



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2026 – 12:31 PM EDT

PDB ID : 36CV / pdb_000036cv
Title : Crystal structure of cyanate bound bovine cytochrome c oxidase
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.
Deposited on : 2026-06-01
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

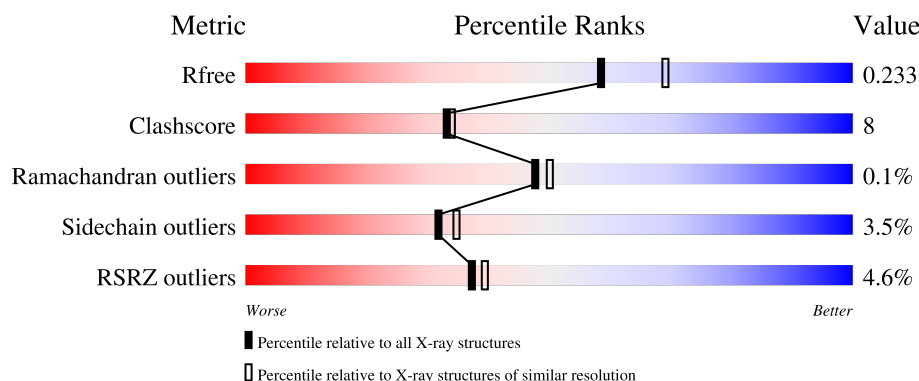
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



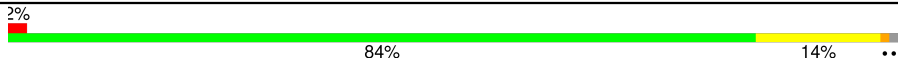
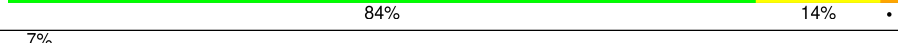
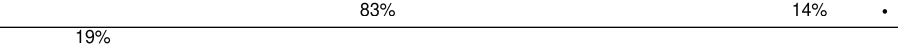
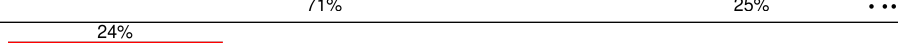
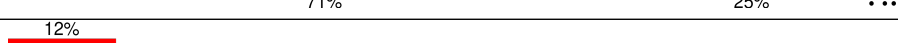
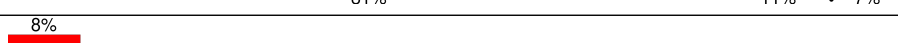
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	86% 13% .
1	N	514	84% 15% .
2	B	227	3% 85% 14% .
2	O	227	5% 83% 15% .
3	C	261	85% 14% .

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	EDO	C	310	-	-	X	-
19	EDO	O	304	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	DMU	C	316	X	-	-	-
26	DMU	G	101	X	-	-	-
26	DMU	G	105	X	-	-	-
26	DMU	M	103	X	-	-	-
26	DMU	P	314	X	-	-	-
26	DMU	Z	102	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32333 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.

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	141	Total	C	N	O	S	0	0	0
			1175	764	193	214	4			

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

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

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

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.

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.

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.

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.

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.

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 (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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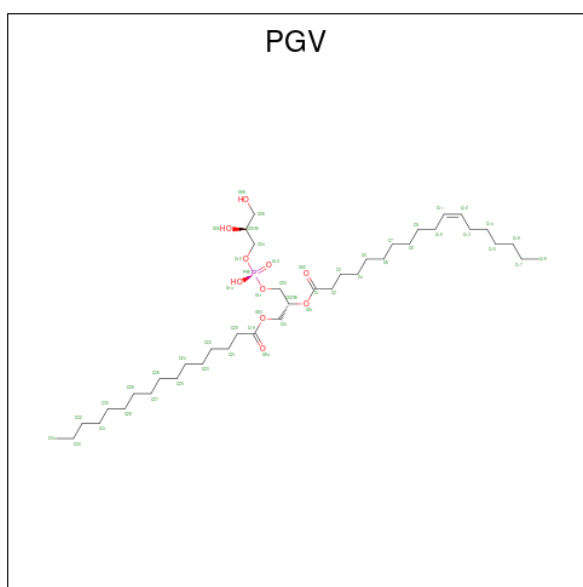
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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 (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



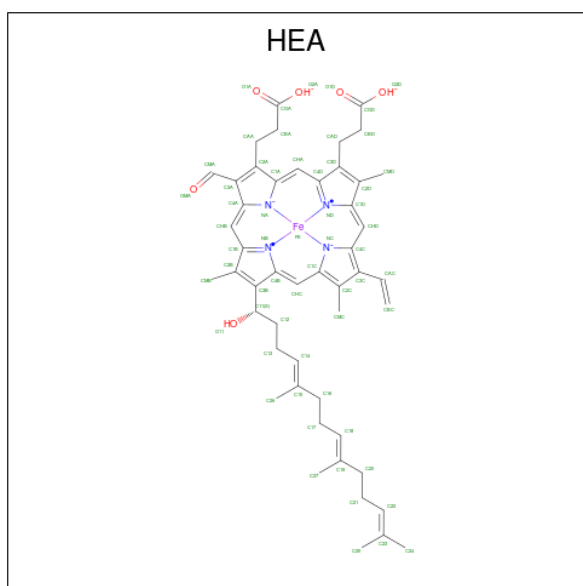
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	M	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		

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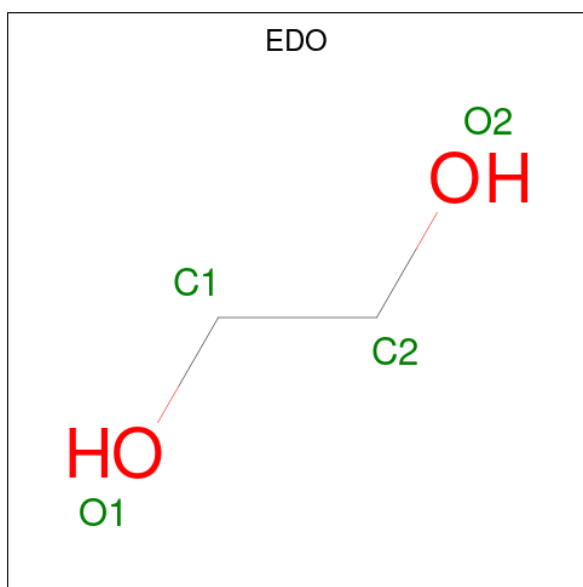
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	Z	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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	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	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	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
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	F	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
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	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	K	1	Total 4	C 2	O 2	0	0
19	L	1	Total 4	C 2	O 2	0	0
19	L	1	Total 4	C 2	O 2	0	0
19	L	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

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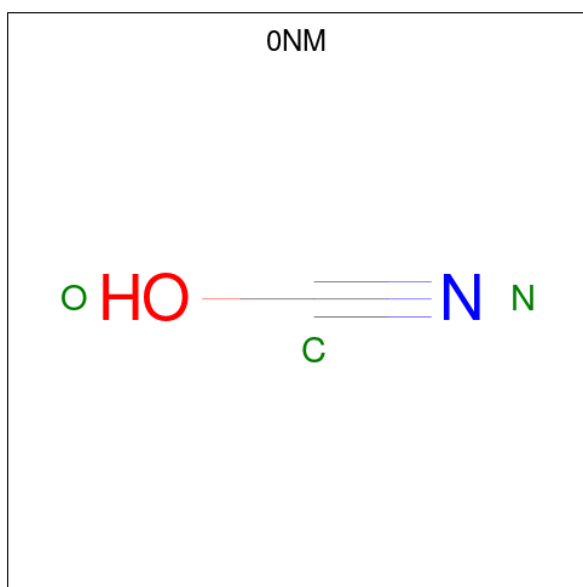
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19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	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	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

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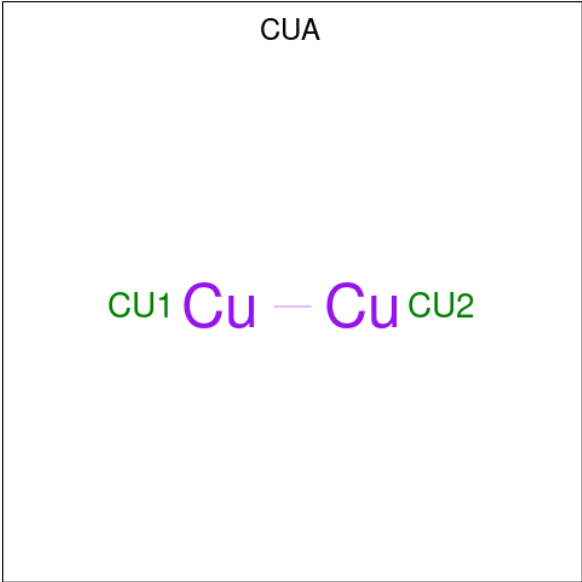
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	V	1	Total	C	O	0	0
			4	2	2		
19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

- Molecule 20 is cyanic acid (CCD ID: 0NM) (formula: CHNO) (labeled as "Ligand of Interest" by depositor).



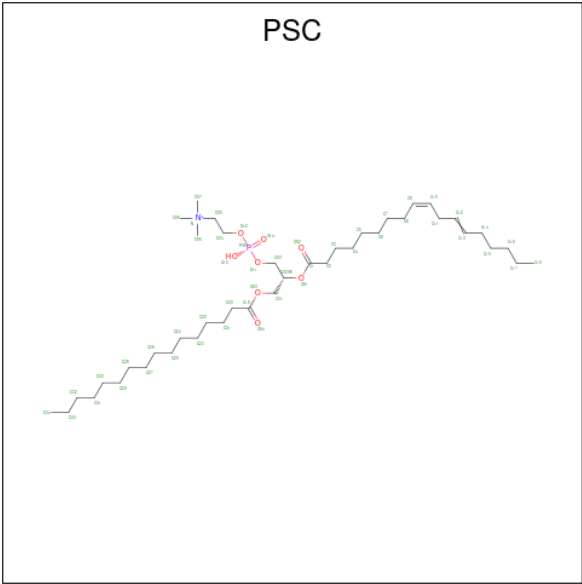
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	N	O	0	0
			3	1	1	1		
20	A	1	Total	C	N	O	0	0
			3	1	1	1		
20	A	1	Total	C	N	O	0	0
			3	1	1	1		
20	C	1	Total	C	N	O	0	0
			3	1	1	1		
20	N	1	Total	C	N	O	0	0
			3	1	1	1		
20	N	1	Total	C	N	O	0	0
			3	1	1	1		
20	N	1	Total	C	N	O	0	0
			3	1	1	1		
20	N	1	Total	C	N	O	0	0
			3	1	1	1		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



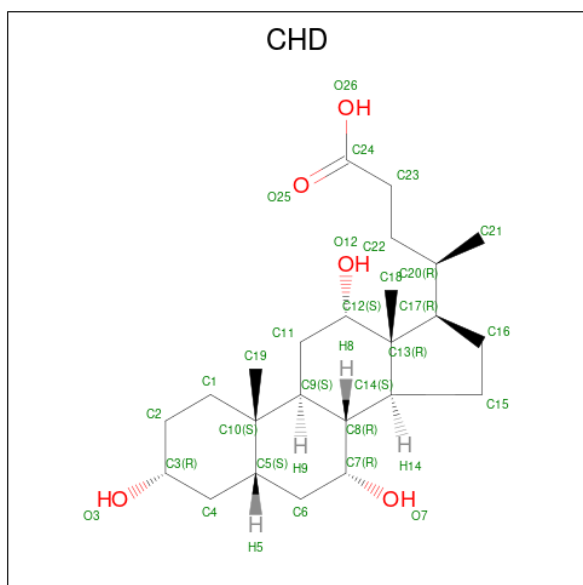
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is (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 (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).



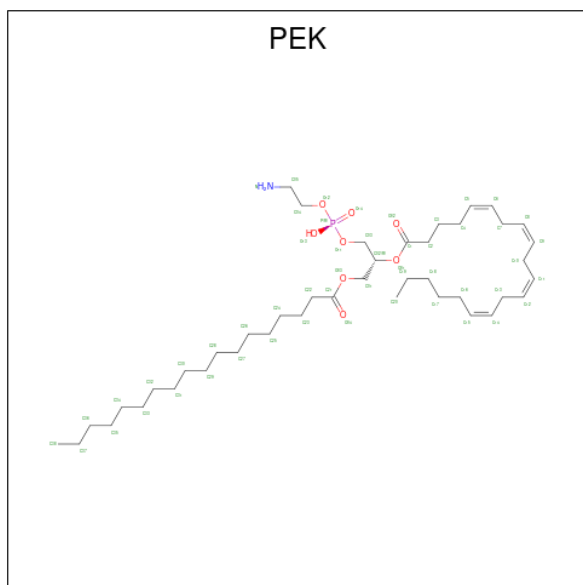
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	G	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	T	1	Total	C	O	0	0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

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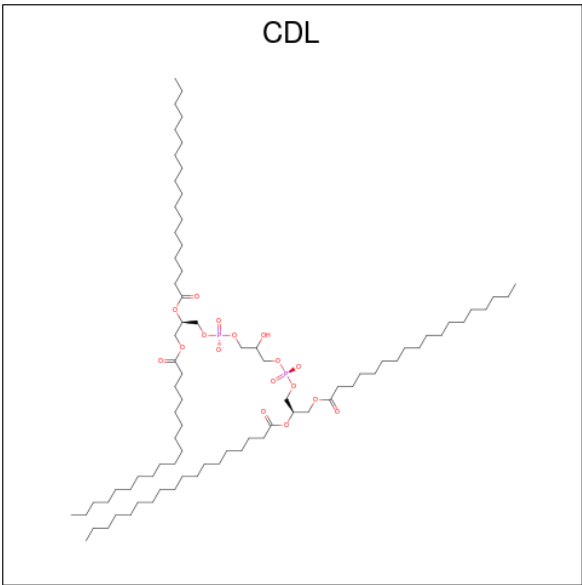
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	Y	1	Total	C	O	0	0
			29	24	5		

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



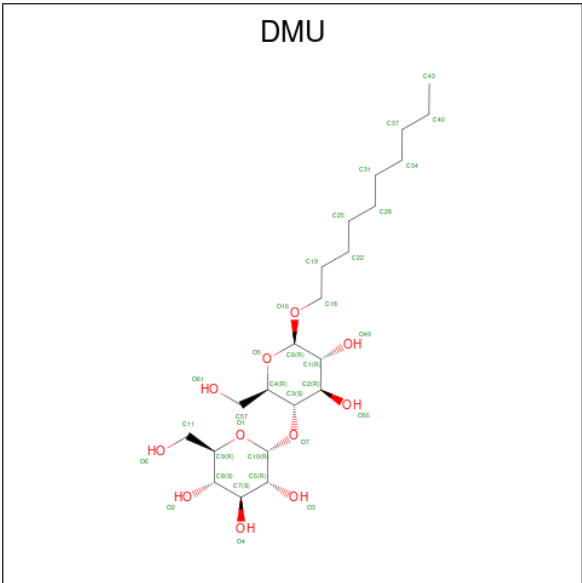
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



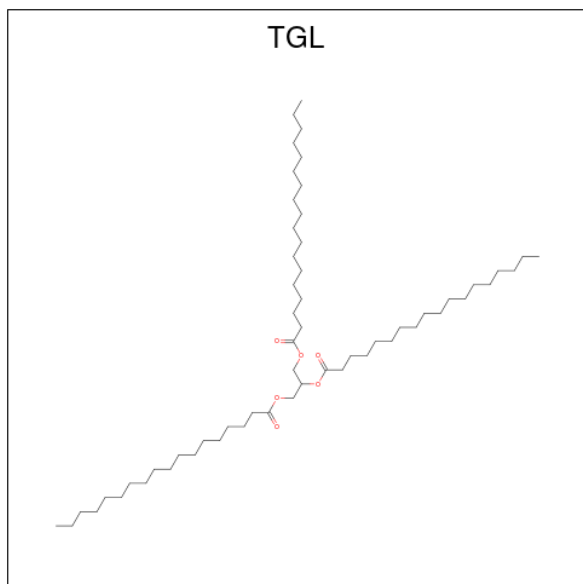
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	D	1	Total	C	O	0	0
			63	57	6		
27	I	1	Total	C	O	0	0
			63	57	6		
27	L	1	Total	C	O	0	0
			63	57	6		
27	N	1	Total	C	O	0	0
			63	57	6		
27	N	1	Total	C	O	0	0
			63	57	6		

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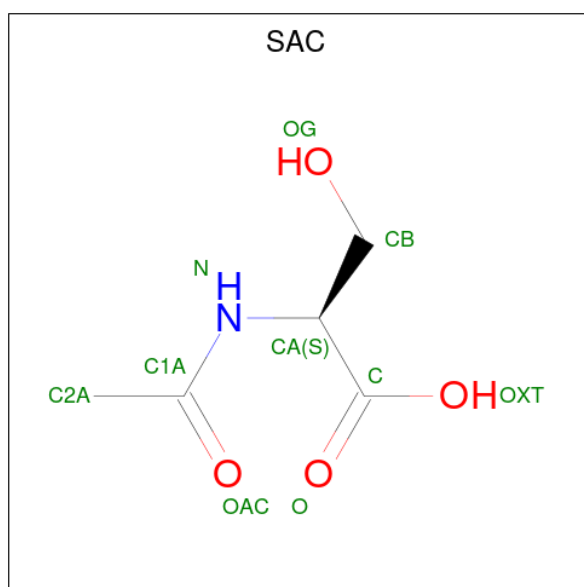
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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 (CCD ID: SAC) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



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	150	Total	O	0	0
			150	150		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	112	Total 112	O 112	0	0
30	C	78	Total 78	O 78	0	0
30	D	34	Total 34	O 34	0	0
30	E	38	Total 38	O 38	0	0
30	F	60	Total 60	O 60	0	0
30	G	42	Total 42	O 42	0	0
30	H	44	Total 44	O 44	0	0
30	I	18	Total 18	O 18	0	0
30	J	19	Total 19	O 19	0	0
30	K	1	Total 1	O 1	0	0
30	L	21	Total 21	O 21	0	0
30	M	13	Total 13	O 13	0	0
30	N	130	Total 130	O 130	0	0
30	O	73	Total 73	O 73	0	0
30	P	69	Total 69	O 69	0	0
30	Q	30	Total 30	O 30	0	0
30	R	34	Total 34	O 34	0	0
30	S	43	Total 43	O 43	0	0
30	T	22	Total 22	O 22	0	0
30	U	35	Total 35	O 35	0	0
30	V	11	Total 11	O 11	0	0

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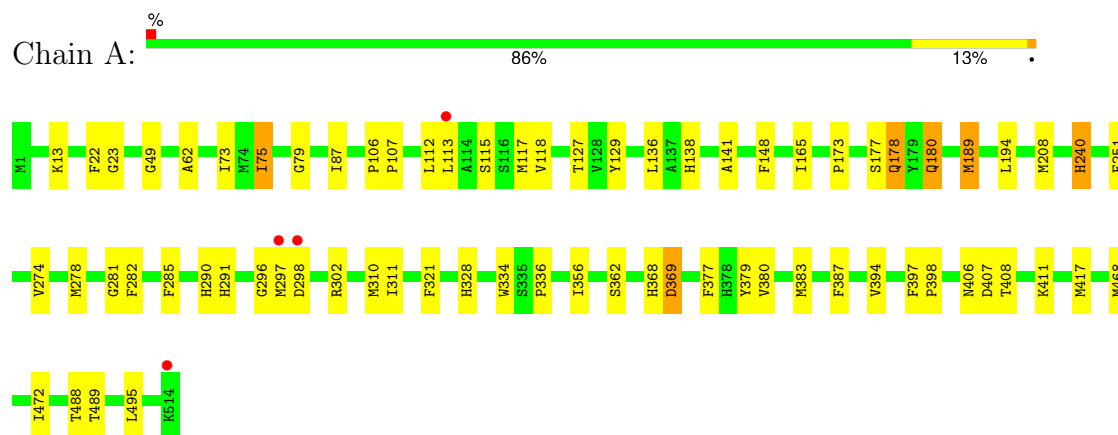
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	W	12	Total 12	O 12	0	0
30	X	3	Total 3	O 3	0	0
30	Y	9	Total 9	O 9	0	0
30	Z	7	Total 7	O 7	0	0

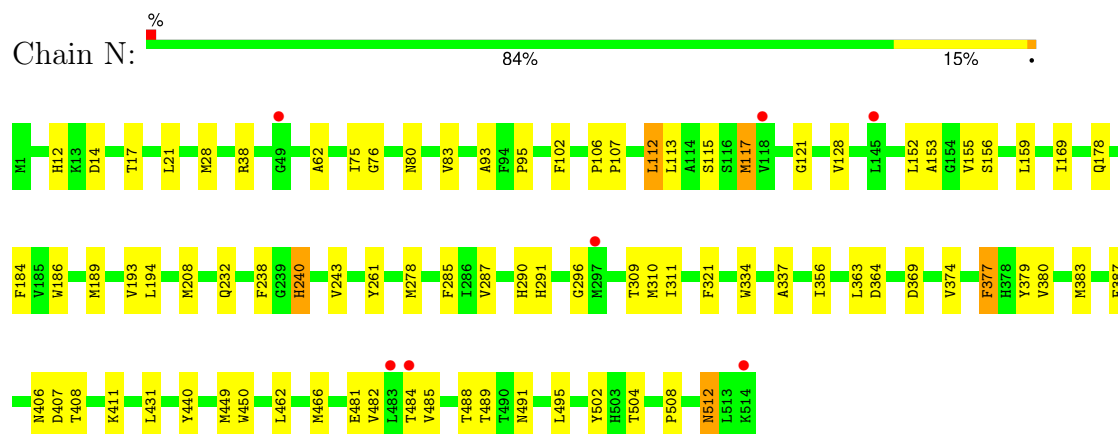
3 Residue-property plots

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

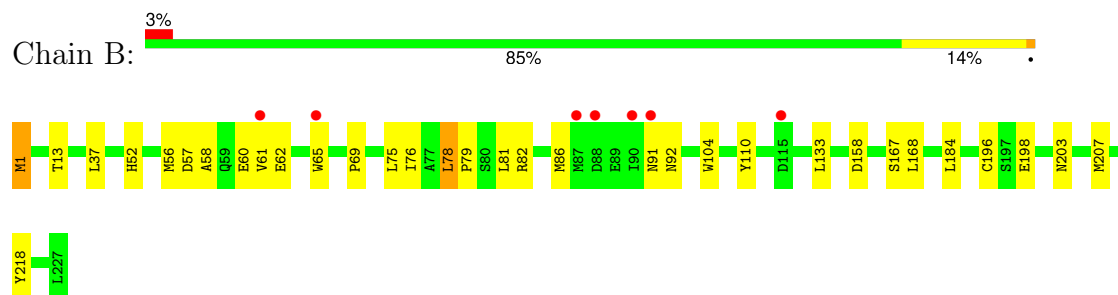
• Molecule 1: Cytochrome c oxidase subunit 1



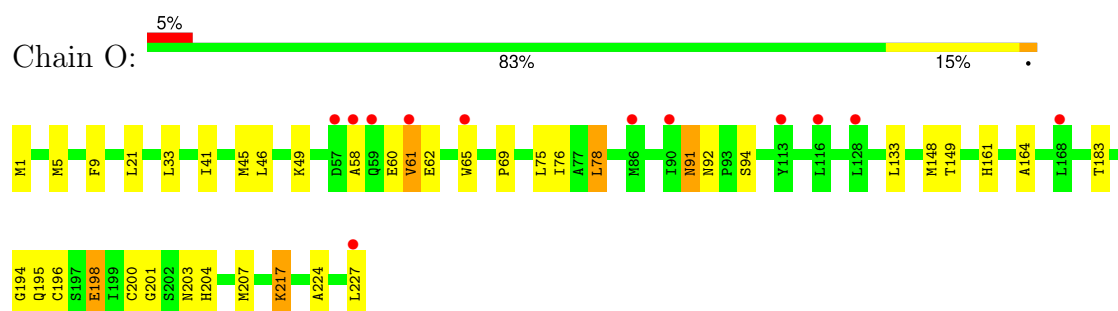
• Molecule 1: Cytochrome c oxidase subunit 1



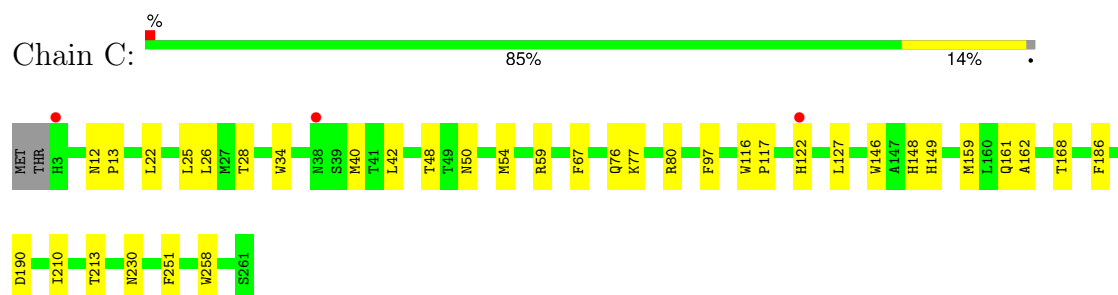
• Molecule 2: Cytochrome c oxidase subunit 2



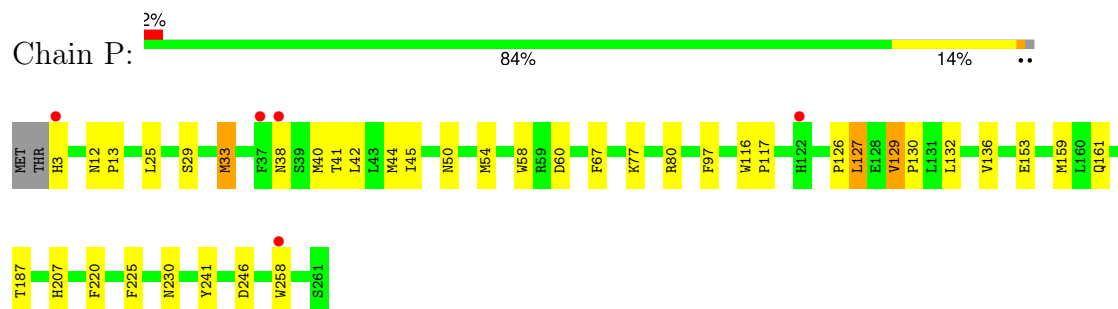
- Molecule 2: Cytochrome c oxidase subunit 2



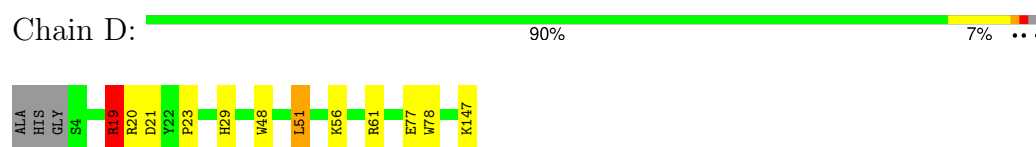
- Molecule 3: Cytochrome c oxidase subunit 3



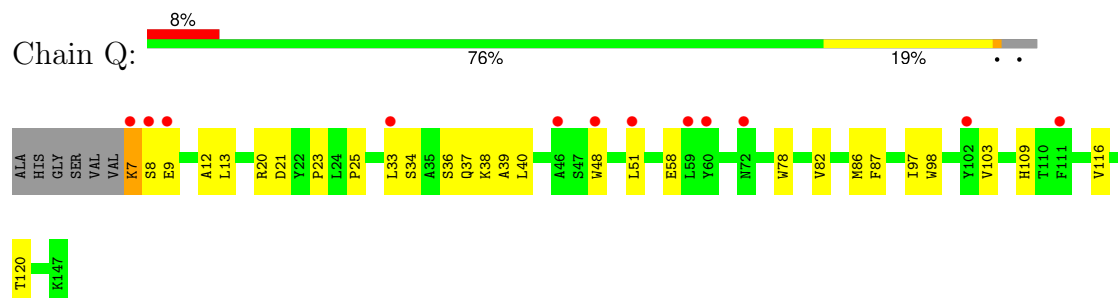
- Molecule 3: Cytochrome c oxidase subunit 3



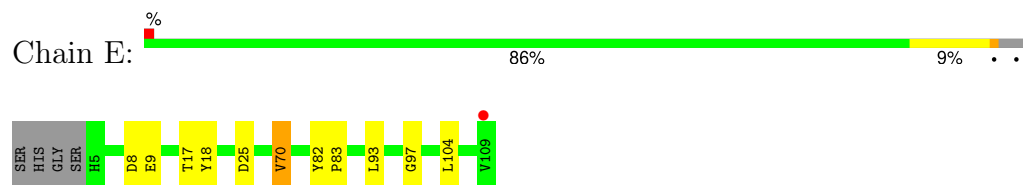
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



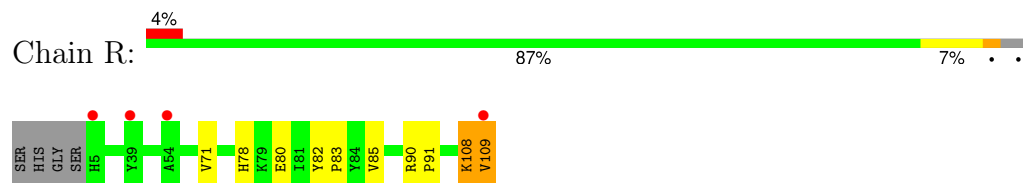
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



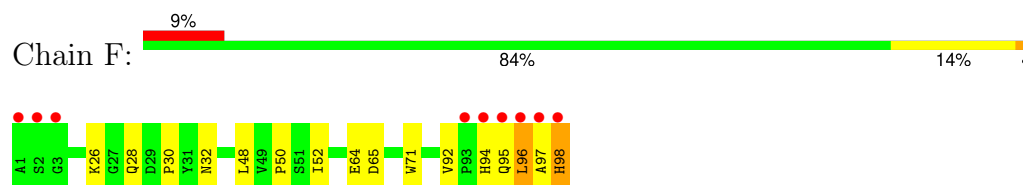
- Molecule 5: Cytochrome c oxidase subunit 5A



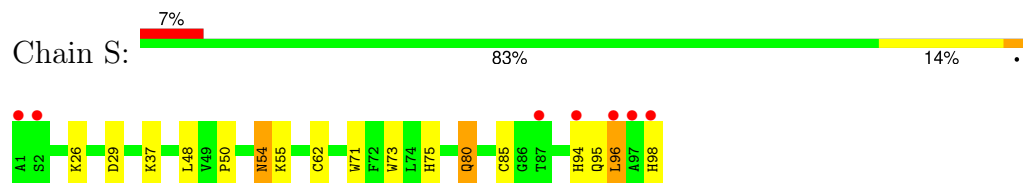
- Molecule 5: Cytochrome c oxidase subunit 5A



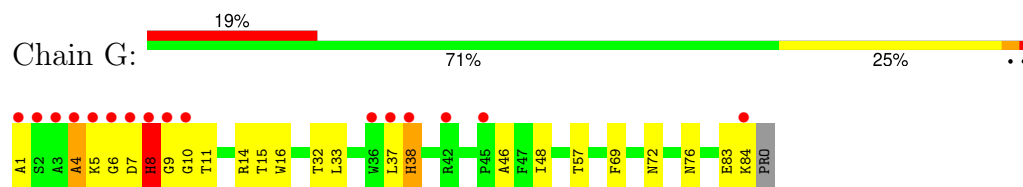
- Molecule 6: Cytochrome c oxidase subunit 5B



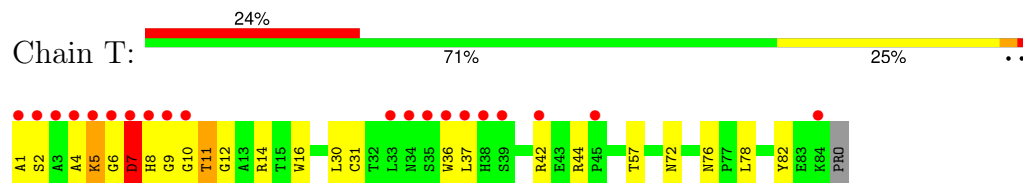
- Molecule 6: Cytochrome c oxidase subunit 5B



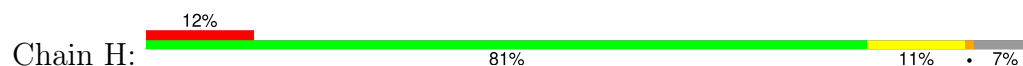
- Molecule 7: Cytochrome c oxidase subunit 6A2

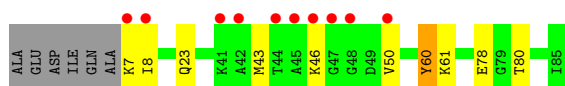


- Molecule 7: Cytochrome c oxidase subunit 6A2

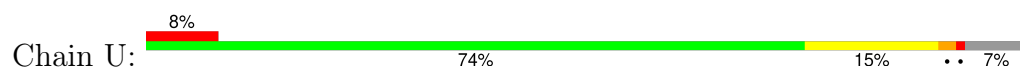


- Molecule 8: Cytochrome c oxidase subunit 6B1





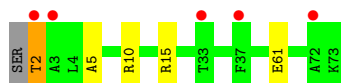
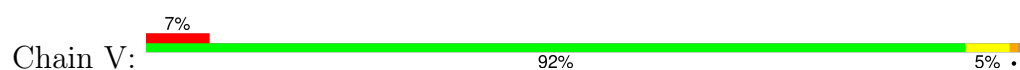
- Molecule 8: Cytochrome c oxidase subunit 6B1



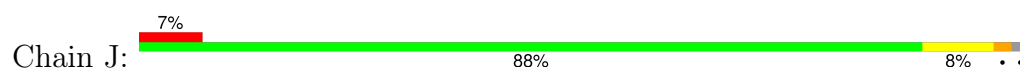
- Molecule 9: Cytochrome c oxidase subunit 6C



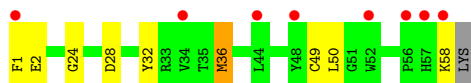
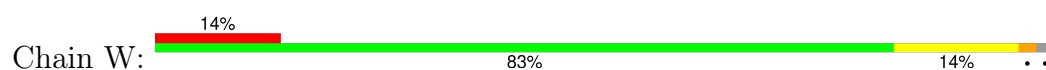
- Molecule 9: Cytochrome c oxidase subunit 6C



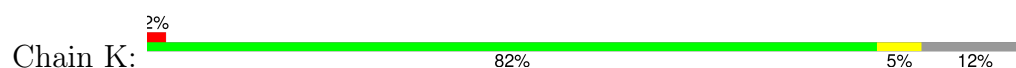
- Molecule 10: Cytochrome c oxidase subunit 7A1



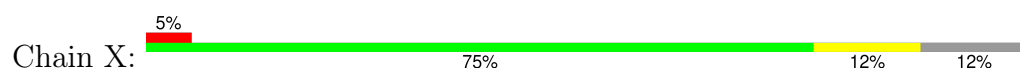
- Molecule 10: Cytochrome c oxidase subunit 7A1



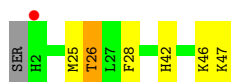
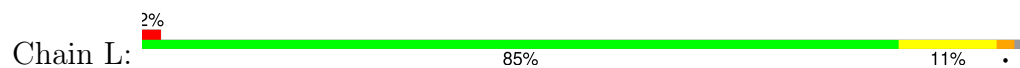
- Molecule 11: Cytochrome c oxidase subunit 7B



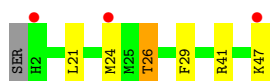
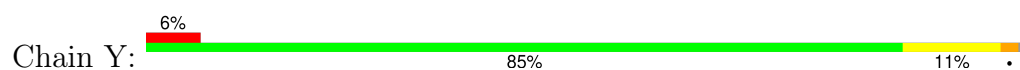
- Molecule 11: Cytochrome c oxidase subunit 7B



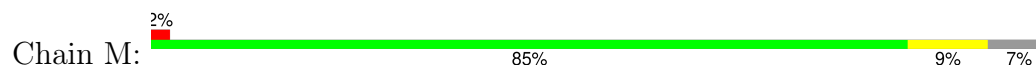
- Molecule 12: Cytochrome c oxidase subunit 7C



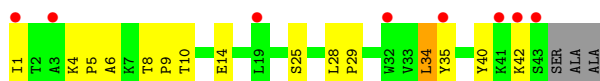
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.29Å 182.82Å 208.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.10) 99.9 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.228 0.201 , 0.233	Depositor DCC
R_{free} test set	20057 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	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	0.96	EDS
Total number of atoms	32333	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0NM, NA, CUA, ZN, TGL, CU, EDO, SAC, CHD, TPO, FME, DMU, CDL, PGV, PEK, MG, HEA, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.09	2/4156 (0.0%)	1.39	7/5678 (0.1%)
1	N	1.18	5/4156 (0.1%)	1.35	13/5678 (0.2%)
2	B	1.11	1/1860 (0.1%)	1.35	1/2534 (0.0%)
2	O	1.06	1/1860 (0.1%)	1.38	5/2534 (0.2%)
3	C	1.03	0/2197	1.33	1/3005 (0.0%)
3	P	1.15	2/2197 (0.1%)	1.23	2/3005 (0.1%)
4	D	1.11	0/1229	1.30	1/1658 (0.1%)
4	Q	1.05	1/1209 (0.1%)	1.35	1/1630 (0.1%)
5	E	1.06	0/871	1.41	6/1182 (0.5%)
5	R	0.99	0/871	1.42	2/1182 (0.2%)
6	F	1.08	0/765	1.32	0/1038
6	S	1.11	0/765	1.30	0/1038
7	G	1.04	1/690 (0.1%)	1.34	2/937 (0.2%)
7	T	1.02	0/690	1.30	1/937 (0.1%)
8	H	0.99	0/682	1.42	0/921
8	U	0.96	0/682	1.48	3/921 (0.3%)
9	I	1.01	0/605	1.35	0/802
9	V	0.99	0/605	1.50	0/802
10	J	0.99	0/471	1.39	1/636 (0.2%)
10	W	1.17	0/471	1.34	0/636
11	K	1.08	0/398	1.39	0/546
11	X	1.10	0/398	1.35	0/546
12	L	0.97	0/393	1.44	2/526 (0.4%)
12	Y	1.10	0/393	1.38	0/526
13	M	1.01	0/345	1.38	0/470
13	Z	1.09	0/345	1.48	0/470
All	All	1.08	13/29304 (0.0%)	1.36	48/39838 (0.1%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	9.67	1.34	1.23
2	O	198	GLU	C-O	8.01	1.32	1.23
3	P	60	ASP	C-O	6.81	1.32	1.24
1	N	240	HIS	CE1-NE2	6.65	1.39	1.32
1	A	240	HIS	CE1-NE2	6.35	1.38	1.32

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	CA-CB-CG	-11.47	102.33	113.80
2	O	92	ASN	CB-CA-C	10.71	120.08	110.44
1	A	240	HIS	CA-CB-CG	-8.91	104.89	113.80
2	B	92	ASN	CB-CA-C	8.09	118.58	110.33
1	N	102	PHE	CA-CB-CG	-6.97	106.83	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	62	0
1	N	4027	0	4001	53	0
2	B	1824	0	1833	23	0
2	O	1824	0	1833	30	0
3	C	2110	0	2027	28	0
3	P	2110	0	2027	25	0
4	D	1195	0	1183	13	0
4	Q	1175	0	1160	26	0
5	E	852	0	845	4	0
5	R	852	0	845	6	0
6	F	748	0	728	21	0
6	S	748	0	728	13	0
7	G	675	0	644	26	0
7	T	675	0	644	27	0
8	H	662	0	623	4	0
8	U	662	0	623	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	592	0	604	4	0
9	V	592	0	604	5	0
10	J	460	0	459	3	0
10	W	460	0	459	7	0
11	K	384	0	366	4	0
11	X	384	0	366	4	0
12	L	380	0	380	6	0
12	Y	380	0	380	11	0
13	M	335	0	352	3	0
13	Z	335	0	352	27	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	51	0	76	0	0
17	C	102	0	152	7	0
17	M	51	0	76	6	0
17	P	153	0	228	5	0
17	Z	51	0	76	20	0
18	A	120	0	108	6	0
18	N	120	0	108	9	0
19	A	36	0	54	3	0
19	B	36	0	54	2	0
19	C	24	0	36	7	0
19	D	16	0	24	0	0
19	E	16	0	24	1	0
19	F	32	0	48	3	0
19	G	16	0	23	1	0
19	I	4	0	6	0	0
19	J	8	0	12	0	0
19	K	4	0	6	0	0
19	L	16	0	24	0	0
19	M	4	0	6	0	0
19	N	56	0	84	5	0
19	O	8	0	12	5	0
19	P	12	0	18	0	0
19	Q	12	0	18	0	0
19	R	8	0	12	2	0
19	S	24	0	36	2	0
19	T	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	V	8	0	12	0	0
19	W	12	0	18	0	0
19	Y	4	0	6	0	0
20	A	9	0	1	1	0
20	C	3	0	1	0	0
20	N	15	0	3	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	10	0
22	O	52	0	80	5	0
23	B	29	0	39	0	0
23	C	58	0	78	1	0
23	G	29	0	39	0	0
23	J	29	0	39	1	0
23	P	58	0	78	2	0
23	T	29	0	39	7	0
23	W	29	0	39	0	0
23	Y	29	0	39	4	0
24	C	159	0	231	16	0
24	P	159	0	231	13	0
25	C	200	0	312	15	0
25	P	200	0	312	12	0
26	C	33	0	42	3	0
26	G	66	0	83	9	0
26	M	33	0	42	0	0
26	P	33	0	42	0	0
26	Z	33	0	42	16	0
27	D	63	0	110	12	0
27	I	63	0	110	3	0
27	L	63	0	110	6	0
27	N	126	0	220	8	0
27	Y	63	0	110	5	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	1	0
29	V	9	0	8	2	0
30	A	150	0	0	1	0
30	B	112	0	0	1	0
30	C	78	0	0	2	0
30	D	34	0	0	1	0
30	E	38	0	0	0	0
30	F	60	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	G	42	0	0	2	0
30	H	44	0	0	0	0
30	I	18	0	0	0	0
30	J	19	0	0	0	0
30	K	1	0	0	1	0
30	L	21	0	0	2	0
30	M	13	0	0	0	0
30	N	130	0	0	4	0
30	O	73	0	0	2	0
30	P	69	0	0	4	0
30	Q	30	0	0	2	0
30	R	34	0	0	3	0
30	S	43	0	0	1	0
30	T	22	0	0	5	0
30	U	35	0	0	3	0
30	V	11	0	0	1	0
30	W	12	0	0	2	0
30	X	3	0	0	1	0
30	Y	9	0	0	2	0
30	Z	7	0	0	0	0
All	All	32333	0	32004	493	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 8.

The worst 5 of 493 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)
13:Z:28:LEU:HD23	26:Z:102:DMU:C19	1.61	1.30
3:C:77:LYS:NZ	30:C:402:HOH:O	1.78	1.14
19:C:310:EDO:O1	24:C:317:PEK:H012	1.47	1.13
13:Z:28:LEU:HD23	26:Z:102:DMU:C18	1.79	1.11
13:Z:28:LEU:HD23	26:Z:102:DMU:H9	1.21	1.09

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%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
2	B	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
2	O	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	30	28
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	139/147 (95%)	130 (94%)	9 (6%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
6	S	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
7	G	81/85 (95%)	72 (89%)	7 (9%)	2 (2%)	4	1
7	T	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	10	7
8	H	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
8	U	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
9	I	70/73 (96%)	70 (100%)	0	0	100	100
9	V	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3499/3614 (97%)	3387 (97%)	108 (3%)	4 (0%)	48	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	T	7	ASP
7	G	8	HIS
3	P	38	ASN

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%)	420 (99%)	6 (1%)	59	67
1	N	426/426 (100%)	415 (97%)	11 (3%)	40	46
2	B	210/210 (100%)	203 (97%)	7 (3%)	33	37
2	O	210/210 (100%)	204 (97%)	6 (3%)	37	42
3	C	224/226 (99%)	221 (99%)	3 (1%)	61	69
3	P	224/226 (99%)	218 (97%)	6 (3%)	39	45
4	D	128/129 (99%)	125 (98%)	3 (2%)	44	51
4	Q	125/129 (97%)	121 (97%)	4 (3%)	34	38
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	37
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	37
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	33
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	10
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	10
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	4
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	63 (89%)	8 (11%)	5	3
9	I	57/58 (98%)	54 (95%)	3 (5%)	20	19
9	V	57/58 (98%)	55 (96%)	2 (4%)	32	35
10	J	49/50 (98%)	46 (94%)	3 (6%)	17	15
10	W	49/50 (98%)	46 (94%)	3 (6%)	17	15
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	21
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	46
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	21
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	18
13	Z	37/38 (97%)	36 (97%)	1 (3%)	39	45
All	All	3037/3084 (98%)	2931 (96%)	106 (4%)	32	35

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	61	VAL
4	Q	58	GLU
10	W	50	LEU
2	O	78	LEU
3	P	129	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	207	HIS
4	Q	143	ASN
3	P	230	ASN
4	Q	76	ASN
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
1	FME	N	1	1	8,9,10	0.47	0	8,9,11	0.74	0
2	FME	O	1	2	8,9,10	0.50	0	8,9,11	0.86	0
7	TPO	G	11	7	8,10,11	0.83	0	10,14,16	0.82	0
1	FME	A	1	1	8,9,10	0.67	0	8,9,11	1.07	0
7	TPO	T	11	7	8,10,11	1.15	1 (12%)	10,14,16	0.83	0
2	FME	B	1	2	8,9,10	0.58	0	8,9,11	1.20	1 (12%)

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
1	FME	N	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	6/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	2/9/11/13	-
2	FME	B	1	2	-	4/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	2.62	1.64	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-2.04	119.69	122.82

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	4	0
7	G	11	TPO	5	0
7	T	11	TPO	2	0
2	B	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 158 ligands modelled in this entry, 8 are monoatomic - leaving 150 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	TGL	I	101	-	62,62,62	0.37	0	65,65,65	0.72	1 (1%)
19	EDO	B	306	-	3,3,3	0.31	0	2,2,2	0.13	0
19	EDO	N	613	-	3,3,3	0.38	0	2,2,2	0.59	0
17	PGV	Z	101	-	50,50,50	0.40	0	53,56,56	0.61	1 (1%)
19	EDO	T	1301	-	3,3,3	0.34	0	2,2,2	0.24	0
19	EDO	B	312	-	3,3,3	0.06	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSC	B	302	-	51,51,51	0.39	0	57,59,59	0.57	1 (1%)
22	PSC	O	302	-	51,51,51	0.40	0	57,59,59	0.53	0
19	EDO	B	307	-	3,3,3	0.16	0	2,2,2	0.24	0
20	ONM	A	615	-	1,2,2	0.14	0	0,1,1	-	-
19	EDO	C	310	-	3,3,3	0.07	0	2,2,2	0.07	0
25	CDL	P	308	-	99,99,99	0.44	0	105,111,111	0.60	2 (1%)
19	EDO	G	104	-	3,3,3	0.20	0	2,2,2	0.02	0
19	EDO	E	201	-	3,3,3	0.15	0	2,2,2	0.11	0
19	EDO	Q	1802	-	3,3,3	0.08	0	2,2,2	0.14	0
23	CHD	J	101	-	32,32,32	0.64	1 (3%)	51,51,51	0.85	1 (1%)
19	EDO	P	310	-	3,3,3	0.06	0	2,2,2	0.17	0
17	PGV	C	305	-	50,50,50	0.40	0	53,56,56	0.49	0
24	PEK	P	304	-	52,52,52	0.36	0	55,57,57	0.68	2 (3%)
19	EDO	A	610	-	3,3,3	0.31	0	2,2,2	0.05	0
18	HEA	A	606	1	67,67,67	2.29	26 (38%)	81,103,103	2.58	33 (40%)
19	EDO	B	310	-	3,3,3	0.09	0	2,2,2	0.25	0
26	DMU	P	314	-	34,34,34	0.52	0	45,45,45	1.45	9 (20%)
25	CDL	C	306	-	99,99,99	0.37	0	105,111,111	0.46	1 (0%)
20	ONM	N	616	-	1,2,2	0.07	0	0,1,1	-	-
19	EDO	D	204	-	3,3,3	0.36	0	2,2,2	0.34	0
19	EDO	F	707	-	3,3,3	0.34	0	2,2,2	0.09	0
19	EDO	F	702	-	3,3,3	0.38	0	2,2,2	0.37	0
19	EDO	F	705	-	3,3,3	0.16	0	2,2,2	0.06	0
29	SAC	V	101	-	7,8,9	0.56	0	7,9,11	1.09	1 (14%)
19	EDO	B	309	-	3,3,3	0.09	0	2,2,2	0.63	0
19	EDO	J	102	-	3,3,3	0.16	0	2,2,2	0.22	0
19	EDO	D	203	-	3,3,3	0.26	0	2,2,2	0.37	0
19	EDO	W	303	-	3,3,3	0.12	0	2,2,2	0.08	0
19	EDO	A	618	-	3,3,3	0.31	0	2,2,2	0.52	0
19	EDO	S	1601	-	3,3,3	0.08	0	2,2,2	0.10	0
24	PEK	P	301	-	52,52,52	0.35	0	55,57,57	0.50	0
19	EDO	E	202	-	3,3,3	0.14	0	2,2,2	0.15	0
19	EDO	E	203	-	3,3,3	0.22	0	2,2,2	0.13	0
19	EDO	C	314	-	3,3,3	0.59	0	2,2,2	0.64	0
19	EDO	N	614	-	3,3,3	0.12	0	2,2,2	0.17	0
24	PEK	C	302	-	52,52,52	0.42	0	55,57,57	0.74	1 (1%)
17	PGV	A	604	-	50,50,50	0.54	0	53,56,56	0.61	0
23	CHD	P	303	-	32,32,32	0.63	1 (3%)	51,51,51	0.77	0
17	PGV	P	302	-	50,50,50	0.44	0	53,56,56	0.60	0
19	EDO	A	616	-	3,3,3	0.12	0	2,2,2	0.21	0
19	EDO	N	626	-	3,3,3	0.21	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	107	-	3,3,3	0.12	0	2,2,2	0.16	0
19	EDO	S	1603	-	3,3,3	0.54	0	2,2,2	0.33	0
19	EDO	F	704	-	3,3,3	0.16	0	2,2,2	0.33	0
17	PGV	M	101	-	50,50,50	0.39	0	53,56,56	0.48	0
27	TGL	L	502	-	62,62,62	0.32	0	65,65,65	0.43	1 (1%)
19	EDO	W	301	-	3,3,3	0.16	0	2,2,2	0.36	0
19	EDO	R	202	-	3,3,3	0.10	0	2,2,2	0.22	0
19	EDO	S	1606	-	3,3,3	0.12	0	2,2,2	0.20	0
19	EDO	N	620	-	3,3,3	0.25	0	2,2,2	0.25	0
19	EDO	S	1605	-	3,3,3	0.06	0	2,2,2	0.17	0
17	PGV	P	307	-	50,50,50	0.34	0	53,56,56	0.46	0
19	EDO	M	102	-	3,3,3	0.14	0	2,2,2	0.32	0
19	EDO	V	102	-	3,3,3	0.12	0	2,2,2	0.23	0
19	EDO	N	611	-	3,3,3	0.22	0	2,2,2	0.05	0
19	EDO	A	611	-	3,3,3	0.26	0	2,2,2	0.45	0
23	CHD	C	307	-	32,32,32	0.54	0	51,51,51	0.77	0
24	PEK	C	317	-	52,52,52	0.42	0	55,57,57	0.82	2 (3%)
19	EDO	C	311	-	3,3,3	0.05	0	2,2,2	0.16	0
19	EDO	F	709	-	3,3,3	0.32	0	2,2,2	0.40	0
21	CUA	B	301	2	0,1,1	-	-	-	-	-
21	CUA	O	301	2	0,1,1	-	-	-	-	-
27	TGL	D	201	-	62,62,62	0.36	0	65,65,65	0.36	0
19	EDO	Q	1801	-	3,3,3	0.26	0	2,2,2	0.07	0
19	EDO	G	102	-	3,3,3	0.17	0	2,2,2	0.43	0
24	PEK	C	303	-	52,52,52	0.36	0	55,57,57	0.49	0
23	CHD	T	1302	-	32,32,32	0.69	0	51,51,51	1.11	2 (3%)
17	PGV	P	306	-	50,50,50	0.45	0	53,56,56	0.51	1 (1%)
19	EDO	A	609	-	3,3,3	0.31	0	2,2,2	0.17	0
19	EDO	A	612	-	3,3,3	0.13	0	2,2,2	0.07	0
23	CHD	B	303	-	32,32,32	0.59	0	51,51,51	1.12	2 (3%)
19	EDO	J	103	-	3,3,3	0.18	0	2,2,2	0.16	0
20	ONM	A	613	18,14	1,2,2	0.09	0	0,1,1	-	-
19	EDO	B	311	-	3,3,3	0.06	0	2,2,2	0.19	0
17	PGV	C	304	-	50,50,50	0.38	0	53,56,56	0.52	0
18	HEA	N	605	20,1	67,67,67	2.15	23 (34%)	81,103,103	2.56	31 (38%)
19	EDO	L	501	-	3,3,3	0.19	0	2,2,2	0.20	0
25	CDL	P	312	-	99,99,99	0.35	0	105,111,111	0.44	0
19	EDO	L	504	-	3,3,3	0.17	0	2,2,2	0.21	0
19	EDO	F	706	-	3,3,3	0.35	0	2,2,2	0.78	0
20	ONM	A	614	-	1,2,2	0.01	0	0,1,1	-	-
19	EDO	N	607	-	3,3,3	0.12	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DMU	M	103	-	34,34,34	0.78	1 (2%)	45,45,45	1.91	15 (33%)
19	EDO	N	610	-	3,3,3	0.28	0	2,2,2	0.50	0
19	EDO	N	608	-	3,3,3	0.27	0	2,2,2	0.11	0
19	EDO	P	311	-	3,3,3	0.09	0	2,2,2	0.16	0
27	TGL	N	622	-	62,62,62	0.34	0	65,65,65	0.39	0
19	EDO	B	304	-	3,3,3	0.21	0	2,2,2	0.41	0
27	TGL	Y	101	-	62,62,62	0.41	0	65,65,65	0.76	2 (3%)
19	EDO	I	103	-	3,3,3	0.30	0	2,2,2	0.24	0
27	TGL	N	604	-	62,62,62	0.37	0	65,65,65	0.67	1 (1%)
23	CHD	C	301	-	32,32,32	0.55	0	51,51,51	0.87	1 (1%)
19	EDO	V	103	-	3,3,3	0.13	0	2,2,2	0.11	0
19	EDO	C	315	-	3,3,3	0.39	0	2,2,2	0.43	0
19	EDO	L	505	-	3,3,3	0.18	0	2,2,2	0.23	0
19	EDO	N	624	-	3,3,3	0.37	0	2,2,2	0.38	0
19	EDO	B	308	-	3,3,3	0.51	0	2,2,2	0.26	0
19	EDO	G	103	-	3,3,3	0.21	0	2,2,2	0.25	0
19	EDO	N	612	-	3,3,3	0.15	0	2,2,2	0.38	0
19	EDO	O	304	-	3,3,3	0.14	0	2,2,2	0.09	0
20	0NM	N	619	-	1,2,2	0.09	0	0,1,1	-	-
20	0NM	N	617	-	1,2,2	0.17	0	0,1,1	-	-
19	EDO	Q	1803	-	3,3,3	0.17	0	2,2,2	0.22	0
23	CHD	G	106	-	32,32,32	0.68	0	51,51,51	0.80	0
19	EDO	O	303	-	3,3,3	0.08	0	2,2,2	0.08	0
18	HEA	A	605	20,1	67,67,67	2.10	24 (35%)	81,103,103	2.61	28 (34%)
19	EDO	N	625	-	3,3,3	0.16	0	2,2,2	0.21	0
19	EDO	A	617	-	3,3,3	0.22	0	2,2,2	0.18	0
19	EDO	K	201	-	3,3,3	0.12	0	2,2,2	0.08	0
26	DMU	G	101	-	34,34,34	0.70	1 (2%)	45,45,45	1.26	3 (6%)
19	EDO	N	621	-	3,3,3	1.74	1 (33%)	2,2,2	1.14	0
19	EDO	A	607	-	3,3,3	0.46	0	2,2,2	0.53	0
19	EDO	A	608	-	3,3,3	0.44	0	2,2,2	0.17	0
19	EDO	L	503	-	3,3,3	0.04	0	2,2,2	0.15	0
20	0NM	N	615	18,14	1,2,2	0.06	0	0,1,1	-	-
19	EDO	B	305	-	3,3,3	0.72	0	2,2,2	0.57	0
19	EDO	Y	102	-	3,3,3	0.09	0	2,2,2	0.24	0
23	CHD	Y	103	-	32,32,32	0.60	0	51,51,51	0.92	0
20	0NM	C	312	-	1,2,2	0.05	0	0,1,1	-	-
19	EDO	T	1303	-	3,3,3	0.23	0	2,2,2	0.03	0
19	EDO	N	609	-	3,3,3	0.24	0	2,2,2	0.42	0
19	EDO	P	313	-	3,3,3	0.47	0	2,2,2	0.58	0
19	EDO	S	1607	-	3,3,3	0.10	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	ONM	N	618	-	1,2,2	0.03	0	0,1,1	-	-
26	DMU	G	105	-	34,34,34	1.09	1 (2%)	45,45,45	1.37	7 (15%)
19	EDO	N	623	-	3,3,3	0.05	0	2,2,2	0.18	0
29	SAC	I	102	-	7,8,9	0.61	0	7,9,11	1.19	1 (14%)
19	EDO	S	1604	-	3,3,3	0.31	0	2,2,2	0.29	0
19	EDO	R	201	-	3,3,3	0.22	0	2,2,2	0.08	0
19	EDO	E	204	-	3,3,3	0.14	0	2,2,2	0.27	0
23	CHD	P	309	-	32,32,32	0.66	0	51,51,51	1.14	2 (3%)
25	CDL	C	313	-	99,99,99	0.49	0	105,111,111	0.49	0
18	HEA	N	606	1	67,67,67	2.36	26 (38%)	81,103,103	2.65	32 (39%)
19	EDO	D	202	-	3,3,3	0.15	0	2,2,2	0.05	0
26	DMU	Z	102	-	34,34,34	0.54	0	45,45,45	1.64	11 (24%)
19	EDO	W	304	-	3,3,3	0.12	0	2,2,2	0.07	0
24	PEK	P	305	-	52,52,52	0.38	0	55,57,57	0.58	1 (1%)
19	EDO	C	308	-	3,3,3	0.32	0	2,2,2	0.17	0
19	EDO	F	708	-	3,3,3	0.10	0	2,2,2	0.26	0
19	EDO	D	205	-	3,3,3	0.12	0	2,2,2	0.11	0
23	CHD	W	302	-	32,32,32	0.60	0	51,51,51	0.89	0
26	DMU	C	316	-	34,34,34	0.66	0	45,45,45	1.17	5 (11%)
19	EDO	C	309	-	3,3,3	0.27	0	2,2,2	0.18	0
19	EDO	F	701	-	3,3,3	0.27	0	2,2,2	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	TGL	I	101	-	-	39/65/65/65	-
19	EDO	B	306	-	-	0/1/1/1	-
19	EDO	N	613	-	-	0/1/1/1	-
17	PGV	Z	101	-	-	26/55/55/55	-
19	EDO	T	1301	-	-	1/1/1/1	-
19	EDO	B	312	-	-	0/1/1/1	-
22	PSC	B	302	-	-	22/55/55/55	-
22	PSC	O	302	-	-	27/55/55/55	-
19	EDO	B	307	-	-	0/1/1/1	-
19	EDO	C	310	-	-	1/1/1/1	-
25	CDL	P	308	-	-	59/110/110/110	-
19	EDO	G	104	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	E	201	-	-	1/1/1/1	-
19	EDO	Q	1802	-	-	1/1/1/1	-
23	CHD	J	101	-	-	2/9/74/74	0/4/4/4
19	EDO	P	310	-	-	1/1/1/1	-
17	PGV	C	305	-	-	28/55/55/55	-
24	PEK	P	304	-	-	16/56/56/56	-
19	EDO	A	610	-	-	1/1/1/1	-
18	HEA	A	606	1	-	2/36/76/76	-
26	DMU	P	314	-	2/2/10/10	9/19/59/59	0/2/2/2
19	EDO	B	310	-	-	1/1/1/1	-
25	CDL	C	306	-	-	57/110/110/110	-
19	EDO	D	204	-	-	1/1/1/1	-
19	EDO	F	707	-	-	0/1/1/1	-
19	EDO	F	702	-	-	1/1/1/1	-
19	EDO	F	705	-	-	0/1/1/1	-
29	SAC	V	101	-	-	2/7/8/10	-
19	EDO	B	309	-	-	0/1/1/1	-
19	EDO	J	102	-	-	0/1/1/1	-
19	EDO	D	203	-	-	1/1/1/1	-
19	EDO	W	303	-	-	1/1/1/1	-
19	EDO	A	618	-	-	0/1/1/1	-
19	EDO	S	1601	-	-	0/1/1/1	-
24	PEK	P	301	-	-	19/56/56/56	-
19	EDO	E	202	-	-	1/1/1/1	-
19	EDO	E	203	-	-	1/1/1/1	-
19	EDO	C	314	-	-	0/1/1/1	-
19	EDO	N	614	-	-	0/1/1/1	-
24	PEK	C	302	-	-	20/56/56/56	-
17	PGV	A	604	-	-	16/55/55/55	-
23	CHD	P	303	-	-	2/9/74/74	0/4/4/4
17	PGV	P	302	-	-	10/55/55/55	-
19	EDO	A	616	-	-	0/1/1/1	-
19	EDO	N	626	-	-	1/1/1/1	-
19	EDO	G	107	-	-	1/1/1/1	-
19	EDO	S	1603	-	-	1/1/1/1	-
19	EDO	F	704	-	-	1/1/1/1	-
17	PGV	M	101	-	-	30/55/55/55	-
27	TGL	L	502	-	-	33/65/65/65	-
19	EDO	W	301	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	R	202	-	-	1/1/1/1	-
19	EDO	S	1606	-	-	1/1/1/1	-
19	EDO	N	620	-	-	1/1/1/1	-
19	EDO	S	1605	-	-	1/1/1/1	-
17	PGV	P	307	-	-	21/55/55/55	-
19	EDO	M	102	-	-	1/1/1/1	-
19	EDO	V	102	-	-	0/1/1/1	-
19	EDO	N	611	-	-	1/1/1/1	-
19	EDO	A	611	-	-	0/1/1/1	-
23	CHD	C	307	-	-	2/9/74/74	0/4/4/4
24	PEK	C	317	-	-	26/56/56/56	-
19	EDO	C	311	-	-	1/1/1/1	-
19	EDO	F	709	-	-	1/1/1/1	-
27	TGL	D	201	-	-	34/65/65/65	-
19	EDO	Q	1801	-	-	1/1/1/1	-
19	EDO	G	102	-	-	1/1/1/1	-
24	PEK	C	303	-	-	28/56/56/56	-
23	CHD	T	1302	-	-	7/9/74/74	0/4/4/4
17	PGV	P	306	-	-	17/55/55/55	-
19	EDO	A	609	-	-	0/1/1/1	-
19	EDO	A	612	-	-	0/1/1/1	-
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
19	EDO	J	103	-	-	1/1/1/1	-
19	EDO	B	311	-	-	0/1/1/1	-
17	PGV	C	304	-	-	19/55/55/55	-
18	HEA	N	605	20,1	-	6/36/76/76	-
19	EDO	L	501	-	-	1/1/1/1	-
25	CDL	P	312	-	-	56/110/110/110	-
19	EDO	L	504	-	-	0/1/1/1	-
19	EDO	F	706	-	-	0/1/1/1	-
19	EDO	N	607	-	-	1/1/1/1	-
26	DMU	M	103	-	2/2/10/10	7/19/59/59	0/2/2/2
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	N	608	-	-	1/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
27	TGL	N	622	-	-	40/65/65/65	-
19	EDO	B	304	-	-	0/1/1/1	-
27	TGL	Y	101	-	-	36/65/65/65	-
19	EDO	I	103	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	TGL	N	604	-	-	31/65/65/65	-
23	CHD	C	301	-	-	2/9/74/74	0/4/4/4
19	EDO	V	103	-	-	1/1/1/1	-
19	EDO	C	315	-	-	1/1/1/1	-
19	EDO	L	505	-	-	1/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
19	EDO	G	103	-	-	0/1/1/1	-
19	EDO	N	624	-	-	1/1/1/1	-
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	O	304	-	-	1/1/1/1	-
19	EDO	Q	1803	-	-	1/1/1/1	-
23	CHD	G	106	-	-	4/9/74/74	0/4/4/4
19	EDO	O	303	-	-	0/1/1/1	-
18	HEA	A	605	20,1	-	6/36/76/76	-
19	EDO	N	625	-	-	1/1/1/1	-
19	EDO	A	617	-	-	1/1/1/1	-
26	DMU	G	101	-	2/2/10/10	12/19/59/59	0/2/2/2
19	EDO	K	201	-	-	1/1/1/1	-
19	EDO	N	621	-	-	0/1/1/1	-
19	EDO	A	607	-	-	1/1/1/1	-
19	EDO	A	608	-	-	0/1/1/1	-
19	EDO	L	503	-	-	1/1/1/1	-
19	EDO	B	305	-	-	1/1/1/1	-
19	EDO	Y	102	-	-	1/1/1/1	-
23	CHD	Y	103	-	-	0/9/74/74	0/4/4/4
19	EDO	T	1303	-	-	1/1/1/1	-
19	EDO	N	609	-	-	1/1/1/1	-
19	EDO	P	313	-	-	1/1/1/1	-
19	EDO	S	1607	-	-	1/1/1/1	-
26	DMU	G	105	-	2/2/10/10	10/19/59/59	0/2/2/2
19	EDO	N	623	-	-	0/1/1/1	-
29	SAC	I	102	-	-	6/7/8/10	-
19	EDO	S	1604	-	-	1/1/1/1	-
19	EDO	R	201	-	-	0/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
23	CHD	P	309	-	-	2/9/74/74	0/4/4/4
25	CDL	C	313	-	-	54/110/110/110	-
18	HEA	N	606	1	-	4/36/76/76	-
19	EDO	D	202	-	-	1/1/1/1	-
26	DMU	Z	102	-	2/2/10/10	14/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	W	304	-	-	1/1/1/1	-
24	PEK	P	305	-	-	33/56/56/56	-
19	EDO	C	308	-	-	1/1/1/1	-
19	EDO	F	708	-	-	1/1/1/1	-
19	EDO	D	205	-	-	0/1/1/1	-
23	CHD	W	302	-	-	1/9/74/74	0/4/4/4
26	DMU	C	316	-	2/2/10/10	14/19/59/59	0/2/2/2
19	EDO	C	309	-	-	0/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	606	HEA	FE-ND	5.85	2.12	1.94
18	A	606	HEA	C4C-NC	-5.50	1.29	1.39
18	N	606	HEA	C1D-ND	-5.49	1.30	1.40
18	N	606	HEA	FE-NB	5.26	2.11	1.94
18	A	606	HEA	CHB-C4A	5.13	1.48	1.38

The worst 5 of 201 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	605	HEA	C2D-C1D-ND	7.21	118.13	109.84
18	A	606	HEA	C3C-C2C-C1C	-7.17	98.71	107.17
18	A	605	HEA	C2D-C1D-ND	7.07	117.97	109.84
18	N	606	HEA	C3D-C4D-ND	6.74	116.87	110.35
18	N	606	HEA	C3A-C2A-C1A	-6.70	100.70	107.05

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	C	316	DMU	C5
26	C	316	DMU	C6
26	G	101	DMU	C5
26	G	101	DMU	C6
26	G	105	DMU	C5

5 of 974 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	305	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
17	M	101	PGV	C03-O11-P-O12
17	M	101	PGV	C03-O11-P-O13
17	M	101	PGV	C03-O11-P-O14
17	M	101	PGV	C04-O12-P-O11

There are no ring outliers.

56 monomers are involved in 221 short contacts:

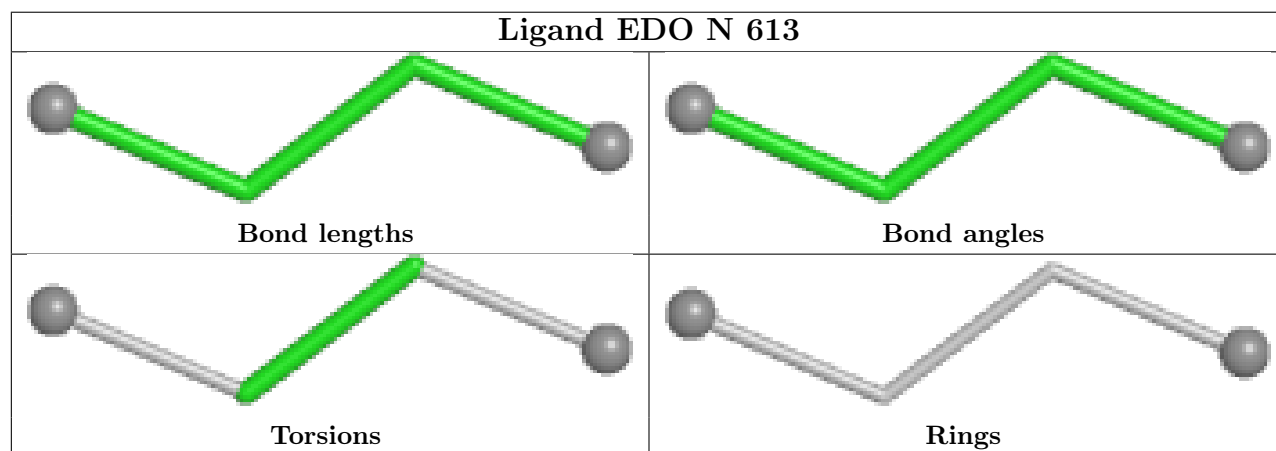
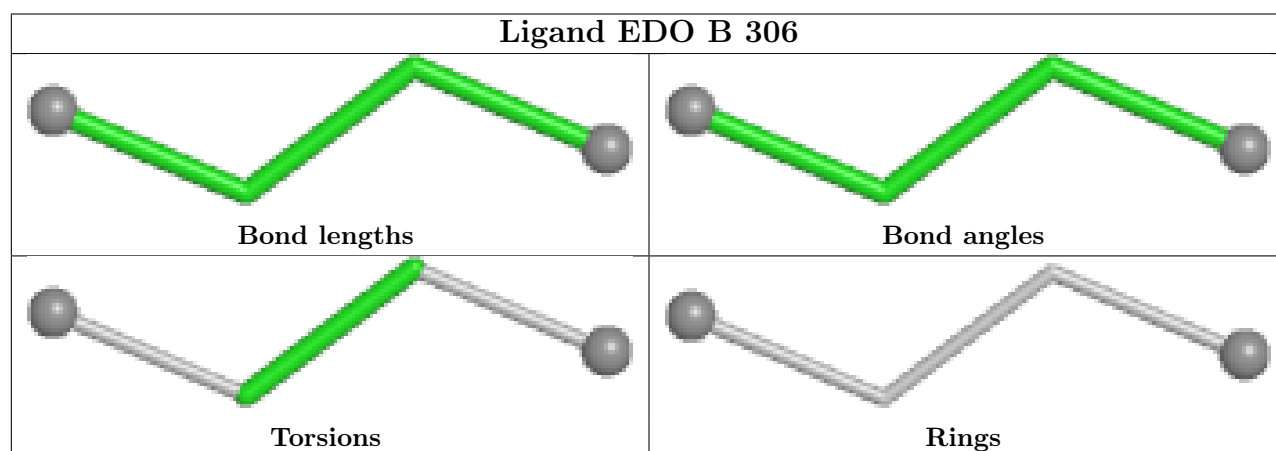
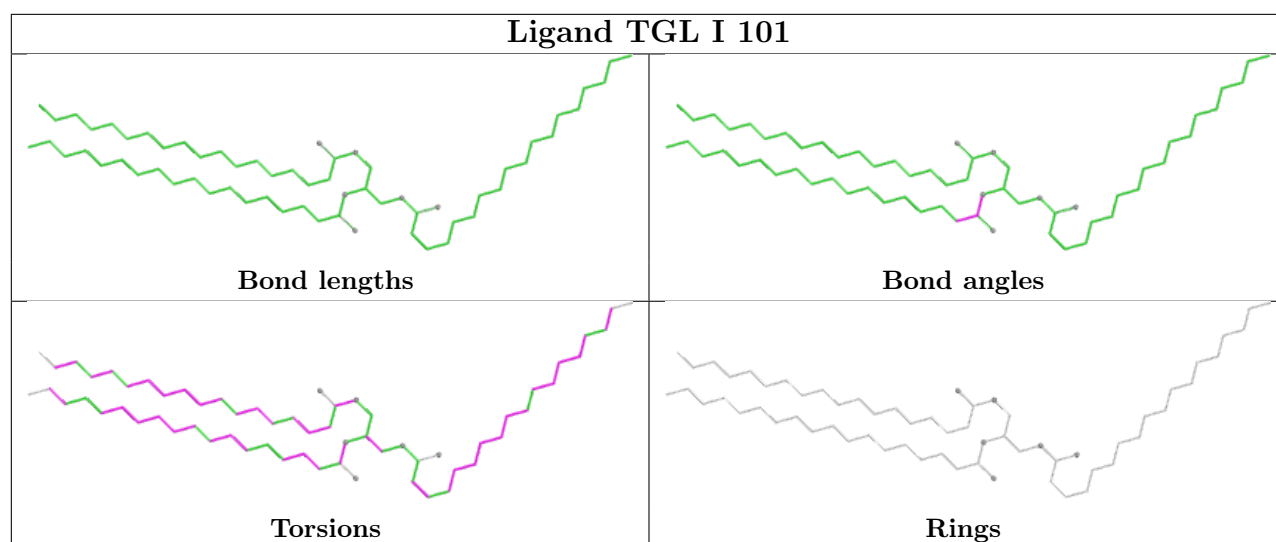
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	I	101	TGL	3	0
19	N	613	EDO	1	0
17	Z	101	PGV	20	0
22	B	302	PSC	10	0
22	O	302	PSC	5	0
20	A	615	0NM	1	0
19	C	310	EDO	6	0
25	P	308	CDL	2	0
19	E	201	EDO	1	0
23	J	101	CHD	1	0
17	C	305	PGV	3	0
24	P	304	PEK	2	0
18	A	606	HEA	4	0
19	B	310	EDO	1	0
25	C	306	CDL	12	0
29	V	101	SAC	2	0
24	P	301	PEK	6	0
24	C	302	PEK	2	0
23	P	303	CHD	1	0
19	A	616	EDO	2	0
19	F	704	EDO	3	0
17	M	101	PGV	6	0
27	L	502	TGL	6	0
19	R	202	EDO	2	0
17	P	307	PGV	3	0
24	C	317	PEK	9	0
27	D	201	TGL	12	0
24	C	303	PEK	5	0
23	T	1302	CHD	7	0
17	P	306	PGV	2	0
19	A	612	EDO	1	0
17	C	304	PGV	4	0
18	N	605	HEA	5	0

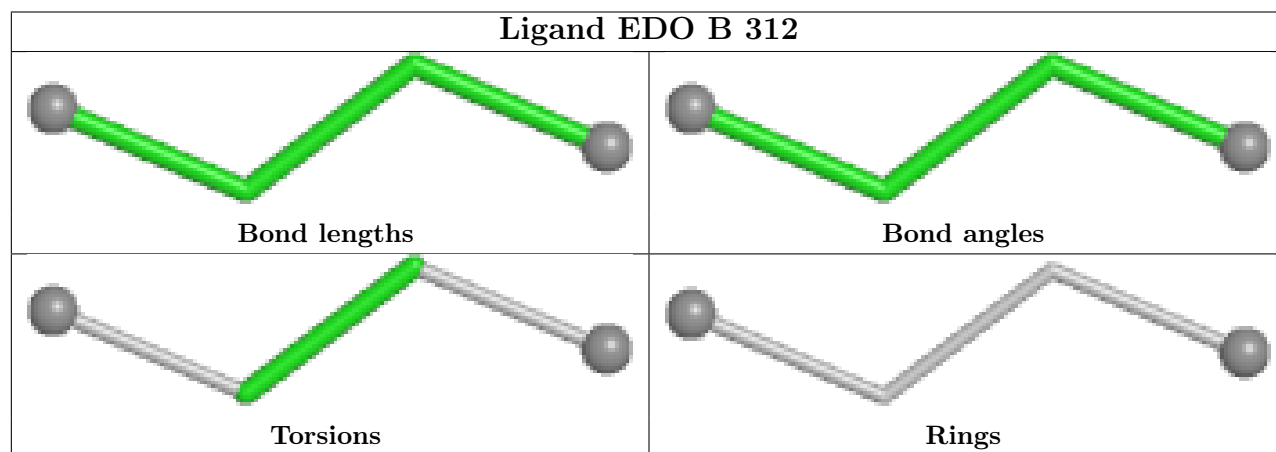
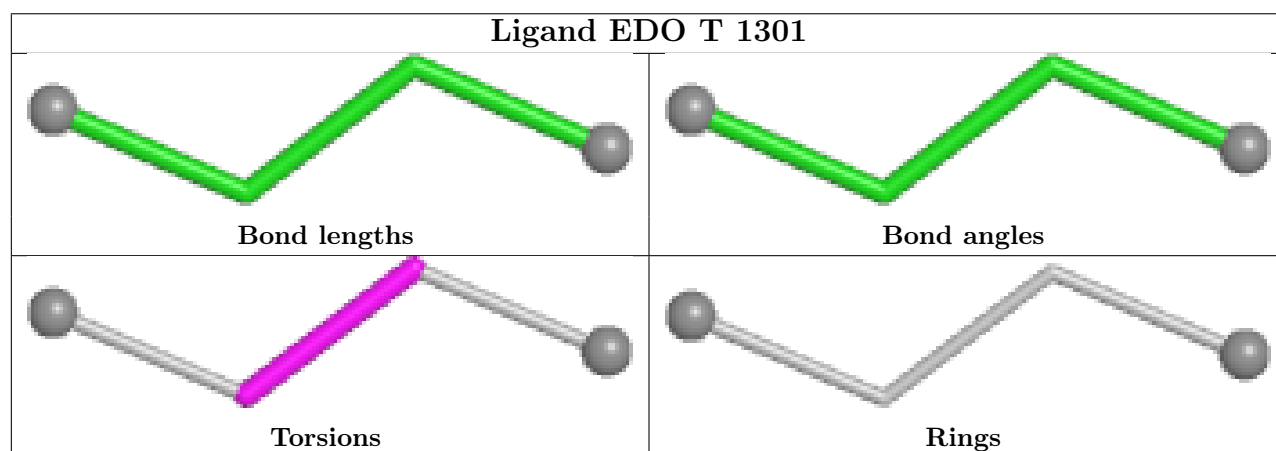
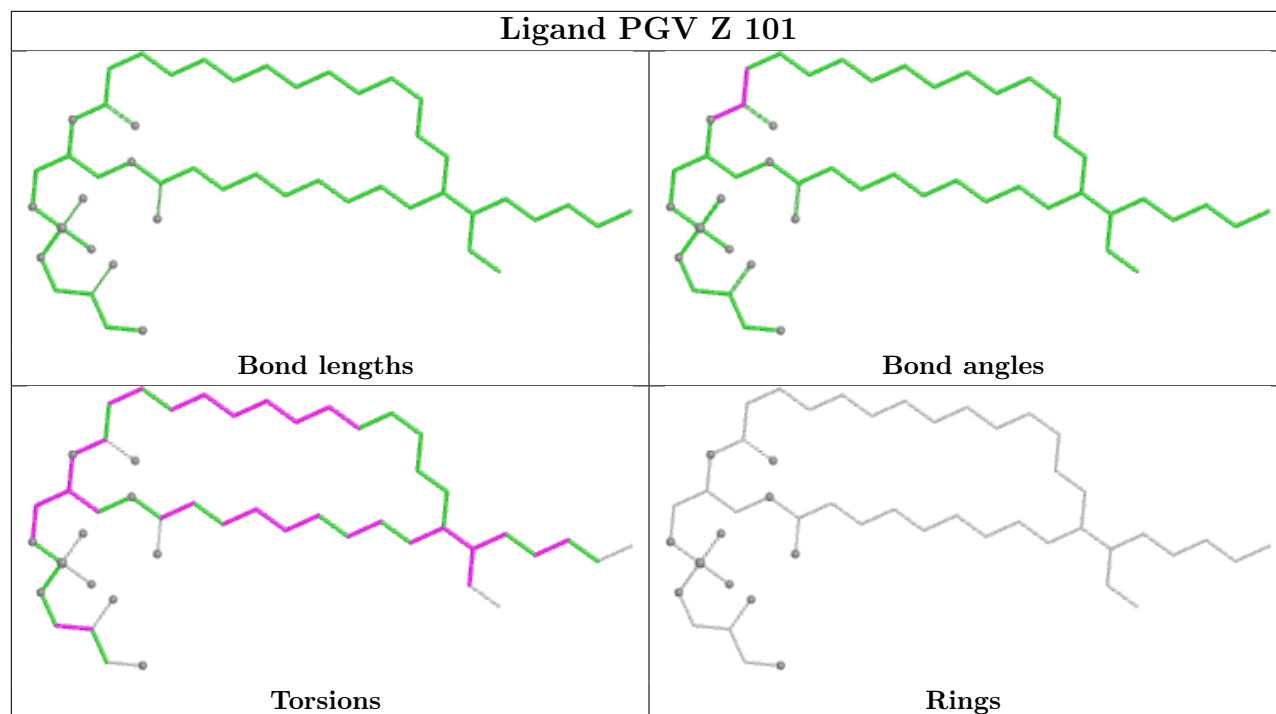
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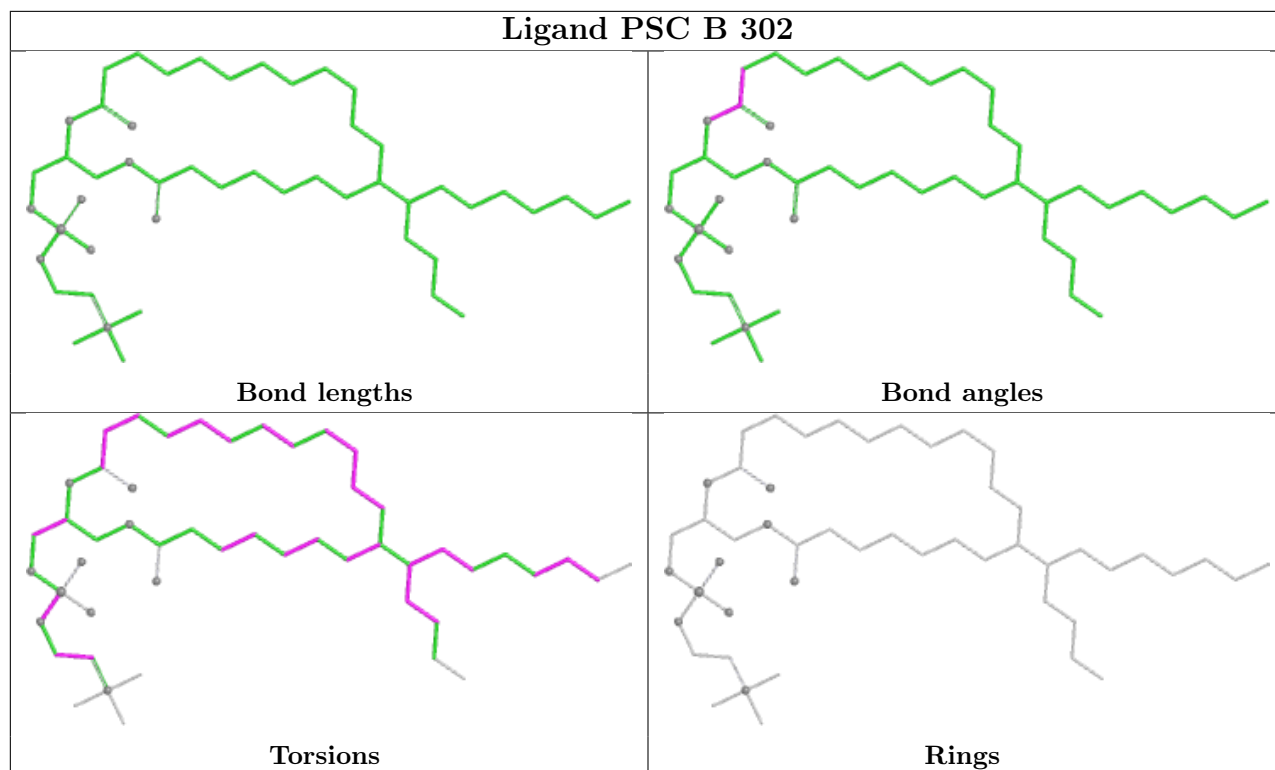
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	312	CDL	10	0
19	N	610	EDO	3	0
27	N	622	TGL	8	0
27	Y	101	TGL	5	0
23	C	301	CHD	1	0
19	C	315	EDO	1	0
19	N	624	EDO	1	0
19	G	103	EDO	1	0
19	O	304	EDO	5	0
18	A	605	HEA	2	0
26	G	101	DMU	1	0
20	N	615	0NM	1	0
19	B	305	EDO	1	0
23	Y	103	CHD	4	0
19	S	1607	EDO	2	0
26	G	105	DMU	8	0
29	I	102	SAC	1	0
23	P	309	CHD	1	0
25	C	313	CDL	3	0
18	N	606	HEA	4	0
26	Z	102	DMU	16	0
24	P	305	PEK	5	0
26	C	316	DMU	3	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.

