



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 06:33 PM EDT

PDB ID : 7KG2
Title : Dihydrodipicolinate synthase (DHDPS) from *C.jejuni*, H59K mutant with pyruvate bound in the active site and L-histidine bound at the allosteric site
Authors : Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.
Deposited on : 2020-10-15
Resolution : 1.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

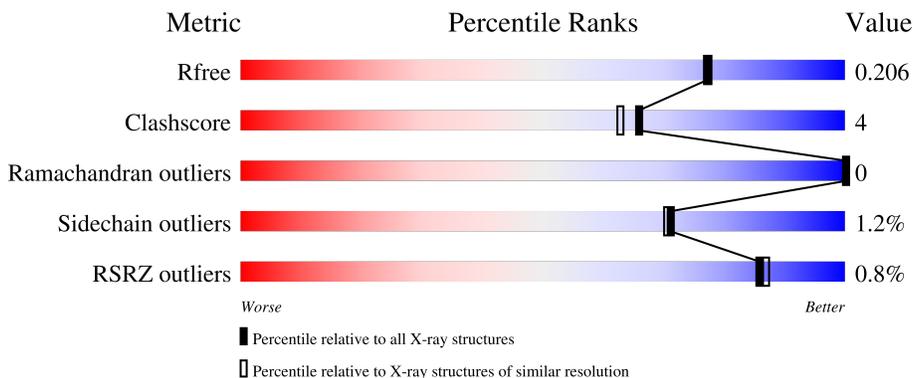
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	 87% 7% • 5%
1	B	310	 86% 8% • 5%
1	C	310	 86% 8% • 5%
1	D	310	 87% 7% • 5%
1	E	310	 85% 10% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	 % 89% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	304	-	-	X	-
2	EDO	C	302	-	-	X	-
2	EDO	E	307	-	-	X	-
8	PEG	E	316	-	X	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 14872 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
			Total	C	N	O	S			
1	A	296	2279	1450	378	438	13	0	0	0
1	B	296	2283	1451	378	441	13	0	2	0
1	C	296	2281	1451	378	439	13	0	1	0
1	D	296	2277	1449	377	438	13	0	0	0
1	E	296	2281	1450	377	441	13	0	2	0
1	F	297	2290	1455	379	443	13	0	1	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP A0A2U0QMK8
A	-10	ARG	-	expression tag	UNP A0A2U0QMK8
A	-9	GLY	-	expression tag	UNP A0A2U0QMK8
A	-8	SER	-	expression tag	UNP A0A2U0QMK8
A	-7	HIS	-	expression tag	UNP A0A2U0QMK8
A	-6	HIS	-	expression tag	UNP A0A2U0QMK8
A	-5	HIS	-	expression tag	UNP A0A2U0QMK8
A	-4	HIS	-	expression tag	UNP A0A2U0QMK8
A	-3	HIS	-	expression tag	UNP A0A2U0QMK8
A	-2	HIS	-	expression tag	UNP A0A2U0QMK8
A	-1	GLY	-	expression tag	UNP A0A2U0QMK8
A	0	SER	-	expression tag	UNP A0A2U0QMK8
A	59	LYS	HIS	engineered mutation	UNP A0A2U0QMK8
B	-11	MET	-	expression tag	UNP A0A2U0QMK8
B	-10	ARG	-	expression tag	UNP A0A2U0QMK8
B	-9	GLY	-	expression tag	UNP A0A2U0QMK8
B	-8	SER	-	expression tag	UNP A0A2U0QMK8

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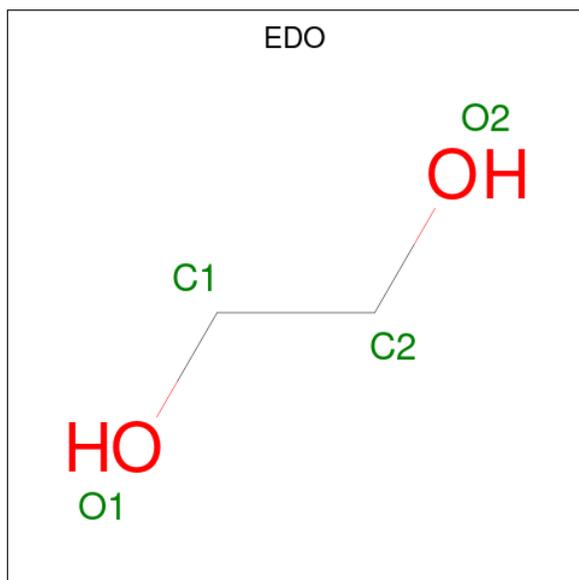
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP A0A2U0QMK8
B	-6	HIS	-	expression tag	UNP A0A2U0QMK8
B	-5	HIS	-	expression tag	UNP A0A2U0QMK8
B	-4	HIS	-	expression tag	UNP A0A2U0QMK8
B	-3	HIS	-	expression tag	UNP A0A2U0QMK8
B	-2	HIS	-	expression tag	UNP A0A2U0QMK8
B	-1	GLY	-	expression tag	UNP A0A2U0QMK8
B	0	SER	-	expression tag	UNP A0A2U0QMK8
B	59	LYS	HIS	engineered mutation	UNP A0A2U0QMK8
C	-11	MET	-	expression tag	UNP A0A2U0QMK8
C	-10	ARG	-	expression tag	UNP A0A2U0QMK8
C	-9	GLY	-	expression tag	UNP A0A2U0QMK8
C	-8	SER	-	expression tag	UNP A0A2U0QMK8
C	-7	HIS	-	expression tag	UNP A0A2U0QMK8
C	-6	HIS	-	expression tag	UNP A0A2U0QMK8
C	-5	HIS	-	expression tag	UNP A0A2U0QMK8
C	-4	HIS	-	expression tag	UNP A0A2U0QMK8
C	-3	HIS	-	expression tag	UNP A0A2U0QMK8
C	-2	HIS	-	expression tag	UNP A0A2U0QMK8
C	-1	GLY	-	expression tag	UNP A0A2U0QMK8
C	0	SER	-	expression tag	UNP A0A2U0QMK8
C	59	LYS	HIS	engineered mutation	UNP A0A2U0QMK8
D	-11	MET	-	expression tag	UNP A0A2U0QMK8
D	-10	ARG	-	expression tag	UNP A0A2U0QMK8
D	-9	GLY	-	expression tag	UNP A0A2U0QMK8
D	-8	SER	-	expression tag	UNP A0A2U0QMK8
D	-7	HIS	-	expression tag	UNP A0A2U0QMK8
D	-6	HIS	-	expression tag	UNP A0A2U0QMK8
D	-5	HIS	-	expression tag	UNP A0A2U0QMK8
D	-4	HIS	-	expression tag	UNP A0A2U0QMK8
D	-3	HIS	-	expression tag	UNP A0A2U0QMK8
D	-2	HIS	-	expression tag	UNP A0A2U0QMK8
D	-1	GLY	-	expression tag	UNP A0A2U0QMK8
D	0	SER	-	expression tag	UNP A0A2U0QMK8
D	59	LYS	HIS	engineered mutation	UNP A0A2U0QMK8
E	-11	MET	-	expression tag	UNP A0A2U0QMK8
E	-10	ARG	-	expression tag	UNP A0A2U0QMK8
E	-9	GLY	-	expression tag	UNP A0A2U0QMK8
E	-8	SER	-	expression tag	UNP A0A2U0QMK8
E	-7	HIS	-	expression tag	UNP A0A2U0QMK8
E	-6	HIS	-	expression tag	UNP A0A2U0QMK8
E	-5	HIS	-	expression tag	UNP A0A2U0QMK8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP A0A2U0QMK8
E	-3	HIS	-	expression tag	UNP A0A2U0QMK8
E	-2	HIS	-	expression tag	UNP A0A2U0QMK8
E	-1	GLY	-	expression tag	UNP A0A2U0QMK8
E	0	SER	-	expression tag	UNP A0A2U0QMK8
E	59	LYS	HIS	engineered mutation	UNP A0A2U0QMK8
F	-11	MET	-	expression tag	UNP A0A2U0QMK8
F	-10	ARG	-	expression tag	UNP A0A2U0QMK8
F	-9	GLY	-	expression tag	UNP A0A2U0QMK8
F	-8	SER	-	expression tag	UNP A0A2U0QMK8
F	-7	HIS	-	expression tag	UNP A0A2U0QMK8
F	-6	HIS	-	expression tag	UNP A0A2U0QMK8
F	-5	HIS	-	expression tag	UNP A0A2U0QMK8
F	-4	HIS	-	expression tag	UNP A0A2U0QMK8
F	-3	HIS	-	expression tag	UNP A0A2U0QMK8
F	-2	HIS	-	expression tag	UNP A0A2U0QMK8
F	-1	GLY	-	expression tag	UNP A0A2U0QMK8
F	0	SER	-	expression tag	UNP A0A2U0QMK8
F	59	LYS	HIS	engineered mutation	UNP A0A2U0QMK8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

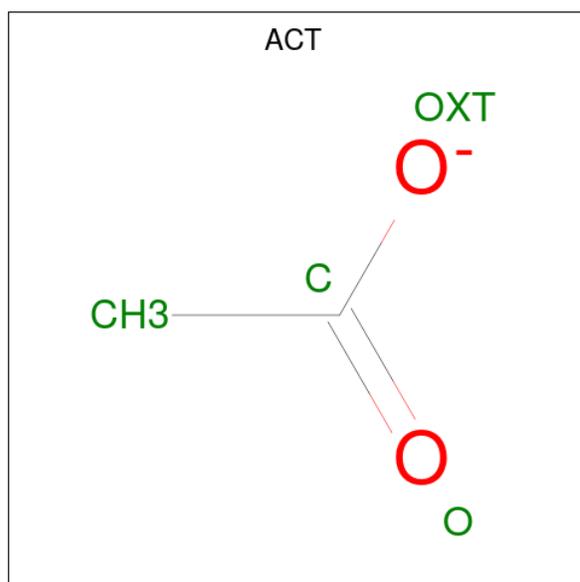
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Mg 5 5	0	0
3	B	2	Total Mg 2 2	0	0
3	C	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	3	Total Mg 3 3	0	0
3	E	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



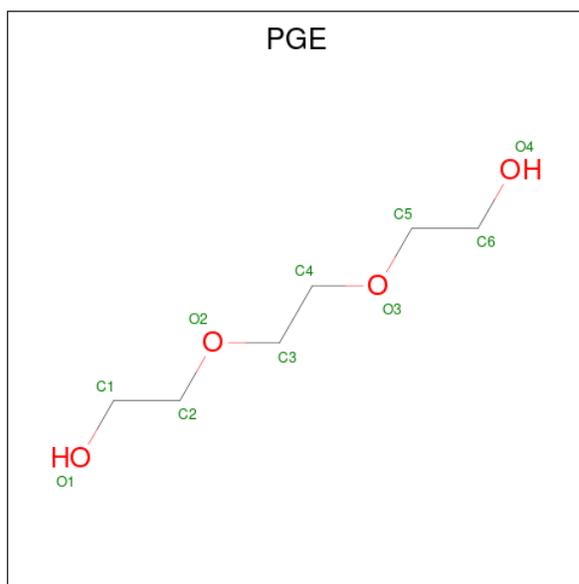
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



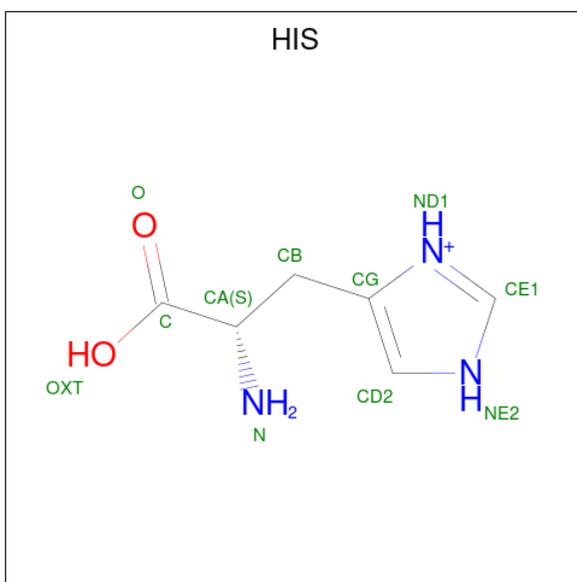
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		

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

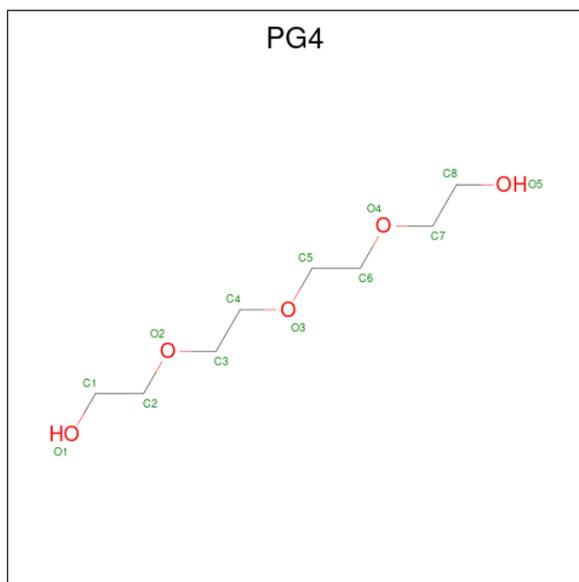
- Molecule 6 is HISTIDINE (three-letter code: HIS) (formula: C₆H₁₀N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	6	3	2		
6	B	1	Total	C	N	O	0	0
			11	6	3	2		
6	C	1	Total	C	N	O	0	0
			11	6	3	2		
6	D	1	Total	C	N	O	0	0
			11	6	3	2		
6	E	1	Total	C	N	O	0	0
			11	6	3	2		
6	F	1	Total	C	N	O	0	0
			11	6	3	2		

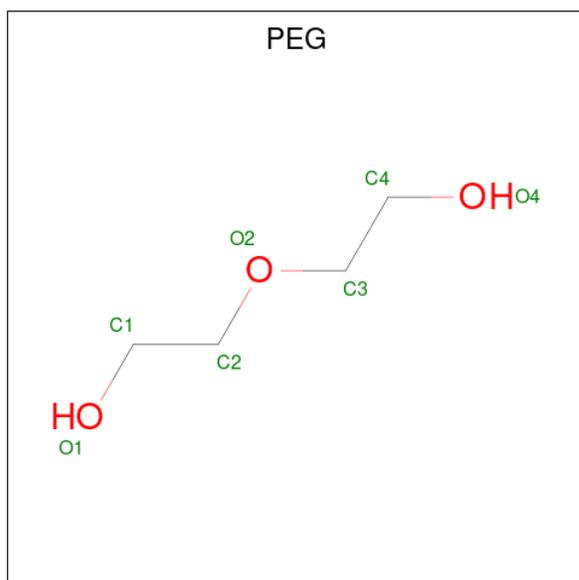
- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			7	4	3		

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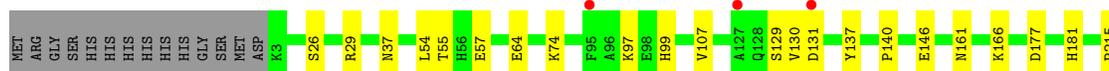
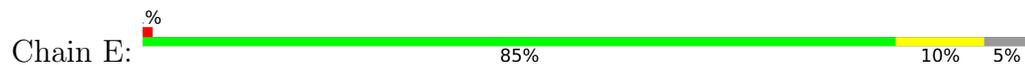
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		
8	E	1	Total	C	O	0	0
			7	4	3		
8	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is water.

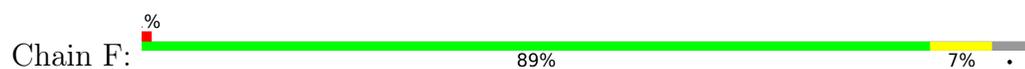
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	136	Total	O	0	0
			136	136		
9	B	126	Total	O	0	0
			126	126		
9	C	128	Total	O	0	0
			128	128		
9	D	128	Total	O	0	0
			128	128		
9	E	110	Total	O	0	0
			110	110		
9	F	133	Total	O	0	0
			133	133		



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.78Å 230.74Å 202.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 1.89 49.63 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.63-1.89) 98.8 (49.63-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.207 0.170 , 0.206	Depositor DCC
R_{free} test set	7806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14872	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, KPI, MG, PG4, PEG, PGE, EDO

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	0.86	2/2302 (0.1%)	0.81	1/3109 (0.0%)
1	B	0.80	0/2316	0.75	0/3129
1	C	0.81	0/2308	0.73	0/3117
1	D	0.76	0/2300	0.77	0/3107
1	E	0.80	0/2315	0.80	3/3127 (0.1%)
1	F	0.78	0/2318	0.71	0/3131
All	All	0.80	2/13859 (0.0%)	0.76	4/18720 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLU	CD-OE1	-6.07	1.19	1.25
1	A	270	GLU	CD-OE2	-5.13	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	216	ASP	CB-CG-OD1	8.84	126.25	118.30
1	E	216	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	E	215	PRO	O-C-N	5.82	132.01	122.70
1	A	273	LEU	CB-CG-CD1	5.26	119.95	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2279	0	2325	16	0
1	B	2283	0	2320	22	0
1	C	2281	0	2326	24	0
1	D	2277	0	2319	18	0
1	E	2281	0	2317	26	0
1	F	2290	0	2330	12	0
2	A	28	0	42	0	0
2	B	20	0	30	7	0
2	C	24	0	36	8	0
2	D	36	0	54	1	0
2	E	28	0	42	10	0
2	F	16	0	24	1	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
4	A	12	0	9	2	0
4	B	12	0	9	0	0
4	C	4	0	3	1	0
4	D	12	0	9	1	0
4	E	8	0	6	0	0
4	F	12	0	9	0	0
5	A	10	0	14	0	0
5	B	20	0	28	0	0
5	C	10	0	14	0	0
5	D	10	0	14	1	0
5	E	30	0	42	1	0
6	A	11	0	6	1	0
6	B	11	0	6	0	0
6	C	11	0	6	0	0
6	D	11	0	6	2	0
6	E	11	0	6	1	0
6	F	11	0	6	1	0
7	D	13	0	18	0	0
8	D	21	0	30	2	0
8	E	14	0	20	4	0
9	A	136	0	0	0	0
9	B	126	0	0	0	0
9	C	128	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	128	0	0	0	0
9	E	110	0	0	1	0
9	F	133	0	0	0	0
All	All	14872	0	14426	115	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 4.

The worst 5 of 115 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:F:273:LEU:H	2:F:302:EDO:H12	1.24	0.98
1:E:29:ARG:HE	2:E:307:EDO:H12	1.32	0.93
1:E:26:SER:HA	2:E:307:EDO:H11	1.52	0.92
1:F:25:GLN:HB3	1:F:29:ARG:NH1	1.93	0.84
1:E:177:ASP:OD1	8:E:316:PEG:H21	1.79	0.82

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	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	B	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
1	C	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	D	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	E	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
1	F	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
All	All	1765/1860 (95%)	1728 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	248/260 (95%)	244 (98%)	4 (2%)	62	60
1	B	249/260 (96%)	244 (98%)	5 (2%)	55	51
1	C	249/260 (96%)	247 (99%)	2 (1%)	81	82
1	D	247/260 (95%)	244 (99%)	3 (1%)	71	70
1	E	249/260 (96%)	247 (99%)	2 (1%)	81	82
1	F	250/260 (96%)	247 (99%)	3 (1%)	71	70
All	All	1492/1560 (96%)	1473 (99%)	19 (1%)	71	68

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	129	SER
1	F	285	LYS
1	F	294	LYS
1	F	74	LYS
1	B	292	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	128	GLN

5.3.3 RNA [i](#)

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	D	166	1	11,13,14	1.16	1 (9%)	10,15,17	3.15	4 (40%)
1	KPI	F	166	1	11,13,14	1.48	2 (18%)	10,15,17	3.17	4 (40%)
1	KPI	A	166	1	11,13,14	1.14	1 (9%)	10,15,17	4.06	5 (50%)
1	KPI	C	166	1	11,13,14	2.02	3 (27%)	10,15,17	3.51	4 (40%)
1	KPI	E	166	1	11,13,14	1.16	0	10,15,17	3.41	3 (30%)
1	KPI	B	166	1	11,13,14	2.09	4 (36%)	10,15,17	3.45	6 (60%)

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	D	166	1	-	1/13/14/16	-
1	KPI	F	166	1	-	1/13/14/16	-
1	KPI	A	166	1	-	1/13/14/16	-
1	KPI	C	166	1	-	1/13/14/16	-
1	KPI	E	166	1	-	1/13/14/16	-
1	KPI	B	166	1	-	1/13/14/16	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	O2-CX2	5.22	1.36	1.22
1	C	166	KPI	O2-CX2	4.70	1.35	1.22
1	C	166	KPI	CX2-CX1	3.36	1.53	1.49
1	F	166	KPI	O-C	3.13	1.32	1.19
1	B	166	KPI	CX2-CX1	2.87	1.53	1.49

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	KPI	C1-CX1-CX2	-10.38	108.08	118.17
1	D	166	KPI	C1-CX1-CX2	-8.19	110.20	118.17
1	F	166	KPI	C1-CX1-CX2	-7.36	111.01	118.17
1	C	166	KPI	C1-CX1-CX2	-7.33	111.04	118.17
1	B	166	KPI	C1-CX1-CX2	-7.21	111.16	118.17

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	C1-CX1-NZ-CE
1	D	166	KPI	C1-CX1-NZ-CE
1	E	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	C1-CX1-NZ-CE

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	166	KPI	1	0
1	A	166	KPI	1	0
1	C	166	KPI	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 14 are monoatomic - leaving 73 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
4	ACT	F	308	-	3,3,3	2.28	1 (33%)	3,3,3	1.37	0
2	EDO	E	302	-	3,3,3	0.44	0	2,2,2	0.28	0
2	EDO	D	305	-	3,3,3	0.48	0	2,2,2	0.07	0
2	EDO	C	304	-	3,3,3	0.51	0	2,2,2	0.22	0
2	EDO	A	306	-	3,3,3	0.63	0	2,2,2	0.50	0
2	EDO	D	309	-	3,3,3	0.41	0	2,2,2	0.71	0
2	EDO	E	307	-	3,3,3	0.23	0	2,2,2	0.63	0
8	PEG	D	319	-	6,6,6	0.47	0	5,5,5	0.58	0
2	EDO	A	307	-	3,3,3	0.65	0	2,2,2	0.13	0
2	EDO	F	301	-	3,3,3	0.64	0	2,2,2	0.38	0
8	PEG	D	318	-	6,6,6	0.45	0	5,5,5	0.77	0
2	EDO	D	308	-	3,3,3	0.52	0	2,2,2	0.27	0
2	EDO	B	301	-	3,3,3	0.72	0	2,2,2	0.31	0
4	ACT	B	308	-	3,3,3	1.72	1 (33%)	3,3,3	1.20	0
2	EDO	F	303	-	3,3,3	0.56	0	2,2,2	0.15	0
4	ACT	B	310	-	3,3,3	1.28	0	3,3,3	1.33	0
2	EDO	D	306	-	3,3,3	0.57	0	2,2,2	0.37	0
4	ACT	D	314	-	3,3,3	1.46	1 (33%)	3,3,3	1.70	1 (33%)
2	EDO	E	305	-	3,3,3	0.29	0	2,2,2	0.44	0
4	ACT	A	313	-	3,3,3	1.27	1 (33%)	3,3,3	1.53	1 (33%)
2	EDO	A	304	-	3,3,3	0.46	0	2,2,2	0.25	0
2	EDO	C	306	-	3,3,3	0.62	0	2,2,2	0.61	0
2	EDO	A	301	-	3,3,3	0.63	0	2,2,2	0.59	0
2	EDO	B	303	-	3,3,3	0.83	0	2,2,2	0.46	0
6	HIS	F	309	-	6,11,11	0.94	1 (16%)	7,14,14	1.51	3 (42%)
4	ACT	F	306	-	3,3,3	1.63	1 (33%)	3,3,3	1.42	0
5	PGE	A	316	-	9,9,9	0.39	0	8,8,8	0.38	0
2	EDO	C	301	-	3,3,3	0.56	0	2,2,2	0.17	0
2	EDO	E	304	-	3,3,3	0.64	0	2,2,2	0.19	0
2	EDO	F	302	-	3,3,3	0.55	0	2,2,2	0.43	0
2	EDO	B	302	-	3,3,3	0.40	0	2,2,2	0.80	0
4	ACT	A	314	-	3,3,3	2.09	1 (33%)	3,3,3	1.22	0
4	ACT	F	307	-	3,3,3	1.98	1 (33%)	3,3,3	1.20	0
5	PGE	C	309	-	9,9,9	0.32	0	8,8,8	0.46	0
6	HIS	C	310	-	6,11,11	1.26	1 (16%)	7,14,14	1.70	3 (42%)
8	PEG	E	315	-	6,6,6	0.53	0	5,5,5	0.34	0
8	PEG	E	316	-	6,6,6	0.37	0	5,5,5	1.87	2 (40%)
2	EDO	B	305	-	3,3,3	0.35	0	2,2,2	0.79	0
2	EDO	E	306	-	3,3,3	0.36	0	2,2,2	0.42	0
7	PG4	D	317	-	12,12,12	1.09	1 (8%)	11,11,11	1.56	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HIS	A	317	-	6,11,11	0.81	0	7,14,14	1.43	2 (28%)
6	HIS	B	313	-	6,11,11	0.96	0	7,14,14	1.59	3 (42%)
2	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.55	0
4	ACT	B	309	-	3,3,3	1.60	1 (33%)	3,3,3	1.37	0
6	HIS	E	317	-	6,11,11	0.84	0	7,14,14	1.54	1 (14%)
4	ACT	E	310	-	3,3,3	1.80	1 (33%)	3,3,3	1.28	0
2	EDO	A	303	-	3,3,3	0.69	0	2,2,2	0.58	0
2	EDO	B	304	3	3,3,3	0.50	0	2,2,2	0.50	0
2	EDO	D	303	-	3,3,3	0.60	0	2,2,2	0.33	0
2	EDO	F	304	-	3,3,3	0.42	0	2,2,2	0.76	0
6	HIS	D	321	-	6,11,11	0.99	0	7,14,14	1.48	2 (28%)
2	EDO	A	305	-	3,3,3	0.43	0	2,2,2	0.53	0
5	PGE	B	312	-	9,9,9	0.33	0	8,8,8	0.43	0
5	PGE	D	316	-	9,9,9	0.37	0	8,8,8	0.59	0
4	ACT	E	311	-	3,3,3	1.85	1 (33%)	3,3,3	1.24	0
2	EDO	A	302	-	3,3,3	0.41	0	2,2,2	0.61	0
2	EDO	D	301	-	3,3,3	0.64	0	2,2,2	0.45	0
2	EDO	D	302	-	3,3,3	0.66	0	2,2,2	0.20	0
5	PGE	E	313	-	9,9,9	0.45	0	8,8,8	0.44	0
2	EDO	E	303	-	3,3,3	0.55	0	2,2,2	0.39	0
2	EDO	C	302	-	3,3,3	0.26	0	2,2,2	0.77	0
4	ACT	D	313	-	3,3,3	1.49	1 (33%)	3,3,3	1.32	0
5	PGE	B	311	-	9,9,9	0.46	0	8,8,8	0.56	0
5	PGE	E	314	-	9,9,9	0.39	0	8,8,8	0.48	0
4	ACT	D	315	-	3,3,3	1.66	1 (33%)	3,3,3	1.28	0
4	ACT	A	315	-	3,3,3	1.99	1 (33%)	3,3,3	1.11	0
2	EDO	C	305	-	3,3,3	0.39	0	2,2,2	0.82	0
2	EDO	E	301	-	3,3,3	0.58	0	2,2,2	0.41	0
4	ACT	C	308	-	3,3,3	1.23	0	3,3,3	1.54	0
2	EDO	D	307	-	3,3,3	0.54	0	2,2,2	0.35	0
5	PGE	E	312	-	9,9,9	0.35	0	8,8,8	0.54	0
8	PEG	D	320	-	6,6,6	0.31	0	5,5,5	0.53	0
2	EDO	D	304	-	3,3,3	0.65	0	2,2,2	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	E	302	-	-	1/1/1/1	-
2	EDO	D	305	-	-	1/1/1/1	-
2	EDO	C	304	-	-	0/1/1/1	-
2	EDO	A	306	-	-	0/1/1/1	-
2	EDO	D	309	-	-	1/1/1/1	-
2	EDO	E	307	-	-	1/1/1/1	-
8	PEG	D	319	-	-	1/4/4/4	-
2	EDO	A	307	-	-	0/1/1/1	-
2	EDO	F	301	-	-	0/1/1/1	-
8	PEG	D	318	-	-	4/4/4/4	-
2	EDO	D	308	-	-	0/1/1/1	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	F	303	-	-	0/1/1/1	-
2	EDO	D	306	-	-	0/1/1/1	-
2	EDO	E	305	-	-	0/1/1/1	-
2	EDO	A	304	-	-	0/1/1/1	-
2	EDO	C	306	-	-	0/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
6	HIS	F	309	-	-	1/8/8/8	0/1/1/1
5	PGE	A	316	-	-	1/7/7/7	-
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	E	304	-	-	0/1/1/1	-
2	EDO	F	302	-	-	1/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
6	HIS	C	310	-	-	3/8/8/8	0/1/1/1
5	PGE	C	309	-	-	0/7/7/7	-
8	PEG	E	315	-	-	2/4/4/4	-
8	PEG	E	316	-	-	4/4/4/4	-
2	EDO	B	305	-	-	0/1/1/1	-
2	EDO	E	306	-	-	1/1/1/1	-
7	PG4	D	317	-	-	3/10/10/10	-
6	HIS	A	317	-	-	2/8/8/8	0/1/1/1
6	HIS	B	313	-	-	1/8/8/8	0/1/1/1
2	EDO	C	303	-	-	1/1/1/1	-
6	HIS	E	317	-	-	1/8/8/8	0/1/1/1
2	EDO	A	303	-	-	0/1/1/1	-
2	EDO	B	304	3	-	0/1/1/1	-
2	EDO	D	303	-	-	0/1/1/1	-
2	EDO	F	304	-	-	1/1/1/1	-
6	HIS	D	321	-	-	1/8/8/8	0/1/1/1
2	EDO	A	305	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	B	312	-	-	3/7/7/7	-
5	PGE	D	316	-	-	2/7/7/7	-
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	D	301	-	-	0/1/1/1	-
2	EDO	D	302	-	-	0/1/1/1	-
5	PGE	E	313	-	-	3/7/7/7	-
2	EDO	E	303	-	-	1/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
5	PGE	B	311	-	-	2/7/7/7	-
5	PGE	E	314	-	-	2/7/7/7	-
2	EDO	C	305	-	-	0/1/1/1	-
2	EDO	E	301	-	-	0/1/1/1	-
2	EDO	D	307	-	-	1/1/1/1	-
5	PGE	E	312	-	-	0/7/7/7	-
8	PEG	D	320	-	-	2/4/4/4	-
2	EDO	D	304	-	-	0/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	308	ACT	CH3-C	3.78	1.65	1.49
4	A	315	ACT	CH3-C	3.28	1.62	1.49
4	A	314	ACT	CH3-C	3.26	1.62	1.49
4	E	310	ACT	CH3-C	2.86	1.61	1.49
6	C	310	HIS	OXT-C	-2.74	1.21	1.30

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	310	HIS	OXT-C-O	-3.11	117.03	124.09
7	D	317	PG4	C5-O3-C4	3.09	126.69	113.29
6	E	317	HIS	OXT-C-O	-2.93	117.44	124.09
8	E	316	PEG	O2-C3-C4	-2.92	97.22	110.07
6	D	321	HIS	OXT-C-O	-2.81	117.70	124.09

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	317	HIS	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
6	C	310	HIS	CA-CB-CG-ND1
6	D	321	HIS	CA-CB-CG-ND1
6	E	317	HIS	CA-CB-CG-ND1
6	F	309	HIS	CA-CB-CG-ND1

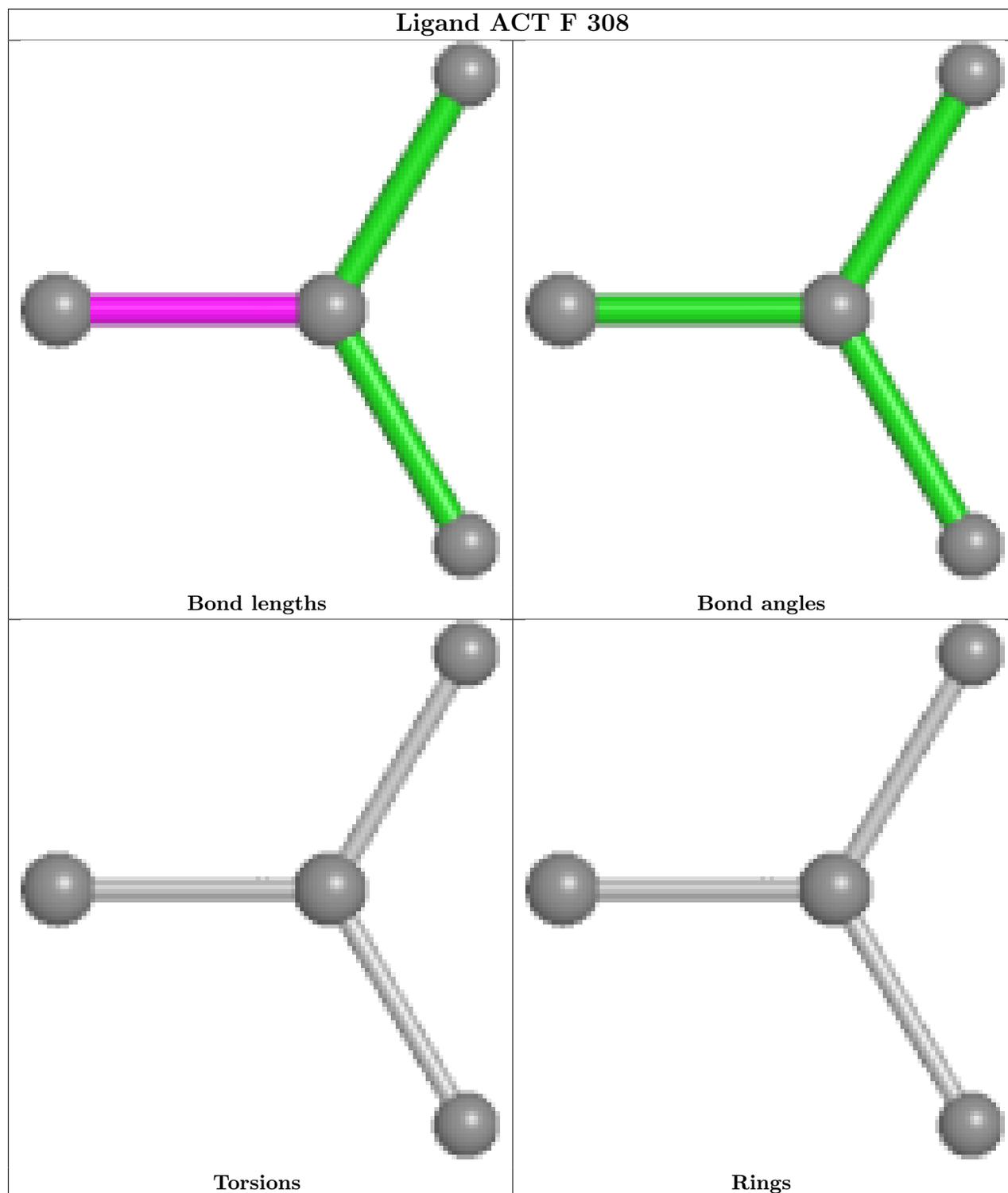
There are no ring outliers.

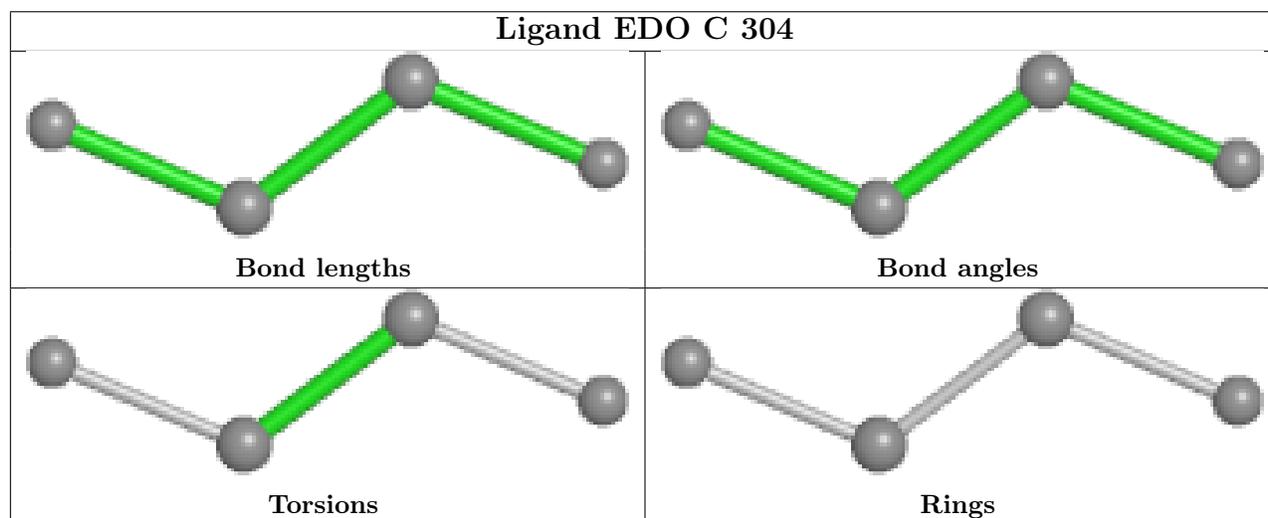
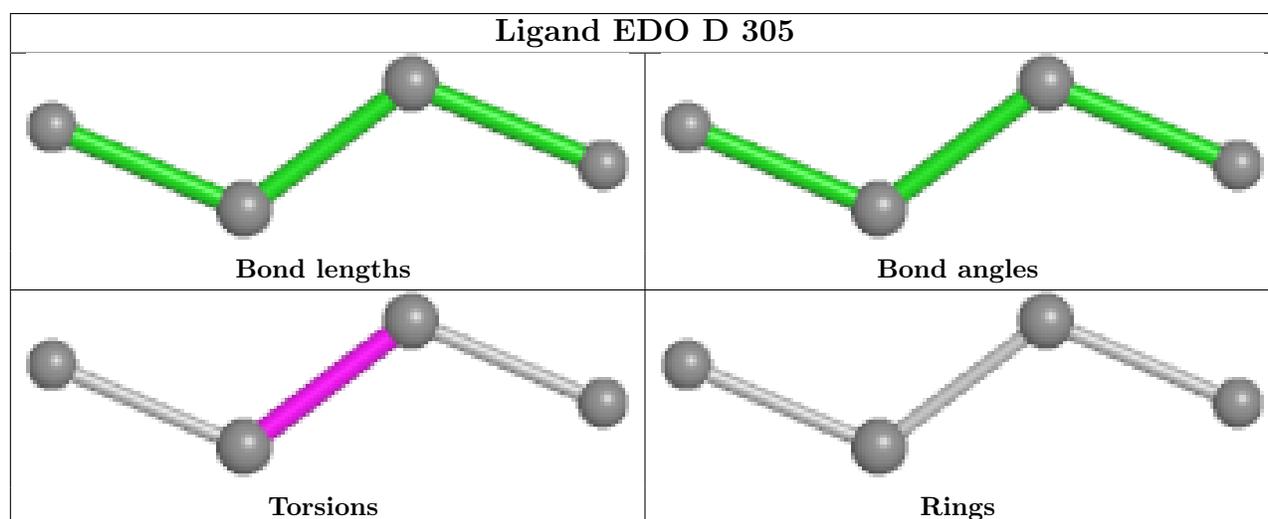
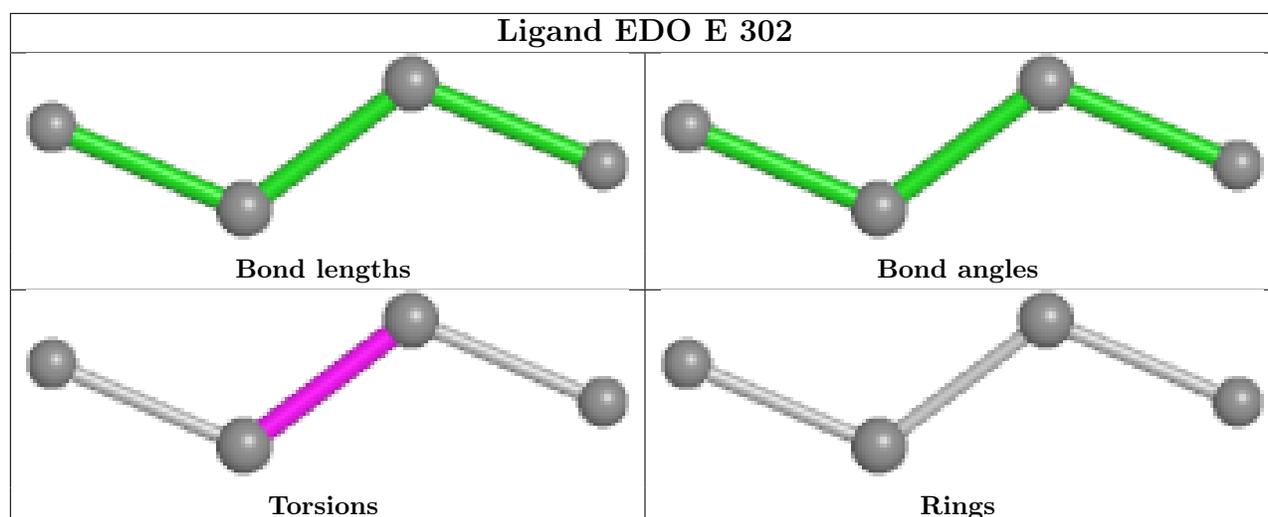
25 monomers are involved in 44 short contacts:

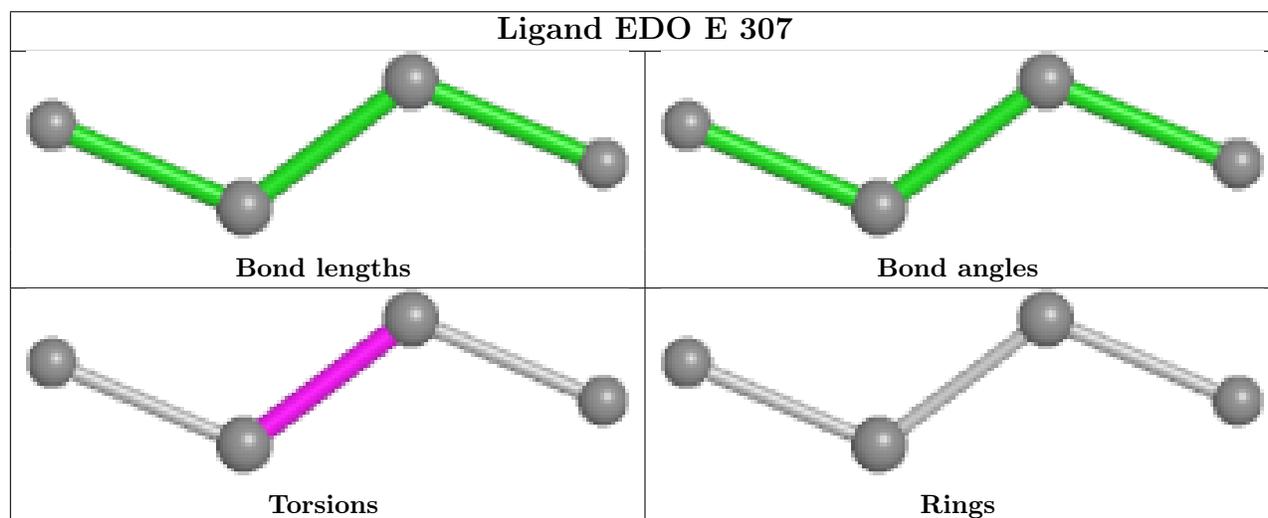
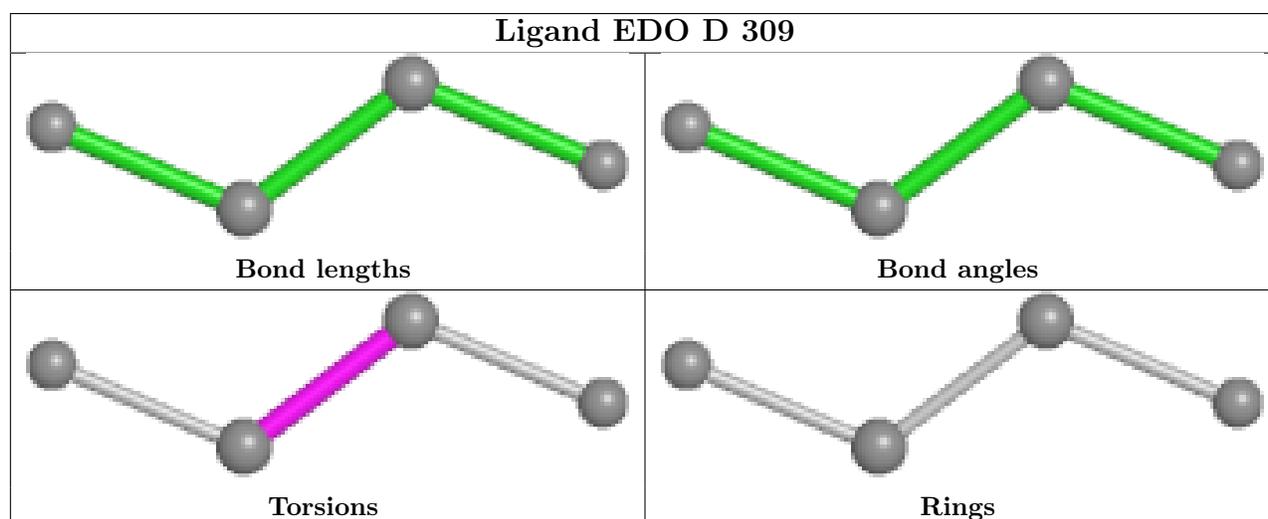
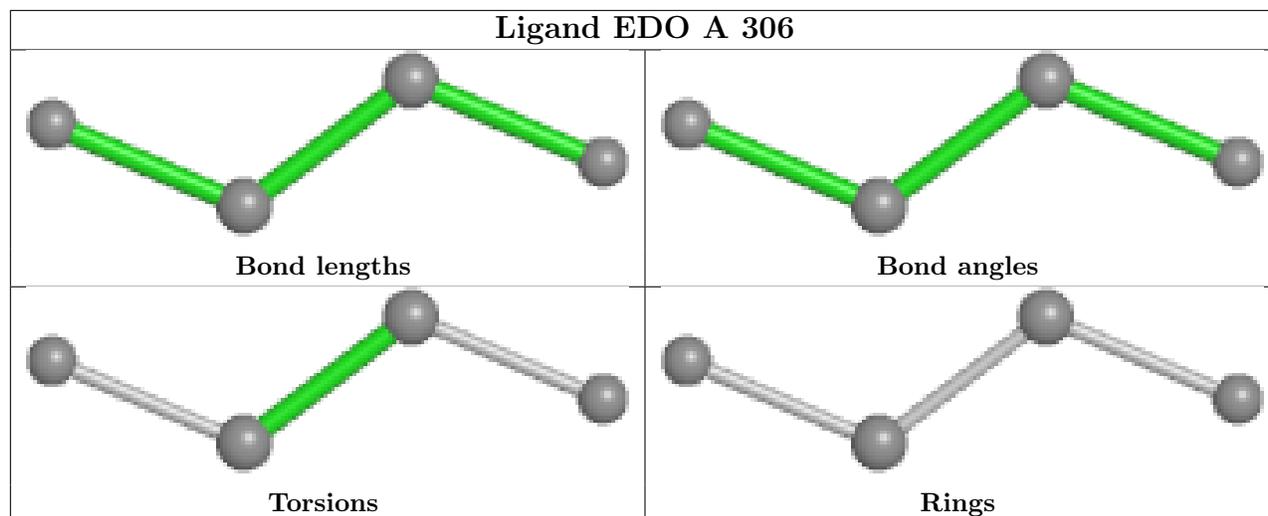
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	304	EDO	1	0
2	D	309	EDO	1	0
2	E	307	EDO	7	0
2	B	301	EDO	1	0
4	A	313	ACT	1	0
2	C	306	EDO	1	0
6	F	309	HIS	1	0
2	E	304	EDO	1	0
2	F	302	EDO	1	0
2	B	302	EDO	1	0
4	A	314	ACT	1	0
8	E	316	PEG	4	0
2	E	306	EDO	2	0
6	A	317	HIS	1	0
2	C	303	EDO	1	0
6	E	317	HIS	1	0
2	B	304	EDO	5	0
6	D	321	HIS	2	0
5	D	316	PGE	1	0
2	C	302	EDO	4	0
4	D	313	ACT	1	0
5	E	314	PGE	1	0
2	C	305	EDO	1	0
4	C	308	ACT	1	0
8	D	320	PEG	2	0

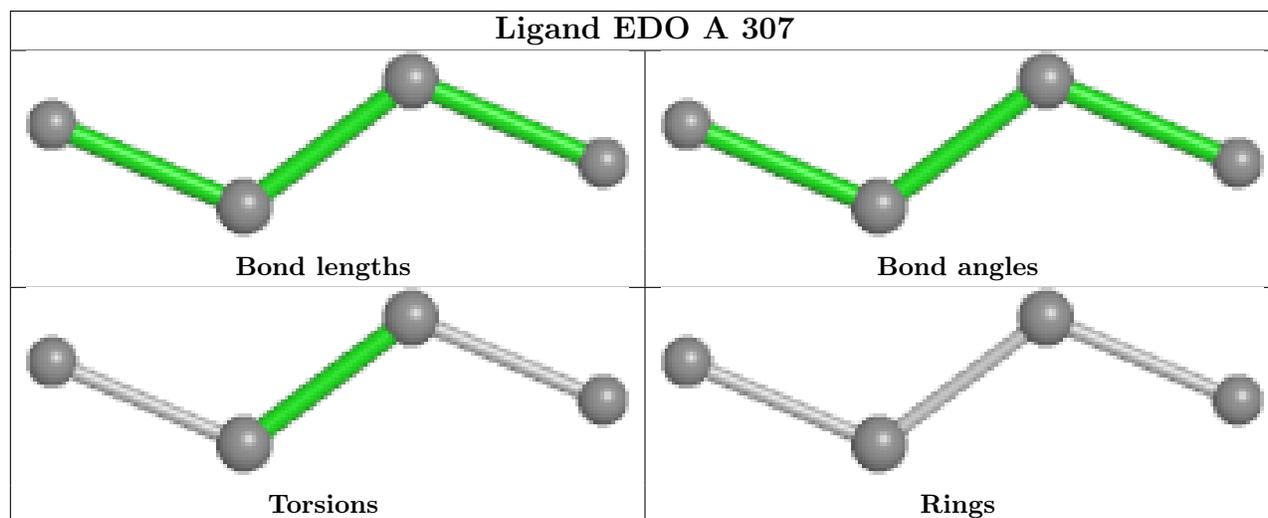
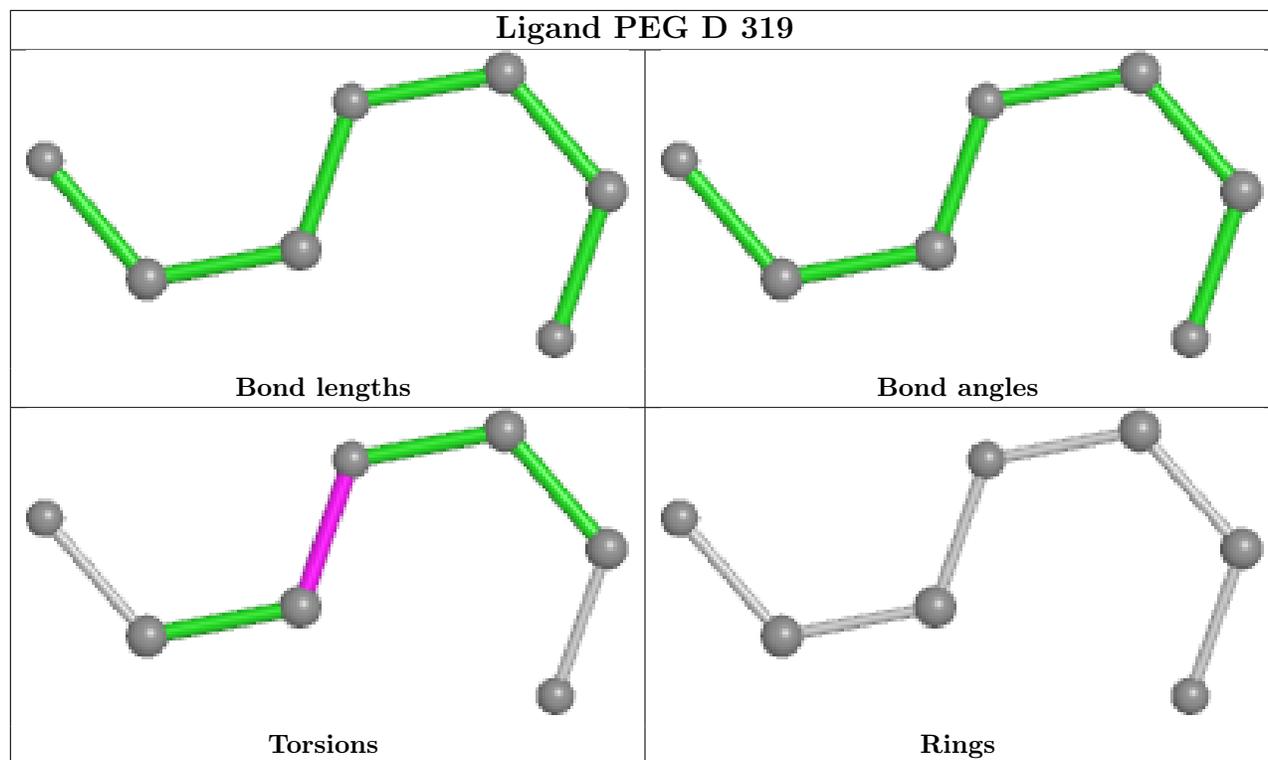
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

