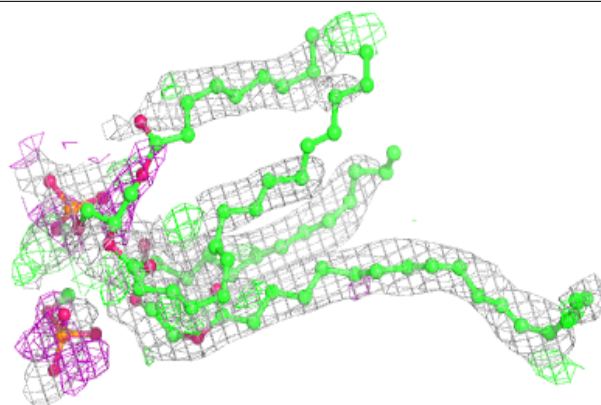
**Electron density around TGL Q 201:**

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

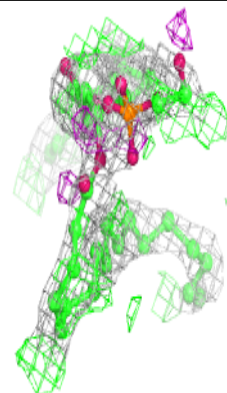
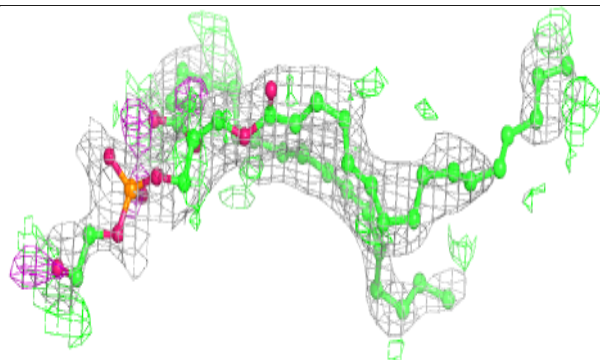
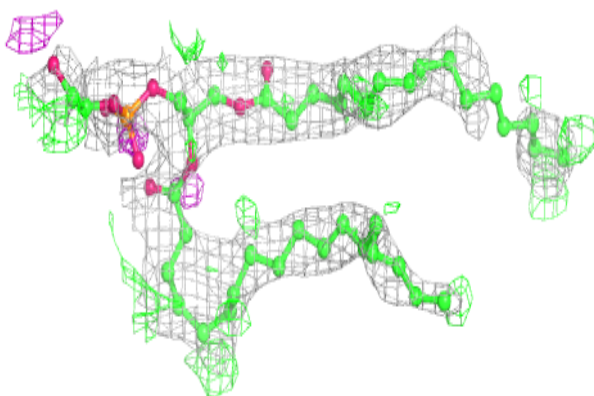


Electron density around CDL P 304:

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

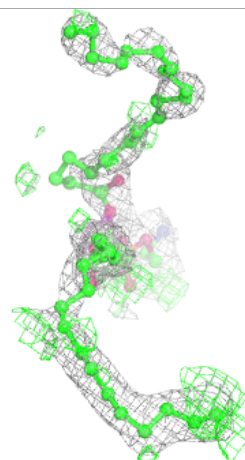
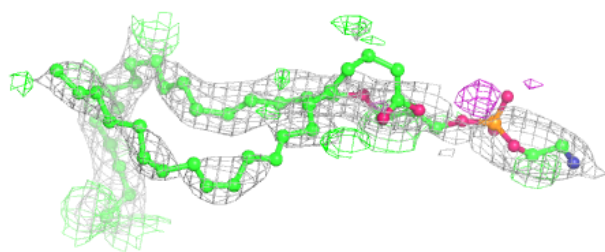
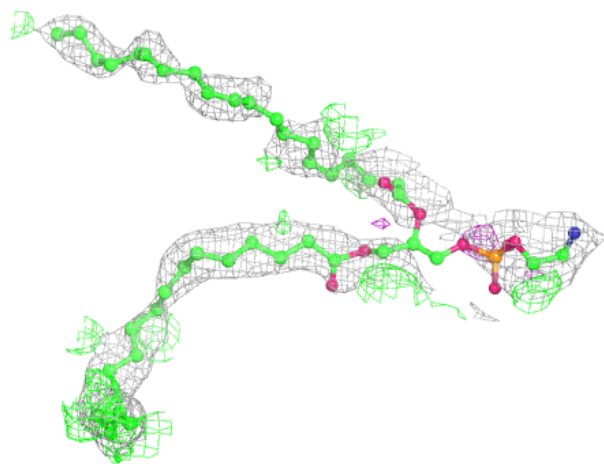
**Electron density around PGV C 308:**

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



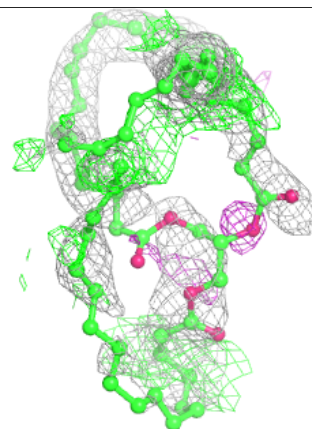
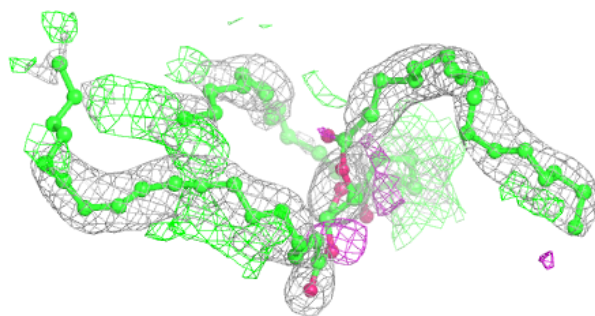
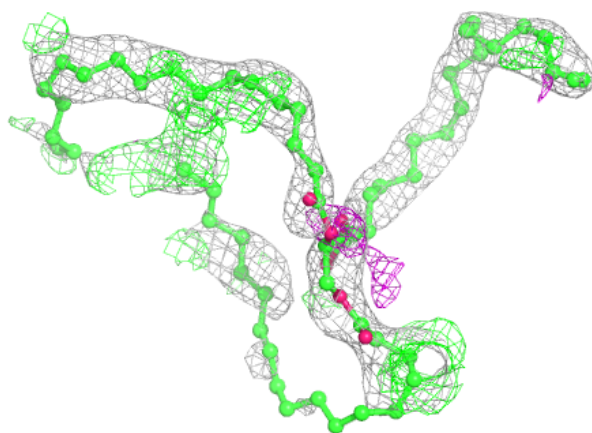
Electron density around PEK C 307:

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

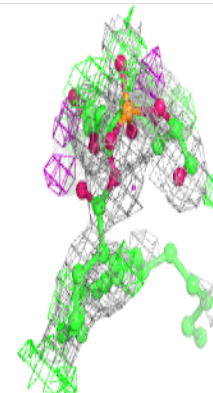
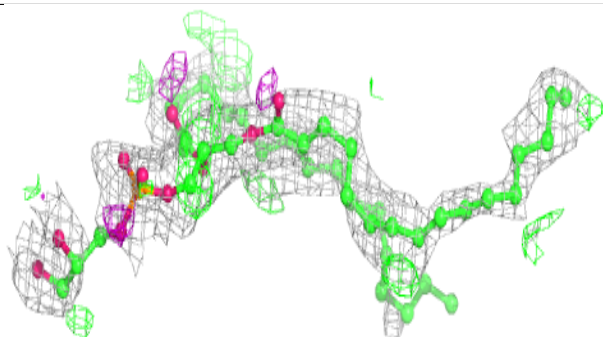
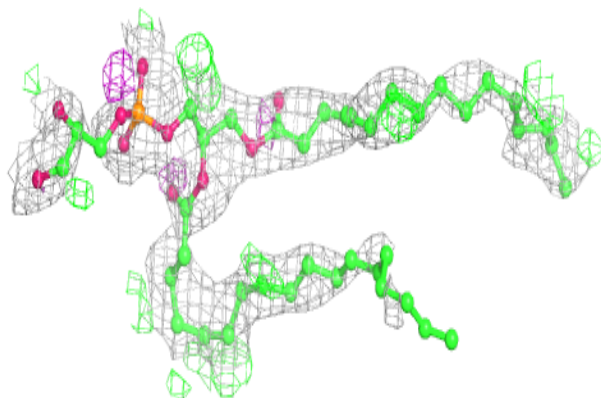