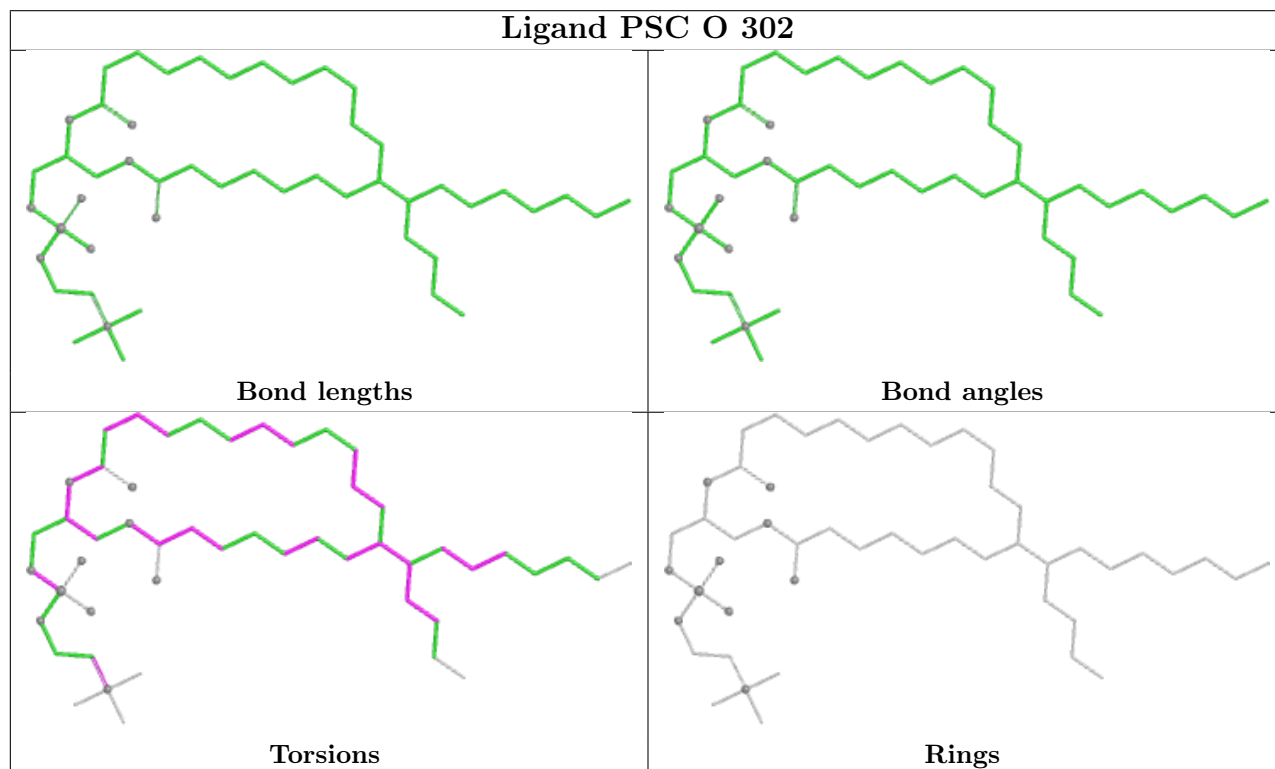


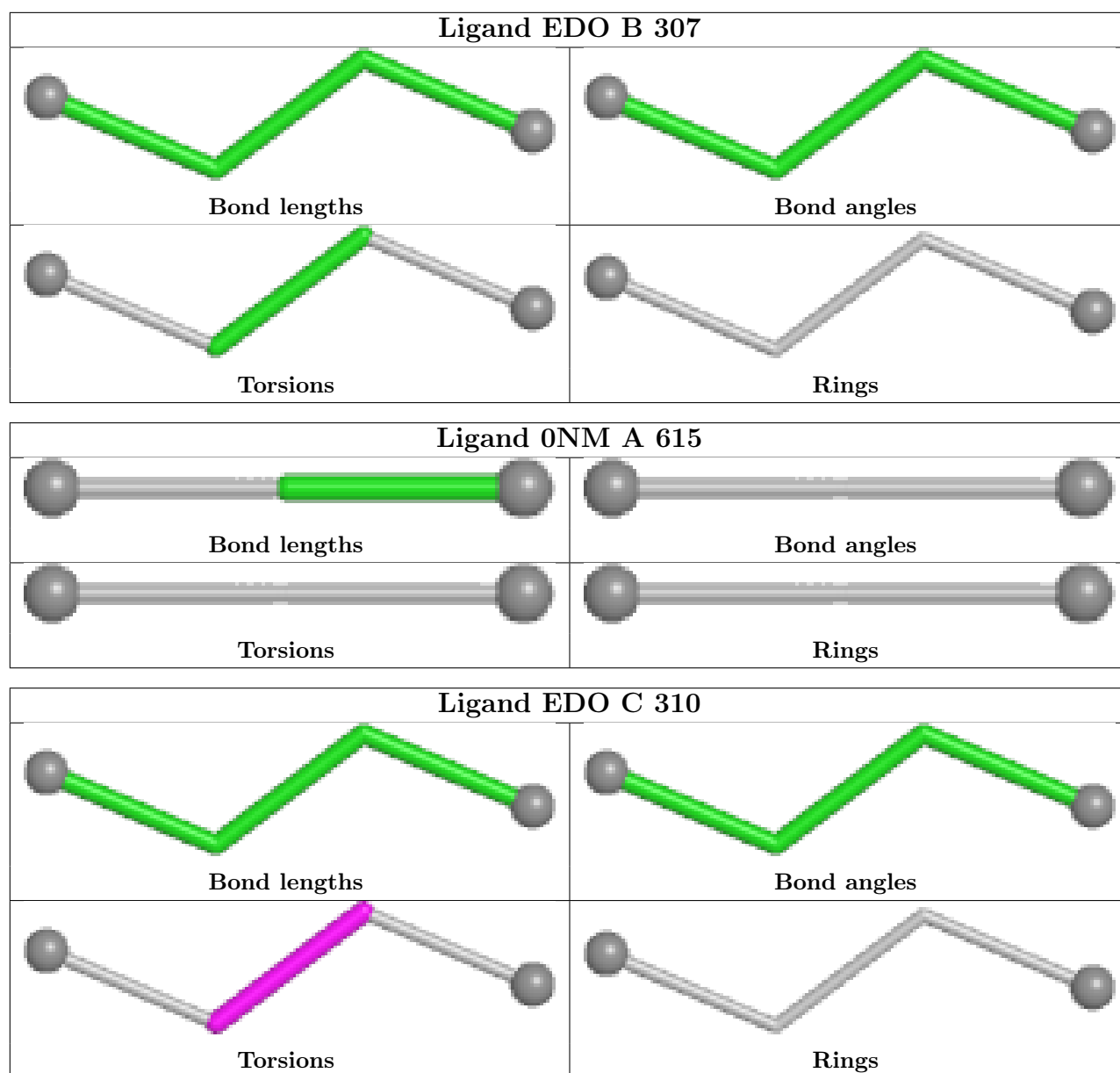


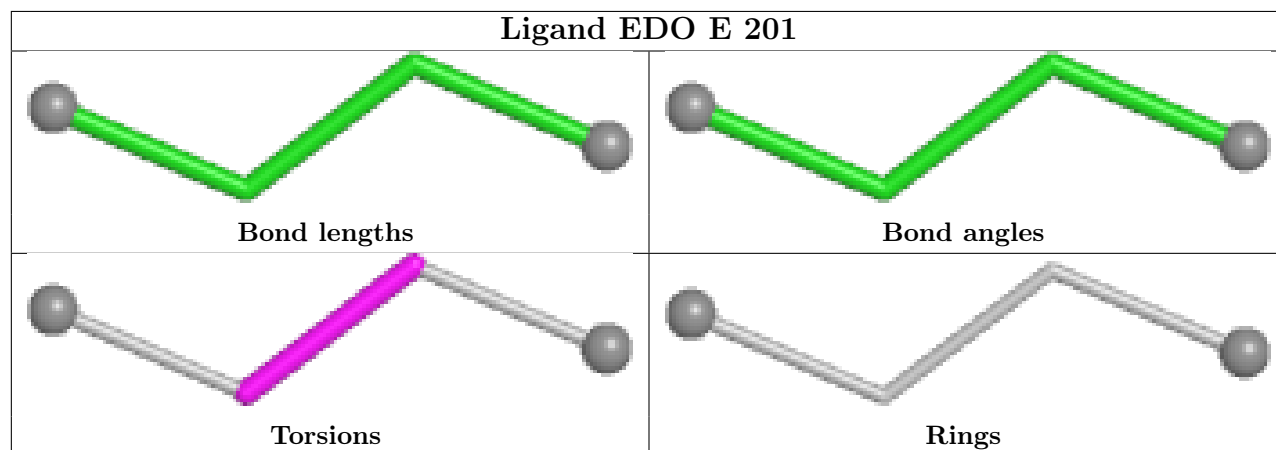
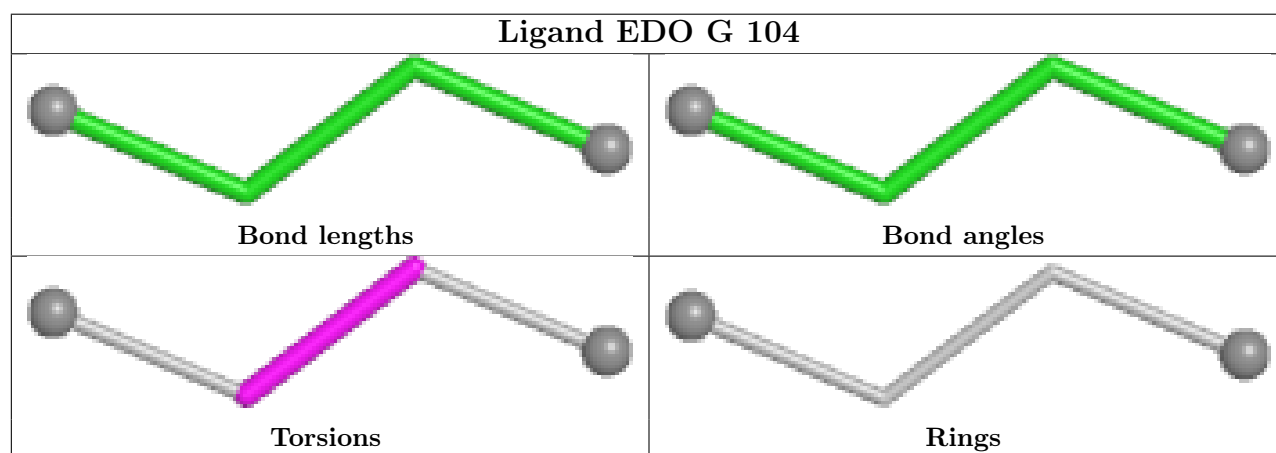
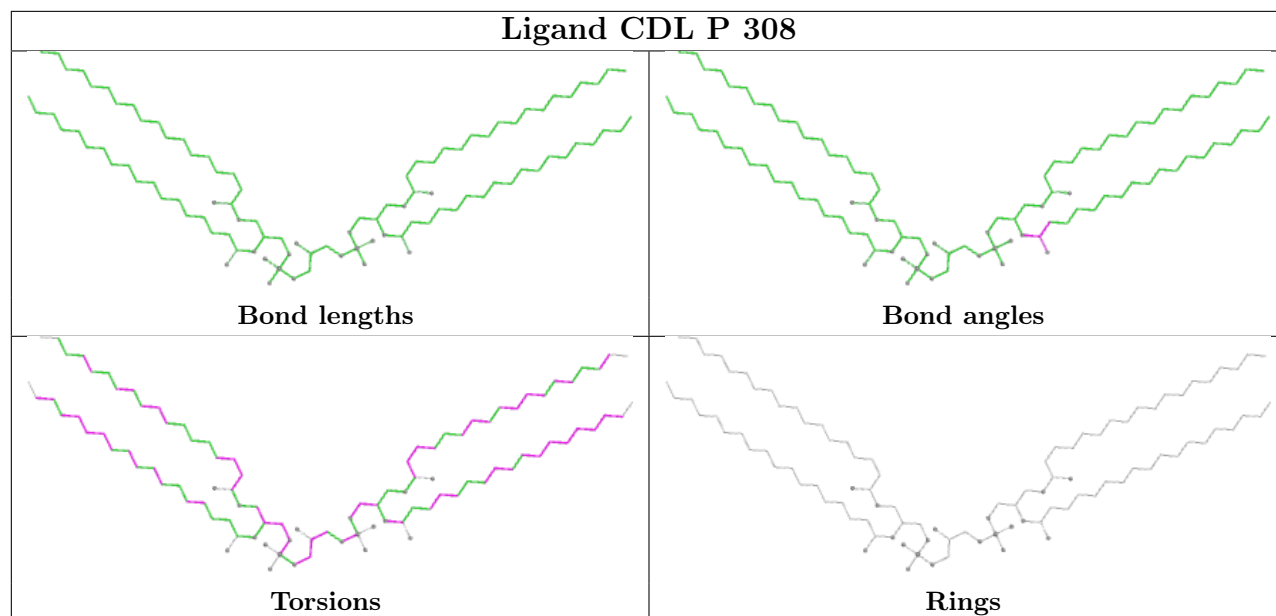
Ligand PSC B 302

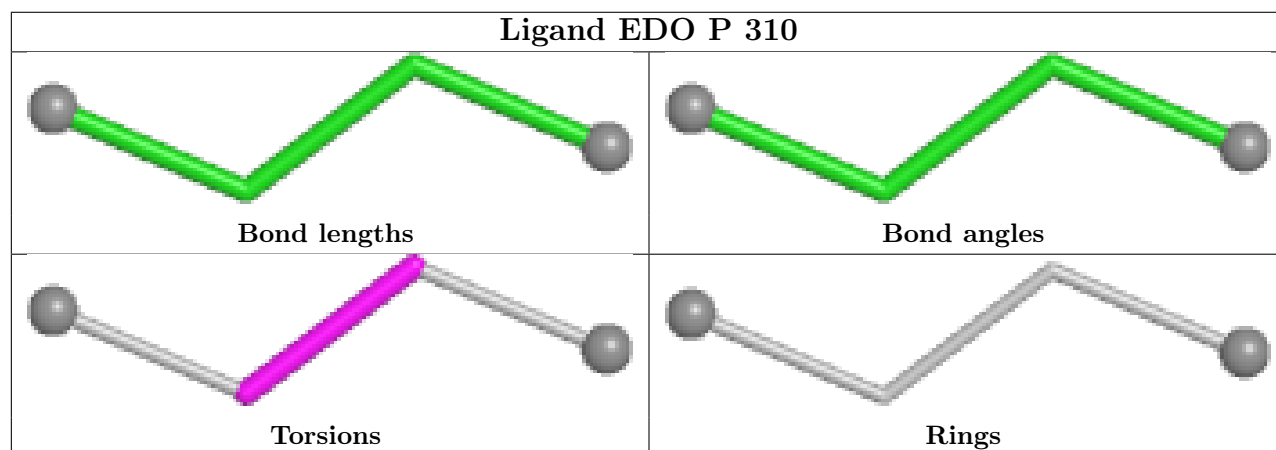
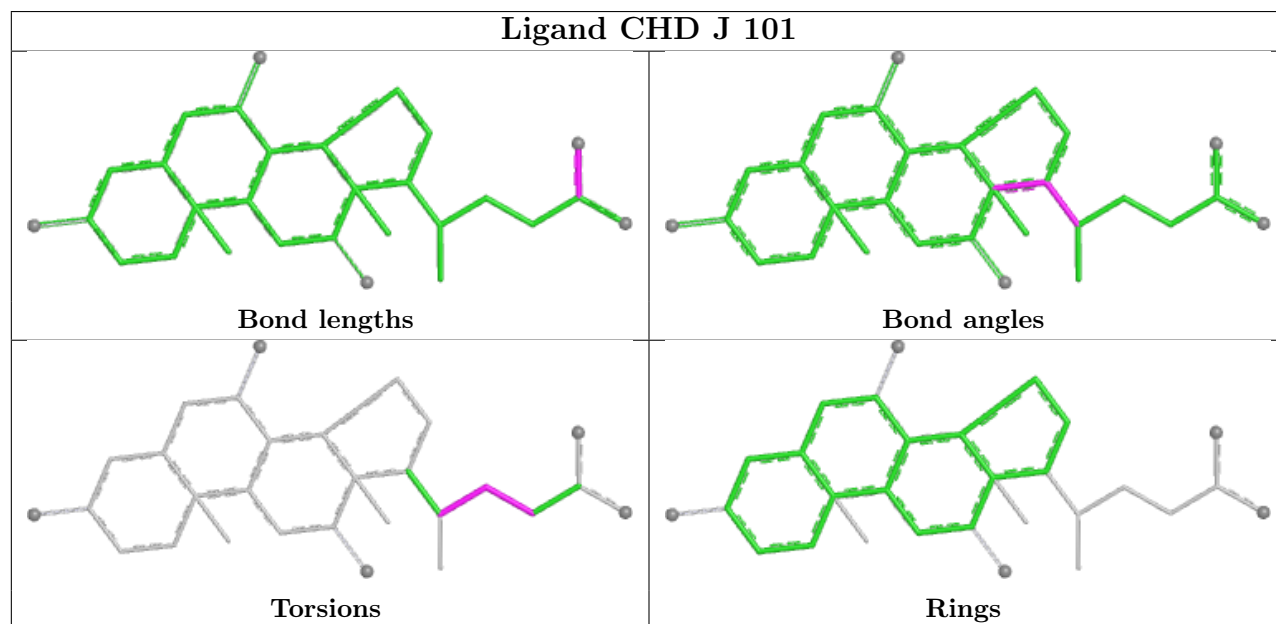
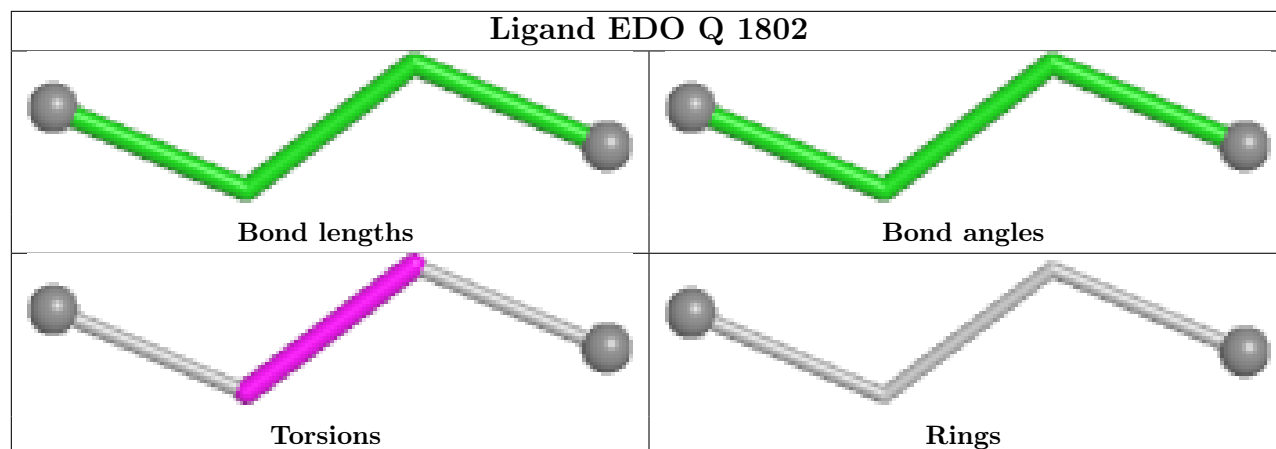


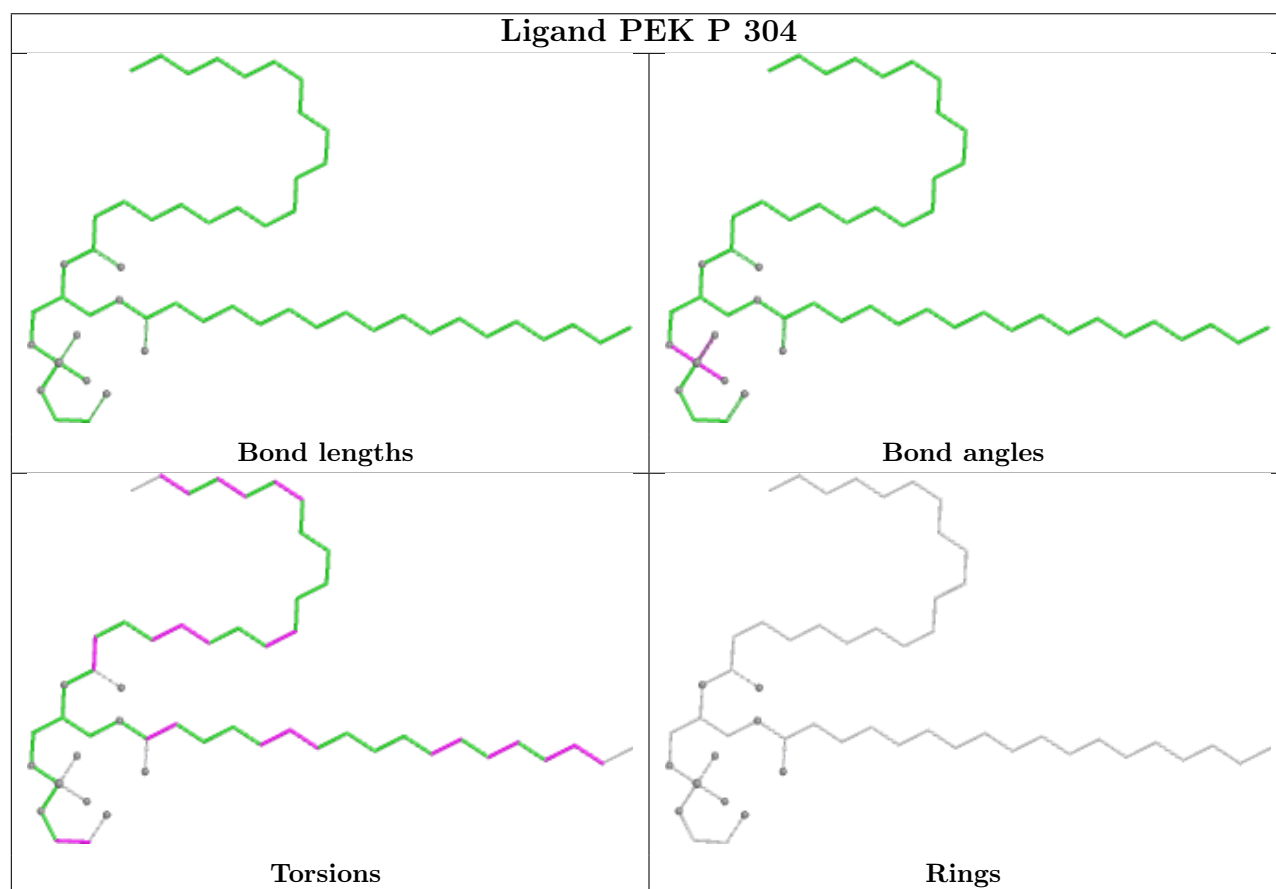
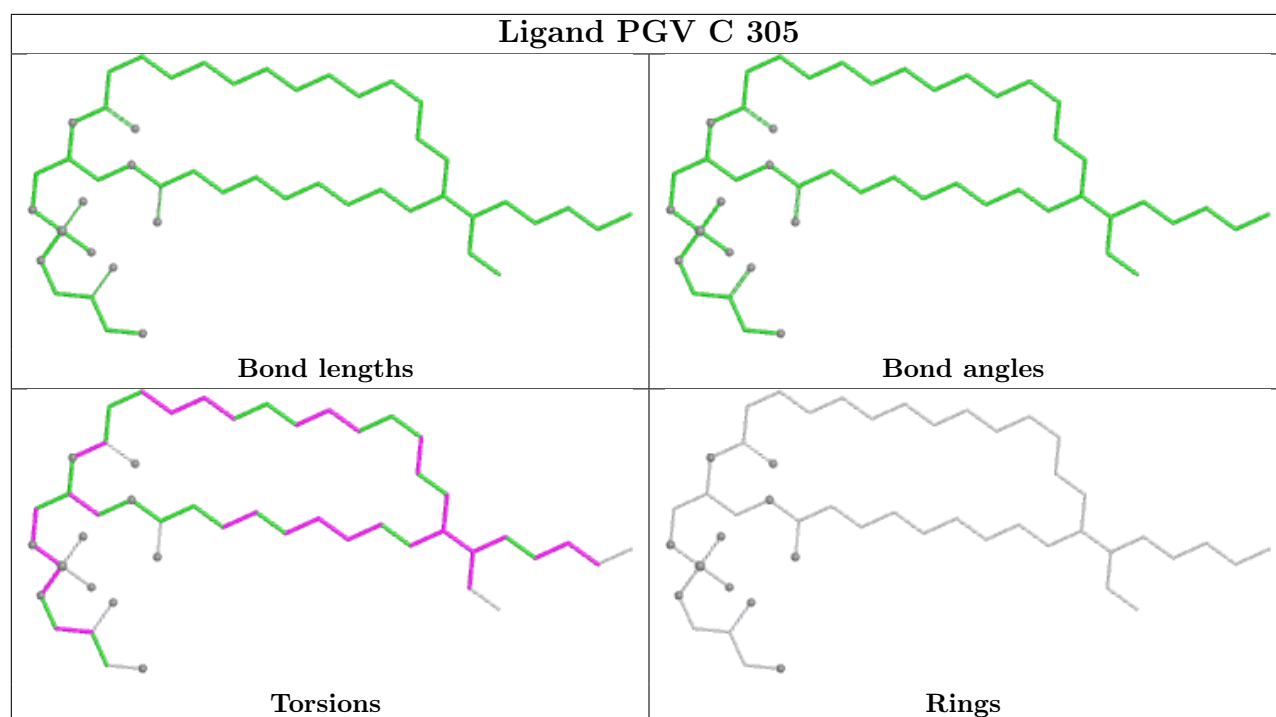
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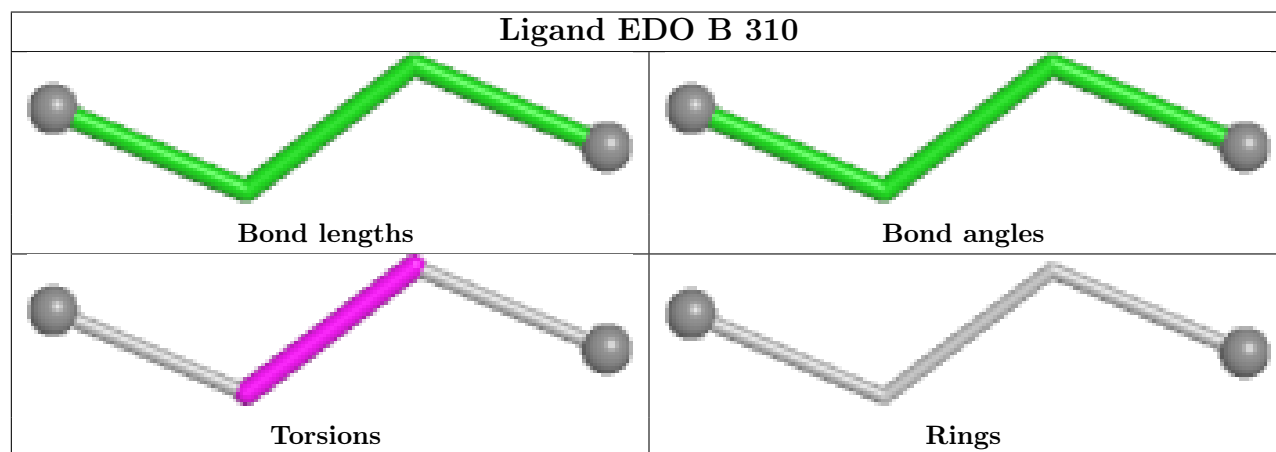
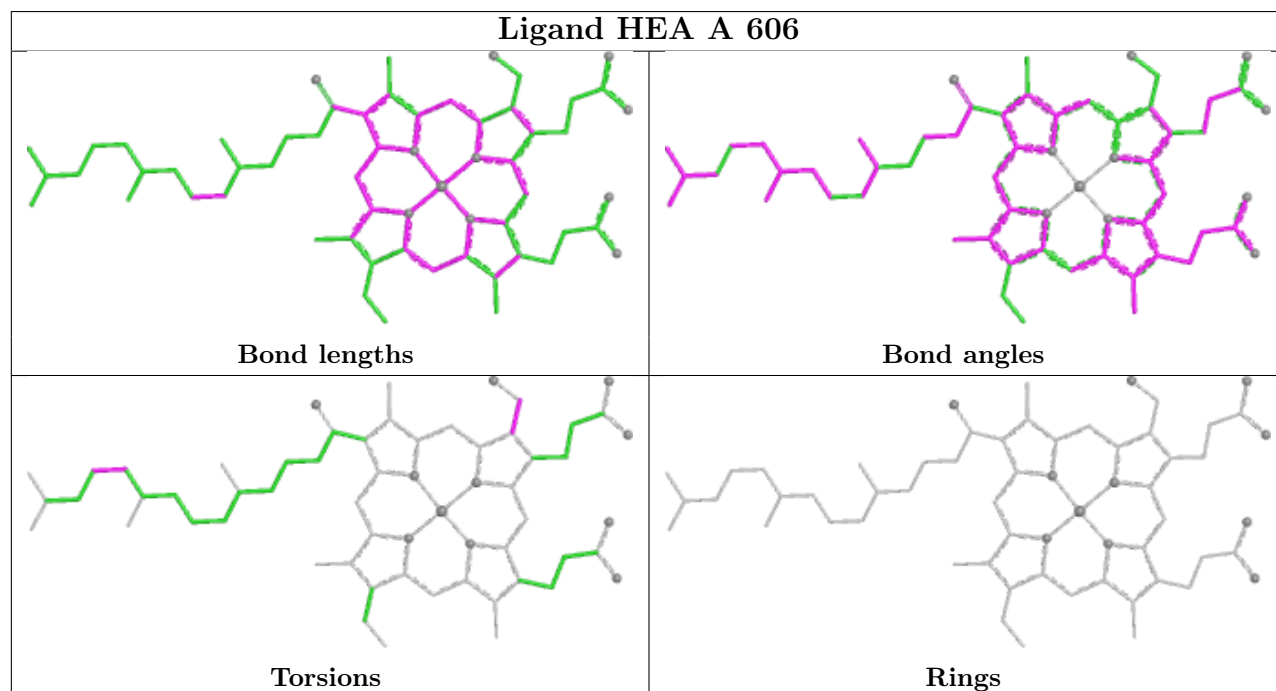
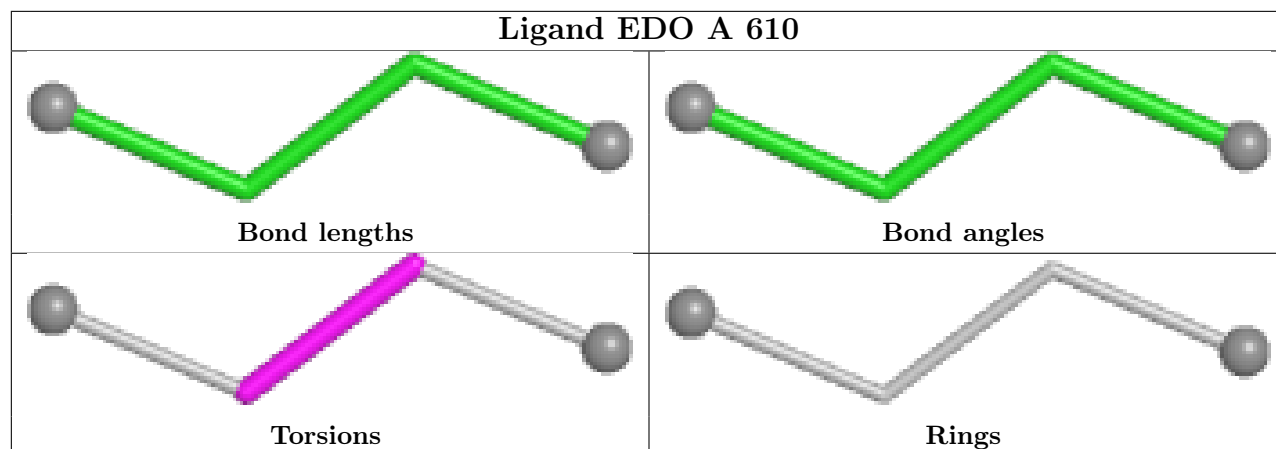


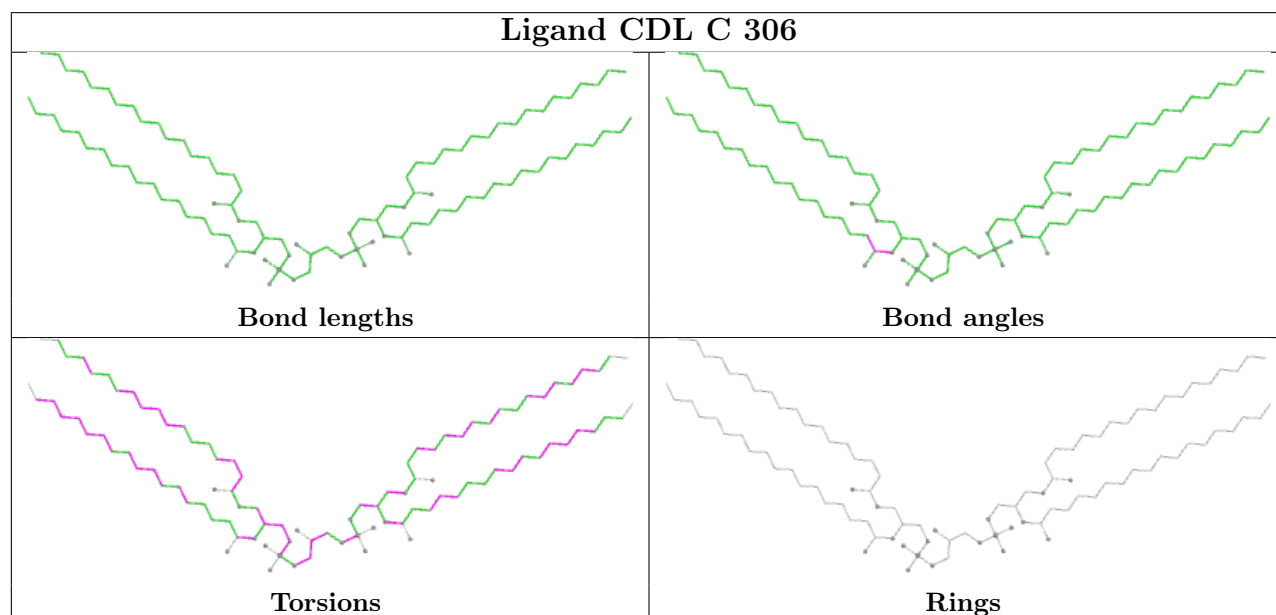
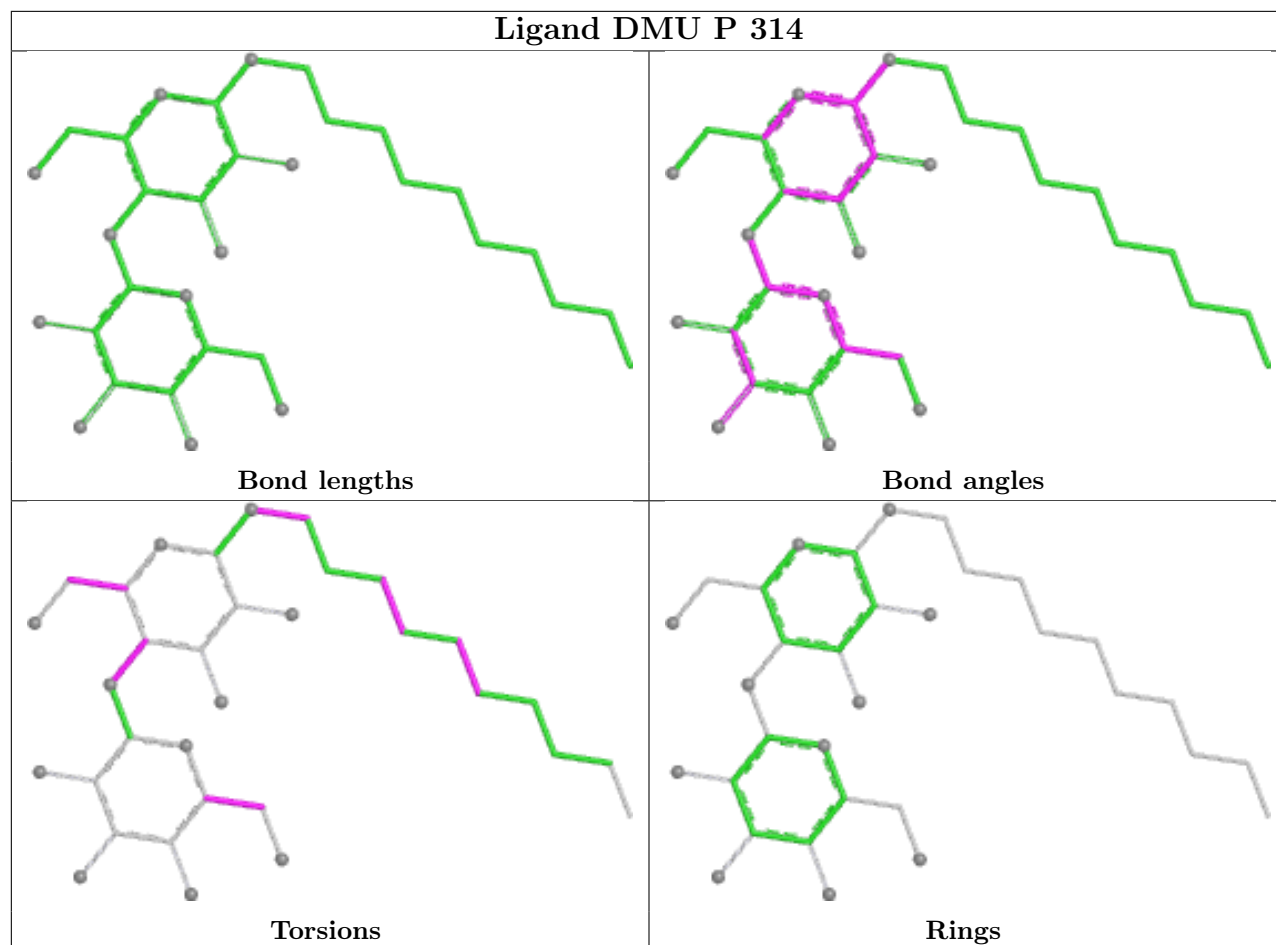


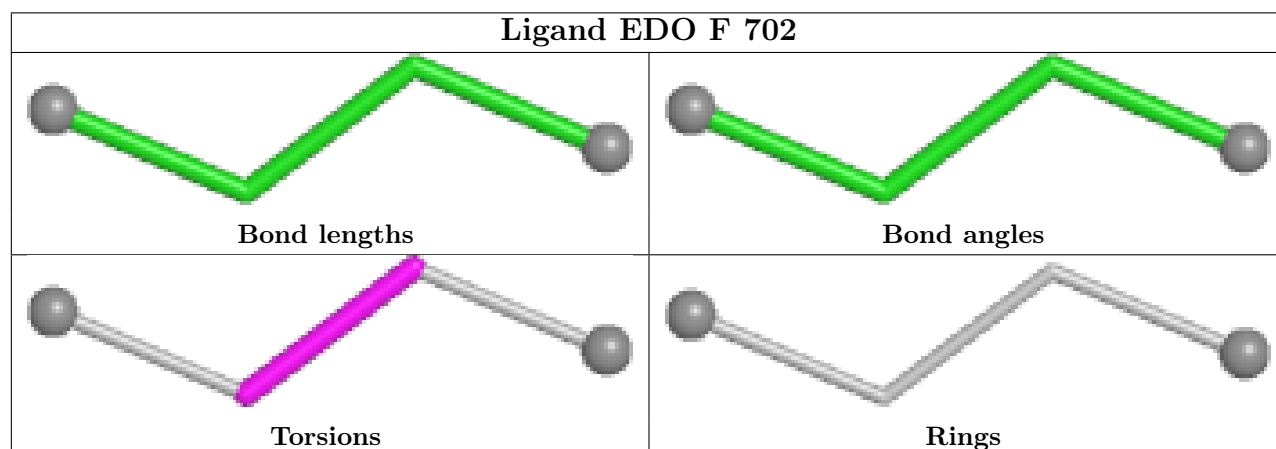
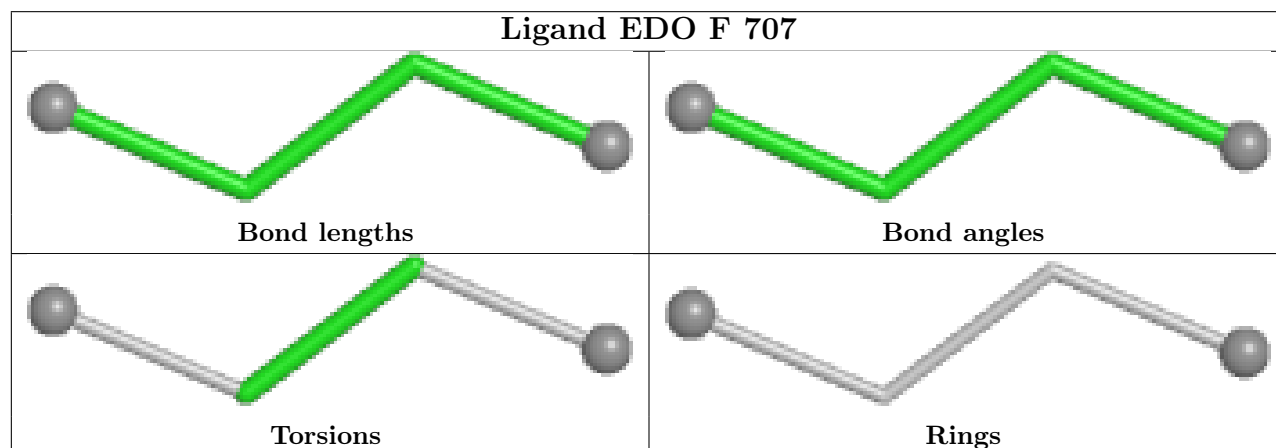
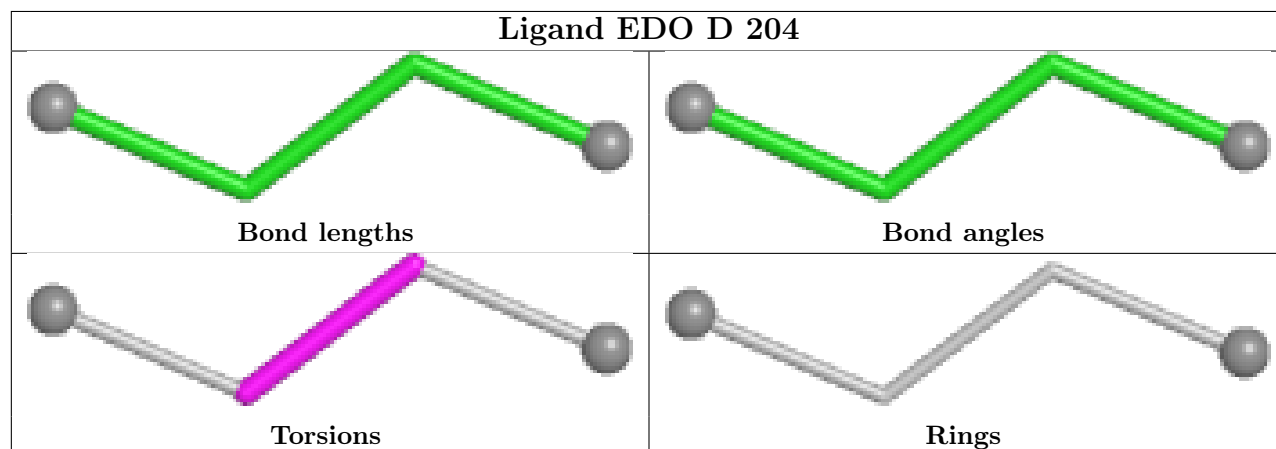
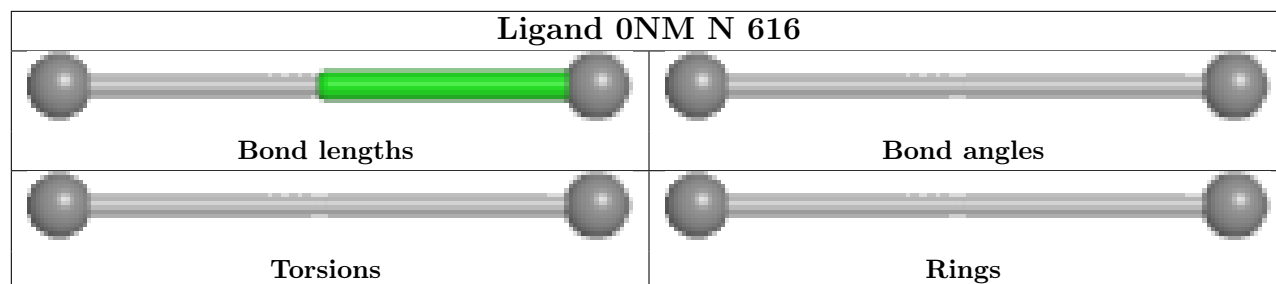


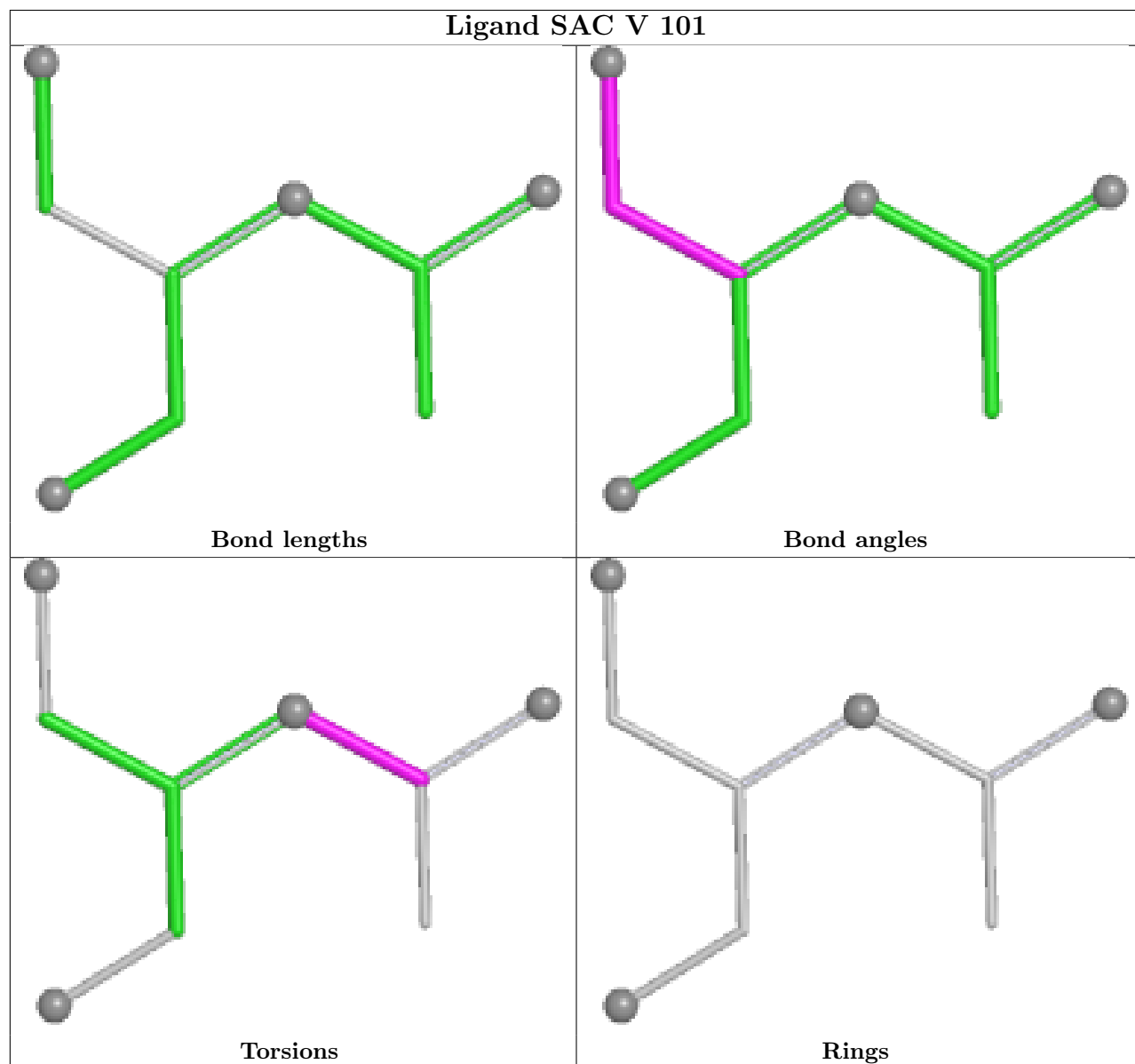
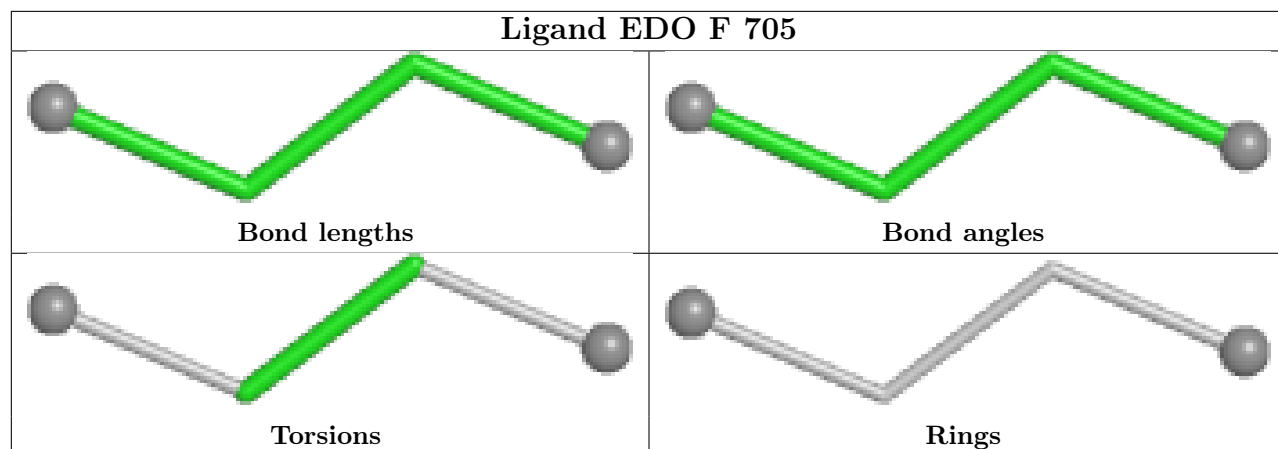


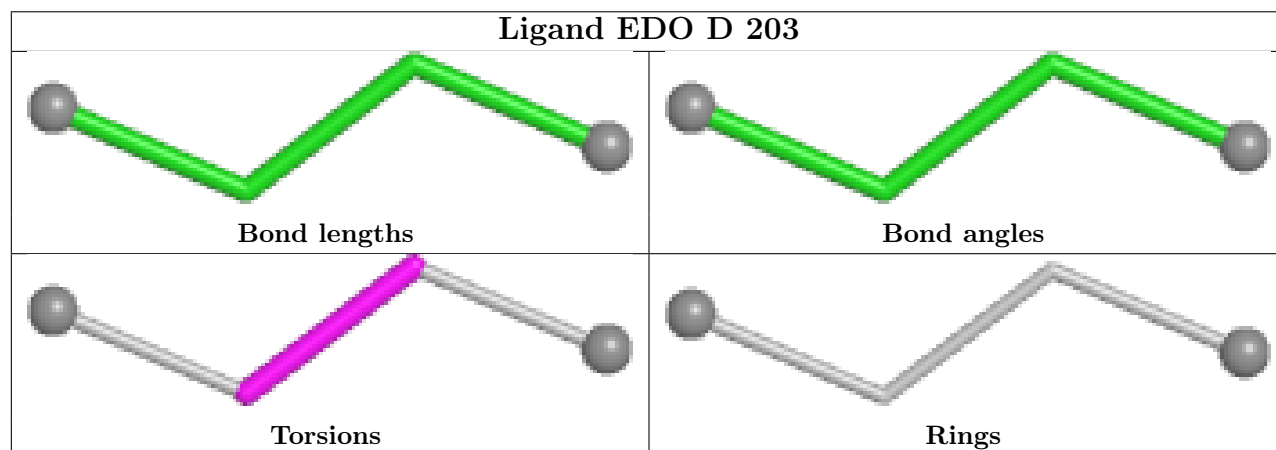
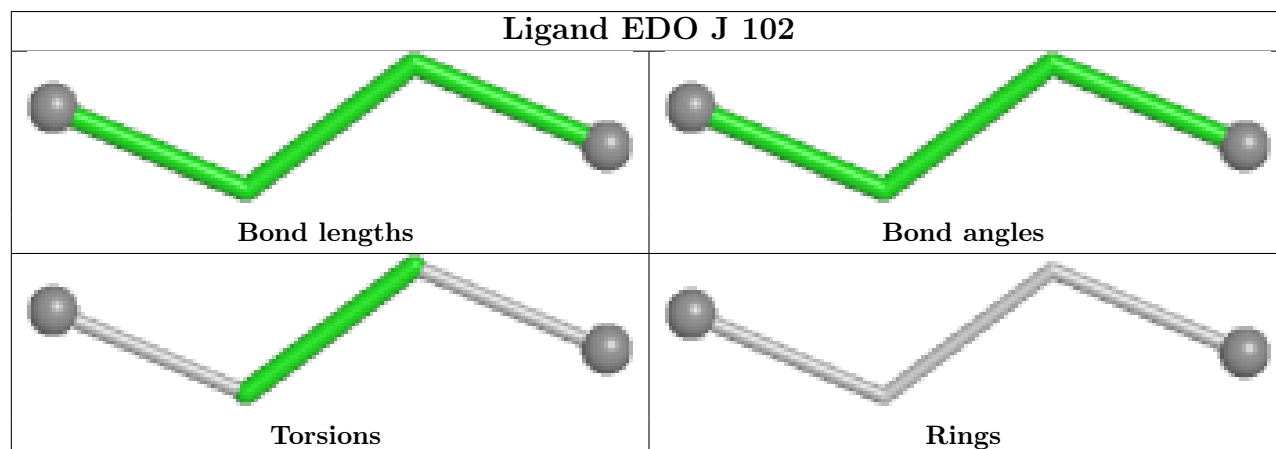
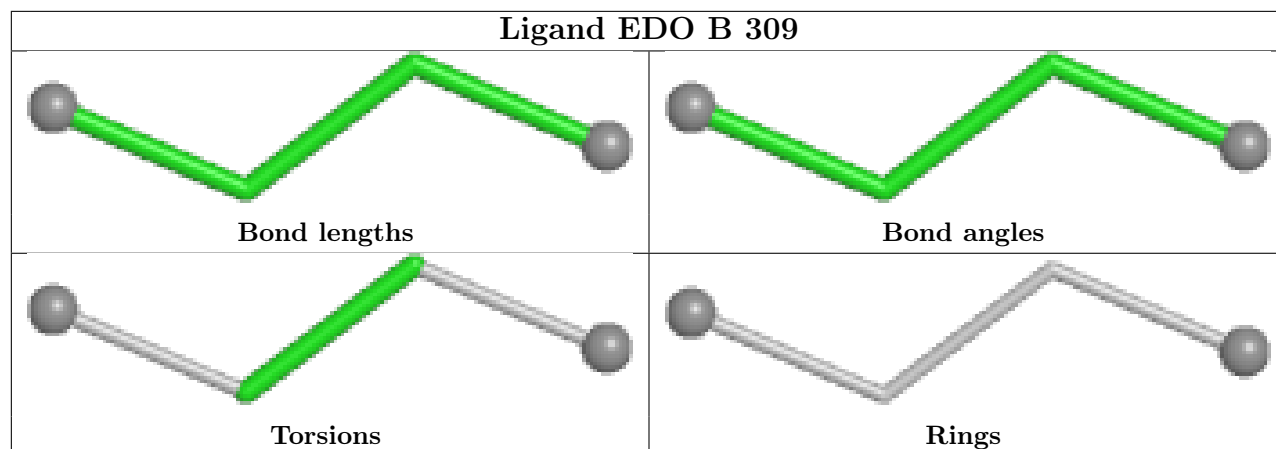


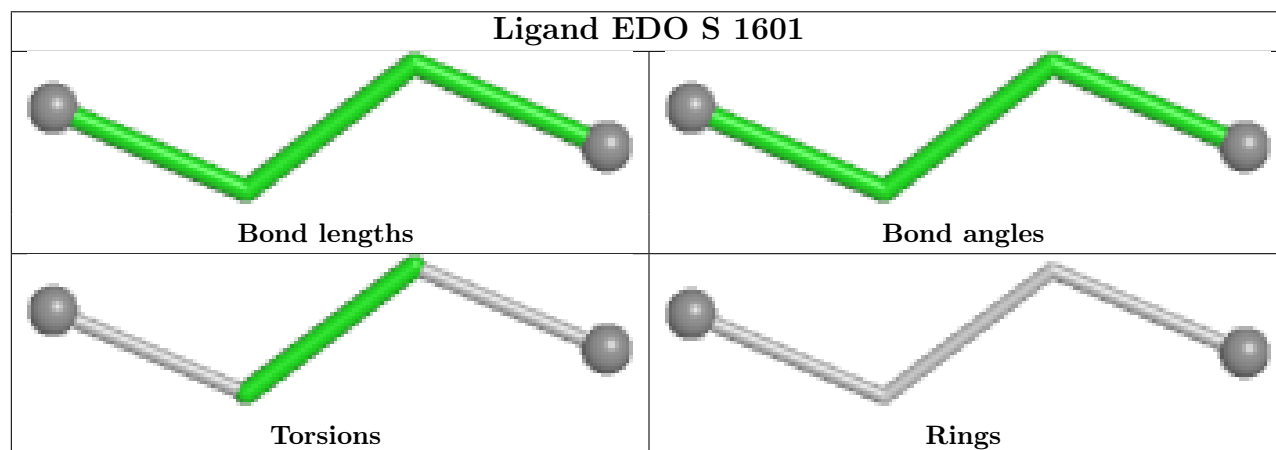
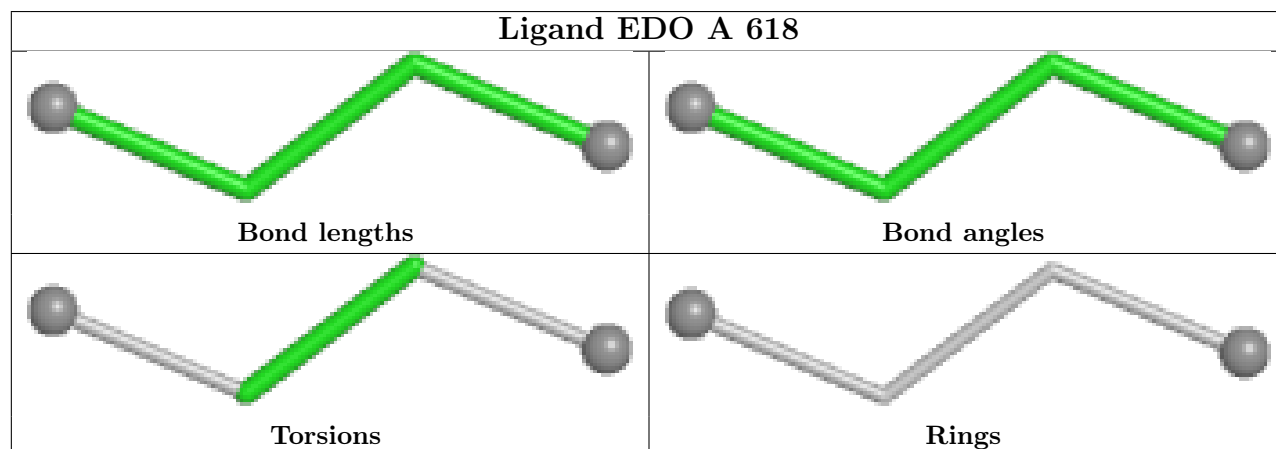
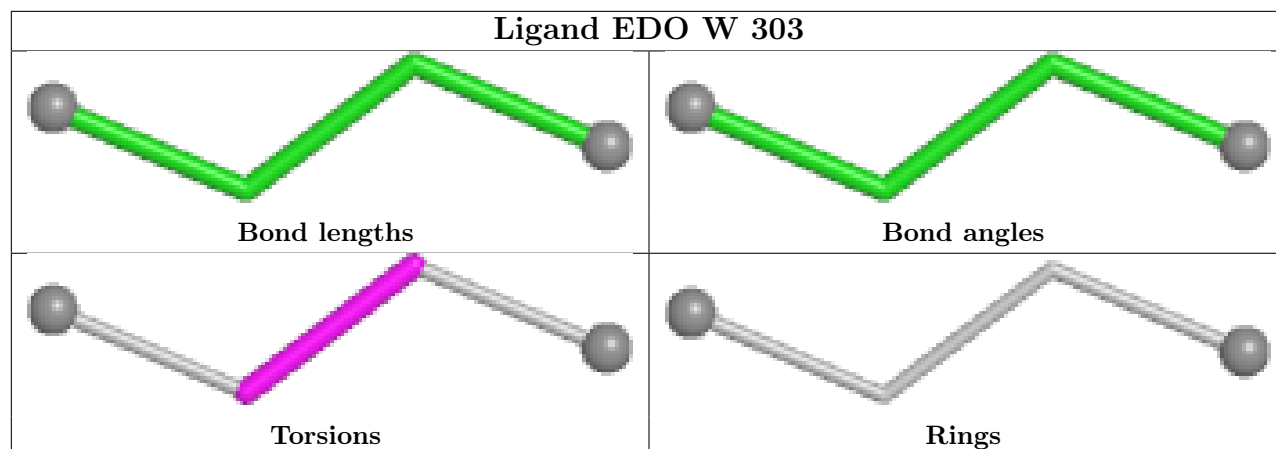




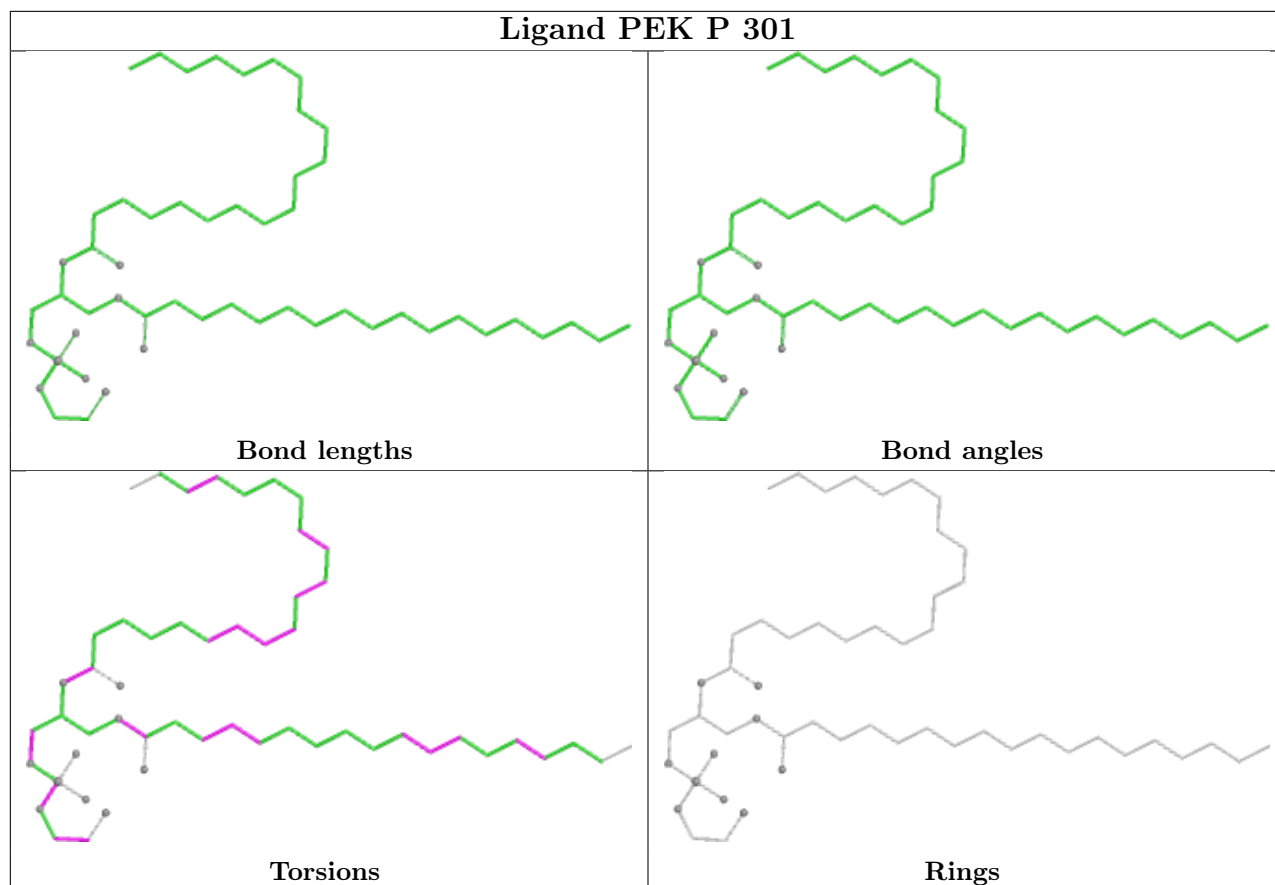




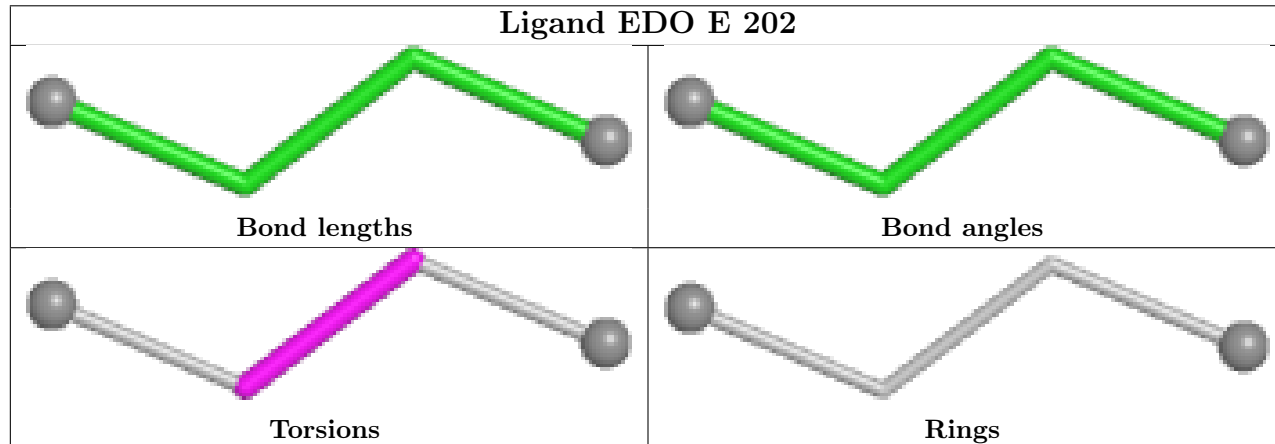


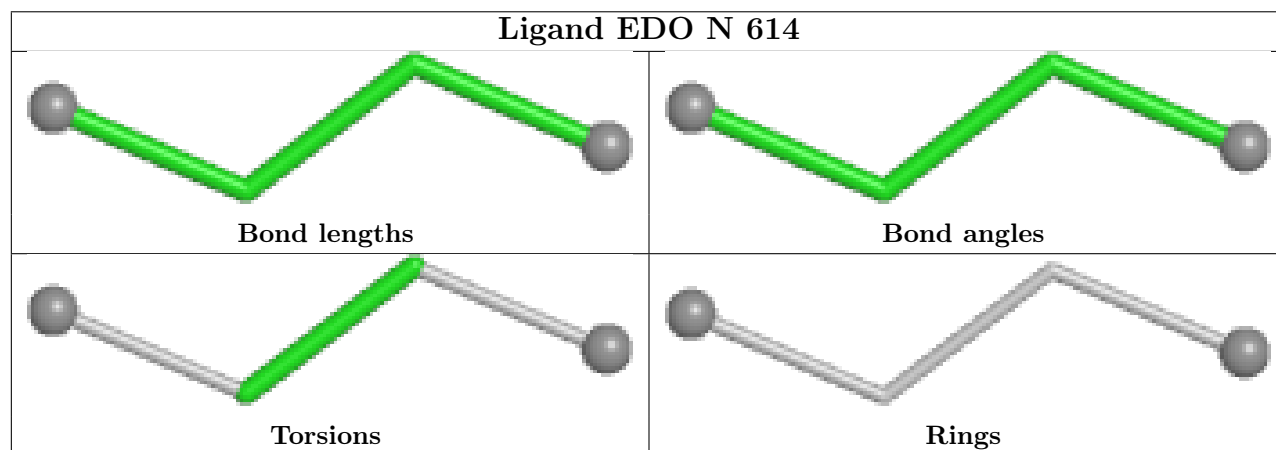
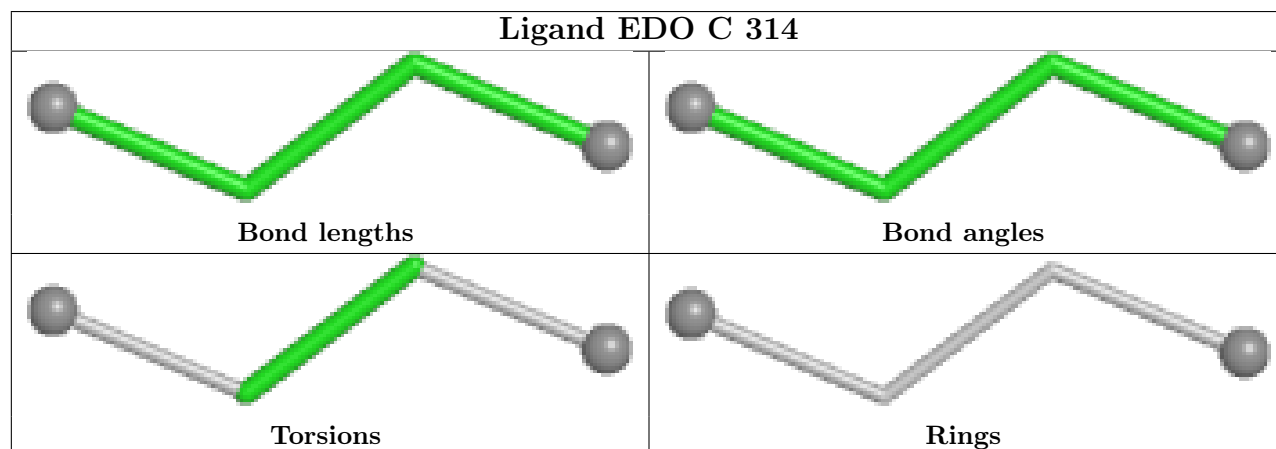
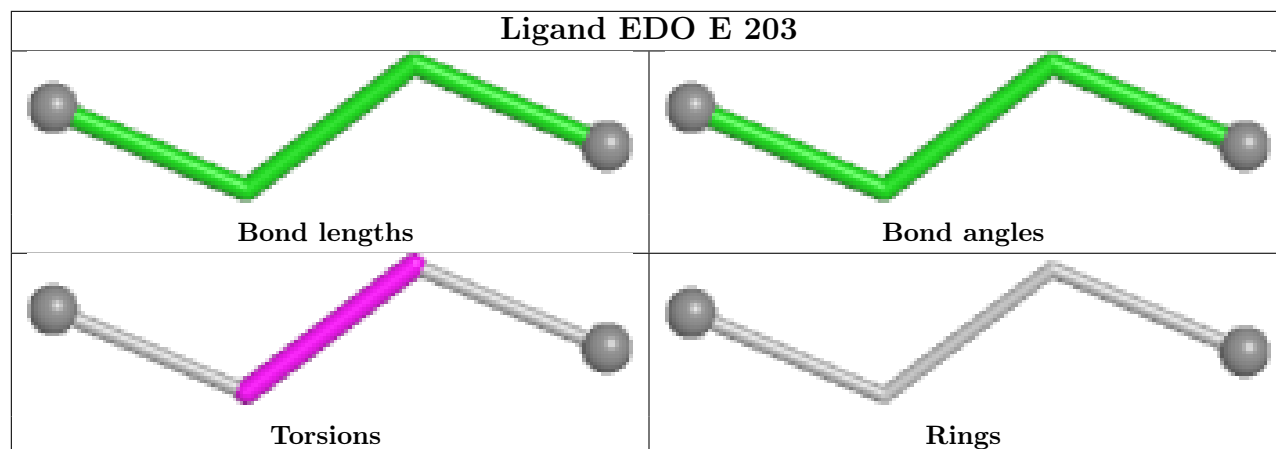


Ligand PEK P 301

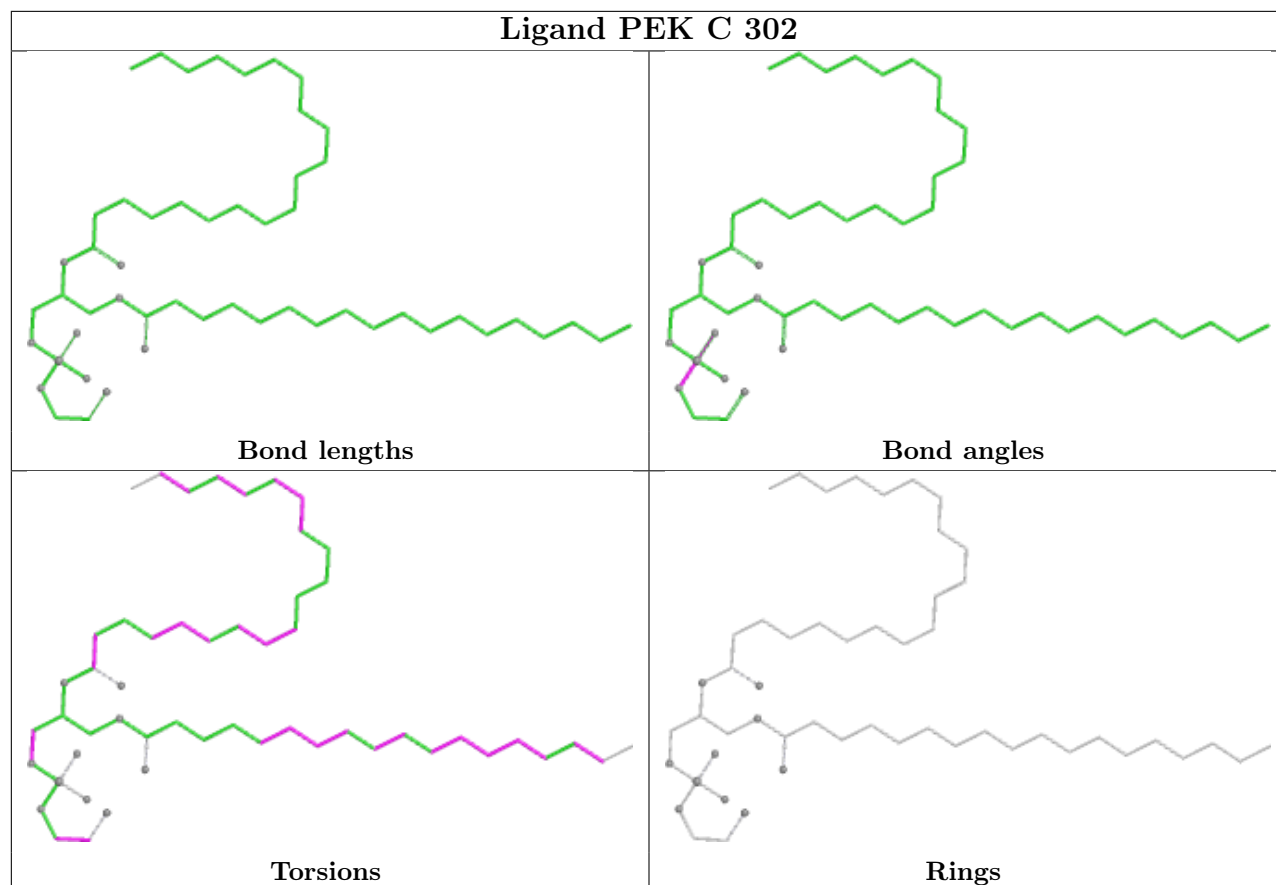


Ligand EDO E 202

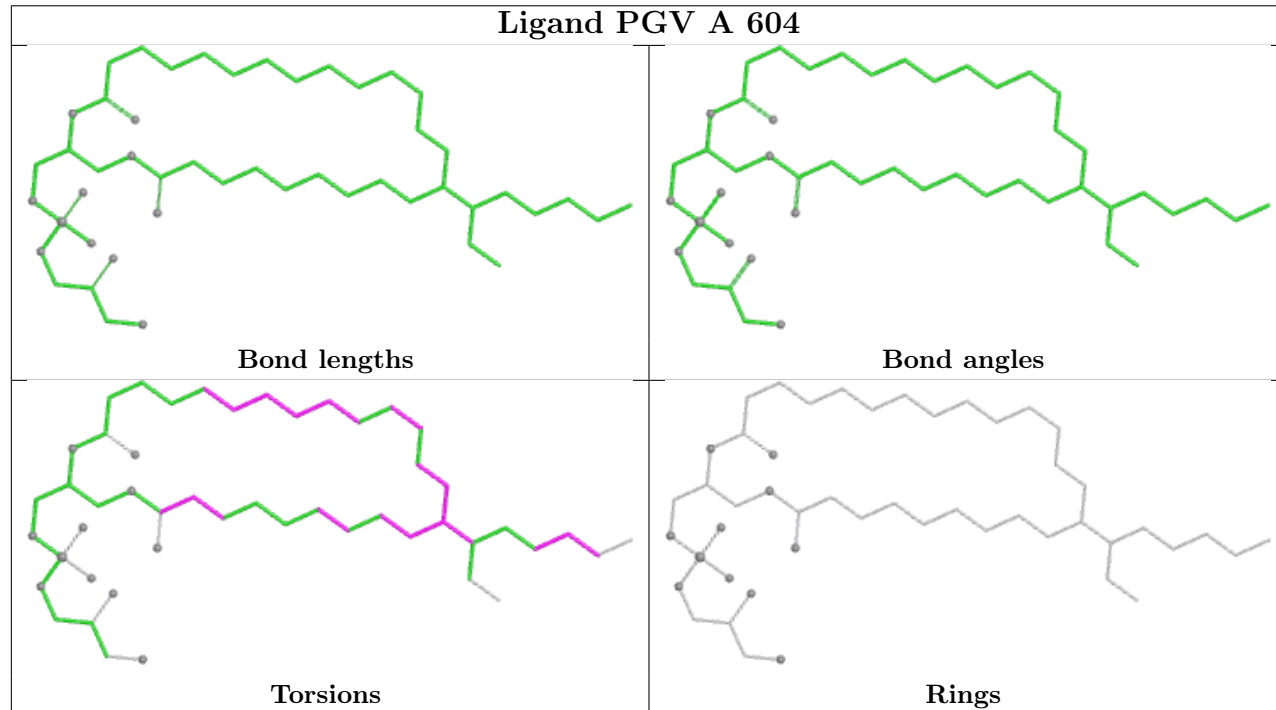


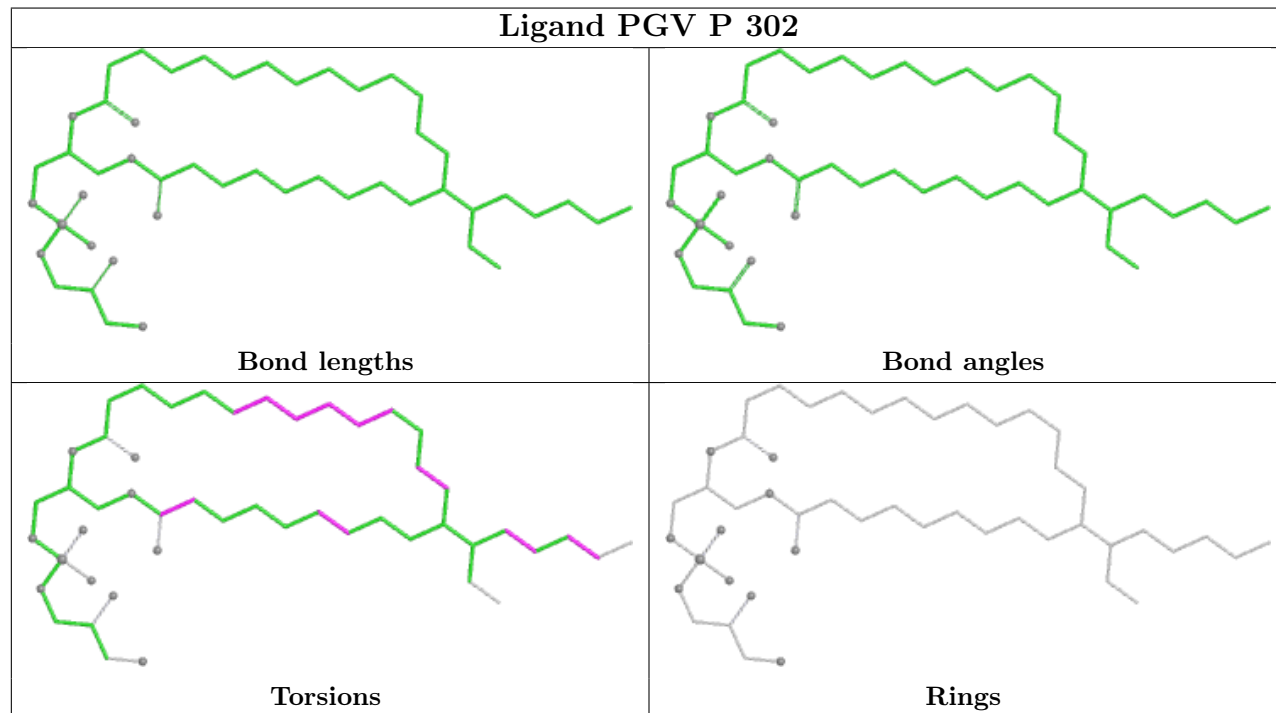
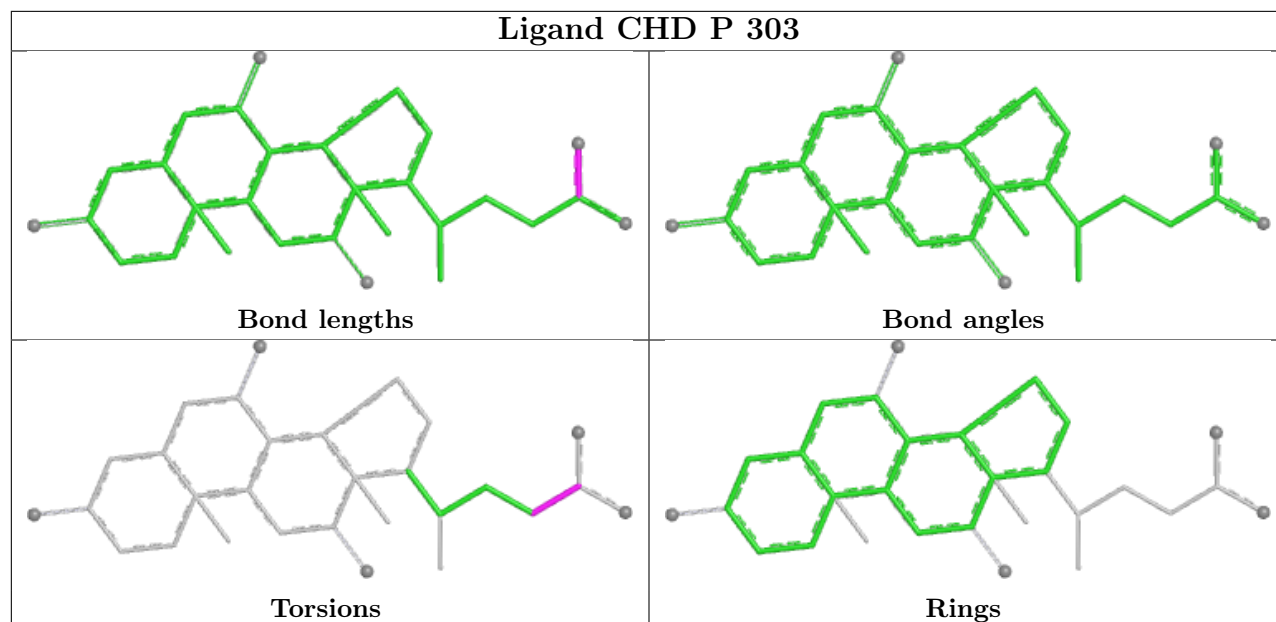


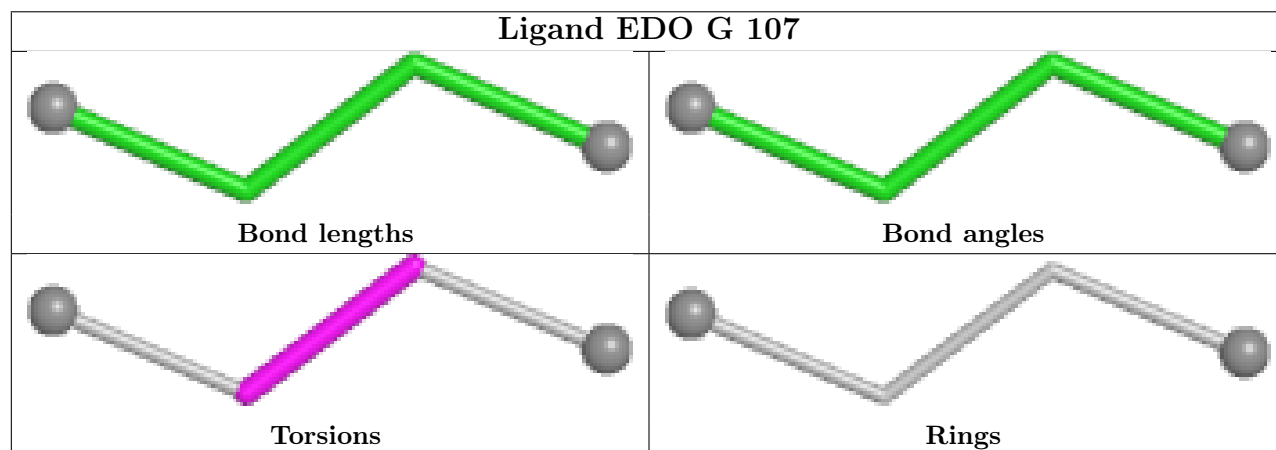
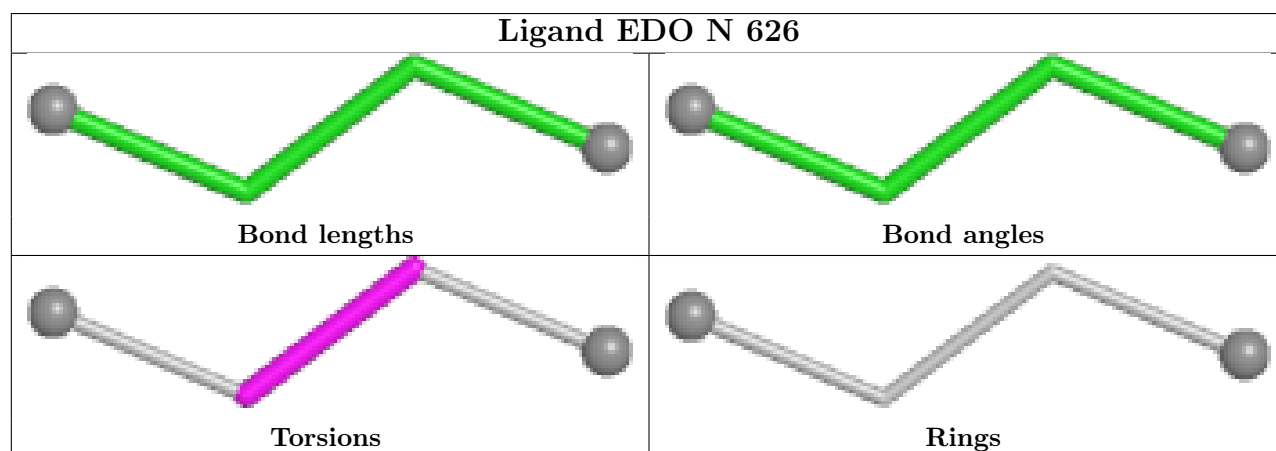
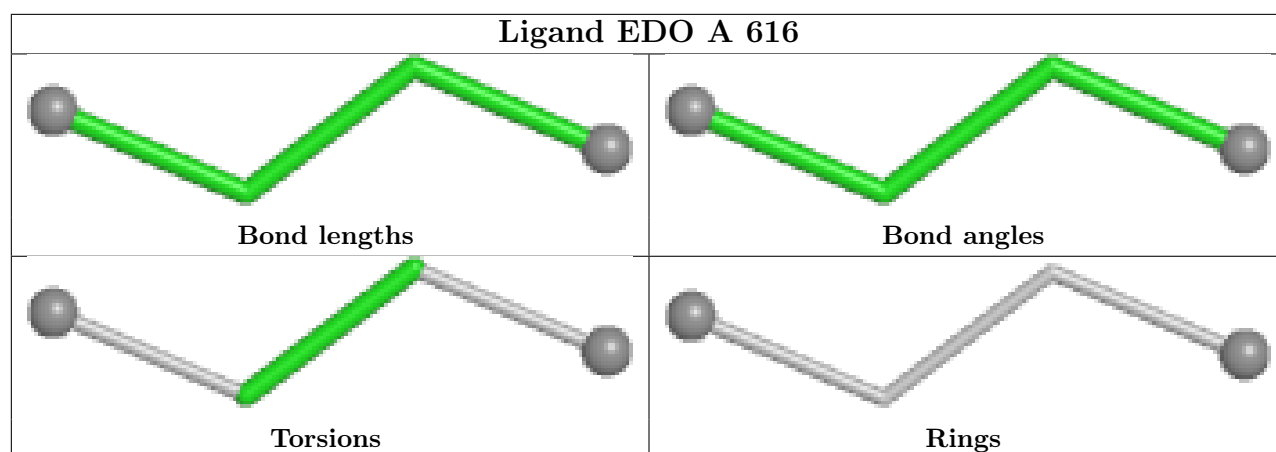
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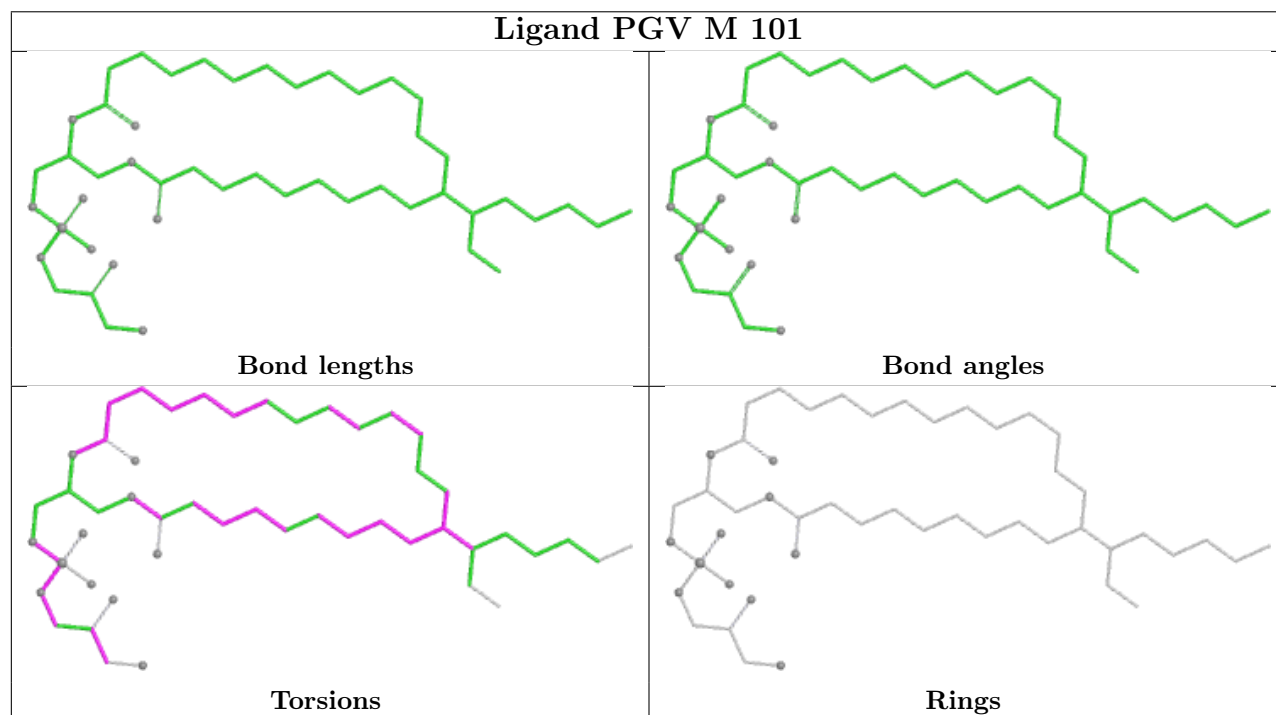
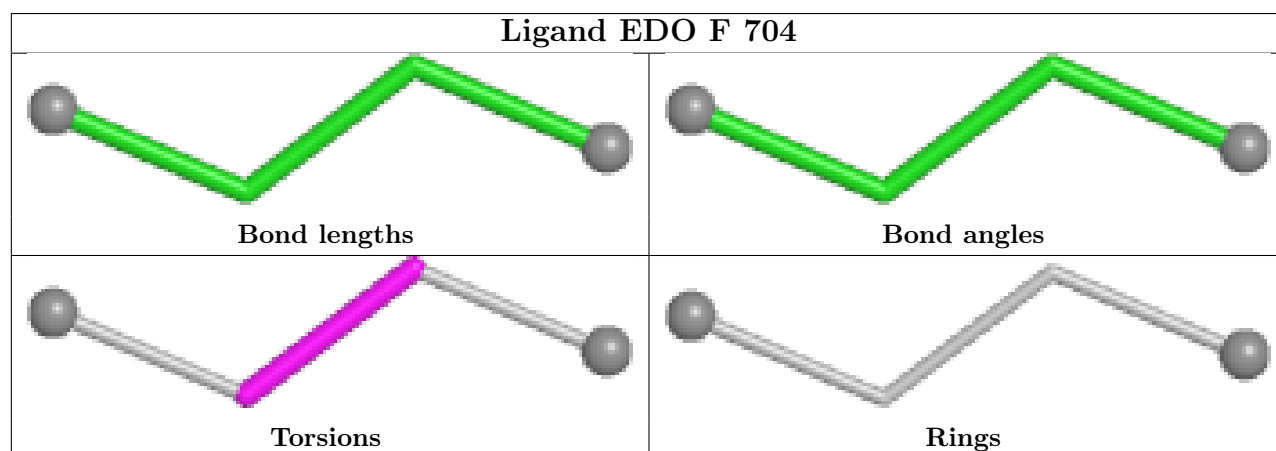
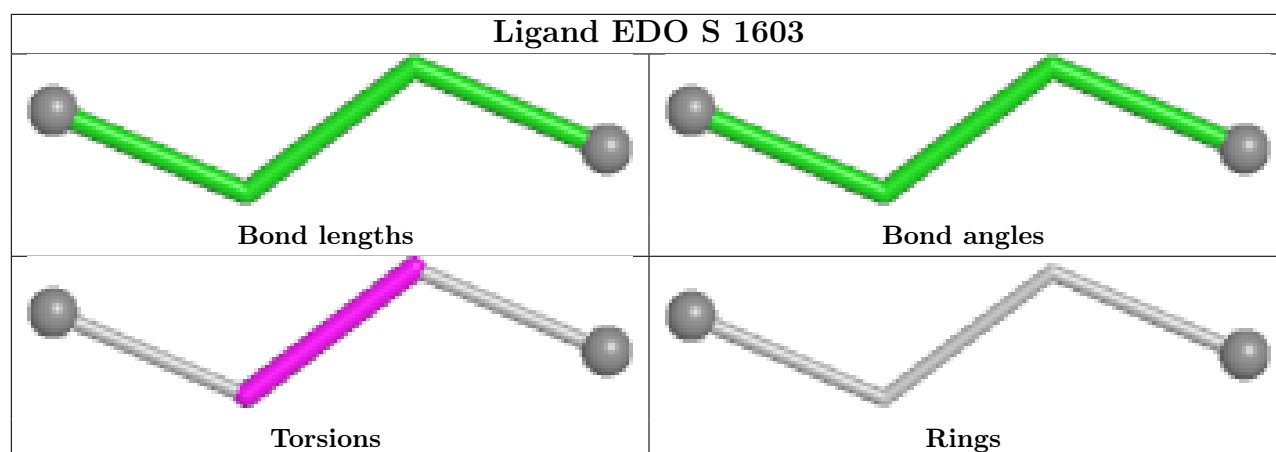


