wwPDB X-ray Structure Validation Summary Report (i)

Mar 12, 2026 – 05:53 PM UTC

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

This is a 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 (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 (i)) were used in the production of this report:

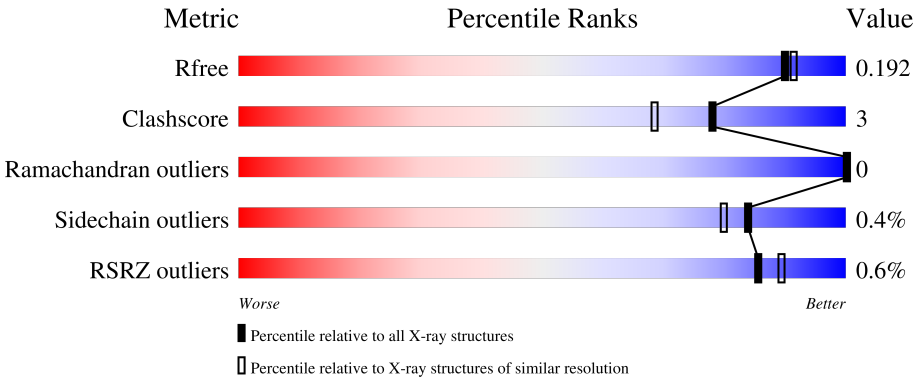
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

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



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

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

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

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Mol	Chain	Length	Quality of chain
1	E	310	
1	F	310	

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

There are 78 discrepancies between the modelled and reference sequences:

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

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

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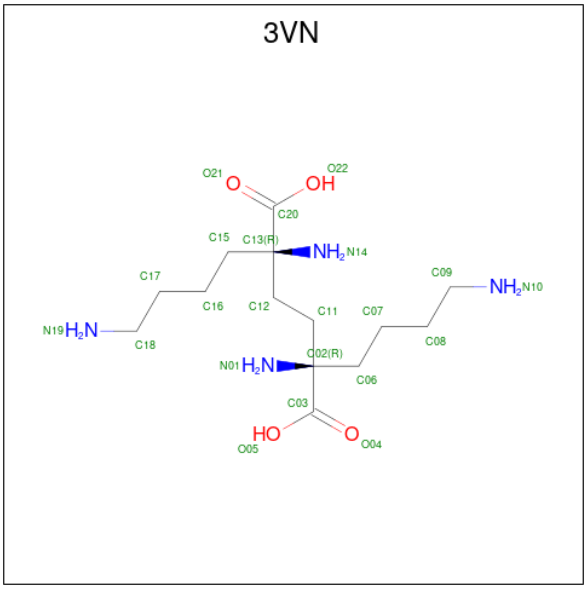
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	56	TRP	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag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

- Molecule 2 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (CCD ID: 3VN) (formula: $C_{14}H_{30}N_4O_4$) (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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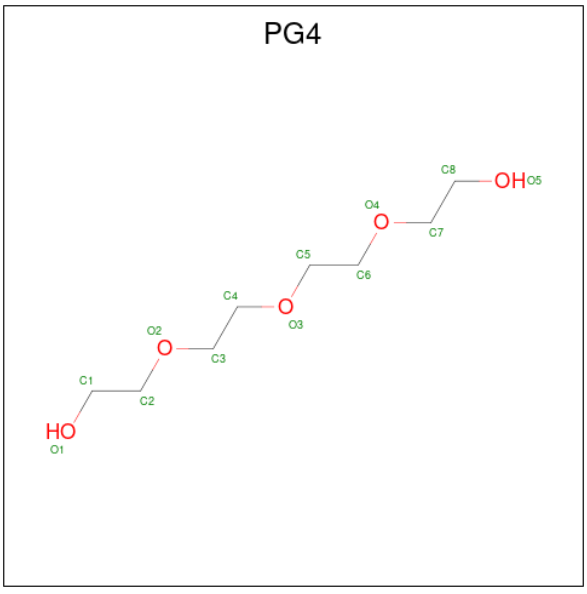
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 22 14 4 4	0	0
2	D	1	Total C N O 22 14 4 4	0	0

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

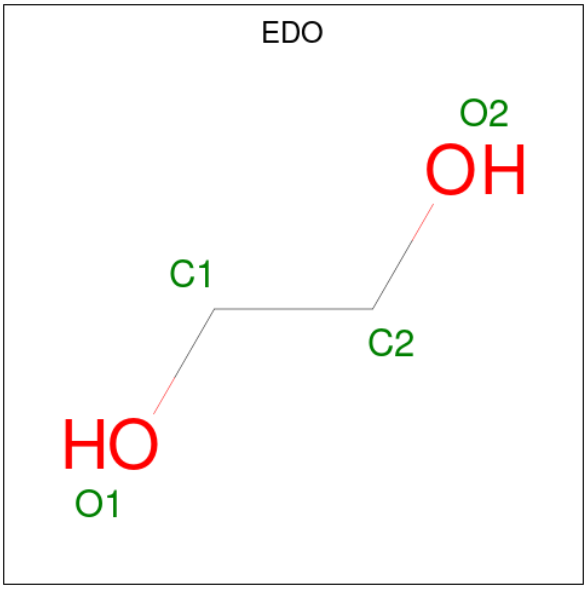
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Mg 4 4	0	0
3	B	3	Total Mg 3 3	0	0
3	C	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	E	5	Total Mg 5 5	0	0
3	F	4	Total Mg 4 4	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$) (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 (CCD ID: EDO) (formula: $C_2H_6O_2$) (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	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

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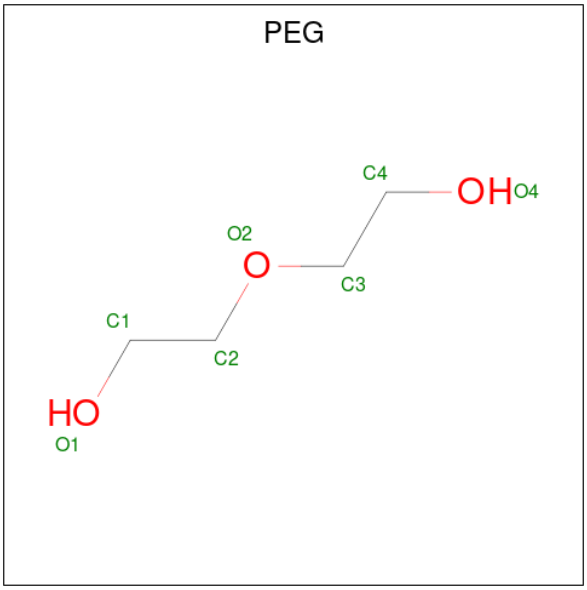
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

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



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

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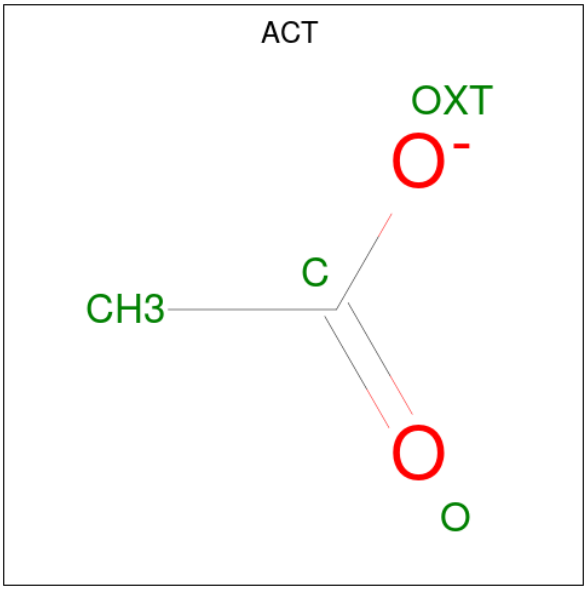
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	E	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0

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



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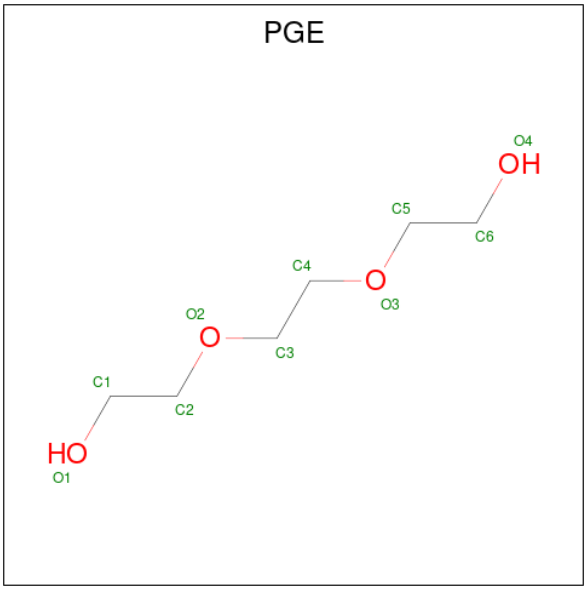
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

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



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

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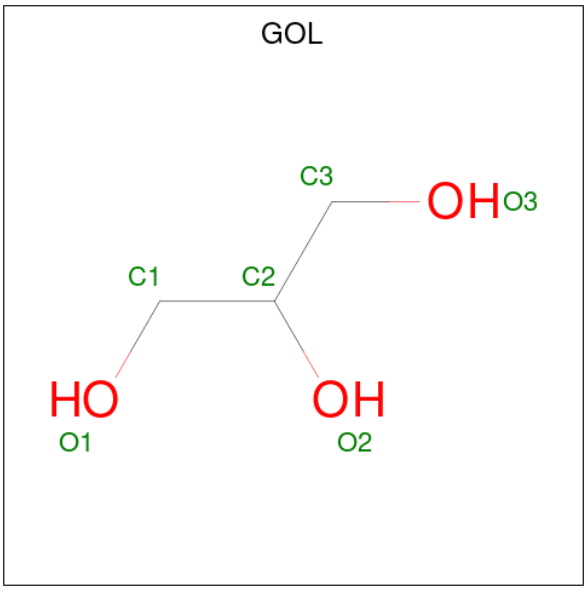
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 10 6 4	0	0

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



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

- Molecule 10 is water.

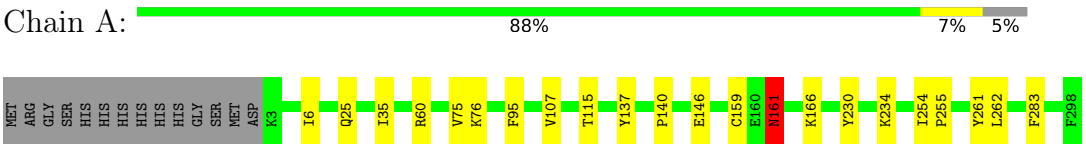
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	184	Total O 184 184	0	0
10	B	192	Total O 192 192	0	0
10	C	170	Total O 170 170	0	0
10	D	201	Total O 201 201	0	0
10	E	198	Total O 198 198	0	0
10	F	171	Total O 171 171	0	0

3 Residue-property plots (i)

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.

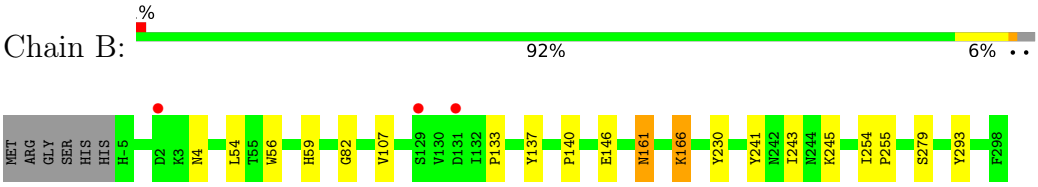
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A:



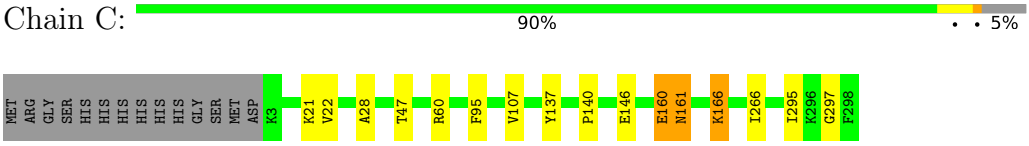
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:



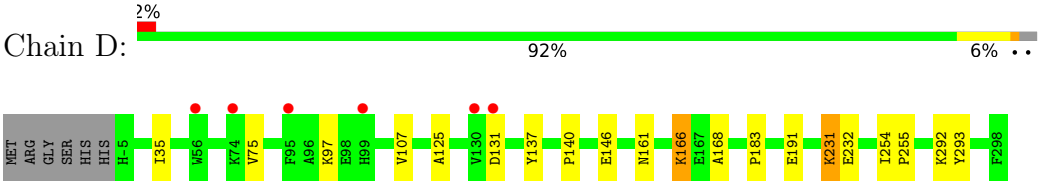
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C:



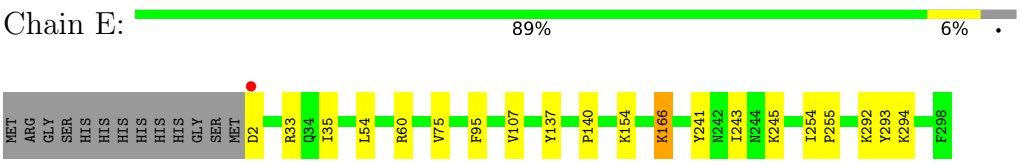
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D:



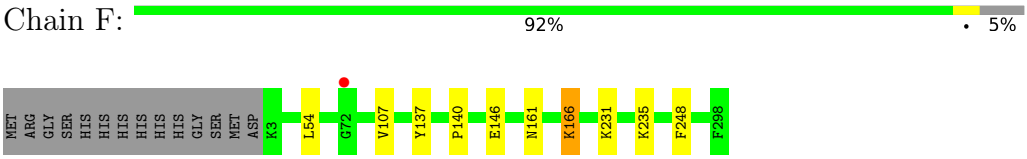
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F:


92%
5%
MET
ARG
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
GLY
SER
MET
ASP
K3
L54
G72
V107
Y137
P140
E146
N161
K166
K231
K235
F248
F298

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	84.41Å 225.29Å 199.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 1.75 48.90 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-1.75) 99.9 (48.90-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.75Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.157 , 0.185 0.165 , 0.192	Depositor DCC
R_{free} test set	9509 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 3VN, PG4, EDO, GOL, PEG, KPI, MG, ACT

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

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	ILE	C-O	-6.00	1.17	1.24
1	C	266	ILE	C-O	-5.90	1.18	1.24
1	C	22	VAL	C-O	-5.58	1.18	1.24
1	D	125	ALA	C-O	-5.46	1.17	1.24
1	C	28	ALA	C-O	-5.46	1.17	1.24

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2286	0	2323	13	0
1	B	2351	0	2375	18	0
1	C	2285	0	2323	7	0
1	D	2363	0	2383	11	0
1	E	2293	0	2327	16	0
1	F	2284	0	2322	8	0
2	A	22	0	28	1	0
2	B	22	0	28	1	0
2	D	22	0	28	1	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	5	0	0	0	0
3	F	4	0	0	0	0
4	A	13	0	18	0	0
4	B	13	0	18	0	0
4	C	13	0	18	0	0
4	D	13	0	18	1	0
4	E	13	0	18	3	0
4	F	13	0	18	0	0
5	A	40	0	60	2	0
5	B	20	0	30	6	0
5	C	24	0	36	0	0
5	D	16	0	24	1	0
5	E	24	0	36	1	0
5	F	8	0	12	1	0
6	A	14	0	20	0	0
6	B	21	0	30	3	0
6	C	7	0	10	2	0
6	D	7	0	10	0	0
6	E	7	0	10	1	0
6	F	14	0	20	0	0
7	A	8	0	6	1	0
7	B	8	0	6	0	0
7	D	16	0	12	0	0
7	E	4	0	3	1	0
7	F	16	0	12	0	0
8	B	10	0	14	0	0
8	D	20	0	28	3	0
8	E	10	0	14	1	0

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

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

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:KPI:H1B	10:B:581:HOH:O	1.73	0.88
1:D:166:KPI:H1A	10:D:444:HOH:O	1.79	0.81
1:B:279:SER:HB3	6:B:313:PEG:H42	1.64	0.80
1:C:160:GLU:CD	1:C:160:GLU:H	1.89	0.80
1:C:166:KPI:H1A	10:C:428:HOH:O	1.86	0.75

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

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

5 of 6 residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	19	ASN
1	F	252	ASN

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Mol	Chain	Res	Type
1	B	128	GLN
1	D	201	ASN
1	E	19	ASN

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	1.40	1 (9%)	9,15,17	3.16	5 (55%)
1	KPI	D	166	1	11,13,14	1.28	1 (9%)	9,15,17	2.56	3 (33%)
1	KPI	E	166	1	11,13,14	2.01	2 (18%)	9,15,17	2.48	1 (11%)
1	KPI	A	166	1	11,13,14	2.03	2 (18%)	9,15,17	2.53	3 (33%)
1	KPI	C	166	1	11,13,14	2.47	2 (18%)	9,15,17	3.02	5 (55%)
1	KPI	F	166	1	11,13,14	1.55	2 (18%)	9,15,17	2.56	2 (22%)

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

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

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	CX2-CX1	7.12	1.58	1.49
1	E	166	KPI	CX2-CX1	5.60	1.56	1.49
1	A	166	KPI	CX2-CX1	5.28	1.56	1.49
1	F	166	KPI	CX2-CX1	3.76	1.54	1.49
1	B	166	KPI	CX2-CX1	3.66	1.54	1.49

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	166	KPI	CE-NZ-CX1	6.62	139.78	121.58
1	F	166	KPI	CE-NZ-CX1	6.26	138.77	121.58
1	D	166	KPI	CE-NZ-CX1	6.18	138.56	121.58
1	C	166	KPI	CE-NZ-CX1	6.05	138.19	121.58
1	A	166	KPI	CE-NZ-CX1	5.60	136.96	121.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ACT	D	310	-	3,3,3	0.81	0	3,3,3	1.39	0
5	EDO	A	315	-	3,3,3	0.39	0	2,2,2	0.51	0
5	EDO	C	307	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	C	308	-	3,3,3	0.46	0	2,2,2	0.21	0
5	EDO	E	311	-	3,3,3	0.57	0	2,2,2	0.11	0
7	ACT	E	314	-	3,3,3	0.84	0	3,3,3	1.45	0
4	PG4	A	306	-	12,12,12	0.54	0	11,11,11	0.29	0
4	PG4	F	305	-	12,12,12	0.55	0	11,11,11	0.35	0
8	PGE	E	315	-	9,9,9	0.37	0	8,8,8	0.54	0
5	EDO	A	316	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	B	310	-	3,3,3	0.44	0	2,2,2	0.23	0
4	PG4	B	305	-	12,12,12	0.52	0	11,11,11	0.21	0
5	EDO	A	307	-	3,3,3	0.56	0	2,2,2	0.39	0
5	EDO	A	309	-	3,3,3	0.39	0	2,2,2	0.38	0
5	EDO	C	309	-	3,3,3	0.46	0	2,2,2	0.50	0
5	EDO	D	307	-	3,3,3	0.45	0	2,2,2	0.65	0
5	EDO	E	310	-	3,3,3	0.51	0	2,2,2	0.33	0
6	PEG	B	313	-	6,6,6	0.52	0	5,5,5	0.31	0
8	PGE	D	313	-	9,9,9	0.33	0	8,8,8	0.34	0
6	PEG	E	313	-	6,6,6	0.53	0	5,5,5	0.33	0
5	EDO	E	307	-	3,3,3	0.44	0	2,2,2	0.44	0
6	PEG	A	317	-	6,6,6	0.50	0	5,5,5	0.32	0
6	PEG	D	308	-	6,6,6	0.46	0	5,5,5	0.23	0
6	PEG	A	318	-	6,6,6	0.45	0	5,5,5	0.41	0
2	3VN	A	301	-	17,21,21	0.78	0	18,28,28	1.11	1 (5%)
5	EDO	E	309	-	3,3,3	0.42	0	2,2,2	0.61	0
6	PEG	B	312	-	6,6,6	0.48	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	308	-	3,3,3	0.39	0	2,2,2	0.62	0
2	3VN	B	301	-	17,21,21	0.80	0	18,28,28	1.13	1 (5%)
7	ACT	F	313	-	3,3,3	0.82	0	3,3,3	1.44	0
5	EDO	B	308	-	3,3,3	0.43	0	2,2,2	0.51	0
5	EDO	A	314	-	3,3,3	0.46	0	2,2,2	0.21	0
7	ACT	F	310	-	3,3,3	0.77	0	3,3,3	1.24	0
4	PG4	C	303	-	12,12,12	0.51	0	11,11,11	0.35	0
2	3VN	D	301	-	17,21,21	0.77	0	18,28,28	1.31	3 (16%)
5	EDO	C	306	-	3,3,3	0.44	0	2,2,2	0.67	0
5	EDO	D	304	-	3,3,3	0.52	0	2,2,2	0.40	0
5	EDO	F	307	-	3,3,3	0.53	0	2,2,2	0.27	0
5	EDO	A	313	-	3,3,3	0.50	0	2,2,2	0.27	0
5	EDO	E	312	-	3,3,3	0.42	0	2,2,2	0.40	0
7	ACT	B	314	-	3,3,3	0.85	0	3,3,3	1.36	0
5	EDO	E	308	-	3,3,3	0.42	0	2,2,2	0.39	0
6	PEG	F	309	-	6,6,6	0.49	0	5,5,5	0.33	0
7	ACT	B	315	-	3,3,3	0.82	0	3,3,3	1.44	0
8	PGE	D	314	-	9,9,9	0.26	0	8,8,8	1.05	1 (12%)
5	EDO	C	305	-	3,3,3	0.39	0	2,2,2	0.66	0
5	EDO	D	306	-	3,3,3	0.61	0	2,2,2	0.08	0
7	ACT	F	311	-	3,3,3	0.81	0	3,3,3	1.44	0
8	PGE	B	316	-	9,9,9	0.36	0	8,8,8	0.43	0
5	EDO	D	305	-	3,3,3	0.38	0	2,2,2	0.40	0
9	GOL	C	311	-	5,5,5	0.23	0	5,5,5	0.49	0
4	PG4	E	306	-	12,12,12	0.52	0	11,11,11	0.44	0
5	EDO	B	306	-	3,3,3	0.51	0	2,2,2	0.13	0
5	EDO	B	307	-	3,3,3	0.43	0	2,2,2	0.47	0
5	EDO	B	309	-	3,3,3	0.42	0	2,2,2	0.51	0
5	EDO	C	304	-	3,3,3	0.42	0	2,2,2	0.39	0
7	ACT	D	309	-	3,3,3	0.85	0	3,3,3	1.29	0
7	ACT	F	312	-	3,3,3	0.88	0	3,3,3	1.44	0
4	PG4	D	303	-	12,12,12	0.53	0	11,11,11	0.21	0
5	EDO	A	312	-	3,3,3	0.48	0	2,2,2	0.28	0
7	ACT	D	312	-	3,3,3	0.82	0	3,3,3	1.37	0
6	PEG	F	308	-	6,6,6	0.53	0	5,5,5	0.24	0
5	EDO	A	311	-	3,3,3	0.39	0	2,2,2	0.66	0
6	PEG	B	311	-	6,6,6	0.49	0	5,5,5	0.41	0
5	EDO	A	310	-	3,3,3	0.45	0	2,2,2	0.39	0
7	ACT	A	319	-	3,3,3	0.76	0	3,3,3	1.18	0
7	ACT	A	320	-	3,3,3	0.80	0	3,3,3	1.42	0
5	EDO	F	306	-	3,3,3	0.45	0	2,2,2	0.47	0
7	ACT	D	311	-	3,3,3	0.82	0	3,3,3	1.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PEG	C	310	-	6,6,6	0.48	0	5,5,5	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	315	-	-	1/1/1/1	-
5	EDO	C	307	-	-	1/1/1/1	-
5	EDO	C	308	-	-	1/1/1/1	-
5	EDO	E	311	-	-	0/1/1/1	-
4	PG4	A	306	-	-	0/10/10/10	-
4	PG4	F	305	-	-	1/10/10/10	-
8	PGE	E	315	-	-	1/7/7/7	-
5	EDO	A	316	-	-	0/1/1/1	-
5	EDO	B	310	-	-	1/1/1/1	-
4	PG4	B	305	-	-	1/10/10/10	-
5	EDO	A	307	-	-	1/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	C	309	-	-	0/1/1/1	-
5	EDO	D	307	-	-	0/1/1/1	-
5	EDO	E	310	-	-	0/1/1/1	-
6	PEG	B	313	-	-	2/4/4/4	-
8	PGE	D	313	-	-	2/7/7/7	-
6	PEG	E	313	-	-	3/4/4/4	-
5	EDO	E	307	-	-	0/1/1/1	-
6	PEG	A	317	-	-	0/4/4/4	-
6	PEG	D	308	-	-	1/4/4/4	-
6	PEG	A	318	-	-	3/4/4/4	-
2	3VN	A	301	-	-	8/31/31/31	-
5	EDO	E	309	-	-	1/1/1/1	-
6	PEG	B	312	-	-	3/4/4/4	-
5	EDO	A	308	-	-	1/1/1/1	-
2	3VN	B	301	-	-	10/31/31/31	-
5	EDO	B	308	-	-	1/1/1/1	-
5	EDO	A	314	-	-	0/1/1/1	-
4	PG4	C	303	-	-	1/10/10/10	-
2	3VN	D	301	-	-	10/31/31/31	-
5	EDO	C	306	-	-	1/1/1/1	-
5	EDO	D	304	-	-	0/1/1/1	-

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

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	314	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
8	D	313	PGE	O2-C3-C4-O3
4	E	306	PG4	C5-C6-O4-C7
6	C	310	PEG	C4-C3-O2-C2
8	B	316	PGE	O2-C3-C4-O3

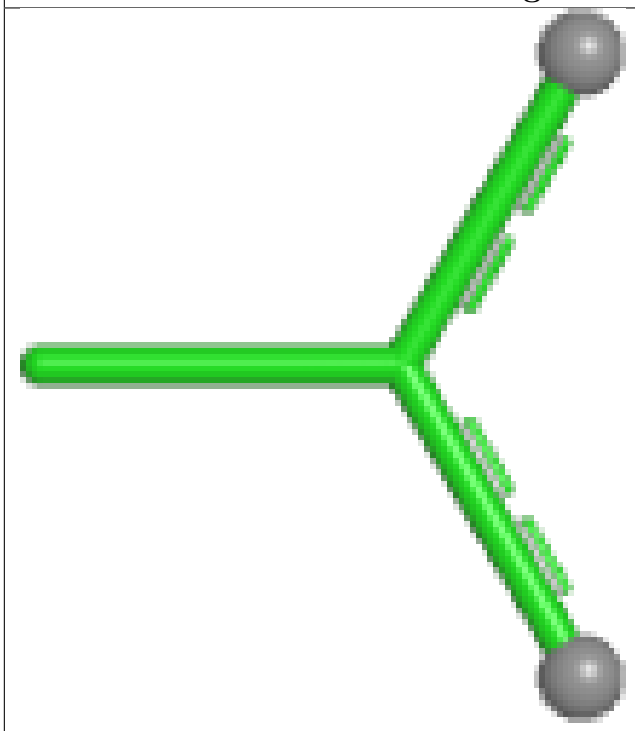
There are no ring outliers.

20 monomers are involved in 29 short contacts:

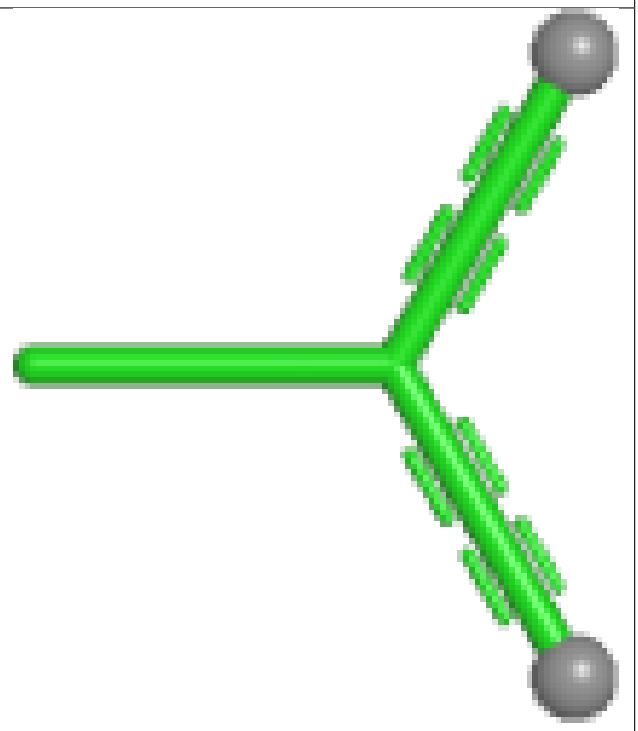
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	314	ACT	1	0
8	E	315	PGE	1	0
5	B	310	EDO	1	0
5	D	307	EDO	1	0
6	B	313	PEG	2	0
6	E	313	PEG	1	0
2	A	301	3VN	1	0
5	E	309	EDO	1	0
5	A	308	EDO	2	0
2	B	301	3VN	1	0
5	B	308	EDO	1	0
2	D	301	3VN	1	0
8	D	314	PGE	3	0
4	E	306	PG4	3	0
5	B	306	EDO	4	0
4	D	303	PG4	1	0
6	B	311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

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

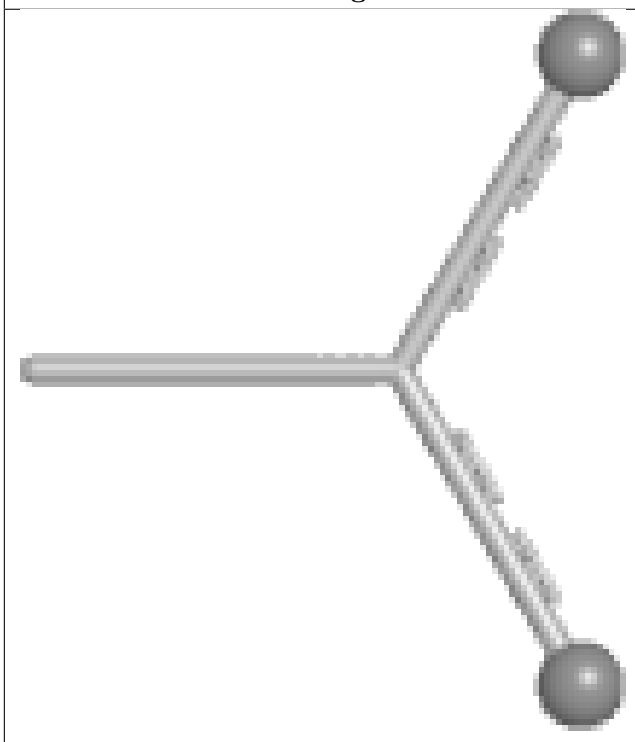
Ligand ACT D 310



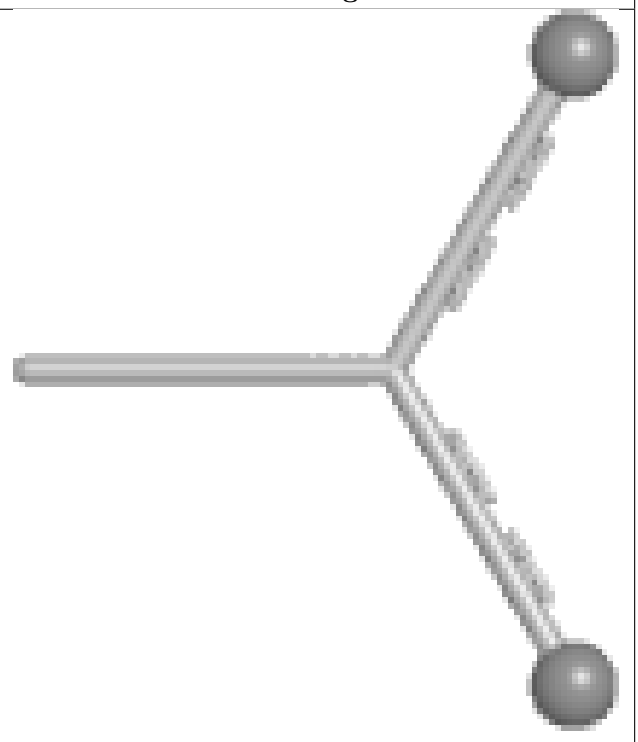
Bond lengths



Bond angles

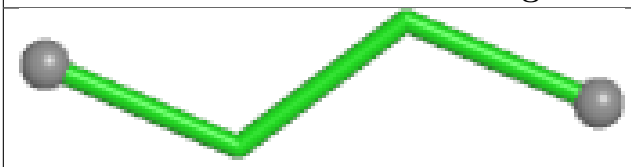


Torsions



Rings

Ligand EDO A 315



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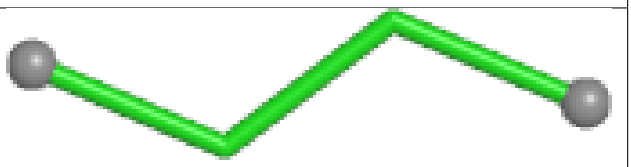

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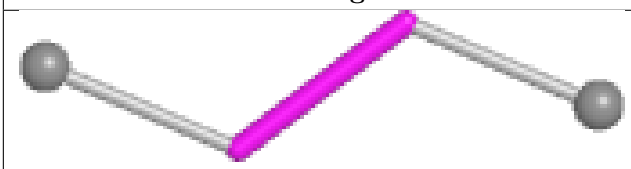

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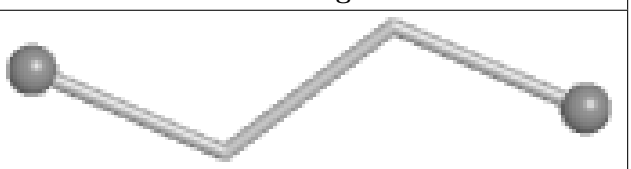
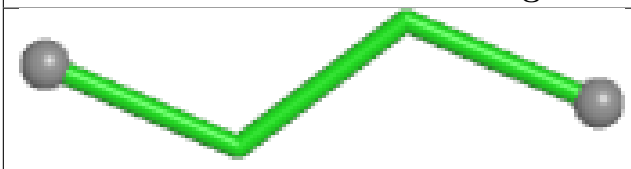


Rings

Ligand EDO C 307



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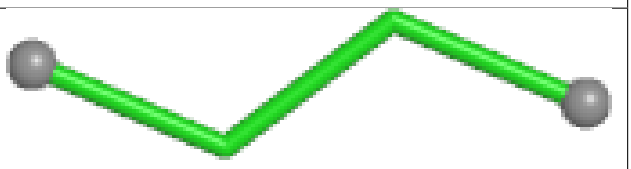

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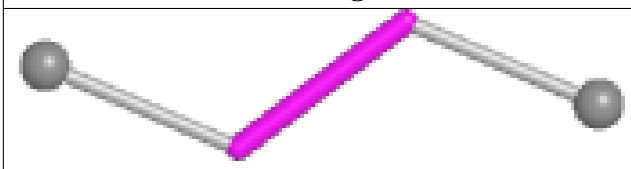

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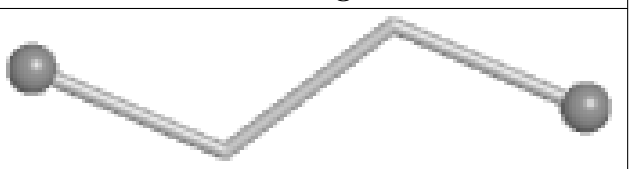
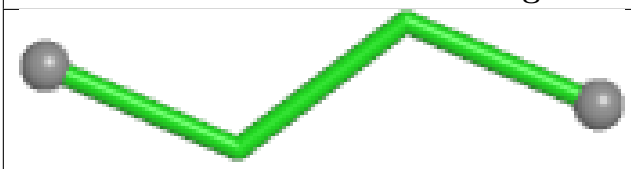


Rings

Ligand EDO C 308



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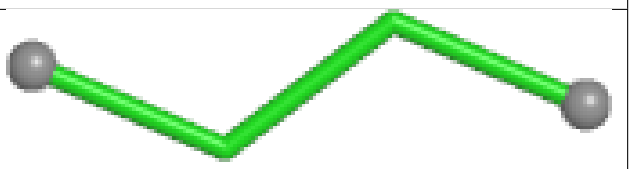

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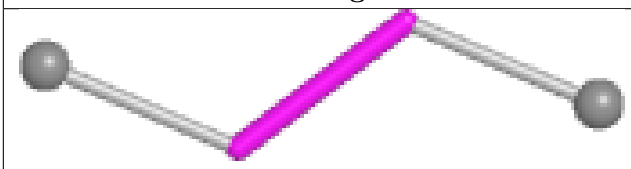

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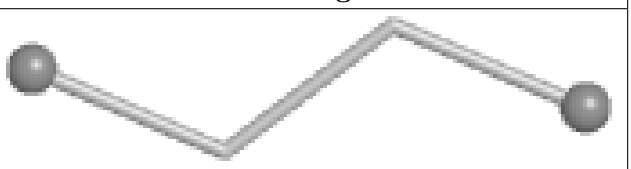
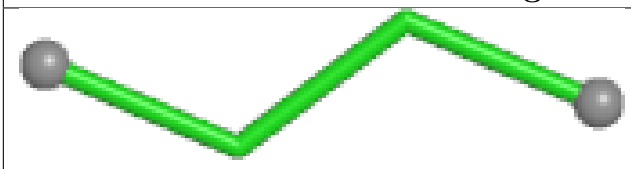


Rings

Ligand EDO E 311



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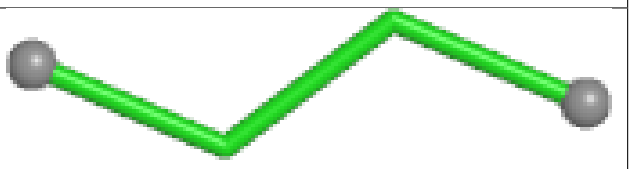

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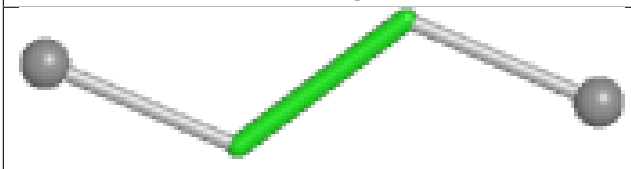
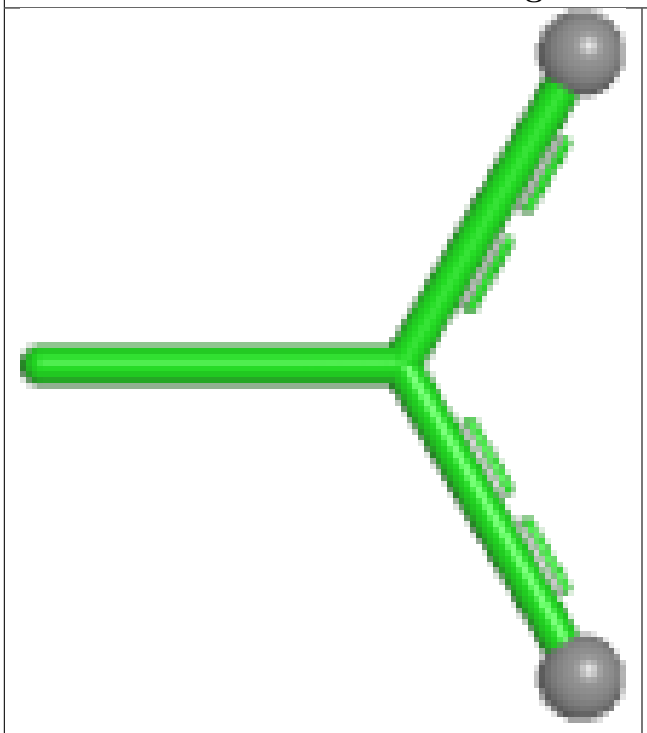


Torsions



Rings

Ligand ACT E 314



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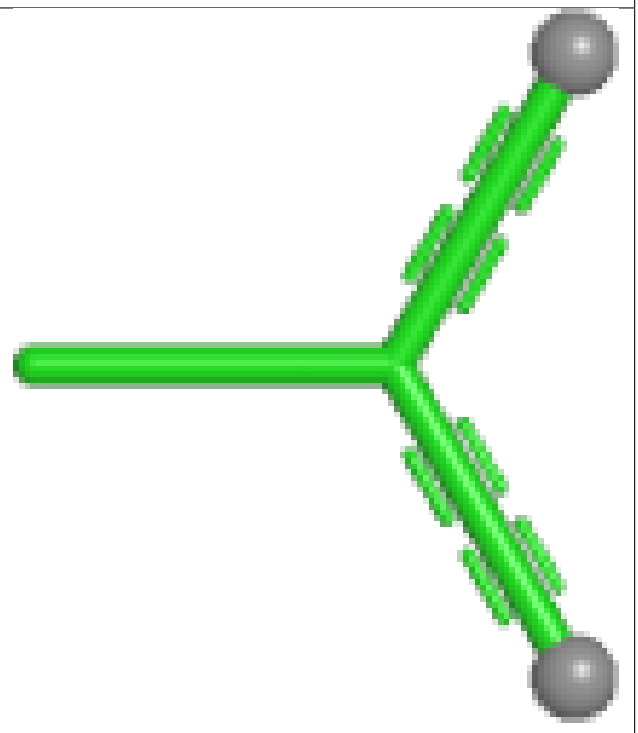

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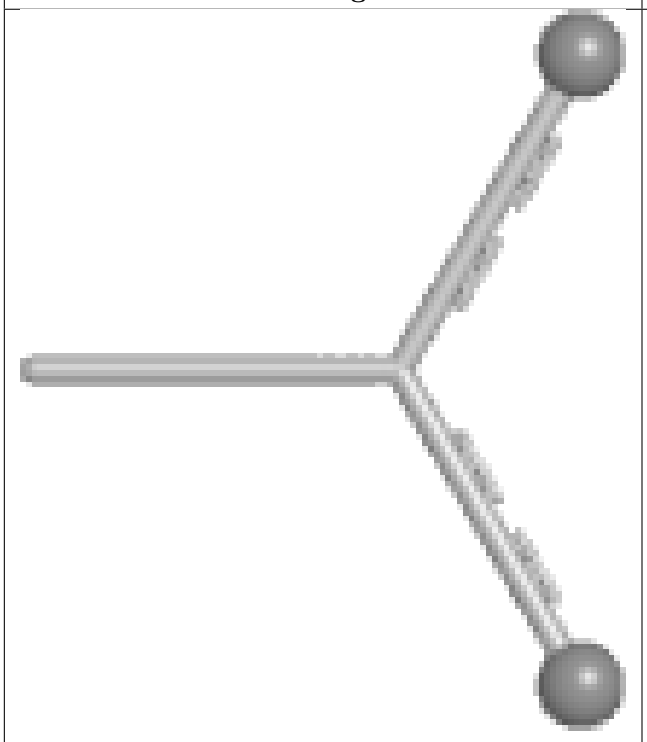

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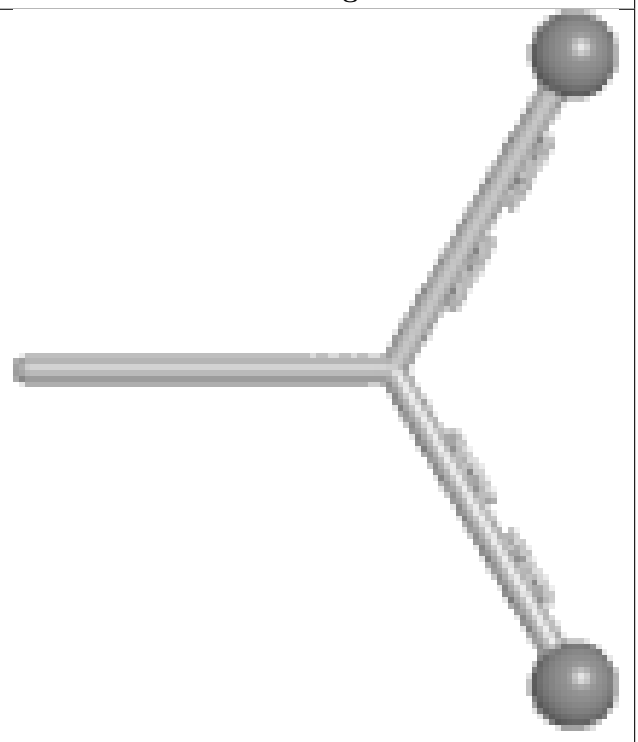
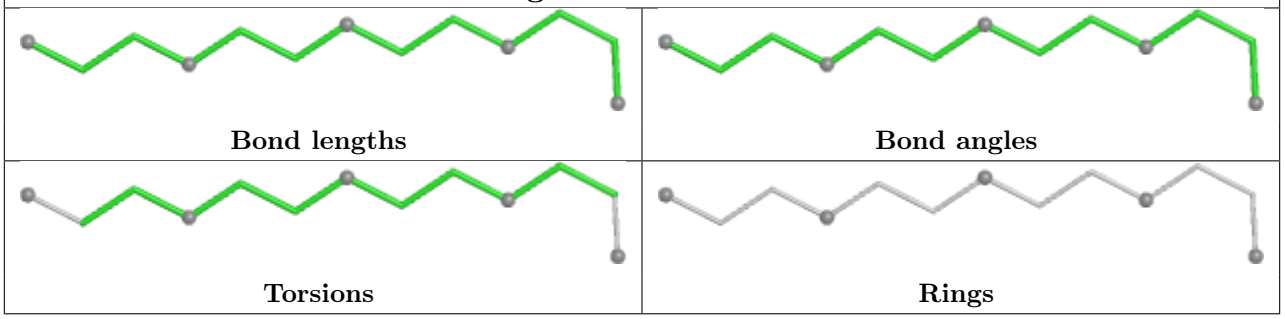


Rings

Ligand PG4 A 306



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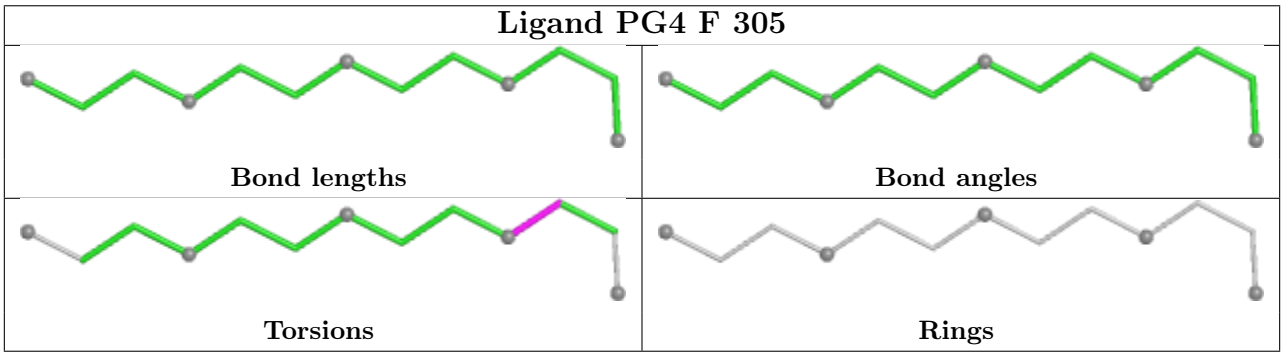
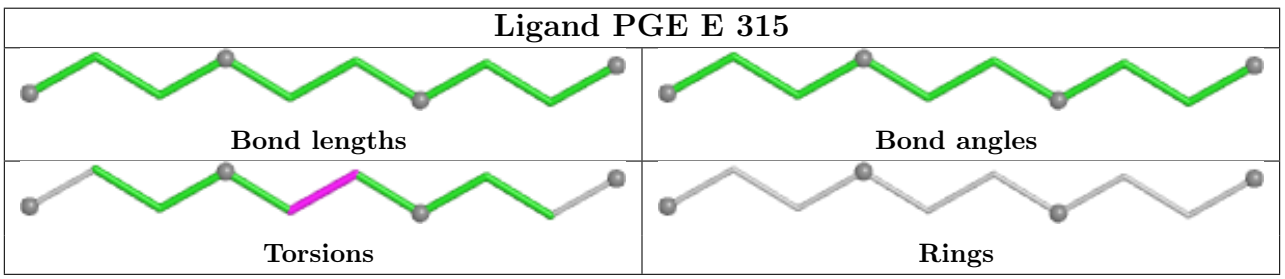


Ligand PGE E 315



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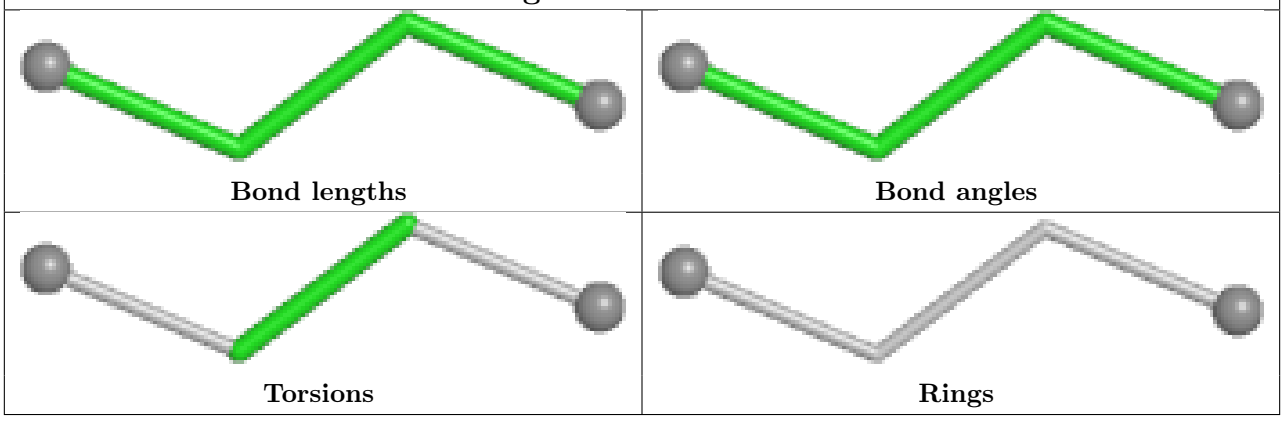

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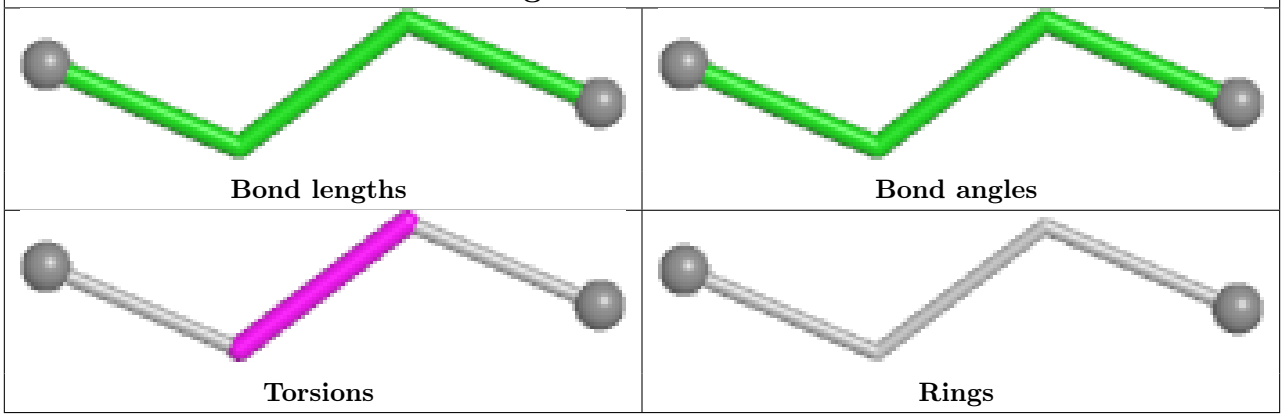

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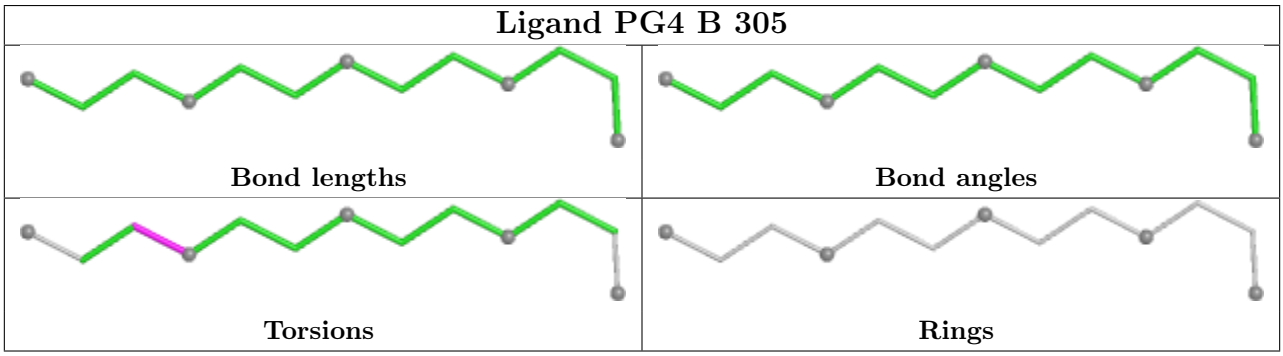

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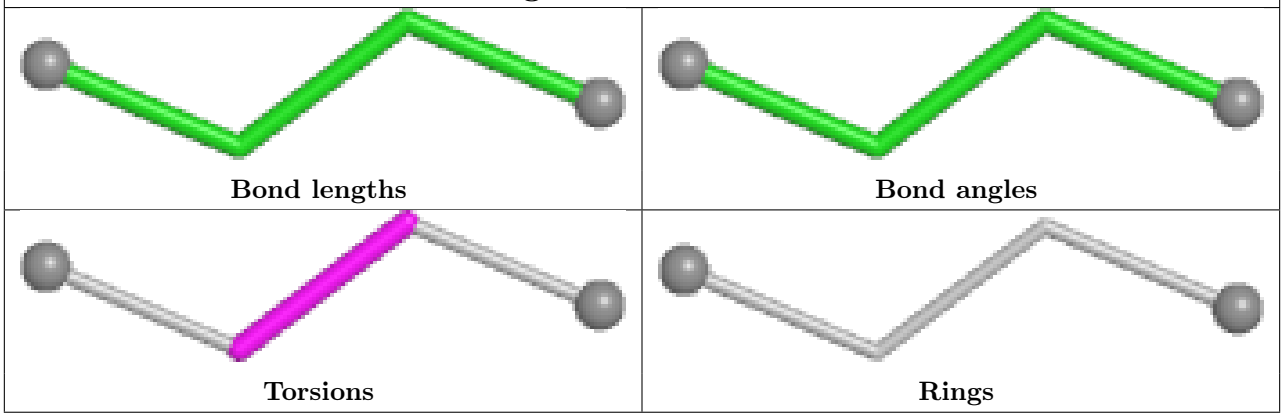

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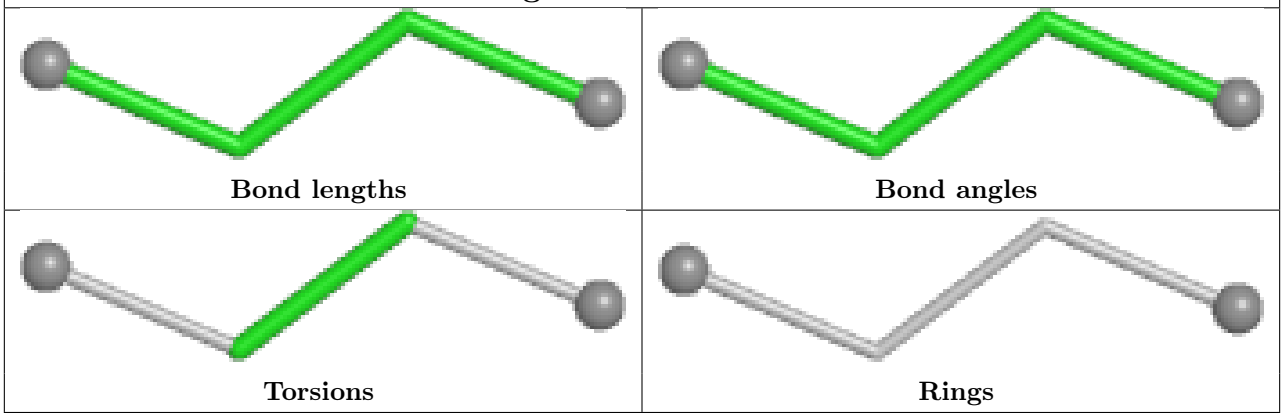

