



Full wwPDB X-ray Structure Validation Report i

Oct 9, 2023 – 07:51 AM EDT

PDB ID : 7KH4

Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H56W mutant with pyruvate bound in the active site and R,R-bislysine bound at the allosteric site

Authors : Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.

Deposited on : 2020-10-19

Resolution : 1.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

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

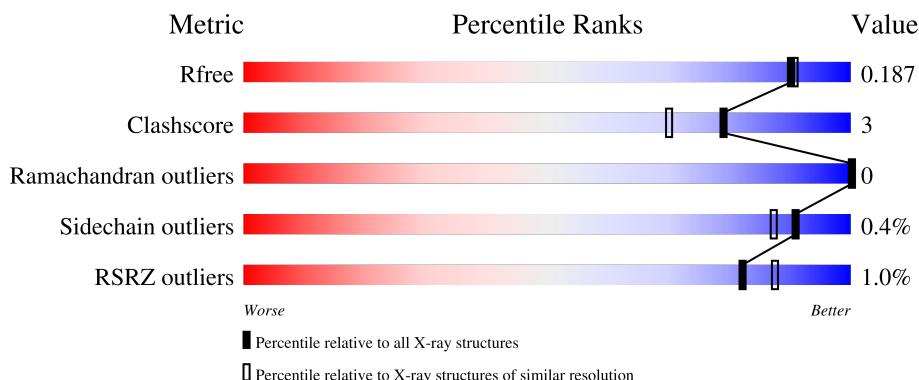
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

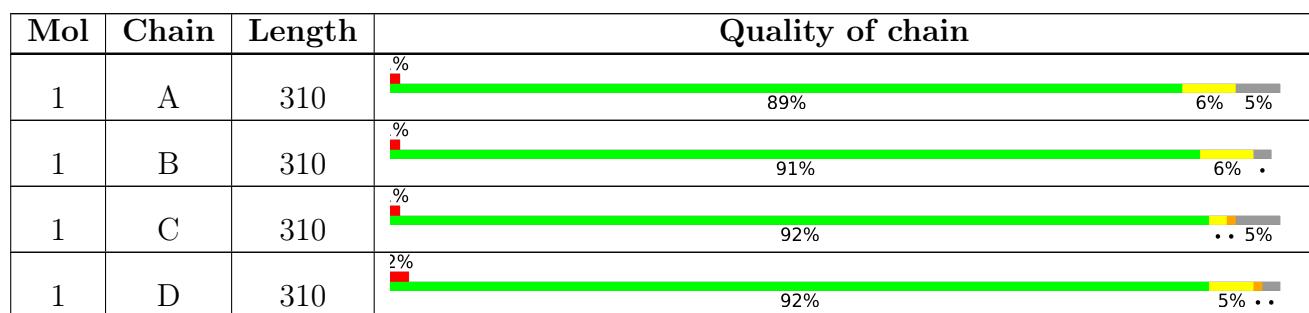
The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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



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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	306	-	-	X	-

2 Entry composition [\(i\)](#)

There are 10 unique types of molecules in this entry. The entry contains 15441 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 4-hydroxy-tetrahydrodipicolinate synthase.

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

There are 78 discrepancies between the modelled and reference sequences:

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

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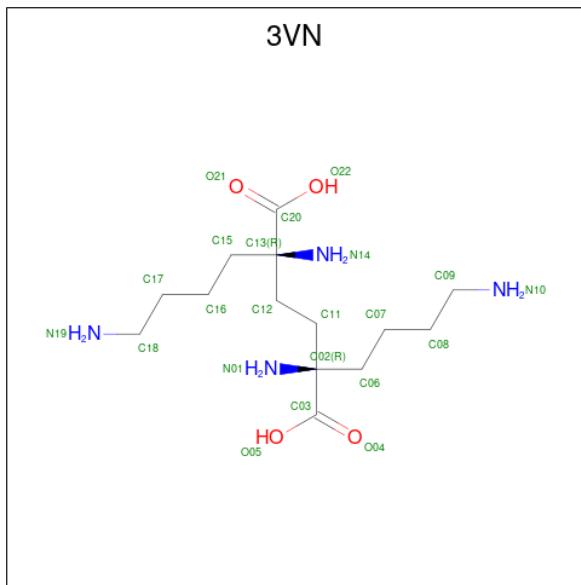
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4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

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

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



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

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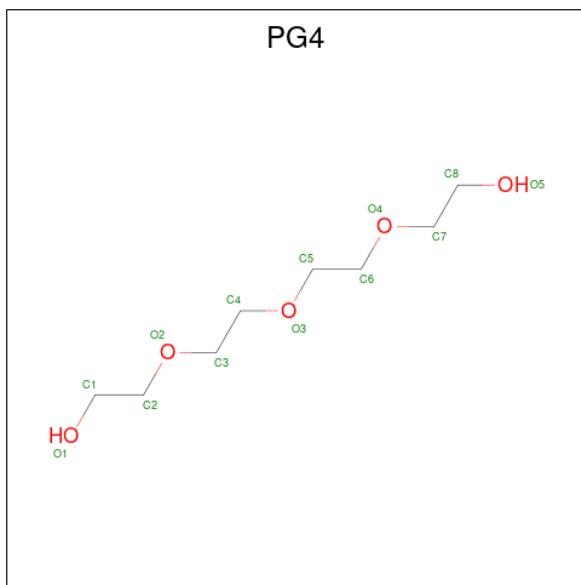
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 22 14 4 4	0	0
2	D	1	Total C N O 22 14 4 4	0	0

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

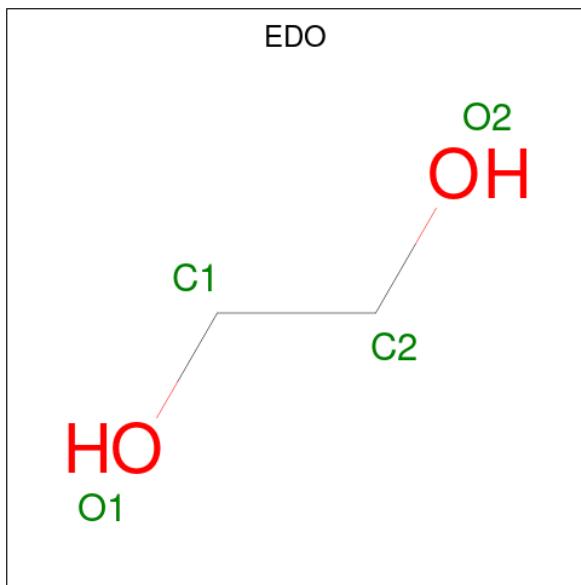
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Mg 4 4	0	0
3	B	3	Total Mg 3 3	0	0
3	C	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	E	5	Total Mg 5 5	0	0
3	F	4	Total Mg 4 4	0	0

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



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

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



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

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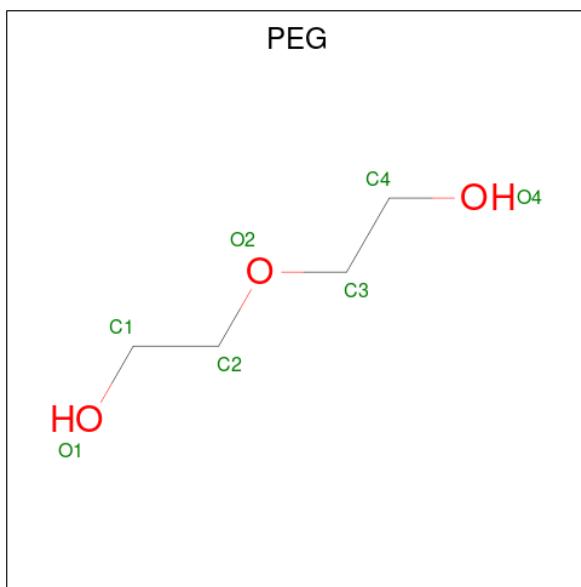
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0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

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

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



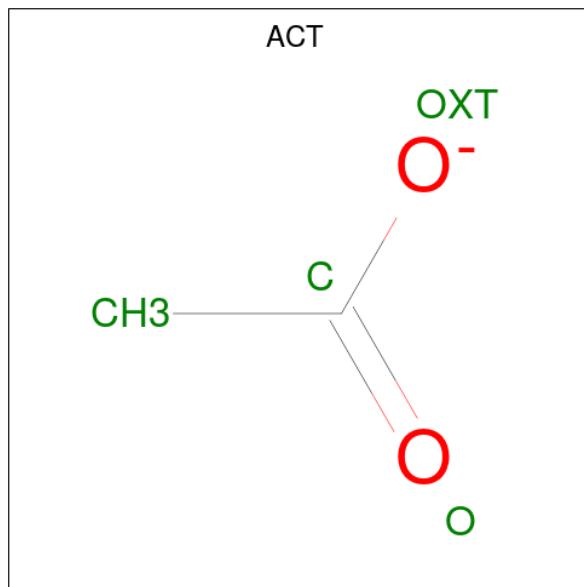
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



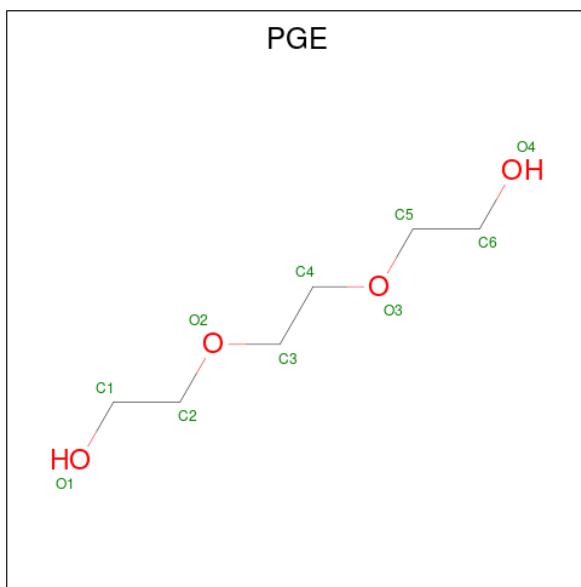
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



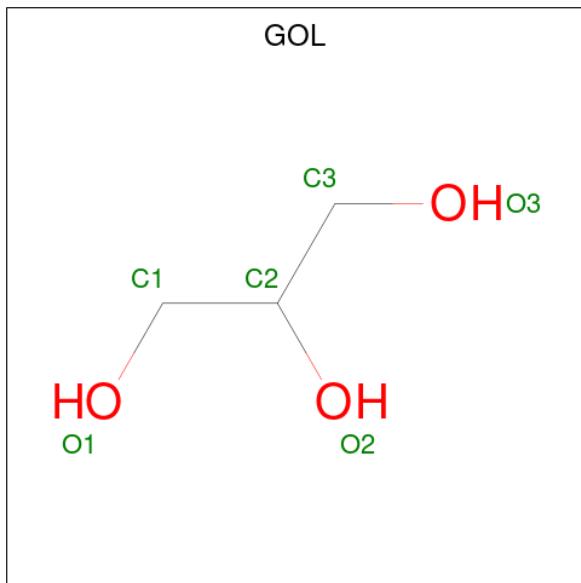
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 10 6 4	0	0
8	D	1	Total C O 10 6 4	0	0
8	D	1	Total C O 10 6 4	0	0

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



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

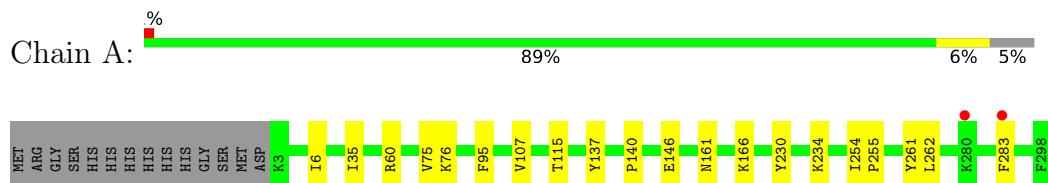
- Molecule 10 is water.

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

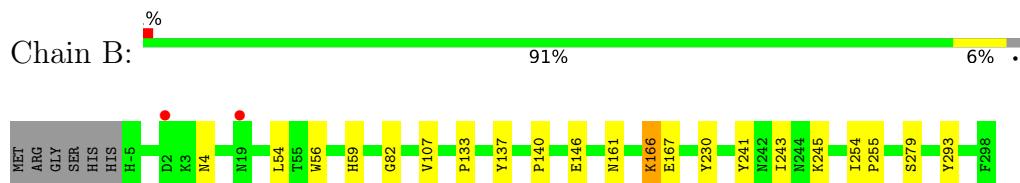
3 Residue-property plots

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

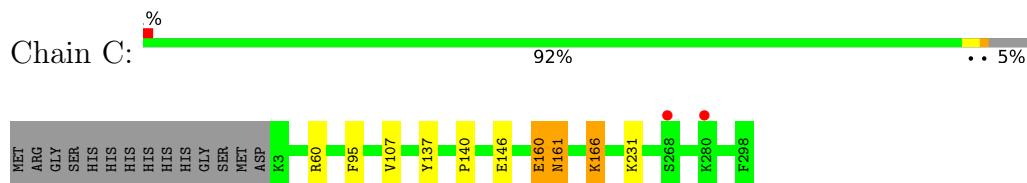
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



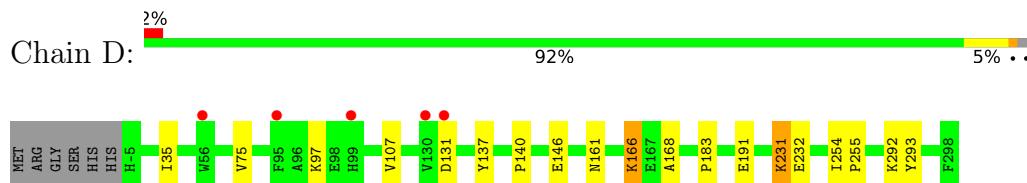
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



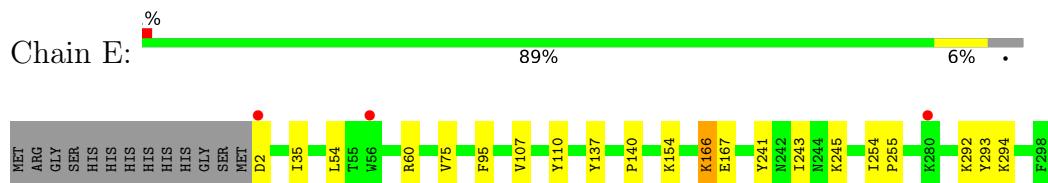
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



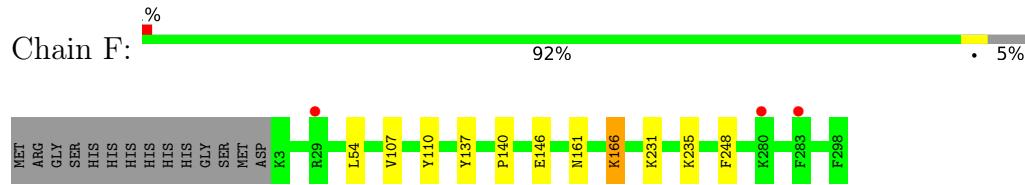
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.41 Å 225.29 Å 199.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 1.75 49.04 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-1.75) 99.9 (49.04-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.90 (at 1.75 Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R , R_{free}	0.157 , 0.185 0.159 , 0.187	Depositor DCC
R_{free} test set	9509 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.1	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15441	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, ACT, 3VN, MG, PG4, GOL, PGE, KPI, 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	0.45	0/2315	0.58	0/3129
1	B	0.46	1/2385 (0.0%)	0.58	0/3223
1	C	0.51	0/2315	0.60	0/3129
1	D	0.47	0/2397	0.60	0/3239
1	E	0.45	1/2323 (0.0%)	0.58	0/3140
1	F	0.42	0/2309	0.60	0/3121
All	All	0.46	2/14044 (0.0%)	0.59	0/18981

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	167	GLU	CD-OE2	-5.37	1.19	1.25
1	B	167	GLU	CD-OE1	-5.11	1.20	1.25

There are no bond angle outliers.

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	2286	0	2322	12	0
1	B	2351	0	2374	18	0
1	C	2285	0	2322	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2363	0	2382	11	0
1	E	2293	0	2326	18	0
1	F	2284	0	2321	8	0
2	A	22	0	28	1	0
2	B	22	0	28	1	0
2	D	22	0	28	1	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	5	0	0	0	0
3	F	4	0	0	0	0
4	A	13	0	18	0	0
4	B	13	0	18	0	0
4	C	13	0	18	0	0
4	D	13	0	18	1	0
4	E	13	0	18	3	0
4	F	13	0	18	0	0
5	A	40	0	60	2	0
5	B	20	0	30	6	0
5	C	24	0	36	0	0
5	D	16	0	24	1	0
5	E	24	0	36	1	0
5	F	8	0	12	1	0
6	A	14	0	20	0	0
6	B	21	0	30	3	0
6	C	7	0	10	2	0
6	D	7	0	10	0	0
6	E	7	0	10	1	0
6	F	14	0	20	0	0
7	A	8	0	6	1	0
7	B	8	0	6	0	0
7	D	16	0	12	0	0
7	E	4	0	3	1	0
7	F	16	0	12	0	0
8	B	10	0	14	0	0
8	D	20	0	28	3	0
8	E	10	0	14	3	0
9	C	6	0	8	0	0
10	A	184	0	0	0	0
10	B	192	0	0	4	0
10	C	170	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	201	0	0	1	0
10	E	198	0	0	4	0
10	F	171	0	0	2	0
All	All	15441	0	14640	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:KPI:H1B	10:B:581:HOH:O	1.73	0.88
1:D:166:KPI:H1A	10:D:444:HOH:O	1.79	0.81
1:B:279:SER:HB3	6:B:313:PEG:H42	1.64	0.80
1:C:160:GLU:CD	1:C:160:GLU:H	1.89	0.75
1:C:166:KPI:H1A	10:C:428:HOH:O	1.86	0.75
1:F:166:KPI:H1A	10:F:432:HOH:O	1.95	0.67
1:D:183:PRO:HD2	8:D:314:PGE:H32	1.78	0.65
1:C:60:ARG:HD3	6:C:310:PEG:H32	1.78	0.64
1:E:154:LYS:HZ2	4:E:306:PG4:H51	1.63	0.62
1:A:261:TYR:O	7:A:319:ACT:H1	2.00	0.62
1:E:294:LYS:HZ2	8:E:315:PGE:H22	1.63	0.61
1:E:166:KPI:H1A	10:E:461:HOH:O	2.00	0.61
8:D:314:PGE:H2	8:D:314:PGE:H52	1.85	0.58
1:A:234:LYS:HD3	5:B:308:EDO:H22	1.86	0.57
1:D:140:PRO:HG3	1:D:146:GLU:OE2	2.05	0.55
1:B:82:GLY:O	5:B:306:EDO:H22	2.07	0.55
1:B:161:ASN:OD1	1:B:161:ASN:N	2.40	0.55
6:E:313:PEG:H32	10:E:519:HOH:O	2.08	0.54
1:B:59:HIS:HE1	5:B:306:EDO:H12	1.72	0.53
5:A:308:EDO:H12	10:F:546:HOH:O	2.07	0.53
1:A:262:LEU:HD21	1:A:283:PHE:CZ	2.44	0.52
1:E:294:LYS:NZ	8:E:315:PGE:H22	2.24	0.52
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.91	0.52
1:B:59:HIS:CE1	5:B:306:EDO:H12	2.46	0.51
1:A:140:PRO:HG3	1:A:146:GLU:OE1	2.11	0.51
1:D:292:LYS:HG2	1:D:293:TYR:CE2	2.46	0.51
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.92	0.51
1:E:60:ARG:HD2	1:E:95:PHE:CE2	2.45	0.51
1:C:161:ASN:OD1	1:C:161:ASN:N	2.40	0.50
1:A:6:ILE:HG12	1:A:76:LYS:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.93	0.50
1:A:161:ASN:OD1	1:A:161:ASN:N	2.41	0.50
1:B:140:PRO:HG3	1:B:146:GLU:OE1	2.12	0.49
1:B:54:LEU:O	2:B:301:3VN:H9	2.13	0.49
1:E:154:LYS:NZ	4:E:306:PG4:H51	2.28	0.48
8:D:314:PGE:H52	8:D:314:PGE:C2	2.43	0.48
4:D:303:PG4:H11	5:D:307:EDO:O1	2.14	0.48
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.95	0.48
1:C:140:PRO:HG3	1:C:146:GLU:OE1	2.14	0.48
1:F:248:PHE:HE2	5:F:306:EDO:H22	1.79	0.47
1:F:140:PRO:HG3	1:F:146:GLU:OE1	2.15	0.47
1:E:2:ASP:N	10:E:405:HOH:O	2.48	0.47
1:F:161:ASN:OD1	1:F:161:ASN:N	2.48	0.47
1:D:231:LYS:HE2	1:D:232:GLU:OE2	2.14	0.46
1:E:294:LYS:HZ2	8:E:315:PGE:C2	2.28	0.46
1:B:4:ASN:HB2	1:B:133:PRO:HG3	1.97	0.46
2:D:301:3VN:H9	1:E:54:LEU:O	2.14	0.46
1:E:60:ARG:HB3	1:E:95:PHE:CZ	2.51	0.46
1:A:60:ARG:HB3	1:A:95:PHE:CZ	2.52	0.45
5:B:306:EDO:H21	10:C:461:HOH:O	2.17	0.45
1:B:56:TRP:HE1	6:B:311:PEG:H21	1.81	0.45
2:A:301:3VN:H23	1:F:54:LEU:O	2.16	0.45
1:D:161:ASN:OD1	1:D:161:ASN:N	2.48	0.45
1:F:231:LYS:C	1:F:231:LYS:HD3	2.38	0.44
1:B:166:KPI:H1A	10:B:439:HOH:O	2.17	0.44
1:E:241:TYR:CE2	1:E:245:LYS:HG3	2.52	0.44
1:E:292:LYS:HD2	1:E:292:LYS:HA	1.70	0.44
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.99	0.44
5:B:310:EDO:H21	10:B:536:HOH:O	2.17	0.44
6:C:310:PEG:H42	6:C:310:PEG:H21	1.61	0.44
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.99	0.44
5:E:309:EDO:H11	10:E:535:HOH:O	2.17	0.43
1:B:243:ILE:HB	1:B:293:TYR:CE2	2.54	0.43
1:B:254:ILE:HB	1:B:255:PRO:HD3	2.00	0.43
1:D:97:LYS:NZ	1:D:131:ASP:OD1	2.29	0.43
1:A:115:THR:HA	5:A:308:EDO:H22	2.00	0.43
1:D:168:ALA:HA	1:D:191:GLU:HG3	2.01	0.43
1:B:279:SER:HB3	6:B:313:PEG:C4	2.41	0.42
1:B:166:KPI:C1	10:B:581:HOH:O	2.49	0.42
1:E:243:ILE:HB	1:E:293:TYR:CE1	2.54	0.42
1:E:35:ILE:HG12	1:E:75:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:PRO:HB2	7:E:314:ACT:H1	2.01	0.42
1:C:60:ARG:HB3	1:C:95:PHE:CZ	2.54	0.42
1:E:254:ILE:HB	1:E:255:PRO:HD3	2.01	0.41
1:F:231:LYS:HE3	1:F:235:LYS:NZ	2.35	0.41
1:D:254:ILE:HB	1:D:255:PRO:HD3	2.02	0.41
1:A:230:TYR:HD2	1:B:230:TYR:CD2	2.39	0.41
1:A:254:ILE:HB	1:A:255:PRO:HD3	2.01	0.41
1:E:154:LYS:HD3	4:E:306:PG4:H22	2.03	0.41
1:D:35:ILE:HG12	1:D:75:VAL:HG21	2.02	0.41
1:B:241:TYR:CE2	1:B:245:LYS:HG3	2.56	0.40
1:A:35:ILE:HG12	1:A:75:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/310 (95%)	289 (98%)	5 (2%)	0	100 100
1	B	302/310 (97%)	297 (98%)	5 (2%)	0	100 100
1	C	294/310 (95%)	289 (98%)	5 (2%)	0	100 100
1	D	303/310 (98%)	298 (98%)	5 (2%)	0	100 100
1	E	295/310 (95%)	291 (99%)	4 (1%)	0	100 100
1	F	293/310 (94%)	287 (98%)	6 (2%)	0	100 100
All	All	1781/1860 (96%)	1751 (98%)	30 (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	249/260 (96%)	249 (100%)	0	100 100
1	B	256/260 (98%)	256 (100%)	0	100 100
1	C	249/260 (96%)	246 (99%)	3 (1%)	71 56
1	D	257/260 (99%)	256 (100%)	1 (0%)	91 87
1	E	250/260 (96%)	249 (100%)	1 (0%)	91 87
1	F	248/260 (95%)	247 (100%)	1 (0%)	91 87
All	All	1509/1560 (97%)	1503 (100%)	6 (0%)	91 87

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

Mol	Chain	Res	Type
1	C	160	GLU
1	C	161	ASN
1	C	231	LYS
1	D	231	LYS
1	E	110	TYR
1	F	110	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	B	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 (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	KPI	B	166	1	11,13,14	1.38	1 (9%)	10,15,17	2.99	5 (50%)
1	KPI	A	166	1	11,13,14	1.98	2 (18%)	10,15,17	2.45	4 (40%)
1	KPI	C	166	1	11,13,14	2.41	2 (18%)	10,15,17	2.95	6 (60%)
1	KPI	F	166	1	11,13,14	1.52	2 (18%)	10,15,17	2.44	2 (20%)
1	KPI	E	166	1	11,13,14	1.97	2 (18%)	10,15,17	2.35	1 (10%)
1	KPI	D	166	1	11,13,14	1.26	1 (9%)	10,15,17	2.42	3 (30%)

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	CX2-CX1	7.03	1.58	1.49
1	E	166	KPI	CX2-CX1	5.54	1.56	1.49
1	A	166	KPI	CX2-CX1	5.23	1.56	1.49
1	F	166	KPI	CX2-CX1	3.74	1.54	1.49
1	B	166	KPI	CX2-CX1	3.64	1.54	1.49
1	D	166	KPI	CX2-CX1	3.16	1.53	1.49
1	A	166	KPI	O2-CX2	2.94	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	O2-CX2	2.78	1.30	1.22
1	E	166	KPI	O2-CX2	2.19	1.28	1.22
1	F	166	KPI	O2-CX2	2.11	1.28	1.22

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	166	KPI	CE-NZ-CX1	6.63	139.78	121.70
1	F	166	KPI	CE-NZ-CX1	6.26	138.77	121.70
1	D	166	KPI	CE-NZ-CX1	6.19	138.56	121.70
1	C	166	KPI	CE-NZ-CX1	6.05	138.19	121.70
1	A	166	KPI	CE-NZ-CX1	5.60	136.96	121.70
1	B	166	KPI	CE-NZ-CX1	5.41	136.45	121.70
1	B	166	KPI	O2-CX2-CX1	-5.35	114.55	121.38
1	C	166	KPI	C1-CX1-CX2	3.54	121.60	118.17
1	A	166	KPI	C1-CX1-CX2	3.44	121.51	118.17
1	B	166	KPI	O1-CX2-CX1	3.20	123.29	116.35
1	C	166	KPI	CX2-CX1-NZ	3.07	122.46	114.98
1	C	166	KPI	O1-CX2-O2	-2.99	116.77	123.61
1	B	166	KPI	C1-CX1-CX2	2.78	120.86	118.17
1	C	166	KPI	C1-CX1-NZ	-2.75	115.92	123.11
1	C	166	KPI	O2-CX2-CX1	2.70	124.82	121.38
1	F	166	KPI	CX2-CX1-NZ	2.58	121.26	114.98
1	B	166	KPI	CX2-CX1-NZ	2.56	121.22	114.98
1	D	166	KPI	O2-CX2-CX1	-2.48	118.21	121.38
1	A	166	KPI	CX2-CX1-NZ	2.44	120.92	114.98
1	D	166	KPI	CX2-CX1-NZ	2.17	120.27	114.98
1	A	166	KPI	C1-CX1-NZ	-2.13	117.54	123.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 89 ligands modelled in this entry, 19 are monoatomic - leaving 70 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	307	-	3,3,3	0.48	0	2,2,2	0.62	0
5	EDO	E	309	-	3,3,3	0.45	0	2,2,2	0.58	0
2	3VN	B	301	-	17,21,21	0.76	0	18,28,28	1.13	1 (5%)
7	ACT	D	310	-	3,3,3	0.77	0	3,3,3	1.39	0
7	ACT	F	310	-	3,3,3	0.72	0	3,3,3	1.24	0
8	PGE	D	313	-	9,9,9	0.32	0	8,8,8	0.34	0
8	PGE	E	315	-	9,9,9	0.36	0	8,8,8	0.55	0
9	GOL	C	311	-	5,5,5	0.23	0	5,5,5	0.45	0
6	PEG	E	313	-	6,6,6	0.52	0	5,5,5	0.33	0
2	3VN	D	301	-	17,21,21	0.73	0	18,28,28	1.30	2 (11%)
6	PEG	D	308	-	6,6,6	0.45	0	5,5,5	0.23	0
5	EDO	A	308	-	3,3,3	0.42	0	2,2,2	0.59	0
5	EDO	C	305	-	3,3,3	0.42	0	2,2,2	0.63	0
5	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.64	0
5	EDO	C	308	-	3,3,3	0.49	0	2,2,2	0.16	0
5	EDO	A	309	-	3,3,3	0.42	0	2,2,2	0.34	0
7	ACT	A	320	-	3,3,3	0.75	0	3,3,3	1.42	0
5	EDO	D	305	-	3,3,3	0.40	0	2,2,2	0.36	0
7	ACT	D	312	-	3,3,3	0.77	0	3,3,3	1.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACT	B	314	-	3,3,3	0.81	0	3,3,3	1.37	0
4	PG4	B	305	-	12,12,12	0.51	0	11,11,11	0.21	0
5	EDO	D	306	-	3,3,3	0.63	0	2,2,2	0.03	0
4	PG4	E	306	-	12,12,12	0.51	0	11,11,11	0.45	0
5	EDO	A	314	-	3,3,3	0.50	0	2,2,2	0.16	0
5	EDO	F	307	-	3,3,3	0.57	0	2,2,2	0.22	0
6	PEG	A	318	-	6,6,6	0.43	0	5,5,5	0.41	0
5	EDO	C	304	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	E	310	-	3,3,3	0.54	0	2,2,2	0.28	0
4	PG4	F	305	-	12,12,12	0.54	0	11,11,11	0.35	0
6	PEG	A	317	-	6,6,6	0.49	0	5,5,5	0.32	0
6	PEG	B	311	-	6,6,6	0.47	0	5,5,5	0.40	0
2	3VN	A	301	-	17,21,21	0.74	0	18,28,28	1.11	1 (5%)
5	EDO	A	311	-	3,3,3	0.42	0	2,2,2	0.64	0
6	PEG	B	313	-	6,6,6	0.51	0	5,5,5	0.31	0
8	PGE	B	316	-	9,9,9	0.35	0	8,8,8	0.44	0
5	EDO	B	306	-	3,3,3	0.53	0	2,2,2	0.08	0
7	ACT	F	313	-	3,3,3	0.77	0	3,3,3	1.45	0
5	EDO	D	304	-	3,3,3	0.55	0	2,2,2	0.36	0
5	EDO	B	310	-	3,3,3	0.46	0	2,2,2	0.18	0
5	EDO	A	312	-	3,3,3	0.51	0	2,2,2	0.23	0
6	PEG	F	309	-	6,6,6	0.47	0	5,5,5	0.33	0
7	ACT	A	319	-	3,3,3	0.71	0	3,3,3	1.18	0
5	EDO	A	310	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	A	316	-	3,3,3	0.46	0	2,2,2	0.35	0
6	PEG	F	308	-	6,6,6	0.52	0	5,5,5	0.25	0
6	PEG	B	312	-	6,6,6	0.47	0	5,5,5	0.39	0
5	EDO	C	309	-	3,3,3	0.49	0	2,2,2	0.47	0
7	ACT	D	309	-	3,3,3	0.80	0	3,3,3	1.30	0
7	ACT	D	311	-	3,3,3	0.77	0	3,3,3	1.33	0
5	EDO	E	308	-	3,3,3	0.44	0	2,2,2	0.36	0
7	ACT	F	312	-	3,3,3	0.83	0	3,3,3	1.44	0
5	EDO	B	309	-	3,3,3	0.45	0	2,2,2	0.47	0
5	EDO	B	308	-	3,3,3	0.45	0	2,2,2	0.47	0
5	EDO	E	312	-	3,3,3	0.45	0	2,2,2	0.36	0
4	PG4	C	303	-	12,12,12	0.50	0	11,11,11	0.36	0
5	EDO	E	307	-	3,3,3	0.47	0	2,2,2	0.40	0
5	EDO	A	313	-	3,3,3	0.53	0	2,2,2	0.24	0
8	PGE	D	314	-	9,9,9	0.25	0	8,8,8	1.06	1 (12%)
6	PEG	C	310	-	6,6,6	0.46	0	5,5,5	0.34	0
7	ACT	B	315	-	3,3,3	0.78	0	3,3,3	1.44	0
4	PG4	D	303	-	12,12,12	0.52	0	11,11,11	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	315	-	3,3,3	0.42	0	2,2,2	0.47	0
5	EDO	F	306	-	3,3,3	0.48	0	2,2,2	0.43	0
7	ACT	E	314	-	3,3,3	0.79	0	3,3,3	1.46	0
7	ACT	F	311	-	3,3,3	0.76	0	3,3,3	1.44	0
5	EDO	B	307	-	3,3,3	0.46	0	2,2,2	0.44	0
5	EDO	C	307	-	3,3,3	0.50	0	2,2,2	0.34	0
5	EDO	E	311	-	3,3,3	0.62	0	2,2,2	0.12	0
5	EDO	A	307	-	3,3,3	0.59	0	2,2,2	0.34	0
4	PG4	A	306	-	12,12,12	0.53	0	11,11,11	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	307	-	-	0/1/1/1	-
5	EDO	E	309	-	-	1/1/1/1	-
2	3VN	B	301	-	-	10/29/31/31	-
8	PGE	D	313	-	-	2/7/7/7	-
8	PGE	E	315	-	-	1/7/7/7	-
9	GOL	C	311	-	-	0/4/4/4	-
6	PEG	E	313	-	-	3/4/4/4	-
2	3VN	D	301	-	-	10/29/31/31	-
6	PEG	D	308	-	-	1/4/4/4	-
5	EDO	A	308	-	-	1/1/1/1	-
5	EDO	C	305	-	-	1/1/1/1	-
5	EDO	C	306	-	-	1/1/1/1	-
5	EDO	C	308	-	-	1/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	D	305	-	-	0/1/1/1	-
4	PG4	B	305	-	-	1/10/10/10	-
5	EDO	D	306	-	-	0/1/1/1	-
4	PG4	E	306	-	-	7/10/10/10	-
5	EDO	A	314	-	-	0/1/1/1	-
5	EDO	F	307	-	-	0/1/1/1	-
6	PEG	A	318	-	-	3/4/4/4	-
5	EDO	C	304	-	-	0/1/1/1	-
5	EDO	E	310	-	-	0/1/1/1	-
4	PG4	F	305	-	-	1/10/10/10	-
6	PEG	A	317	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	B	311	-	-	1/4/4/4	-
2	3VN	A	301	-	-	8/29/31/31	-
5	EDO	A	311	-	-	0/1/1/1	-
6	PEG	B	313	-	-	2/4/4/4	-
8	PGE	B	316	-	-	3/7/7/7	-
5	EDO	B	306	-	-	1/1/1/1	-
5	EDO	D	304	-	-	0/1/1/1	-
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	A	312	-	-	0/1/1/1	-
6	PEG	F	309	-	-	1/4/4/4	-
5	EDO	A	310	-	-	0/1/1/1	-
5	EDO	A	316	-	-	0/1/1/1	-
6	PEG	F	308	-	-	0/4/4/4	-
6	PEG	B	312	-	-	3/4/4/4	-
5	EDO	C	309	-	-	0/1/1/1	-
5	EDO	E	308	-	-	1/1/1/1	-
5	EDO	B	309	-	-	0/1/1/1	-
5	EDO	B	308	-	-	1/1/1/1	-
5	EDO	E	312	-	-	1/1/1/1	-
4	PG4	C	303	-	-	1/10/10/10	-
5	EDO	E	307	-	-	0/1/1/1	-
5	EDO	A	313	-	-	1/1/1/1	-
8	PGE	D	314	-	-	4/7/7/7	-
6	PEG	C	310	-	-	4/4/4/4	-
4	PG4	D	303	-	-	0/10/10/10	-
5	EDO	A	315	-	-	1/1/1/1	-
5	EDO	F	306	-	-	1/1/1/1	-
5	EDO	B	307	-	-	1/1/1/1	-
5	EDO	C	307	-	-	1/1/1/1	-
5	EDO	E	311	-	-	0/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-
4	PG4	A	306	-	-	0/10/10/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	314	PGE	O4-C6-C5	-2.68	96.25	111.81
2	D	301	3VN	O05-C03-C02	2.48	120.36	113.70
2	B	301	3VN	C15-C16-C17	-2.42	105.97	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	3VN	O05-C03-C02	2.12	119.39	113.70
2	D	301	3VN	C16-C15-C13	-2.03	111.60	115.20

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	314	PGE	C3-C4-O3-C5
8	D	313	PGE	O2-C3-C4-O3
4	E	306	PG4	C5-C6-O4-C7
6	C	310	PEG	C4-C3-O2-C2
4	E	306	PG4	O2-C3-C4-O3
8	B	316	PGE	O2-C3-C4-O3
6	A	318	PEG	C4-C3-O2-C2
6	C	310	PEG	O2-C3-C4-O4
5	C	306	EDO	O1-C1-C2-O2
6	B	313	PEG	O1-C1-C2-O2
6	A	318	PEG	O1-C1-C2-O2
5	B	306	EDO	O1-C1-C2-O2
5	C	307	EDO	O1-C1-C2-O2
5	E	308	EDO	O1-C1-C2-O2
5	E	312	EDO	O1-C1-C2-O2
4	E	306	PG4	O1-C1-C2-O2
4	E	306	PG4	O4-C7-C8-O5
5	F	306	EDO	O1-C1-C2-O2
8	E	315	PGE	O2-C3-C4-O3
2	B	301	3VN	C16-C17-C18-N19
2	D	301	3VN	C15-C16-C17-C18
5	B	310	EDO	O1-C1-C2-O2
6	E	313	PEG	O1-C1-C2-O2
6	E	313	PEG	O2-C3-C4-O4
4	B	305	PG4	C8-C7-O4-C6
6	B	312	PEG	C4-C3-O2-C2
4	F	305	PG4	C1-C2-O2-C3
6	D	308	PEG	C4-C3-O2-C2
6	E	313	PEG	C1-C2-O2-C3
6	B	313	PEG	O2-C3-C4-O4
2	A	301	3VN	C06-C02-C03-O05
2	A	301	3VN	C11-C02-C03-O04
2	A	301	3VN	C11-C02-C03-O05
2	A	301	3VN	C12-C13-C20-O21
2	A	301	3VN	C12-C13-C20-O22

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Mol	Chain	Res	Type	Atoms
2	B	301	3VN	C11-C02-C03-O04
2	B	301	3VN	C11-C02-C03-O05
2	B	301	3VN	C12-C13-C20-O21
2	B	301	3VN	C12-C13-C20-O22
2	B	301	3VN	C15-C13-C20-O22
2	D	301	3VN	C11-C02-C03-O04
2	D	301	3VN	C11-C02-C03-O05
2	D	301	3VN	C12-C13-C20-O21
2	D	301	3VN	C12-C13-C20-O22
6	A	318	PEG	O2-C3-C4-O4
5	C	308	EDO	O1-C1-C2-O2
8	D	314	PGE	O2-C3-C4-O3
6	B	312	PEG	O1-C1-C2-O2
8	D	314	PGE	O3-C5-C6-O4
6	B	311	PEG	C4-C3-O2-C2
5	A	307	EDO	O1-C1-C2-O2
5	A	313	EDO	O1-C1-C2-O2
8	D	314	PGE	C4-C3-O2-C2
4	E	306	PG4	C1-C2-O2-C3
4	C	303	PG4	O4-C7-C8-O5
4	E	306	PG4	C3-C4-O3-C5
6	C	310	PEG	C1-C2-O2-C3
6	C	310	PEG	O1-C1-C2-O2
6	F	309	PEG	O2-C3-C4-O4
6	B	312	PEG	O2-C3-C4-O4
2	B	301	3VN	C15-C16-C17-C18
5	A	315	EDO	O1-C1-C2-O2
5	B	307	EDO	O1-C1-C2-O2
5	B	308	EDO	O1-C1-C2-O2
5	E	309	EDO	O1-C1-C2-O2
8	D	313	PGE	C1-C2-O2-C3
8	B	316	PGE	C3-C4-O3-C5
8	B	316	PGE	O3-C5-C6-O4
2	A	301	3VN	C06-C02-C03-O04
2	A	301	3VN	C15-C13-C20-O21
2	A	301	3VN	C15-C13-C20-O22
2	B	301	3VN	C06-C02-C03-O04
2	B	301	3VN	C06-C02-C03-O05
2	B	301	3VN	C15-C13-C20-O21
2	D	301	3VN	C06-C02-C03-O04
2	D	301	3VN	C06-C02-C03-O05
2	D	301	3VN	C15-C13-C20-O21

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Mol	Chain	Res	Type	Atoms
2	D	301	3VN	C15-C13-C20-O22
5	A	308	EDO	O1-C1-C2-O2
5	C	305	EDO	O1-C1-C2-O2
2	D	301	3VN	C16-C17-C18-N19
4	E	306	PG4	O3-C5-C6-O4

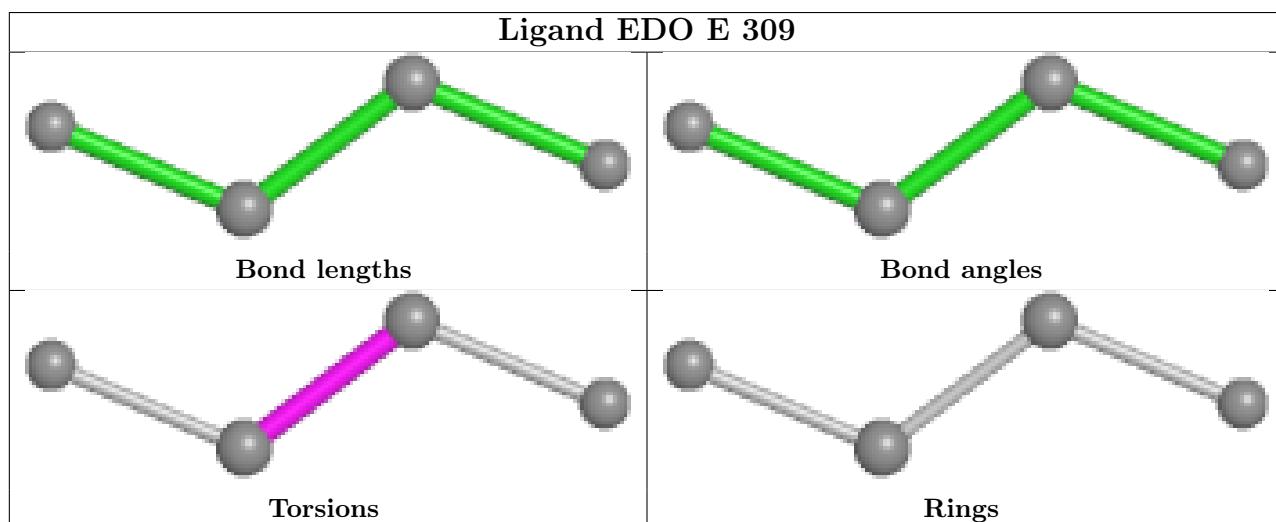
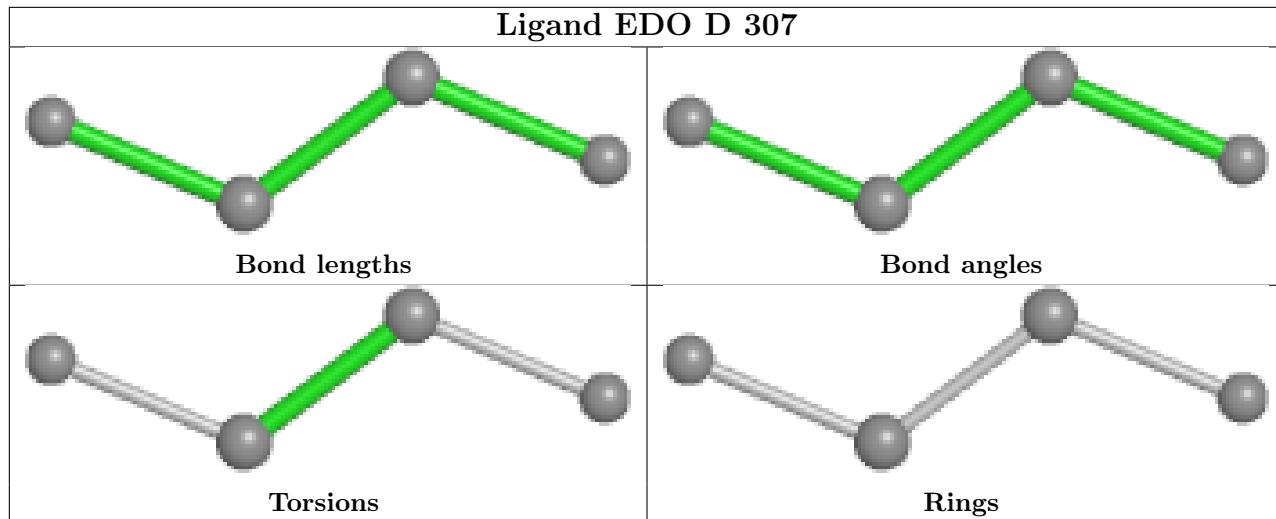
There are no ring outliers.

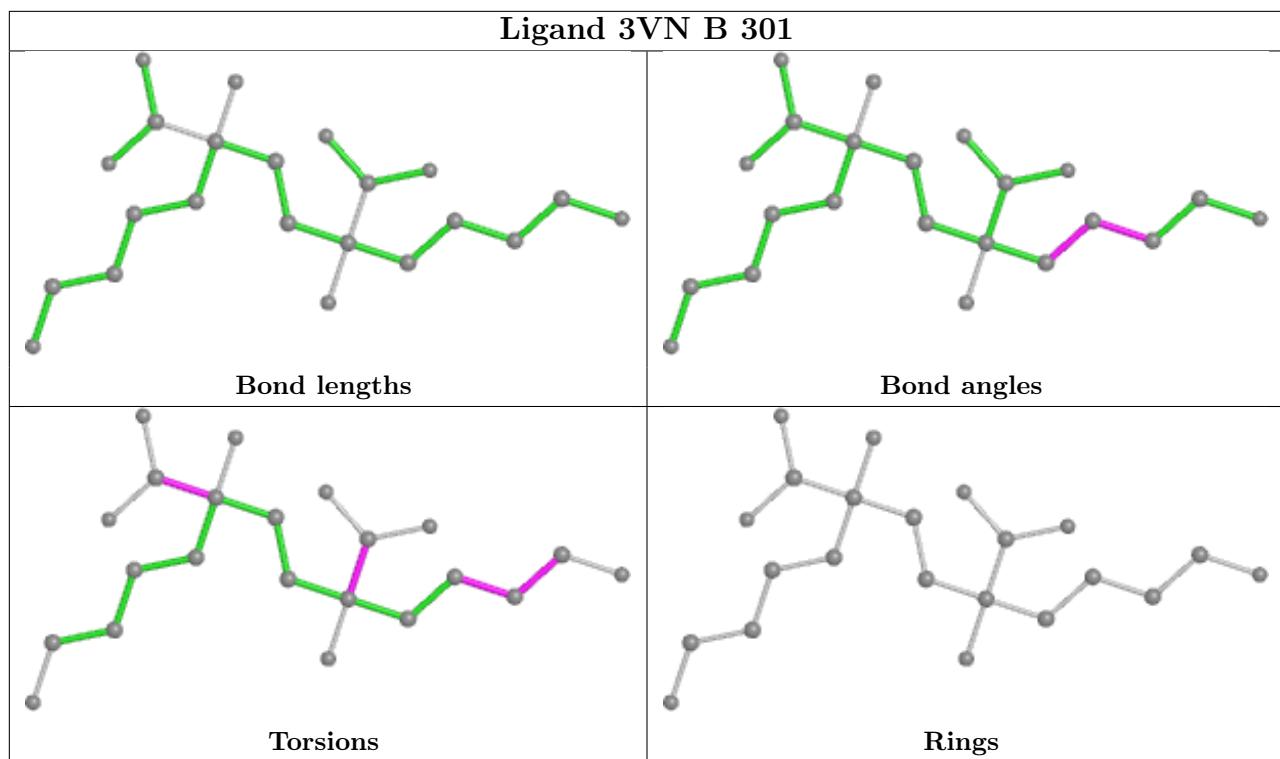
20 monomers are involved in 31 short contacts:

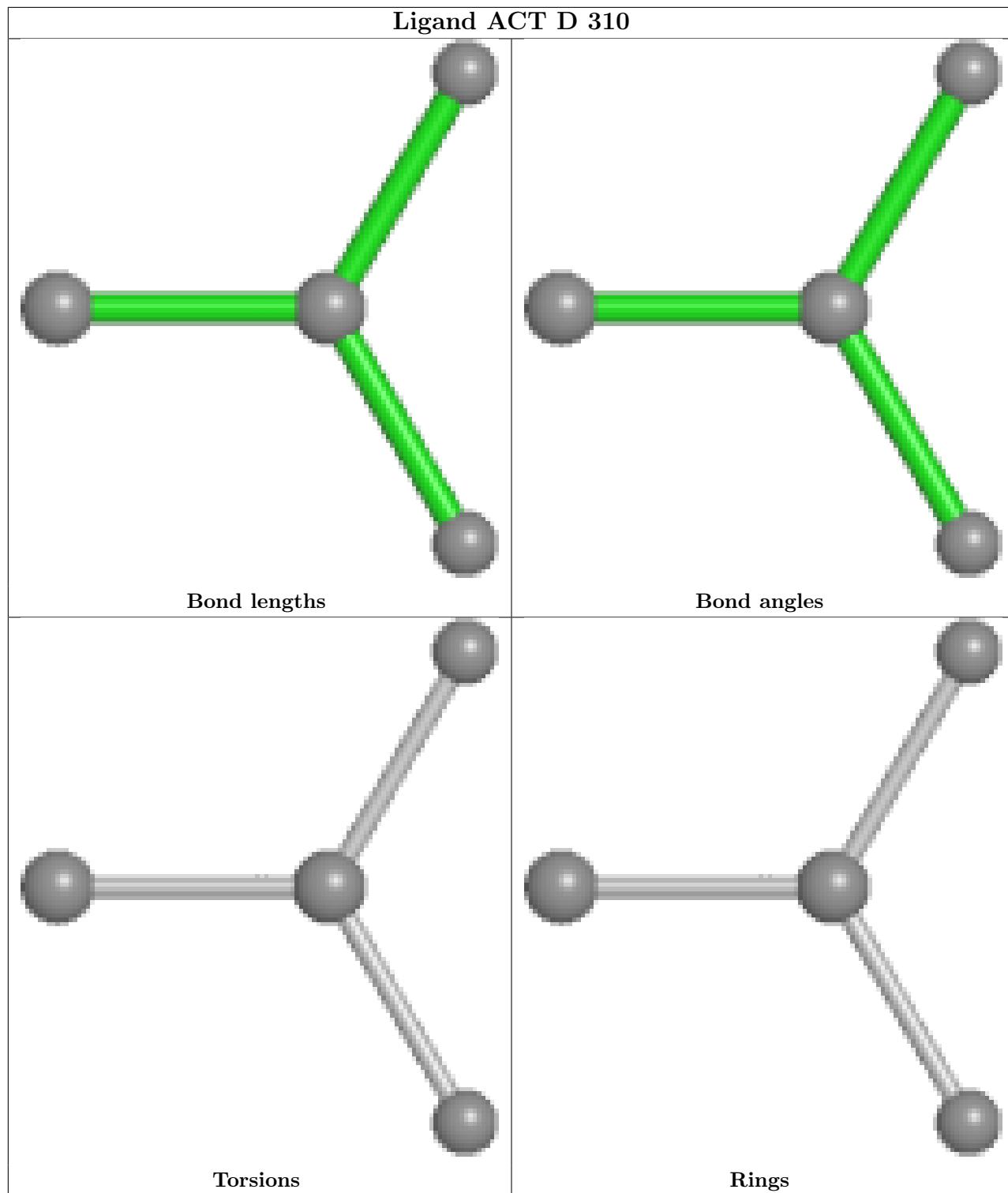
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	307	EDO	1	0
5	E	309	EDO	1	0
2	B	301	3VN	1	0
8	E	315	PGE	3	0
6	E	313	PEG	1	0
2	D	301	3VN	1	0
5	A	308	EDO	2	0
4	E	306	PG4	3	0
6	B	311	PEG	1	0
2	A	301	3VN	1	0
6	B	313	PEG	2	0
5	B	306	EDO	4	0
5	B	310	EDO	1	0
7	A	319	ACT	1	0
5	B	308	EDO	1	0
8	D	314	PGE	3	0
6	C	310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

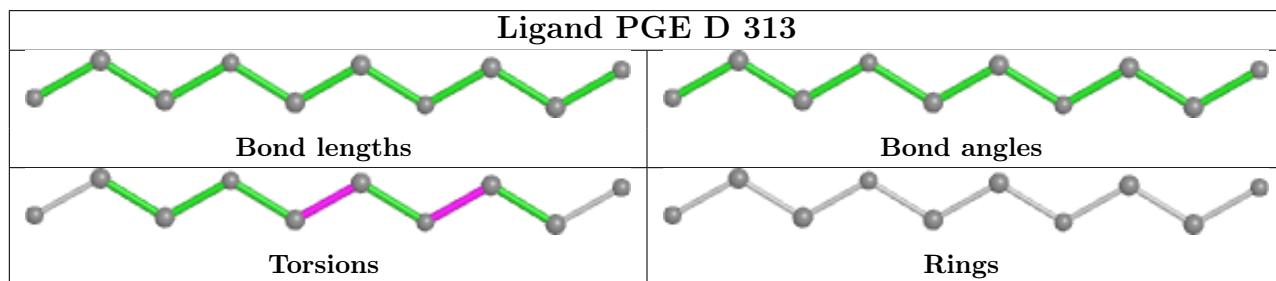
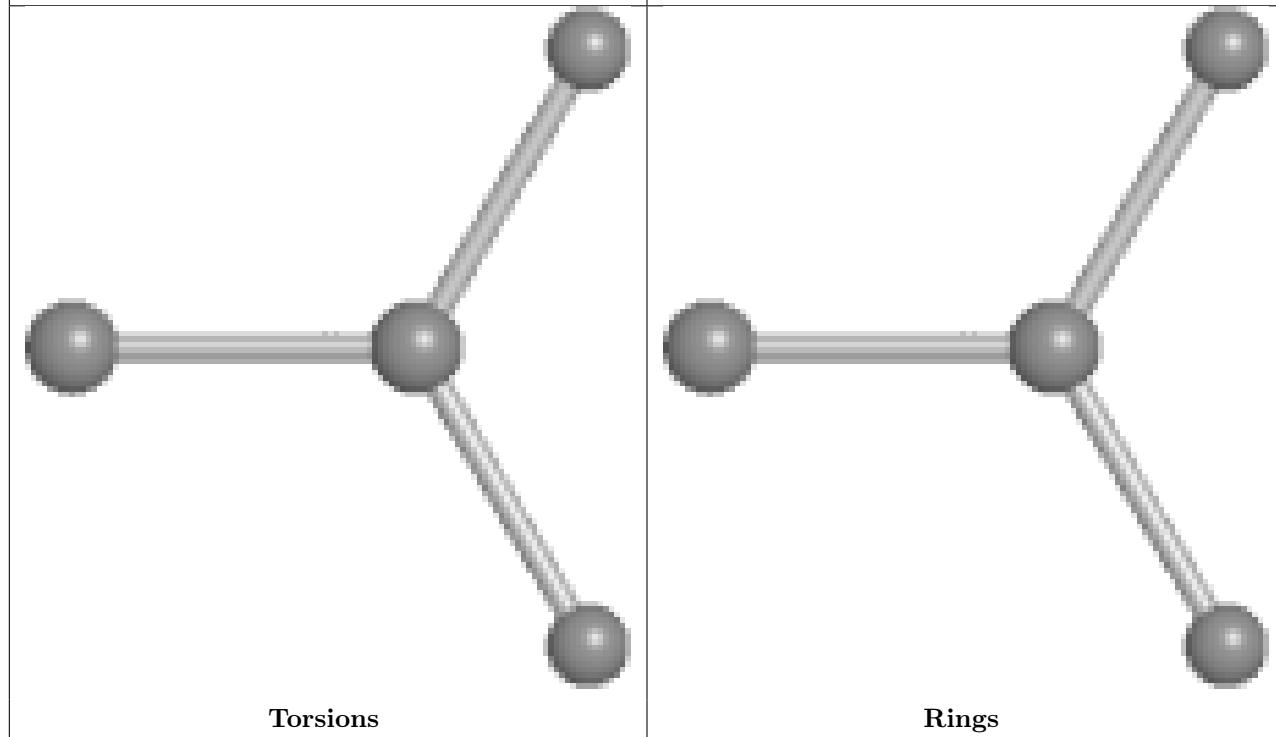
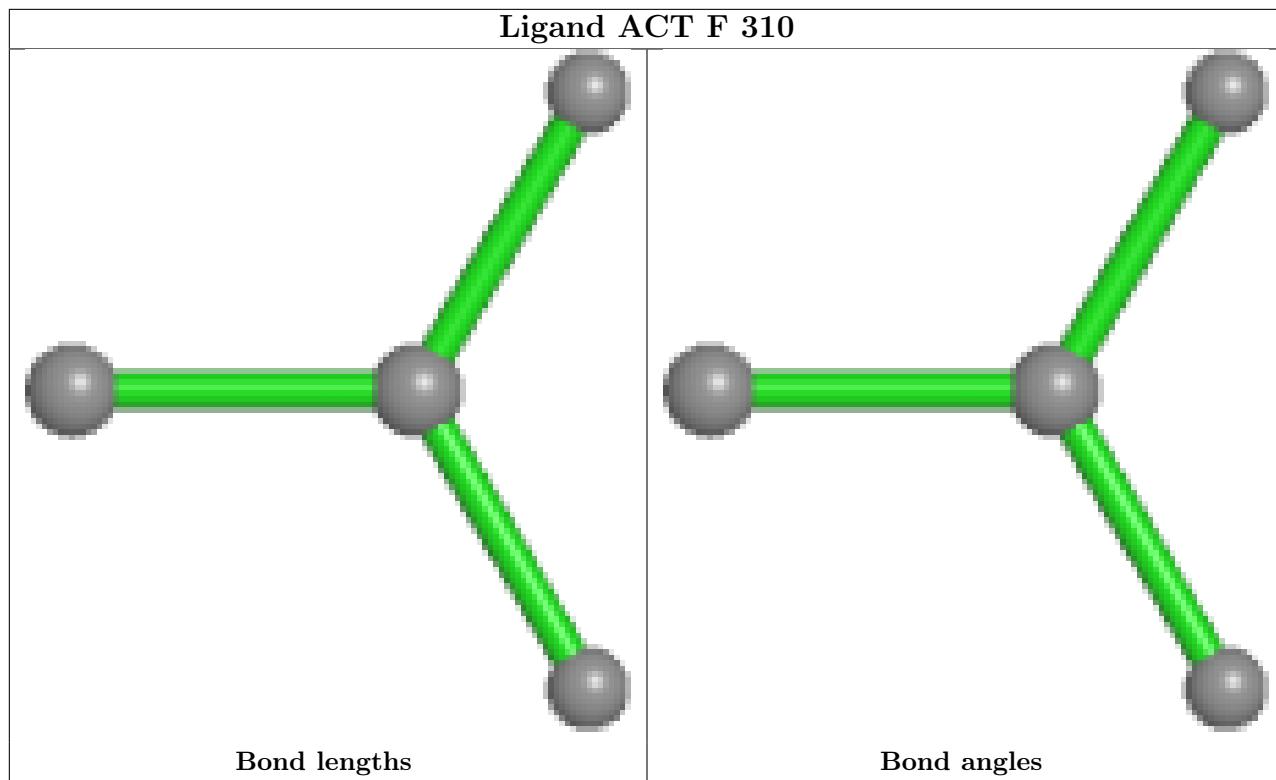
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

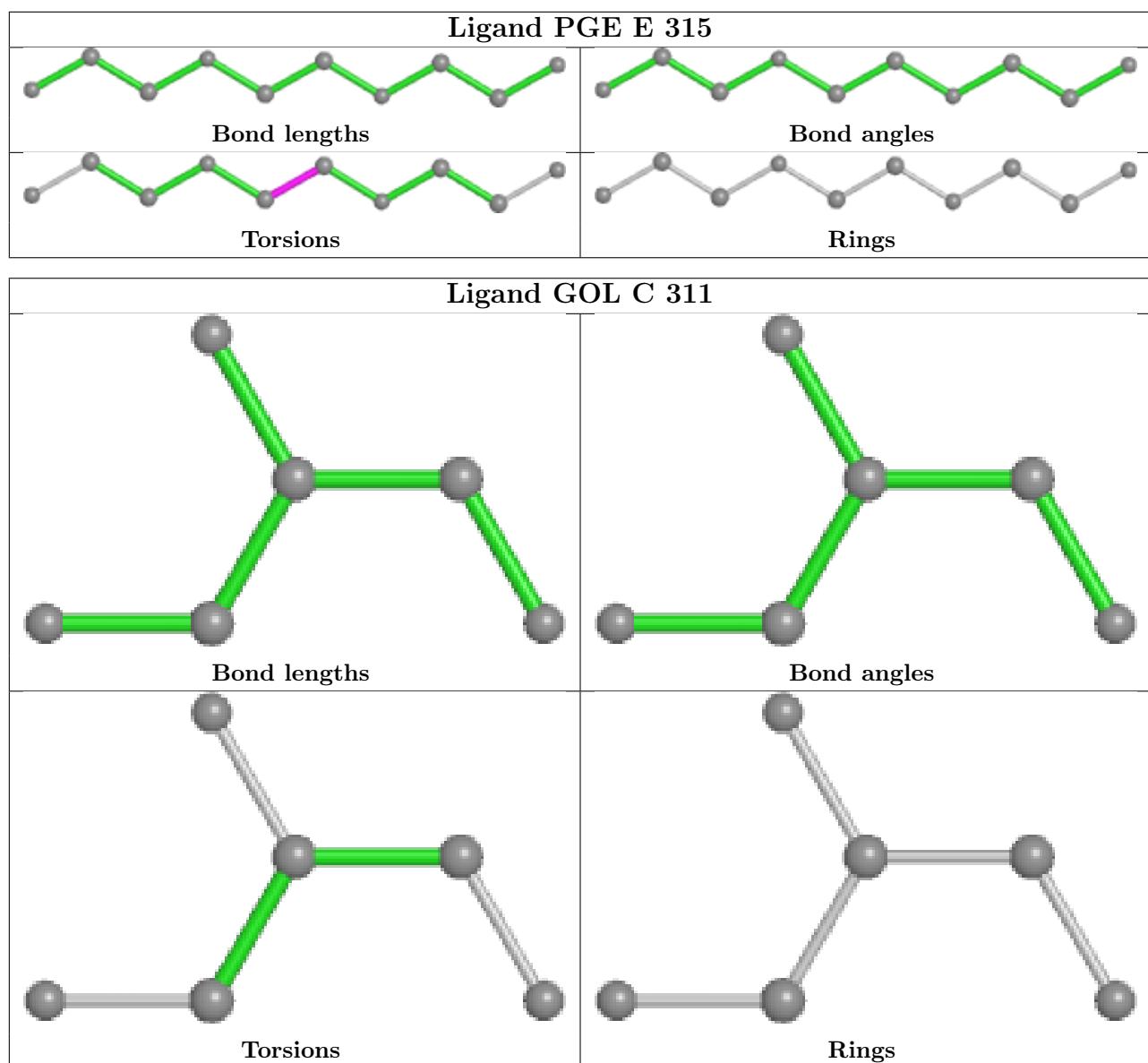
equivalents in the CSD to analyse the geometry.