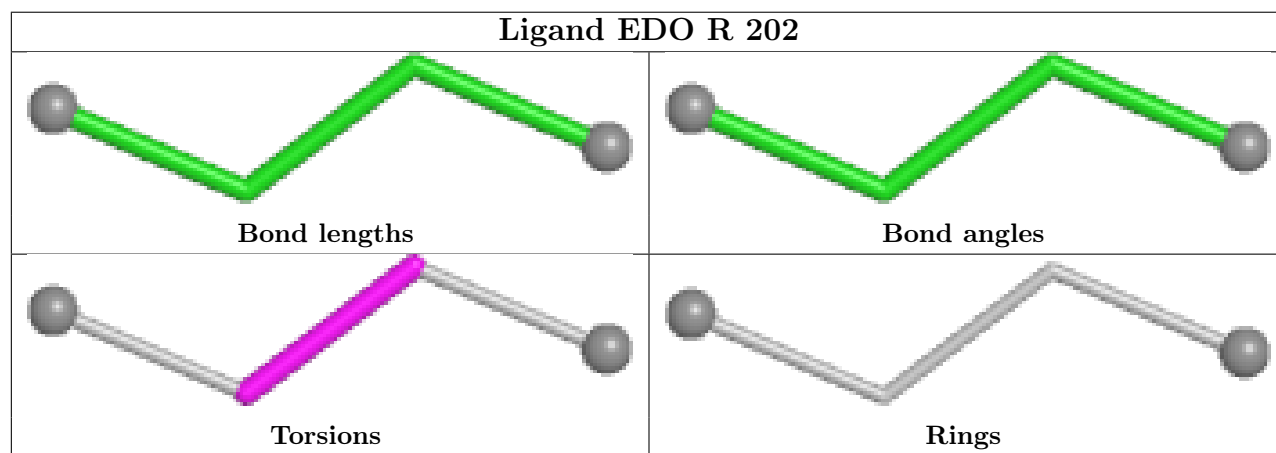
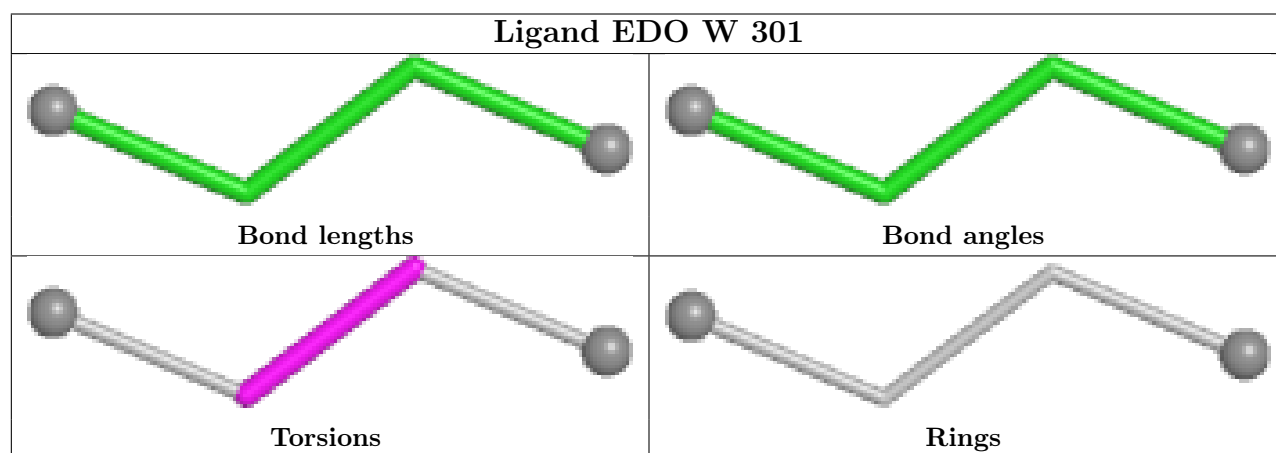
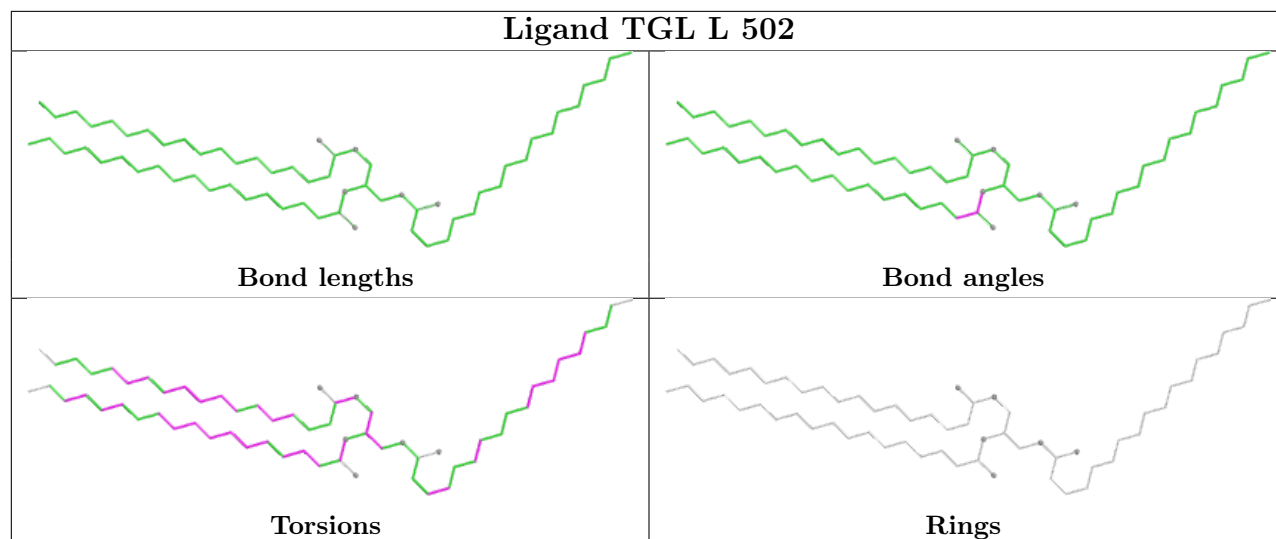
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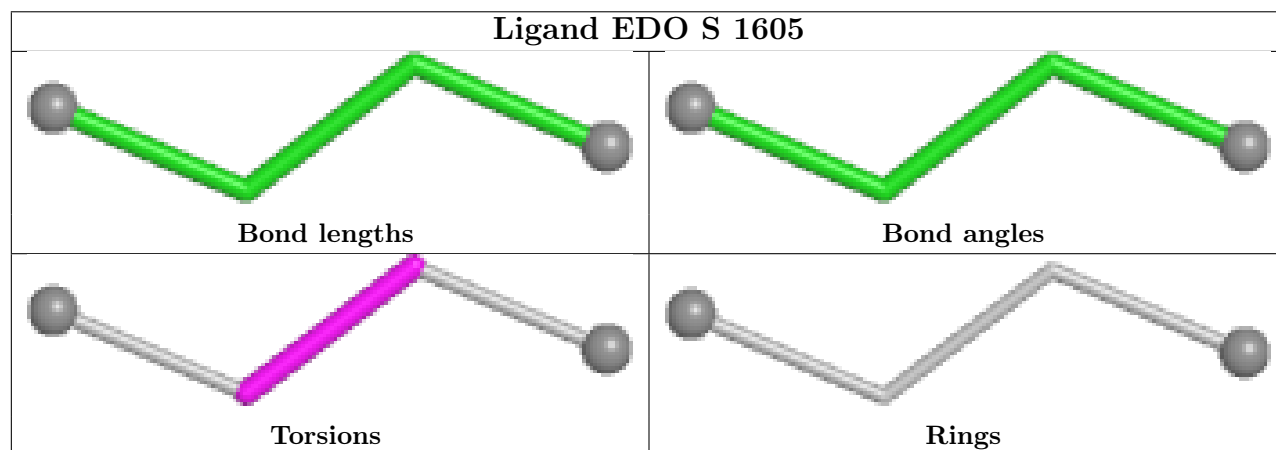
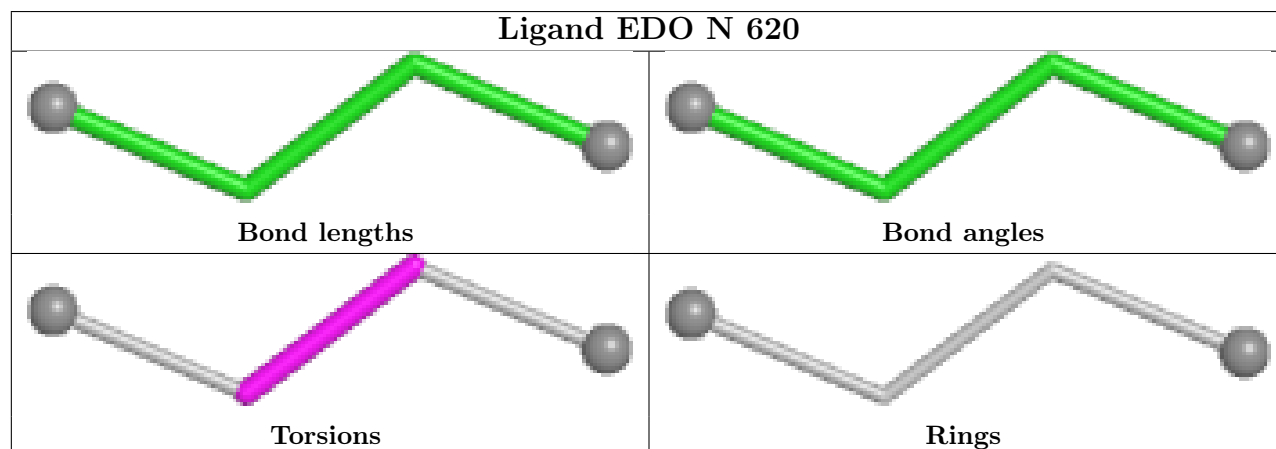
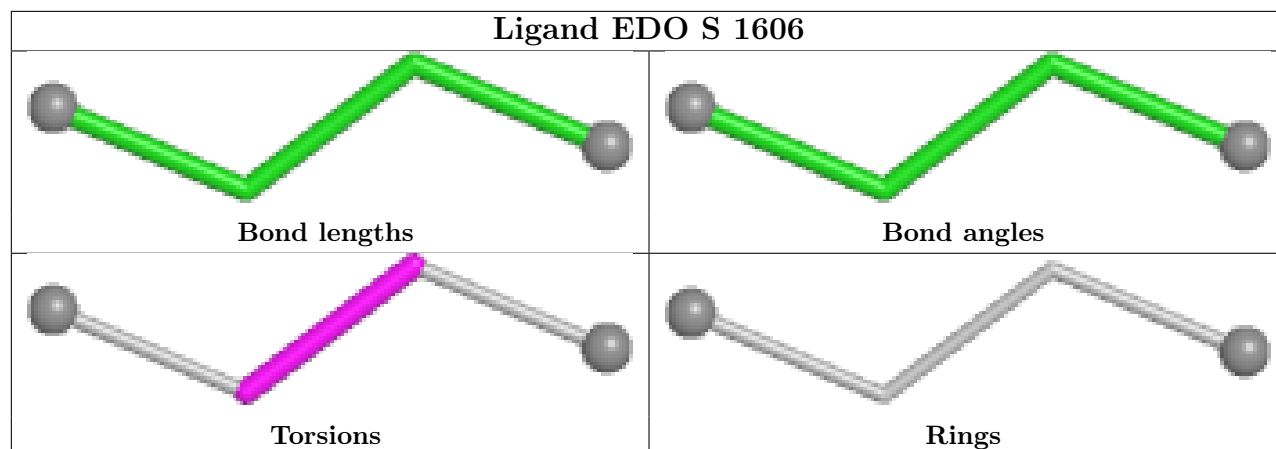


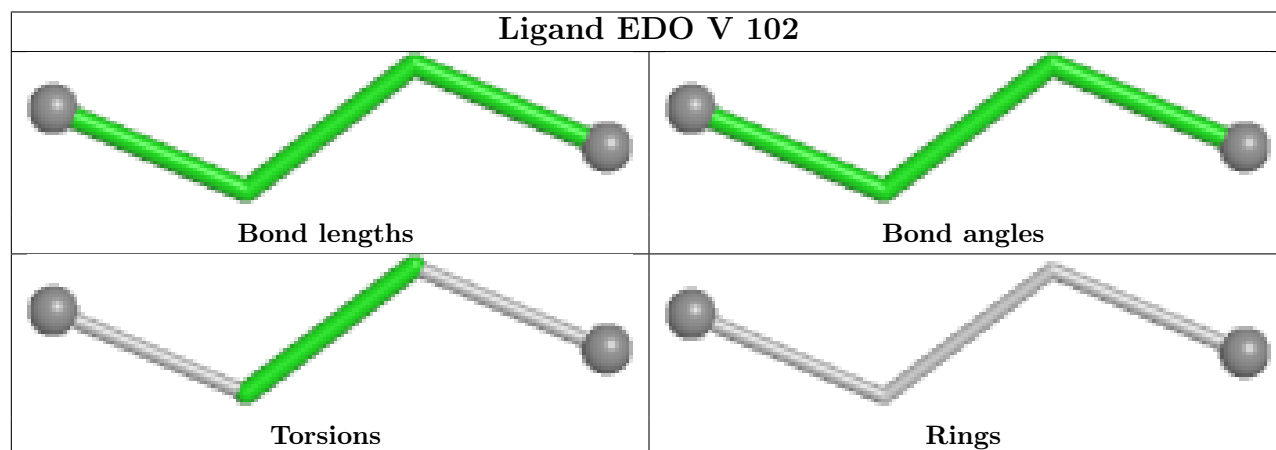
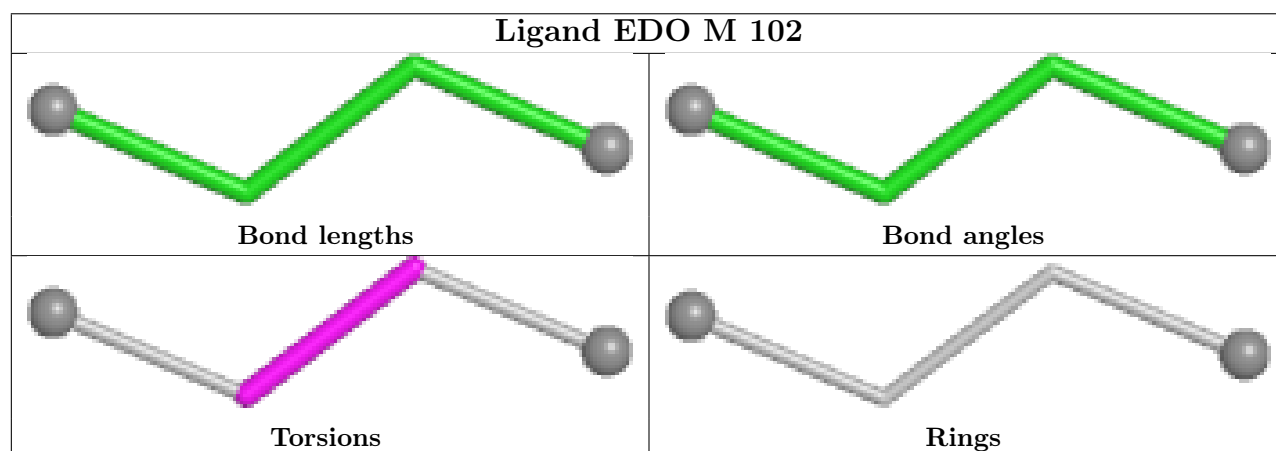
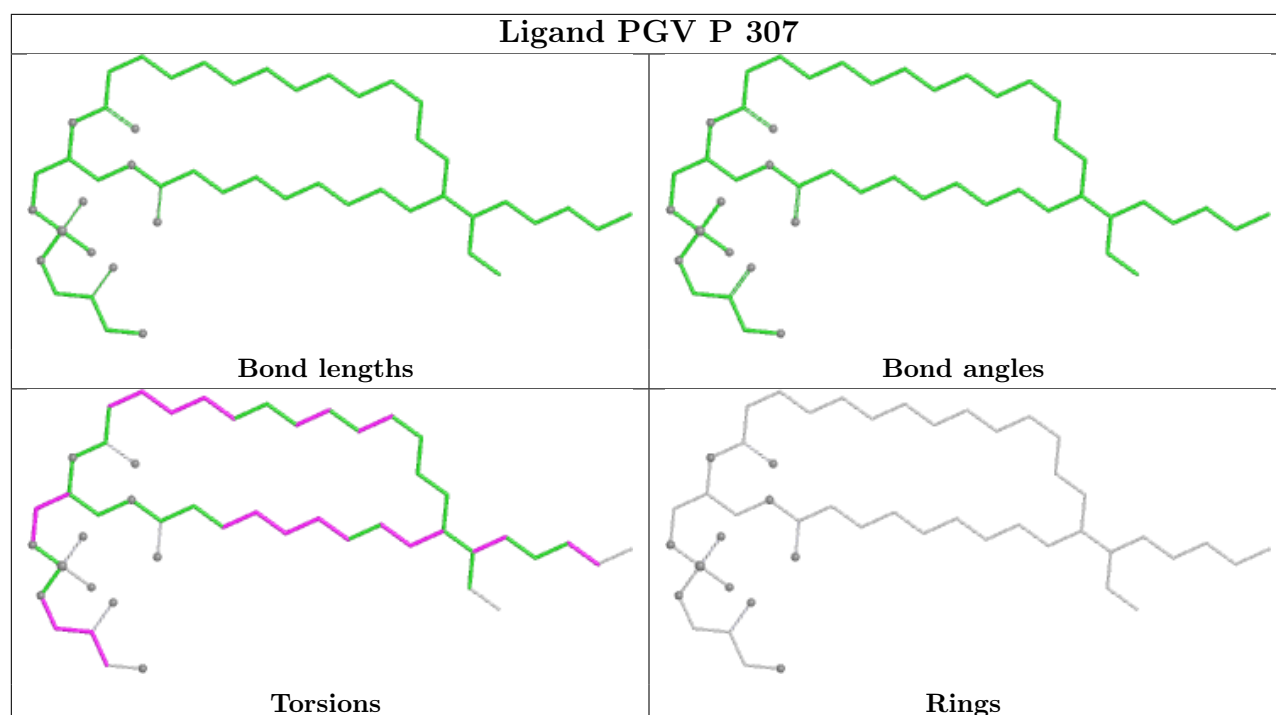


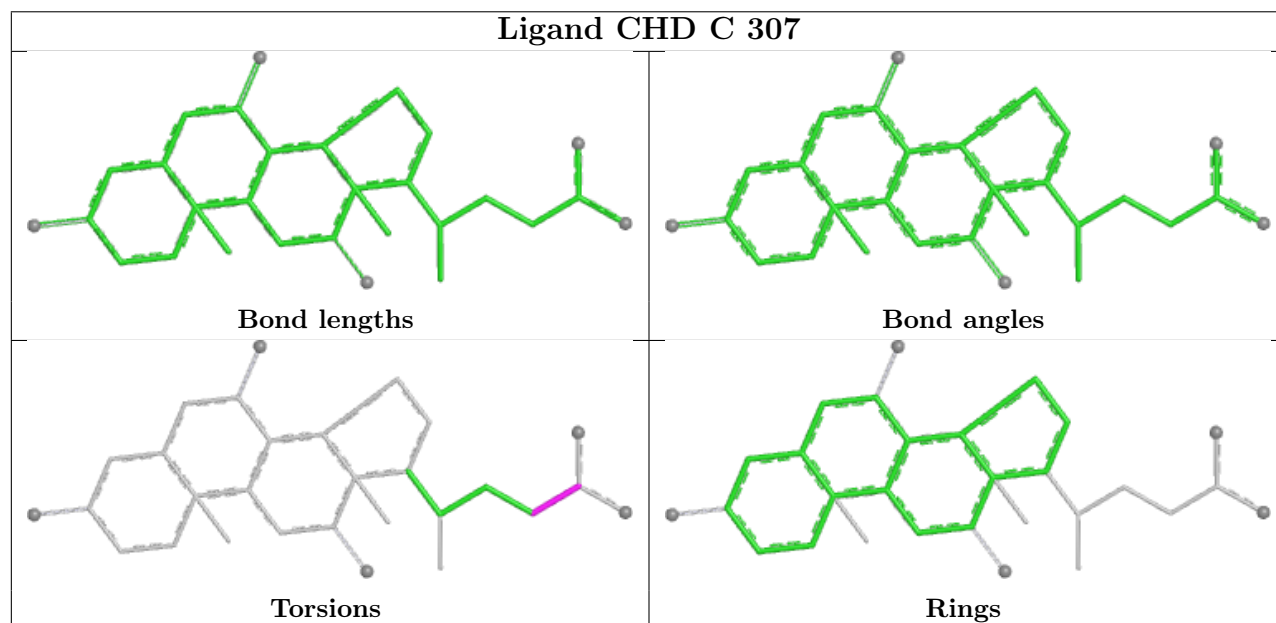
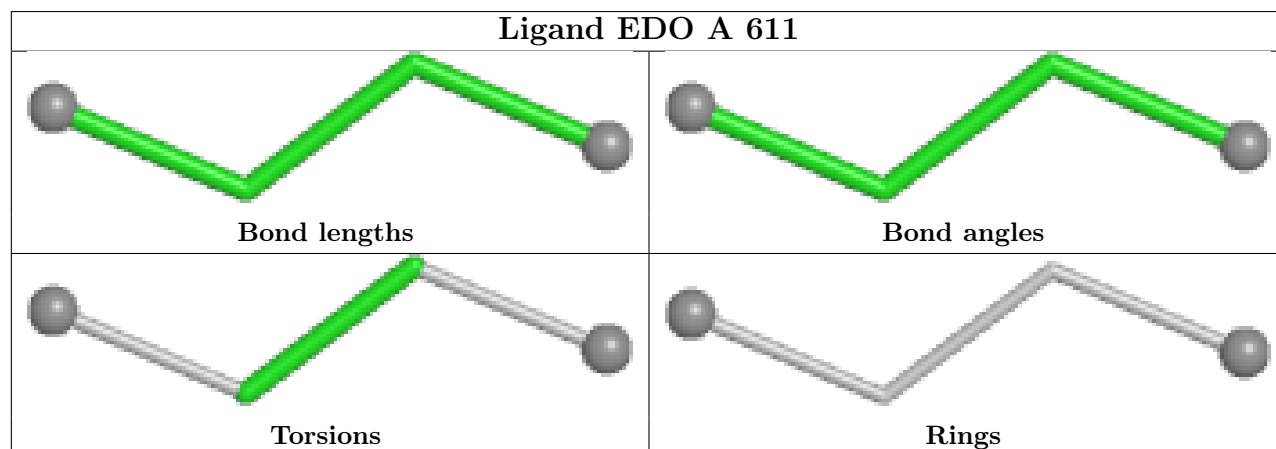
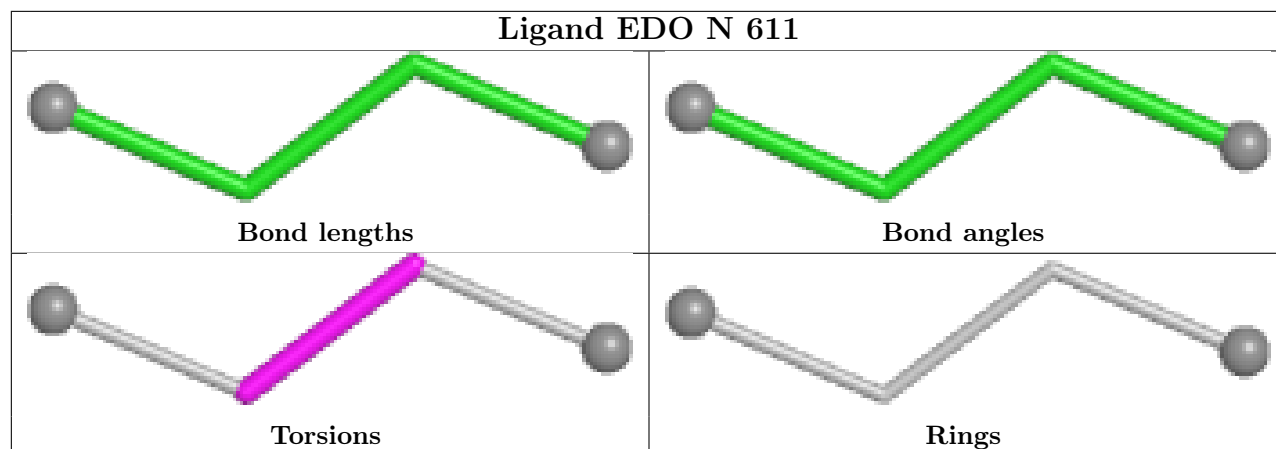


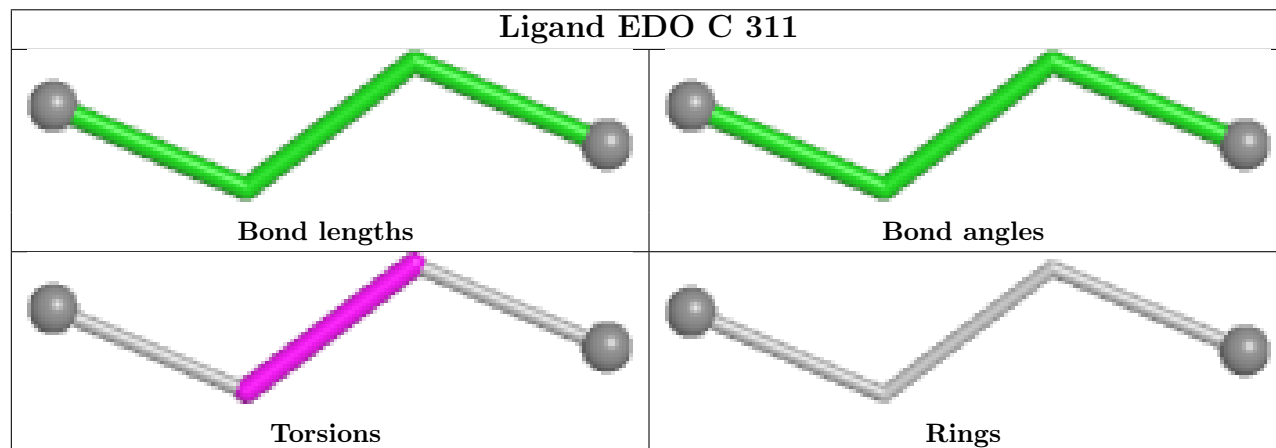
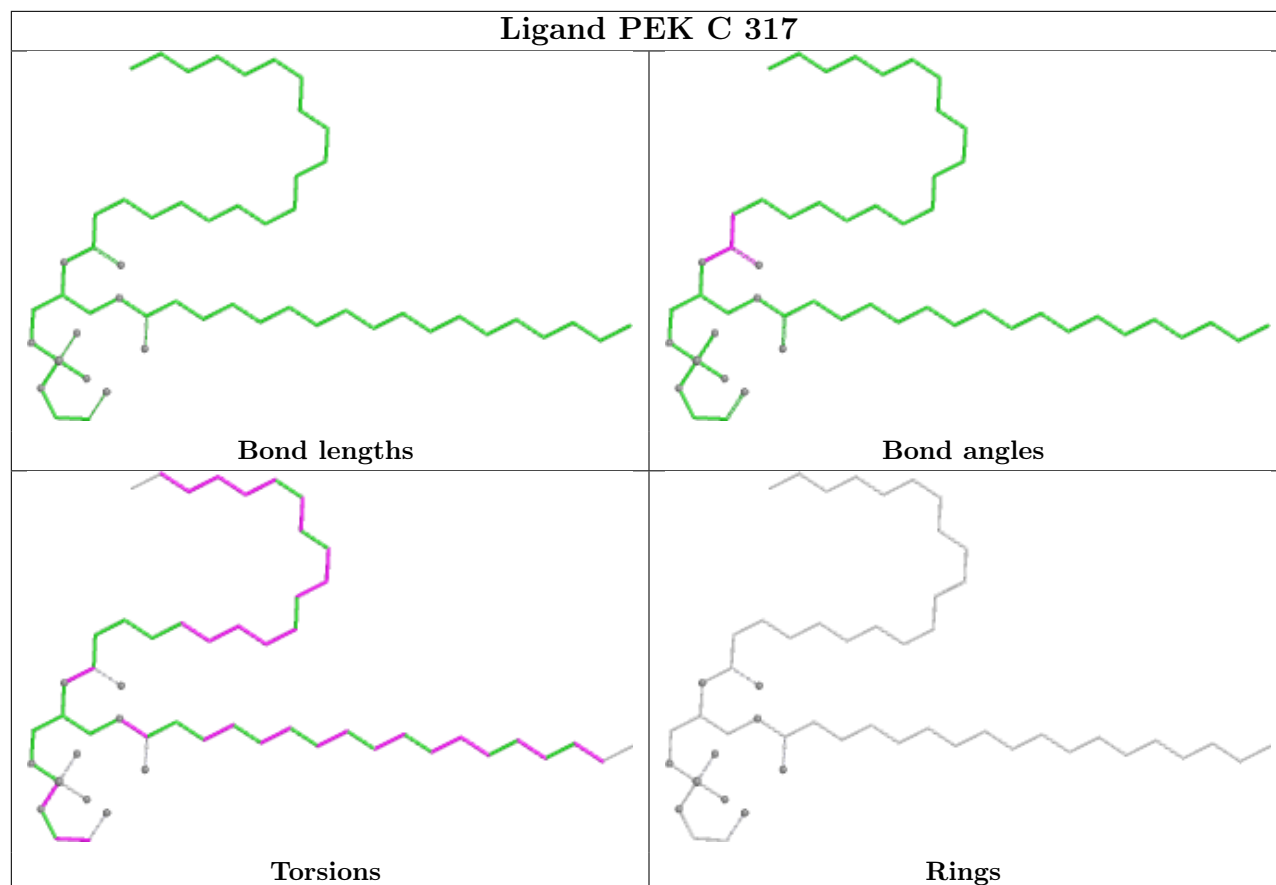


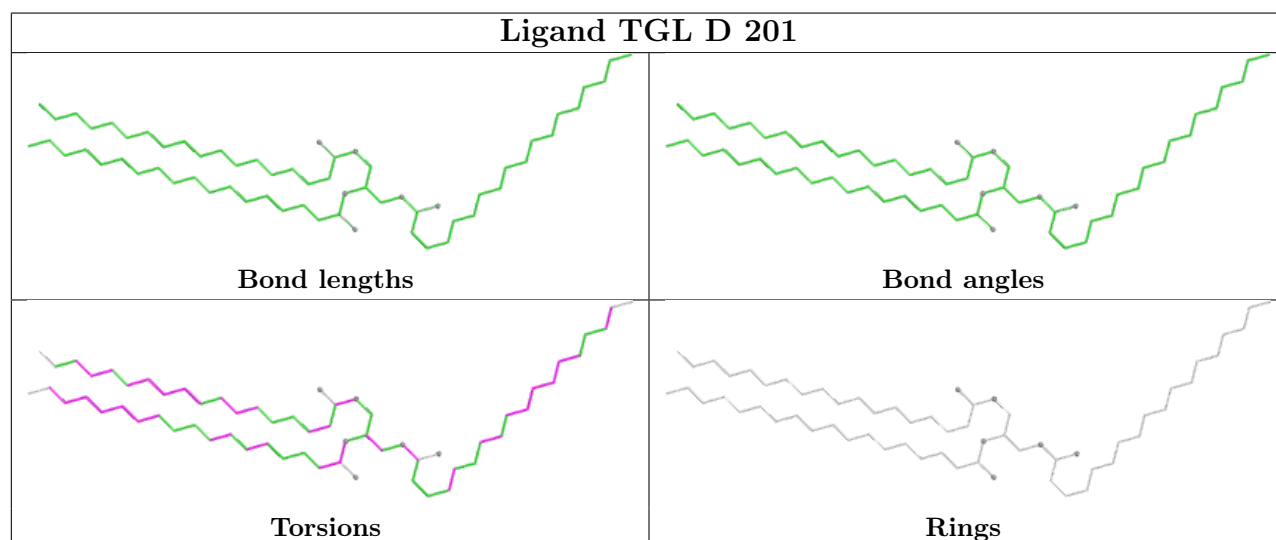
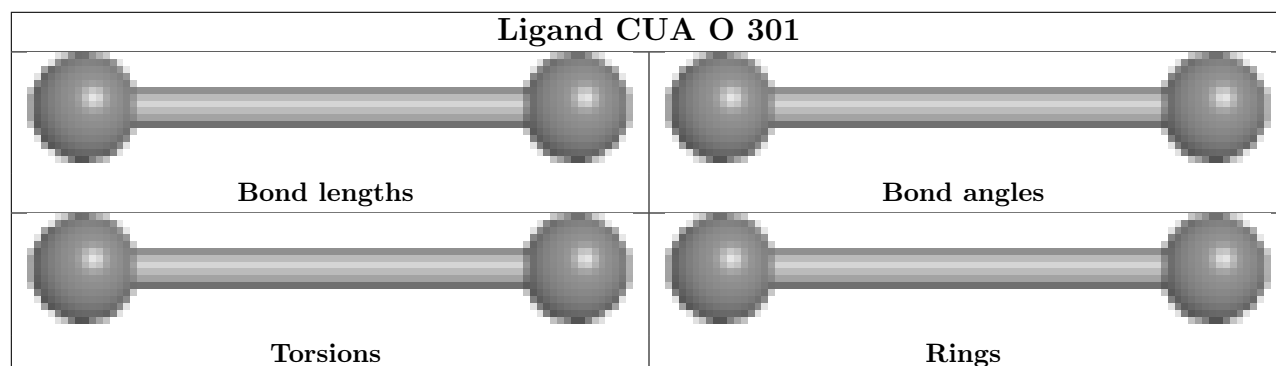
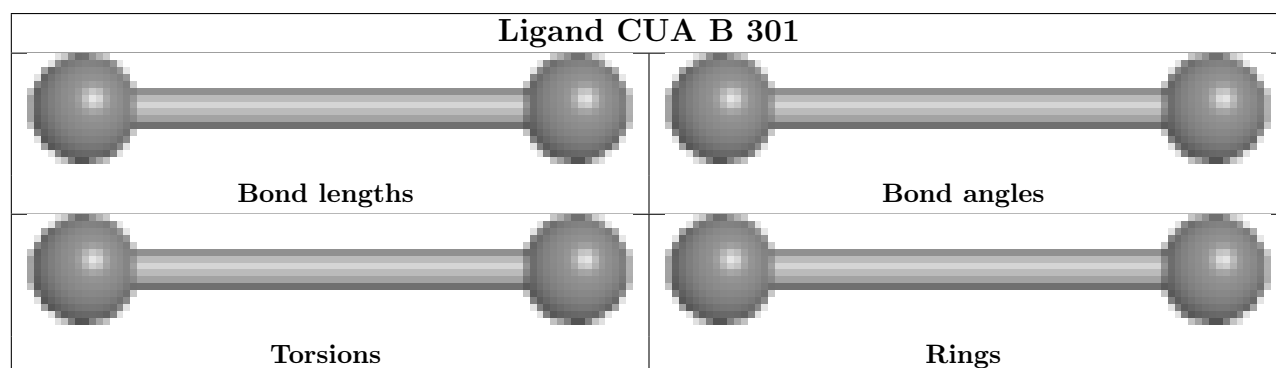
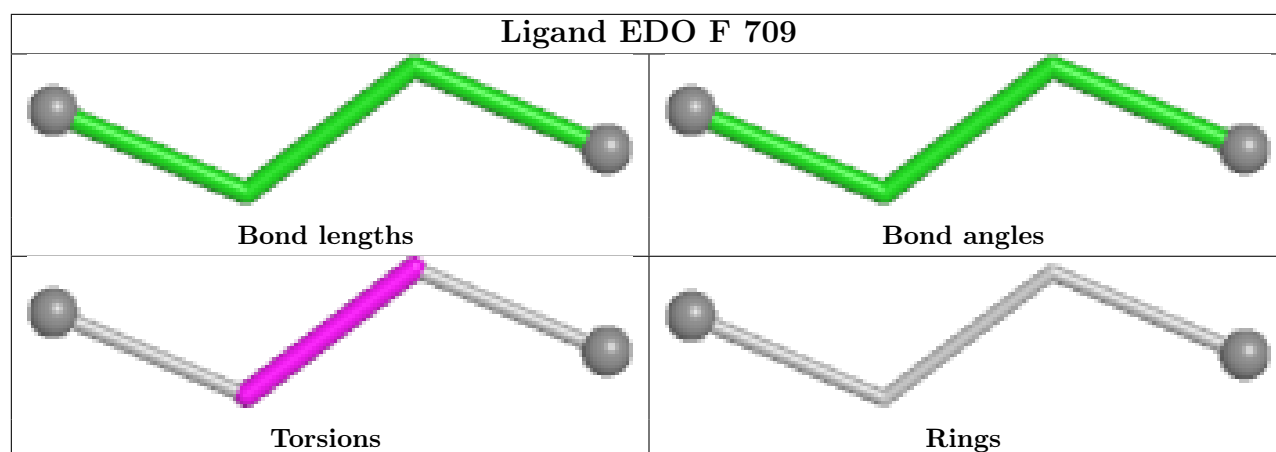


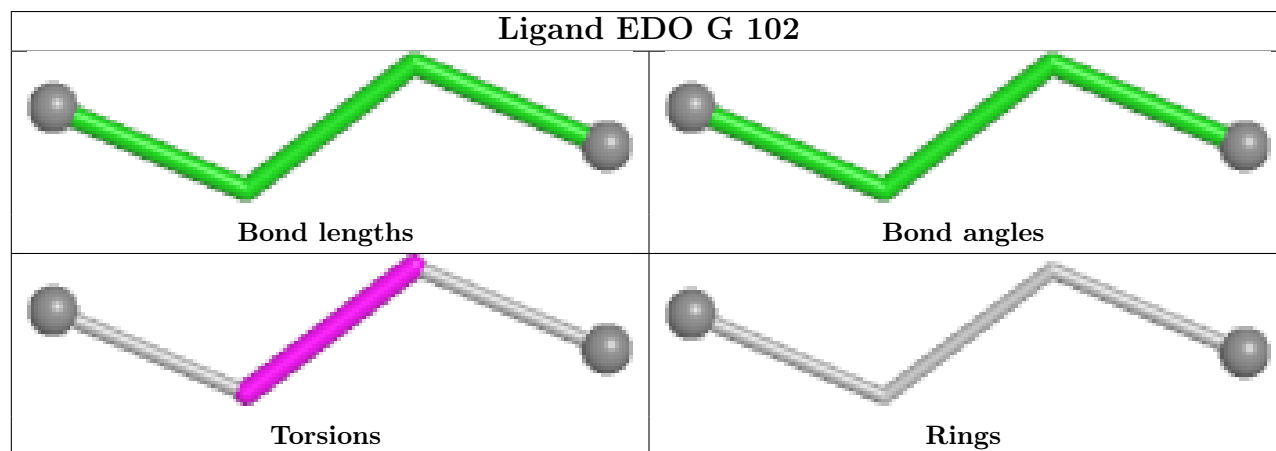
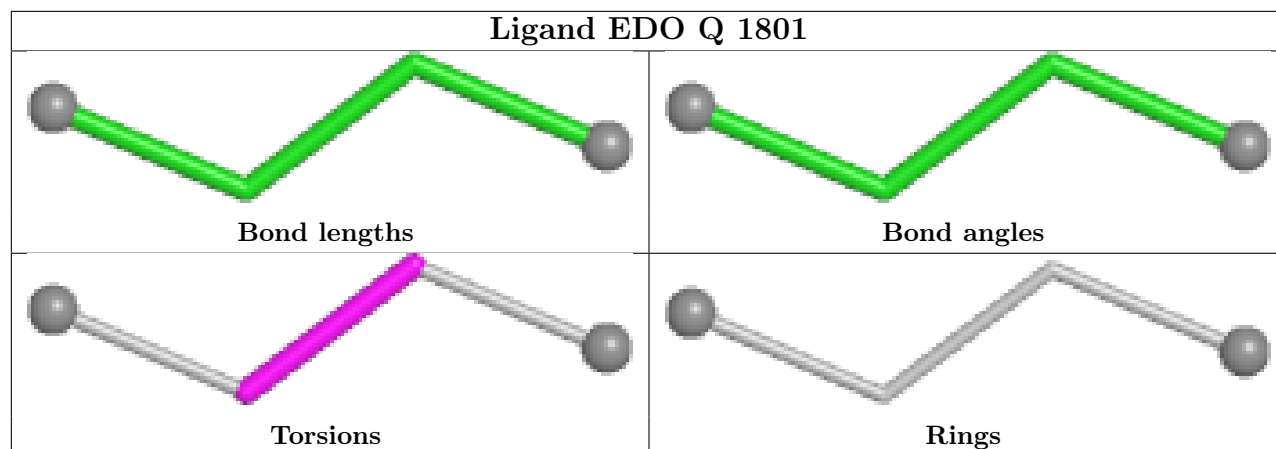




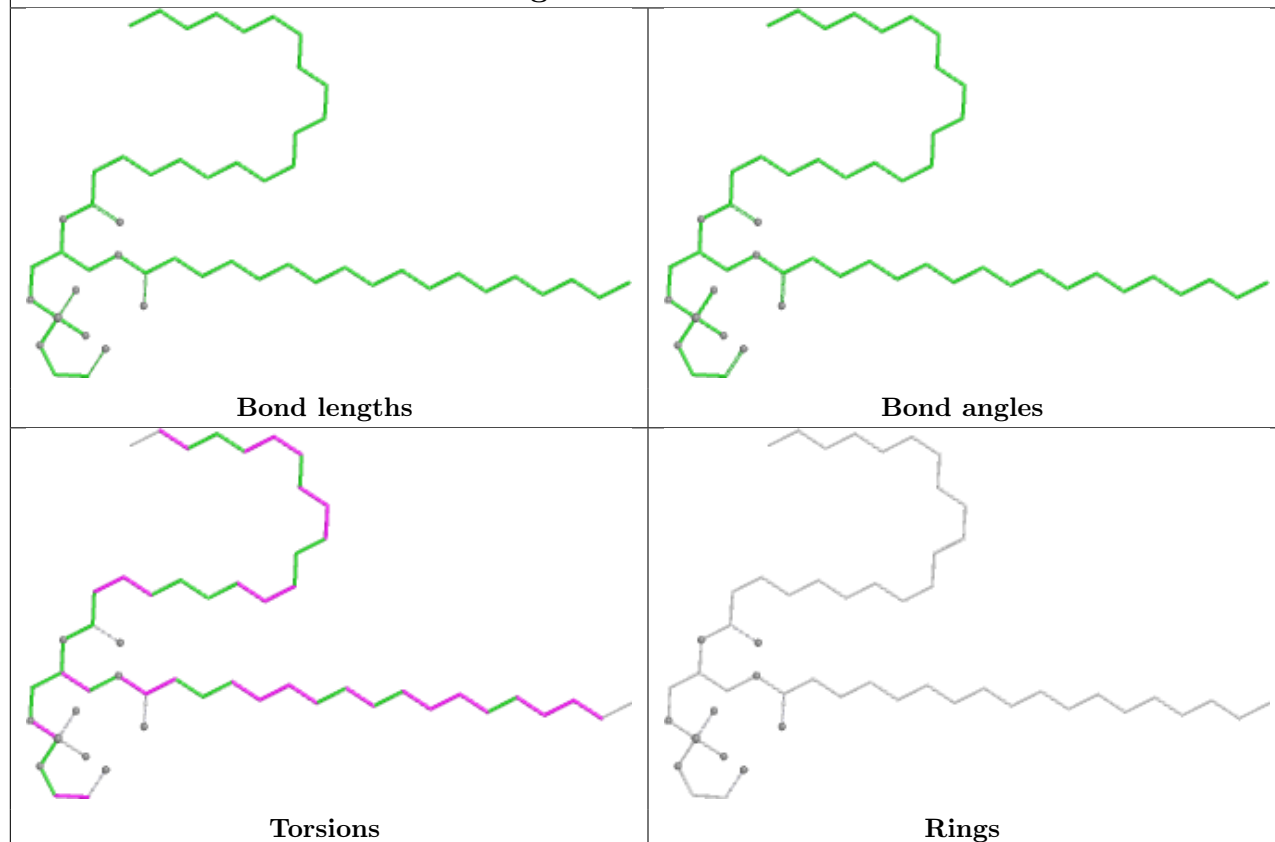




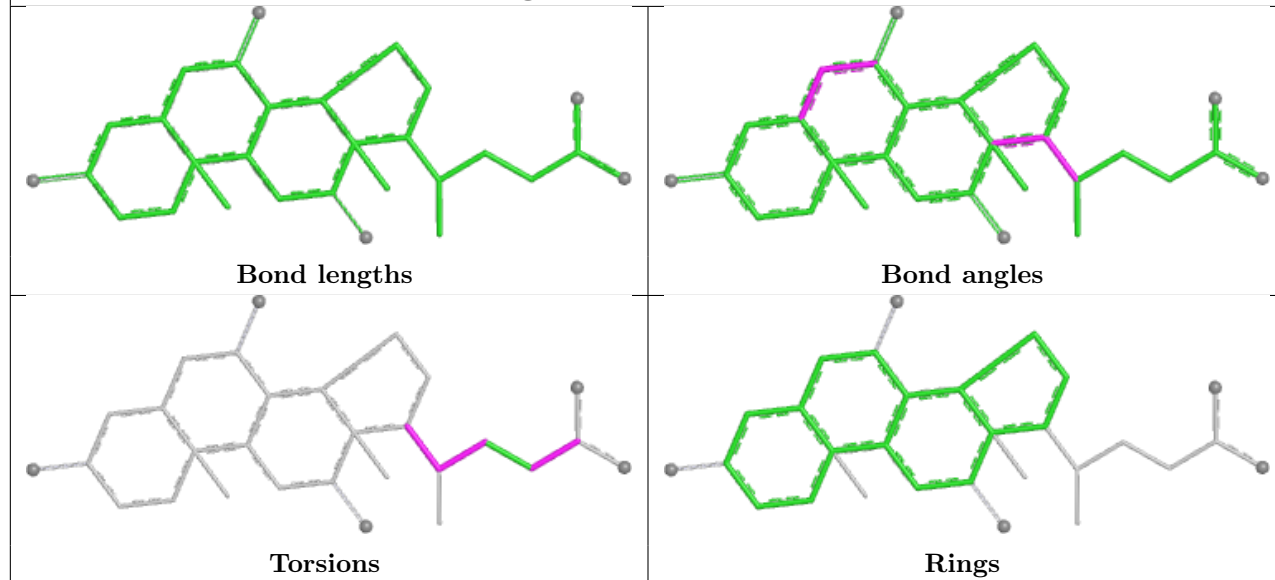


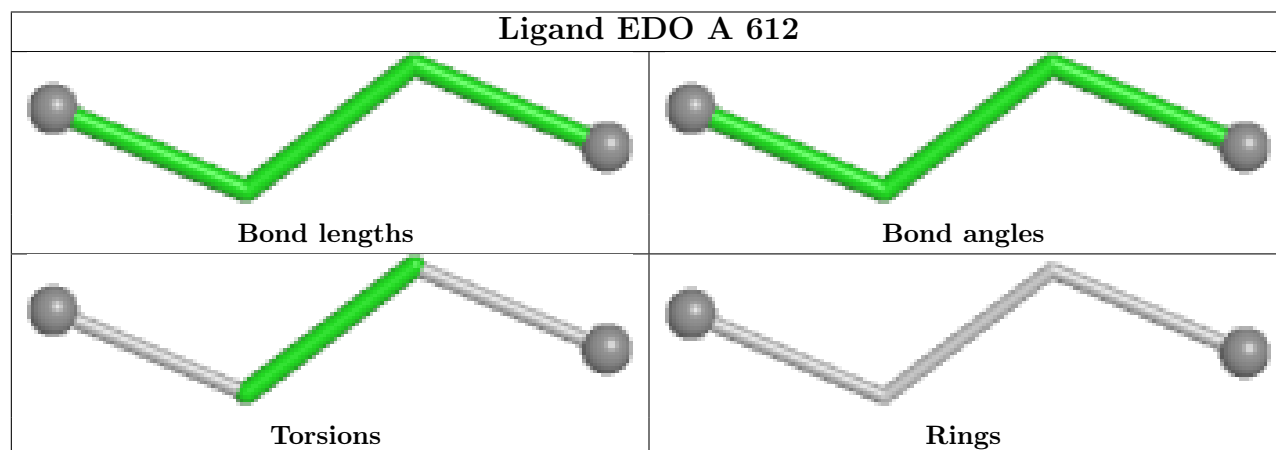
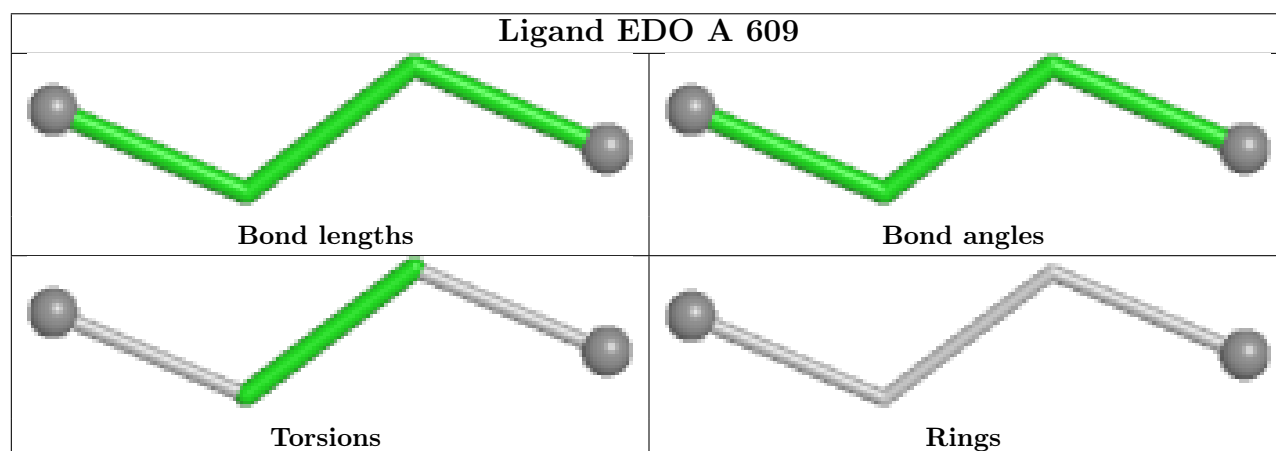
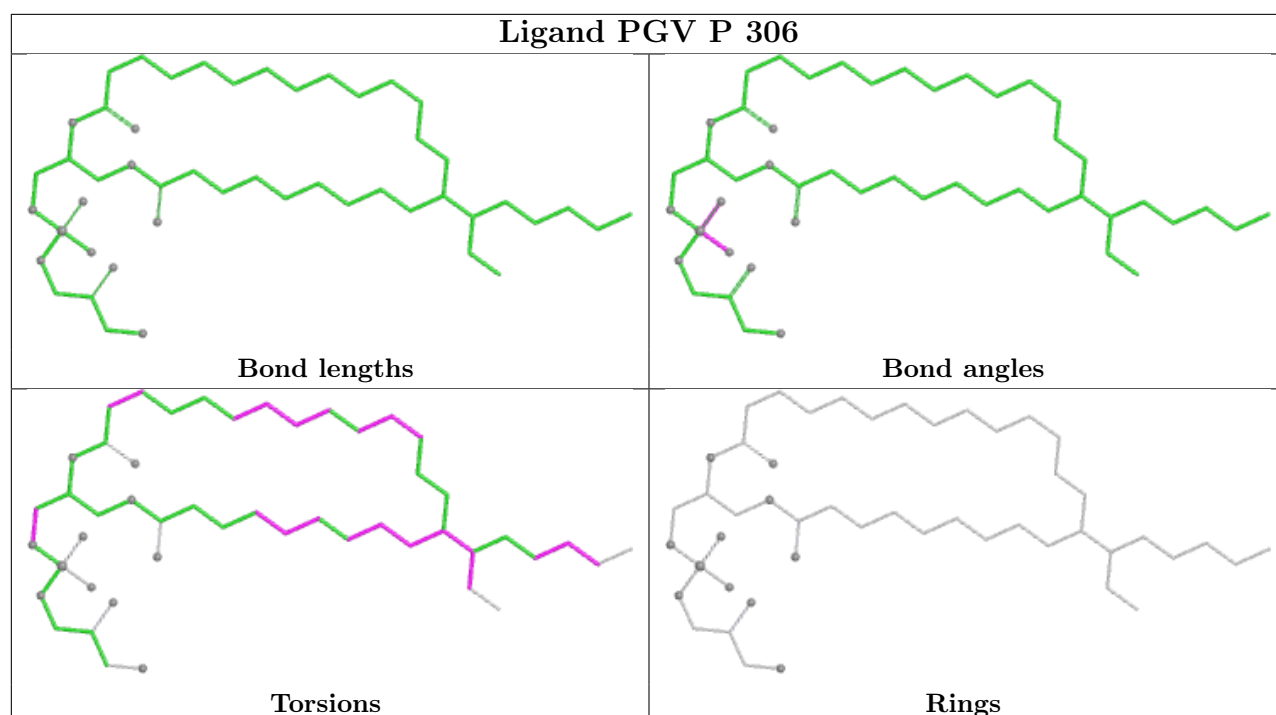


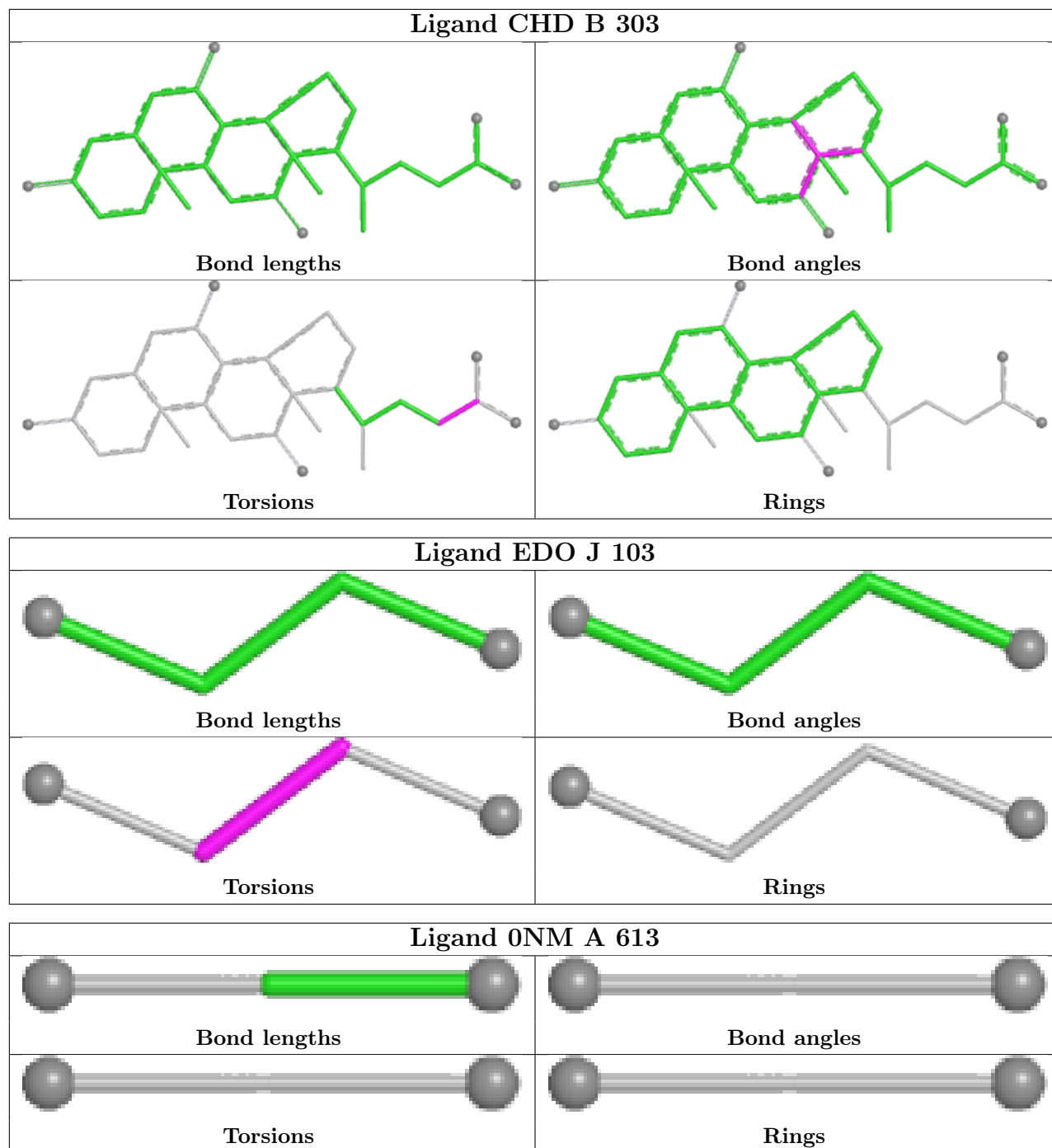
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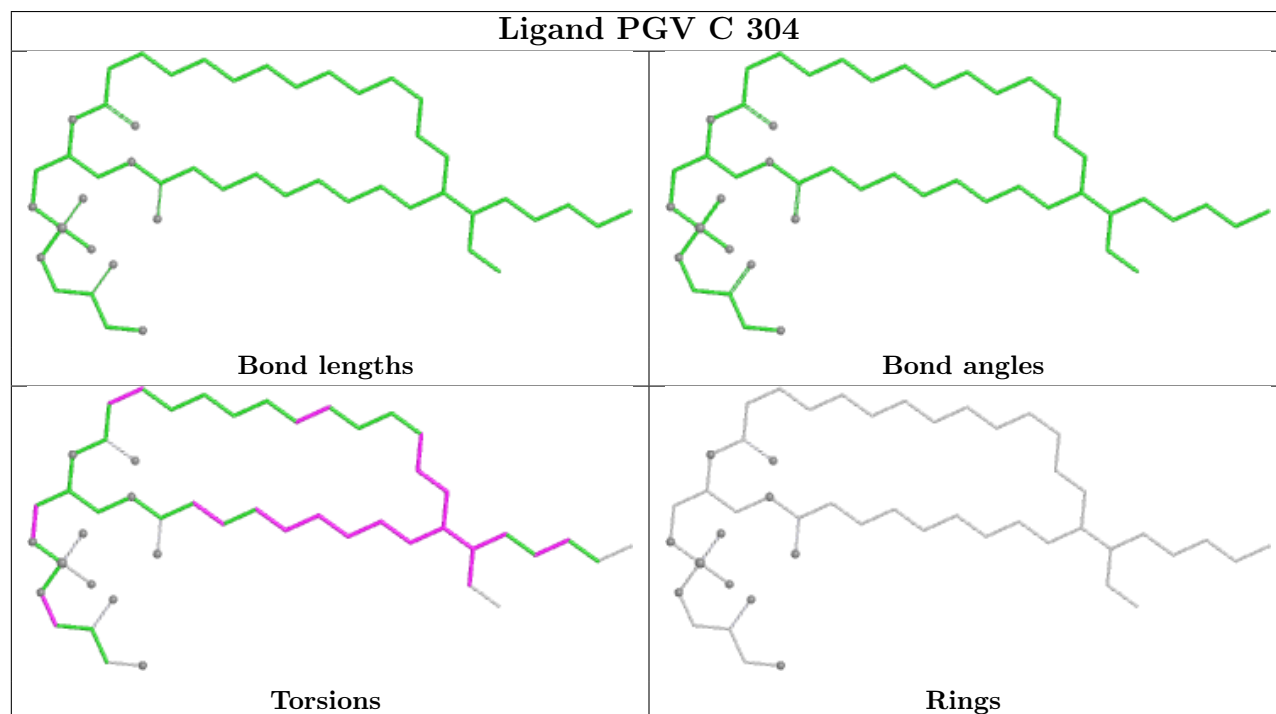
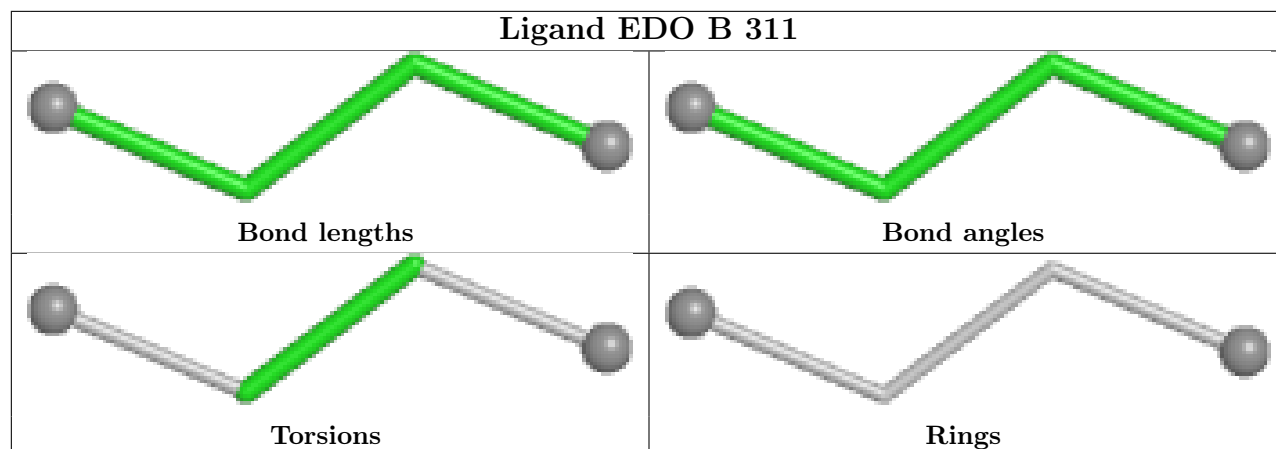


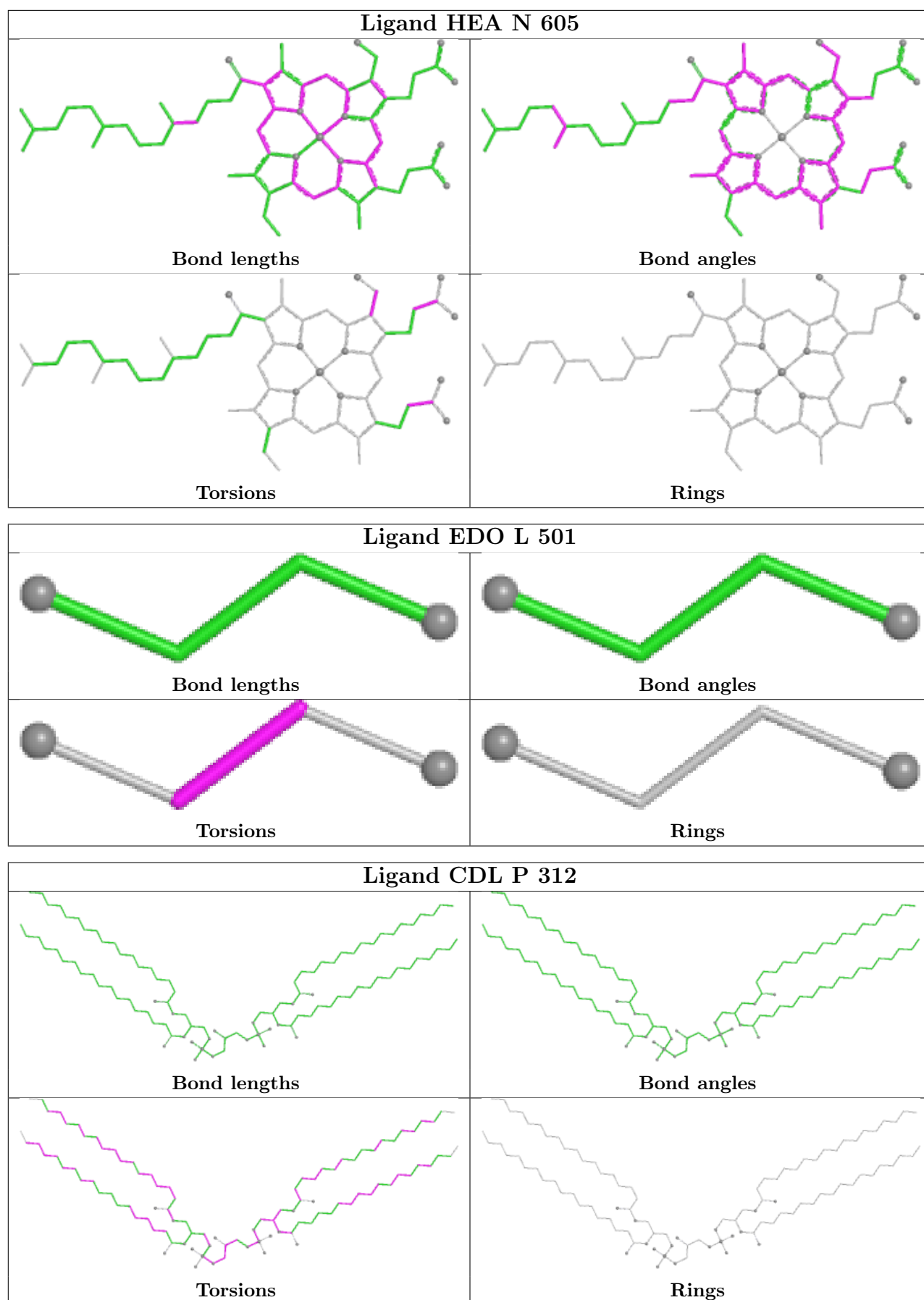
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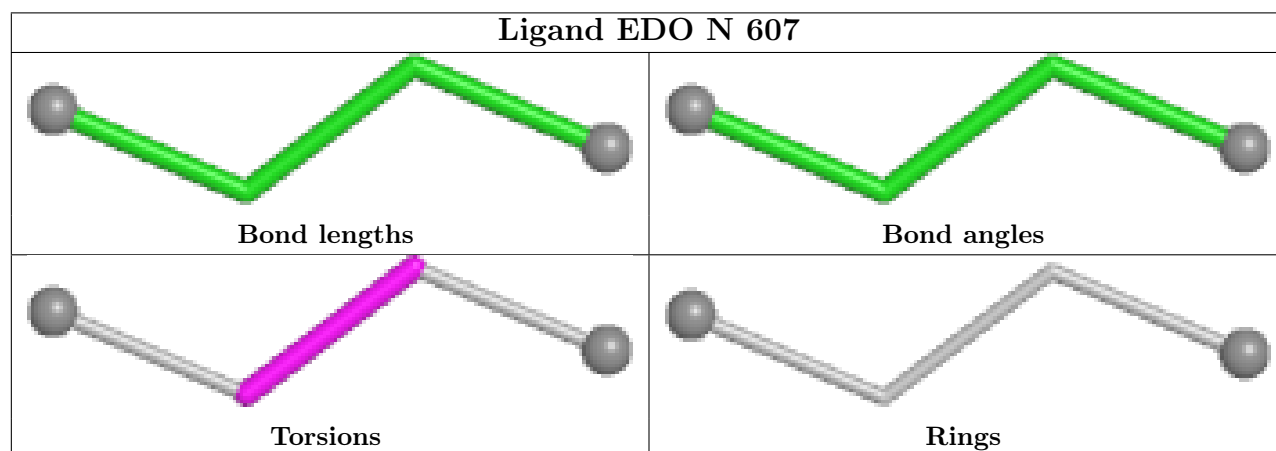
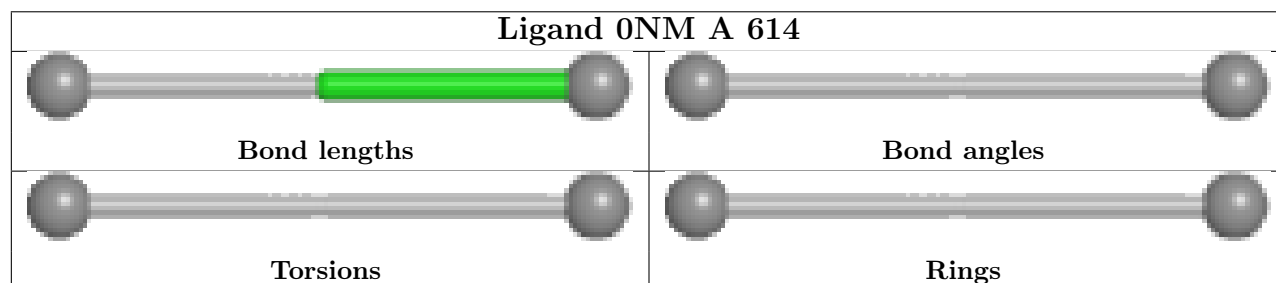
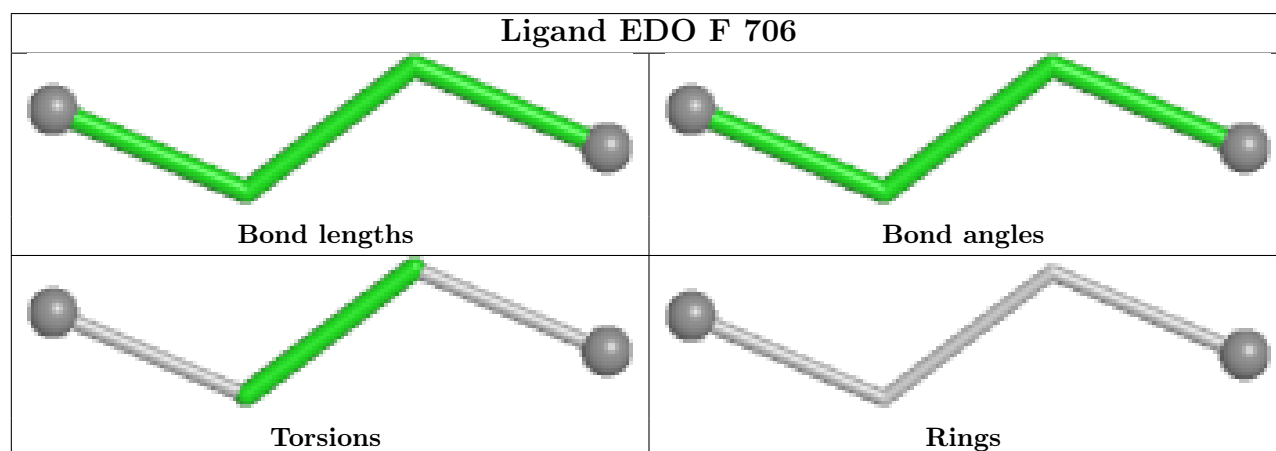
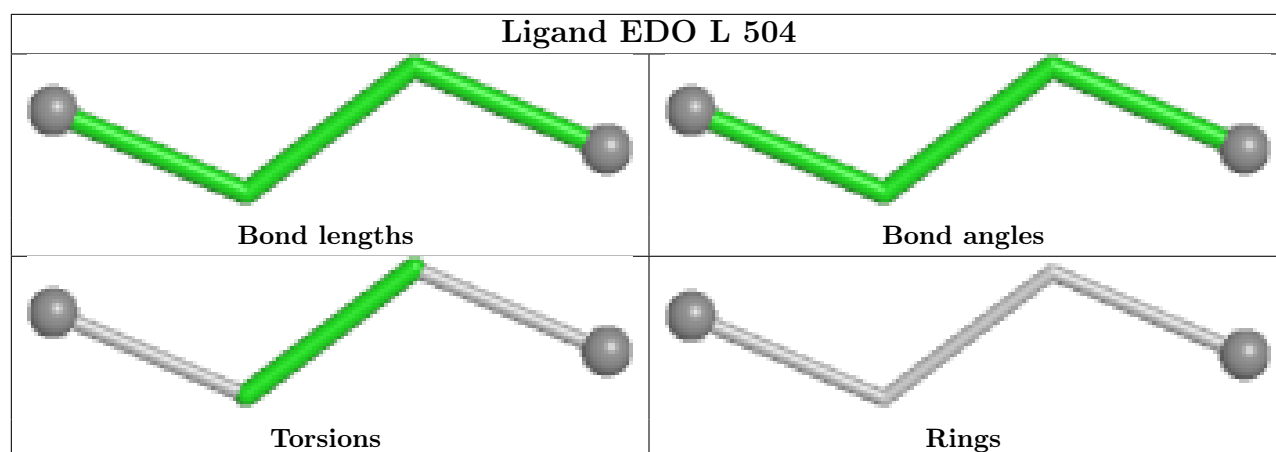




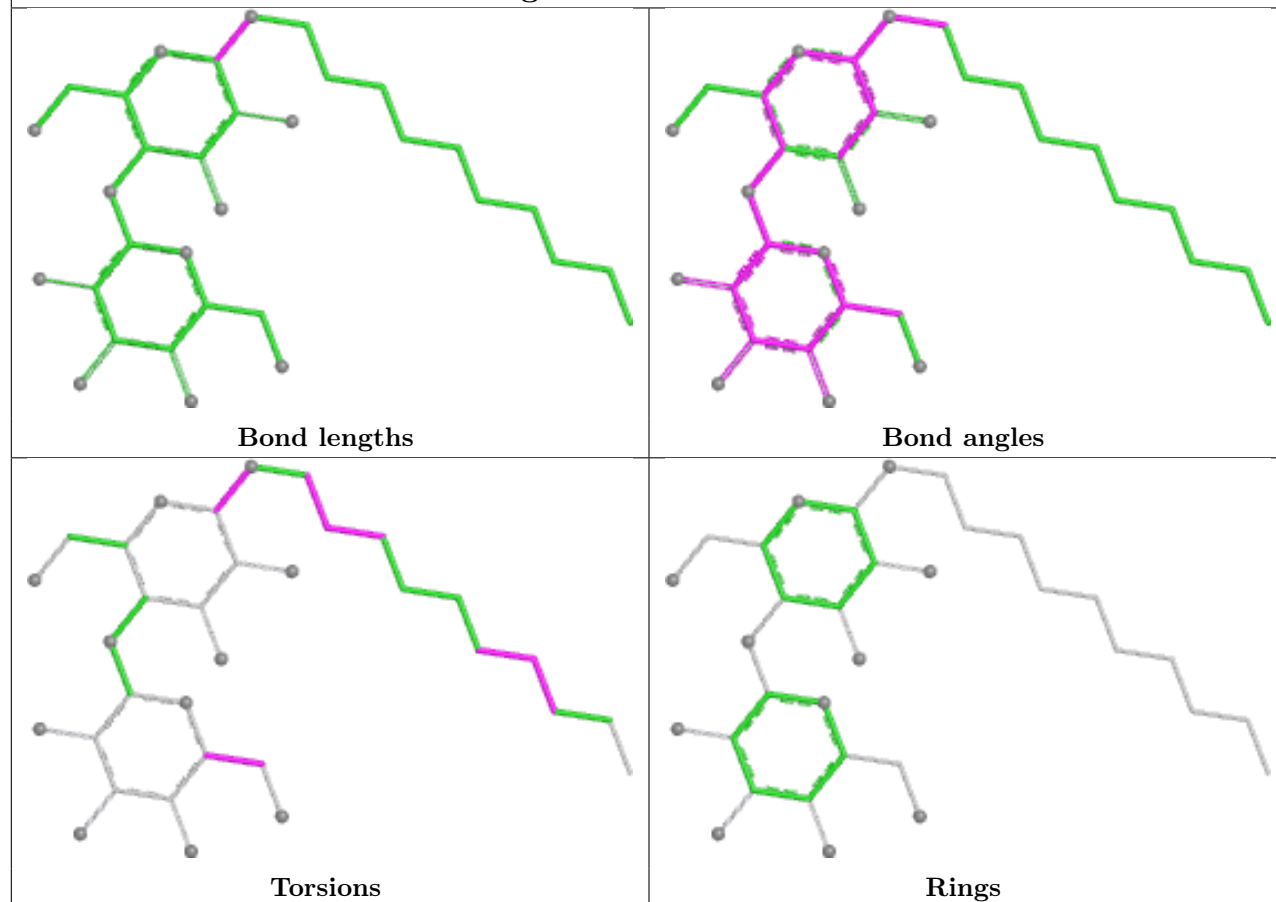




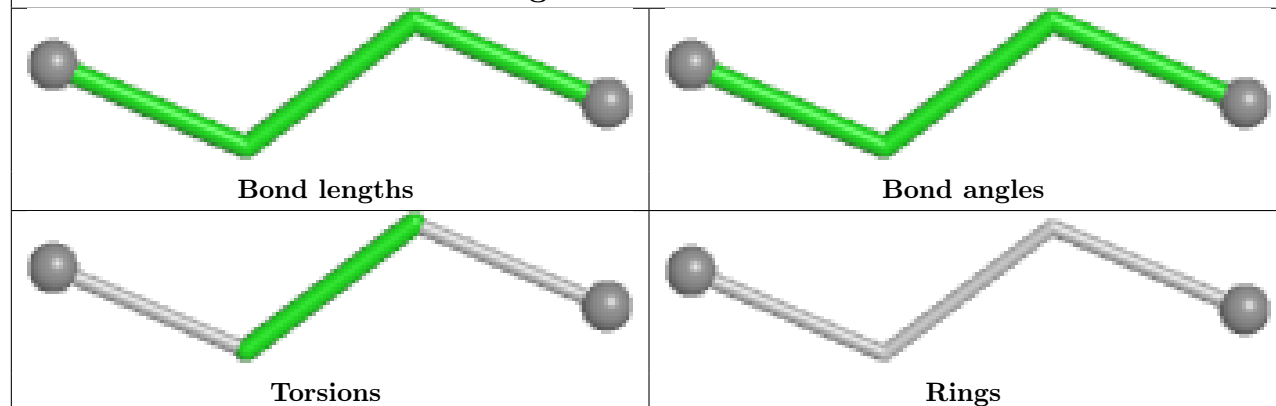


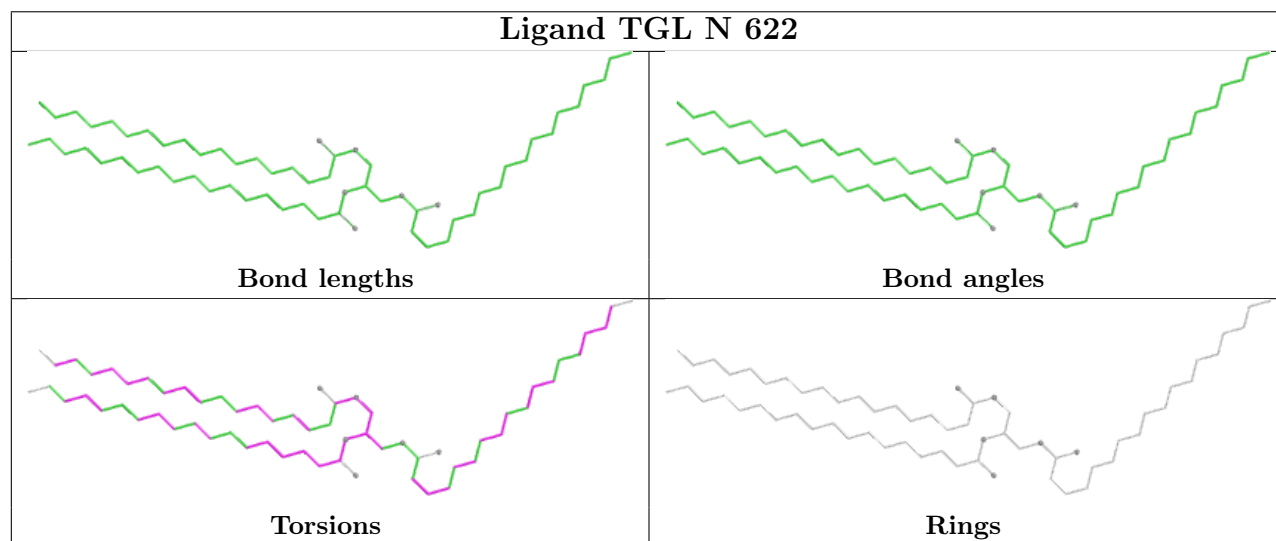
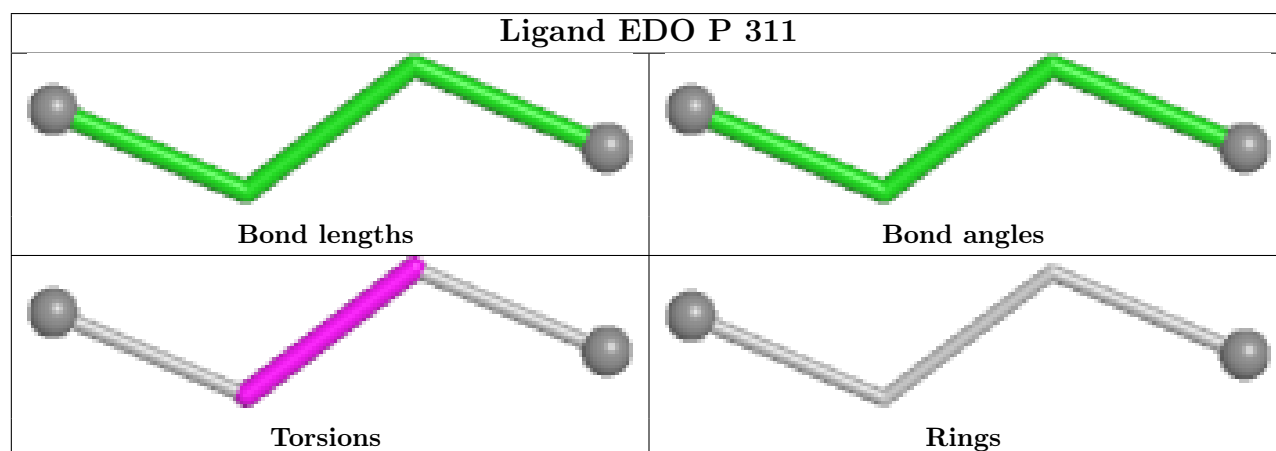
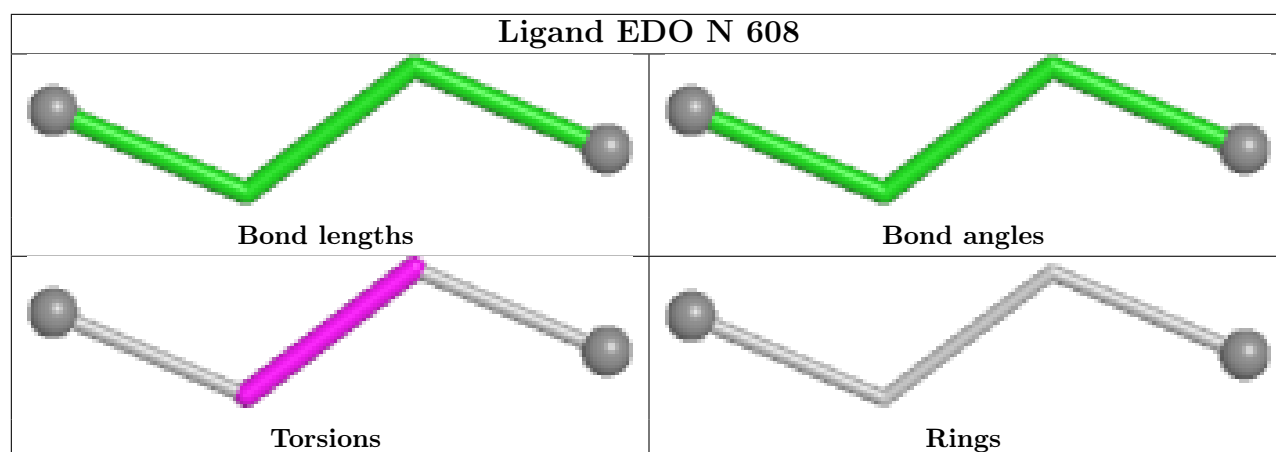


