



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:59 PM UTC

PDB ID : 7KH4 / pdb_00007kh4
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H56W mutant with pyruvate bound in the active site and R,R-bislysine bound at the allosteric site
Authors : Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.
Deposited on : 2020-10-19
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

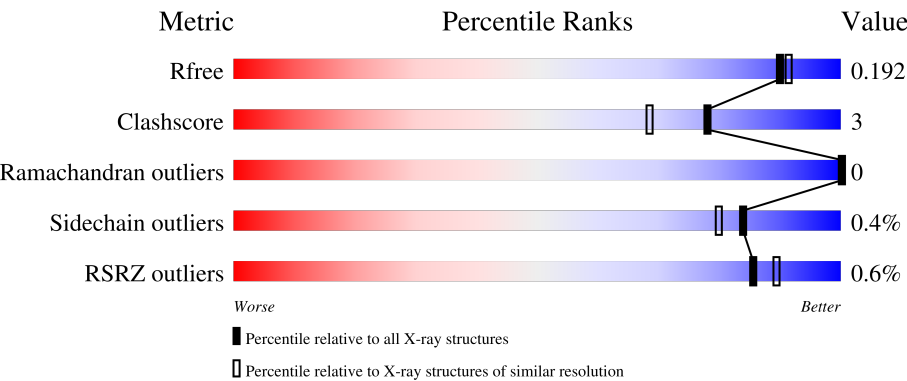
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.



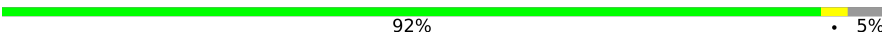
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	310	88%7%5%
1	B	310	% 92%6%..
1	C	310	90%..5%
1	D	310	2% 92%6%..

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Mol	Chain	Length	Quality of chain
1	E	310	 89% 6% •
1	F	310	 92% • 5%

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
5	EDO	B	306	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15441 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2286	1456	378	439	13			
1	B	304	Total	C	N	O	S	0	1	0
			2351	1493	394	450	14			
1	C	296	Total	C	N	O	S	0	1	0
			2285	1455	378	439	13			
1	D	304	Total	C	N	O	S	0	2	0
			2363	1503	395	451	14			
1	E	297	Total	C	N	O	S	0	1	0
			2293	1459	379	442	13			
1	F	296	Total	C	N	O	S	0	0	0
			2284	1455	378	438	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	56	TRP	HIS	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

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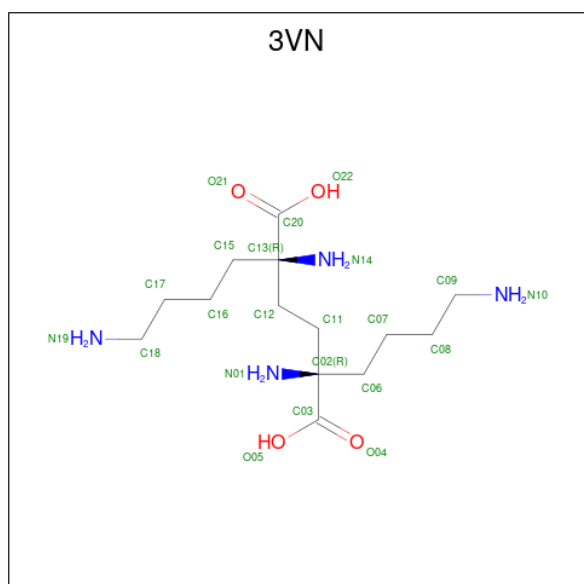
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	56	TRP	HIS	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	56	TRP	HIS	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	56	TRP	HIS	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	56	TRP	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	56	TRP	HIS	engineered mutation	UNP Q9PPB4

- Molecule 2 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (CCD ID: 3VN) (formula: C₁₄H₃₀N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	O	
			22	14	4	4	
							0
							0

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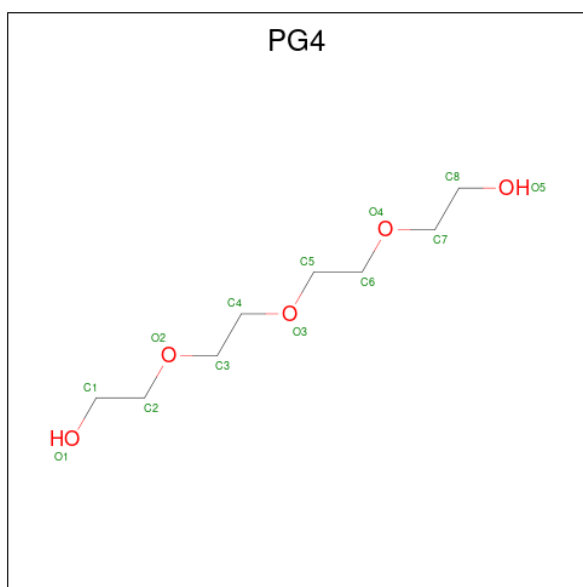
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			22	14	4	4		
2	D	1	Total	C	N	O	0	0
			22	14	4	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

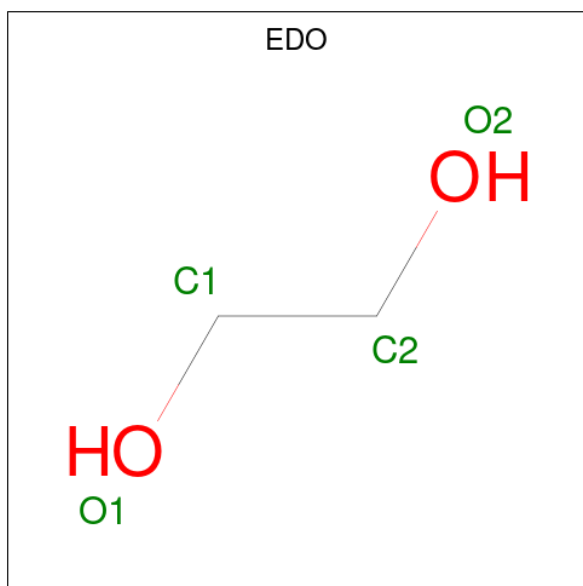
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		
3	B	3	Total	Mg	0	0
			3	3		
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		
3	E	5	Total	Mg	0	0
			5	5		
3	F	4	Total	Mg	0	0
			4	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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

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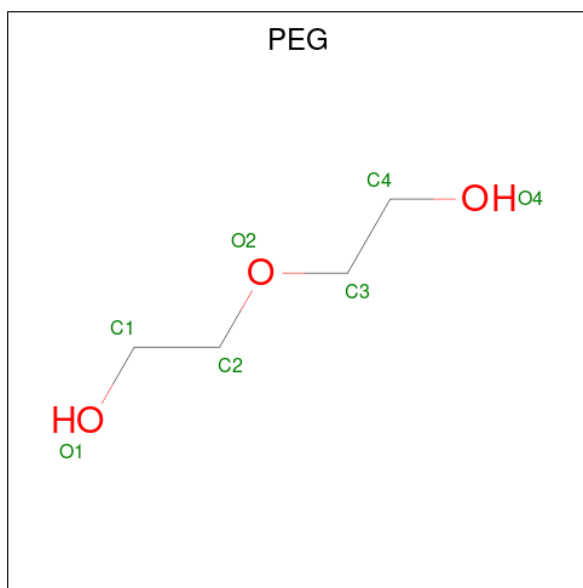
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



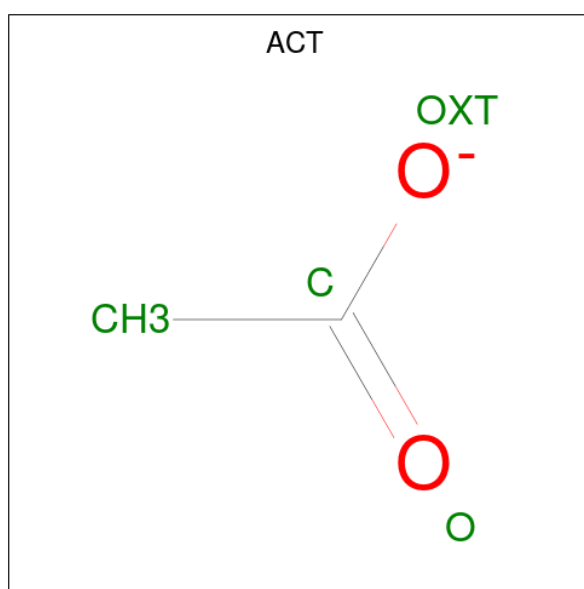
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		
6	E	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



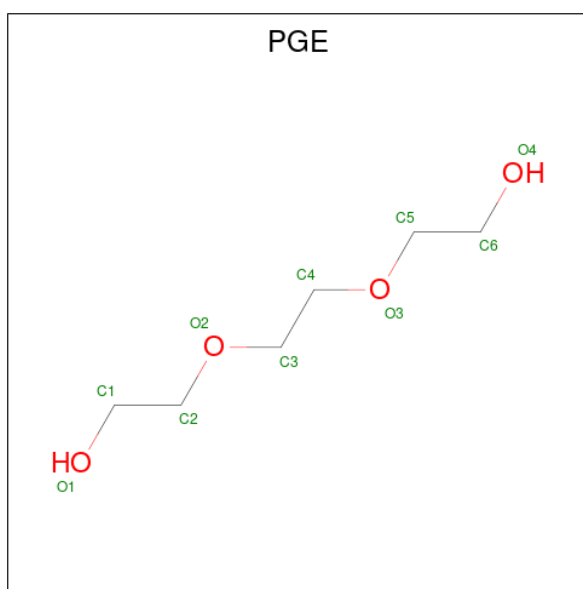
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



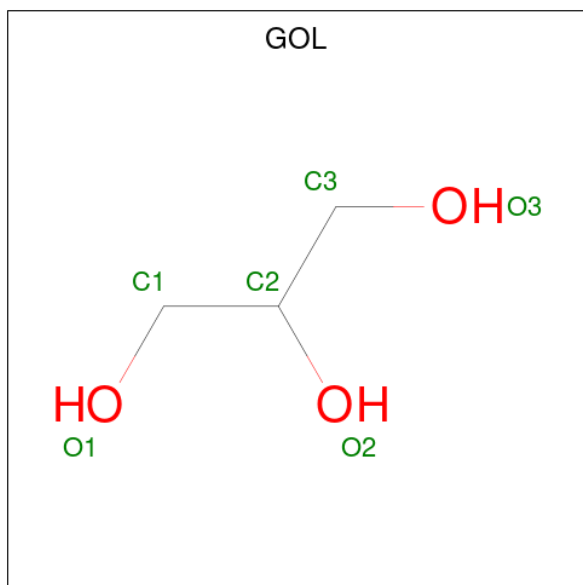
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 10 6 4	0	0
8	D	1	Total C O 10 6 4	0	0
8	D	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	184	Total	O	0	0
			184	184		
10	B	192	Total	O	0	0
			192	192		
10	C	170	Total	O	0	0
			170	170		
10	D	201	Total	O	0	0
			201	201		
10	E	198	Total	O	0	0
			198	198		
10	F	171	Total	O	0	0
			171	171		

Chain F:  92% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.41Å 225.29Å 199.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 1.75 48.90 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-1.75) 99.9 (48.90-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.75Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.157 , 0.185 0.165 , 0.192	Depositor DCC
R_{free} test set	9509 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15441	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: PGE, 3VN, PG4, EDO, GOL, PEG, KPI, MG, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	1/2315 (0.0%)	0.56	1/3129 (0.0%)
1	B	0.42	0/2385	0.57	0/3223
1	C	0.55	6/2315 (0.3%)	0.59	0/3129
1	D	0.44	1/2397 (0.0%)	0.58	0/3239
1	E	0.42	1/2323 (0.0%)	0.55	0/3140
1	F	0.35	0/2309	0.56	0/3121
All	All	0.44	9/14044 (0.1%)	0.57	1/18981 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	ILE	C-O	-6.00	1.17	1.24
1	C	266	ILE	C-O	-5.90	1.18	1.24
1	C	22	VAL	C-O	-5.58	1.18	1.24
1	D	125	ALA	C-O	-5.46	1.17	1.24
1	C	28	ALA	C-O	-5.46	1.17	1.24
1	C	297	GLY	C-O	-5.41	1.17	1.24
1	A	159	CYS	C-O	-5.36	1.18	1.24
1	C	21	LYS	C-O	-5.25	1.17	1.23
1	E	33	ARG	C-O	-5.24	1.18	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASN	N-CA-C	5.01	119.24	113.18

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	2286	0	2323	13	0
1	B	2351	0	2375	18	0
1	C	2285	0	2323	7	0
1	D	2363	0	2383	11	0
1	E	2293	0	2327	16	0
1	F	2284	0	2322	8	0
2	A	22	0	28	1	0
2	B	22	0	28	1	0
2	D	22	0	28	1	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	5	0	0	0	0
3	F	4	0	0	0	0
4	A	13	0	18	0	0
4	B	13	0	18	0	0
4	C	13	0	18	0	0
4	D	13	0	18	1	0
4	E	13	0	18	3	0
4	F	13	0	18	0	0
5	A	40	0	60	2	0
5	B	20	0	30	6	0
5	C	24	0	36	0	0
5	D	16	0	24	1	0
5	E	24	0	36	1	0
5	F	8	0	12	1	0
6	A	14	0	20	0	0
6	B	21	0	30	3	0
6	C	7	0	10	2	0
6	D	7	0	10	0	0
6	E	7	0	10	1	0
6	F	14	0	20	0	0
7	A	8	0	6	1	0
7	B	8	0	6	0	0
7	D	16	0	12	0	0
7	E	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	16	0	12	0	0
8	B	10	0	14	0	0
8	D	20	0	28	3	0
8	E	10	0	14	1	0
9	C	6	0	8	0	0
10	A	184	0	0	0	0
10	B	192	0	0	4	0
10	C	170	0	0	2	0
10	D	201	0	0	1	0
10	E	198	0	0	4	0
10	F	171	0	0	2	0
All	All	15441	0	14646	81	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 3.

All (81) 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)
1:B:166:KPI:H1B	10:B:581:HOH:O	1.73	0.88
1:D:166:KPI:H1A	10:D:444:HOH:O	1.79	0.81
1:B:279:SER:HB3	6:B:313:PEG:H42	1.64	0.80
1:C:160:GLU:CD	1:C:160:GLU:H	1.89	0.80
1:C:166:KPI:H1A	10:C:428:HOH:O	1.86	0.75
1:F:166:KPI:H1A	10:F:432:HOH:O	1.95	0.67
1:D:183:PRO:HD2	8:D:314:PGE:H32	1.78	0.65
1:C:60:ARG:HD3	6:C:310:PEG:H32	1.78	0.64
1:A:261:TYR:O	7:A:319:ACT:H1	2.00	0.62
1:E:166:KPI:H1A	10:E:461:HOH:O	2.00	0.61
1:E:154:LYS:HZ2	4:E:306:PG4:H51	1.65	0.60
8:D:314:PGE:H2	8:D:314:PGE:H52	1.85	0.58
1:A:234:LYS:HD3	5:B:308:EDO:H22	1.86	0.57
1:D:140:PRO:HG3	1:D:146:GLU:OE2	2.05	0.55
1:B:82:GLY:O	5:B:306:EDO:H22	2.07	0.55
1:B:161:ASN:OD1	1:B:161:ASN:N	2.40	0.55
6:E:313:PEG:H32	10:E:519:HOH:O	2.08	0.54
1:B:59:HIS:HE1	5:B:306:EDO:H12	1.72	0.53
5:A:308:EDO:H12	10:F:546:HOH:O	2.07	0.53
1:E:294:LYS:NZ	8:E:315:PGE:H22	2.24	0.53
1:A:262:LEU:HD21	1:A:283:PHE:CZ	2.44	0.52
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:HIS:CE1	5:B:306:EDO:H12	2.46	0.51
1:A:140:PRO:HG3	1:A:146:GLU:OE1	2.11	0.51
1:D:292:LYS:HG2	1:D:293:TYR:CE2	2.46	0.51
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.92	0.51
1:E:60:ARG:HD2	1:E:95:PHE:CE2	2.45	0.51
1:C:161:ASN:OD1	1:C:161:ASN:N	2.40	0.50
1:A:6:ILE:HG12	1:A:76:LYS:HD3	1.92	0.50
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.93	0.50
1:A:161:ASN:OD1	1:A:161:ASN:N	2.41	0.50
1:B:140:PRO:HG3	1:B:146:GLU:OE1	2.12	0.49
1:F:231:LYS:C	1:F:231:LYS:HD3	2.38	0.49
1:B:54:LEU:O	2:B:301:3VN:H9	2.13	0.49
1:E:154:LYS:NZ	4:E:306:PG4:H51	2.28	0.48
8:D:314:PGE:H52	8:D:314:PGE:C2	2.43	0.48
4:D:303:PG4:H11	5:D:307:EDO:O1	2.14	0.48
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.95	0.48
1:C:140:PRO:HG3	1:C:146:GLU:OE1	2.14	0.48
1:F:248:PHE:HE2	5:F:306:EDO:H22	1.79	0.47
1:F:140:PRO:HG3	1:F:146:GLU:OE1	2.15	0.47
1:E:2:ASP:N	10:E:405:HOH:O	2.48	0.47
1:F:161:ASN:OD1	1:F:161:ASN:N	2.48	0.47
1:D:231:LYS:HE2	1:D:232:GLU:OE2	2.14	0.46
1:B:4:ASN:HB2	1:B:133:PRO:HG3	1.97	0.46
2:D:301:3VN:H9	1:E:54:LEU:O	2.14	0.46
1:E:60:ARG:HB3	1:E:95:PHE:CZ	2.51	0.46
1:A:60:ARG:HB3	1:A:95:PHE:CZ	2.52	0.45
5:B:306:EDO:H21	10:C:461:HOH:O	2.17	0.45
1:B:56:TRP:HE1	6:B:311:PEG:H21	1.81	0.45
2:A:301:3VN:H23	1:F:54:LEU:O	2.16	0.45
1:D:161:ASN:OD1	1:D:161:ASN:N	2.48	0.45
1:B:166:KPI:H1A	10:B:439:HOH:O	2.17	0.44
1:E:241:TYR:CE2	1:E:245:LYS:HG3	2.52	0.44
1:E:292:LYS:HD2	1:E:292:LYS:HA	1.70	0.44
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.99	0.44
5:B:310:EDO:H21	10:B:536:HOH:O	2.17	0.44
6:C:310:PEG:H42	6:C:310:PEG:H21	1.61	0.44
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.99	0.44
1:A:25:GLN:N	1:A:25:GLN:CD	2.76	0.44
5:E:309:EDO:H11	10:E:535:HOH:O	2.17	0.43
1:B:243:ILE:HB	1:B:293:TYR:CE2	2.54	0.43
1:B:254:ILE:HB	1:B:255:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:LYS:NZ	1:D:131:ASP:OD1	2.29	0.43
1:A:115:THR:HA	5:A:308:EDO:H22	2.00	0.43
1:D:168:ALA:HA	1:D:191:GLU:HG3	2.01	0.43
1:B:279:SER:HB3	6:B:313:PEG:C4	2.41	0.42
1:B:166:KPI:C1	10:B:581:HOH:O	2.49	0.42
1:E:243:ILE:HB	1:E:293:TYR:CE1	2.54	0.42
1:E:35:ILE:HG12	1:E:75:VAL:HG21	2.01	0.42
1:E:140:PRO:HB2	7:E:314:ACT:H1	2.01	0.42
1:C:60:ARG:HB3	1:C:95:PHE:CZ	2.54	0.42
1:E:254:ILE:HB	1:E:255:PRO:HD3	2.01	0.41
1:F:231:LYS:HE3	1:F:235:LYS:NZ	2.35	0.41
1:D:254:ILE:HB	1:D:255:PRO:HD3	2.02	0.41
1:A:230:TYR:HD2	1:B:230:TYR:CD2	2.39	0.41
1:A:254:ILE:HB	1:A:255:PRO:HD3	2.01	0.41
1:E:154:LYS:HD3	4:E:306:PG4:H22	2.03	0.41
1:D:35:ILE:HG12	1:D:75:VAL:HG21	2.02	0.41
1:B:241:TYR:CE2	1:B:245:LYS:HG3	2.56	0.40
1:A:35:ILE:HG12	1:A:75:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
1	B	302/310 (97%)	297 (98%)	5 (2%)	0	100	100
1	C	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
1	D	303/310 (98%)	298 (98%)	5 (2%)	0	100	100
1	E	295/310 (95%)	291 (99%)	4 (1%)	0	100	100
1	F	293/310 (94%)	287 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1781/1860 (96%)	1751 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	249/260 (96%)	248 (100%)	1 (0%)	84	80
1	B	256/260 (98%)	255 (100%)	1 (0%)	84	80
1	C	249/260 (96%)	246 (99%)	3 (1%)	63	49
1	D	257/260 (99%)	256 (100%)	1 (0%)	84	80
1	E	250/260 (96%)	250 (100%)	0	100	100
1	F	248/260 (95%)	248 (100%)	0	100	100
All	All	1509/1560 (97%)	1503 (100%)	6 (0%)	84	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	B	161	ASN
1	C	47	THR
1	C	160	GLU
1	C	161	ASN
1	D	231	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	25	GLN
1	B	116	GLN

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Mol	Chain	Res	Type
1	B	128	GLN
1	D	201	ASN
1	E	19	ASN
1	E	201	ASN
1	F	19	ASN
1	F	252	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	KPI	B	166	1	11,13,14	1.40	1 (9%)	9,15,17	3.16	5 (55%)
1	KPI	D	166	1	11,13,14	1.28	1 (9%)	9,15,17	2.56	3 (33%)
1	KPI	E	166	1	11,13,14	2.01	2 (18%)	9,15,17	2.48	1 (11%)
1	KPI	A	166	1	11,13,14	2.03	2 (18%)	9,15,17	2.53	3 (33%)
1	KPI	C	166	1	11,13,14	2.47	2 (18%)	9,15,17	3.02	5 (55%)
1	KPI	F	166	1	11,13,14	1.55	2 (18%)	9,15,17	2.56	2 (22%)

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	KPI	B	166	1	-	2/13/14/16	-
1	KPI	D	166	1	-	0/13/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	E	166	1	-	0/13/14/16	-
1	KPI	A	166	1	-	0/13/14/16	-
1	KPI	C	166	1	-	0/13/14/16	-
1	KPI	F	166	1	-	2/13/14/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	CX2-CX1	7.12	1.58	1.49
1	E	166	KPI	CX2-CX1	5.60	1.56	1.49
1	A	166	KPI	CX2-CX1	5.28	1.56	1.49
1	F	166	KPI	CX2-CX1	3.76	1.54	1.49
1	B	166	KPI	CX2-CX1	3.66	1.54	1.49
1	A	166	KPI	O2-CX2	3.19	1.30	1.22
1	D	166	KPI	CX2-CX1	3.16	1.53	1.49
1	C	166	KPI	O2-CX2	3.02	1.30	1.22
1	E	166	KPI	O2-CX2	2.39	1.28	1.22
1	F	166	KPI	O2-CX2	2.31	1.28	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	166	KPI	CE-NZ-CX1	6.62	139.78	121.58
1	F	166	KPI	CE-NZ-CX1	6.26	138.77	121.58
1	D	166	KPI	CE-NZ-CX1	6.18	138.56	121.58
1	C	166	KPI	CE-NZ-CX1	6.05	138.19	121.58
1	A	166	KPI	CE-NZ-CX1	5.60	136.96	121.58
1	B	166	KPI	O2-CX2-CX1	-5.57	114.55	121.35
1	B	166	KPI	CE-NZ-CX1	5.41	136.45	121.58
1	C	166	KPI	C1-CX1-CX2	3.70	121.60	118.11
1	A	166	KPI	C1-CX1-CX2	3.60	121.51	118.11
1	C	166	KPI	CX2-CX1-NZ	3.22	122.46	114.88
1	B	166	KPI	O1-CX2-CX1	3.19	123.29	116.50
1	C	166	KPI	O1-CX2-O2	-2.99	116.77	123.90
1	B	166	KPI	C1-CX1-CX2	2.92	120.86	118.11
1	C	166	KPI	O2-CX2-CX1	2.85	124.82	121.35
1	F	166	KPI	CX2-CX1-NZ	2.71	121.26	114.88
1	B	166	KPI	CX2-CX1-NZ	2.69	121.22	114.88
1	D	166	KPI	O2-CX2-CX1	-2.57	118.21	121.35
1	A	166	KPI	CX2-CX1-NZ	2.56	120.92	114.88
1	D	166	KPI	CX2-CX1-NZ	2.29	120.27	114.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	166	KPI	NZ-CX1-CX2-O1
1	B	166	KPI	NZ-CX1-CX2-O2
1	F	166	KPI	NZ-CX1-CX2-O2
1	F	166	KPI	NZ-CX1-CX2-O1

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	166	KPI	3	0
1	D	166	KPI	1	0
1	E	166	KPI	1	0
1	C	166	KPI	1	0
1	F	166	KPI	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 19 are monoatomic - leaving 70 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	$\# Z > 2$
7	ACT	D	310	-	3,3,3	0.81	0	3,3,3	1.39	0
5	EDO	A	315	-	3,3,3	0.39	0	2,2,2	0.51	0
5	EDO	C	307	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	C	308	-	3,3,3	0.46	0	2,2,2	0.21	0
5	EDO	E	311	-	3,3,3	0.57	0	2,2,2	0.11	0
7	ACT	E	314	-	3,3,3	0.84	0	3,3,3	1.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PG4	A	306	-	12,12,12	0.54	0	11,11,11	0.29	0
4	PG4	F	305	-	12,12,12	0.55	0	11,11,11	0.35	0
8	PGE	E	315	-	9,9,9	0.37	0	8,8,8	0.54	0
5	EDO	A	316	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	B	310	-	3,3,3	0.44	0	2,2,2	0.23	0
4	PG4	B	305	-	12,12,12	0.52	0	11,11,11	0.21	0
5	EDO	A	307	-	3,3,3	0.56	0	2,2,2	0.39	0
5	EDO	A	309	-	3,3,3	0.39	0	2,2,2	0.38	0
5	EDO	C	309	-	3,3,3	0.46	0	2,2,2	0.50	0
5	EDO	D	307	-	3,3,3	0.45	0	2,2,2	0.65	0
5	EDO	E	310	-	3,3,3	0.51	0	2,2,2	0.33	0
6	PEG	B	313	-	6,6,6	0.52	0	5,5,5	0.31	0
8	PGE	D	313	-	9,9,9	0.33	0	8,8,8	0.34	0
6	PEG	E	313	-	6,6,6	0.53	0	5,5,5	0.33	0
5	EDO	E	307	-	3,3,3	0.44	0	2,2,2	0.44	0
6	PEG	A	317	-	6,6,6	0.50	0	5,5,5	0.32	0
6	PEG	D	308	-	6,6,6	0.46	0	5,5,5	0.23	0
6	PEG	A	318	-	6,6,6	0.45	0	5,5,5	0.41	0
2	3VN	A	301	-	17,21,21	0.78	0	18,28,28	1.11	1 (5%)
5	EDO	E	309	-	3,3,3	0.42	0	2,2,2	0.61	0
6	PEG	B	312	-	6,6,6	0.48	0	5,5,5	0.38	0
5	EDO	A	308	-	3,3,3	0.39	0	2,2,2	0.62	0
2	3VN	B	301	-	17,21,21	0.80	0	18,28,28	1.13	1 (5%)
7	ACT	F	313	-	3,3,3	0.82	0	3,3,3	1.44	0
5	EDO	B	308	-	3,3,3	0.43	0	2,2,2	0.51	0
5	EDO	A	314	-	3,3,3	0.46	0	2,2,2	0.21	0
7	ACT	F	310	-	3,3,3	0.77	0	3,3,3	1.24	0
4	PG4	C	303	-	12,12,12	0.51	0	11,11,11	0.35	0
2	3VN	D	301	-	17,21,21	0.77	0	18,28,28	1.31	3 (16%)
5	EDO	C	306	-	3,3,3	0.44	0	2,2,2	0.67	0
5	EDO	D	304	-	3,3,3	0.52	0	2,2,2	0.40	0
5	EDO	F	307	-	3,3,3	0.53	0	2,2,2	0.27	0
5	EDO	A	313	-	3,3,3	0.50	0	2,2,2	0.27	0
5	EDO	E	312	-	3,3,3	0.42	0	2,2,2	0.40	0
7	ACT	B	314	-	3,3,3	0.85	0	3,3,3	1.36	0
5	EDO	E	308	-	3,3,3	0.42	0	2,2,2	0.39	0
6	PEG	F	309	-	6,6,6	0.49	0	5,5,5	0.33	0
7	ACT	B	315	-	3,3,3	0.82	0	3,3,3	1.44	0
8	PGE	D	314	-	9,9,9	0.26	0	8,8,8	1.05	1 (12%)
5	EDO	C	305	-	3,3,3	0.39	0	2,2,2	0.66	0
5	EDO	D	306	-	3,3,3	0.61	0	2,2,2	0.08	0
7	ACT	F	311	-	3,3,3	0.81	0	3,3,3	1.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PGE	B	316	-	9,9,9	0.36	0	8,8,8	0.43	0
5	EDO	D	305	-	3,3,3	0.38	0	2,2,2	0.40	0
9	GOL	C	311	-	5,5,5	0.23	0	5,5,5	0.49	0
4	PG4	E	306	-	12,12,12	0.52	0	11,11,11	0.44	0
5	EDO	B	306	-	3,3,3	0.51	0	2,2,2	0.13	0
5	EDO	B	307	-	3,3,3	0.43	0	2,2,2	0.47	0
5	EDO	B	309	-	3,3,3	0.42	0	2,2,2	0.51	0
5	EDO	C	304	-	3,3,3	0.42	0	2,2,2	0.39	0
7	ACT	D	309	-	3,3,3	0.85	0	3,3,3	1.29	0
7	ACT	F	312	-	3,3,3	0.88	0	3,3,3	1.44	0
4	PG4	D	303	-	12,12,12	0.53	0	11,11,11	0.21	0
5	EDO	A	312	-	3,3,3	0.48	0	2,2,2	0.28	0
7	ACT	D	312	-	3,3,3	0.82	0	3,3,3	1.37	0
6	PEG	F	308	-	6,6,6	0.53	0	5,5,5	0.24	0
5	EDO	A	311	-	3,3,3	0.39	0	2,2,2	0.66	0
6	PEG	B	311	-	6,6,6	0.49	0	5,5,5	0.41	0
5	EDO	A	310	-	3,3,3	0.45	0	2,2,2	0.39	0
7	ACT	A	319	-	3,3,3	0.76	0	3,3,3	1.18	0
7	ACT	A	320	-	3,3,3	0.80	0	3,3,3	1.42	0
5	EDO	F	306	-	3,3,3	0.45	0	2,2,2	0.47	0
7	ACT	D	311	-	3,3,3	0.82	0	3,3,3	1.32	0
6	PEG	C	310	-	6,6,6	0.48	0	5,5,5	0.34	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
5	EDO	A	315	-	-	1/1/1/1	-
5	EDO	C	307	-	-	1/1/1/1	-
5	EDO	C	308	-	-	1/1/1/1	-
5	EDO	E	311	-	-	0/1/1/1	-
4	PG4	A	306	-	-	0/10/10/10	-
4	PG4	F	305	-	-	1/10/10/10	-
8	PGE	E	315	-	-	1/7/7/7	-
5	EDO	A	316	-	-	0/1/1/1	-
5	EDO	B	310	-	-	1/1/1/1	-
4	PG4	B	305	-	-	1/10/10/10	-
5	EDO	A	307	-	-	1/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	C	309	-	-	0/1/1/1	-
5	EDO	D	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	310	-	-	0/1/1/1	-
6	PEG	B	313	-	-	2/4/4/4	-
8	PGE	D	313	-	-	2/7/7/7	-
6	PEG	E	313	-	-	3/4/4/4	-
5	EDO	E	307	-	-	0/1/1/1	-
6	PEG	A	317	-	-	0/4/4/4	-
6	PEG	D	308	-	-	1/4/4/4	-
6	PEG	A	318	-	-	3/4/4/4	-
2	3VN	A	301	-	-	8/31/31/31	-
5	EDO	E	309	-	-	1/1/1/1	-
6	PEG	B	312	-	-	3/4/4/4	-
5	EDO	A	308	-	-	1/1/1/1	-
2	3VN	B	301	-	-	10/31/31/31	-
5	EDO	B	308	-	-	1/1/1/1	-
5	EDO	A	314	-	-	0/1/1/1	-
4	PG4	C	303	-	-	1/10/10/10	-
2	3VN	D	301	-	-	10/31/31/31	-
5	EDO	C	306	-	-	1/1/1/1	-
5	EDO	D	304	-	-	0/1/1/1	-
5	EDO	F	307	-	-	0/1/1/1	-
5	EDO	A	313	-	-	1/1/1/1	-
5	EDO	E	312	-	-	1/1/1/1	-
5	EDO	E	308	-	-	1/1/1/1	-
6	PEG	F	309	-	-	1/4/4/4	-
8	PGE	D	314	-	-	4/7/7/7	-
5	EDO	C	305	-	-	1/1/1/1	-
5	EDO	D	306	-	-	0/1/1/1	-
8	PGE	B	316	-	-	3/7/7/7	-
5	EDO	D	305	-	-	0/1/1/1	-
9	GOL	C	311	-	-	0/4/4/4	-
4	PG4	E	306	-	-	6/10/10/10	-
5	EDO	B	306	-	-	1/1/1/1	-
5	EDO	B	307	-	-	1/1/1/1	-
5	EDO	B	309	-	-	0/1/1/1	-
5	EDO	C	304	-	-	0/1/1/1	-
4	PG4	D	303	-	-	0/10/10/10	-
5	EDO	A	312	-	-	0/1/1/1	-
6	PEG	F	308	-	-	0/4/4/4	-
5	EDO	A	311	-	-	0/1/1/1	-
6	PEG	B	311	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	310	-	-	0/1/1/1	-
5	EDO	F	306	-	-	1/1/1/1	-
6	PEG	C	310	-	-	4/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	314	PGE	O4-C6-C5	-2.64	96.25	111.82
2	D	301	3VN	O05-C03-C02	2.50	120.36	113.69
2	B	301	3VN	C15-C16-C17	-2.42	105.97	113.19
2	A	301	3VN	O05-C03-C02	2.13	119.39	113.69
2	D	301	3VN	O22-C20-C13	2.01	119.06	113.69
2	D	301	3VN	C16-C15-C13	-2.01	111.60	115.16

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	314	PGE	C3-C4-O3-C5
8	D	313	PGE	O2-C3-C4-O3
4	E	306	PG4	C5-C6-O4-C7
6	C	310	PEG	C4-C3-O2-C2
8	B	316	PGE	O2-C3-C4-O3
4	E	306	PG4	O2-C3-C4-O3
6	A	318	PEG	C4-C3-O2-C2
6	B	313	PEG	O1-C1-C2-O2
6	C	310	PEG	O2-C3-C4-O4
6	A	318	PEG	O1-C1-C2-O2
5	C	306	EDO	O1-C1-C2-O2
4	E	306	PG4	O1-C1-C2-O2
4	E	306	PG4	O4-C7-C8-O5
5	B	306	EDO	O1-C1-C2-O2
5	C	307	EDO	O1-C1-C2-O2
5	E	308	EDO	O1-C1-C2-O2
5	E	312	EDO	O1-C1-C2-O2
2	B	301	3VN	C16-C17-C18-N19
8	E	315	PGE	O2-C3-C4-O3
5	F	306	EDO	O1-C1-C2-O2
2	D	301	3VN	C15-C16-C17-C18
4	B	305	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
4	F	305	PG4	C1-C2-O2-C3
6	D	308	PEG	C4-C3-O2-C2
6	E	313	PEG	C1-C2-O2-C3
6	B	313	PEG	O2-C3-C4-O4
6	E	313	PEG	O1-C1-C2-O2
6	E	313	PEG	O2-C3-C4-O4
6	A	318	PEG	O2-C3-C4-O4
6	B	312	PEG	C4-C3-O2-C2
2	A	301	3VN	C06-C02-C03-O05
2	A	301	3VN	C11-C02-C03-O04
2	A	301	3VN	C11-C02-C03-O05
2	A	301	3VN	C12-C13-C20-O21
2	A	301	3VN	C12-C13-C20-O22
2	B	301	3VN	C11-C02-C03-O04
2	B	301	3VN	C11-C02-C03-O05
2	B	301	3VN	C12-C13-C20-O21
2	B	301	3VN	C12-C13-C20-O22
2	B	301	3VN	C15-C13-C20-O22
2	D	301	3VN	C11-C02-C03-O04
2	D	301	3VN	C11-C02-C03-O05
2	D	301	3VN	C12-C13-C20-O21
2	D	301	3VN	C12-C13-C20-O22
6	B	312	PEG	O1-C1-C2-O2
8	D	314	PGE	O3-C5-C6-O4
8	D	314	PGE	O2-C3-C4-O3
6	B	311	PEG	C4-C3-O2-C2
8	D	314	PGE	C4-C3-O2-C2
4	E	306	PG4	C1-C2-O2-C3
5	A	307	EDO	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
4	C	303	PG4	O4-C7-C8-O5
4	E	306	PG4	C3-C4-O3-C5
5	C	308	EDO	O1-C1-C2-O2
6	C	310	PEG	O1-C1-C2-O2
6	F	309	PEG	O2-C3-C4-O4
6	C	310	PEG	C1-C2-O2-C3
5	A	313	EDO	O1-C1-C2-O2
5	A	315	EDO	O1-C1-C2-O2
5	B	308	EDO	O1-C1-C2-O2
6	B	312	PEG	O2-C3-C4-O4
5	A	308	EDO	O1-C1-C2-O2
5	C	305	EDO	O1-C1-C2-O2

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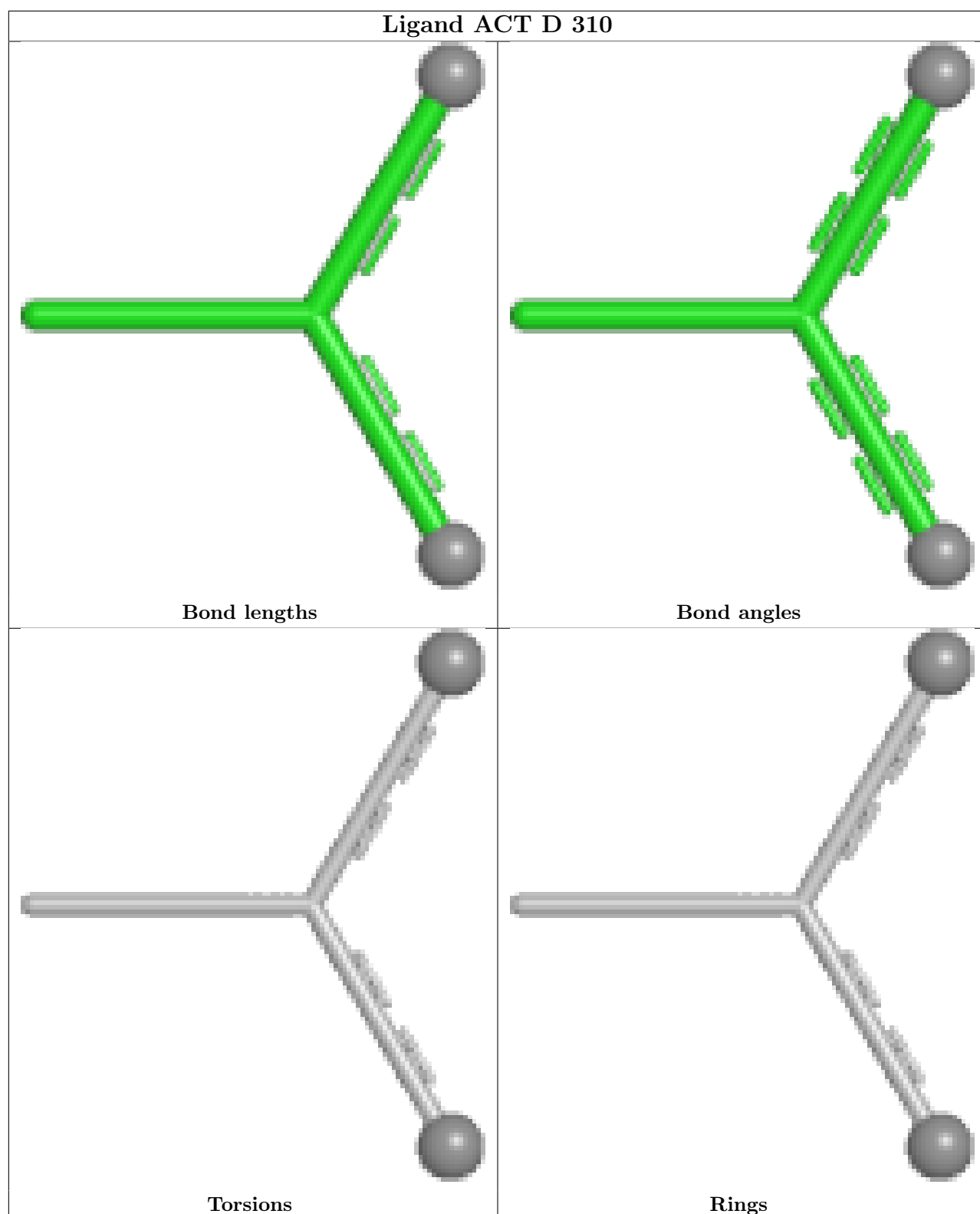
Mol	Chain	Res	Type	Atoms
5	E	309	EDO	O1-C1-C2-O2
2	B	301	3VN	C15-C16-C17-C18
8	B	316	PGE	C3-C4-O3-C5
8	D	313	PGE	C1-C2-O2-C3
8	B	316	PGE	O3-C5-C6-O4
5	B	307	EDO	O1-C1-C2-O2
2	A	301	3VN	C06-C02-C03-O04
2	A	301	3VN	C15-C13-C20-O21
2	A	301	3VN	C15-C13-C20-O22
2	B	301	3VN	C06-C02-C03-O04
2	B	301	3VN	C06-C02-C03-O05
2	B	301	3VN	C15-C13-C20-O21
2	D	301	3VN	C06-C02-C03-O04
2	D	301	3VN	C06-C02-C03-O05
2	D	301	3VN	C15-C13-C20-O21
2	D	301	3VN	C15-C13-C20-O22
2	D	301	3VN	C16-C17-C18-N19

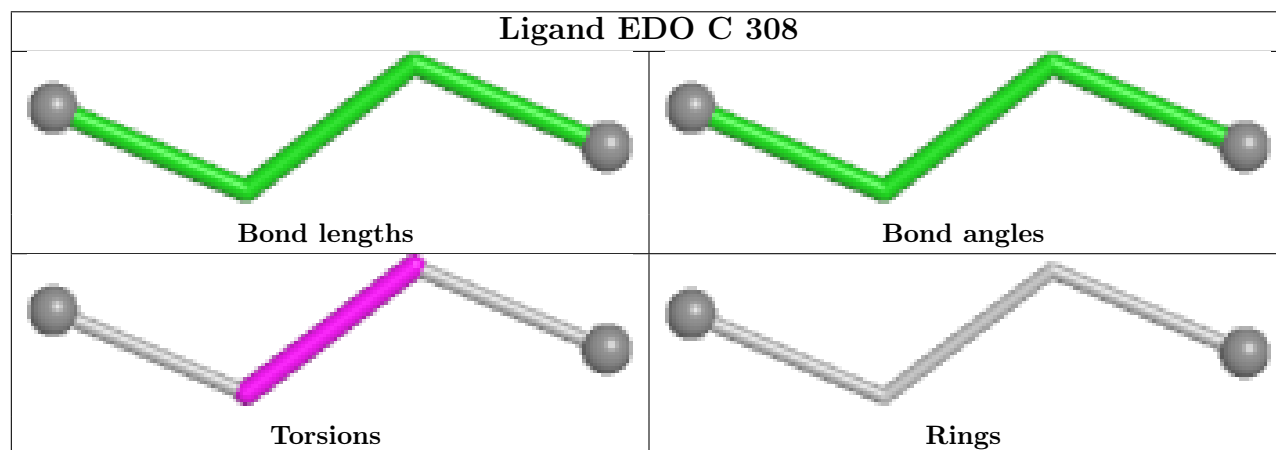
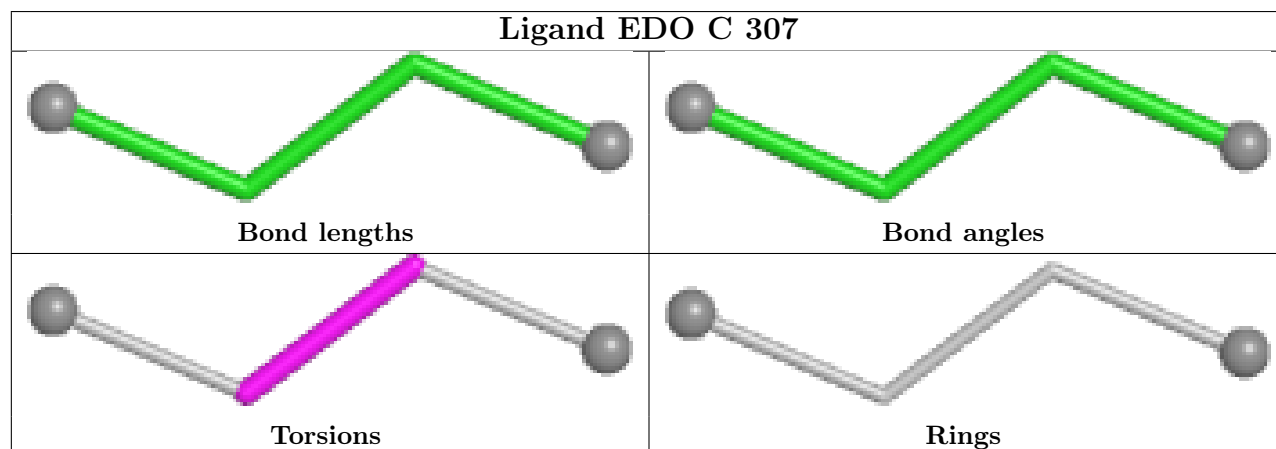
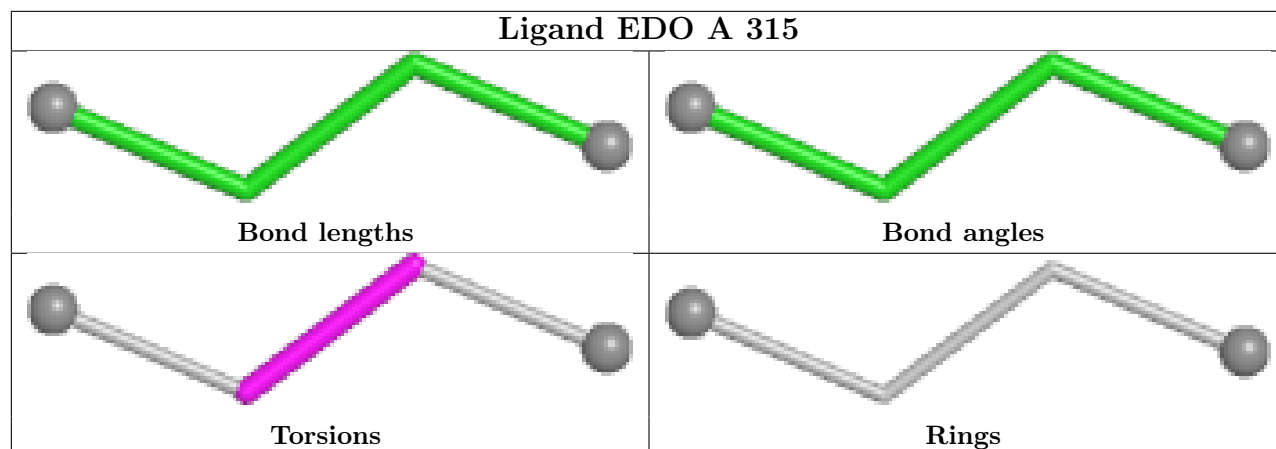
There are no ring outliers.