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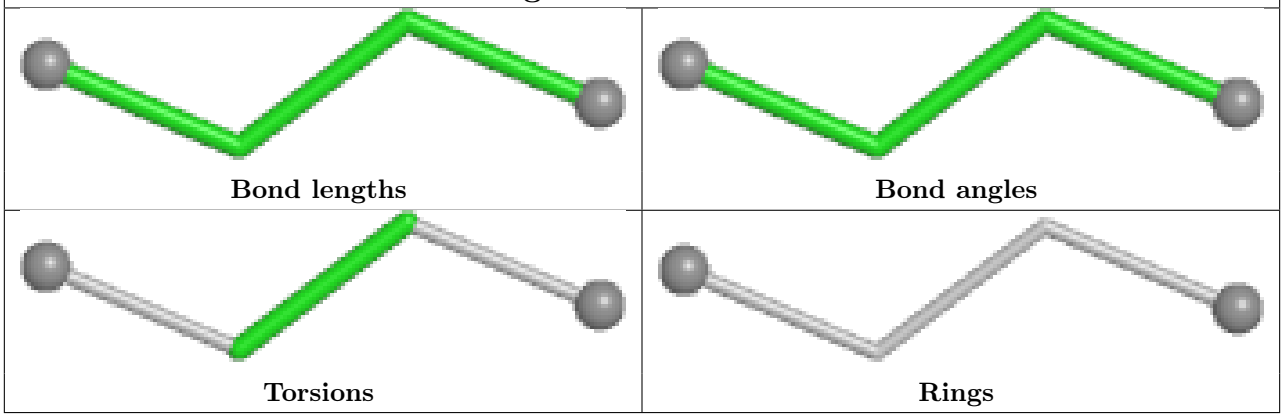
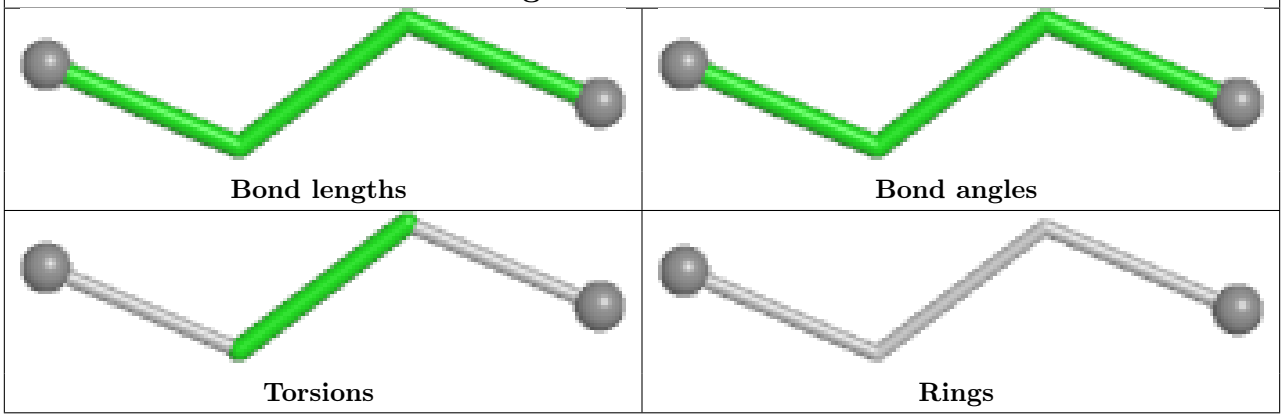


Ligand EDO D 307



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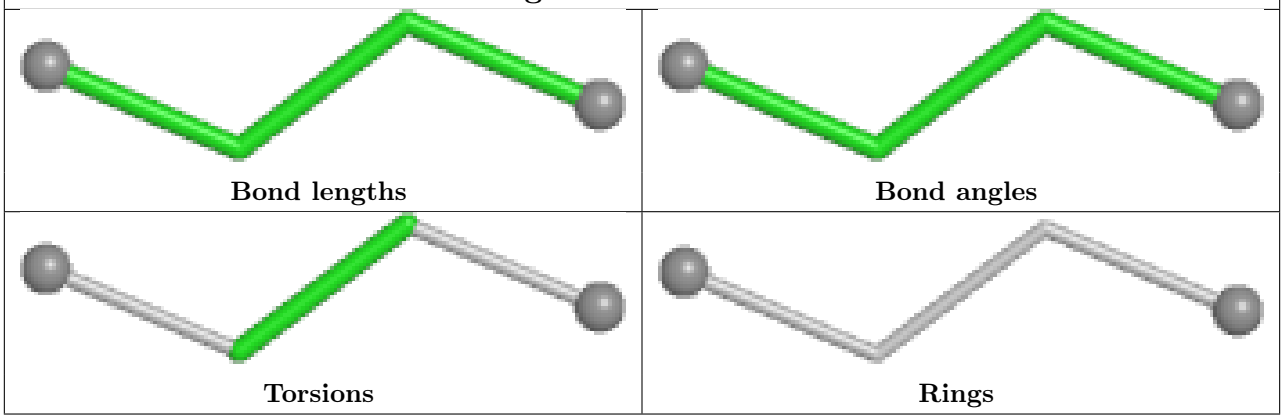

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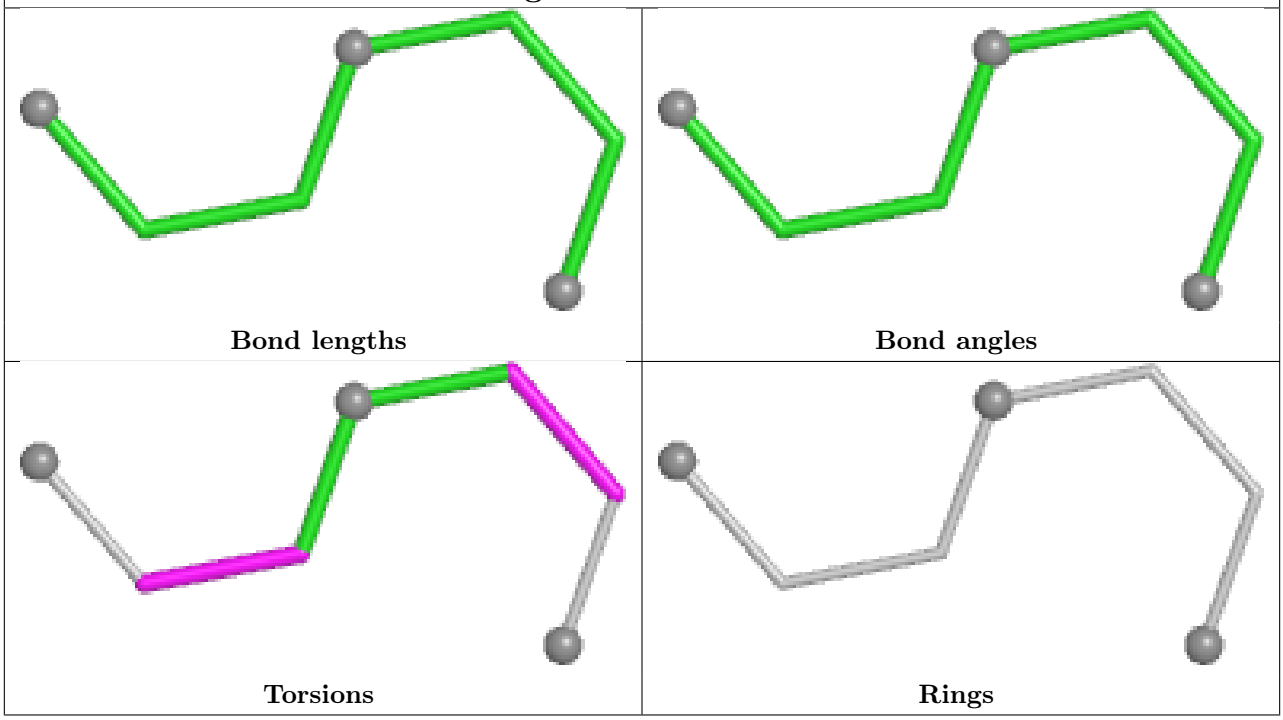

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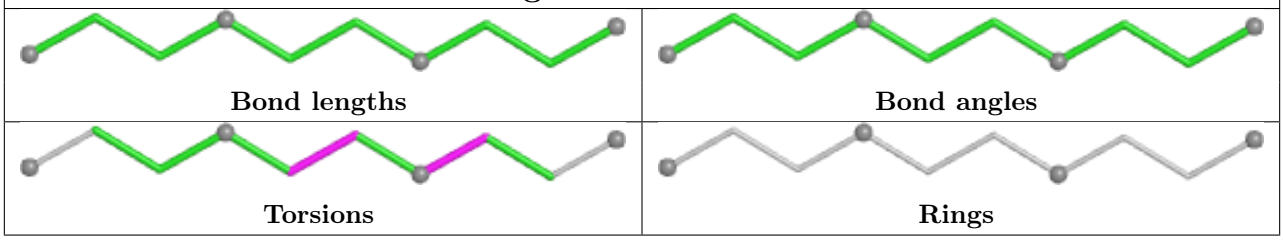

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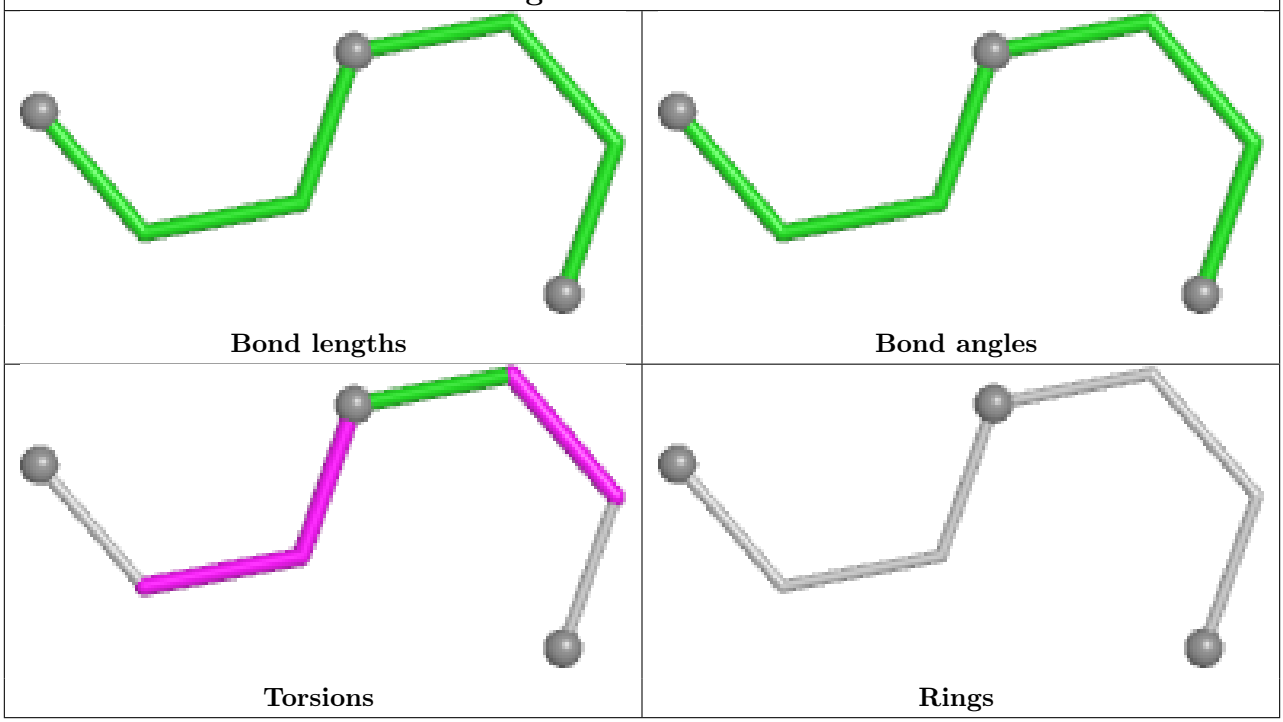

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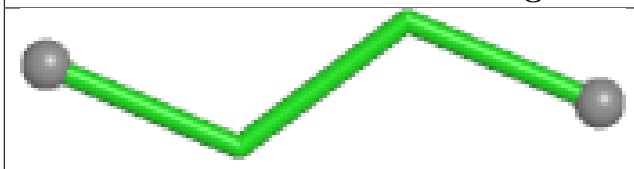

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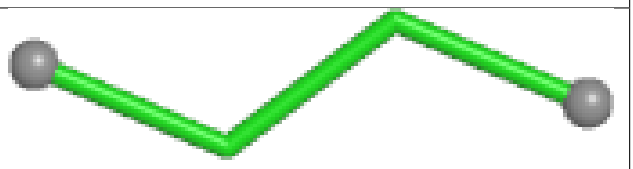
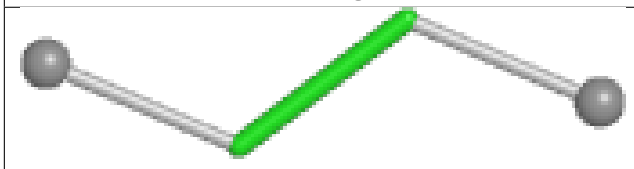


Bond angles

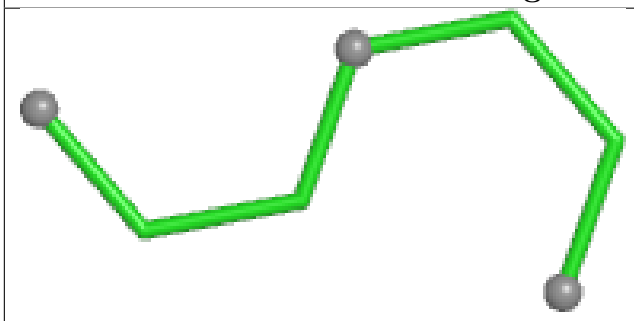


Torsions



Rings

Ligand PEG A 317



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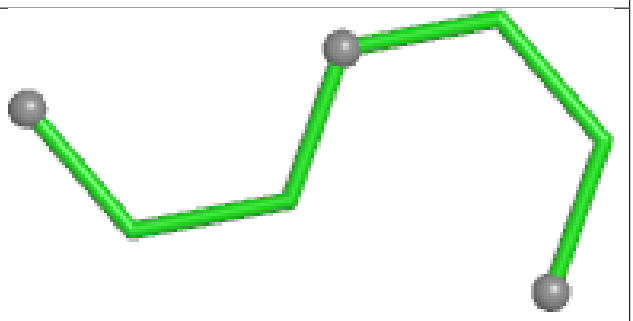
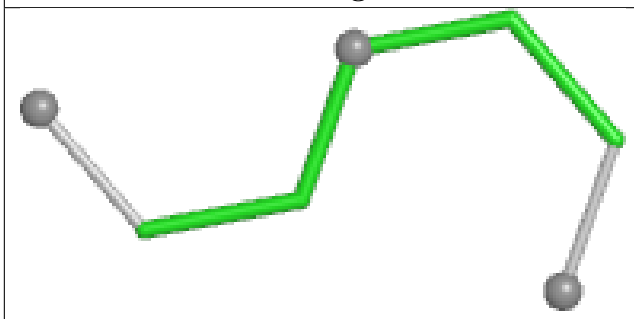
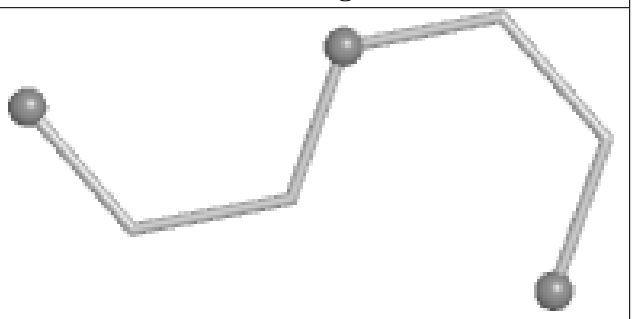


Bond angles

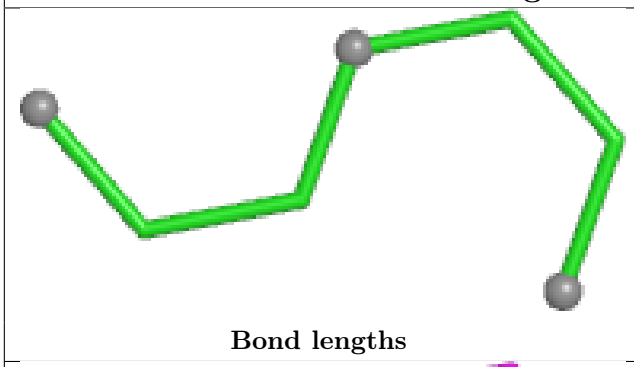


Torsions



Rings

Ligand PEG D 308



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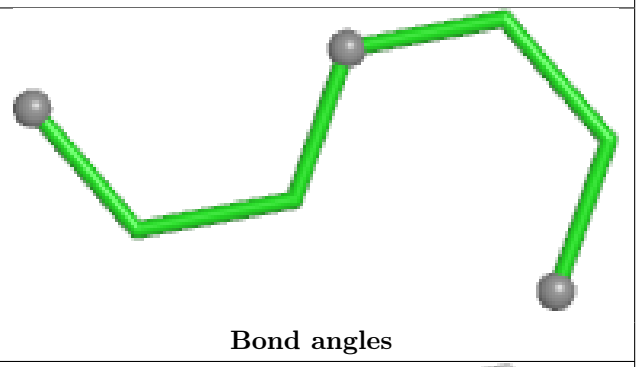
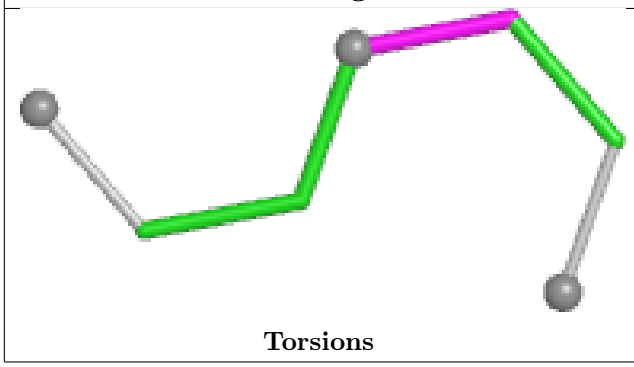


Bond angles



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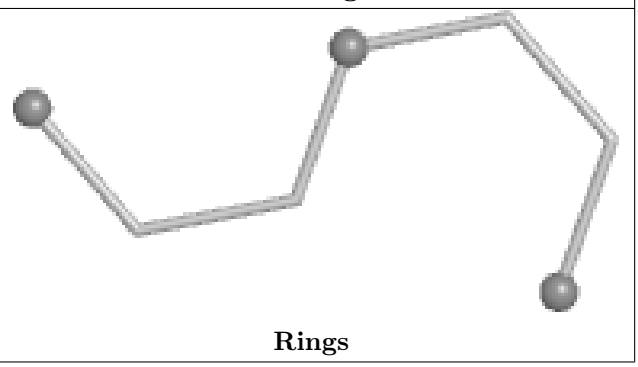
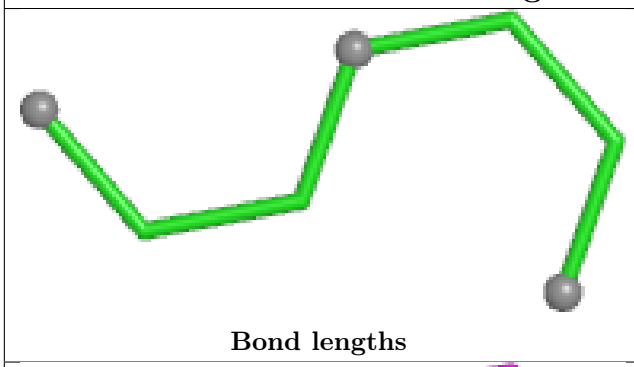
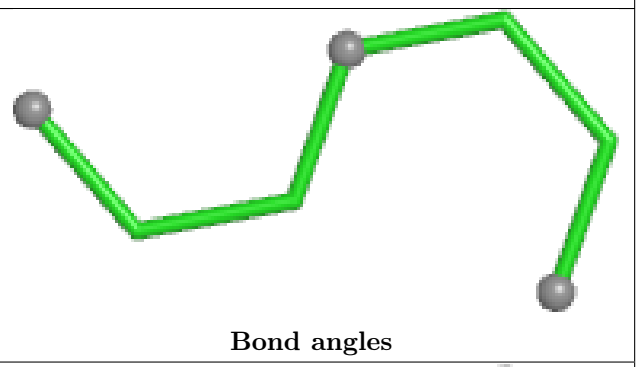


Rings

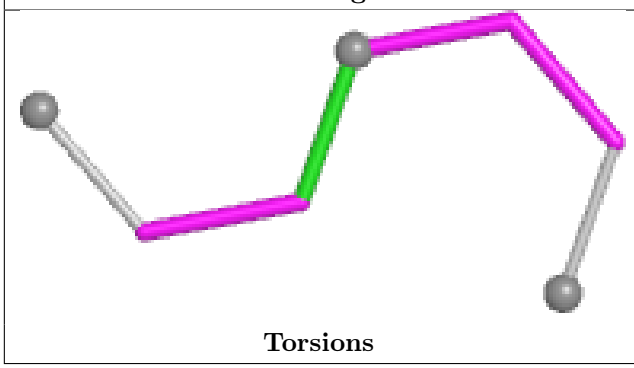
Ligand PEG A 318



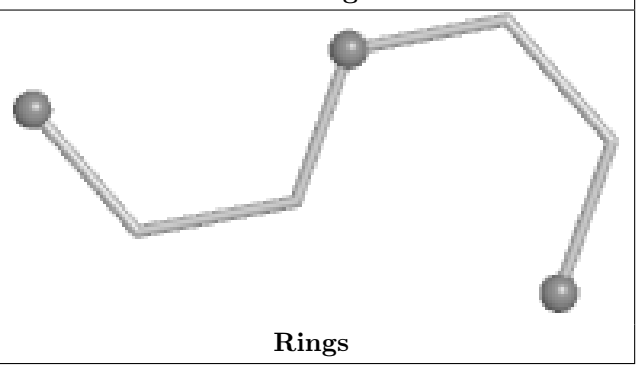
Bond lengths



Bond angles

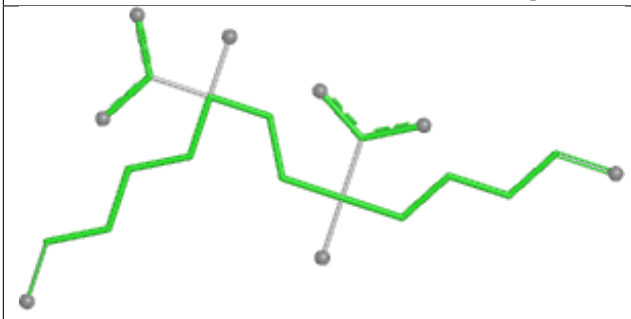


Torsions



Rings

Ligand 3VN A 301



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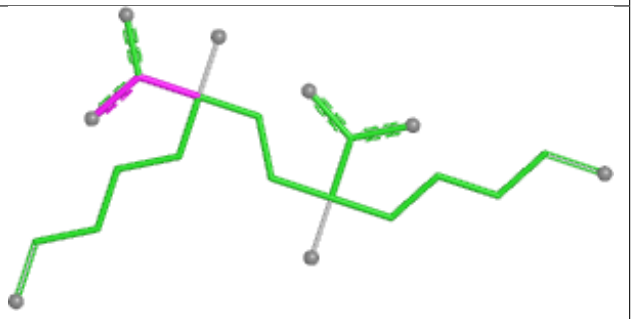

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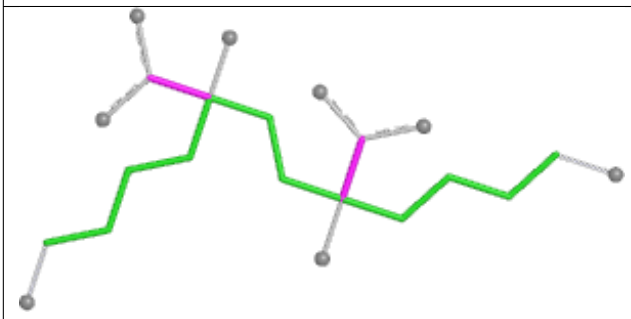

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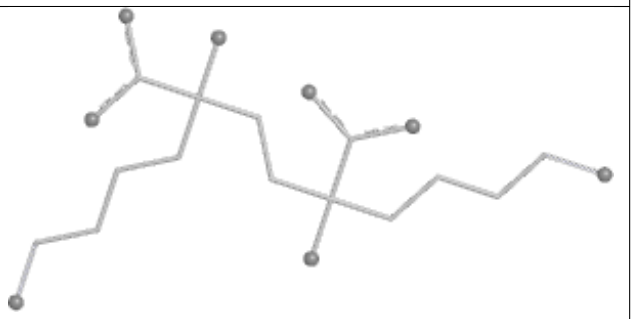
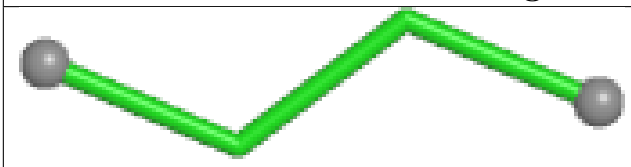


Rings

Ligand EDO E 309



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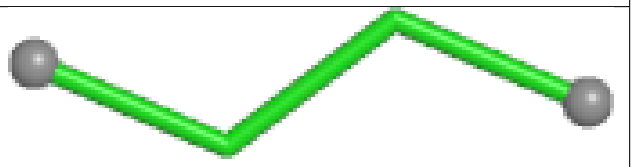

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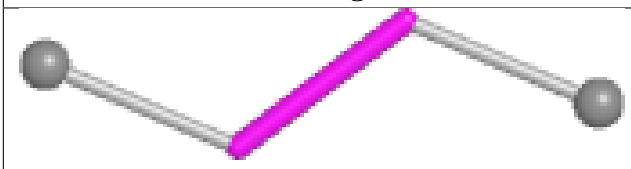

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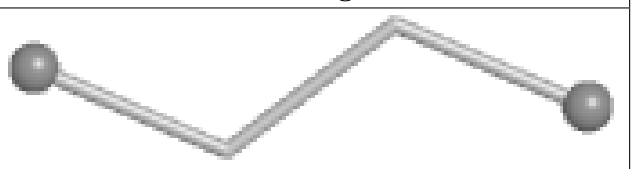
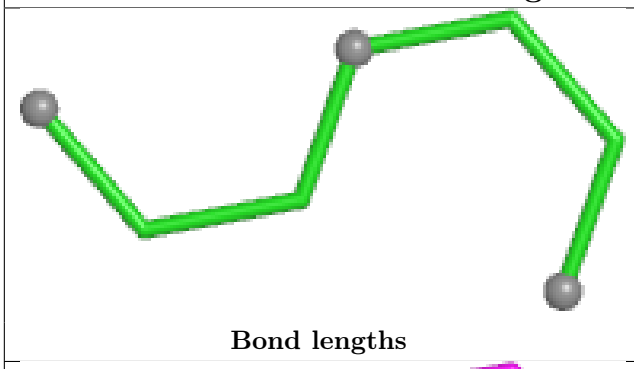


Rings

Ligand PEG B 312



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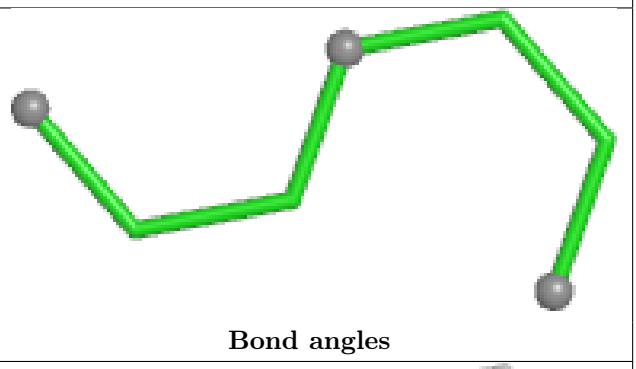
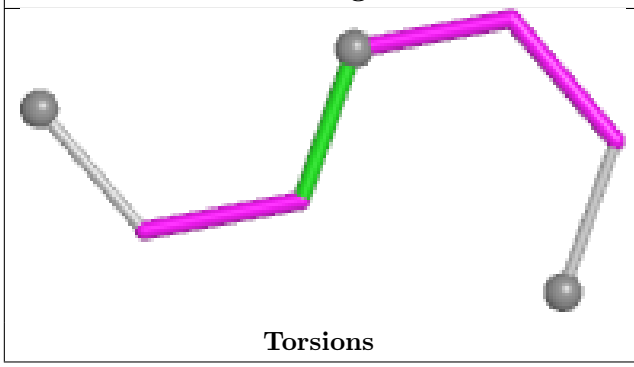


Bond angles



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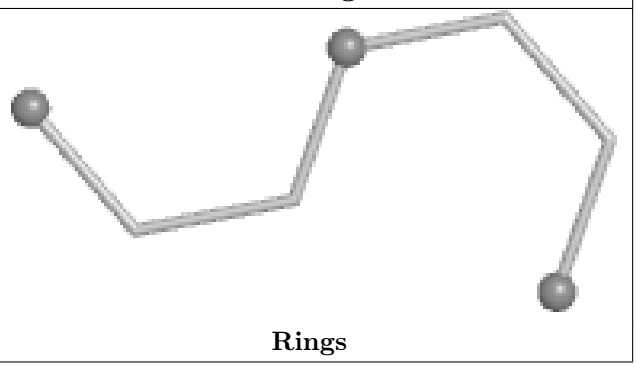
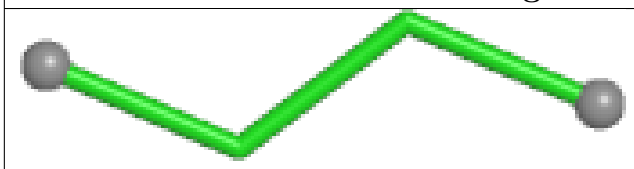


Rings

Ligand EDO A 308



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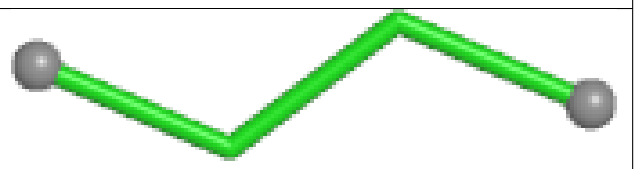

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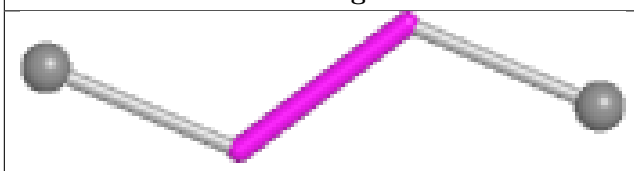

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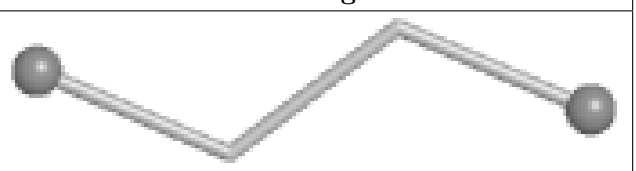
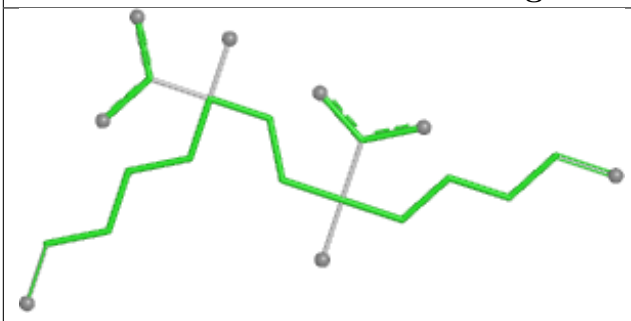


Rings

Ligand 3VN B 301



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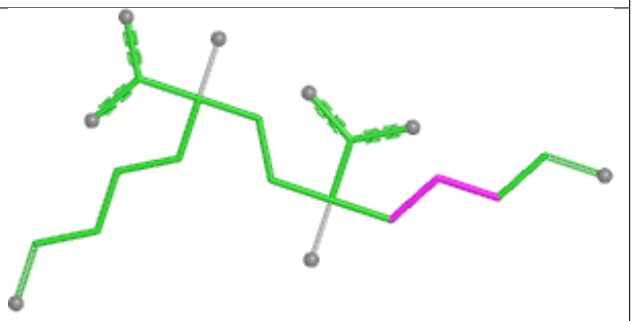

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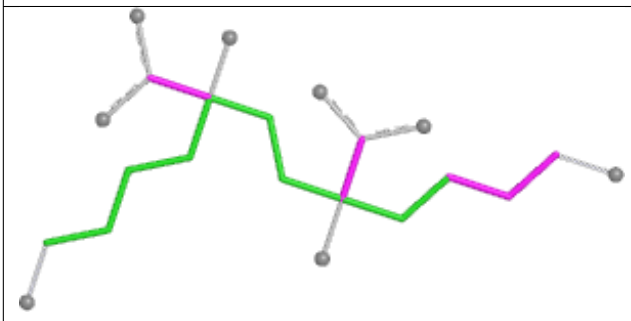

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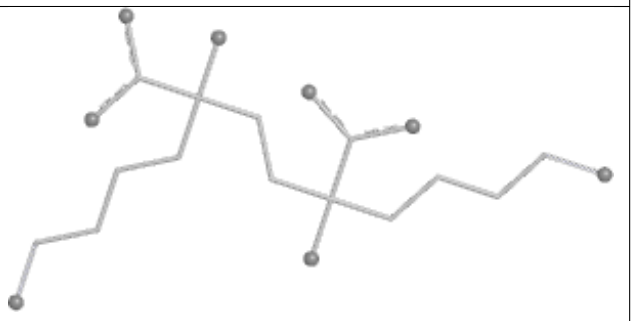
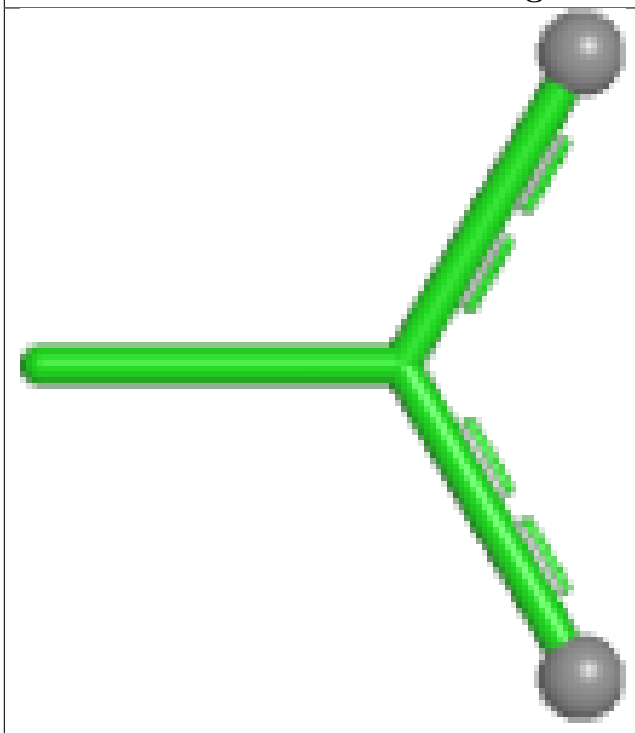


Rings

Ligand ACT F 313



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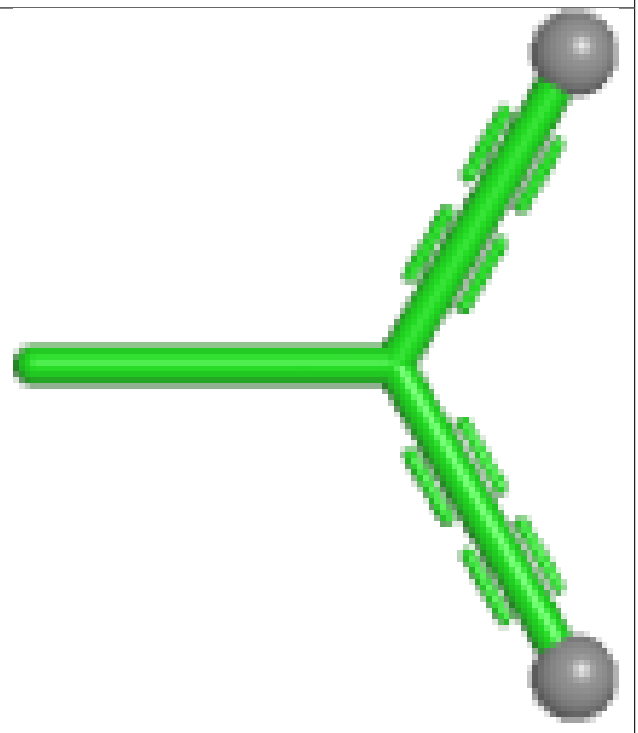
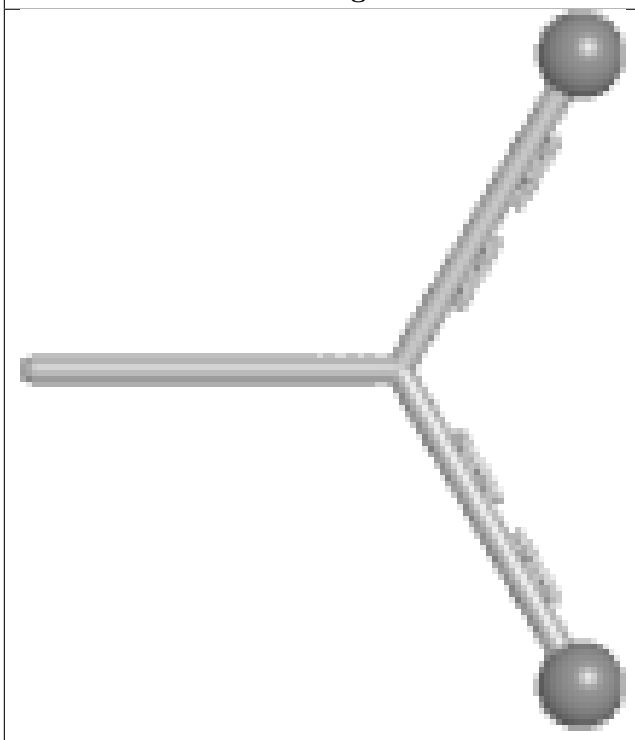


Bond angles



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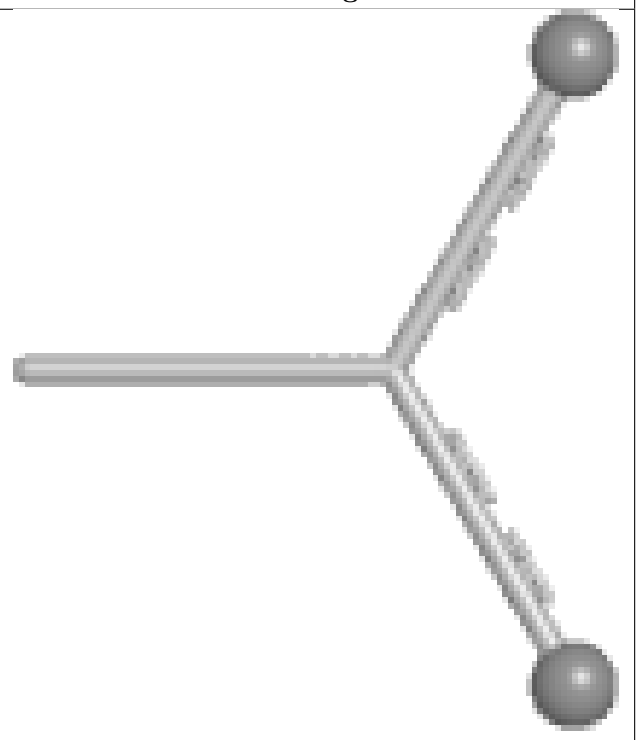
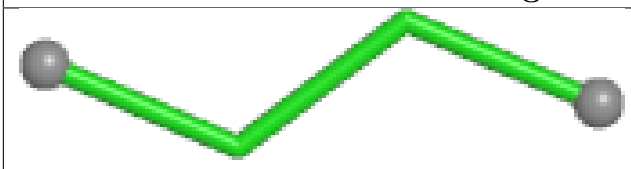
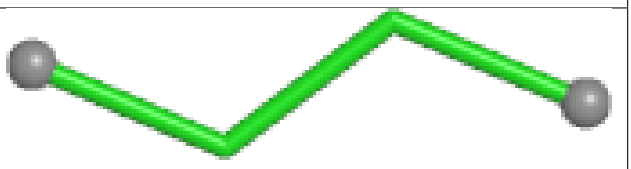
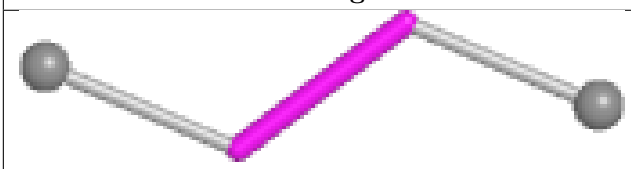
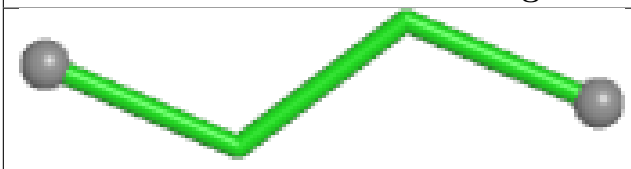
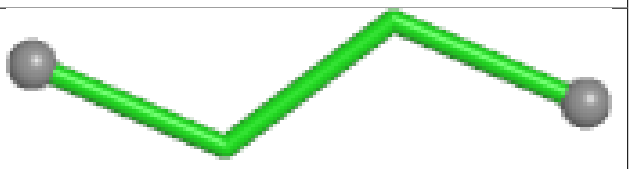
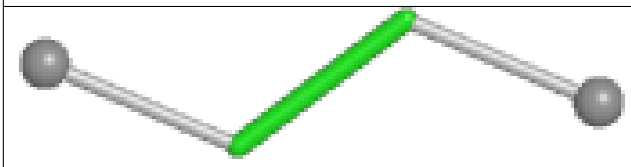
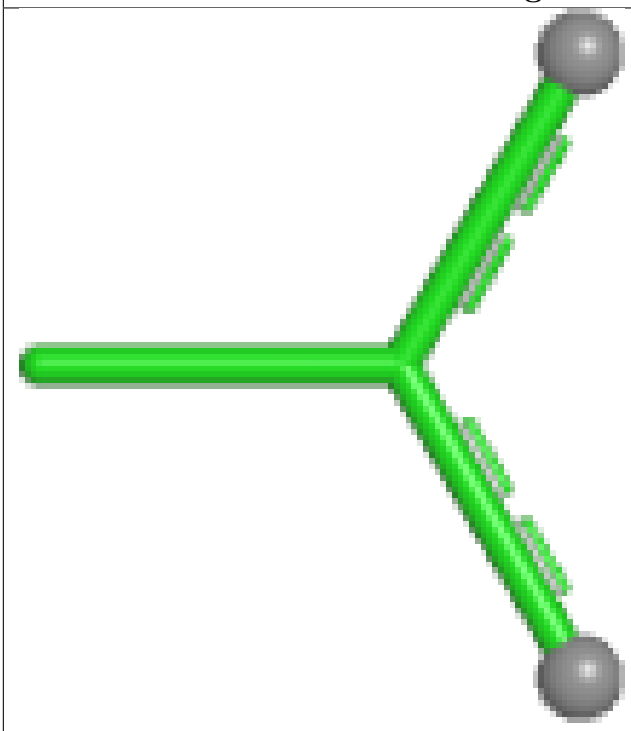


Rings

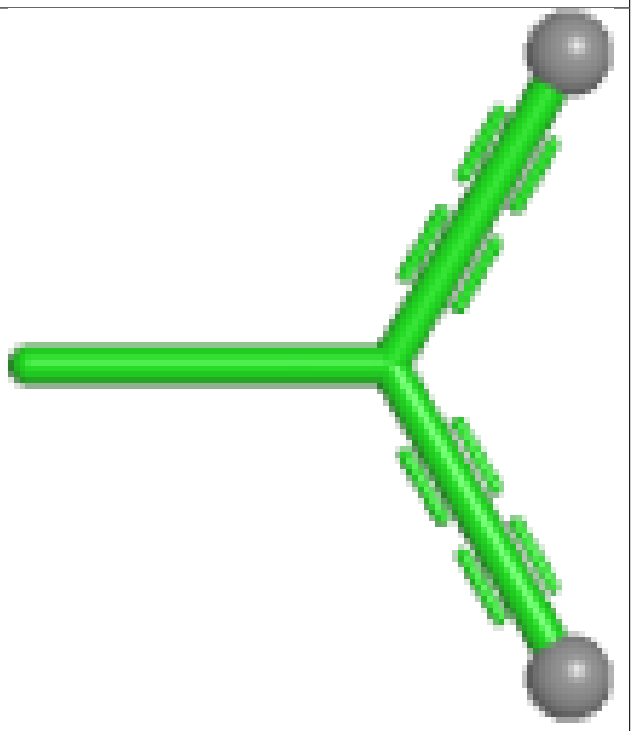
Ligand EDO B 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO A 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

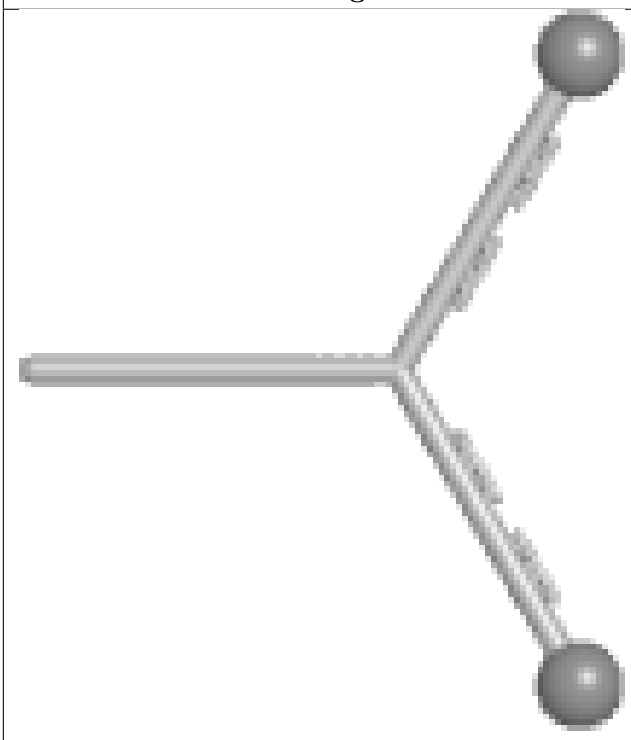
Ligand ACT F 310



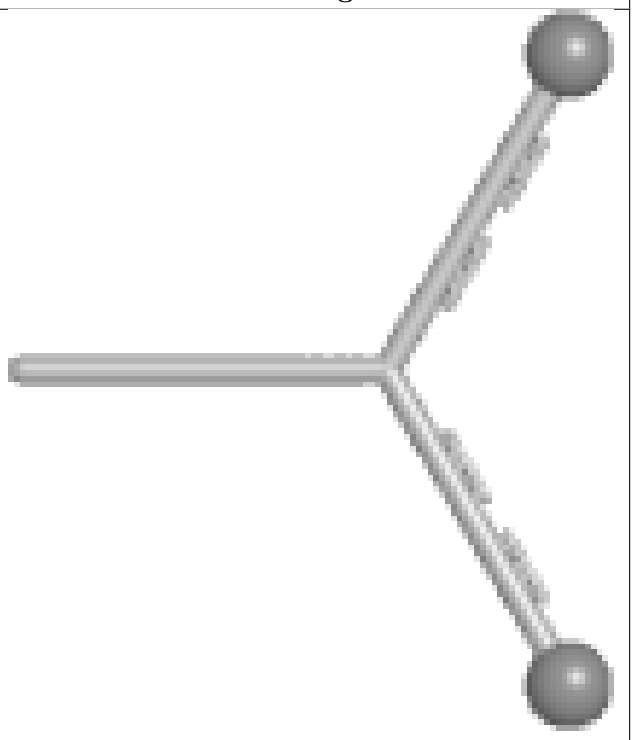
Bond lengths



Bond angles

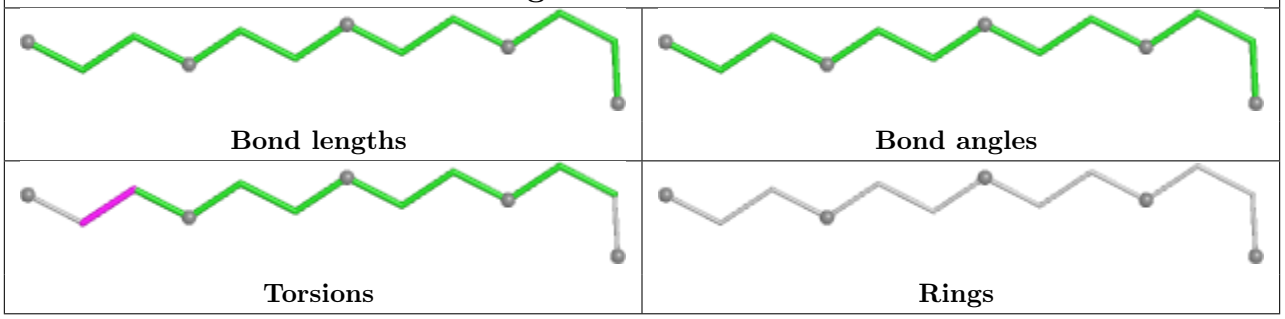


Torsions

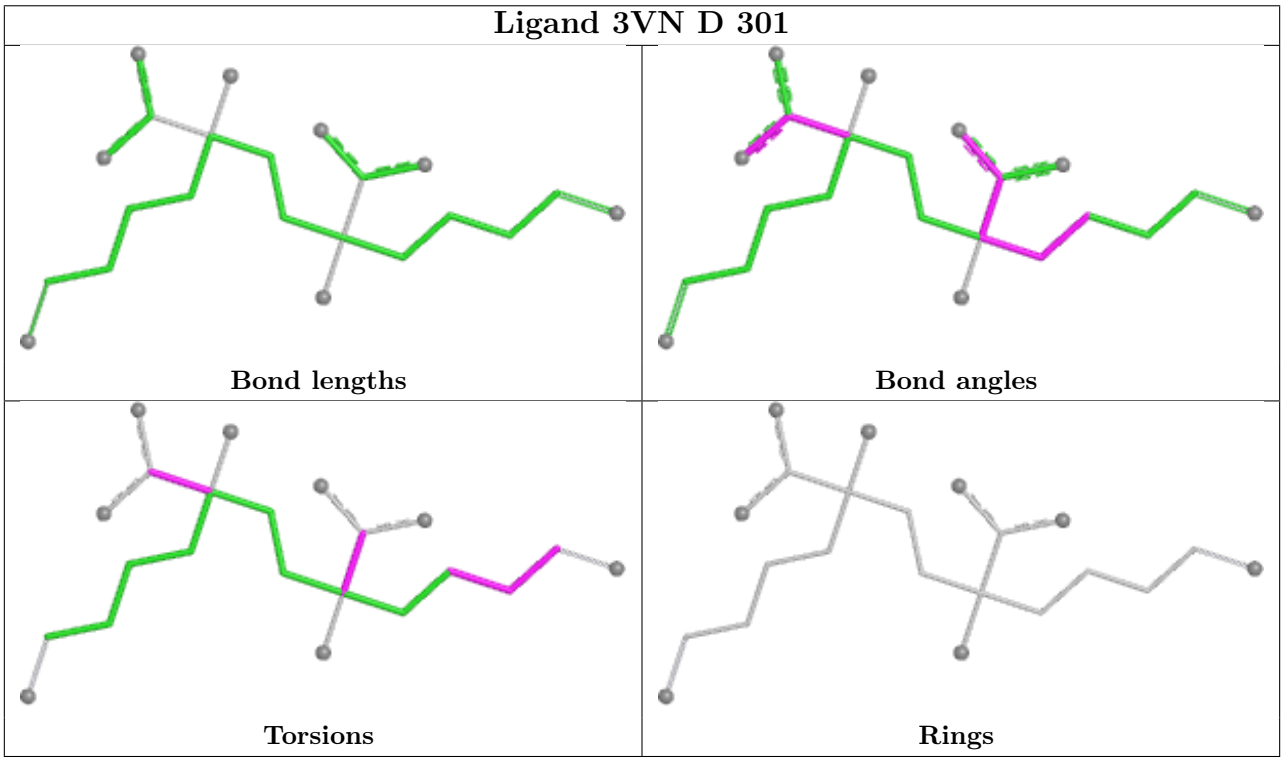


Rings

Ligand PG4 C 303



Ligand 3VN D 301



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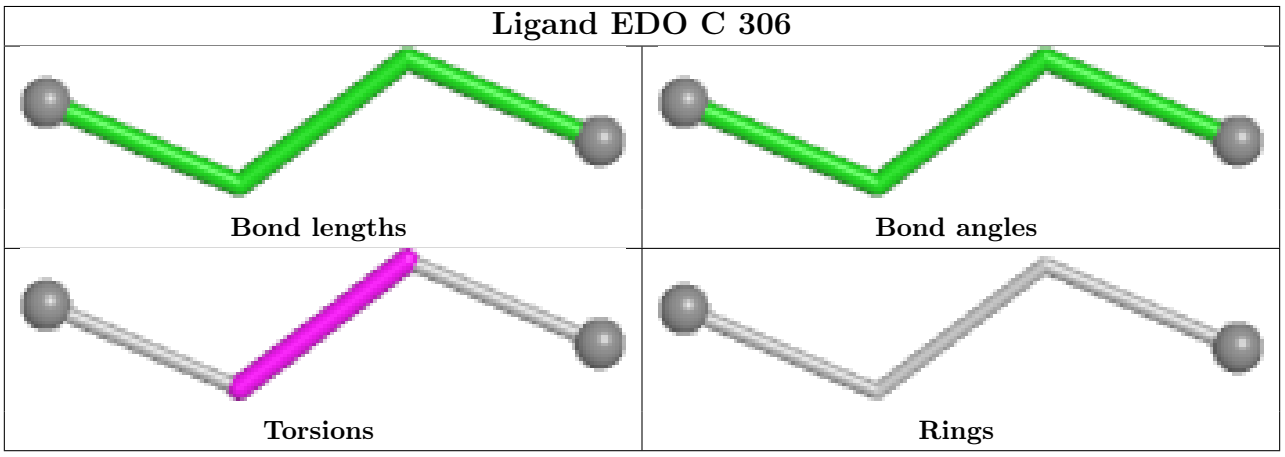

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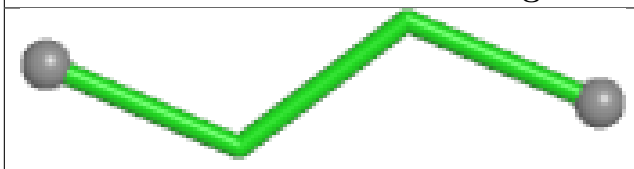
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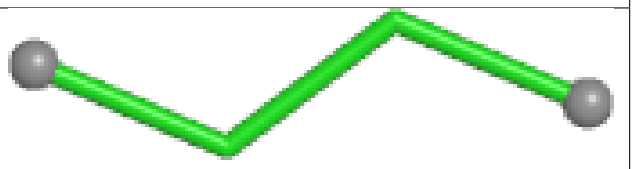
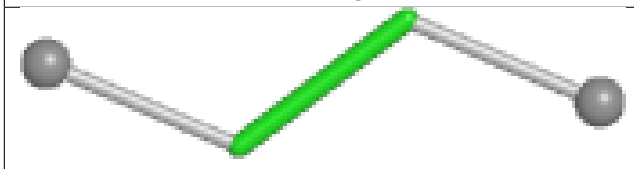
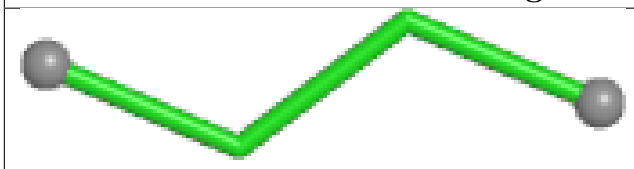

Bond angles


Torsions


Rings

Ligand EDO F 307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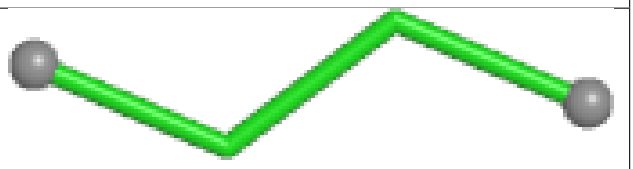
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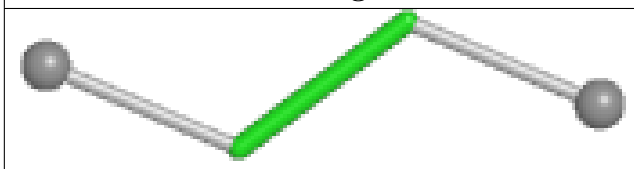
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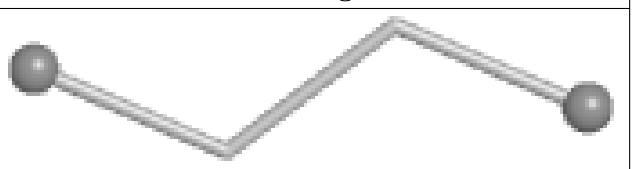
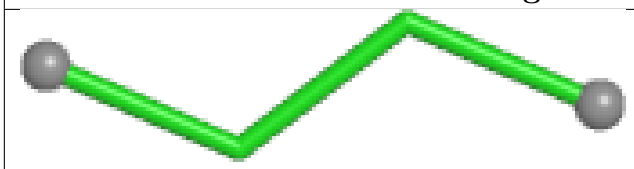

Rings

Ligand EDO A 313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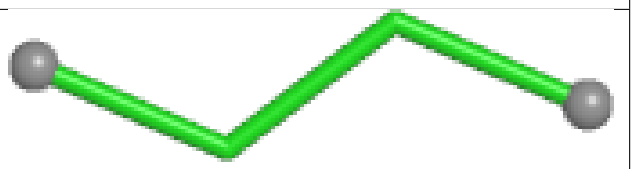
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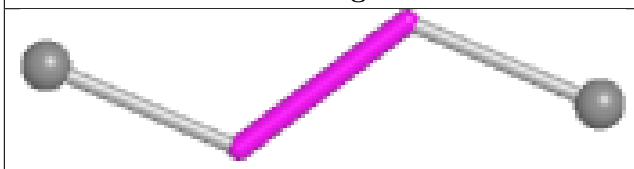
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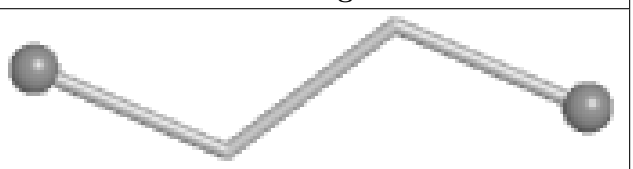
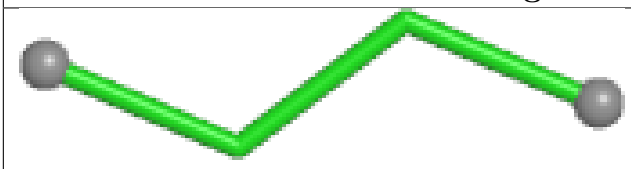

