wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 05:36 AM EDT

PDB ID	:	7KLY
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H59N mutant with pyruvate bound in the active site and L-lysine bound at the allosteric site
Authors	:	Saran, S.; Sanders, D.A.R.
Deposited on	:	2020-11-01
Resolution	:	1.67 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:

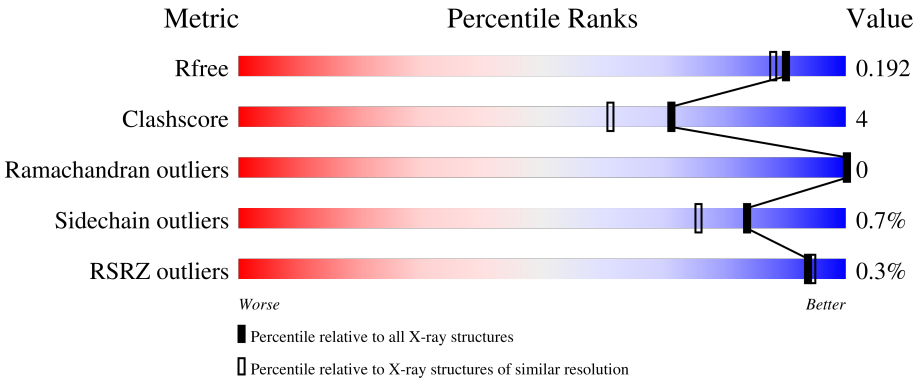
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.67 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	% 90% 5% 5%
1	B	310	88% 7% 5%
1	C	310	88% 6% • 5%
1	D	310	87% 8% 5%
1	E	310	89% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	92%

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
3	PG4	A	302	-	-	X	-
3	PG4	C	302	-	-	X	-
4	EDO	D	306	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15100 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
			2281	1449	380	439	13			
1	B	296	Total	C	N	O	S	0	0	0
			2278	1448	378	439	13			
1	C	296	Total	C	N	O	S	0	5	0
			2287	1451	382	441	13			
1	D	296	Total	C	N	O	S	0	4	0
			2291	1453	382	443	13			
1	E	295	Total	C	N	O	S	0	1	0
			2275	1444	380	438	13			
1	F	297	Total	C	N	O	S	0	3	0
			2293	1454	382	444	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	59	ASN	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	59	ASN	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	59	ASN	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	59	ASN	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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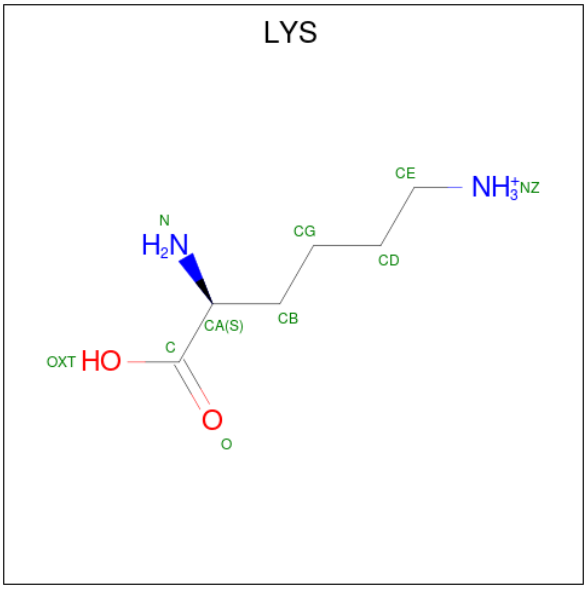
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	59	ASN	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	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	59	ASN	HIS	engineered mutation	UNP Q9PPB4

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		

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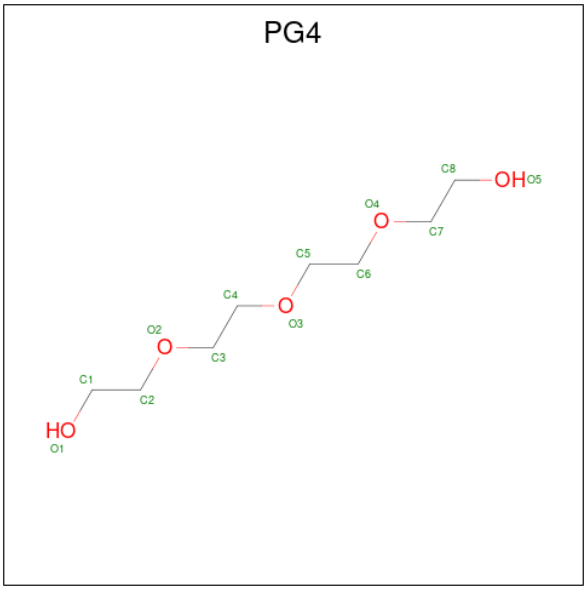
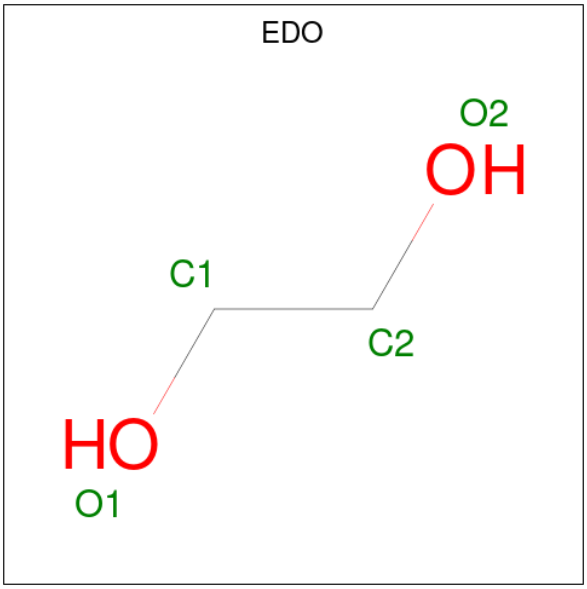
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 10 6 2 2	0	0
2	C	1	Total C N O 10 6 2 2	0	0
2	D	1	Total C N O 10 6 2 2	0	0
2	E	1	Total C N O 10 6 2 2	0	0
2	F	1	Total C N O 10 6 2 2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

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

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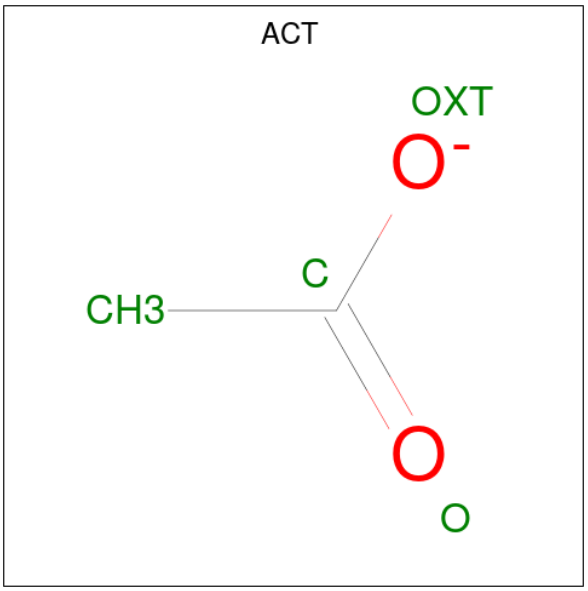
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



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

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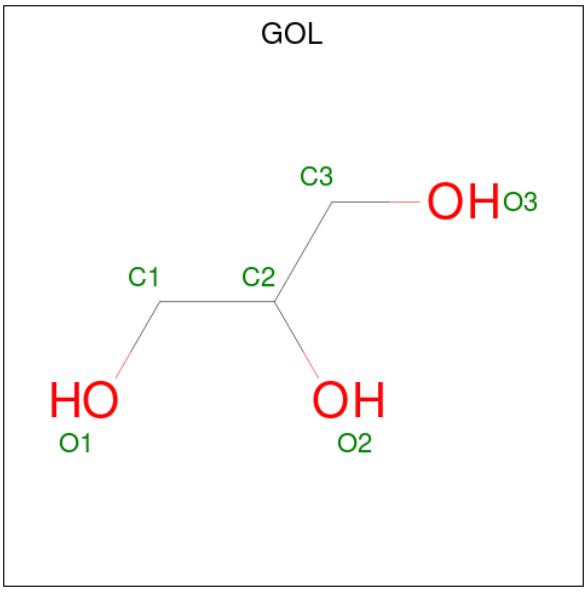
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

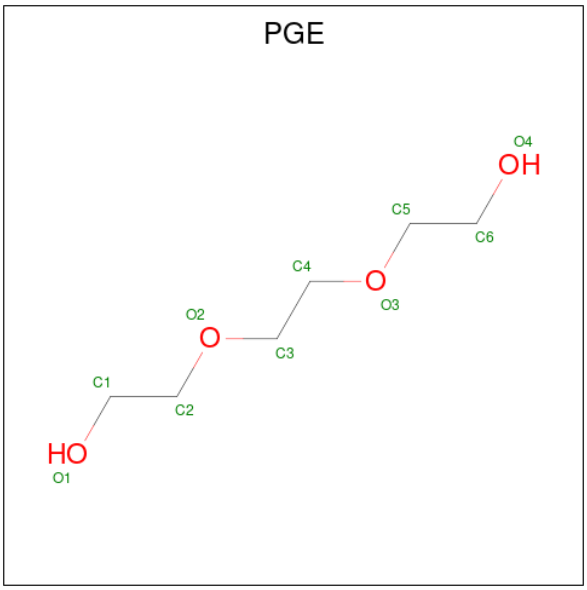
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0
6	B	6	Total Mg 6 6	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



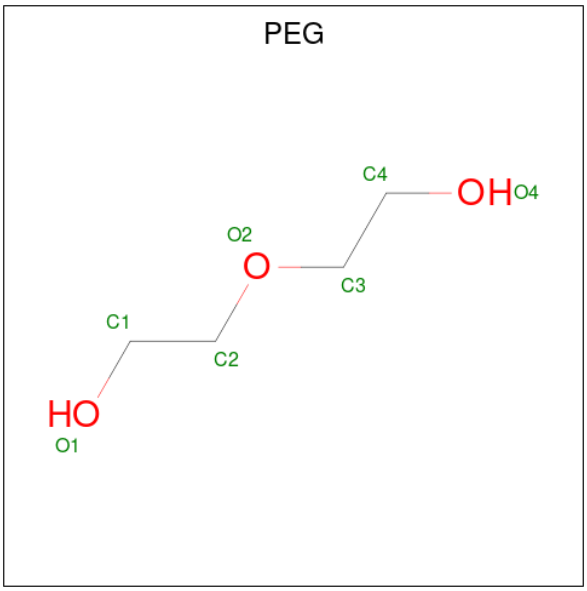
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: 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	C	1	Total C O 10 6 4	0	0
8	C	1	Total C O 10 6 4	0	0
8	D	1	Total C O 10 6 4	0	0
8	E	1	Total C O 10 6 4	0	0
8	F	1	Total C O 10 6 4	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is water.

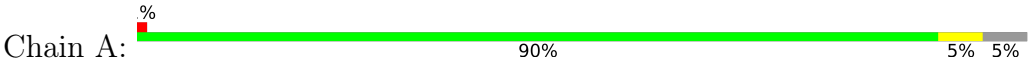
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	163	Total O 163 163	0	0
10	B	164	Total O 164 164	0	0
10	C	163	Total O 163 163	0	0
10	D	146	Total O 146 146	0	0
10	E	151	Total O 151 151	0	0
10	F	170	Total O 170 170	0	0

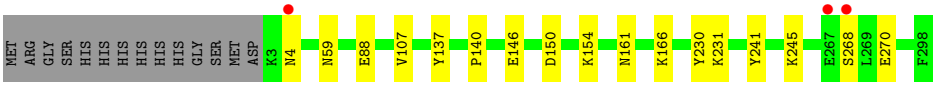
3 Residue-property plots (i)

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:



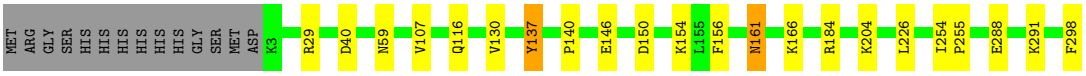


• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:

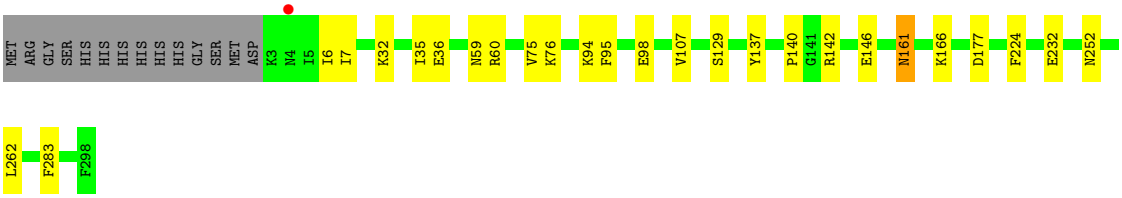
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C:



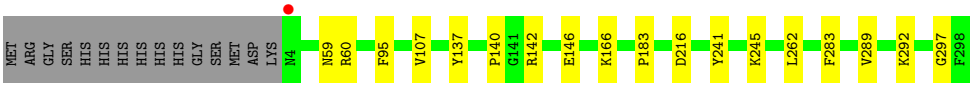
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D:



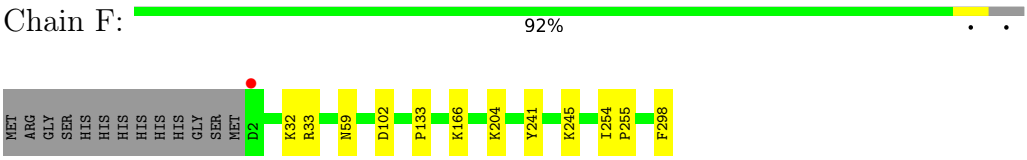
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.52Å 231.49Å 201.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 1.67 49.79 – 1.67	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.14-1.67) 100.0 (49.79-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 1.67Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.163 , 0.192 0.163 , 0.192	Depositor DCC
R_{free} test set	11485 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15100	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: PEG, PG4, KPI, MG, GOL, PGE, EDO, 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	0.54	0/2310	0.64	0/3121
1	B	0.59	0/2301	0.67	0/3109
1	C	0.60	0/2334	0.66	0/3154
1	D	0.54	0/2335	0.64	0/3154
1	E	0.55	0/2303	0.66	2/3112 (0.1%)
1	F	0.56	0/2330	0.64	0/3149
All	All	0.56	0/13913	0.66	2/18799 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	216	ASP	CB-CG-OD1	9.31	126.68	118.30
1	E	216	ASP	CB-CG-OD2	-5.10	113.71	118.30

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	2281	0	2323	19	0
1	B	2278	0	2318	16	0
1	C	2287	0	2324	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2291	0	2328	21	0
1	E	2275	0	2313	14	0
1	F	2293	0	2319	8	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
2	C	10	0	12	0	0
2	D	10	0	12	0	0
2	E	10	0	12	0	0
2	F	10	0	12	0	0
3	A	13	0	18	7	0
3	B	13	0	18	0	0
3	C	13	0	18	8	0
3	D	13	0	18	0	0
3	E	13	0	18	0	0
3	F	13	0	18	0	0
4	A	24	0	36	3	0
4	B	12	0	18	1	0
4	C	28	0	42	8	0
4	D	24	0	36	7	0
4	E	28	0	42	2	0
4	F	28	0	42	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	16	0	12	2	0
5	D	12	0	9	1	0
5	E	4	0	3	0	0
5	F	8	0	6	0	0
6	A	2	0	0	0	0
6	B	6	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	6	0	8	1	0
7	B	6	0	8	1	0
7	D	6	0	8	0	0
7	F	6	0	8	1	0
8	B	10	0	14	0	0
8	C	20	0	28	1	0
8	D	10	0	14	2	0
8	E	10	0	14	1	0
8	F	10	0	14	1	0
9	C	7	0	10	1	0
9	D	7	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	163	0	0	1	0
10	B	164	0	0	2	0
10	C	163	0	0	3	0
10	D	146	0	0	0	0
10	E	151	0	0	0	0
10	F	170	0	0	0	0
All	All	15100	0	14493	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 101 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:E:289:VAL:HA	1:E:292:LYS:NZ	1.84	0.93
1:A:154:LYS:HZ2	3:A:302:PG4:H51	1.34	0.92
1:C:154:LYS:HZ3	3:C:302:PG4:H42	1.35	0.88
1:E:289:VAL:HA	1:E:292:LYS:HZ2	1.46	0.77
1:D:76:LYS:HD2	4:D:306:EDO:H12	1.67	0.76

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%)	290 (99%)	4 (1%)	0	100	100
1	B	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	C	298/310 (96%)	294 (99%)	4 (1%)	0	100	100
1	D	297/310 (96%)	293 (99%)	4 (1%)	0	100	100
1	E	293/310 (94%)	289 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	297/310 (96%)	293 (99%)	4 (1%)	0	100	100
All	All	1772/1860 (95%)	1748 (99%)	24 (1%)	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%)	91	86
1	B	248/260 (95%)	246 (99%)	2 (1%)	81	72
1	C	252/260 (97%)	248 (98%)	4 (2%)	62	46
1	D	252/260 (97%)	249 (99%)	3 (1%)	71	57
1	E	248/260 (95%)	247 (100%)	1 (0%)	91	86
1	F	251/260 (96%)	250 (100%)	1 (0%)	91	86
All	All	1500/1560 (96%)	1488 (99%)	12 (1%)	84	72

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	59	ASN
1	D	161[A]	ASN
1	F	59	ASN
1	D	161[B]	ASN
1	C	59	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	A	166	1	11,13,14	1.82	3 (27%)	10,15,17	3.75	5 (50%)
1	KPI	E	166	1	11,13,14	0.76	0	10,15,17	3.16	4 (40%)
1	KPI	D	166	1	11,13,14	1.39	1 (9%)	10,15,17	3.19	4 (40%)
1	KPI	F	166	1	11,13,14	1.52	2 (18%)	10,15,17	3.32	5 (50%)
1	KPI	C	166	1	11,13,14	1.99	4 (36%)	10,15,17	3.71	5 (50%)
1	KPI	B	166	1	11,13,14	1.38	1 (9%)	10,15,17	2.82	4 (40%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	O2-CX2	4.69	1.35	1.22
1	A	166	KPI	O2-CX2	4.55	1.34	1.22
1	B	166	KPI	O-C	3.52	1.34	1.19
1	D	166	KPI	O-C	3.45	1.33	1.19
1	F	166	KPI	O-C	3.37	1.33	1.19

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	KPI	C1-CX1-CX2	-7.87	110.52	118.17
1	F	166	KPI	O2-CX2-CX1	7.73	131.25	121.38
1	C	166	KPI	C1-CX1-CX2	-7.46	110.91	118.17
1	D	166	KPI	C1-CX1-CX2	-7.32	111.05	118.17
1	E	166	KPI	O2-CX2-CX1	6.49	129.66	121.38

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 82 ligands modelled in this entry, 10 are monoatomic - leaving 72 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	GOL	F	313	-	5,5,5	0.40	0	5,5,5	0.26	0
5	ACT	C	312	-	3,3,3	0.76	0	3,3,3	1.32	0
4	EDO	C	307	-	3,3,3	0.41	0	2,2,2	0.39	0
4	EDO	F	303	-	3,3,3	0.54	0	2,2,2	0.10	0
2	LYS	E	301	-	8,9,9	0.67	0	9,10,10	1.04	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LYS	A	301	-	8,9,9	1.10	1 (12%)	9,10,10	0.84	0
4	EDO	D	304	-	3,3,3	0.48	0	2,2,2	0.66	0
4	EDO	C	306	-	3,3,3	0.51	0	2,2,2	0.49	0
4	EDO	E	305	-	3,3,3	0.57	0	2,2,2	0.14	0
4	EDO	E	307	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	F	305	-	3,3,3	0.56	0	2,2,2	0.38	0
4	EDO	C	303	-	3,3,3	0.58	0	2,2,2	0.29	0
4	EDO	F	306	-	3,3,3	0.43	0	2,2,2	0.36	0
5	ACT	C	313	-	3,3,3	0.75	0	3,3,3	1.41	0
8	PGE	D	312	-	9,9,9	0.32	0	8,8,8	0.37	0
4	EDO	F	309	-	3,3,3	0.57	0	2,2,2	0.18	0
8	PGE	B	307	-	9,9,9	0.33	0	8,8,8	0.38	0
4	EDO	D	306	-	3,3,3	0.28	0	2,2,2	1.03	0
4	EDO	F	308	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	304	-	3,3,3	0.49	0	2,2,2	0.43	0
3	PG4	D	302	-	12,12,12	0.50	0	11,11,11	0.25	0
4	EDO	D	308	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	D	307	-	3,3,3	0.43	0	2,2,2	0.49	0
3	PG4	C	302	-	12,12,12	0.51	0	11,11,11	0.45	0
4	EDO	D	303	-	3,3,3	0.60	0	2,2,2	0.32	0
4	EDO	D	305	-	3,3,3	0.38	0	2,2,2	0.62	0
4	EDO	E	304	-	3,3,3	0.46	0	2,2,2	0.42	0
9	PEG	D	315	-	6,6,6	0.52	0	5,5,5	0.50	0
4	EDO	A	303	-	3,3,3	0.55	0	2,2,2	0.27	0
7	GOL	B	314	-	5,5,5	0.46	0	5,5,5	0.23	0
4	EDO	C	305	-	3,3,3	0.46	0	2,2,2	0.53	0
5	ACT	E	310	-	3,3,3	0.87	0	3,3,3	1.36	0
8	PGE	C	314	-	9,9,9	0.33	0	8,8,8	0.38	0
4	EDO	E	309	-	3,3,3	0.44	0	2,2,2	0.27	0
5	ACT	B	306	-	3,3,3	0.80	0	3,3,3	1.34	0
7	GOL	A	312	-	5,5,5	0.41	0	5,5,5	0.12	0
3	PG4	E	302	-	12,12,12	0.53	0	11,11,11	0.12	0
4	EDO	E	306	-	3,3,3	0.41	0	2,2,2	0.57	0
4	EDO	E	303	-	3,3,3	0.43	0	2,2,2	0.50	0
3	PG4	F	302	-	12,12,12	0.53	0	11,11,11	0.32	0
4	EDO	F	307	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	C	309	-	3,3,3	0.47	0	2,2,2	0.41	0
4	EDO	A	306	-	3,3,3	0.40	0	2,2,2	0.33	0
5	ACT	A	309	-	3,3,3	0.76	0	3,3,3	1.45	0
2	LYS	F	301	-	8,9,9	1.02	0	9,10,10	0.74	0
4	EDO	C	304	-	3,3,3	0.41	0	2,2,2	0.14	0
4	EDO	B	303	-	3,3,3	0.35	0	2,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LYS	C	301	-	8,9,9	0.91	0	9,10,10	1.12	1 (11%)
3	PG4	B	302	-	12,12,12	0.51	0	11,11,11	0.35	0
5	ACT	C	311	-	3,3,3	0.70	0	3,3,3	1.24	0
7	GOL	D	314	-	5,5,5	0.38	0	5,5,5	0.17	0
4	EDO	E	308	-	3,3,3	0.51	0	2,2,2	0.15	0
5	ACT	D	310	-	3,3,3	0.83	0	3,3,3	1.16	0
8	PGE	F	312	-	9,9,9	0.30	0	8,8,8	0.49	0
2	LYS	D	301	-	8,9,9	0.92	0	9,10,10	0.95	1 (11%)
4	EDO	B	305	-	3,3,3	0.50	0	2,2,2	0.29	0
4	EDO	A	305	-	3,3,3	0.53	0	2,2,2	0.33	0
5	ACT	D	309	-	3,3,3	0.86	0	3,3,3	1.56	1 (33%)
5	ACT	C	310	-	3,3,3	0.79	0	3,3,3	1.21	0
9	PEG	C	317	-	6,6,6	0.47	0	5,5,5	0.33	0
2	LYS	B	301	-	8,9,9	0.80	0	9,10,10	1.02	0
5	ACT	D	311	-	3,3,3	0.77	0	3,3,3	1.48	0
8	PGE	C	315	-	9,9,9	0.33	0	8,8,8	0.38	0
4	EDO	A	307	-	3,3,3	0.41	0	2,2,2	0.68	0
5	ACT	F	311	-	3,3,3	0.77	0	3,3,3	1.34	0
8	PGE	E	311	-	9,9,9	0.34	0	8,8,8	0.30	0
4	EDO	C	308	-	3,3,3	0.53	0	2,2,2	0.62	0
5	ACT	F	310	-	3,3,3	0.75	0	3,3,3	1.44	0
3	PG4	A	302	-	12,12,12	0.51	0	11,11,11	0.51	0
4	EDO	B	304	-	3,3,3	0.61	0	2,2,2	0.27	0
4	EDO	F	304	-	3,3,3	0.51	0	2,2,2	0.18	0
4	EDO	A	308	-	3,3,3	0.42	0	2,2,2	0.52	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
7	GOL	F	313	-	-	4/4/4/4	-
4	EDO	C	307	-	-	0/1/1/1	-
4	EDO	F	303	-	-	0/1/1/1	-
2	LYS	E	301	-	-	0/9/9/9	-
2	LYS	A	301	-	-	0/9/9/9	-
4	EDO	D	304	-	-	1/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	E	305	-	-	1/1/1/1	-
4	EDO	E	307	-	-	1/1/1/1	-
4	EDO	F	305	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	F	306	-	-	0/1/1/1	-
9	PEG	C	317	-	-	0/4/4/4	-
8	PGE	D	312	-	-	2/7/7/7	-
4	EDO	F	309	-	-	1/1/1/1	-
8	PGE	B	307	-	-	4/7/7/7	-
4	EDO	D	306	-	-	1/1/1/1	-
4	EDO	F	308	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
3	PG4	D	302	-	-	1/10/10/10	-
4	EDO	D	308	-	-	1/1/1/1	-
4	EDO	D	307	-	-	0/1/1/1	-
3	PG4	C	302	-	-	7/10/10/10	-
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	D	305	-	-	1/1/1/1	-
4	EDO	E	304	-	-	0/1/1/1	-
9	PEG	D	315	-	-	3/4/4/4	-
4	EDO	A	303	-	-	0/1/1/1	-
7	GOL	B	314	-	-	4/4/4/4	-
4	EDO	C	305	-	-	0/1/1/1	-
8	PGE	C	314	-	-	2/7/7/7	-
4	EDO	E	309	-	-	0/1/1/1	-
7	GOL	A	312	-	-	2/4/4/4	-
3	PG4	E	302	-	-	2/10/10/10	-
4	EDO	E	306	-	-	0/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
3	PG4	F	302	-	-	0/10/10/10	-
4	EDO	F	307	-	-	1/1/1/1	-
4	EDO	C	309	-	-	1/1/1/1	-
4	EDO	A	306	-	-	0/1/1/1	-
2	LYS	F	301	-	-	0/9/9/9	-
4	EDO	C	304	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
2	LYS	C	301	-	-	0/9/9/9	-
3	PG4	B	302	-	-	0/10/10/10	-
7	GOL	D	314	-	-	4/4/4/4	-
4	EDO	E	308	-	-	0/1/1/1	-
8	PGE	F	312	-	-	1/7/7/7	-
2	LYS	D	301	-	-	0/9/9/9	-
4	EDO	B	305	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	305	-	-	1/1/1/1	-
2	LYS	B	301	-	-	0/9/9/9	-
8	PGE	C	315	-	-	5/7/7/7	-
4	EDO	A	307	-	-	1/1/1/1	-
8	PGE	E	311	-	-	2/7/7/7	-
4	EDO	C	308	-	-	0/1/1/1	-
3	PG4	A	302	-	-	5/10/10/10	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	F	304	-	-	0/1/1/1	-
4	EDO	A	308	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	LYS	OXT-C	-2.11	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	LYS	OXT-C-O	-2.32	118.83	124.09
2	E	301	LYS	OXT-C-CA	2.15	120.69	113.38
2	D	301	LYS	OXT-C-CA	2.09	120.50	113.38
5	D	309	ACT	OXT-C-O	-2.06	114.47	122.05

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	312	GOL	O1-C1-C2-C3
7	B	314	GOL	O1-C1-C2-C3
7	D	314	GOL	C1-C2-C3-O3
7	D	314	GOL	O2-C2-C3-O3
7	F	313	GOL	O1-C1-C2-C3

There are no ring outliers.

24 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	313	GOL	1	0
4	C	307	EDO	2	0

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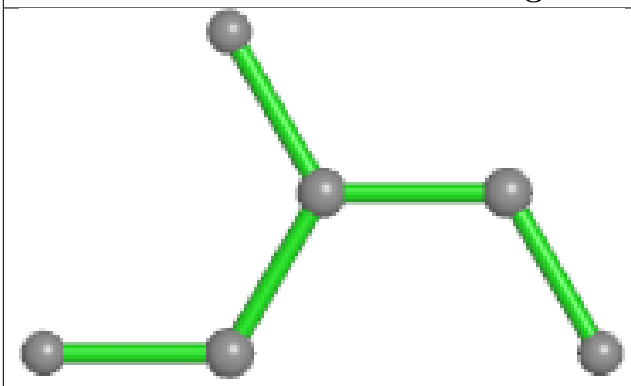
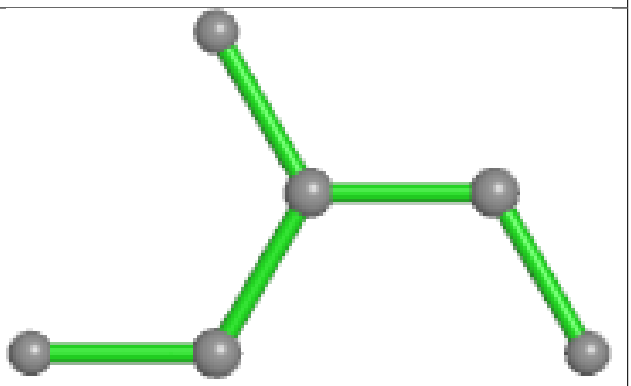
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	306	EDO	1	0
4	F	306	EDO	3	0
5	C	313	ACT	1	0
8	D	312	PGE	2	0
4	D	306	EDO	4	0
3	C	302	PG4	8	0
4	D	305	EDO	3	0
9	D	315	PEG	3	0
4	A	303	EDO	3	0
7	B	314	GOL	1	0
8	C	314	PGE	1	0
7	A	312	GOL	1	0
4	E	306	EDO	2	0
4	C	309	EDO	3	0
4	C	304	EDO	2	0
5	C	311	ACT	1	0
5	D	310	ACT	1	0
8	F	312	PGE	1	0
4	B	305	EDO	1	0
9	C	317	PEG	1	0
8	E	311	PGE	1	0
3	A	302	PG4	7	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.

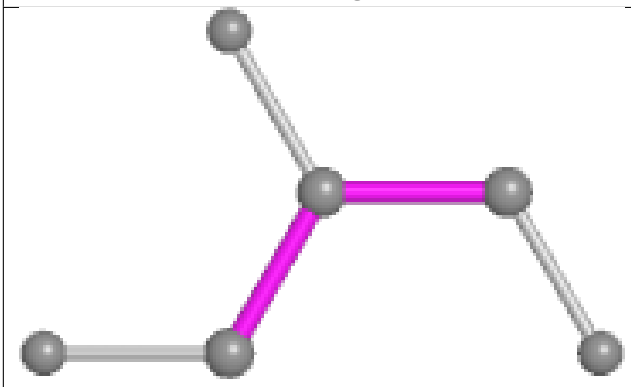
Ligand GOL F 313



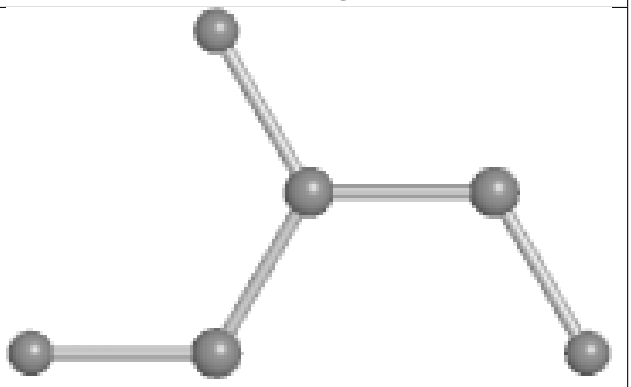
Bond lengths



Bond angles

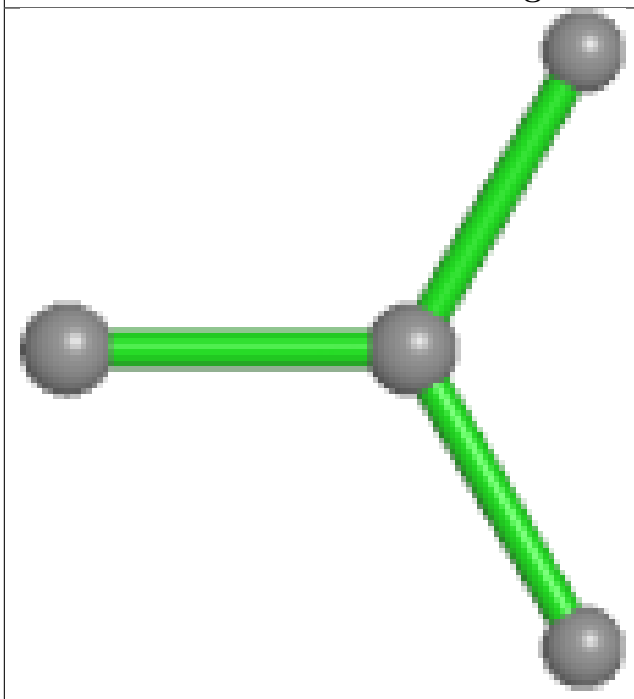


Torsions

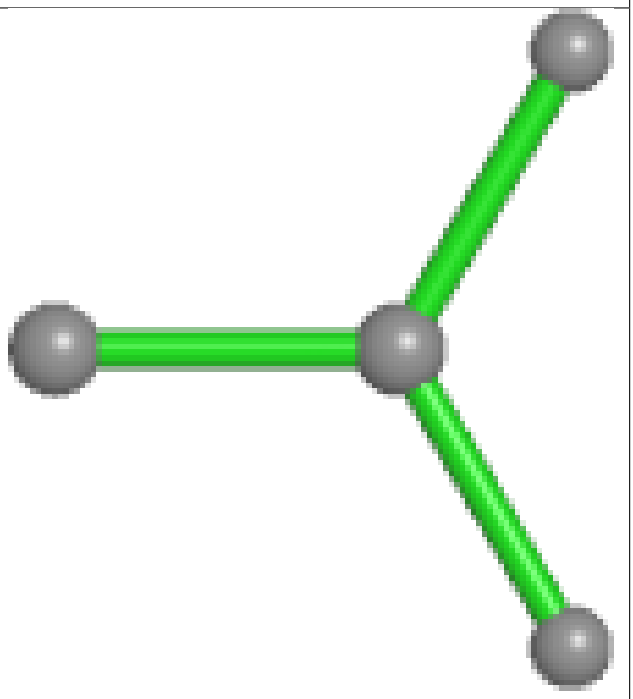


Rings

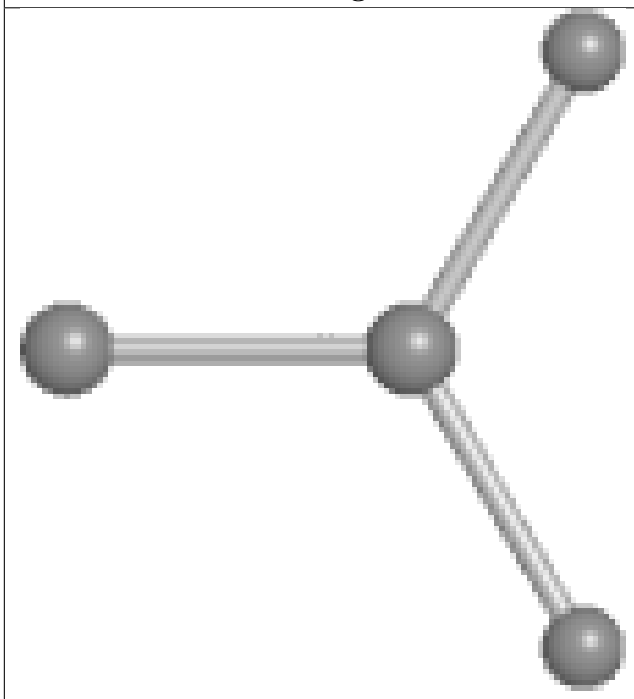
Ligand ACT C 312



Bond lengths



Bond angles



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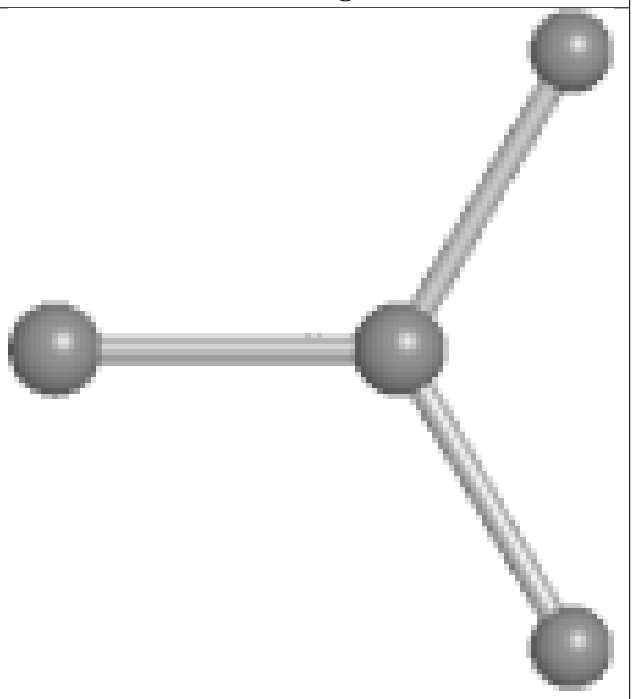
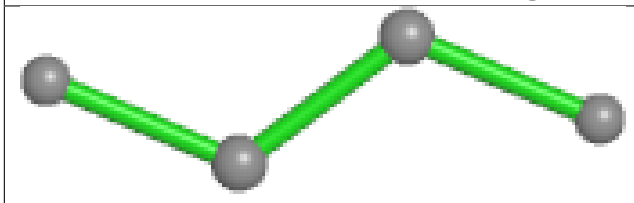


Rings

Ligand EDO C 307



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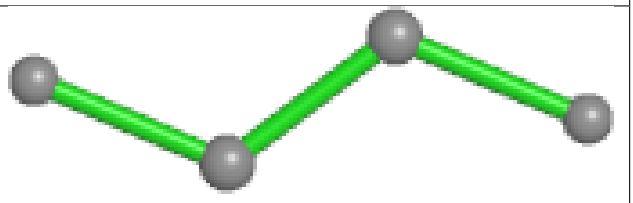
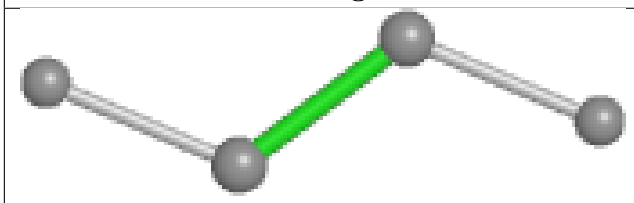


Bond angles



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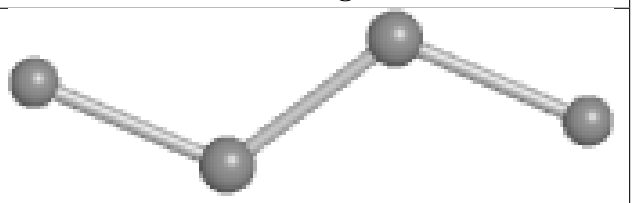
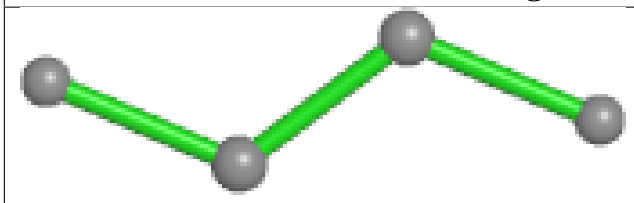


Rings

Ligand EDO F 303



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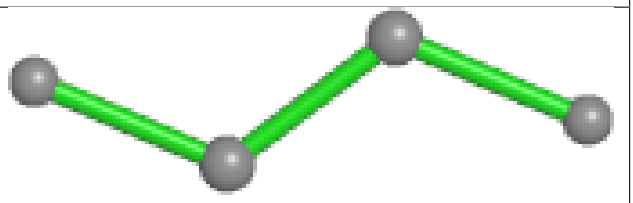
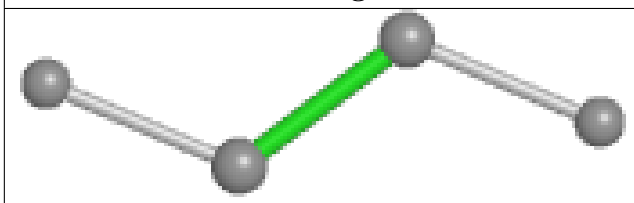


Bond angles



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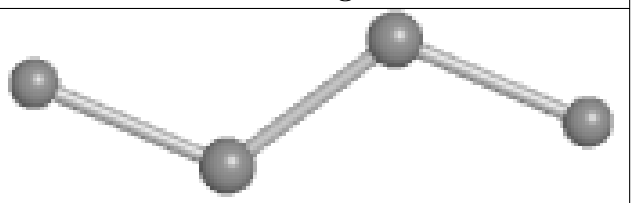
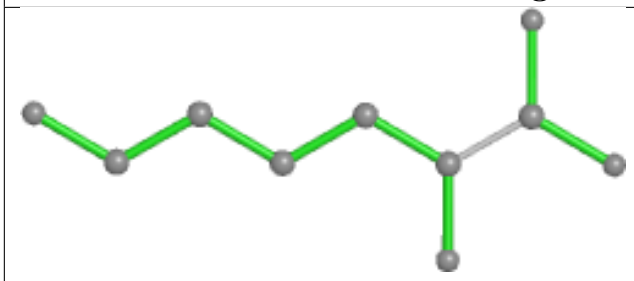


Rings

Ligand LYS E 301



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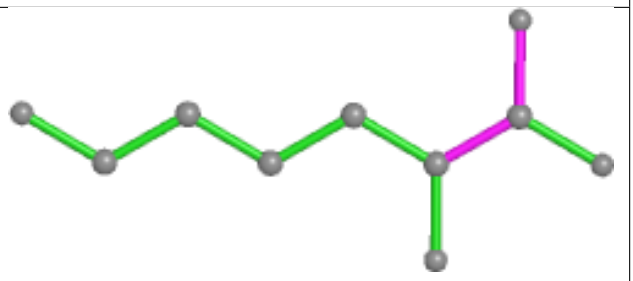

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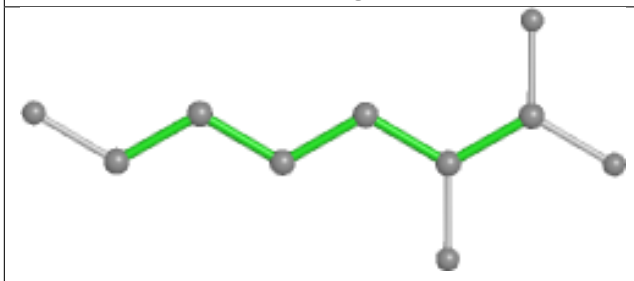