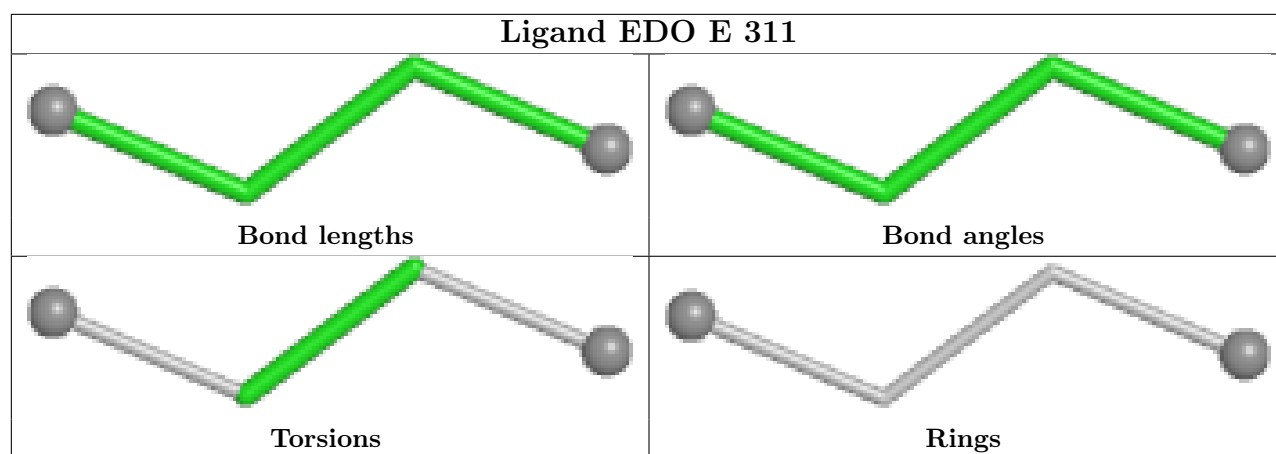
20 monomers are involved in 29 short contacts:

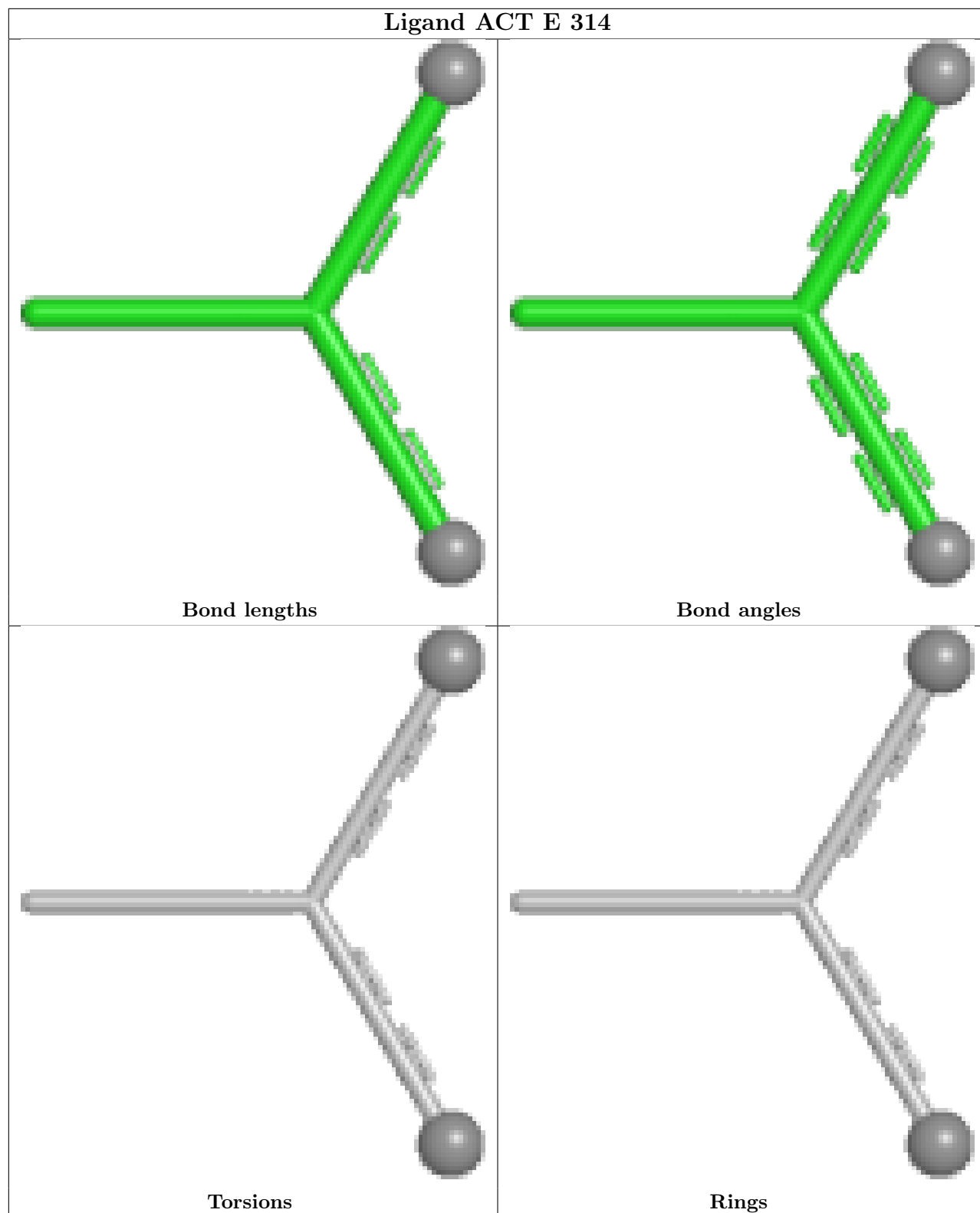
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	314	ACT	1	0
8	E	315	PGE	1	0
5	B	310	EDO	1	0
5	D	307	EDO	1	0
6	B	313	PEG	2	0
6	E	313	PEG	1	0
2	A	301	3VN	1	0
5	E	309	EDO	1	0
5	A	308	EDO	2	0
2	B	301	3VN	1	0
5	B	308	EDO	1	0
2	D	301	3VN	1	0
8	D	314	PGE	3	0
4	E	306	PG4	3	0
5	B	306	EDO	4	0
4	D	303	PG4	1	0
6	B	311	PEG	1	0
7	A	319	ACT	1	0
5	F	306	EDO	1	0
6	C	310	PEG	2	0

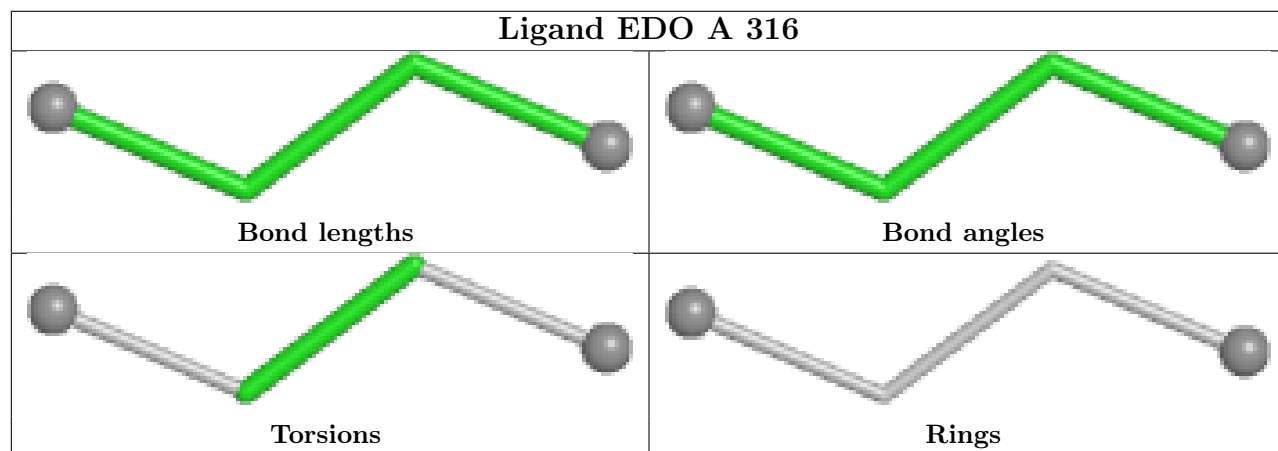
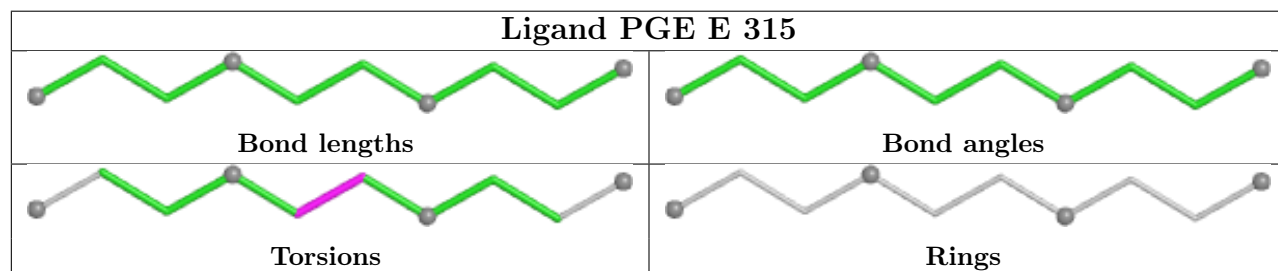
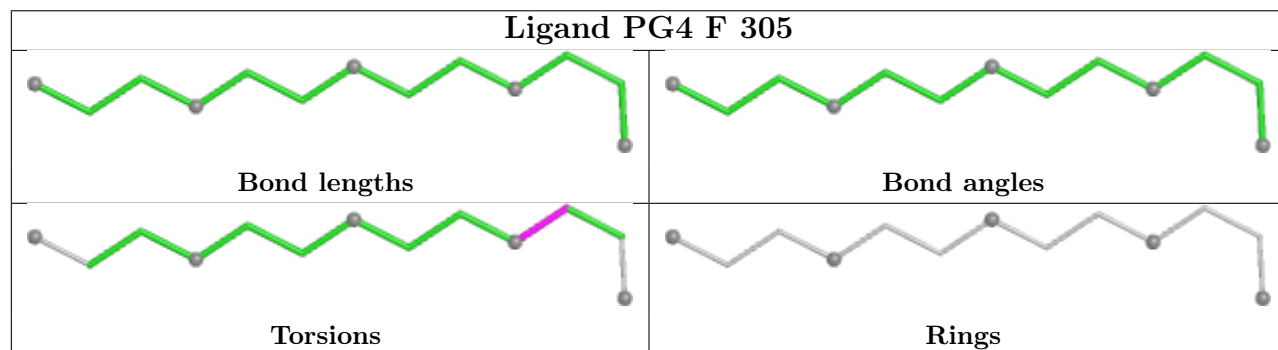
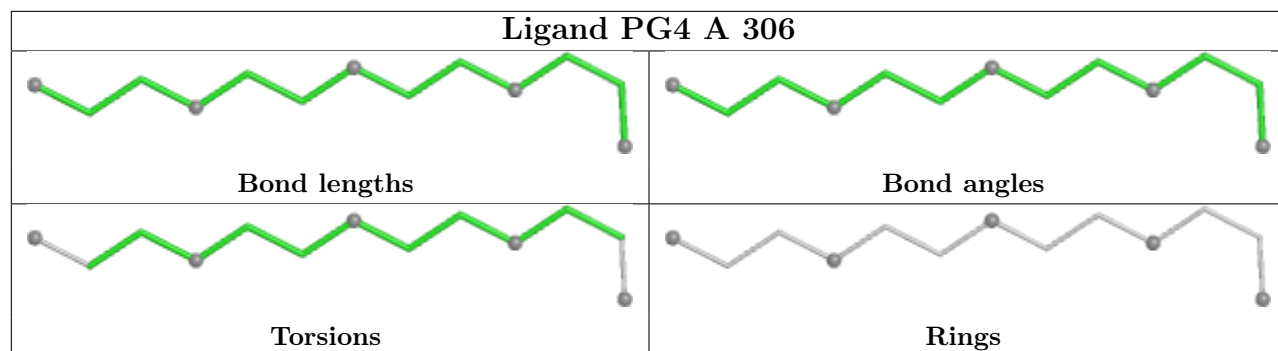
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

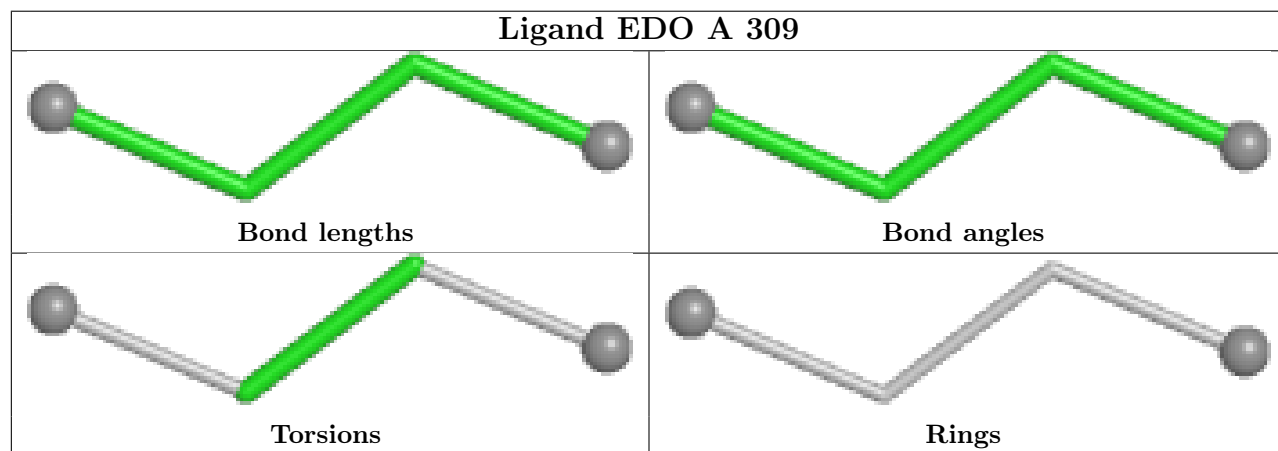
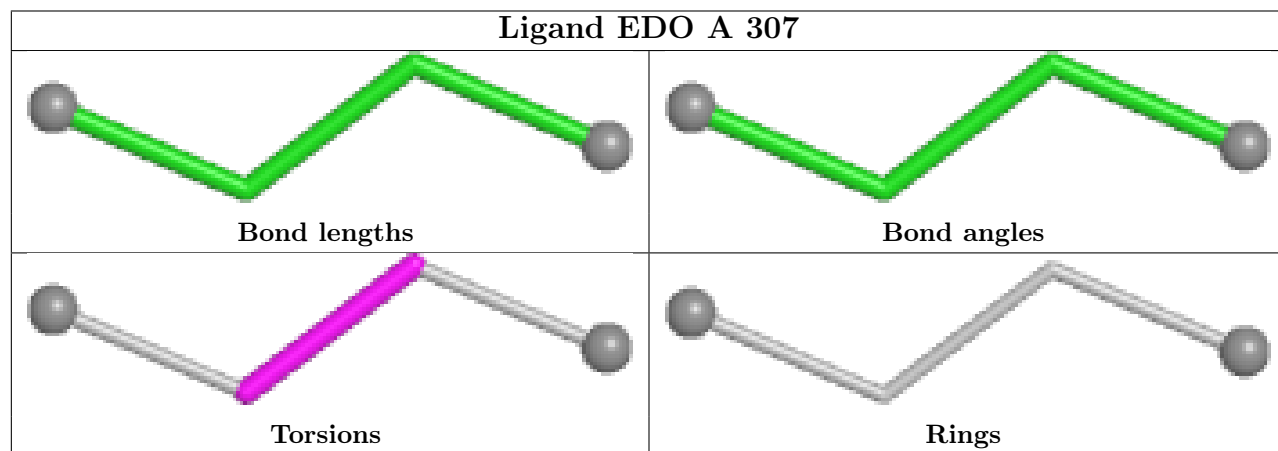
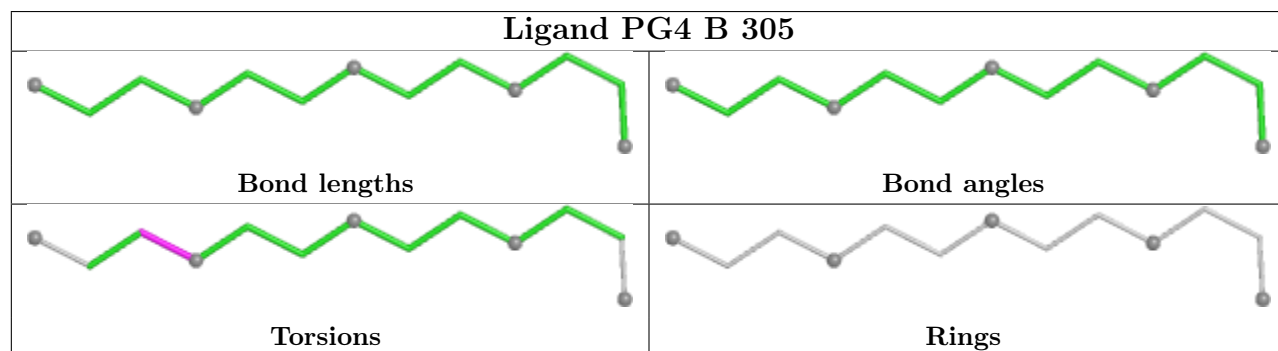
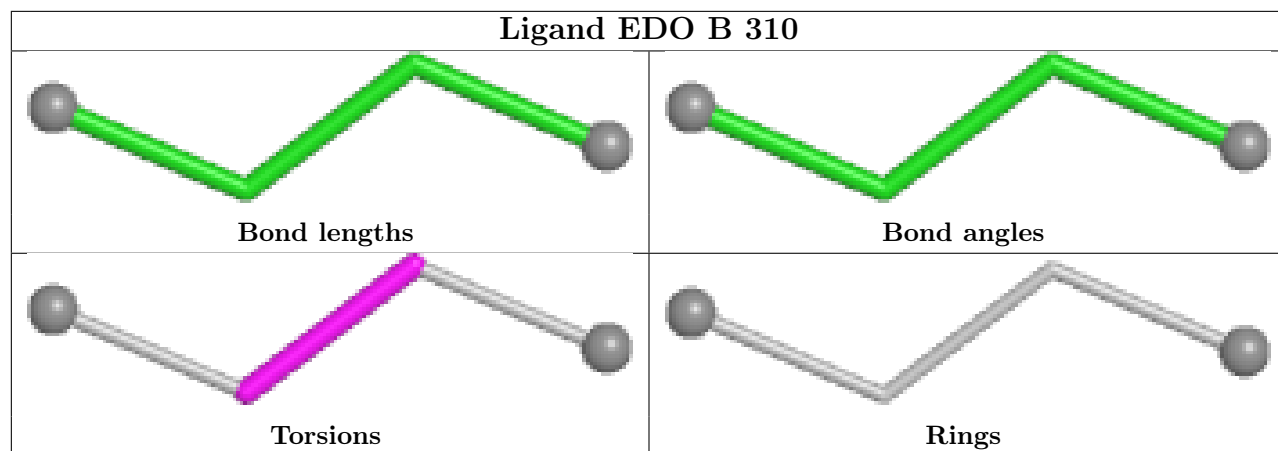


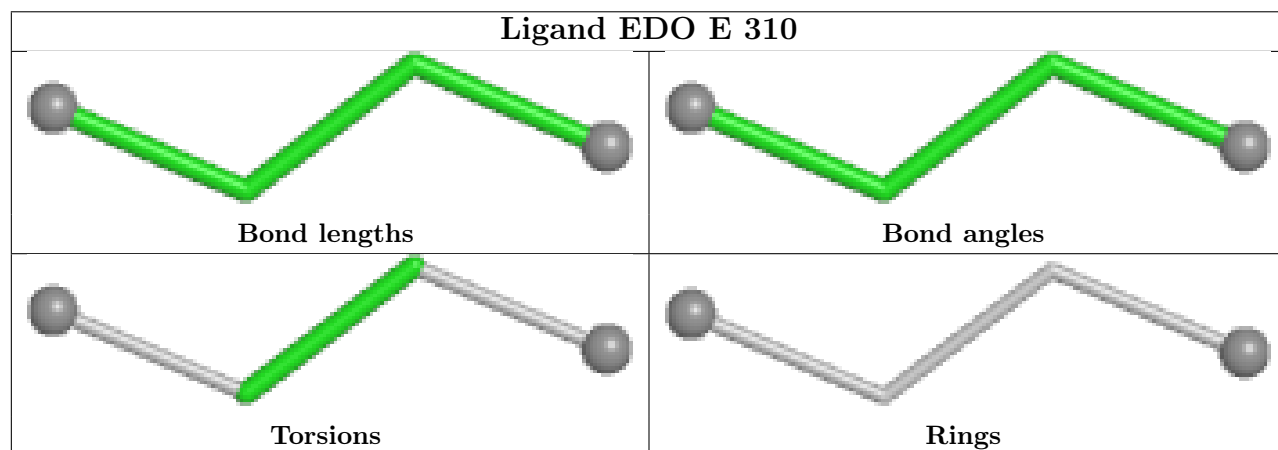
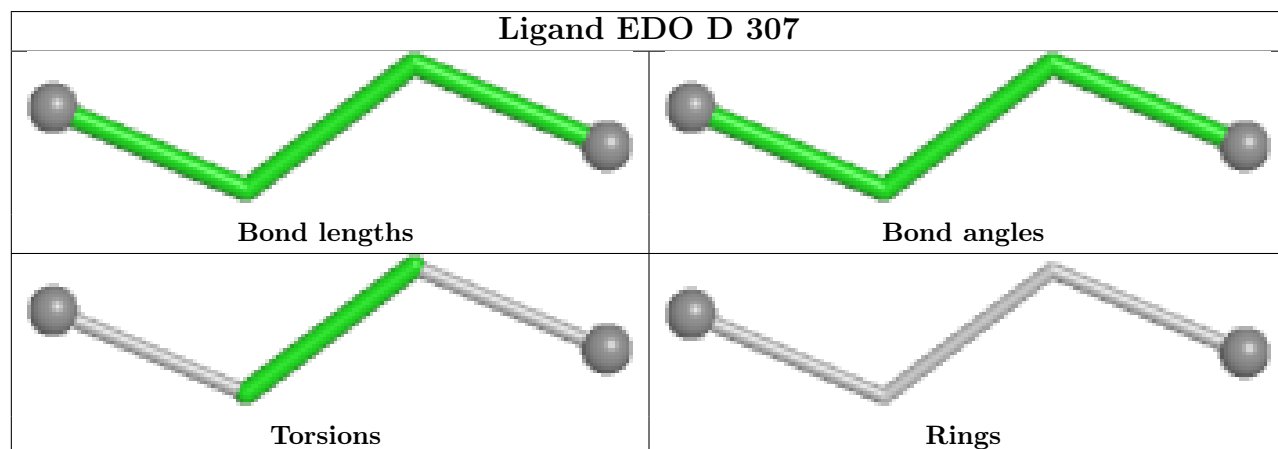
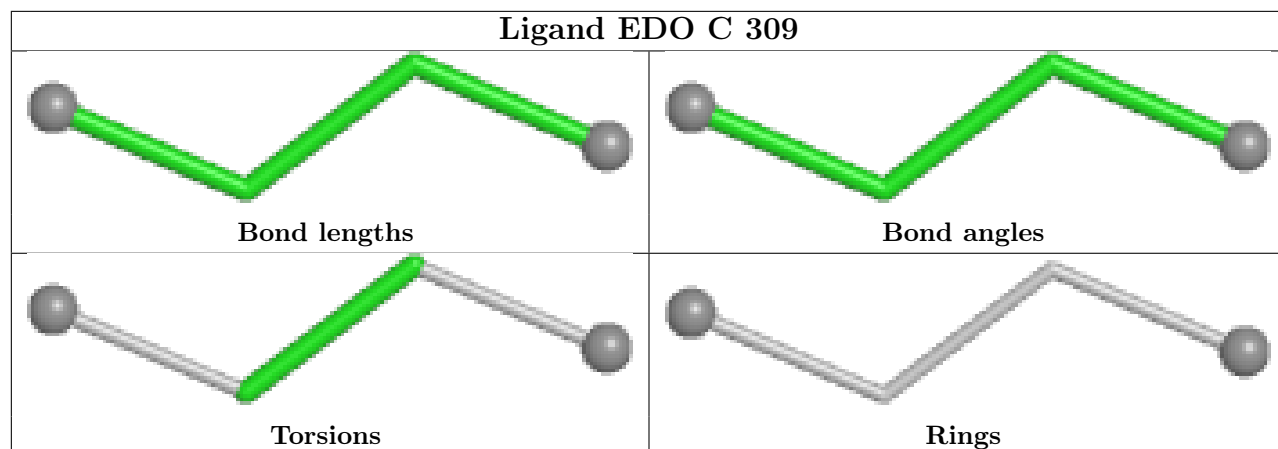


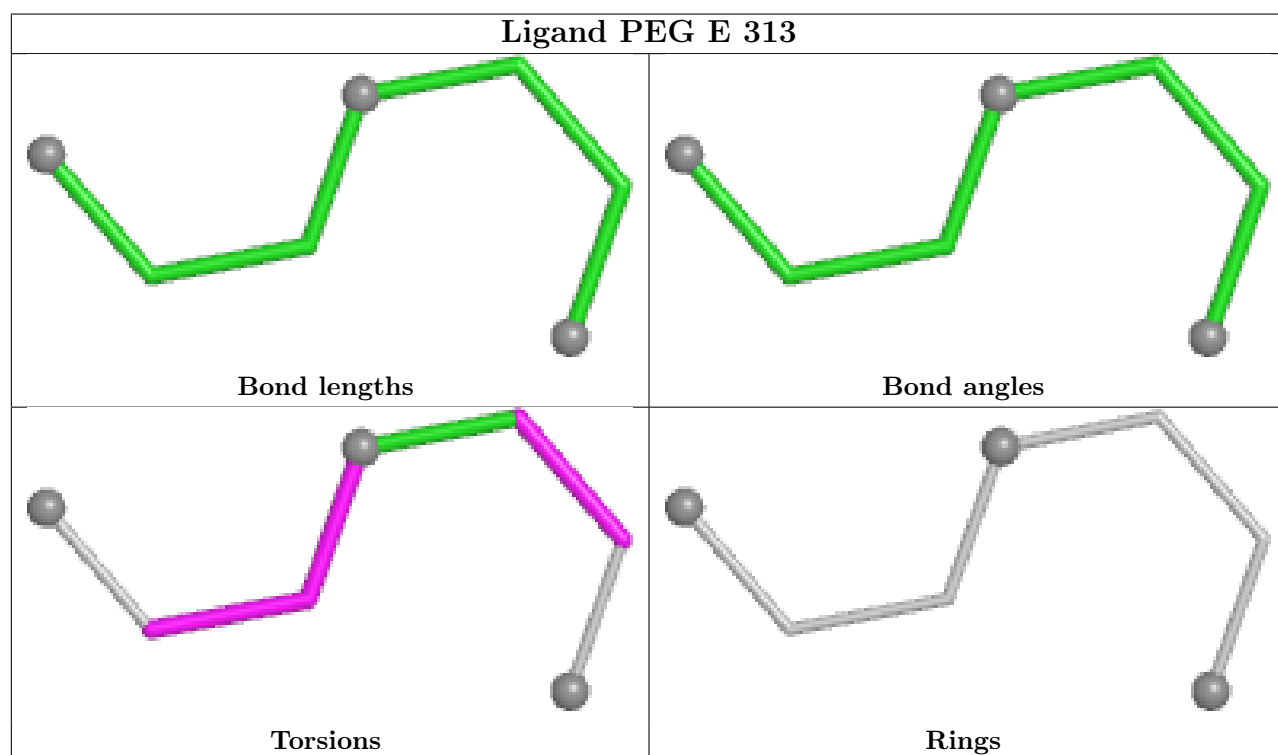
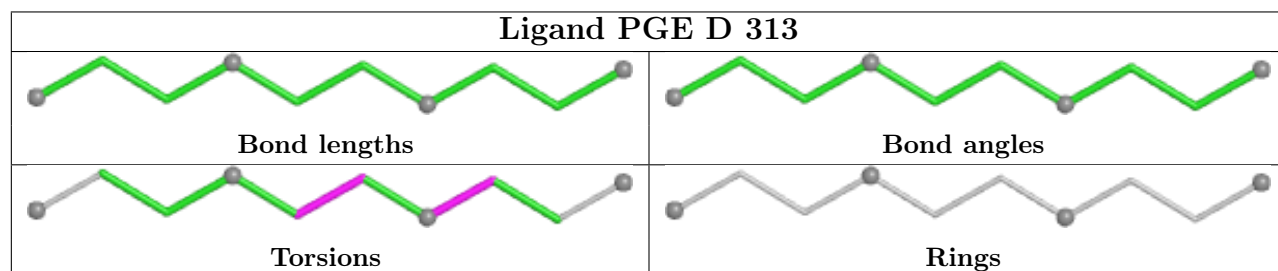
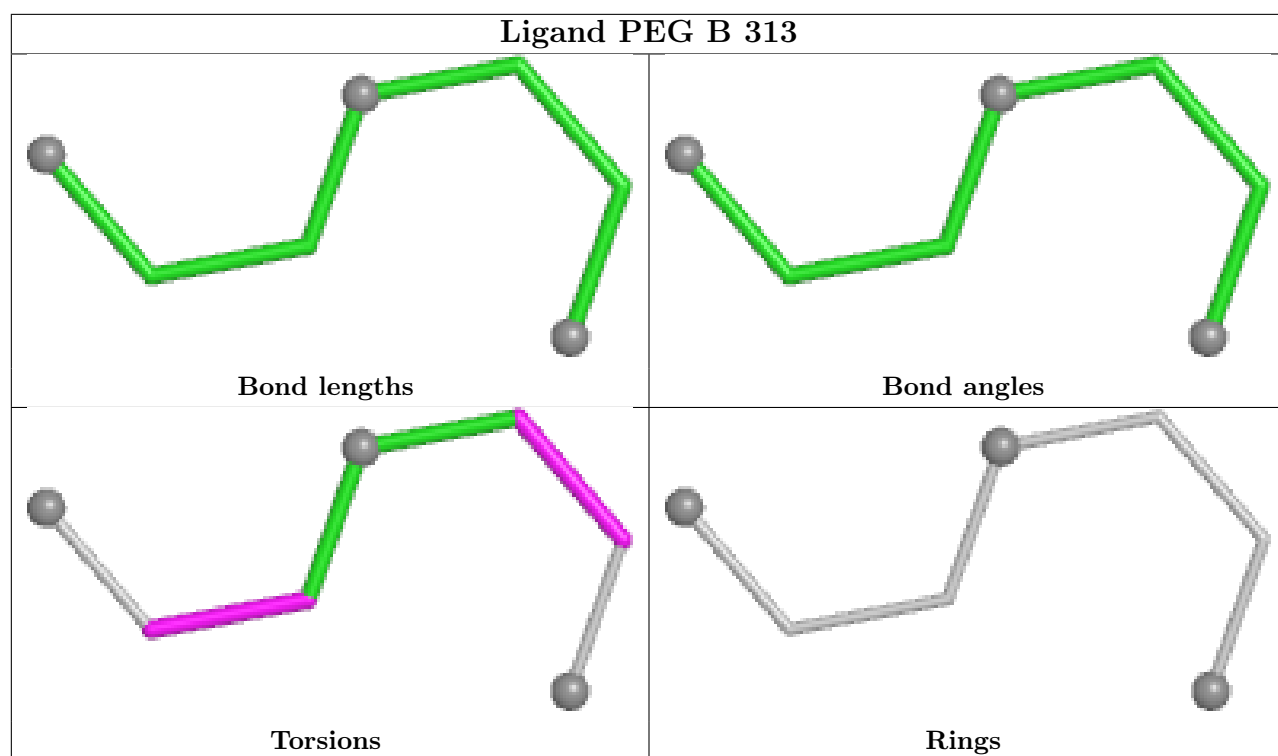


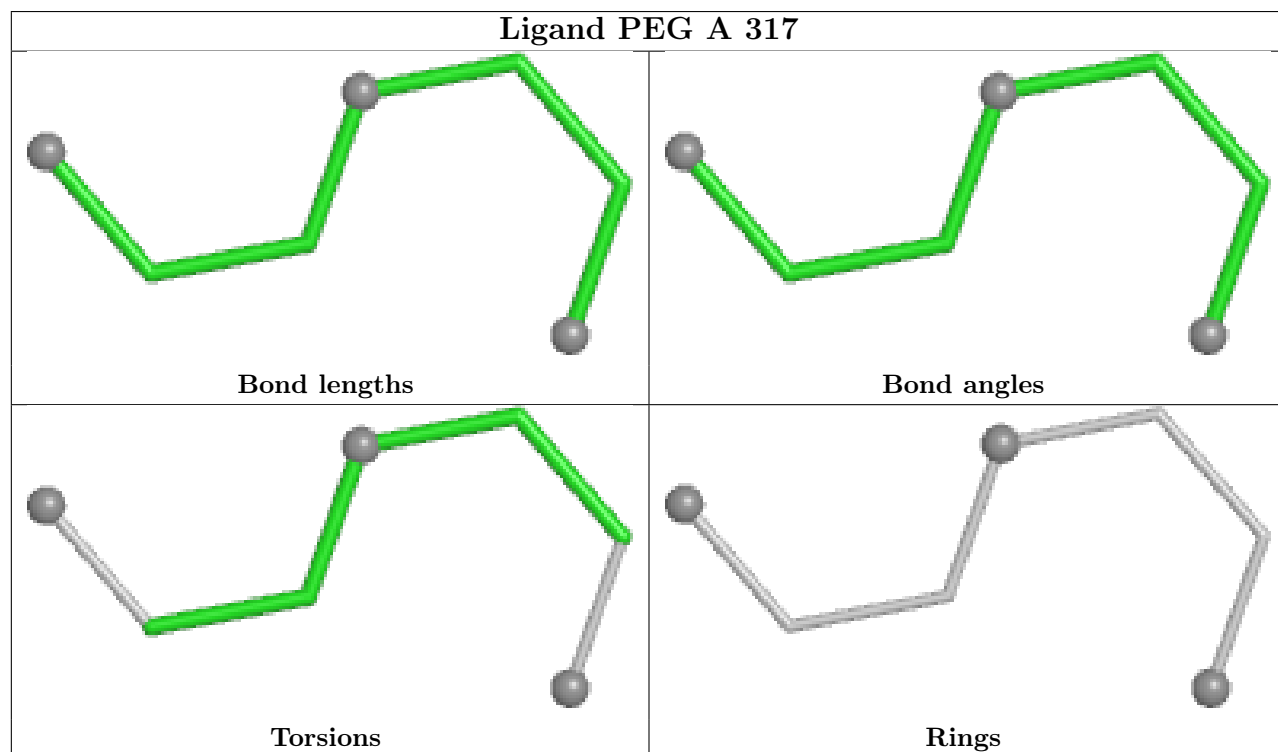
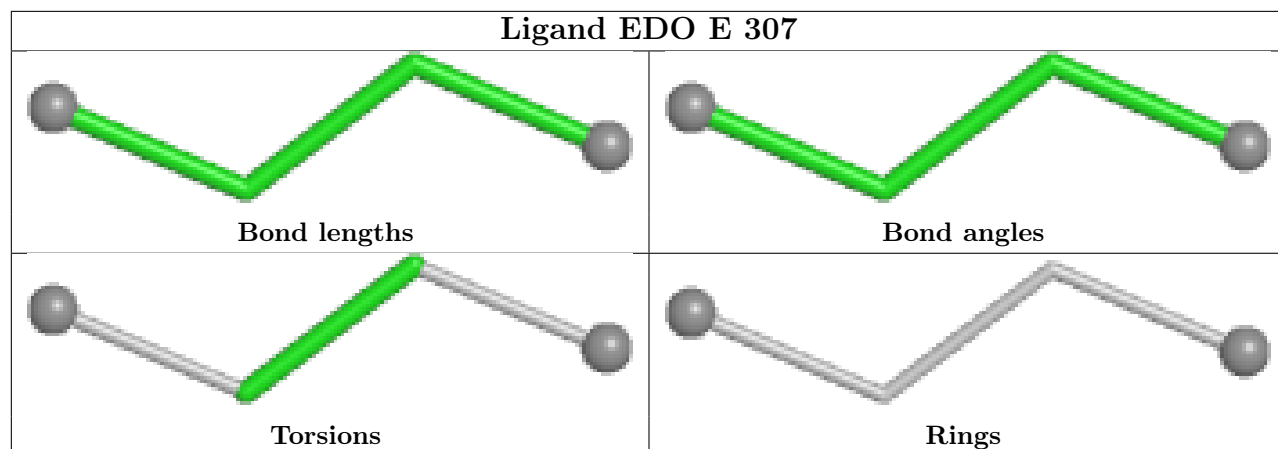


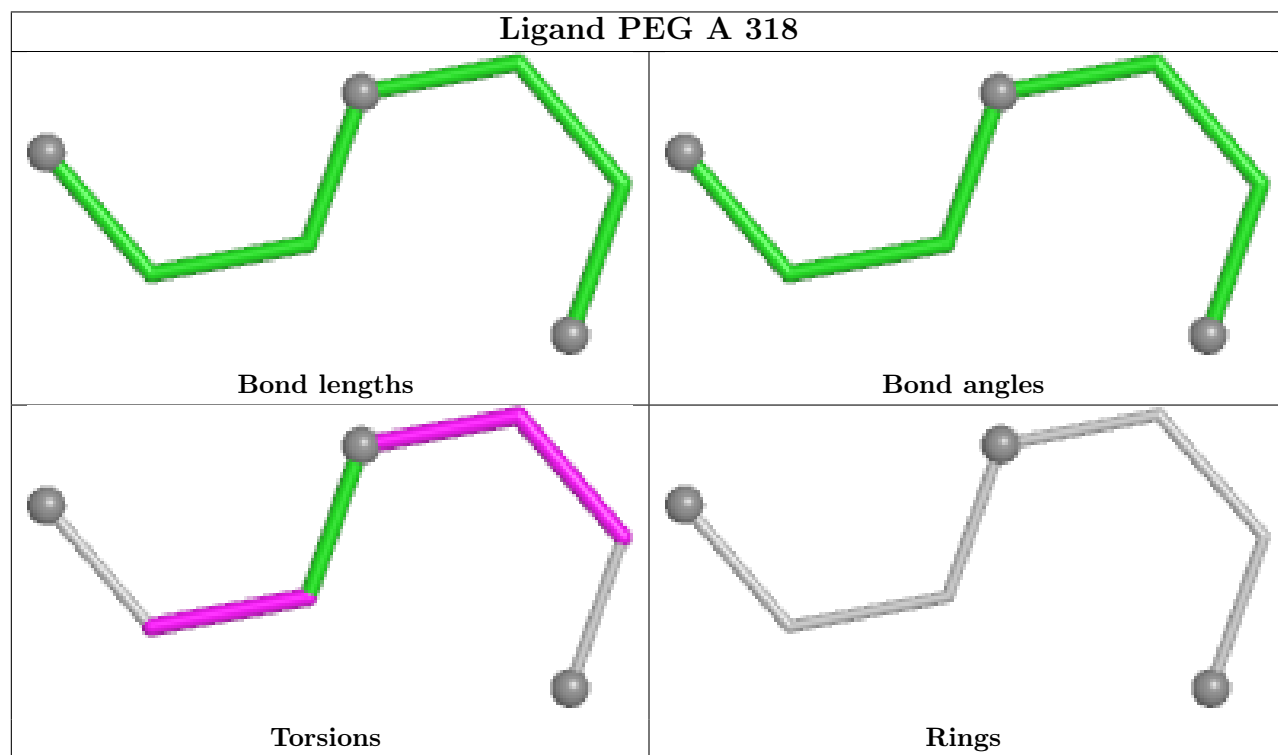
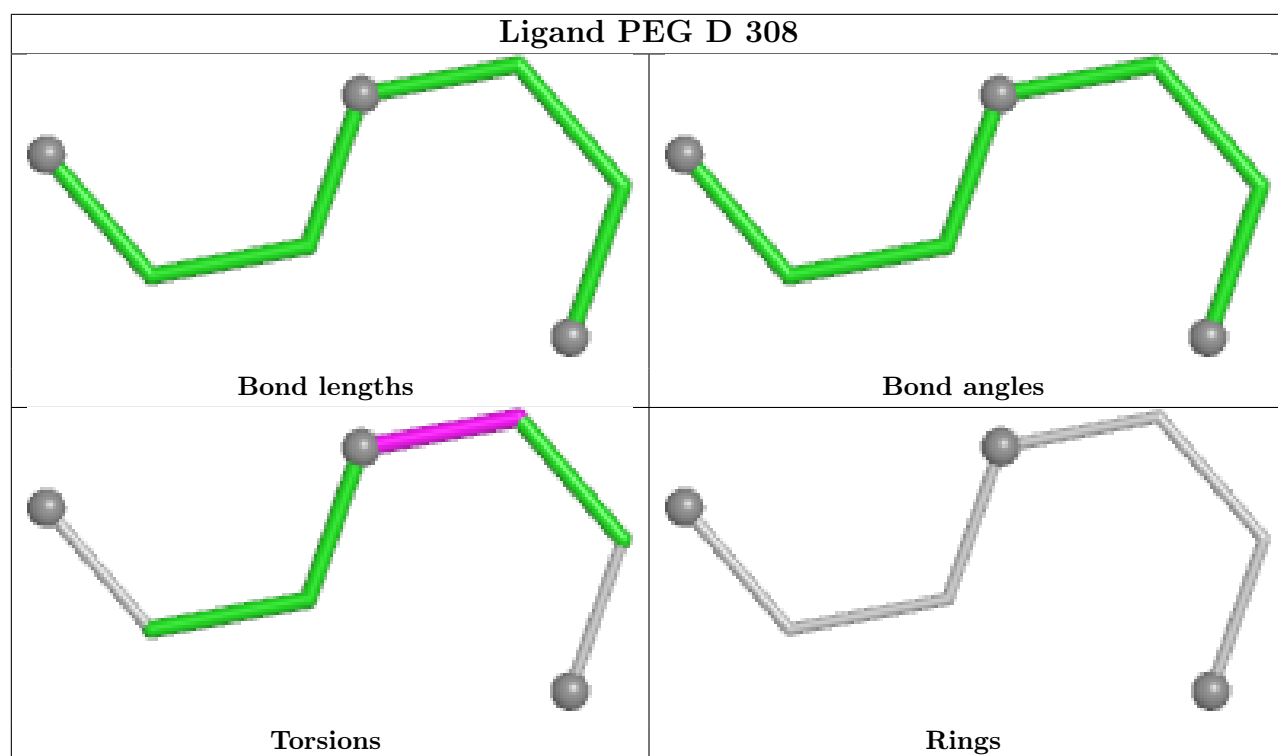




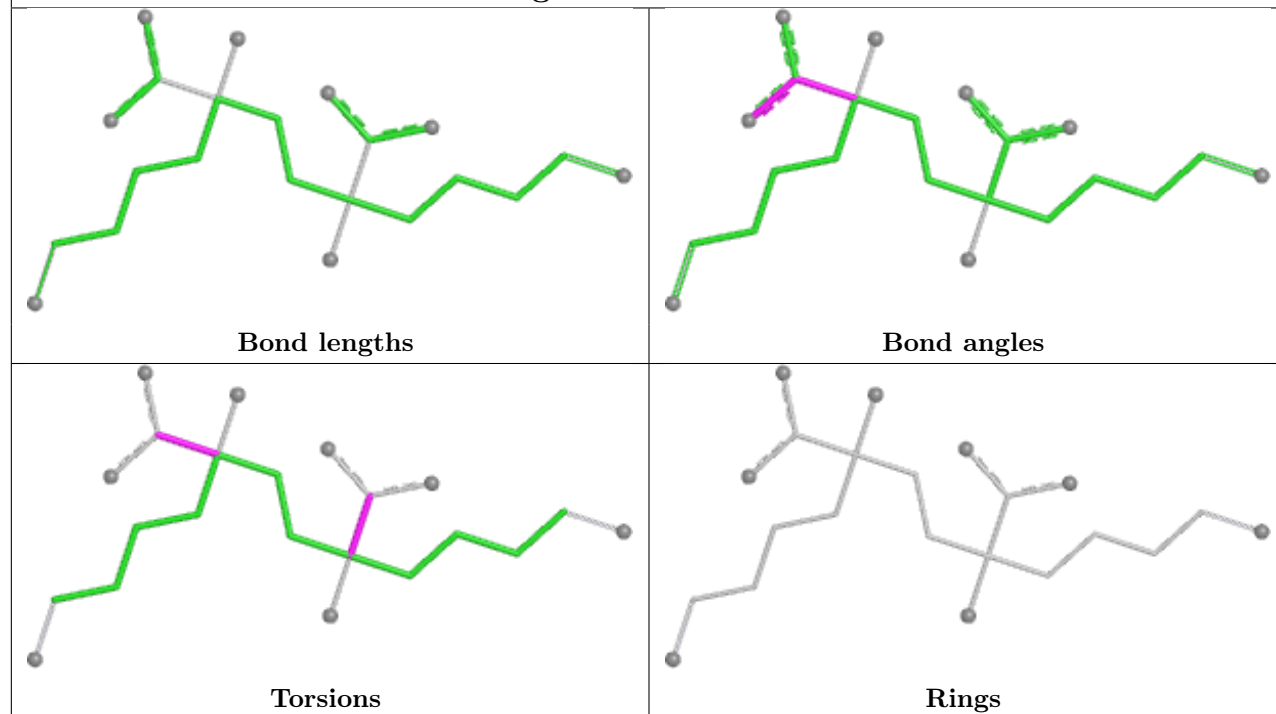




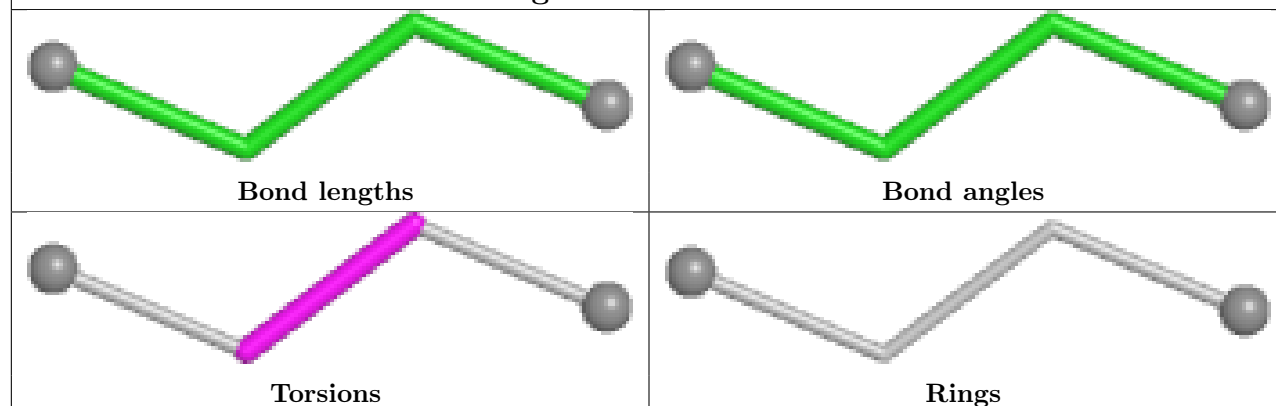


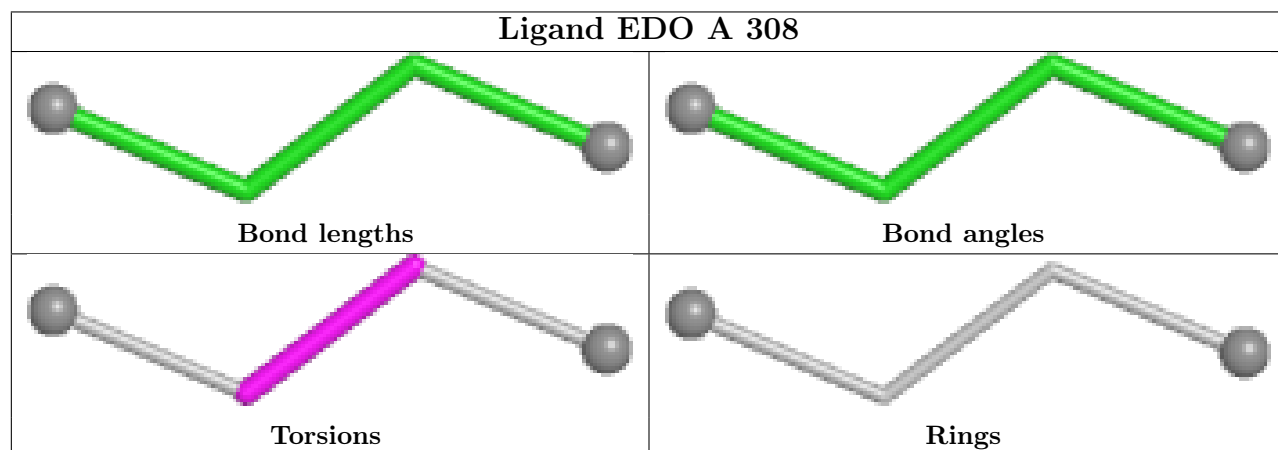
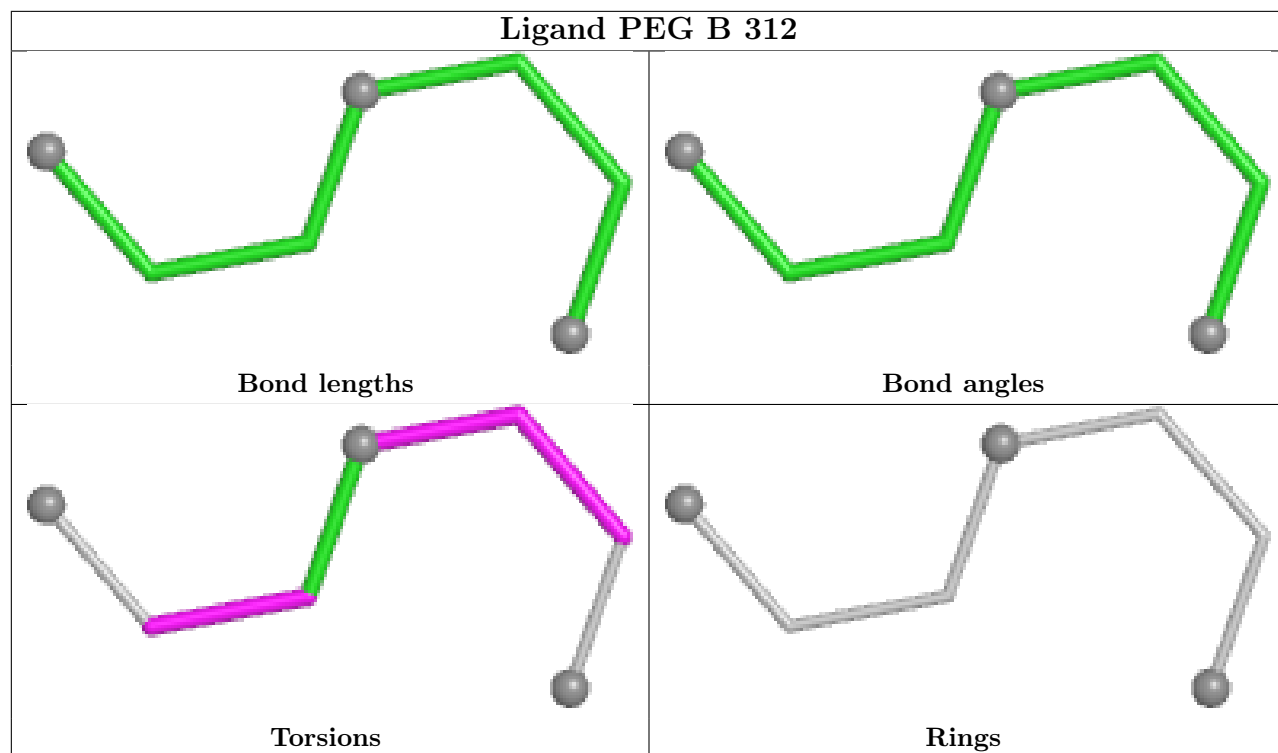


