



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 5, 2022 – 10:19 AM EDT

PDB ID : 7TIH
Title : Structure of oxidized bovine cytochrome c oxidase with reduced metal centers induced by synchrotron X-ray exposure
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.; Russi, S.; Cohen, A.
Deposited on : 2022-01-13
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

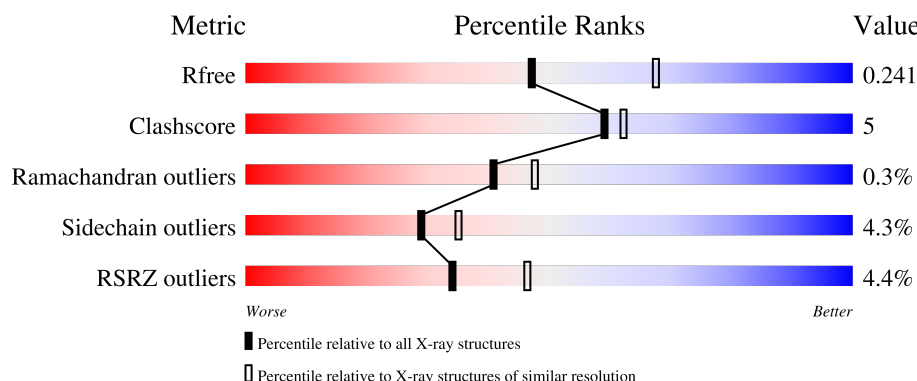
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.

















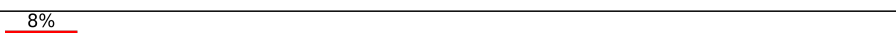
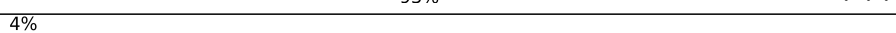





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>0.2%</div> <div>89% 11%</div> </div>
1	N	514	<div> <div>86% 13%</div> </div>
2	B	227	<div> <div>0.2%</div> <div>82% 17%</div> </div>
2	O	227	<div> <div>2%</div> <div>84% 16%</div> </div>
3	C	261	<div> <div>92% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	 90% 9% .
4	D	147	 90% 7% ..
4	Q	147	 10% 86% 11% ..
5	E	109	 3% 87% 9% .
5	R	109	 4% 85% 11% .
6	F	98	 6% 87% 12% .
6	S	98	 6% 72% 23% .
7	G	85	 18% 80% 18% ..
7	T	85	 25% 78% 13% 8% .
8	H	85	 12% 76% 14% .. 7%
8	U	85	 11% 79% 13% . 7%
9	I	73	 16% 92% 7% .
9	V	73	 14% 90% 7% ..
10	J	59	 8% 90% 7% ..
10	W	59	 8% 93% . . .
11	K	56	 4% 80% 7% 12%
11	X	56	 11% 80% 7% 12%
12	L	47	 87% 11% .
12	Y	47	 4% 70% 23% . .
13	M	46	 4% 80% 11% . 7%
13	Z	46	 13% 70% 24% 7%

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
18	HEA	A	606	X	-	-	-
18	HEA	A	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	605	X	-	-	-
18	HEA	N	606	X	-	-	-
19	EDO	A	617	-	-	-	X
19	EDO	D	205	-	-	-	X
19	EDO	N	608	-	-	-	X
19	EDO	N	614	-	-	-	X
23	PSC	R	201	X	-	-	-
26	DMU	G	101	-	-	-	X
29	SAC	I	101	-	-	-	X
29	SAC	V	101	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32721 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- 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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	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	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

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

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

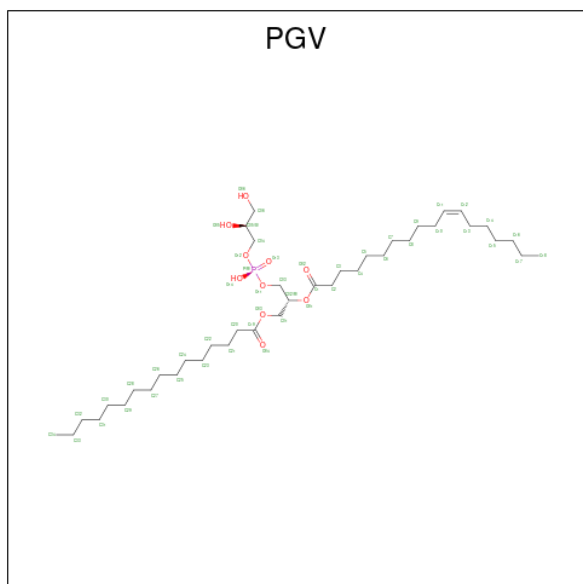
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

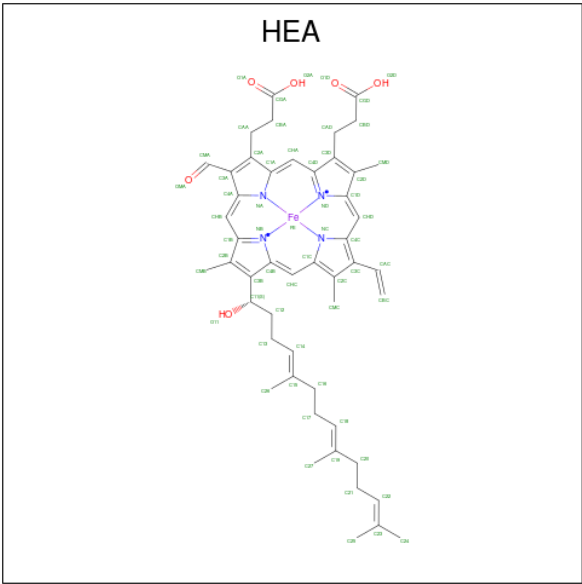
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



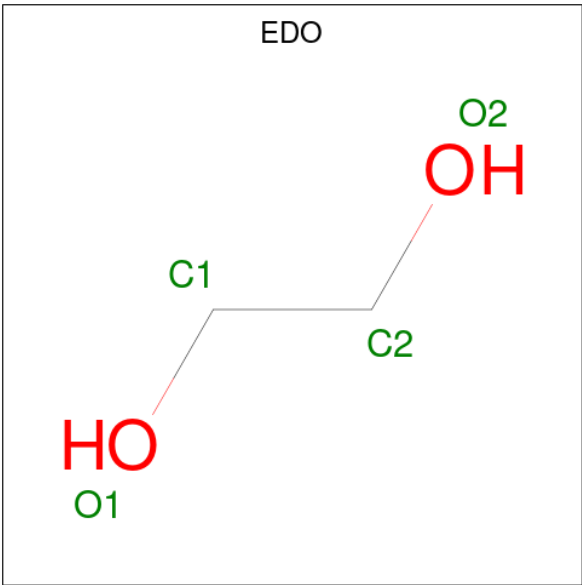
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0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

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	L	1	Total 4	C 2	O 2	0	0
19	M	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0

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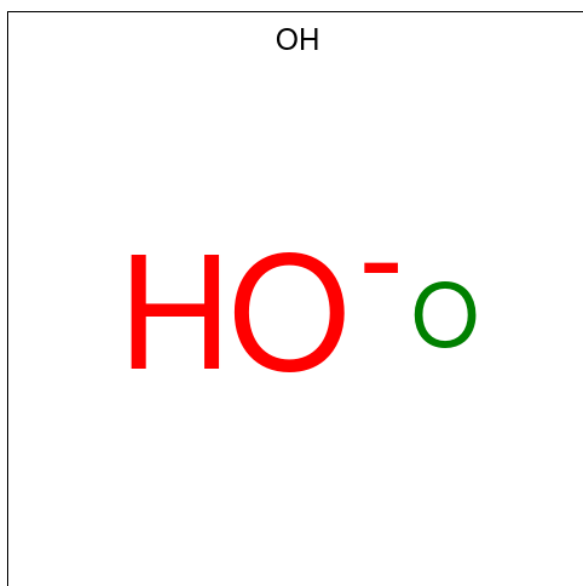
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	O	1	Total 4	C 2	O 2	0	0
19	O	1	Total 4	C 2	O 2	0	0
19	P	1	Total 4	C 2	O 2	0	0
19	P	1	Total 4	C 2	O 2	0	0
19	P	1	Total 4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

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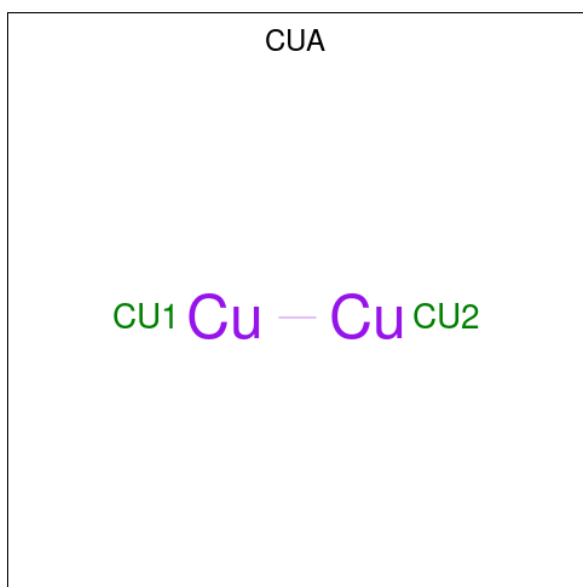
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	V	1	Total	C	O	0	0
			4	2	2		
19	V	1	Total	C	O	0	0
			4	2	2		
19	W	1	Total	C	O	0	0
			4	2	2		
19	W	1	Total	C	O	0	0
			4	2	2		
19	Z	1	Total	C	O	0	0
			4	2	2		

- Molecule 20 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



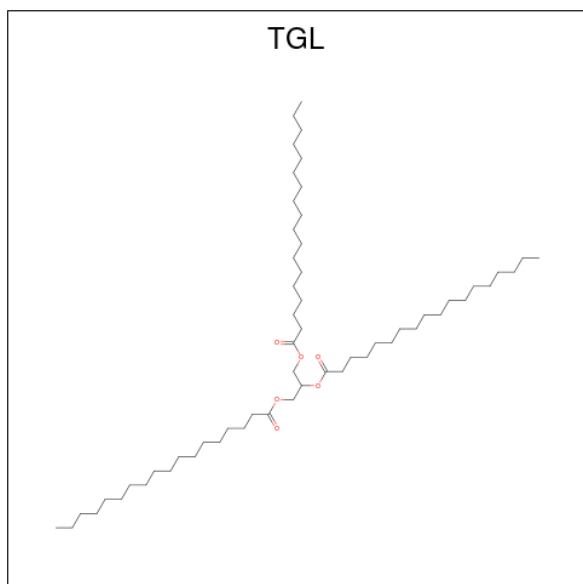
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	O	0	0
			1	1		
20	N	1	Total	O	0	0
			1	1		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$) (labeled as "Ligand of Interest" by depositor).



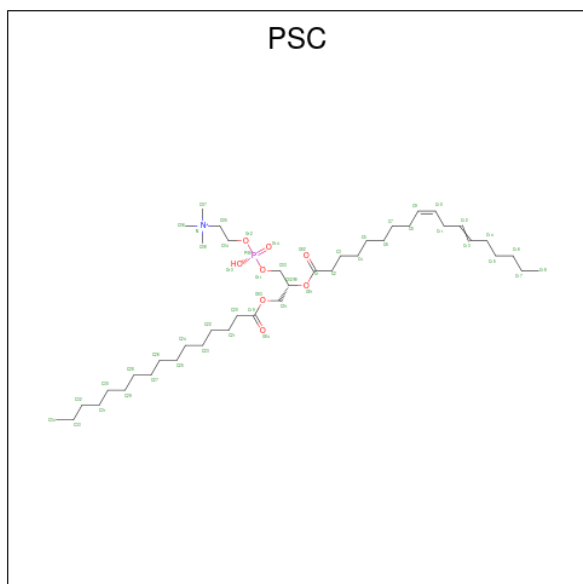
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		

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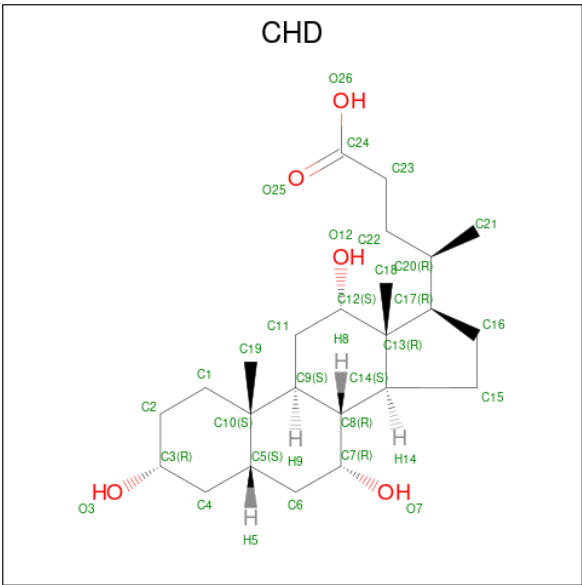
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	D	1	Total	C	O	0	0
			63	57	6		
22	L	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	Q	1	Total	C	O	0	0
			63	57	6		
22	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



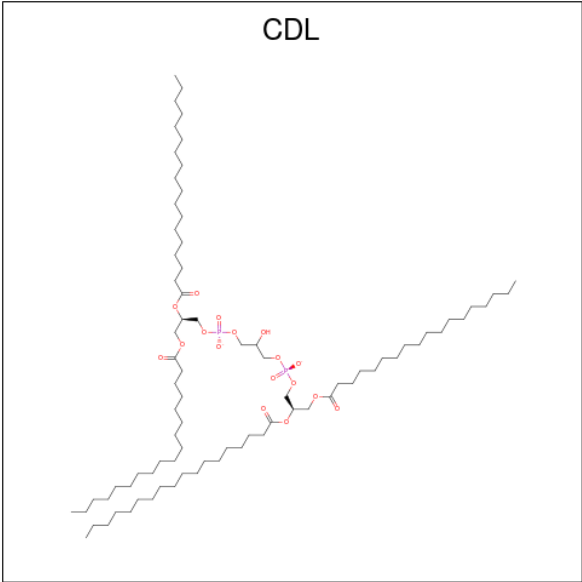
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



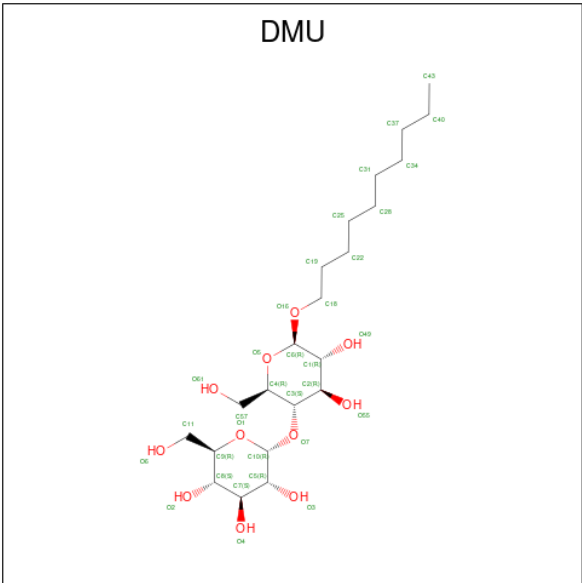
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	J	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	T	1	Total	C	O	0	0
			29	24	5		
24	T	1	Total	C	O	0	0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

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



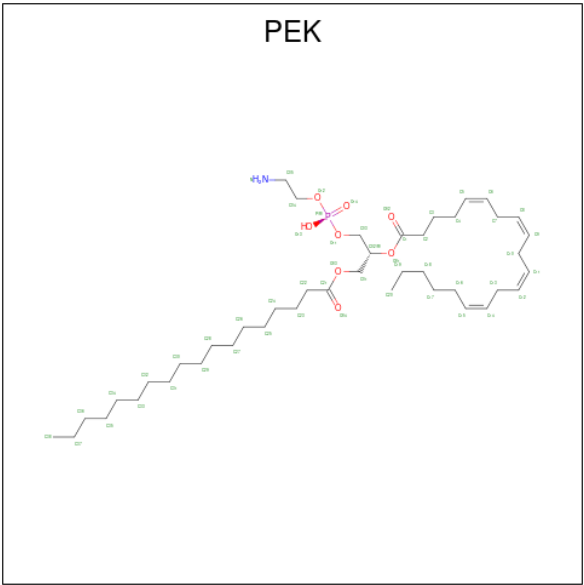
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	C	1	Total	C	O	0	0
			33	22	11		
26	D	1	Total	C	O	0	0
			33	22	11		
26	G	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	Q	1	Total	C	O	0	0
			33	22	11		

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



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

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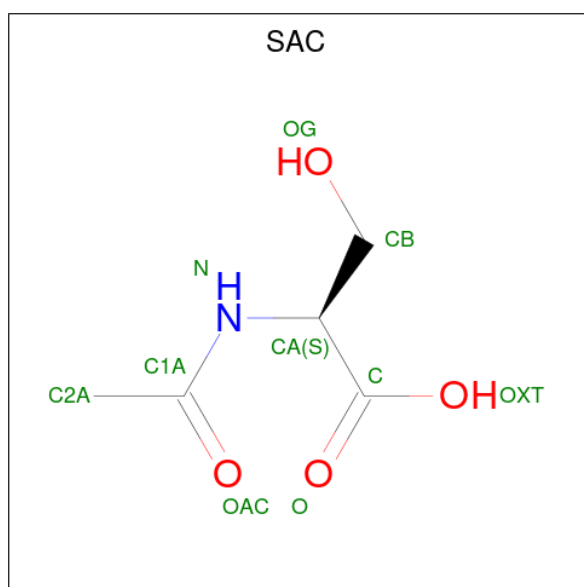
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

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

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	I	1	Total	C	N	O	0	0
			9	5	1	3		
29	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	188	Total	O	0	0
			188	188		
30	B	107	Total	O	0	0
			107	107		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	C	107	Total 107	O 107	0	0
30	D	89	Total 89	O 89	0	0
30	E	71	Total 71	O 71	0	0
30	F	68	Total 68	O 68	0	0
30	G	32	Total 32	O 32	0	0
30	H	41	Total 41	O 41	0	0
30	I	31	Total 31	O 31	0	0
30	J	23	Total 23	O 23	0	0
30	K	19	Total 19	O 19	0	0
30	L	25	Total 25	O 25	0	0
30	M	18	Total 18	O 18	0	0
30	N	167	Total 167	O 167	0	0
30	O	90	Total 90	O 90	0	0
30	P	105	Total 105	O 105	0	0
30	Q	69	Total 69	O 69	0	0
30	R	52	Total 52	O 52	0	0
30	S	81	Total 81	O 81	0	0
30	T	43	Total 43	O 43	0	0
30	U	34	Total 34	O 34	0	0
30	V	17	Total 17	O 17	0	0
30	W	26	Total 26	O 26	0	0

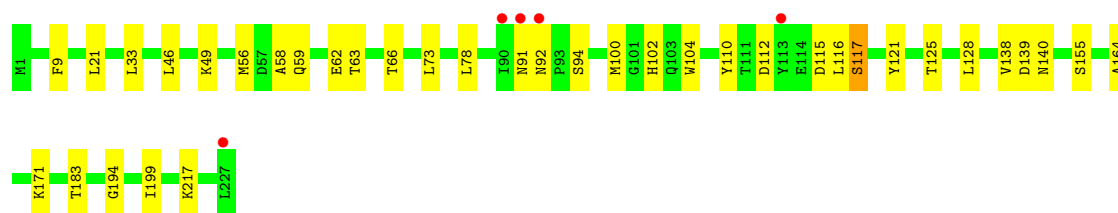
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	14	Total 14	O 14	0	0
30	Y	4	Total 4	O 4	0	0
30	Z	8	Total 8	O 8	0	0

- Molecule 1: Cytochrome c oxidase subunit 1





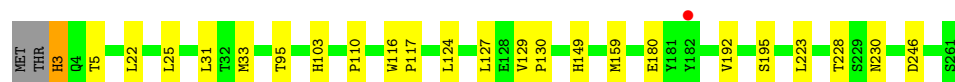
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 92% 8% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 90% 9% .



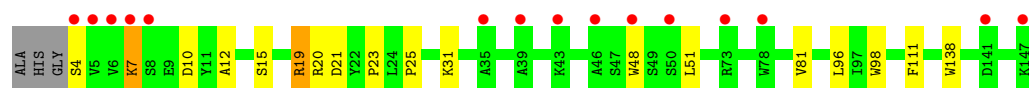
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 90% 7% ..



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

Chain Q: 10% 86% 11% ..



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

Chain E: 3% 87% 9% .

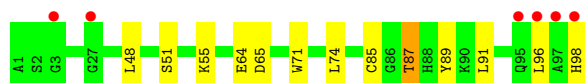
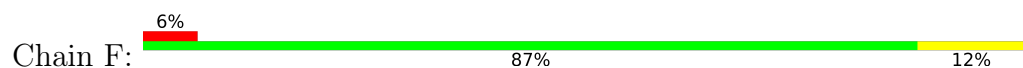


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

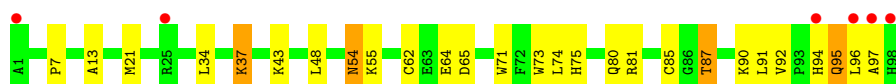
Chain R: 4% 85% 11% .



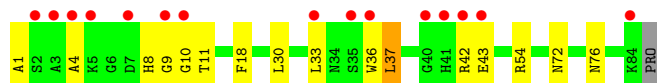
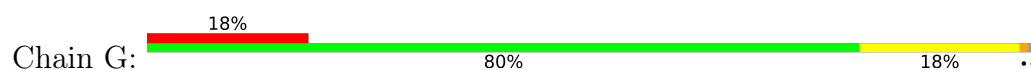
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



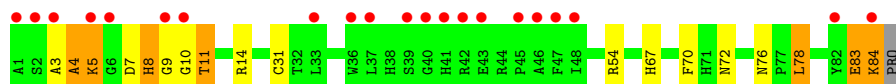
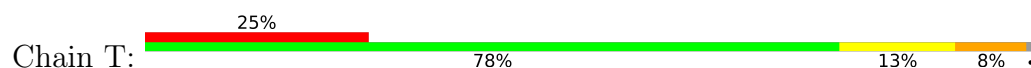
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



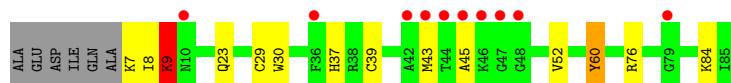
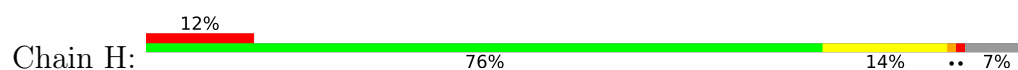
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



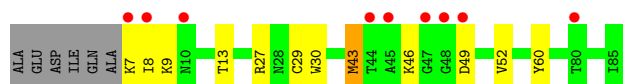
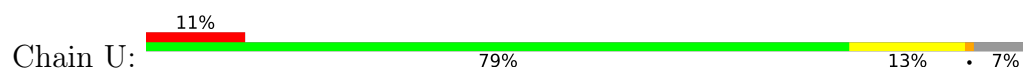
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



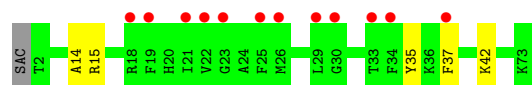
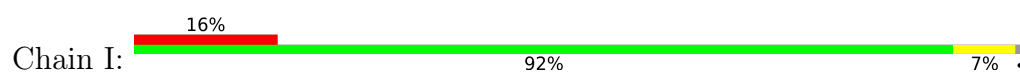
- Molecule 8: Cytochrome c oxidase subunit 6B1



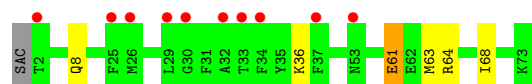
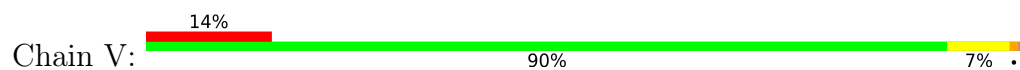
- Molecule 8: Cytochrome c oxidase subunit 6B1



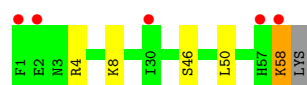
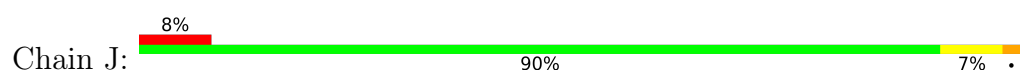
- Molecule 9: Cytochrome c oxidase subunit 6C



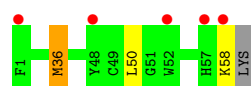
- Molecule 9: Cytochrome c oxidase subunit 6C



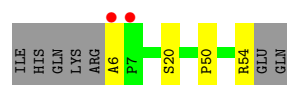
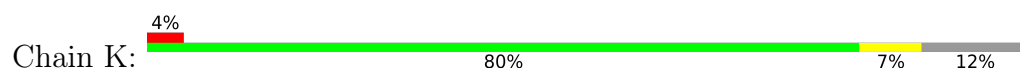
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



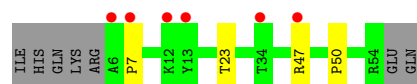
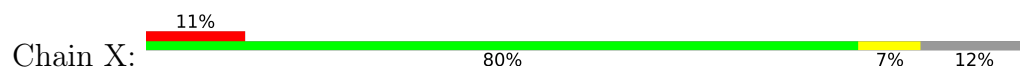
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



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



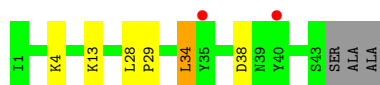
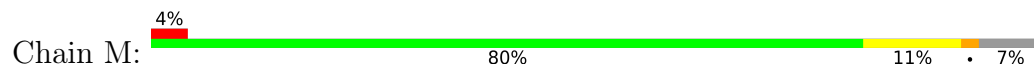
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



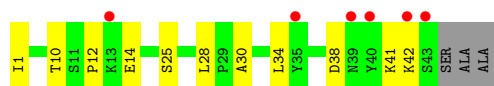
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.04Å 182.70Å 205.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.35 39.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.34-2.35) 99.9 (39.31-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.235 0.203 , 0.241	Depositor DCC
R_{free} test set	13603 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32721	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.66	0/4156	0.78	0/5678
1	N	0.66	0/4156	0.77	0/5678
2	B	0.68	0/1860	0.85	0/2534
2	O	0.67	0/1860	0.84	0/2534
3	C	0.63	0/2197	0.75	0/3005
3	P	0.66	0/2197	0.77	0/3005
4	D	0.69	0/1229	0.77	0/1658
4	Q	0.68	0/1229	0.78	0/1658
5	E	0.67	0/871	0.78	0/1182
5	R	0.67	0/871	0.78	0/1182
6	F	0.70	0/765	0.85	0/1038
6	S	0.71	0/765	0.83	0/1038
7	G	0.65	0/690	0.85	0/937
7	T	0.64	0/690	0.84	0/937
8	H	0.66	0/682	0.81	0/921
8	U	0.67	0/682	0.87	0/921
9	I	0.66	0/605	0.83	0/802
9	V	0.65	0/605	0.82	0/802
10	J	0.66	0/471	0.78	0/636
10	W	0.67	0/471	0.74	0/636
11	K	0.68	0/398	0.80	0/546
11	X	0.67	0/398	0.81	0/546
12	L	0.60	0/393	0.74	0/526
12	Y	0.63	0/393	0.77	0/526
13	M	0.65	0/345	0.79	0/470
13	Z	0.64	0/345	0.75	0/470
All	All	0.66	0/29324	0.79	0/39866

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	T	0	1
8	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	9	LYS	Peptide
7	T	83	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	41	0
1	N	4027	0	4001	43	0
2	B	1824	0	1833	21	0
2	O	1824	0	1833	19	0
3	C	2110	0	2027	11	0
3	P	2110	0	2027	18	0
4	D	1195	0	1183	8	0
4	Q	1195	0	1183	12	0
5	E	852	0	845	5	0
5	R	852	0	845	4	0
6	F	748	0	728	6	0
6	S	748	0	728	16	0
7	G	675	0	643	10	0
7	T	675	0	644	20	0
8	H	662	0	623	7	0
8	U	662	0	623	7	0
9	I	592	0	604	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	592	0	604	2	0
10	J	460	0	459	2	0
10	W	460	0	459	1	0
11	K	384	0	366	2	0
11	X	384	0	366	1	0
12	L	380	0	380	5	0
12	Y	380	0	380	10	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	102	0	152	1	0
17	C	102	0	152	3	0
17	N	51	0	76	4	0
17	P	153	0	228	3	0
18	A	120	0	108	6	0
18	N	120	0	108	12	0
19	A	40	0	60	3	0
19	B	32	0	48	1	0
19	C	16	0	24	1	0
19	D	24	0	36	0	0
19	E	20	0	30	0	0
19	F	12	0	18	0	0
19	G	20	0	30	0	0
19	I	8	0	12	0	0
19	J	16	0	24	0	0
19	K	8	0	12	0	0
19	L	4	0	6	0	0
19	M	4	0	6	0	0
19	N	40	0	60	4	0
19	O	8	0	12	0	0
19	P	20	0	30	0	0
19	Q	16	0	24	2	0
19	R	8	0	12	0	0
19	S	16	0	24	1	0
19	T	4	0	6	0	0
19	V	8	0	12	0	0
19	W	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	4	0	6	0	0
20	A	1	0	0	1	0
20	N	1	0	0	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	63	0	110	0	0
22	D	63	0	110	3	0
22	L	63	0	110	2	0
22	N	63	0	110	0	0
22	Q	63	0	110	1	0
22	Y	63	0	110	2	0
23	B	52	0	80	3	0
23	R	52	0	80	2	0
24	C	58	0	78	1	0
24	G	29	0	39	0	0
24	J	29	0	39	1	0
24	P	58	0	78	1	0
24	T	58	0	78	12	0
24	W	29	0	39	1	0
24	Y	29	0	39	3	0
25	C	200	0	312	4	0
25	P	100	0	156	2	0
25	T	100	0	156	6	0
26	C	66	0	84	2	0
26	D	33	0	42	3	0
26	G	33	0	42	0	0
26	P	33	0	42	0	0
26	Q	33	0	42	2	0
27	C	53	0	77	1	0
27	G	106	0	154	5	0
27	P	106	0	154	4	0
27	T	53	0	77	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	0	0
29	V	9	0	8	2	0
30	A	188	0	0	6	0
30	B	107	0	0	0	0
30	C	107	0	0	1	0
30	D	89	0	0	2	0
30	E	71	0	0	0	0
30	F	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	G	32	0	0	0	0
30	H	41	0	0	1	0
30	I	31	0	0	1	0
30	J	23	0	0	1	0
30	K	19	0	0	1	0
30	L	25	0	0	1	0
30	M	18	0	0	0	0
30	N	167	0	0	6	0
30	O	90	0	0	0	0
30	P	105	0	0	5	0
30	Q	69	0	0	1	0
30	R	52	0	0	0	0
30	S	81	0	0	1	0
30	T	43	0	0	3	0
30	U	34	0	0	1	0
30	V	17	0	0	0	0
30	W	26	0	0	0	0
30	X	14	0	0	0	0
30	Y	4	0	0	1	0
30	Z	8	0	0	1	0
All	All	32721	0	31981	295	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 295 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)
12:Y:24:MET:SD	22:Y:101:TGL:HC42	2.14	0.87
27:P:305:PEK:H381	25:T:103:CDL:H271	1.56	0.85
7:G:76:ASN:HD21	27:G:102:PEK:HN2	1.21	0.85
20:A:618:OH:O	30:A:701:HOH:O	1.99	0.81
20:N:618:OH:O	30:N:701:HOH:O	1.98	0.81

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	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
1	N	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
2	B	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
2	O	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	131 (92%)	11 (8%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
6	S	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	7	4
7	G	81/85 (95%)	69 (85%)	10 (12%)	2 (2%)	5	3
7	T	81/85 (95%)	66 (82%)	13 (16%)	2 (2%)	5	3
8	H	77/85 (91%)	68 (88%)	7 (9%)	2 (3%)	5	3
8	U	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	12	10
9	I	70/73 (96%)	70 (100%)	0	0	100	100
9	V	70/73 (96%)	66 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	44 (94%)	2 (4%)	1 (2%)	7	4
12	L	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	6	4
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3502/3614 (97%)	3351 (96%)	140 (4%)	11 (0%)	41	47

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	8	ILE
8	H	45	ALA
7	G	43	GLU
12	Y	46	LYS
6	S	95	GLN

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	426/426 (100%)	419 (98%)	7 (2%)	62	75
1	N	426/426 (100%)	416 (98%)	10 (2%)	50	61
2	B	210/210 (100%)	201 (96%)	9 (4%)	29	35
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	19
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	55
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	55
4	D	128/129 (99%)	122 (95%)	6 (5%)	26	31
4	Q	128/129 (99%)	123 (96%)	5 (4%)	32	40
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	46
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	35
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	29
6	S	81/81 (100%)	73 (90%)	8 (10%)	8	7
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	6
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	8
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	15
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	26
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	26
10	J	49/50 (98%)	45 (92%)	4 (8%)	11	11
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	20
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	27
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	27
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	6
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	11
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	6
All	All	3040/3082 (99%)	2908 (96%)	132 (4%)	29	35