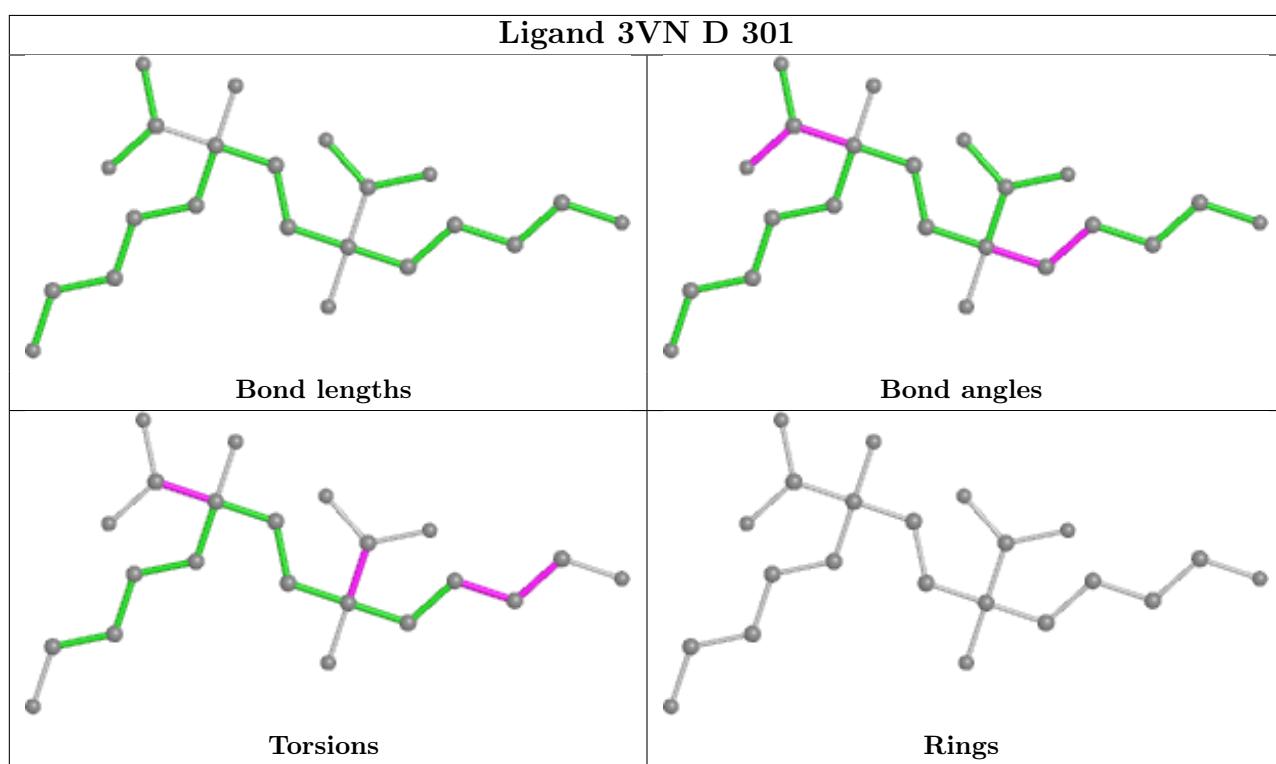
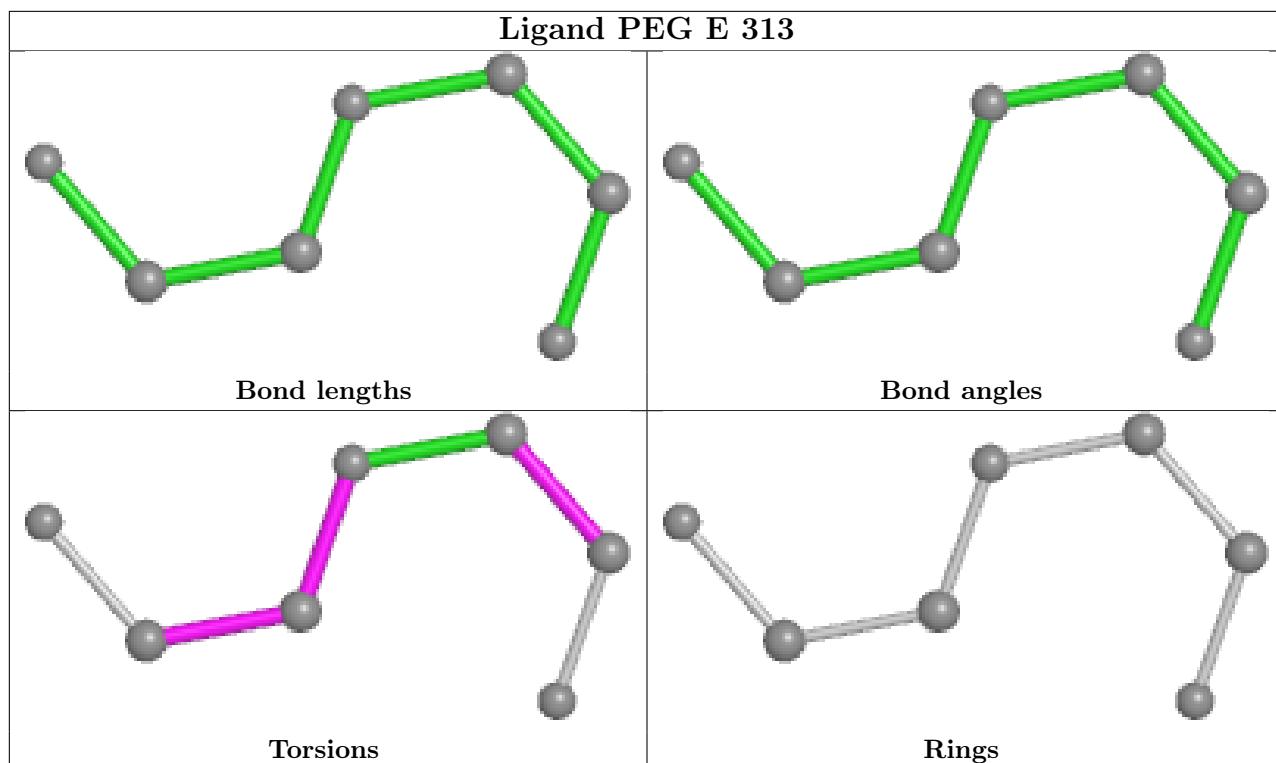


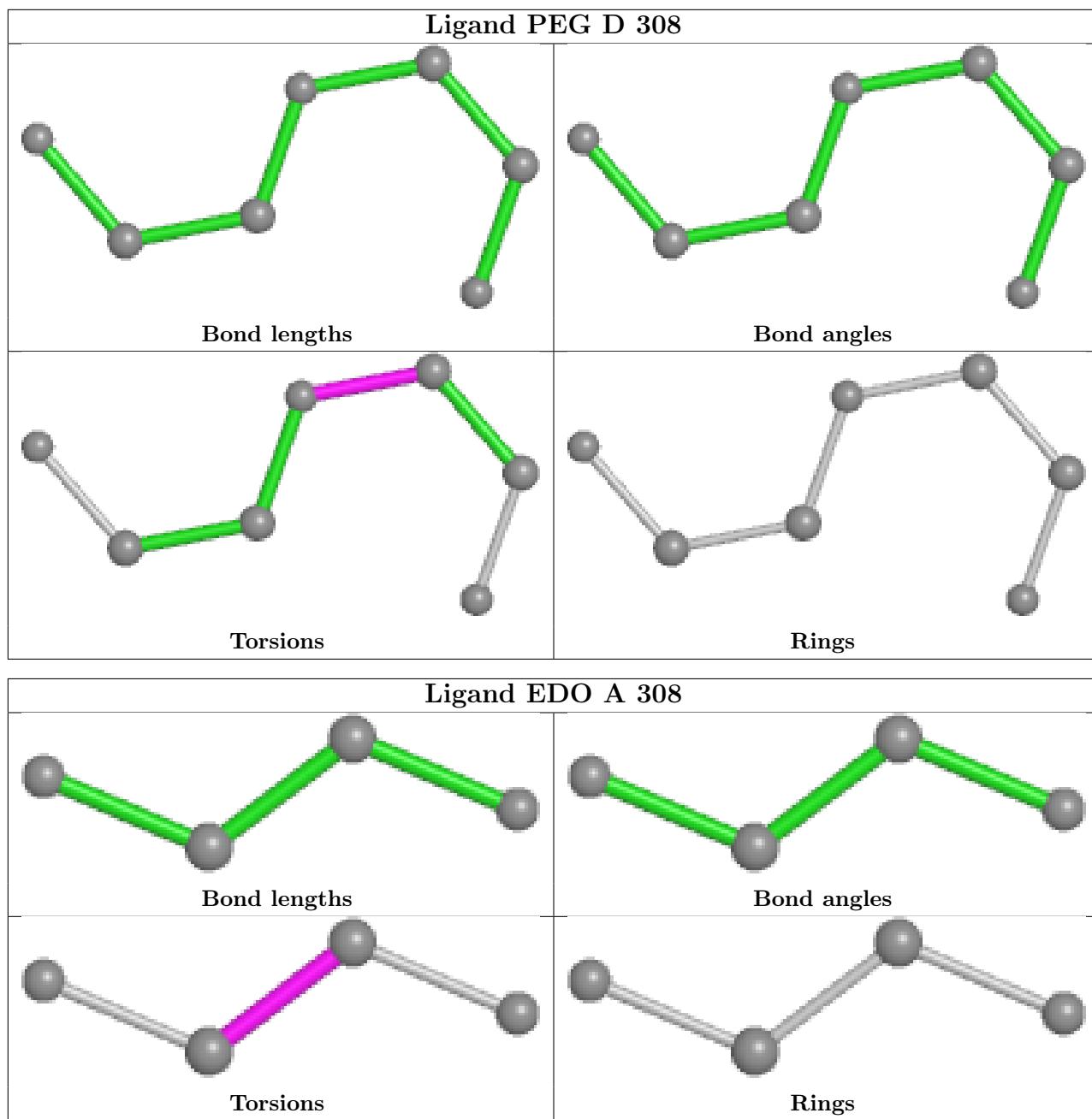


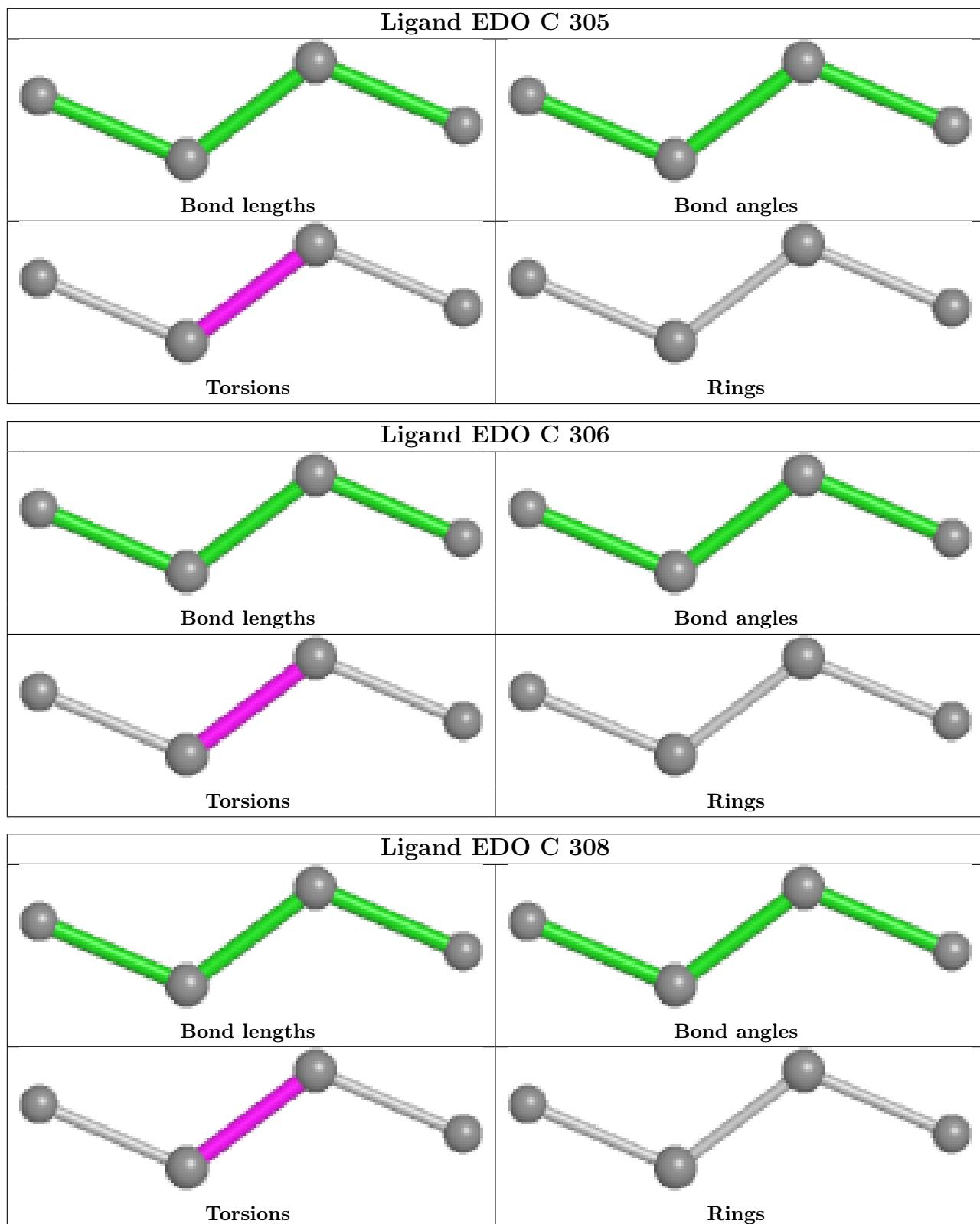


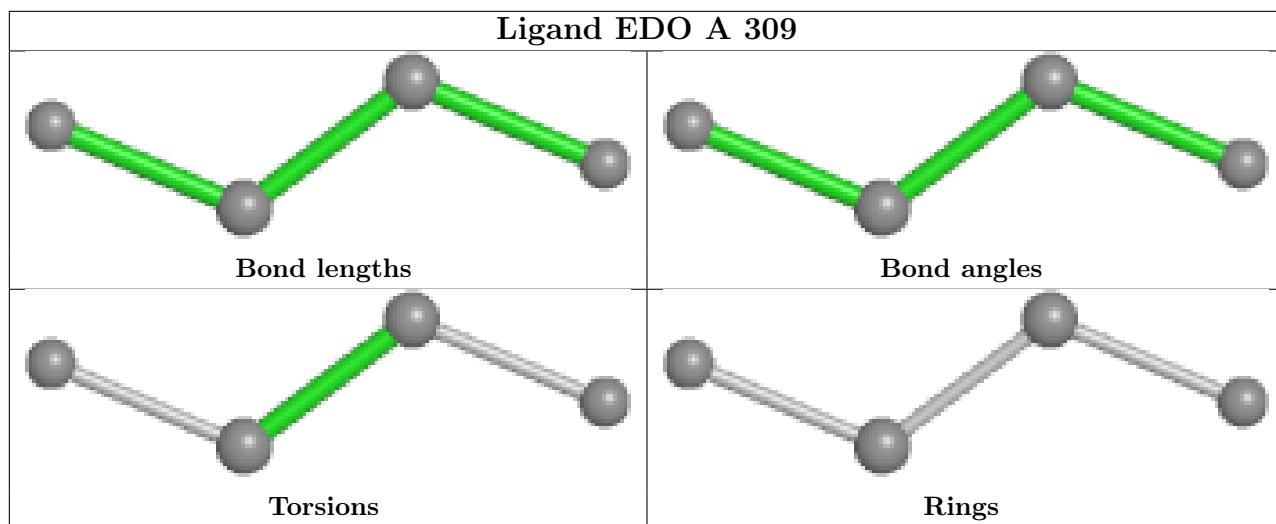


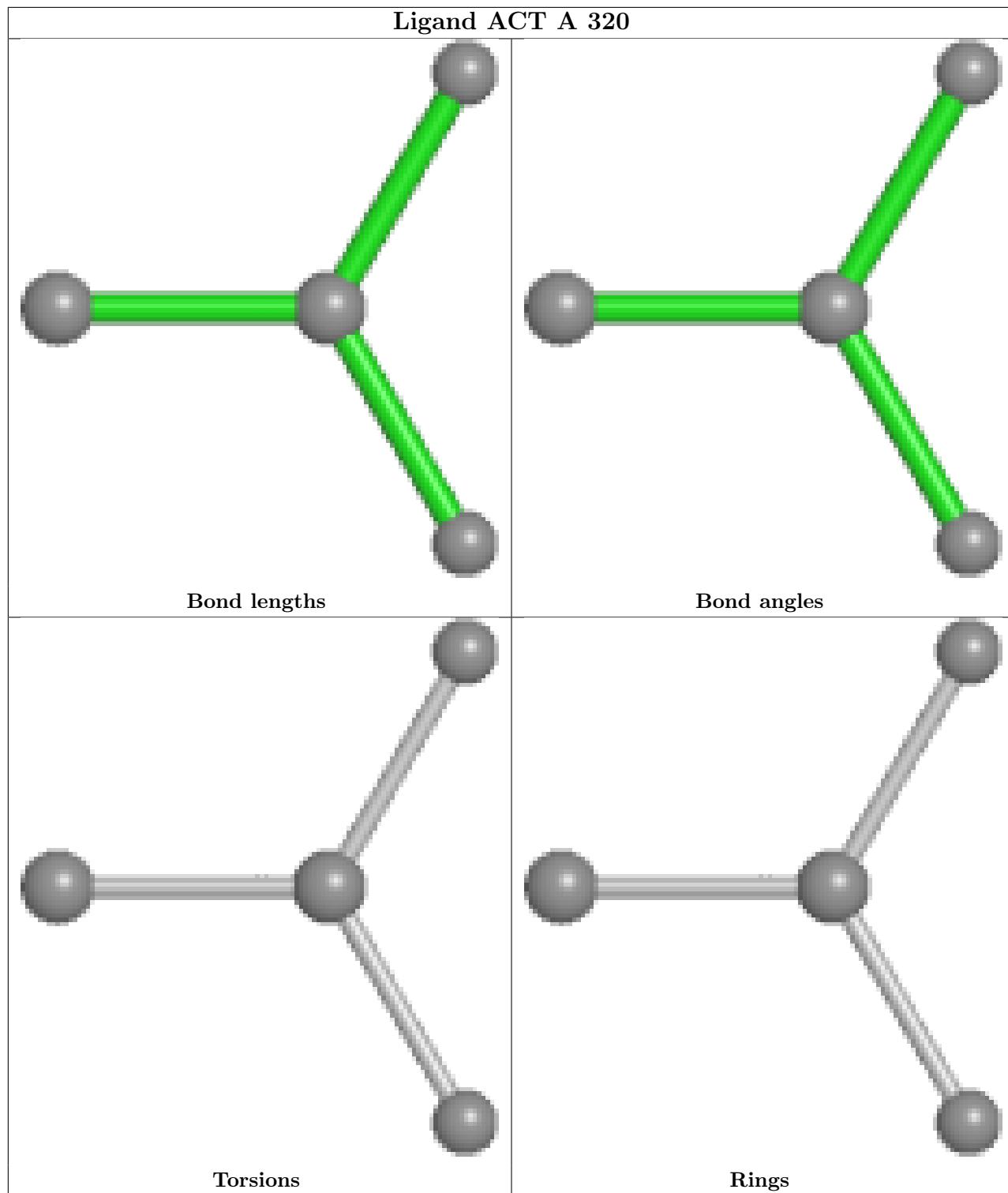


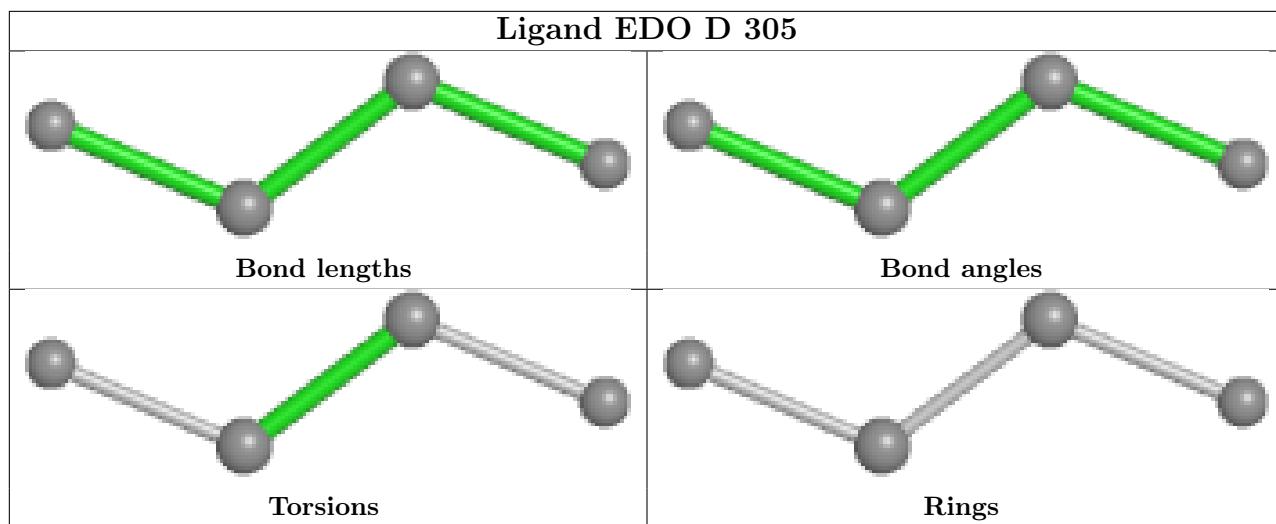


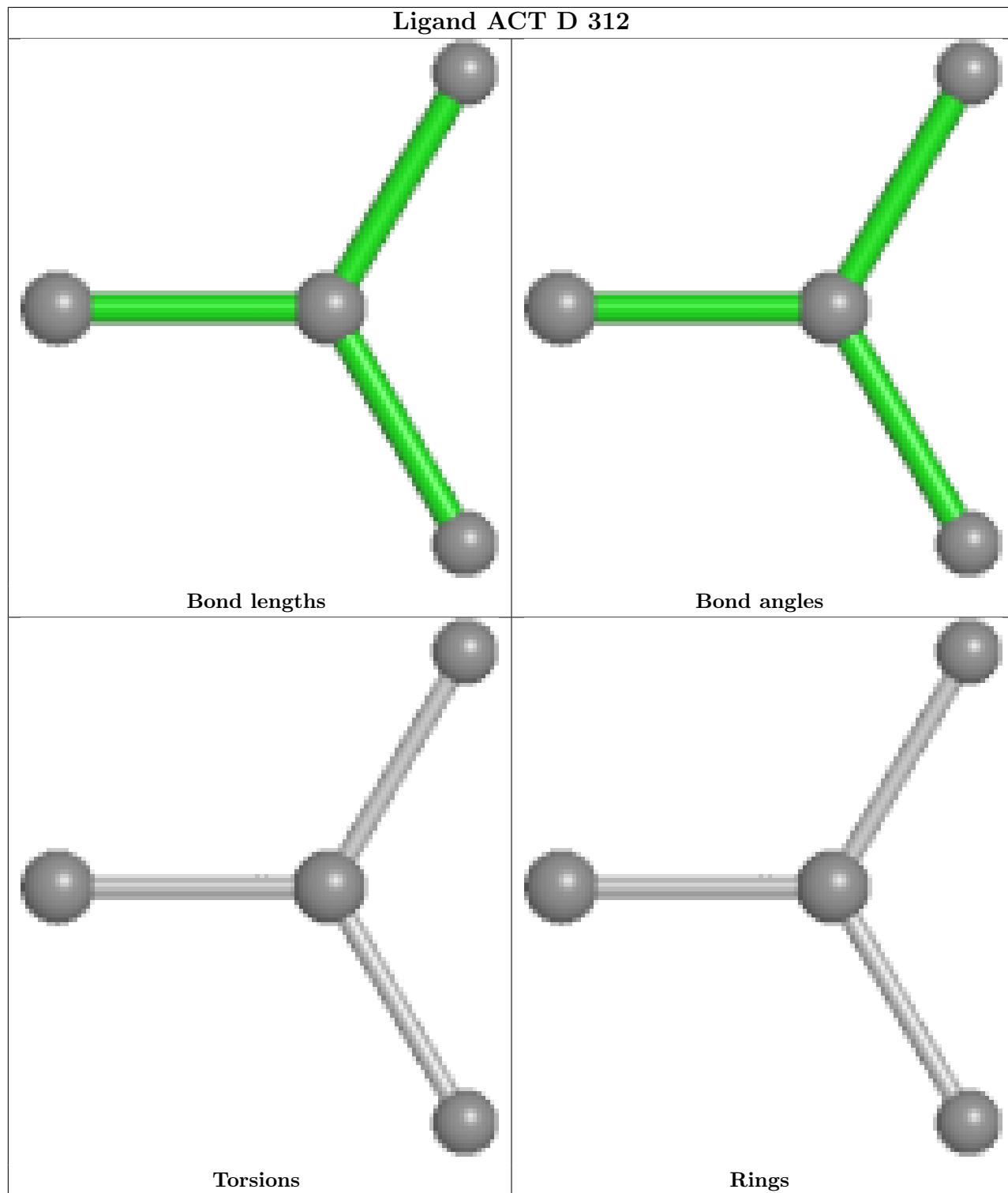


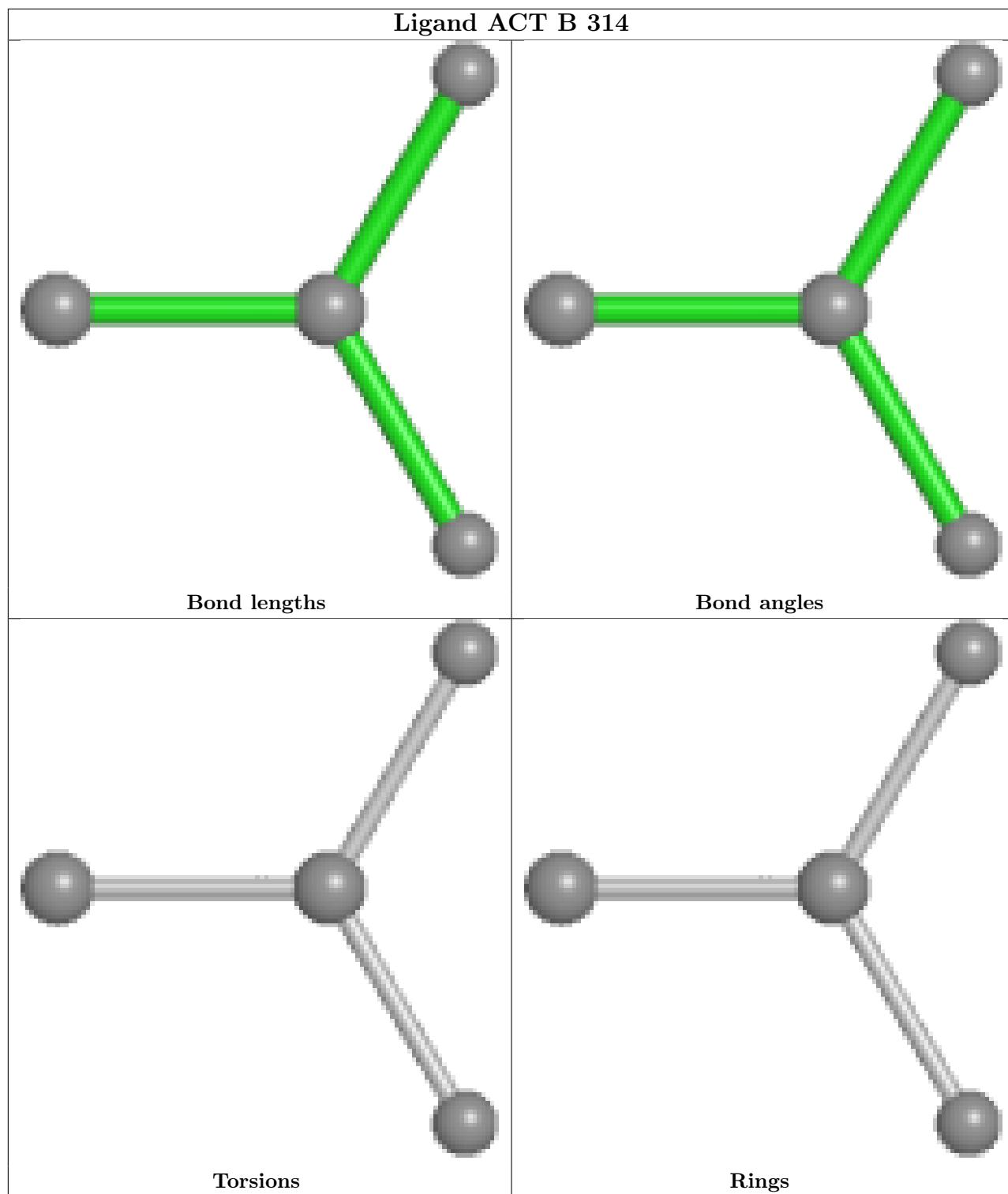


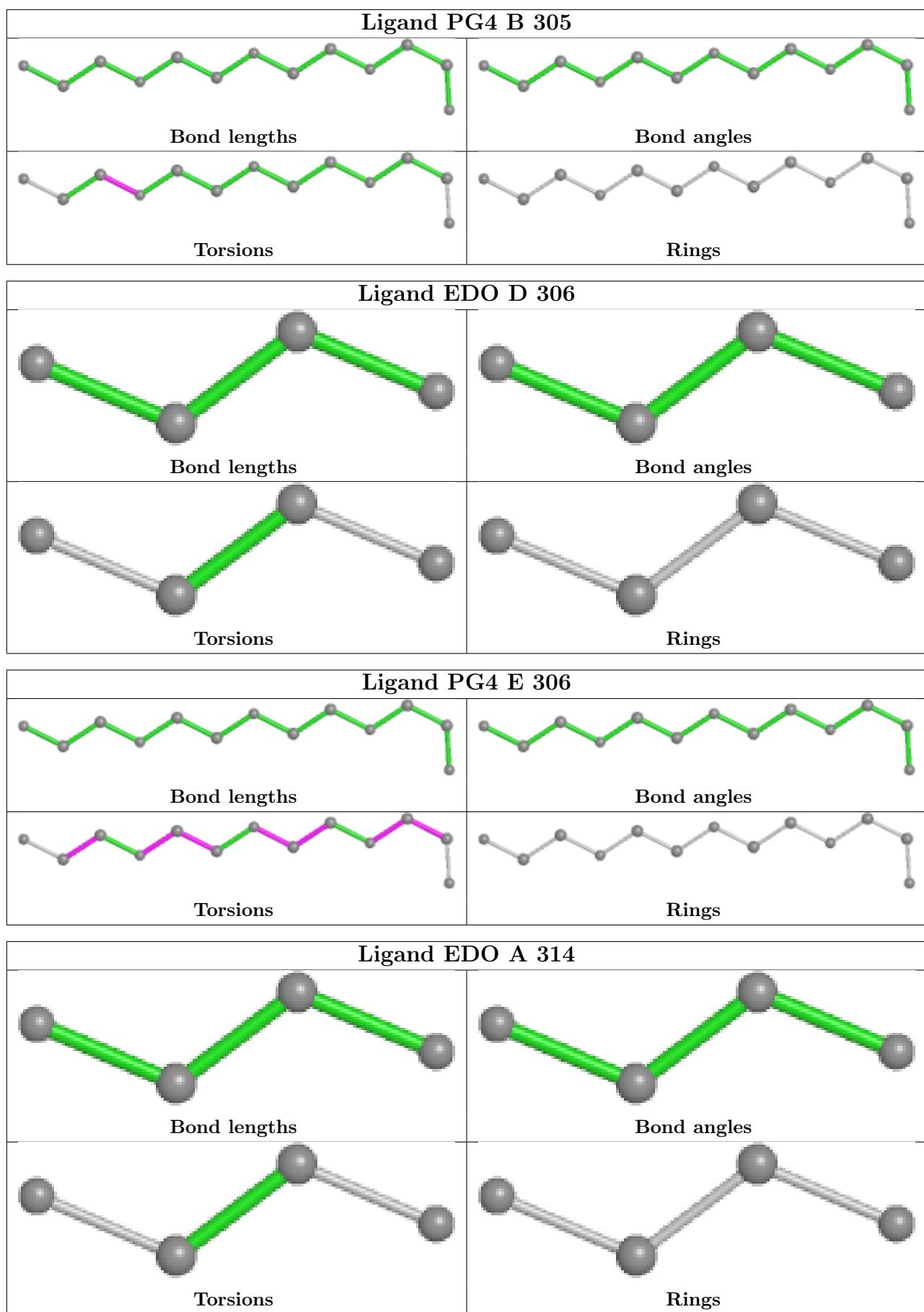


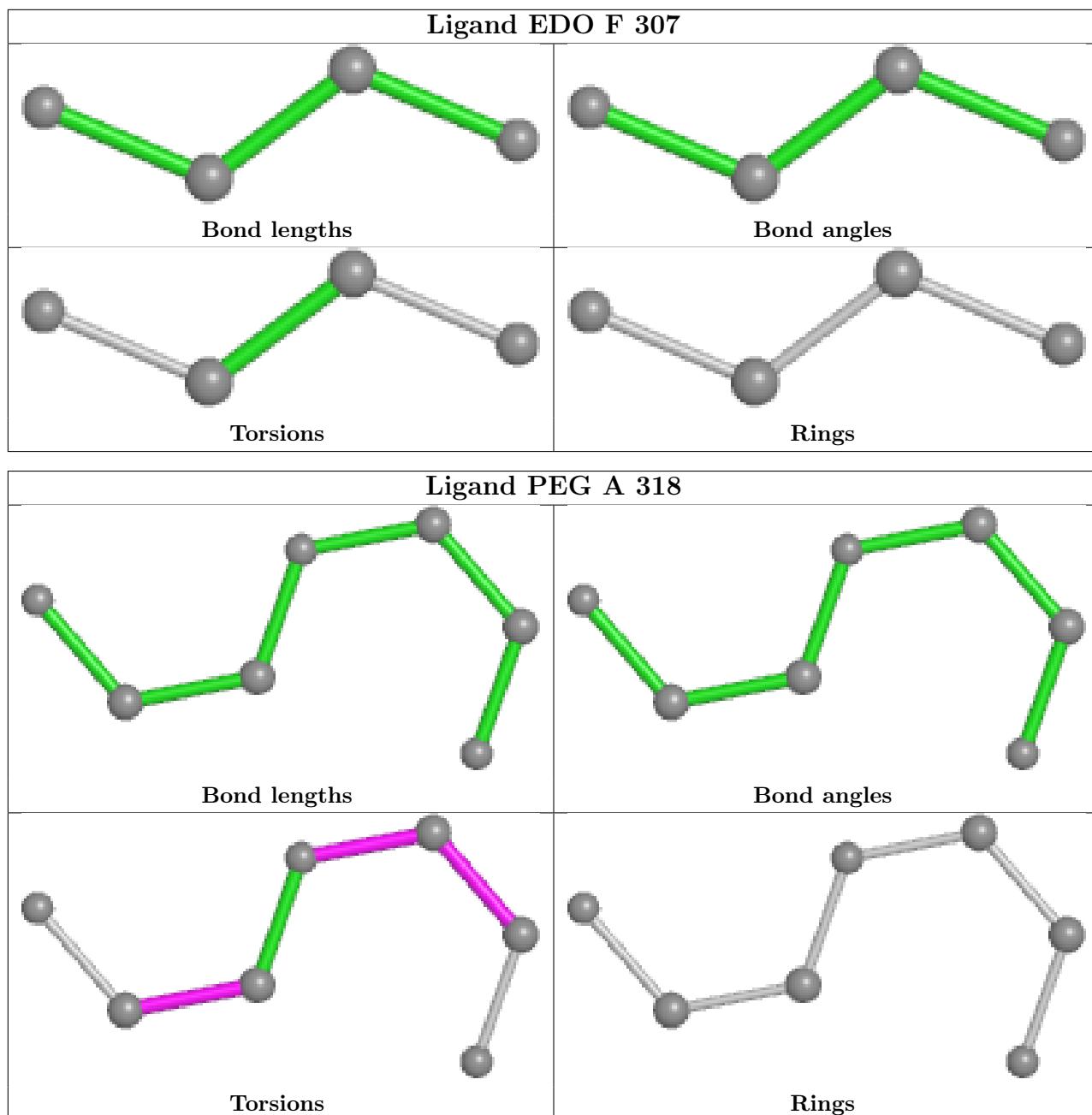


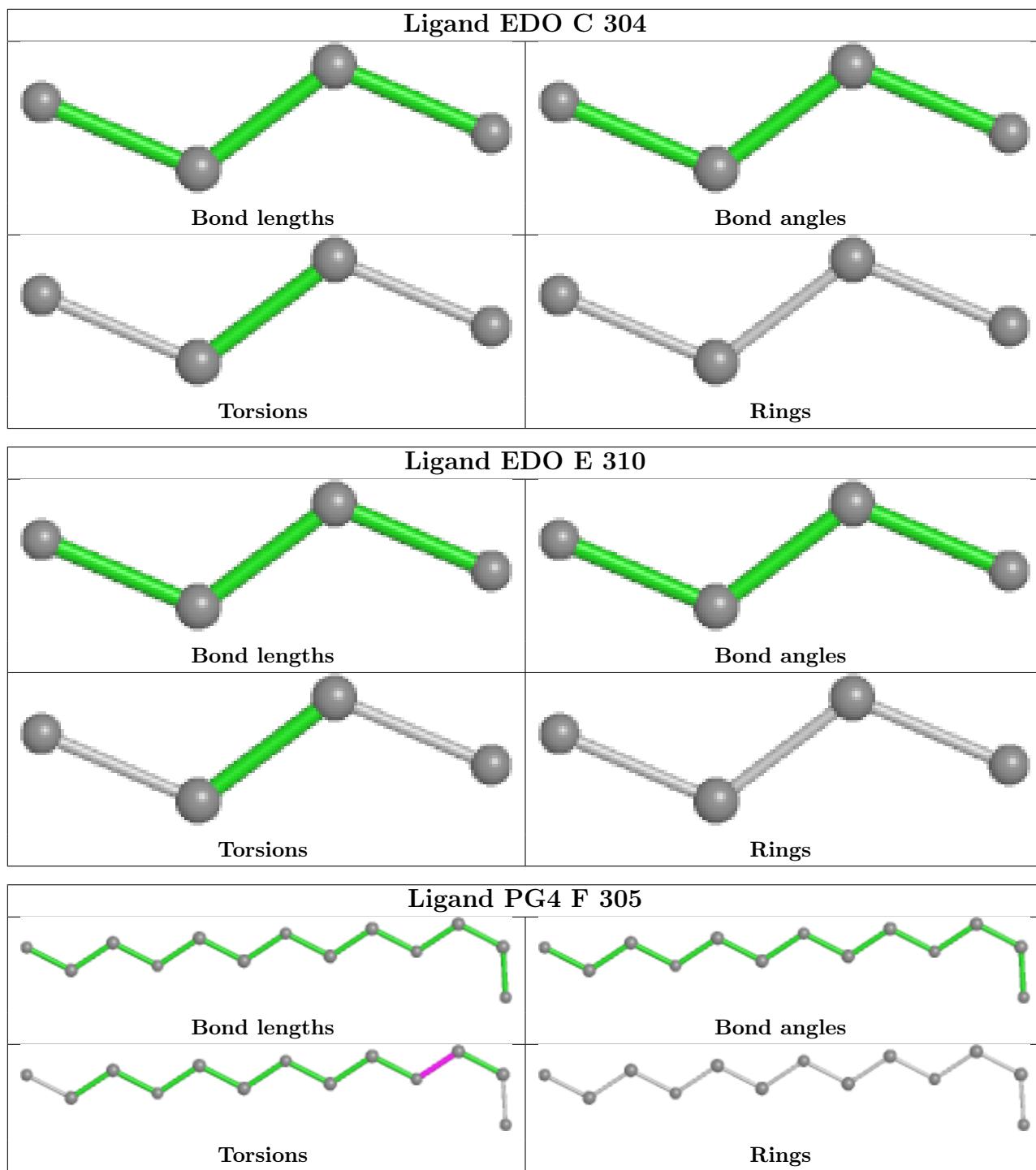


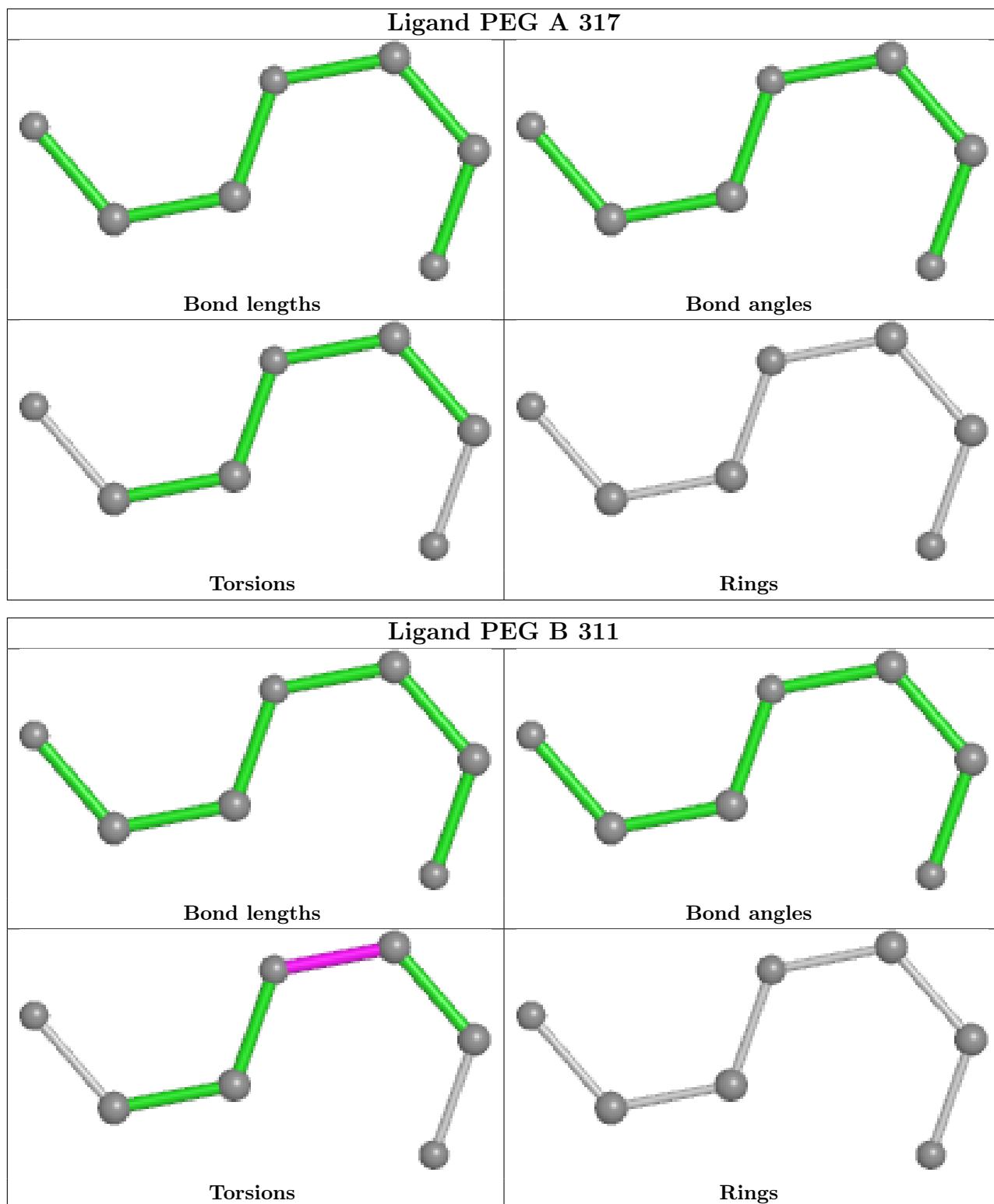


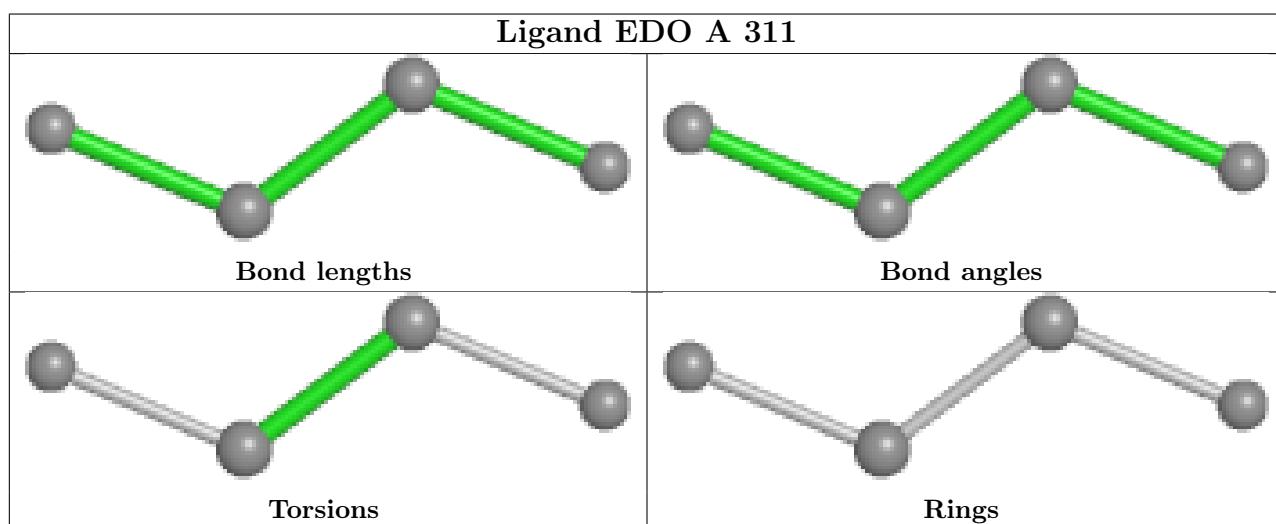
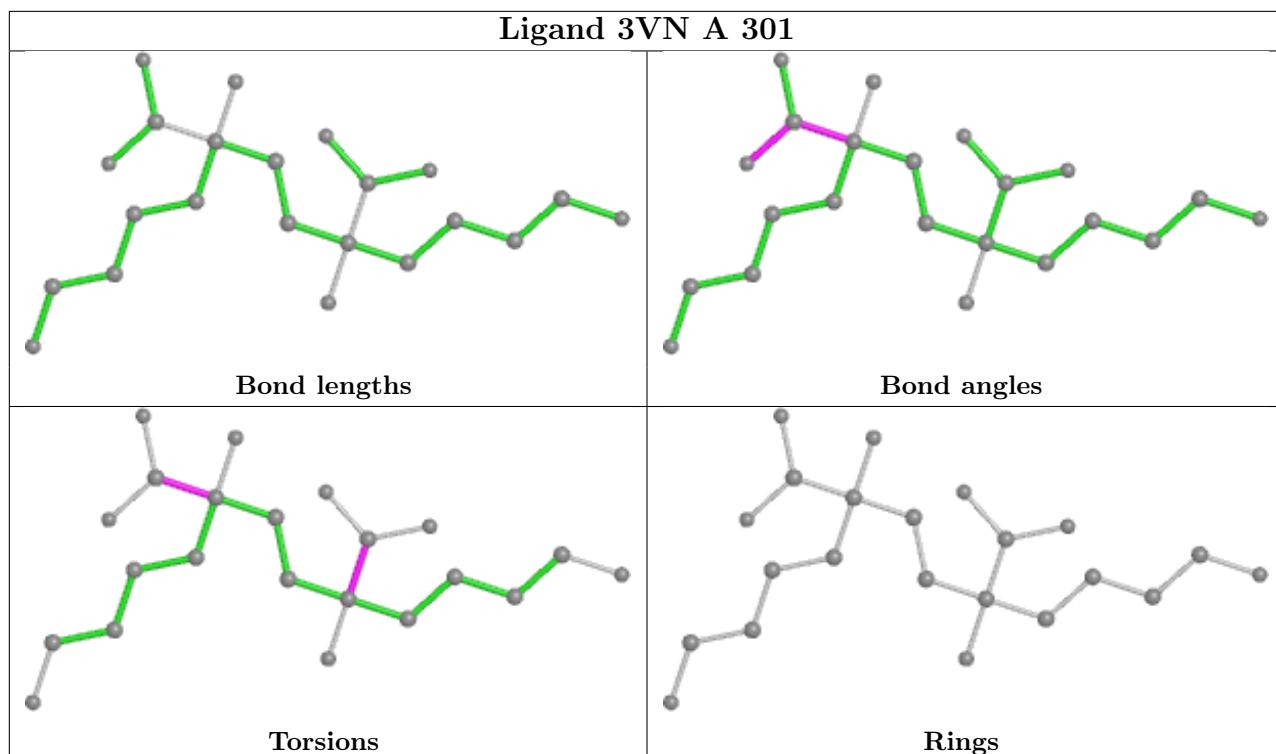