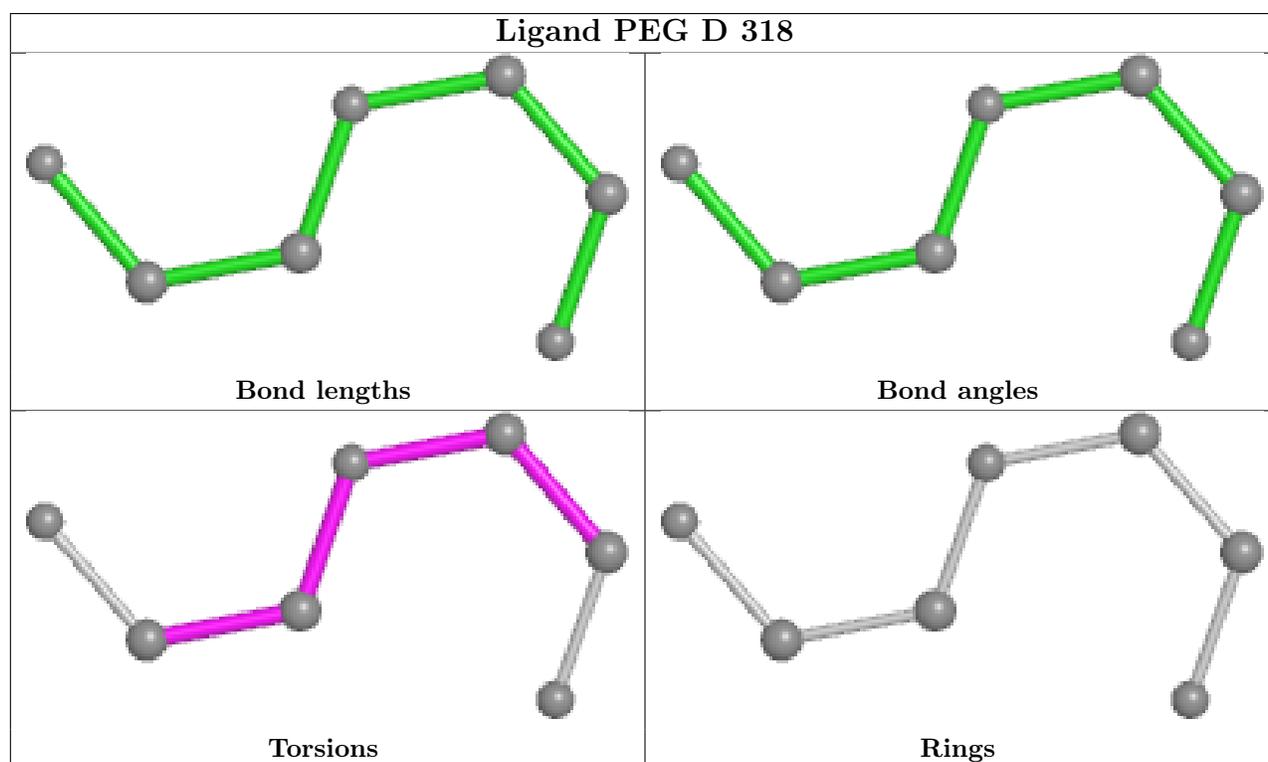
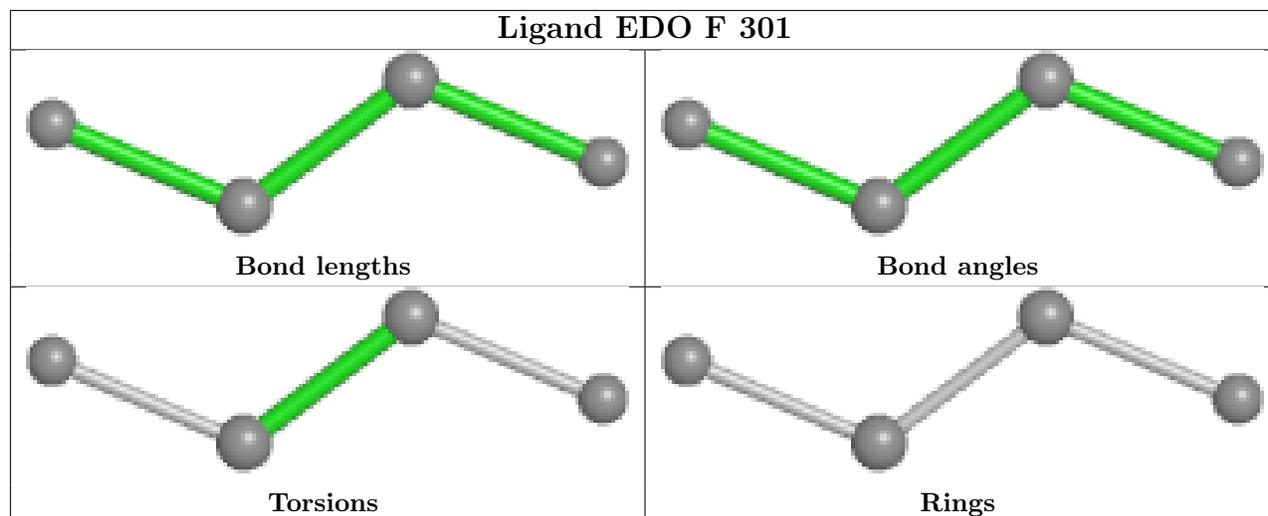
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

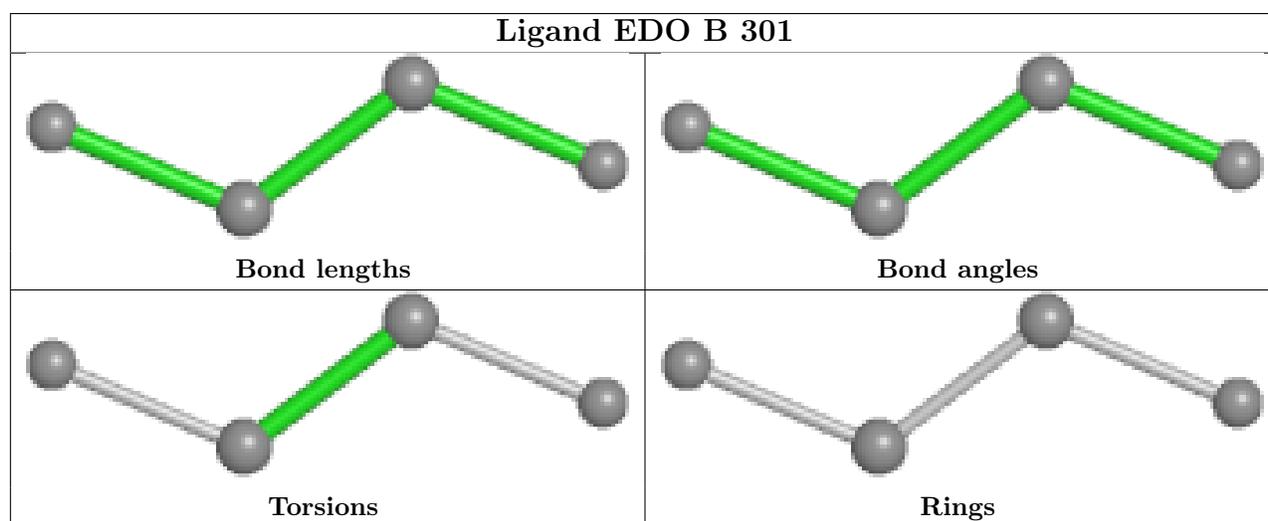
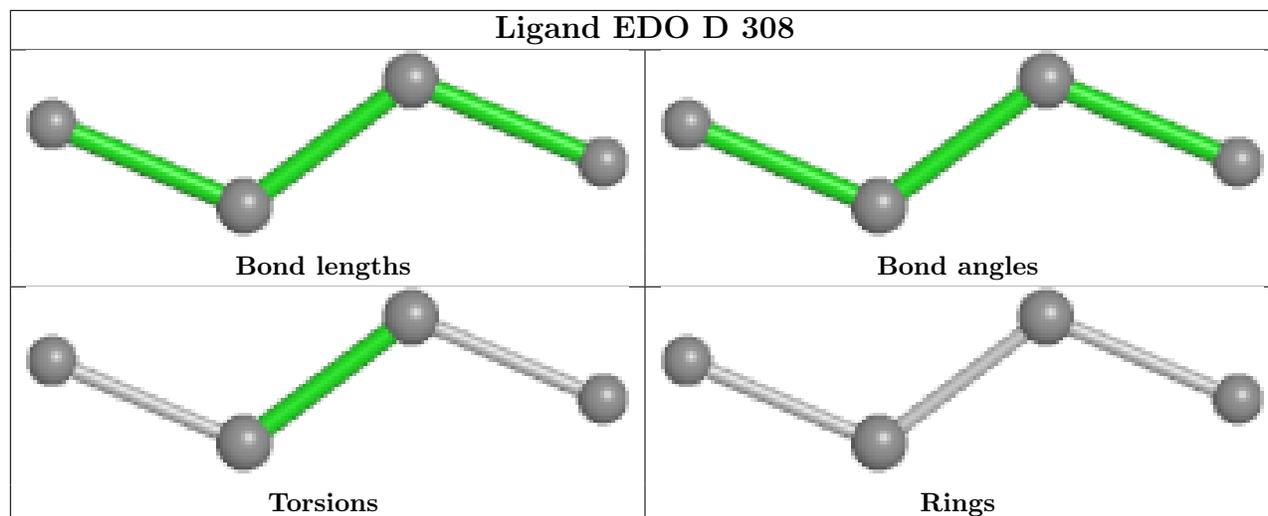


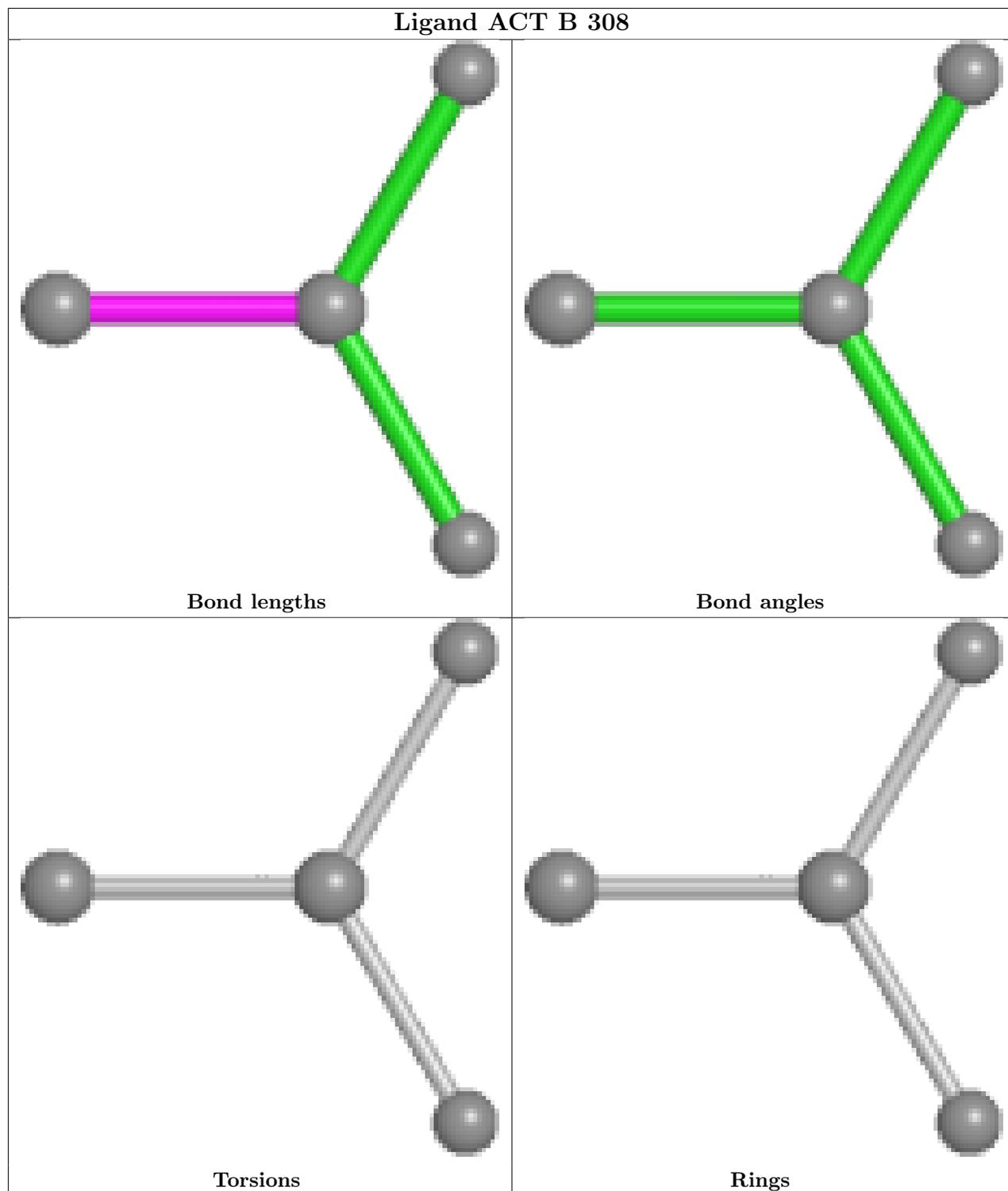


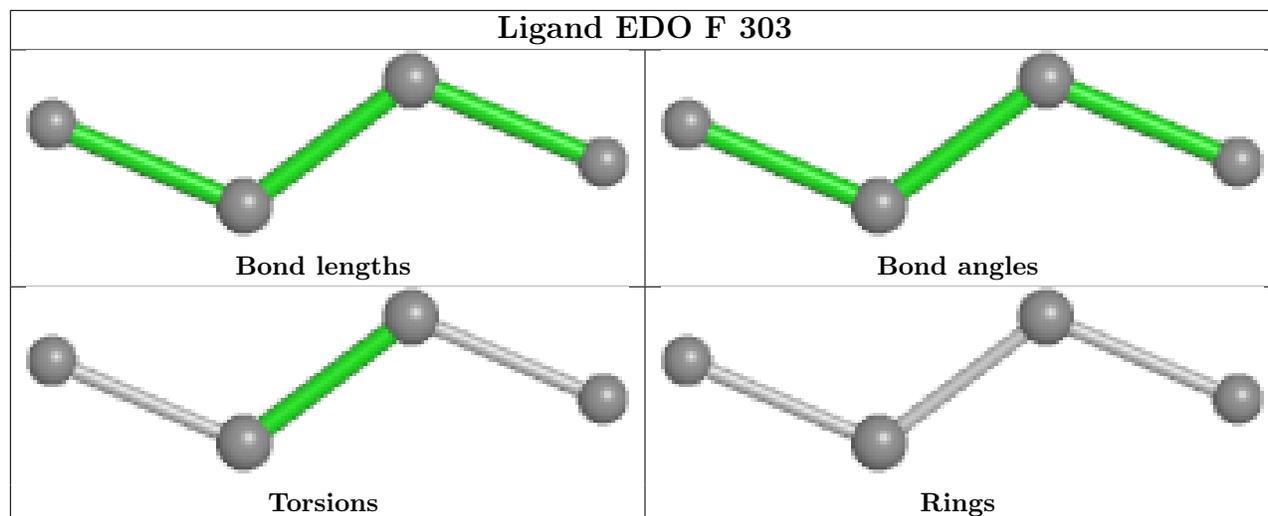


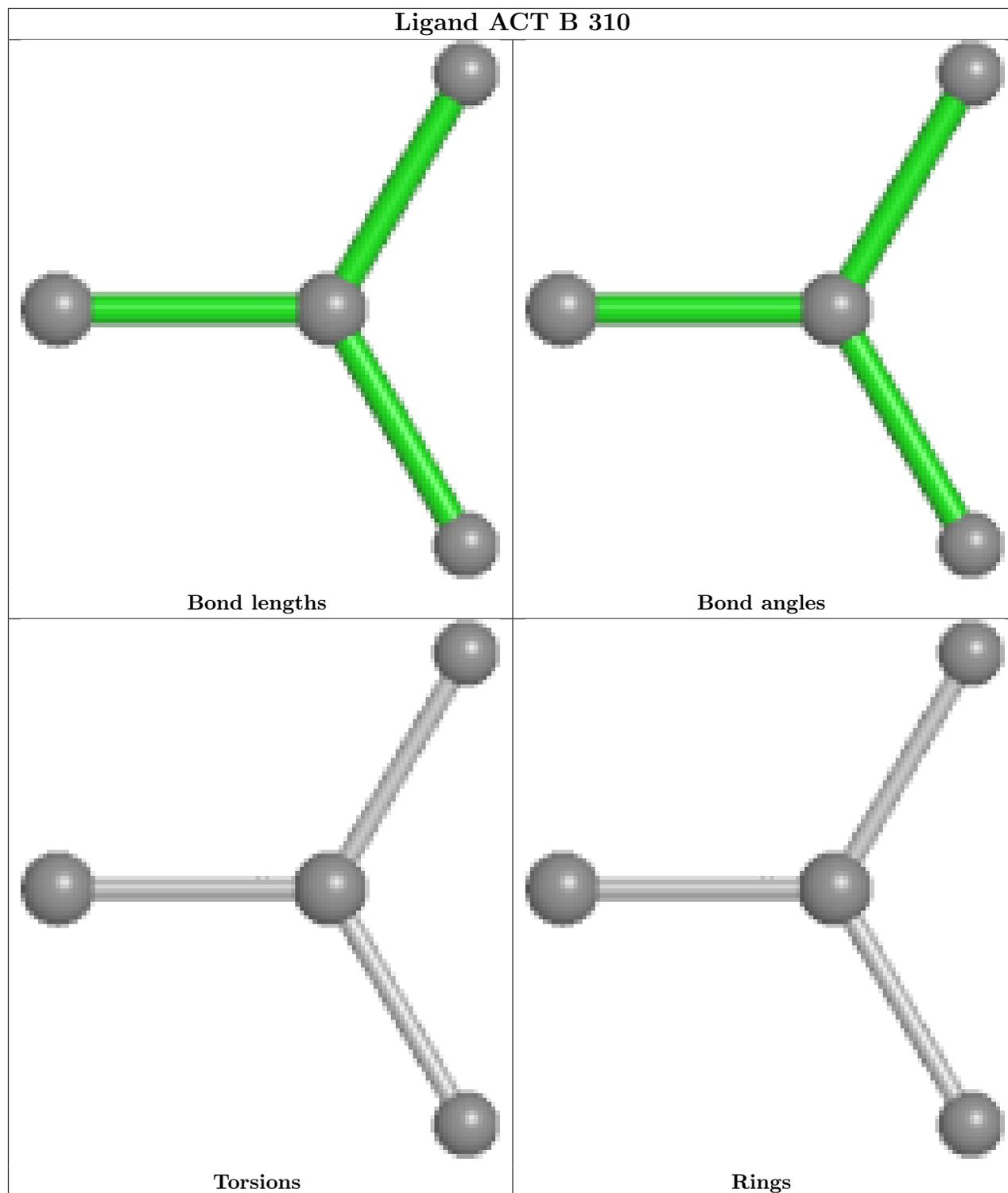


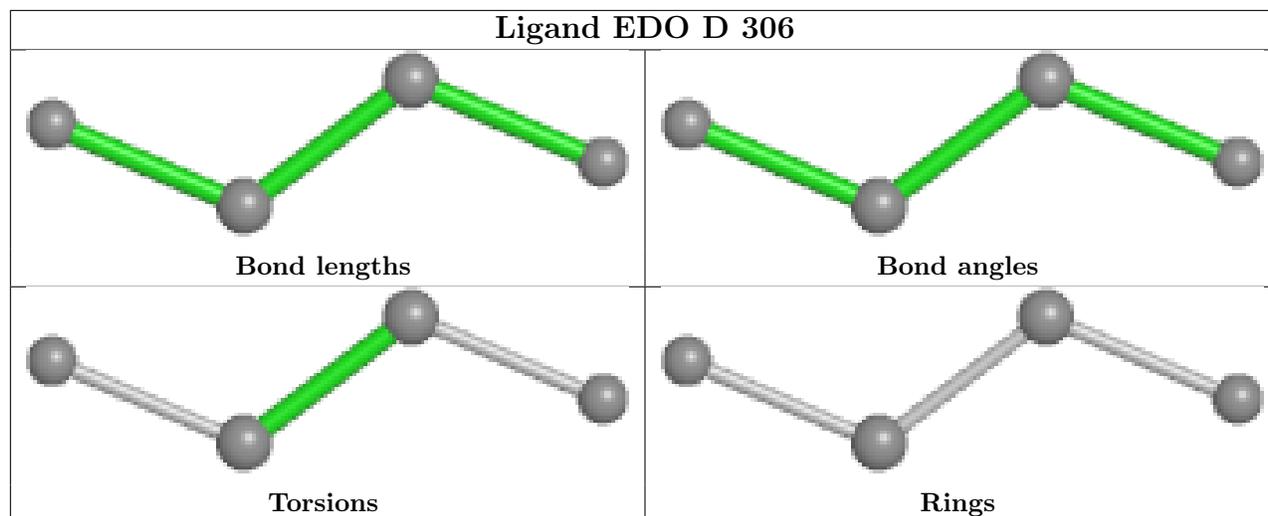


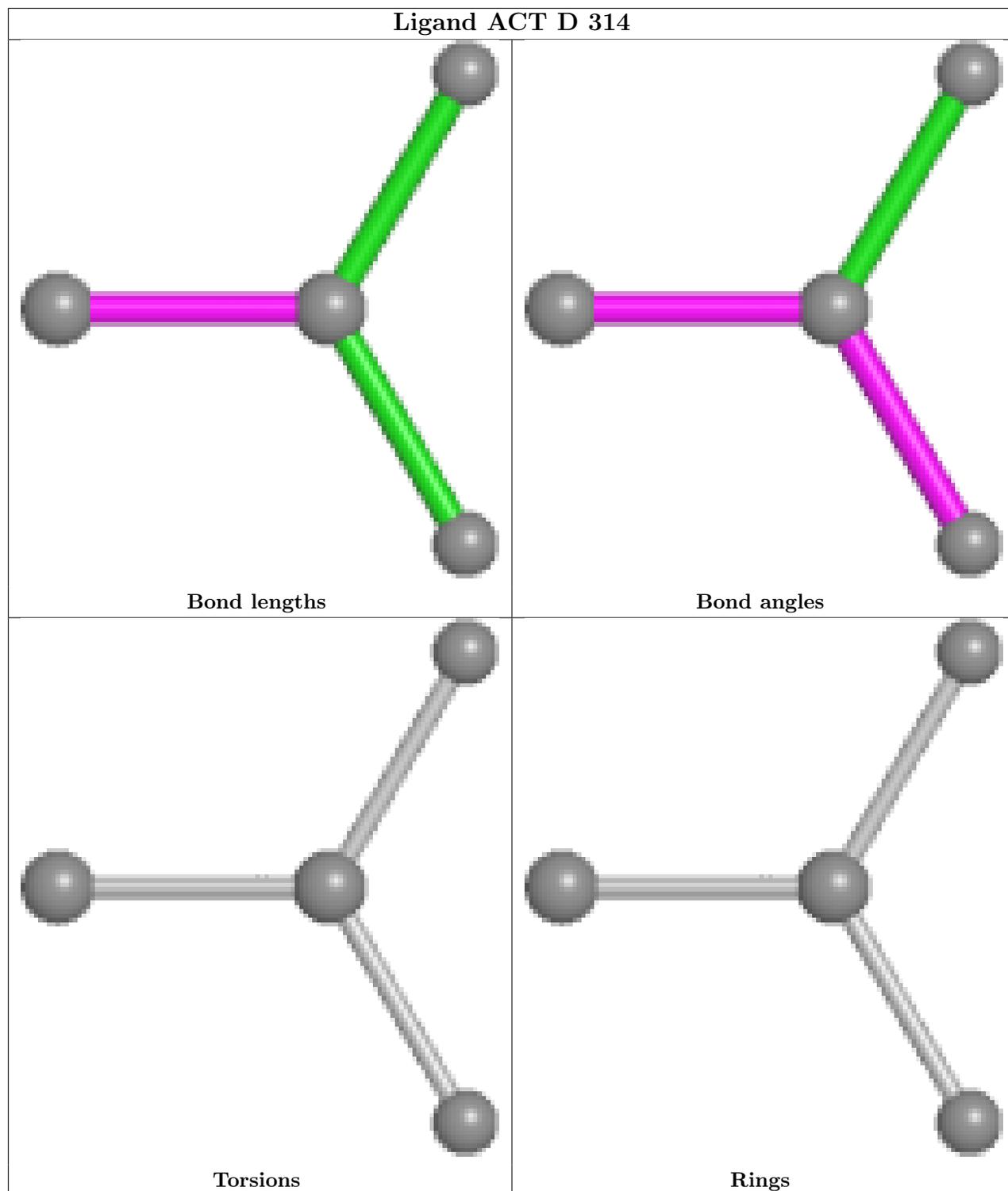


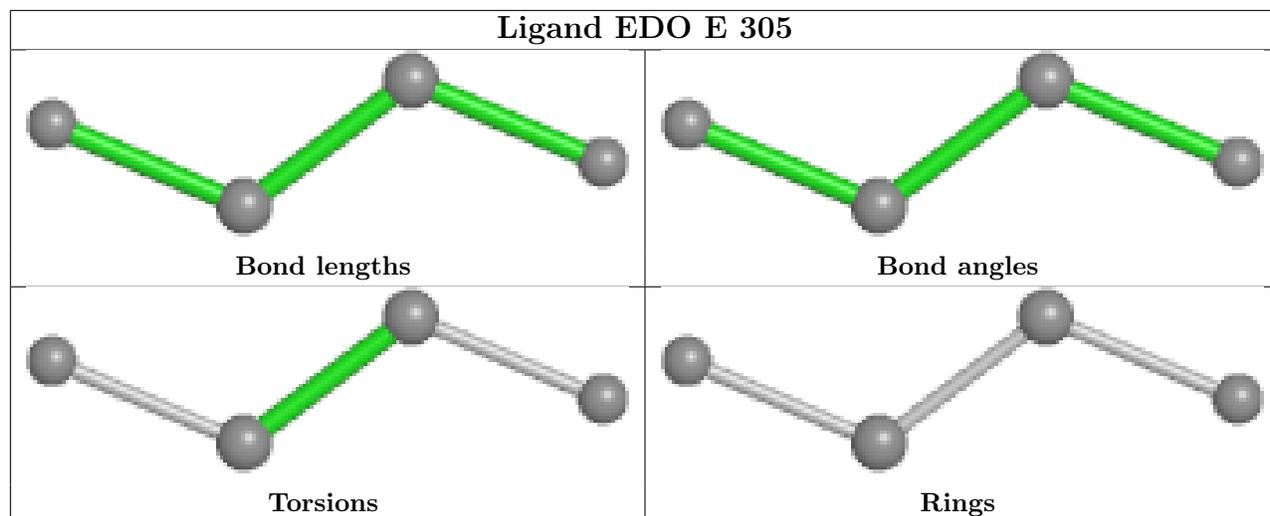


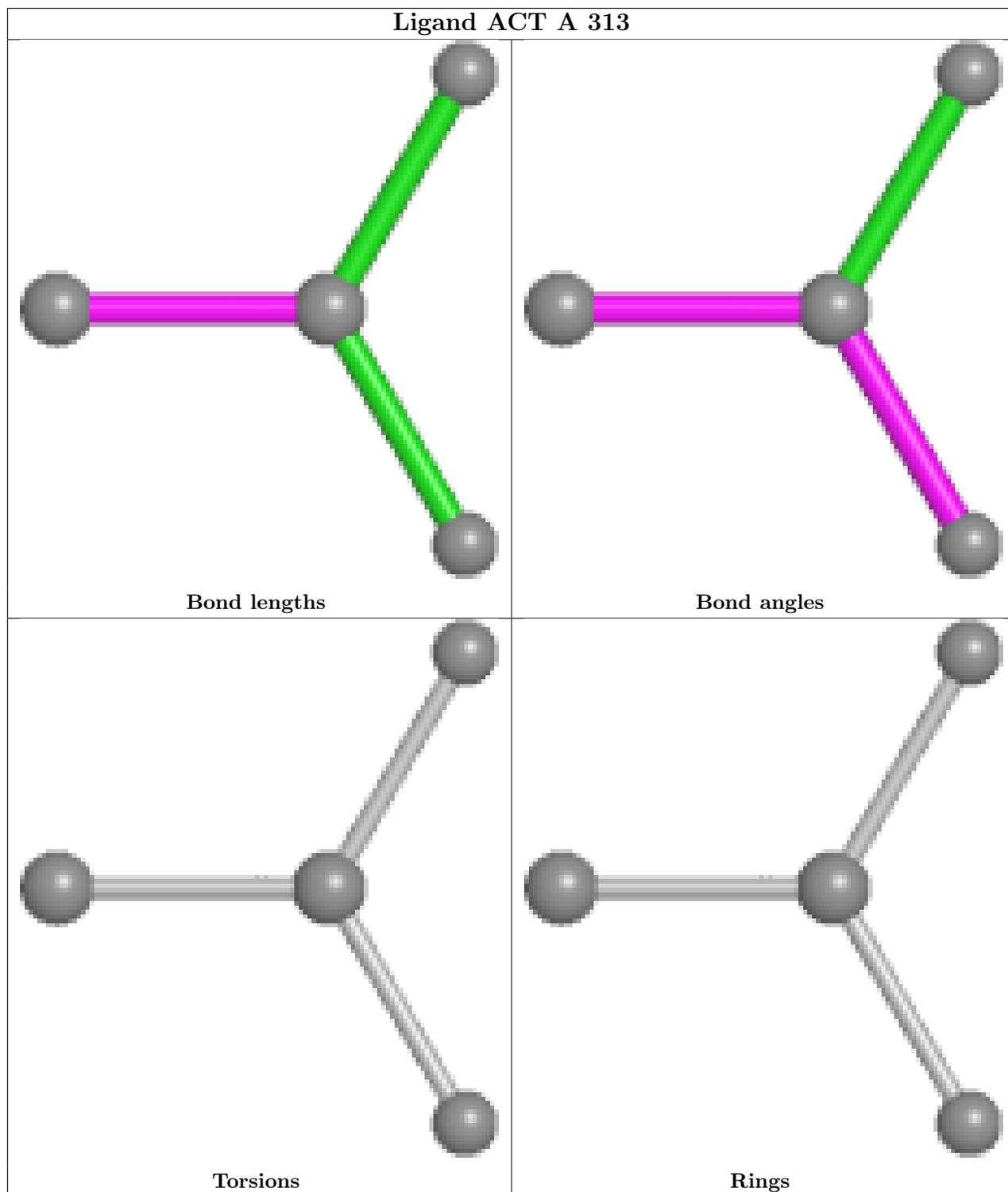


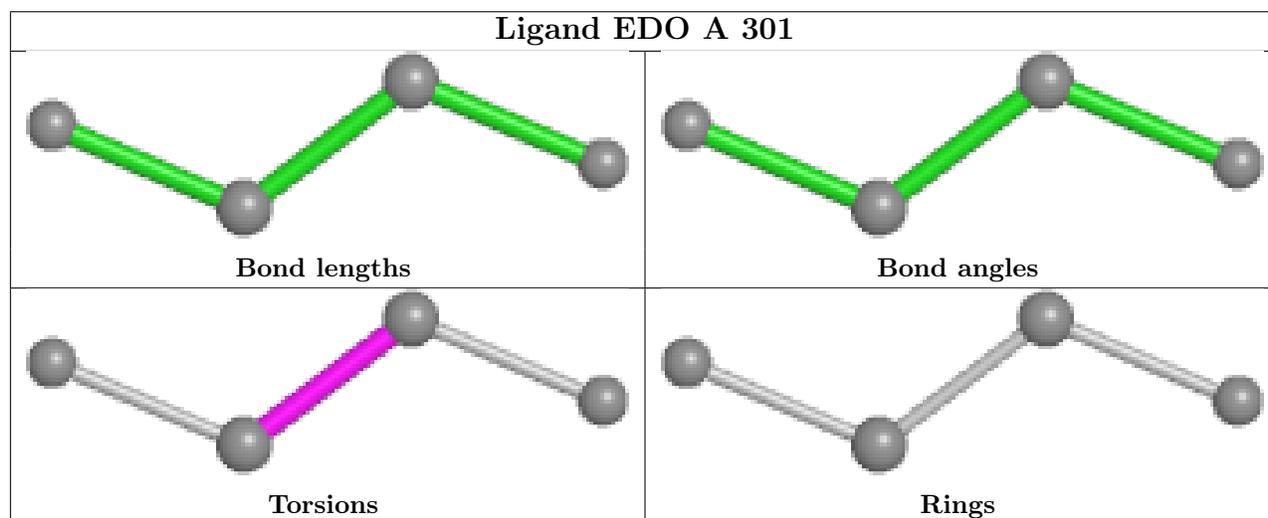
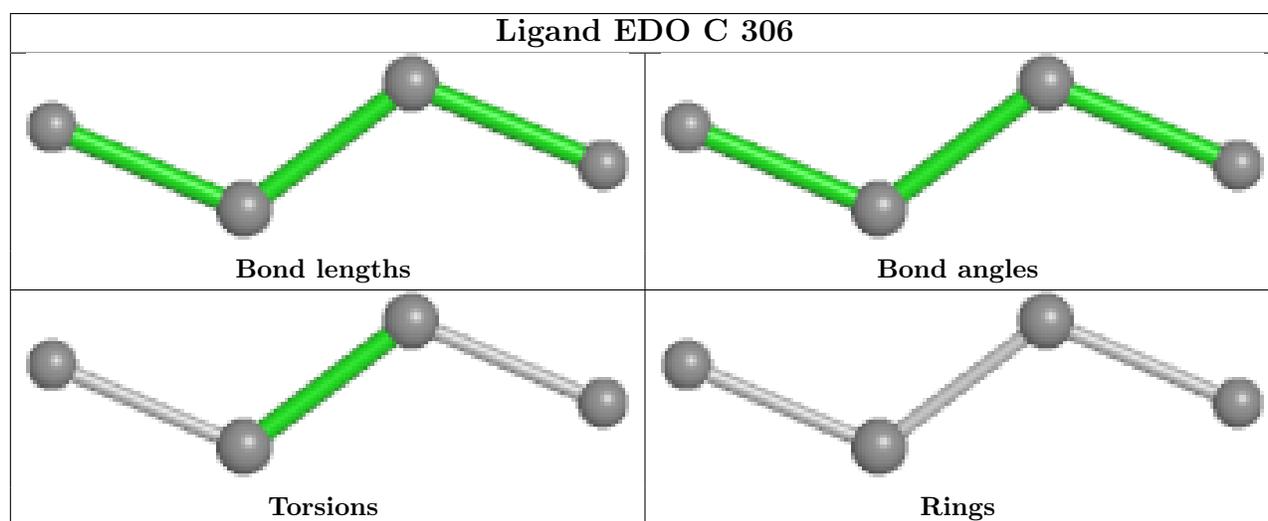
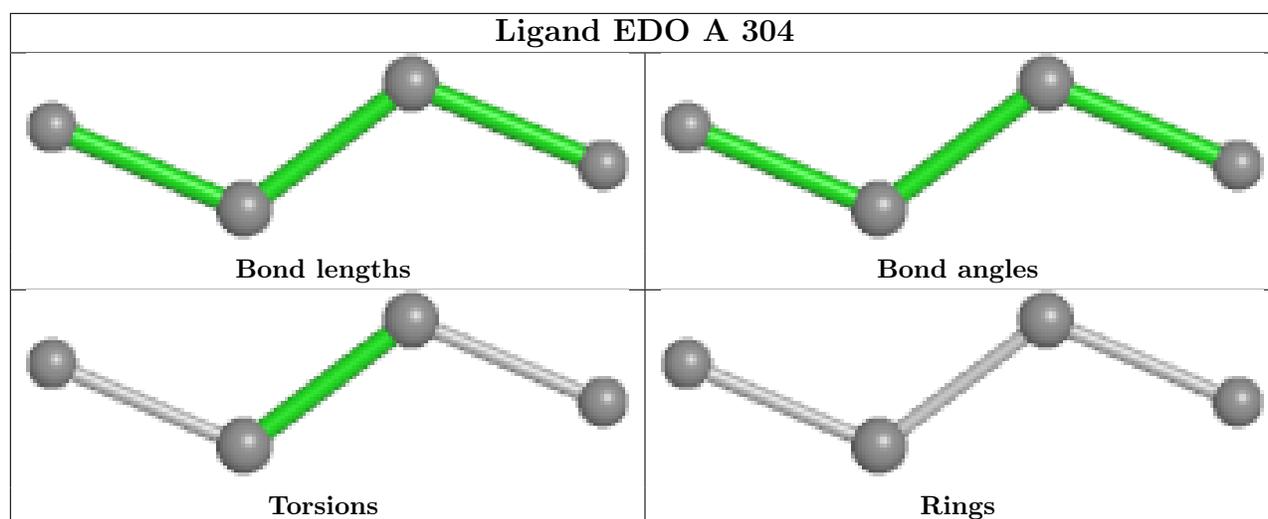


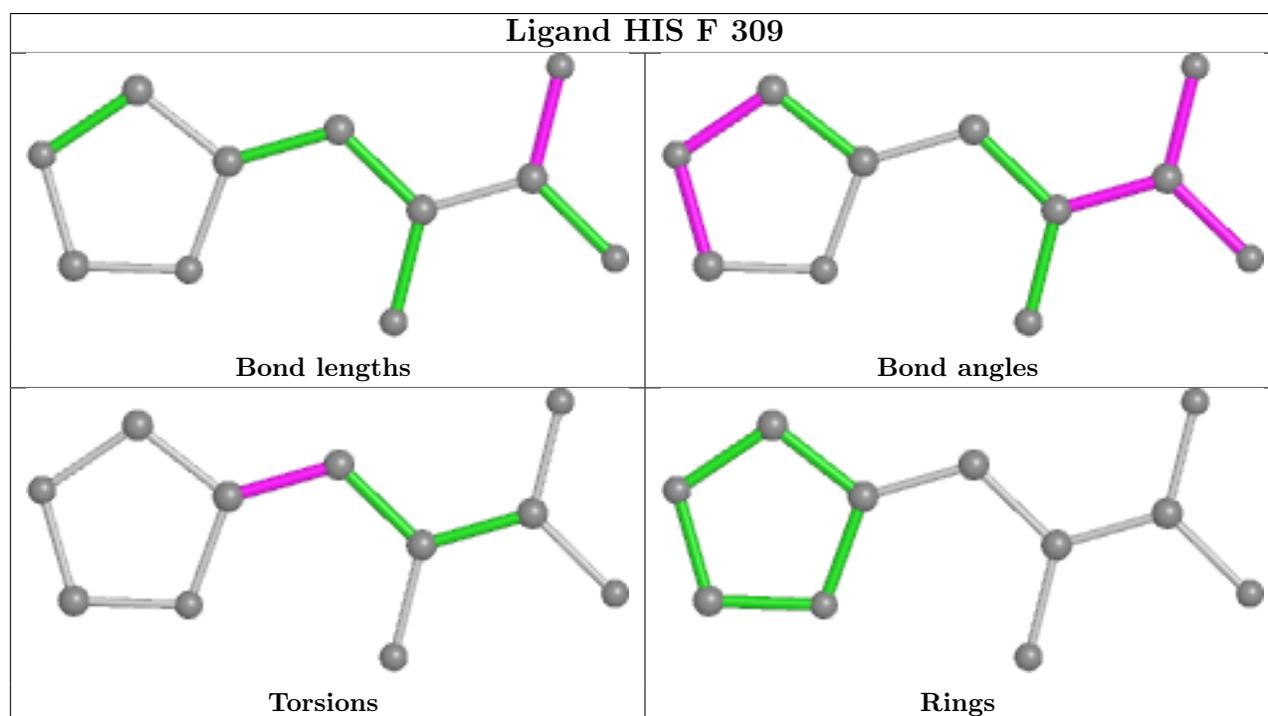
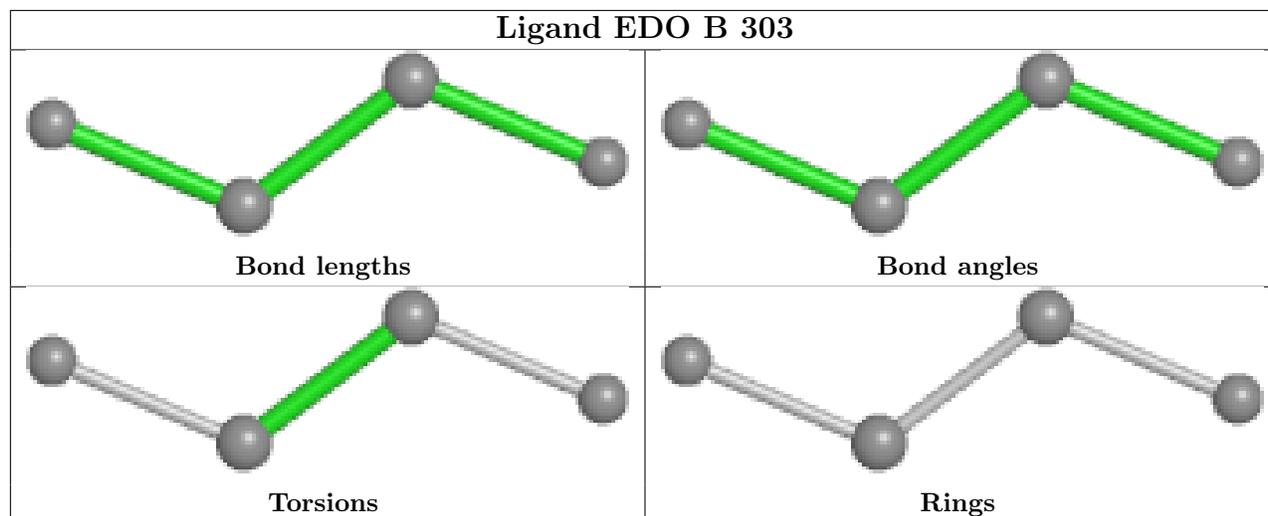


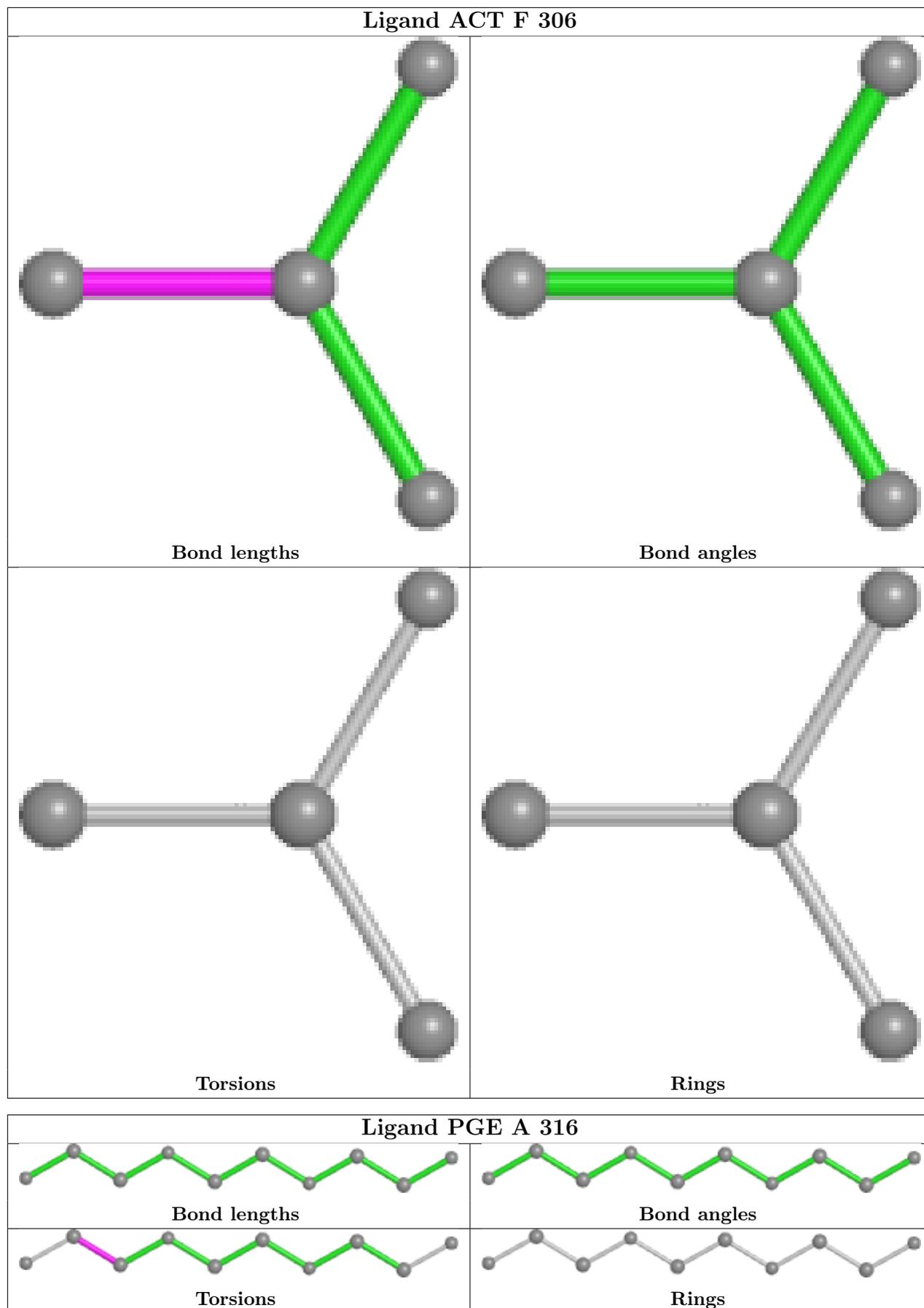


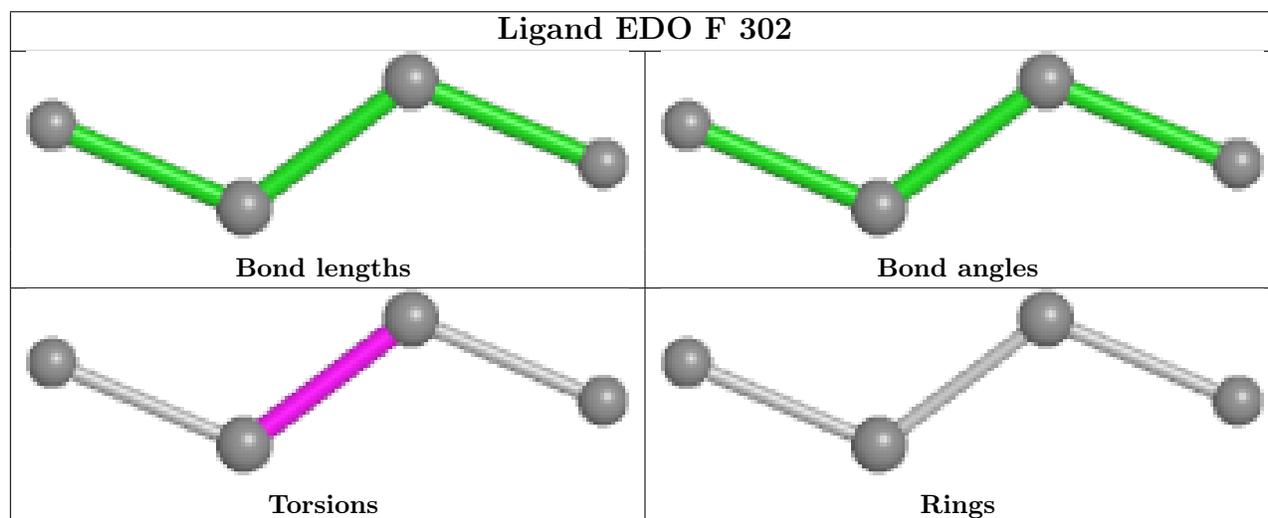
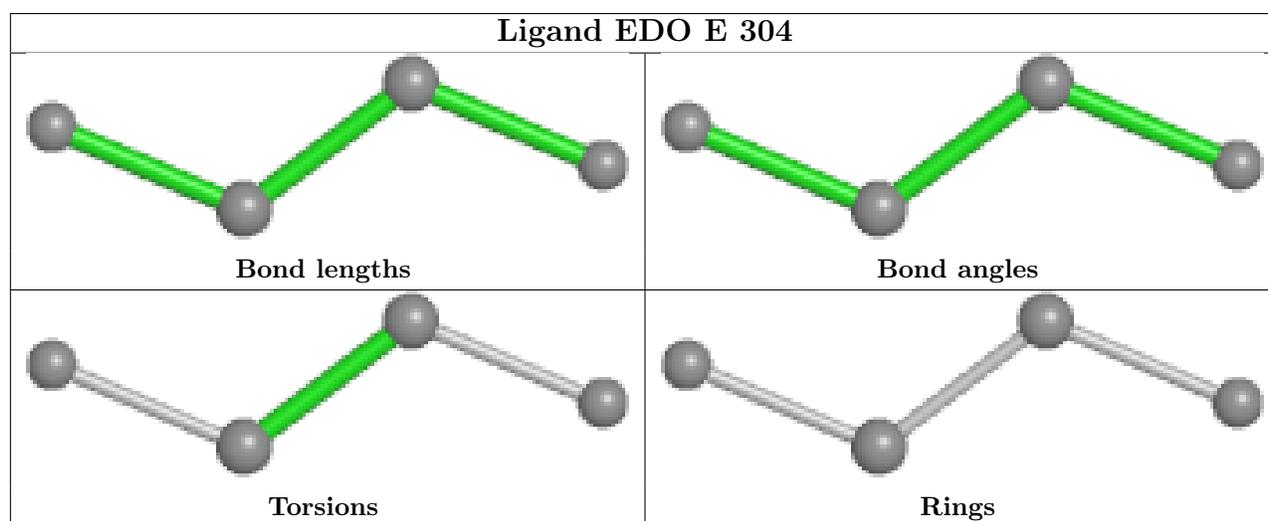
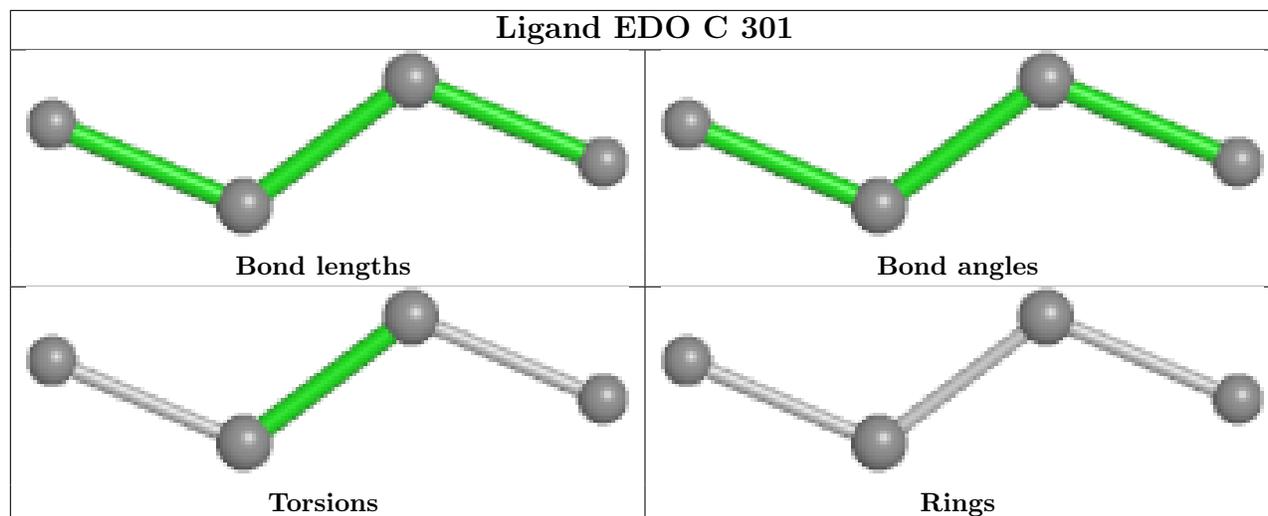