Rings

Ligand EDO E 312



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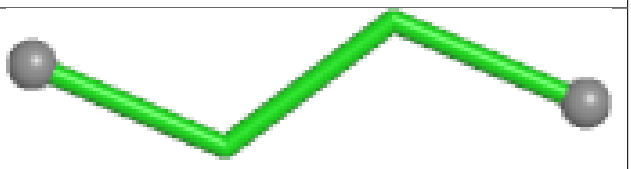
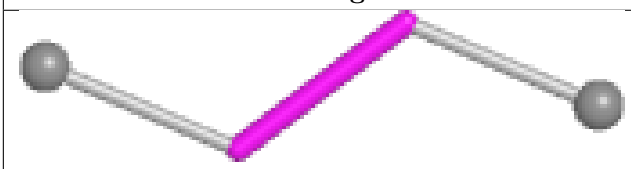


Bond angles

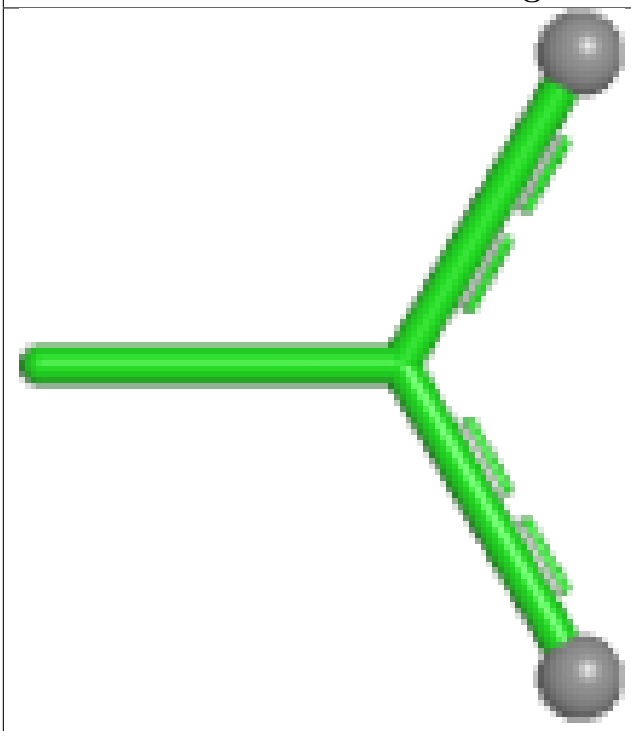


Torsions



Rings

Ligand ACT B 314



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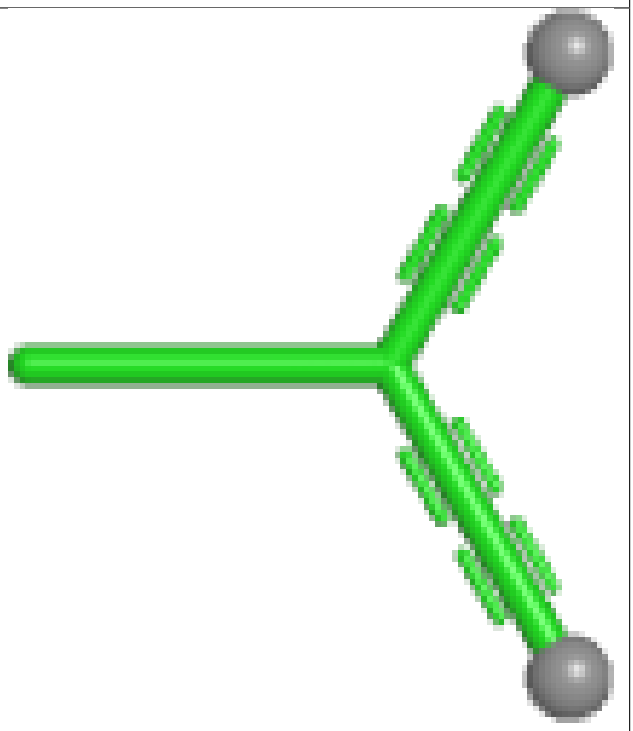
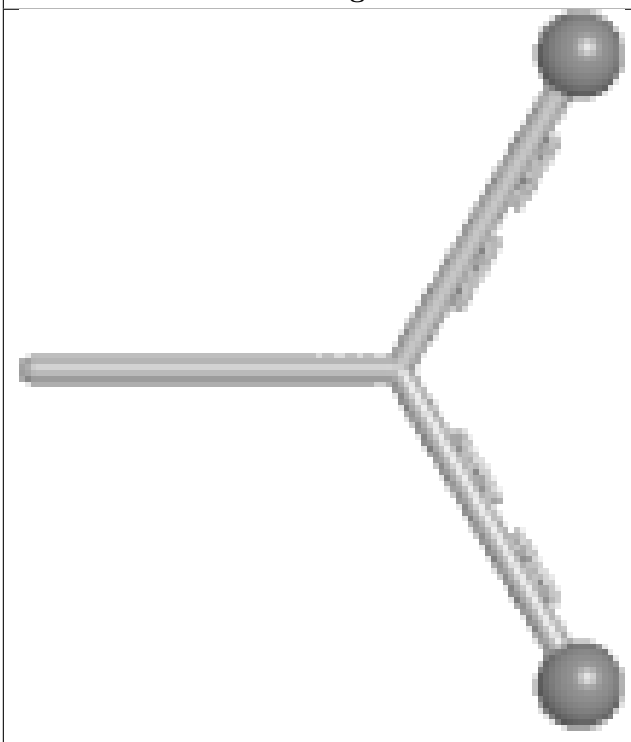


Bond angles



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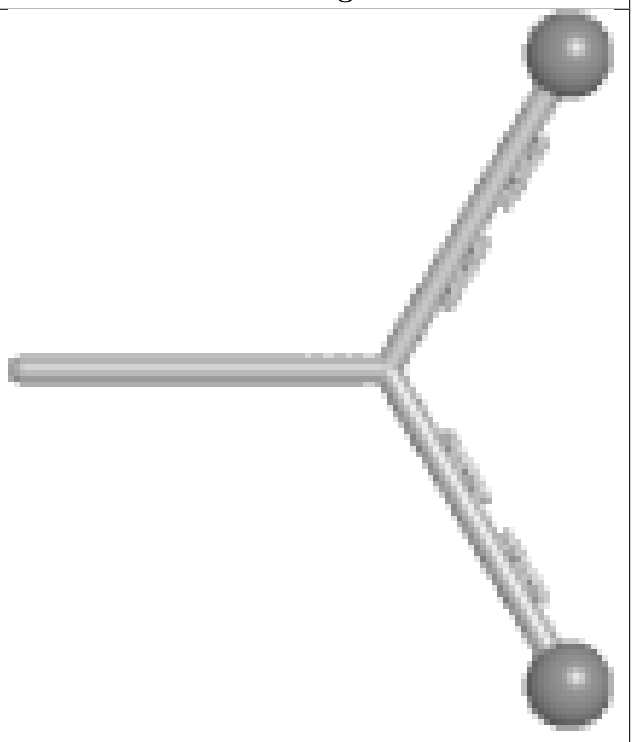
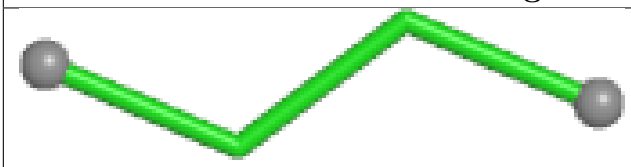
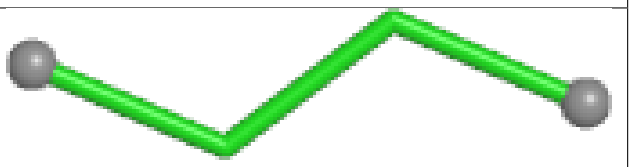


Rings

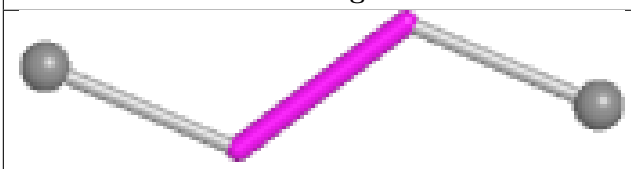
Ligand EDO E 308



Bond lengths



Bond angles

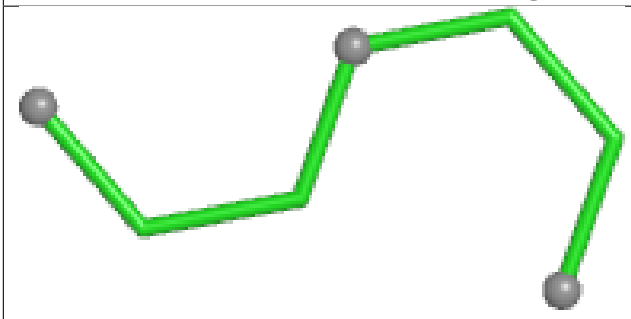


Torsions



Rings

Ligand PEG F 309



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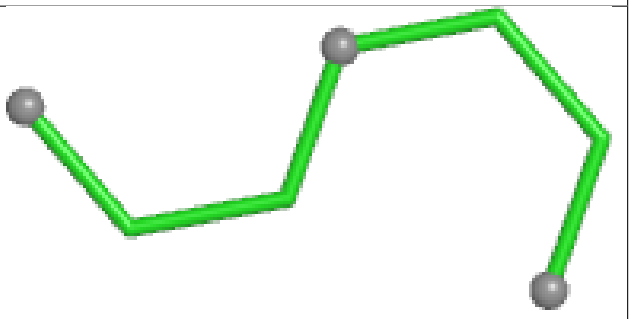

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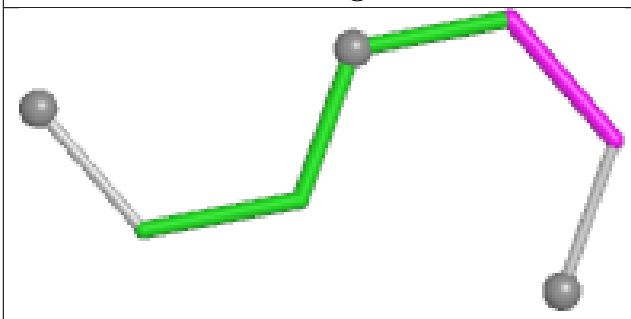
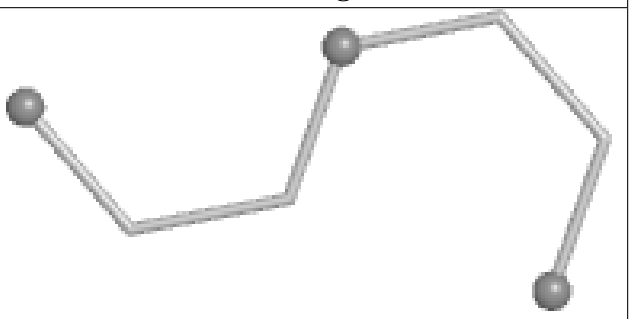
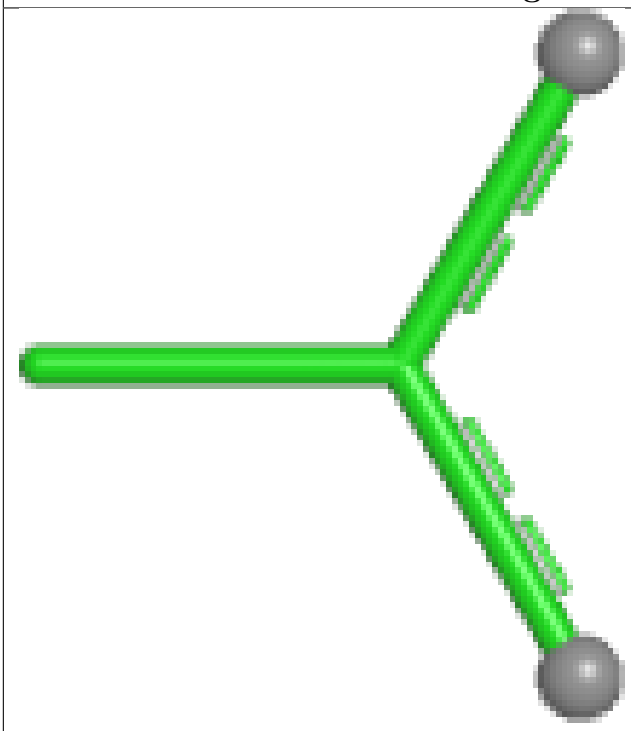


Torsions



Rings

Ligand ACT B 315



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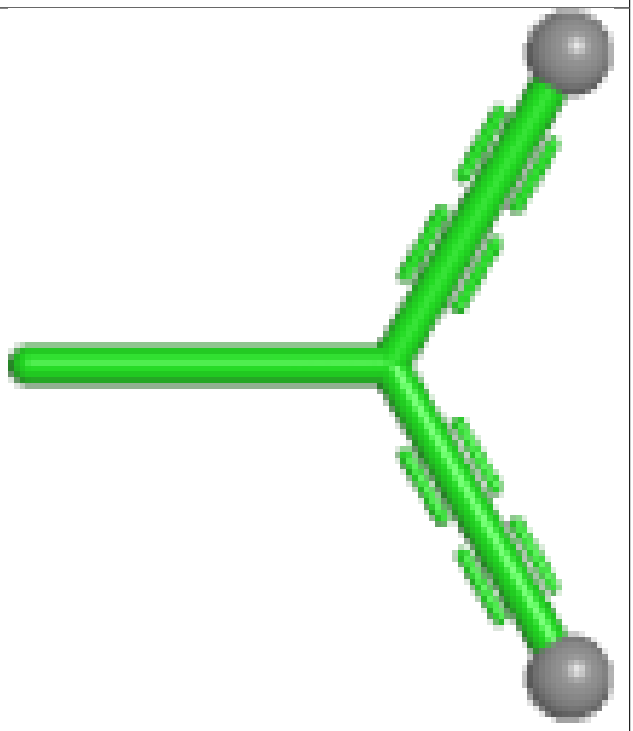
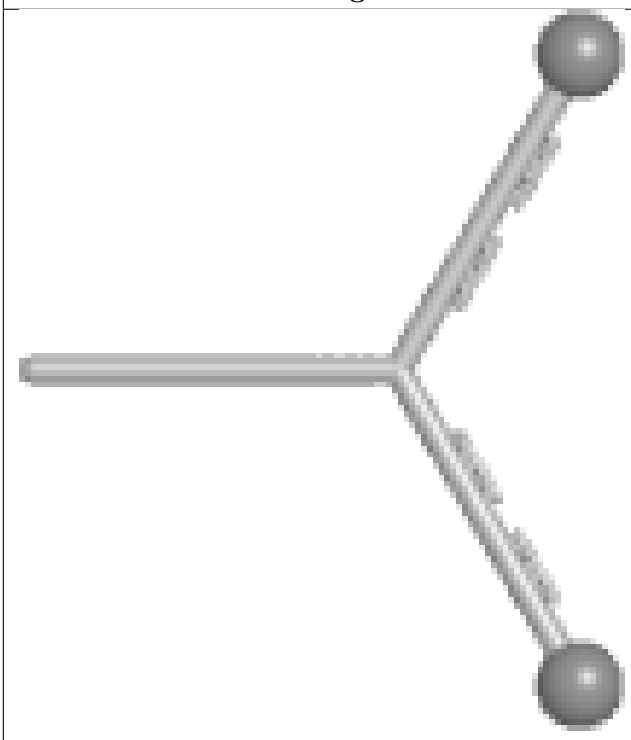


Bond angles



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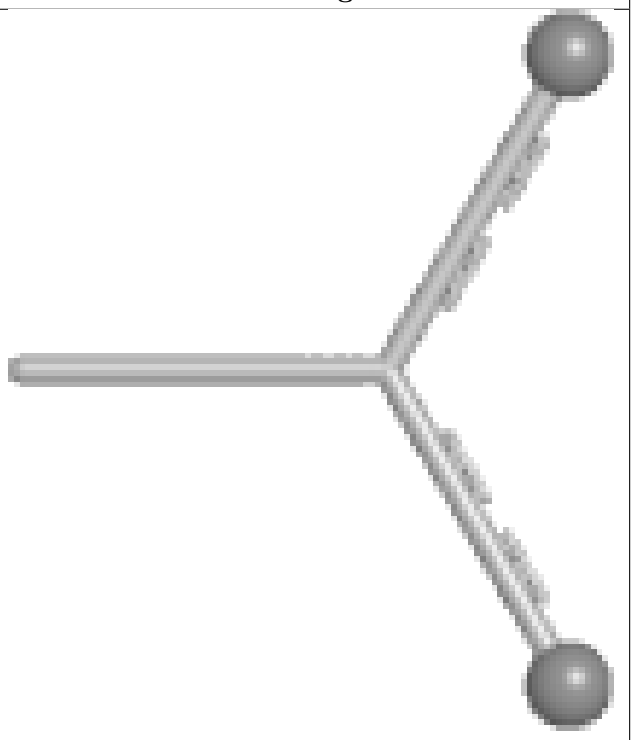
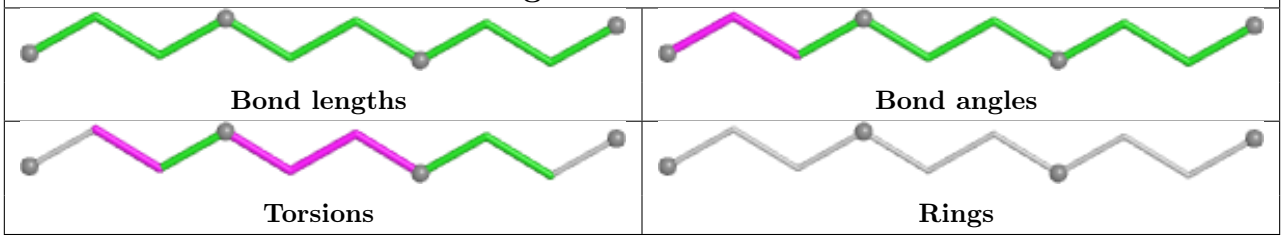
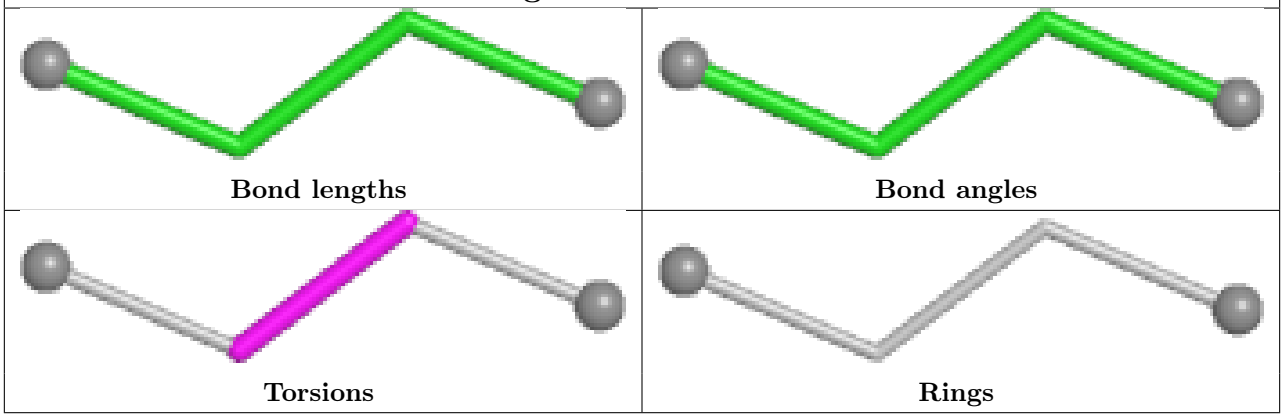


Rings

Ligand PGE D 314



Ligand EDO C 305



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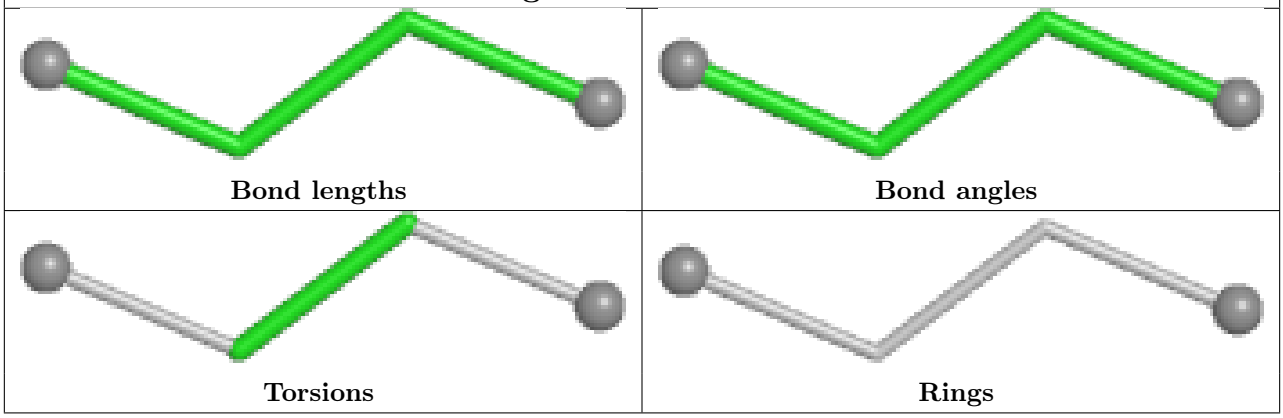
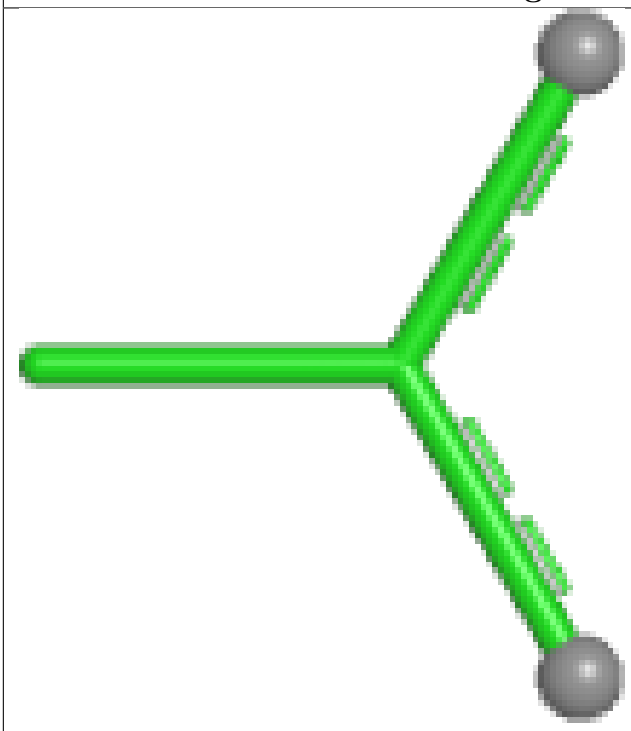
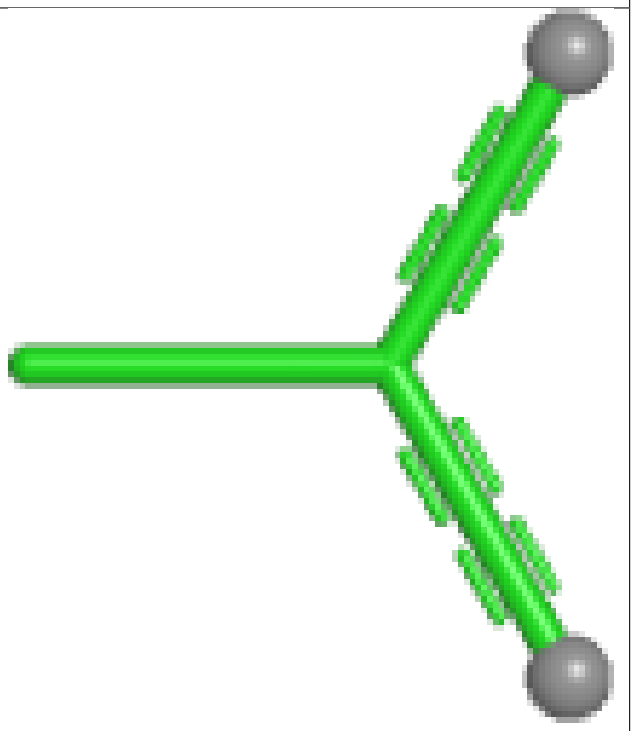


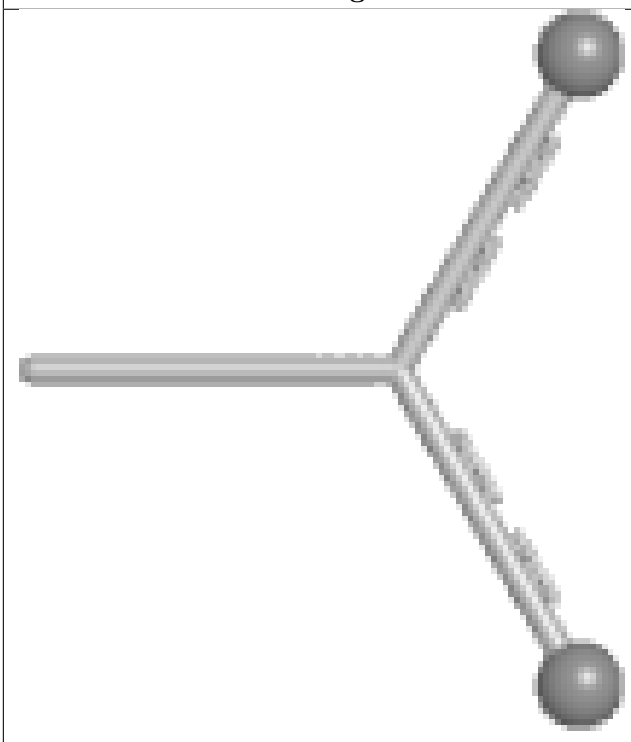
Ligand ACT F 311



Bond lengths



Bond angles



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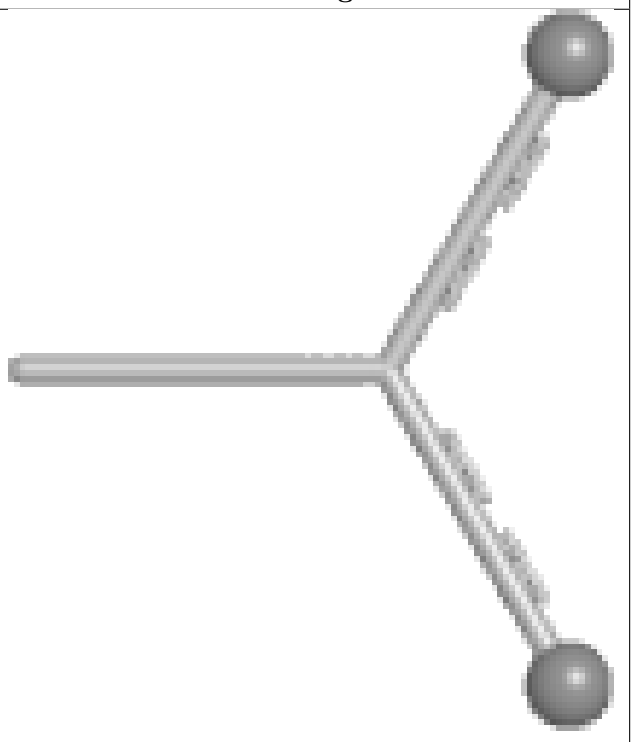
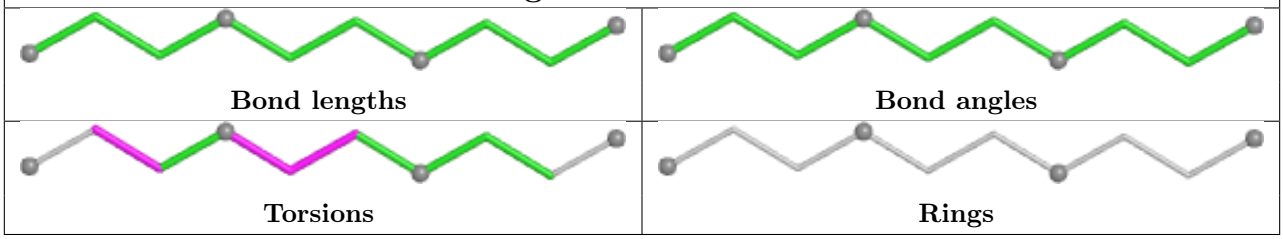
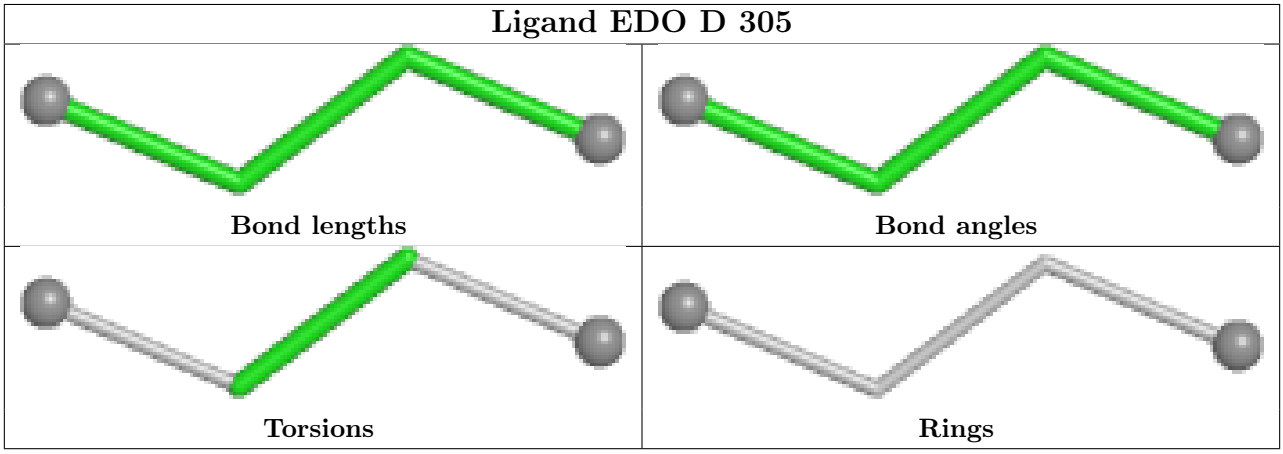


Rings

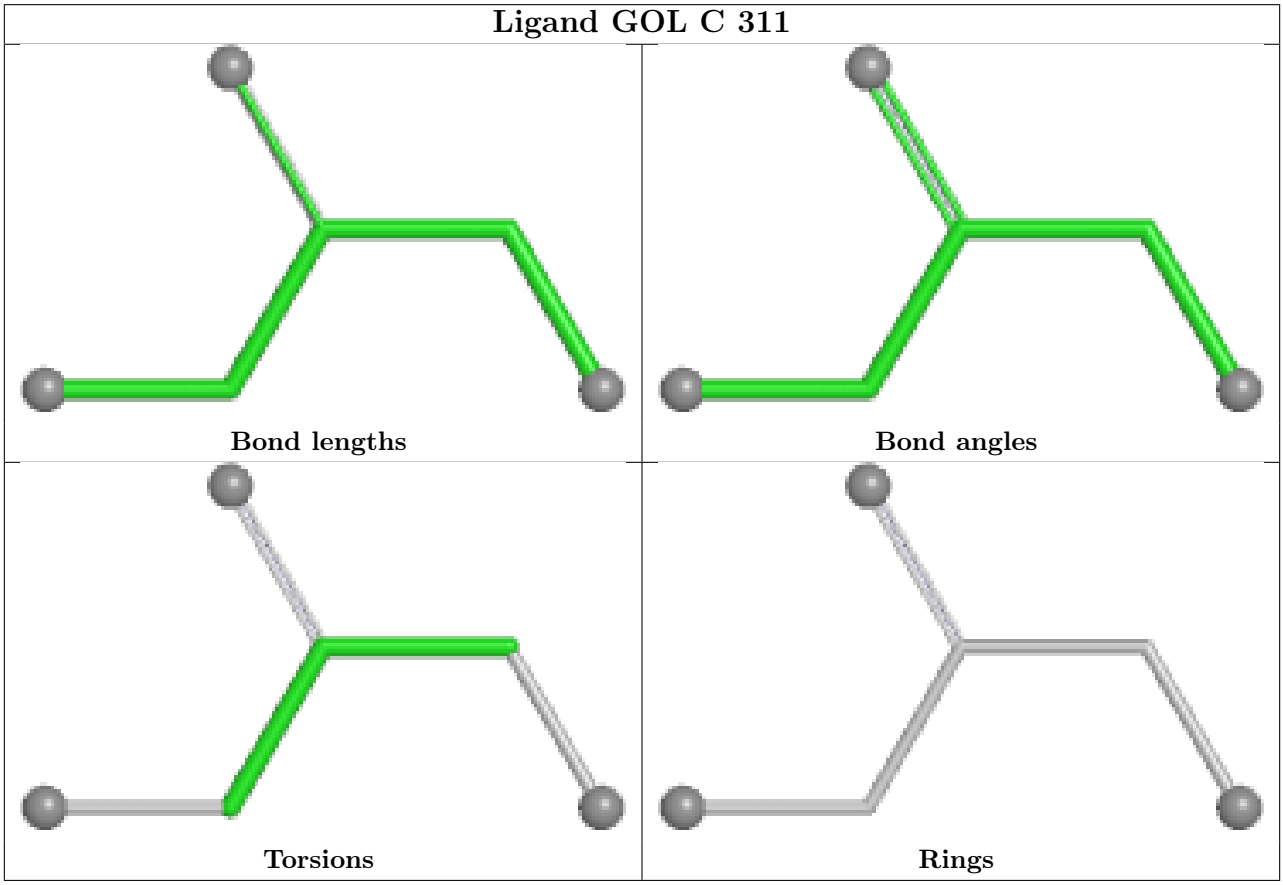
Ligand PGE B 316



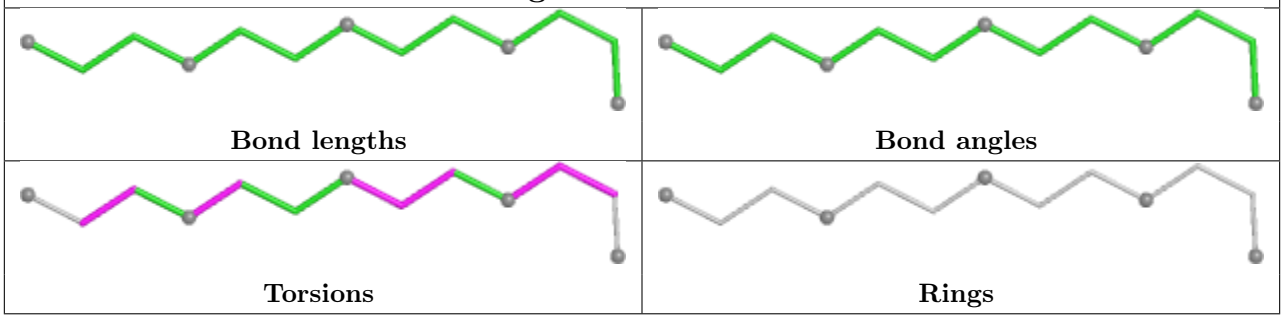
Ligand EDO D 305



Ligand GOL C 311



Ligand PG4 E 306



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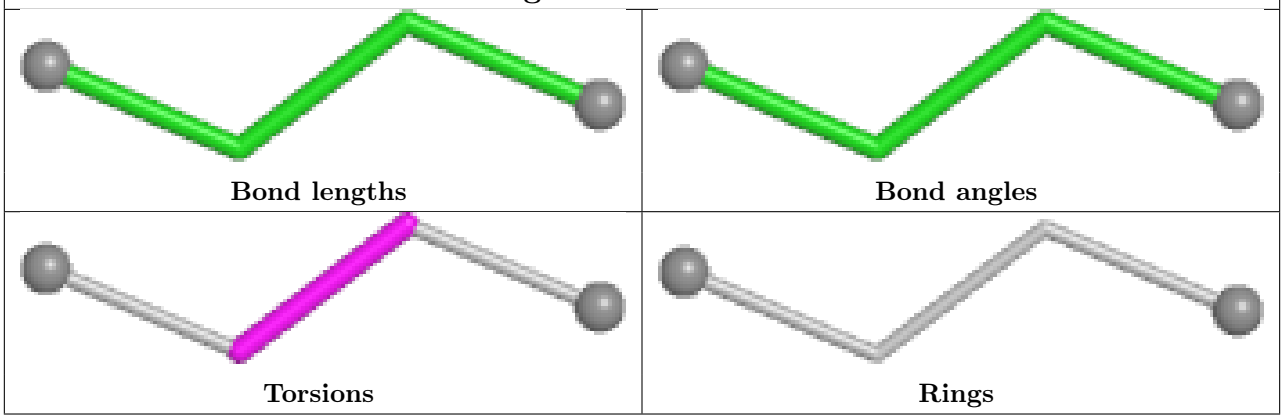

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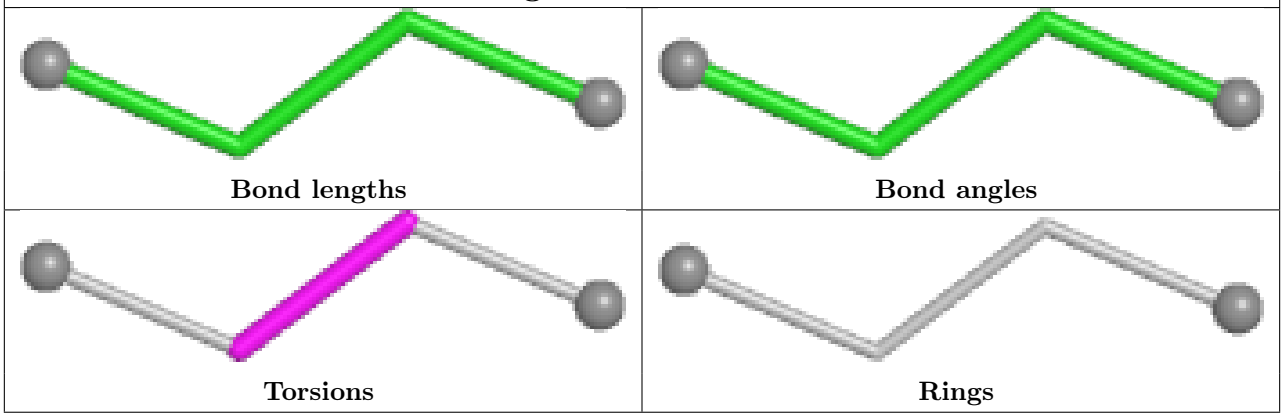

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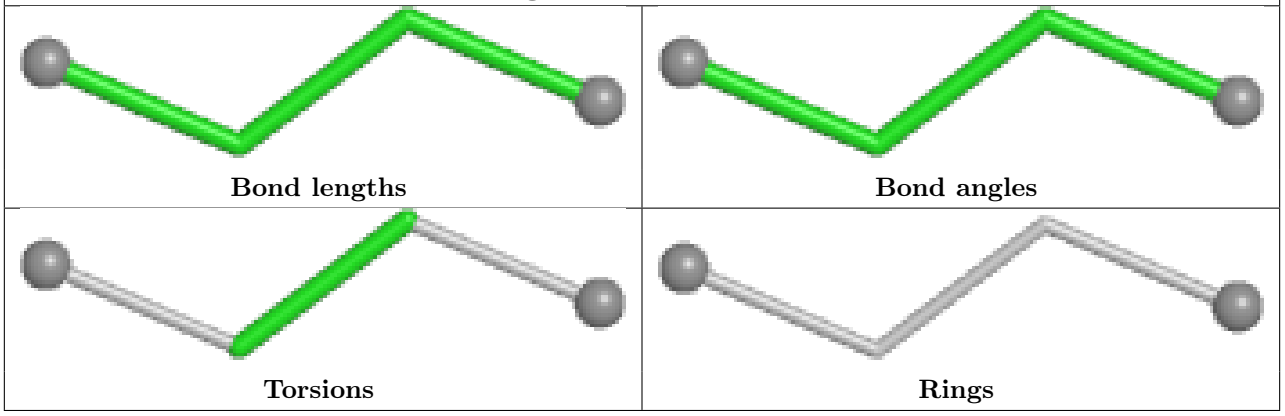

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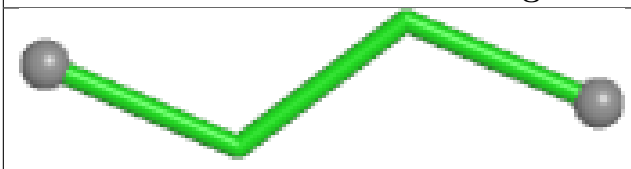
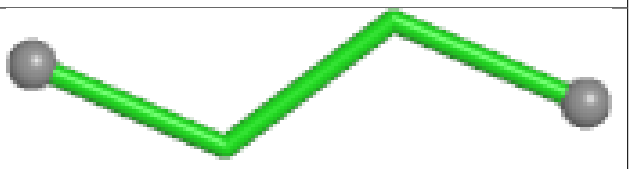
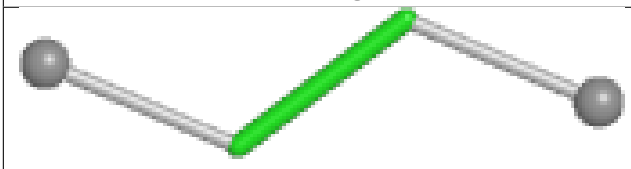


Bond lengths



Bond angles

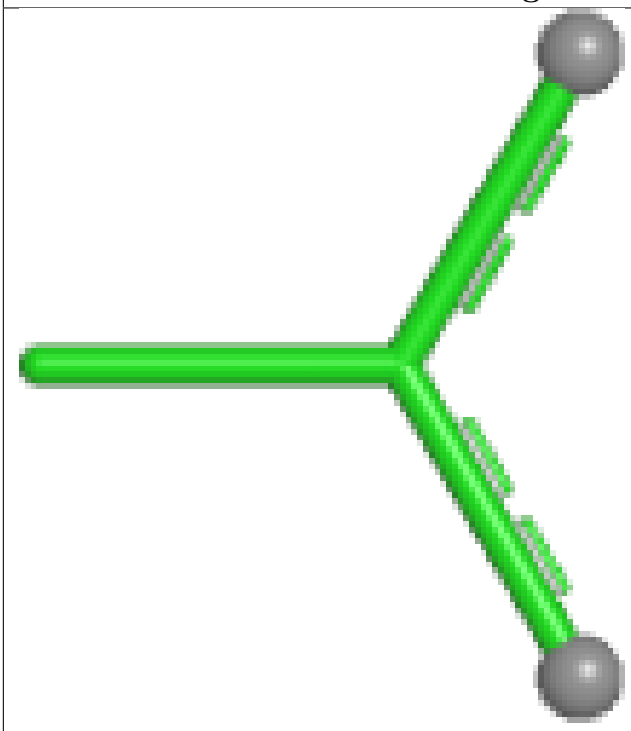


Torsions



Rings

Ligand ACT D 309



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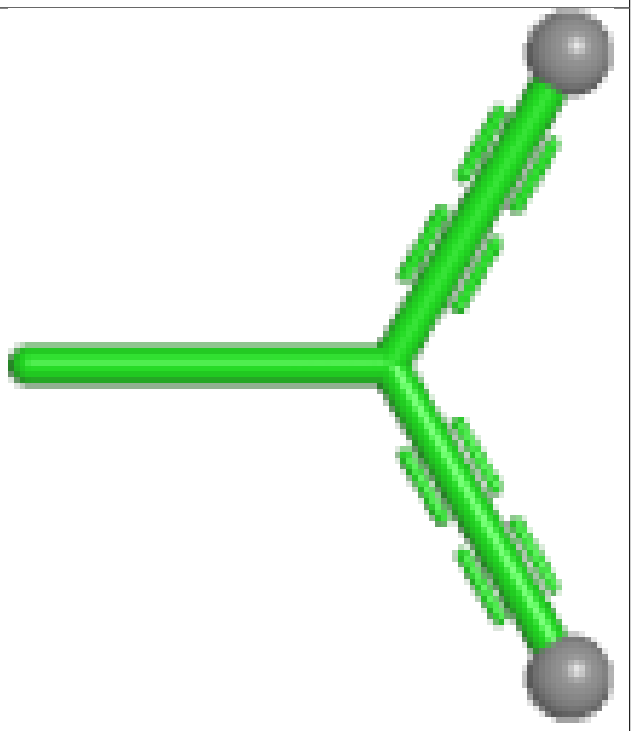
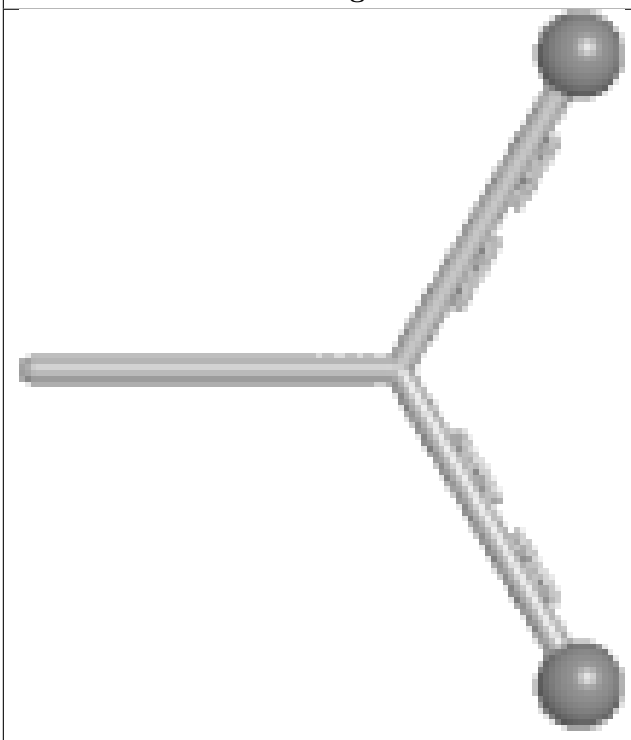
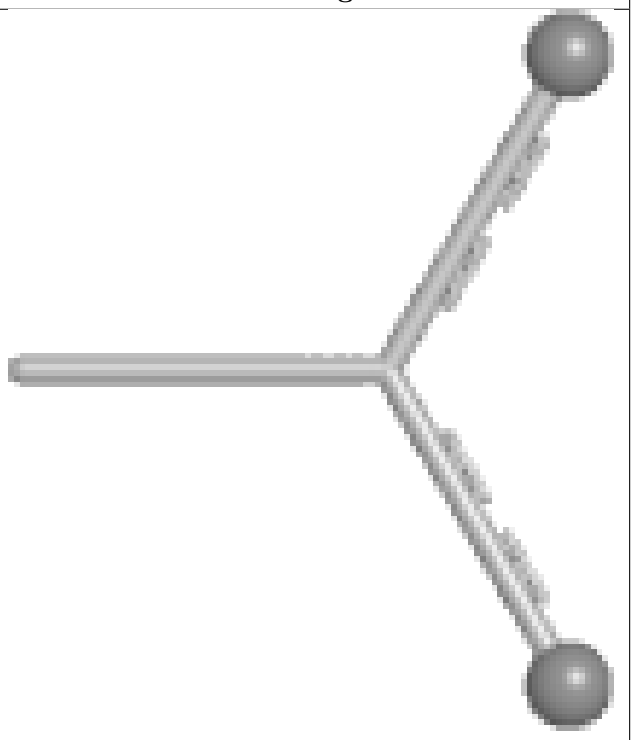


Bond angles

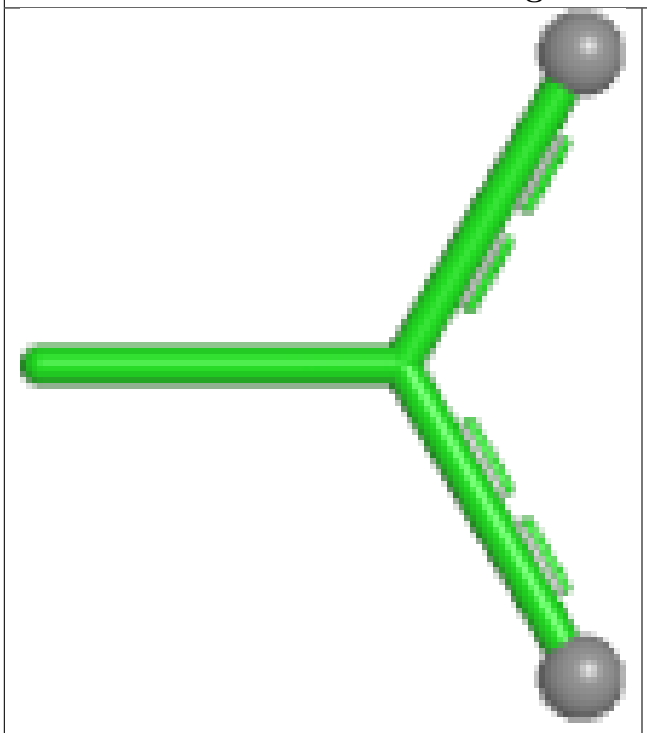


Torsions



Rings

Ligand ACT F 312



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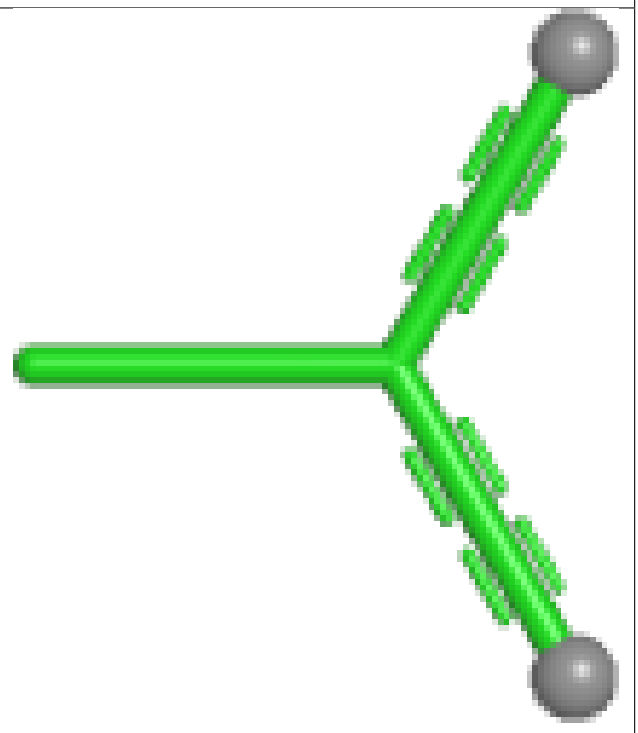
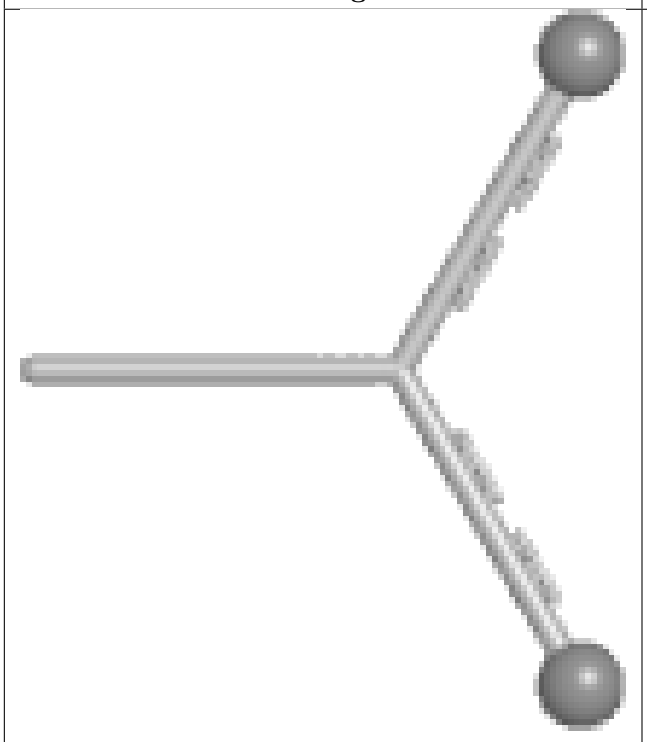


Bond angles



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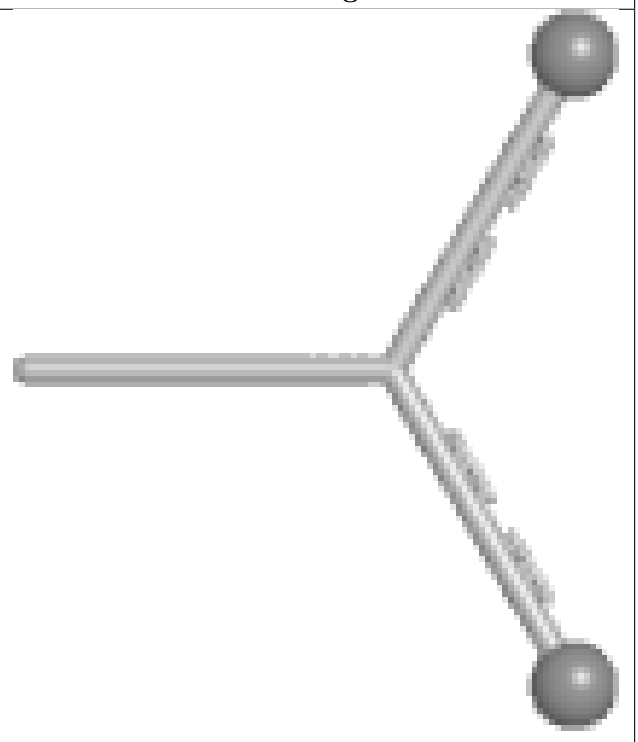
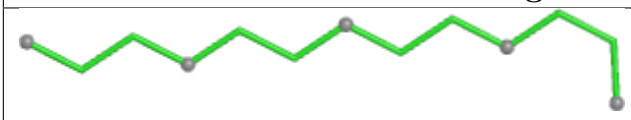


Rings

Ligand PG4 D 303



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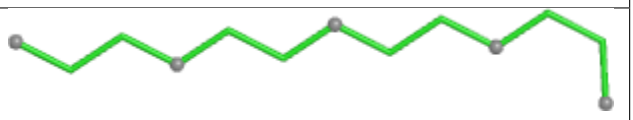
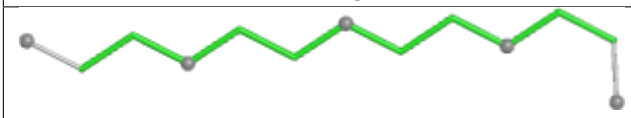


Bond angles



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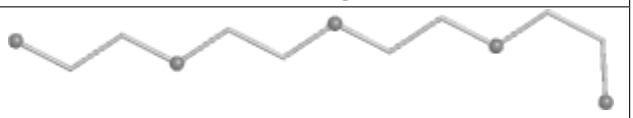
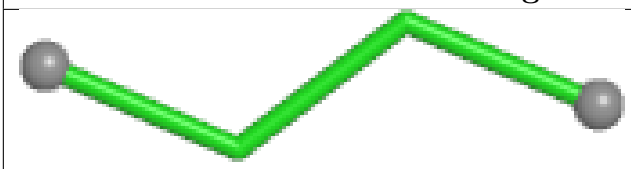


Rings

Ligand EDO A 312



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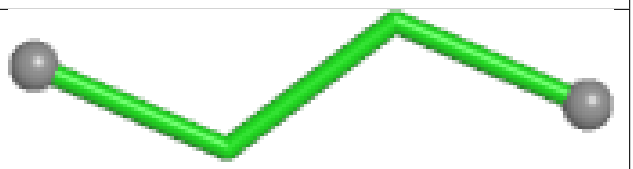
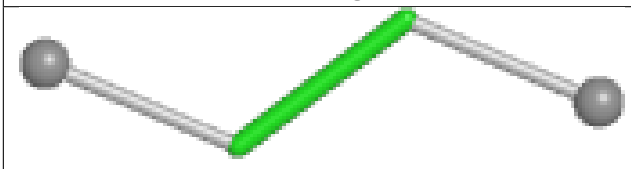


Bond angles



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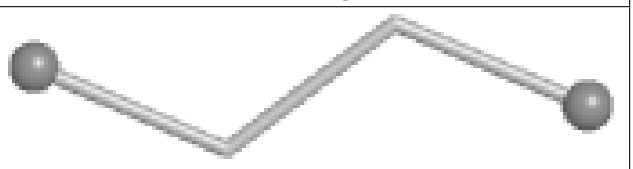
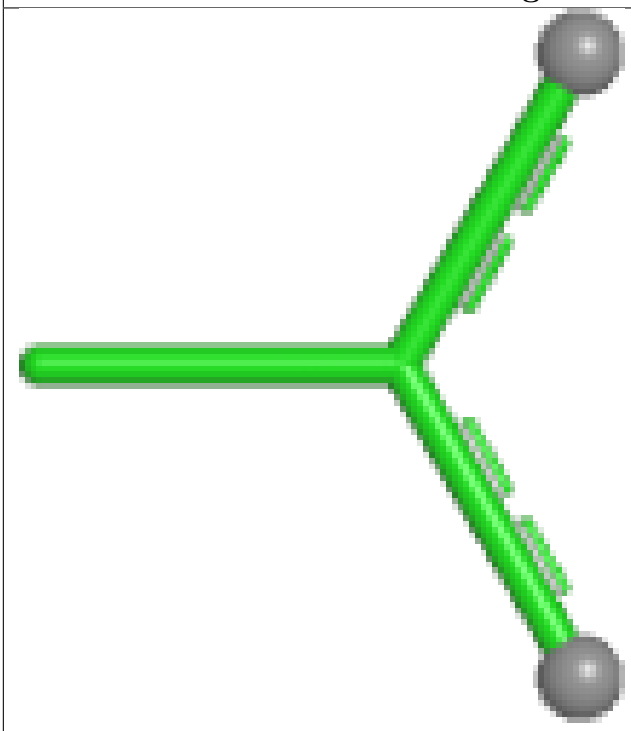