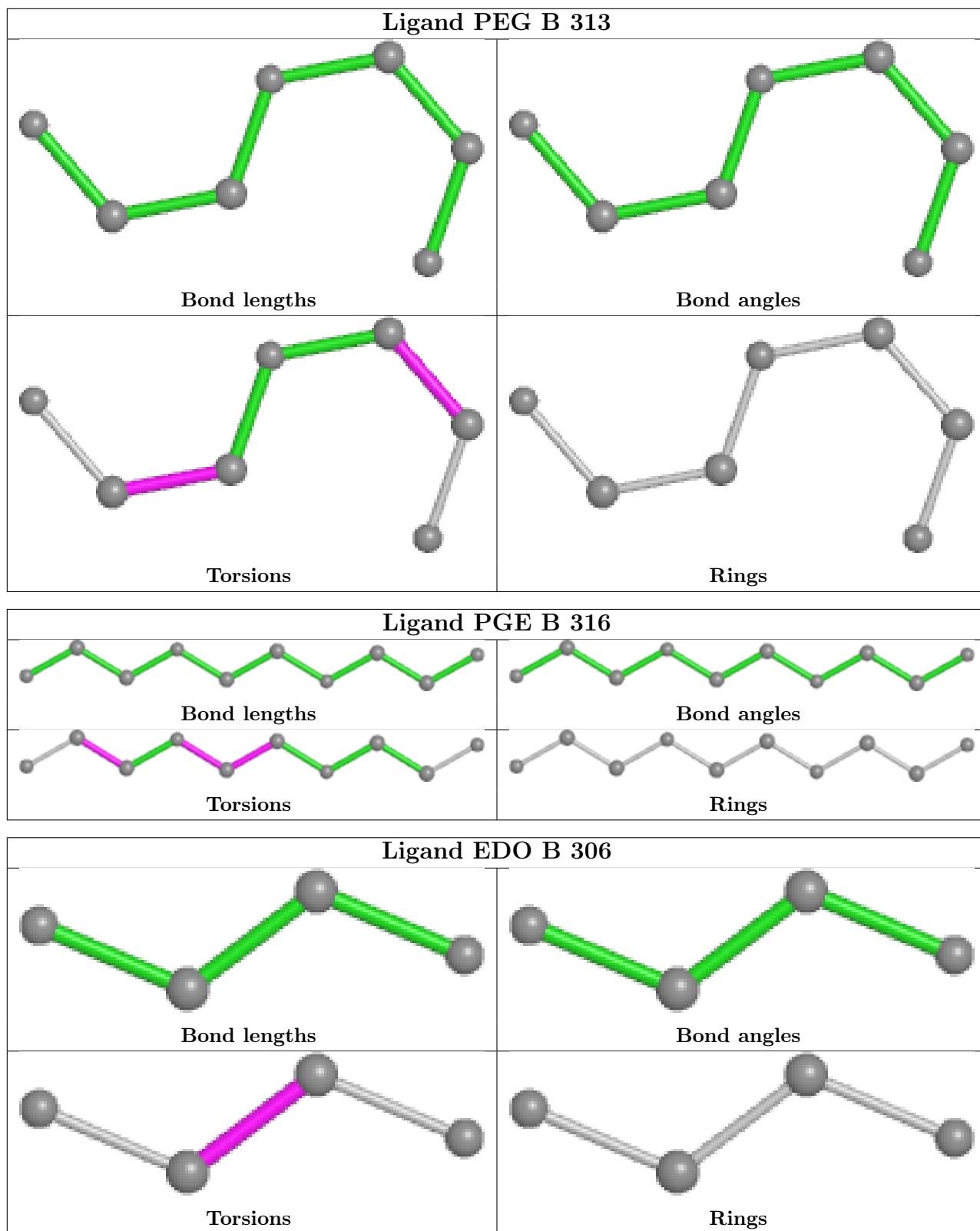


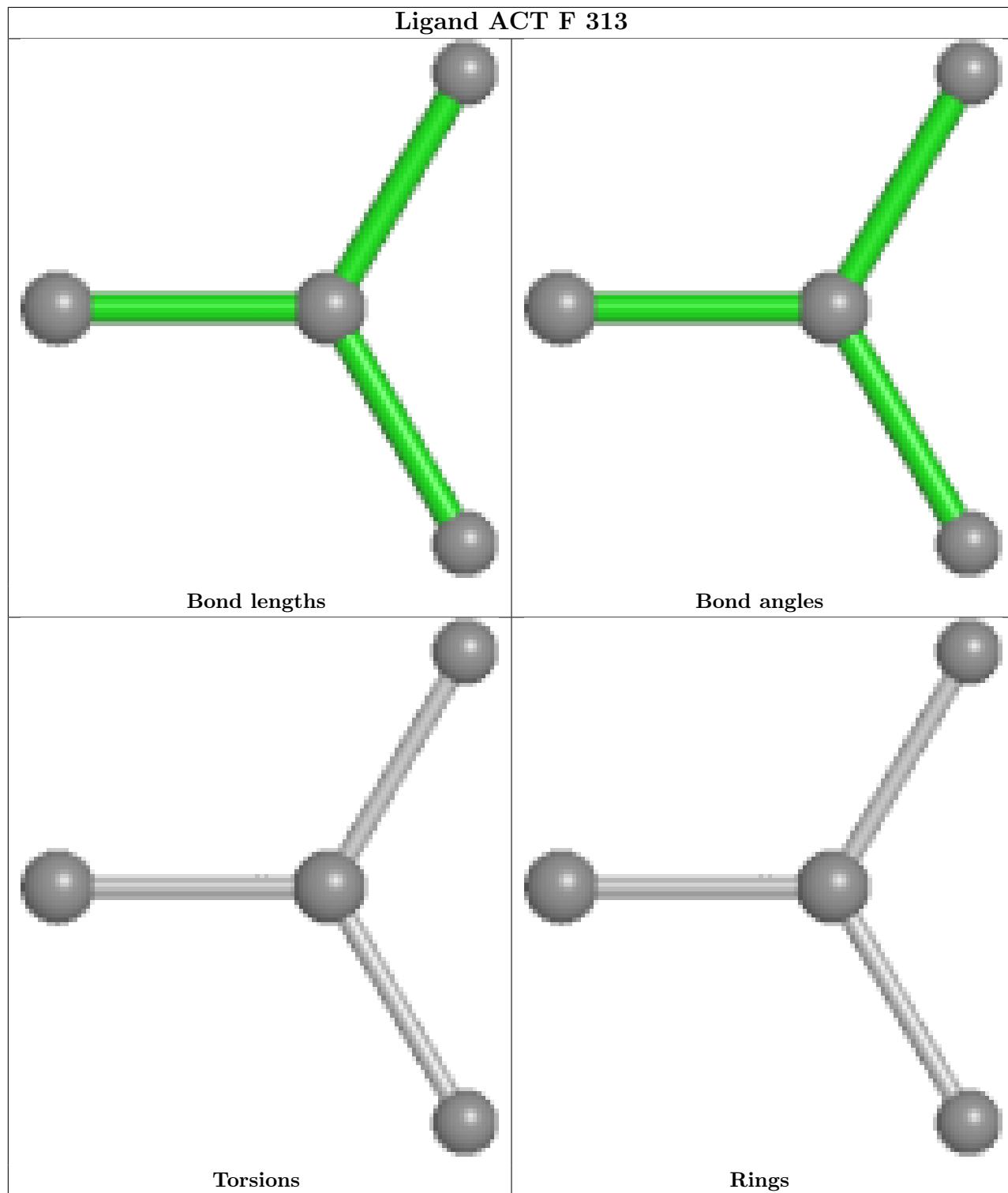


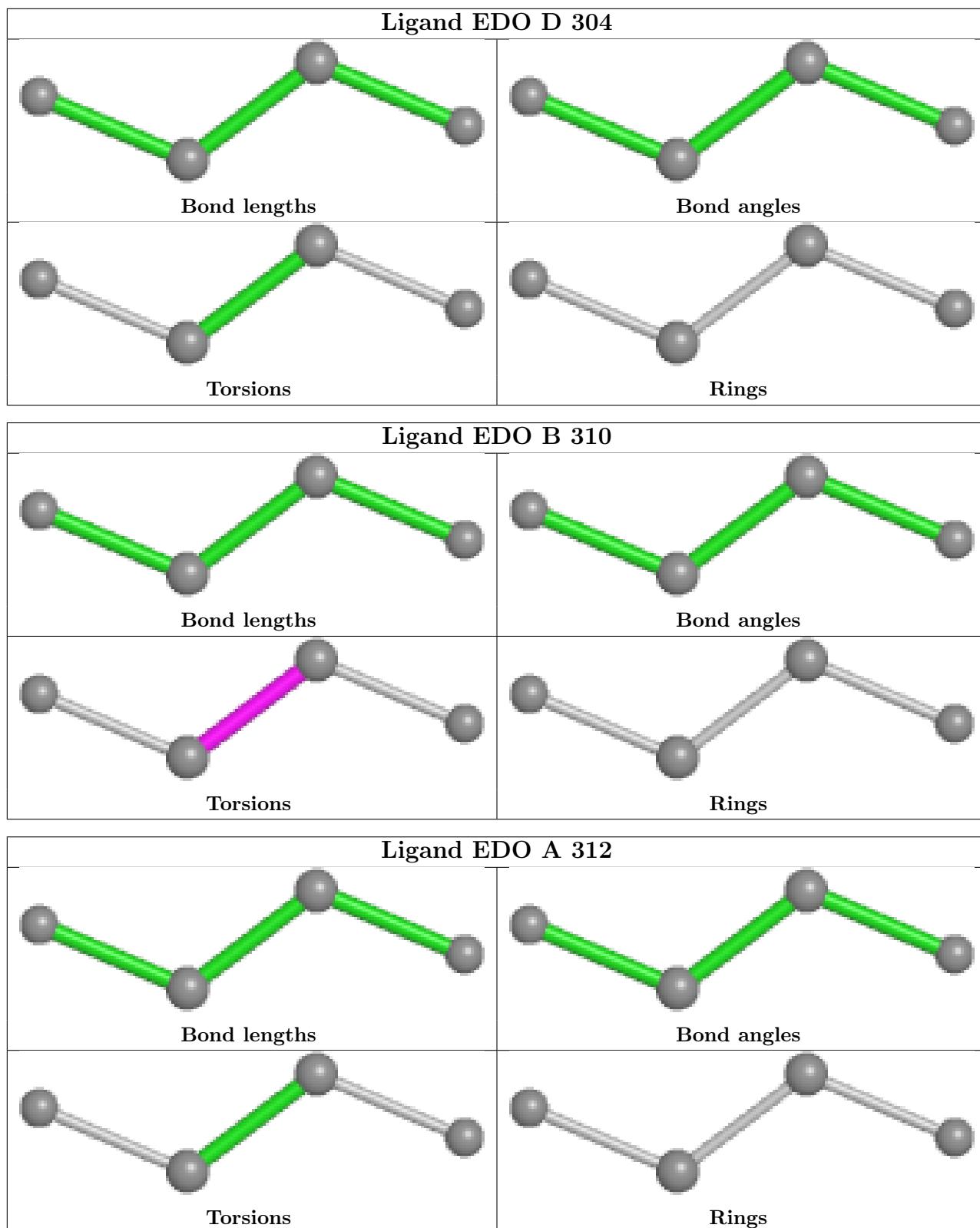


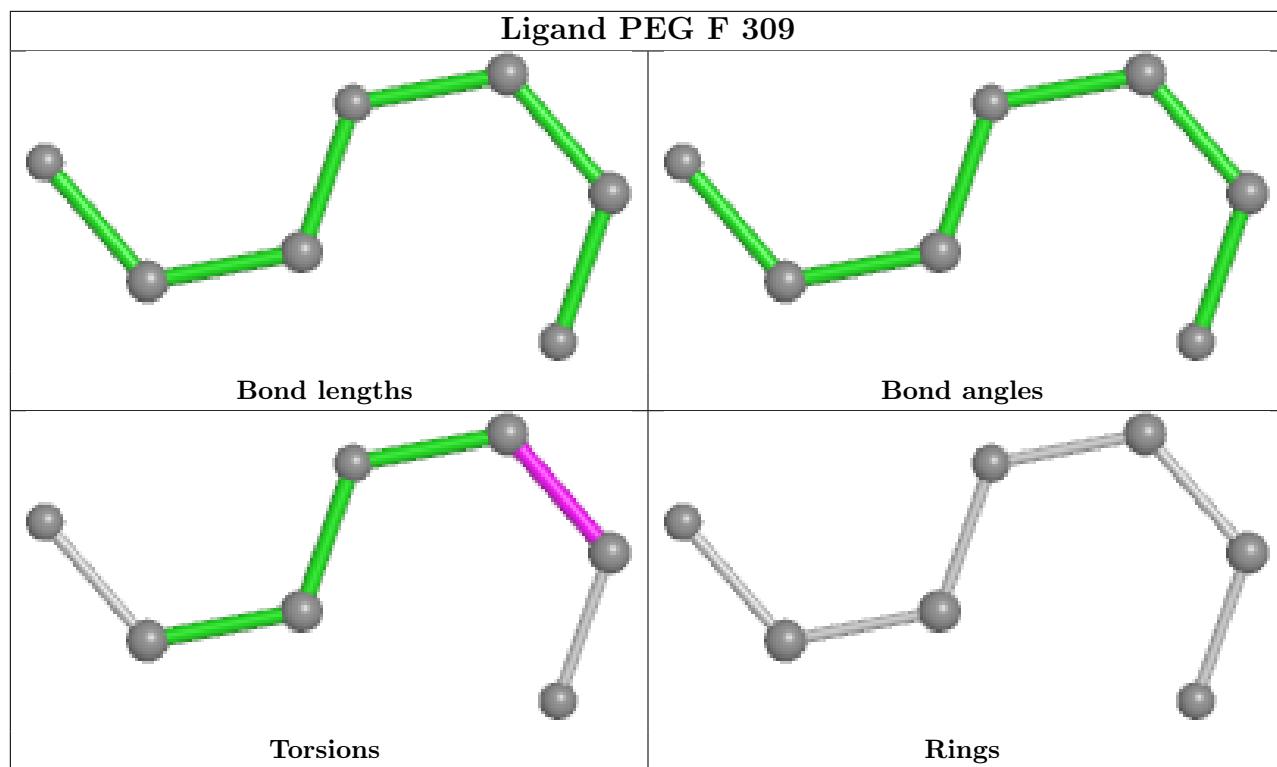


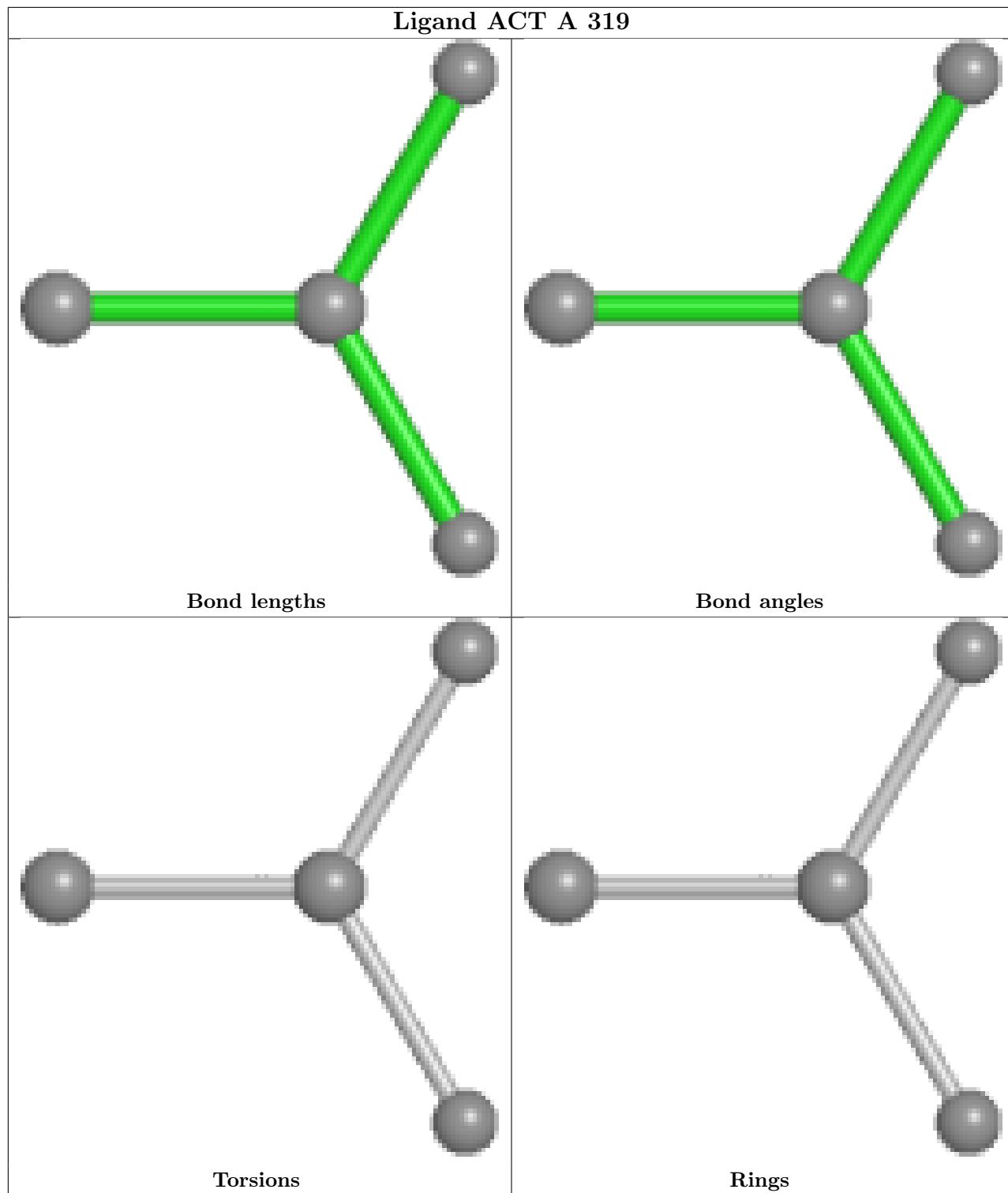


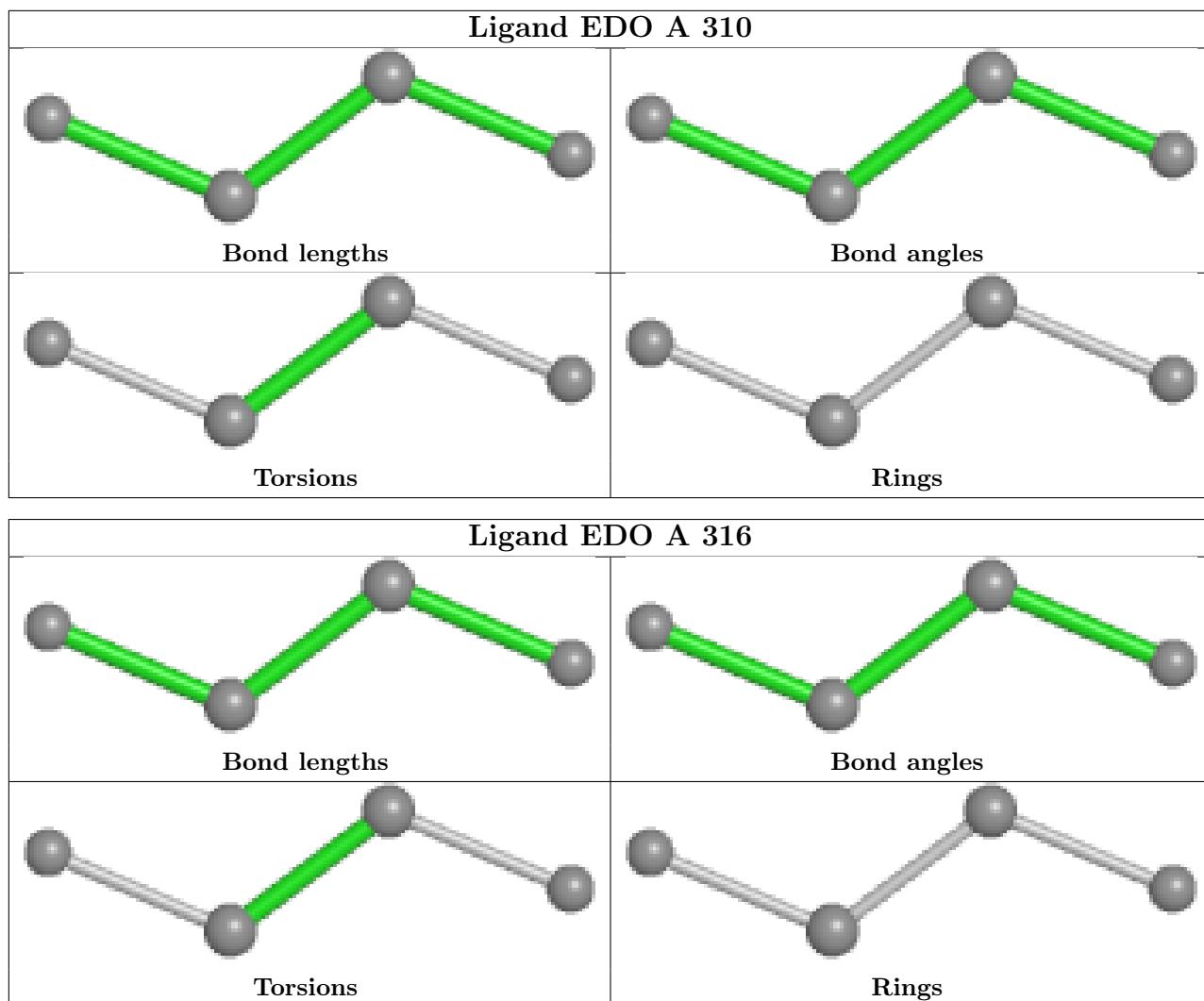


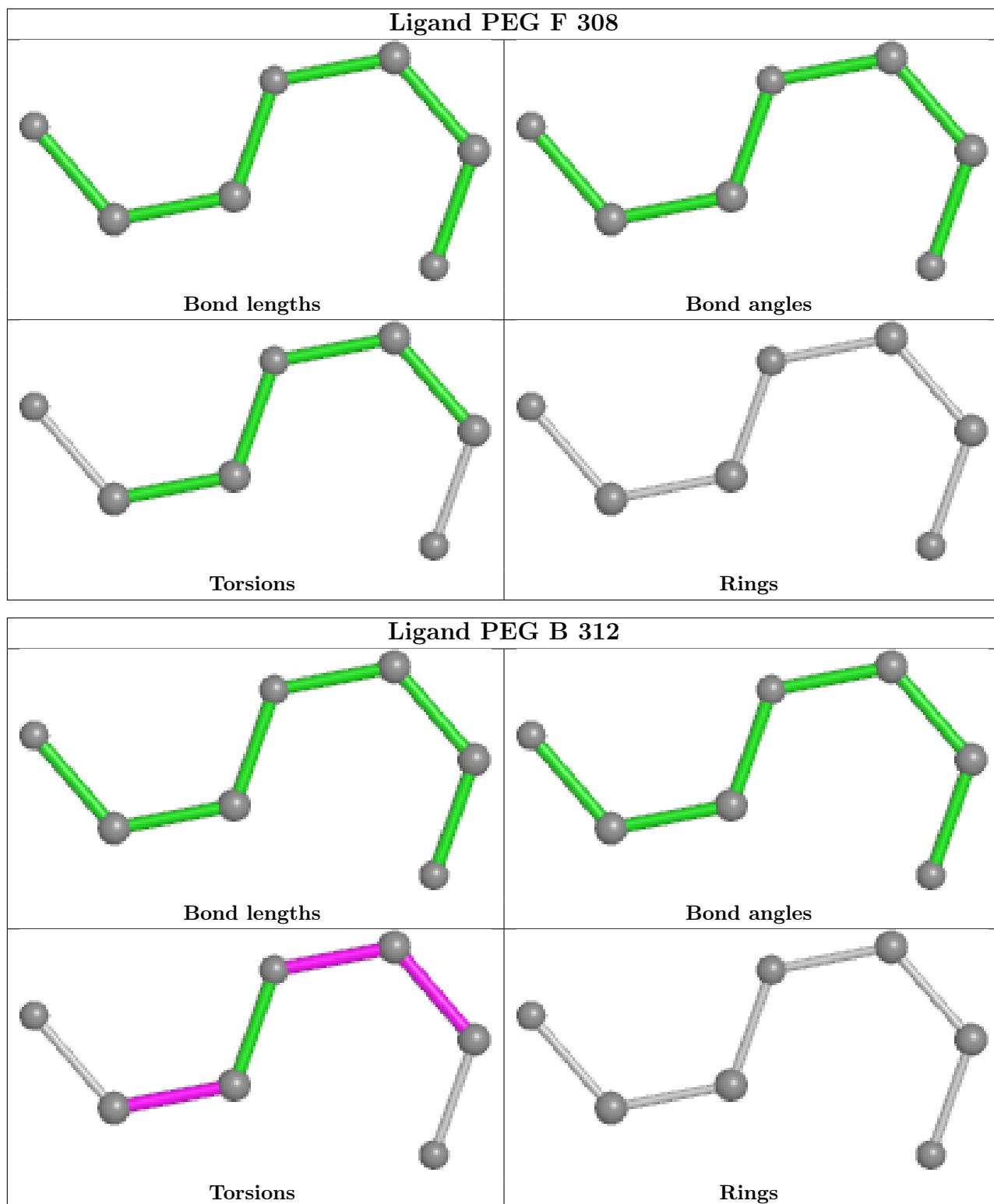


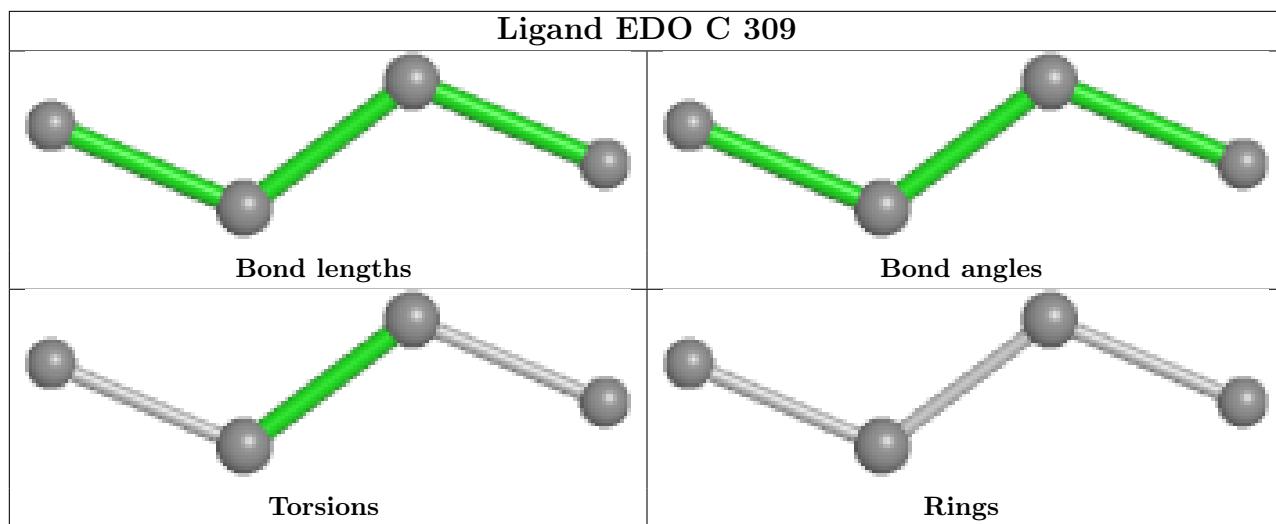


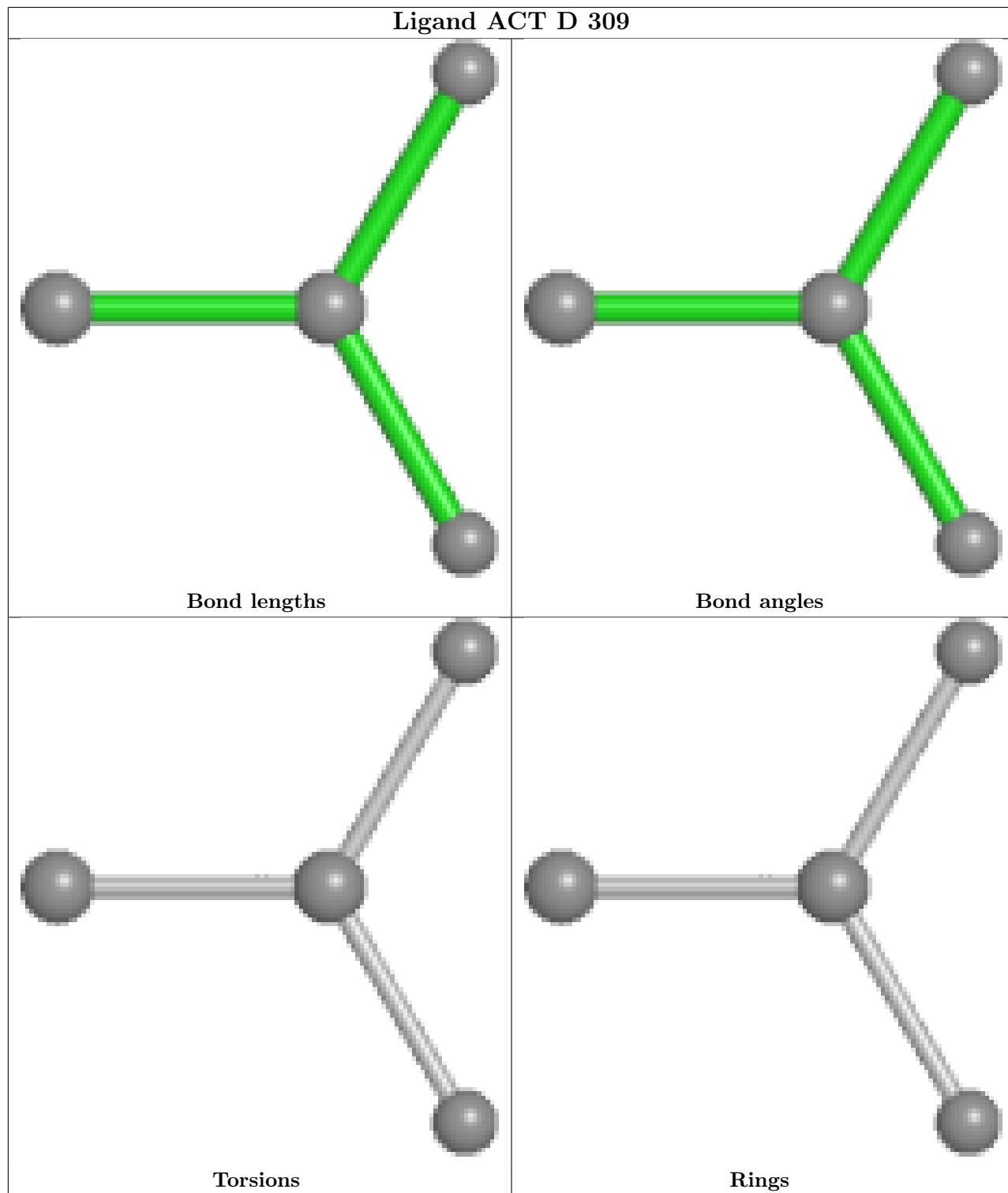


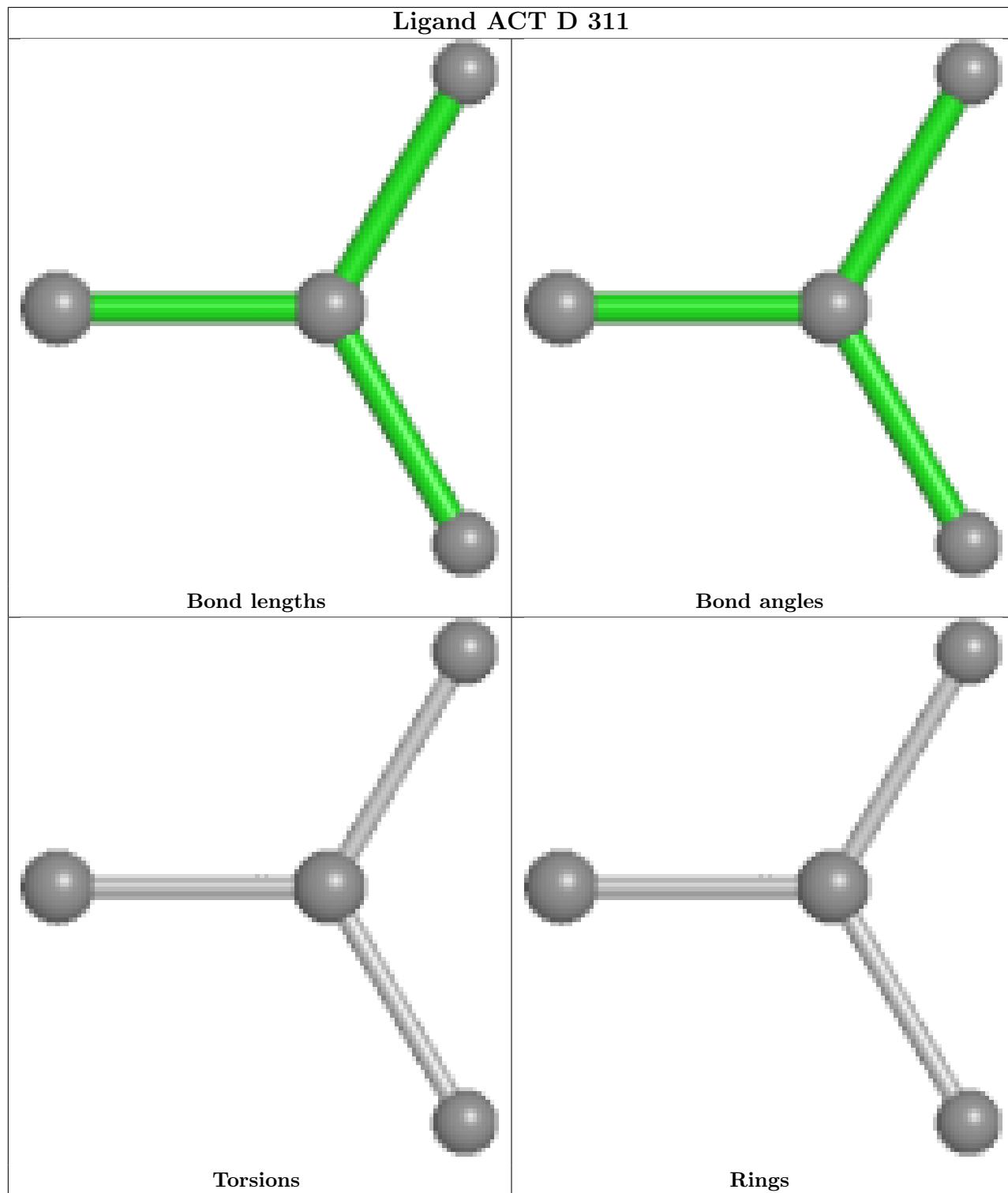


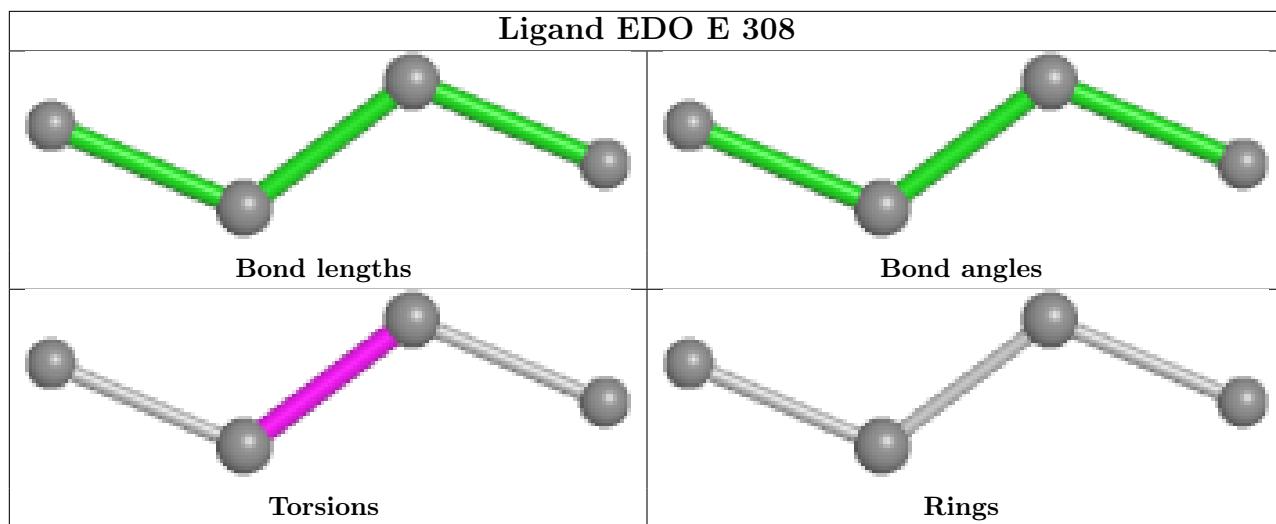


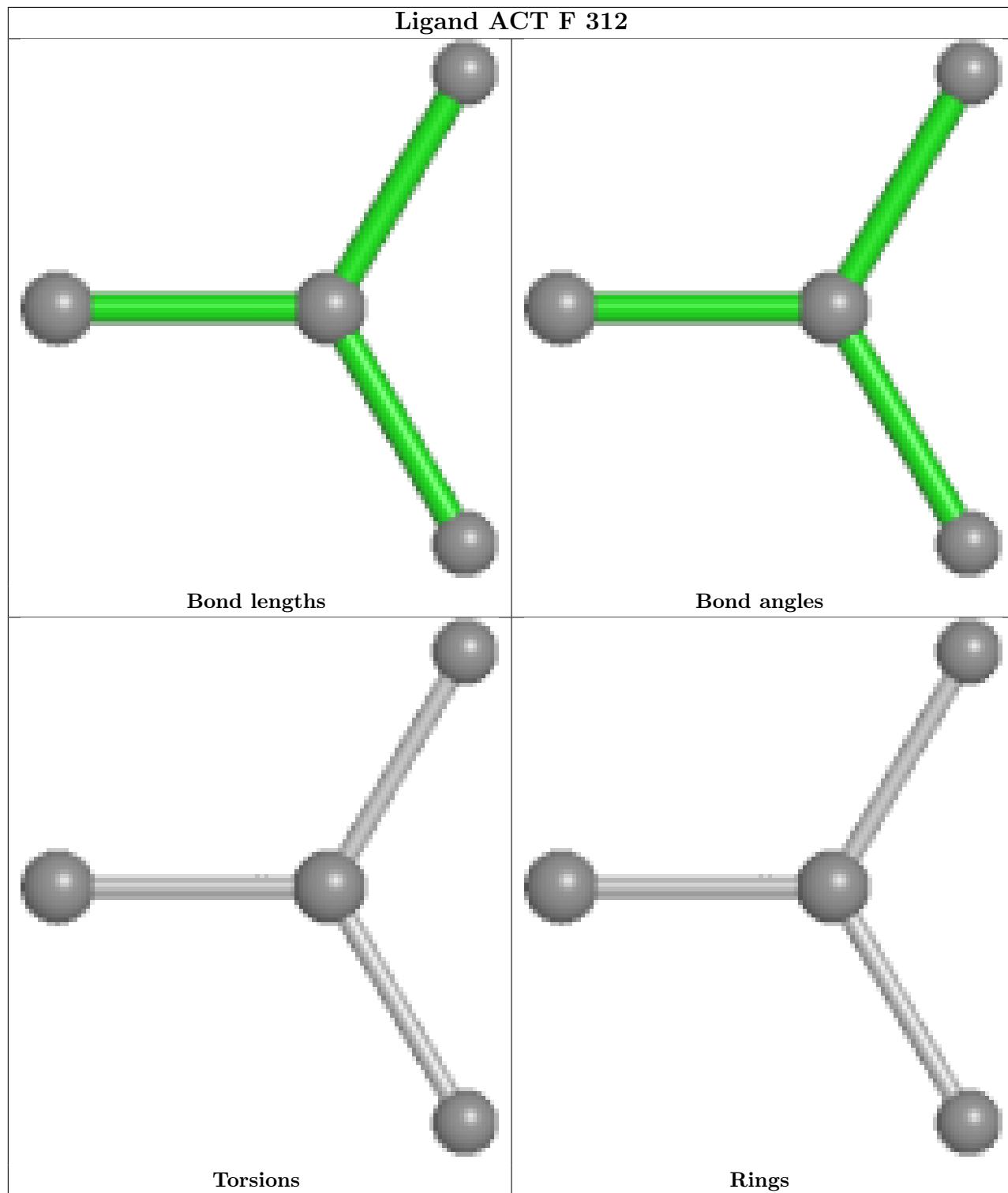


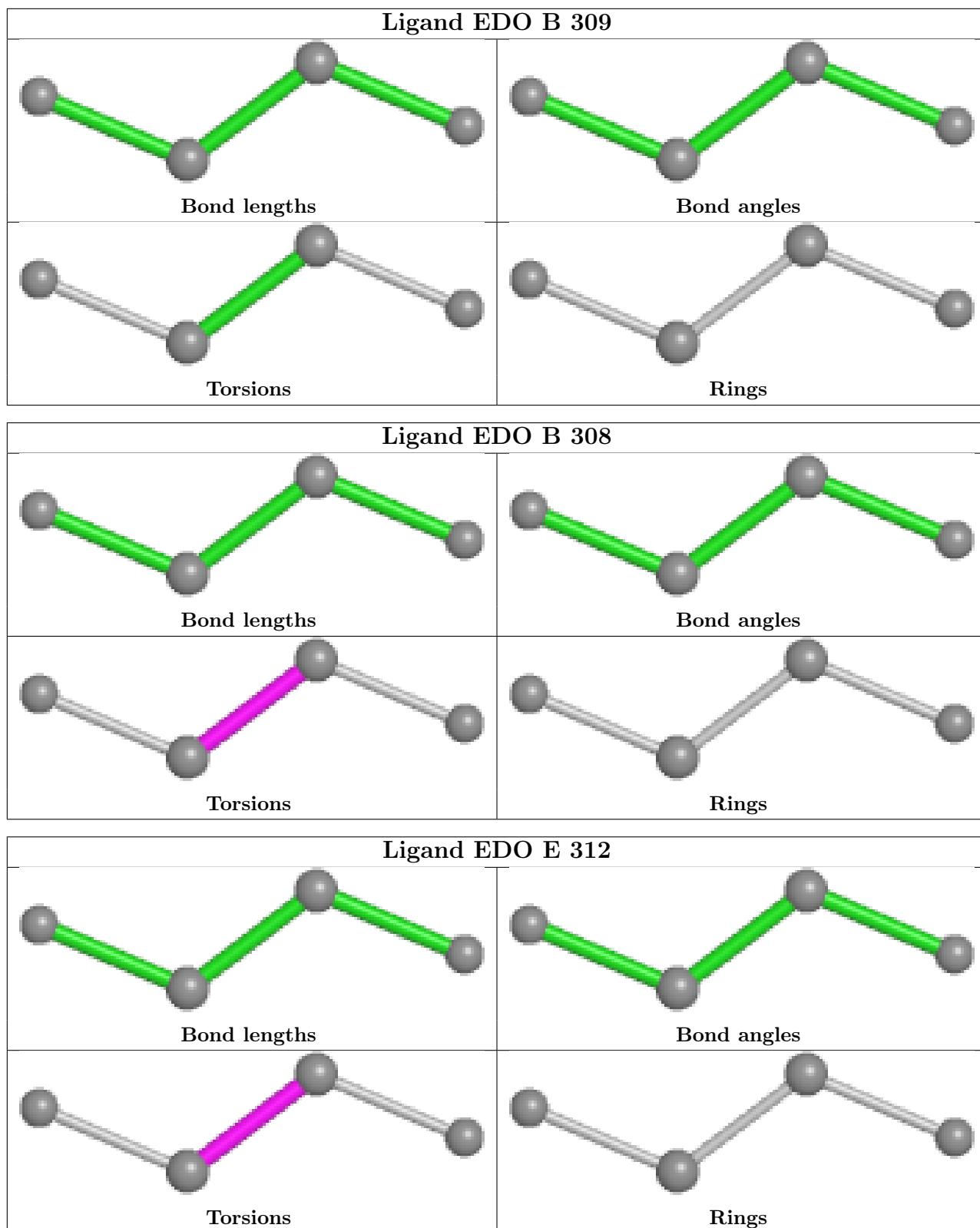


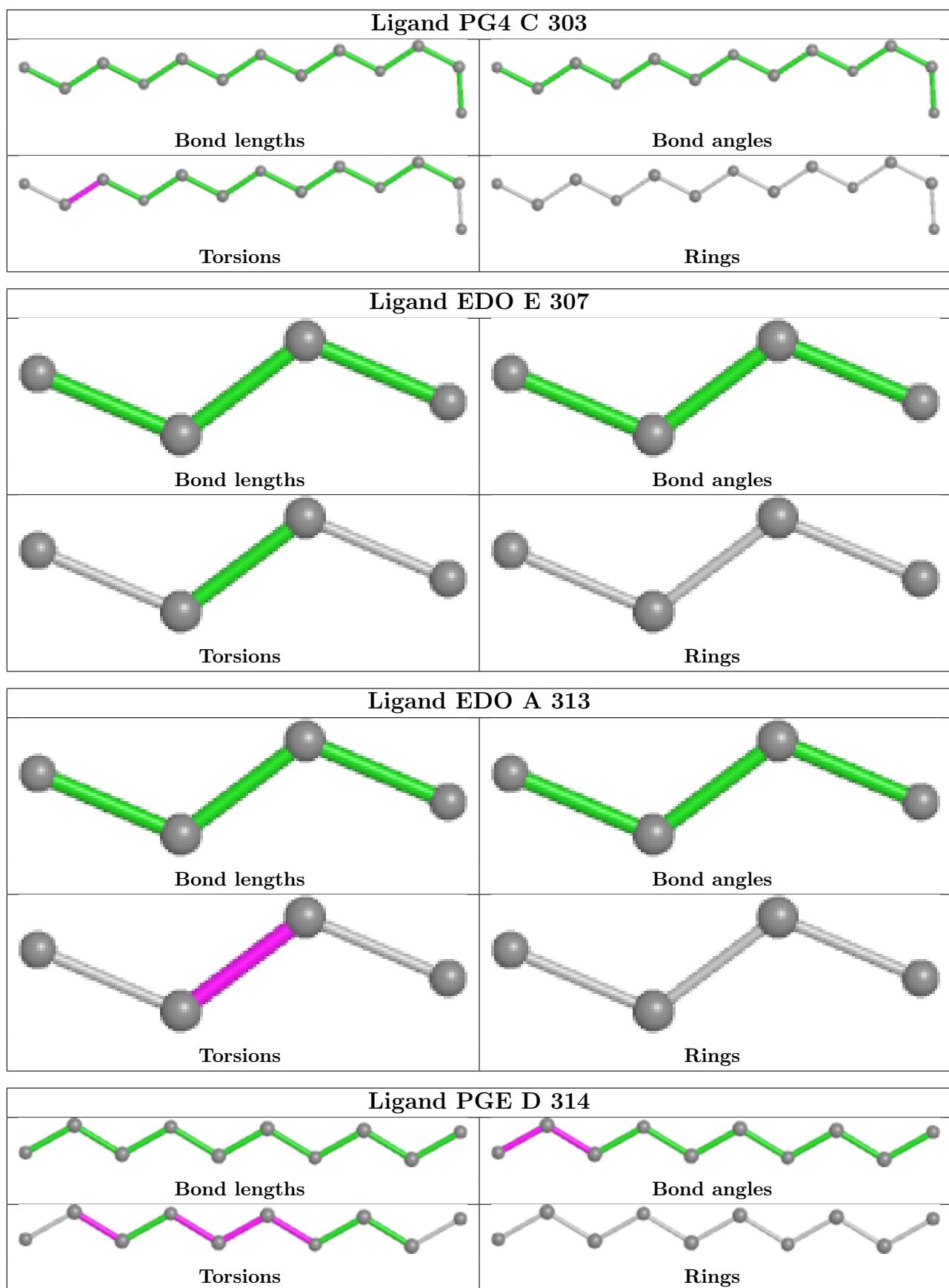


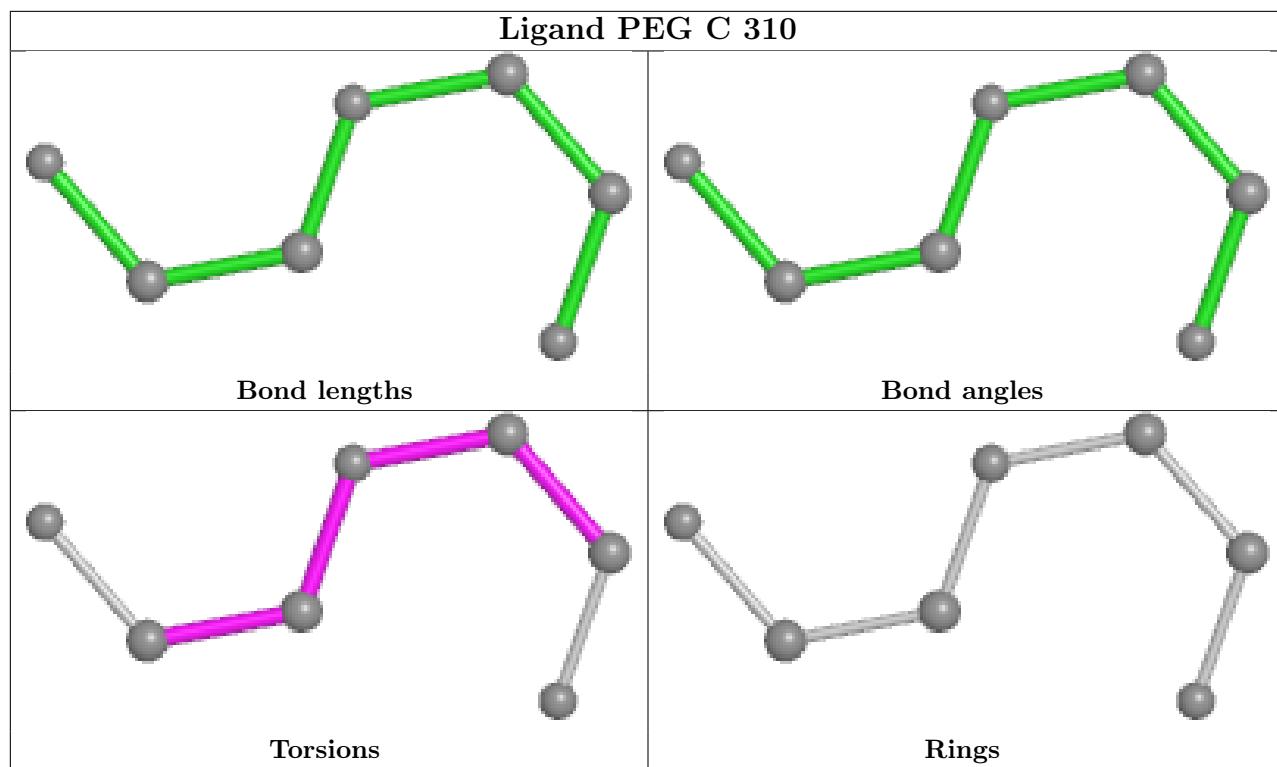


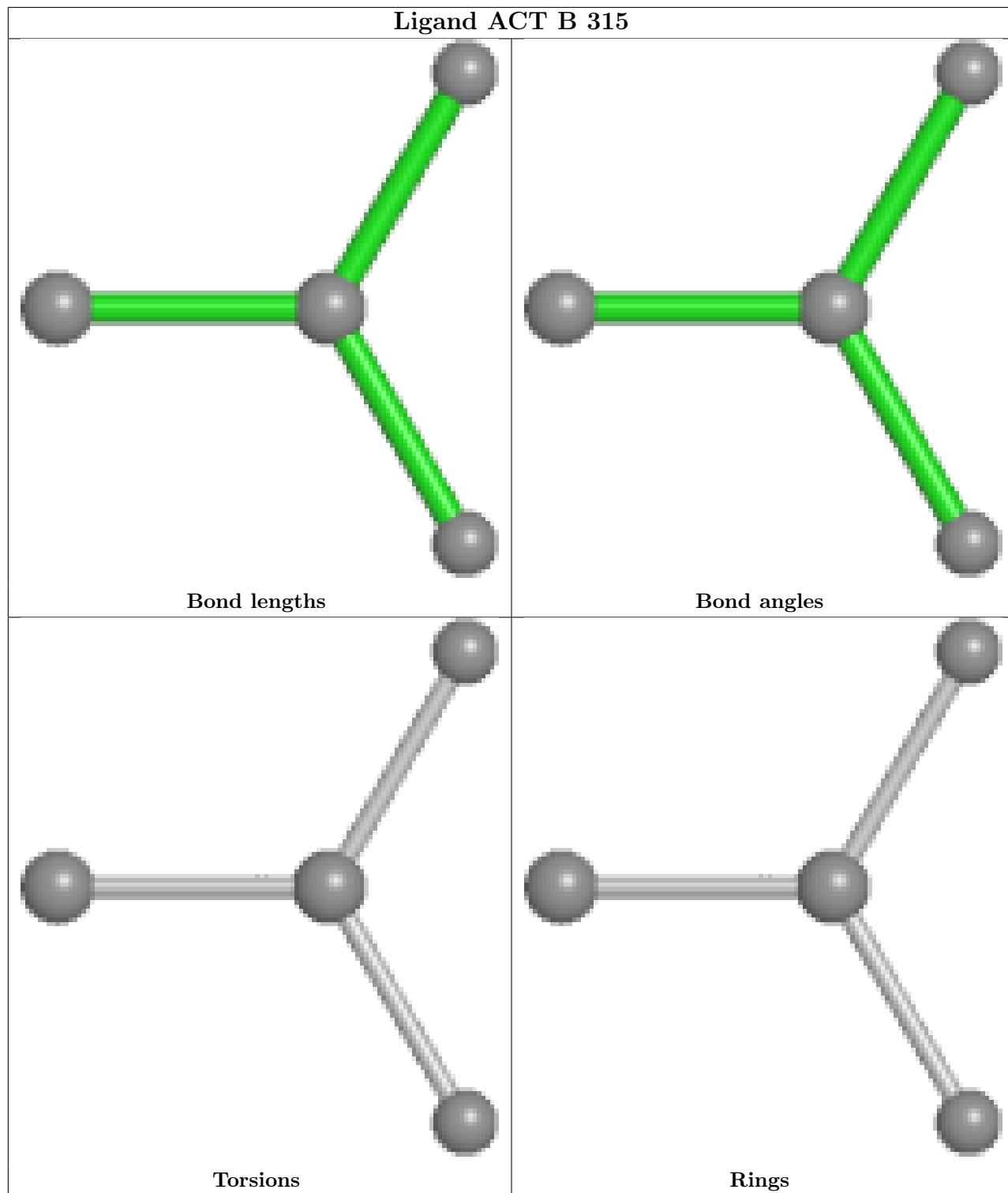


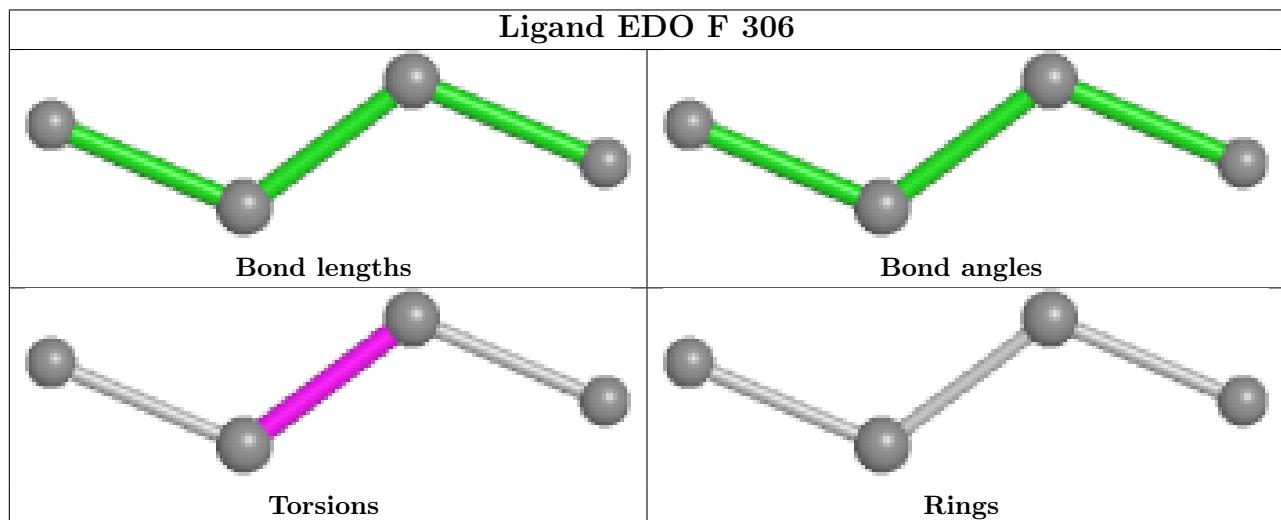
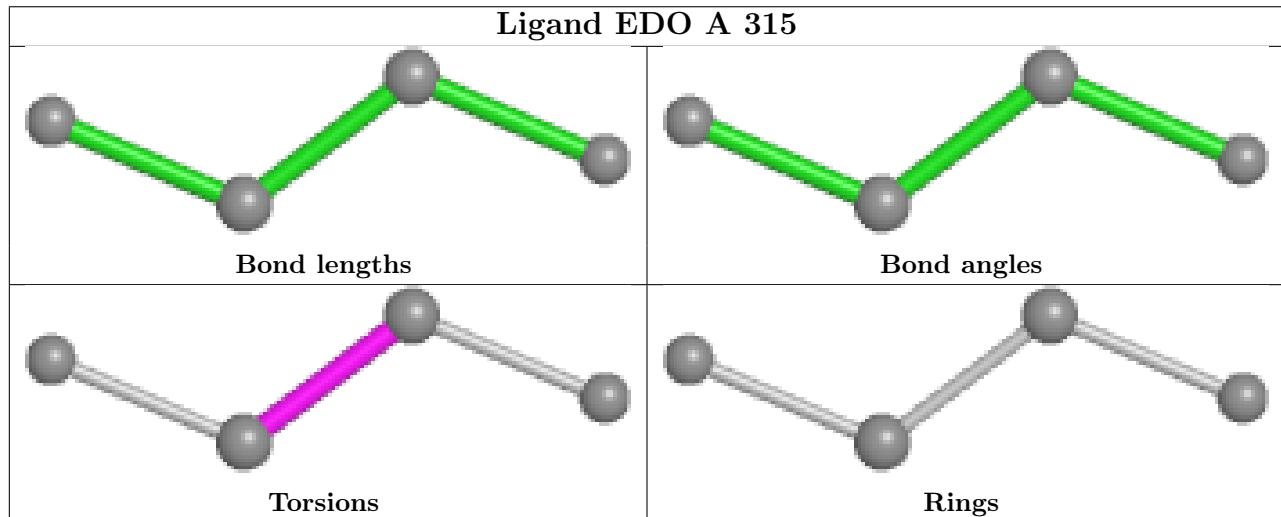
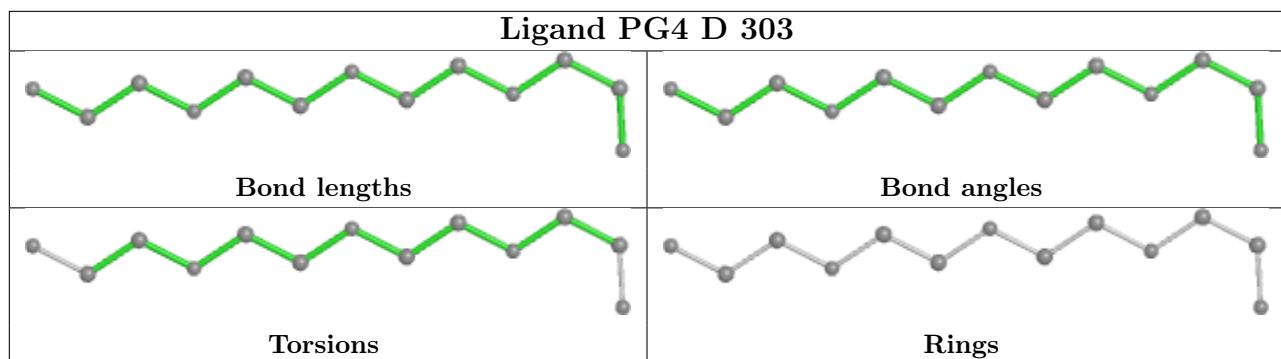