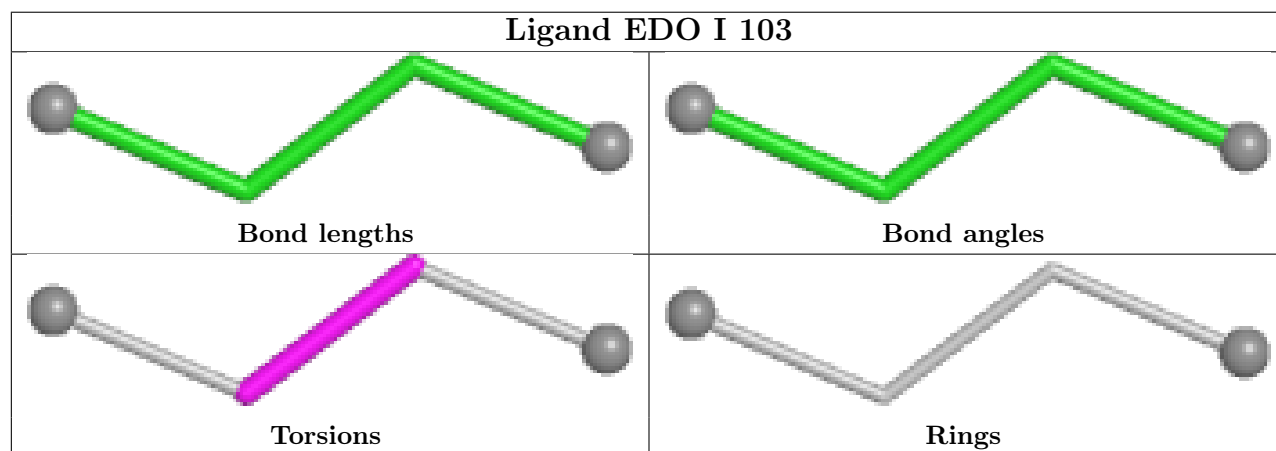
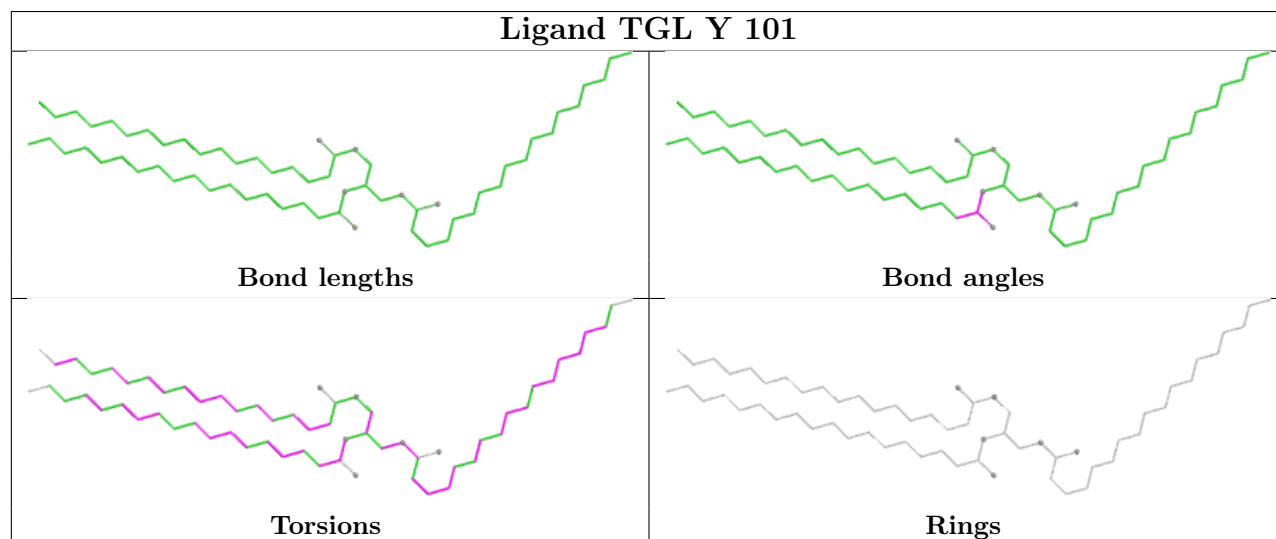
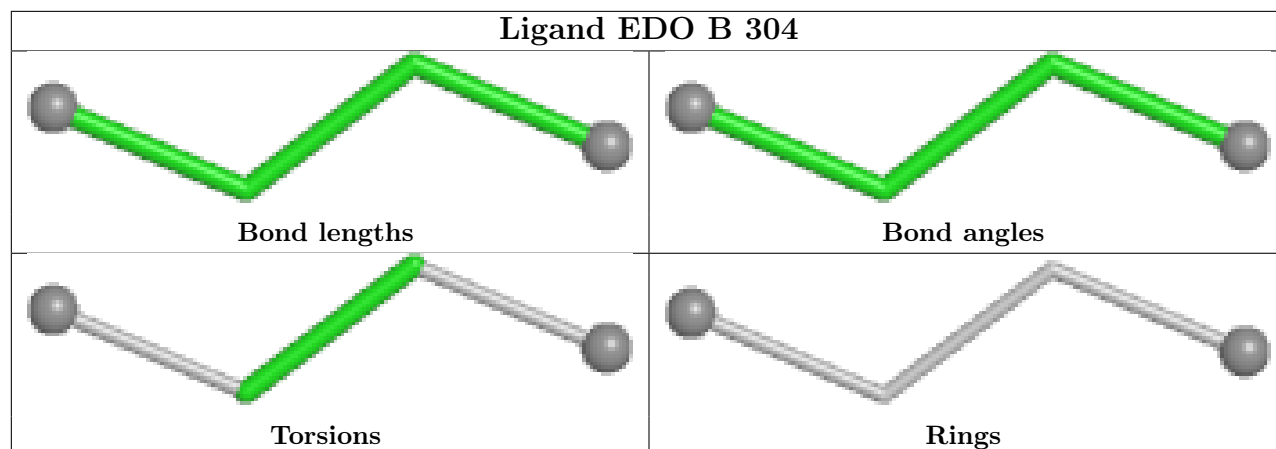
Ligand DMU M 103

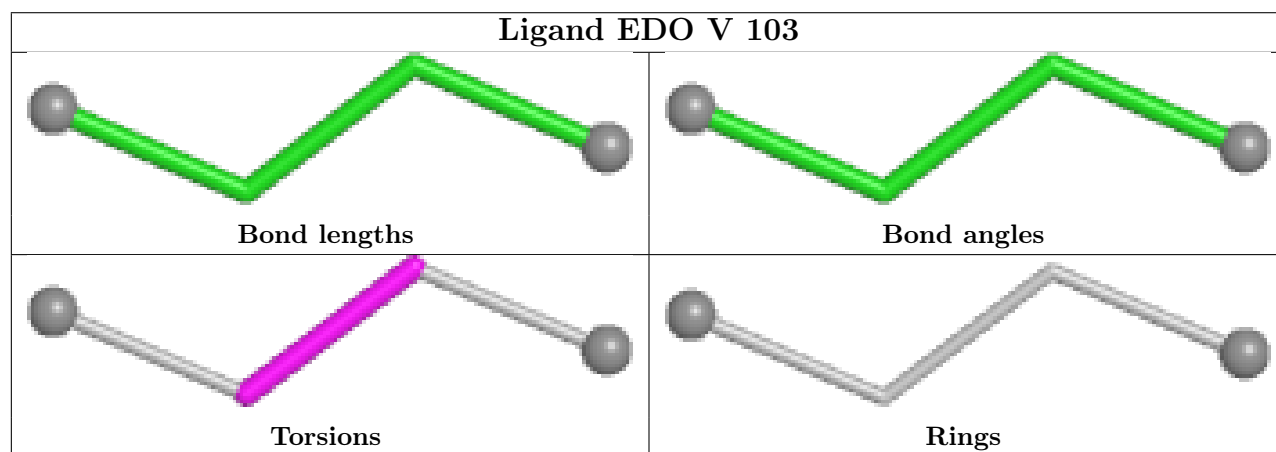
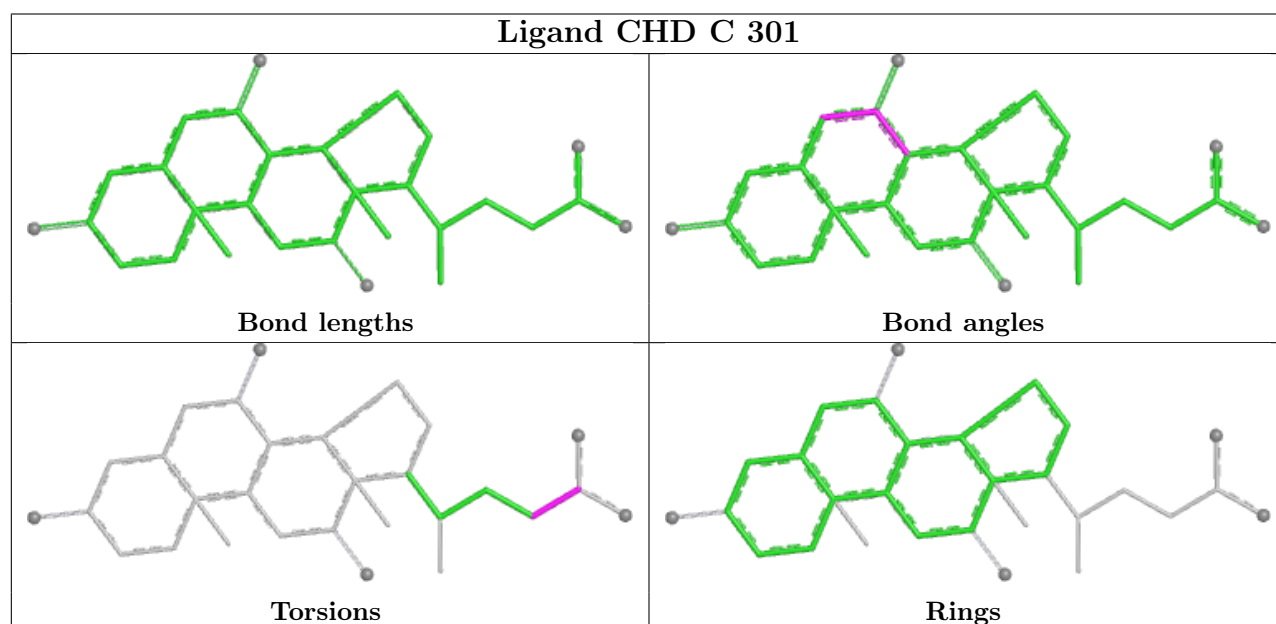
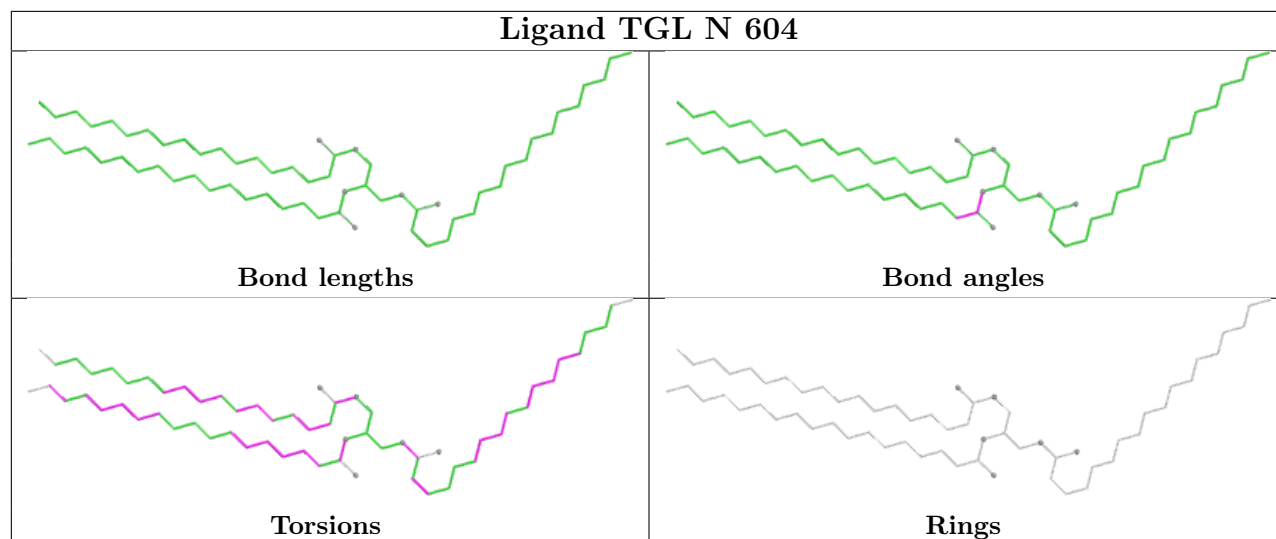


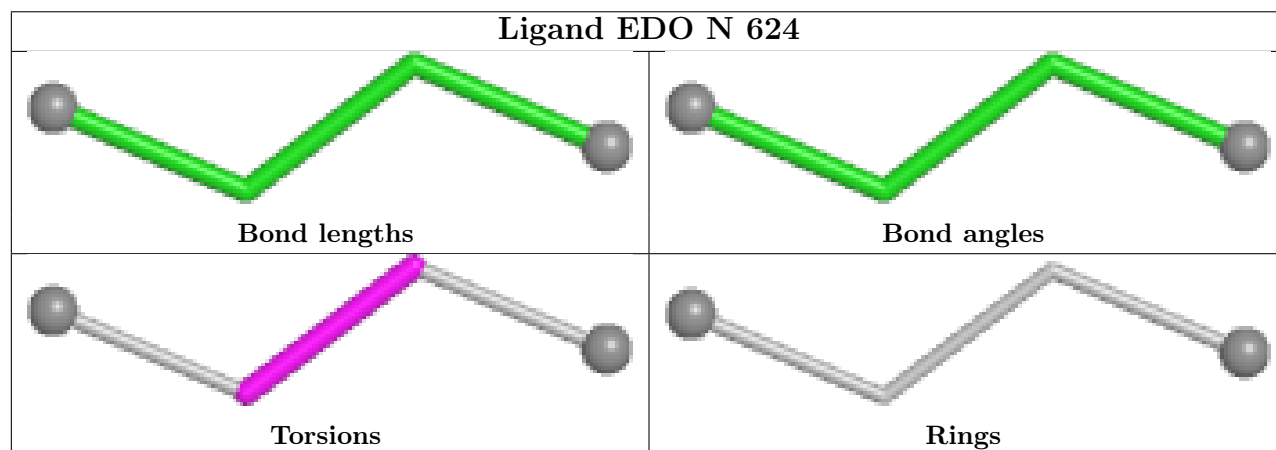
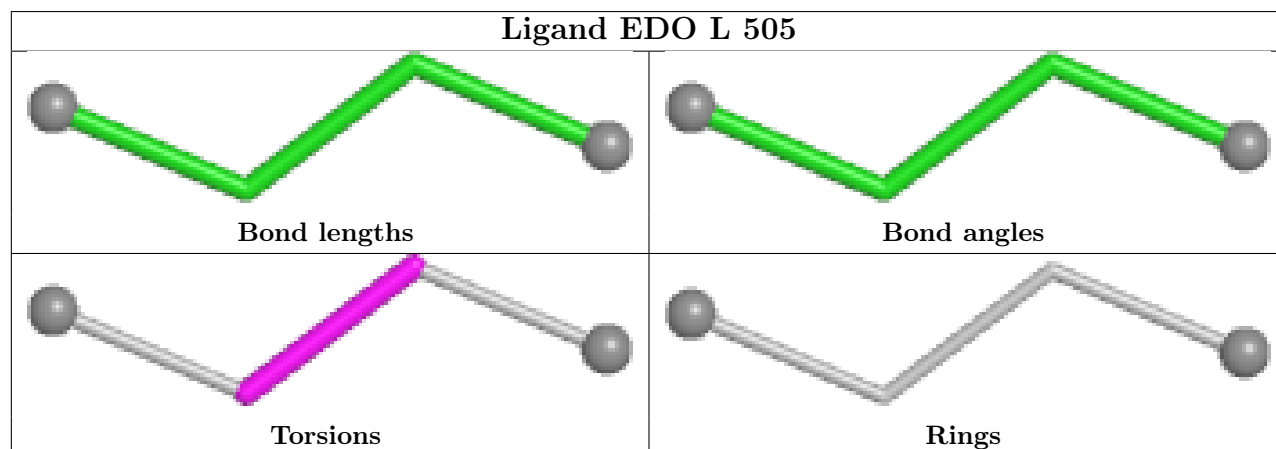
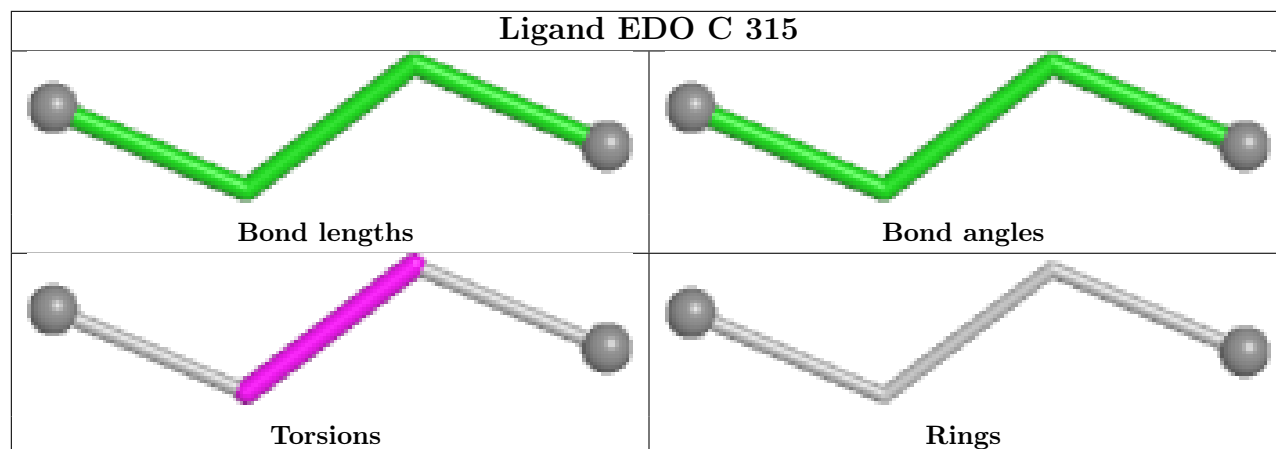
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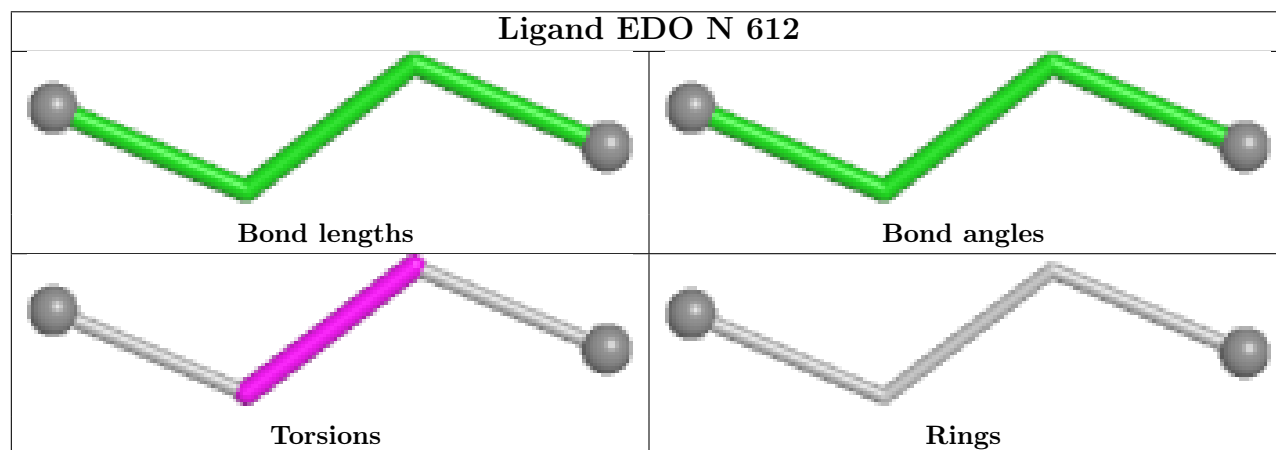
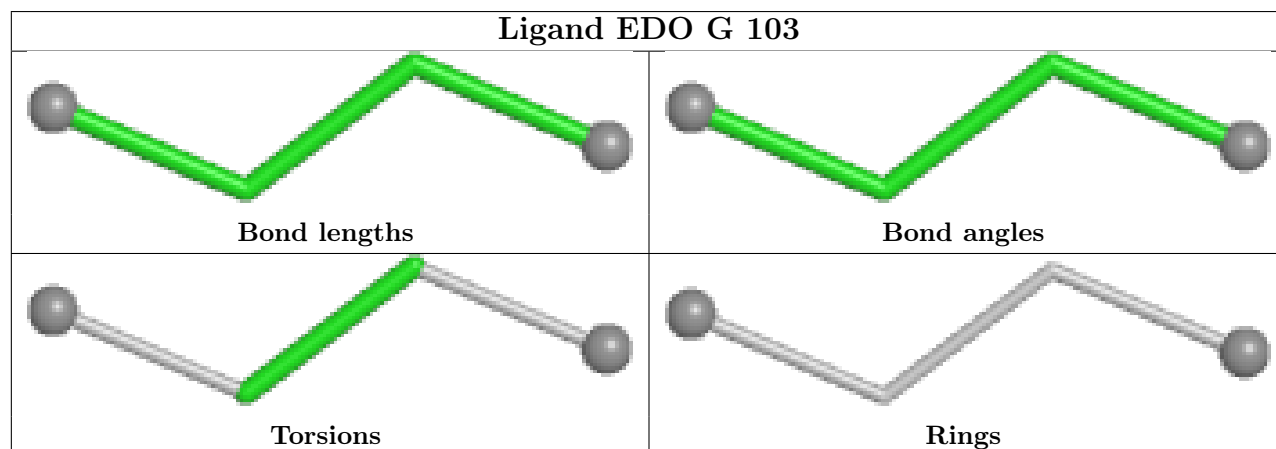
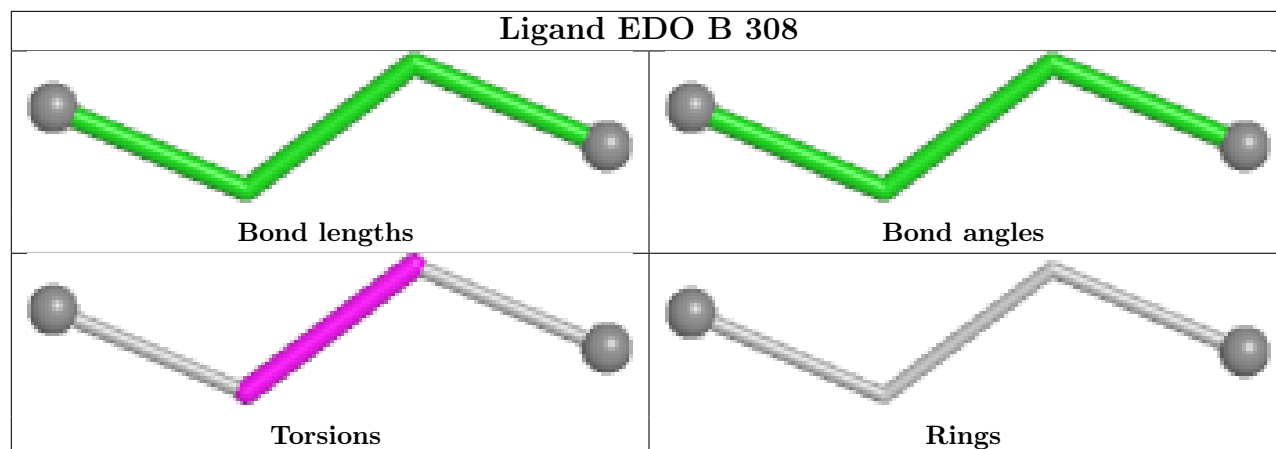


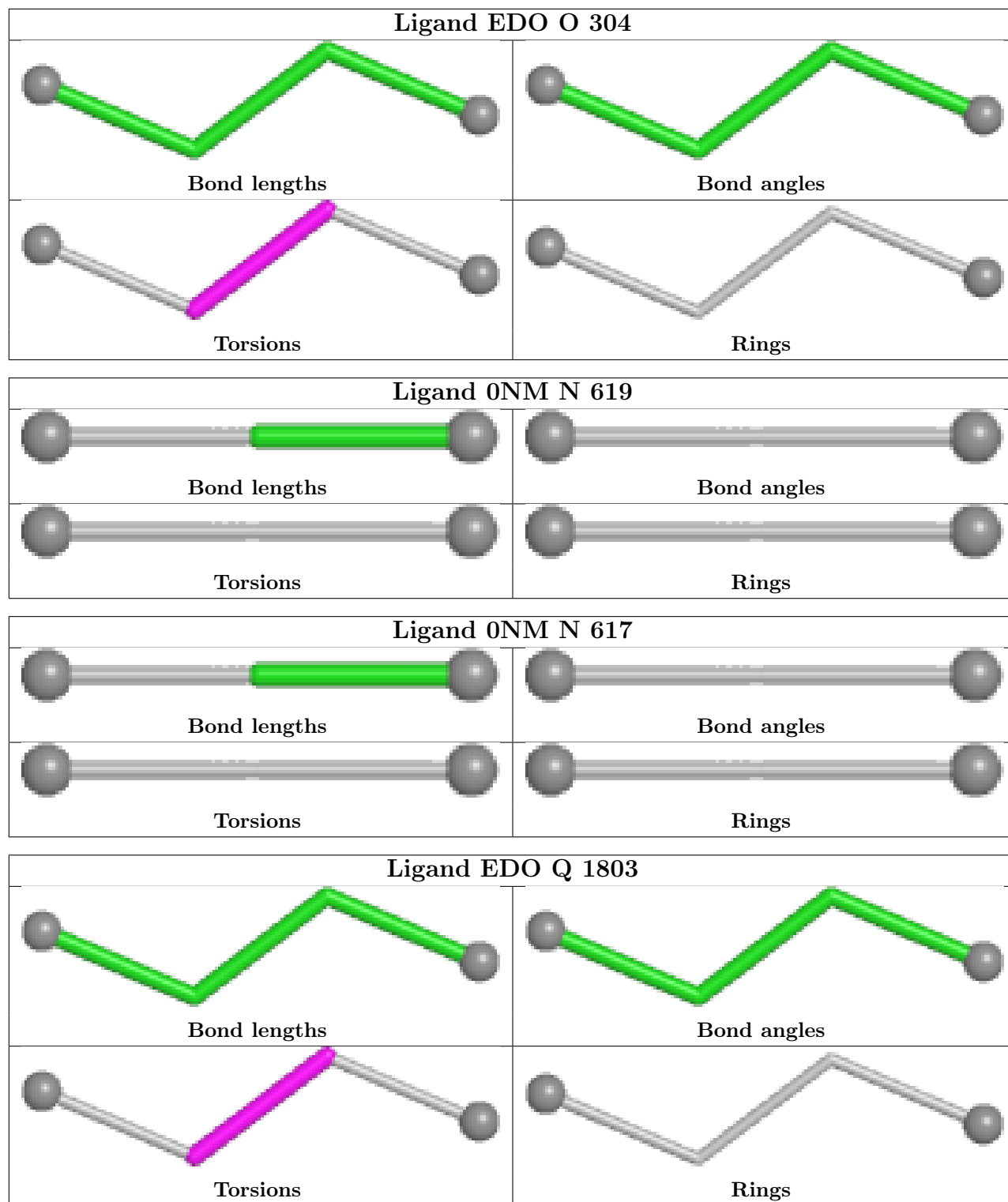


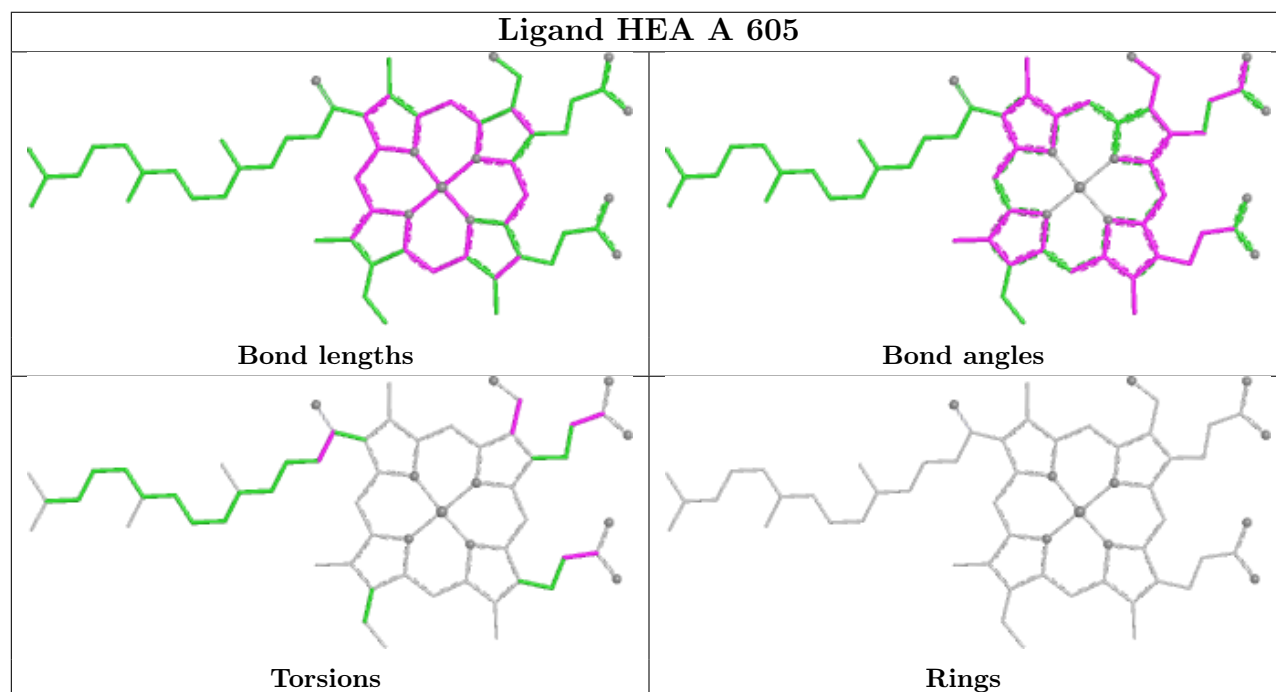
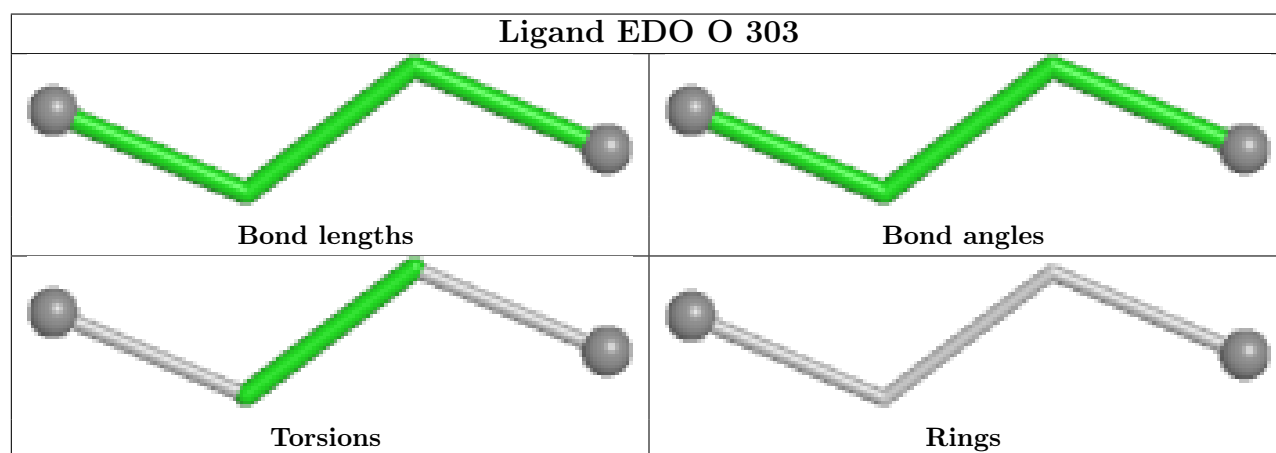
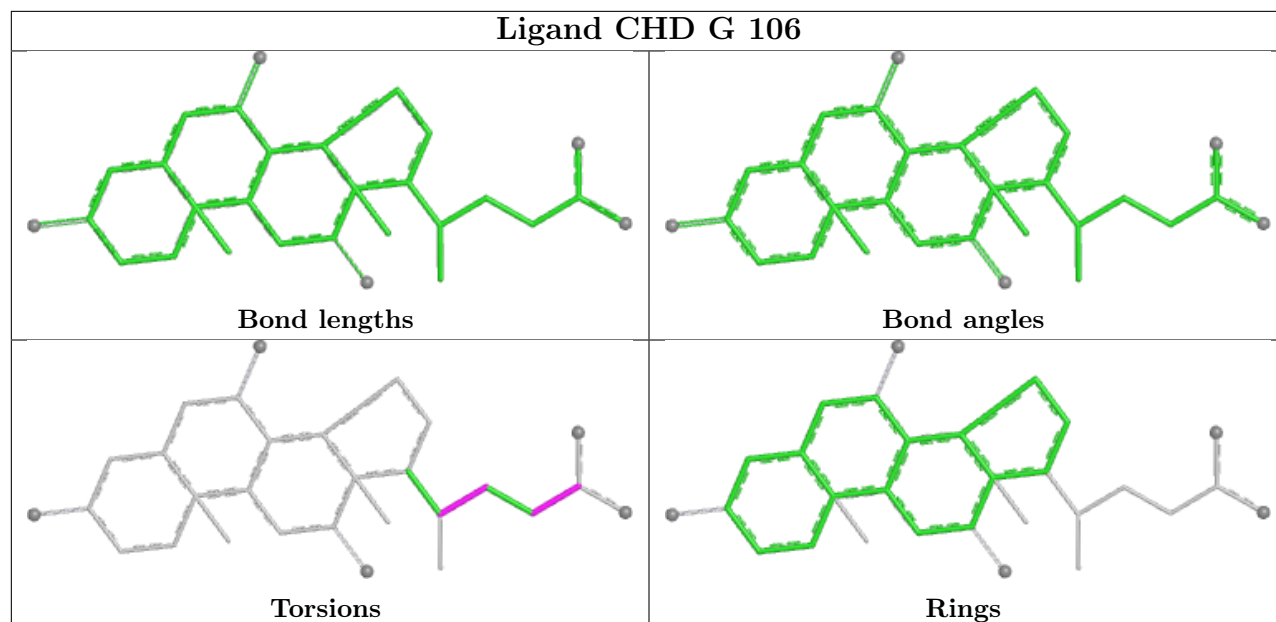


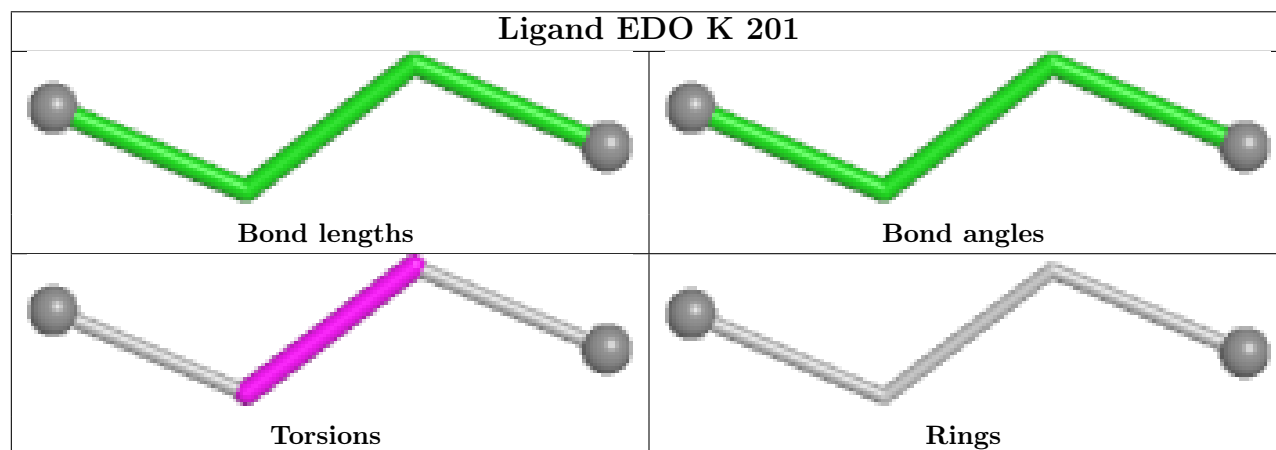
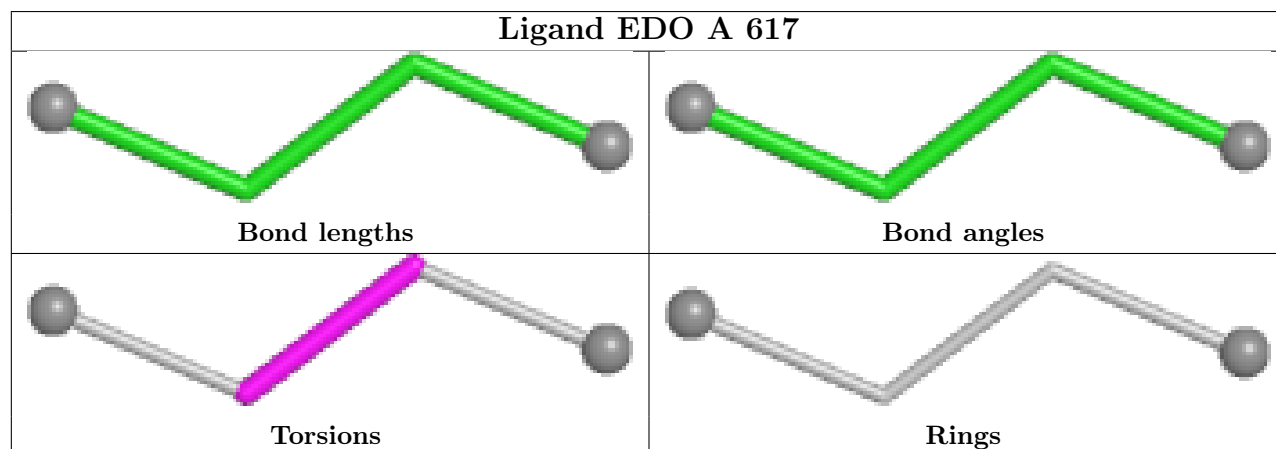
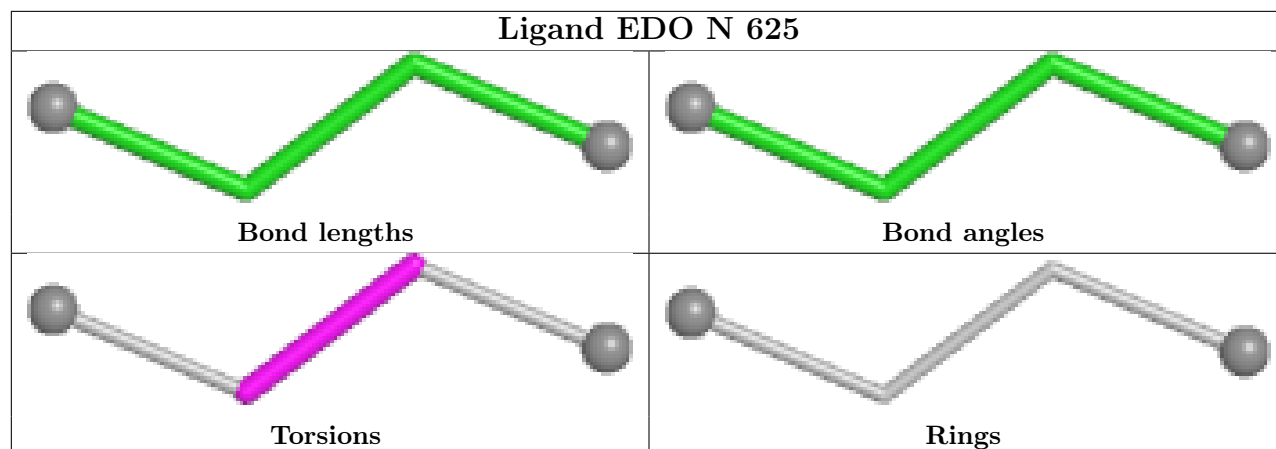


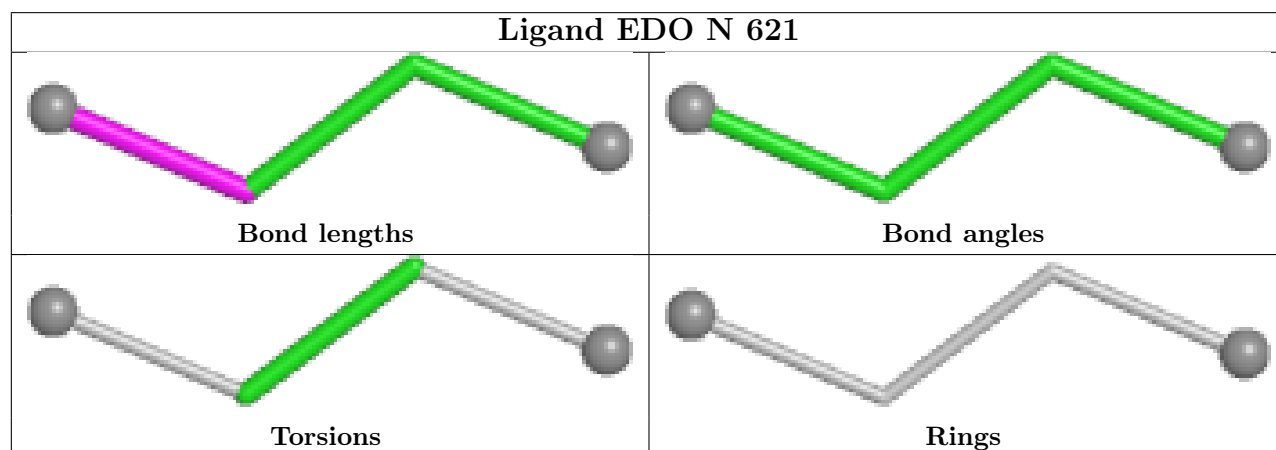
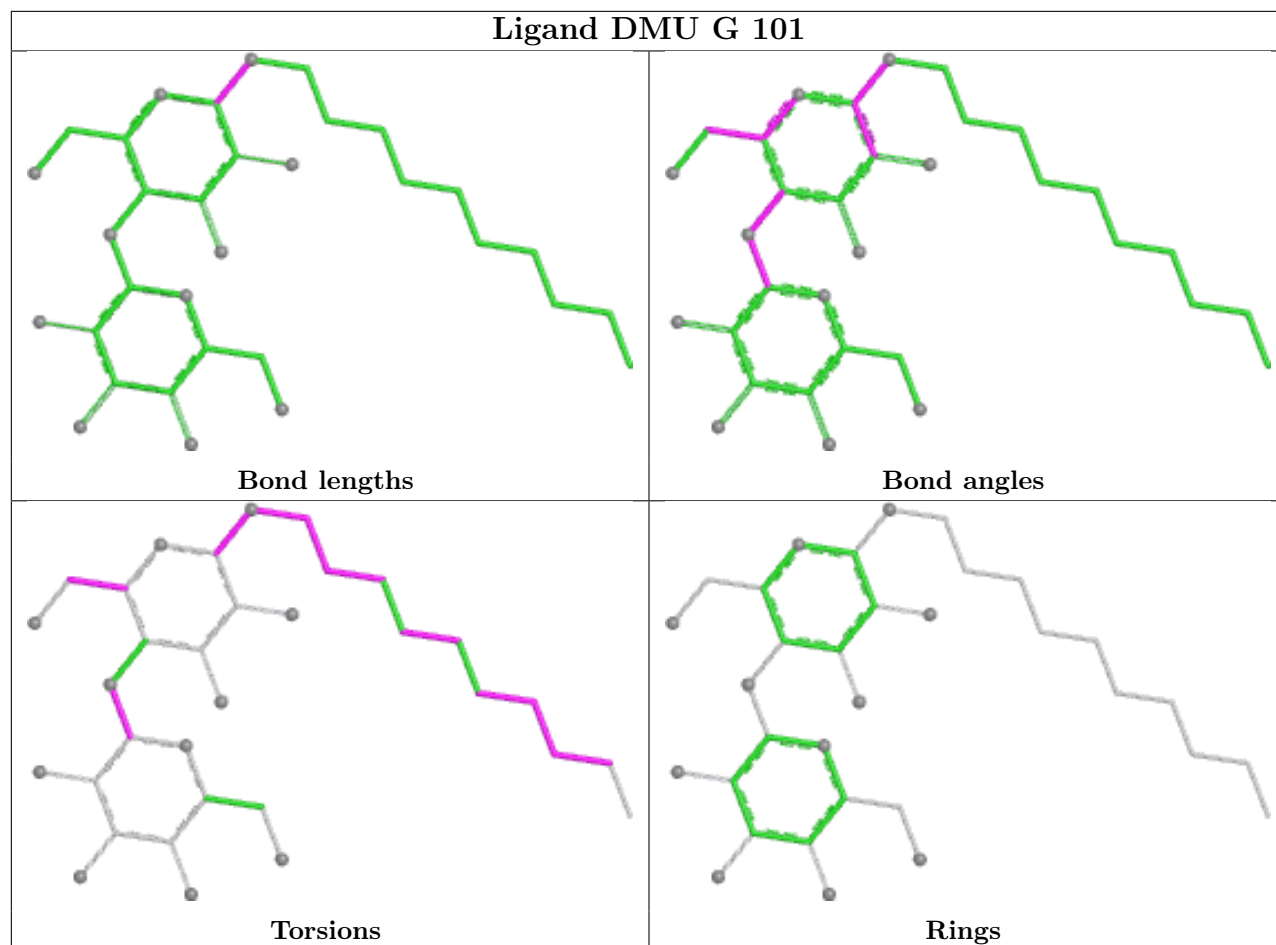


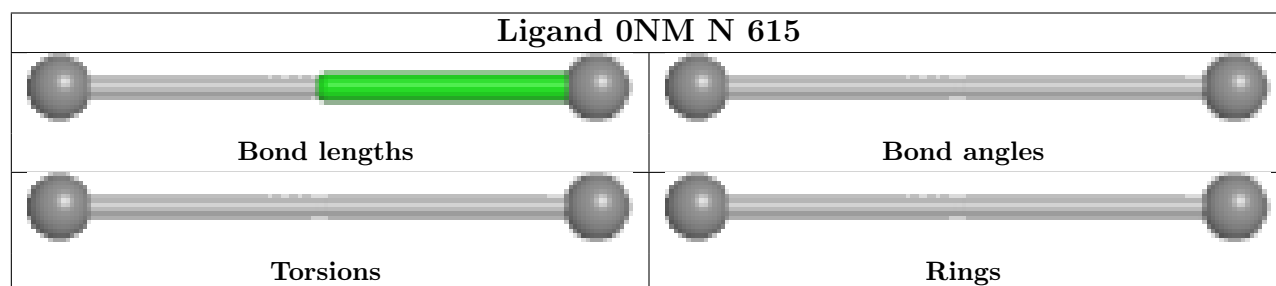
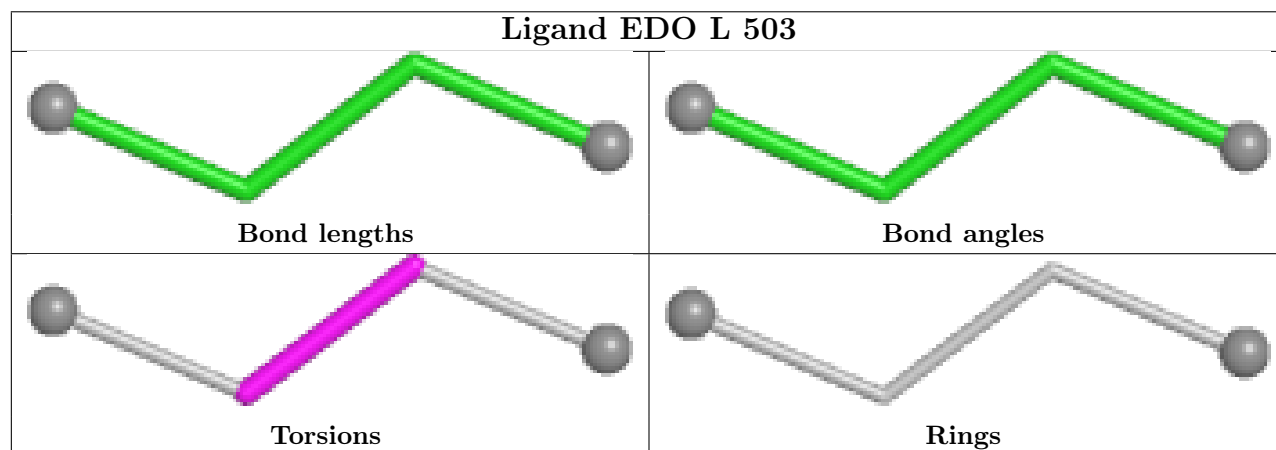
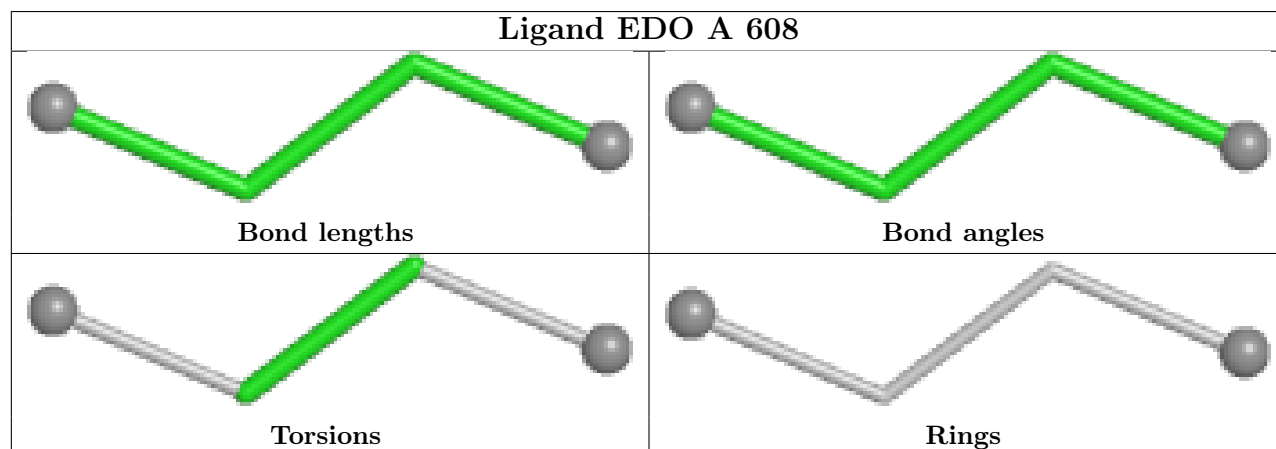
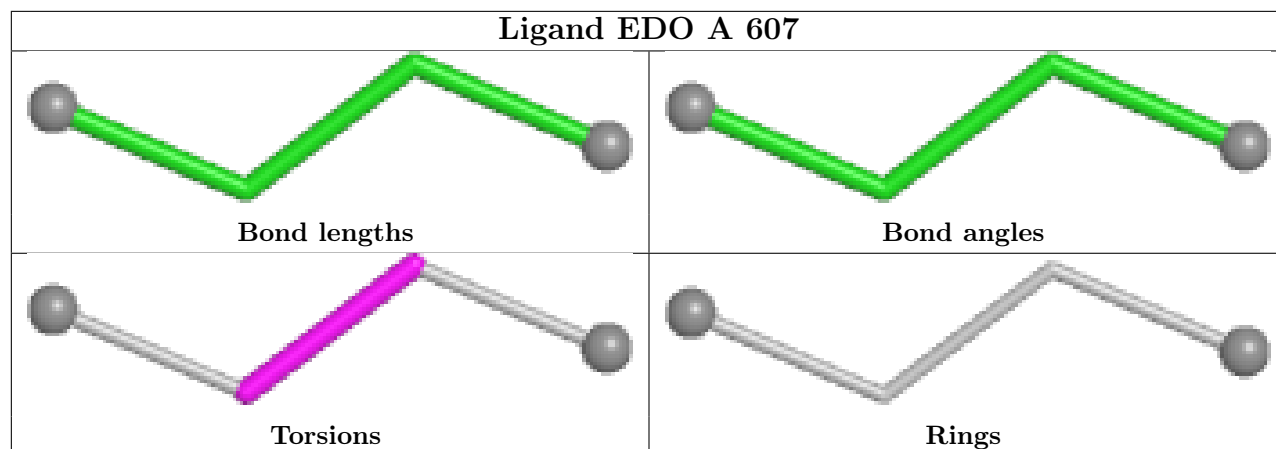


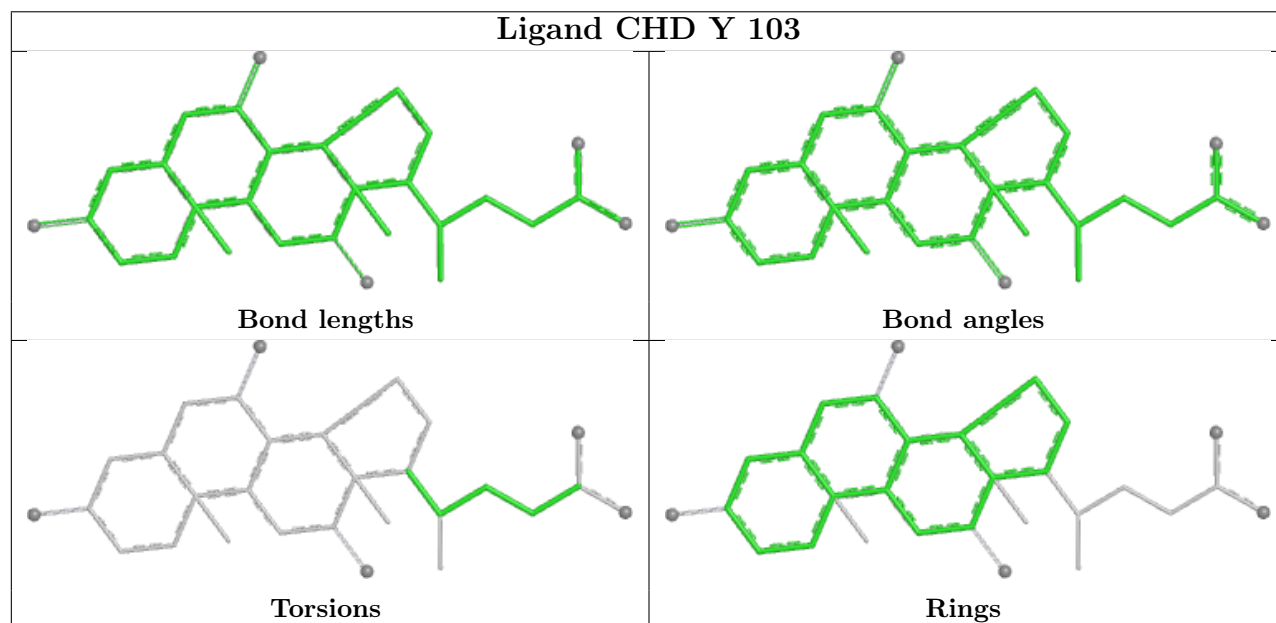
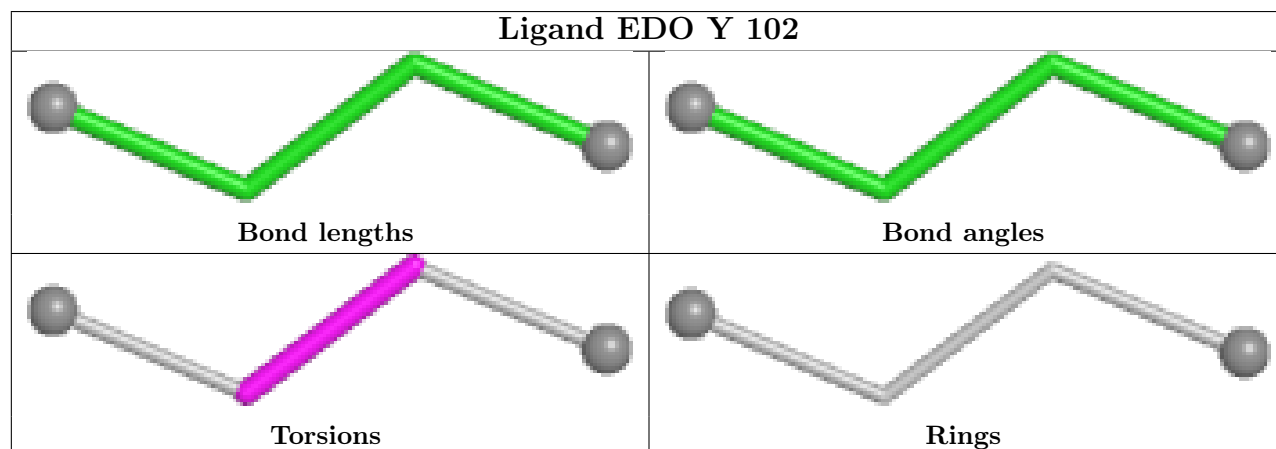
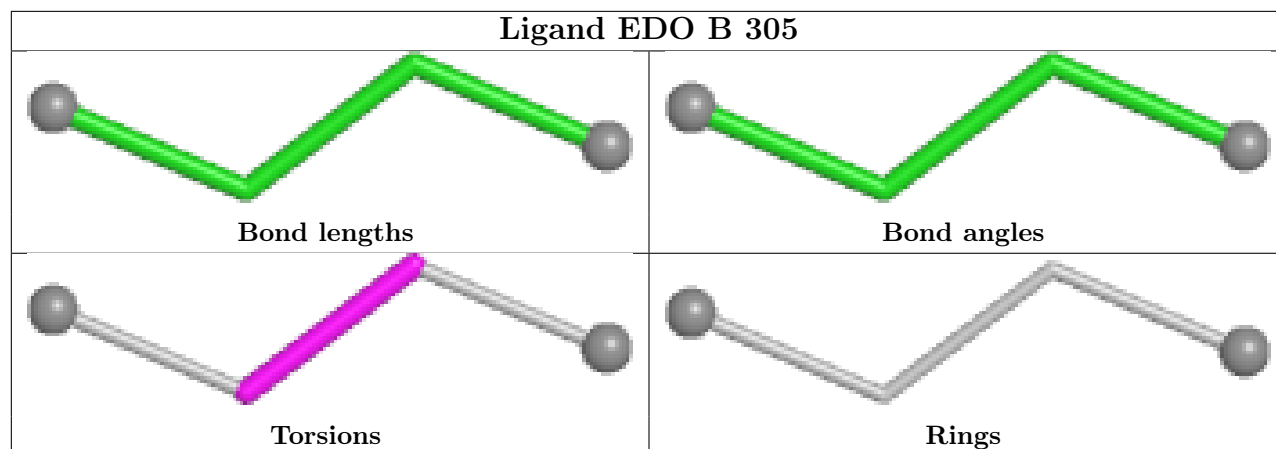


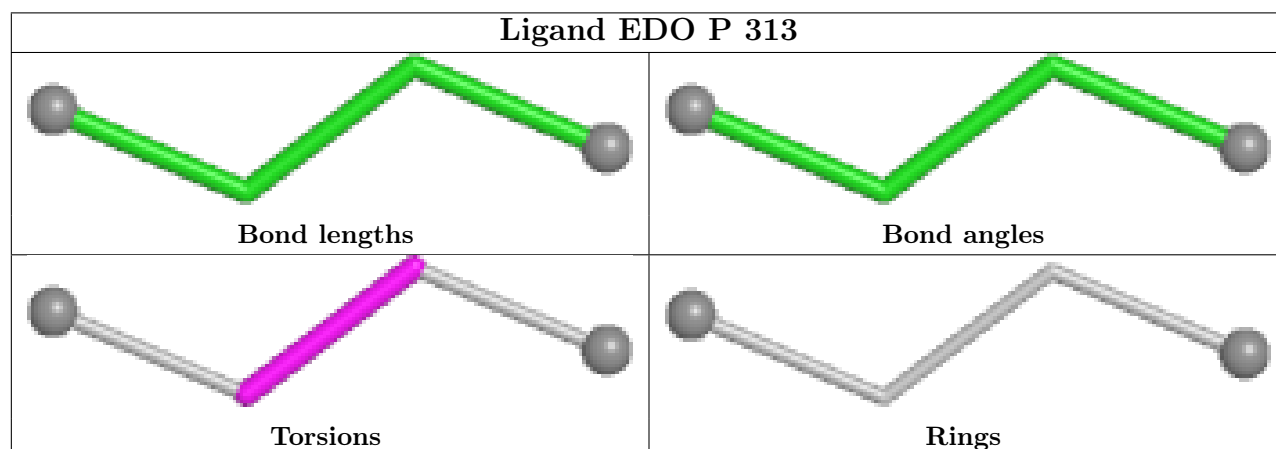
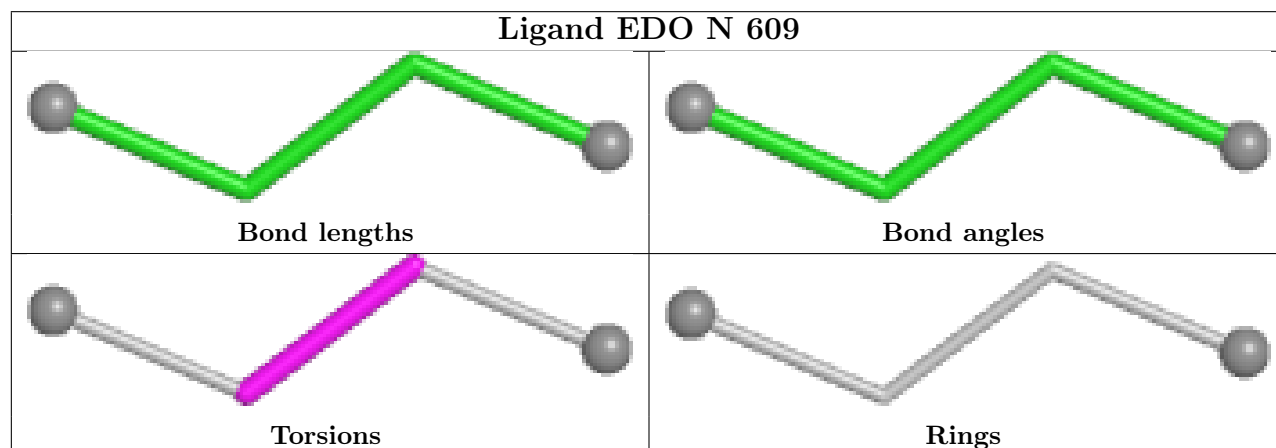
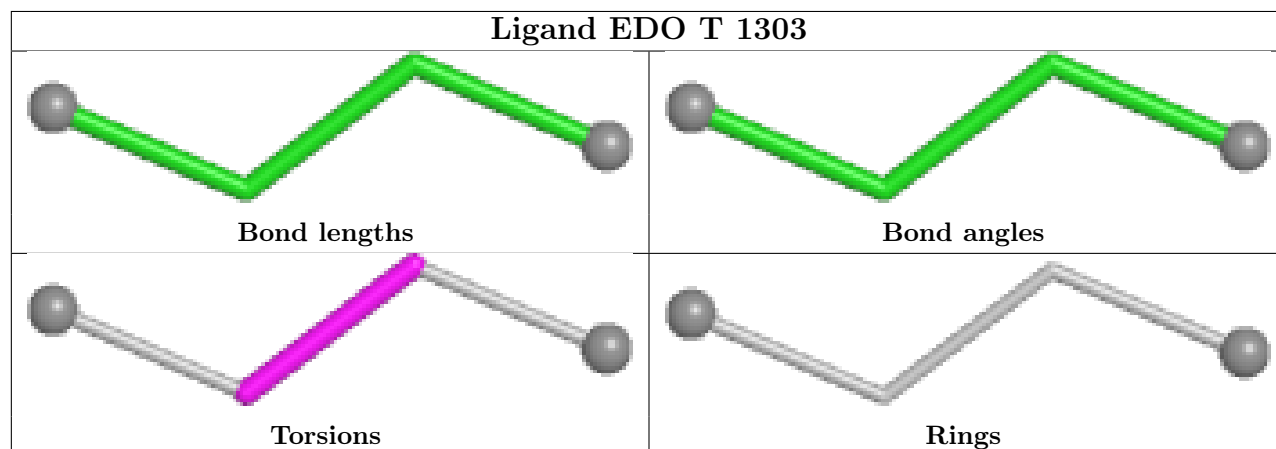
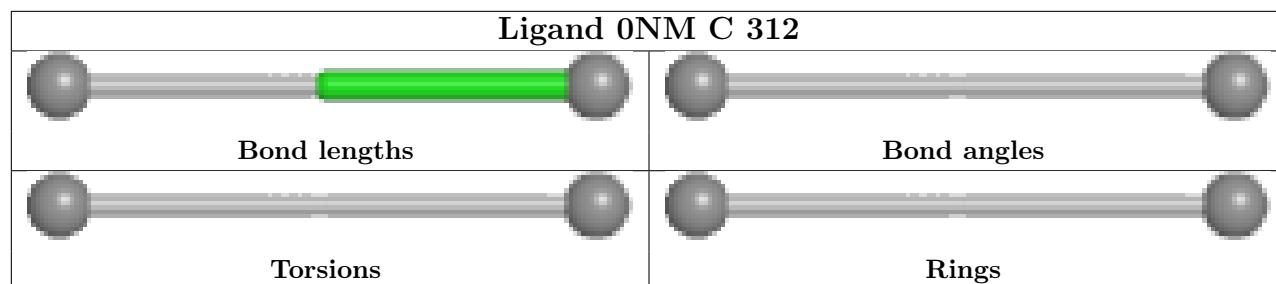


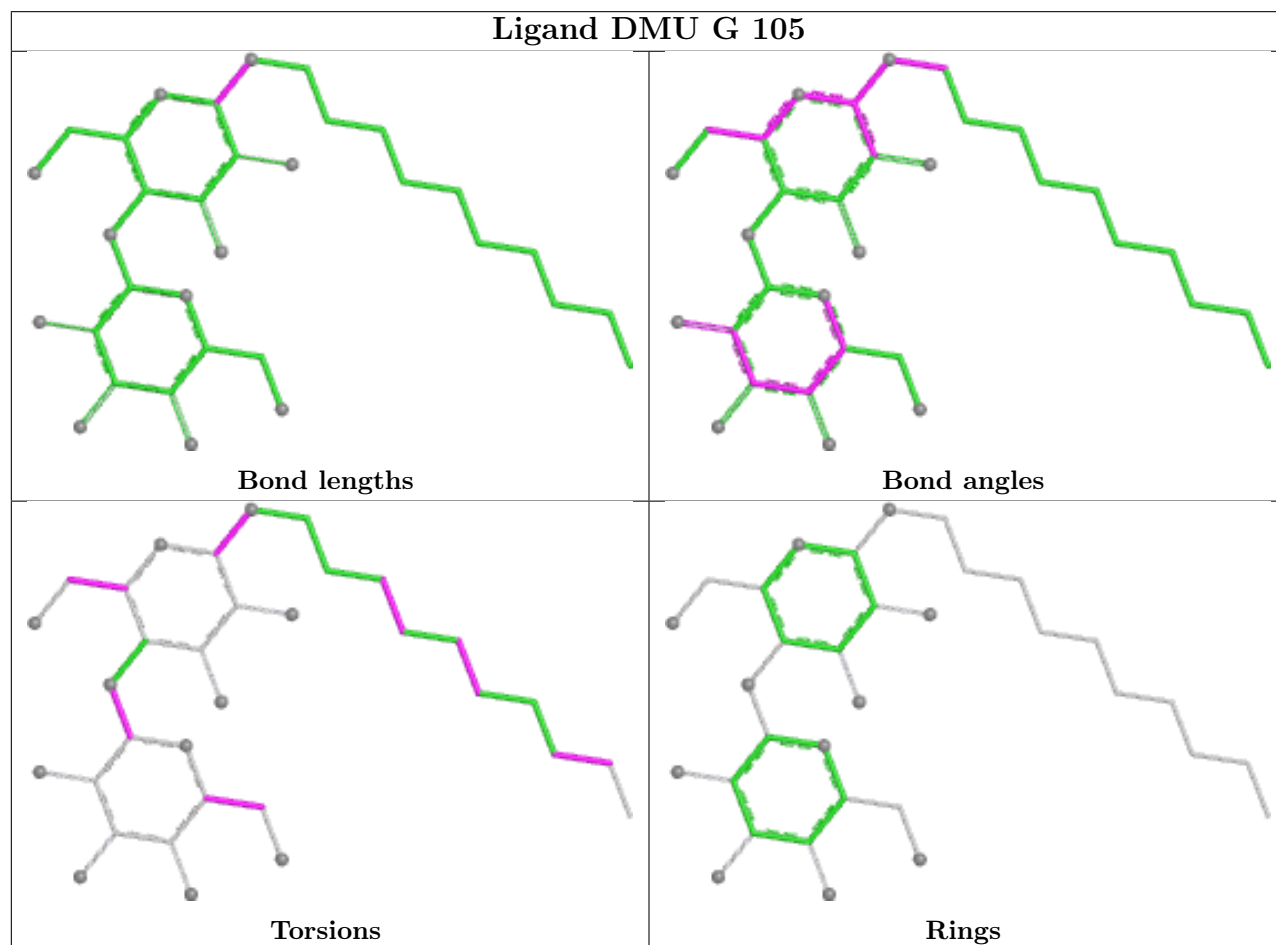
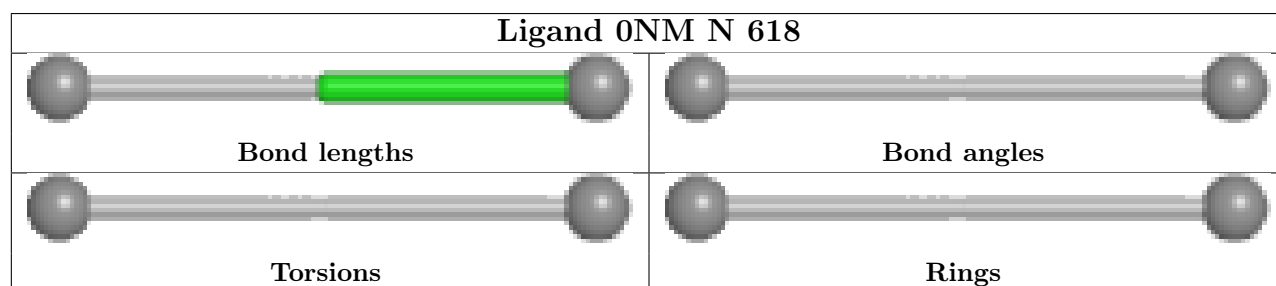
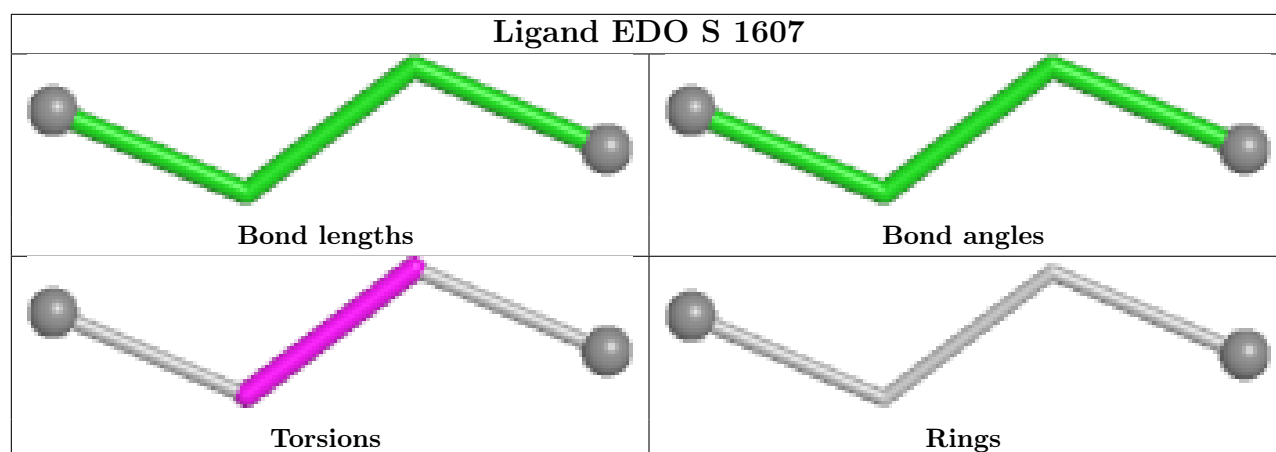


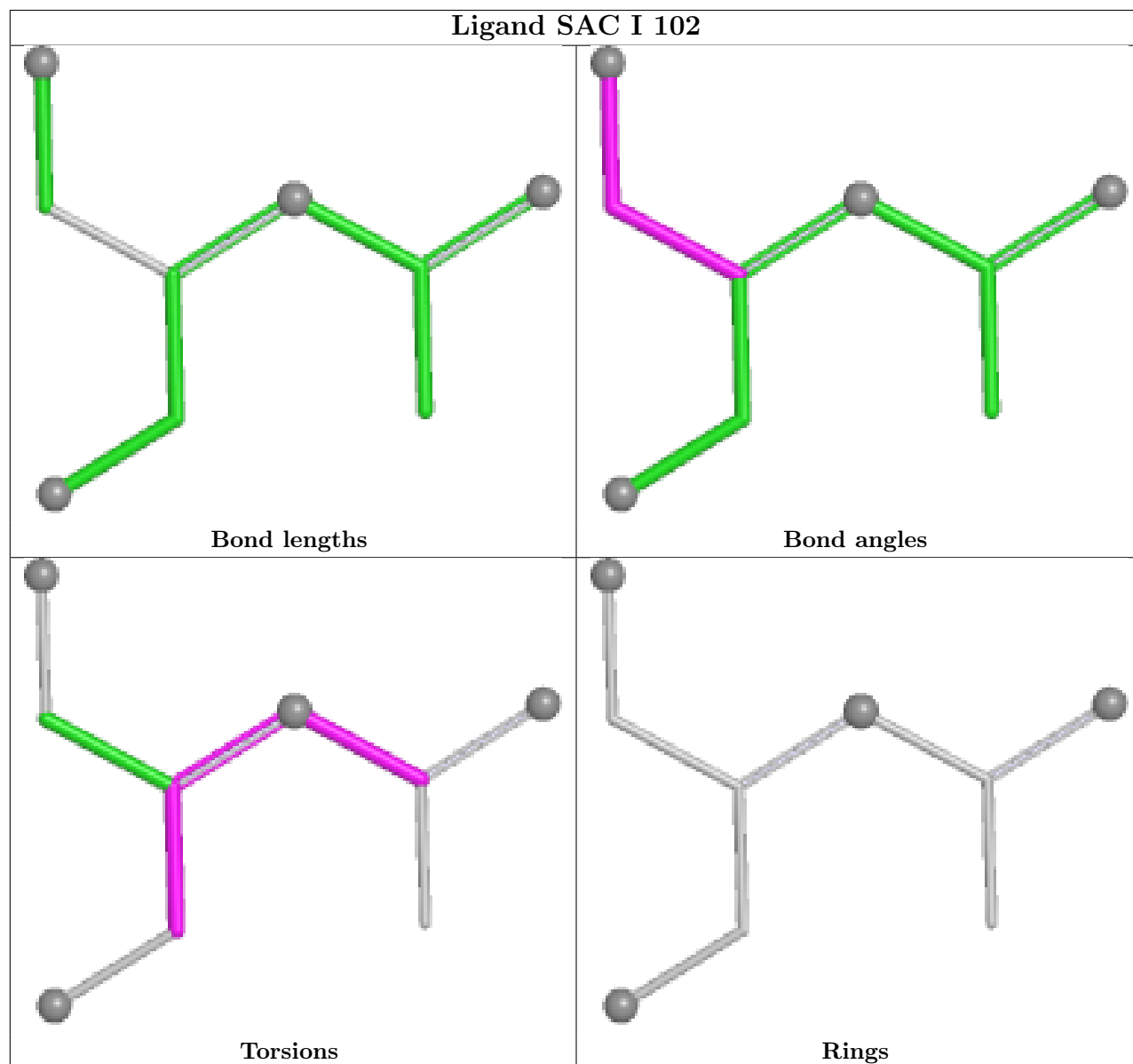
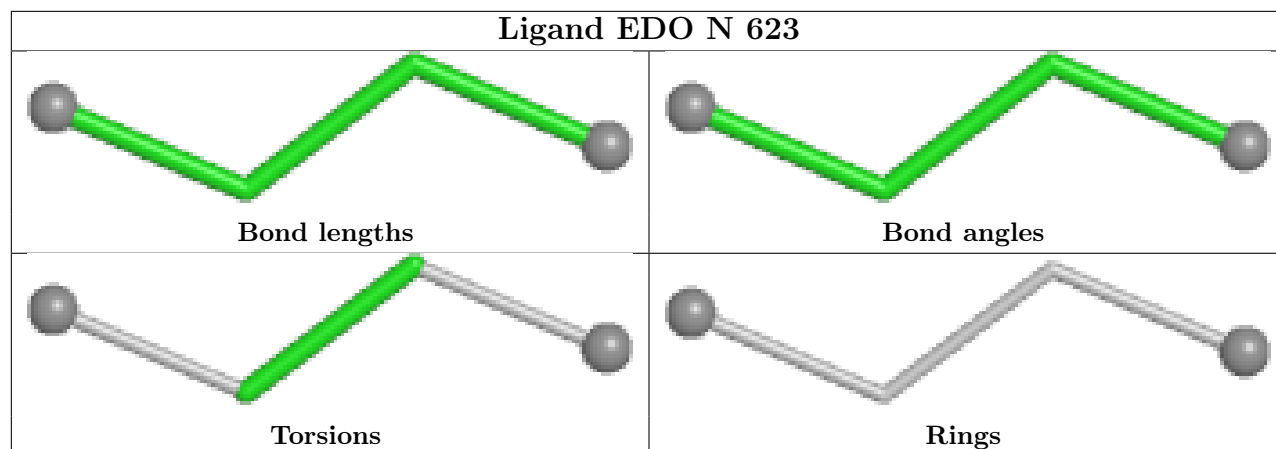


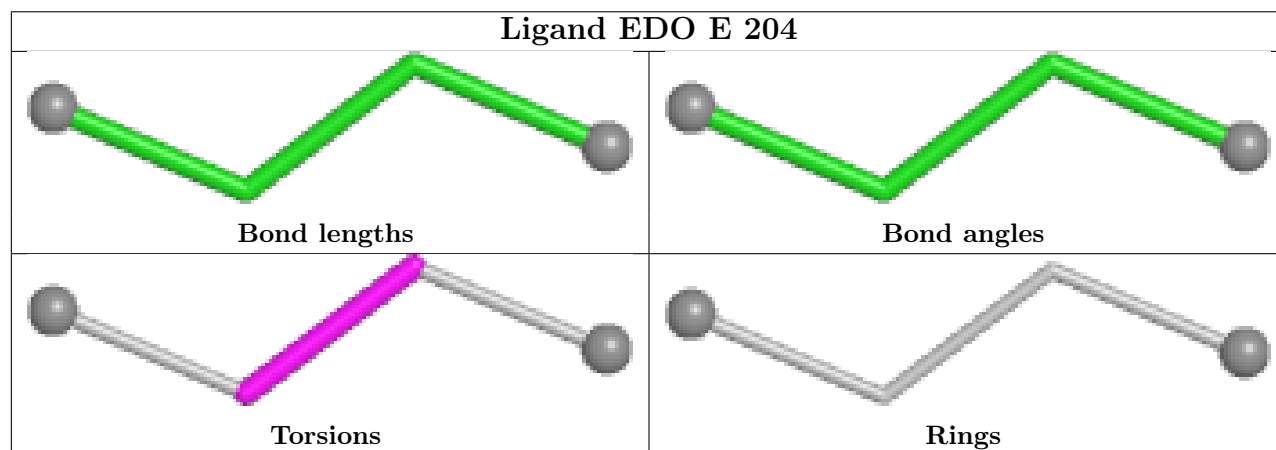
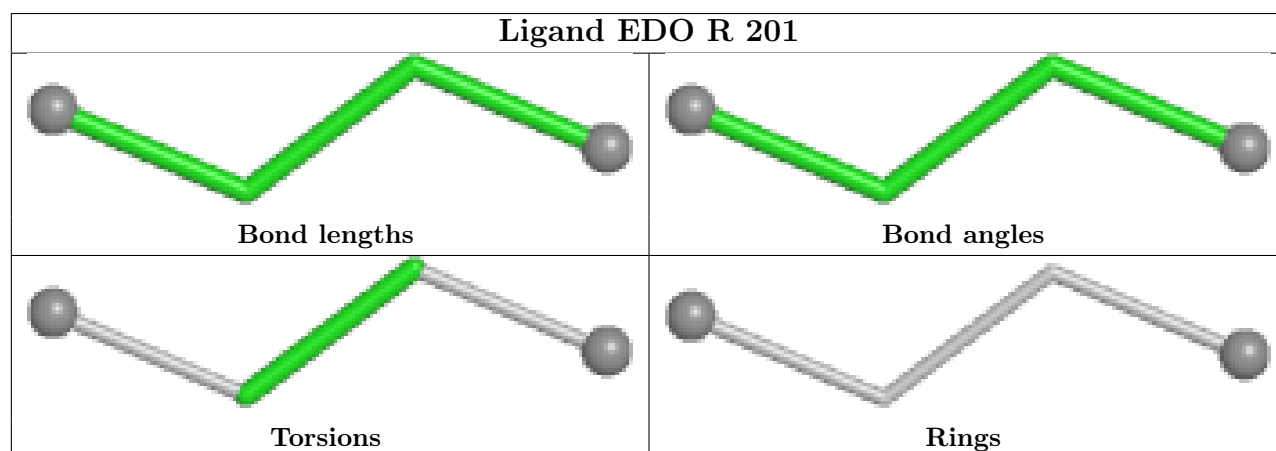
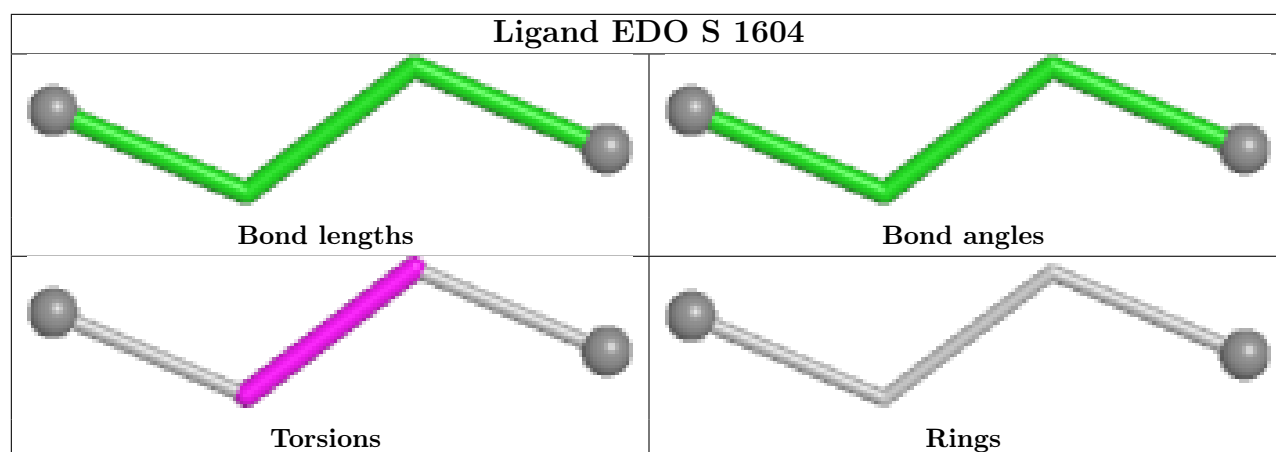


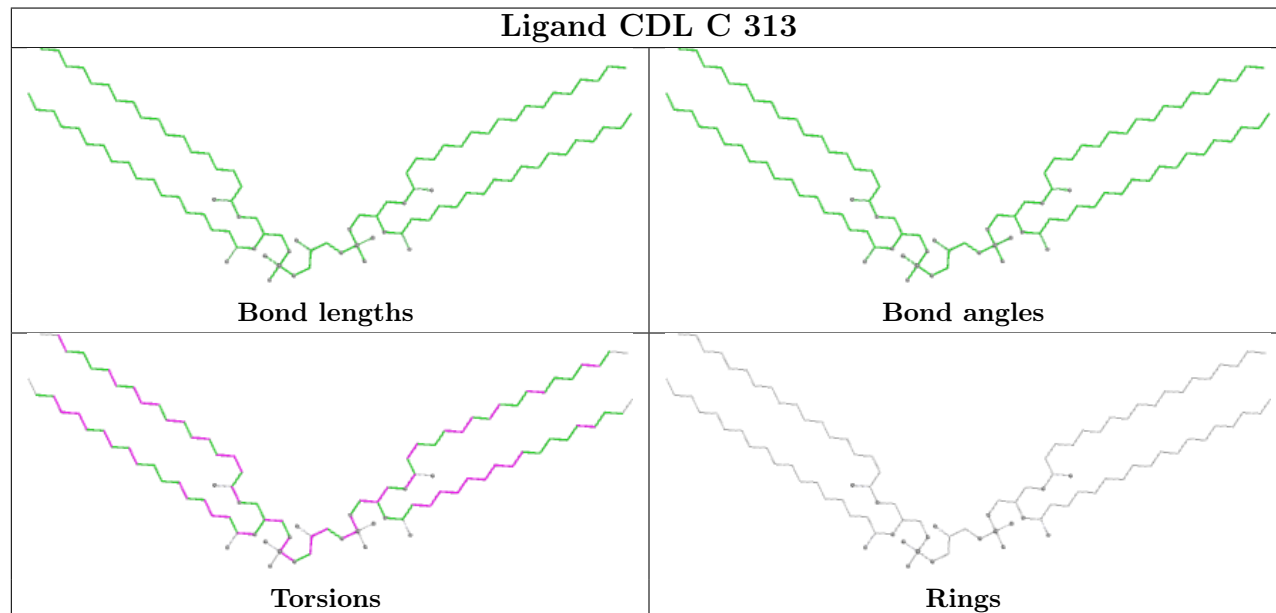
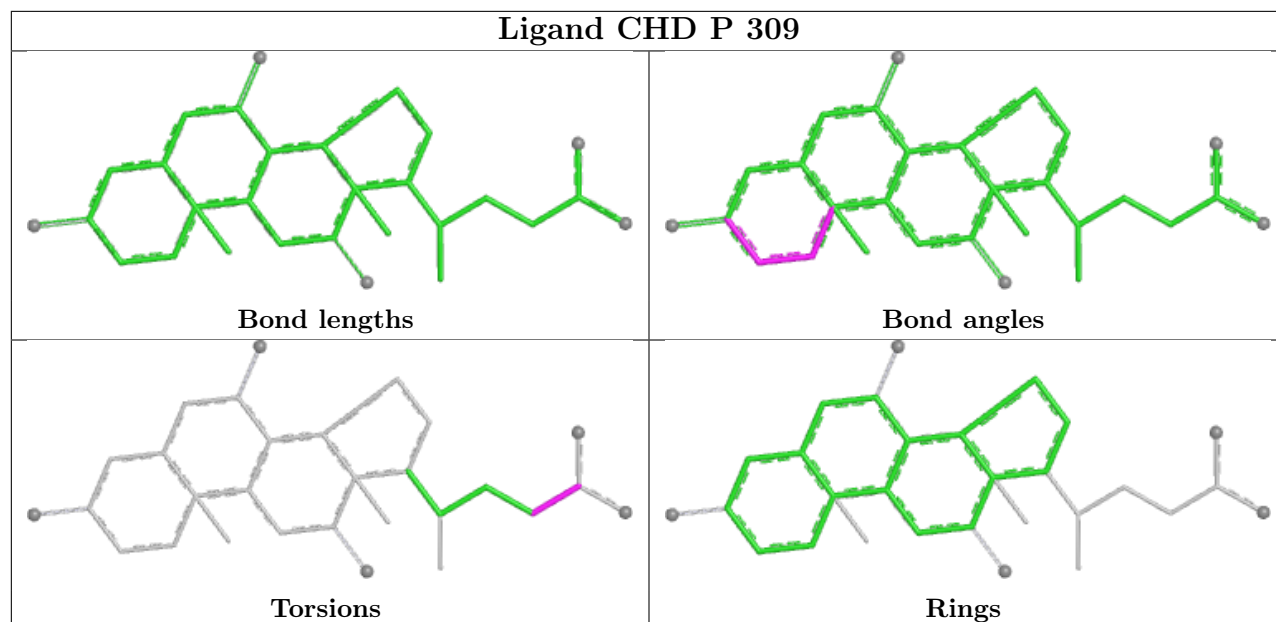