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	60	TYR
10	W	36	MET
13	Z	41	LYS
9	I	37	PHE
9	I	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	59	GLN
6	S	94	HIS
2	O	195	GLN
9	V	70	GLN
5	R	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	O	1	2	8,9,10	0.51	0	7,9,11	0.78	0
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	0.95	0
2	FME	B	1	2	8,9,10	0.59	0	7,9,11	0.99	1 (14%)
1	FME	A	1	1	8,9,10	0.69	0	7,9,11	0.82	0
7	TPO	T	11	7	8,10,11	0.95	1 (12%)	10,14,16	0.80	0
7	TPO	G	11	7	8,10,11	0.94	1 (12%)	10,14,16	0.72	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
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	4/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	7/9/11/13	-
7	TPO	G	11	7	-	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	2.14	1.63	1.59
7	T	11	TPO	P-OG1	2.04	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	C-CA-N	2.18	113.66	109.73

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 134 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	$\# Z > 2$
19	EDO	A	608	-	3,3,3	0.71	0	2,2,2	0.93	0
19	EDO	A	614	-	3,3,3	0.08	0	2,2,2	0.18	0
19	EDO	Q	202	-	3,3,3	0.09	0	2,2,2	0.23	0
19	EDO	E	205	-	3,3,3	0.06	0	2,2,2	0.11	0
19	EDO	V	103	-	3,3,3	0.19	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	G	106	-	3,3,3	0.12	0	2,2,2	0.30	0
24	CHD	C	301	-	32,32,32	0.53	0	51,51,51	0.70	1 (1%)
24	CHD	G	108	-	32,32,32	0.61	0	51,51,51	0.83	0
23	PSC	B	303	-	51,51,51	0.33	0	57,59,59	0.39	0
19	EDO	P	314	-	3,3,3	0.09	0	2,2,2	0.22	0
19	EDO	J	104	-	3,3,3	0.17	0	2,2,2	0.28	0
19	EDO	B	307	-	3,3,3	0.07	0	2,2,2	0.18	0
19	EDO	P	313	-	3,3,3	0.13	0	2,2,2	0.04	0
26	DMU	C	311	-	34,34,34	2.09	8 (23%)	45,45,45	1.76	9 (20%)
19	EDO	F	704	-	3,3,3	0.25	0	2,2,2	0.35	0
22	TGL	Y	101	-	62,62,62	0.28	0	65,65,65	0.40	1 (1%)
19	EDO	D	206	-	3,3,3	0.24	0	2,2,2	0.44	0
17	PGV	C	302	-	50,50,50	0.39	0	53,56,56	0.51	0
27	PEK	G	102	-	52,52,52	0.32	0	55,57,57	0.57	0
24	CHD	T	101	-	32,32,32	0.65	0	51,51,51	1.06	2 (3%)
19	EDO	G	105	-	3,3,3	0.20	0	2,2,2	0.30	0
19	EDO	L	102	-	3,3,3	0.24	0	2,2,2	0.39	0
19	EDO	D	203	-	3,3,3	0.08	0	2,2,2	0.06	0
19	EDO	O	303	-	3,3,3	0.22	0	2,2,2	0.50	0
19	EDO	E	203	-	3,3,3	0.17	0	2,2,2	0.33	0
27	PEK	C	313	-	52,52,52	0.40	0	55,57,57	0.54	1 (1%)
26	DMU	D	208	-	34,34,34	1.07	3 (8%)	45,45,45	2.75	8 (17%)
26	DMU	C	312	-	34,34,34	1.19	3 (8%)	45,45,45	1.31	6 (13%)
25	CDL	T	103	-	99,99,99	0.41	0	105,111,111	0.48	1 (0%)
19	EDO	C	306	-	3,3,3	0.73	0	2,2,2	0.85	0
19	EDO	T	104	-	3,3,3	0.16	0	2,2,2	0.23	0
19	EDO	K	101	-	3,3,3	0.10	0	2,2,2	0.16	0
19	EDO	D	207	-	3,3,3	0.24	0	2,2,2	0.29	0
19	EDO	A	615	-	3,3,3	0.11	0	2,2,2	0.23	0
19	EDO	N	608	-	3,3,3	0.73	0	2,2,2	0.67	0
19	EDO	B	304	-	3,3,3	0.05	0	2,2,2	0.07	0
19	EDO	C	308	-	3,3,3	0.14	0	2,2,2	0.28	0
22	TGL	L	101	-	62,62,62	0.32	0	65,65,65	0.37	0
27	PEK	P	301	-	52,52,52	0.37	0	55,57,57	0.49	0
19	EDO	K	102	-	3,3,3	0.18	0	2,2,2	0.27	0
22	TGL	N	604	-	62,62,62	0.32	0	65,65,65	0.53	1 (1%)
27	PEK	G	103	-	52,52,52	0.36	0	55,57,57	0.50	0
18	HEA	A	607	1	57,67,67	2.06	13 (22%)	61,103,103	2.46	24 (39%)
19	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.39	0
19	EDO	G	107	-	3,3,3	0.05	0	2,2,2	0.15	0
19	EDO	I	102	-	3,3,3	0.08	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	E	201	-	3,3,3	0.13	0	2,2,2	0.26	0
19	EDO	N	615	-	3,3,3	0.14	0	2,2,2	0.20	0
19	EDO	E	202	-	3,3,3	0.15	0	2,2,2	0.18	0
29	SAC	V	101	-	7,8,9	0.50	0	8,9,11	1.39	1 (12%)
26	DMU	P	303	-	34,34,34	1.70	8 (23%)	45,45,45	1.53	9 (20%)
19	EDO	N	616	-	3,3,3	0.04	0	2,2,2	0.35	0
19	EDO	G	104	-	3,3,3	0.27	0	2,2,2	0.40	0
17	PGV	N	617	-	50,50,50	0.36	0	53,56,56	0.46	0
19	EDO	N	611	-	3,3,3	0.16	0	2,2,2	0.18	0
19	EDO	P	312	-	3,3,3	0.11	0	2,2,2	0.32	0
24	CHD	C	305	-	32,32,32	0.62	0	51,51,51	0.92	1 (1%)
23	PSC	R	201	-	51,51,51	0.34	0	57,59,59	0.49	0
19	EDO	B	309	-	3,3,3	0.38	0	2,2,2	0.50	0
21	CUA	B	301	2	0,1,1	-	-	-	-	-
17	PGV	A	605	-	50,50,50	0.40	0	53,56,56	0.56	0
19	EDO	W	301	-	3,3,3	0.09	0	2,2,2	0.18	0
19	EDO	C	307	-	3,3,3	0.15	0	2,2,2	0.17	0
24	CHD	P	304	-	32,32,32	0.57	0	51,51,51	0.68	0
24	CHD	Y	102	-	32,32,32	0.68	0	51,51,51	1.21	7 (13%)
19	EDO	S	104	-	3,3,3	0.07	0	2,2,2	0.07	0
19	EDO	A	609	-	3,3,3	0.24	0	2,2,2	0.27	0
21	CUA	O	301	2	0,1,1	-	-	-	-	-
17	PGV	C	303	-	50,50,50	0.42	0	53,56,56	0.55	1 (1%)
19	EDO	J	102	-	3,3,3	0.12	0	2,2,2	0.13	0
19	EDO	A	611	-	3,3,3	0.33	0	2,2,2	0.45	0
26	DMU	G	101	-	34,34,34	2.39	9 (26%)	45,45,45	2.03	10 (22%)
19	EDO	D	204	-	3,3,3	0.13	0	2,2,2	0.13	0
19	EDO	S	102	-	3,3,3	0.35	0	2,2,2	0.43	0
19	EDO	F	703	-	3,3,3	0.13	0	2,2,2	0.11	0
19	EDO	M	701	-	3,3,3	0.09	0	2,2,2	0.19	0
19	EDO	N	614	-	3,3,3	0.61	0	2,2,2	0.83	0
19	EDO	O	302	-	3,3,3	0.23	0	2,2,2	0.42	0
19	EDO	E	204	-	3,3,3	0.25	0	2,2,2	0.29	0
19	EDO	N	609	-	3,3,3	0.18	0	2,2,2	0.53	0
19	EDO	A	613	-	3,3,3	0.09	0	2,2,2	0.16	0
19	EDO	B	305	-	3,3,3	0.32	0	2,2,2	0.48	0
19	EDO	Q	205	-	3,3,3	0.16	0	2,2,2	0.33	0
19	EDO	W	303	-	3,3,3	0.11	0	2,2,2	0.14	0
19	EDO	I	103	-	3,3,3	0.13	0	2,2,2	0.14	0
25	CDL	C	310	-	99,99,99	0.37	0	105,111,111	0.44	0
26	DMU	Q	206	-	34,34,34	1.02	1 (2%)	45,45,45	1.19	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	F	701	-	3,3,3	0.11	0	2,2,2	0.55	0
24	CHD	P	309	-	32,32,32	0.53	0	51,51,51	0.86	1 (1%)
19	EDO	B	306	-	3,3,3	0.11	0	2,2,2	0.11	0
19	EDO	B	310	-	3,3,3	0.20	0	2,2,2	0.33	0
19	EDO	P	311	-	3,3,3	0.15	0	2,2,2	0.43	0
24	CHD	T	105	-	32,32,32	0.68	0	51,51,51	1.28	5 (9%)
29	SAC	I	101	-	7,8,9	0.54	0	8,9,11	1.21	1 (12%)
19	EDO	G	109	-	3,3,3	0.10	0	2,2,2	0.31	0
17	PGV	A	604	-	50,50,50	0.38	0	53,56,56	0.51	0
19	EDO	D	205	-	3,3,3	0.11	0	2,2,2	0.22	0
17	PGV	P	302	-	50,50,50	0.36	0	53,56,56	0.61	0
19	EDO	A	616	-	3,3,3	0.09	0	2,2,2	0.37	0
19	EDO	V	102	-	3,3,3	0.13	0	2,2,2	0.23	0
19	EDO	B	308	-	3,3,3	0.25	0	2,2,2	0.33	0
19	EDO	B	311	-	3,3,3	0.11	0	2,2,2	0.12	0
19	EDO	A	617	-	3,3,3	0.17	0	2,2,2	0.32	0
27	PEK	P	305	-	52,52,52	0.36	0	55,57,57	0.57	0
19	EDO	J	105	-	3,3,3	0.05	0	2,2,2	0.25	0
25	CDL	P	308	-	99,99,99	0.38	0	105,111,111	0.52	1 (0%)
19	EDO	N	607	-	3,3,3	0.14	0	2,2,2	0.26	0
25	CDL	C	304	-	99,99,99	0.35	0	105,111,111	0.51	0
18	HEA	A	606	1	57,67,67	1.94	14 (24%)	61,103,103	2.39	22 (36%)
18	HEA	N	605	1	57,67,67	1.90	14 (24%)	61,103,103	2.32	25 (40%)
19	EDO	R	203	-	3,3,3	0.12	0	2,2,2	0.16	0
22	TGL	B	302	-	62,62,62	0.38	0	65,65,65	0.41	1 (1%)
17	PGV	P	307	-	50,50,50	0.33	0	53,56,56	0.42	0
19	EDO	Q	204	-	3,3,3	0.26	0	2,2,2	0.40	0
24	CHD	J	101	-	32,32,32	0.65	1 (3%)	51,51,51	0.78	1 (1%)
27	PEK	T	102	-	52,52,52	0.31	0	55,57,57	0.58	1 (1%)
24	CHD	W	302	-	32,32,32	0.63	0	51,51,51	0.86	0
19	EDO	N	612	-	3,3,3	0.27	0	2,2,2	0.58	0
19	EDO	D	202	-	3,3,3	0.27	0	2,2,2	0.51	0
19	EDO	Q	203	-	3,3,3	0.20	0	2,2,2	0.22	0
18	HEA	N	606	1	57,67,67	1.98	16 (28%)	61,103,103	2.54	25 (40%)
19	EDO	A	610	-	3,3,3	0.19	0	2,2,2	0.25	0
17	PGV	P	306	-	50,50,50	0.34	0	53,56,56	0.50	0
22	TGL	Q	201	-	62,62,62	0.34	0	65,65,65	0.38	0
19	EDO	J	103	-	3,3,3	0.79	0	2,2,2	0.88	0
19	EDO	P	310	-	3,3,3	0.12	0	2,2,2	0.23	0
22	TGL	D	201	-	62,62,62	0.34	0	65,65,65	0.32	0
19	EDO	S	103	-	3,3,3	0.09	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	S	105	-	3,3,3	0.19	0	2,2,2	0.36	0
19	EDO	Z	1601	-	3,3,3	0.19	0	2,2,2	0.34	0
19	EDO	R	202	-	3,3,3	0.14	0	2,2,2	0.28	0
19	EDO	C	309	-	3,3,3	0.10	0	2,2,2	0.15	0
19	EDO	N	610	-	3,3,3	0.25	0	2,2,2	0.26	0
19	EDO	N	613	-	3,3,3	0.15	0	2,2,2	0.27	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
19	EDO	A	608	-	-	0/1/1/1	-
19	EDO	A	614	-	-	1/1/1/1	-
19	EDO	Q	202	-	-	1/1/1/1	-
19	EDO	E	205	-	-	0/1/1/1	-
19	EDO	V	103	-	-	1/1/1/1	-
19	EDO	G	106	-	-	0/1/1/1	-
24	CHD	C	301	-	-	0/9/74/74	0/4/4/4
24	CHD	G	108	-	-	2/9/74/74	0/4/4/4
23	PSC	B	303	-	-	30/55/55/55	-
19	EDO	P	314	-	-	1/1/1/1	-
19	EDO	J	104	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-
19	EDO	P	313	-	-	1/1/1/1	-
26	DMU	C	311	-	-	9/19/59/59	0/2/2/2
19	EDO	F	704	-	-	0/1/1/1	-
22	TGL	Y	101	-	-	36/65/65/65	-
19	EDO	D	206	-	-	1/1/1/1	-
17	PGV	C	302	-	-	17/55/55/55	-
27	PEK	G	102	-	-	22/56/56/56	-
24	CHD	T	101	-	-	3/9/74/74	0/4/4/4
19	EDO	G	105	-	-	1/1/1/1	-
19	EDO	L	102	-	-	0/1/1/1	-
19	EDO	D	203	-	-	1/1/1/1	-
19	EDO	O	303	-	-	1/1/1/1	-
19	EDO	E	203	-	-	0/1/1/1	-
27	PEK	C	313	-	-	25/56/56/56	-
26	DMU	D	208	-	-	10/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DMU	C	312	-	-	9/19/59/59	0/2/2/2
25	CDL	T	103	-	-	55/110/110/110	-
19	EDO	C	306	-	-	0/1/1/1	-
19	EDO	T	104	-	-	0/1/1/1	-
19	EDO	K	101	-	-	1/1/1/1	-
19	EDO	D	207	-	-	0/1/1/1	-
19	EDO	A	615	-	-	0/1/1/1	-
19	EDO	N	608	-	-	0/1/1/1	-
19	EDO	B	304	-	-	0/1/1/1	-
19	EDO	C	308	-	-	1/1/1/1	-
22	TGL	L	101	-	-	29/65/65/65	-
27	PEK	P	301	-	-	26/56/56/56	-
19	EDO	K	102	-	-	1/1/1/1	-
22	TGL	N	604	-	-	31/65/65/65	-
27	PEK	G	103	-	-	27/56/56/56	-
18	HEA	A	607	1	3/3/7/16	4/32/76/76	-
19	EDO	A	612	-	-	1/1/1/1	-
19	EDO	G	107	-	-	1/1/1/1	-
19	EDO	I	102	-	-	0/1/1/1	-
19	EDO	E	201	-	-	0/1/1/1	-
19	EDO	N	615	-	-	1/1/1/1	-
19	EDO	E	202	-	-	1/1/1/1	-
29	SAC	V	101	-	-	6/7/8/10	-
26	DMU	P	303	-	-	9/19/59/59	0/2/2/2
19	EDO	N	616	-	-	0/1/1/1	-
19	EDO	G	104	-	-	1/1/1/1	-
17	PGV	N	617	-	-	30/55/55/55	-
19	EDO	N	611	-	-	0/1/1/1	-
19	EDO	P	312	-	-	1/1/1/1	-
24	CHD	C	305	-	-	2/9/74/74	0/4/4/4
23	PSC	R	201	-	1/1/5/9	30/55/55/55	-
19	EDO	B	309	-	-	0/1/1/1	-
17	PGV	A	605	-	-	15/55/55/55	-
19	EDO	W	301	-	-	1/1/1/1	-
19	EDO	C	307	-	-	1/1/1/1	-
24	CHD	P	304	-	-	1/9/74/74	0/4/4/4
24	CHD	Y	102	-	-	4/9/74/74	2/4/4/4
19	EDO	S	104	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PGV	C	303	-	-	33/55/55/55	-
19	EDO	J	102	-	-	1/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-
26	DMU	G	101	-	-	6/19/59/59	0/2/2/2
19	EDO	D	204	-	-	0/1/1/1	-
19	EDO	S	102	-	-	0/1/1/1	-
19	EDO	F	703	-	-	1/1/1/1	-
19	EDO	M	701	-	-	0/1/1/1	-
19	EDO	N	614	-	-	1/1/1/1	-
19	EDO	O	302	-	-	1/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
19	EDO	N	609	-	-	0/1/1/1	-
19	EDO	A	613	-	-	1/1/1/1	-
19	EDO	B	305	-	-	1/1/1/1	-
19	EDO	Q	205	-	-	1/1/1/1	-
19	EDO	W	303	-	-	1/1/1/1	-
19	EDO	I	103	-	-	1/1/1/1	-
25	CDL	C	310	-	-	56/110/110/110	-
26	DMU	Q	206	-	-	10/19/59/59	0/2/2/2
19	EDO	F	701	-	-	0/1/1/1	-
24	CHD	P	309	-	-	3/9/74/74	1/4/4/4
19	EDO	B	306	-	-	0/1/1/1	-
19	EDO	B	310	-	-	1/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
24	CHD	T	105	-	-	7/9/74/74	1/4/4/4
29	SAC	I	101	-	-	4/7/8/10	-
19	EDO	G	109	-	-	1/1/1/1	-
17	PGV	A	604	-	-	31/55/55/55	-
19	EDO	D	205	-	-	1/1/1/1	-
17	PGV	P	302	-	-	15/55/55/55	-
19	EDO	A	616	-	-	0/1/1/1	-
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
19	EDO	B	311	-	-	1/1/1/1	-
19	EDO	A	617	-	-	0/1/1/1	-
27	PEK	P	305	-	-	28/56/56/56	-
19	EDO	J	105	-	-	1/1/1/1	-
25	CDL	P	308	-	-	54/110/110/110	-
19	EDO	N	607	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	C	304	-	-	53/110/110/110	-
18	HEA	N	605	1	3/3/7/16	6/32/76/76	-
18	HEA	A	606	1	3/3/7/16	6/32/76/76	-
19	EDO	R	203	-	-	1/1/1/1	-
22	TGL	B	302	-	-	34/65/65/65	-
17	PGV	P	307	-	-	27/55/55/55	-
19	EDO	Q	204	-	-	1/1/1/1	-
24	CHD	J	101	-	-	1/9/74/74	0/4/4/4
27	PEK	T	102	-	-	16/56/56/56	-
24	CHD	W	302	-	-	2/9/74/74	0/4/4/4
19	EDO	N	612	-	-	0/1/1/1	-
19	EDO	D	202	-	-	1/1/1/1	-
19	EDO	Q	203	-	-	0/1/1/1	-
18	HEA	N	606	1	3/3/7/16	5/32/76/76	-
19	EDO	A	610	-	-	0/1/1/1	-
17	PGV	P	306	-	-	11/55/55/55	-
22	TGL	Q	201	-	-	38/65/65/65	-
19	EDO	J	103	-	-	0/1/1/1	-
19	EDO	P	310	-	-	0/1/1/1	-
22	TGL	D	201	-	-	41/65/65/65	-
19	EDO	S	103	-	-	0/1/1/1	-
19	EDO	S	105	-	-	1/1/1/1	-
19	EDO	Z	1601	-	-	1/1/1/1	-
19	EDO	R	202	-	-	0/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	610	-	-	1/1/1/1	-
19	EDO	N	613	-	-	1/1/1/1	-

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	311	DMU	O16-C6	7.82	1.53	1.40
26	G	101	DMU	O16-C6	7.82	1.53	1.40
18	A	607	HEA	C3C-C2C	5.36	1.47	1.40
18	N	606	HEA	C3B-C2B	5.33	1.46	1.34
18	N	605	HEA	C3D-C2D	5.01	1.47	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	208	DMU	C18-O16-C6	15.73	139.93	113.84
18	N	605	HEA	C3B-C4B-NB	6.09	117.05	109.84
18	N	606	HEA	C3D-C4D-ND	5.99	116.16	110.36
18	N	606	HEA	C1D-C2D-C3D	-5.97	100.68	106.96
26	G	101	DMU	O5-C4-C57	5.70	120.62	106.44

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	606	HEA	NB
18	A	606	HEA	NA
18	A	606	HEA	ND
18	A	607	HEA	NB
18	A	607	HEA	NA

5 of 970 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O13
17	A	604	PGV	C04-O12-P-O11
17	A	604	PGV	O12-C04-C05-O05
17	C	303	PGV	C03-O11-P-O14
17	C	303	PGV	O01-C02-C03-O11

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	P	309	CHD	C1-C10-C2-C3-C4-C5
24	Y	102	CHD	C10-C5-C6-C7-C8-C9
24	Y	102	CHD	C1-C10-C2-C3-C4-C5
24	T	105	CHD	C1-C10-C2-C3-C4-C5

46 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	608	EDO	3	0
24	C	301	CHD	1	0
23	B	303	PSC	3	0
26	C	311	DMU	1	0
22	Y	101	TGL	2	0
17	C	302	PGV	1	0
27	G	102	PEK	4	0
24	T	101	CHD	1	0

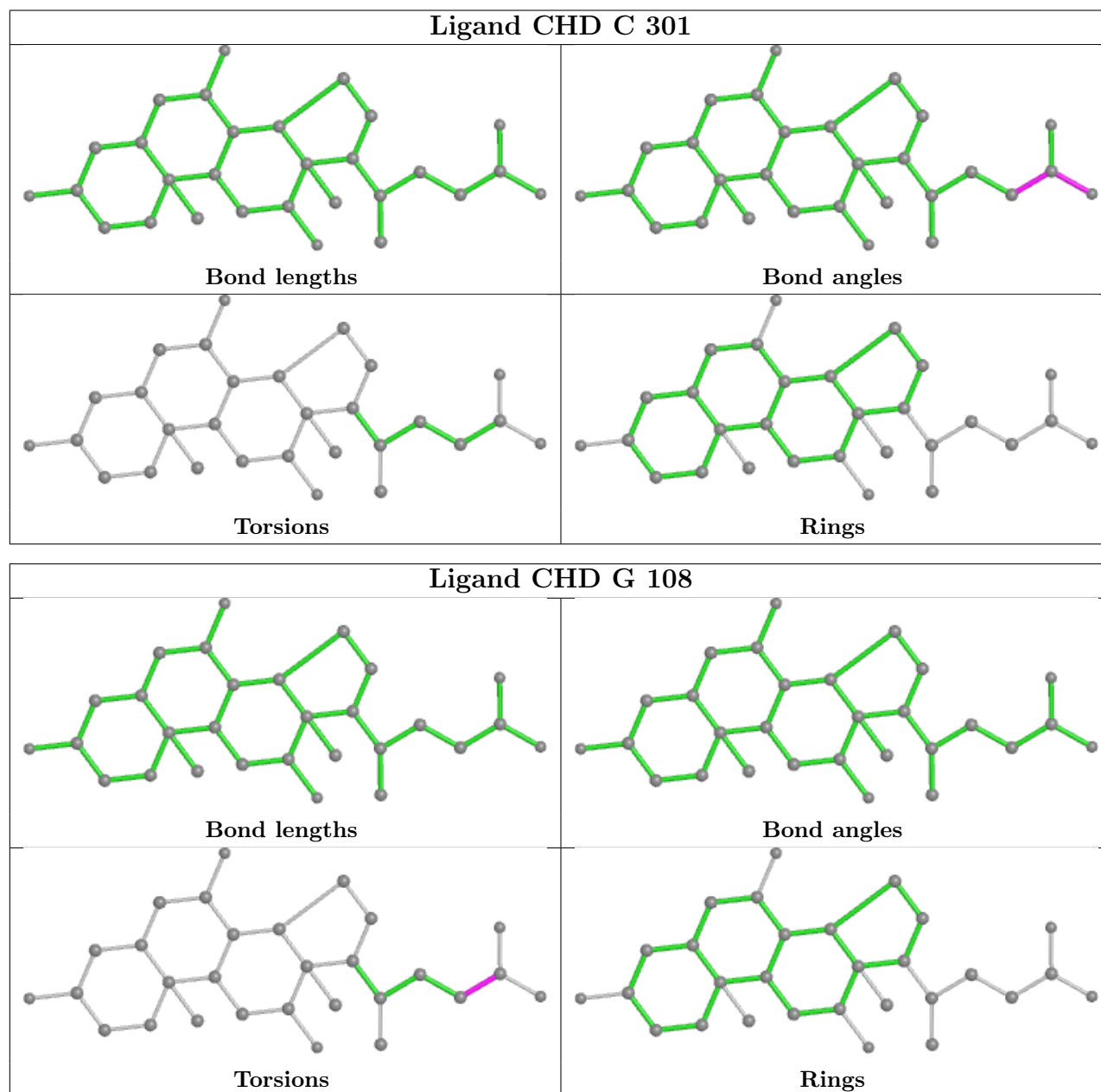
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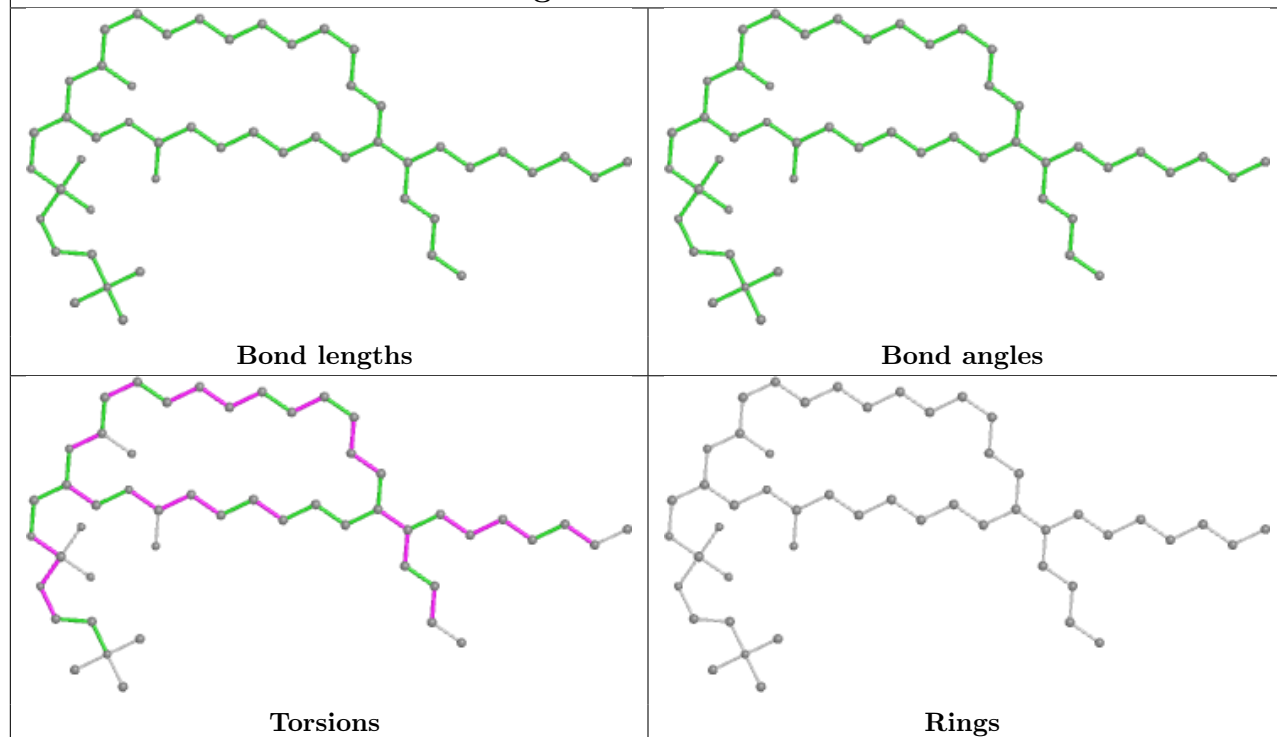
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	313	PEK	1	0
26	D	208	DMU	3	0
26	C	312	DMU	1	0
25	T	103	CDL	6	0
19	C	306	EDO	1	0
22	L	101	TGL	2	0
27	P	301	PEK	2	0
27	G	103	PEK	1	0
18	A	607	HEA	3	0
29	V	101	SAC	2	0
17	N	617	PGV	4	0
19	N	611	EDO	1	0
23	R	201	PSC	2	0
24	Y	102	CHD	3	0
17	C	303	PGV	2	0
19	N	614	EDO	1	0
19	B	305	EDO	1	0
19	Q	205	EDO	1	0
25	C	310	CDL	1	0
26	Q	206	DMU	2	0
24	P	309	CHD	1	0
24	T	105	CHD	11	0
17	A	604	PGV	1	0
27	P	305	PEK	2	0
25	P	308	CDL	2	0
25	C	304	CDL	3	0
18	A	606	HEA	3	0
18	N	605	HEA	6	0
17	P	307	PGV	3	0
19	Q	204	EDO	1	0
24	J	101	CHD	1	0
27	T	102	PEK	4	0
24	W	302	CHD	1	0
19	N	612	EDO	2	0
18	N	606	HEA	6	0
22	Q	201	TGL	1	0
22	D	201	TGL	3	0
19	S	105	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

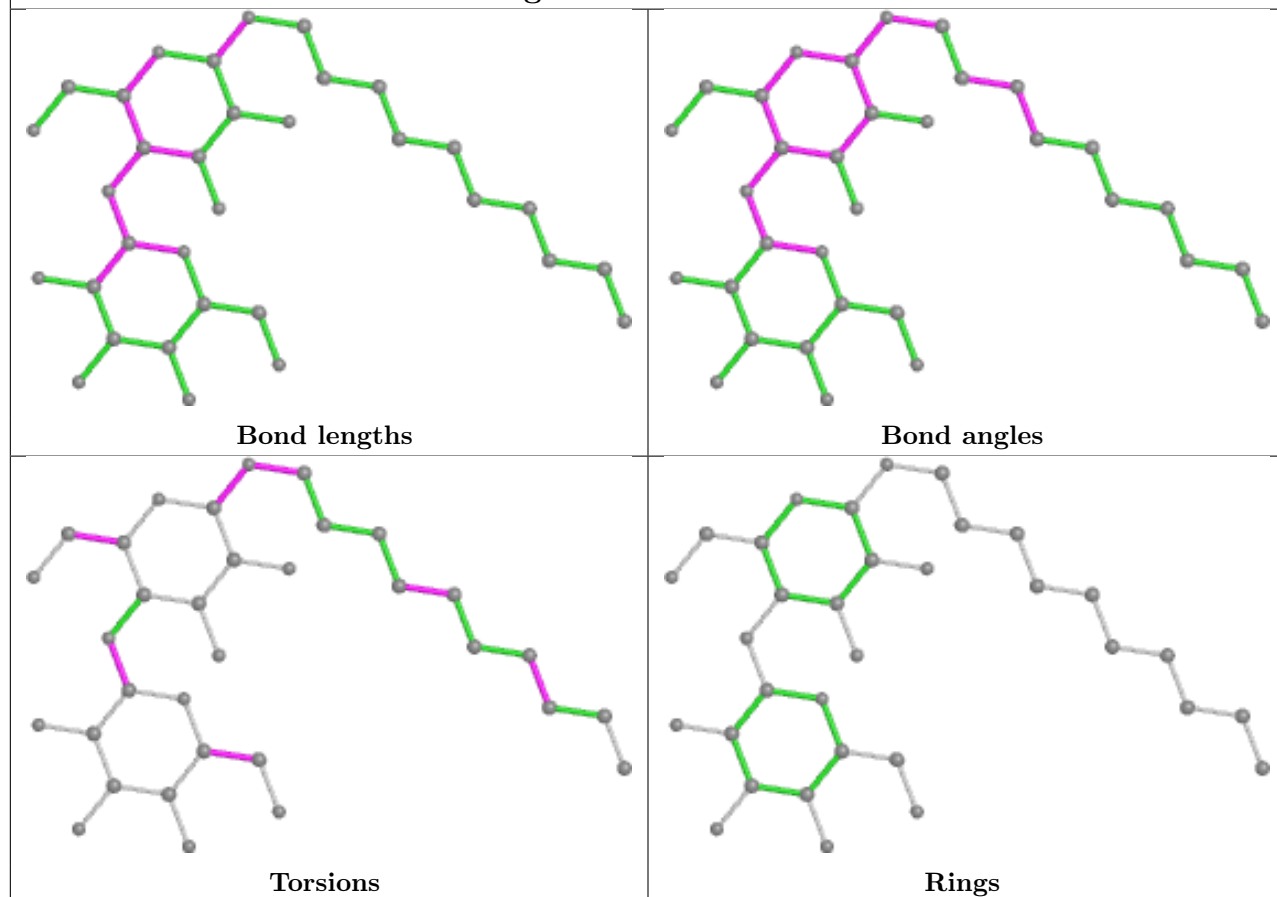
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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