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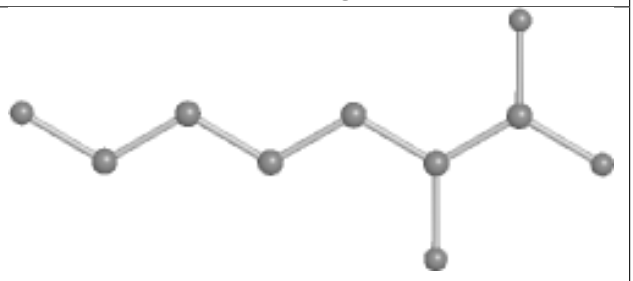

Rings

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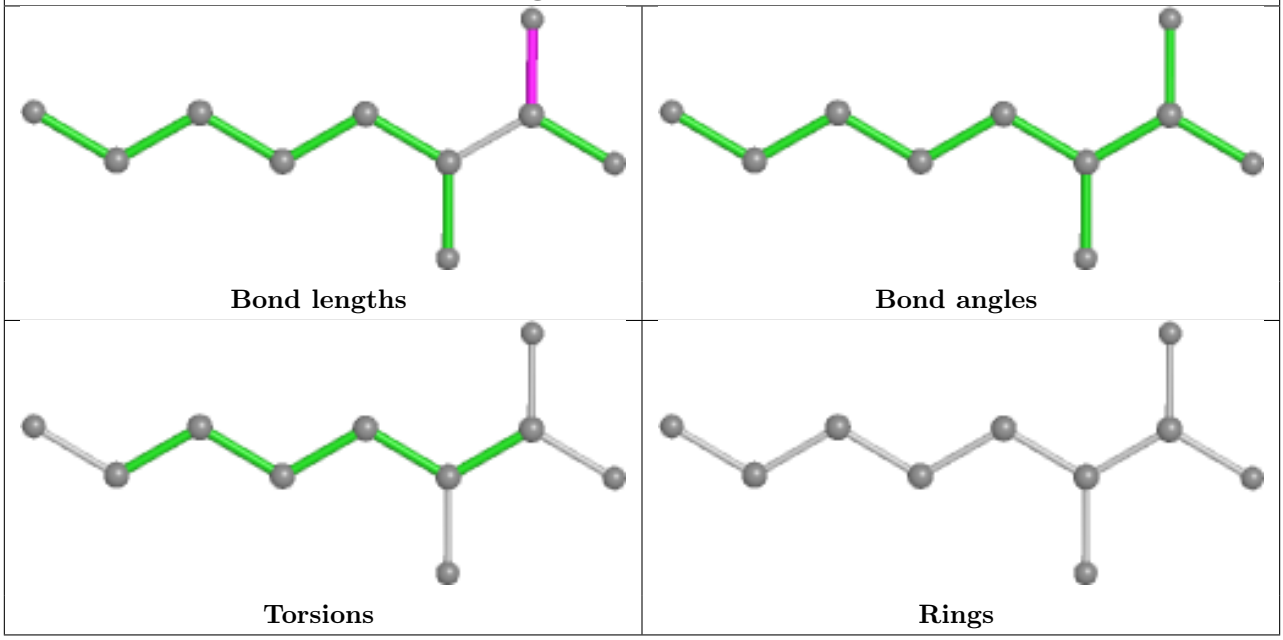
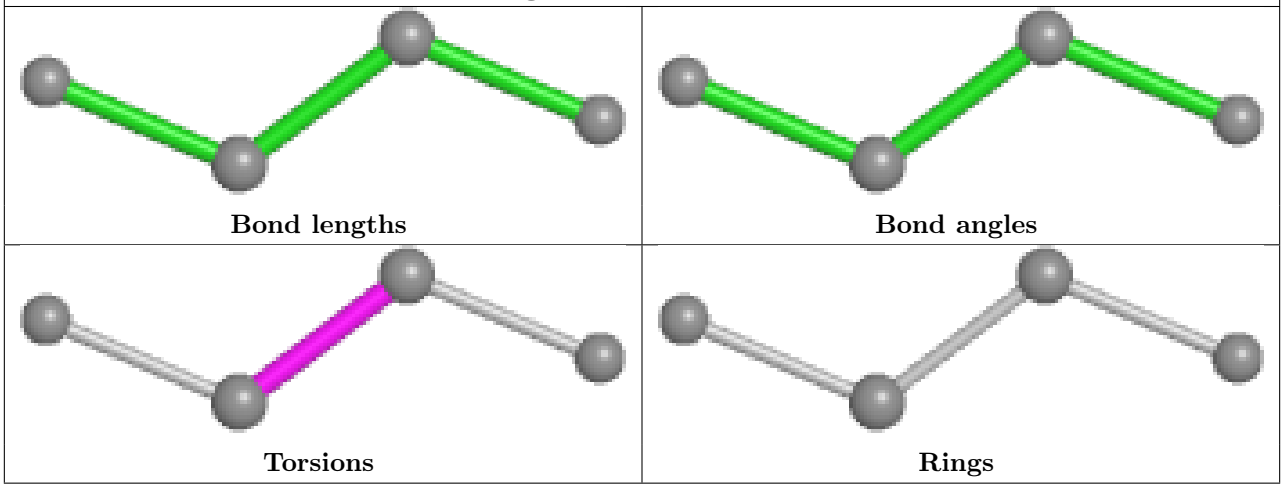
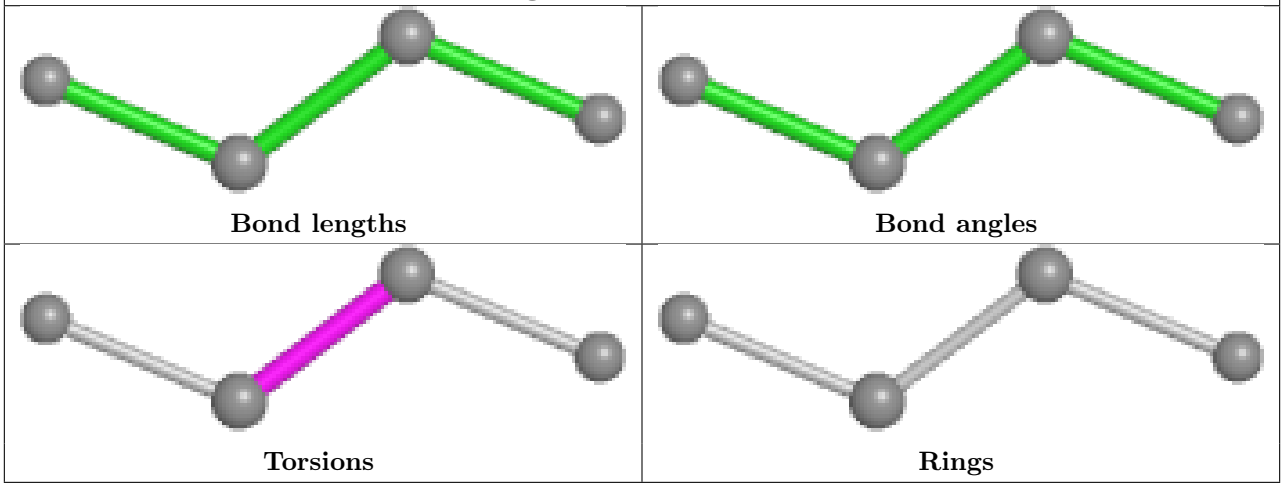


Ligand EDO D 304



Ligand EDO C 306



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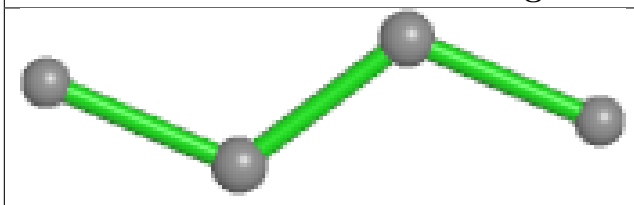
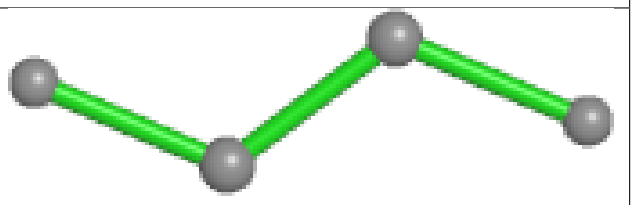
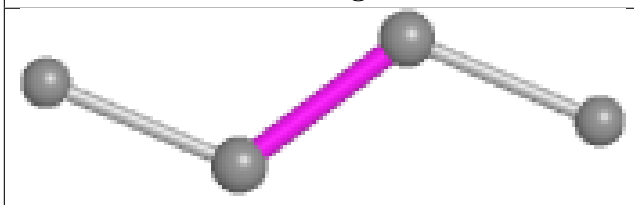


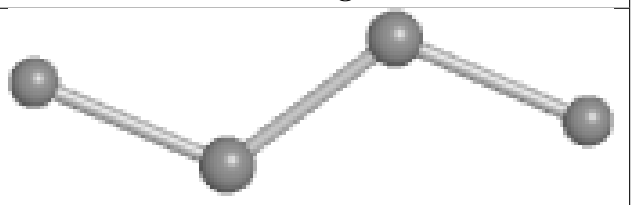
Bond lengths



Bond angles



Torsions



Rings

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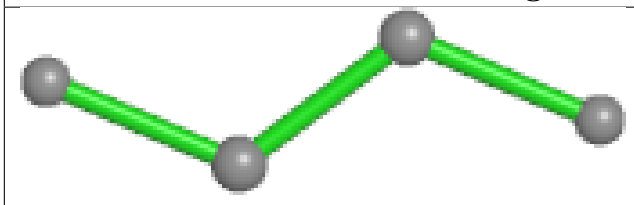

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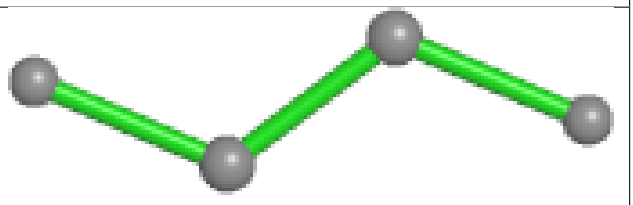
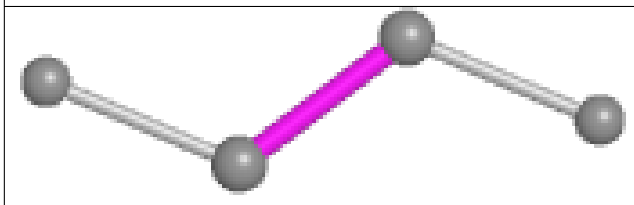


Bond angles



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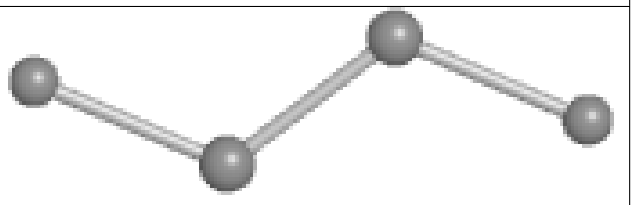
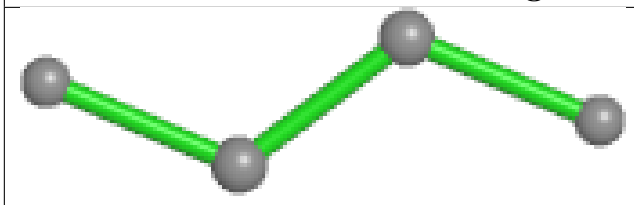


Rings

Ligand EDO F 305



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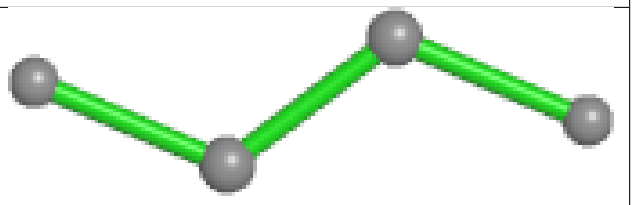
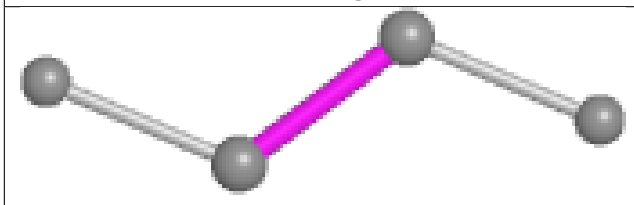
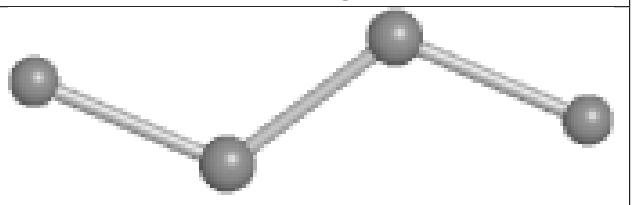


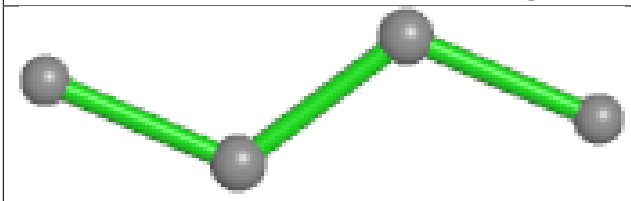
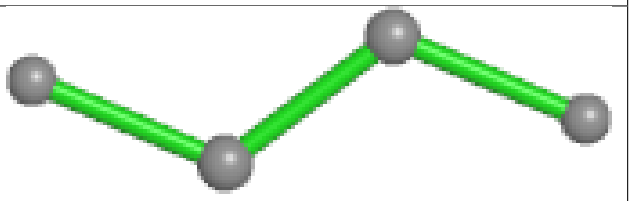
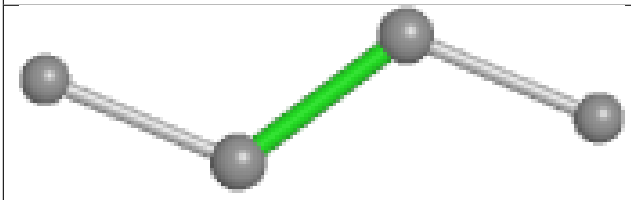
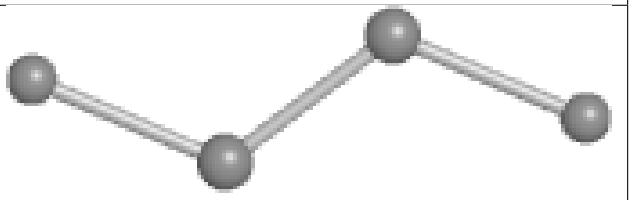
Bond angles



Torsions



Rings

Ligand EDO C 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

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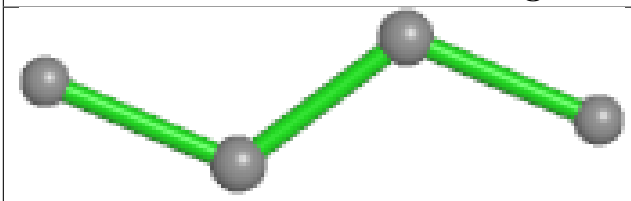
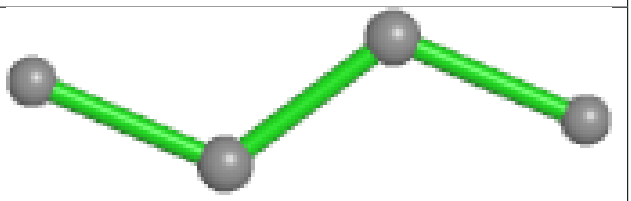
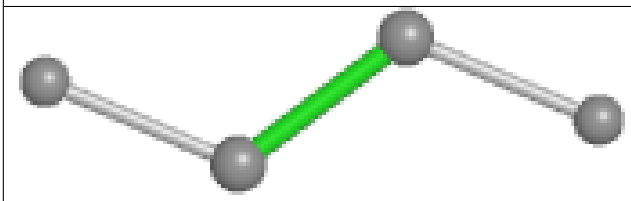
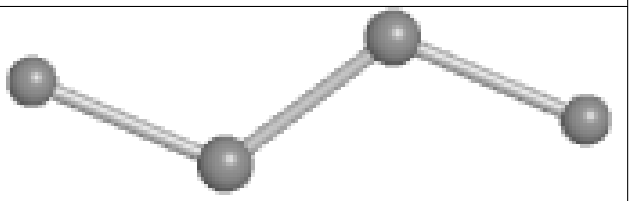
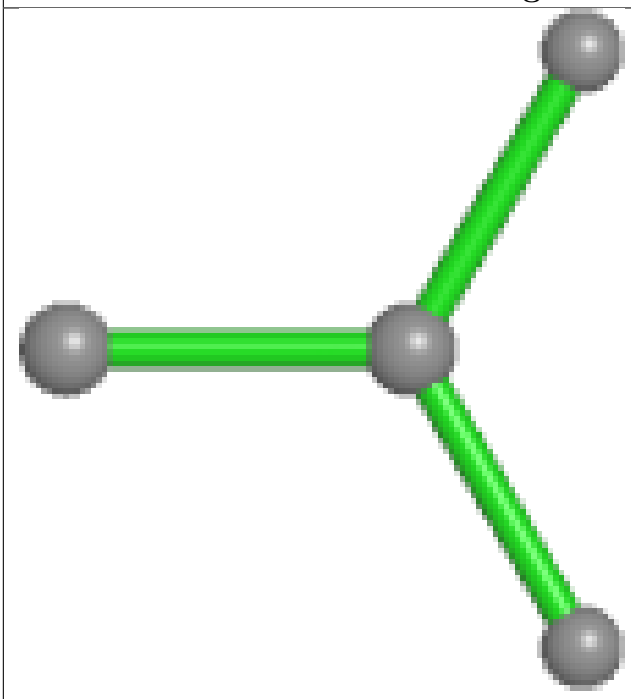
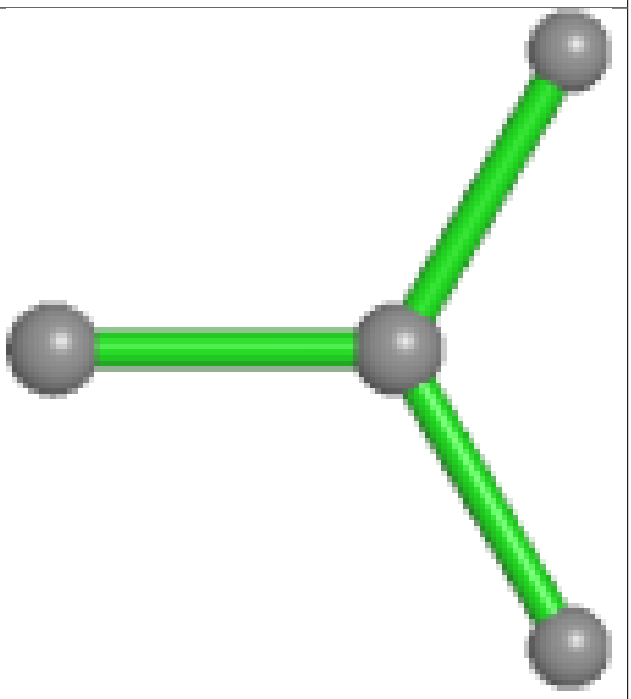
	
Bond lengths	Bond angles
	
Torsions	Rings

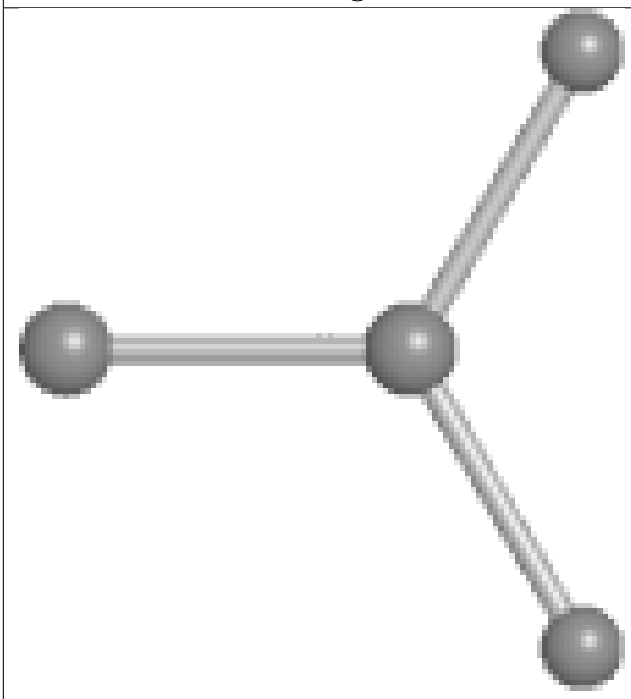
Ligand ACT C 313



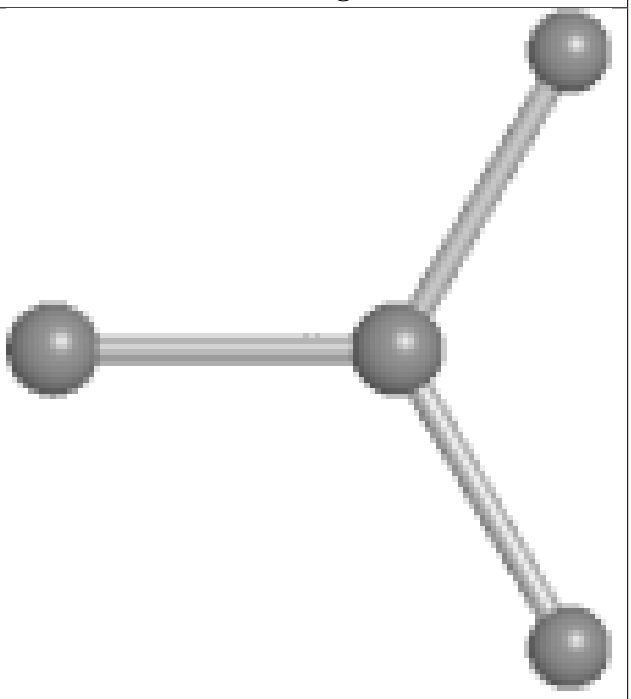
Bond lengths



Bond angles



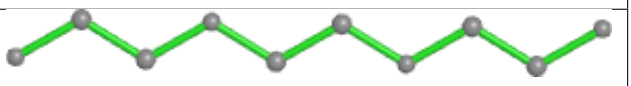
Torsions



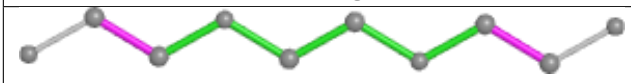
Rings

Ligand PGE D 312

Bond lengths



Bond angles



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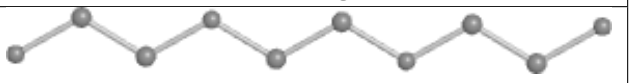
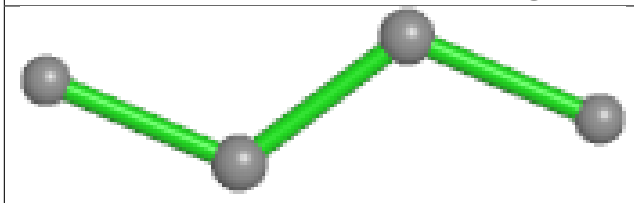


Rings

Ligand EDO F 309



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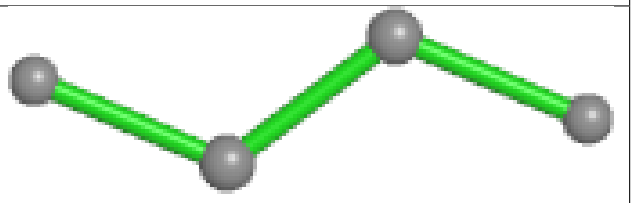
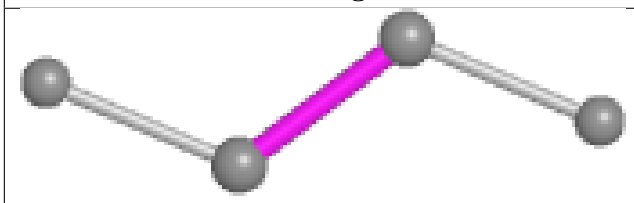


Bond angles



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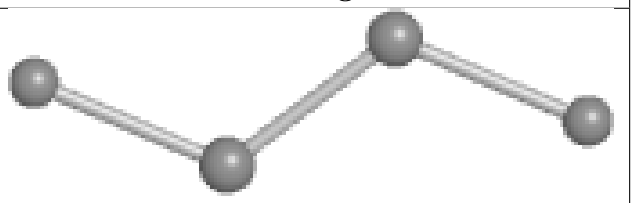
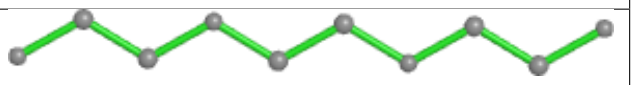


Rings

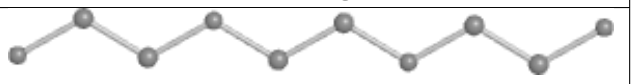
Ligand PGE B 307

Bond lengths



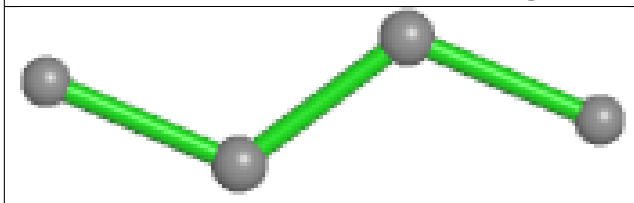
Bond angles

Torsions

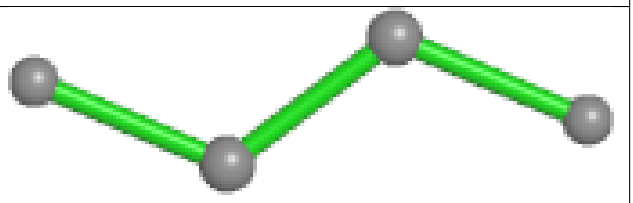


Rings

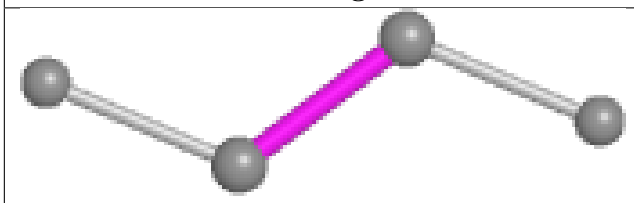
Ligand EDO D 306



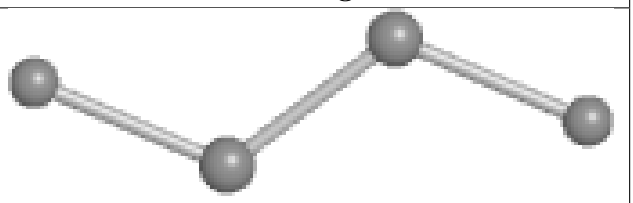
Bond lengths



Bond angles

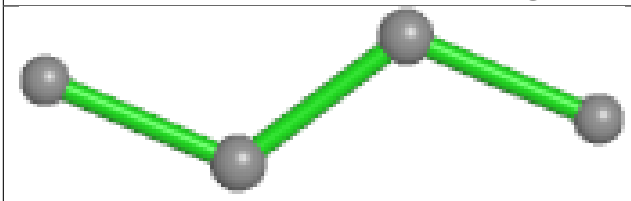


Torsions



Rings

Ligand EDO F 308



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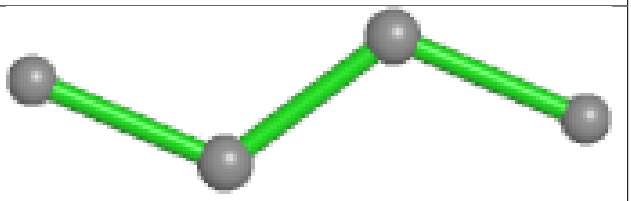
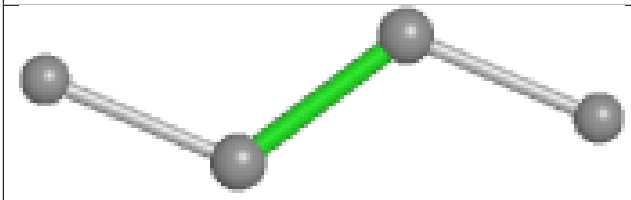


Bond angles



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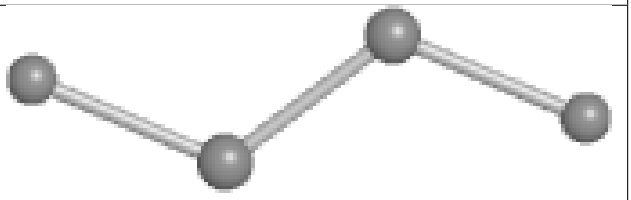
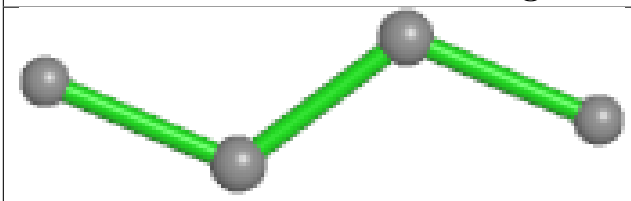


Rings

Ligand EDO A 304



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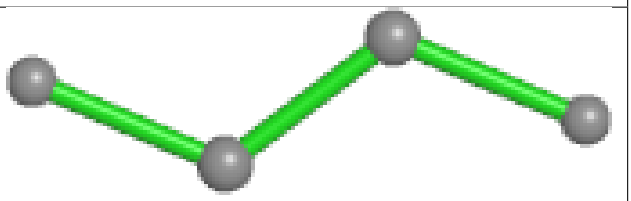
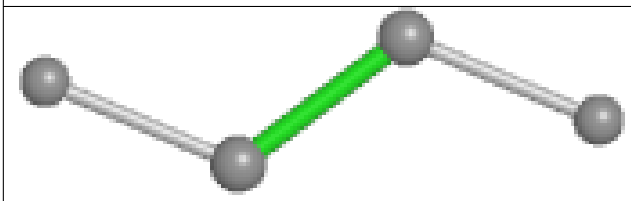


Bond angles



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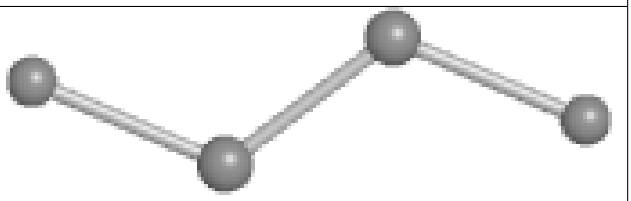
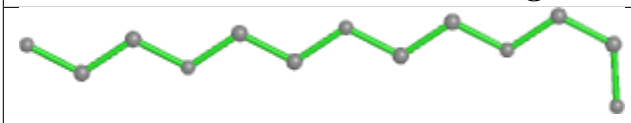
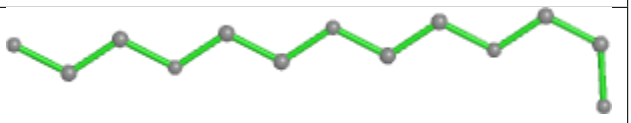


Rings

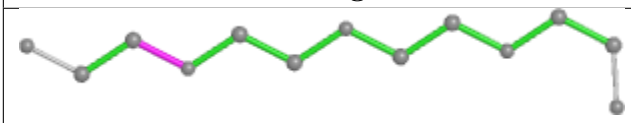
Ligand PG4 D 302



Bond lengths



Bond angles



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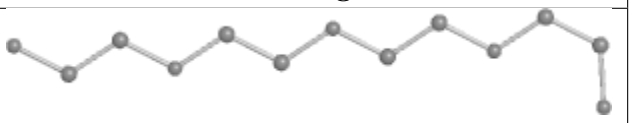
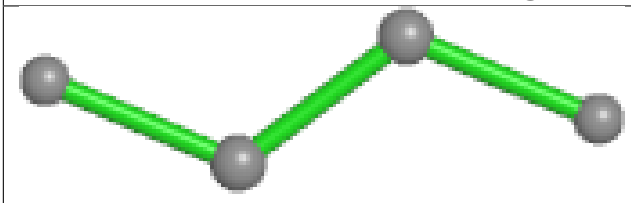


Rings

Ligand EDO D 308



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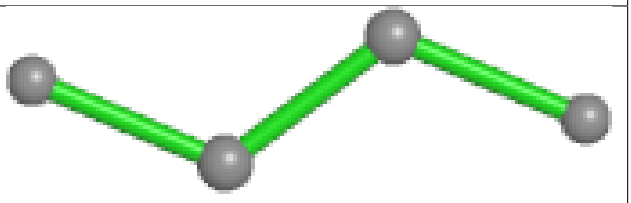
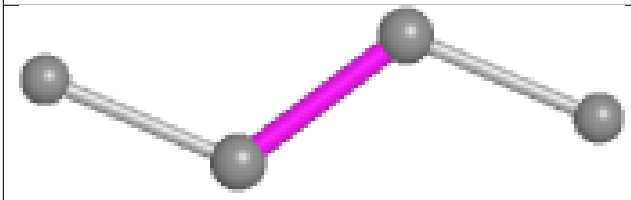


Bond angles



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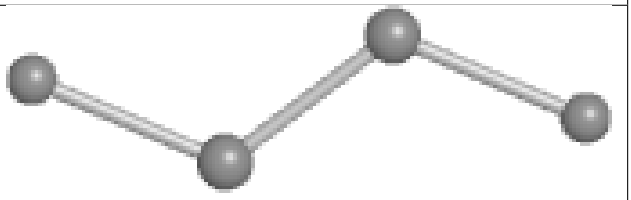
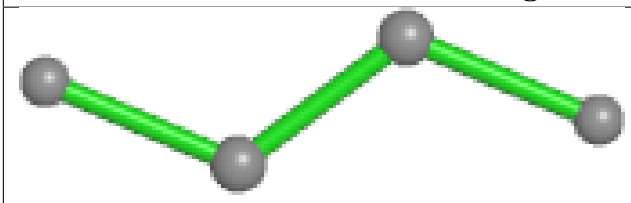
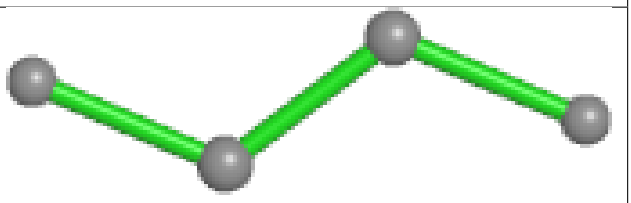


Rings

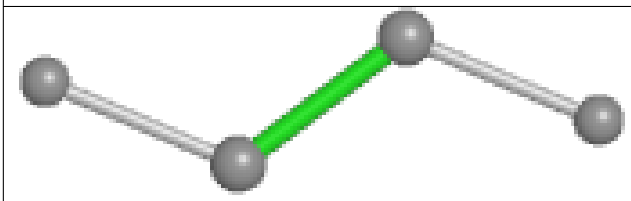
Ligand EDO D 307



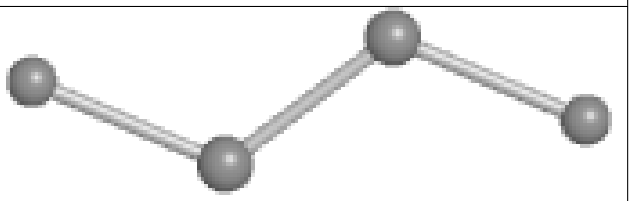
Bond lengths



Bond angles

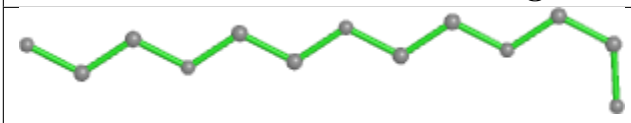


Torsions



Rings

Ligand PG4 C 302



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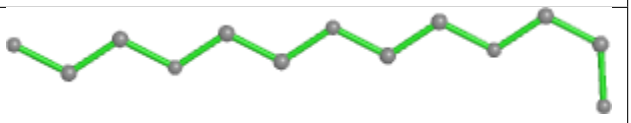
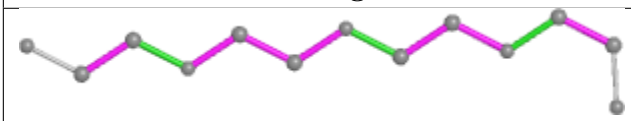
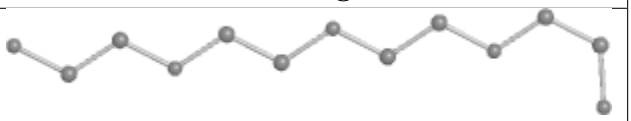


Bond angles

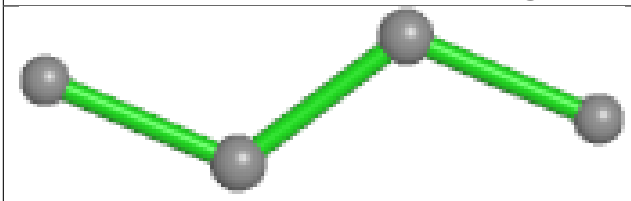


Torsions



Rings

Ligand EDO D 303



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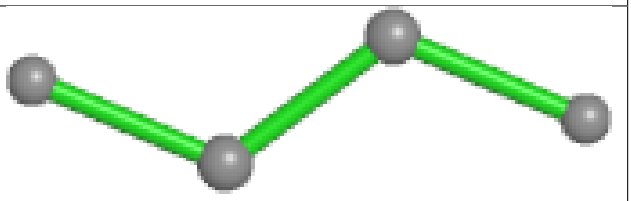
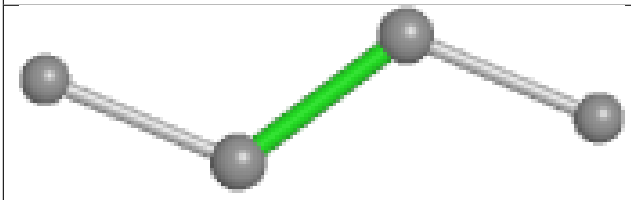


Bond angles



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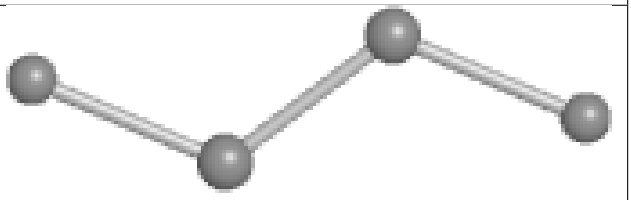
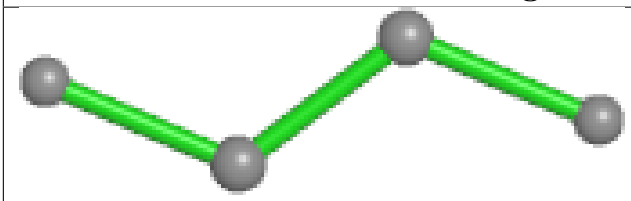


Rings

Ligand EDO D 305



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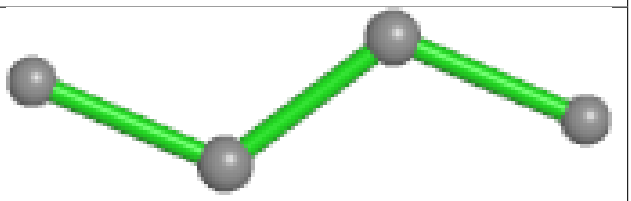
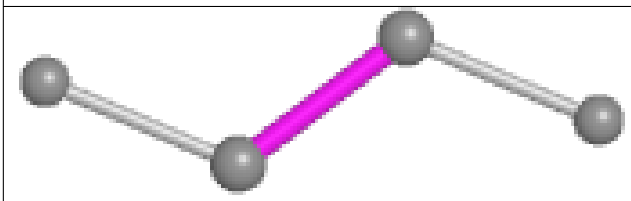


Bond angles



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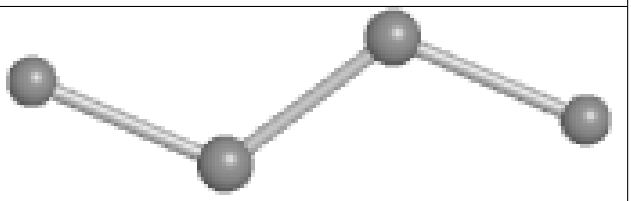
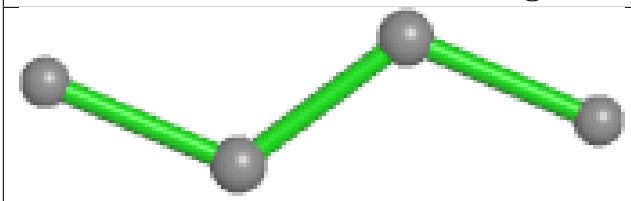


Rings

Ligand EDO E 304



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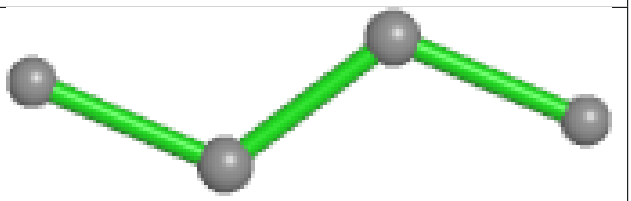
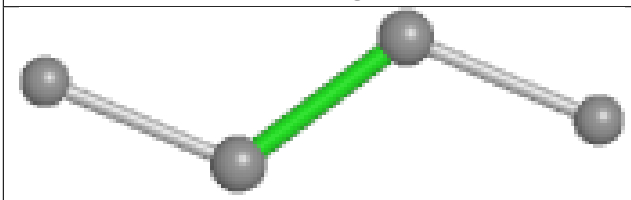
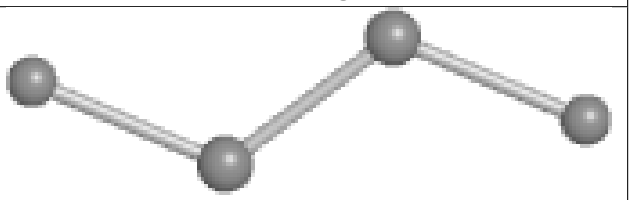