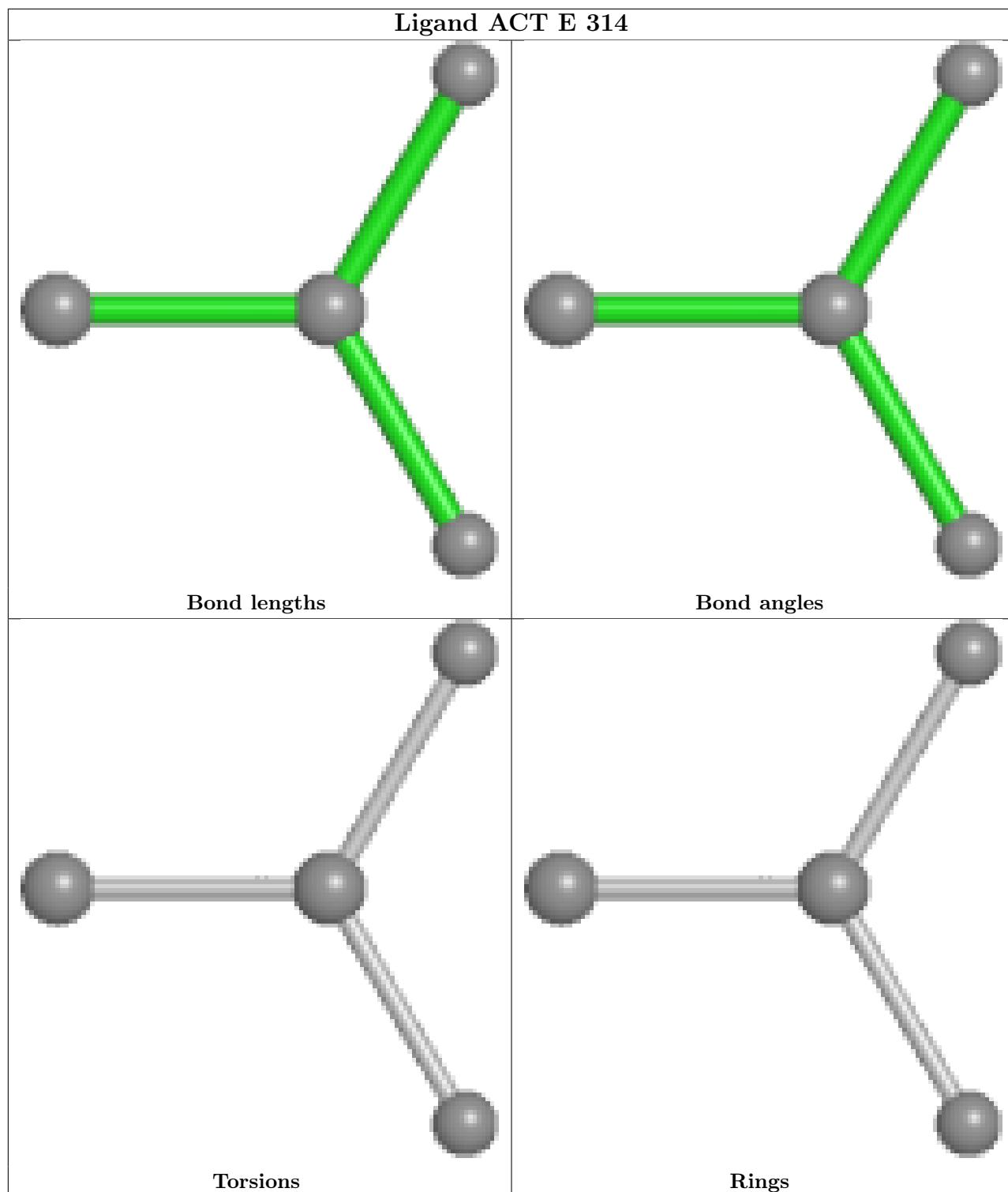


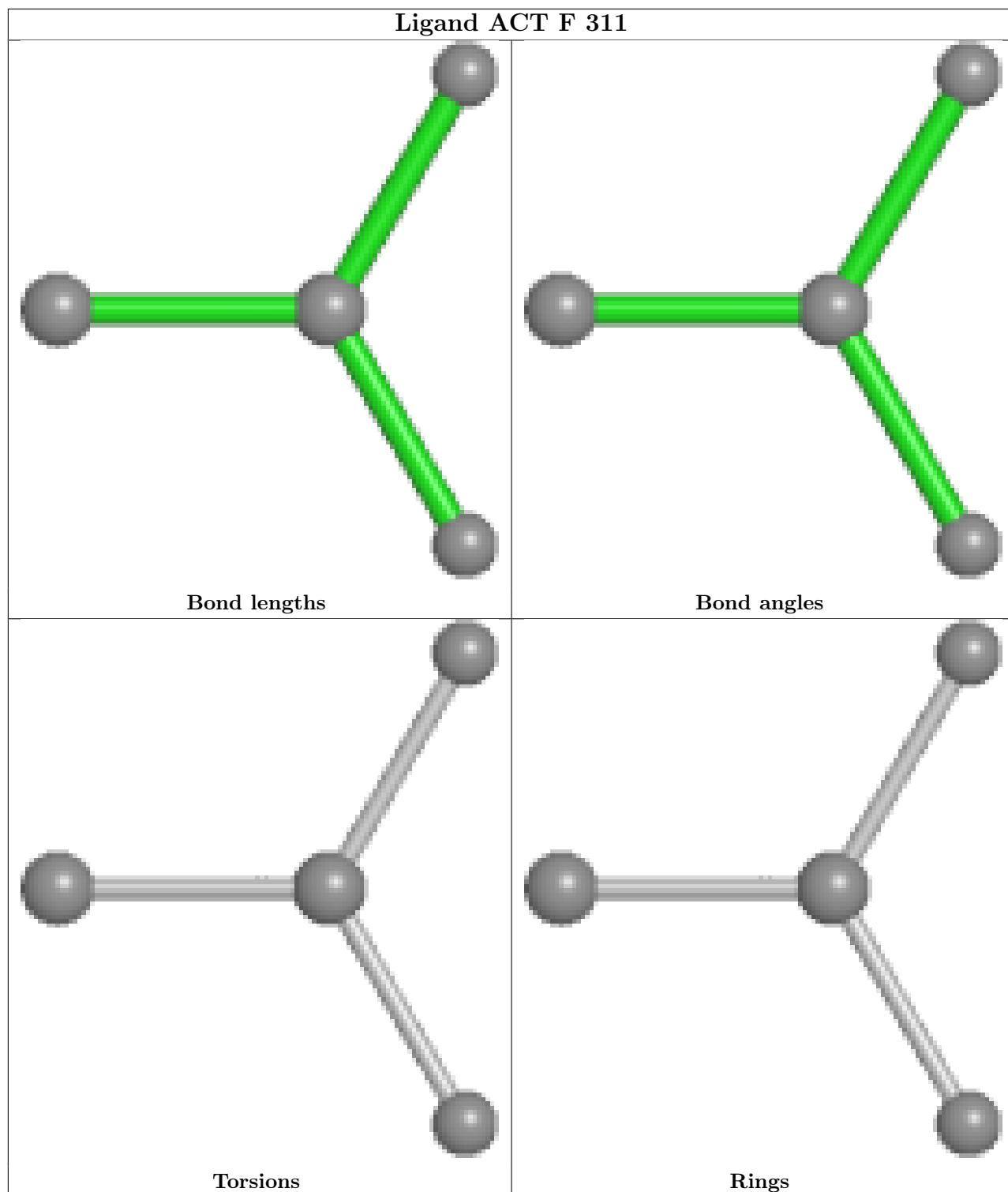


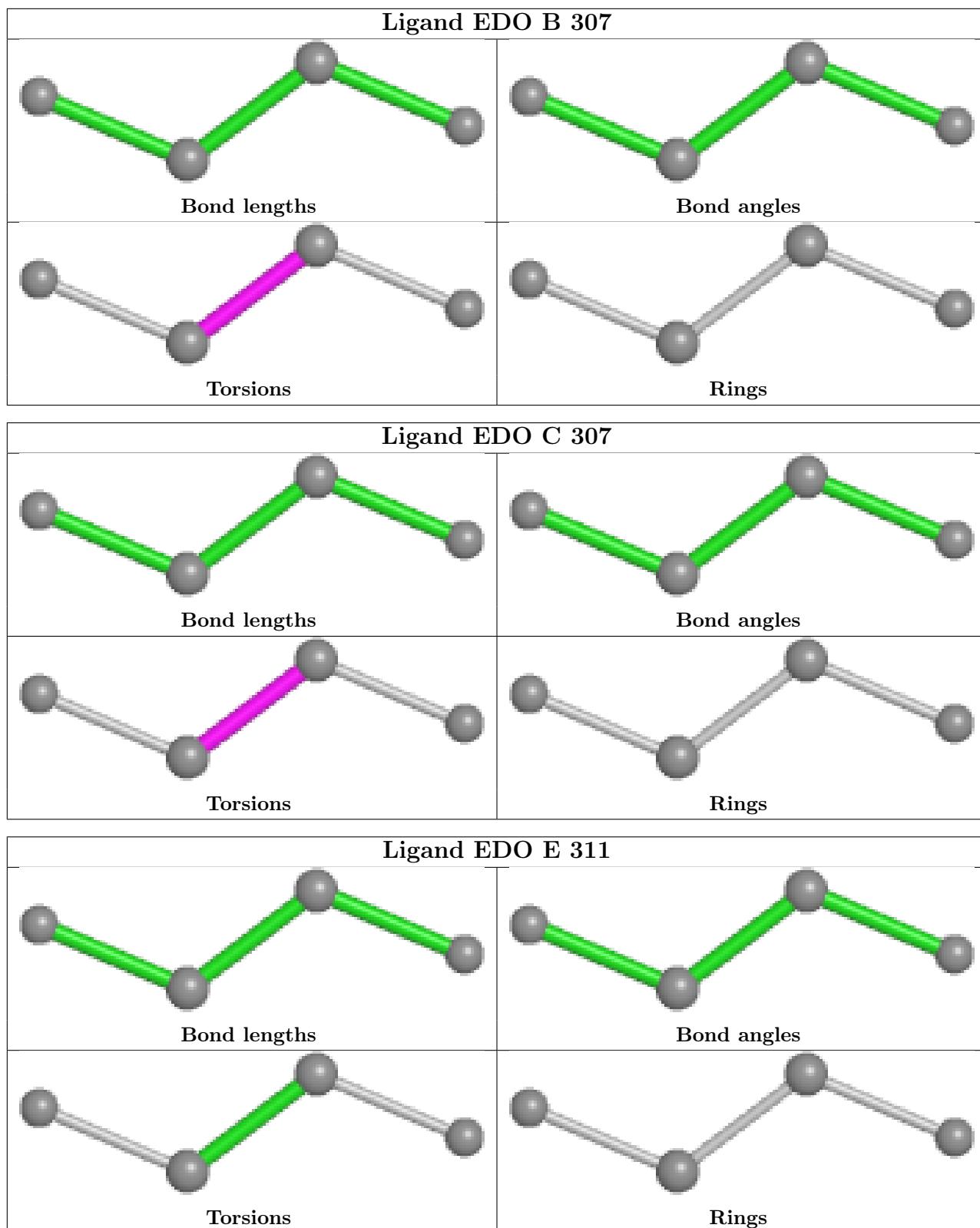


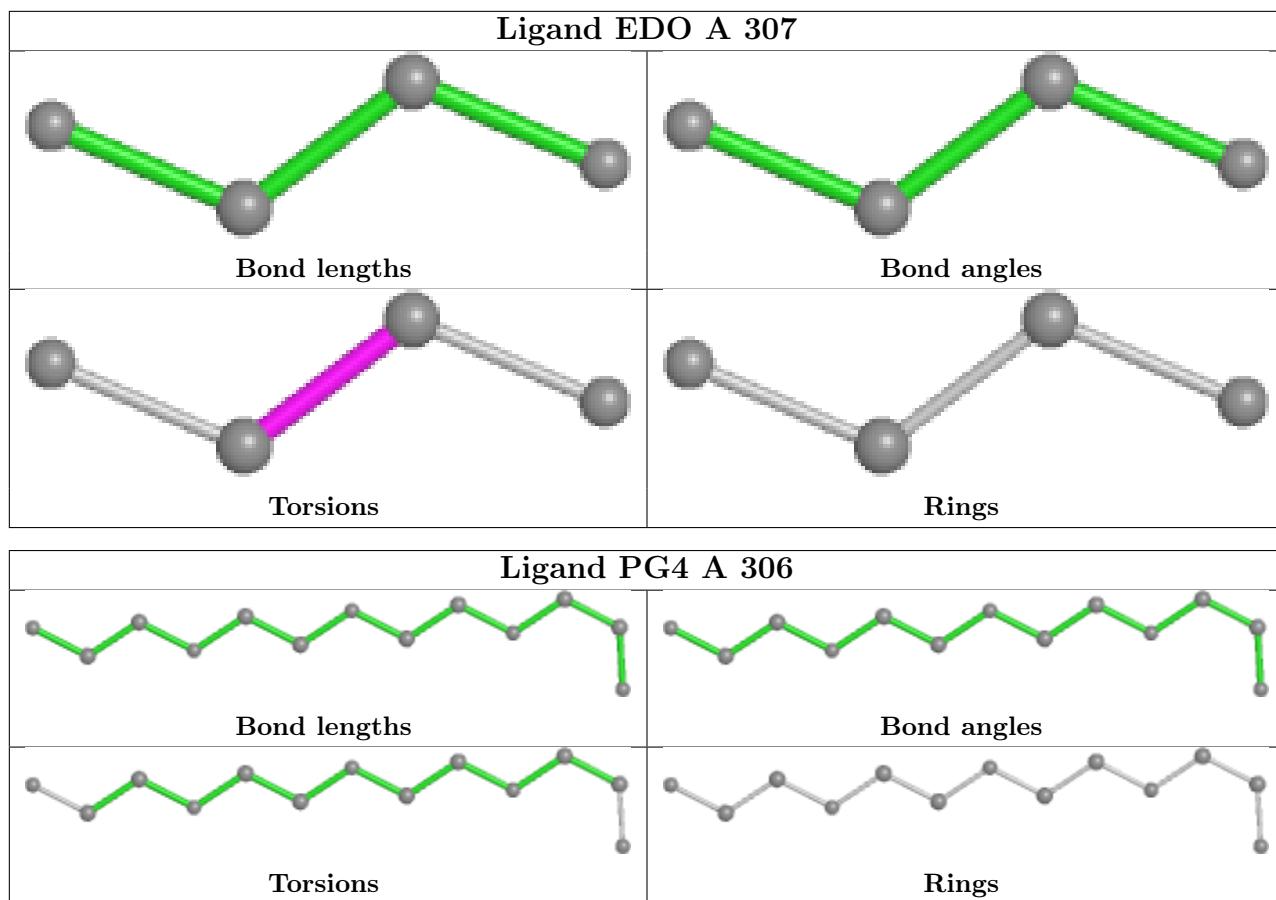












5.7 Other polymers [\(i\)](#)

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%)	0.01	2 (0%) 87 92	13, 18, 30, 46	0
1	B	303/310 (97%)	0.04	2 (0%) 87 92	14, 19, 34, 44	0
1	C	295/310 (95%)	0.12	2 (0%) 87 92	15, 20, 34, 44	0
1	D	303/310 (97%)	-0.00	5 (1%) 70 77	14, 19, 33, 43	0
1	E	296/310 (95%)	-0.03	3 (1%) 82 87	14, 18, 31, 45	0
1	F	295/310 (95%)	0.13	3 (1%) 82 87	15, 20, 34, 47	0
All	All	1787/1860 (96%)	0.04	17 (0%) 82 87	13, 19, 33, 47	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	ASP	3.1
1	D	130	VAL	3.1
1	F	283	PHE	3.0
1	E	56	TRP	2.8
1	B	2	ASP	2.5
1	D	56	TRP	2.5
1	D	95[A]	PHE	2.5
1	A	283	PHE	2.4
1	D	99	HIS	2.3
1	F	29	ARG	2.2
1	C	268	SER	2.2
1	B	19	ASN	2.1
1	E	280	LYS	2.1
1	F	280	LYS	2.1
1	A	280	LYS	2.1
1	D	131	ASP	2.1
1	C	280	LYS	2.0

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	A	166	14/15	0.64	0.23	20,20,20,20	0
1	KPI	B	166	14/15	0.65	0.22	20,20,20,20	0
1	KPI	C	166	14/15	0.65	0.24	20,20,20,20	0
1	KPI	D	166	14/15	0.66	0.22	20,20,20,20	0
1	KPI	E	166	14/15	0.68	0.20	20,20,20,20	0
1	KPI	F	166	14/15	0.75	0.19	20,20,20,20	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
7	ACT	D	309	4/4	0.47	0.28	40,40,42,46	0
7	ACT	A	319	4/4	0.48	0.29	20,39,43,44	0
6	PEG	E	313	7/7	0.66	0.26	25,31,45,48	0
7	ACT	D	310	4/4	0.69	0.20	36,40,42,44	0
5	EDO	E	312	4/4	0.72	0.17	38,43,45,48	0
7	ACT	F	312	4/4	0.72	0.26	37,44,47,49	0
9	GOL	C	311	6/6	0.72	0.17	30,34,36,49	0
8	PGE	D	313	10/10	0.73	0.16	40,45,48,51	0
5	EDO	E	310	4/4	0.76	0.13	33,36,44,44	0
3	MG	E	305	1/1	0.76	0.19	41,41,41,41	0
5	EDO	D	306	4/4	0.76	0.18	24,28,31,36	0
5	EDO	A	307	4/4	0.77	0.15	29,31,37,38	0
5	EDO	F	306	4/4	0.77	0.16	32,35,38,45	0
8	PGE	E	315	10/10	0.77	0.17	31,36,41,55	0
5	EDO	B	306	4/4	0.77	0.34	27,34,36,48	0
3	MG	B	304	1/1	0.78	0.28	50,50,50,50	0

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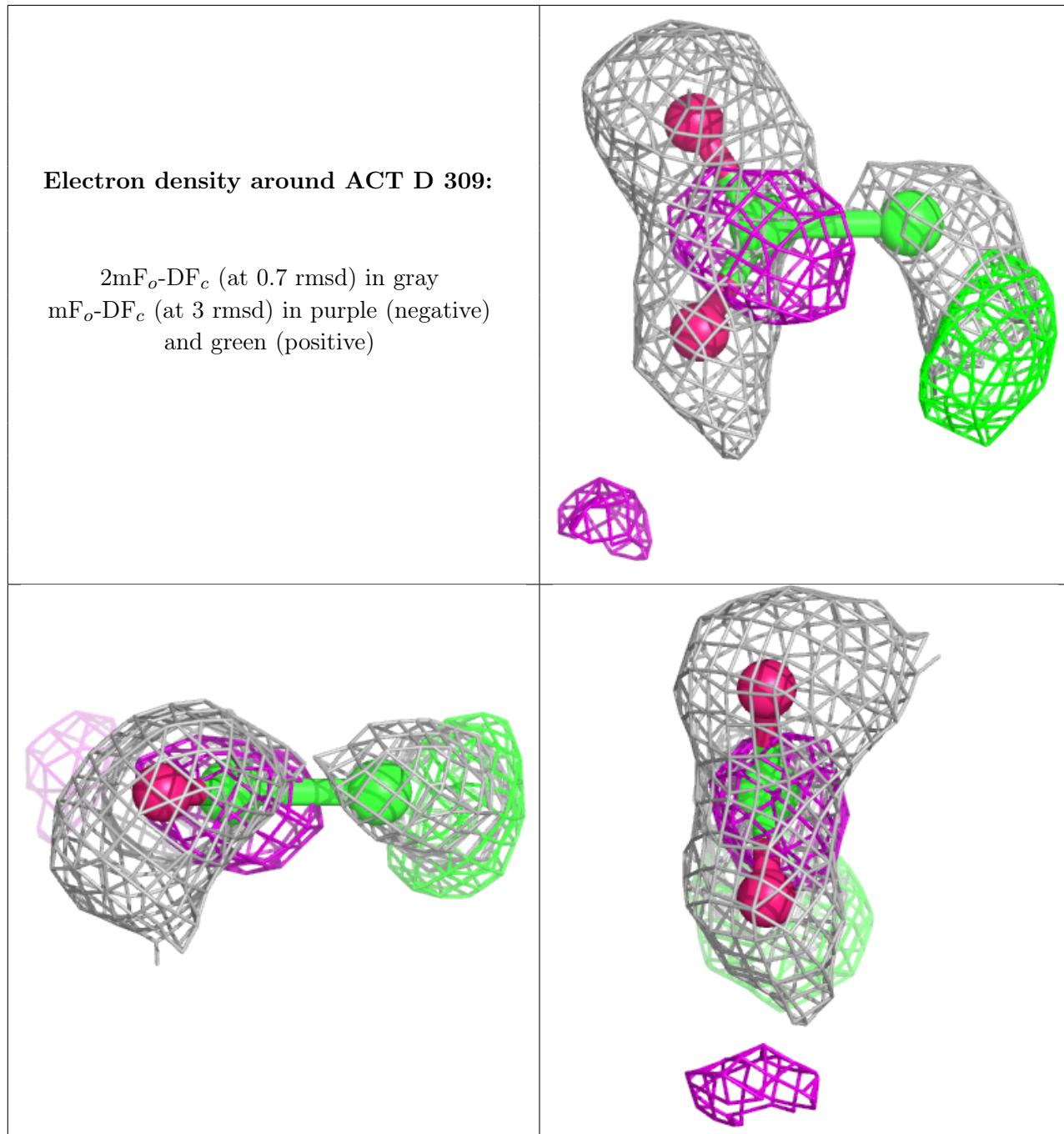
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	F	308	7/7	0.80	0.12	33,38,47,47	0
8	PGE	B	316	10/10	0.81	0.26	24,46,58,62	0
5	EDO	A	313	4/4	0.82	0.15	26,26,34,36	0
3	MG	B	303	1/1	0.82	0.22	46,46,46,46	0
7	ACT	D	311	4/4	0.82	0.14	34,37,44,51	0
6	PEG	B	312	7/7	0.82	0.16	29,36,48,50	0
5	EDO	C	306	4/4	0.84	0.16	38,38,38,39	0
5	EDO	A	310	4/4	0.84	0.14	39,41,46,46	0
5	EDO	E	308	4/4	0.84	0.19	26,30,30,31	0
6	PEG	B	311	7/7	0.84	0.17	31,39,47,48	0
6	PEG	B	313	7/7	0.85	0.54	32,34,43,52	0
5	EDO	D	305	4/4	0.85	0.20	27,31,33,48	0
8	PGE	D	314	10/10	0.85	0.19	22,34,39,46	0
3	MG	A	302	1/1	0.85	0.16	41,41,41,41	0
5	EDO	E	307	4/4	0.85	0.14	38,43,46,46	0
6	PEG	A	318	7/7	0.86	0.15	37,41,45,51	0
7	ACT	F	311	4/4	0.86	0.14	33,40,47,51	0
4	PG4	E	306	13/13	0.86	0.15	24,36,50,51	0
5	EDO	B	308	4/4	0.86	0.14	23,31,37,37	0
5	EDO	C	309	4/4	0.87	0.26	33,41,43,50	0
3	MG	E	304	1/1	0.87	0.13	49,49,49,49	0
5	EDO	A	311	4/4	0.87	0.22	39,40,47,52	0
5	EDO	C	304	4/4	0.87	0.26	35,37,38,43	0
4	PG4	B	305	13/13	0.87	0.16	25,33,50,51	0
7	ACT	A	320	4/4	0.88	0.16	36,42,49,52	0
7	ACT	B	315	4/4	0.88	0.21	36,39,43,44	0
6	PEG	A	317	7/7	0.88	0.13	28,38,44,52	0
4	PG4	C	303	13/13	0.88	0.13	26,33,47,48	0
5	EDO	A	309	4/4	0.89	0.09	30,32,34,40	0
7	ACT	B	314	4/4	0.89	0.13	40,44,46,52	0
7	ACT	E	314	4/4	0.89	0.20	33,36,47,50	0
5	EDO	D	307	4/4	0.89	0.19	26,36,37,42	0
6	PEG	D	308	7/7	0.89	0.16	29,31,43,43	0
6	PEG	F	309	7/7	0.90	0.19	40,46,53,64	0
7	ACT	F	310	4/4	0.90	0.15	35,36,41,41	0
5	EDO	E	309	4/4	0.90	0.23	34,40,42,45	0
5	EDO	B	309	4/4	0.90	0.14	37,42,48,49	0
7	ACT	F	313	4/4	0.90	0.09	38,48,52,54	0
5	EDO	A	316	4/4	0.90	0.11	39,43,47,52	0
6	PEG	C	310	7/7	0.90	0.17	31,41,46,50	0
5	EDO	A	312	4/4	0.90	0.20	30,35,39,42	0
5	EDO	C	307	4/4	0.90	0.20	29,35,36,55	0

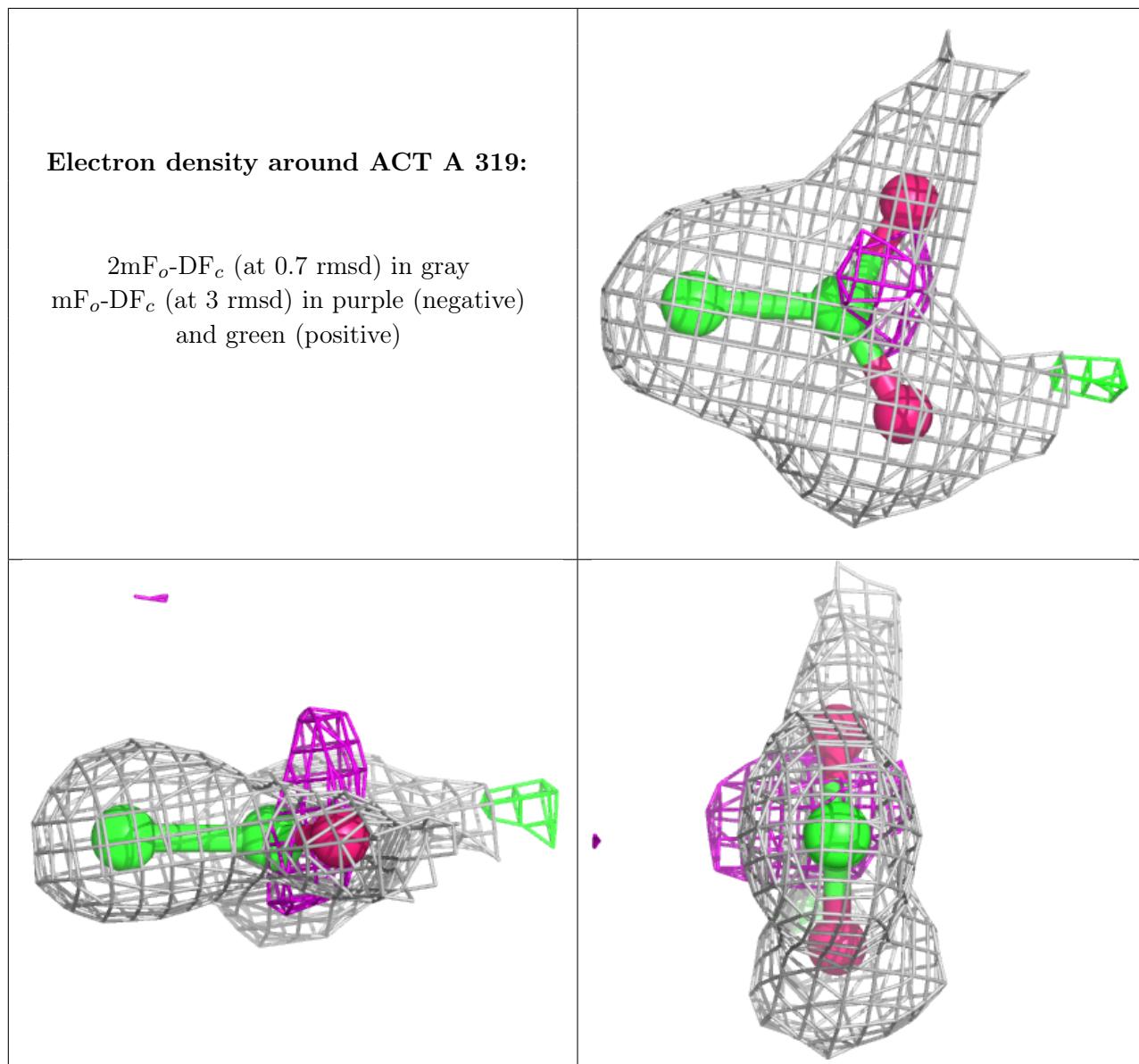
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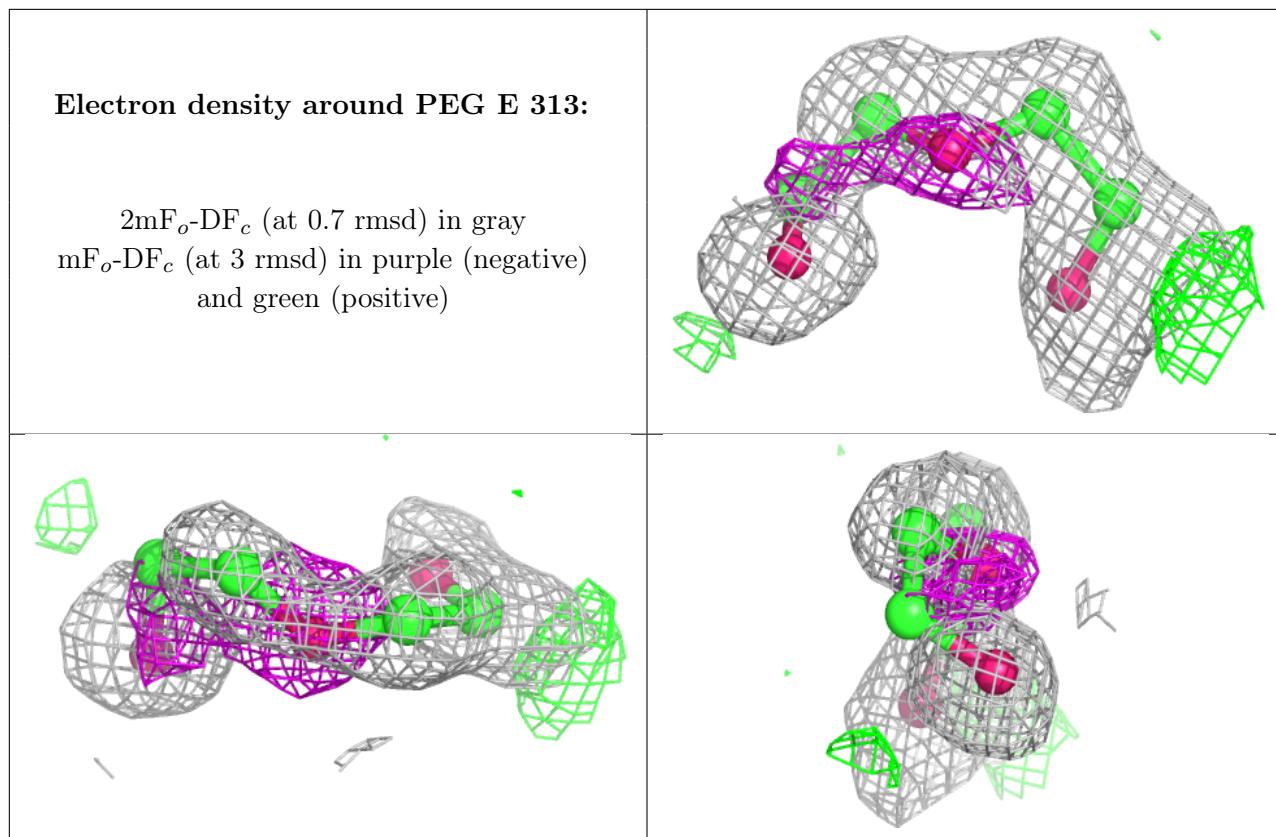
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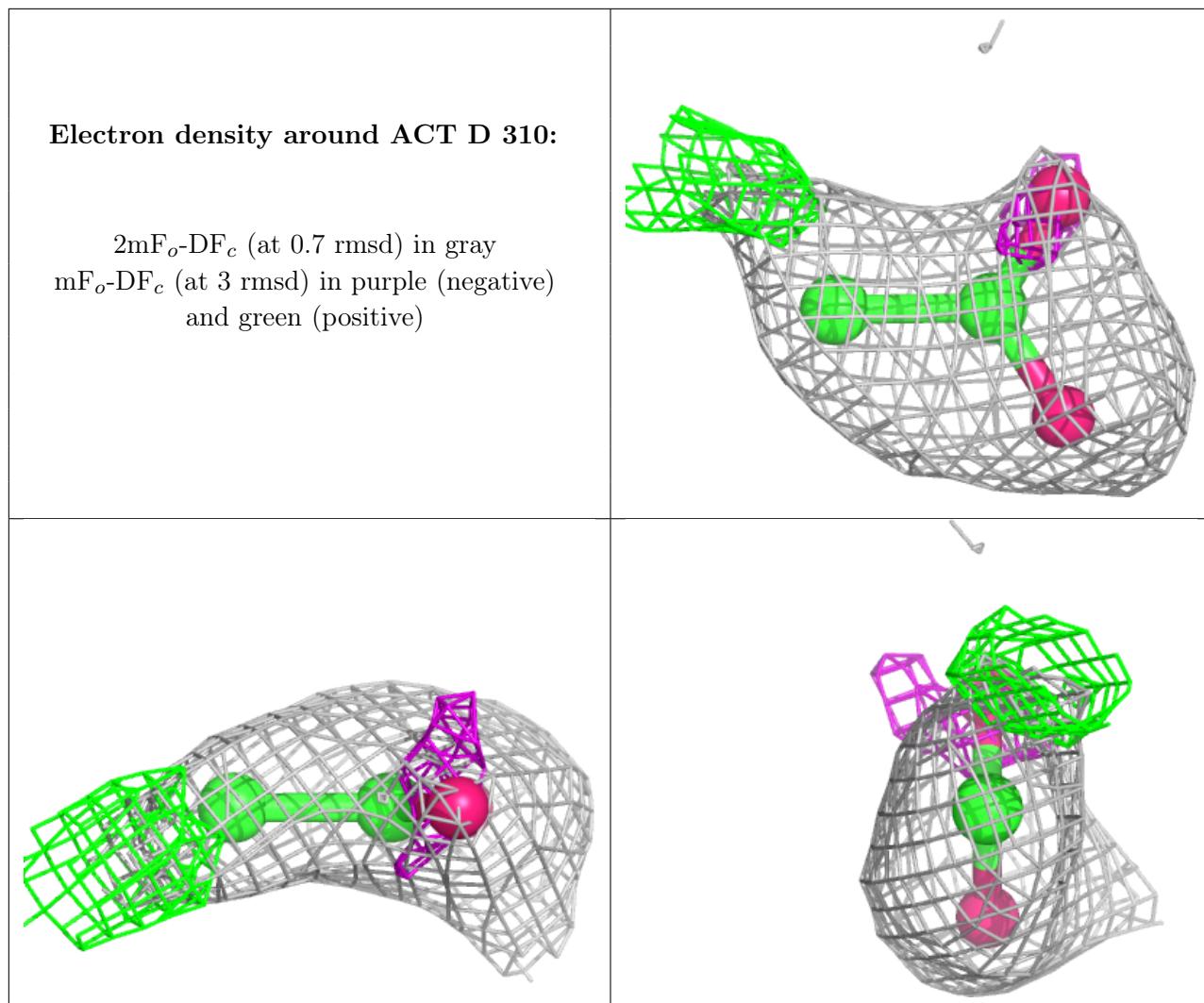
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	305	1/1	0.90	0.10	53,53,53,53	0
5	EDO	A	315	4/4	0.91	0.11	34,38,39,51	0
3	MG	F	304	1/1	0.91	0.10	47,47,47,47	1
4	PG4	F	305	13/13	0.91	0.13	27,32,51,51	0
5	EDO	A	308	4/4	0.92	0.19	22,30,35,36	0
3	MG	C	301	1/1	0.92	0.06	34,34,34,34	0
5	EDO	C	308	4/4	0.92	0.09	35,39,40,48	0
5	EDO	C	305	4/4	0.92	0.12	26,28,32,41	0
4	PG4	D	303	13/13	0.93	0.13	25,31,44,47	0
2	3VN	A	301	22/22	0.93	0.13	14,17,23,25	0
2	3VN	B	301	22/22	0.93	0.11	15,17,23,27	0
5	EDO	B	307	4/4	0.93	0.13	39,40,40,43	0
3	MG	C	302	1/1	0.93	0.09	33,33,33,33	0
7	ACT	D	312	4/4	0.93	0.23	42,43,47,47	0
2	3VN	D	301	22/22	0.93	0.10	14,16,23,26	0
5	EDO	D	304	4/4	0.93	0.10	30,31,33,35	0
5	EDO	F	307	4/4	0.94	0.11	20,25,33,36	0
4	PG4	A	306	13/13	0.95	0.11	26,32,44,49	0
5	EDO	A	314	4/4	0.95	0.09	23,26,26,32	0
5	EDO	B	310	4/4	0.95	0.24	24,30,36,51	0
3	MG	F	303	1/1	0.96	0.15	34,34,34,34	0
3	MG	D	302	1/1	0.97	0.18	30,30,30,30	0
3	MG	E	301	1/1	0.97	0.09	28,28,28,28	0
5	EDO	E	311	4/4	0.98	0.09	18,19,20,20	0
3	MG	E	302	1/1	0.98	0.07	33,33,33,33	0
3	MG	F	301	1/1	0.98	0.17	23,23,23,23	0
3	MG	A	304	1/1	0.98	0.07	19,19,19,19	0
3	MG	A	303	1/1	0.99	0.07	17,17,17,17	0
3	MG	E	303	1/1	0.99	0.08	36,36,36,36	0
3	MG	F	302	1/1	0.99	0.16	29,29,29,29	0
3	MG	B	302	1/1	0.99	0.11	29,29,29,29	0

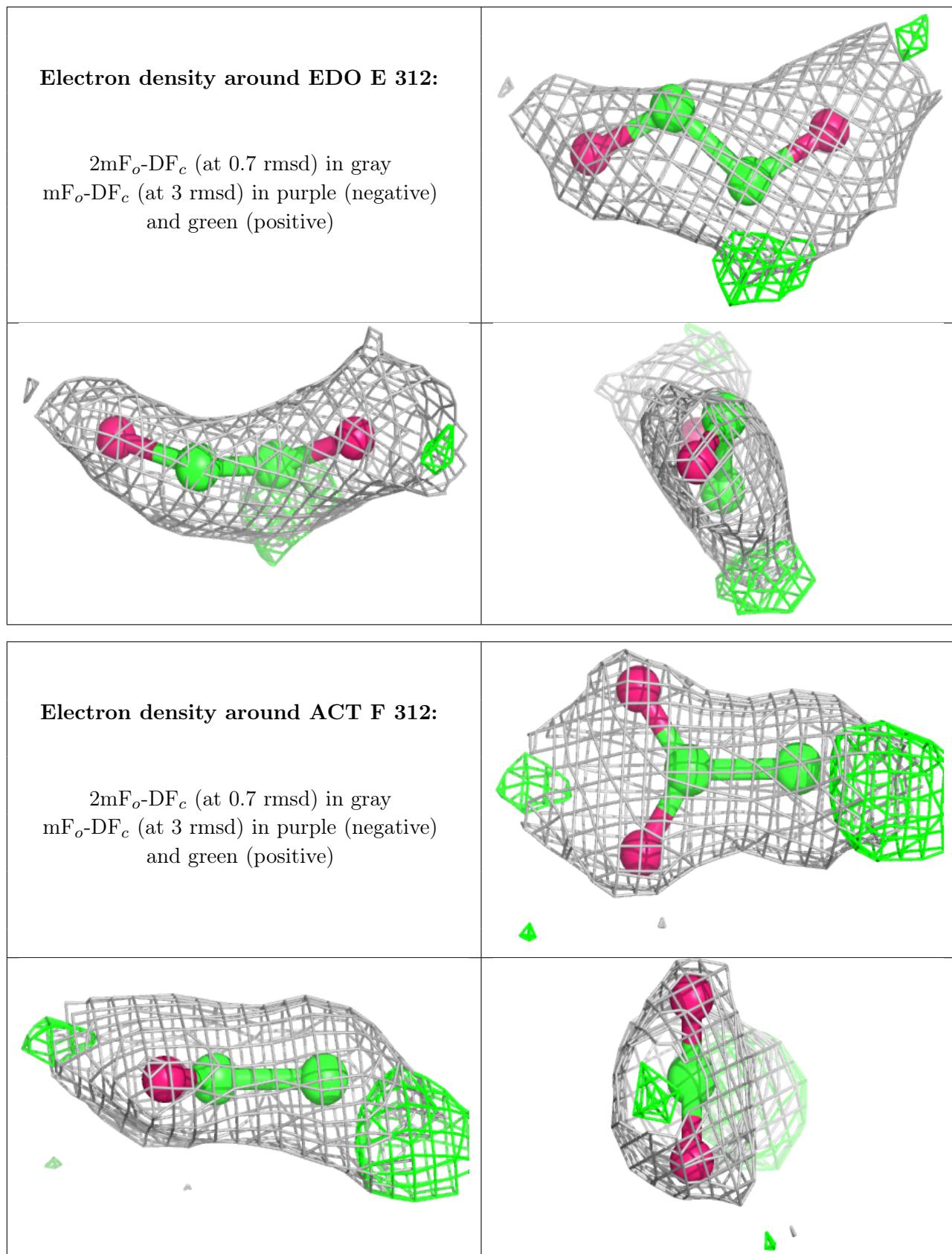
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