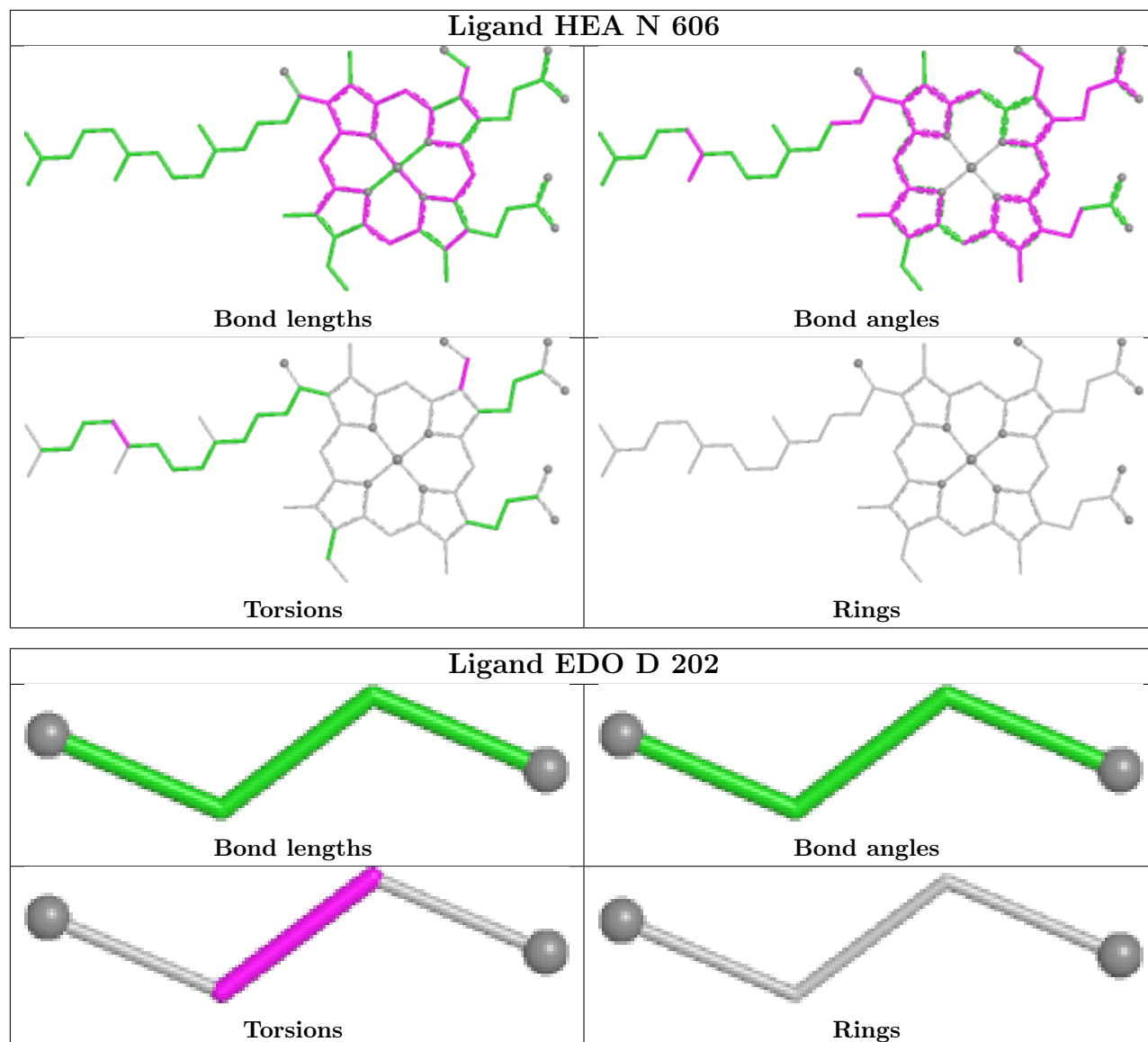


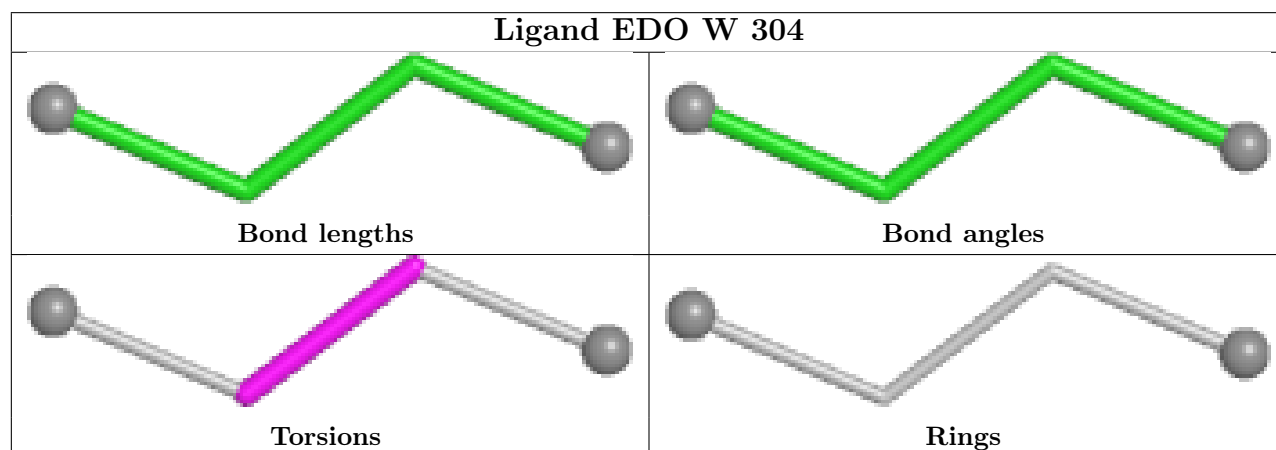
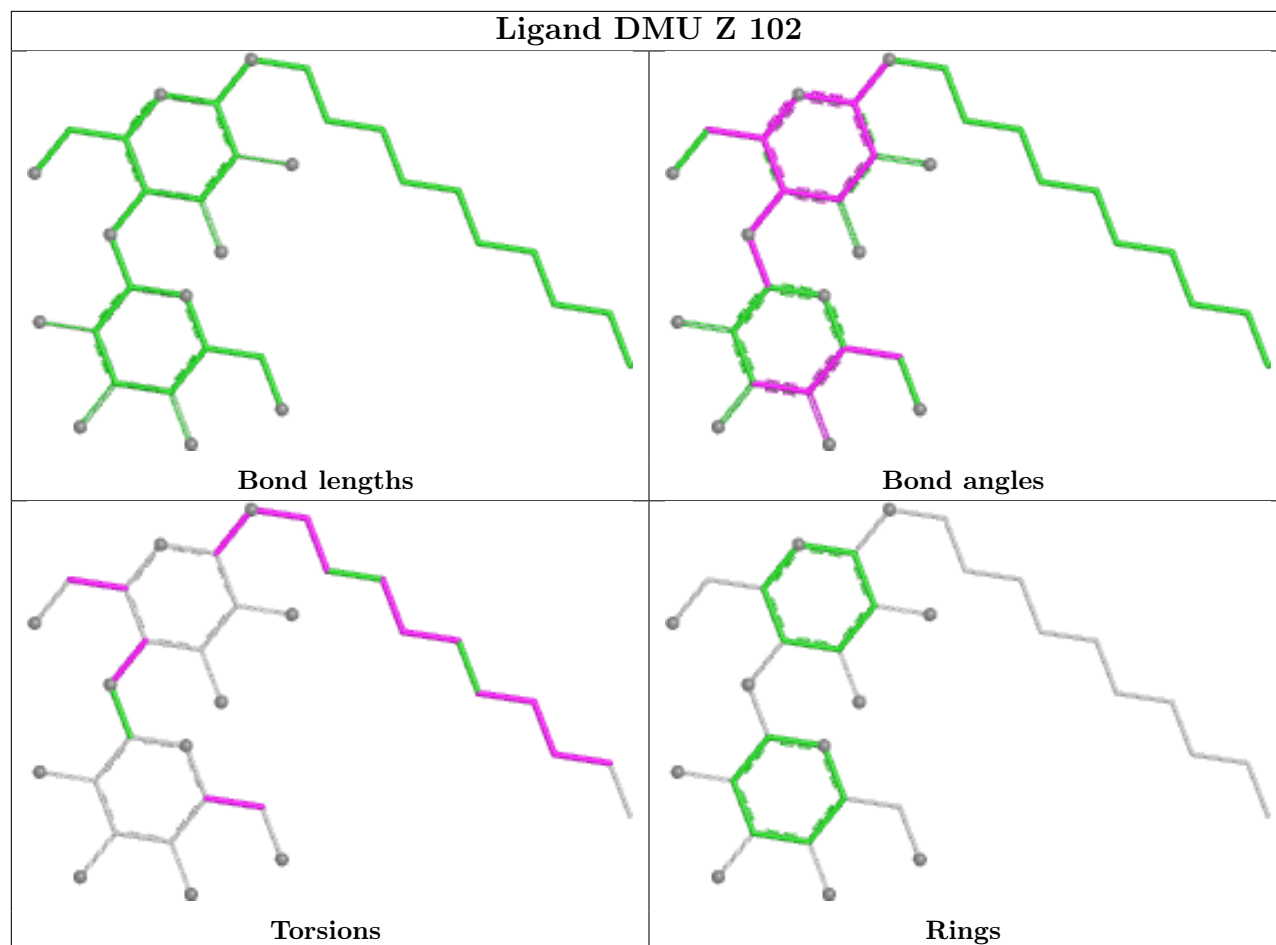




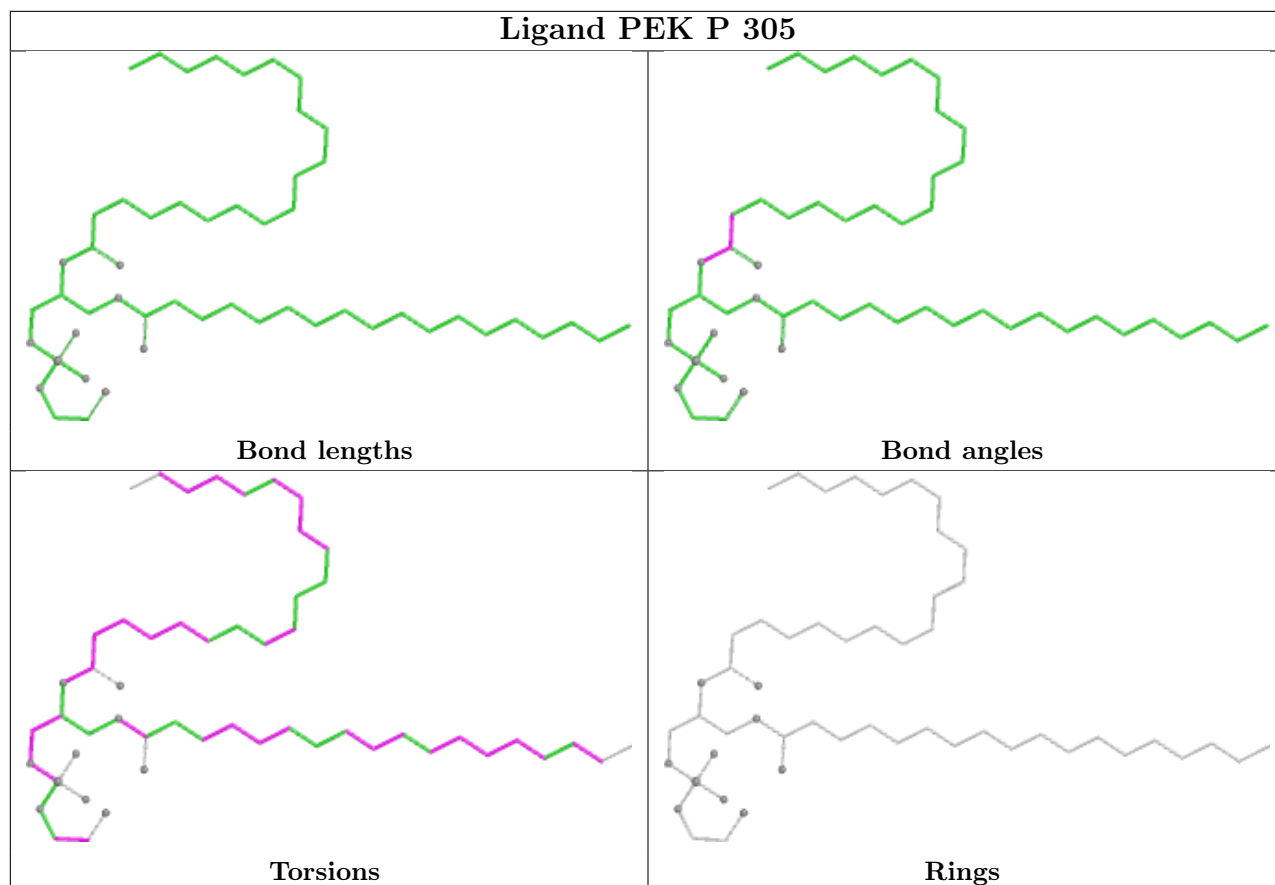




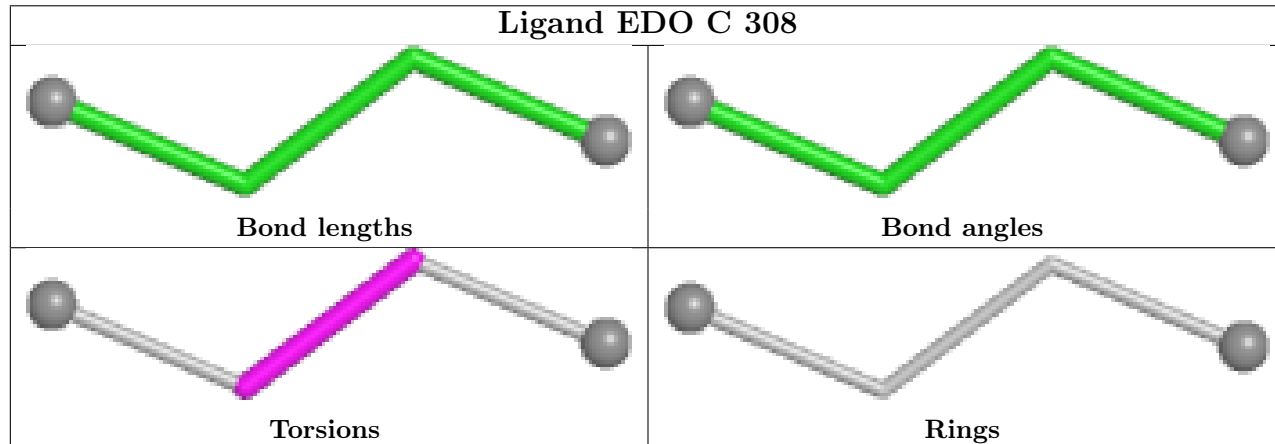


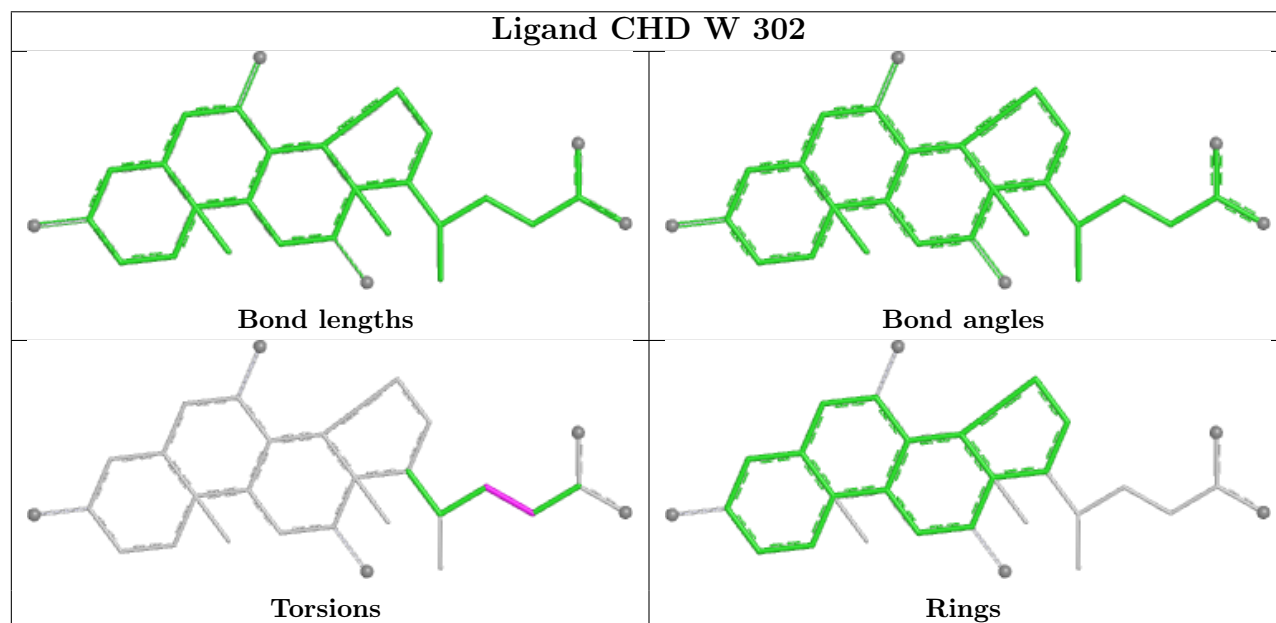
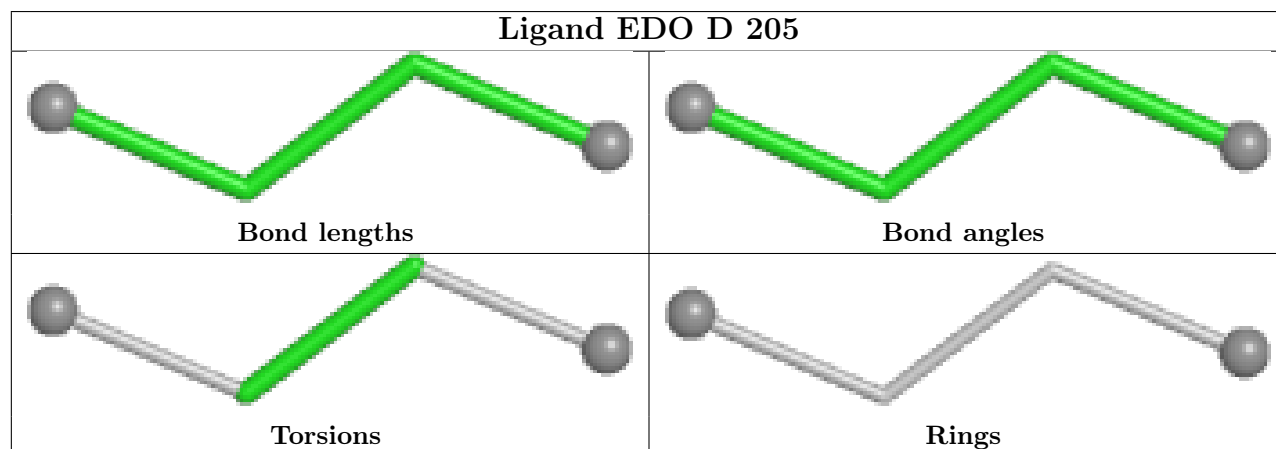
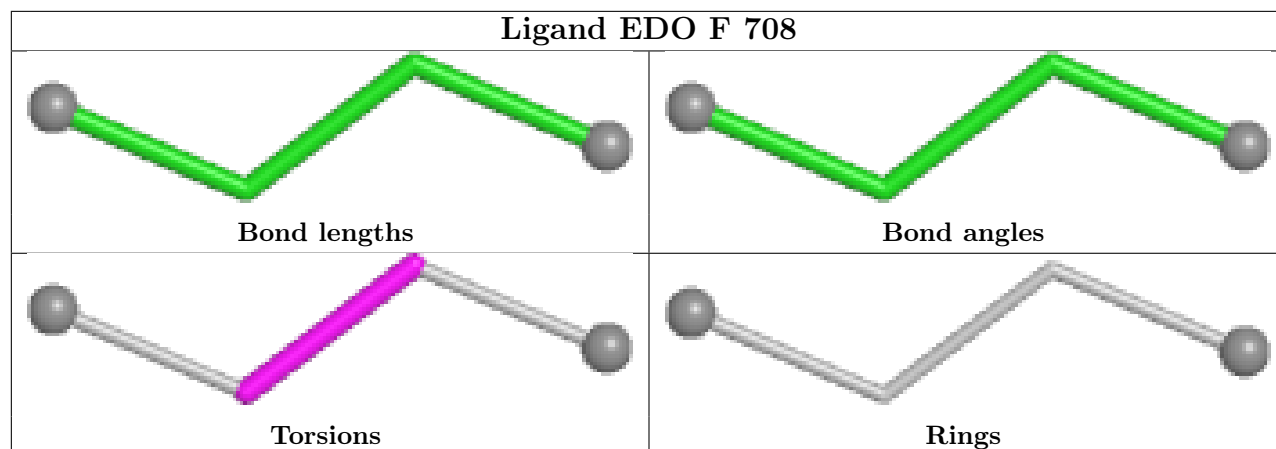


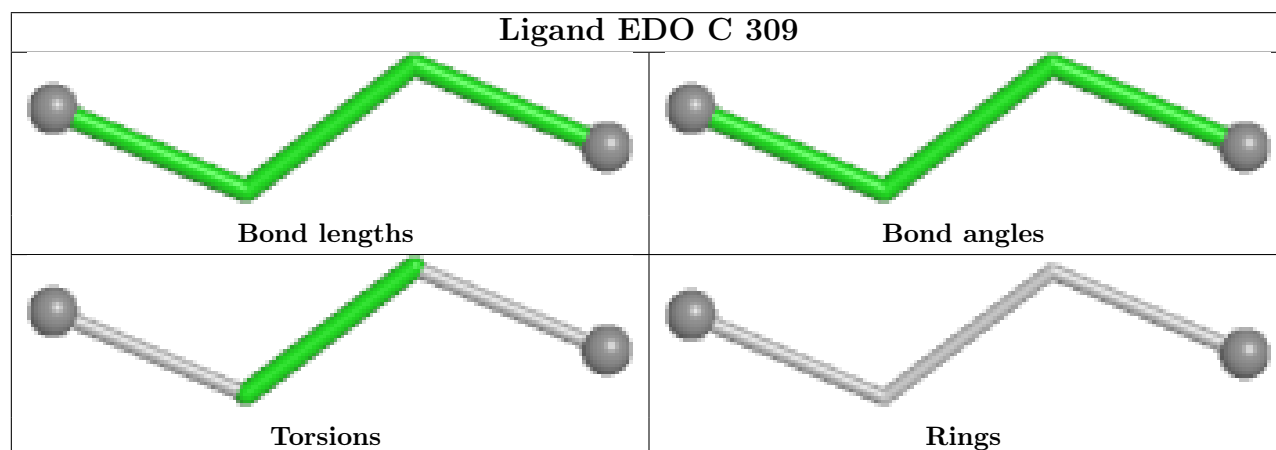
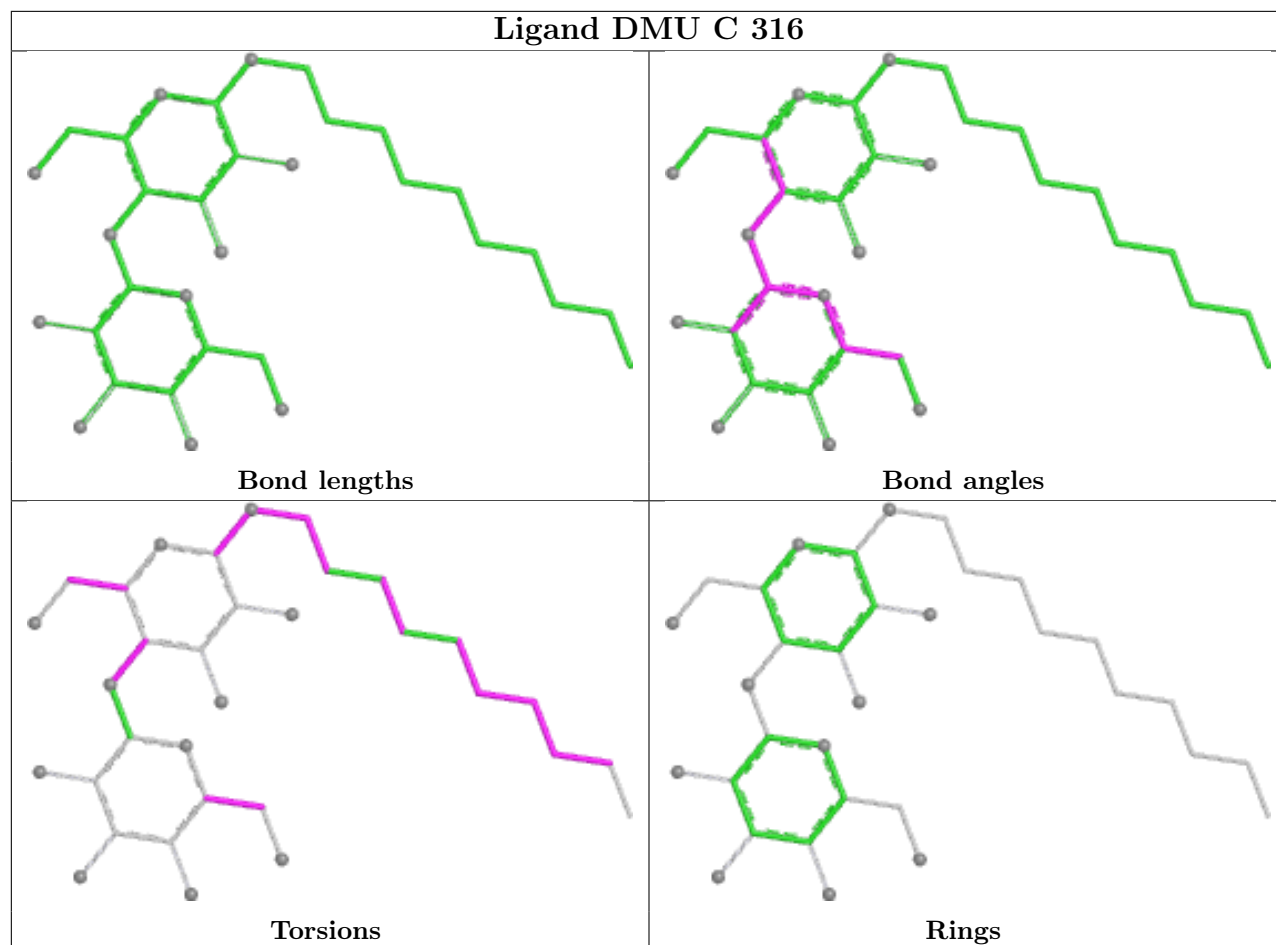
Ligand PEK P 305

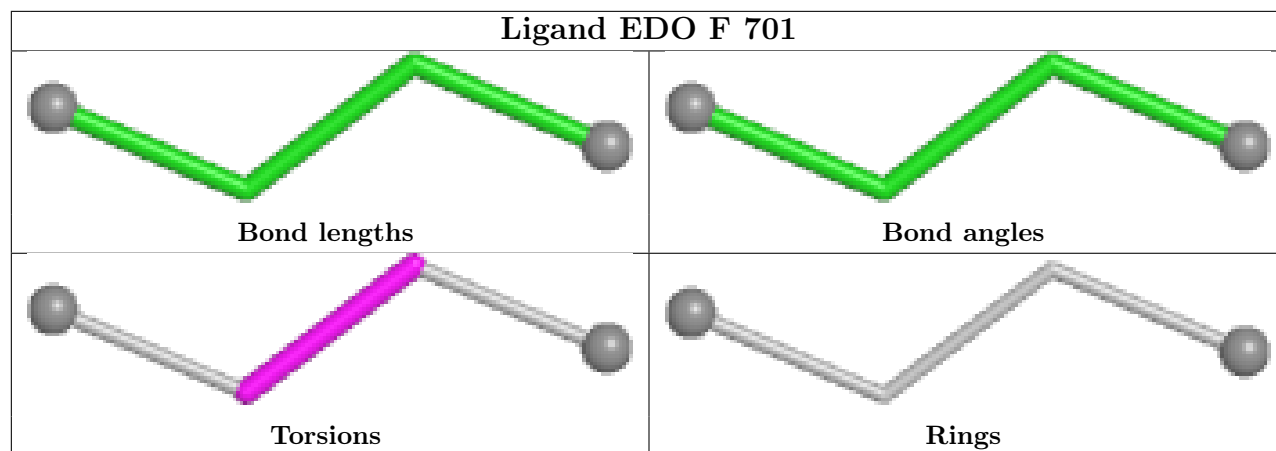


Ligand EDO C 308









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%)	-0.39	4 (0%) 82 84	26, 33, 42, 73	0
1	N	513/514 (99%)	0.21	7 (1%) 73 75	33, 43, 55, 84	0
2	B	226/227 (99%)	0.08	7 (3%) 51 54	29, 39, 69, 93	0
2	O	226/227 (99%)	0.54	12 (5%) 32 34	38, 51, 80, 103	0
3	C	259/261 (99%)	-0.20	3 (1%) 76 78	30, 37, 49, 88	0
3	P	259/261 (99%)	0.13	5 (1%) 66 69	34, 43, 57, 90	0
4	D	144/147 (97%)	0.08	0 100 100	34, 43, 58, 87	0
4	Q	141/147 (95%)	1.04	12 (8%) 16 17	47, 63, 86, 103	0
5	E	105/109 (96%)	0.05	1 (0%) 79 81	37, 46, 69, 117	0
5	R	105/109 (96%)	0.68	4 (3%) 44 46	46, 58, 75, 117	0
6	F	98/98 (100%)	0.40	9 (9%) 14 15	34, 44, 93, 151	0
6	S	98/98 (100%)	0.67	7 (7%) 22 23	40, 53, 93, 149	0
7	G	83/85 (97%)	0.97	16 (19%) 3 3	34, 44, 115, 146	0
7	T	83/85 (97%)	1.26	20 (24%) 2 2	36, 52, 110, 123	0
8	H	79/85 (92%)	0.59	10 (12%) 8 8	34, 49, 88, 98	0
8	U	79/85 (92%)	0.71	7 (8%) 15 16	44, 56, 106, 118	0
9	I	72/73 (98%)	0.40	6 (8%) 17 18	35, 51, 76, 81	0
9	V	72/73 (98%)	0.67	5 (6%) 23 24	41, 61, 82, 101	0
10	J	58/59 (98%)	0.38	4 (6%) 23 24	35, 47, 72, 123	0
10	W	58/59 (98%)	0.98	8 (13%) 6 6	46, 56, 83, 128	0
11	K	49/56 (87%)	0.56	1 (2%) 65 67	33, 45, 64, 82	0
11	X	49/56 (87%)	1.04	3 (6%) 27 29	56, 63, 86, 116	0
12	L	46/47 (97%)	0.04	1 (2%) 62 65	34, 40, 62, 93	0
12	Y	46/47 (97%)	0.93	3 (6%) 25 26	46, 56, 82, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.19	1 (2%) 61 64	34, 40, 67, 90	0
13	Z	43/46 (93%)	1.17	8 (18%) 3 3	51, 60, 86, 114	0
All	All	3547/3614 (98%)	0.28	164 (4%) 37 39	26, 44, 78, 151	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	4	ALA	9.7
7	G	3	ALA	9.6
6	F	96	LEU	8.0
8	H	45	ALA	7.6
7	G	1	ALA	6.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	T	11	11/12	0.49	0.32	63,91,147,165	0
7	TPO	G	11	11/12	0.62	0.24	54,91,144,148	0
1	FME	N	1	10/11	0.88	0.15	55,63,89,89	0
1	FME	A	1	10/11	0.91	0.14	43,51,95,99	0
2	FME	O	1	10/11	0.95	0.13	46,54,64,70	0
2	FME	B	1	10/11	0.97	0.08	33,38,50,60	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	EDO	W	304	4/4	0.13	0.22	114,117,118,123	0
29	SAC	V	101	9/10	0.36	0.18	103,122,133,133	0
23	CHD	Y	103	29/29	0.64	0.22	99,135,142,153	0
23	CHD	T	1302	29/29	0.67	0.26	71,129,153,158	0
26	DMU	Z	102	33/33	0.68	0.20	67,91,110,120	0
25	CDL	C	313	100/100	0.69	0.31	67,94,143,160	0
26	DMU	G	101	33/33	0.69	0.19	73,114,131,141	0
29	SAC	I	102	9/10	0.70	0.17	79,93,108,110	0
19	EDO	D	204	4/4	0.70	0.26	67,82,89,93	0
24	PEK	C	317	53/53	0.72	0.26	66,83,124,129	0
19	EDO	N	621	4/4	0.72	0.32	49,55,55,58	0
19	EDO	L	504	4/4	0.73	0.18	60,68,70,73	0
26	DMU	P	314	33/33	0.74	0.17	71,94,112,116	0
24	PEK	C	303	53/53	0.74	0.26	65,88,140,165	0
19	EDO	F	702	4/4	0.74	0.27	64,89,91,93	0
26	DMU	G	105	33/33	0.74	0.18	55,90,112,113	0
19	EDO	G	103	4/4	0.75	0.22	87,95,108,110	0
26	DMU	C	316	33/33	0.75	0.17	55,86,100,104	0
19	EDO	Q	1801	4/4	0.76	0.26	69,70,73,87	0
27	TGL	N	604	63/63	0.76	0.28	66,92,112,114	0
17	PGV	M	101	51/51	0.76	0.24	45,82,124,145	0
22	PSC	B	302	52/52	0.76	0.25	52,94,153,161	0
17	PGV	C	305	51/51	0.77	0.23	55,87,130,154	0
19	EDO	V	103	4/4	0.78	0.23	80,87,88,96	0
27	TGL	I	101	63/63	0.78	0.26	54,76,109,116	0
24	PEK	P	301	53/53	0.78	0.22	59,84,139,158	0
19	EDO	J	102	4/4	0.78	0.20	77,79,83,86	0
25	CDL	P	312	100/100	0.78	0.28	62,99,162,190	0
17	PGV	Z	101	51/51	0.79	0.26	53,94,153,166	0
27	TGL	D	201	63/63	0.79	0.25	48,78,104,116	0
24	PEK	P	305	53/53	0.79	0.25	60,87,146,165	0
25	CDL	P	308	100/100	0.80	0.23	51,89,124,143	0
22	PSC	O	302	52/52	0.80	0.24	49,101,159,170	0
17	PGV	P	307	51/51	0.80	0.22	66,95,121,138	0
20	ONM	N	618	3/3	0.81	0.23	59,59,65,68	0
19	EDO	N	613	4/4	0.82	0.24	61,62,73,74	0
19	EDO	Y	102	4/4	0.82	0.27	92,97,99,101	0
19	EDO	L	505	4/4	0.82	0.20	77,77,81,87	0
20	ONM	N	619	3/3	0.83	0.31	53,53,58,62	0
25	CDL	C	306	100/100	0.83	0.22	49,84,115,124	0
19	EDO	B	311	4/4	0.83	0.21	73,81,83,98	0
27	TGL	Y	101	63/63	0.83	0.26	57,82,128,138	0
19	EDO	T	1301	4/4	0.83	0.20	61,66,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	EDO	N	626	4/4	0.83	0.21	70,71,73,84	0
19	EDO	B	308	4/4	0.84	0.26	52,66,74,76	0
19	EDO	G	104	4/4	0.85	0.19	66,67,67,70	0
19	EDO	Q	1803	4/4	0.85	0.16	69,83,84,85	0
19	EDO	R	202	4/4	0.85	0.17	63,69,75,82	0
19	EDO	G	107	4/4	0.85	0.13	85,86,88,90	0
27	TGL	N	622	63/63	0.86	0.21	69,86,100,108	0
19	EDO	S	1604	4/4	0.86	0.20	61,70,77,78	0
19	EDO	B	312	4/4	0.86	0.17	86,94,95,95	0
19	EDO	C	309	4/4	0.86	0.16	68,76,77,78	0
19	EDO	V	102	4/4	0.87	0.23	86,87,87,94	0
27	TGL	L	502	63/63	0.87	0.20	44,71,100,109	0
19	EDO	B	305	4/4	0.87	0.18	54,57,59,60	0
19	EDO	F	709	4/4	0.87	0.18	53,74,89,99	0
19	EDO	N	610	4/4	0.87	0.21	66,75,79,87	0
19	EDO	S	1606	4/4	0.87	0.21	50,61,72,75	0
19	EDO	N	612	4/4	0.87	0.23	70,76,84,85	0
19	EDO	A	610	4/4	0.88	0.14	47,55,62,65	0
19	EDO	A	616	4/4	0.88	0.17	48,64,68,71	0
23	CHD	W	302	29/29	0.88	0.14	69,80,103,104	0
19	EDO	S	1605	4/4	0.88	0.16	59,63,63,72	0
19	EDO	N	625	4/4	0.88	0.18	71,72,75,85	0
20	0NM	N	616	3/3	0.89	0.31	52,52,62,69	0
19	EDO	S	1607	4/4	0.89	0.14	72,74,76,81	0
19	EDO	C	315	4/4	0.89	0.18	54,69,71,74	0
19	EDO	N	611	4/4	0.89	0.14	69,73,75,82	0
19	EDO	F	704	4/4	0.89	0.20	59,71,72,78	0
26	DMU	M	103	33/33	0.89	0.12	48,58,74,88	0
19	EDO	P	311	4/4	0.89	0.18	61,67,76,80	0
19	EDO	E	204	4/4	0.89	0.25	76,77,86,88	0
19	EDO	N	623	4/4	0.90	0.16	51,57,64,68	0
23	CHD	J	101	29/29	0.90	0.12	54,67,82,88	0
19	EDO	N	624	4/4	0.90	0.13	54,55,56,65	0
19	EDO	S	1601	4/4	0.90	0.17	53,67,67,68	0
19	EDO	A	609	4/4	0.90	0.15	39,40,46,50	0
19	EDO	A	611	4/4	0.90	0.15	54,55,61,68	0
19	EDO	N	620	4/4	0.90	0.19	49,71,81,91	0
19	EDO	E	203	4/4	0.90	0.15	60,68,70,88	0
19	EDO	Q	1802	4/4	0.90	0.21	75,80,82,99	0
19	EDO	A	612	4/4	0.91	0.27	62,64,65,68	0
19	EDO	B	307	4/4	0.91	0.14	59,67,72,73	0
20	0NM	C	312	3/3	0.91	0.23	43,43,52,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	EDO	F	705	4/4	0.91	0.14	66,68,71,71	0
20	ONM	N	617	3/3	0.91	0.21	66,66,69,74	0
19	EDO	L	501	4/4	0.91	0.15	53,61,68,73	0
19	EDO	P	313	4/4	0.91	0.13	45,46,48,55	0
19	EDO	C	311	4/4	0.91	0.15	71,74,75,78	0
19	EDO	C	314	4/4	0.91	0.17	53,57,60,66	0
19	EDO	N	609	4/4	0.91	0.17	62,62,65,68	0
23	CHD	P	309	29/29	0.91	0.10	51,59,66,68	0
19	EDO	R	201	4/4	0.91	0.13	50,52,53,54	0
19	EDO	D	203	4/4	0.92	0.17	67,68,70,78	0
19	EDO	I	103	4/4	0.92	0.16	62,63,66,72	0
24	PEK	P	304	53/53	0.92	0.16	45,62,98,106	0
19	EDO	A	618	4/4	0.92	0.17	62,68,68,71	0
19	EDO	W	301	4/4	0.92	0.15	61,77,77,80	0
19	EDO	W	303	4/4	0.92	0.18	68,79,81,82	0
19	EDO	J	103	4/4	0.92	0.14	57,61,62,74	0
19	EDO	B	309	4/4	0.92	0.14	65,67,67,68	0
19	EDO	N	614	4/4	0.92	0.18	53,65,73,74	0
19	EDO	B	310	4/4	0.92	0.14	54,65,68,72	0
19	EDO	D	202	4/4	0.92	0.12	55,66,69,70	0
19	EDO	F	708	4/4	0.93	0.14	52,55,62,63	0
19	EDO	M	102	4/4	0.93	0.14	69,76,78,82	0
19	EDO	O	303	4/4	0.93	0.16	69,71,72,78	0
19	EDO	O	304	4/4	0.93	0.19	58,62,64,67	0
23	CHD	C	307	29/29	0.93	0.08	48,55,60,61	0
19	EDO	P	310	4/4	0.93	0.13	70,72,76,85	0
19	EDO	C	310	4/4	0.93	0.11	71,74,77,83	0
20	ONM	A	614	3/3	0.93	0.14	49,49,57,67	0
19	EDO	A	617	4/4	0.93	0.15	53,56,57,61	0
19	EDO	A	607	4/4	0.93	0.14	45,46,58,63	0
19	EDO	F	707	4/4	0.93	0.09	44,50,51,52	0
24	PEK	C	302	53/53	0.94	0.14	37,56,92,105	0
19	EDO	S	1603	4/4	0.94	0.11	37,42,42,47	0
20	ONM	A	615	3/3	0.94	0.15	62,62,65,72	0
19	EDO	N	608	4/4	0.94	0.12	45,47,52,55	0
17	PGV	P	302	51/51	0.94	0.13	34,55,83,92	0
19	EDO	B	306	4/4	0.94	0.10	44,45,48,51	0
19	EDO	K	201	4/4	0.95	0.10	65,65,67,73	0
23	CHD	C	301	29/29	0.95	0.07	33,36,42,44	0
19	EDO	E	201	4/4	0.95	0.09	46,47,47,49	0
19	EDO	L	503	4/4	0.95	0.13	66,66,69,77	0
19	EDO	E	202	4/4	0.95	0.10	47,54,56,57	0

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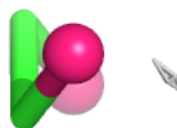
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	PGV	A	604	51/51	0.95	0.12	29,45,74,79	0
19	EDO	D	205	4/4	0.95	0.14	58,64,66,66	0
19	EDO	T	1303	4/4	0.95	0.12	42,45,45,49	0
15	MG	N	602	1/1	0.96	0.05	44,44,44,44	0
23	CHD	P	303	29/29	0.96	0.07	36,40,43,46	0
19	EDO	C	308	4/4	0.96	0.10	43,52,56,56	0
17	PGV	P	306	51/51	0.96	0.11	35,48,86,92	0
19	EDO	G	102	4/4	0.96	0.09	36,38,45,47	0
19	EDO	B	304	4/4	0.96	0.10	30,30,31,37	0
19	EDO	A	608	4/4	0.96	0.07	32,33,33,34	0
23	CHD	B	303	29/29	0.96	0.07	36,40,44,51	0
15	MG	A	602	1/1	0.96	0.05	34,34,34,34	0
19	EDO	F	706	4/4	0.96	0.08	28,31,33,33	0
16	NA	N	603	1/1	0.97	0.05	46,46,46,46	0
17	PGV	C	304	51/51	0.97	0.11	31,44,94,106	0
19	EDO	N	607	4/4	0.97	0.07	40,41,44,48	0
19	EDO	F	701	4/4	0.97	0.07	42,43,43,48	0
23	CHD	G	106	29/29	0.97	0.06	33,42,48,50	0
18	HEA	N	605	60/60	0.98	0.07	30,38,46,60	0
20	ONM	N	615	3/3	0.98	0.09	54,54,61,67	0
18	HEA	N	606	60/60	0.98	0.08	32,40,55,56	0
16	NA	A	603	1/1	0.98	0.08	31,31,31,31	0
18	HEA	A	605	60/60	0.98	0.06	25,30,40,45	0
18	HEA	A	606	60/60	0.98	0.07	25,29,57,65	0
20	ONM	A	613	3/3	0.99	0.11	35,35,36,37	0
28	ZN	S	1602	1/1	0.99	0.02	46,46,46,46	0
21	CUA	B	301	2/2	0.99	0.02	29,29,29,30	0
21	CUA	O	301	2/2	0.99	0.03	41,41,41,43	0
14	CU	A	601	1/1	1.00	0.01	31,31,31,31	0
14	CU	N	601	1/1	1.00	0.02	40,40,40,40	0
28	ZN	F	703	1/1	1.00	0.03	38,38,38,38	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.

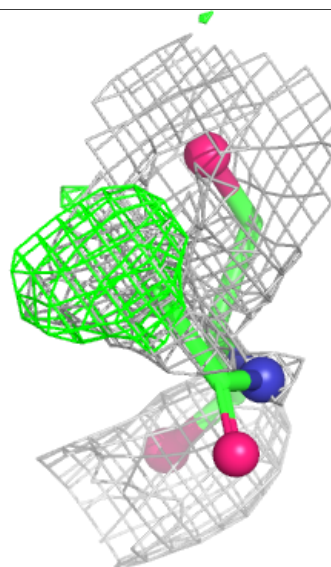
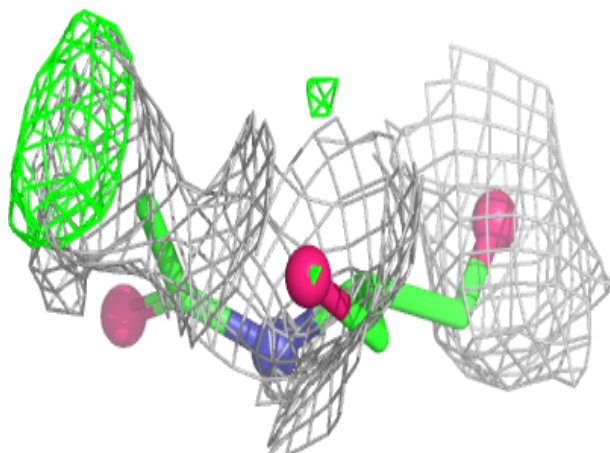
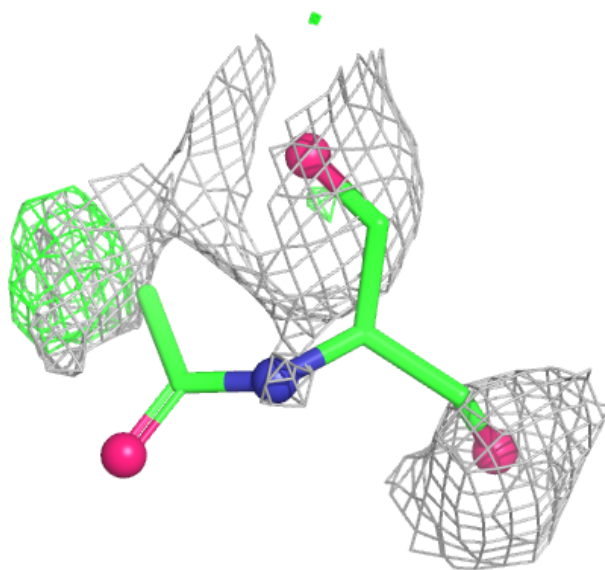
Electron density around EDO W 304:

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



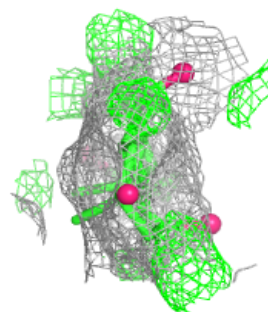
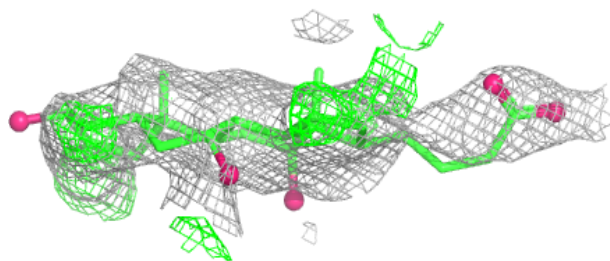
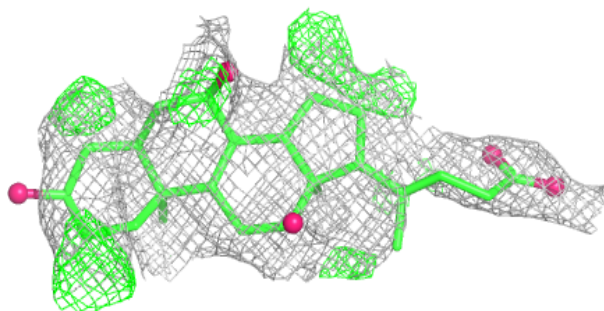
Electron density around SAC V 101:

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

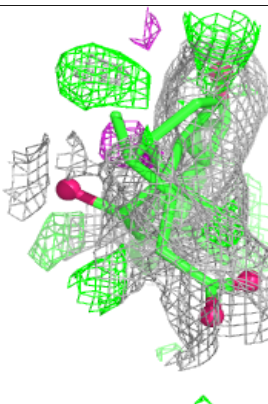
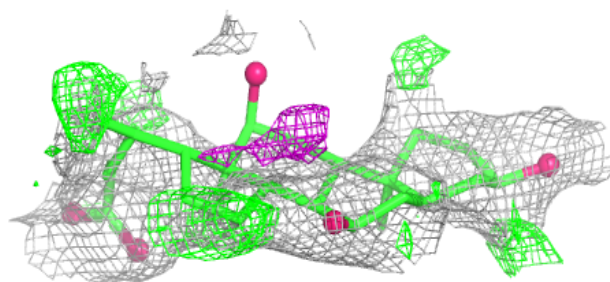
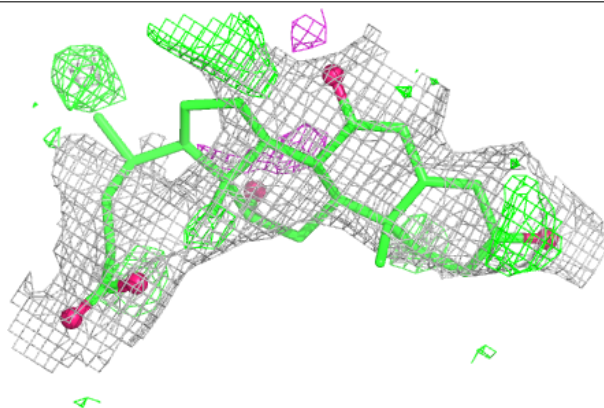


Electron density around CHD Y 103:

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

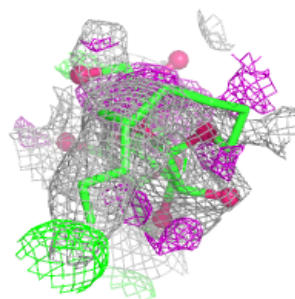
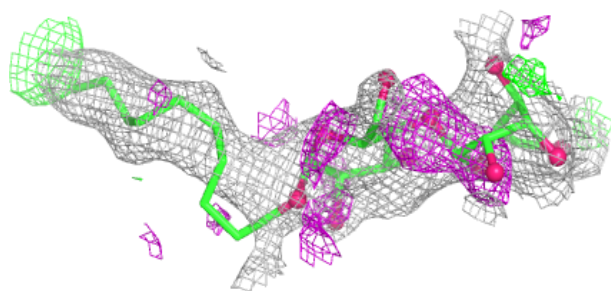
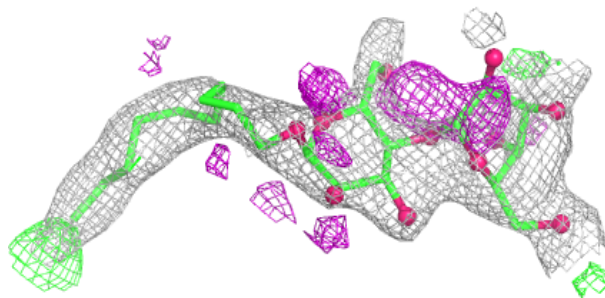
**Electron density around CHD T 1302:**

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

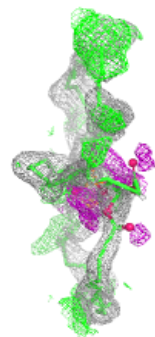
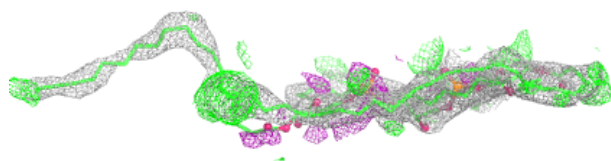
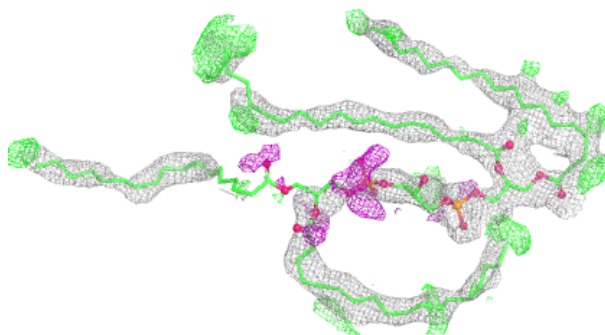


Electron density around DMU Z 102:

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

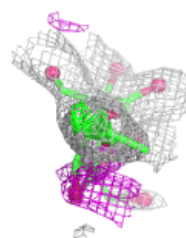
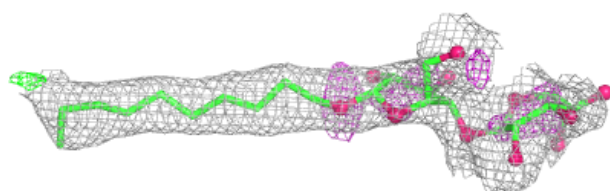
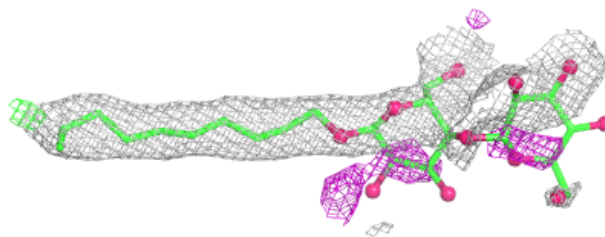
**Electron density around CDL C 313:**

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



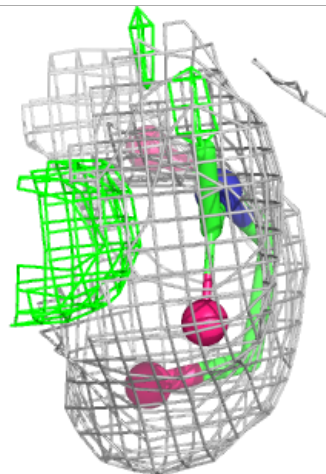
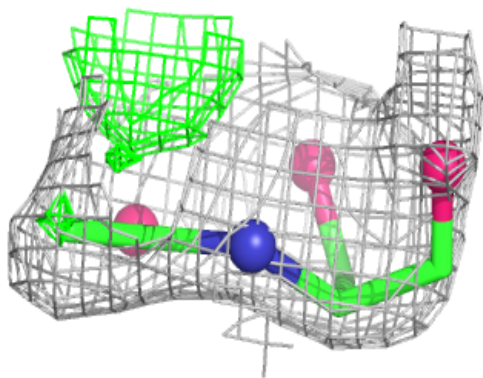
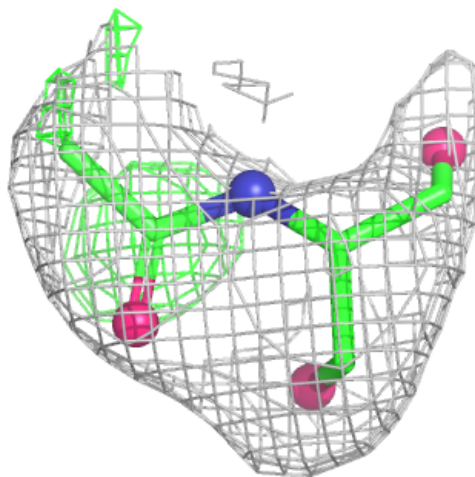
Electron density around DMU G 101:

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



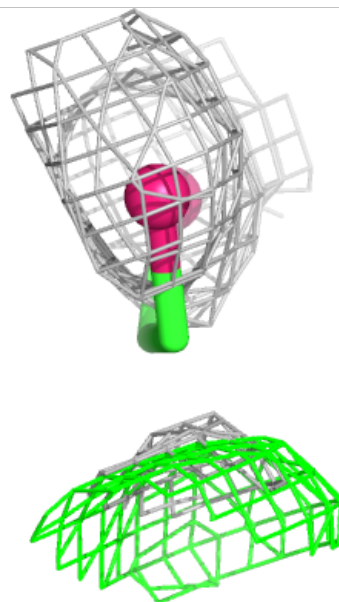
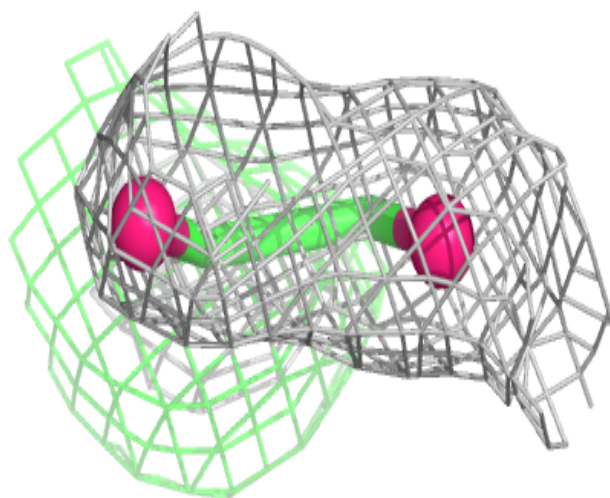
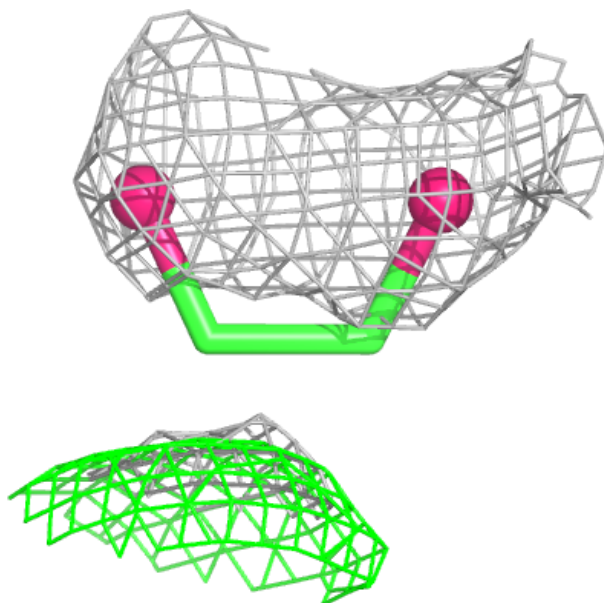
Electron density around SAC I 102:

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



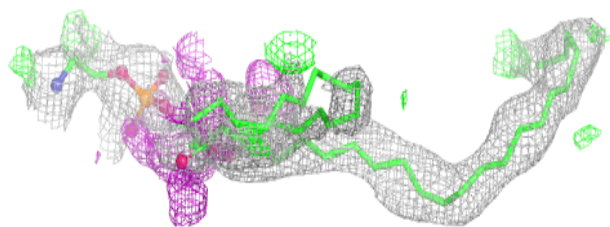
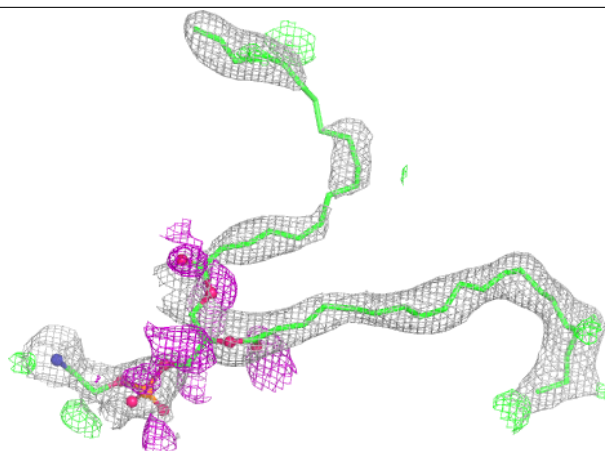
Electron density around EDO D 204:

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



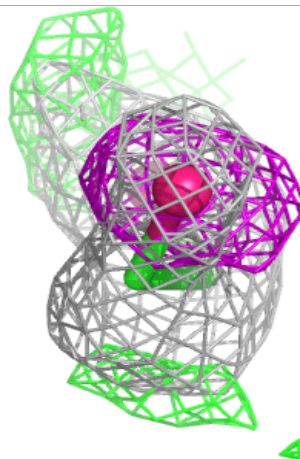
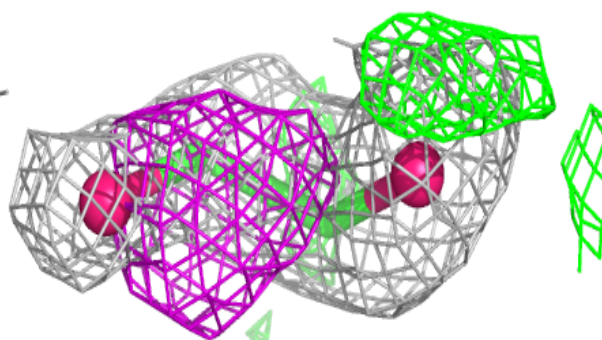
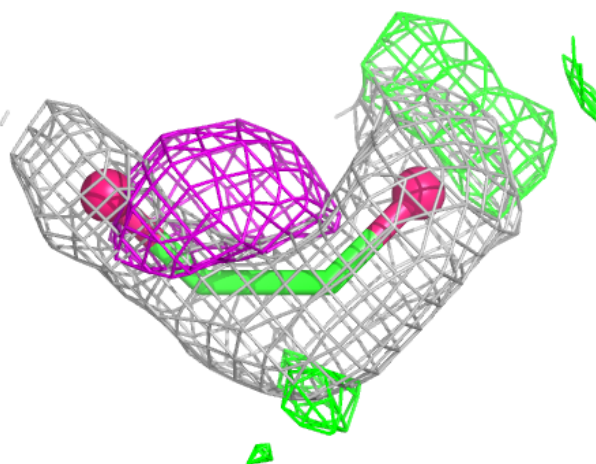
Electron density around PEK C 317:

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



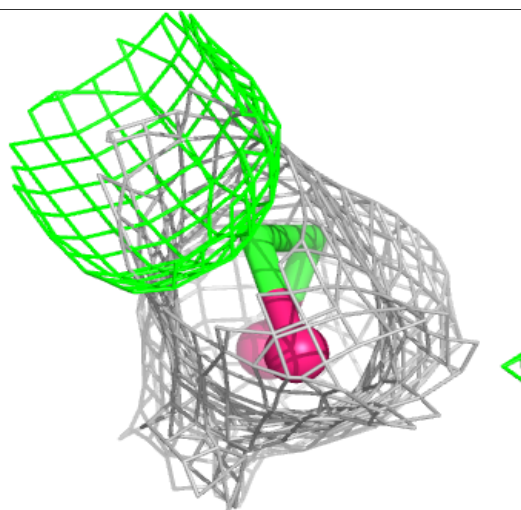
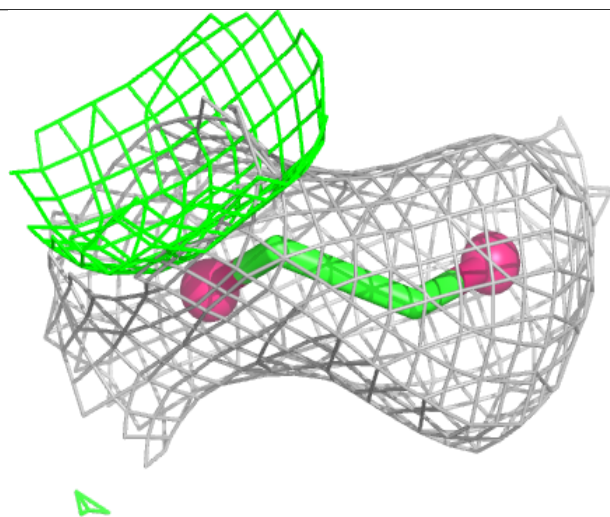
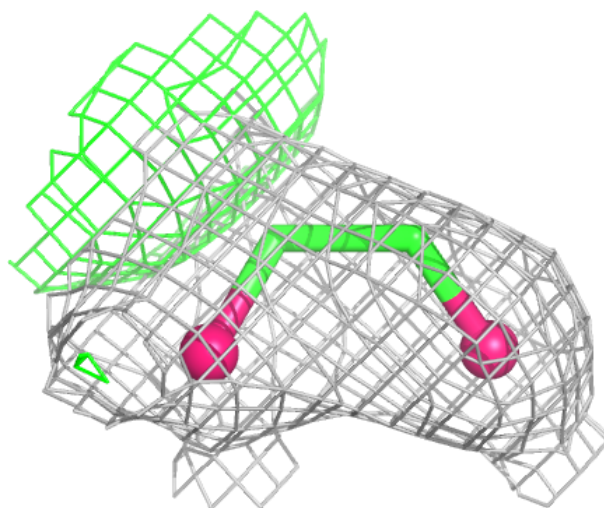
Electron density around EDO N 621:

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



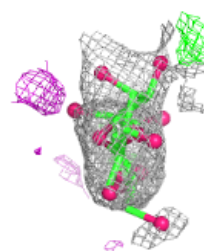
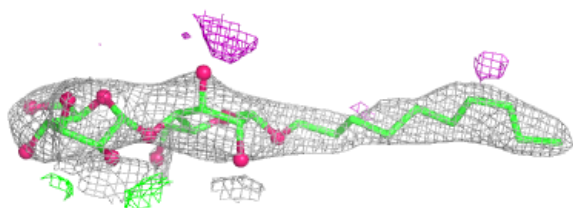
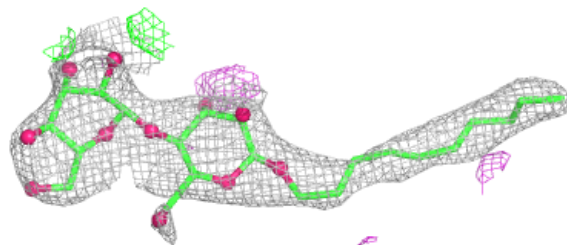
Electron density around EDO L 504:

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

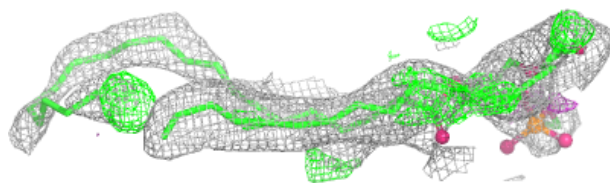
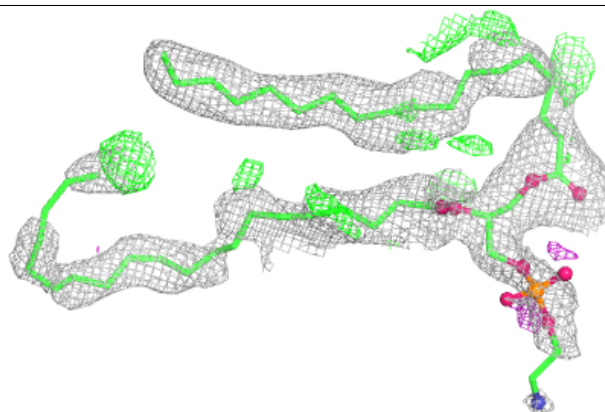


Electron density around DMU P 314:

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

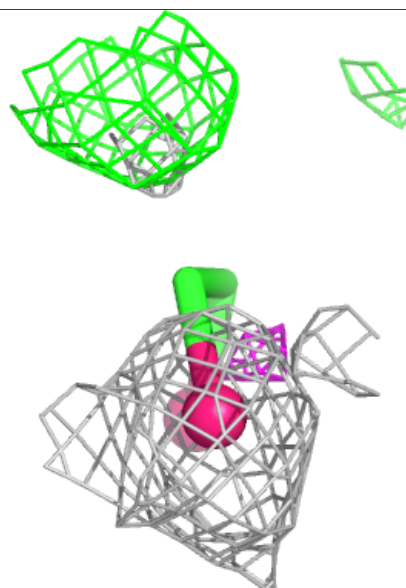
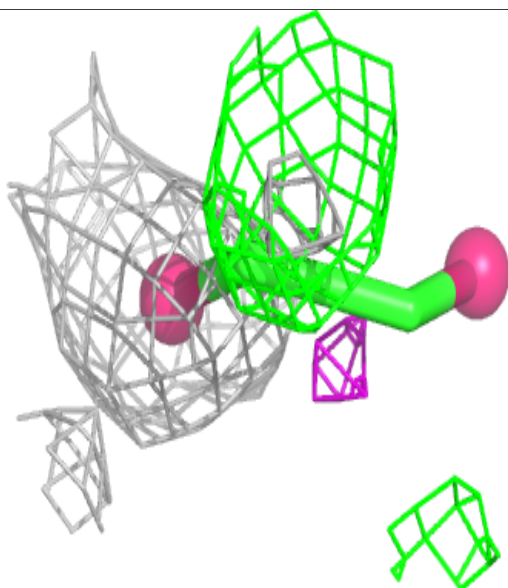
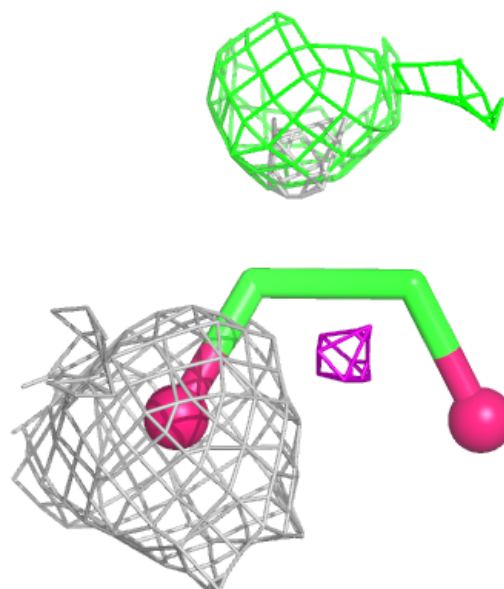
**Electron density around PEK C 303:**

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



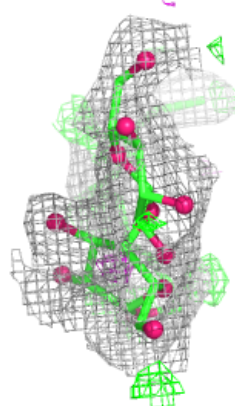
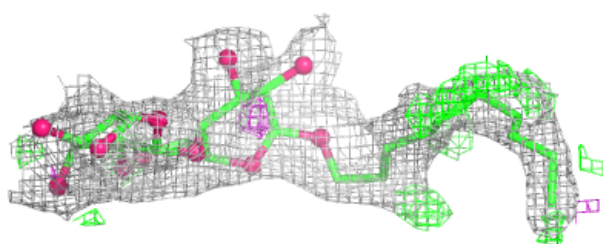
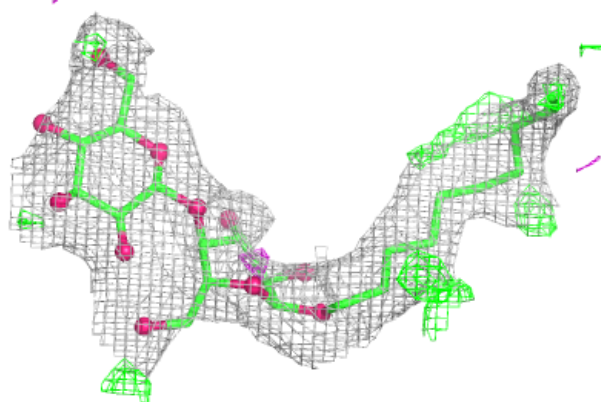
Electron density around EDO F 702:

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

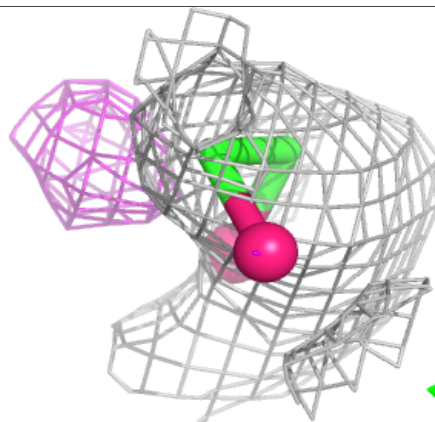
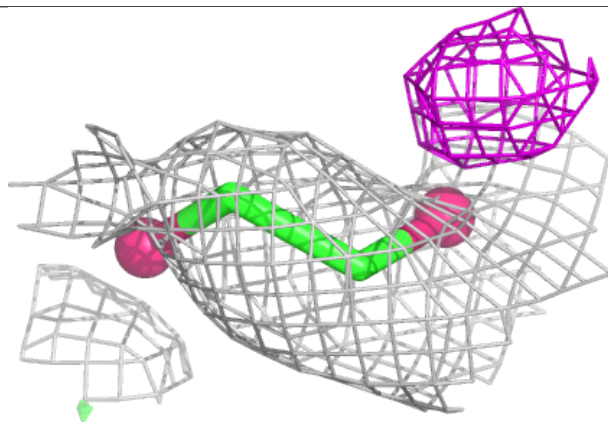
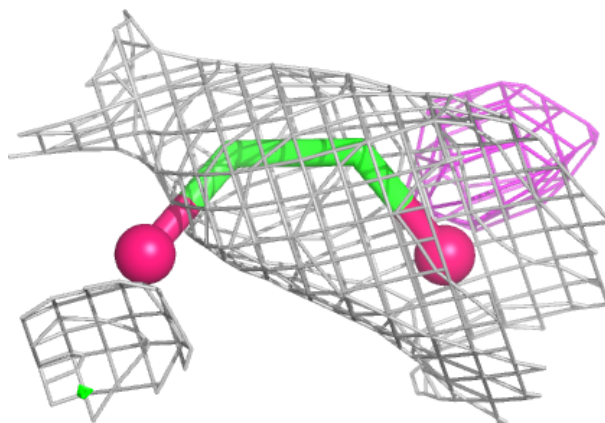


Electron density around DMU G 105:

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

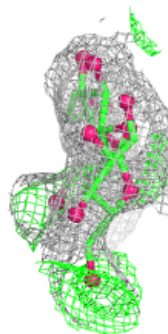
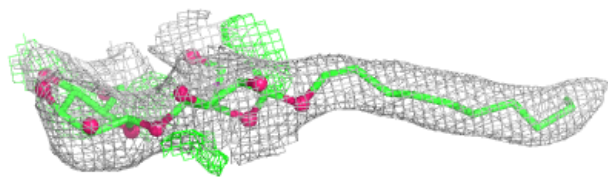
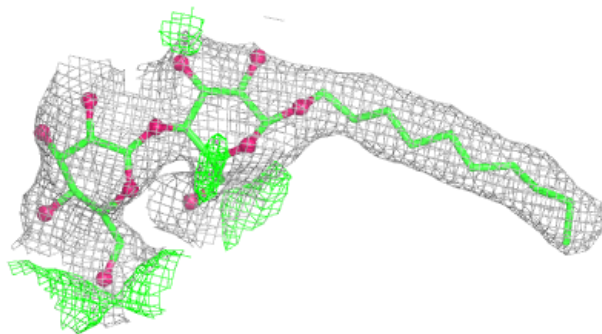
**Electron density around EDO G 103:**

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



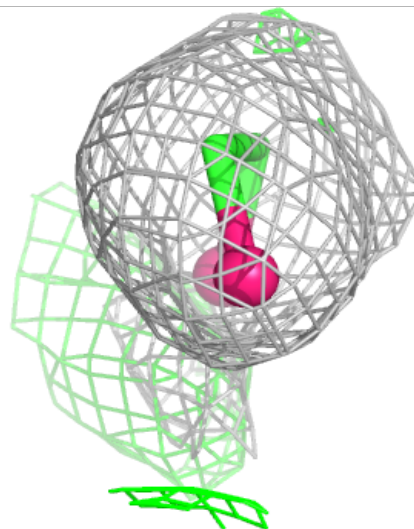
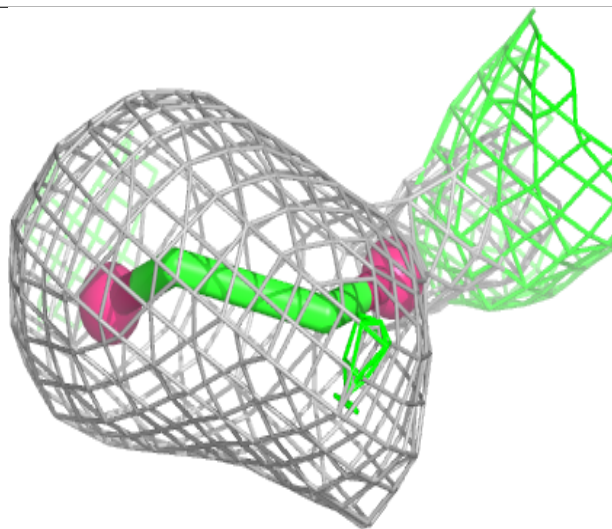
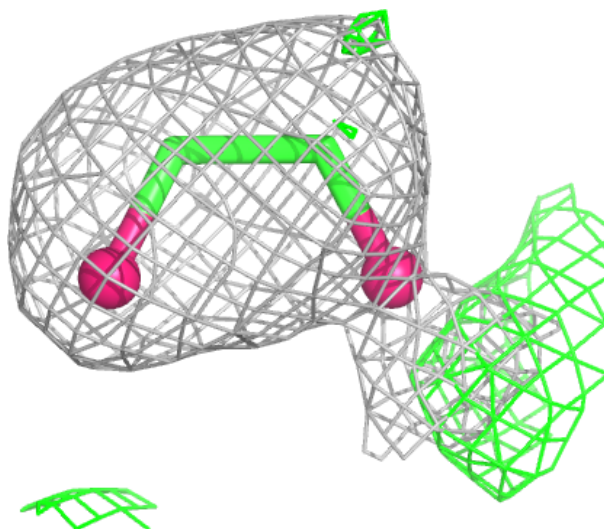
Electron density around DMU C 316:

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



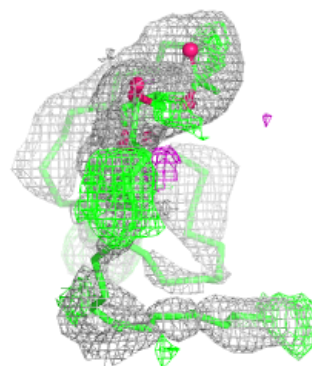
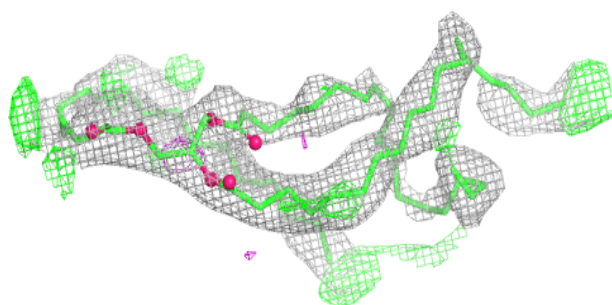
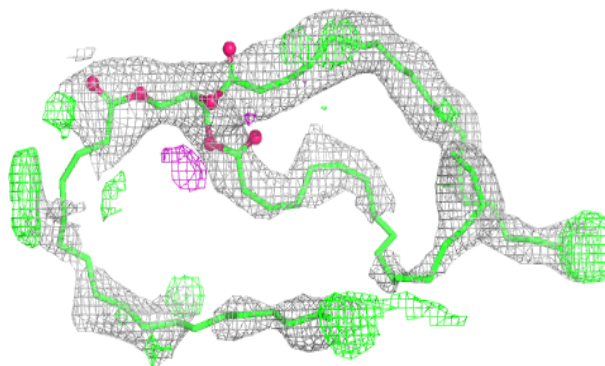
Electron density around EDO Q 1801:

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

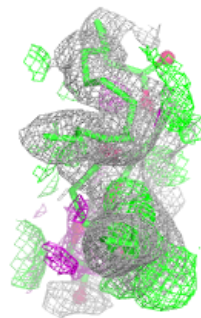
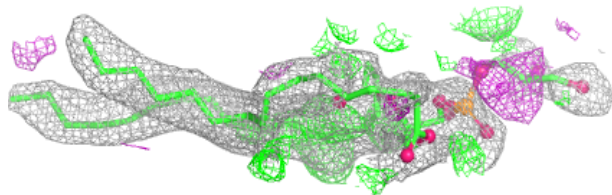
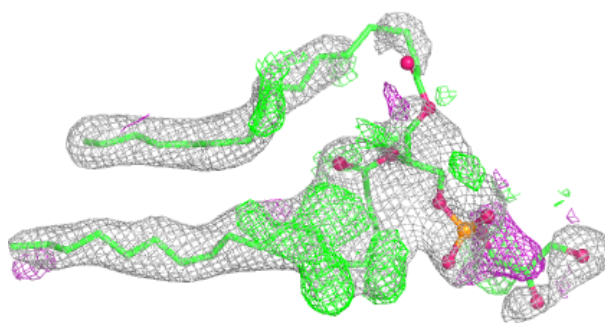


Electron density around TGL N 604:

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

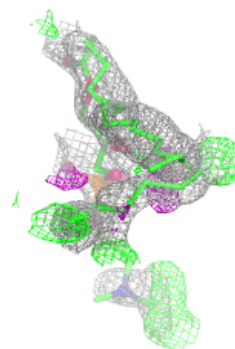
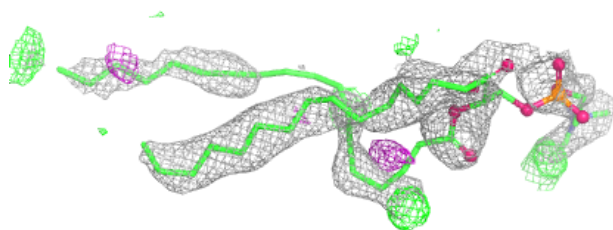
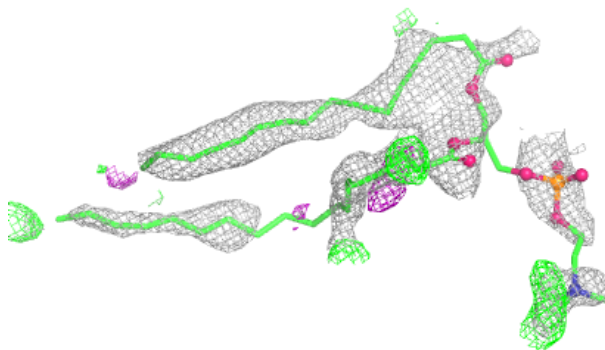
**Electron density around PGV M 101:**

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

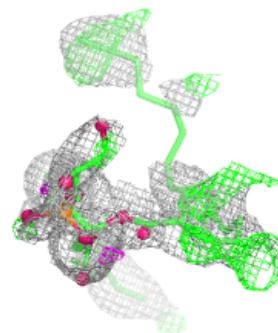
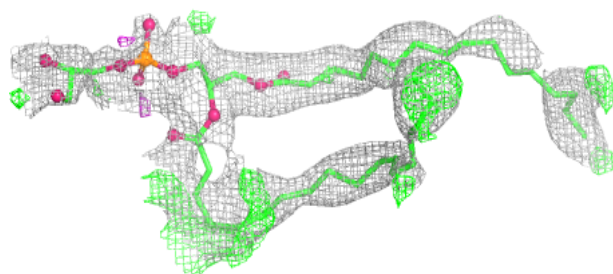
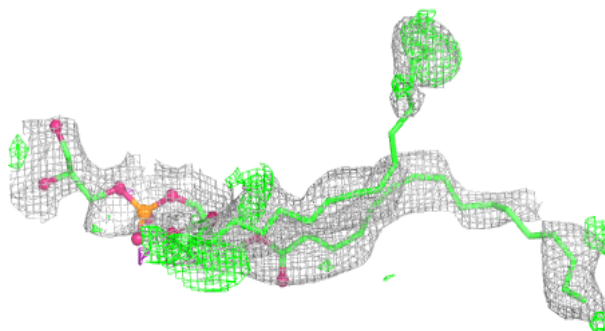


Electron density around PSC B 302:

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

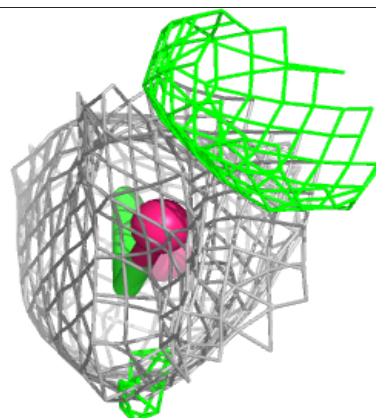
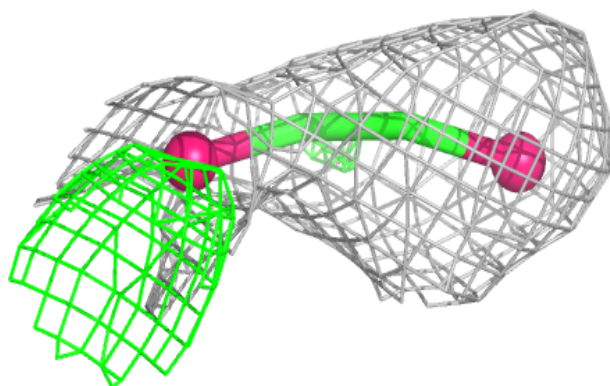
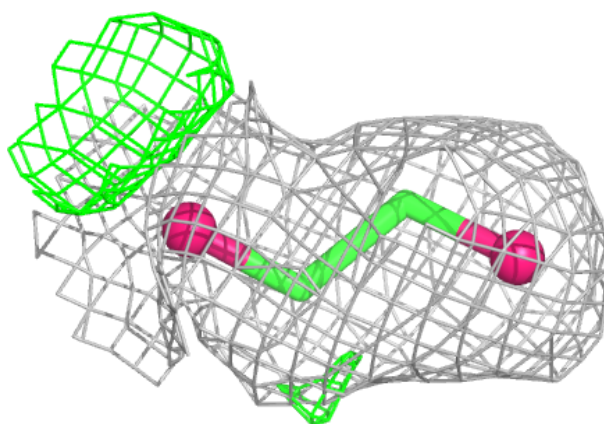
**Electron density around PGV C 305:**

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

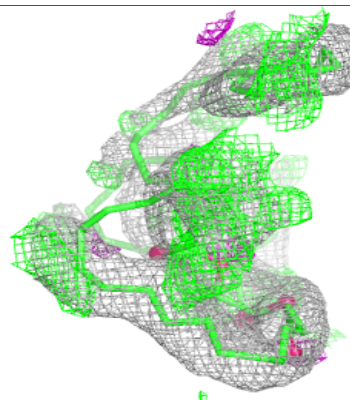
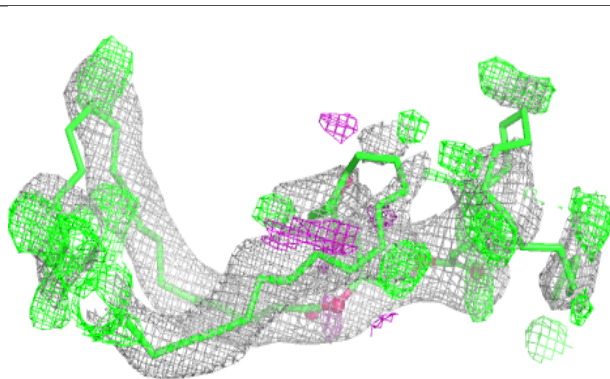
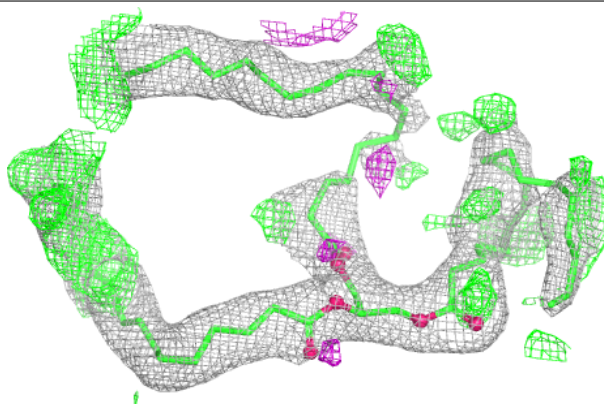


Electron density around EDO V 103:

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

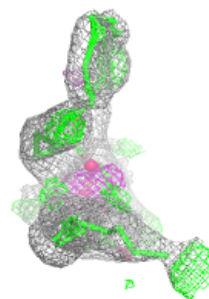
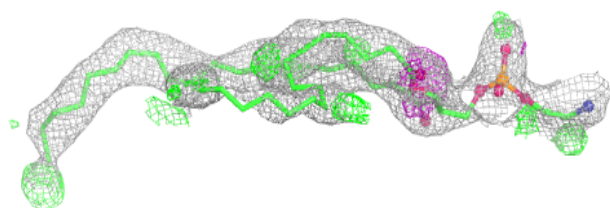
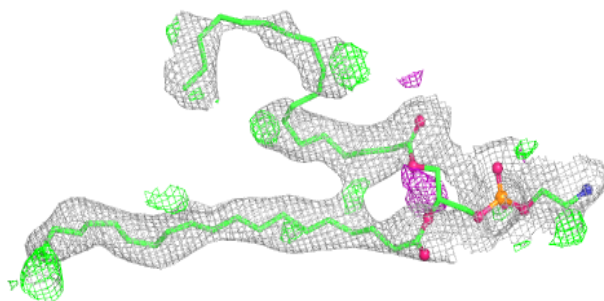
**Electron density around TGL I 101:**