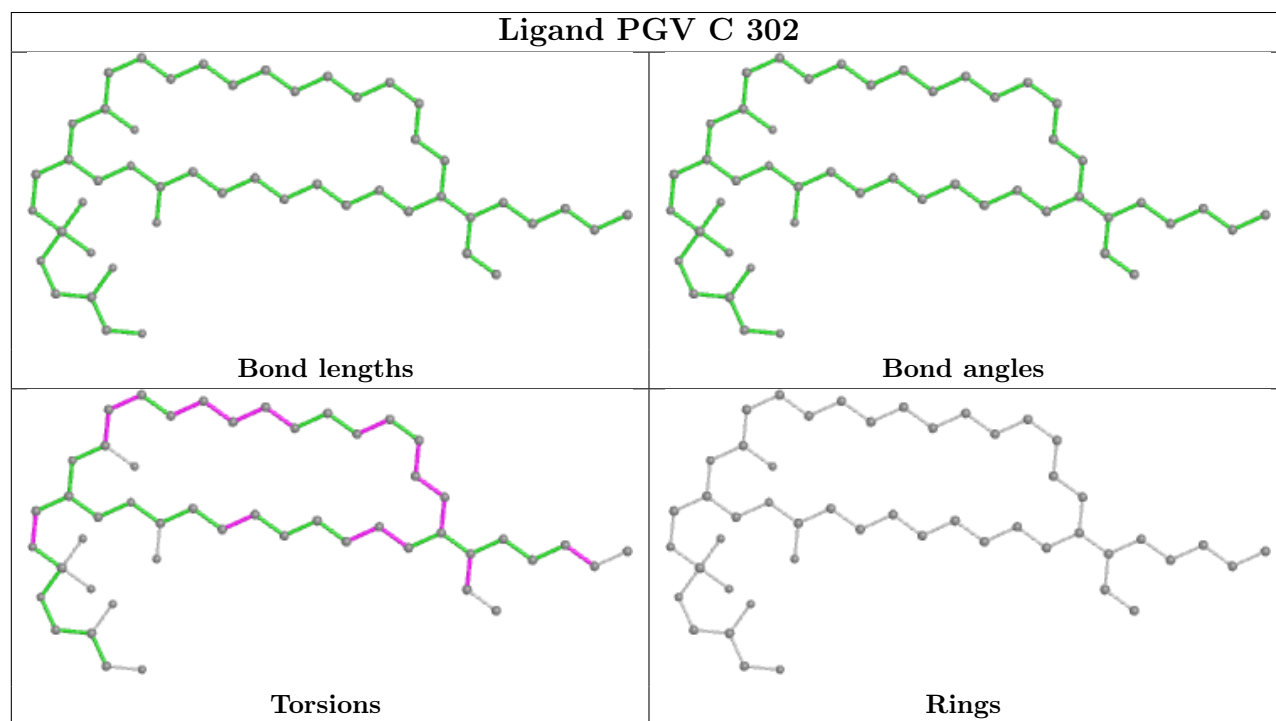
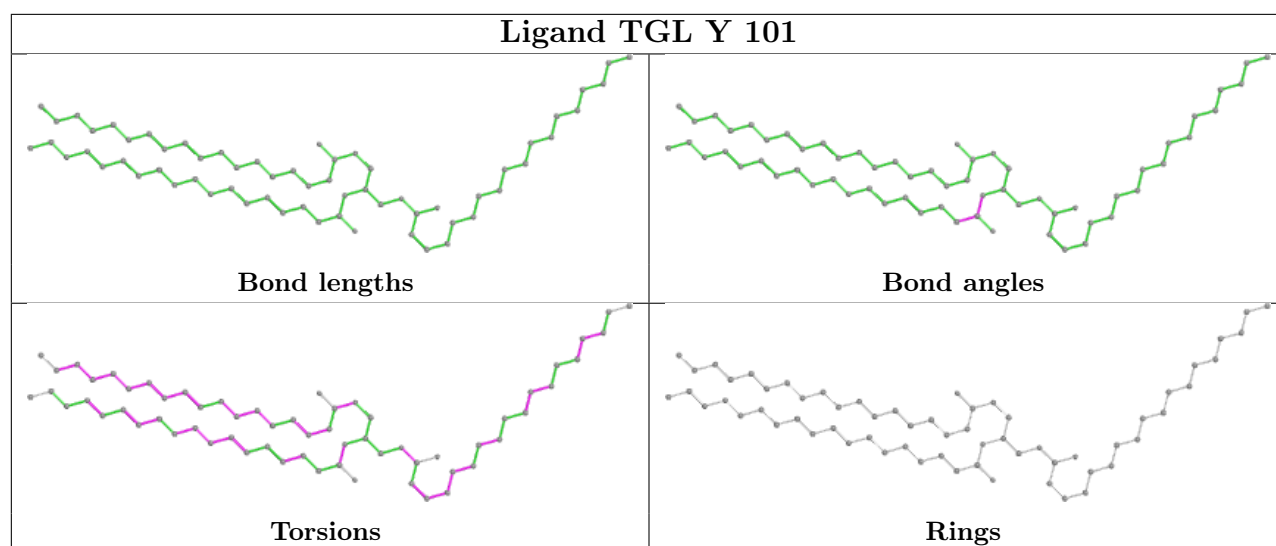


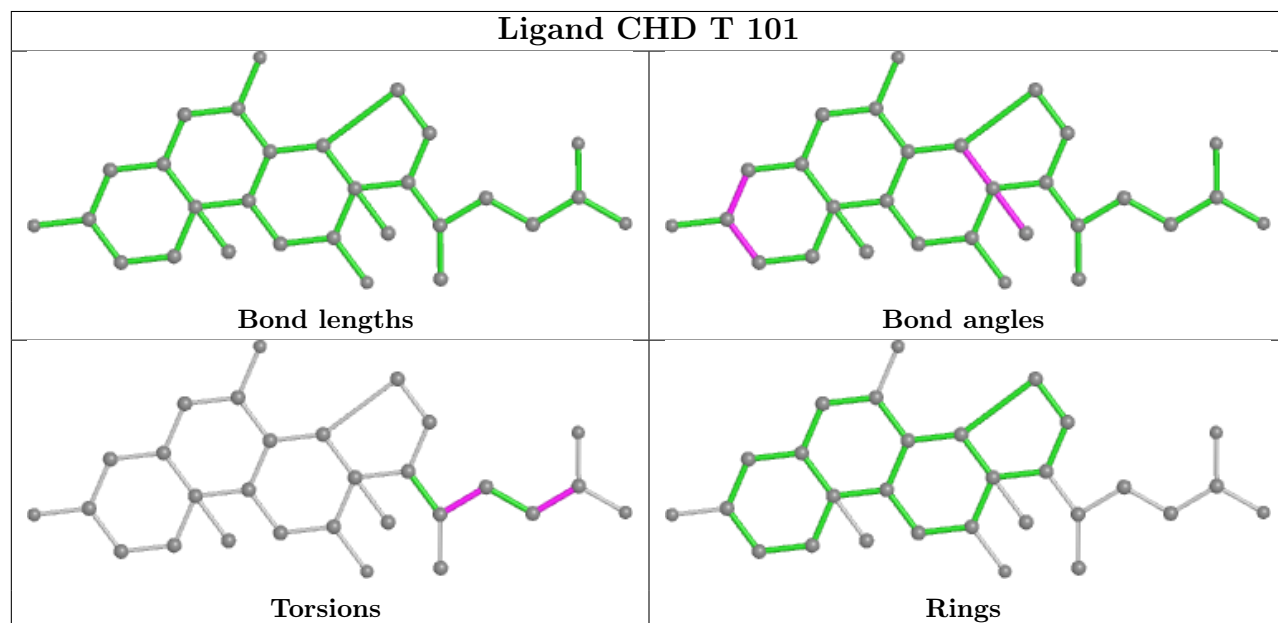
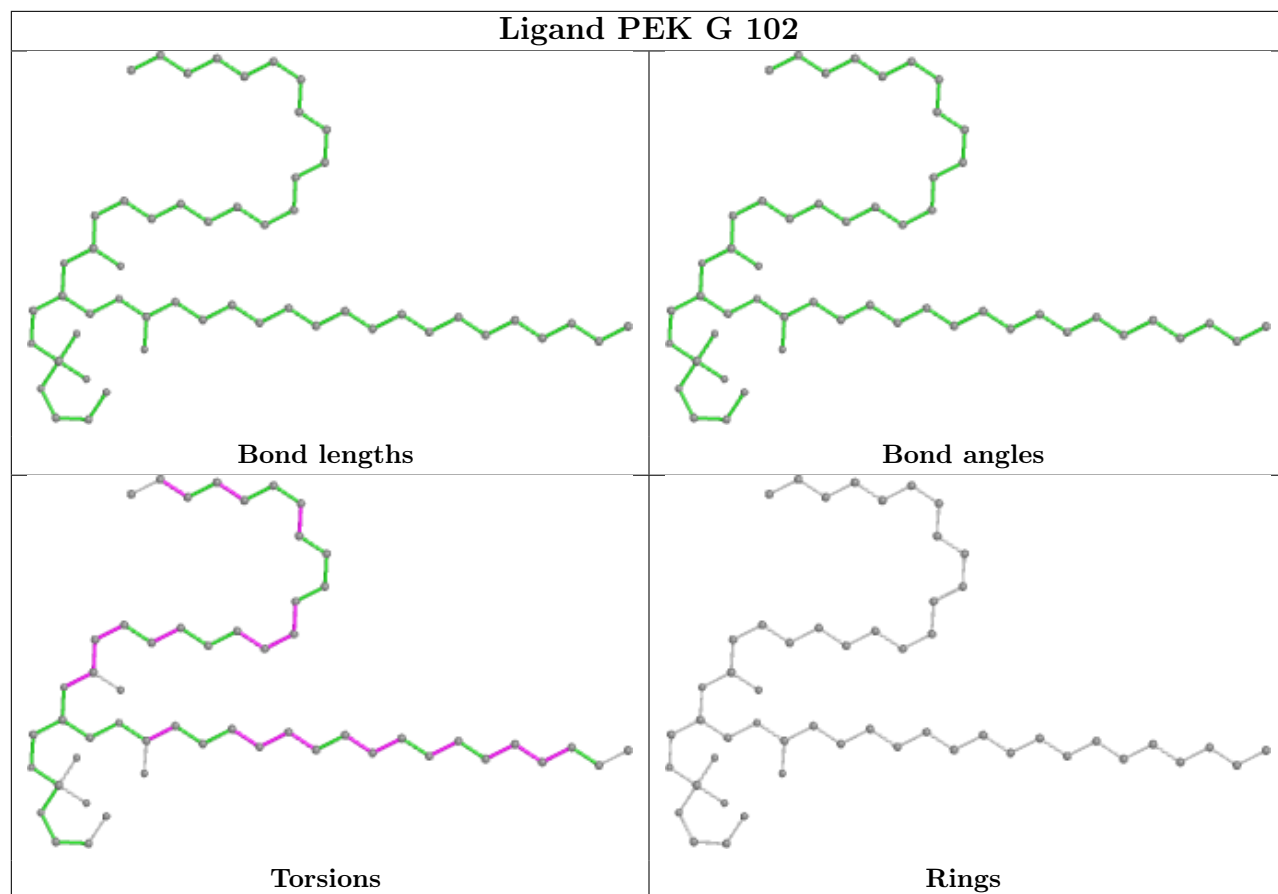
Ligand PSC B 303

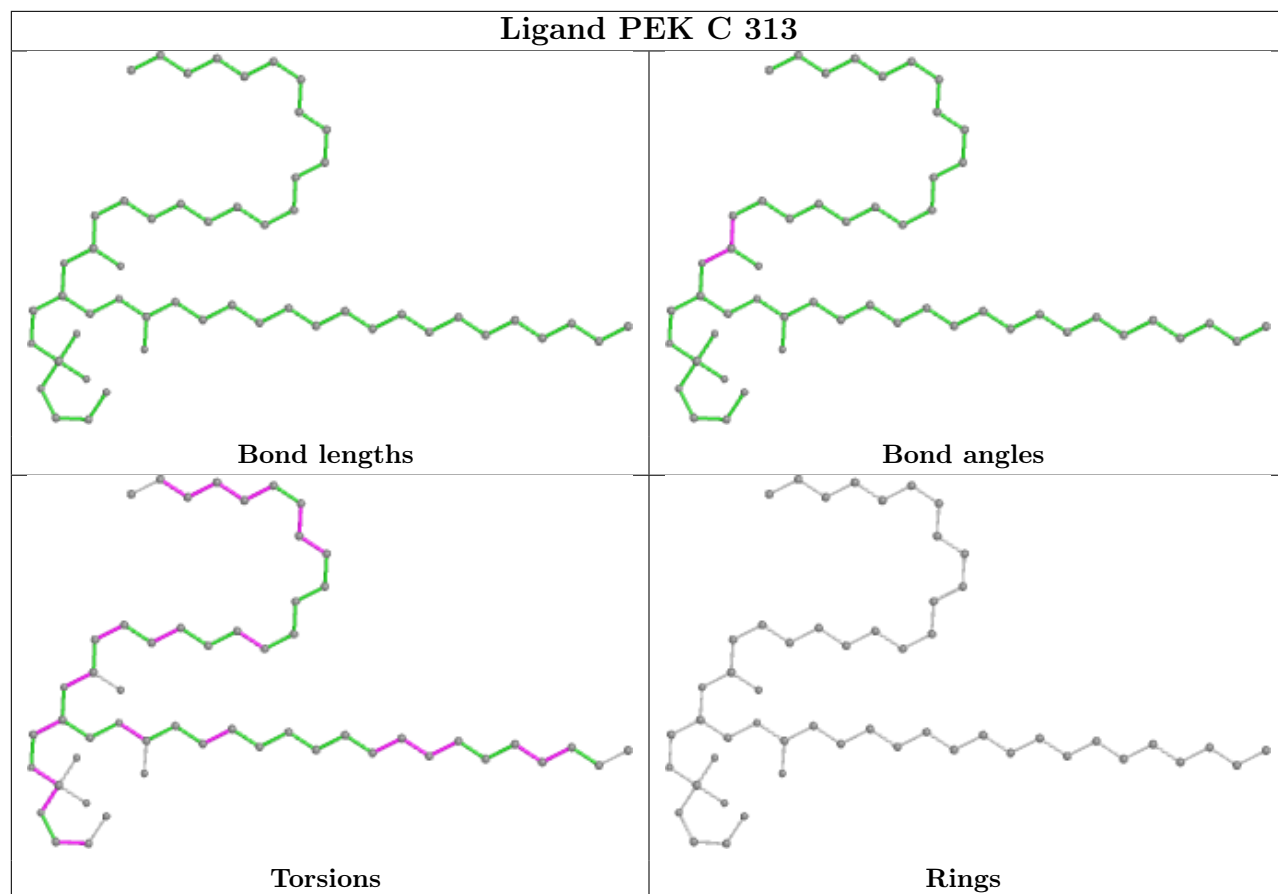


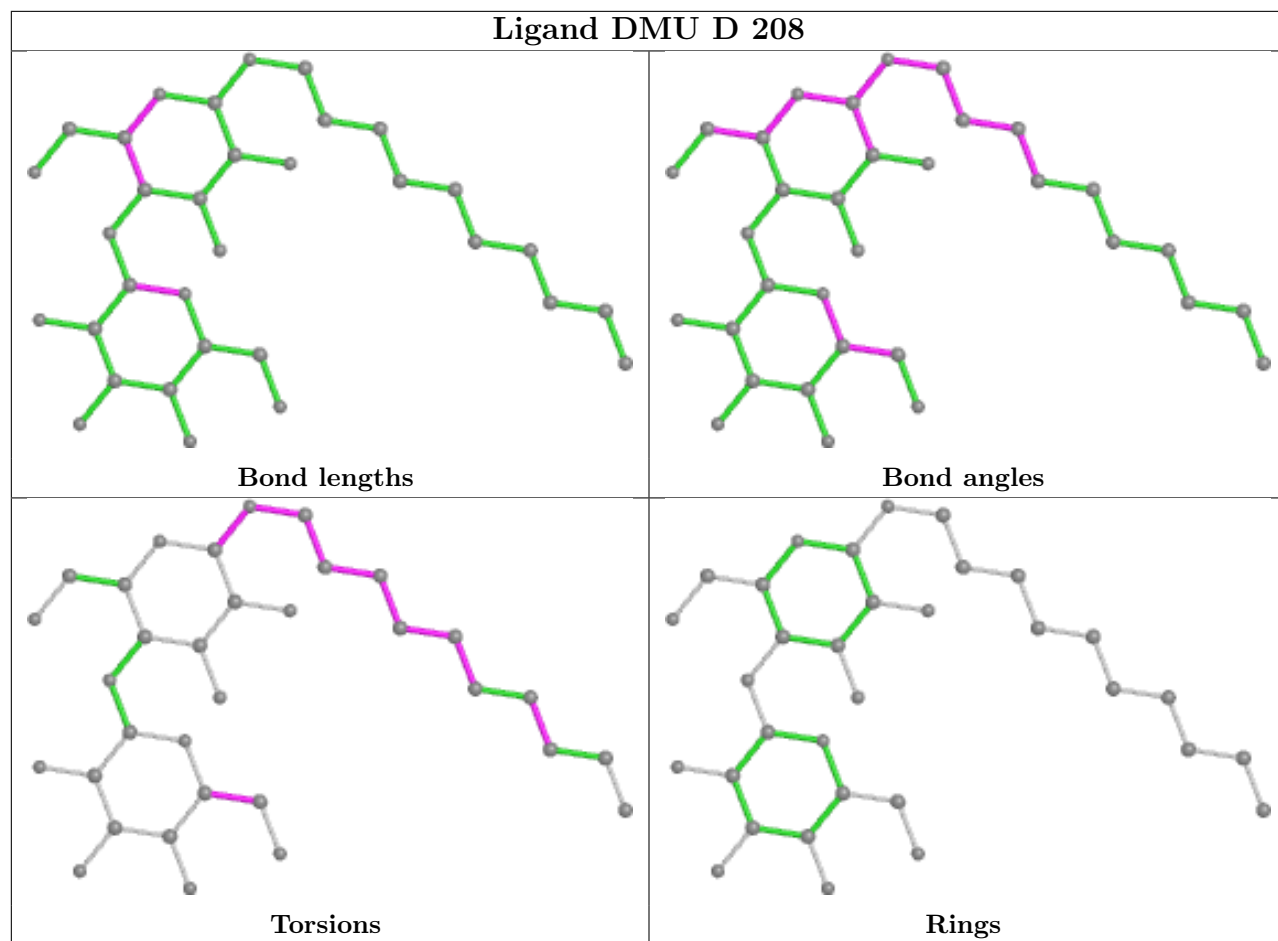
Ligand DMU C 311

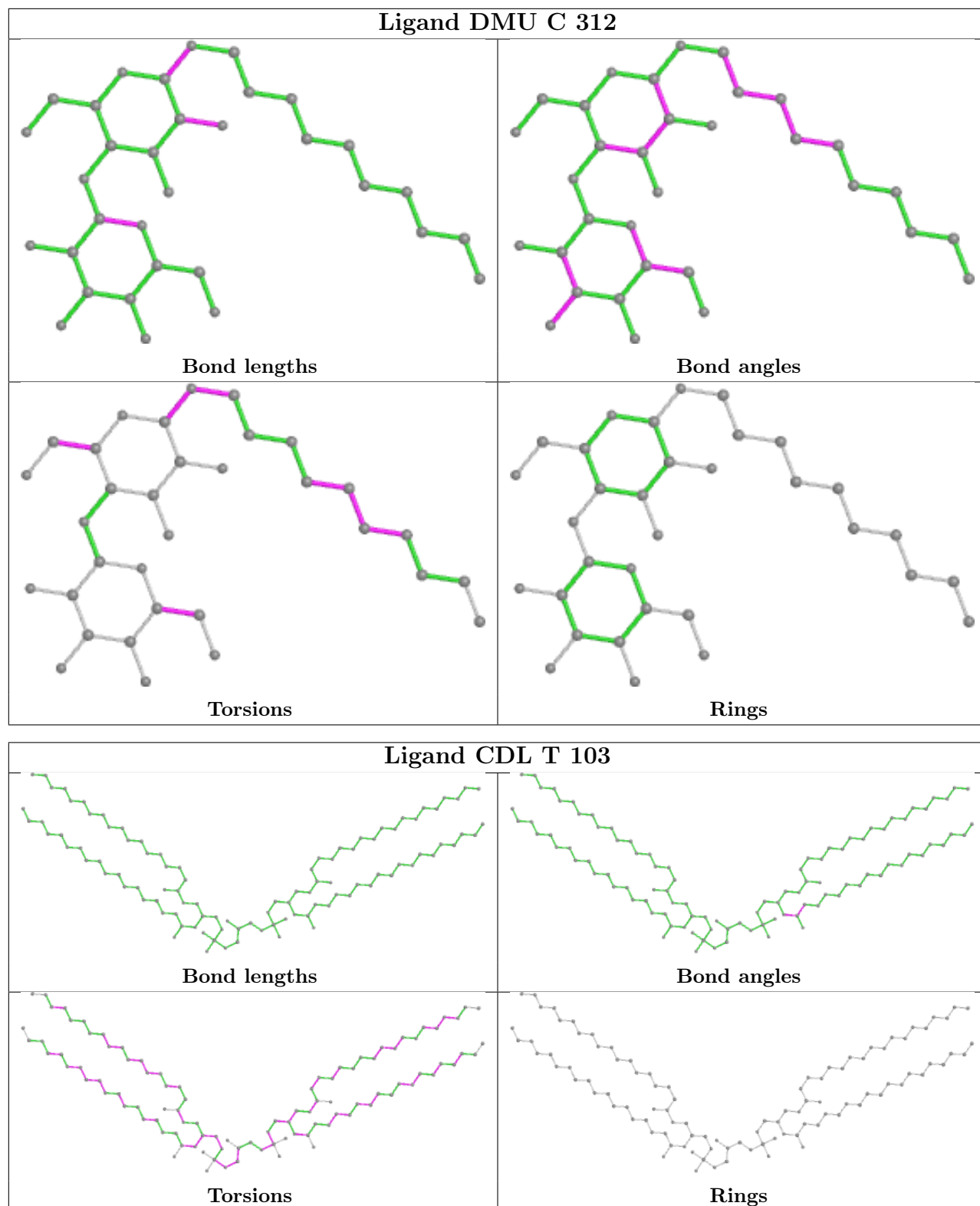


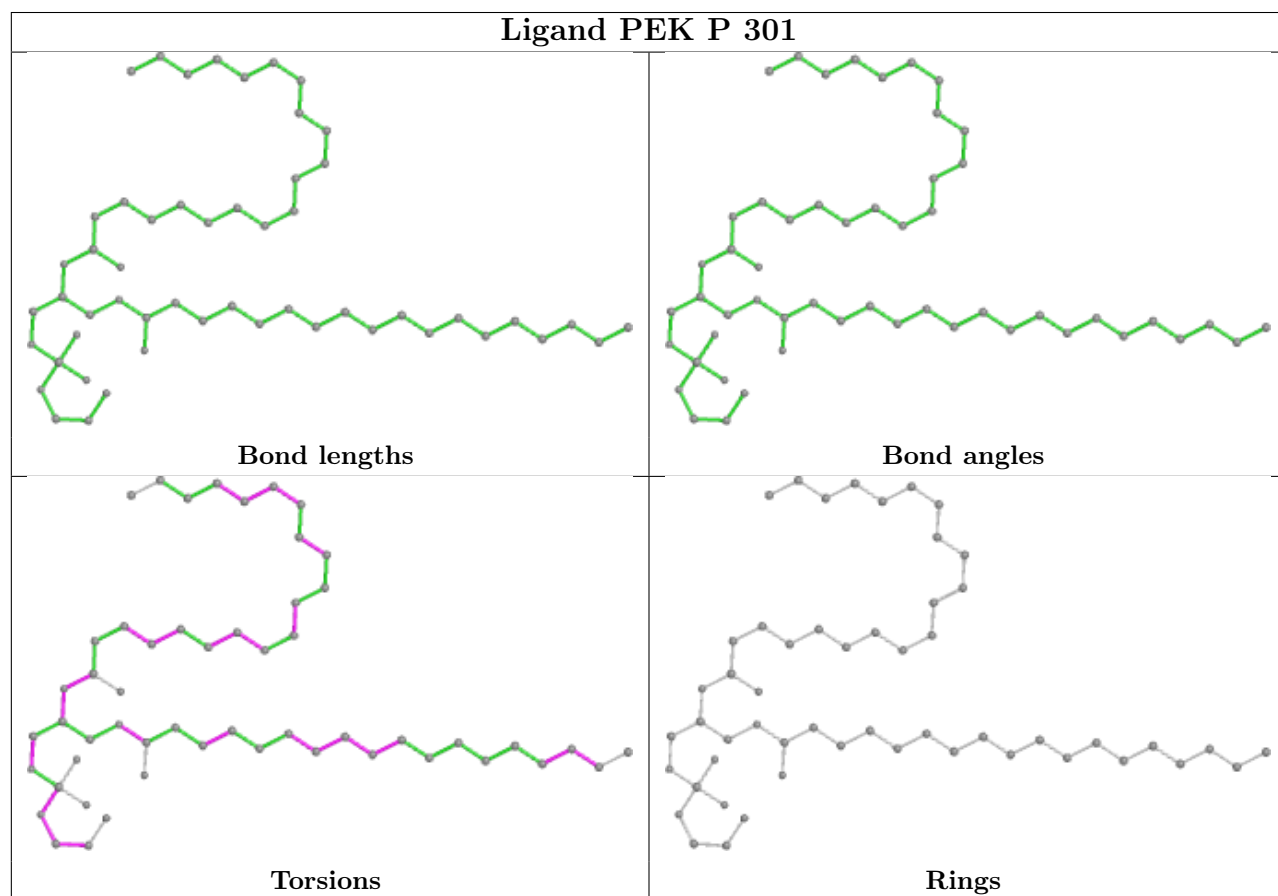
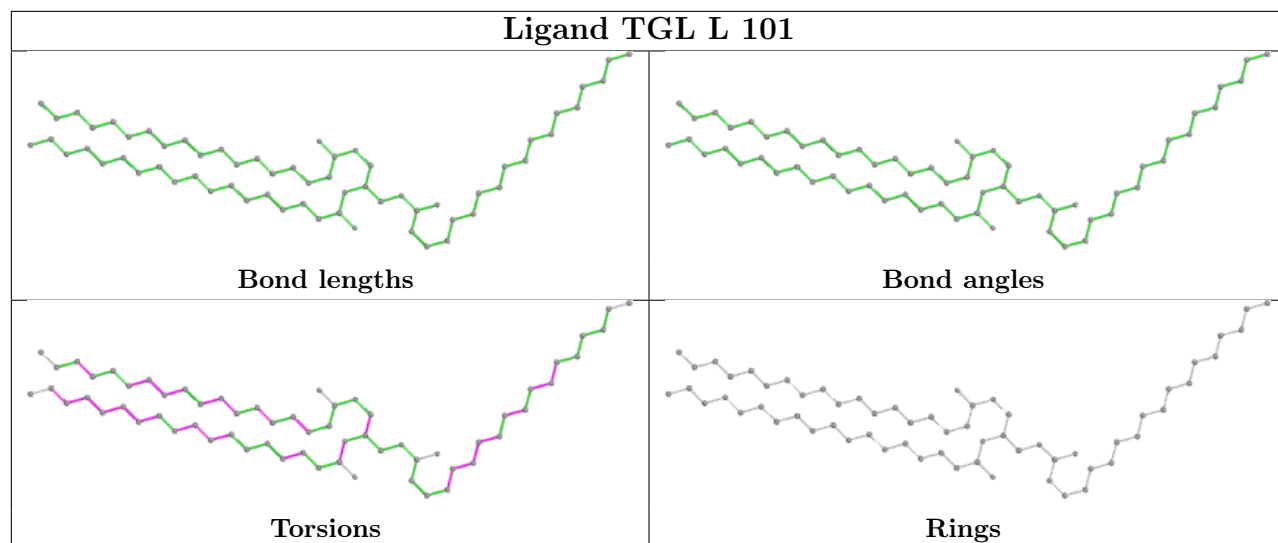


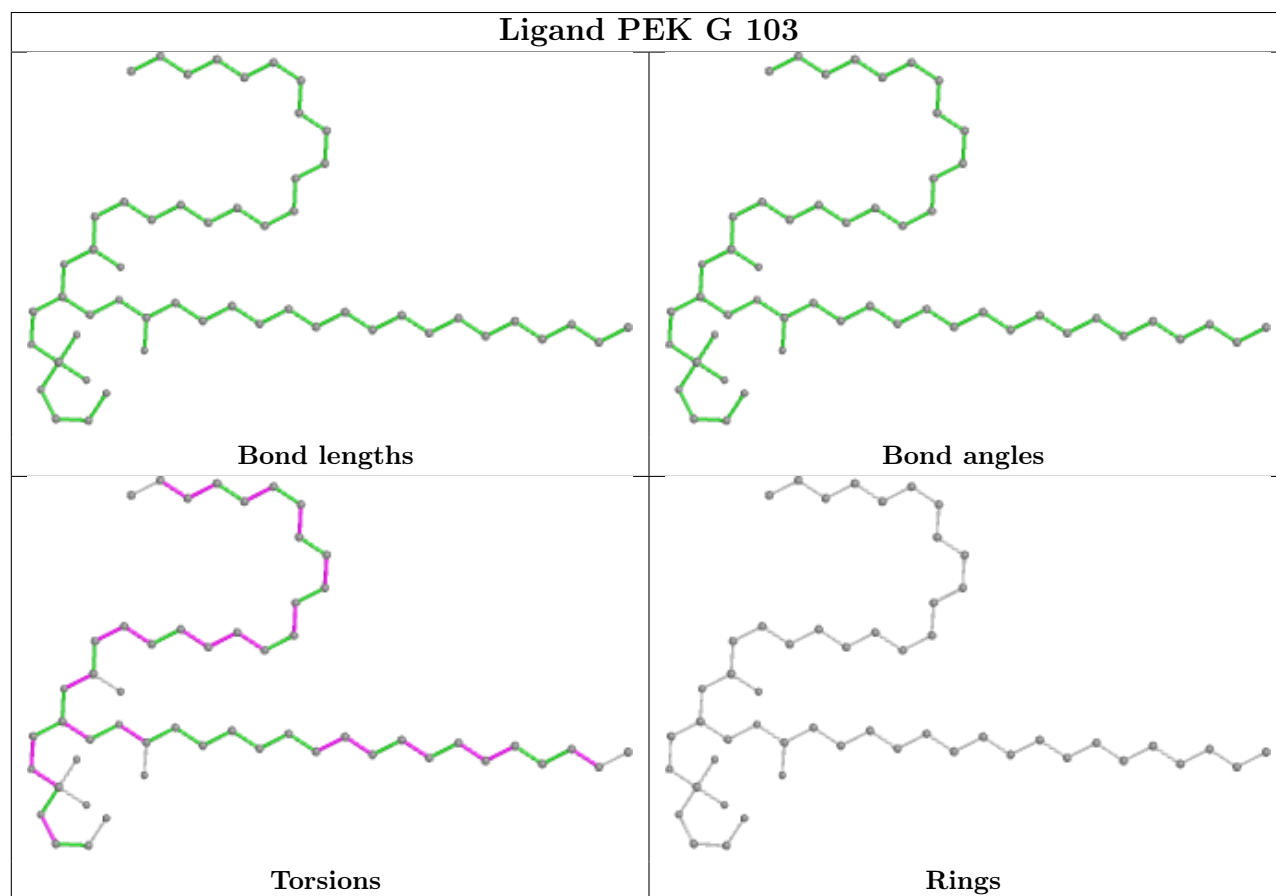
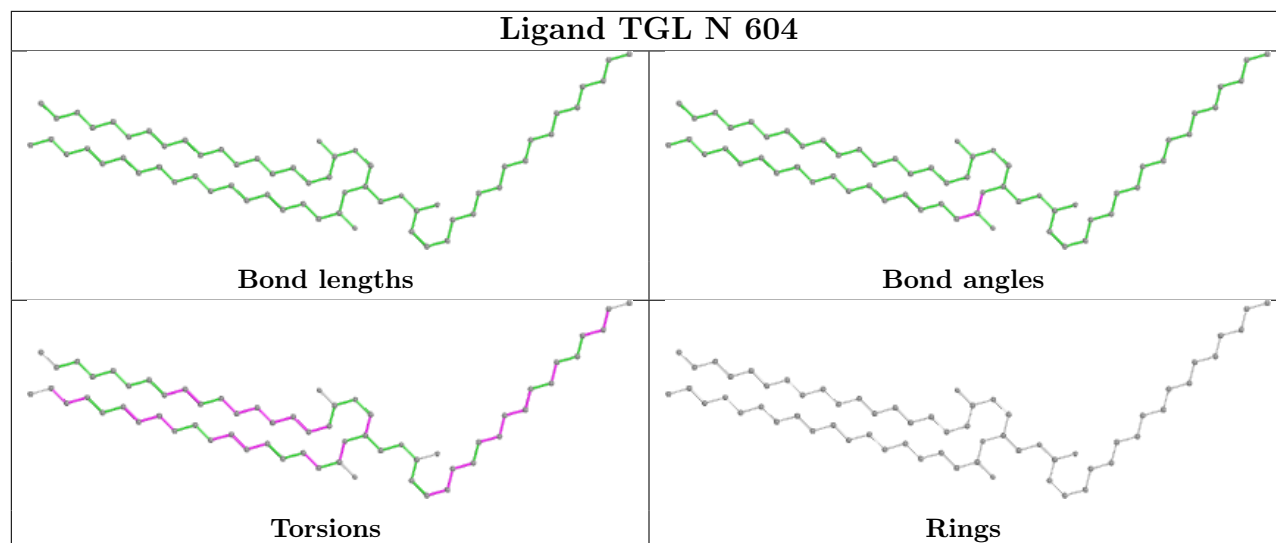


