



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2021 – 10:29 AM JST

PDB ID : 7D5W  
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate of O at 1.84 angstrom resolution  
Authors : Tsukihara, T.; Shimada, A.  
Deposited on : 2020-09-28  
Resolution : 1.84 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](mailto: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.

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

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

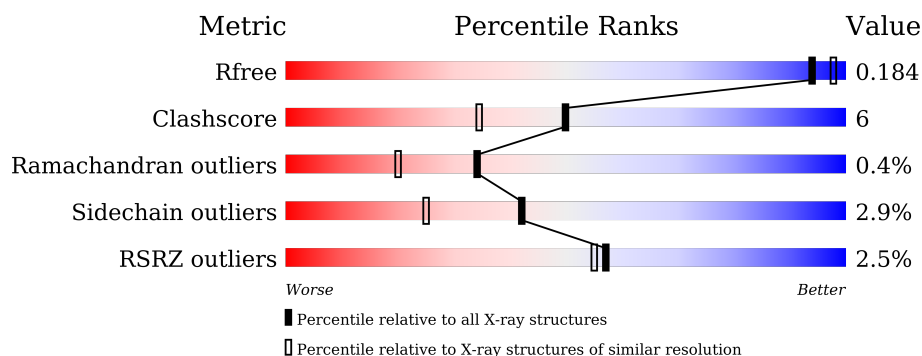
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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.





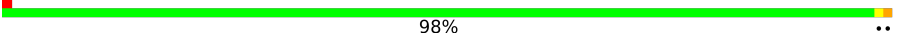














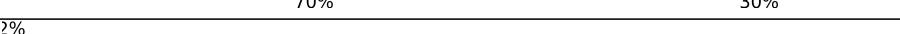


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>90%</div> <div>10%</div> </div>
1	N	514	<div> <div>88%</div> <div>12%</div> </div>
2	B	227	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>
2	O	227	<div> <div>%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>
3	C	259	<div> <div>90%</div> <div>10%</div> </div>
3	P	259	<div> <div>89%</div> <div>11%</div> </div>

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	602	X	-	-	-
14	HEA	N	602[A]	X	-	-	-
14	HEA	N	602[B]	X	-	-	-
14	HEA	N	602[C]	X	-	-	-
14	HEA	N	603	X	-	-	-
23	DMU	X	104	-	-	-	X
25	CHD	J	101	-	-	-	X
9	SAC	V	1	-	-	-	X

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	34	0
			4193	2793	646	714	40			
1	N	514	Total	C	N	O	S	0	38	0
			4199	2799	644	714	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	8	0
			1851	1202	281	347	21			
2	O	227	Total	C	N	O	S	0	12	0
			1872	1217	288	346	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	11	0
			2144	1430	340	359	15			
3	P	259	Total	C	N	O	S	0	11	0
			2143	1431	341	357	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	3	0
			1209	788	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1197	779	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			858	547	147	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	5	0
			731	451	129	145	6			
6	S	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	S	0	5	0
			690	445	130	114	1			
7	T	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	1	0
			665	418	122	120	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	1	0
			605	392	107	102	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	1	0
			462	297	78	84	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	3	0
			390	254	65	69	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

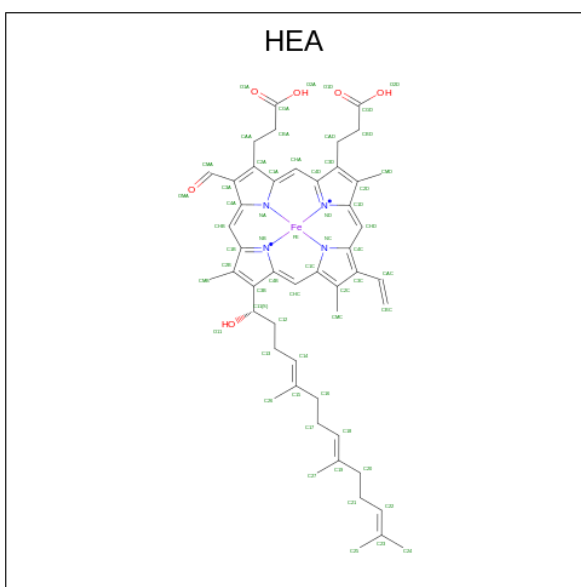
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	2	0
			386	259	64	60	3			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			336	223	53	60			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

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

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

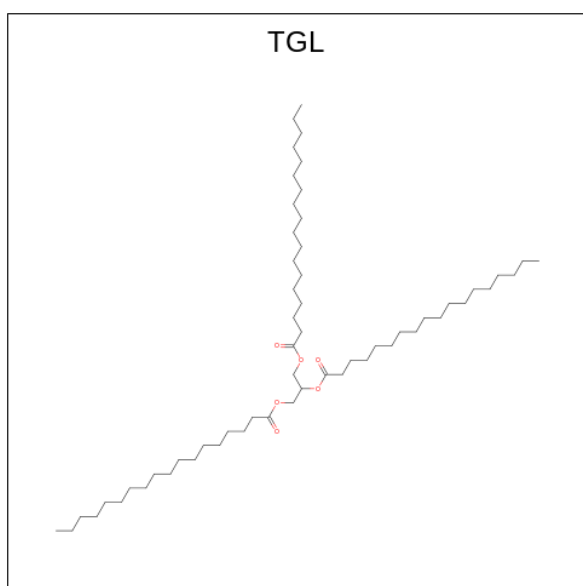
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

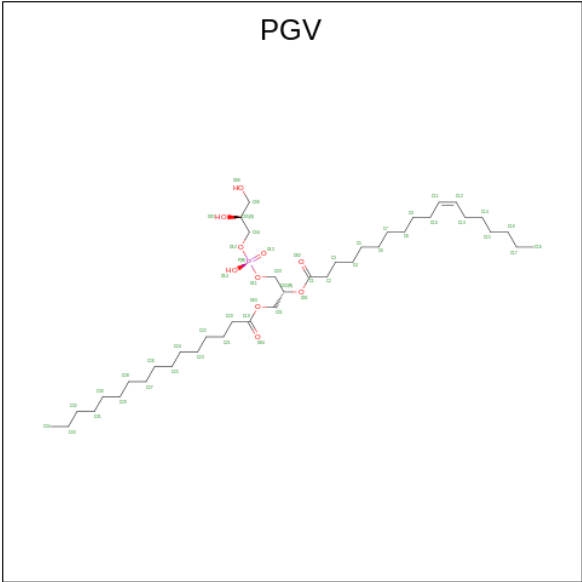
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



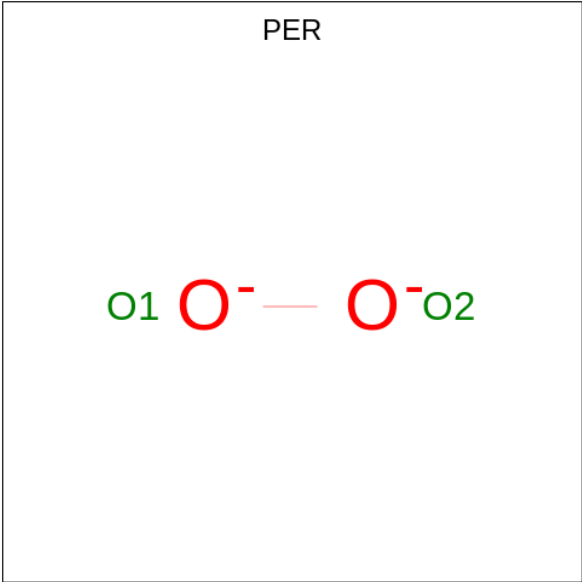
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	A	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			55	53	2		
18	N	1	Total	C	O	0	0
			55	53	2		

- 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: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



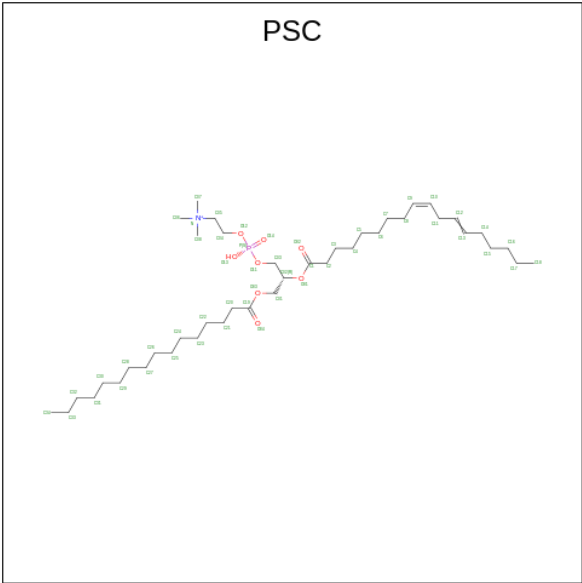
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 34 32 2	0	0
19	A	1	Total C O P 51 40 10 1	0	0
19	C	1	Total C O P 48 37 10 1	0	0
19	C	1	Total C O 36 32 4	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	P	1	Total C O P 51 40 10 1	0	0
19	P	1	Total C O 31 29 2	0	0

- Molecule 20 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



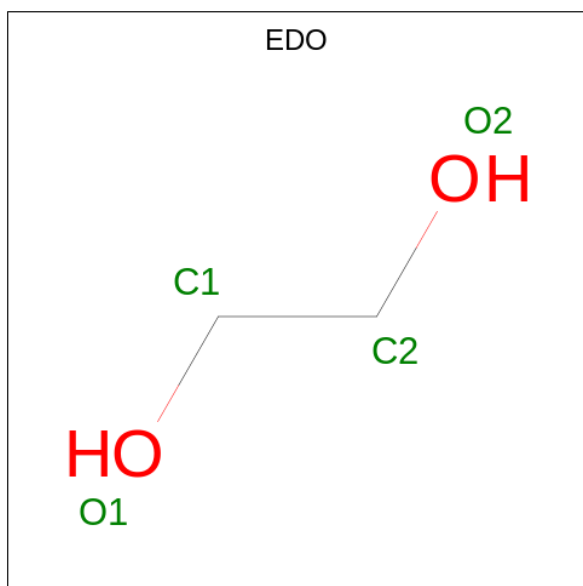
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	C	0	0
			25	25		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			31	29	2		

- Molecule 22 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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

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

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

- 
- The chemical structure of DMU (1,3-bis(4-hydroxyphenyl)urea) is shown. The molecule consists of a central urea group (-NH-CO-NH-) linked to two 4-hydroxyphenyl rings. The atoms are labeled as follows: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814, C815, C816, C817, C818, C819, C820, C821, C822,

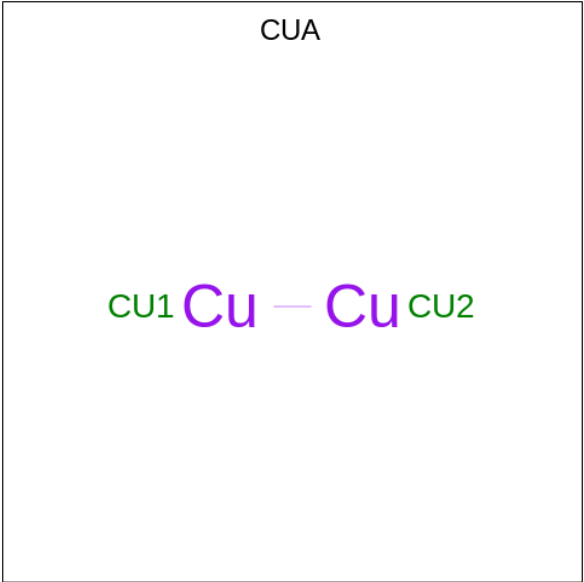
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total 11	C 10	O 1	0	0
23	C	1	Total 33	C 22	O 11	0	0
23	C	1	Total 12	C 11	O 1	0	0
23	D	1	Total 33	C 22	O 11	0	0

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

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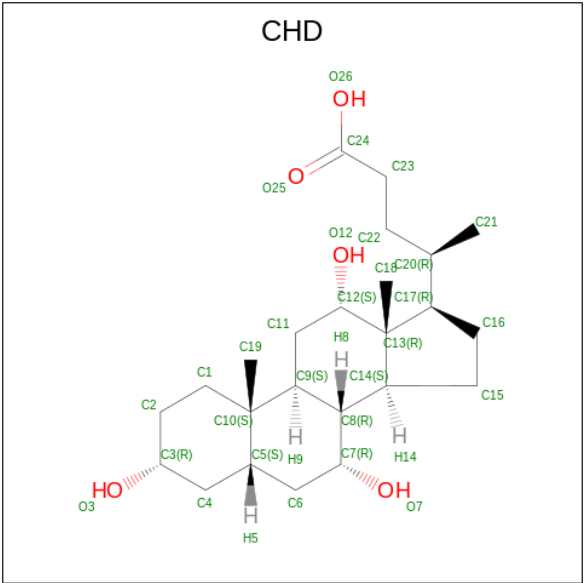
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D	1	Total C O 11 10 1	0	0
23	J	1	Total C O 11 10 1	0	0
23	K	1	Total C 8 8	0	0
23	K	1	Total C O 11 10 1	0	0
23	K	1	Total C 10 10	0	0
23	K	1	Total C O 11 10 1	0	0
23	K	1	Total C 9 9	0	0
23	L	1	Total C O 21 16 5	0	0
23	M	1	Total C O 33 22 11	0	0
23	O	1	Total C O 13 11 2	0	0
23	P	1	Total C O 33 22 11	0	0
23	P	1	Total C O 21 16 5	0	0
23	P	1	Total C O 32 21 11	0	0
23	Q	1	Total C O 11 10 1	0	0
23	X	1	Total C 10 10	0	0
23	X	1	Total C 9 9	0	0
23	X	1	Total C 9 9	0	0
23	X	1	Total C O 22 16 6	0	0
23	Z	1	Total C O 33 22 11	0	0

- Molecule 24 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 25 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



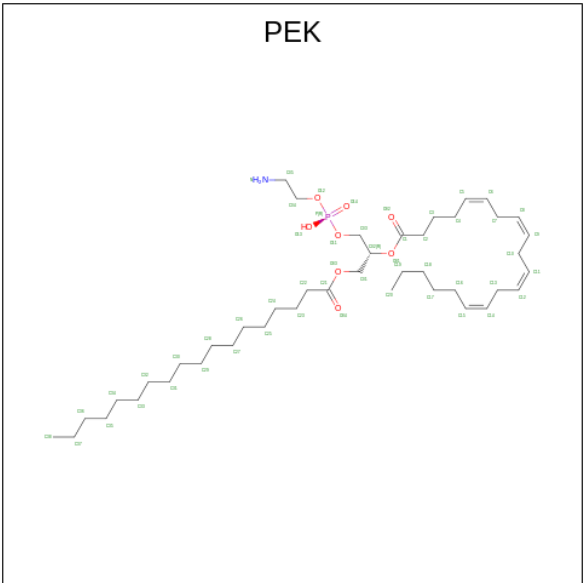
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			29	24	5		
25	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



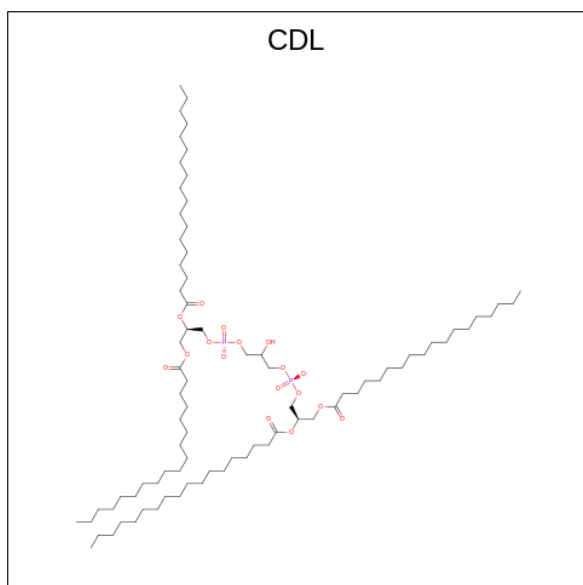
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
26	C	1	Total	C	N	O	P	0	0	
			45	35	1	8	1			
26	C	1	Total	C	N	O	P	0	0	
			52	42	1	8	1			
26	C	1	Total		C				0	0
			36		36					
26	P	1	Total	C	N	O	P	0	0	
			38	28	1	8	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	P	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	T	1	Total	C	O			0	0
			37	35	2				

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).

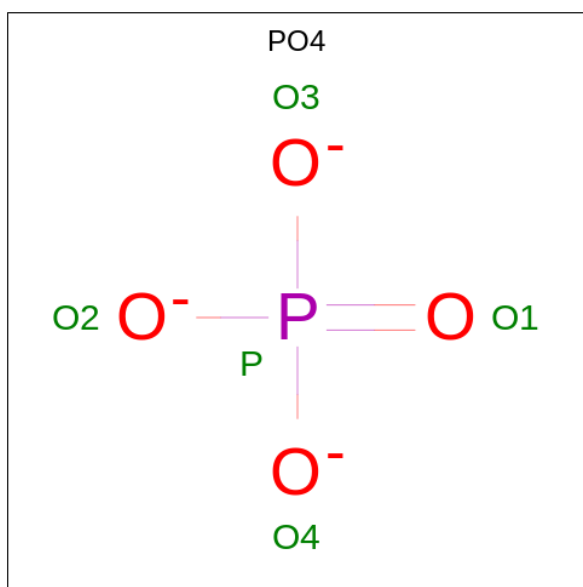


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			65	61	4		
27	N	1	Total	C	O	0	0
			62	60	2		
27	P	1	Total	C	O	0	0
			68	64	4		
27	T	1	Total	C	O	0	0
			61	59	2		

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

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

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	274	Total	O	0	14
			274	274		
30	B	229	Total	O	0	4
			229	229		
30	C	153	Total	O	0	0
			153	153		
30	D	206	Total	O	0	2
			207	207		
30	E	162	Total	O	0	0
			162	162		
30	F	161	Total	O	0	0
			161	161		
30	G	87	Total	O	0	0
			87	87		
30	H	92	Total	O	0	0
			92	92		
30	I	71	Total	O	0	0
			71	71		
30	J	61	Total	O	0	0
			61	61		

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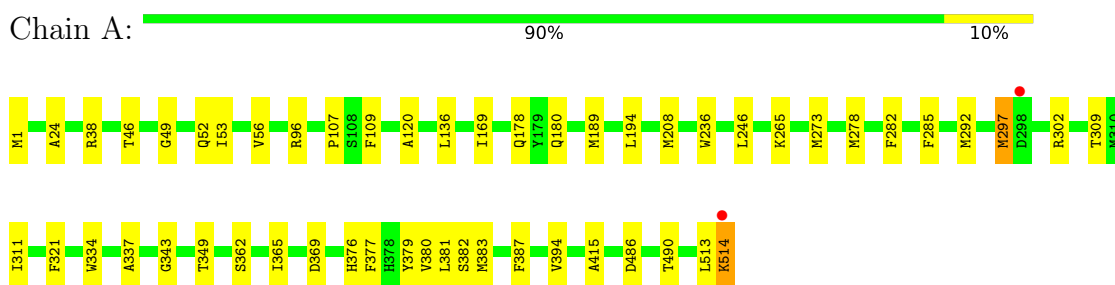
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	45	Total 45	O 45	0	0
30	L	40	Total 40	O 40	0	1
30	M	37	Total 37	O 37	0	0
30	N	282	Total 282	O 282	0	10
30	O	199	Total 199	O 199	0	2
30	P	161	Total 161	O 161	0	3
30	Q	119	Total 119	O 119	0	0
30	R	112	Total 113	O 113	0	1
30	S	141	Total 141	O 141	0	0
30	T	66	Total 66	O 66	0	0
30	U	96	Total 96	O 96	0	0
30	V	65	Total 66	O 66	0	1
30	W	41	Total 41	O 41	0	0
30	X	33	Total 33	O 33	0	0
30	Y	31	Total 31	O 31	0	1
30	Z	28	Total 28	O 28	0	0

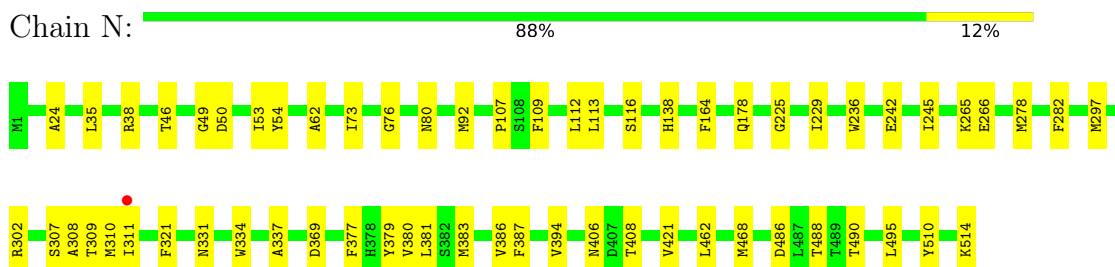
### 3 Residue-property plots

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

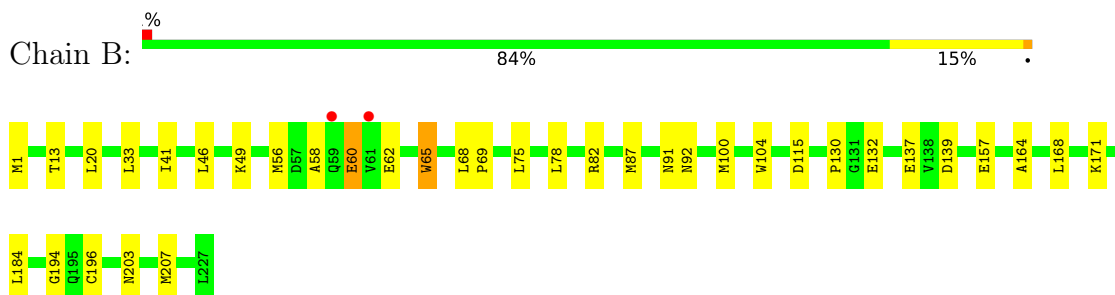
#### • Molecule 1: Cytochrome c oxidase subunit 1



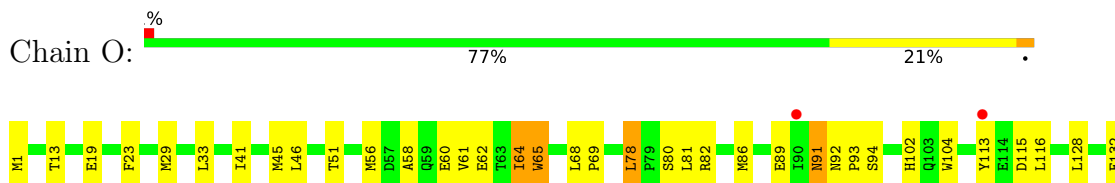
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • Molecule 2: Cytochrome c oxidase subunit 2

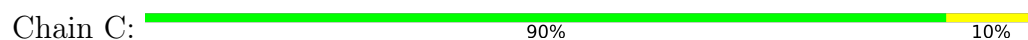


#### • Molecule 2: Cytochrome c oxidase subunit 2

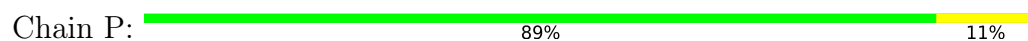




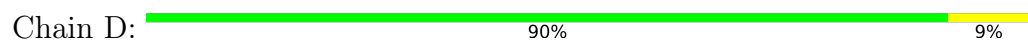
- Molecule 3: Cytochrome c oxidase subunit 3



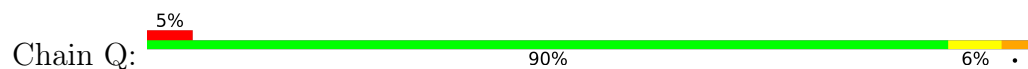
- Molecule 3: Cytochrome c oxidase subunit 3



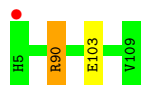
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



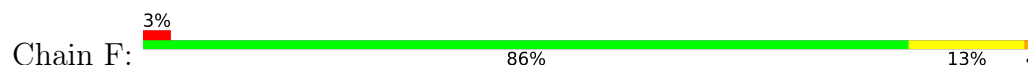
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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

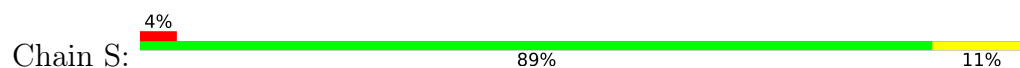


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

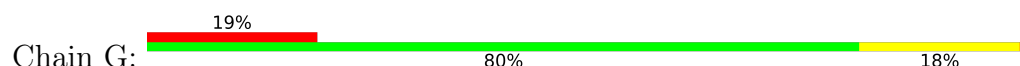




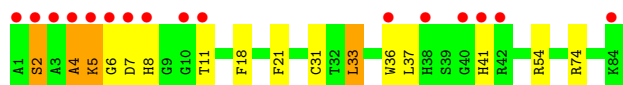
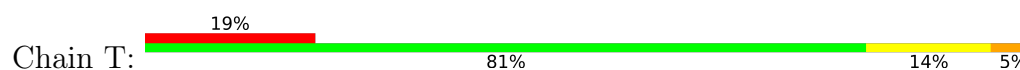
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



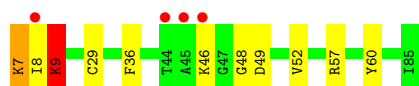
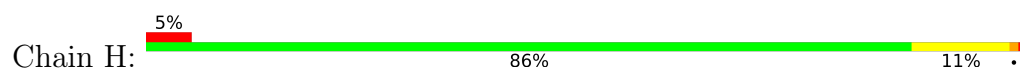
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



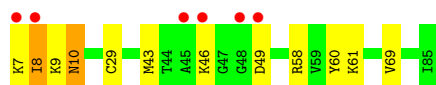
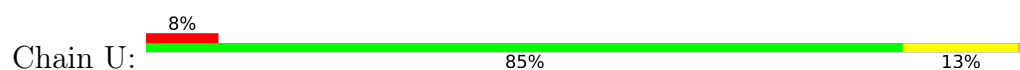
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1



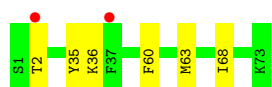
- Molecule 8: Cytochrome c oxidase subunit 6B1



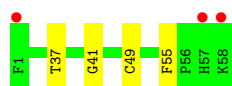
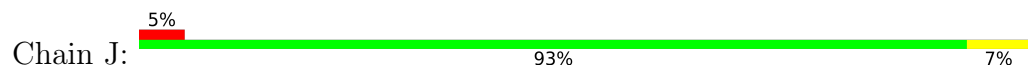
- Molecule 9: Cytochrome c oxidase subunit 6C



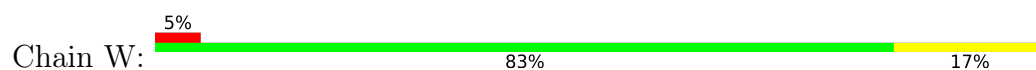
- Molecule 9: Cytochrome c oxidase subunit 6C



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



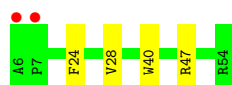
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



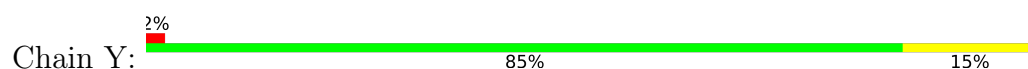
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial




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

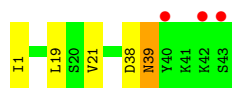


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial




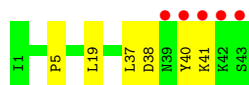
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  7% 88% 9% .



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

Chain Z:  12% 86% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.44Å 203.09Å 177.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.84 133.77 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-1.84) 99.8 (133.77-1.84)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.154 , 0.184 0.154 , 0.184	Depositor DCC
$R_{free}$ test set	28294 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 82.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CDL, PER, FME, PO4, PEK, NA, EDO, CUA, CU, PGV, TGL, ZN, HEA, PSC, MG, DMU, SAC, CHD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.81	0/4432	0.78	3/6043 (0.0%)
1	N	0.76	0/4457	0.74	1/6082 (0.0%)
2	B	0.74	0/1928	0.80	2/2623 (0.1%)
2	O	0.62	0/1973	0.76	2/2686 (0.1%)
3	C	0.73	2/2288 (0.1%)	0.67	0/3125
3	P	0.69	0/2287	0.65	0/3124
4	D	0.68	0/1259	0.68	0/1698
4	Q	0.48	0/1236	0.59	0/1668
5	E	0.62	0/871	0.71	0/1182
5	R	0.52	0/882	0.62	0/1196
6	F	0.67	0/773	0.70	0/1048
6	S	0.68	0/732	0.72	0/993
7	G	0.63	0/743	0.70	0/1009
7	T	0.53	0/699	0.73	1/950 (0.1%)
8	H	0.64	0/690	0.66	0/932
8	U	0.60	1/682 (0.1%)	0.69	0/921
9	I	0.52	0/614	0.63	0/814
9	V	0.48	0/605	0.62	0/802
10	J	0.52	0/478	0.60	0/644
10	W	0.47	0/472	0.59	0/636
11	K	0.57	0/419	0.65	1/574 (0.2%)
11	X	0.50	0/398	0.57	0/544
12	L	0.67	0/409	0.62	0/547
12	Y	0.58	0/393	0.60	0/526
13	M	0.69	0/346	0.66	0/470
13	Z	0.54	0/345	0.60	0/470
All	All	0.68	3/30411 (0.0%)	0.71	10/41307 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246[A]	ASP	CB-CG	6.16	1.64	1.51
3	C	246[B]	ASP	CB-CG	6.16	1.64	1.51
8	U	69	VAL	CB-CG1	5.04	1.63	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	MET	CG-SD-CE	-7.68	87.90	100.20
1	N	310	MET	CG-SD-CE	-7.37	88.41	100.20
2	O	65[A]	TRP	CA-CB-CG	6.37	125.81	113.70
2	O	65[B]	TRP	CA-CB-CG	6.37	125.81	113.70
1	A	96	ARG	NE-CZ-NH2	-6.24	117.18	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	51	0
1	N	4199	0	4190	58	0
2	B	1851	0	1858	22	0
2	O	1872	0	1876	29	0
3	C	2144	0	2062	24	0
3	P	2143	0	2069	24	0
4	D	1209	0	1202	14	0
4	Q	1197	0	1188	11	0
5	E	852	0	845	1	0
5	R	858	0	854	5	0
6	F	731	0	709	13	0
6	S	716	0	697	8	0
7	G	690	0	669	10	0
7	T	672	0	645	13	0
8	H	665	0	625	6	0
8	U	662	0	623	7	0
9	I	605	0	615	2	0
9	V	601	0	613	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	462	0	460	5	0
10	W	461	0	459	5	0
11	K	390	0	377	6	0
11	X	384	0	366	3	0
12	L	386	0	392	19	0
12	Y	380	0	380	5	0
13	M	336	0	352	7	0
13	Z	335	0	352	5	0
14	A	141	0	115	9	0
14	N	141	0	115	10	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	126	0	220	17	0
18	L	63	0	110	15	0
18	N	173	0	312	11	0
19	A	85	0	136	2	0
19	C	84	0	121	3	0
19	N	102	0	152	4	0
19	P	82	0	130	2	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	A	25	0	44	3	0
21	O	31	0	52	4	0
22	A	44	0	66	5	0
22	B	16	0	24	0	0
22	C	40	0	60	2	0
22	D	20	0	30	5	0
22	E	12	0	18	0	0
22	F	32	0	48	0	0
22	G	4	0	6	0	0
22	J	8	0	12	0	0
22	L	8	0	12	0	0
22	M	4	0	6	0	0
22	N	40	0	60	2	0
22	O	12	0	18	0	0
22	P	28	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Q	4	0	6	0	0
22	S	24	0	36	1	0
22	T	12	0	18	0	0
22	W	8	0	12	0	0
22	Y	4	0	6	1	0
23	A	11	0	21	0	0
23	C	45	0	63	3	0
23	D	44	0	63	3	0
23	J	11	0	21	1	0
23	K	49	0	93	2	0
23	L	21	0	30	6	0
23	M	33	0	42	2	0
23	O	13	0	21	0	0
23	P	86	0	109	5	0
23	Q	11	0	21	2	0
23	X	50	0	84	2	0
23	Z	33	0	42	1	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	B	29	0	39	0	0
25	C	58	0	78	2	0
25	G	29	0	39	1	0
25	J	29	0	39	2	0
25	L	29	0	39	2	0
25	P	29	0	39	0	0
25	Y	29	0	39	0	0
26	C	133	0	192	7	0
26	P	90	0	116	2	0
26	T	37	0	59	6	0
27	C	65	0	113	7	0
27	N	62	0	109	5	0
27	P	68	0	119	7	0
27	T	61	0	110	9	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	274	0	0	7	0
30	B	229	0	0	1	0
30	C	153	0	0	5	0
30	D	207	0	0	0	0
30	E	162	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	F	161	0	0	2	0
30	G	87	0	0	1	0
30	H	92	0	0	0	0
30	I	71	0	0	1	0
30	J	61	0	0	0	0
30	K	45	0	0	0	0
30	L	40	0	0	2	0
30	M	37	0	0	0	0
30	N	282	0	0	7	0
30	O	199	0	0	1	0
30	P	161	0	0	0	0
30	Q	119	0	0	2	0
30	R	113	0	0	1	0
30	S	141	0	0	2	0
30	T	66	0	0	1	0
30	U	96	0	0	1	0
30	V	66	0	0	0	0
30	W	41	0	0	0	0
30	X	33	0	0	0	0
30	Y	31	0	0	0	0
30	Z	28	0	0	0	0
All	All	34545	0	32367	372	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 372 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:609[A]:PER:O2	20:A:609[A]:PER:O1	1.55	1.24
20:N:611[A]:PER:O2	20:N:611[A]:PER:O1	1.55	1.21
12:L:20:ARG:HH22	18:L:101:TGL:HC52	1.31	0.95
1:N:113:LEU:HB2	18:N:608:TGL:H301	1.58	0.85
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.16	0.85

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	548/514 (107%)	529 (96%)	19 (4%)	0	100	100
1	N	553/514 (108%)	534 (97%)	19 (3%)	0	100	100
2	B	233/227 (103%)	227 (97%)	5 (2%)	1 (0%)	34	20
2	O	237/227 (104%)	230 (97%)	5 (2%)	2 (1%)	19	7
3	C	268/259 (104%)	263 (98%)	5 (2%)	0	100	100
3	P	268/259 (104%)	263 (98%)	5 (2%)	0	100	100
4	D	145/144 (101%)	142 (98%)	3 (2%)	0	100	100
4	Q	143/144 (99%)	138 (96%)	3 (2%)	2 (1%)	11	3
5	E	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
5	R	104/105 (99%)	103 (99%)	1 (1%)	0	100	100
6	F	97/94 (103%)	95 (98%)	2 (2%)	0	100	100
6	S	92/94 (98%)	90 (98%)	1 (1%)	1 (1%)	14	4
7	G	87/84 (104%)	77 (88%)	8 (9%)	2 (2%)	6	1
7	T	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	2	0
8	H	78/79 (99%)	73 (94%)	3 (4%)	2 (3%)	5	0
8	U	77/79 (98%)	72 (94%)	3 (4%)	2 (3%)	5	0
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	57/58 (98%)	57 (100%)	0	0	100	100
10	W	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
11	K	50/49 (102%)	49 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	46/46 (100%)	44 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
All	All	3640/3550 (102%)	3522 (97%)	102 (3%)	16 (0%)	34	20

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	T	2	SER
8	U	8	ILE
6	S	2	SER
8	H	9	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/426 (108%)	445 (97%)	13 (3%)	43	26
1	N	463/426 (109%)	459 (99%)	4 (1%)	78	71
2	B	218/210 (104%)	207 (95%)	11 (5%)	24	8
2	O	221/210 (105%)	209 (95%)	12 (5%)	22	7
3	C	235/224 (105%)	230 (98%)	5 (2%)	53	38
3	P	235/224 (105%)	231 (98%)	4 (2%)	60	47
4	D	131/128 (102%)	128 (98%)	3 (2%)	50	34
4	Q	129/128 (101%)	124 (96%)	5 (4%)	32	14
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	64
5	R	93/92 (101%)	93 (100%)	0	100	100
6	F	83/78 (106%)	80 (96%)	3 (4%)	35	17
6	S	78/78 (100%)	78 (100%)	0	100	100
7	G	73/68 (107%)	63 (86%)	10 (14%)	3	0
7	T	68/68 (100%)	61 (90%)	7 (10%)	7	1
8	H	72/71 (101%)	68 (94%)	4 (6%)	21	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/71 (100%)	68 (96%)	3 (4%)	30	12
9	I	58/57 (102%)	57 (98%)	1 (2%)	60	47
9	V	57/57 (100%)	56 (98%)	1 (2%)	59	44
10	J	50/49 (102%)	50 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	13
11	K	42/39 (108%)	41 (98%)	1 (2%)	49	32
11	X	39/39 (100%)	38 (97%)	1 (3%)	46	29
12	L	41/39 (105%)	40 (98%)	1 (2%)	49	32
12	Y	39/39 (100%)	37 (95%)	2 (5%)	24	8
13	M	37/37 (100%)	35 (95%)	2 (5%)	22	7
13	Z	37/37 (100%)	36 (97%)	1 (3%)	44	28
All	All	3169/3036 (104%)	3072 (97%)	97 (3%)	42	23

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	138	HIS
3	P	3	HIS
2	O	33	LEU
2	O	94	SER
4	Q	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	195	GLN
3	P	158	HIS
8	U	31	GLN
4	Q	109	HIS
7	T	8	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SAC	I	1	9	7,8,9	0.63	0	8,9,11	1.02	1 (12%)
9	SAC	V	1	9	7,8,9	0.60	0	8,9,11	0.80	0
2	FME	B	1	2	8,9,10	0.76	0	7,9,11	2.24	1 (14%)
1	FME	A	1	1	8,9,10	0.43	0	7,9,11	1.47	2 (28%)
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	1.53	2 (28%)
1	FME	N	1	1	8,9,10	0.43	0	7,9,11	1.31	0

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

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

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.65	100.04	112.95
2	O	1	FME	CG-CB-CA	-3.17	104.15	112.95
1	A	1	FME	C-CA-N	2.40	114.06	109.73
9	I	1	SAC	O-C-CA	-2.16	119.11	124.78
1	A	1	FME	O1-CN-N	-2.12	119.69	125.27