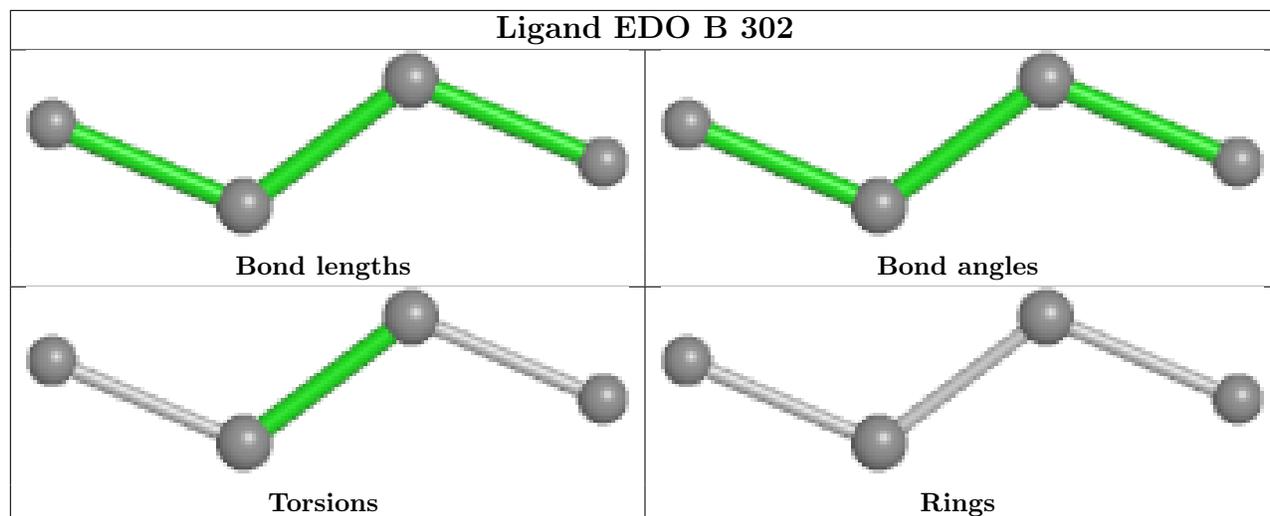


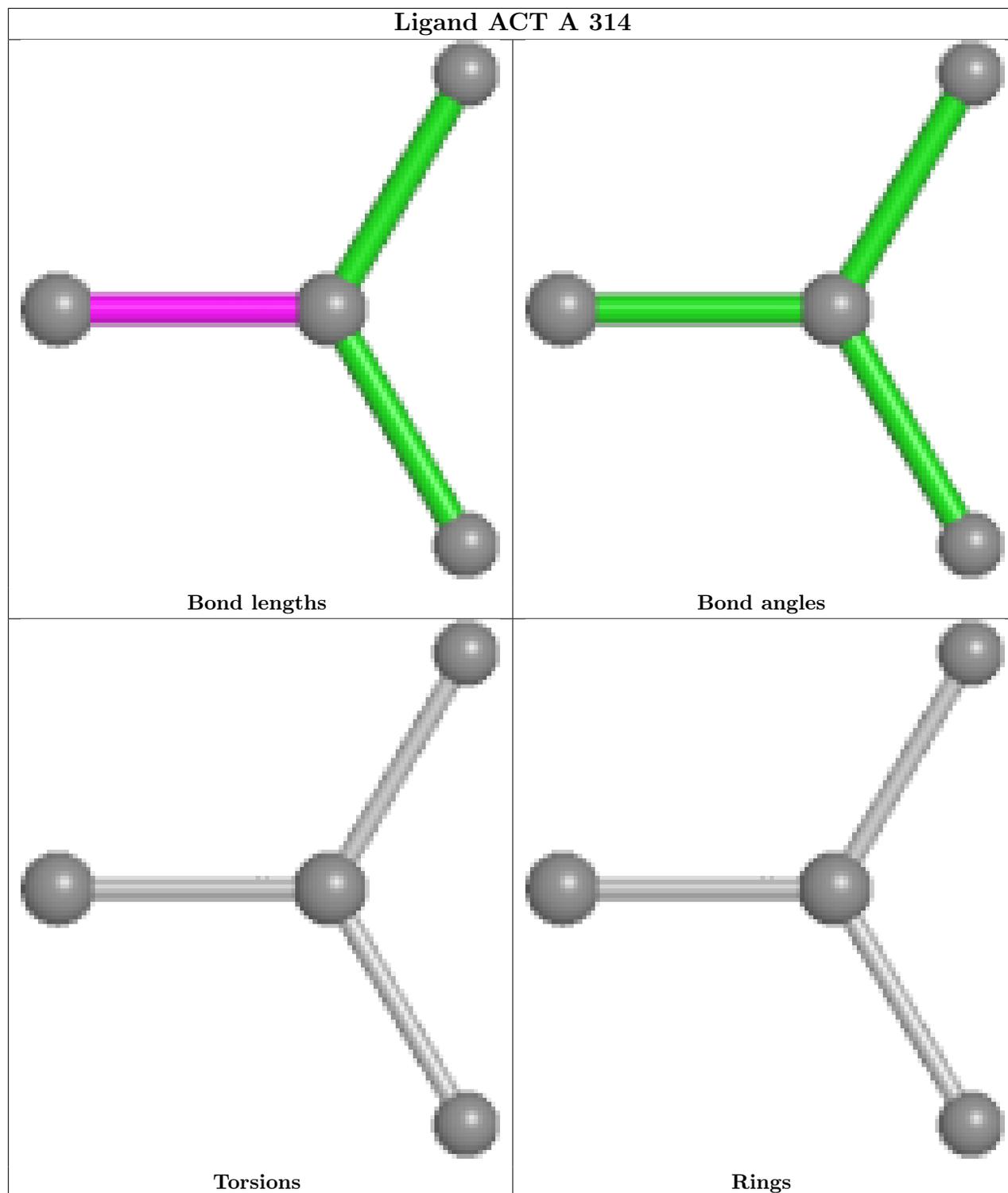


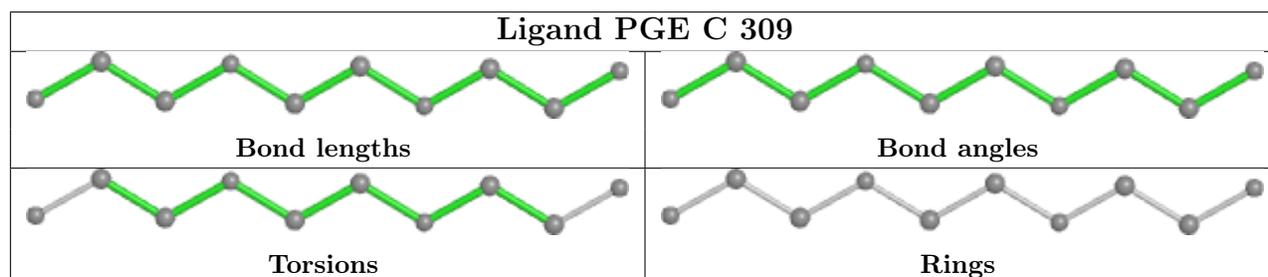
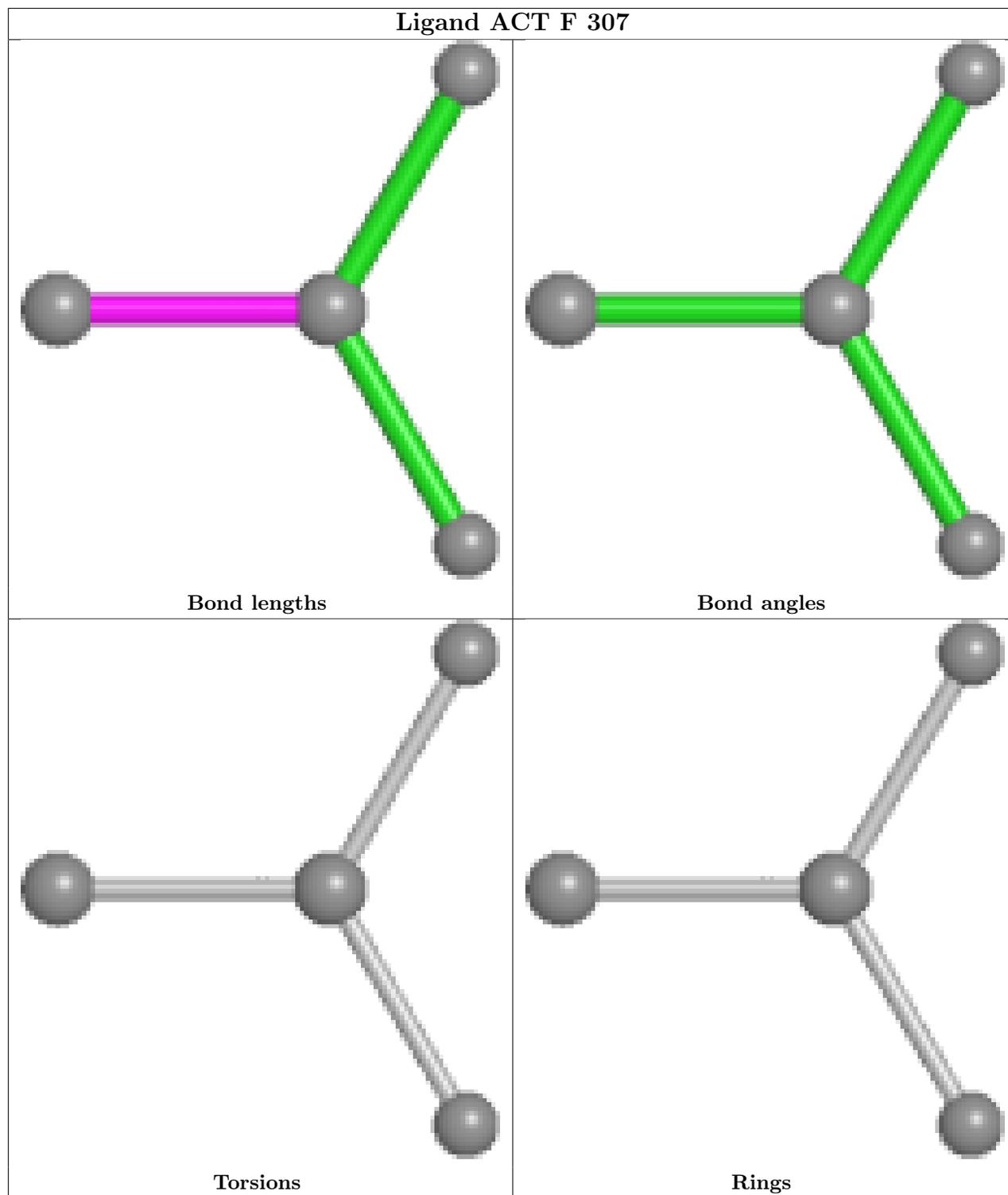


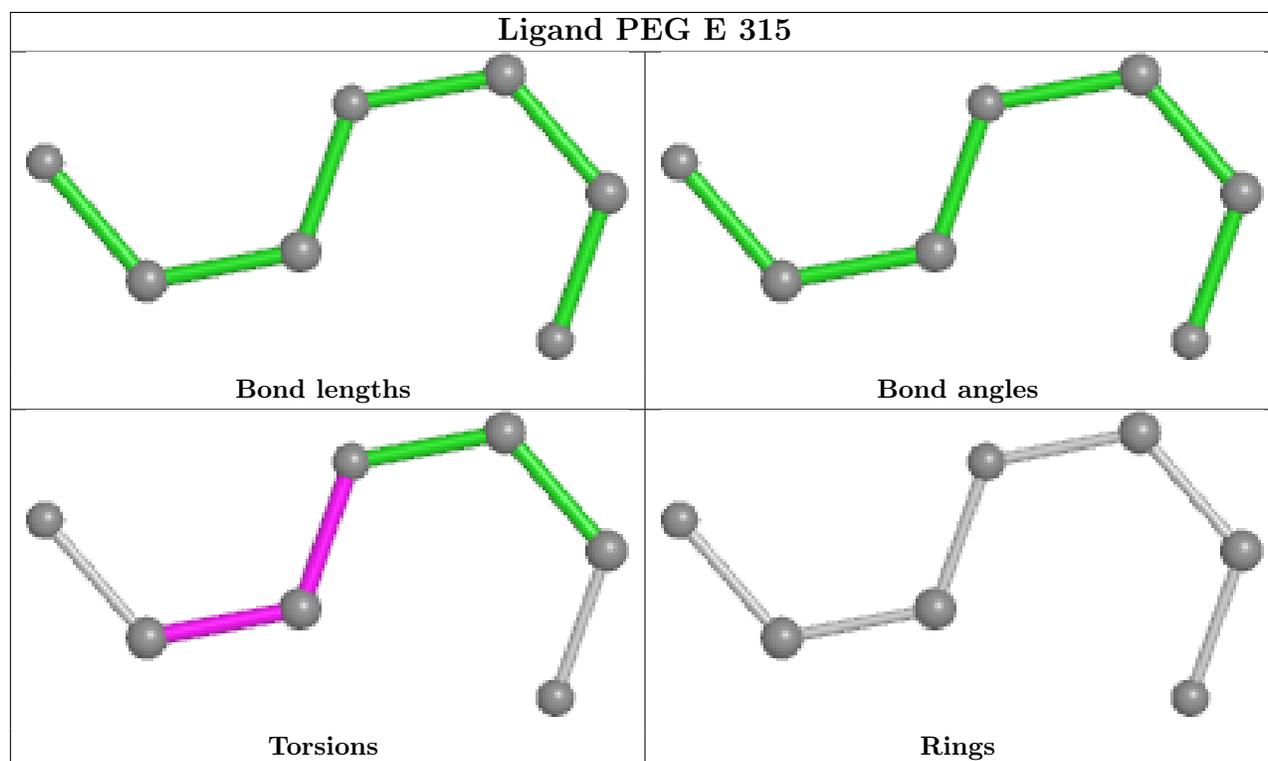
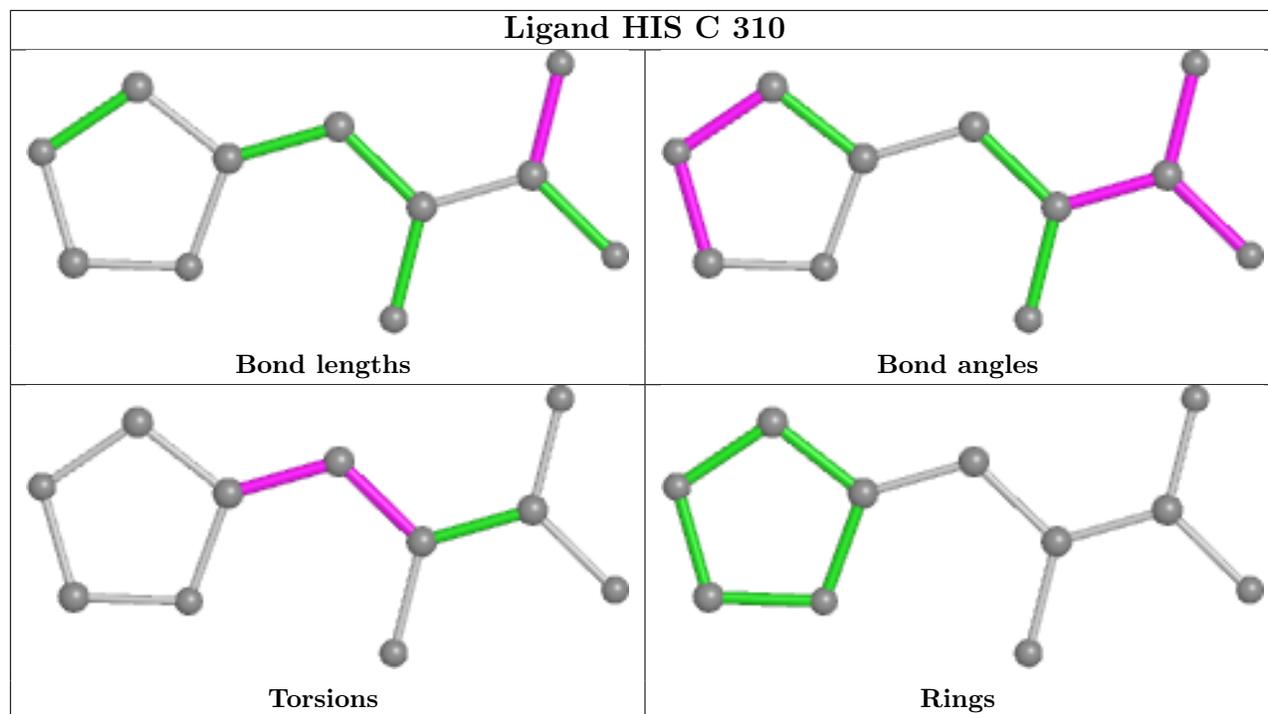


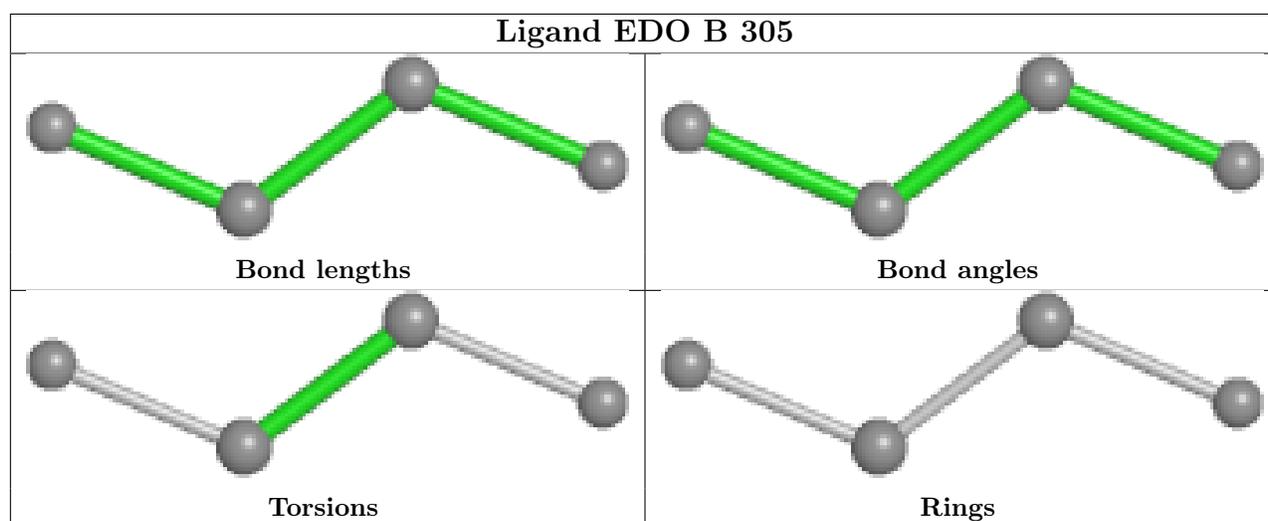
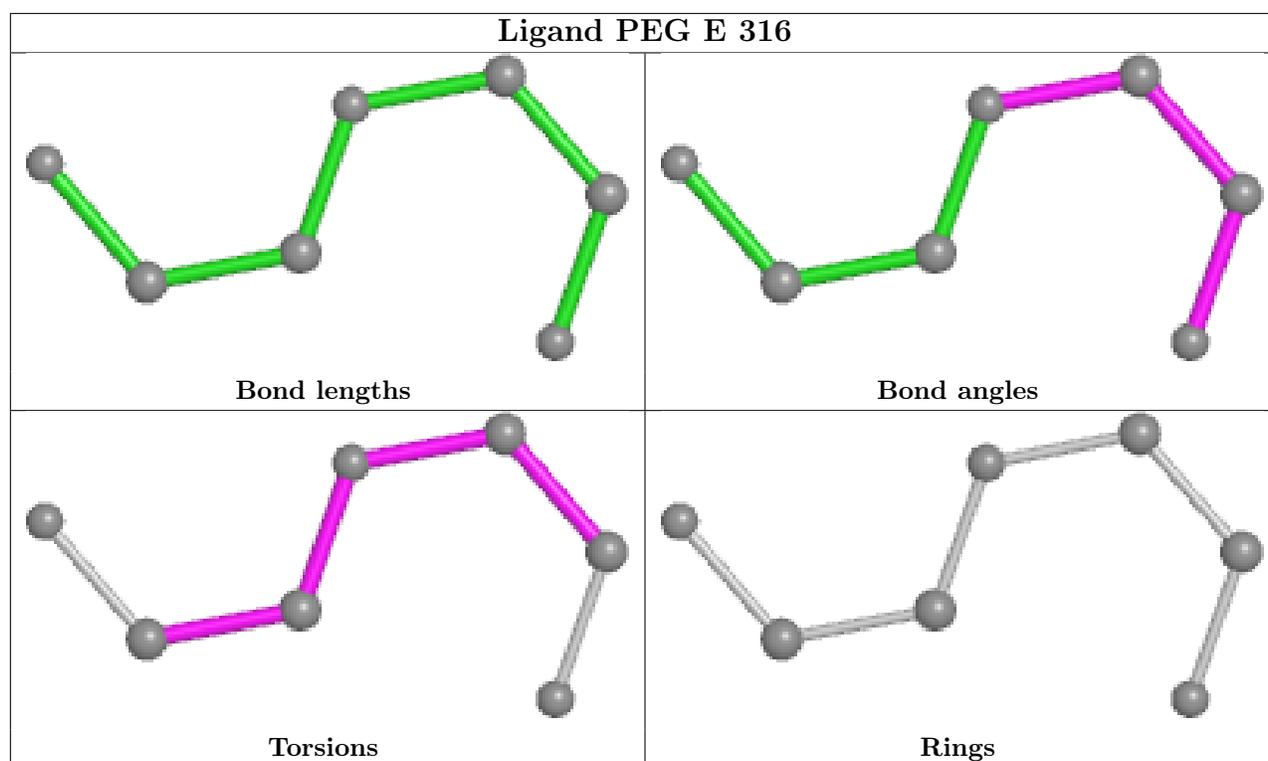


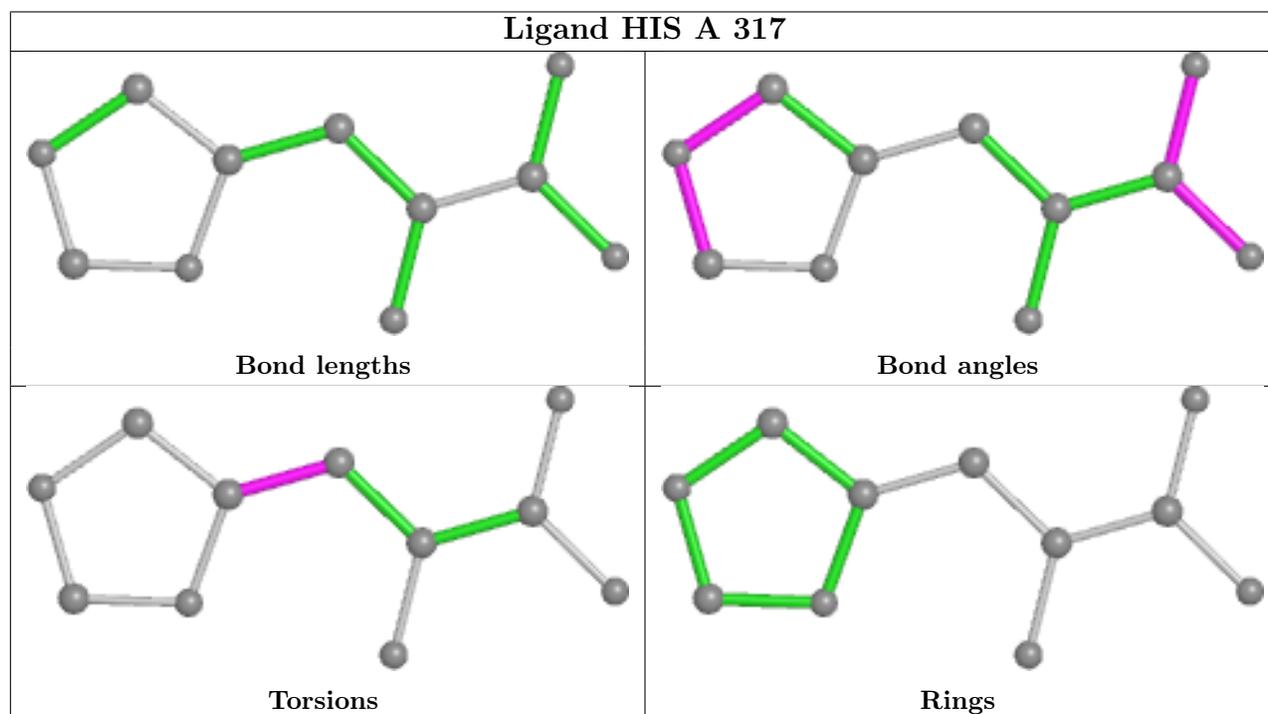
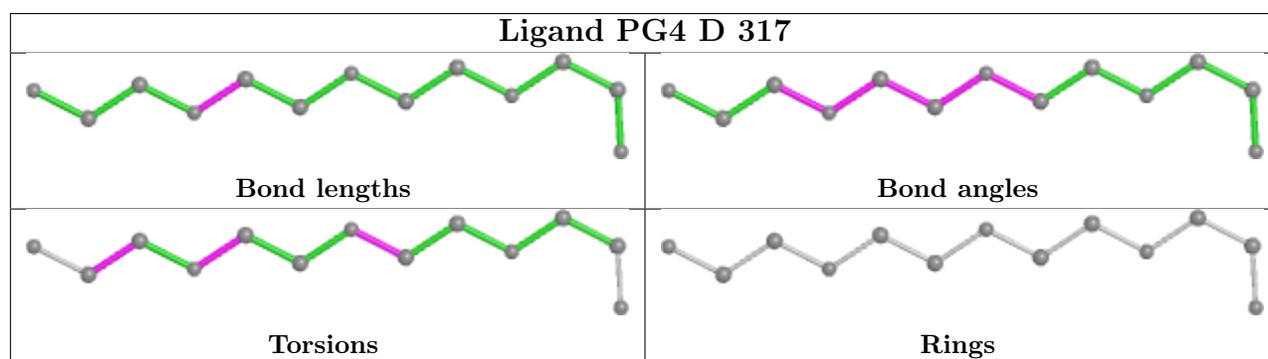
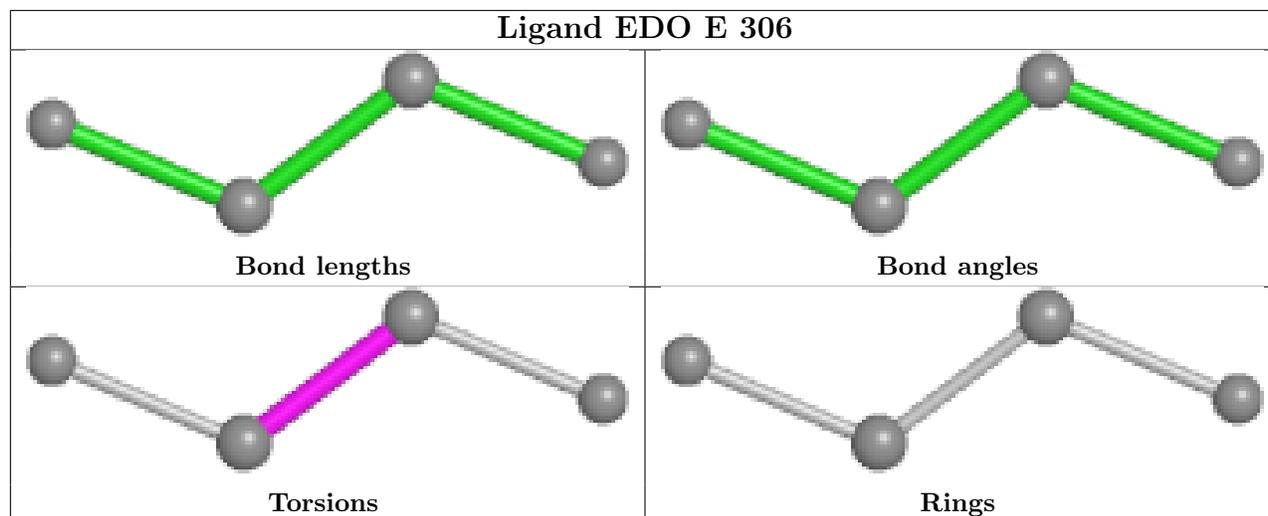


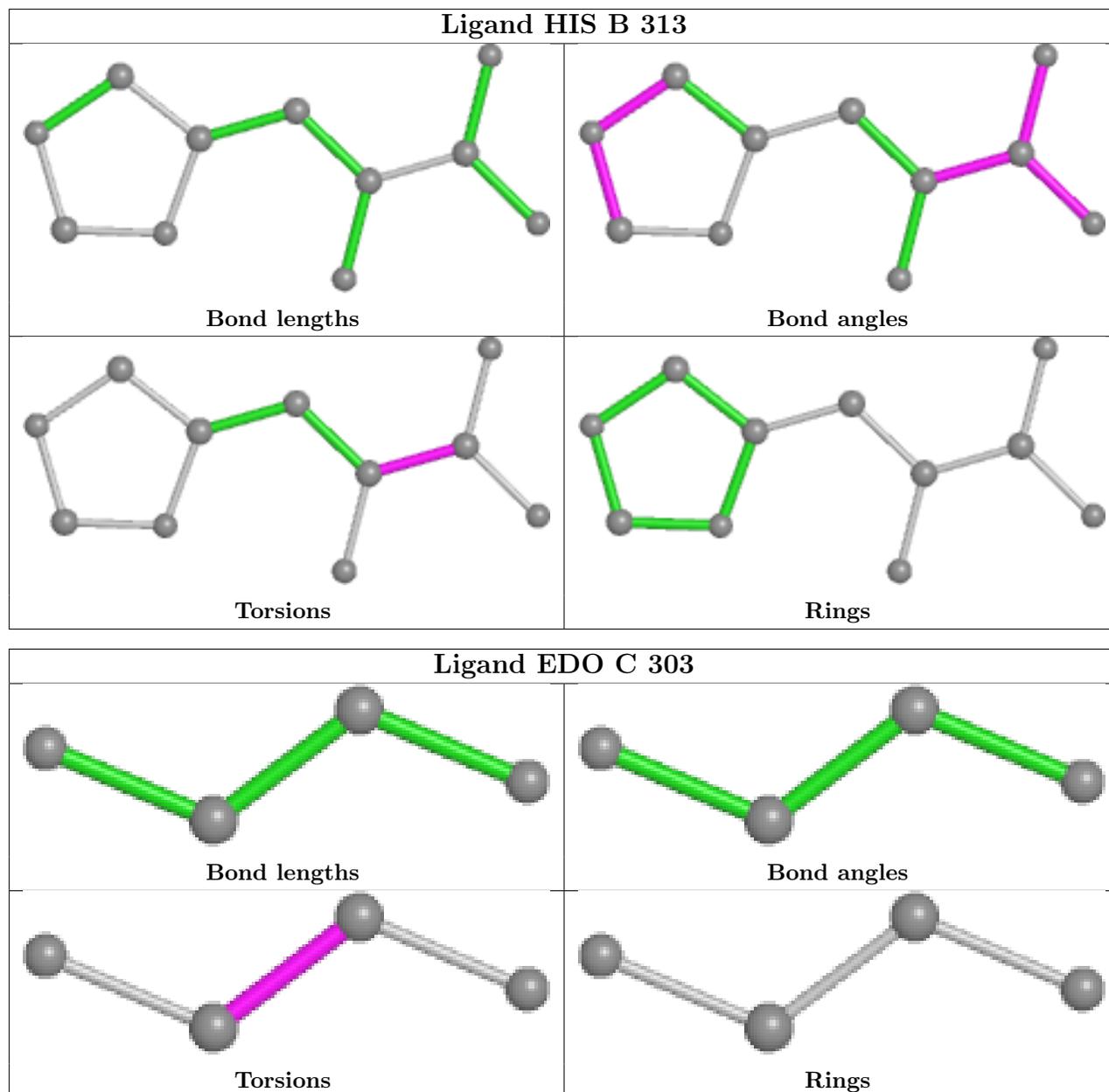


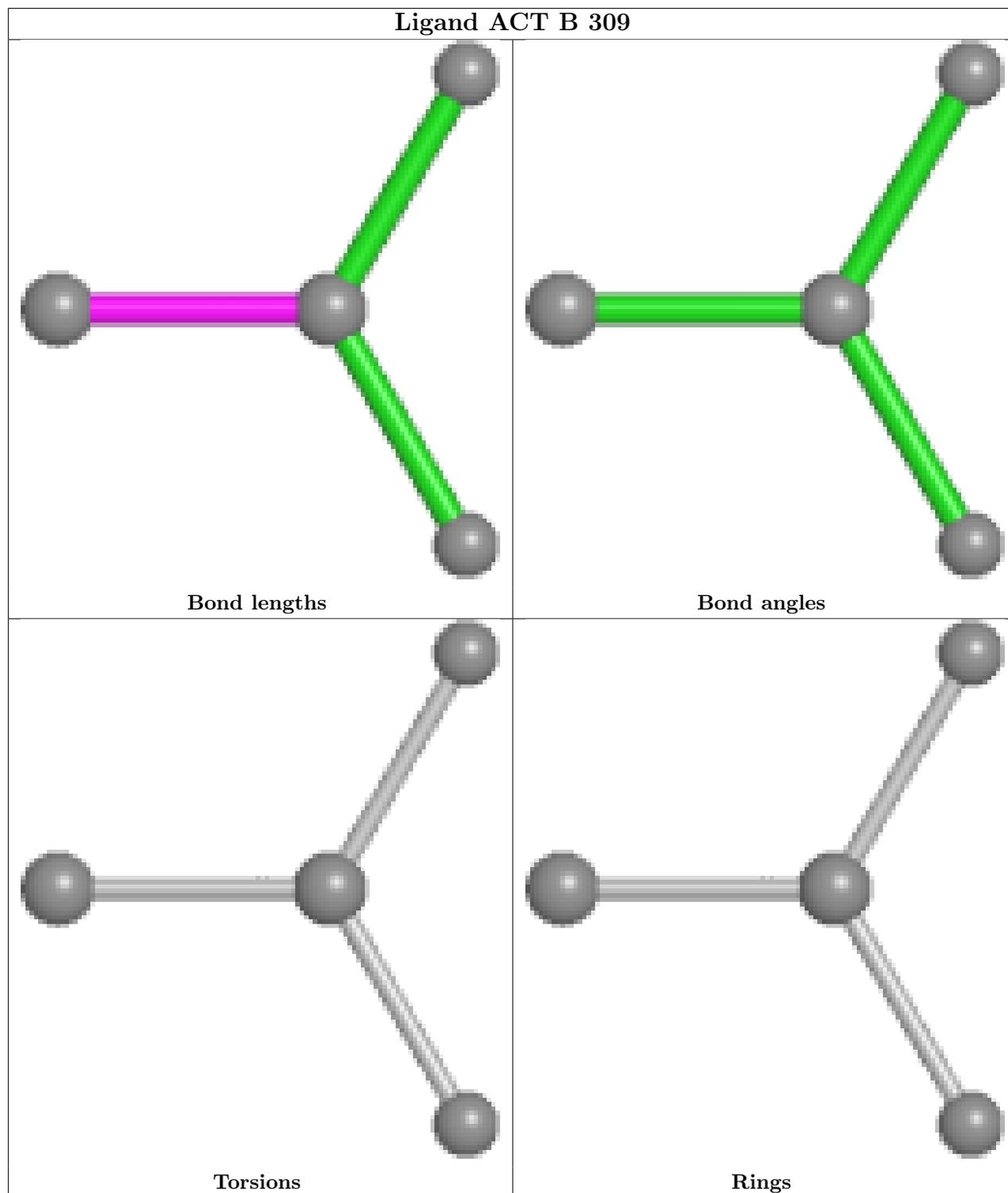


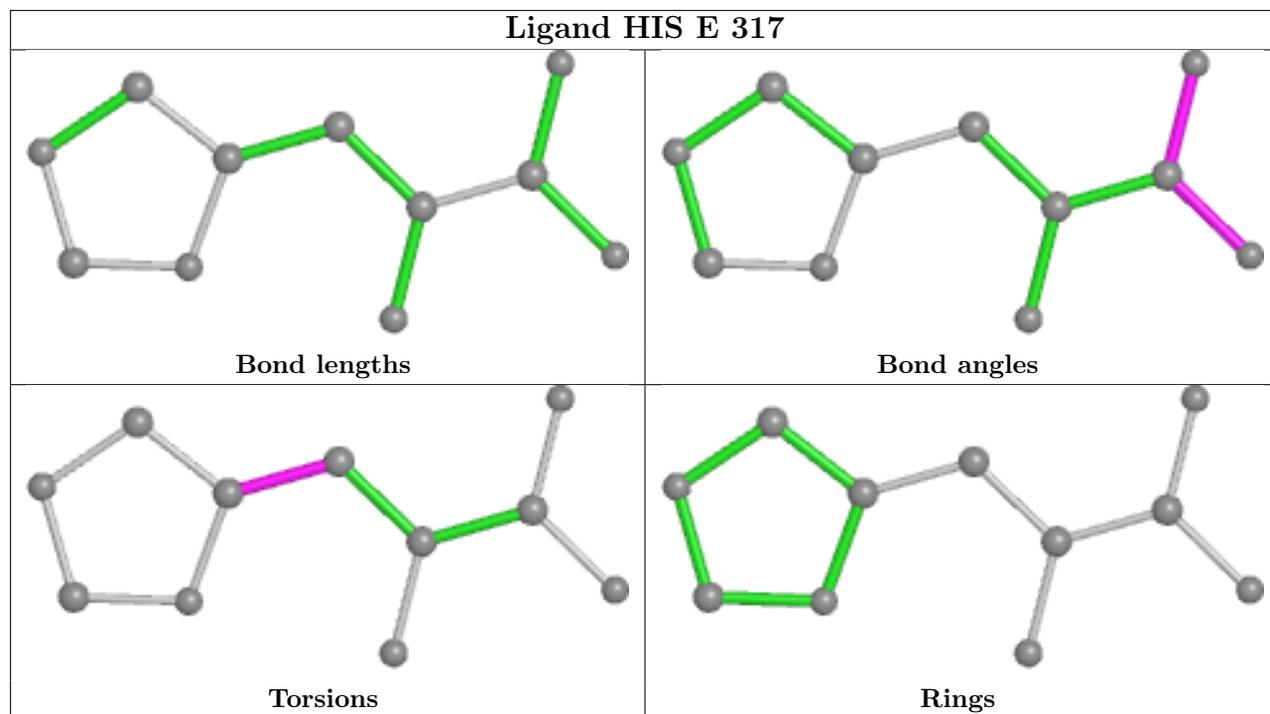


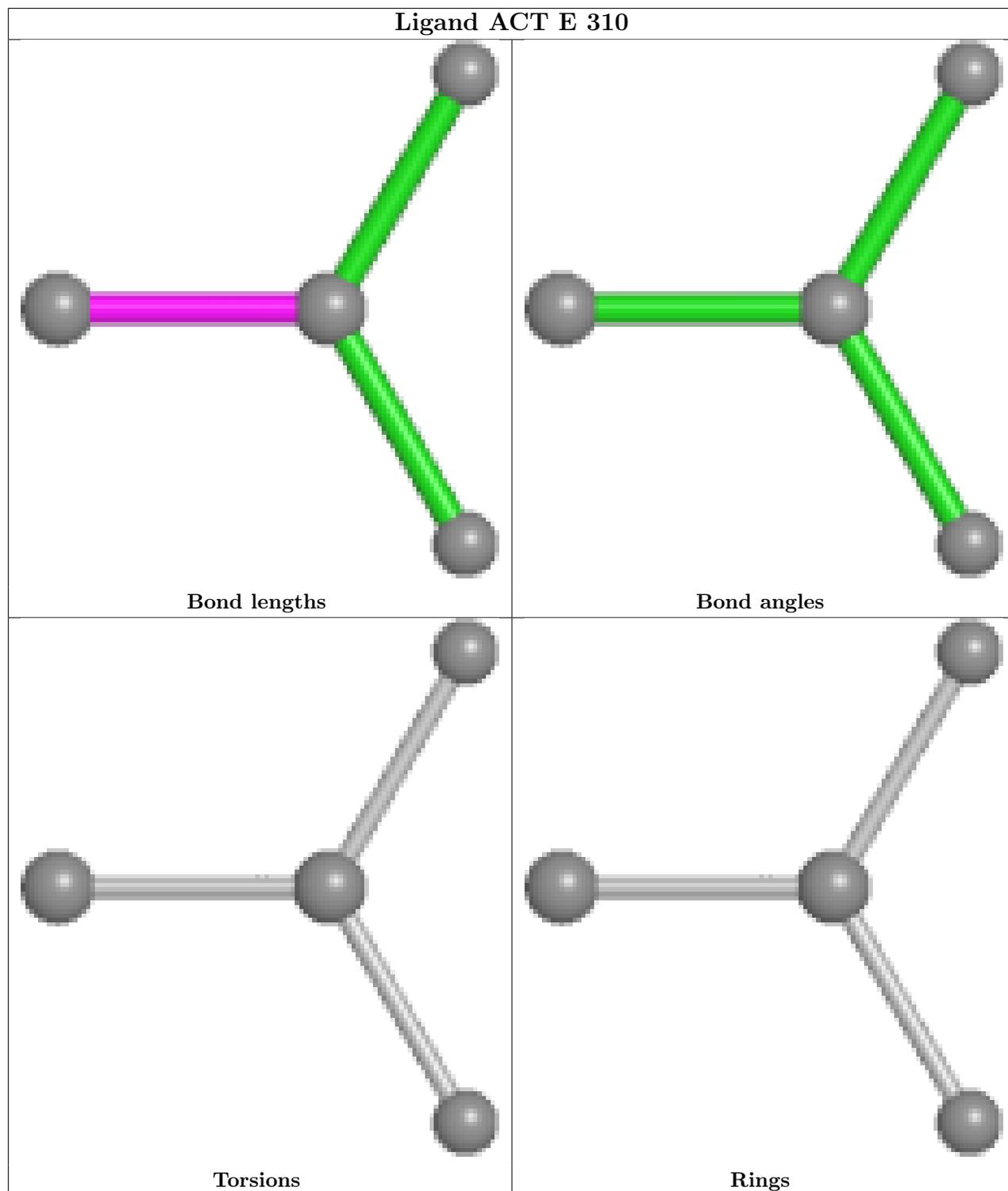


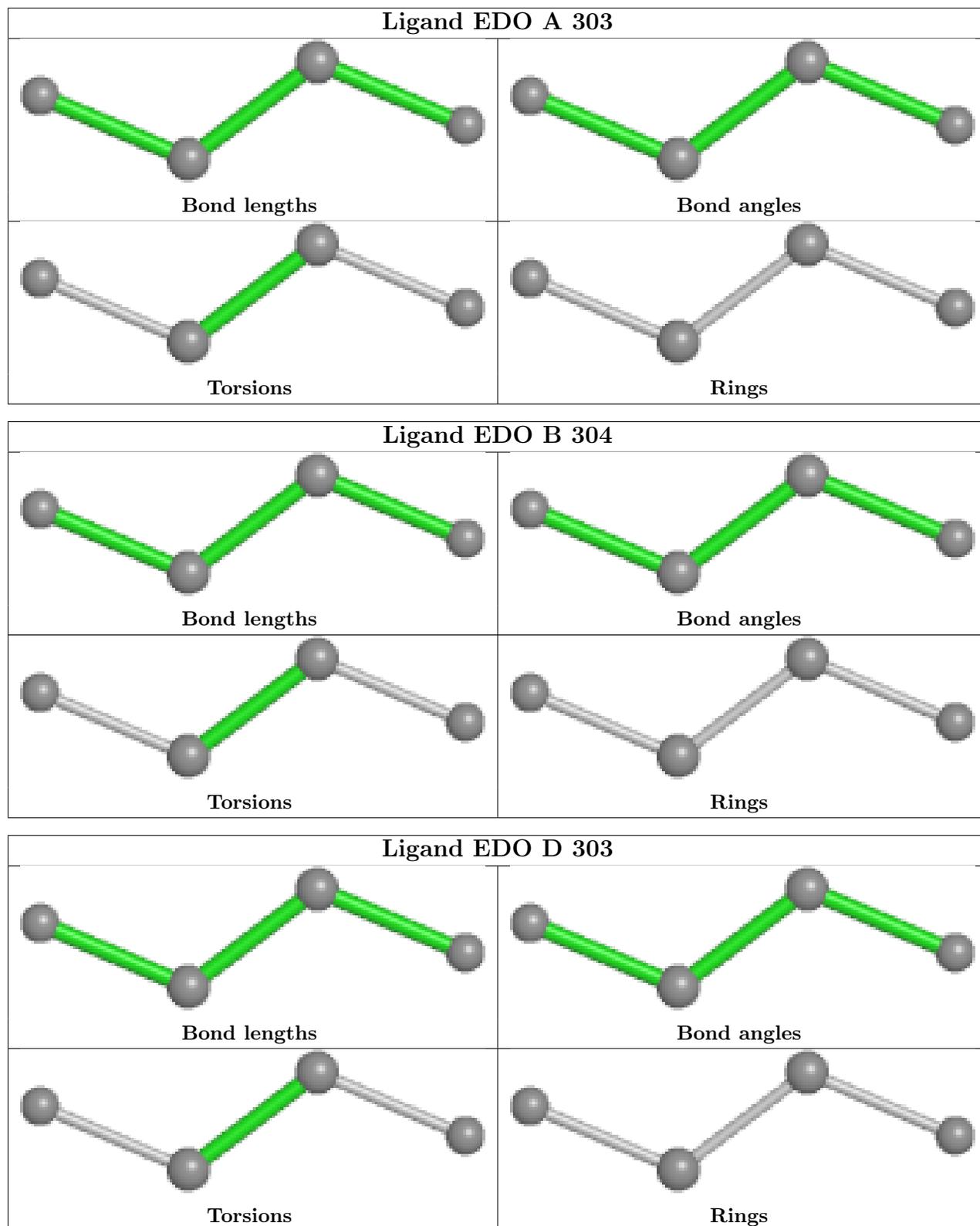


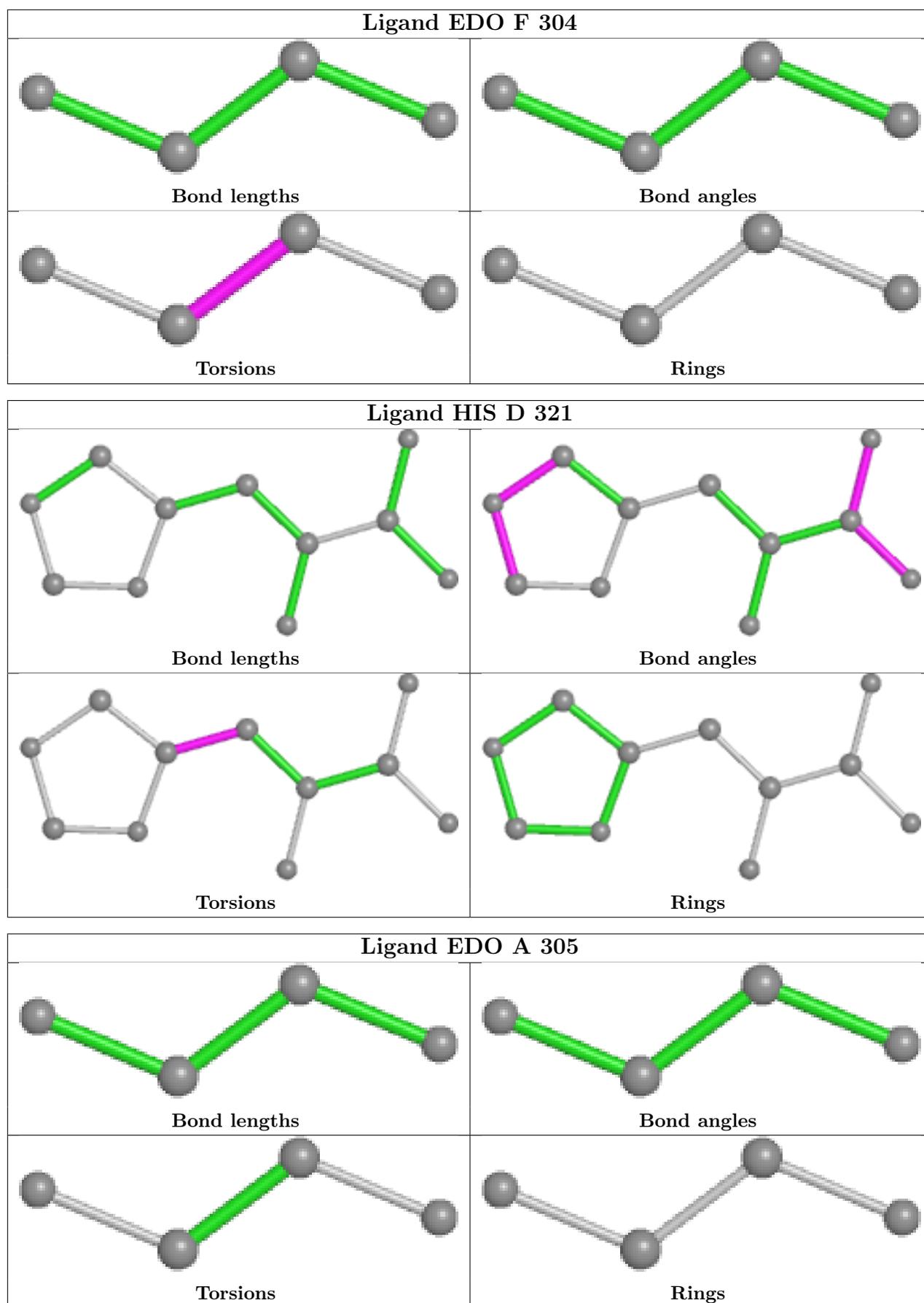


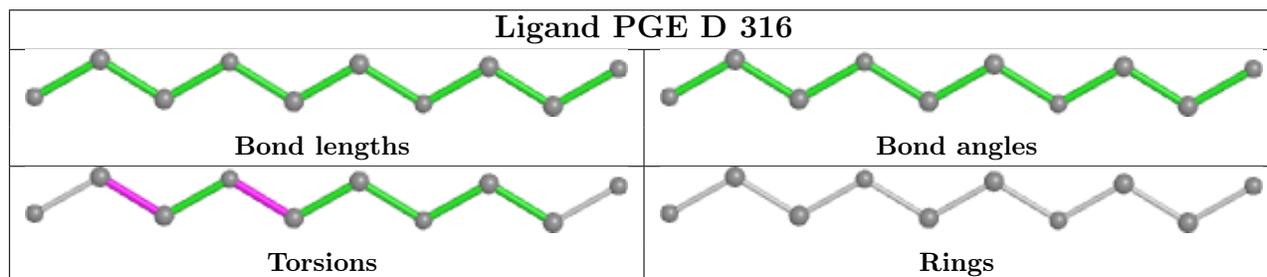
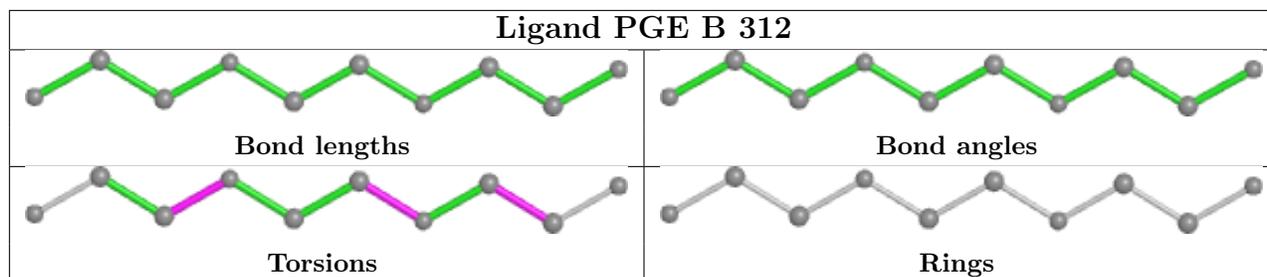


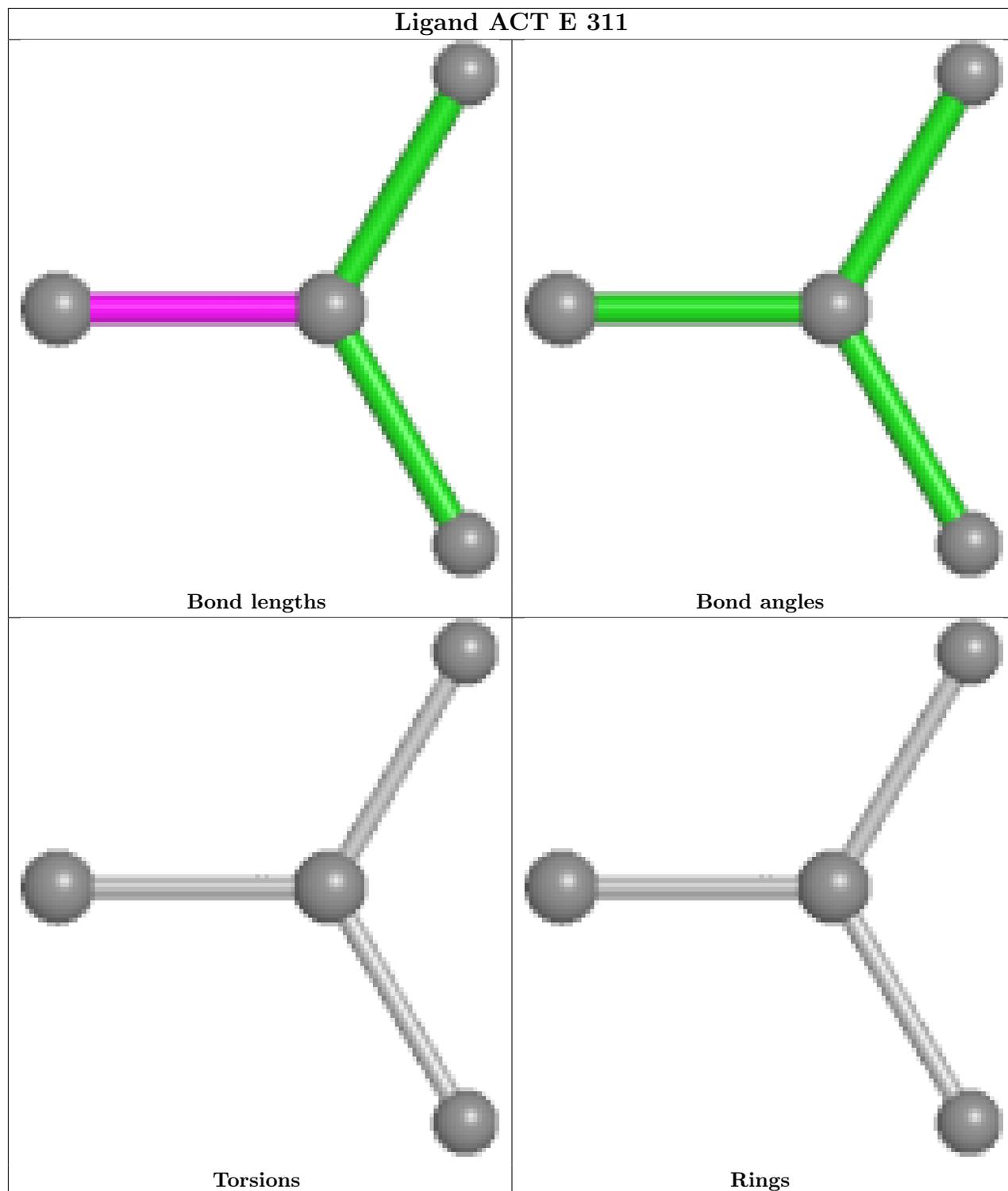


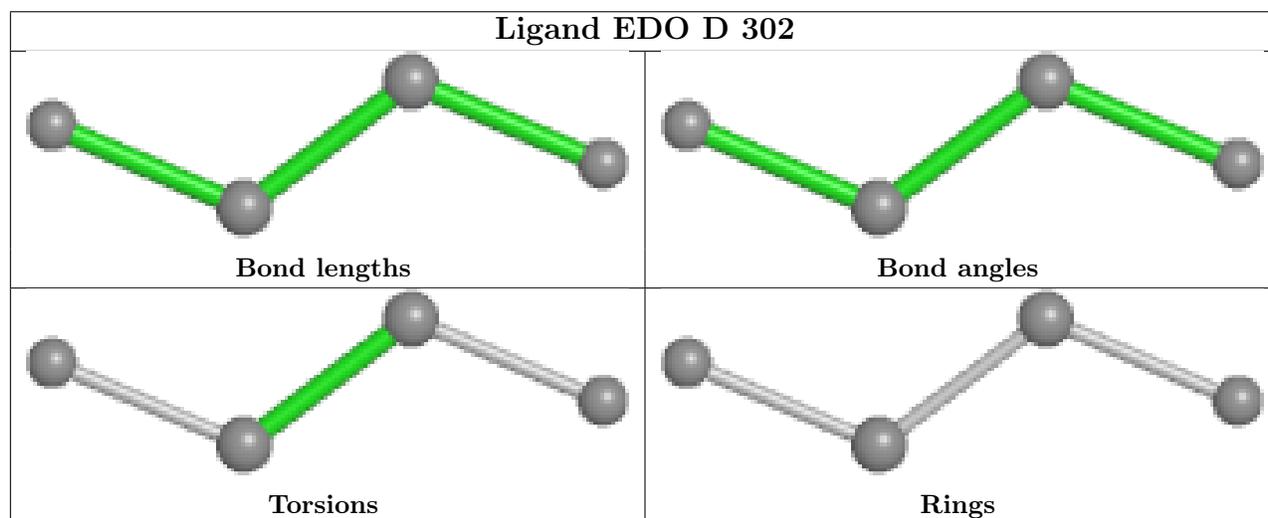
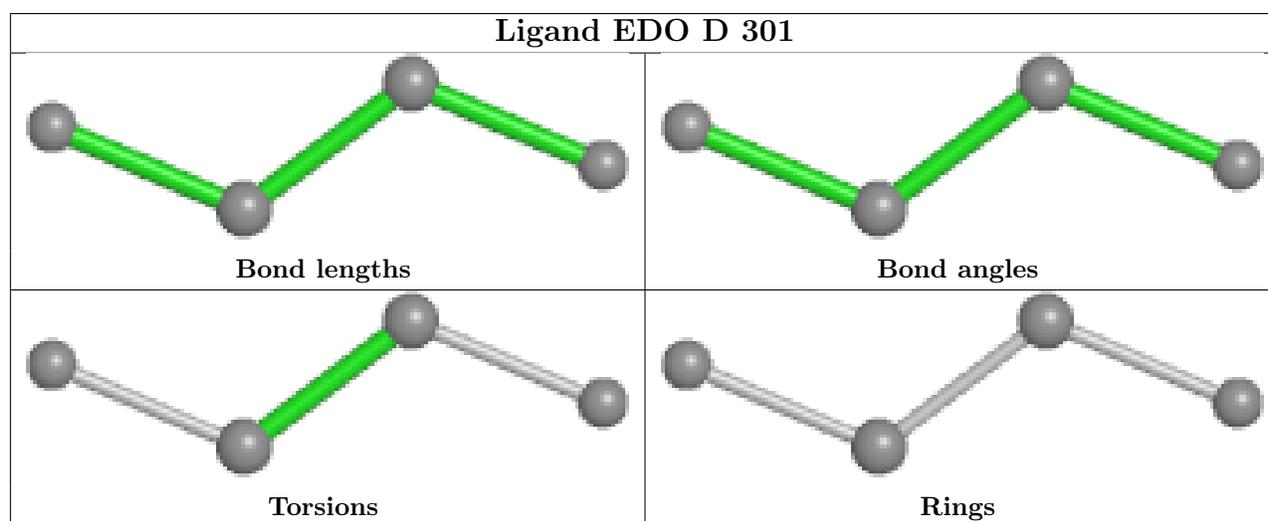
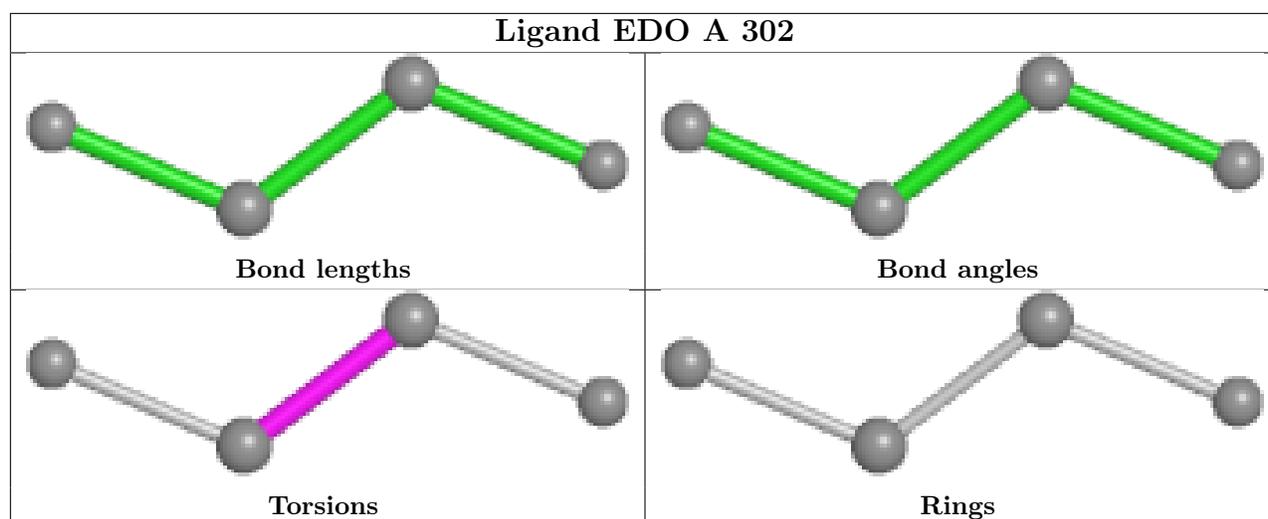