Bond angles

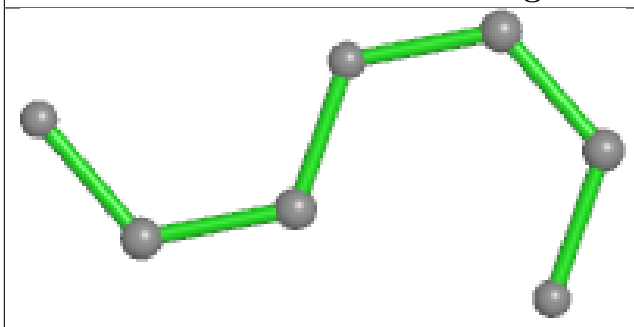


Torsions



Rings

Ligand PEG D 315



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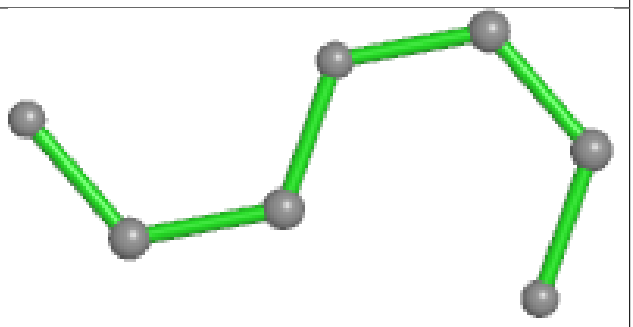
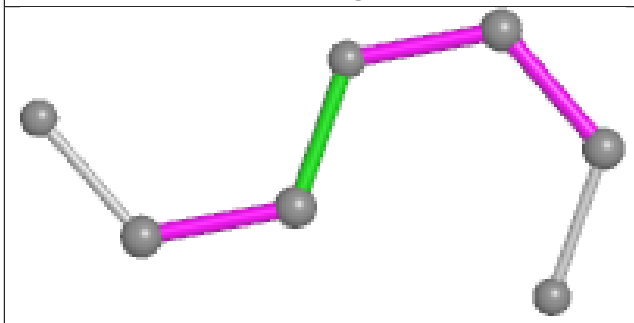
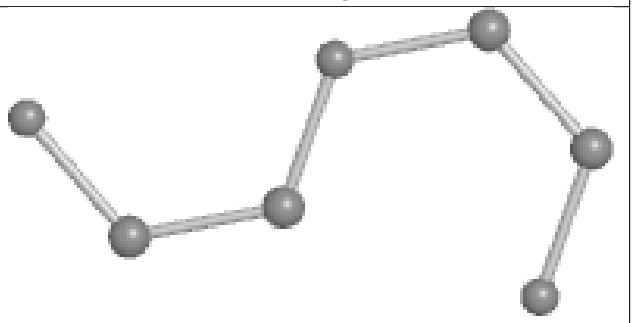


Bond angles

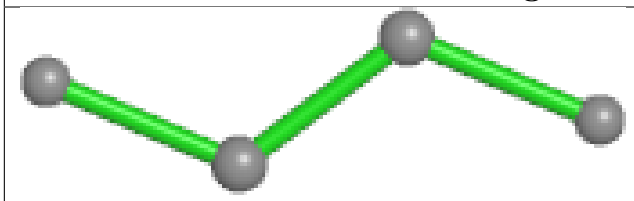


Torsions

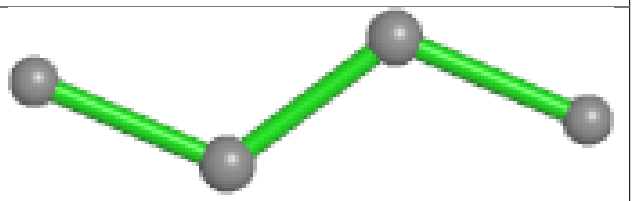


Rings

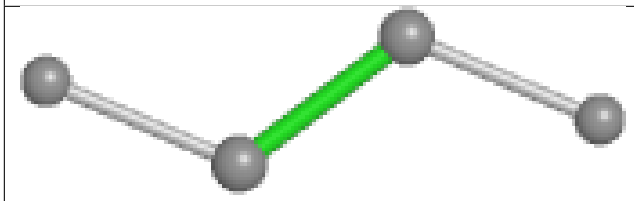
Ligand EDO A 303



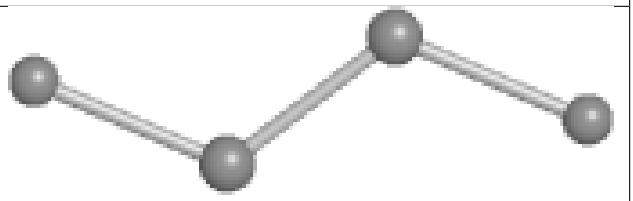
Bond lengths



Bond angles

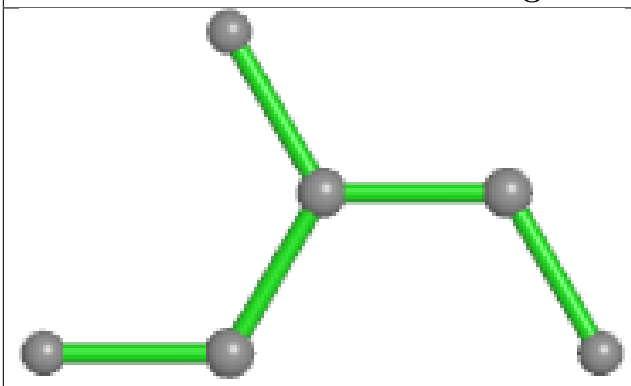


Torsions



Rings

Ligand GOL B 314



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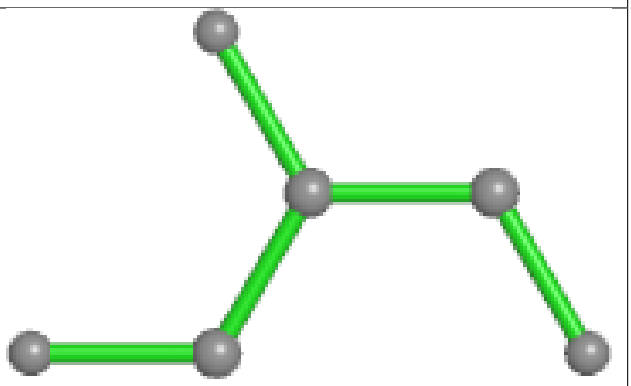
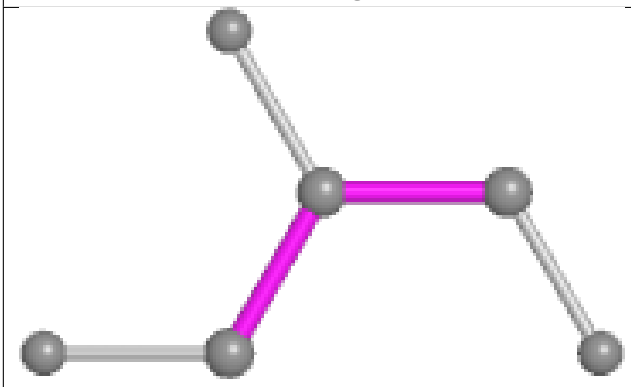
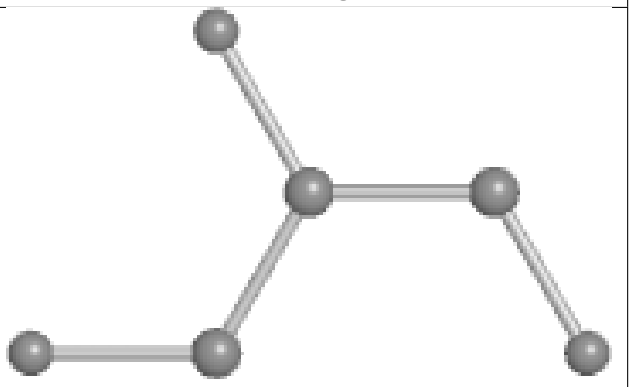


Bond angles

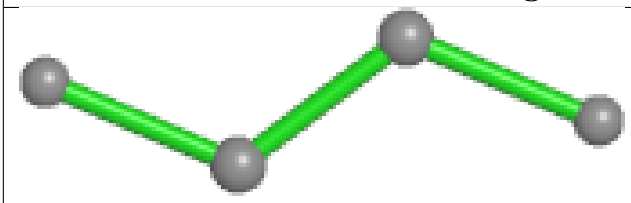


Torsions

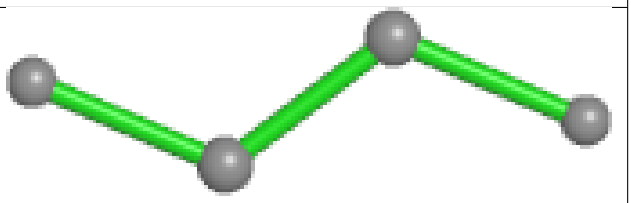


Rings

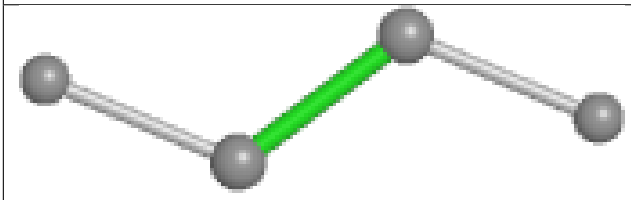
Ligand EDO C 305



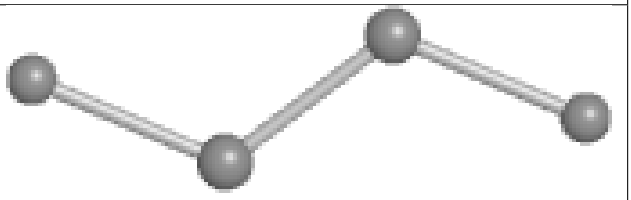
Bond lengths



Bond angles

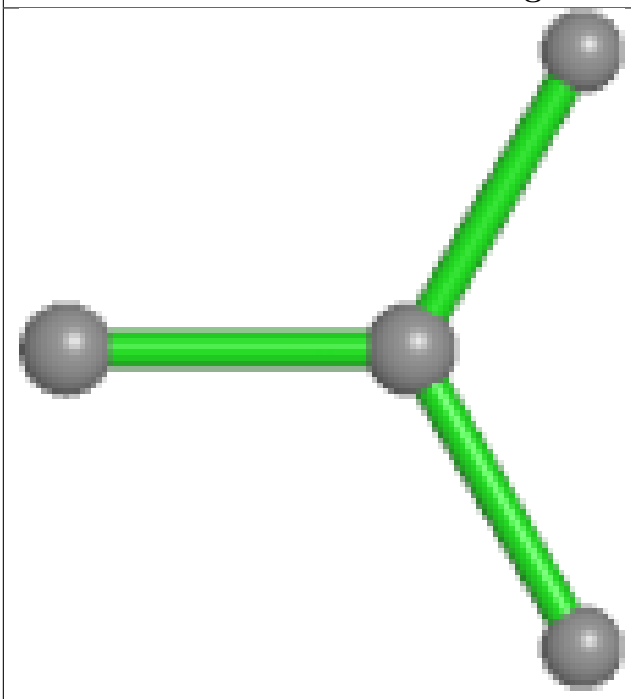


Torsions

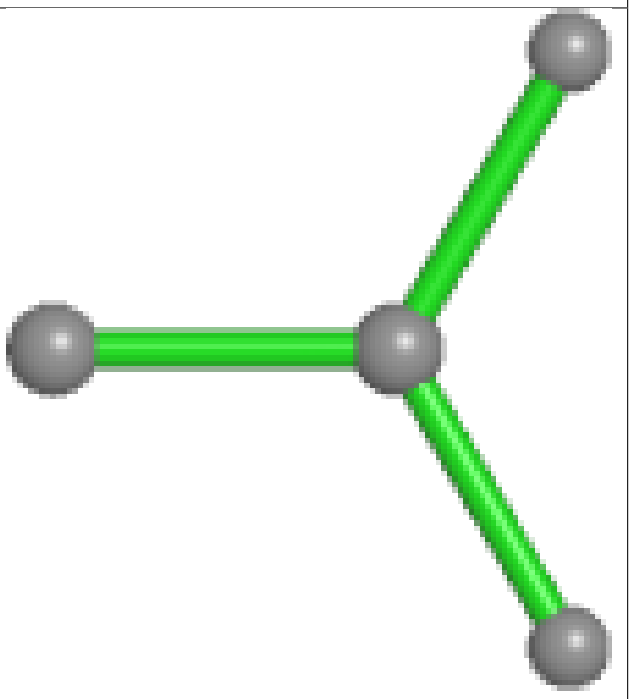


Rings

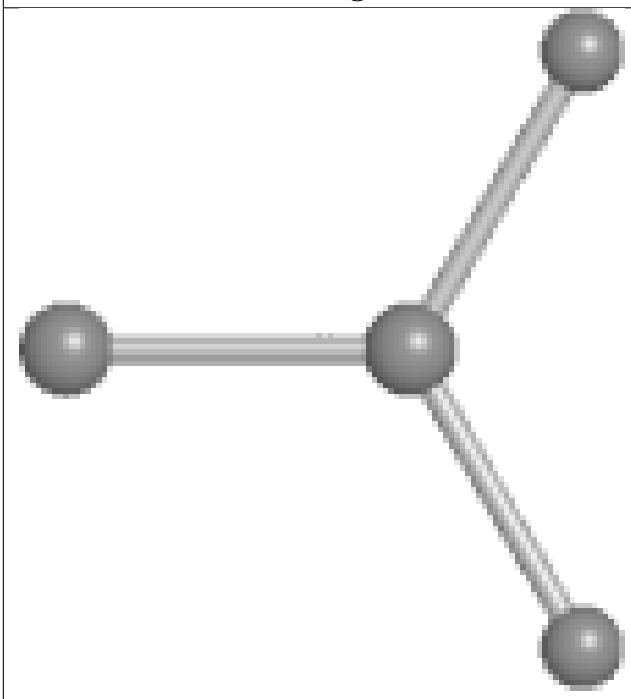
Ligand ACT E 310



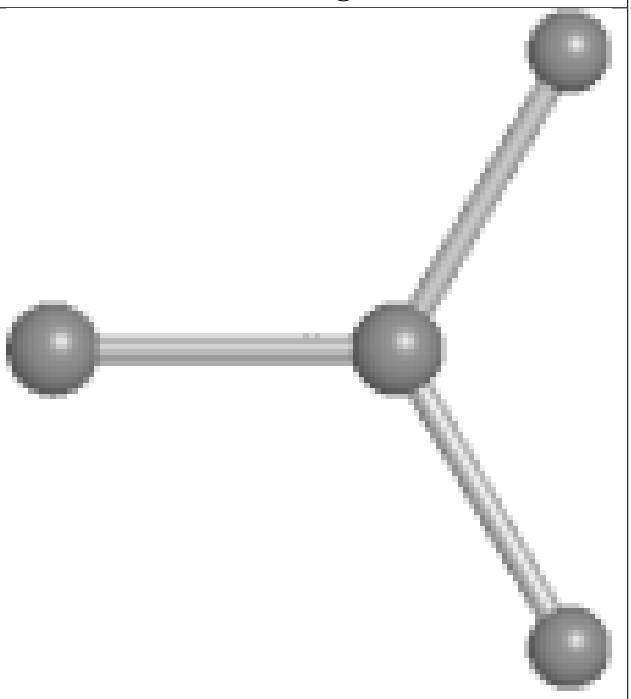
Bond lengths



Bond angles



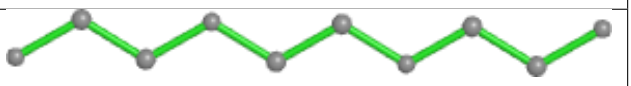
Torsions



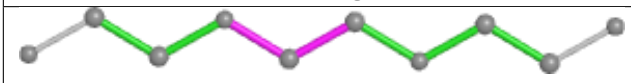
Rings

Ligand PGE C 314

Bond lengths



Bond angles



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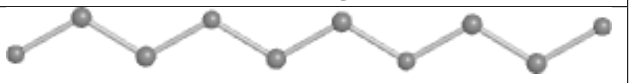
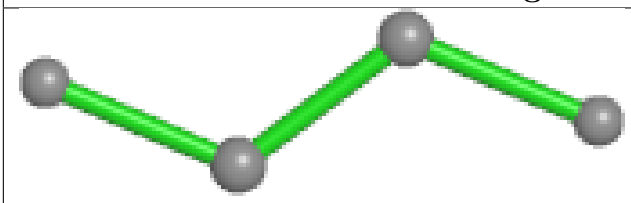
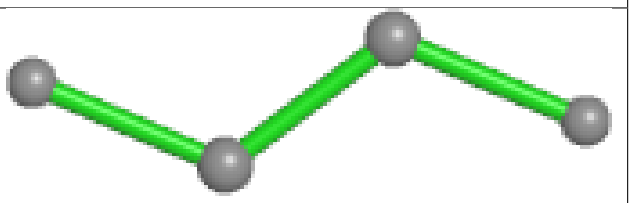


Rings

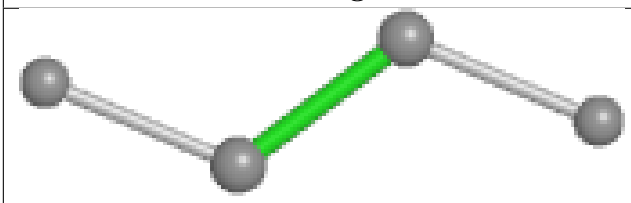
Ligand EDO E 309



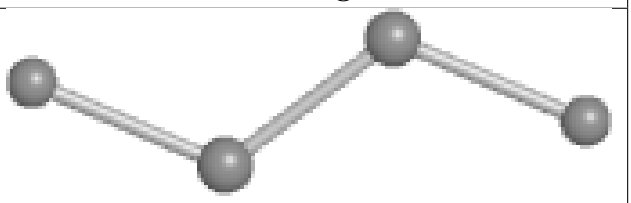
Bond lengths



Bond angles

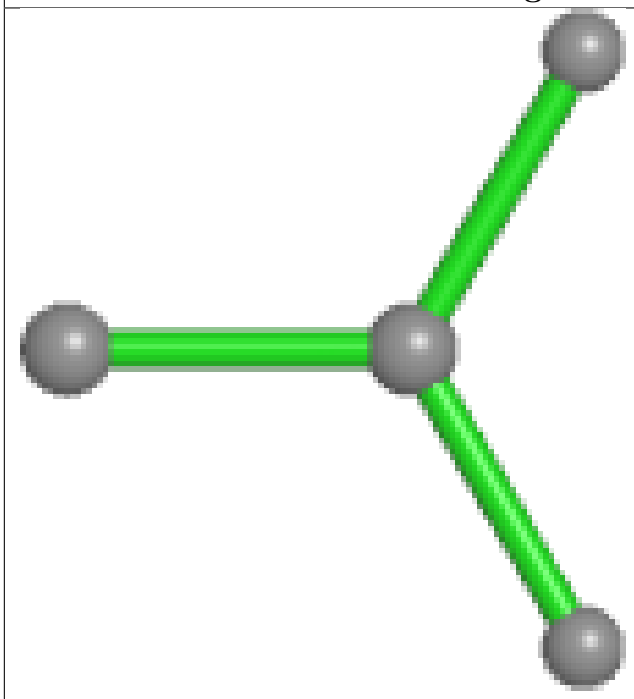


Torsions

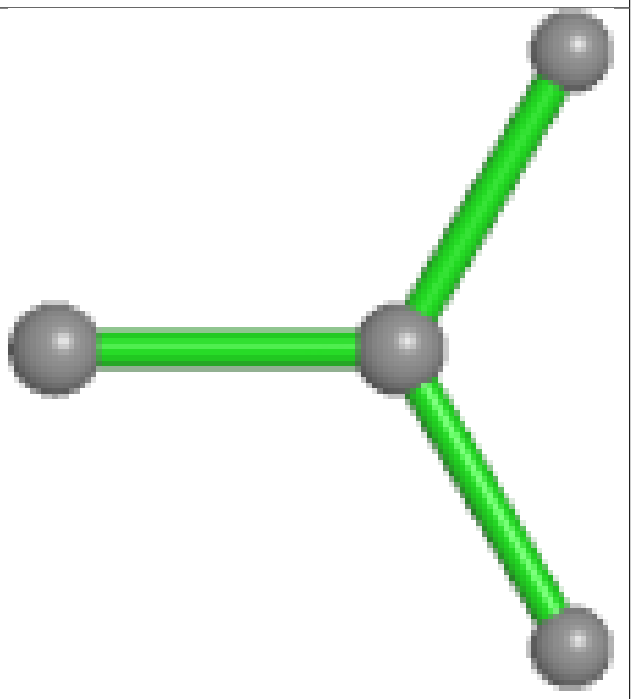


Rings

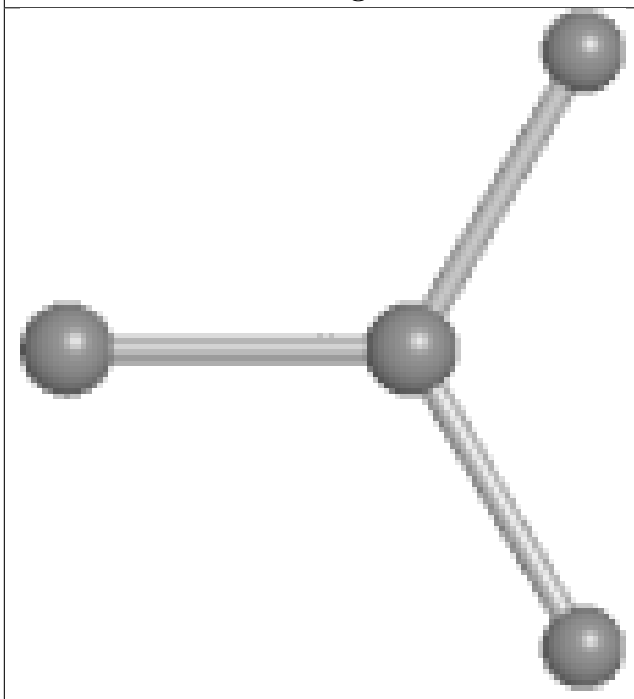
Ligand ACT B 306



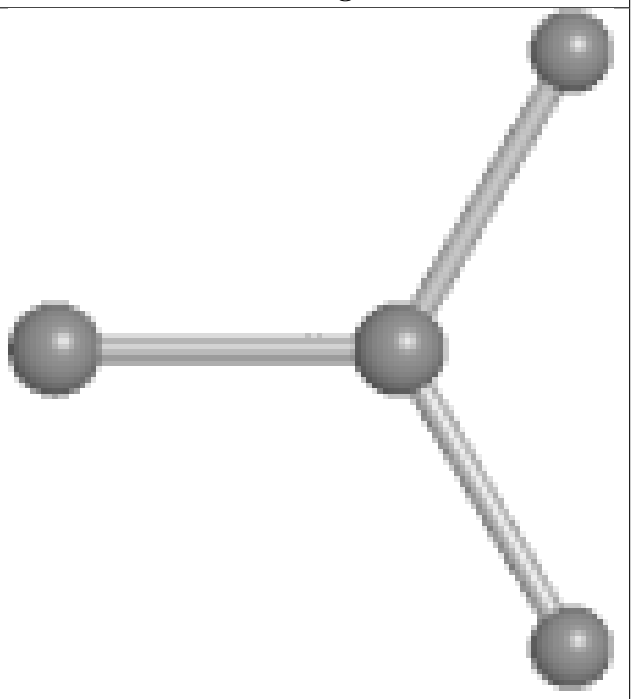
Bond lengths



Bond angles

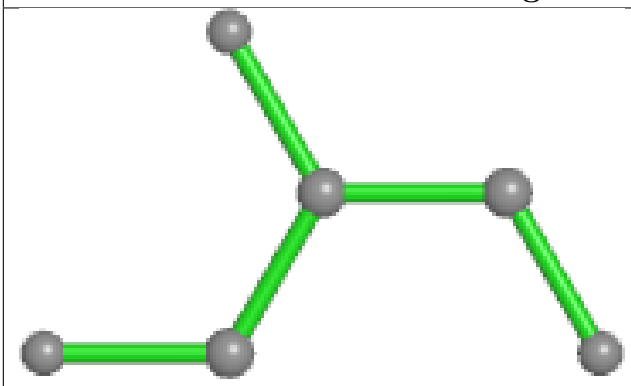


Torsions

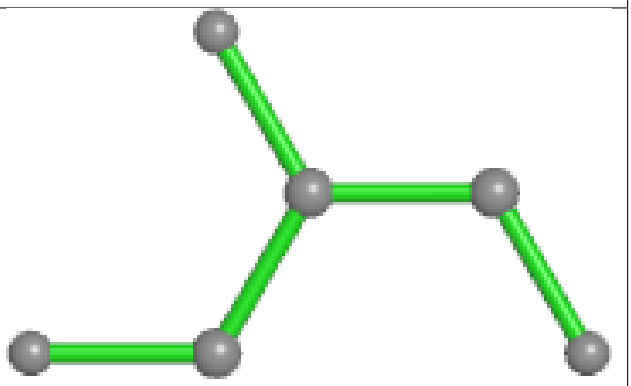


Rings

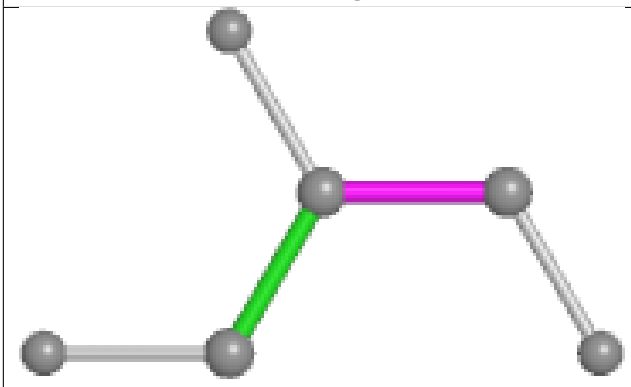
Ligand GOL A 312



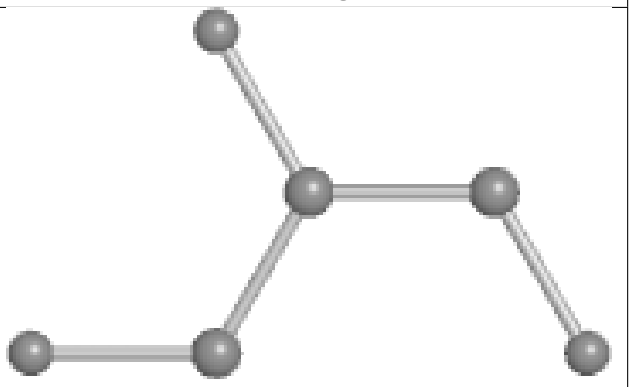
Bond lengths



Bond angles

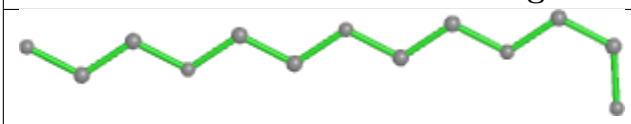


Torsions

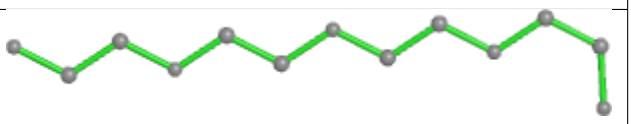


Rings

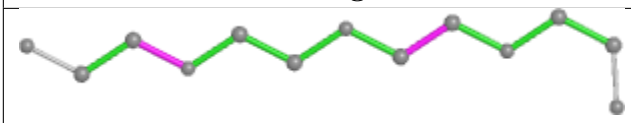
Ligand PG4 E 302



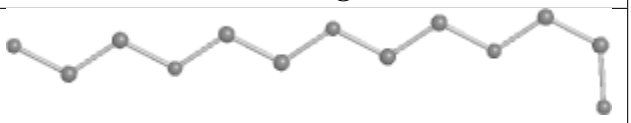
Bond lengths



Bond angles

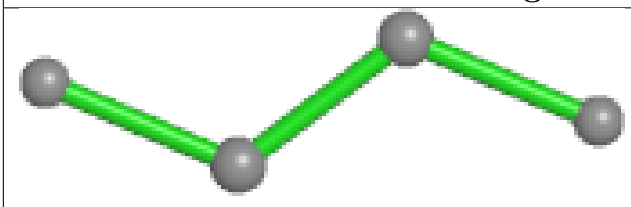


Torsions

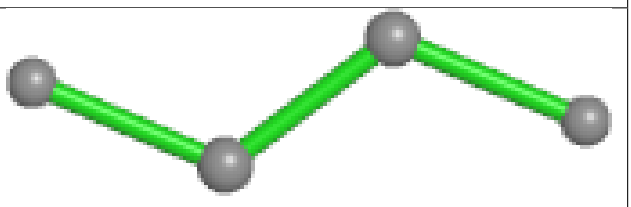


Rings

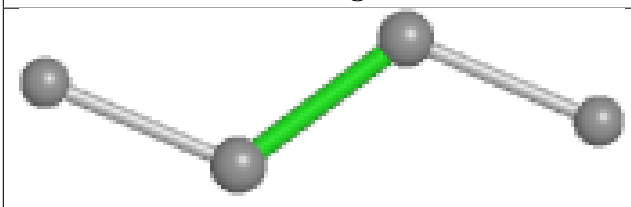
Ligand EDO E 306



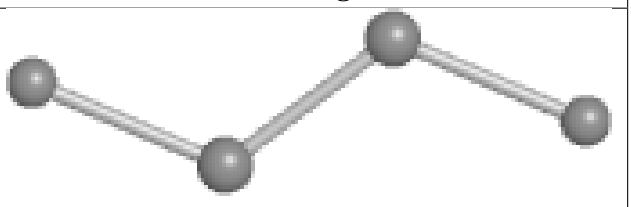
Bond lengths



Bond angles

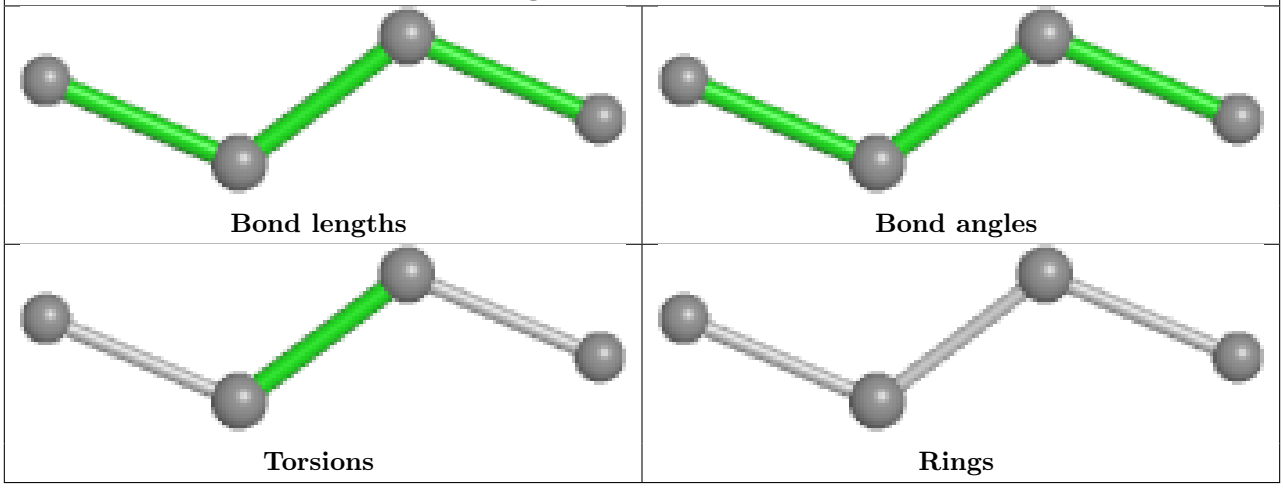


Torsions

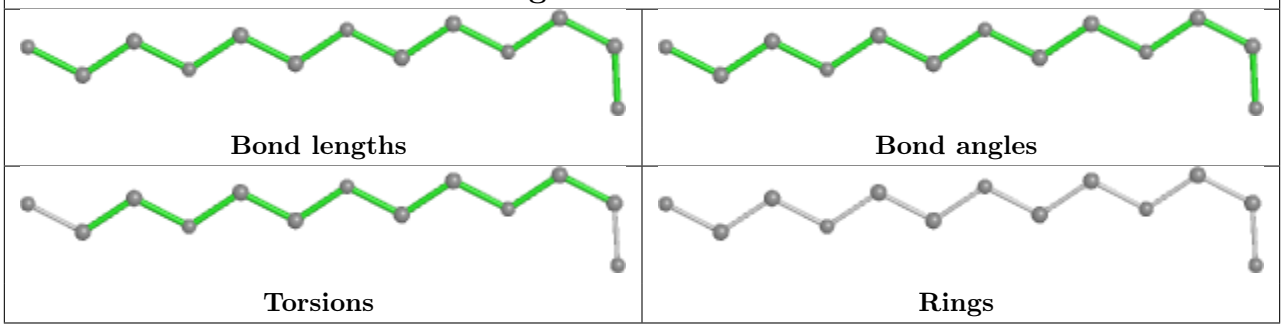


Rings

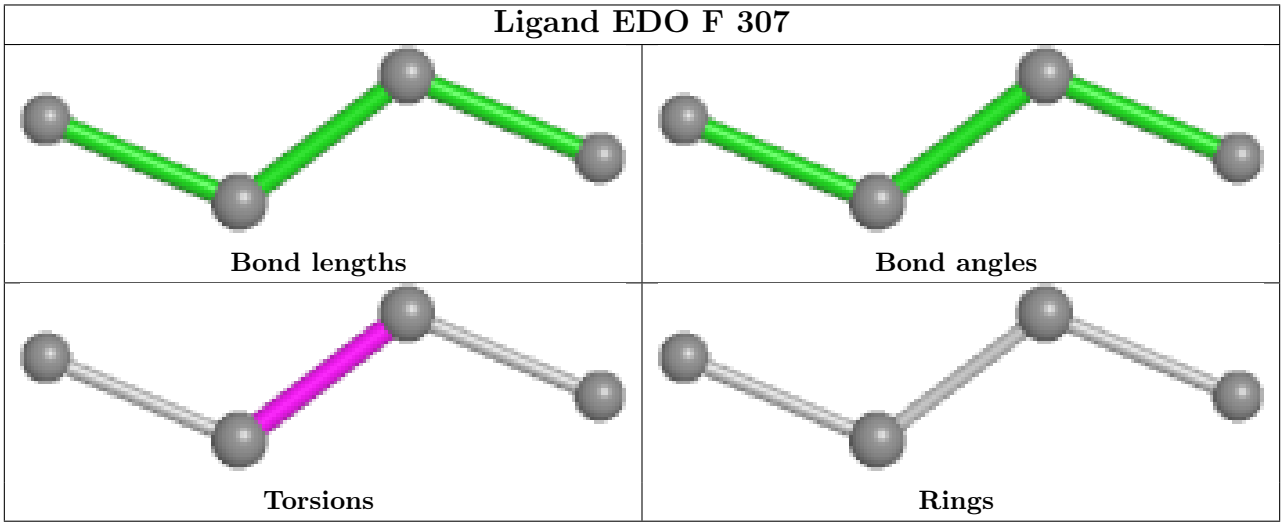
Ligand EDO E 303

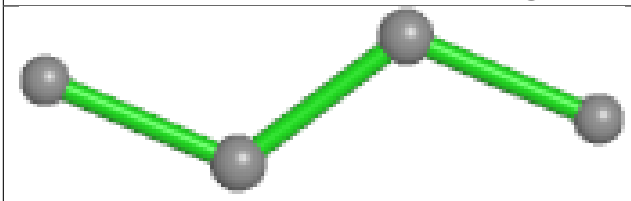
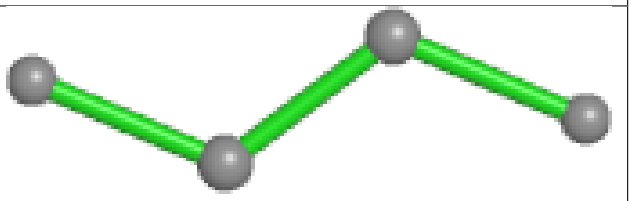
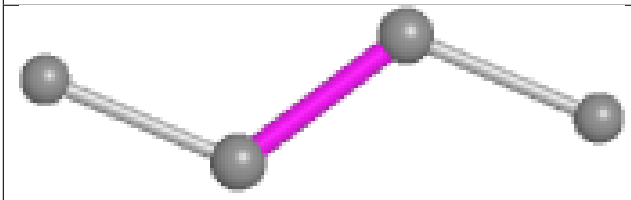
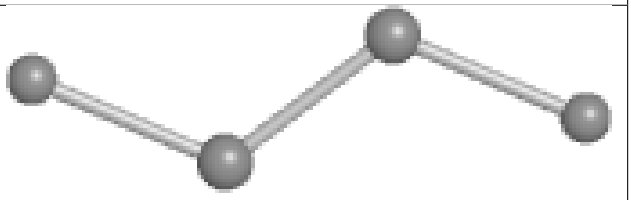


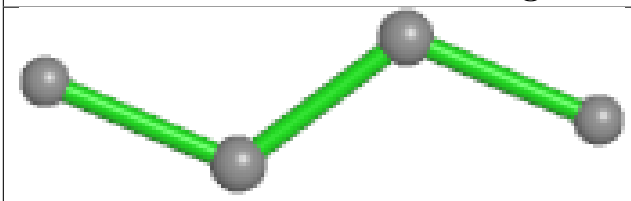
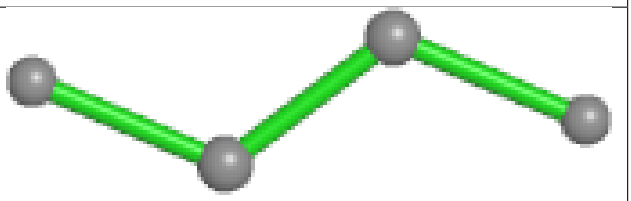
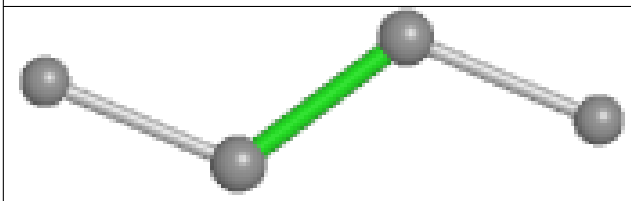
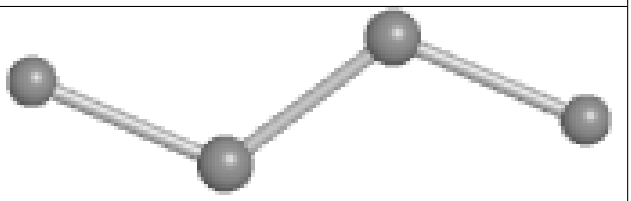
Ligand PG4 F 302



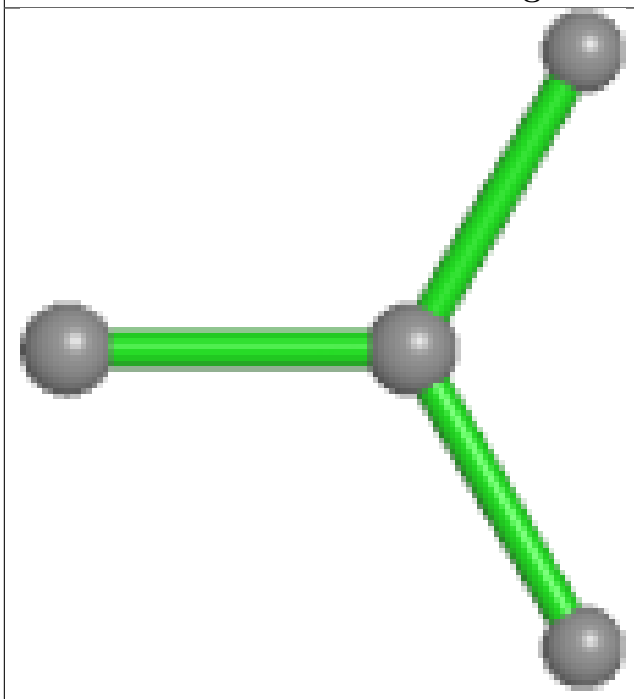
Ligand EDO F 307



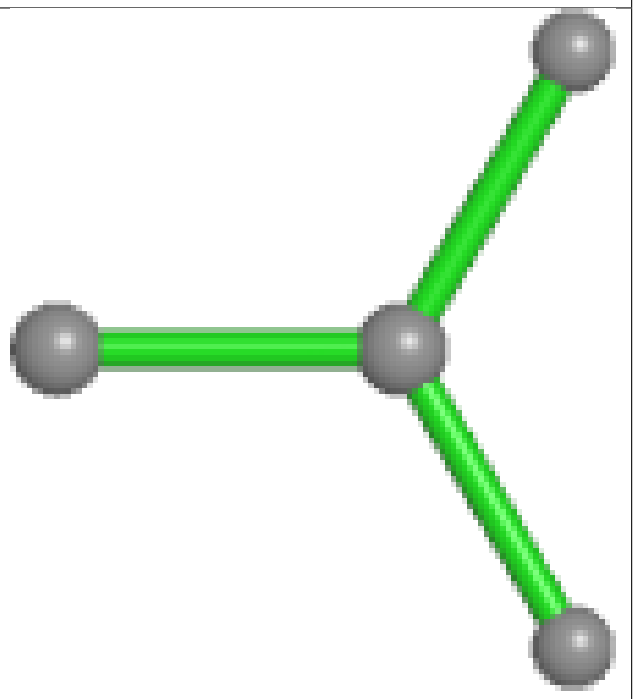
Ligand EDO C 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO A 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