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 10 are monoatomic - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
23	DMU	Q	201	-	10,10,34	0.36	0	9,9,45	0.36	0
22	EDO	P	315	-	3,3,3	0.53	0	2,2,2	0.13	0
22	EDO	N	615	-	3,3,3	0.54	0	2,2,2	0.34	0
22	EDO	O	305	-	3,3,3	0.55	0	2,2,2	0.11	0
14	HEA	N	602[A]	-	44,67,67	0.95	2 (4%)	37,103,103	2.02	7 (18%)
25	CHD	B	302	-	29,32,32	0.81	0	48,51,51	1.40	6 (12%)
26	PEK	C	303	-	44,44,52	1.21	2 (4%)	47,49,57	1.41	8 (17%)
18	TGL	L	101	-	62,62,62	1.12	3 (4%)	65,65,65	1.39	7 (10%)
22	EDO	S	103	-	3,3,3	0.59	0	2,2,2	0.12	0
22	EDO	F	103	-	3,3,3	0.47	0	2,2,2	0.52	0
23	DMU	D	207	-	10,10,34	0.33	0	9,9,45	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	TGL	N	608	-	52,52,62	0.73	1 (1%)	50,50,65	0.88	2 (4%)
22	EDO	F	106	-	3,3,3	0.61	0	2,2,2	0.54	0
22	EDO	N	617	-	3,3,3	0.46	0	2,2,2	0.15	0
22	EDO	A	612	-	3,3,3	0.71	0	2,2,2	0.35	0
22	EDO	A	614	-	3,3,3	0.45	0	2,2,2	0.28	0
14	HEA	N	603	20,1,30	44,67,67	1.03	2 (4%)	37,103,103	1.61	10 (27%)
24	CUA	B	301	2	0,1,1	0.00	-	-		
22	EDO	S	106	-	3,3,3	0.37	0	2,2,2	0.91	0
22	EDO	W	101	-	3,3,3	0.38	0	2,2,2	0.45	0
25	CHD	L	102	-	29,32,32	0.63	0	48,51,51	2.49	23 (47%)
22	EDO	T	104	-	3,3,3	0.49	0	2,2,2	0.28	0
23	DMU	C	321	-	11,11,34	0.40	0	10,10,45	0.32	0
25	CHD	C	309	-	29,32,32	0.69	0	48,51,51	1.30	7 (14%)
22	EDO	Y	101	-	3,3,3	0.46	0	2,2,2	0.17	0
22	EDO	B	306	-	3,3,3	0.57	0	2,2,2	0.32	0
22	EDO	A	620	-	3,3,3	0.67	0	2,2,2	0.14	0
23	DMU	L	105	-	21,21,34	0.90	1 (4%)	24,25,45	2.08	5 (20%)
22	EDO	A	613	-	3,3,3	0.79	0	2,2,2	0.68	0
22	EDO	P	309	-	3,3,3	0.53	0	2,2,2	0.21	0
22	EDO	A	622	-	3,3,3	0.56	0	2,2,2	0.61	0
22	EDO	B	303	-	3,3,3	0.72	0	2,2,2	0.30	0
25	CHD	P	301	-	29,32,32	0.64	0	48,51,51	1.42	10 (20%)
20	PER	A	609[A]	15,14	0,1,1	0.00	-	-		
14	HEA	A	602	20,1,30	44,67,67	1.00	2 (4%)	37,103,103	1.89	14 (37%)
22	EDO	N	621	-	3,3,3	0.34	0	2,2,2	0.50	0
22	EDO	J	102	-	3,3,3	0.51	0	2,2,2	0.16	0
27	CDL	N	601	-	58,58,99	1.30	9 (15%)	55,55,111	0.98	4 (7%)
22	EDO	M	102	-	3,3,3	0.45	0	2,2,2	0.34	0
18	TGL	A	607	-	62,62,62	1.08	3 (4%)	65,65,65	1.11	6 (9%)
19	PGV	N	610	-	50,50,50	0.96	2 (4%)	53,56,56	1.06	3 (5%)
22	EDO	A	617	-	3,3,3	0.50	0	2,2,2	0.59	0
23	DMU	Z	101	-	34,34,34	0.46	0	45,45,45	0.82	2 (4%)
22	EDO	P	313	-	3,3,3	0.43	0	2,2,2	0.97	0
22	EDO	A	621	-	3,3,3	0.61	0	2,2,2	0.51	0
19	PGV	A	608	-	31,31,50	0.41	0	29,29,56	0.58	0
22	EDO	E	203	-	3,3,3	0.46	0	2,2,2	0.40	0
27	CDL	T	102	-	57,57,99	1.26	8 (14%)	54,54,111	0.87	1 (1%)
23	DMU	D	206	-	34,34,34	0.70	1 (2%)	45,45,45	1.40	8 (17%)
29	PO4	H	101	-	4,4,4	0.75	0	6,6,6	0.74	0
21	PSC	O	302	-	27,27,51	0.77	1 (3%)	25,25,59	0.72	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	N	614	-	3,3,3	0.65	0	2,2,2	0.18	0
23	DMU	X	102	-	8,8,34	0.29	0	7,7,45	0.48	0
26	PEK	C	305	-	34,34,52	0.32	0	32,32,57	0.58	0
27	CDL	C	308	-	62,62,99	1.32	8 (12%)	61,61,111	1.41	11 (18%)
19	PGV	C	307	-	35,35,50	1.31	2 (5%)	37,37,56	1.95	9 (24%)
22	EDO	D	203	-	3,3,3	0.50	0	2,2,2	0.22	0
22	EDO	N	620	-	3,3,3	0.58	0	2,2,2	0.15	0
22	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.53	0
22	EDO	S	105	-	3,3,3	0.64	0	2,2,2	0.71	0
22	EDO	T	105	-	3,3,3	0.62	0	2,2,2	0.32	0
22	EDO	W	102	-	3,3,3	0.49	0	2,2,2	0.45	0
22	EDO	S	107	-	3,3,3	0.52	0	2,2,2	0.58	0
22	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.17	0
29	PO4	U	101	-	4,4,4	1.06	0	6,6,6	0.56	0
22	EDO	G	102	-	3,3,3	0.83	0	2,2,2	0.50	0
21	PSC	A	610	-	23,23,51	0.84	1 (4%)	20,21,59	0.79	0
22	EDO	C	312	-	3,3,3	0.63	0	2,2,2	0.34	0
22	EDO	P	311	-	3,3,3	0.70	0	2,2,2	0.18	0
22	EDO	J	103	-	3,3,3	0.36	0	2,2,2	0.76	0
22	EDO	C	317	-	3,3,3	0.54	0	2,2,2	0.15	0
22	EDO	F	102	-	3,3,3	0.56	0	2,2,2	0.43	0
26	PEK	C	304	-	51,51,52	0.80	2 (3%)	54,56,57	1.16	4 (7%)
22	EDO	D	202	-	3,3,3	0.50	0	2,2,2	0.31	0
22	EDO	N	613	-	3,3,3	0.63	0	2,2,2	0.64	0
24	CUA	O	301	2	0,1,1	0.00	-	-	-	-
23	DMU	M	101	-	34,34,34	0.44	0	45,45,45	1.03	1 (2%)
22	EDO	A	618	-	3,3,3	0.75	0	2,2,2	0.29	0
22	EDO	L	104	-	3,3,3	0.59	0	2,2,2	0.49	0
25	CHD	C	301	-	29,32,32	0.59	0	48,51,51	1.60	9 (18%)
19	PGV	C	306	-	47,47,50	0.84	2 (4%)	50,53,56	0.90	3 (6%)
22	EDO	T	103	-	3,3,3	0.73	0	2,2,2	0.36	0
22	EDO	A	619	-	3,3,3	0.48	0	2,2,2	0.16	0
22	EDO	F	107	-	3,3,3	0.50	0	2,2,2	0.38	0
25	CHD	J	101	-	29,32,32	0.63	0	48,51,51	2.82	18 (37%)
19	PGV	P	306	-	26,29,50	0.40	0	24,28,56	0.58	0
19	PGV	P	305	-	50,50,50	0.76	2 (4%)	53,56,56	1.00	1 (1%)
22	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.50	0
22	EDO	P	312	-	3,3,3	0.44	0	2,2,2	0.97	0
22	EDO	P	310	-	3,3,3	0.54	0	2,2,2	0.19	0
23	DMU	K	101	-	7,7,34	0.25	0	6,6,45	0.37	0
22	EDO	O	303	-	3,3,3	0.76	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	C	313	-	3,3,3	0.80	0	2,2,2	0.35	0
22	EDO	Q	202	-	3,3,3	0.54	0	2,2,2	0.39	0
22	EDO	F	109	-	3,3,3	0.61	0	2,2,2	0.75	0
23	DMU	O	306	-	11,11,34	0.22	0	9,9,45	0.65	0
18	TGL	N	609	-	52,52,62	0.69	1 (1%)	50,50,65	0.69	2 (4%)
22	EDO	C	318	-	3,3,3	0.56	0	2,2,2	0.35	0
23	DMU	C	310	-	34,34,34	0.55	1 (2%)	45,45,45	1.20	6 (13%)
22	EDO	N	618	-	3,3,3	0.53	0	2,2,2	0.32	0
20	PER	N	611[A]	15,14	0,1,1	0.00	-	-		
23	DMU	X	101	-	9,9,34	0.31	0	8,8,45	0.51	0
25	CHD	Y	102	-	29,32,32	0.62	0	48,51,51	2.25	16 (33%)
23	DMU	K	104	-	10,10,34	0.25	0	9,9,45	0.52	0
23	DMU	J	104	-	10,10,34	0.33	0	9,9,45	0.41	0
22	EDO	L	103	-	3,3,3	0.24	0	2,2,2	1.02	0
26	PEK	P	304	-	51,51,52	0.77	2 (3%)	54,56,57	1.07	4 (7%)
18	TGL	N	607	-	62,62,62	1.04	3 (4%)	65,65,65	1.20	4 (6%)
22	EDO	N	616	-	3,3,3	0.40	0	2,2,2	0.69	0
22	EDO	F	105	-	3,3,3	0.62	0	2,2,2	0.23	0
22	EDO	E	201	-	3,3,3	0.56	0	2,2,2	0.25	0
23	DMU	P	308	-	34,34,34	0.51	0	45,45,45	1.21	7 (15%)
23	DMU	P	316	-	21,21,34	0.61	1 (4%)	24,25,45	0.81	1 (4%)
22	EDO	P	314	-	3,3,3	0.57	0	2,2,2	0.14	0
23	DMU	K	105	-	8,8,34	0.30	0	7,7,45	0.57	0
23	DMU	X	103	-	8,8,34	0.30	0	7,7,45	0.61	0
19	PGV	A	611	-	50,50,50	0.90	3 (6%)	53,56,56	1.20	4 (7%)
22	EDO	B	305	-	3,3,3	0.71	0	2,2,2	0.10	0
22	EDO	C	315	-	3,3,3	0.56	0	2,2,2	0.18	0
22	EDO	D	201	-	3,3,3	0.57	0	2,2,2	0.29	0
22	EDO	S	104	-	3,3,3	0.49	0	2,2,2	0.77	0
22	EDO	D	204	-	3,3,3	0.50	0	2,2,2	0.46	0
23	DMU	X	104	-	22,22,34	0.57	1 (4%)	27,27,45	0.77	0
27	CDL	P	307	-	65,65,99	1.37	9 (13%)	64,64,111	1.24	6 (9%)
25	CHD	G	101	-	29,32,32	0.72	1 (3%)	48,51,51	1.14	3 (6%)
22	EDO	F	108	-	3,3,3	0.48	0	2,2,2	0.37	0
23	DMU	A	623	-	10,10,34	0.31	0	9,9,45	0.48	0
22	EDO	S	102	-	3,3,3	0.77	0	2,2,2	0.72	0
26	PEK	T	101	-	35,35,52	0.86	1 (2%)	34,34,57	1.07	3 (8%)
19	PGV	N	612	-	50,50,50	0.89	3 (6%)	53,56,56	1.12	6 (11%)
18	TGL	A	606	-	62,62,62	1.04	3 (4%)	65,65,65	1.28	5 (7%)
22	EDO	C	314	-	3,3,3	0.34	0	2,2,2	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	D	205	-	3,3,3	0.37	0	2,2,2	0.39	0
22	EDO	E	202	-	3,3,3	0.45	0	2,2,2	0.12	0
22	EDO	N	619	-	3,3,3	0.56	0	2,2,2	0.13	0
14	HEA	A	601[A]	-	44,67,67	1.11	2 (4%)	37,103,103	2.08	10 (27%)
22	EDO	A	615	-	3,3,3	0.68	0	2,2,2	0.98	0
22	EDO	O	304	-	3,3,3	0.65	0	2,2,2	0.08	0
22	EDO	C	316	-	3,3,3	0.38	0	2,2,2	0.35	0
23	DMU	K	102	-	10,10,34	0.34	0	9,9,45	0.62	0
22	EDO	C	319	-	3,3,3	0.60	0	2,2,2	0.31	0
23	DMU	P	317	-	33,33,34	0.73	1 (3%)	44,44,45	1.66	8 (18%)
22	EDO	N	622	-	3,3,3	0.75	0	2,2,2	0.28	0
23	DMU	K	103	-	9,9,34	0.34	0	8,8,45	0.34	0
22	EDO	F	104	-	3,3,3	0.58	0	2,2,2	0.33	0
22	EDO	C	320	-	3,3,3	0.71	0	2,2,2	0.45	0
26	PEK	P	303	-	37,37,52	1.14	2 (5%)	40,42,57	1.27	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	DMU	Q	201	-	-	4/8/8/59	-
22	EDO	P	315	-	-	0/1/1/1	-
22	EDO	N	615	-	-	0/1/1/1	-
22	EDO	O	305	-	-	0/1/1/1	-
14	HEA	N	602[A]	-	3/3/7/16	0/24/76/76	-
25	CHD	B	302	-	-	0/7/74/74	0/4/4/4
26	PEK	C	303	-	-	19/48/48/56	-
18	TGL	L	101	-	-	39/65/65/65	-
22	EDO	S	103	-	-	0/1/1/1	-
22	EDO	F	103	-	-	0/1/1/1	-
23	DMU	D	207	-	-	4/8/8/59	-
18	TGL	N	608	-	-	22/47/47/65	-
22	EDO	F	106	-	-	0/1/1/1	-
22	EDO	N	617	-	-	0/1/1/1	-
22	EDO	A	612	-	-	1/1/1/1	-
22	EDO	A	614	-	-	1/1/1/1	-
14	HEA	N	603	20,1,30	3/3/7/16	1/24/76/76	-
22	EDO	S	106	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	W	101	-	-	1/1/1/1	-
25	CHD	L	102	-	-	5/7/74/74	0/4/4/4
22	EDO	T	104	-	-	1/1/1/1	-
23	DMU	C	321	-	-	0/9/9/59	-
25	CHD	C	309	-	-	3/7/74/74	0/4/4/4
22	EDO	Y	101	-	-	0/1/1/1	-
22	EDO	B	306	-	-	0/1/1/1	-
22	EDO	A	620	-	-	1/1/1/1	-
23	DMU	L	105	-	-	8/13/29/59	0/1/1/2
22	EDO	A	613	-	-	0/1/1/1	-
22	EDO	P	309	-	-	0/1/1/1	-
22	EDO	A	622	-	-	0/1/1/1	-
22	EDO	B	303	-	-	0/1/1/1	-
25	CHD	P	301	-	-	0/7/74/74	0/4/4/4
14	HEA	A	602	20,1,30	3/3/7/16	0/24/76/76	-
22	EDO	N	621	-	-	0/1/1/1	-
22	EDO	J	102	-	-	1/1/1/1	-
27	CDL	N	601	-	-	16/51/51/110	-
22	EDO	M	102	-	-	1/1/1/1	-
18	TGL	A	607	-	-	26/65/65/65	-
19	PGV	N	610	-	-	14/55/55/55	-
22	EDO	A	617	-	-	1/1/1/1	-
23	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
22	EDO	P	313	-	-	1/1/1/1	-
22	EDO	A	621	-	-	0/1/1/1	-
19	PGV	A	608	-	-	9/26/27/55	-
22	EDO	E	203	-	-	0/1/1/1	-
27	CDL	T	102	-	-	18/50/50/110	-
23	DMU	D	206	-	-	6/19/59/59	0/2/2/2
21	PSC	O	302	-	-	5/23/23/55	-
22	EDO	N	614	-	-	0/1/1/1	-
23	DMU	X	102	-	-	2/6/6/59	-
26	PEK	C	305	-	-	13/30/30/56	-
27	CDL	C	308	-	-	17/55/58/110	-
19	PGV	C	307	-	-	16/36/36/55	-
22	EDO	D	203	-	-	0/1/1/1	-
22	EDO	N	620	-	-	0/1/1/1	-
22	EDO	B	304	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	S	105	-	-	0/1/1/1	-
22	EDO	T	105	-	-	1/1/1/1	-
22	EDO	W	102	-	-	1/1/1/1	-
22	EDO	S	107	-	-	0/1/1/1	-
22	EDO	C	311	-	-	0/1/1/1	-
22	EDO	G	102	-	-	0/1/1/1	-
21	PSC	A	610	-	-	11/19/19/55	-
22	EDO	C	312	-	-	0/1/1/1	-
22	EDO	P	311	-	-	0/1/1/1	-
22	EDO	J	103	-	-	1/1/1/1	-
22	EDO	C	317	-	-	0/1/1/1	-
22	EDO	F	102	-	-	0/1/1/1	-
26	PEK	C	304	-	-	17/55/55/56	-
22	EDO	D	202	-	-	1/1/1/1	-
22	EDO	N	613	-	-	0/1/1/1	-
23	DMU	M	101	-	-	4/19/59/59	0/2/2/2
22	EDO	A	618	-	-	1/1/1/1	-
22	EDO	L	104	-	-	1/1/1/1	-
25	CHD	C	301	-	-	0/7/74/74	0/4/4/4
19	PGV	C	306	-	-	13/52/52/55	-
22	EDO	T	103	-	-	0/1/1/1	-
22	EDO	A	619	-	-	1/1/1/1	-
22	EDO	F	107	-	-	0/1/1/1	-
25	CHD	J	101	-	-	6/7/74/74	0/4/4/4
19	PGV	P	306	-	-	5/23/25/55	-
19	PGV	P	305	-	-	6/55/55/55	-
22	EDO	A	616	-	-	0/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
22	EDO	P	310	-	-	0/1/1/1	-
23	DMU	K	101	-	-	1/5/5/59	-
22	EDO	O	303	-	-	0/1/1/1	-
22	EDO	C	313	-	-	0/1/1/1	-
14	HEA	A	601[C]	-	3/3/5/16	-	-
22	EDO	Q	202	-	-	0/1/1/1	-
22	EDO	F	109	-	-	0/1/1/1	-
23	DMU	O	306	-	-	1/8/8/59	-
18	TGL	N	609	-	-	20/47/47/65	-
22	EDO	C	318	-	-	0/1/1/1	-
23	DMU	C	310	-	-	3/19/59/59	0/2/2/2
22	EDO	N	618	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	DMU	X	101	-	-	2/7/7/59	-
25	CHD	Y	102	-	-	3/7/74/74	0/4/4/4
23	DMU	K	104	-	-	3/8/8/59	-
14	HEA	A	601[B]	-	3/3/5/16	-	-
23	DMU	J	104	-	-	2/8/8/59	-
22	EDO	L	103	-	-	1/1/1/1	-
26	PEK	P	304	-	-	10/55/55/56	-
18	TGL	N	607	-	-	31/65/65/65	-
22	EDO	N	616	-	-	0/1/1/1	-
14	HEA	N	602[C]	-	3/3/5/16	-	-
22	EDO	F	105	-	-	0/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
23	DMU	P	308	-	-	8/19/59/59	0/2/2/2
23	DMU	P	316	-	-	5/13/29/59	0/1/1/2
22	EDO	P	314	-	-	0/1/1/1	-
23	DMU	K	105	-	-	0/6/6/59	-
23	DMU	X	103	-	-	0/6/6/59	-
19	PGV	A	611	-	-	4/55/55/55	-
22	EDO	B	305	-	-	0/1/1/1	-
22	EDO	C	315	-	-	0/1/1/1	-
22	EDO	D	201	-	-	0/1/1/1	-
22	EDO	S	104	-	-	0/1/1/1	-
22	EDO	D	204	-	-	1/1/1/1	-
23	DMU	X	104	-	-	2/13/33/59	0/1/1/2
14	HEA	N	602[B]	-	3/3/5/16	-	-
27	CDL	P	307	-	-	27/61/61/110	-
25	CHD	G	101	-	-	0/7/74/74	0/4/4/4
22	EDO	F	108	-	-	1/1/1/1	-
23	DMU	A	623	-	-	0/8/8/59	-
22	EDO	S	102	-	-	0/1/1/1	-
26	PEK	T	101	-	-	14/32/32/56	-
19	PGV	N	612	-	-	6/55/55/55	-
18	TGL	A	606	-	-	37/65/65/65	-
22	EDO	C	314	-	-	0/1/1/1	-
22	EDO	D	205	-	-	1/1/1/1	-
22	EDO	E	202	-	-	1/1/1/1	-
22	EDO	N	619	-	-	1/1/1/1	-
14	HEA	A	601[A]	-	3/3/7/16	0/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	A	615	-	-	0/1/1/1	-
22	EDO	O	304	-	-	0/1/1/1	-
22	EDO	C	316	-	-	0/1/1/1	-
23	DMU	K	102	-	-	4/8/8/59	-
22	EDO	C	319	-	-	0/1/1/1	-
23	DMU	P	317	-	-	3/18/58/59	0/2/2/2
22	EDO	N	622	-	-	0/1/1/1	-
23	DMU	K	103	-	-	2/7/7/59	-
22	EDO	F	104	-	-	0/1/1/1	-
22	EDO	C	320	-	-	1/1/1/1	-
26	PEK	P	303	-	-	13/41/41/56	-

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	307	PGV	O03-C19	5.47	1.49	1.33
26	C	303	PEK	O03-C21	5.28	1.48	1.33
18	L	101	TGL	OG2-CB1	5.01	1.48	1.34
27	N	601	CDL	OB8-CB7	4.91	1.47	1.33
27	P	307	CDL	OB6-CB5	4.82	1.47	1.33

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	101	CHD	C10-C9-C8	7.54	119.92	111.82
25	J	101	CHD	C14-C8-C9	-7.45	99.48	109.71
25	J	101	CHD	C14-C8-C7	7.39	121.60	111.81
14	N	602[A]	HEA	C13-C12-C11	-7.03	103.78	114.35
18	A	606	TGL	OG2-CB1-CB2	6.40	125.30	111.50

5 of 24 chirality outliers are listed below:

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

5 of 543 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	607	TGL	OB1-CB1-OG2-CG2
18	L	101	TGL	CB2-CB1-OG2-CG2
18	L	101	TGL	OB1-CB1-OG2-CG2
18	N	609	TGL	CC2-CC1-OG3-CG3
19	A	608	PGV	C1-C2-C3-C4

There are no ring outliers.

64 monomers are involved in 173 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Q	201	DMU	2	0
14	N	602[A]	HEA	2	0
26	C	303	PEK	1	0
18	L	101	TGL	15	0
18	N	608	TGL	7	0
22	A	612	EDO	2	0
14	N	603	HEA	5	0
22	S	106	EDO	1	0
25	L	102	CHD	2	0
25	C	309	CHD	2	0
22	Y	101	EDO	1	0
22	A	620	EDO	1	0
23	L	105	DMU	6	0
20	A	609[A]	PER	1	0
14	A	602	HEA	5	0
22	N	621	EDO	1	0
27	N	601	CDL	5	0
18	A	607	TGL	13	0
19	N	610	PGV	3	0
23	Z	101	DMU	1	0
19	A	608	PGV	1	0
27	T	102	CDL	9	0
23	D	206	DMU	3	0
21	O	302	PSC	4	0
23	X	102	DMU	2	0
26	C	305	PEK	1	0
27	C	308	CDL	7	0
19	C	307	PGV	1	0
22	N	620	EDO	1	0
21	A	610	PSC	3	0
26	C	304	PEK	5	0
23	M	101	DMU	2	0
22	A	618	EDO	1	0

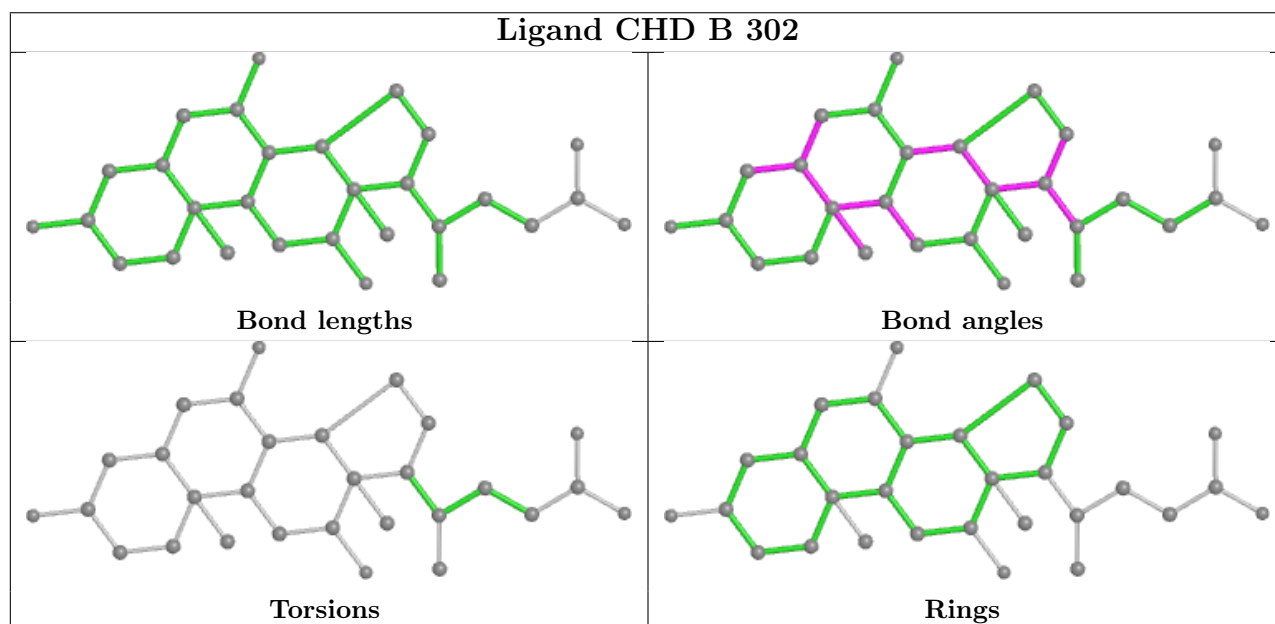
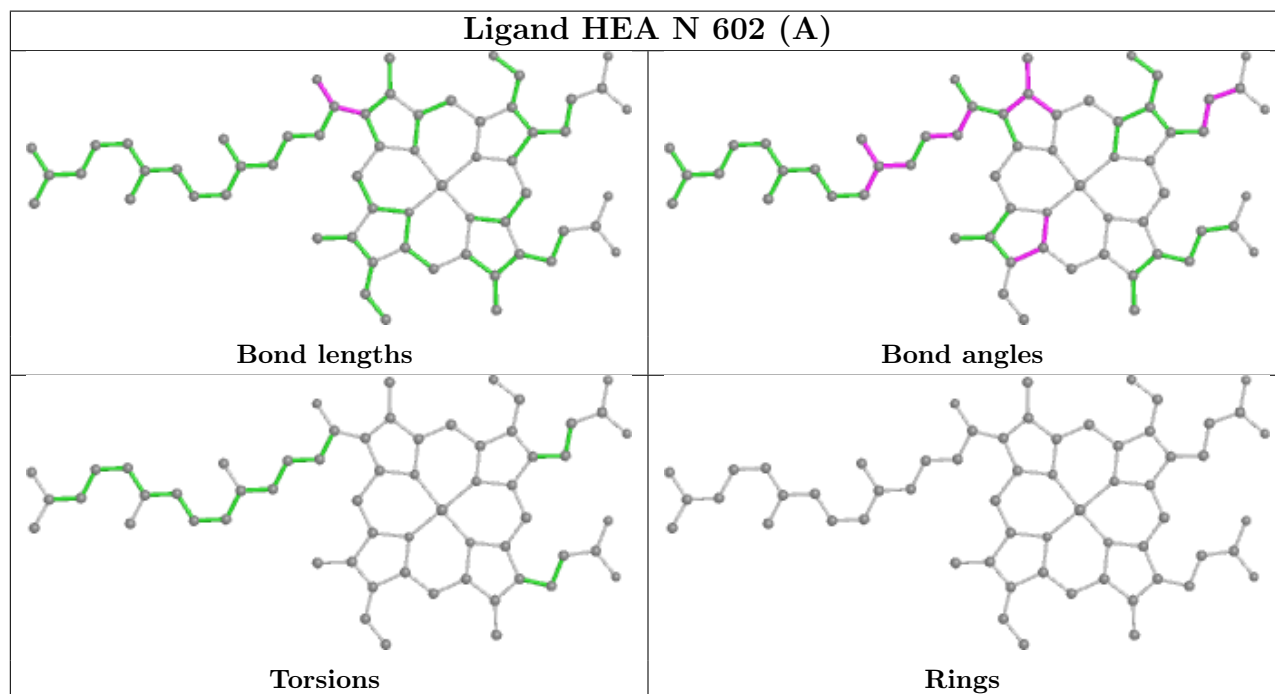
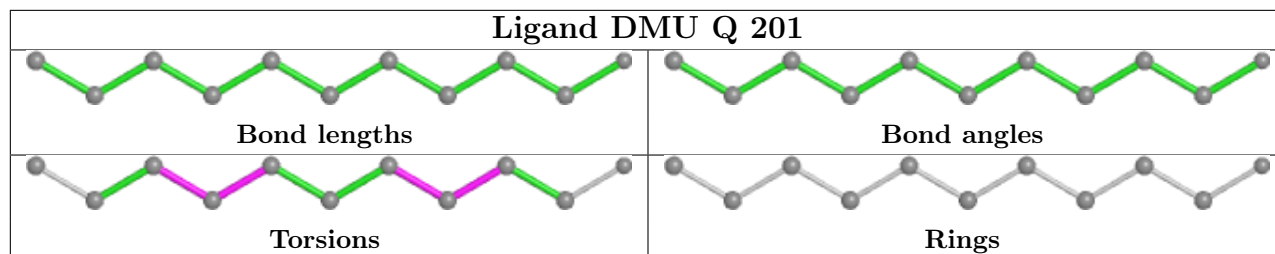
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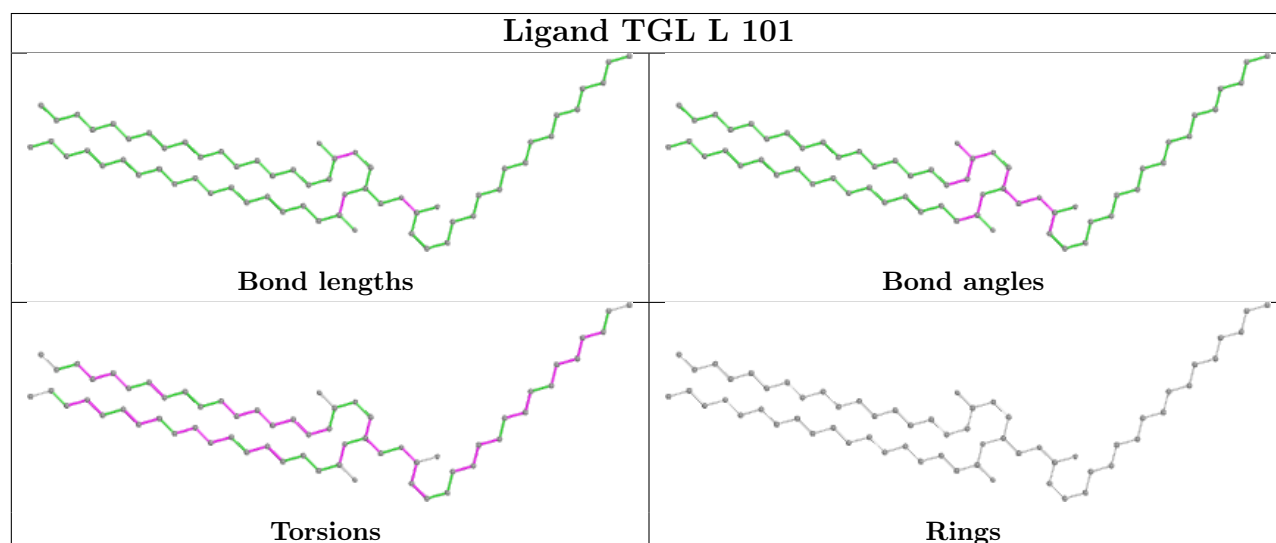
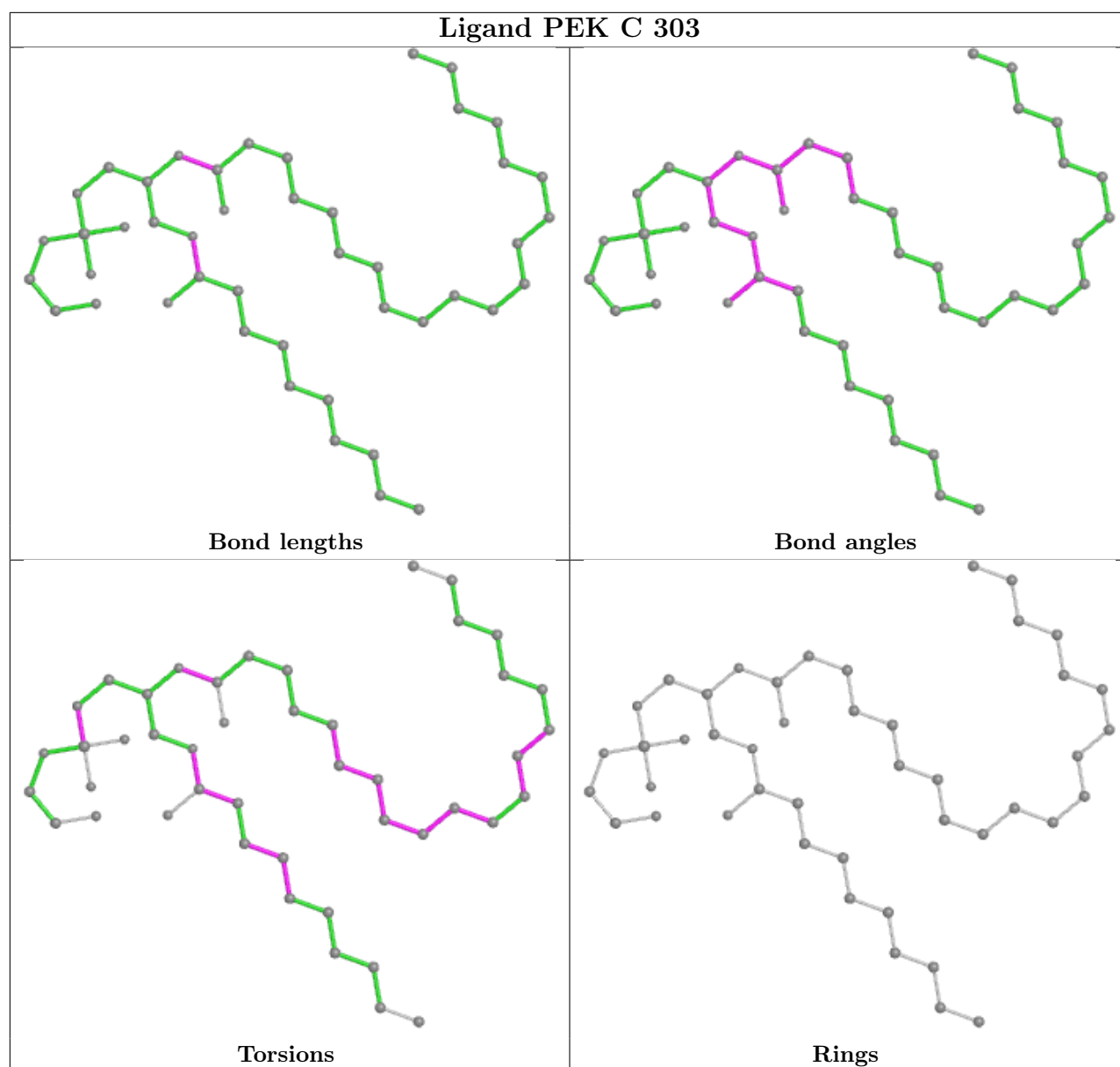
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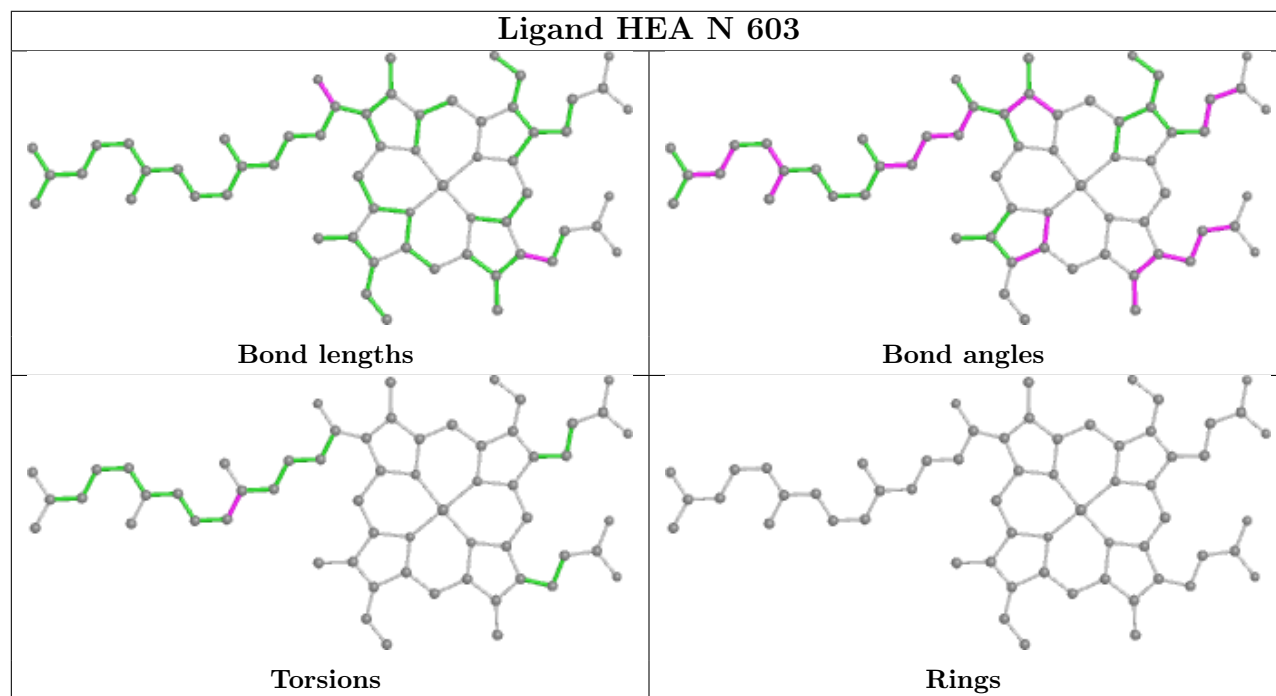
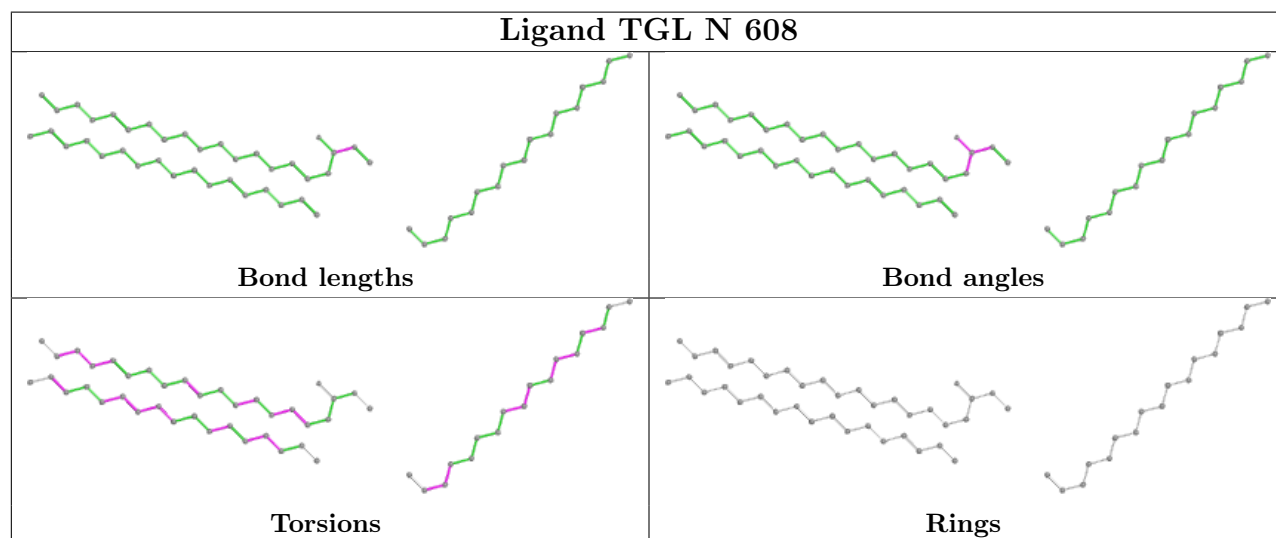
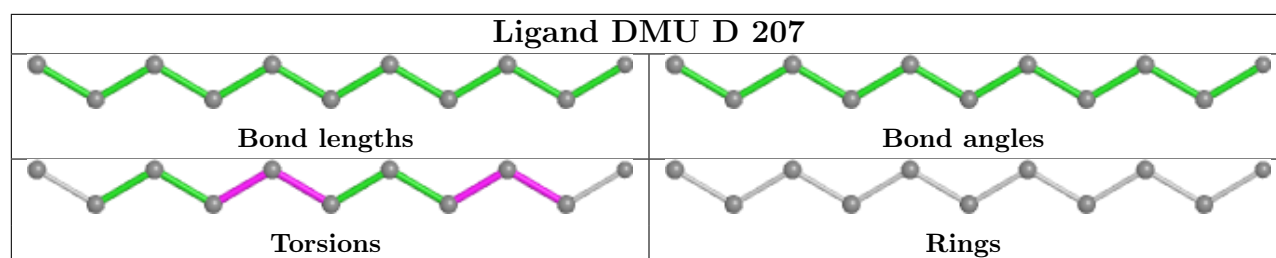
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	306	PGV	2	0
25	J	101	CHD	2	0
19	P	306	PGV	1	0
19	P	305	PGV	1	0
22	A	616	EDO	1	0
23	K	101	DMU	1	0
14	A	601[C]	HEA	1	0
18	N	609	TGL	1	0
22	C	318	EDO	1	0
23	C	310	DMU	3	0
20	N	611[A]	PER	1	0
14	A	601[B]	HEA	1	0
23	J	104	DMU	1	0
26	P	304	PEK	2	0
18	N	607	TGL	3	0
14	N	602[C]	HEA	2	0
23	P	308	DMU	3	0
23	P	316	DMU	2	0
19	A	611	PGV	1	0
22	C	315	EDO	1	0
22	D	204	EDO	3	0
14	N	602[B]	HEA	1	0
27	P	307	CDL	7	0
25	G	101	CHD	1	0
26	T	101	PEK	6	0
19	N	612	PGV	1	0
18	A	606	TGL	4	0
22	D	205	EDO	2	0
14	A	601[A]	HEA	2	0
23	K	102	DMU	1	0
23	K	103	DMU	1	0