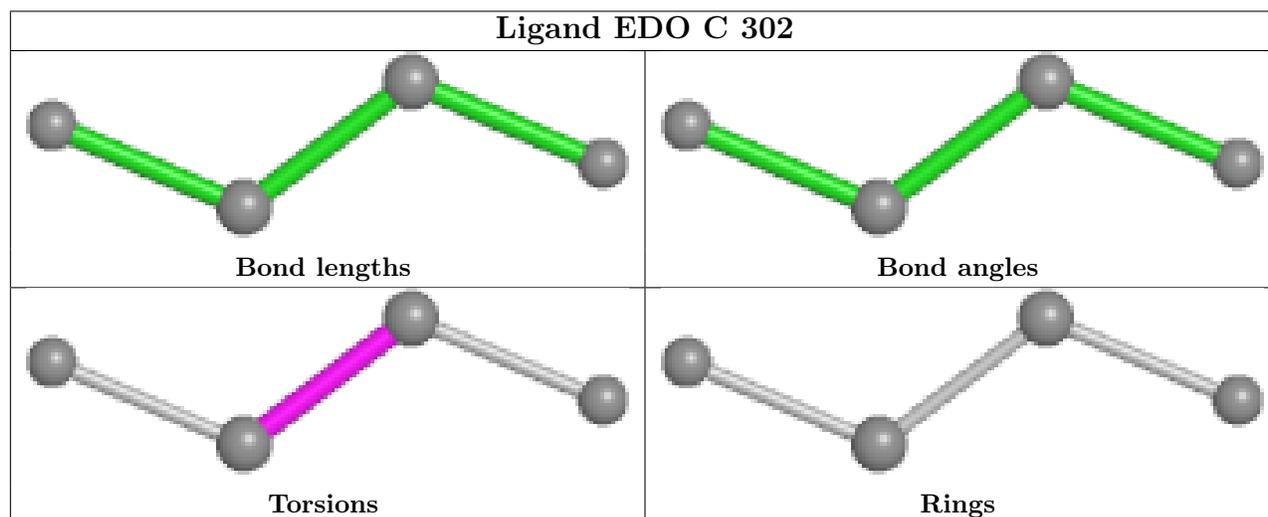
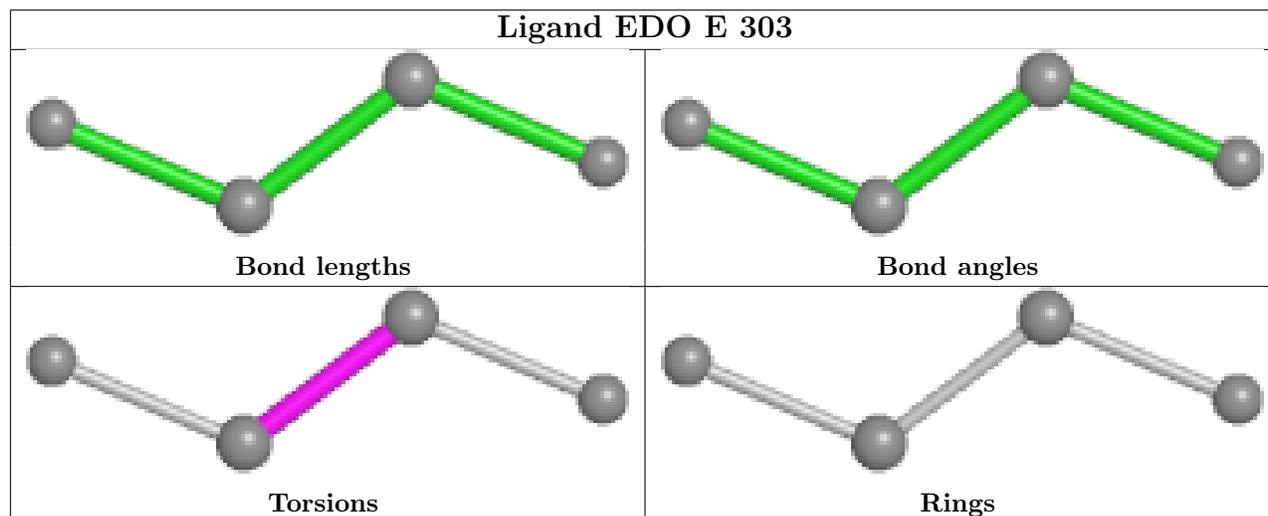
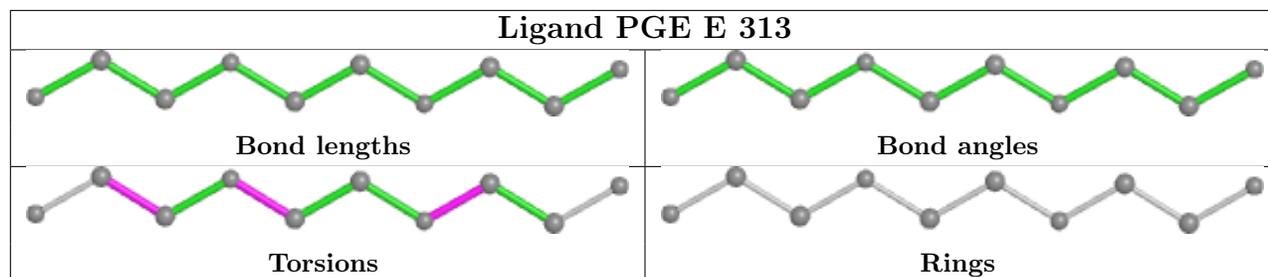


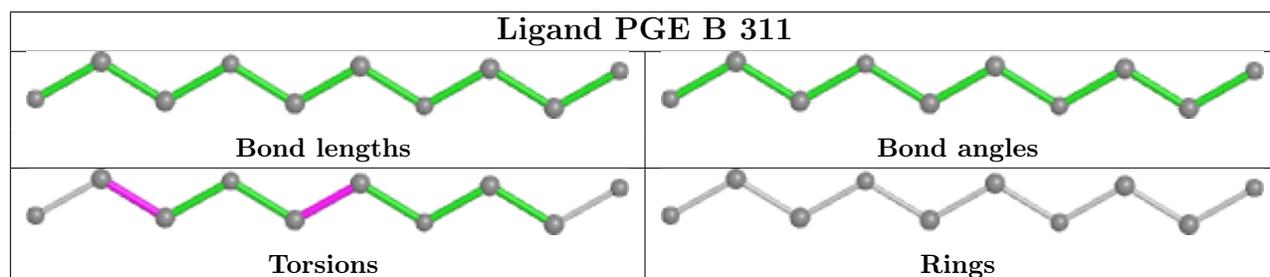
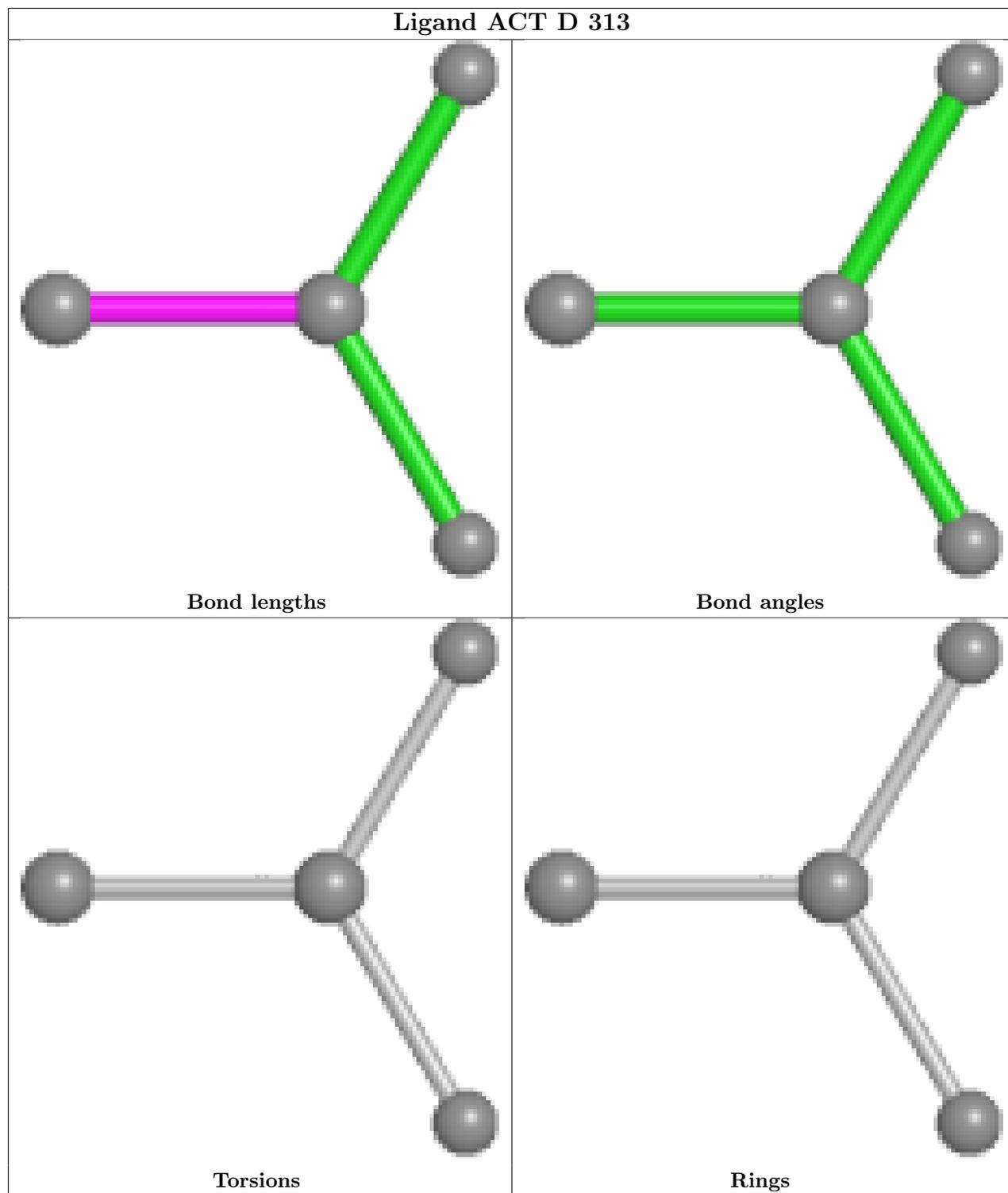


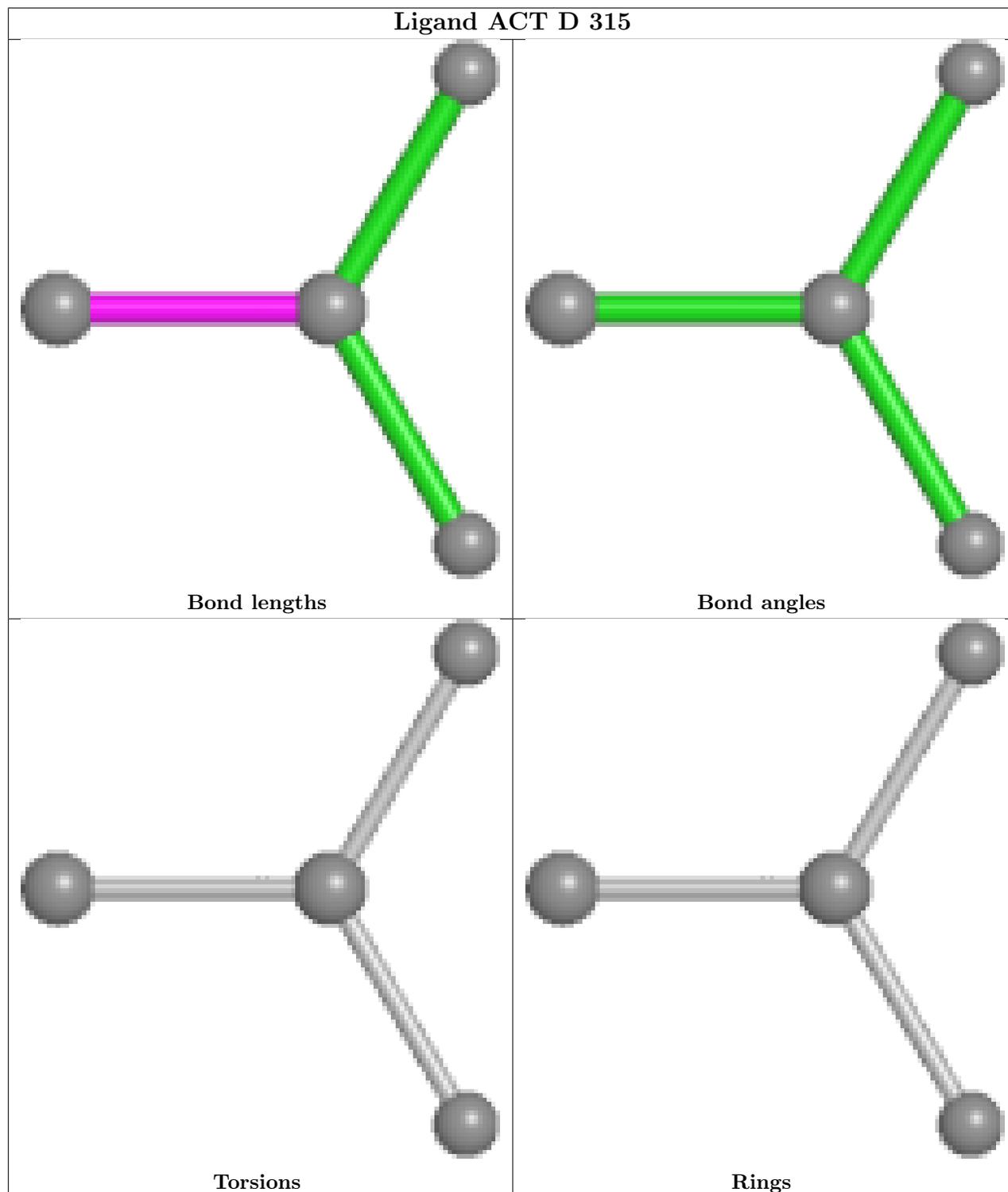
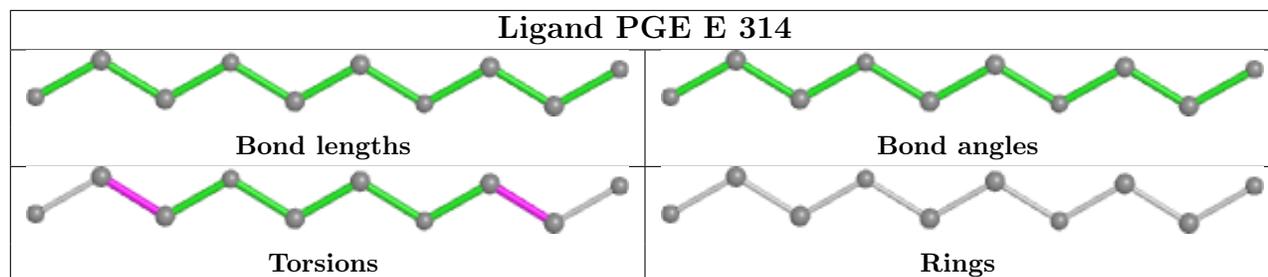


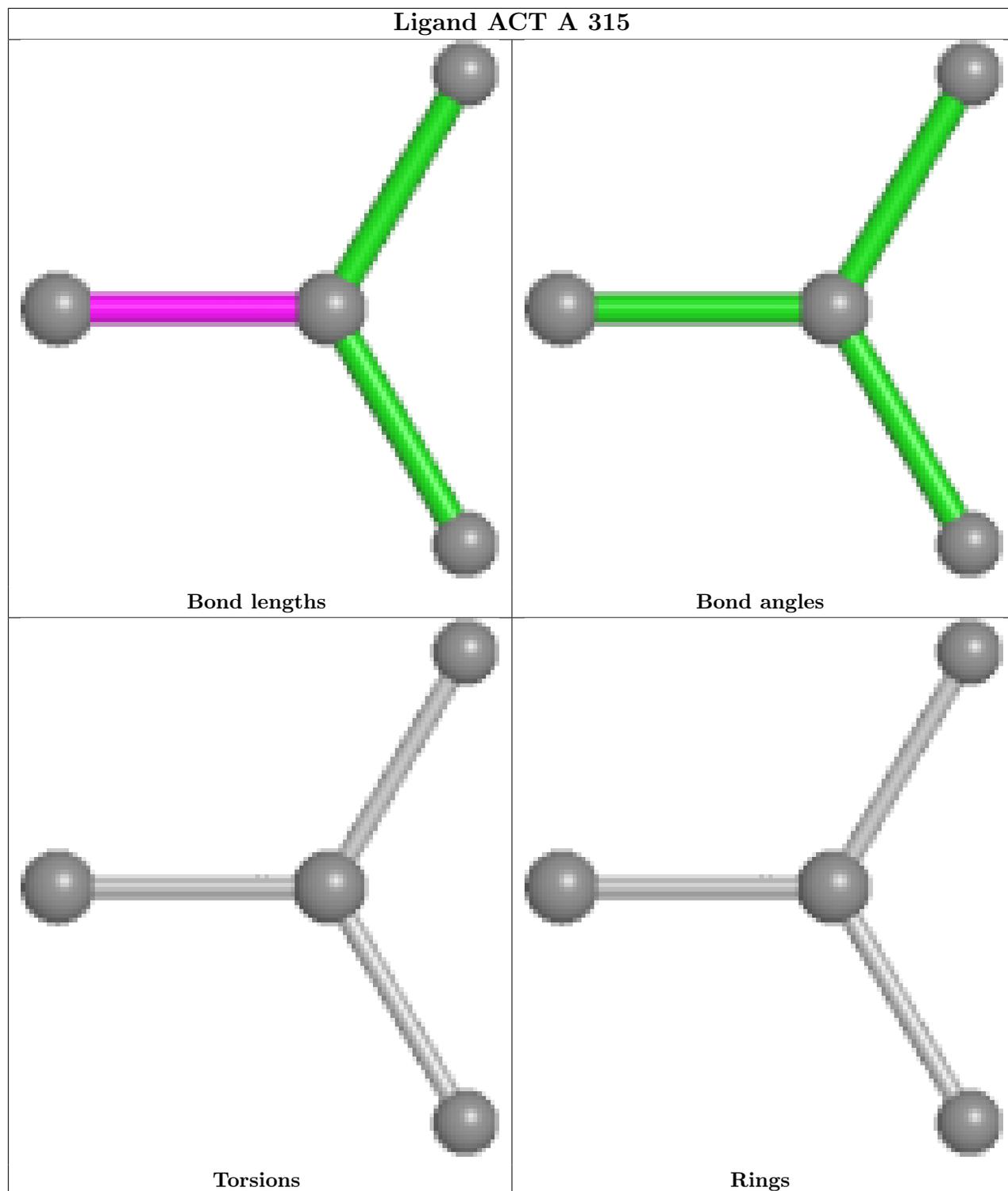


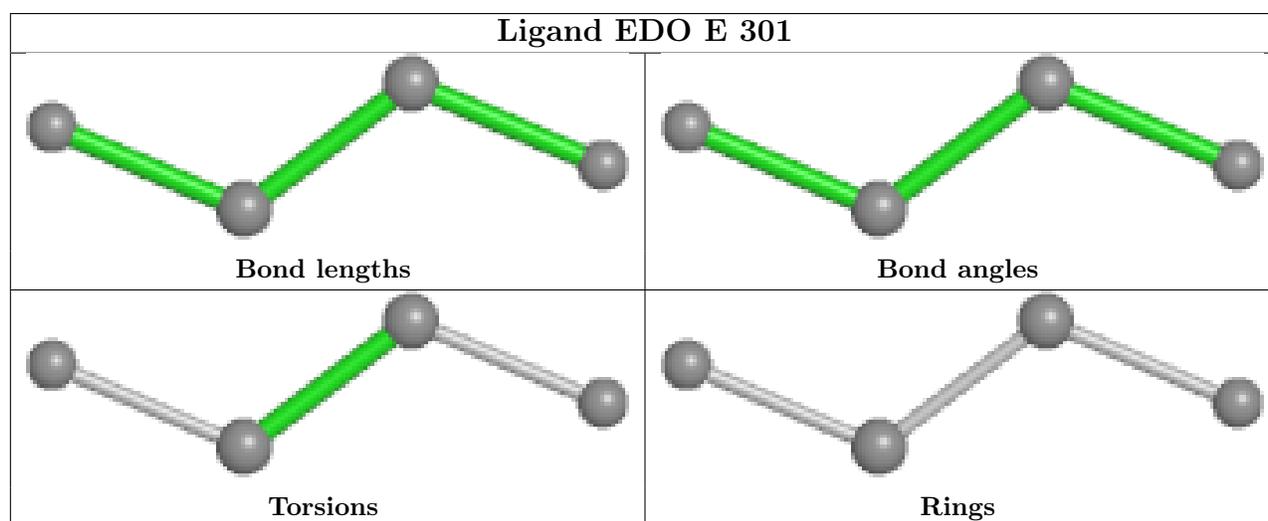
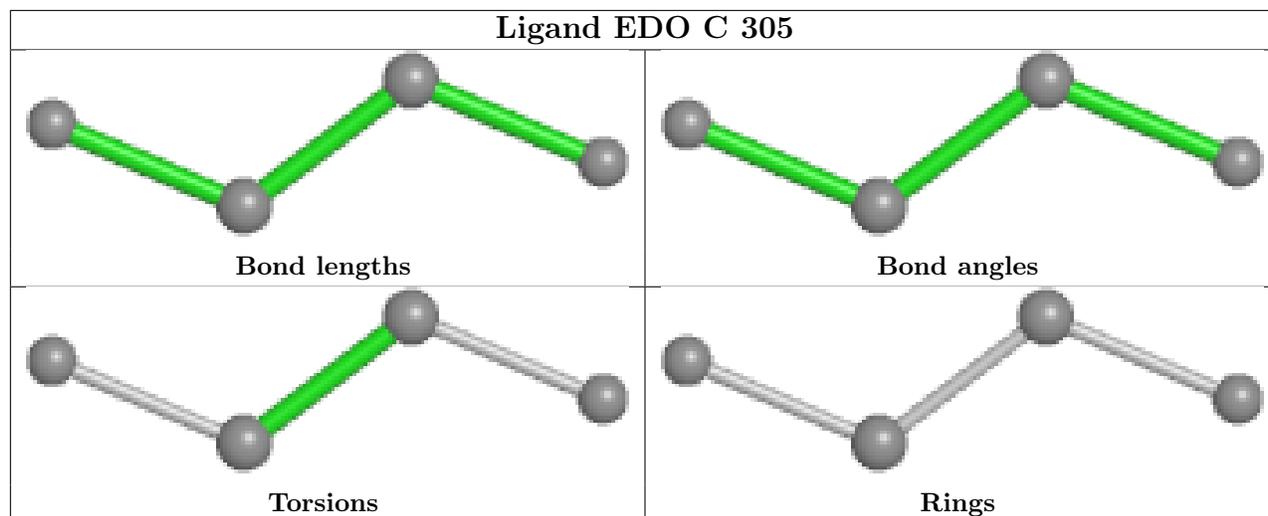


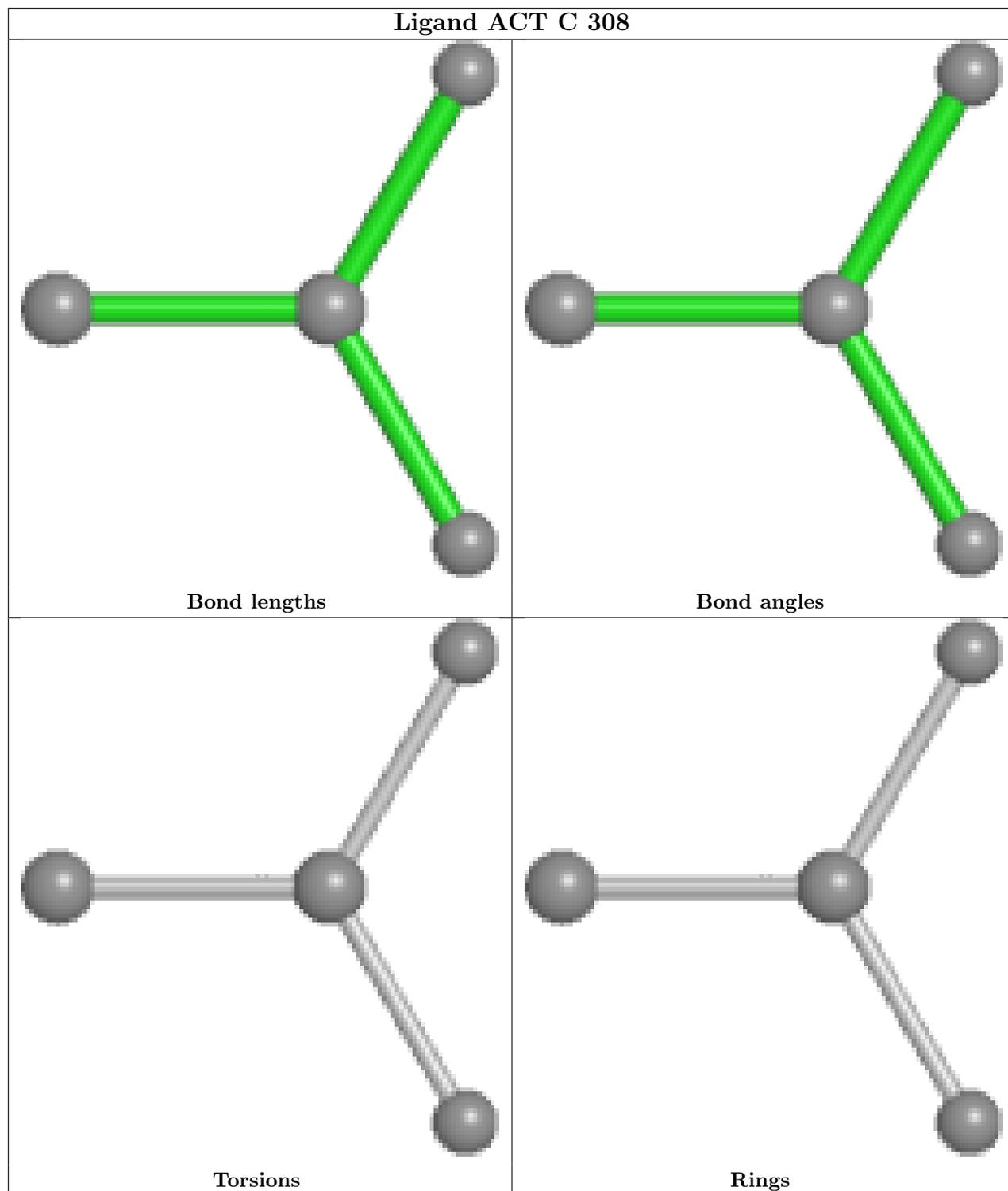


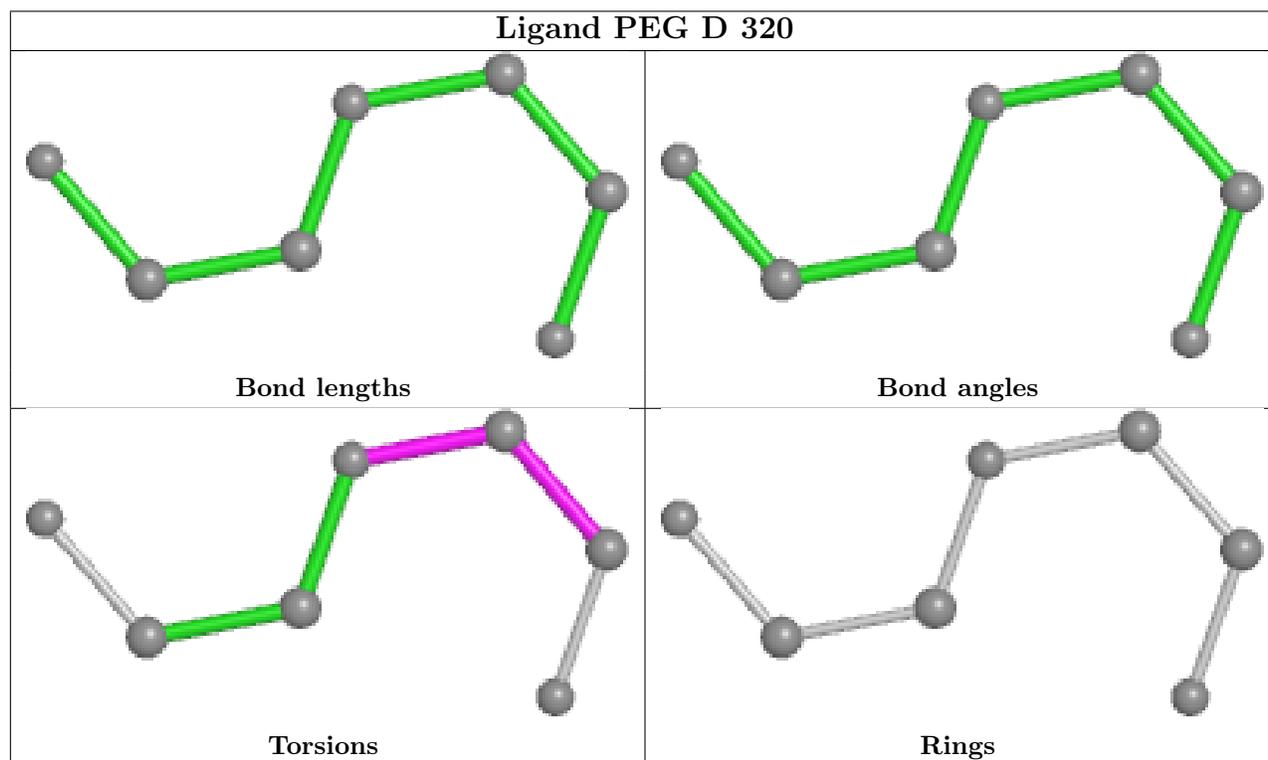
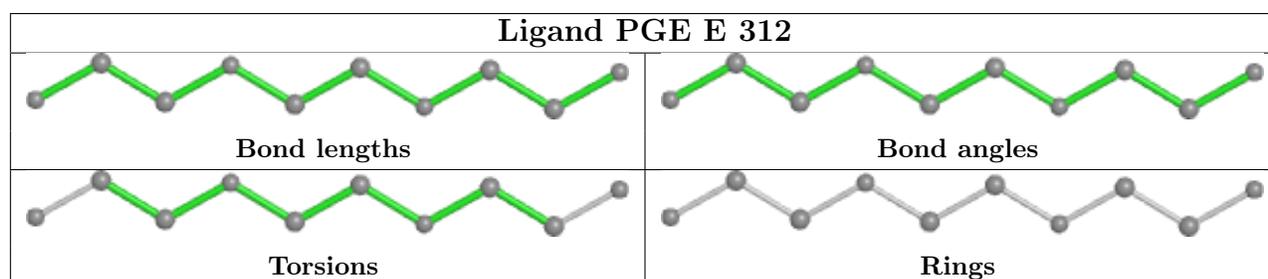
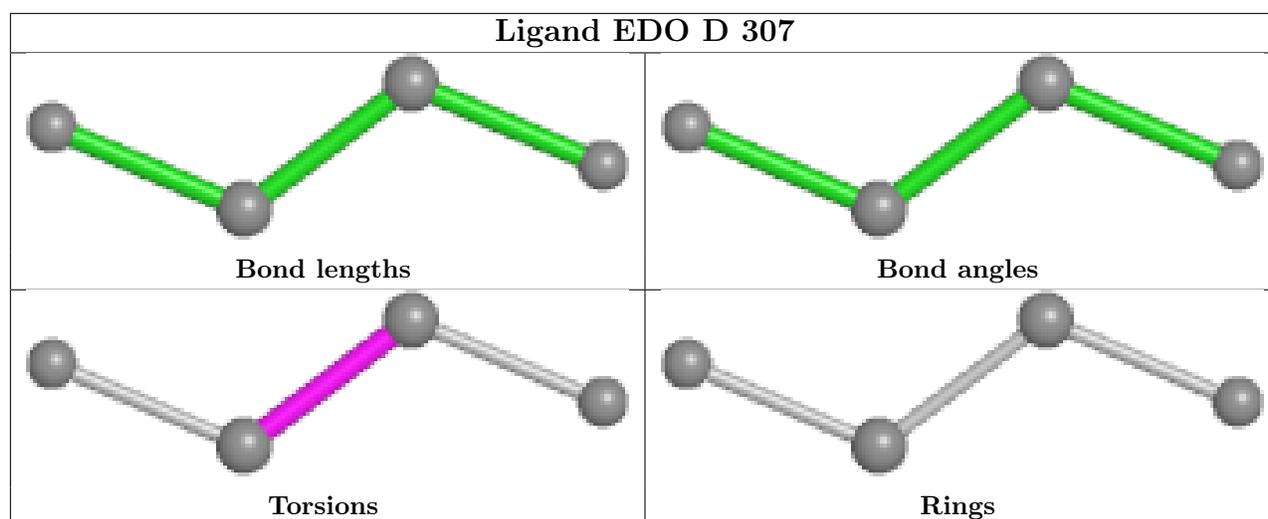


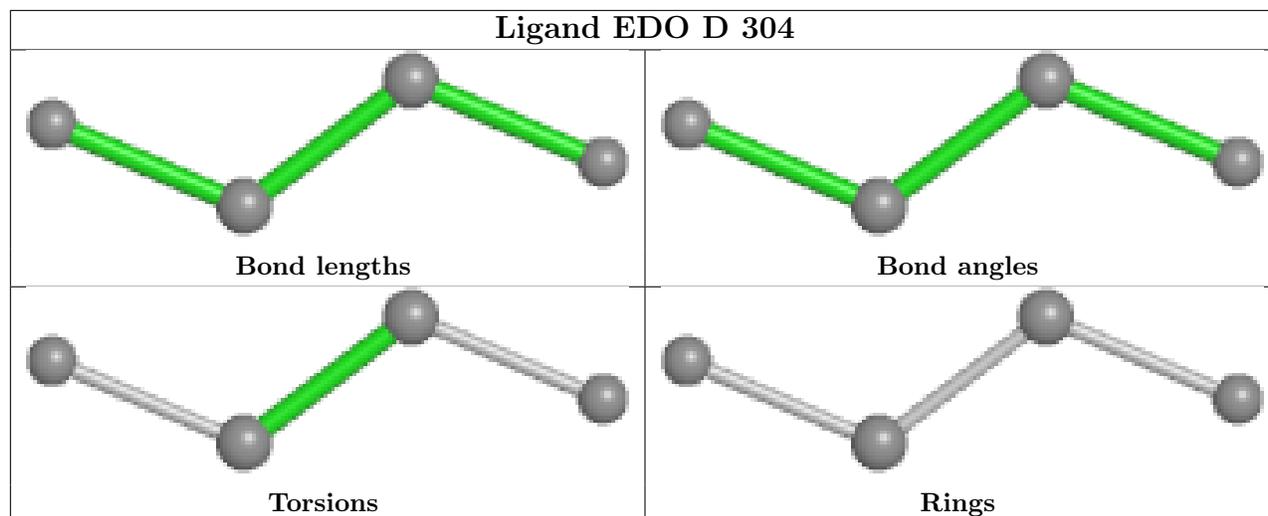












5.7 Other polymers [i](#)

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%)	-0.02	3 (1%) 82 84	19, 25, 42, 54	0
1	B	295/310 (95%)	0.07	3 (1%) 82 84	19, 27, 45, 58	0
1	C	295/310 (95%)	0.09	0 100 100	20, 27, 44, 54	0
1	D	295/310 (95%)	0.10	2 (0%) 87 88	20, 27, 44, 51	0
1	E	295/310 (95%)	-0.04	3 (1%) 82 84	19, 28, 45, 59	0
1	F	296/310 (95%)	0.06	3 (1%) 82 84	19, 28, 47, 56	0
All	All	1771/1860 (95%)	0.04	14 (0%) 86 87	19, 27, 45, 59	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ASN	3.3
1	B	267	GLU	2.9
1	F	29	ARG	2.9
1	E	131	ASP	2.7
1	F	261	TYR	2.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KPI	F	166	14/15	0.93	0.13	19,25,31,31	0
1	KPI	E	166	14/15	0.94	0.10	23,24,28,28	0
1	KPI	C	166	14/15	0.95	0.15	15,24,28,29	0
1	KPI	D	166	14/15	0.96	0.12	20,25,29,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KPI	B	166	14/15	0.96	0.11	16,21,30,31	0
1	KPI	A	166	14/15	0.96	0.11	18,21,28,29	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	A	307	4/4	0.24	0.36	63,66,66,69	0
4	ACT	A	314	4/4	0.69	0.21	37,38,50,59	0
4	ACT	D	314	4/4	0.69	0.17	49,51,53,54	0
8	PEG	D	318	7/7	0.70	0.32	45,46,55,59	0
4	ACT	E	311	4/4	0.75	0.29	36,42,45,55	0
4	ACT	D	315	4/4	0.77	0.19	38,49,51,53	0
3	MG	A	312	1/1	0.78	0.12	56,56,56,56	0
3	MG	E	308	1/1	0.80	0.15	59,59,59,59	0
4	ACT	F	308	4/4	0.80	0.18	42,44,48,53	0
5	PGE	E	314	10/10	0.80	0.40	20,20,20,20	0
2	EDO	B	303	4/4	0.80	0.25	35,36,48,54	0
5	PGE	B	312	10/10	0.81	0.17	44,50,56,58	0
8	PEG	E	316	7/7	0.81	0.42	20,20,20,20	0
2	EDO	D	308	4/4	0.82	0.25	43,45,48,49	0
4	ACT	A	315	4/4	0.83	0.19	32,35,40,46	0
2	EDO	F	302	4/4	0.83	0.20	27,43,47,49	0
8	PEG	D	319	7/7	0.83	0.15	39,47,52,55	0
2	EDO	C	303	4/4	0.83	0.15	51,54,58,59	0
3	MG	A	311	1/1	0.84	0.40	54,54,54,54	0
4	ACT	B	308	4/4	0.84	0.25	37,38,39,44	0
4	ACT	D	313	4/4	0.84	0.22	35,39,42,44	0
4	ACT	E	310	4/4	0.85	0.16	31,36,38,40	0
5	PGE	E	313	10/10	0.86	0.14	41,44,50,58	0
2	EDO	A	305	4/4	0.86	0.13	39,43,50,53	0
3	MG	F	305	1/1	0.86	0.23	54,54,54,54	0
2	EDO	B	304	4/4	0.86	0.20	29,34,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	D	320	7/7	0.86	0.47	20,20,20,20	0
2	EDO	E	306	4/4	0.86	0.35	20,20,20,20	0
7	PG4	D	317	13/13	0.87	0.14	32,45,49,56	0
3	MG	D	311	1/1	0.87	0.09	41,41,41,41	0
2	EDO	C	305	4/4	0.87	0.20	32,33,37,44	0
3	MG	E	309	1/1	0.87	0.29	54,54,54,54	0
2	EDO	B	302	4/4	0.87	0.12	39,44,48,50	0
2	EDO	B	301	4/4	0.88	0.12	38,41,42,45	0
4	ACT	B	309	4/4	0.88	0.11	41,47,49,49	0
2	EDO	E	302	4/4	0.89	0.16	36,41,42,57	0
2	EDO	C	304	4/4	0.89	0.14	45,47,48,59	0
2	EDO	E	307	4/4	0.89	0.37	20,20,20,20	0
4	ACT	A	313	4/4	0.89	0.15	34,40,40,47	0
2	EDO	C	301	4/4	0.89	0.12	43,46,48,51	0
3	MG	A	308	1/1	0.89	0.24	47,47,47,47	0
6	HIS	B	313	11/11	0.89	0.13	27,33,39,41	0
3	MG	A	309	1/1	0.89	0.18	57,57,57,57	0
2	EDO	D	304	4/4	0.89	0.19	35,40,45,54	0
2	EDO	D	306	4/4	0.89	0.11	39,41,49,50	0
3	MG	D	310	1/1	0.89	0.14	41,41,41,41	0
2	EDO	A	306	4/4	0.89	0.10	34,37,42,45	0
4	ACT	F	307	4/4	0.90	0.13	38,39,47,48	0
3	MG	C	307	1/1	0.90	0.25	52,52,52,52	0
5	PGE	B	311	10/10	0.90	0.12	31,34,44,45	0
2	EDO	E	301	4/4	0.90	0.10	34,34,36,42	0
5	PGE	D	316	10/10	0.91	0.12	37,39,44,54	0
2	EDO	D	305	4/4	0.91	0.10	39,39,49,52	0
2	EDO	E	305	4/4	0.91	0.35	20,20,20,20	0
2	EDO	B	305	4/4	0.91	0.14	39,41,42,50	0
6	HIS	C	310	11/11	0.91	0.15	24,30,37,37	0
6	HIS	D	321	11/11	0.91	0.12	27,31,37,38	0
6	HIS	E	317	11/11	0.91	0.12	27,32,35,36	0
4	ACT	F	306	4/4	0.91	0.17	38,38,44,48	0
2	EDO	C	306	4/4	0.91	0.34	33,40,43,51	0
4	ACT	B	310	4/4	0.91	0.11	46,51,54,56	0
3	MG	B	307	1/1	0.91	0.15	42,42,42,42	0
8	PEG	E	315	7/7	0.91	0.12	36,45,54,55	0
2	EDO	A	303	4/4	0.91	0.11	33,37,44,46	0
2	EDO	F	303	4/4	0.92	0.16	33,39,40,50	0
2	EDO	A	301	4/4	0.92	0.12	25,29,32,39	0
2	EDO	E	304	4/4	0.92	0.12	29,30,36,43	0
4	ACT	C	308	4/4	0.92	0.21	34,36,40,45	0

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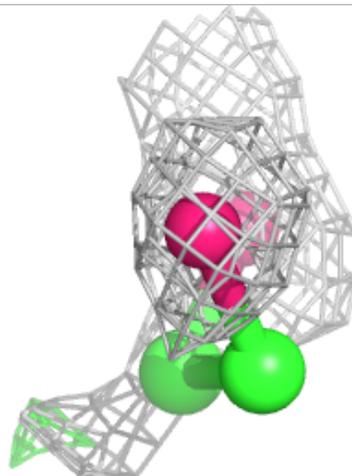
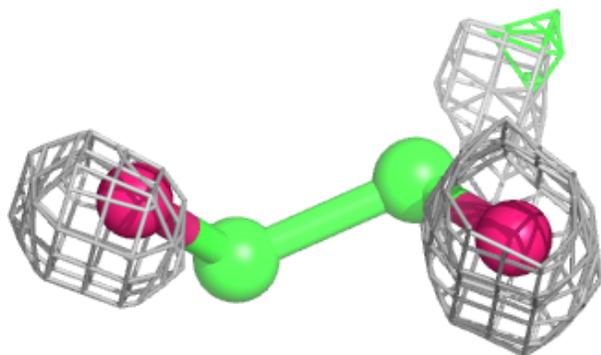
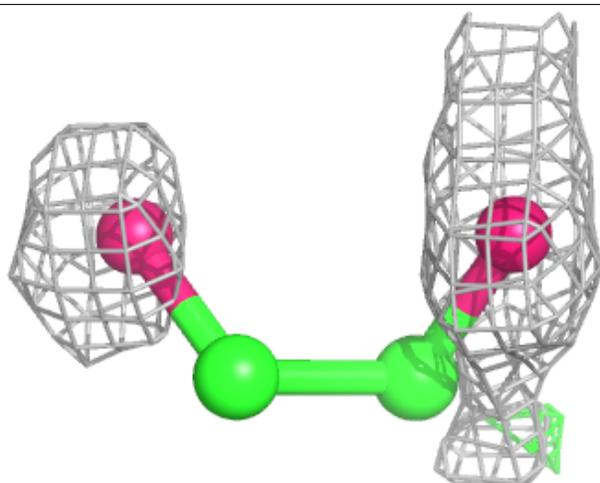
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGE	A	316	10/10	0.92	0.10	31,38,45,47	0
2	EDO	D	303	4/4	0.93	0.13	41,42,42,52	0
6	HIS	A	317	11/11	0.93	0.14	26,31,38,39	0
5	PGE	E	312	10/10	0.93	0.17	37,41,46,53	0
5	PGE	C	309	10/10	0.93	0.09	32,37,41,57	0
2	EDO	E	303	4/4	0.94	0.11	41,41,41,49	0
3	MG	A	310	1/1	0.94	0.08	33,33,33,33	0
2	EDO	D	309	4/4	0.94	0.11	42,43,47,47	0
2	EDO	D	307	4/4	0.94	0.14	31,35,40,51	0
2	EDO	D	301	4/4	0.94	0.13	27,35,40,45	0
2	EDO	A	304	4/4	0.95	0.08	41,42,52,56	0
2	EDO	D	302	4/4	0.96	0.11	28,28,29,35	0
2	EDO	C	302	4/4	0.96	0.17	30,31,38,39	0
2	EDO	F	304	4/4	0.96	0.17	29,35,43,51	0
6	HIS	F	309	11/11	0.96	0.12	29,34,39,43	0
2	EDO	A	302	4/4	0.96	0.20	31,42,43,49	0
3	MG	B	306	1/1	0.97	0.10	28,28,28,28	0
2	EDO	F	301	4/4	0.98	0.15	22,25,26,31	0
3	MG	D	312	1/1	0.99	0.10	39,39,39,39	0

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

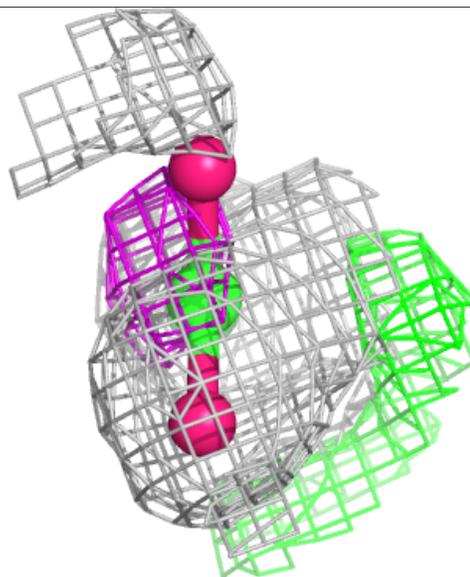
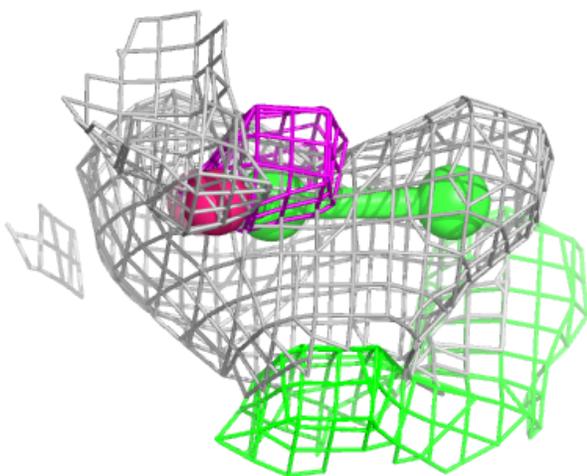
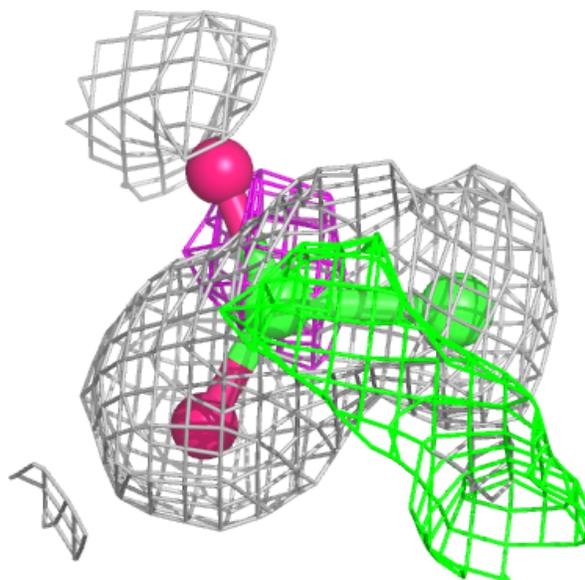
Electron density around EDO A 307:

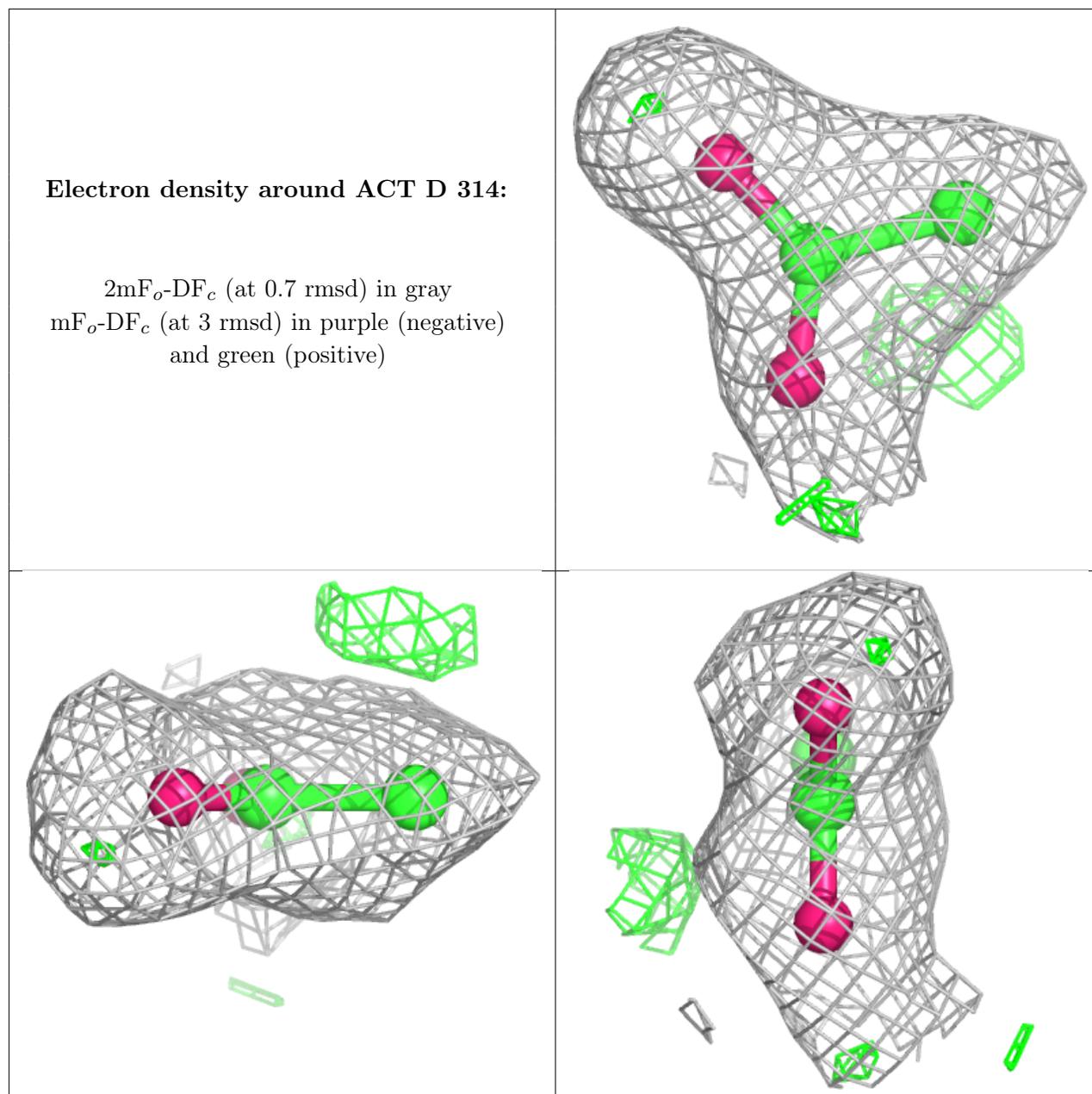
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

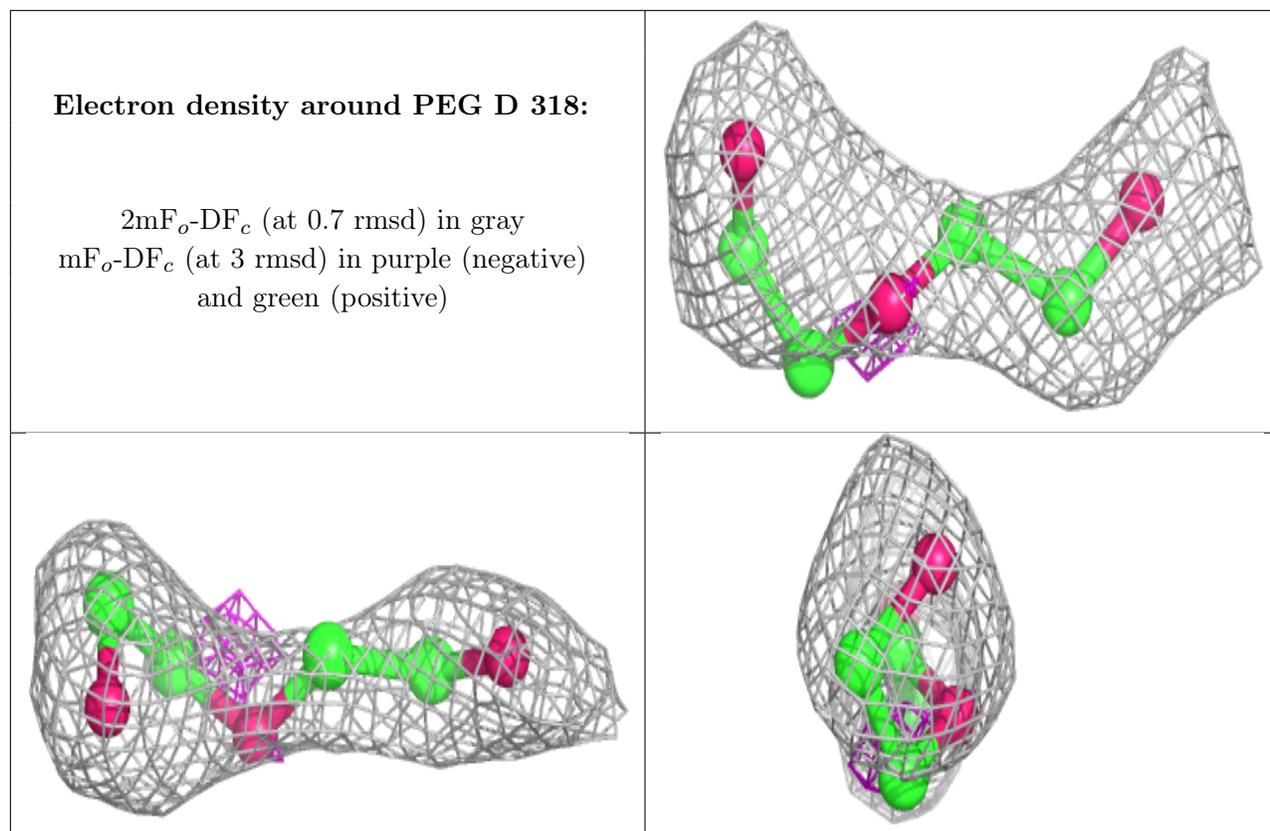


Electron density around ACT A 314:

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and green (positive)

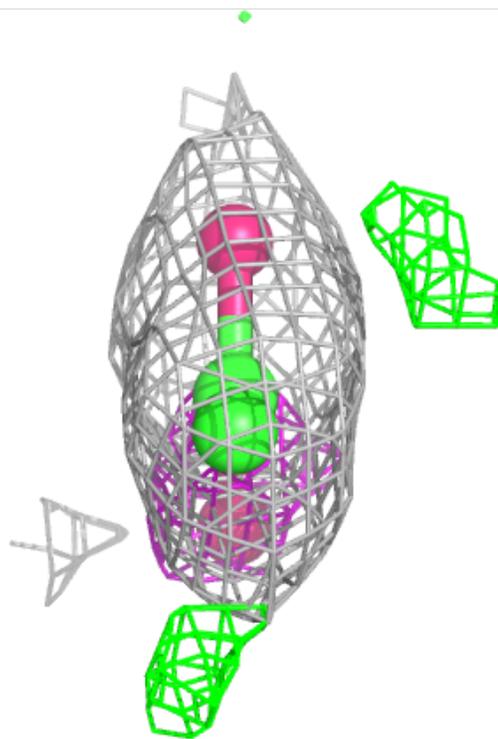
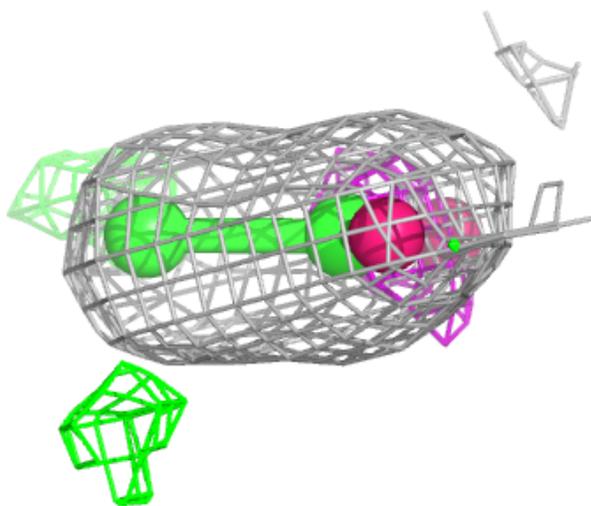
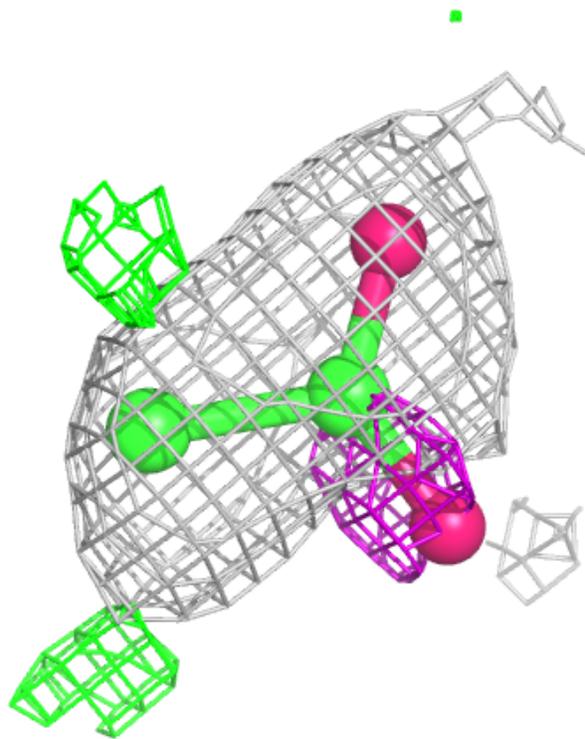






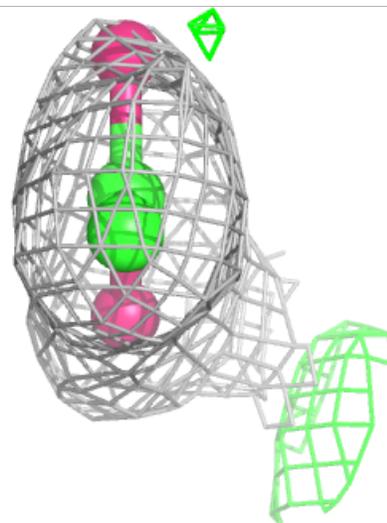
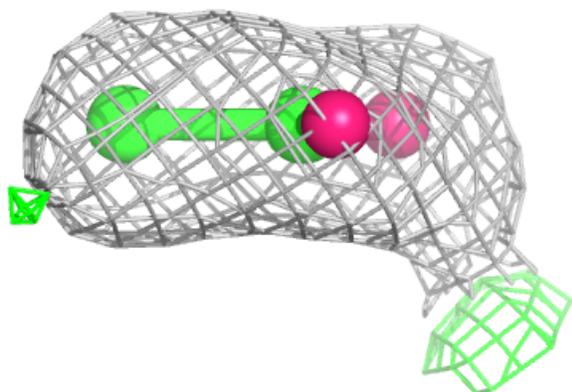
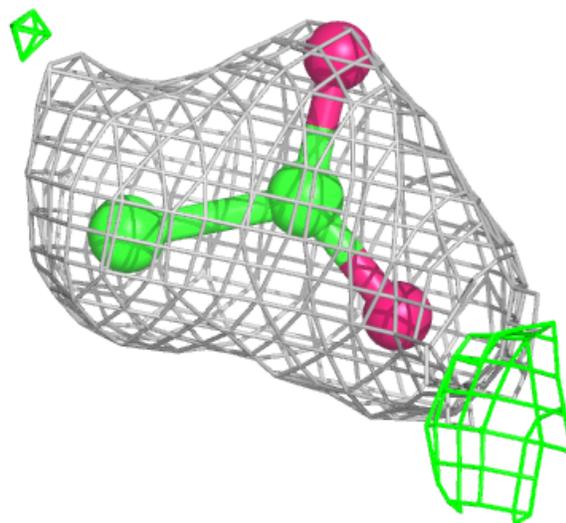
Electron density around ACT E 311:

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



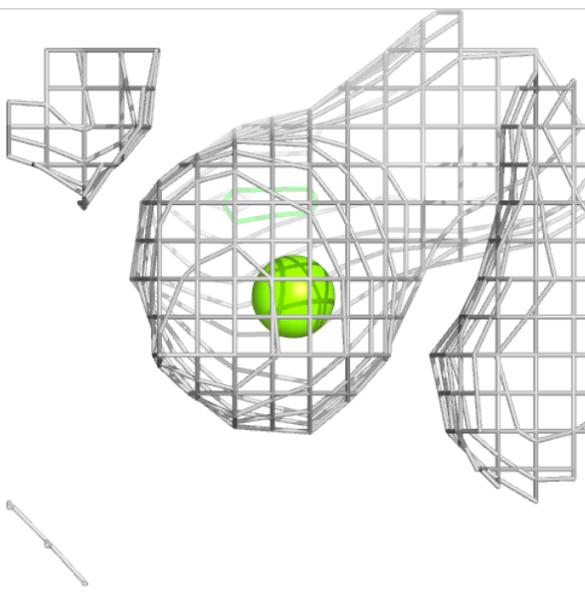
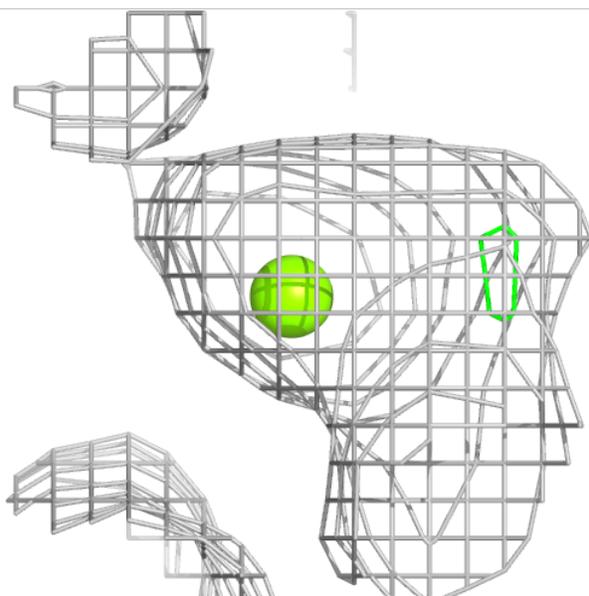
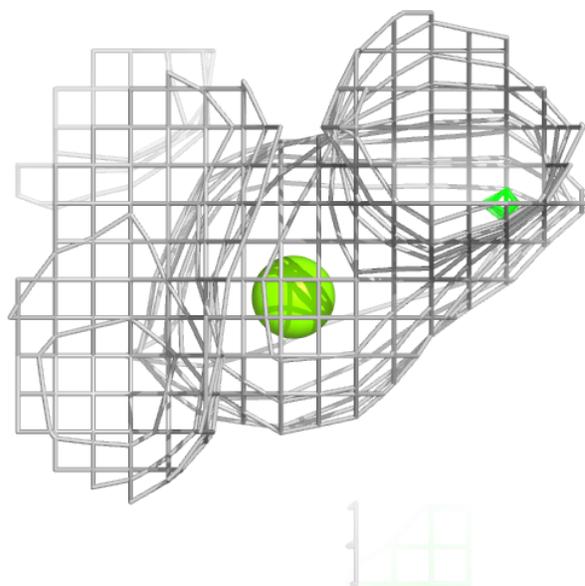
Electron density around ACT D 315:

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



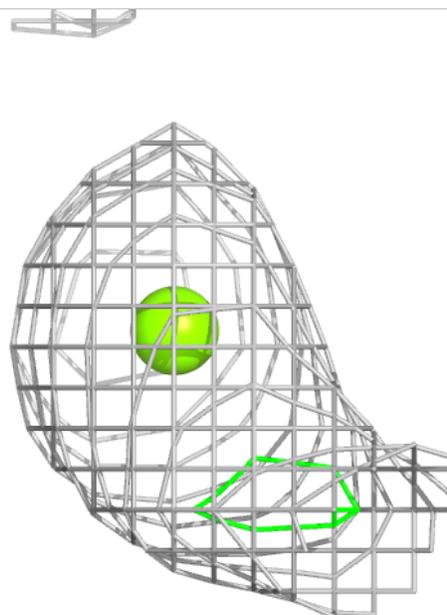
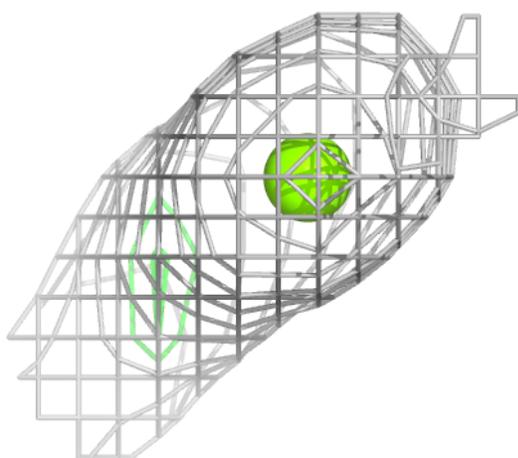
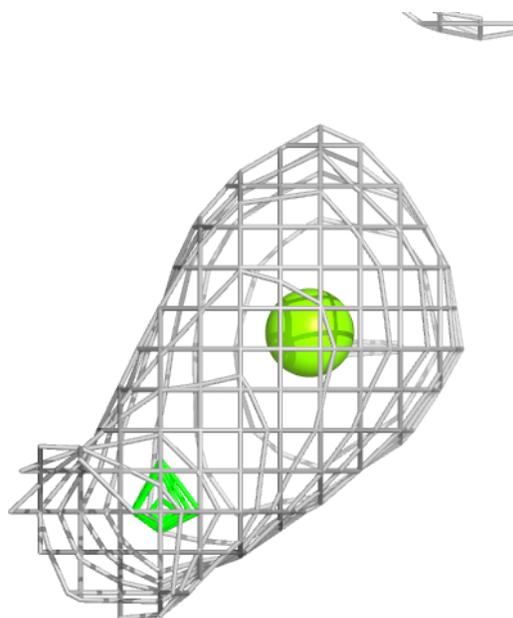
Electron density around MG A 312:

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and green (positive)



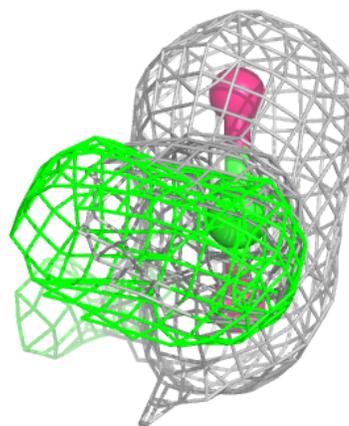
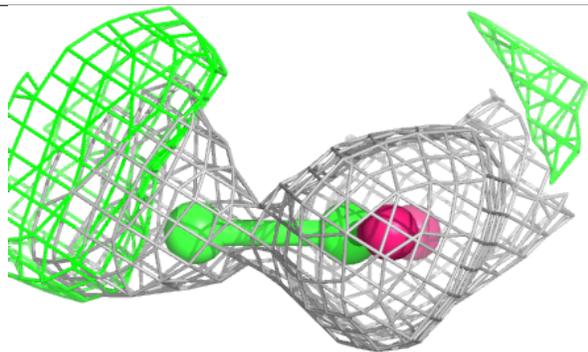
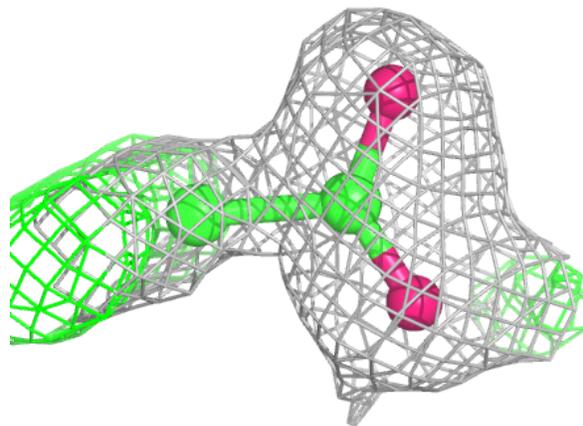
Electron density around MG E 308:

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



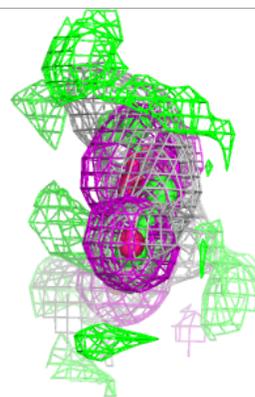
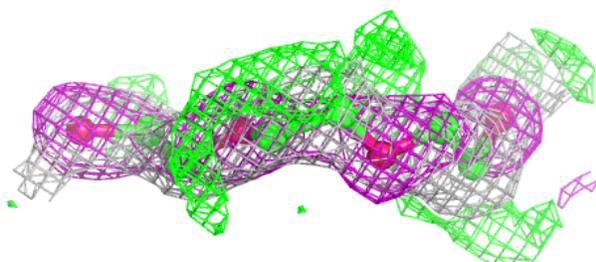
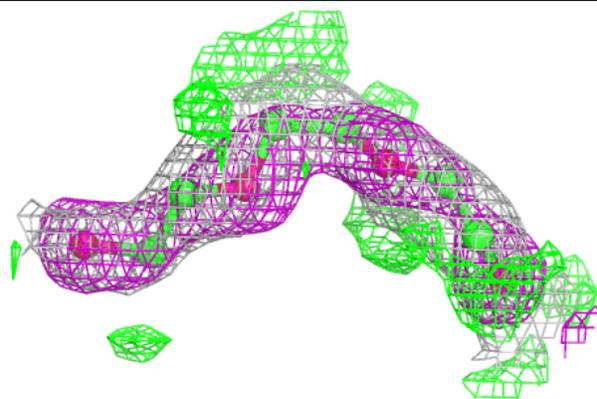
Electron density around ACT F 308:

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

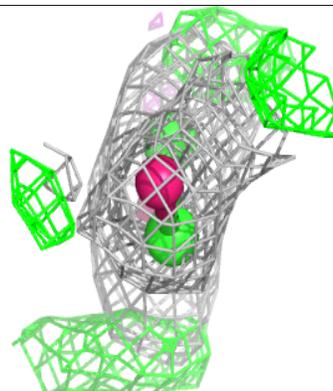
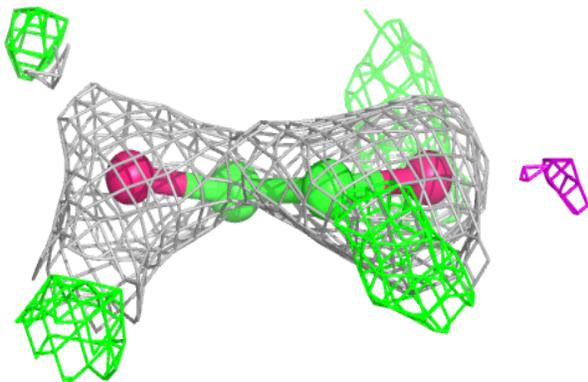
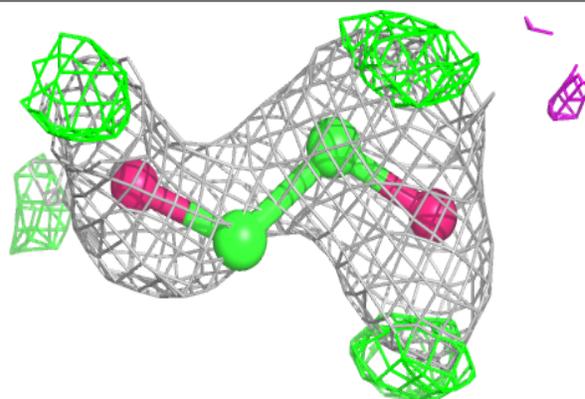


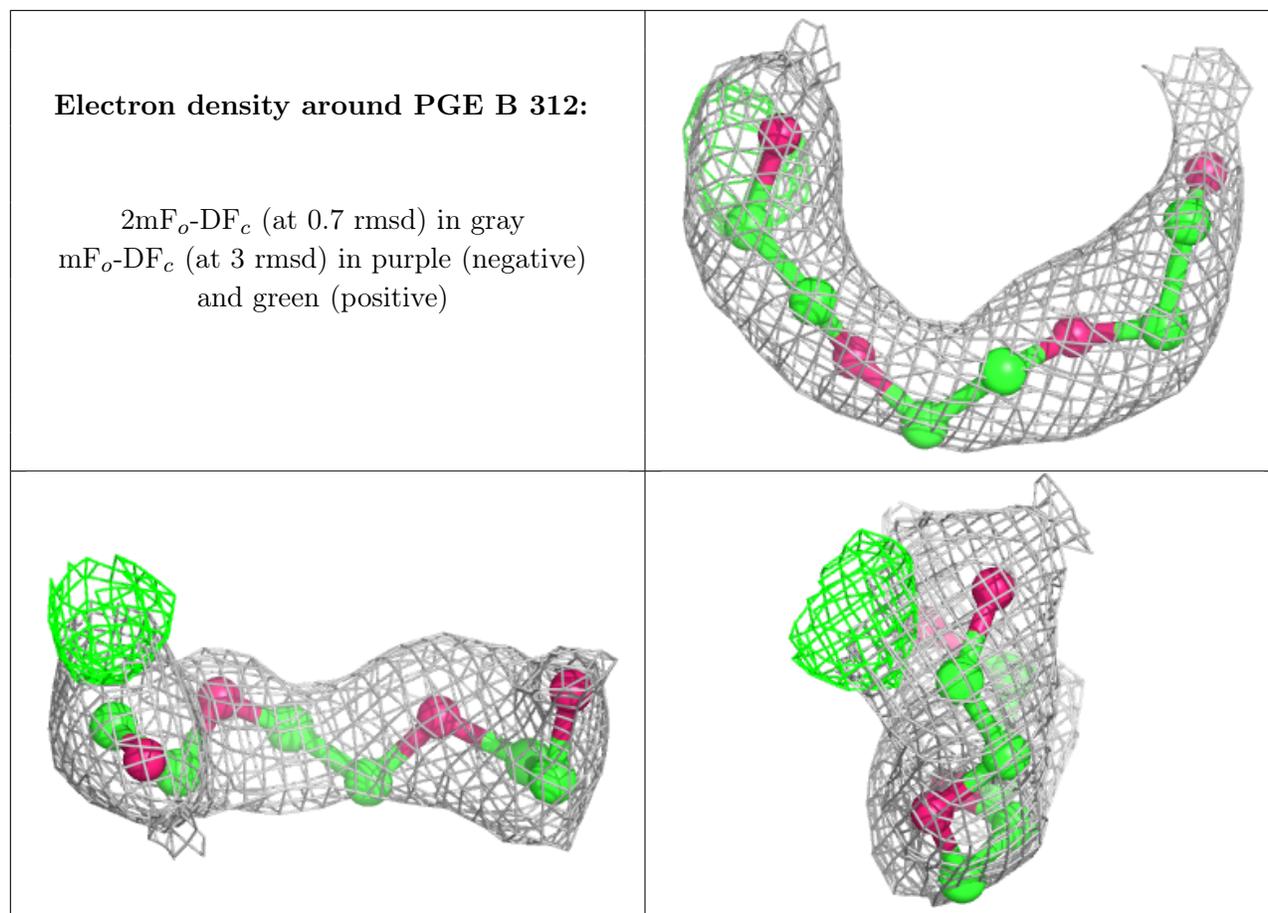
Electron density around PGE E 314:

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and green (positive)

**Electron density around EDO B 303:**

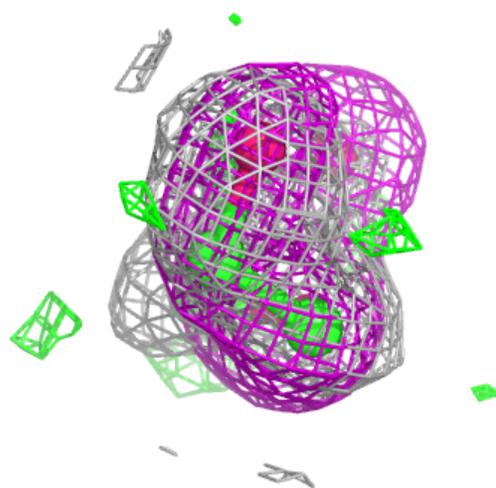
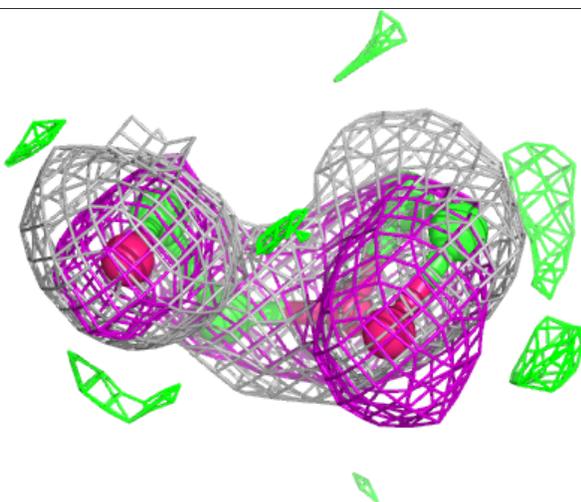
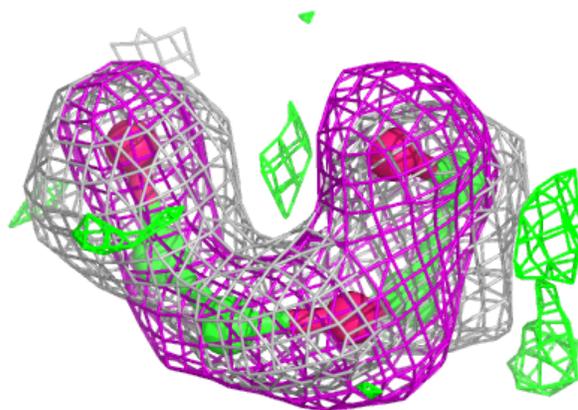
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





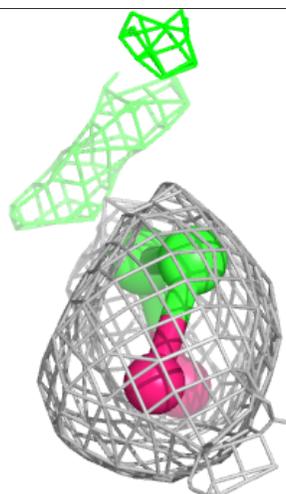
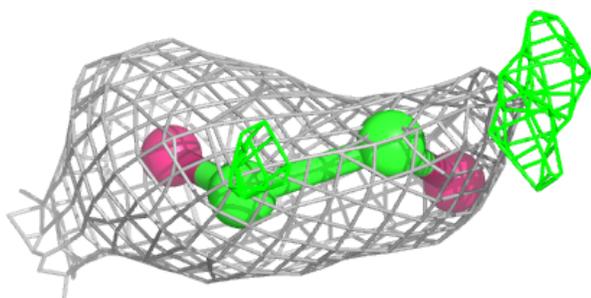
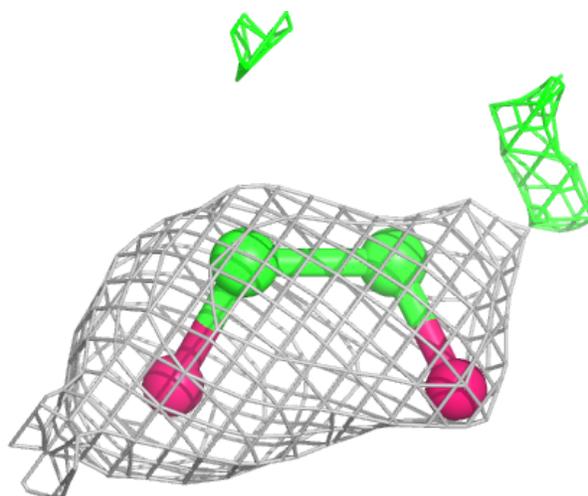
Electron density around PEG E 316:

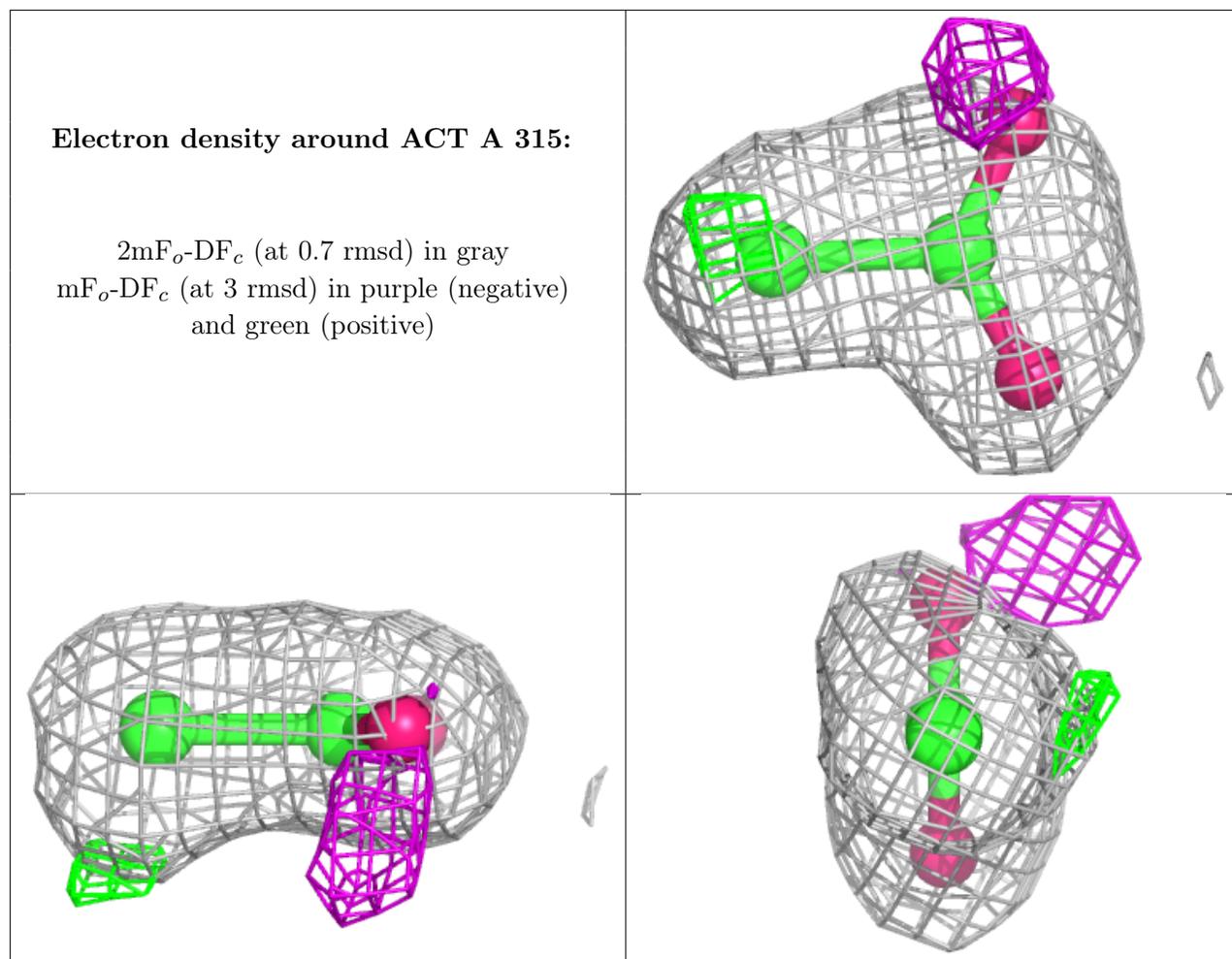
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EDO D 308:

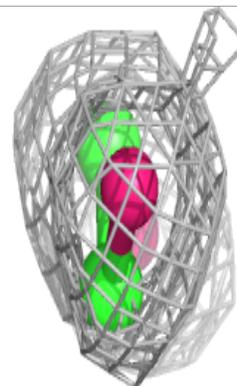
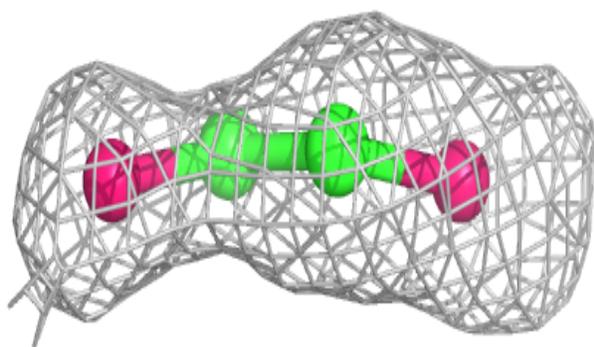
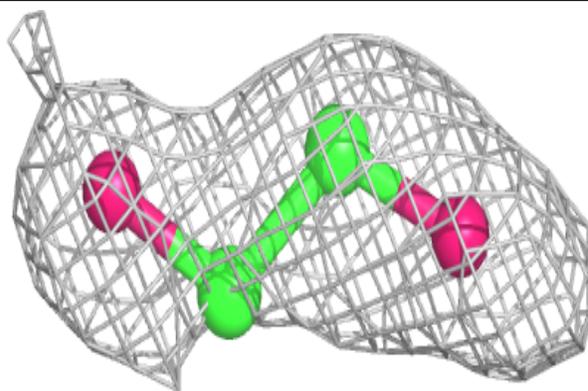
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



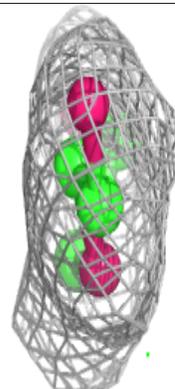
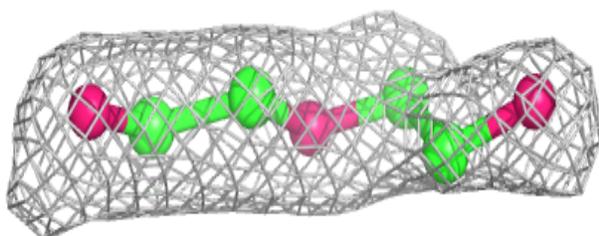
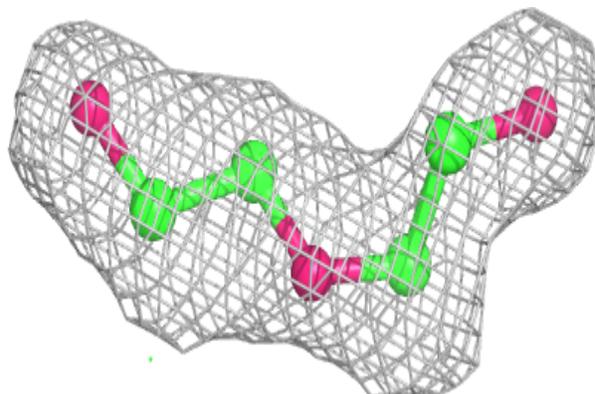


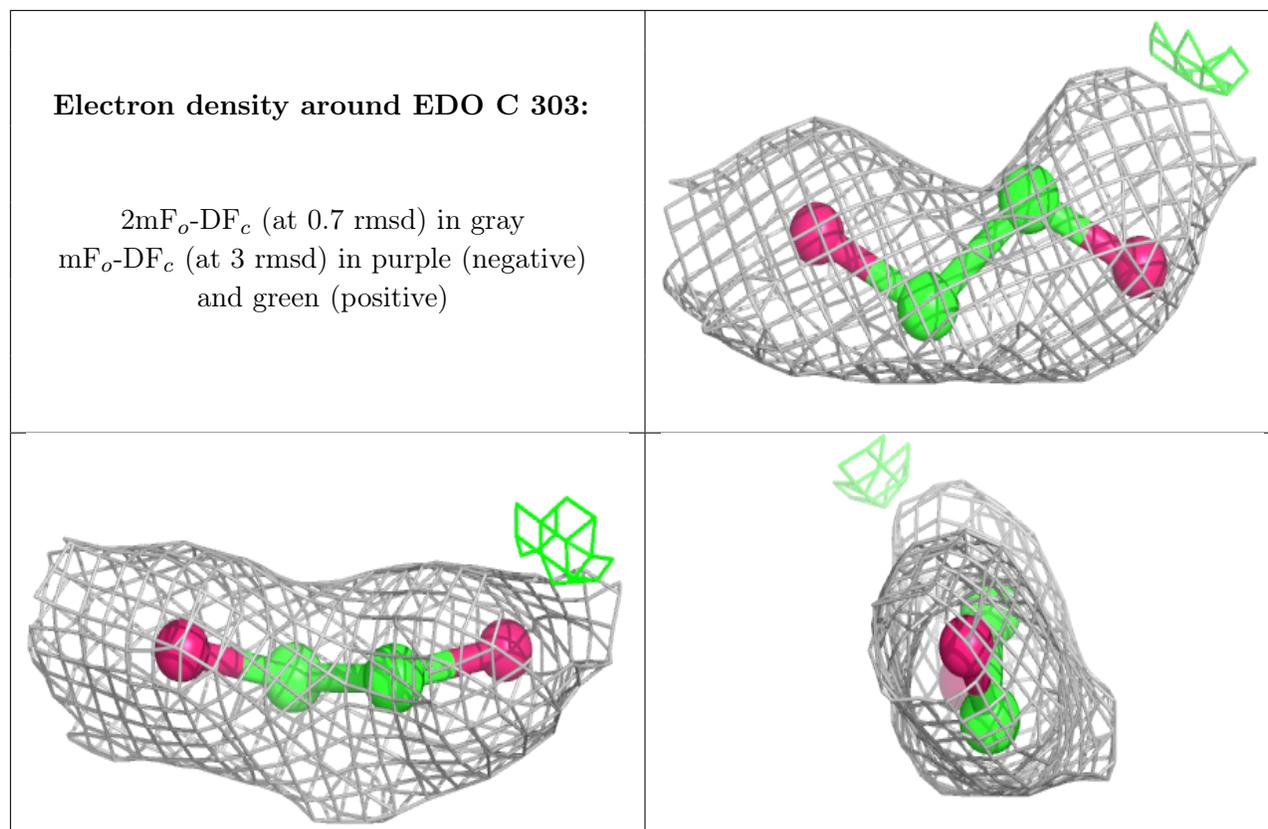
Electron density around EDO F 302:

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

**Electron density around PEG D 319:**

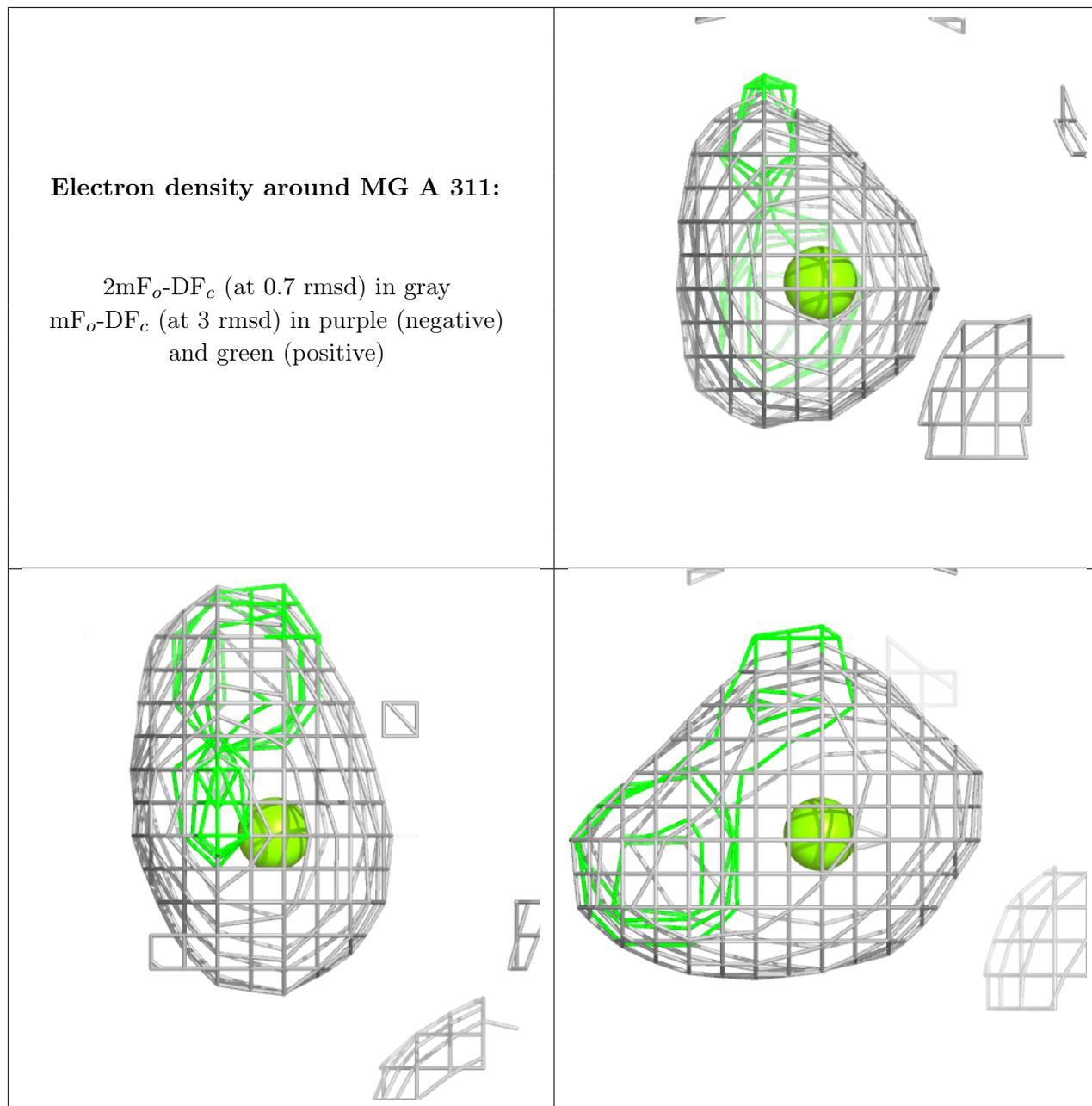
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

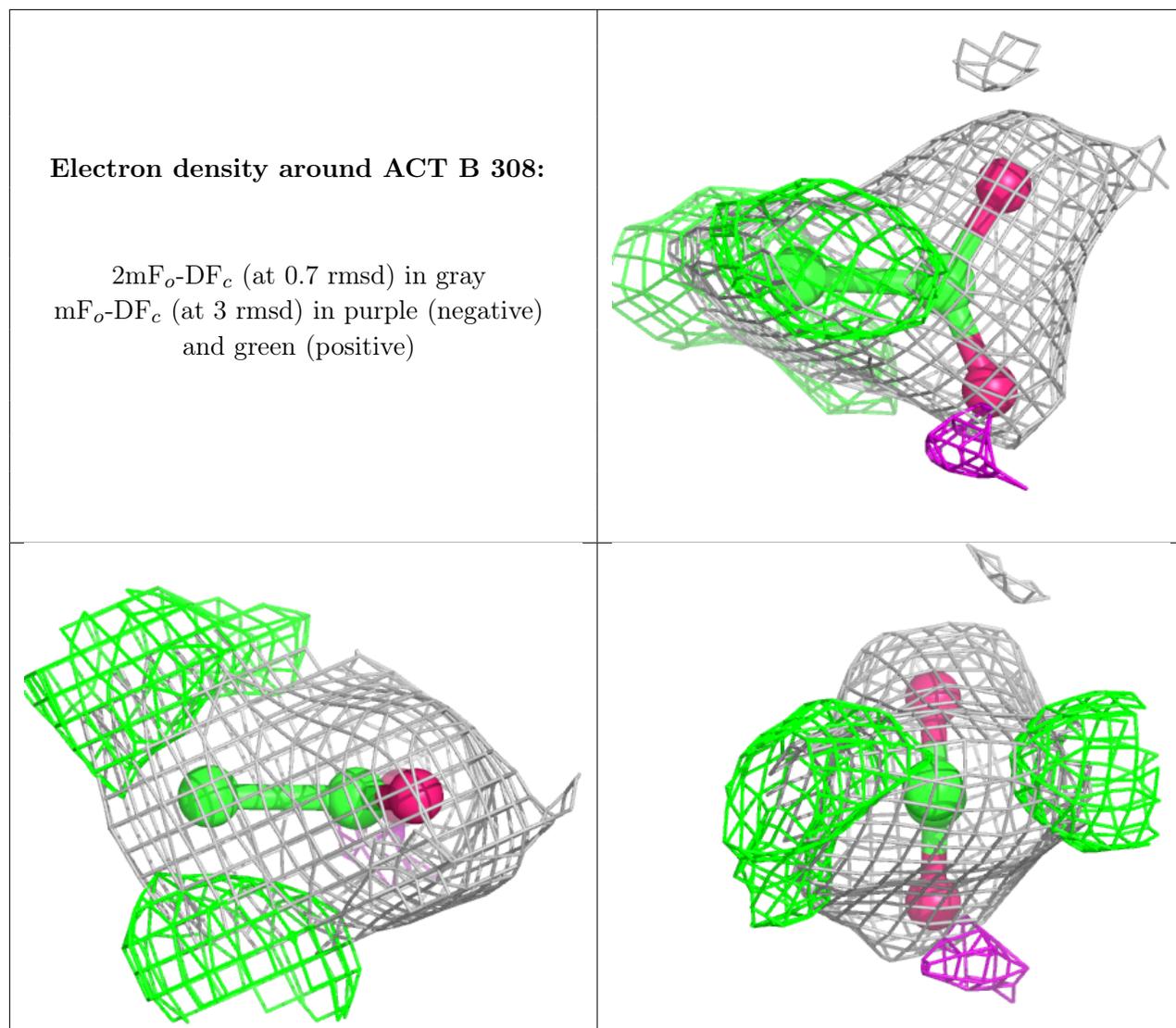




Electron density around MG A 311:

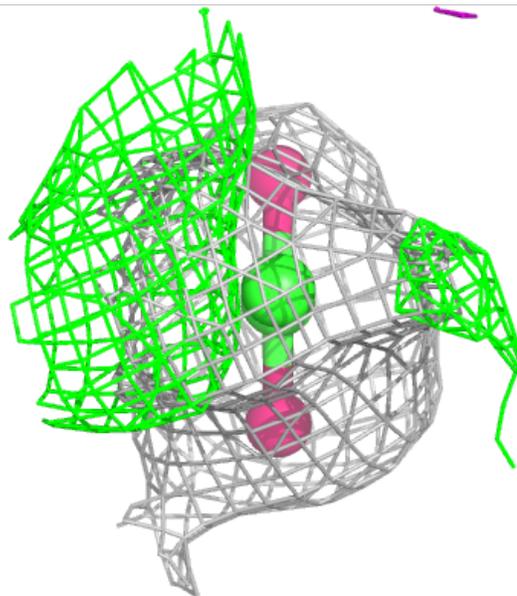
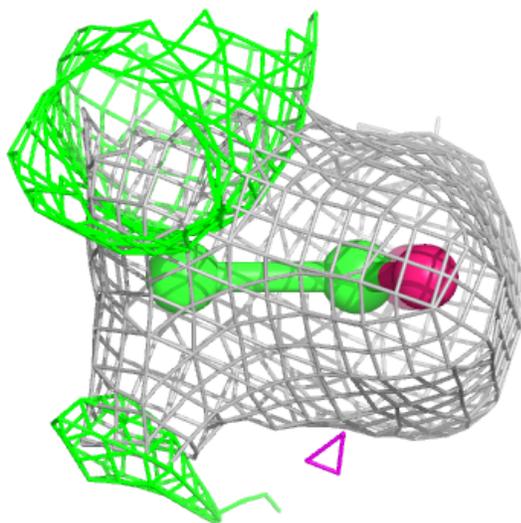
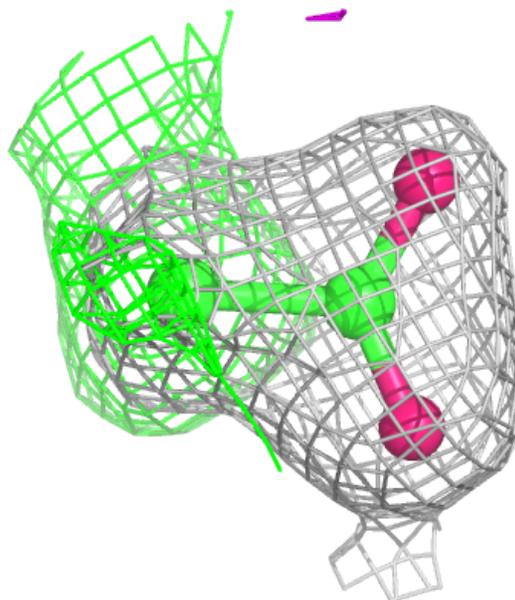
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





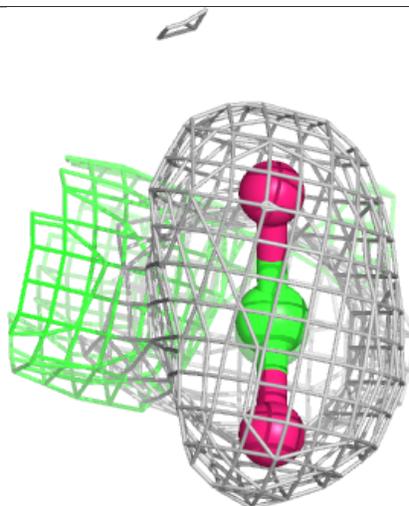
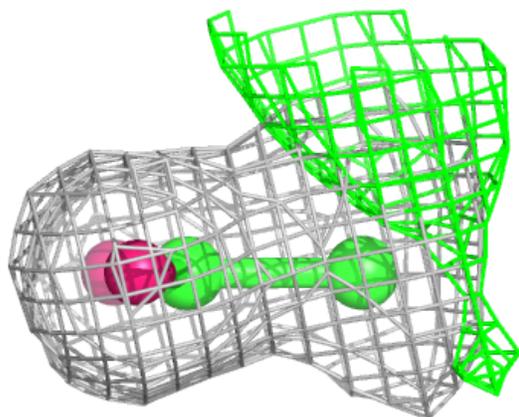
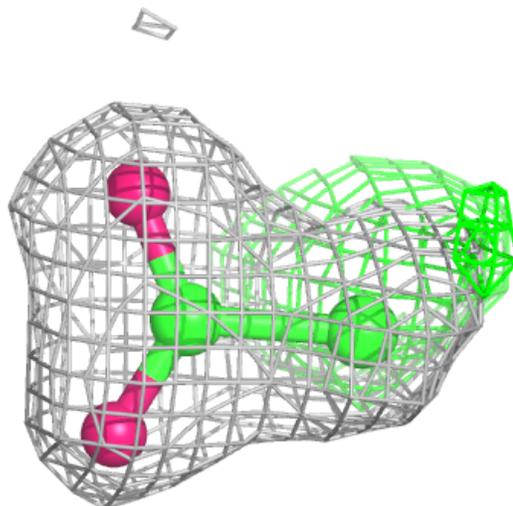
Electron density around ACT D 313:

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



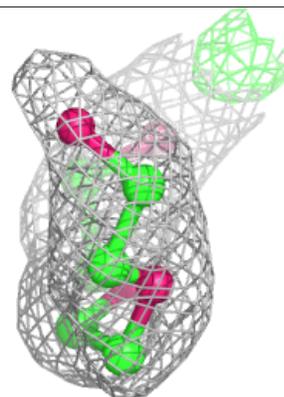
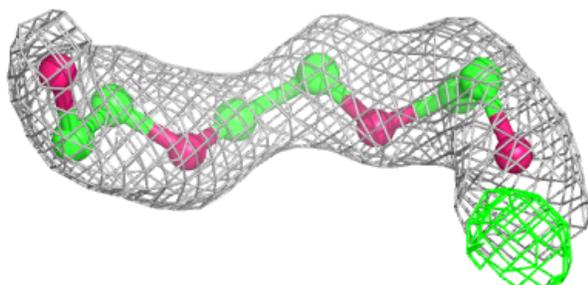
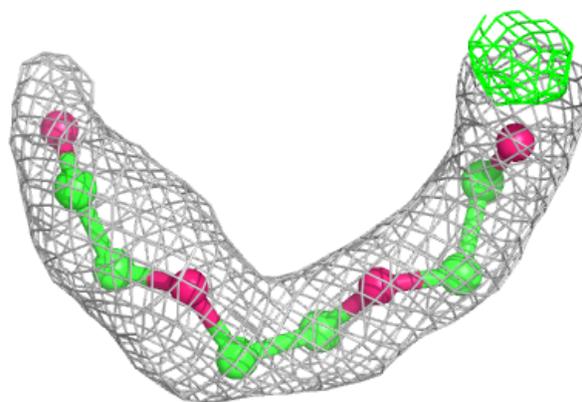
Electron density around ACT E 310:

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and green (positive)

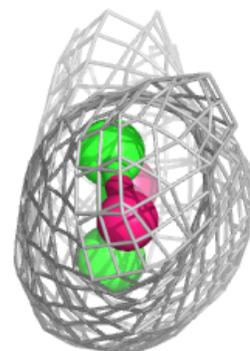
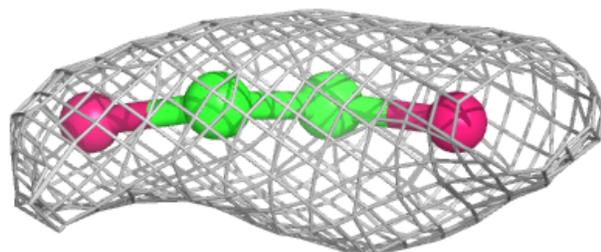
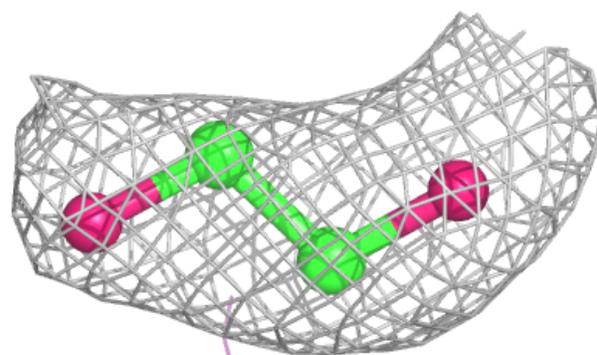


Electron density around PGE E 313:

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and green (positive)

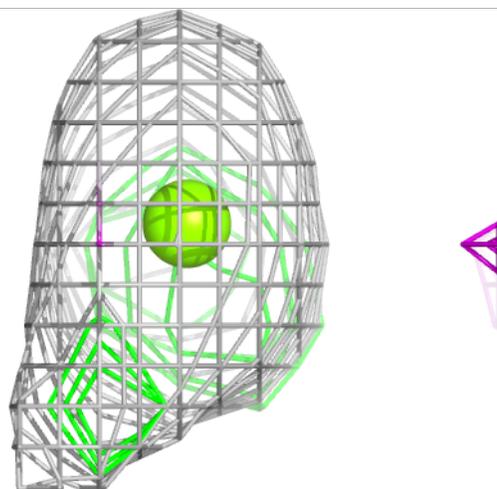
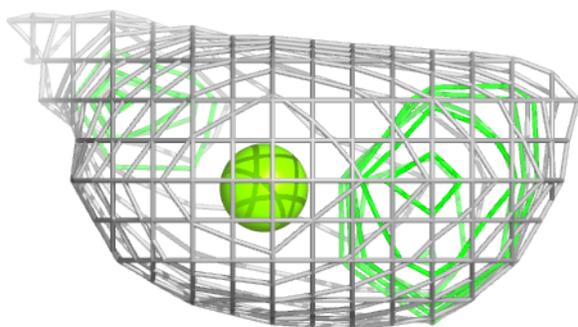
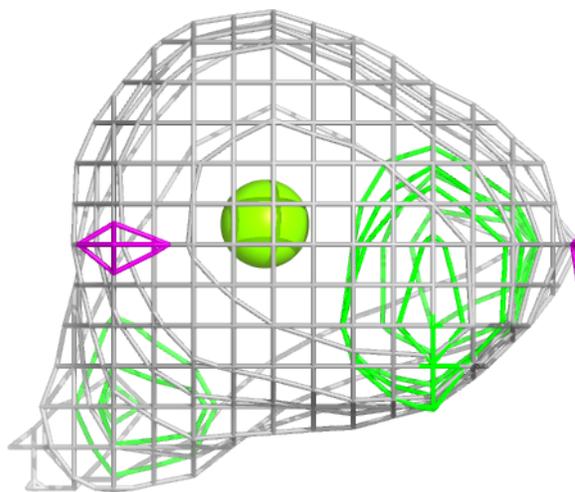
**Electron density around EDO A 305:**