Electron density around TGL Y 101:

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

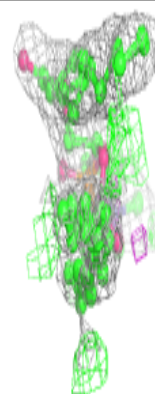
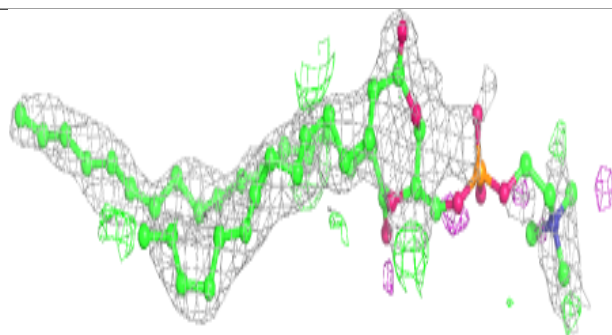
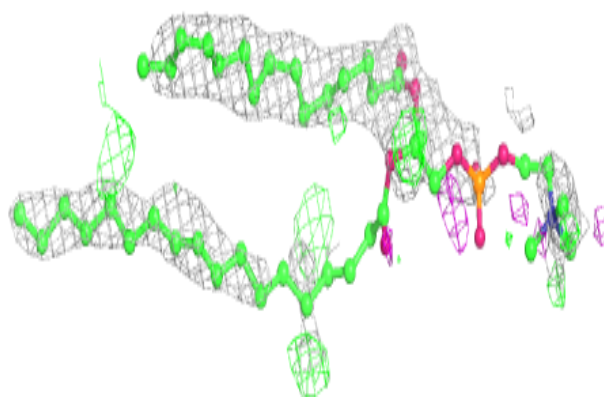
**Electron density around PGV G 104:**

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

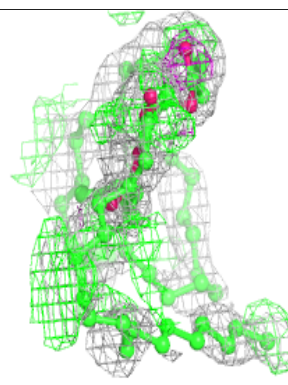
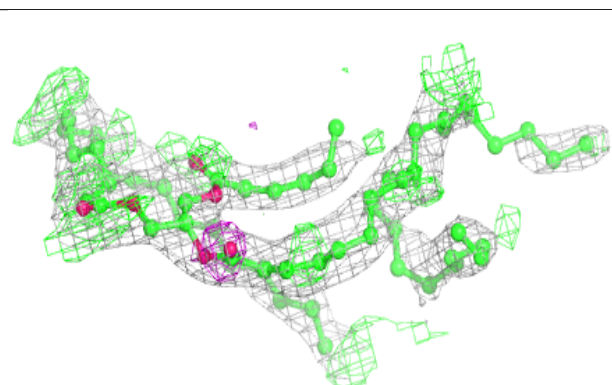
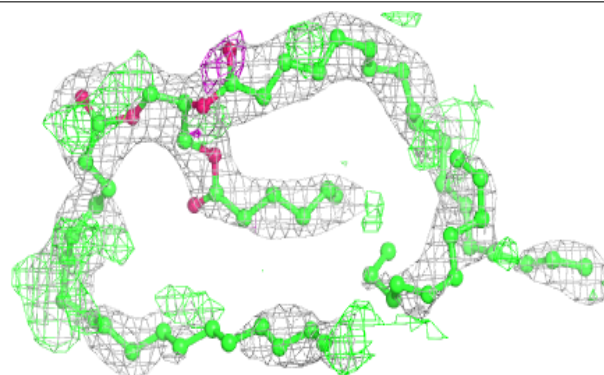


Electron density around PSC O 302:

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

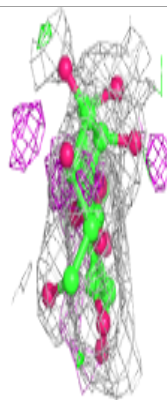
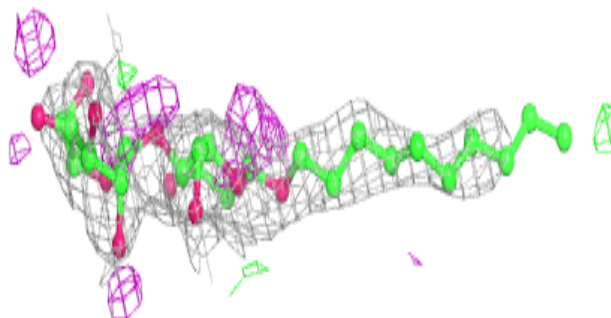
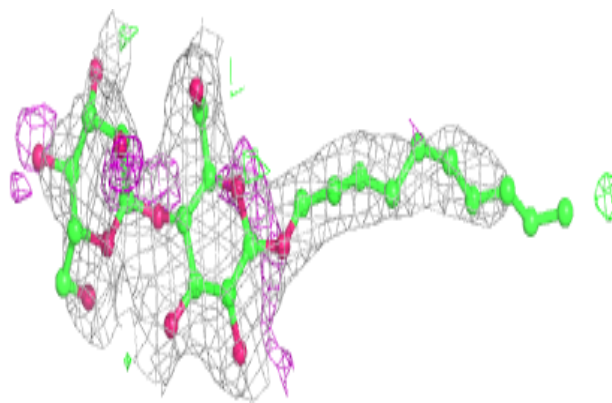
**Electron density around TGL N 610:**

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

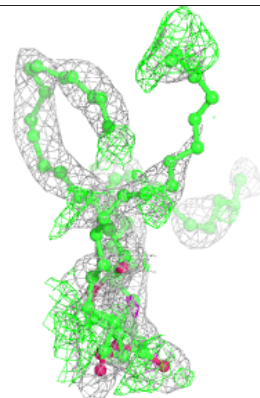
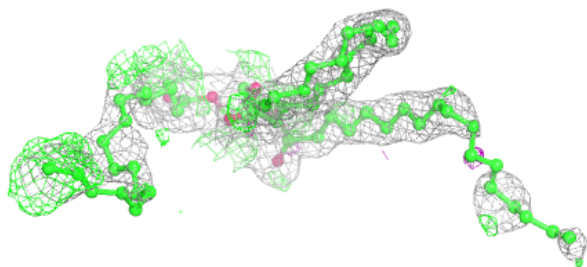
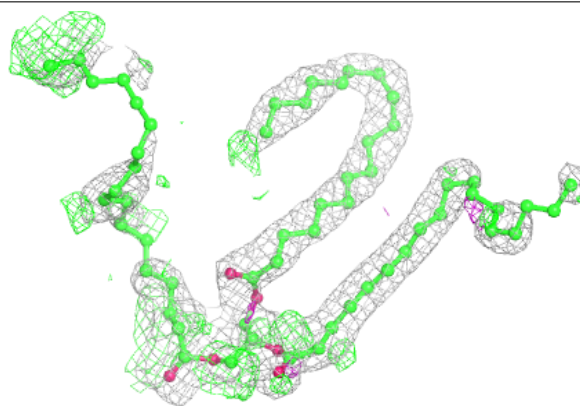


Electron density around DMU C 309:

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

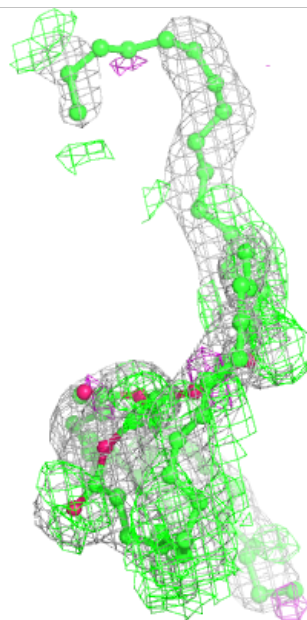
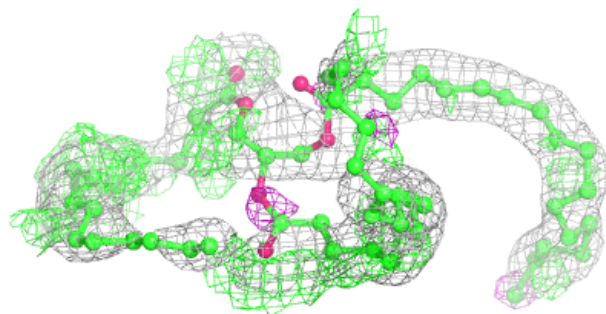
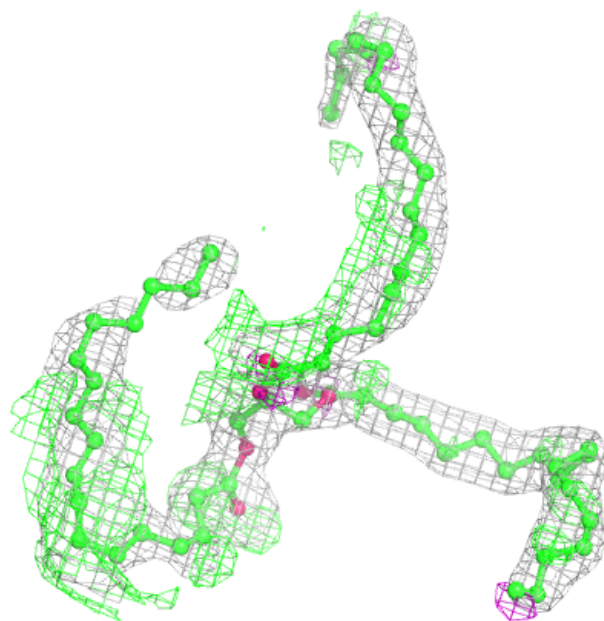
**Electron density around TGL D 201:**

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



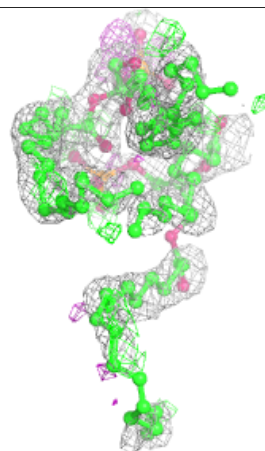
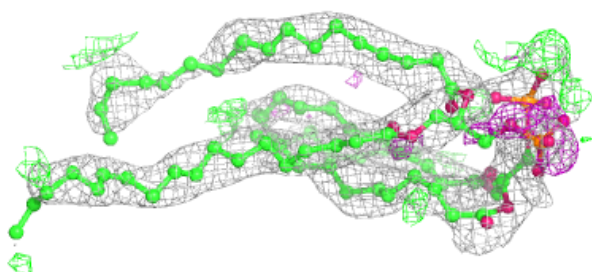
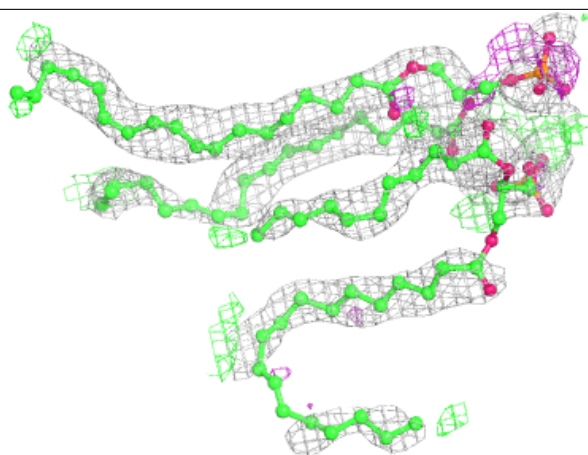
Electron density around TGL L 101:

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

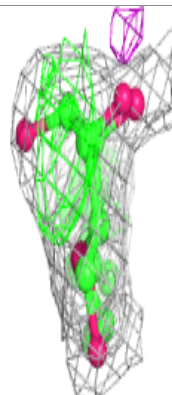
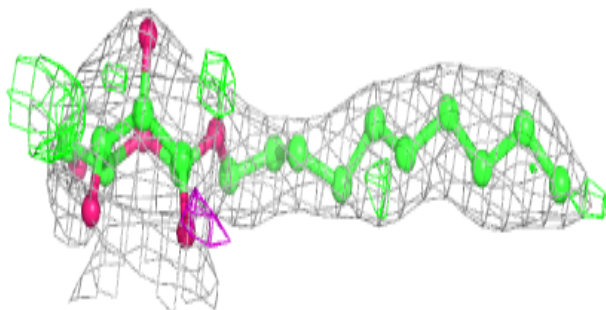
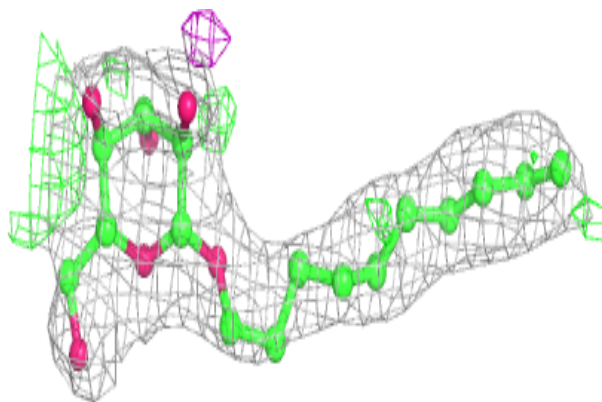


Electron density around CDL C 305:

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

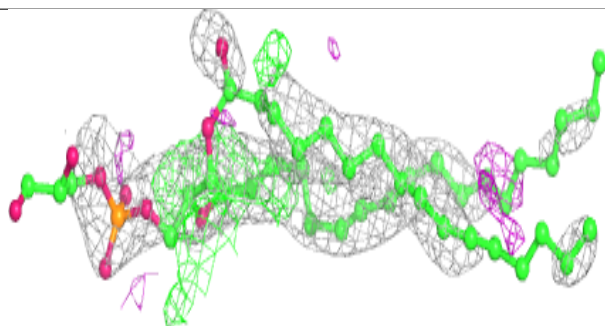
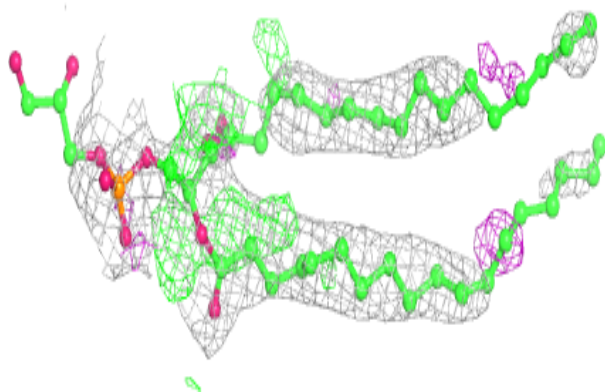
**Electron density around DMU C 310:**

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

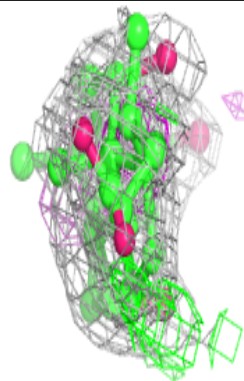
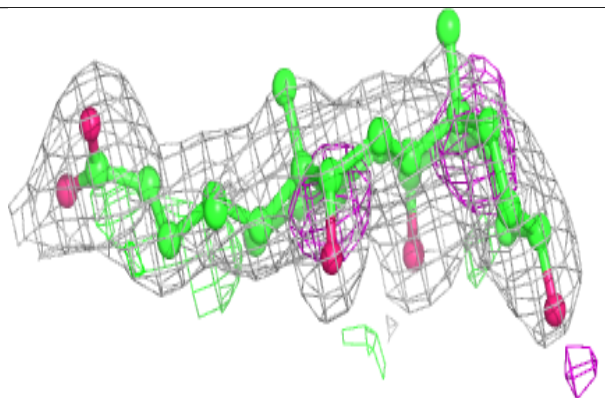
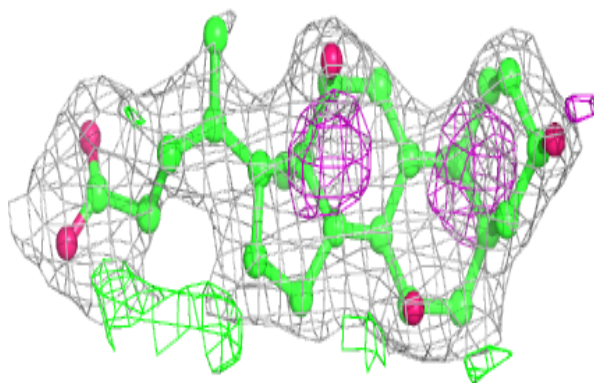