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

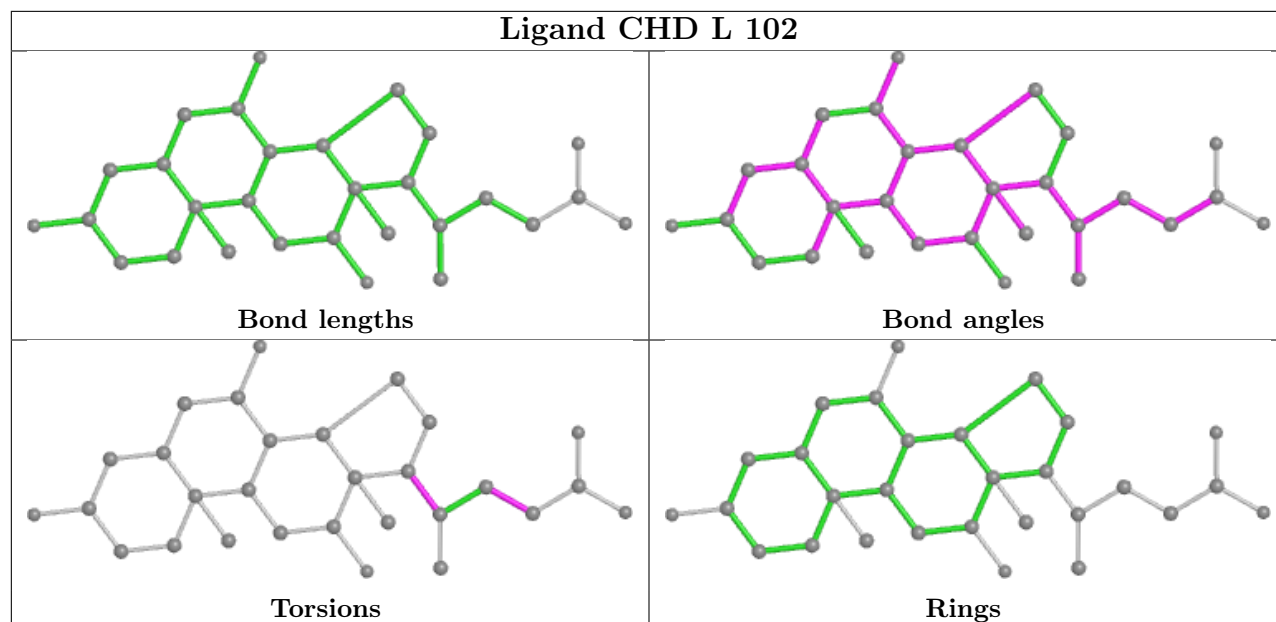
equivalents in the CSD to analyse the geometry.



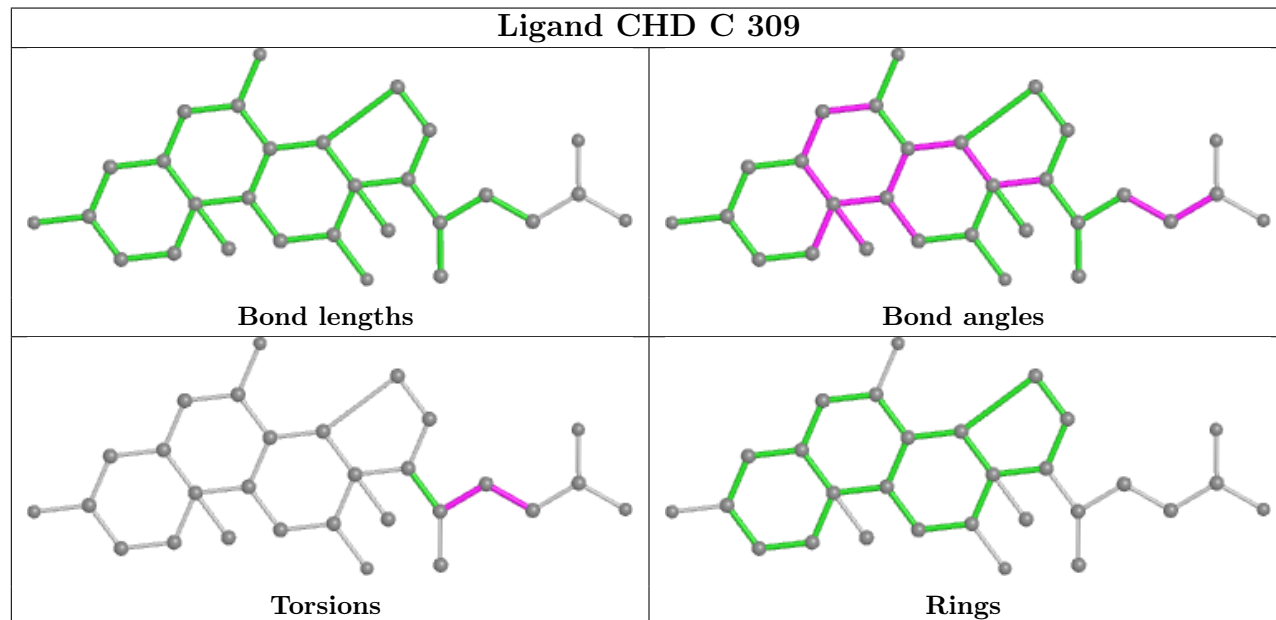


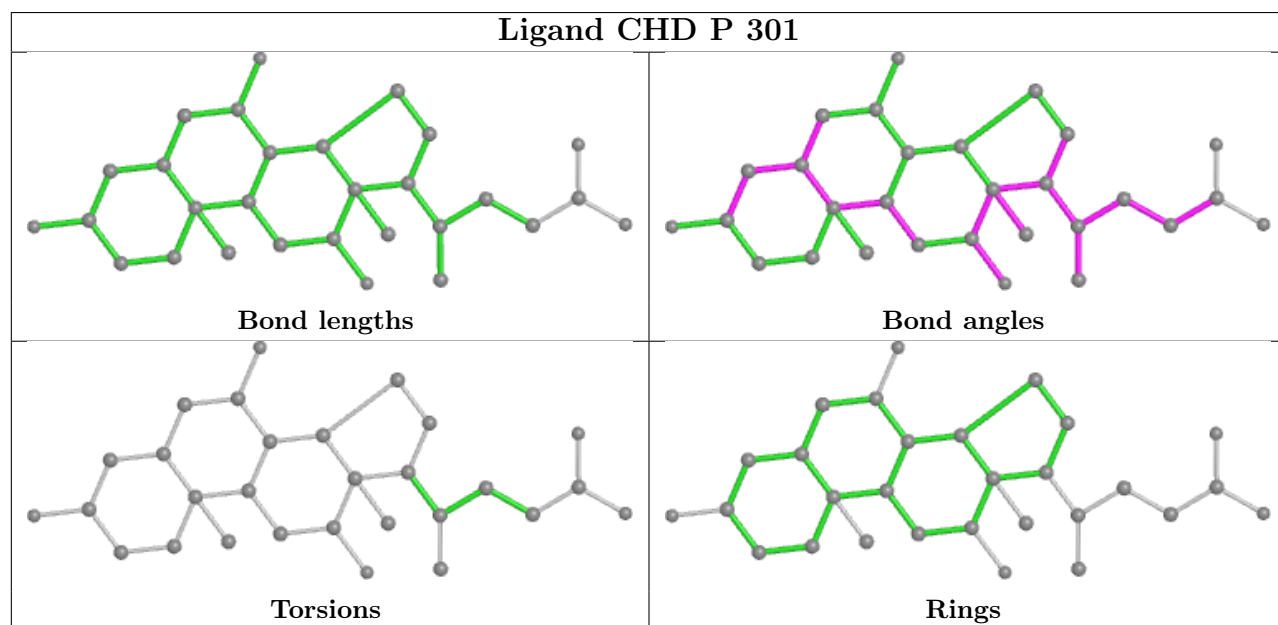
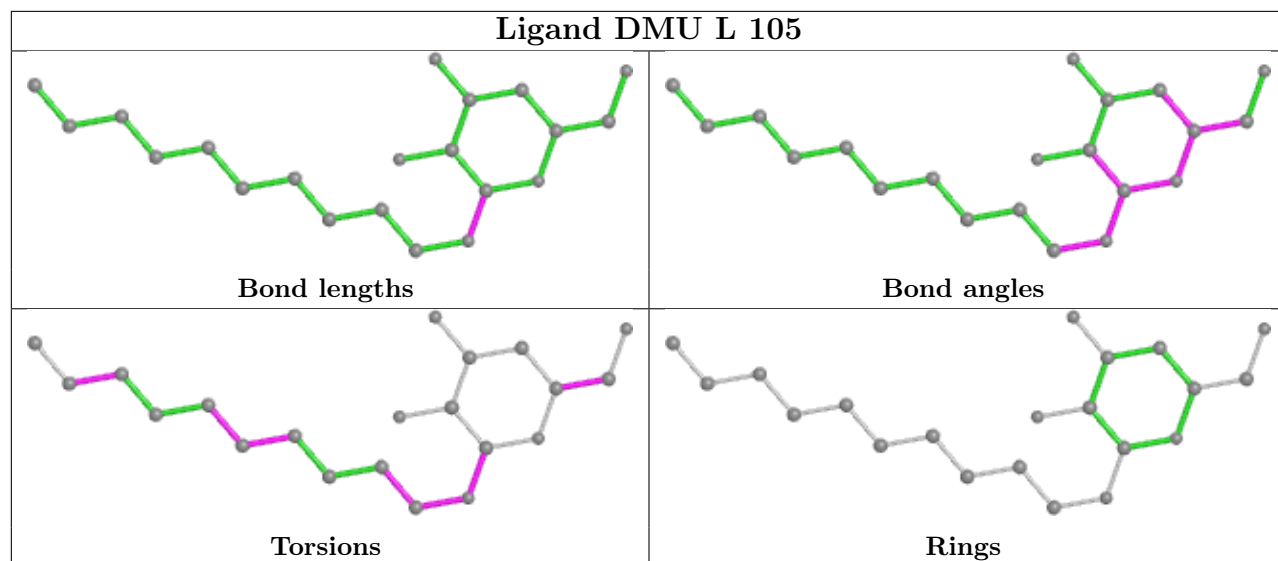


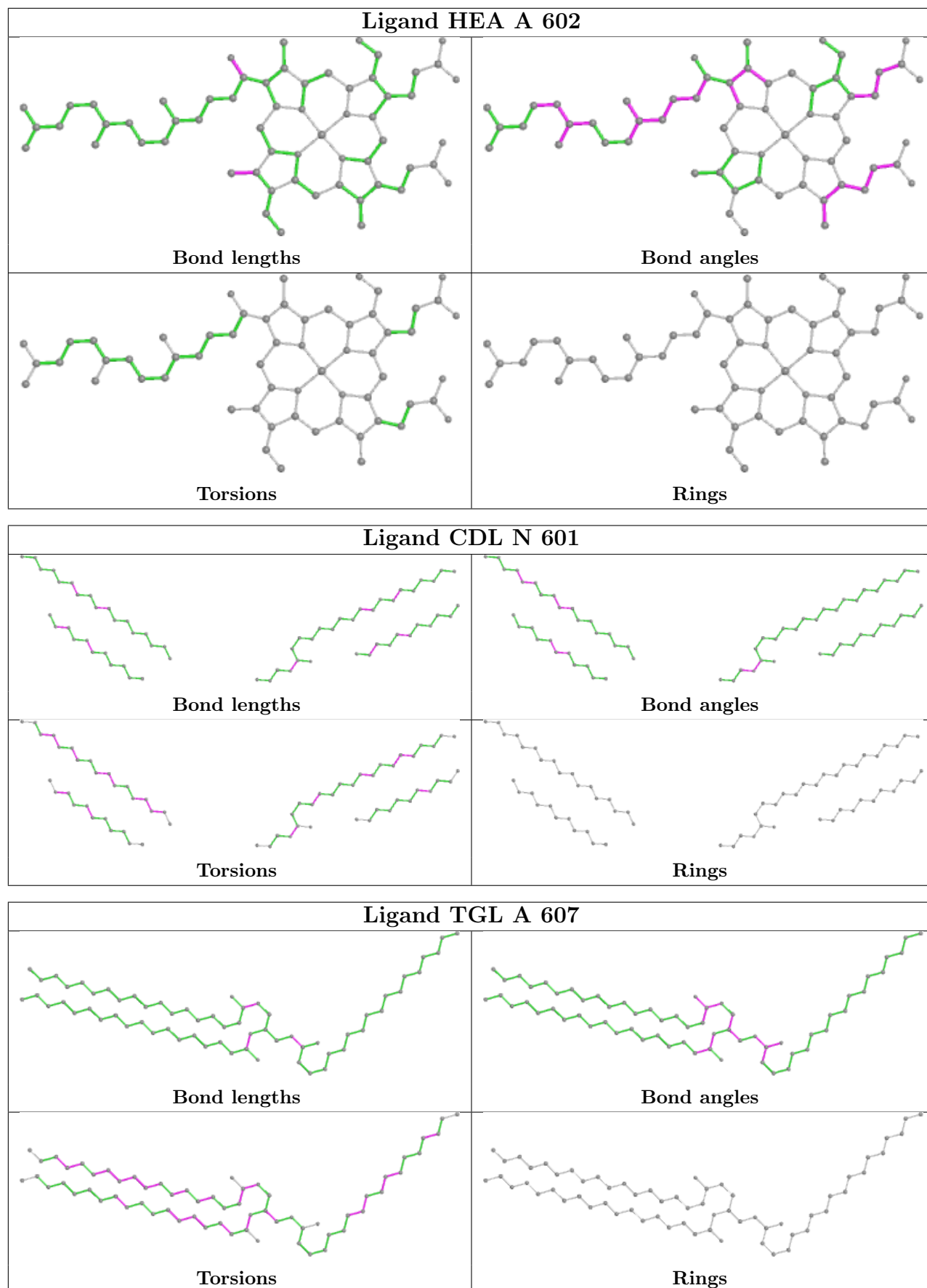
## Ligand CHD L 102

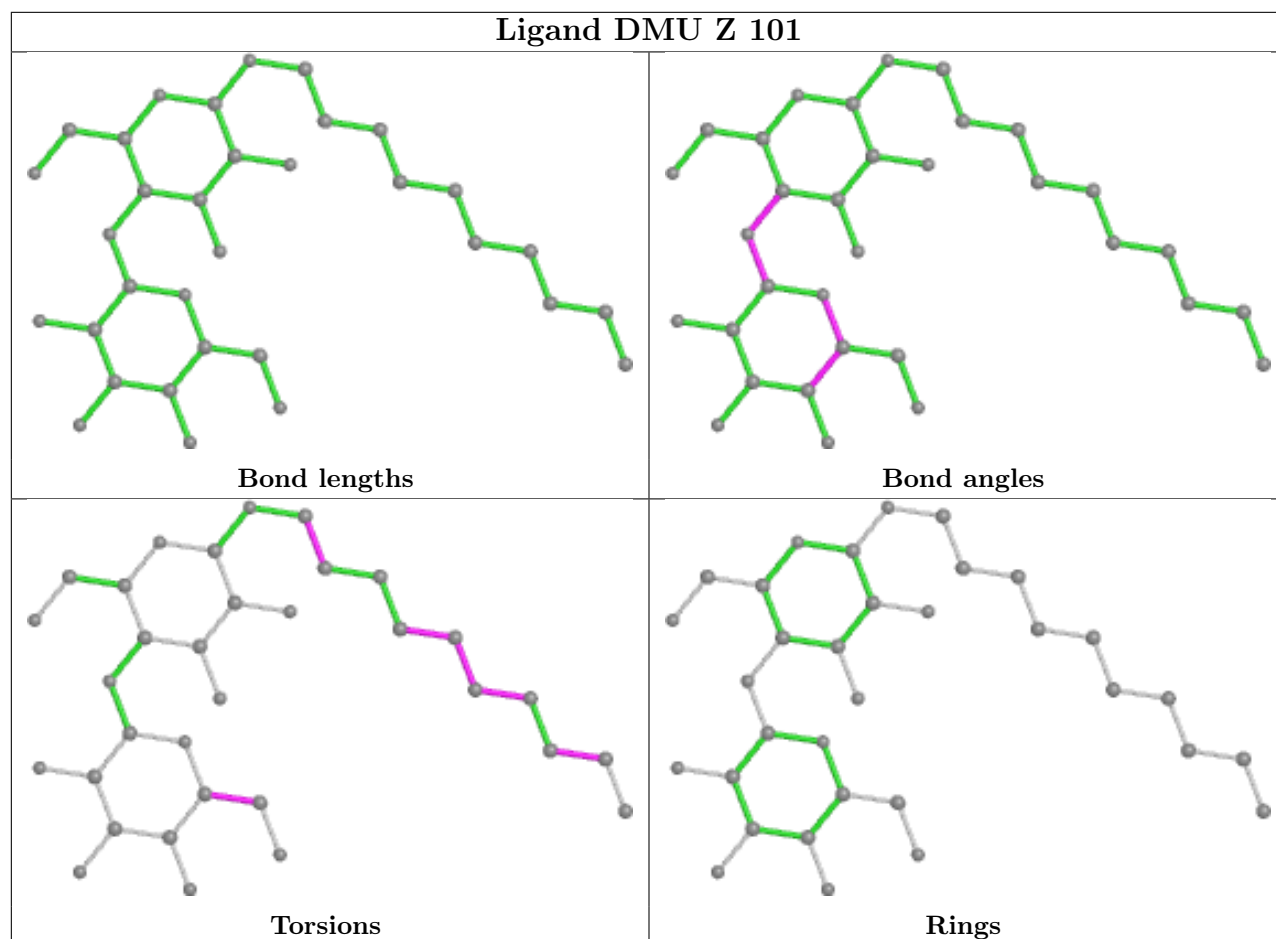
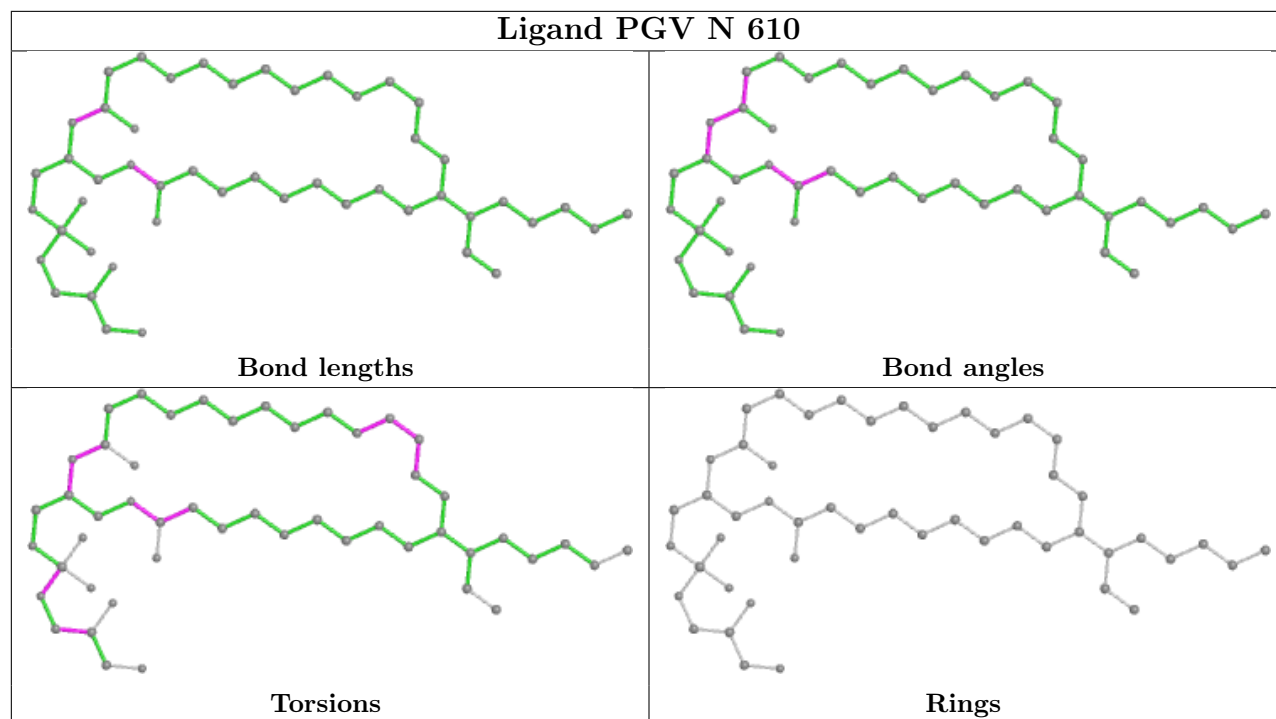


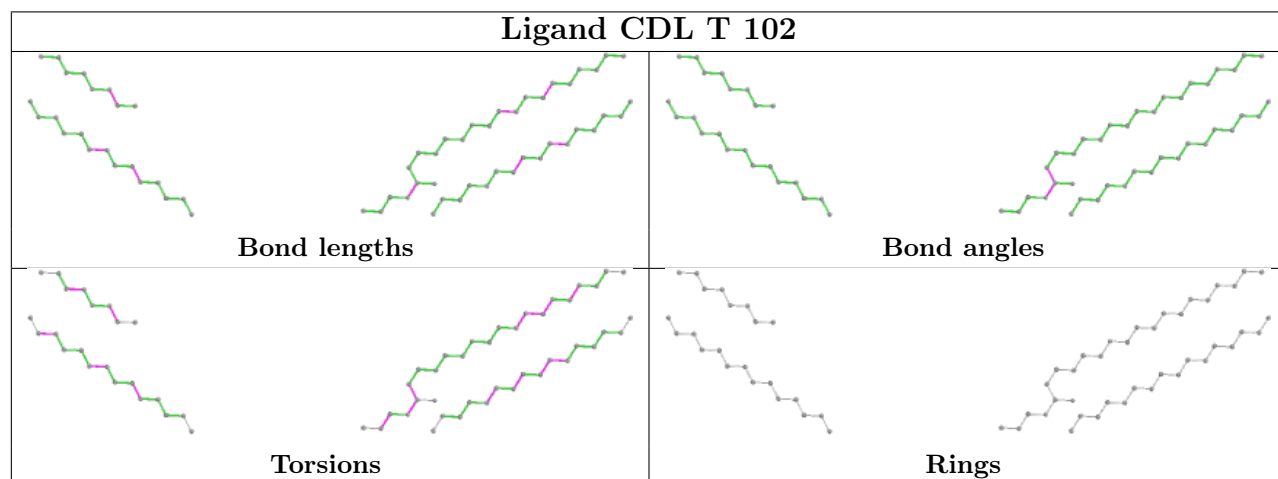
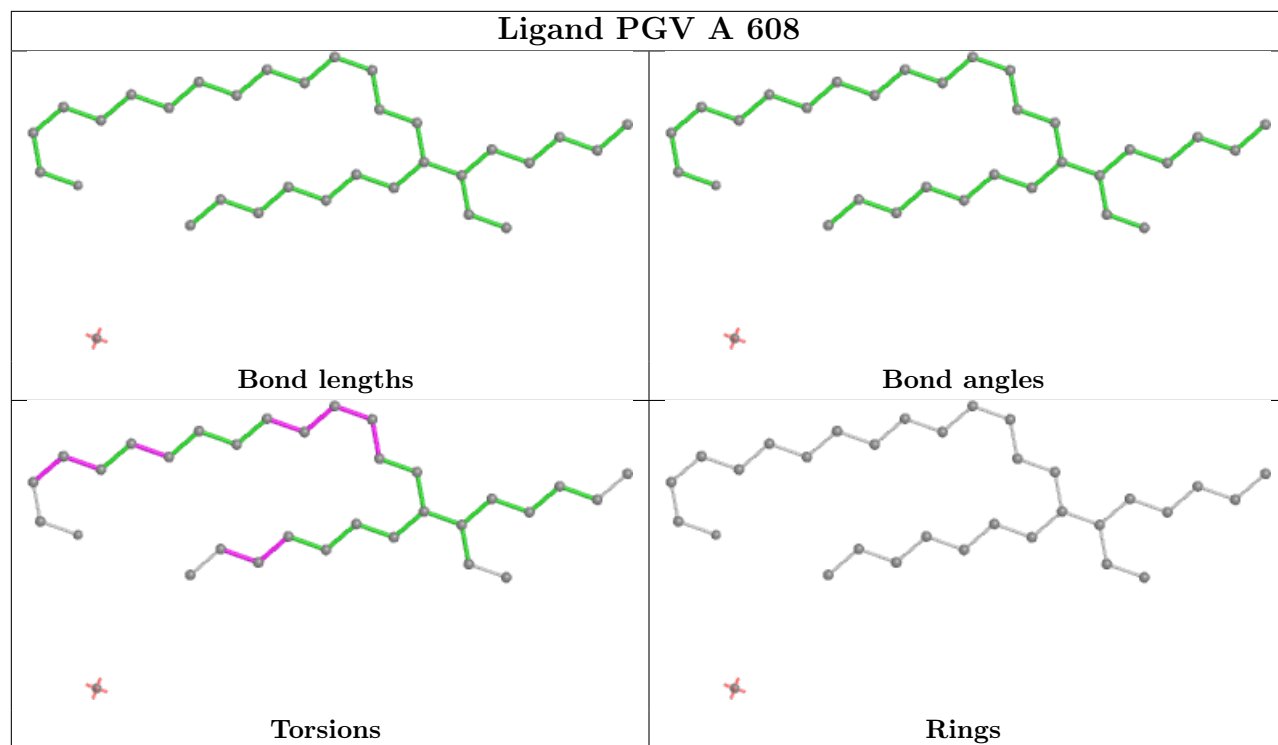
## Ligand CHD C 309

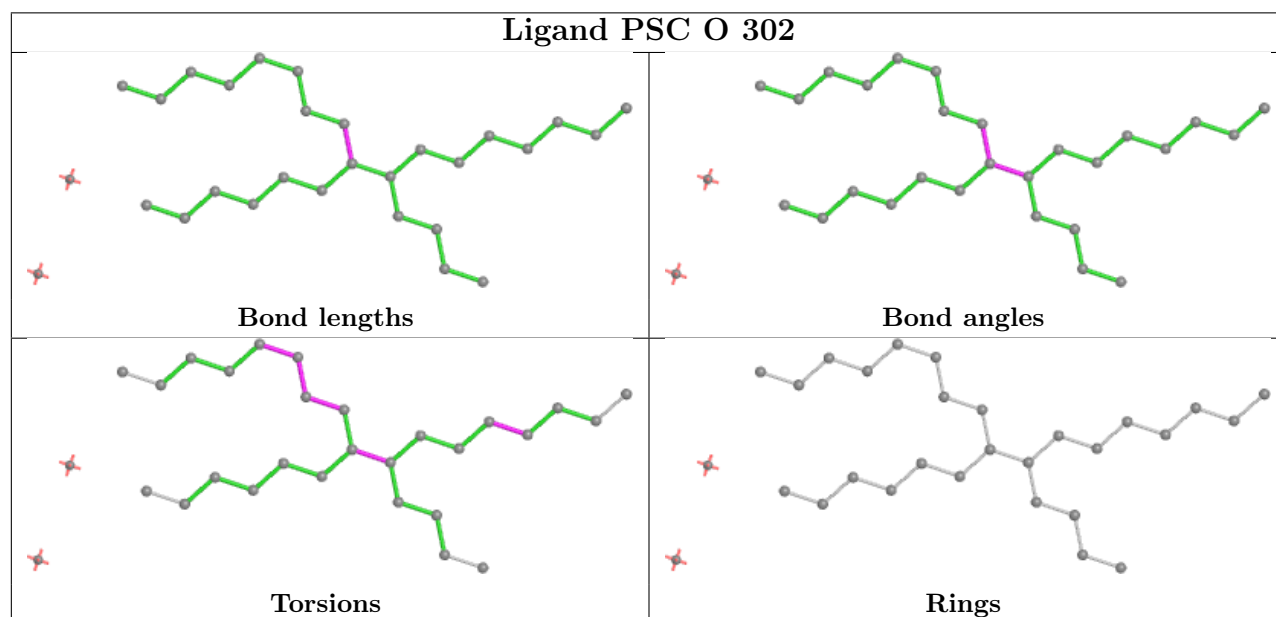
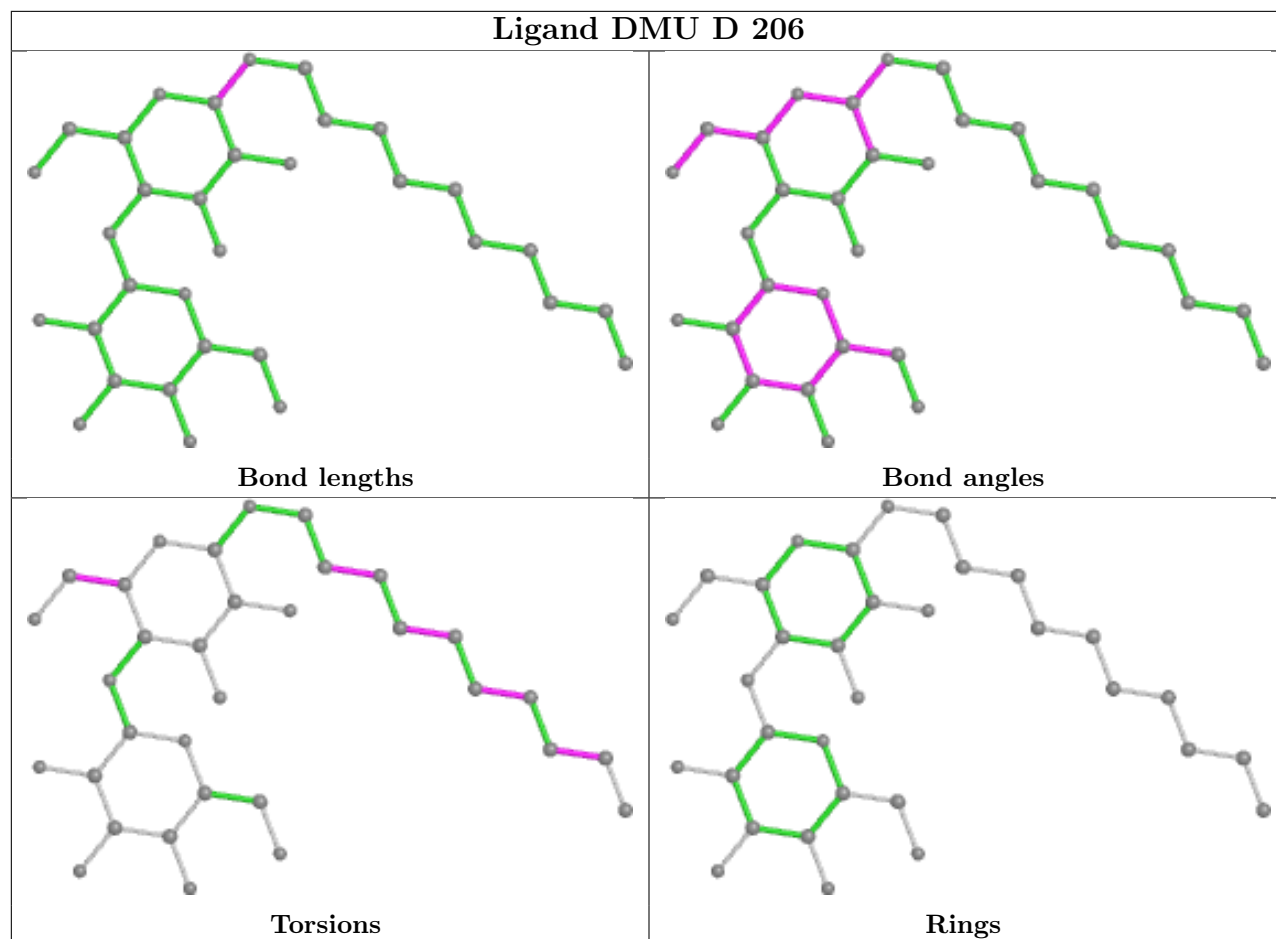


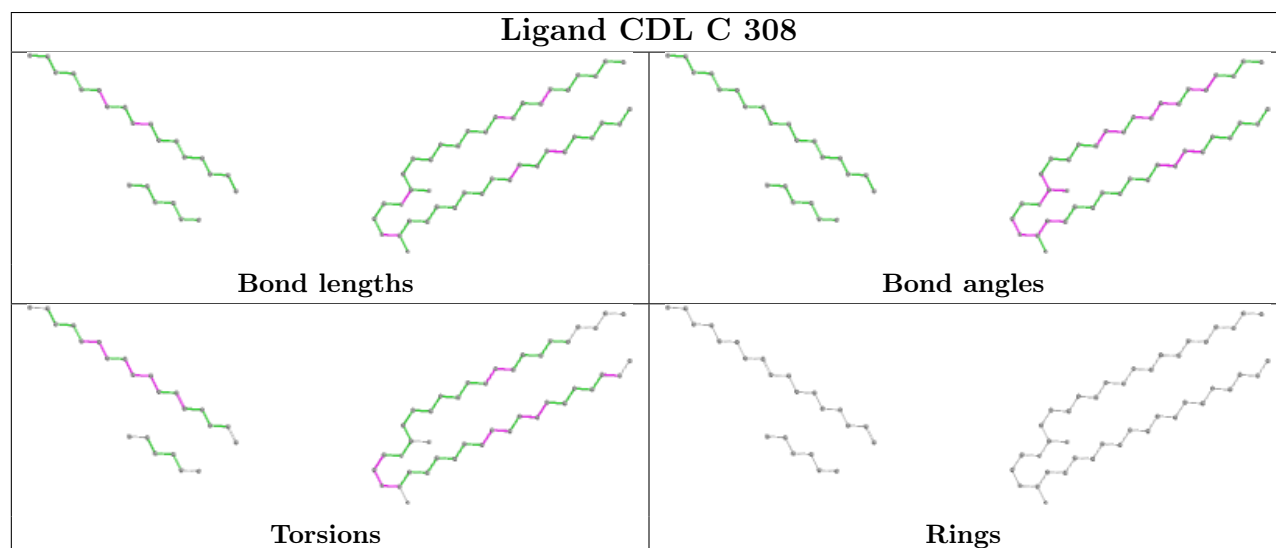
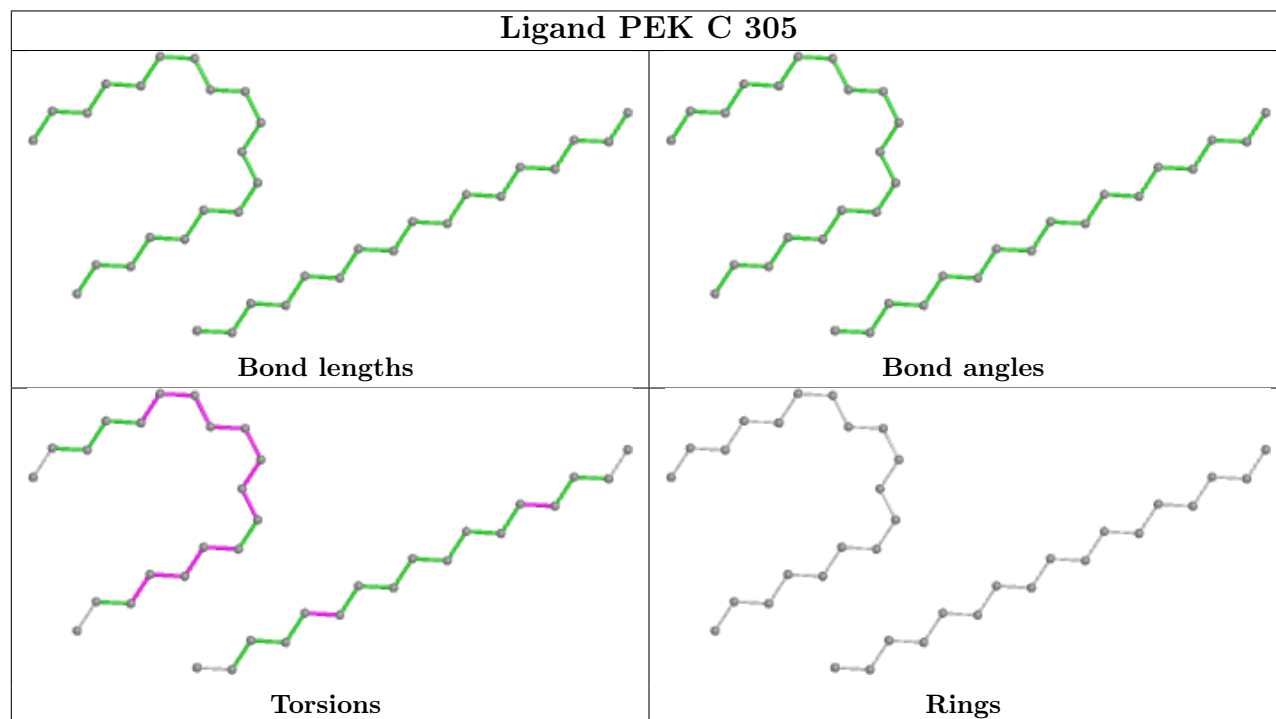
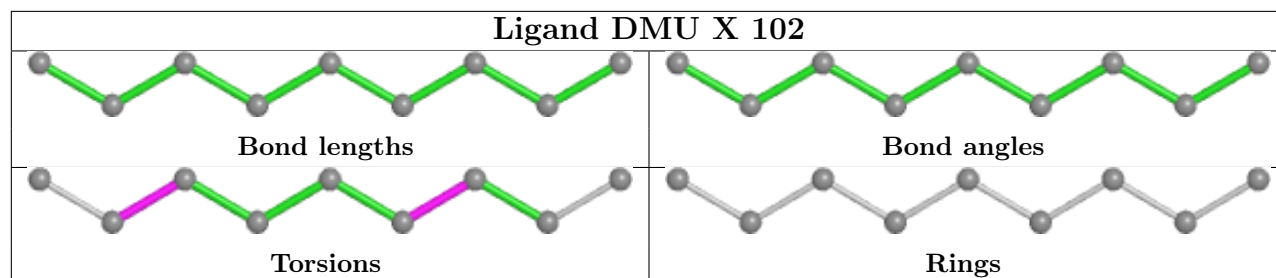