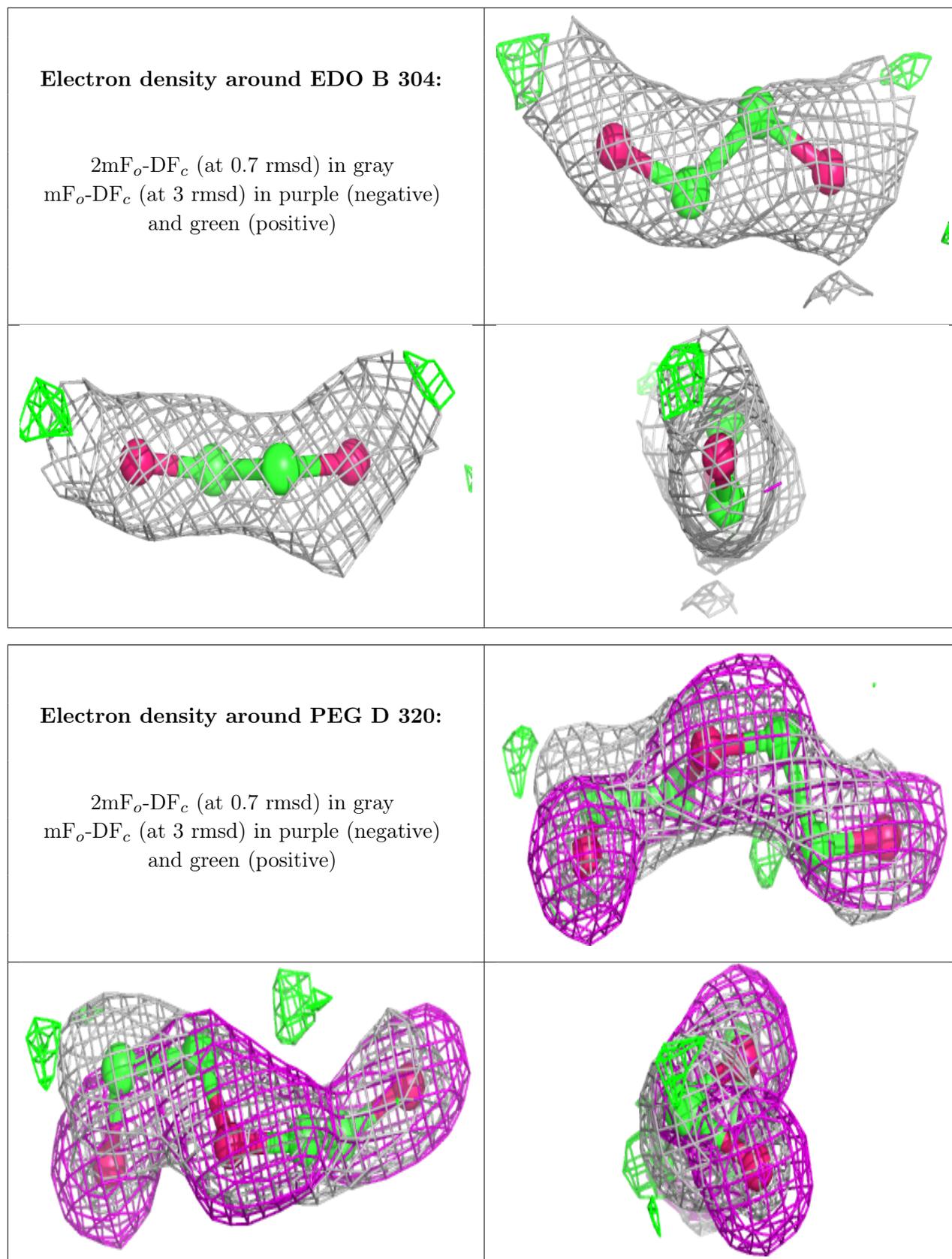
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

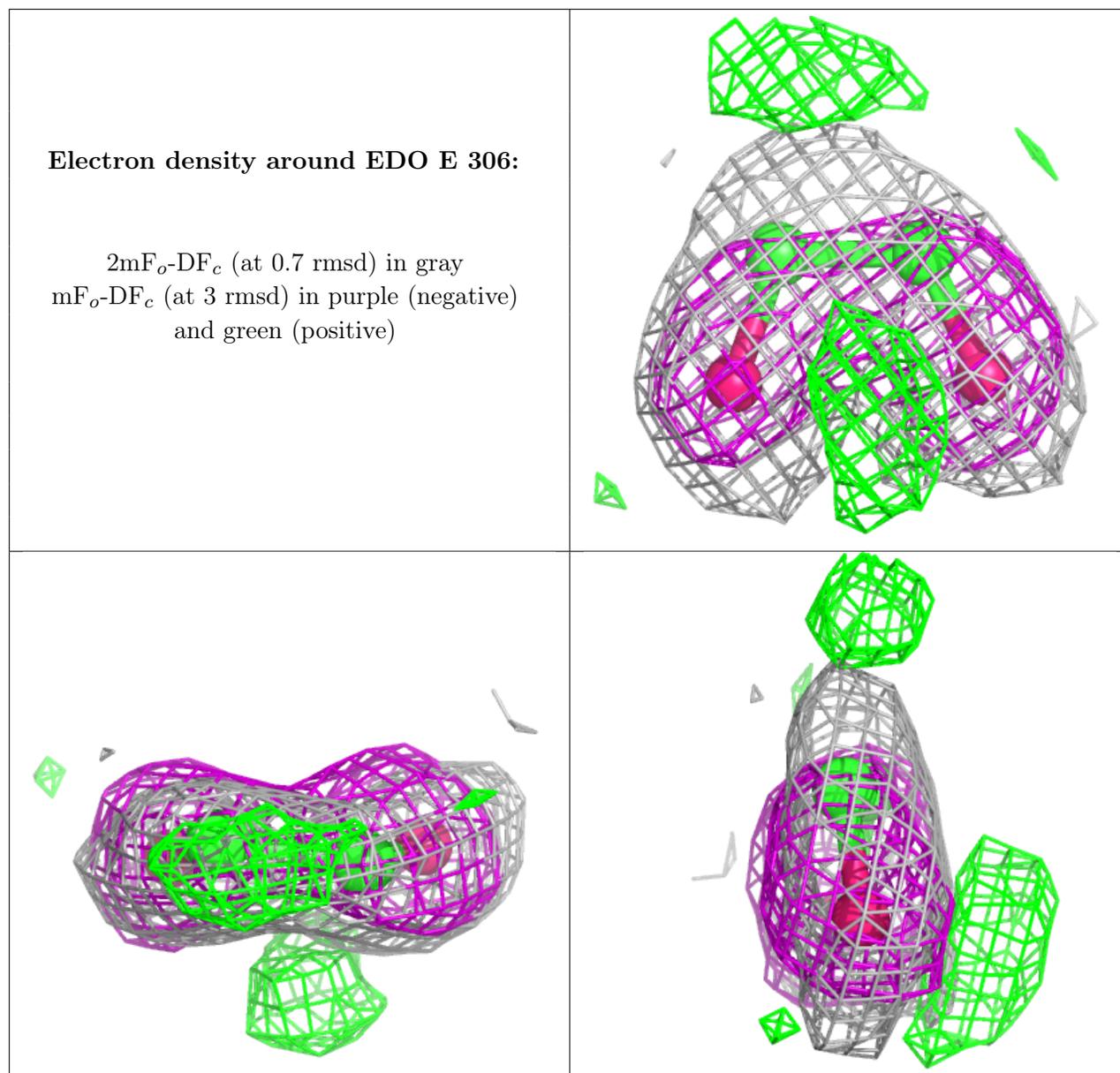


Electron density around MG F 305:

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

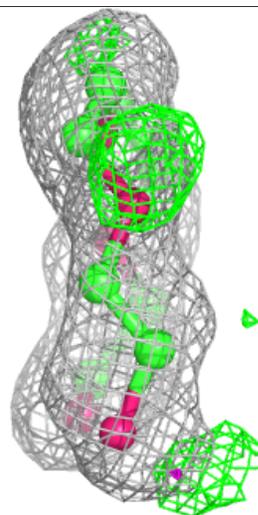
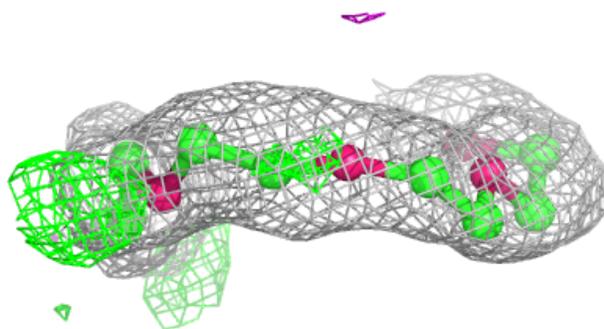
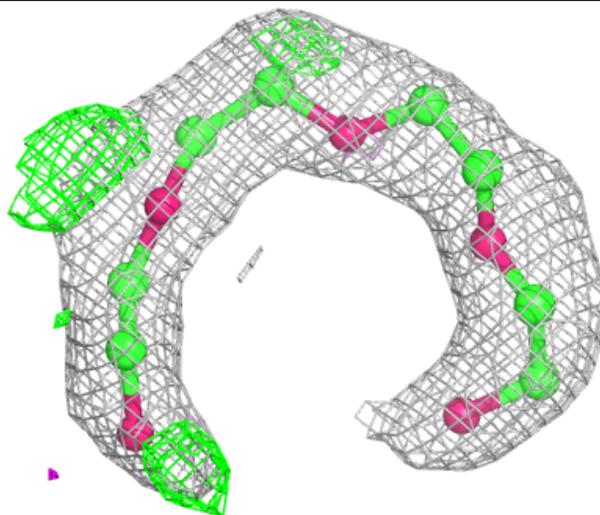






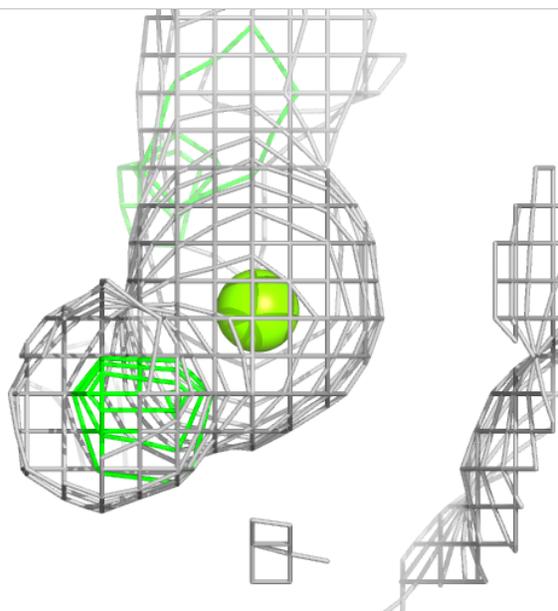
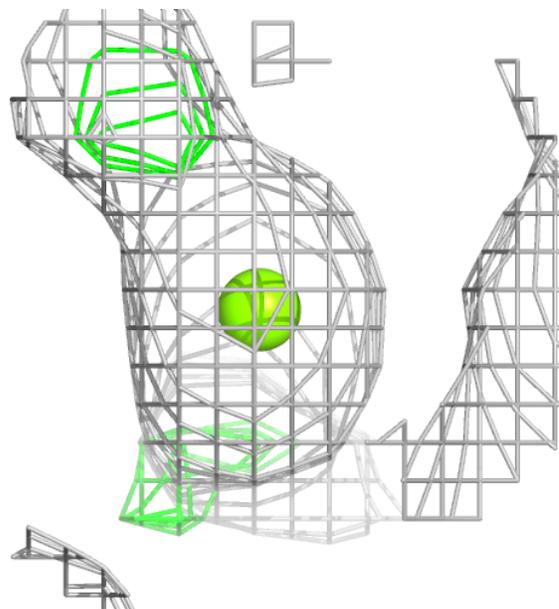
Electron density around PG4 D 317:

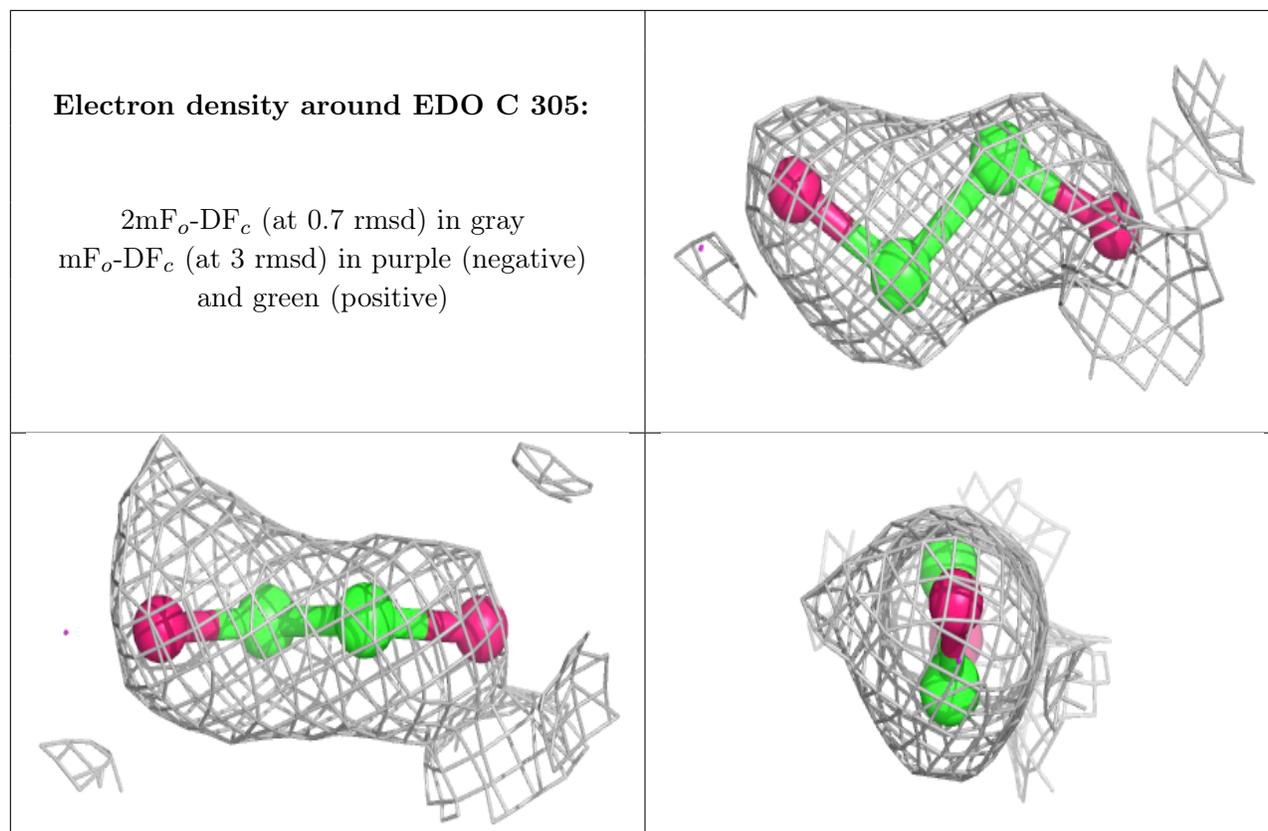
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 311:

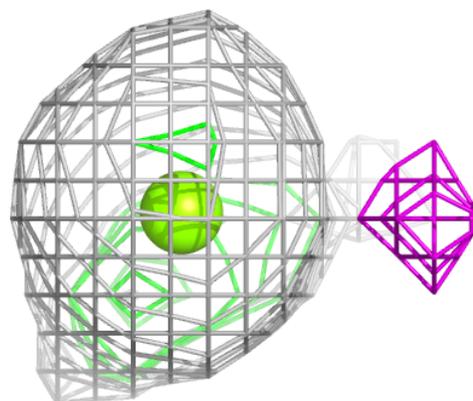
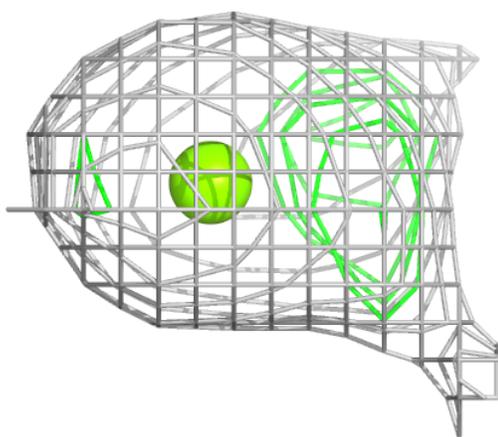
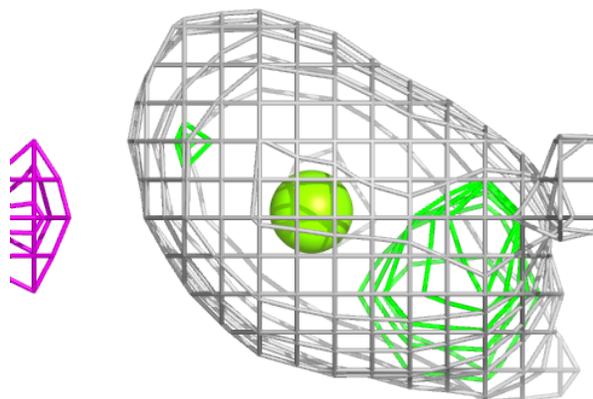
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

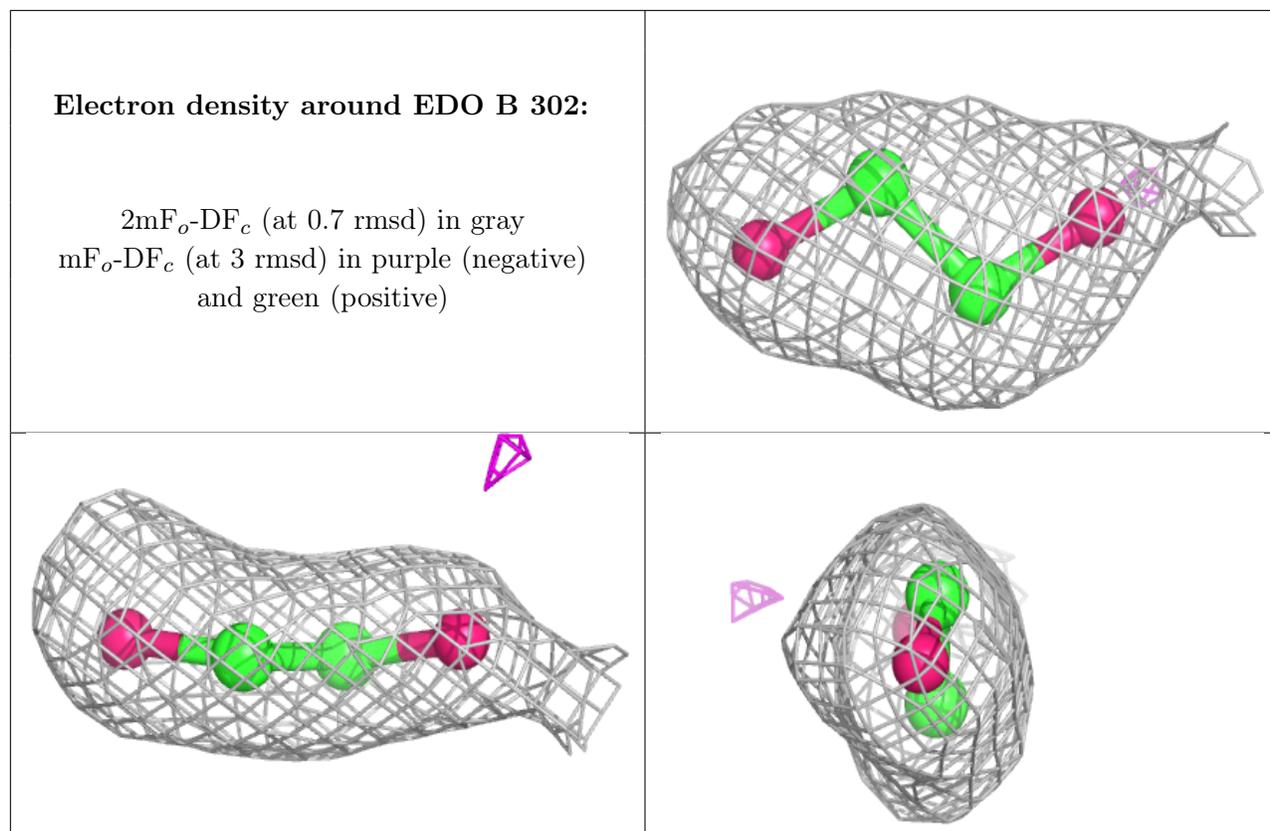




Electron density around MG E 309:

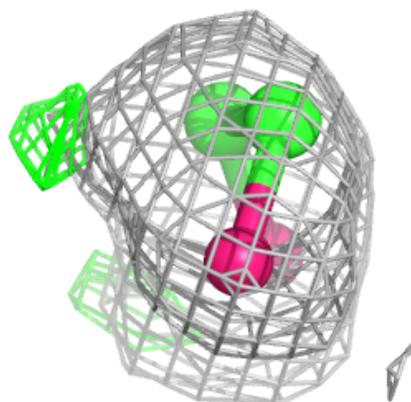
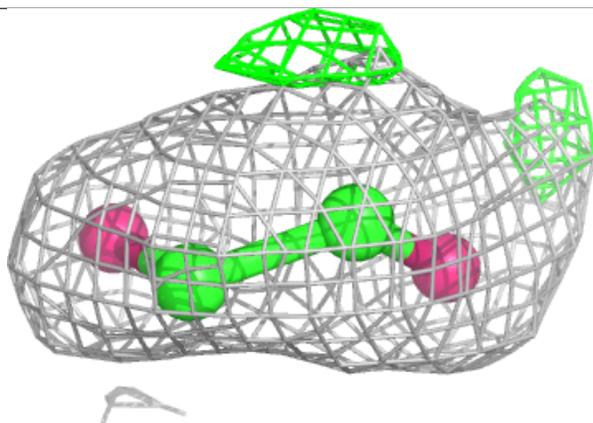
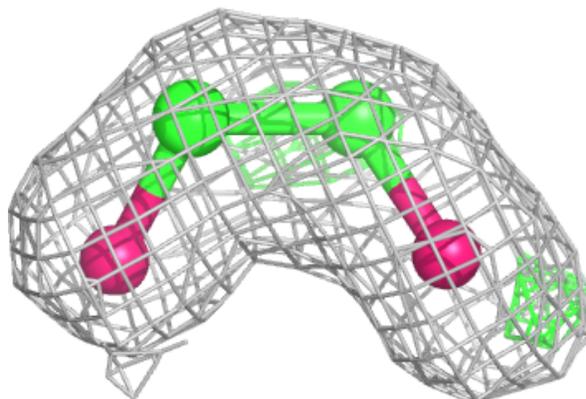
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





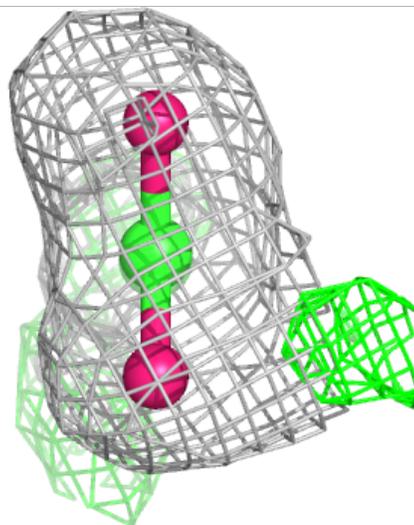
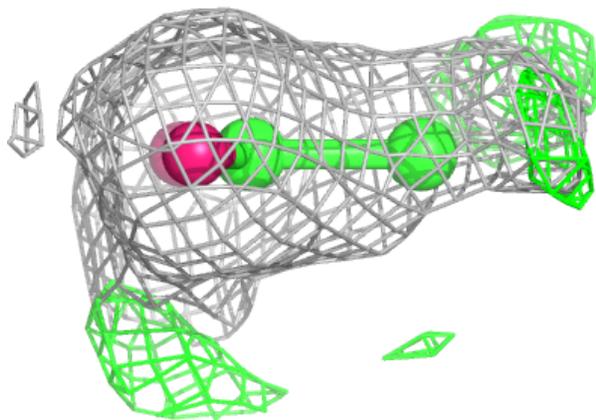
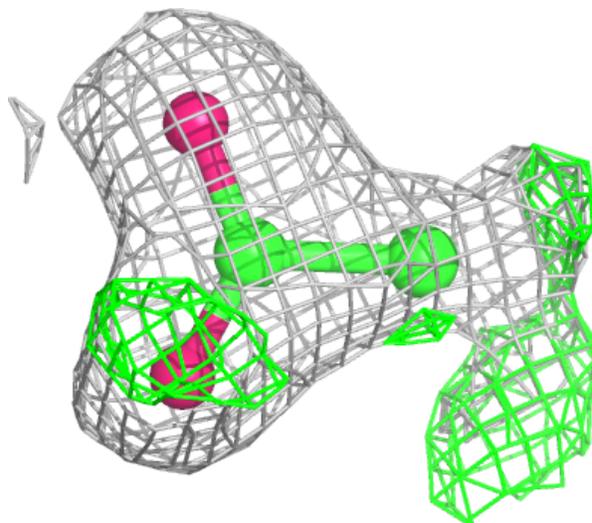
Electron density around EDO B 301:

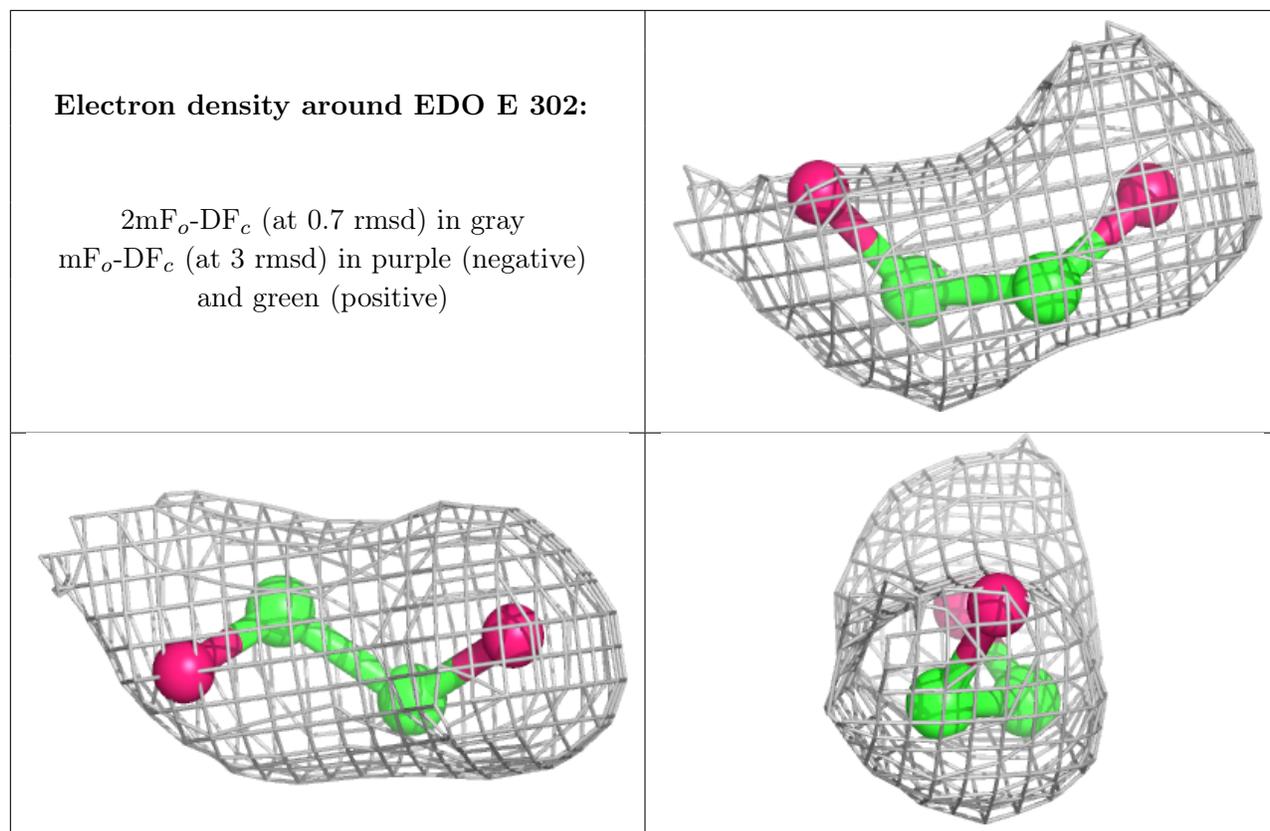
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ACT B 309:

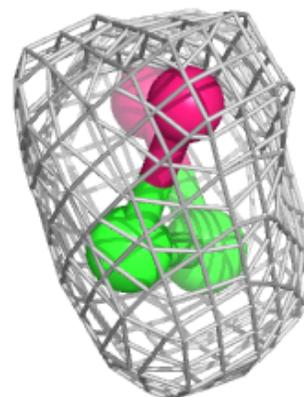
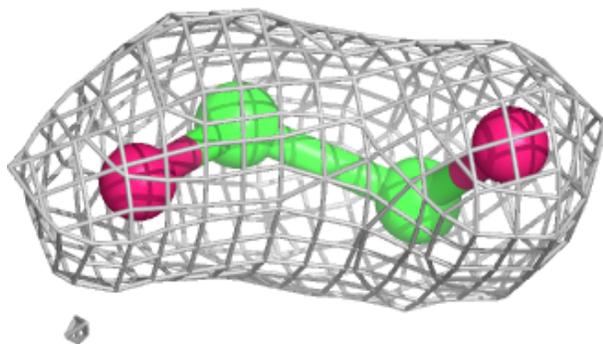
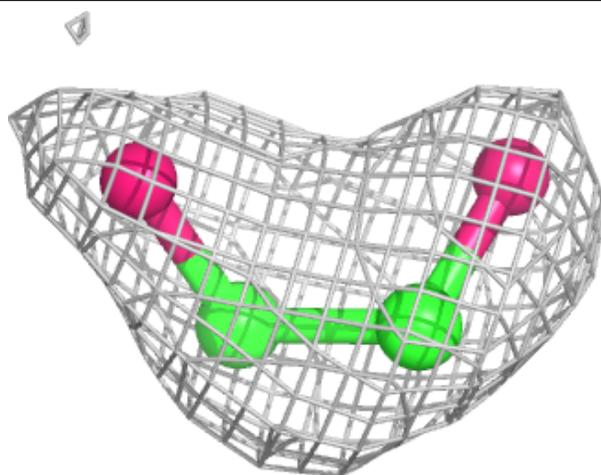
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

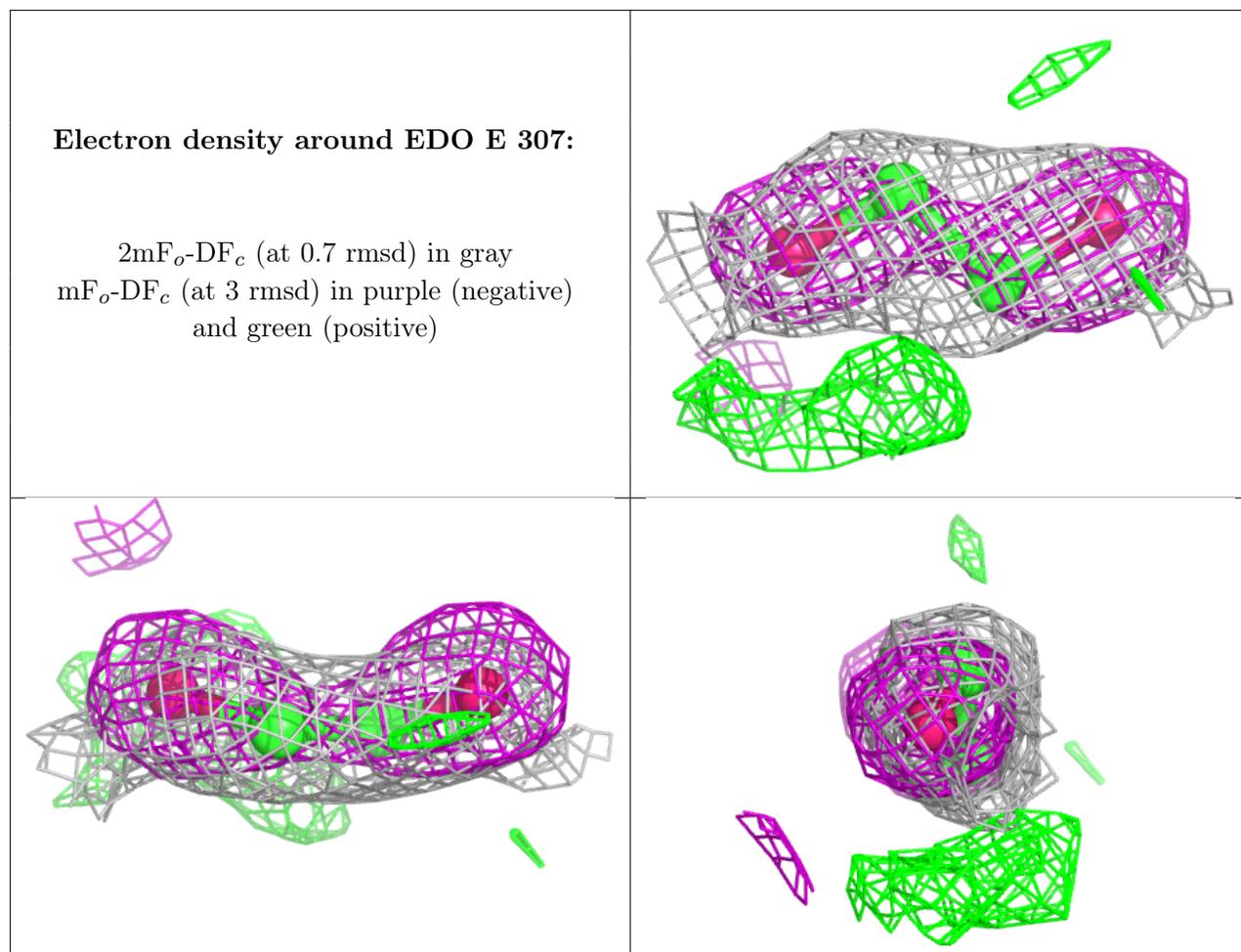




Electron density around EDO C 304:

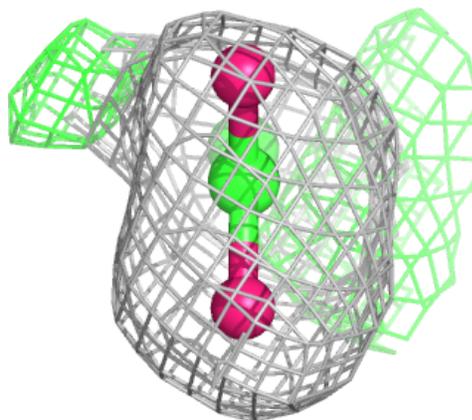
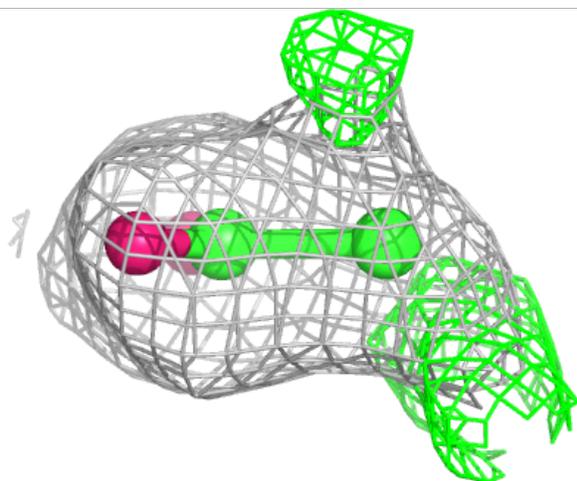
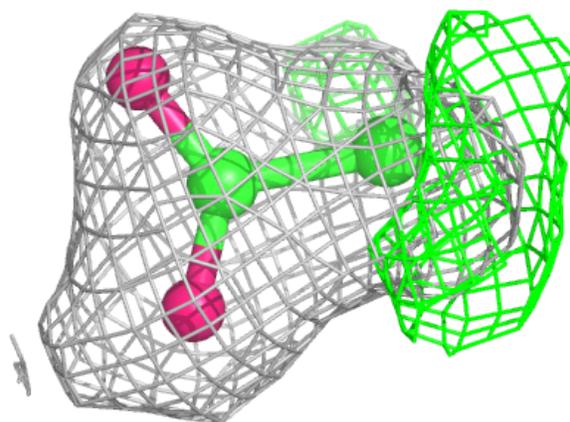
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

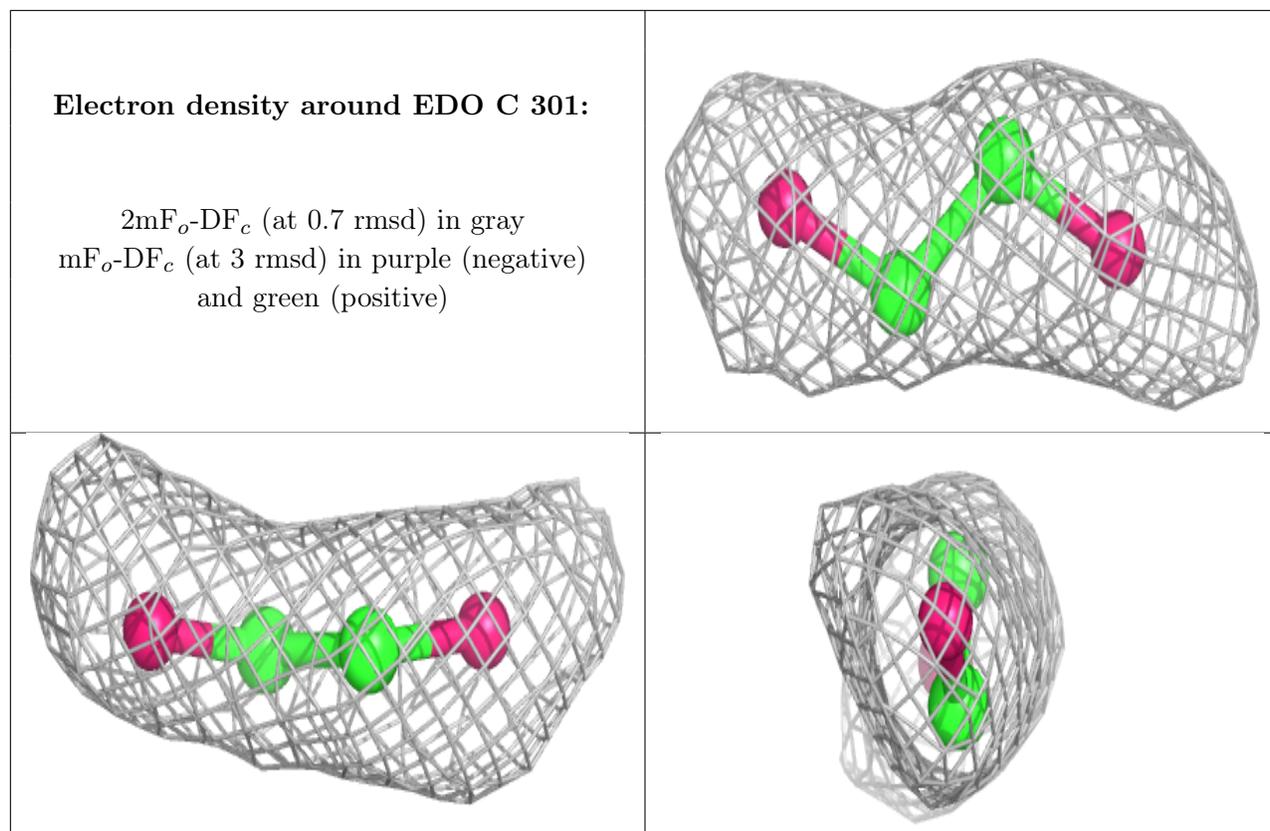




Electron density around ACT A 313:

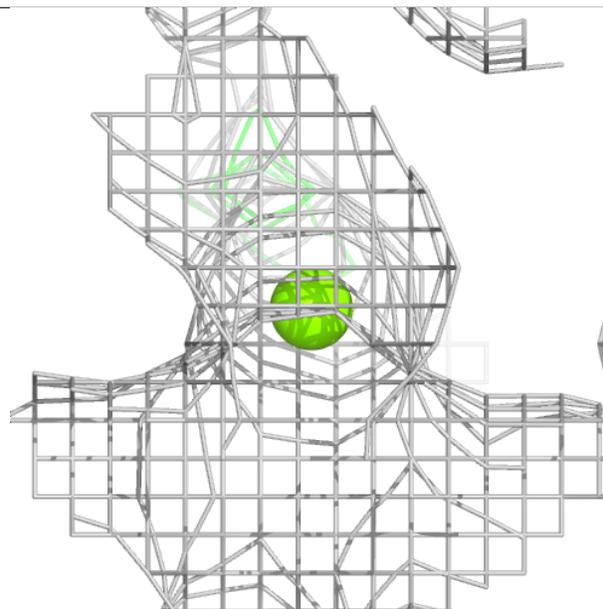
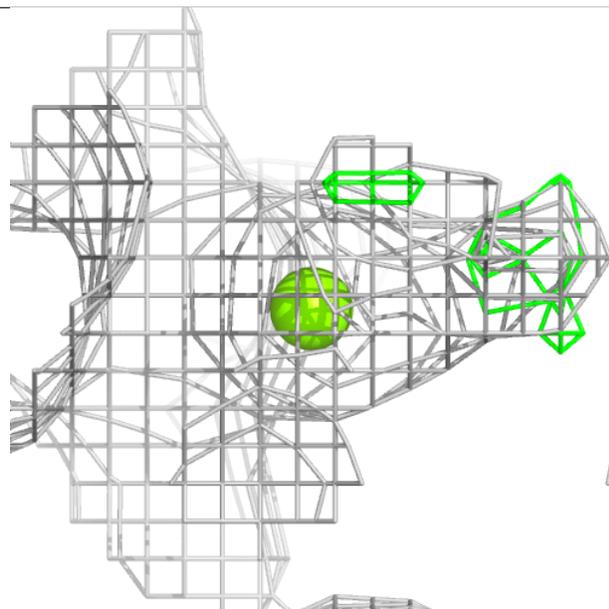
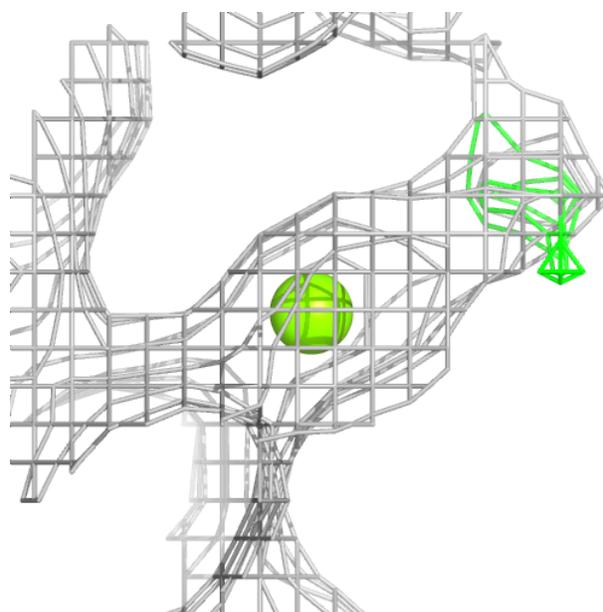
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





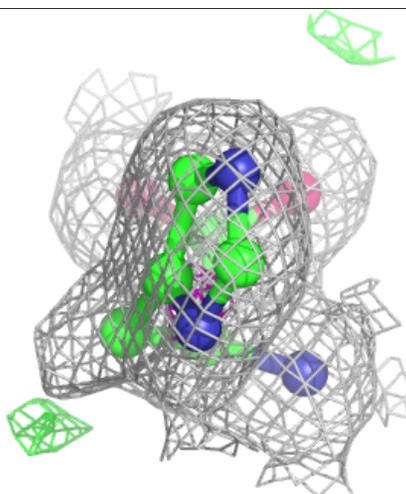
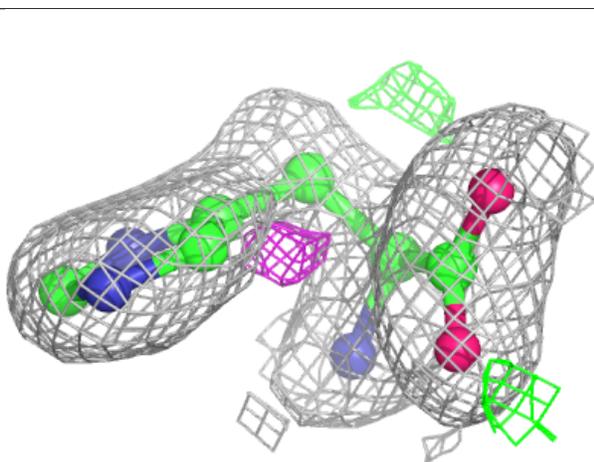
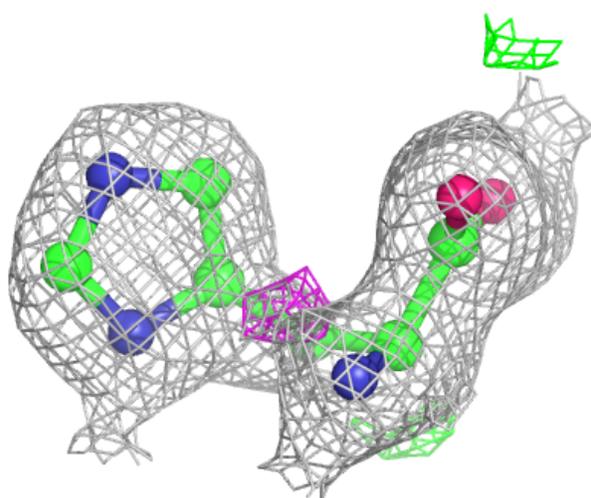
Electron density around MG A 308:

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



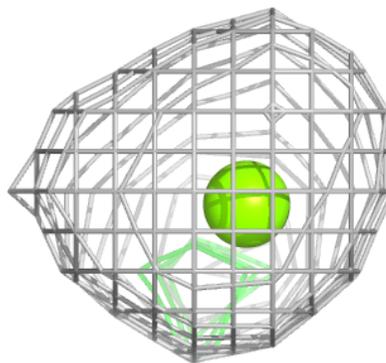
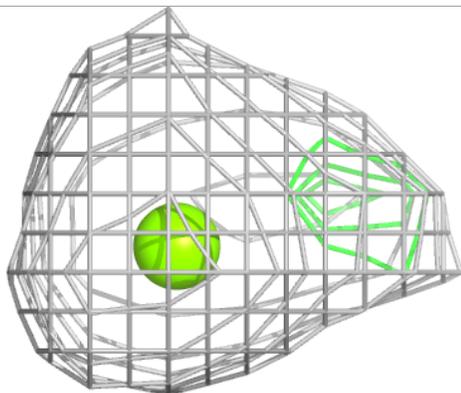
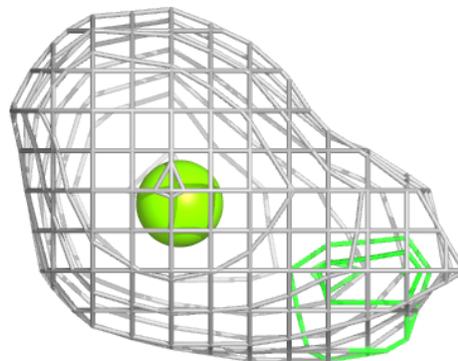
Electron density around HIS B 313:

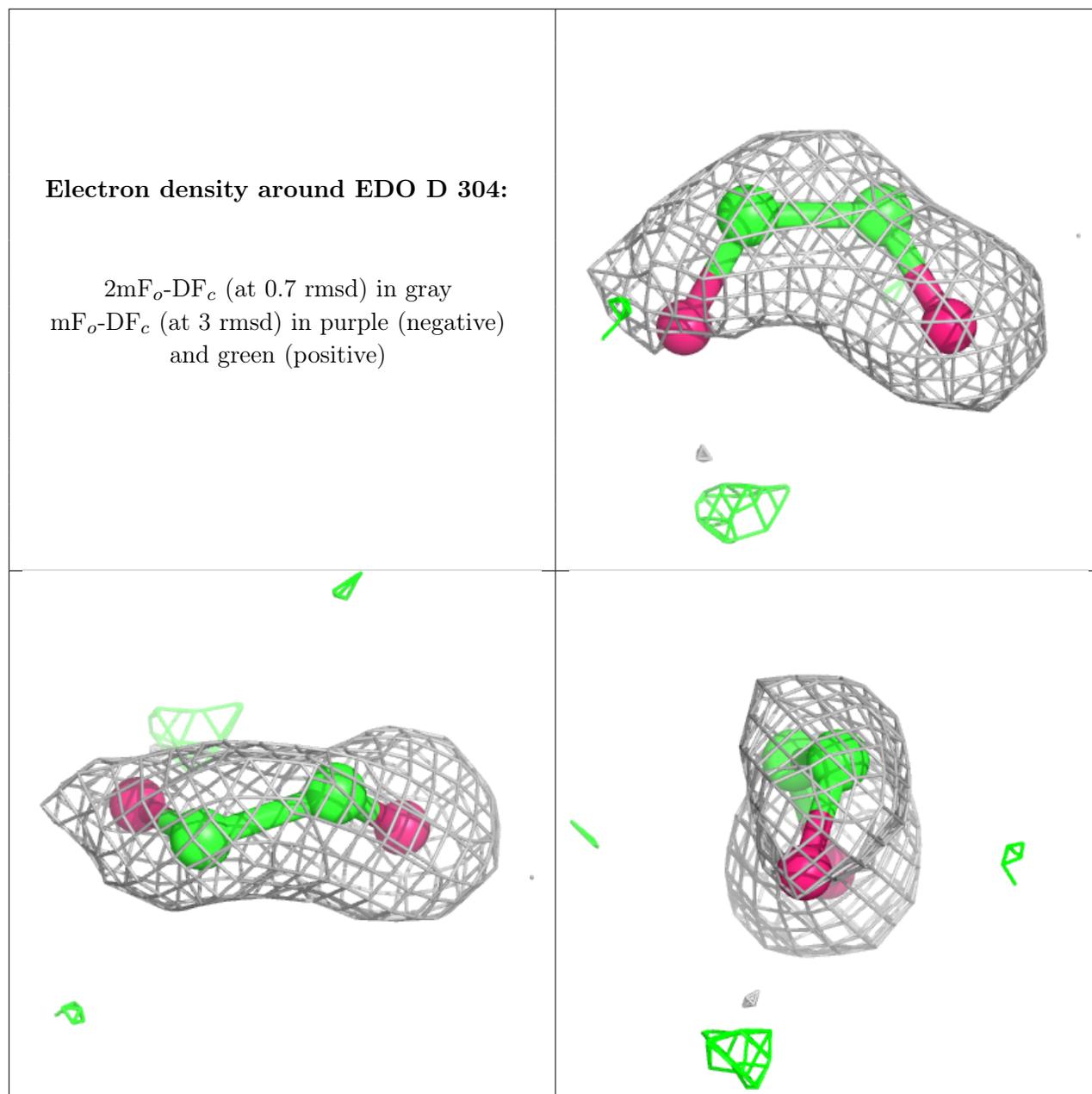
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 309:

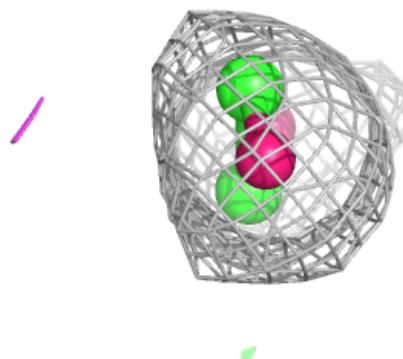
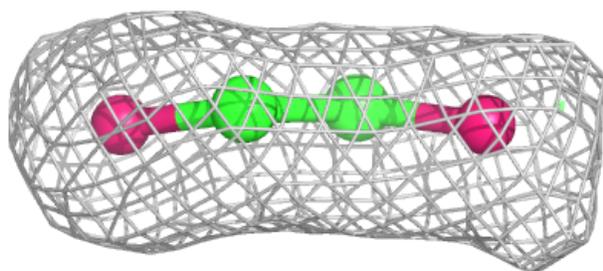
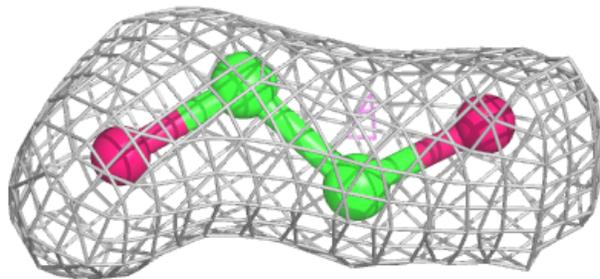
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





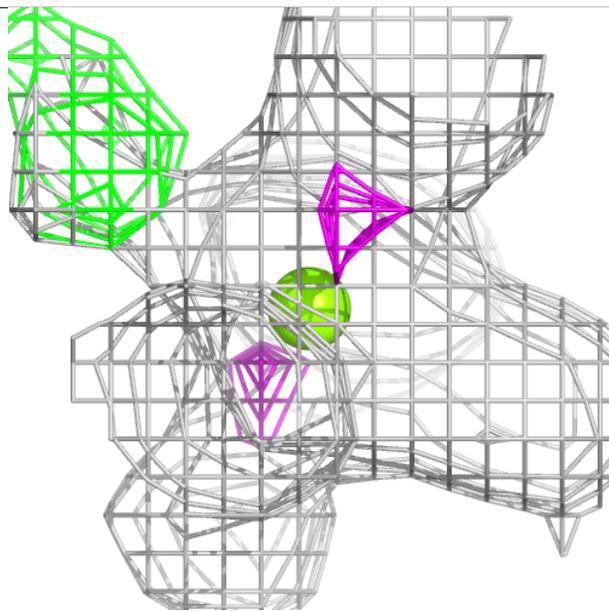
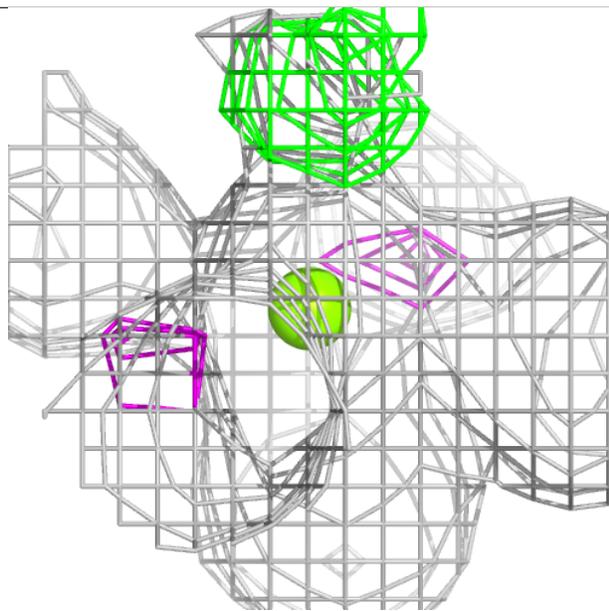
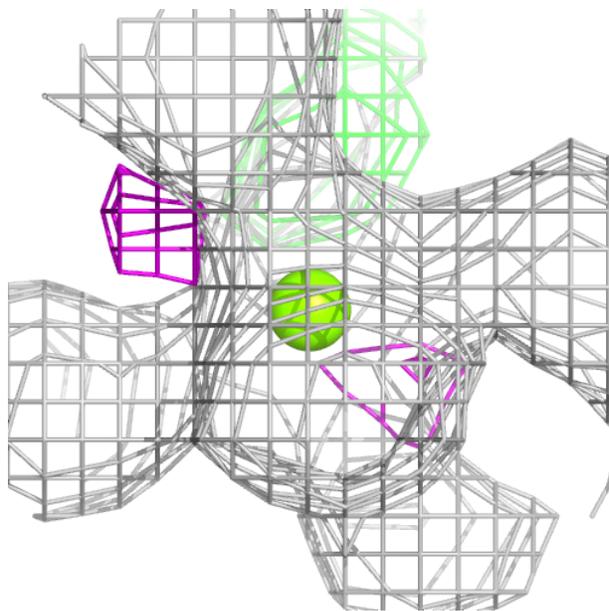
Electron density around EDO D 306:

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



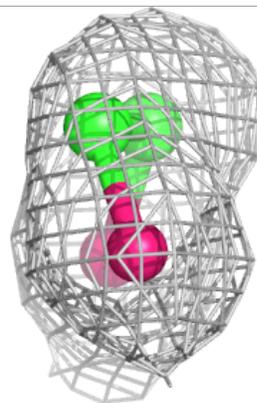
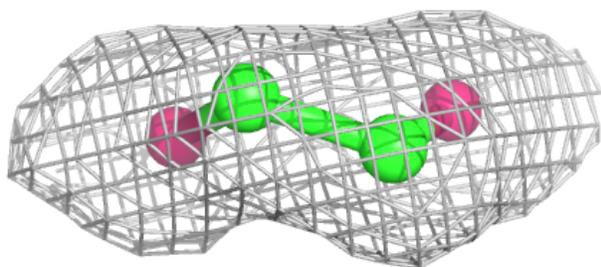
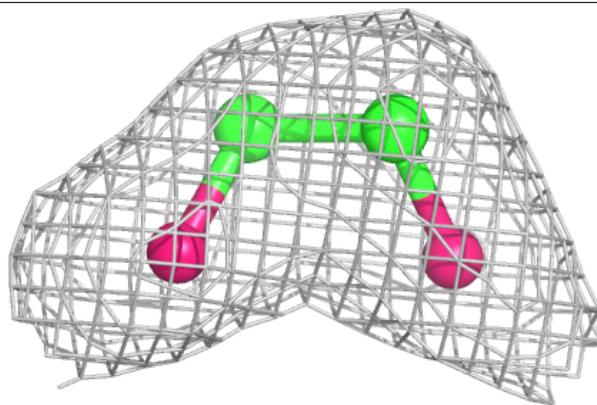
Electron density around MG D 310:

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



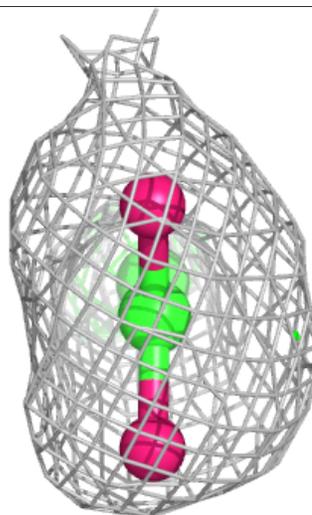
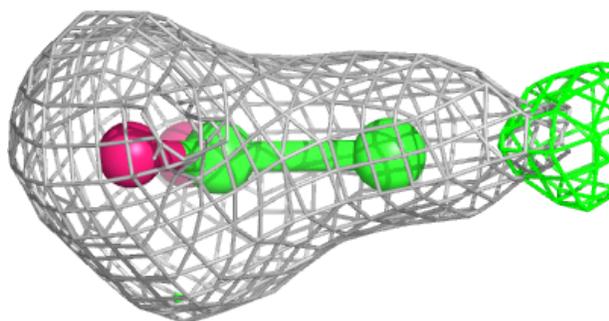
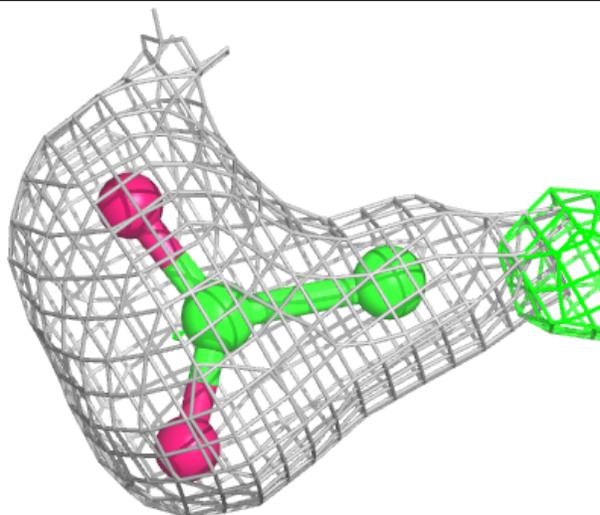
Electron density around EDO A 306:

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



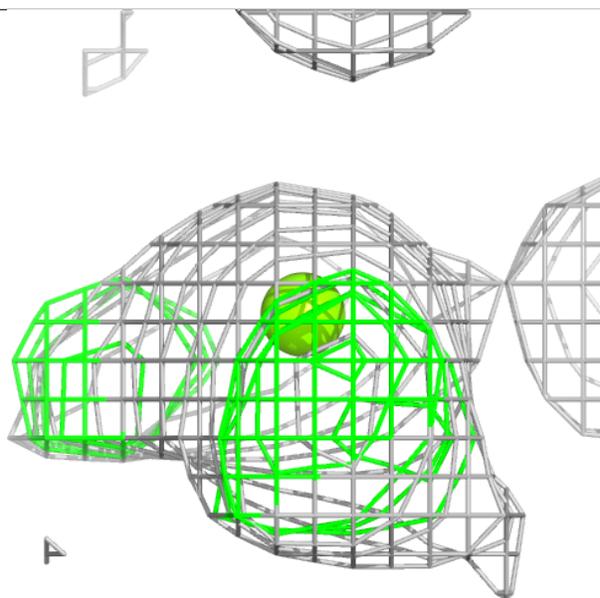
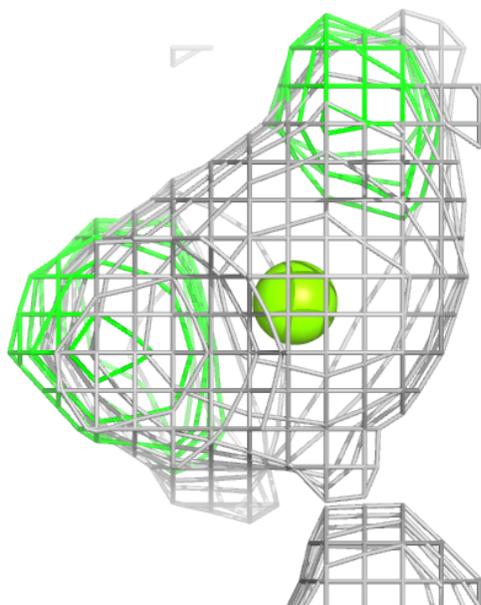
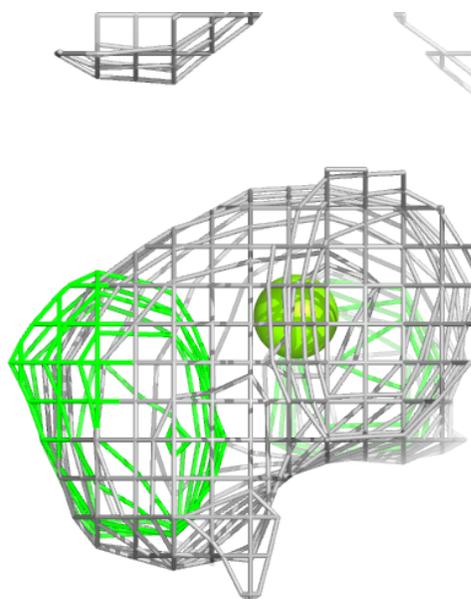
Electron density around ACT F 307:

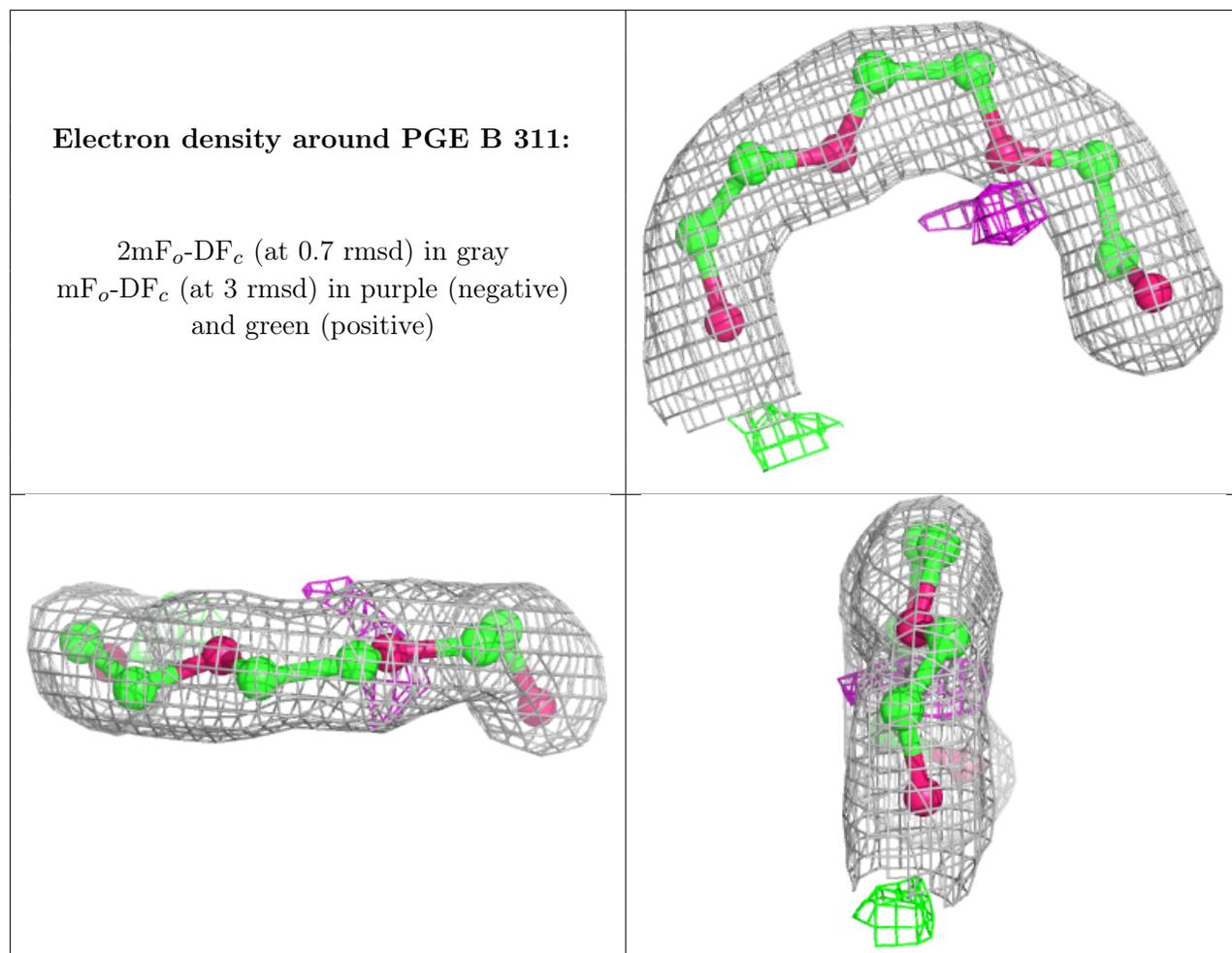
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

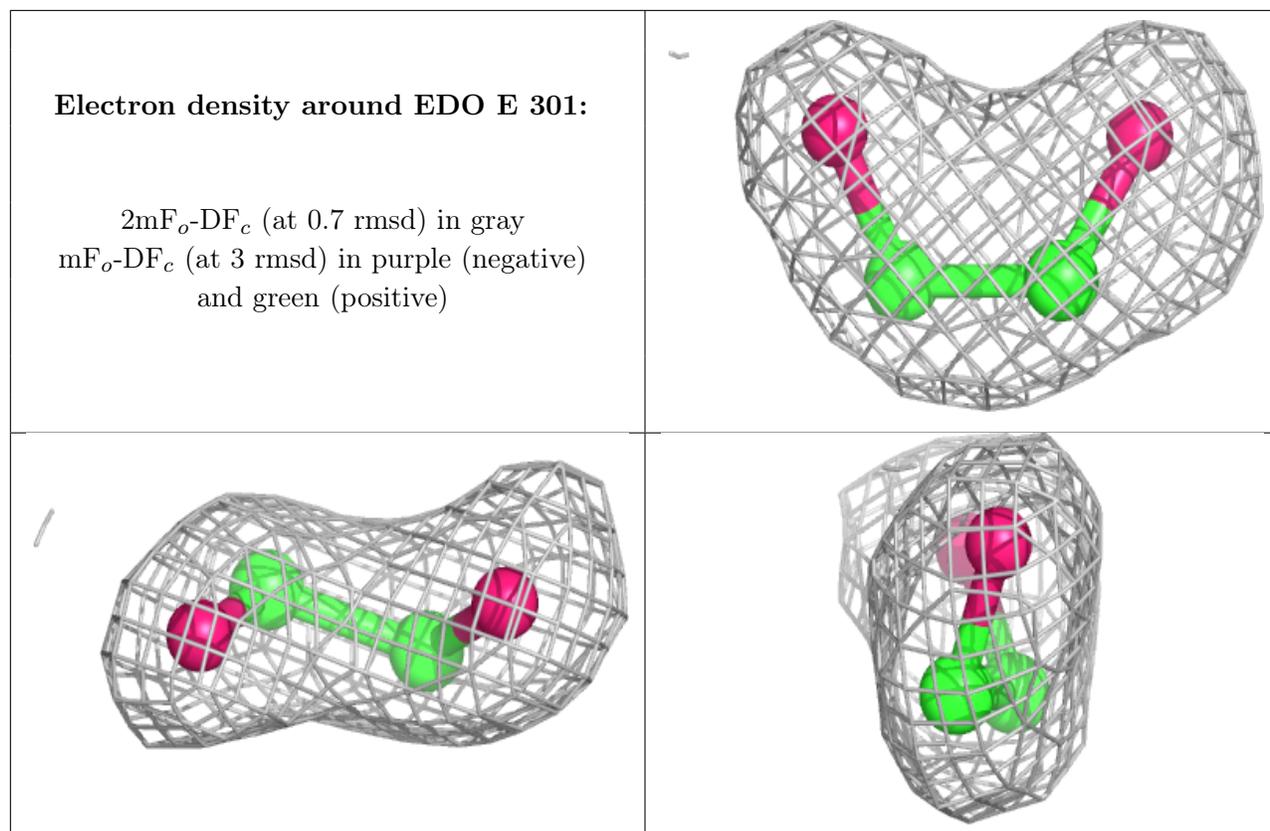


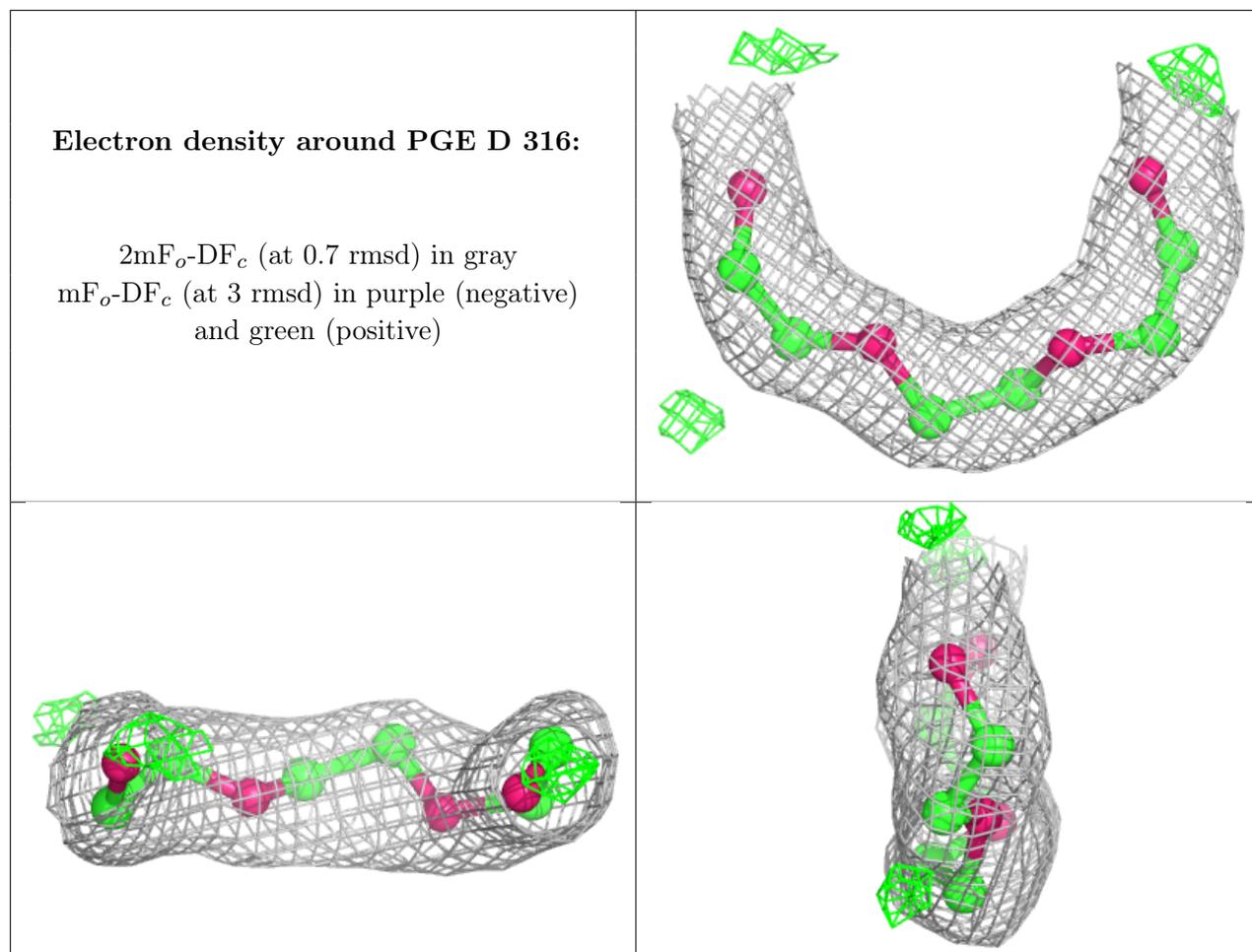
Electron density around MG C 307:

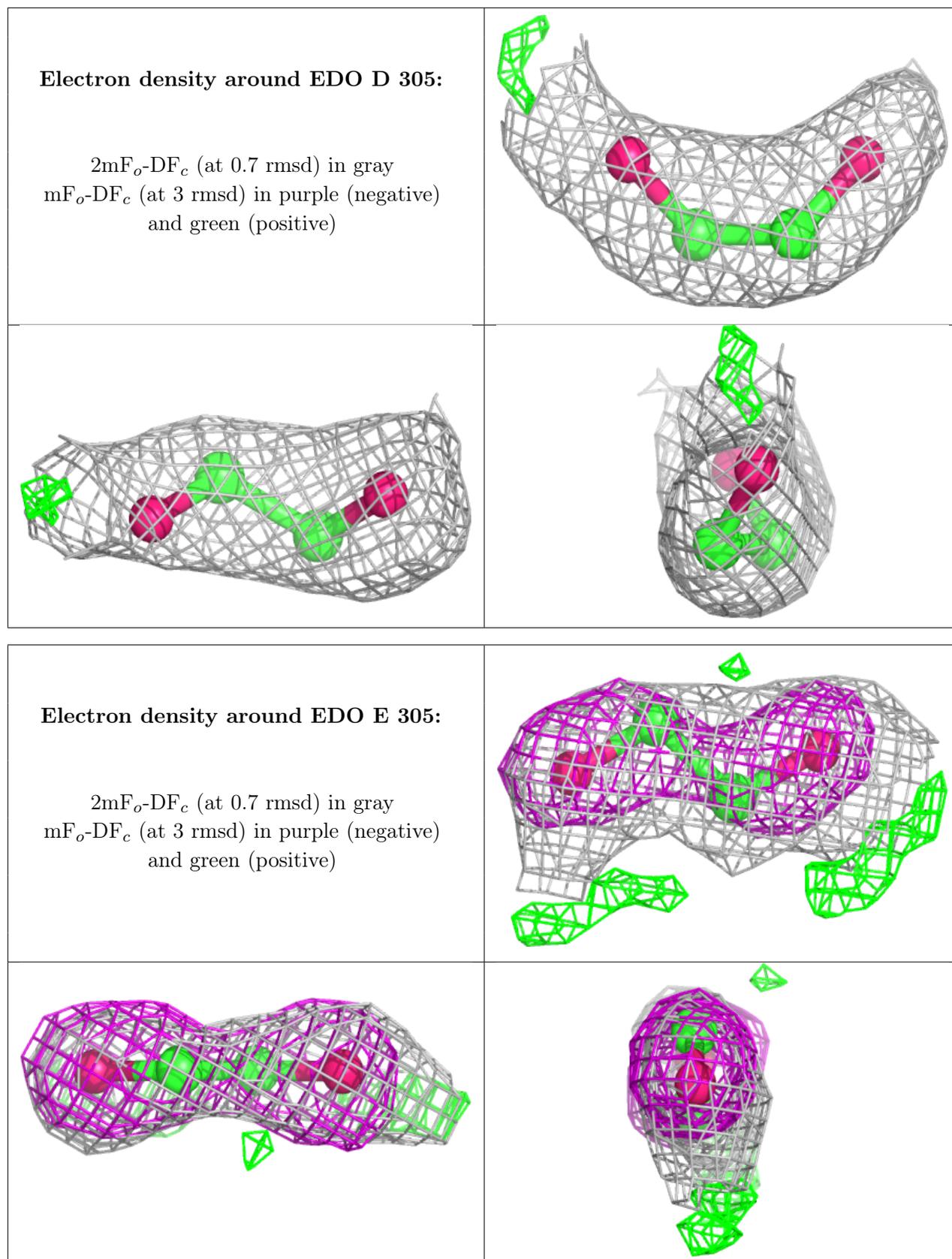
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

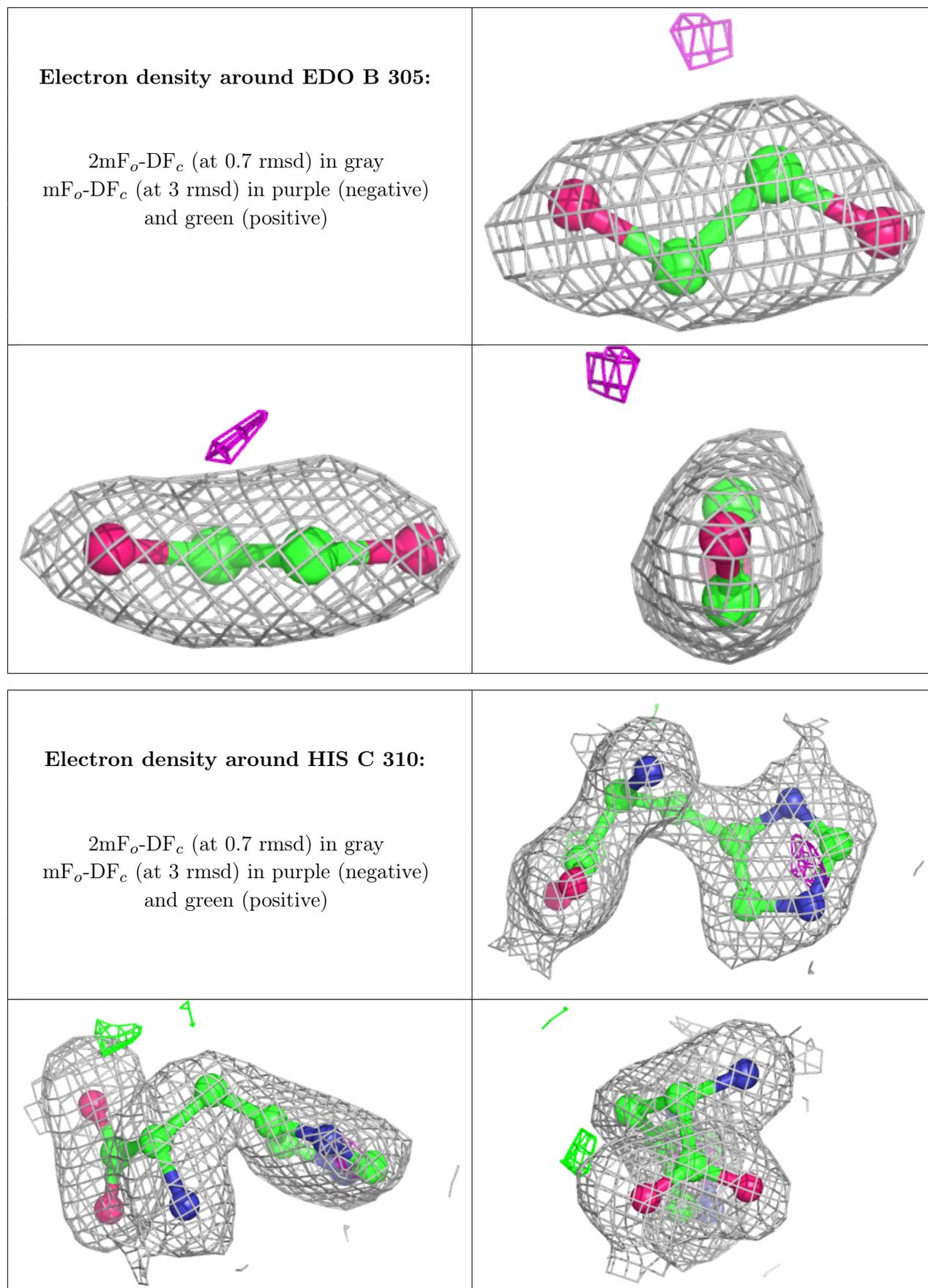






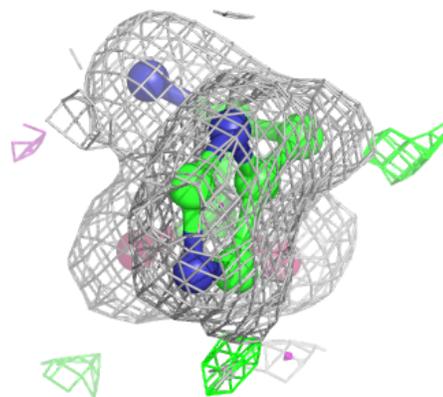
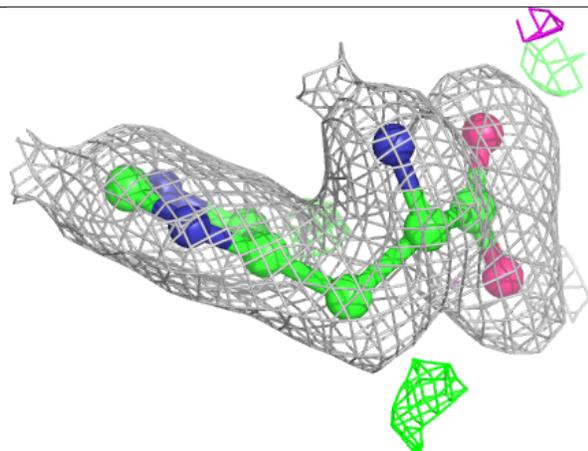
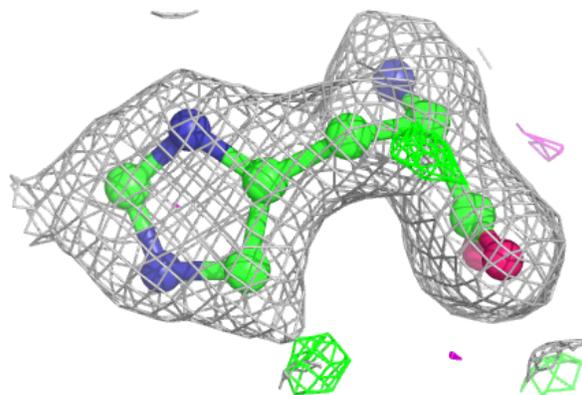






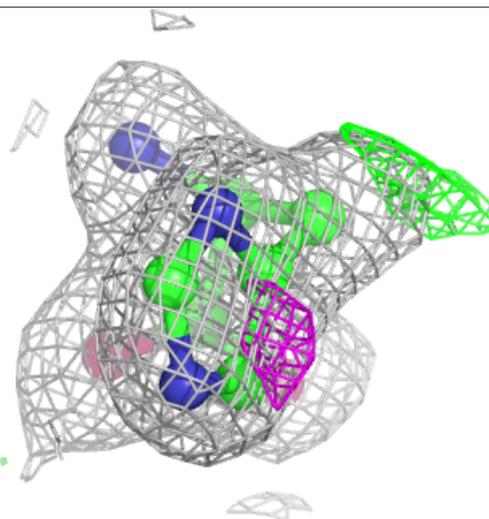
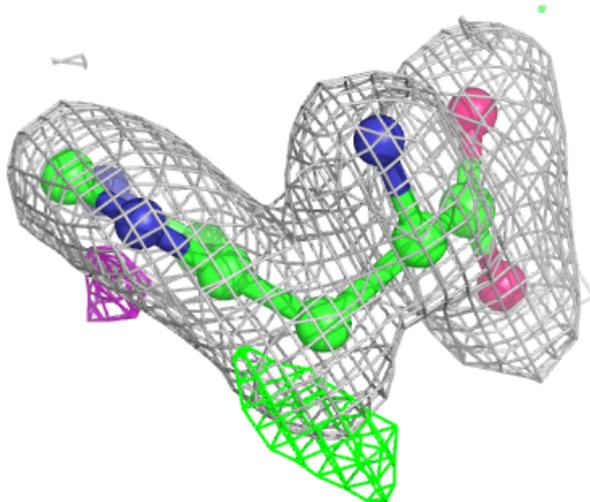
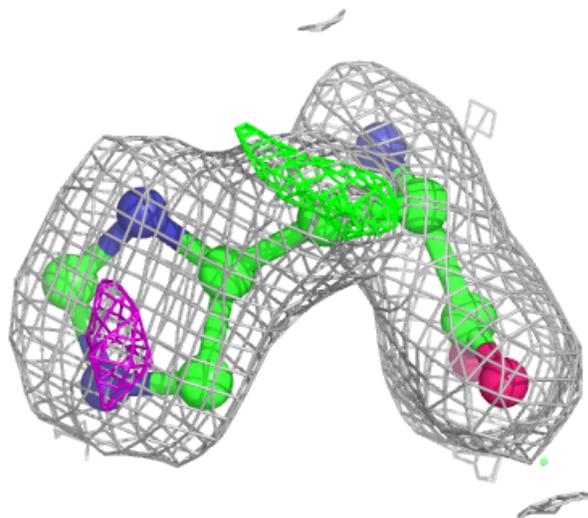
Electron density around HIS D 321:

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



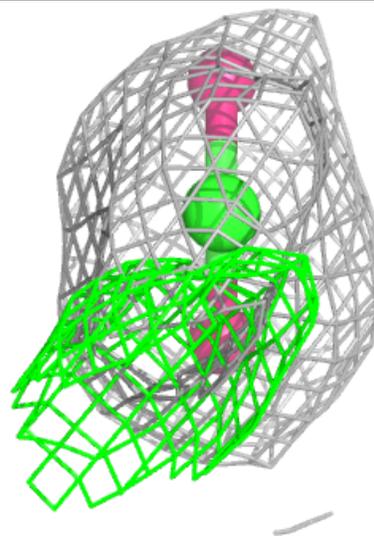
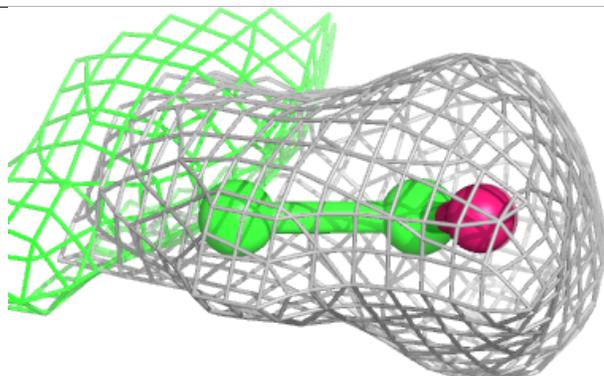
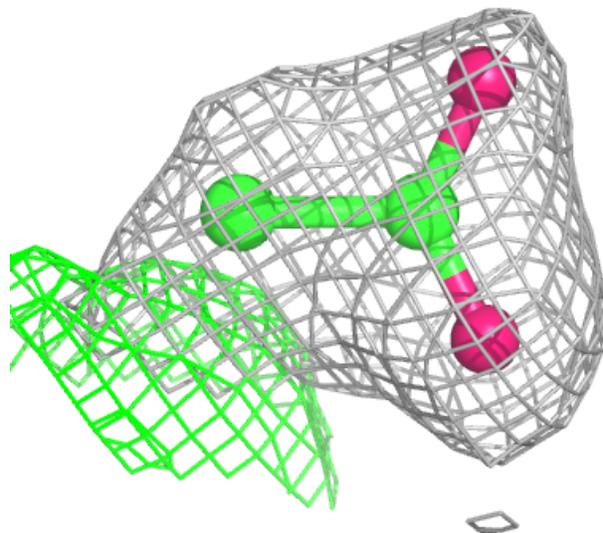
Electron density around HIS E 317:

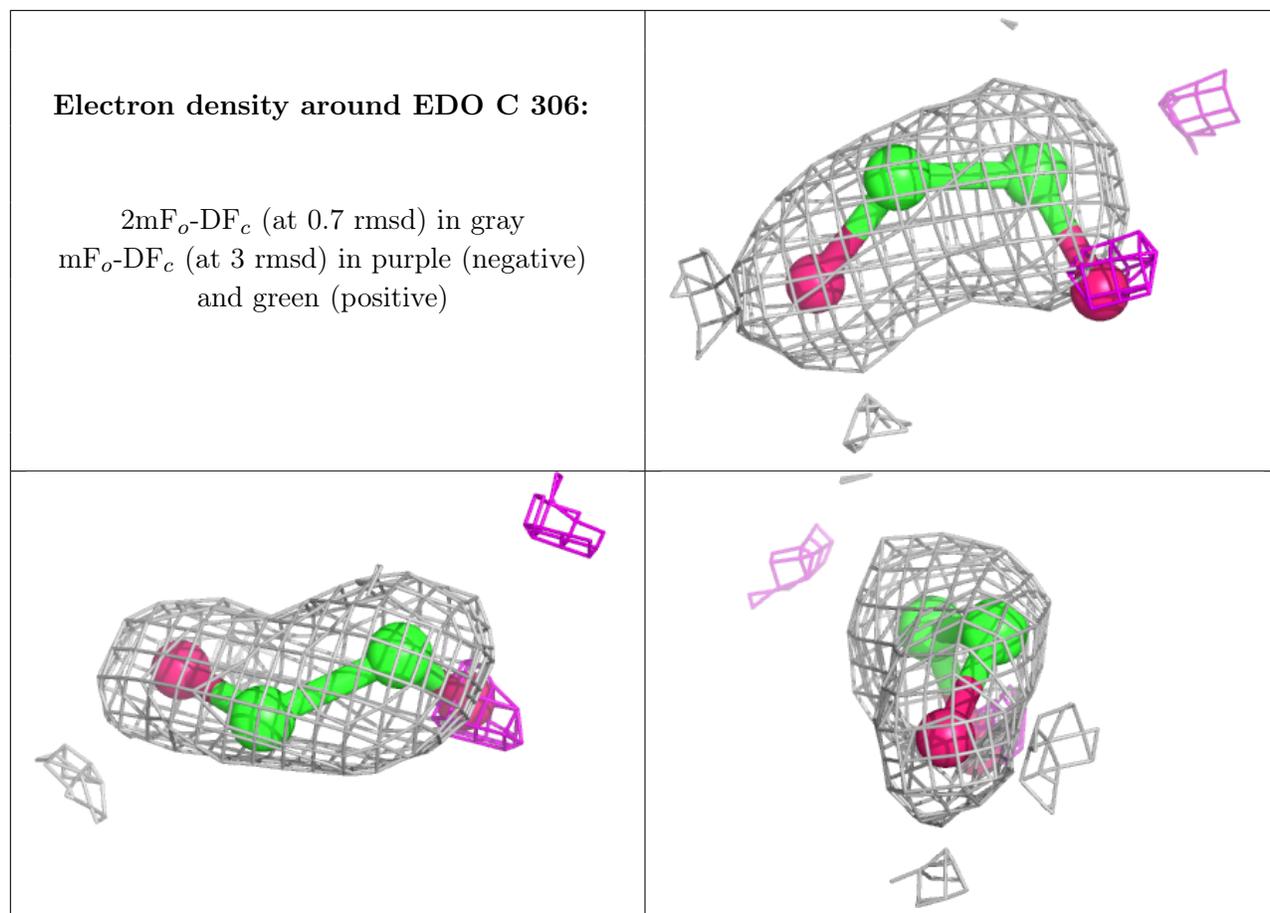
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

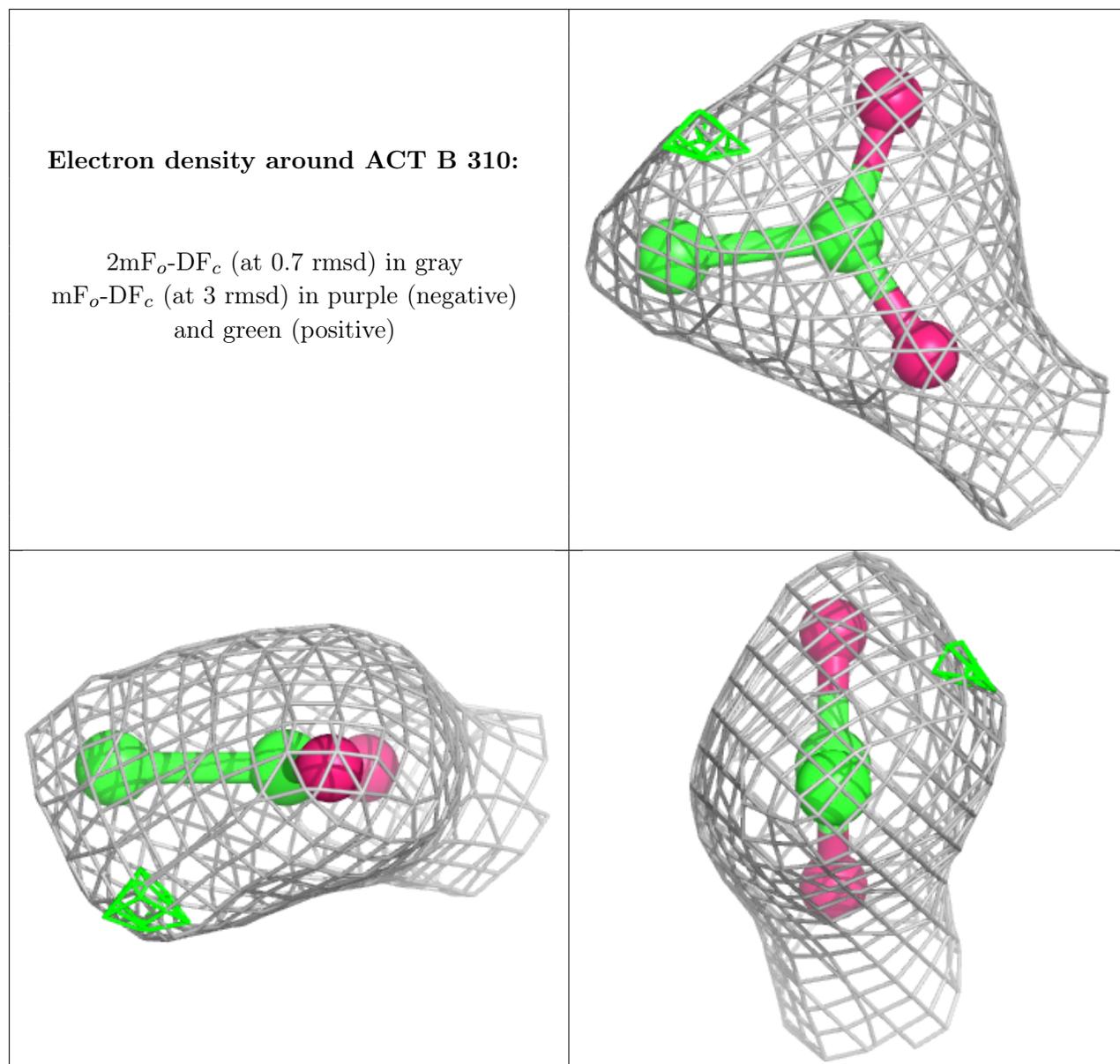


Electron density around ACT F 306:

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

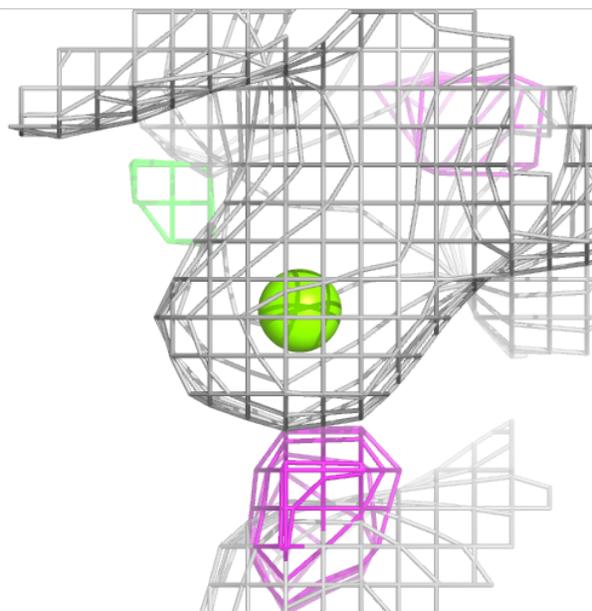
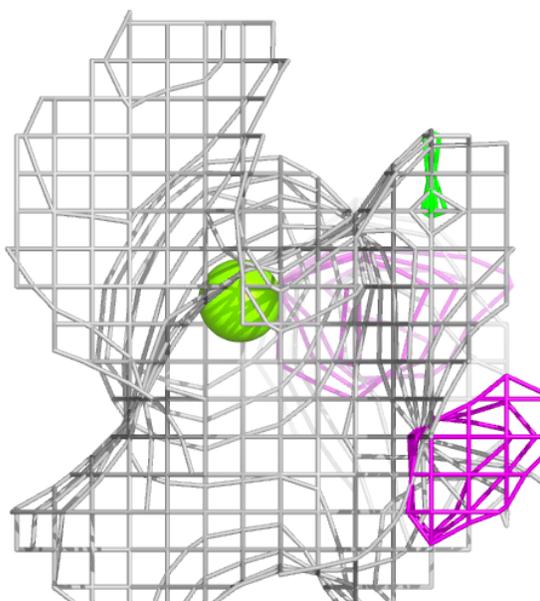
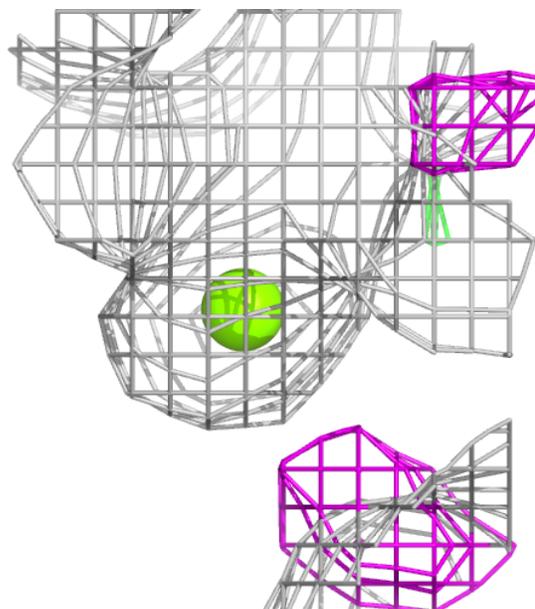






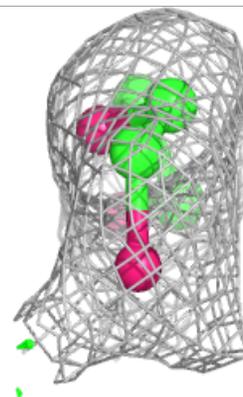
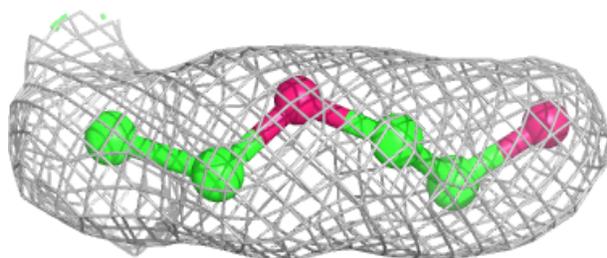
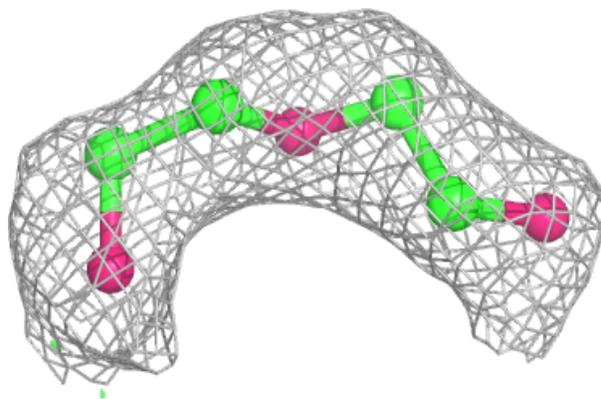
Electron density around MG B 307:

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



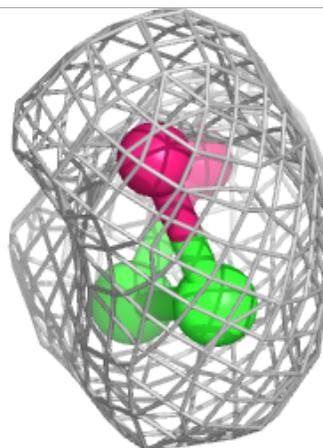
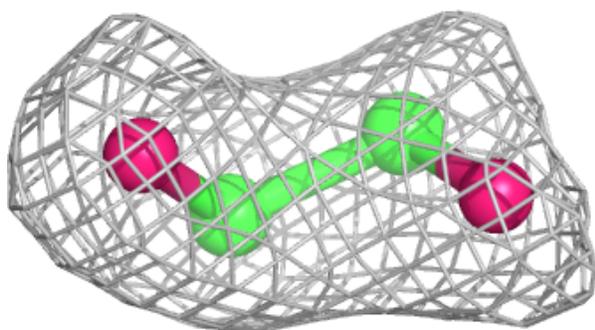
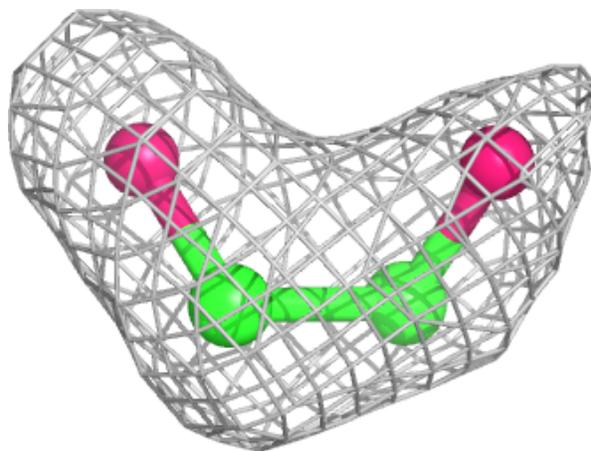
Electron density around PEG E 315:

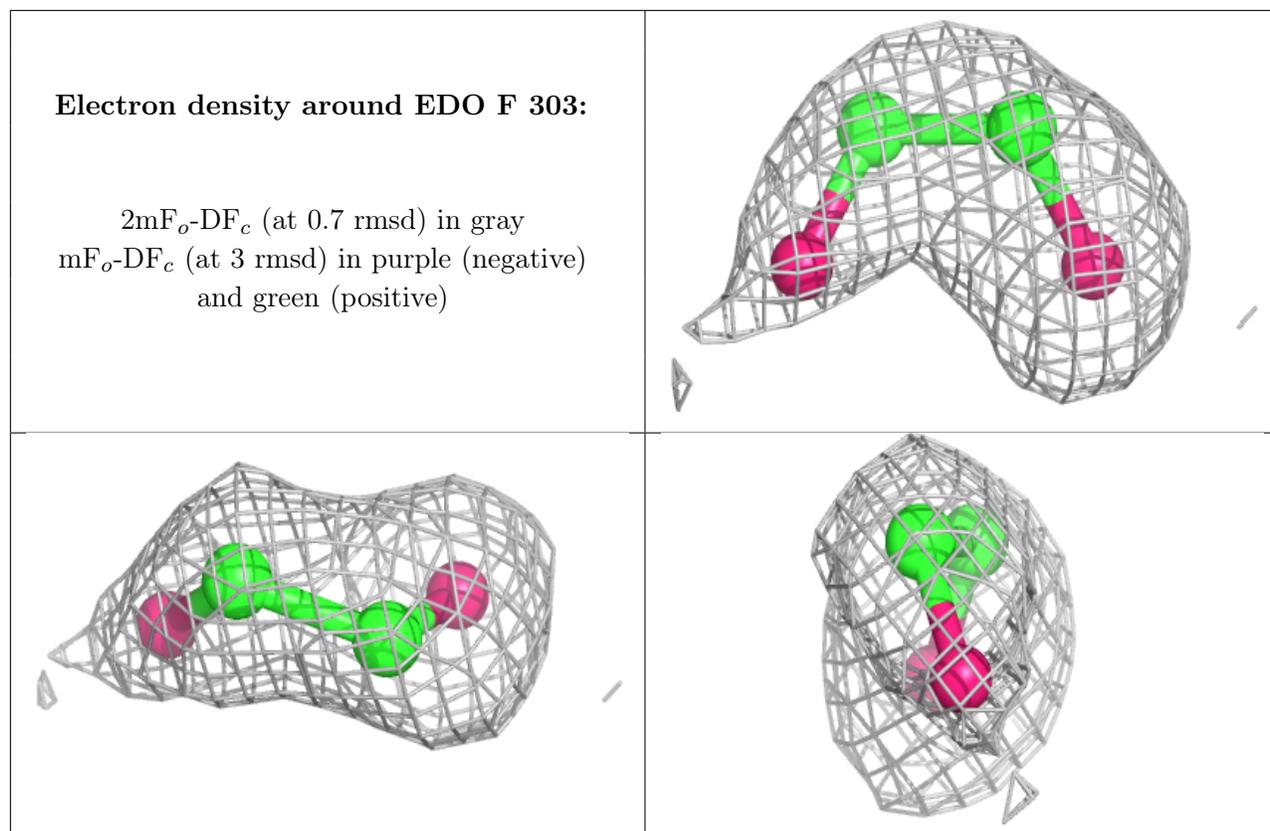
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

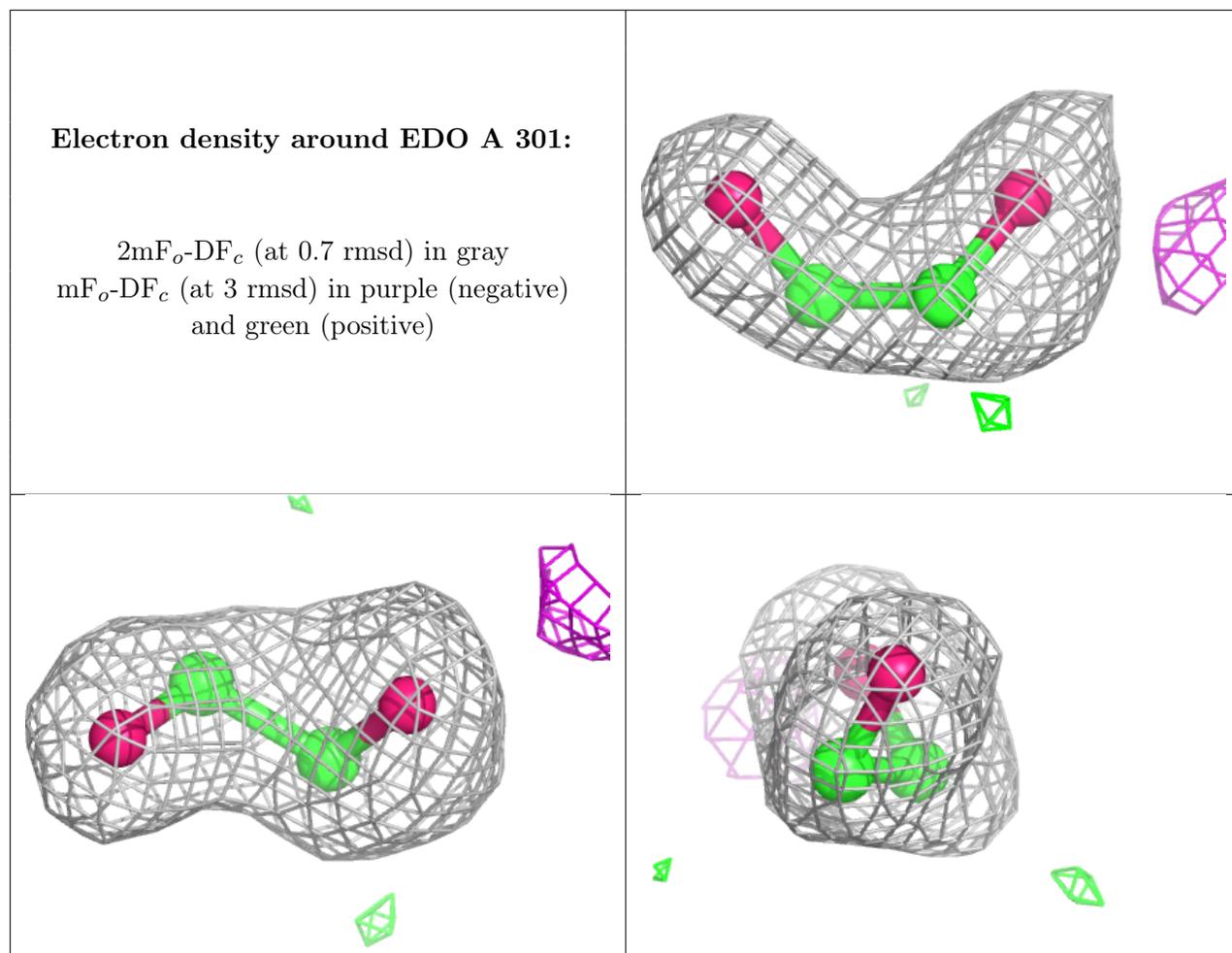


Electron density around EDO A 303:

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

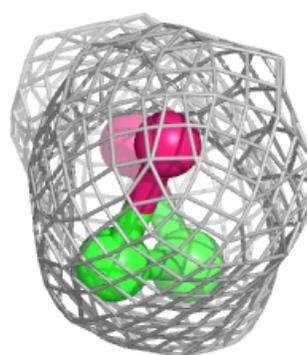
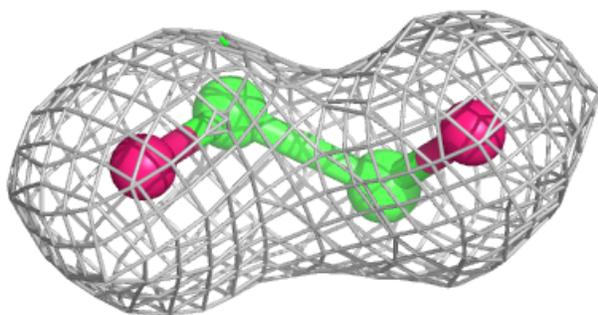
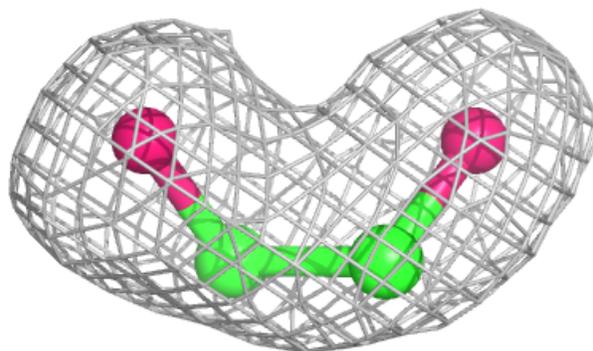