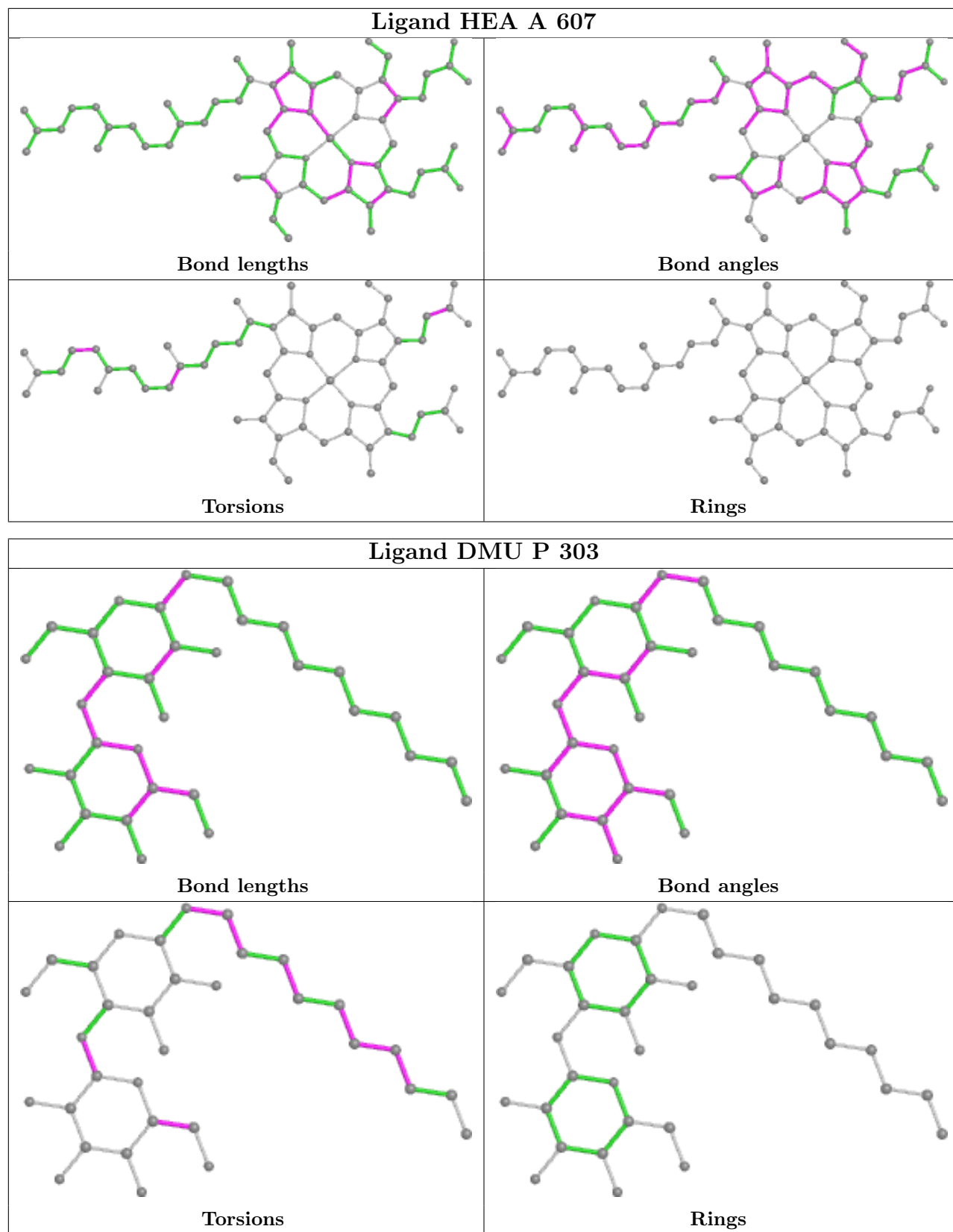


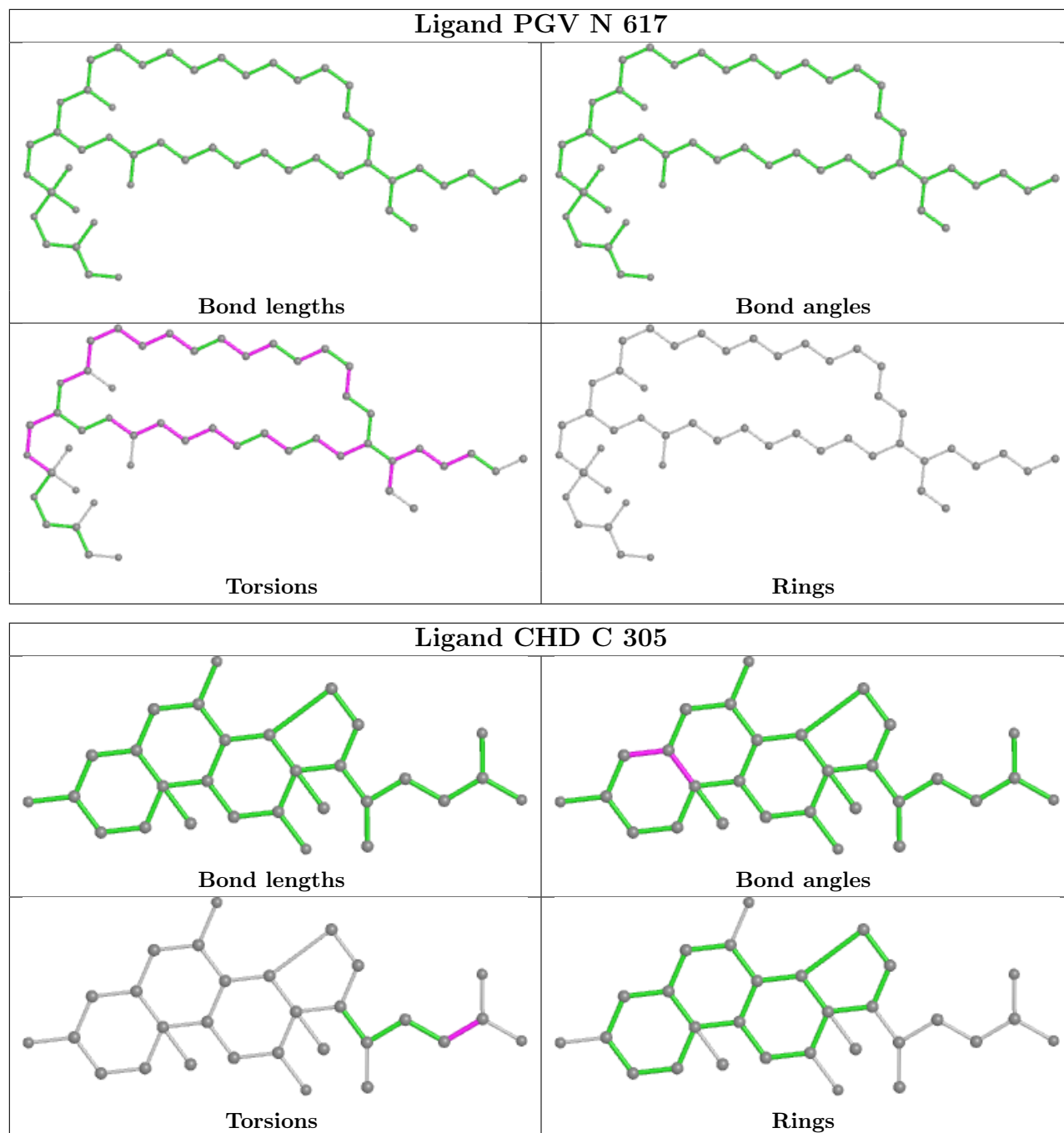




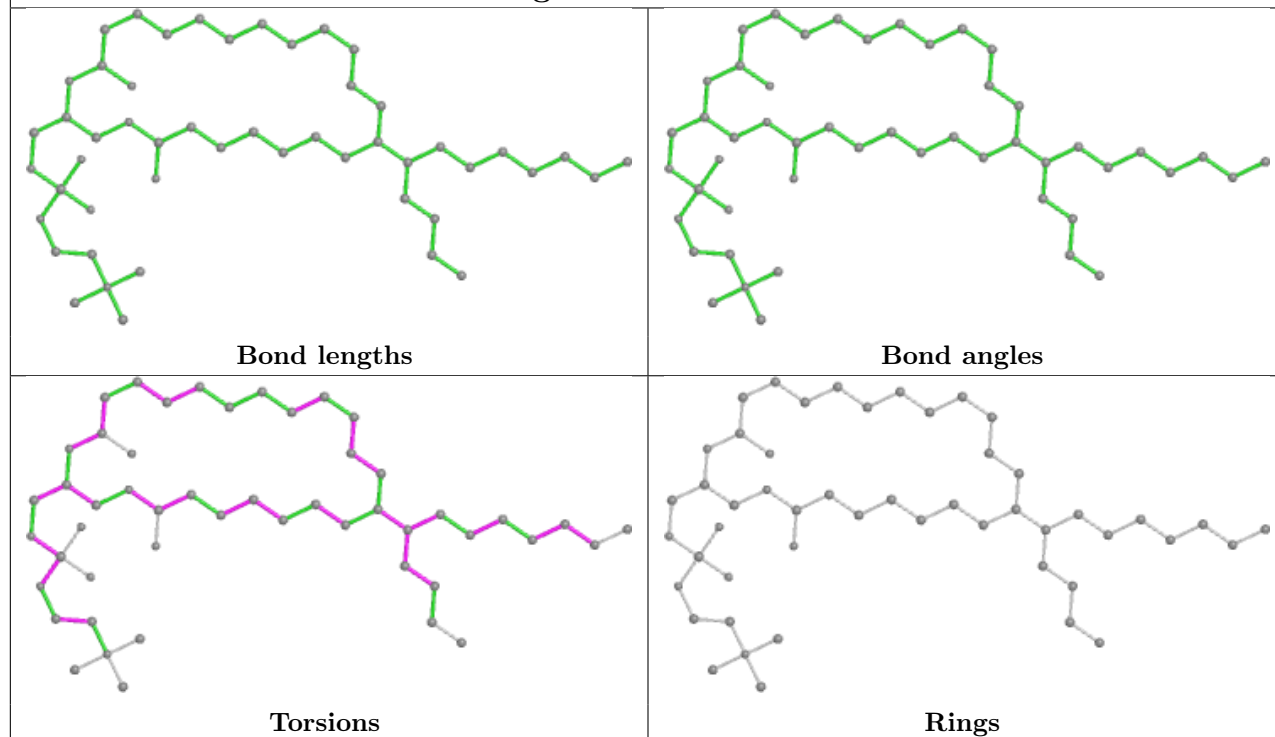




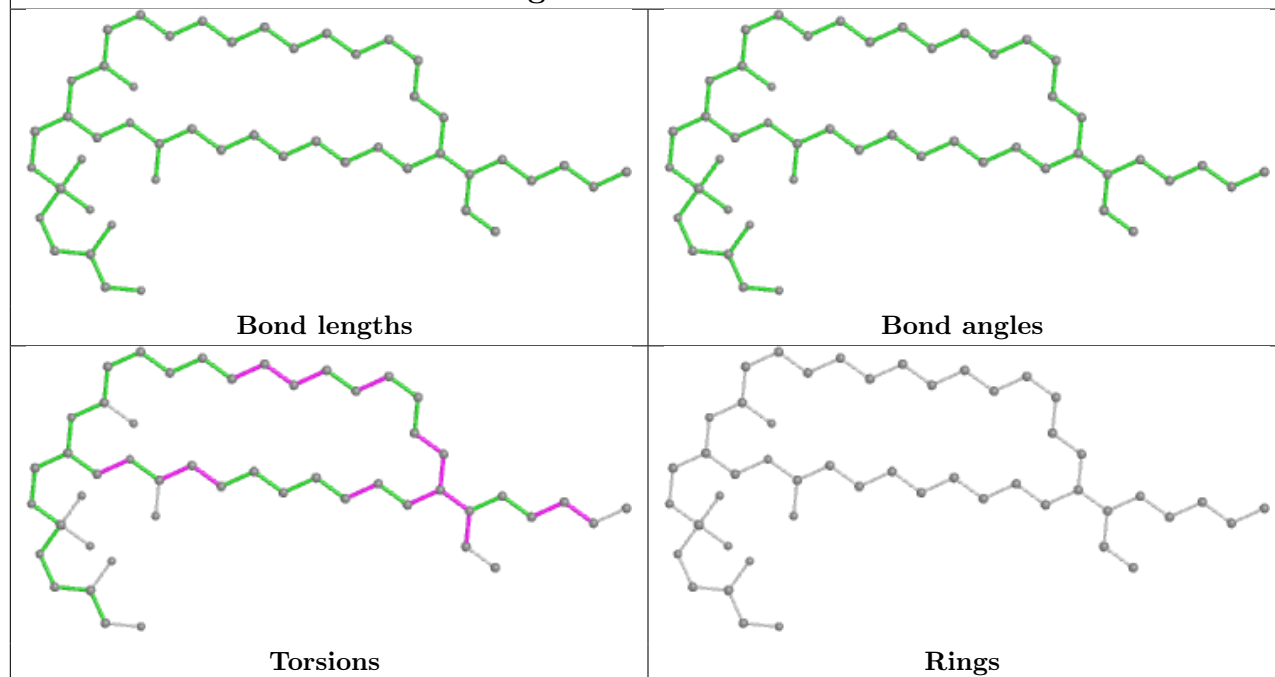


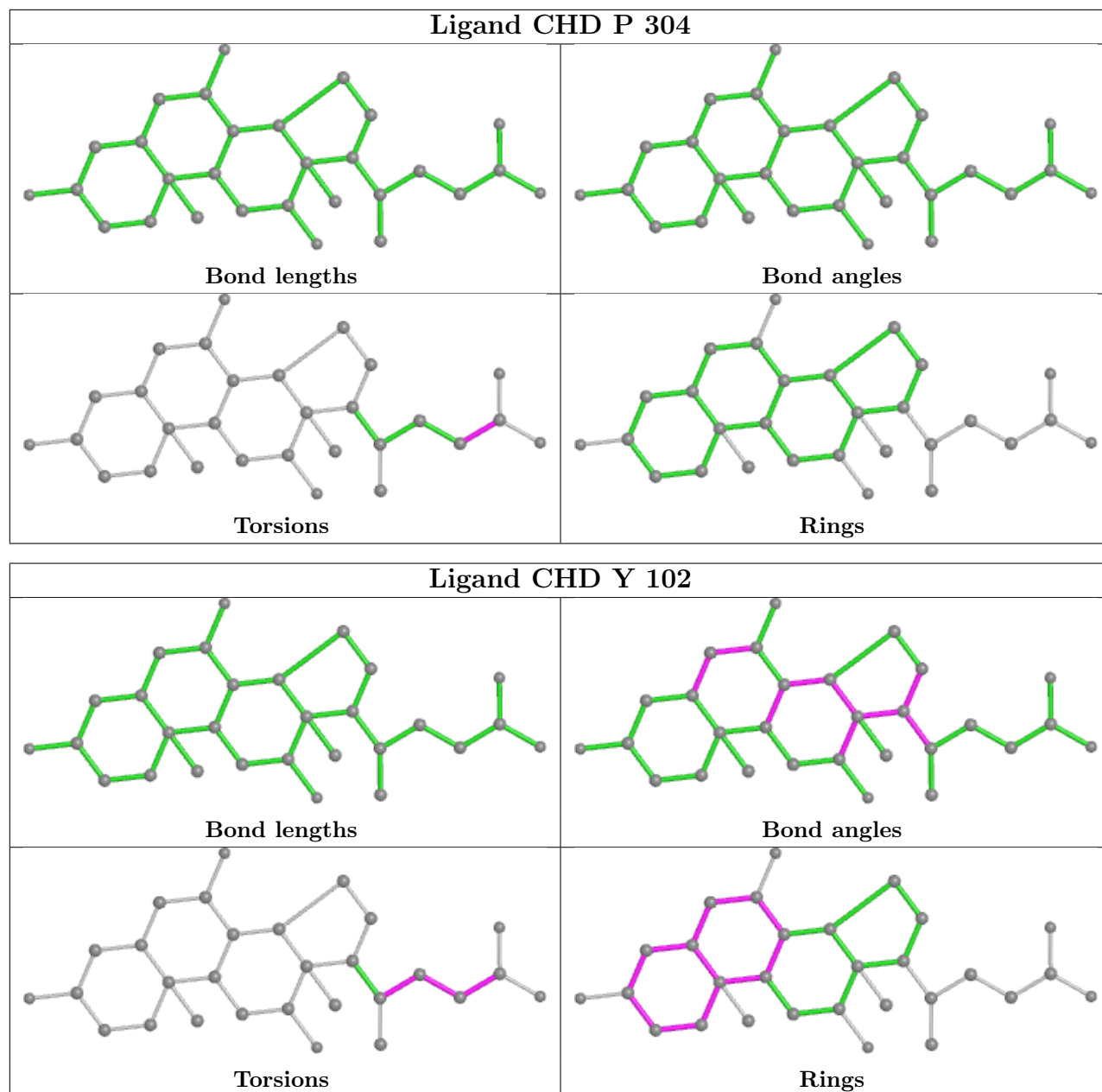


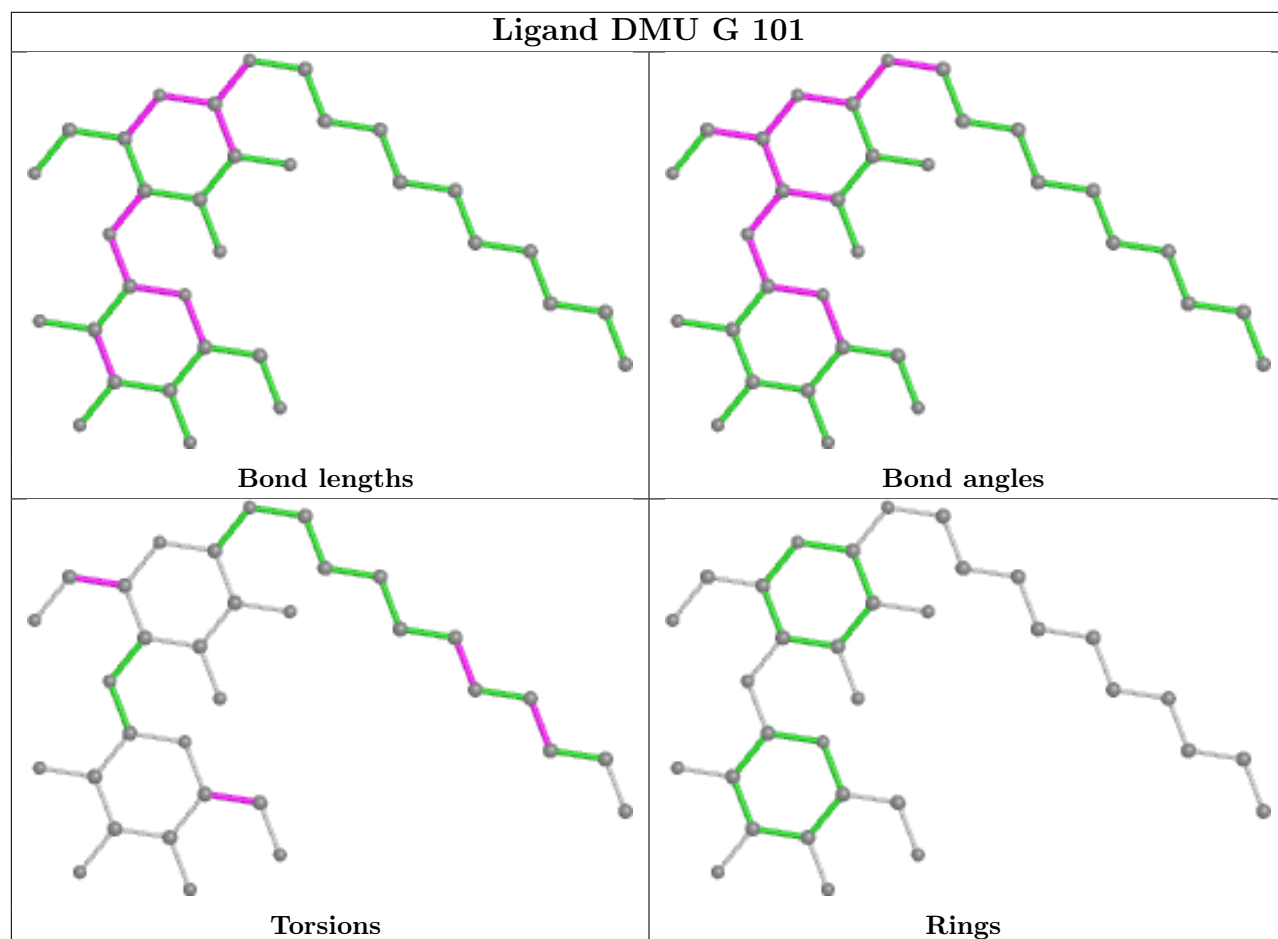
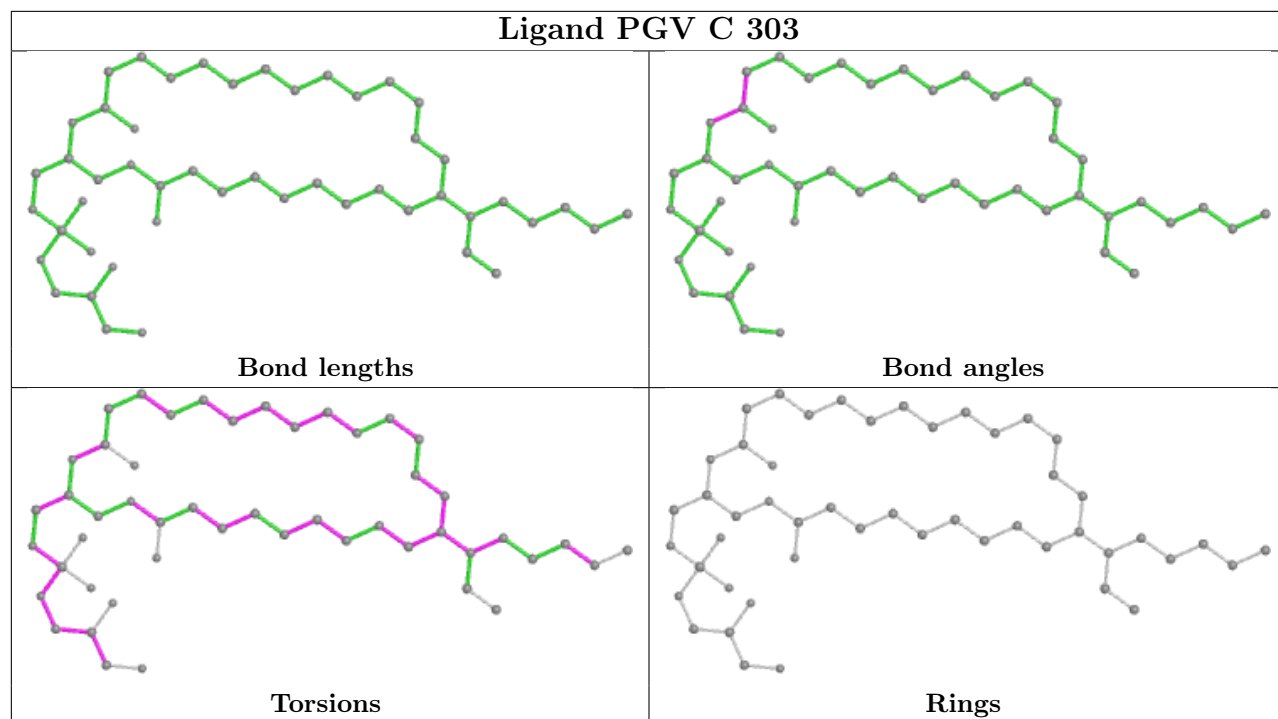
Ligand PSC R 201

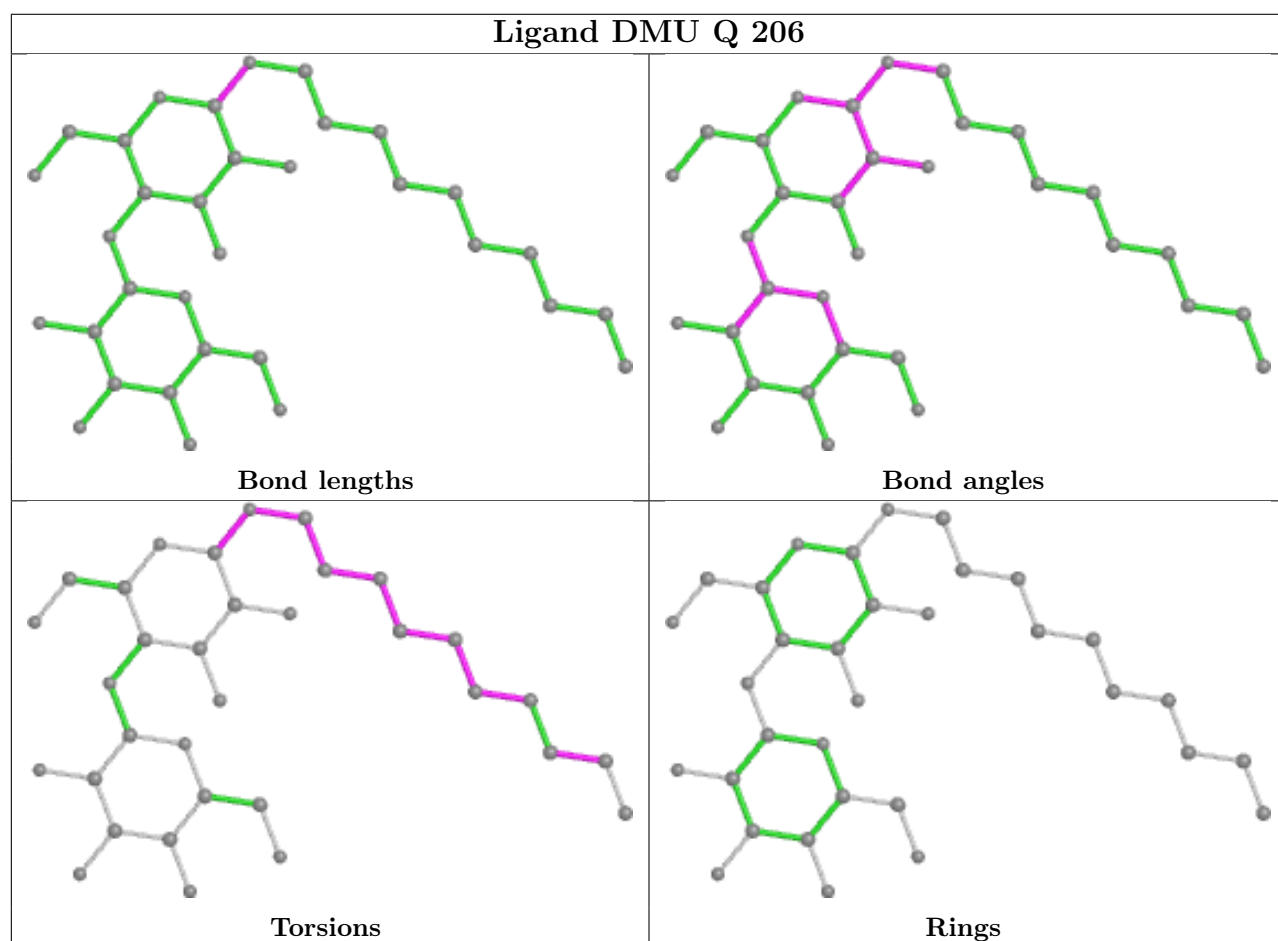
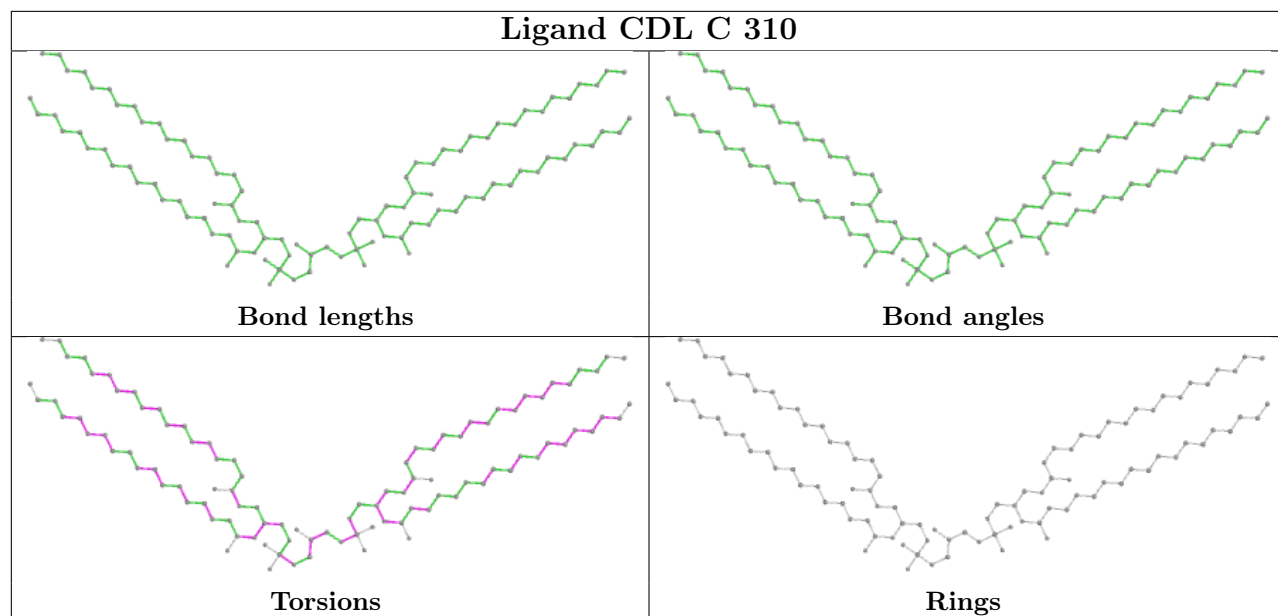