Electron density around PGV N 619:

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

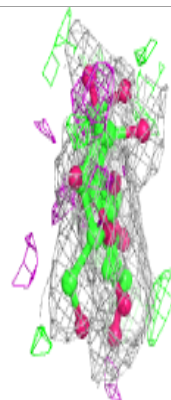
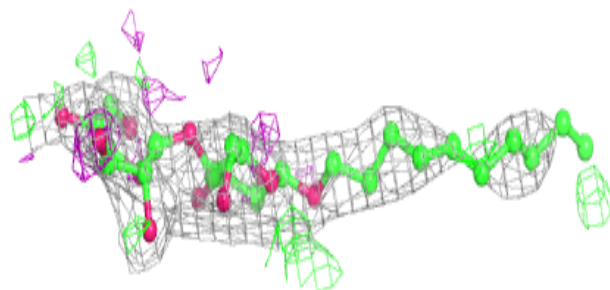
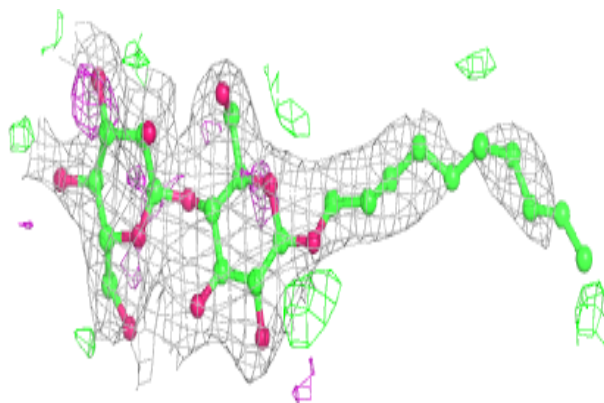
**Electron density around CHD P 305:**

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

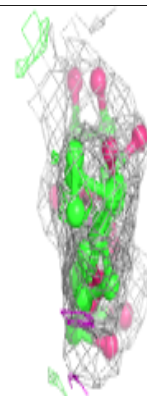
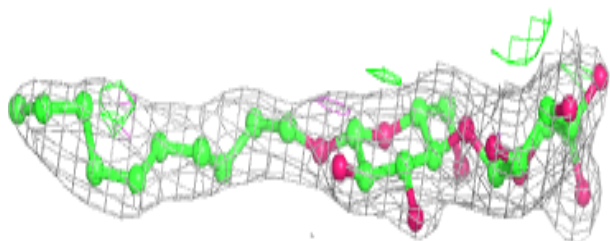
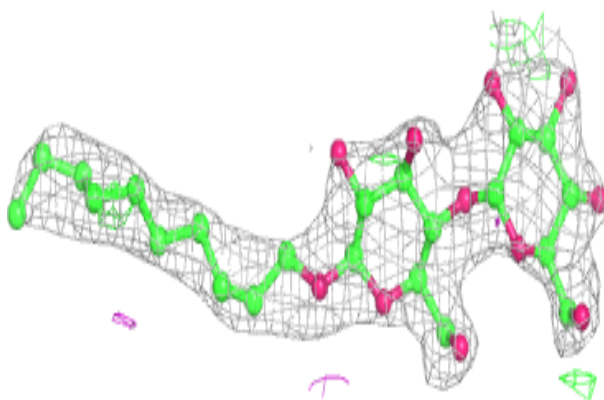


Electron density around DMU P 307:

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

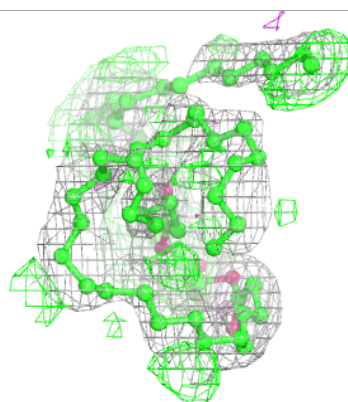
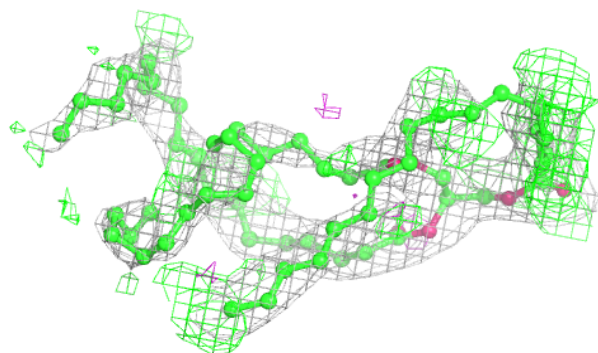
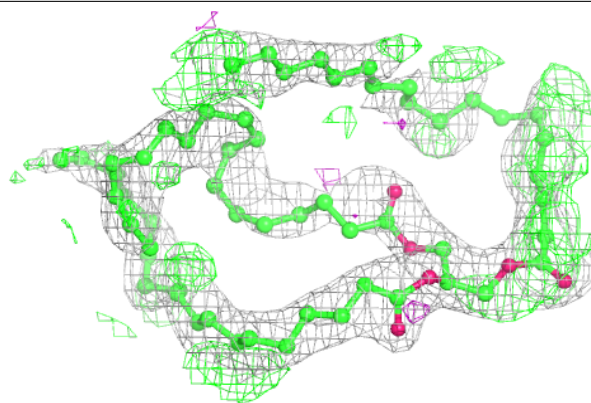
**Electron density around DMU P 308:**

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

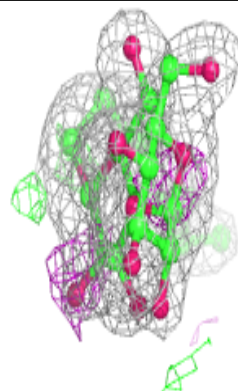
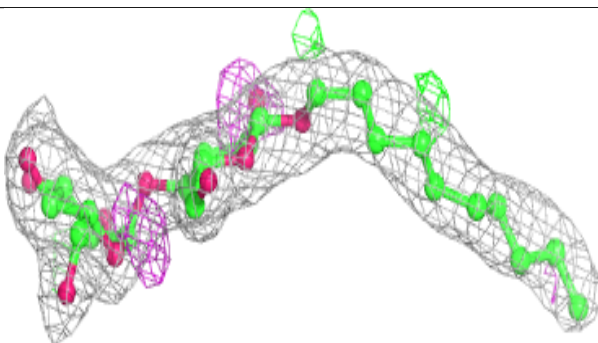
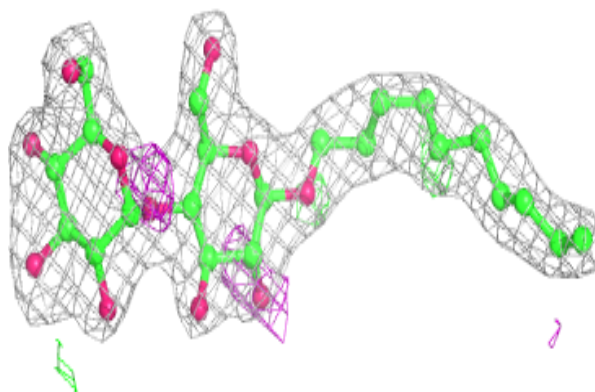


Electron density around TGL B 301:

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

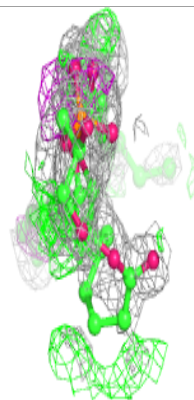
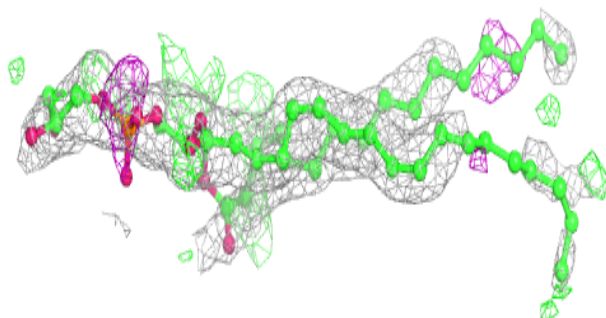
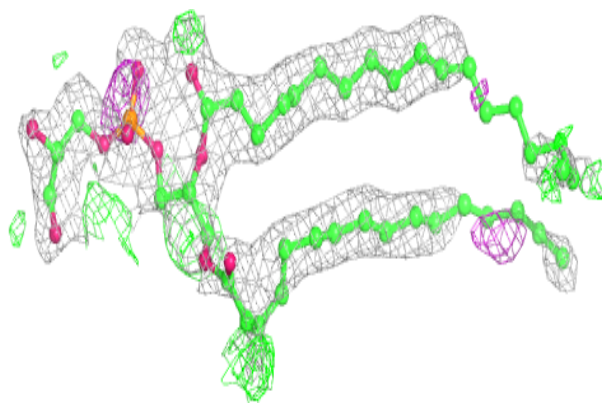
**Electron density around DMU Z 101:**