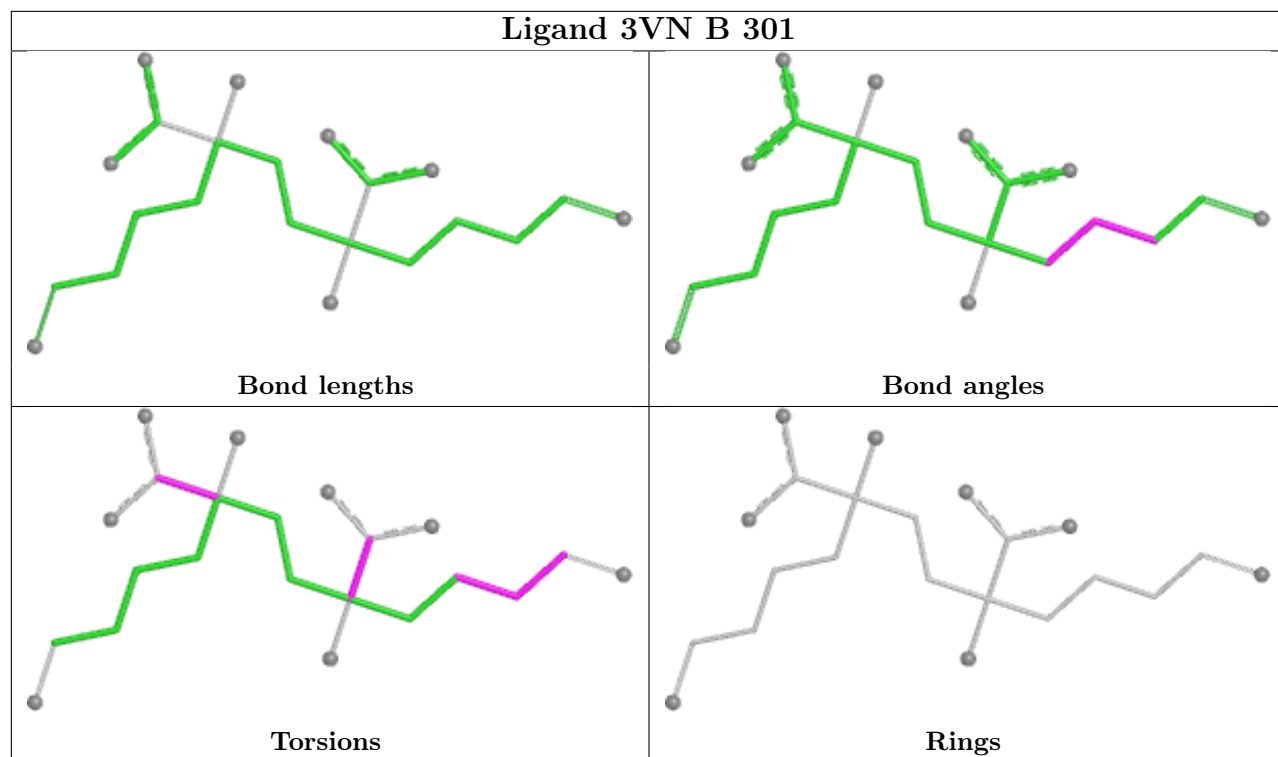
Ligand 3VN A 301

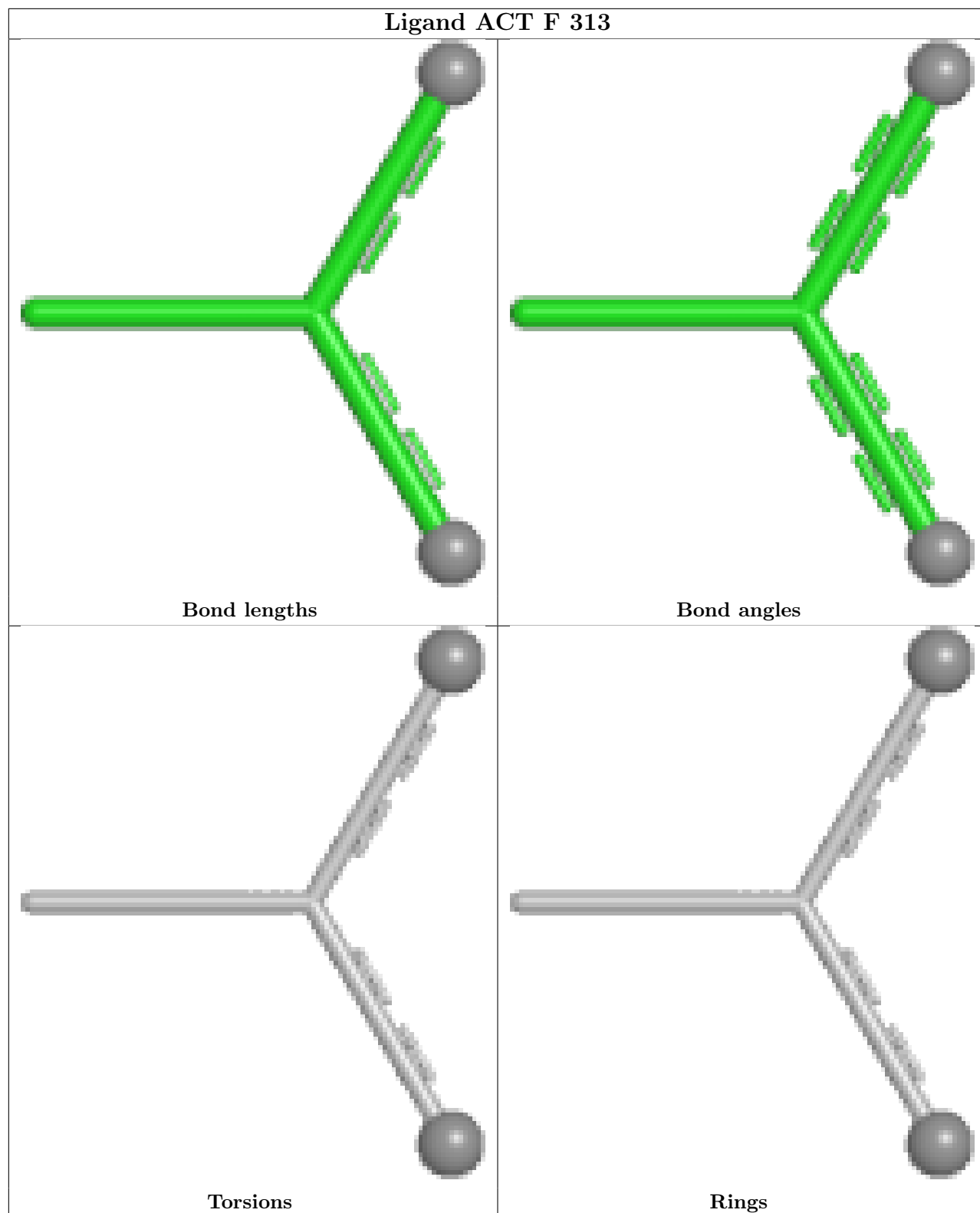


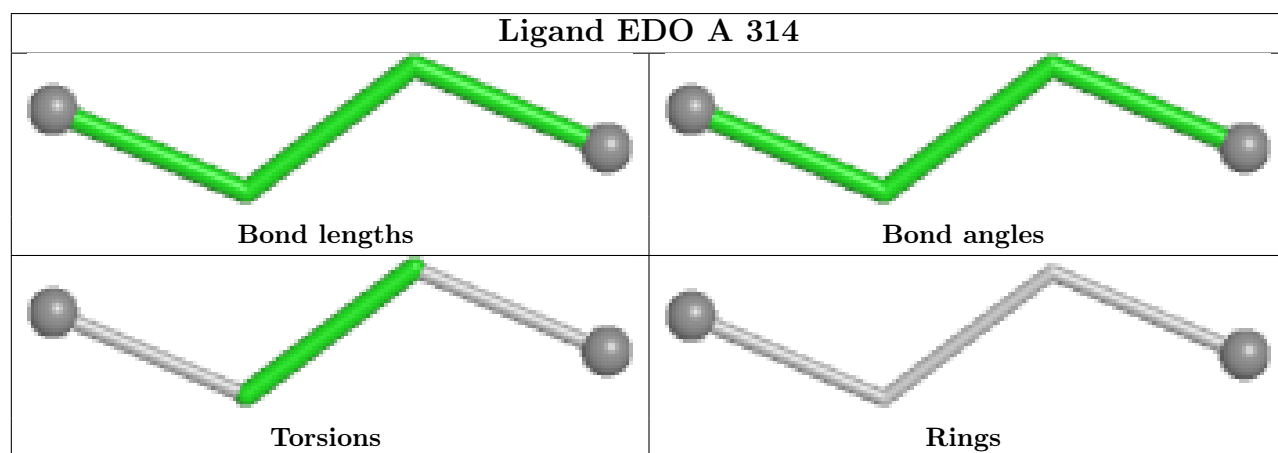
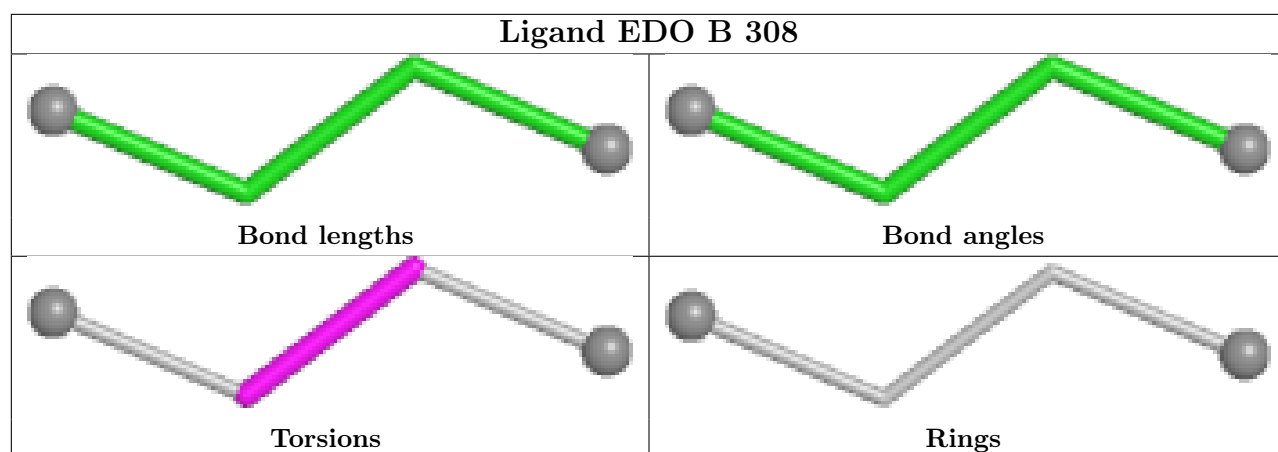
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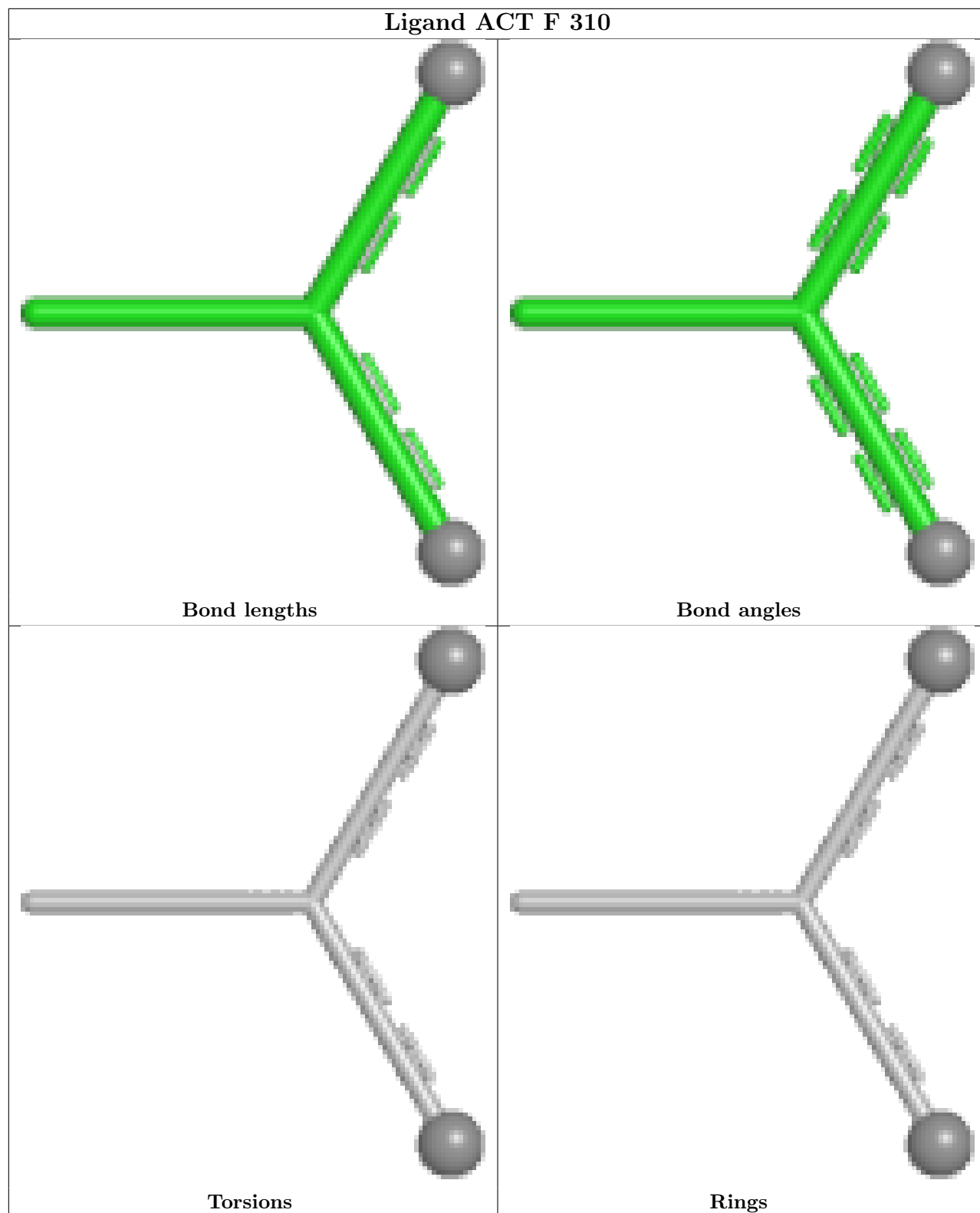


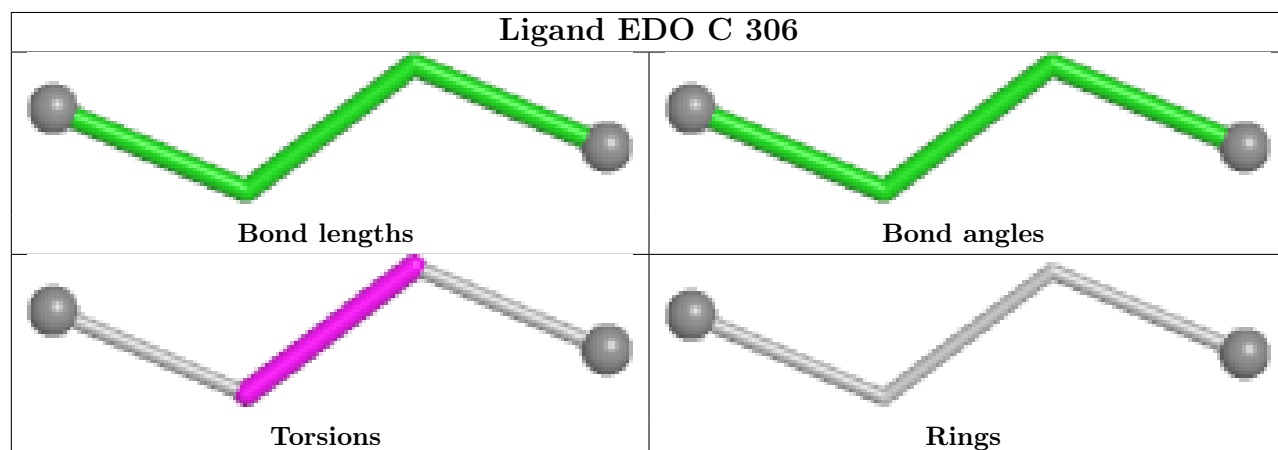
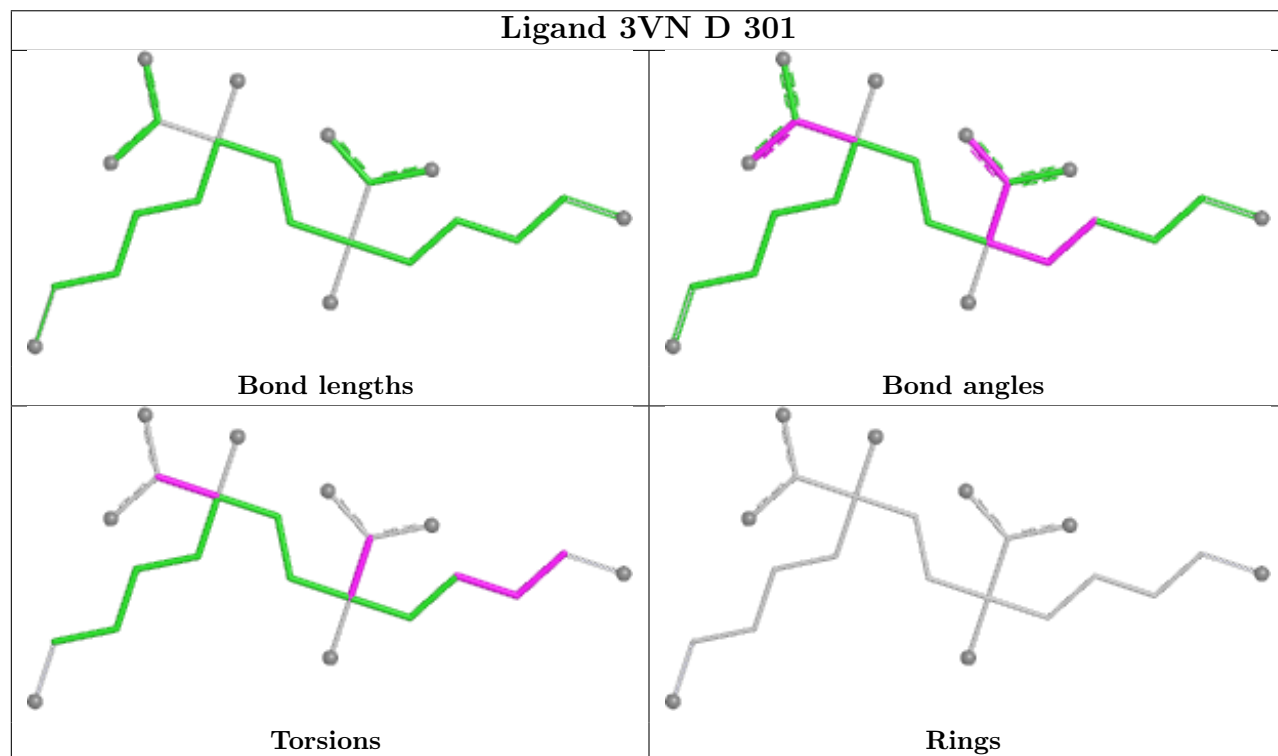
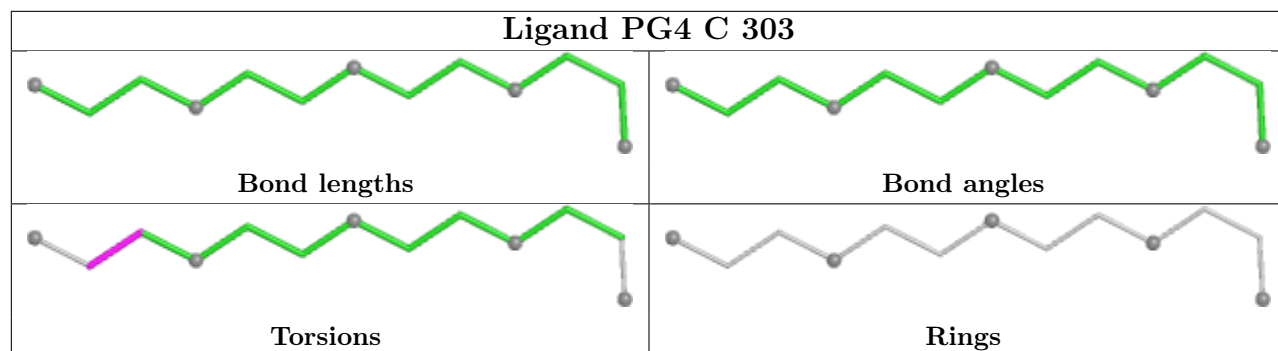


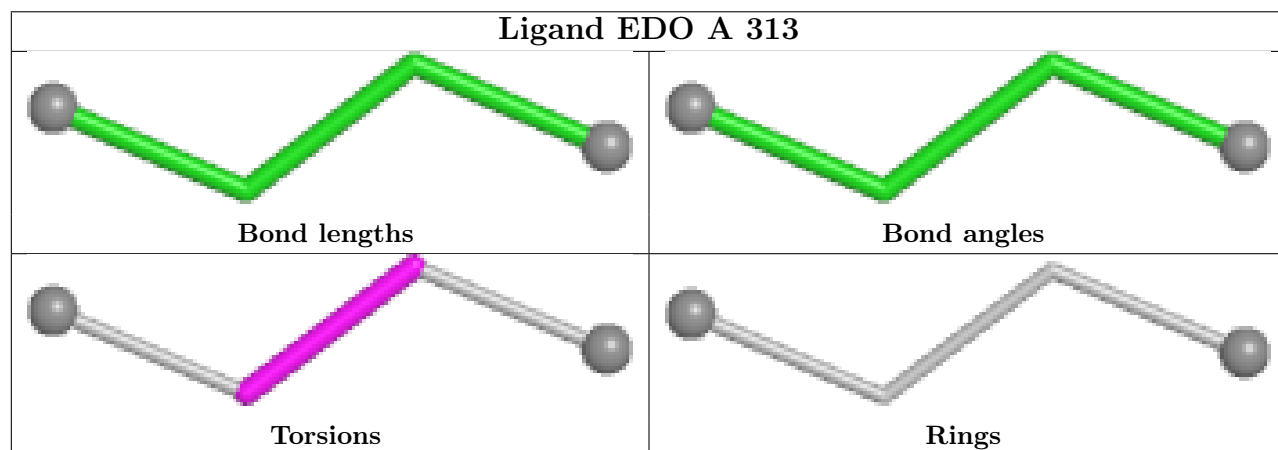
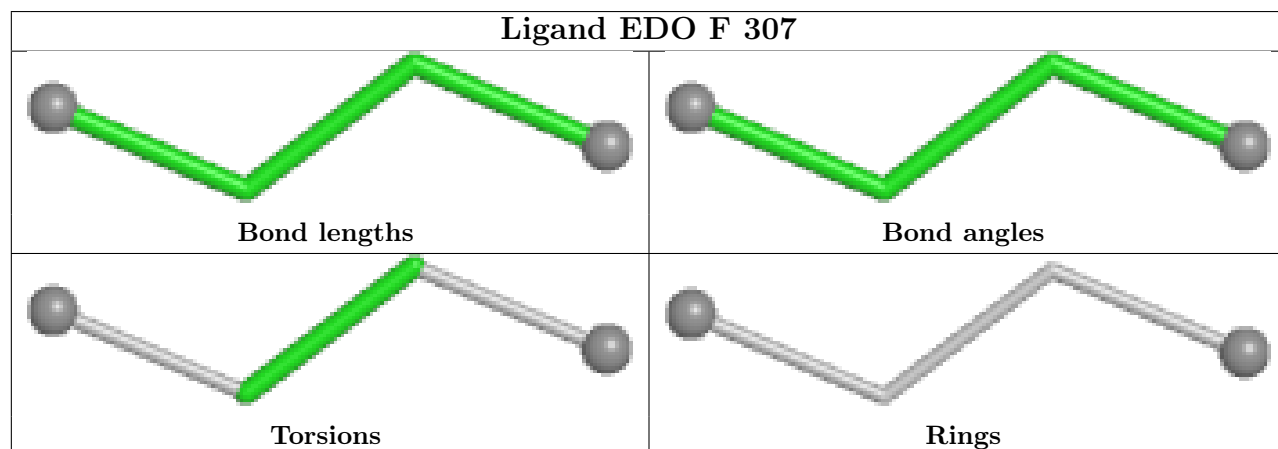
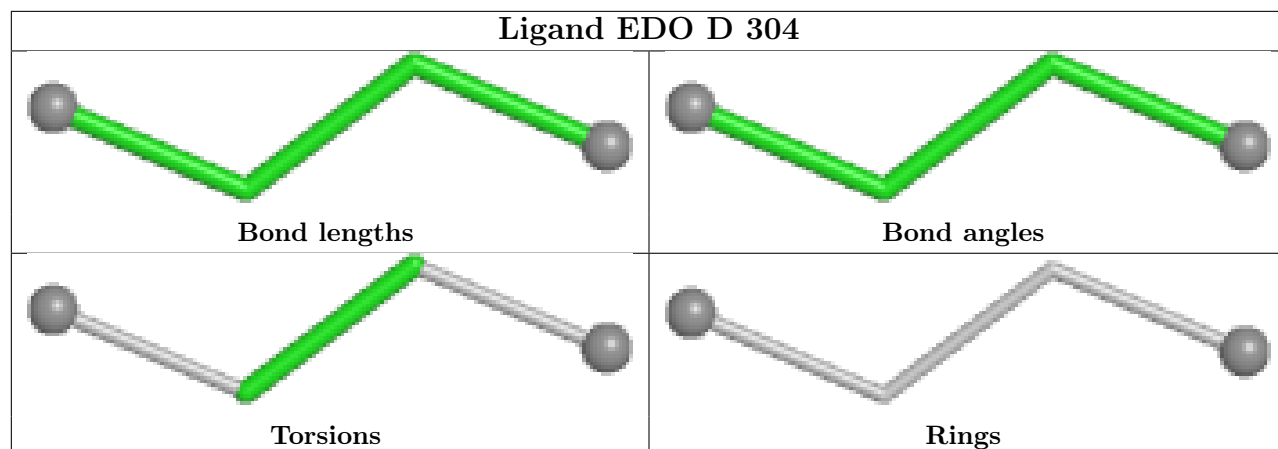


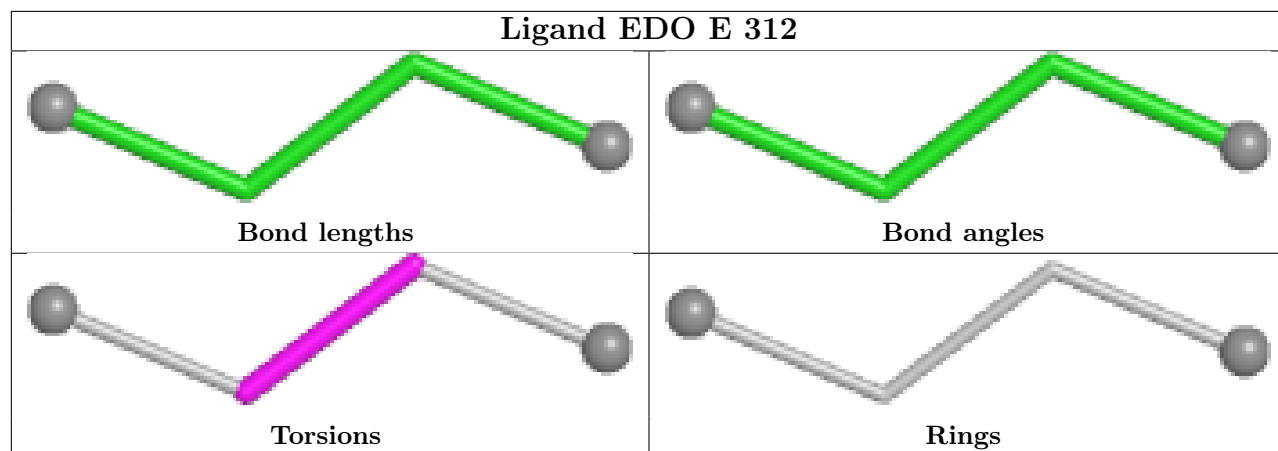


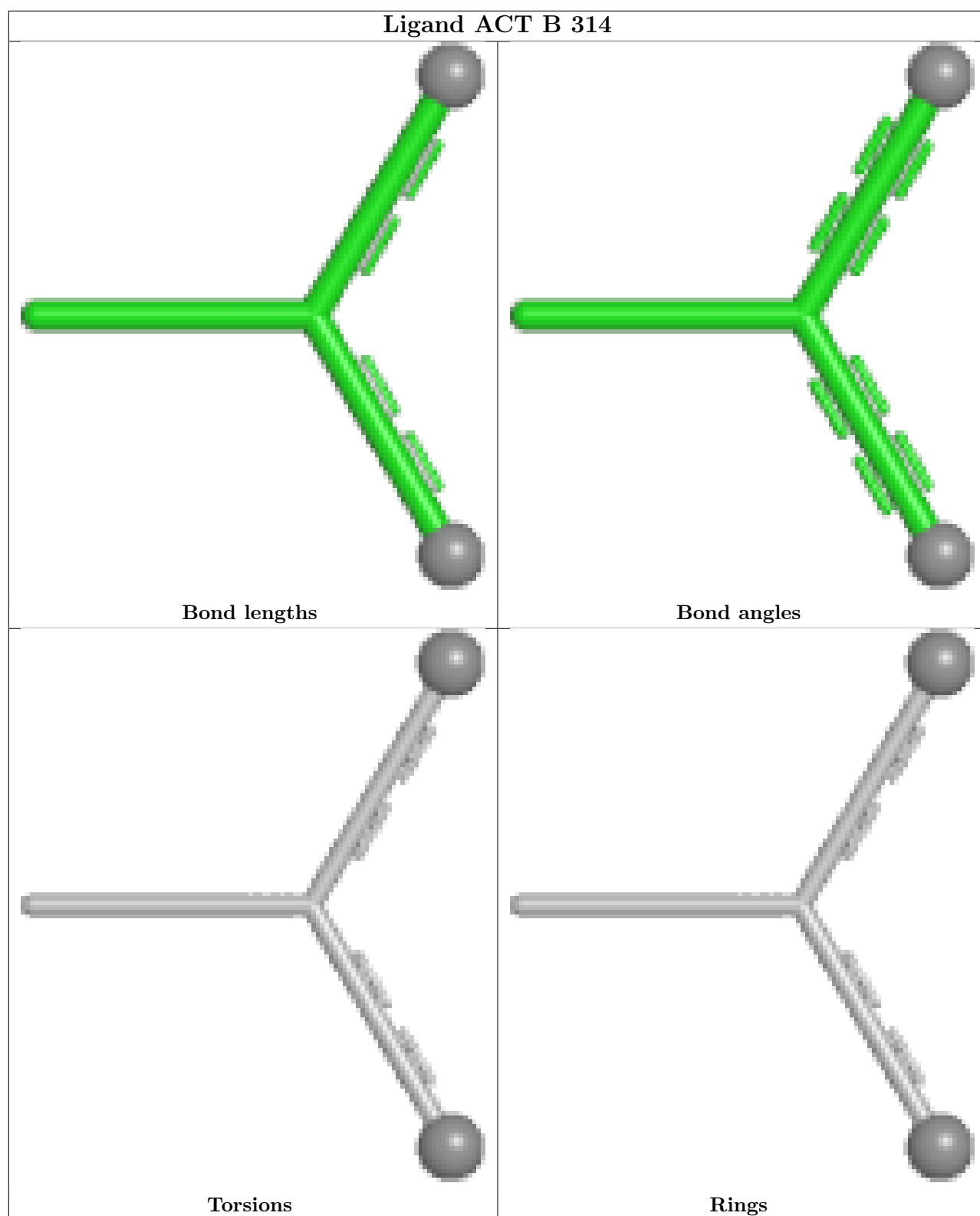


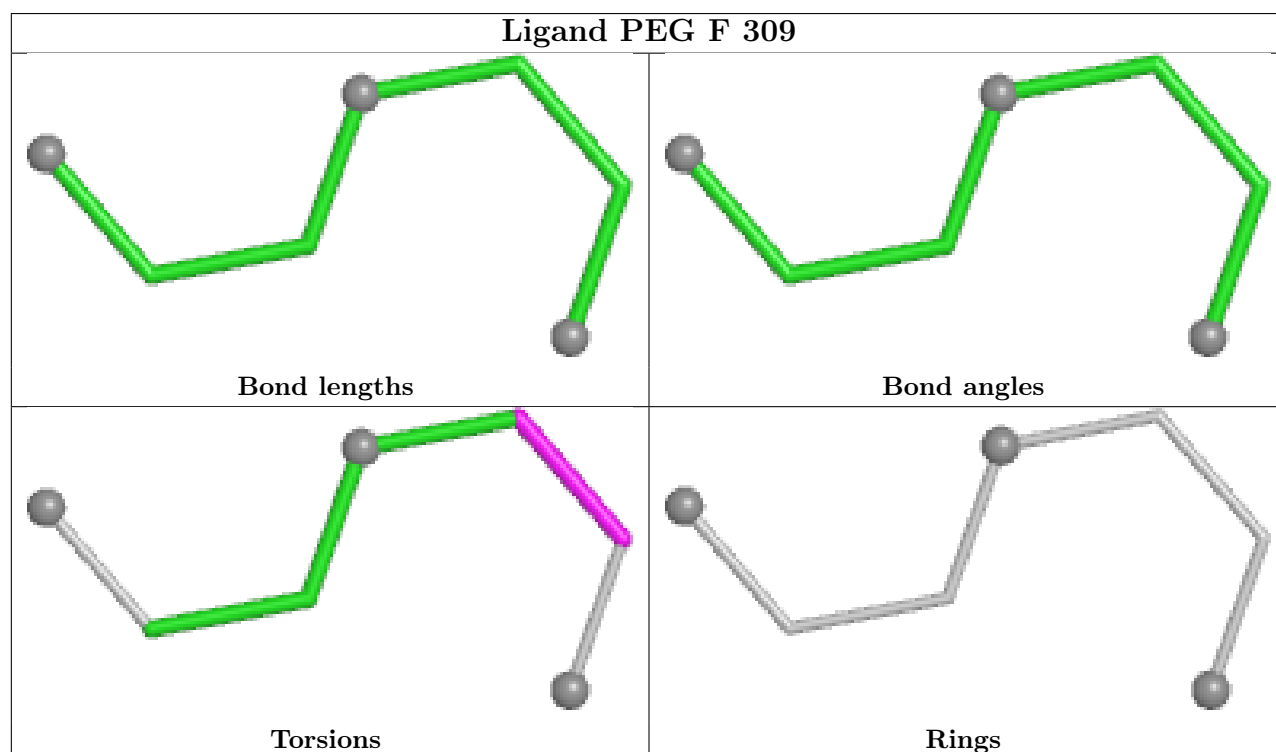
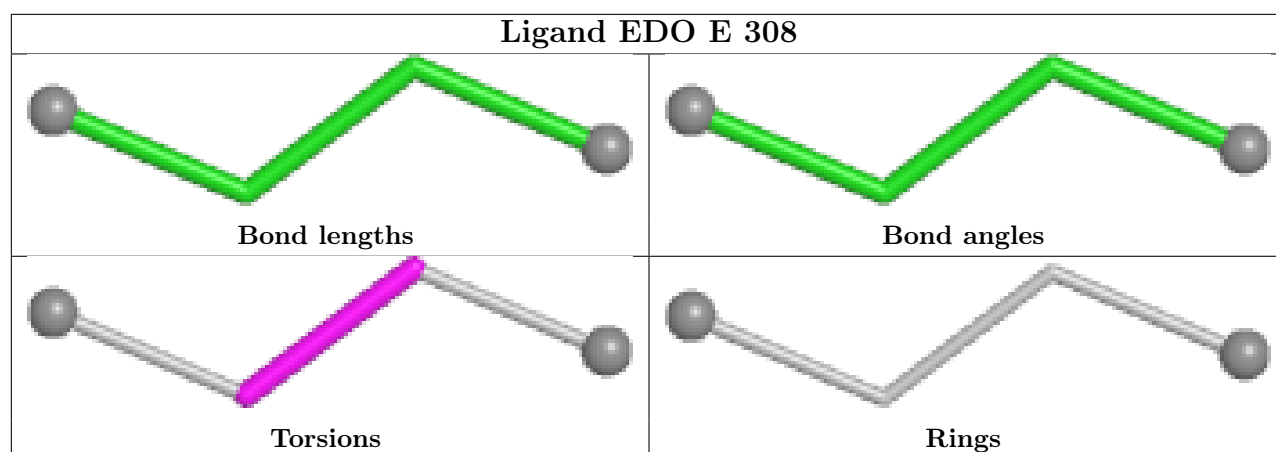


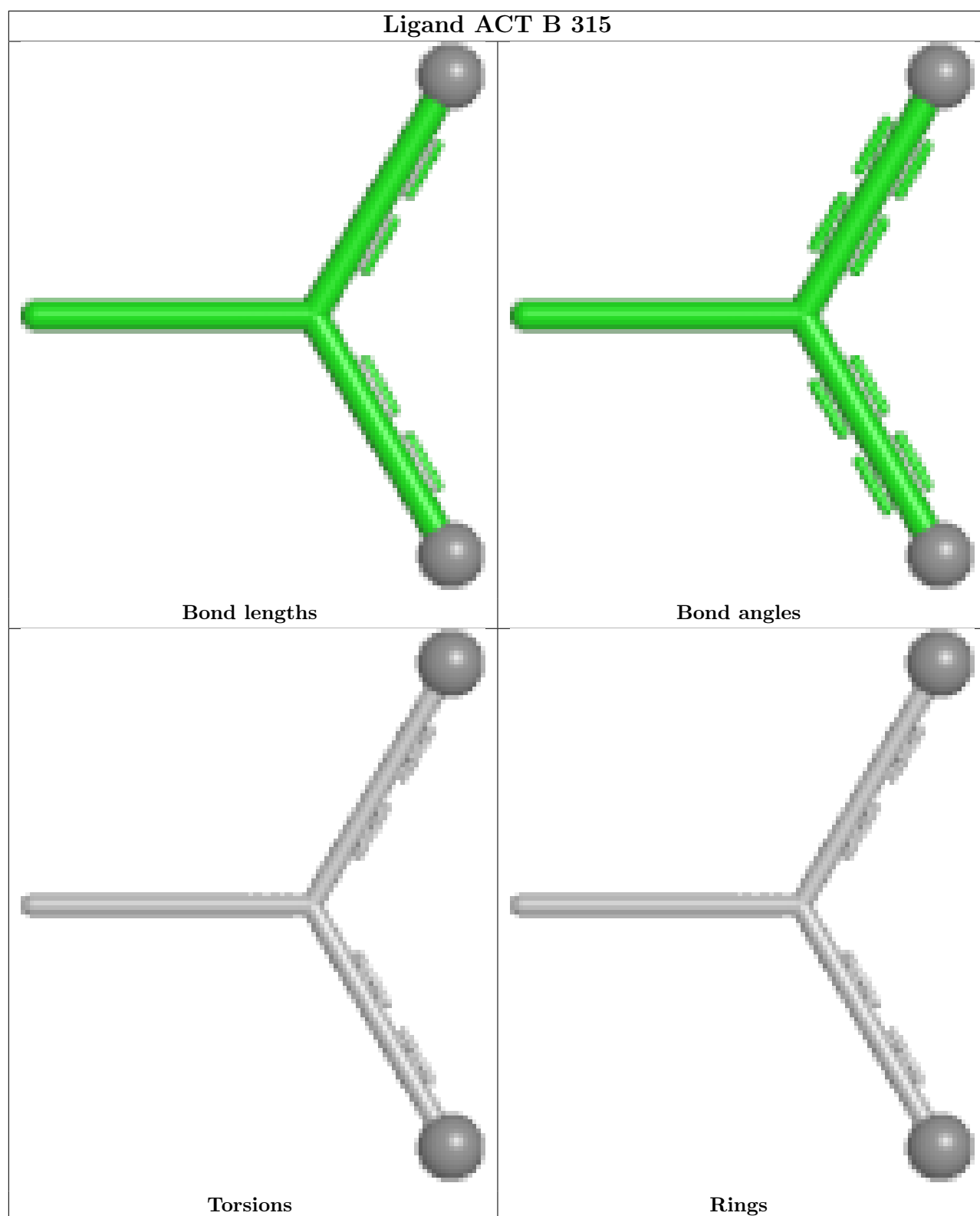


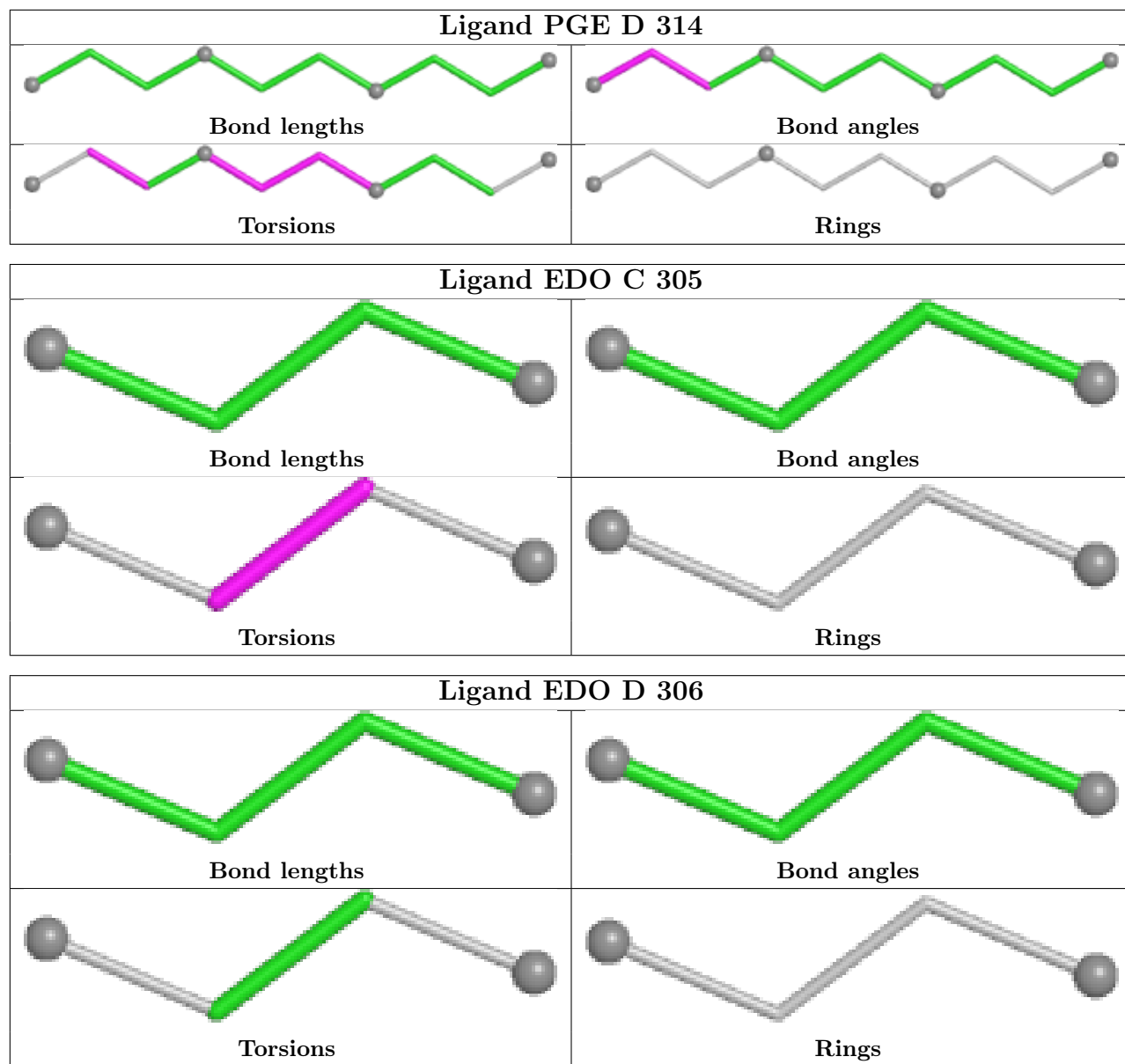


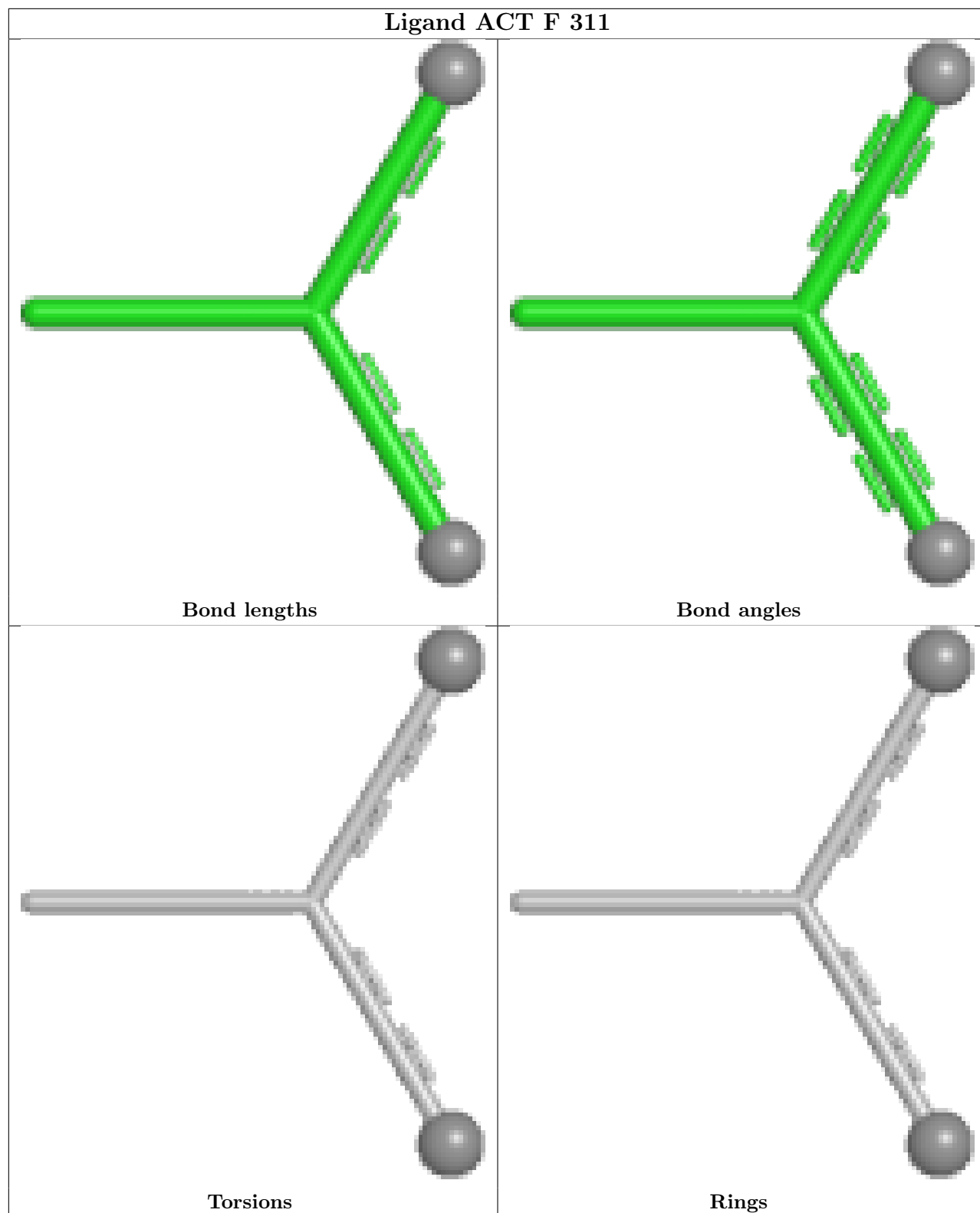


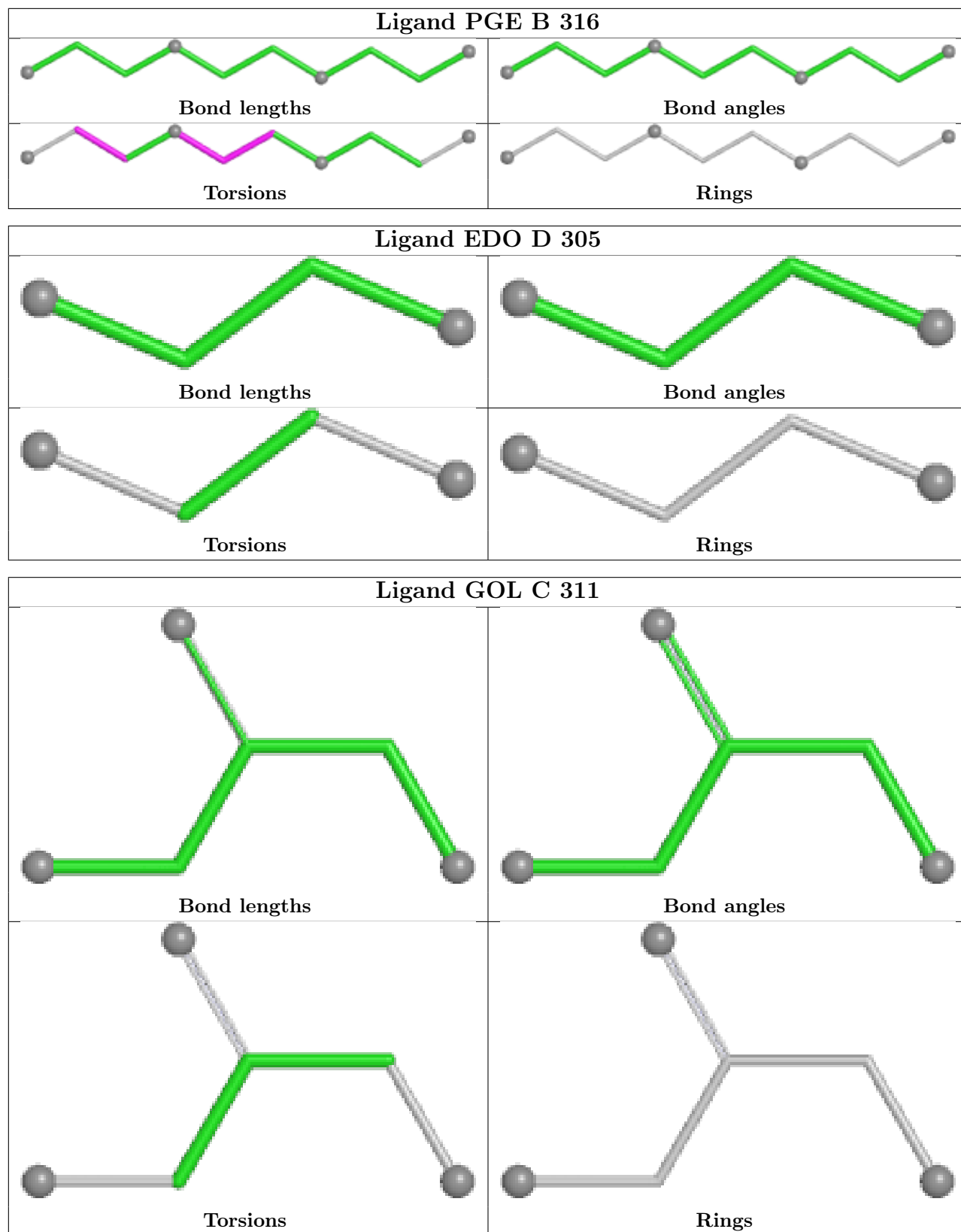


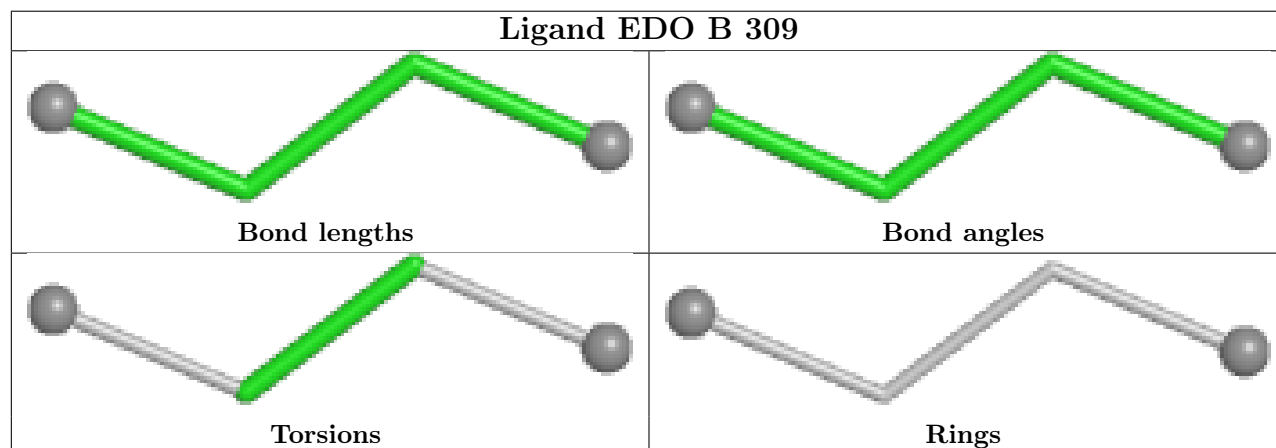
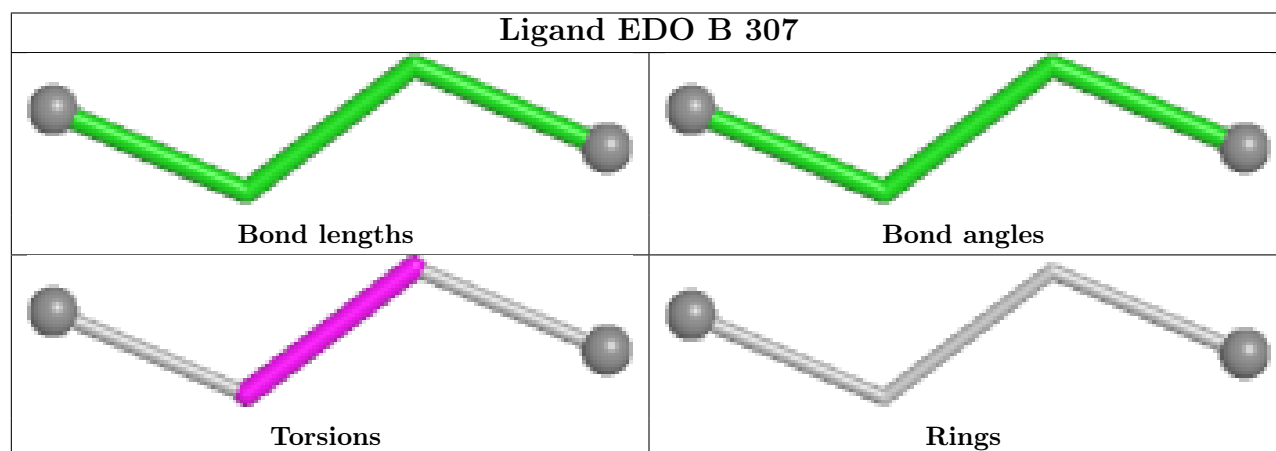
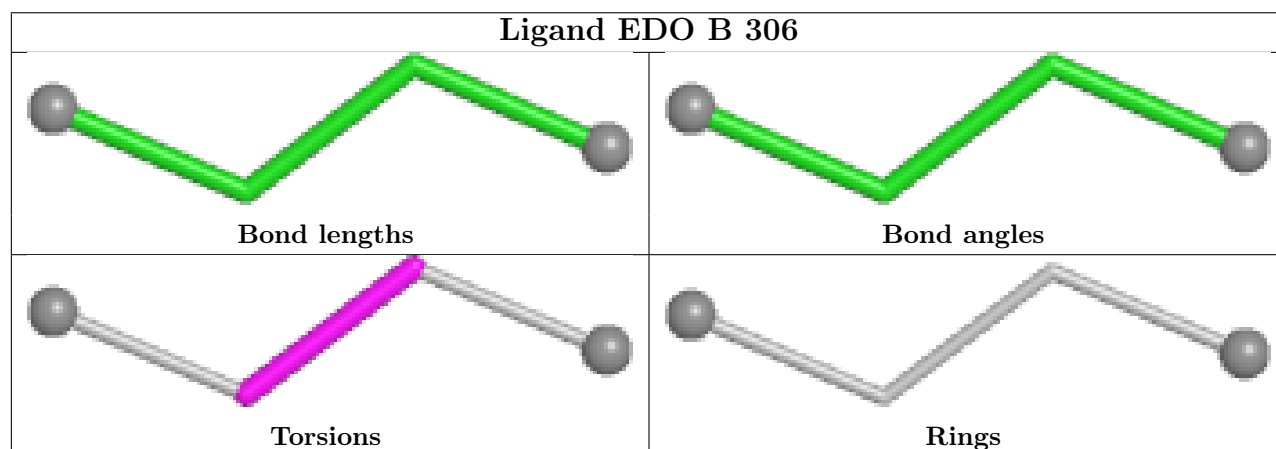
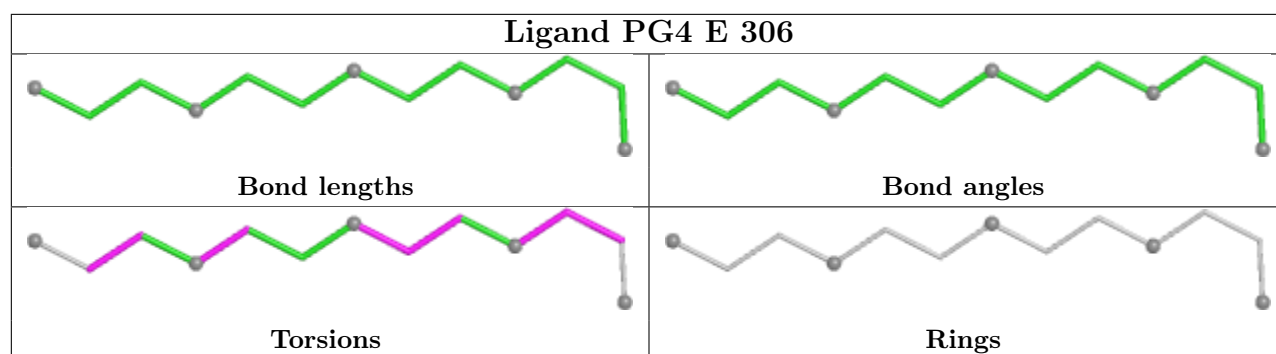