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



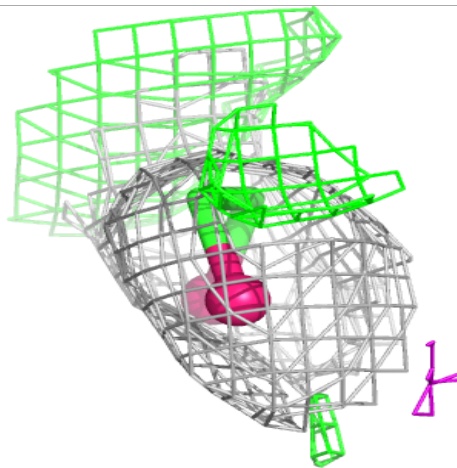
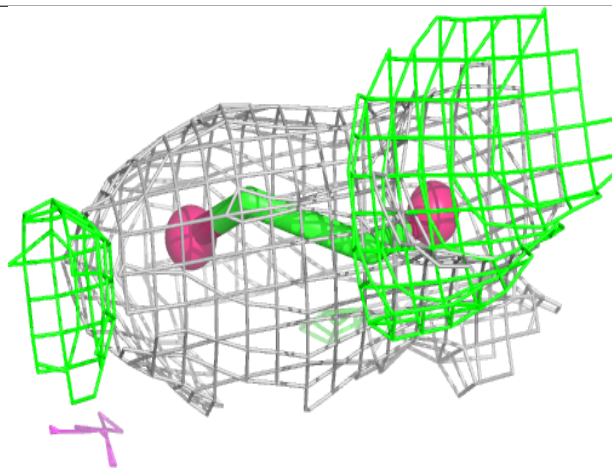
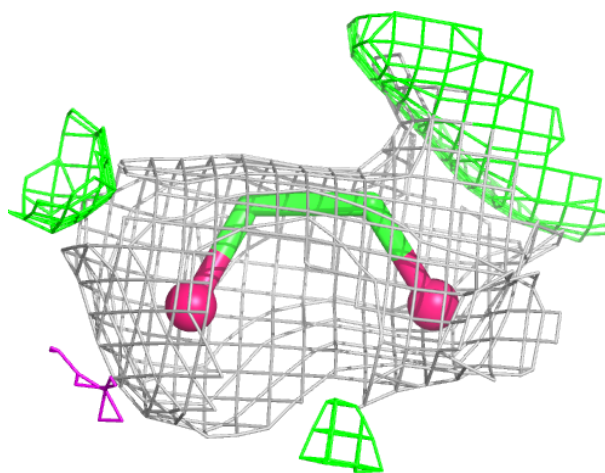
Electron density around PEK P 301:

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



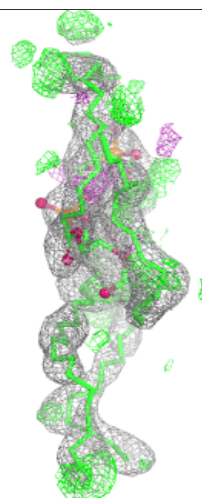
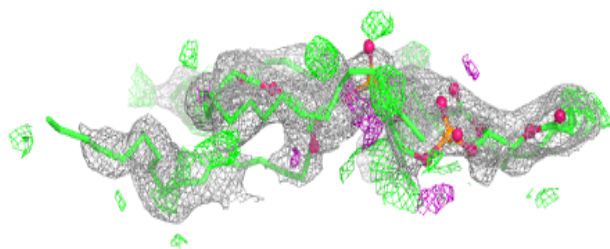
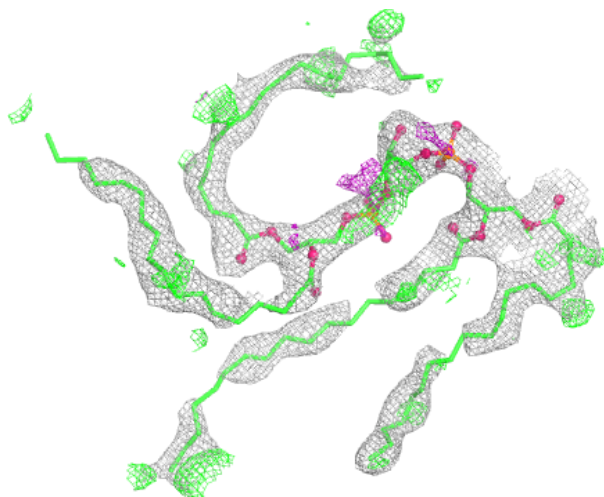
Electron density around EDO J 102:

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



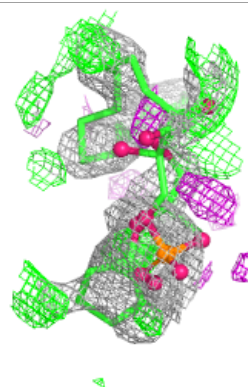
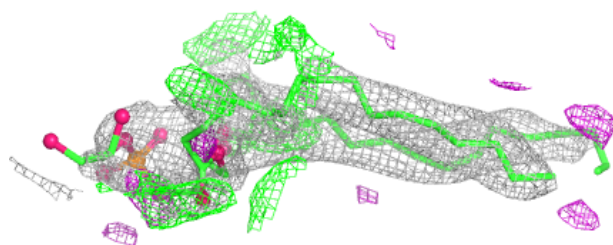
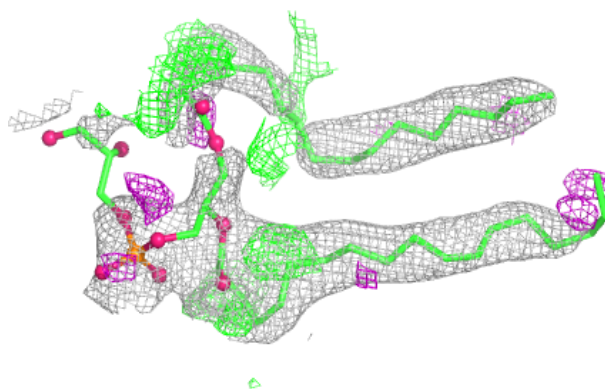
Electron density around CDL P 312:

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



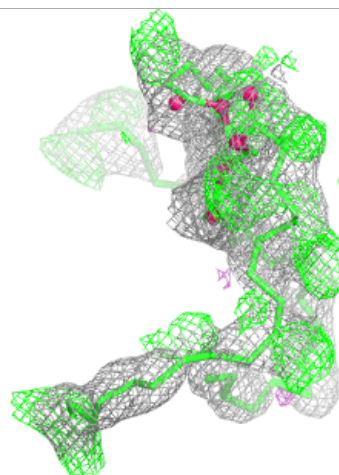
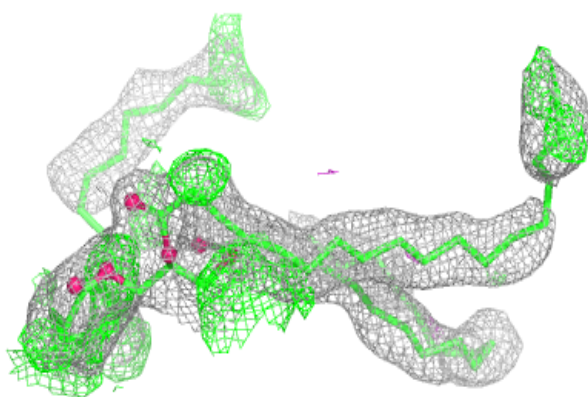
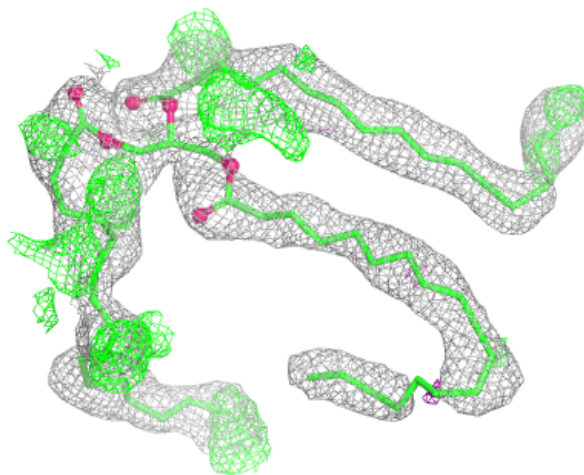
Electron density around PGV Z 101:

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



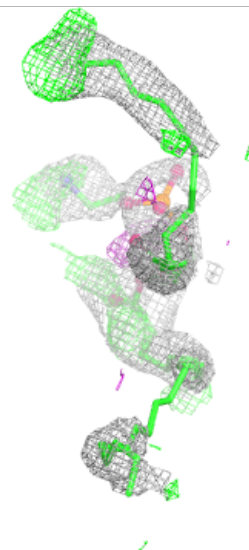
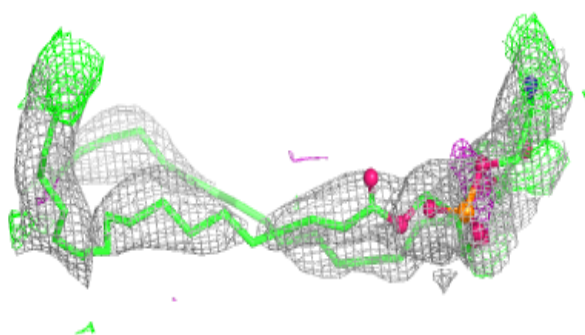
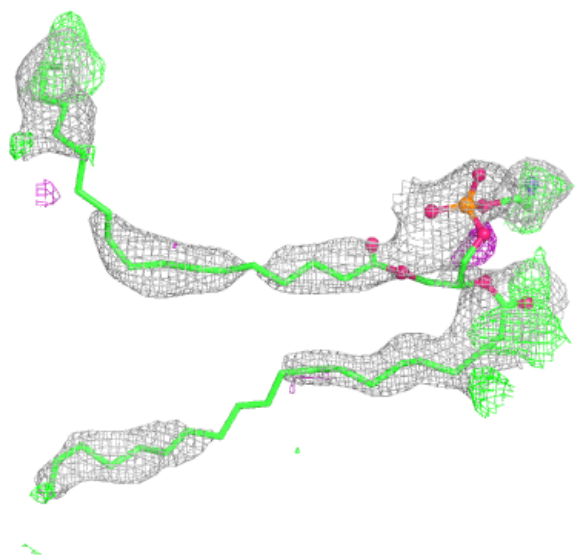
Electron density around TGL D 201:

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



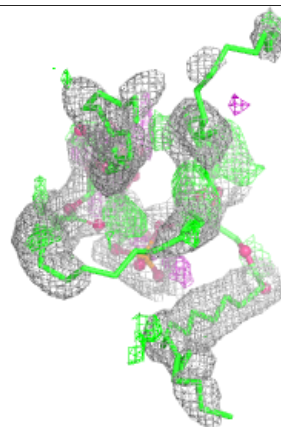
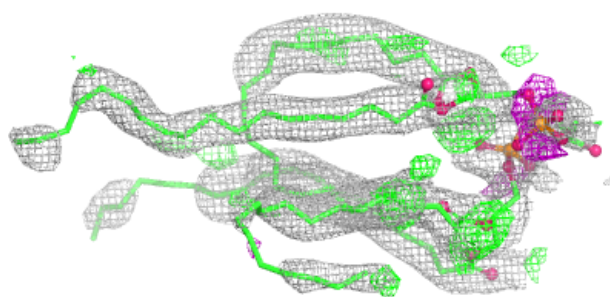
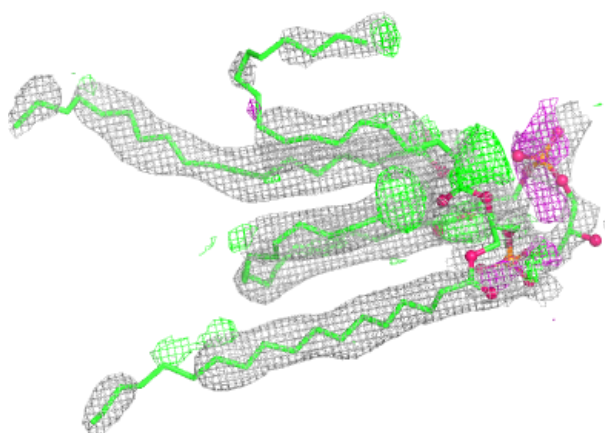
Electron density around PEK P 305:

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

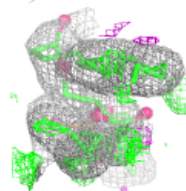
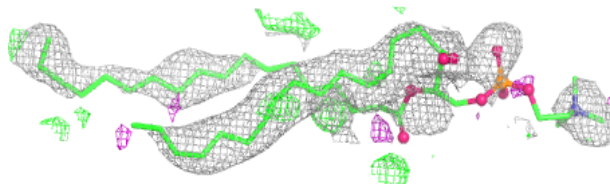
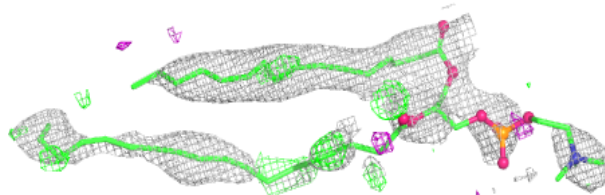


Electron density around CDL P 308:

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

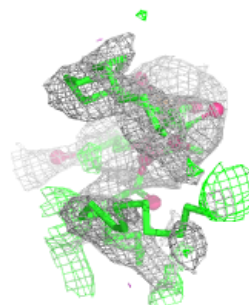
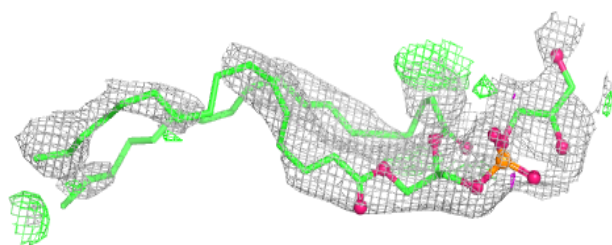
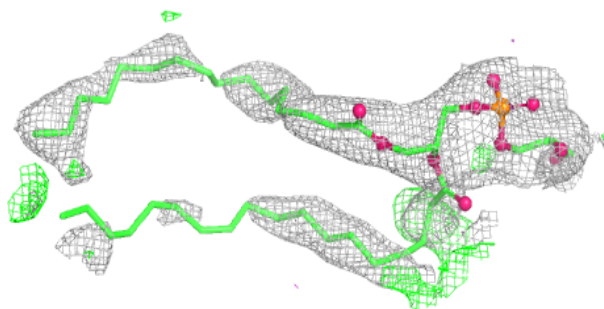
**Electron density around PSC O 302:**

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

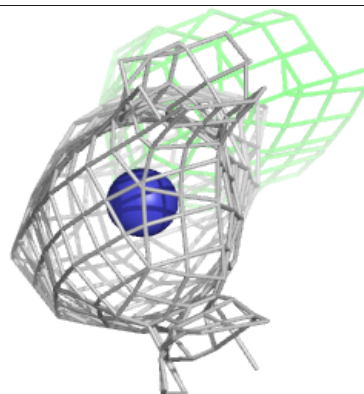
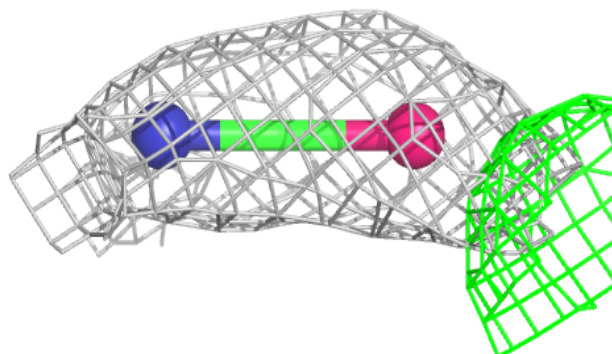
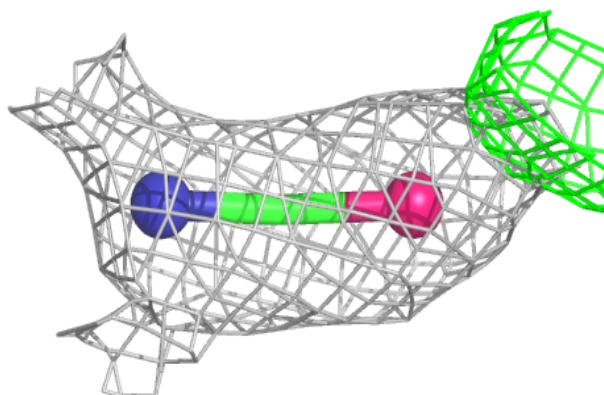


Electron density around PGV P 307:

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

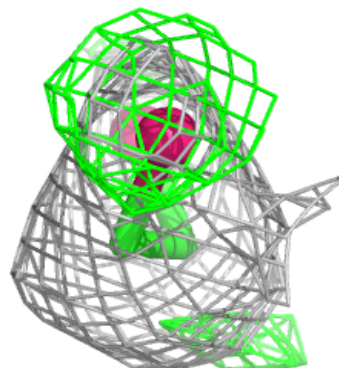
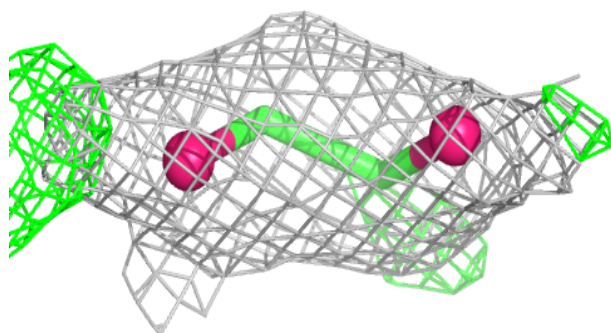
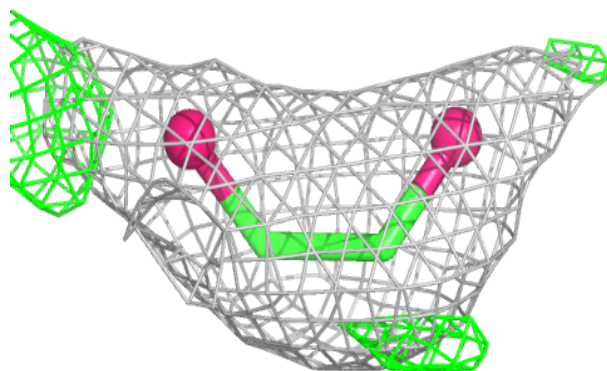
**Electron density around 0NM N 618:**

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

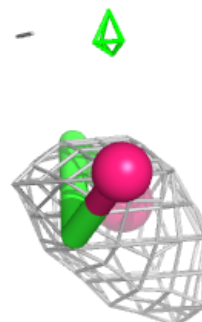
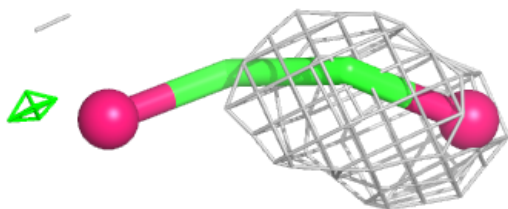
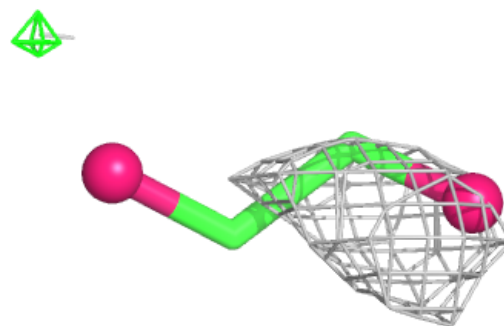


Electron density around EDO N 613:

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

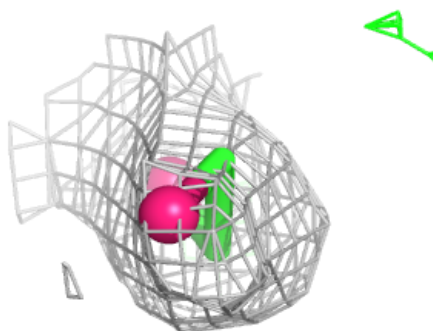
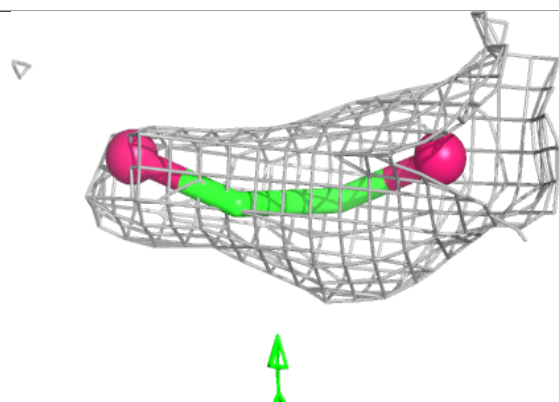
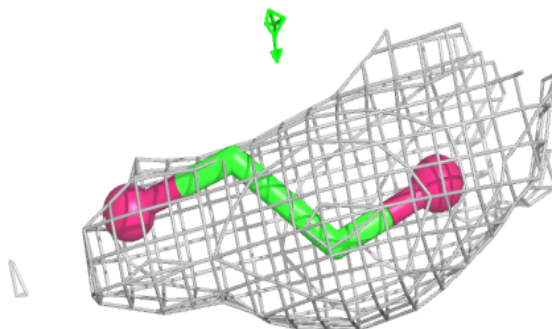
**Electron density around EDO Y 102:**

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

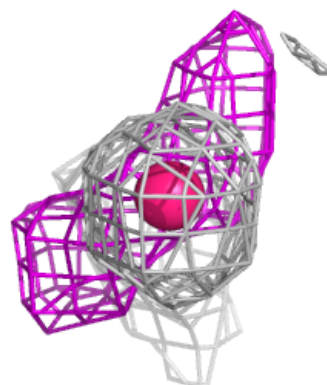
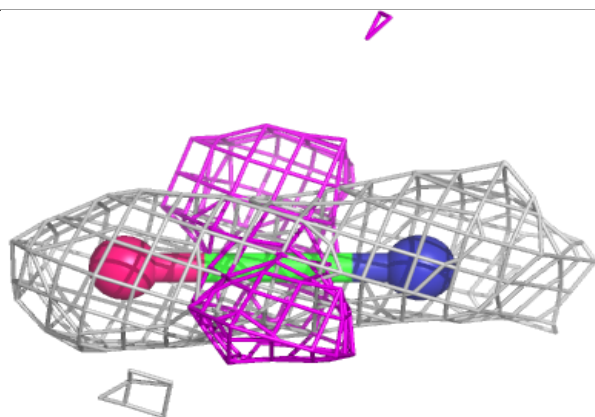
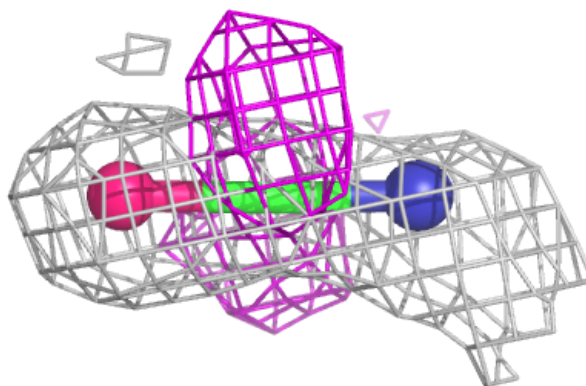


Electron density around EDO L 505:

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

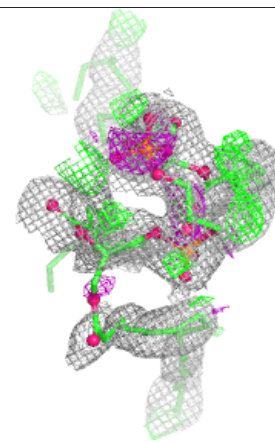
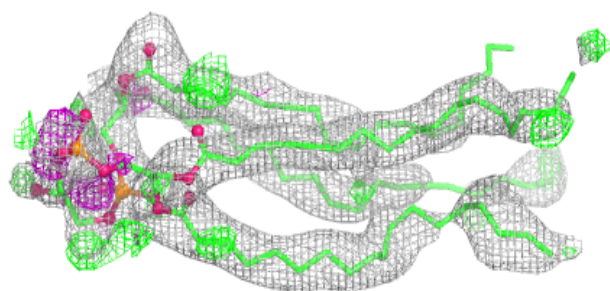
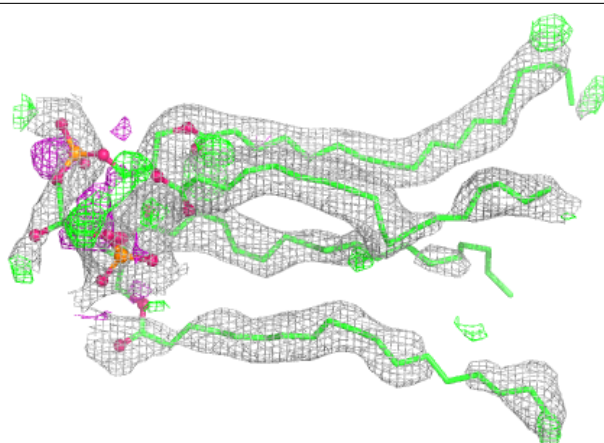
**Electron density around ONM N 619:**

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

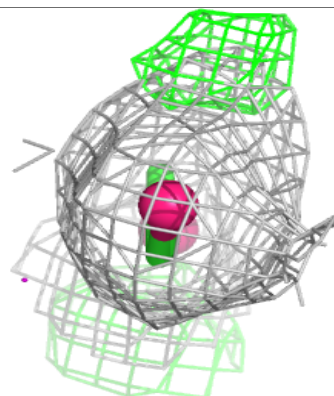
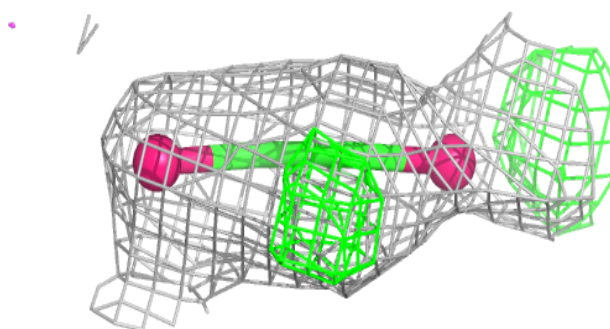
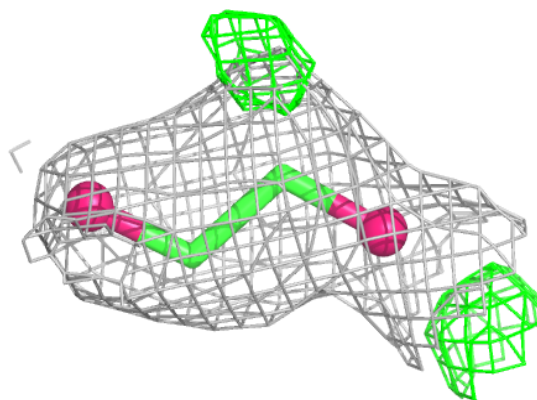


Electron density around CDL C 306:

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

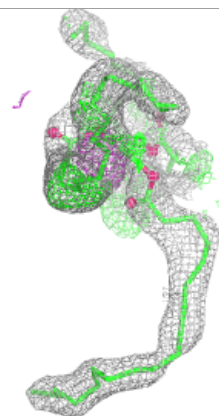
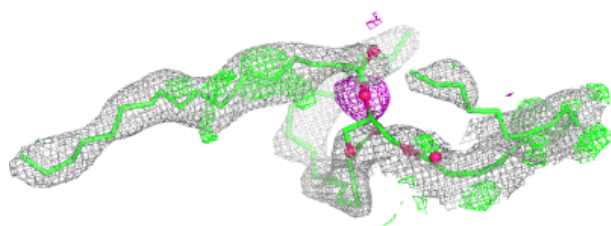
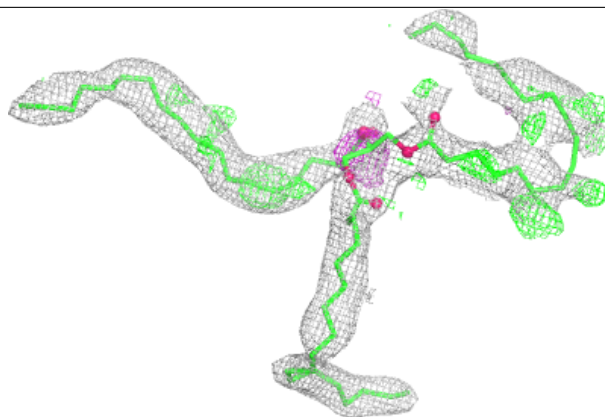
**Electron density around EDO B 311:**

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



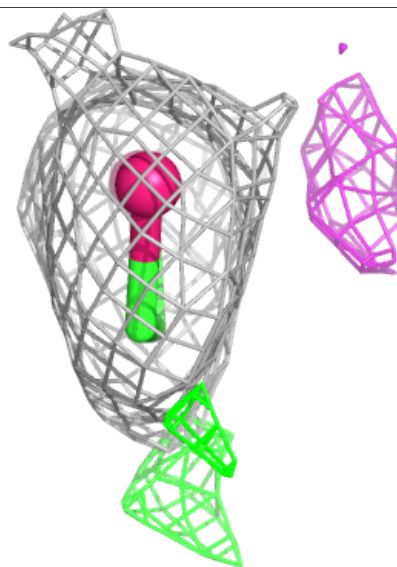
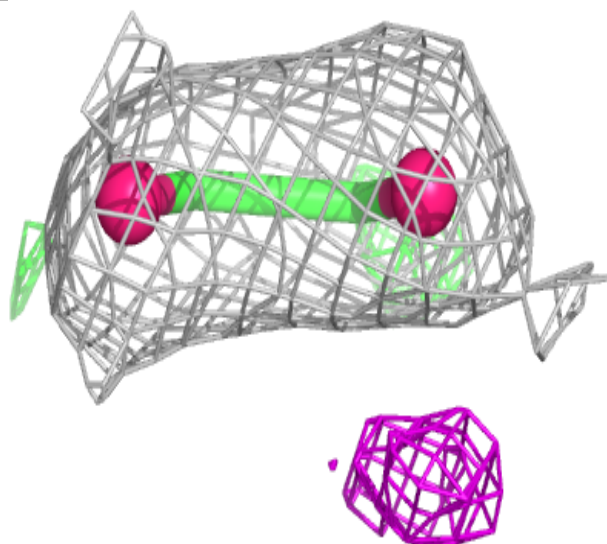
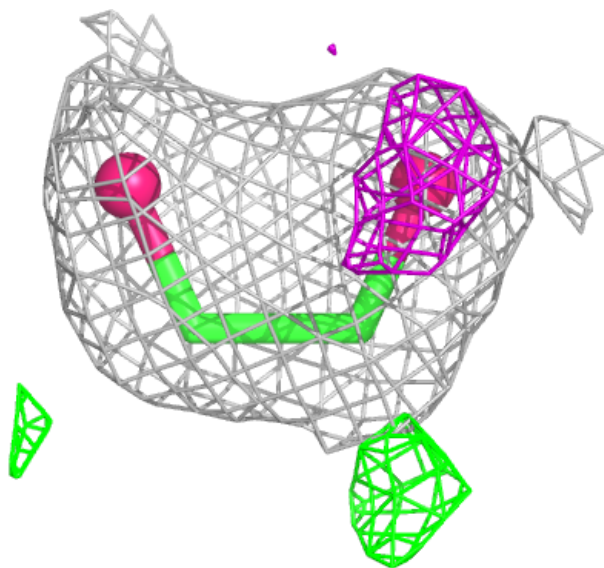
Electron density around TGL Y 101:

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



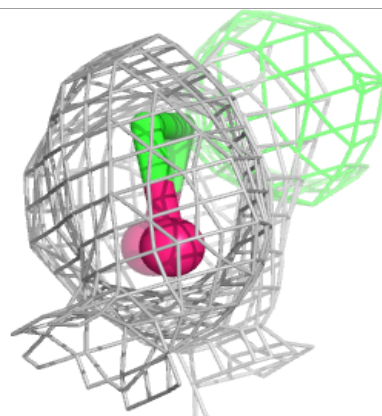
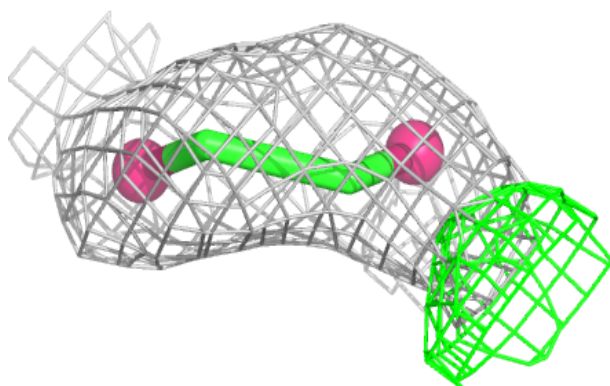
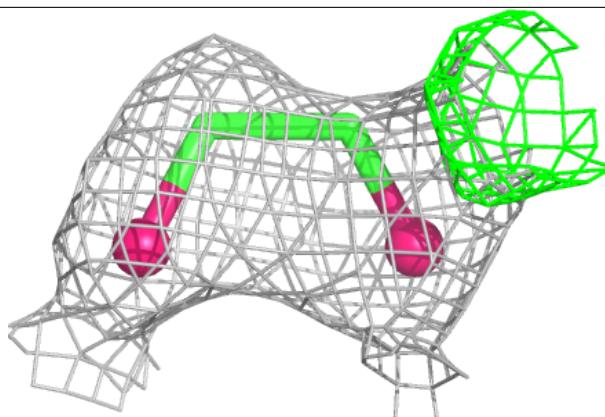
Electron density around EDO T 1301:

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

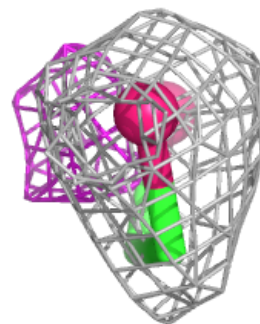
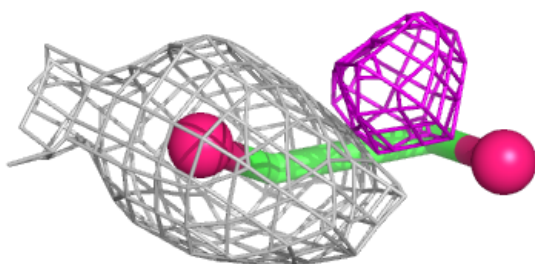
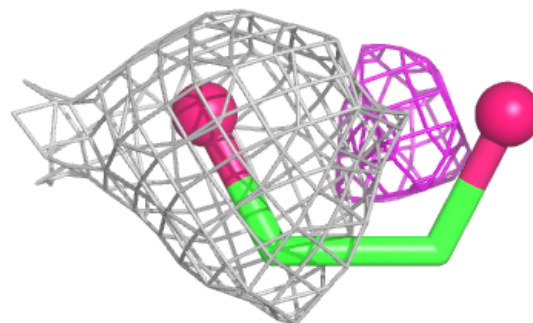


Electron density around EDO N 626:

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

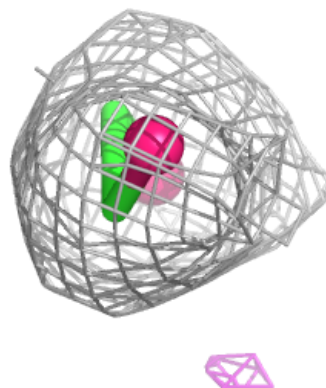
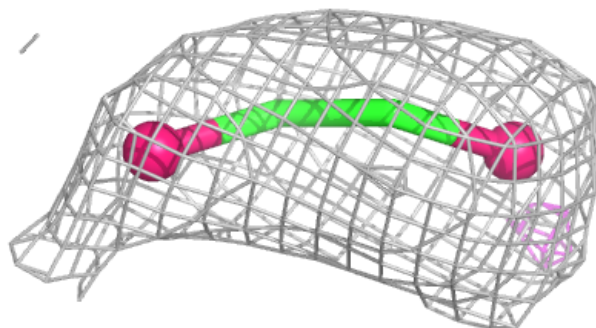
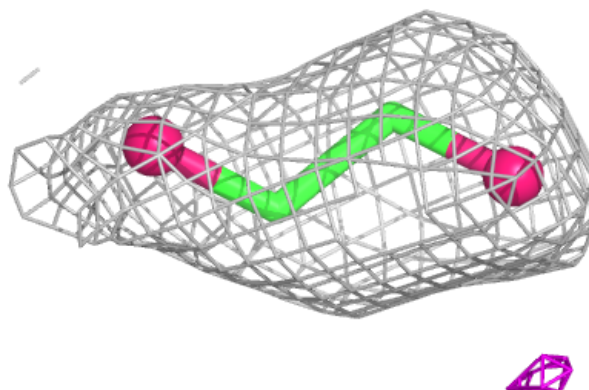
**Electron density around EDO B 308:**

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

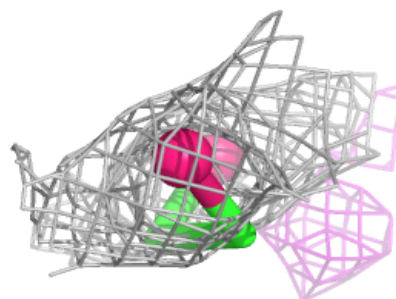
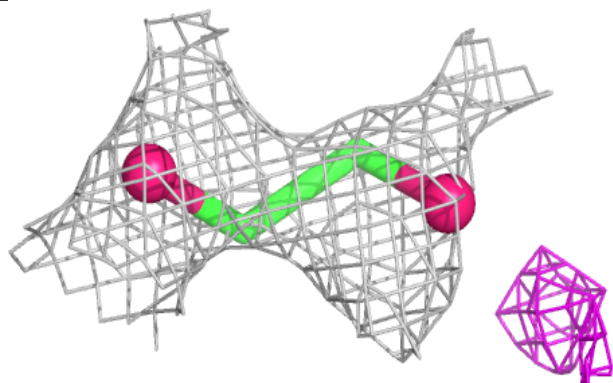
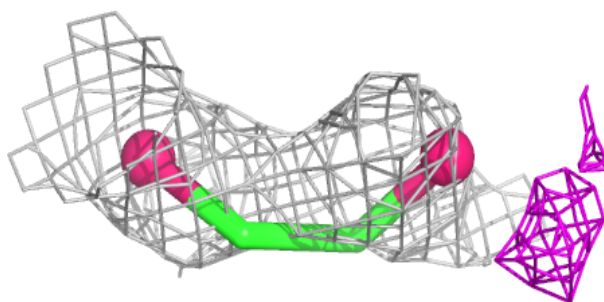


Electron density around EDO G 104:

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

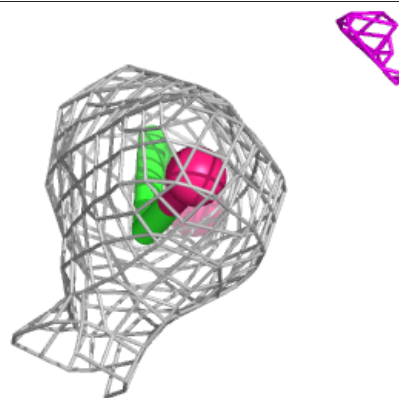
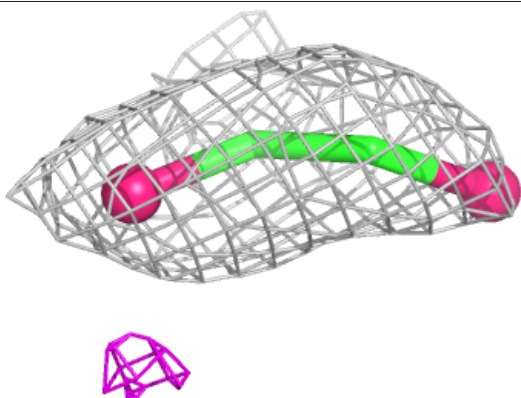
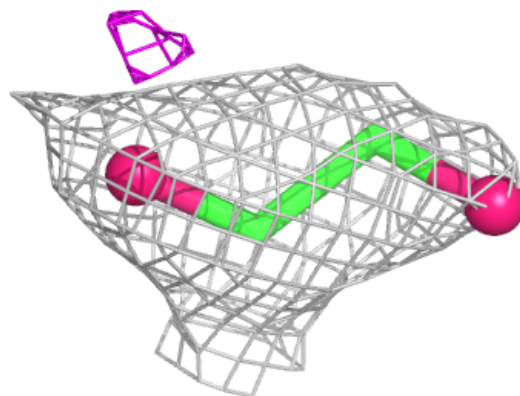
**Electron density around EDO Q 1803:**

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

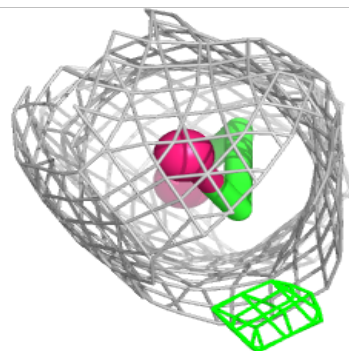
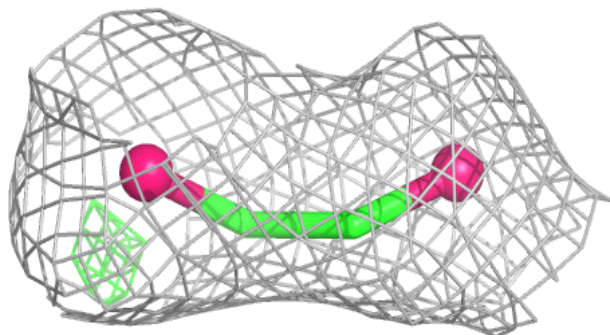
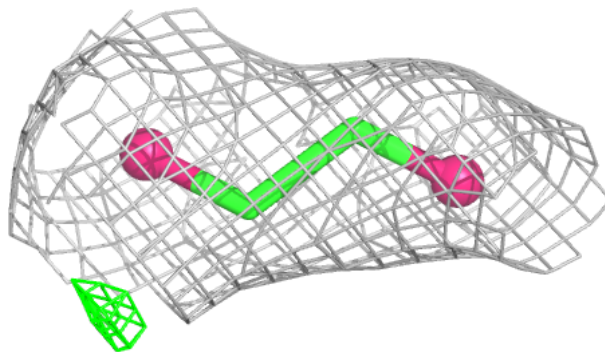


Electron density around EDO R 202:

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

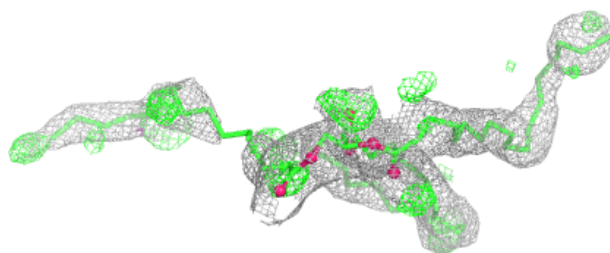
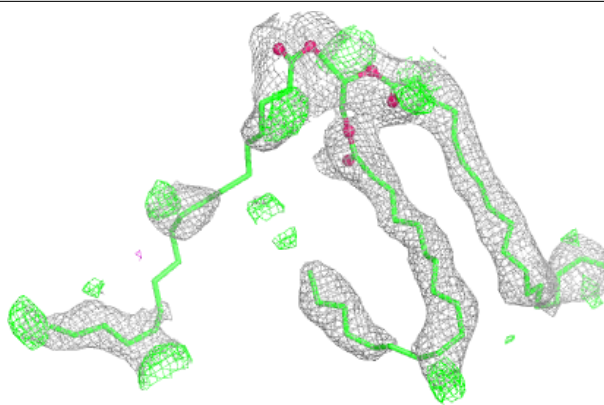
**Electron density around EDO G 107:**

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



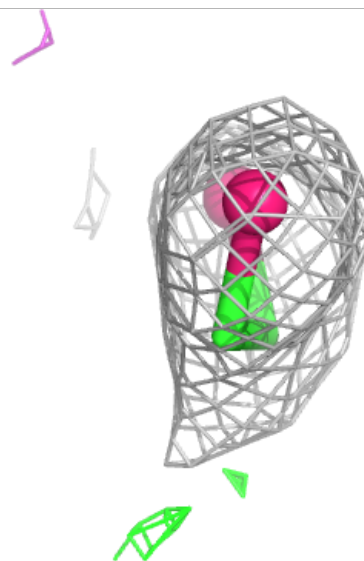
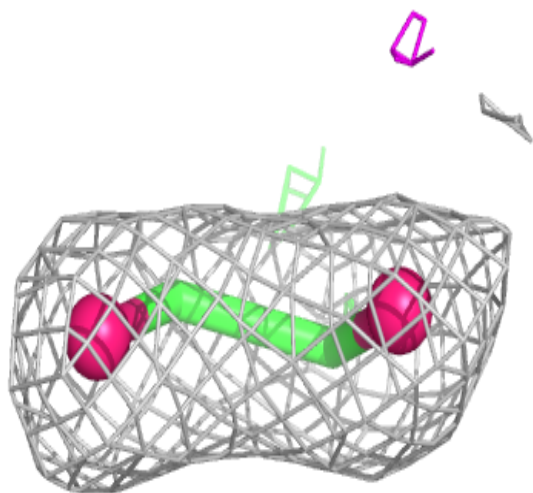
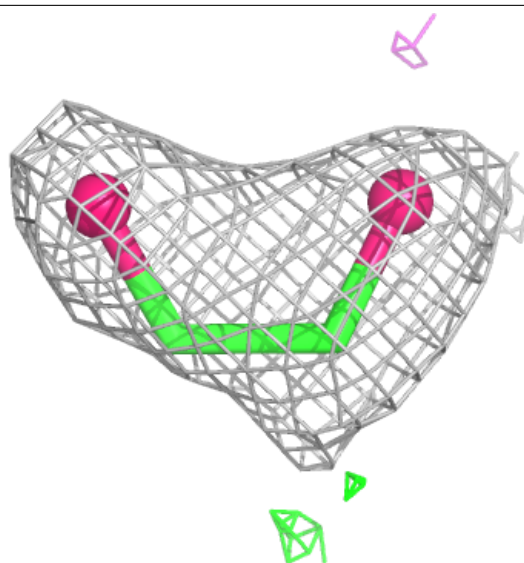
Electron density around TGL N 622:

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



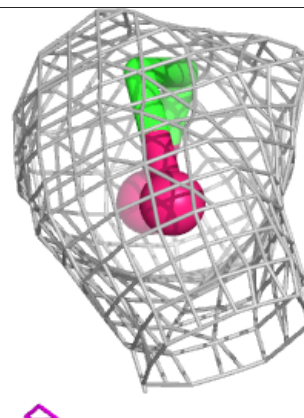
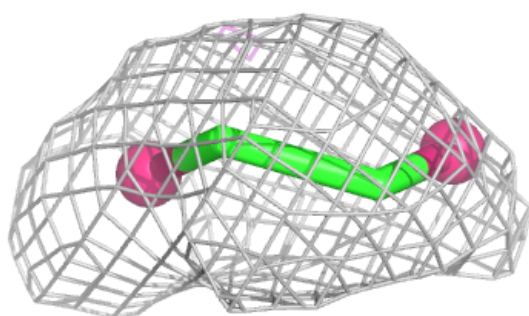
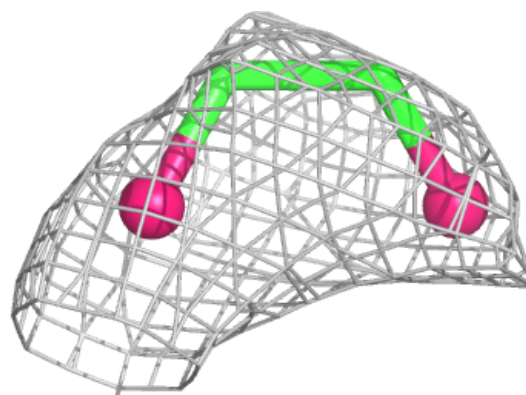
Electron density around EDO S 1604:

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

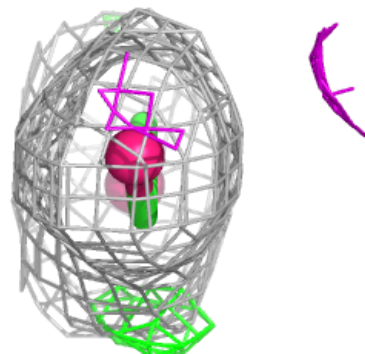
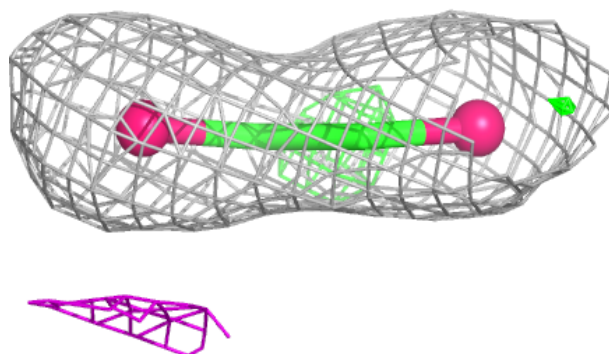
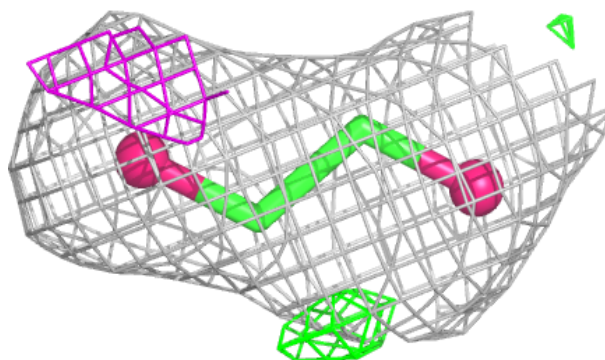


Electron density around EDO B 312:

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

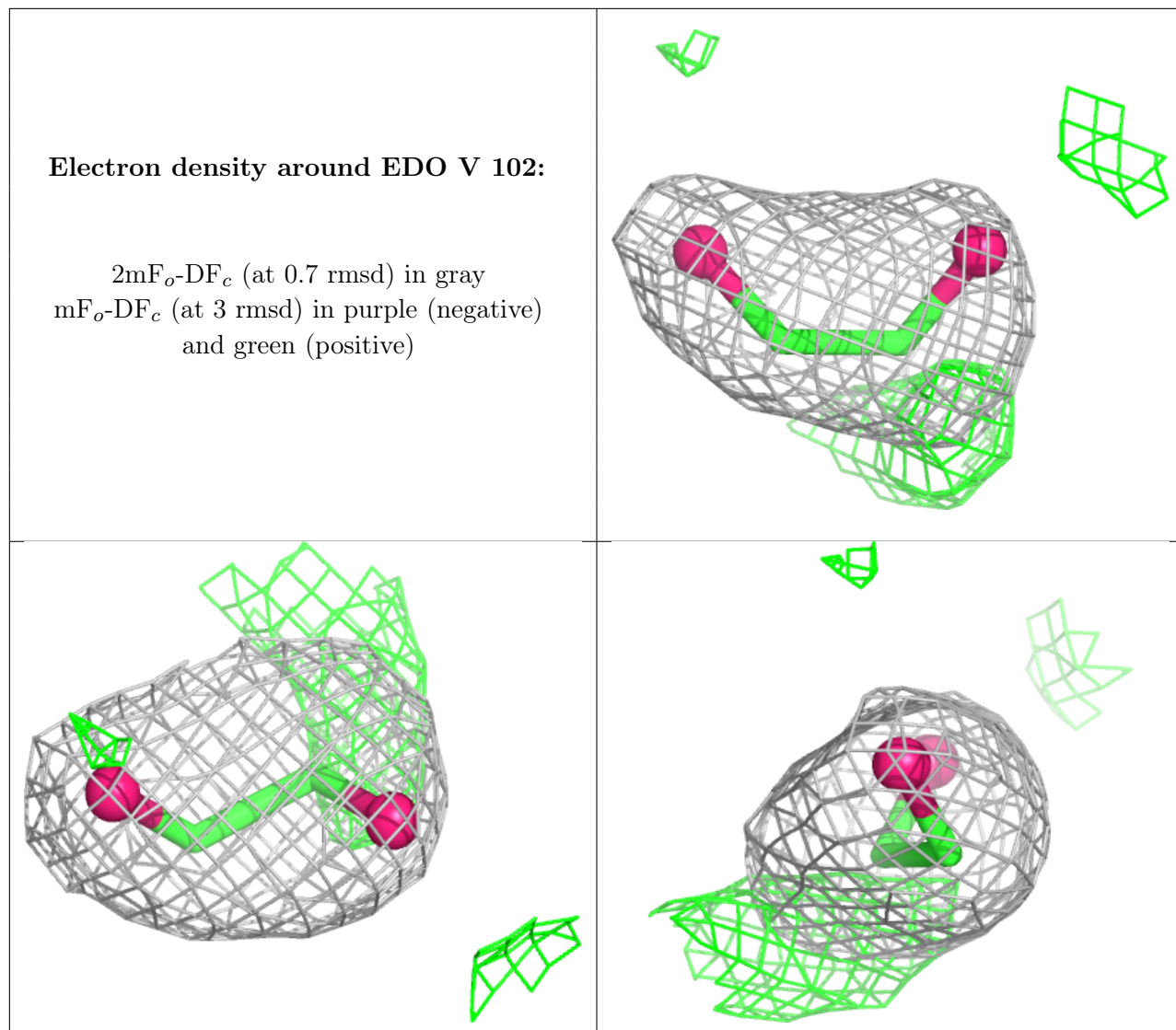
**Electron density around EDO C 309:**

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



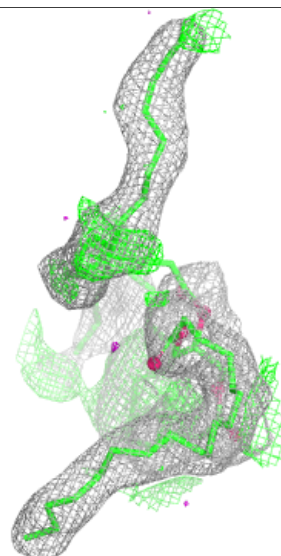
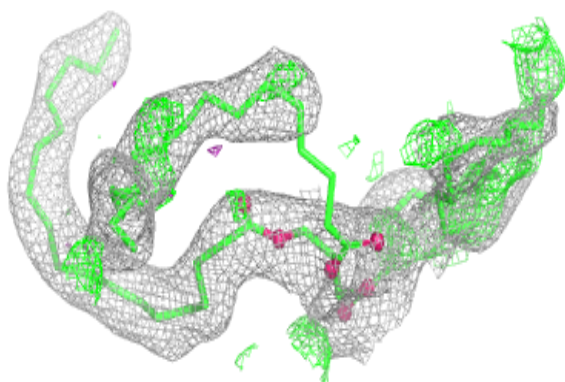
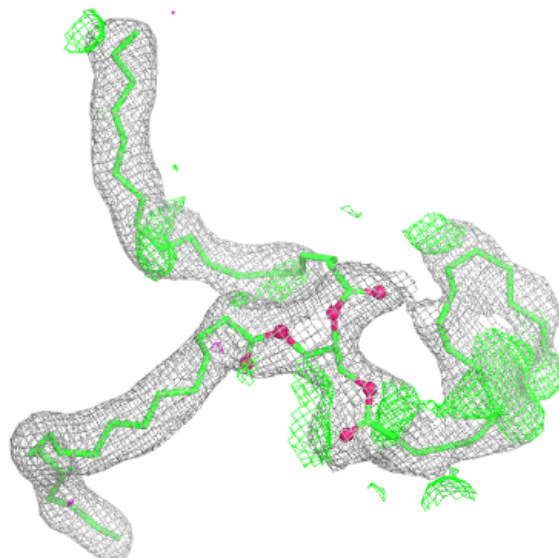
Electron density around EDO V 102:

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



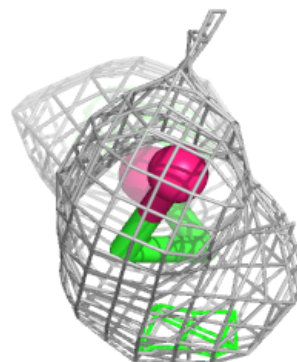
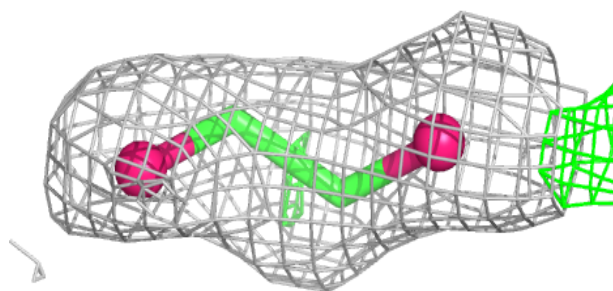
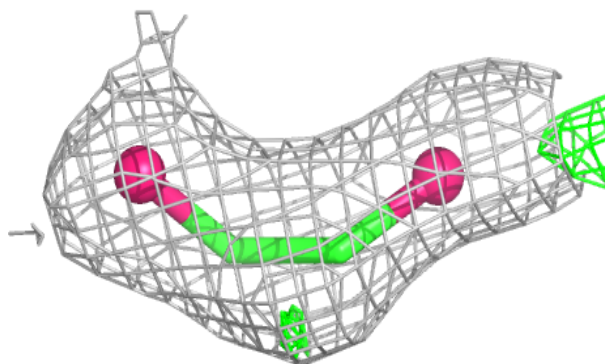
Electron density around TGL L 502:

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

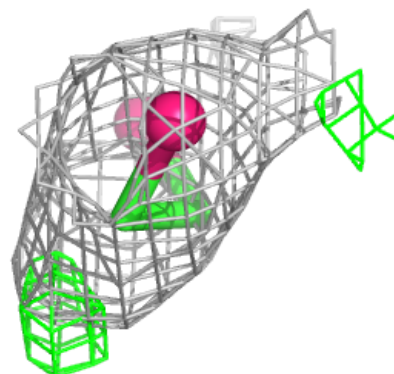
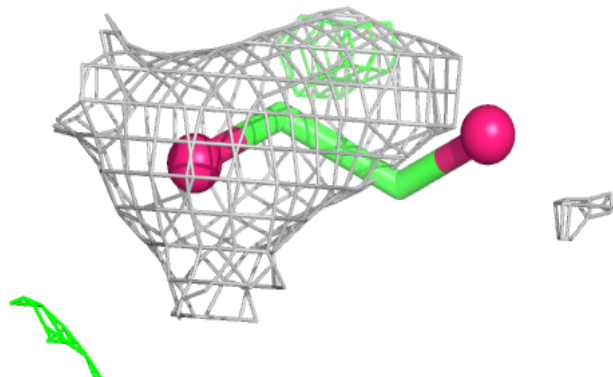
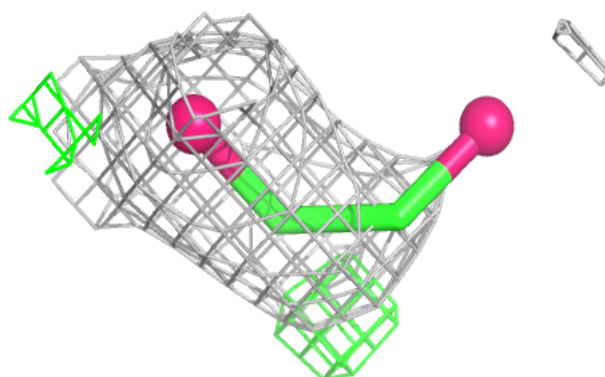


Electron density around EDO B 305:

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

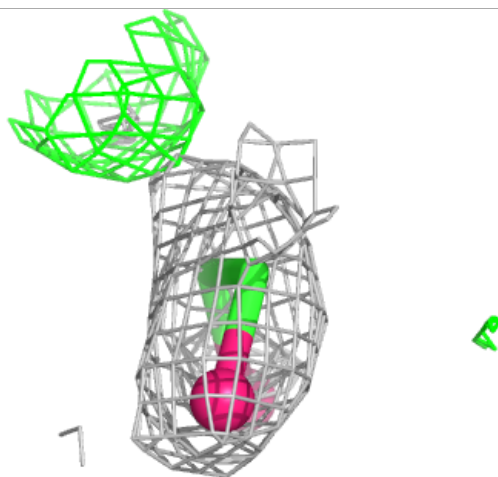
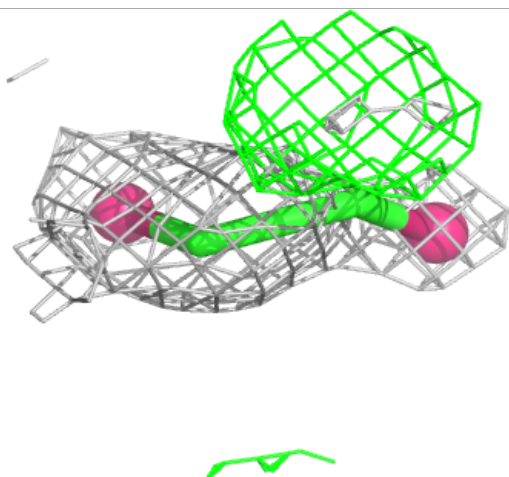
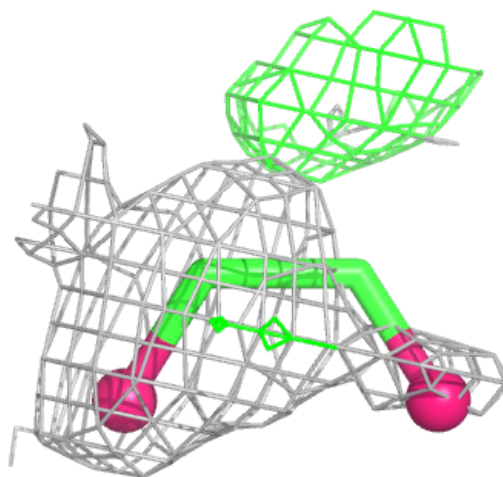
**Electron density around EDO F 709:**

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



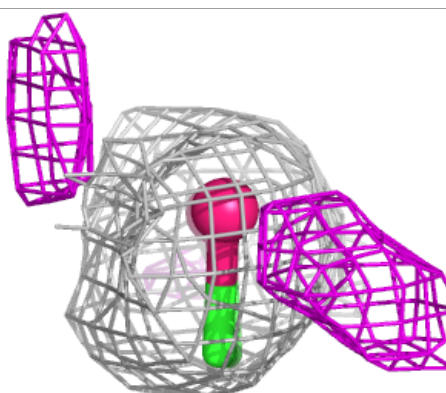
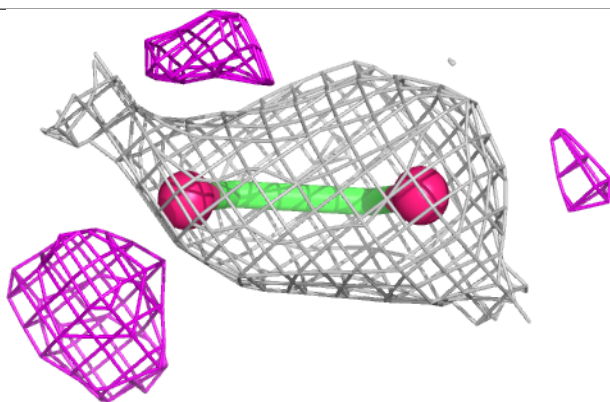
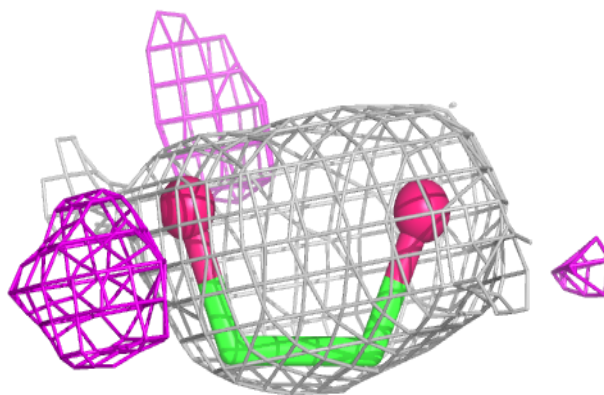
Electron density around EDO N 610:

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

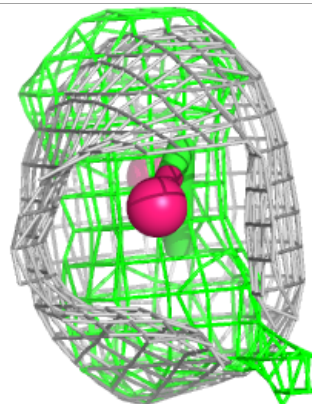
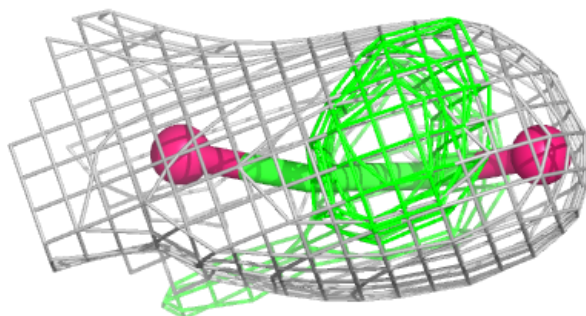
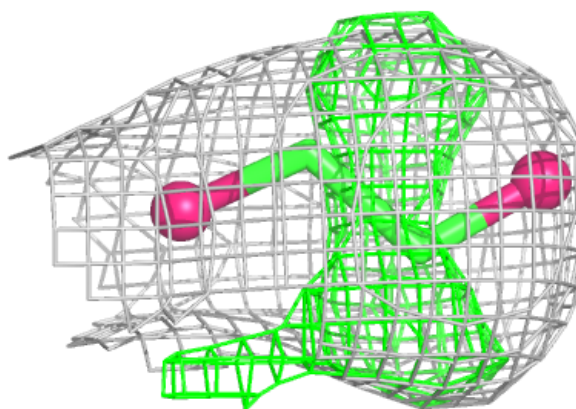


Electron density around EDO S 1606:

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

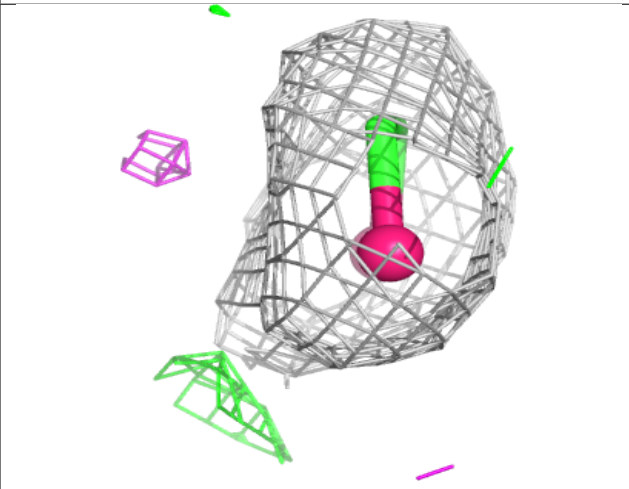
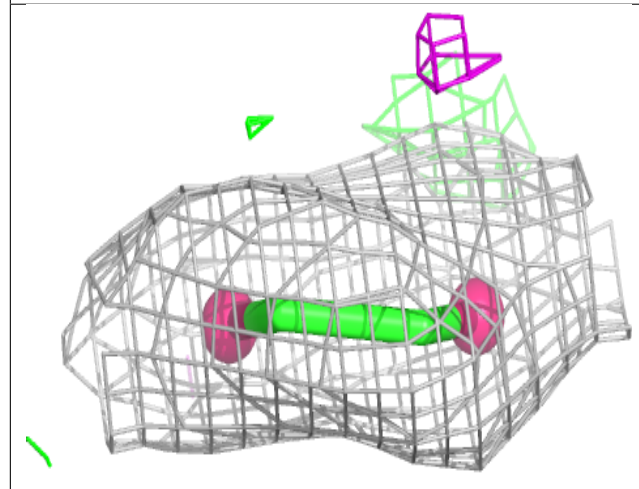
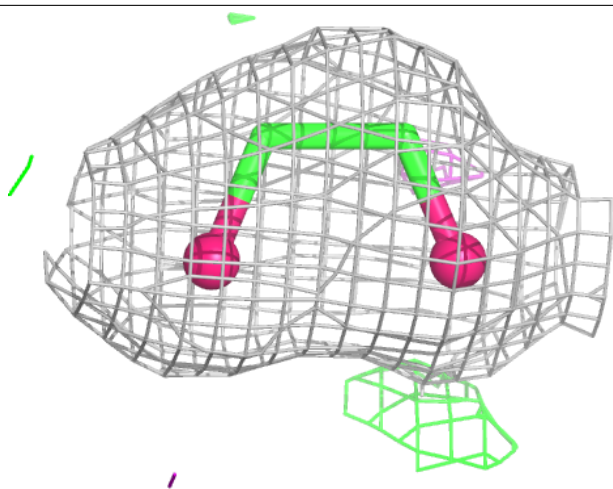
**Electron density around EDO N 612:**

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



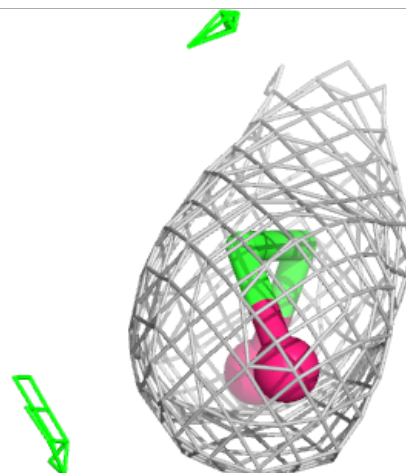
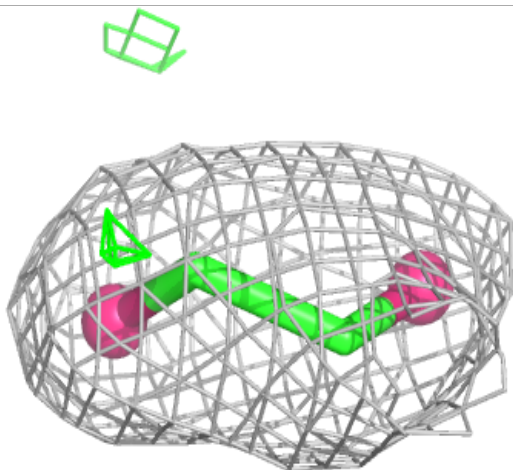
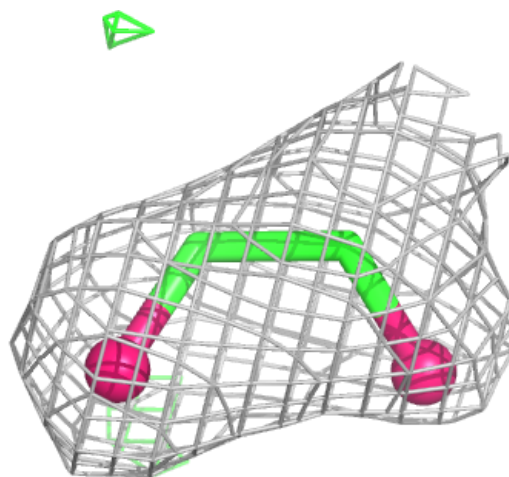
Electron density around EDO A 610:

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



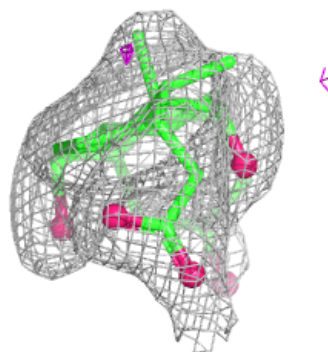
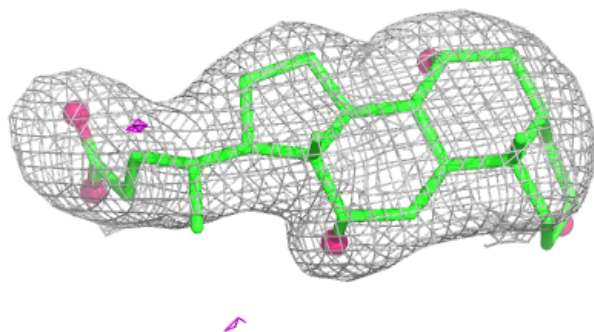
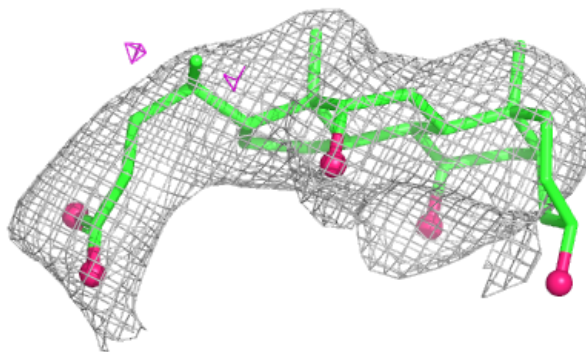
Electron density around EDO A 616:

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

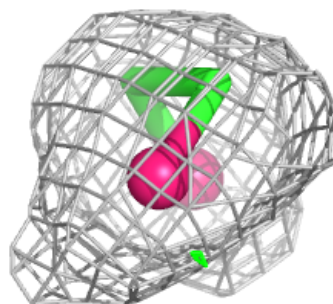
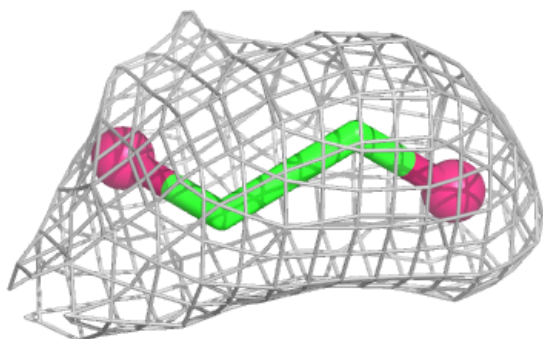
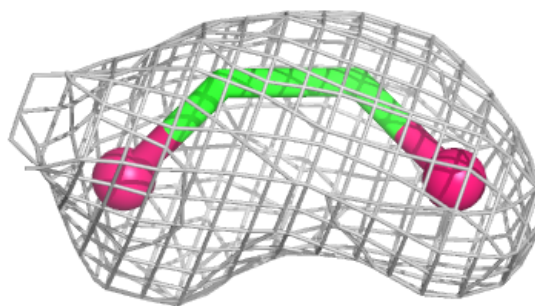


Electron density around CHD W 302:

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

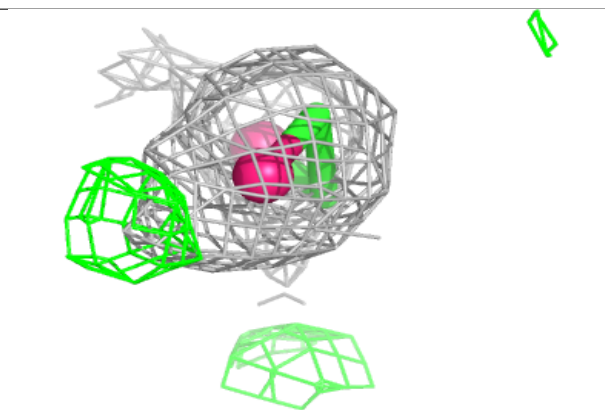
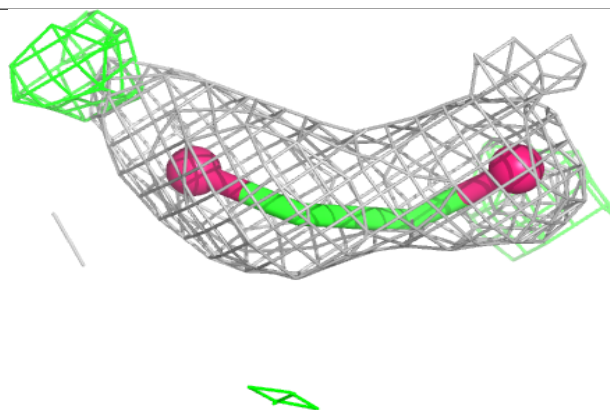
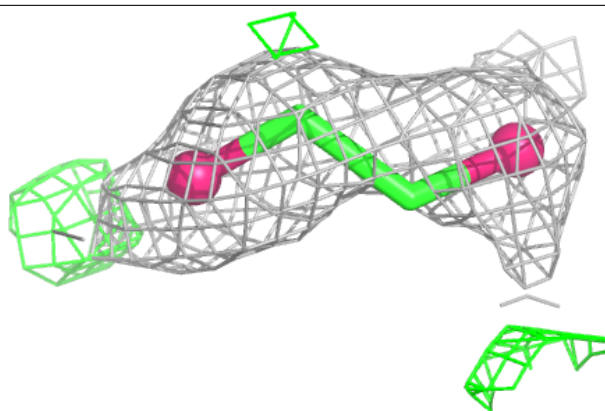
**Electron density around EDO S 1605:**

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

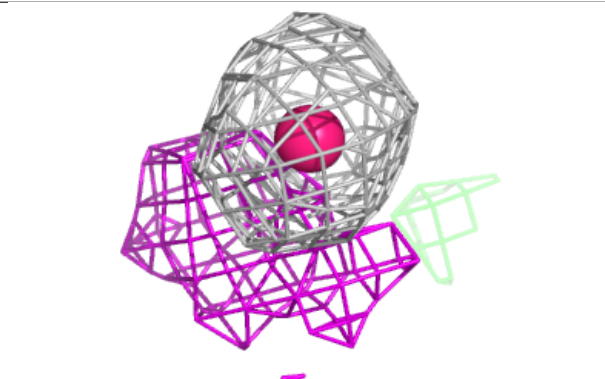
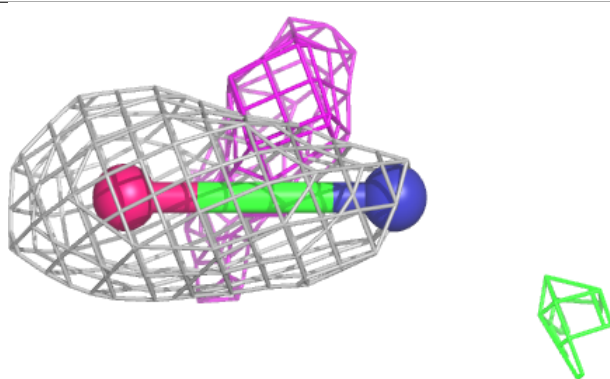
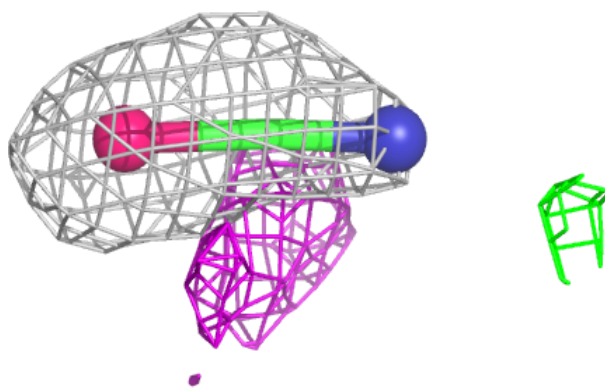


Electron density around EDO N 625:

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

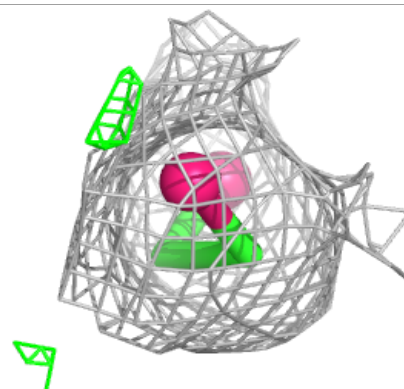
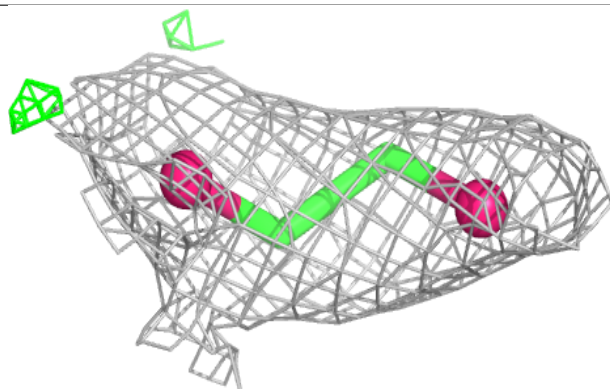
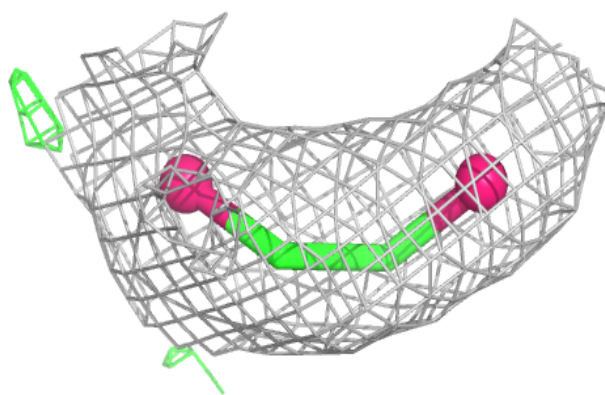
**Electron density around ONM N 616:**

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

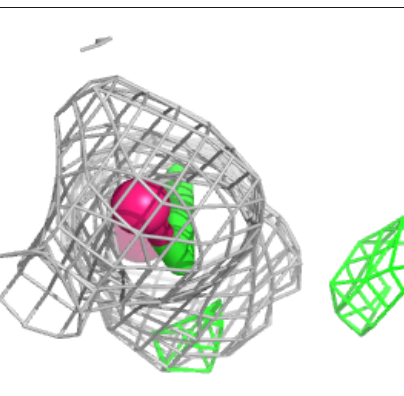
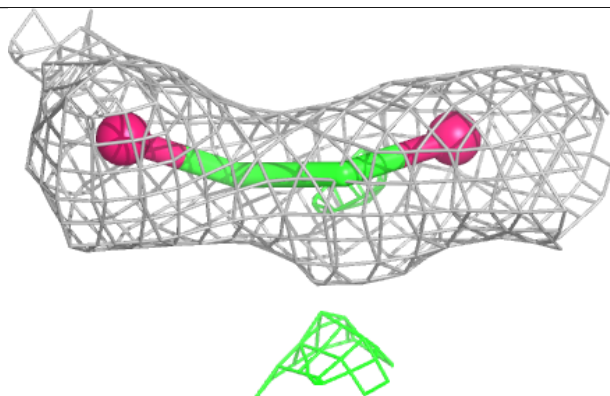
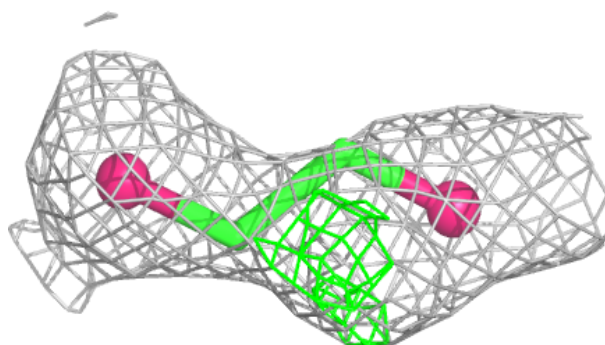


Electron density around EDO S 1607:

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

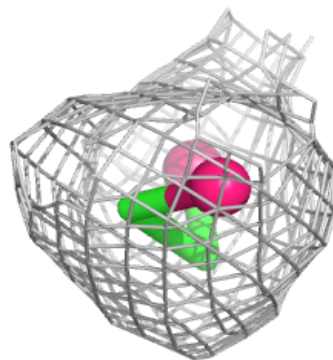
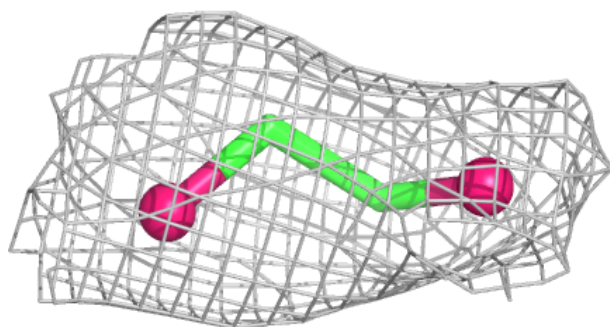
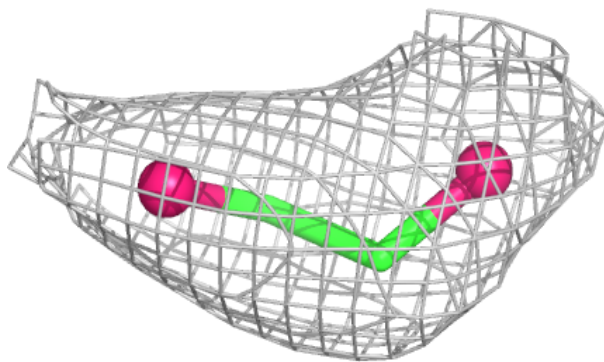
**Electron density around EDO C 315:**

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



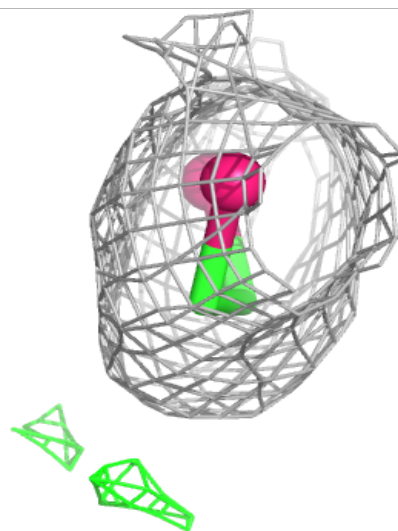
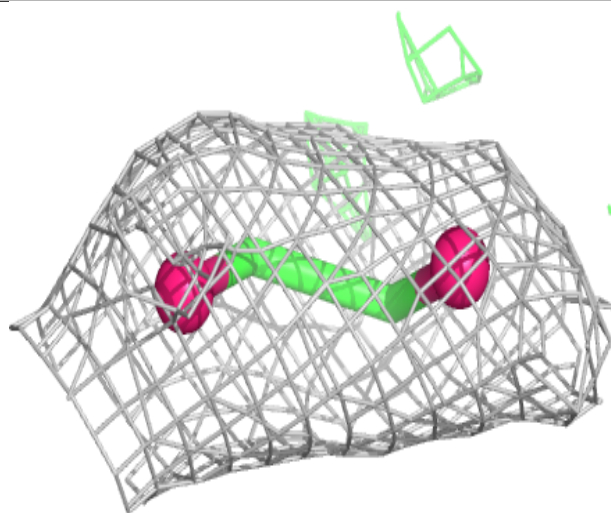
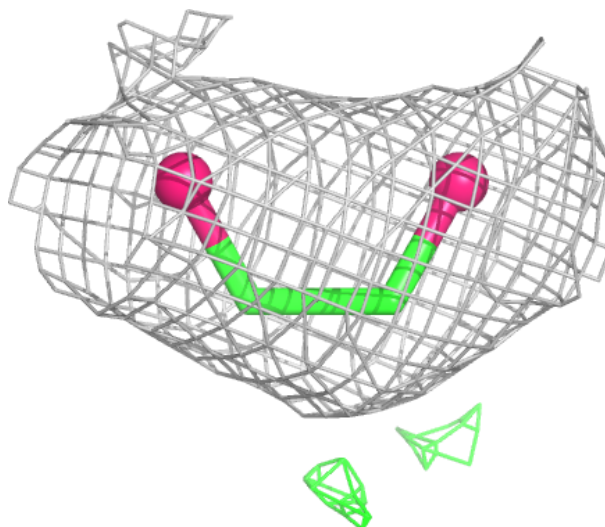
Electron density around EDO N 611:

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



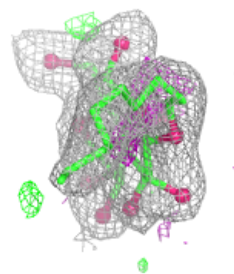
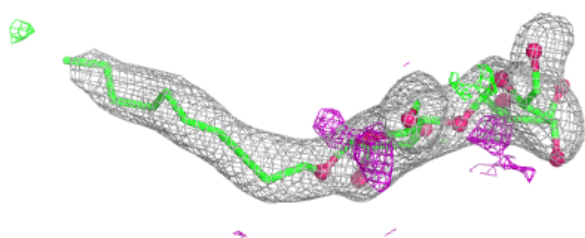
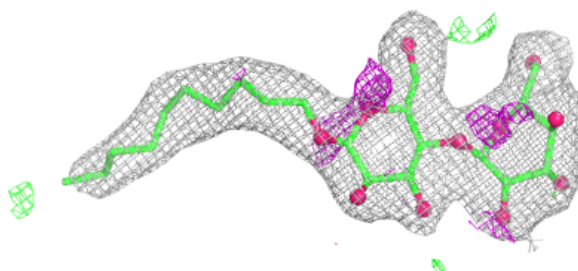
Electron density around EDO F 704:

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



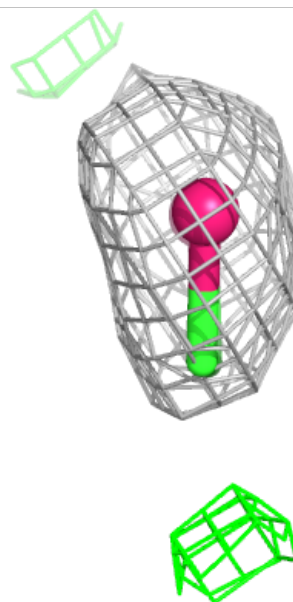
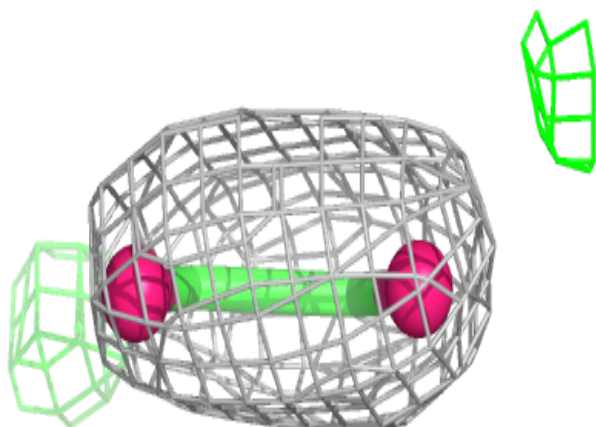
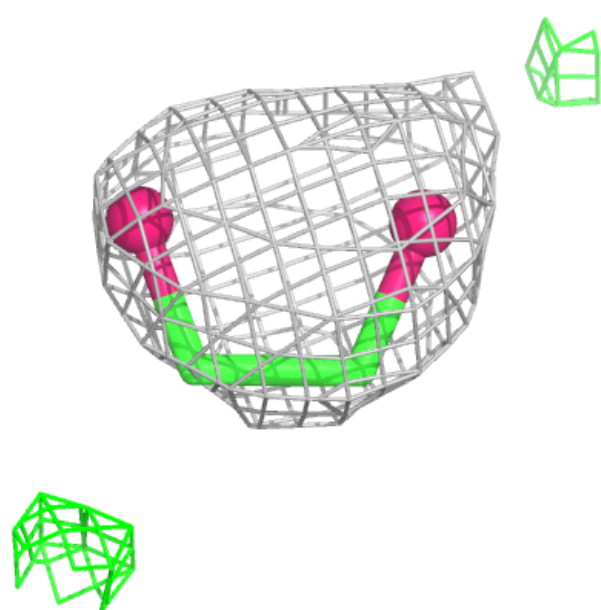
Electron density around DMU M 103:

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



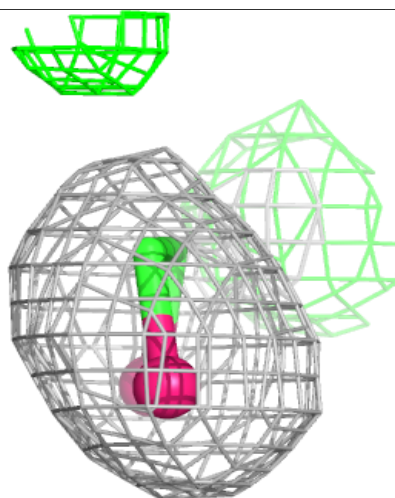
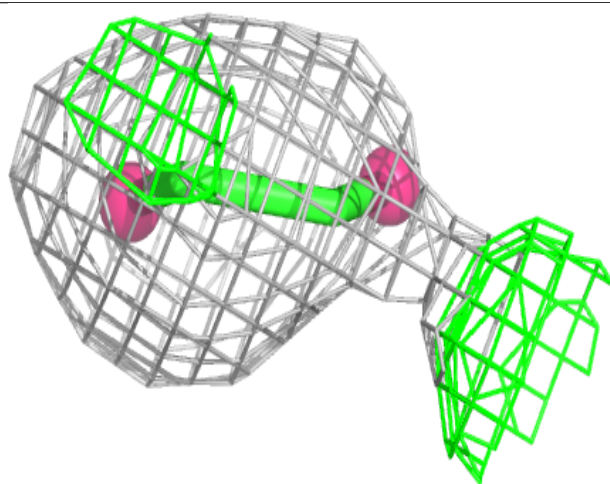
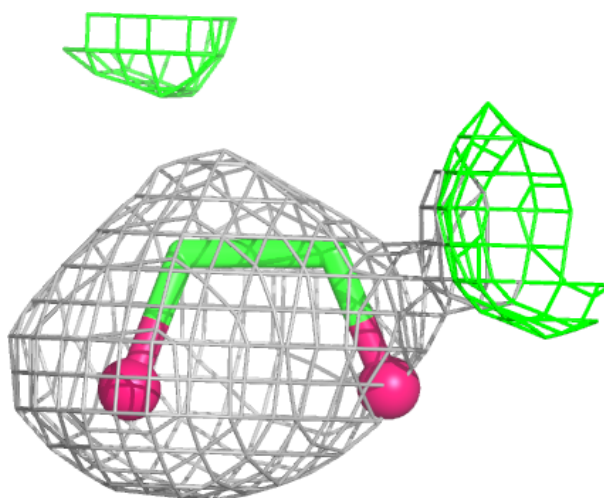
Electron density around EDO P 311:

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



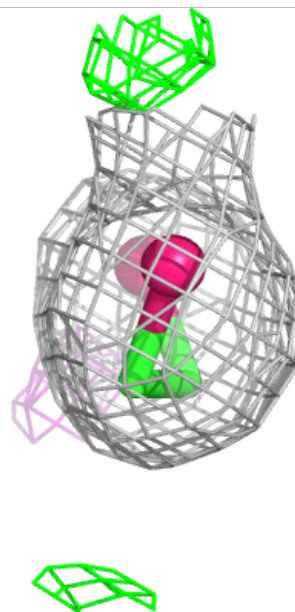
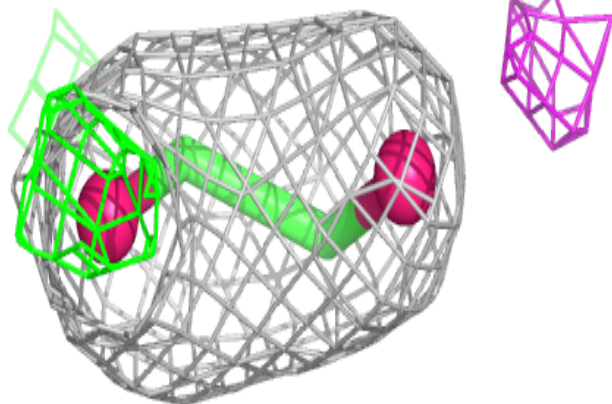
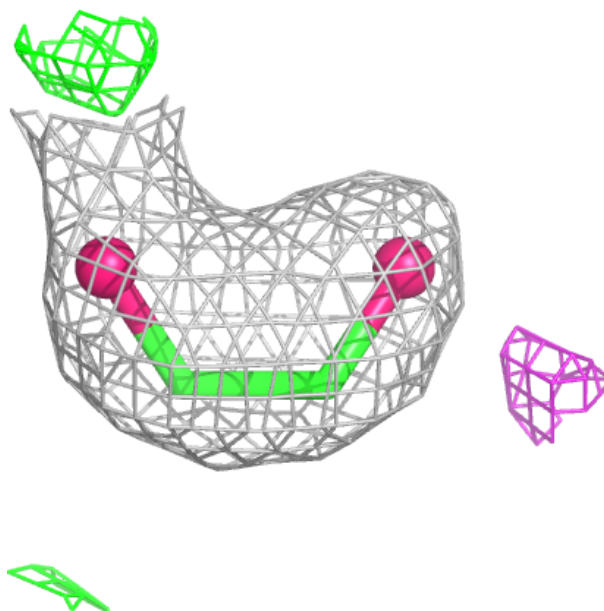
Electron density around EDO E 204:

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



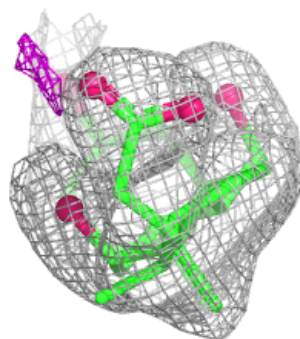
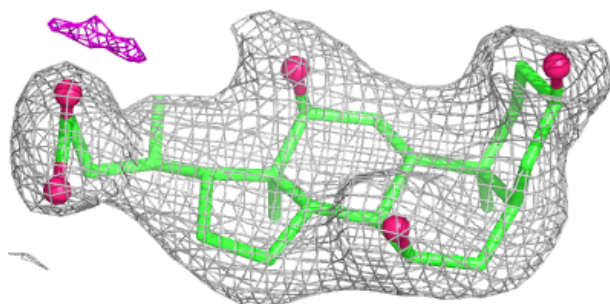
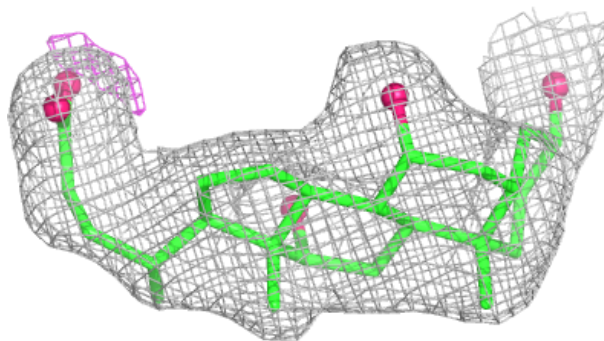
Electron density around EDO N 623:

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

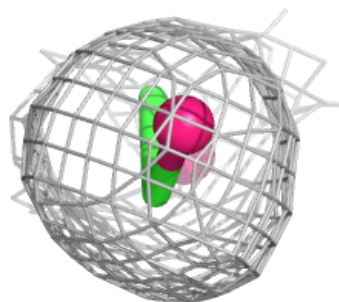
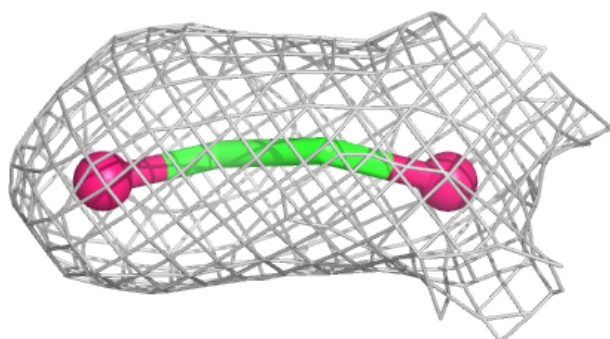
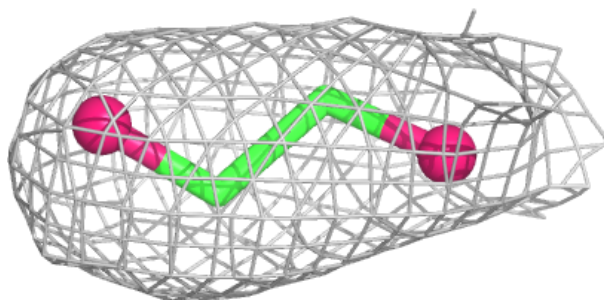


Electron density around CHD J 101:

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

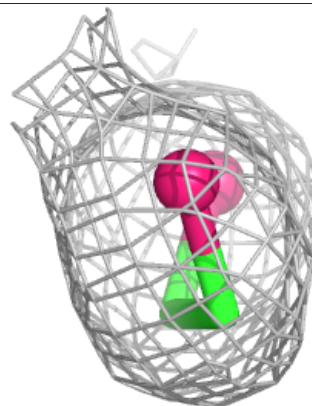
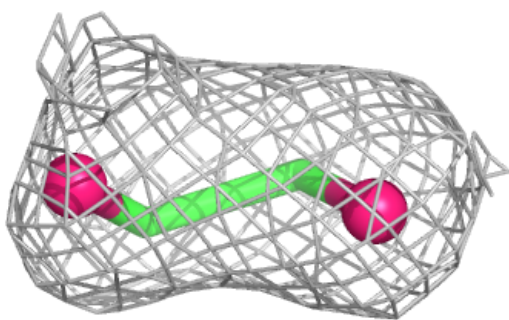
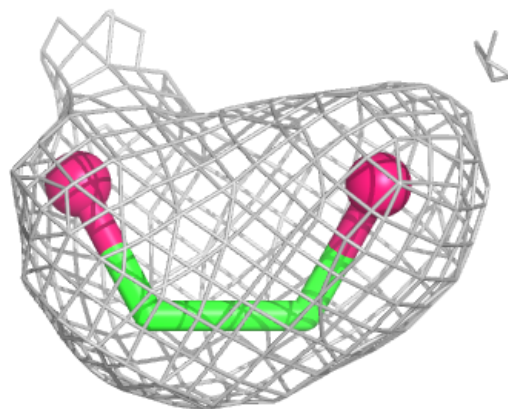
**Electron density around EDO N 624:**

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



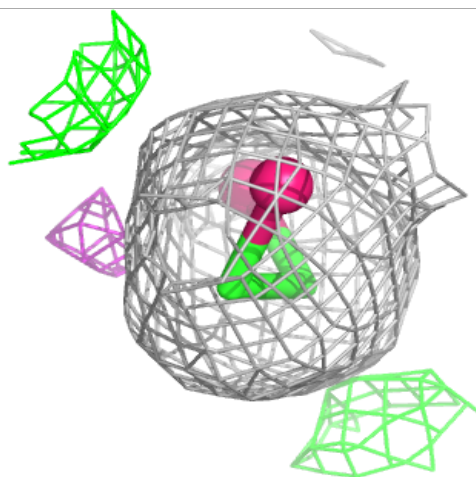
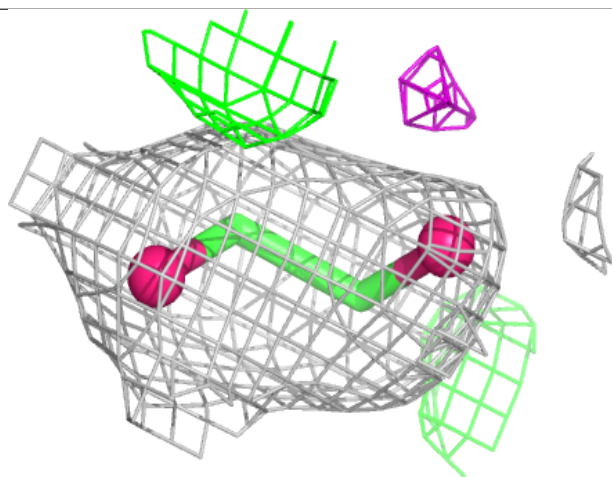
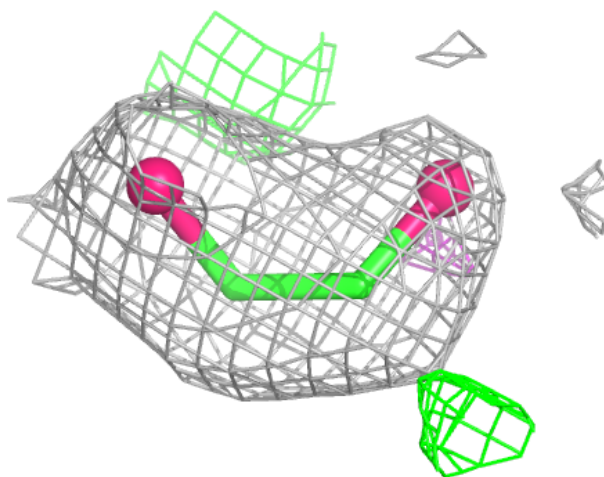
Electron density around EDO S 1601:

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



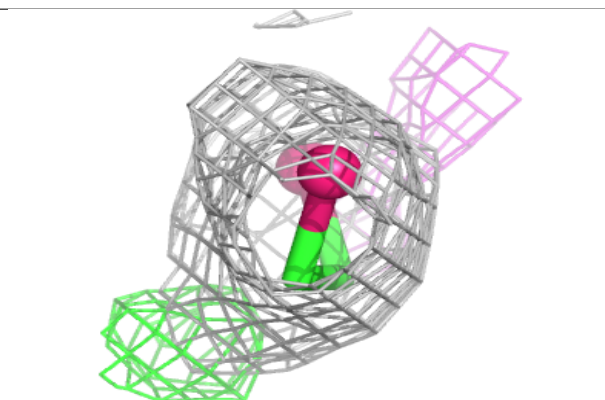
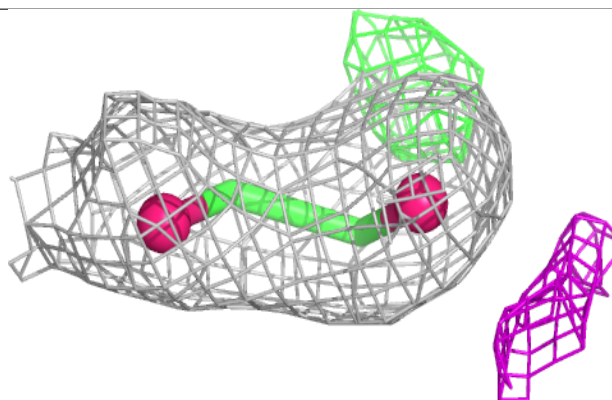
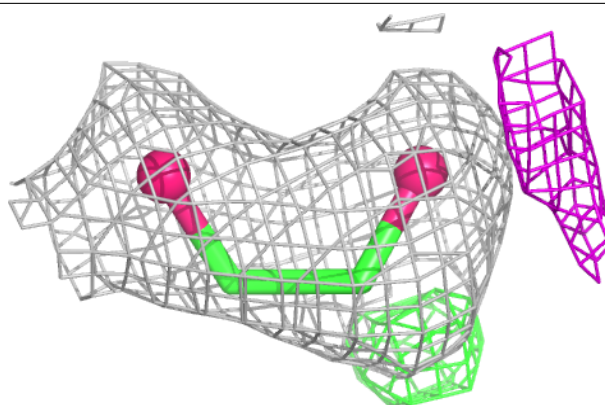
Electron density around EDO A 609:

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

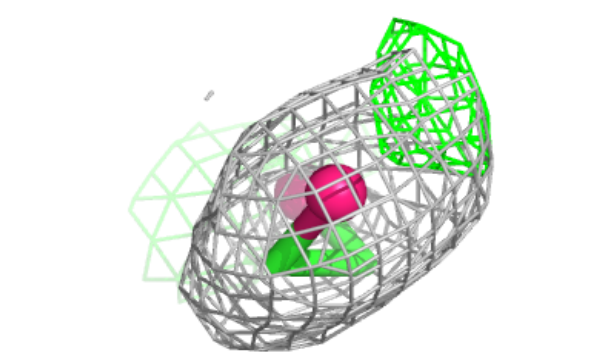
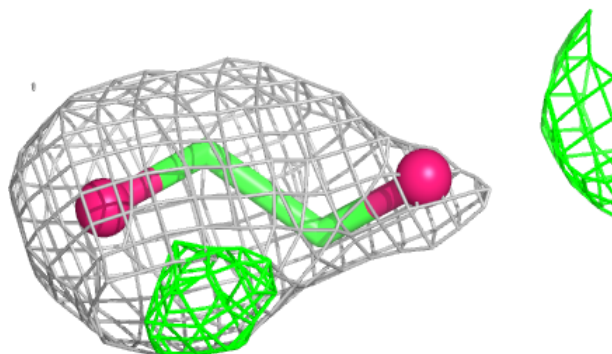
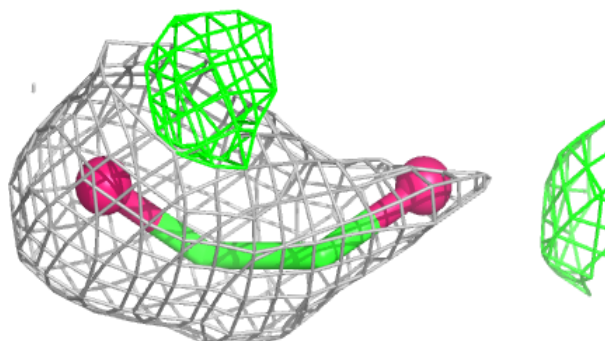


Electron density around EDO A 611:

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

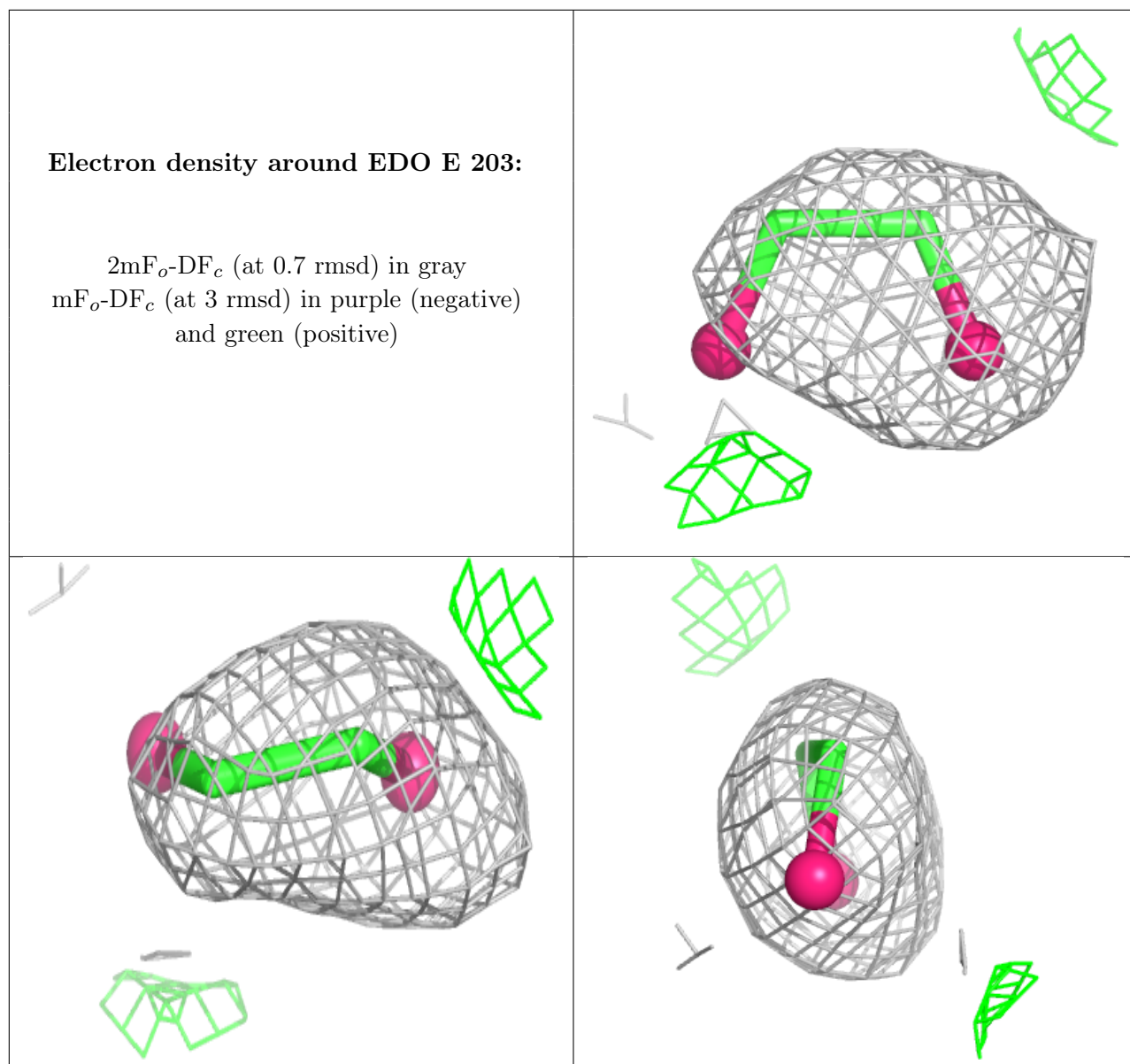
**Electron density around EDO N 620:**

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



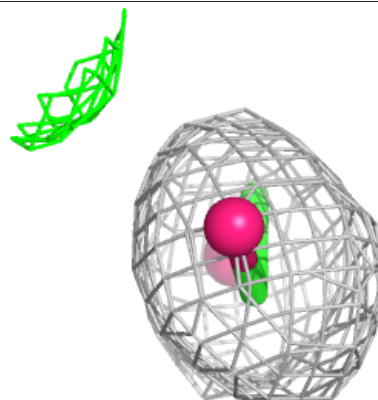
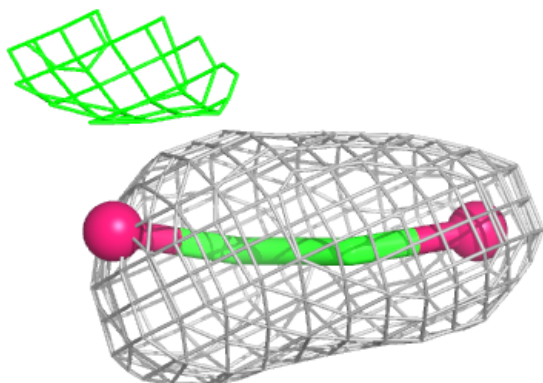
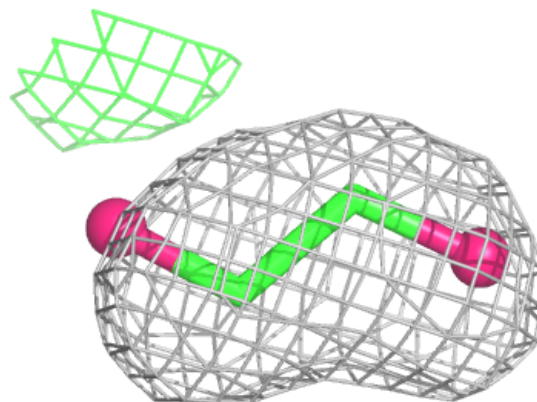
Electron density around EDO E 203:

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

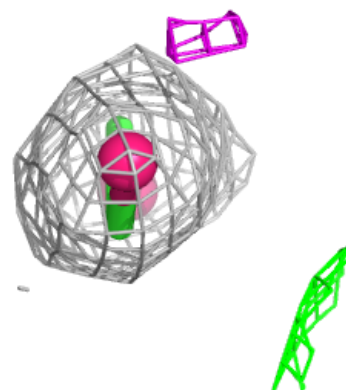
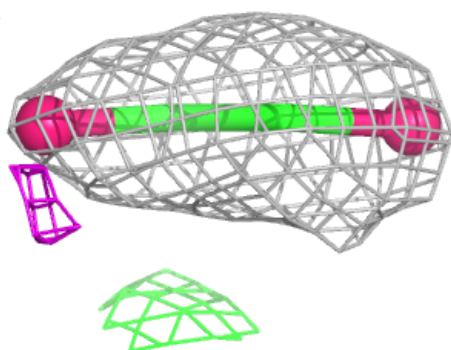
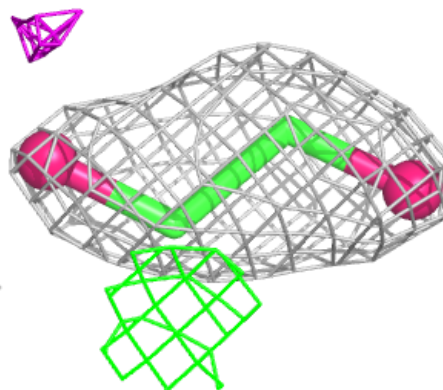


Electron density around EDO Q 1802:

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

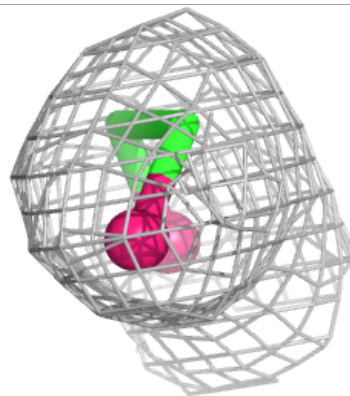
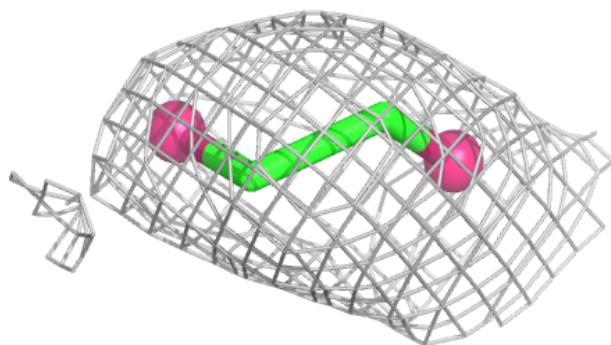
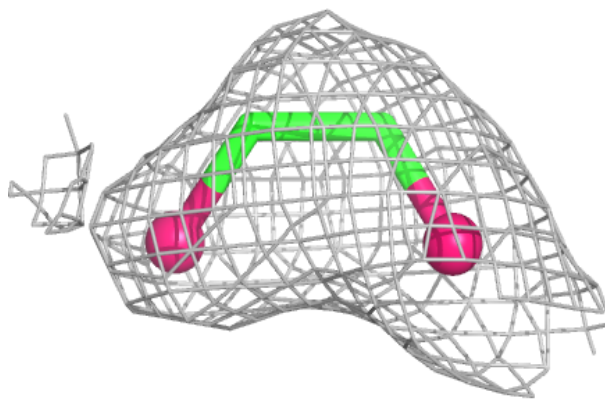
**Electron density around EDO A 612:**

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



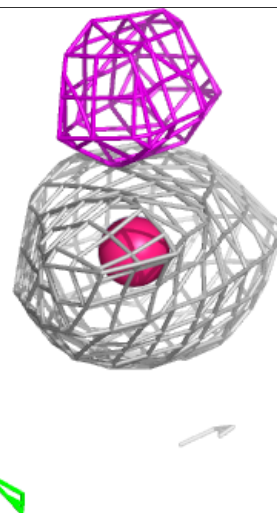
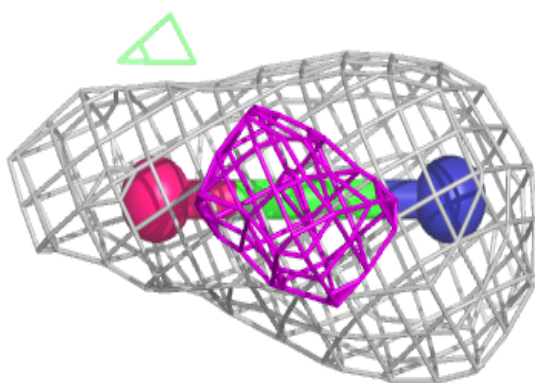
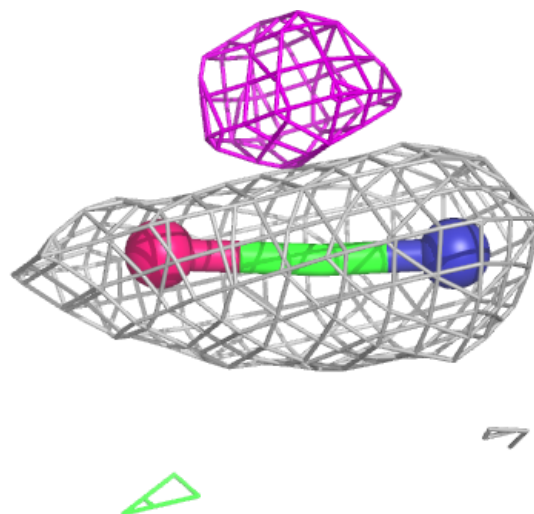
Electron density around EDO B 307:

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



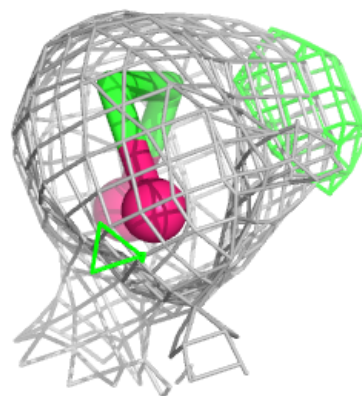
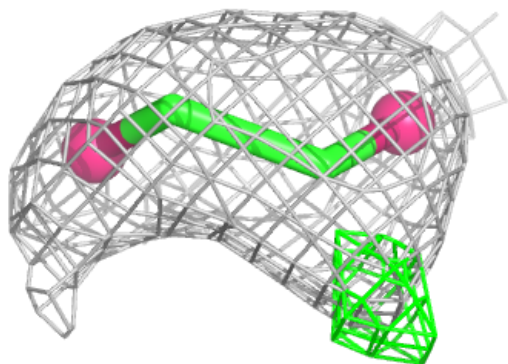
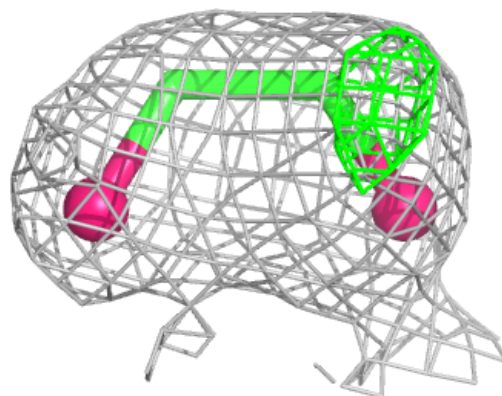
Electron density around 0NM C 312:

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

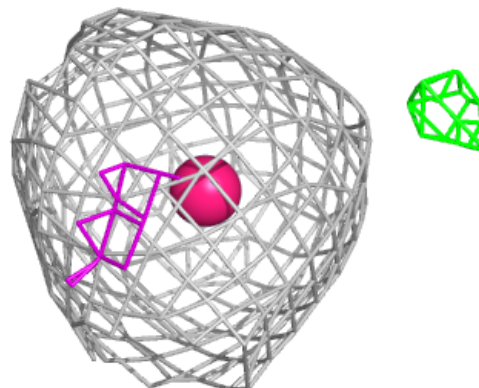
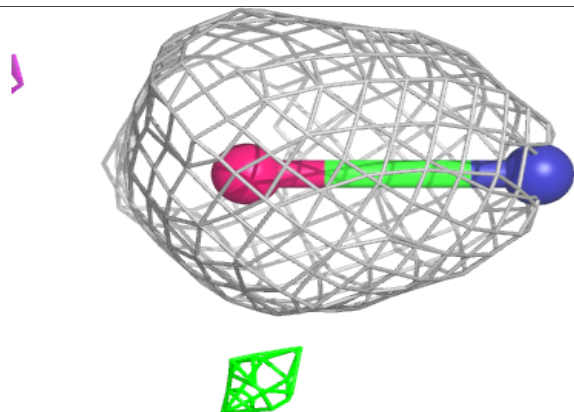
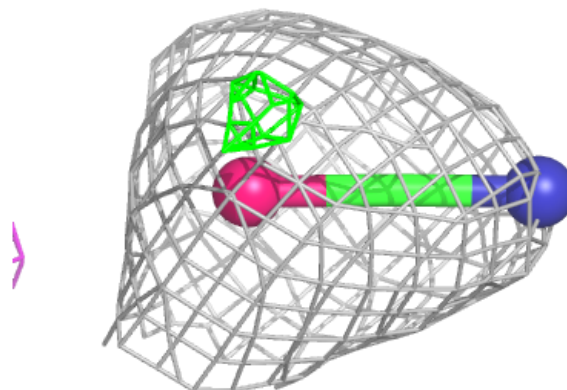


Electron density around EDO F 705:

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

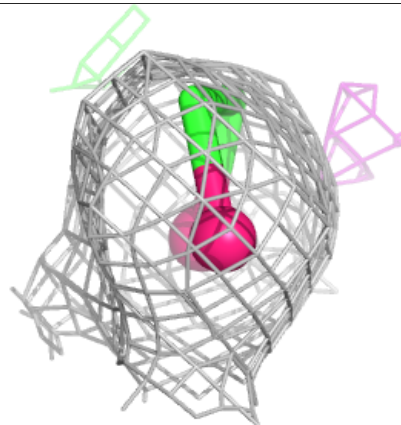
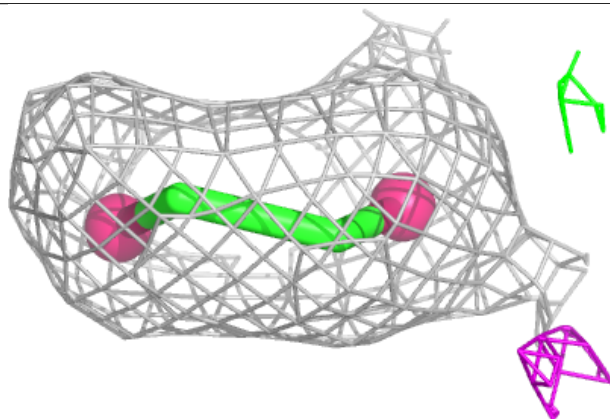
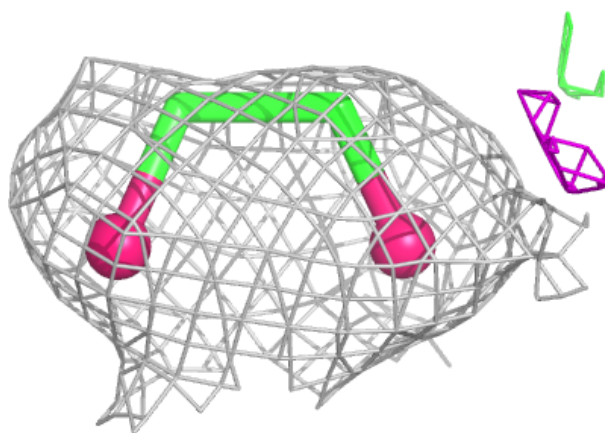
**Electron density around 0NM N 617:**

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

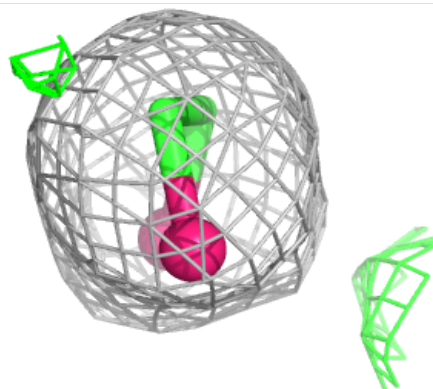
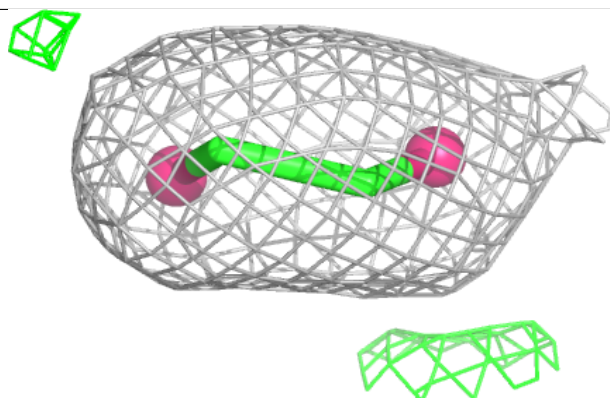
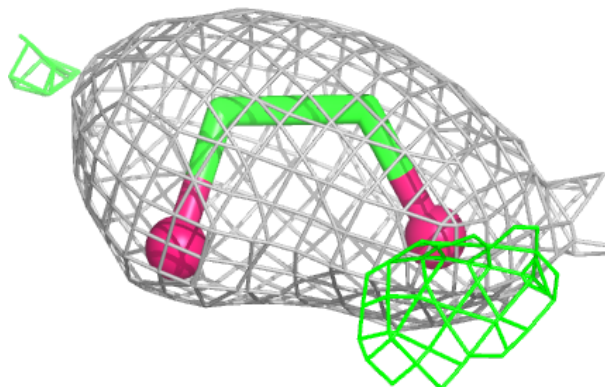


Electron density around EDO L 501:

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

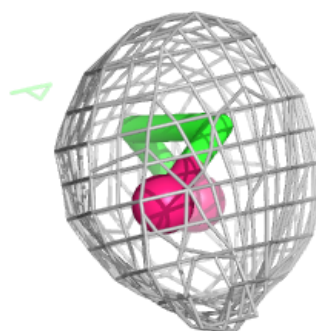
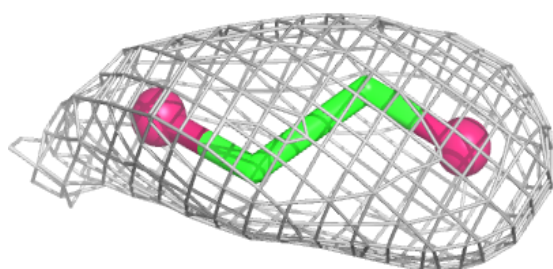
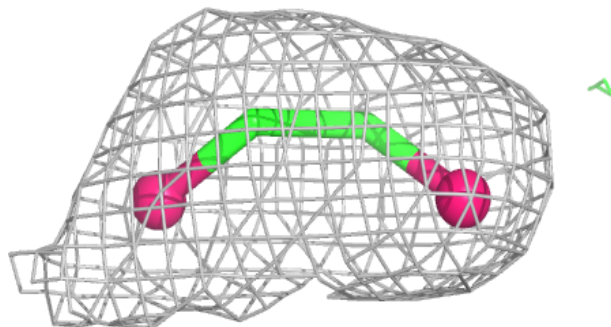
**Electron density around EDO P 313:**

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

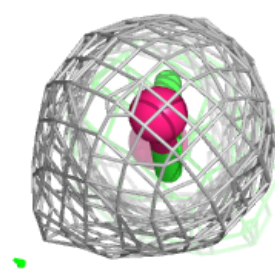
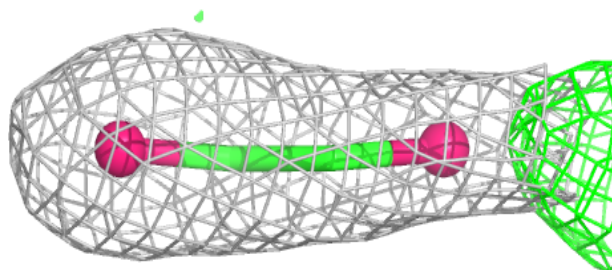
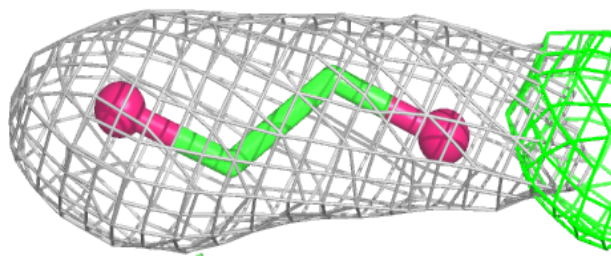


Electron density around EDO C 311:

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

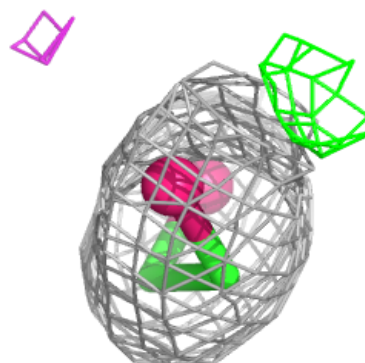
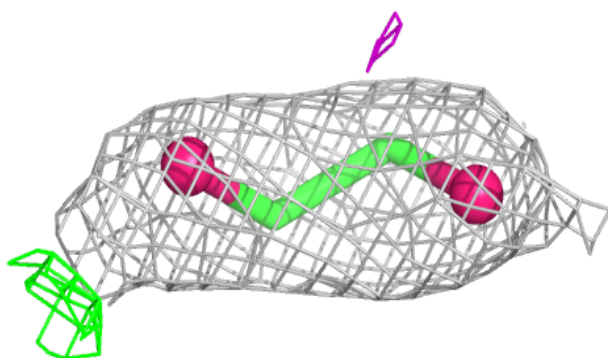
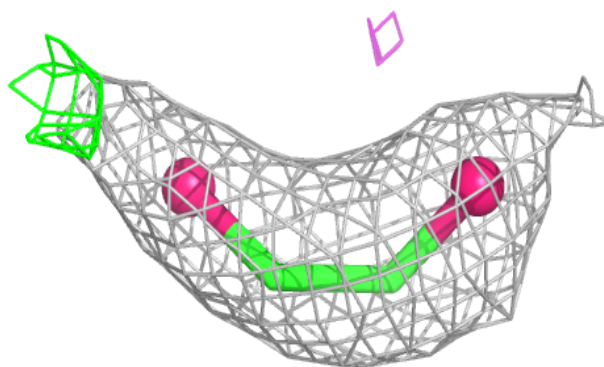
**Electron density around EDO C 314:**

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

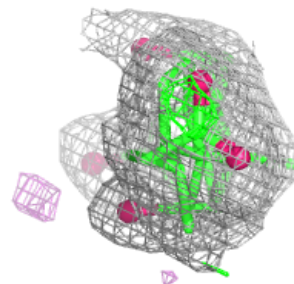
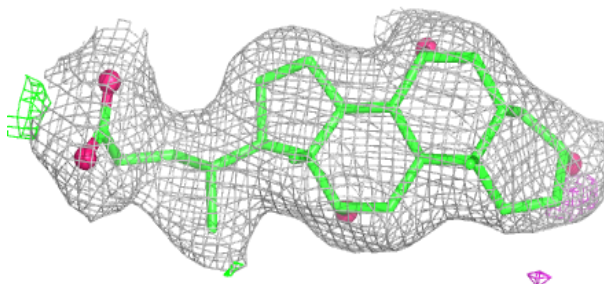


Electron density around EDO N 609:

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

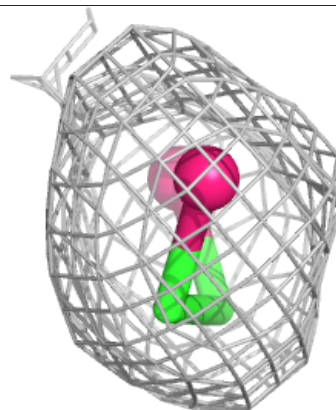
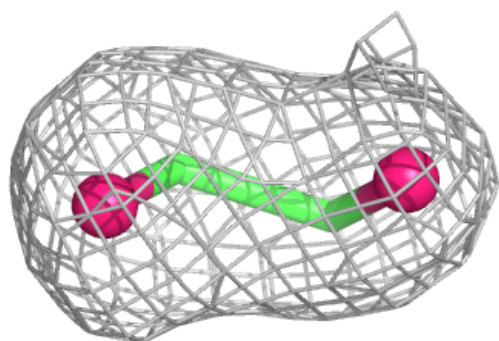
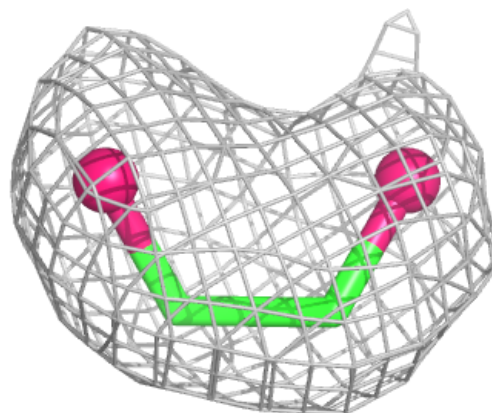
**Electron density around CHD P 309:**

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

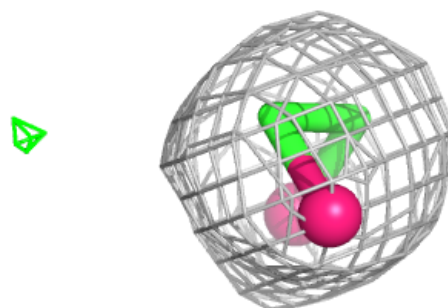
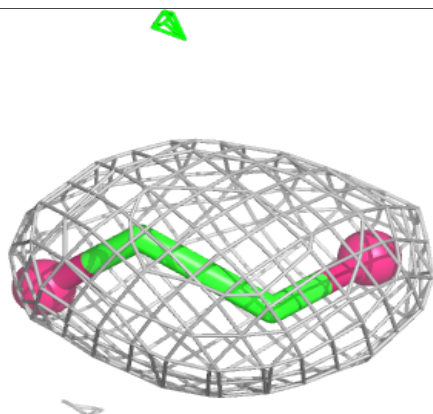
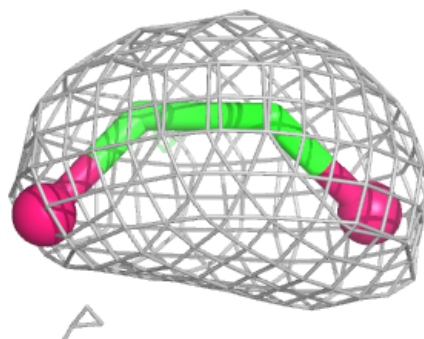


Electron density around EDO R 201:

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

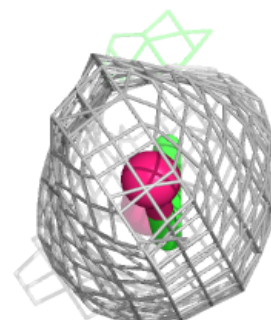
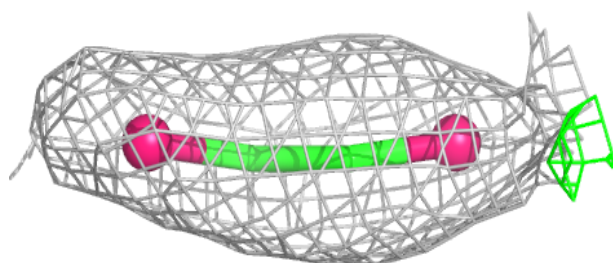
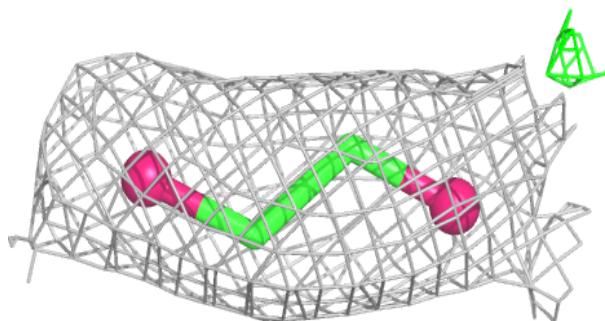
**Electron density around EDO D 203:**

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

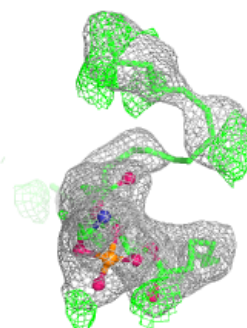
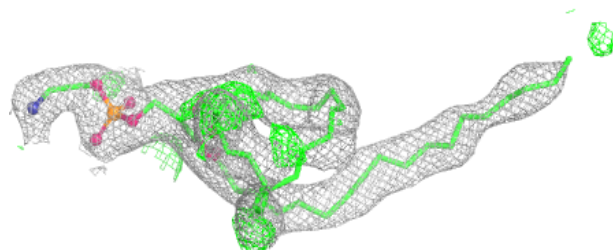
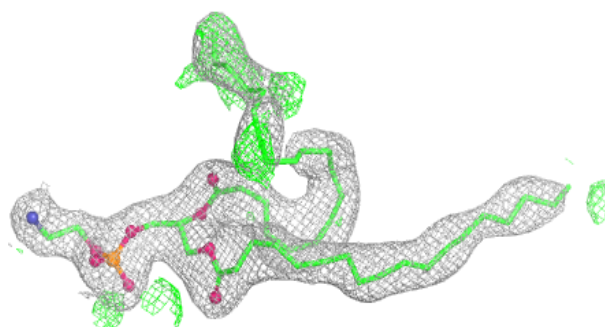


Electron density around EDO I 103:

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

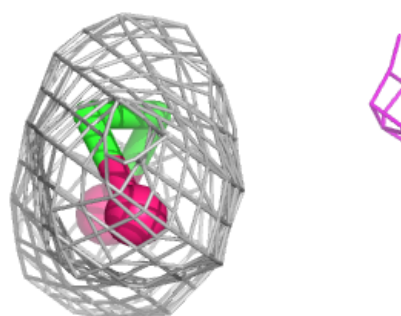
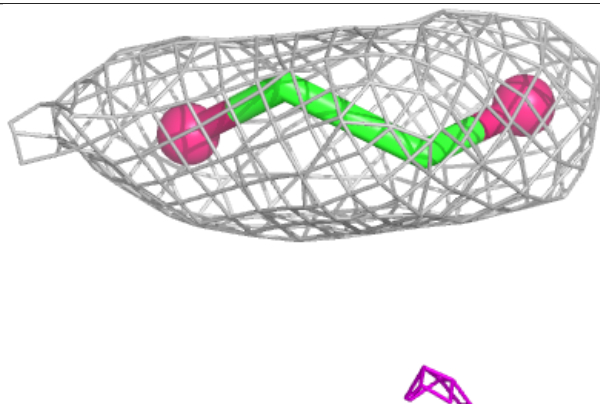
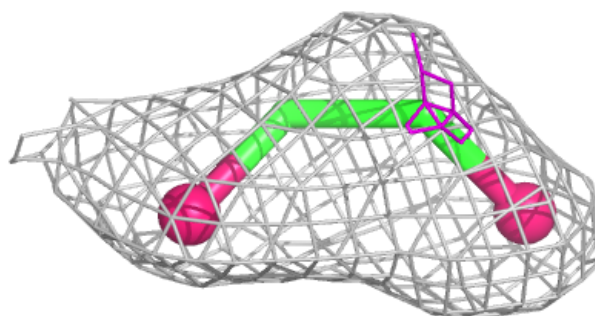
**Electron density around PEK P 304:**

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

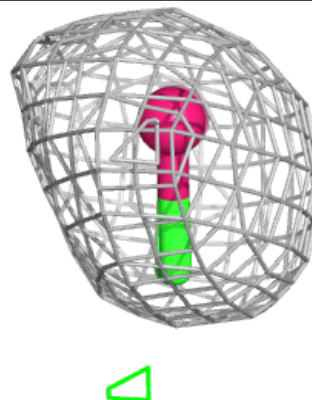
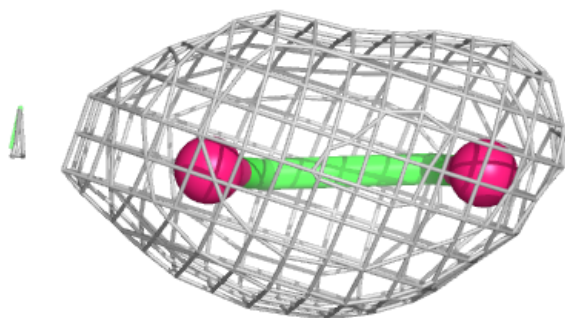
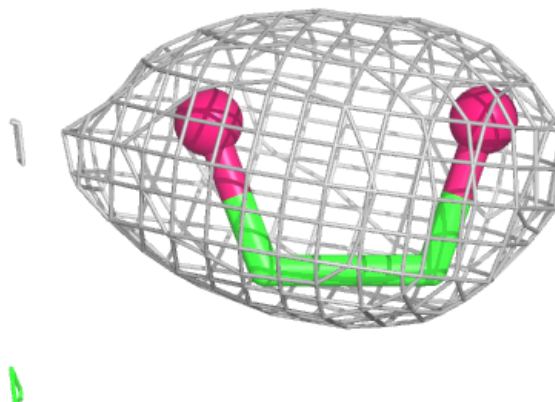


Electron density around EDO A 618:

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

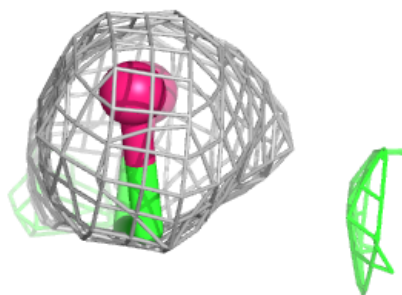
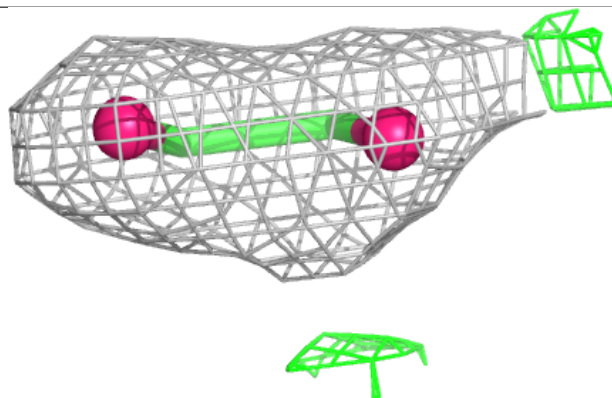
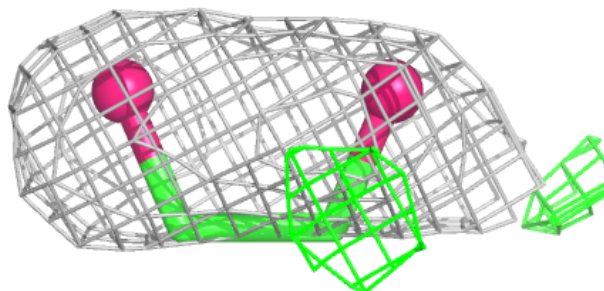
**Electron density around EDO W 301:**

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



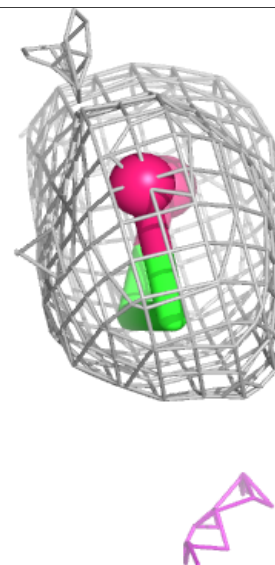
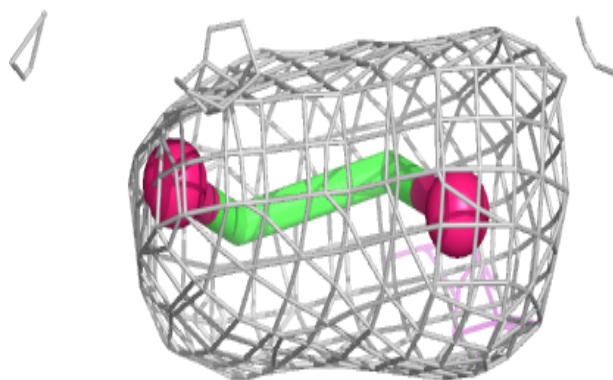
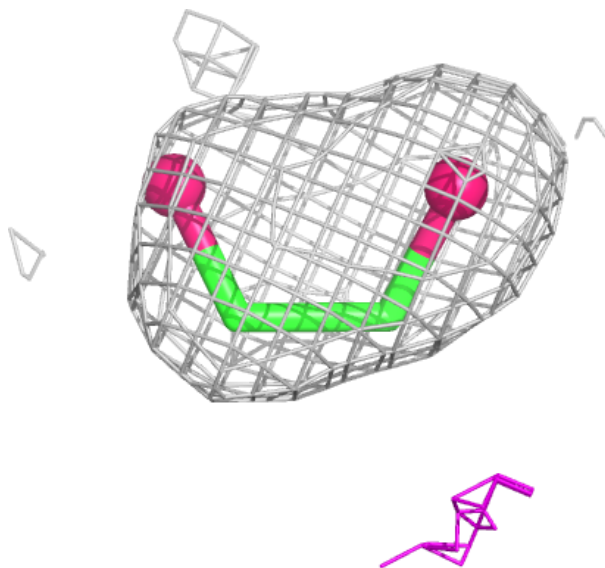
Electron density around EDO W 303:

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



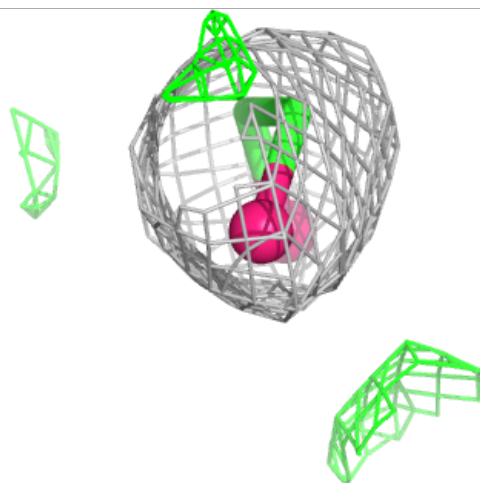
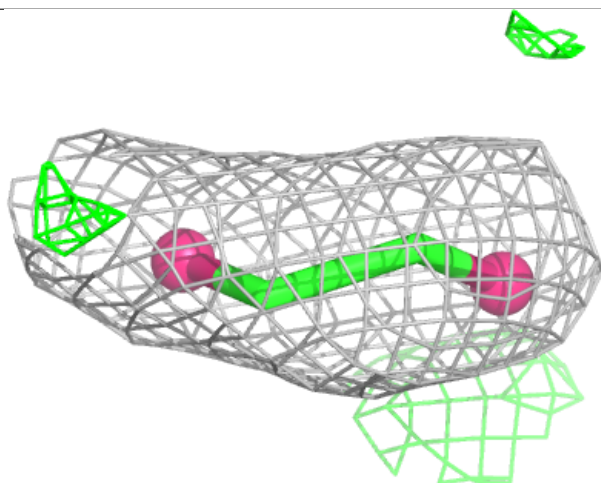
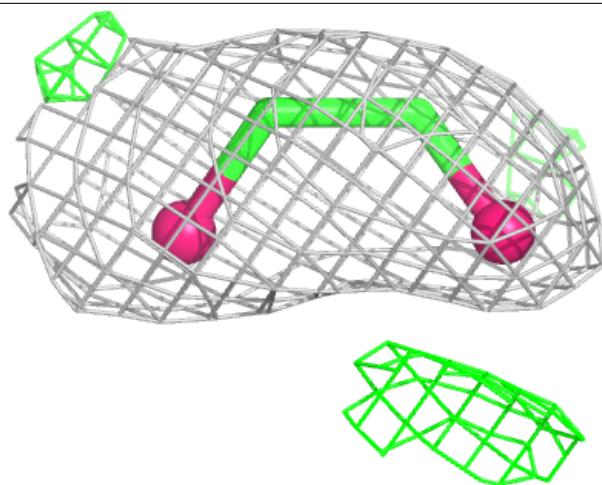
Electron density around EDO J 103:

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



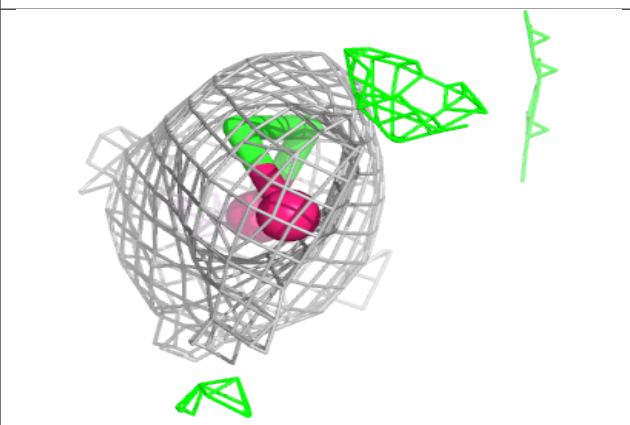
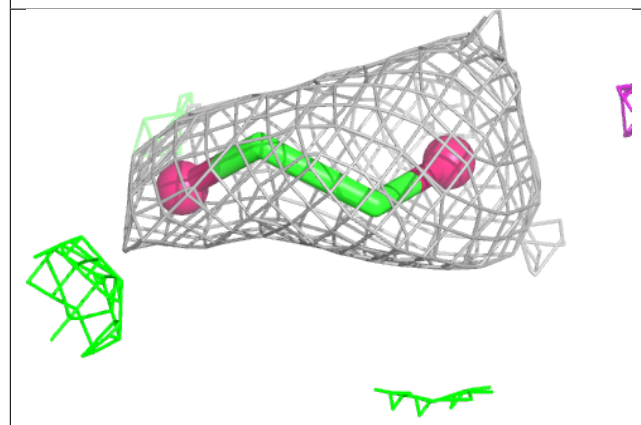
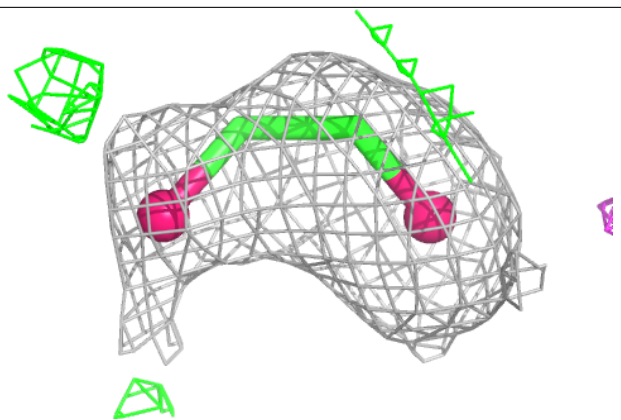
Electron density around EDO B 309:

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

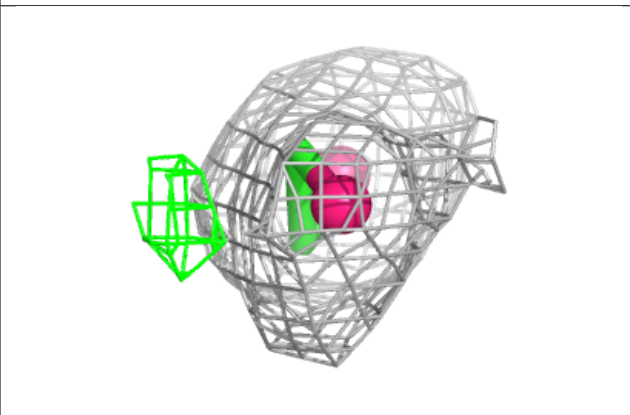
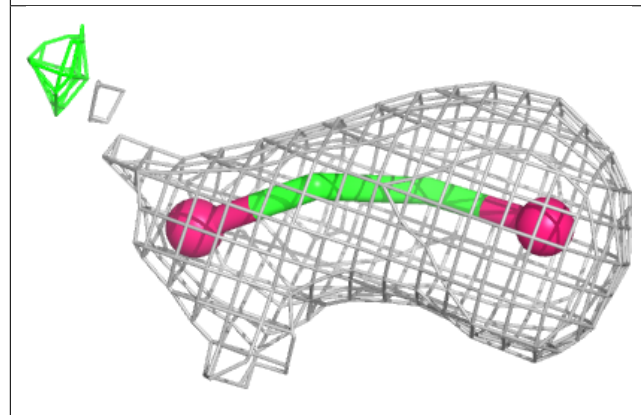
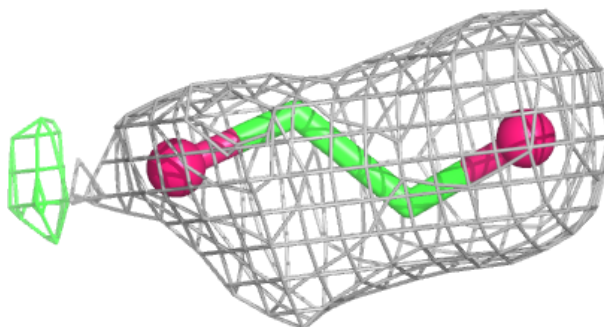


Electron density around EDO N 614:

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

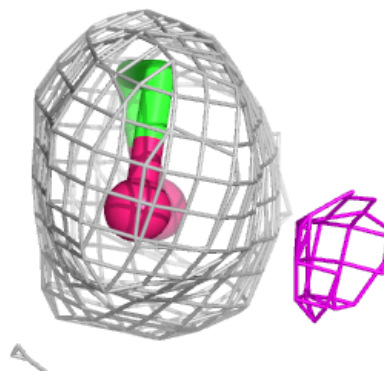
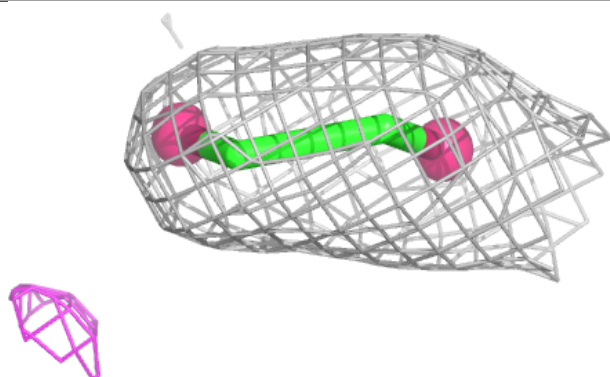
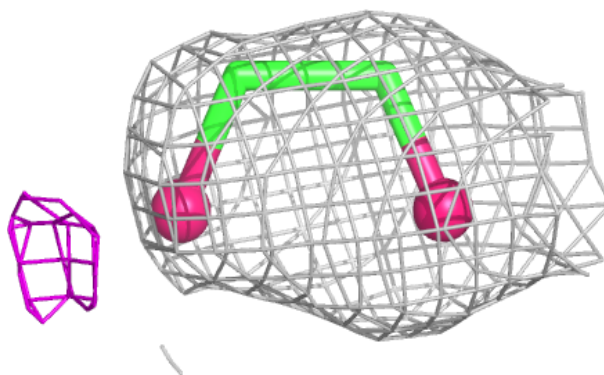
**Electron density around EDO B 310:**

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

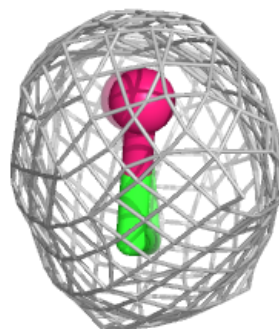
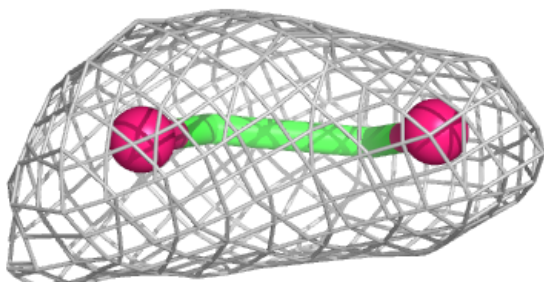
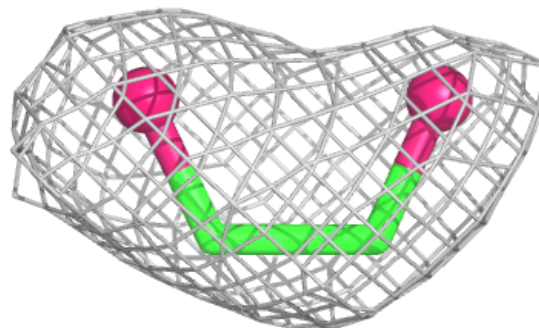


Electron density around EDO D 202:

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

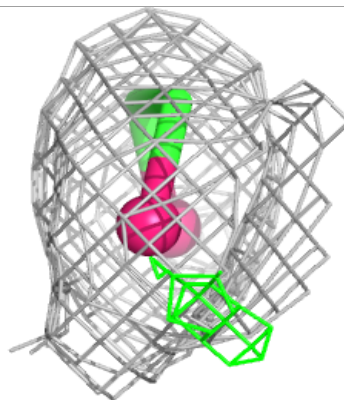
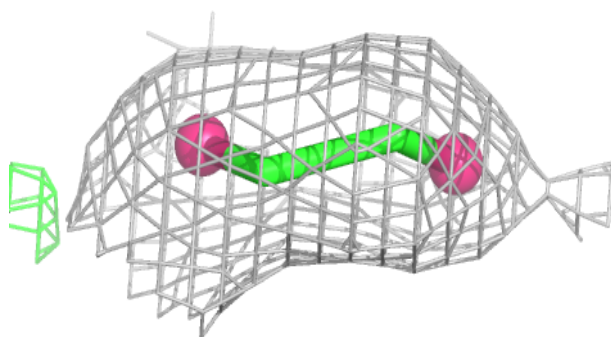
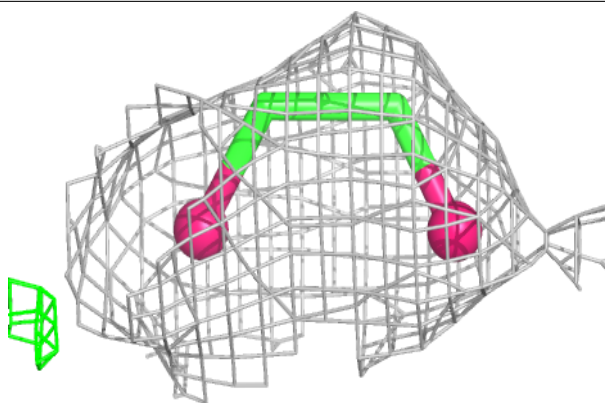
**Electron density around EDO F 708:**

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

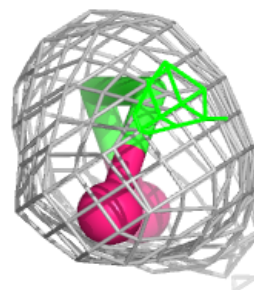
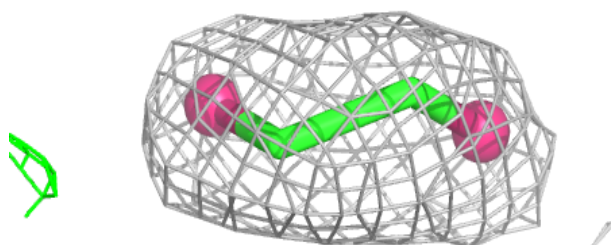
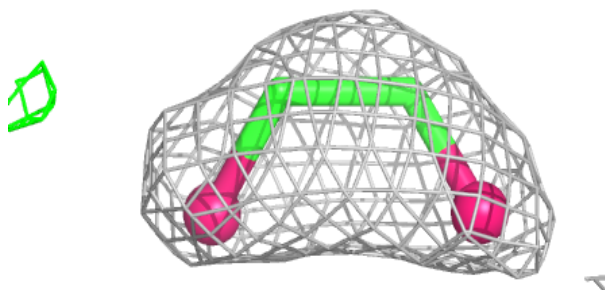


Electron density around EDO M 102:

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

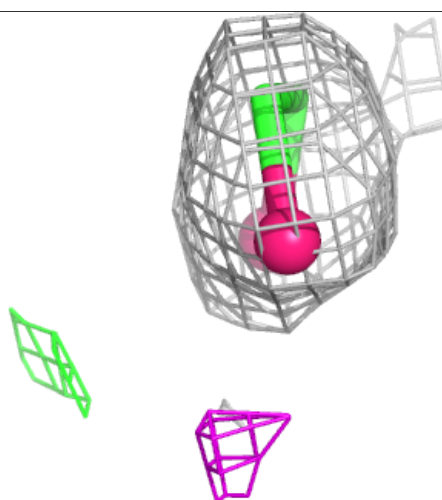
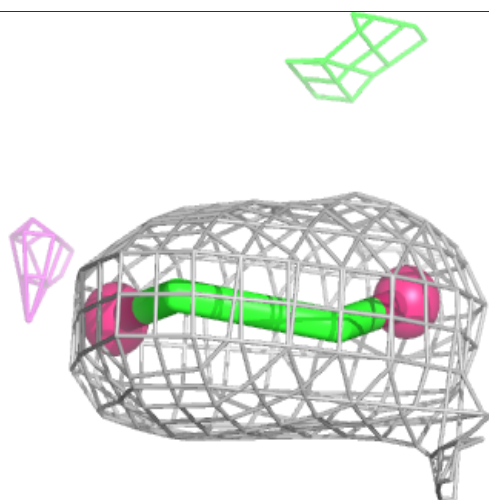
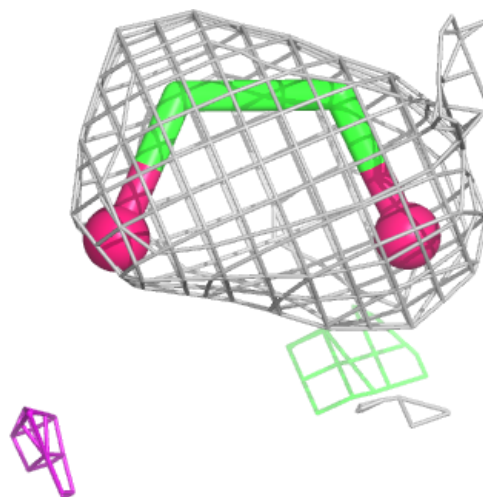
**Electron density around EDO O 303:**

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



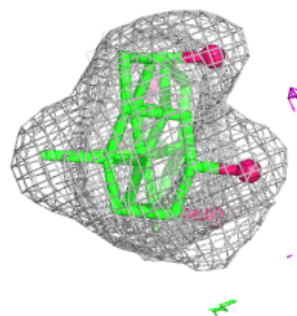
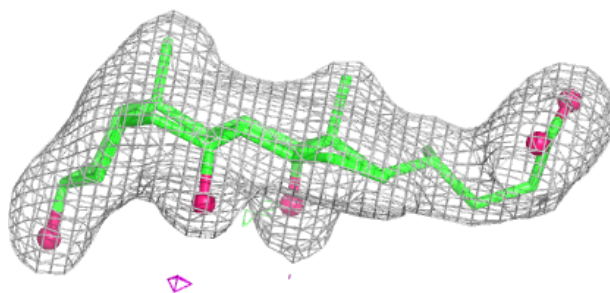
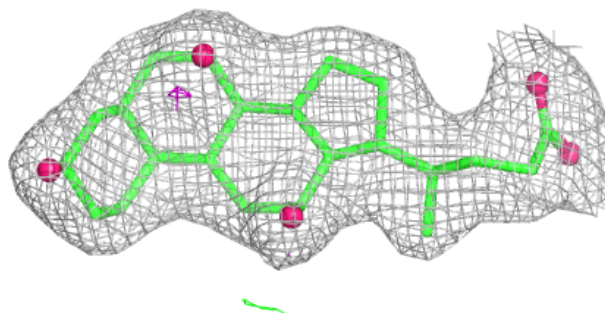
Electron density around EDO O 304:

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

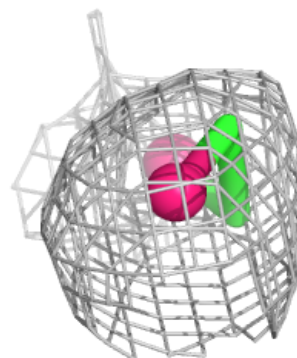
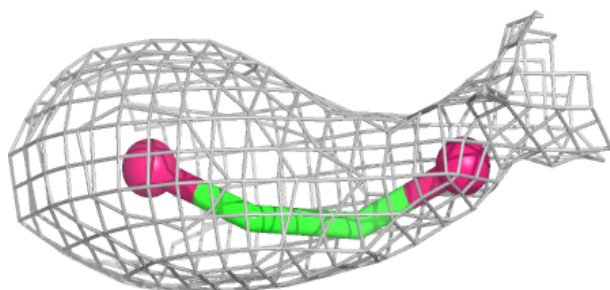
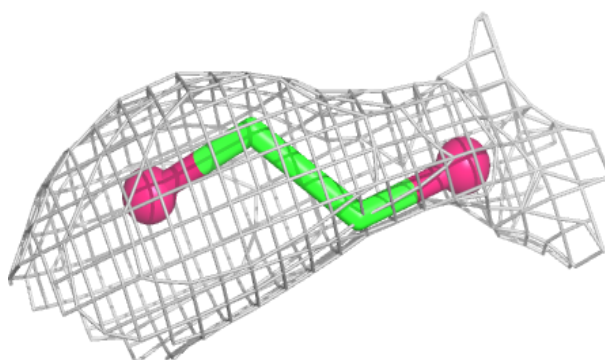


Electron density around CHD C 307:

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

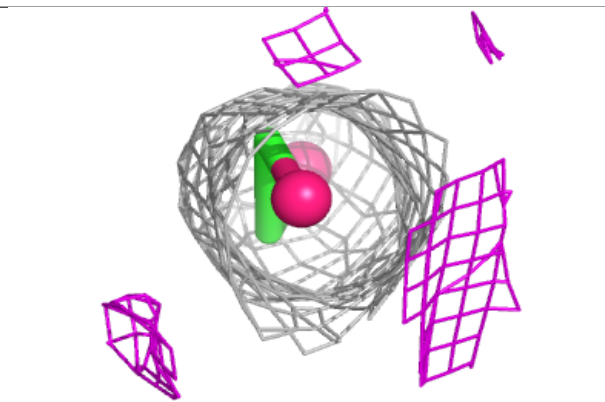
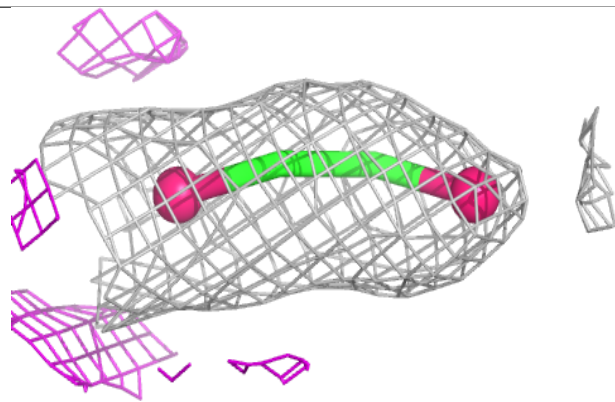
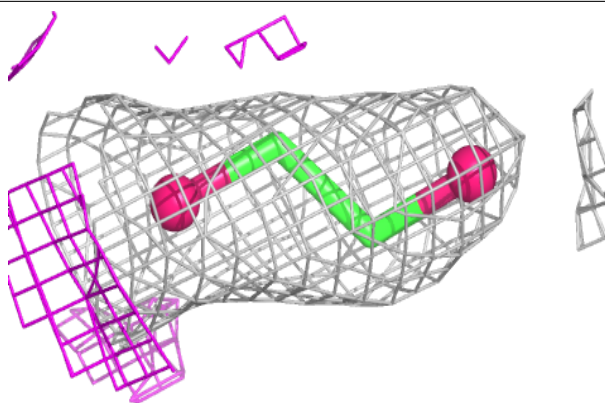
**Electron density around EDO P 310:**

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

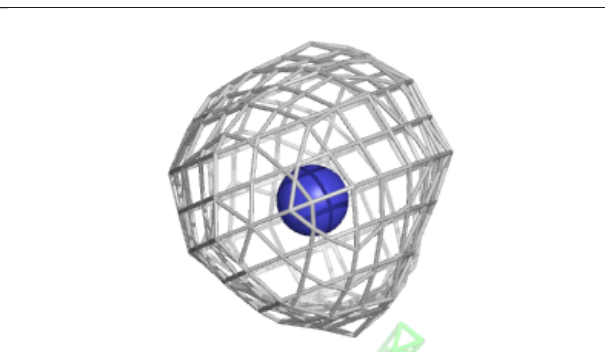
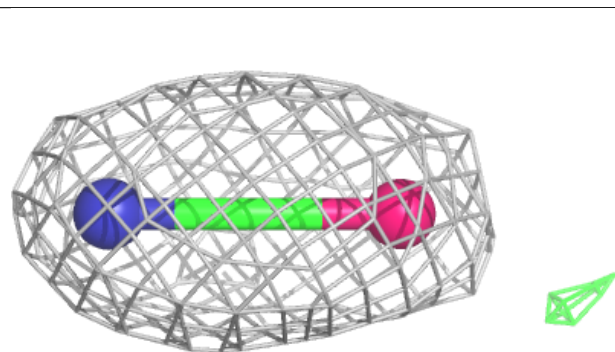
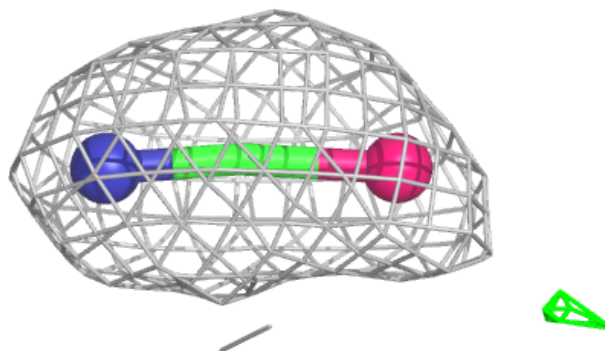


Electron density around EDO C 310:

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

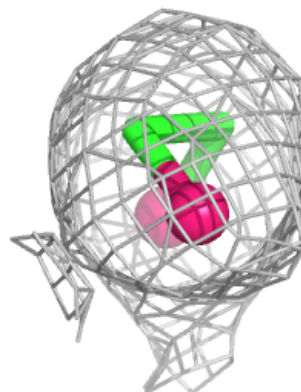
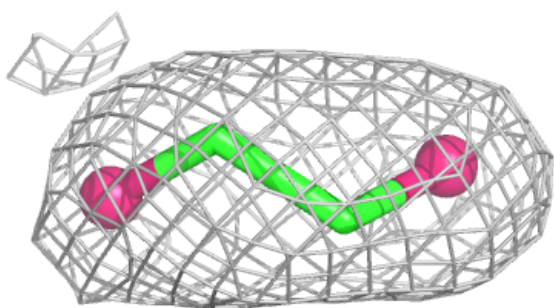
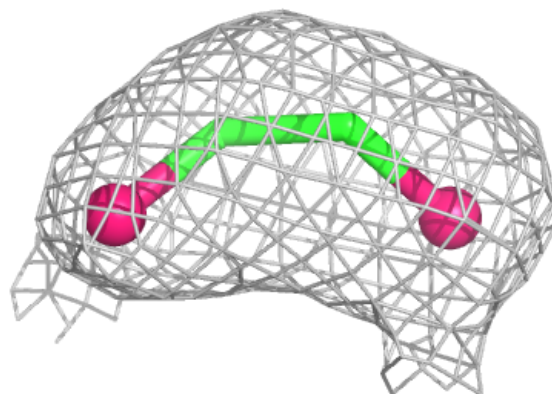
**Electron density around ONM A 614:**

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

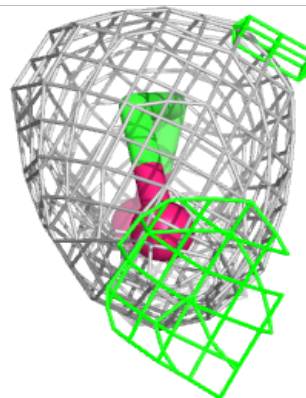
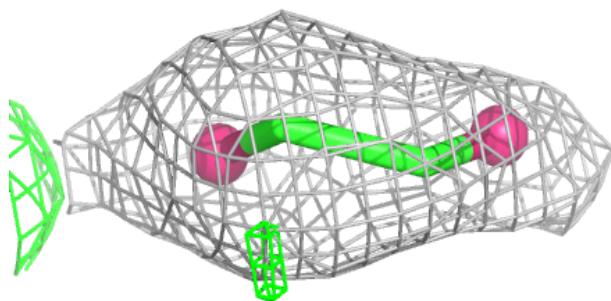
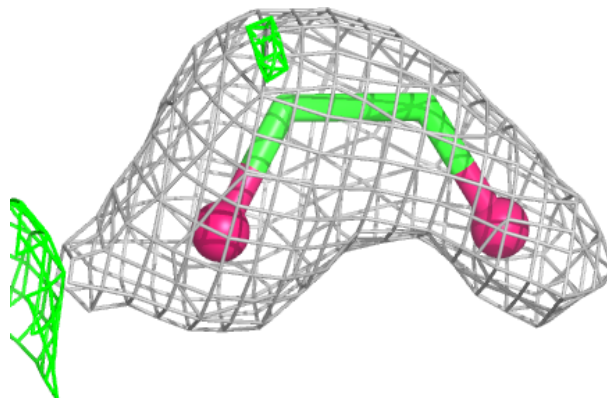


Electron density around EDO A 617:

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

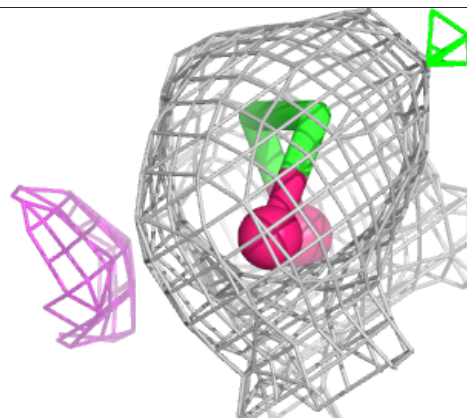
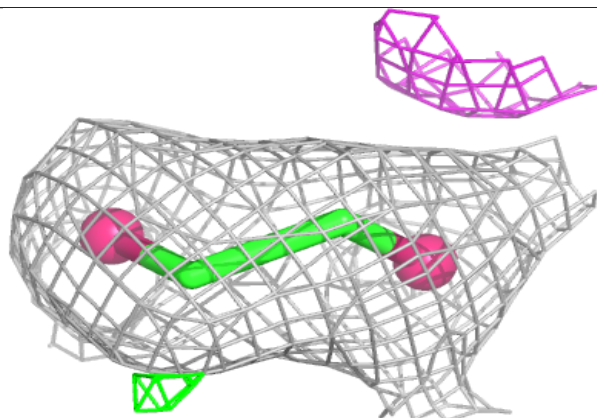
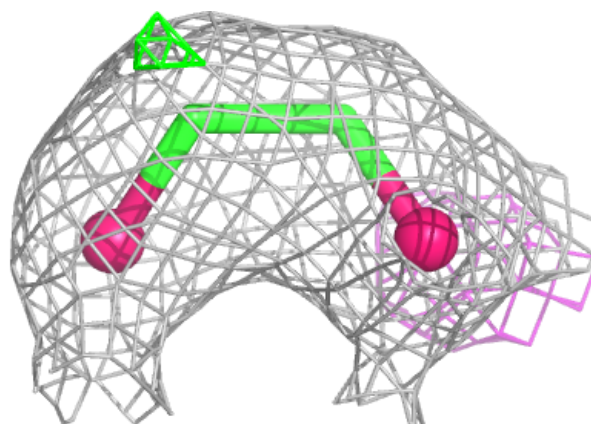
**Electron density around EDO A 607:**