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

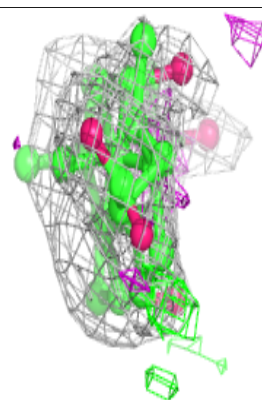
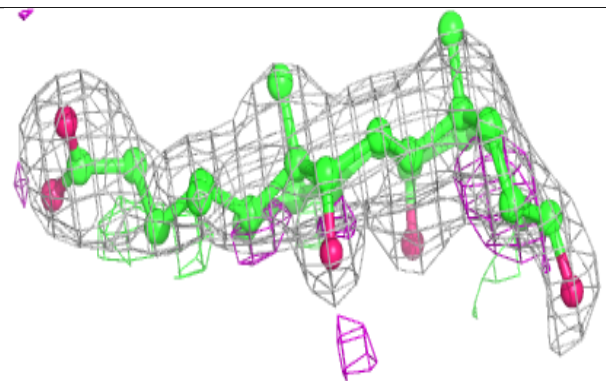
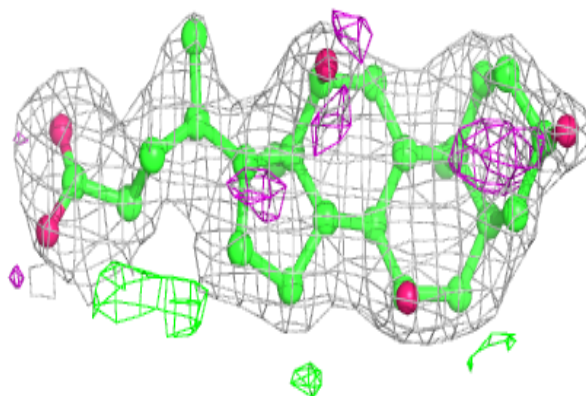


Electron density around PGV A 609:

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

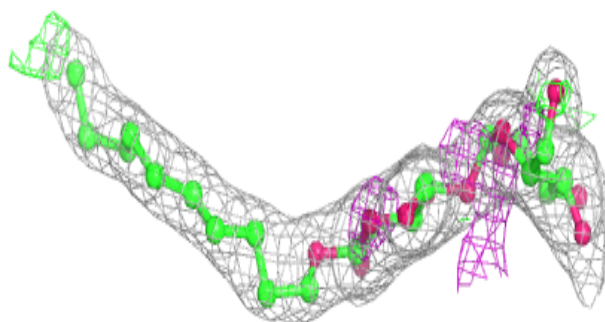
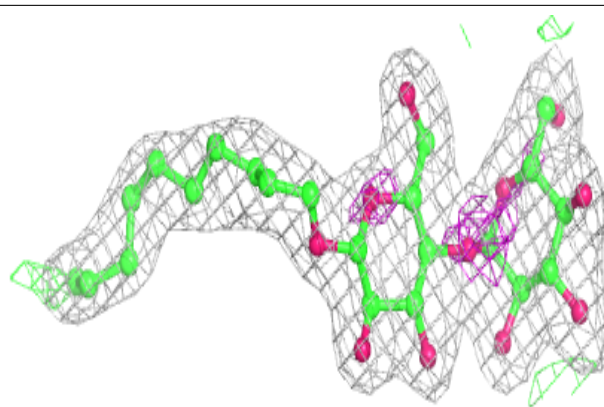
**Electron density around CHD C 306:**

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

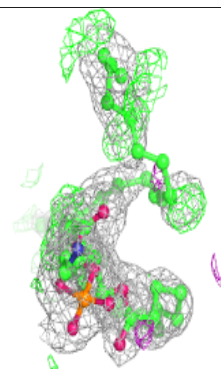
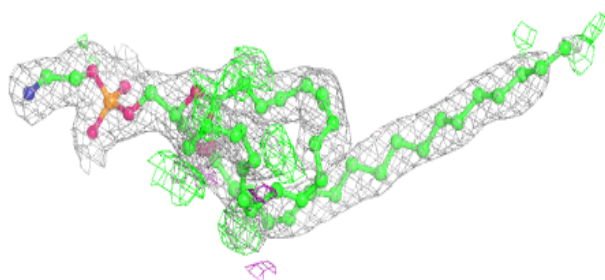
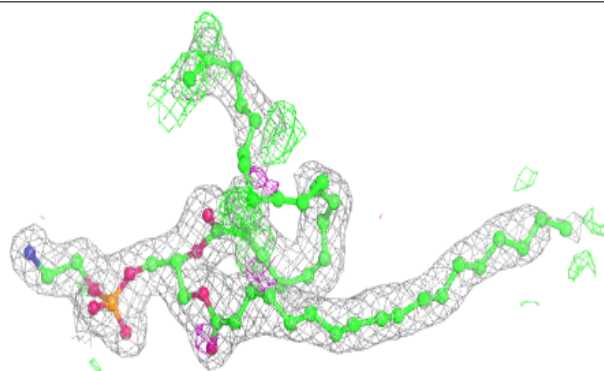


Electron density around DMU M 101:

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

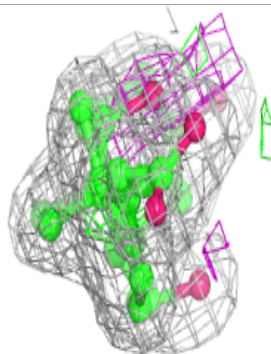
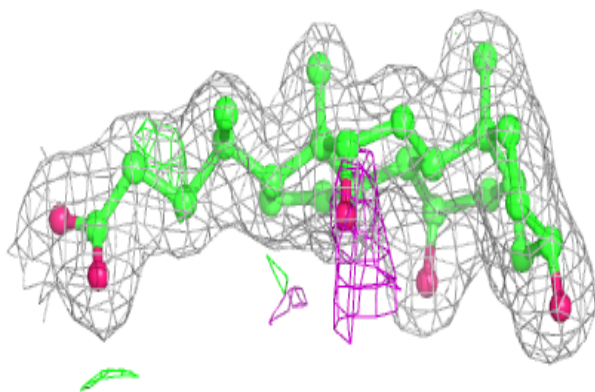
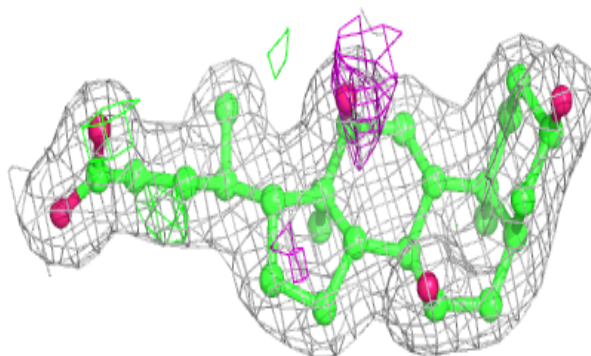
**Electron density around PEK P 312:**