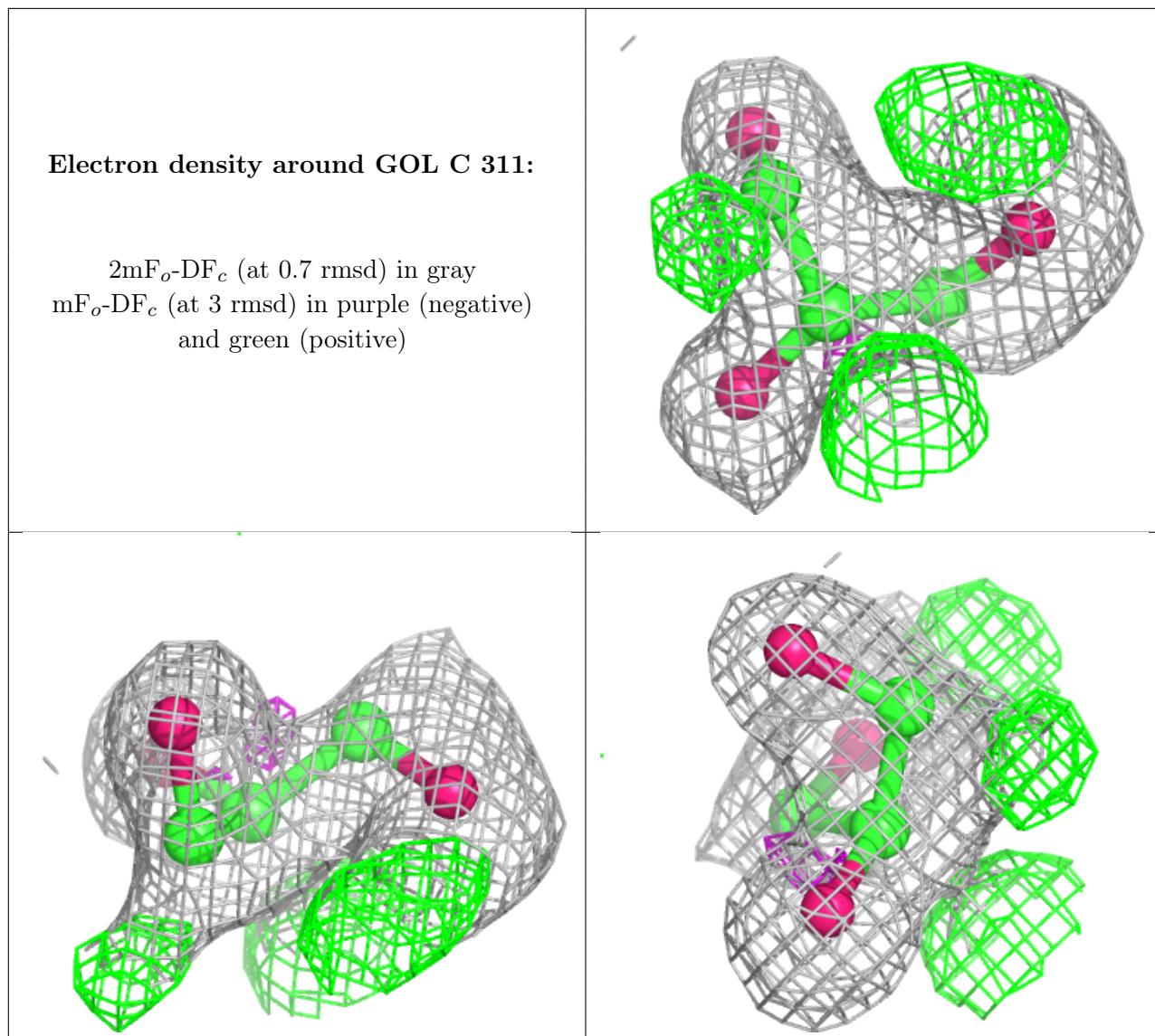


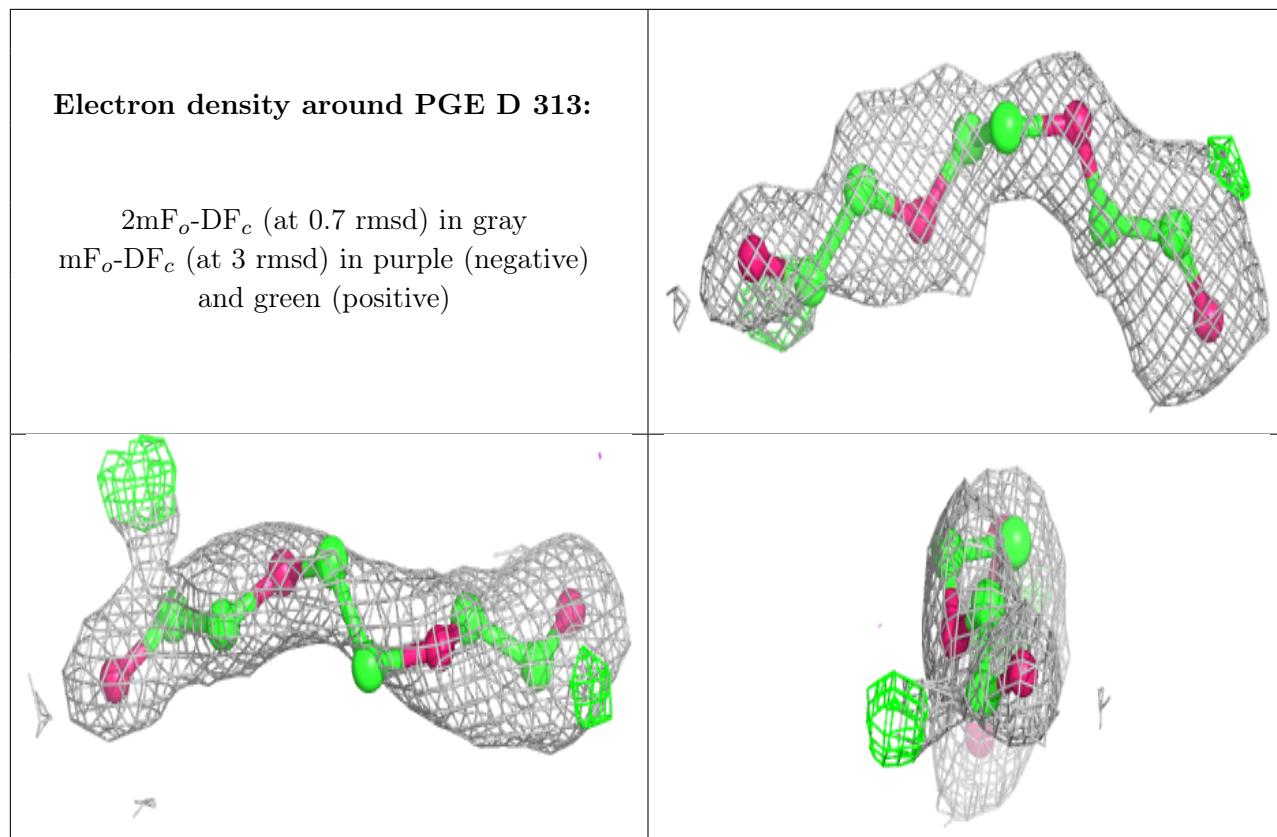


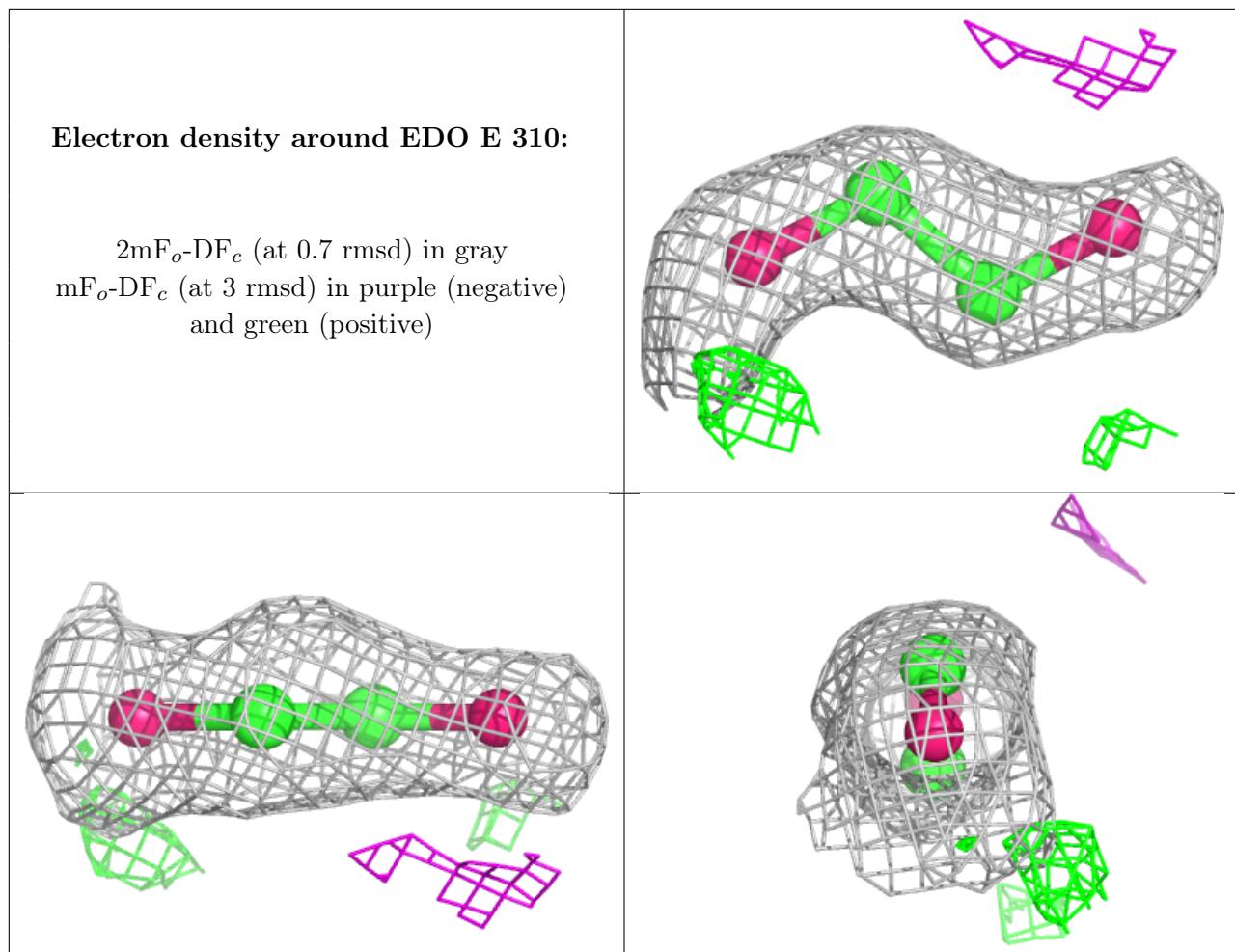


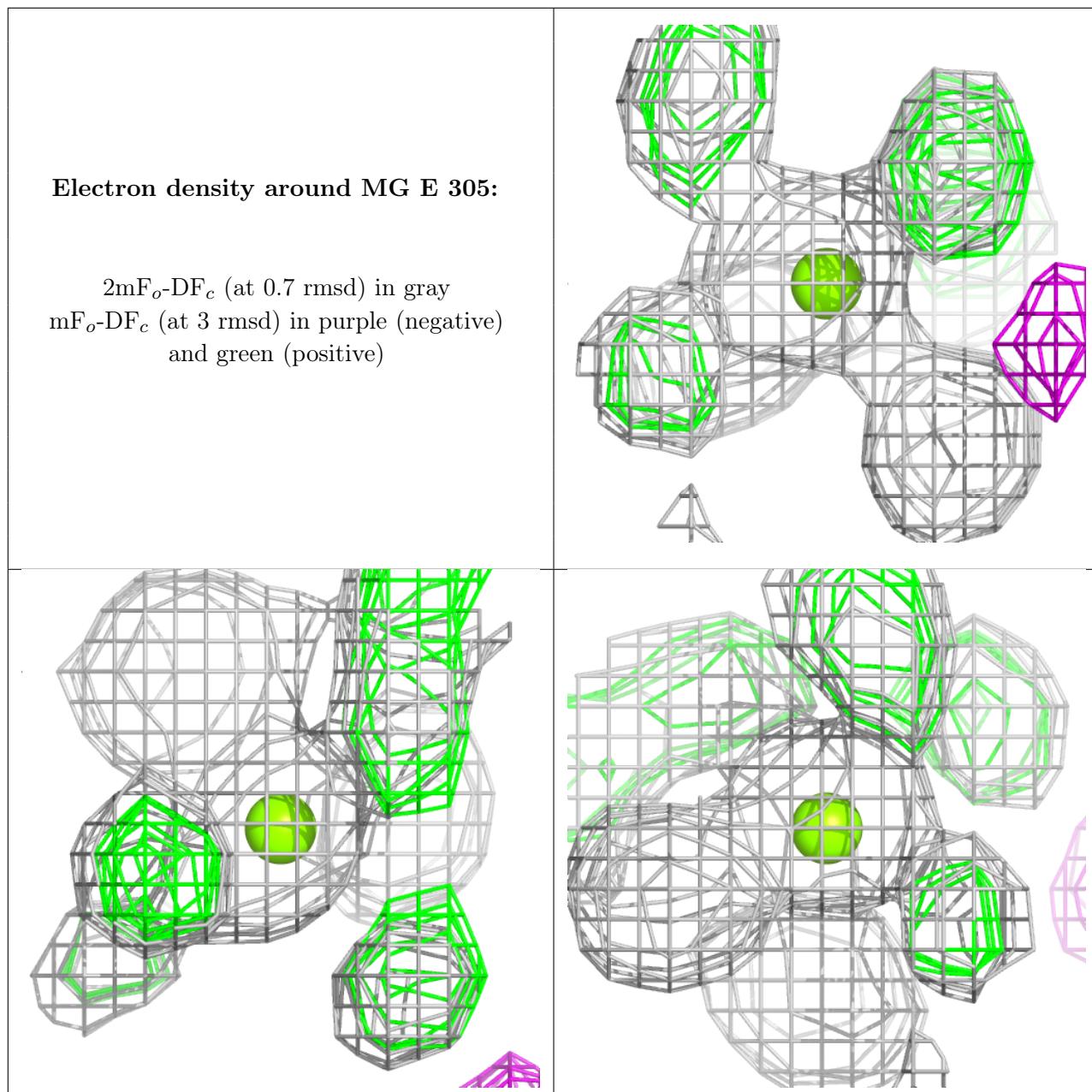


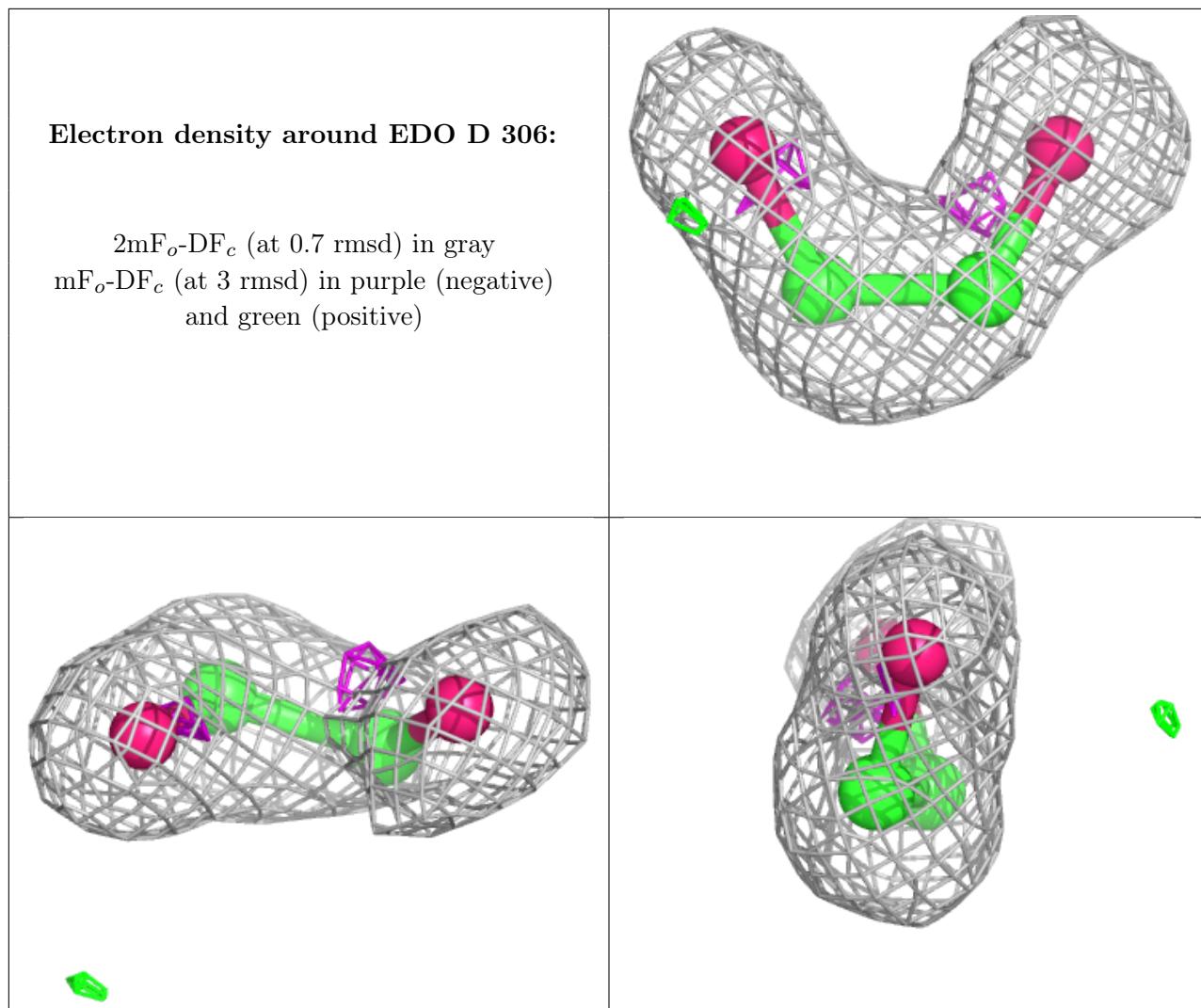


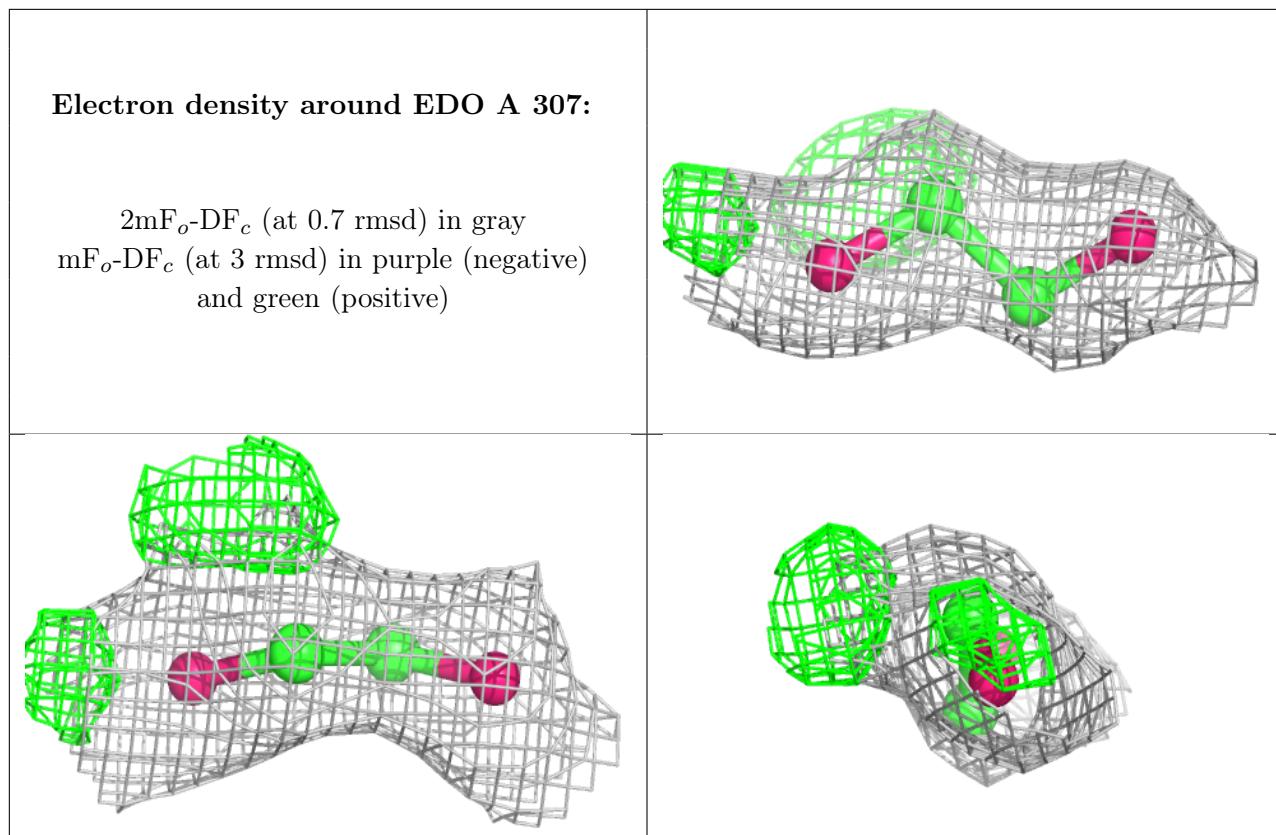


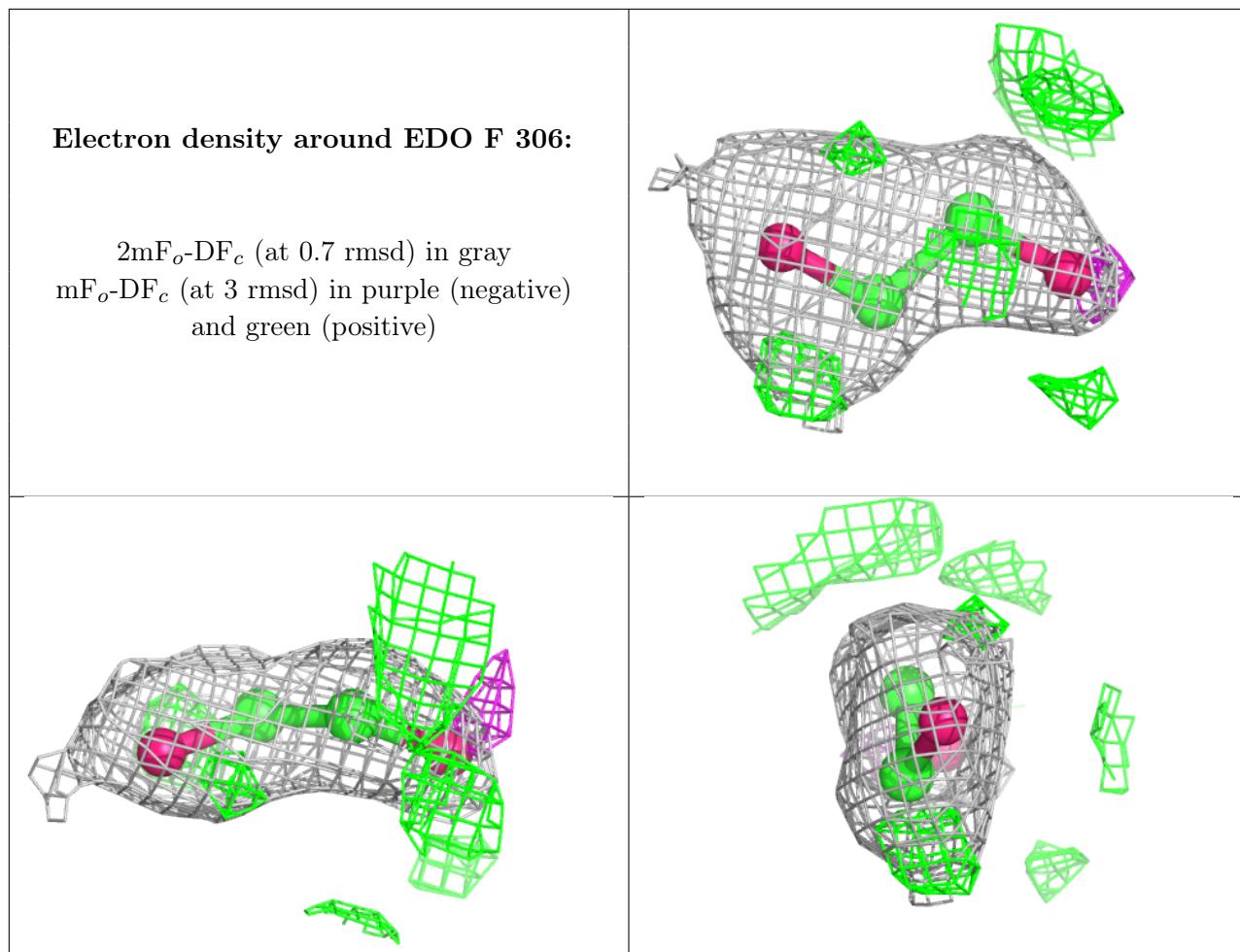


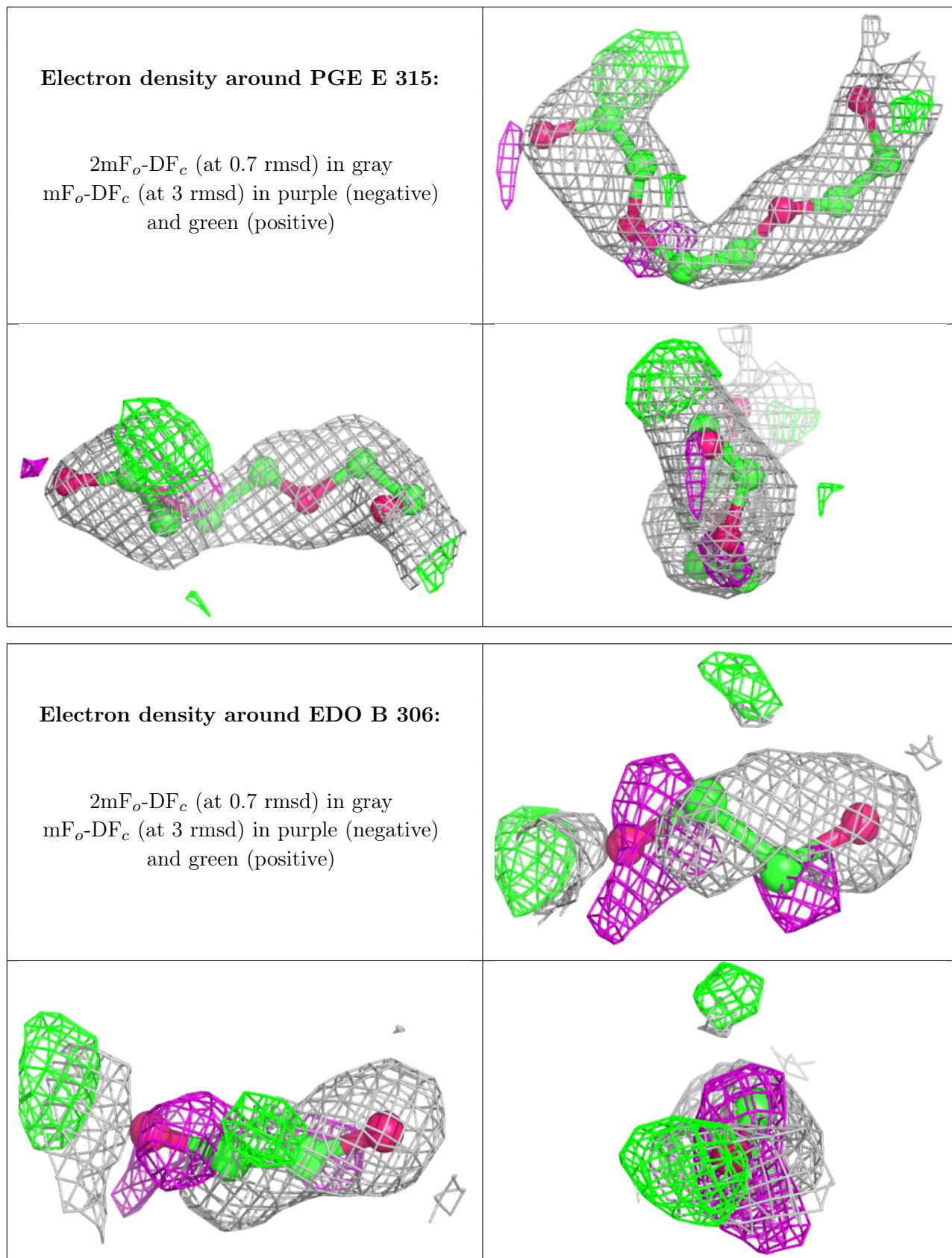


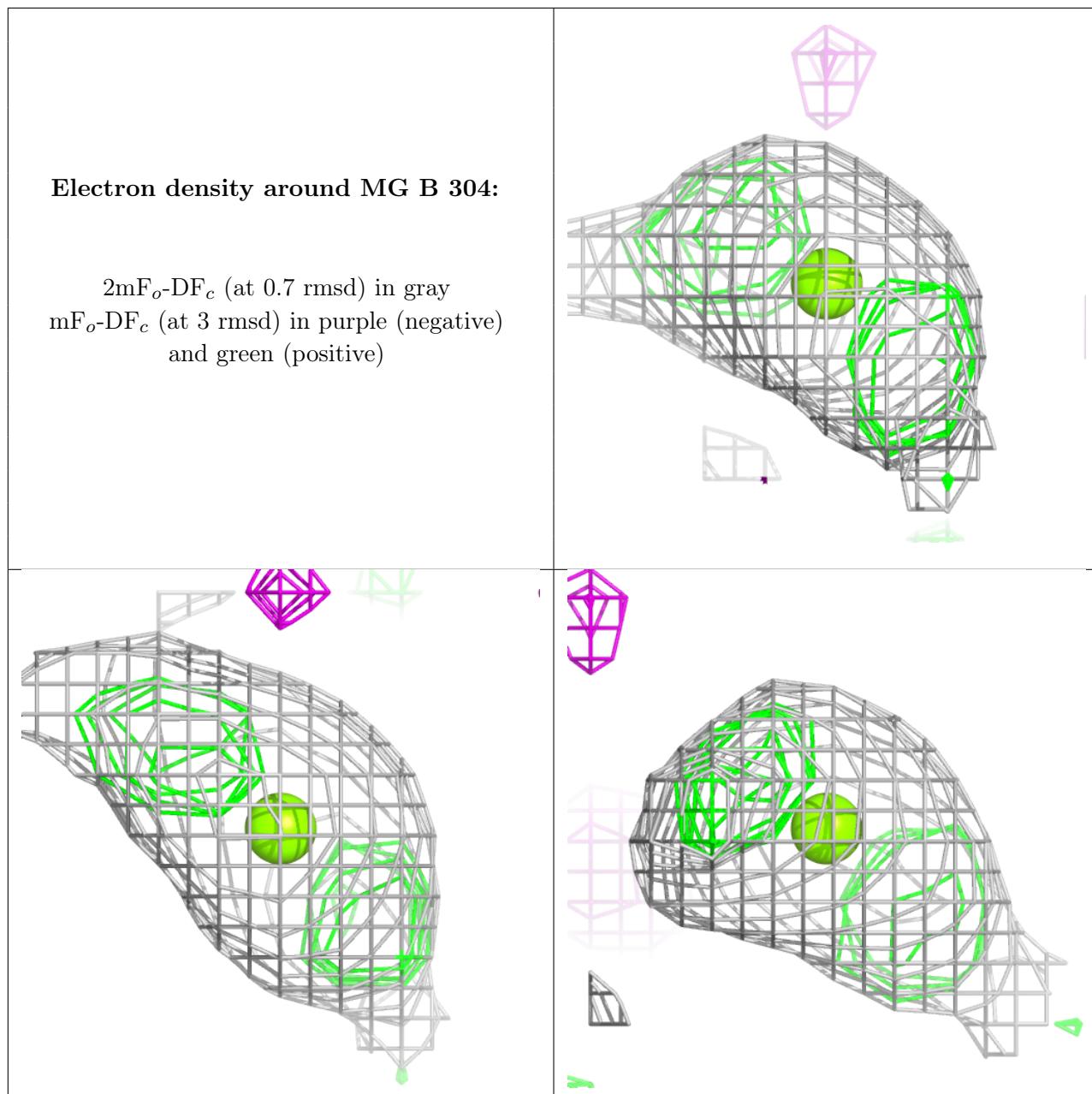


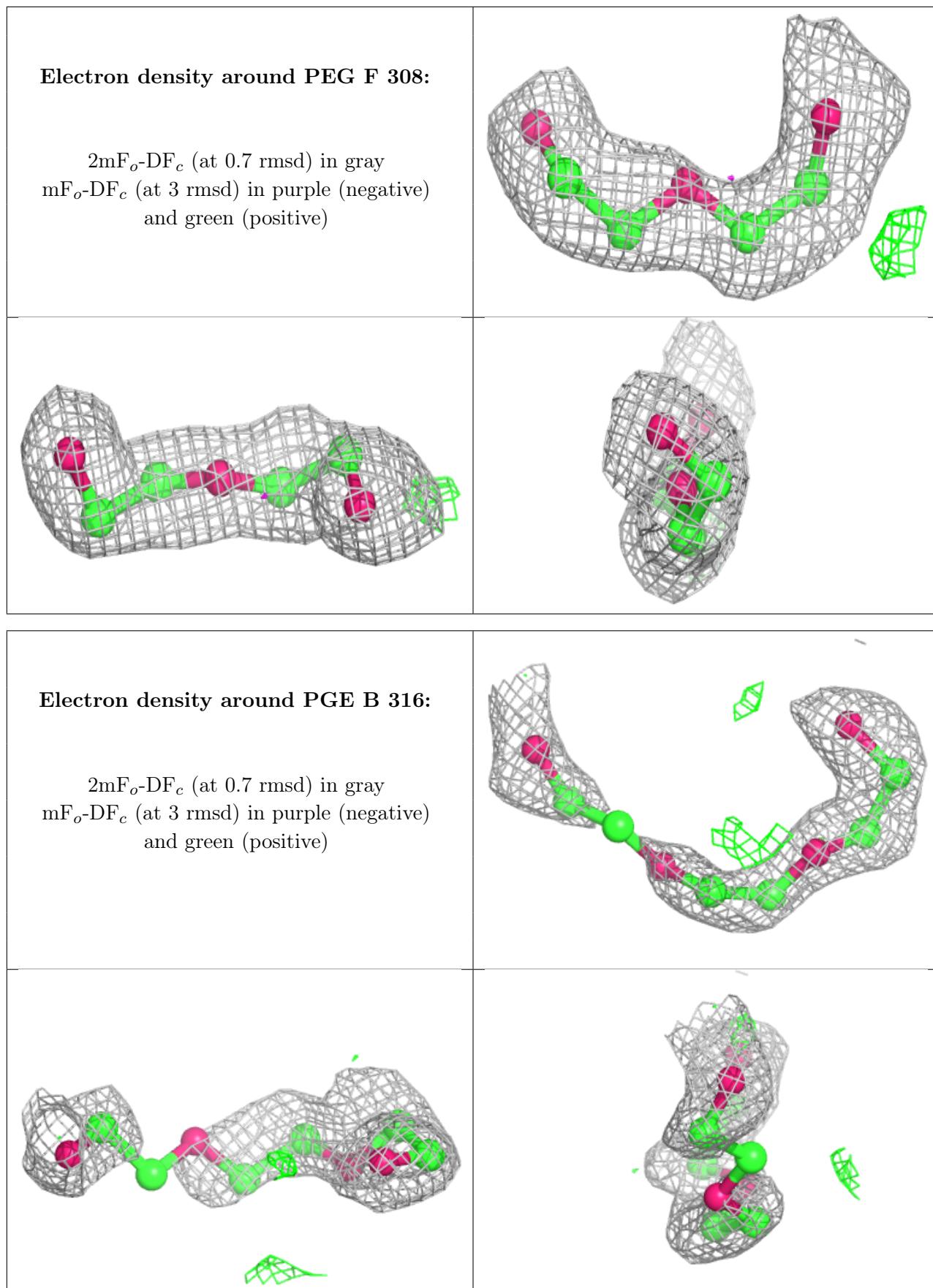


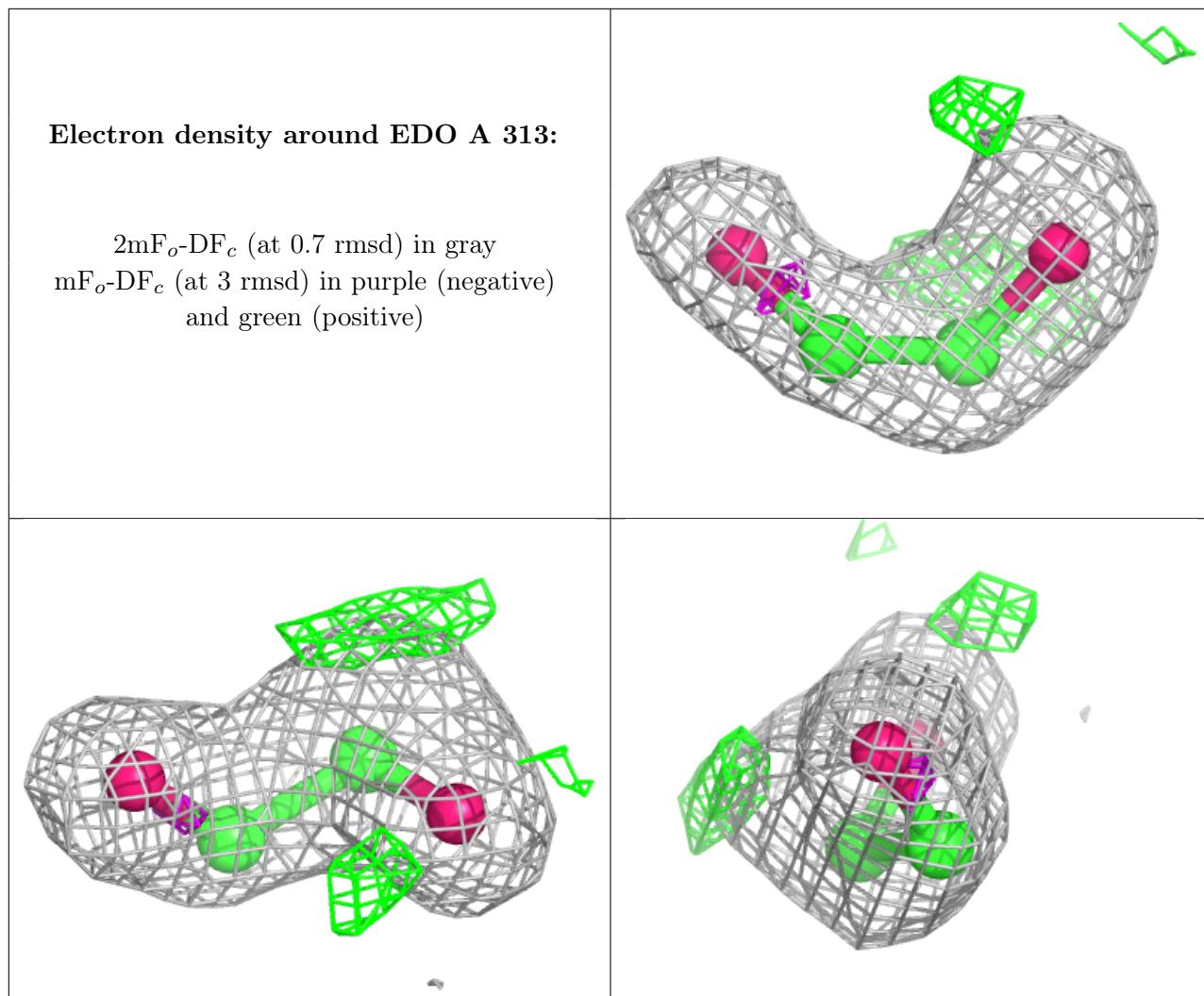


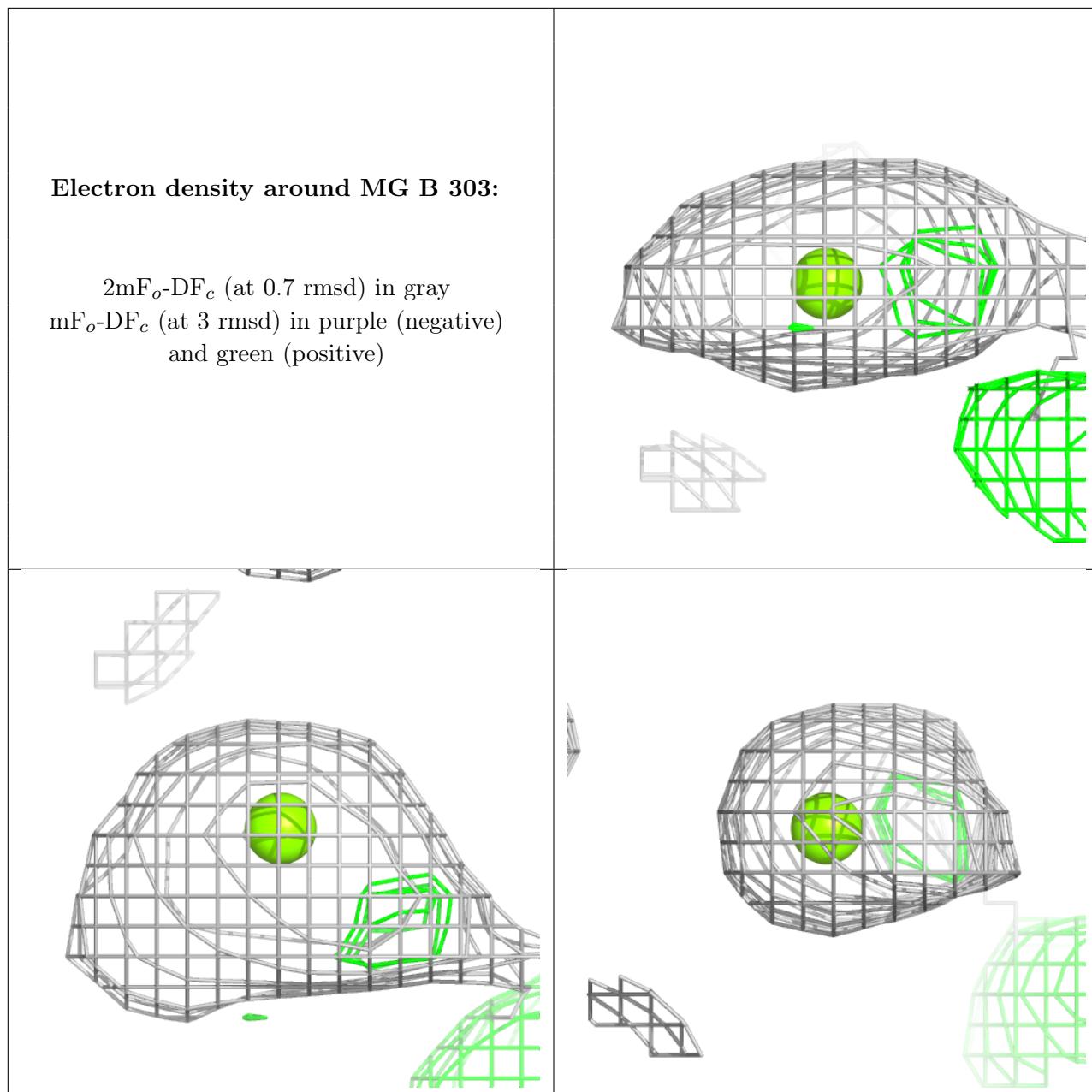


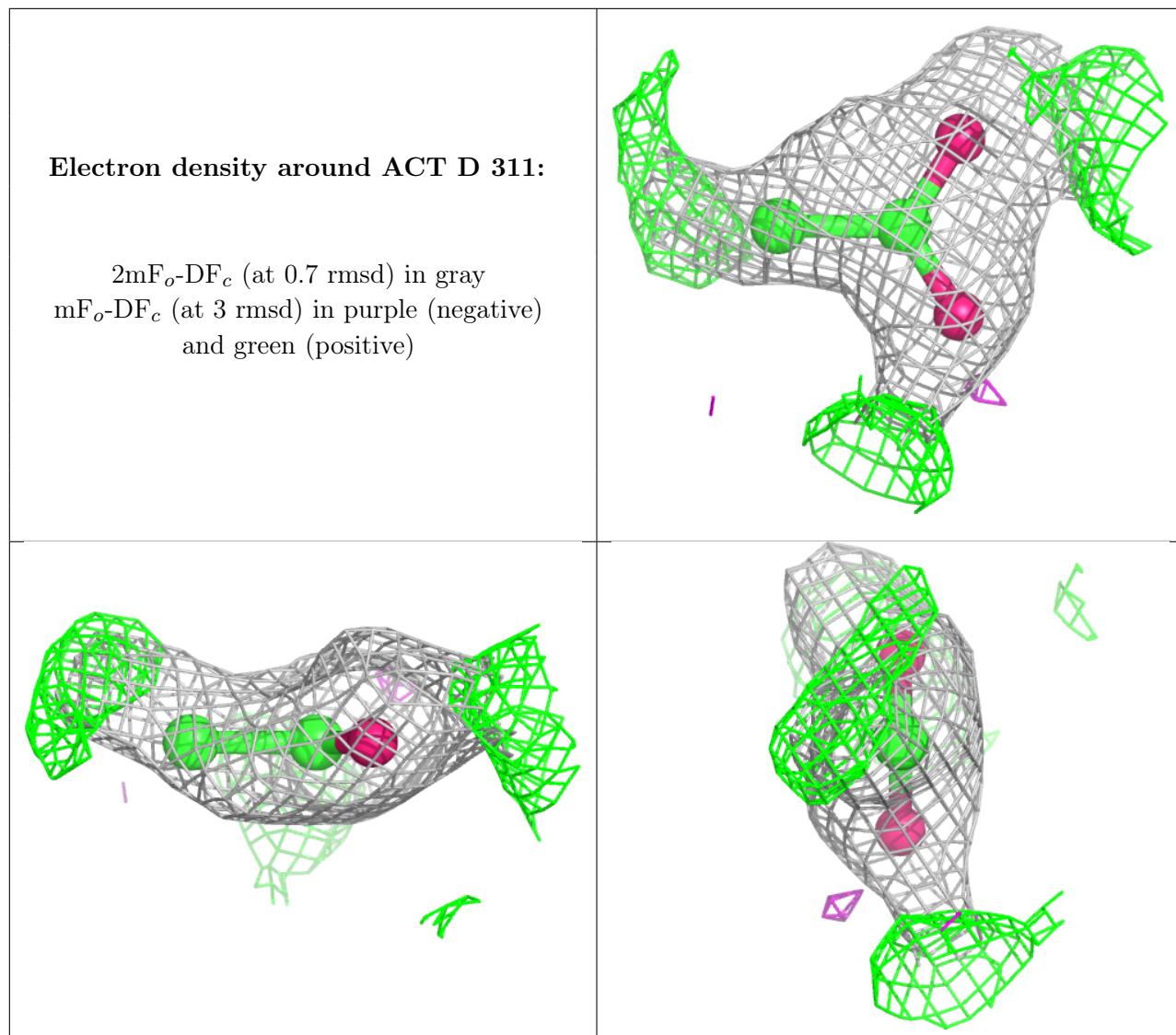


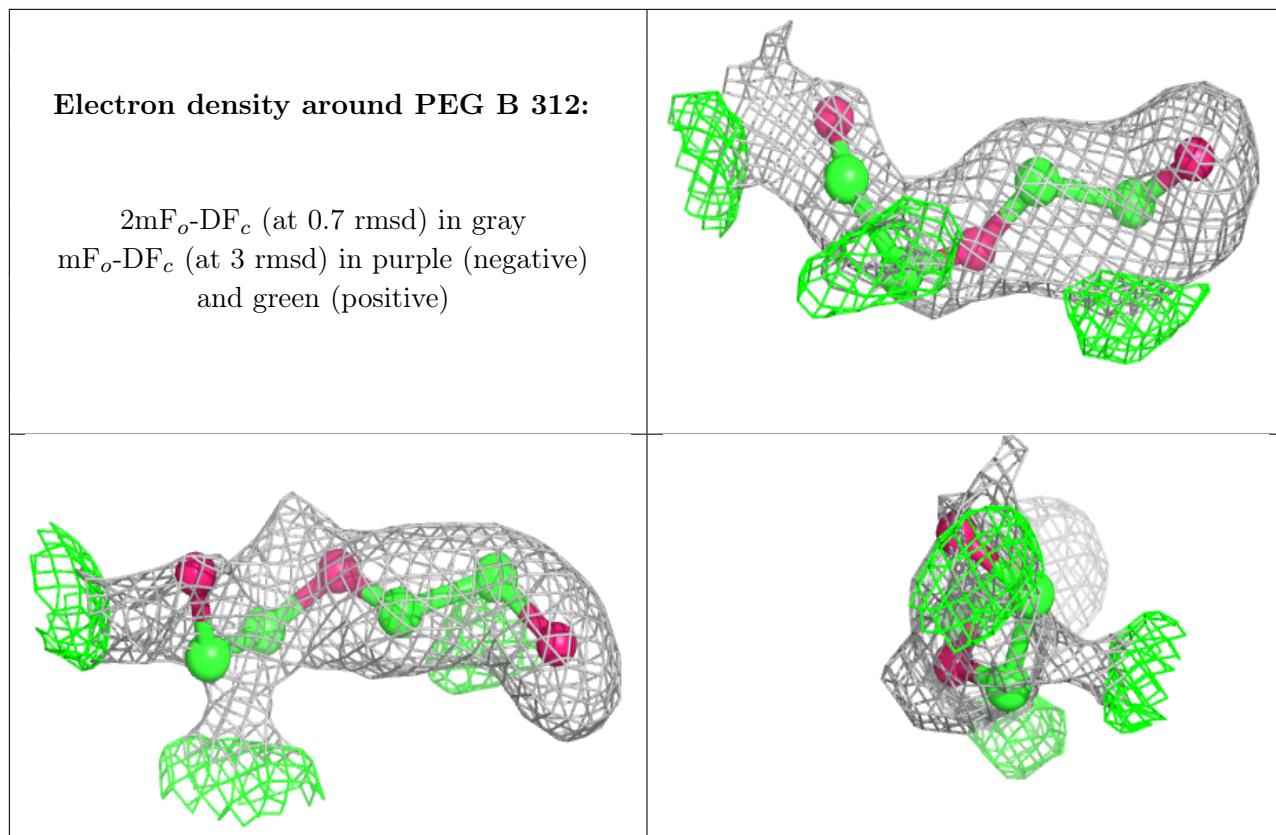


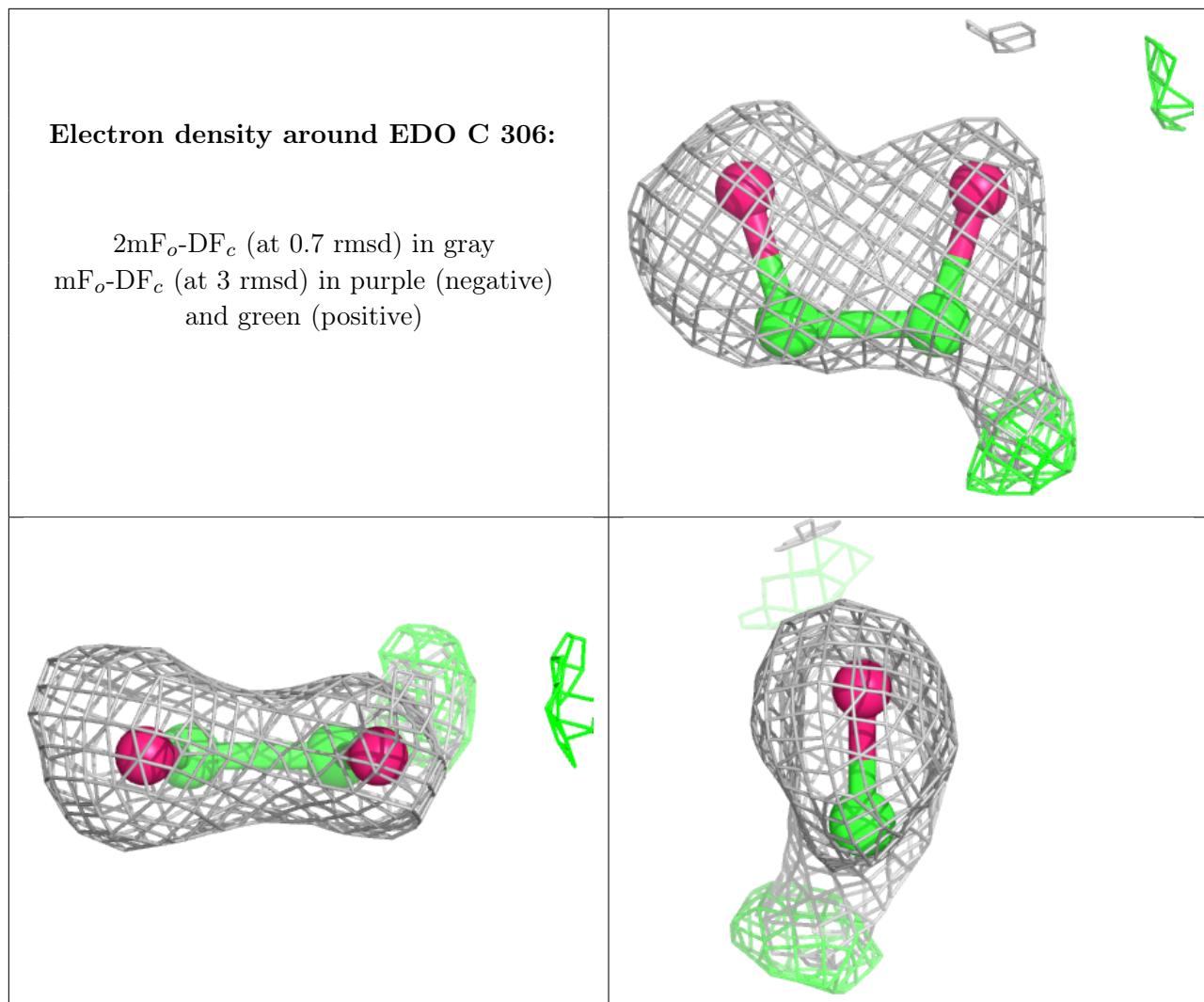


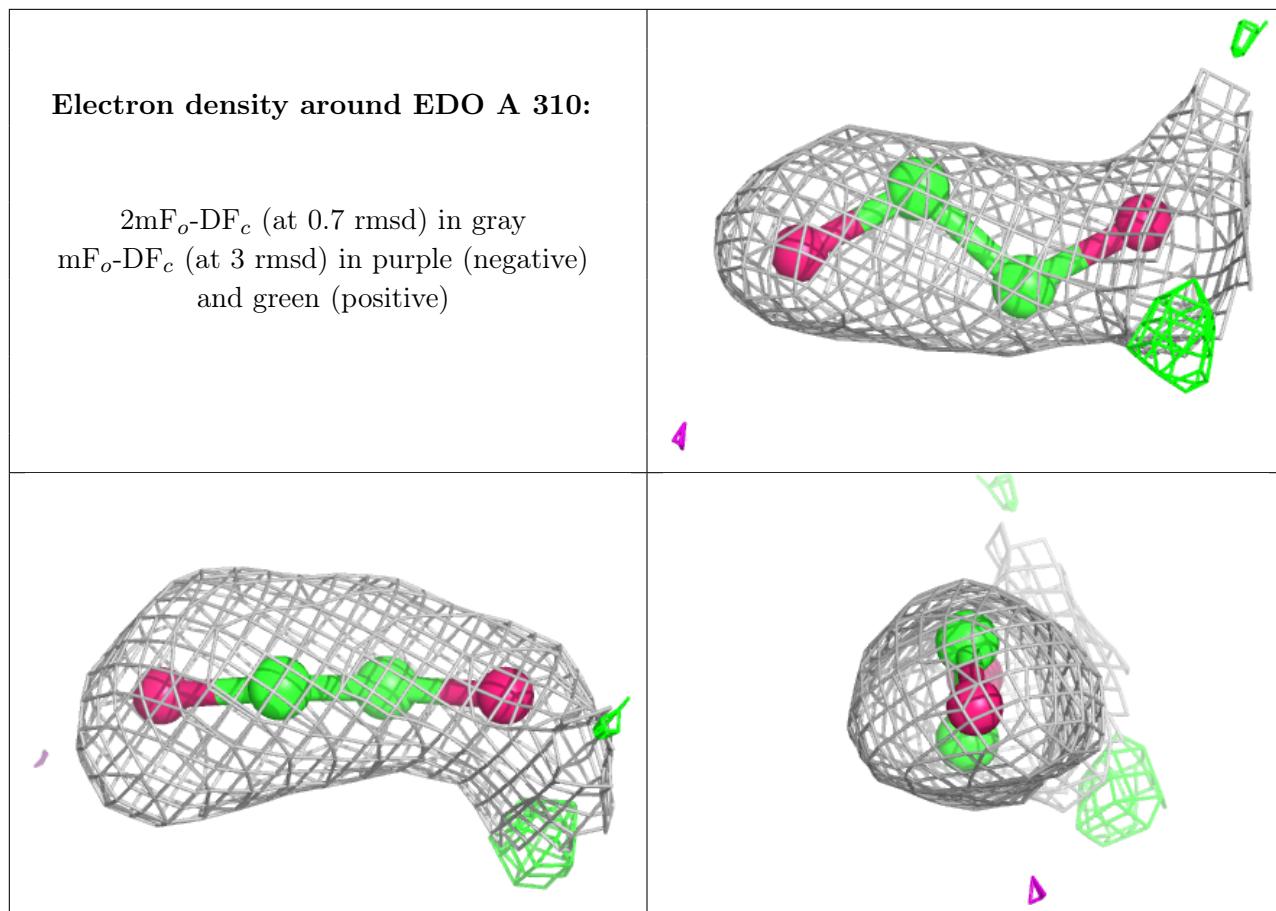


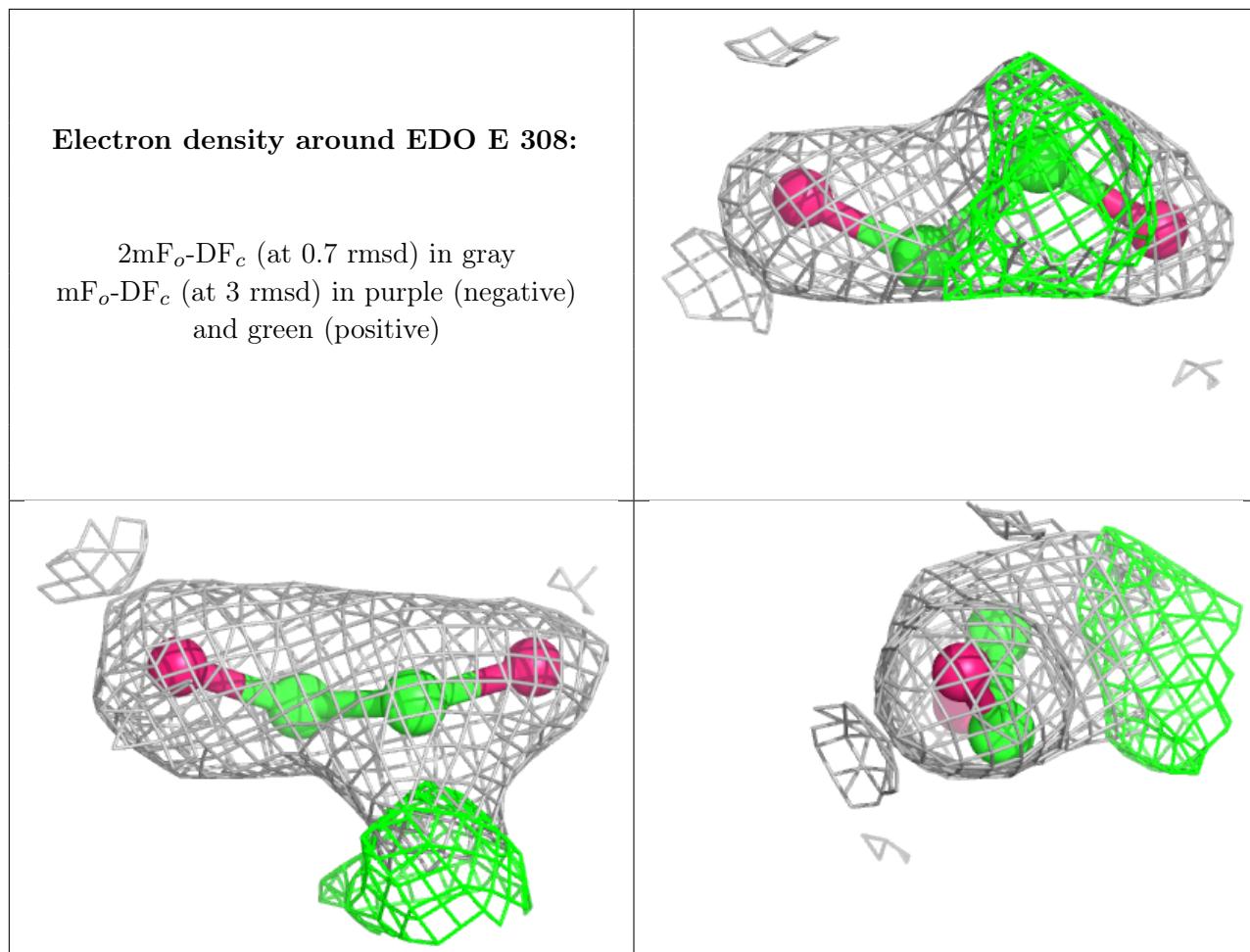


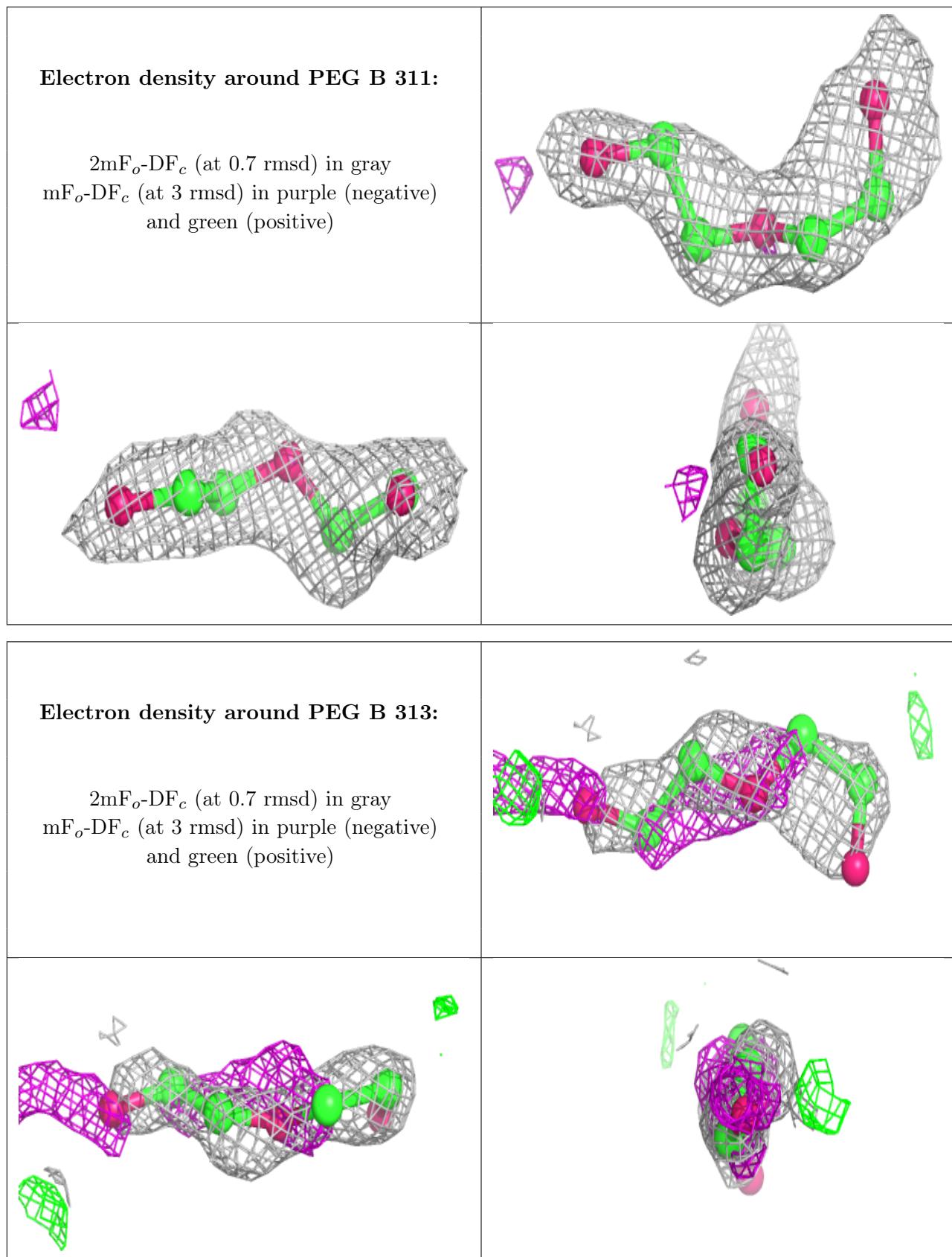


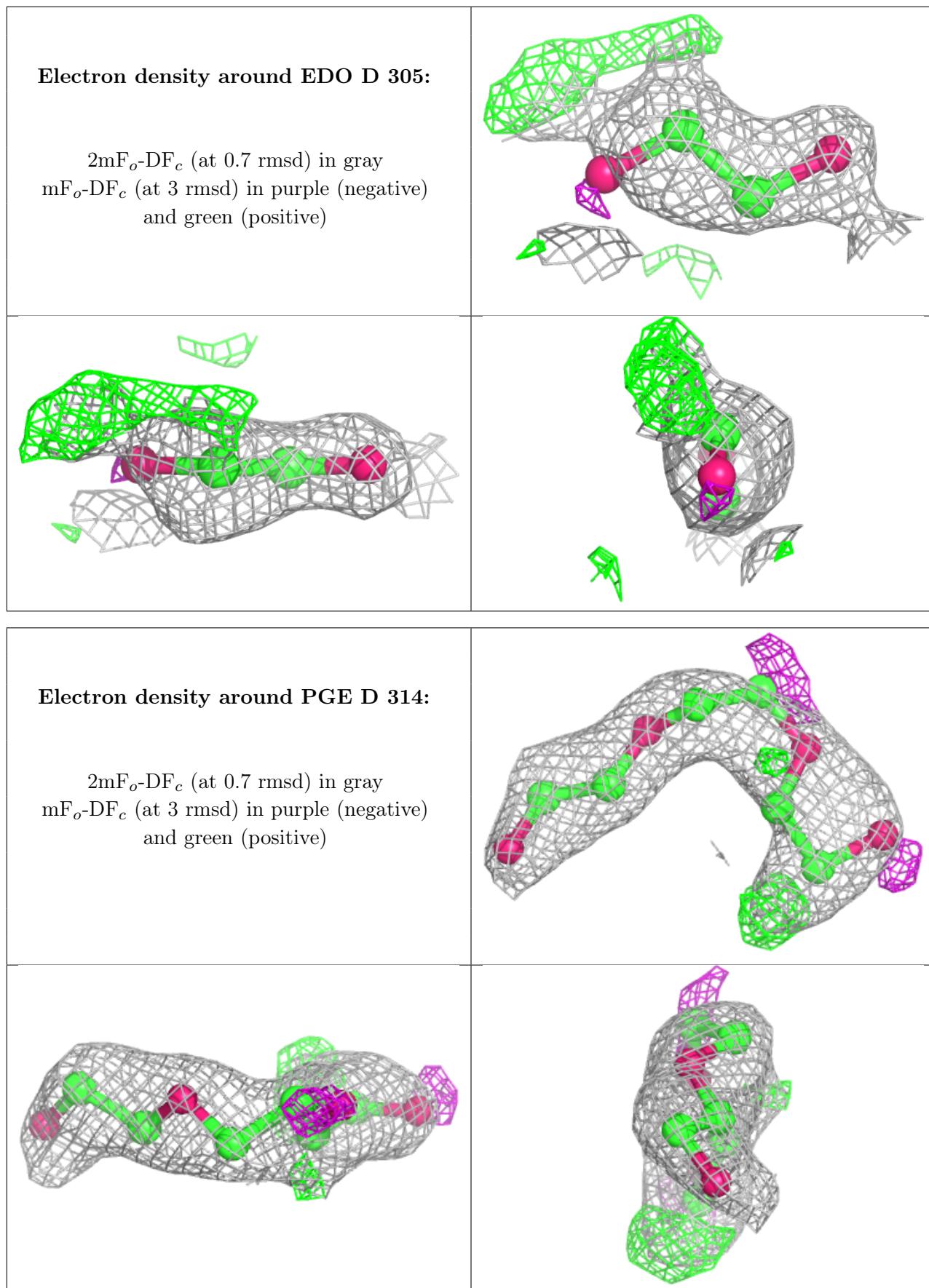