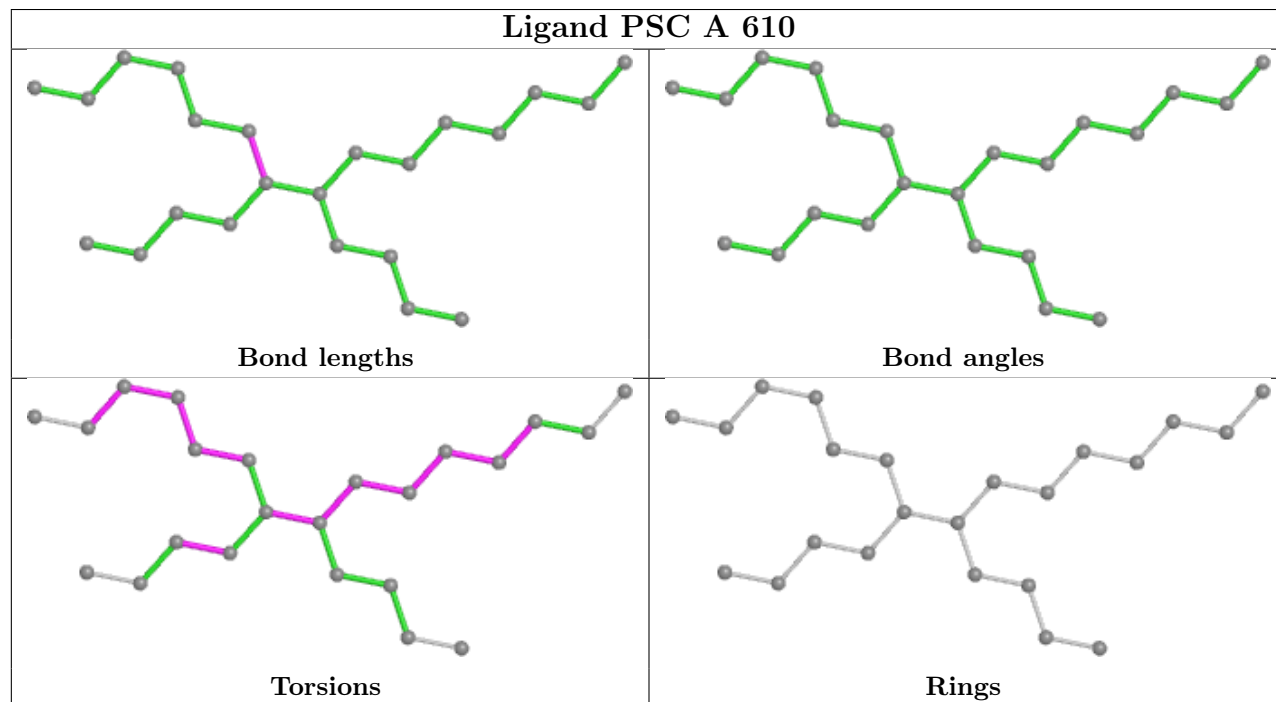
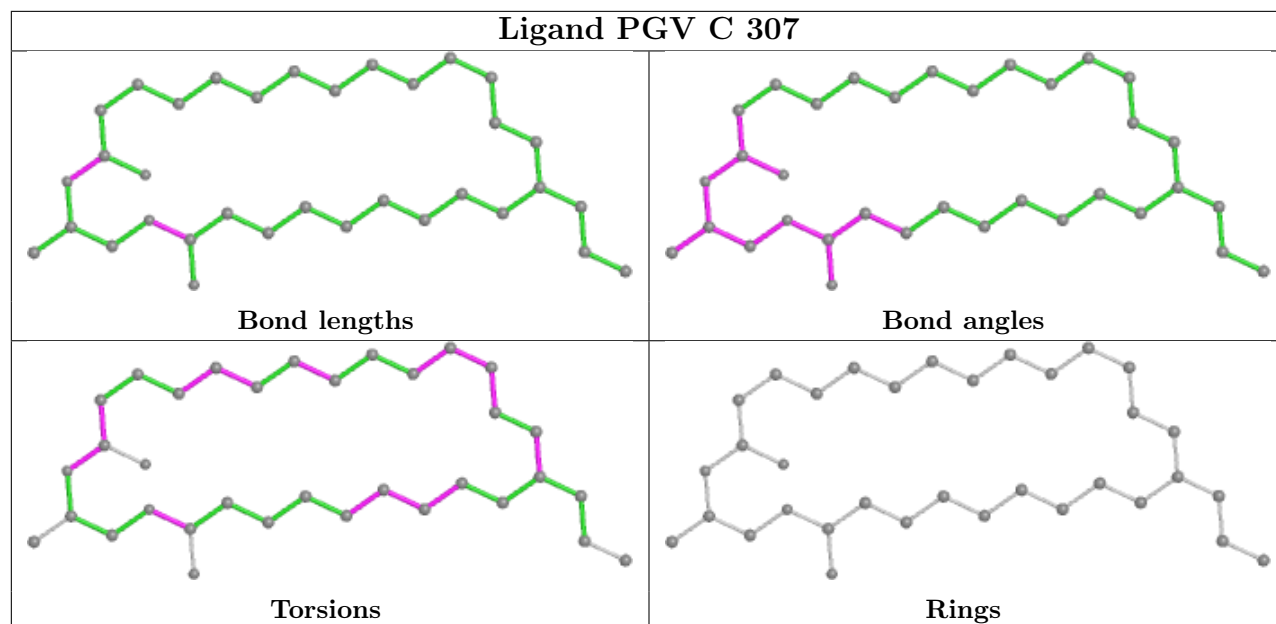


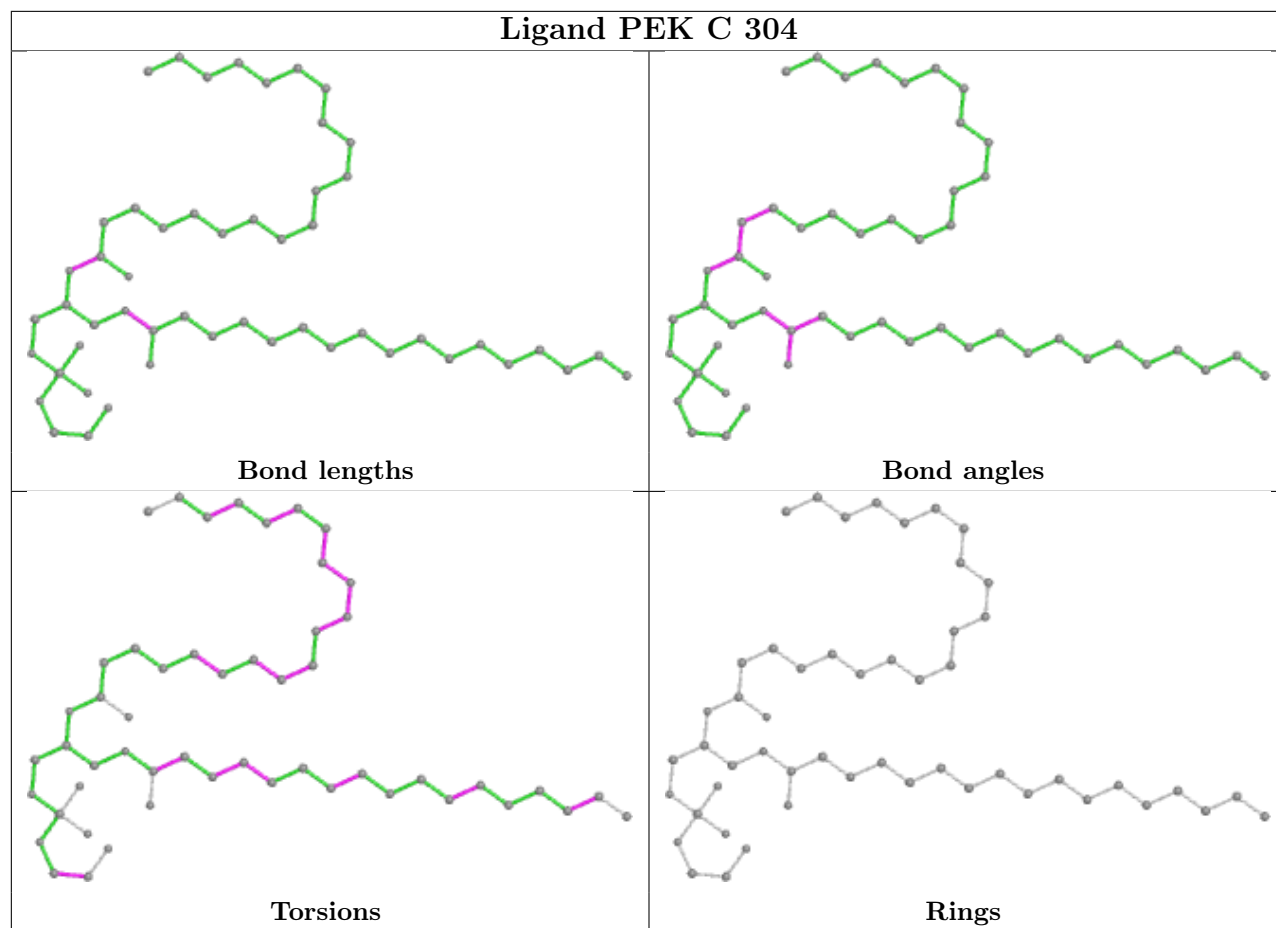




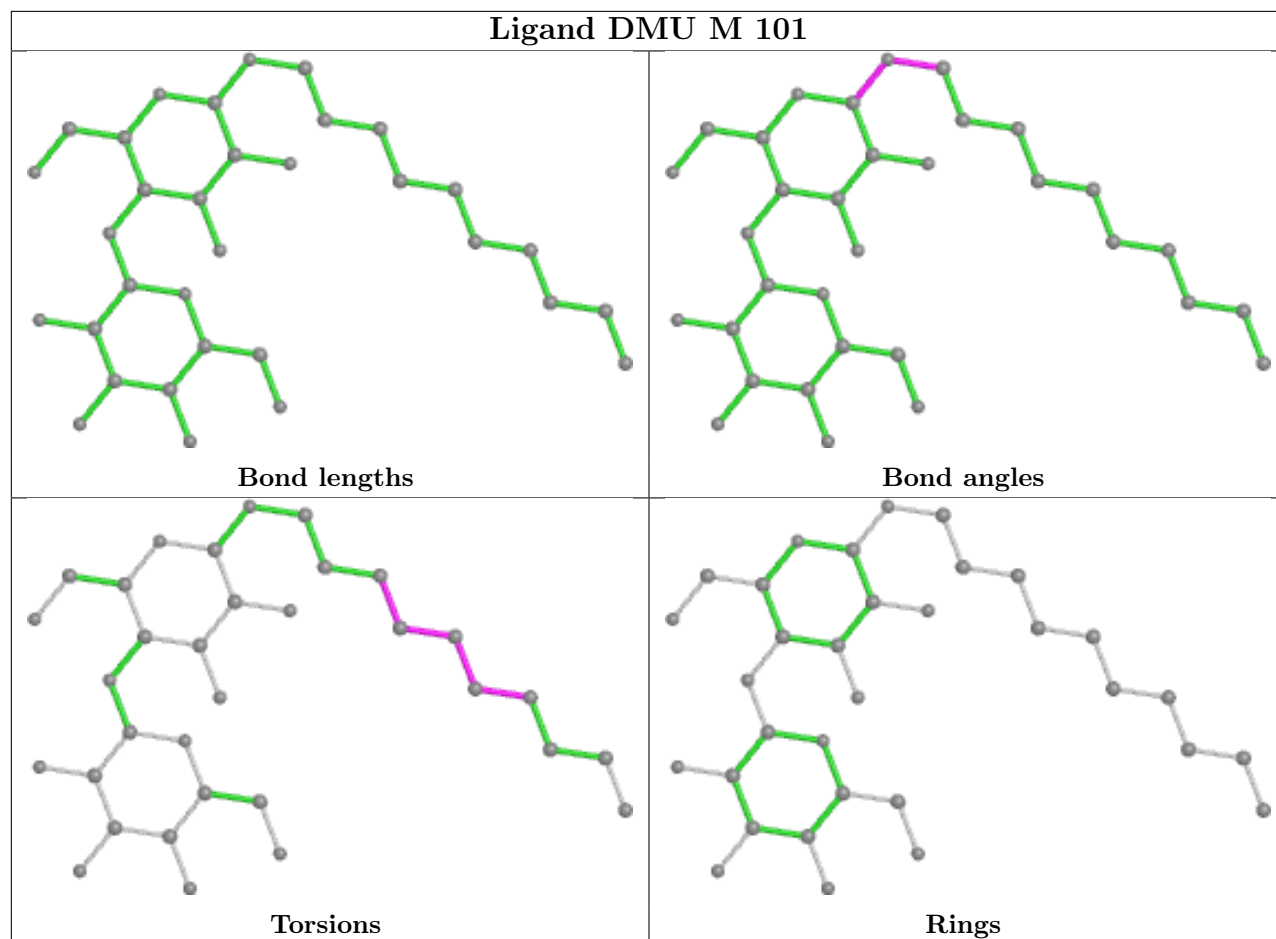




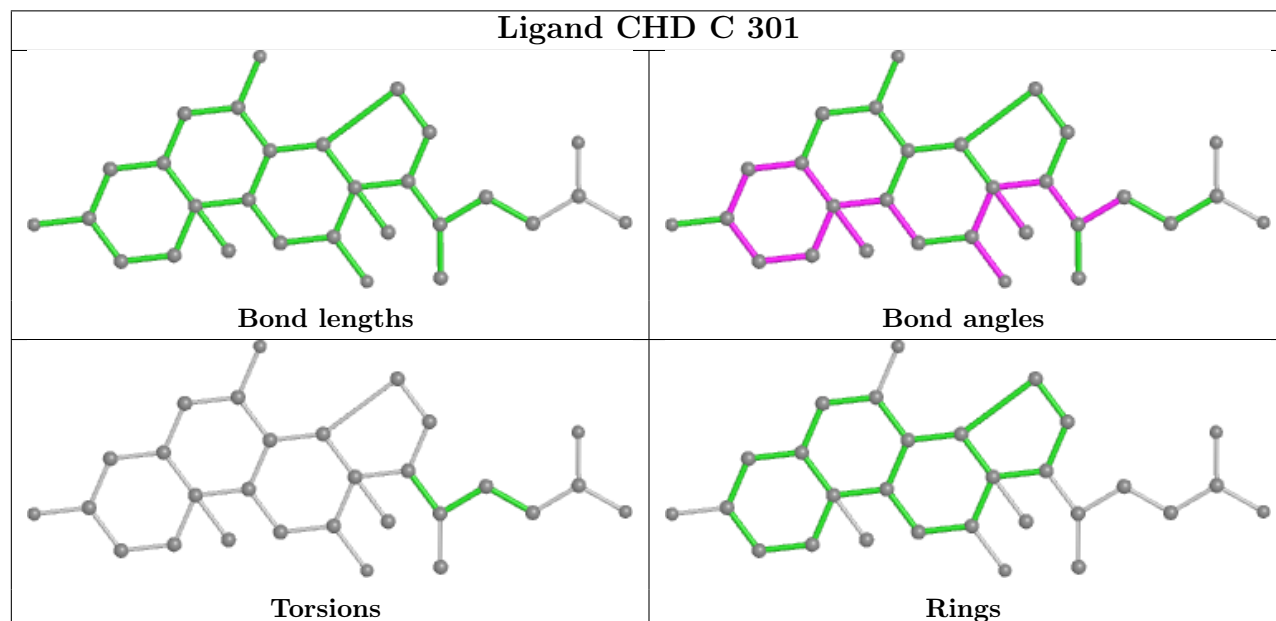


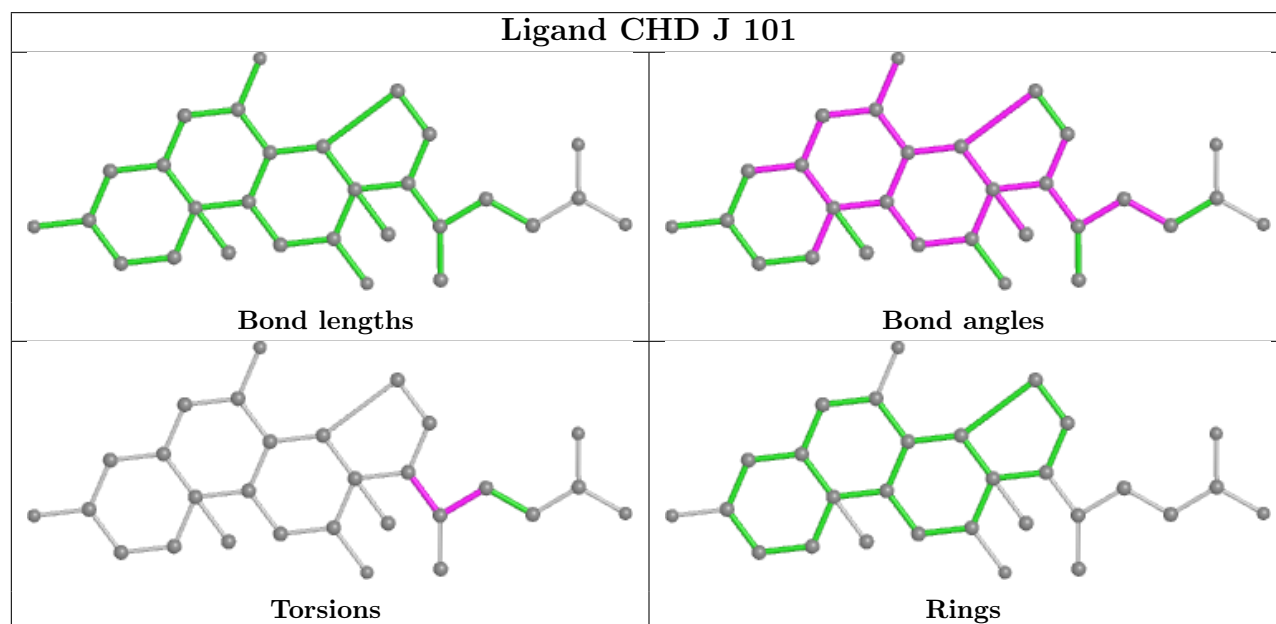
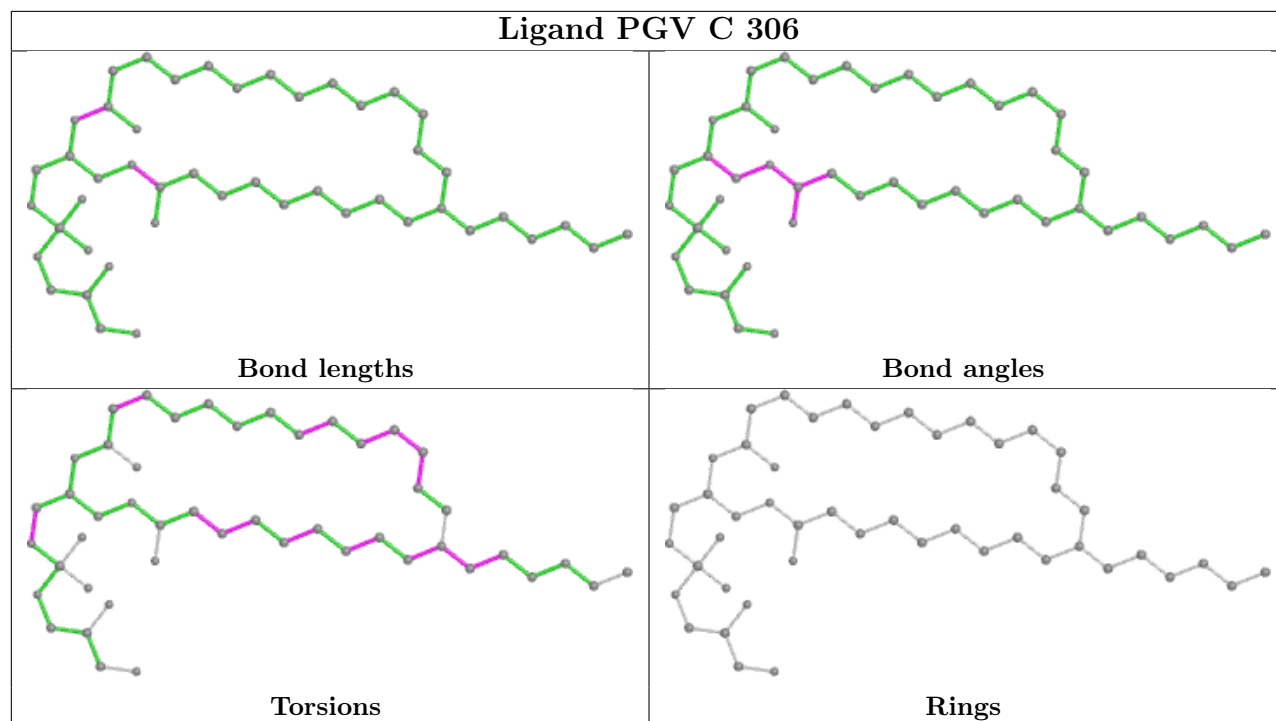


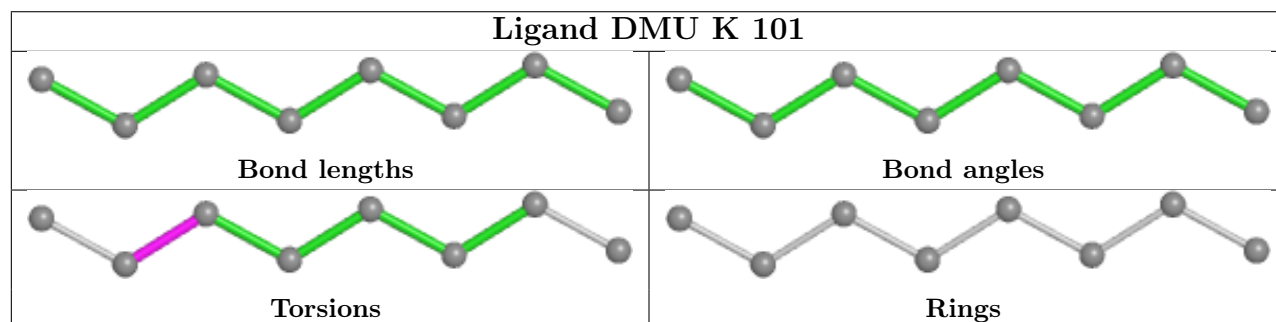
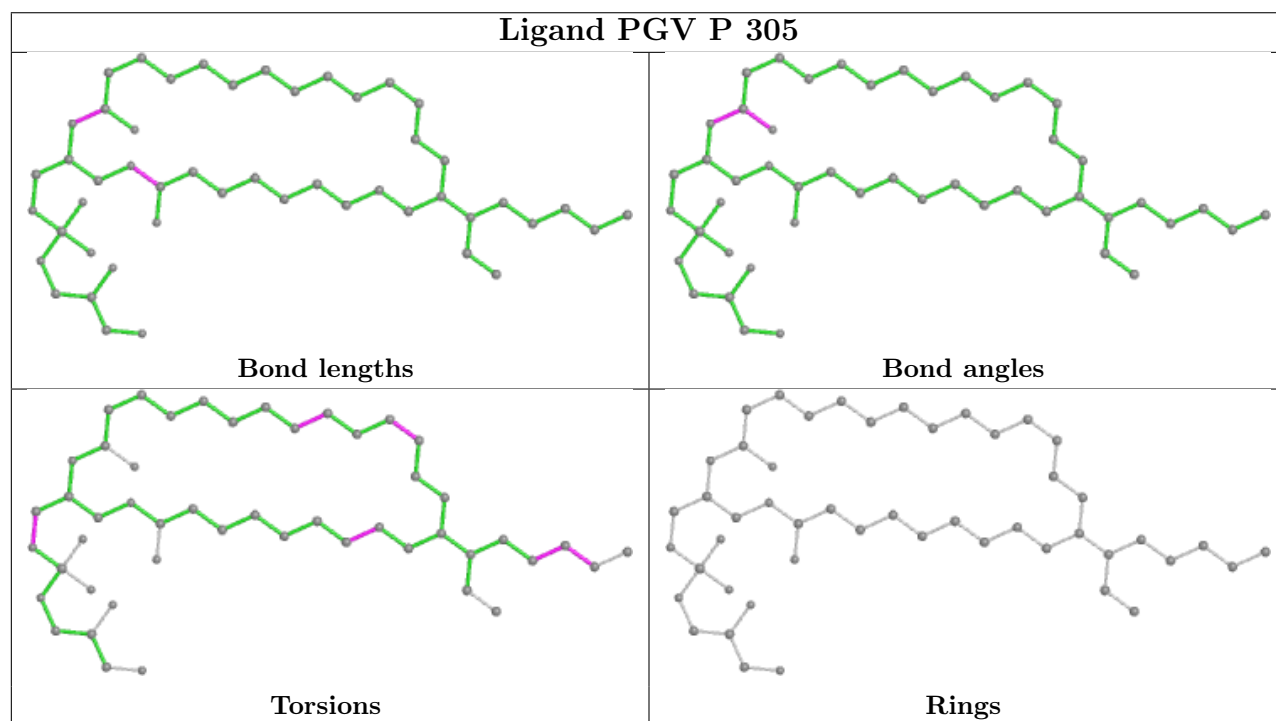
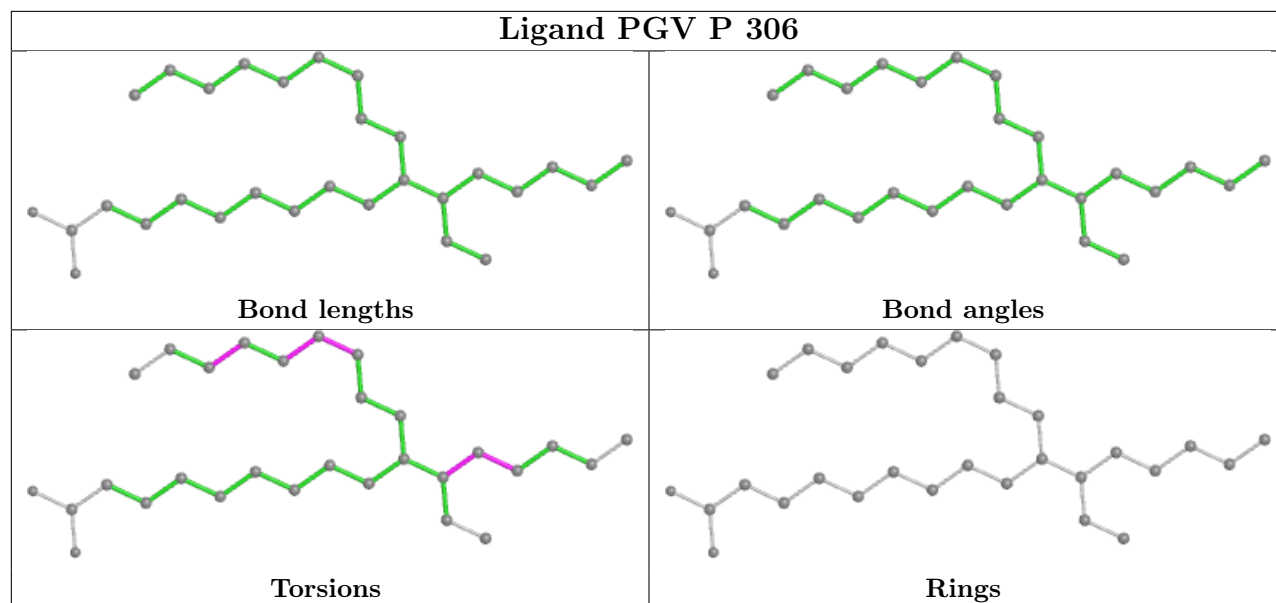
## Ligand DMU M 101

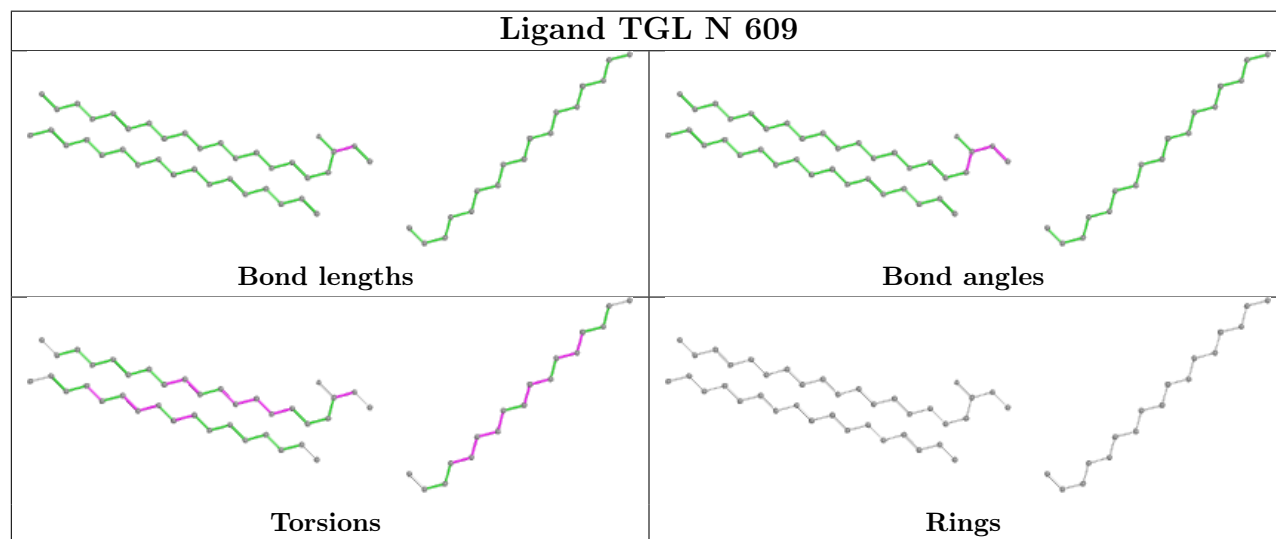
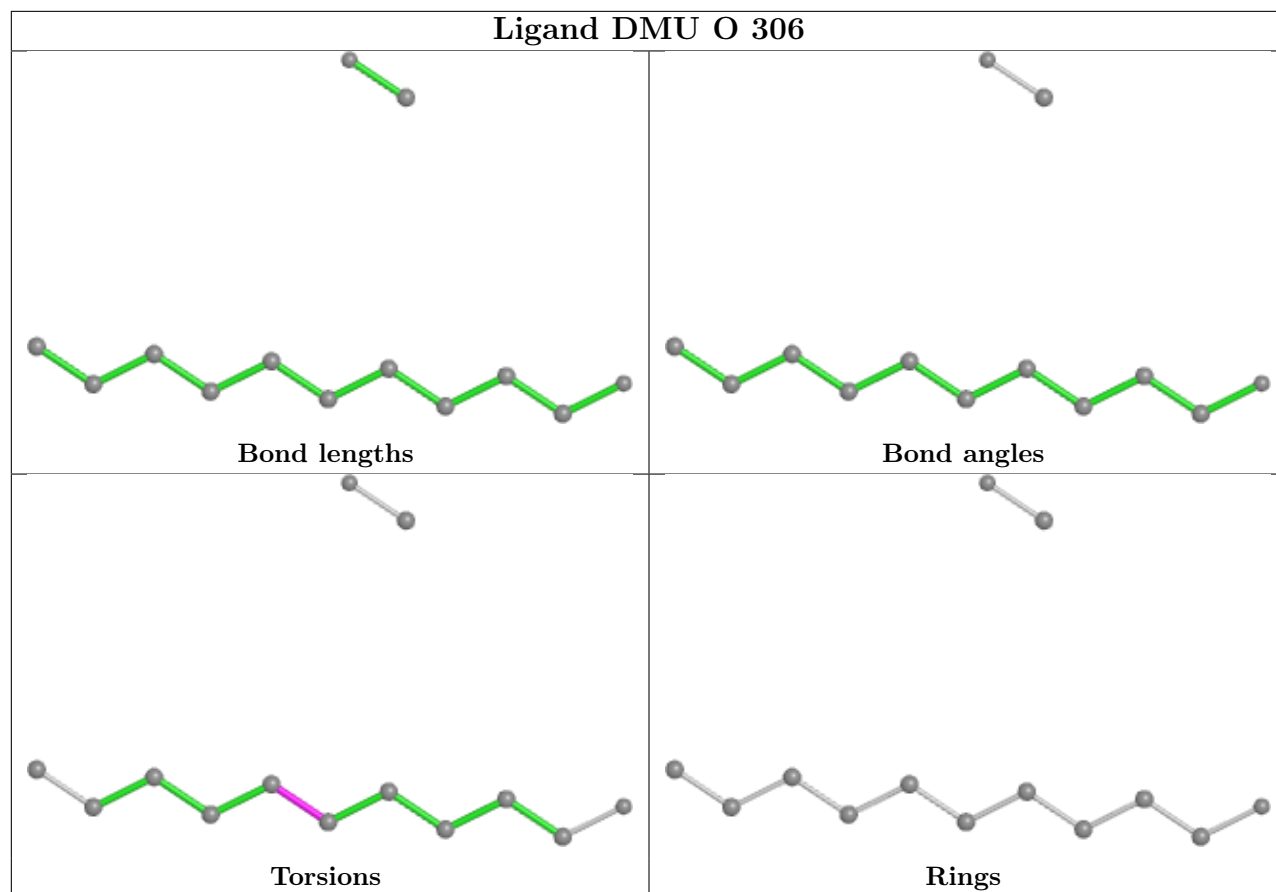