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

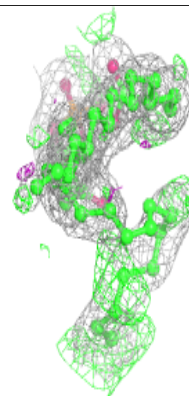
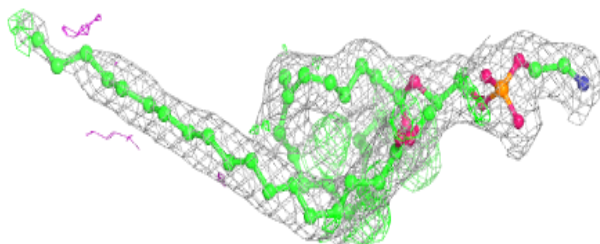
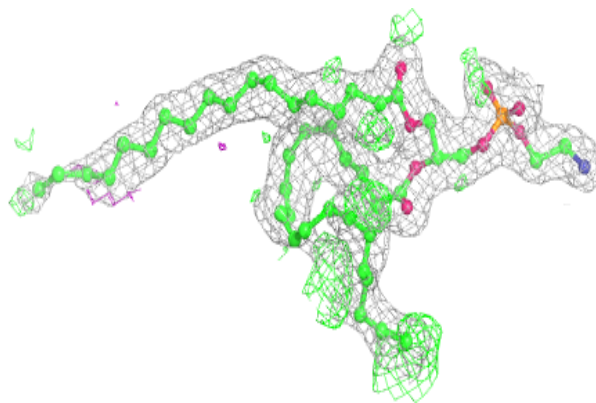


Electron density around CHD C 301:

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

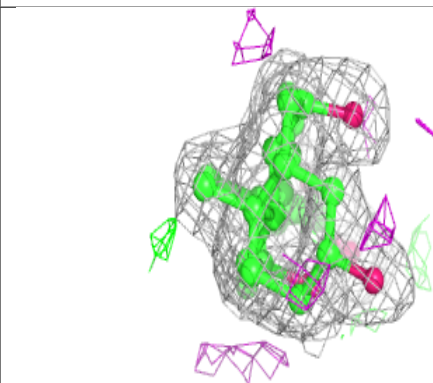
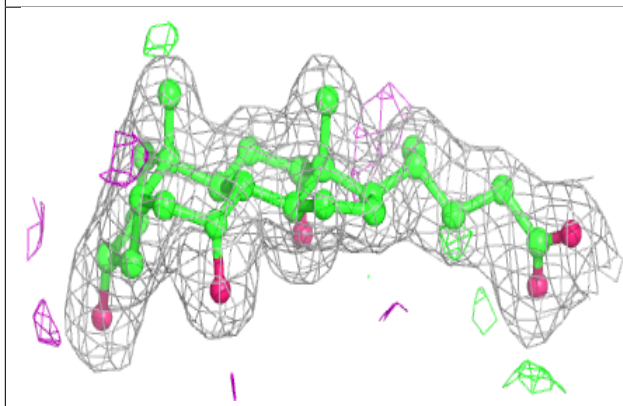
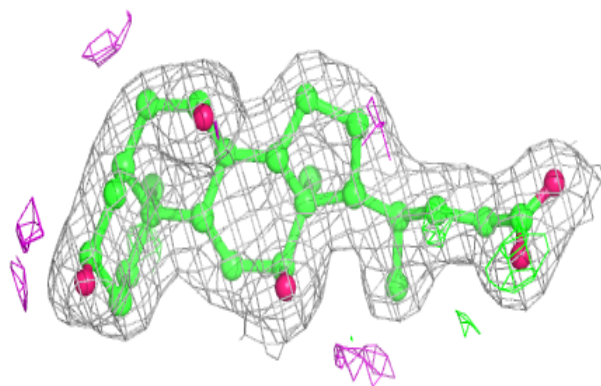
**Electron density around PEK G 101:**

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

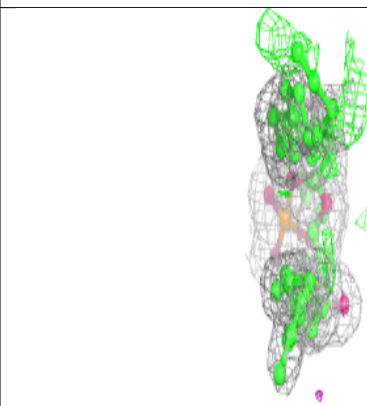
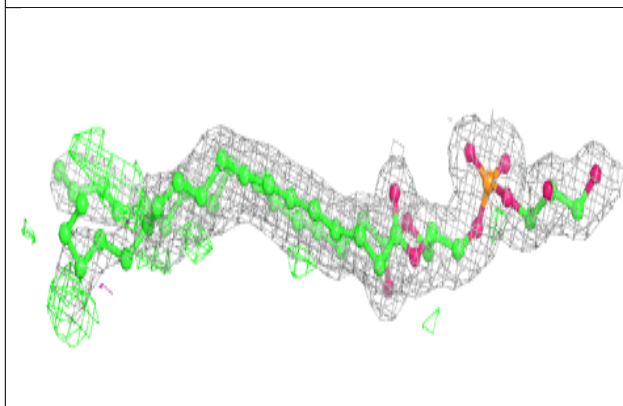
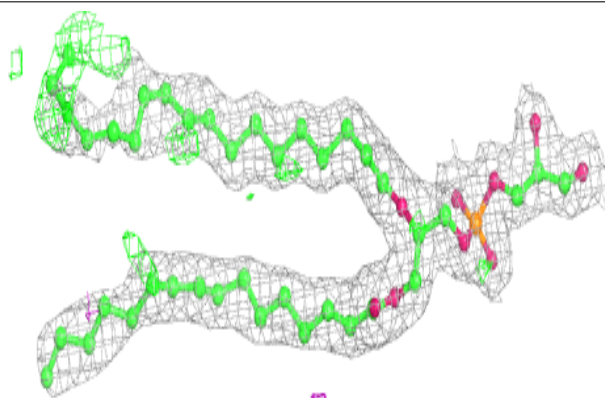


Electron density around CHD P 301:

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

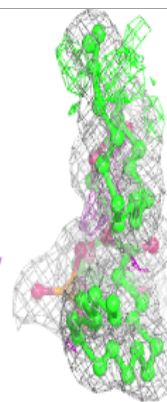
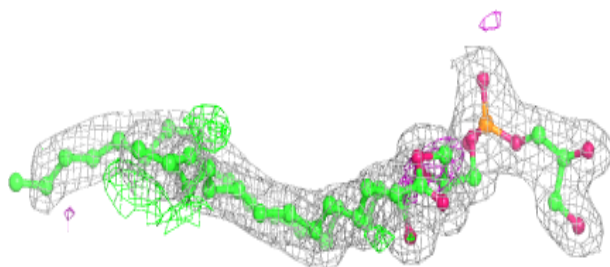
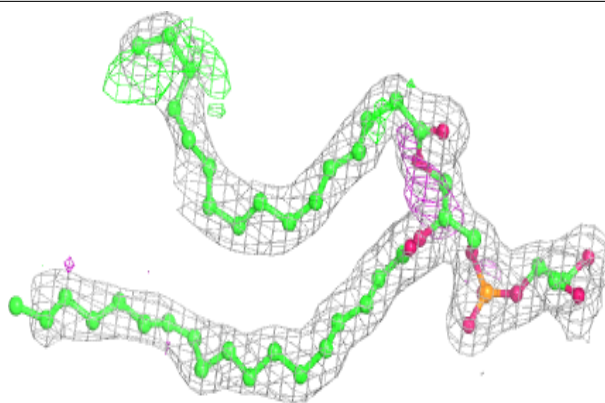
**Electron density around PGV C 304:**

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

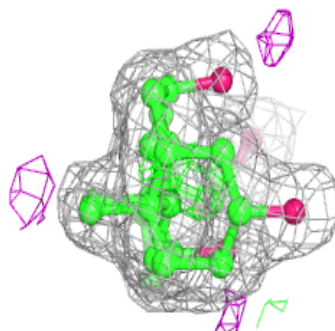
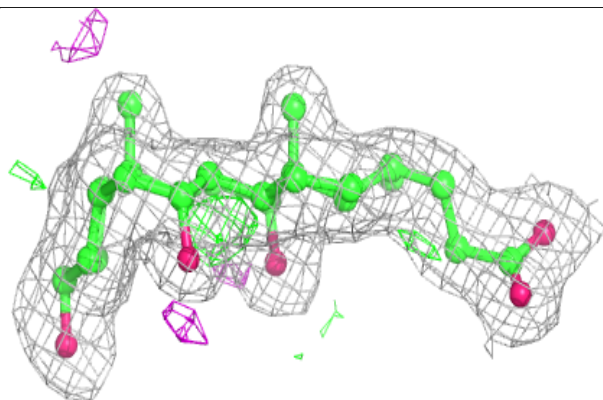
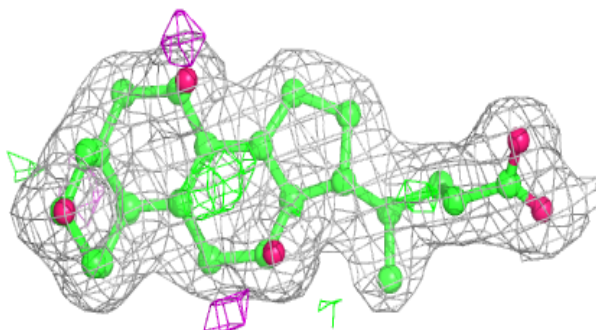