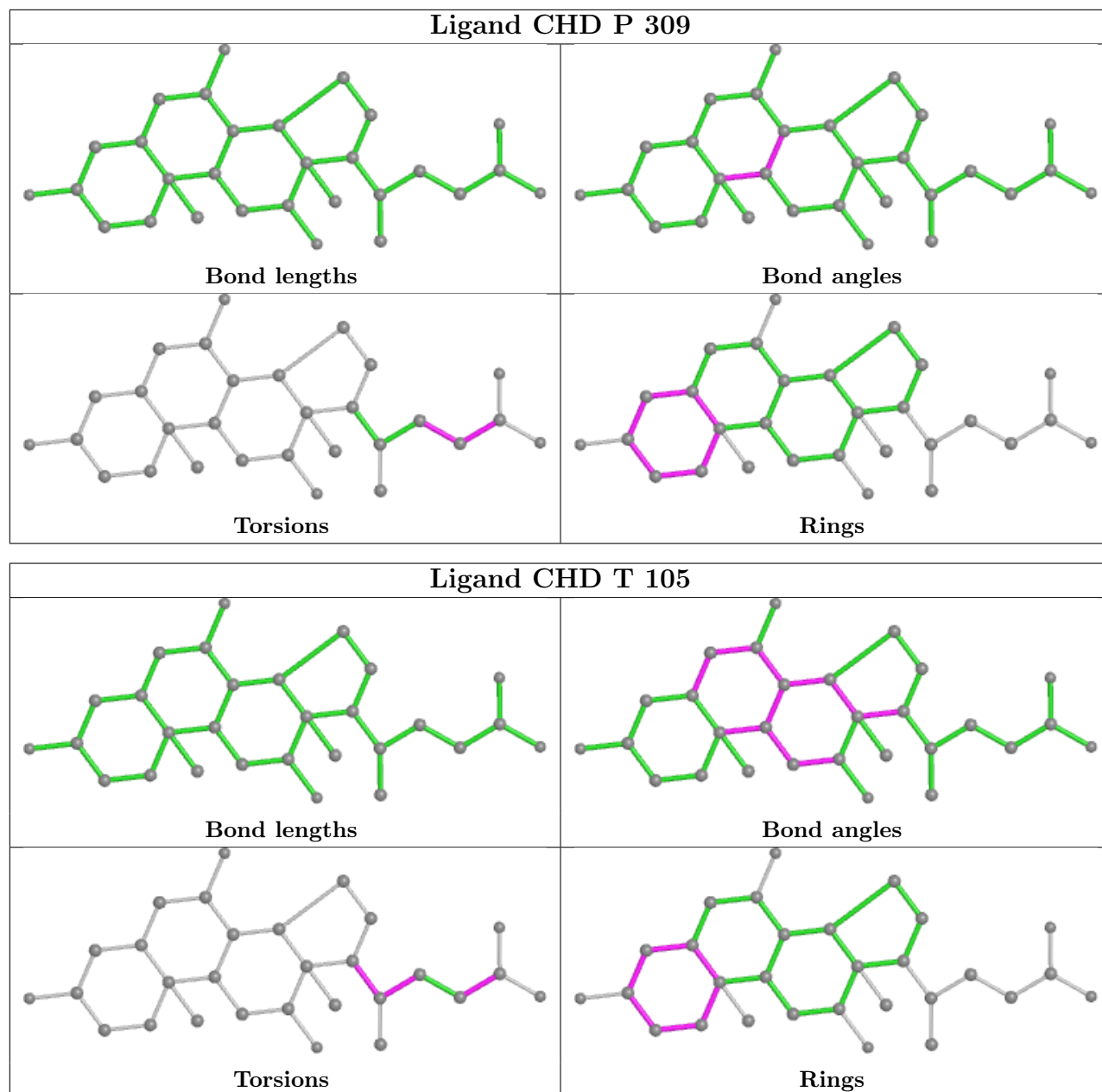
Ligand PGV A 605

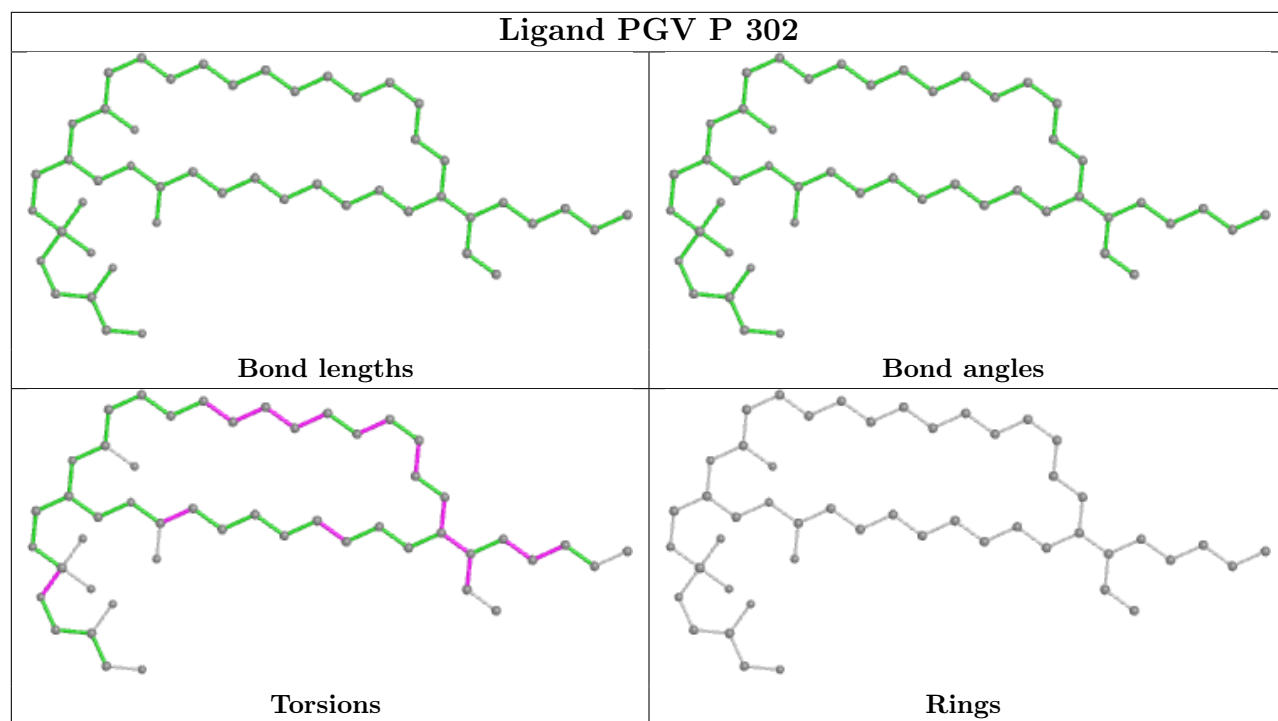
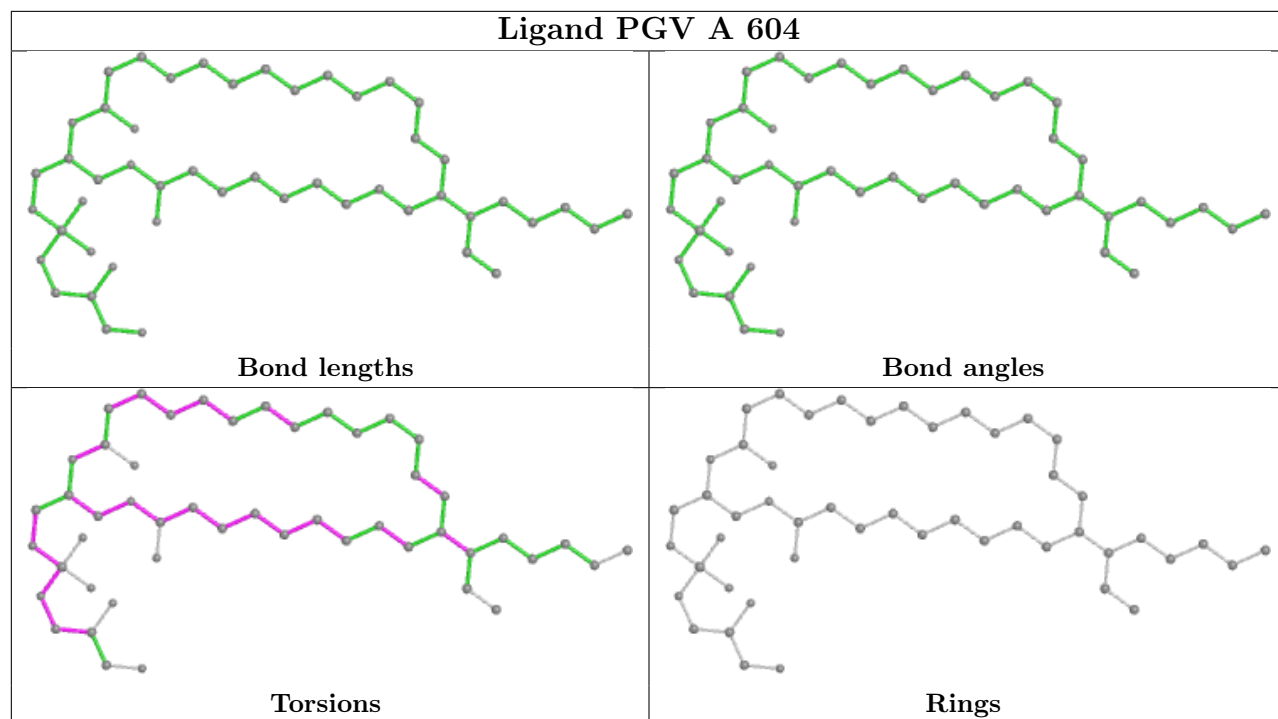


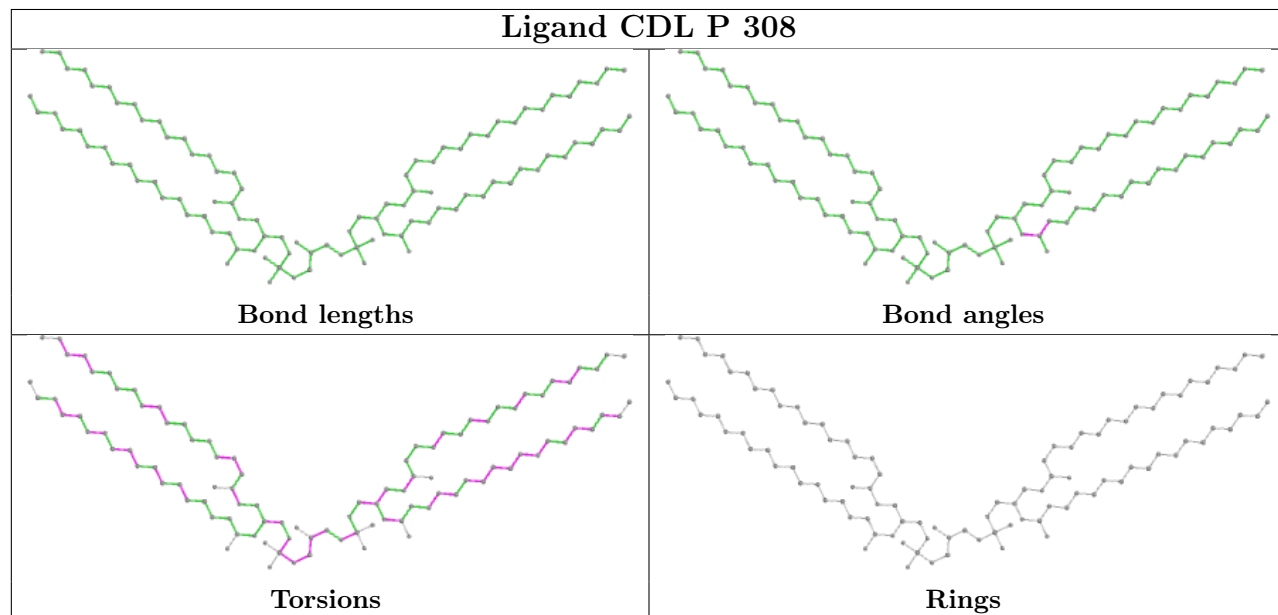
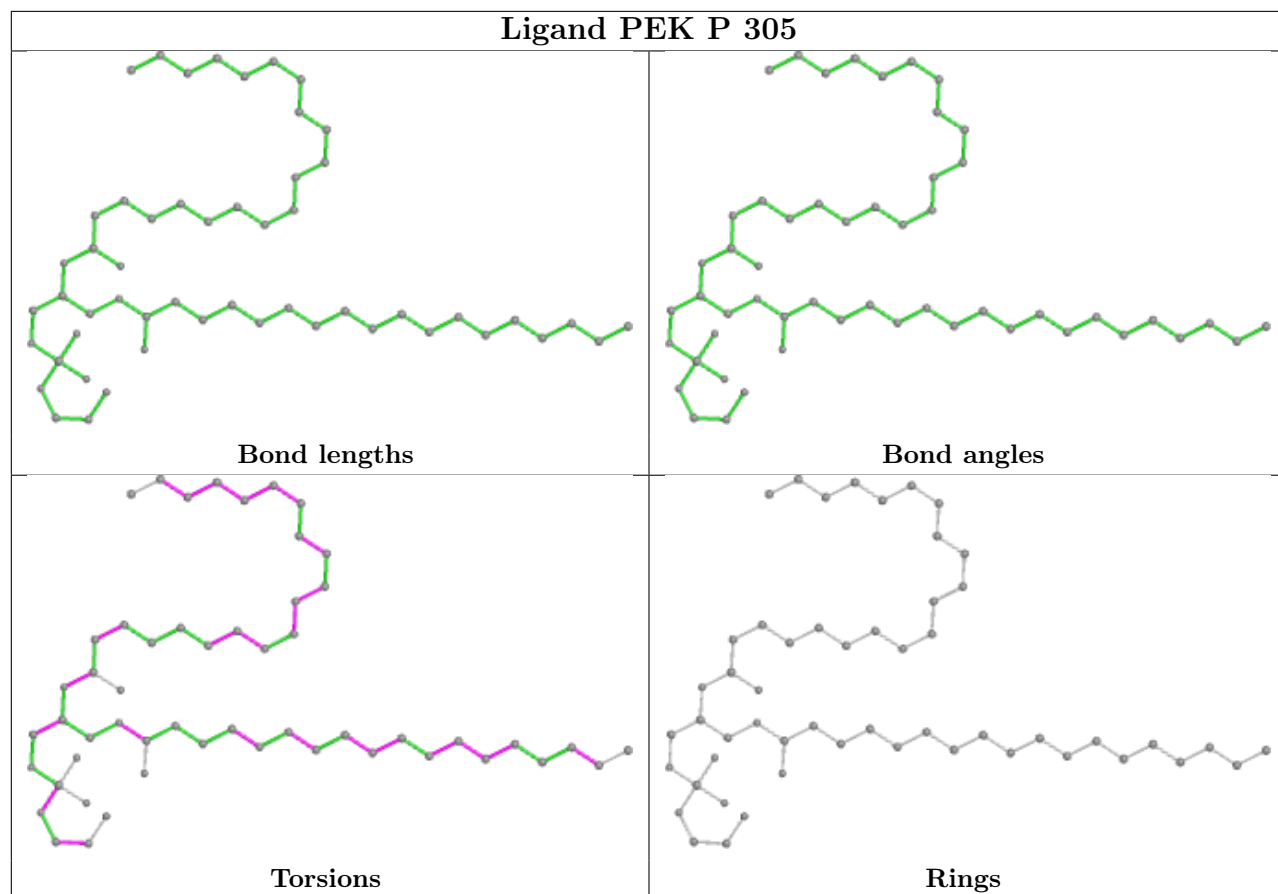


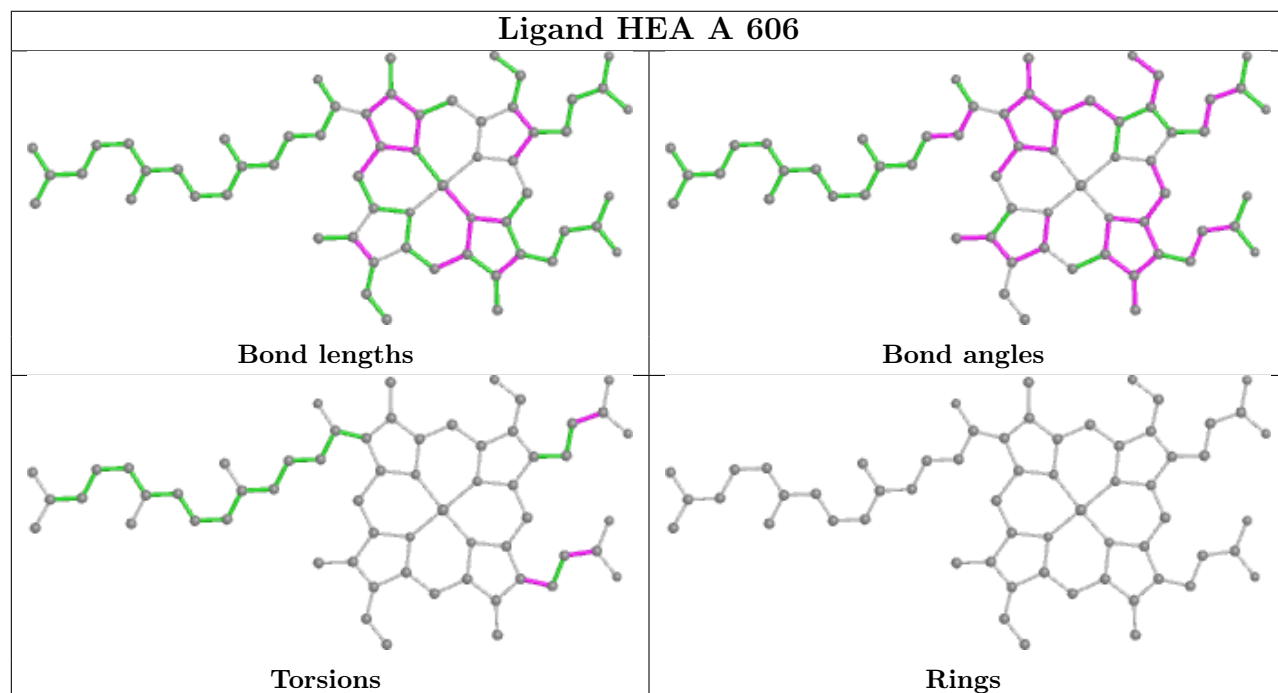
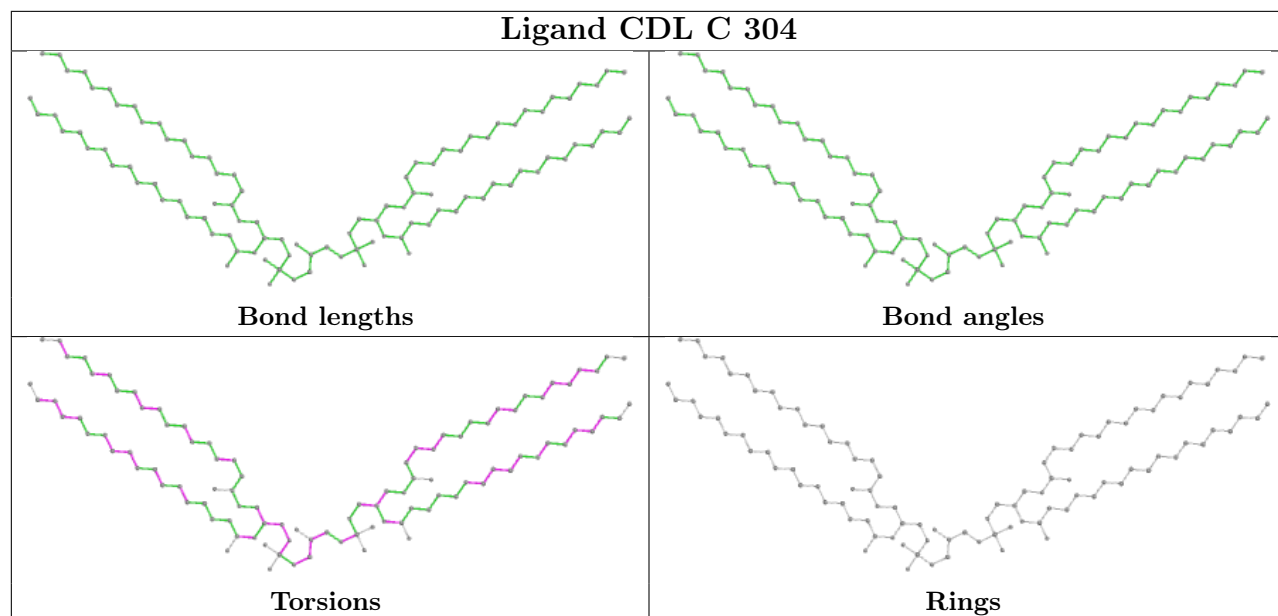


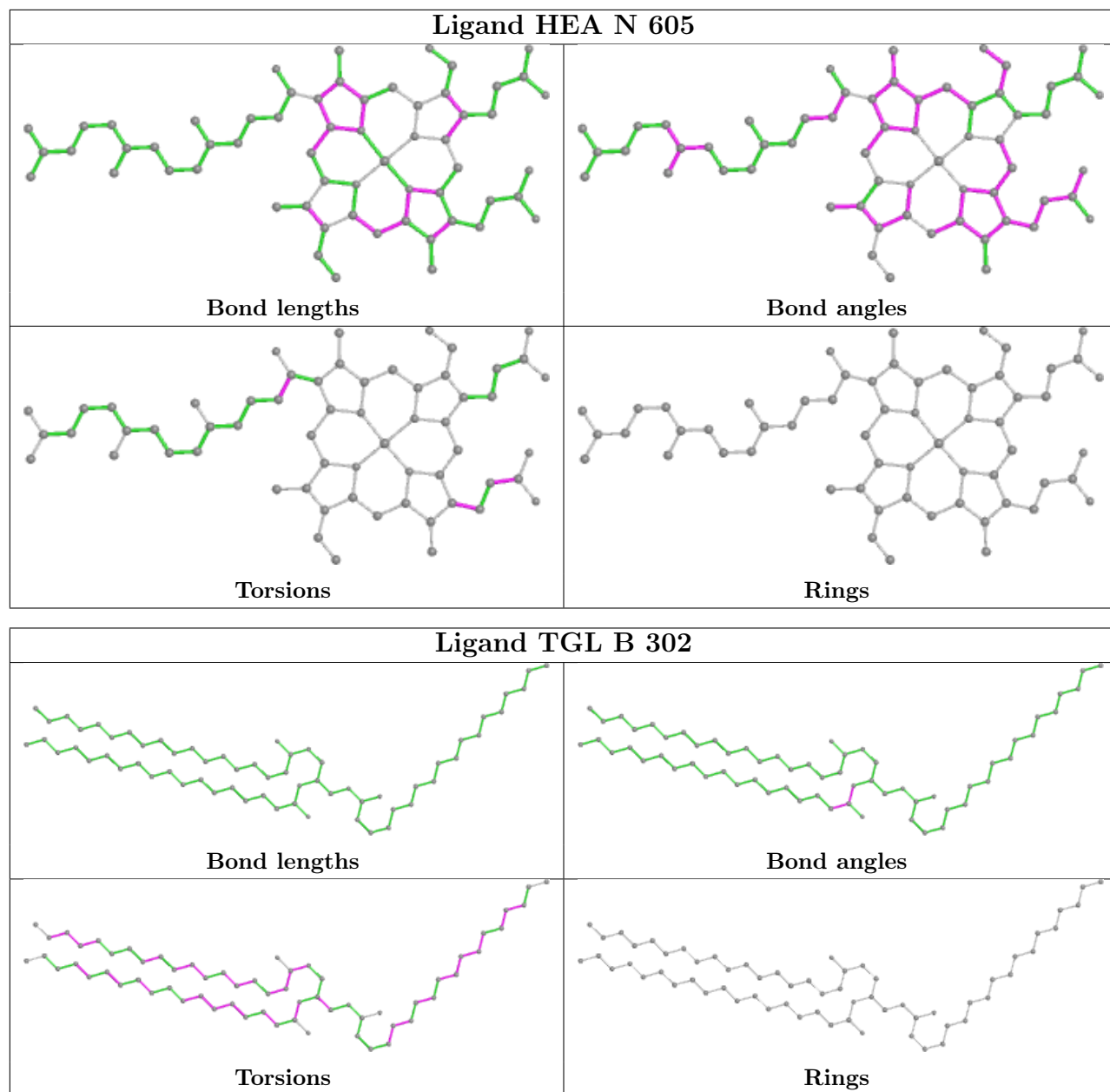


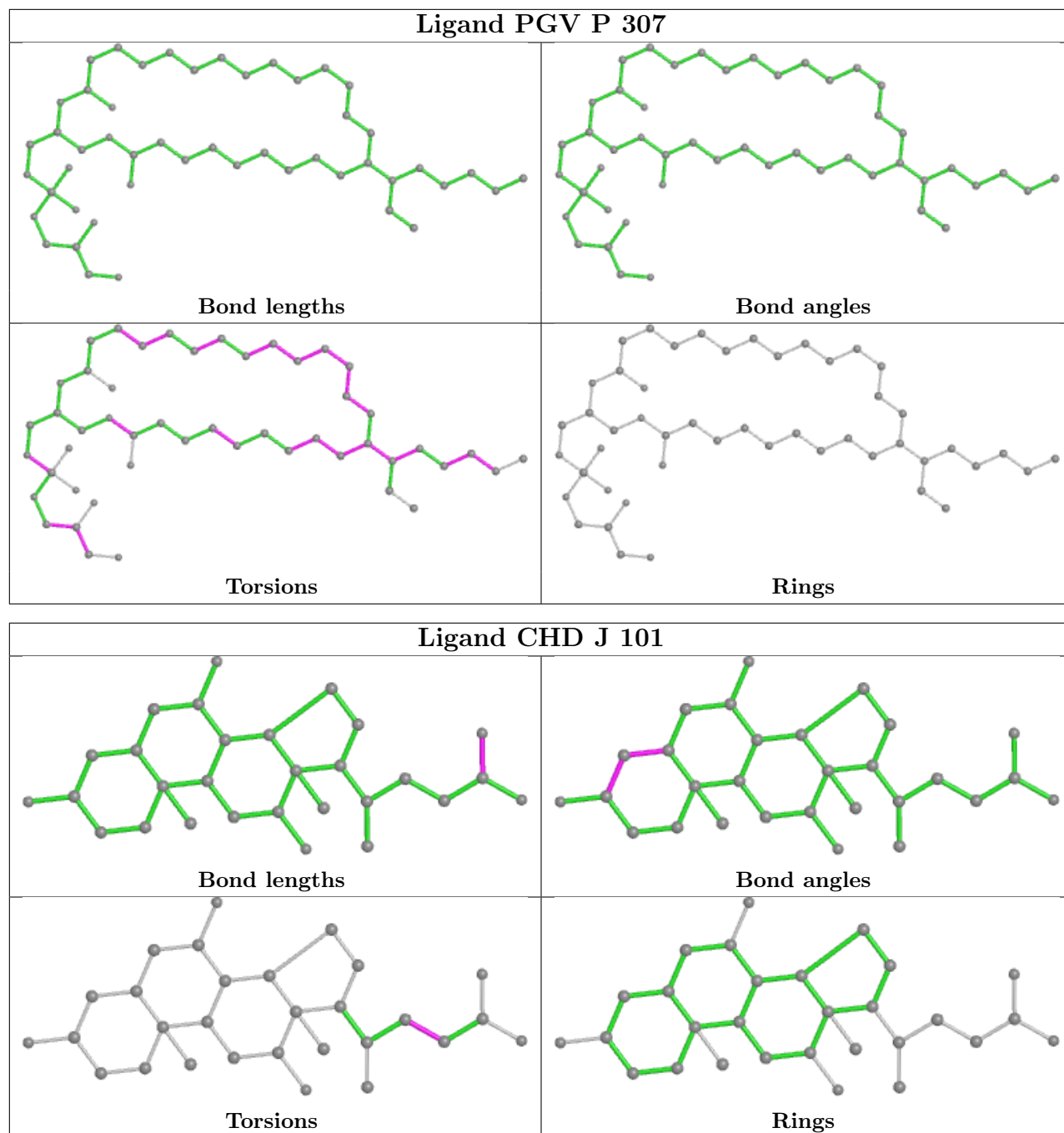




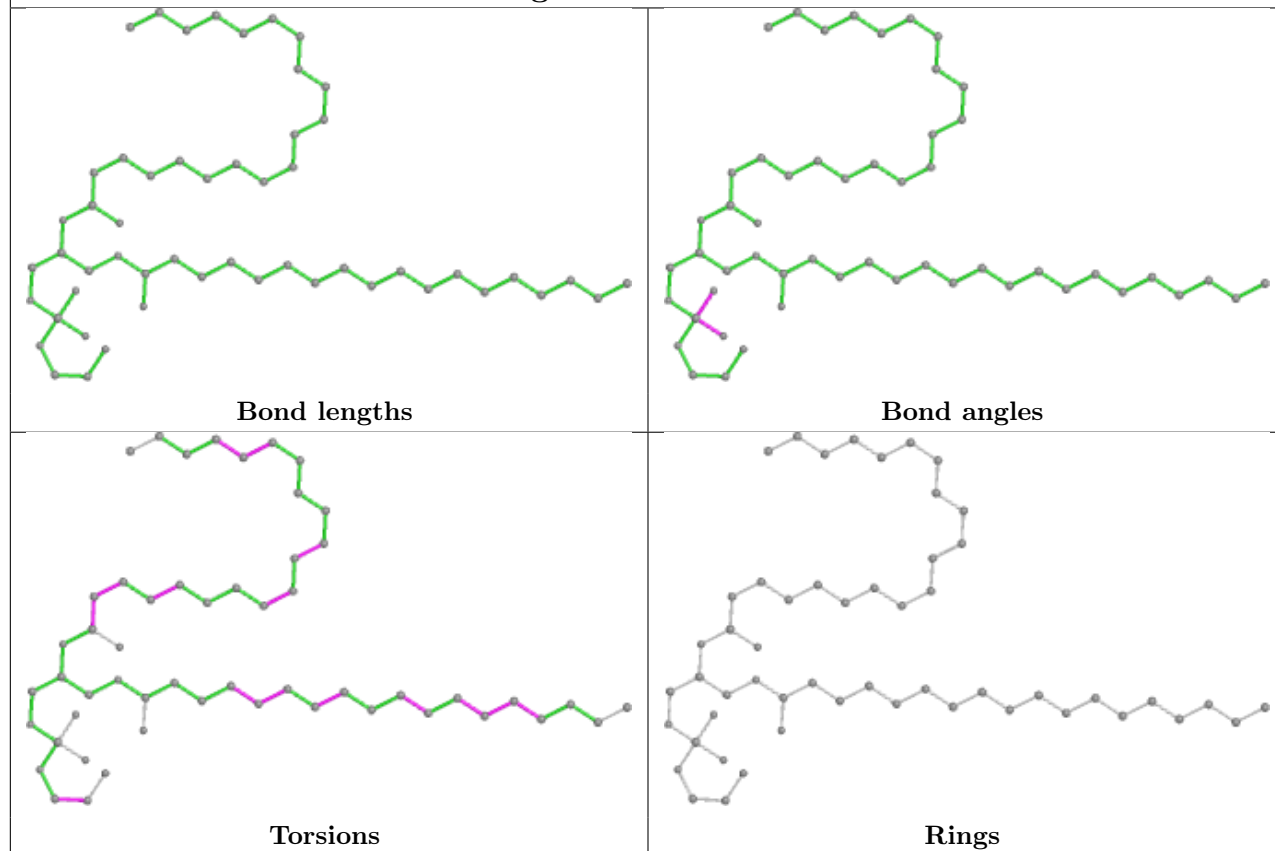




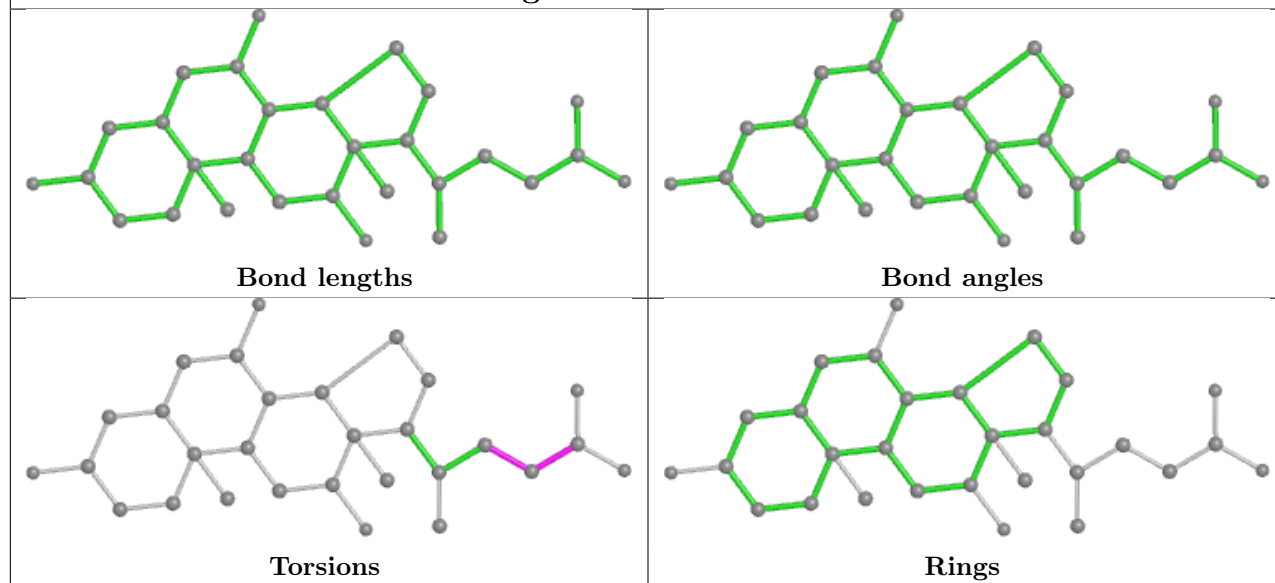


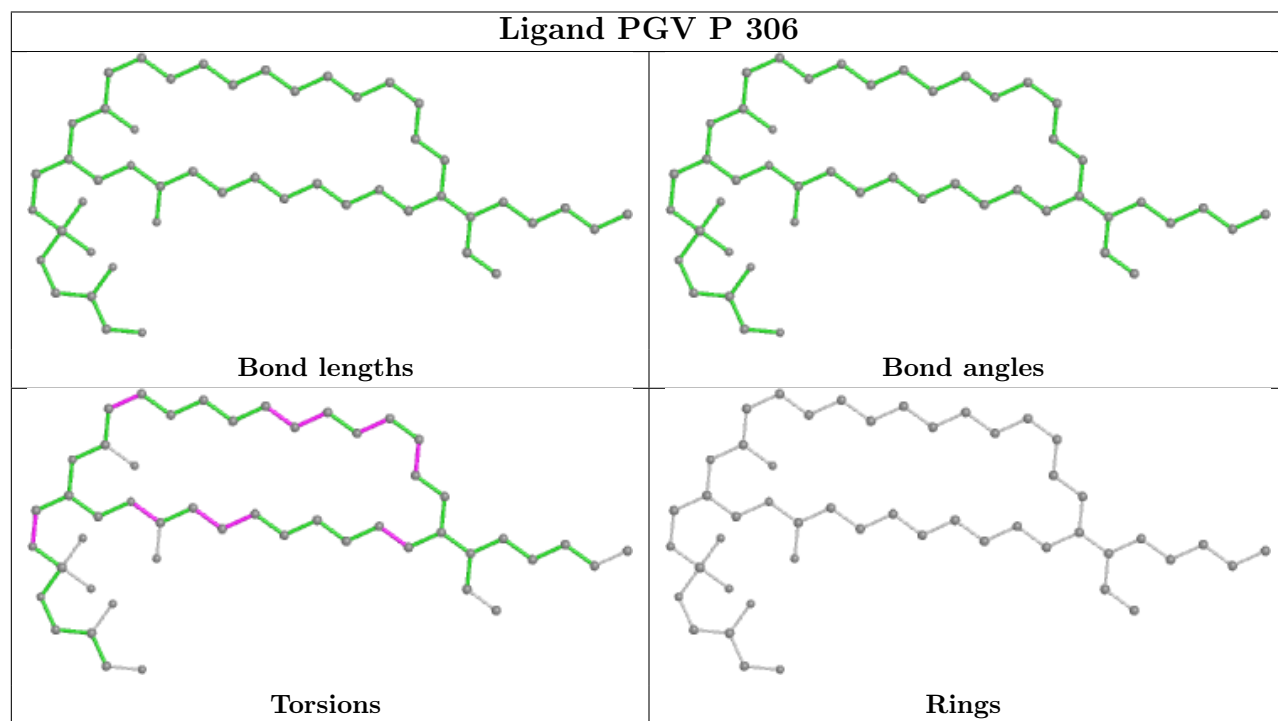
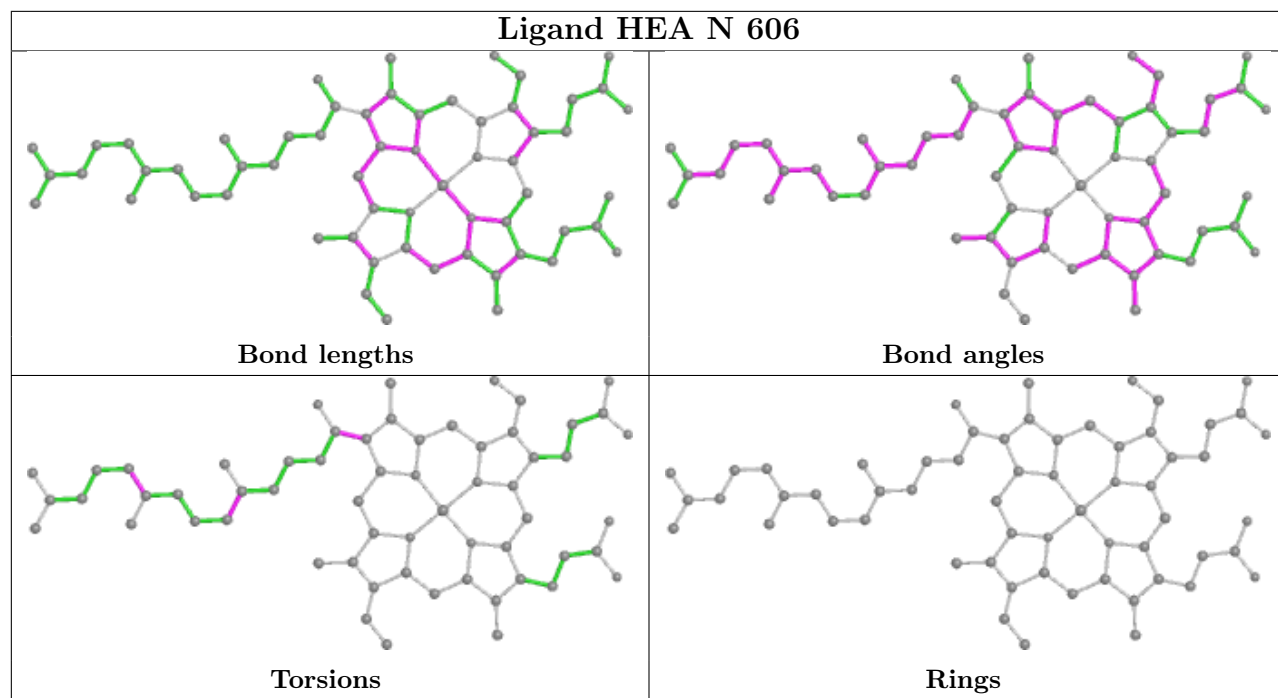