Rings

Ligand ACT D 312



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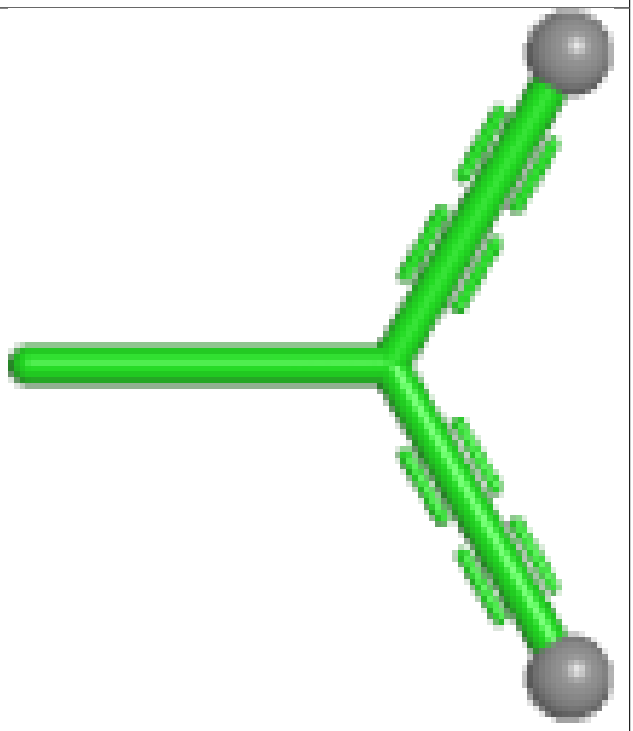
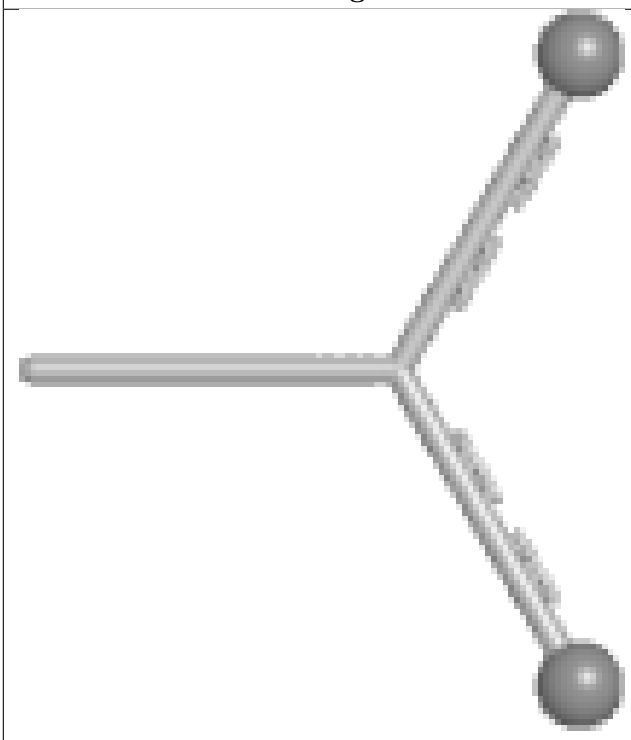


Bond angles



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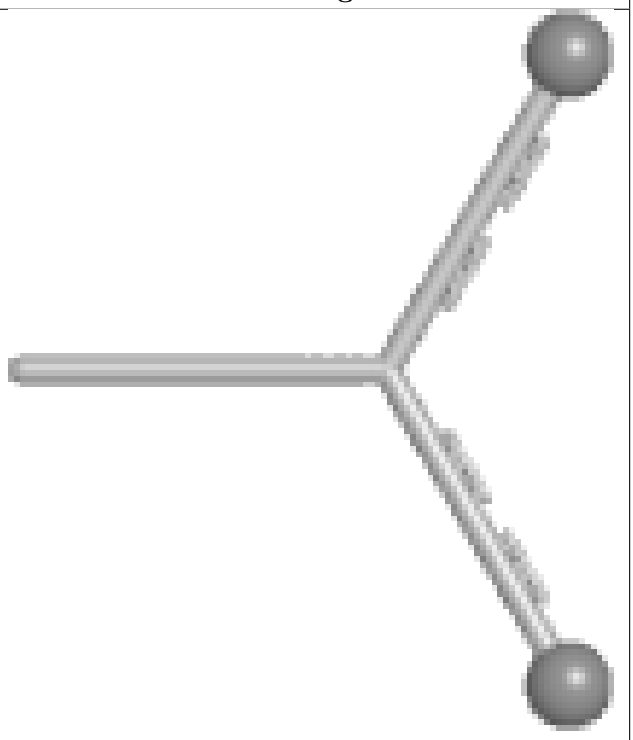
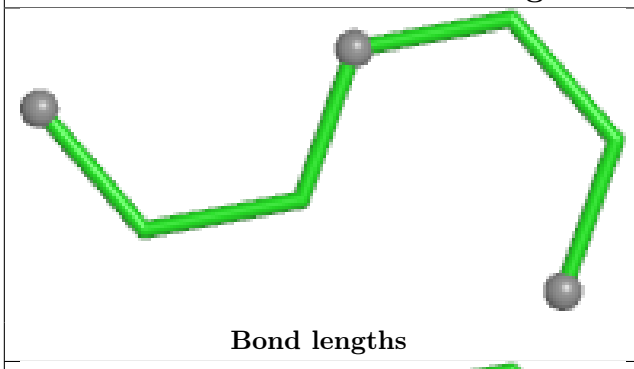
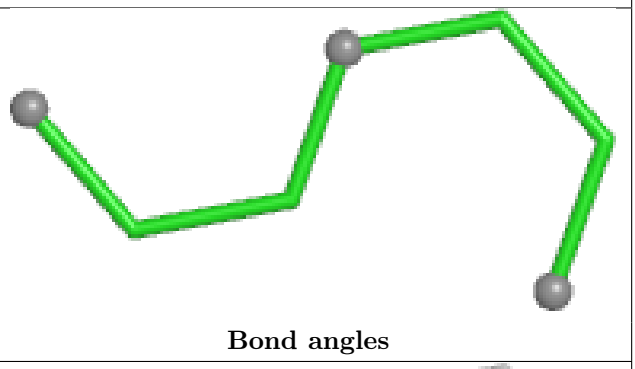


Rings

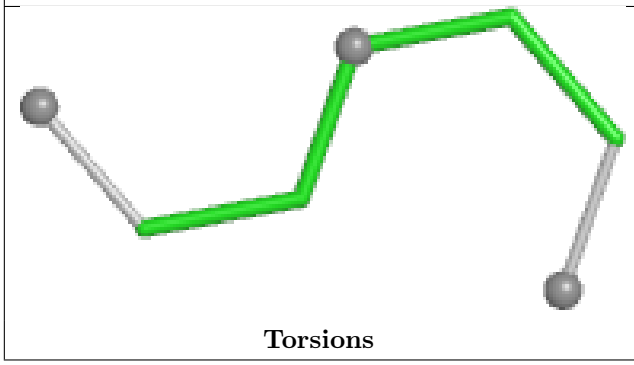
Ligand PEG F 308



Bond lengths



Bond angles



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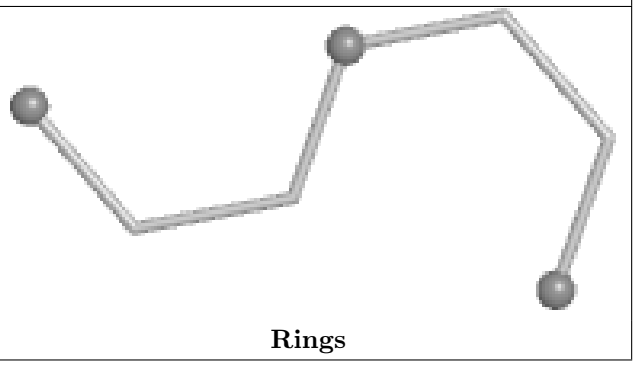
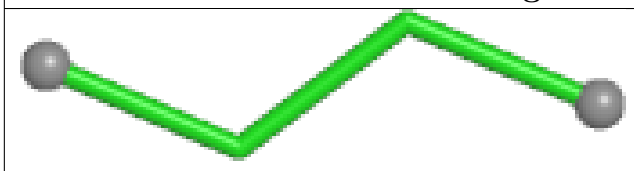


Rings

Ligand EDO A 311



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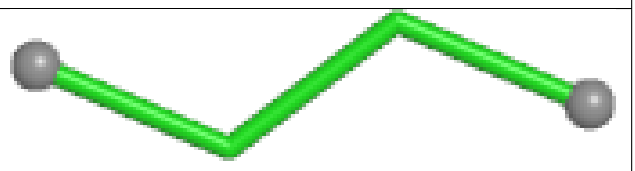
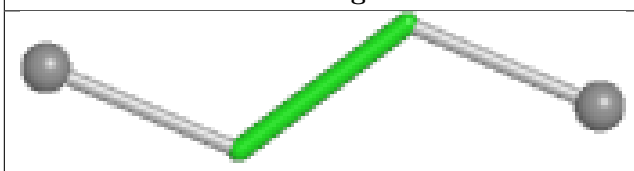


Bond angles



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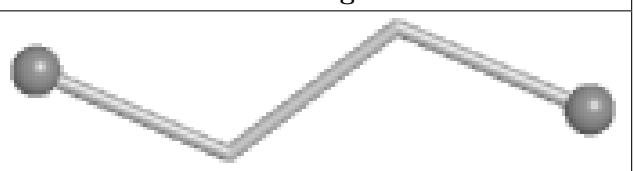
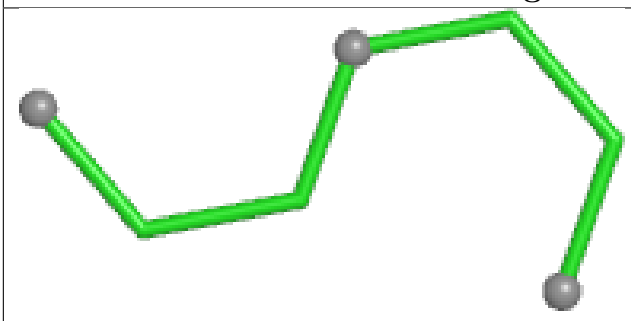
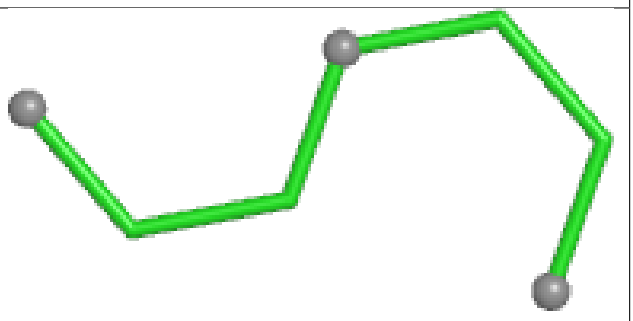
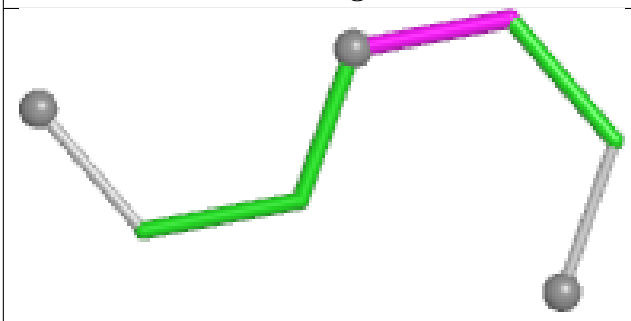
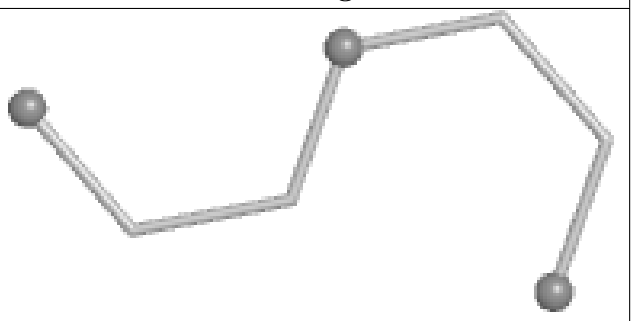
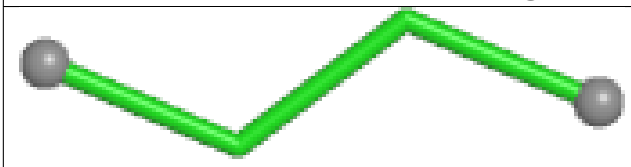
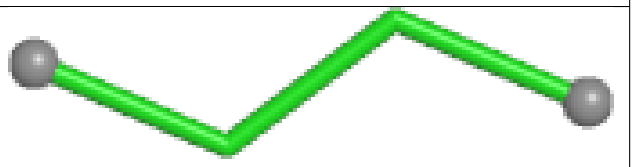
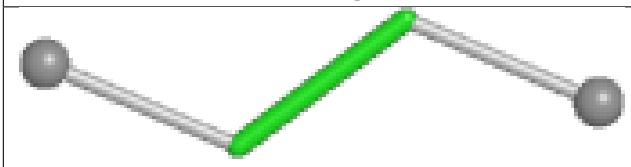
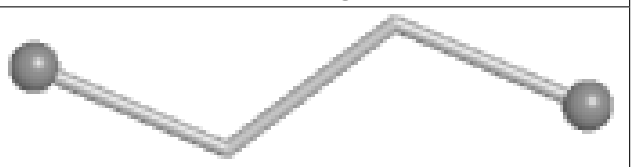
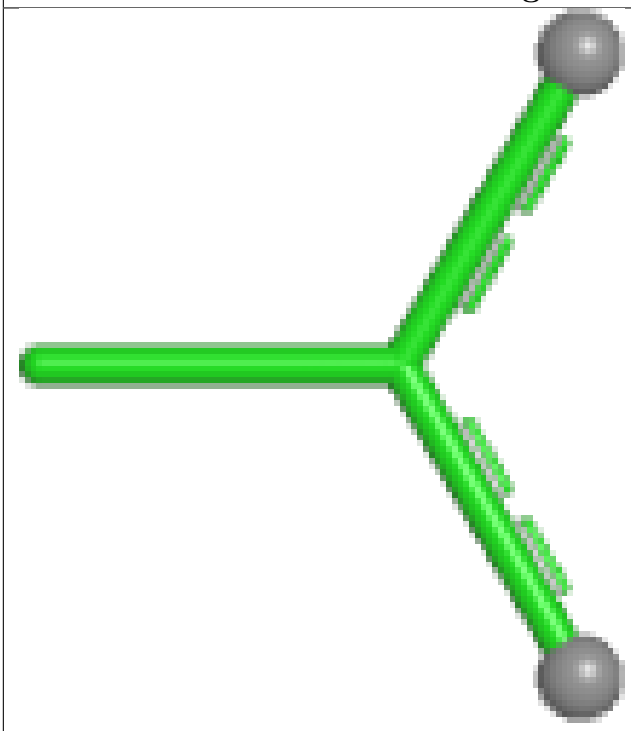


Rings

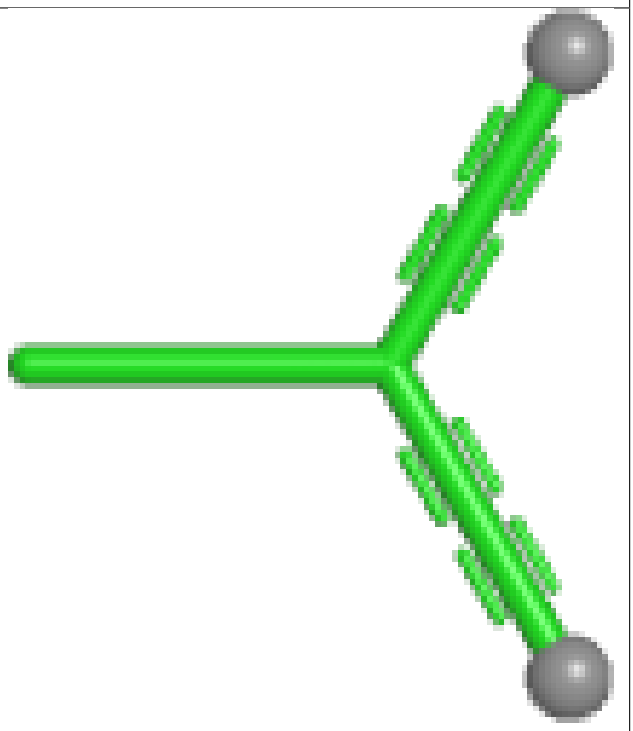
Ligand PEG B 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO A 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

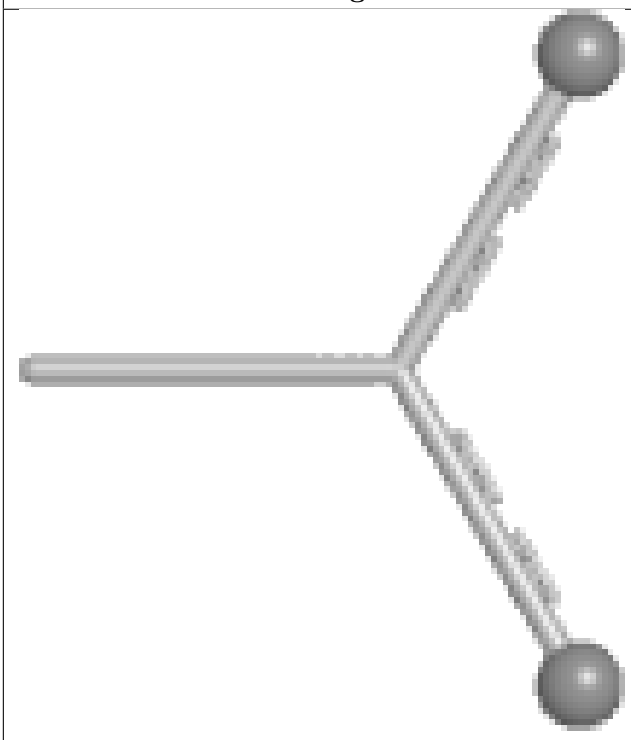
Ligand ACT A 319



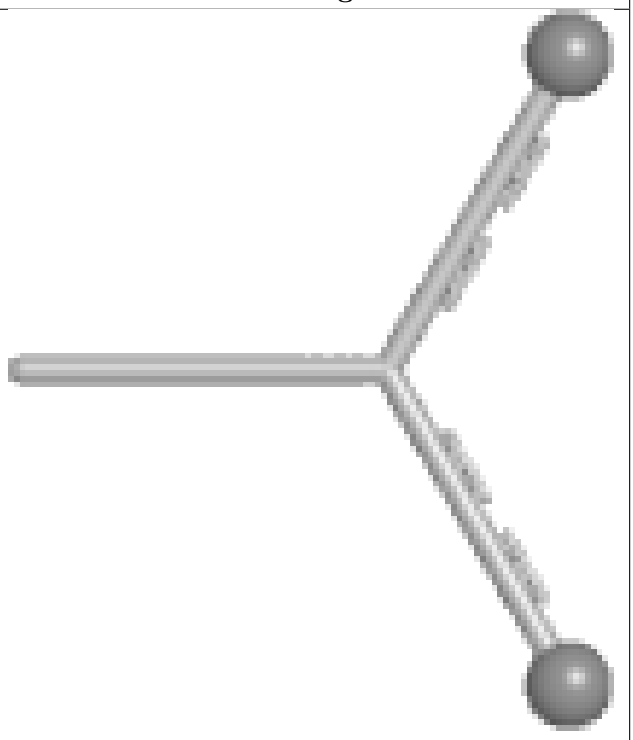
Bond lengths



Bond angles

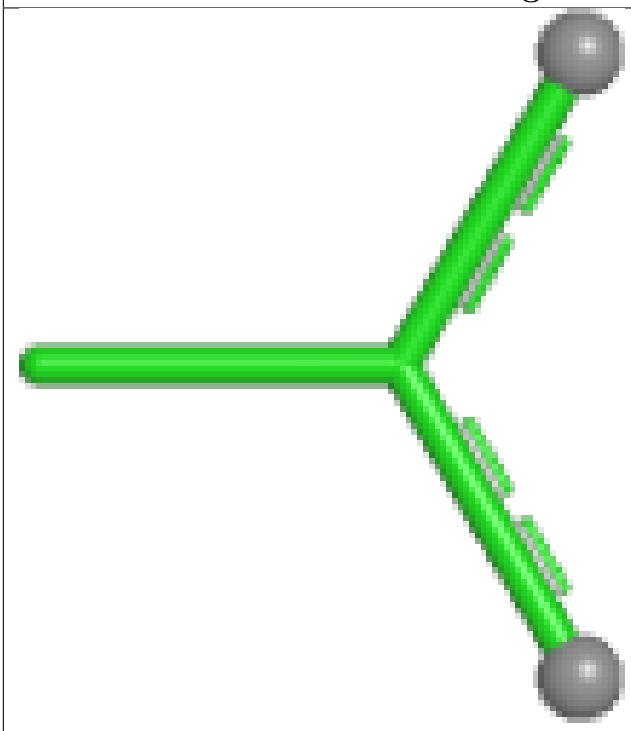


Torsions

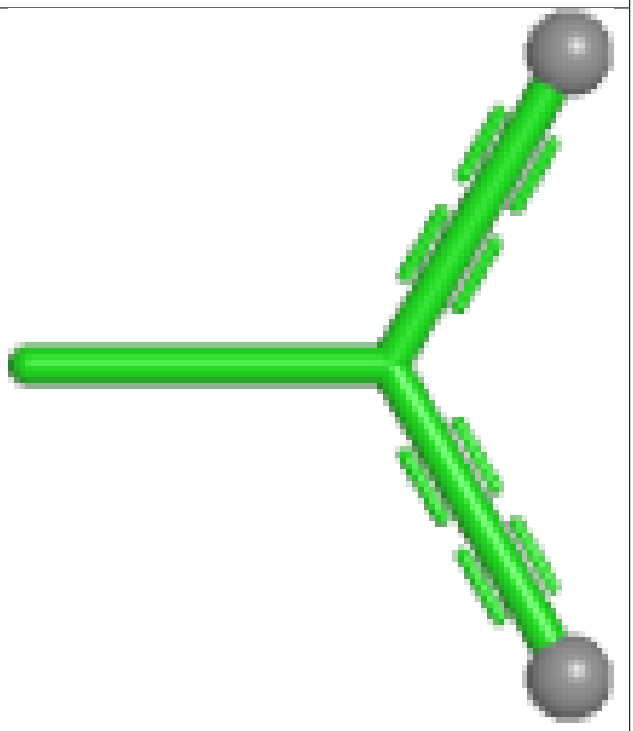


Rings

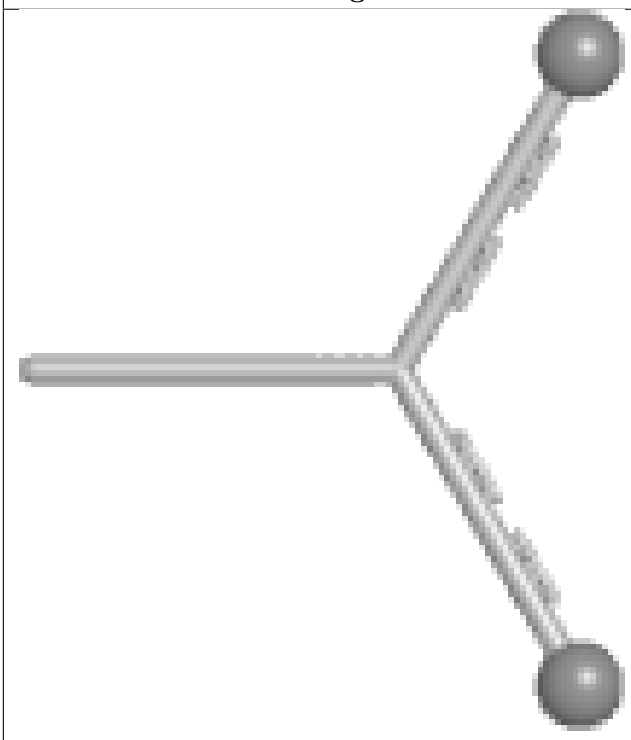
Ligand ACT A 320



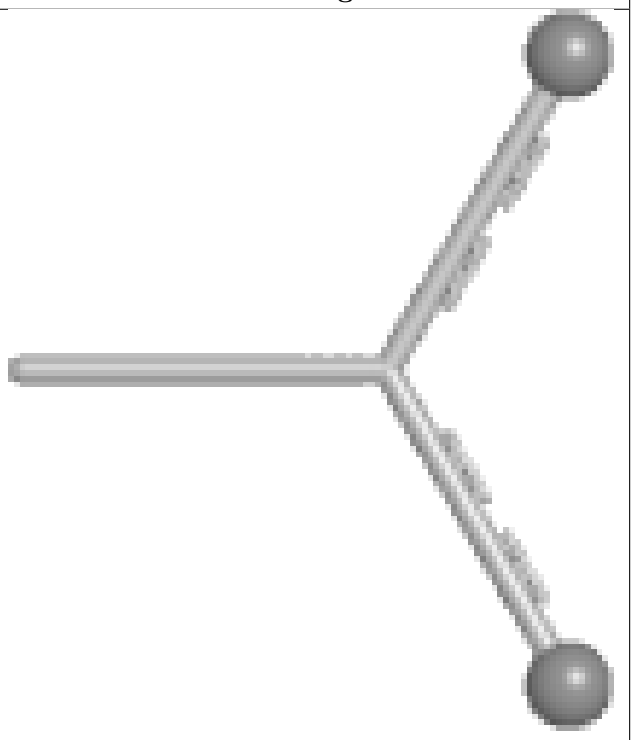
Bond lengths



Bond angles

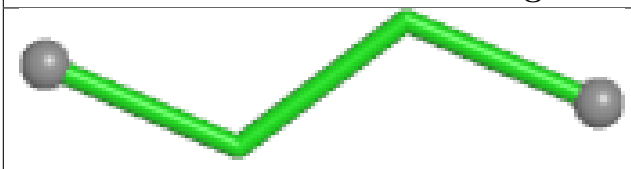


Torsions

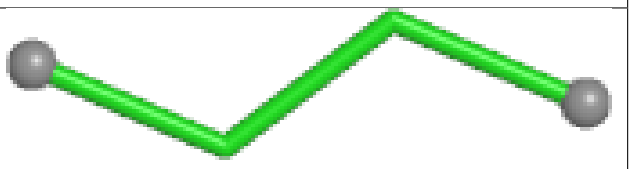


Rings

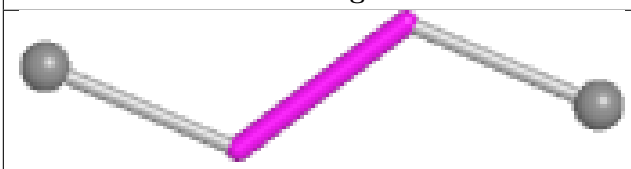
Ligand EDO F 306



Bond lengths



Bond angles

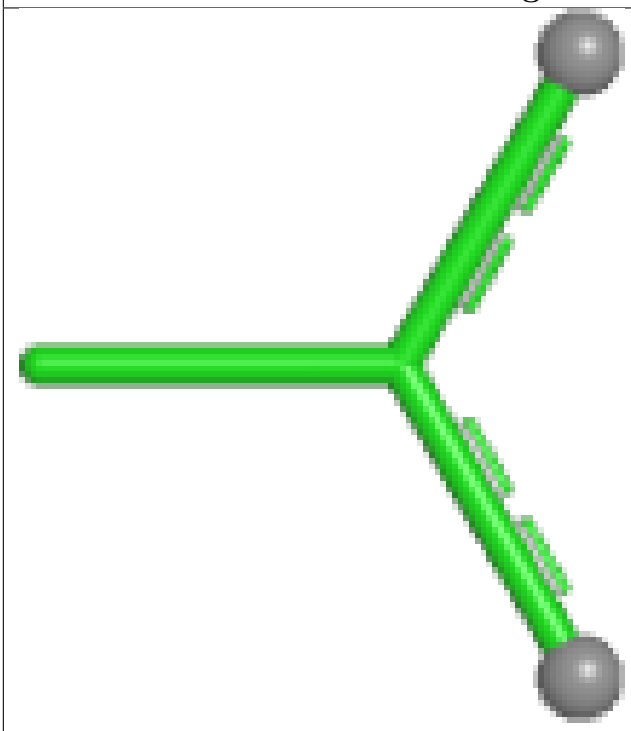


Torsions

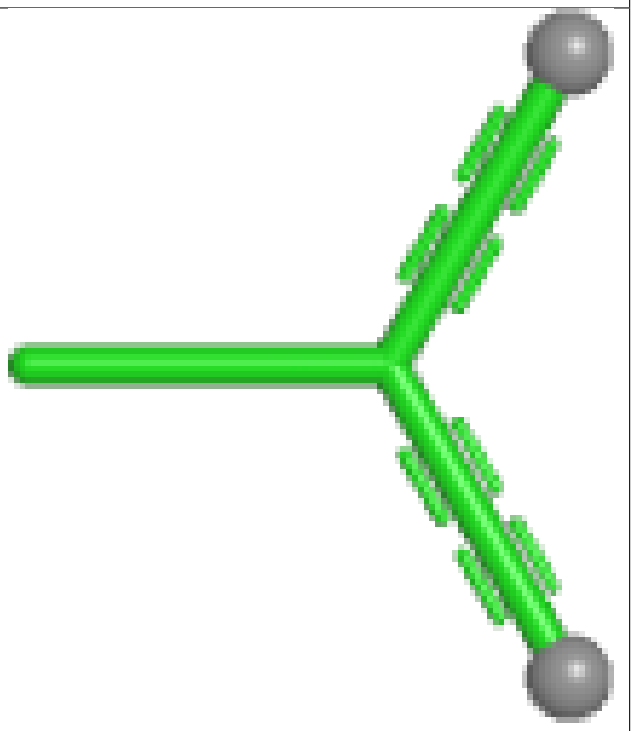


Rings

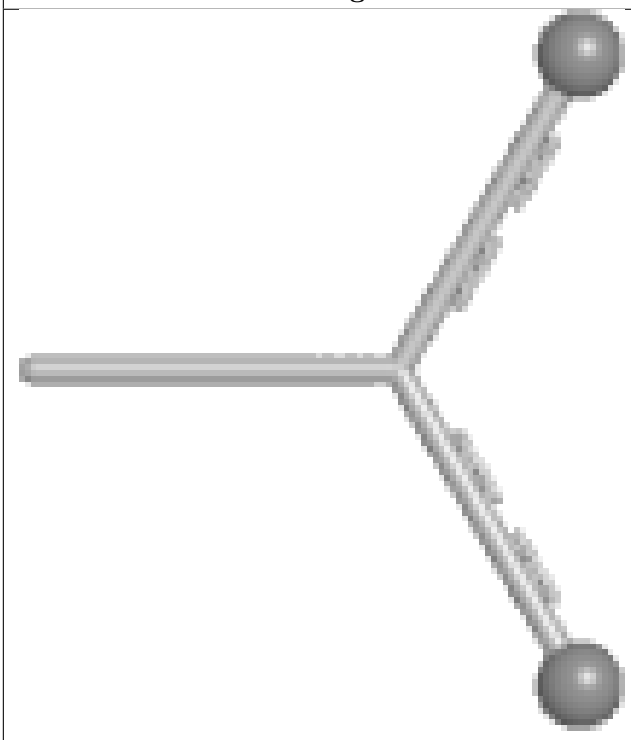
Ligand ACT D 311



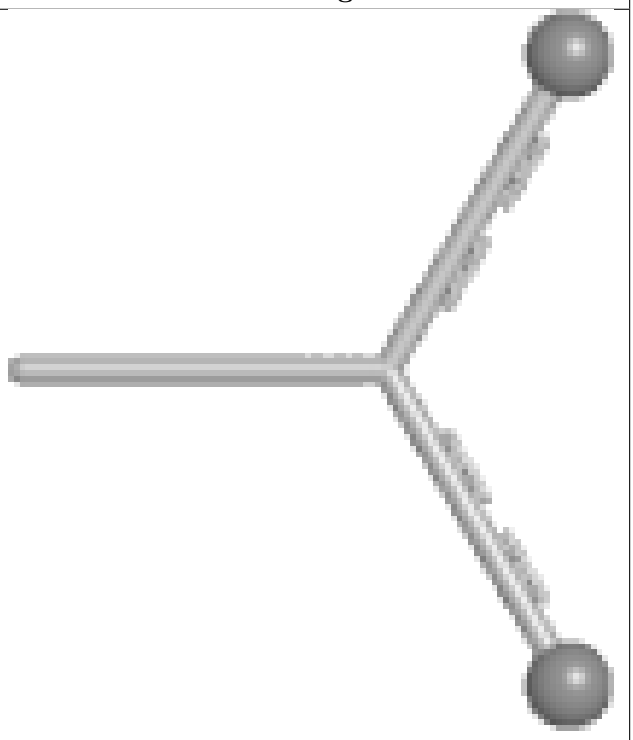
Bond lengths



Bond angles

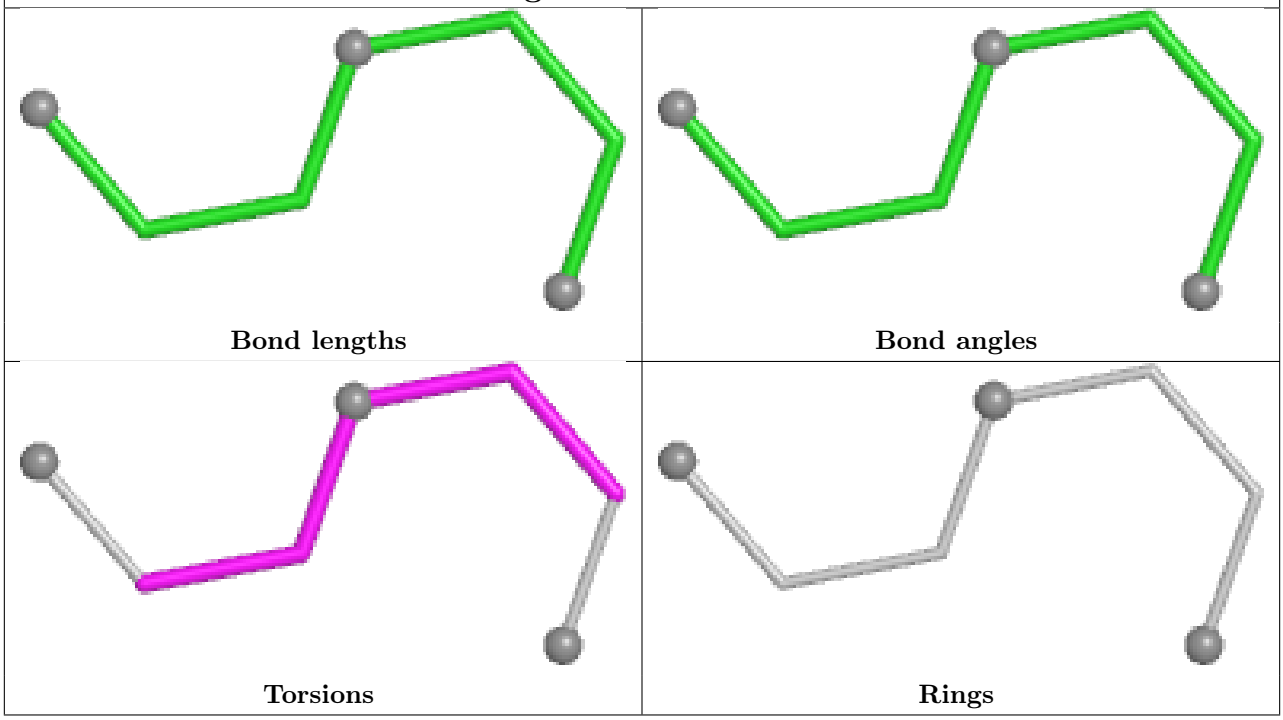


Torsions



Rings

Ligand PEG C 310



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	295/310 (95%)	-0.44	0 100 100	12, 18, 30, 46	1 (0%)
1	B	303/310 (97%)	-0.31	3 (0%) 79 84	14, 19, 34, 44	1 (0%)
1	C	295/310 (95%)	-0.31	0 100 100	15, 20, 34, 44	1 (0%)
1	D	303/310 (97%)	-0.32	6 (1%) 65 71	13, 19, 33, 43	2 (0%)
1	E	296/310 (95%)	-0.43	1 (0%) 90 92	14, 18, 31, 45	1 (0%)
1	F	295/310 (95%)	-0.31	1 (0%) 90 92	15, 20, 34, 47	0
All	All	1787/1860 (96%)	-0.35	11 (0%) 85 89	12, 19, 33, 47	6 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	95[A]	PHE	3.6
1	D	56	TRP	2.9
1	D	99	HIS	2.8
1	D	131	ASP	2.7
1	B	2	ASP	2.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	C	166	14/15	0.71	0.16	20,20,20,20	0
1	KPI	A	166	14/15	0.73	0.16	20,20,20,20	0
1	KPI	D	166	14/15	0.76	0.16	20,20,20,20	0
1	KPI	E	166	14/15	0.76	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	F	166	14/15	0.77	0.14	20,20,20,20	0
1	KPI	B	166	14/15	0.79	0.14	20,20,20,20	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ACT	F	312	4/4	0.63	0.18	37,44,47,49	0
7	ACT	F	313	4/4	0.68	0.16	38,48,52,54	0
7	ACT	D	309	4/4	0.70	0.22	40,40,42,46	0
7	ACT	D	310	4/4	0.70	0.19	36,40,42,44	0
5	EDO	B	306	4/4	0.72	0.29	27,34,36,48	0
5	EDO	A	315	4/4	0.73	0.16	34,38,39,51	0
7	ACT	E	314	4/4	0.73	0.17	33,36,47,50	0
7	ACT	D	311	4/4	0.74	0.18	34,37,44,51	0
7	ACT	A	320	4/4	0.74	0.18	36,42,49,52	0
8	PGE	D	313	10/10	0.74	0.16	40,45,48,51	0
5	EDO	A	311	4/4	0.75	0.16	39,40,47,52	0
5	EDO	E	312	4/4	0.75	0.15	38,43,45,48	0
9	GOL	C	311	6/6	0.76	0.16	30,34,36,49	0
7	ACT	B	315	4/4	0.77	0.18	36,39,43,44	0
5	EDO	F	306	4/4	0.77	0.16	32,35,38,45	0
7	ACT	B	314	4/4	0.77	0.17	40,44,46,52	0
5	EDO	D	305	4/4	0.78	0.18	27,31,33,48	0
8	PGE	E	315	10/10	0.78	0.16	31,36,41,55	0
7	ACT	F	311	4/4	0.78	0.18	33,40,47,51	0
6	PEG	B	313	7/7	0.79	0.14	32,34,43,52	0
6	PEG	E	313	7/7	0.79	0.15	25,31,45,48	0
5	EDO	C	306	4/4	0.79	0.14	38,38,38,39	0
5	EDO	B	310	4/4	0.80	0.23	24,30,36,51	0
6	PEG	A	318	7/7	0.81	0.14	37,41,45,51	0
8	PGE	B	316	10/10	0.82	0.16	24,46,58,62	0
6	PEG	B	312	7/7	0.82	0.14	29,36,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	F	309	7/7	0.82	0.14	40,46,53,64	0
5	EDO	B	309	4/4	0.82	0.15	37,42,48,49	0
7	ACT	A	319	4/4	0.83	0.16	20,39,43,44	0
8	PGE	D	314	10/10	0.83	0.15	22,34,39,46	0
6	PEG	F	308	7/7	0.83	0.14	33,38,47,47	0
5	EDO	A	316	4/4	0.83	0.14	39,43,47,52	0
7	ACT	D	312	4/4	0.84	0.13	42,43,47,47	0
5	EDO	A	307	4/4	0.84	0.12	29,31,37,38	0
3	MG	A	305	1/1	0.84	0.23	53,53,53,53	0
3	MG	E	304	1/1	0.84	0.14	49,49,49,49	0
4	PG4	E	306	13/13	0.84	0.14	24,36,50,51	0
5	EDO	E	310	4/4	0.85	0.13	33,36,44,44	0
5	EDO	B	307	4/4	0.85	0.14	39,40,40,43	0
5	EDO	E	309	4/4	0.86	0.14	34,40,42,45	0
6	PEG	B	311	7/7	0.86	0.12	31,39,47,48	0
5	EDO	A	310	4/4	0.86	0.14	39,41,46,46	0
3	MG	B	304	1/1	0.87	0.23	50,50,50,50	0
5	EDO	E	308	4/4	0.87	0.13	26,30,30,31	0
5	EDO	C	309	4/4	0.87	0.12	33,41,43,50	0
5	EDO	C	304	4/4	0.88	0.13	35,37,38,43	0
3	MG	E	305	1/1	0.88	0.10	41,41,41,41	0
6	PEG	C	310	7/7	0.88	0.10	31,41,46,50	0
6	PEG	D	308	7/7	0.88	0.12	29,31,43,43	0
5	EDO	C	307	4/4	0.88	0.13	29,35,36,55	0
5	EDO	A	313	4/4	0.88	0.12	26,26,34,36	0
5	EDO	A	308	4/4	0.89	0.14	22,30,35,36	0
4	PG4	F	305	13/13	0.89	0.11	27,32,51,51	0
5	EDO	E	307	4/4	0.89	0.11	38,43,46,46	0
6	PEG	A	317	7/7	0.89	0.11	28,38,44,52	0
5	EDO	B	308	4/4	0.89	0.12	23,31,37,37	0
3	MG	F	304	1/1	0.89	0.13	47,47,47,47	1
5	EDO	C	308	4/4	0.90	0.10	35,39,40,48	0
7	ACT	F	310	4/4	0.90	0.11	35,36,41,41	0
5	EDO	D	306	4/4	0.91	0.12	24,28,31,36	0
4	PG4	D	303	13/13	0.91	0.09	25,31,44,47	0
5	EDO	A	312	4/4	0.91	0.11	30,35,39,42	0
3	MG	B	303	1/1	0.91	0.18	46,46,46,46	0
4	PG4	B	305	13/13	0.91	0.10	25,33,50,51	0
5	EDO	C	305	4/4	0.92	0.10	26,28,32,41	0
5	EDO	D	307	4/4	0.92	0.14	26,36,37,42	0
3	MG	A	302	1/1	0.92	0.08	41,41,41,41	0
5	EDO	A	309	4/4	0.92	0.09	30,32,34,40	0

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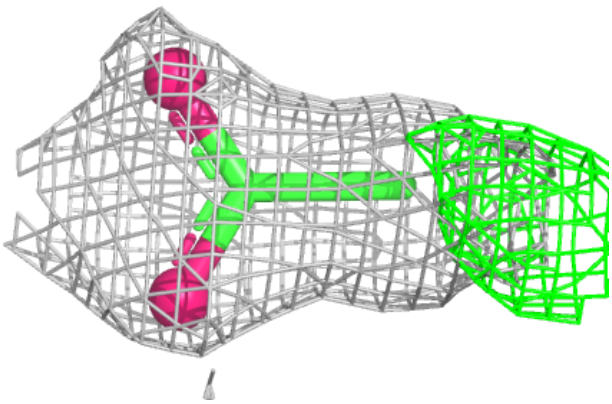
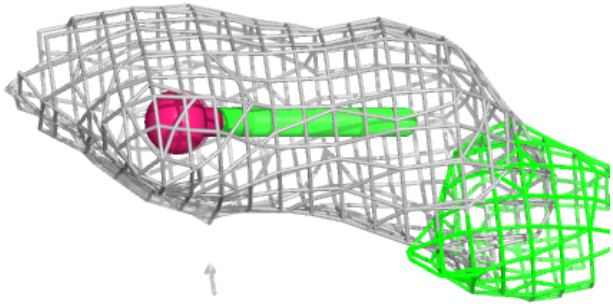
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG4	C	303	13/13	0.93	0.10	26,33,47,48	0
5	EDO	D	304	4/4	0.95	0.07	30,31,33,35	0
3	MG	C	301	1/1	0.95	0.04	34,34,34,34	0
4	PG4	A	306	13/13	0.96	0.07	26,32,44,49	0
5	EDO	F	307	4/4	0.96	0.08	20,25,33,36	0
5	EDO	A	314	4/4	0.96	0.07	23,26,26,32	0
2	3VN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

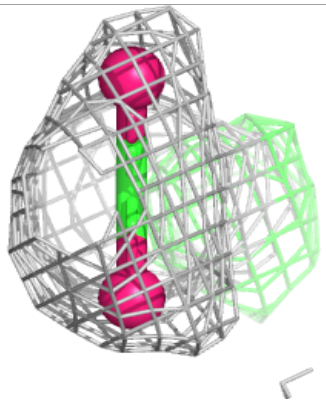
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACT F 312:

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

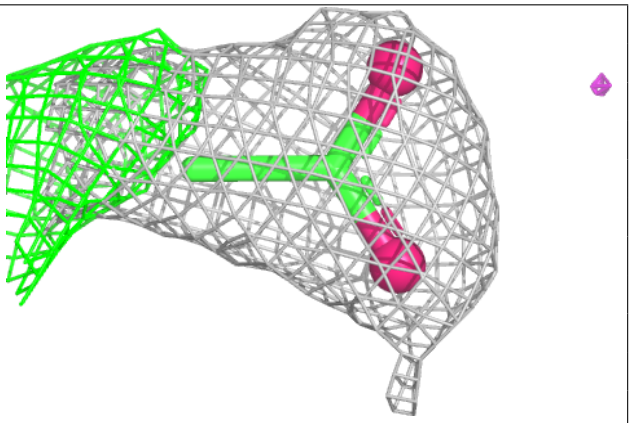


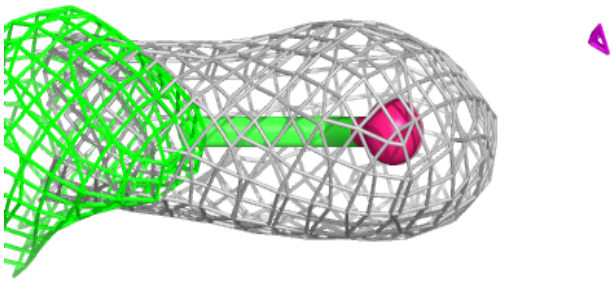


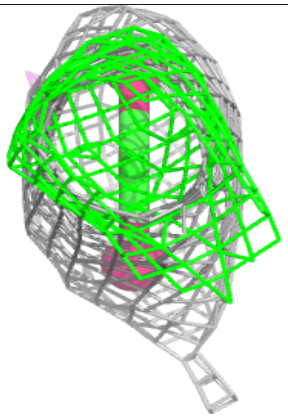


Electron density around ACT F 313:

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

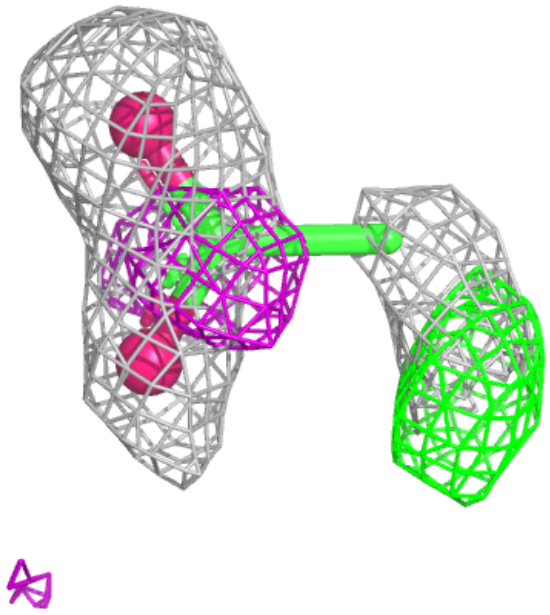


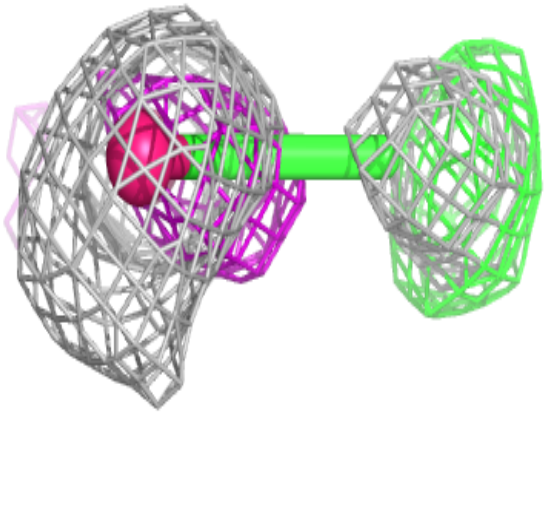


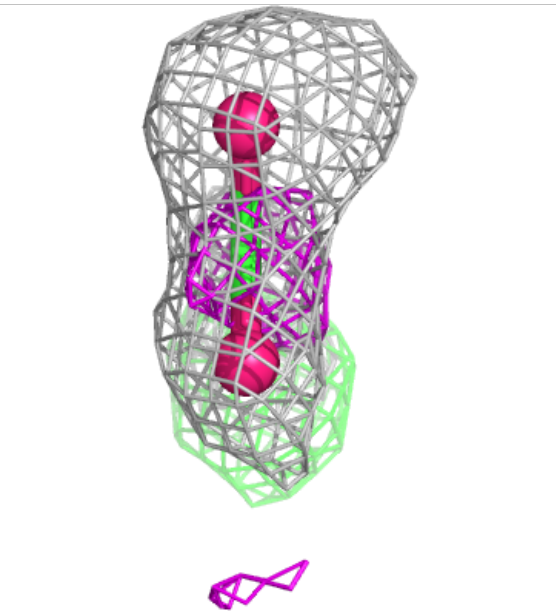


Electron density around ACT D 309:

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

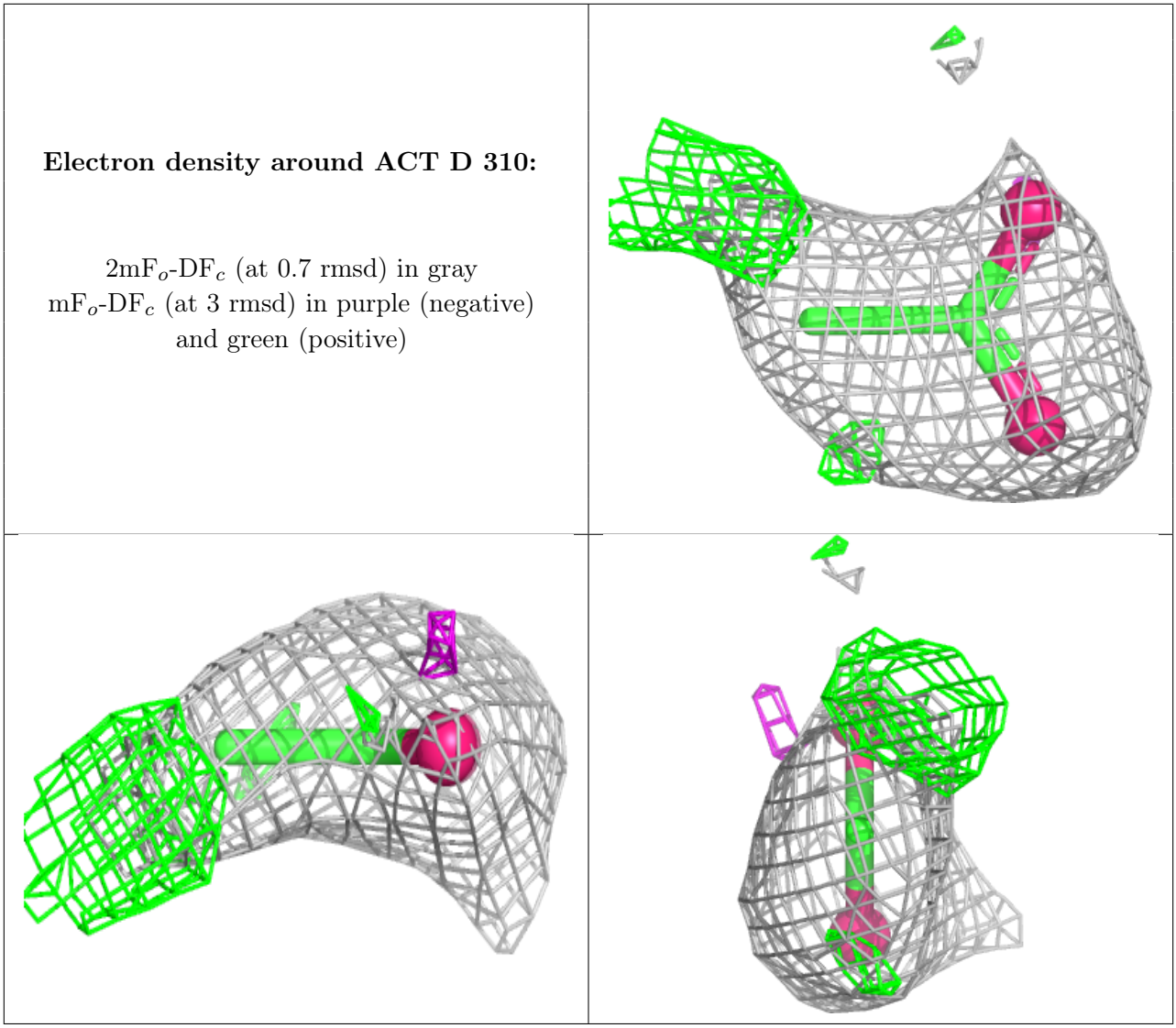






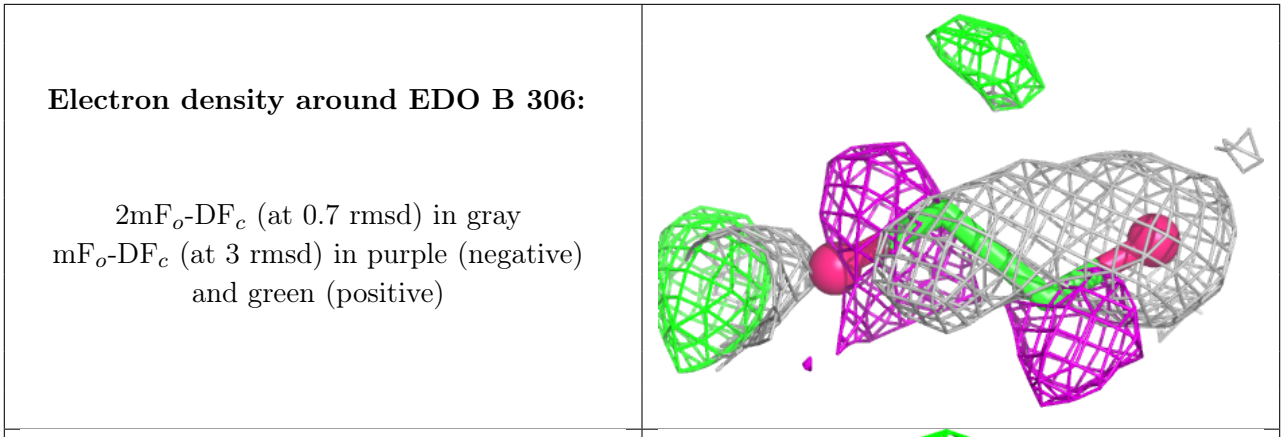
Electron density around ACT D 310:

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



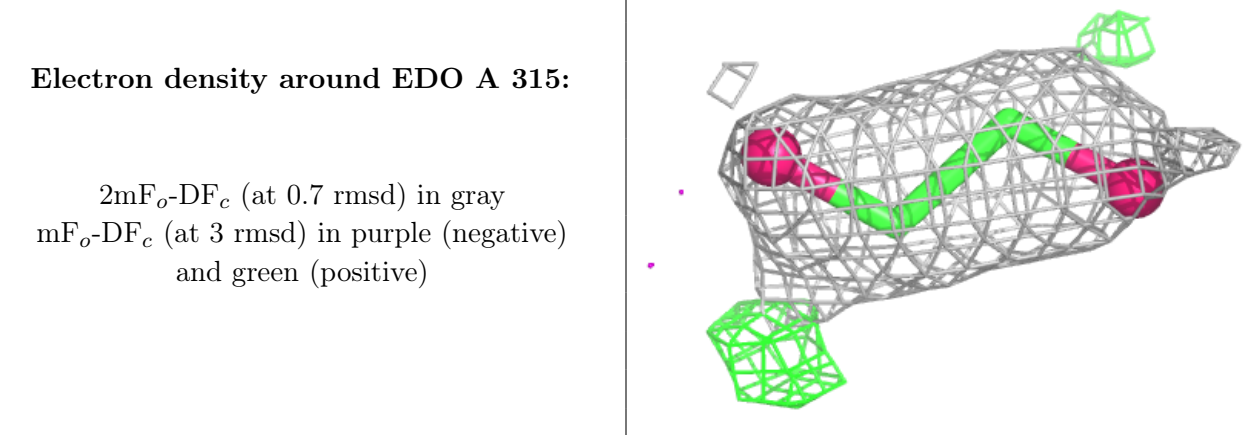
Electron density around EDO B 306:

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



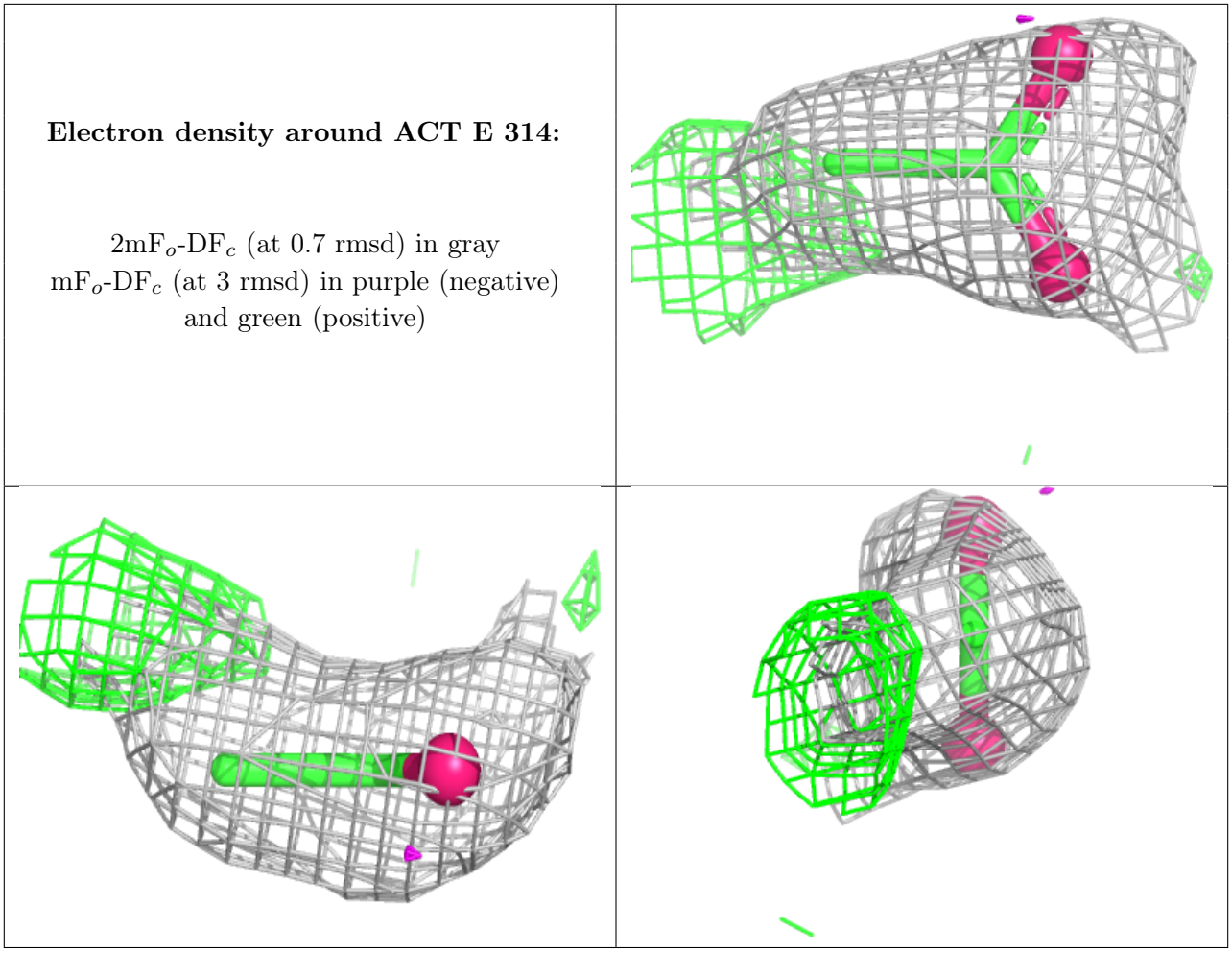
Electron density around EDO A 315:

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



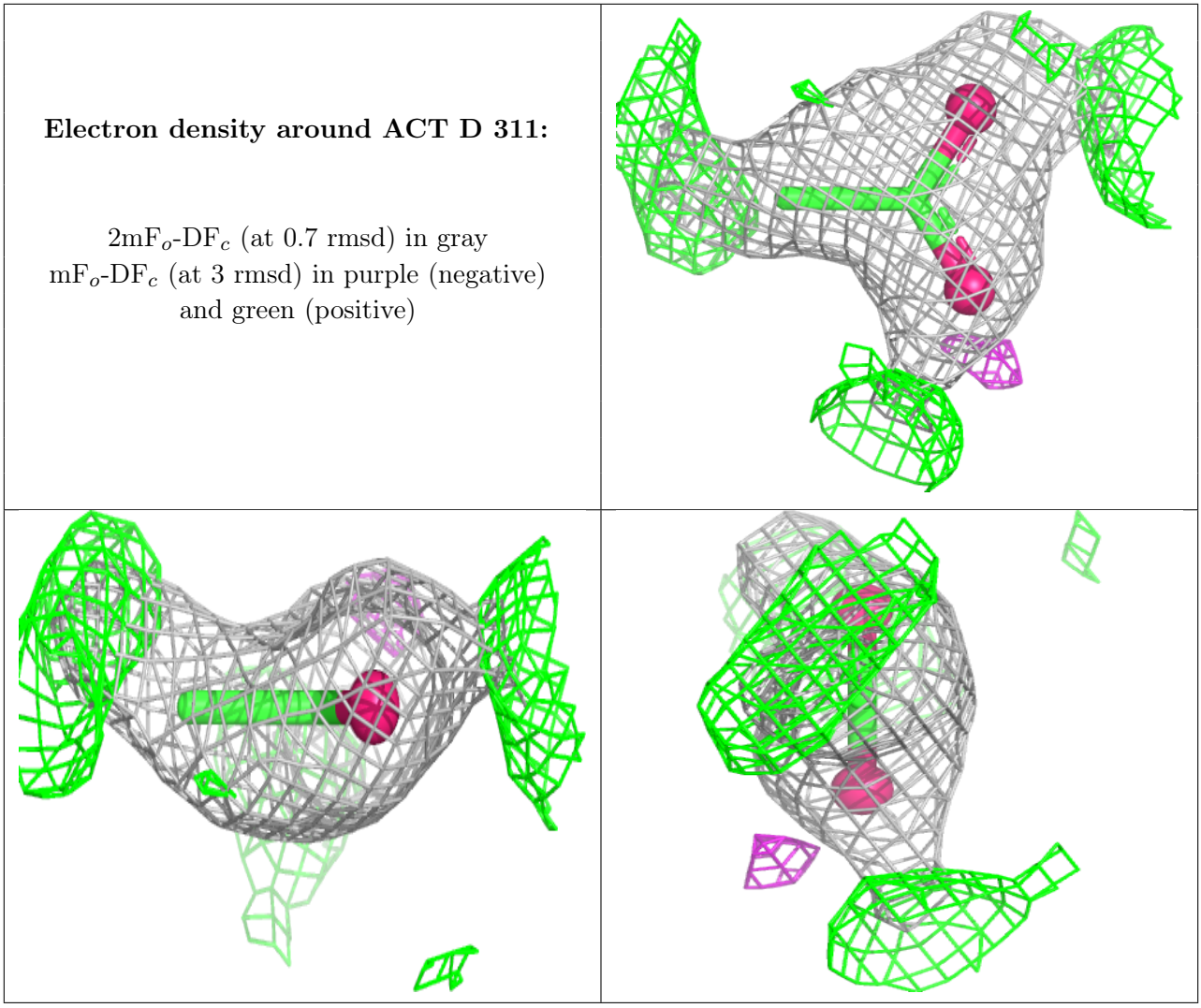
Electron density around ACT E 314:

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



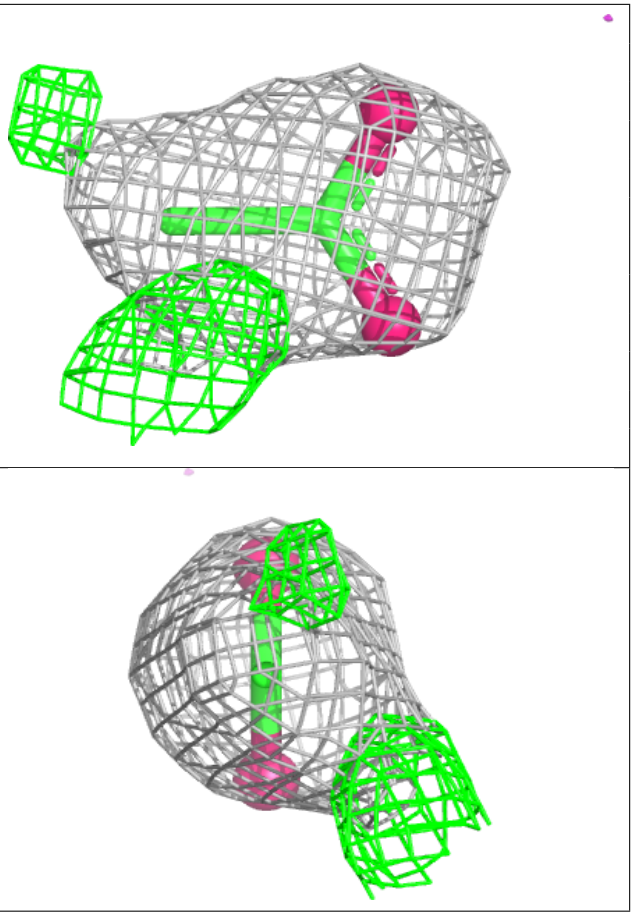
Electron density around ACT D 311:

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



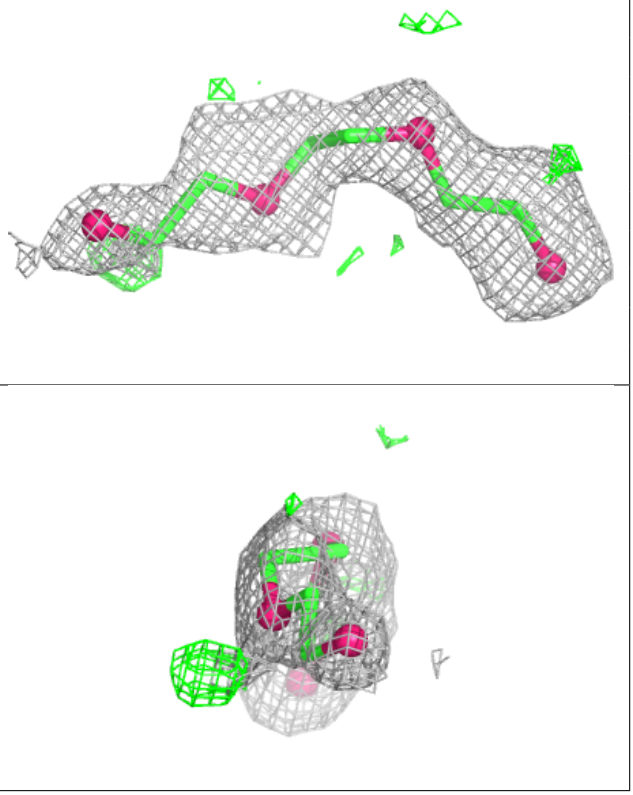
Electron density around ACT A 320:

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



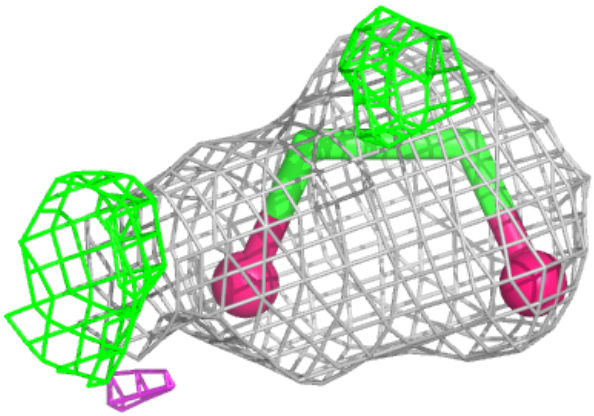
Electron density around PGE D 313:

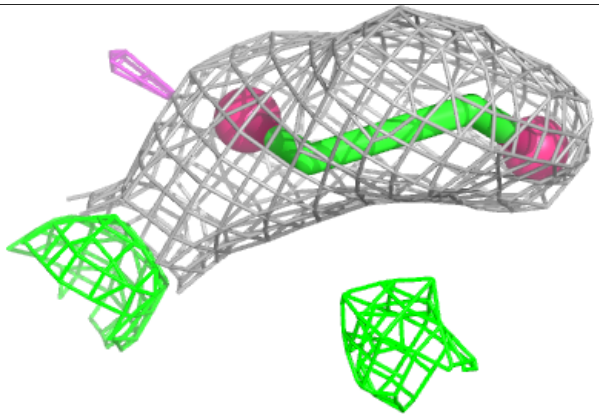
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

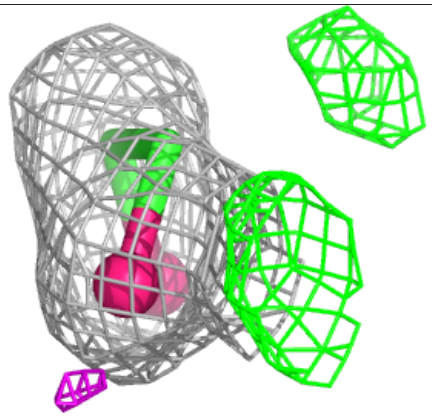


Electron density around EDO A 311:

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

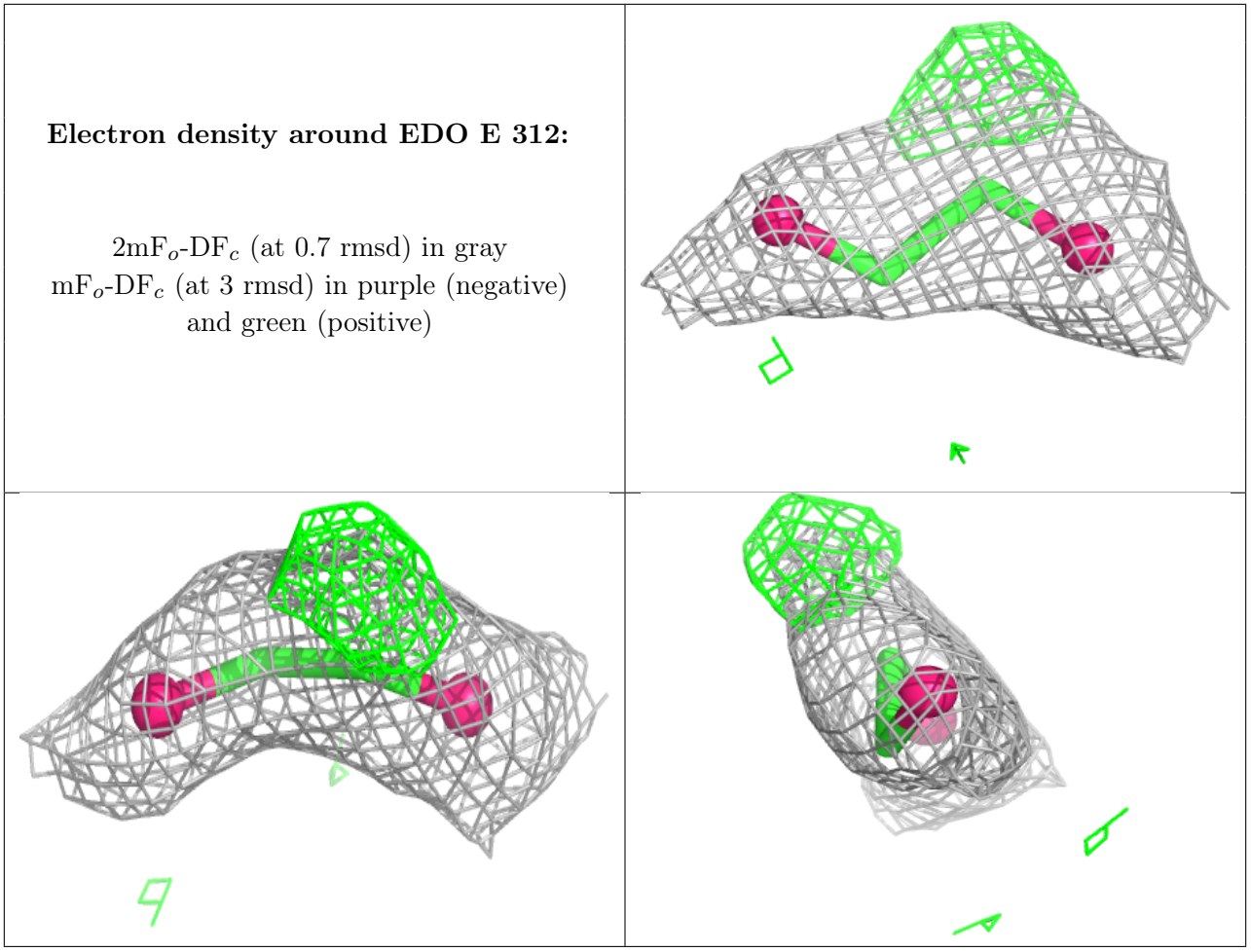






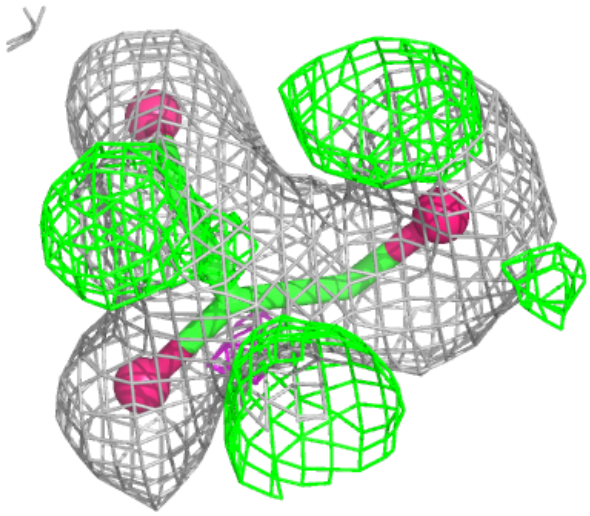
Electron density around EDO E 312:

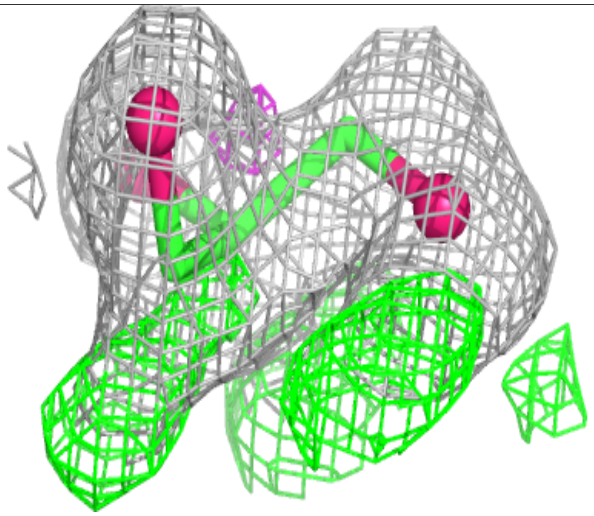
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

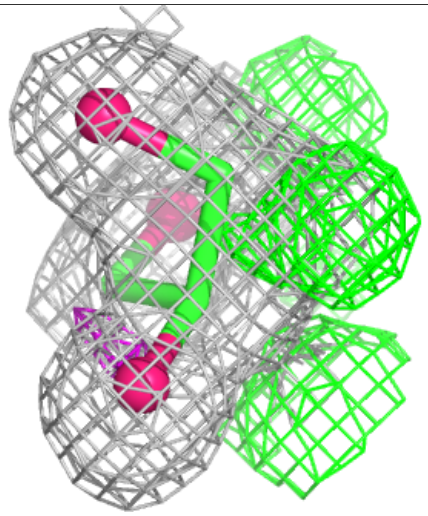


Electron density around GOL C 311:

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

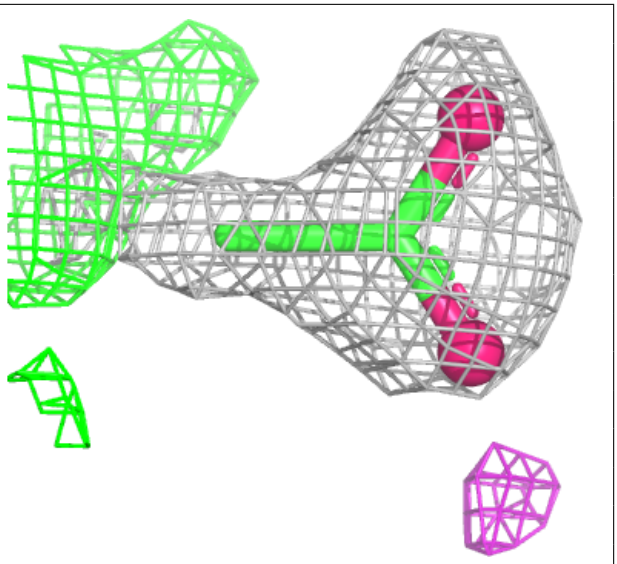


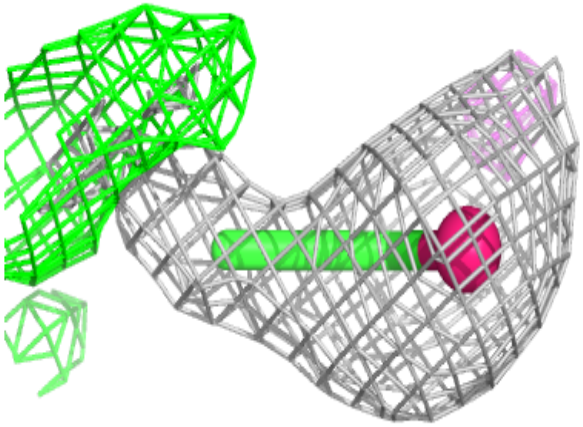


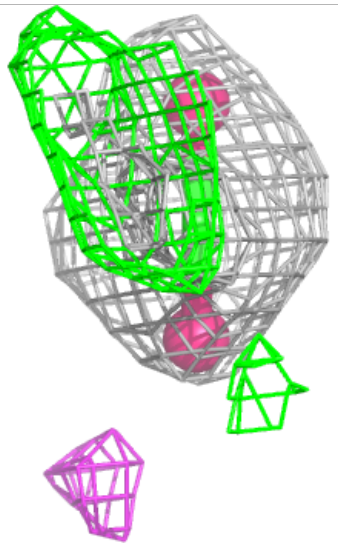


Electron density around ACT B 315:

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

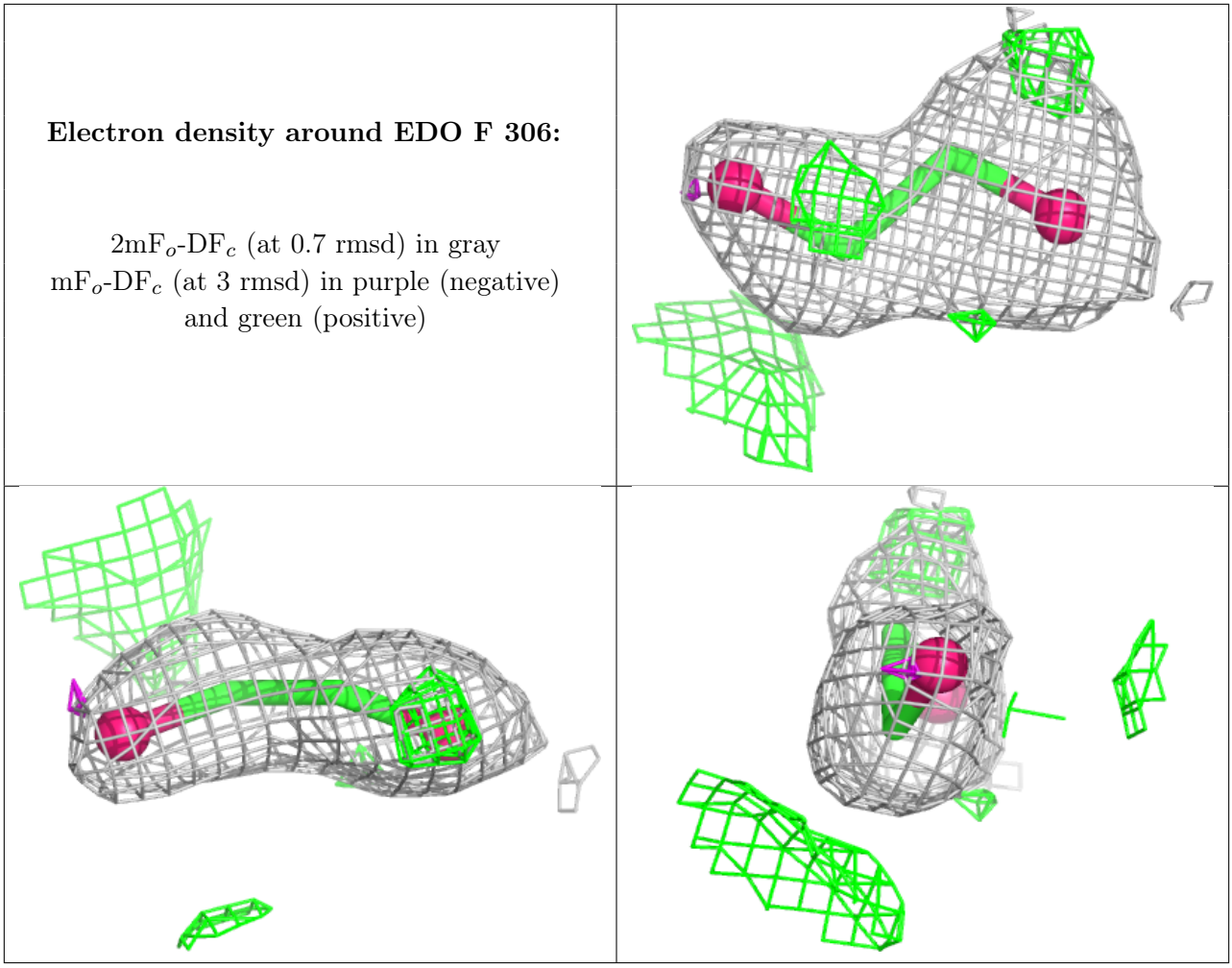






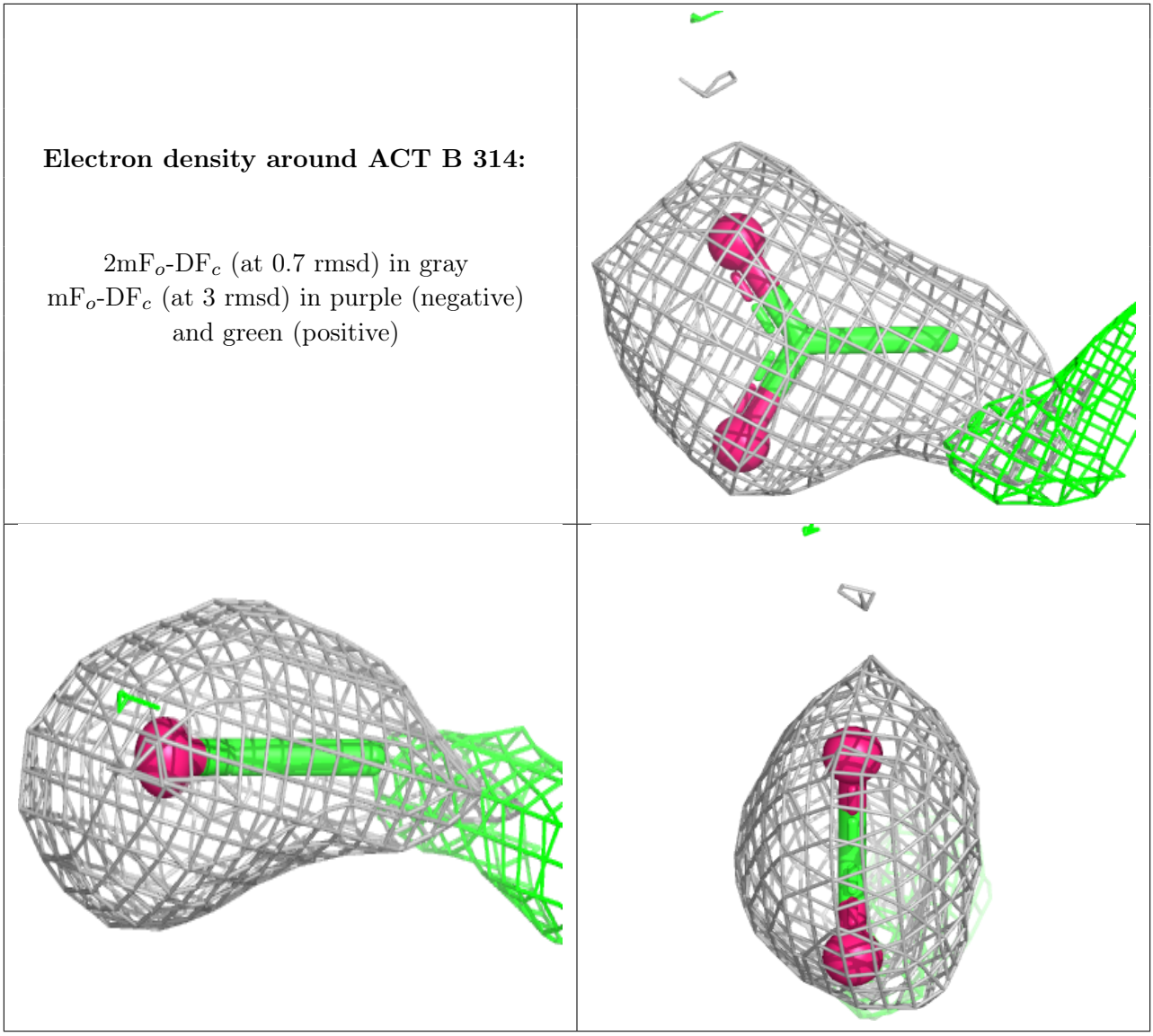
Electron density around EDO F 306:

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



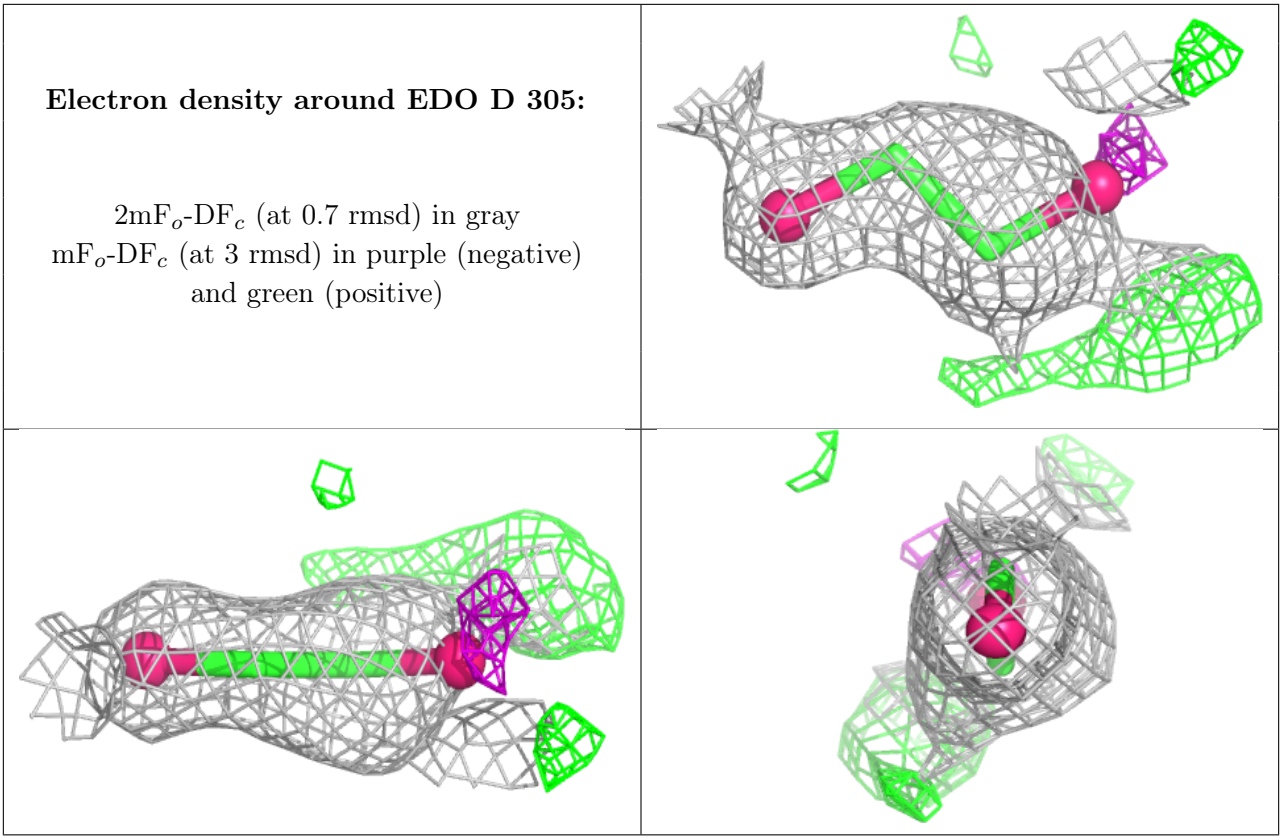
Electron density around ACT B 314:

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



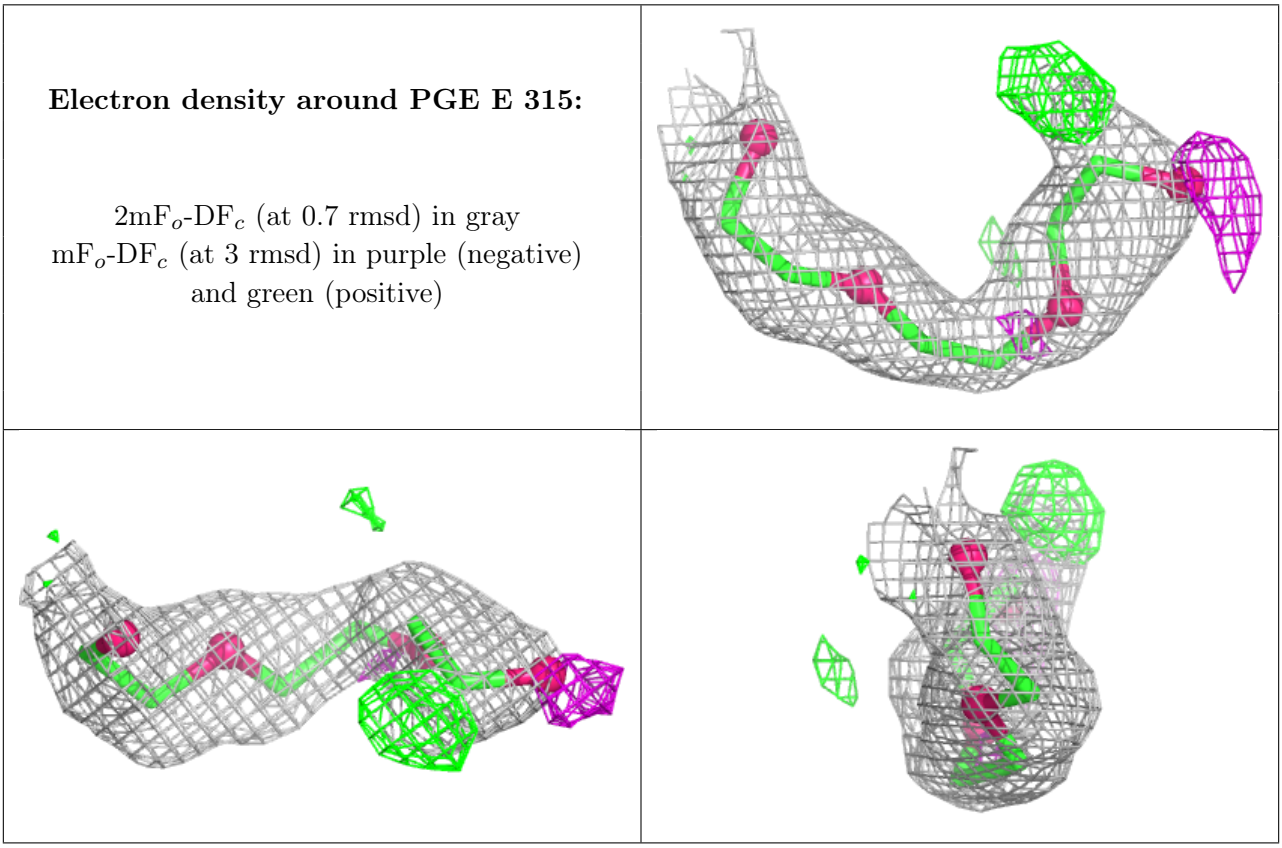
Electron density around EDO D 305:

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



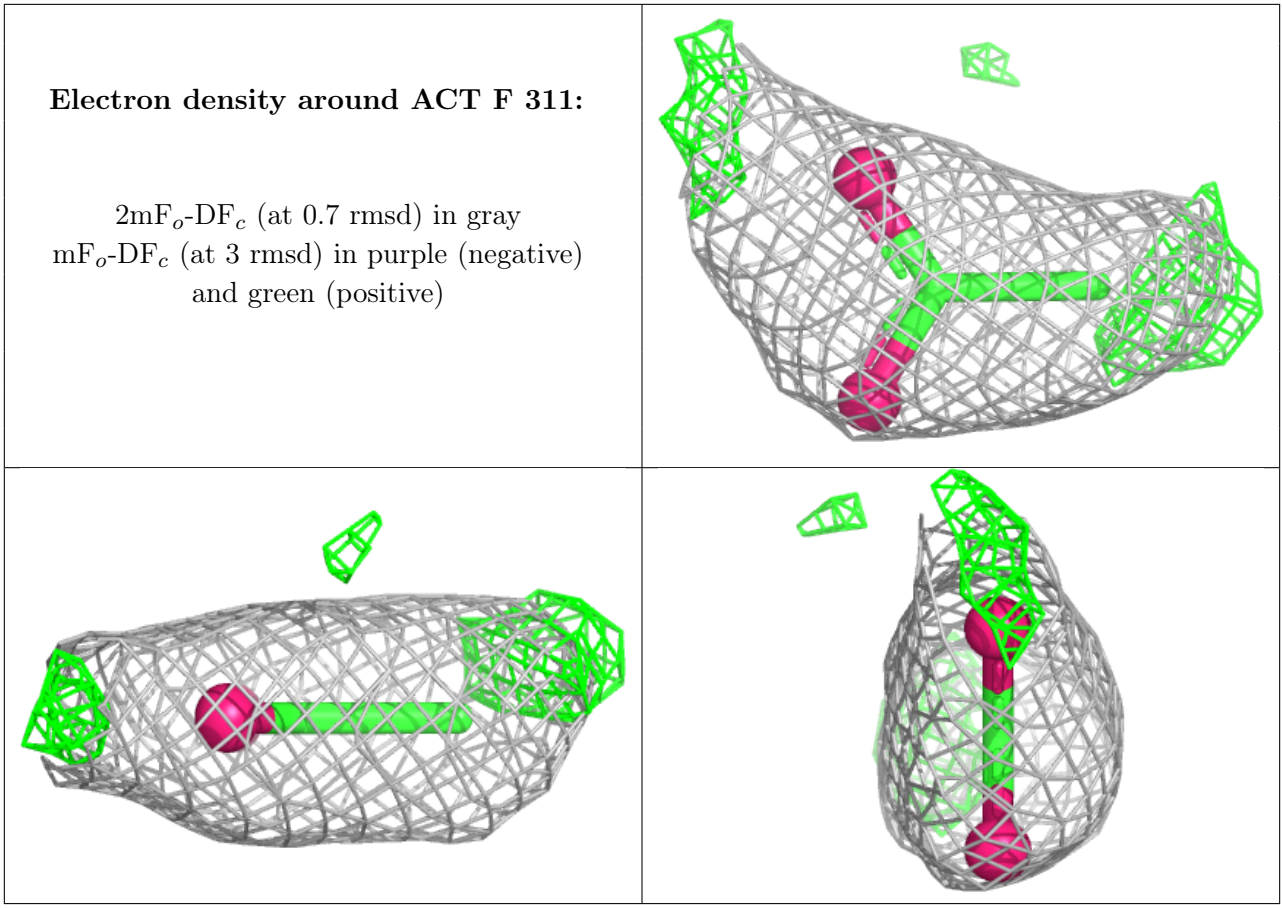
Electron density around PGE E 315:

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



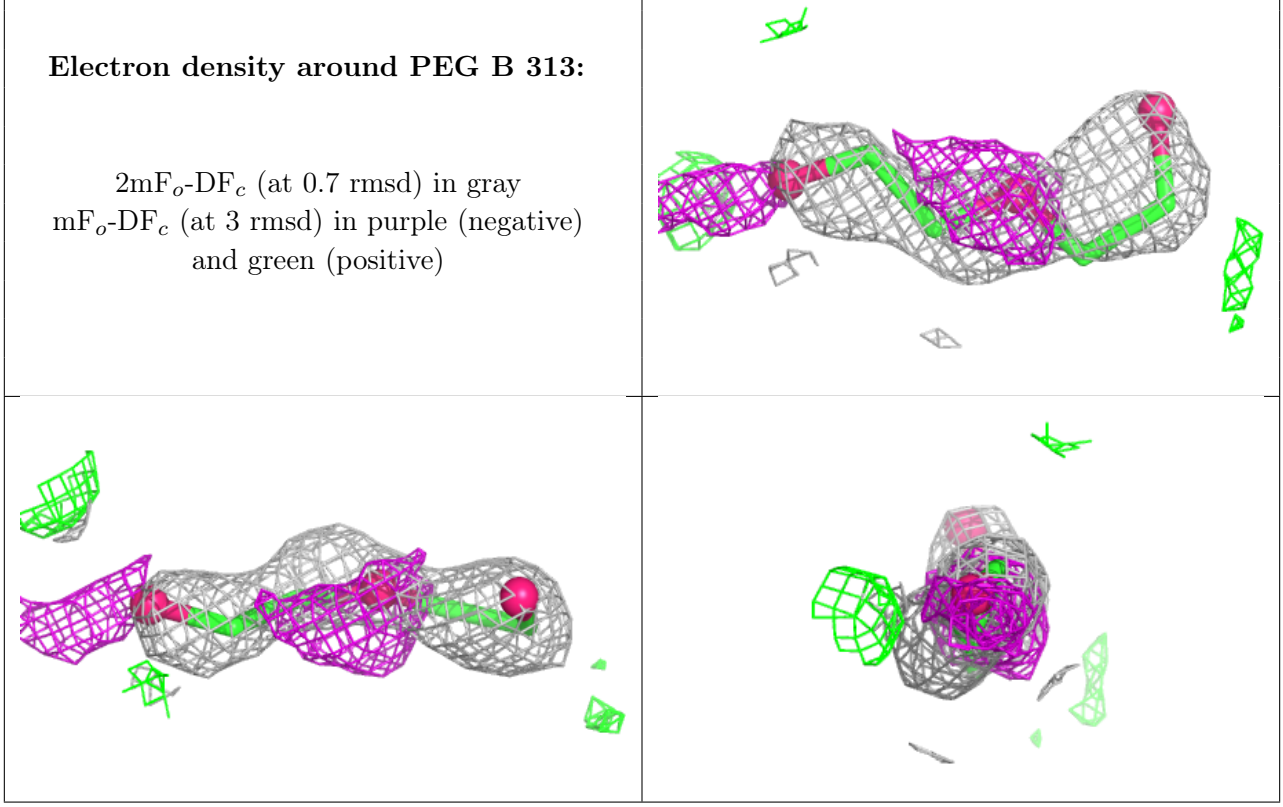
Electron density around ACT F 311:

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



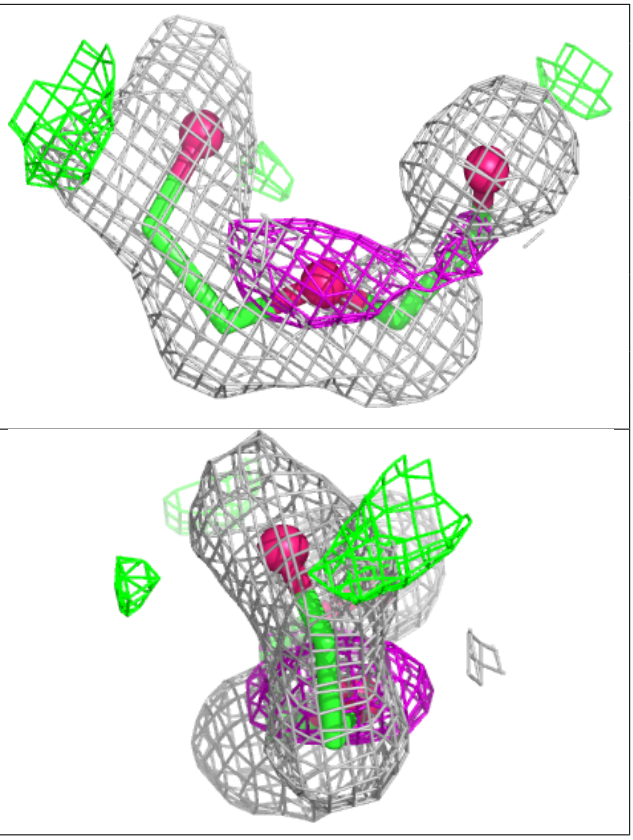
Electron density around PEG B 313:

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



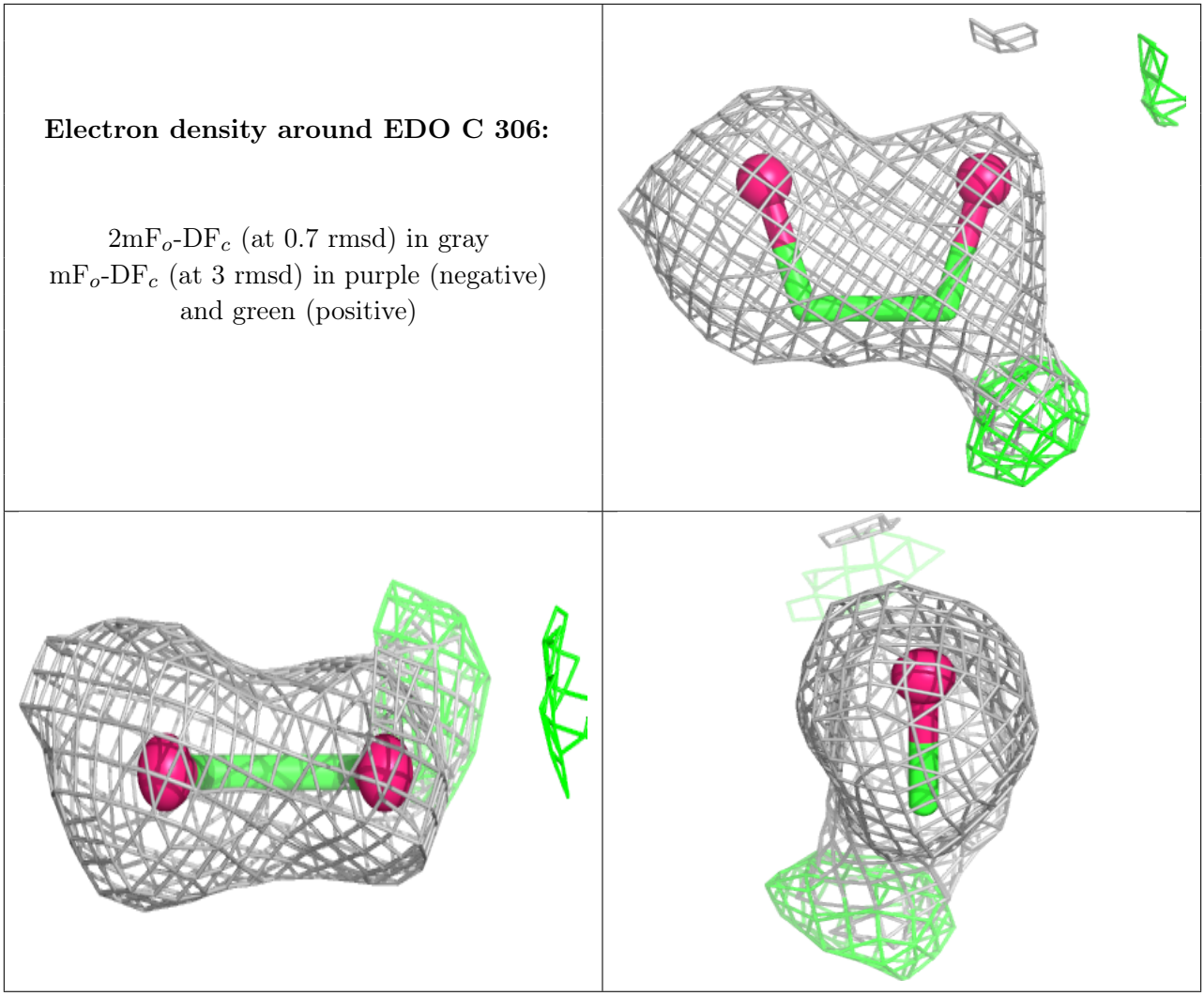
Electron density around PEG E 313:

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



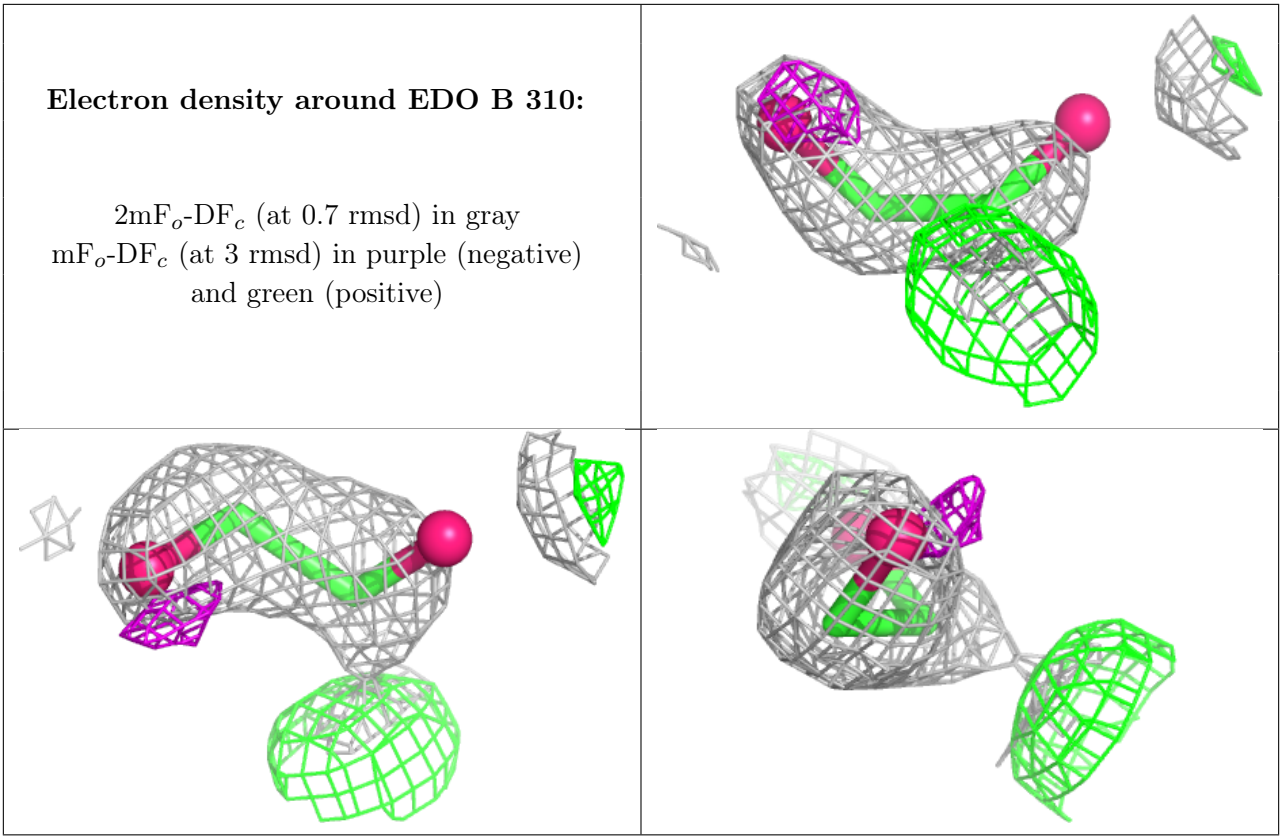
Electron density around EDO C 306:

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



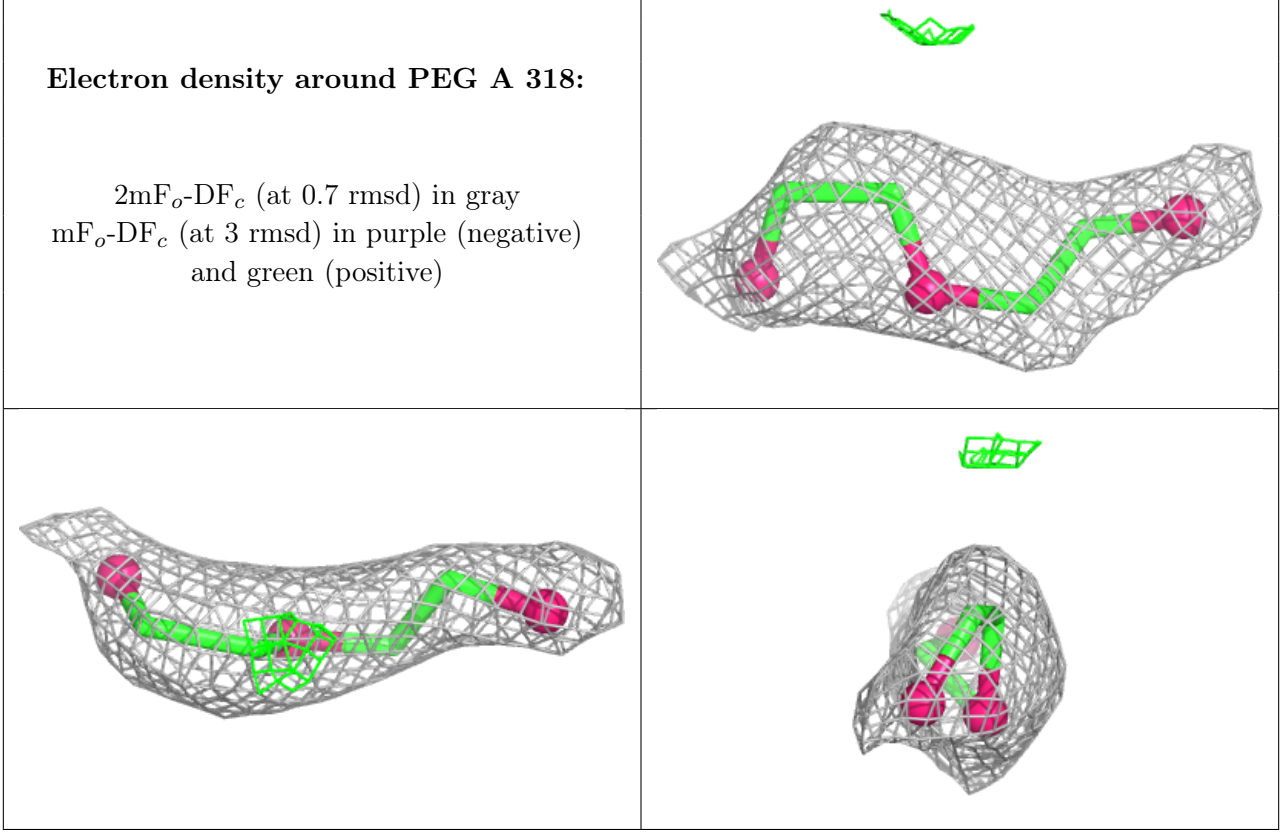
Electron density around EDO B 310:

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



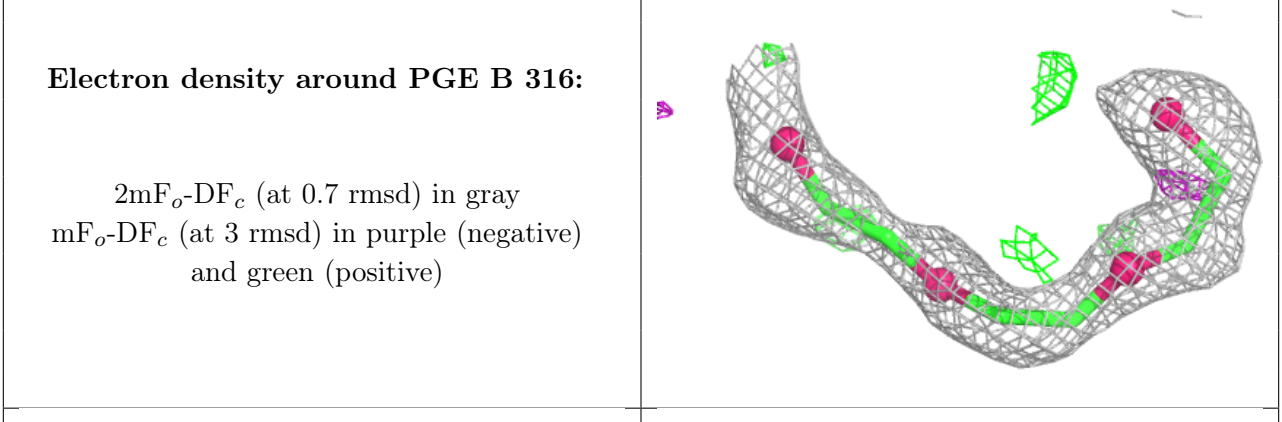
Electron density around PEG A 318:

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



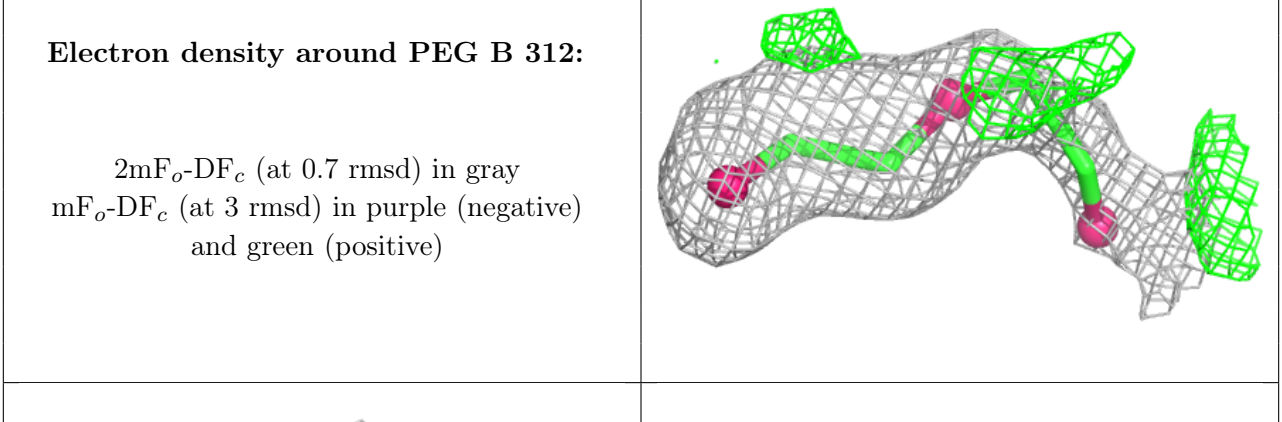
Electron density around PGE B 316:

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



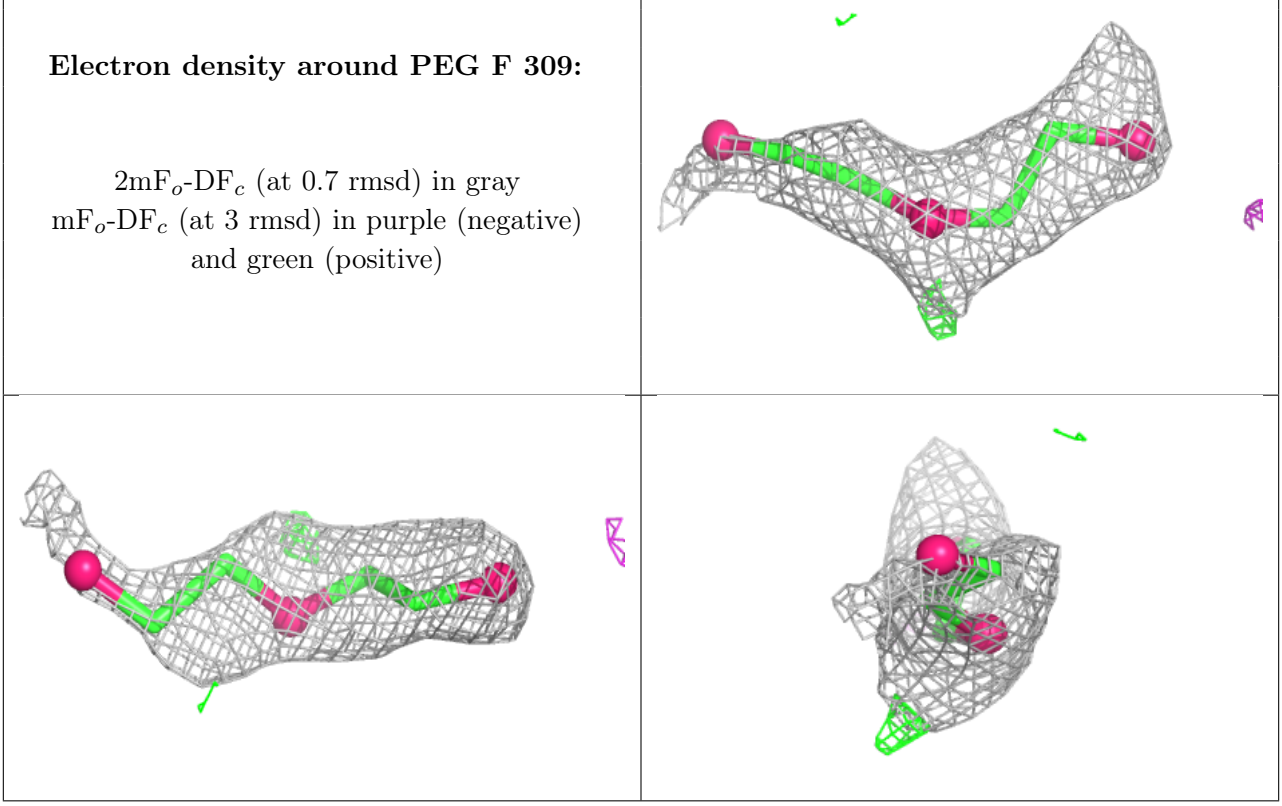
Electron density around PEG B 312:

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



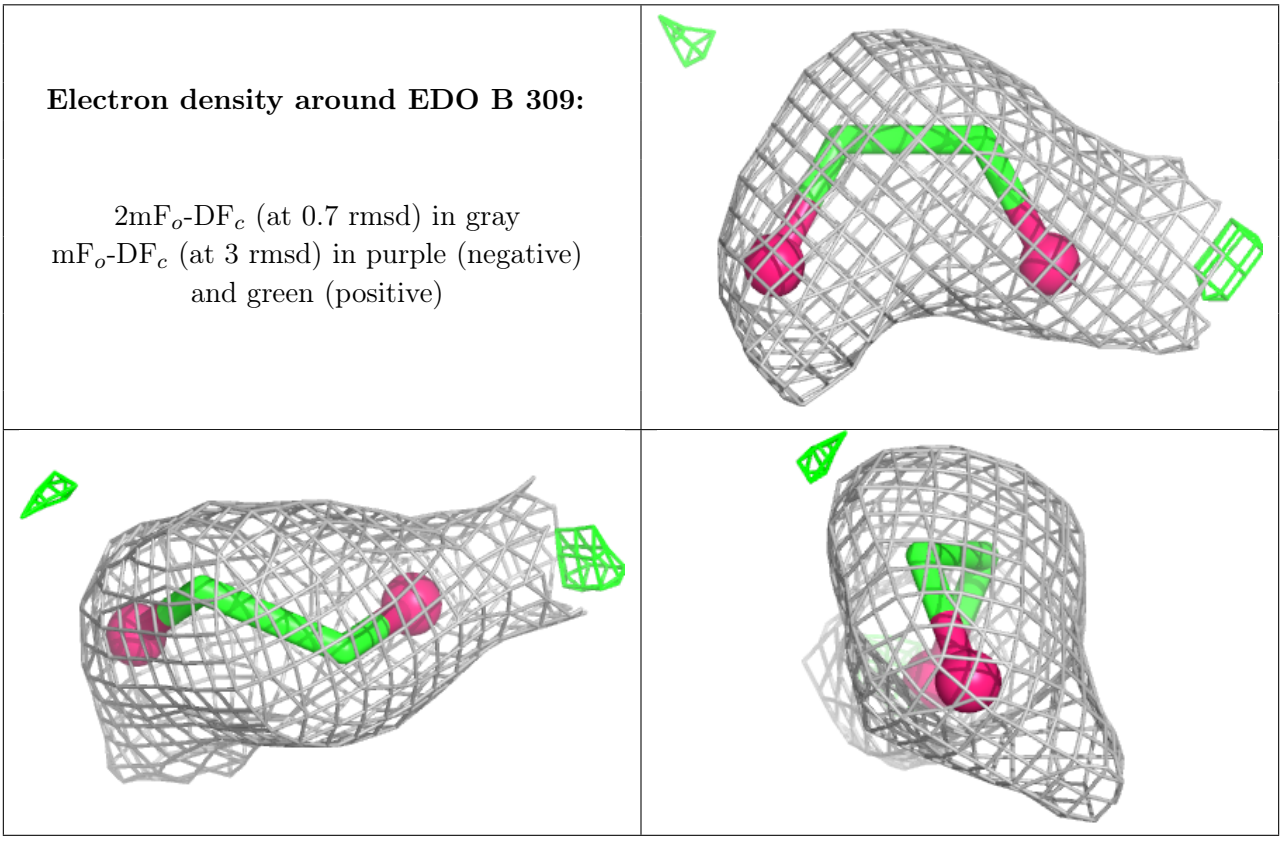
Electron density around PEG F 309:

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



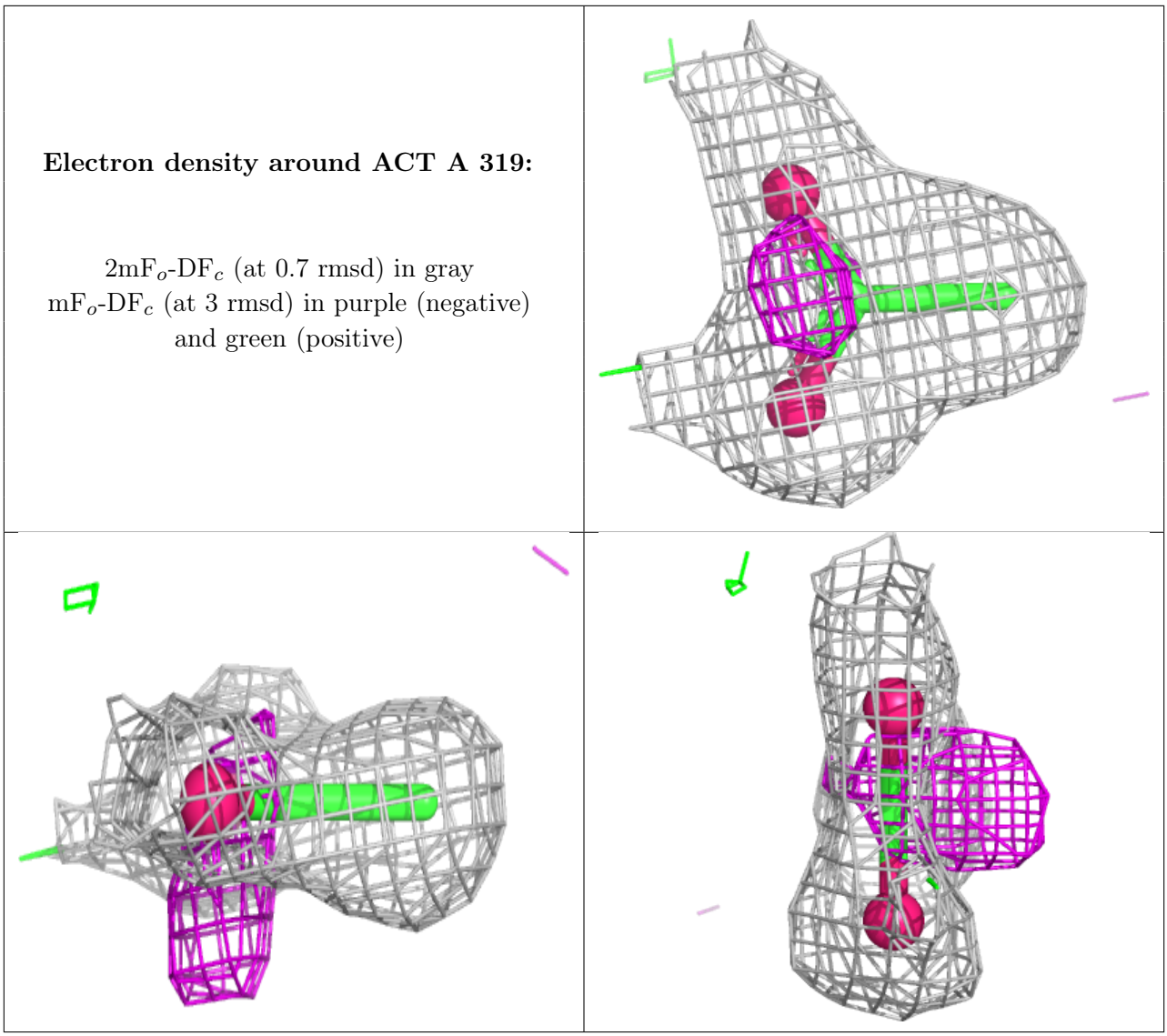
Electron density around EDO B 309:

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



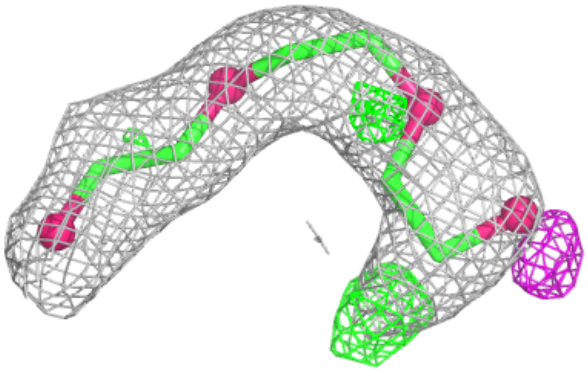
Electron density around ACT A 319:

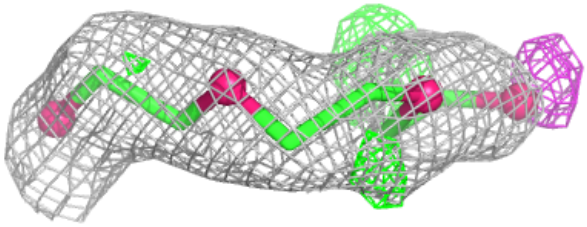
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

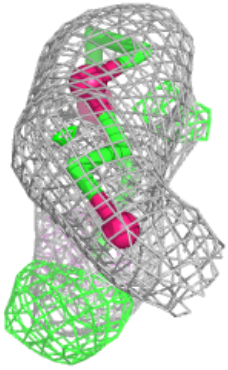


Electron density around PGE D 314:

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

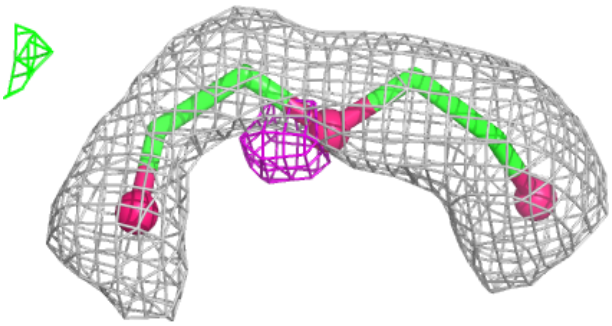


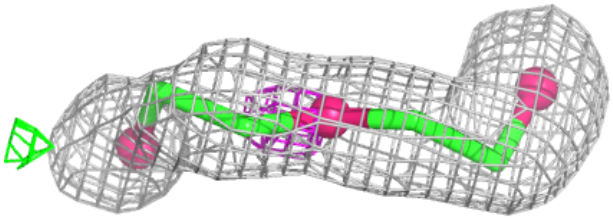


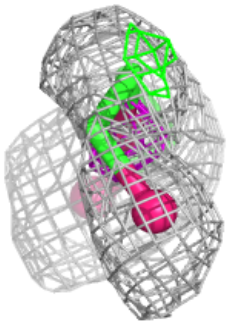


Electron density around PEG F 308:

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

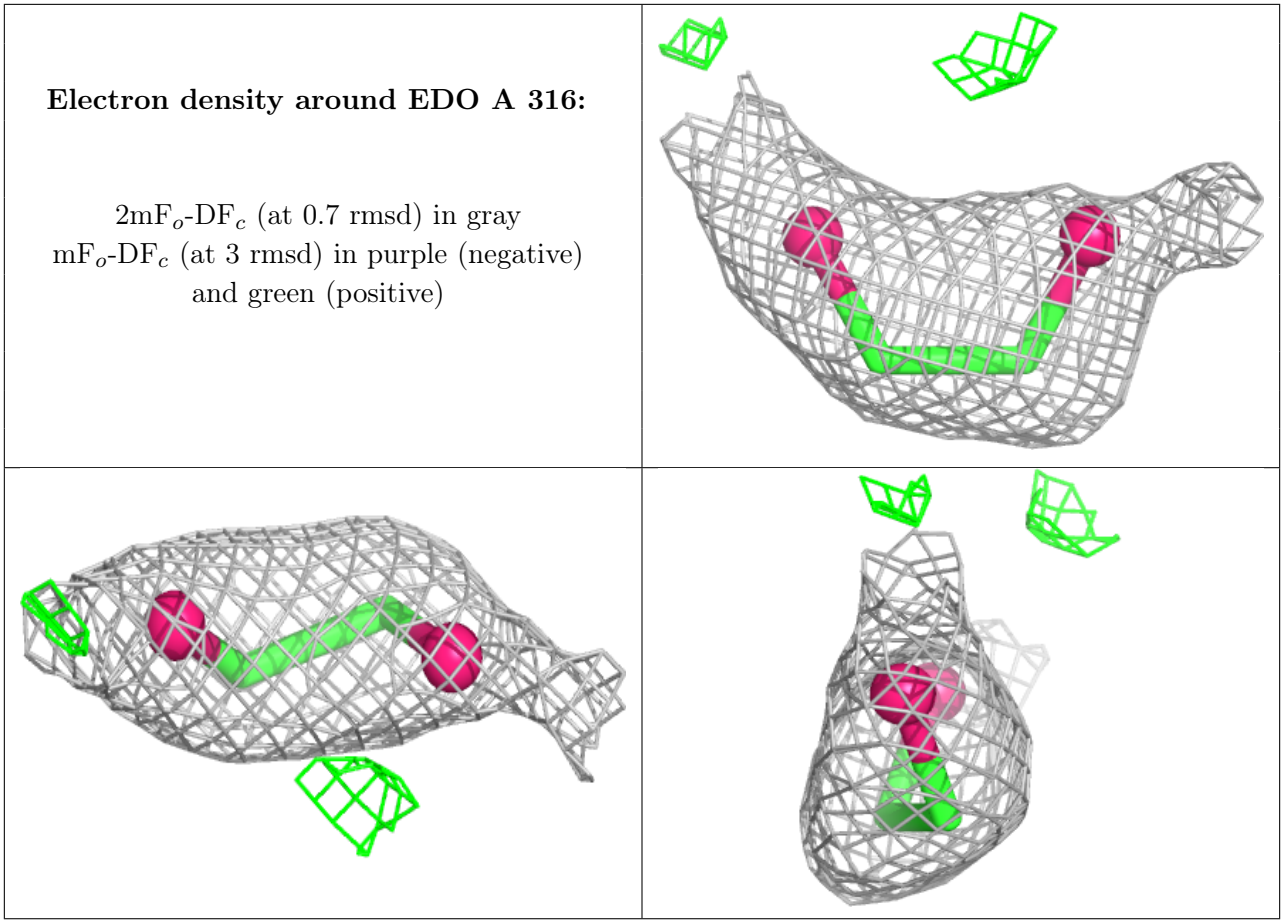






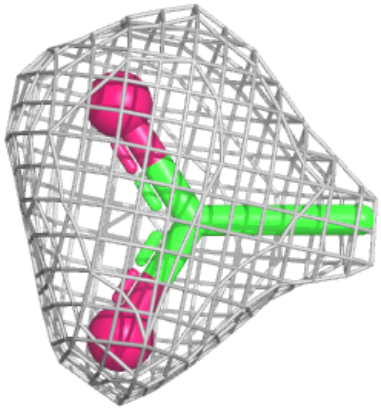
Electron density around EDO A 316:

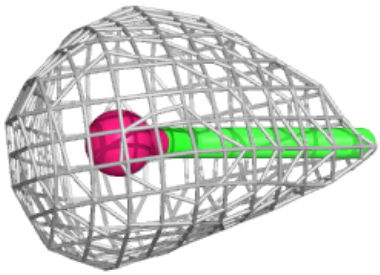
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

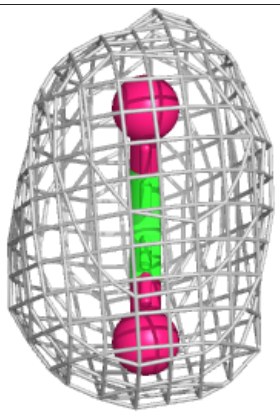


Electron density around ACT D 312:

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

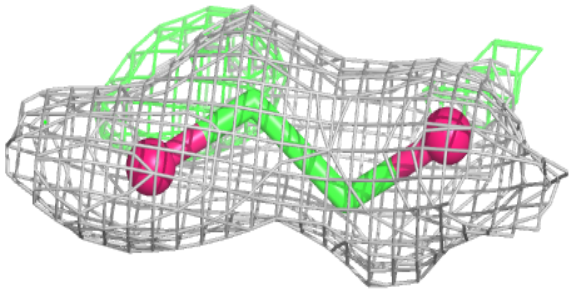


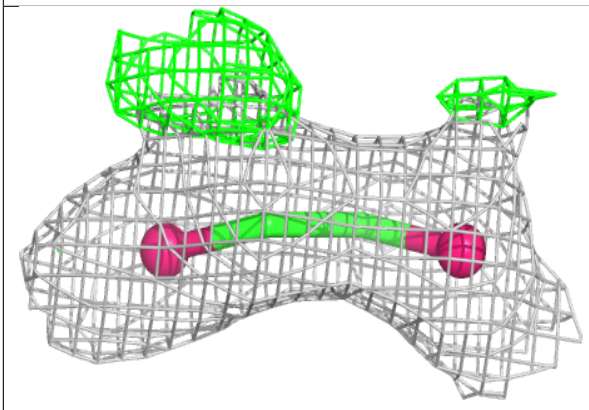


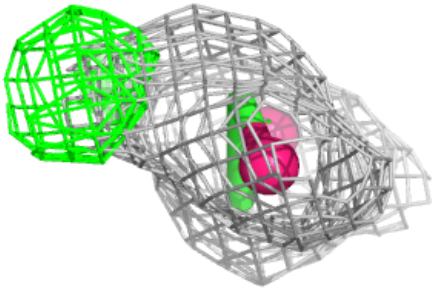


Electron density around EDO A 307:

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

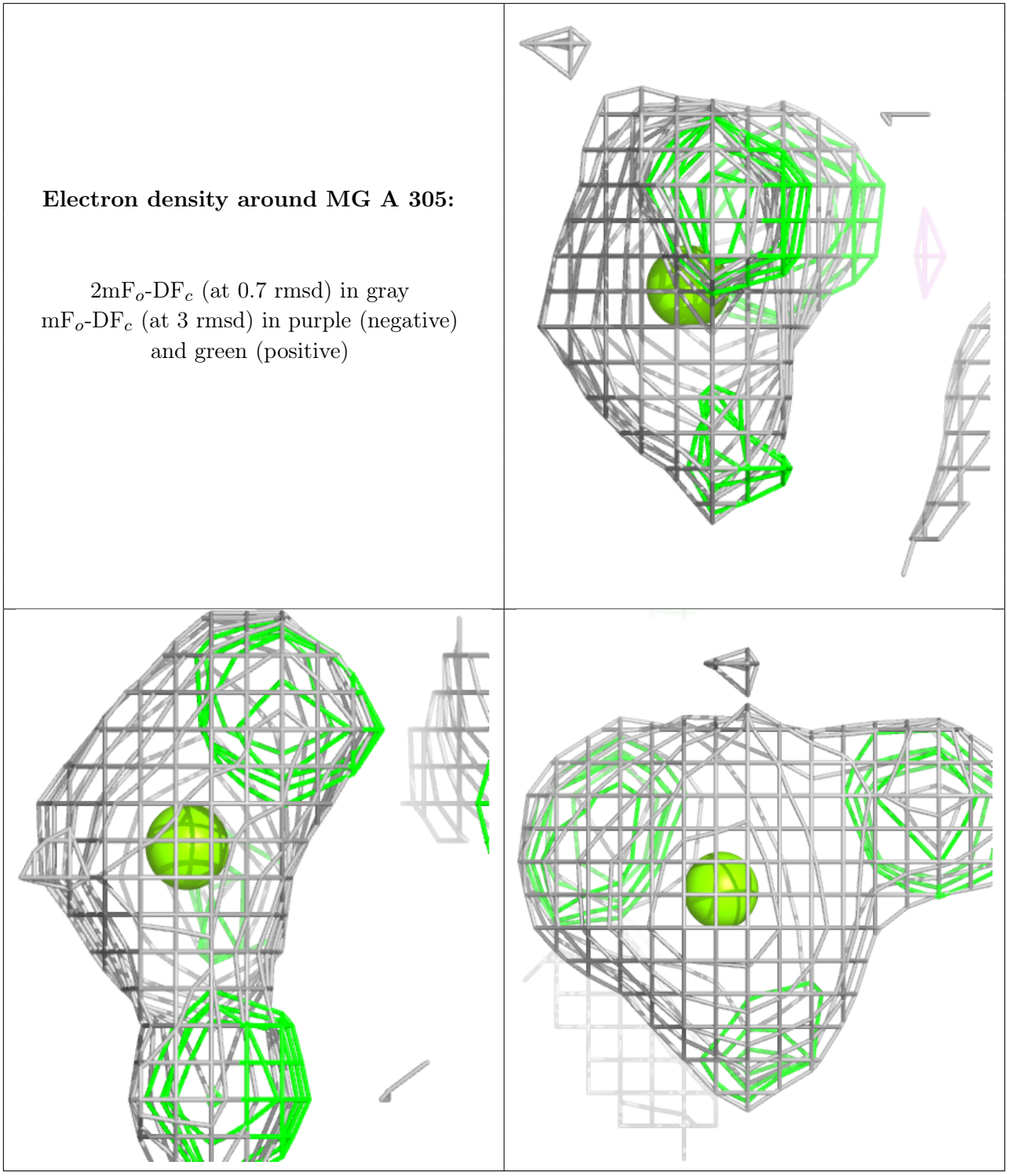






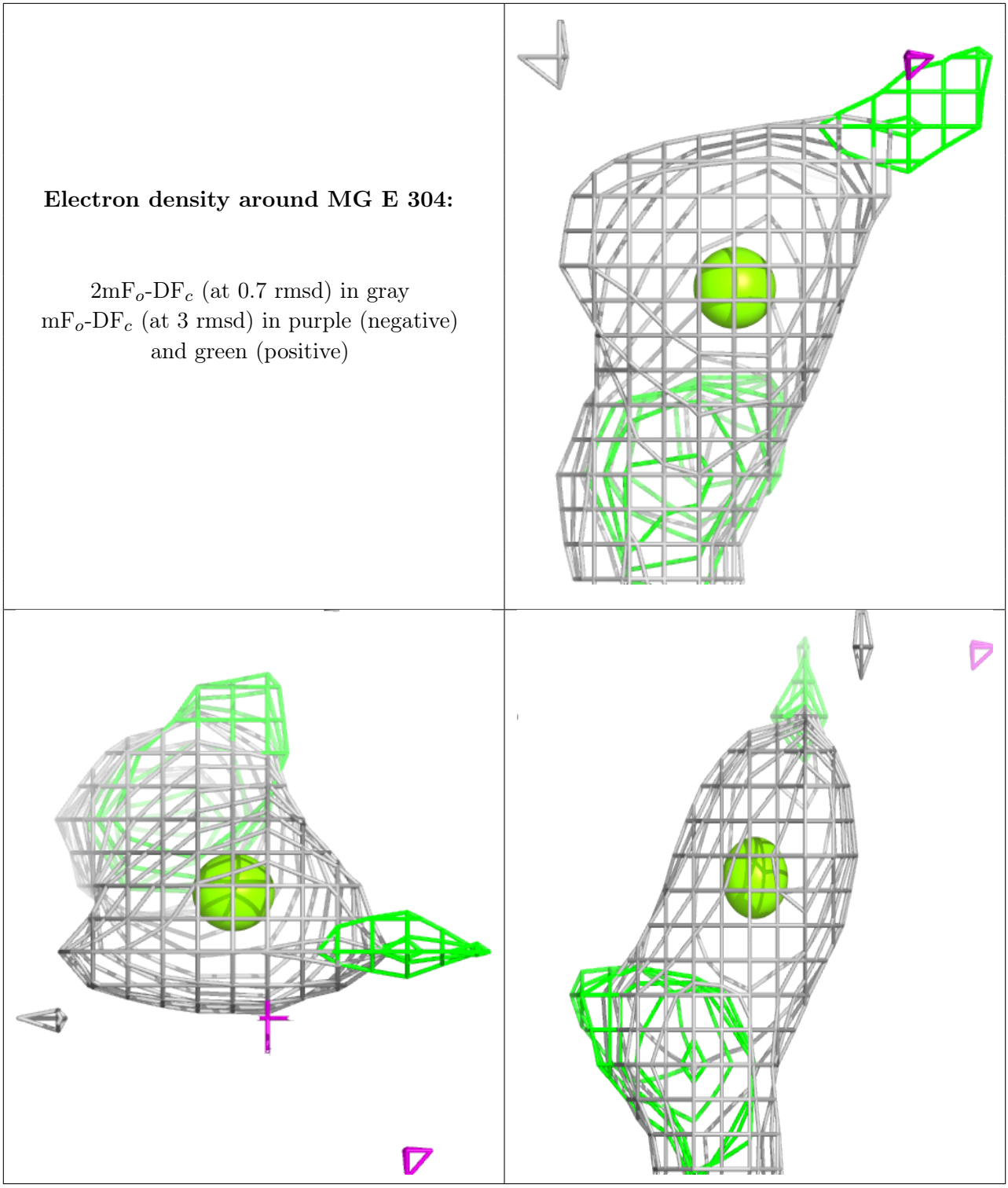
Electron density around MG A 305:

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



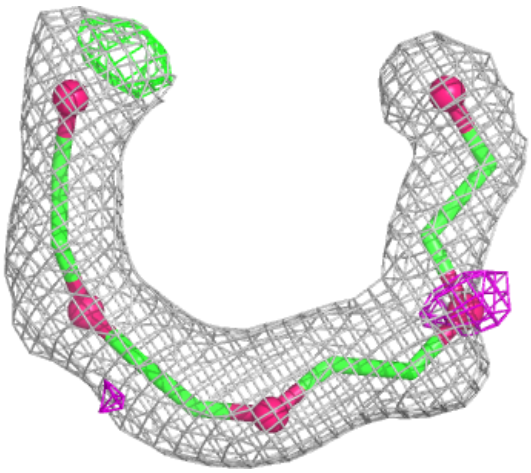
Electron density around MG E 304:

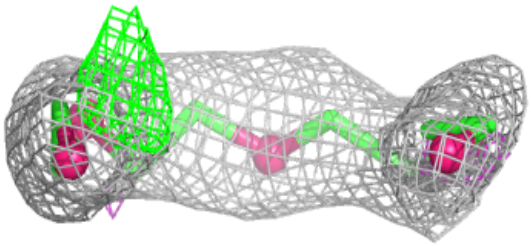
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

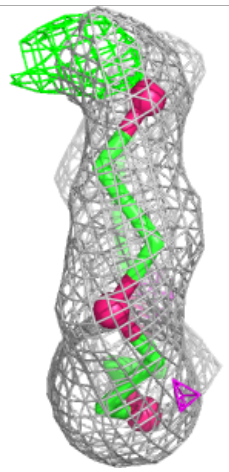


Electron density around PG4 E 306:

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

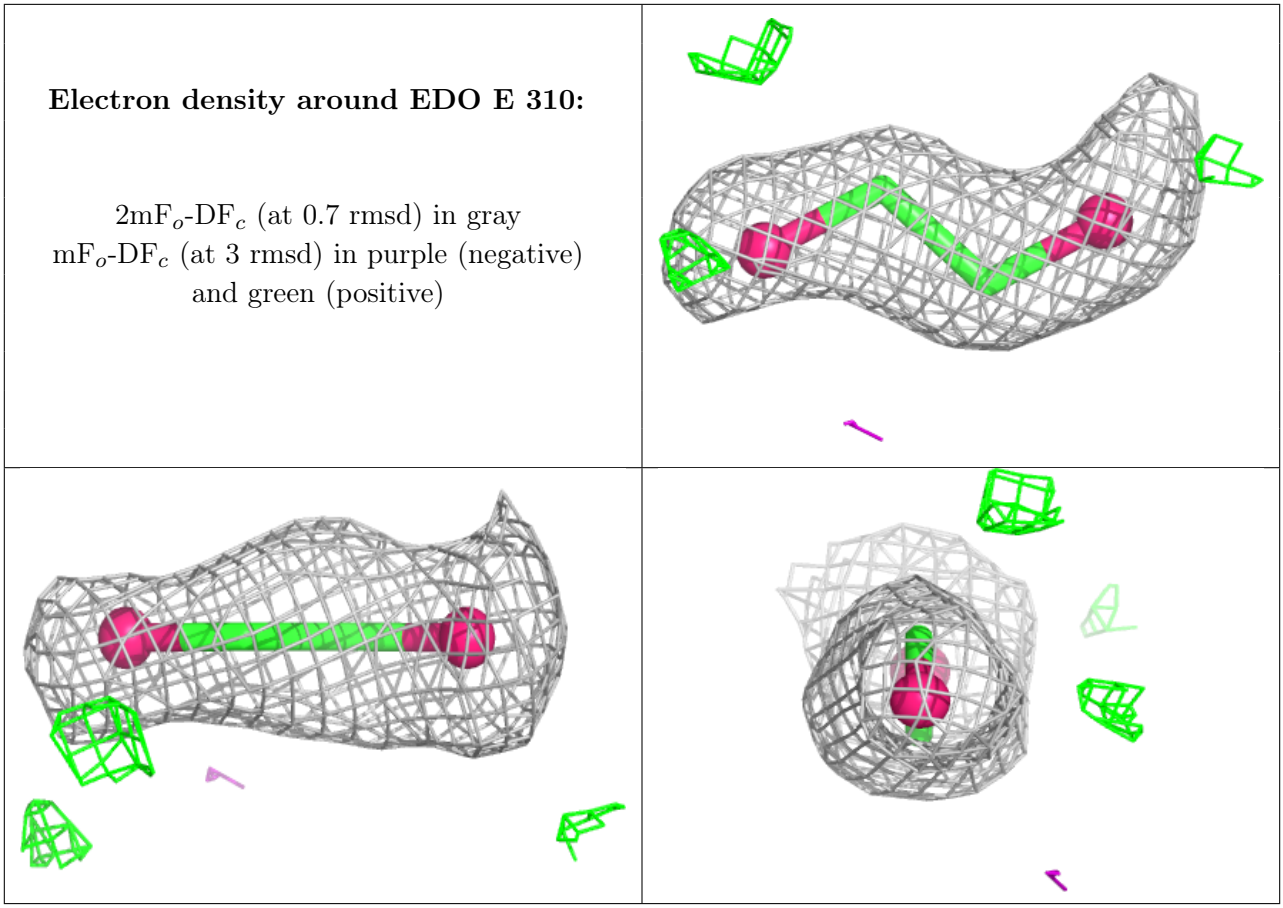






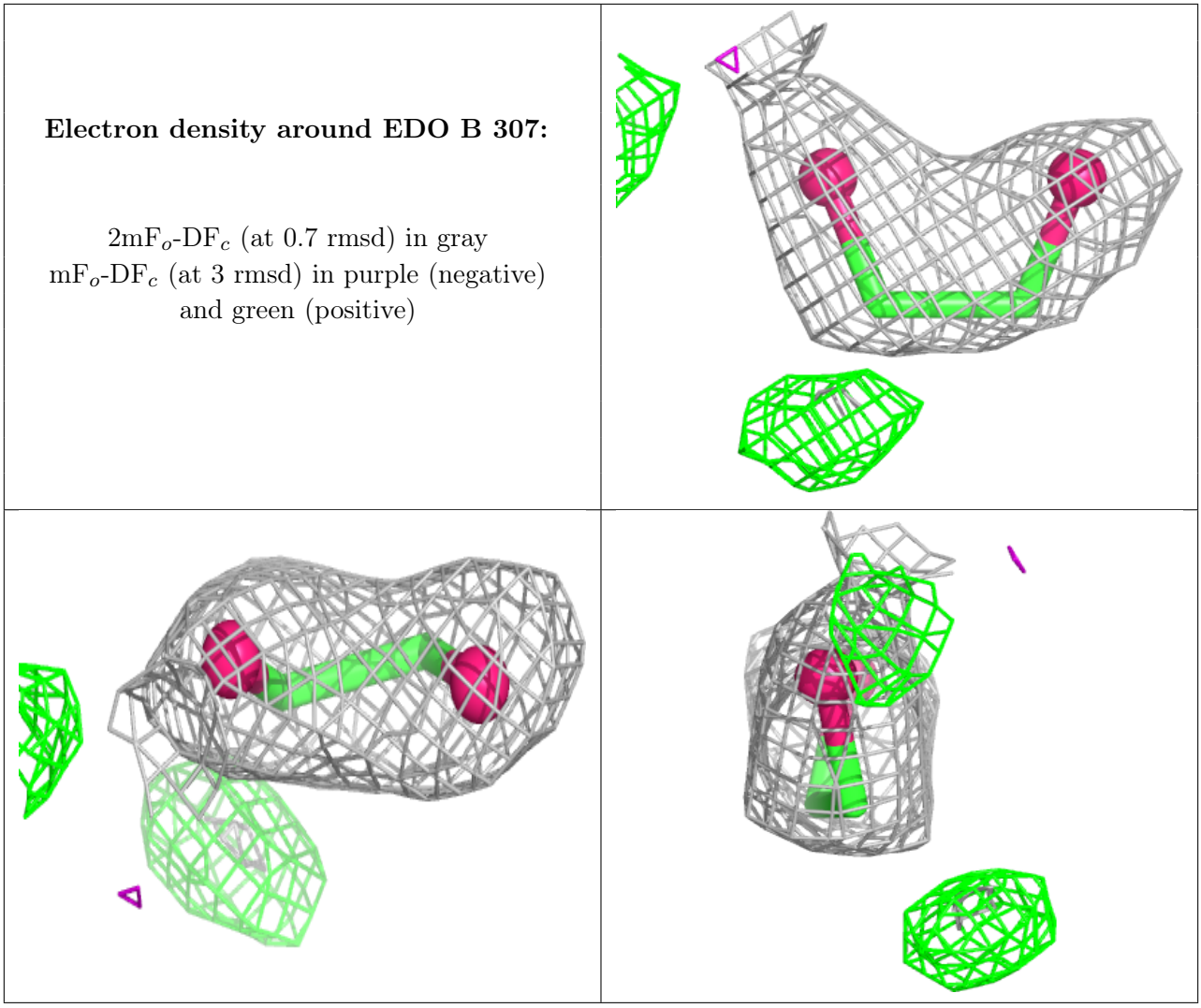
Electron density around EDO E 310:

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



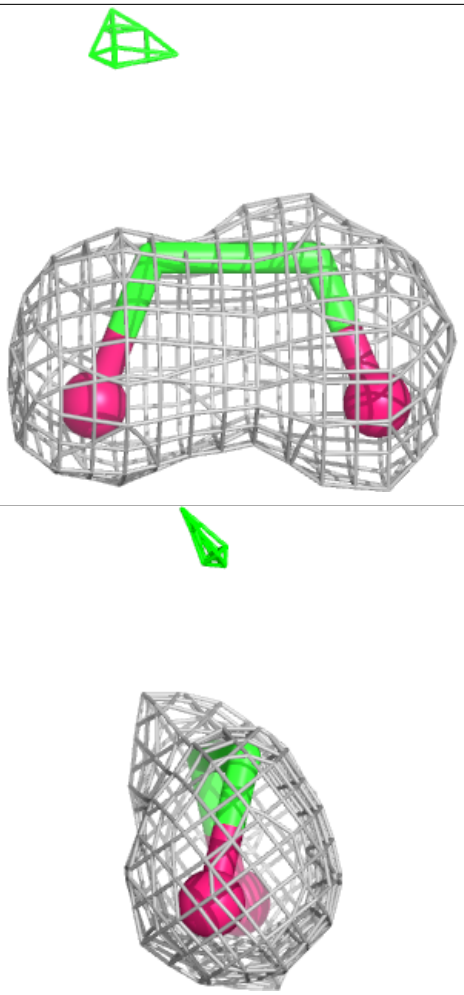
Electron density around EDO B 307:

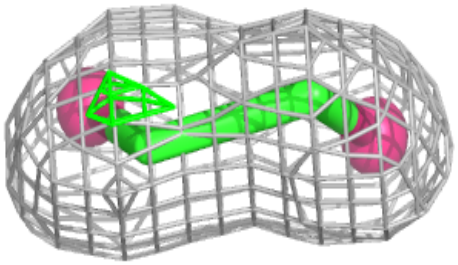
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO E 309:

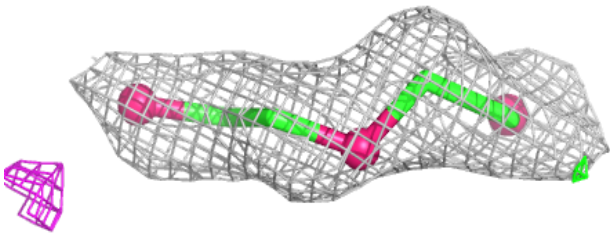
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

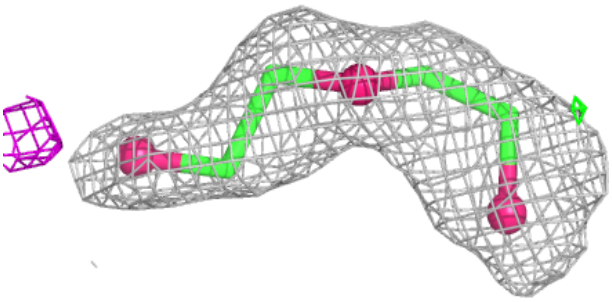


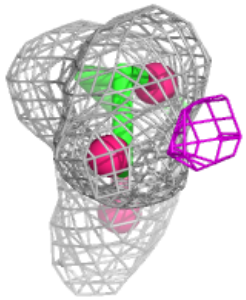


Electron density around PEG B 311:

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

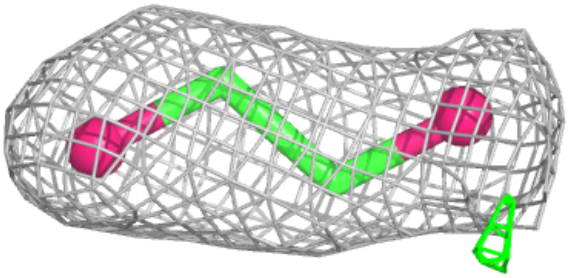


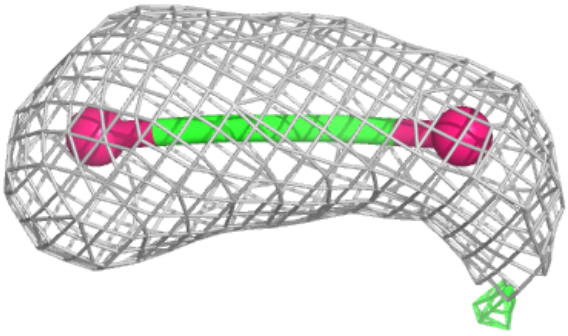


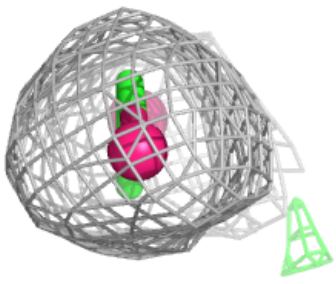


Electron density around EDO A 310:

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

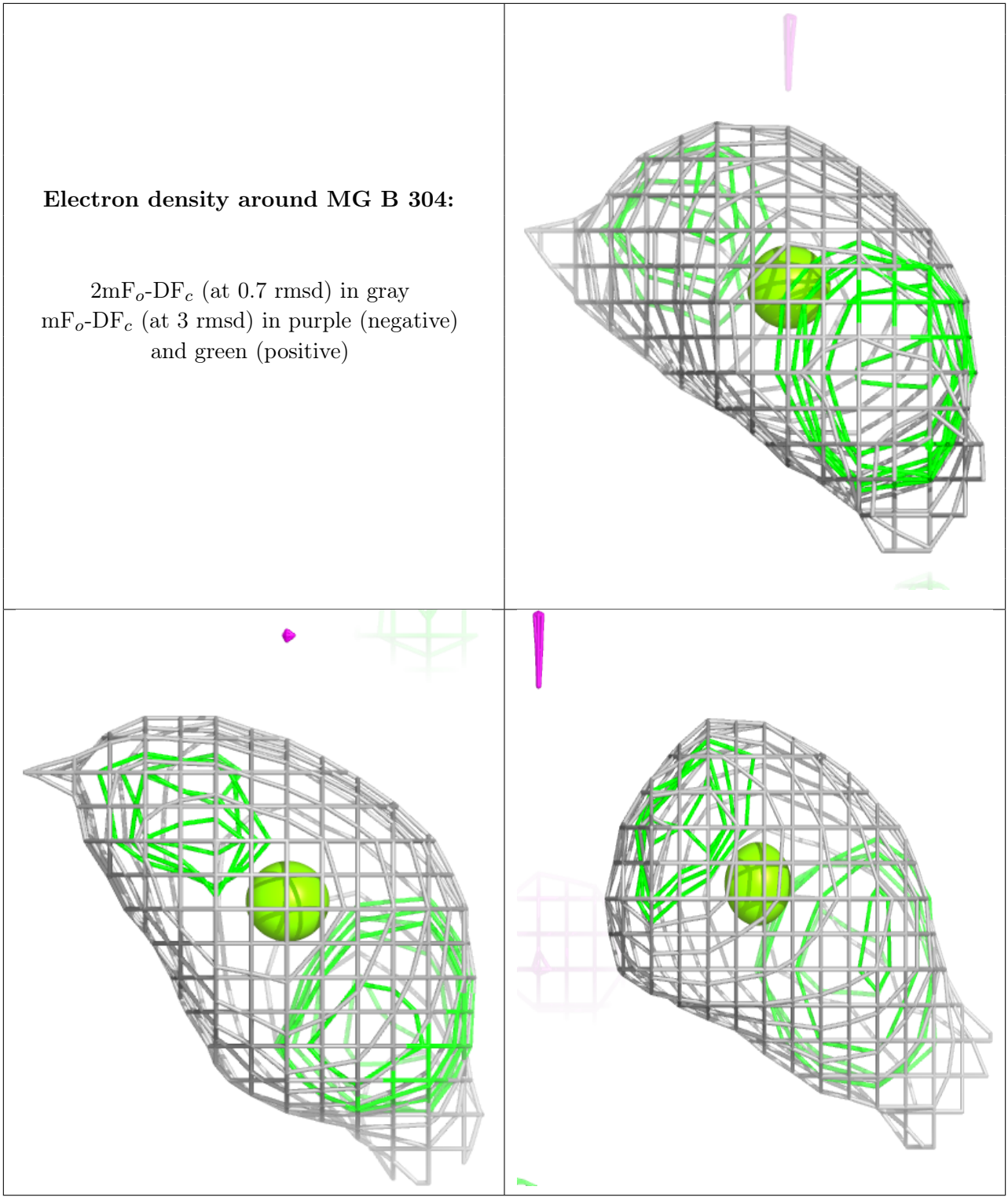






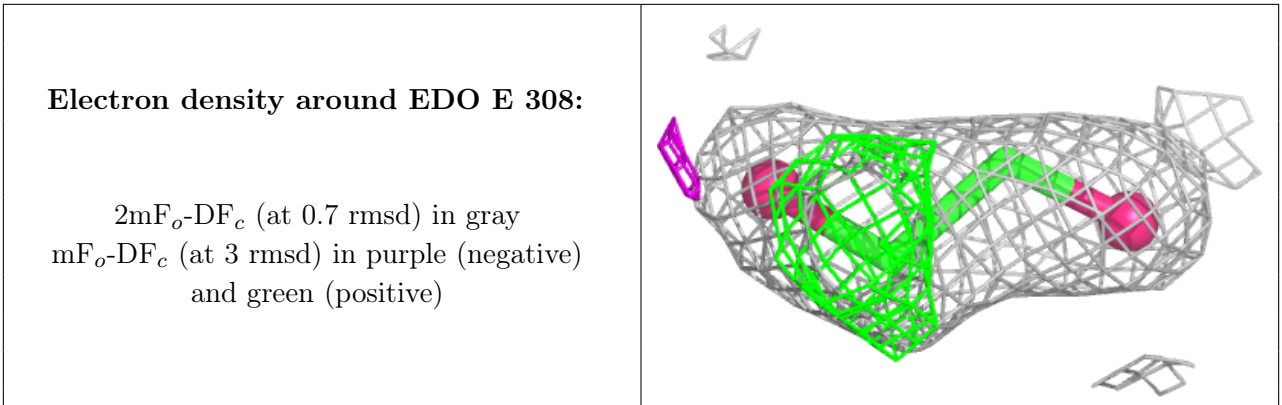
Electron density around MG B 304:

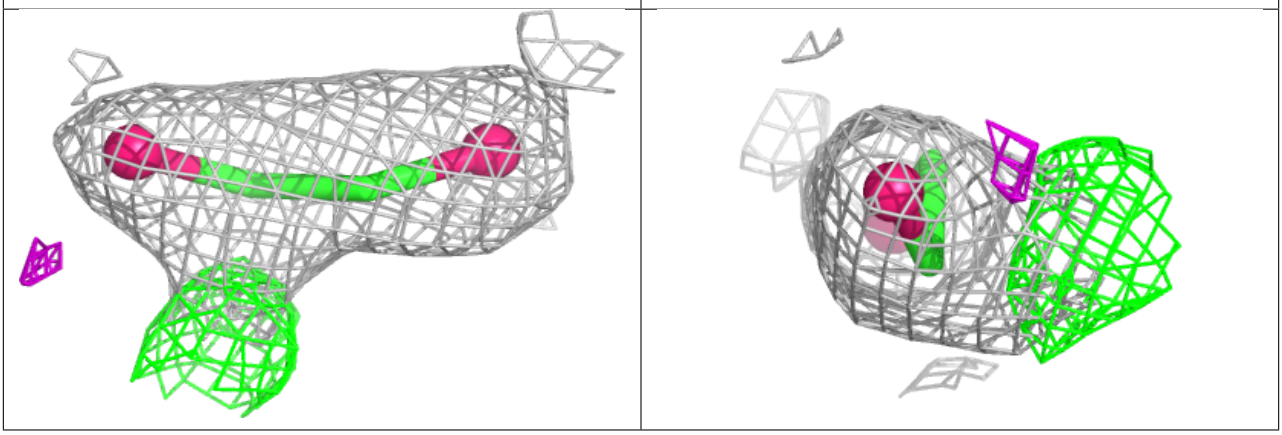
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO E 308:

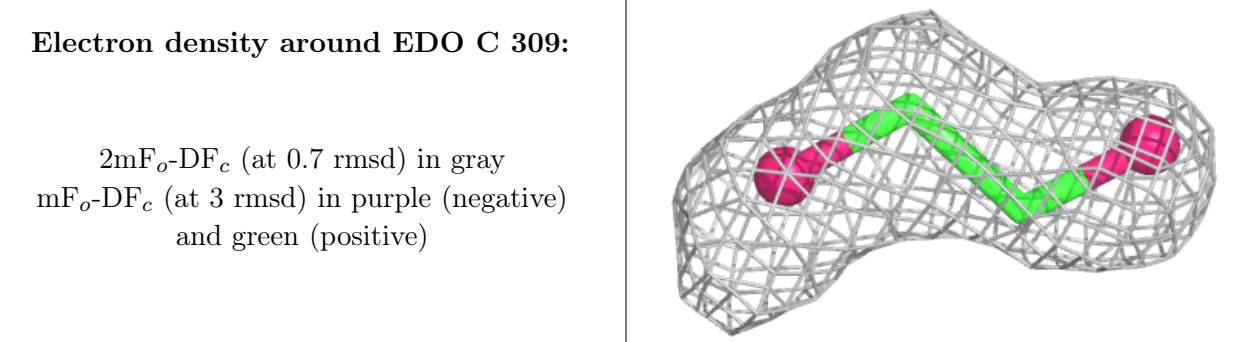
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

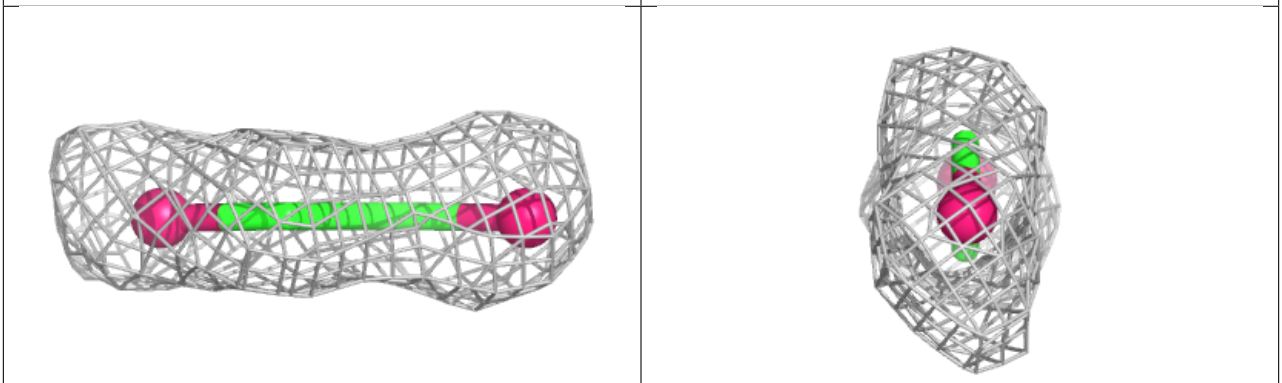




Electron density around EDO C 309:

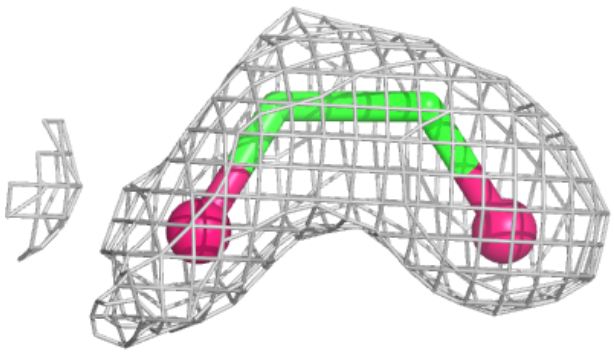
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

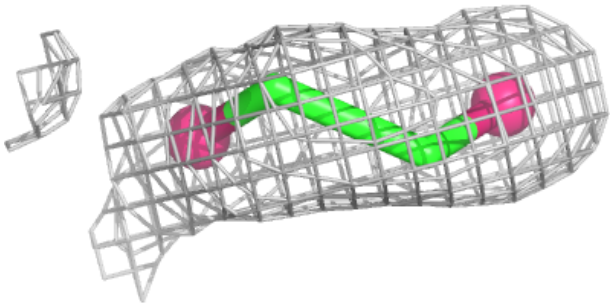


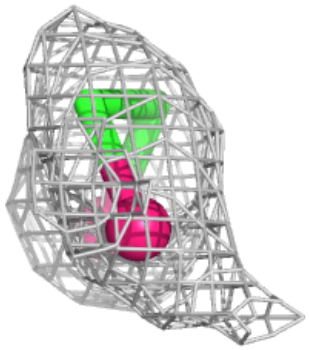


Electron density around EDO C 304:

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

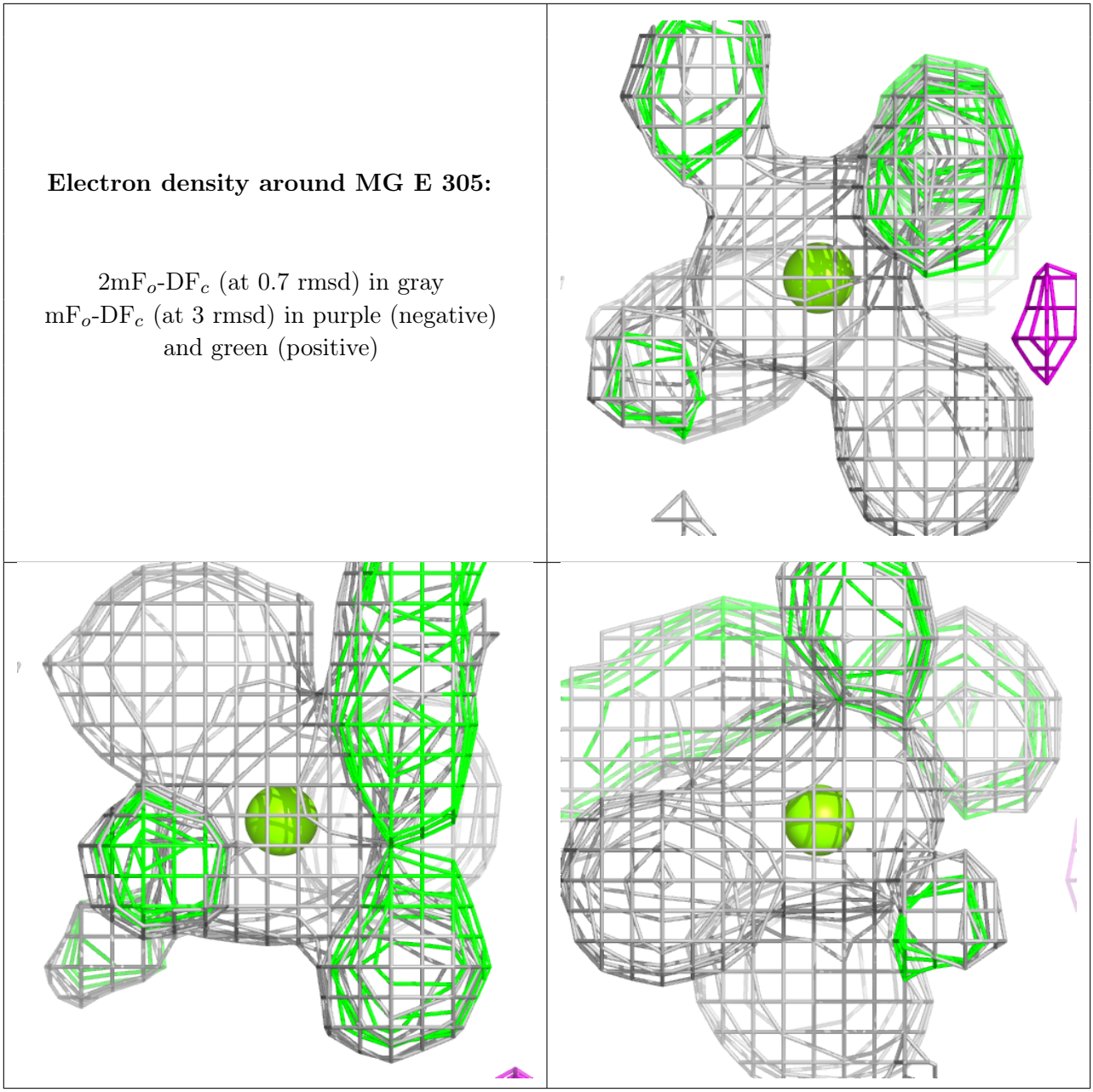






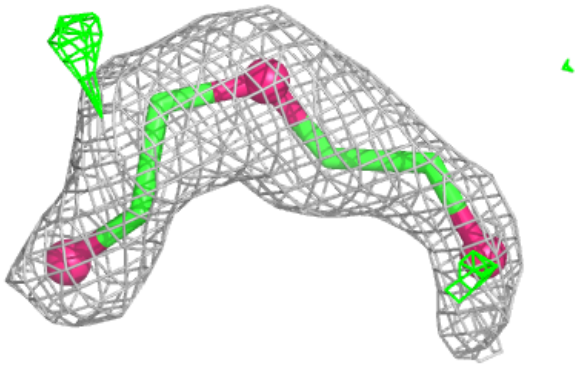
Electron density around MG E 305:

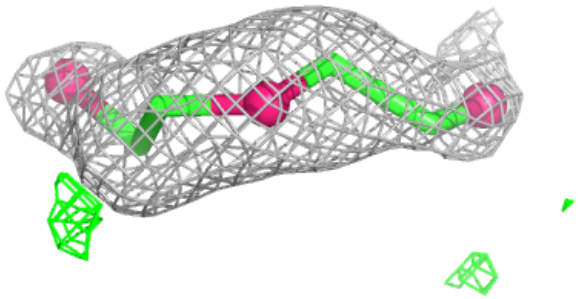
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

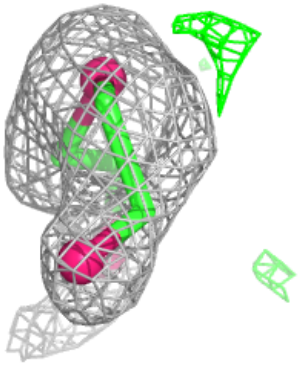


Electron density around PEG C 310:

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

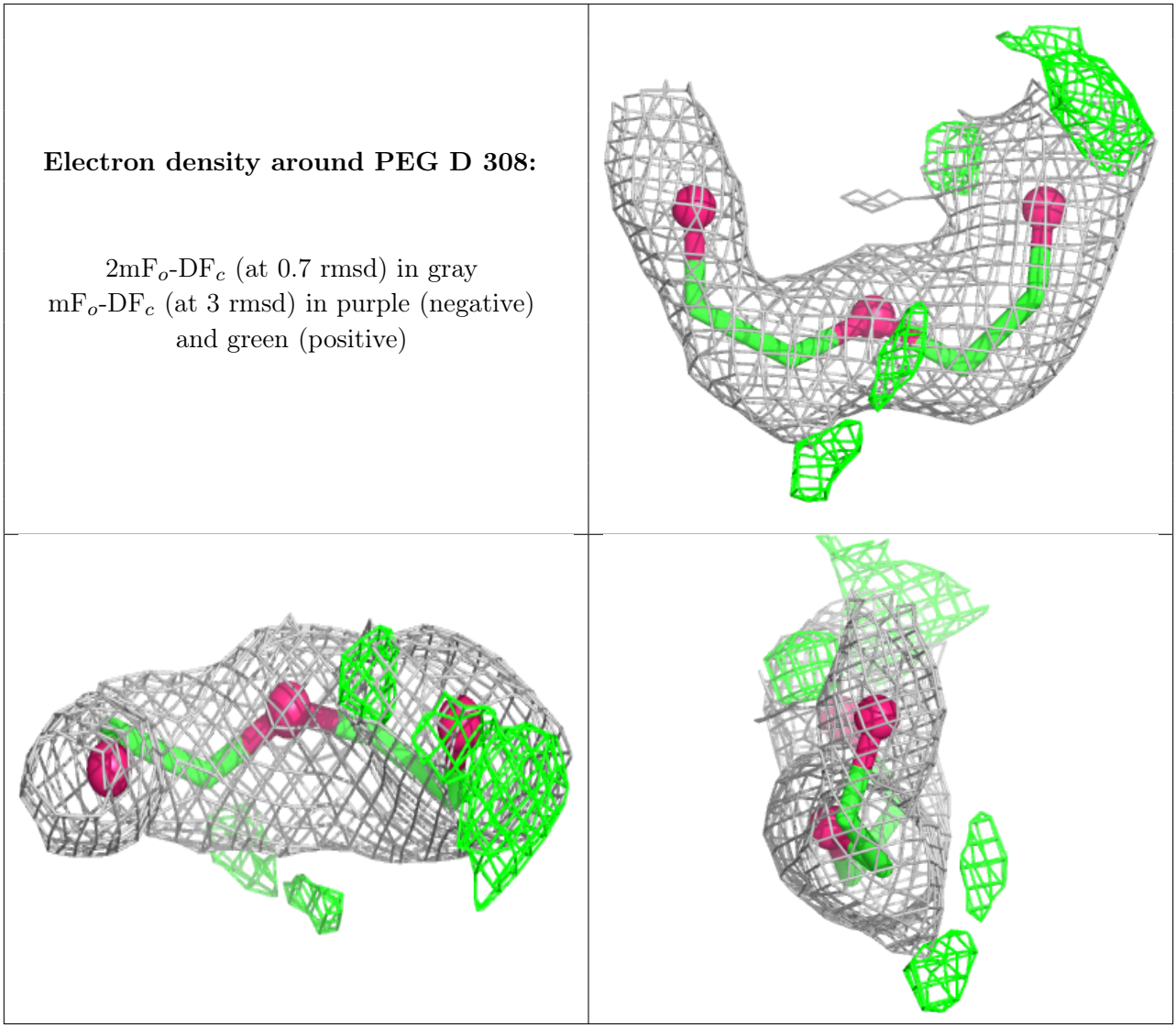






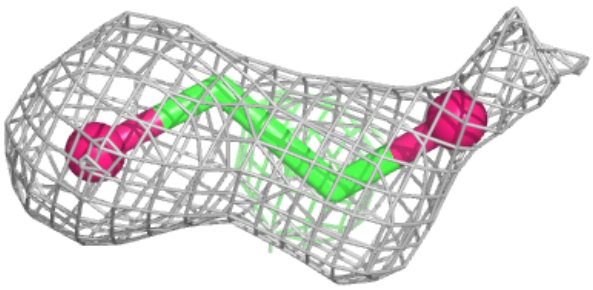
Electron density around PEG D 308:

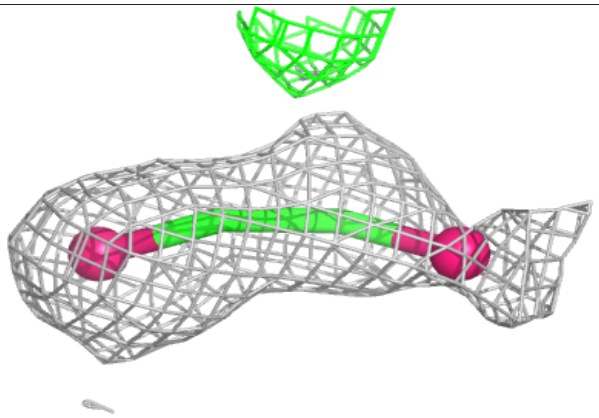
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

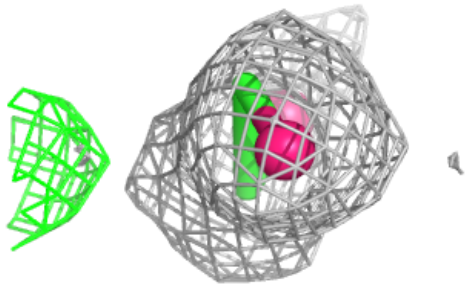


Electron density around EDO C 307:

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

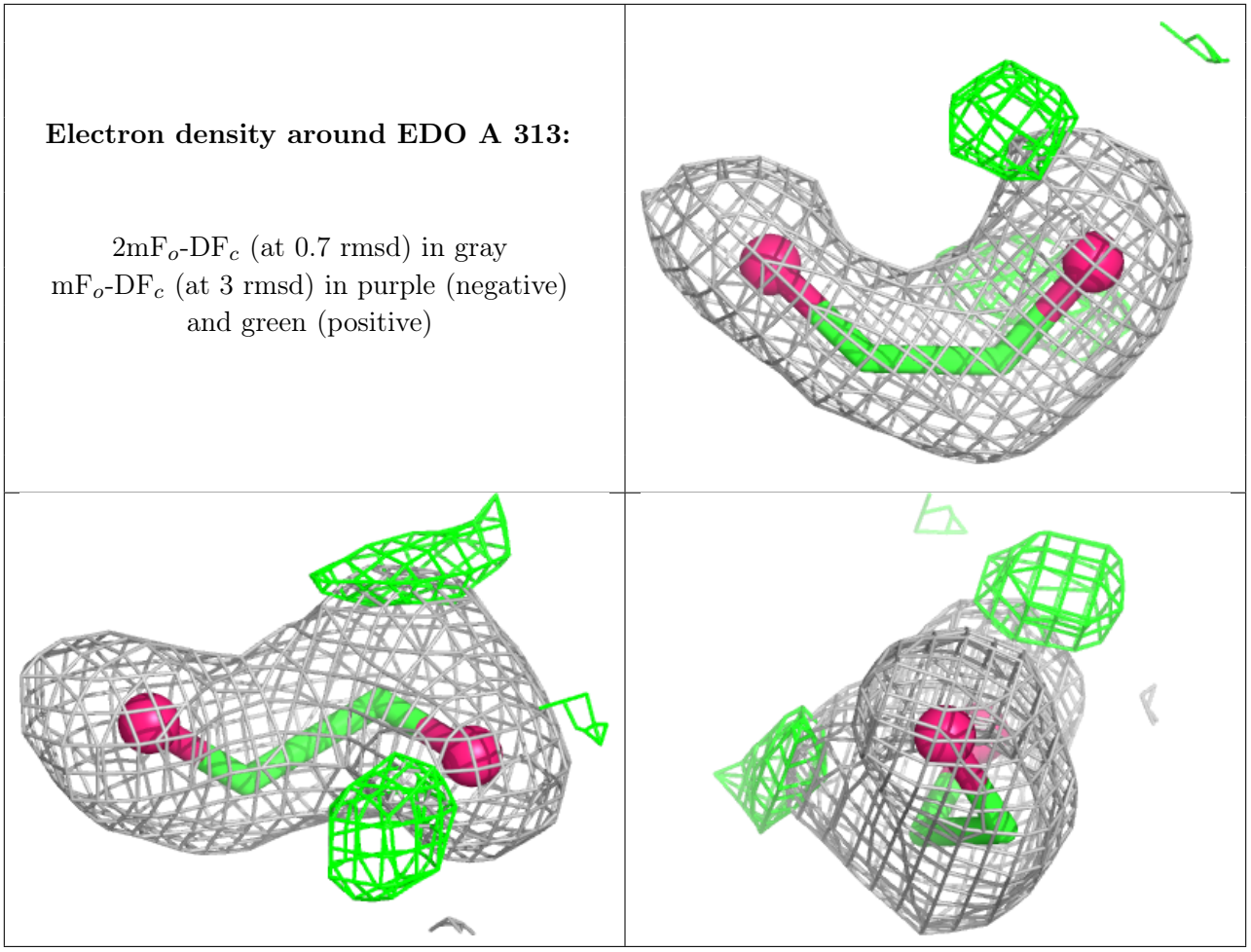






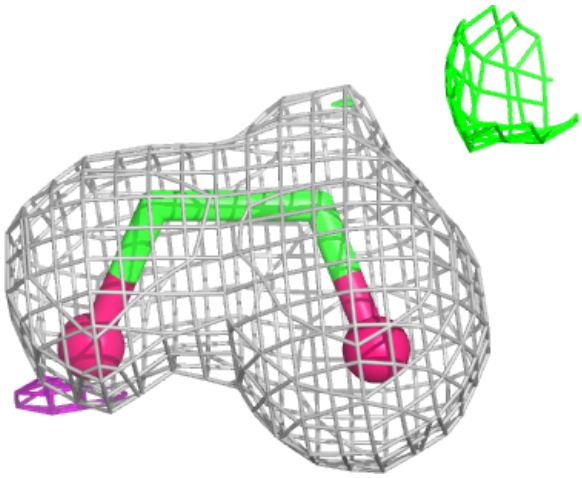
Electron density around EDO A 313:

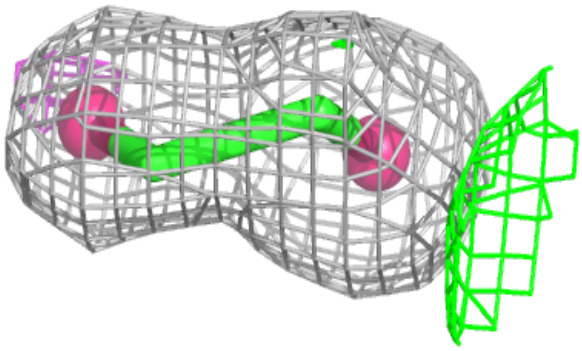
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

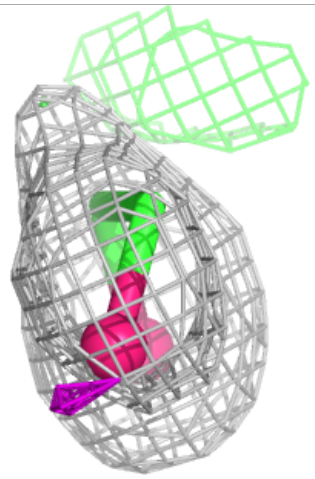


Electron density around EDO A 308:

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

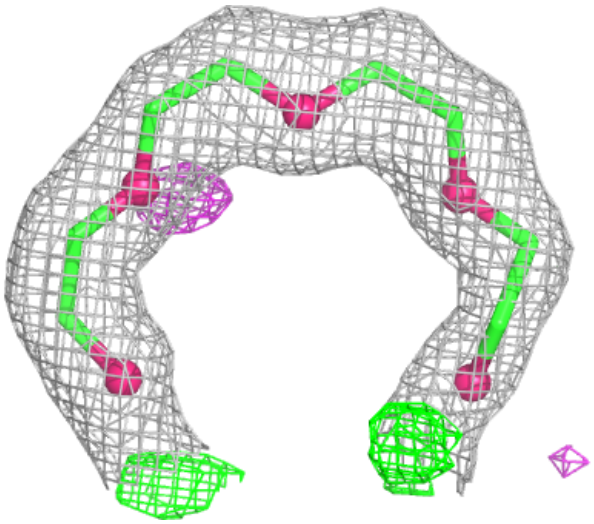


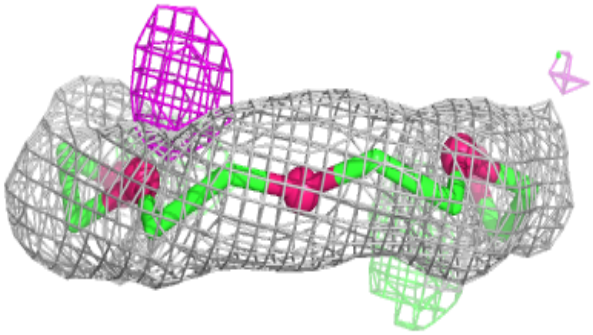


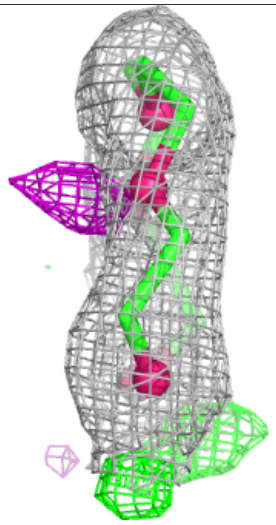


Electron density around PG4 F 305:

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

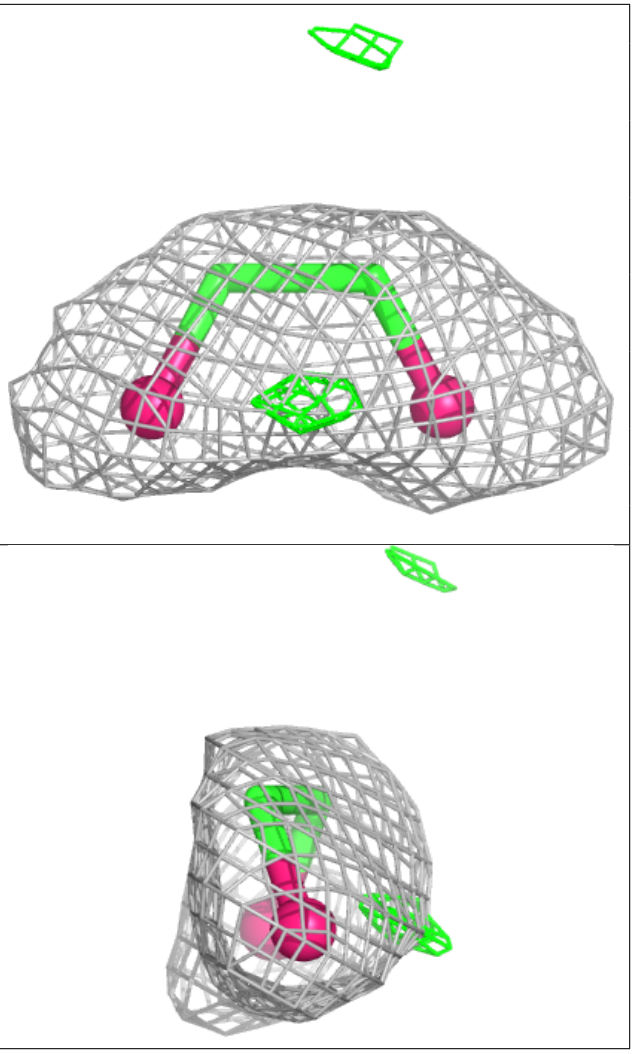






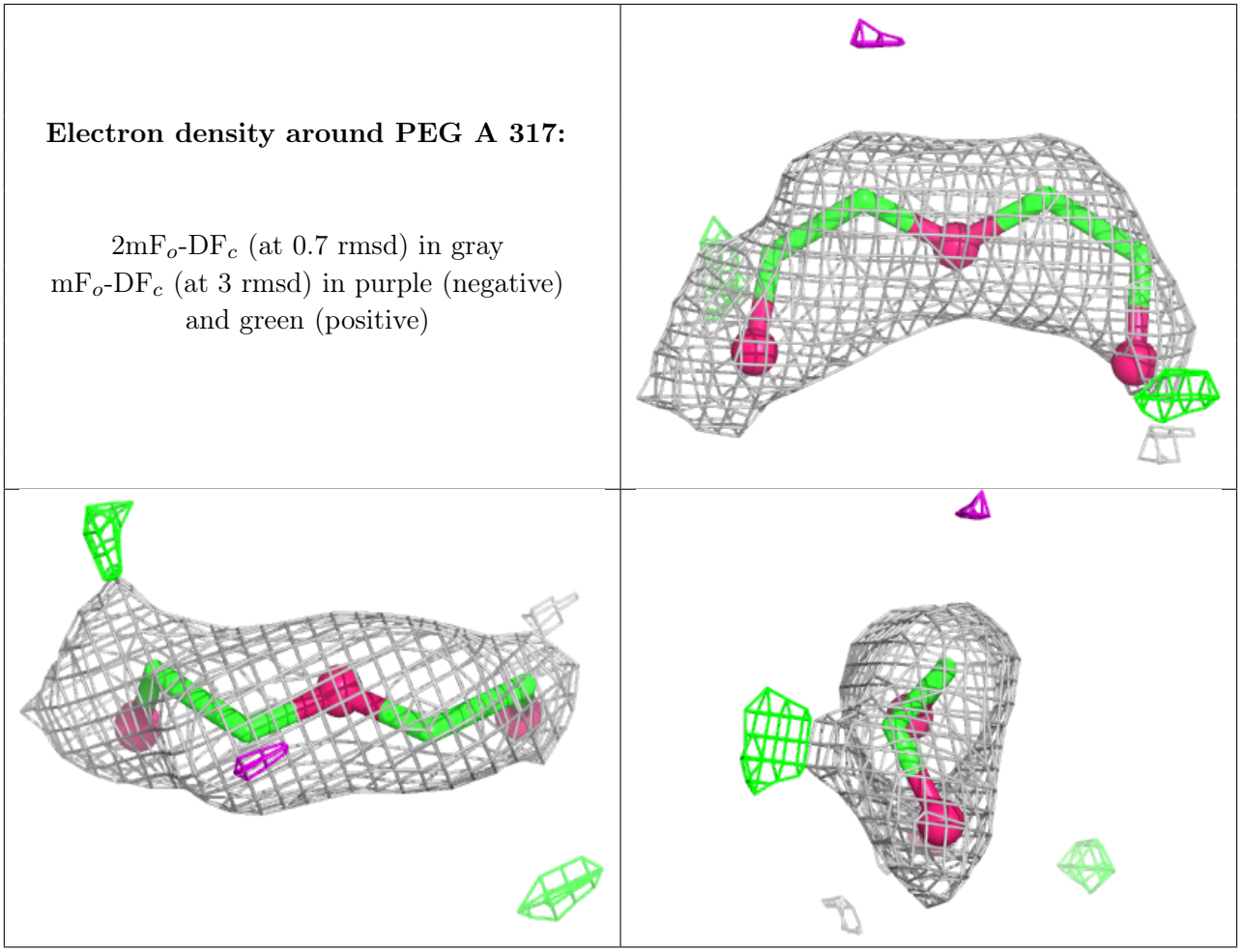
Electron density around EDO E 307:

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



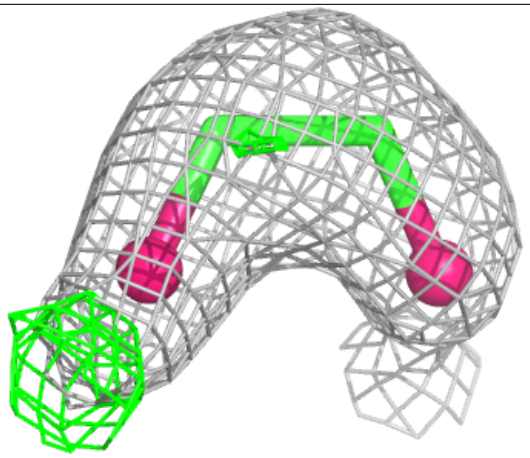
Electron density around PEG A 317:

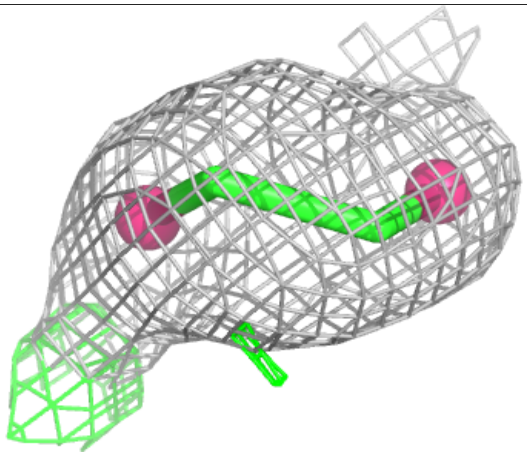
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

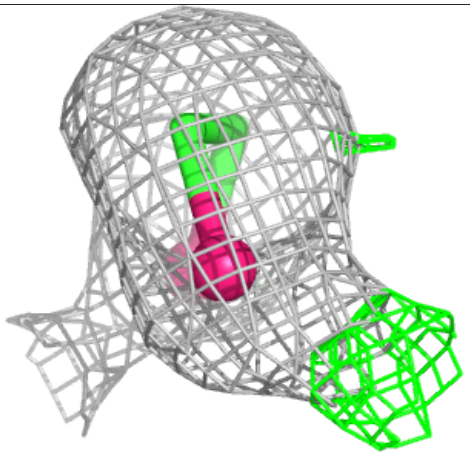


Electron density around EDO B 308:

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

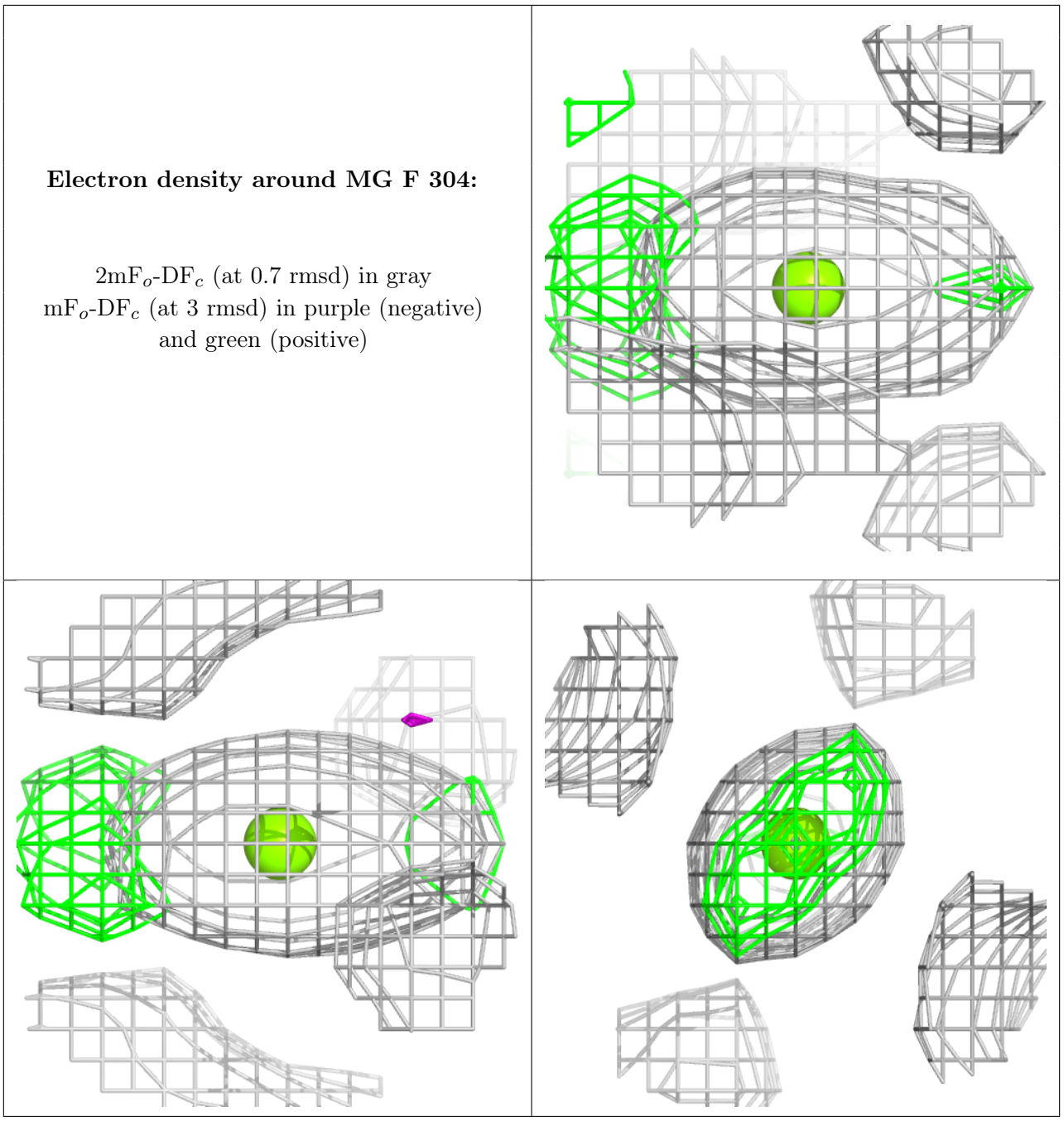






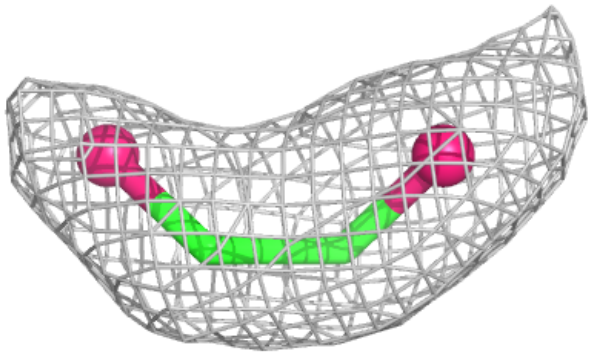
Electron density around MG F 304:

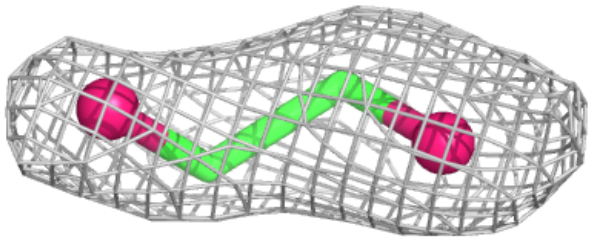
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

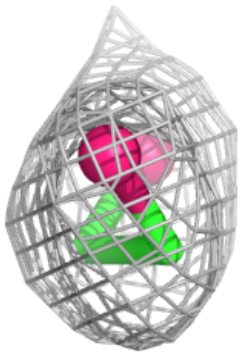


Electron density around EDO C 308:

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

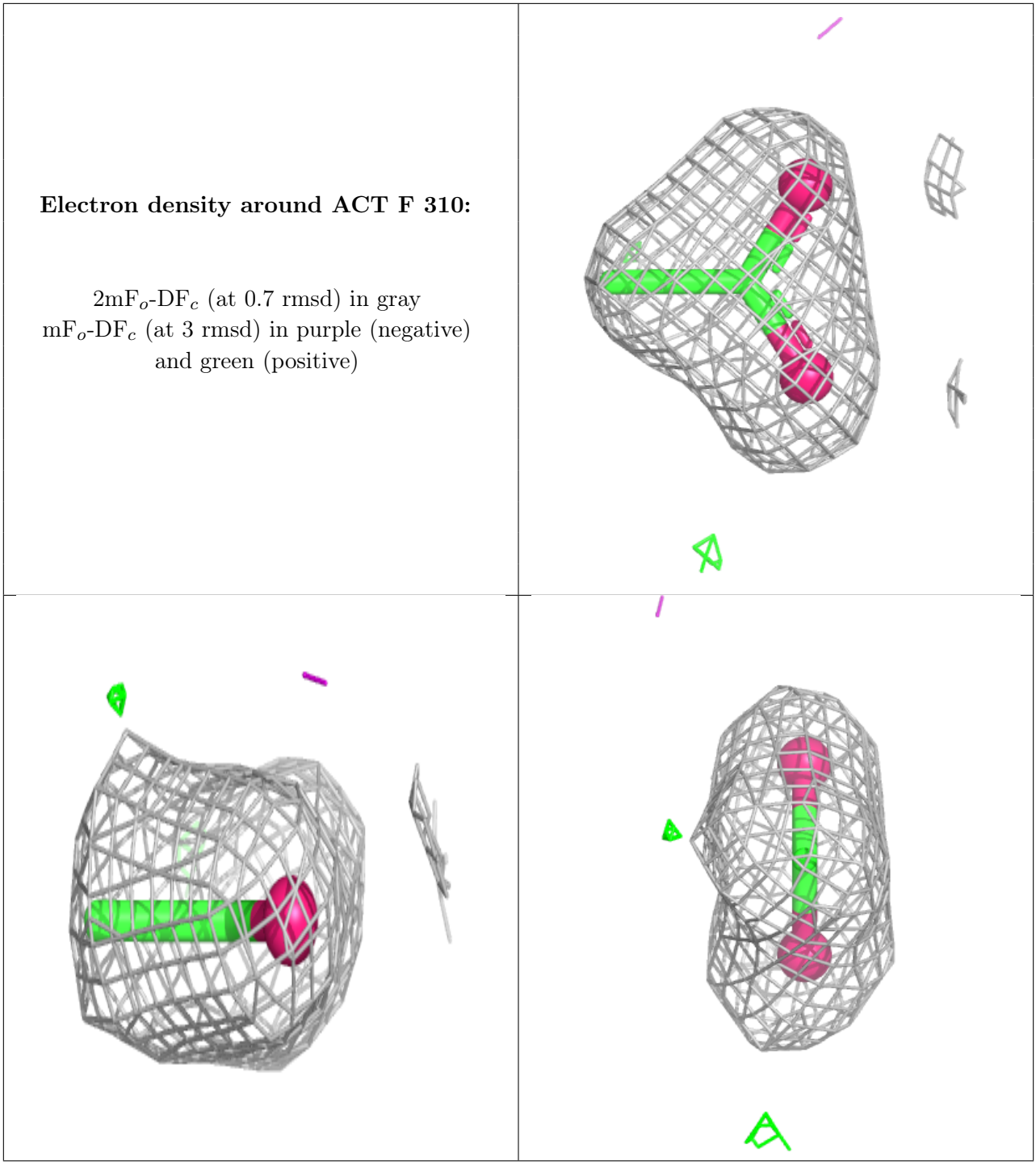






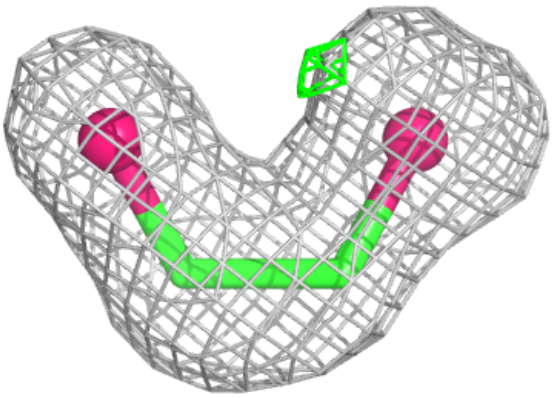
Electron density around ACT F 310:

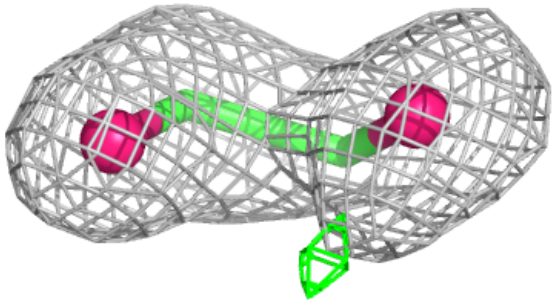
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

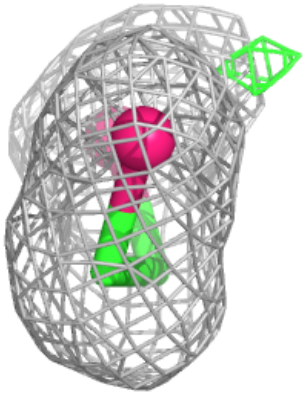


Electron density around EDO D 306:

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

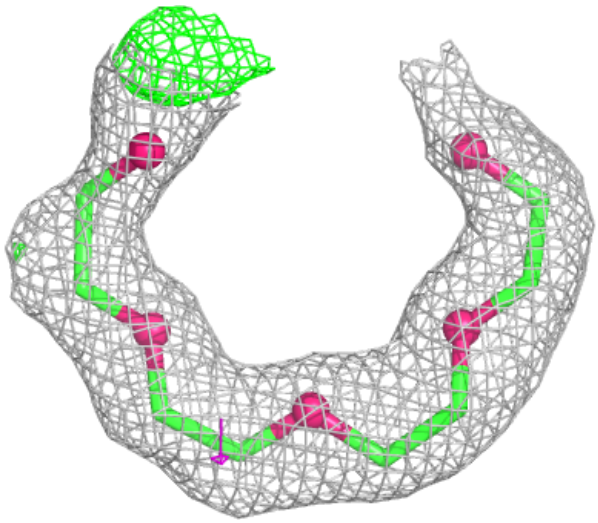


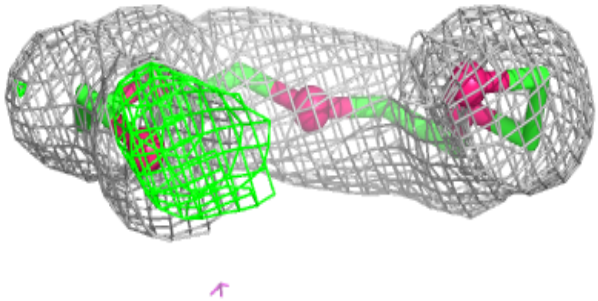


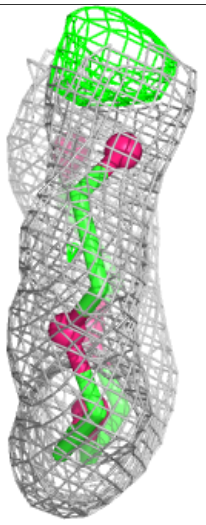


Electron density around PG4 D 303:

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

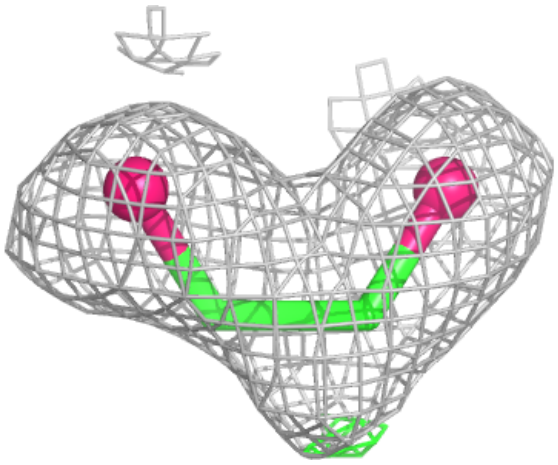


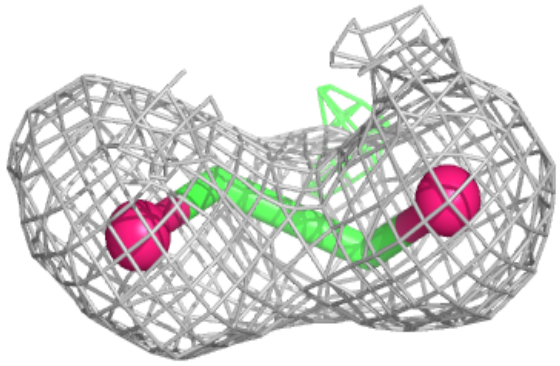


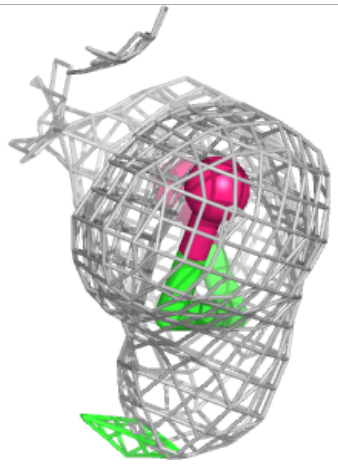


Electron density around EDO A 312:

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

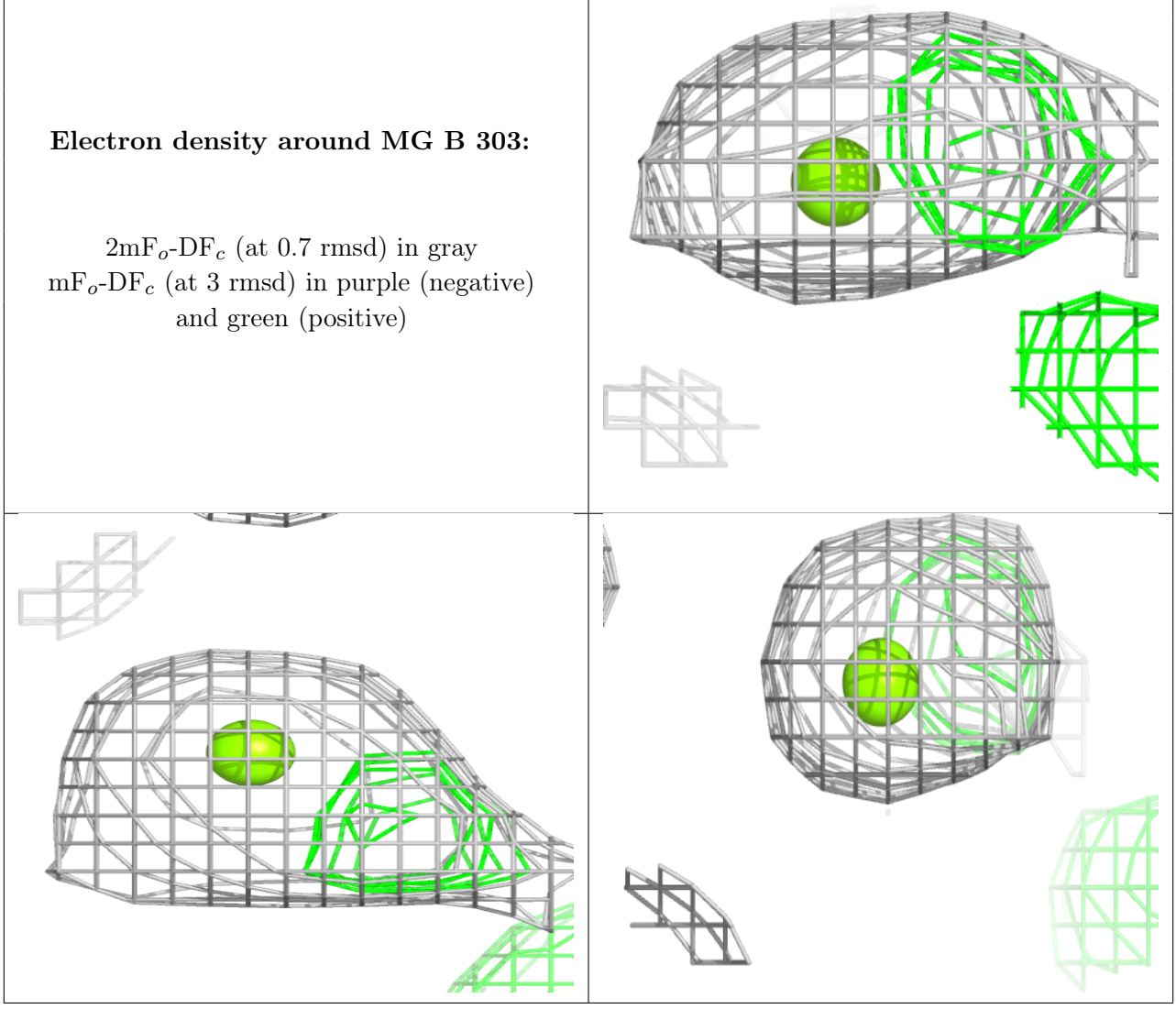






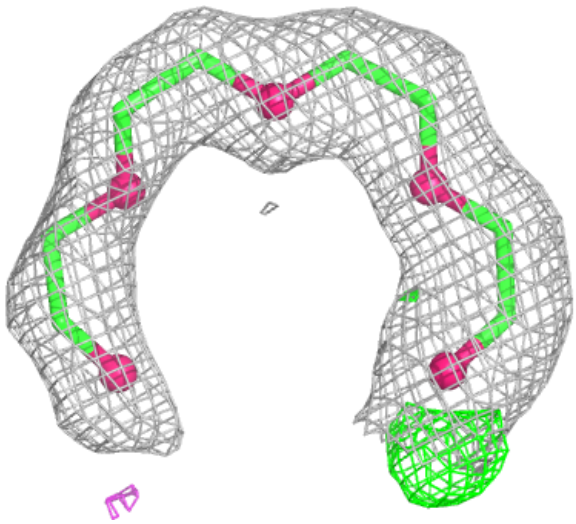
Electron density around MG B 303:

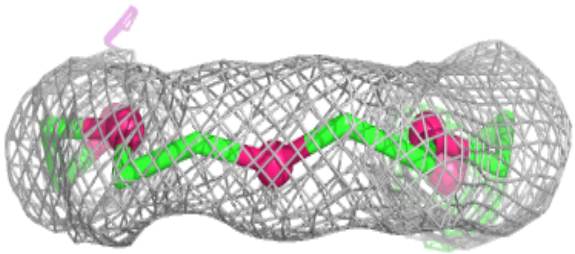
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

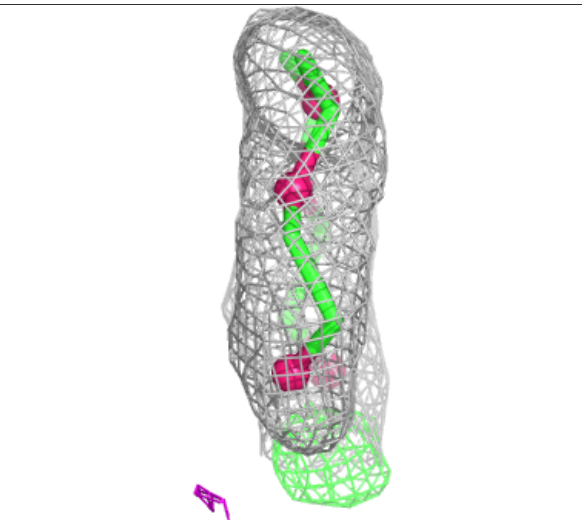


Electron density around PG4 B 305:

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

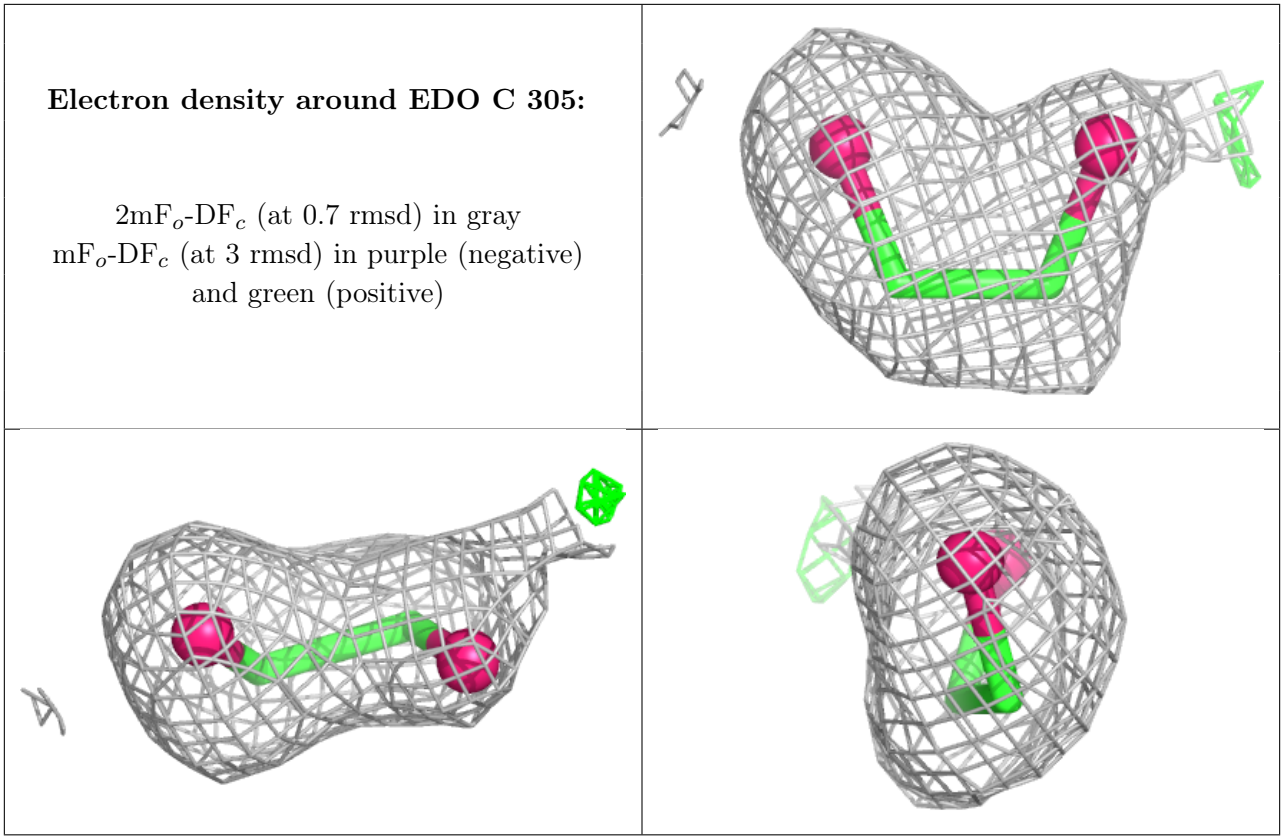






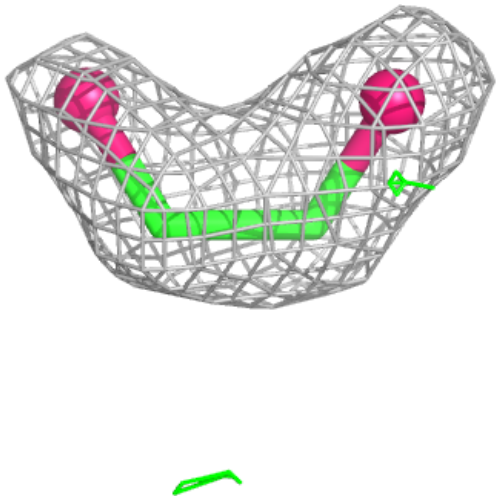
Electron density around EDO C 305:

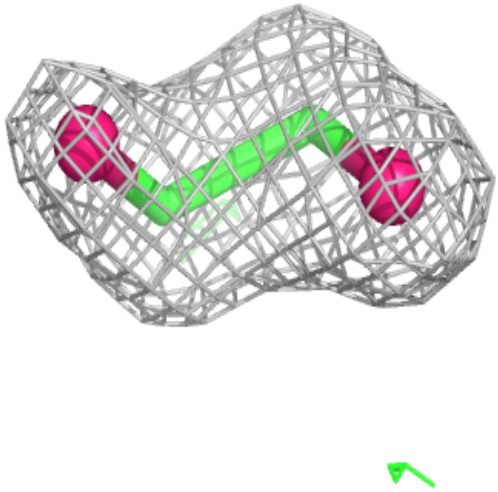
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

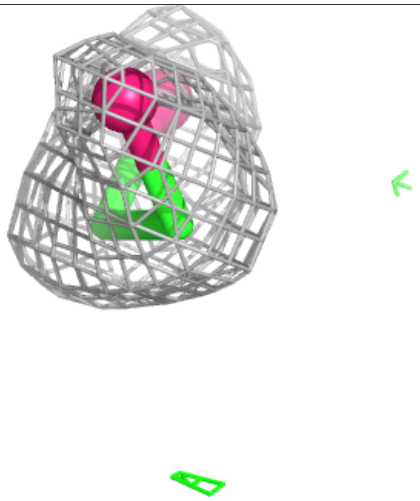


Electron density around EDO D 307:

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

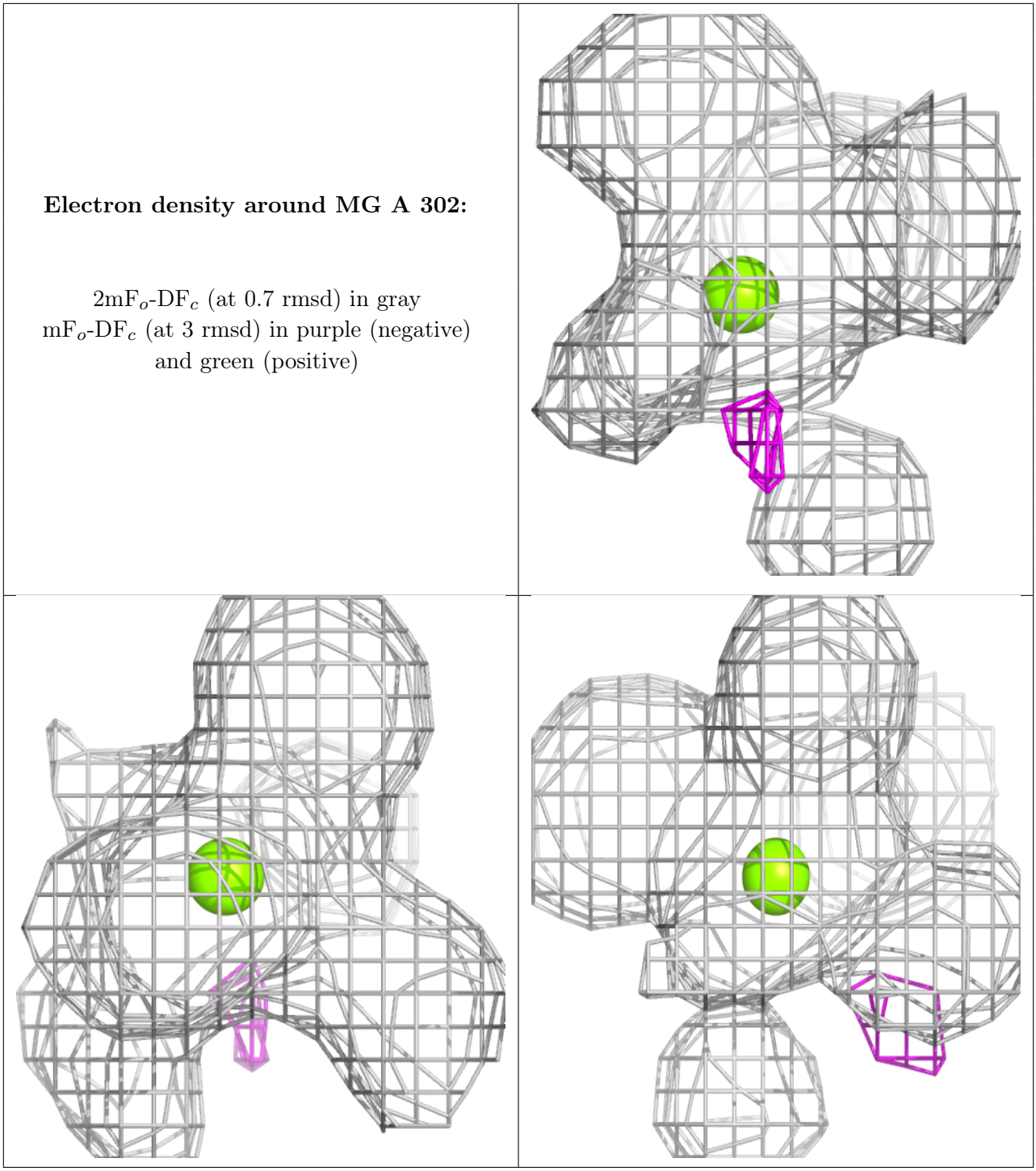






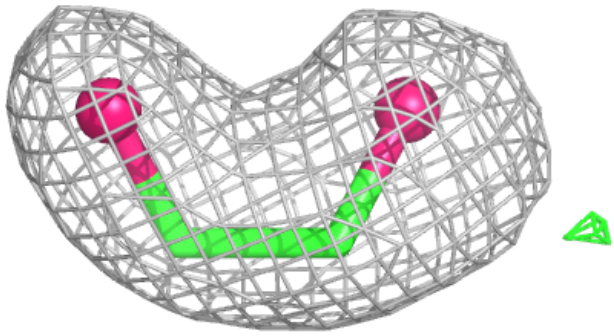
Electron density around MG A 302:

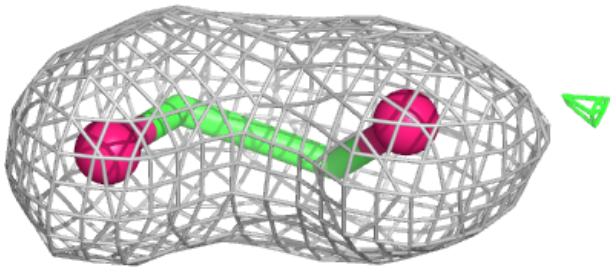
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

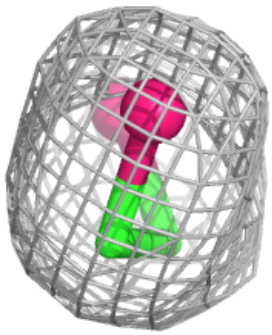


Electron density around EDO A 309:

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

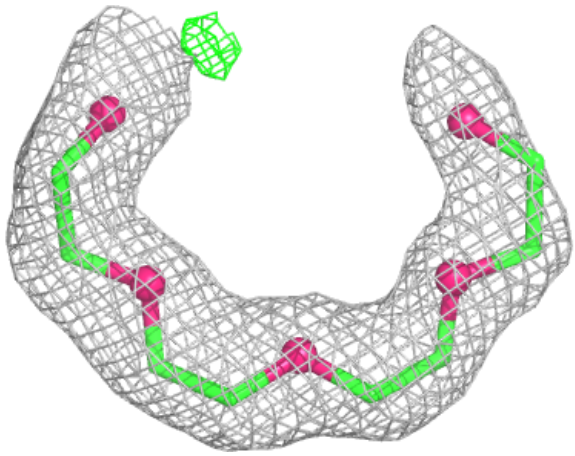


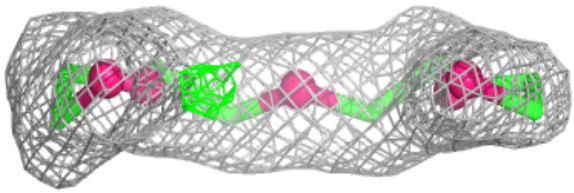


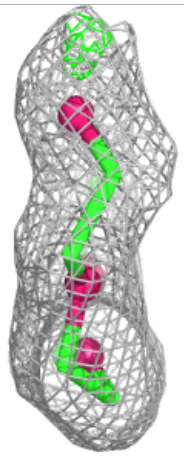


Electron density around PG4 C 303:

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

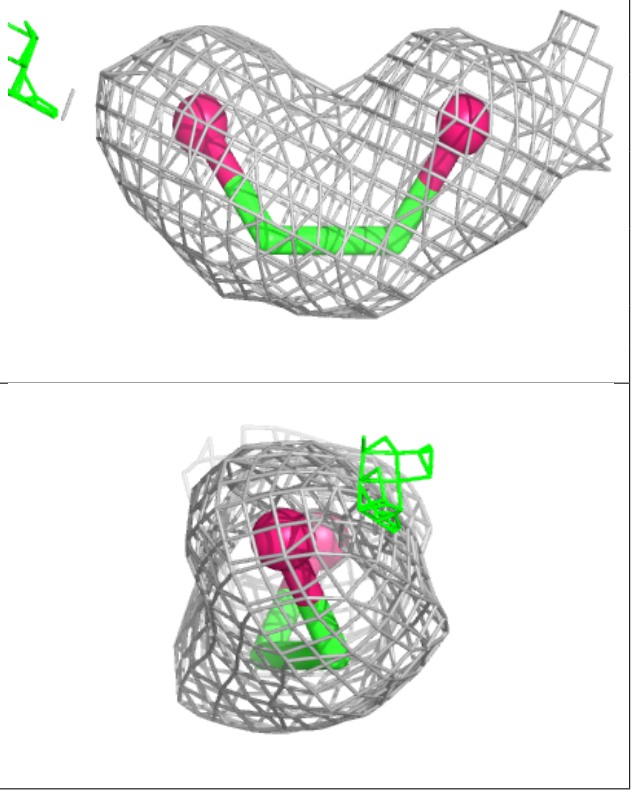






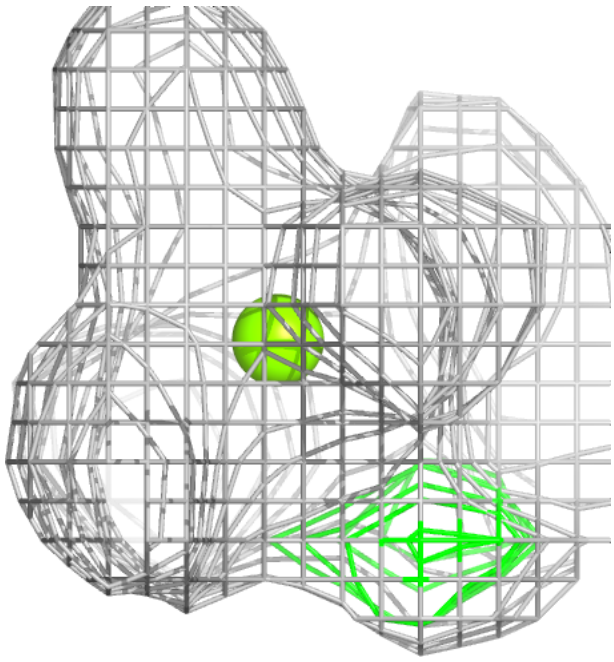
Electron density around EDO D 304:

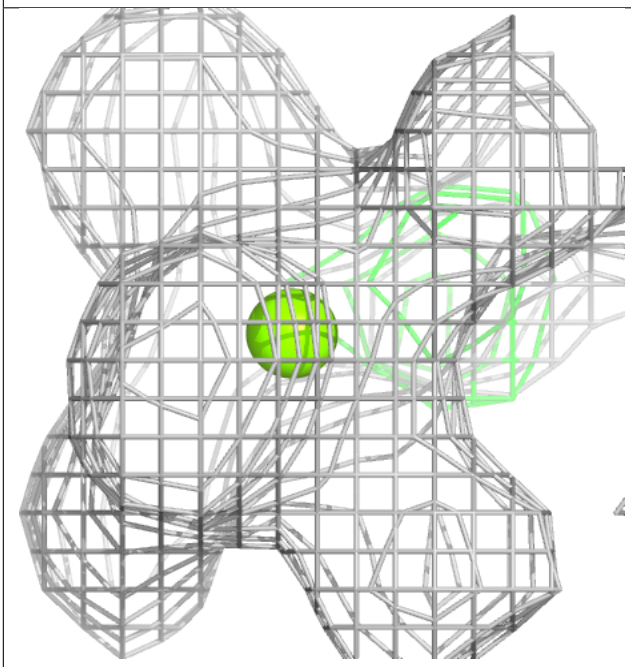
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

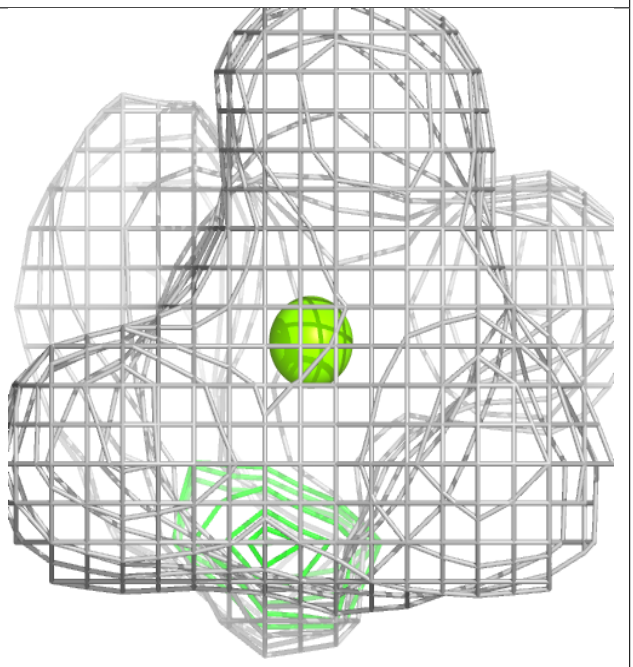


Electron density around MG C 301:

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

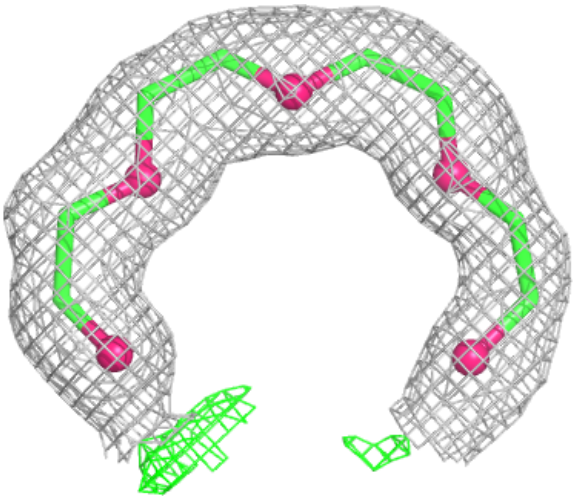


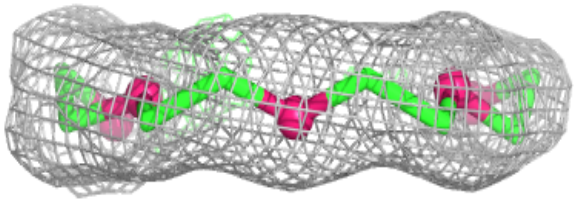


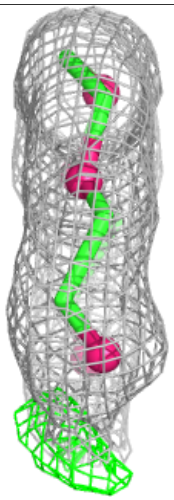


Electron density around PG4 A 306:

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

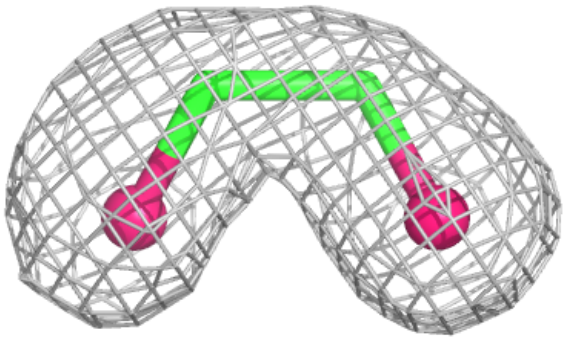


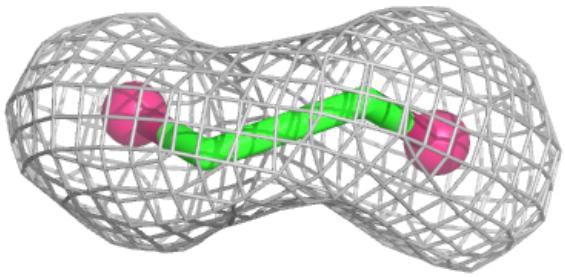


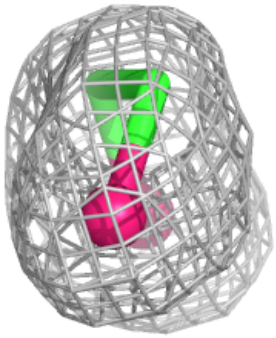


Electron density around EDO F 307:

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

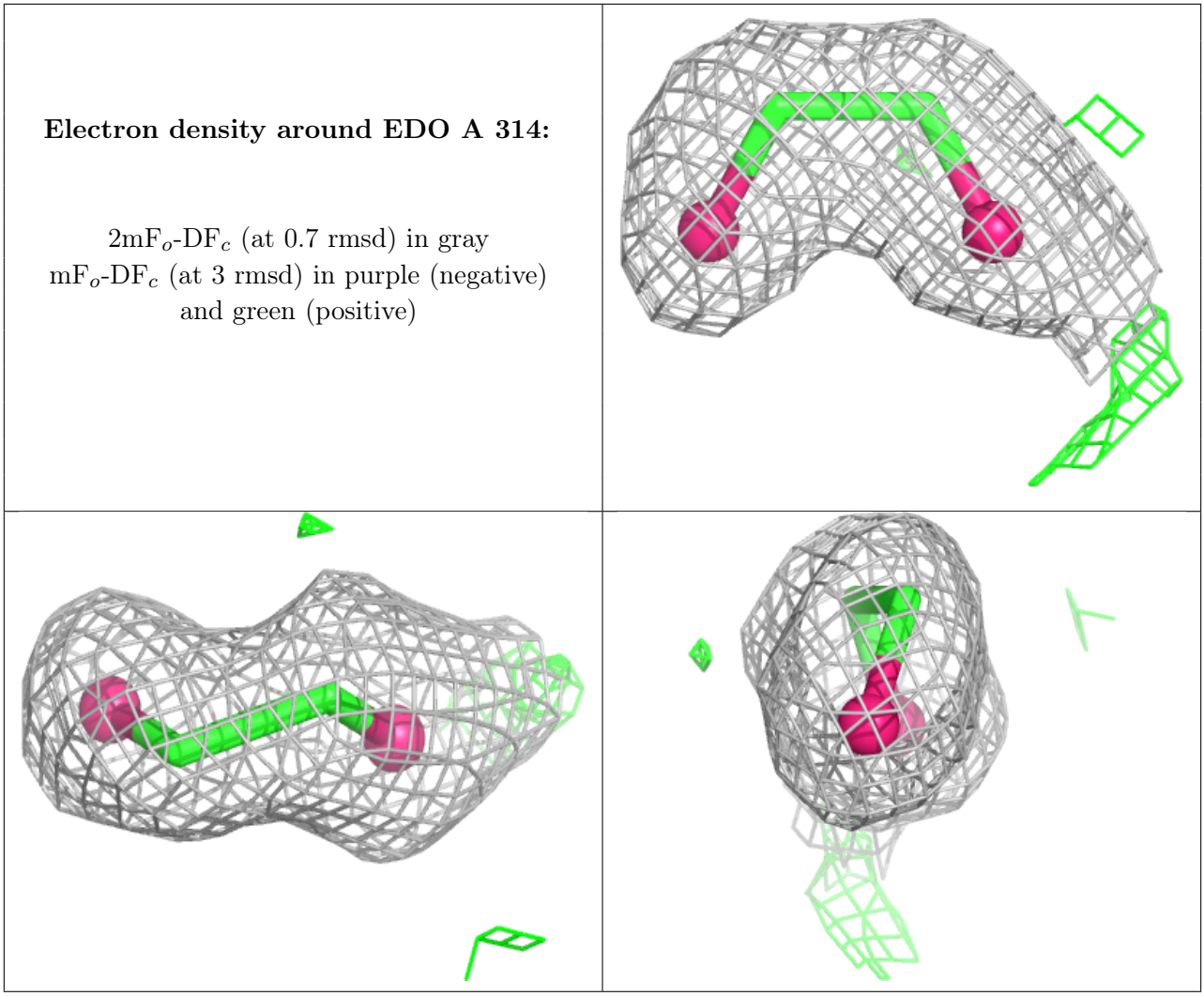






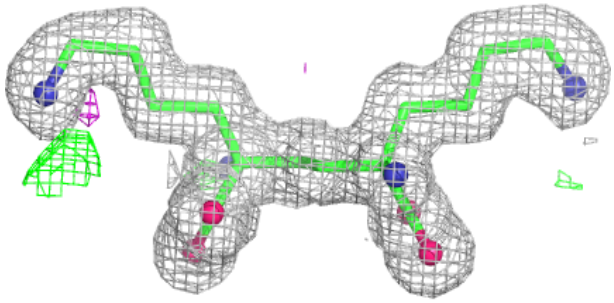
Electron density around EDO A 314:

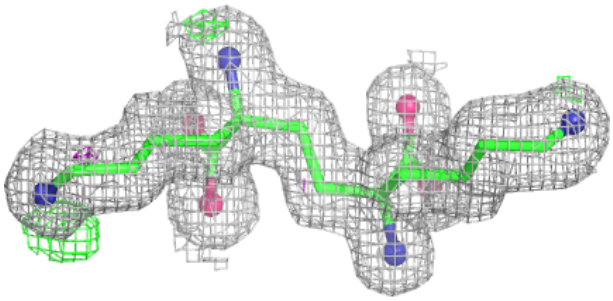
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

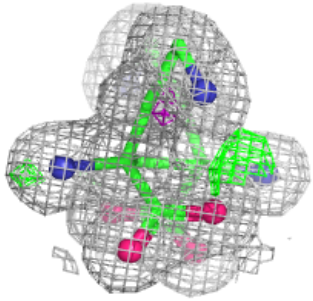


Electron density around 3VN A 301:

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

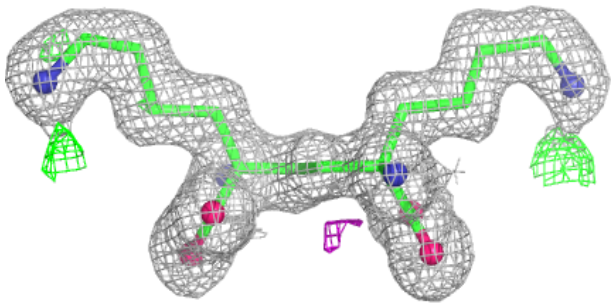


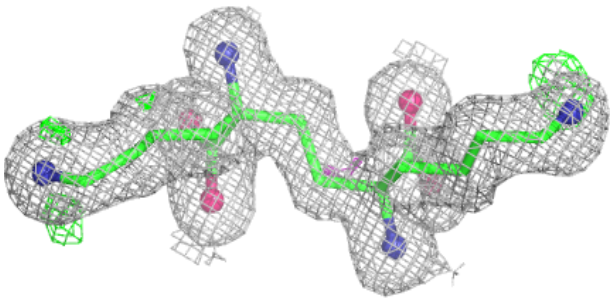


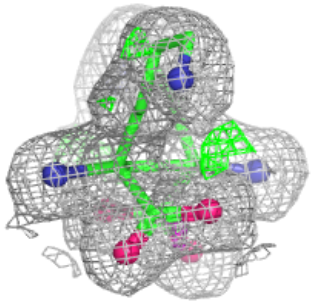


Electron density around 3VN B 301:

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

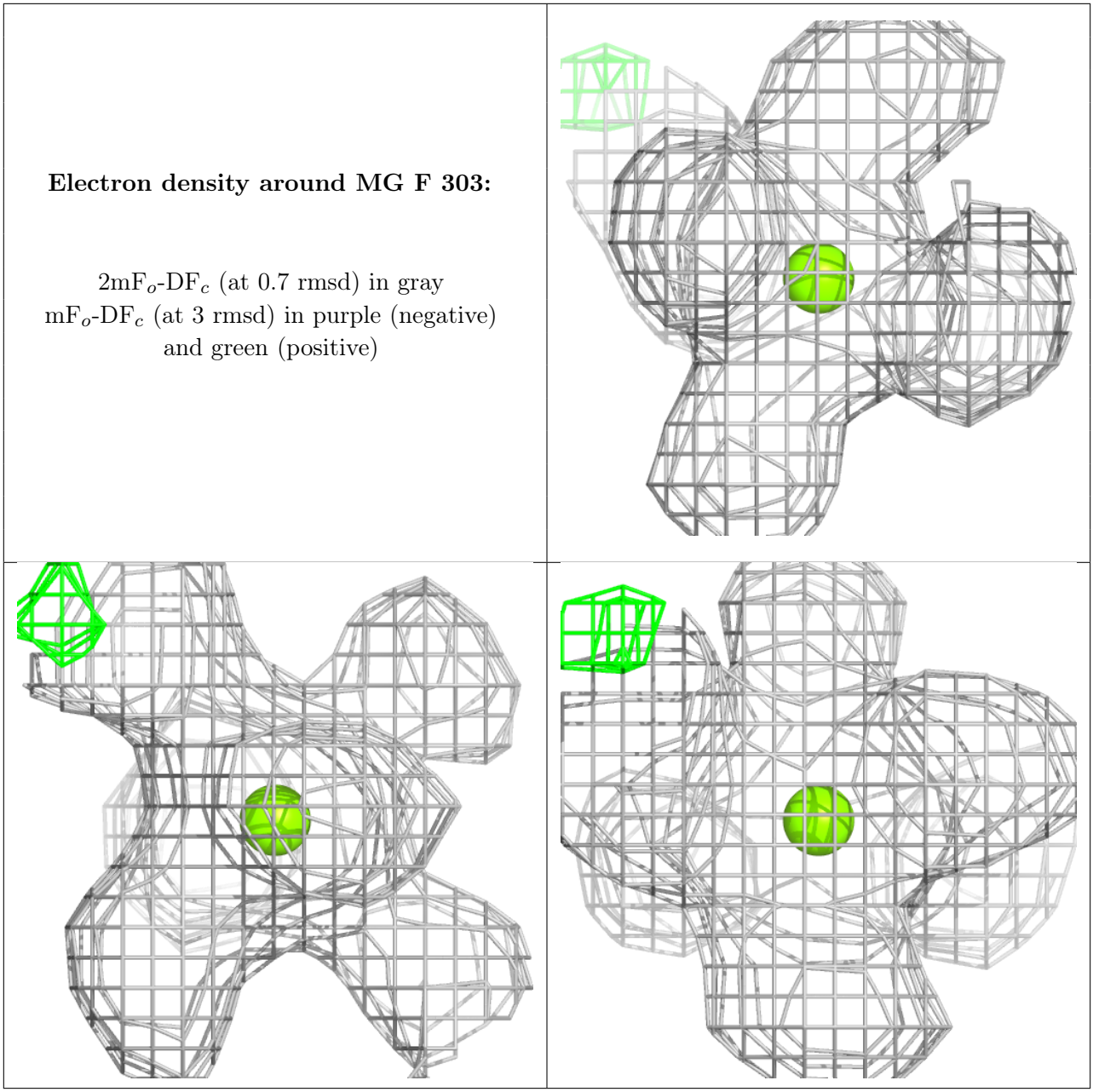






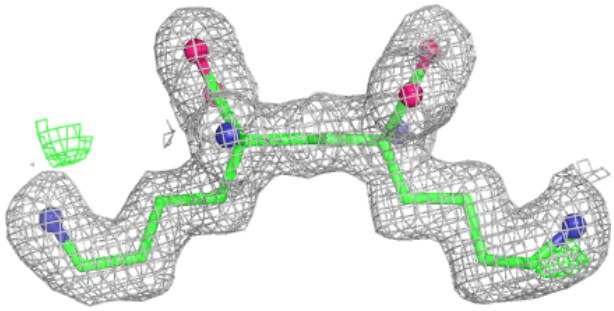
Electron density around MG F 303:

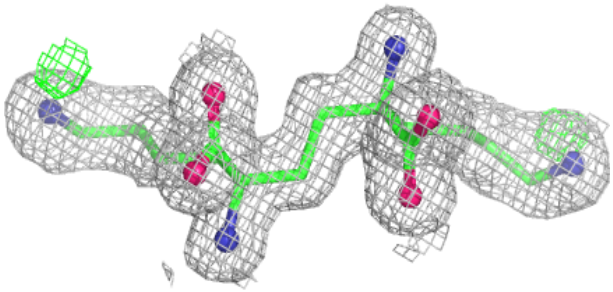
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

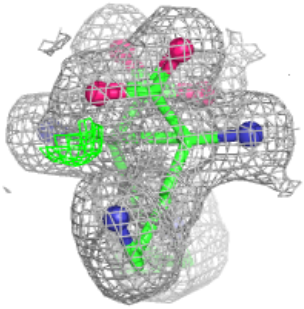


Electron density around 3VN D 301:

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

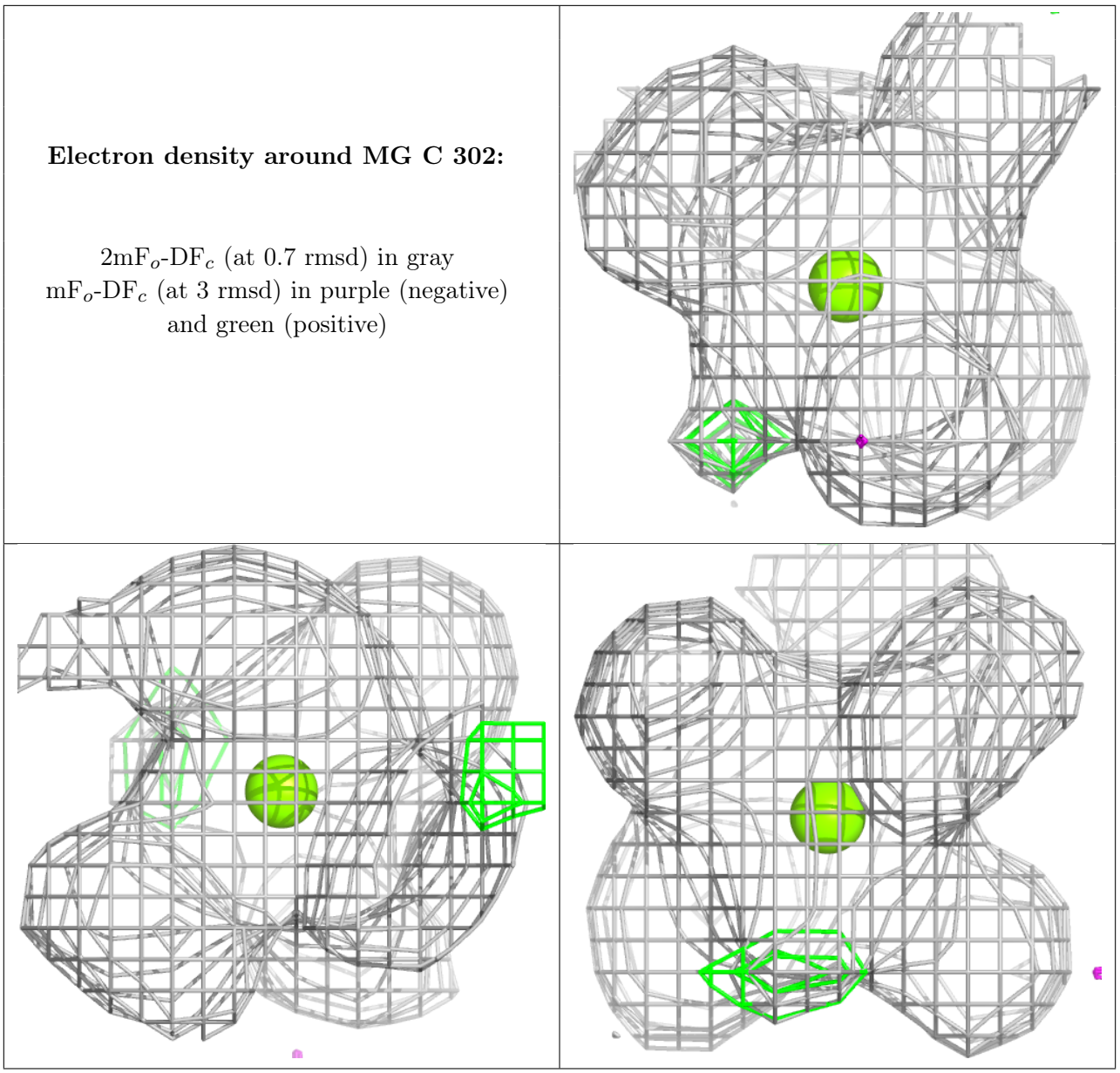






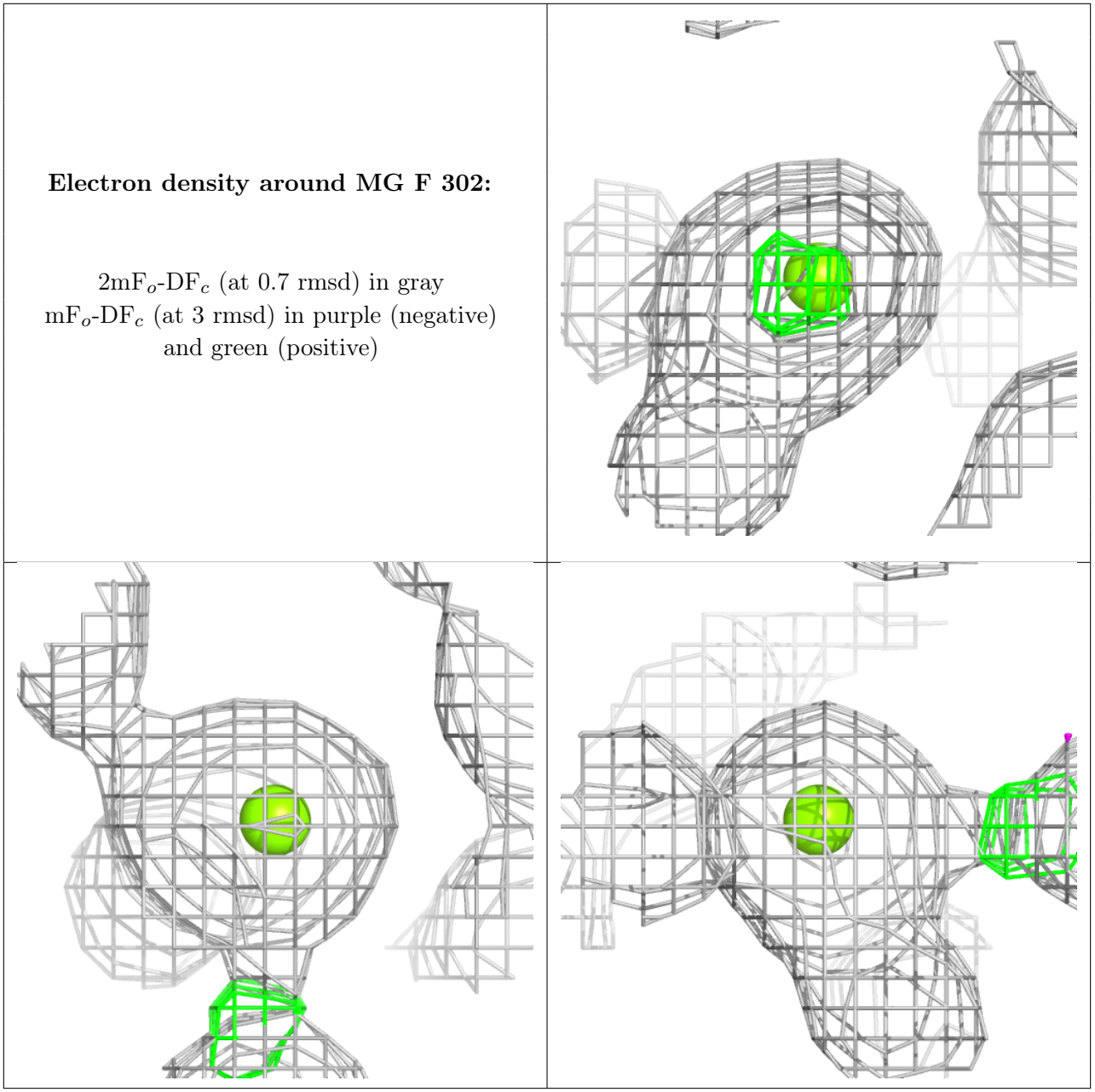
Electron density around MG C 302:

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



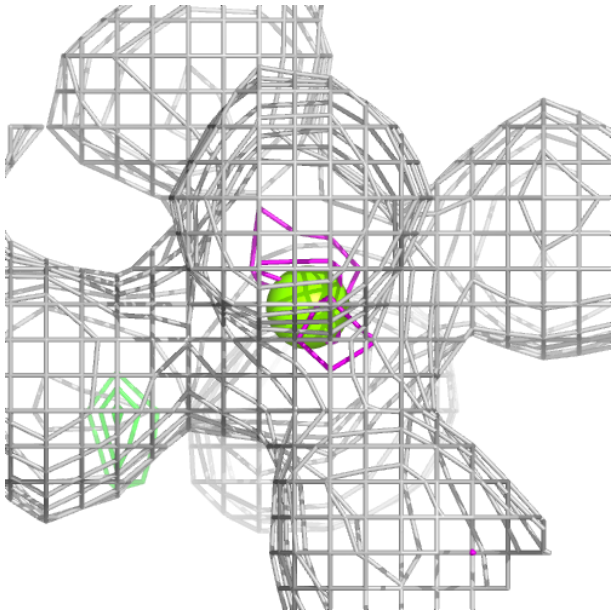
Electron density around MG F 302:

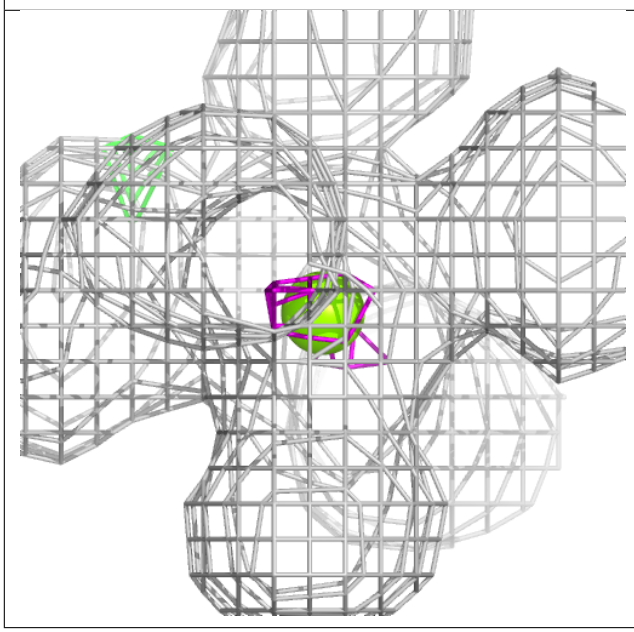
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

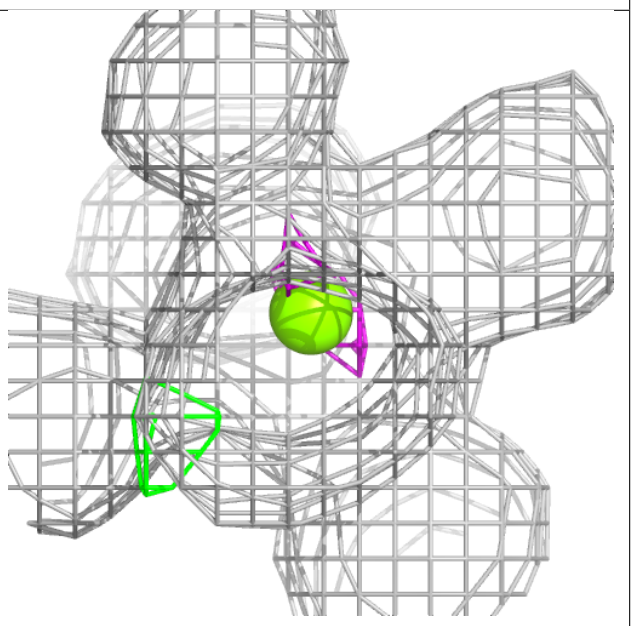


Electron density around MG F 301:

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

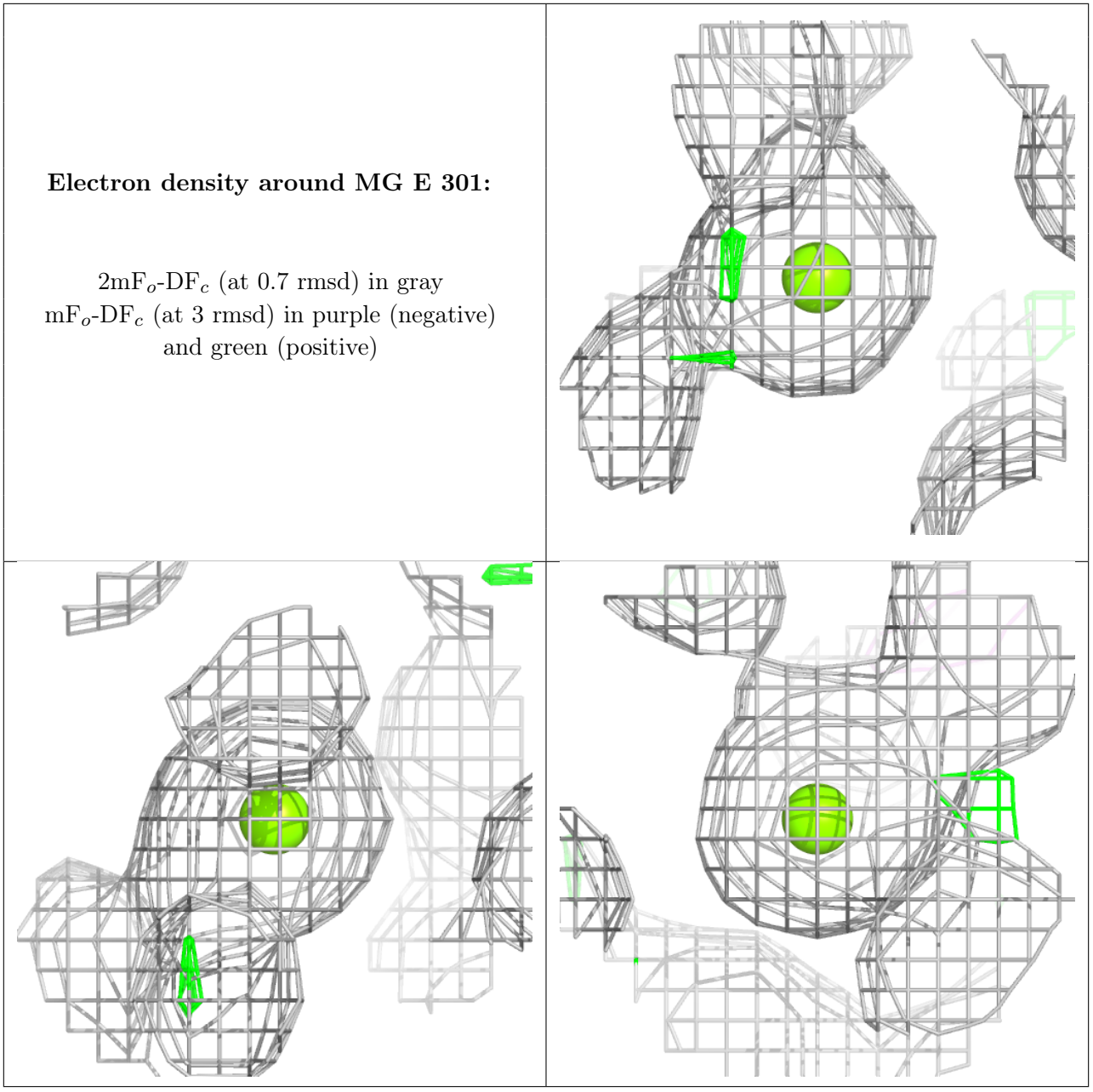






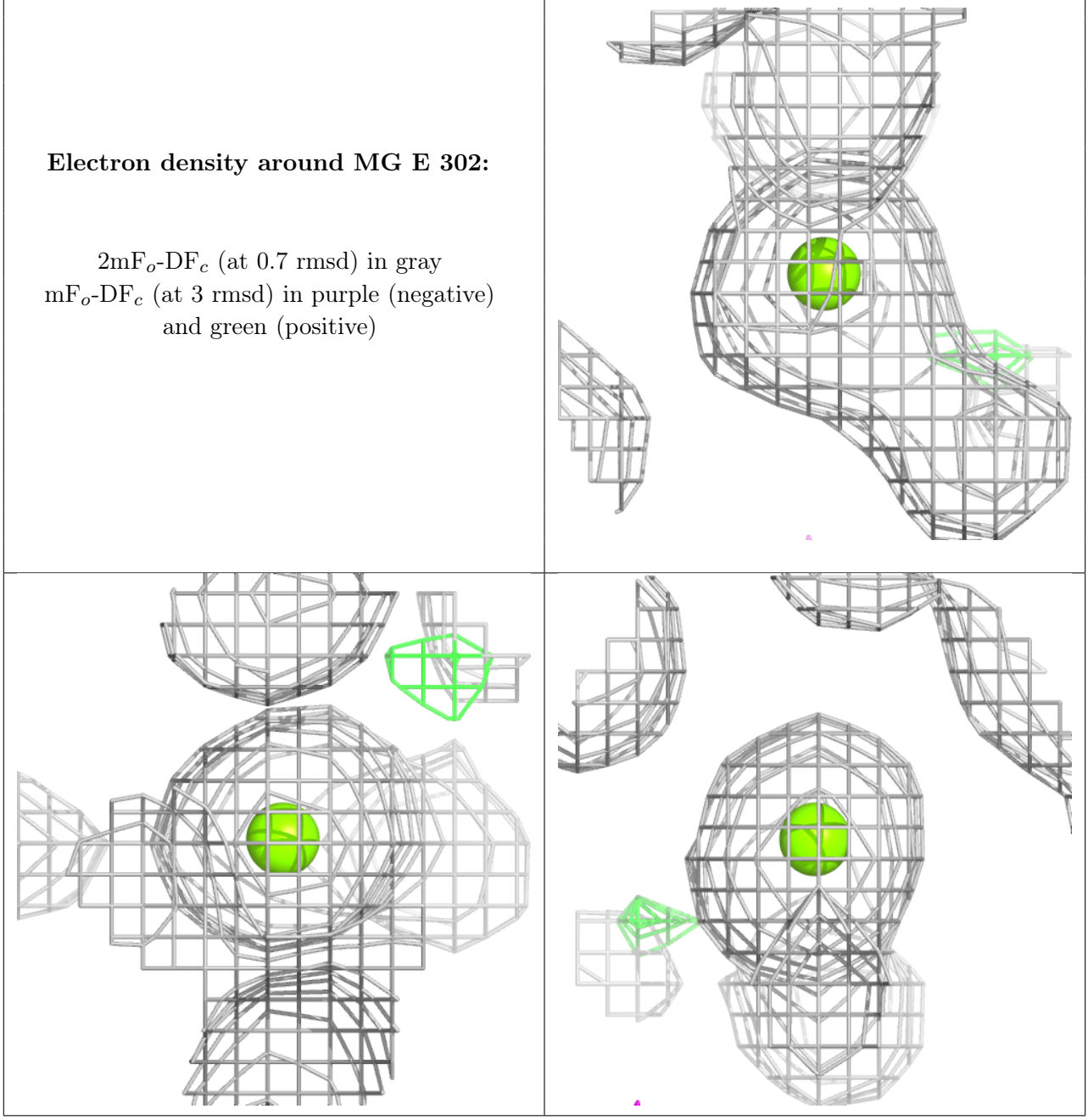
Electron density around MG E 301:

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



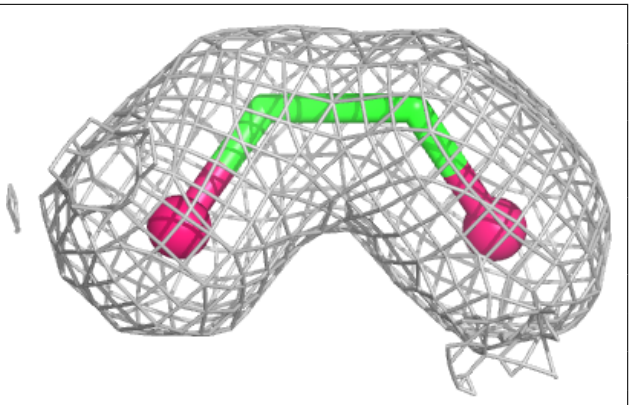
Electron density around MG E 302:

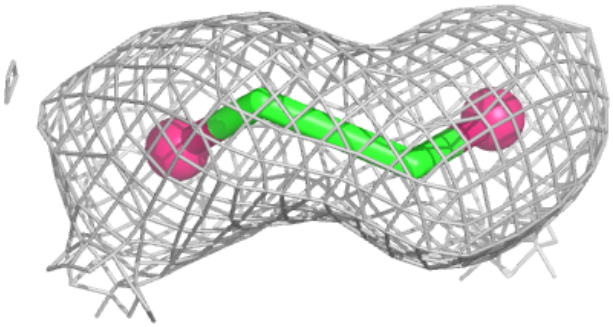
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

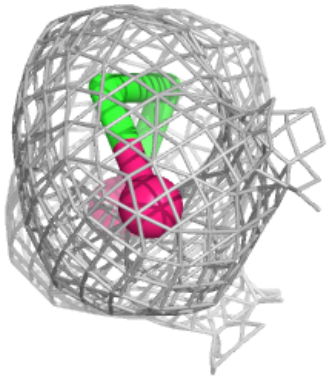


Electron density around EDO E 311:

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

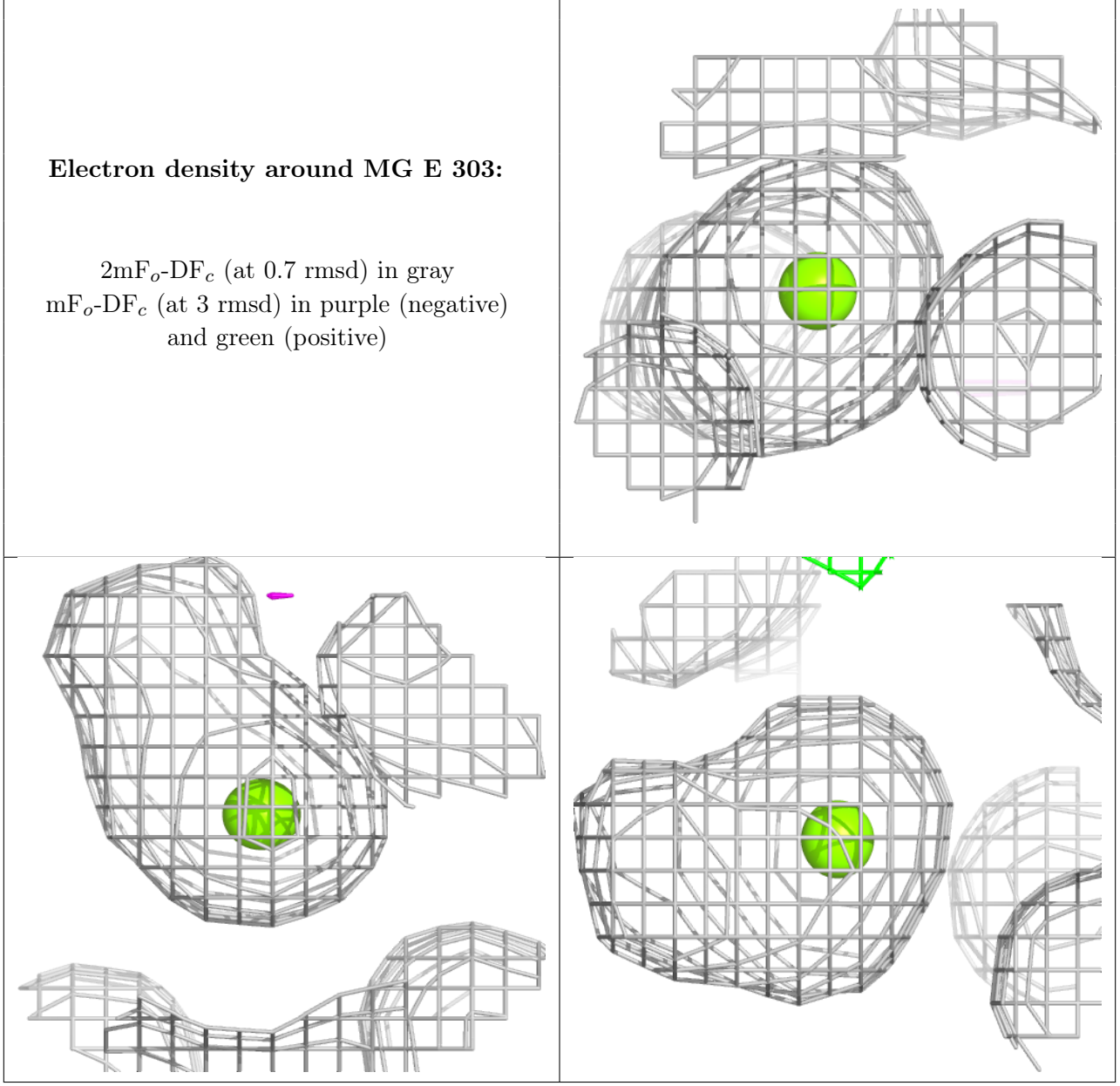






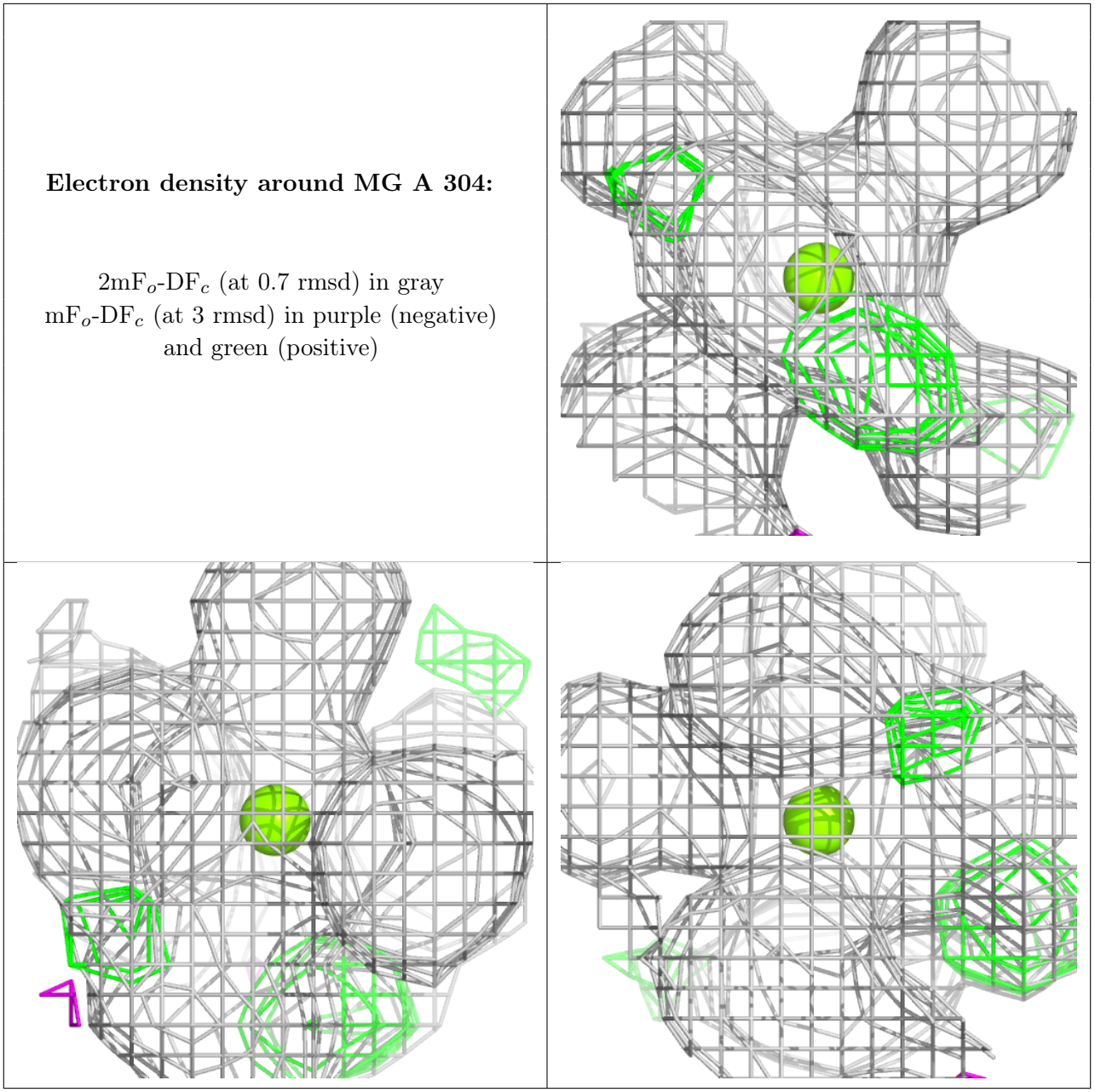
Electron density around MG E 303:

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



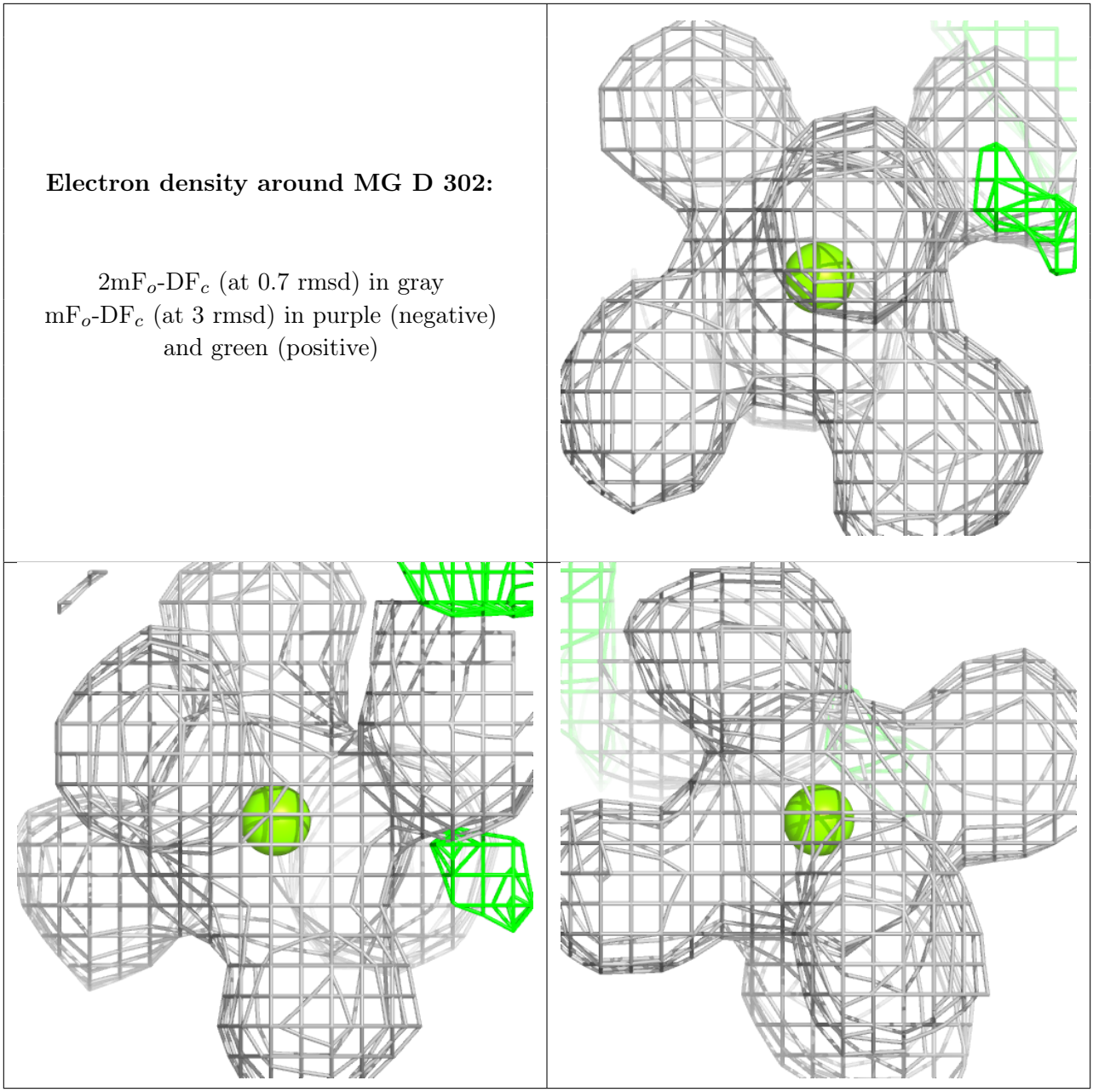
Electron density around MG A 304:

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



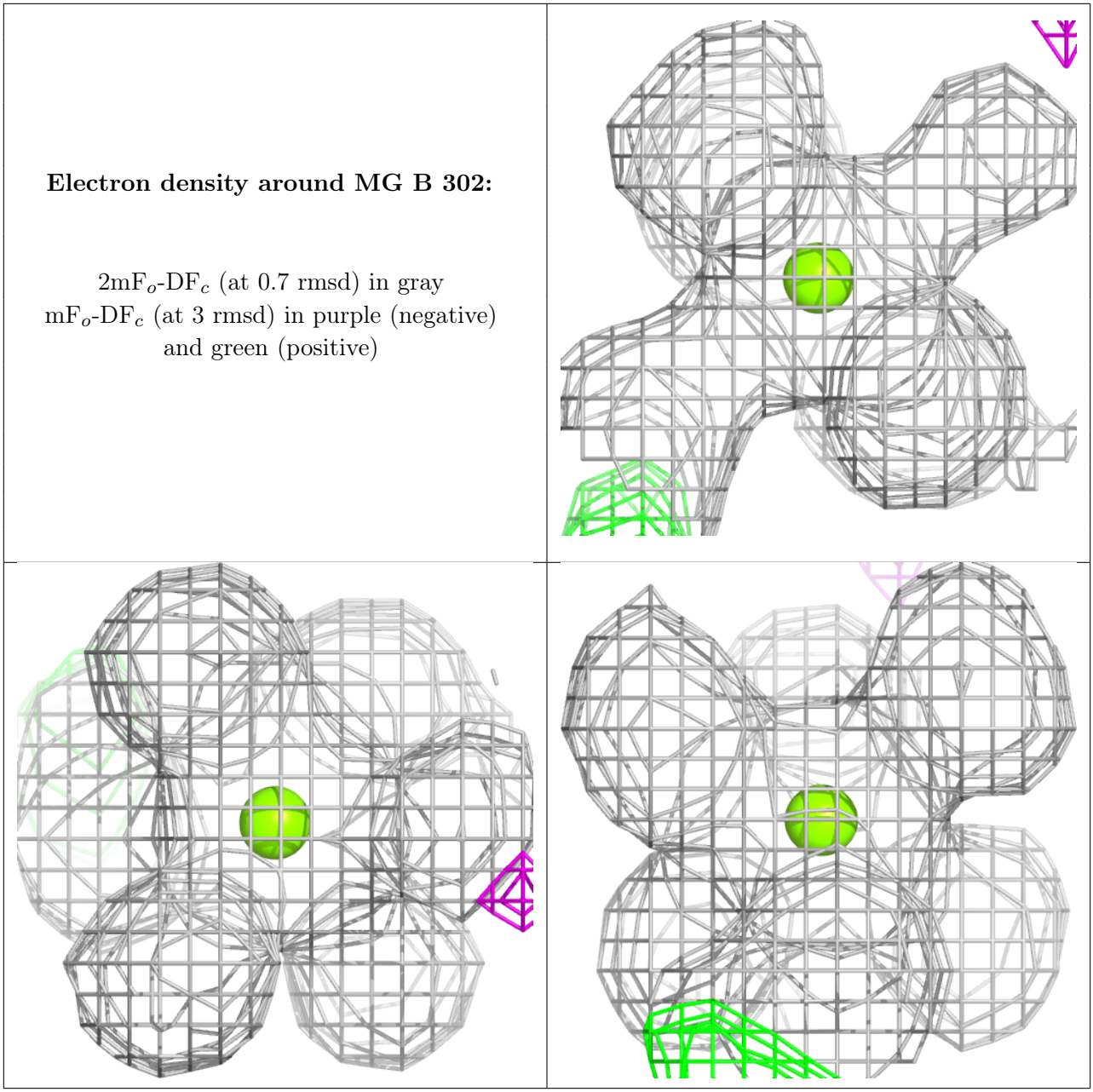
Electron density around MG D 302:

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



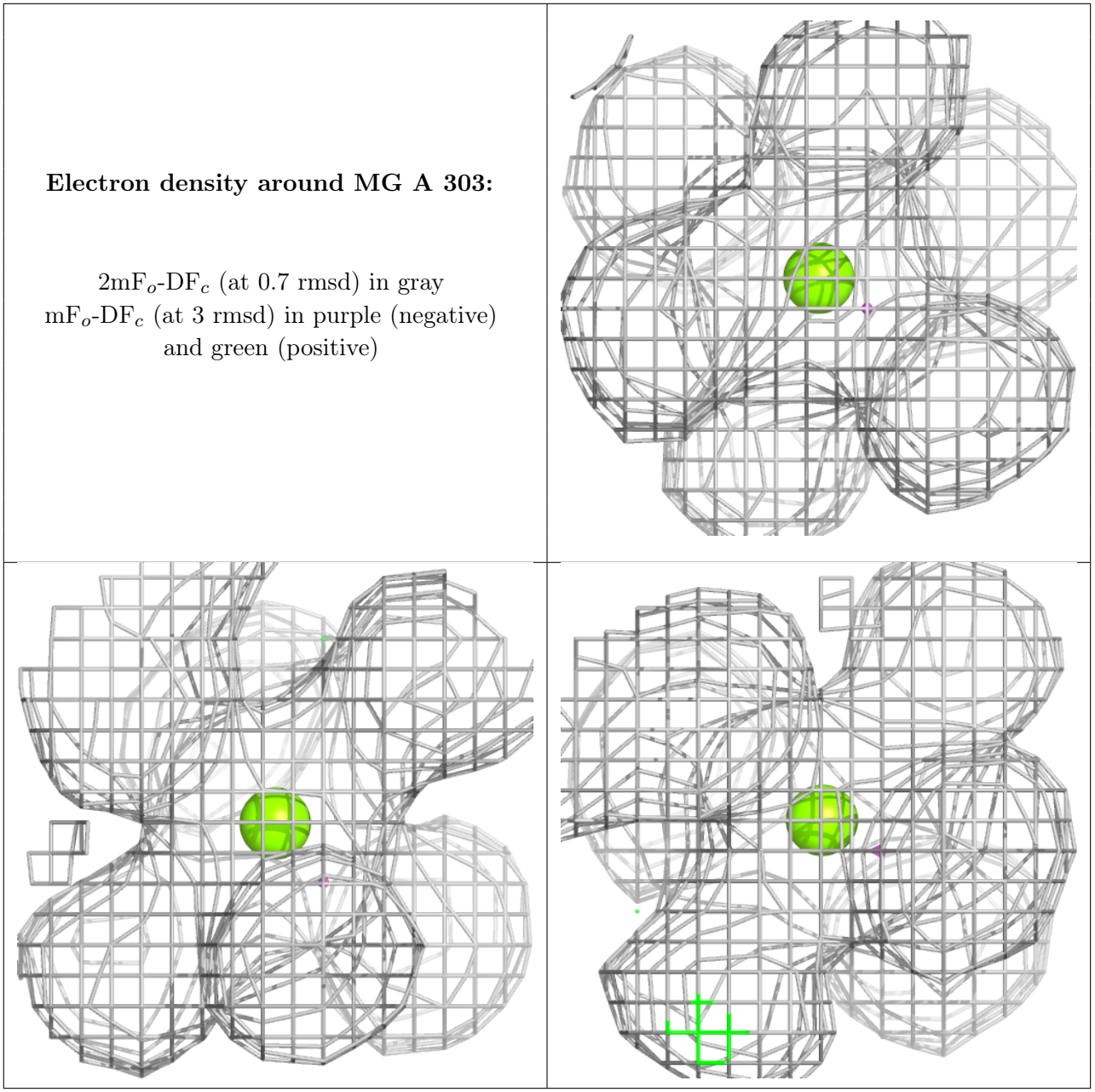
Electron density around MG B 302:

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



Electron density around MG A 303:

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



6.5 Other polymers

There are no such residues in this entry.