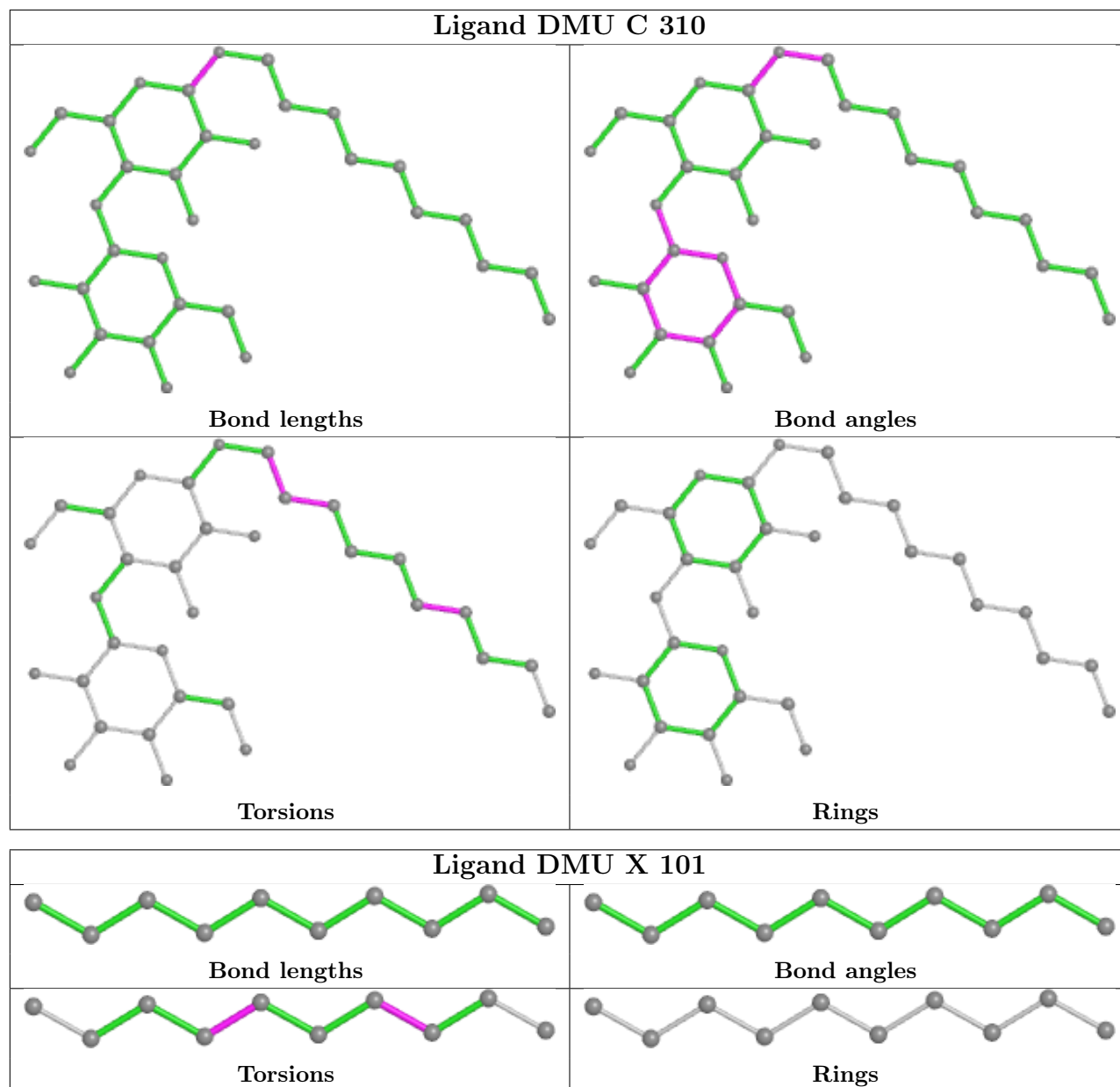
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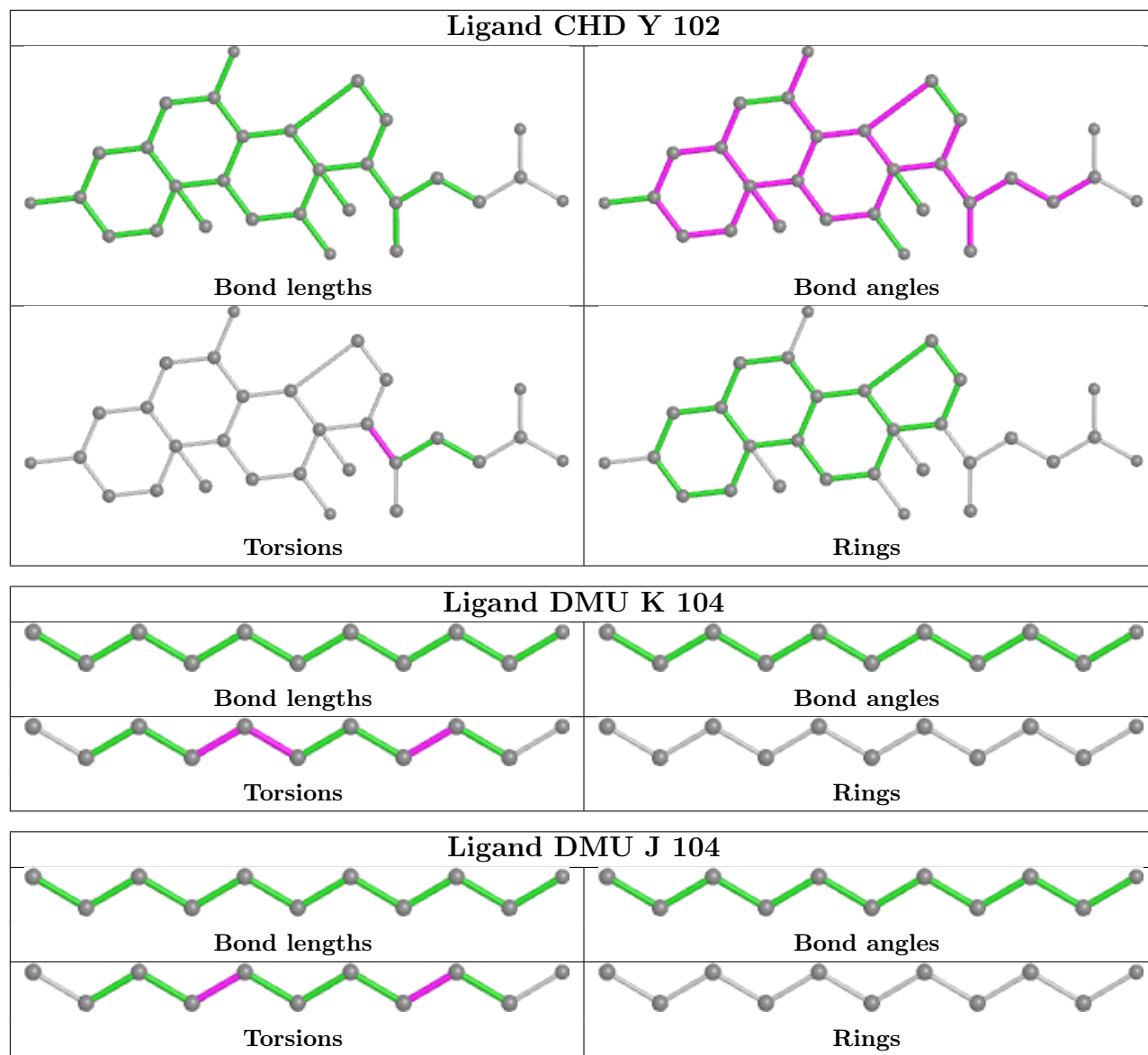




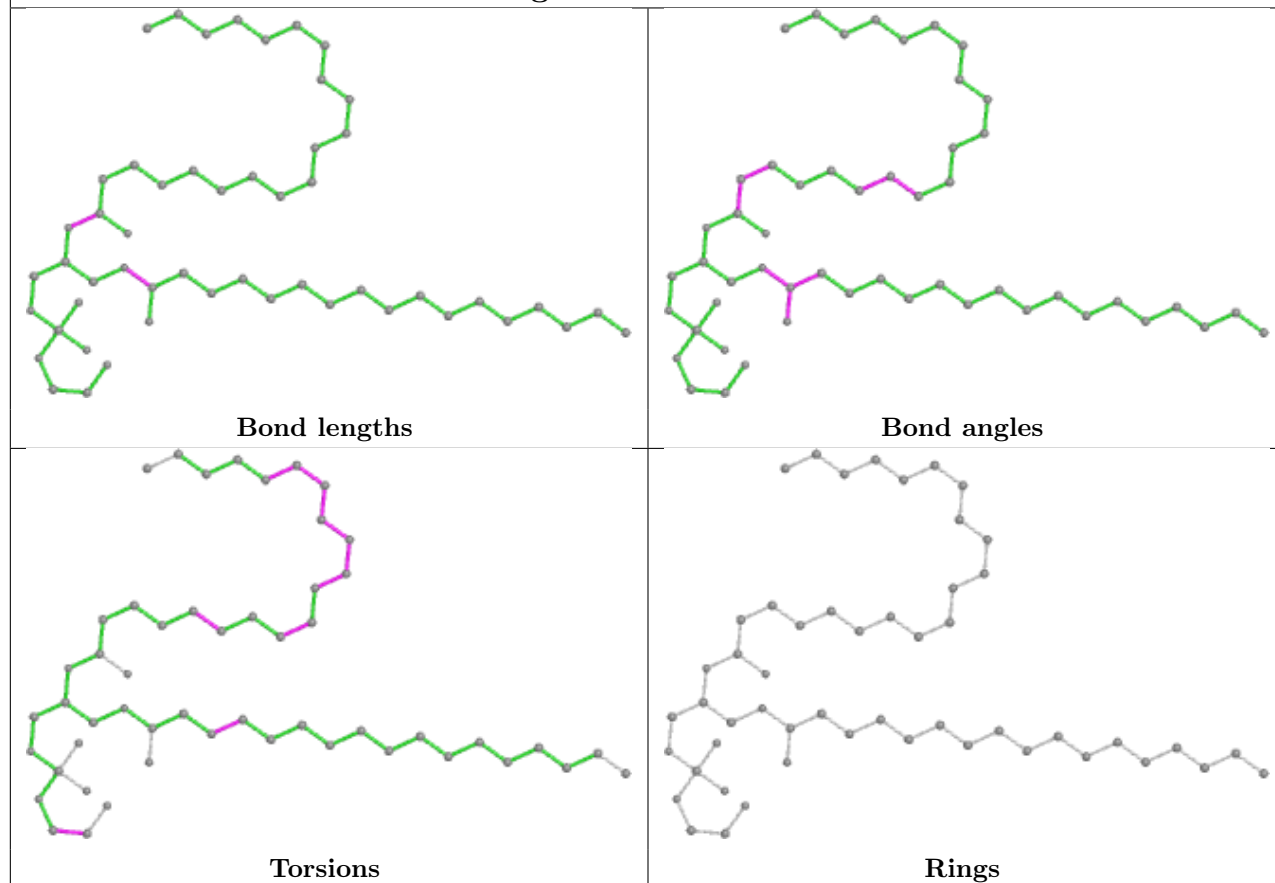




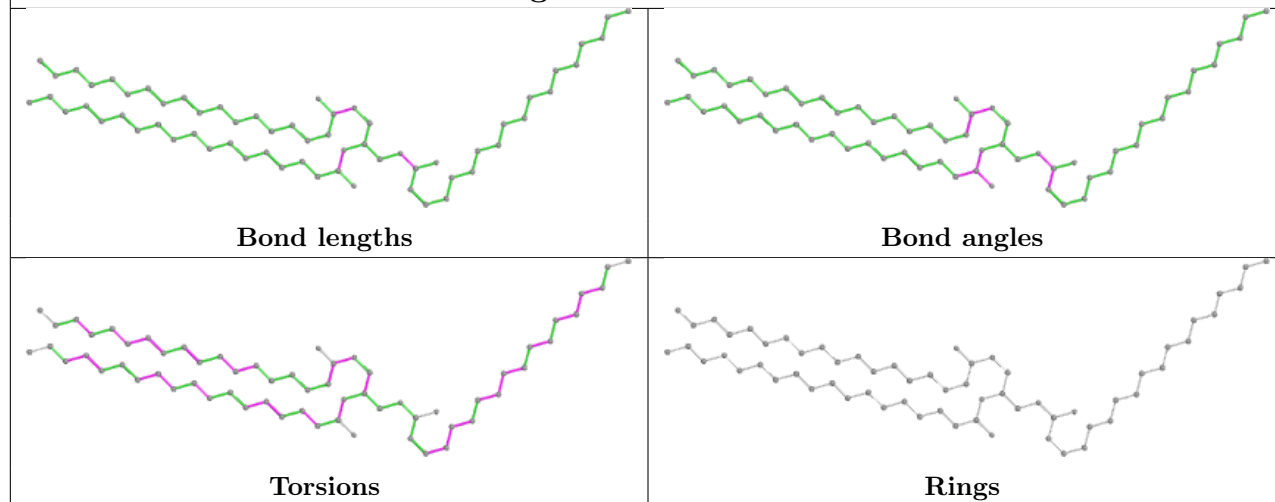


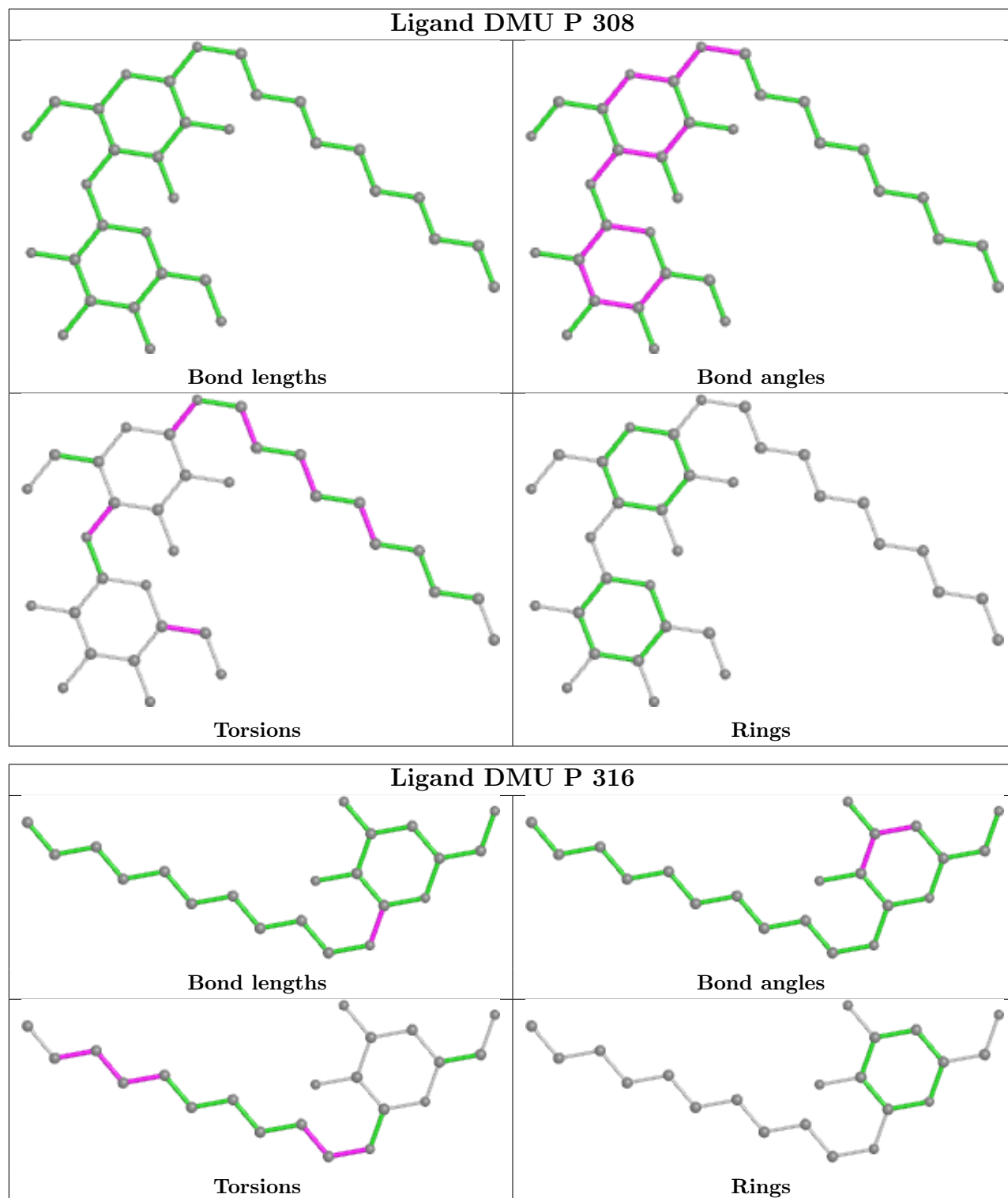


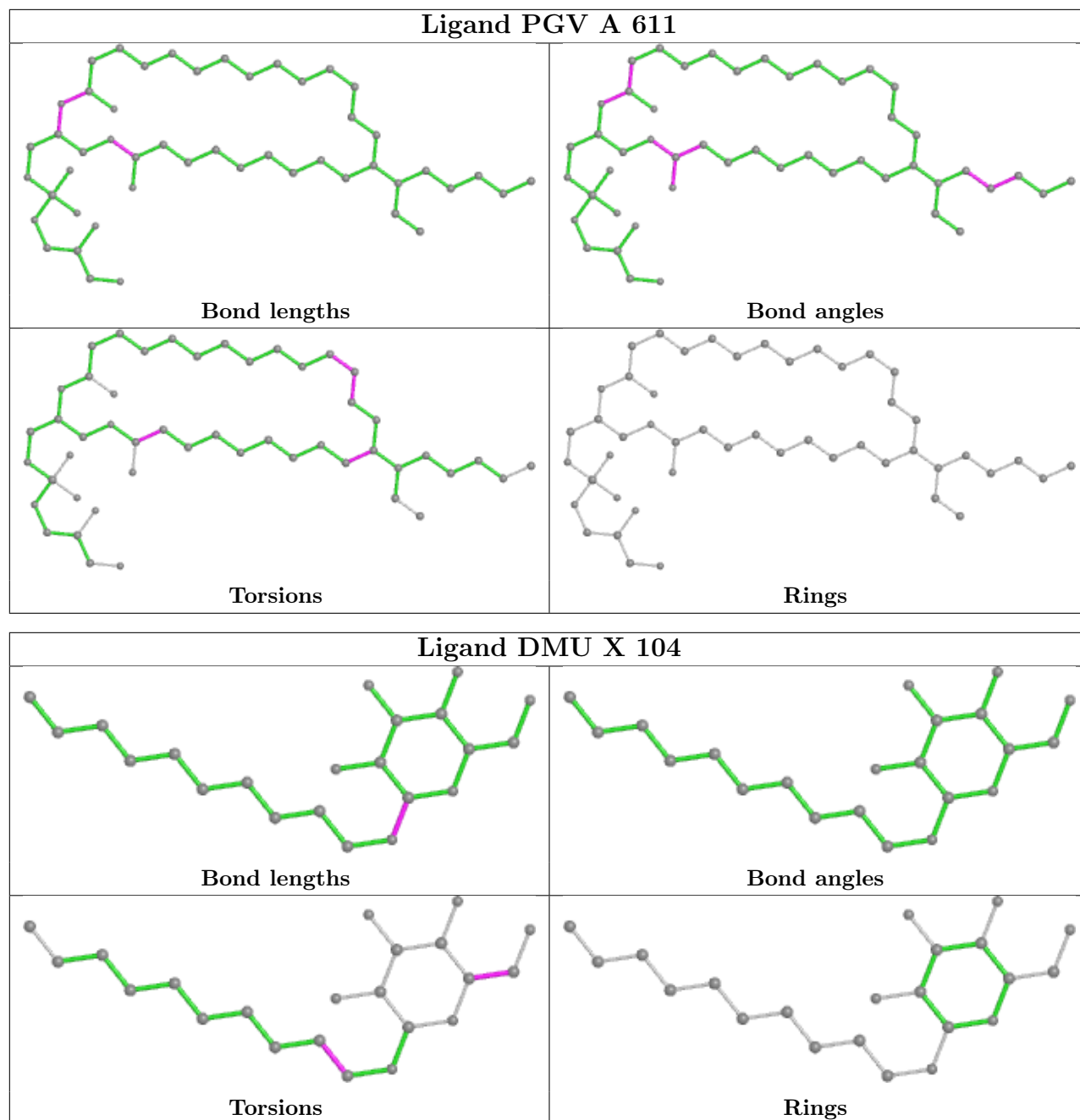
## Ligand PEK P 304

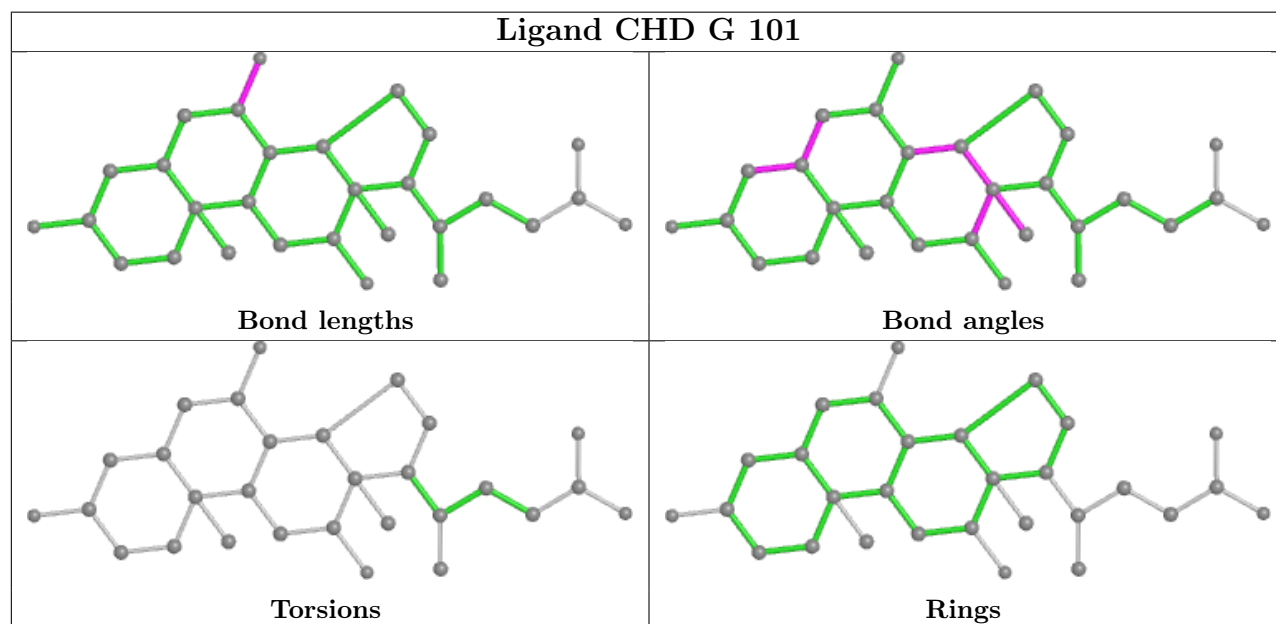
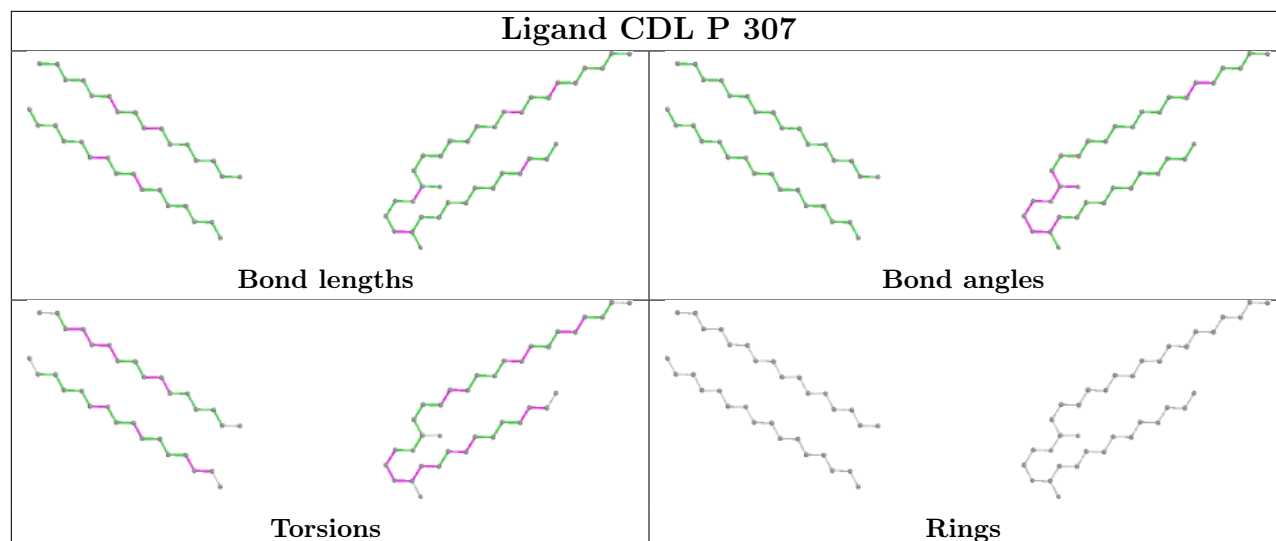


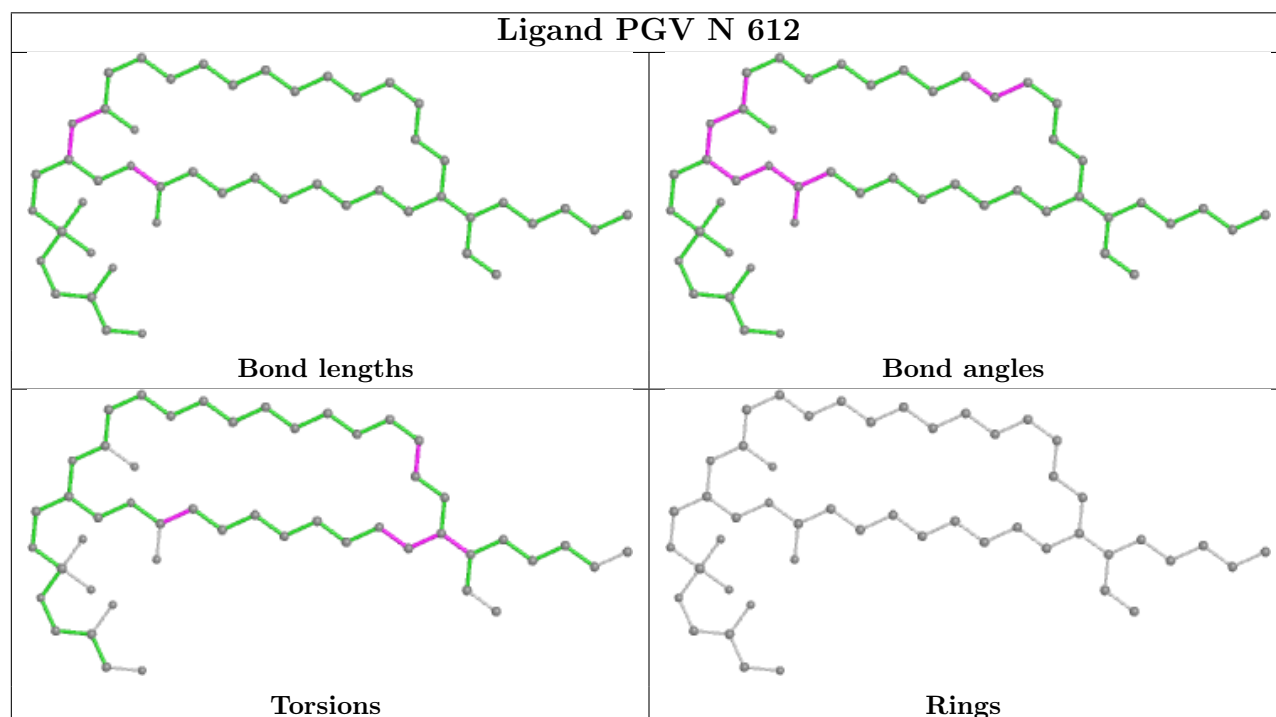
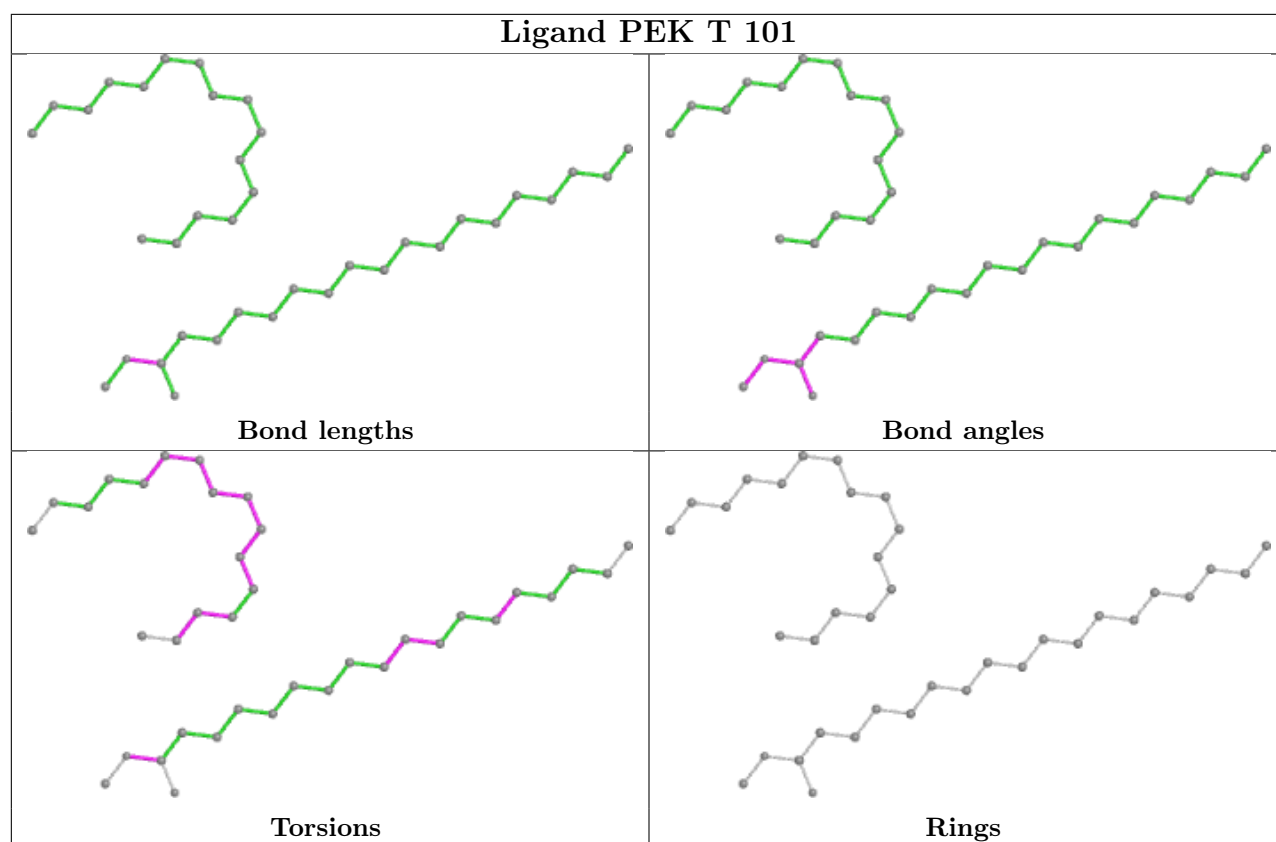
## Ligand TGL N 607

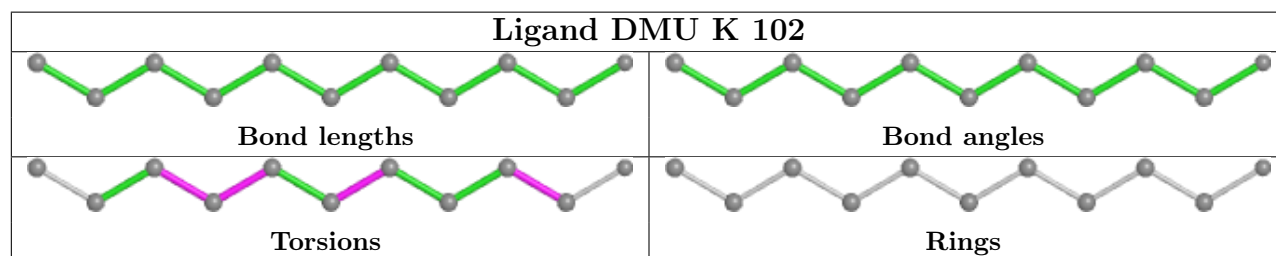
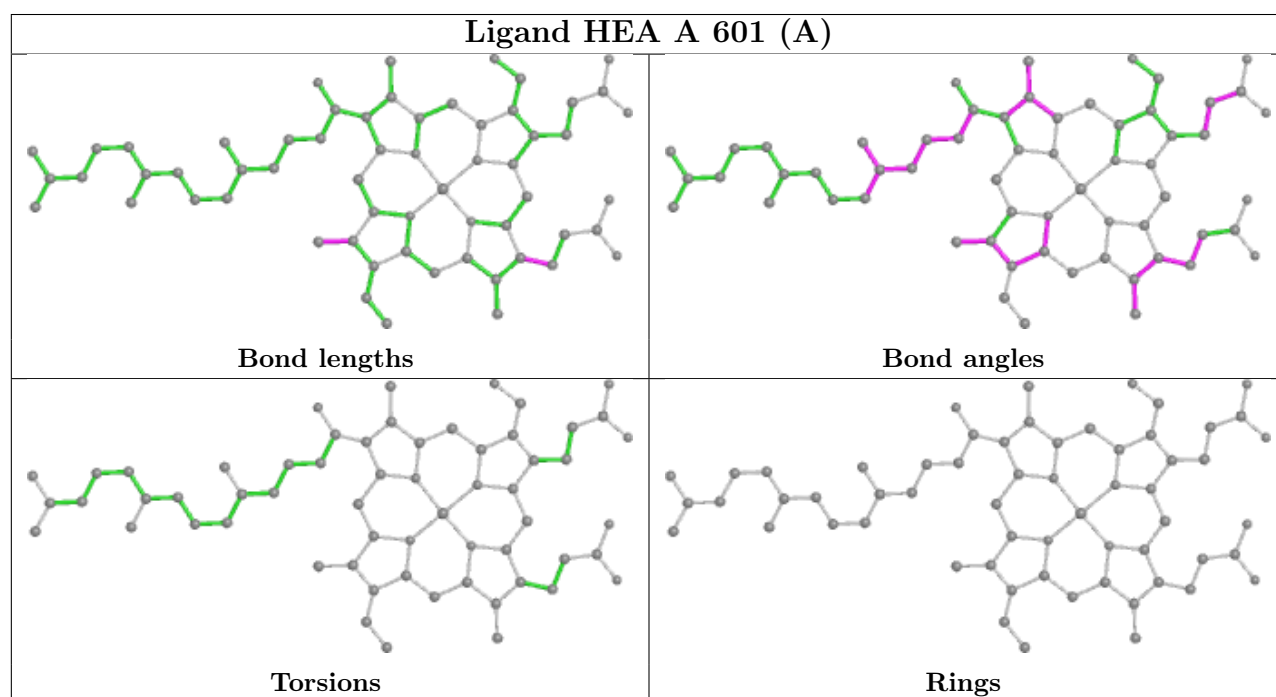
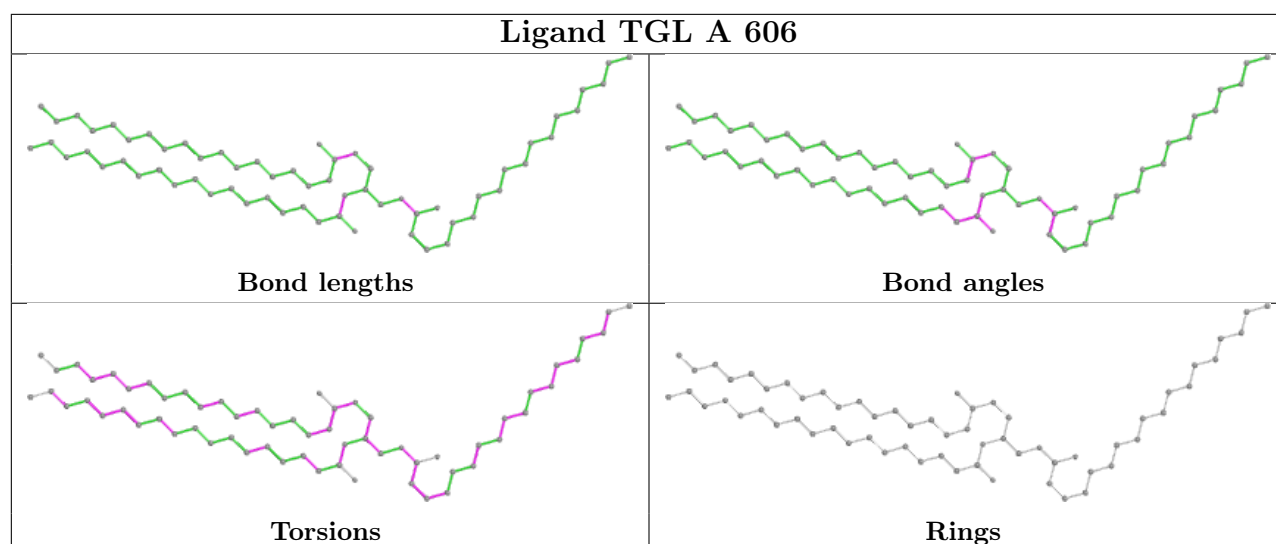