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

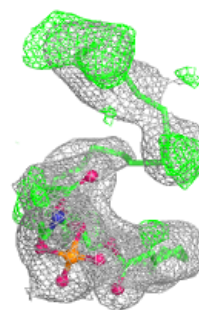
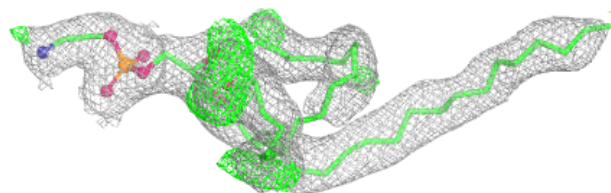
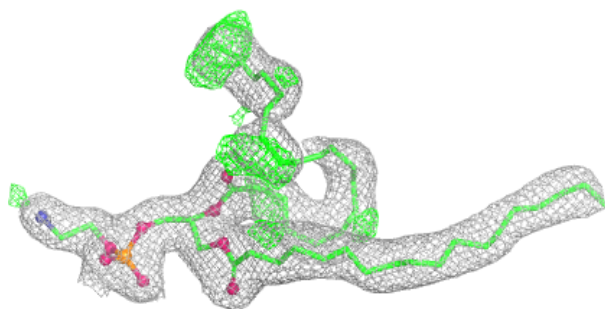


Electron density around EDO F 707:

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

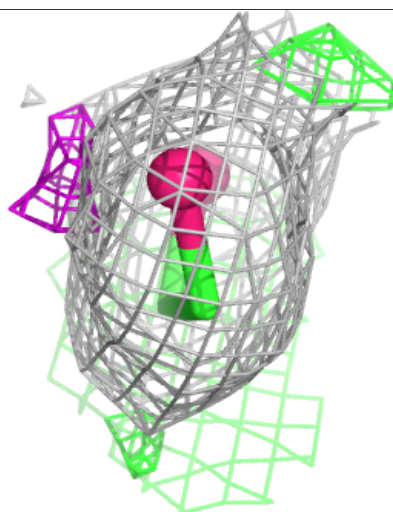
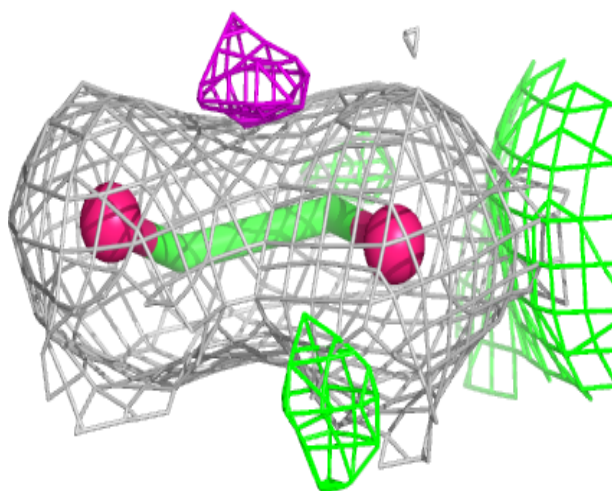
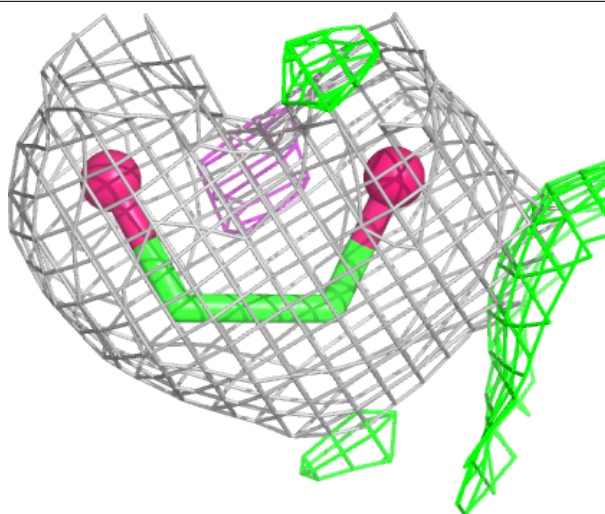
**Electron density around PEK C 302:**

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



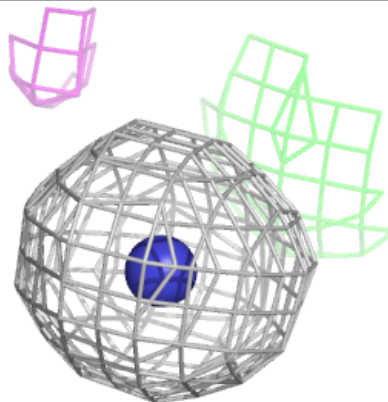
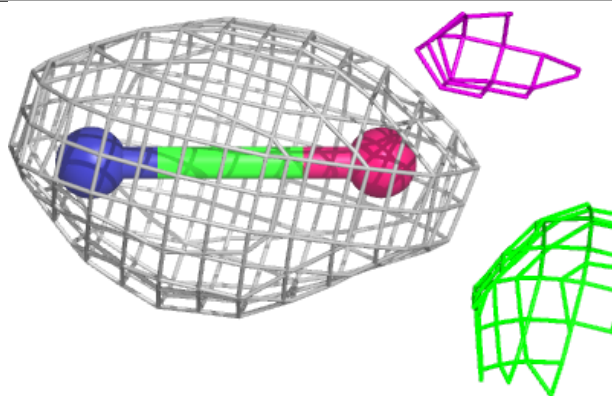
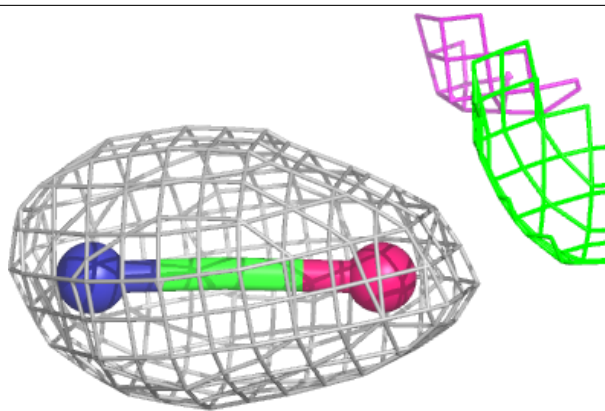
Electron density around EDO S 1603:

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



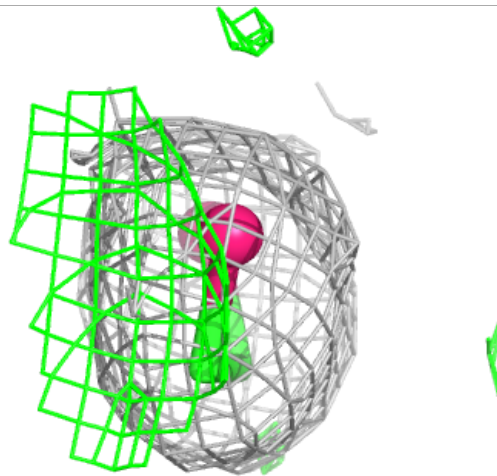
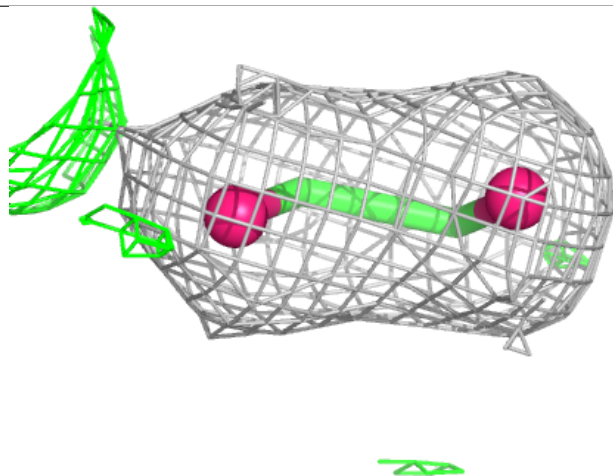
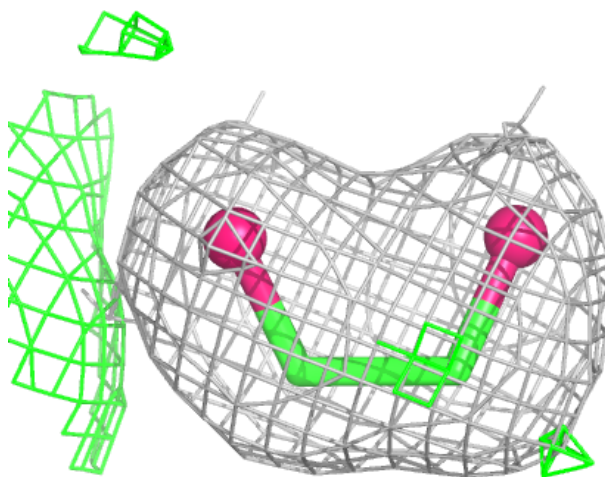
Electron density around 0NM A 615:

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



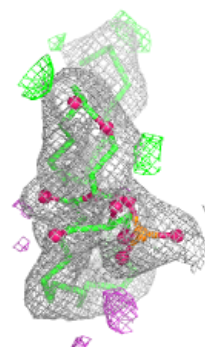
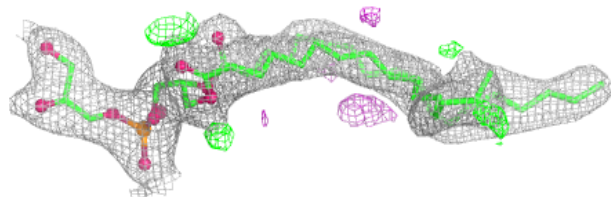
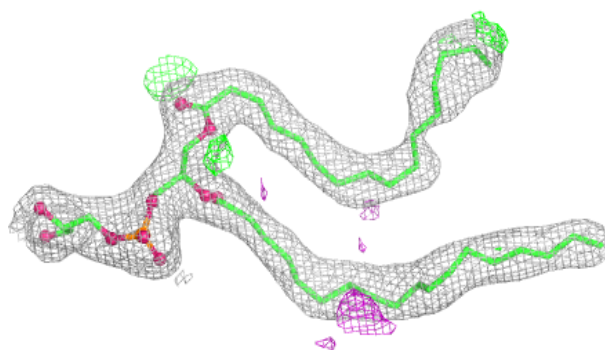
Electron density around EDO N 608:

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

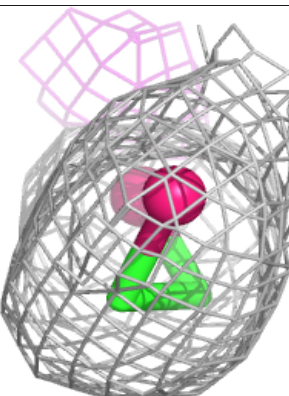
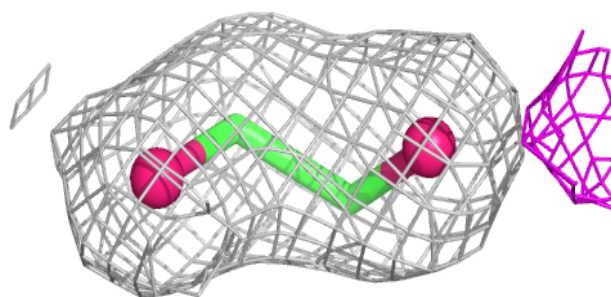
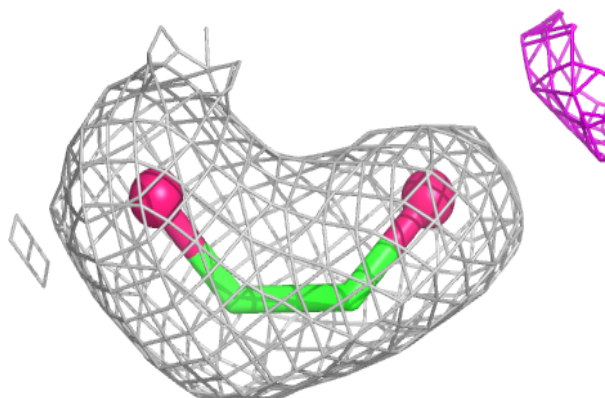


Electron density around PGV P 302:

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

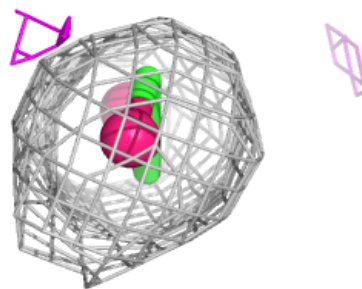
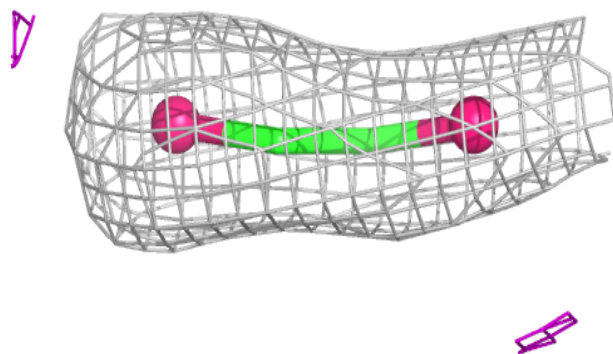
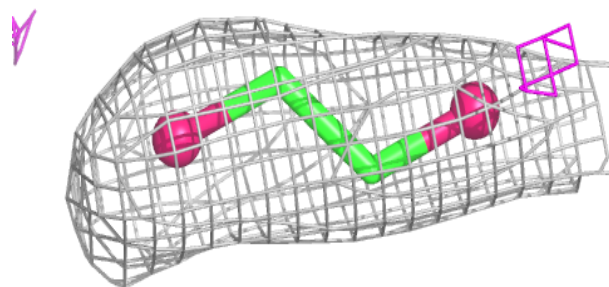
**Electron density around EDO B 306:**

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

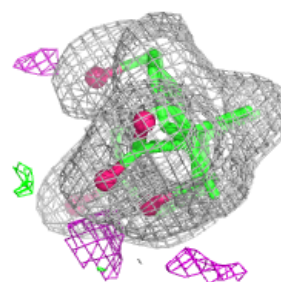
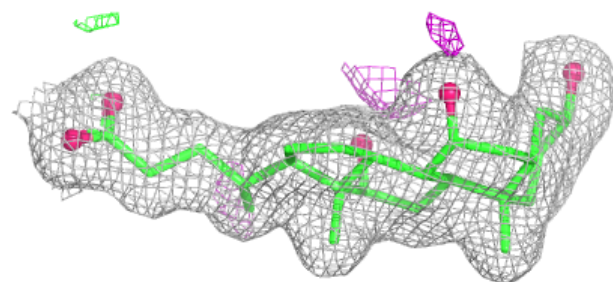
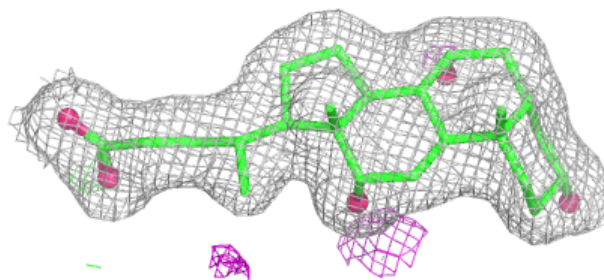


Electron density around EDO K 201:

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

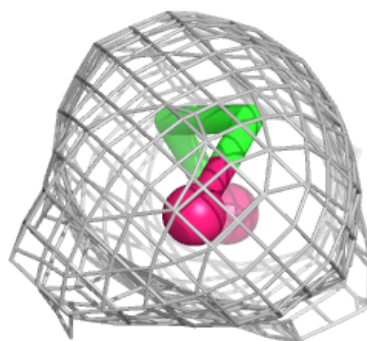
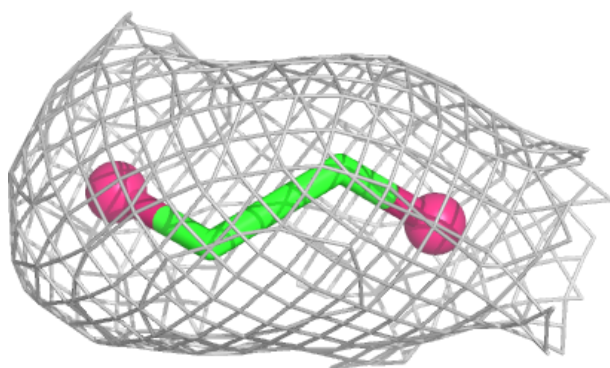
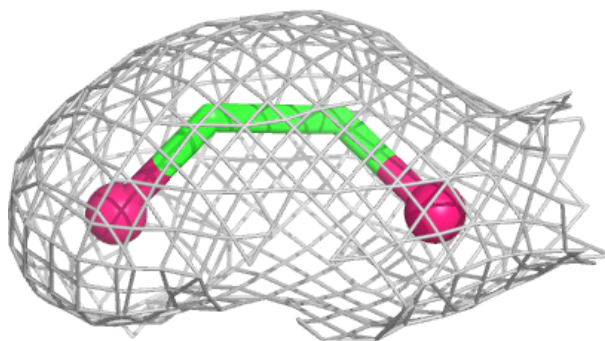
**Electron density around CHD C 301:**

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

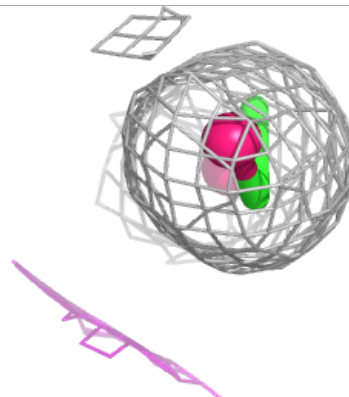
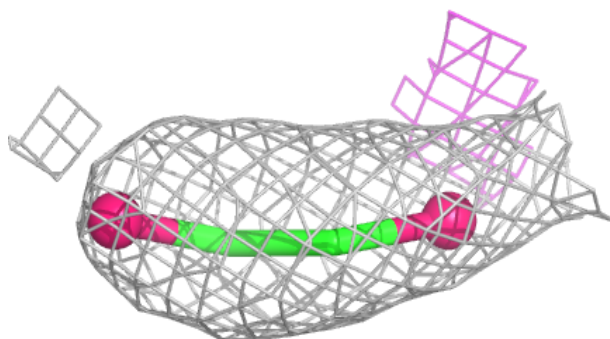
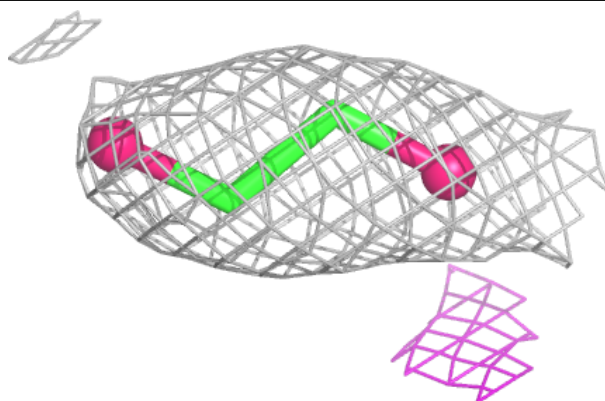


Electron density around EDO E 201:

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

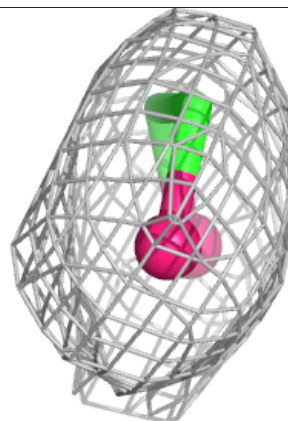
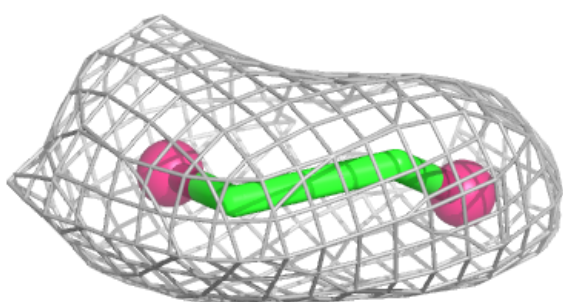
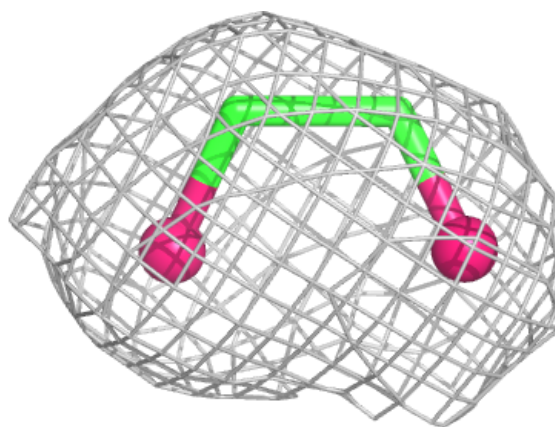
**Electron density around EDO L 503:**

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

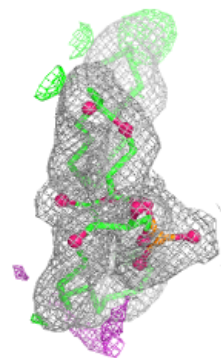
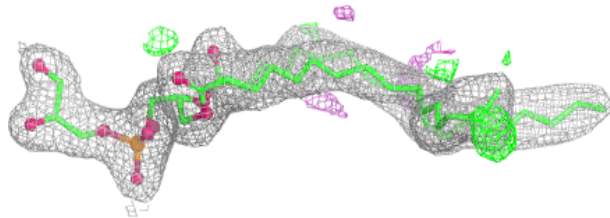
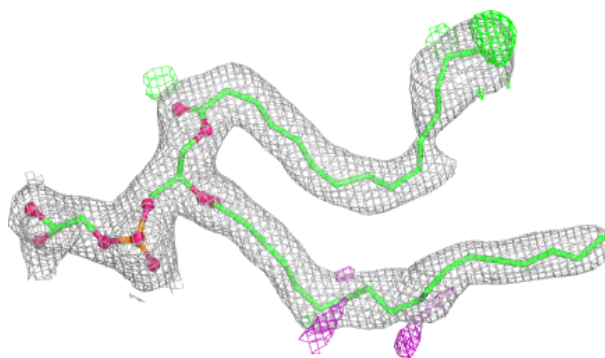


Electron density around EDO E 202:

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

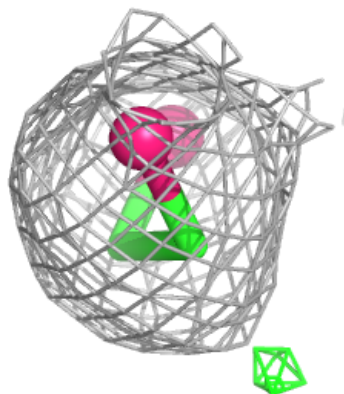
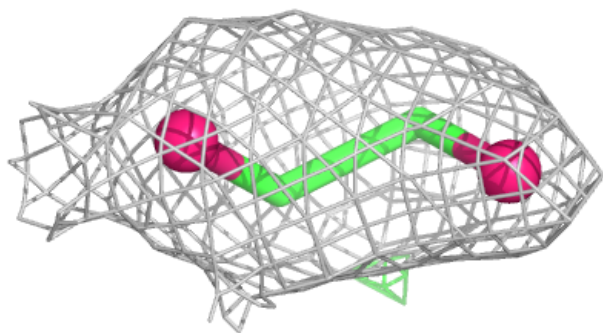
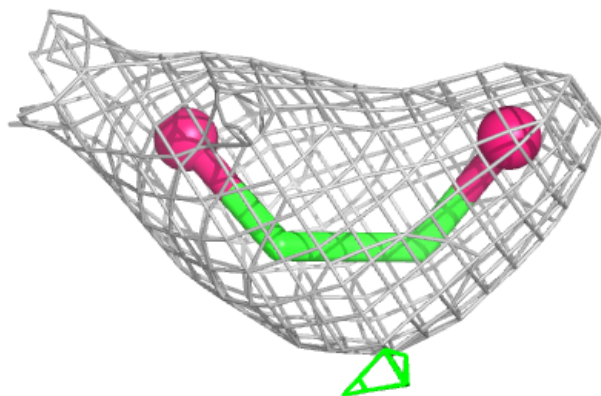
**Electron density around PGV A 604:**

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



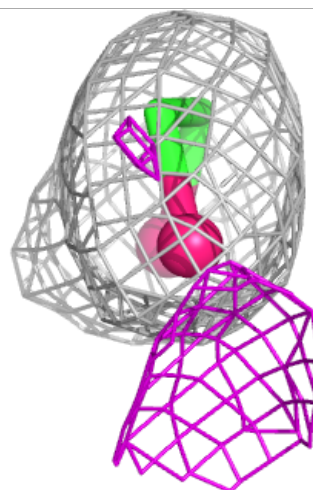
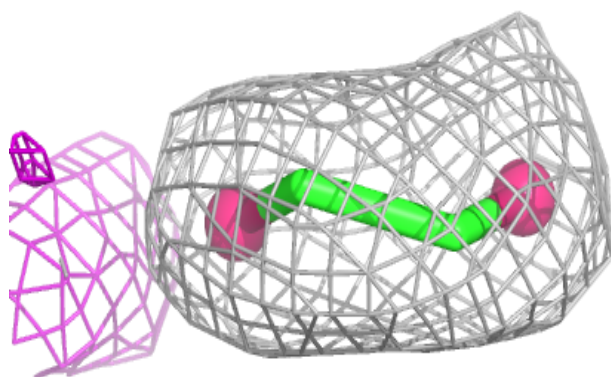
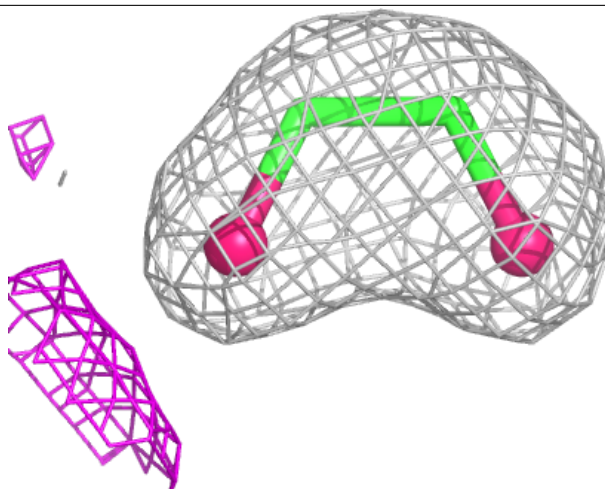
Electron density around EDO D 205:

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



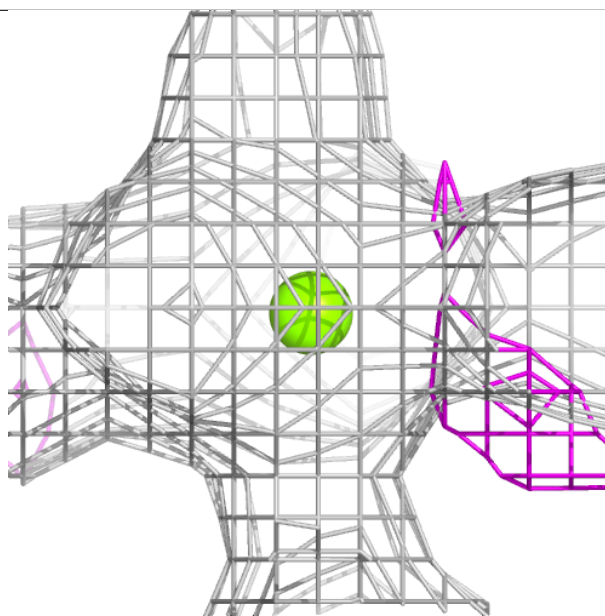
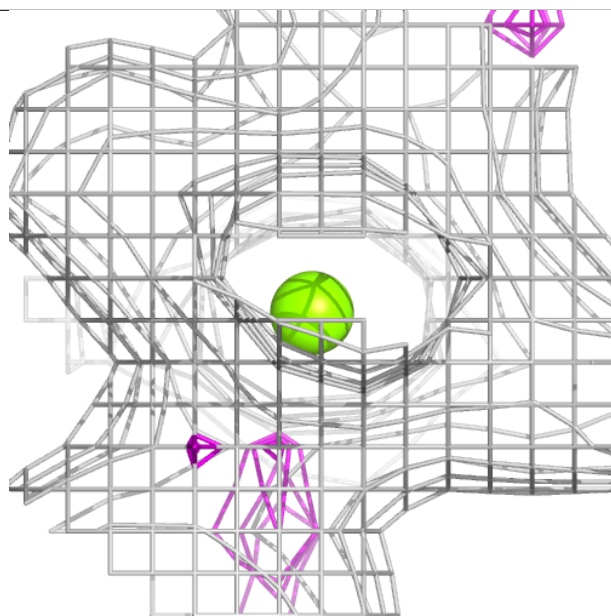
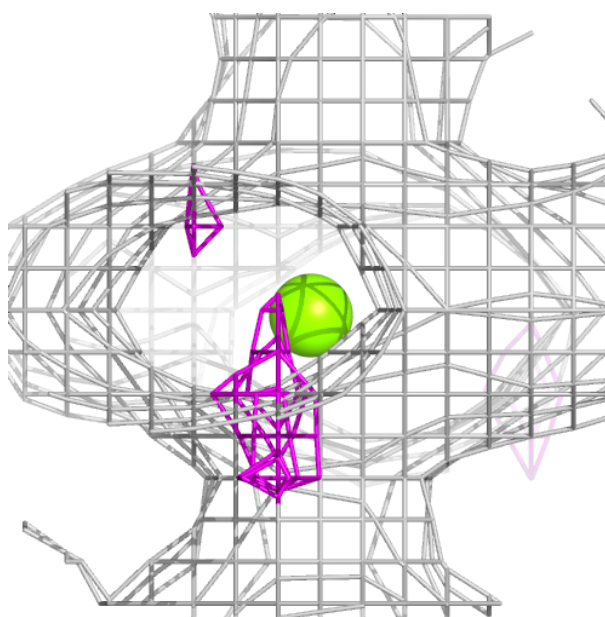
Electron density around EDO T 1303:

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



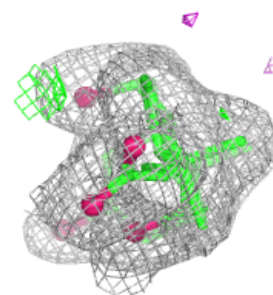
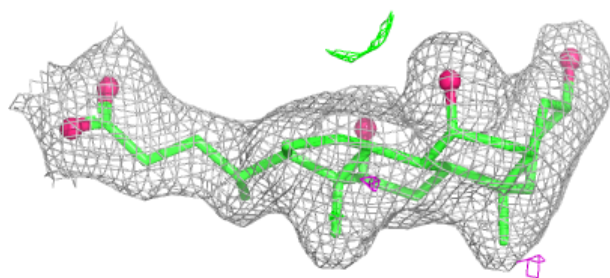
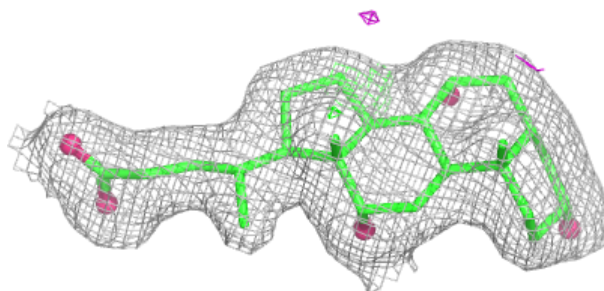
Electron density around MG N 602:

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

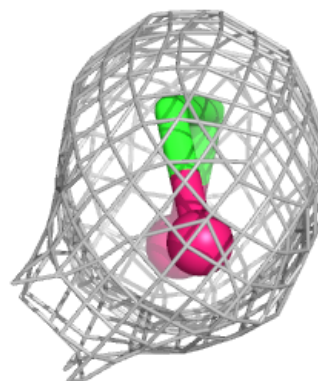
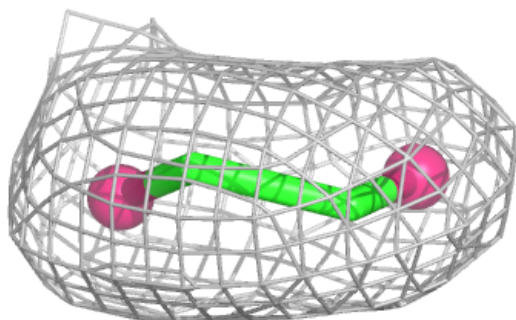
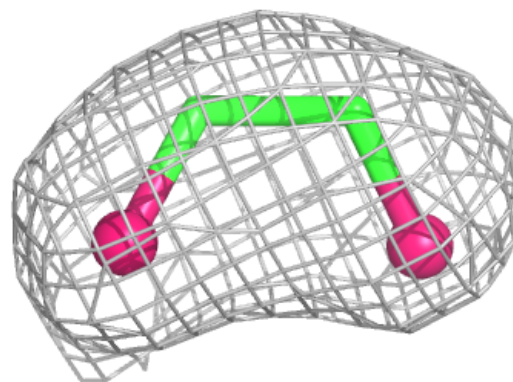


Electron density around CHD P 303:

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

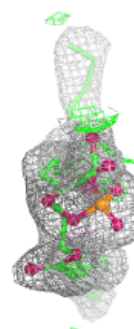
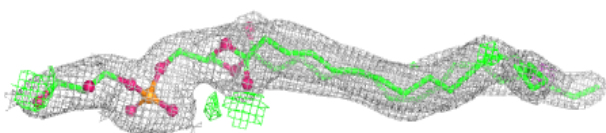
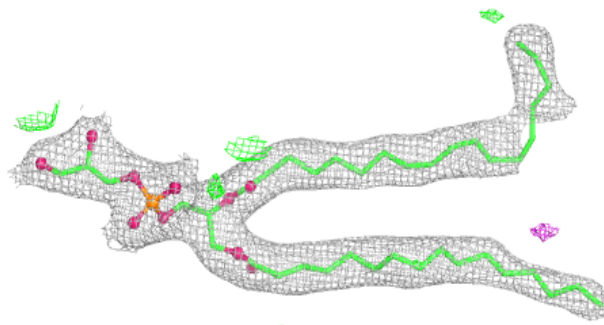
**Electron density around EDO C 308:**

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

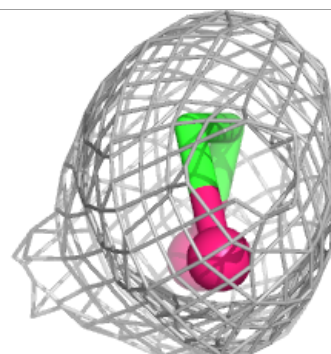
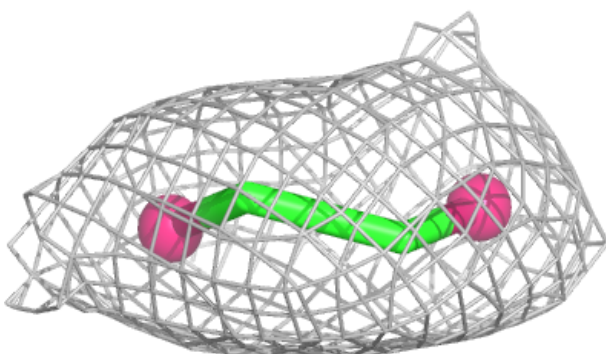
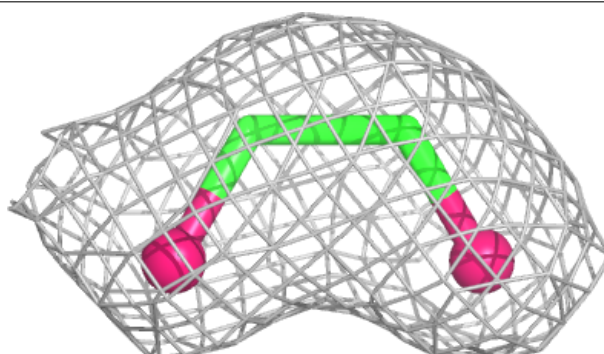


Electron density around PGV P 306:

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

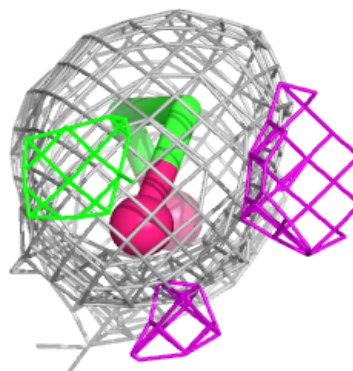
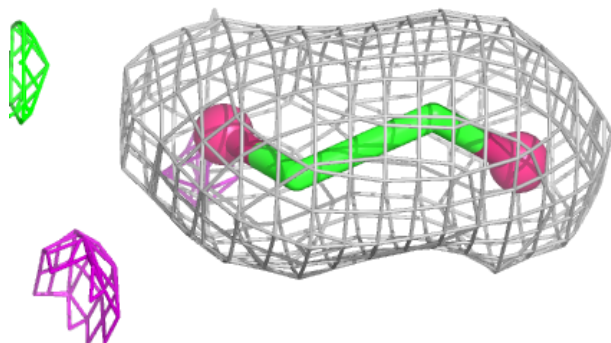
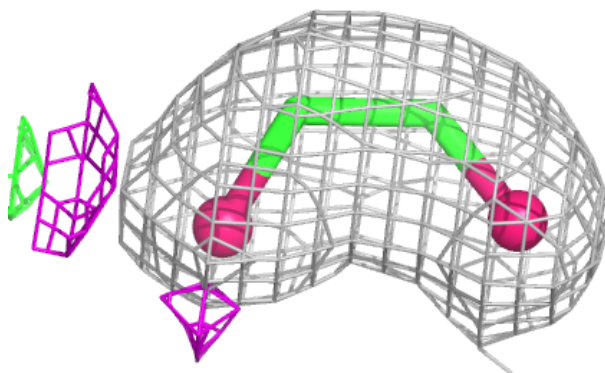
**Electron density around EDO G 102:**

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

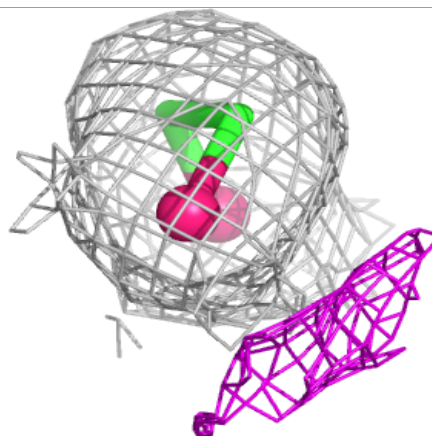
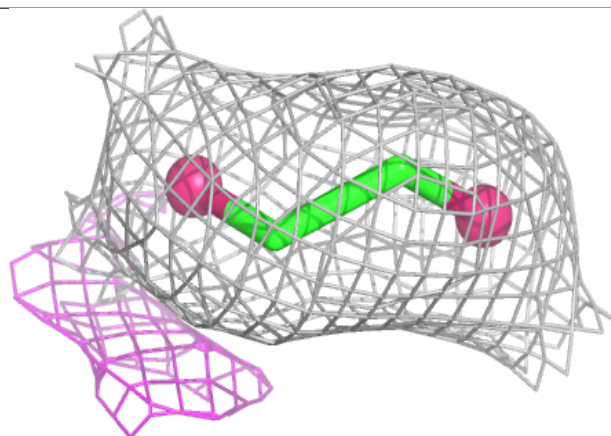
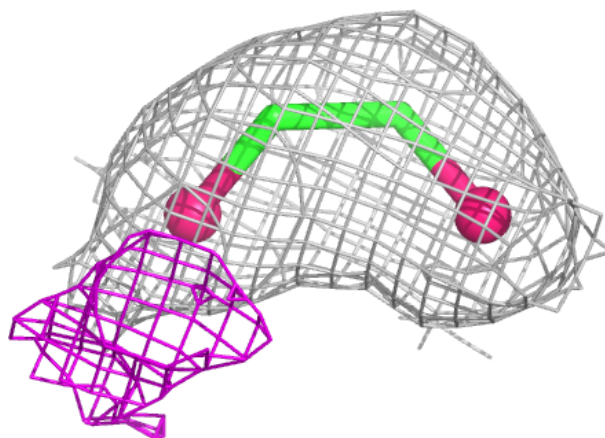


Electron density around EDO B 304:

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

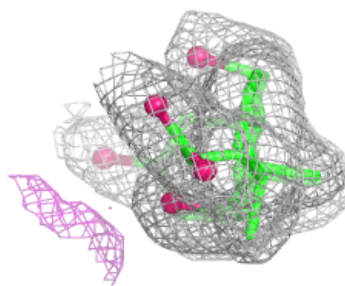
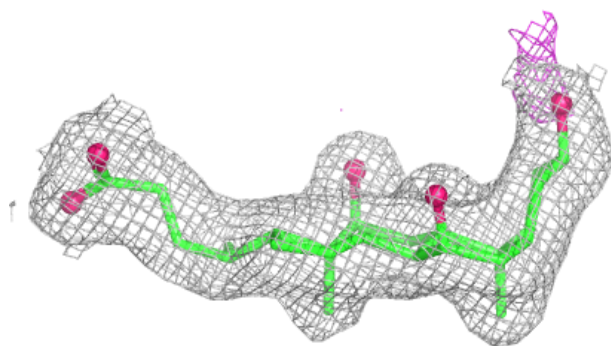
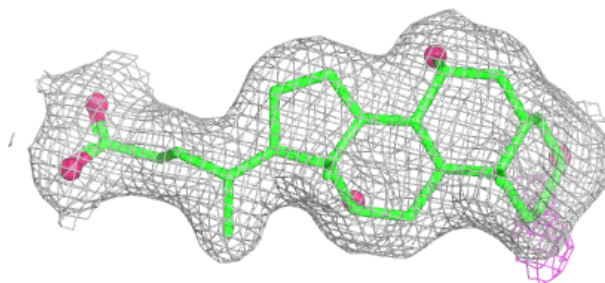
**Electron density around EDO A 608:**

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



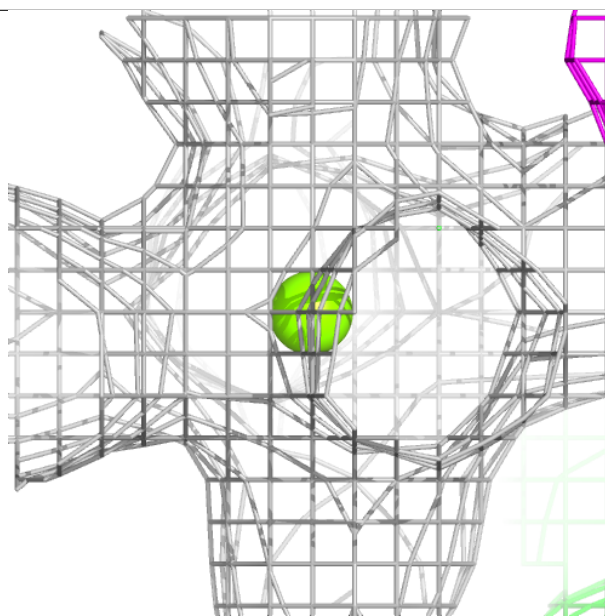
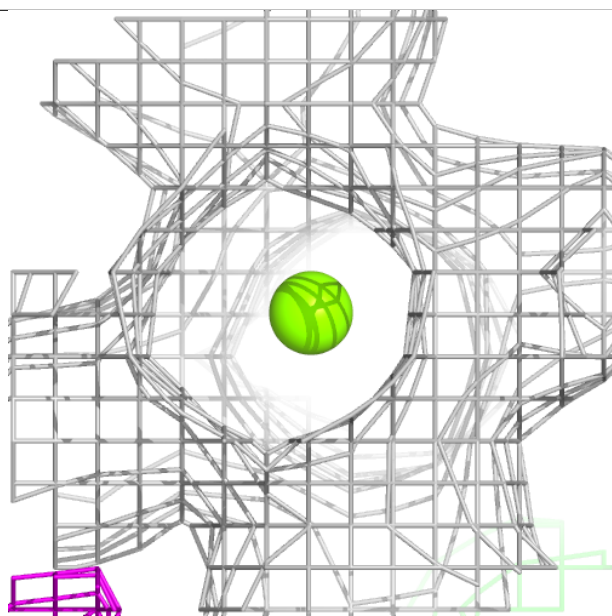
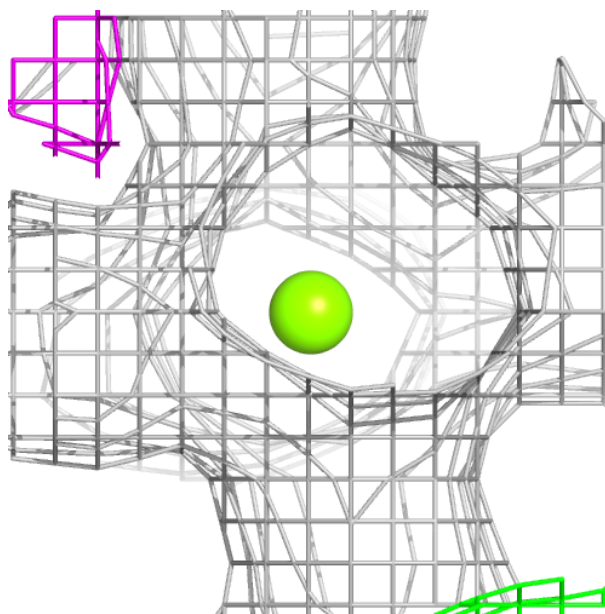
Electron density around CHD B 303:

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



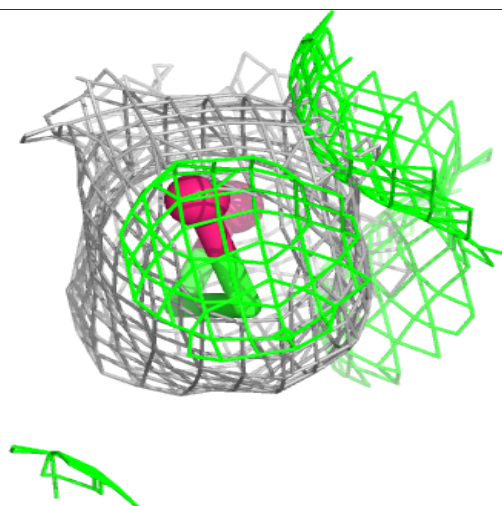
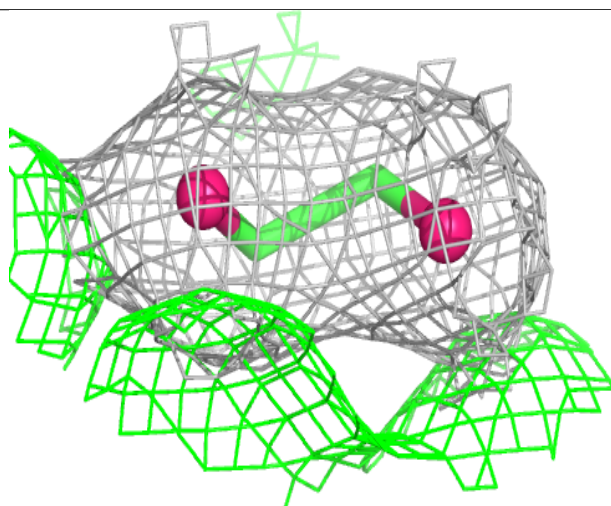
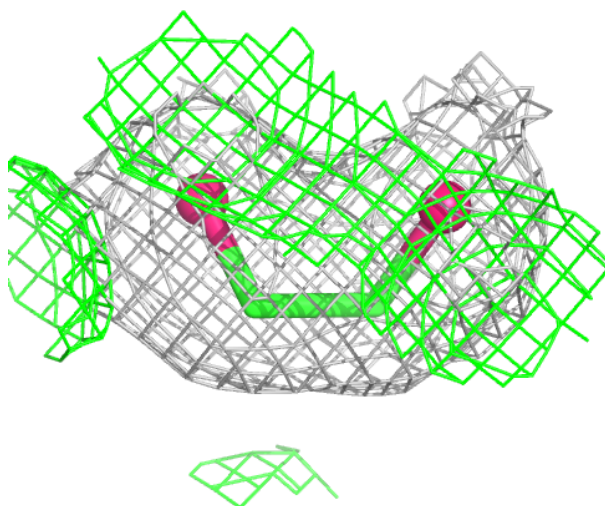
Electron density around MG A 602:

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



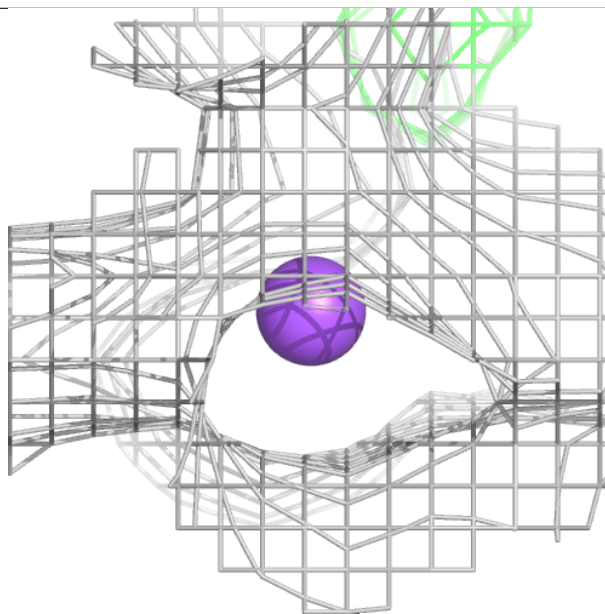
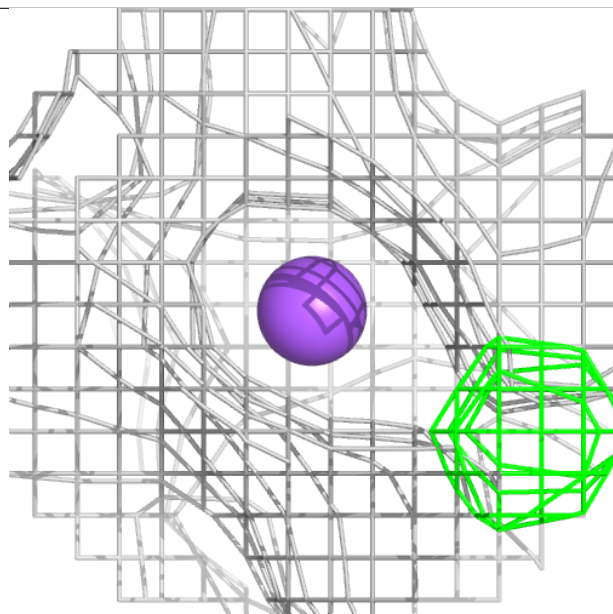
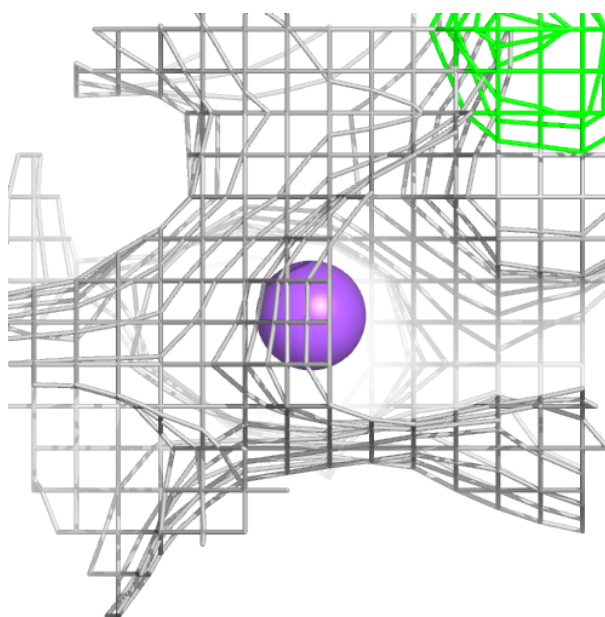
Electron density around EDO F 706:

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



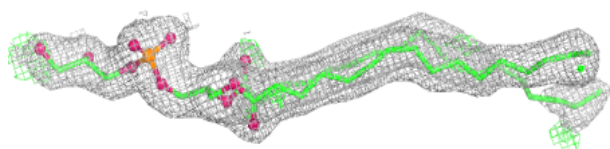
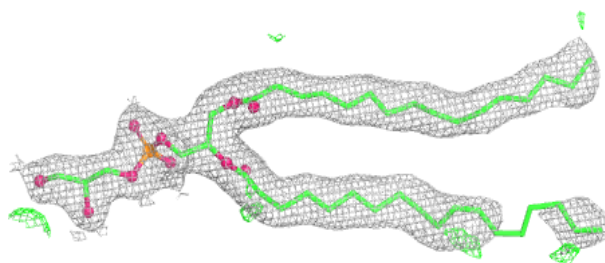
Electron density around NA N 603:

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

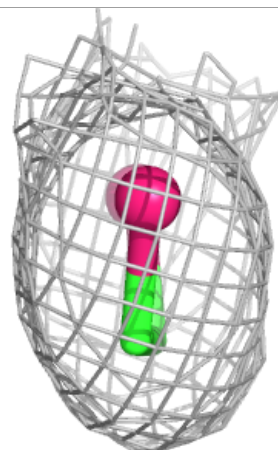
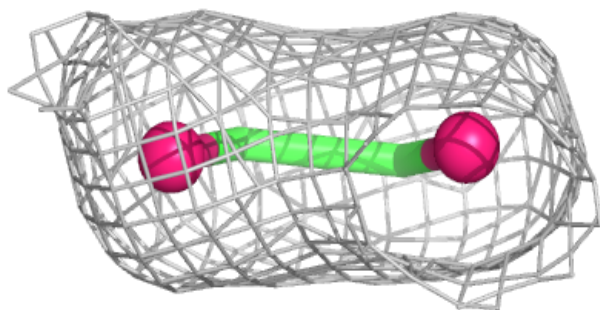
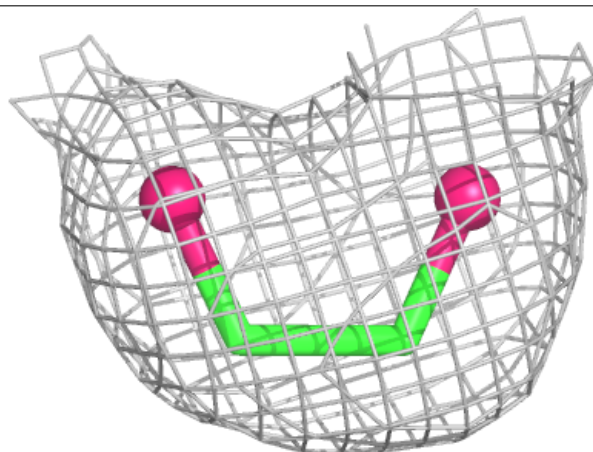


Electron density around PGV C 304:

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

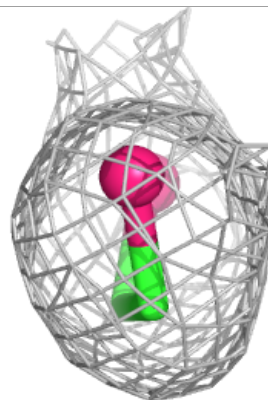
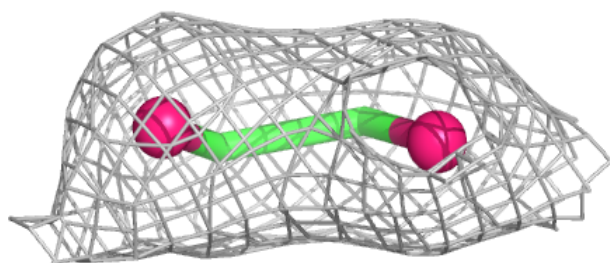
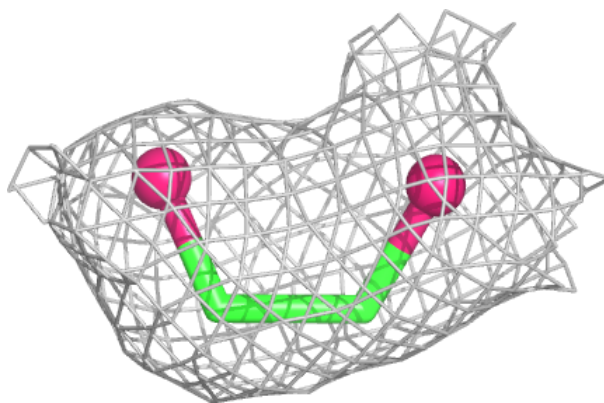
**Electron density around EDO N 607:**

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

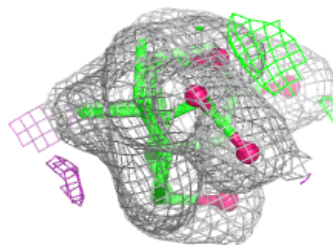
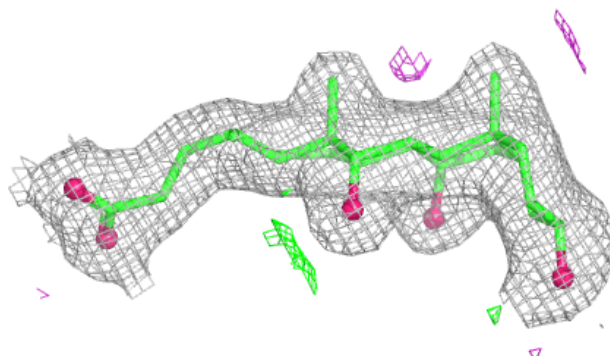
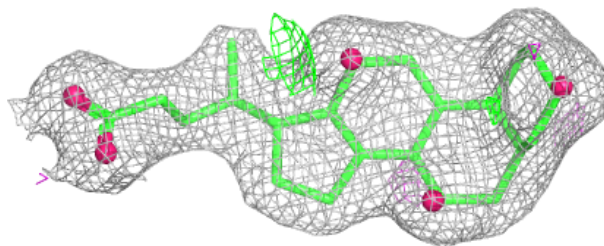


Electron density around EDO F 701:

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

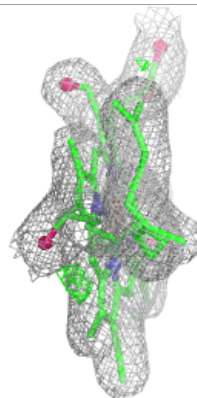
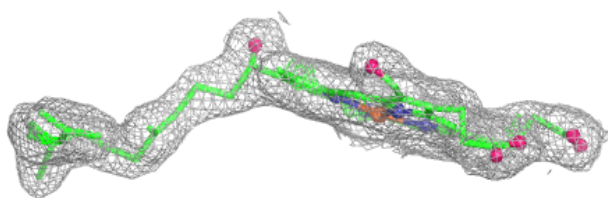
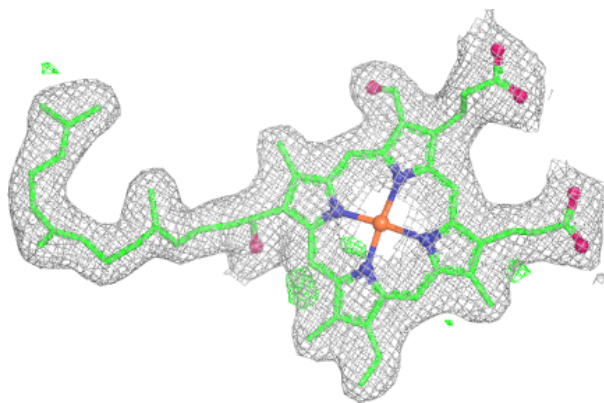
**Electron density around CHD G 106:**

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

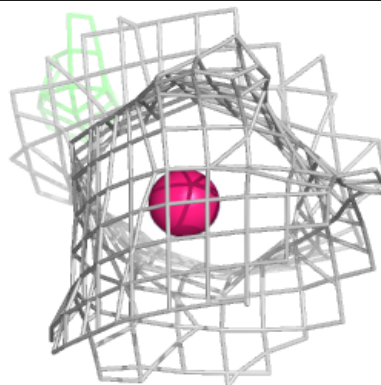
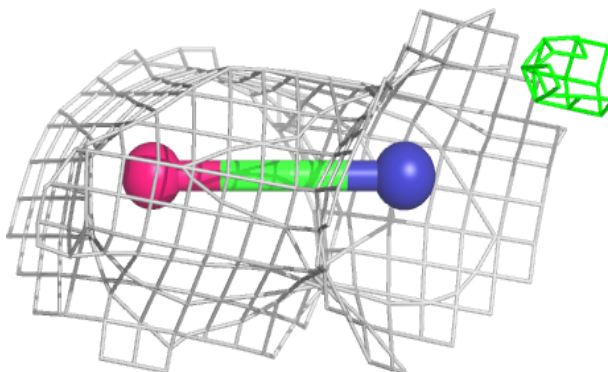
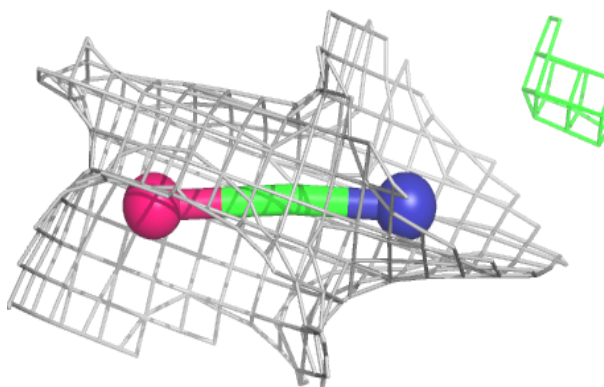


Electron density around HEA N 605:

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

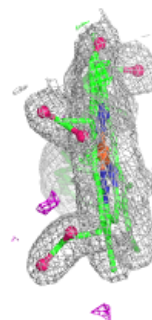
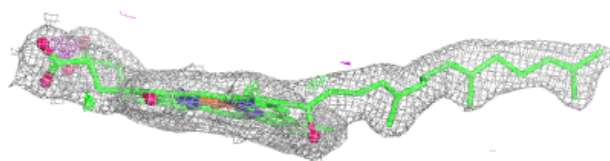
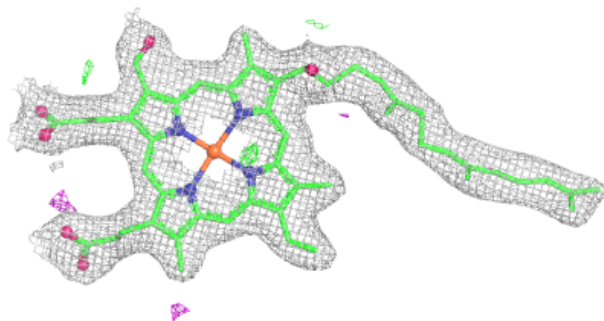
**Electron density around 0NM N 615:**

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



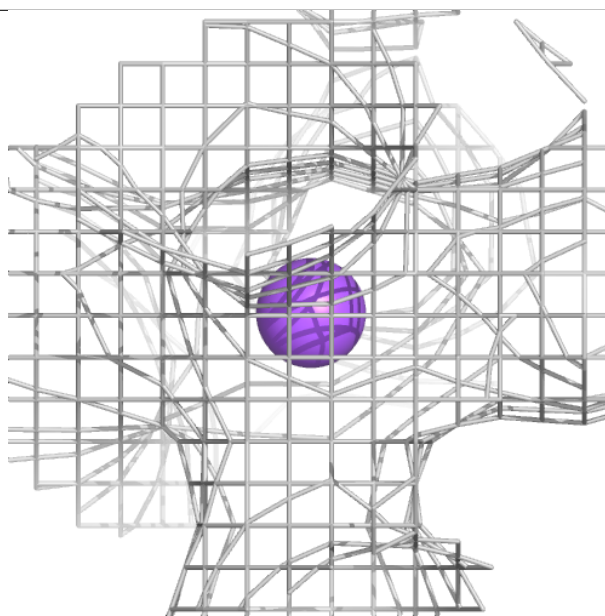
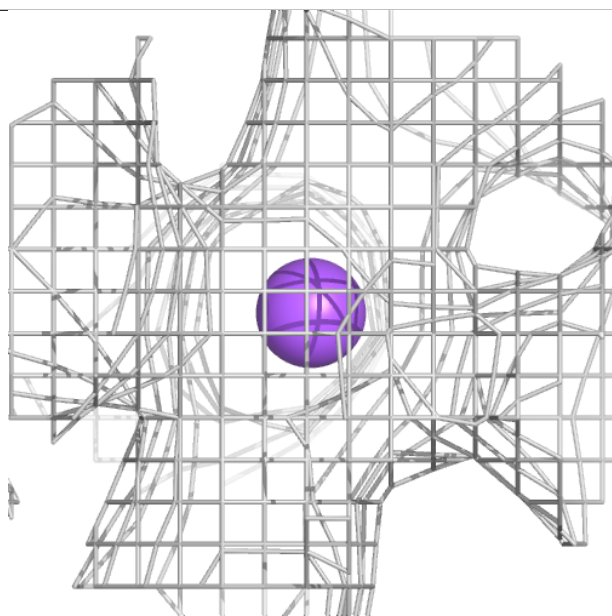
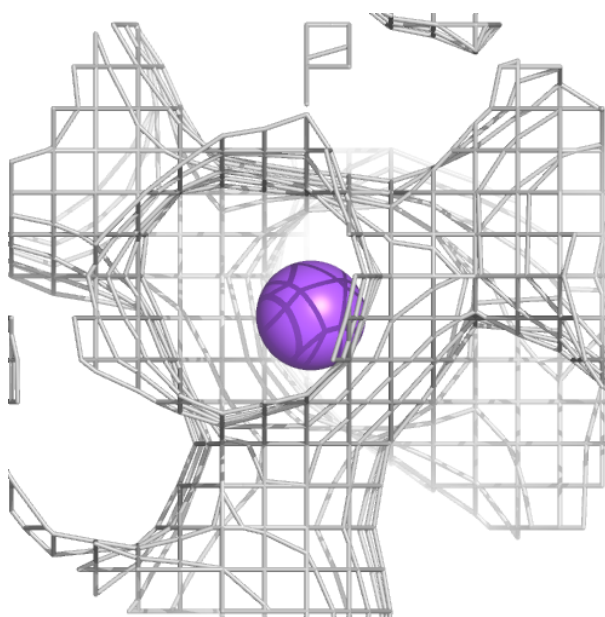
Electron density around HEA N 606:

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



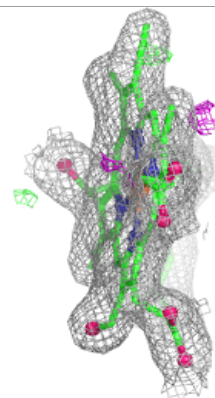
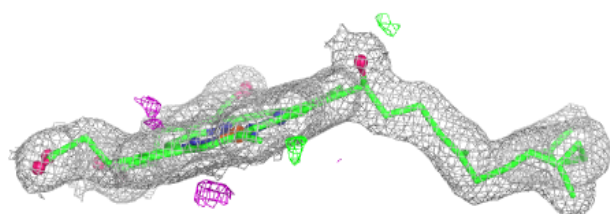
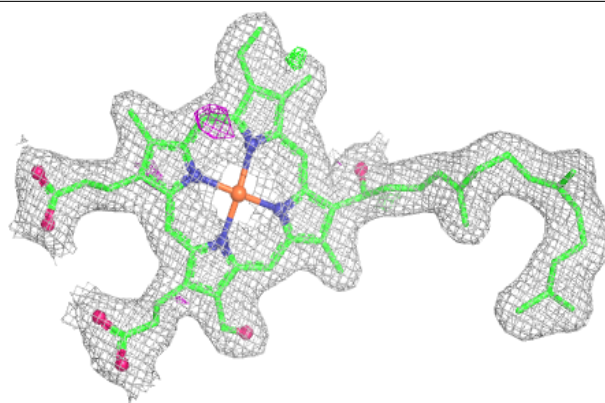
Electron density around NA A 603:

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

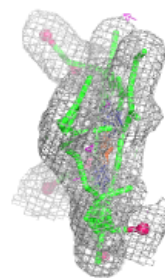
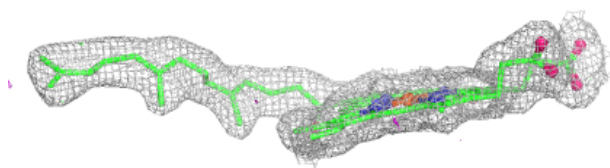
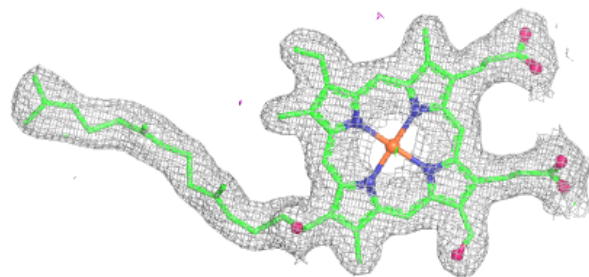


Electron density around HEA A 605:

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

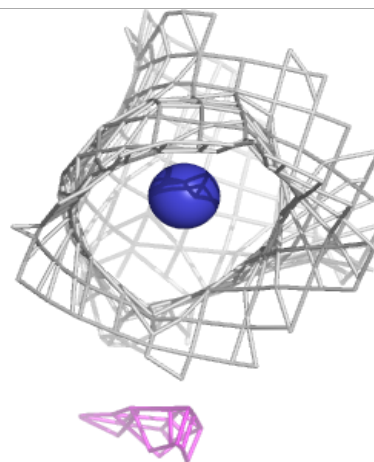
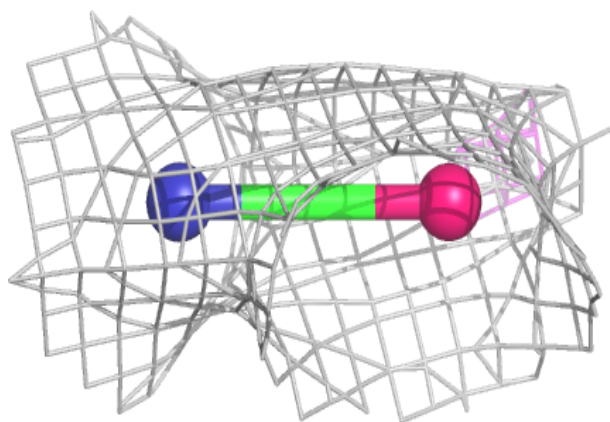
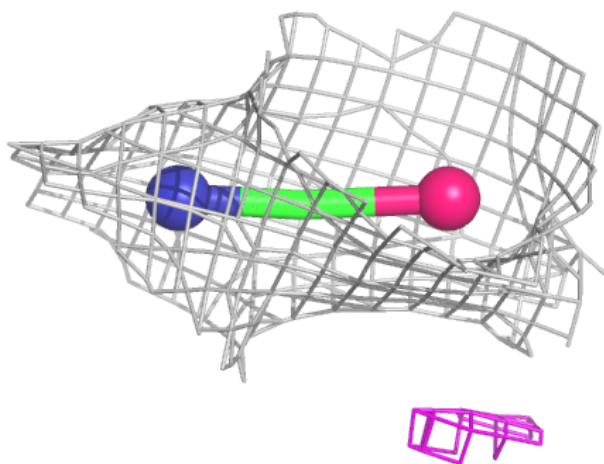
**Electron density around HEA A 606:**

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



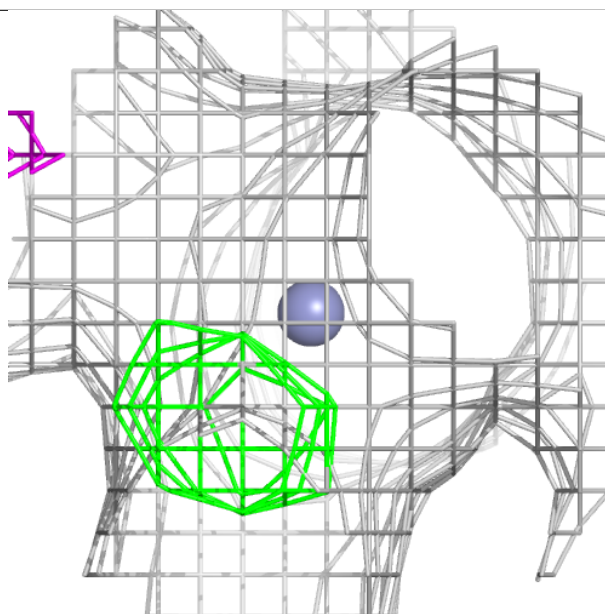
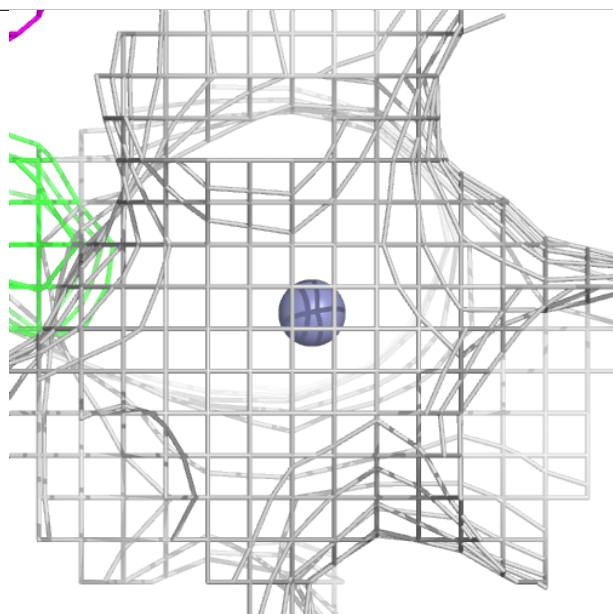
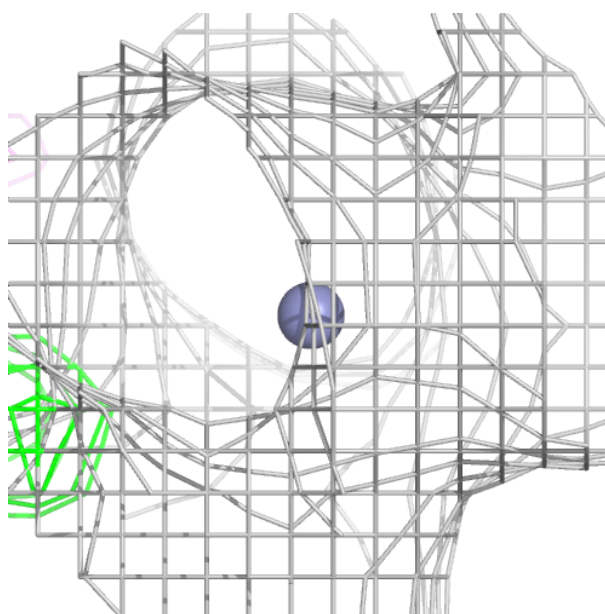
Electron density around 0NM A 613:

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



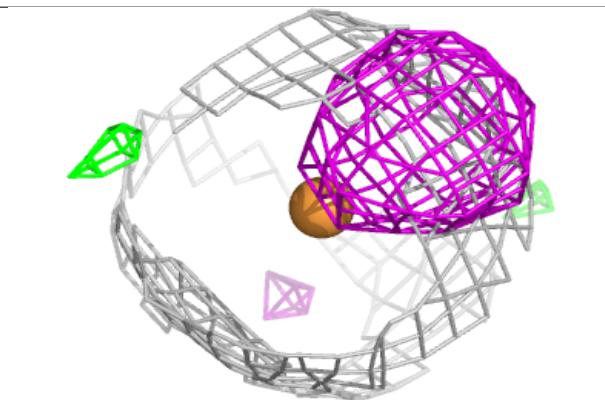
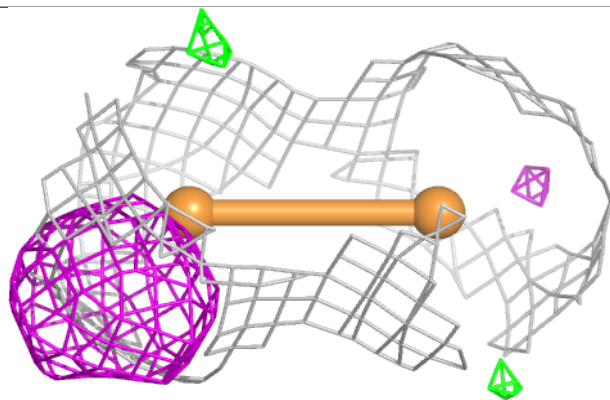
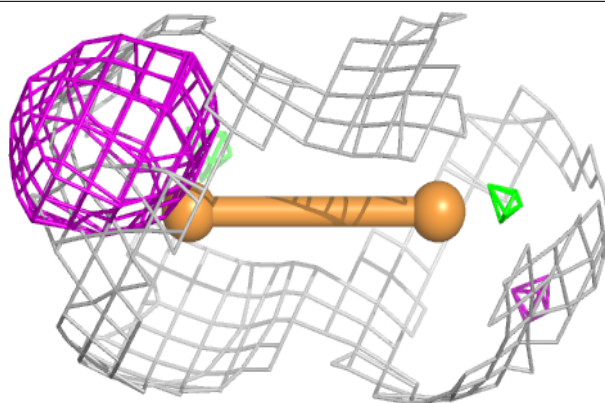
Electron density around ZN S 1602:

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

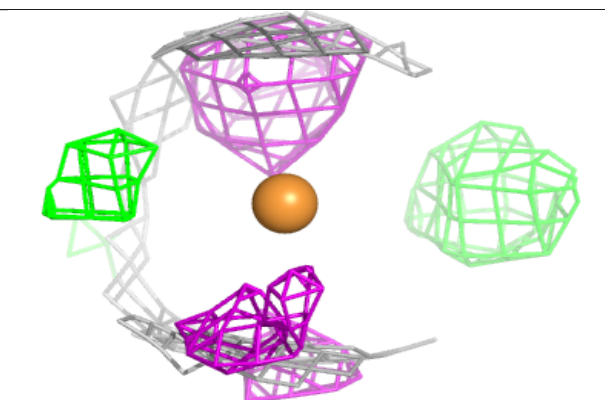
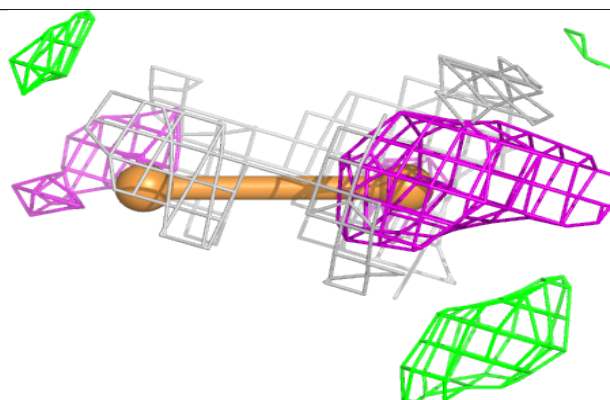
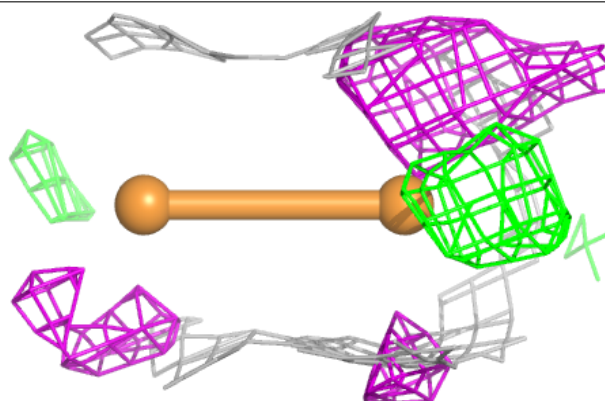


Electron density around CUA B 301:

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

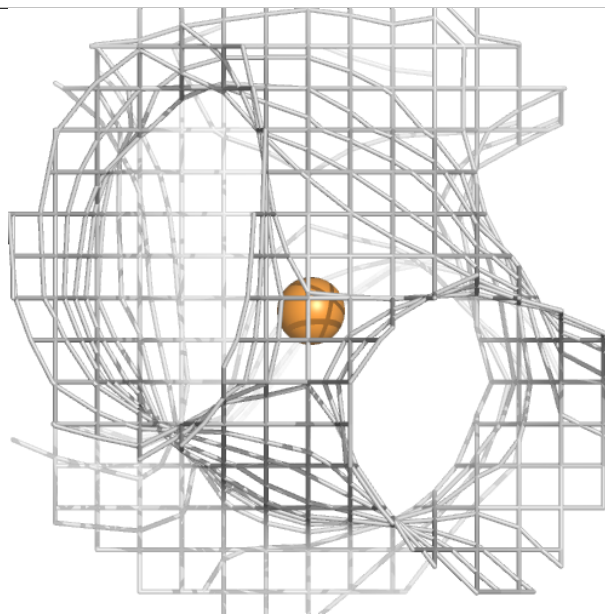
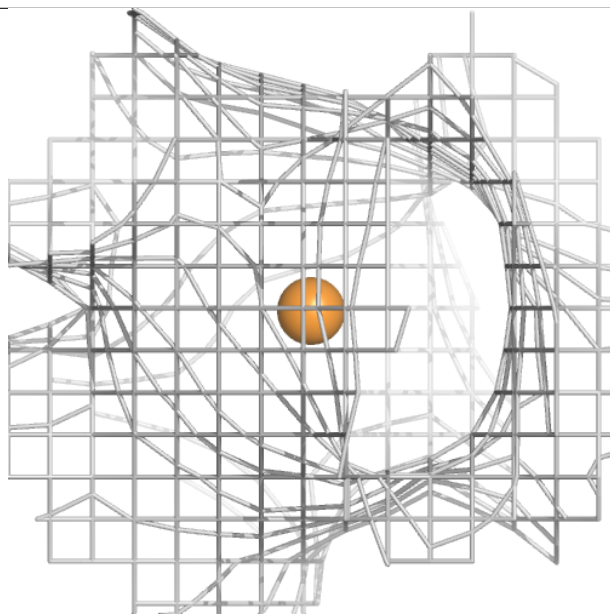
**Electron density around CUA O 301:**

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



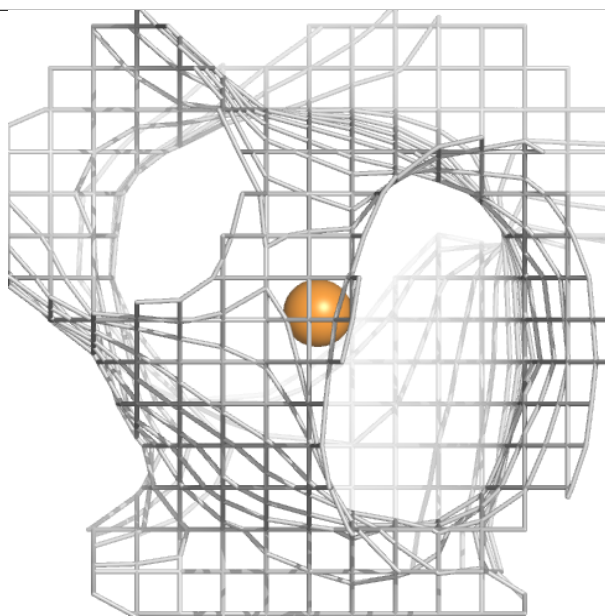
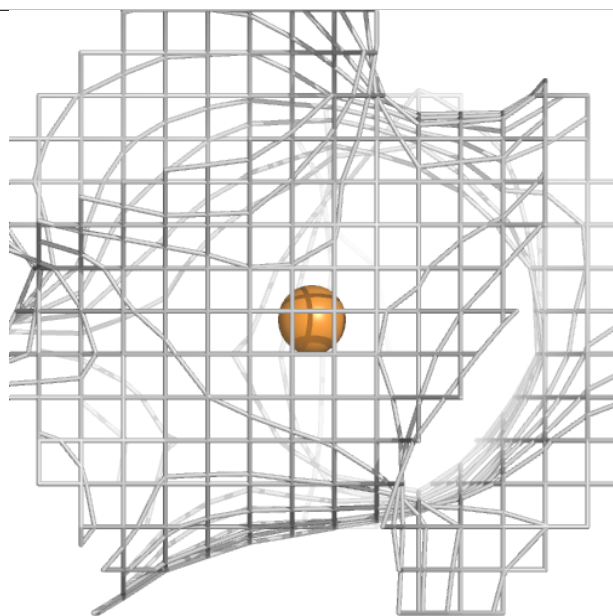
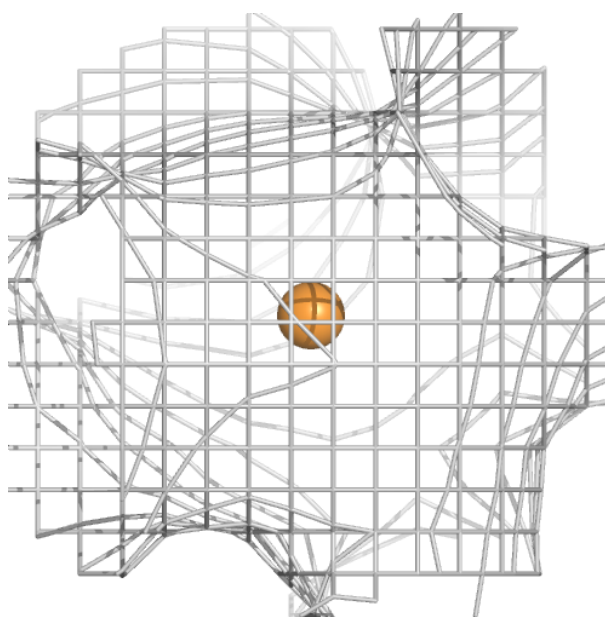
Electron density around CU A 601:

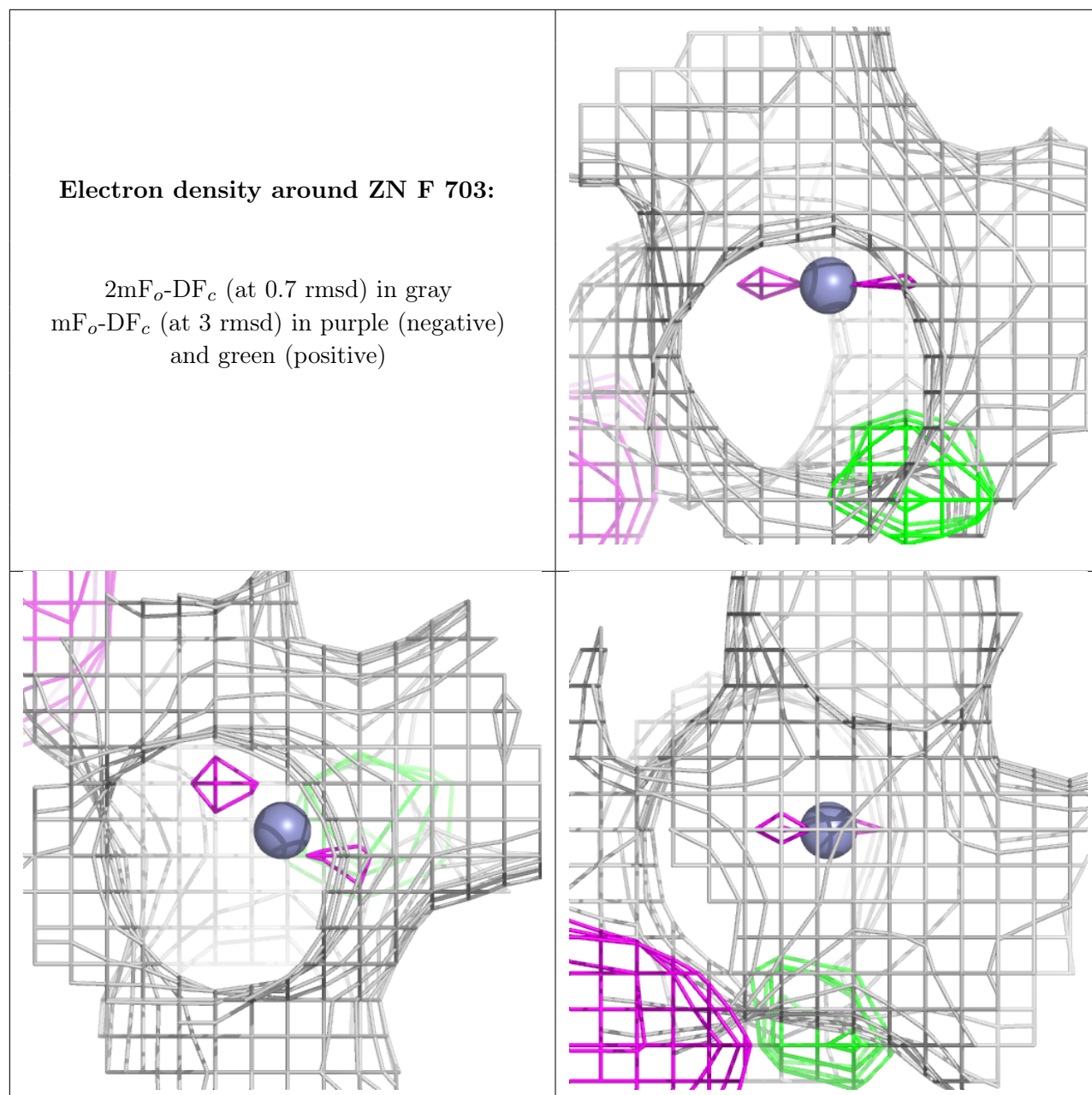
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU N 601:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.