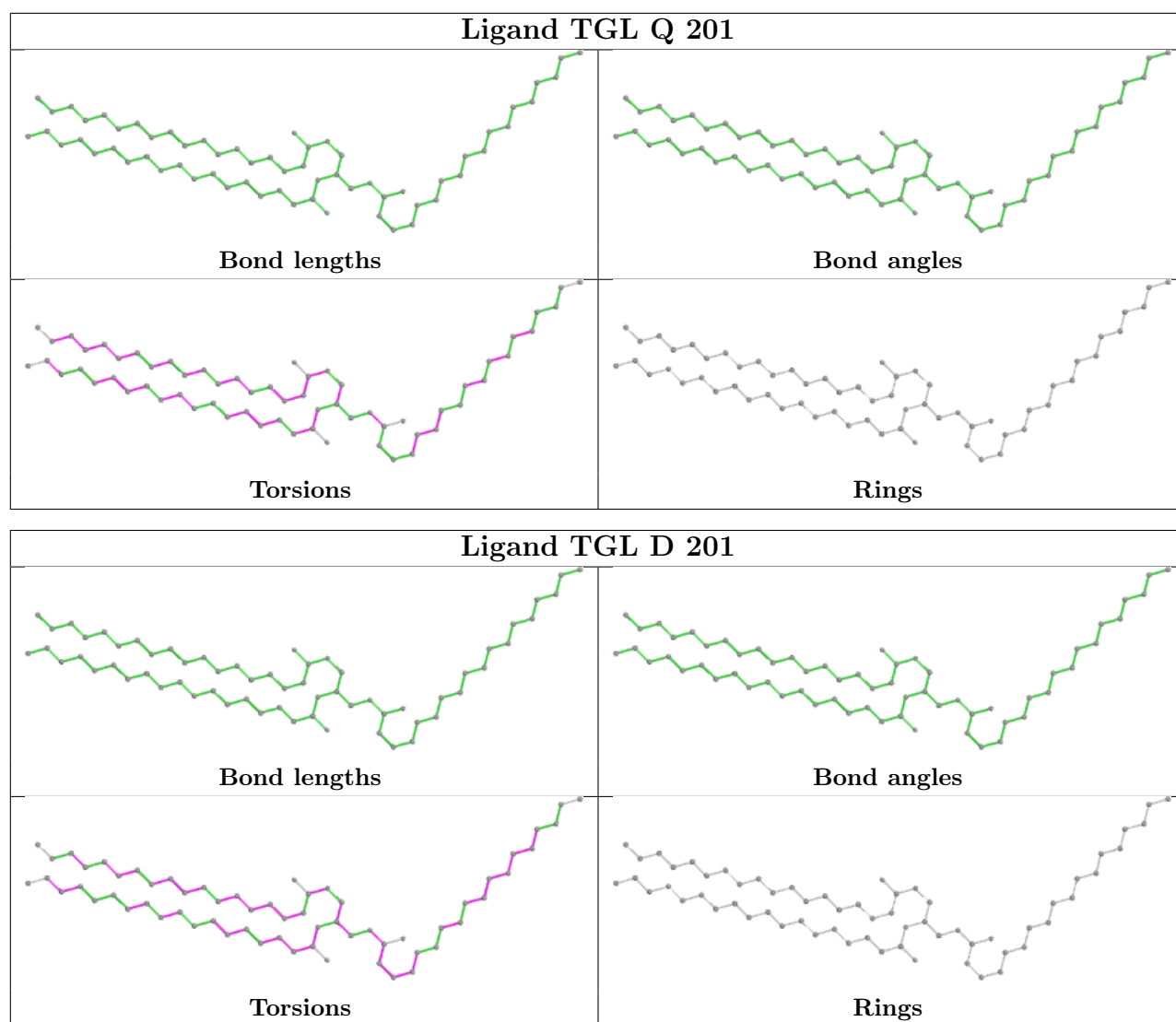
Ligand PEK T 102



Ligand CHD W 302







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.08	4 (0%) 86 91	26, 32, 41, 78	0
1	N	513/514 (99%)	-0.11	2 (0%) 92 96	28, 36, 47, 75	0
2	B	226/227 (99%)	-0.38	2 (0%) 84 90	27, 39, 73, 116	0
2	O	226/227 (99%)	-0.25	5 (2%) 62 72	32, 45, 76, 100	0
3	C	259/261 (99%)	-0.57	0 100 100	27, 36, 49, 93	0
3	P	259/261 (99%)	-0.59	1 (0%) 92 96	30, 37, 54, 93	0
4	D	144/147 (97%)	-0.45	2 (1%) 75 83	31, 41, 63, 89	0
4	Q	144/147 (97%)	0.47	15 (10%) 6 10	39, 56, 89, 170	0
5	E	105/109 (96%)	-0.38	3 (2%) 51 62	33, 42, 68, 114	0
5	R	105/109 (96%)	-0.19	4 (3%) 40 53	38, 50, 73, 112	0
6	F	98/98 (100%)	0.34	6 (6%) 21 31	31, 41, 94, 178	0
6	S	98/98 (100%)	-0.05	6 (6%) 21 31	32, 43, 99, 135	0
7	G	83/85 (97%)	0.63	15 (18%) 1 2	32, 44, 113, 120	0
7	T	83/85 (97%)	0.81	21 (25%) 0 1	33, 48, 112, 144	0
8	H	79/85 (92%)	0.39	10 (12%) 3 6	32, 45, 104, 110	0
8	U	79/85 (92%)	0.36	9 (11%) 5 7	37, 51, 110, 154	0
9	I	72/73 (98%)	0.60	12 (16%) 1 2	34, 51, 82, 107	0
9	V	72/73 (98%)	0.54	10 (13%) 2 4	40, 58, 82, 98	0
10	J	58/59 (98%)	-0.03	5 (8%) 10 16	35, 46, 73, 110	0
10	W	58/59 (98%)	0.19	5 (8%) 10 16	38, 51, 86, 128	0
11	K	49/56 (87%)	0.05	2 (4%) 37 49	33, 45, 64, 70	0
11	X	49/56 (87%)	0.74	6 (12%) 4 7	45, 55, 81, 110	0
12	L	46/47 (97%)	-0.42	0 100 100	30, 37, 56, 112	0
12	Y	46/47 (97%)	-0.29	2 (4%) 35 47	36, 47, 78, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.15	2 (4%) 31 44	31, 38, 74, 96	0
13	Z	43/46 (93%)	0.18	6 (13%) 2 4	40, 48, 83, 126	0
All	All	3550/3614 (98%)	-0.08	155 (4%) 34 46	26, 40, 77, 178	0

The worst 5 of 155 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	18.6
6	F	97	ALA	11.9
4	Q	5	VAL	11.3
4	Q	4	SER	9.8
6	F	96	LEU	9.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	T	11	11/12	0.69	0.26	86,110,136,136	0
7	TPO	G	11	11/12	0.71	0.24	65,112,161,163	0
1	FME	A	1	10/11	0.92	0.16	44,54,81,85	0
2	FME	O	1	10/11	0.95	0.15	43,47,55,60	0
1	FME	N	1	10/11	0.96	0.18	49,54,81,82	0
2	FME	B	1	10/11	0.98	0.13	38,39,50,58	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	A	617	4/4	0.17	0.64	94,103,106,110	0
29	SAC	V	101	9/10	0.25	0.90	113,120,131,132	0
29	SAC	I	101	9/10	0.27	0.41	98,111,125,128	0
26	DMU	G	101	33/33	0.41	0.47	78,110,150,153	0
19	EDO	G	109	4/4	0.46	0.34	91,103,104,105	0
19	EDO	G	105	4/4	0.57	0.31	76,80,85,86	0
19	EDO	Z	1601	4/4	0.61	0.17	77,84,85,86	0
26	DMU	C	311	33/33	0.62	0.27	82,113,128,132	0
27	PEK	C	313	53/53	0.62	0.32	60,84,139,156	0
23	PSC	B	303	52/52	0.64	0.35	59,111,180,194	0
25	CDL	C	310	100/100	0.65	0.28	61,107,147,165	0
17	PGV	C	303	51/51	0.66	0.26	66,98,125,151	0
24	CHD	T	105	29/29	0.66	0.26	88,161,180,184	0
19	EDO	D	205	4/4	0.67	0.46	91,98,101,105	0
19	EDO	B	309	4/4	0.69	0.23	65,72,78,81	0
22	TGL	Q	201	63/63	0.69	0.26	66,92,121,137	0
27	PEK	P	305	53/53	0.70	0.26	63,98,164,174	0
19	EDO	N	614	4/4	0.70	0.41	63,63,67,73	0
19	EDO	V	103	4/4	0.70	0.23	82,90,92,93	0
22	TGL	Y	101	63/63	0.71	0.27	52,69,126,140	0
19	EDO	N	608	4/4	0.71	0.49	47,51,52,56	0
26	DMU	C	312	33/33	0.72	0.35	70,103,119,133	0
25	CDL	T	103	100/100	0.72	0.29	59,107,145,164	0
27	PEK	G	103	53/53	0.73	0.27	65,97,166,172	0
27	PEK	P	301	53/53	0.73	0.24	59,87,135,155	0
19	EDO	B	311	4/4	0.73	0.28	91,92,93,96	0
23	PSC	R	201	52/52	0.73	0.36	56,99,184,199	0
19	EDO	E	204	4/4	0.73	0.20	64,64,64,70	0
19	EDO	N	612	4/4	0.74	0.38	78,79,85,87	0
19	EDO	Q	204	4/4	0.74	0.35	68,76,83,84	0
19	EDO	A	608	4/4	0.75	0.28	47,56,59,61	0
17	PGV	P	307	51/51	0.76	0.29	69,104,132,144	0
22	TGL	D	201	63/63	0.77	0.24	48,82,100,115	0
25	CDL	P	308	100/100	0.77	0.25	51,90,120,128	0
19	EDO	P	314	4/4	0.77	0.26	67,74,77,79	0
17	PGV	N	617	51/51	0.78	0.32	51,90,145,155	0
19	EDO	L	102	4/4	0.79	0.26	63,64,64,65	0
22	TGL	L	101	63/63	0.79	0.22	43,70,121,131	0
22	TGL	N	604	63/63	0.79	0.27	58,91,131,137	0
19	EDO	J	103	4/4	0.79	0.21	52,57,63,64	0
26	DMU	P	303	33/33	0.81	0.31	54,103,121,129	0
26	DMU	Q	206	33/33	0.81	0.28	53,68,83,92	0
19	EDO	O	302	4/4	0.81	0.20	68,74,75,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	S	105	4/4	0.81	0.21	67,68,70,71	0
19	EDO	P	310	4/4	0.81	0.24	61,67,71,78	0
19	EDO	D	202	4/4	0.81	0.22	53,67,72,74	0
24	CHD	Y	102	29/29	0.81	0.29	82,140,163,186	0
25	CDL	C	304	100/100	0.81	0.26	52,92,118,123	0
19	EDO	D	206	4/4	0.82	0.26	55,56,57,61	0
19	EDO	J	102	4/4	0.82	0.20	74,77,77,79	0
19	EDO	N	610	4/4	0.83	0.28	66,69,69,72	0
19	EDO	K	101	4/4	0.83	0.20	58,60,61,61	0
19	EDO	O	303	4/4	0.83	0.25	69,73,77,81	0
22	TGL	B	302	63/63	0.83	0.25	49,85,110,116	0
19	EDO	C	306	4/4	0.84	0.17	44,45,48,49	0
19	EDO	S	104	4/4	0.84	0.20	71,79,81,82	0
19	EDO	N	616	4/4	0.84	0.25	70,70,73,74	0
17	PGV	A	604	51/51	0.85	0.24	48,83,126,130	0
19	EDO	C	309	4/4	0.85	0.22	78,78,78,81	0
19	EDO	J	104	4/4	0.85	0.21	67,74,78,79	0
19	EDO	V	102	4/4	0.85	0.25	72,80,81,88	0
26	DMU	D	208	33/33	0.85	0.23	42,53,75,76	0
19	EDO	I	102	4/4	0.85	0.10	60,65,66,68	0
19	EDO	K	102	4/4	0.85	0.20	62,64,64,66	0
19	EDO	B	308	4/4	0.86	0.28	63,65,72,74	0
19	EDO	B	310	4/4	0.86	0.14	57,60,62,64	0
19	EDO	W	303	4/4	0.86	0.11	82,85,85,86	0
19	EDO	G	106	4/4	0.86	0.18	54,60,62,69	0
19	EDO	G	107	4/4	0.86	0.21	60,62,62,62	0
24	CHD	W	302	29/29	0.87	0.30	66,74,96,98	0
19	EDO	B	305	4/4	0.87	0.16	55,62,66,67	0
24	CHD	J	101	29/29	0.88	0.30	53,72,92,93	0
19	EDO	R	203	4/4	0.88	0.18	64,65,66,68	0
19	EDO	A	612	4/4	0.88	0.14	54,63,65,65	0
15	MG	N	602	1/1	0.88	0.11	35,35,35,35	0
19	EDO	F	703	4/4	0.89	0.22	53,69,73,77	0
19	EDO	S	103	4/4	0.89	0.23	73,74,74,77	0
19	EDO	P	311	4/4	0.89	0.21	68,72,74,76	0
19	EDO	C	308	4/4	0.90	0.12	74,78,79,80	0
19	EDO	I	103	4/4	0.91	0.21	61,62,67,68	0
19	EDO	D	207	4/4	0.91	0.25	64,65,68,73	0
19	EDO	A	610	4/4	0.91	0.26	41,42,45,49	0
19	EDO	Q	205	4/4	0.91	0.21	61,69,79,83	0
19	EDO	N	613	4/4	0.92	0.15	51,64,70,75	0
19	EDO	D	203	4/4	0.92	0.17	53,57,61,62	0

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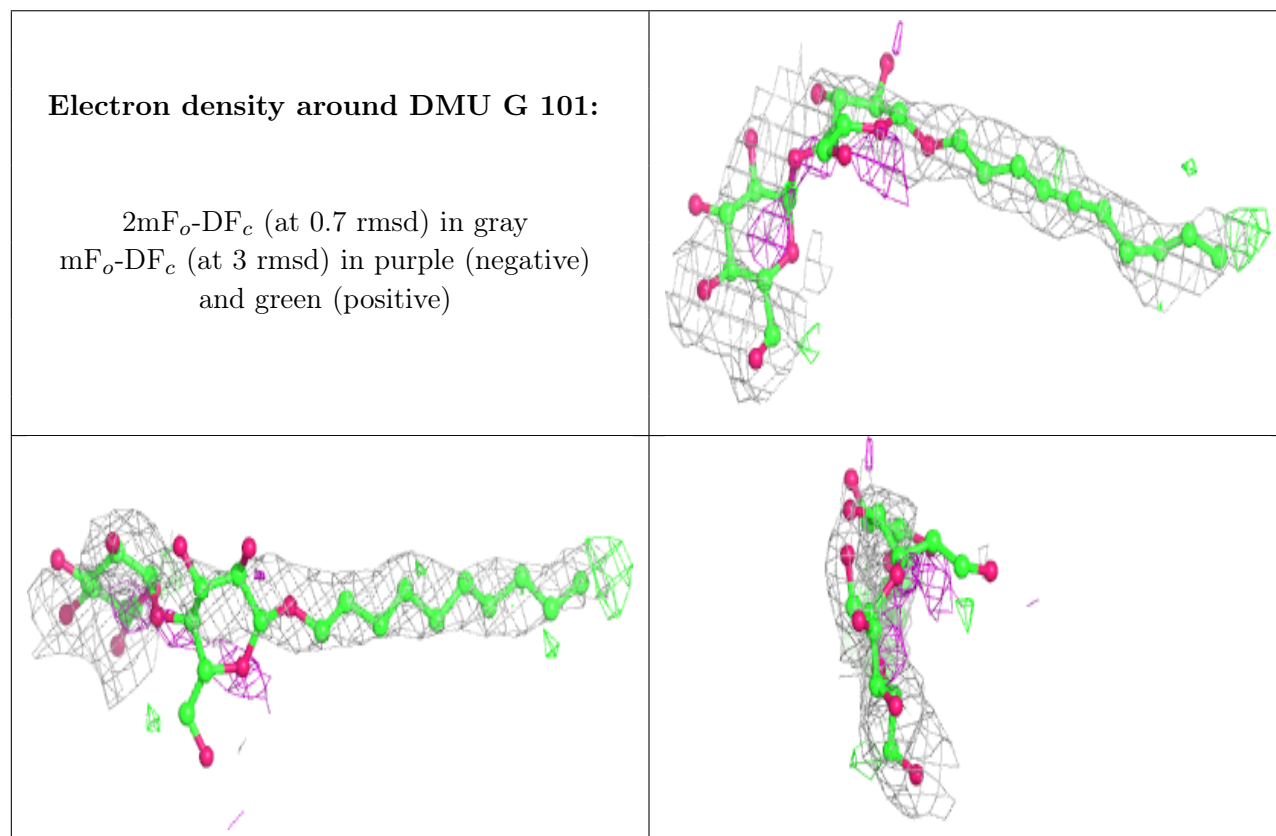
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	M	701	4/4	0.92	0.20	67,69,70,75	0
19	EDO	J	105	4/4	0.92	0.14	58,62,62,66	0
19	EDO	W	301	4/4	0.92	0.27	69,75,80,80	0
27	PEK	T	102	53/53	0.92	0.22	35,54,100,105	0
19	EDO	D	204	4/4	0.92	0.17	65,67,69,70	0
19	EDO	A	613	4/4	0.92	0.18	56,65,70,76	0
19	EDO	B	306	4/4	0.93	0.18	55,59,62,65	0
19	EDO	Q	202	4/4	0.93	0.16	61,64,68,76	0
24	CHD	C	305	29/29	0.93	0.22	53,55,59,63	0
19	EDO	A	611	4/4	0.93	0.14	64,65,67,68	0
19	EDO	N	615	4/4	0.93	0.20	56,57,60,60	0
19	EDO	R	202	4/4	0.93	0.19	57,58,60,60	0
19	EDO	A	616	4/4	0.93	0.24	68,69,72,72	0
19	EDO	S	102	4/4	0.93	0.15	37,38,39,39	0
19	EDO	E	205	4/4	0.94	0.24	60,69,70,70	0
19	EDO	C	307	4/4	0.94	0.14	66,66,70,76	0
19	EDO	P	312	4/4	0.94	0.28	53,56,57,58	0
19	EDO	P	313	4/4	0.94	0.13	51,52,54,59	0
19	EDO	N	611	4/4	0.94	0.20	65,68,70,73	0
19	EDO	E	203	4/4	0.94	0.16	54,55,58,59	0
15	MG	A	602	1/1	0.94	0.11	31,31,31,31	0
17	PGV	C	302	51/51	0.95	0.23	30,44,100,102	0
19	EDO	B	307	4/4	0.95	0.08	64,68,70,70	0
19	EDO	T	104	4/4	0.95	0.32	58,60,63,64	0
24	CHD	P	309	29/29	0.95	0.21	55,63,68,74	0
19	EDO	A	614	4/4	0.95	0.22	55,56,57,57	0
19	EDO	A	615	4/4	0.95	0.19	61,66,67,68	0
24	CHD	T	101	29/29	0.96	0.10	32,38,43,47	0
27	PEK	G	102	53/53	0.96	0.21	32,53,88,100	0
19	EDO	A	609	4/4	0.96	0.18	30,33,33,35	0
19	EDO	B	304	4/4	0.96	0.17	32,35,36,39	0
19	EDO	F	704	4/4	0.96	0.17	37,39,41,42	0
19	EDO	G	104	4/4	0.96	0.26	37,39,40,42	0
19	EDO	Q	203	4/4	0.96	0.07	58,62,64,66	0
17	PGV	A	605	51/51	0.96	0.23	28,44,72,73	0
18	HEA	N	606	60/60	0.97	0.17	25,37,47,59	0
17	PGV	P	306	51/51	0.97	0.17	30,45,87,88	0
19	EDO	N	607	4/4	0.97	0.15	35,35,36,36	0
24	CHD	C	301	29/29	0.97	0.10	35,37,40,44	0
19	EDO	F	701	4/4	0.97	0.17	43,44,45,46	0
19	EDO	N	609	4/4	0.97	0.12	51,52,53,53	0
24	CHD	P	304	29/29	0.97	0.10	31,35,38,40	0

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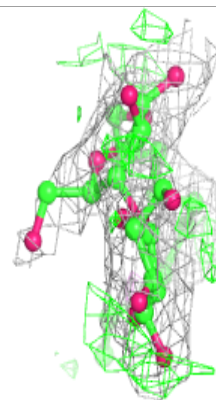
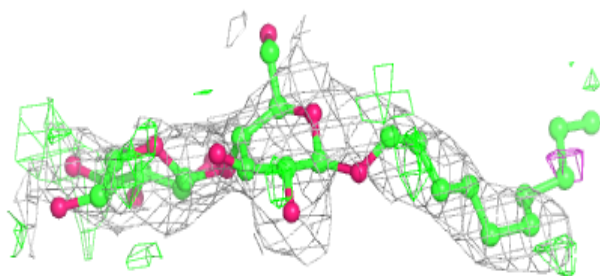
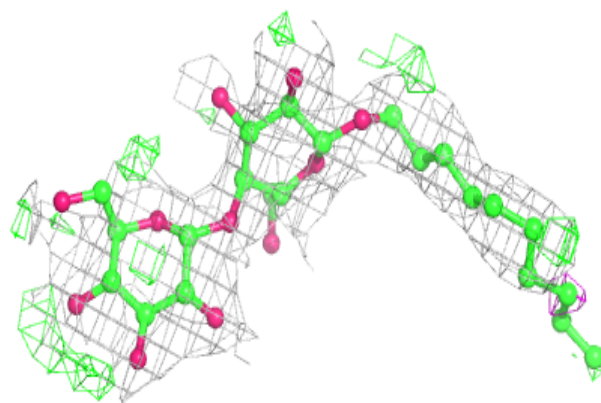
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	E	201	4/4	0.97	0.14	47,48,49,49	0
19	EDO	E	202	4/4	0.97	0.16	49,53,54,54	0
17	PGV	P	302	51/51	0.97	0.22	28,51,74,75	0
18	HEA	A	607	60/60	0.98	0.16	25,31,54,63	0
18	HEA	N	605	60/60	0.98	0.13	28,31,38,40	0
16	NA	A	603	1/1	0.98	0.08	30,30,30,30	0
21	CUA	O	301	2/2	0.98	0.08	35,35,35,37	0
24	CHD	G	108	29/29	0.98	0.08	32,35,39,41	0
18	HEA	A	606	60/60	0.98	0.13	25,28,37,40	0
21	CUA	B	301	2/2	0.99	0.07	30,30,30,31	0
16	NA	N	603	1/1	0.99	0.06	32,32,32,32	0
20	OH	A	618	1/1	1.00	0.13	21,21,21,21	1
20	OH	N	618	1/1	1.00	0.13	18,18,18,18	1
28	ZN	F	702	1/1	1.00	0.06	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.05	39,39,39,39	0
14	CU	A	601	1/1	1.00	0.12	31,31,31,31	0
14	CU	N	601	1/1	1.00	0.12	33,33,33,33	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.

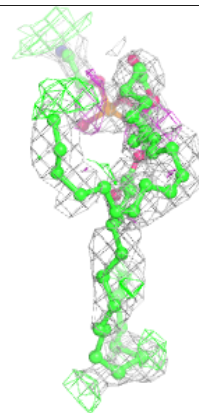
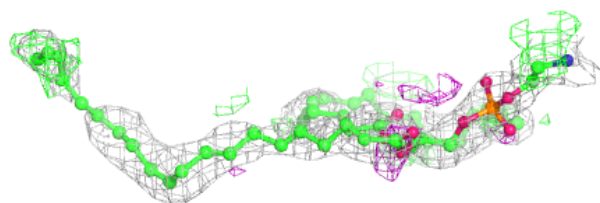
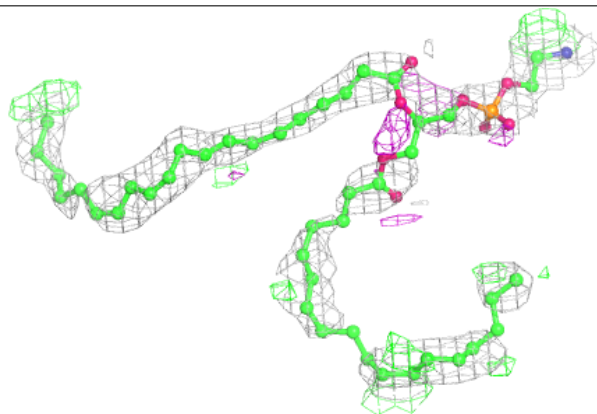


Electron density around DMU C 311:

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

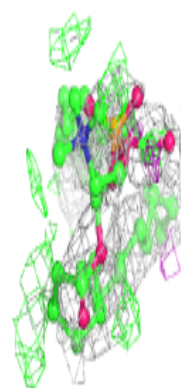
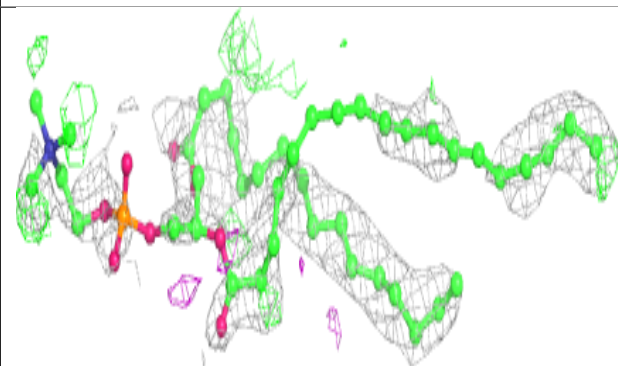
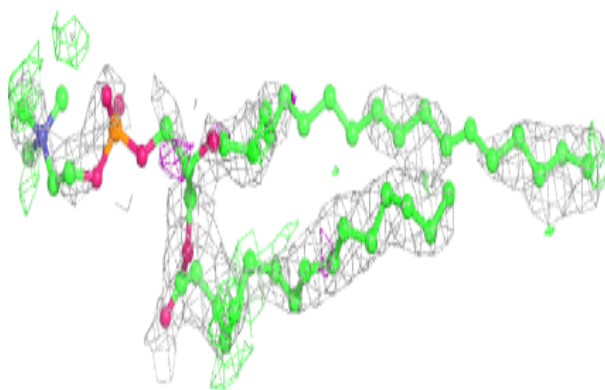
**Electron density around PEK C 313:**

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

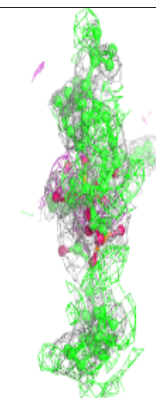
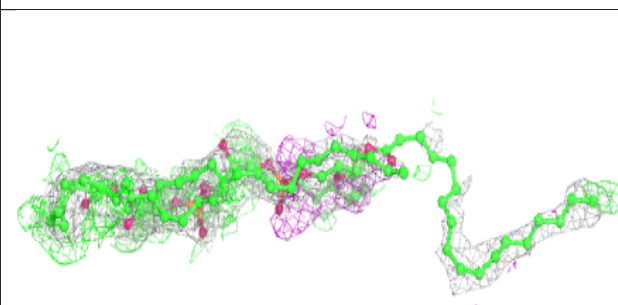
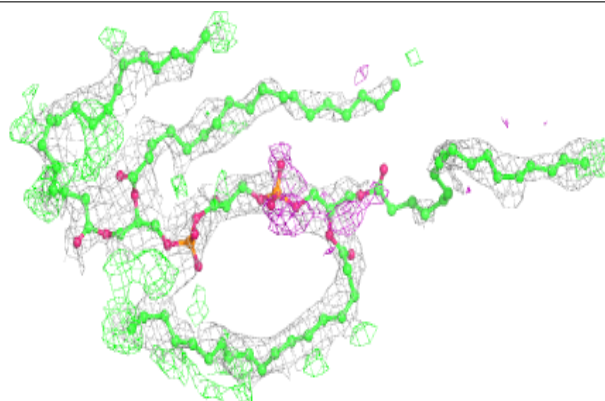


Electron density around PSC B 303:

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

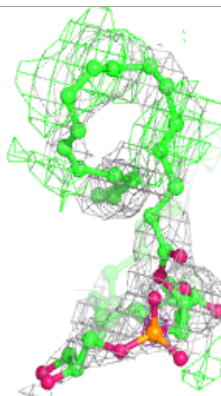
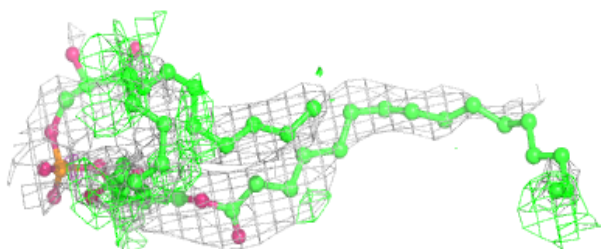
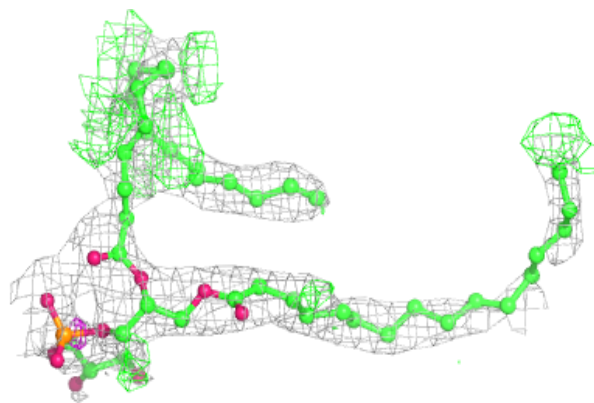
**Electron density around CDL C 310:**