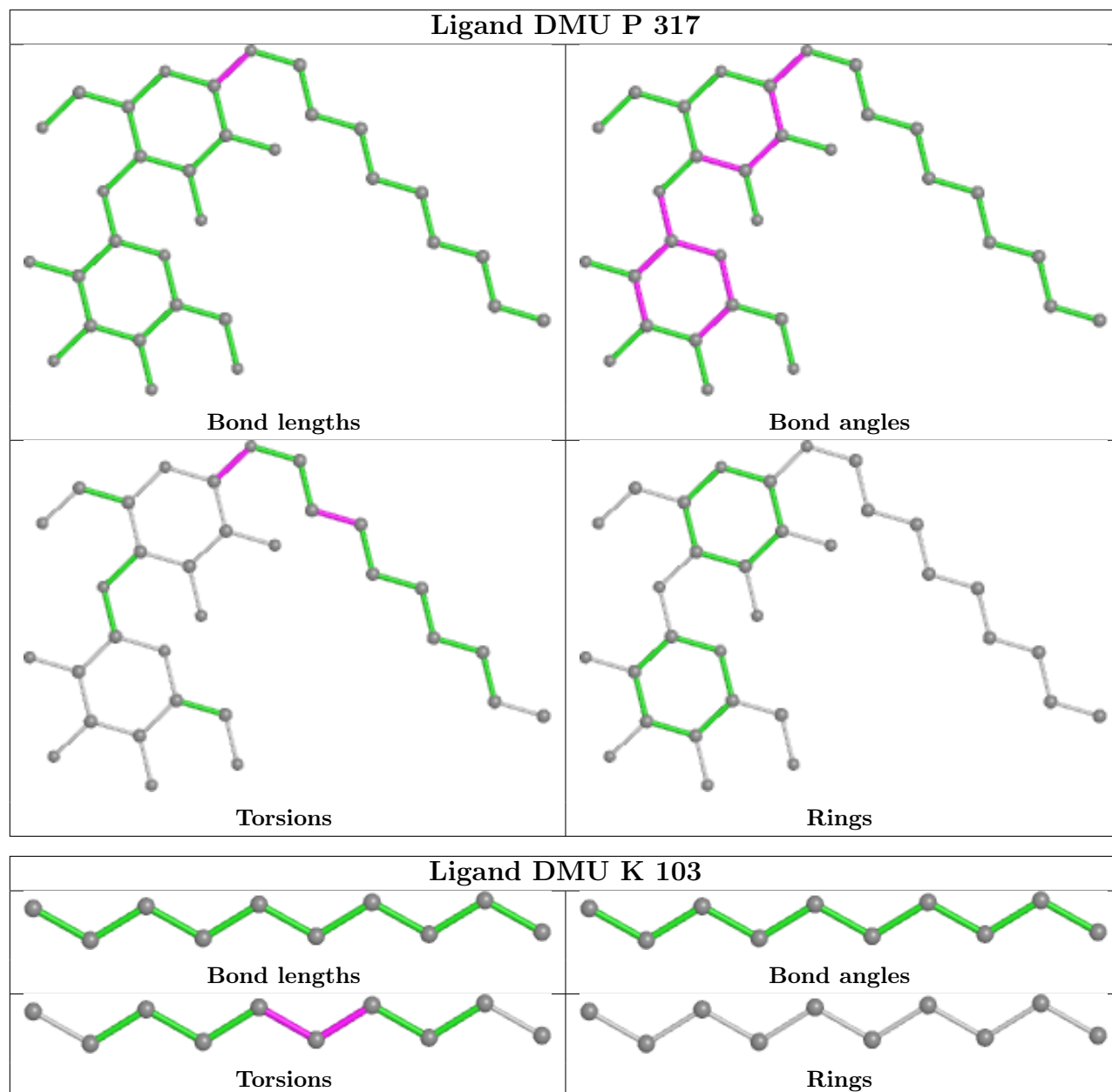


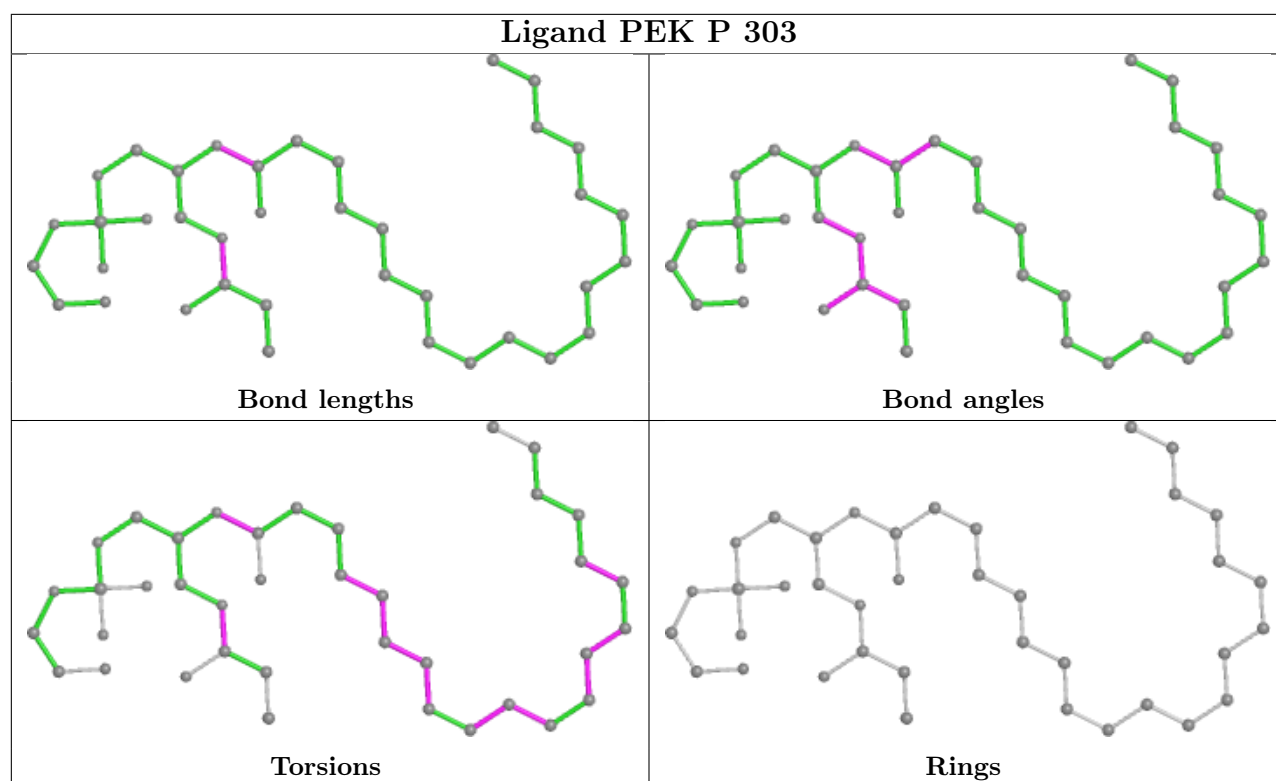












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-0.12	2 (0%) 92 92	19, 24, 33, 82	0
1	N	513/514 (99%)	-0.13	1 (0%) 95 94	19, 26, 35, 80	0
2	B	226/227 (99%)	-0.10	2 (0%) 84 84	22, 32, 61, 110	0
2	O	226/227 (99%)	-0.13	2 (0%) 84 84	25, 36, 73, 115	0
3	C	259/259 (100%)	-0.15	0 100 100	21, 27, 40, 93	0
3	P	259/259 (100%)	-0.13	0 100 100	21, 28, 43, 90	0
4	D	144/144 (100%)	-0.28	0 100 100	25, 34, 56, 93	0
4	Q	144/144 (100%)	0.34	7 (4%) 29 27	31, 48, 96, 243	0
5	E	105/105 (100%)	-0.26	1 (0%) 82 82	27, 33, 69, 156	0
5	R	105/105 (100%)	-0.17	2 (1%) 66 65	29, 42, 77, 169	0
6	F	94/94 (100%)	-0.05	3 (3%) 47 44	23, 34, 65, 130	0
6	S	94/94 (100%)	-0.02	4 (4%) 35 32	22, 31, 66, 125	0
7	G	84/84 (100%)	0.88	16 (19%) 1 1	25, 35, 140, 183	0
7	T	84/84 (100%)	0.73	16 (19%) 1 1	25, 39, 127, 194	0
8	H	79/79 (100%)	0.15	4 (5%) 28 25	26, 38, 112, 179	0
8	U	79/79 (100%)	0.16	6 (7%) 13 12	31, 42, 117, 215	0
9	I	72/73 (98%)	0.14	1 (1%) 75 75	30, 48, 86, 102	0
9	V	72/73 (98%)	0.17	2 (2%) 53 51	29, 55, 95, 161	0
10	J	58/58 (100%)	0.17	3 (5%) 27 24	27, 38, 88, 175	0
10	W	58/58 (100%)	0.04	3 (5%) 27 24	28, 39, 86, 171	0
11	K	49/49 (100%)	-0.11	0 100 100	30, 38, 59, 72	0
11	X	49/49 (100%)	0.10	2 (4%) 37 34	36, 47, 86, 100	0
12	L	46/46 (100%)	-0.18	1 (2%) 62 60	25, 30, 56, 105	0
12	Y	46/46 (100%)	-0.19	1 (2%) 62 60	28, 36, 74, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/43 (100%)	-0.03	3 (6%) 16 14	25, 30, 86, 141	0
13	Z	43/43 (100%)	0.09	5 (11%) 4 4	33, 38, 122, 190	0
All	All	3544/3550 (99%)	-0.03	87 (2%) 57 55	19, 31, 77, 243	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	17.4
10	J	58	LYS	13.6
6	F	1	ALA	13.1
4	Q	6	VAL	12.9
4	Q	5	VAL	12.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.19	0.53	201,217,238,247	0
9	SAC	I	1	9/10	0.73	0.32	129,147,176,183	0
1	FME	N	1	10/11	0.95	0.10	36,45,97,109	0
2	FME	B	1	10/11	0.96	0.11	28,31,40,126	0
1	FME	A	1	10/11	0.96	0.10	37,51,85,99	0
2	FME	O	1	10/11	0.97	0.12	31,36,44,111	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
23	DMU	X	102	9/33	0.52	0.31	65,70,82,86	0
27	CDL	N	601	62/100	0.52	0.35	44,76,103,117	0
22	EDO	P	310	4/4	0.54	0.17	71,72,75,80	0
23	DMU	X	104	22/33	0.56	0.43	58,94,150,157	0
22	EDO	A	618	4/4	0.58	0.26	52,59,65,85	0
23	DMU	A	623	11/33	0.64	0.37	62,76,106,114	0
22	EDO	F	105	4/4	0.66	0.18	56,58,67,70	0
22	EDO	C	315	4/4	0.66	0.23	65,78,87,99	0
25	CHD	J	101	29/29	0.68	0.41	50,120,146,151	0
23	DMU	L	105	21/33	0.68	0.20	54,80,107,120	0
23	DMU	D	207	11/33	0.69	0.33	58,81,115,120	0
23	DMU	P	317	32/33	0.69	0.22	52,107,133,136	0
23	DMU	Q	201	11/33	0.70	0.22	49,70,93,95	0
22	EDO	C	317	4/4	0.71	0.18	60,67,70,80	0
23	DMU	K	103	10/33	0.73	0.26	62,75,106,112	0
26	PEK	C	303	45/53	0.73	0.33	44,95,175,209	0
23	DMU	D	206	33/33	0.73	0.23	46,95,141,151	0
27	CDL	T	102	61/100	0.74	0.27	42,77,110,117	0
26	PEK	P	303	38/53	0.75	0.25	49,79,163,172	0
23	DMU	P	308	33/33	0.76	0.29	37,102,137,160	0
26	PEK	C	305	36/53	0.77	0.23	42,76,101,118	0
22	EDO	O	305	4/4	0.77	0.19	49,61,62,105	0
25	CHD	Y	102	29/29	0.78	0.24	56,91,135,152	0
23	DMU	K	102	11/33	0.78	0.24	55,70,95,105	0
23	DMU	X	103	9/33	0.78	0.23	56,62,103,104	0
22	EDO	T	104	4/4	0.78	0.26	56,73,98,107	0
22	EDO	P	315	4/4	0.78	0.17	66,95,100,113	0
25	CHD	L	102	29/29	0.78	0.30	51,95,117,134	0
22	EDO	C	311	4/4	0.79	0.16	44,65,68,73	0
22	EDO	C	320	4/4	0.79	0.35	33,68,70,73	0
18	TGL	N	609	55/63	0.79	0.21	46,72,112,119	0
22	EDO	N	620	4/4	0.80	0.20	52,52,53,80	0
19	PGV	P	306	31/51	0.80	0.25	32,72,96,109	0
21	PSC	O	302	31/52	0.80	0.23	36,62,106,153	0
26	PEK	T	101	37/53	0.80	0.26	43,75,105,131	0
22	EDO	A	612	4/4	0.80	0.24	51,51,71,101	0
22	EDO	L	103	4/4	0.80	0.22	42,49,64,119	0
23	DMU	P	316	21/33	0.81	0.17	51,81,126,136	0
22	EDO	A	617	4/4	0.81	0.27	57,70,72,73	0
22	EDO	L	104	4/4	0.81	0.24	50,51,79,128	0
25	CHD	C	309	29/29	0.83	0.27	47,86,113,140	0
22	EDO	P	314	4/4	0.83	0.14	37,53,55,74	0
21	PSC	A	610	25/52	0.83	0.22	44,70,88,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	PGV	N	610	51/51	0.83	0.28	40,83,151,204	0
18	TGL	A	607	63/63	0.83	0.21	32,68,117,128	0
19	PGV	A	608	34/51	0.84	0.23	32,57,110,126	0
18	TGL	N	608	55/63	0.84	0.20	38,64,110,123	0
22	EDO	A	620	4/4	0.84	0.19	44,52,61,82	0
18	TGL	L	101	63/63	0.85	0.21	25,60,114,165	0
18	TGL	N	607	63/63	0.85	0.24	40,79,108,125	0
23	DMU	O	306	13/33	0.85	0.19	45,66,128,139	0
27	CDL	C	308	65/100	0.85	0.24	37,69,123,156	0
19	PGV	C	307	36/51	0.85	0.25	41,74,140,164	0
18	TGL	A	606	63/63	0.85	0.17	39,72,108,119	0
22	EDO	N	619	4/4	0.86	0.15	40,78,80,94	0
22	EDO	F	102	4/4	0.86	0.11	33,36,53,121	0
27	CDL	P	307	68/100	0.86	0.24	39,76,127,157	0
23	DMU	C	310	33/33	0.86	0.24	35,81,151,167	0
22	EDO	B	305	4/4	0.87	0.14	28,36,44,63	0
22	EDO	P	309	4/4	0.87	0.18	60,63,63,69	0
23	DMU	K	104	11/33	0.87	0.20	50,68,100,112	0
23	DMU	J	104	11/33	0.87	0.17	49,60,84,99	0
22	EDO	J	103	4/4	0.88	0.26	59,62,62,75	0
22	EDO	C	319	4/4	0.88	0.25	43,47,61,111	0
22	EDO	F	103	4/4	0.88	0.14	44,51,53,59	0
22	EDO	C	313	4/4	0.88	0.14	30,39,40,49	0
23	DMU	C	321	12/33	0.89	0.13	51,66,84,89	0
23	DMU	X	101	10/33	0.89	0.15	41,60,84,103	0
22	EDO	W	101	4/4	0.89	0.18	54,56,71,77	0
22	EDO	S	104	4/4	0.89	0.13	44,46,48,54	0
22	EDO	A	614	4/4	0.89	0.19	51,61,65,80	0
23	DMU	Z	101	33/33	0.89	0.11	37,47,68,72	0
22	EDO	C	312	4/4	0.90	0.12	32,33,33,82	0
22	EDO	M	102	4/4	0.90	0.33	68,86,88,93	0
22	EDO	C	316	4/4	0.90	0.13	49,55,70,77	0
23	DMU	K	101	8/33	0.90	0.18	48,63,77,85	0
22	EDO	D	205	4/4	0.90	0.33	53,58,59,61	0
22	EDO	A	616	4/4	0.90	0.32	31,40,42,78	0
22	EDO	P	313	4/4	0.91	0.18	49,54,61,76	0
23	DMU	M	101	33/33	0.91	0.11	35,41,54,65	0
22	EDO	B	306	4/4	0.92	0.15	38,47,48,48	0
22	EDO	Q	202	4/4	0.92	0.17	41,46,48,52	0
22	EDO	J	102	4/4	0.92	0.17	48,48,91,98	0
22	EDO	D	201	4/4	0.92	0.21	39,49,70,82	0
22	EDO	P	311	4/4	0.92	0.13	33,37,37,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	W	102	4/4	0.92	0.24	46,63,67,113	0
22	EDO	D	204	4/4	0.92	0.32	41,43,50,59	0
22	EDO	O	304	4/4	0.92	0.13	46,46,48,52	0
29	PO4	U	101	5/5	0.92	0.20	51,53,120,124	0
22	EDO	N	622	4/4	0.93	0.18	30,34,50,92	0
22	EDO	N	614	4/4	0.93	0.11	38,39,40,40	0
22	EDO	F	109	4/4	0.93	0.19	35,36,71,71	0
22	EDO	A	621	4/4	0.93	0.17	37,40,40,52	0
23	DMU	K	105	9/33	0.93	0.16	38,52,70,105	0
22	EDO	F	108	4/4	0.94	0.16	37,42,79,101	0
22	EDO	S	106	4/4	0.94	0.14	37,52,72,76	0
22	EDO	C	318	4/4	0.94	0.20	40,60,68,94	0
17	NA	C	302	1/1	0.94	0.09	36,36,36,36	0
22	EDO	E	203	4/4	0.94	0.12	49,49,49,75	0
22	EDO	Y	101	4/4	0.94	0.15	48,51,53,64	0
22	EDO	A	622	4/4	0.95	0.22	32,37,42,42	0
22	EDO	N	615	4/4	0.95	0.09	38,41,42,58	0
22	EDO	T	103	4/4	0.95	0.11	30,30,38,40	0
25	CHD	C	301	29/29	0.95	0.09	26,29,39,44	0
22	EDO	N	616	4/4	0.95	0.16	33,40,44,86	0
22	EDO	T	105	4/4	0.95	0.15	37,48,58,62	0
22	EDO	F	107	4/4	0.95	0.15	45,50,81,119	0
25	CHD	P	301	29/29	0.95	0.09	26,30,35,44	0
22	EDO	C	314	4/4	0.95	0.18	31,35,53,60	0
20	PER	A	609[A]	2/2	0.96	0.12	20,20,20,24	2
22	EDO	A	615	4/4	0.96	0.11	26,26,28,33	0
25	CHD	G	101	29/29	0.96	0.10	20,26,34,40	0
19	PGV	N	612	51/51	0.96	0.13	24,31,73,93	0
22	EDO	D	203	4/4	0.96	0.14	37,40,57,68	0
26	PEK	P	304	52/53	0.96	0.13	28,43,96,117	0
22	EDO	N	613	4/4	0.97	0.10	24,27,28,32	0
17	NA	P	302	1/1	0.97	0.10	38,38,38,38	0
22	EDO	P	312	4/4	0.97	0.11	28,39,39,57	0
16	MG	A	604	1/1	0.97	0.06	18,18,18,18	0
20	PER	N	611[A]	2/2	0.97	0.15	20,20,20,31	2
22	EDO	G	102	4/4	0.97	0.07	25,32,32,34	0
26	PEK	C	304	52/53	0.97	0.13	25,42,97,111	0
19	PGV	A	611	51/51	0.97	0.13	19,30,73,90	0
22	EDO	S	103	4/4	0.97	0.08	32,33,43,43	0
22	EDO	N	621	4/4	0.97	0.29	39,41,43,116	0
22	EDO	S	105	4/4	0.97	0.14	29,31,32,32	0
22	EDO	B	304	4/4	0.97	0.14	33,43,55,80	0

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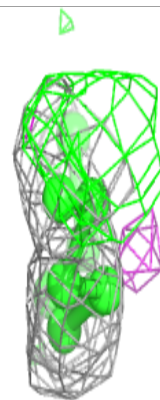
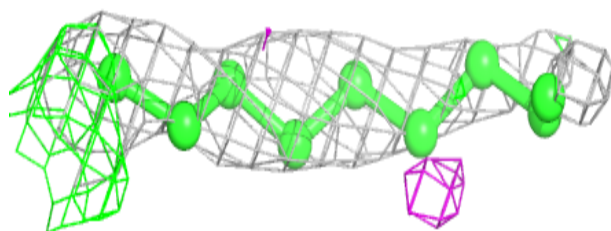
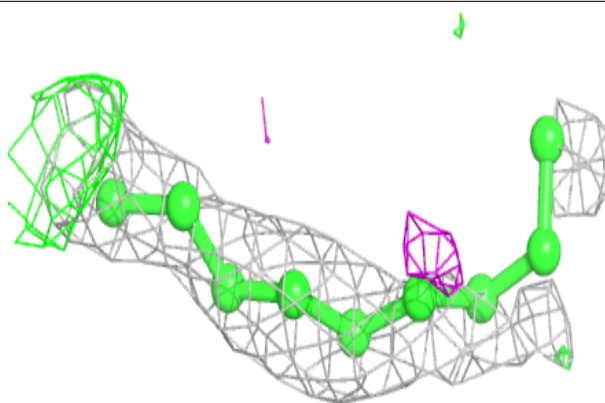
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	PGV	P	305	51/51	0.97	0.14	22,31,87,120	0
25	CHD	B	302	29/29	0.97	0.09	21,27,36,50	0
22	EDO	D	202	4/4	0.97	0.15	43,43,57,86	0
29	PO4	H	101	5/5	0.97	0.22	62,62,77,101	0
22	EDO	F	106	4/4	0.97	0.11	30,31,32,32	0
14	HEA	A	602	60/60	0.98	0.10	16,21,30,37	0
22	EDO	E	201	4/4	0.98	0.13	38,39,40,40	0
22	EDO	E	202	4/4	0.98	0.11	37,37,41,43	0
14	HEA	N	602[A]	60/60	0.98	0.12	18,24,38,44	18
14	HEA	N	602[B]	54/60	0.98	0.12	15,24,33,40	12
22	EDO	S	102	4/4	0.98	0.12	20,22,22,24	0
14	HEA	N	602[C]	51/60	0.98	0.12	16,24,28,33	9
22	EDO	N	617	4/4	0.98	0.12	20,26,28,31	0
22	EDO	N	618	4/4	0.98	0.16	29,42,46,46	0
22	EDO	A	619	4/4	0.98	0.12	28,42,71,95	0
22	EDO	S	107	4/4	0.98	0.18	28,45,48,62	0
14	HEA	N	603	60/60	0.98	0.10	18,23,28,37	0
14	HEA	A	601[A]	60/60	0.98	0.13	17,21,40,61	18
14	HEA	A	601[B]	54/60	0.98	0.13	9,20,29,45	12
22	EDO	O	303	4/4	0.98	0.11	25,29,30,31	0
22	EDO	B	303	4/4	0.98	0.09	21,25,26,32	0
17	NA	N	606	1/1	0.98	0.07	30,30,30,30	0
19	PGV	C	306	48/51	0.98	0.13	21,28,66,92	0
22	EDO	A	613	4/4	0.98	0.14	21,24,30,30	0
14	HEA	A	601[C]	51/60	0.98	0.13	9,20,24,40	9
16	MG	N	605	1/1	0.99	0.05	21,21,21,21	0
28	ZN	S	101	1/1	0.99	0.11	25,25,25,25	0
17	NA	A	605	1/1	0.99	0.08	24,24,24,24	0
22	EDO	F	104	4/4	0.99	0.13	22,24,25,27	0
15	CU	A	603	1/1	1.00	0.15	23,23,23,23	0
28	ZN	F	101	1/1	1.00	0.11	26,26,26,26	0
24	CUA	B	301	2/2	1.00	0.13	22,22,22,23	0
24	CUA	O	301	2/2	1.00	0.12	26,26,26,26	0
15	CU	N	604	1/1	1.00	0.14	24,24,24,24	0

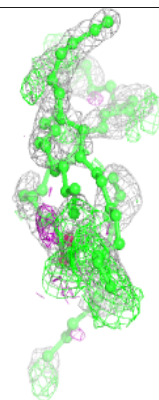
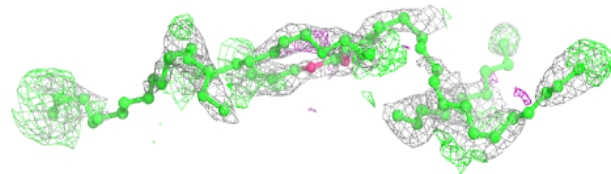
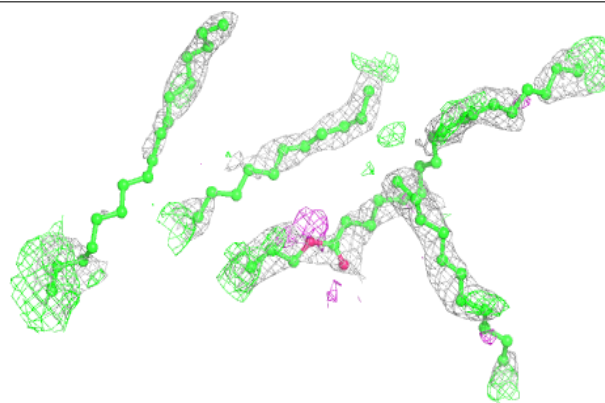
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DMU X 102:**

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

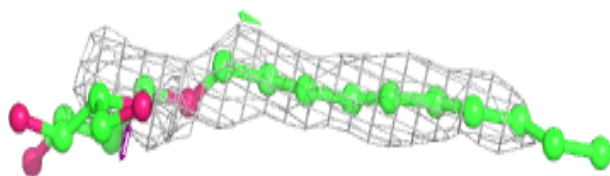
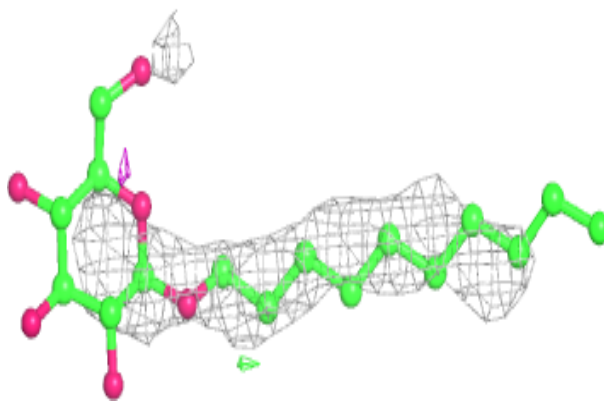
**Electron density around CDL N 601:**

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



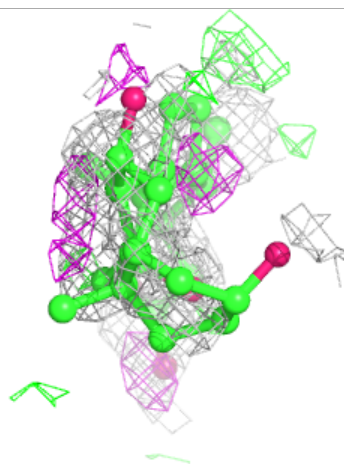
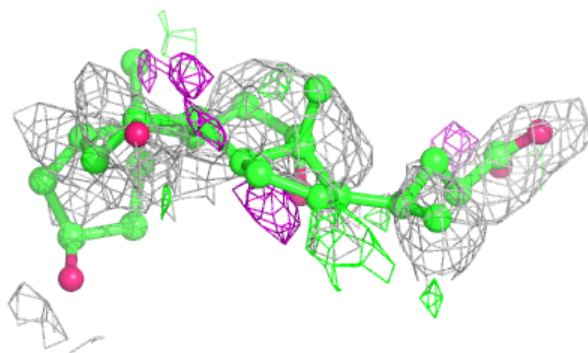
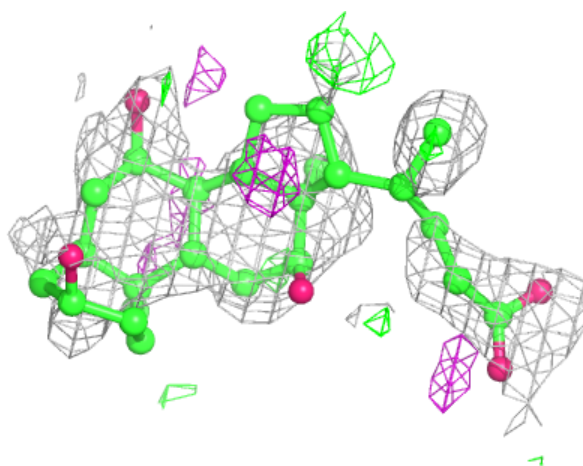
**Electron density around DMU X 104:**

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



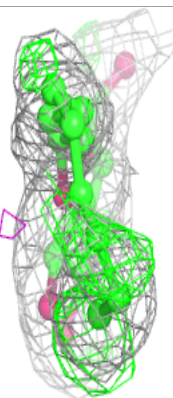
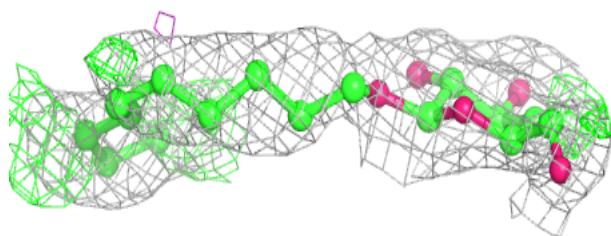
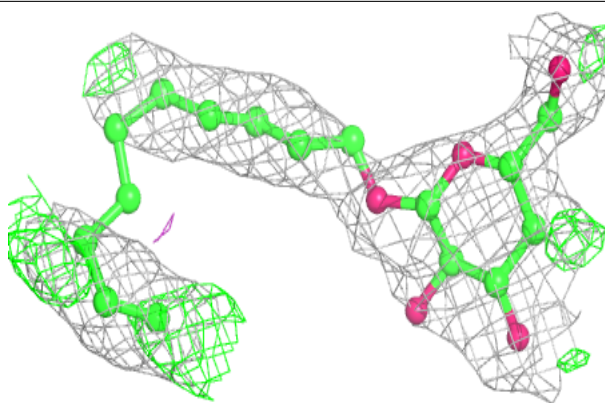
**Electron density around CHD J 101:**

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

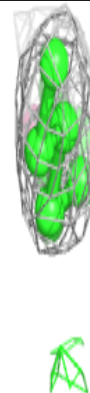
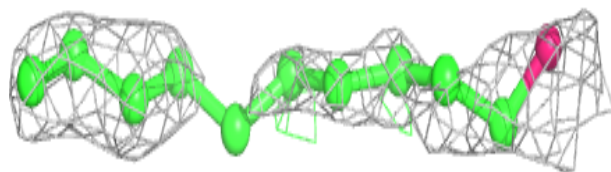
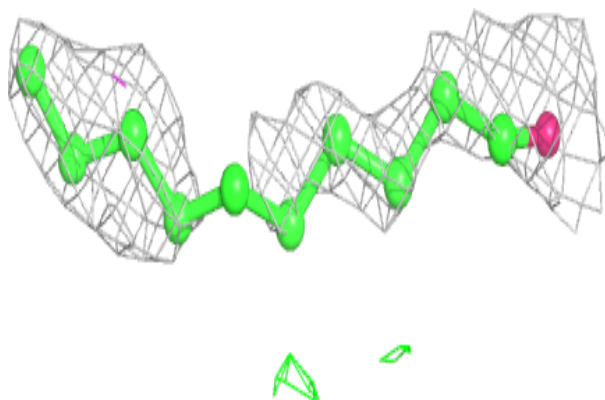


**Electron density around DMU L 105:**

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

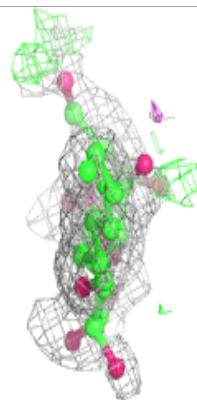
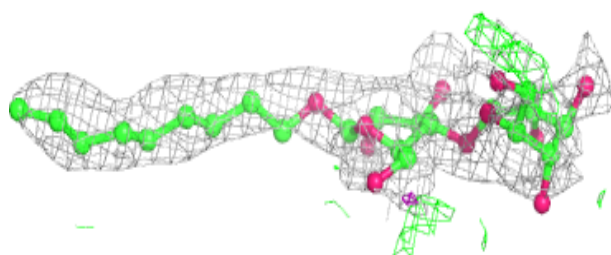
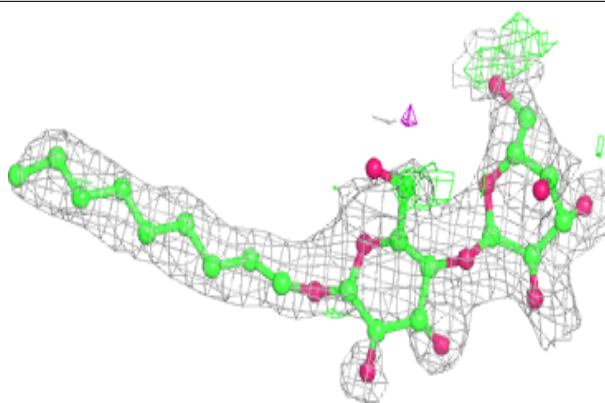
**Electron density around DMU D 207:**

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

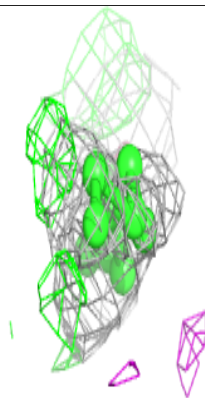
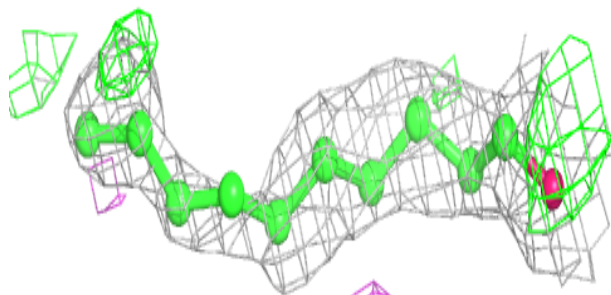
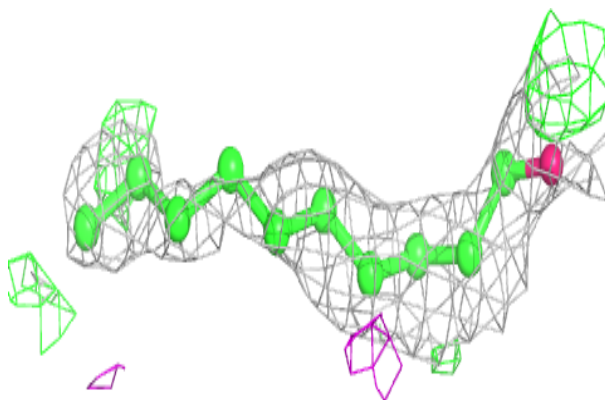


**Electron density around DMU P 317:**

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

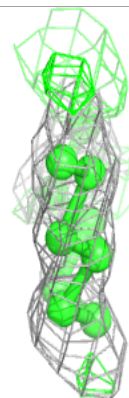
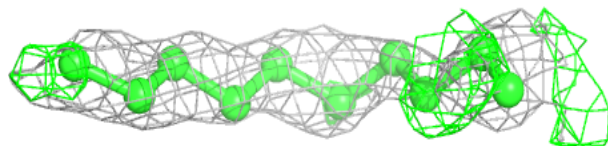
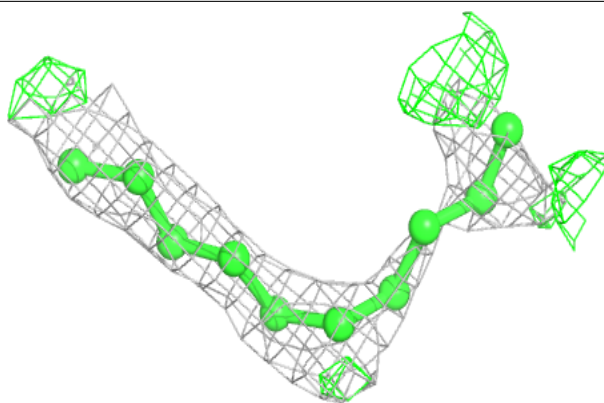
**Electron density around DMU Q 201:**

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



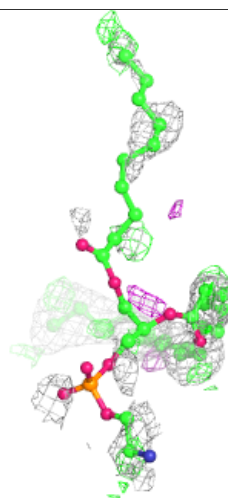
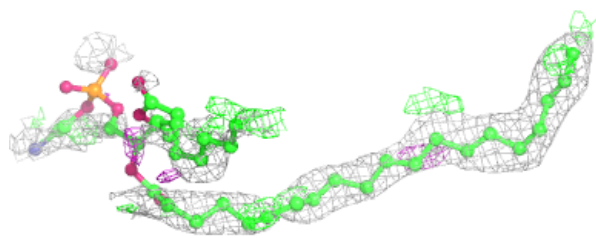
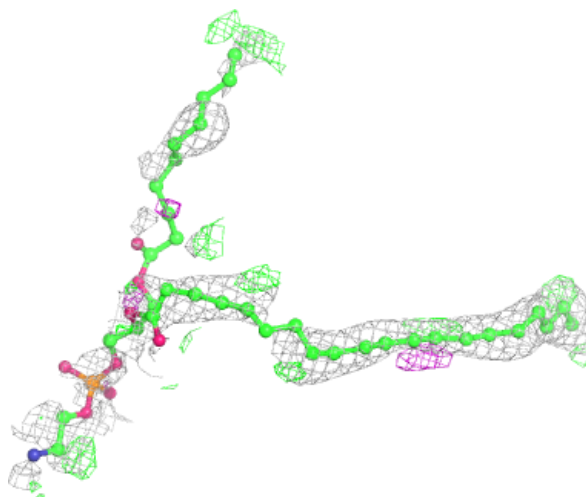
**Electron density around DMU K 103:**

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



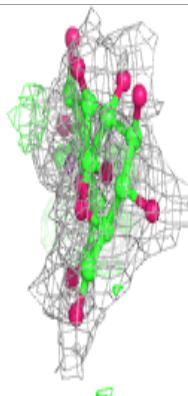
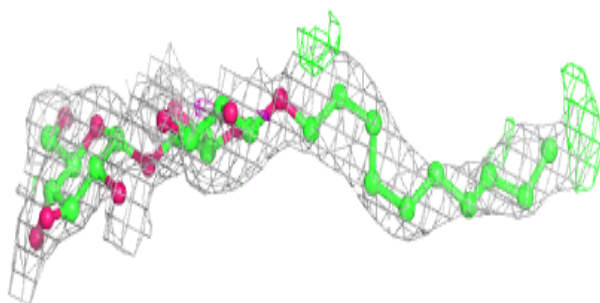
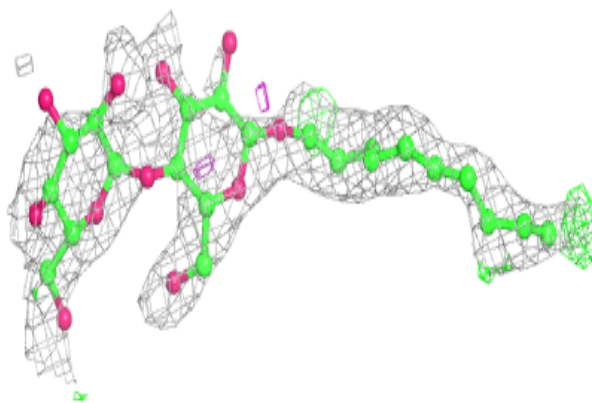
**Electron density around PEK C 303:**

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

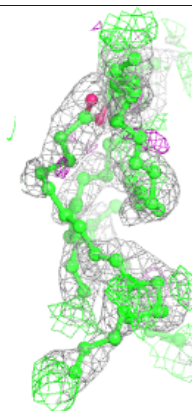
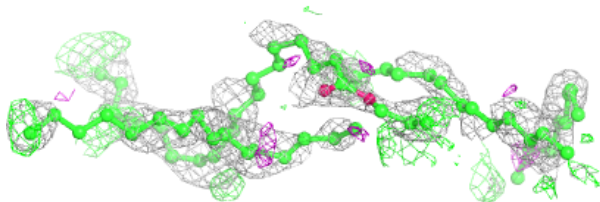
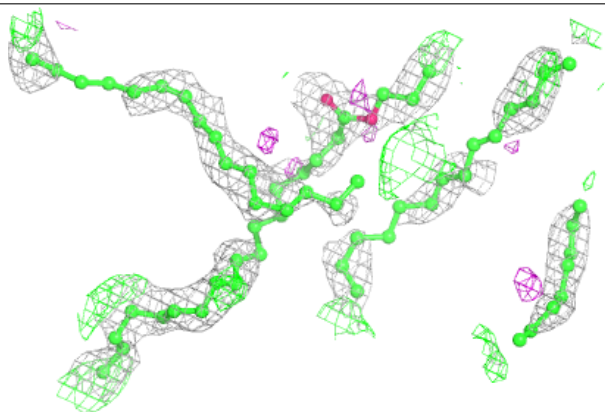


**Electron density around DMU D 206:**

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

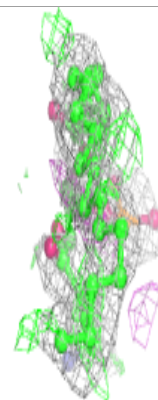
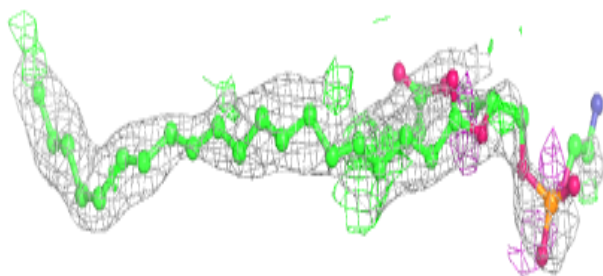
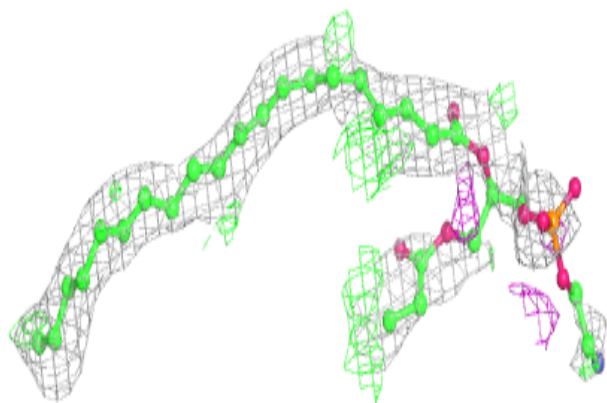
**Electron density around CDL T 102:**