Electron density around PGV N 609:

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

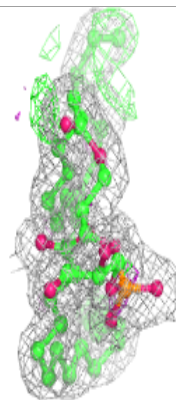
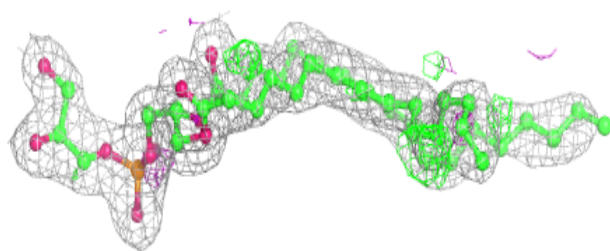
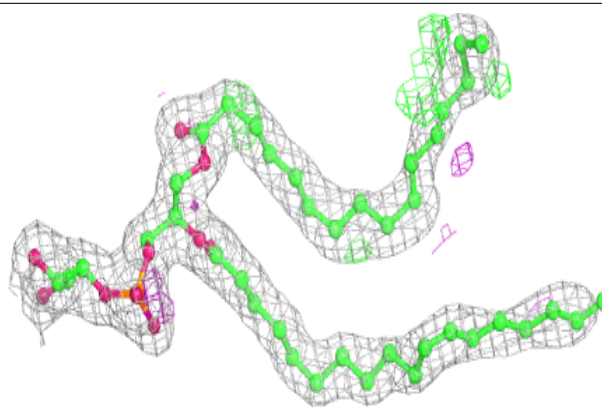
**Electron density around CHD B 302:**

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

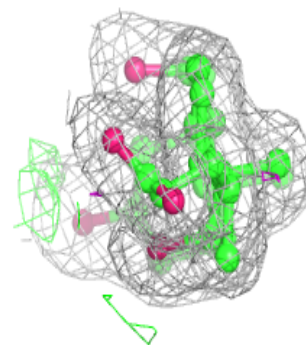
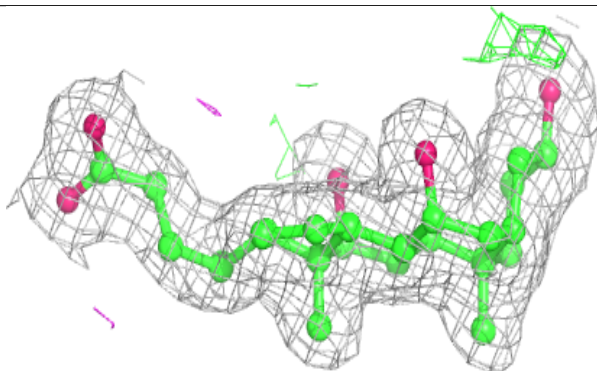
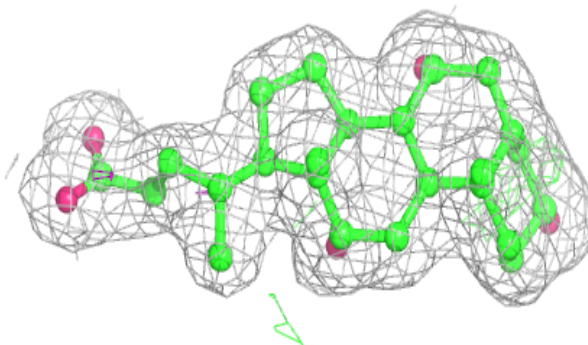


Electron density around PGV A 608:

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

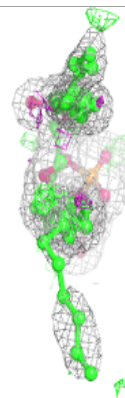
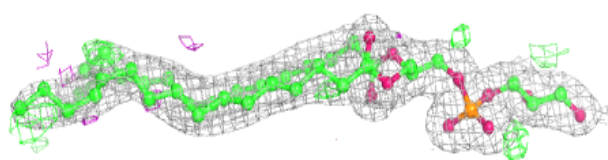
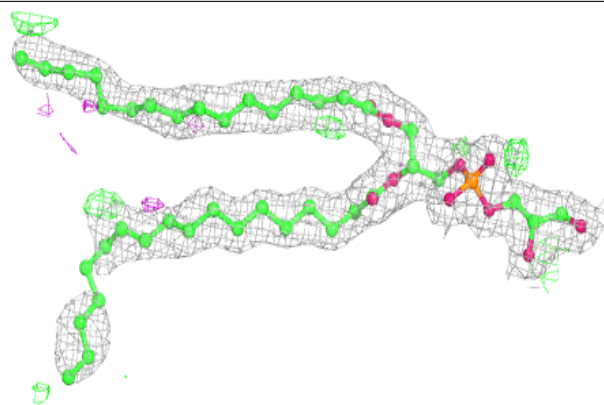
**Electron density around CHD G 102:**

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

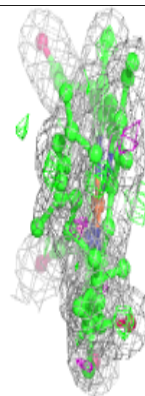
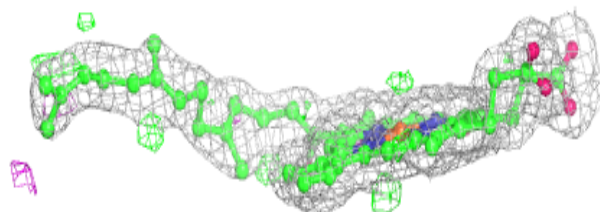
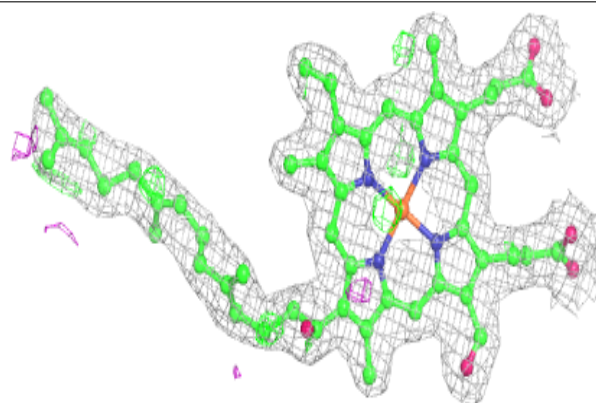


Electron density around PGV P 303:

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

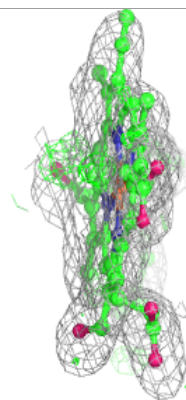
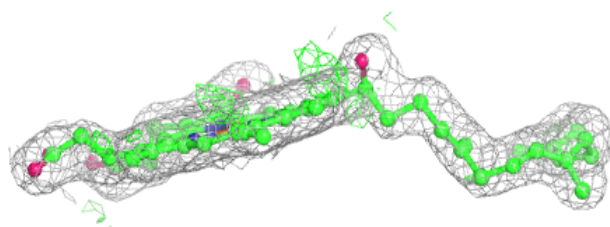
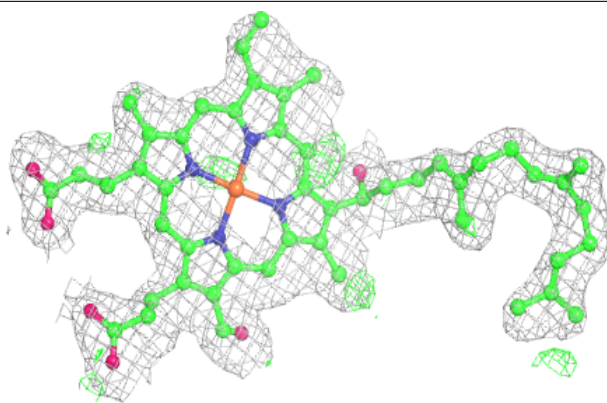
**Electron density around HEA N 602:**