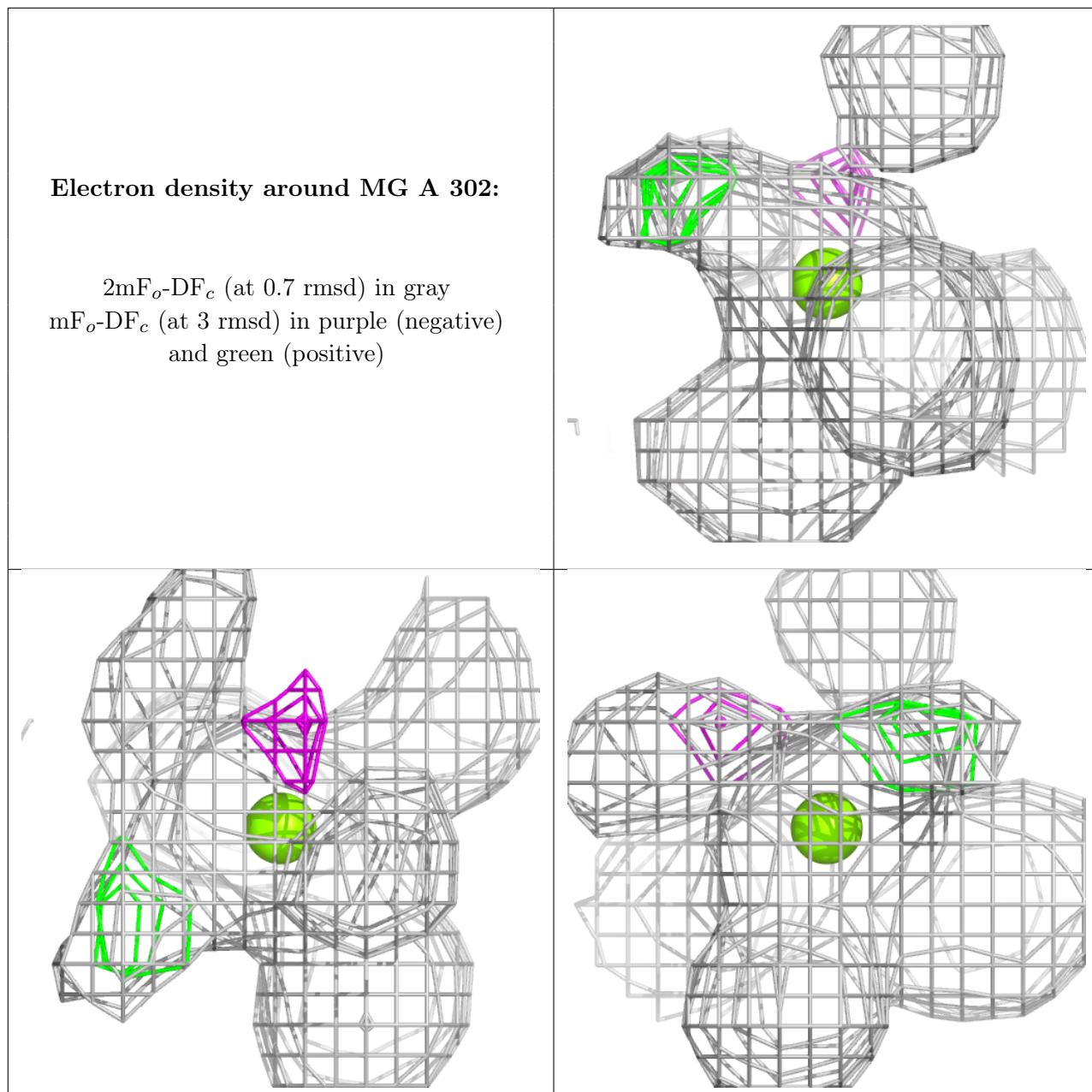


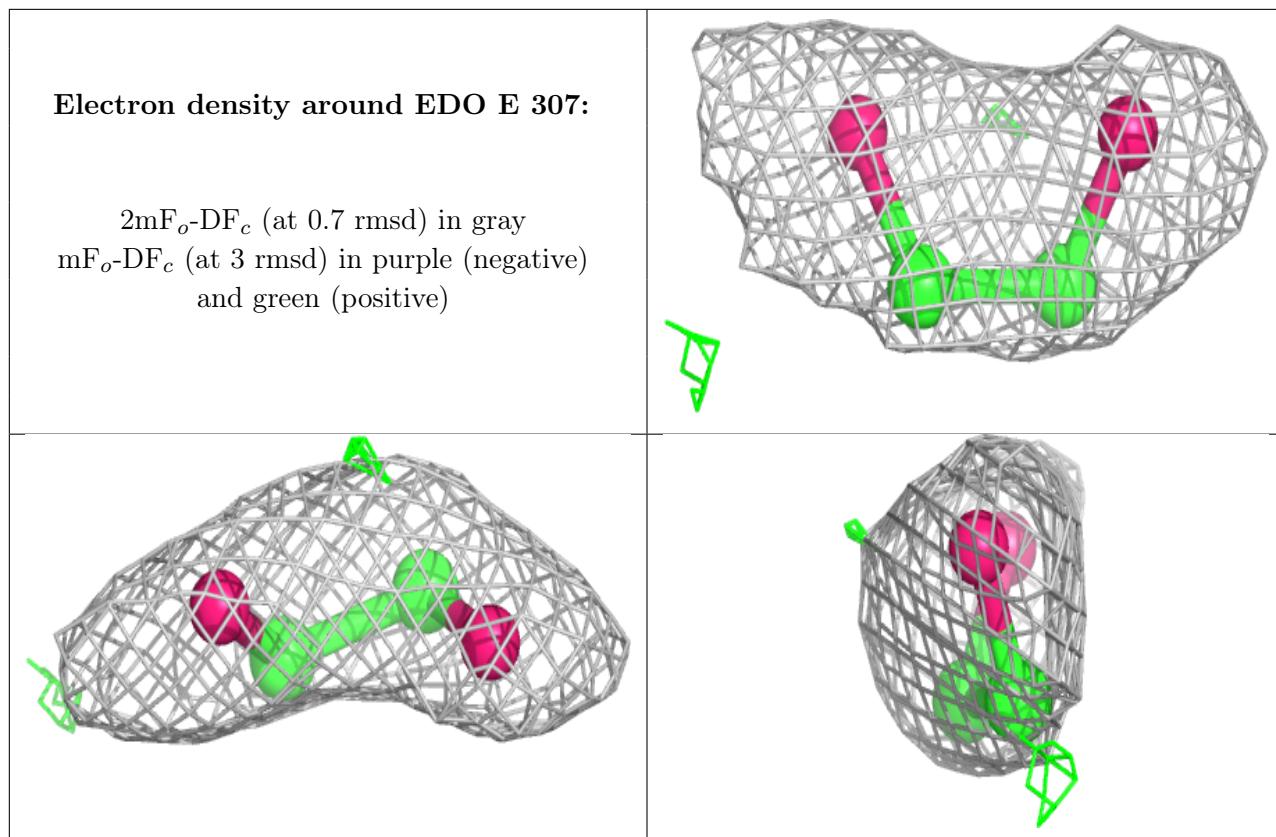


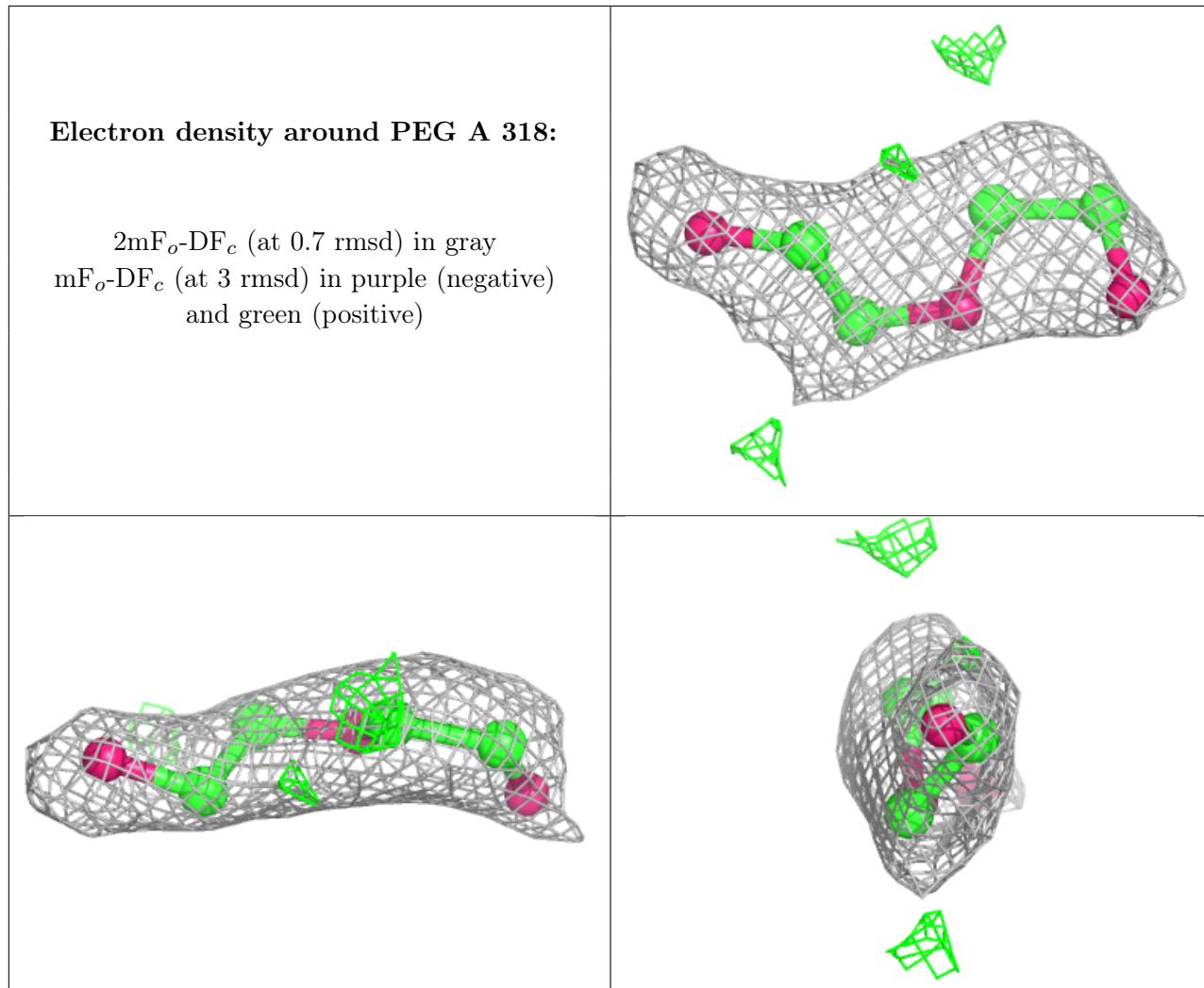


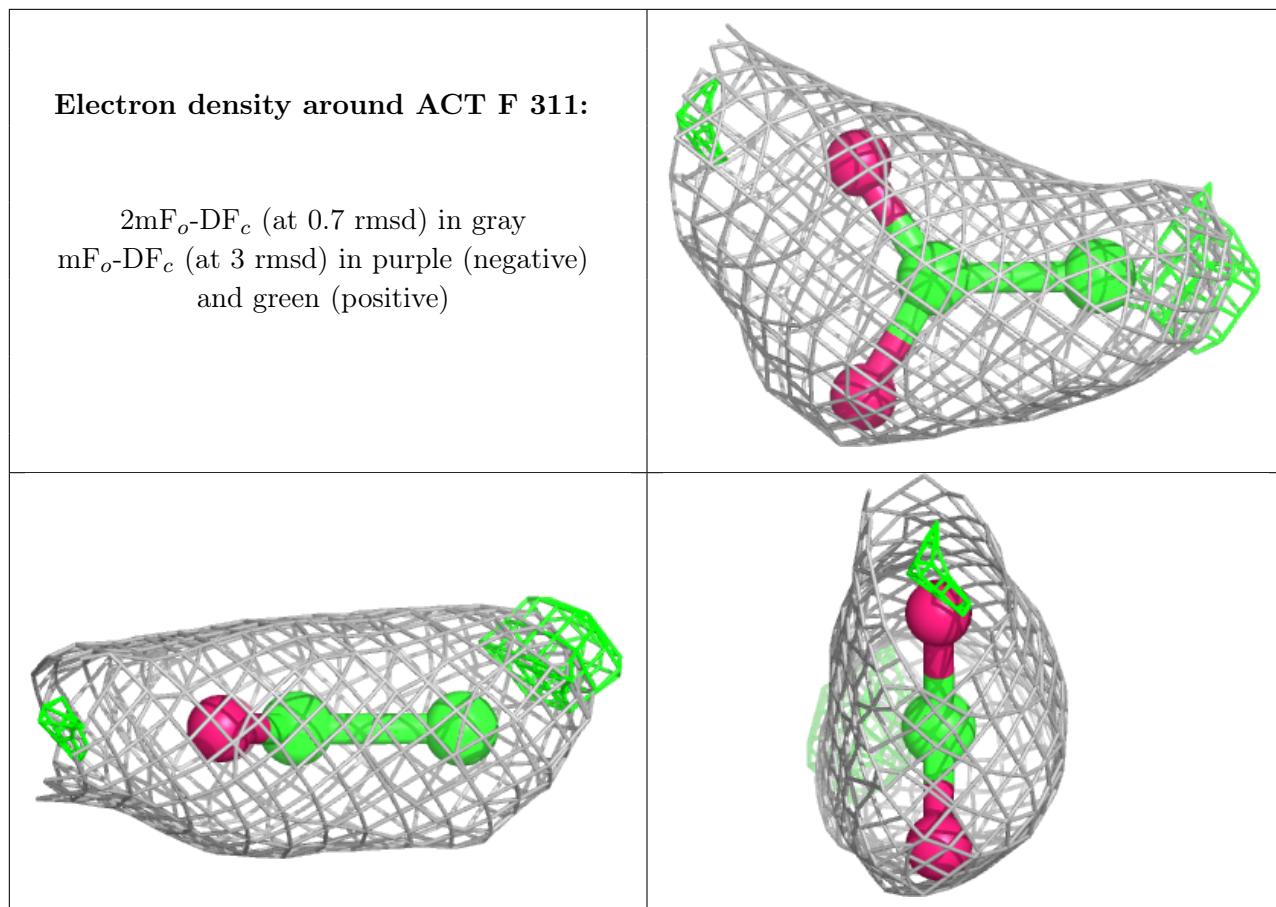


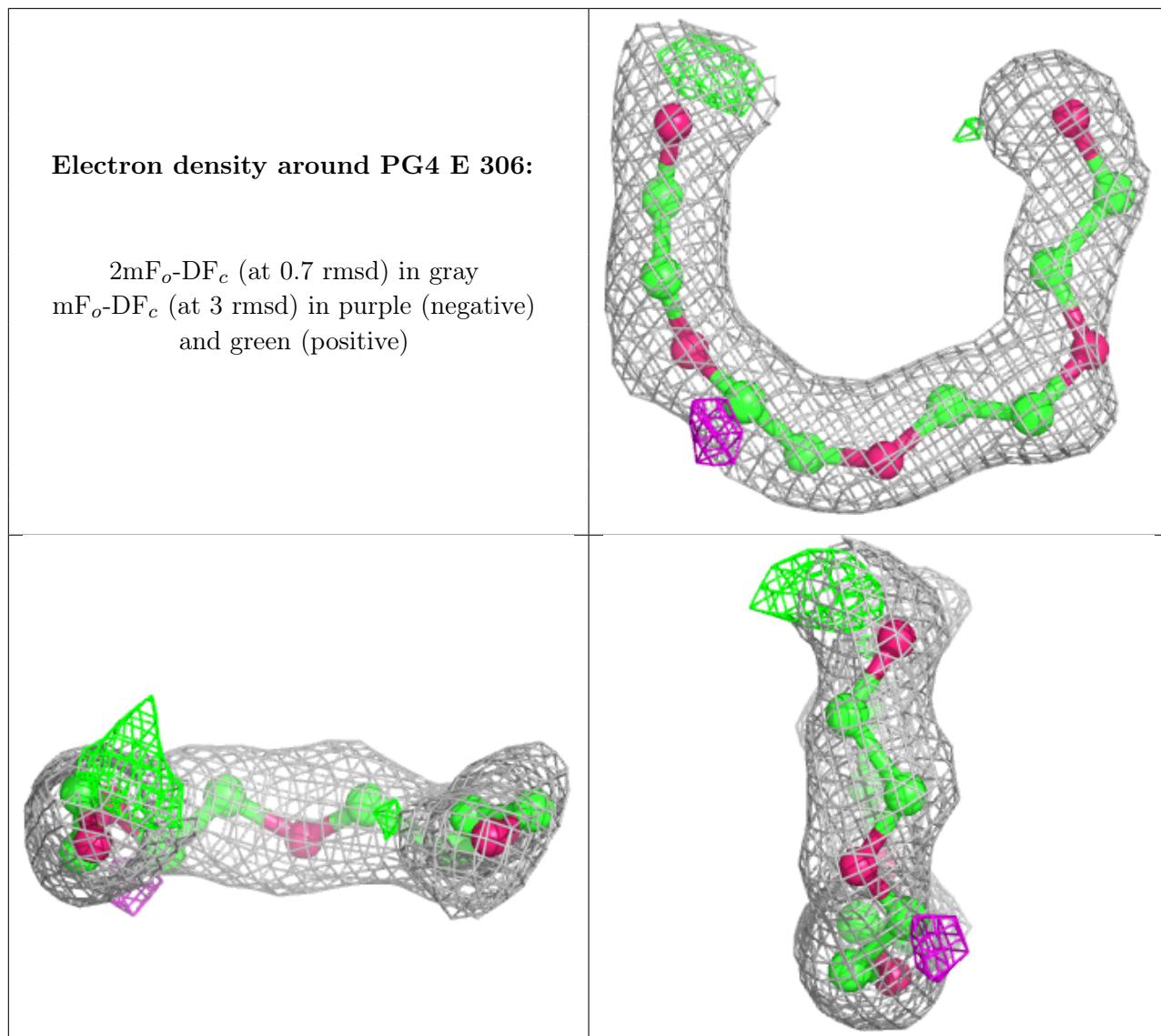


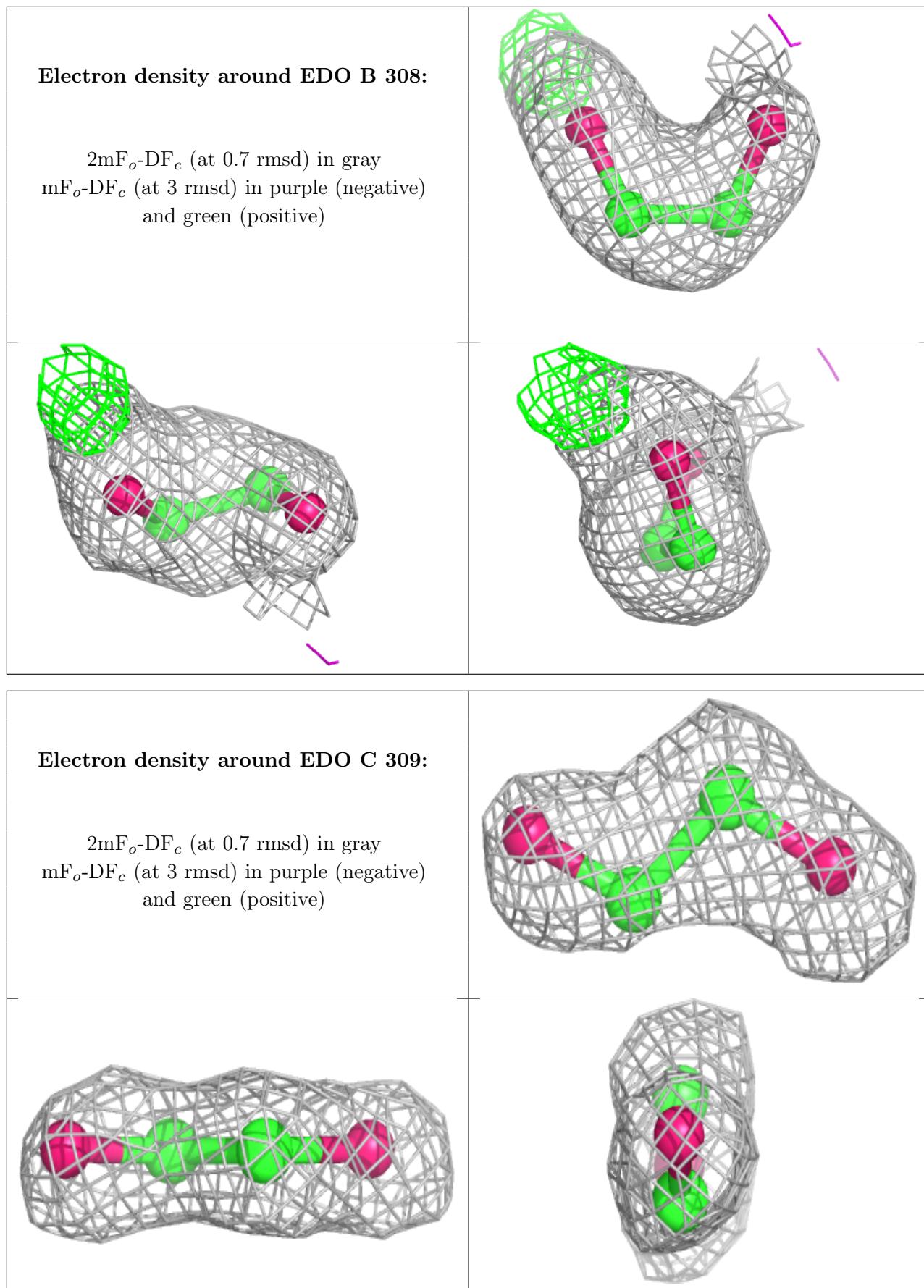


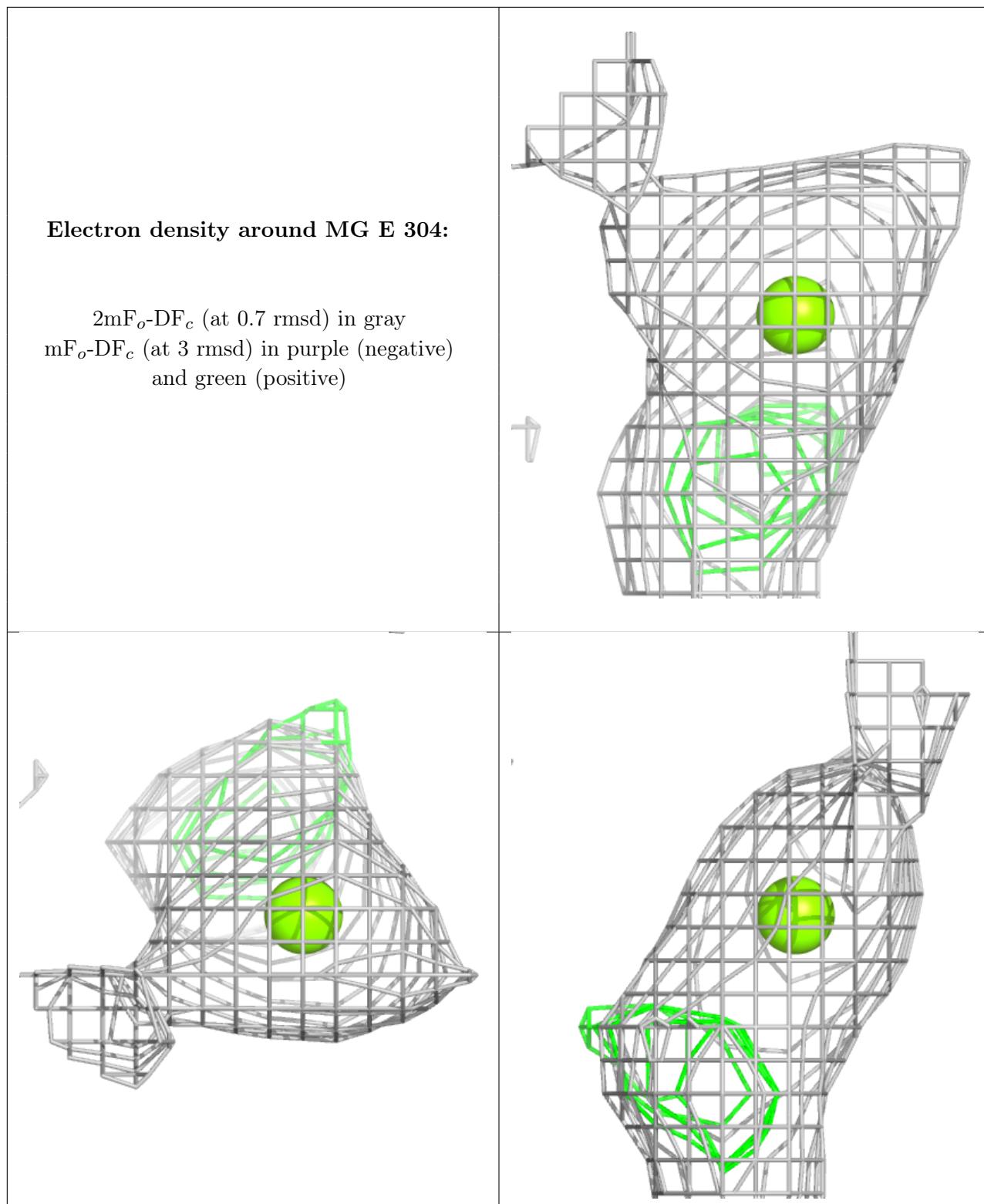


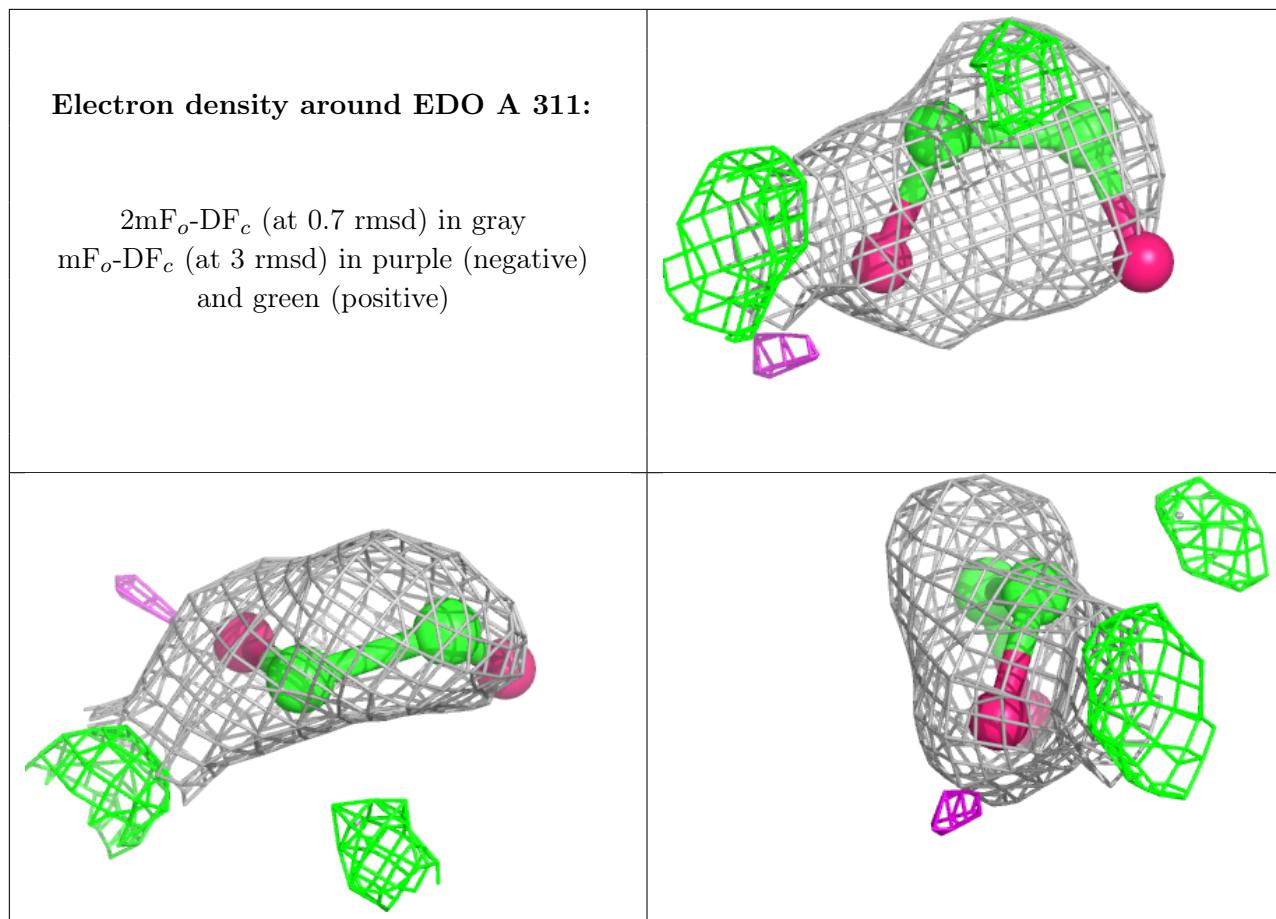


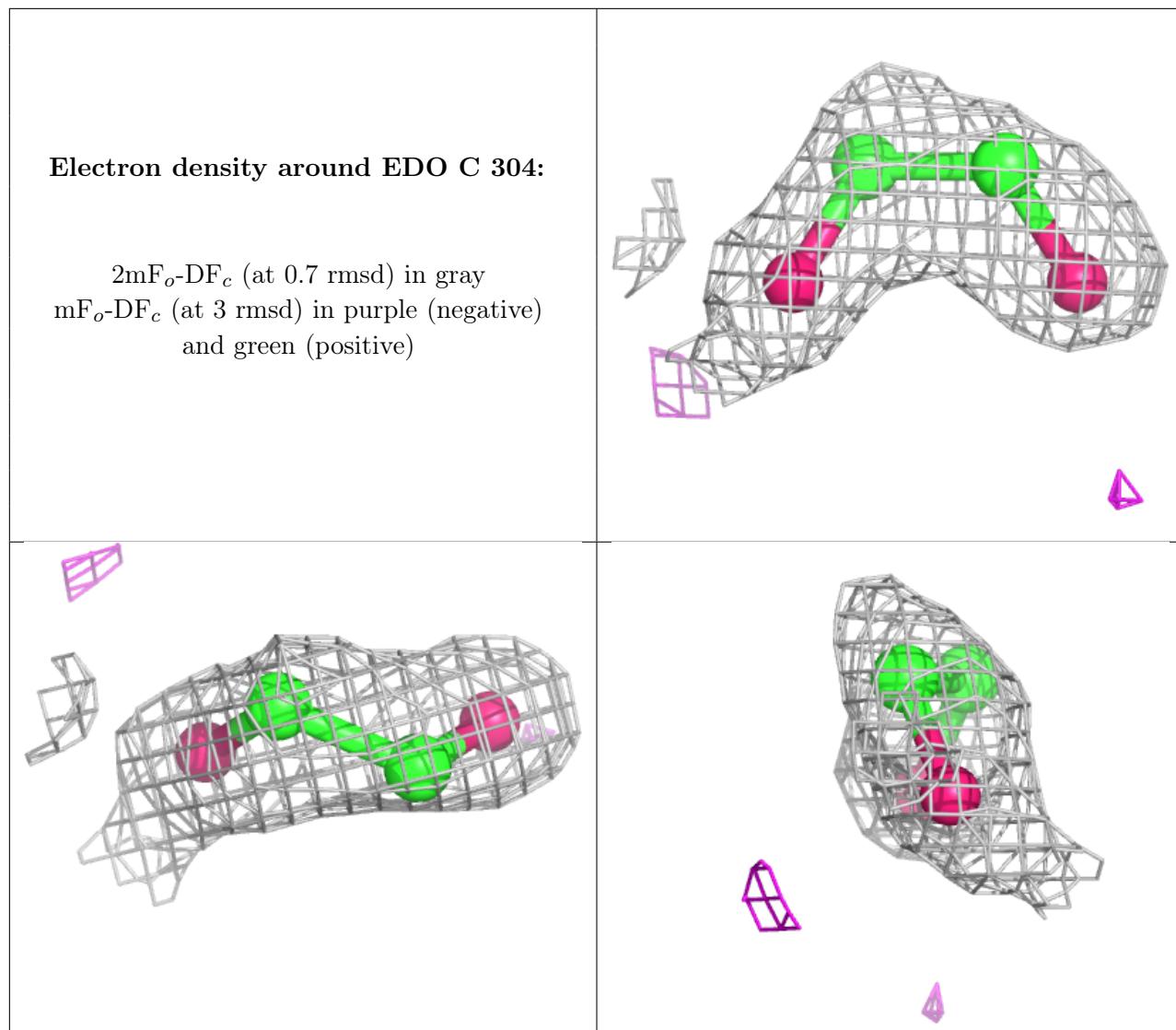


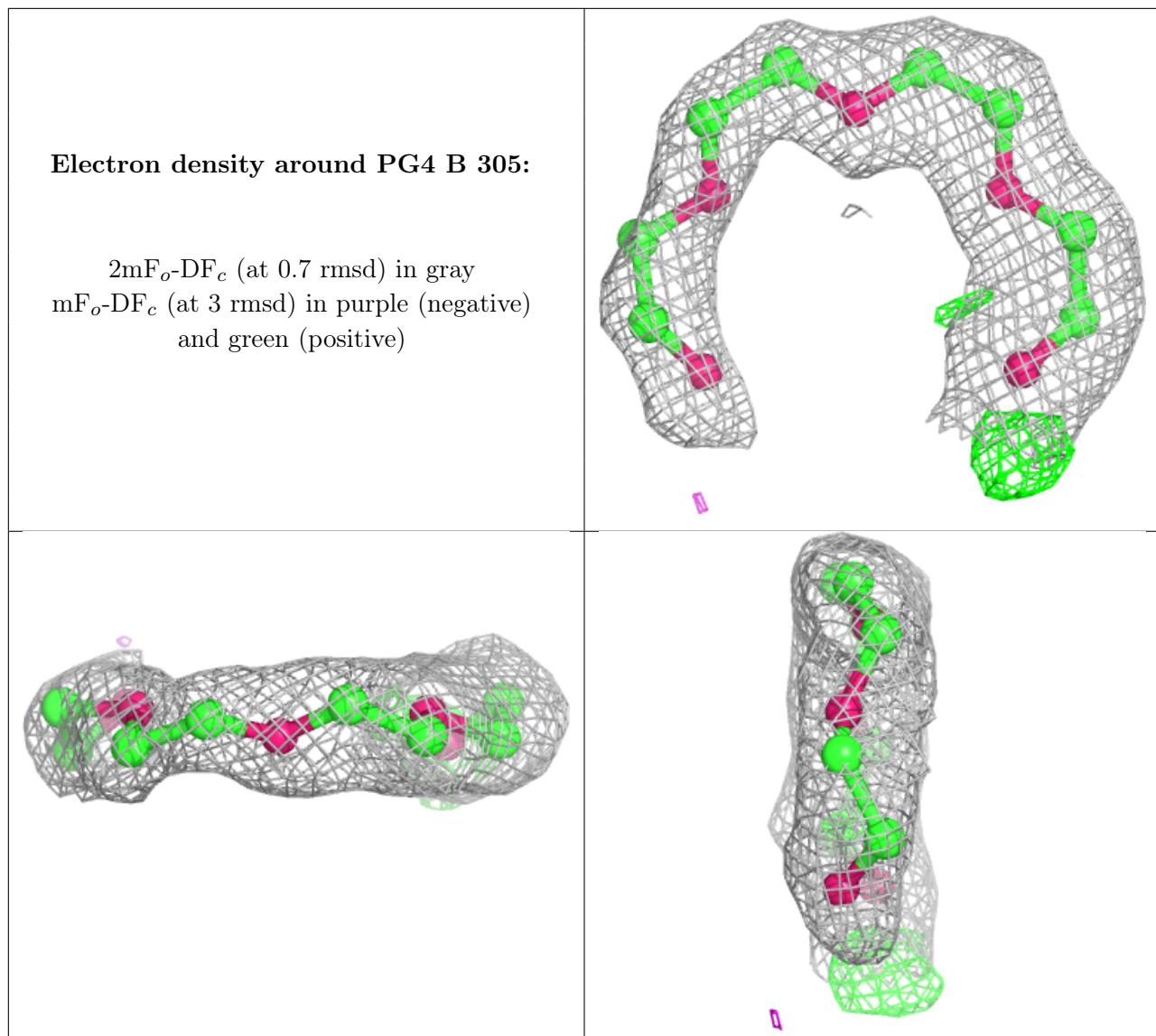


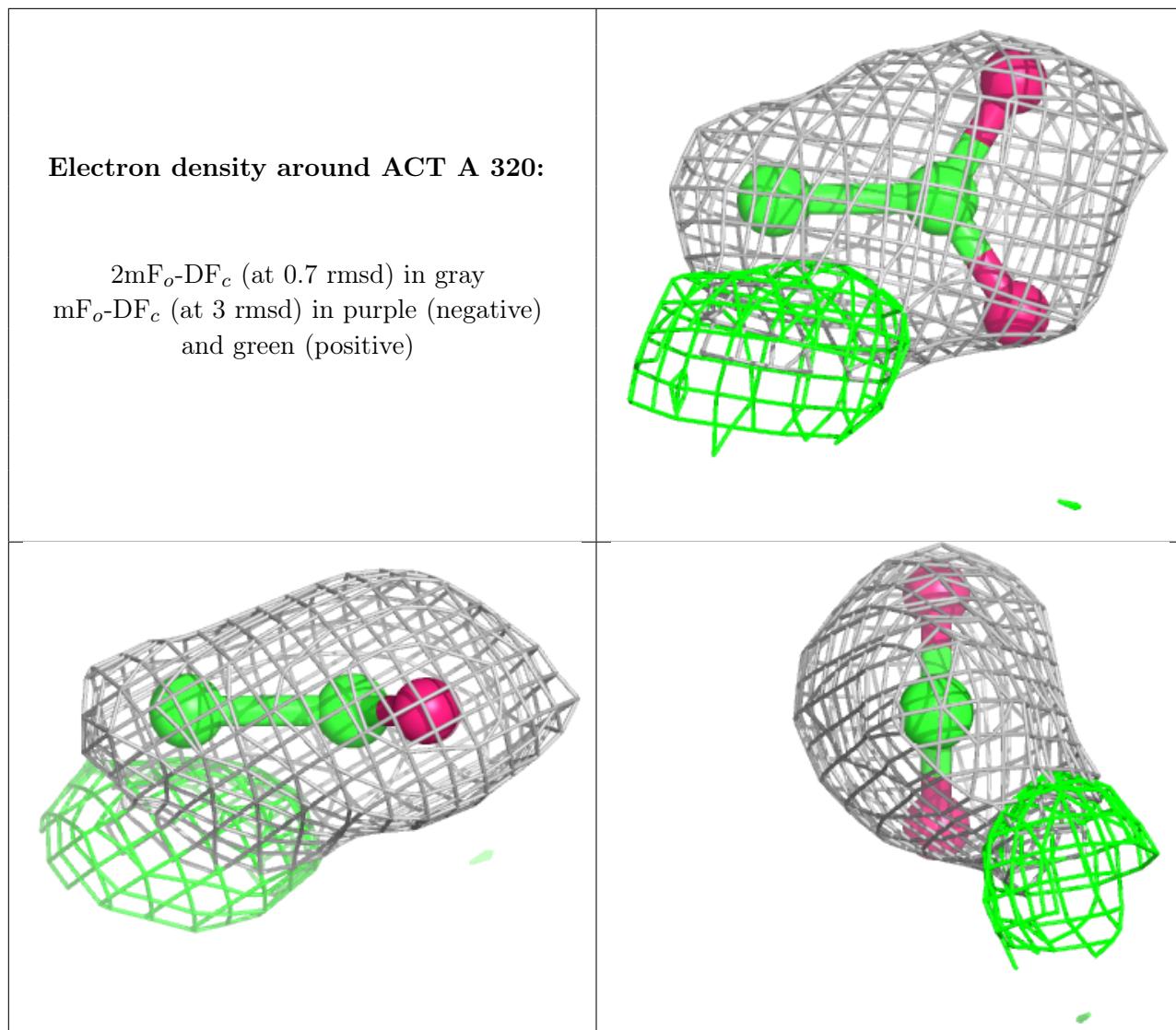


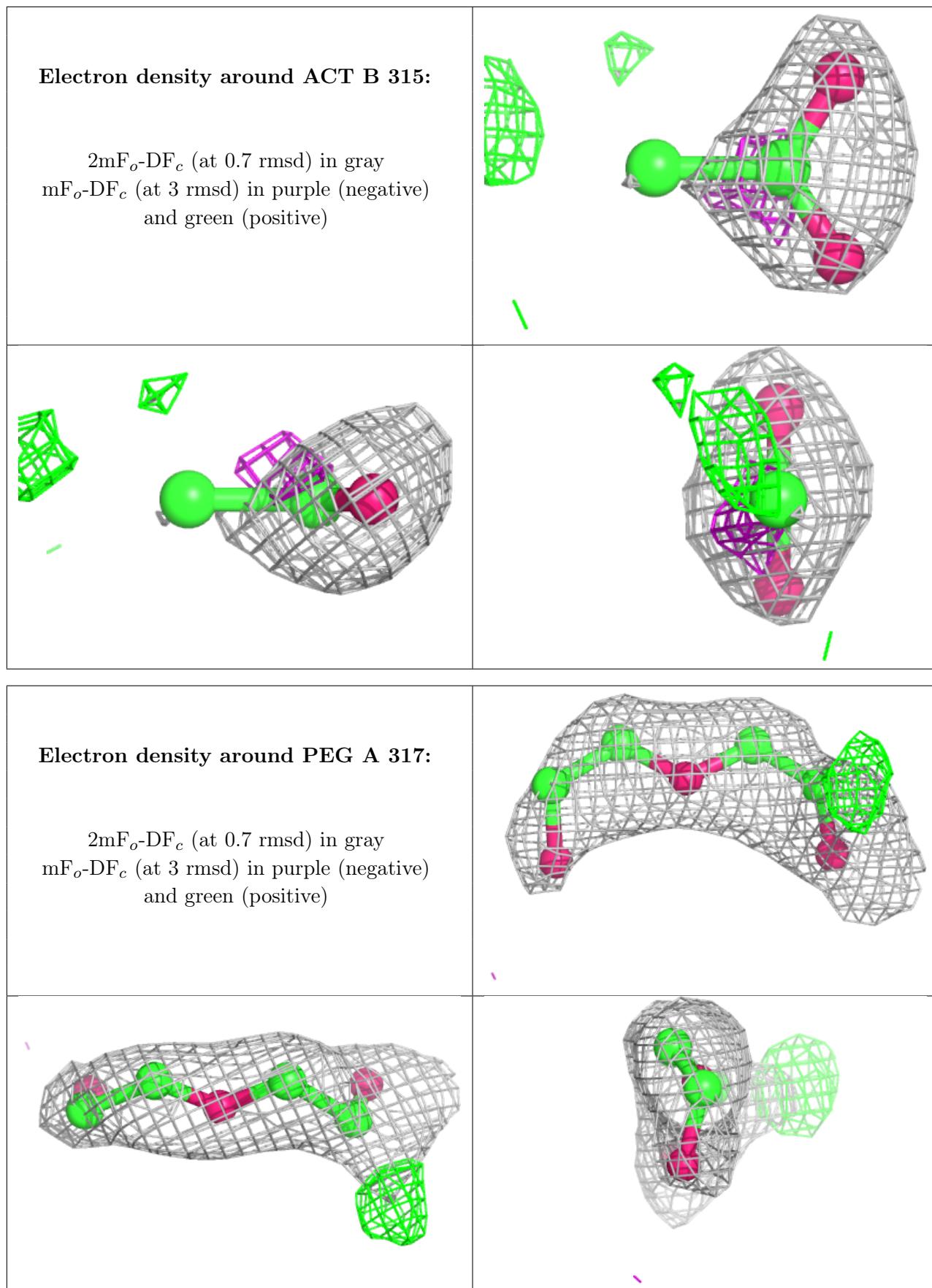


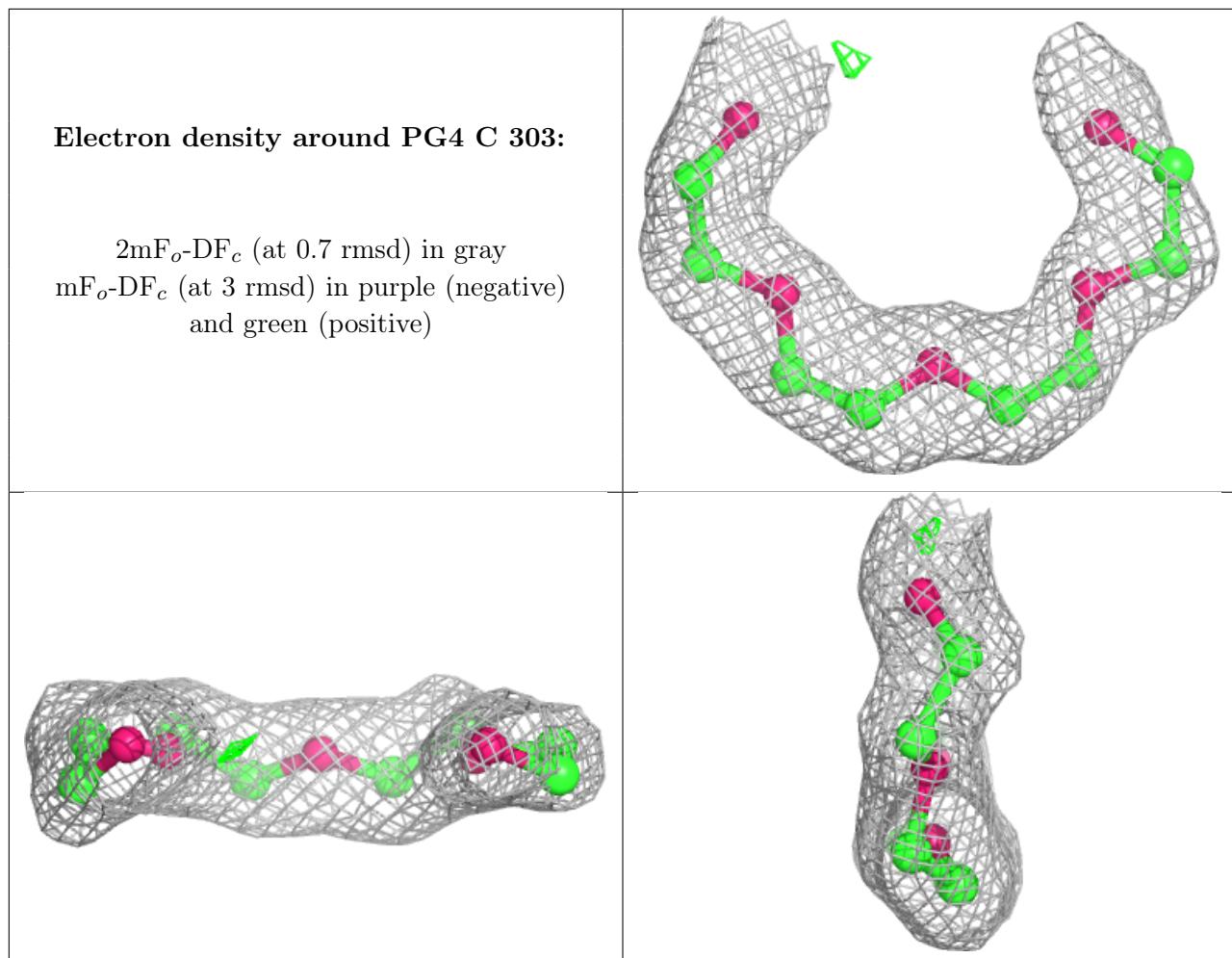


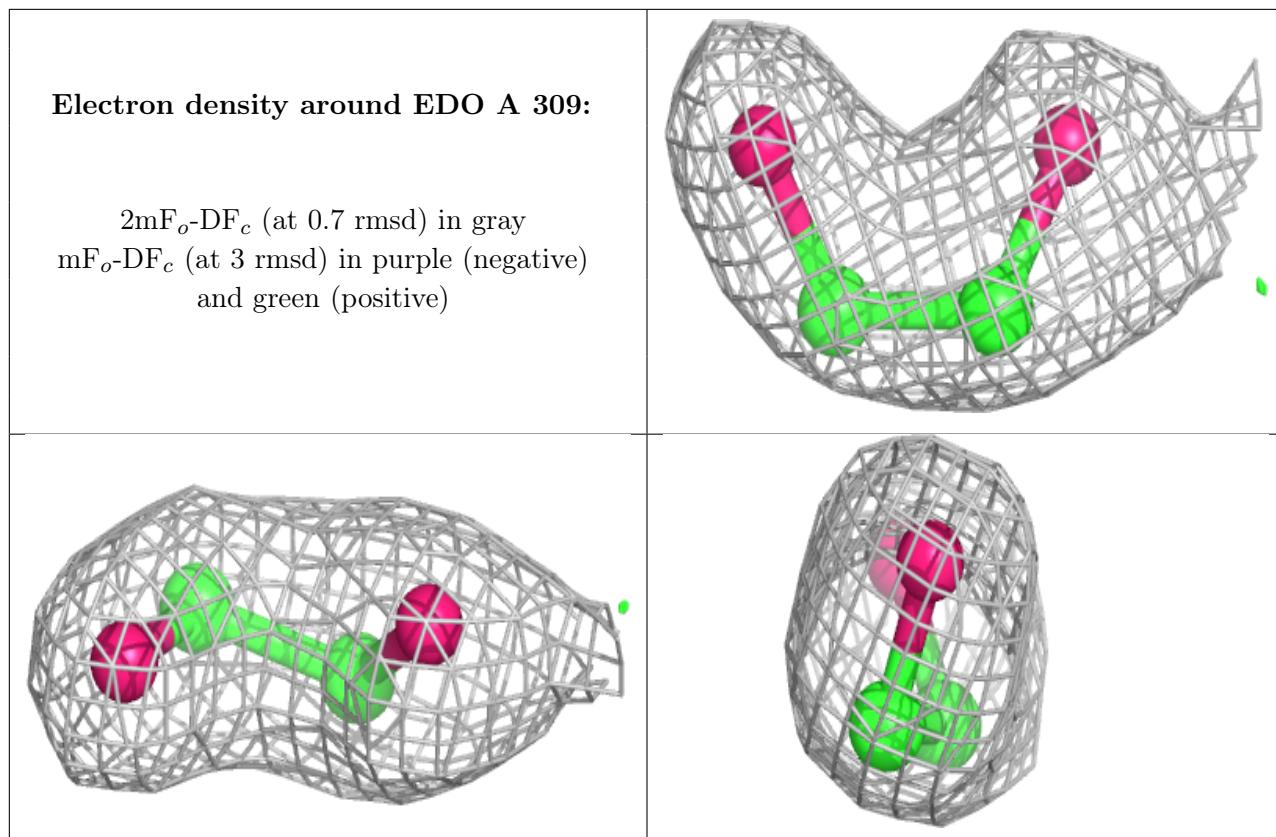


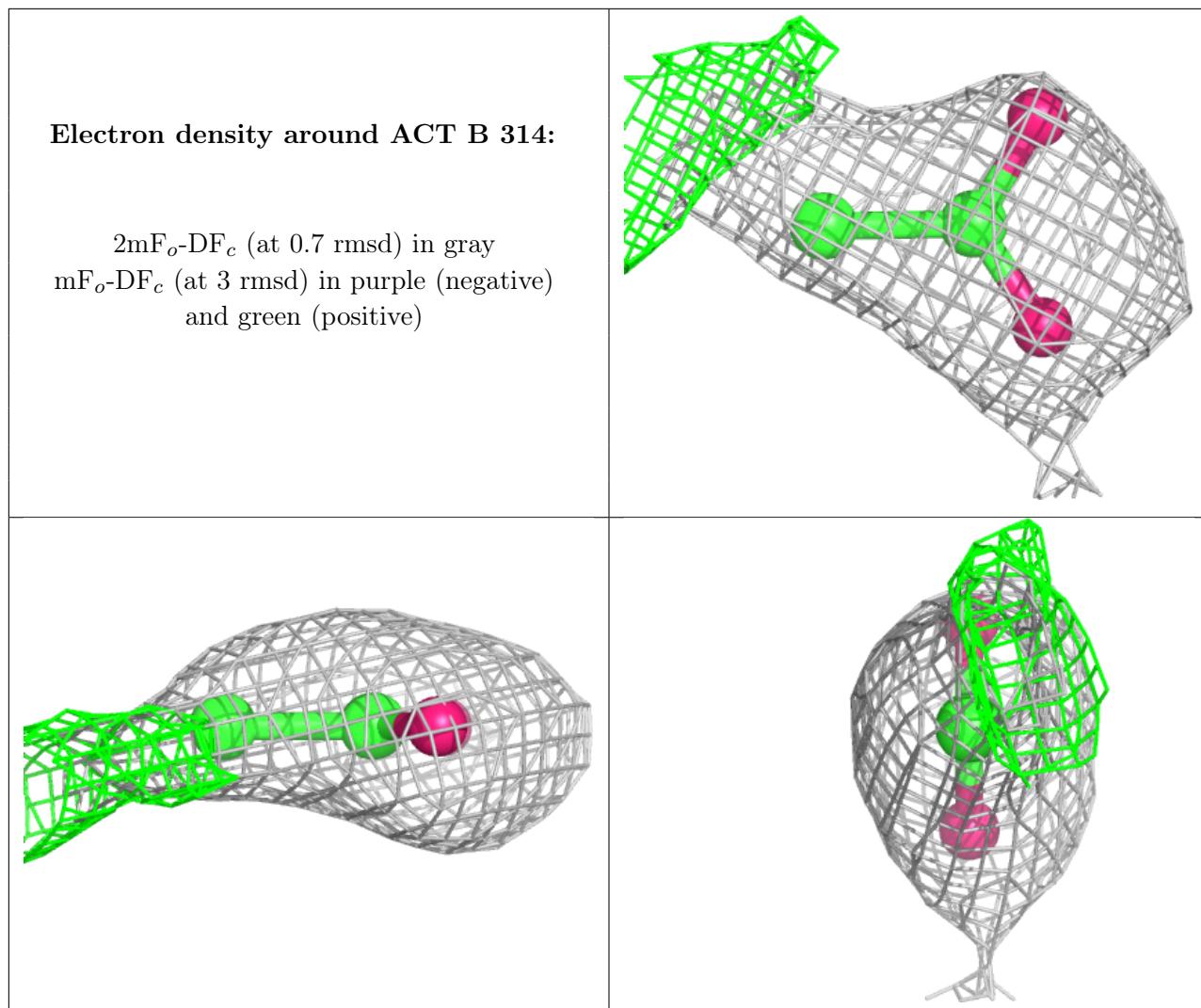


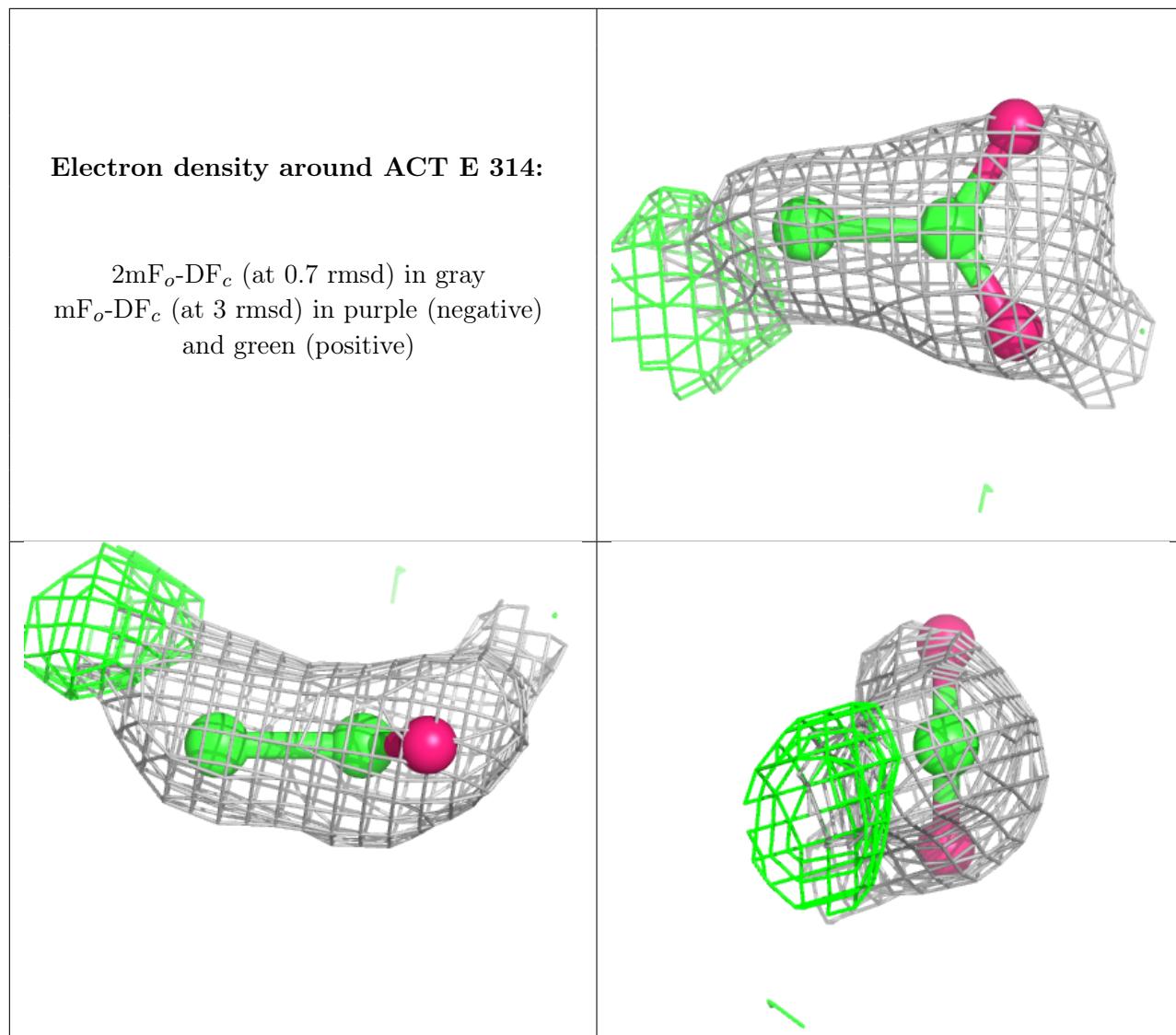


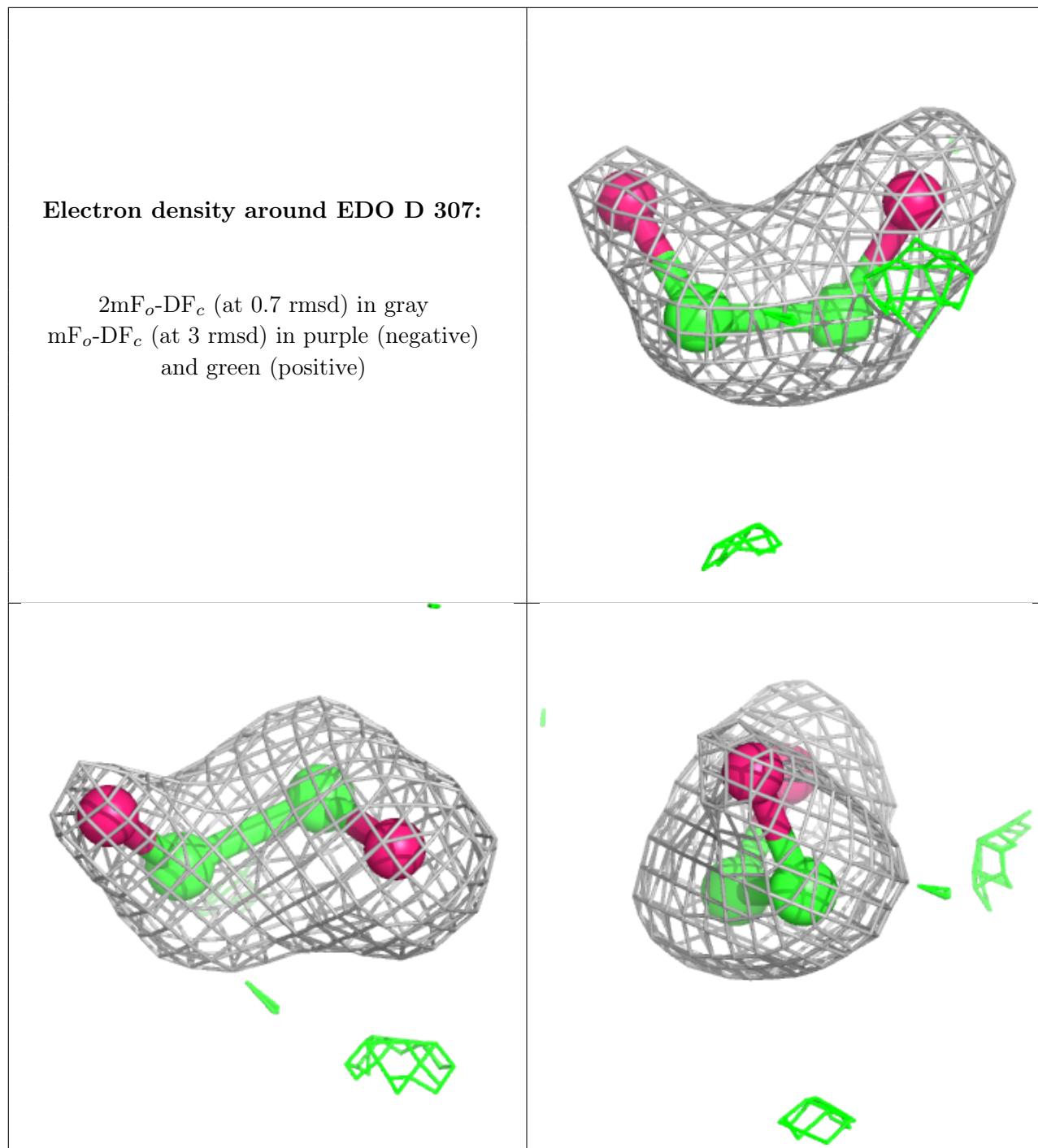


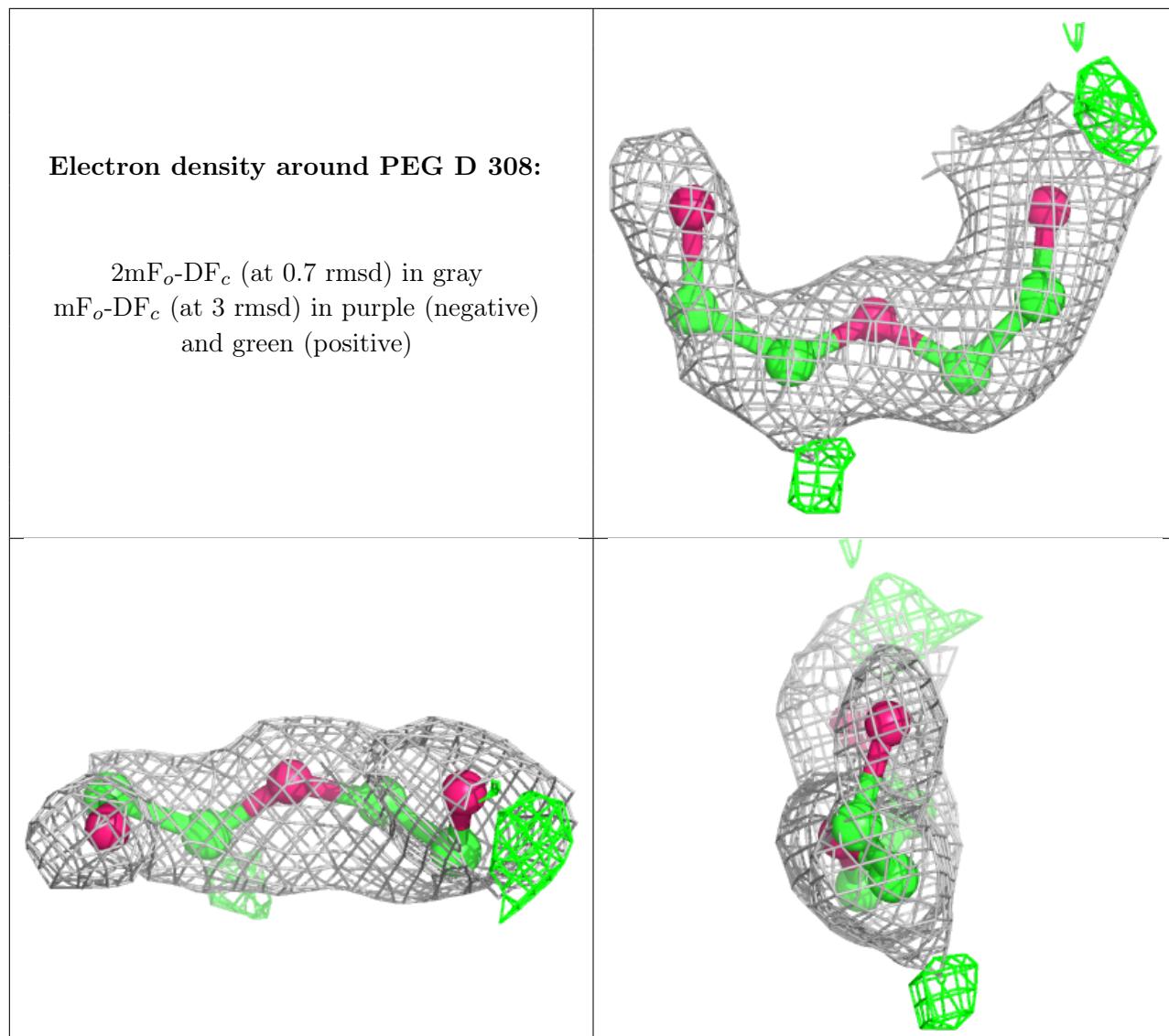