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

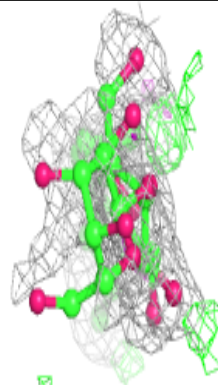
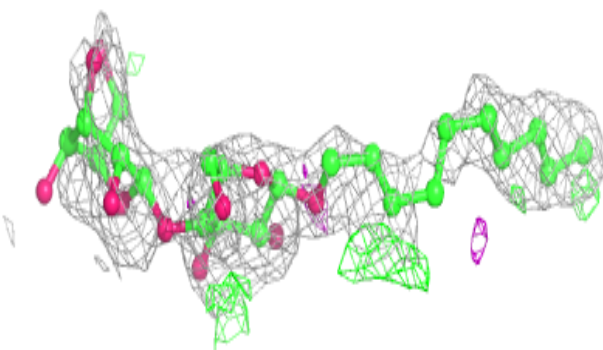
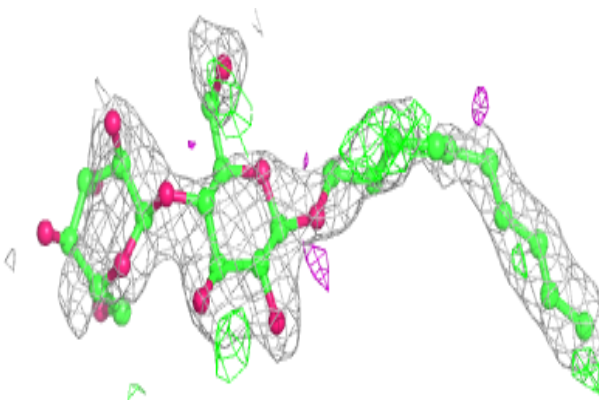


**Electron density around PEK P 303:**

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

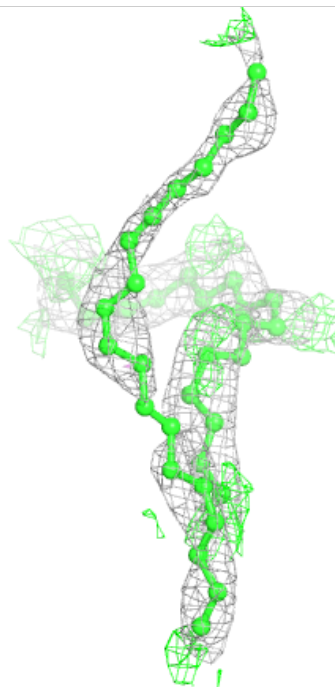
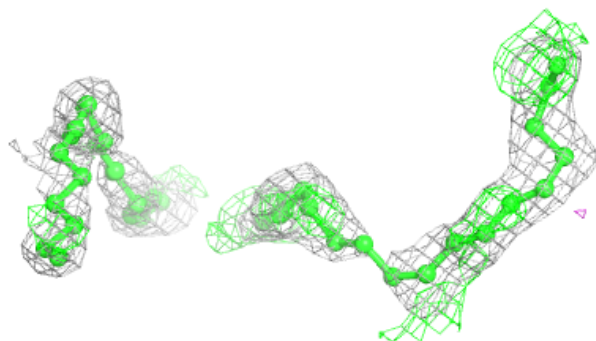
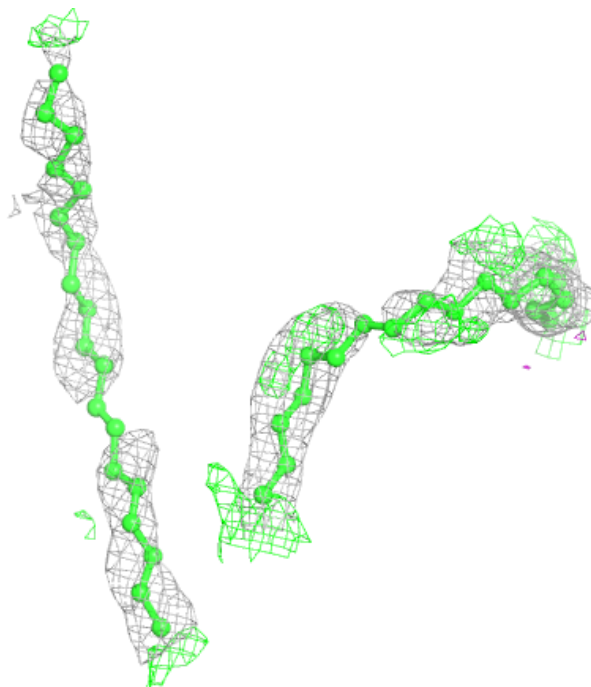
**Electron density around DMU P 308:**

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



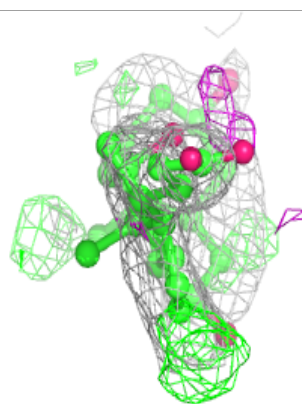
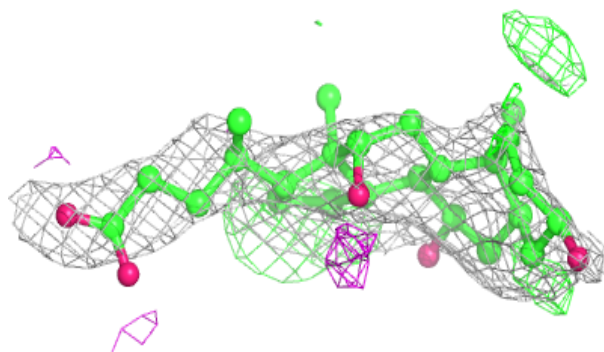
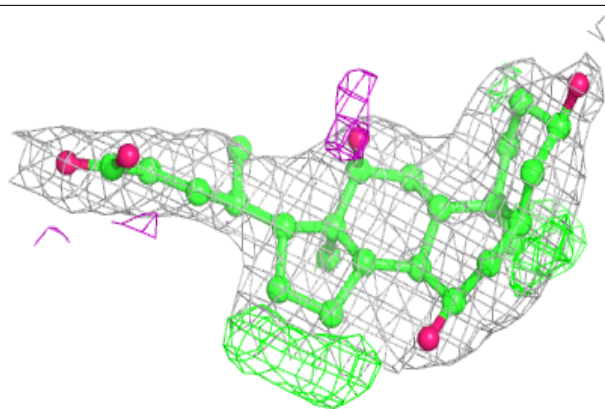
**Electron density around PEK C 305:**

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

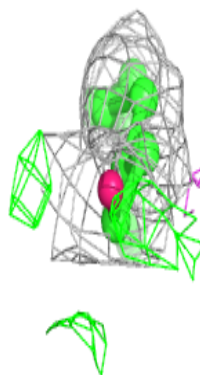
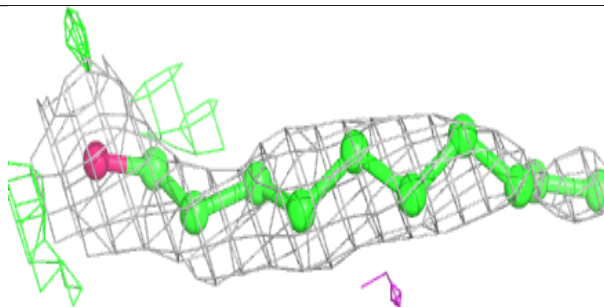
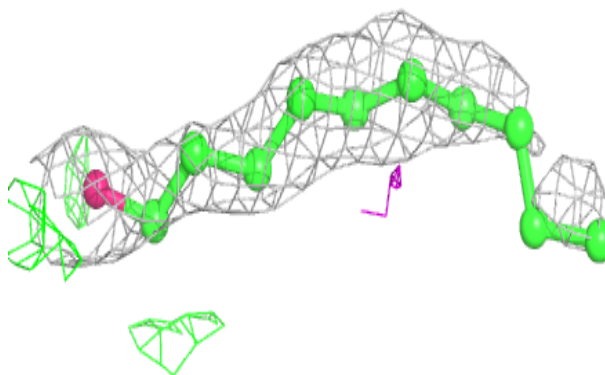


**Electron density around CHD Y 102:**

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

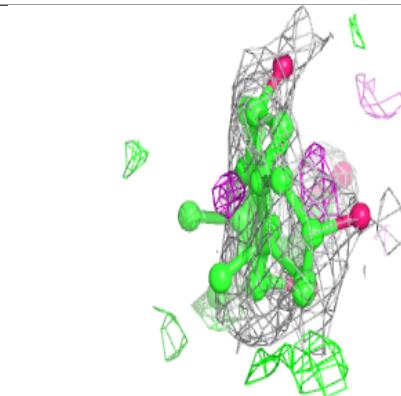
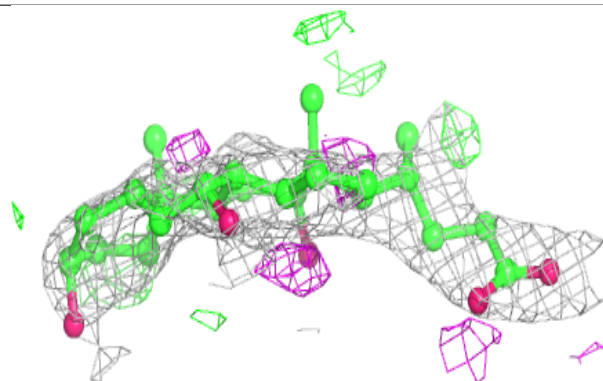
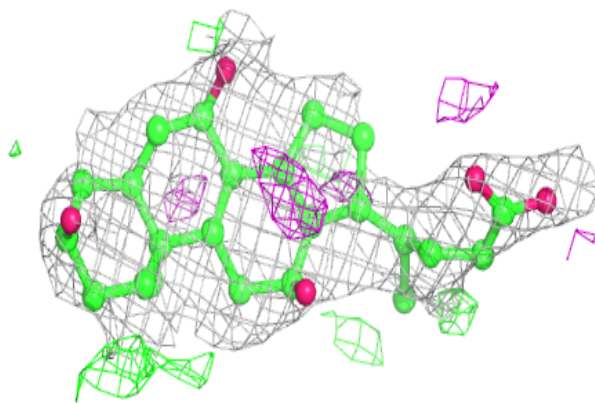
**Electron density around DMU K 102:**

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

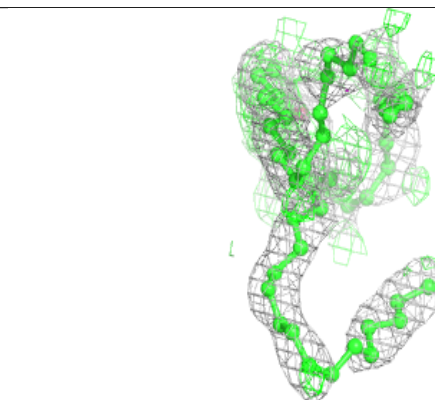
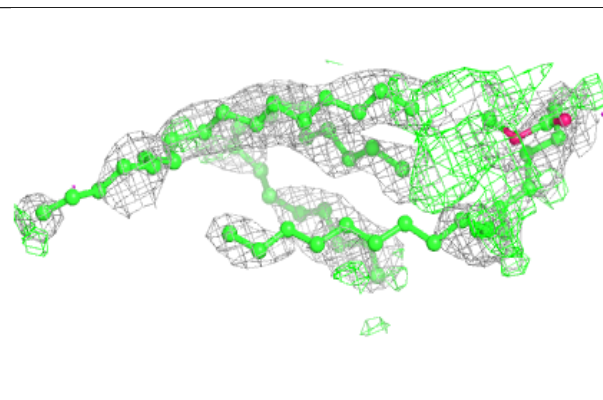
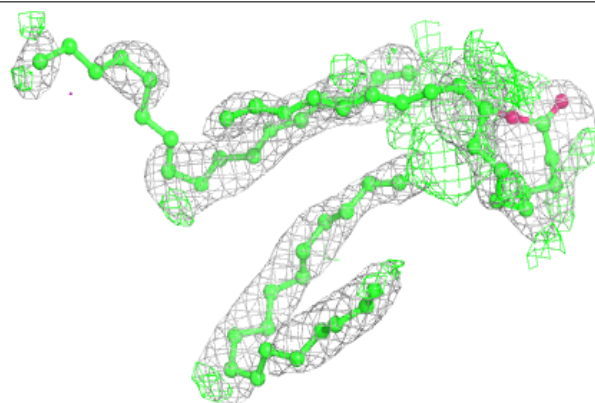


**Electron density around CHD L 102:**

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

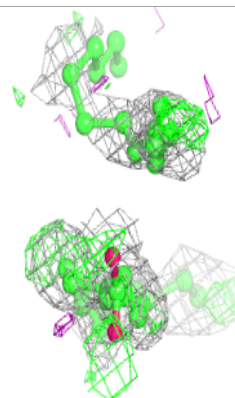
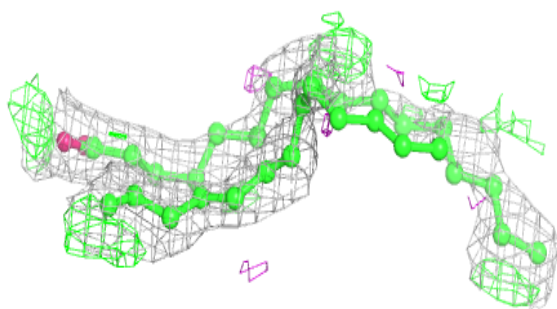
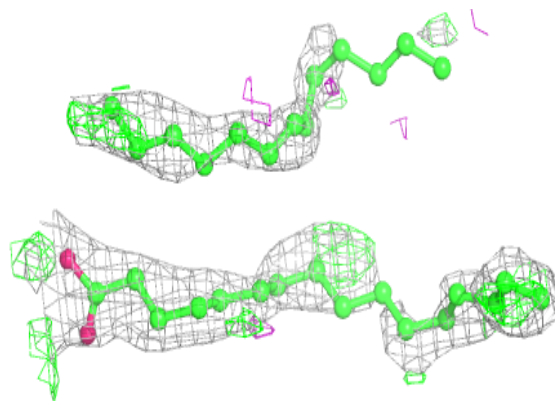
**Electron density around TGL N 609:**

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

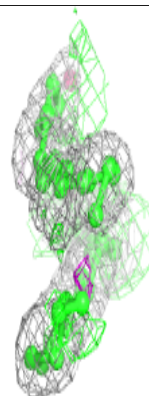
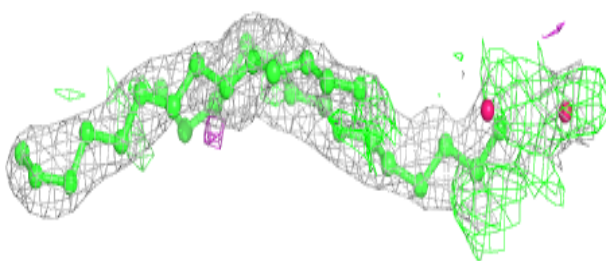
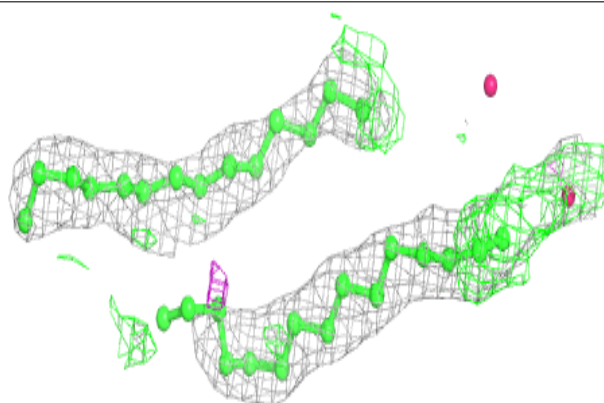


**Electron density around PGV P 306:**

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

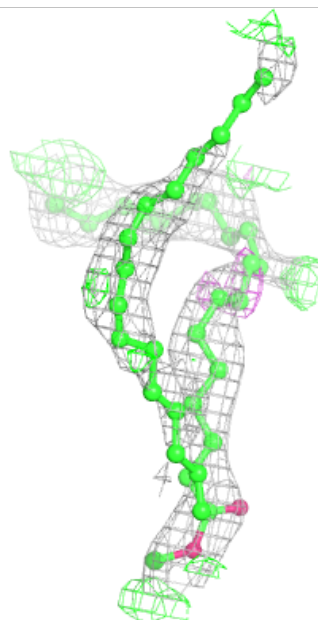
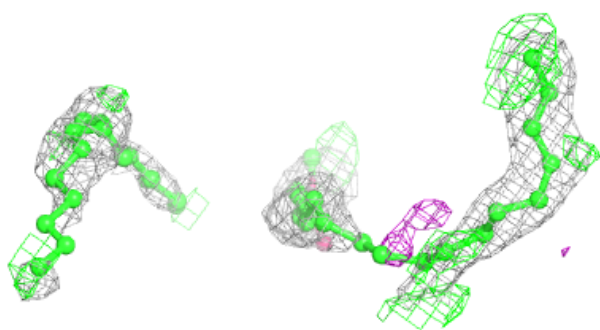
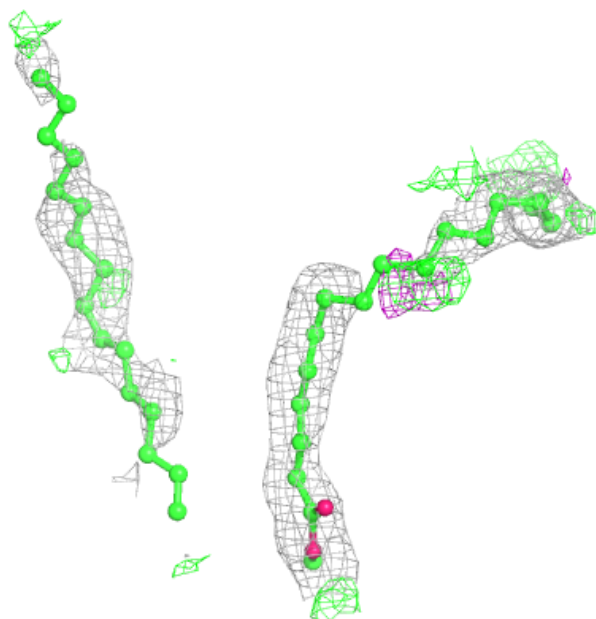
**Electron density around PSC O 302:**

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



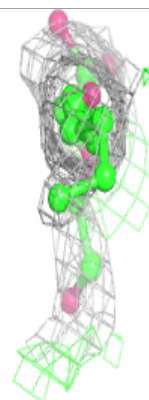
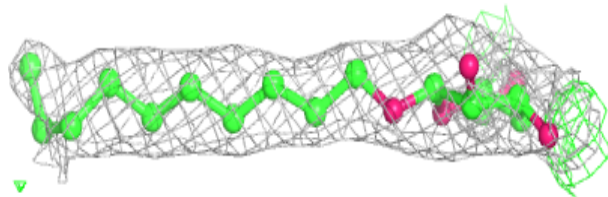
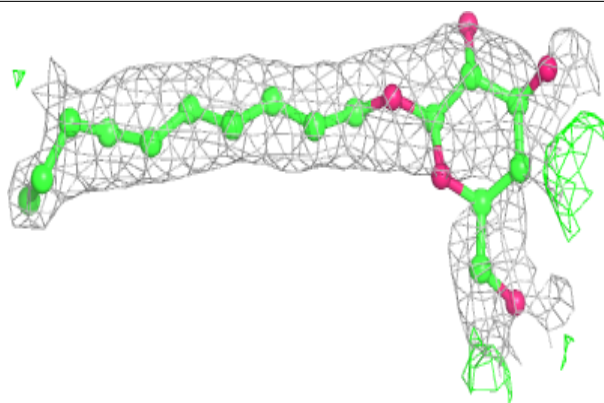
**Electron density around PEK T 101:**

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

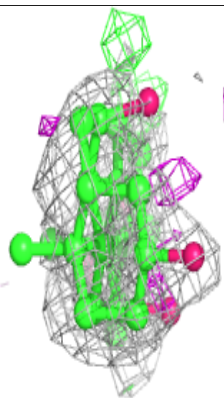
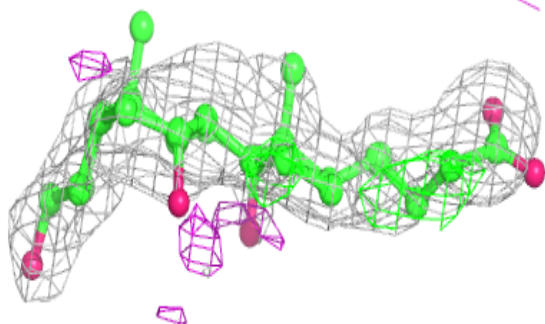
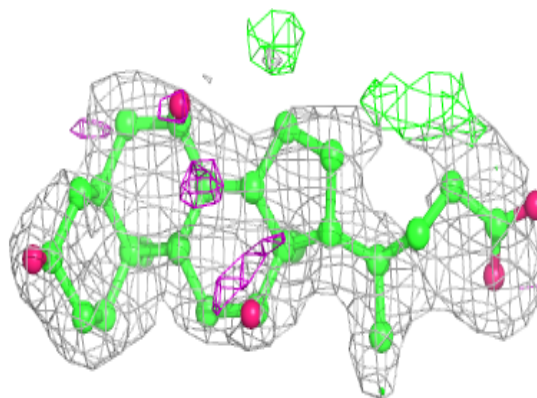


**Electron density around DMU P 316:**

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

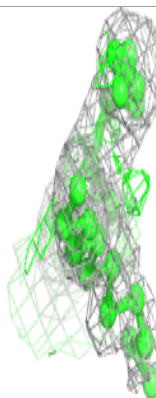
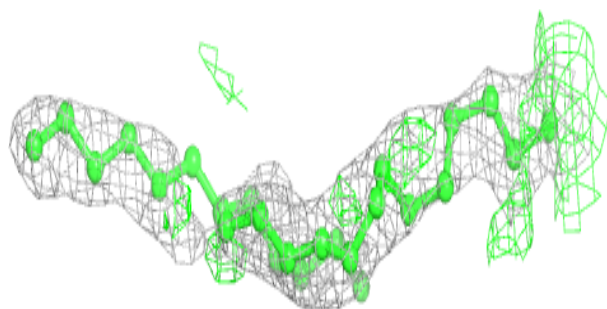
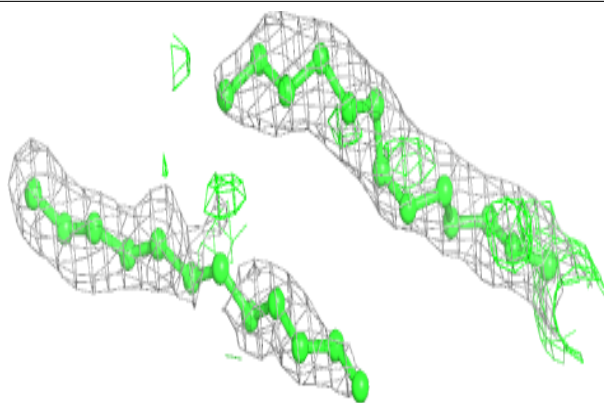
**Electron density around CHD C 309:**

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

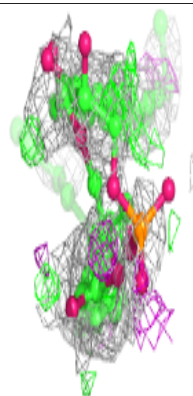
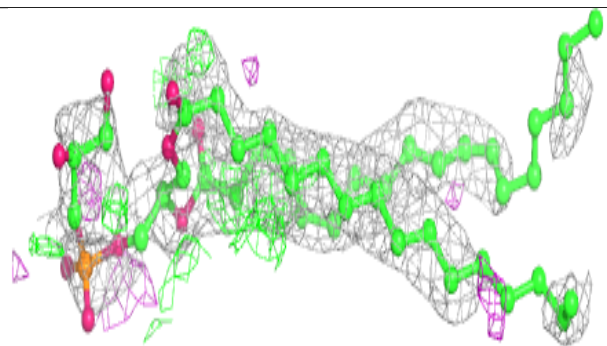
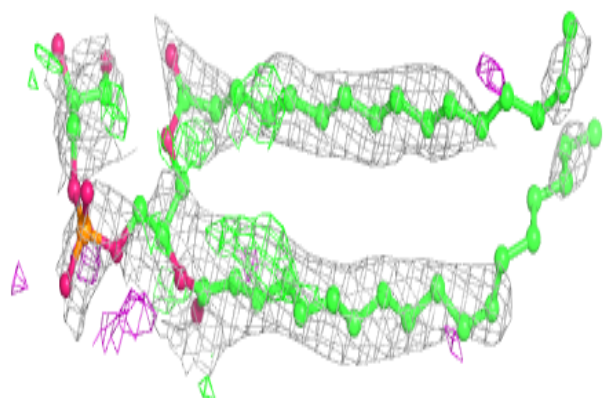


**Electron density around PSC A 610:**

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

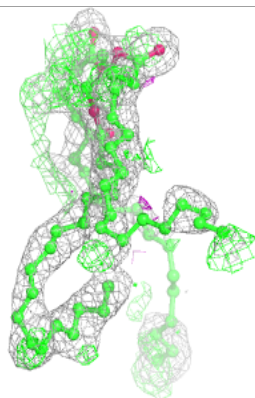
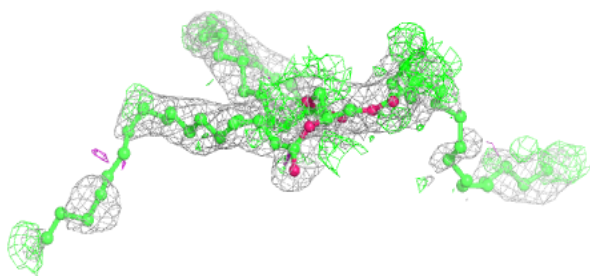
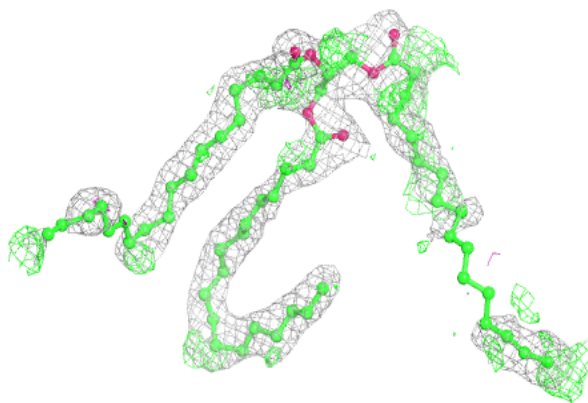
**Electron density around PGV N 610:**

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

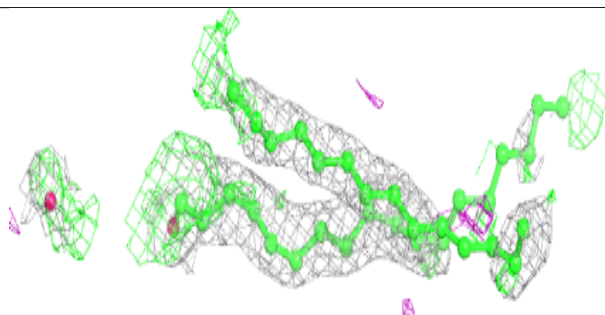
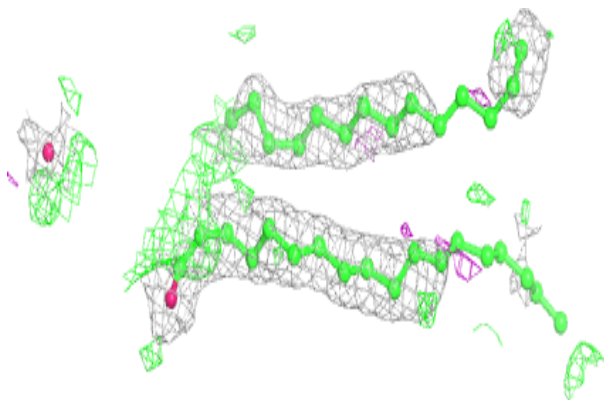


**Electron density around TGL A 607:**

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

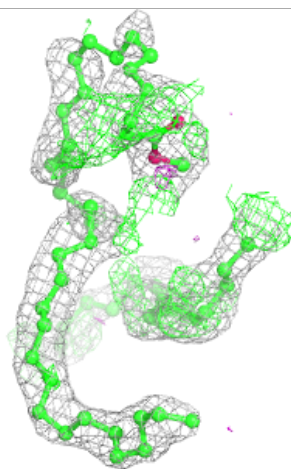
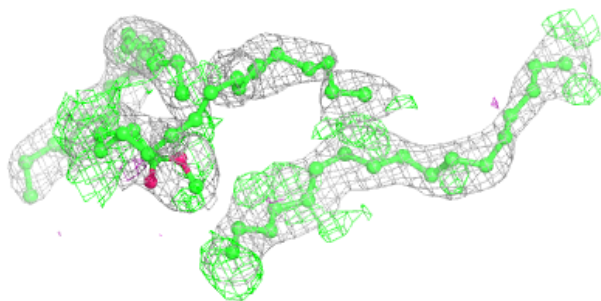
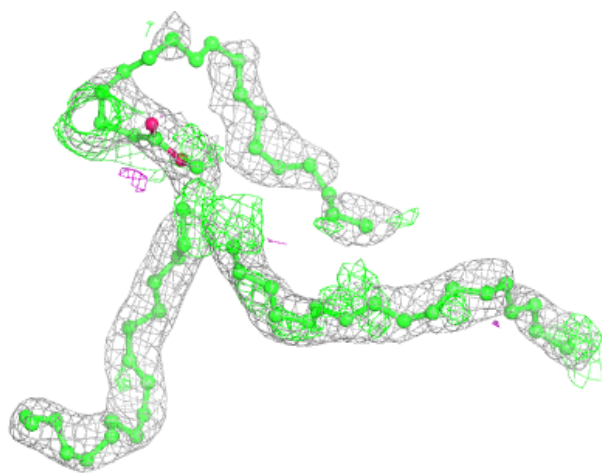
**Electron density around PGV A 608:**

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



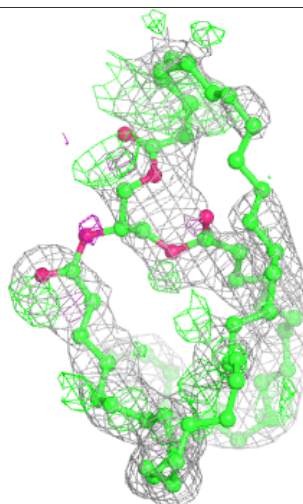
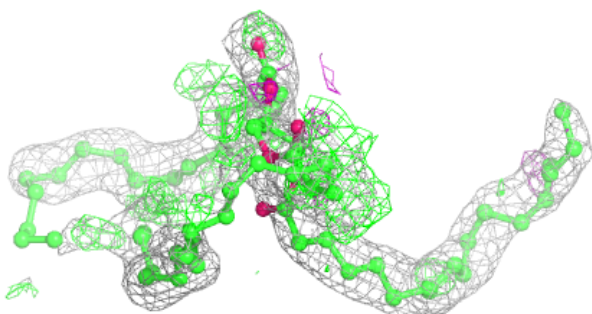
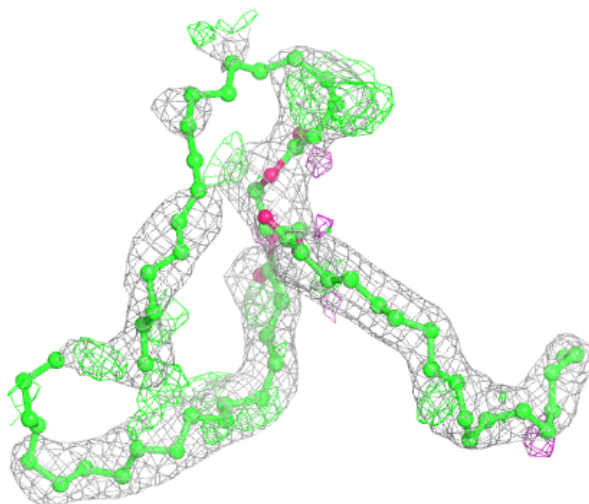
**Electron density around TGL N 608:**

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



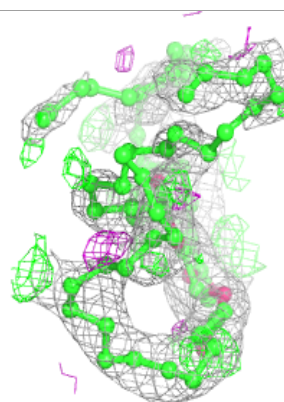
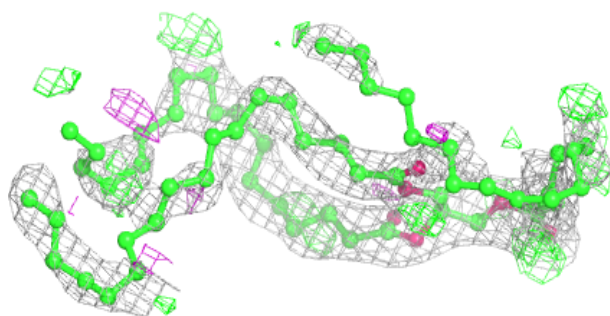
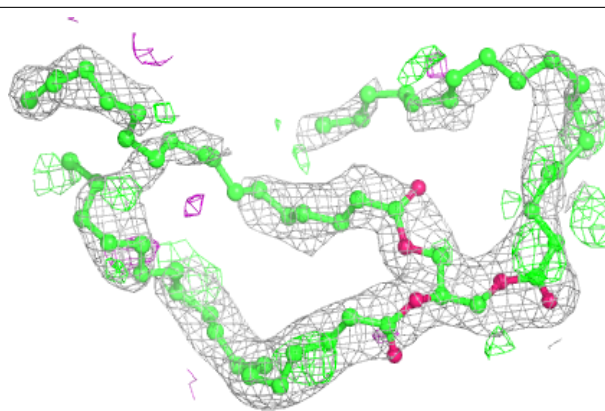
**Electron density around TGL L 101:**

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

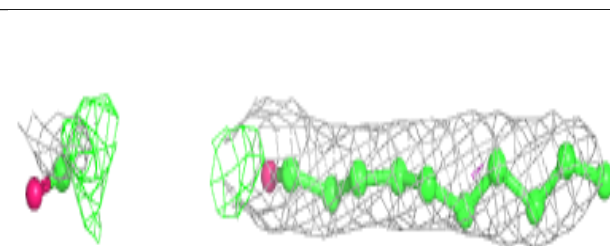
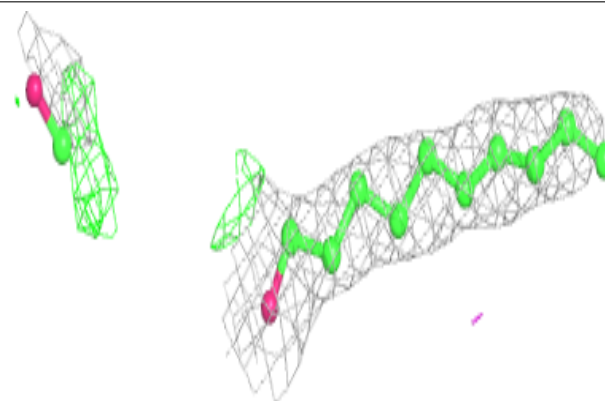


**Electron density around TGL N 607:**

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

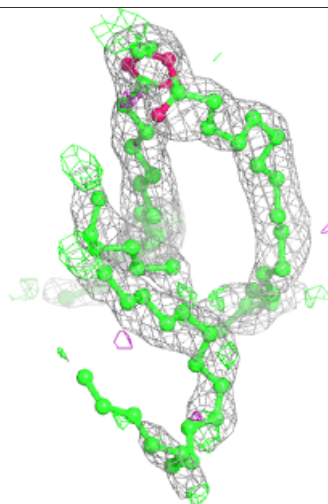
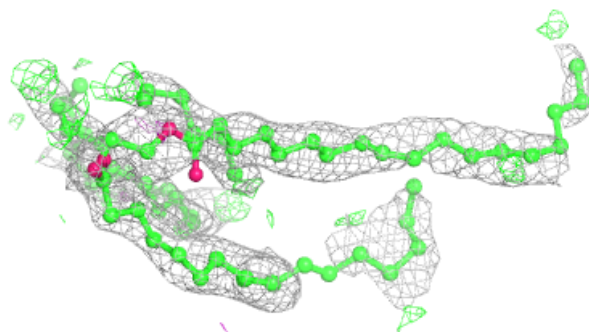
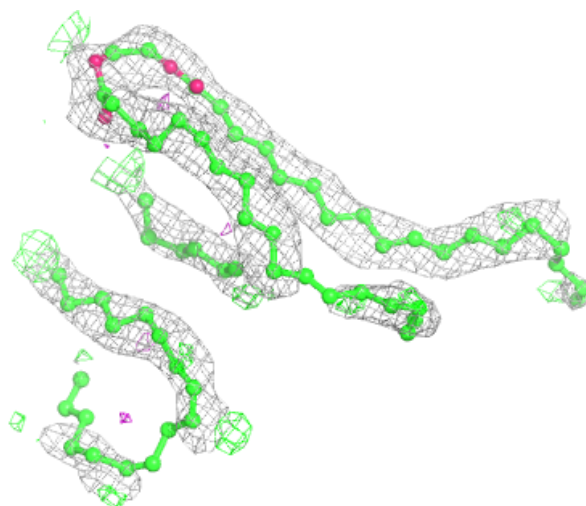
**Electron density around DMU O 306:**

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



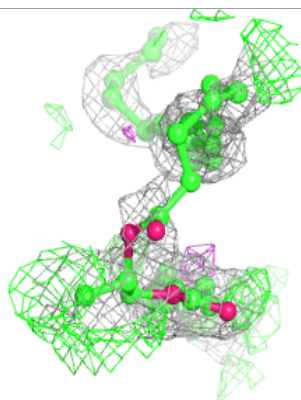
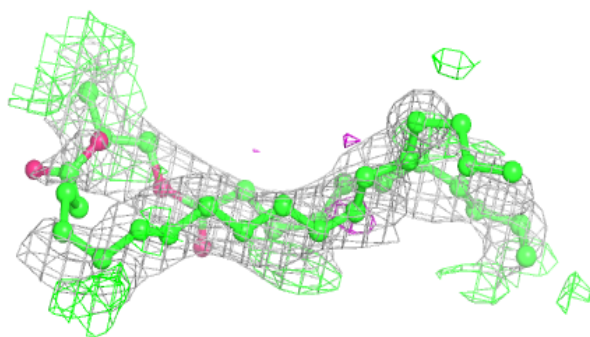
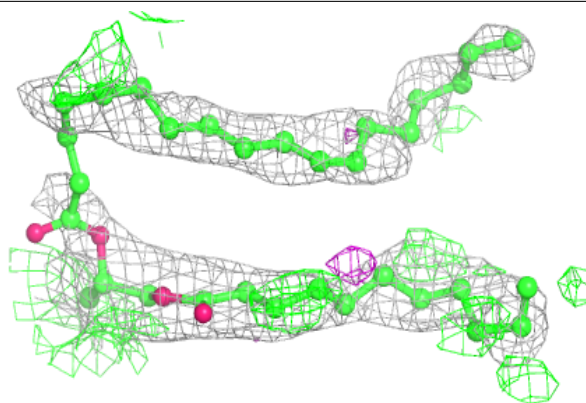
**Electron density around CDL C 308:**