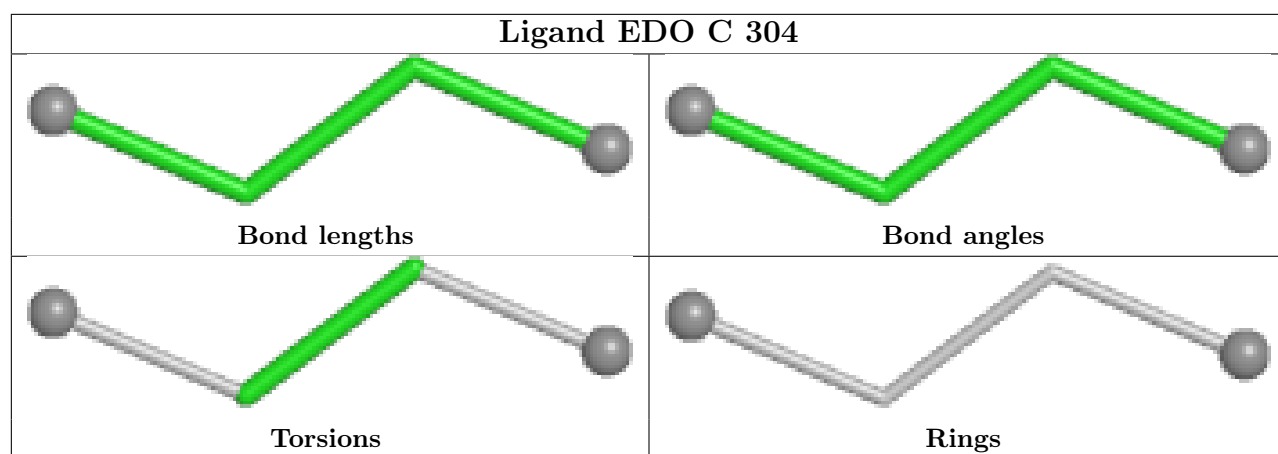


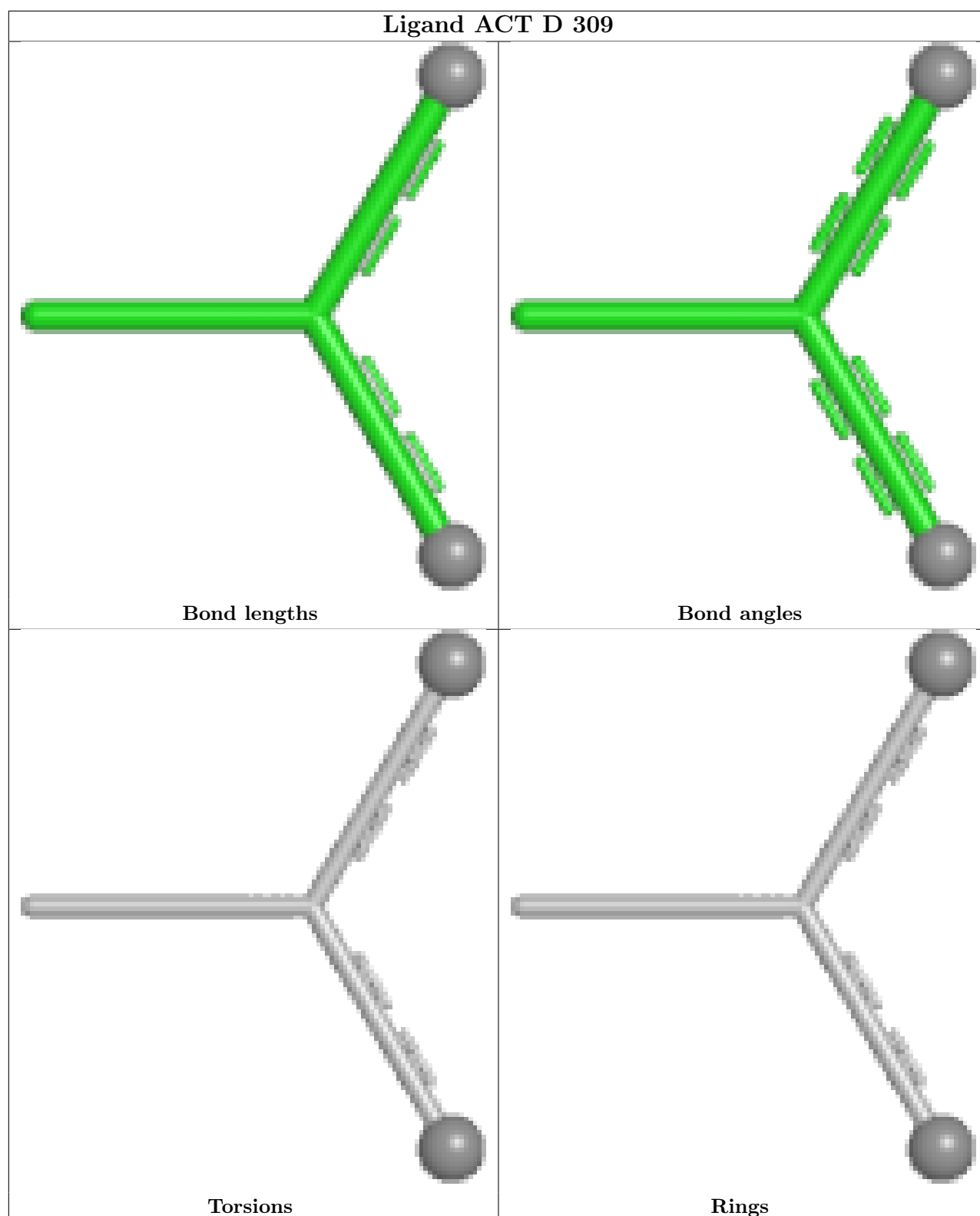


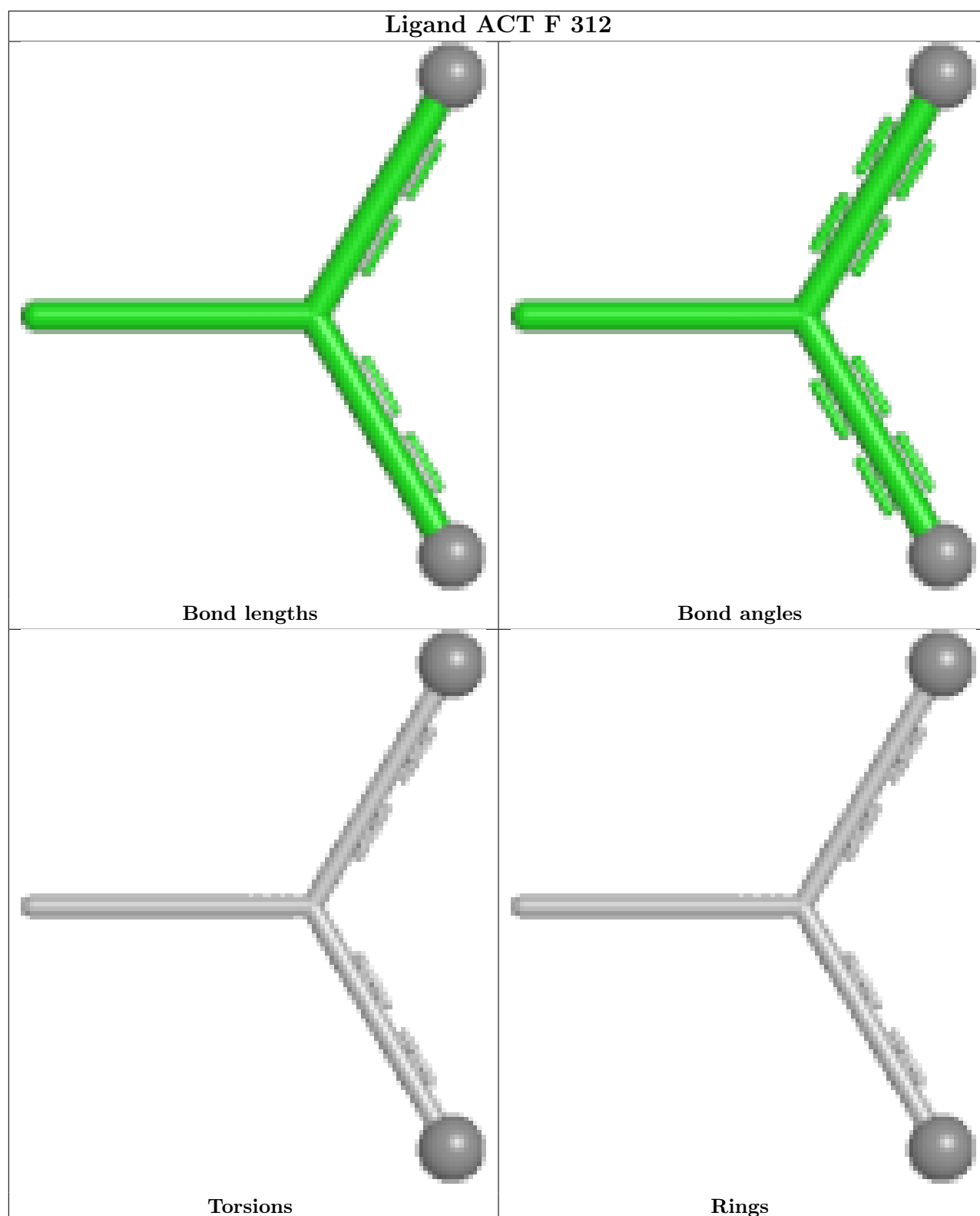


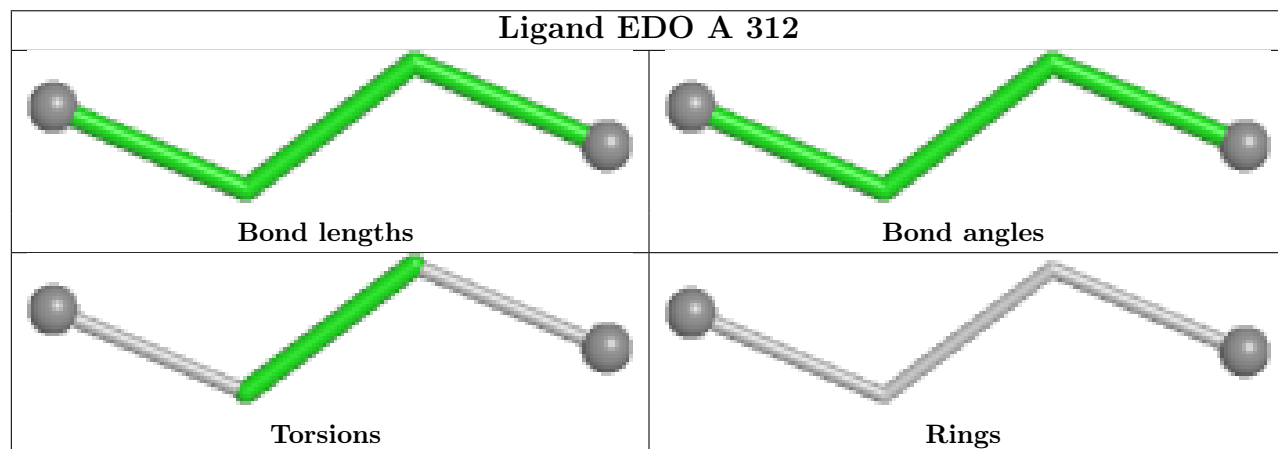
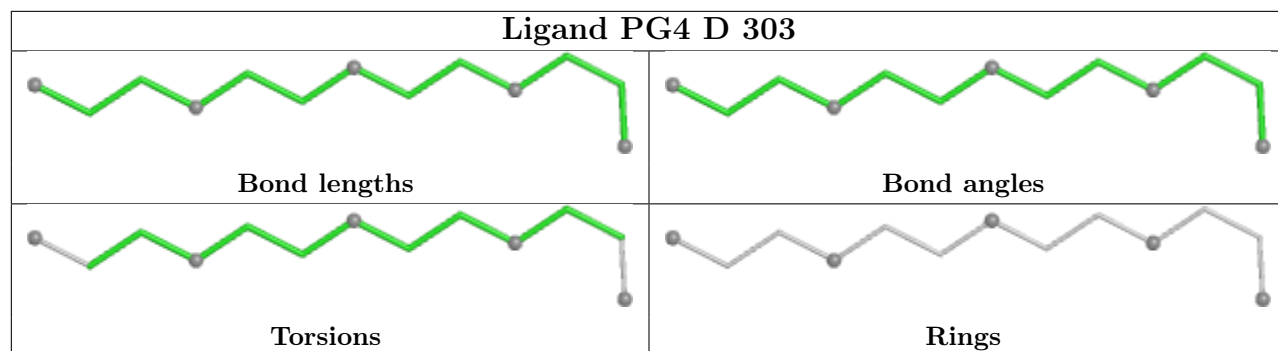


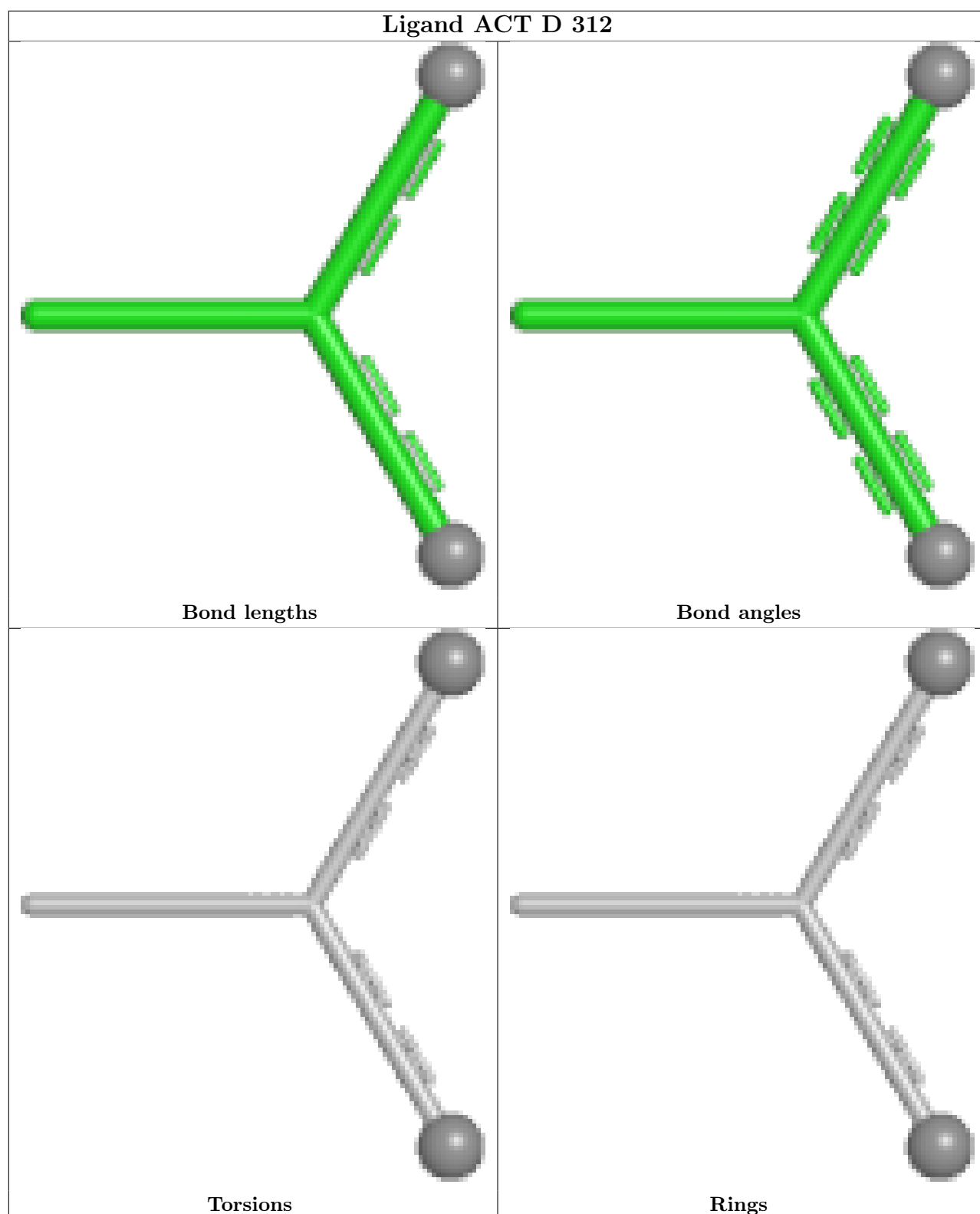


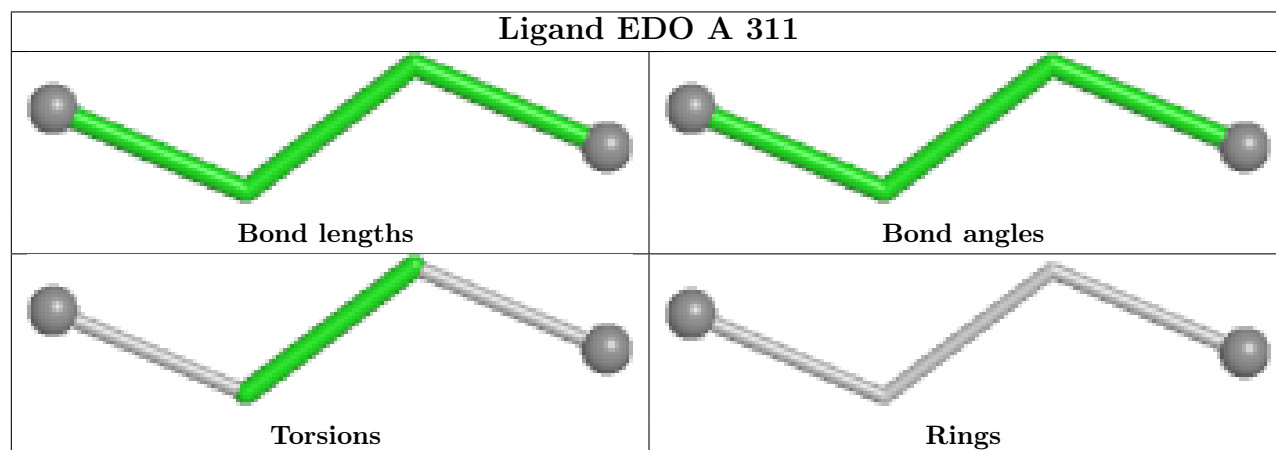
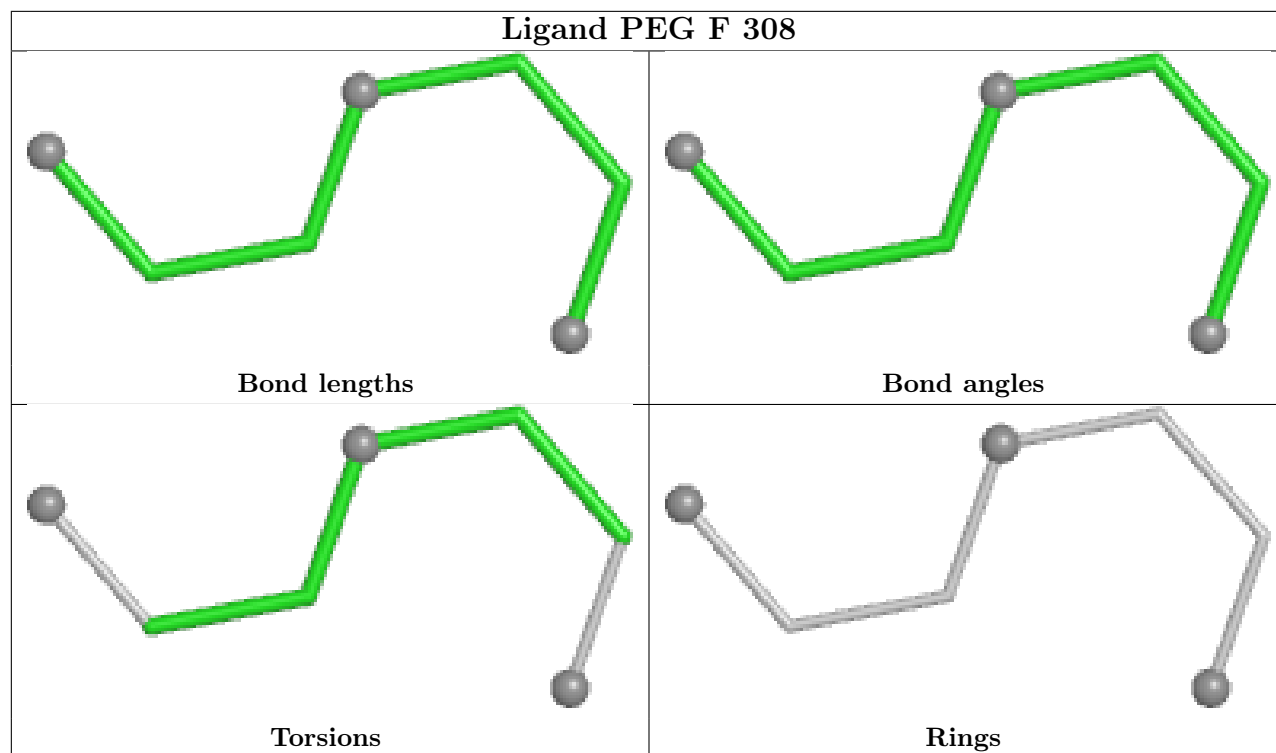


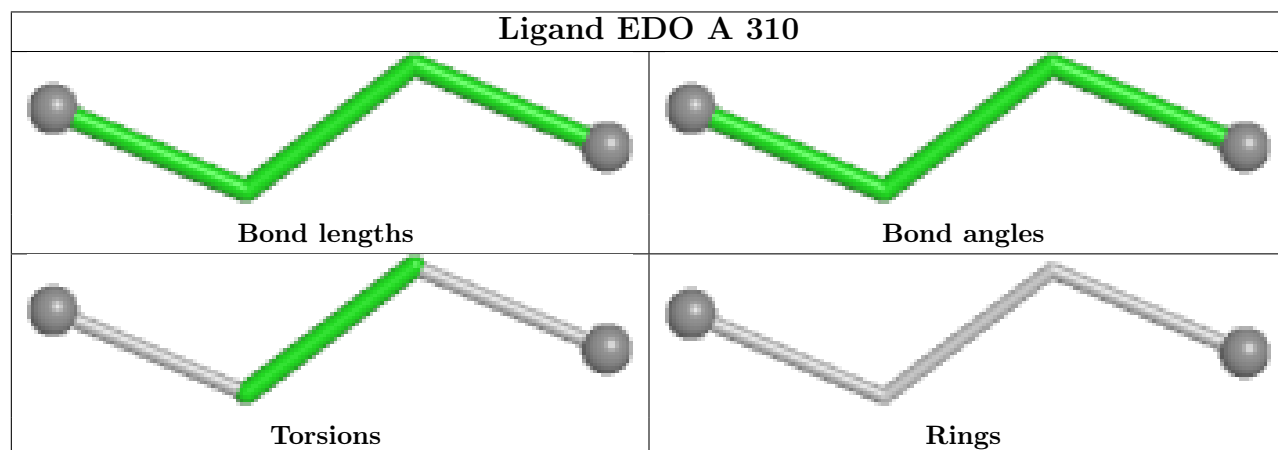
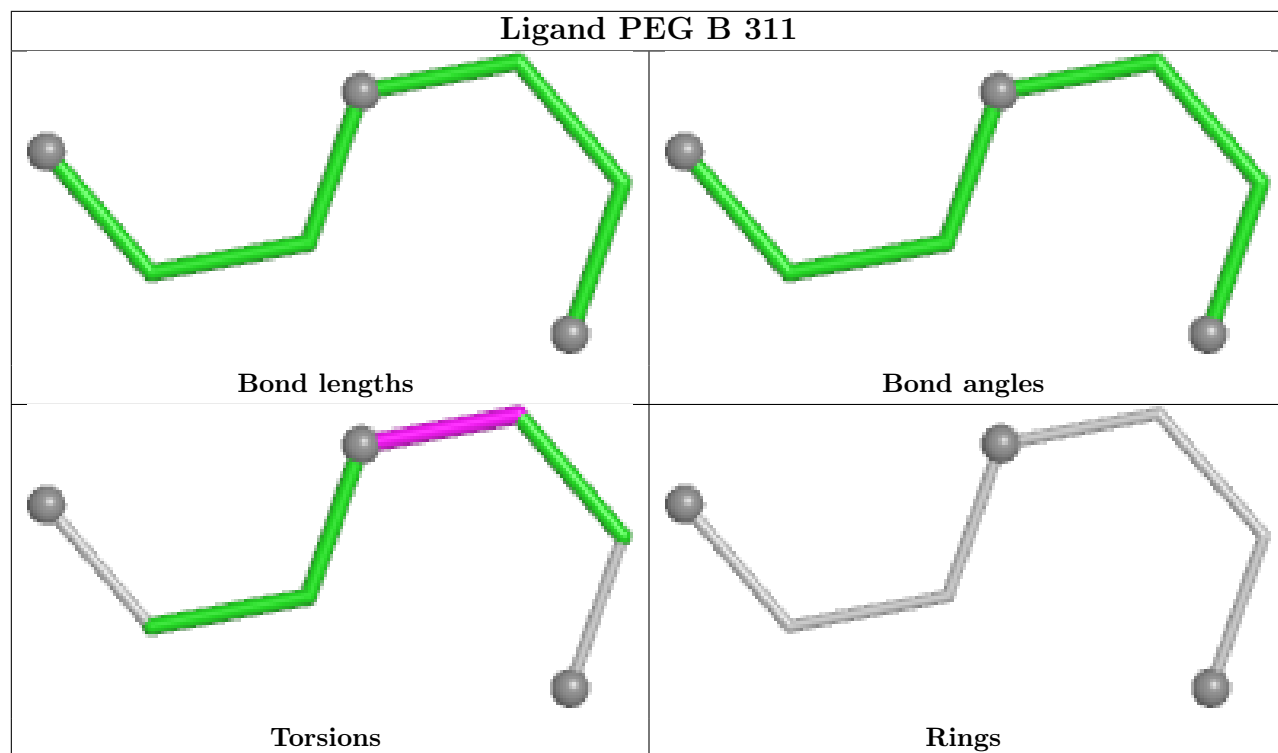


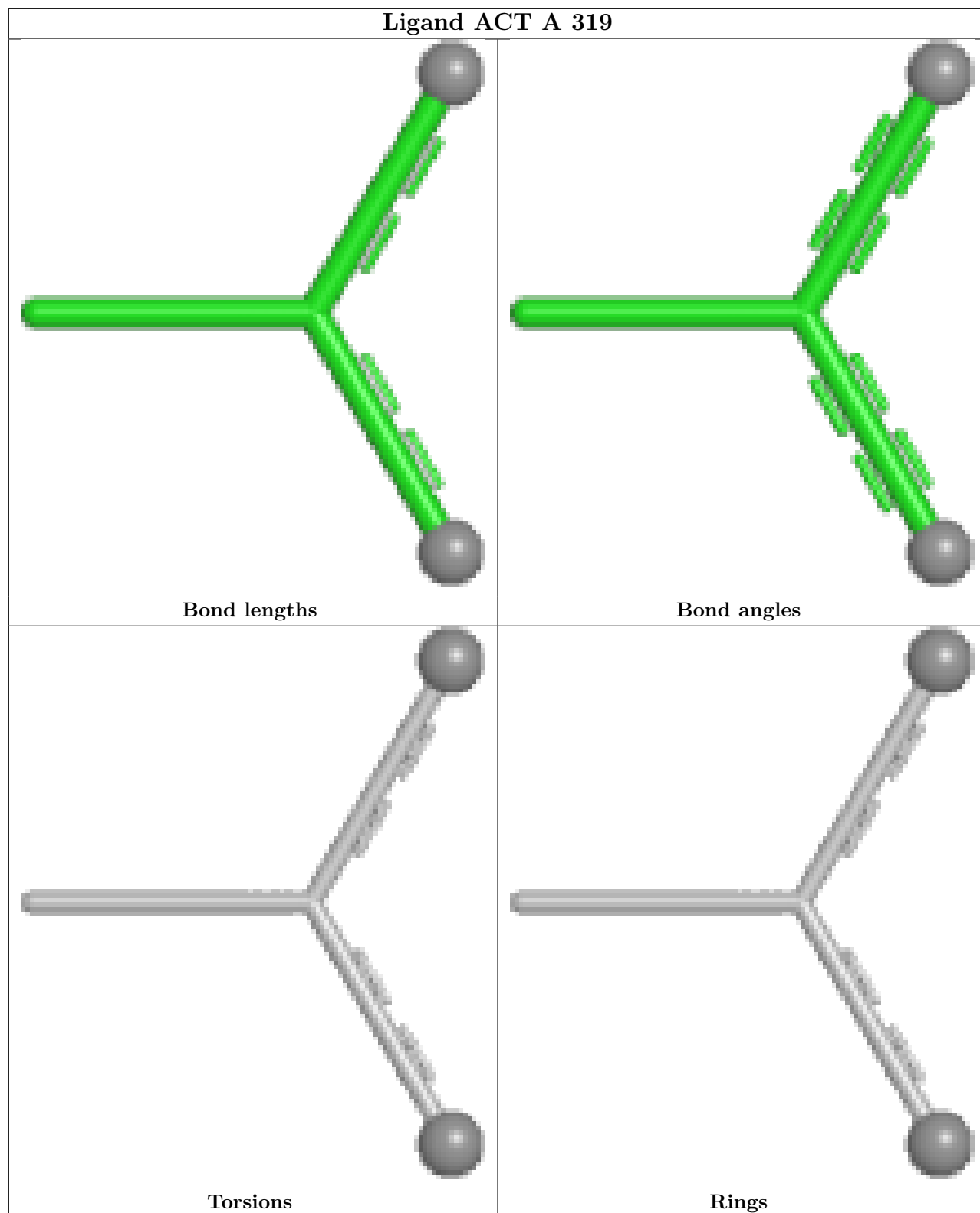


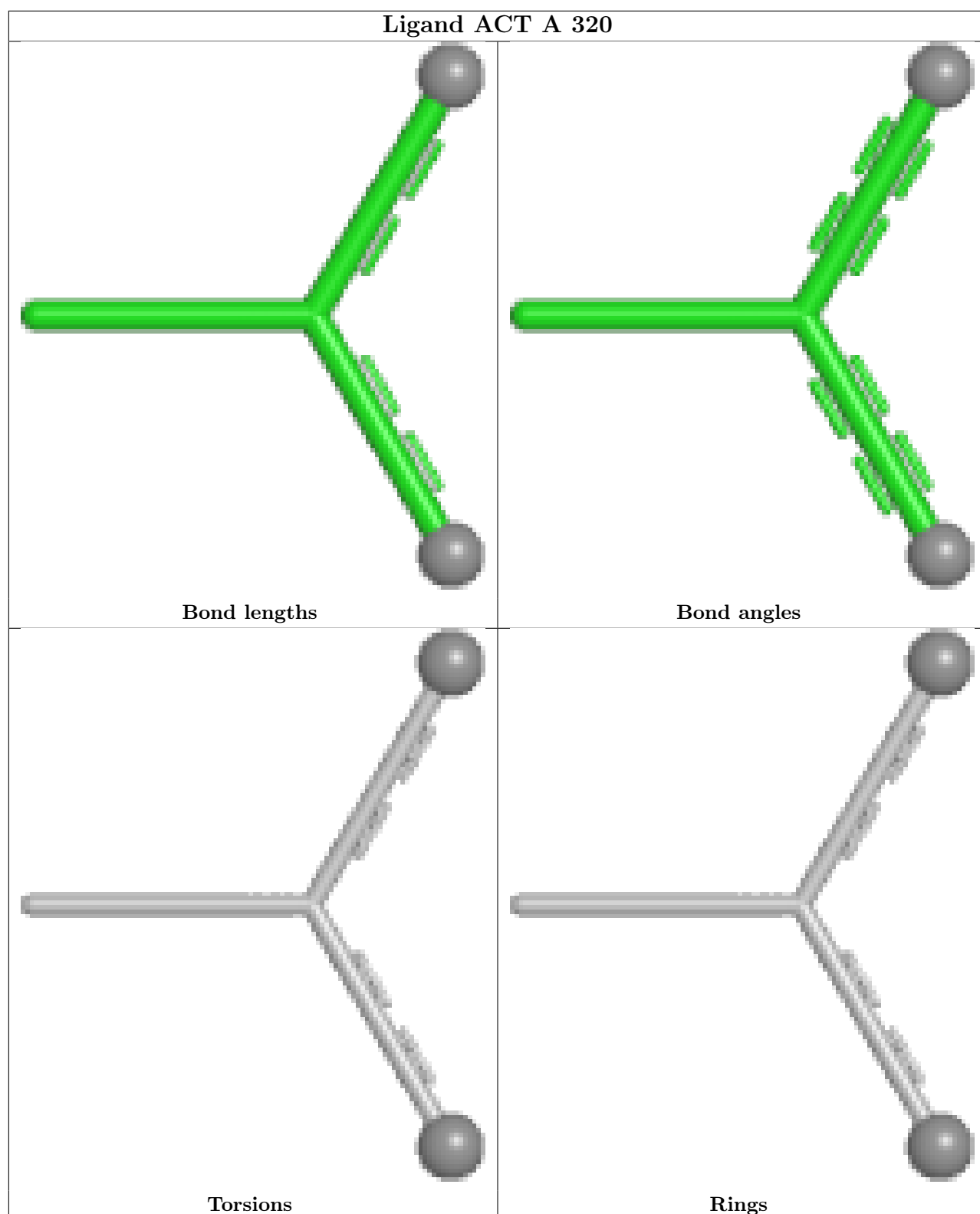


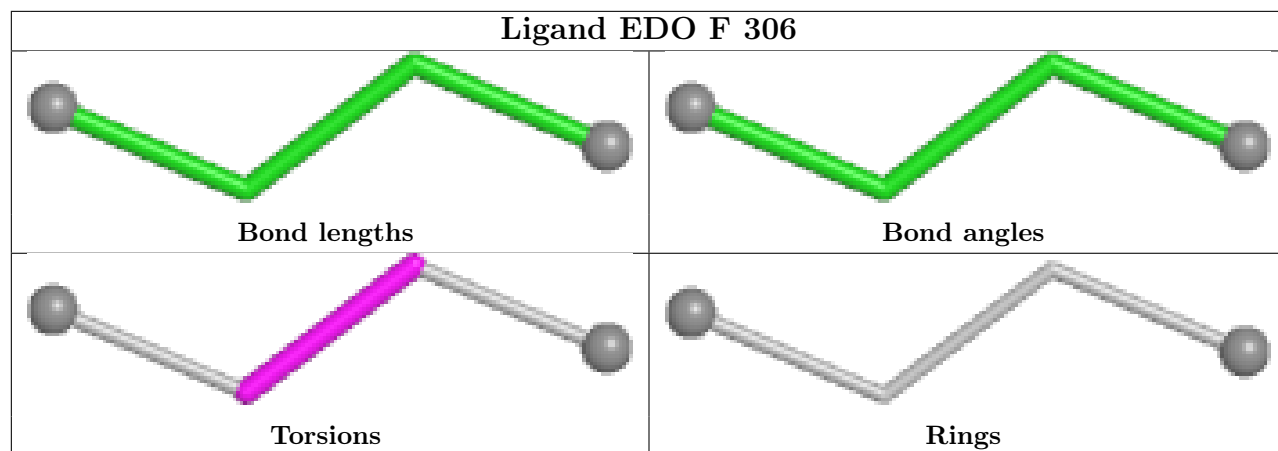


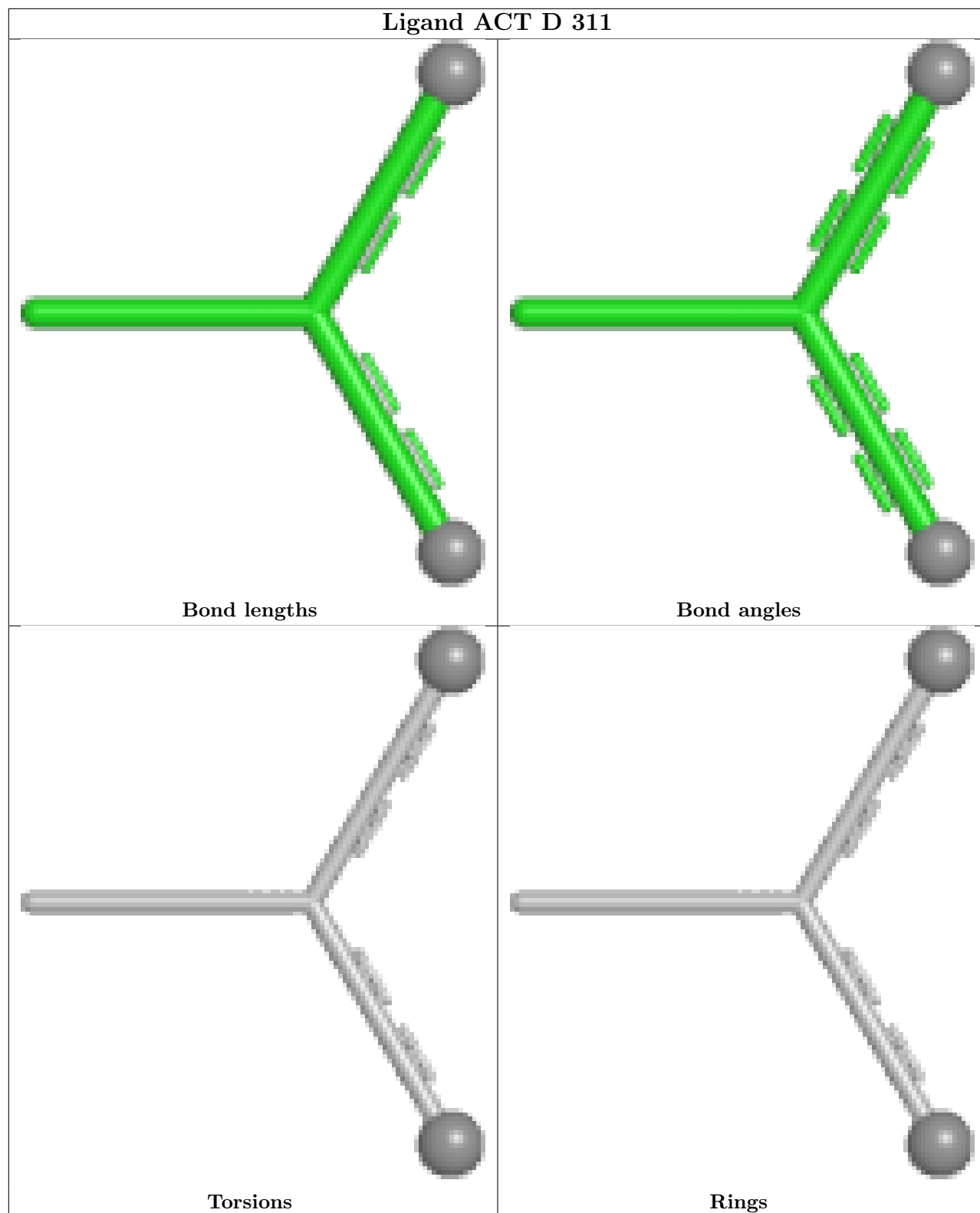


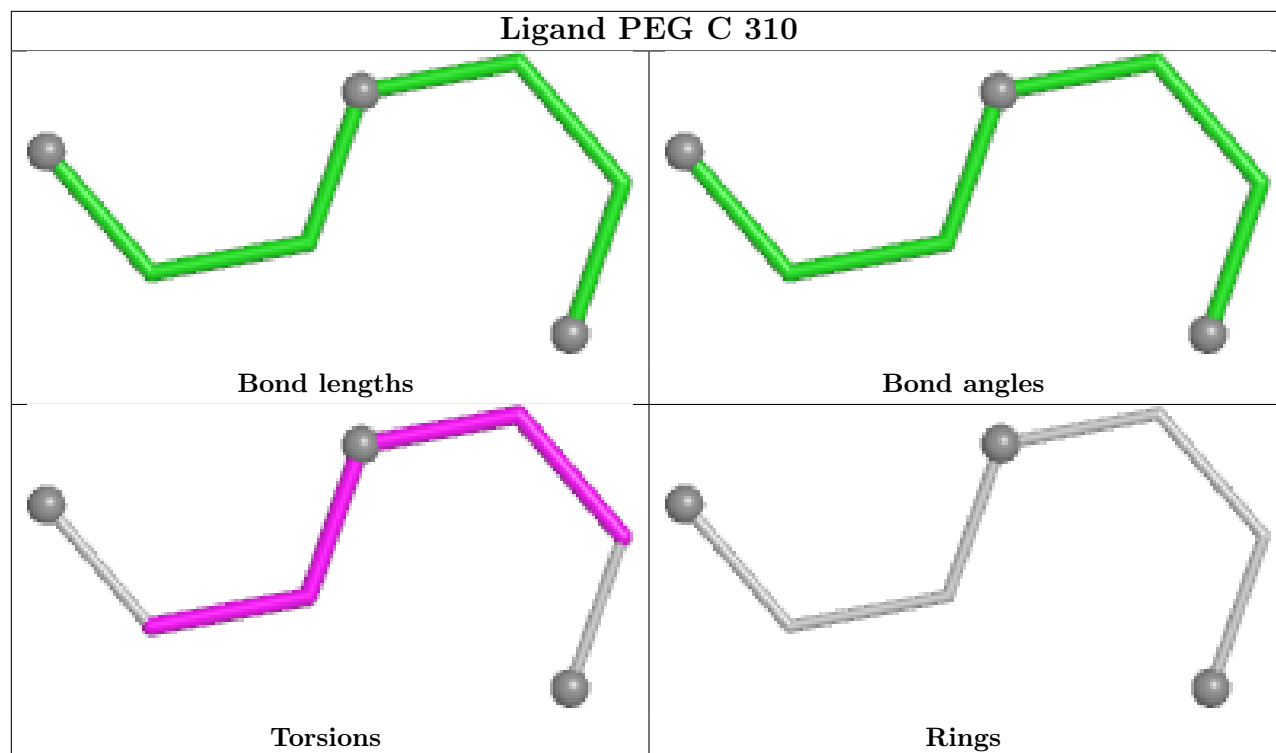












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	295/310 (95%)	-0.44	0 100 100	12, 18, 30, 46	1 (0%)
1	B	303/310 (97%)	-0.31	3 (0%) 79 84	14, 19, 34, 44	1 (0%)
1	C	295/310 (95%)	-0.31	0 100 100	15, 20, 34, 44	1 (0%)
1	D	303/310 (97%)	-0.32	6 (1%) 65 71	13, 19, 33, 43	2 (0%)
1	E	296/310 (95%)	-0.43	1 (0%) 90 92	14, 18, 31, 45	1 (0%)
1	F	295/310 (95%)	-0.31	1 (0%) 90 92	15, 20, 34, 47	0
All	All	1787/1860 (96%)	-0.35	11 (0%) 85 89	12, 19, 33, 47	6 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	95[A]	PHE	3.6
1	D	56	TRP	2.9
1	D	99	HIS	2.8
1	D	131	ASP	2.7
1	B	2	ASP	2.5
1	F	72	GLY	2.4
1	D	74	LYS	2.4
1	E	2	ASP	2.3
1	B	129	SER	2.3
1	B	131	ASP	2.2
1	D	130	VAL	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KPI	C	166	14/15	0.71	0.16	20,20,20,20	0
1	KPI	A	166	14/15	0.73	0.16	20,20,20,20	0
1	KPI	D	166	14/15	0.76	0.16	20,20,20,20	0
1	KPI	E	166	14/15	0.76	0.14	20,20,20,20	0
1	KPI	F	166	14/15	0.77	0.14	20,20,20,20	0
1	KPI	B	166	14/15	0.79	0.14	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ACT	F	312	4/4	0.63	0.18	37,44,47,49	0
7	ACT	F	313	4/4	0.68	0.16	38,48,52,54	0
7	ACT	D	309	4/4	0.70	0.22	40,40,42,46	0
7	ACT	D	310	4/4	0.70	0.19	36,40,42,44	0
5	EDO	B	306	4/4	0.72	0.29	27,34,36,48	0
5	EDO	A	315	4/4	0.73	0.16	34,38,39,51	0
7	ACT	E	314	4/4	0.73	0.17	33,36,47,50	0
7	ACT	D	311	4/4	0.74	0.18	34,37,44,51	0
7	ACT	A	320	4/4	0.74	0.18	36,42,49,52	0
8	PGE	D	313	10/10	0.74	0.16	40,45,48,51	0
5	EDO	A	311	4/4	0.75	0.16	39,40,47,52	0
5	EDO	E	312	4/4	0.75	0.15	38,43,45,48	0
9	GOL	C	311	6/6	0.76	0.16	30,34,36,49	0
7	ACT	B	315	4/4	0.77	0.18	36,39,43,44	0
5	EDO	F	306	4/4	0.77	0.16	32,35,38,45	0
7	ACT	B	314	4/4	0.77	0.17	40,44,46,52	0
5	EDO	D	305	4/4	0.78	0.18	27,31,33,48	0
8	PGE	E	315	10/10	0.78	0.16	31,36,41,55	0
7	ACT	F	311	4/4	0.78	0.18	33,40,47,51	0
6	PEG	B	313	7/7	0.79	0.14	32,34,43,52	0
6	PEG	E	313	7/7	0.79	0.15	25,31,45,48	0
5	EDO	C	306	4/4	0.79	0.14	38,38,38,39	0
5	EDO	B	310	4/4	0.80	0.23	24,30,36,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	A	318	7/7	0.81	0.14	37,41,45,51	0
8	PGE	B	316	10/10	0.82	0.16	24,46,58,62	0
6	PEG	B	312	7/7	0.82	0.14	29,36,48,50	0
6	PEG	F	309	7/7	0.82	0.14	40,46,53,64	0
5	EDO	B	309	4/4	0.82	0.15	37,42,48,49	0
7	ACT	A	319	4/4	0.83	0.16	20,39,43,44	0
8	PGE	D	314	10/10	0.83	0.15	22,34,39,46	0
6	PEG	F	308	7/7	0.83	0.14	33,38,47,47	0
5	EDO	A	316	4/4	0.83	0.14	39,43,47,52	0
7	ACT	D	312	4/4	0.84	0.13	42,43,47,47	0
5	EDO	A	307	4/4	0.84	0.12	29,31,37,38	0
3	MG	A	305	1/1	0.84	0.23	53,53,53,53	0
3	MG	E	304	1/1	0.84	0.14	49,49,49,49	0
4	PG4	E	306	13/13	0.84	0.14	24,36,50,51	0
5	EDO	E	310	4/4	0.85	0.13	33,36,44,44	0
5	EDO	B	307	4/4	0.85	0.14	39,40,40,43	0
5	EDO	E	309	4/4	0.86	0.14	34,40,42,45	0
6	PEG	B	311	7/7	0.86	0.12	31,39,47,48	0
5	EDO	A	310	4/4	0.86	0.14	39,41,46,46	0
3	MG	B	304	1/1	0.87	0.23	50,50,50,50	0
5	EDO	E	308	4/4	0.87	0.13	26,30,30,31	0
5	EDO	C	309	4/4	0.87	0.12	33,41,43,50	0
5	EDO	C	304	4/4	0.88	0.13	35,37,38,43	0
3	MG	E	305	1/1	0.88	0.10	41,41,41,41	0
6	PEG	C	310	7/7	0.88	0.10	31,41,46,50	0
6	PEG	D	308	7/7	0.88	0.12	29,31,43,43	0
5	EDO	C	307	4/4	0.88	0.13	29,35,36,55	0
5	EDO	A	313	4/4	0.88	0.12	26,26,34,36	0
5	EDO	A	308	4/4	0.89	0.14	22,30,35,36	0
4	PG4	F	305	13/13	0.89	0.11	27,32,51,51	0
5	EDO	E	307	4/4	0.89	0.11	38,43,46,46	0
6	PEG	A	317	7/7	0.89	0.11	28,38,44,52	0
5	EDO	B	308	4/4	0.89	0.12	23,31,37,37	0
3	MG	F	304	1/1	0.89	0.13	47,47,47,47	1
5	EDO	C	308	4/4	0.90	0.10	35,39,40,48	0
7	ACT	F	310	4/4	0.90	0.11	35,36,41,41	0
5	EDO	D	306	4/4	0.91	0.12	24,28,31,36	0
4	PG4	D	303	13/13	0.91	0.09	25,31,44,47	0
5	EDO	A	312	4/4	0.91	0.11	30,35,39,42	0
3	MG	B	303	1/1	0.91	0.18	46,46,46,46	0
4	PG4	B	305	13/13	0.91	0.10	25,33,50,51	0
5	EDO	C	305	4/4	0.92	0.10	26,28,32,41	0