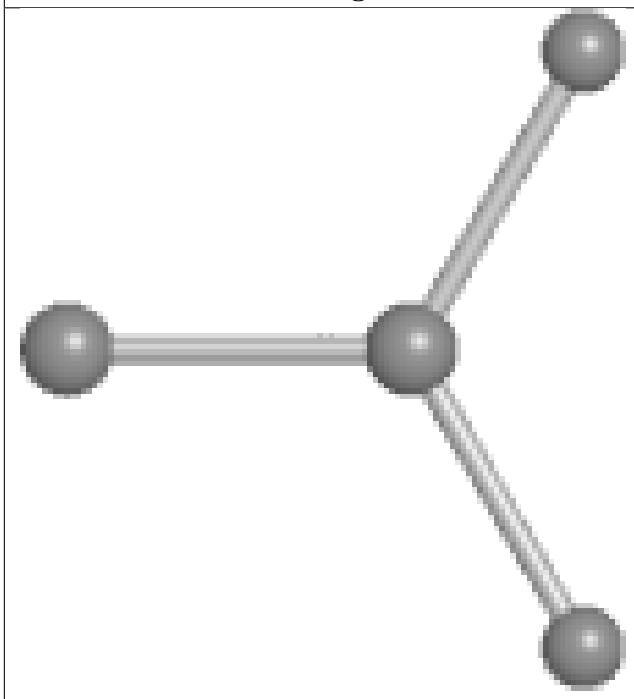
Ligand ACT A 309



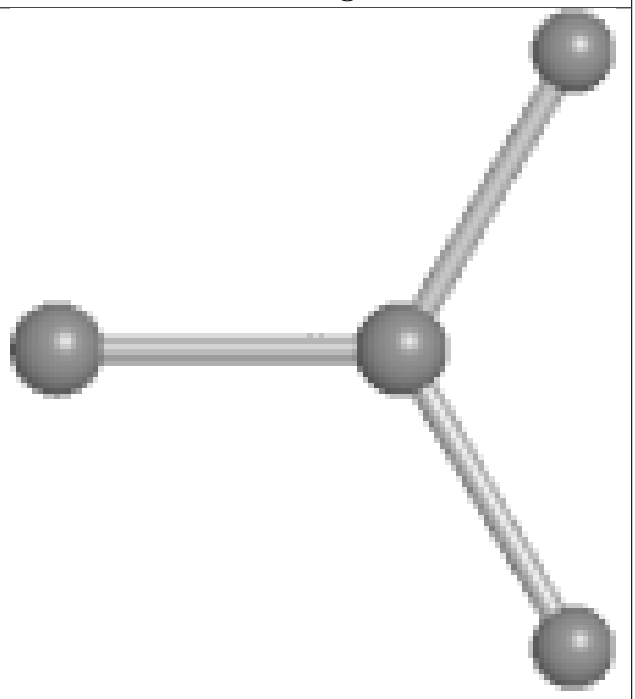
Bond lengths



Bond angles

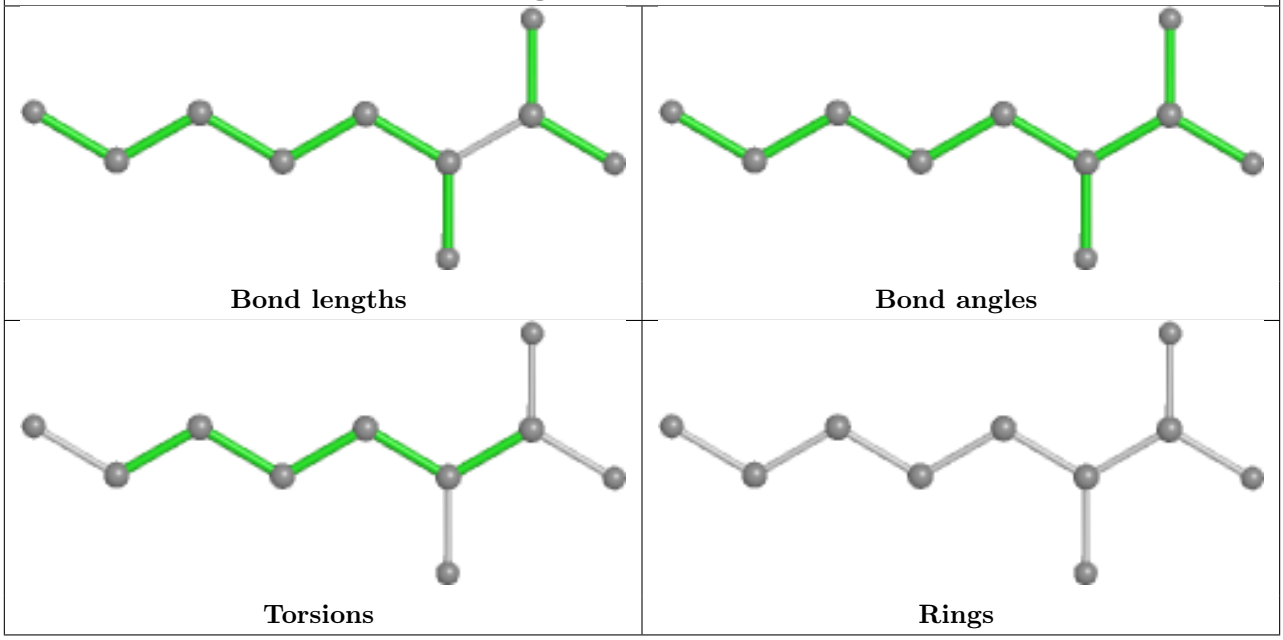


Torsions

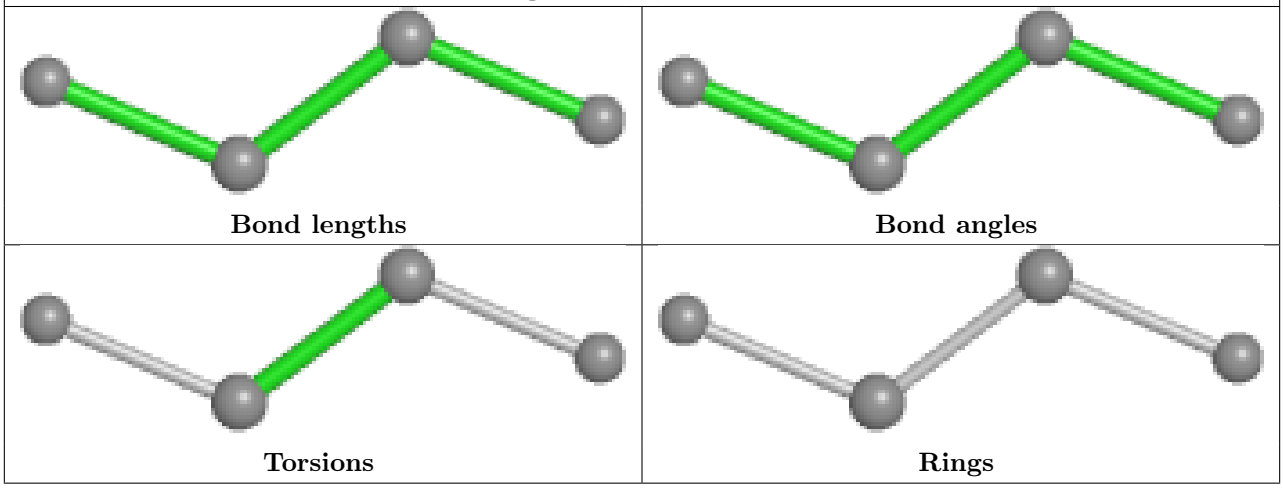


Rings

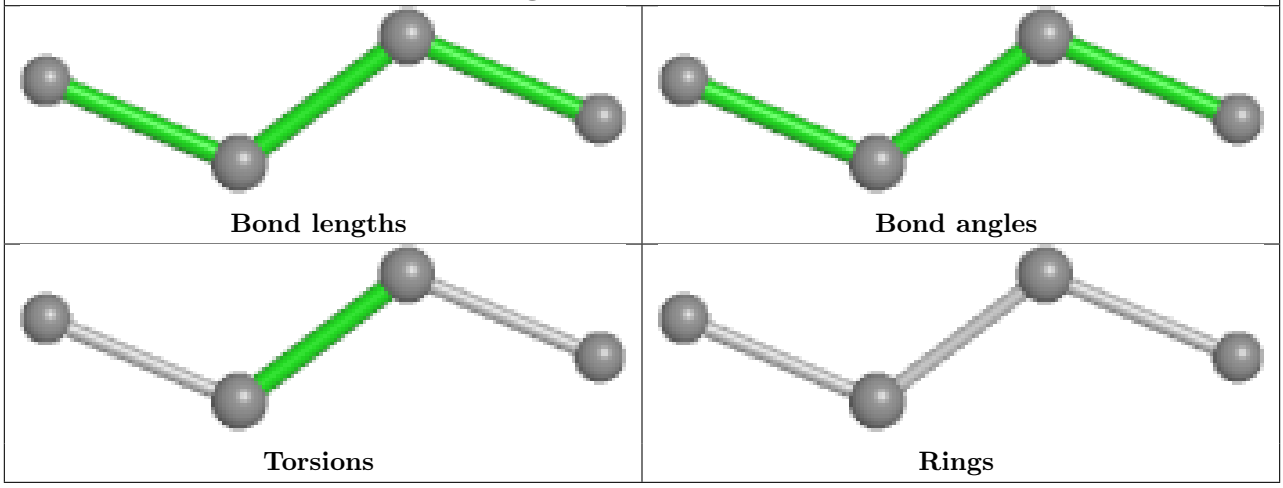
Ligand LYS F 301



Ligand EDO C 304



Ligand EDO B 303



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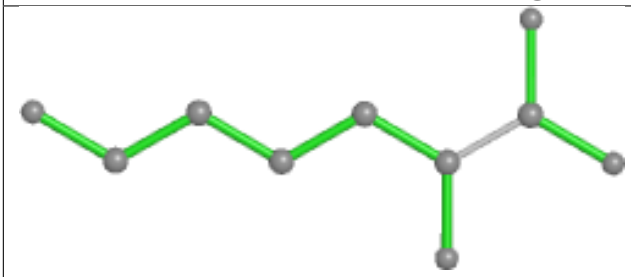
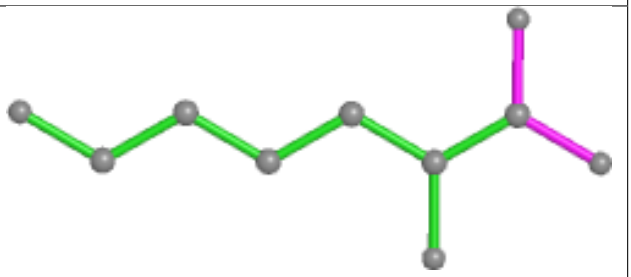
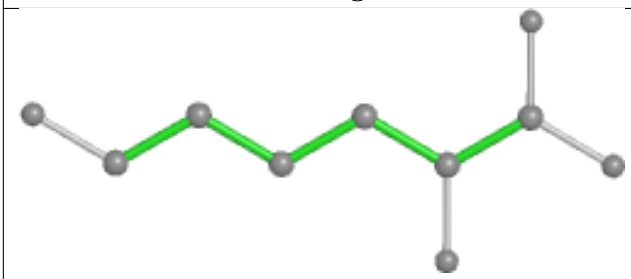


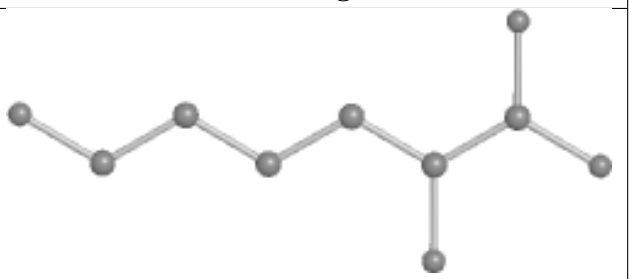
Bond lengths



Bond angles

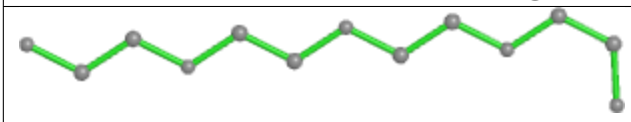


Torsions



Rings

Ligand PG4 B 302



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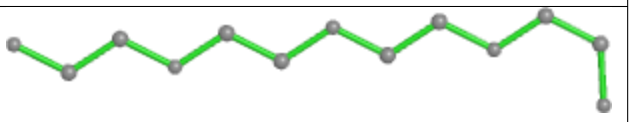
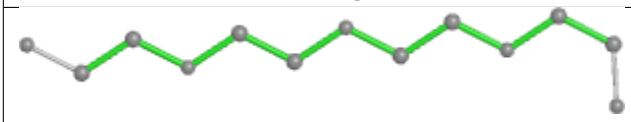
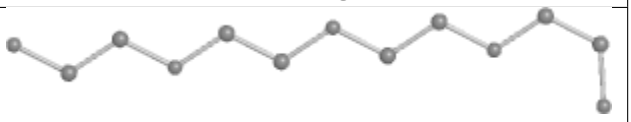


Bond angles

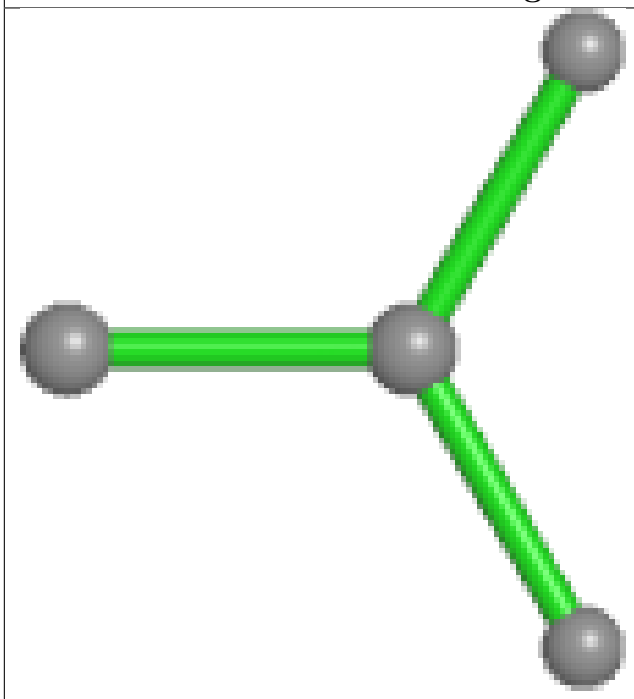


Torsions

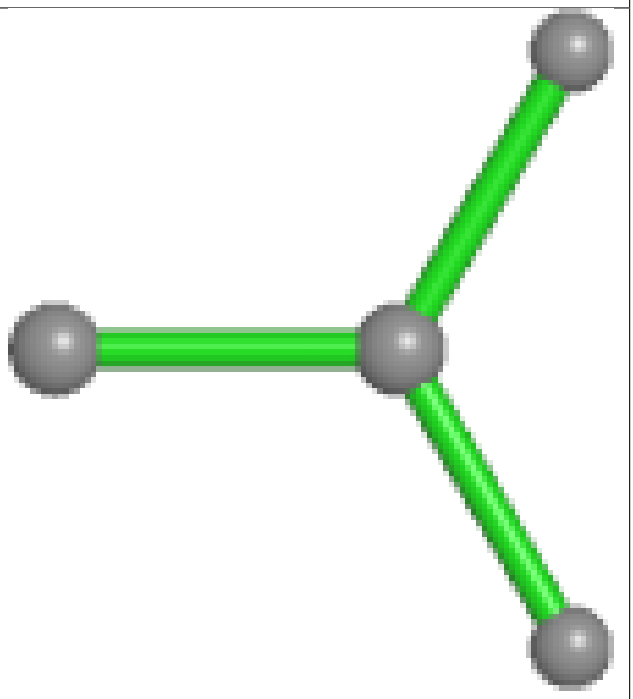


Rings

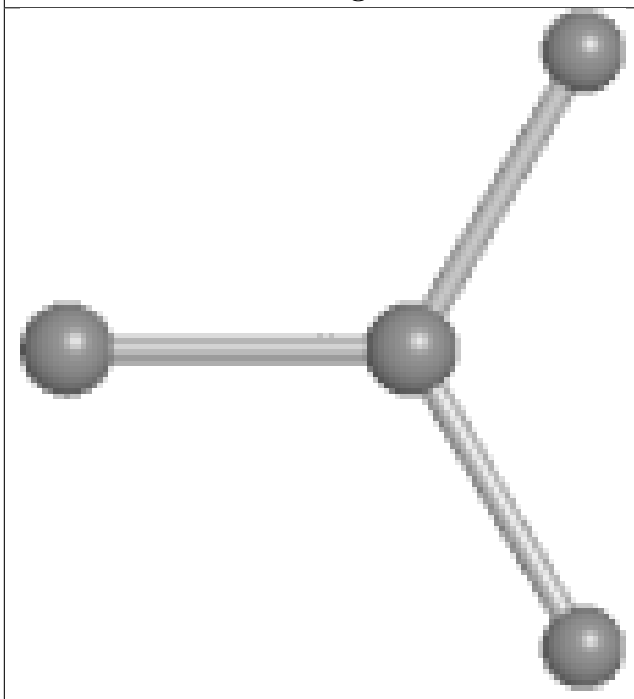
Ligand ACT C 311



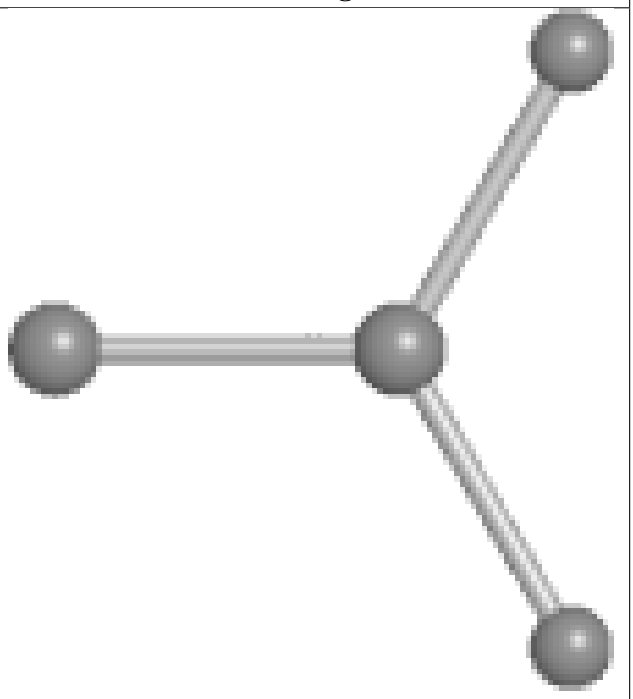
Bond lengths



Bond angles

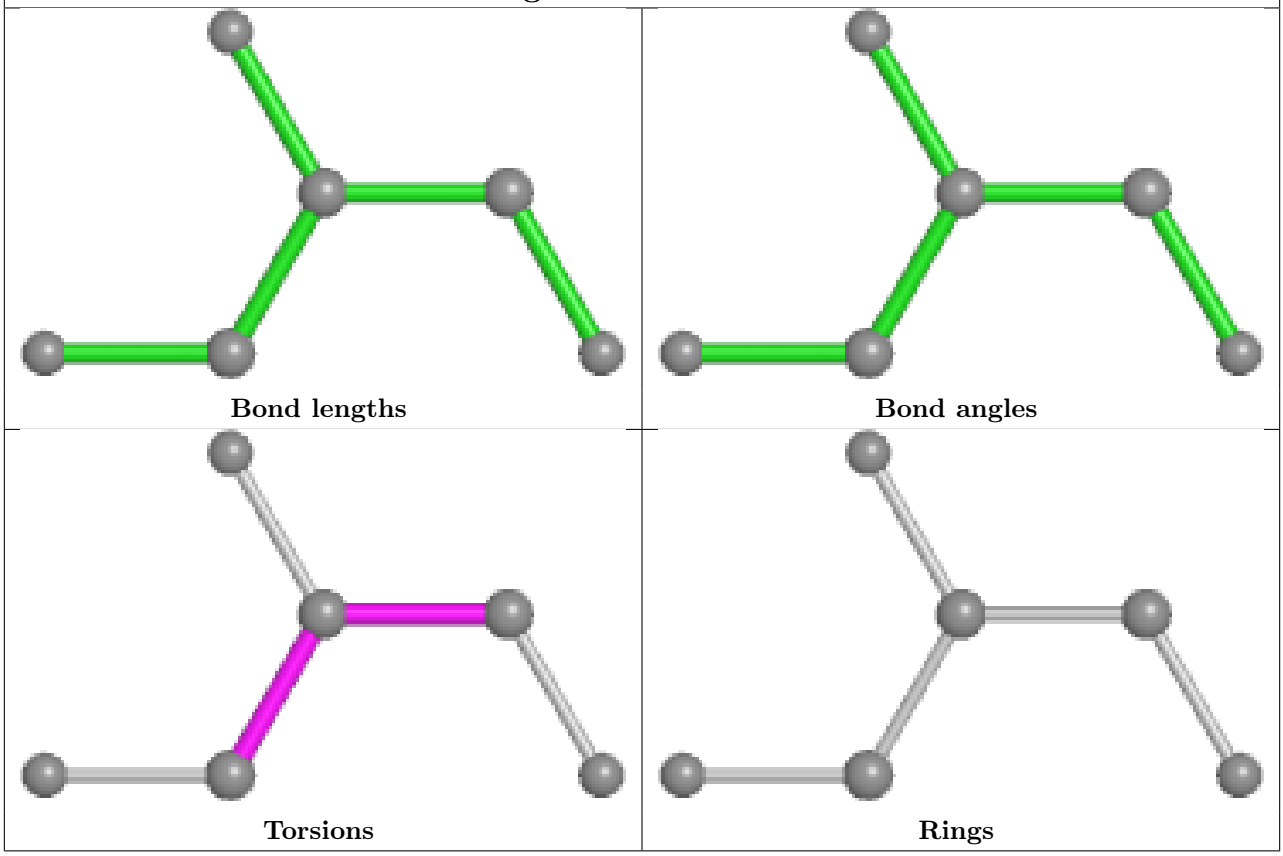


Torsions

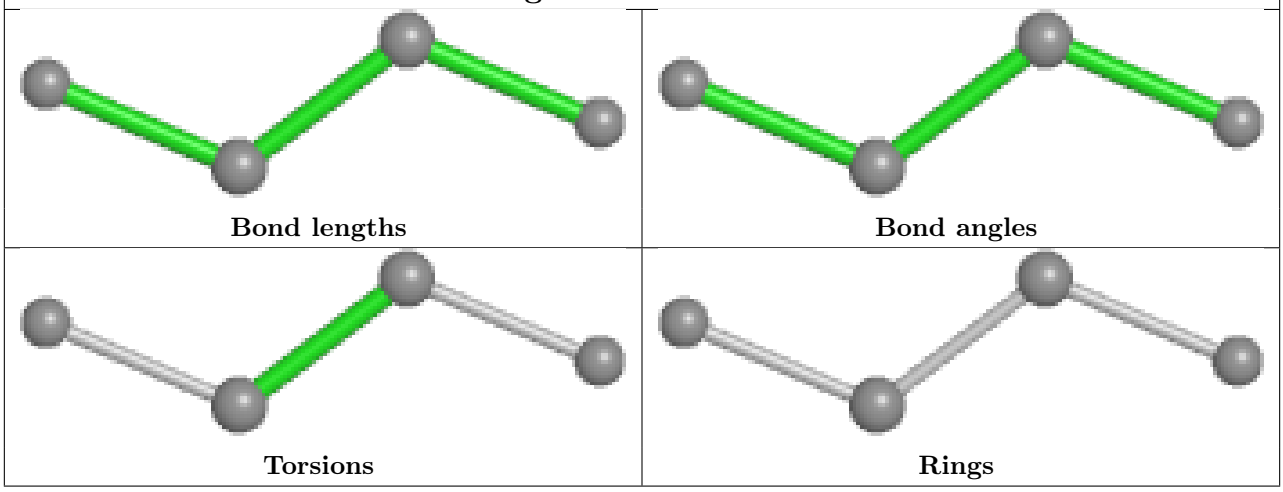


Rings

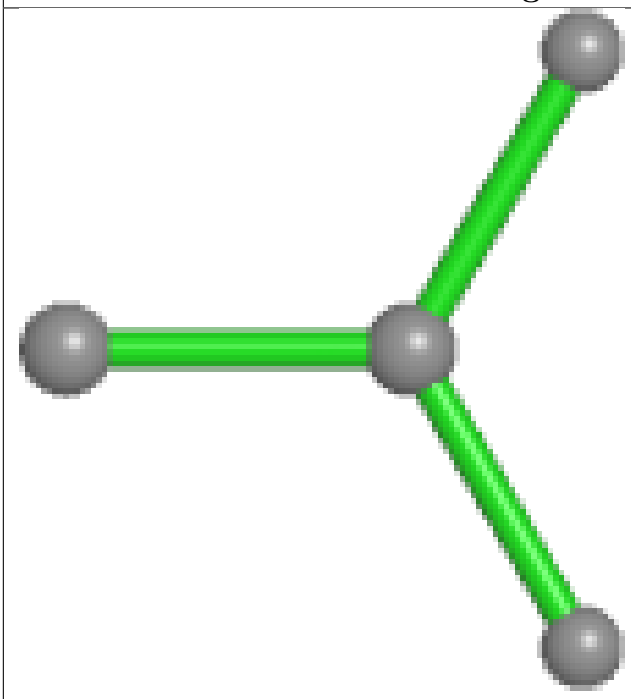
Ligand GOL D 314



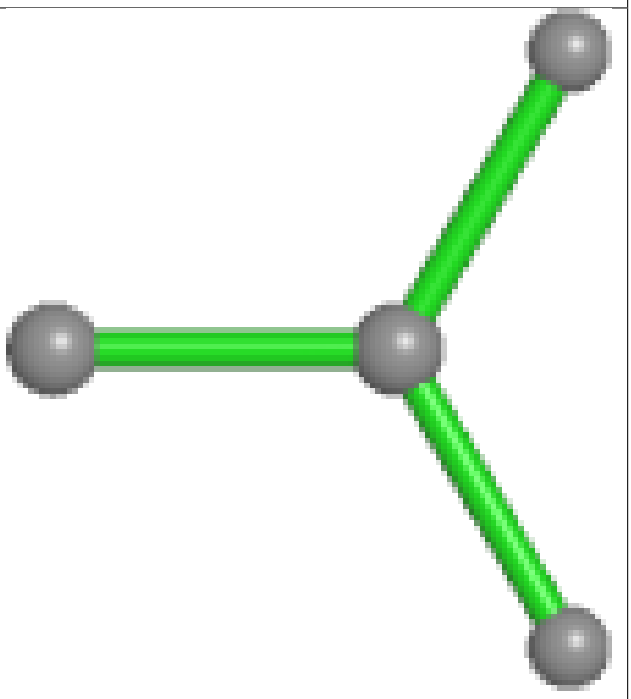
Ligand EDO E 308



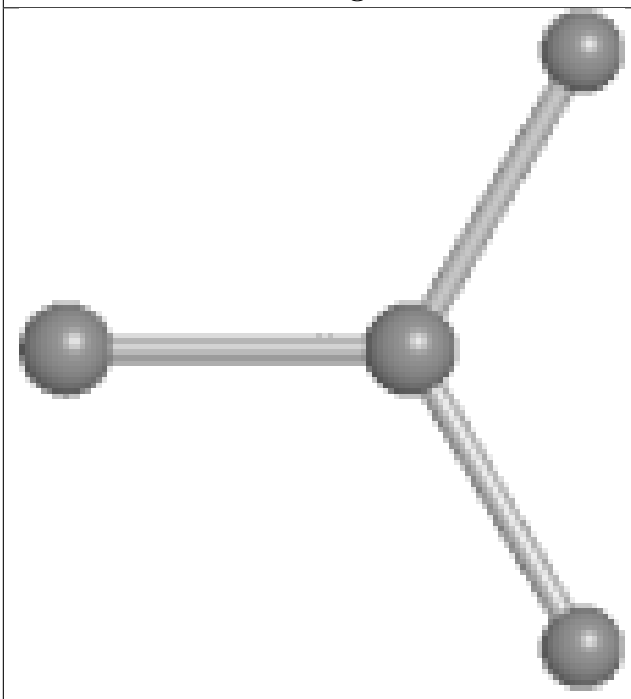
Ligand ACT D 310



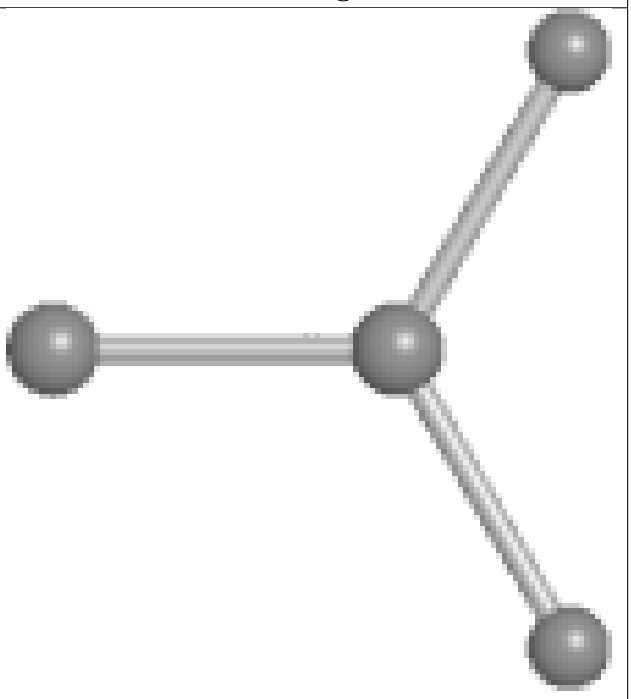
Bond lengths



Bond angles



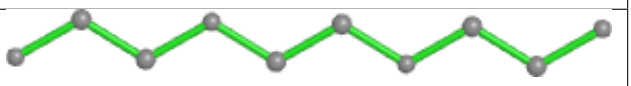
Torsions



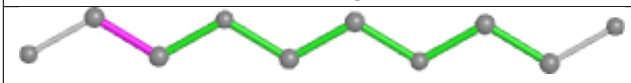
Rings

Ligand PGE F 312

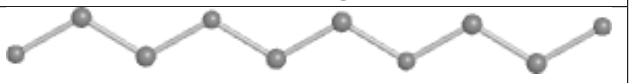
Bond lengths



Bond angles

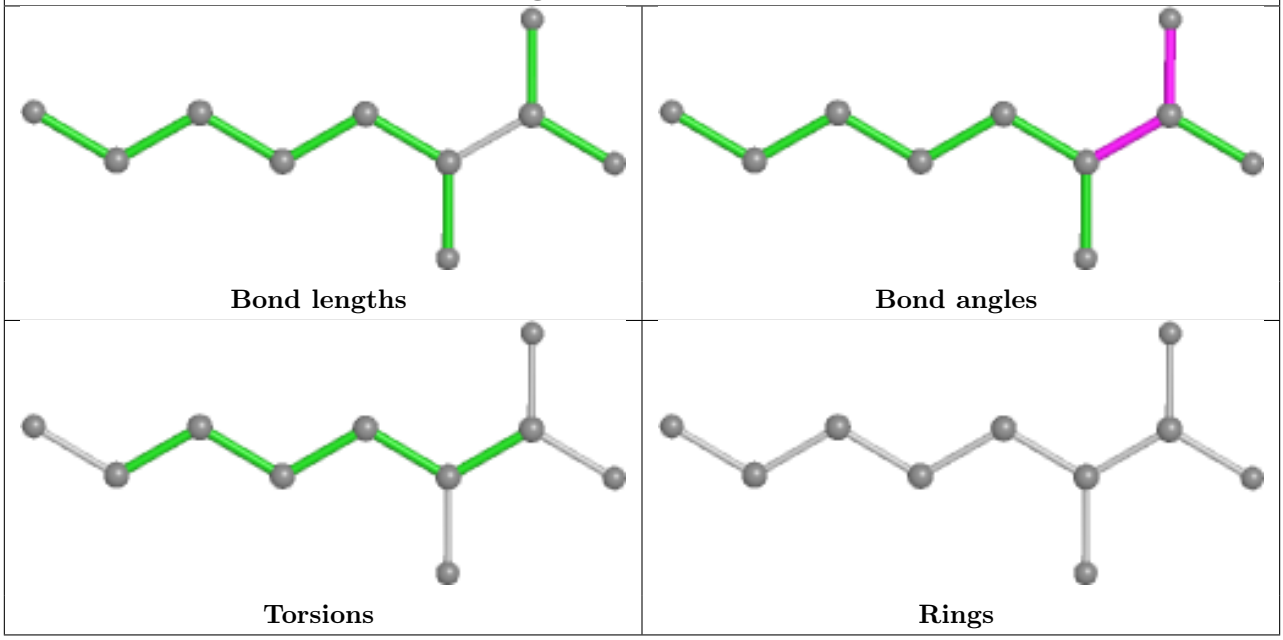


Torsions

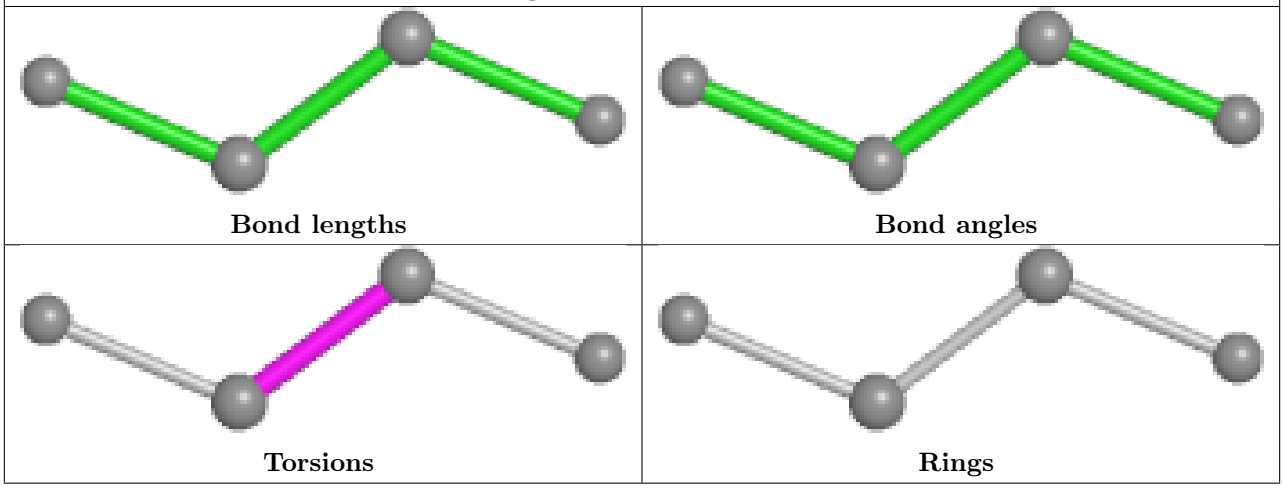


Rings

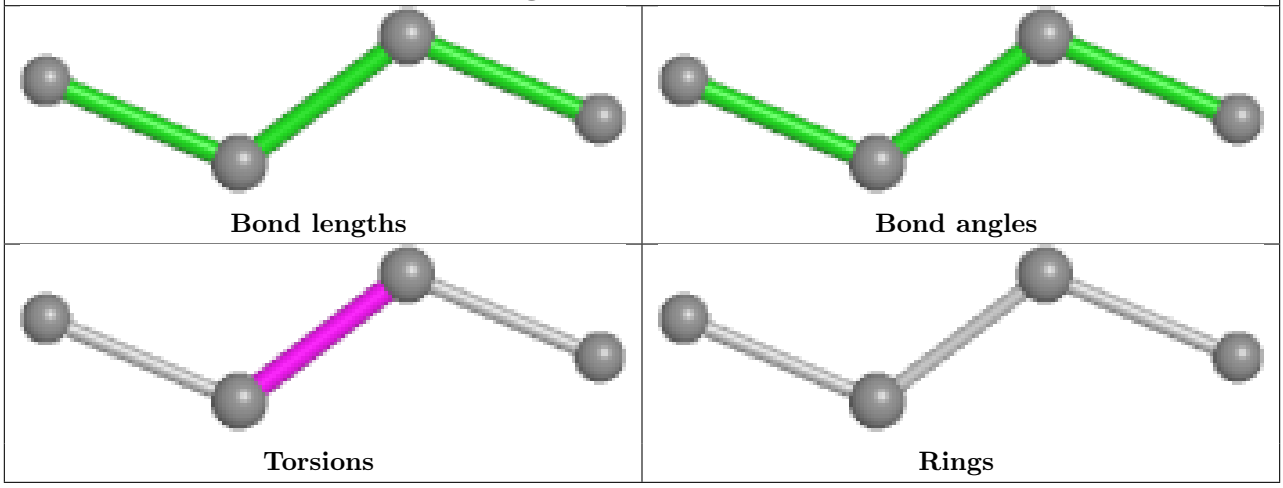
Ligand LYS D 301



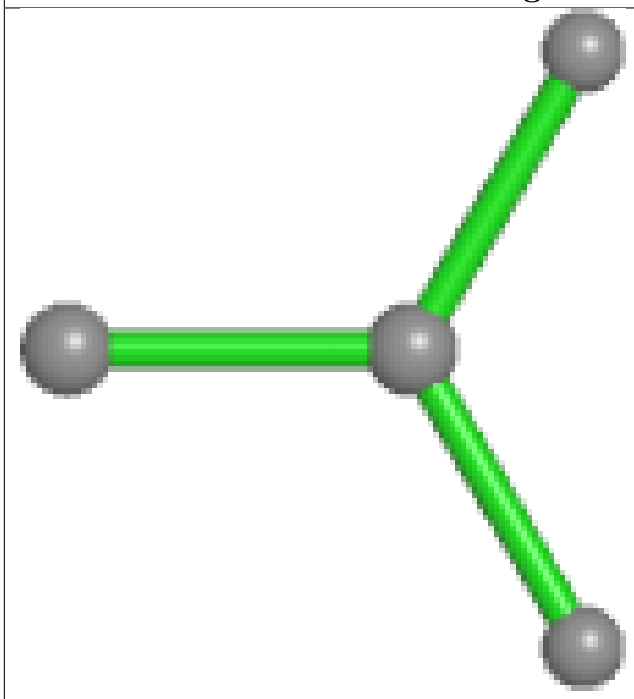
Ligand EDO B 305



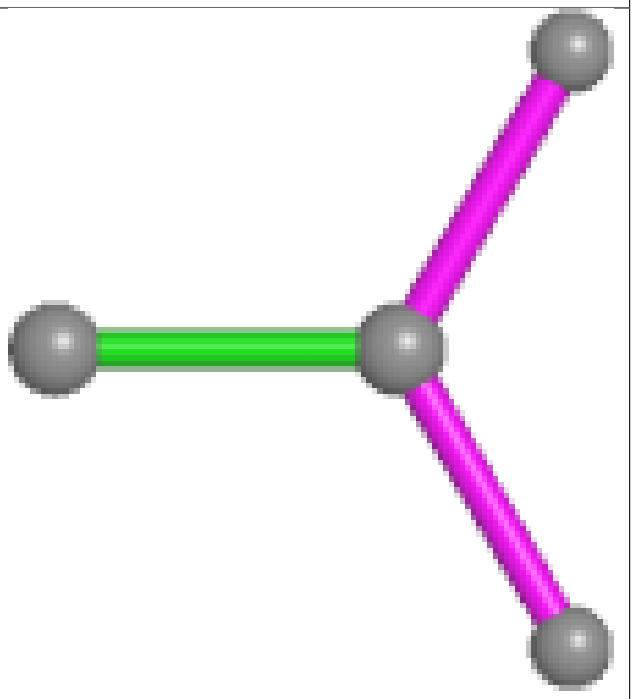
Ligand EDO A 305



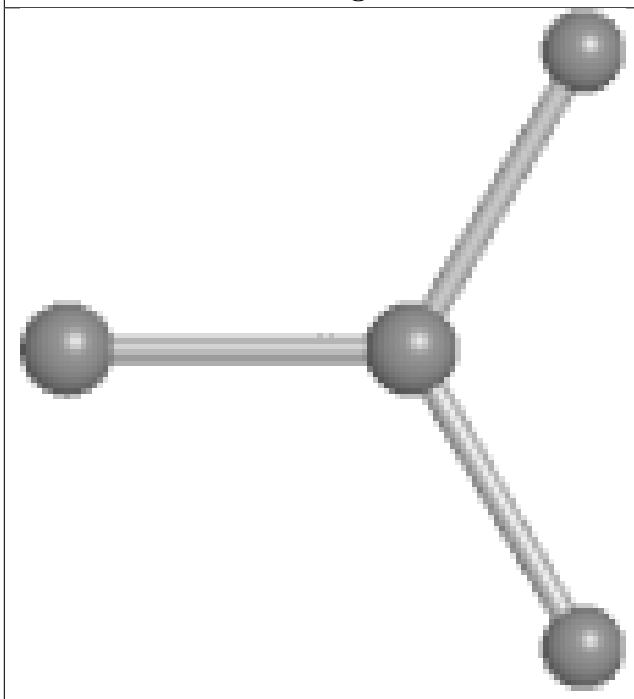
Ligand ACT D 309



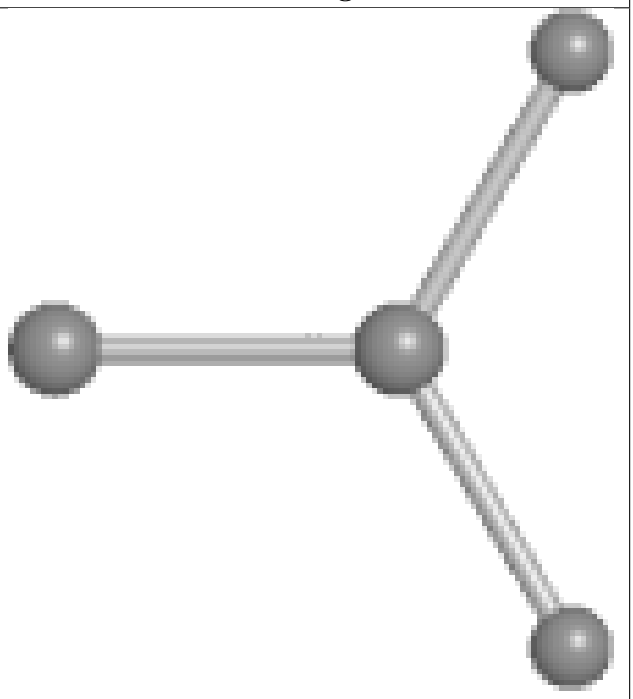
Bond lengths



Bond angles

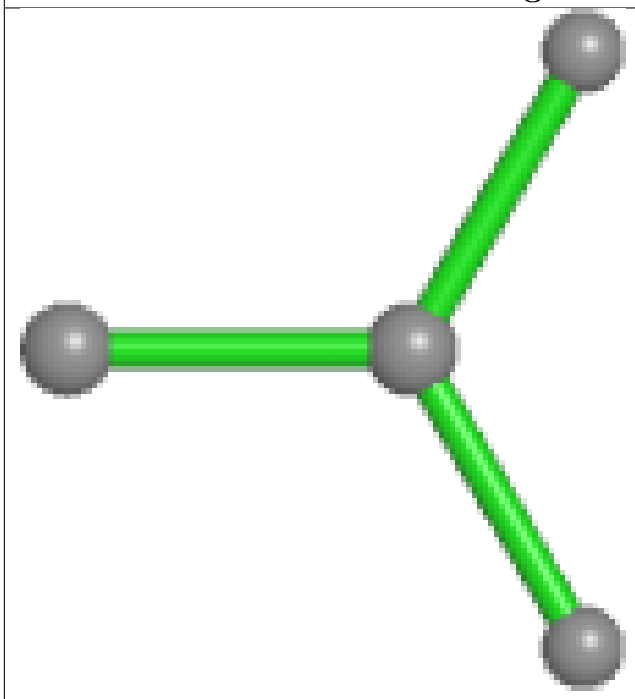


Torsions



Rings

Ligand ACT C 310



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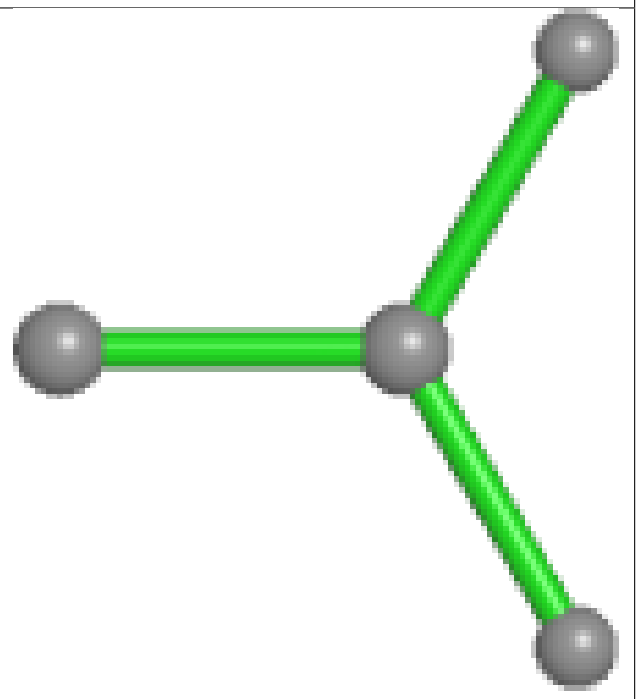
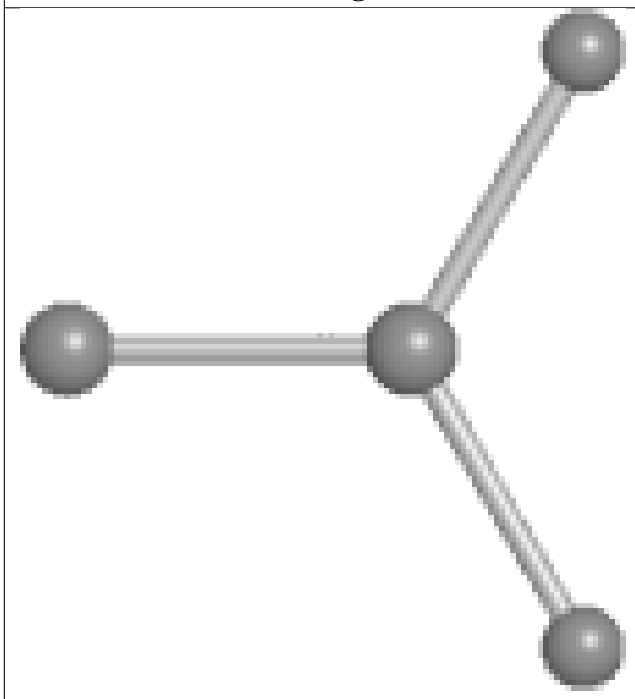
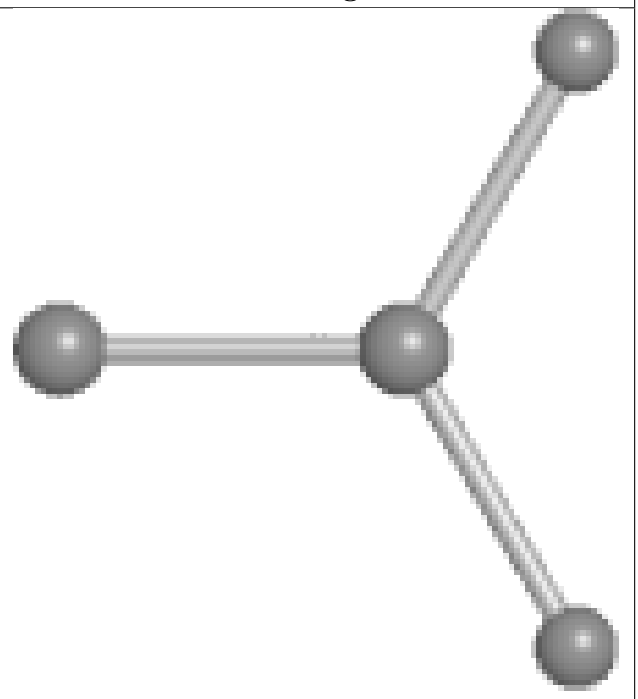