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

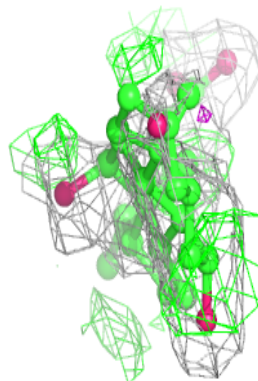
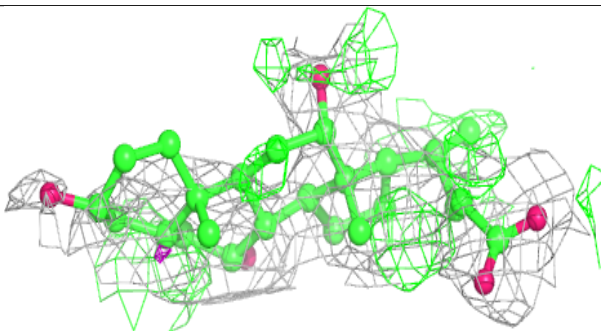
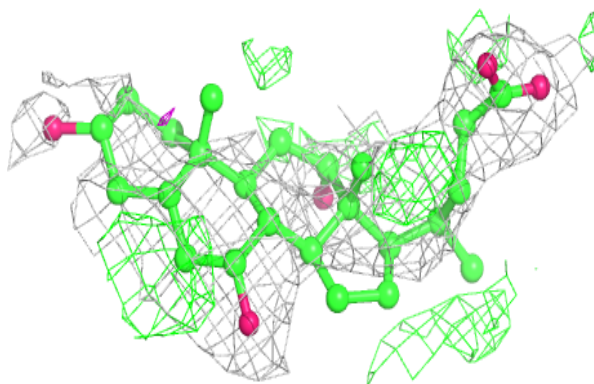


Electron density around PGV C 303:

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

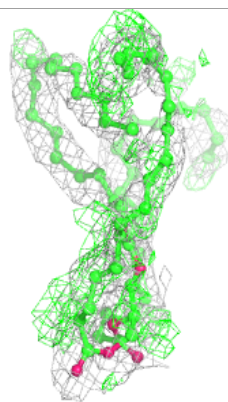
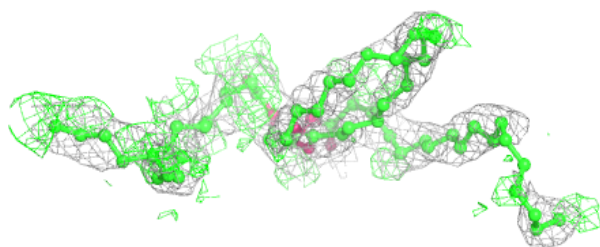
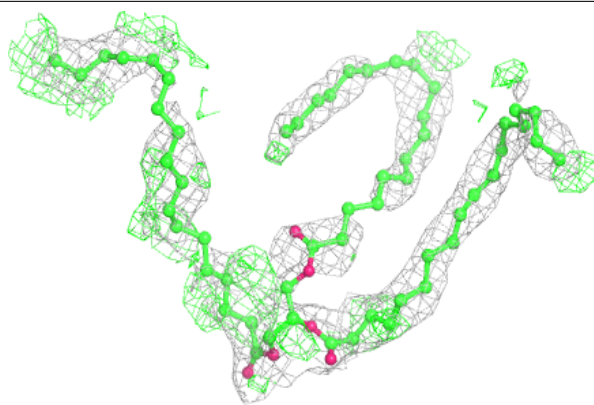
**Electron density around CHD T 105:**

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

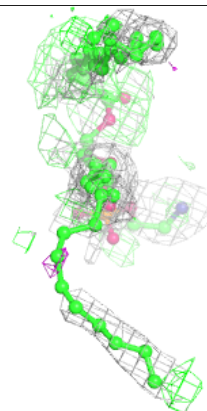
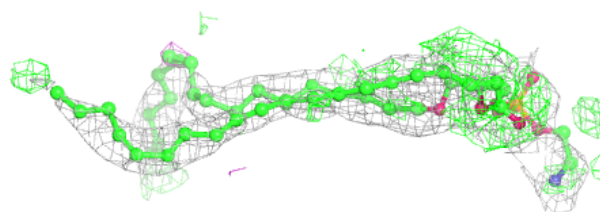
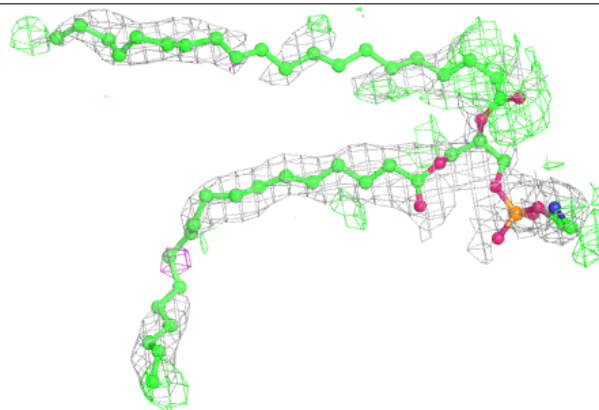


Electron density around TGL Q 201:

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

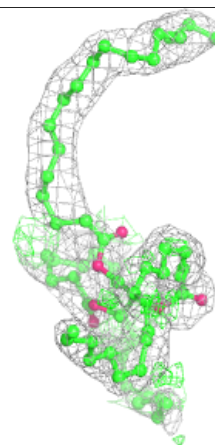
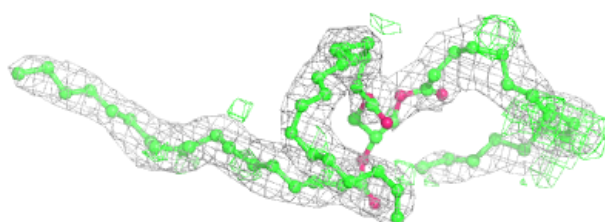
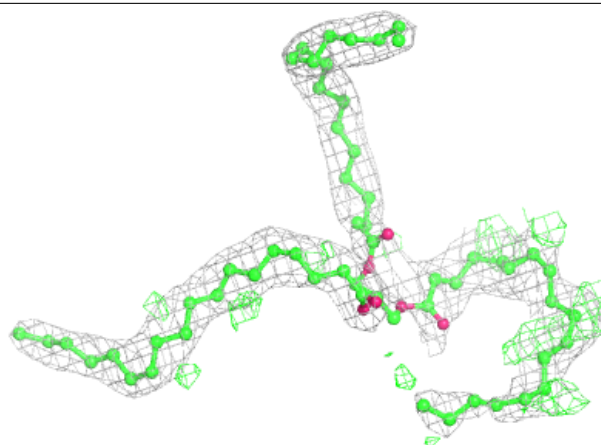
**Electron density around PEK P 305:**

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

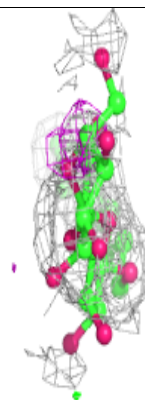
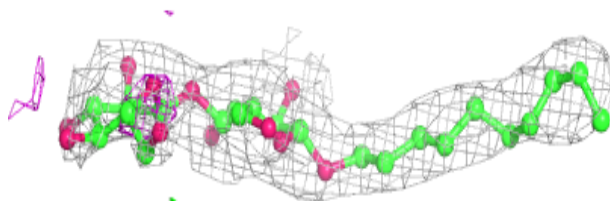
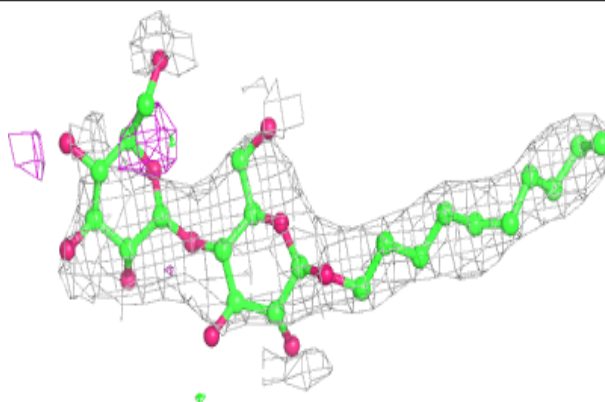


Electron density around TGL Y 101:

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

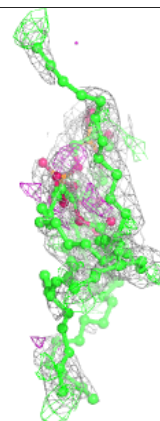
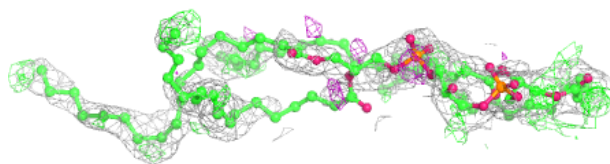
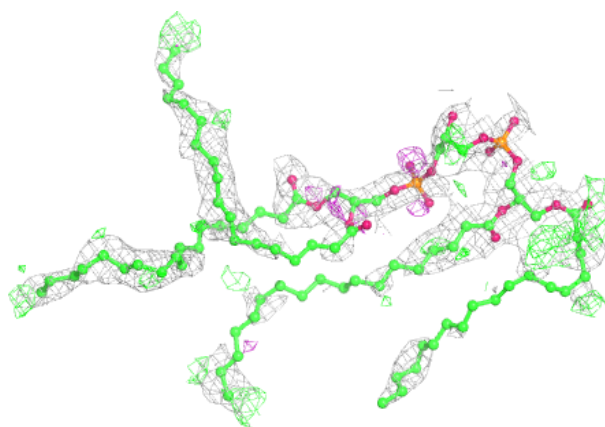
**Electron density around DMU C 312:**

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

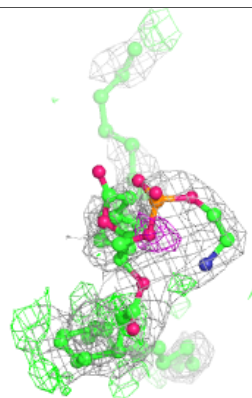
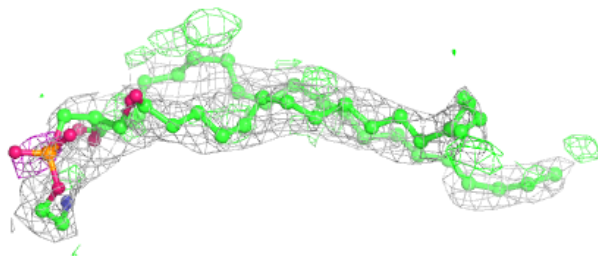
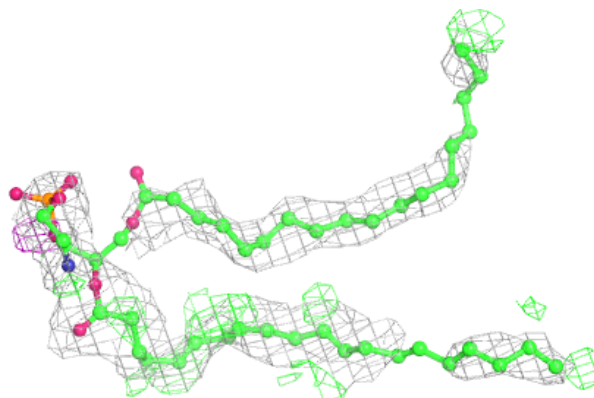


Electron density around CDL T 103:

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

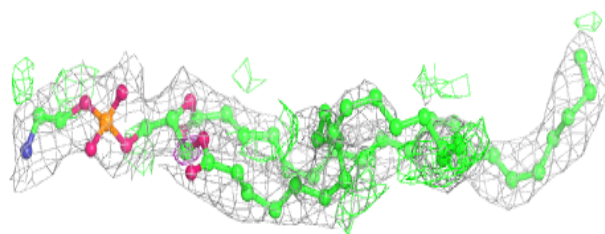
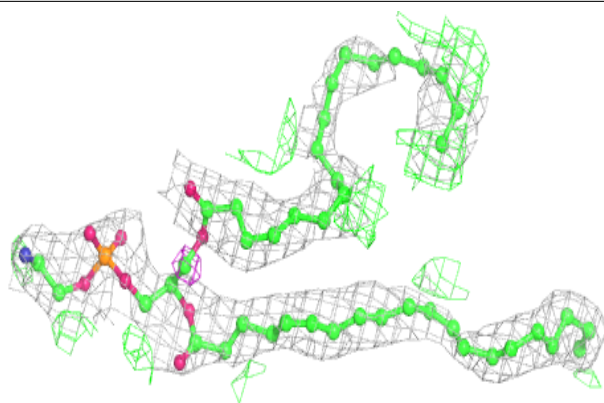
**Electron density around PEK G 103:**

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

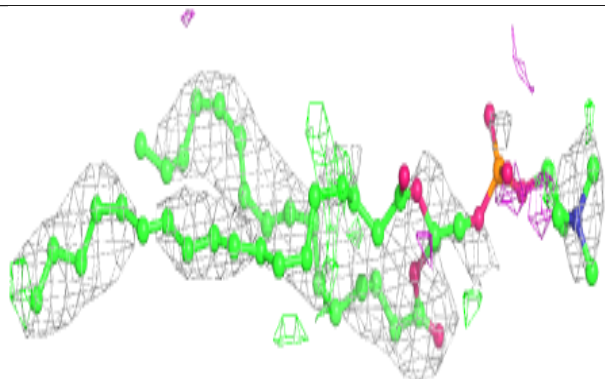
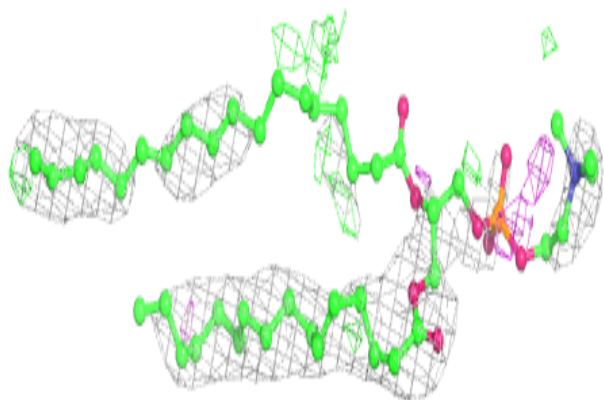


Electron density around PEK P 301:

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

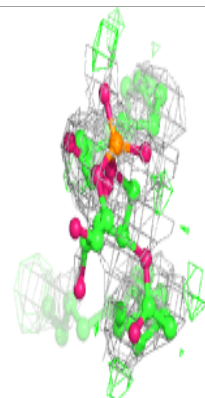
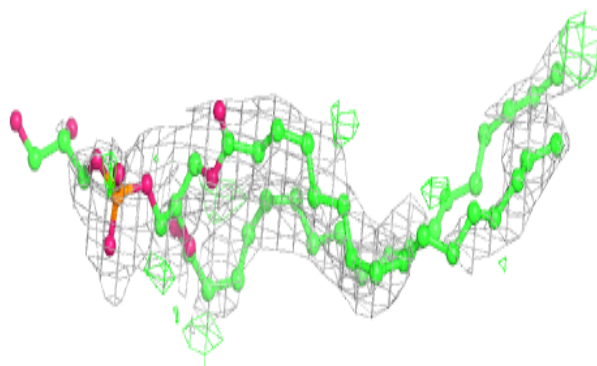
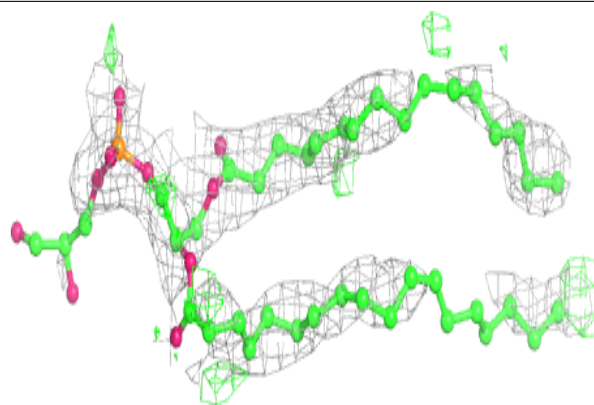
**Electron density around PSC R 201:**

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

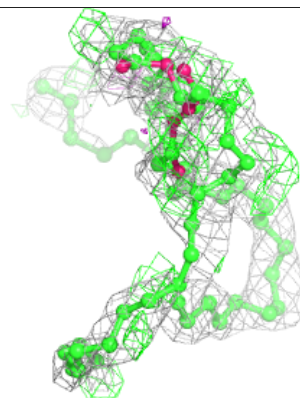
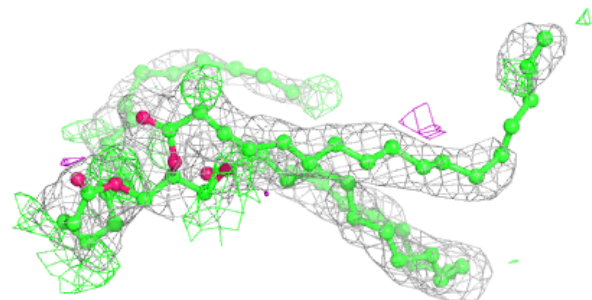
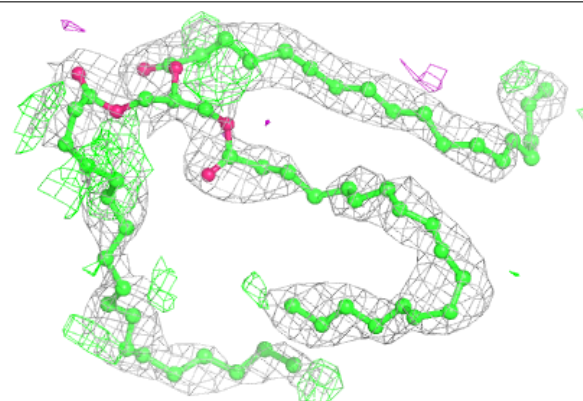


Electron density around PGV P 307:

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

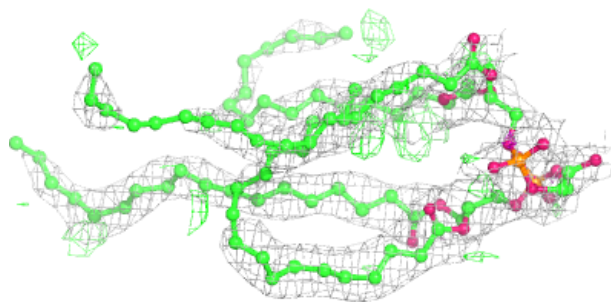
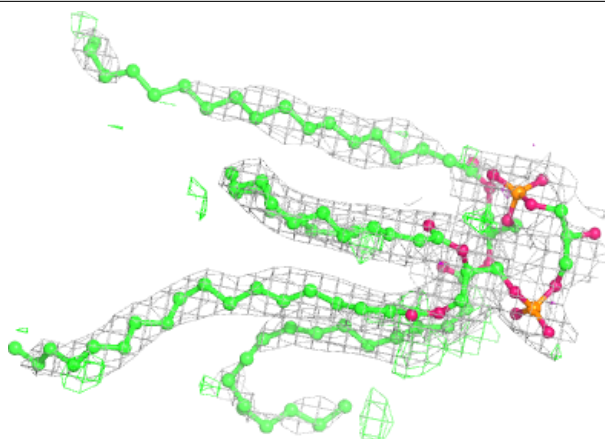
**Electron density around TGL D 201:**

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

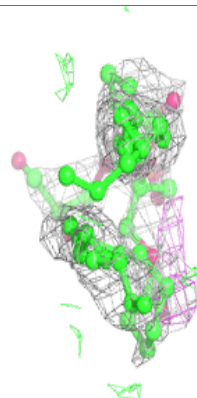
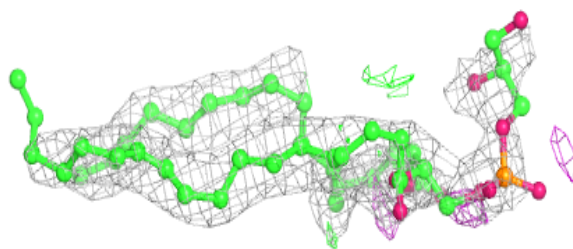
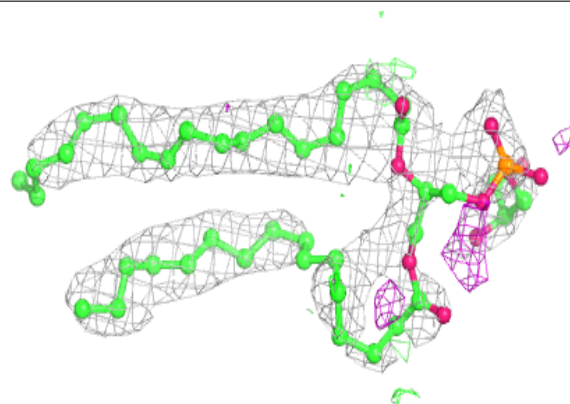


Electron density around CDL P 308:

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

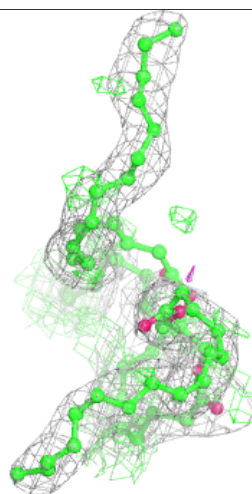
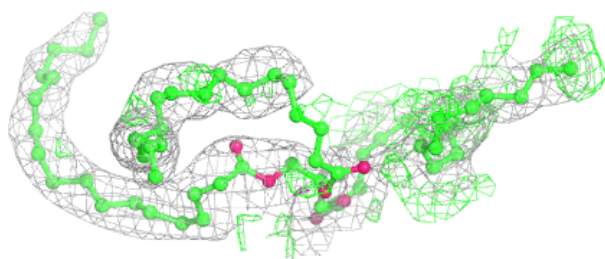
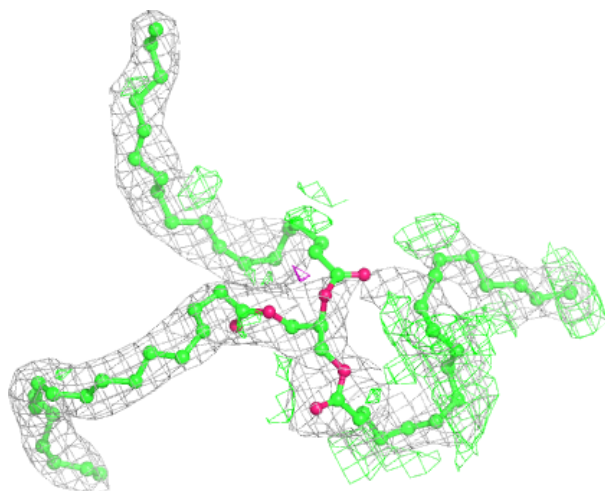
**Electron density around PGV N 617:**

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



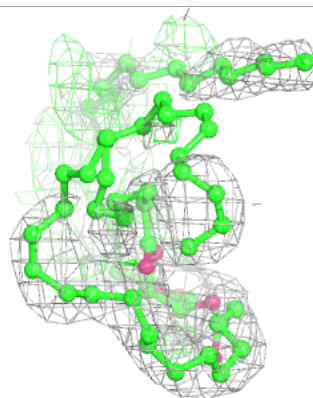
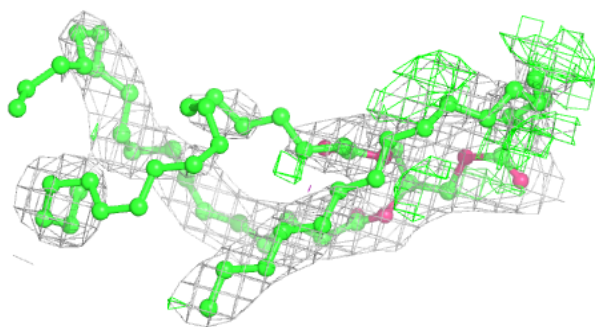
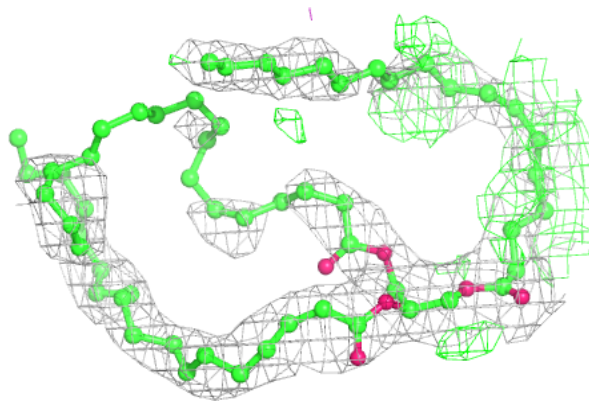
Electron density around TGL L 101:

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

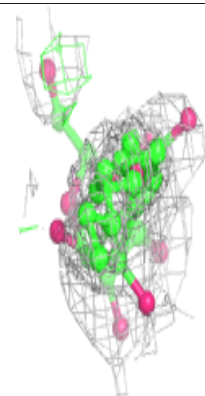
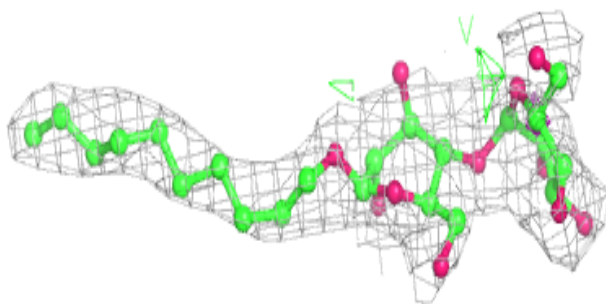
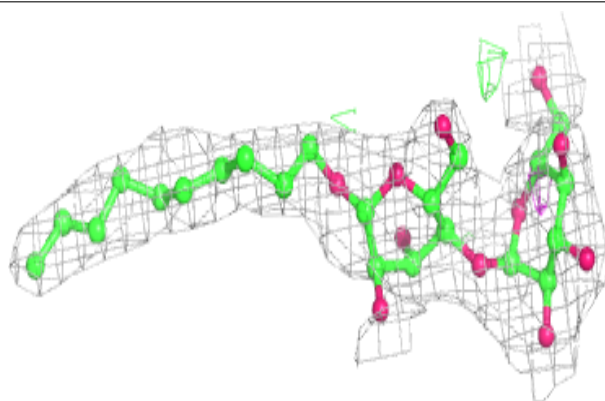


Electron density around TGL N 604:

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

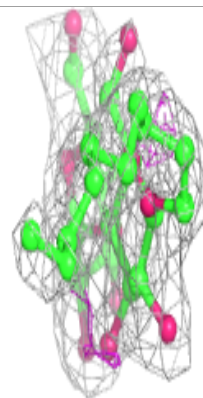
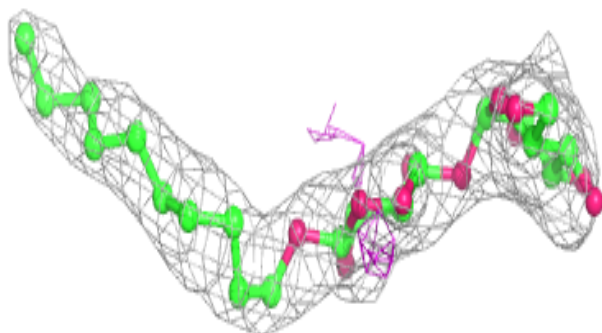
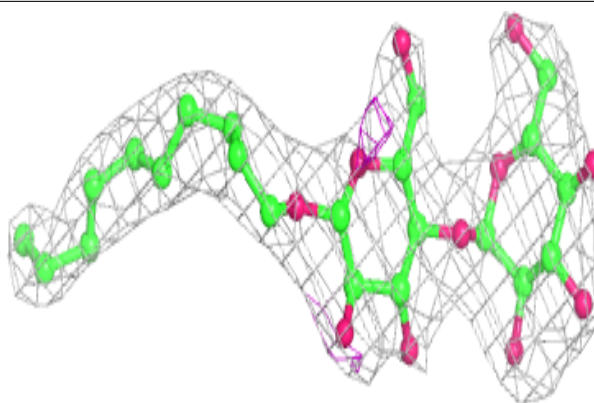
**Electron density around DMU P 303:**

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

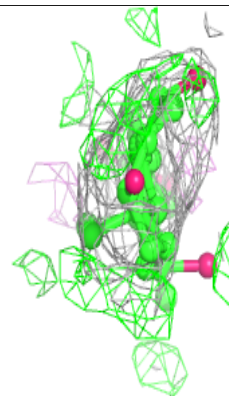
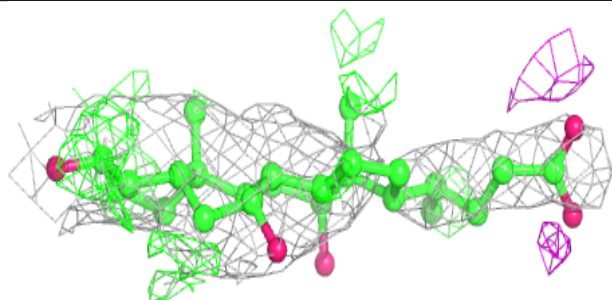
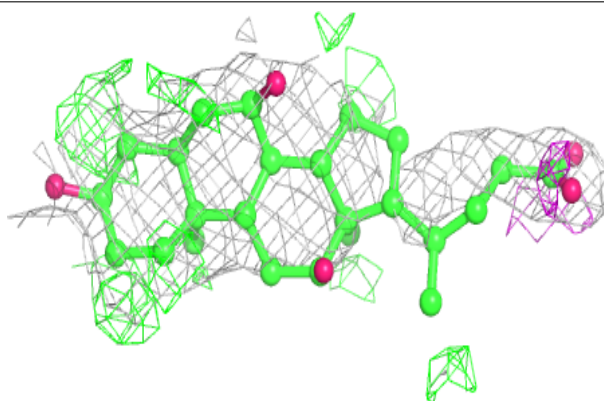


Electron density around DMU Q 206:

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

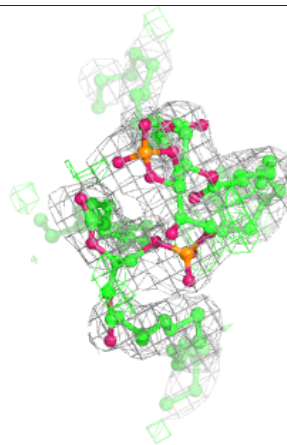
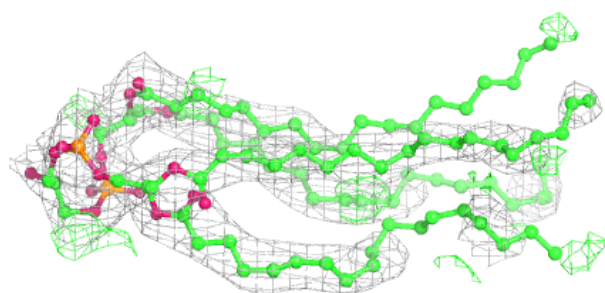
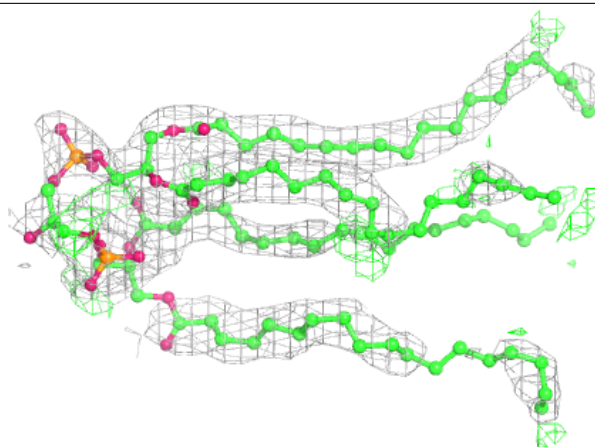
**Electron density around CHD Y 102:**

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

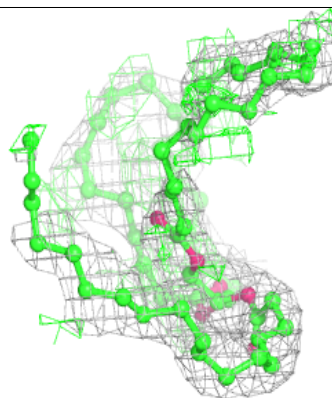
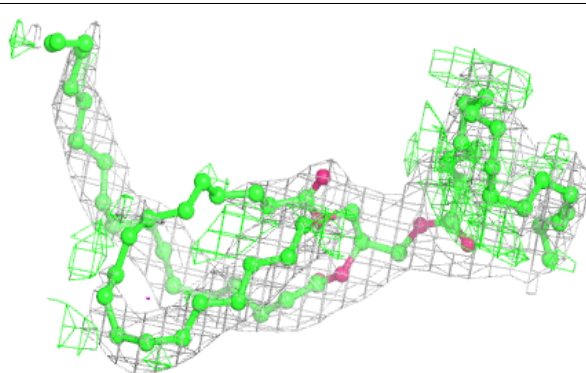
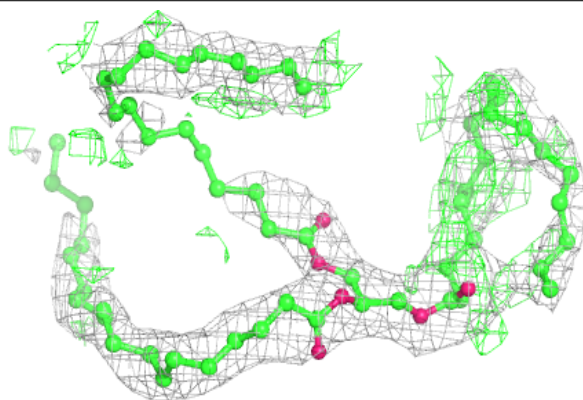