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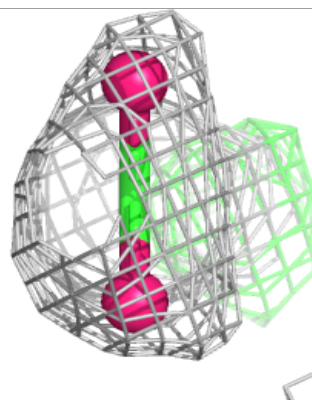
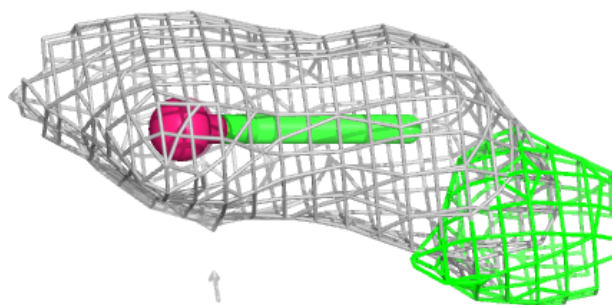
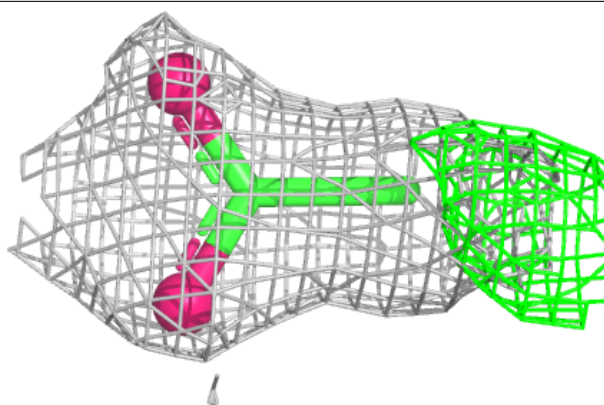
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	D	307	4/4	0.92	0.14	26,36,37,42	0
3	MG	A	302	1/1	0.92	0.08	41,41,41,41	0
5	EDO	A	309	4/4	0.92	0.09	30,32,34,40	0
4	PG4	C	303	13/13	0.93	0.10	26,33,47,48	0
5	EDO	D	304	4/4	0.95	0.07	30,31,33,35	0
3	MG	C	301	1/1	0.95	0.04	34,34,34,34	0
4	PG4	A	306	13/13	0.96	0.07	26,32,44,49	0
5	EDO	F	307	4/4	0.96	0.08	20,25,33,36	0
5	EDO	A	314	4/4	0.96	0.07	23,26,26,32	0
2	3VN	A	301	22/22	0.96	0.06	14,17,23,25	0
2	3VN	B	301	22/22	0.96	0.07	15,17,23,27	0
3	MG	F	303	1/1	0.97	0.06	34,34,34,34	0
2	3VN	D	301	22/22	0.97	0.06	14,16,23,26	0
3	MG	C	302	1/1	0.97	0.04	33,33,33,33	0
3	MG	F	302	1/1	0.97	0.06	29,29,29,29	0
3	MG	F	301	1/1	0.98	0.11	23,23,23,23	0
3	MG	E	301	1/1	0.98	0.04	28,28,28,28	0
3	MG	E	302	1/1	0.98	0.04	33,33,33,33	0
5	EDO	E	311	4/4	0.98	0.05	18,19,20,20	0
3	MG	E	303	1/1	0.98	0.05	36,36,36,36	0
3	MG	A	304	1/1	0.98	0.05	19,19,19,19	0
3	MG	D	302	1/1	0.98	0.07	30,30,30,30	0
3	MG	B	302	1/1	0.99	0.08	29,29,29,29	0
3	MG	A	303	1/1	0.99	0.07	17,17,17,17	0

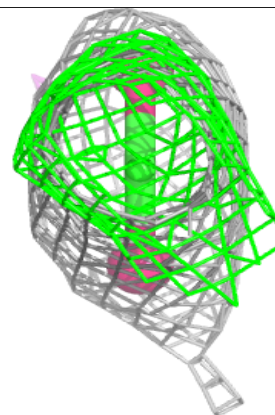
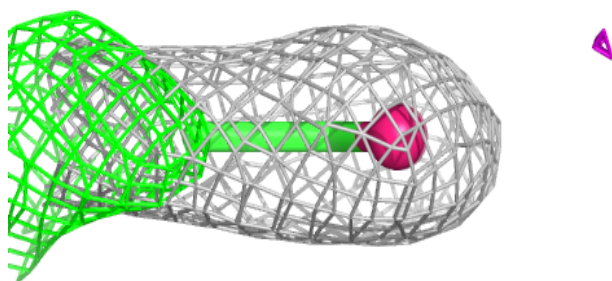
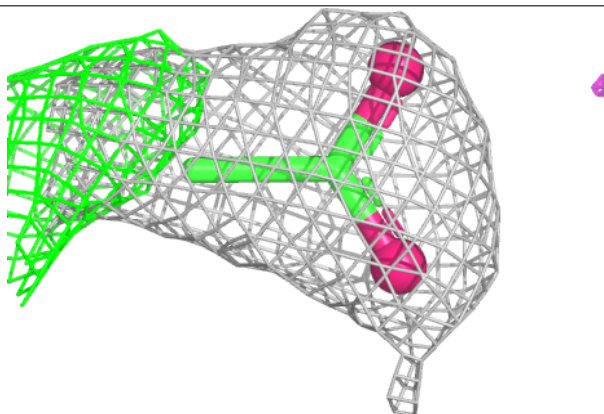
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACT F 312:

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

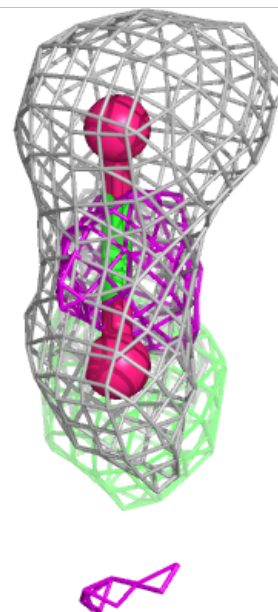
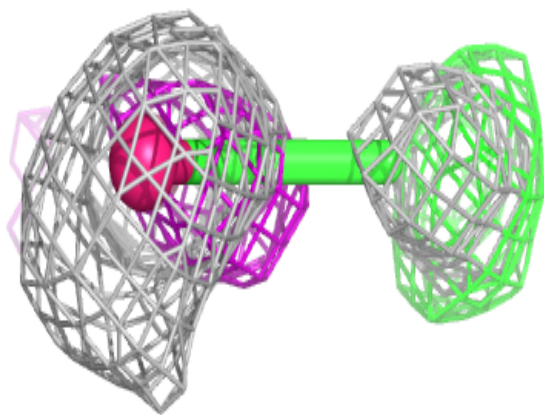
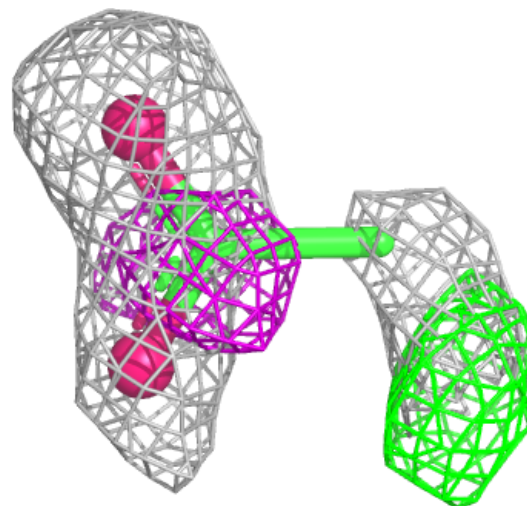
**Electron density around ACT F 313:**

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



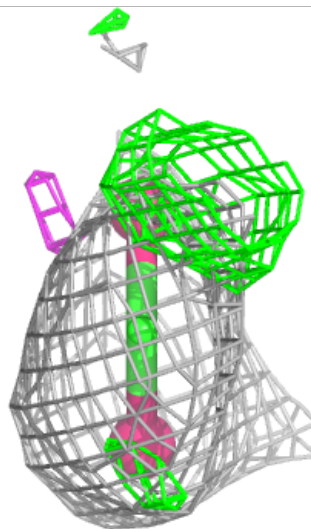
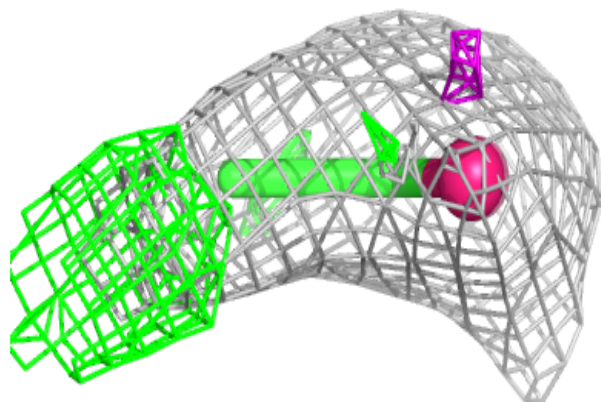
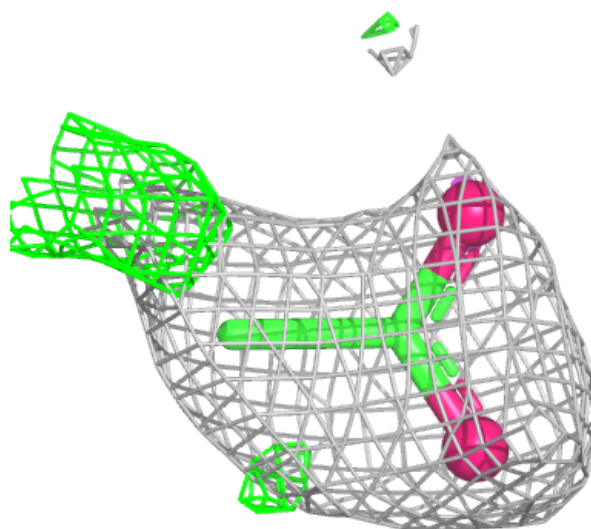
Electron density around ACT D 309:

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



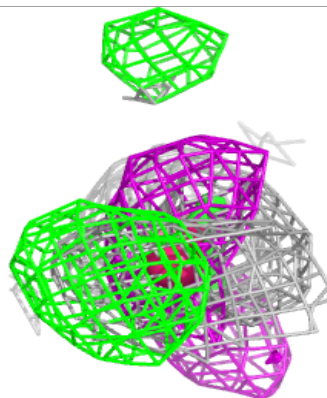
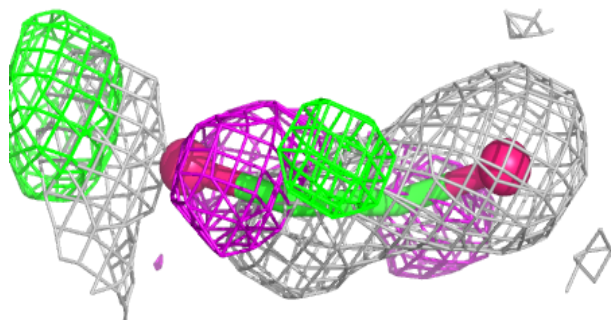
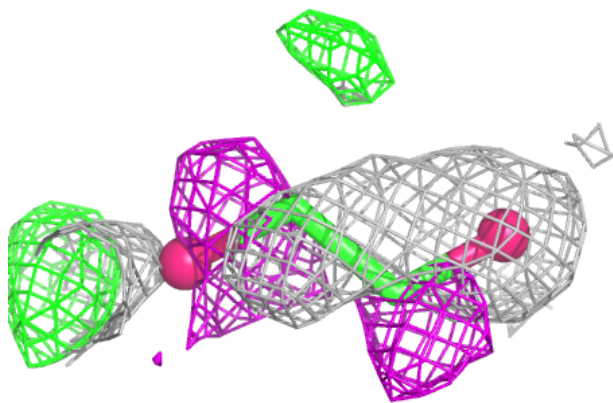
Electron density around ACT D 310:

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

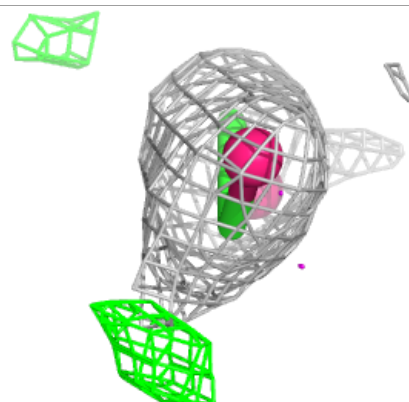
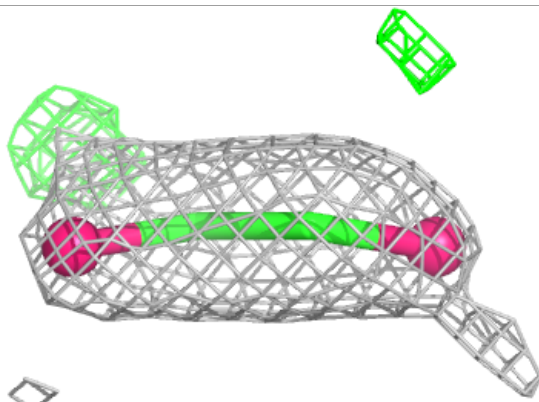
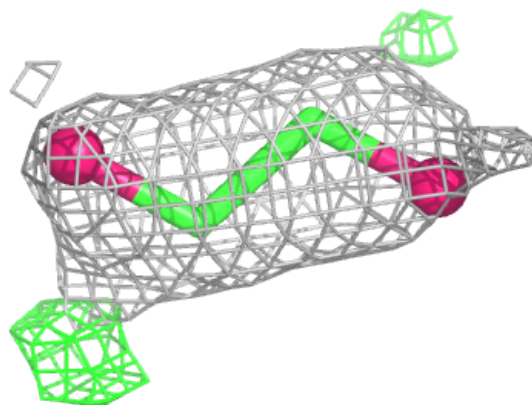


Electron density around EDO B 306:

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

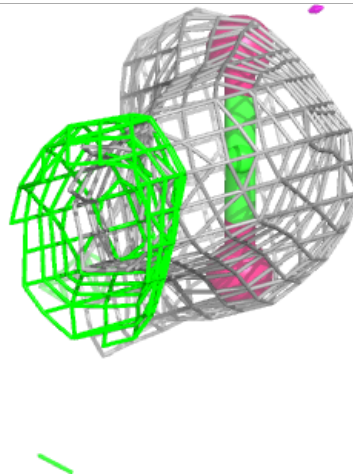
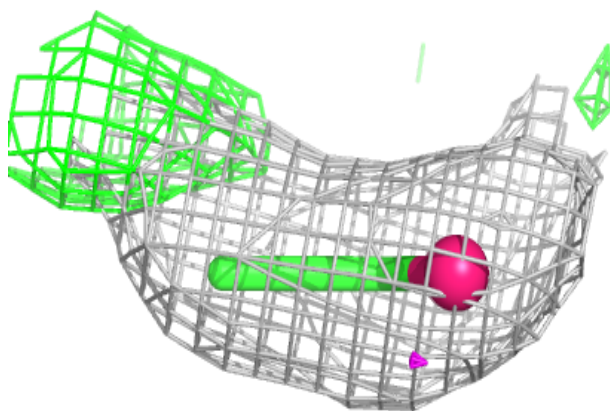
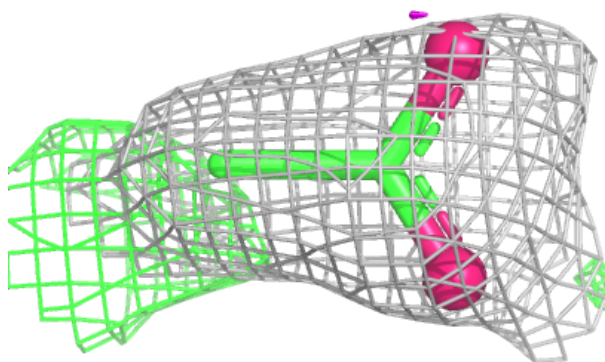
**Electron density around EDO A 315:**

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



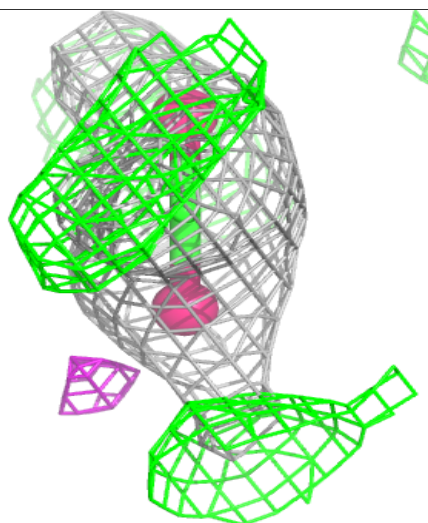
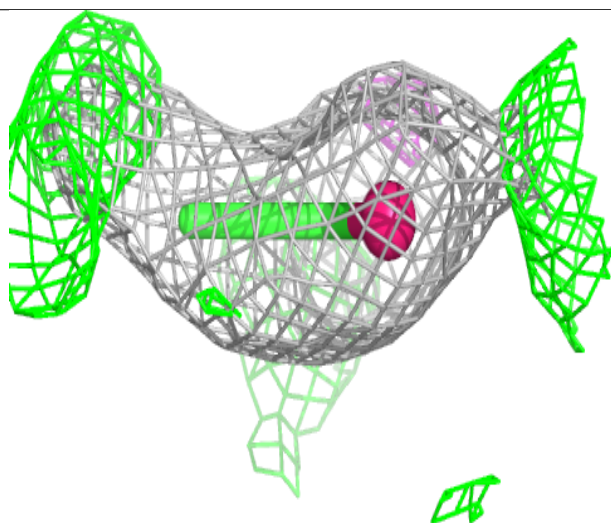
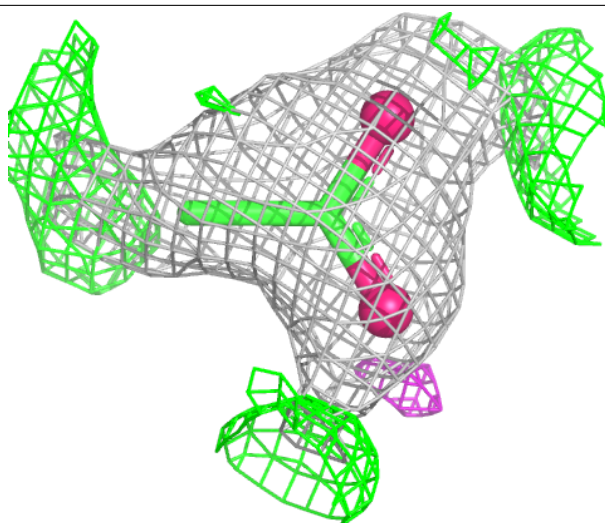
Electron density around ACT E 314:

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



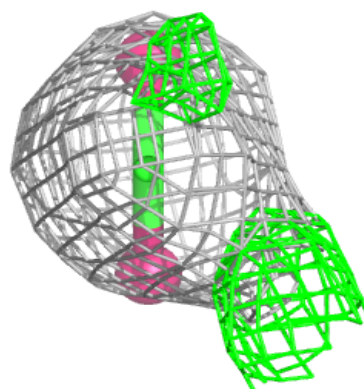
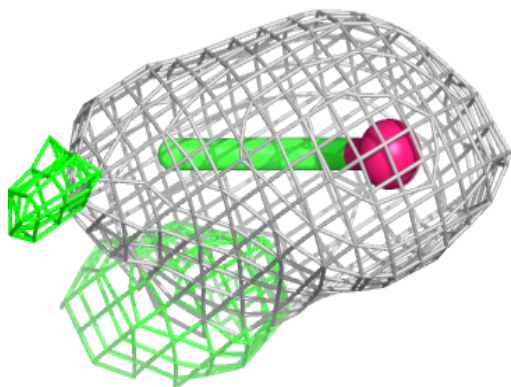
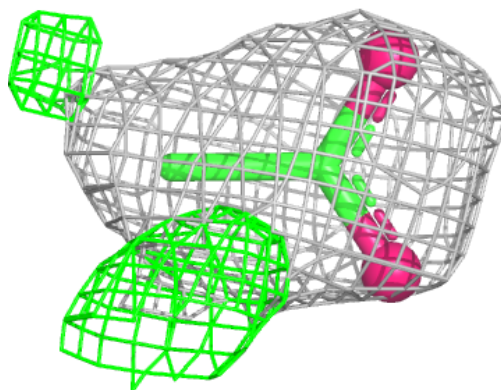
Electron density around ACT D 311:

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

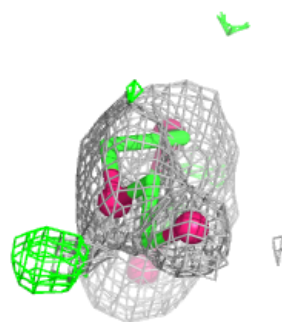
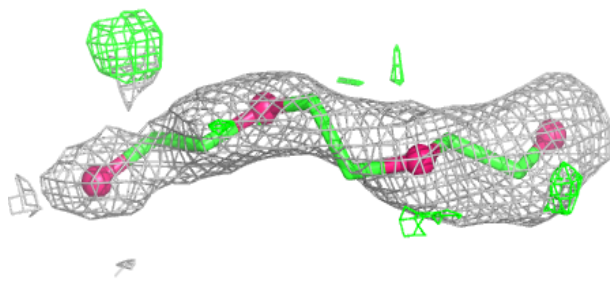
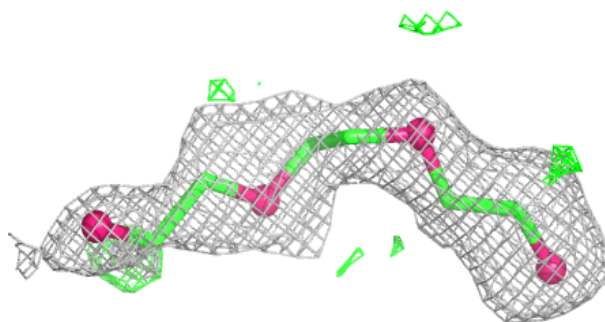


Electron density around ACT A 320:

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

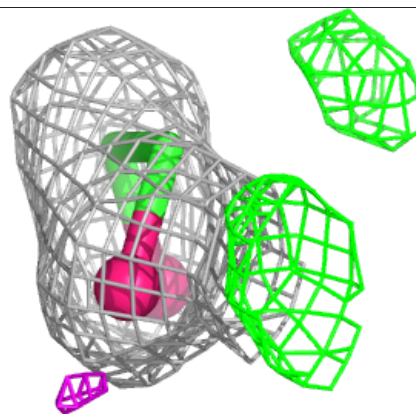
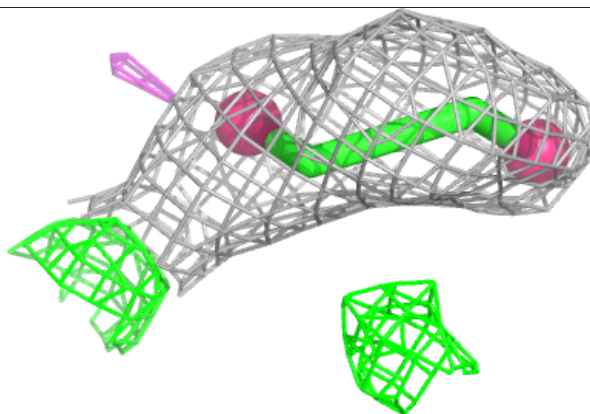
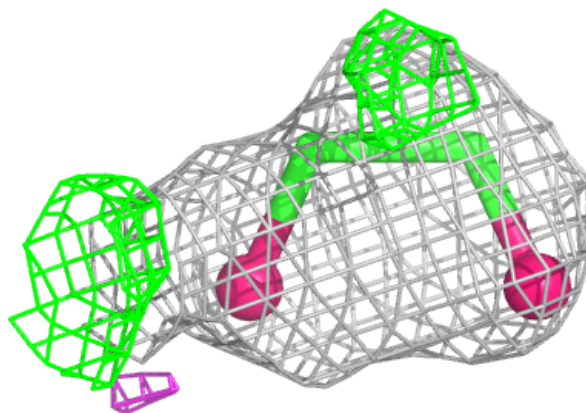
**Electron density around PGE D 313:**

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



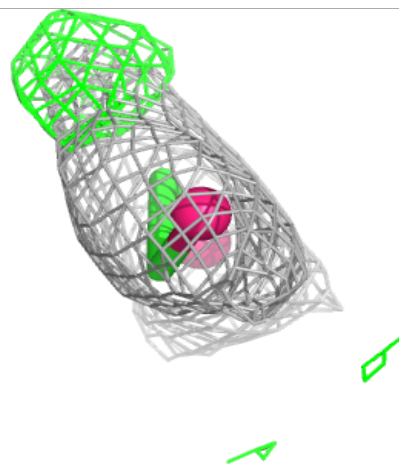
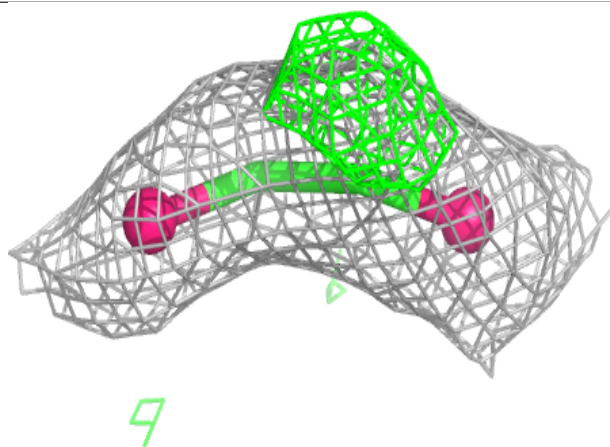
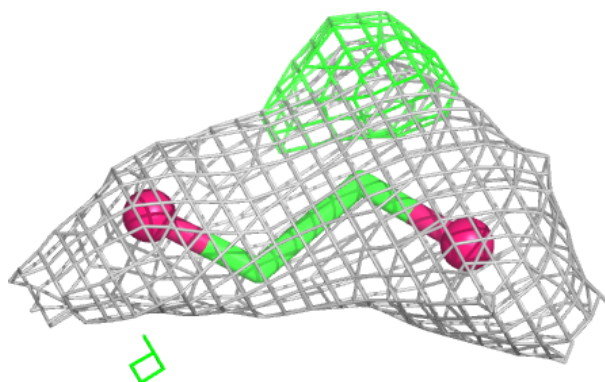
Electron density around EDO A 311:

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



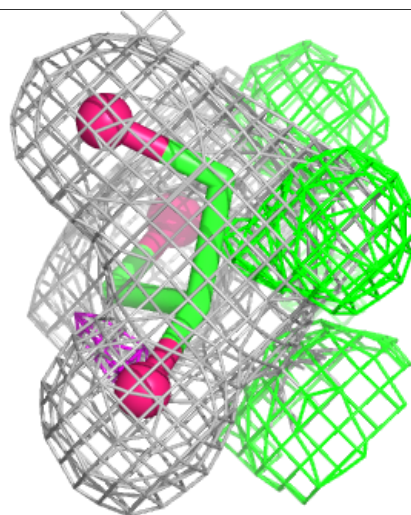
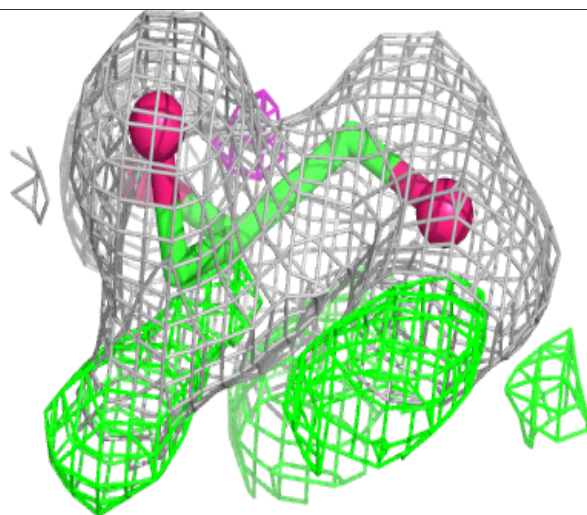
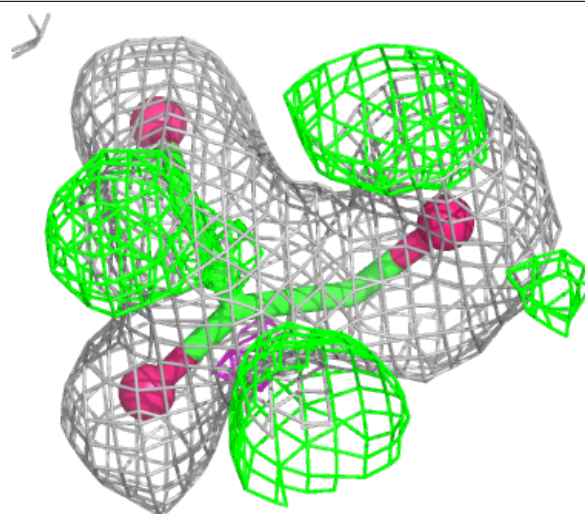
Electron density around EDO E 312:

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



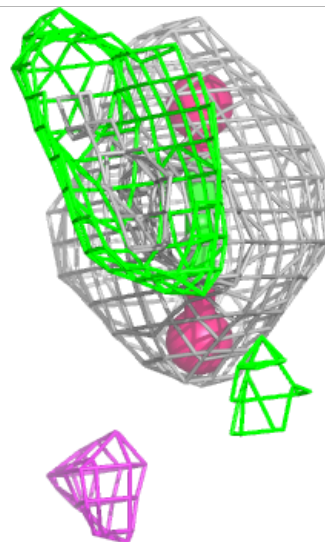
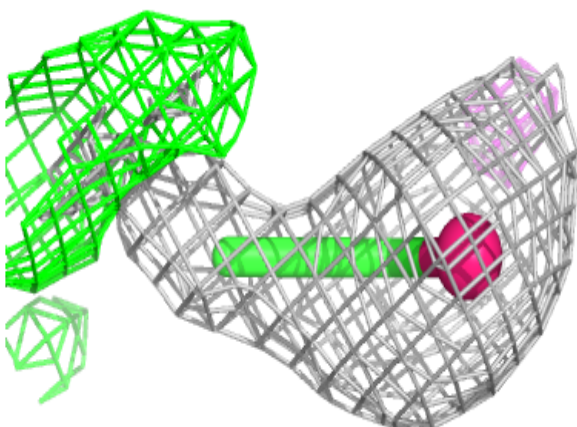
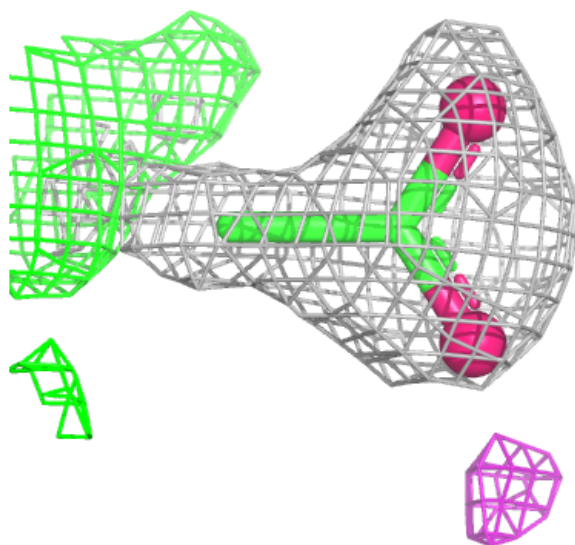
Electron density around GOL C 311:

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



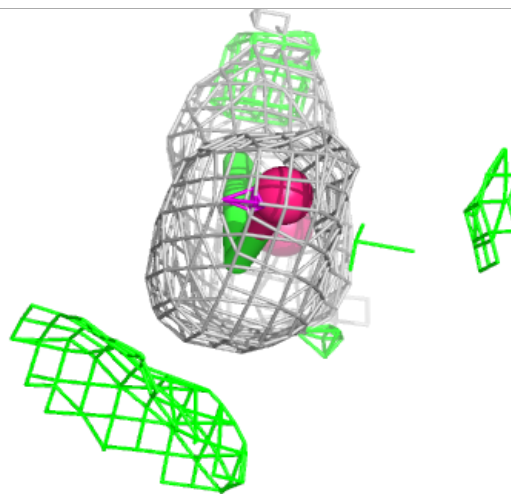
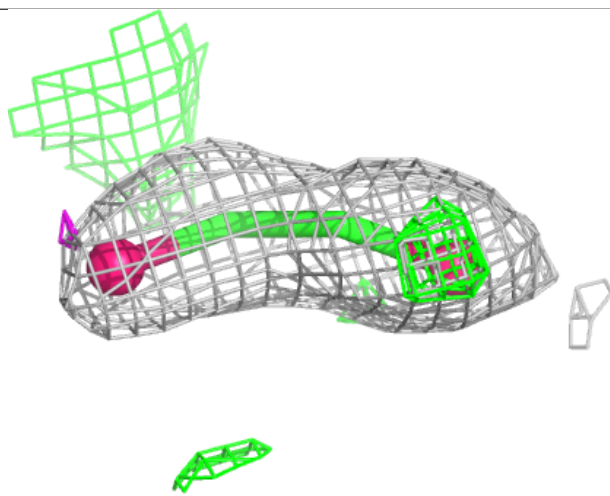
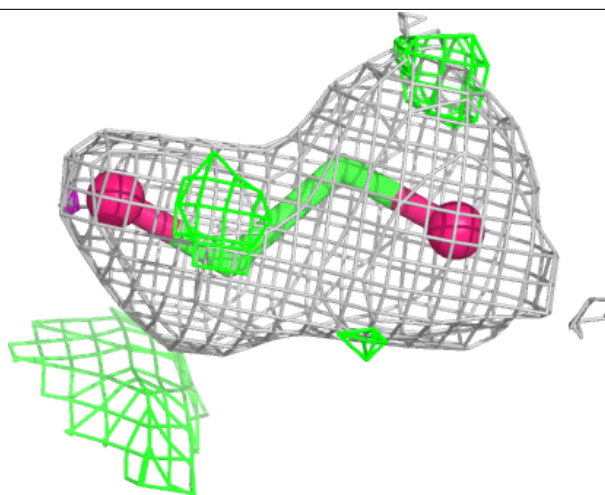
Electron density around ACT B 315:

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



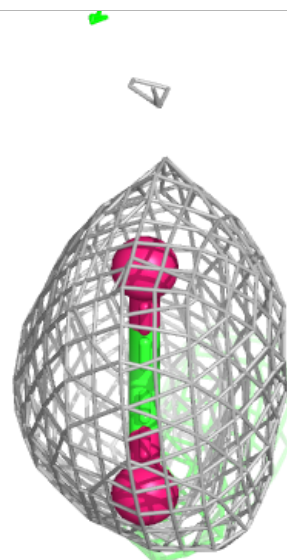
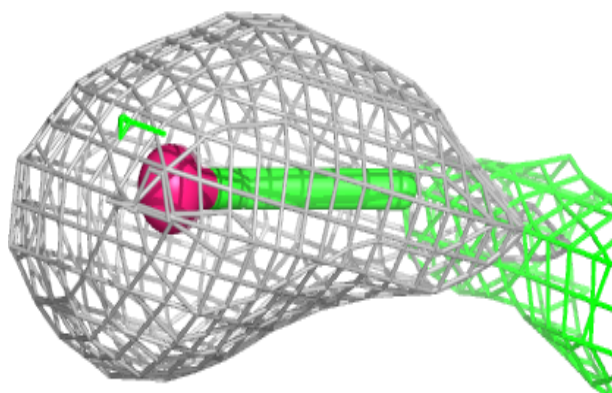
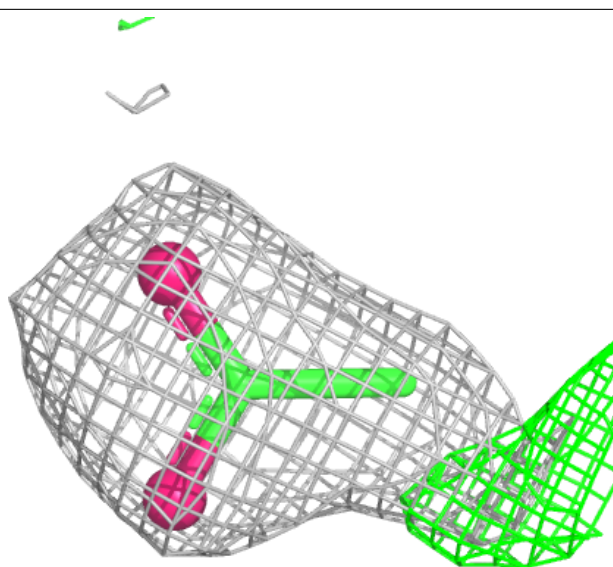
Electron density around EDO F 306:

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



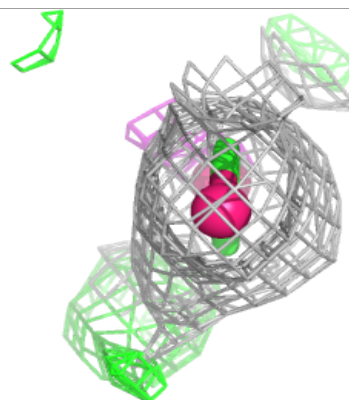
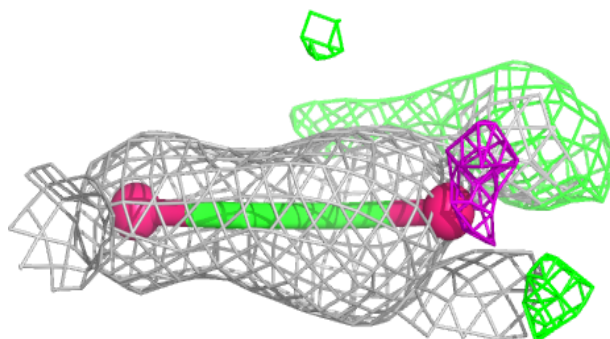
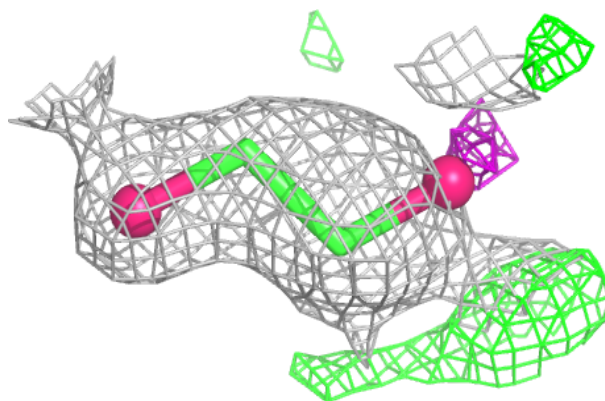
Electron density around ACT B 314:

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

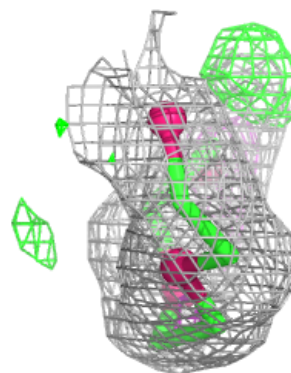
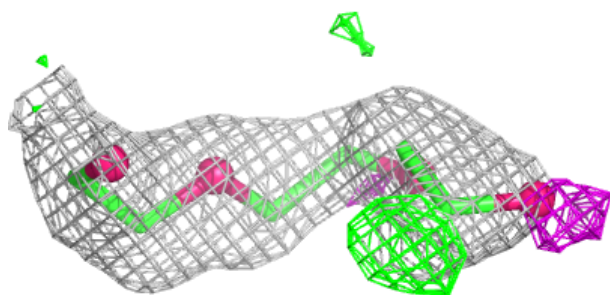
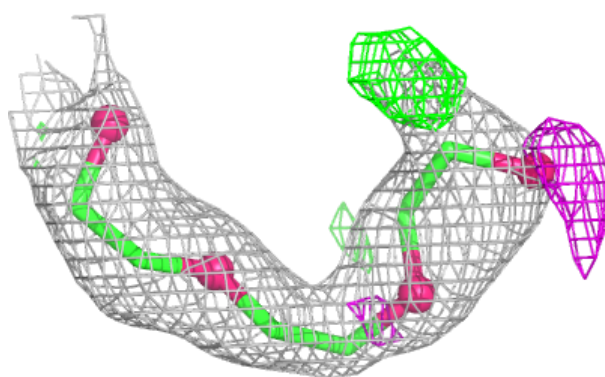


Electron density around EDO D 305:

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

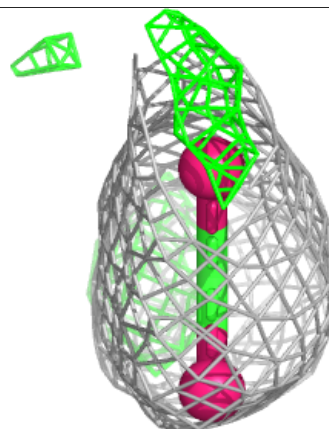
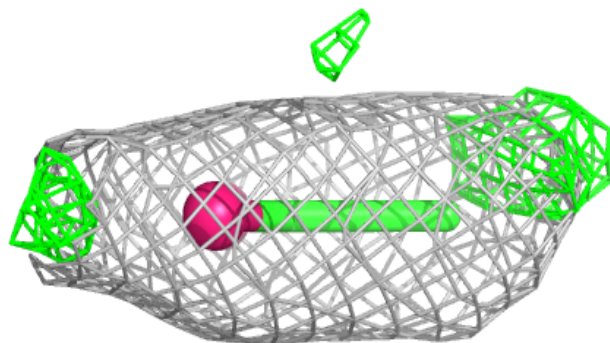
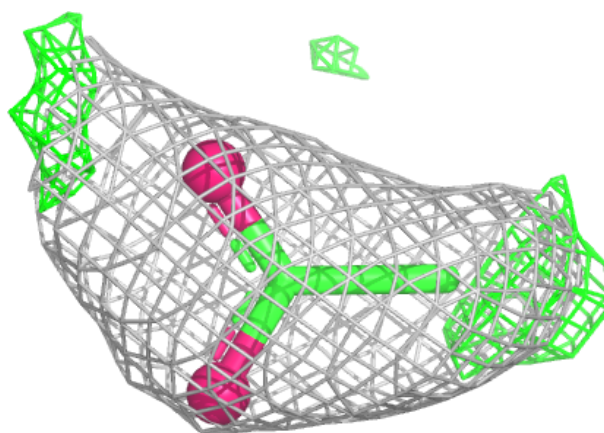
**Electron density around PGE E 315:**

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

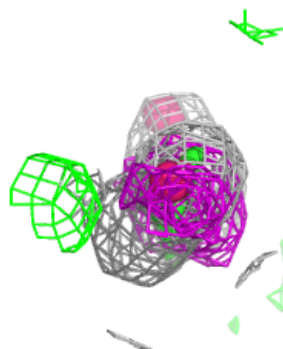
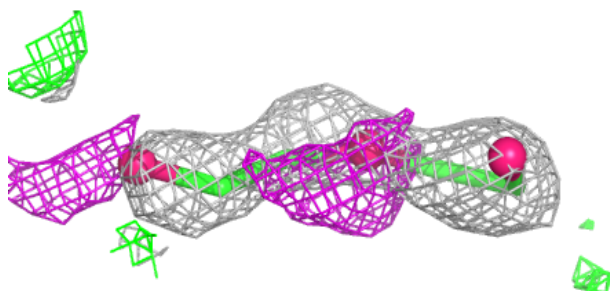
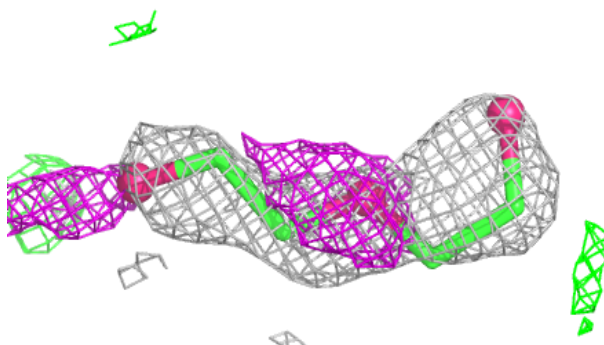


Electron density around ACT F 311:

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

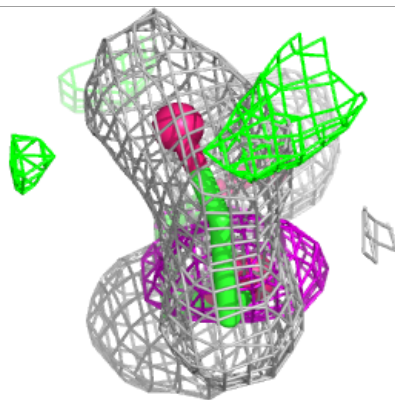
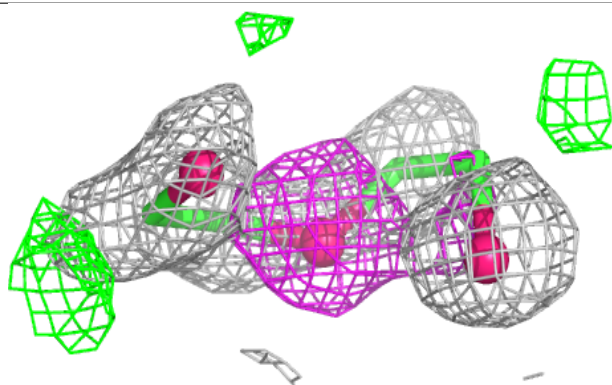
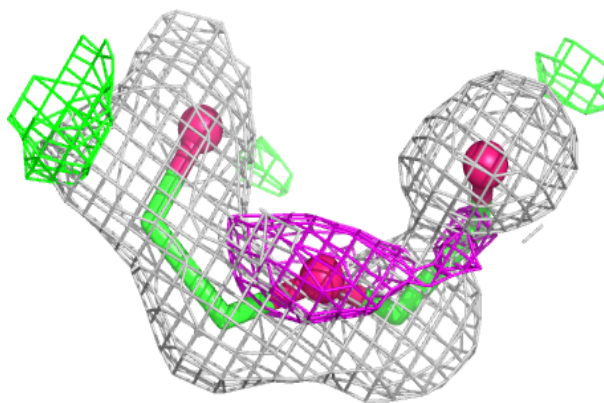
**Electron density around PEG B 313:**

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



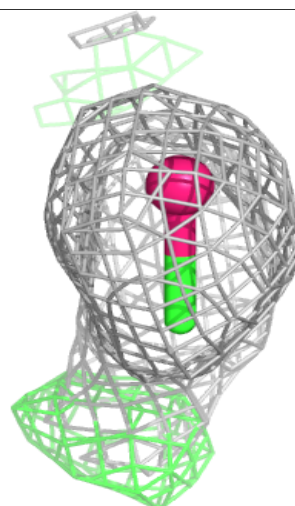
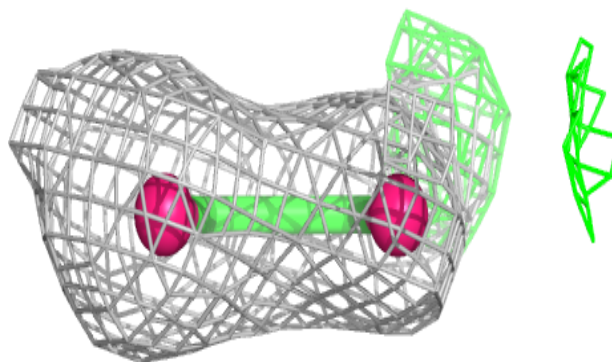
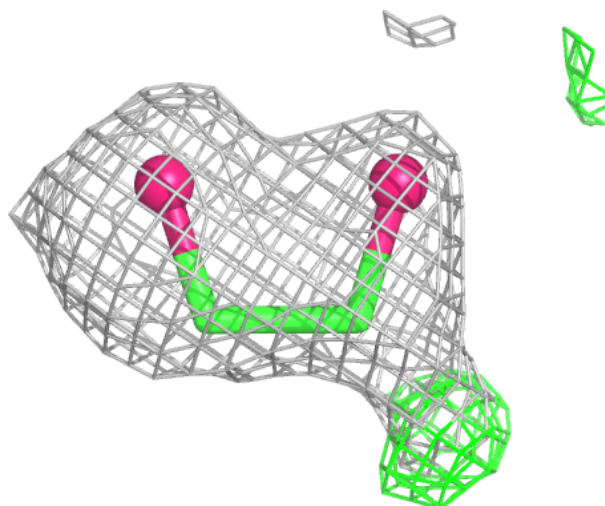
Electron density around PEG E 313:

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



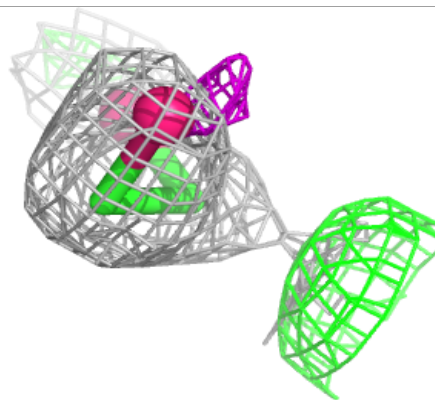
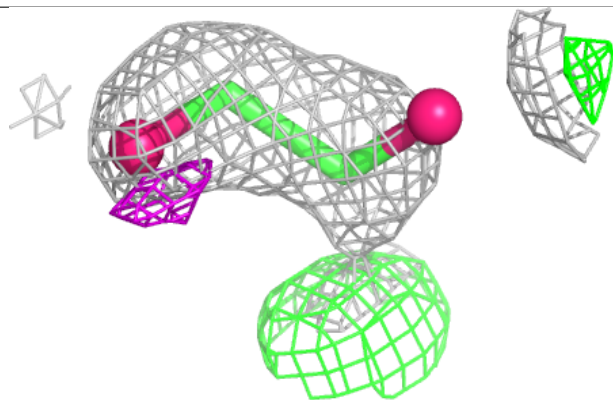
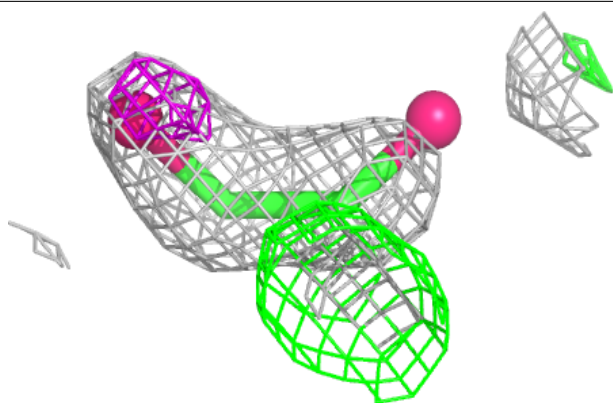
Electron density around EDO C 306:

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

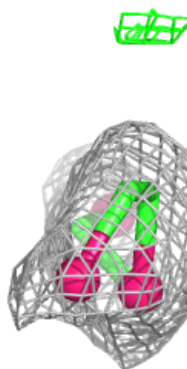
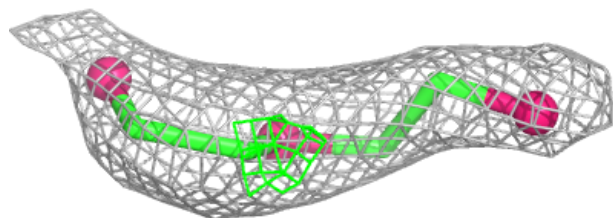
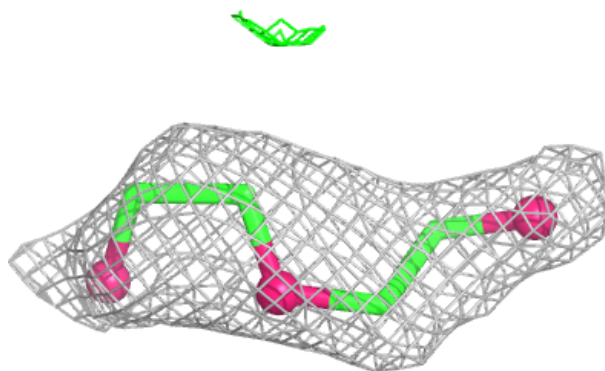


Electron density around EDO B 310:

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

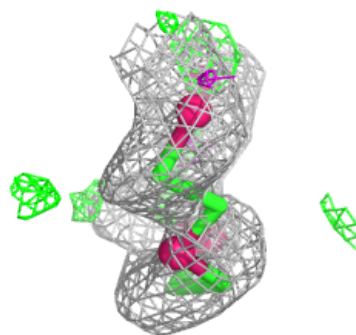
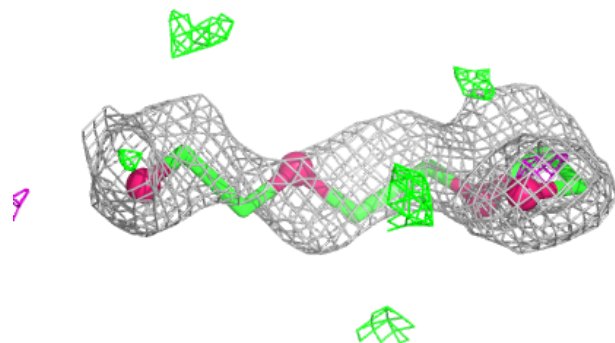
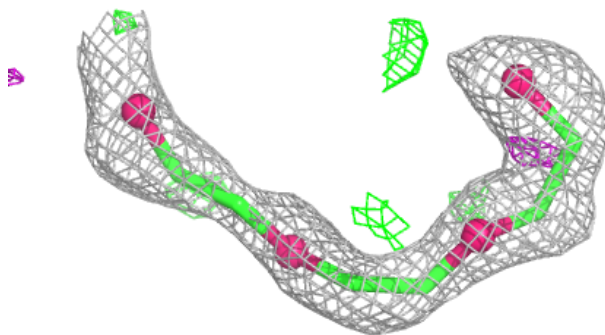
**Electron density around PEG A 318:**

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

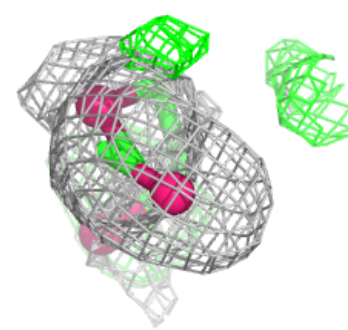
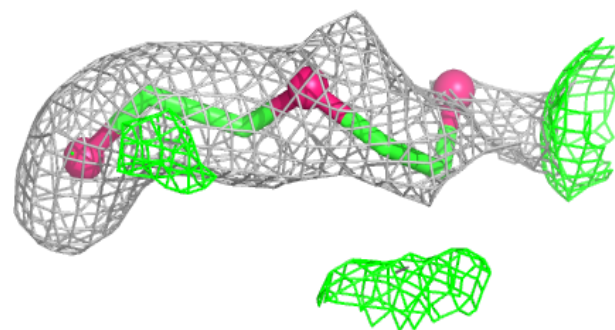
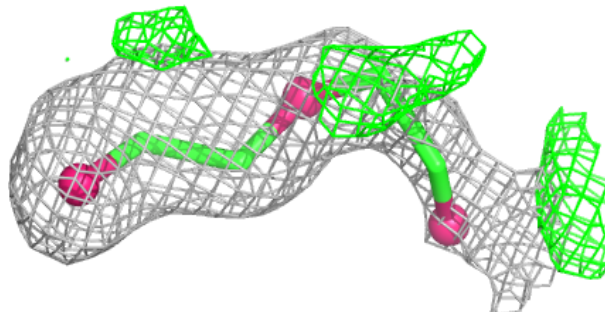


Electron density around PGE B 316:

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

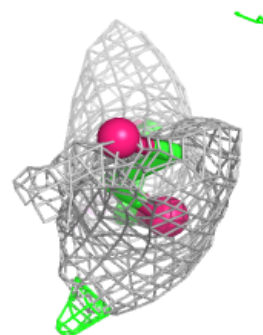
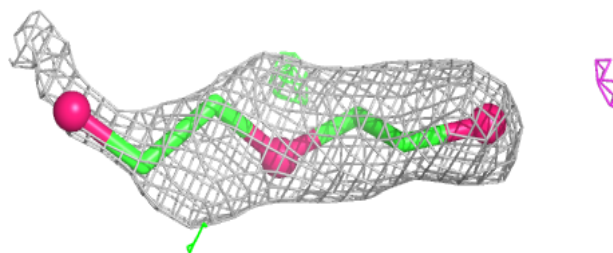
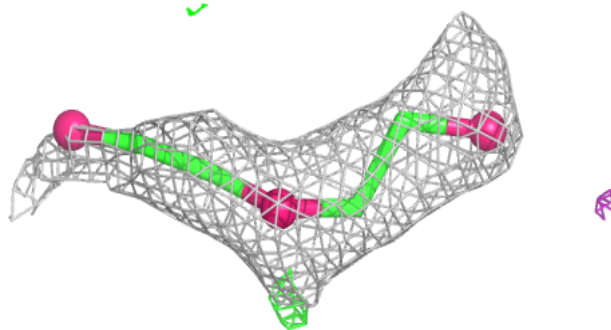
**Electron density around PEG B 312:**

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

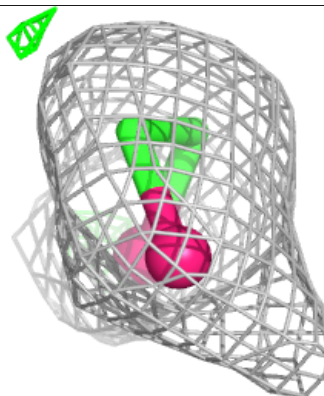
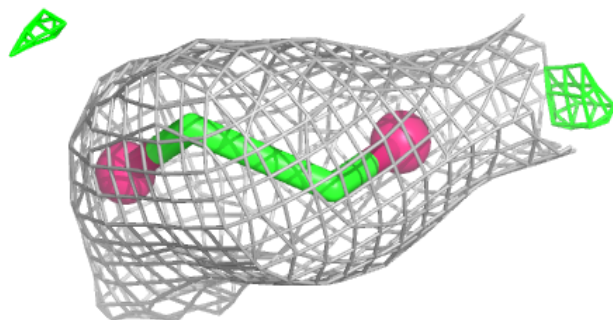
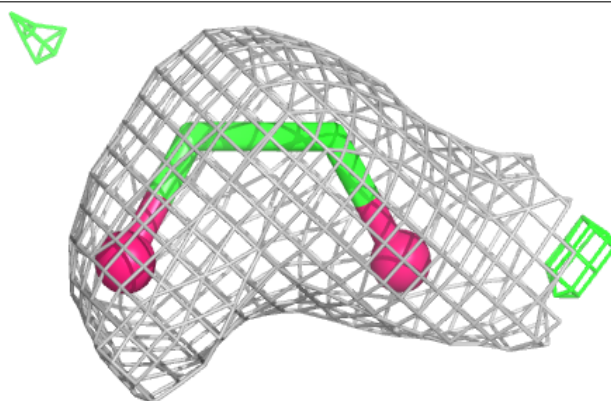


Electron density around PEG F 309:

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

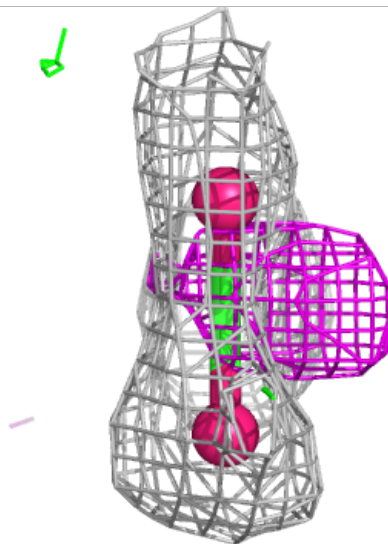
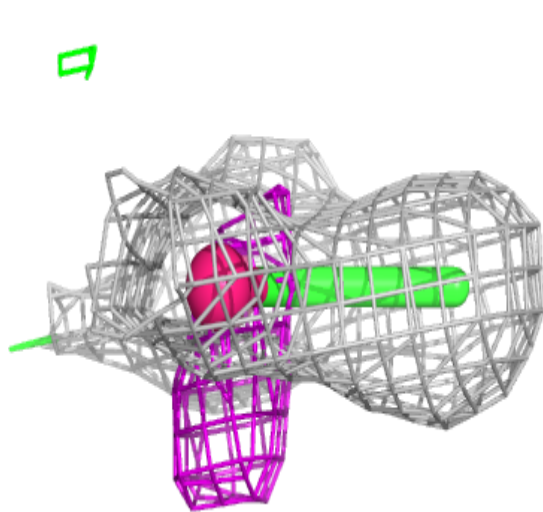
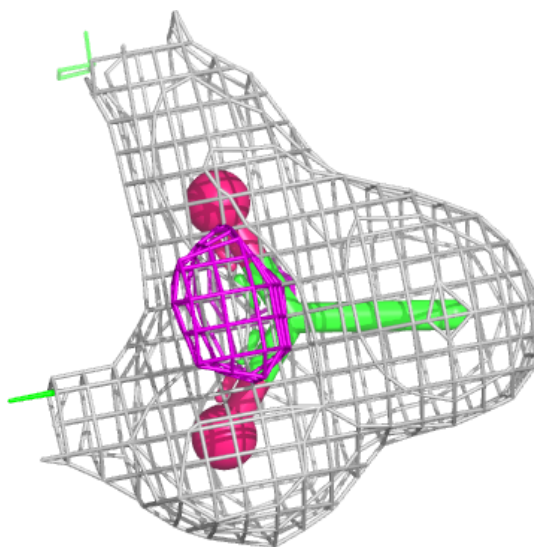
**Electron density around EDO B 309:**

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



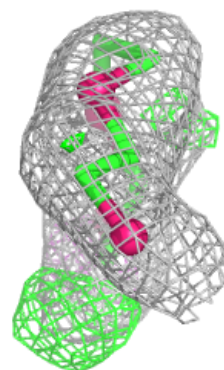
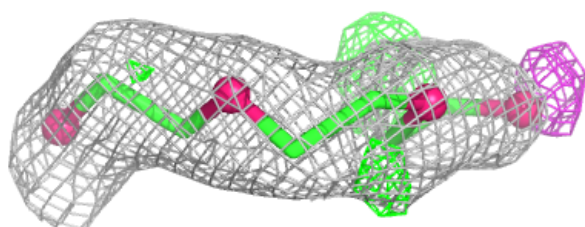
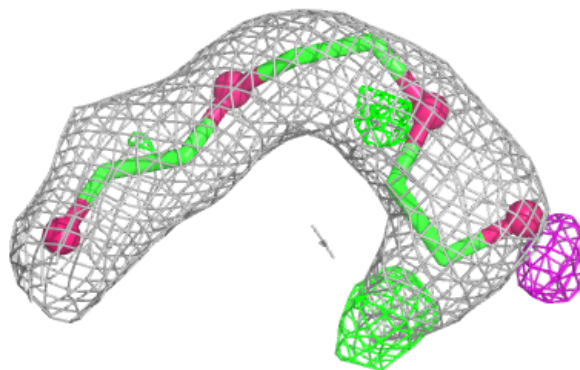
Electron density around ACT A 319:

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

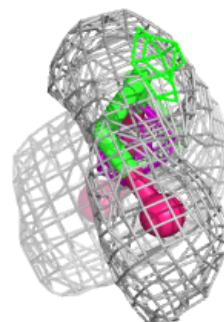
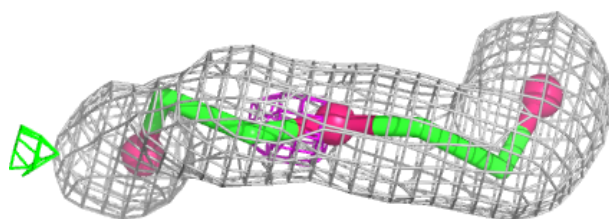
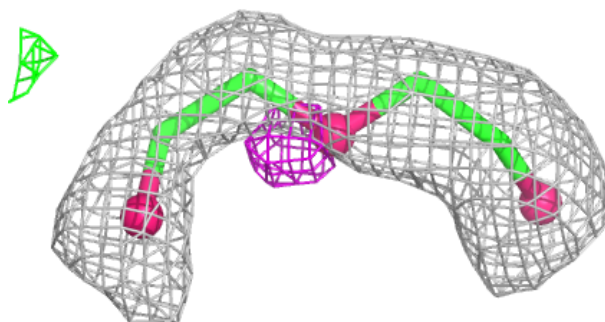


Electron density around PGE D 314:

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

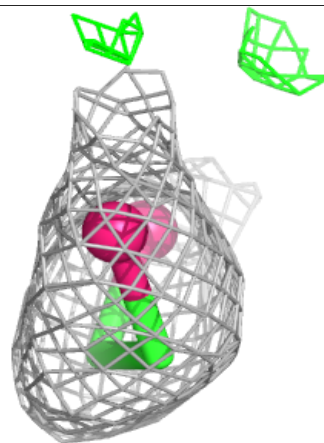
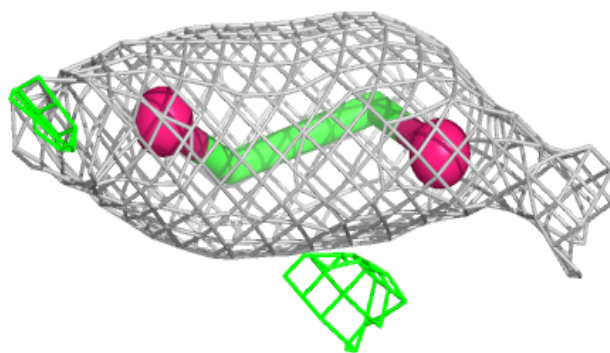
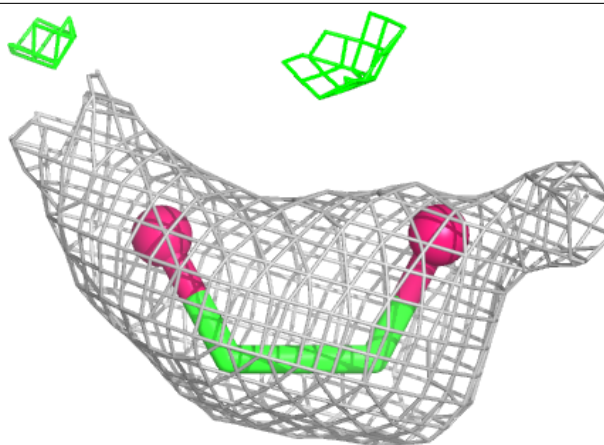
**Electron density around PEG F 308:**

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



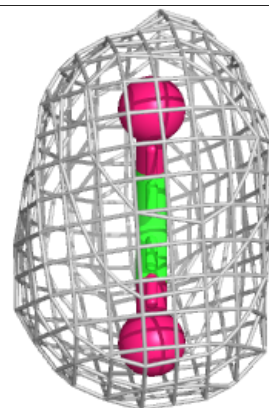
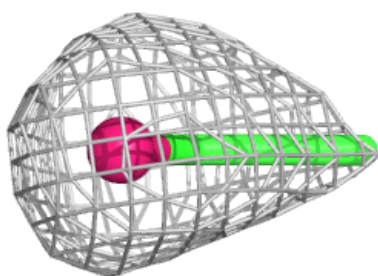
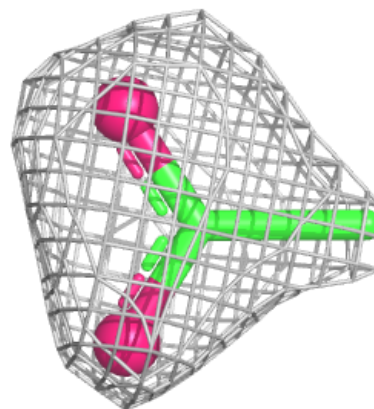
Electron density around EDO A 316:

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

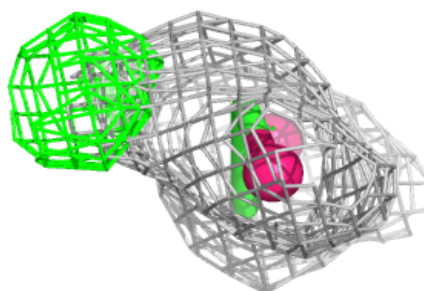
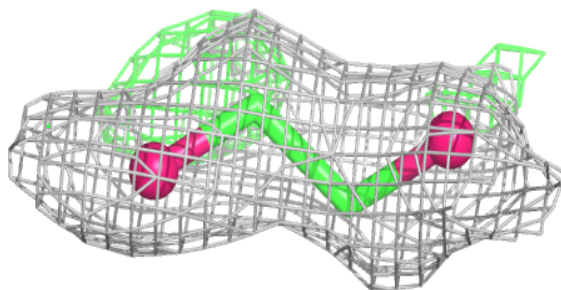


Electron density around ACT D 312:

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

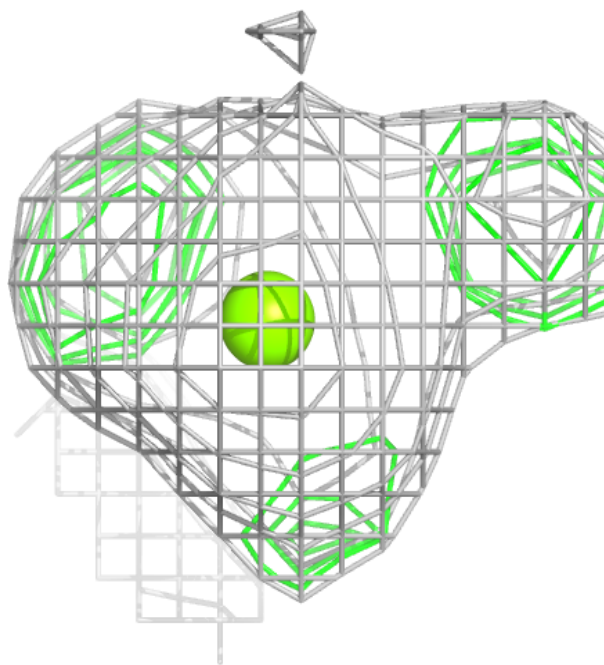
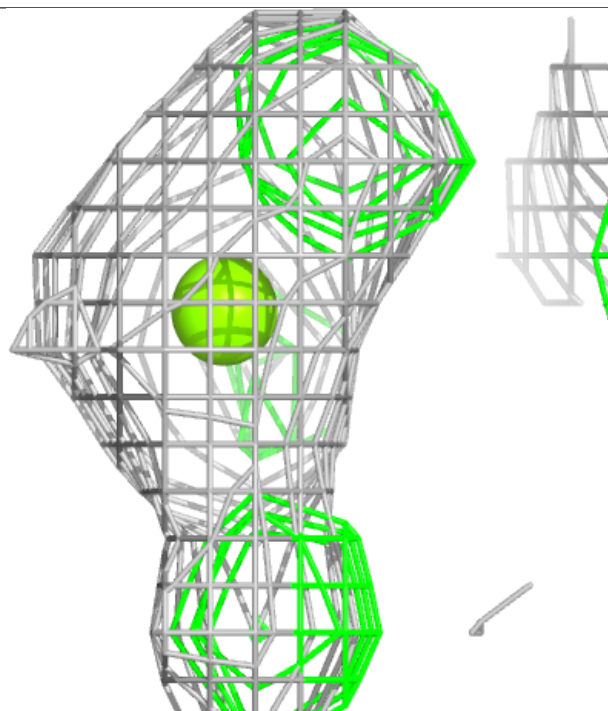
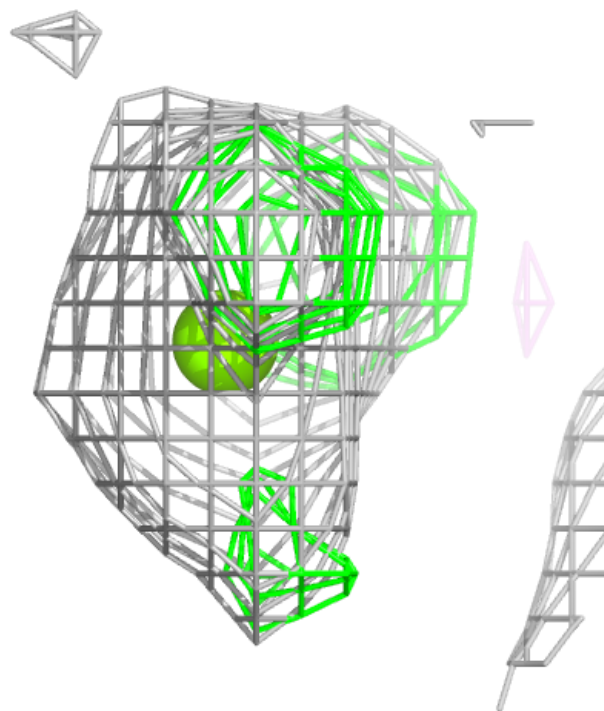
**Electron density around EDO A 307:**

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



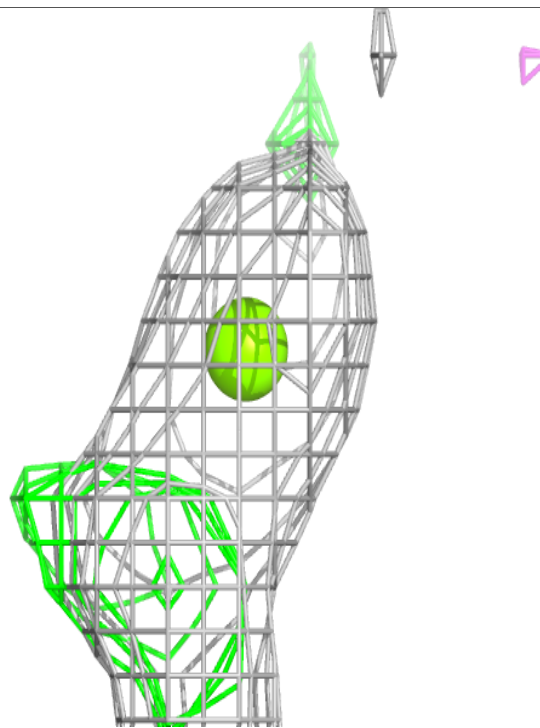
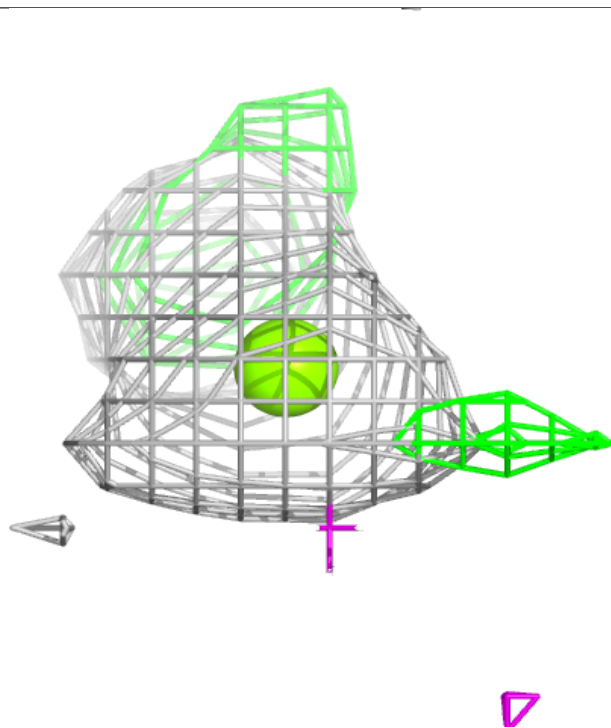
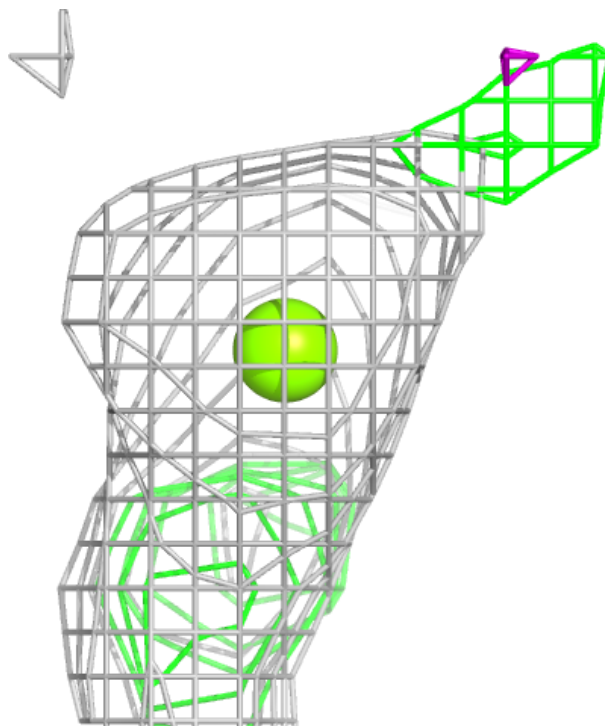
Electron density around MG A 305:

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



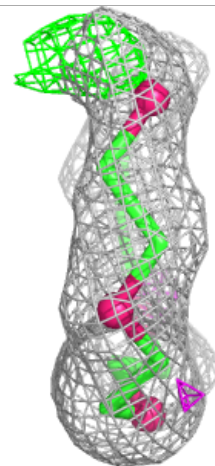
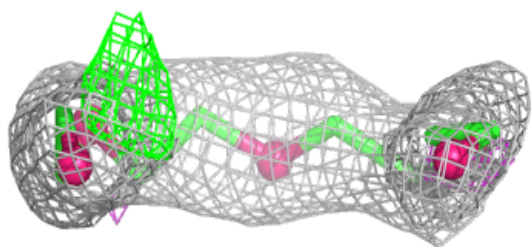
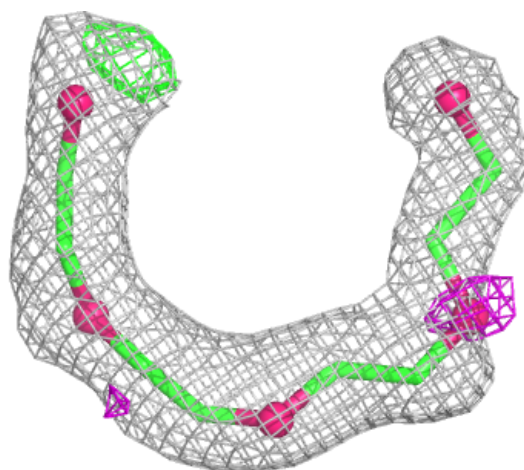
Electron density around MG E 304:

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



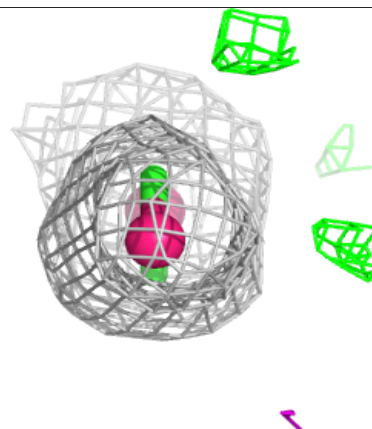
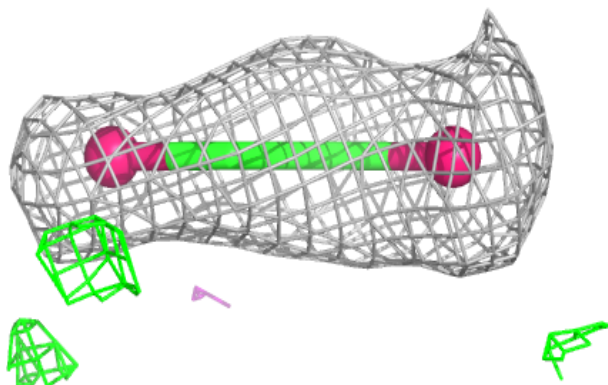
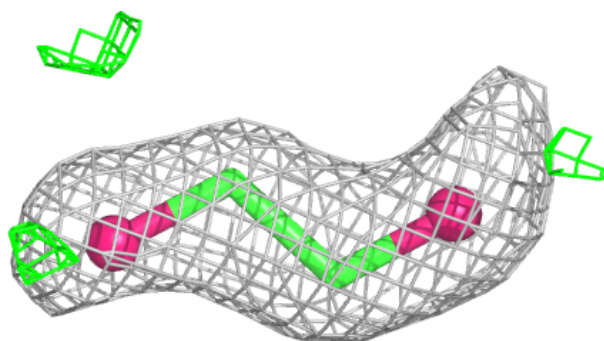
Electron density around PG4 E 306:

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



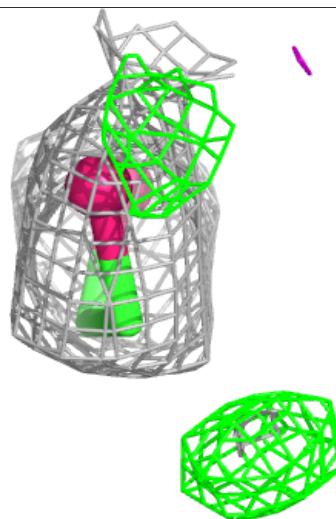
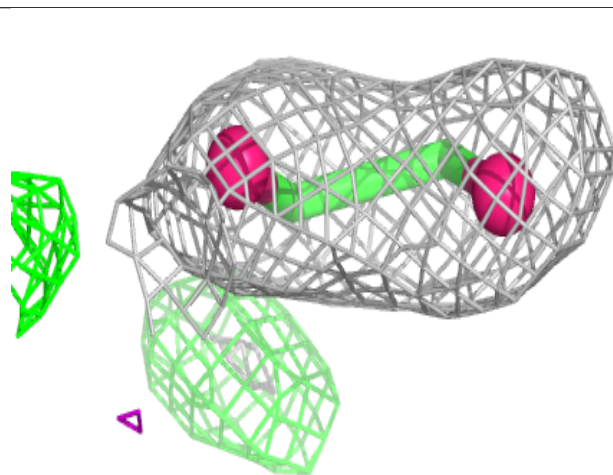
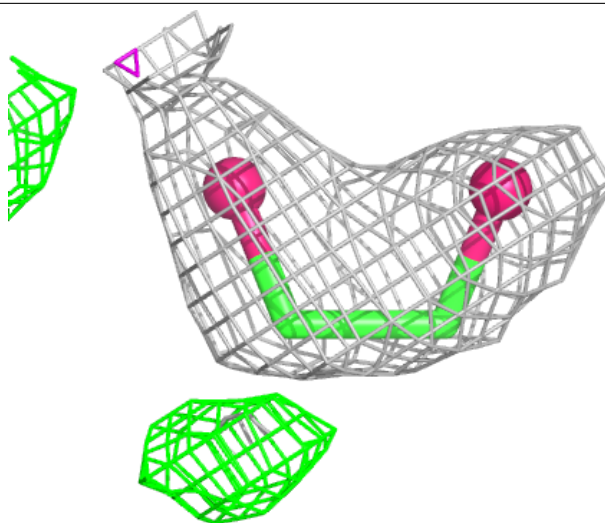
Electron density around EDO E 310:

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



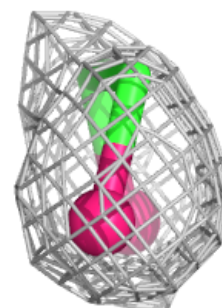
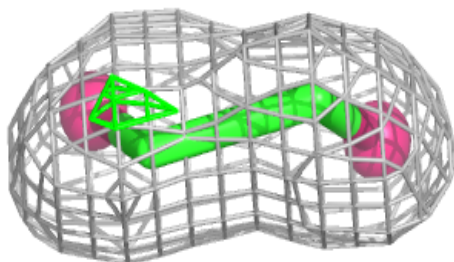
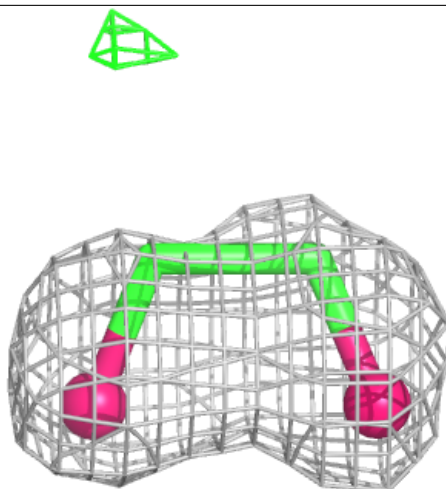
Electron density around EDO B 307:

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



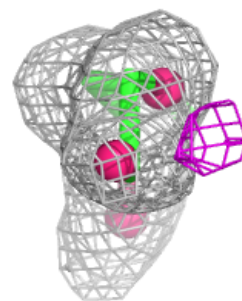
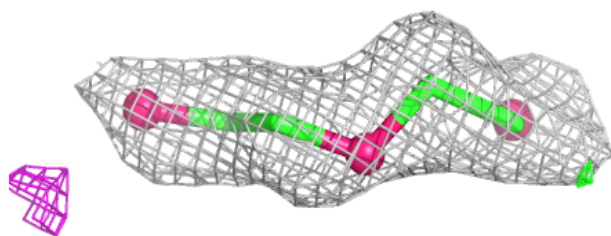
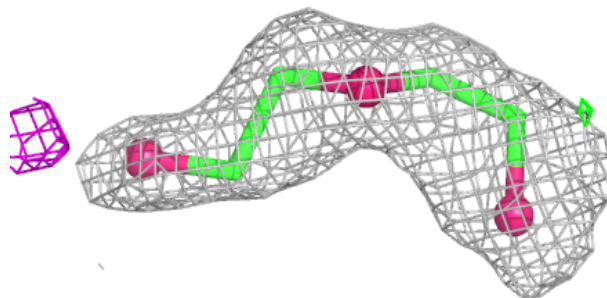
Electron density around EDO E 309:

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

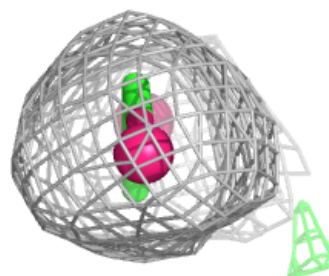
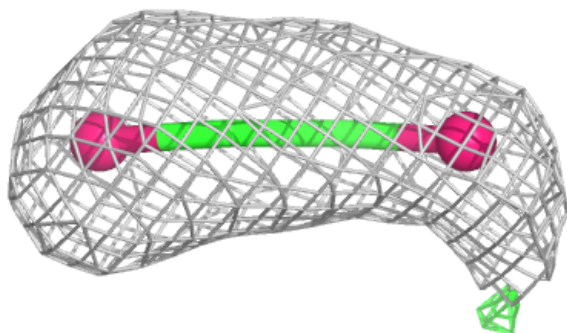
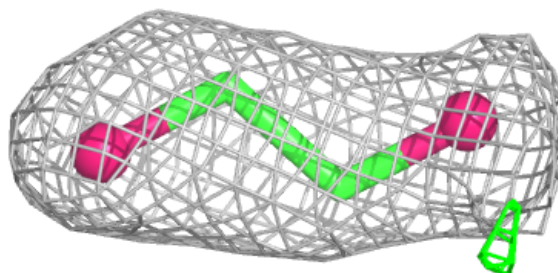


Electron density around PEG B 311:

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

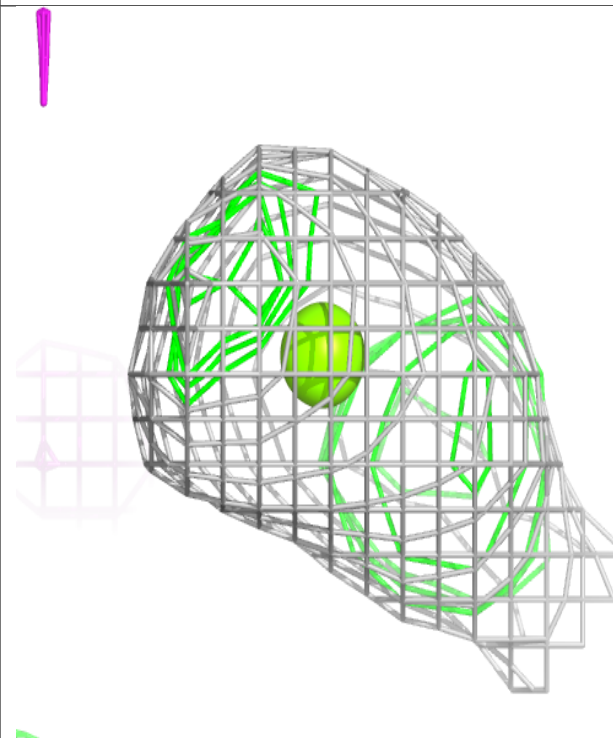
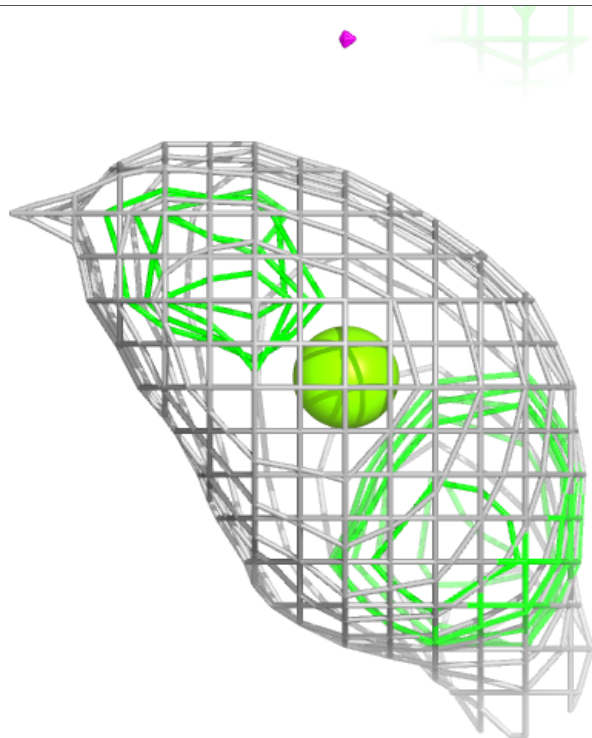
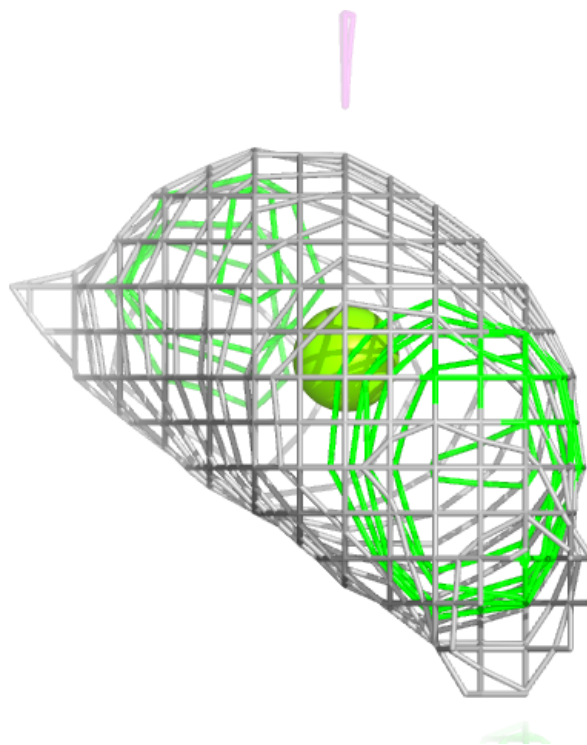
**Electron density around EDO A 310:**

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



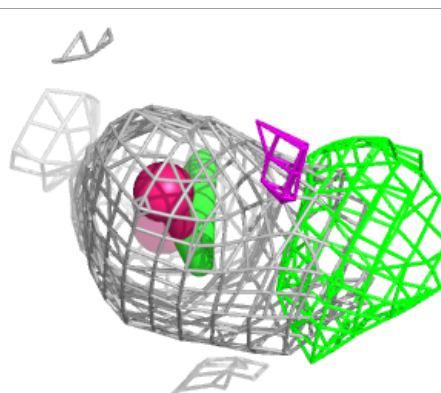
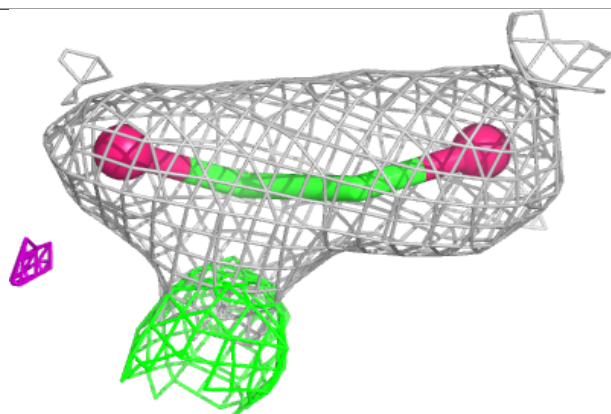
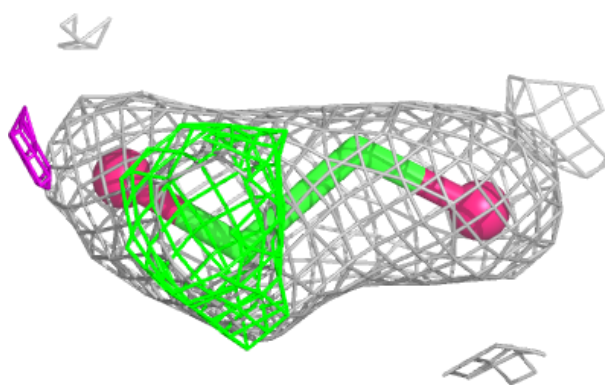
Electron density around MG B 304:

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

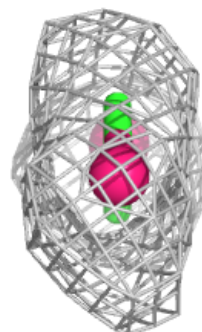
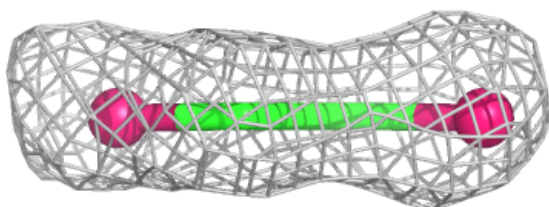
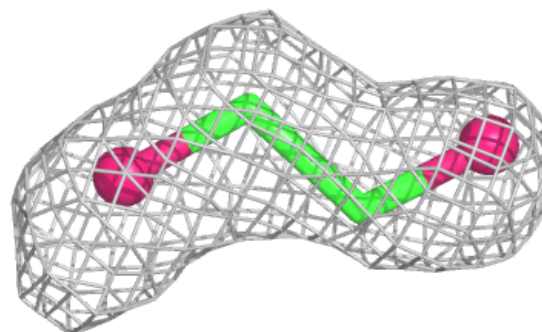


Electron density around EDO E 308:

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

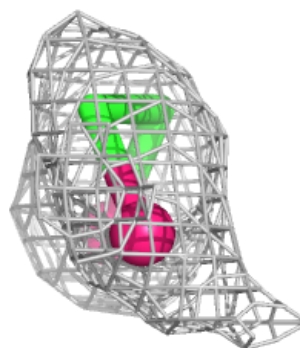
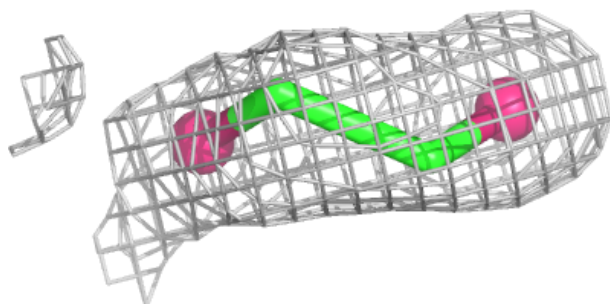
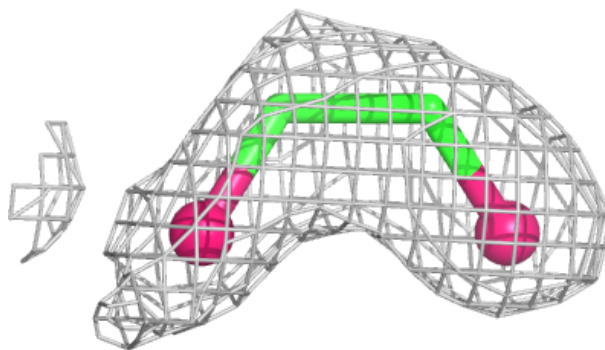
**Electron density around EDO C 309:**

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



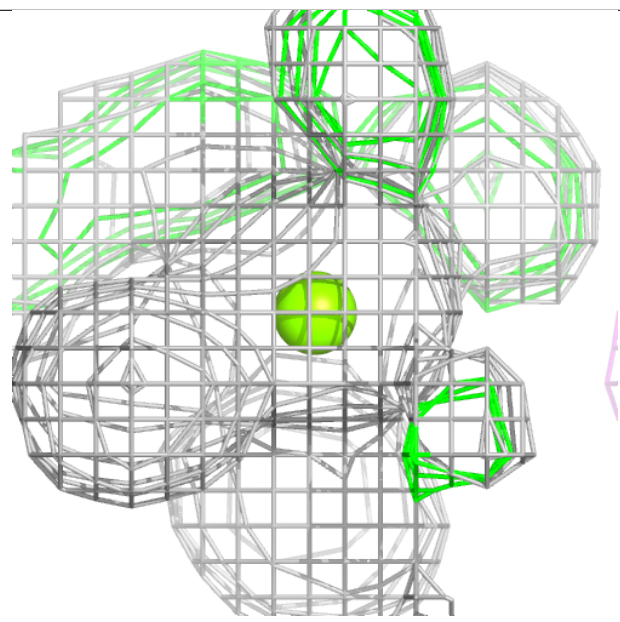
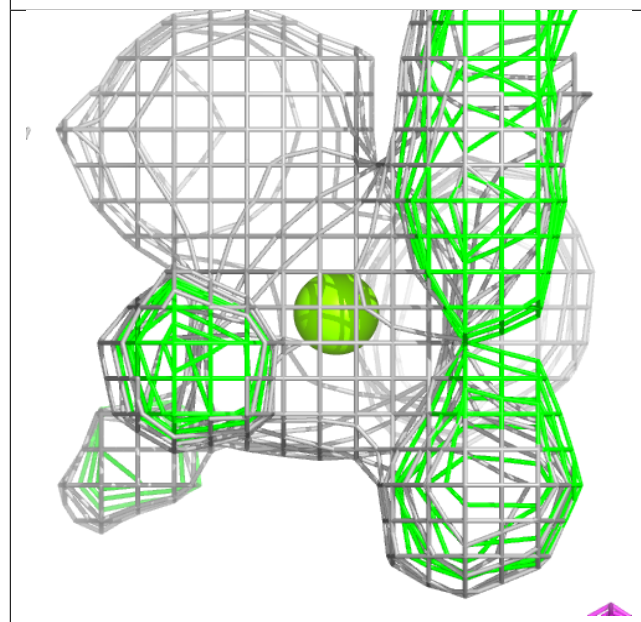
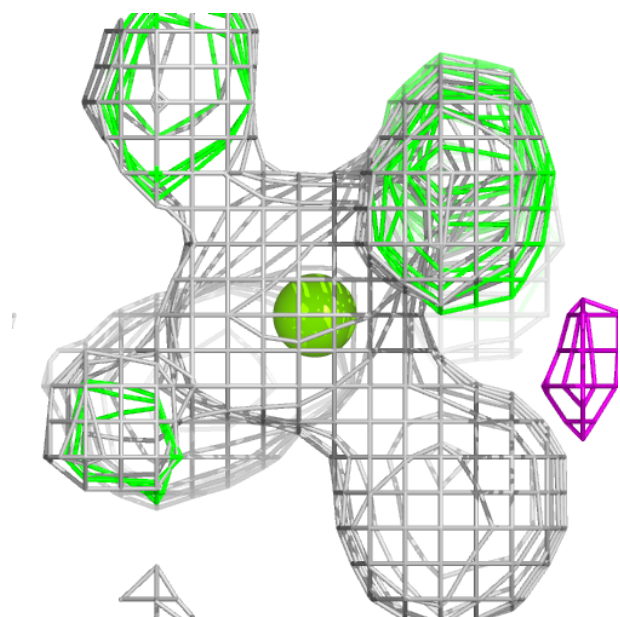
Electron density around EDO C 304:

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



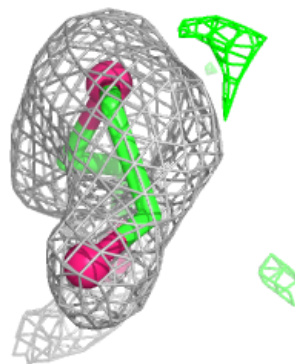
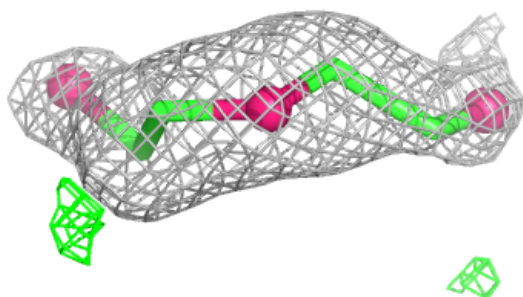
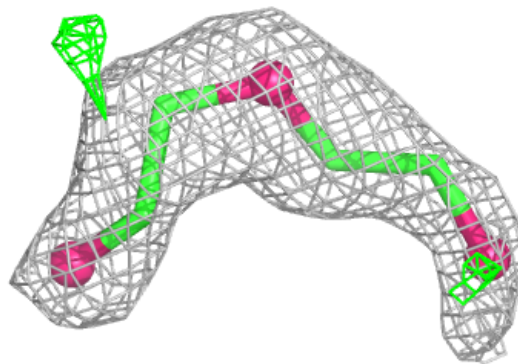
Electron density around MG E 305:

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



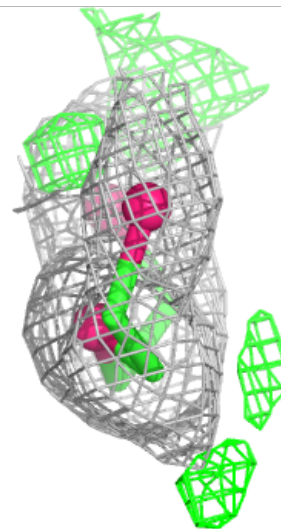
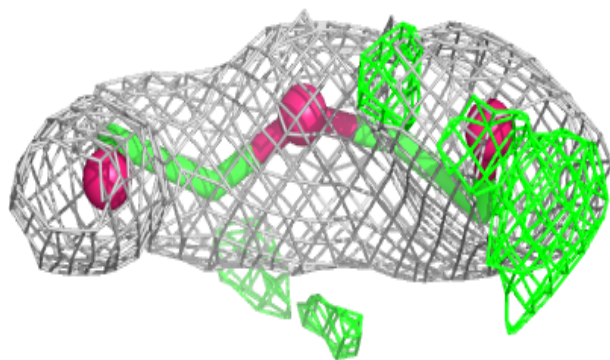
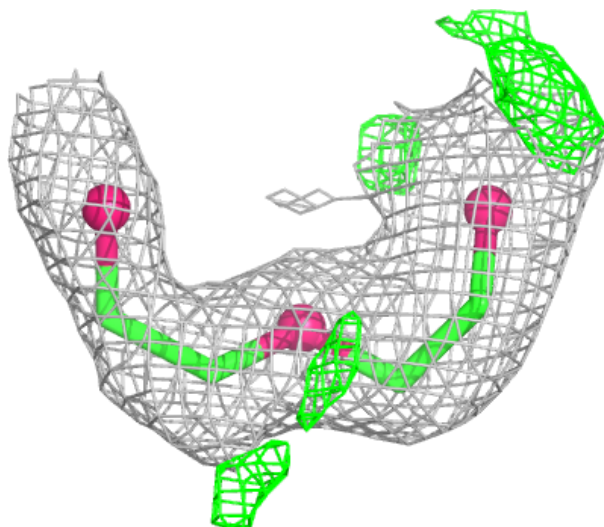
Electron density around PEG C 310:

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



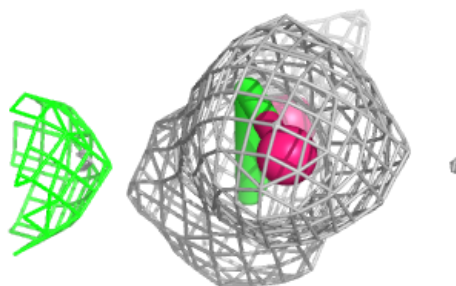
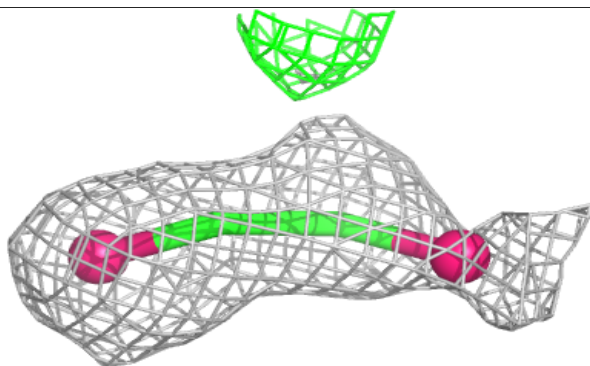
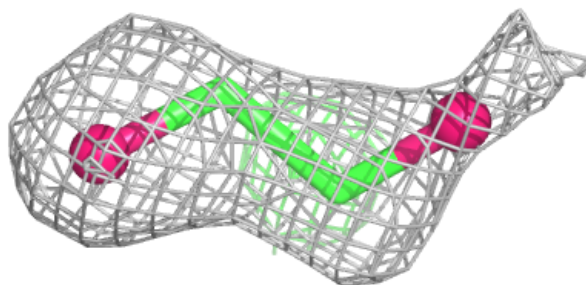
Electron density around PEG D 308:

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



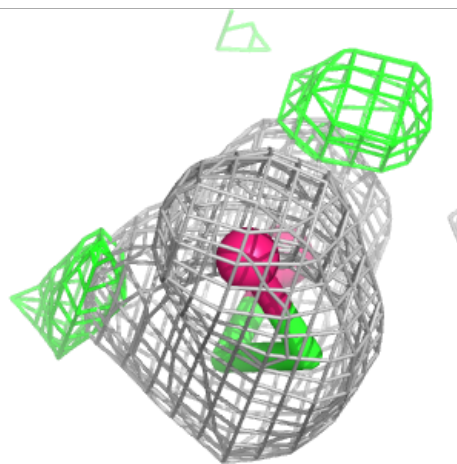
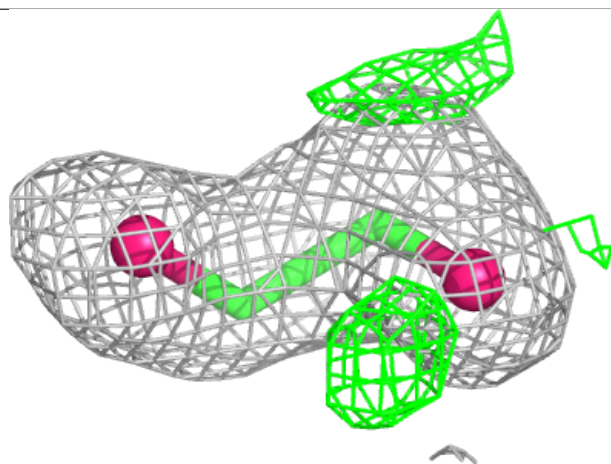
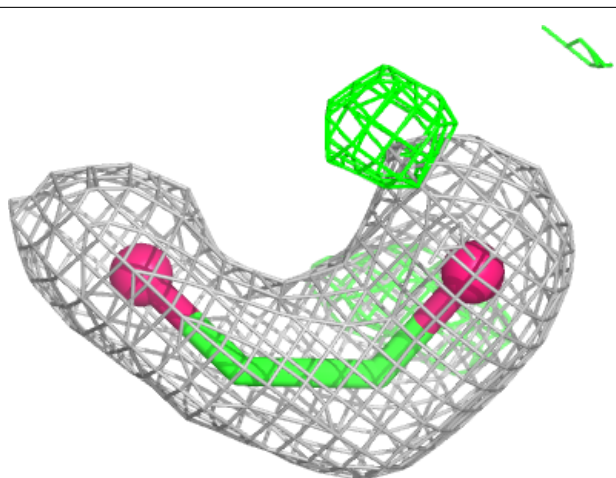
Electron density around EDO C 307:

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



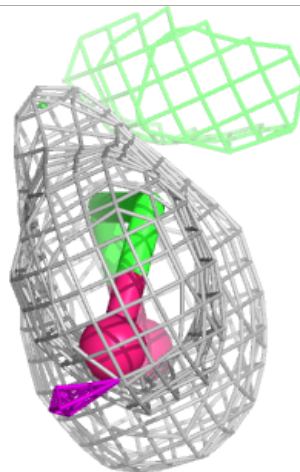
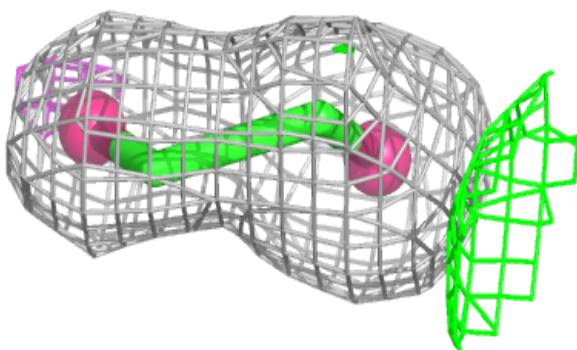
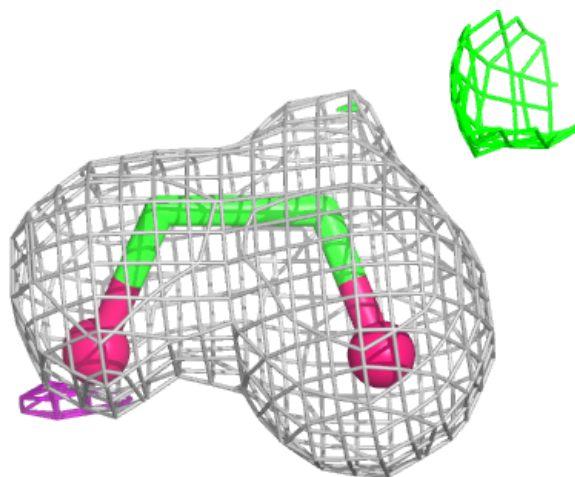
Electron density around EDO A 313:

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



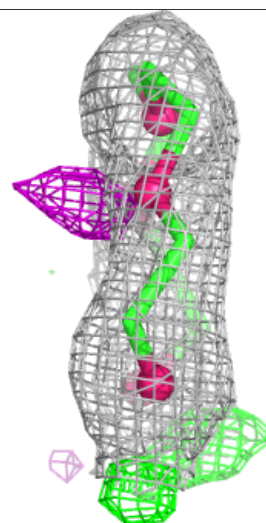
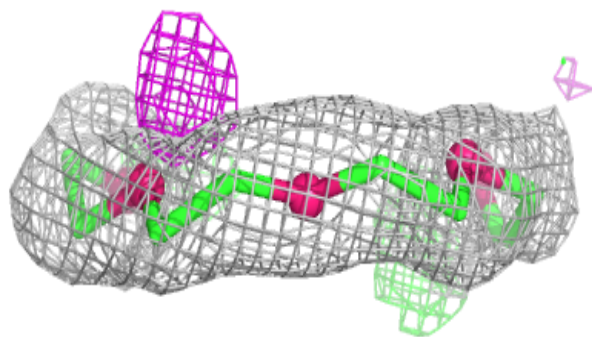
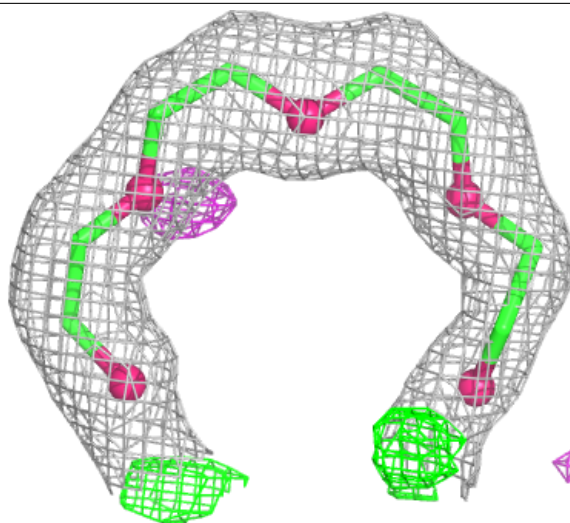
Electron density around EDO A 308:

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



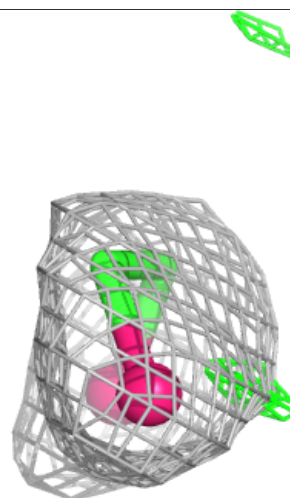
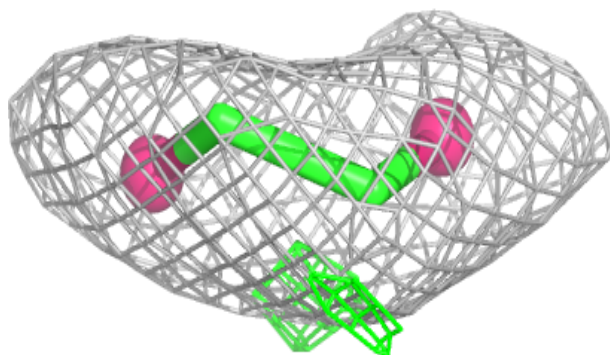
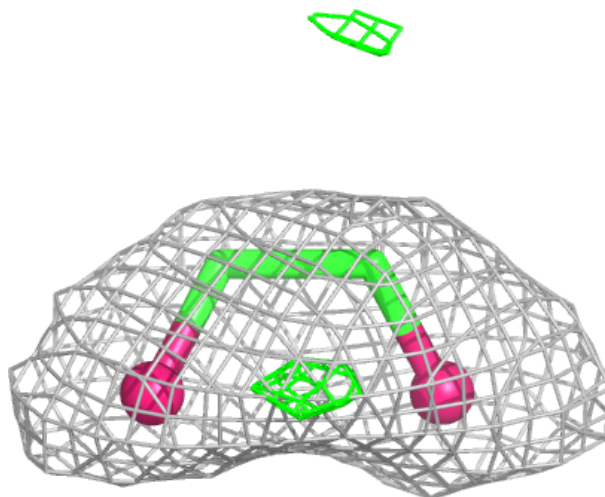
Electron density around PG4 F 305:

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



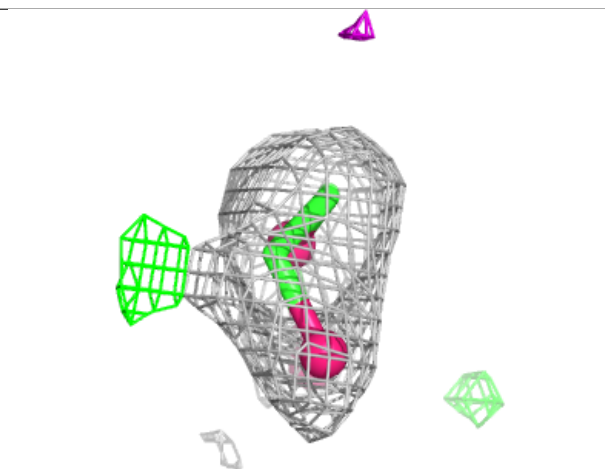
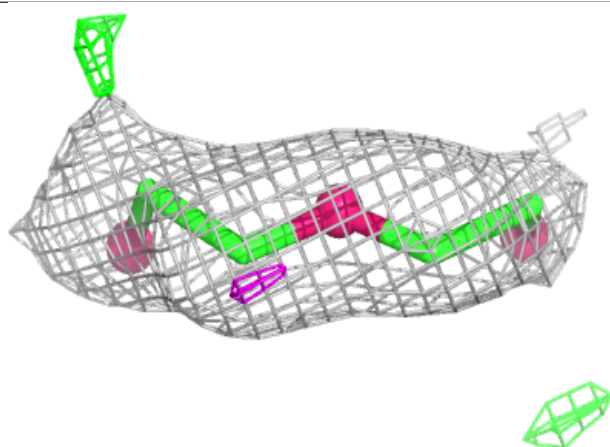
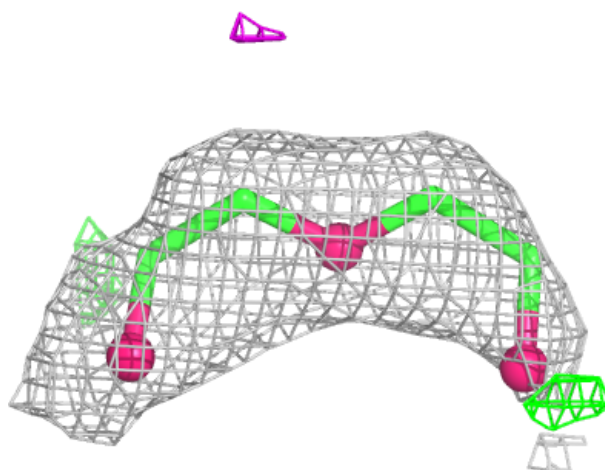
Electron density around EDO E 307:

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



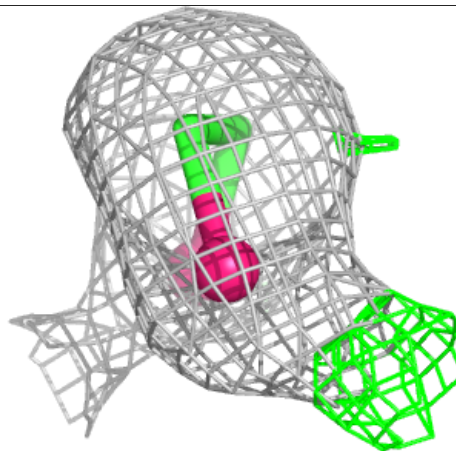
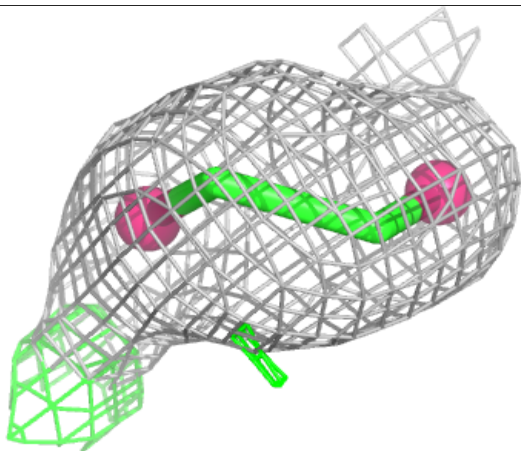
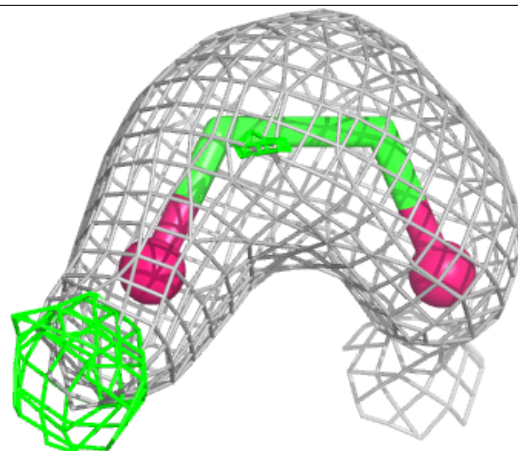
Electron density around PEG A 317:

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



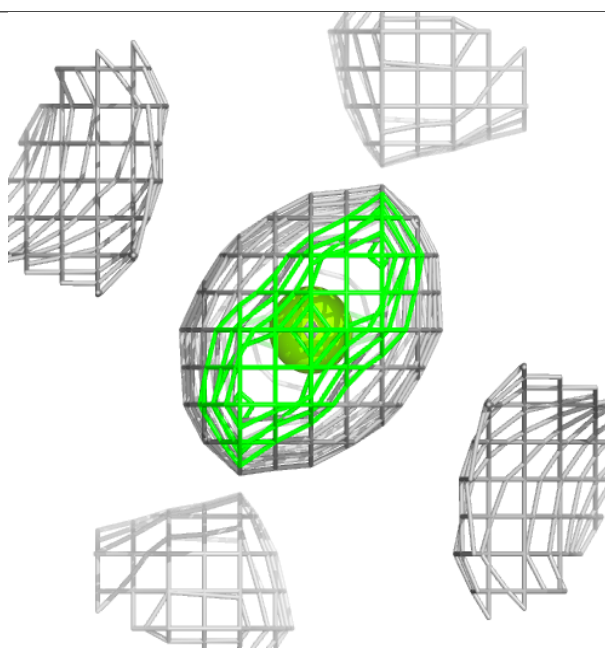
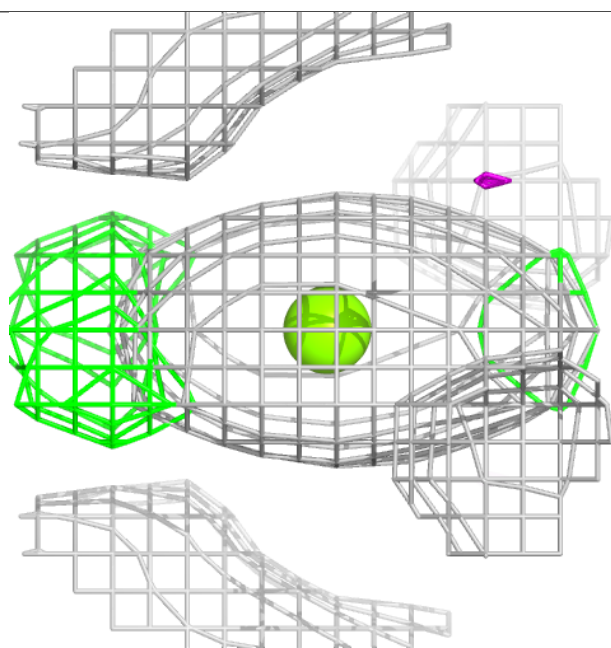
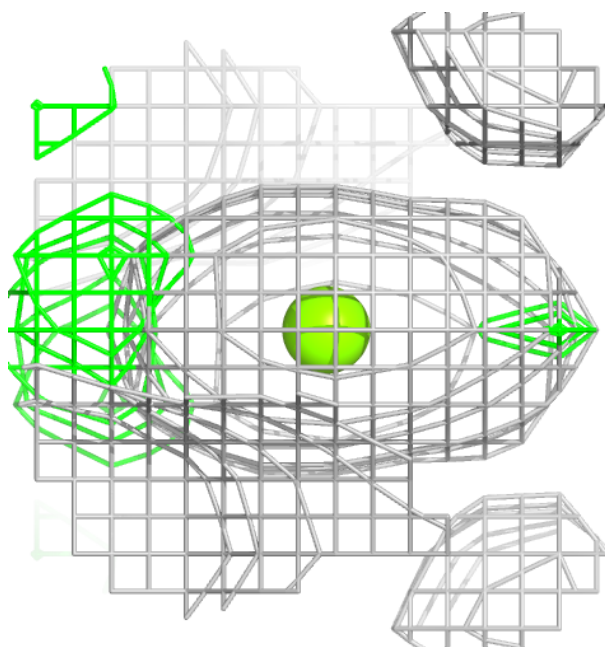
Electron density around EDO B 308:

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



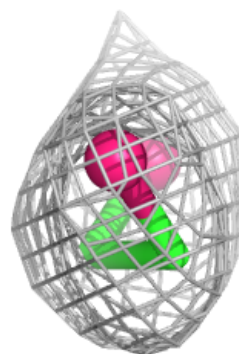
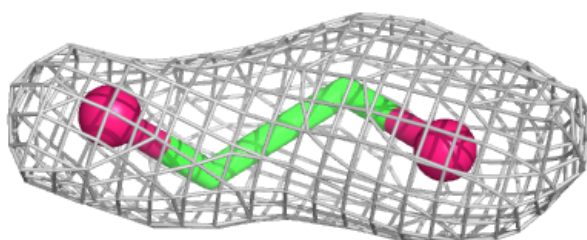
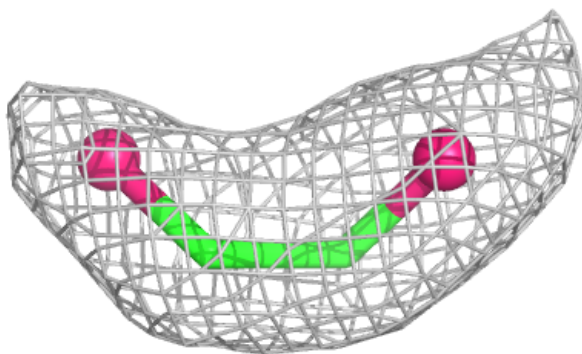
Electron density around MG F 304:

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



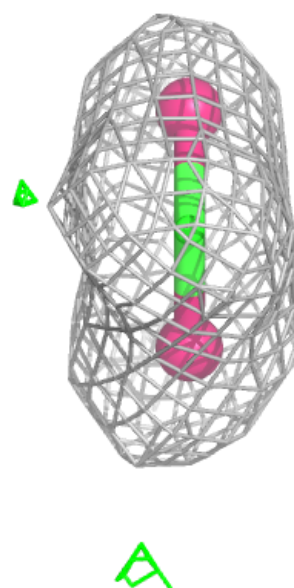
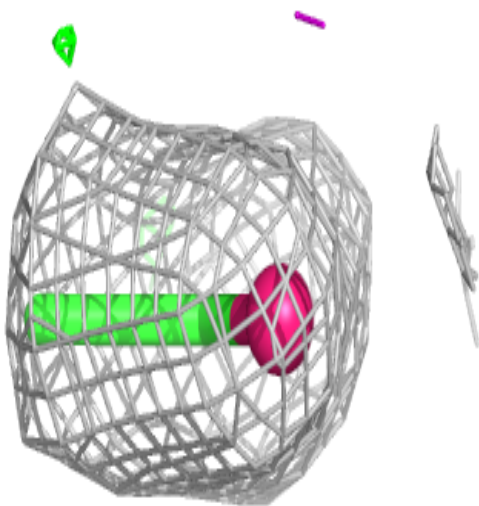
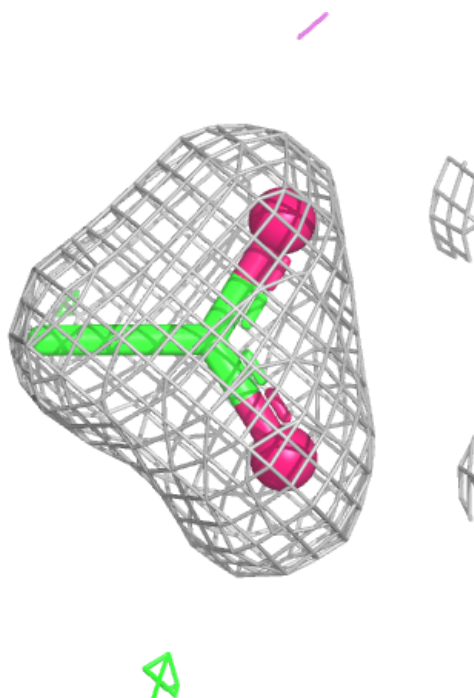
Electron density around EDO C 308:

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



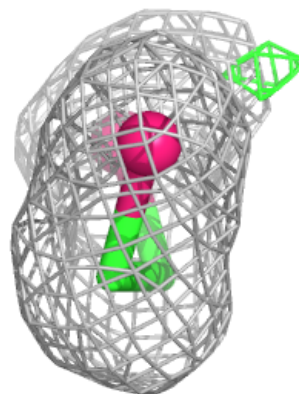
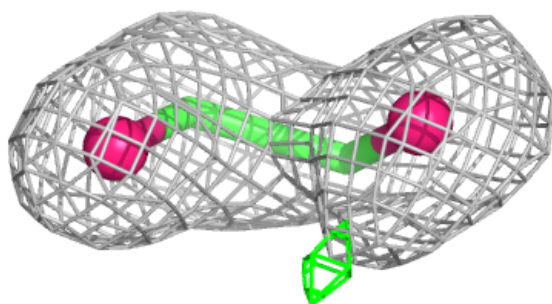
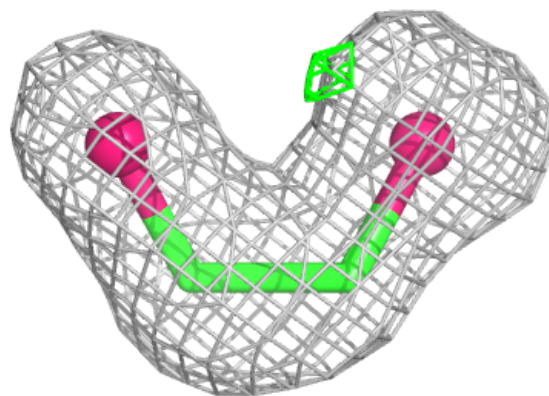
Electron density around ACT F 310:

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



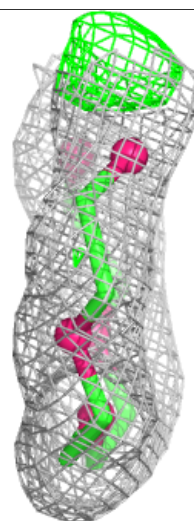
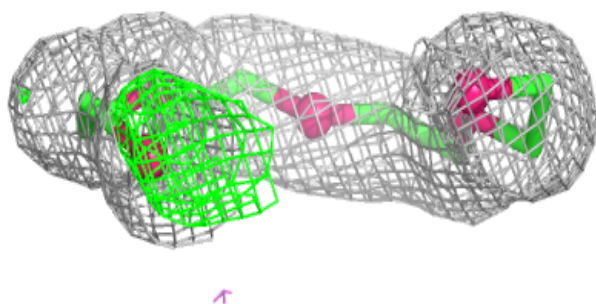
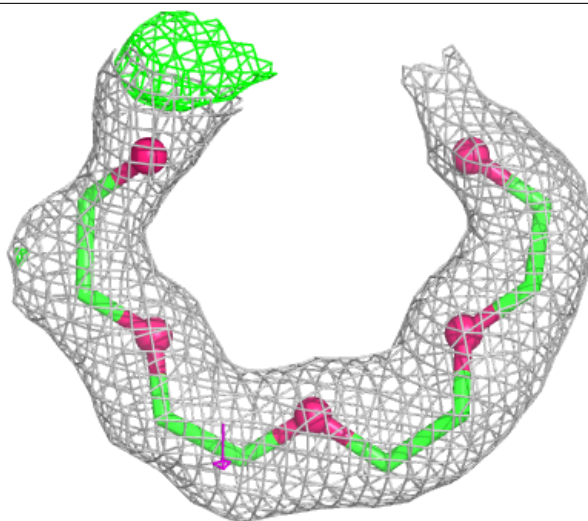
Electron density around EDO D 306:

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



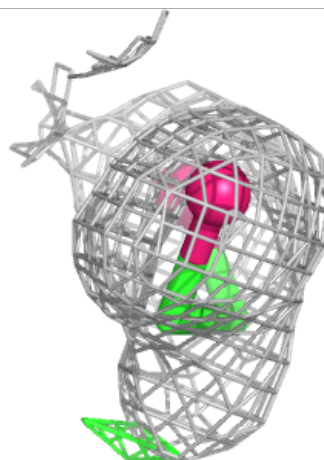
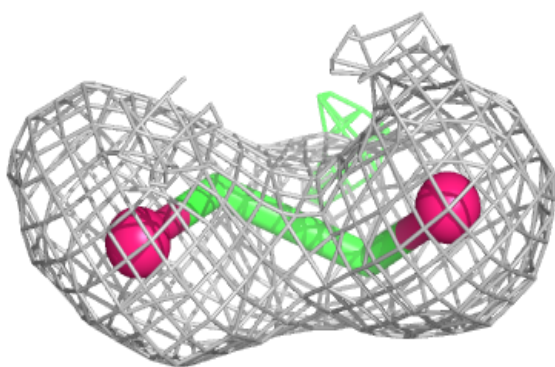
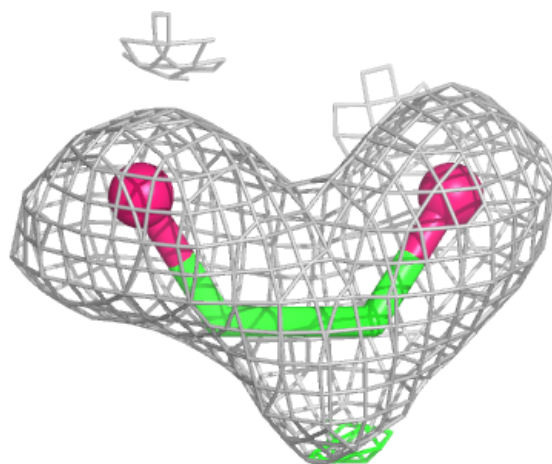
Electron density around PG4 D 303:

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



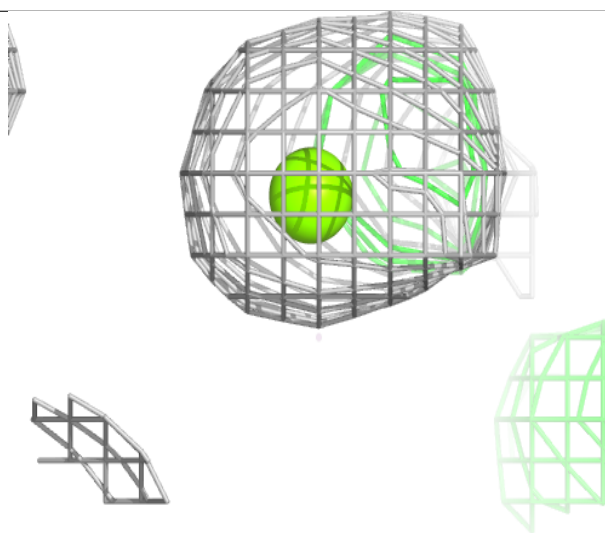
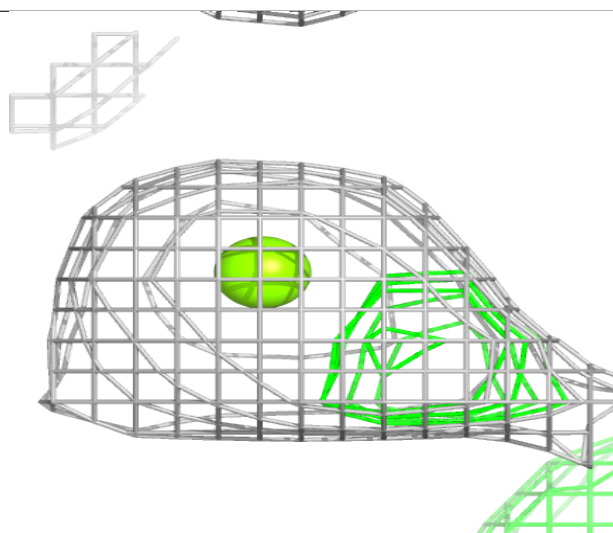
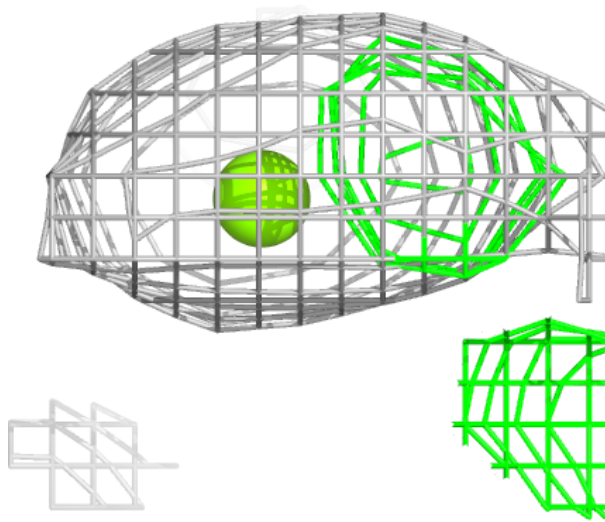
Electron density around EDO A 312:

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



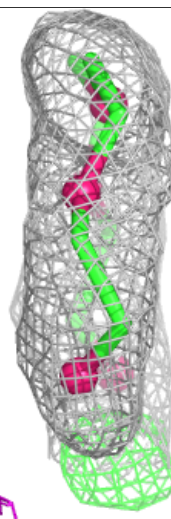
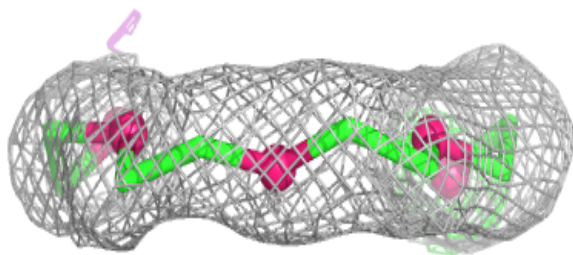
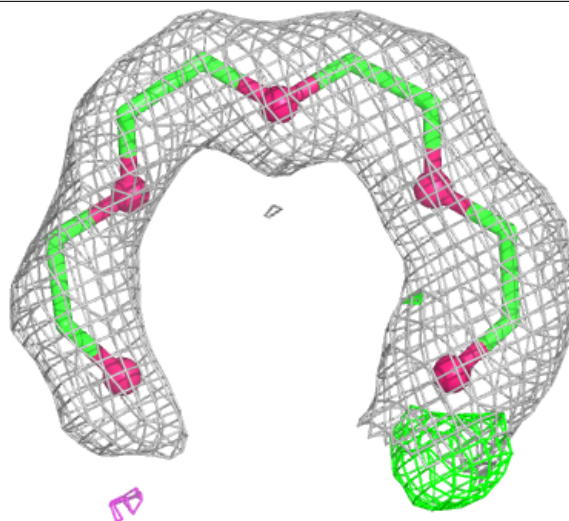
Electron density around MG B 303:

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



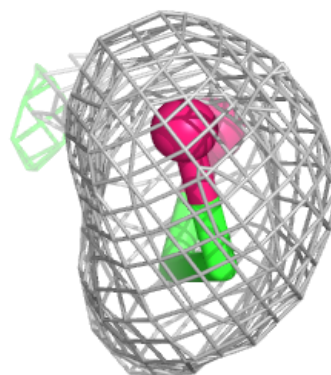
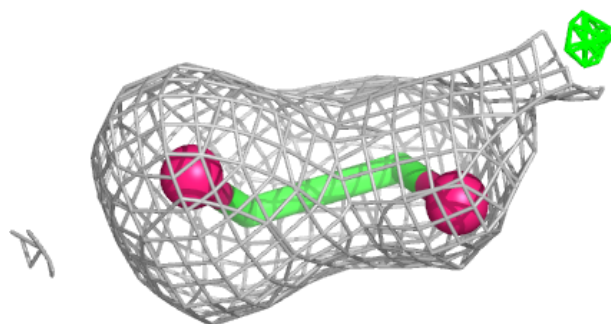
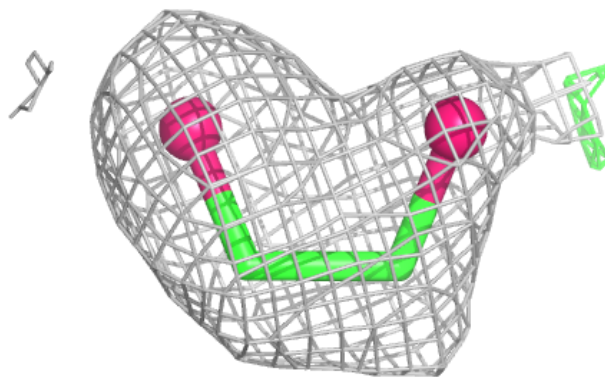
Electron density around PG4 B 305:

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



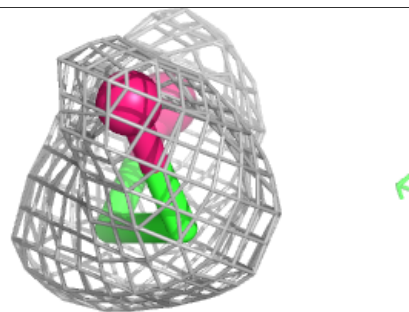
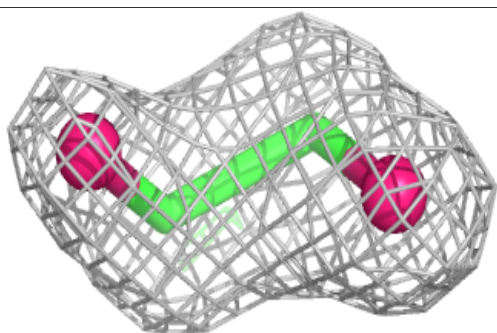
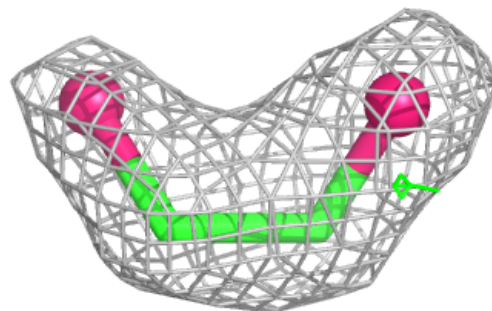
Electron density around EDO C 305:

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



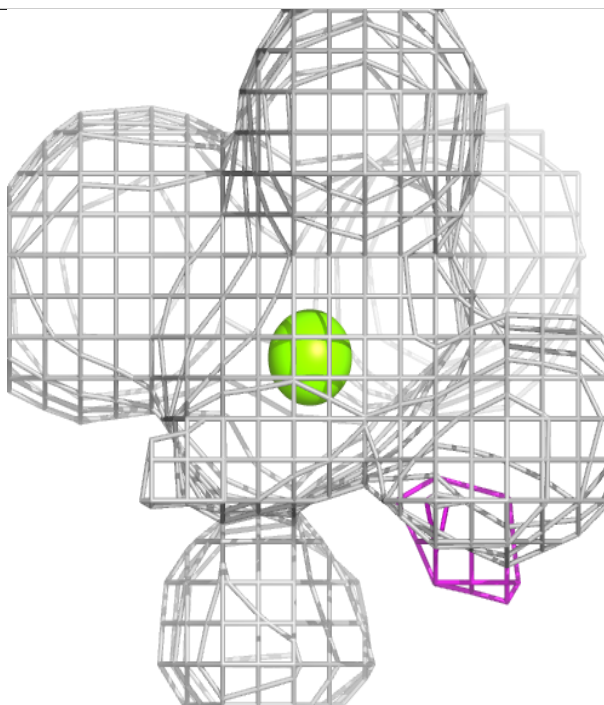
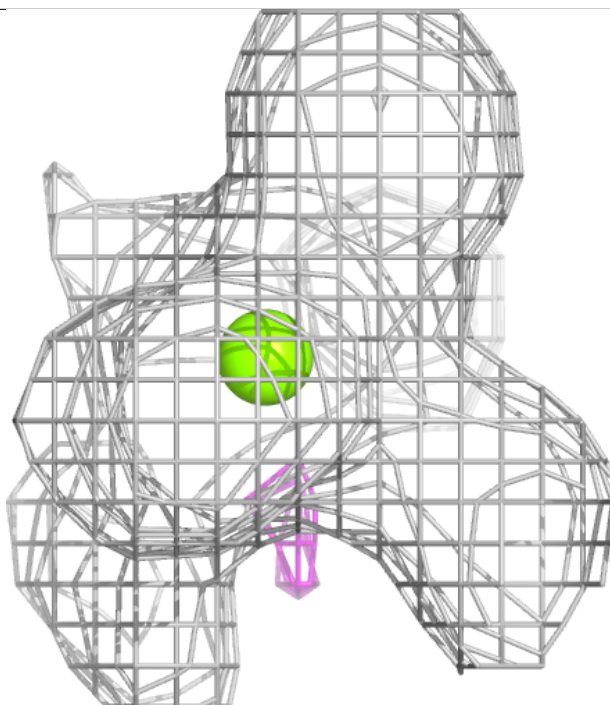
Electron density around EDO D 307:

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



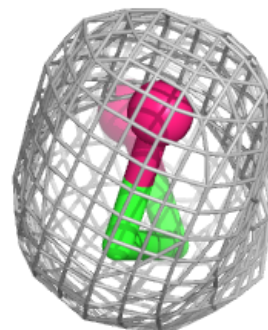
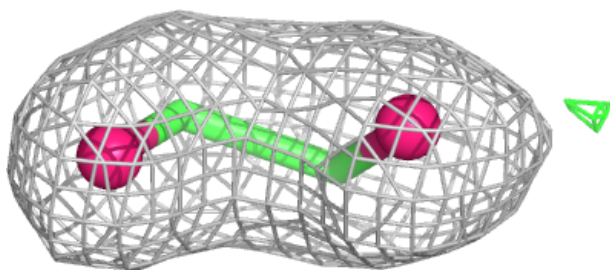
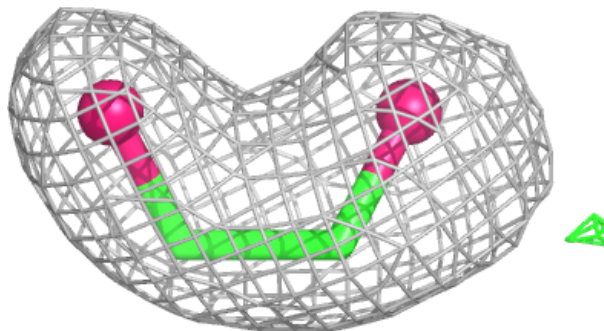
Electron density around MG A 302:

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



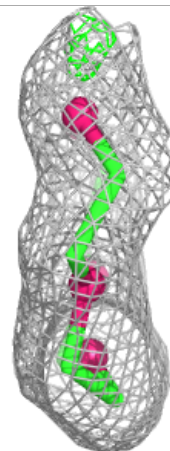
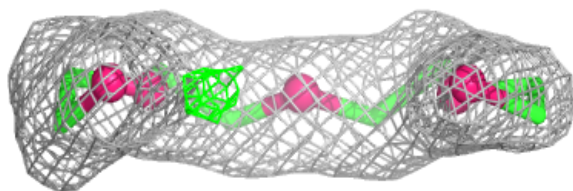
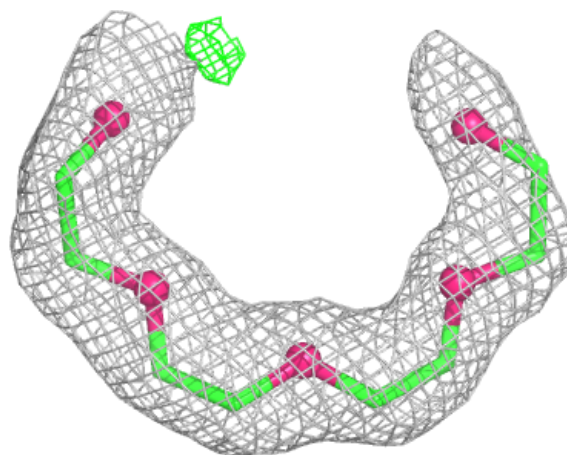
Electron density around EDO A 309:

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



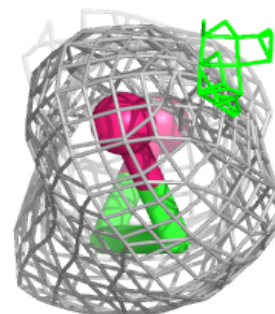
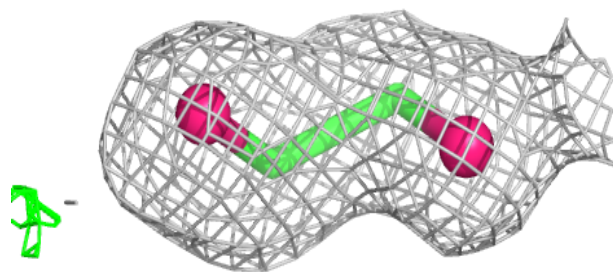
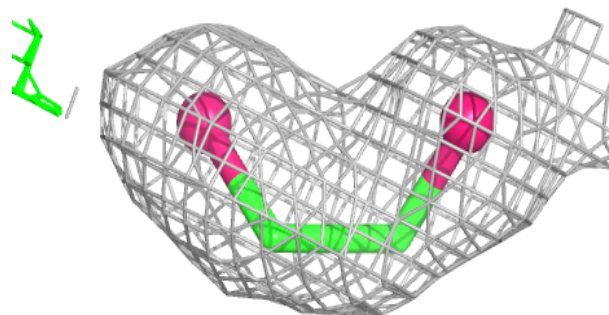
Electron density around PG4 C 303:

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



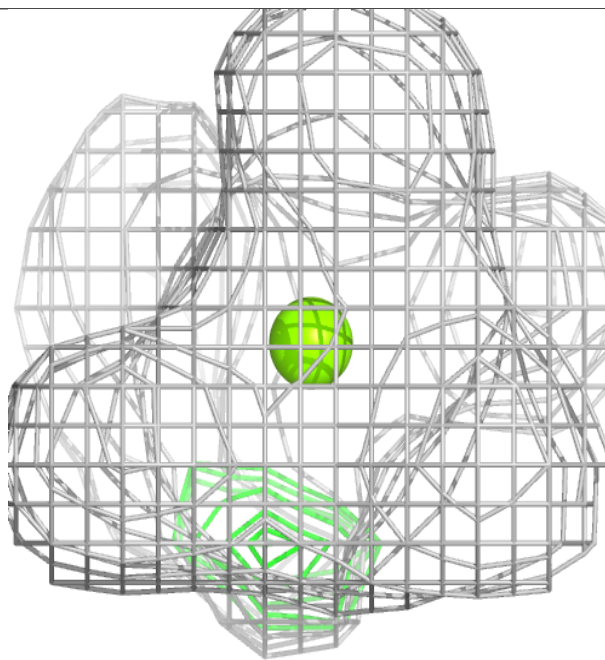
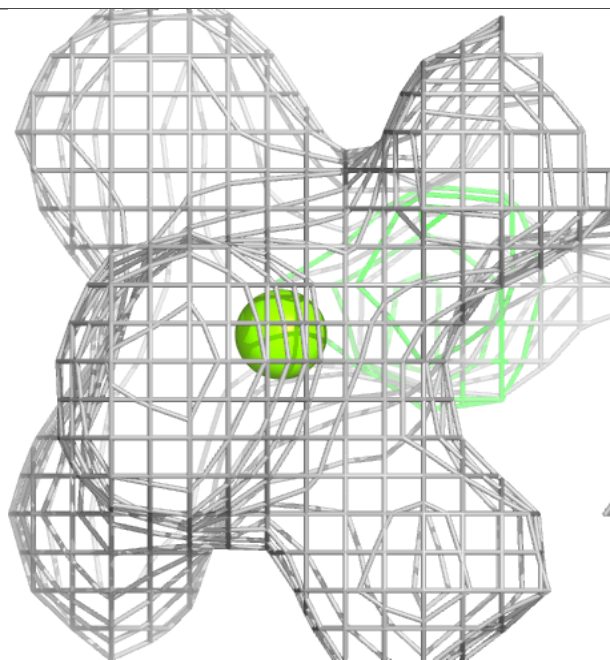
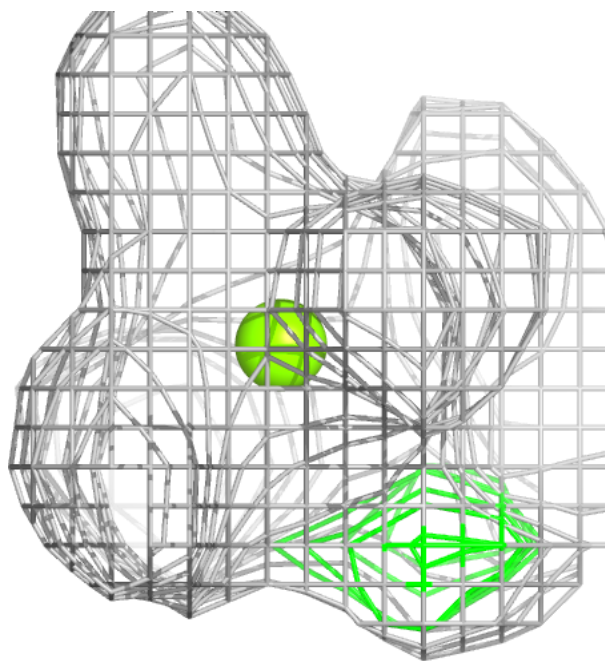
Electron density around EDO D 304:

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



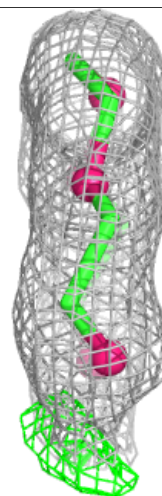
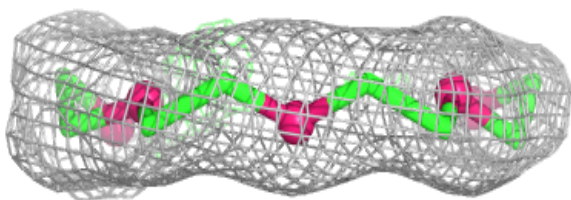
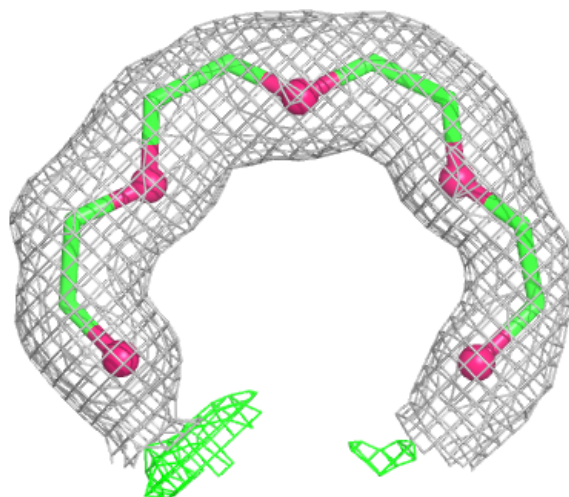
Electron density around MG C 301:

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



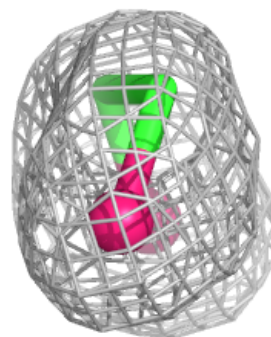
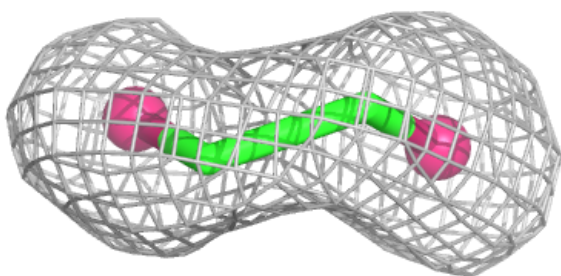
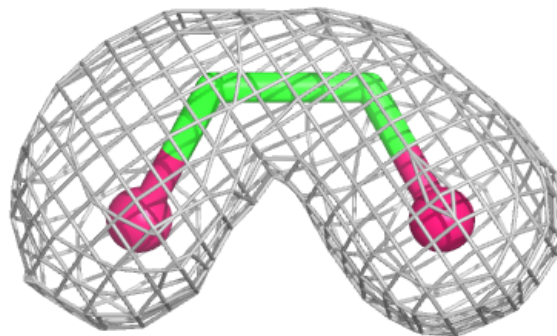
Electron density around PG4 A 306:

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



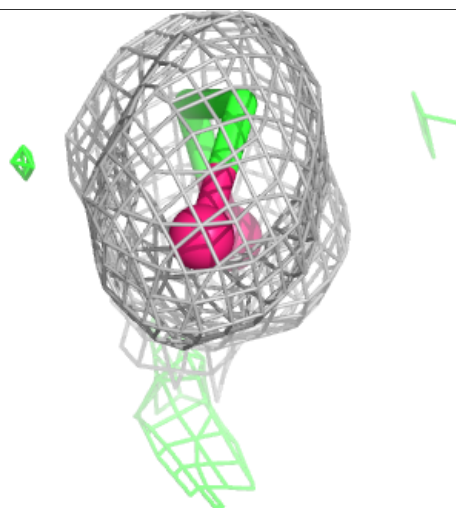
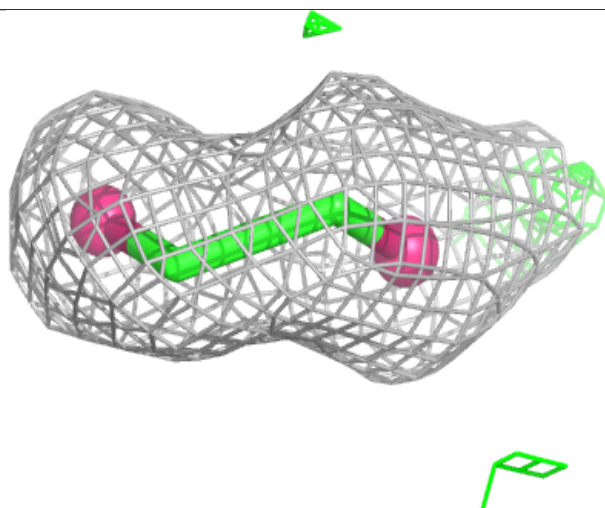
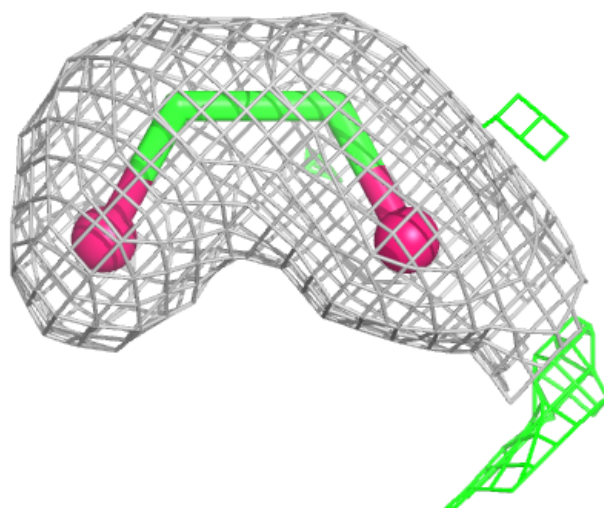
Electron density around EDO F 307:

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



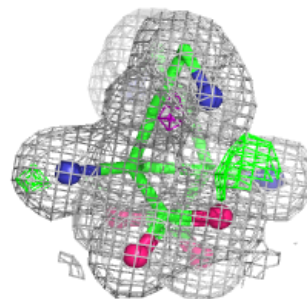
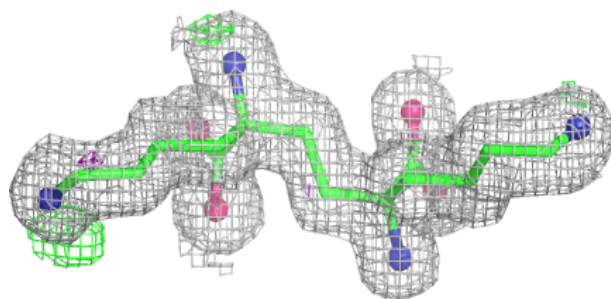
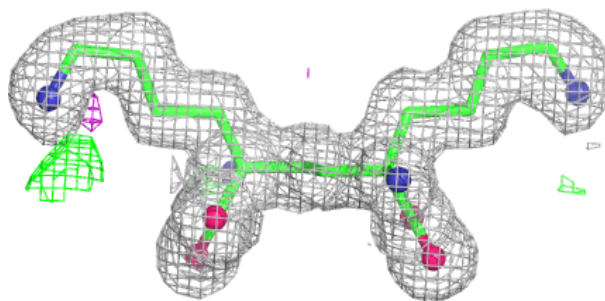
Electron density around EDO A 314:

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

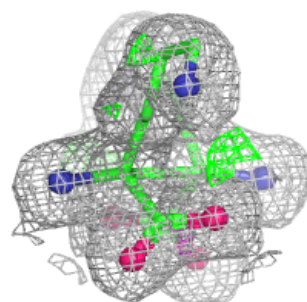
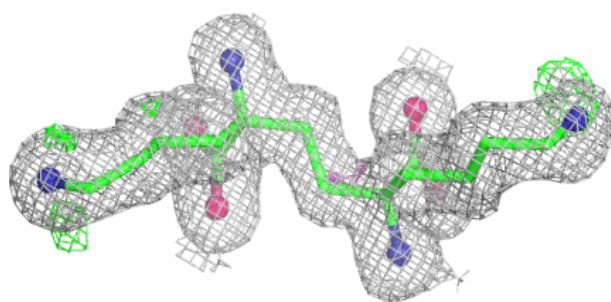
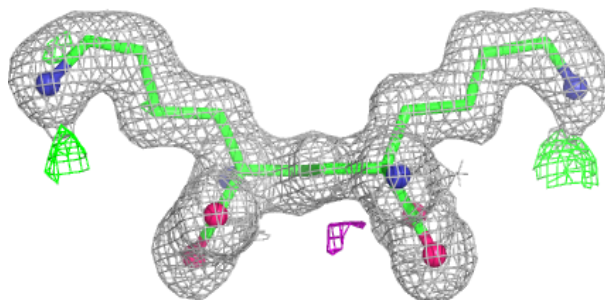


Electron density around 3VN A 301:

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

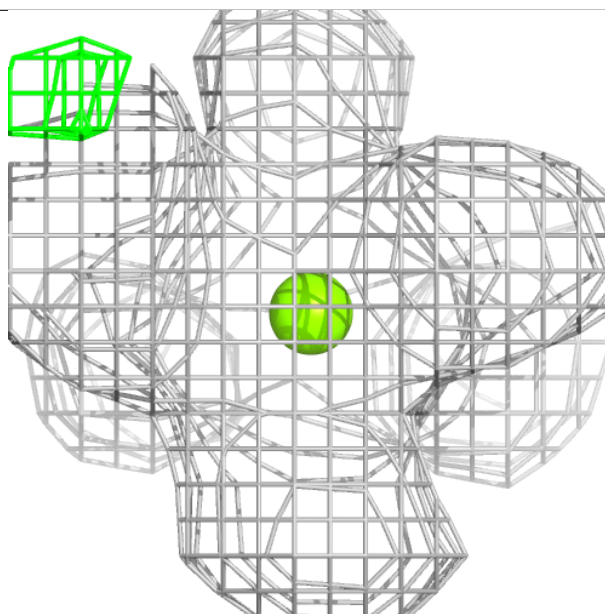
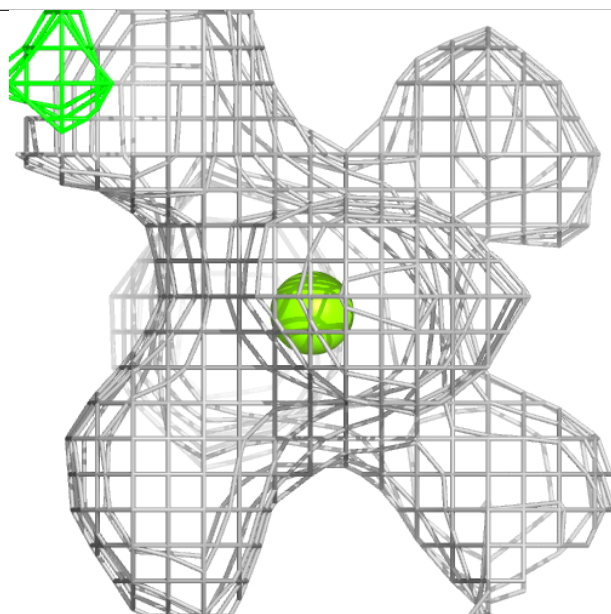
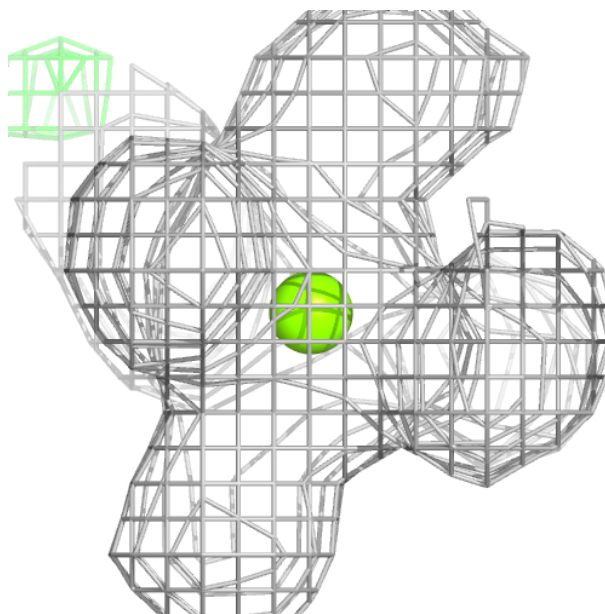
**Electron density around 3VN B 301:**

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



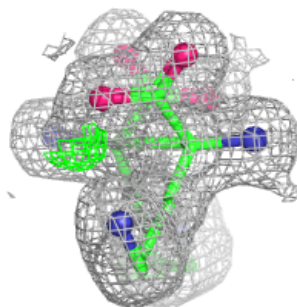
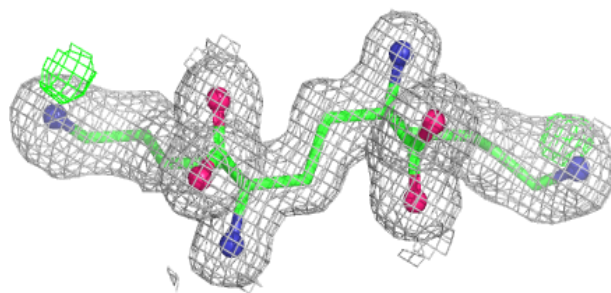
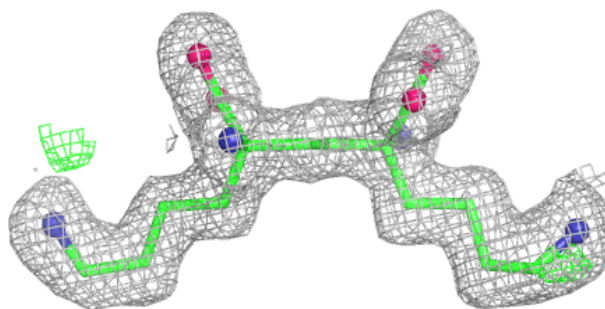
Electron density around MG F 303:

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



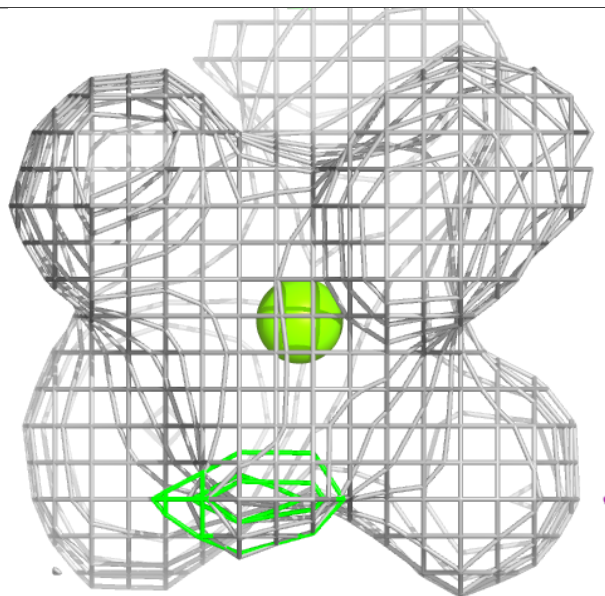
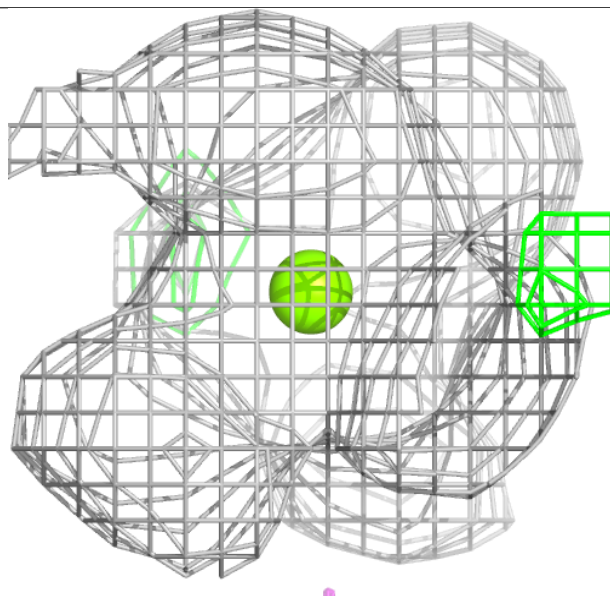
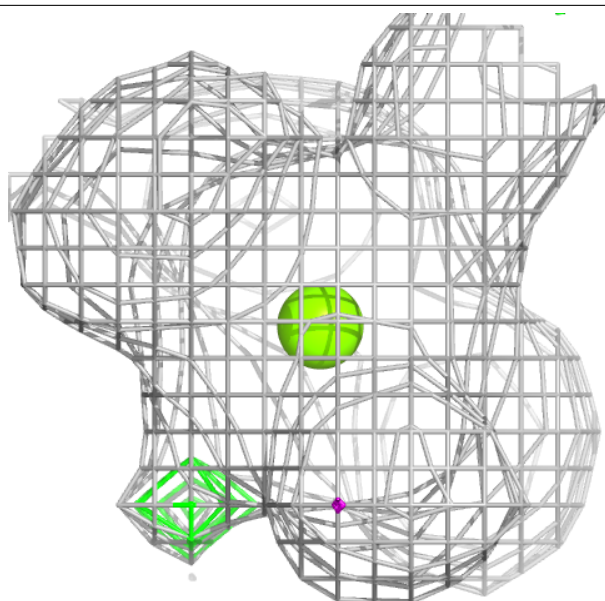
Electron density around 3VN D 301:

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



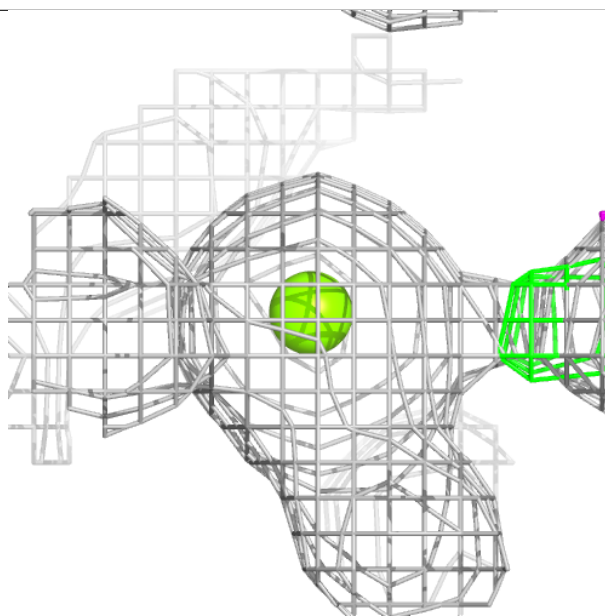
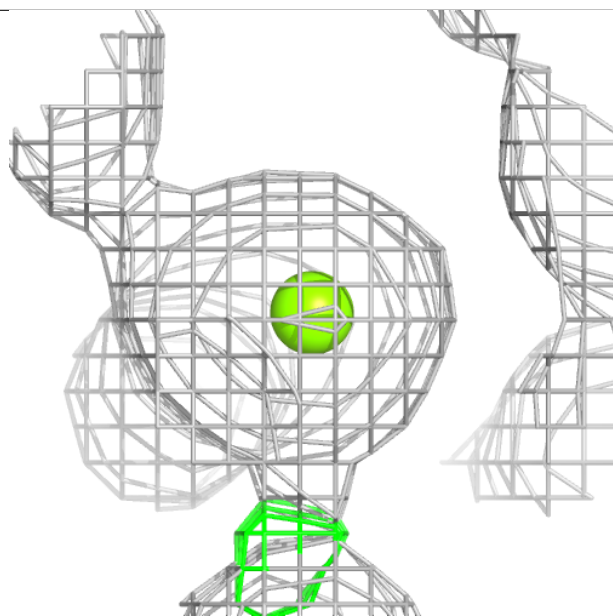
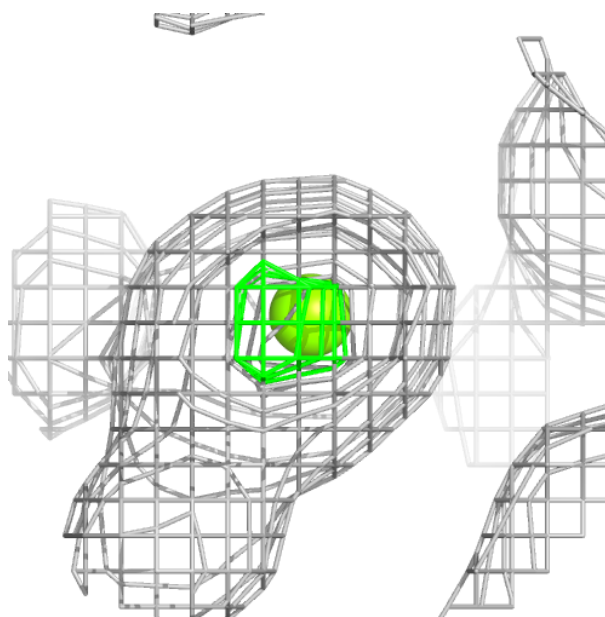
Electron density around MG C 302:

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



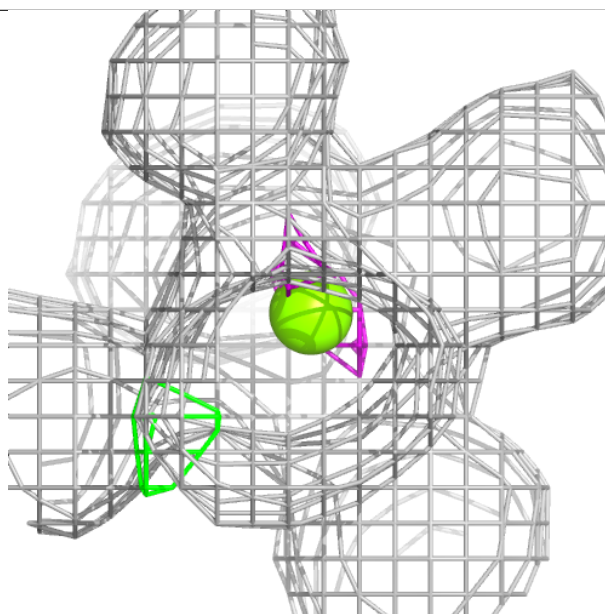
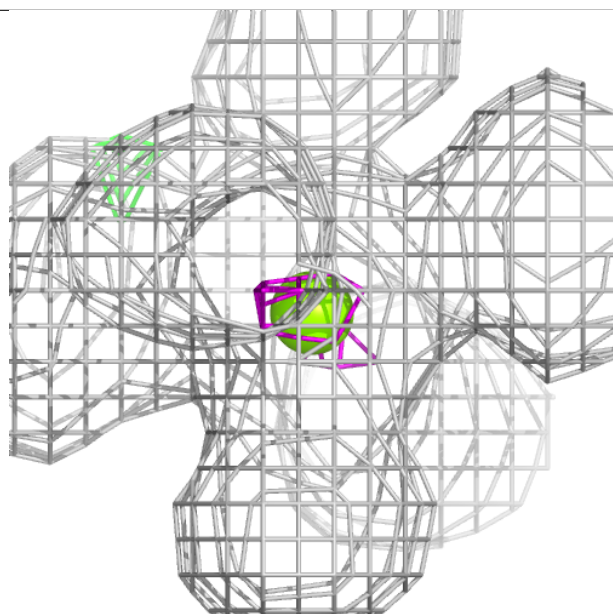
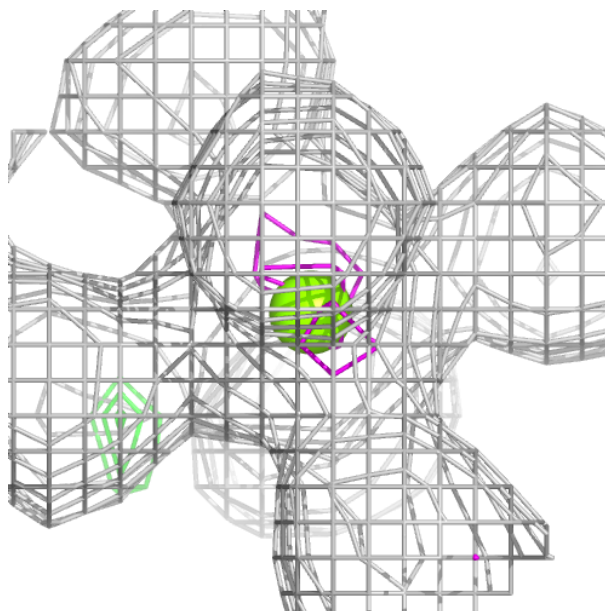
Electron density around MG F 302:

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



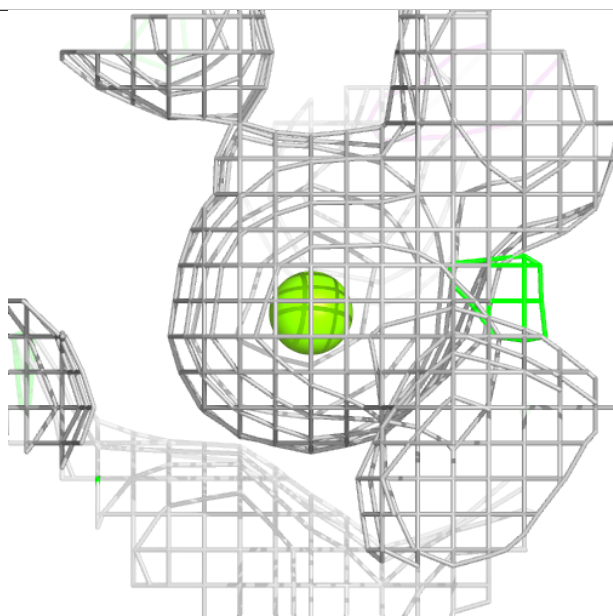
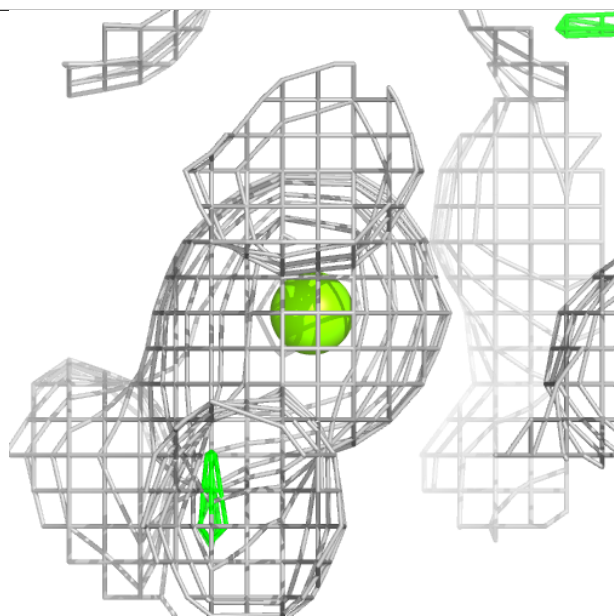
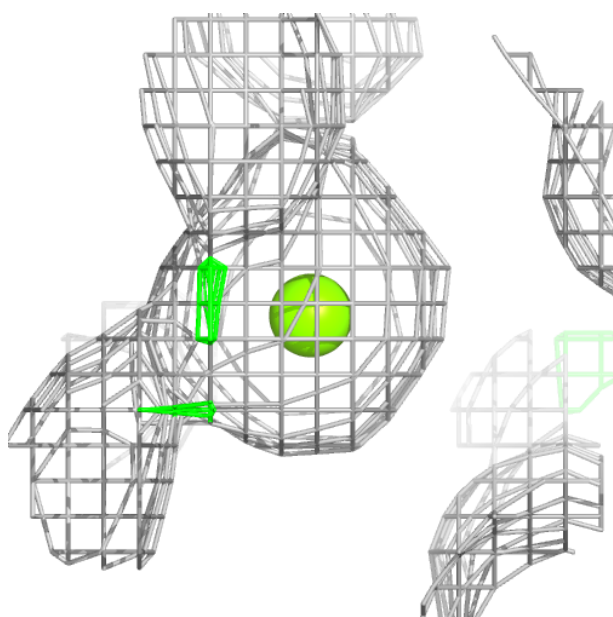
Electron density around MG F 301:

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



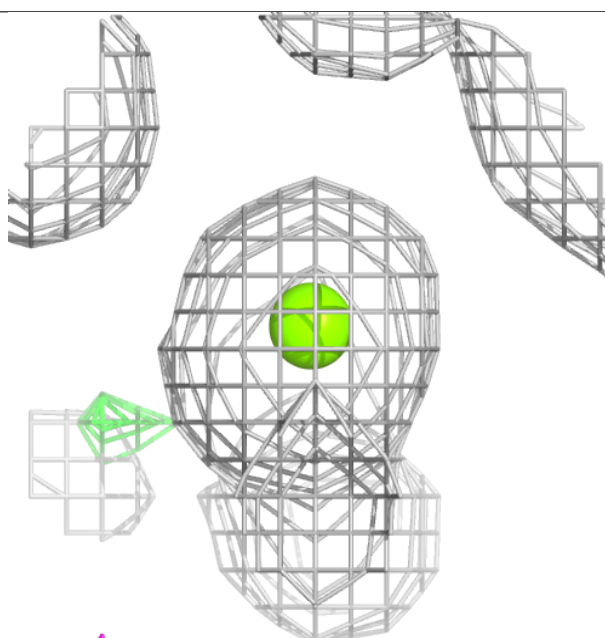
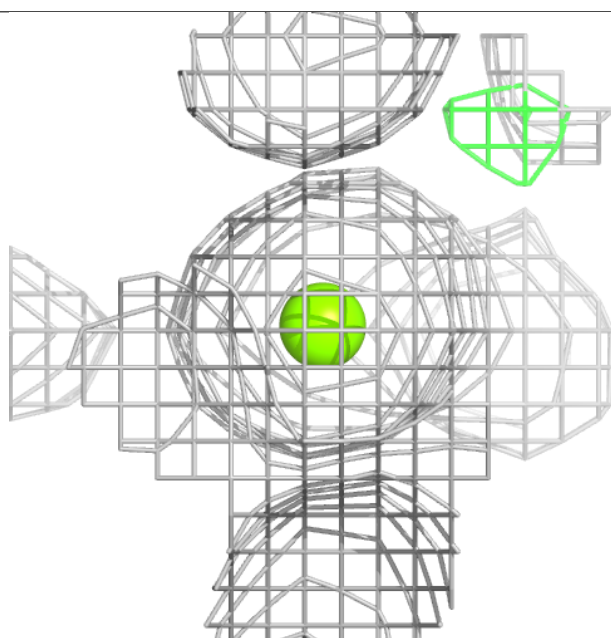
Electron density around MG E 301:

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



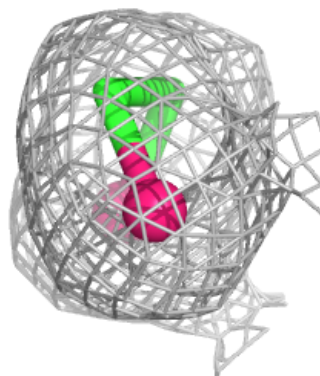
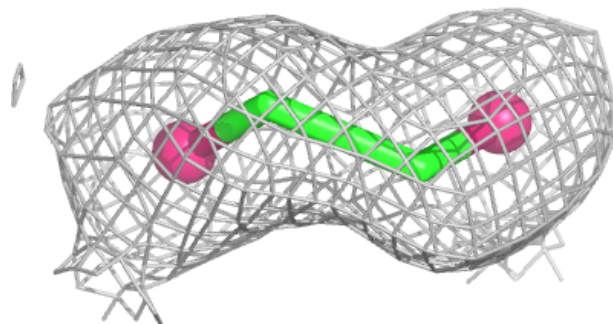
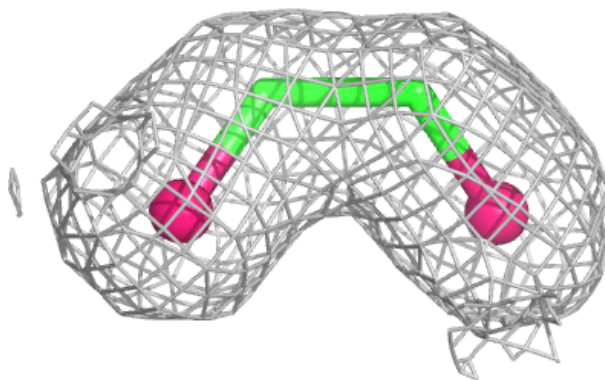
Electron density around MG E 302:

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



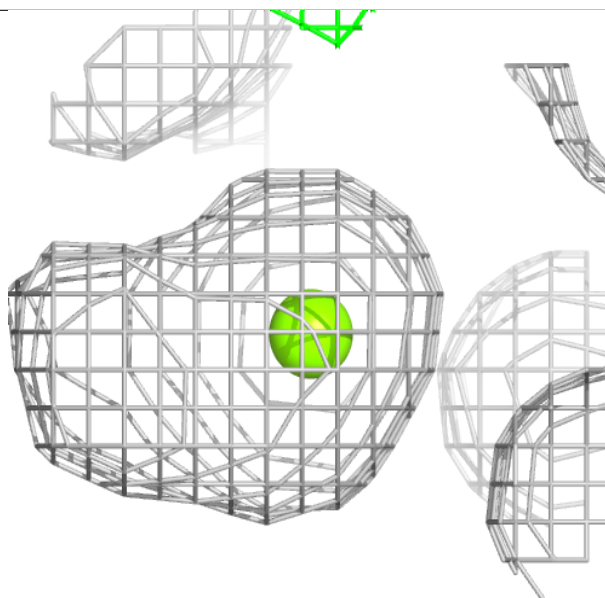
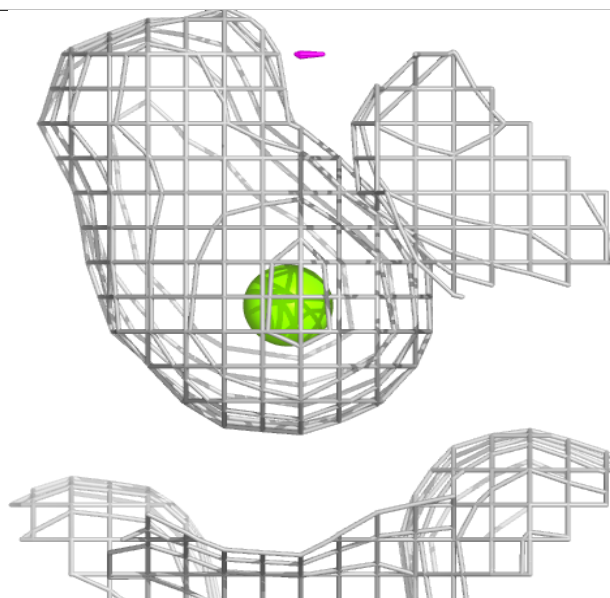
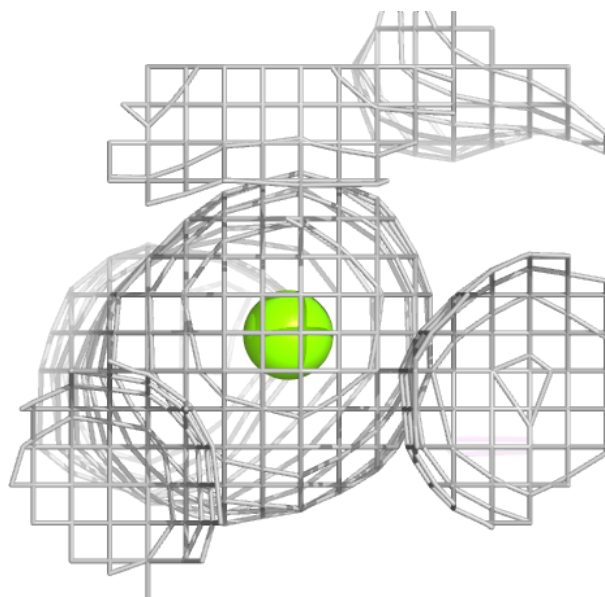
Electron density around EDO E 311:

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



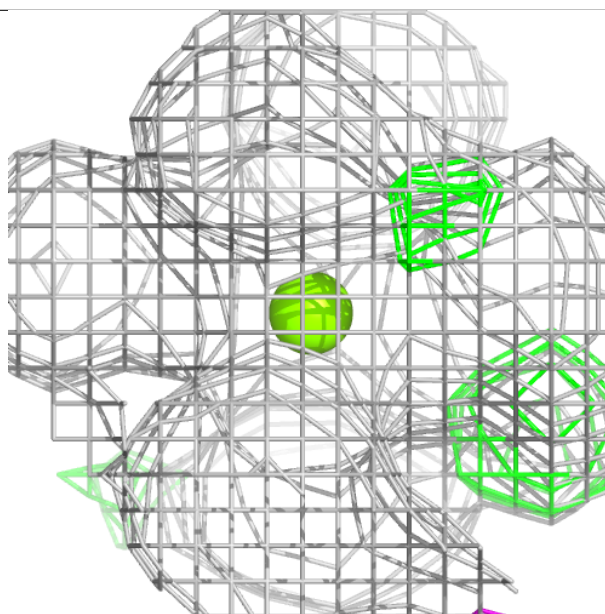
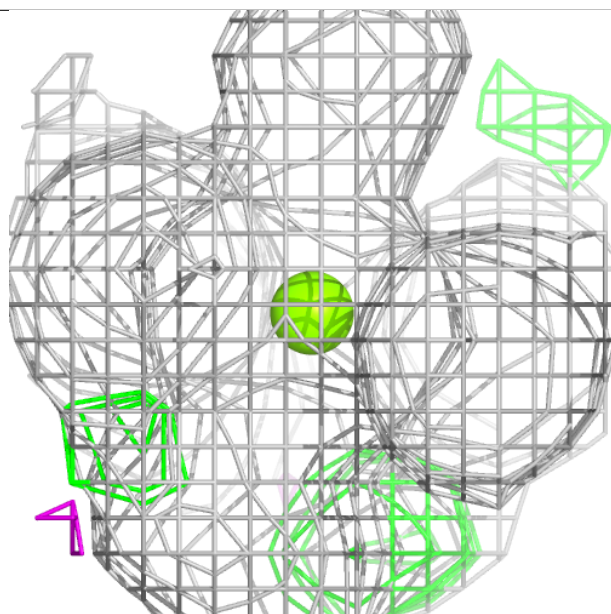
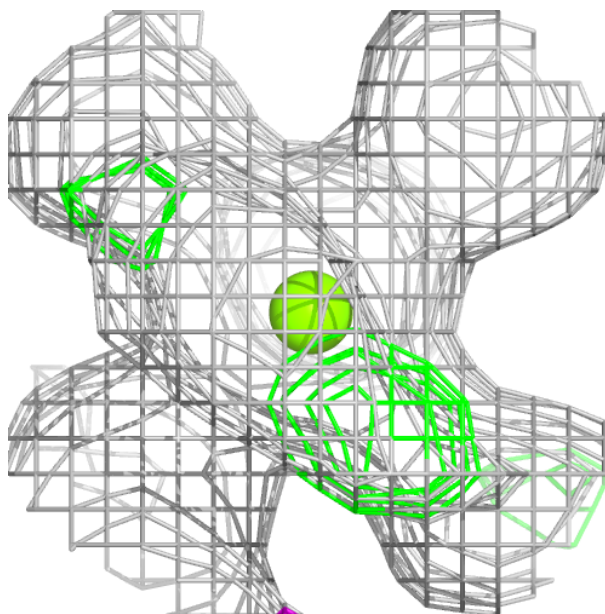
Electron density around MG E 303:

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



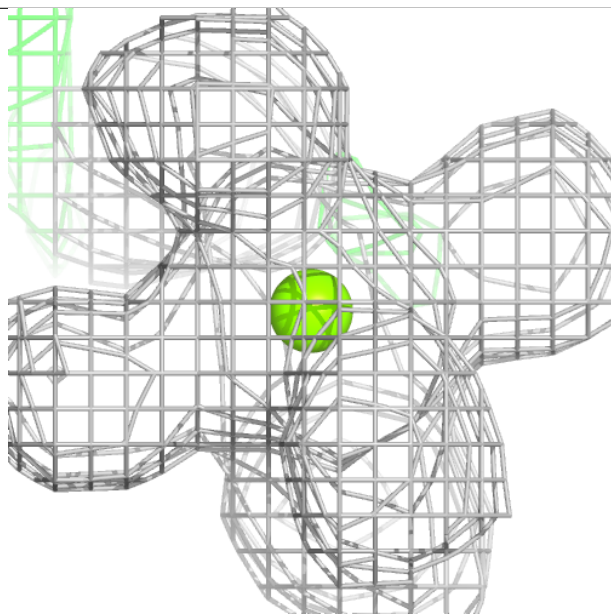
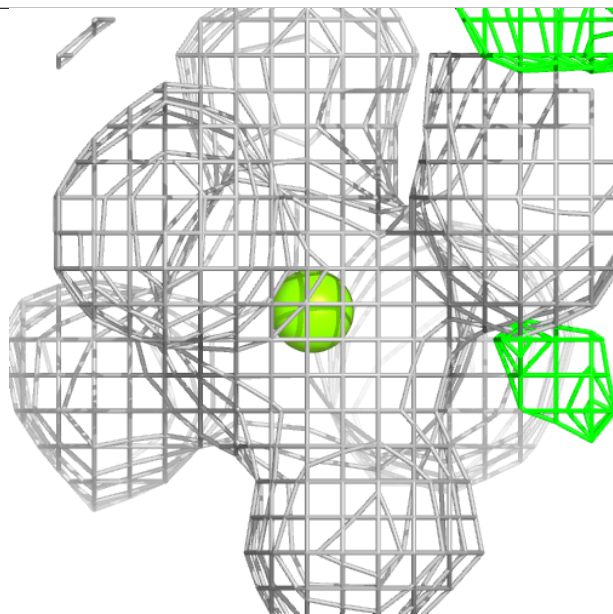
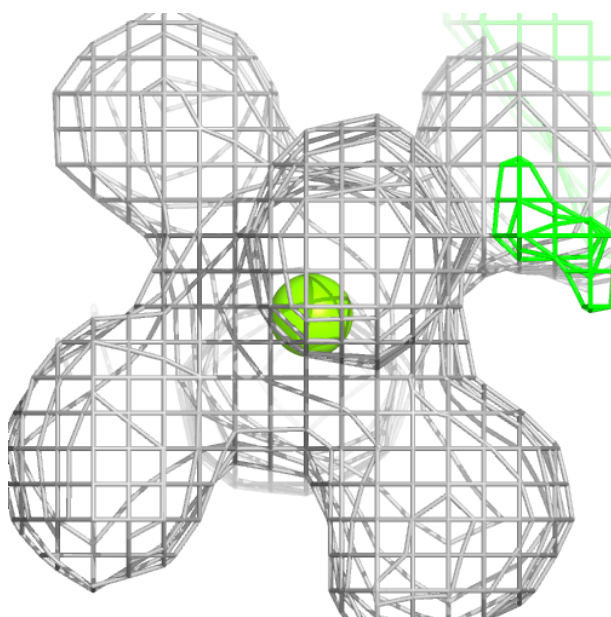
Electron density around MG A 304:

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



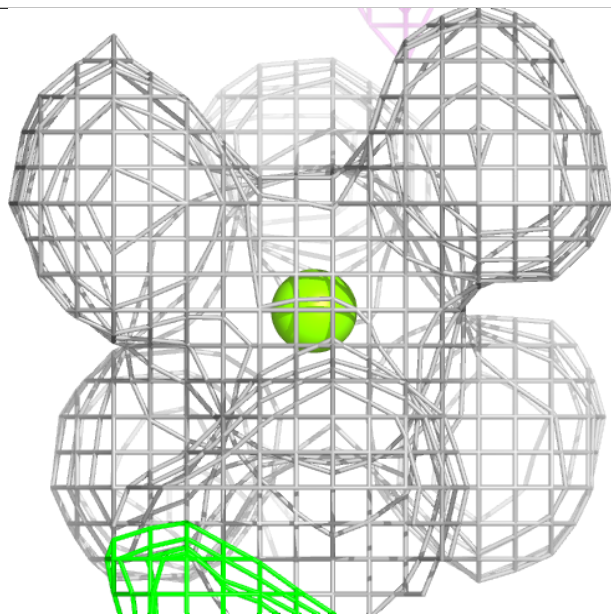
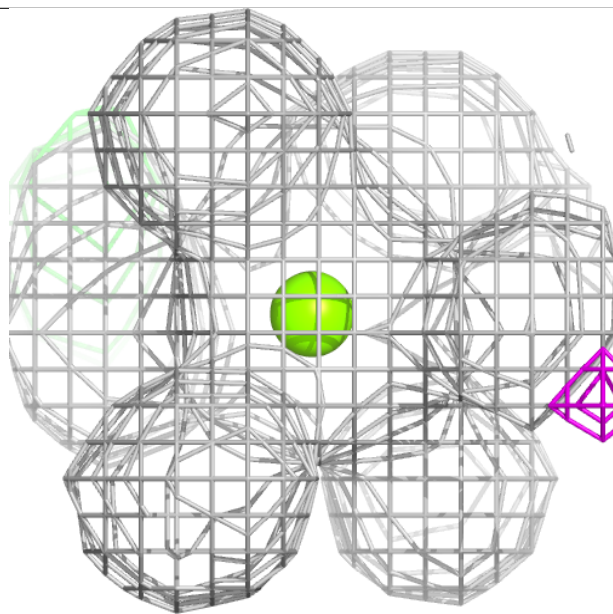
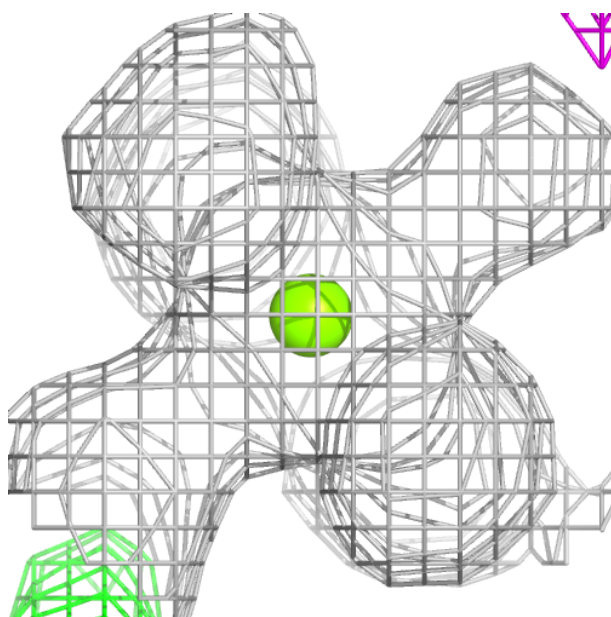
Electron density around MG D 302:

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



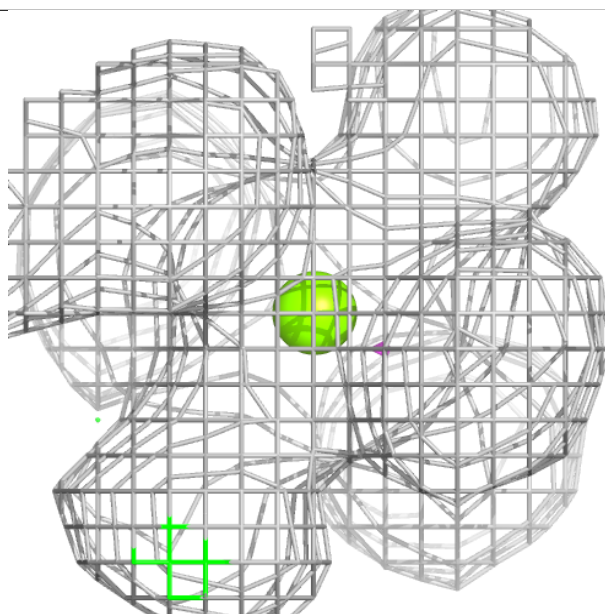
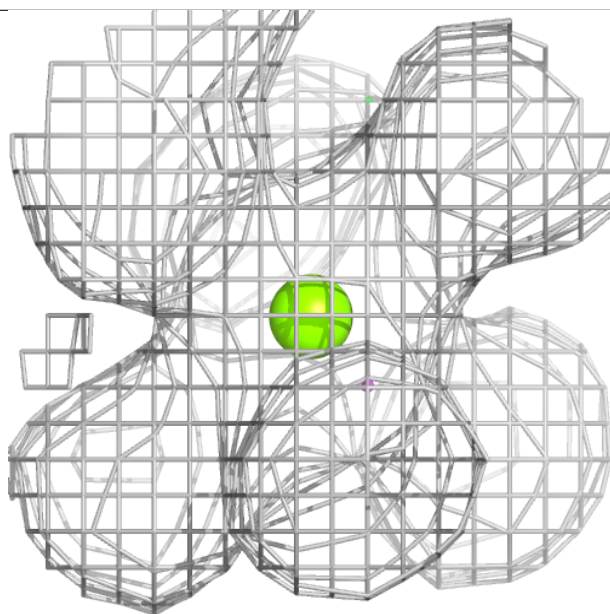
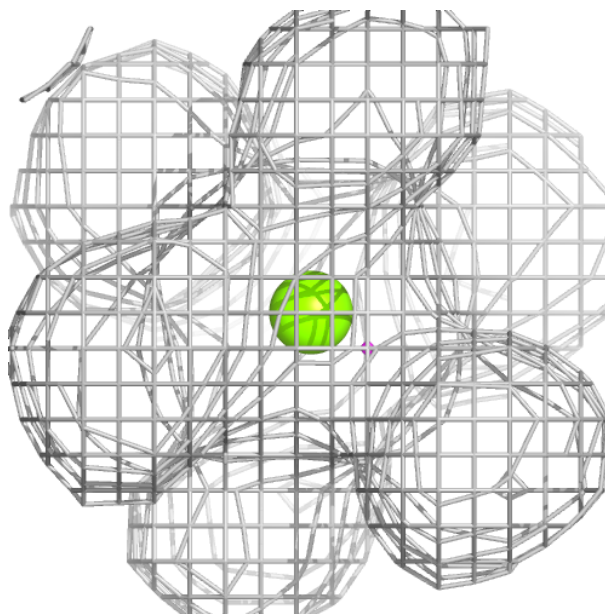
Electron density around MG B 302:

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



Electron density around MG A 303:

$2mF_o-DF_c$ (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.