Bond angles

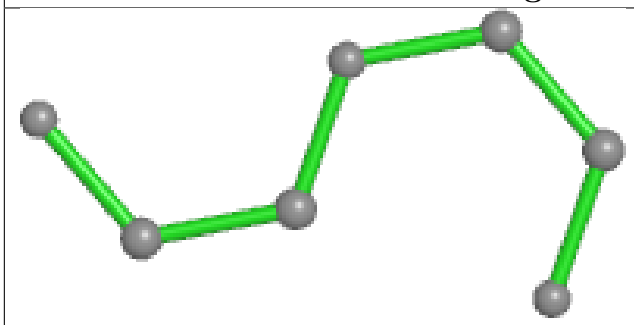


Torsions

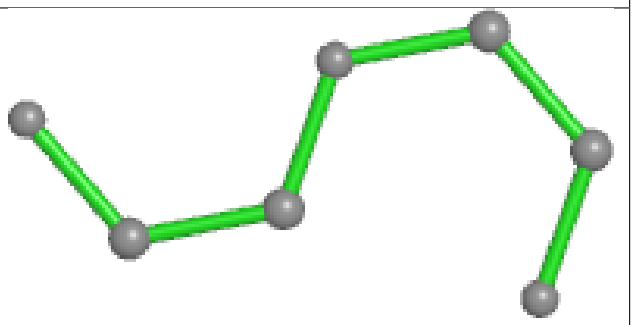


Rings

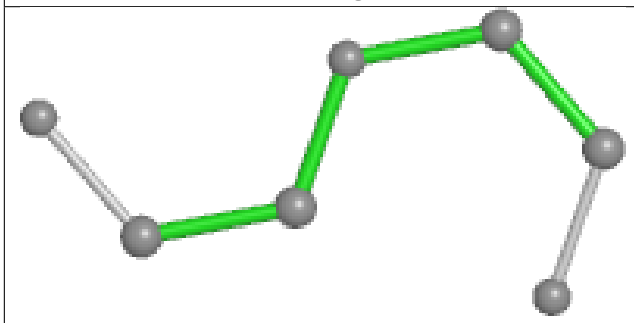
Ligand PEG C 317



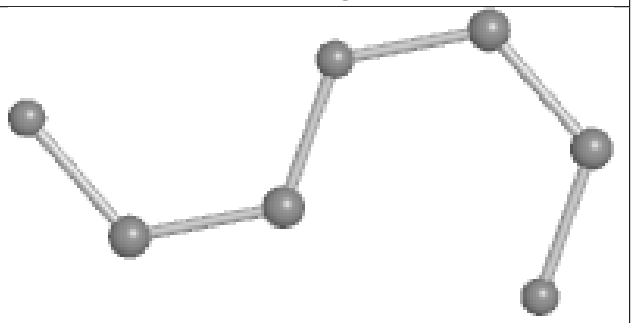
Bond lengths



Bond angles

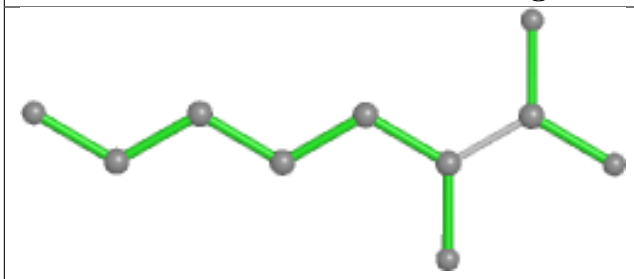


Torsions



Rings

Ligand LYS B 301



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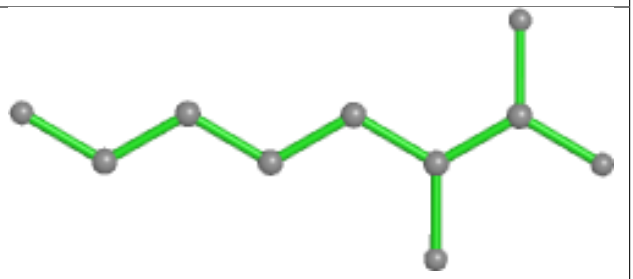
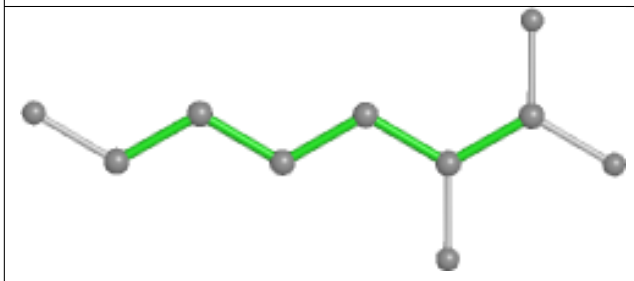
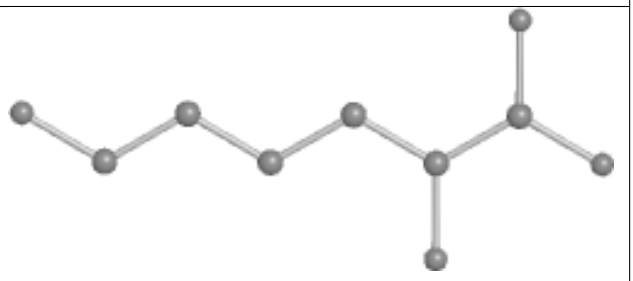


Bond angles

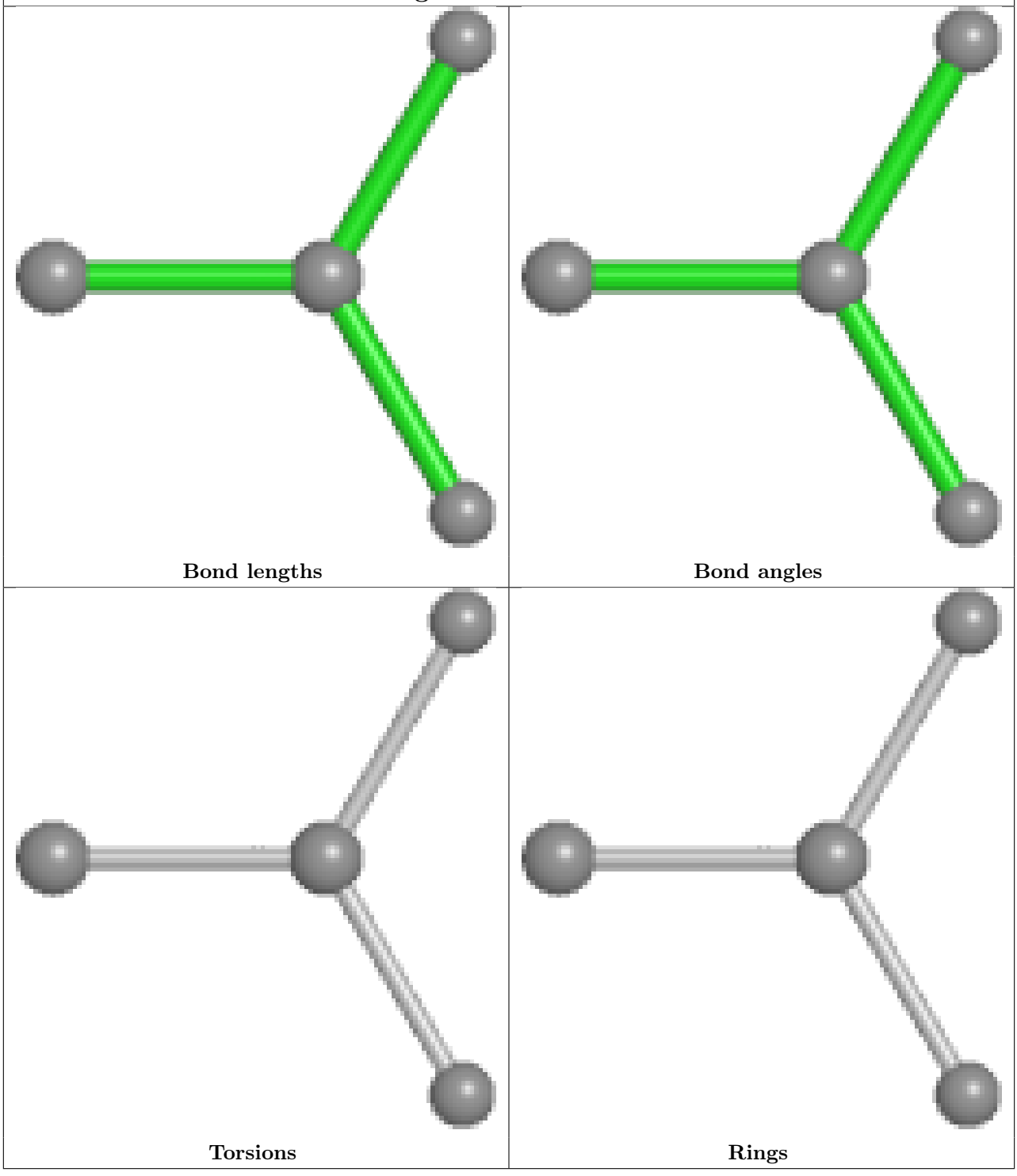


Torsions

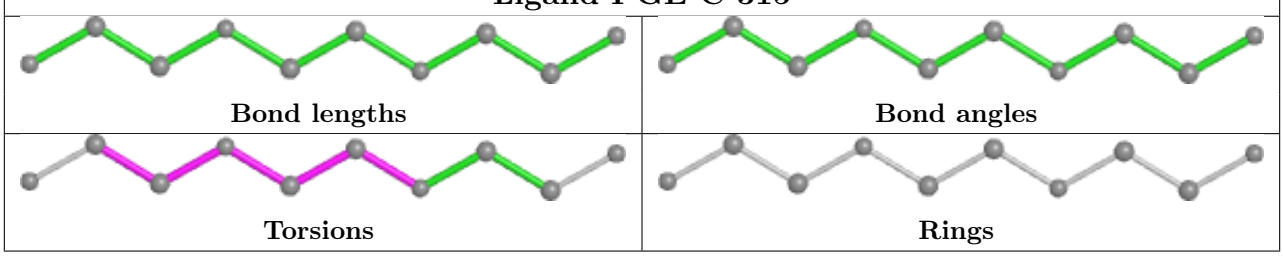


Rings

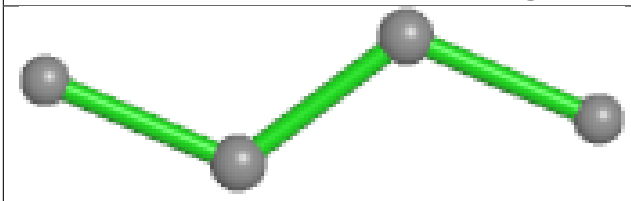
Ligand ACT D 311



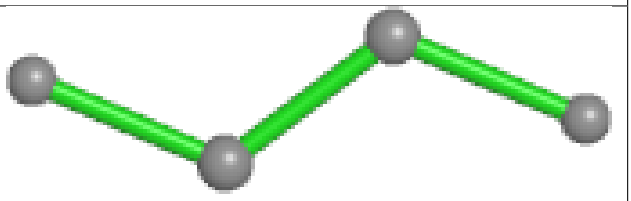
Ligand PGE C 315



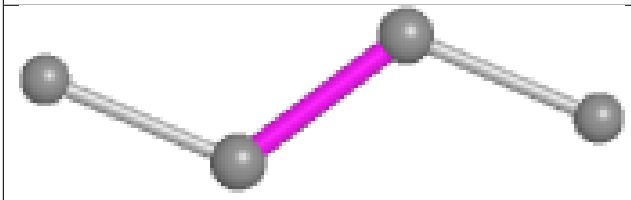
Ligand EDO A 307



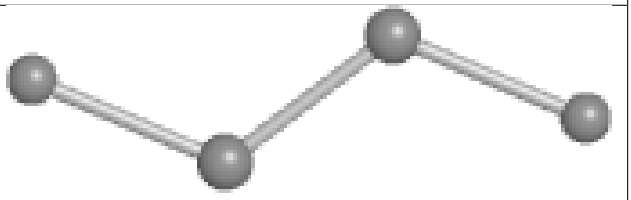
Bond lengths



Bond angles

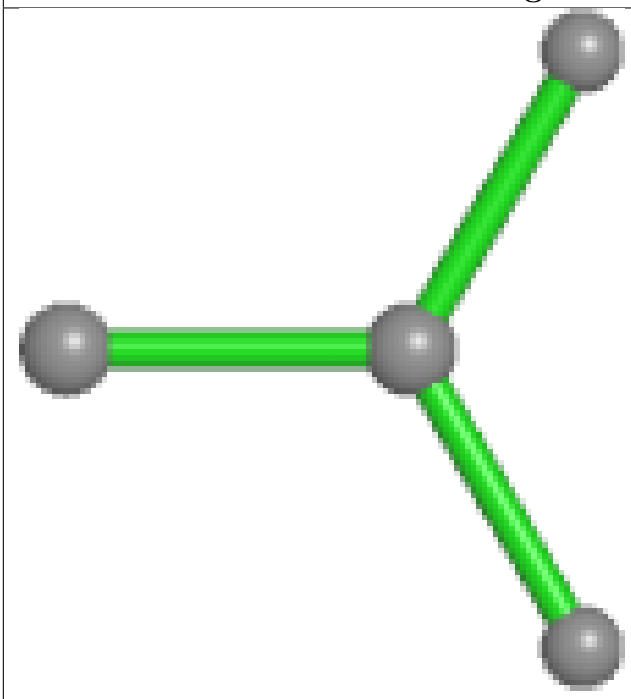


Torsions

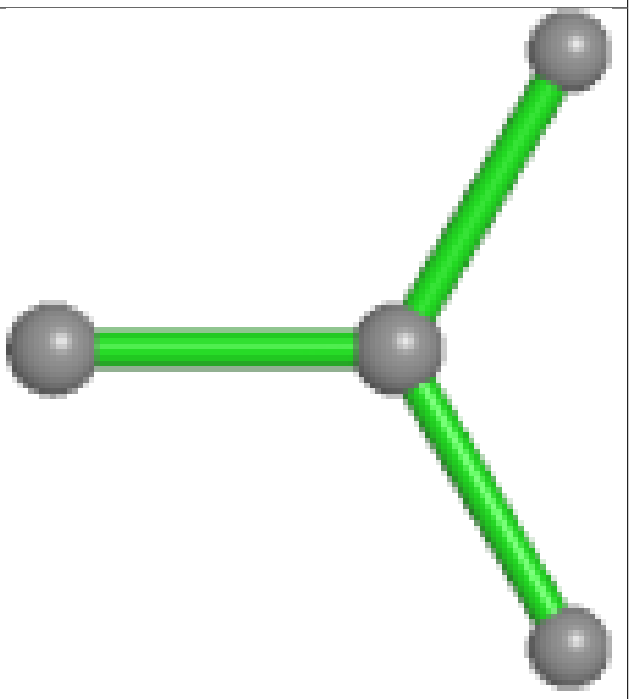


Rings

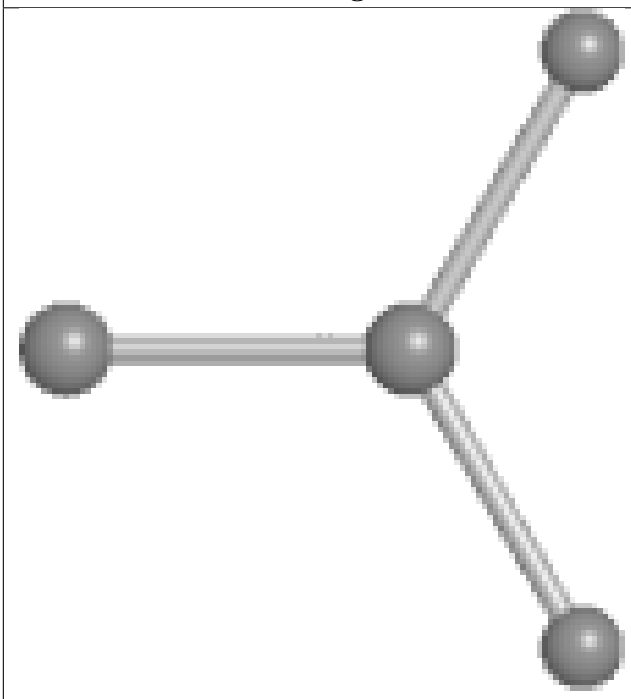
Ligand ACT F 311



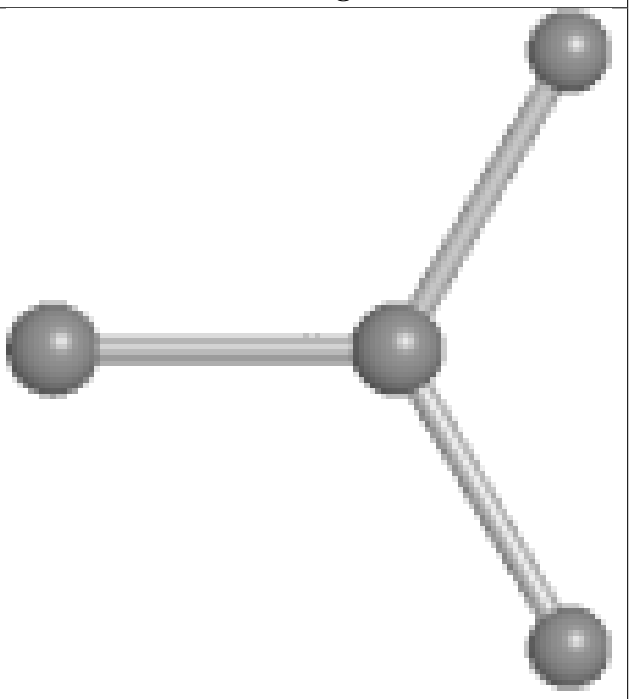
Bond lengths



Bond angles



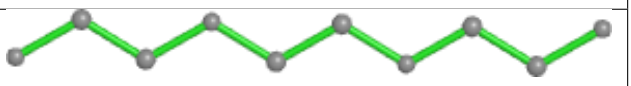
Torsions



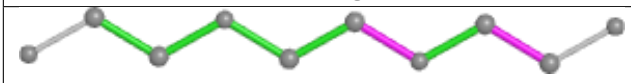
Rings

Ligand PGE E 311

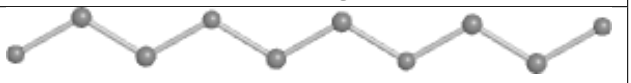
Bond lengths



Bond angles

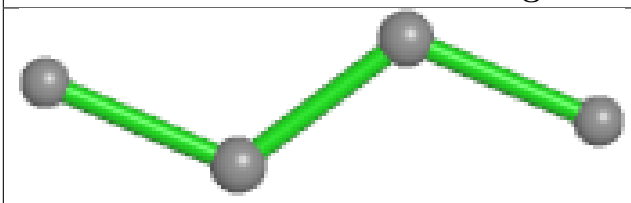


Torsions

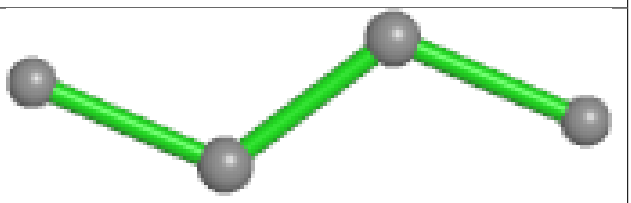


Rings

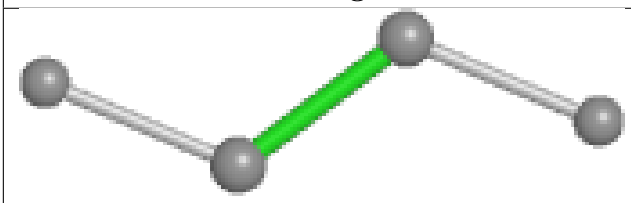
Ligand EDO C 308



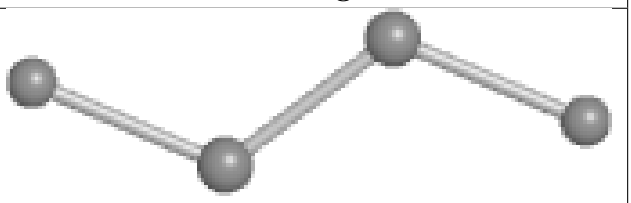
Bond lengths



Bond angles

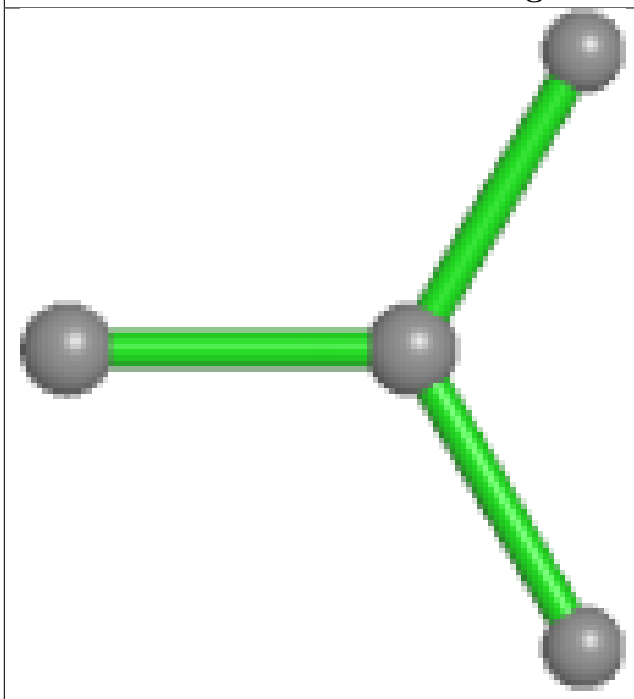


Torsions

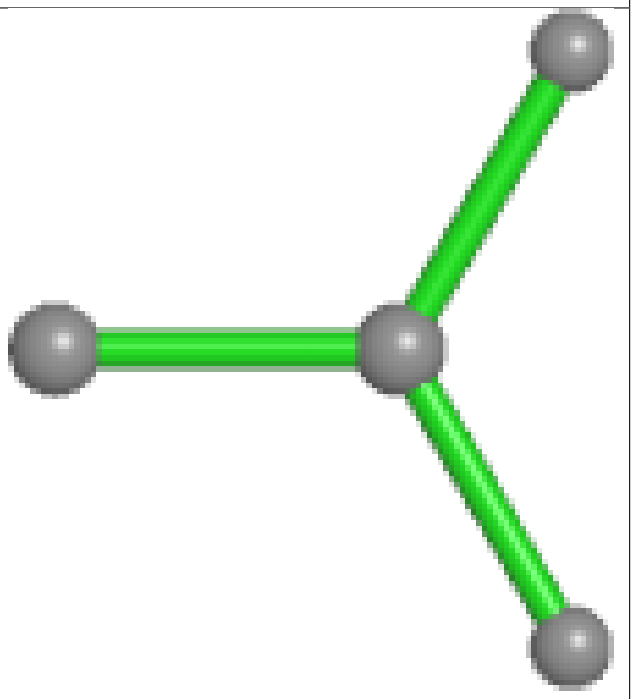


Rings

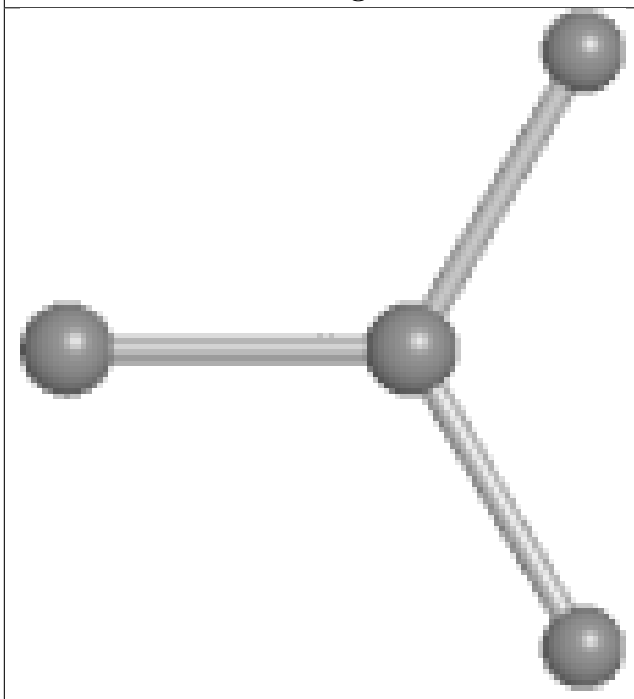
Ligand ACT F 310



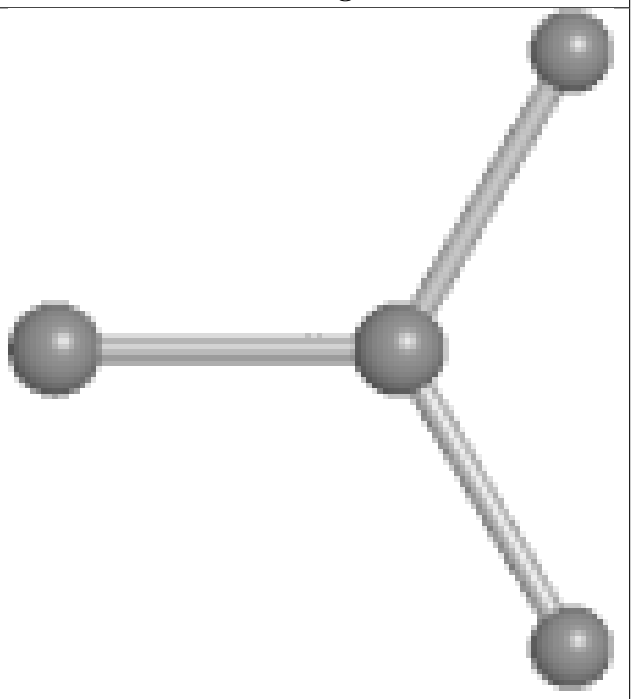
Bond lengths



Bond angles

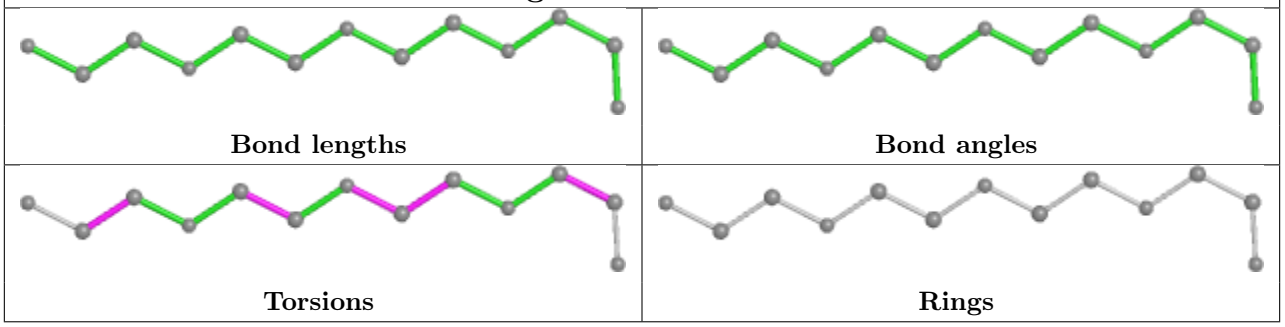


Torsions

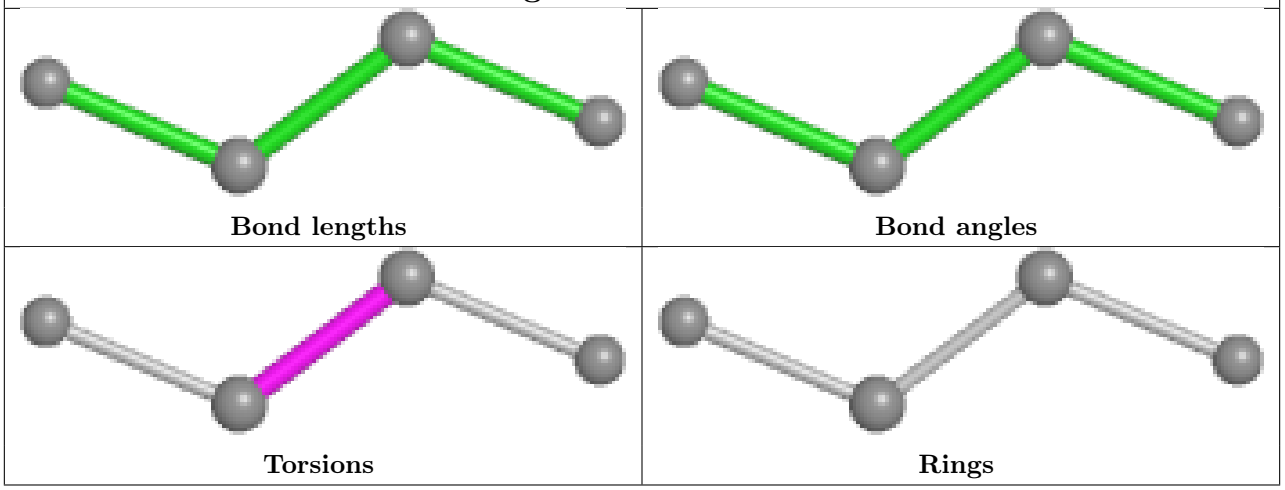


Rings

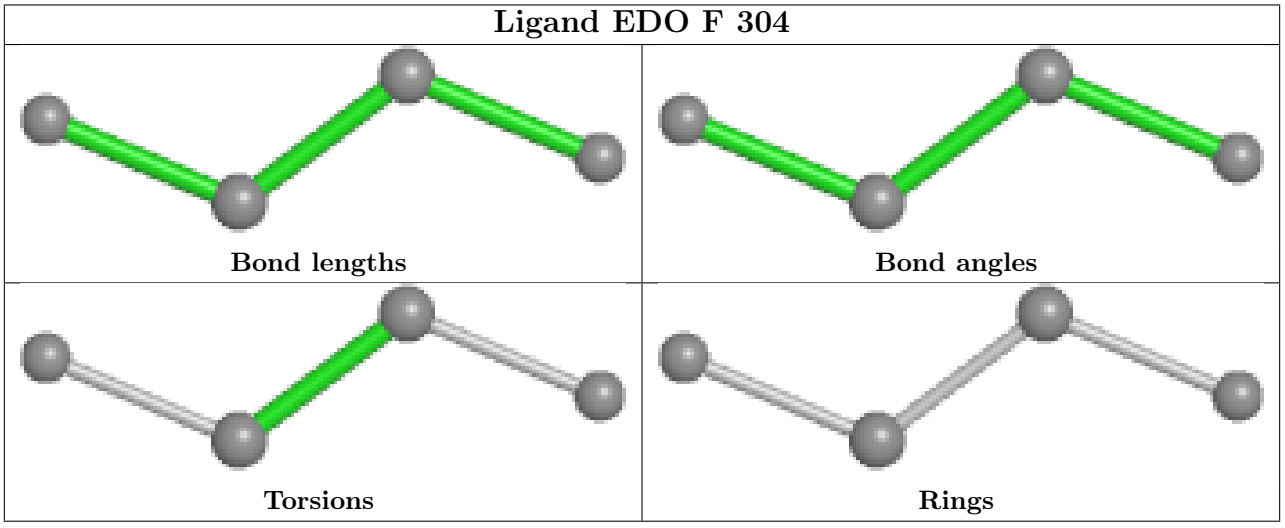
Ligand PG4 A 302

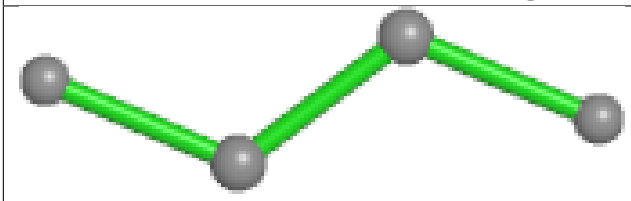
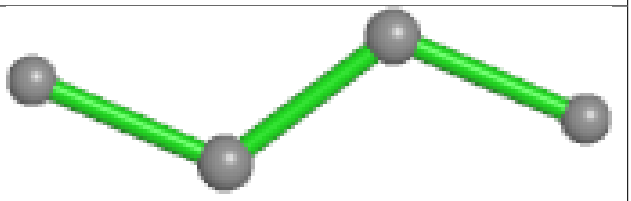
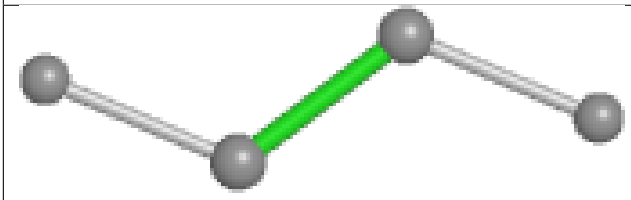
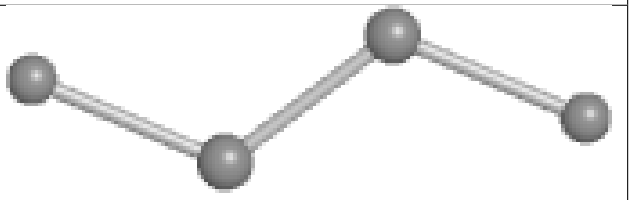


Ligand EDO B 304



Ligand EDO F 304



Ligand EDO A 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95^{th} 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%)	-0.29	3 (1%) 82 85	15, 21, 38, 46	0
1	B	295/310 (95%)	-0.44	0 100 100	15, 20, 37, 47	0
1	C	295/310 (95%)	-0.29	0 100 100	15, 21, 38, 54	0
1	D	295/310 (95%)	-0.22	1 (0%) 94 94	16, 21, 40, 54	0
1	E	294/310 (94%)	-0.35	1 (0%) 94 94	16, 23, 40, 51	0
1	F	296/310 (95%)	-0.27	1 (0%) 94 94	15, 23, 41, 56	0
All	All	1770/1860 (95%)	-0.31	6 (0%) 94 94	15, 21, 39, 56	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	ASP	2.8
1	A	268	SER	2.6
1	D	4	ASN	2.4
1	E	4	ASN	2.2
1	A	267	GLU	2.1

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, 95^{th} 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	0.94	0.11	12,16,20,22	0
1	KPI	E	166	14/15	0.95	0.09	16,18,26,28	0
1	KPI	A	166	14/15	0.96	0.08	13,16,24,26	0
1	KPI	B	166	14/15	0.96	0.08	13,16,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	D	166	14/15	0.97	0.09	15,17,23,23	0
1	KPI	F	166	14/15	0.97	0.09	13,16,25,26	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	C	313	4/4	0.61	0.22	41,58,58,61	0
6	MG	B	308	1/1	0.66	0.09	53,53,53,53	0
6	MG	B	313	1/1	0.68	0.10	51,51,51,51	0
9	PEG	D	315	7/7	0.71	0.32	40,46,66,71	0
5	ACT	D	310	4/4	0.74	0.16	38,49,51,59	0
5	ACT	F	310	4/4	0.75	0.36	41,55,57,63	0
8	PGE	E	311	10/10	0.75	0.16	38,48,57,60	0
4	EDO	E	307	4/4	0.75	0.15	41,43,48,54	0
8	PGE	C	315	10/10	0.76	0.13	28,42,55,61	0
5	ACT	C	311	4/4	0.76	0.20	33,48,51,54	0
7	GOL	D	314	6/6	0.76	0.14	46,50,53,54	0
6	MG	B	311	1/1	0.78	0.15	51,51,51,51	0
4	EDO	C	308	4/4	0.79	0.14	34,35,44,45	0
8	PGE	C	314	10/10	0.80	0.28	36,48,60,67	0
7	GOL	F	313	6/6	0.80	0.15	45,54,59,60	0
4	EDO	D	308	4/4	0.81	0.14	38,45,46,49	0
4	EDO	A	304	4/4	0.83	0.13	31,39,45,52	0
4	EDO	F	309	4/4	0.84	0.21	29,33,44,63	0
5	ACT	C	310	4/4	0.85	0.16	31,47,51,55	0
6	MG	B	312	1/1	0.85	0.19	58,58,58,58	0
9	PEG	C	317	7/7	0.85	0.12	42,49,60,61	0
4	EDO	A	308	4/4	0.85	0.11	38,43,48,58	0
8	PGE	B	307	10/10	0.86	0.12	42,48,54,63	0
5	ACT	D	309	4/4	0.86	0.11	37,43,45,47	0
4	EDO	F	308	4/4	0.86	0.12	44,45,46,47	0
5	ACT	D	311	4/4	0.86	0.20	37,44,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PGE	F	312	10/10	0.86	0.20	35,50,54,54	0
4	EDO	C	309	4/4	0.86	0.17	30,32,42,50	0
5	ACT	A	309	4/4	0.86	0.13	40,42,52,52	0
6	MG	C	316	1/1	0.87	0.13	53,53,53,53	0
8	PGE	D	312	10/10	0.87	0.20	41,45,67,68	0
3	PG4	E	302	13/13	0.87	0.17	36,44,56,56	0
4	EDO	F	305	4/4	0.87	0.09	29,32,32,48	0
4	EDO	E	303	4/4	0.87	0.22	38,39,44,52	0
4	EDO	E	304	4/4	0.87	0.09	38,45,48,49	0
4	EDO	B	304	4/4	0.88	0.10	21,32,34,44	0
5	ACT	E	310	4/4	0.88	0.27	39,49,50,54	0
4	EDO	E	308	4/4	0.88	0.11	40,41,45,50	0
7	GOL	B	314	6/6	0.88	0.35	40,51,62,71	0
6	MG	A	311	1/1	0.88	0.08	52,52,52,52	0
4	EDO	E	305	4/4	0.88	0.11	33,34,35,57	0
4	EDO	F	307	4/4	0.88	0.09	38,38,50,56	0
4	EDO	C	303	4/4	0.89	0.33	28,35,37,52	0
4	EDO	E	309	4/4	0.89	0.10	42,50,54,58	0
5	ACT	F	311	4/4	0.89	0.11	41,46,56,60	0
3	PG4	D	302	13/13	0.89	0.14	34,39,56,60	0
5	ACT	C	312	4/4	0.89	0.14	40,43,46,52	0
4	EDO	C	305	4/4	0.90	0.16	38,38,40,49	0
4	EDO	E	306	4/4	0.90	0.11	33,34,37,50	0
3	PG4	C	302	13/13	0.90	0.12	24,37,54,54	0
3	PG4	A	302	13/13	0.90	0.17	25,40,52,52	0
4	EDO	D	304	4/4	0.90	0.27	31,36,47,53	0
4	EDO	D	307	4/4	0.90	0.11	29,29,34,34	0
3	PG4	B	302	13/13	0.90	0.12	31,38,52,55	0
4	EDO	B	305	4/4	0.90	0.11	28,38,40,50	0
6	MG	D	313	1/1	0.90	0.26	33,33,33,33	0
3	PG4	F	302	13/13	0.90	0.11	25,39,55,55	0
7	GOL	A	312	6/6	0.91	0.40	28,41,50,52	0
6	MG	A	310	1/1	0.91	0.13	47,47,47,47	0
4	EDO	D	306	4/4	0.92	0.31	24,41,42,42	0
4	EDO	C	304	4/4	0.92	0.24	34,34,45,47	0
4	EDO	A	306	4/4	0.92	0.17	36,41,44,48	0
4	EDO	C	307	4/4	0.92	0.12	34,36,49,56	0
4	EDO	D	305	4/4	0.92	0.10	29,34,43,51	0
5	ACT	B	306	4/4	0.92	0.23	45,49,51,64	0
4	EDO	A	303	4/4	0.93	0.08	25,33,43,47	0
4	EDO	A	307	4/4	0.93	0.11	31,39,41,54	0
4	EDO	A	305	4/4	0.93	0.10	24,29,31,42	0

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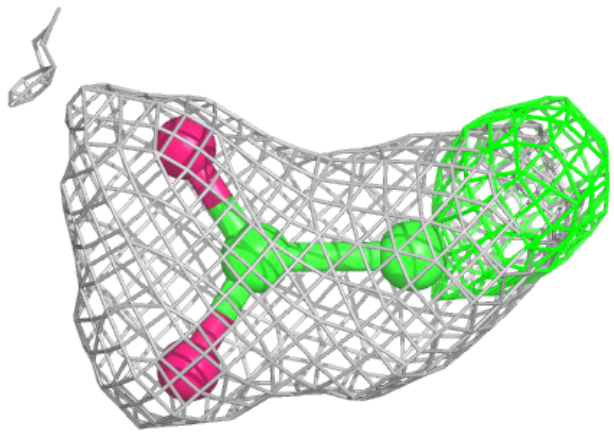
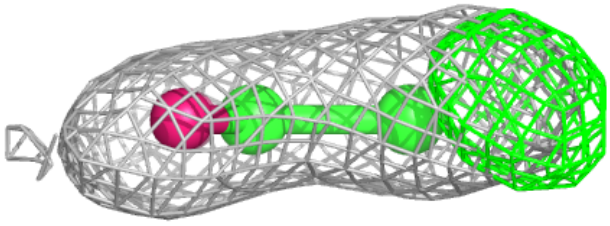
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	303	4/4	0.93	0.12	30,41,46,46	0
4	EDO	C	306	4/4	0.94	0.08	28,32,35,45	0
4	EDO	D	303	4/4	0.94	0.08	20,27,32,43	0
4	EDO	F	304	4/4	0.94	0.14	30,39,40,55	0
4	EDO	F	306	4/4	0.95	0.35	36,39,40,48	0
2	LYS	A	301	10/10	0.95	0.09	16,18,23,27	0
6	MG	B	310	1/1	0.96	0.09	19,19,19,19	0
2	LYS	F	301	10/10	0.96	0.09	15,19,24,27	0
6	MG	B	309	1/1	0.96	0.07	20,20,20,20	0
2	LYS	B	301	10/10	0.97	0.09	14,18,23,26	0
2	LYS	C	301	10/10	0.97	0.10	14,17,22,28	0
2	LYS	D	301	10/10	0.97	0.09	18,20,25,29	0
2	LYS	E	301	10/10	0.97	0.07	16,21,25,30	0
4	EDO	F	303	4/4	0.98	0.06	19,23,24,24	0