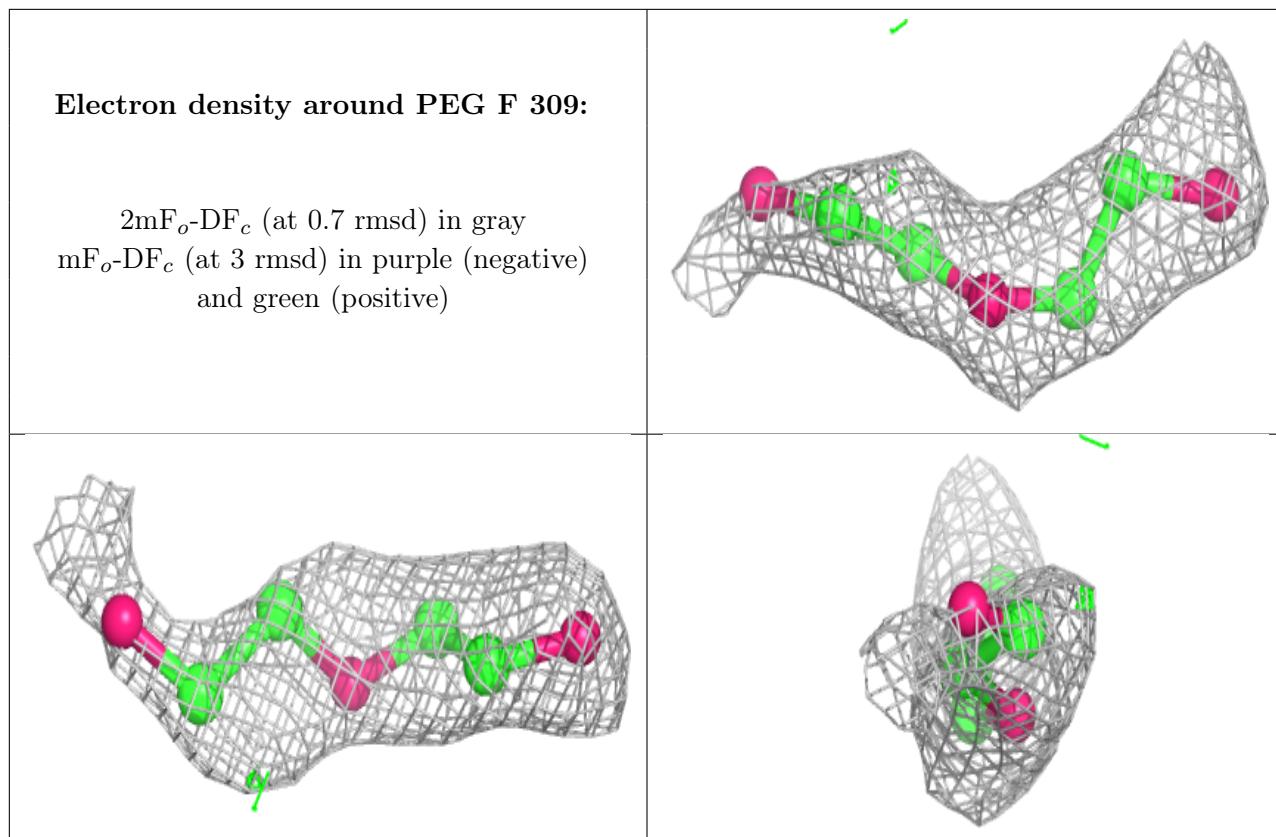


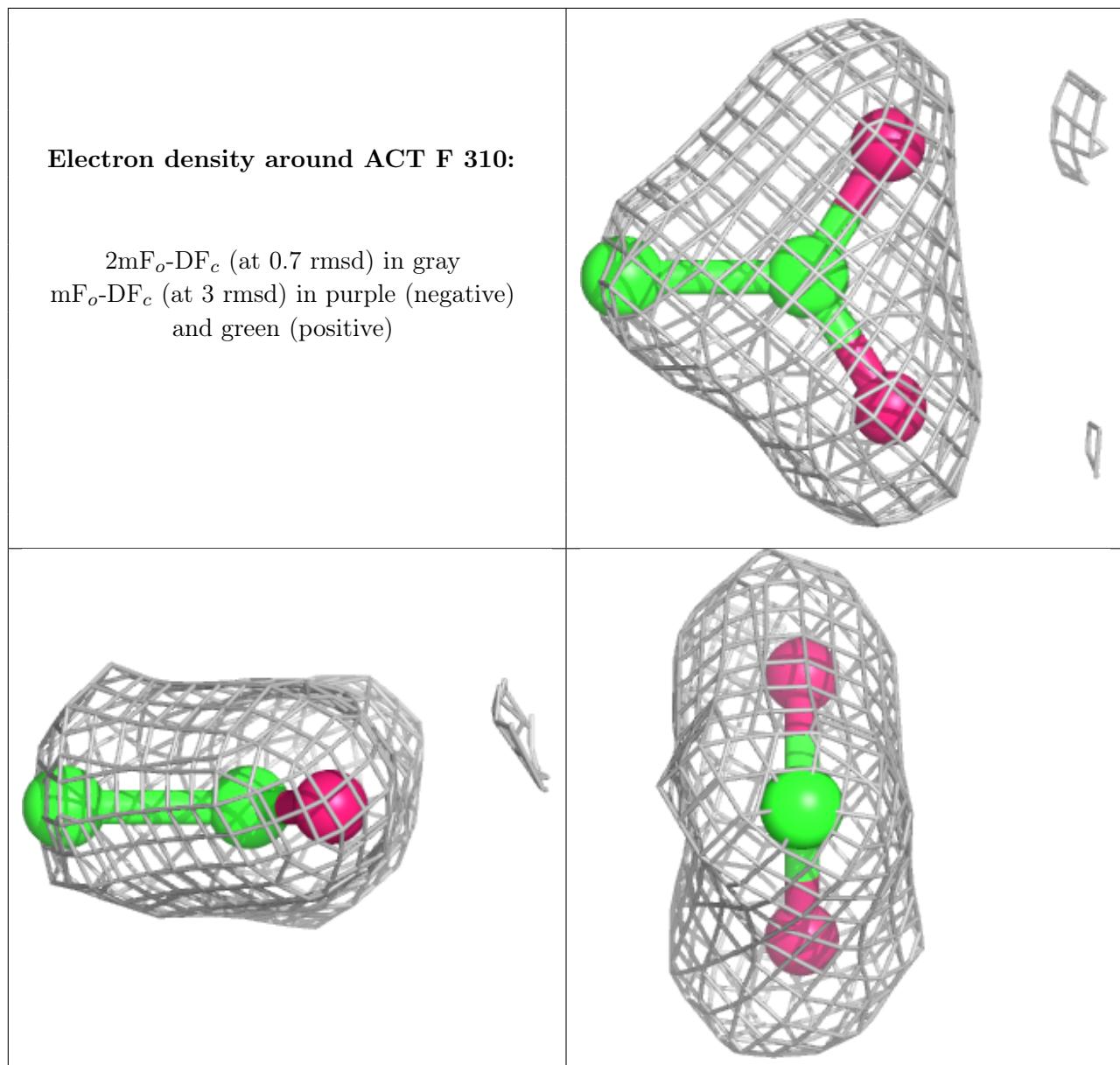


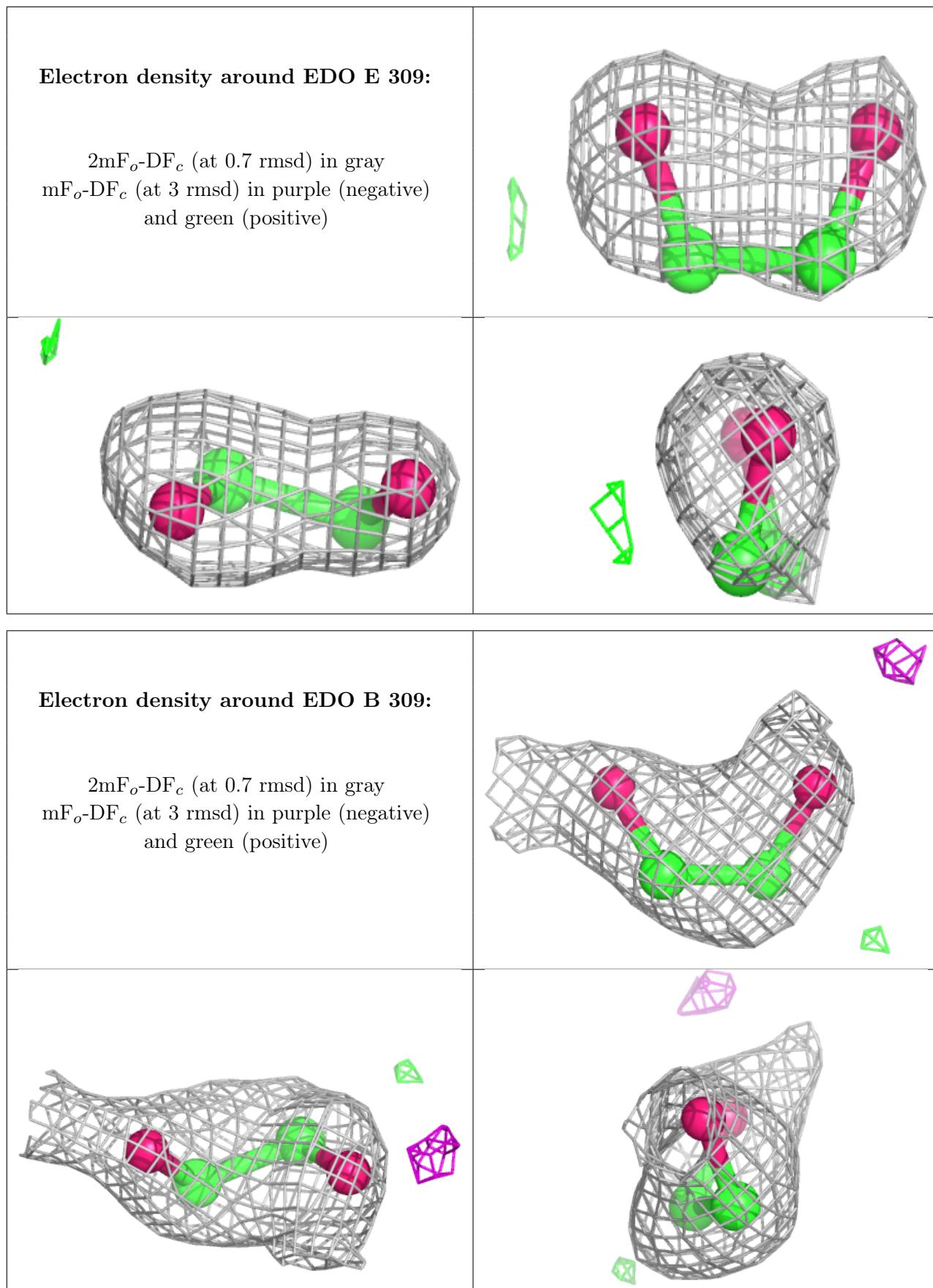


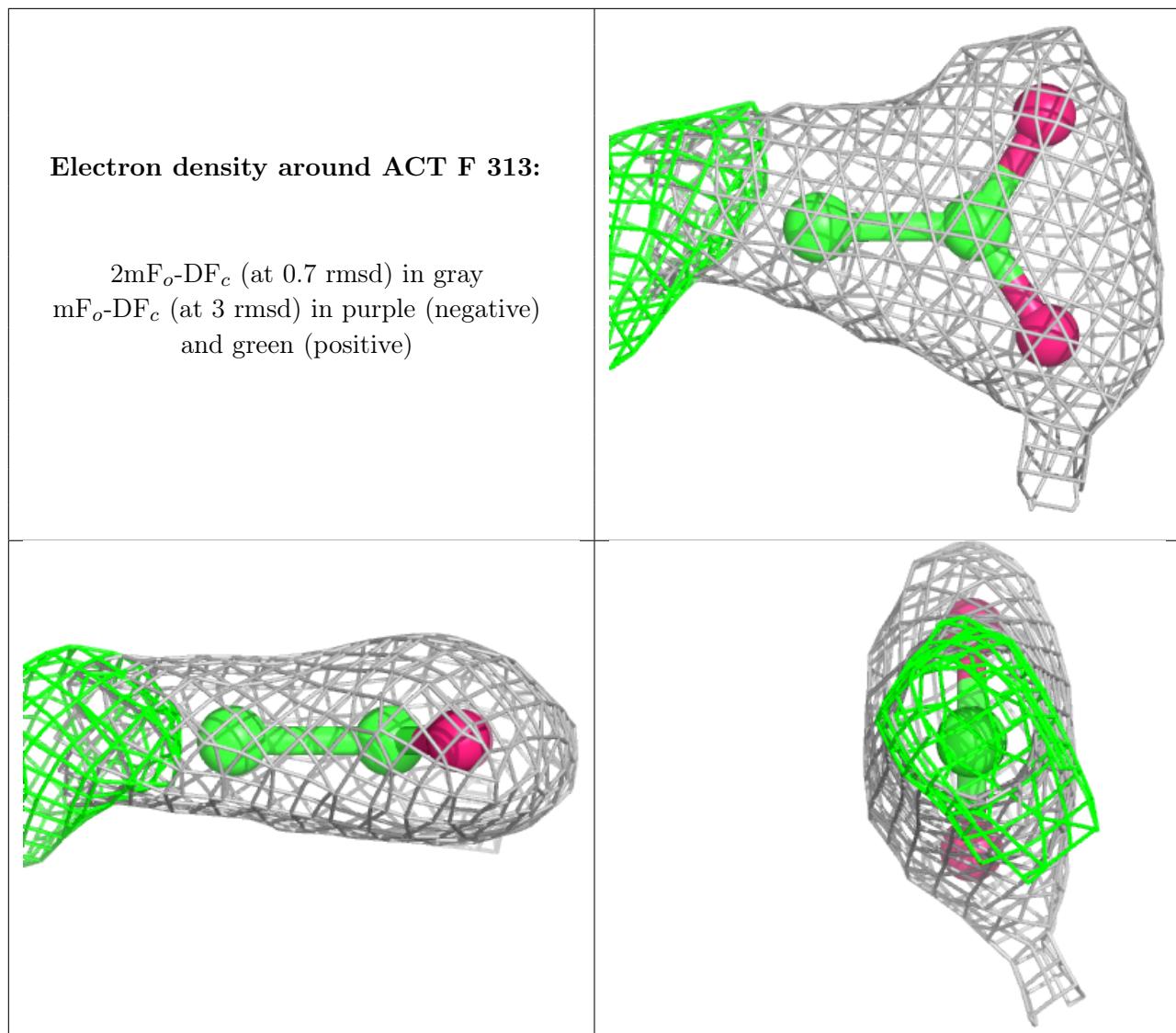


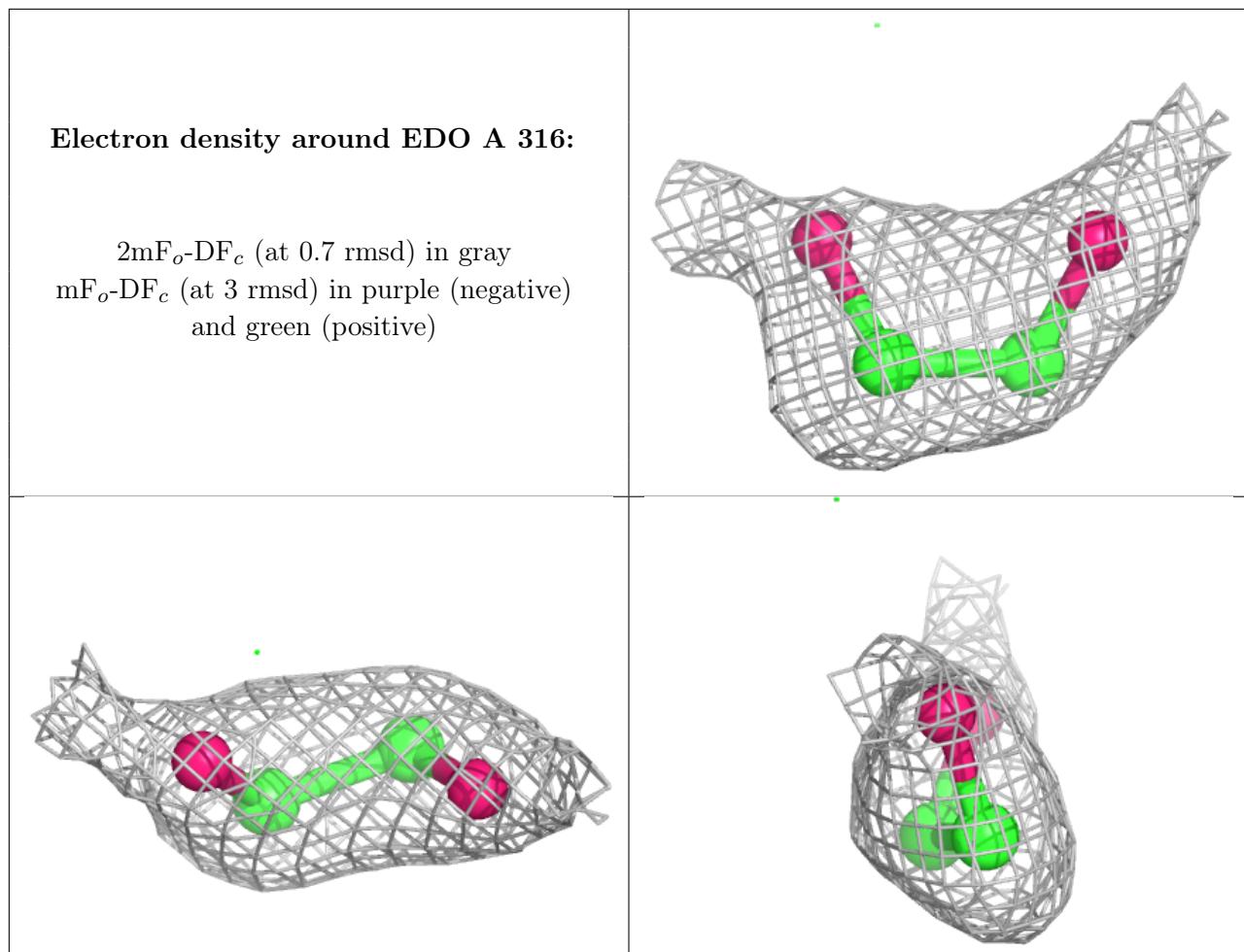


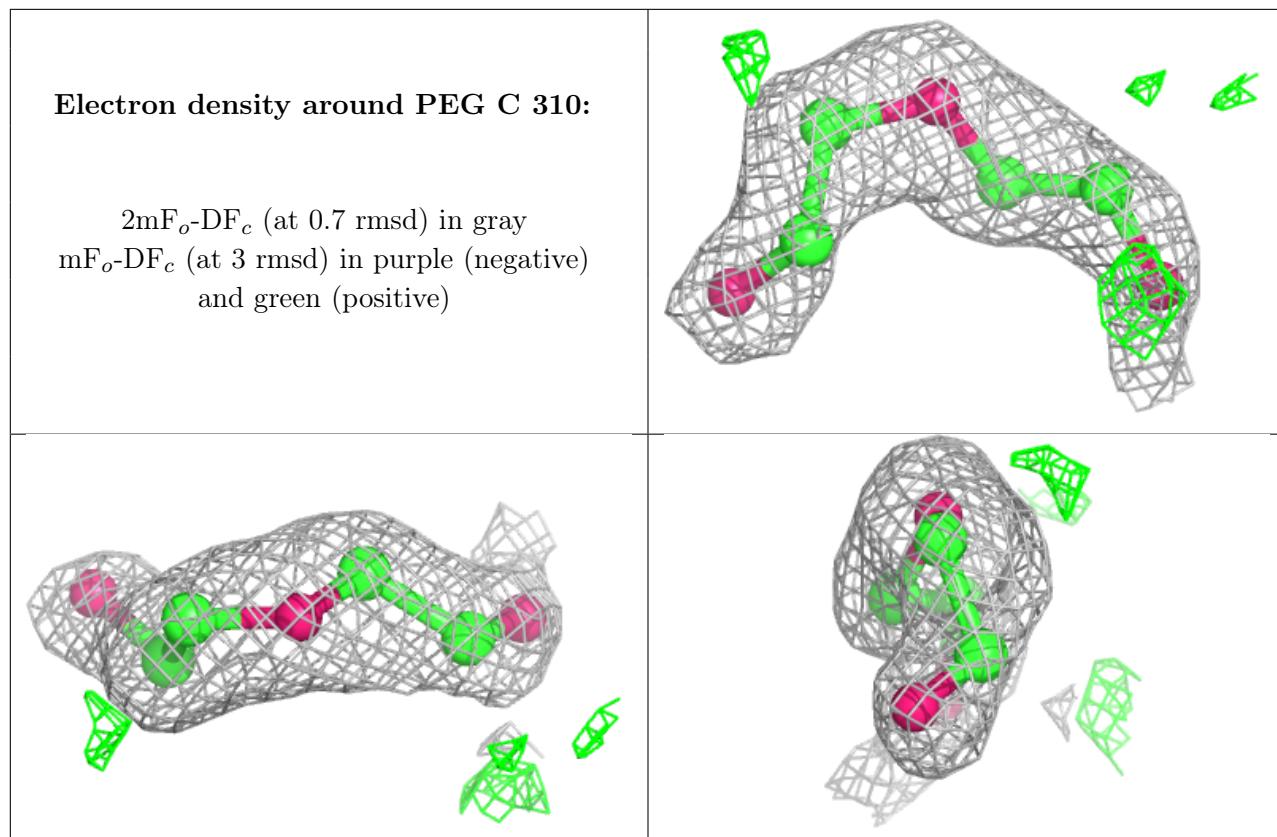


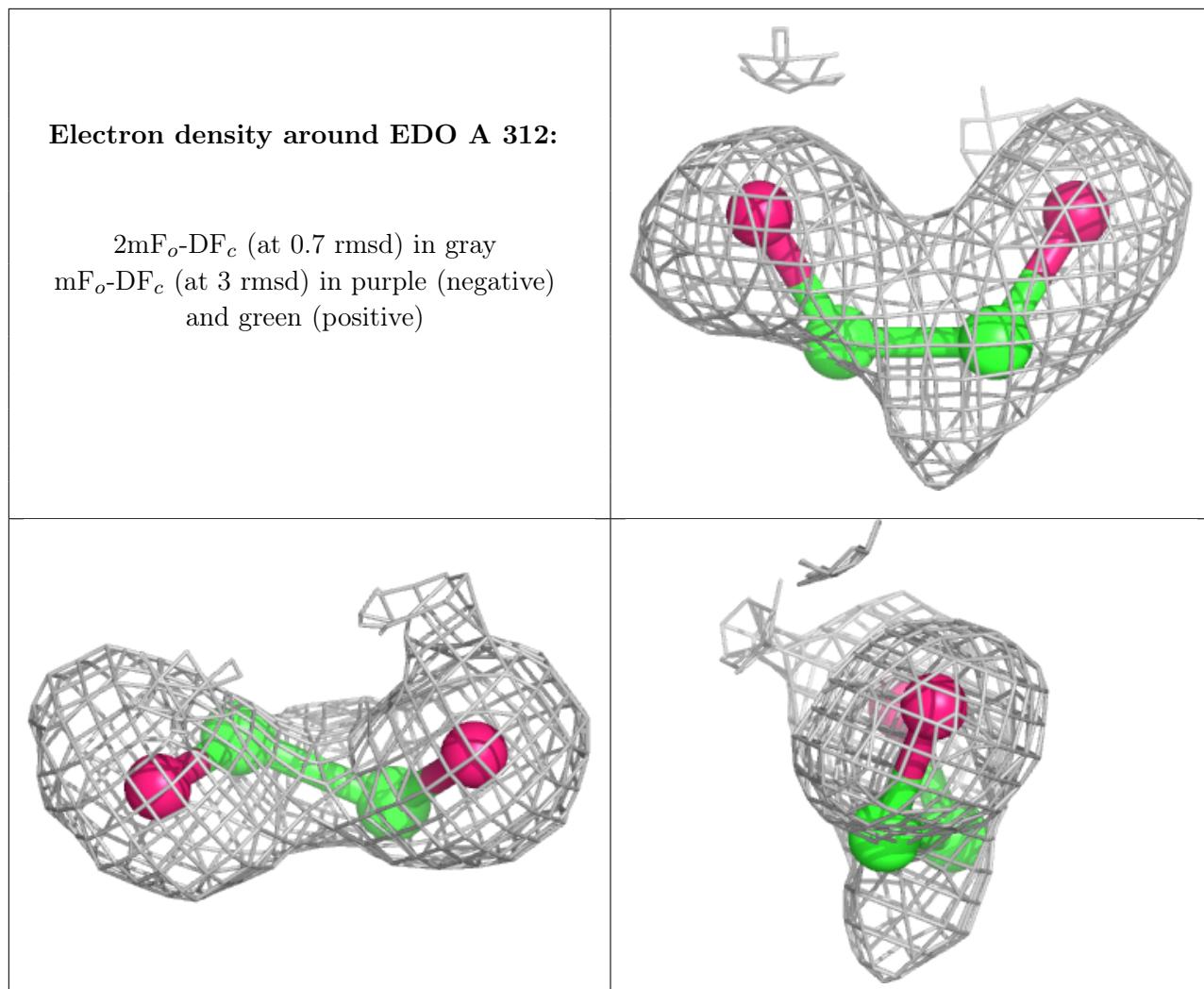


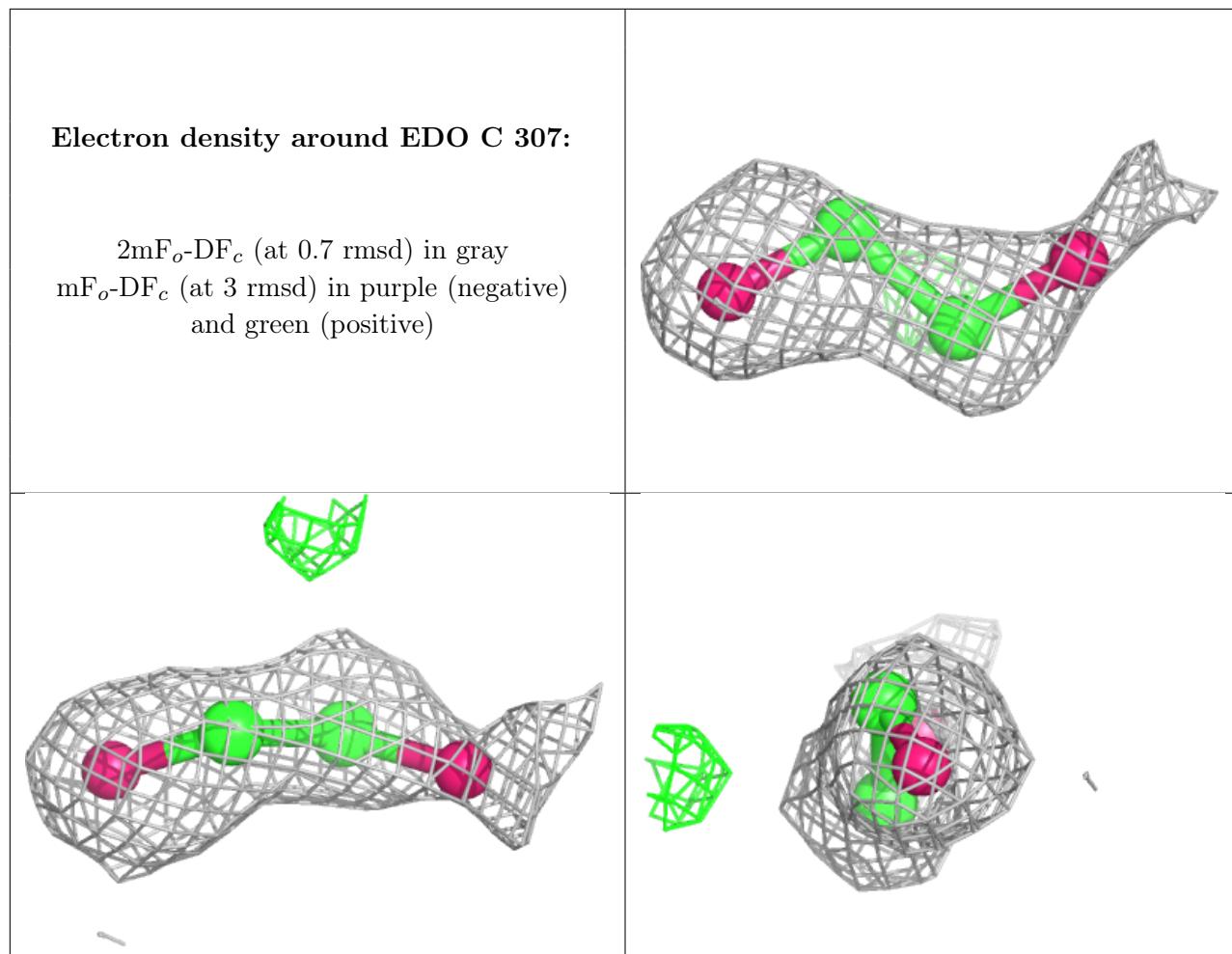


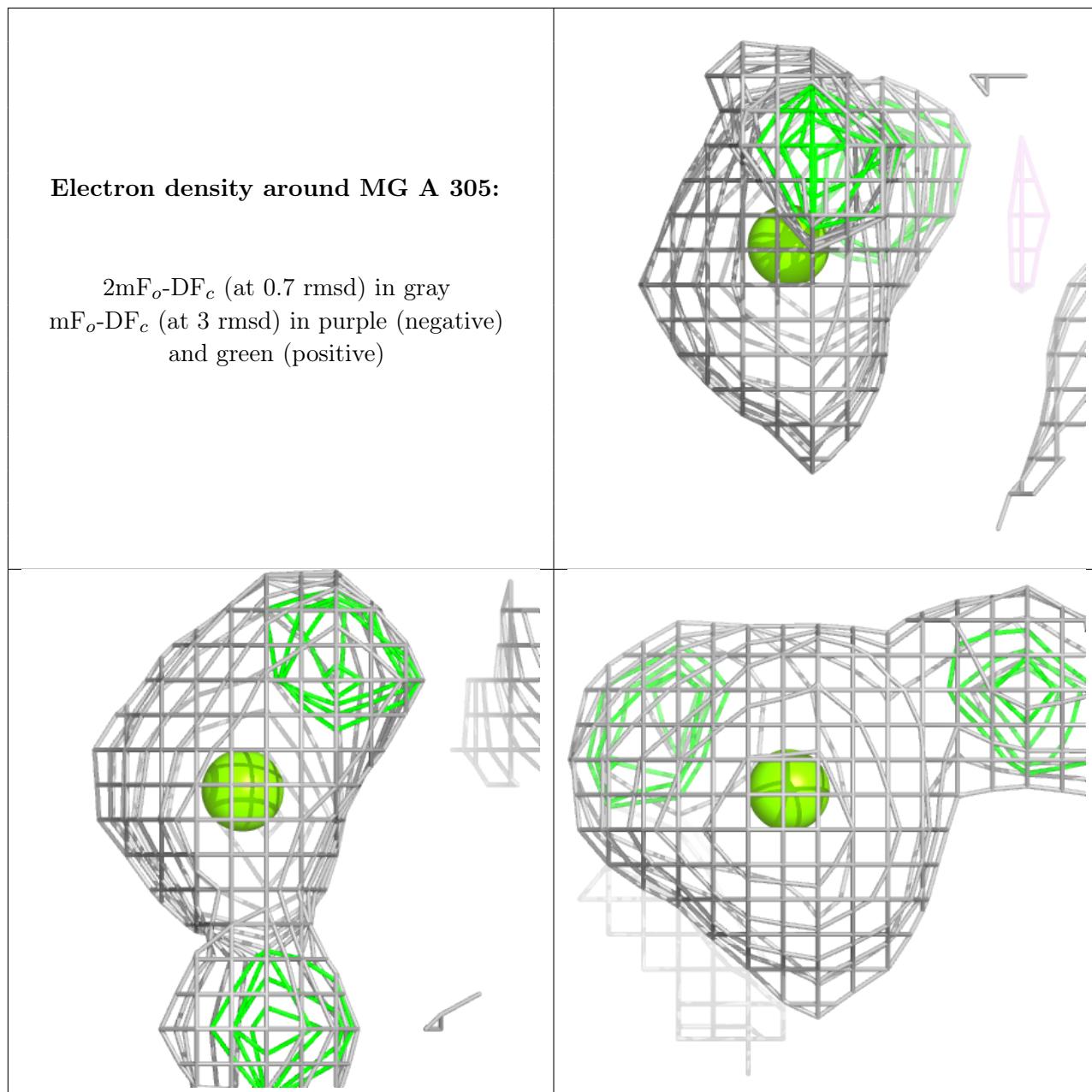


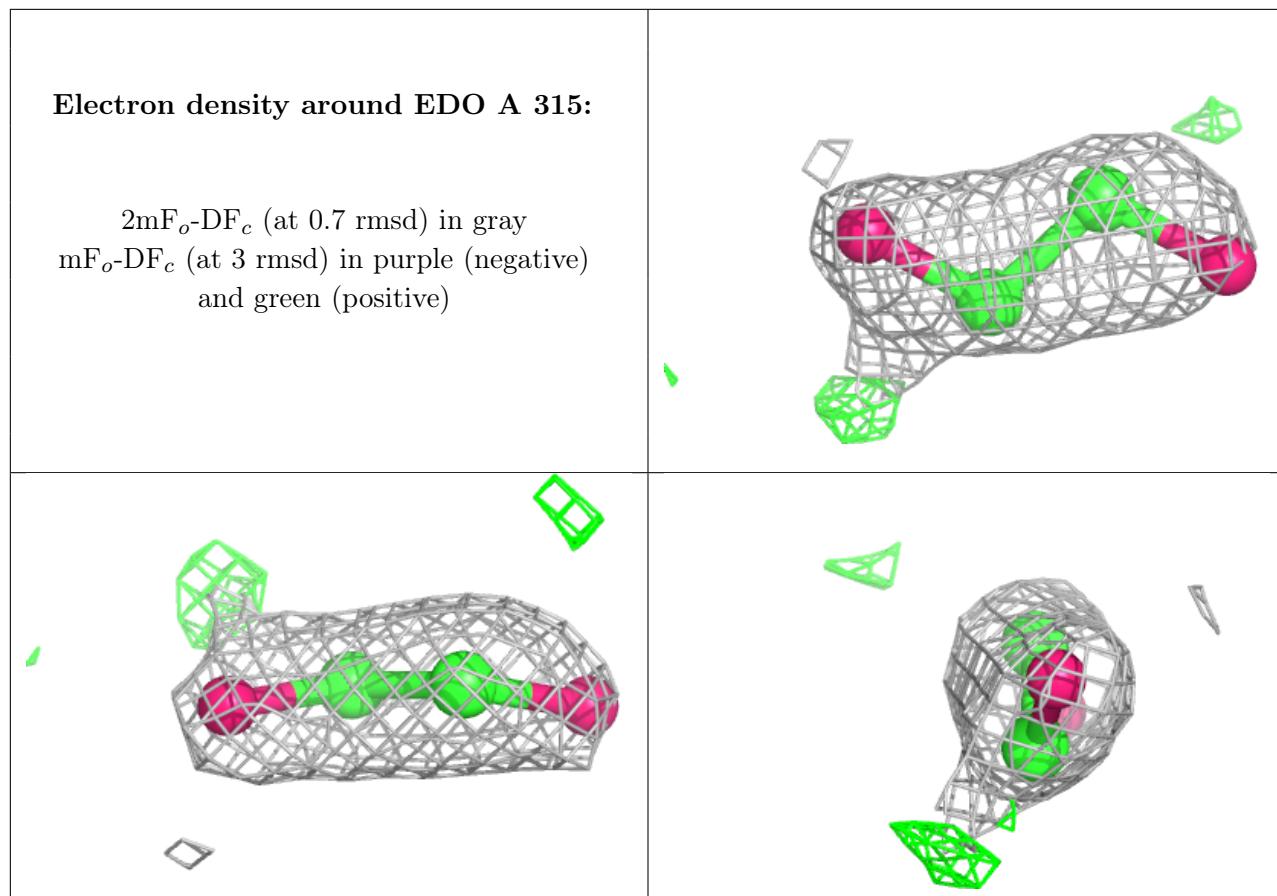


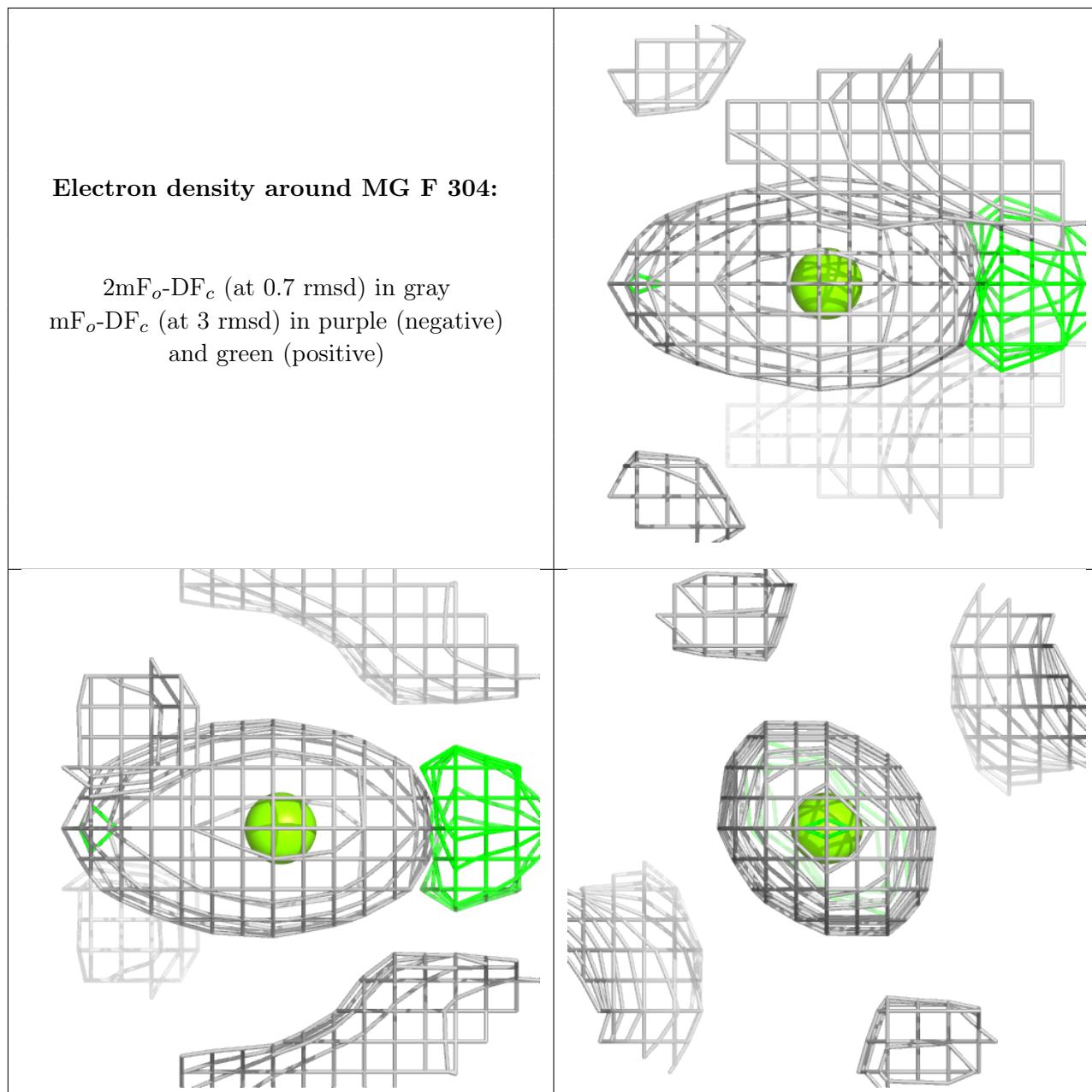


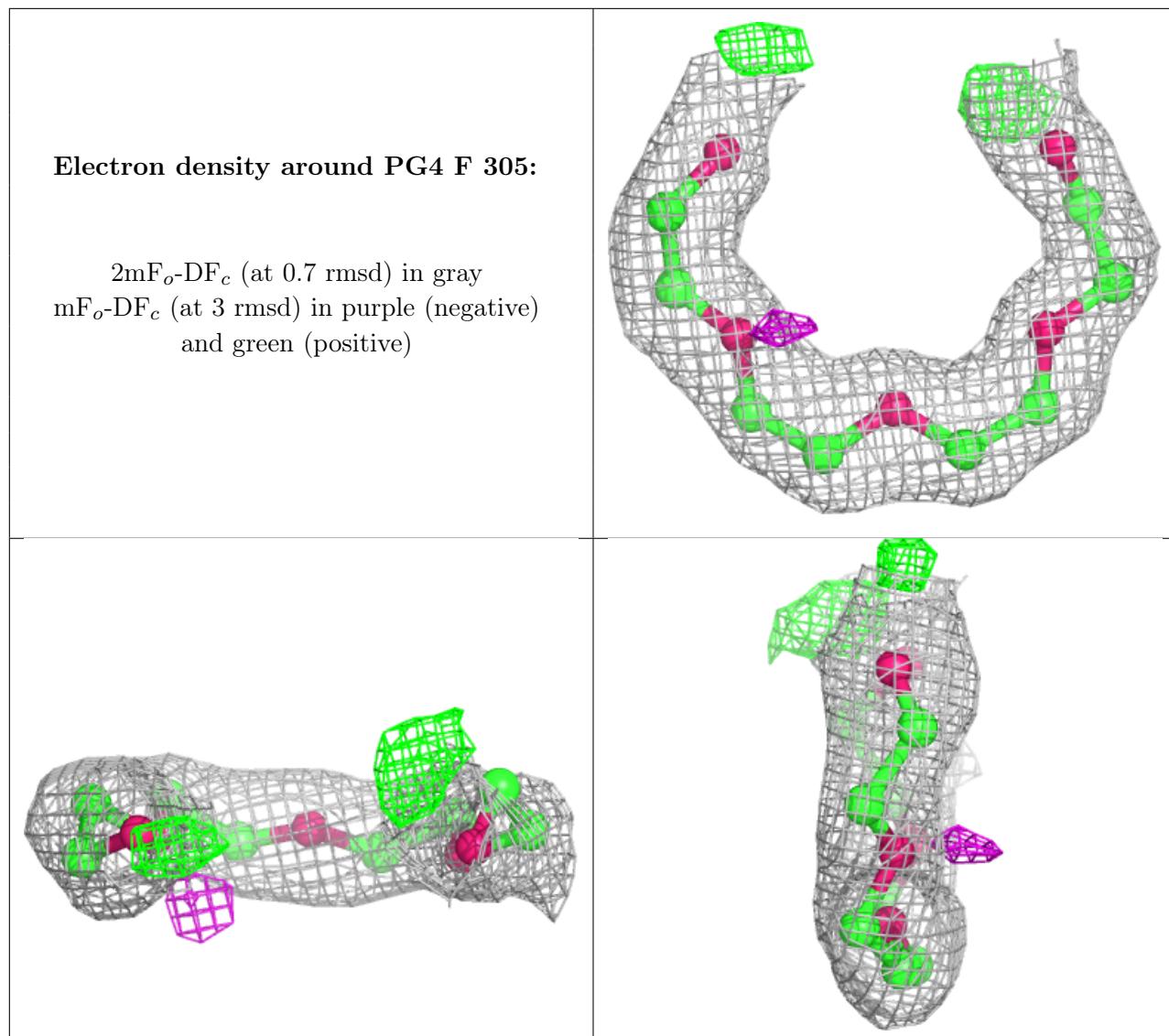


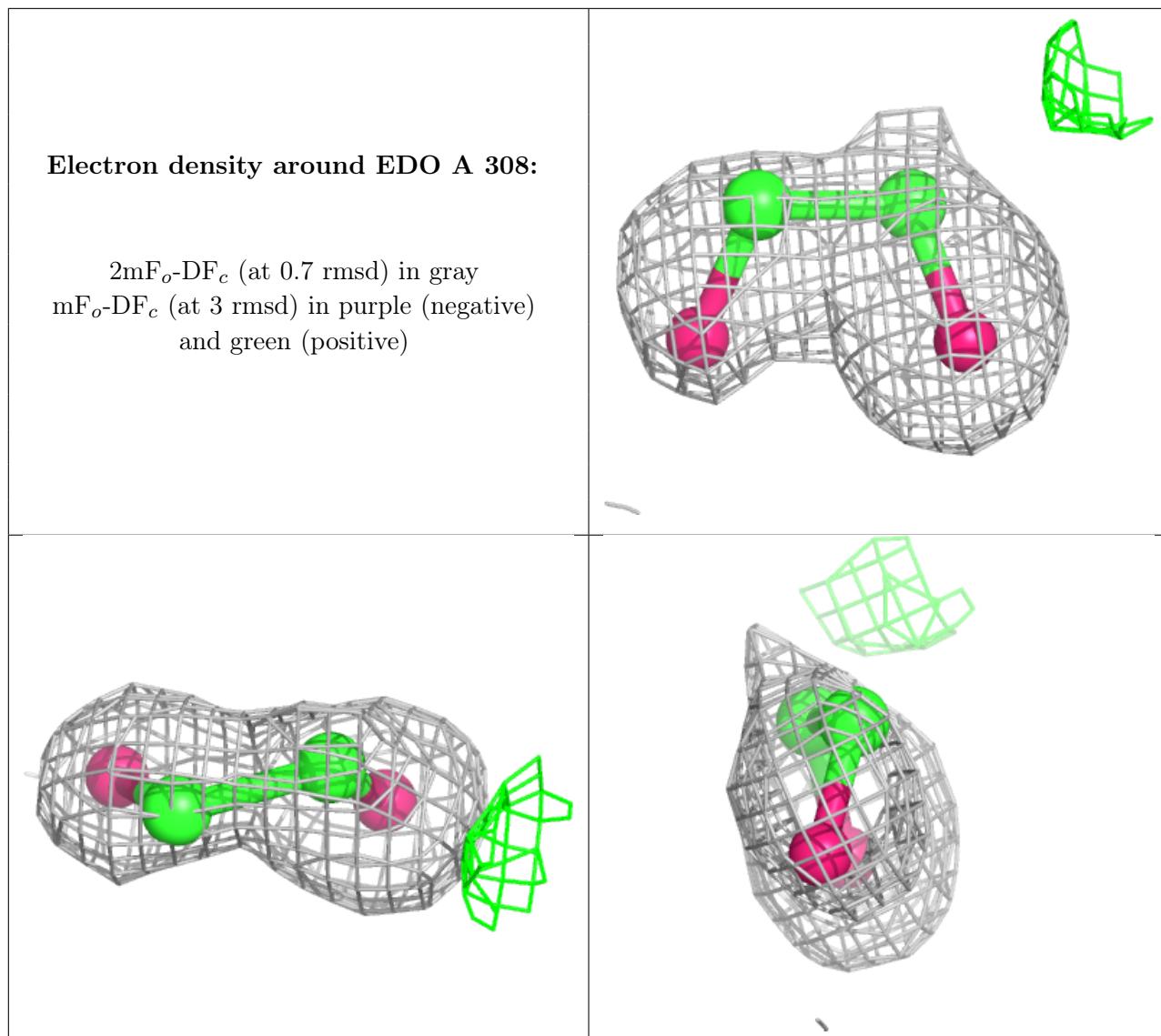


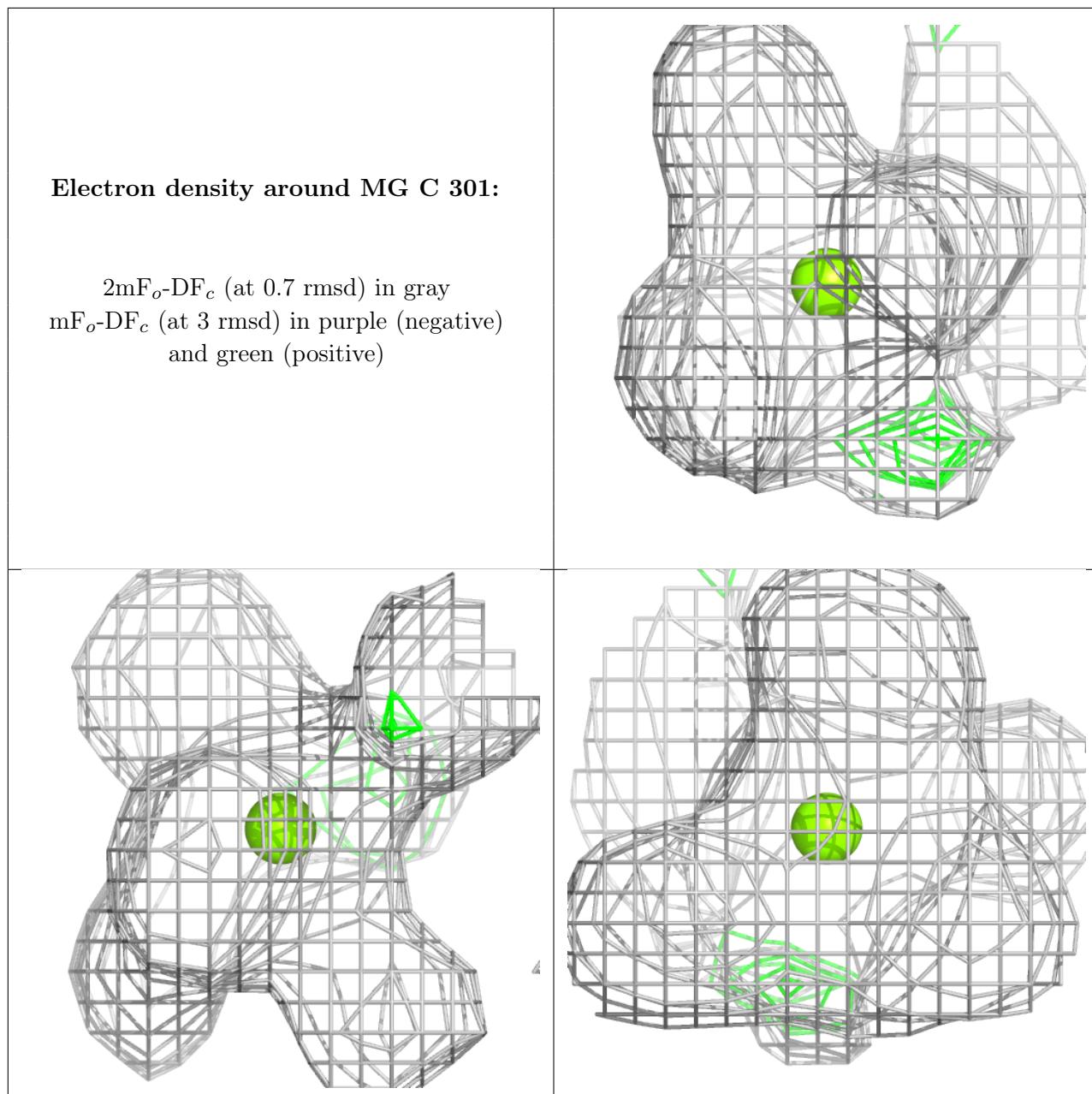


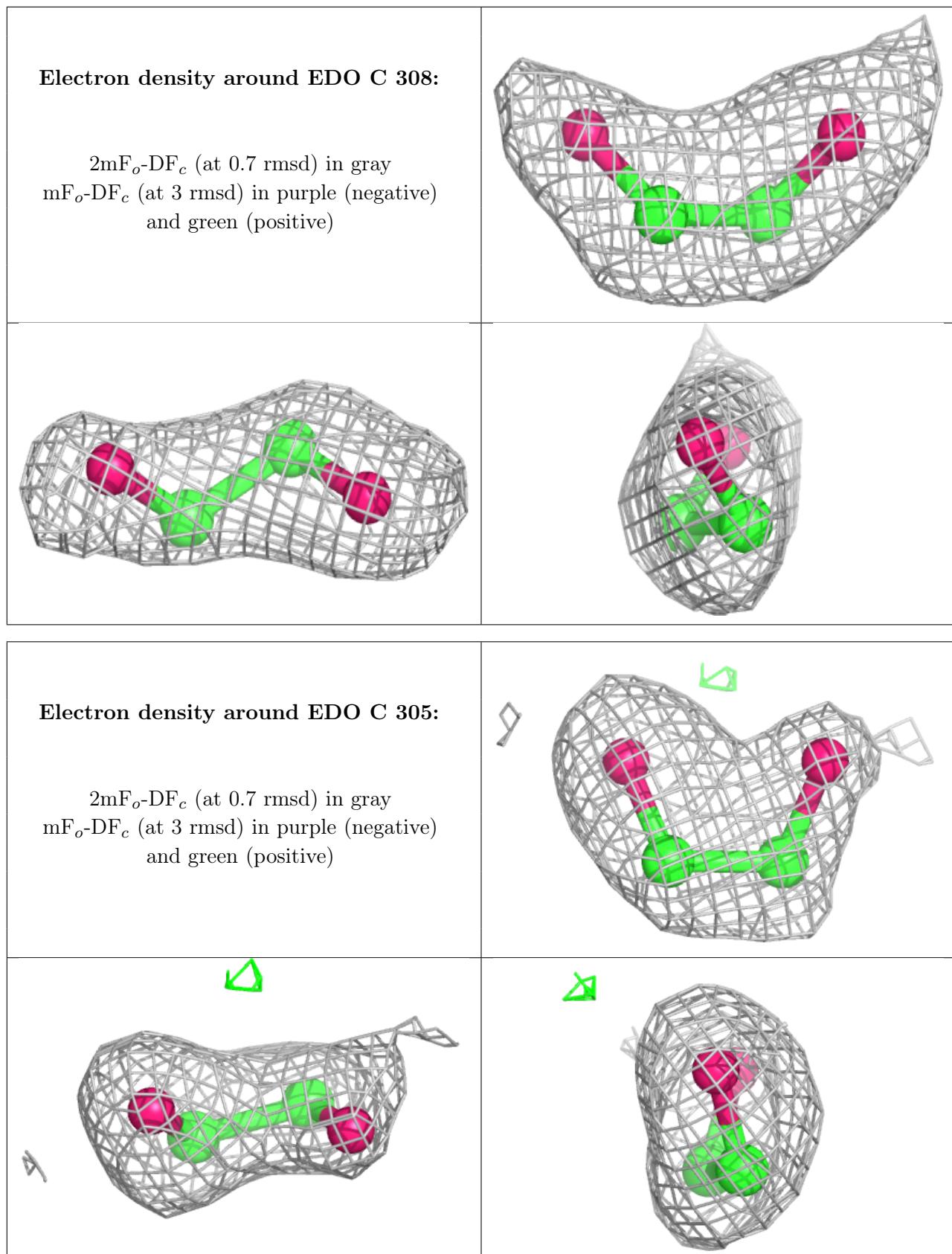


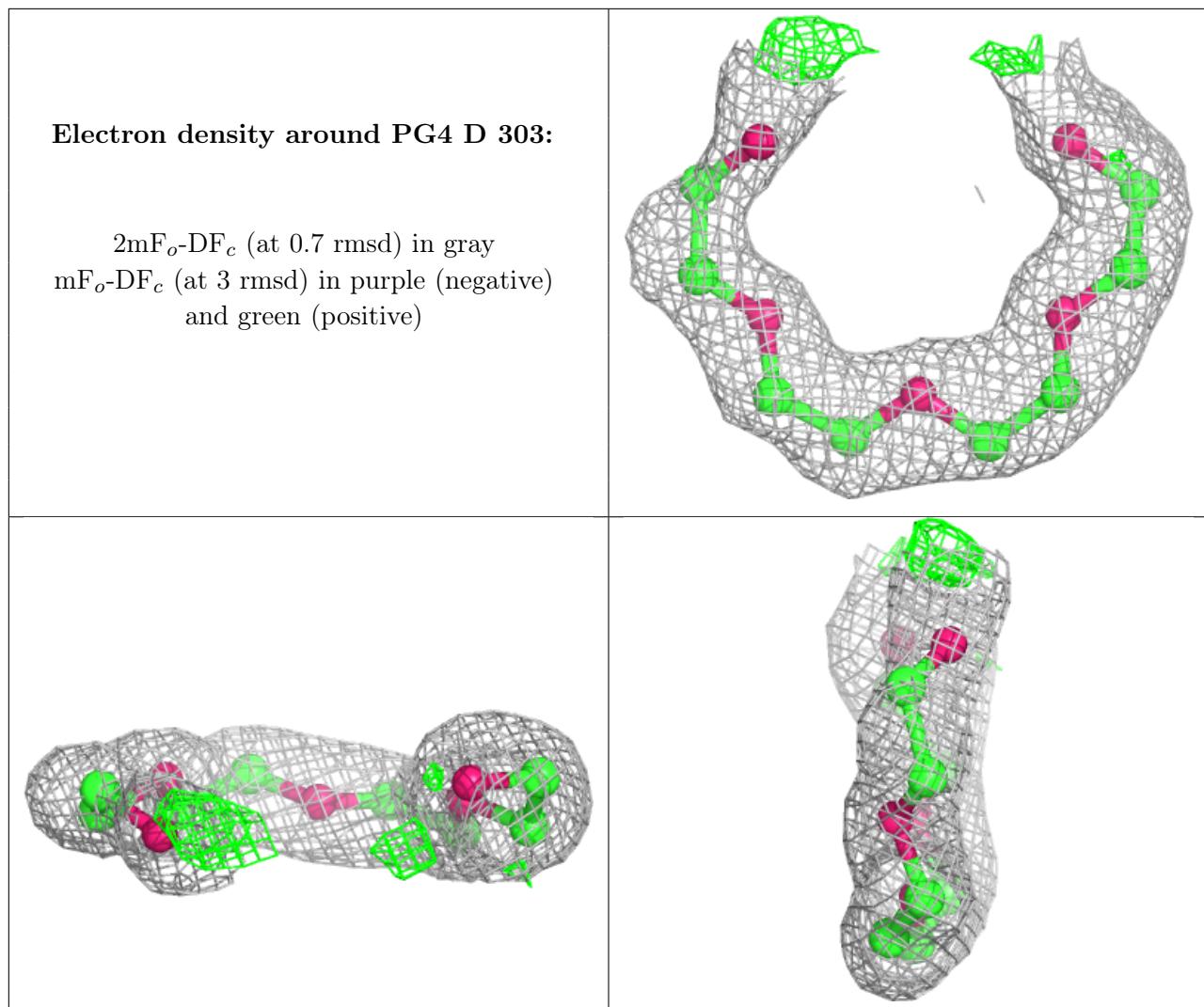


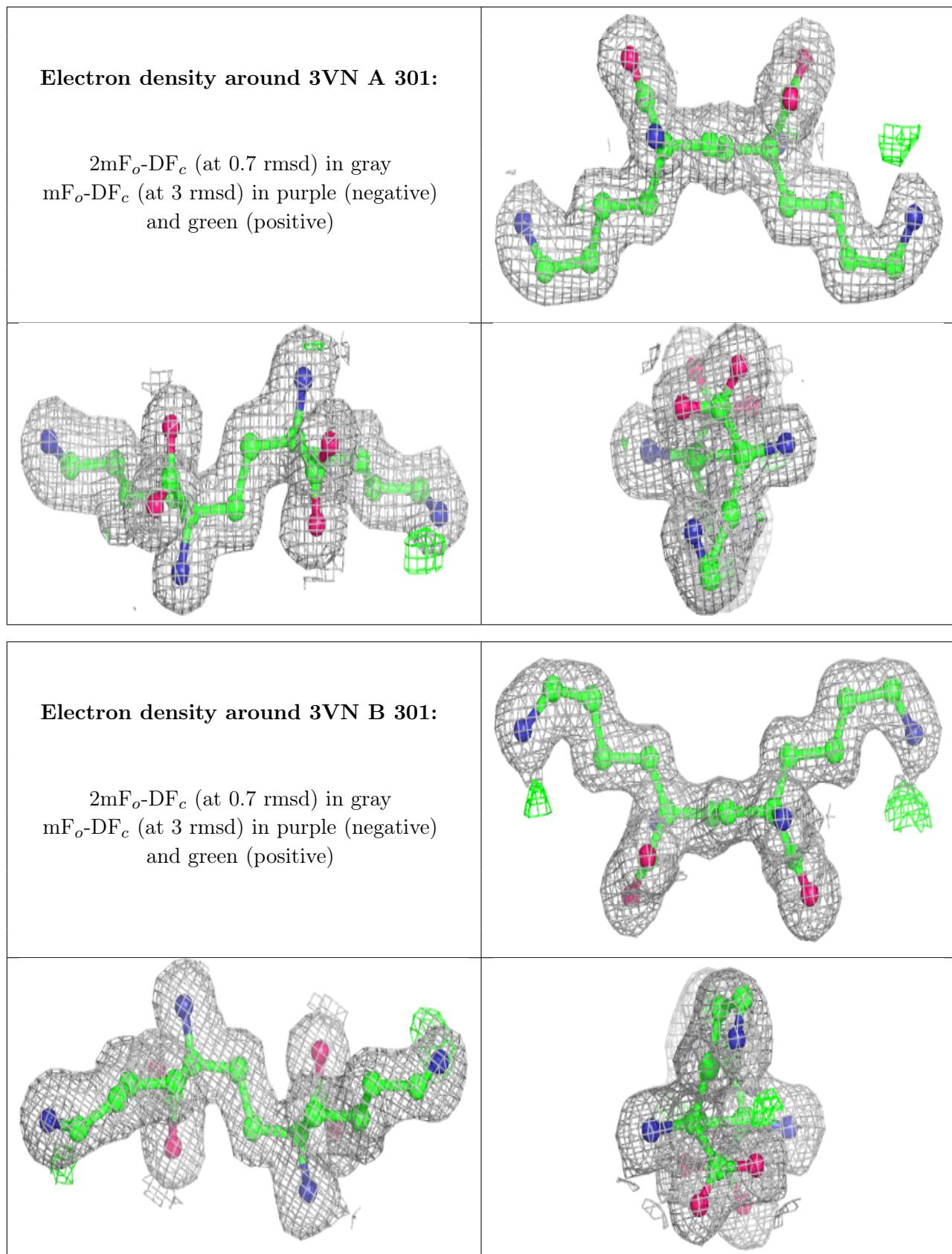


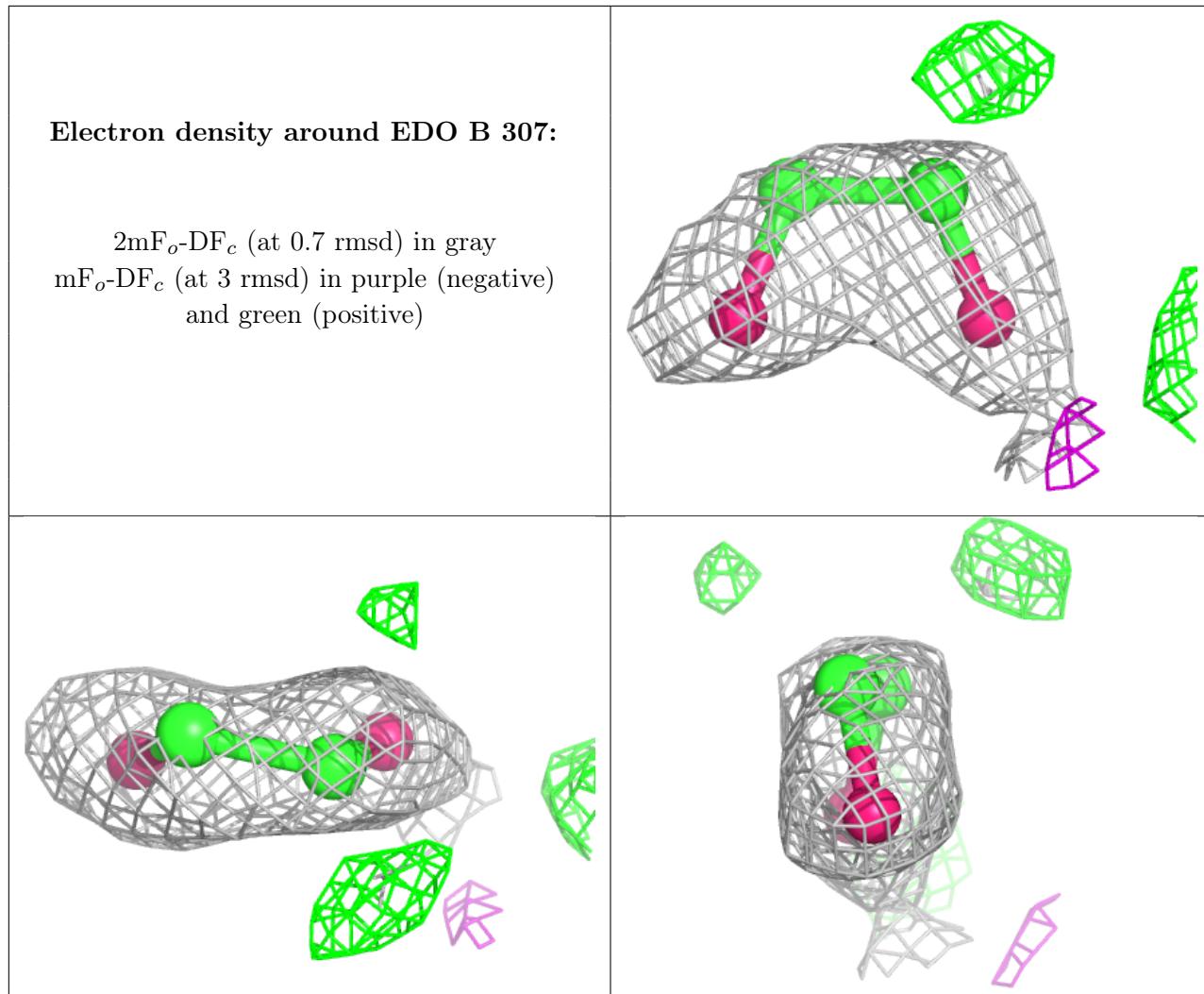


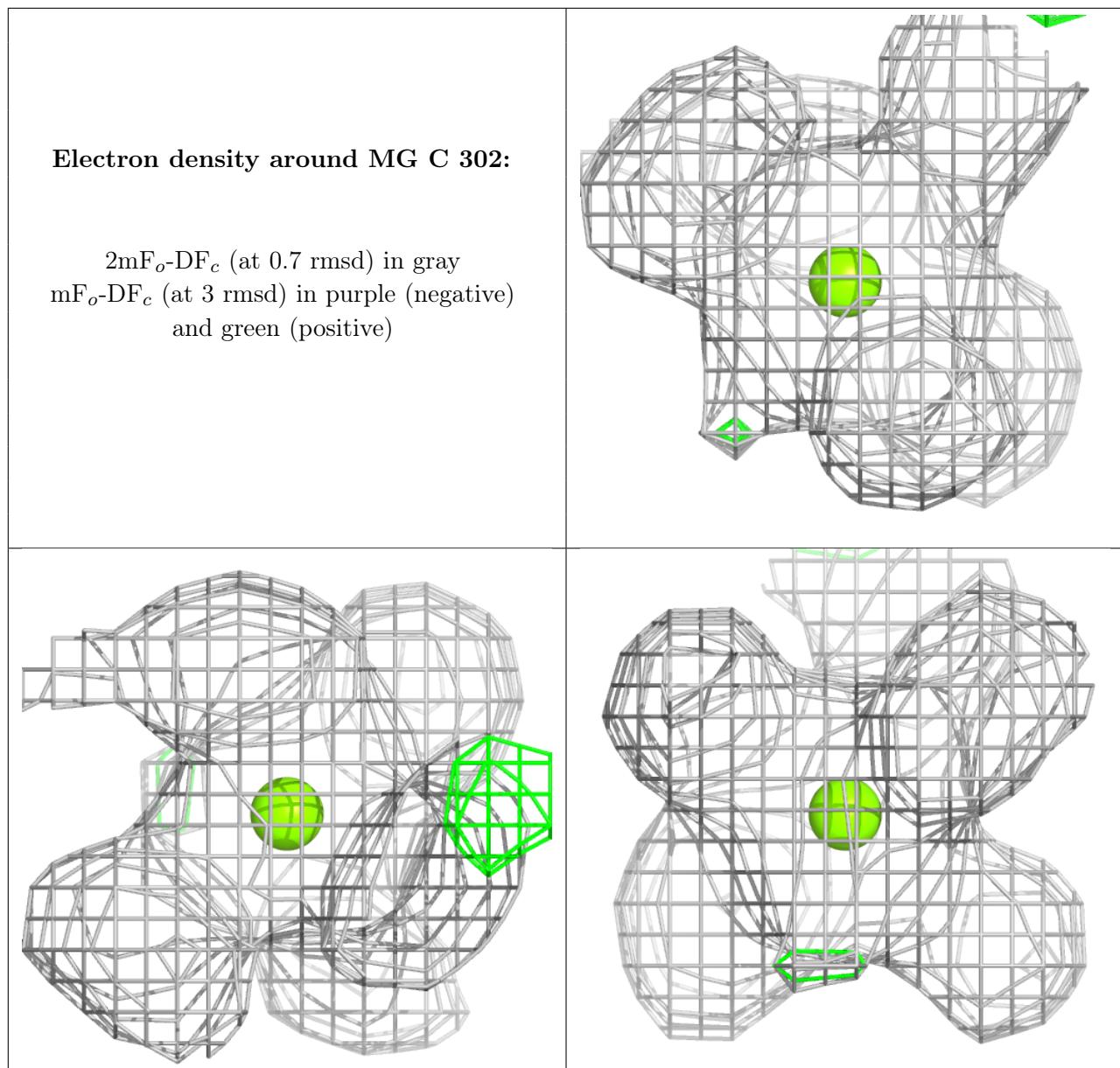