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

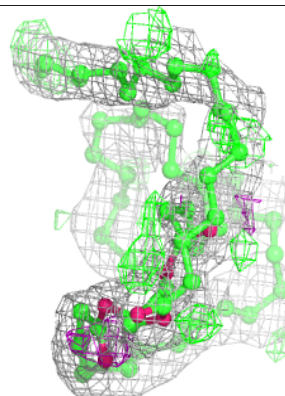
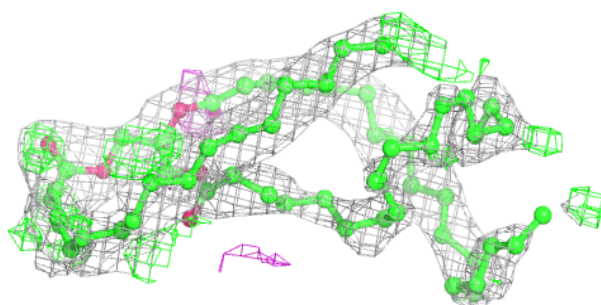
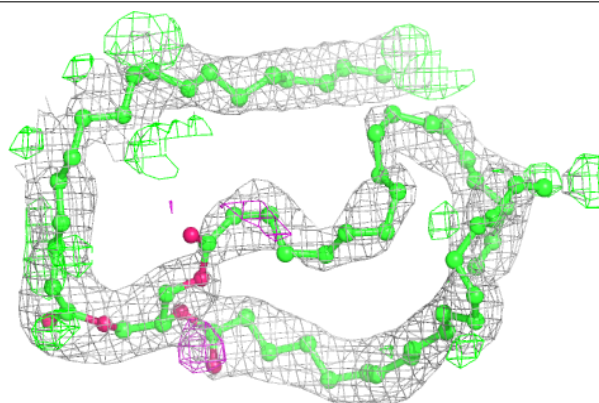


**Electron density around PGV C 307:**

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

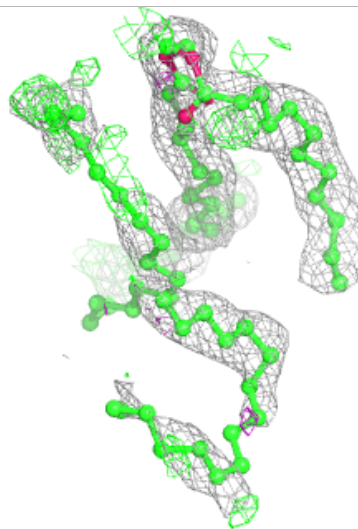
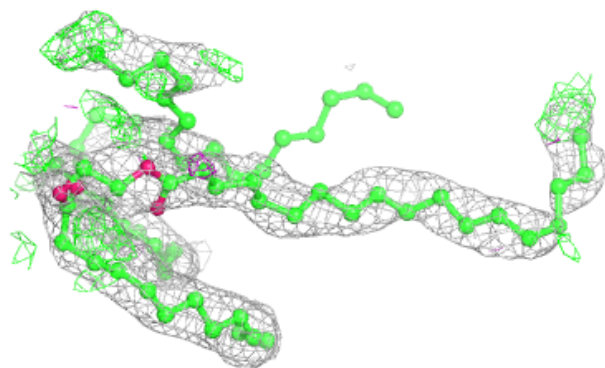
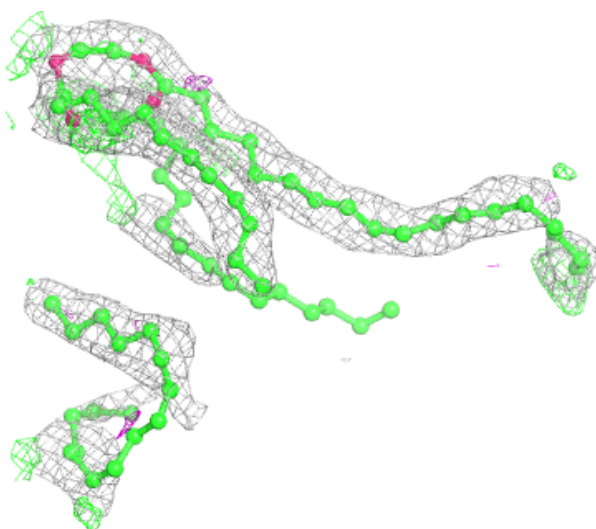
**Electron density around TGL A 606:**

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



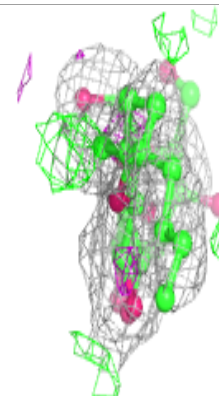
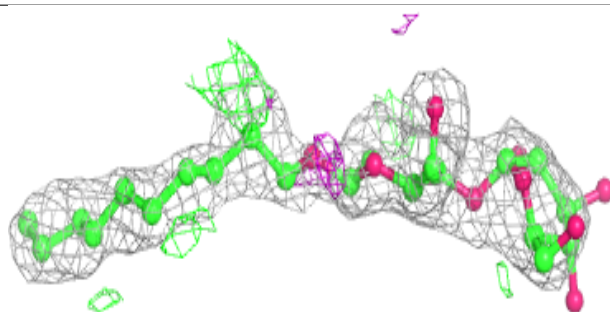
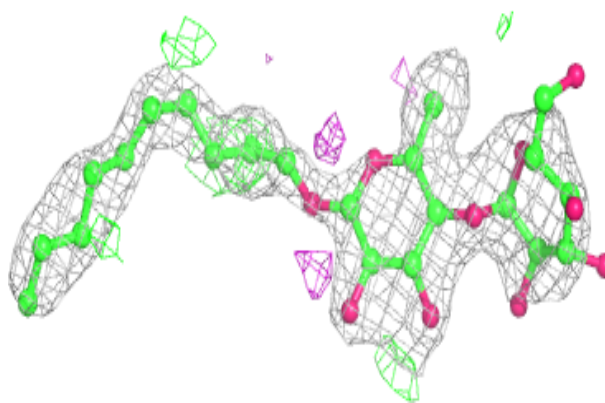
**Electron density around CDL P 307:**

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

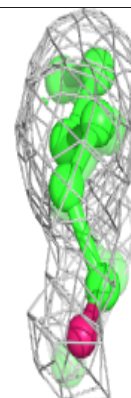
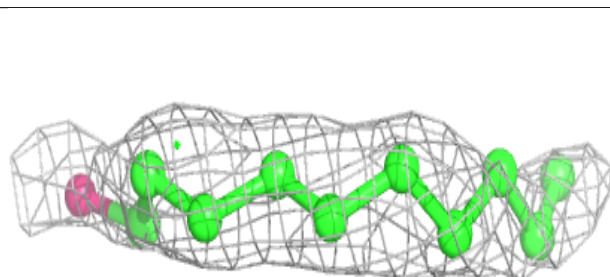
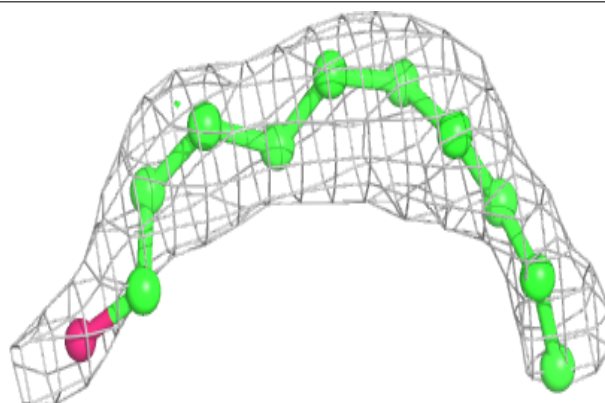


**Electron density around DMU C 310:**

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

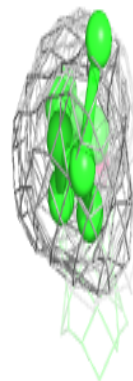
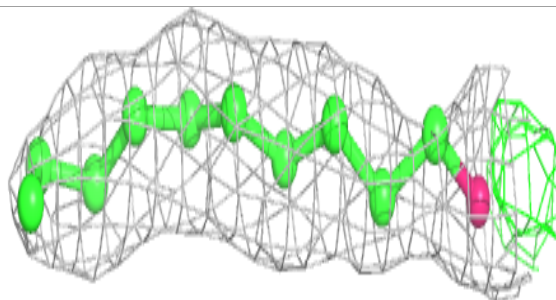
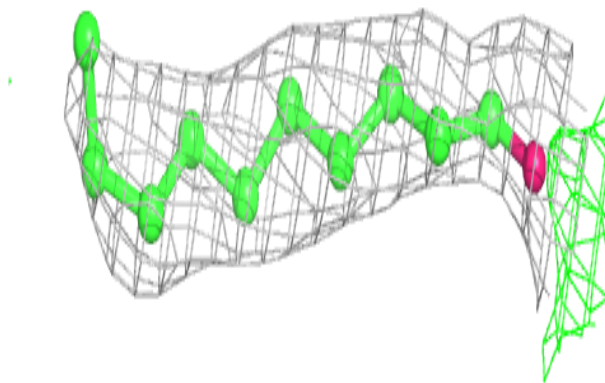
**Electron density around DMU K 104:**

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

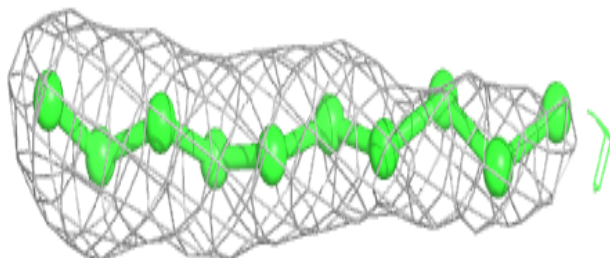
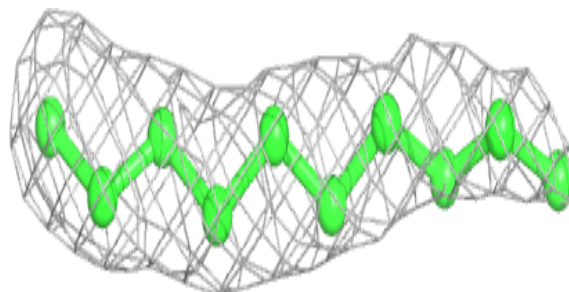


**Electron density around DMU J 104:**

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

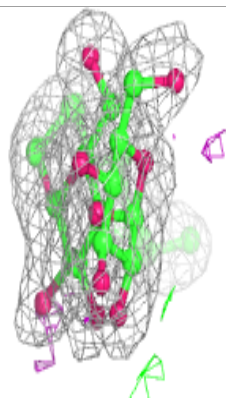
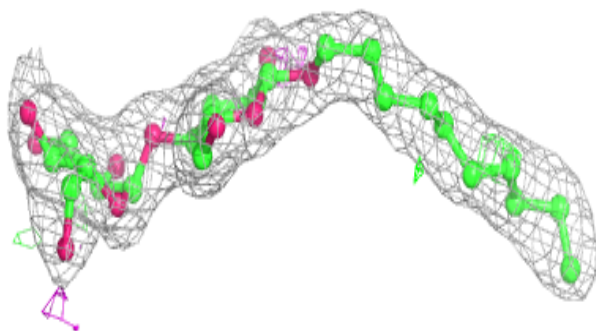
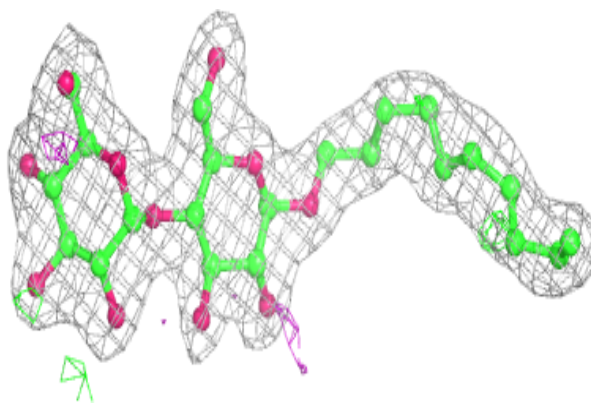
**Electron density around DMU X 101:**

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

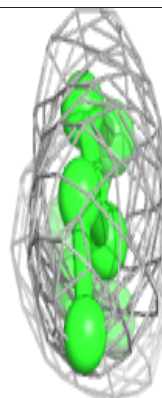
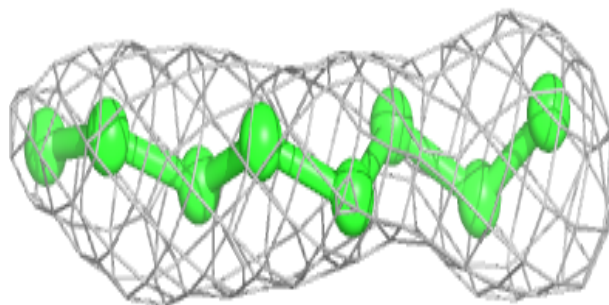
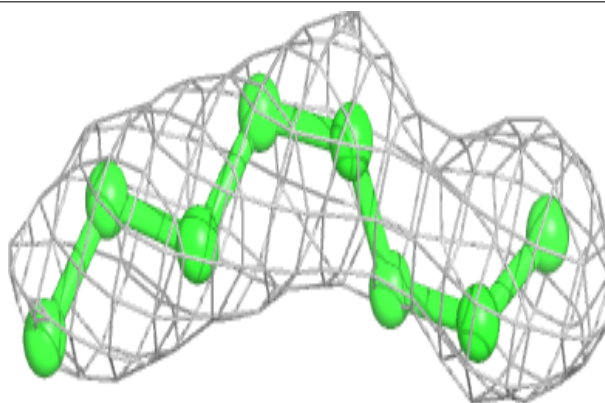


**Electron density around DMU Z 101:**

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

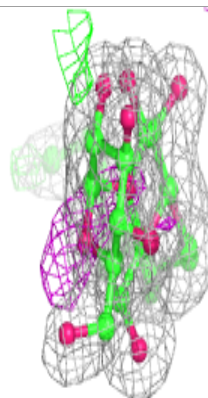
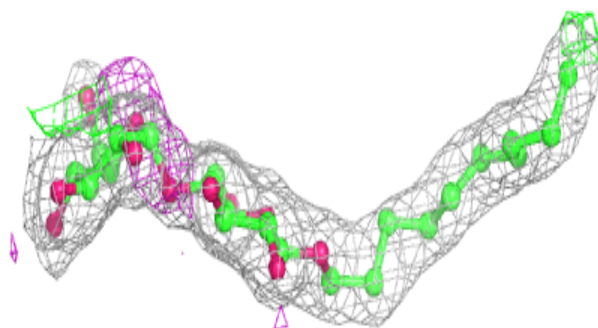
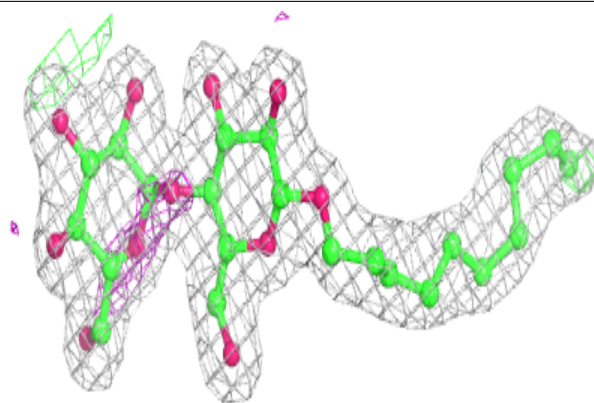
**Electron density around DMU K 101:**

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

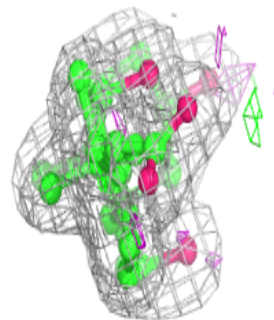
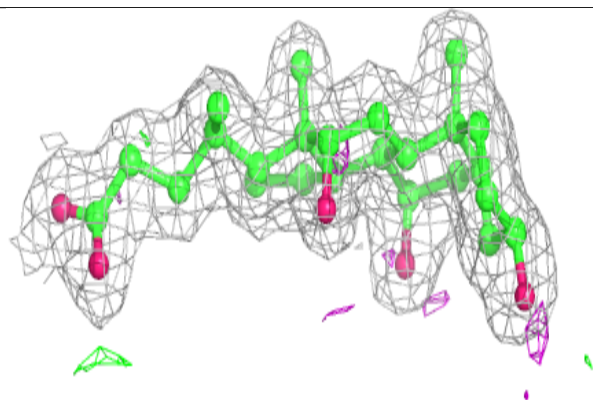
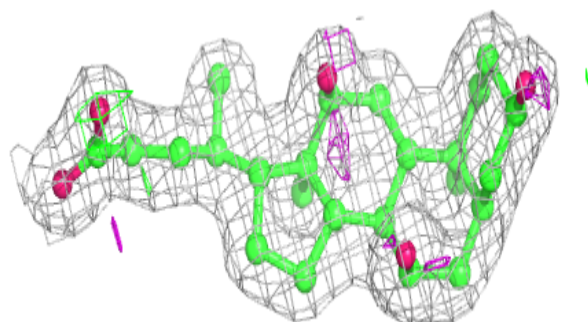


**Electron density around DMU M 101:**

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

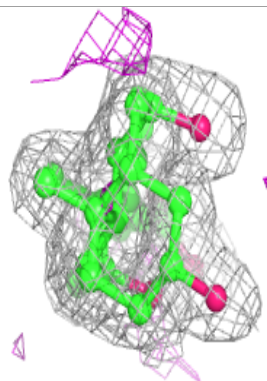
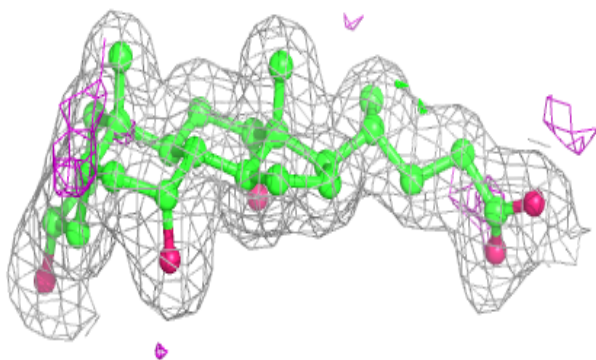
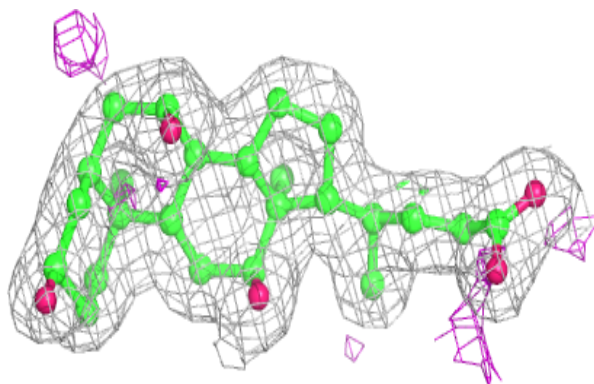
**Electron density around CHD C 301:**

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

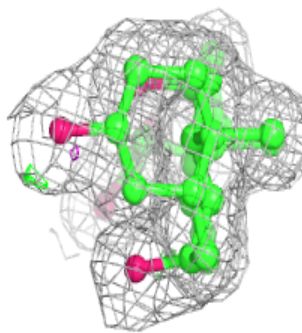
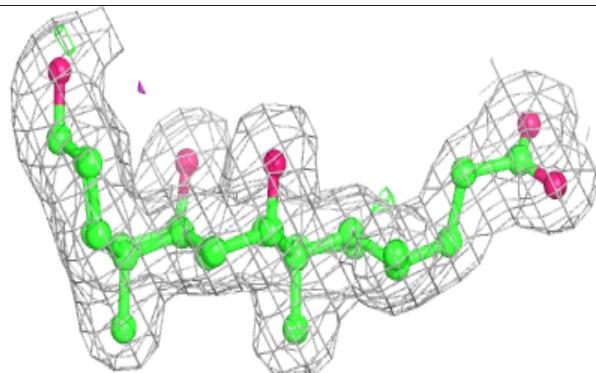
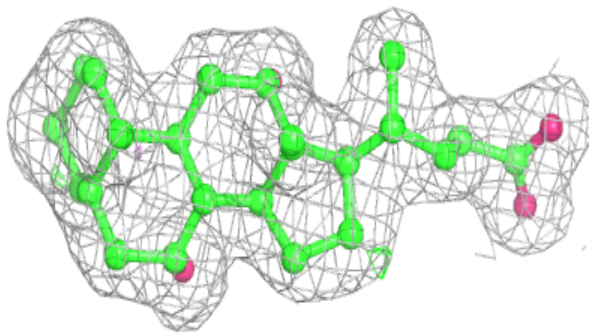


**Electron density around CHD P 301:**

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

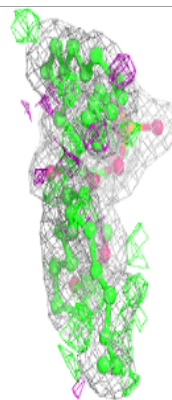
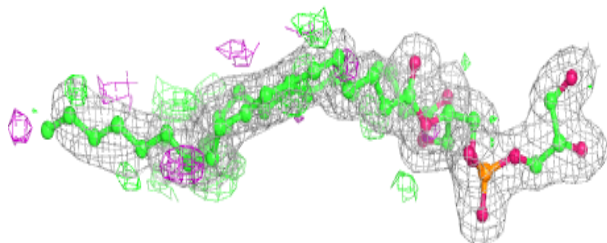
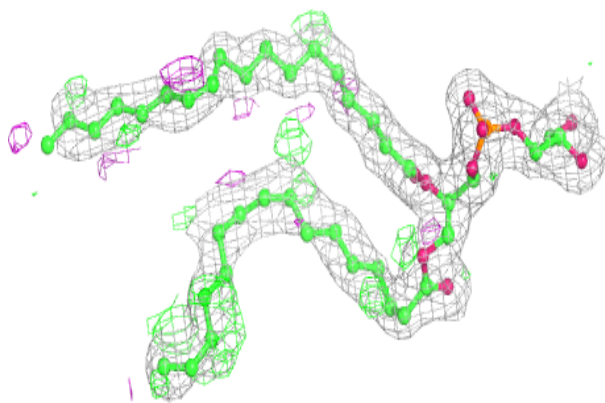
**Electron density around CHD G 101:**

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

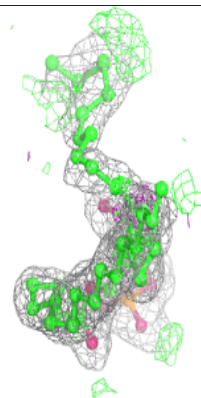
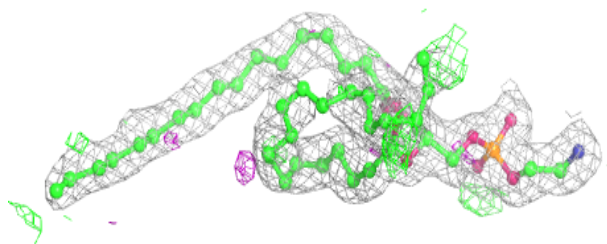
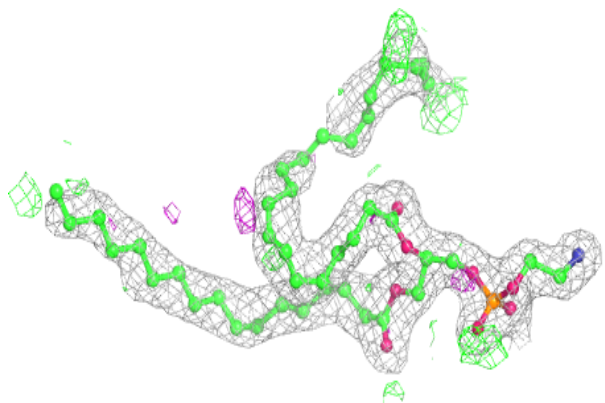


**Electron density around PGV N 612:**

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

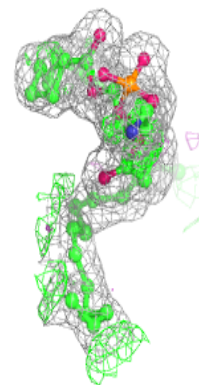
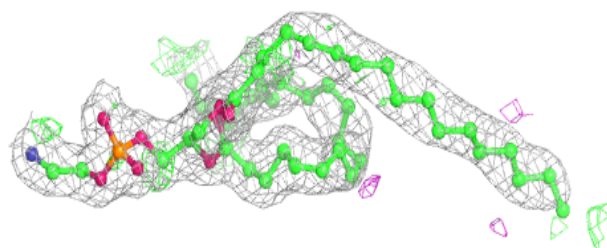
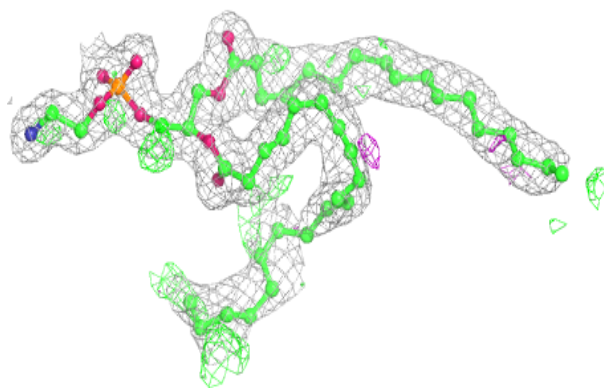
**Electron density around PEK P 304:**

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

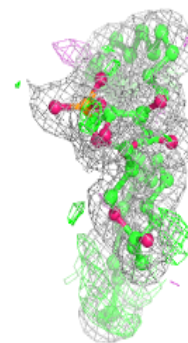
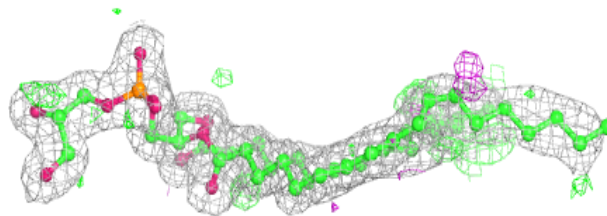
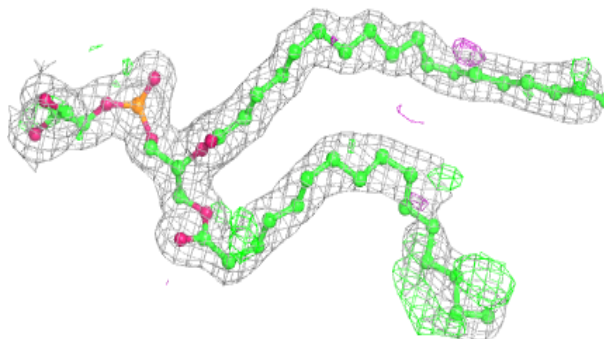


**Electron density around PEK C 304:**

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

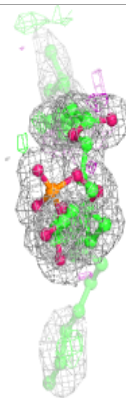
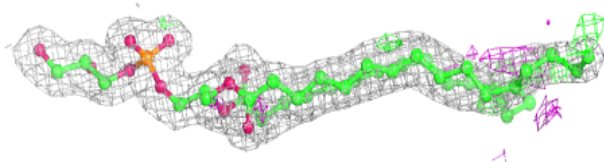
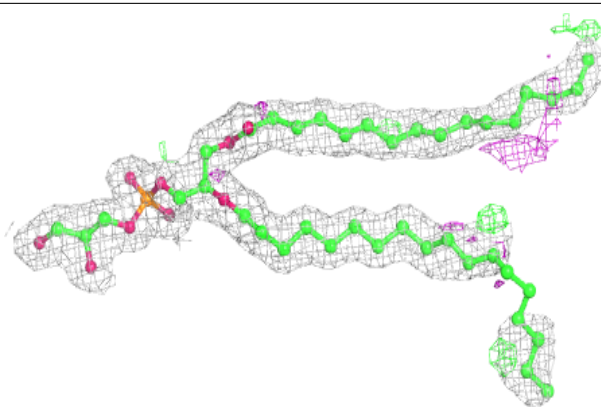
**Electron density around PGV A 611:**

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

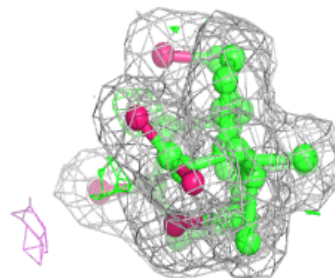
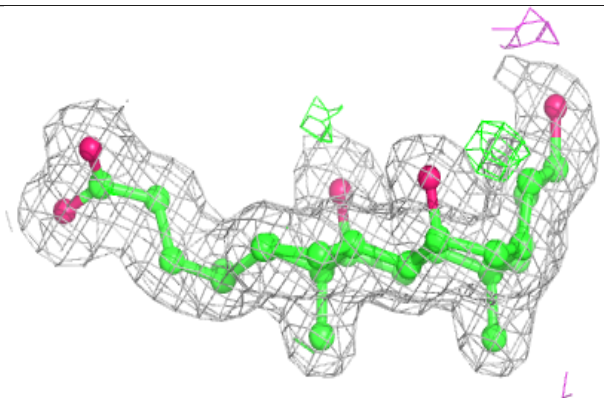
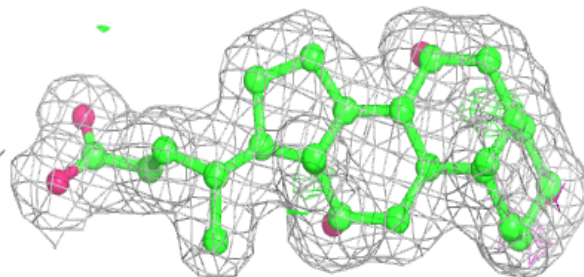


**Electron density around PGV P 305:**

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

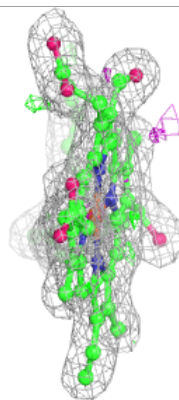
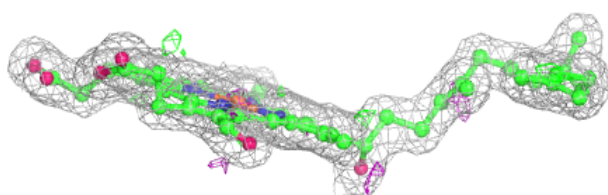
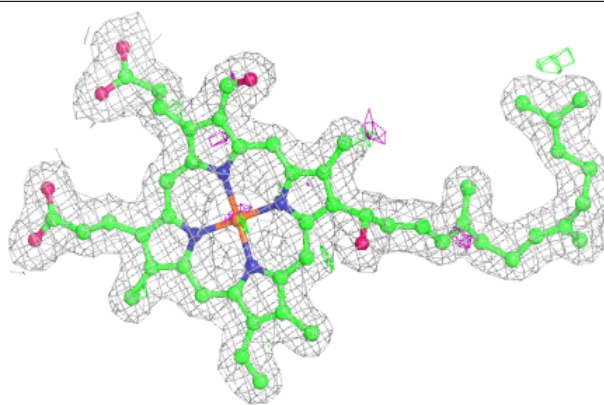
**Electron density around CHD B 302:**

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

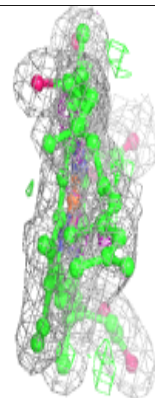
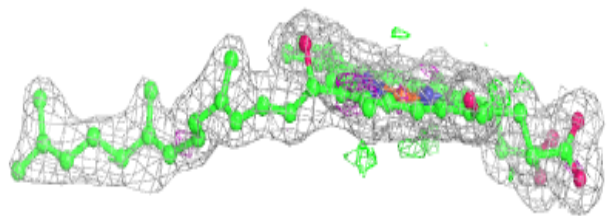
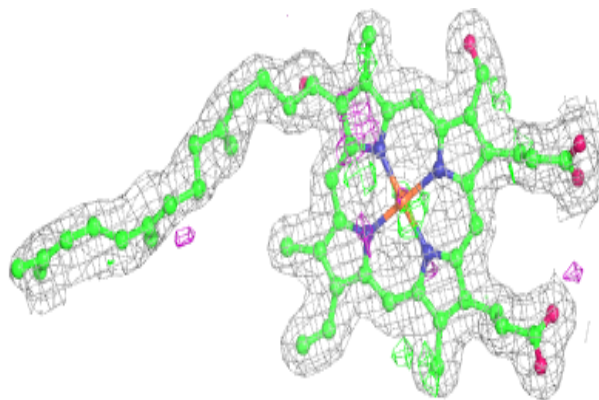


**Electron density around HEA A 602:**

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

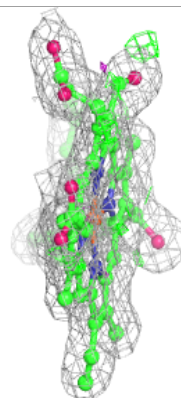
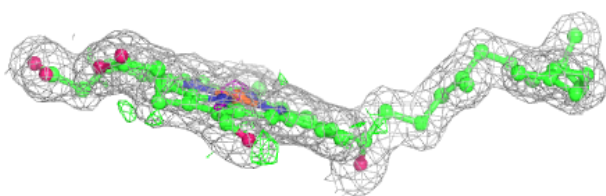
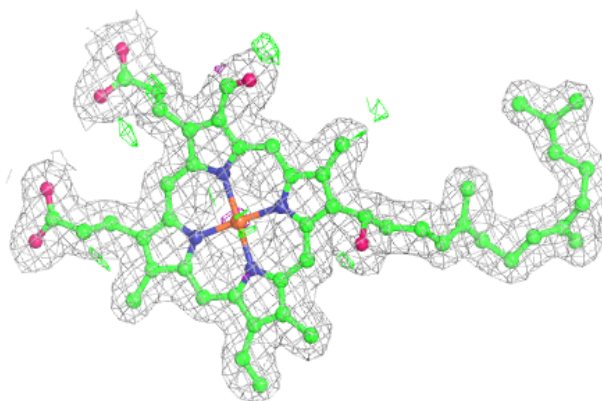
**Electron density around HEA N 602 (A):**

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

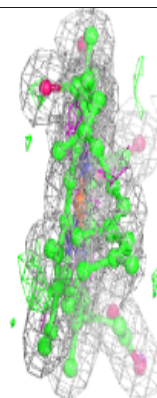
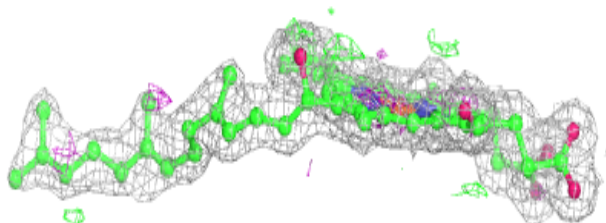
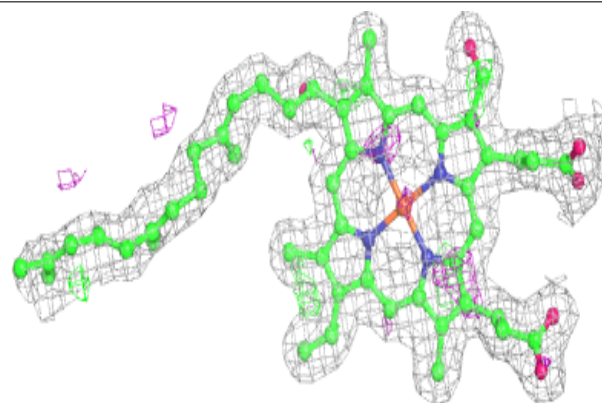


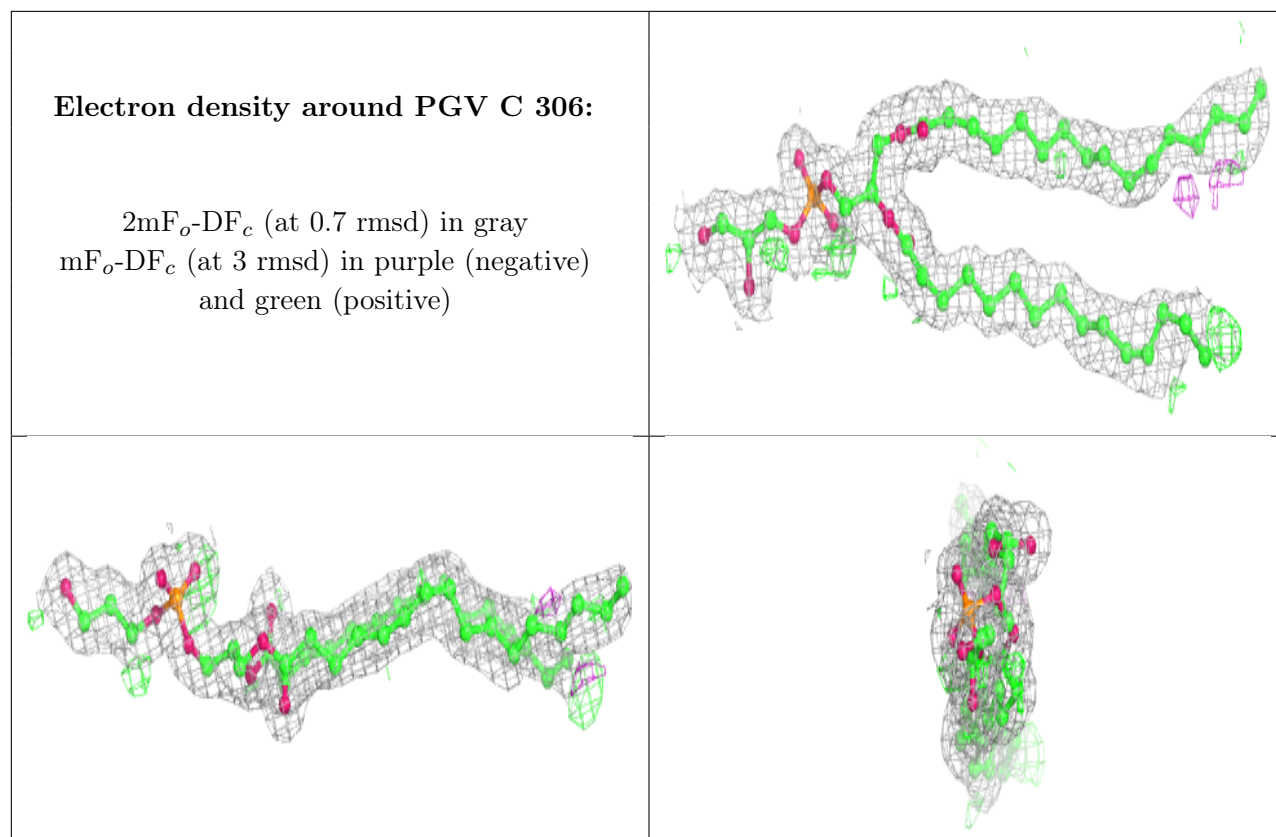
**Electron density around HEA N 603:**

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

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

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.