Electron density around CDL C 304:

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

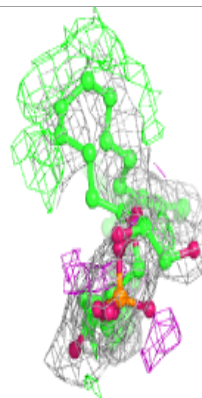
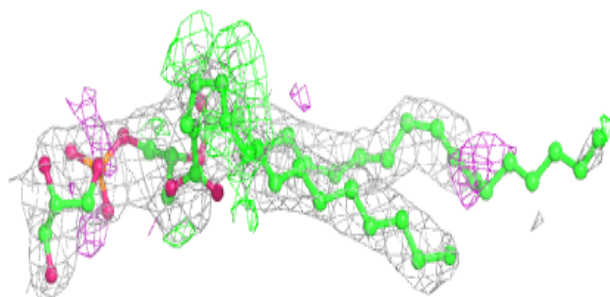
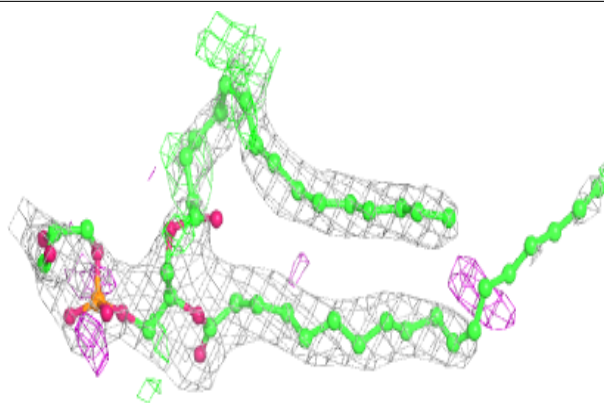
**Electron density around TGL B 302:**

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

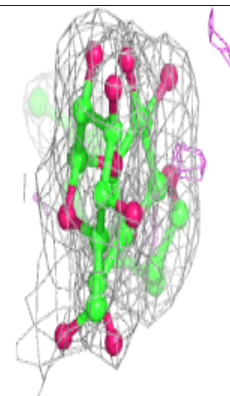
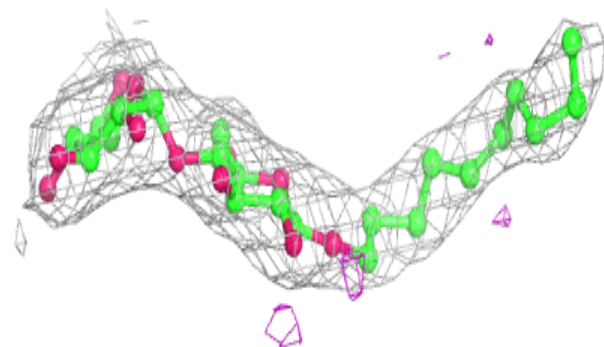
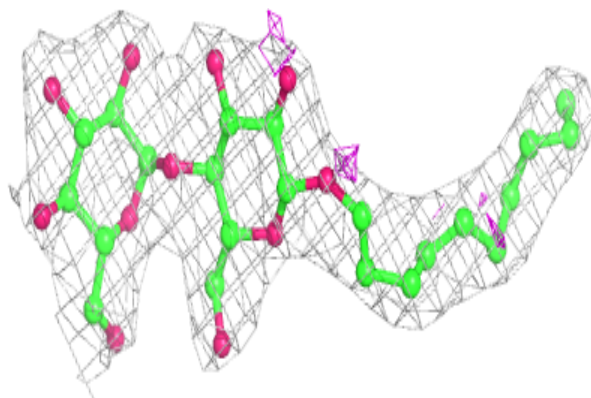


Electron density around PGV A 604:

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

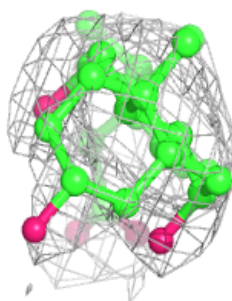
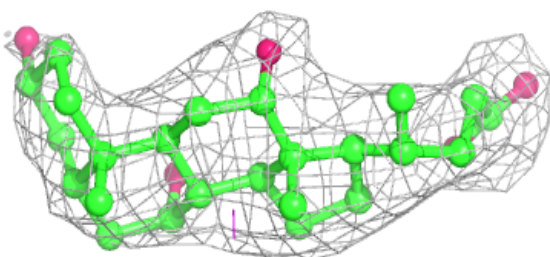
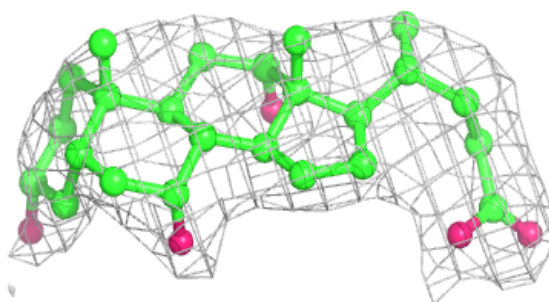
**Electron density around DMU D 208:**

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

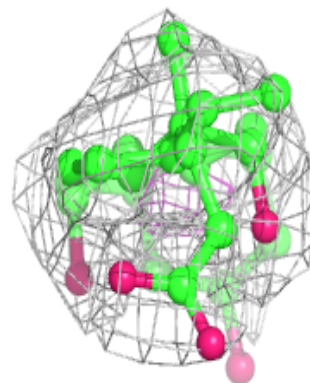
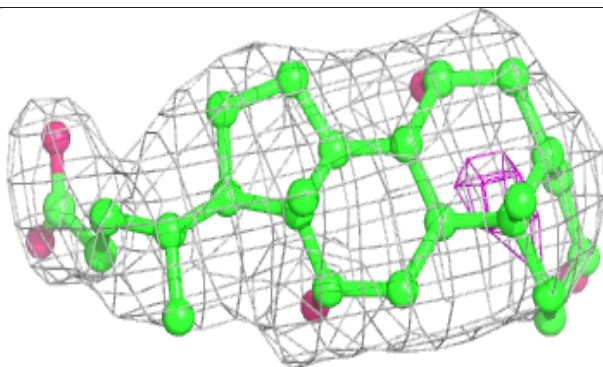
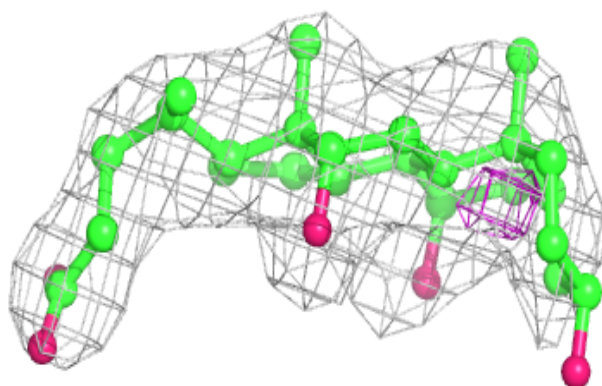


Electron density around CHD W 302:

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

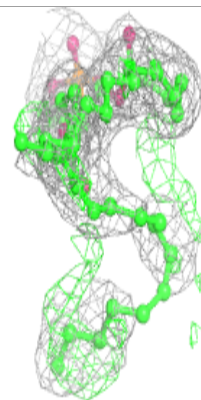
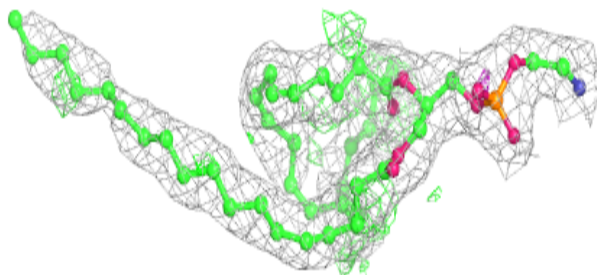
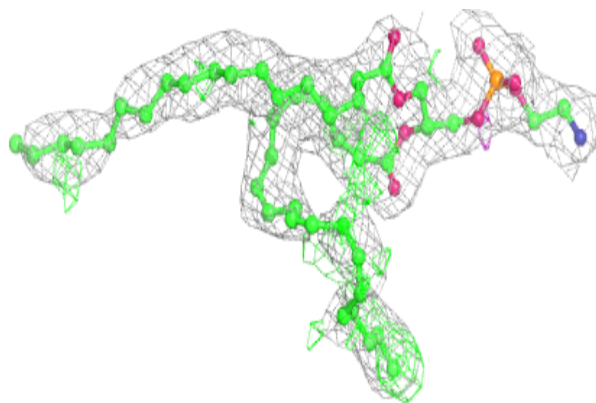
**Electron density around CHD J 101:**

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

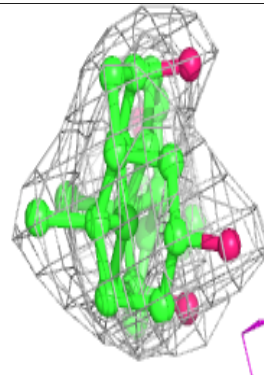
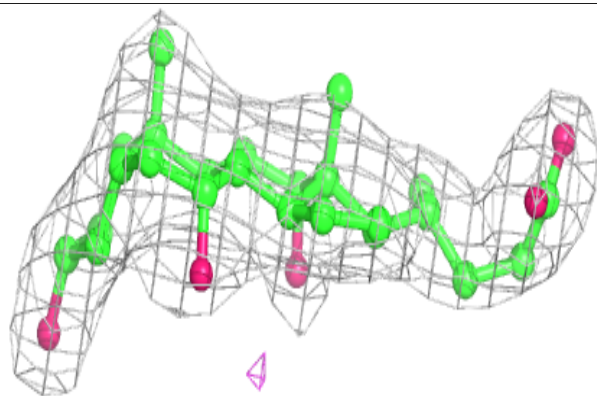
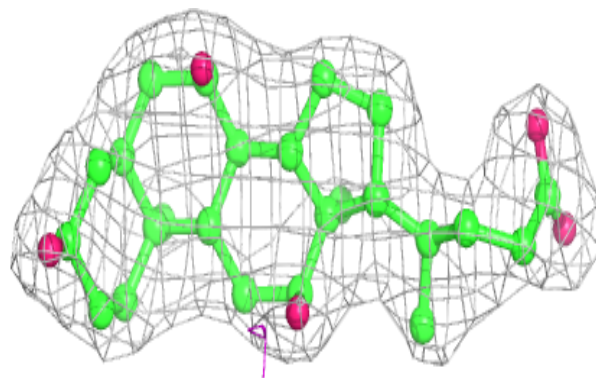


Electron density around PEK T 102:

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

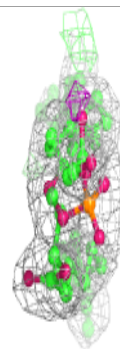
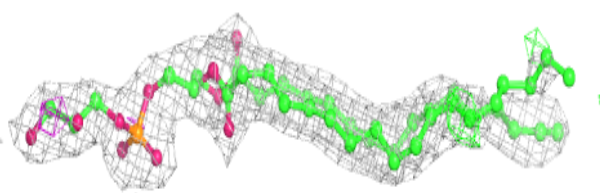
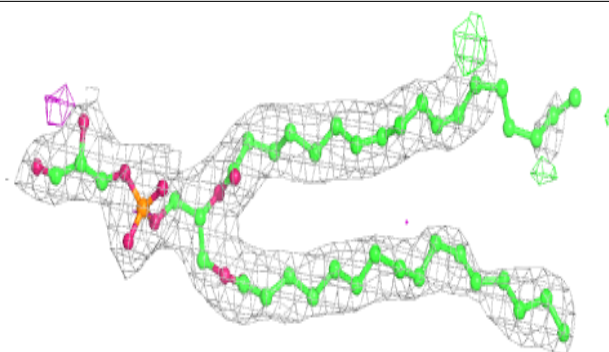
**Electron density around CHD C 305:**

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

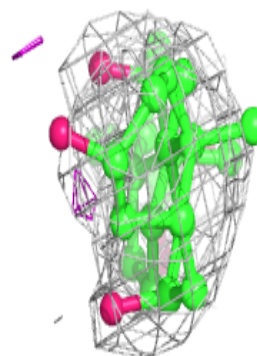
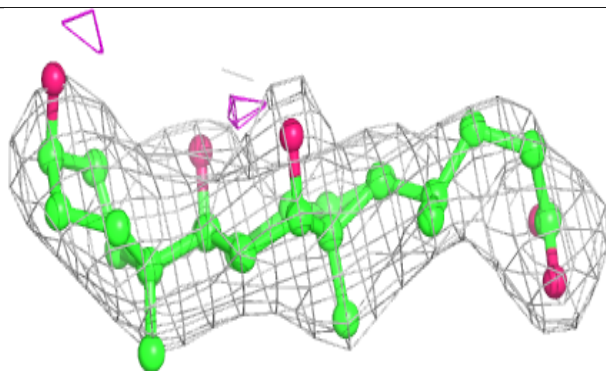
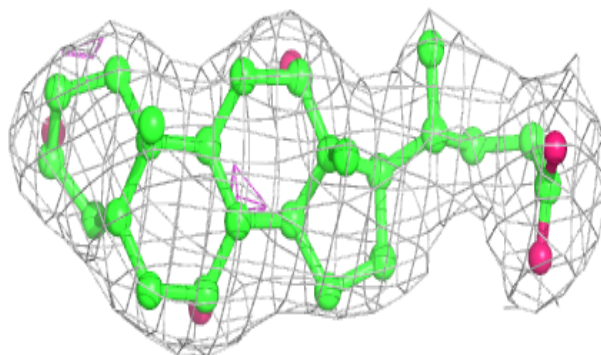


Electron density around PGV C 302:

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

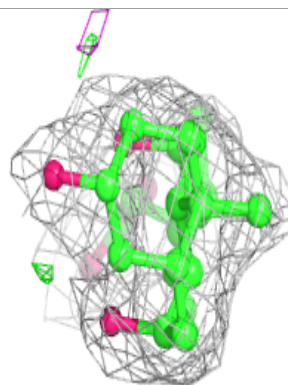
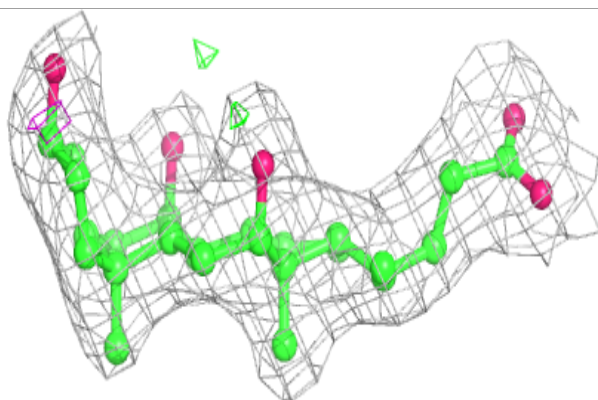
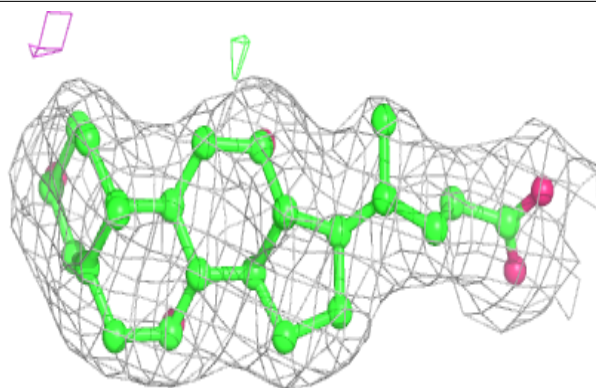
**Electron density around CHD P 309:**

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

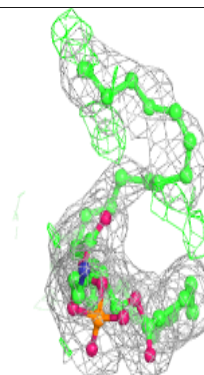
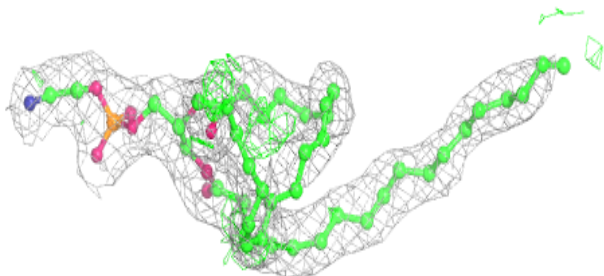
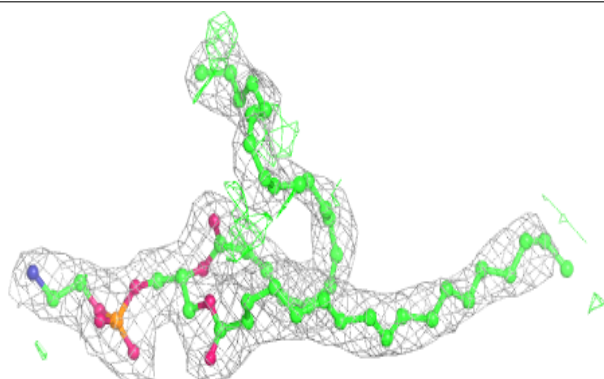


Electron density around CHD T 101:

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

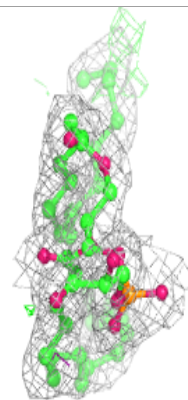
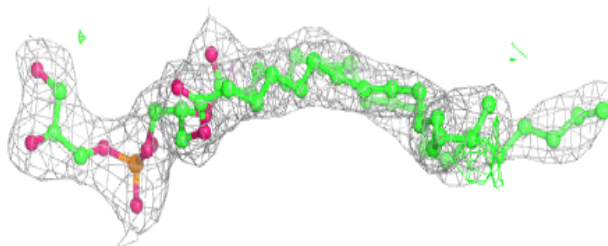
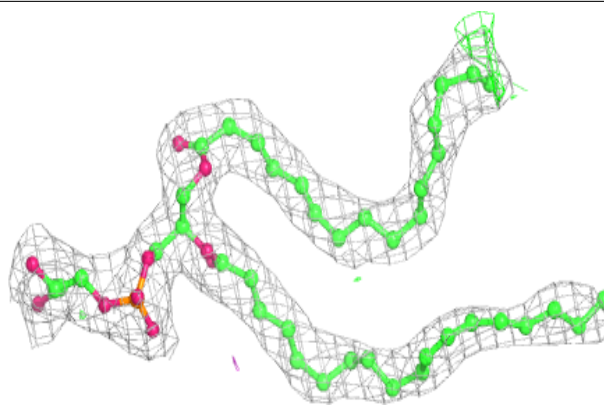
**Electron density around PEK G 102:**

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

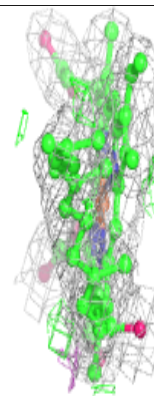
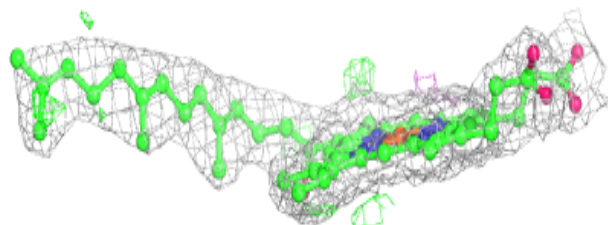
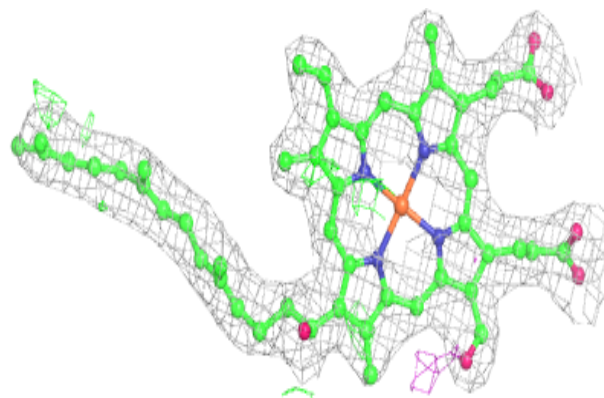


Electron density around PGV A 605:

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

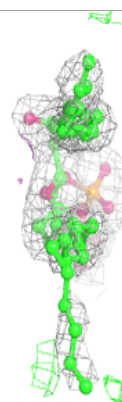
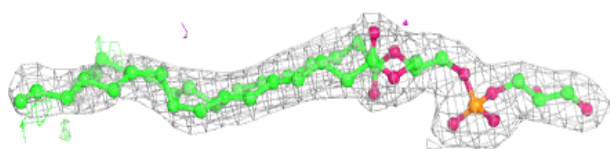
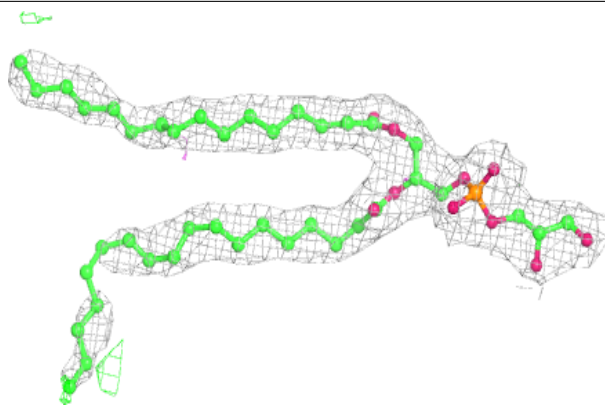
**Electron density around HEA N 606:**

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

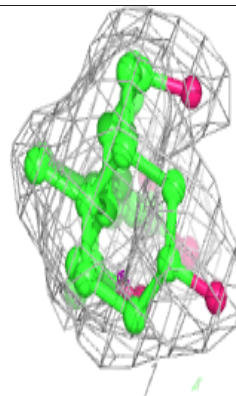
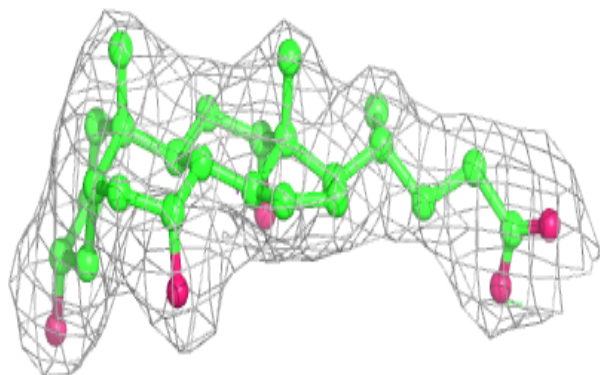
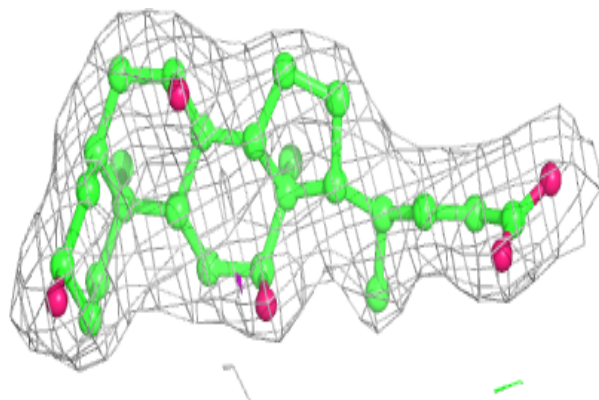


Electron density around PGV P 306:

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

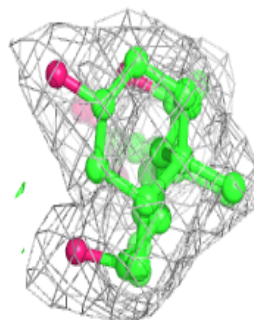
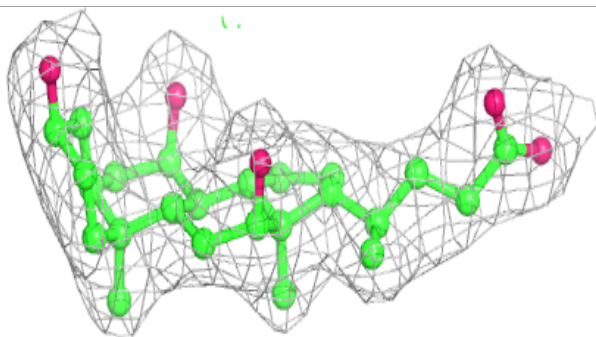
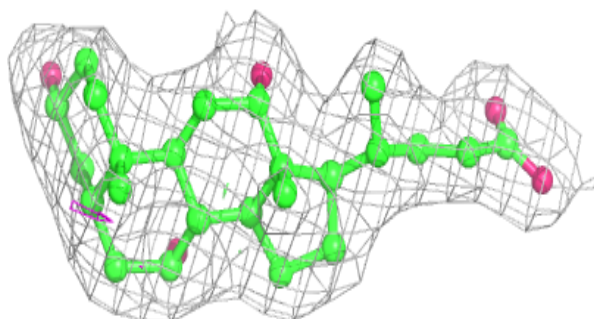
**Electron density around CHD C 301:**

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

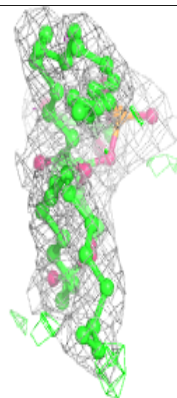
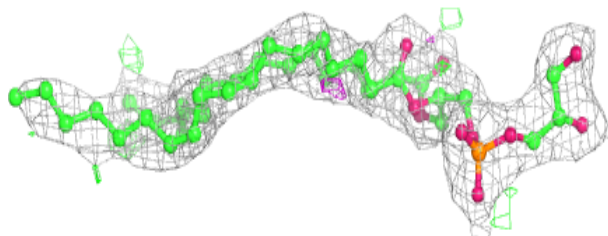
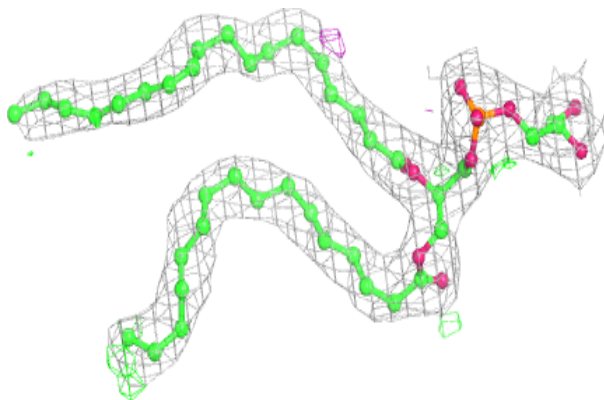


Electron density around CHD P 304:

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

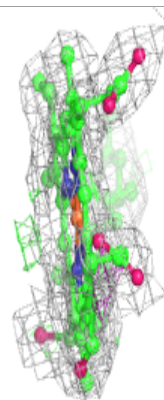
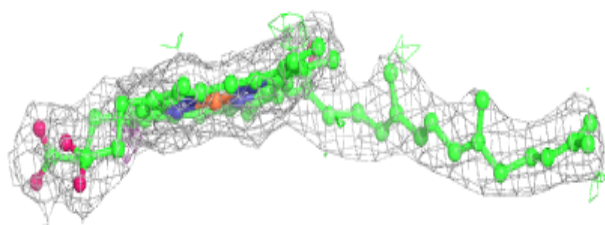
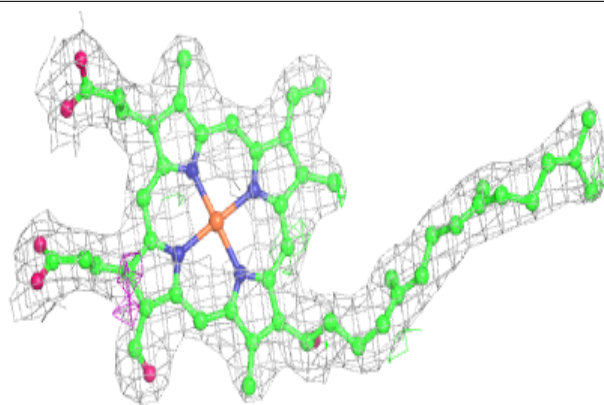
**Electron density around PGV P 302:**

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

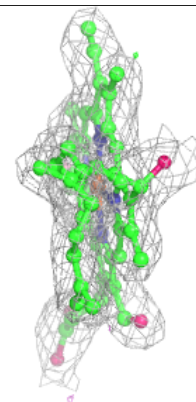
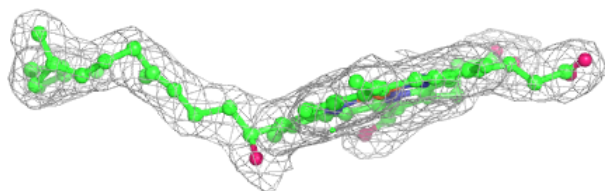
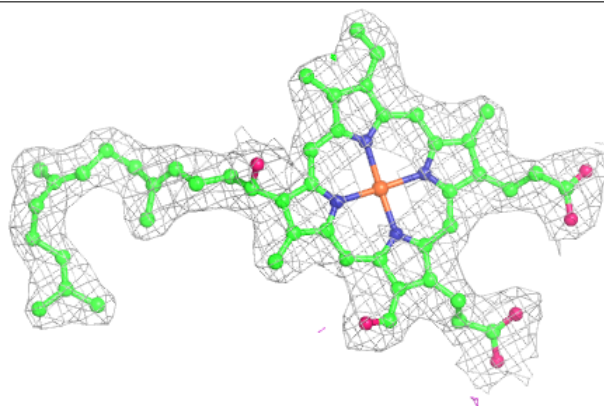


Electron density around HEA A 607:

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

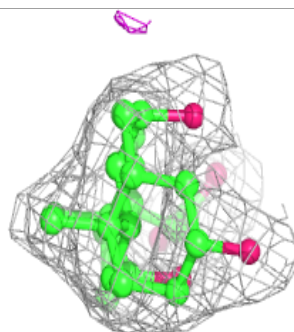
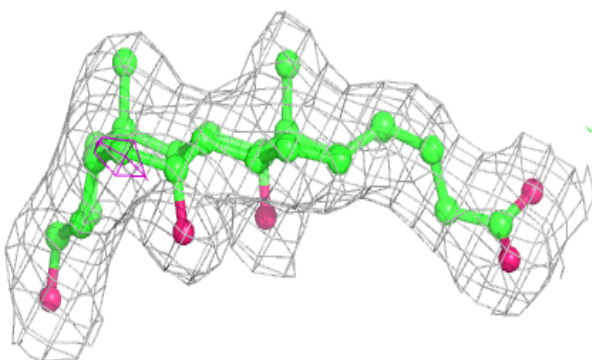
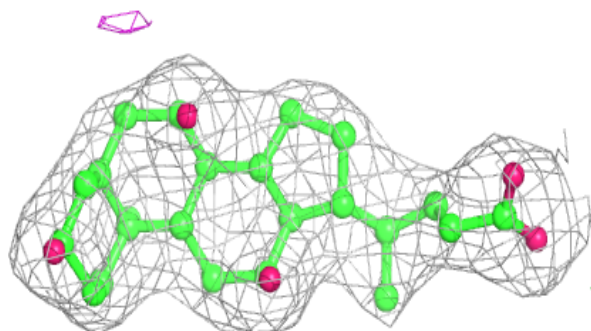
**Electron density around HEA N 605:**

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

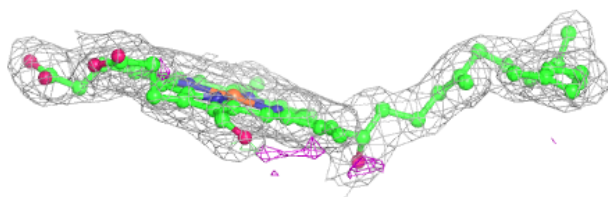
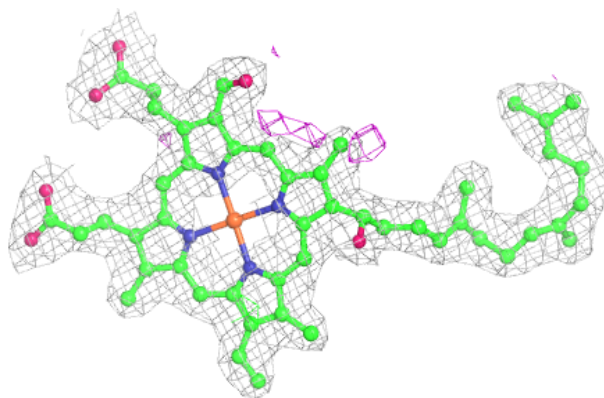


Electron density around CHD G 108:

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

**Electron density around HEA A 606:**

$2mF_o-DF_c$ (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.