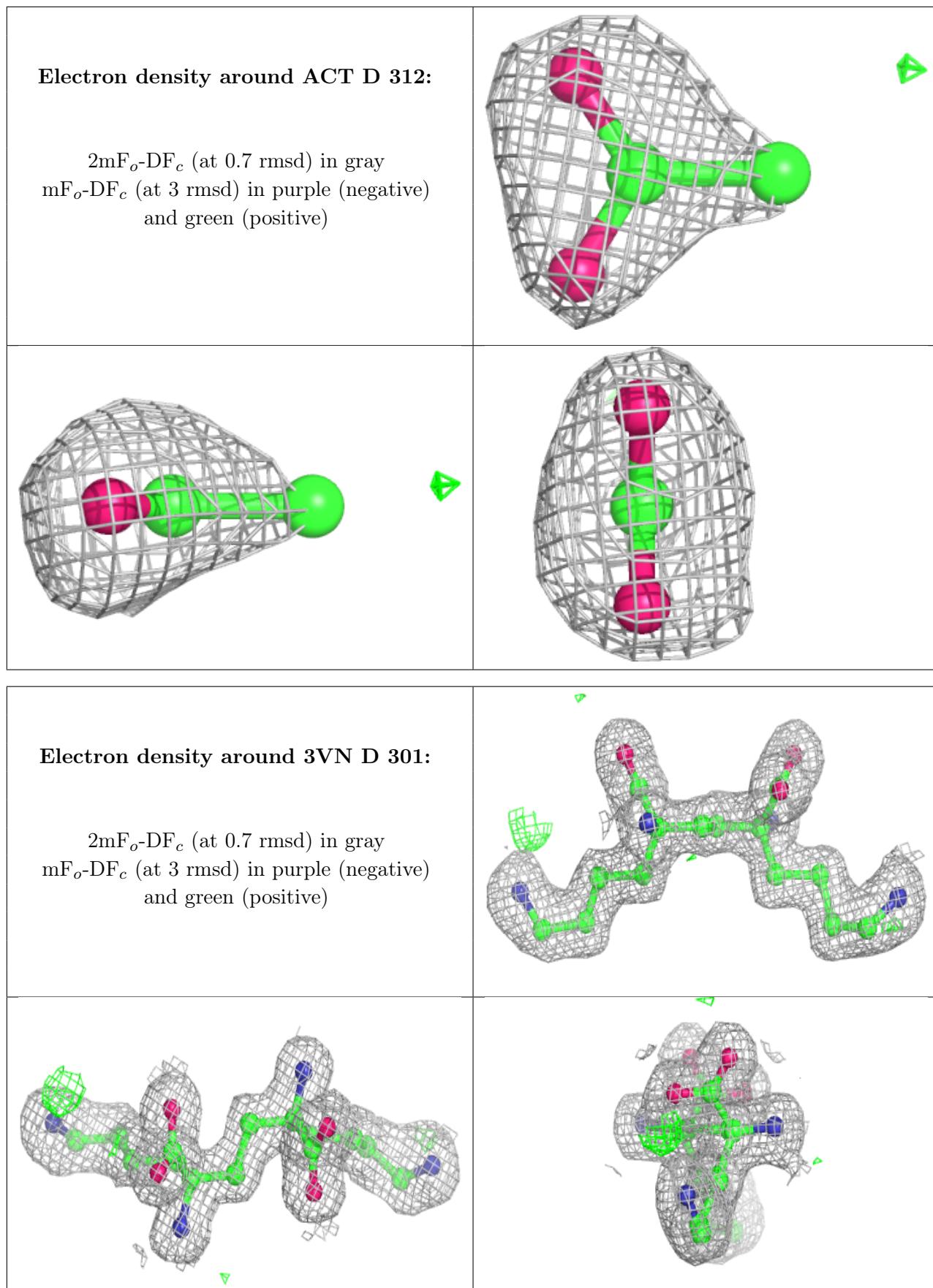


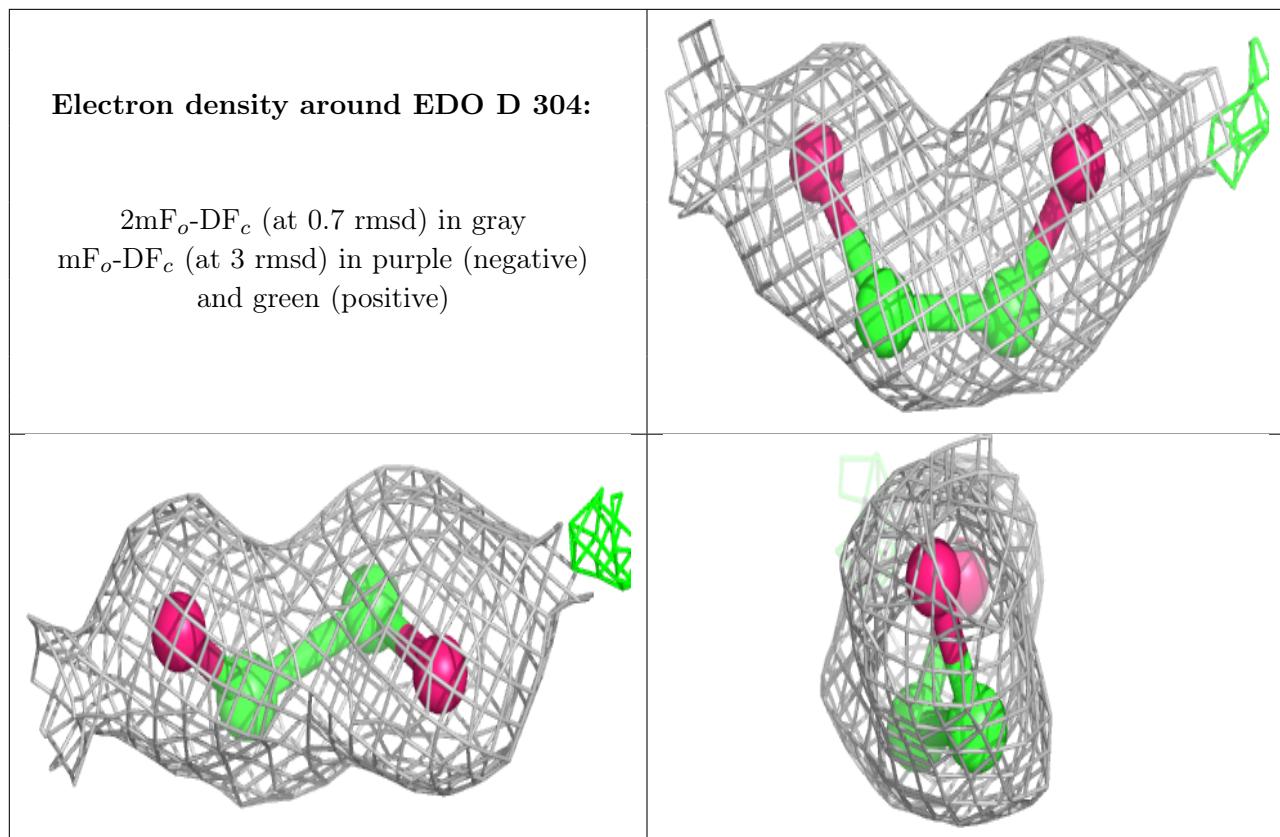


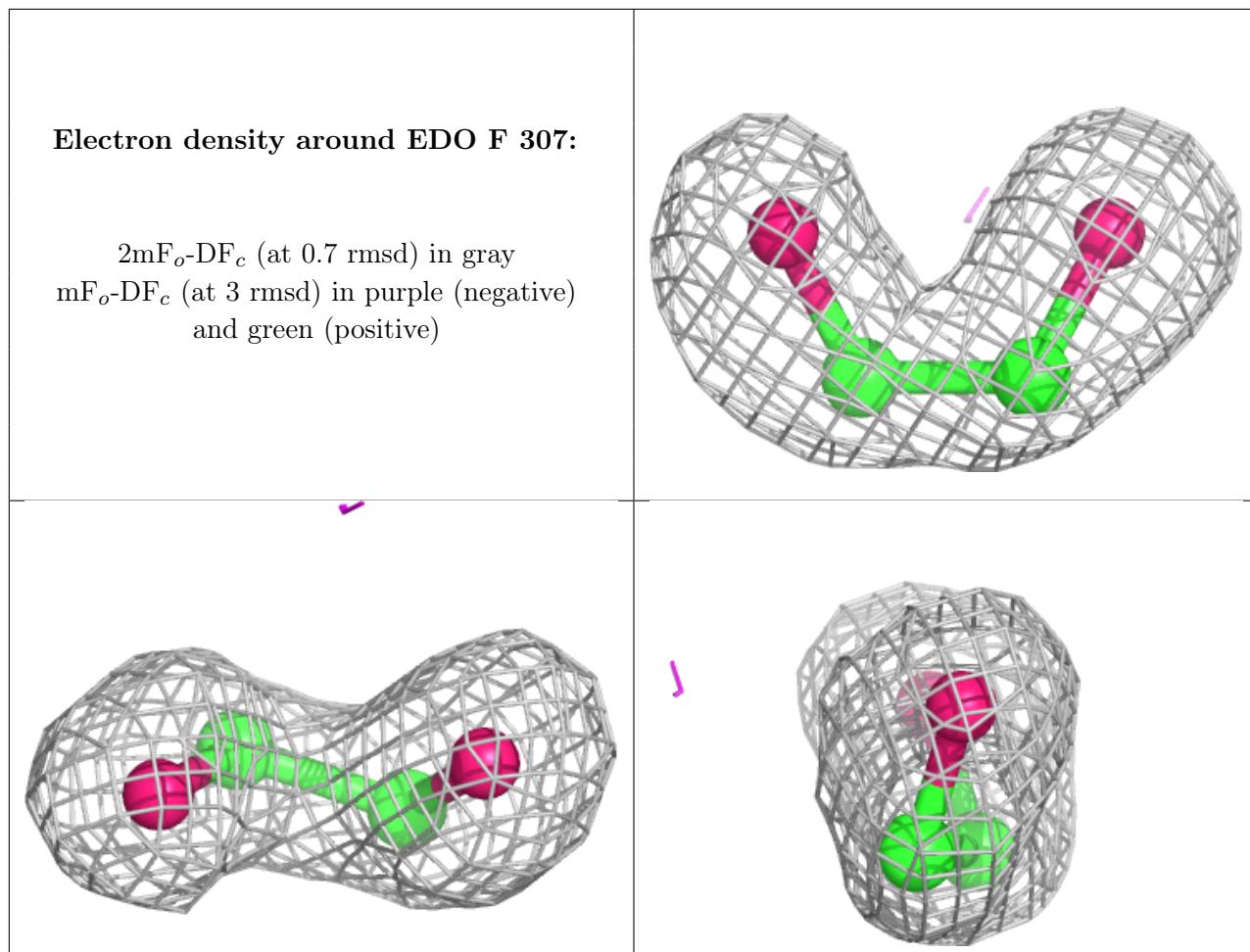


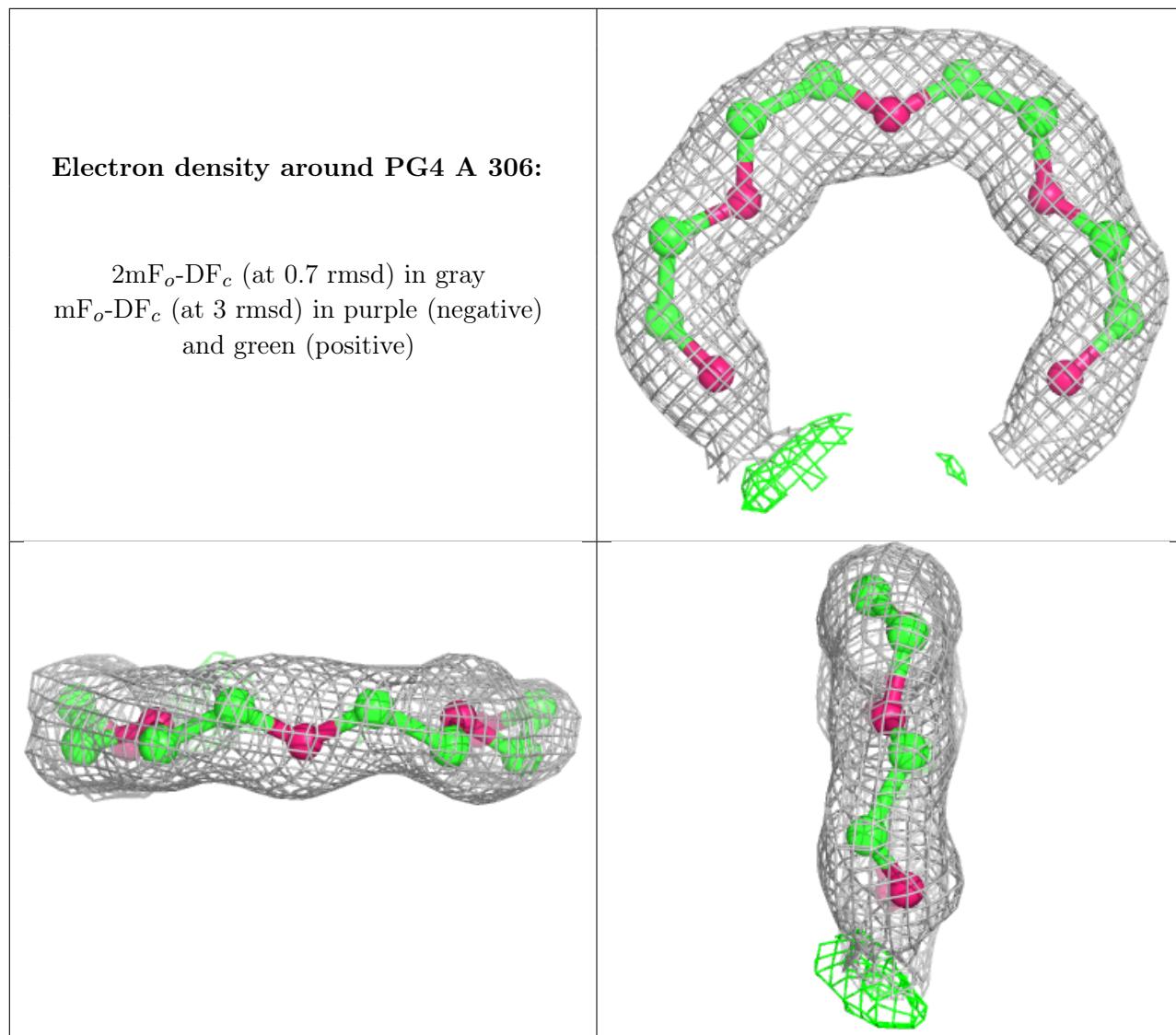


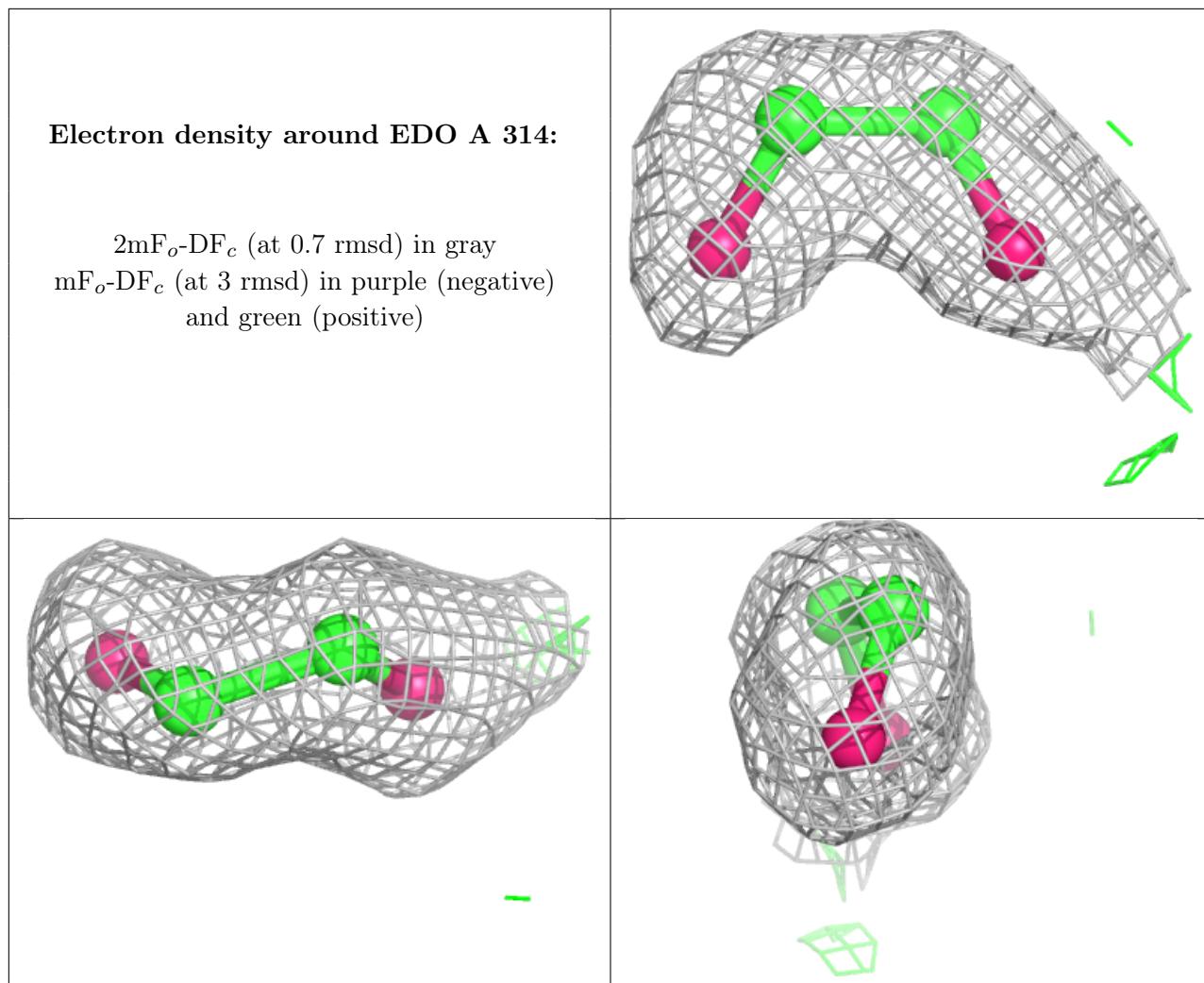


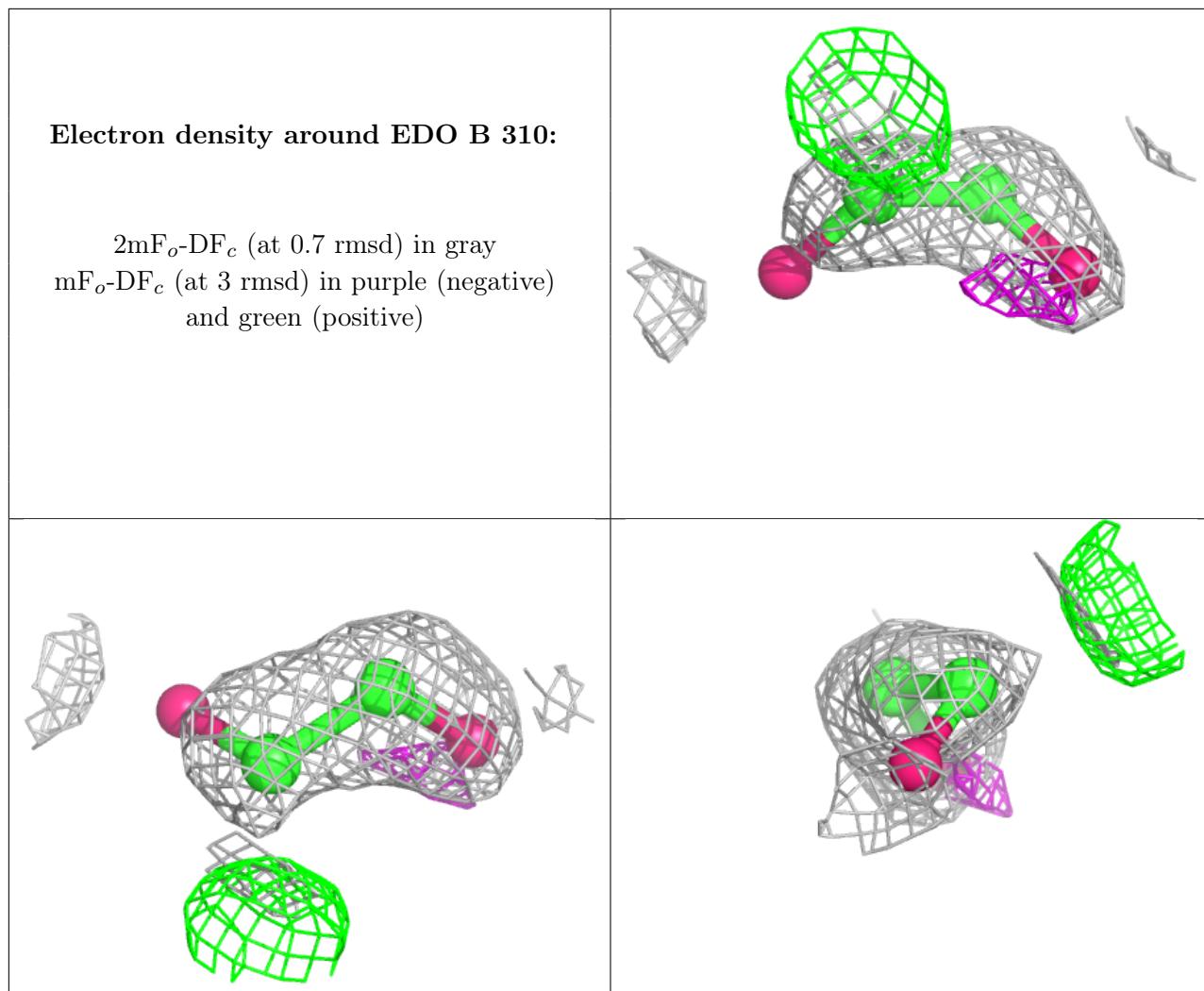


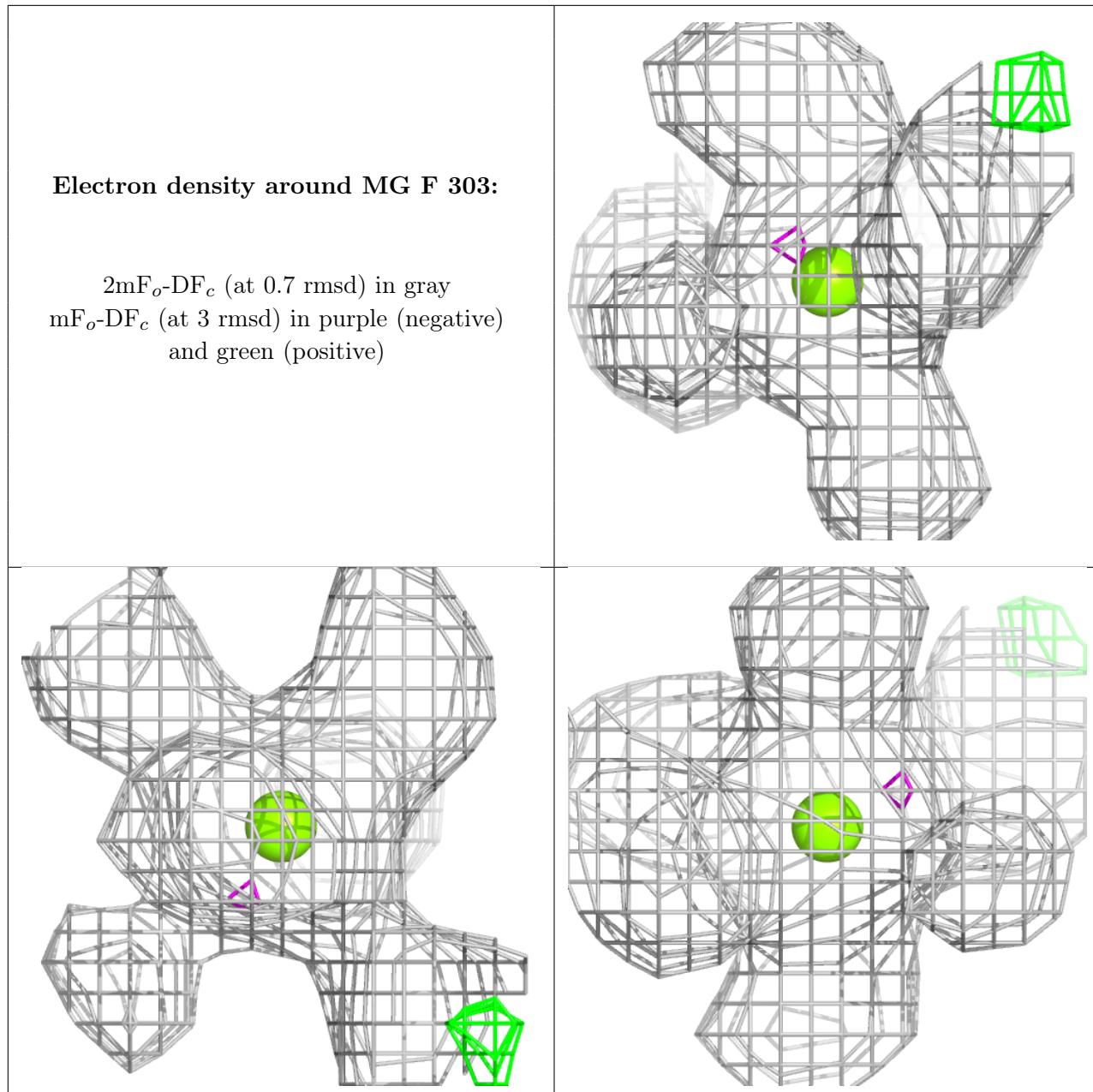


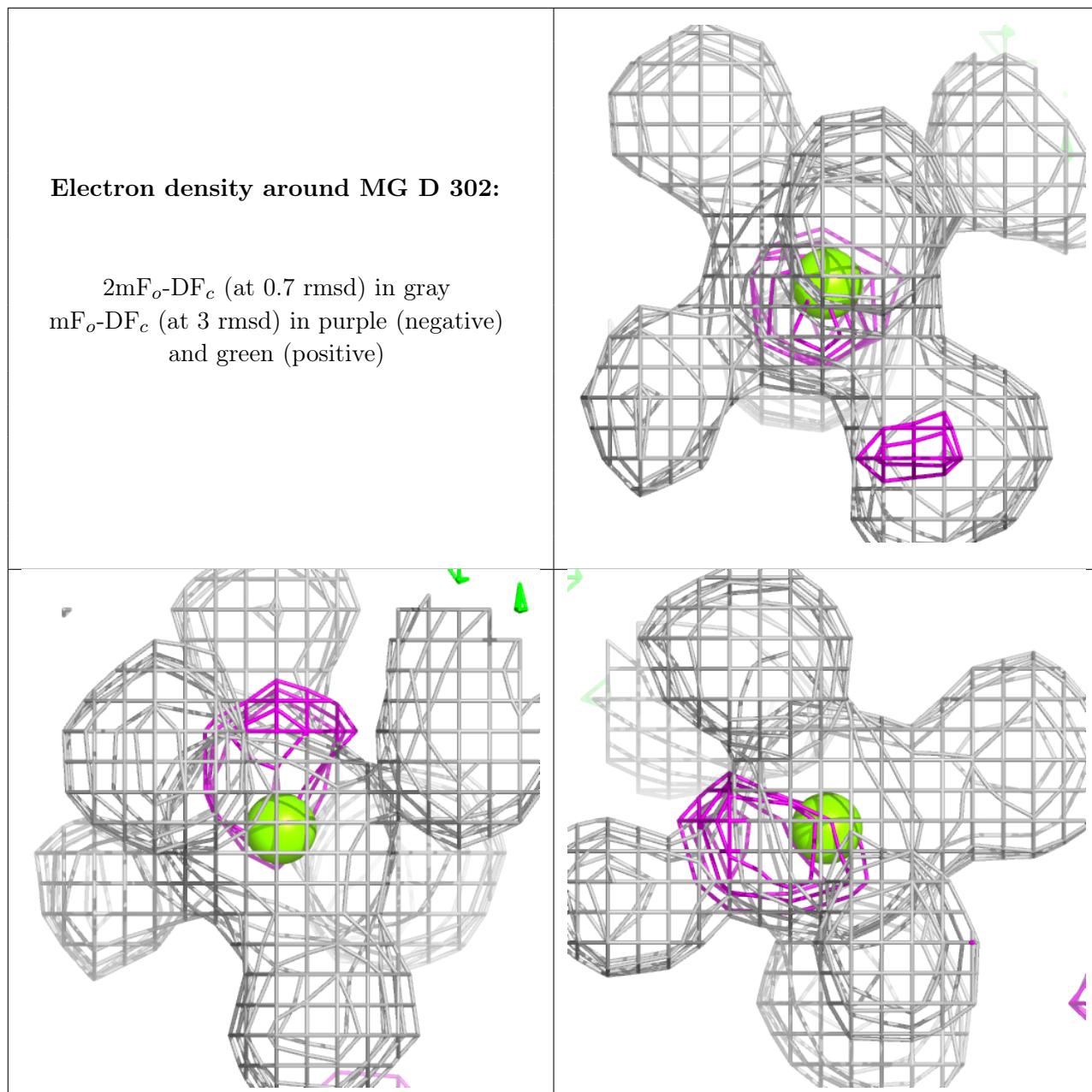


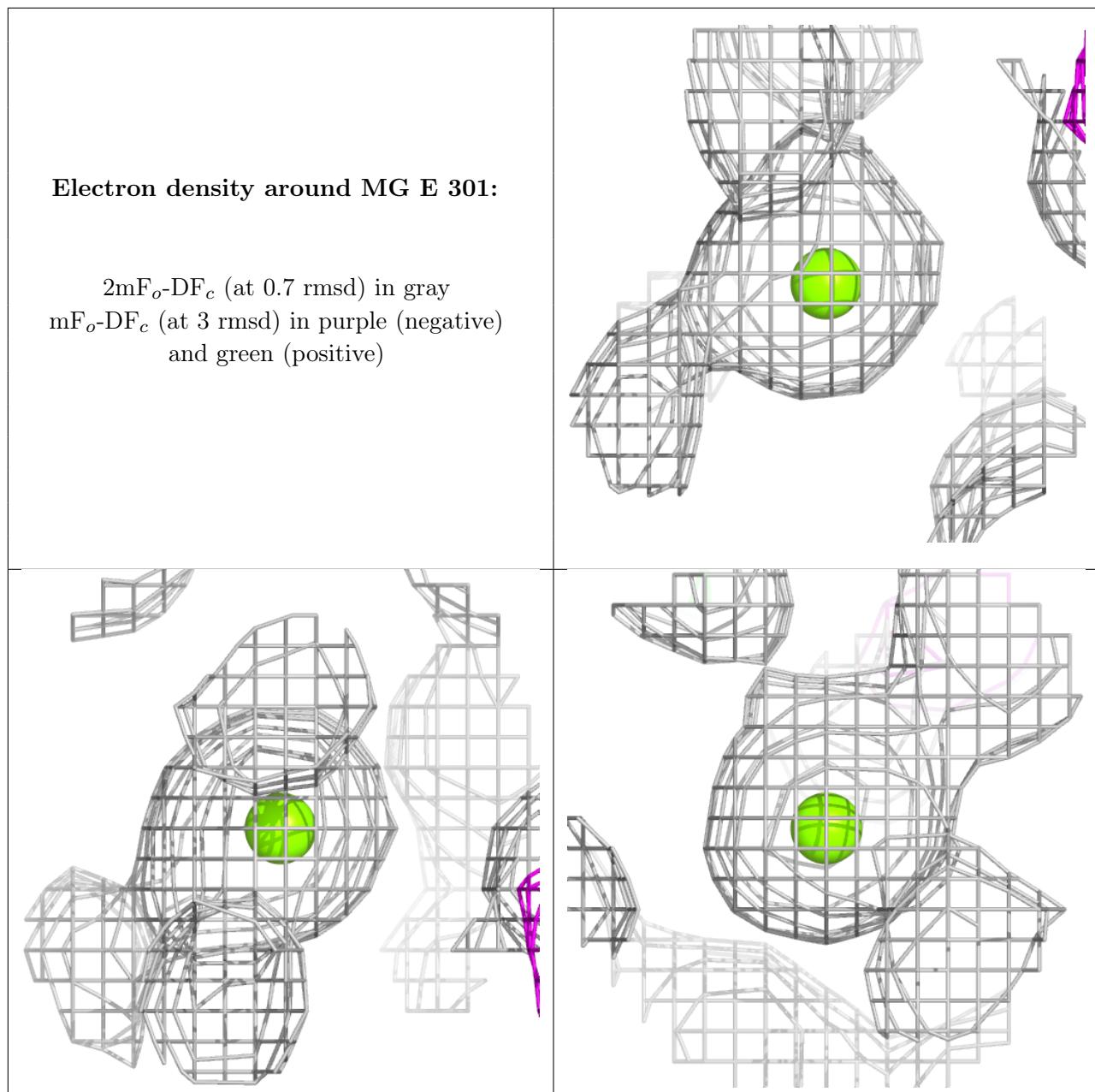


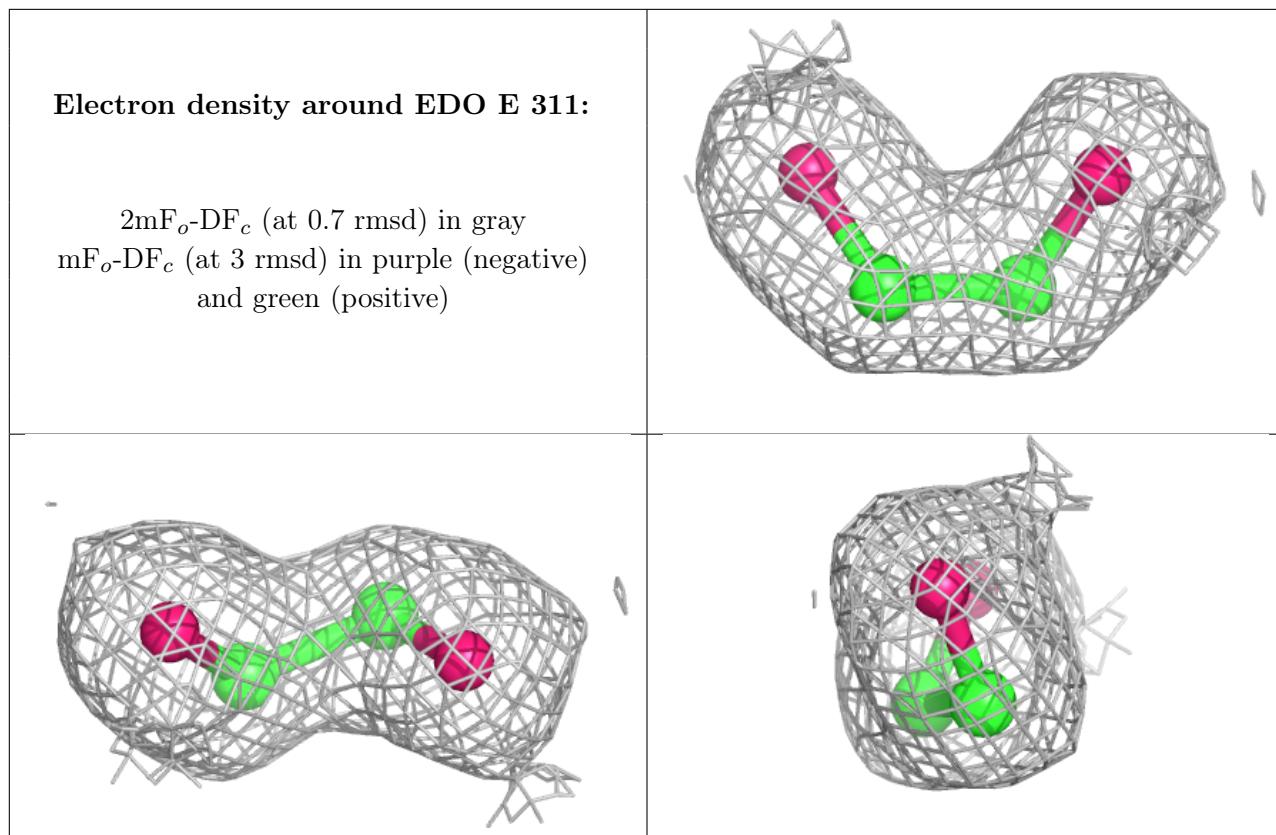


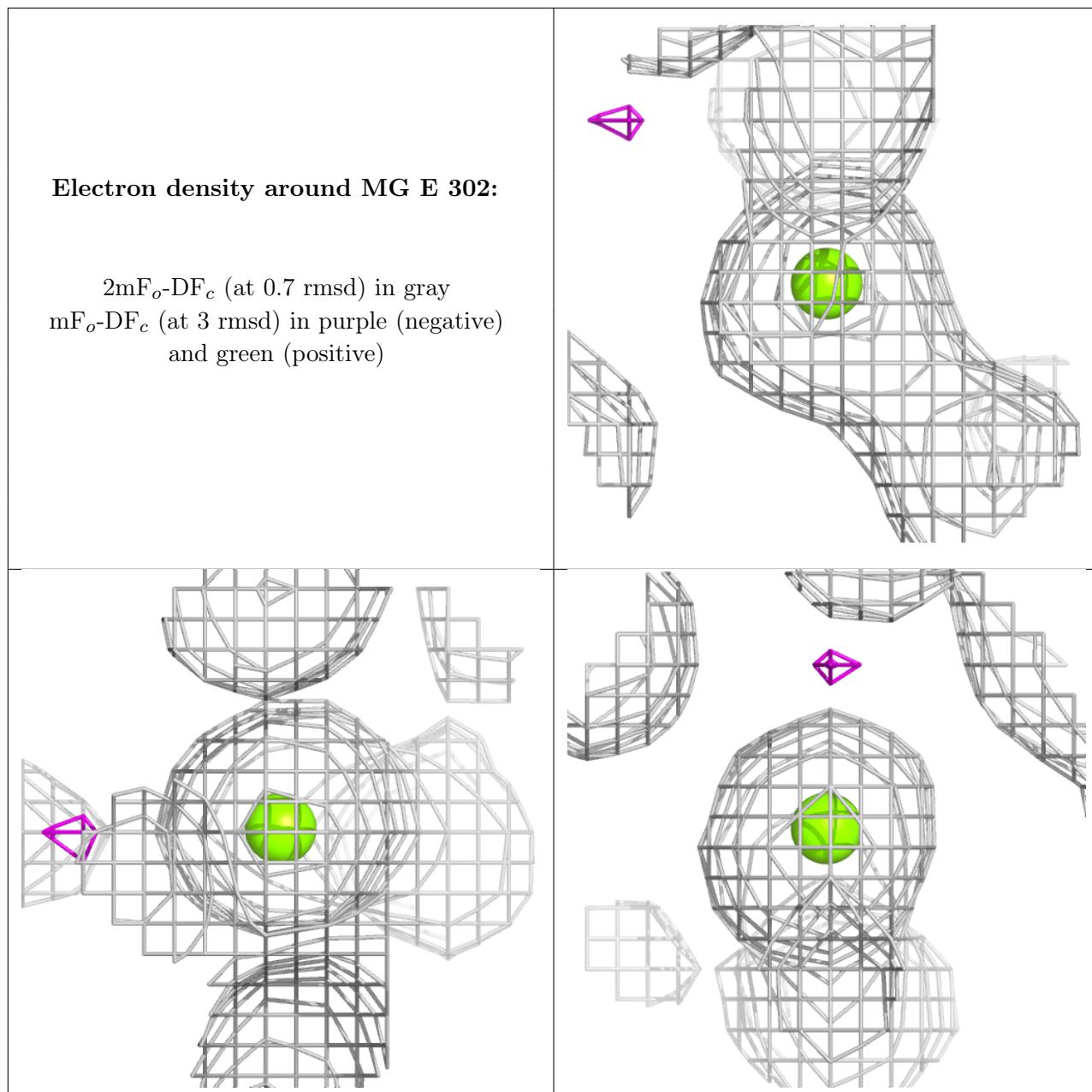


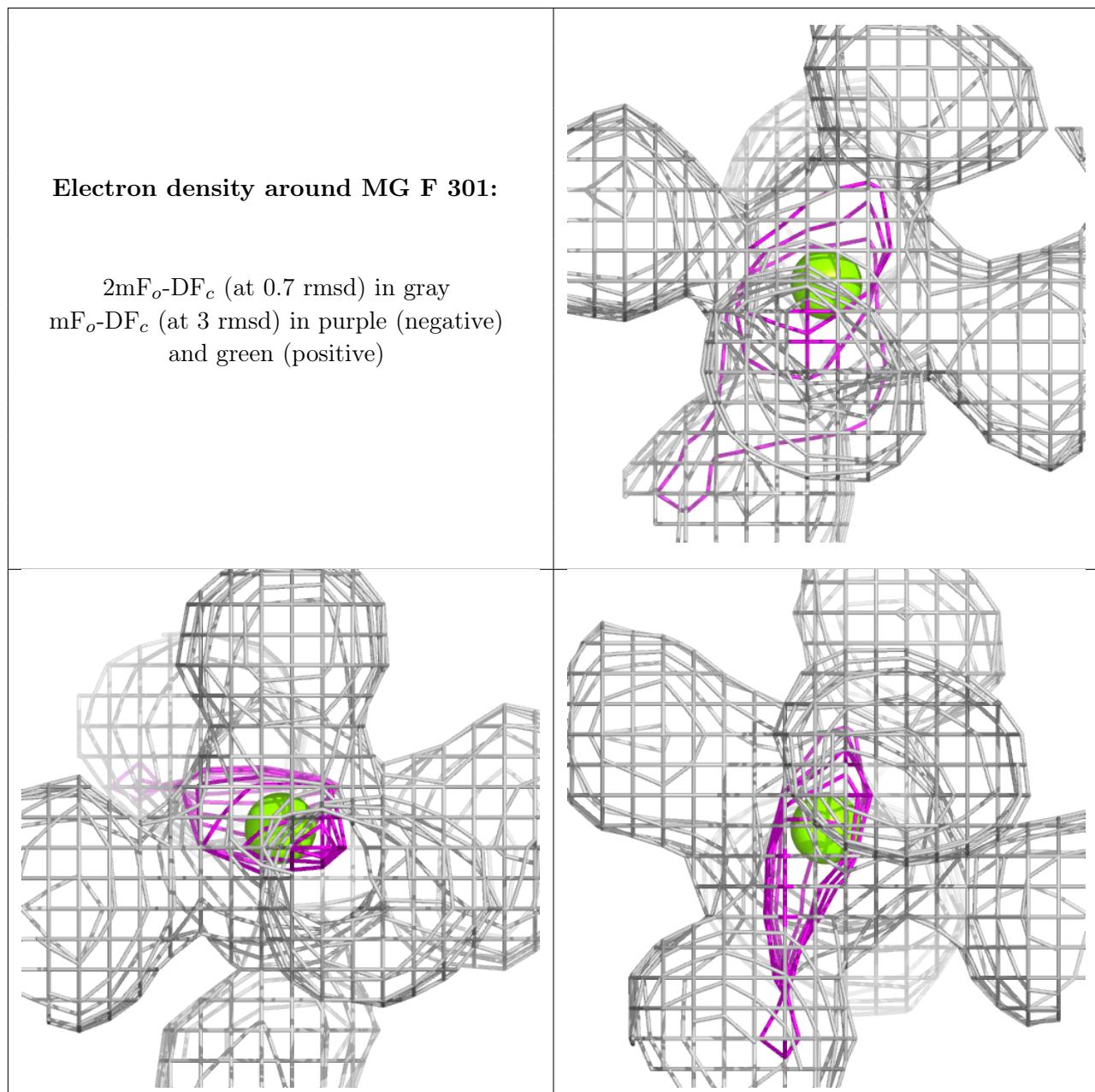


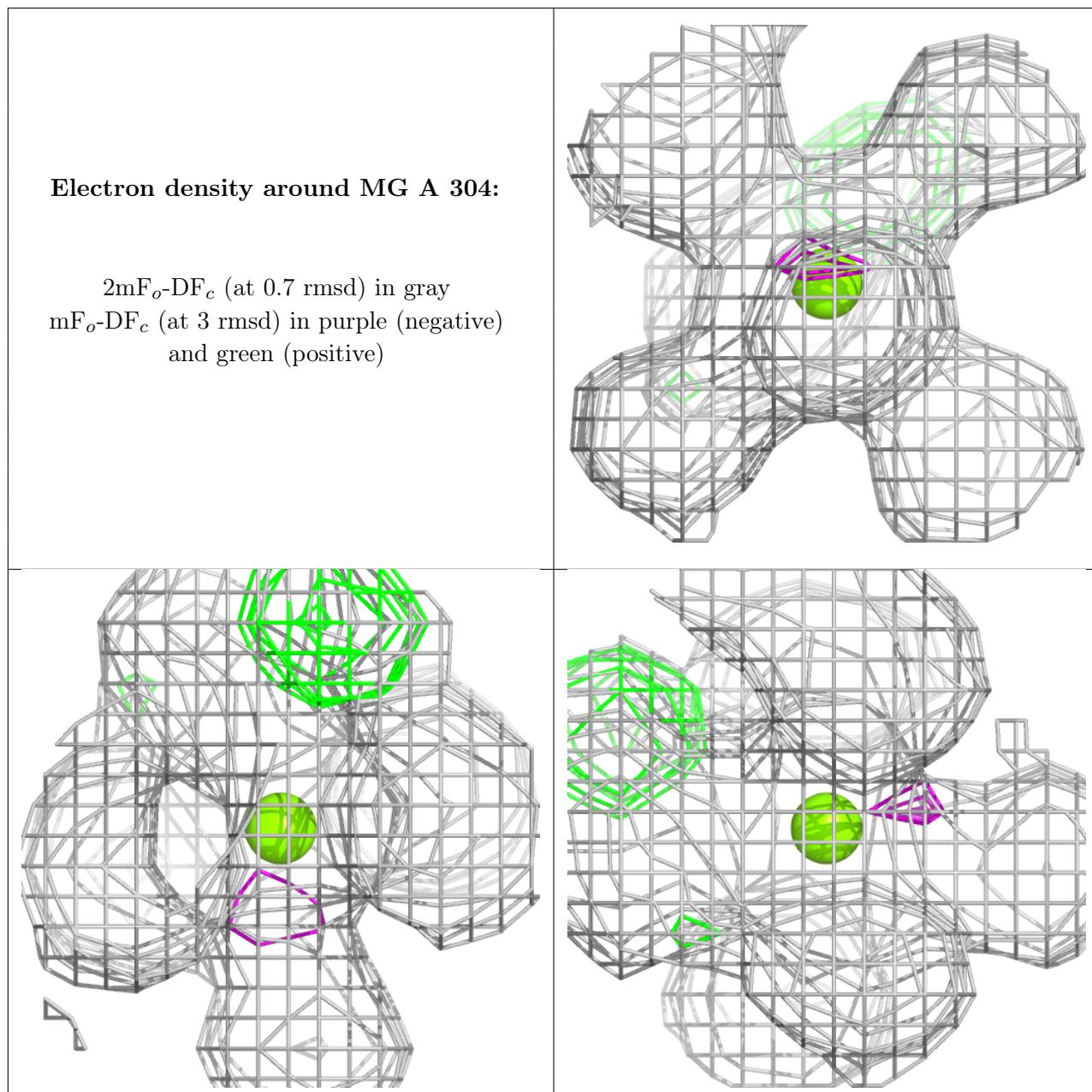


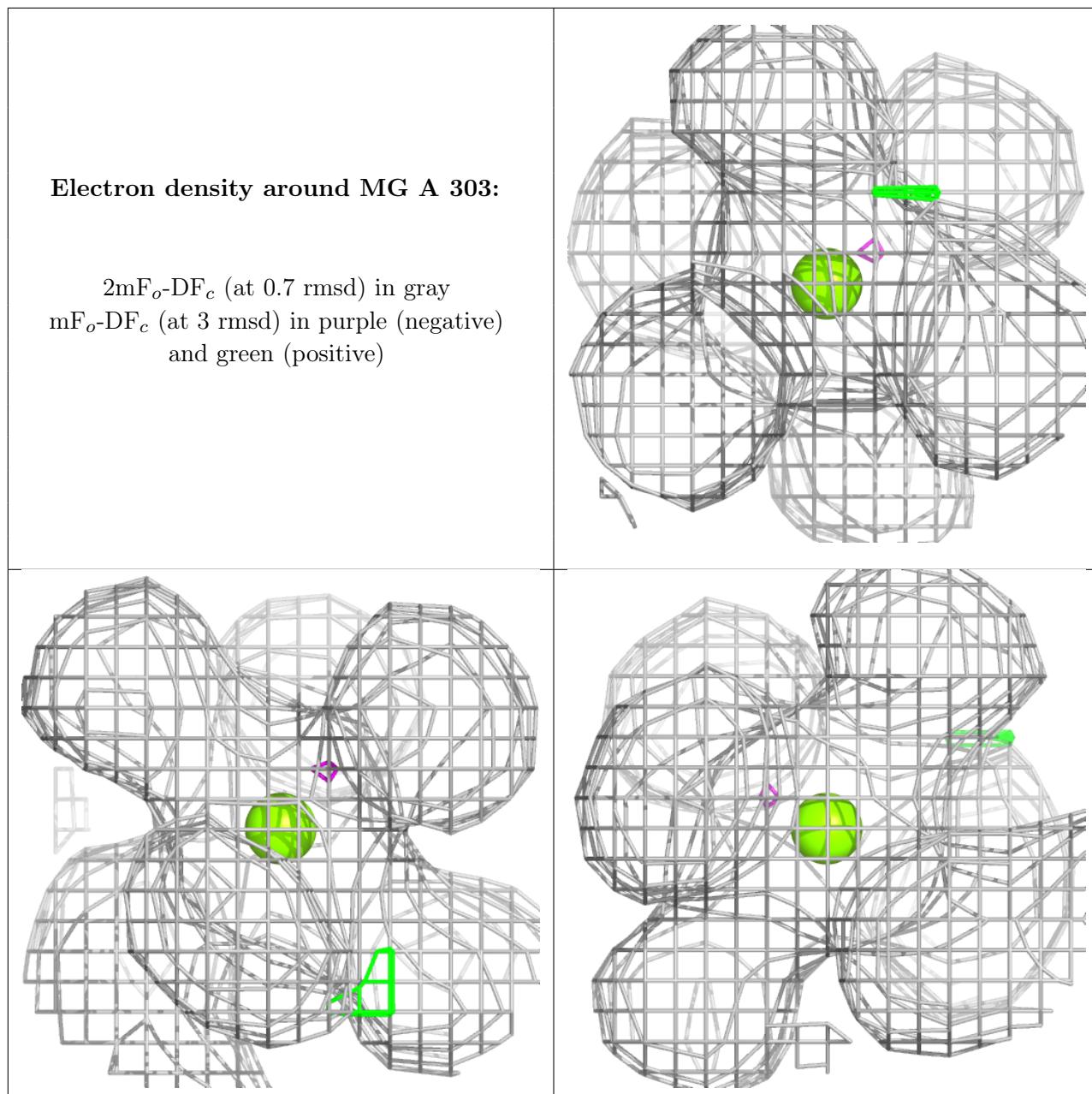


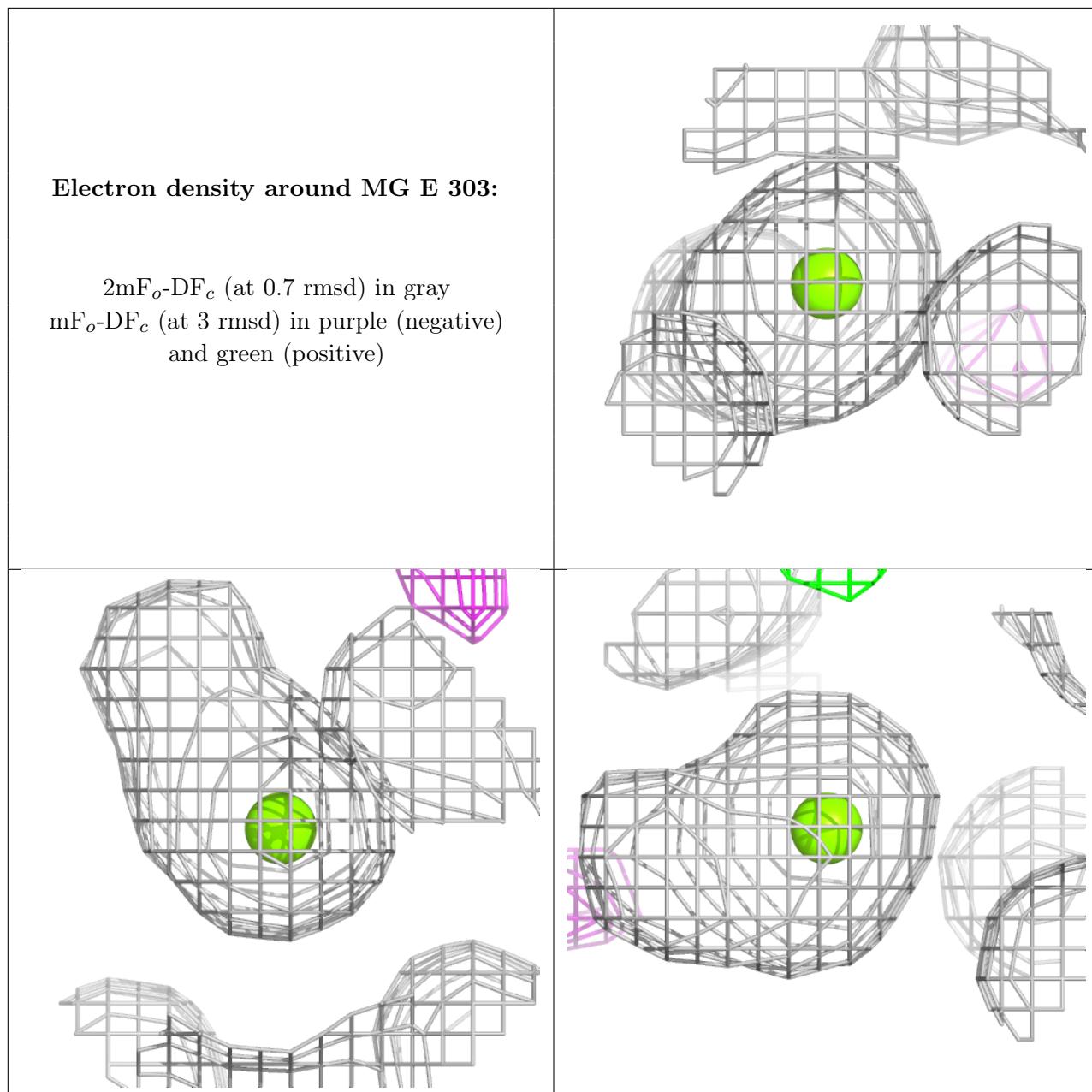


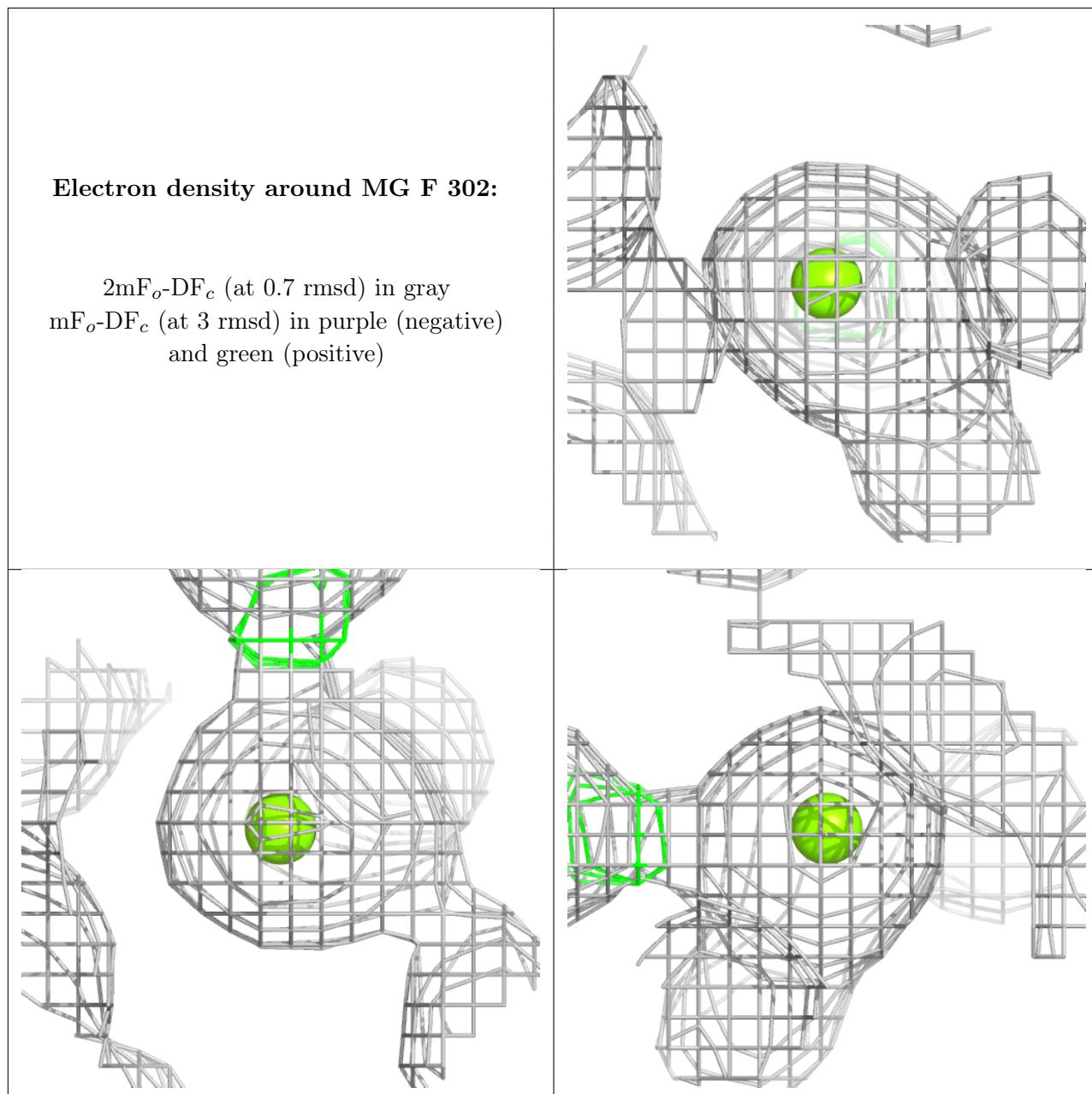


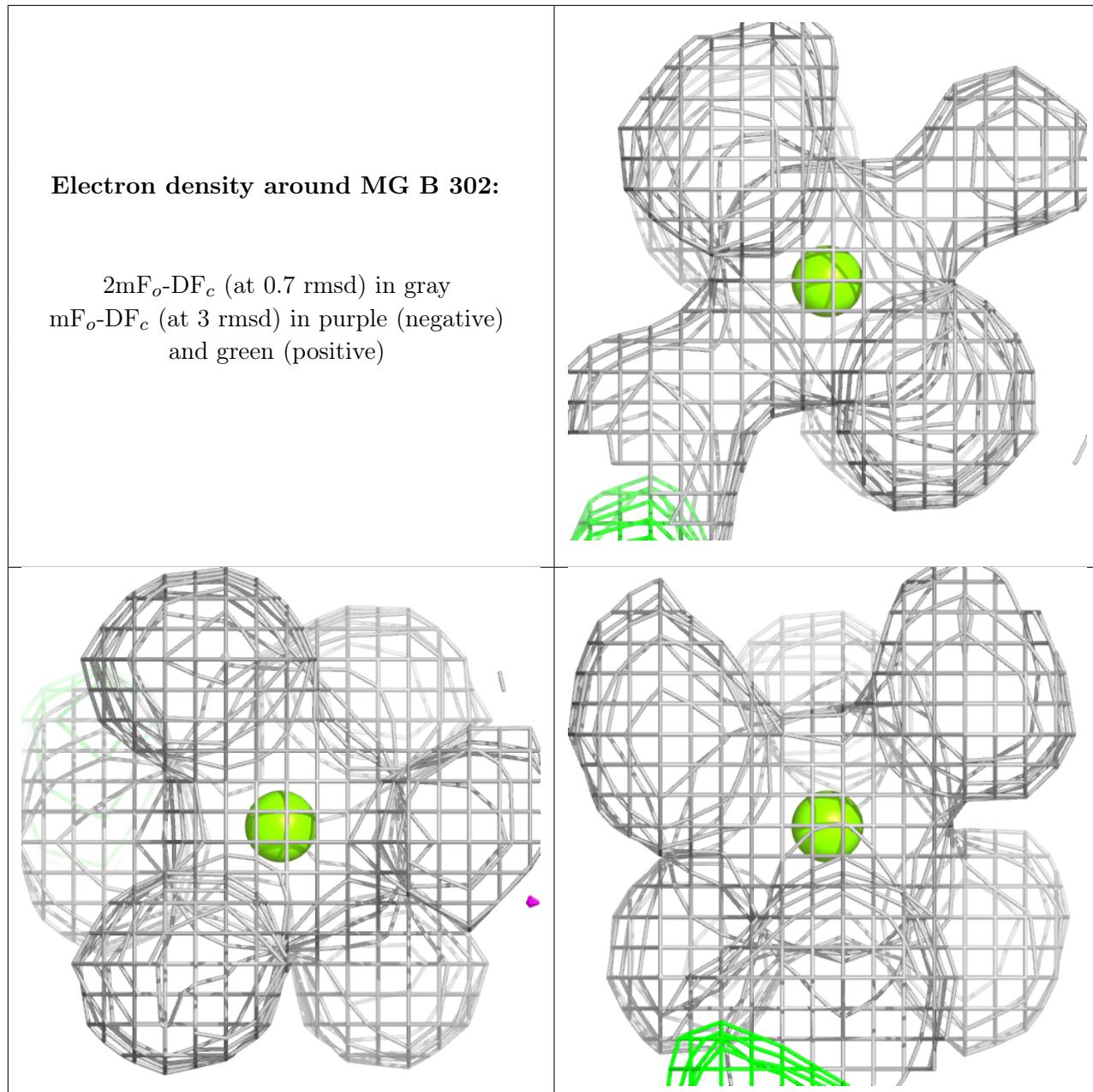












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.