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

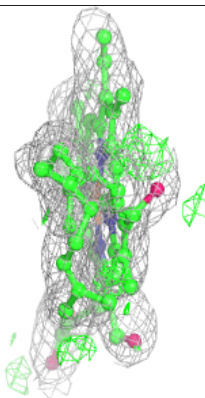
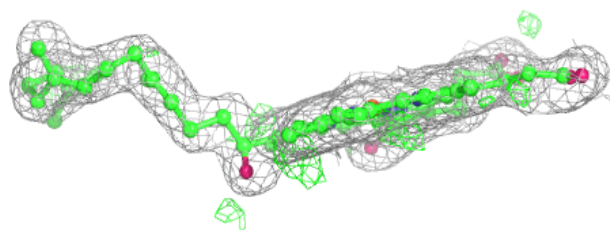
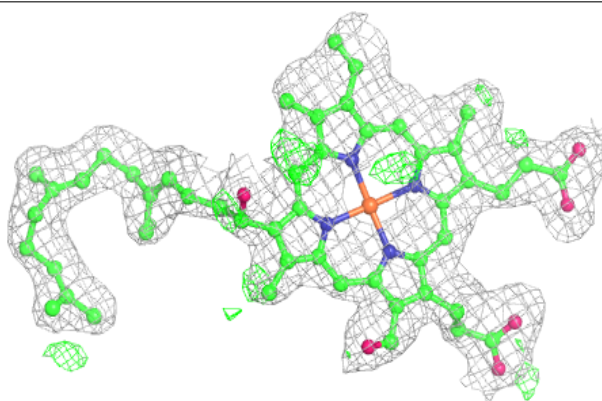


Electron density around HEA N 603 (A):

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

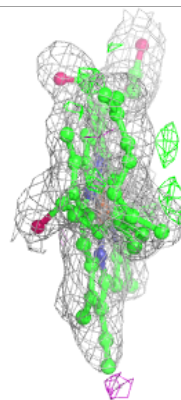
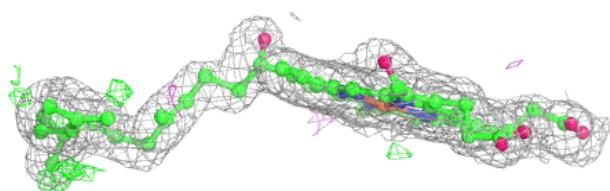
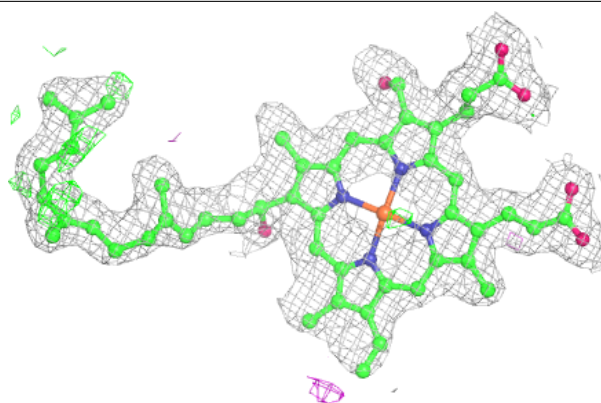
**Electron density around HEA N 603 (B):**

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

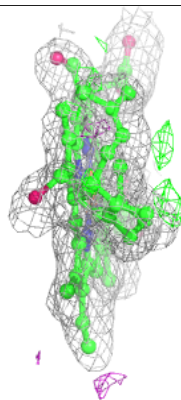
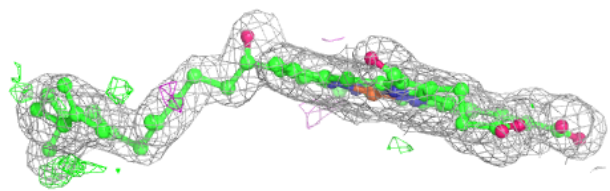
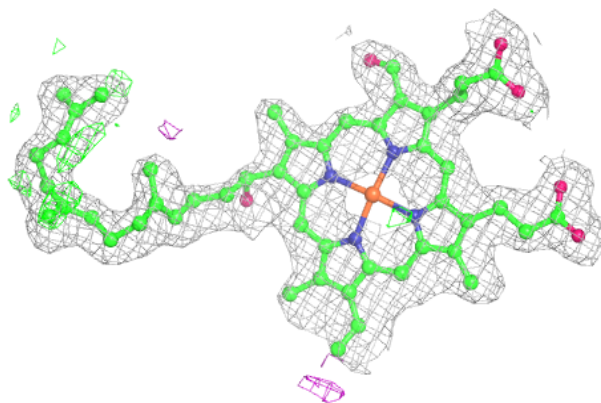


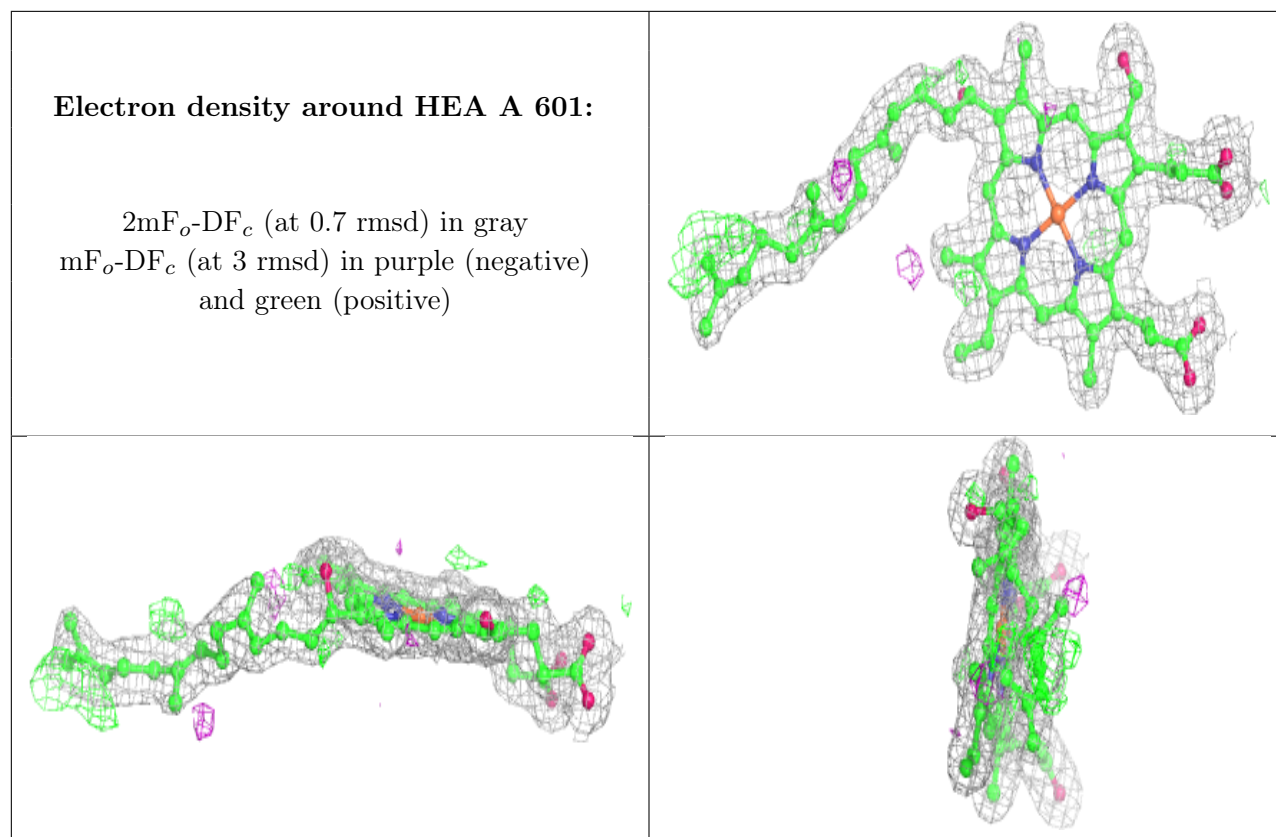
Electron density around HEA A 602 (A):

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

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

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





6.5 Other polymers [i](#)

There are no such residues in this entry.