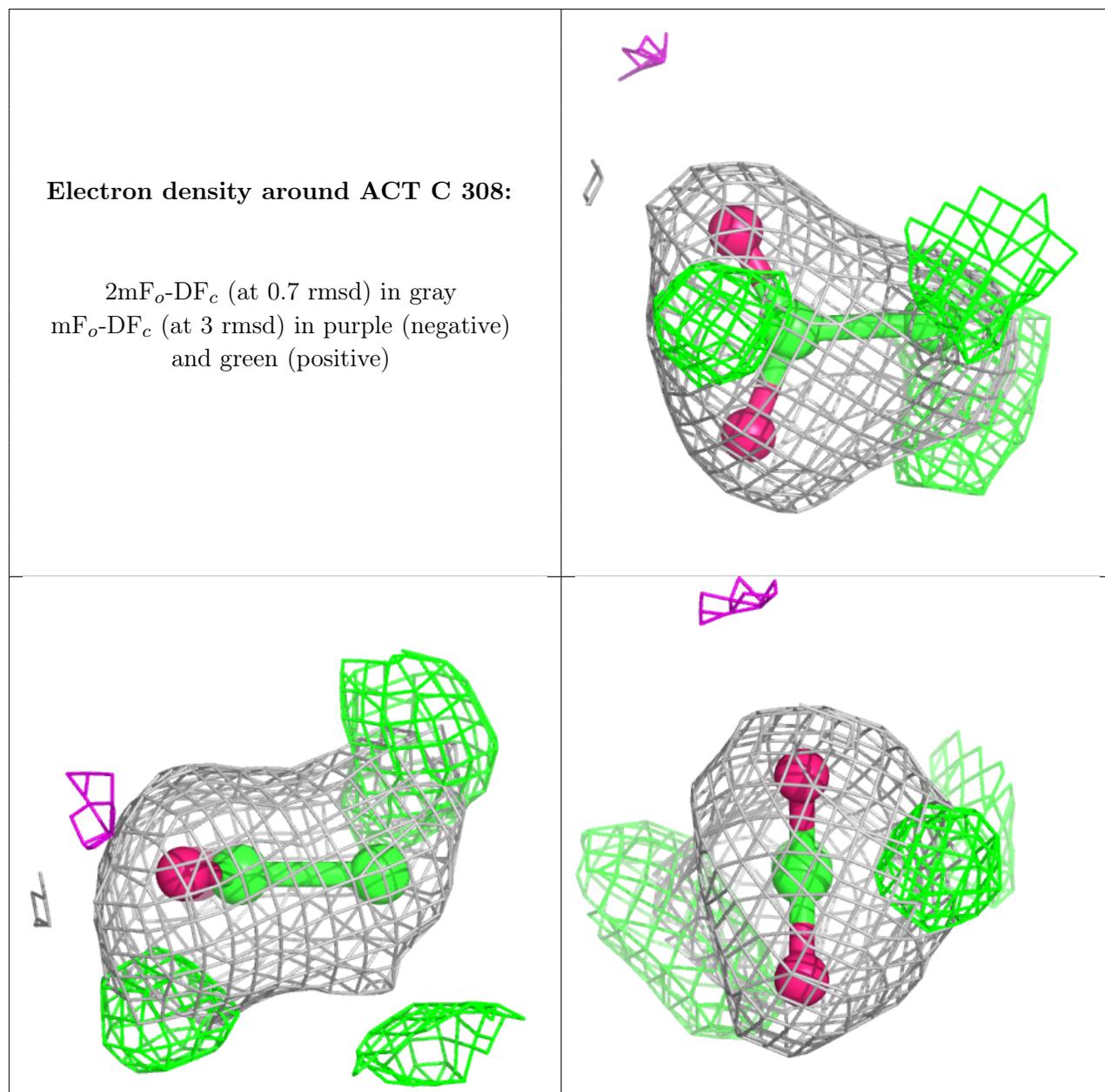


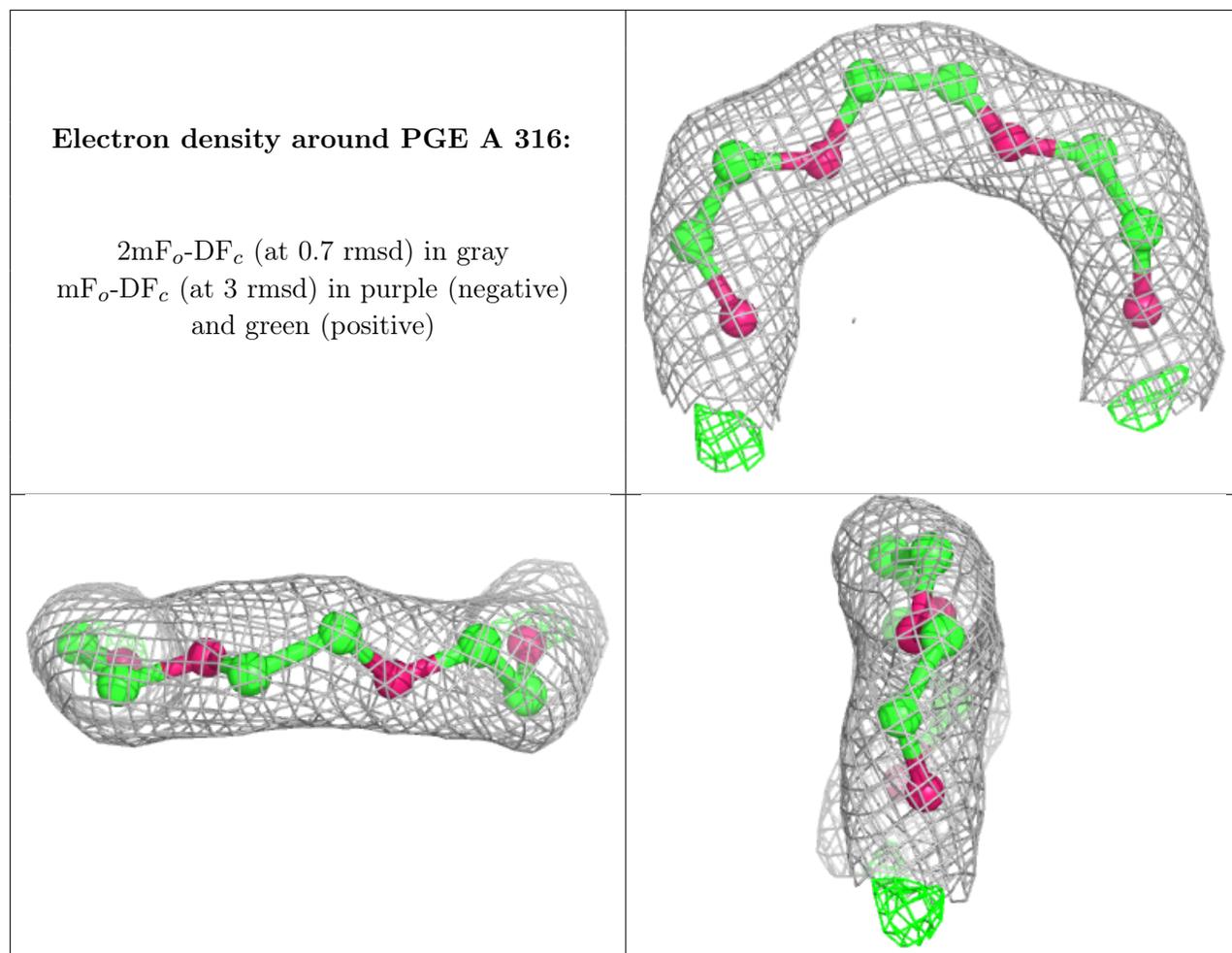


Electron density around EDO E 304:

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

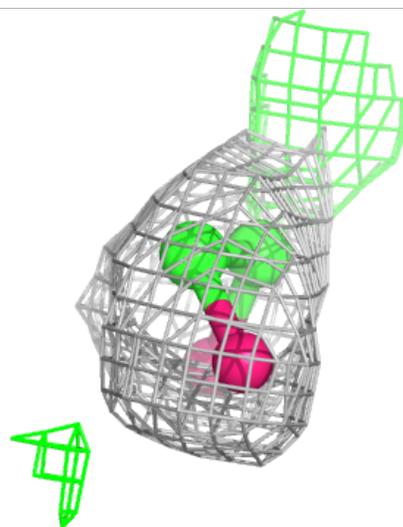
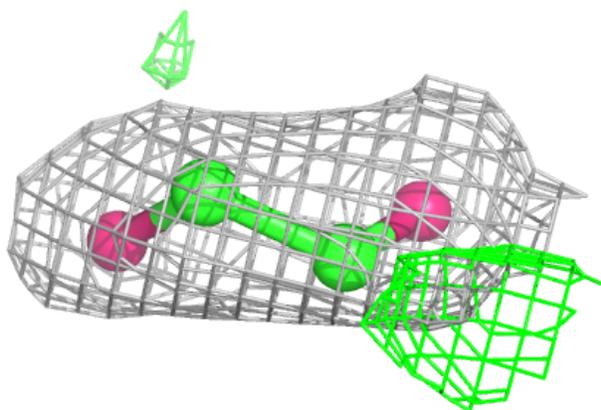
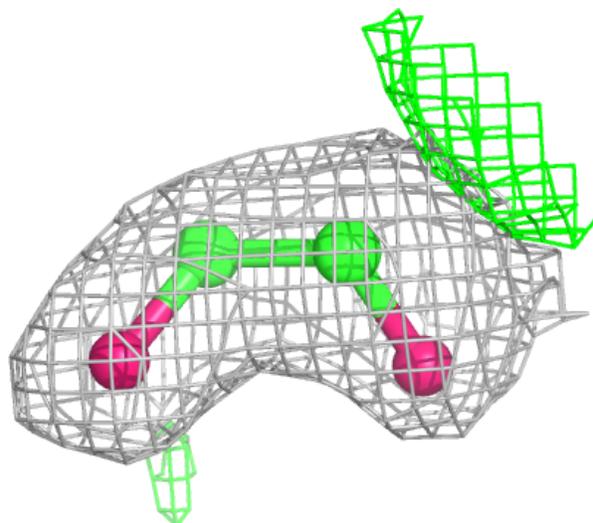






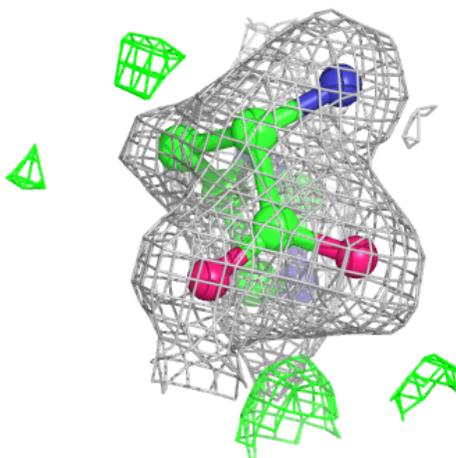
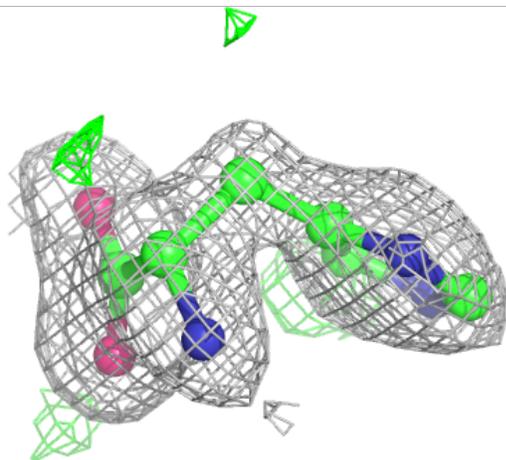
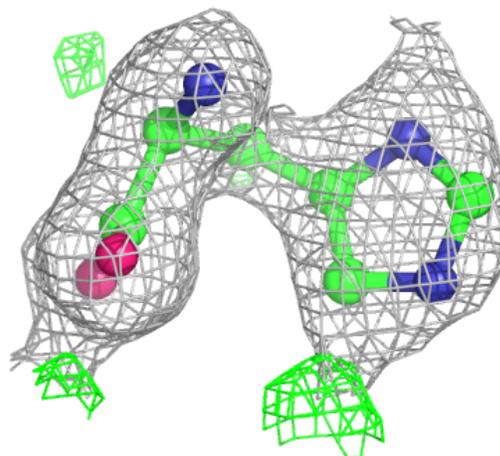
Electron density around EDO D 303:

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



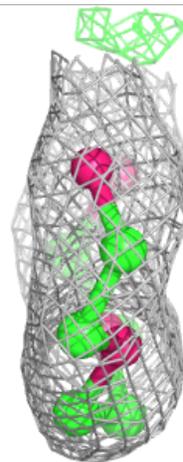
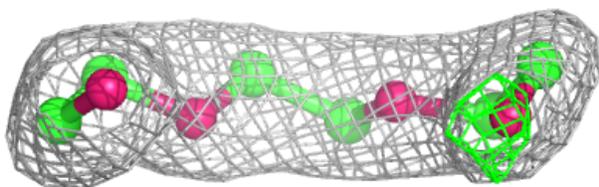
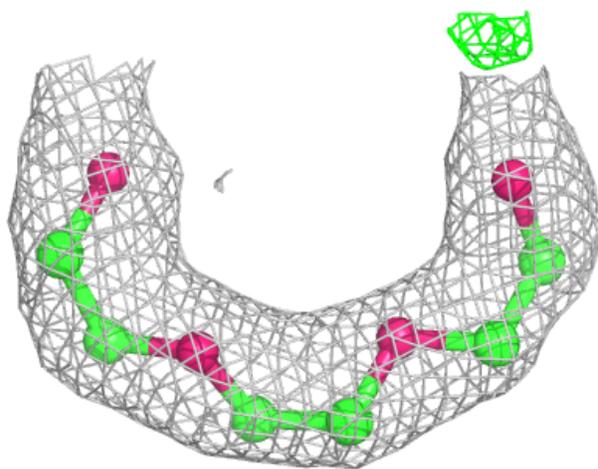
Electron density around HIS A 317:

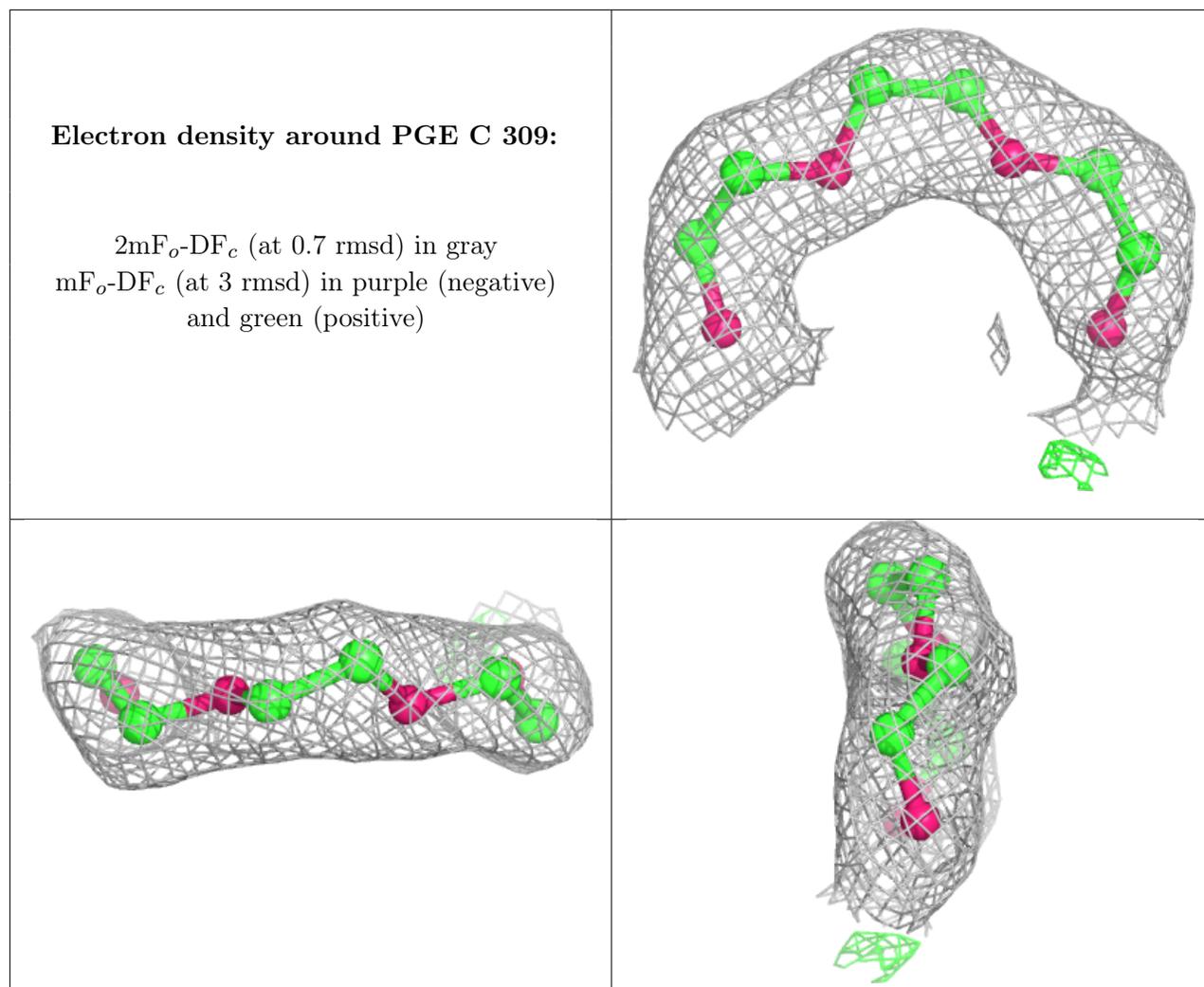
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

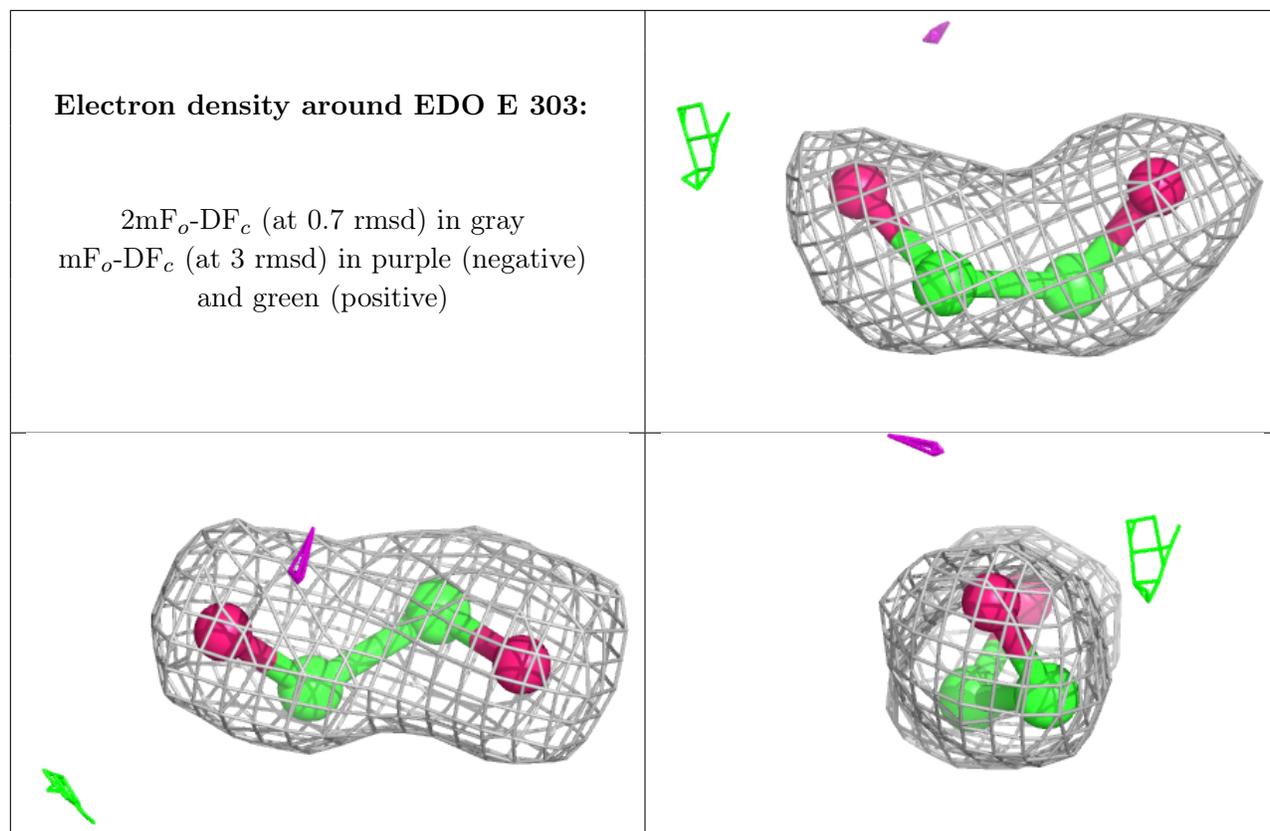


Electron density around PGE E 312:

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

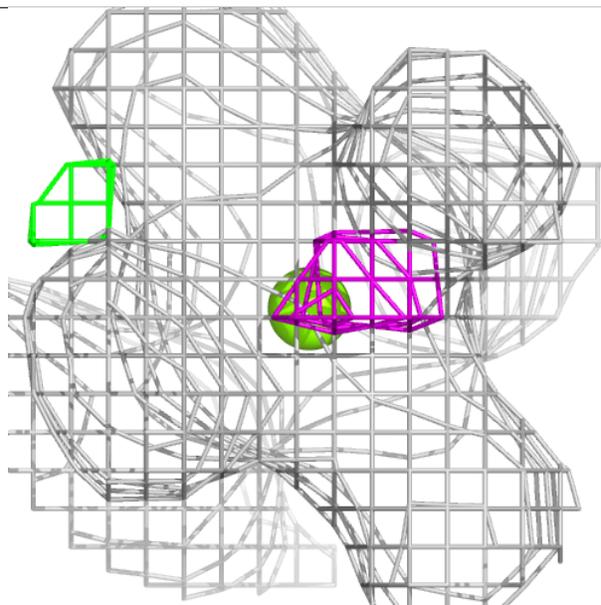
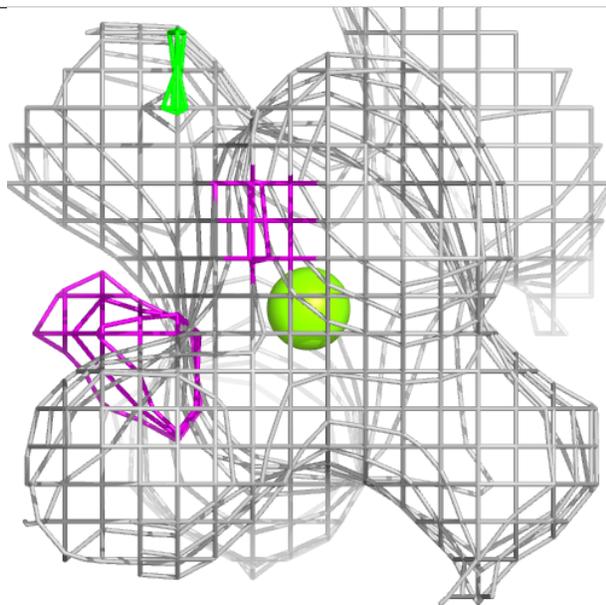
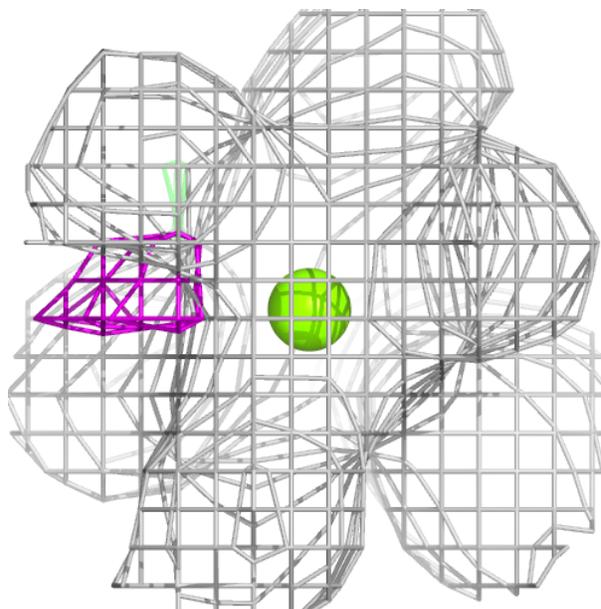






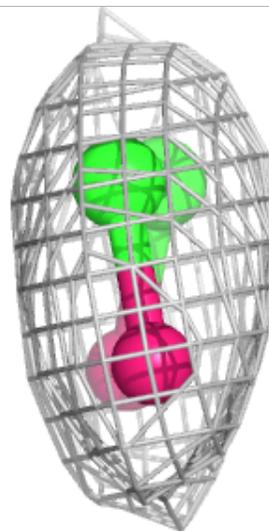
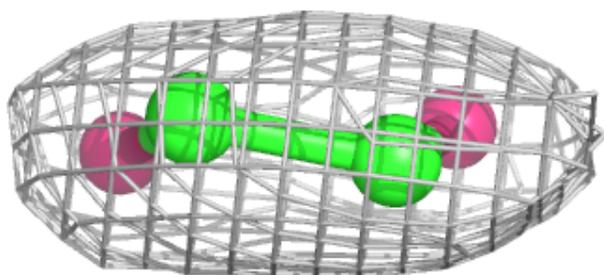
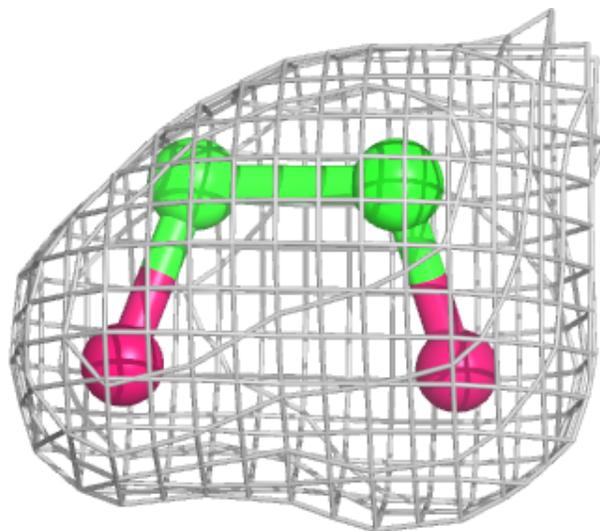
Electron density around MG A 310:

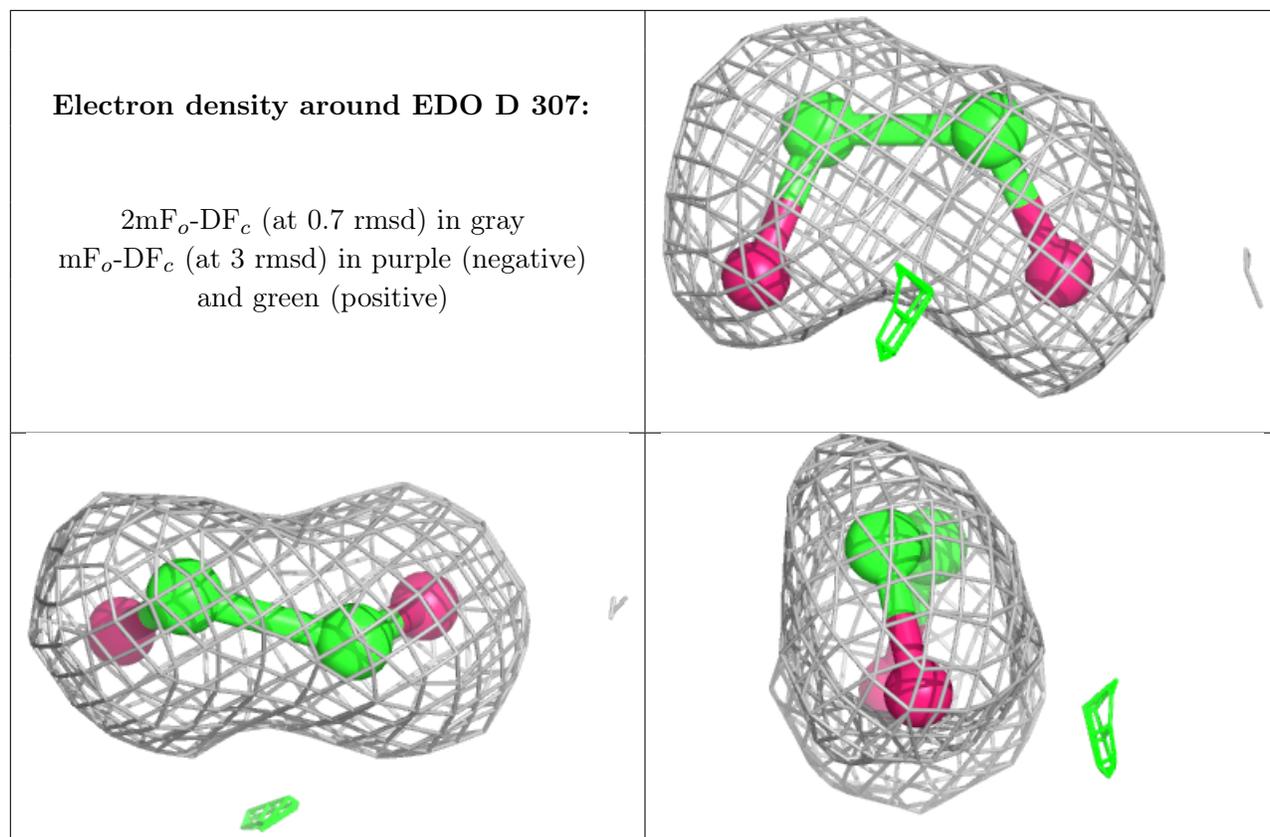
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

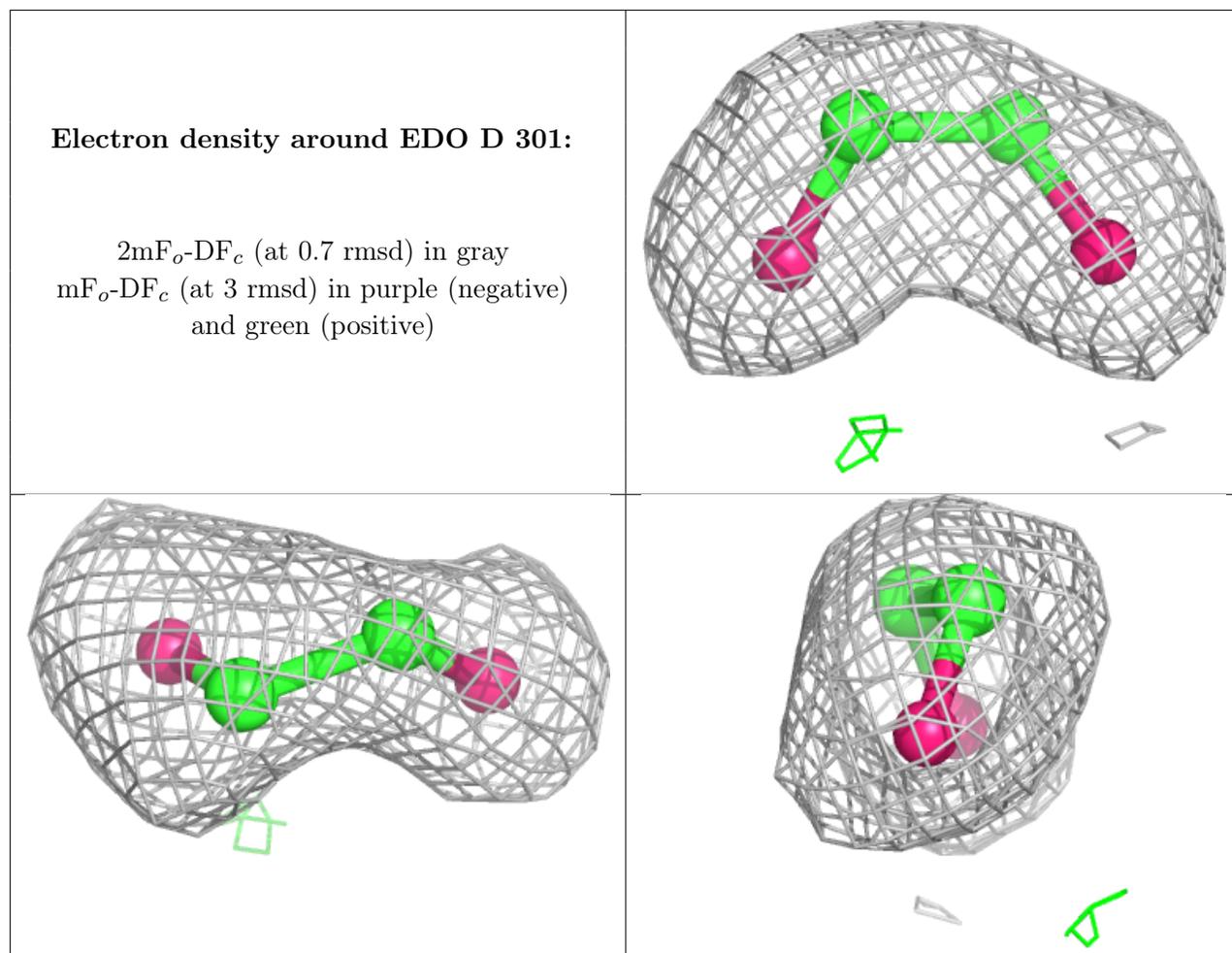


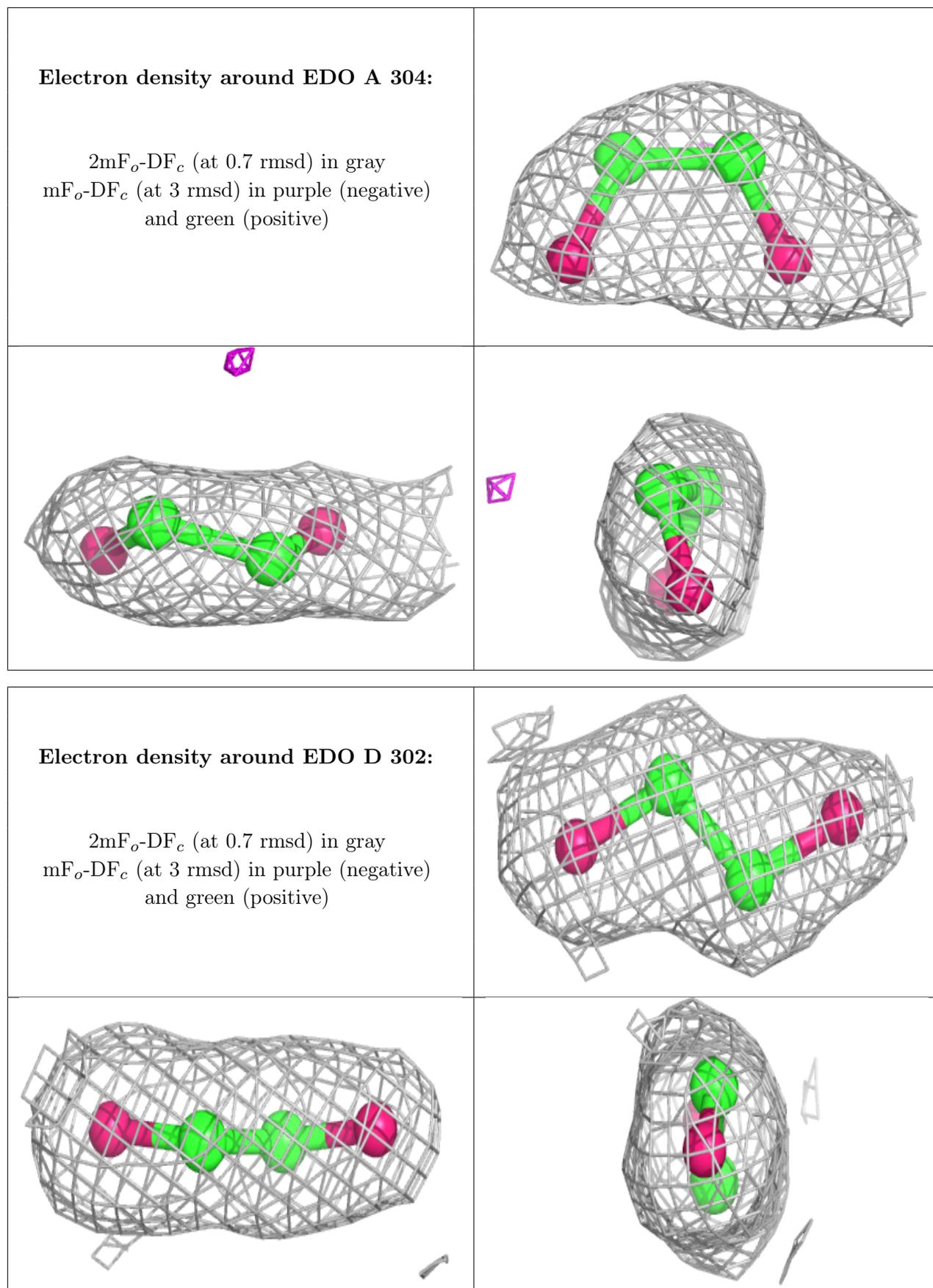
Electron density around EDO D 309:

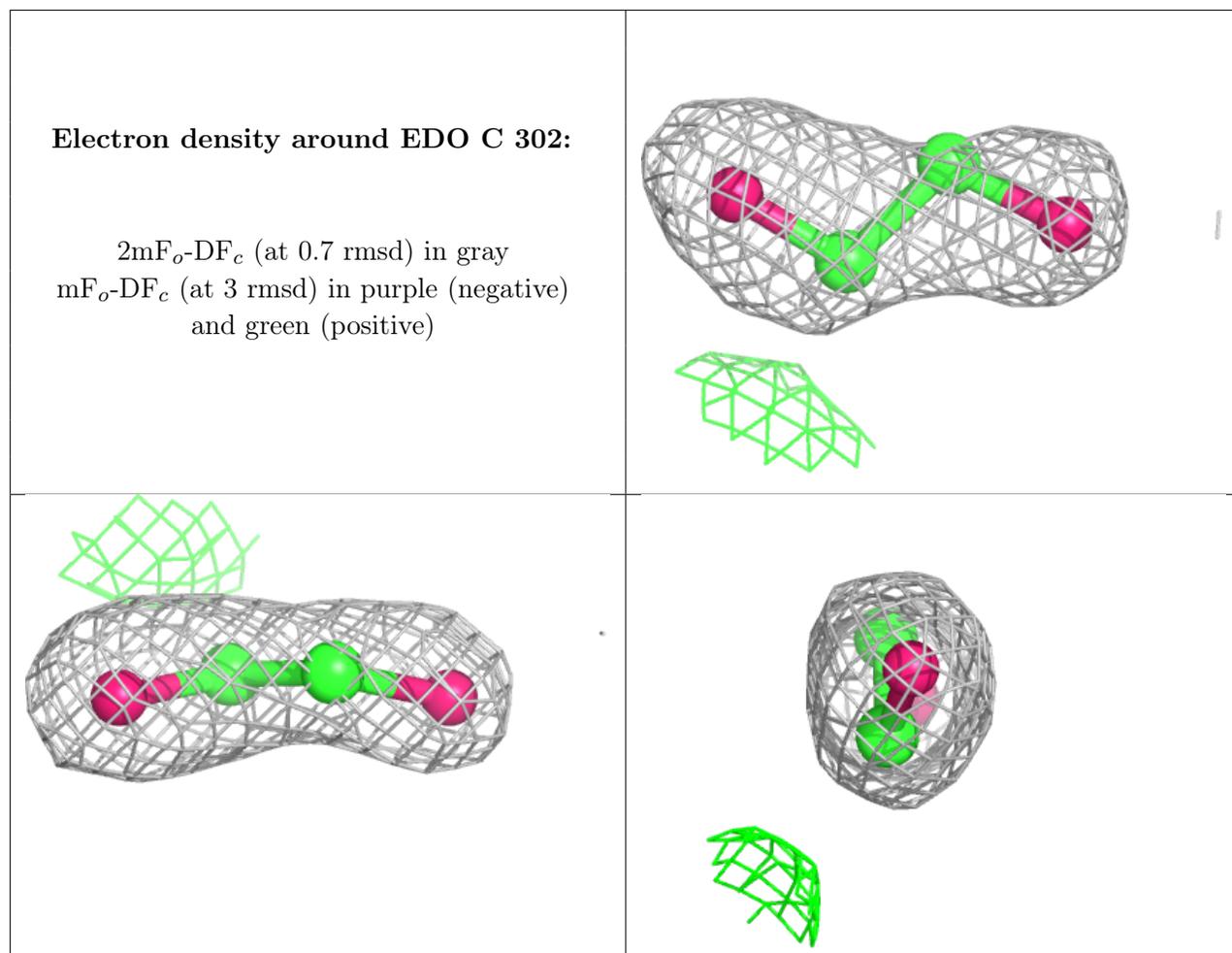
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





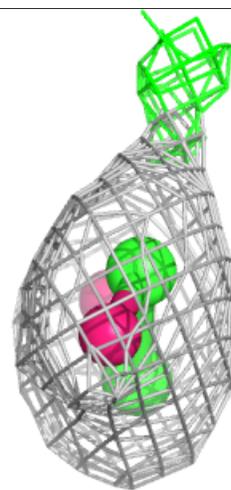
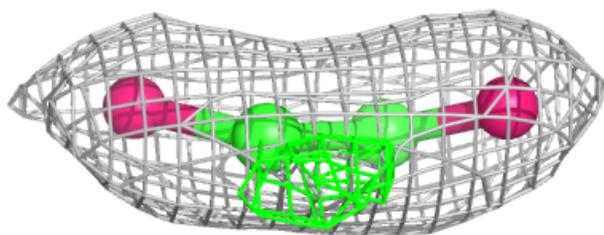
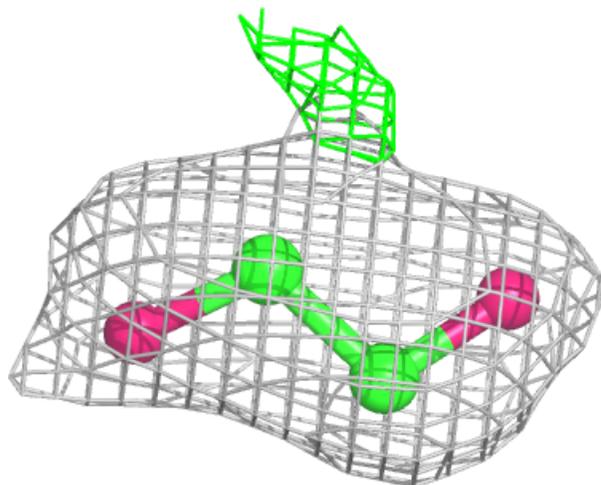






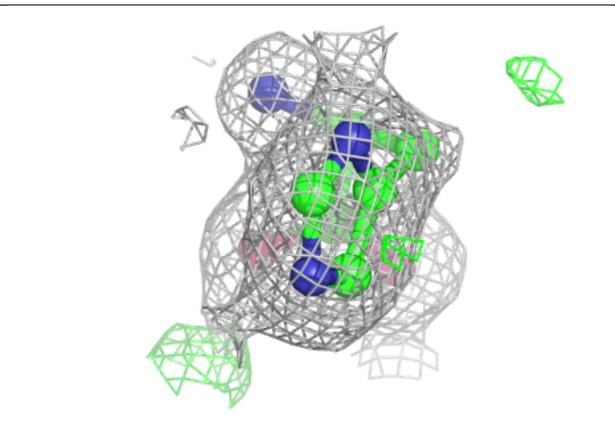
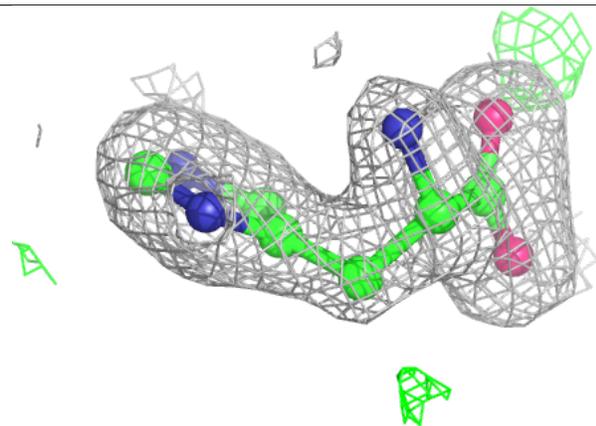
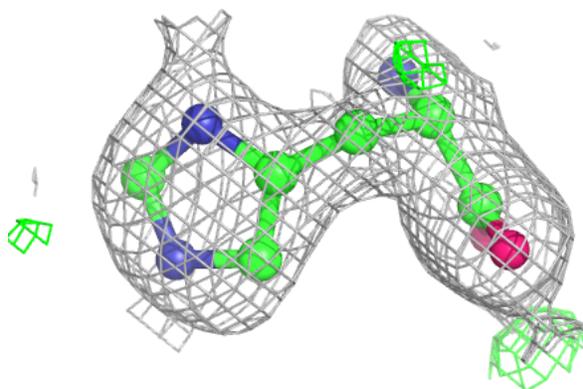
Electron density around EDO F 304:

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

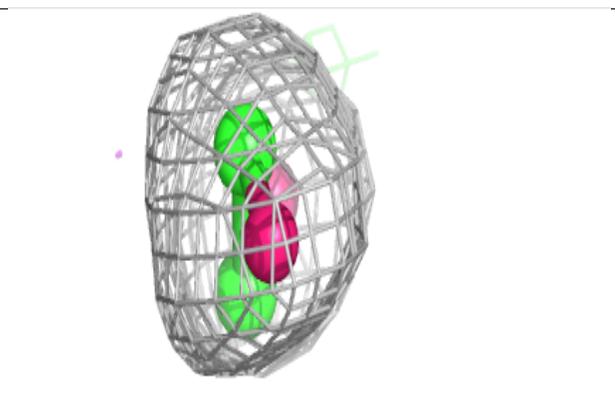
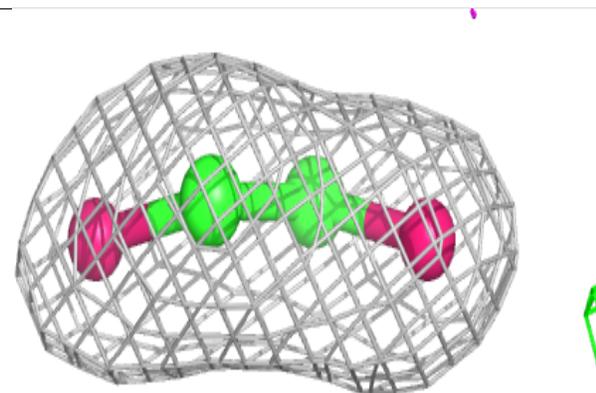
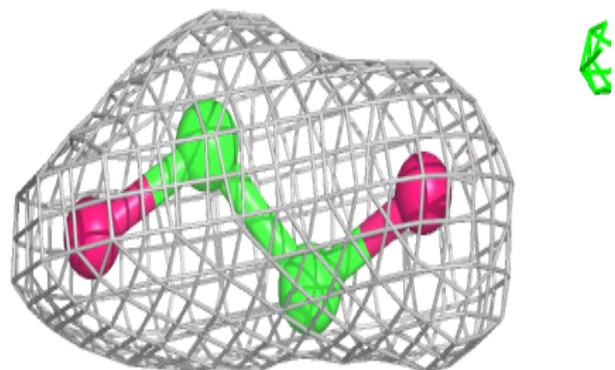


Electron density around HIS F 309:

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

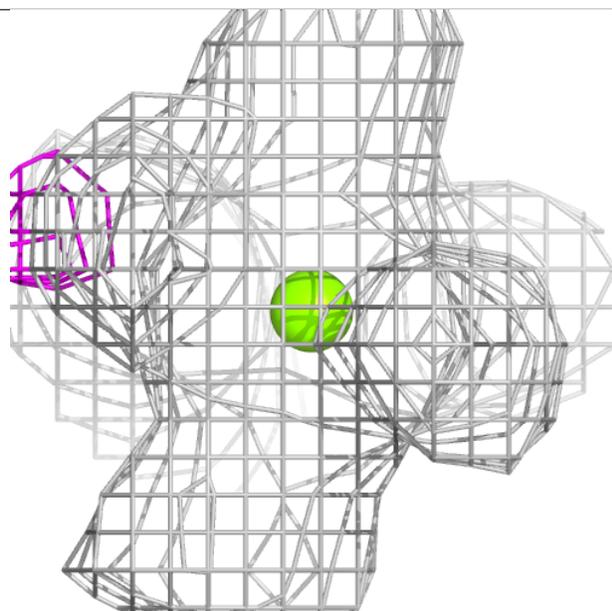
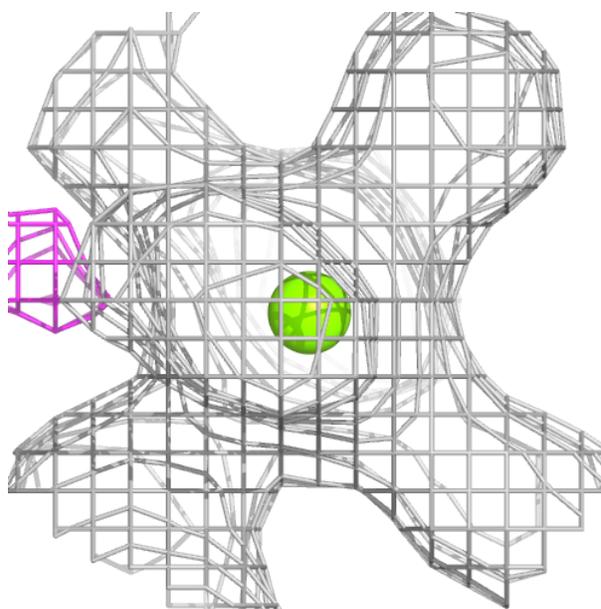
**Electron density around EDO A 302:**

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



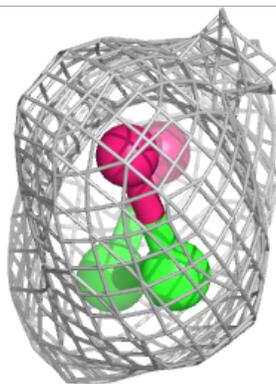
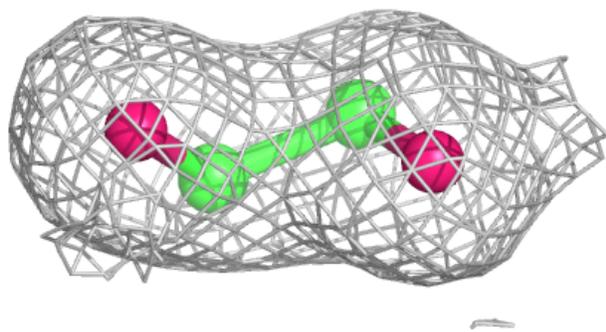
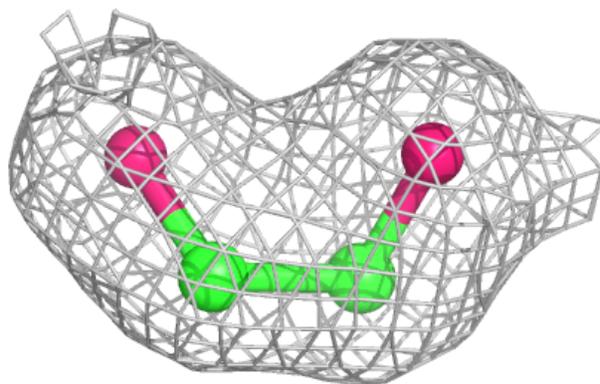
Electron density around MG B 306:

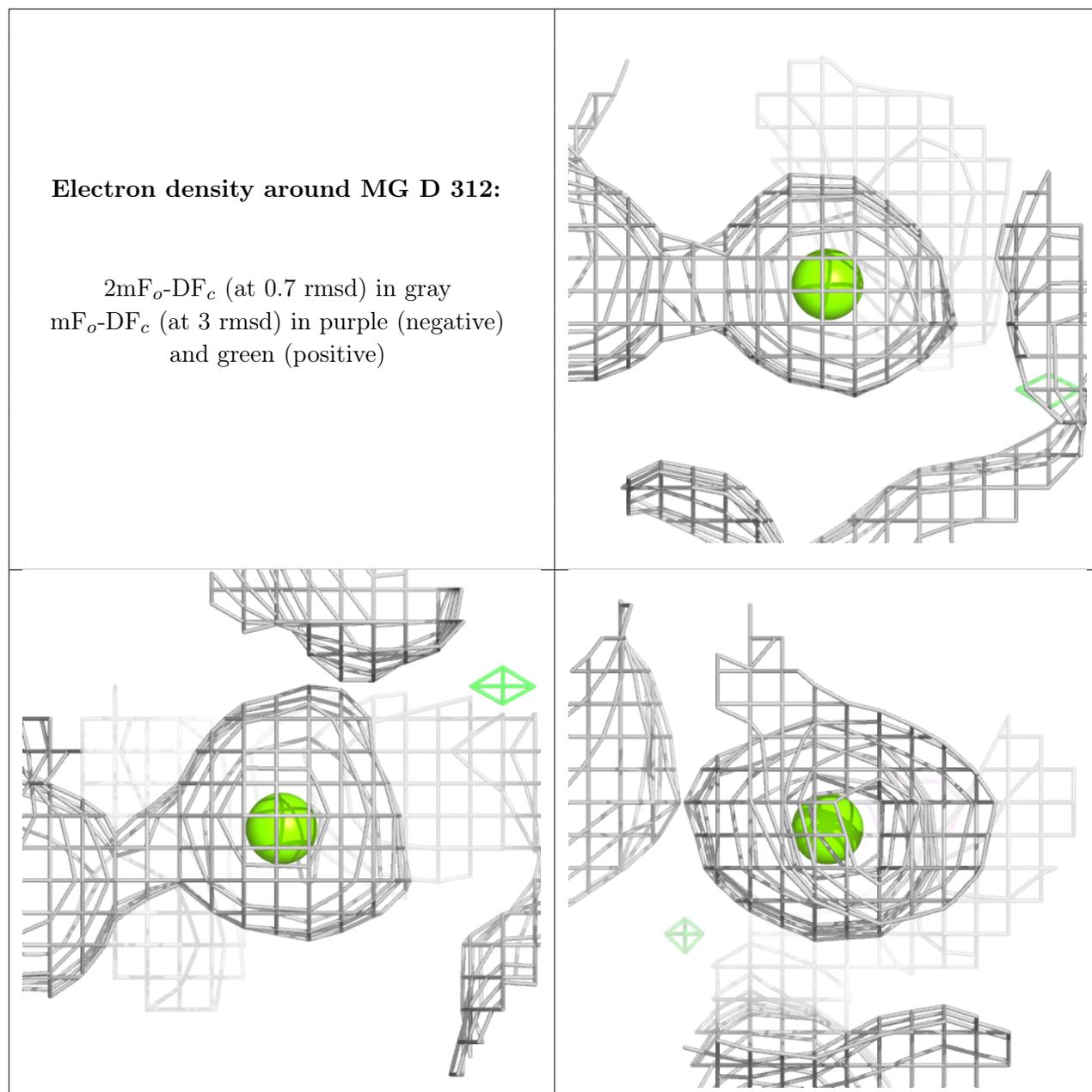
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EDO 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.