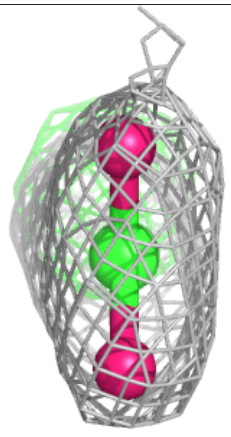
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACT C 313:

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

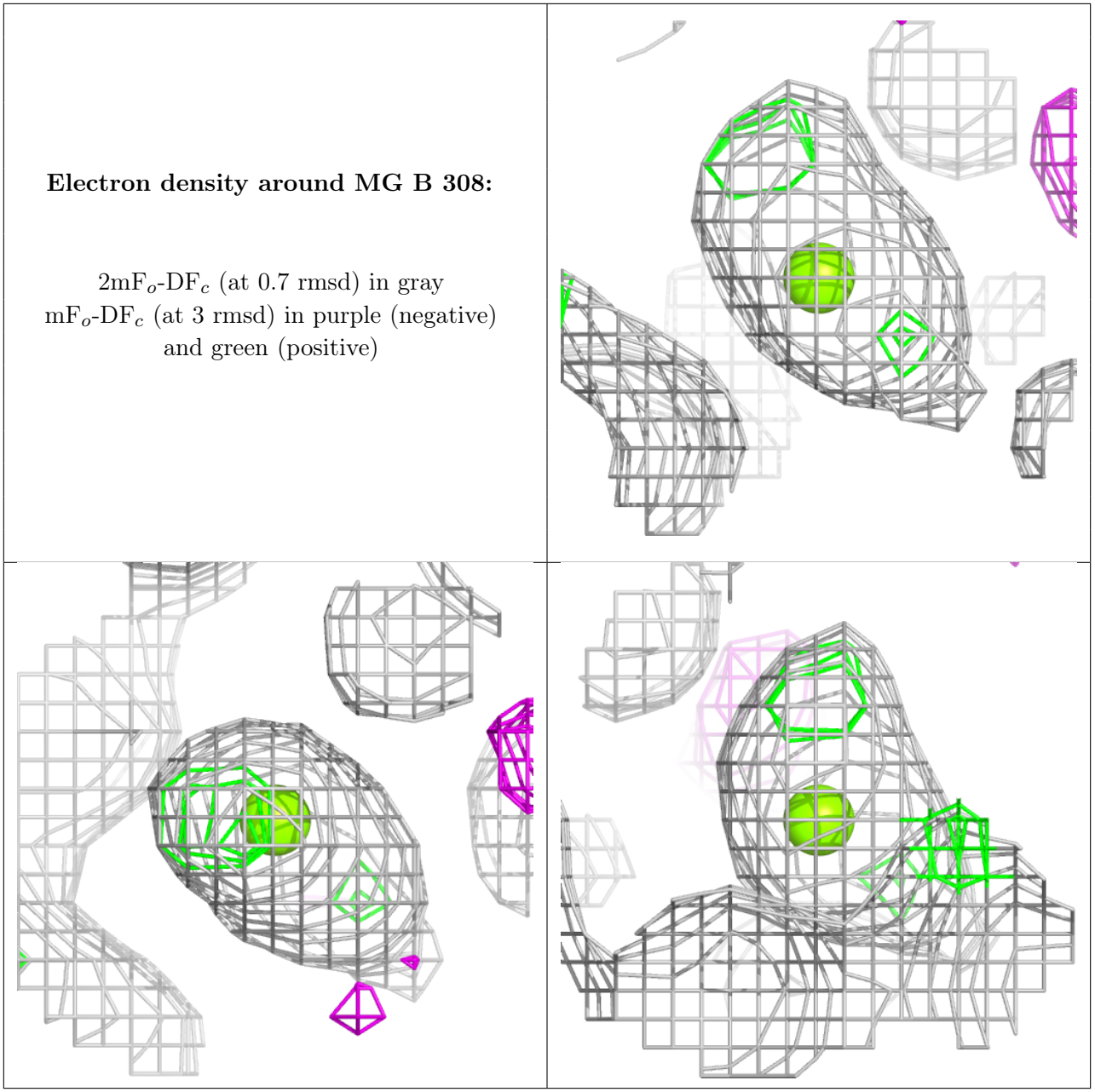






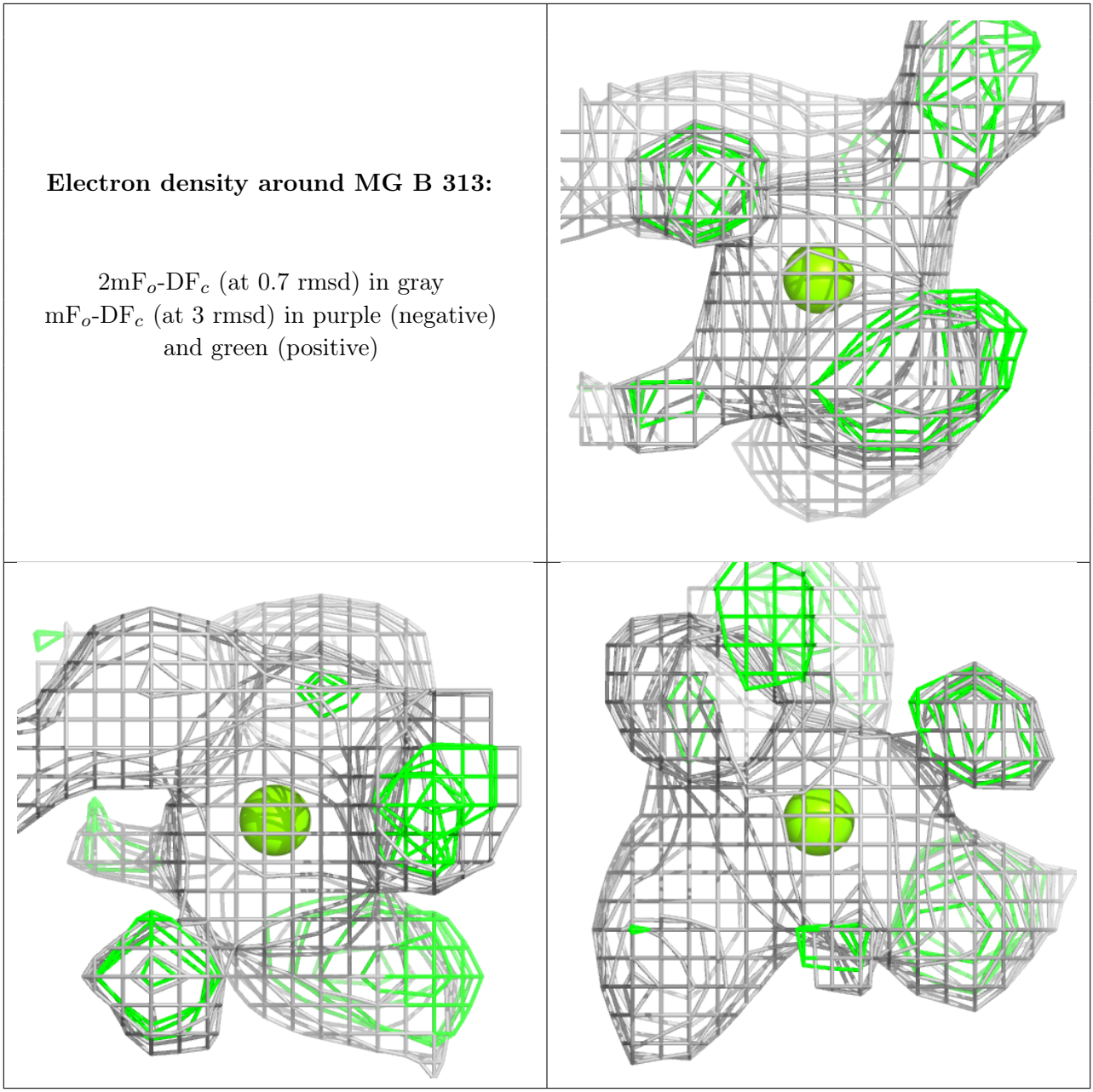
Electron density around MG B 308:

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



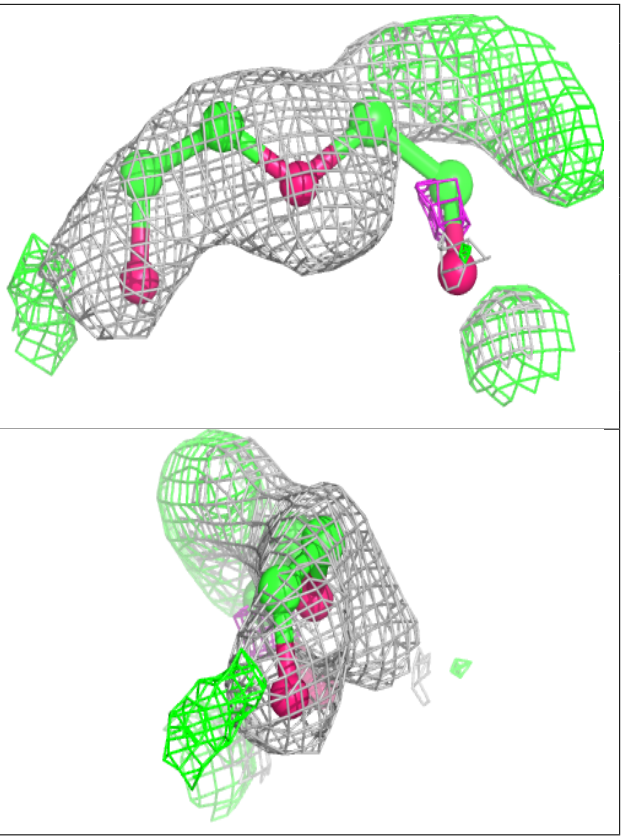
Electron density around MG B 313:

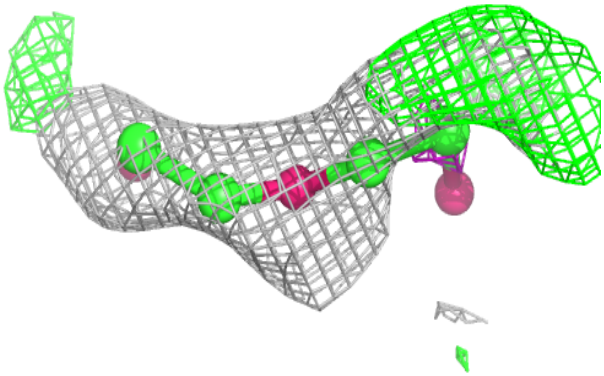
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PEG D 315:

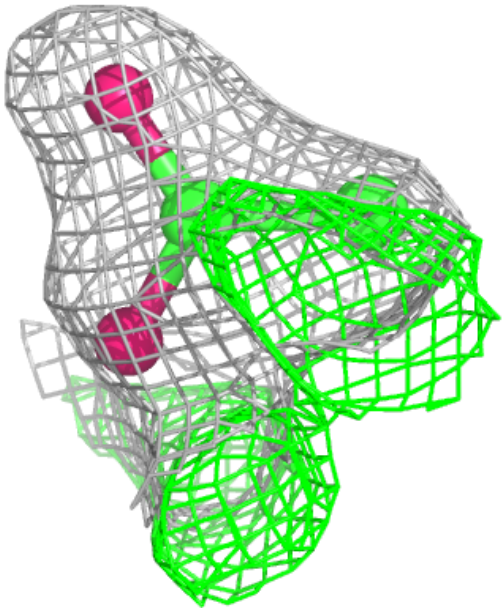
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

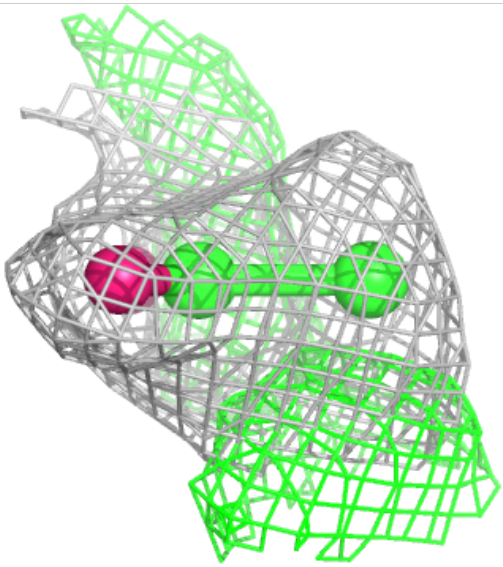


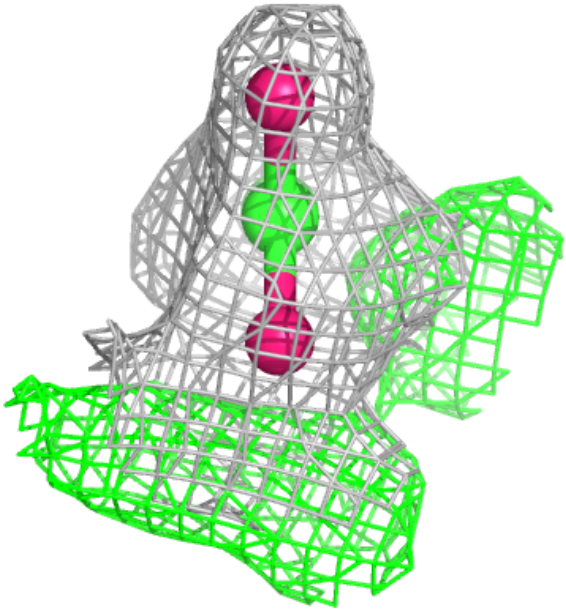


Electron density around ACT D 310:

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

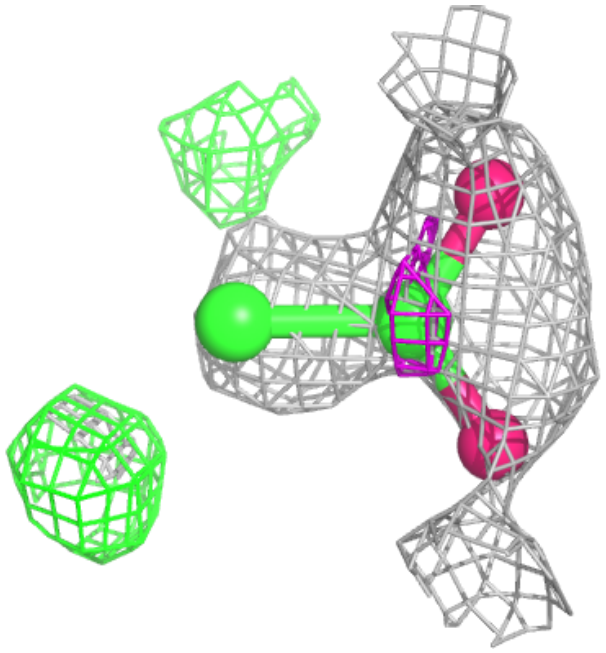


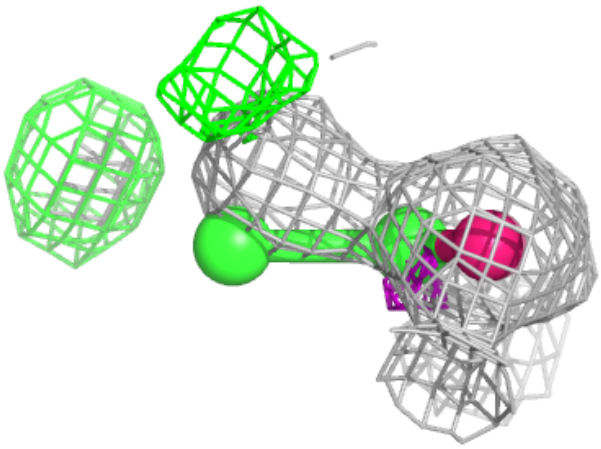


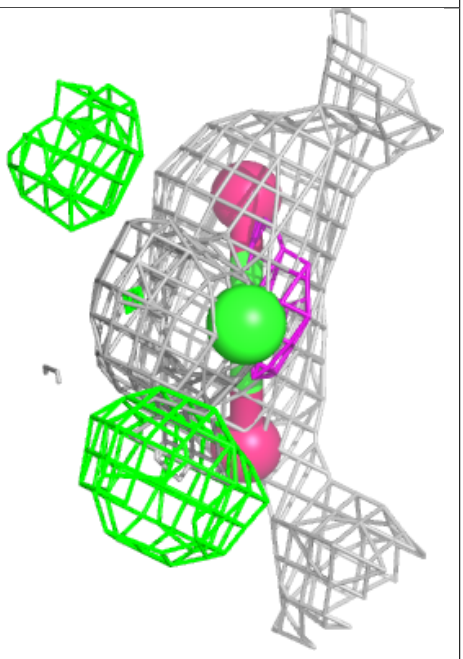


Electron density around ACT F 310:

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

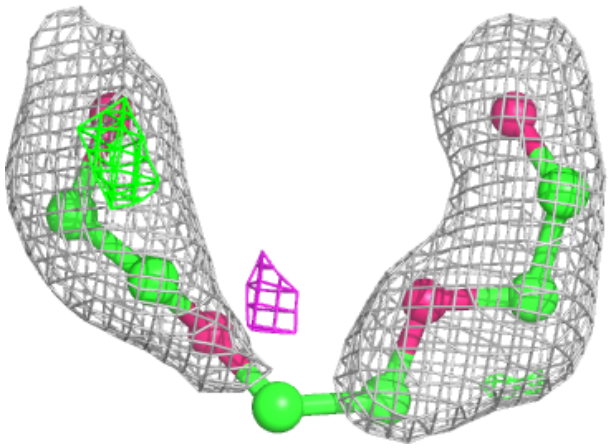


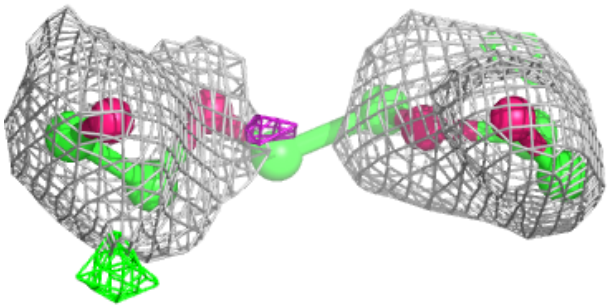


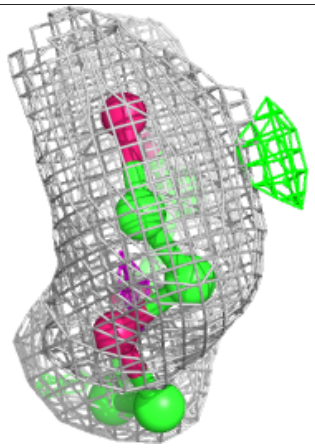


Electron density around PGE E 311:

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

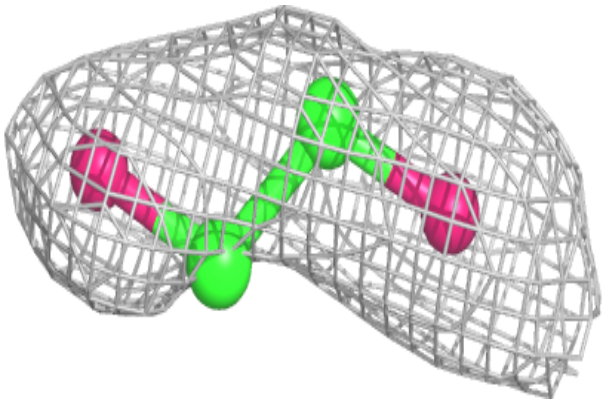


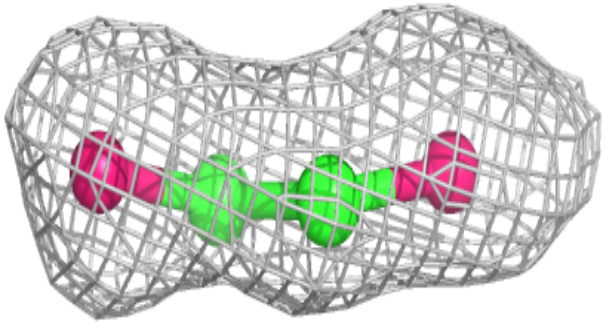


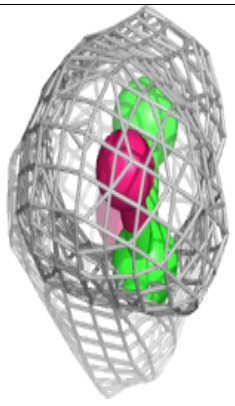


Electron density around EDO E 307:

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

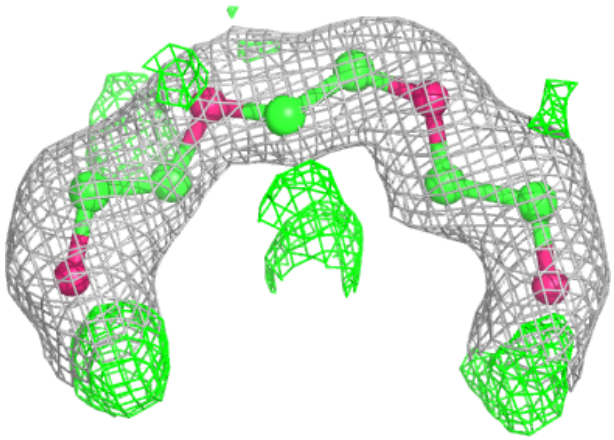


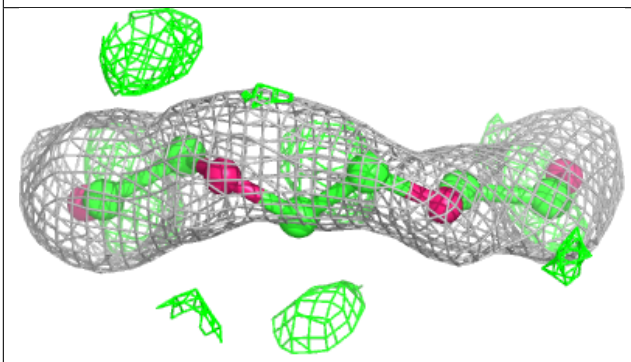


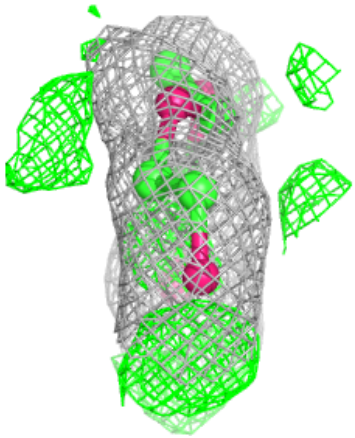


Electron density around PGE C 315:

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

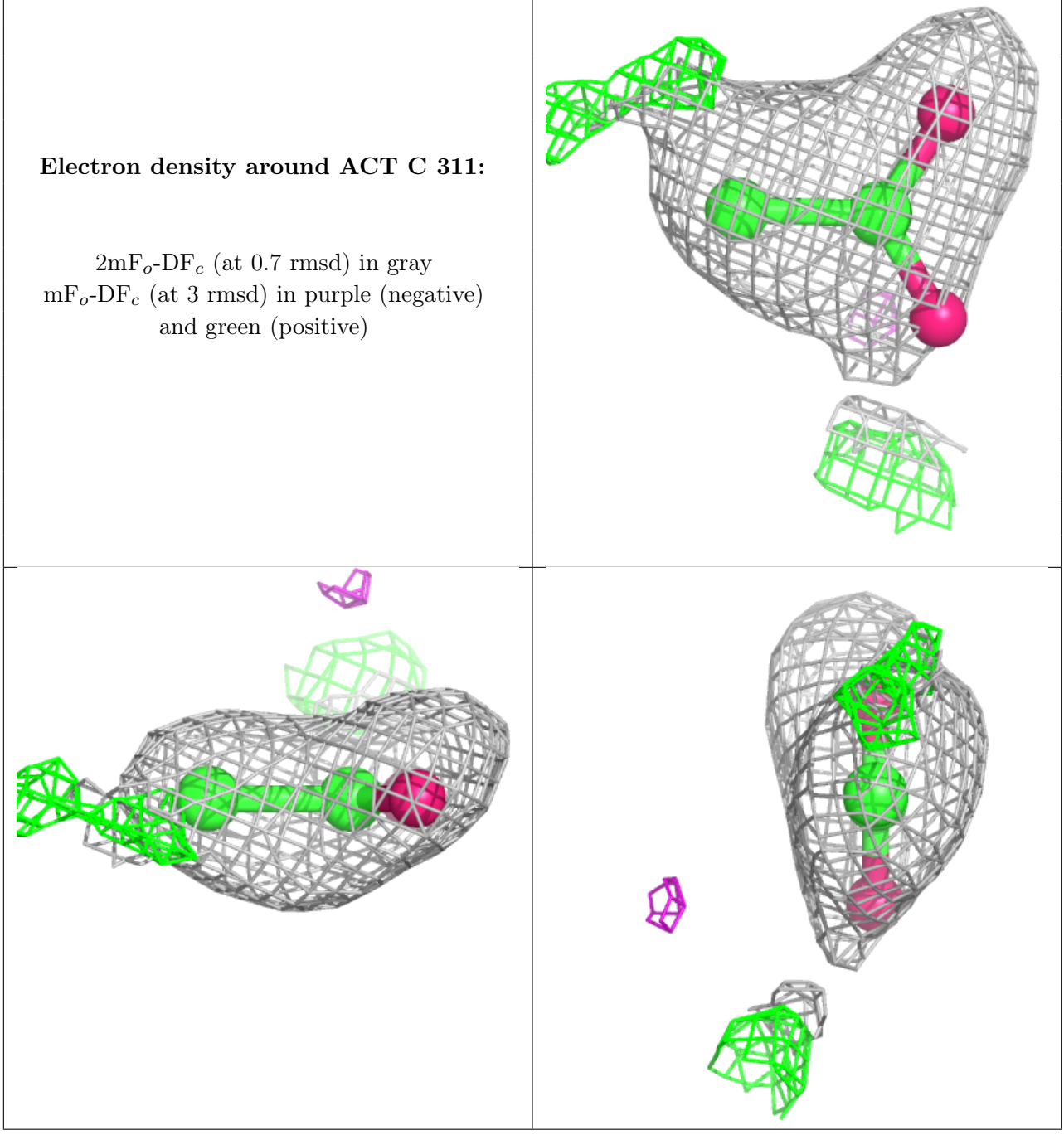






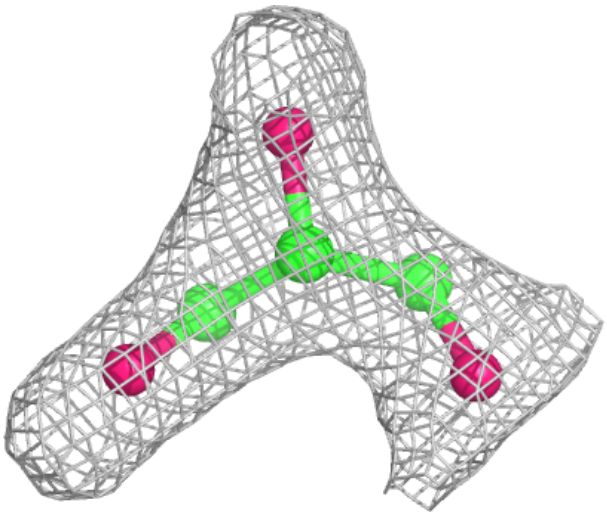
Electron density around ACT C 311:

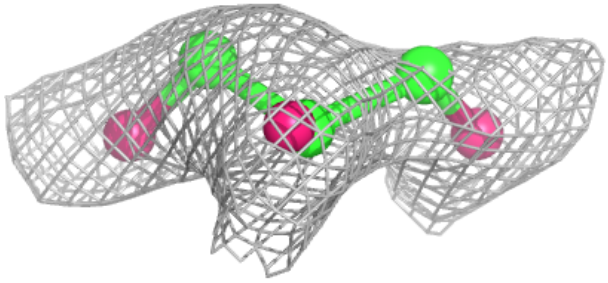
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

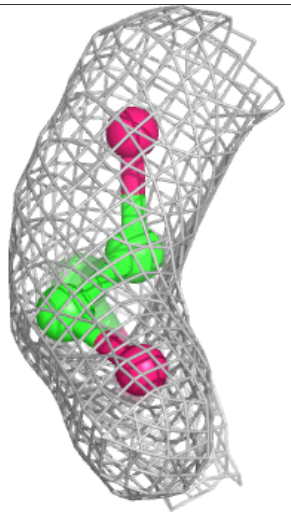


Electron density around GOL D 314:

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

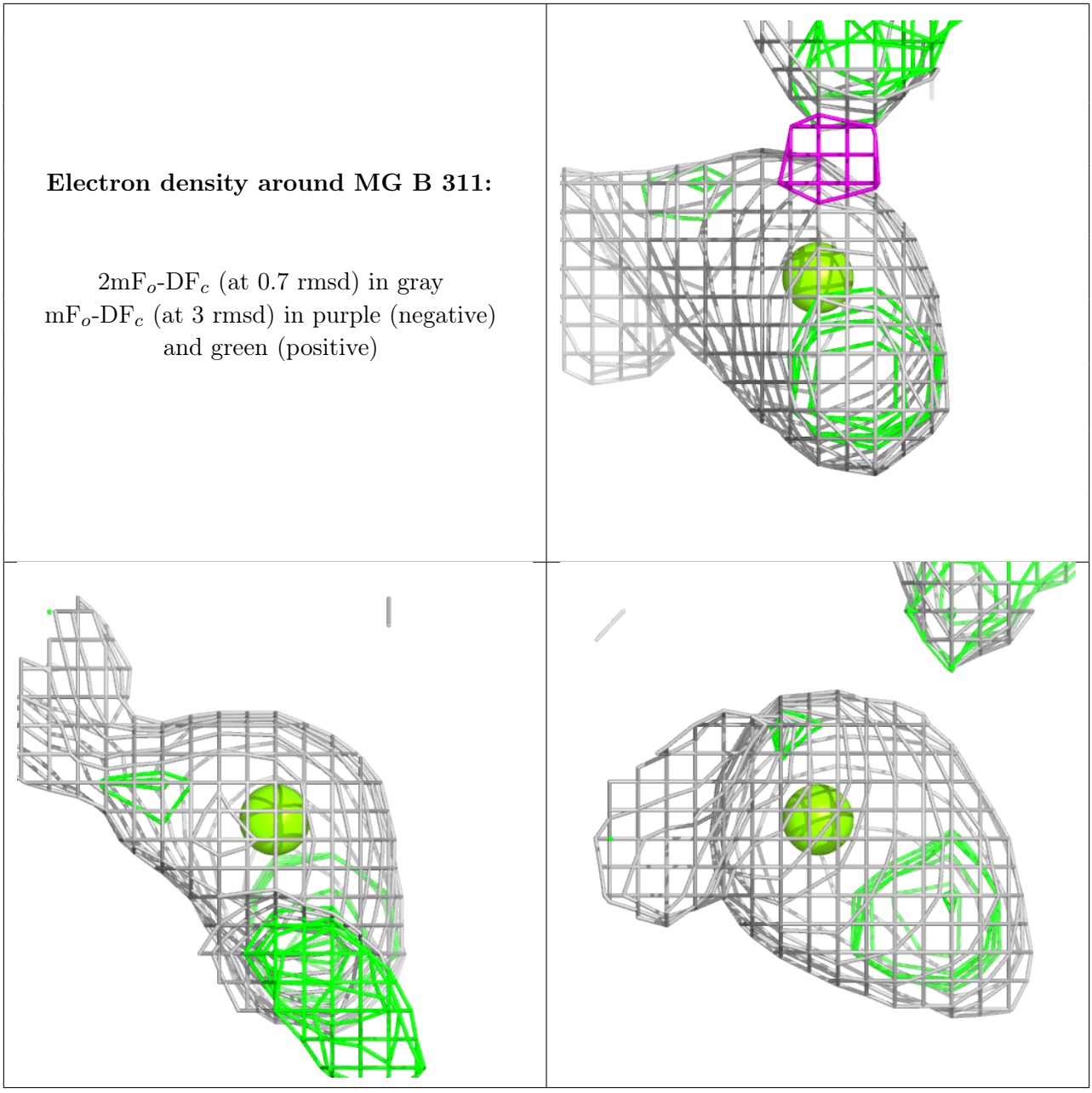






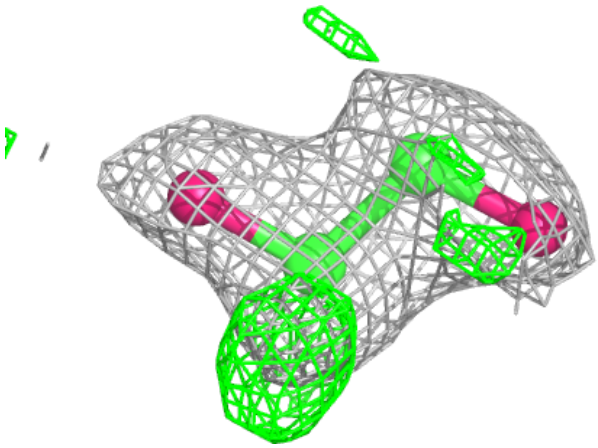
Electron density around MG B 311:

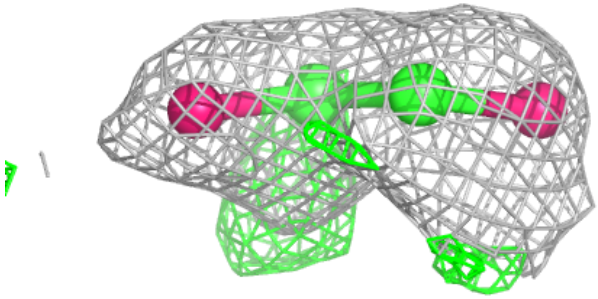
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

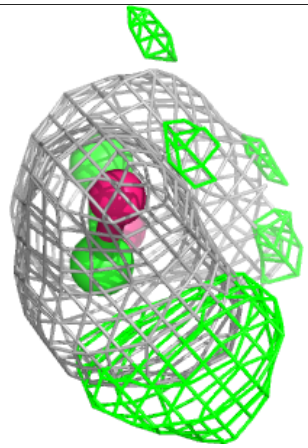


Electron density around EDO C 308:

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

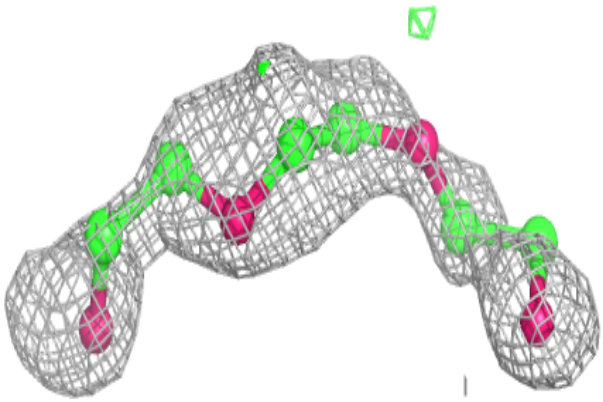


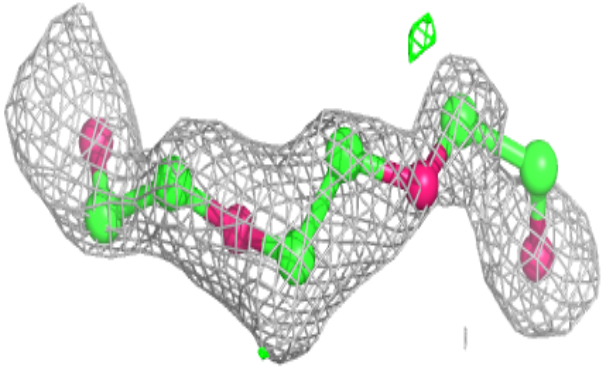


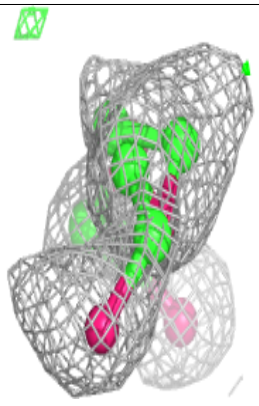


Electron density around PGE C 314:

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

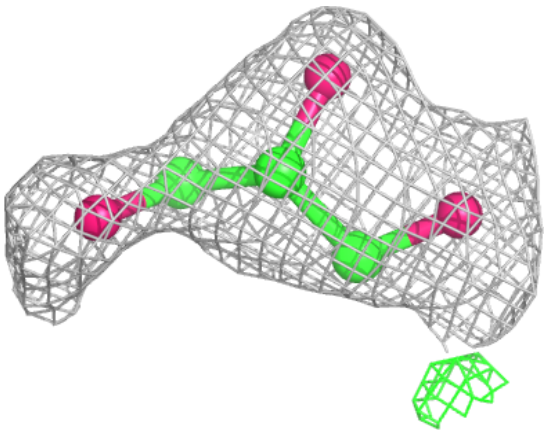


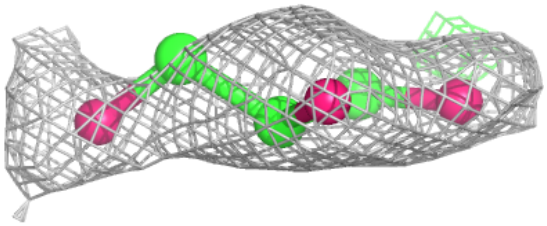


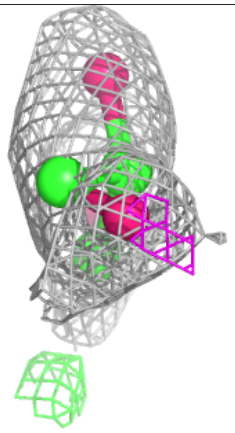


Electron density around GOL F 313:

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

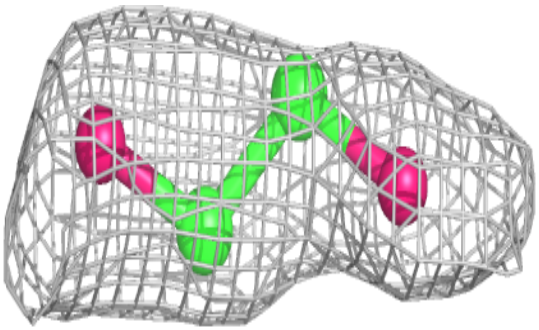


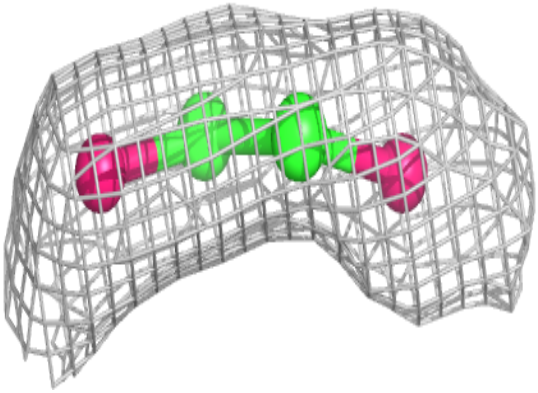


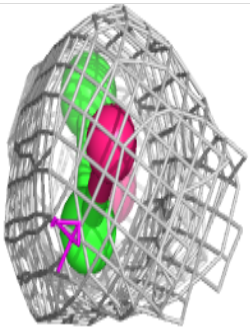


Electron density around EDO D 308:

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

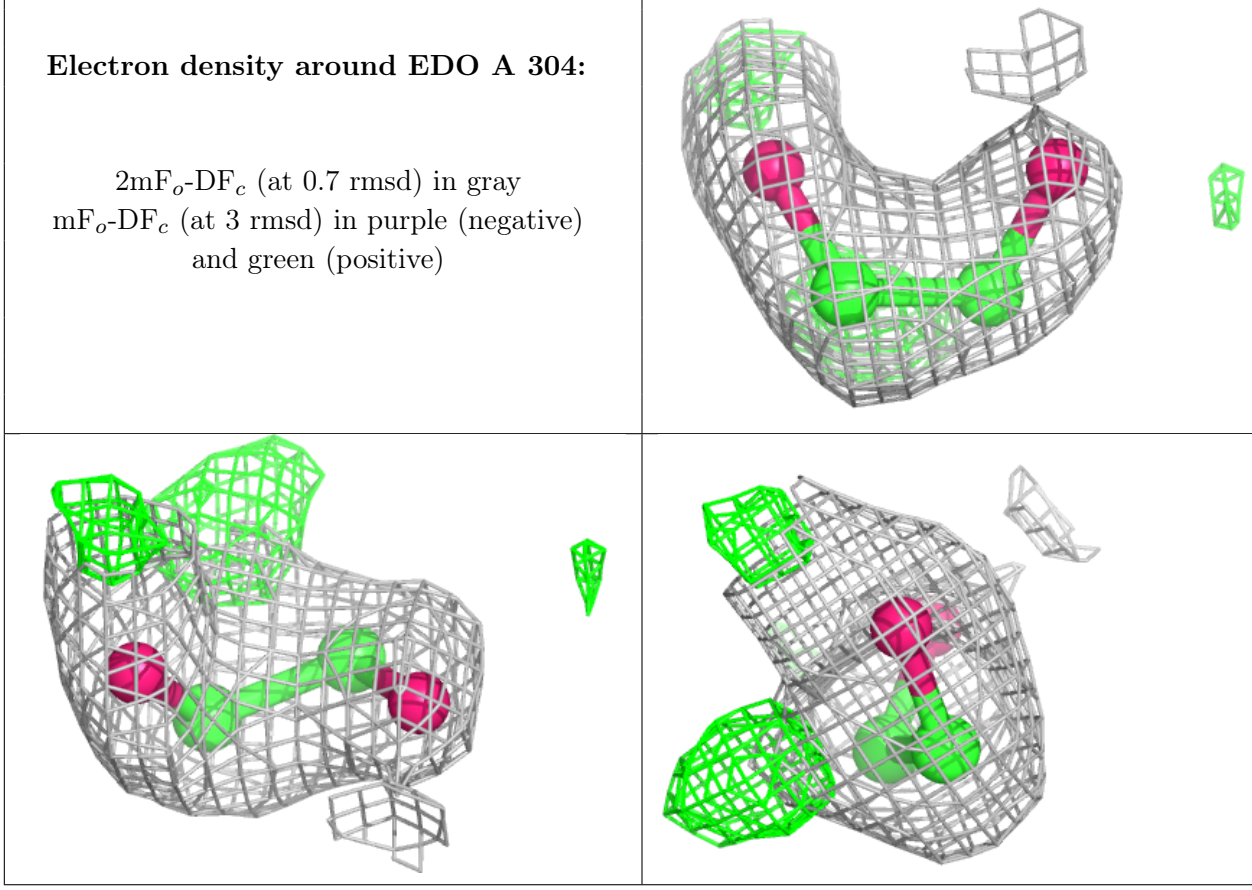






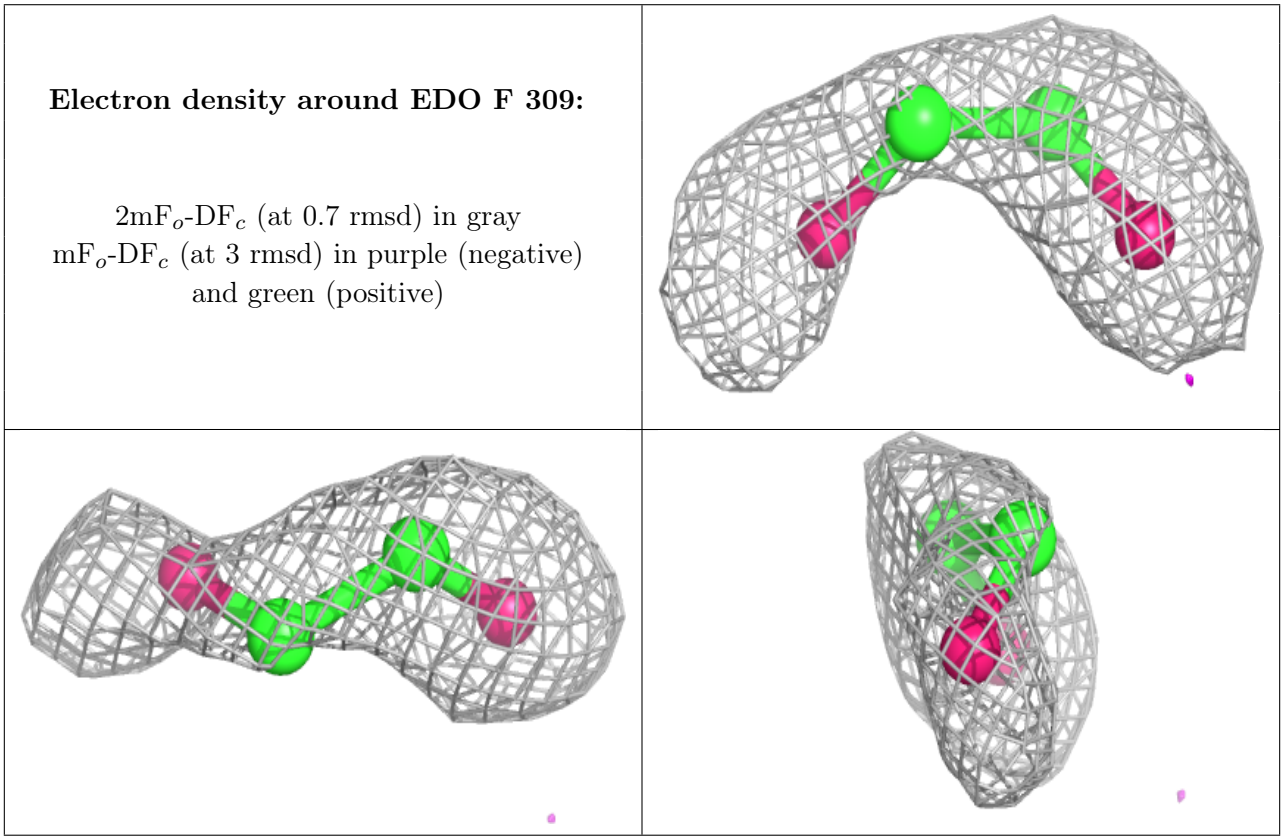
Electron density around EDO A 304:

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



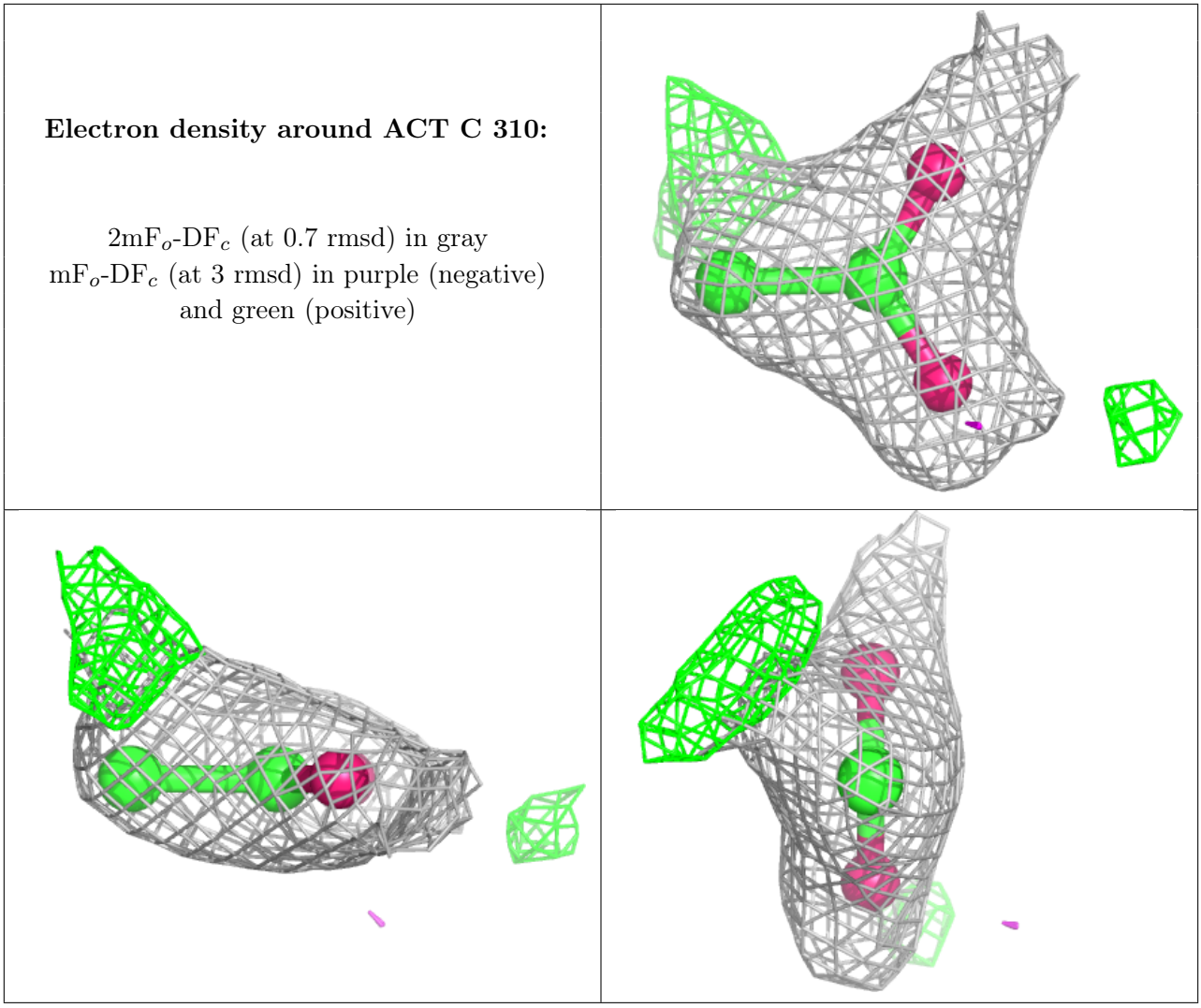
Electron density around EDO F 309:

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



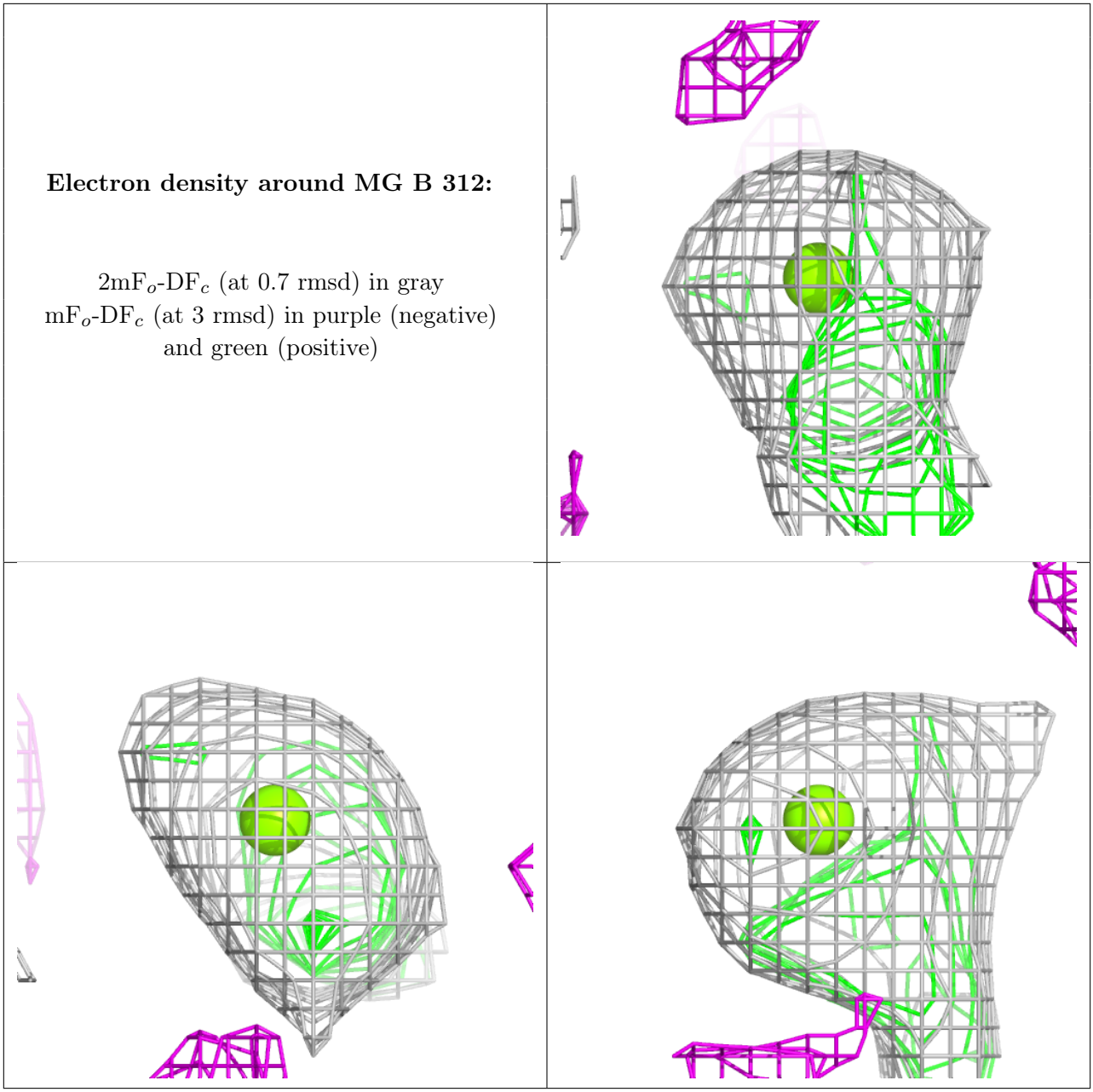
Electron density around ACT C 310:

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



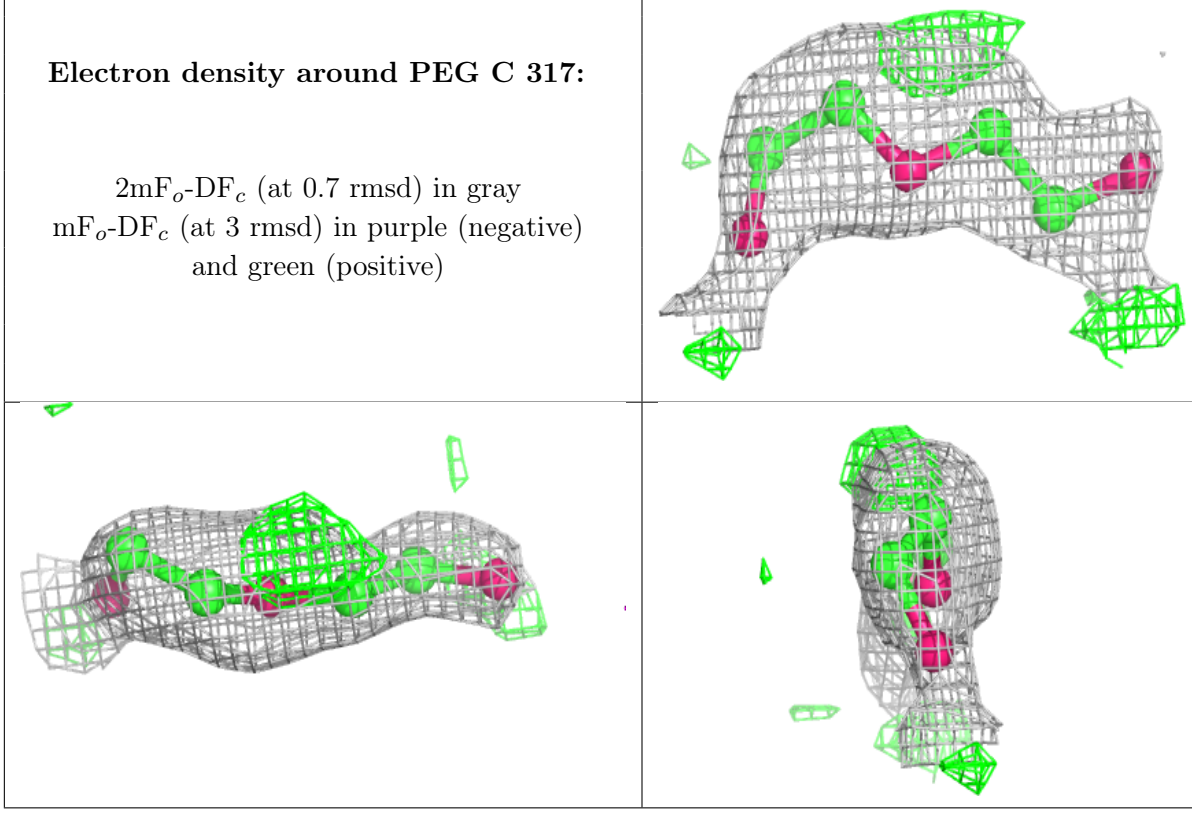
Electron density around MG B 312:

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



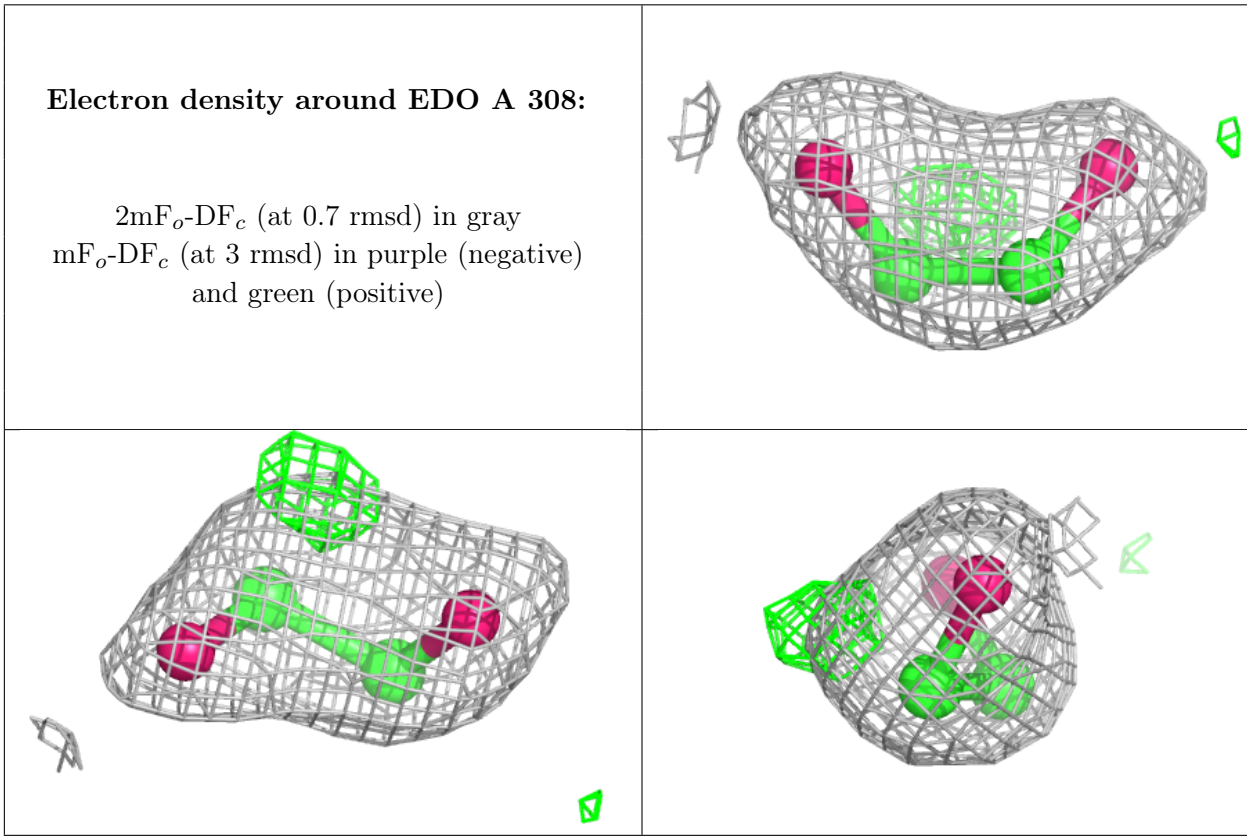
Electron density around PEG C 317:

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



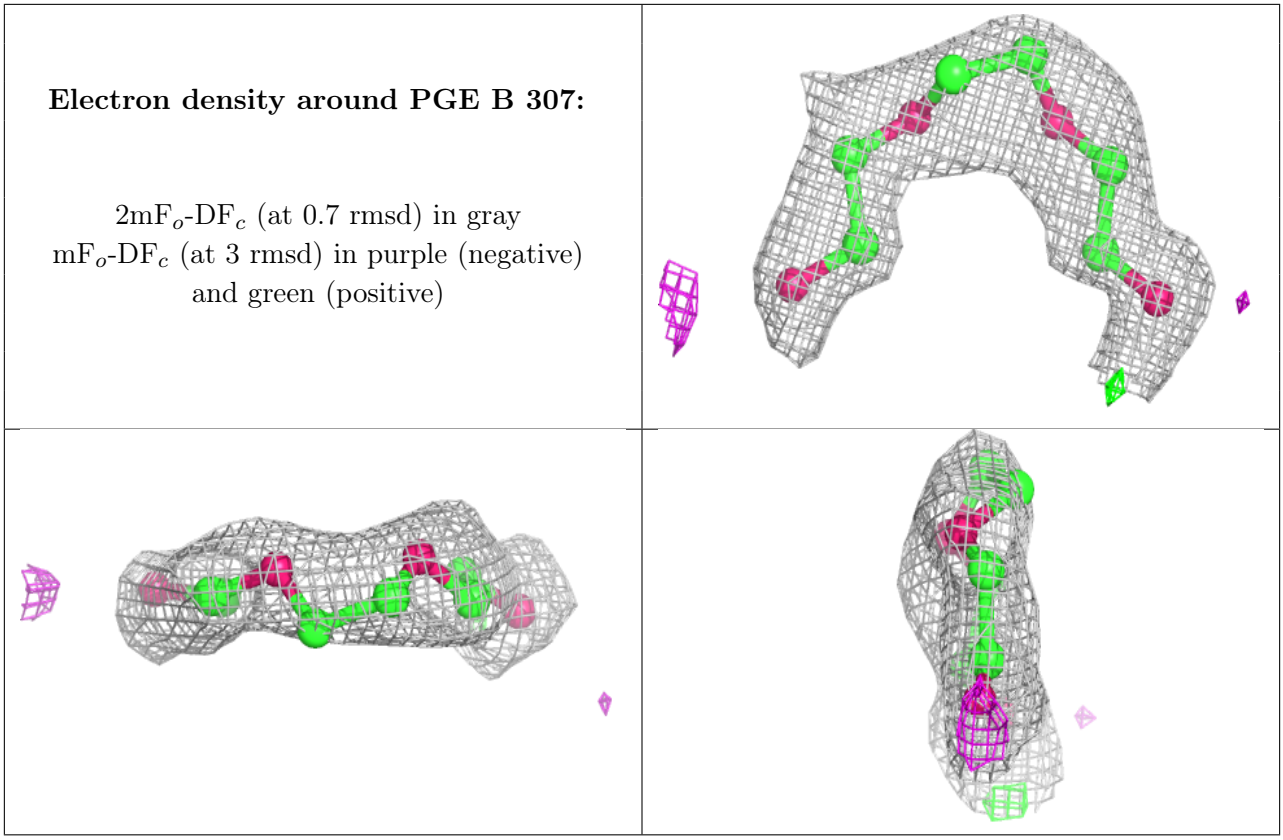
Electron density around EDO A 308:

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



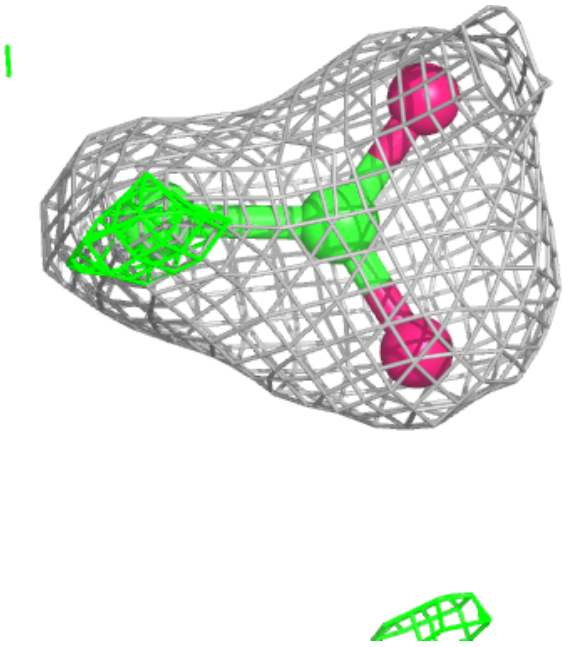
Electron density around PGE B 307:

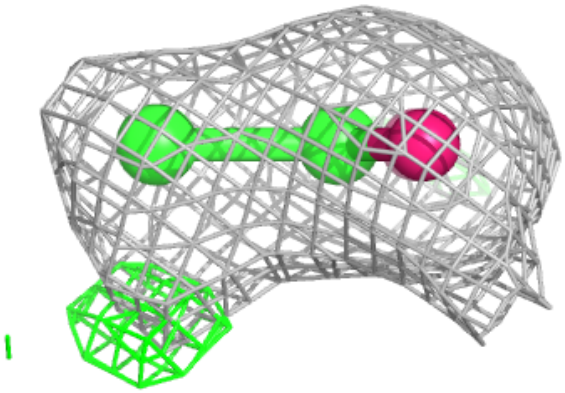
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

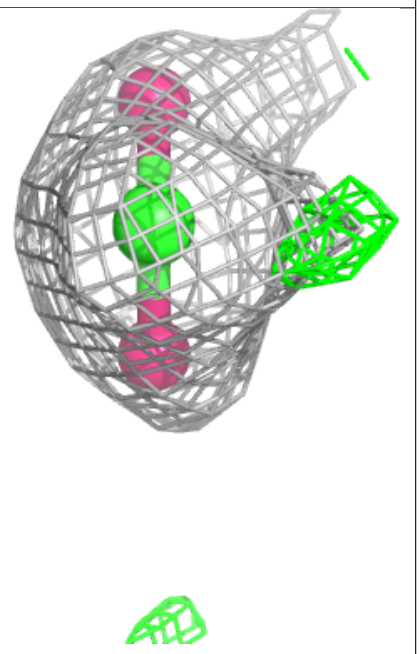


Electron density around ACT D 309:

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

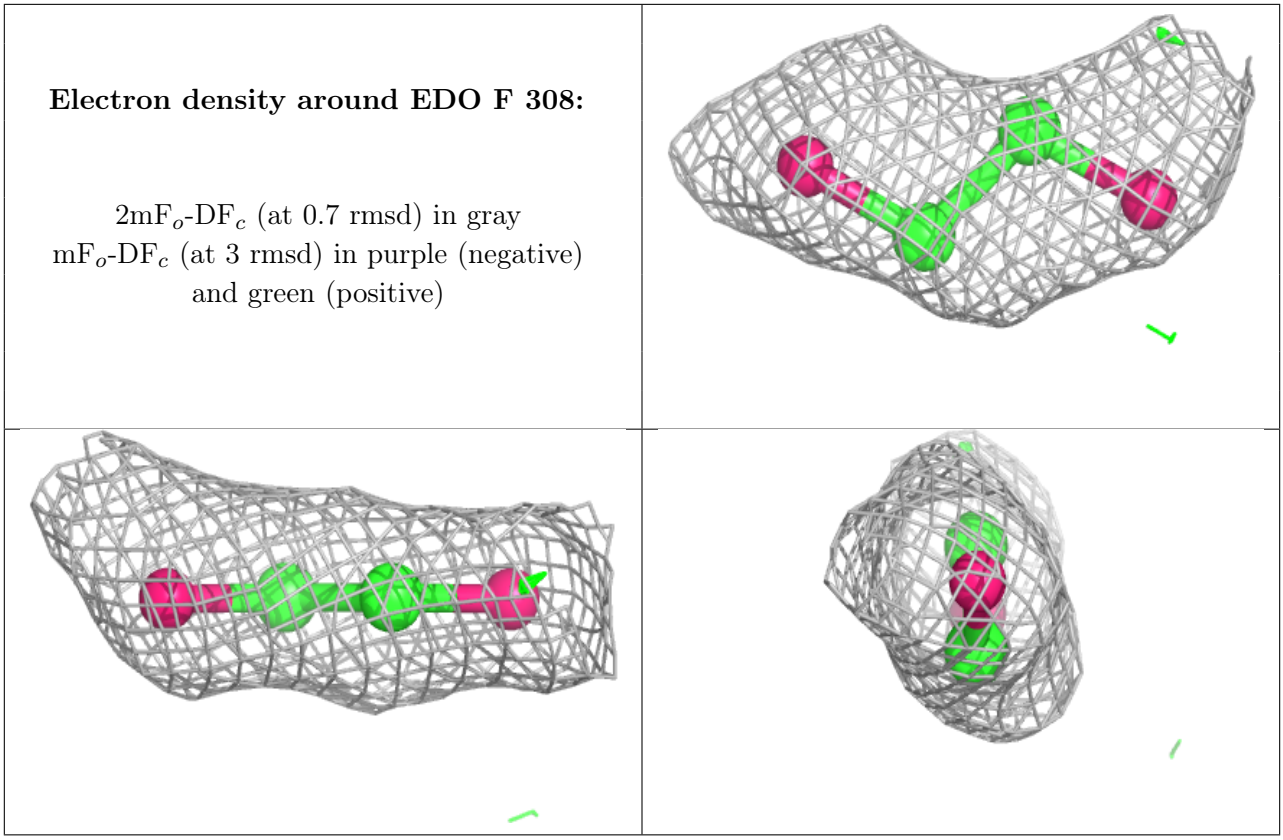






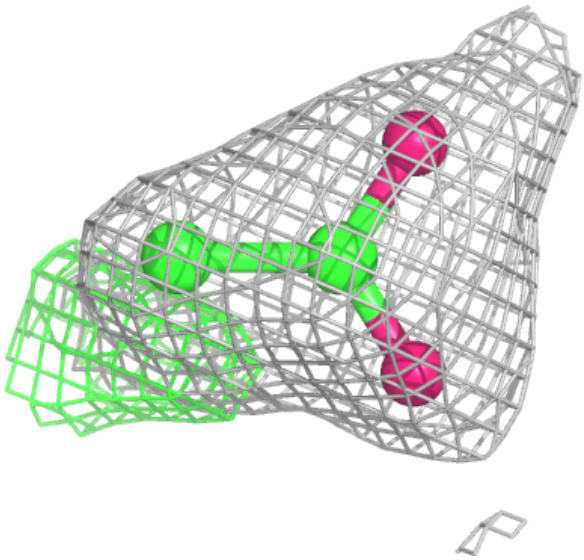
Electron density around EDO F 308:

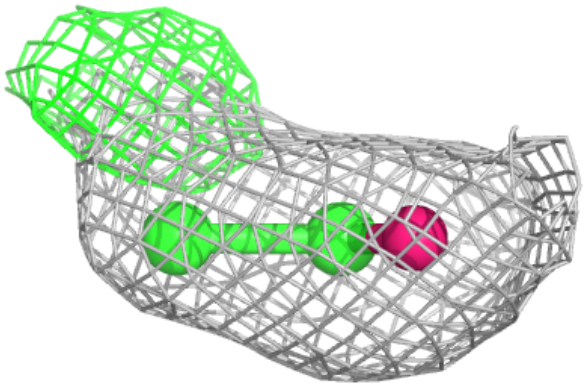
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

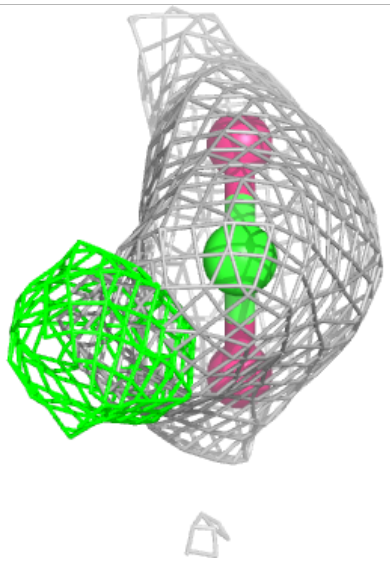


Electron density around ACT D 311:

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

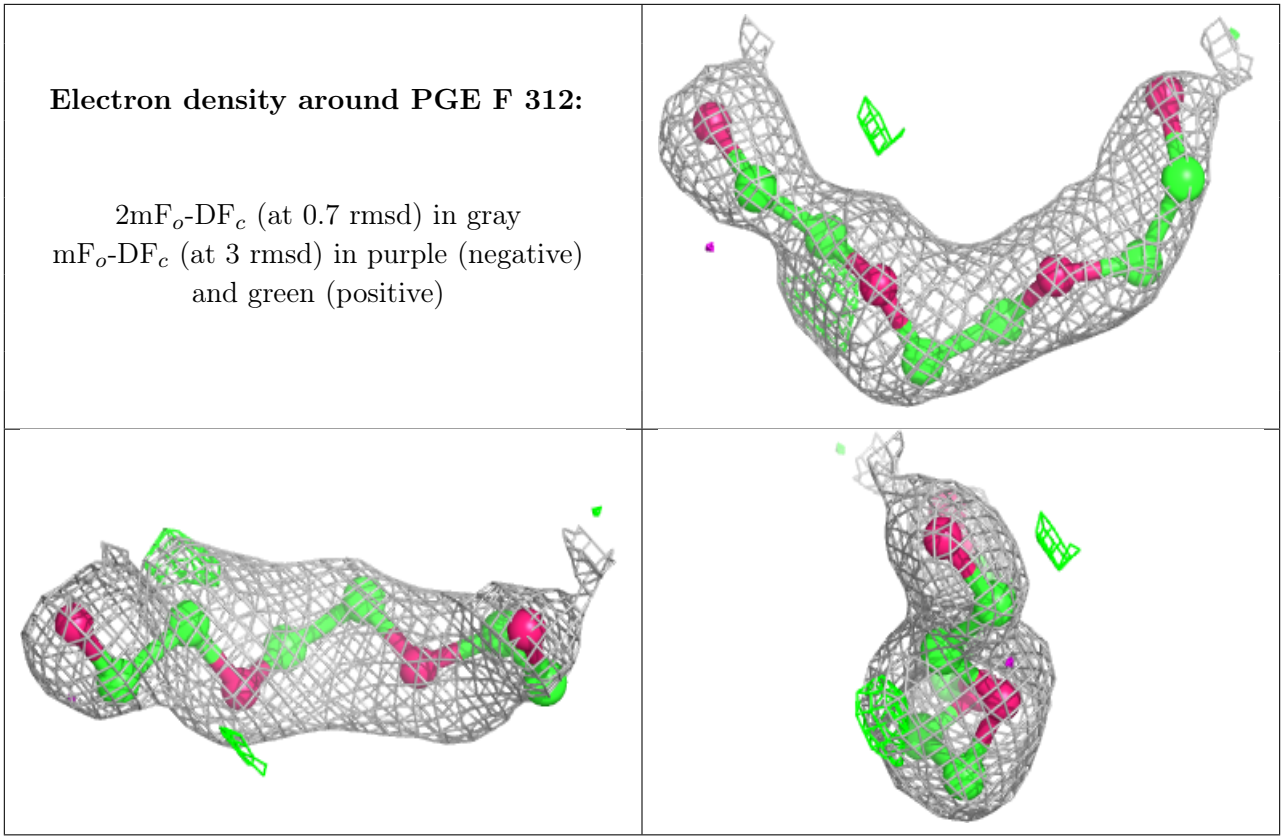






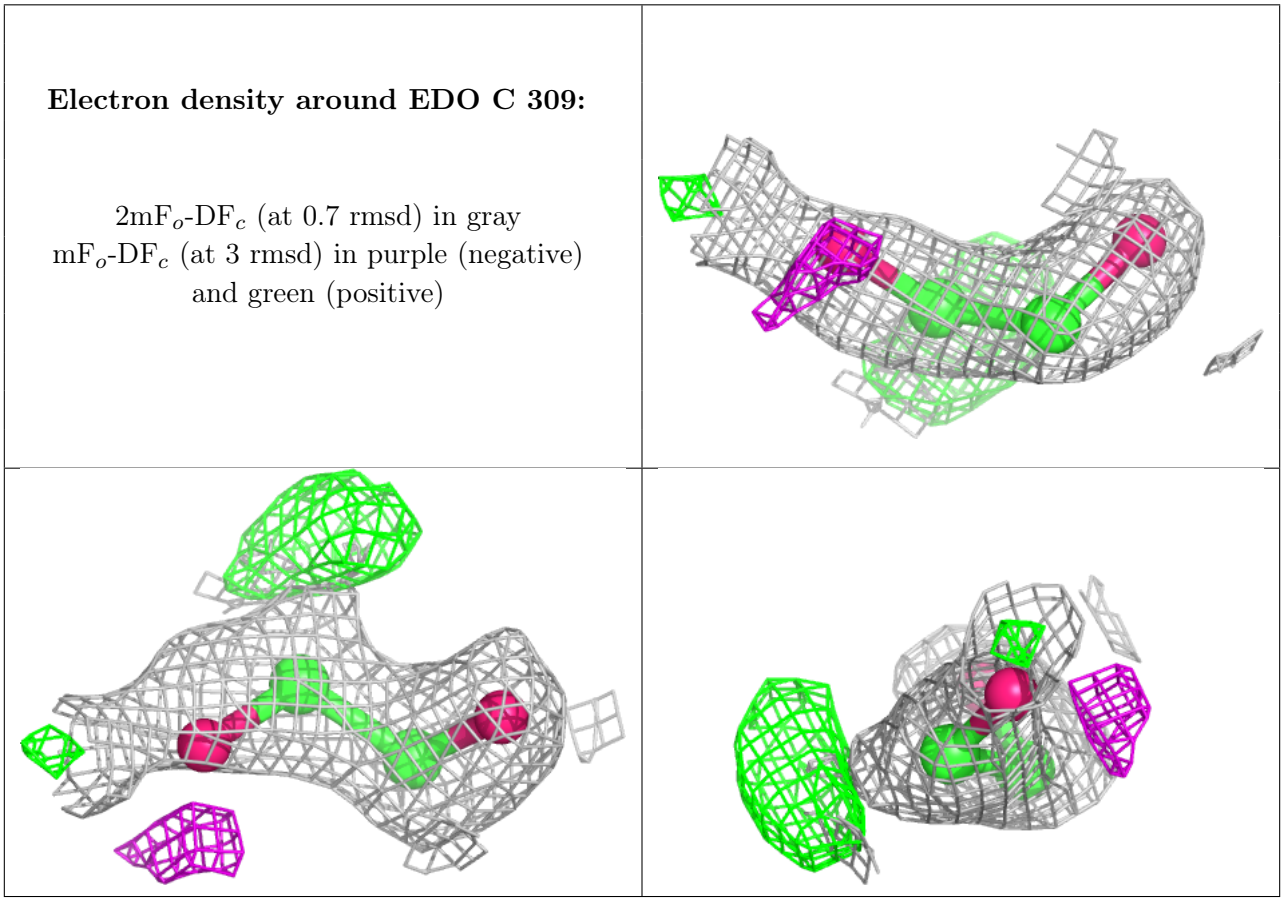
Electron density around PGE F 312:

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



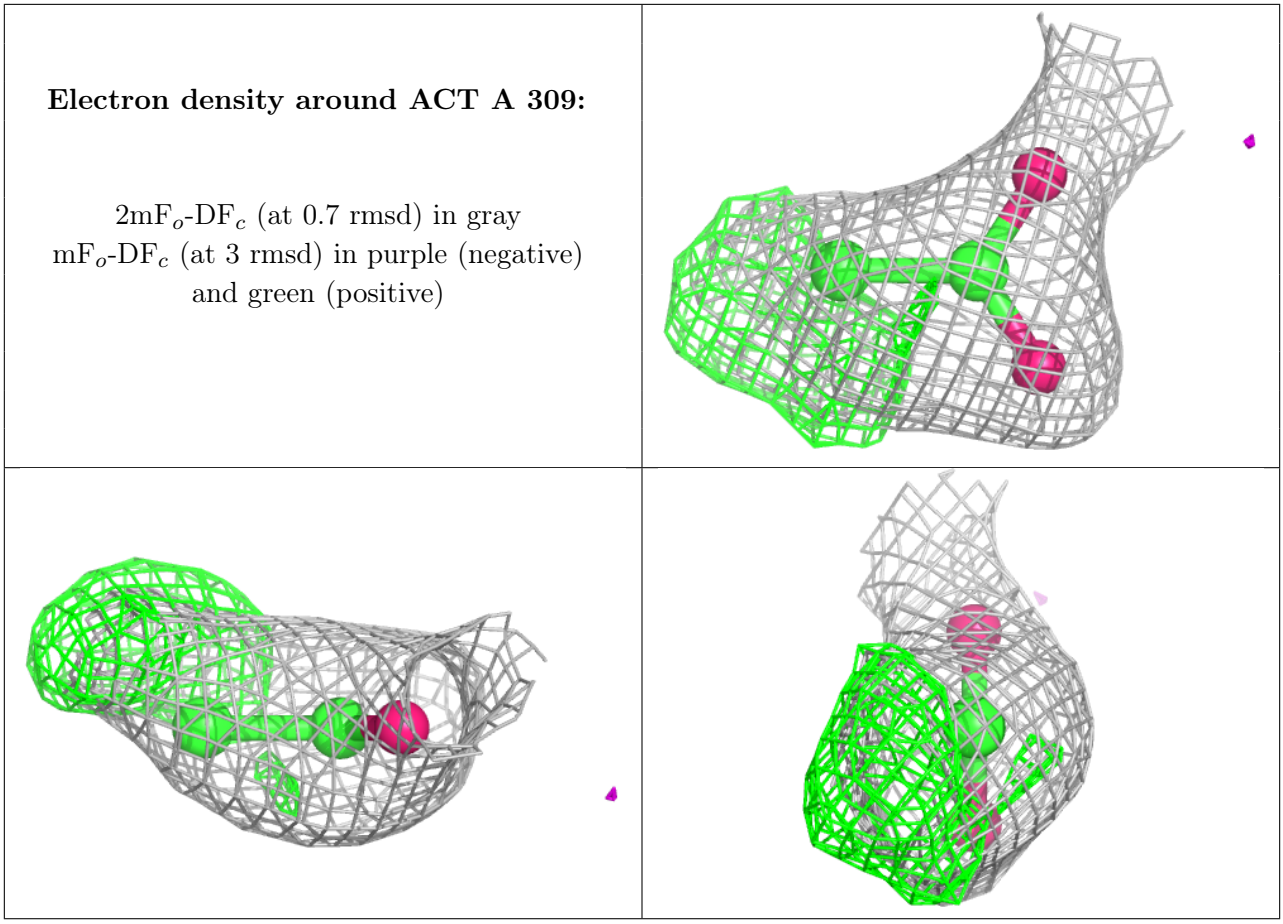
Electron density around EDO C 309:

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



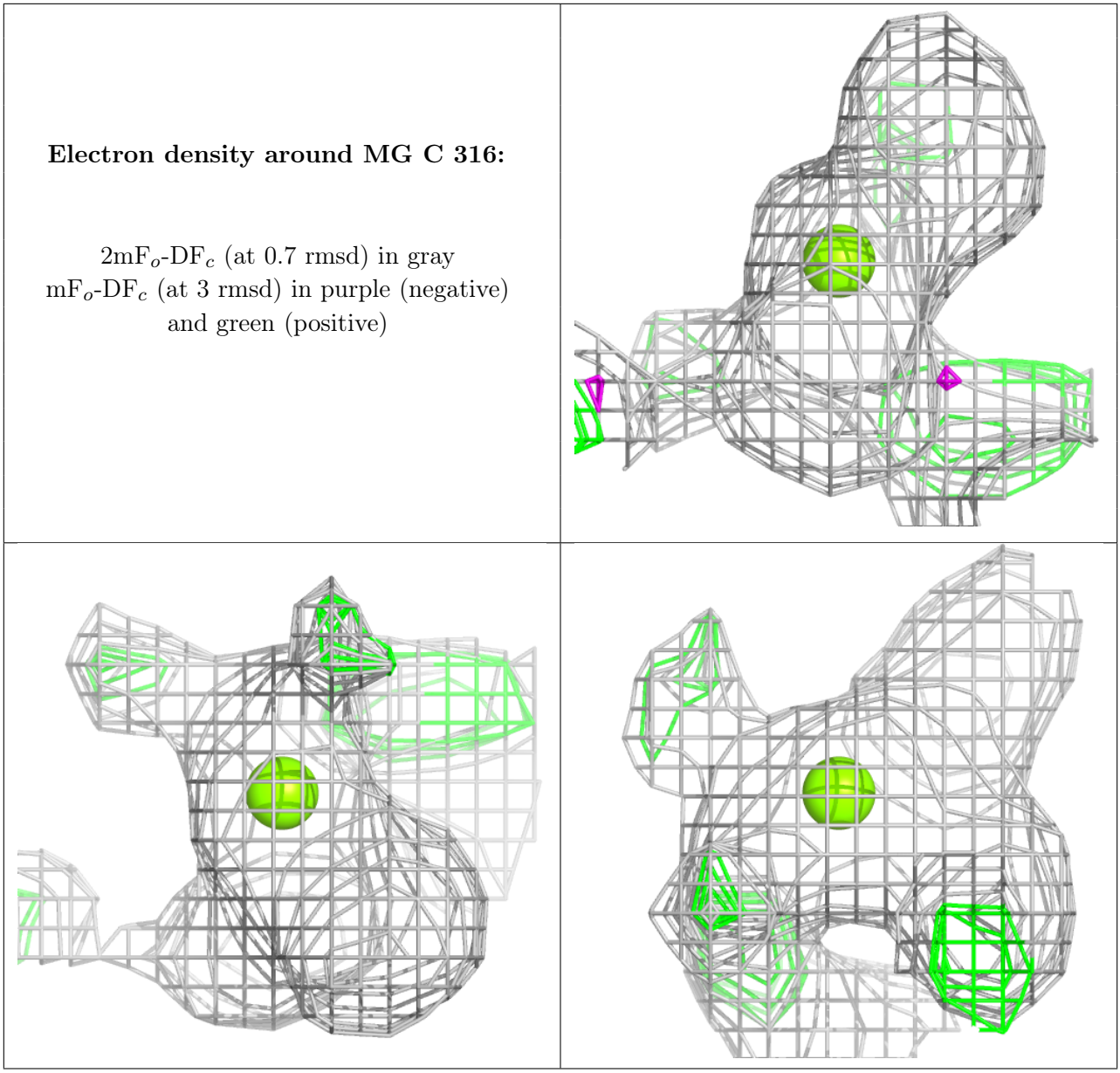
Electron density around ACT A 309:

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



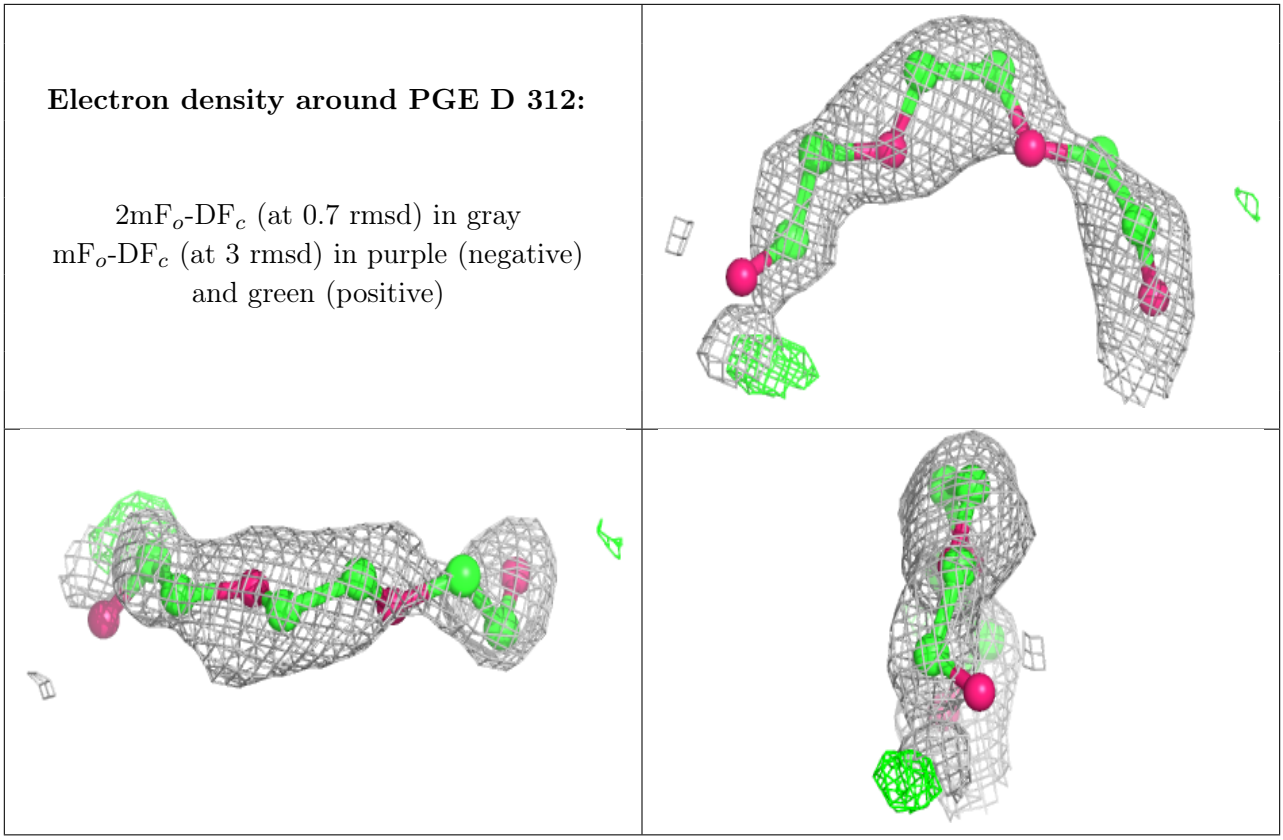
Electron density around MG C 316:

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



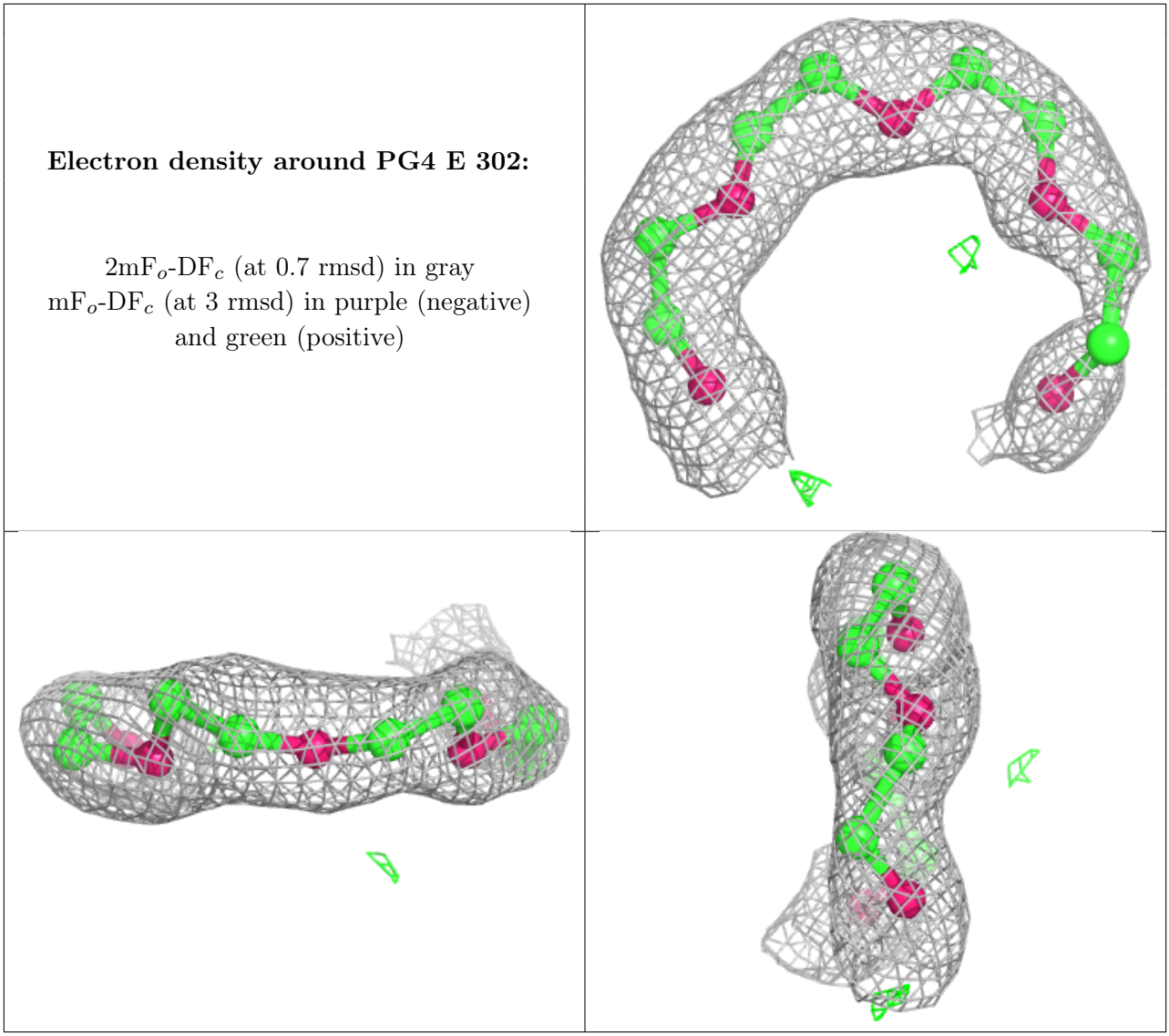
Electron density around PGE D 312:

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



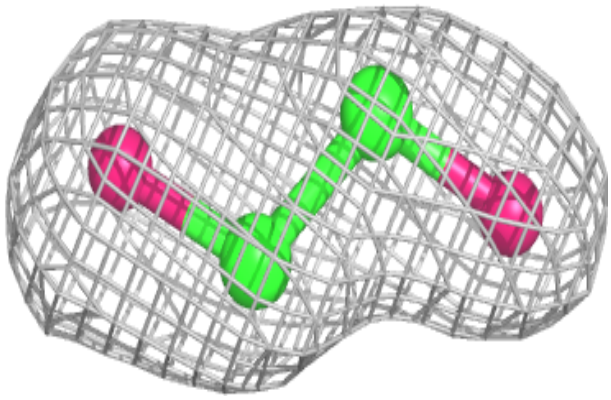
Electron density around PG4 E 302:

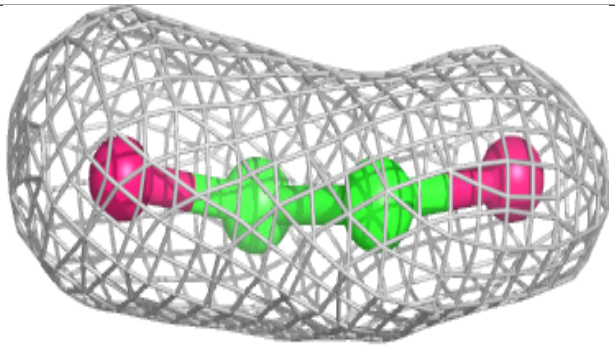
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

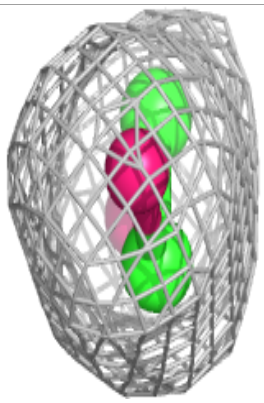


Electron density around EDO F 305:

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

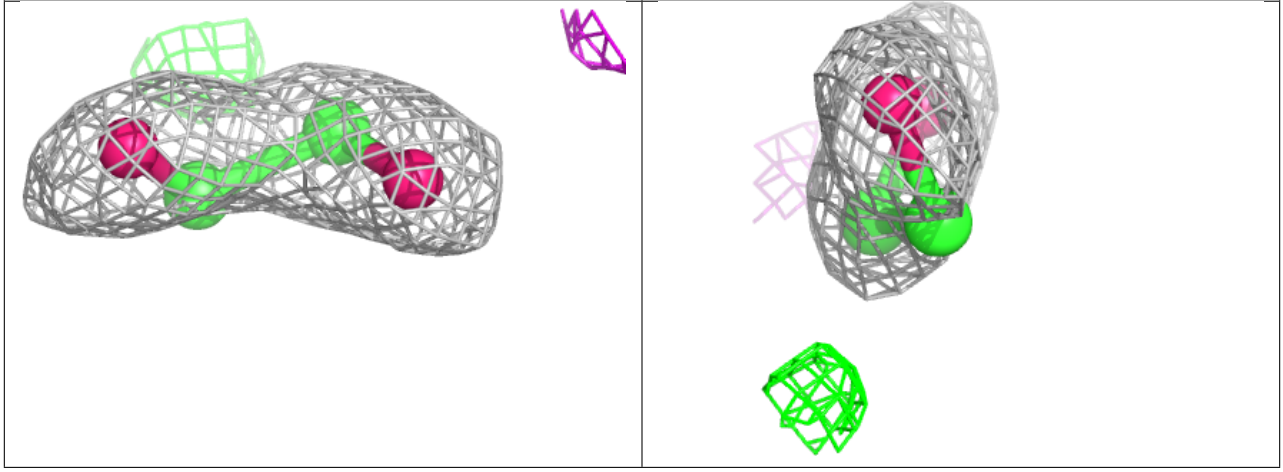






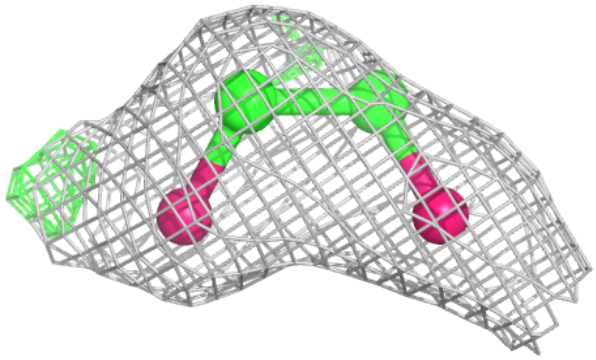
Electron density around EDO E 303:

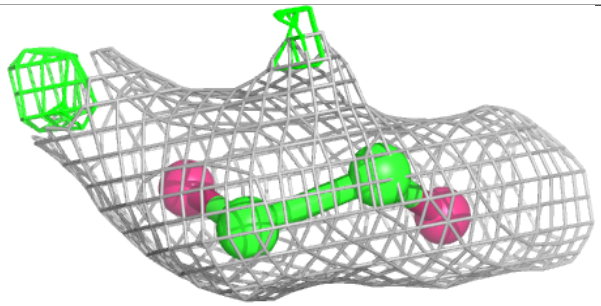
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

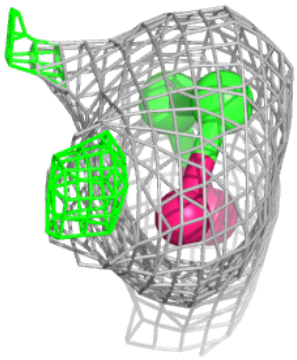


Electron density around EDO E 304:

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

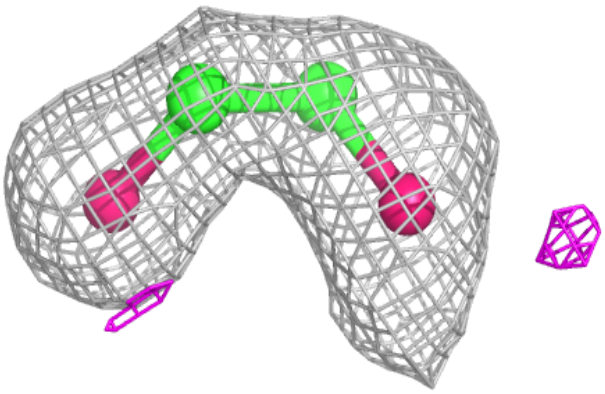


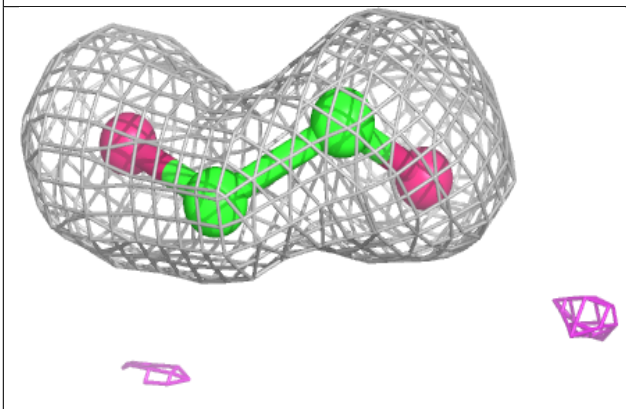


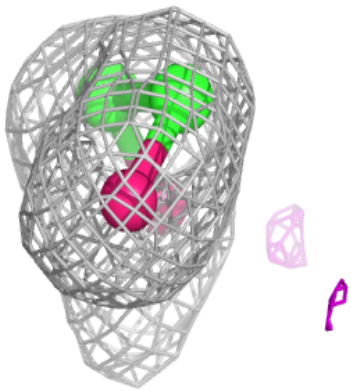


Electron density around EDO B 304:

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

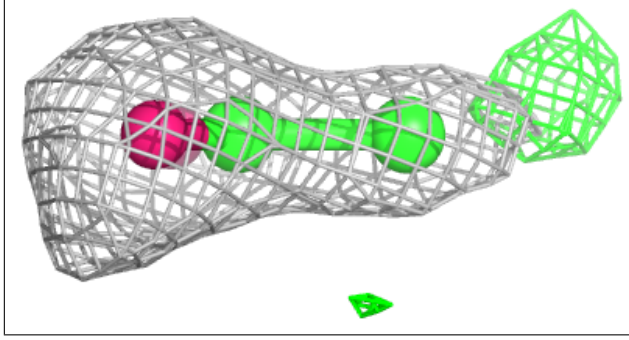


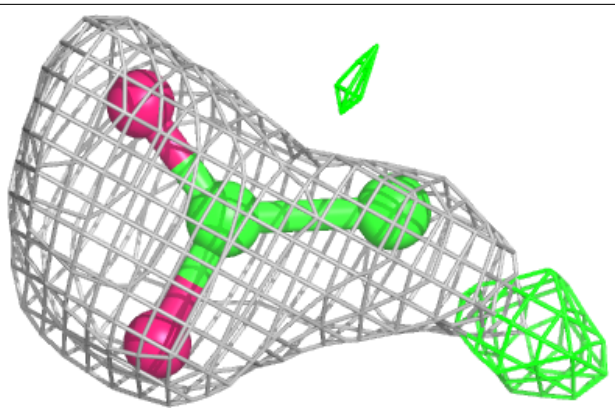


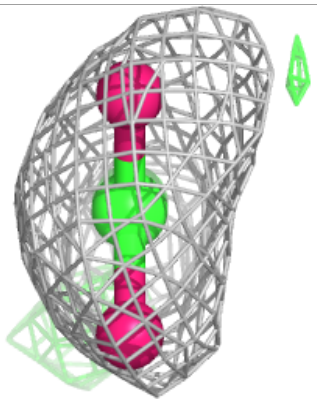


Electron density around ACT E 310:

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

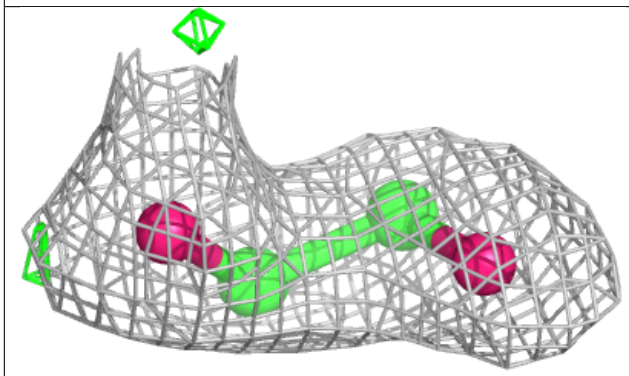


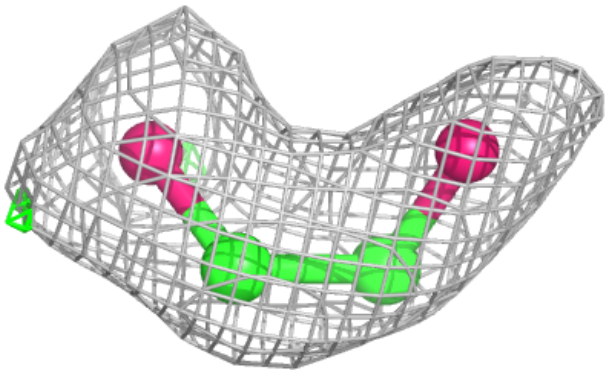


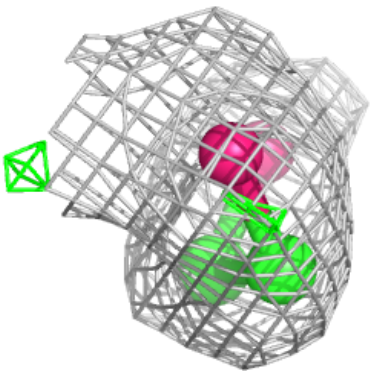


Electron density around EDO E 308:

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

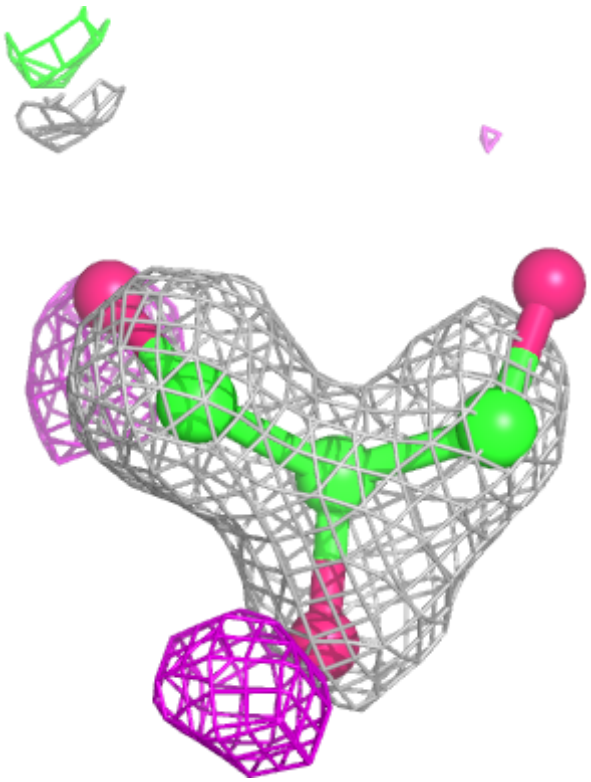


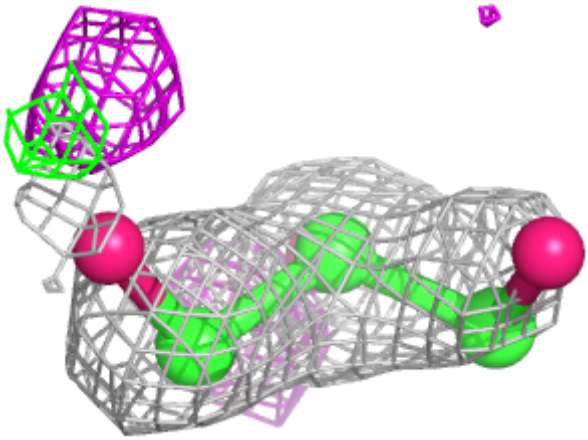


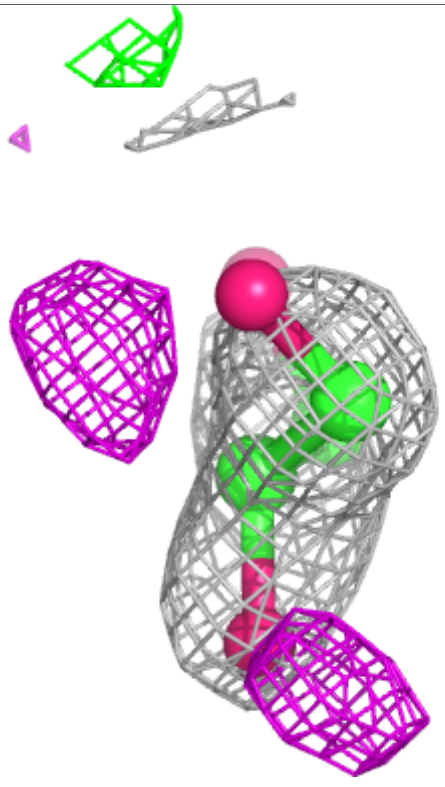


Electron density around GOL B 314:

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

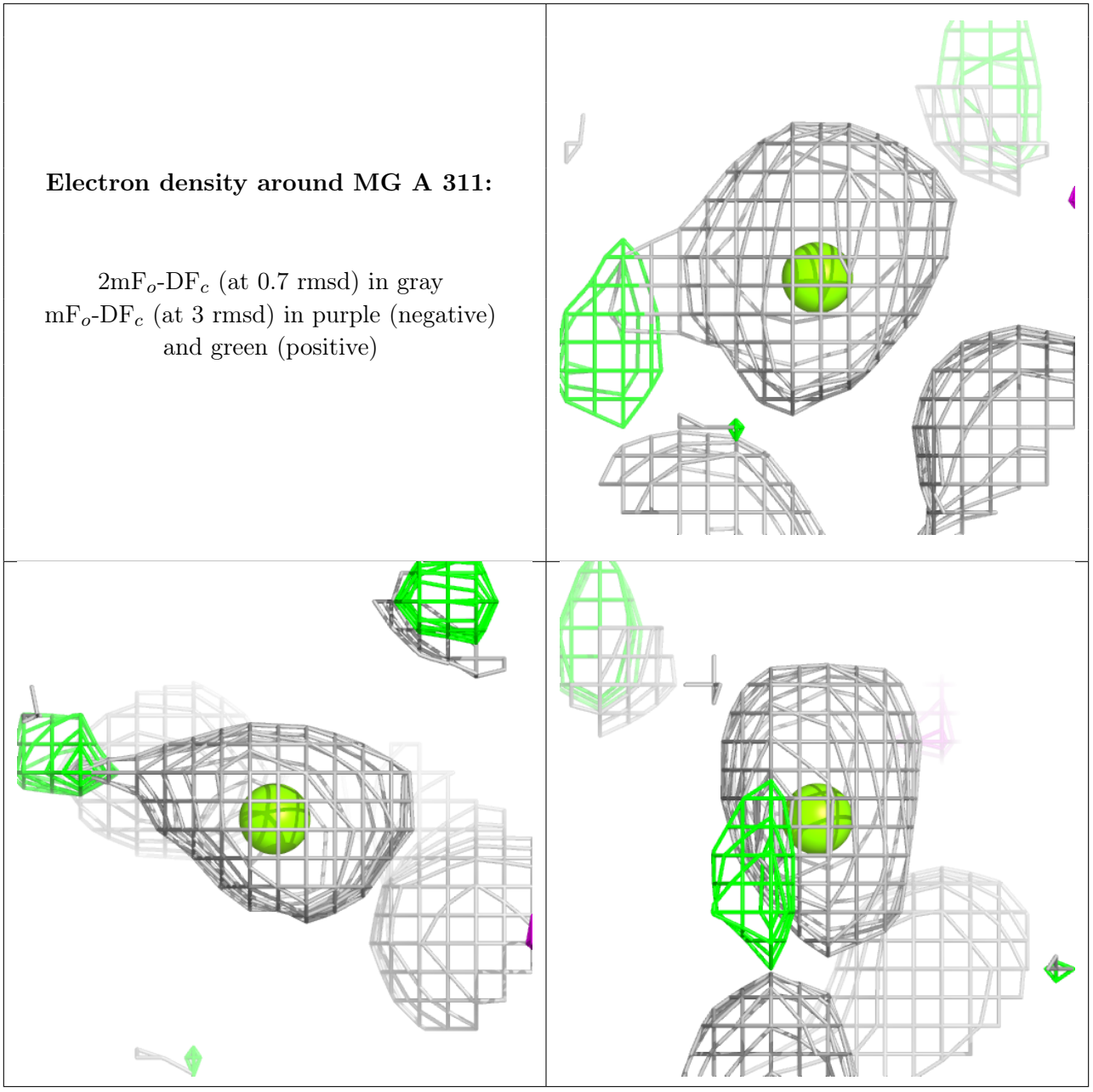






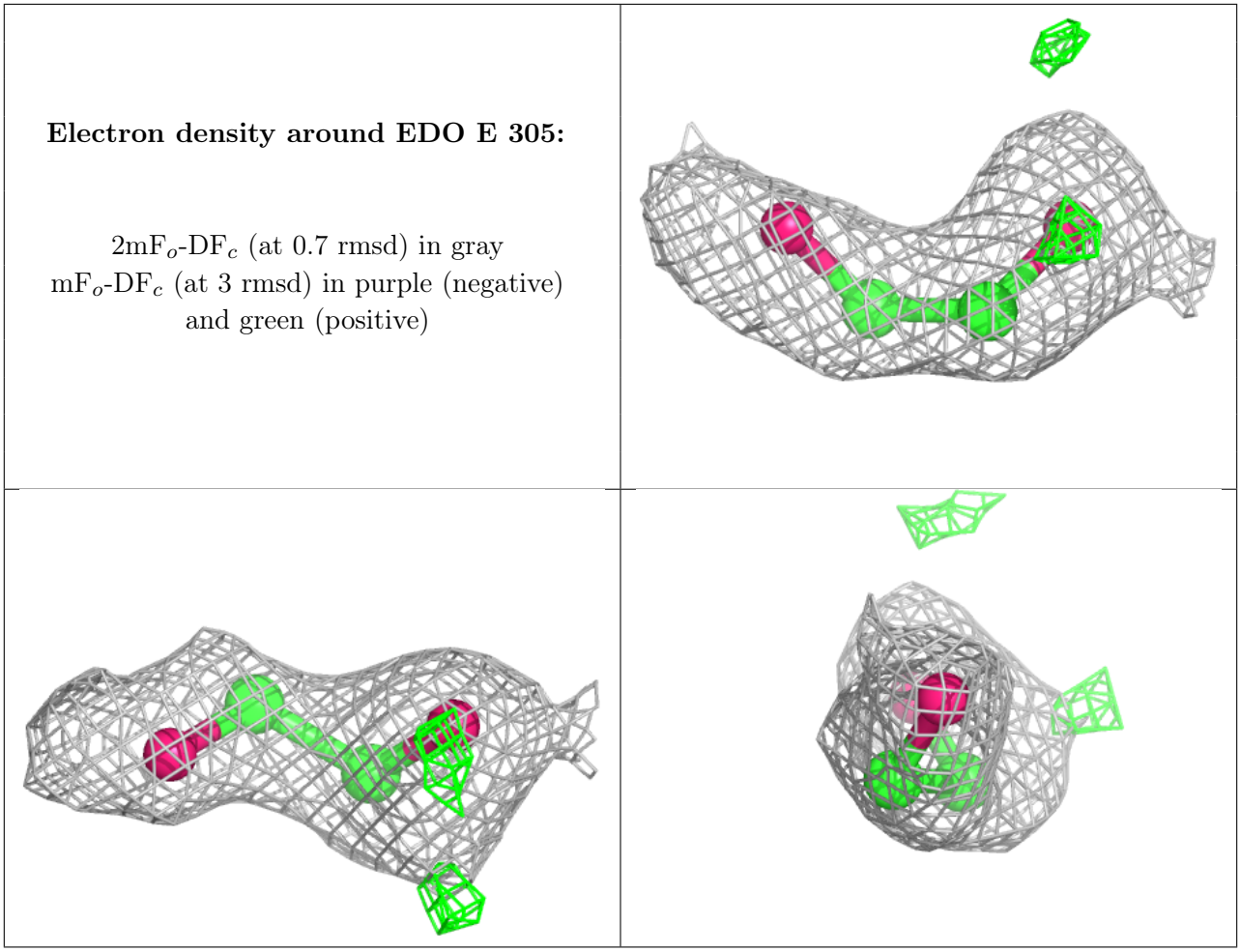
Electron density around MG A 311:

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



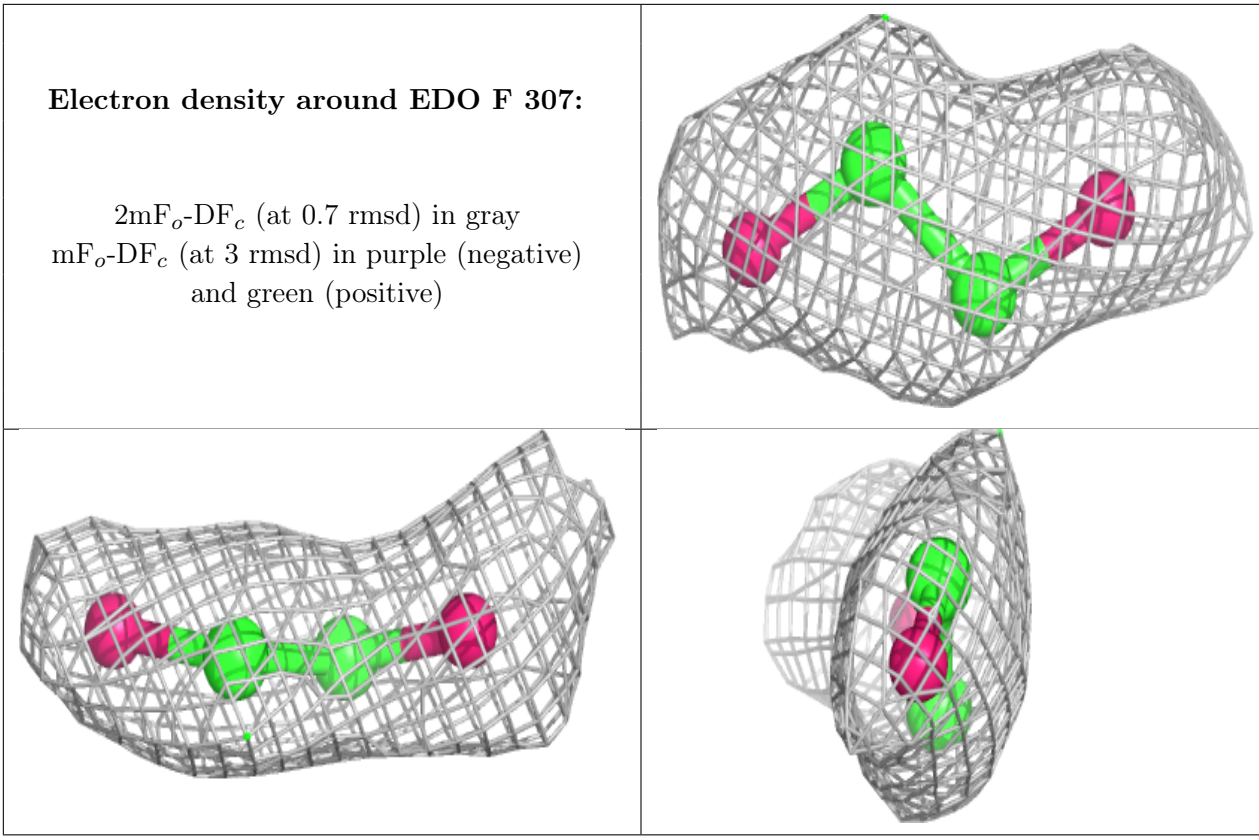
Electron density around EDO E 305:

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



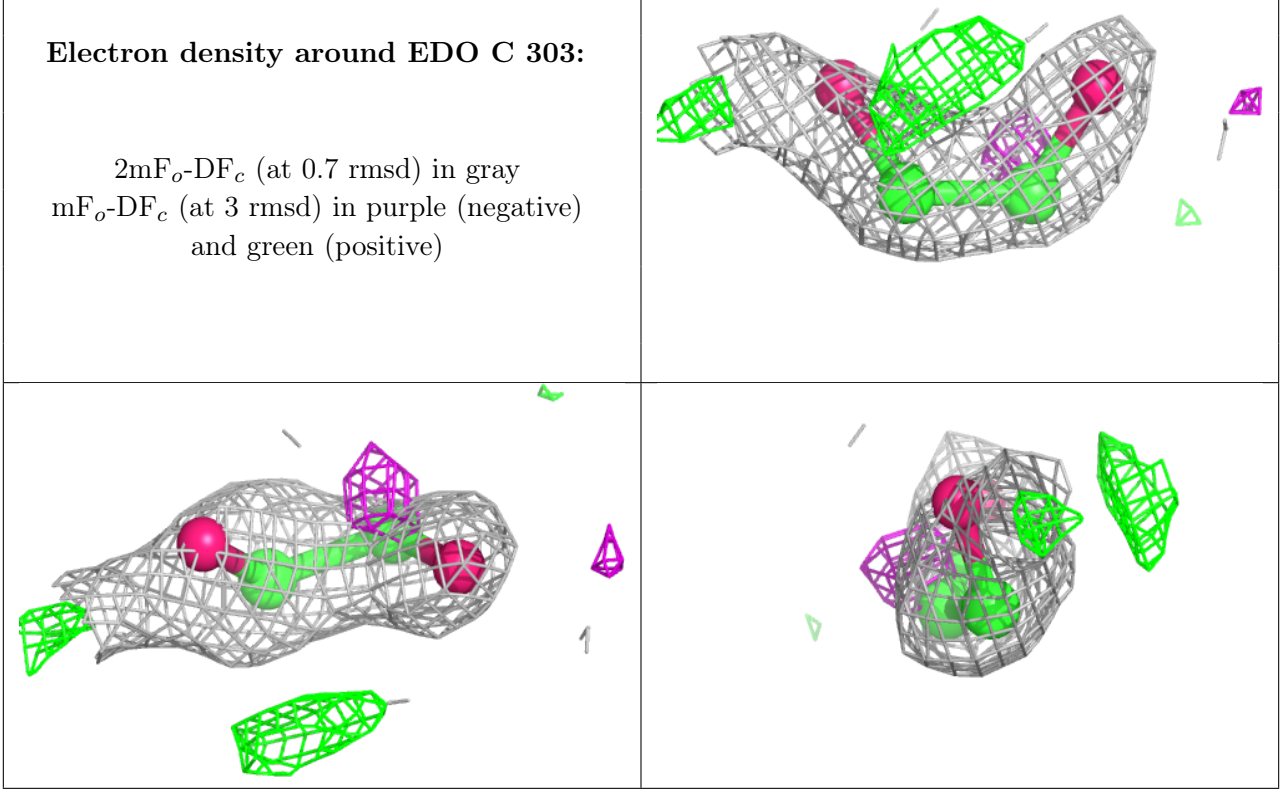
Electron density around EDO F 307:

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



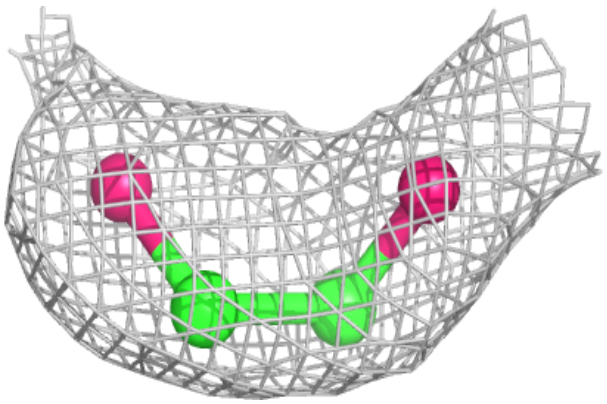
Electron density around EDO C 303:

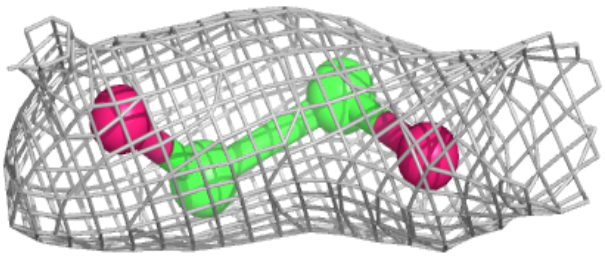
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

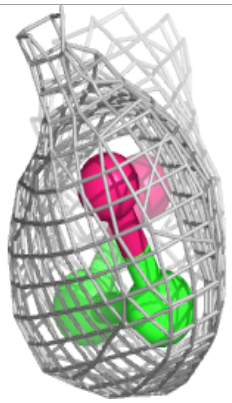


Electron density around EDO E 309:

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

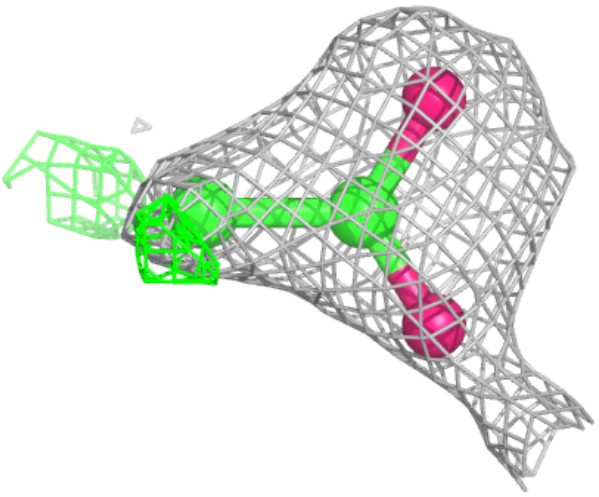


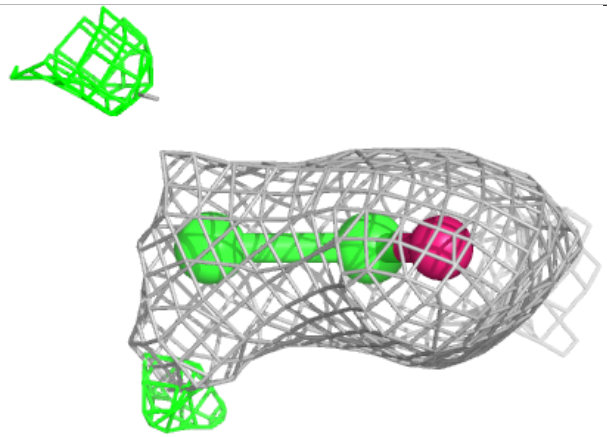


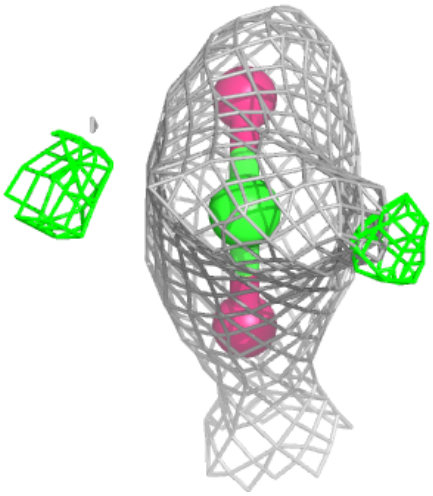


Electron density around ACT F 311:

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

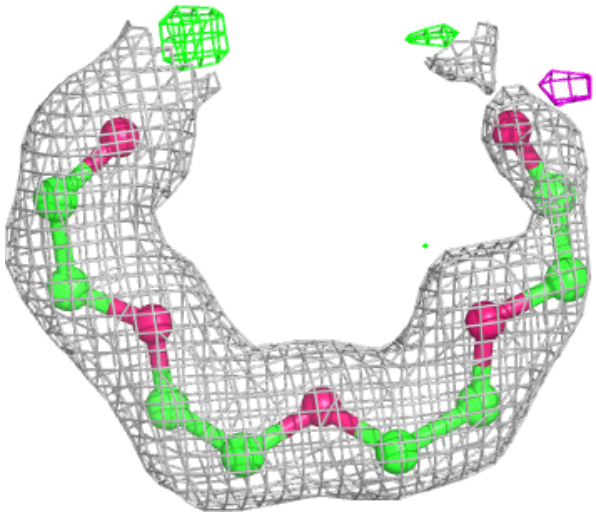


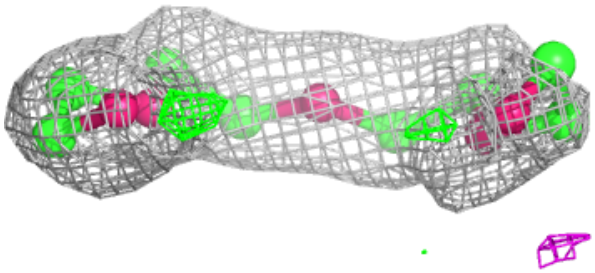


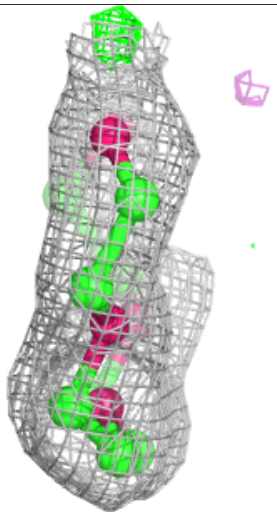


Electron density around PG4 D 302:

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

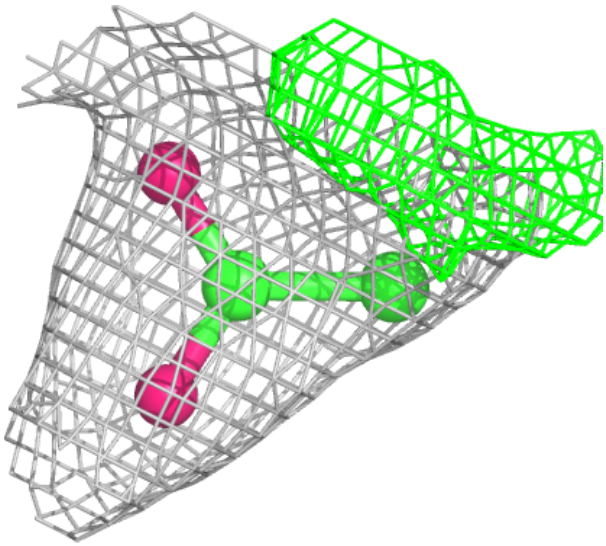


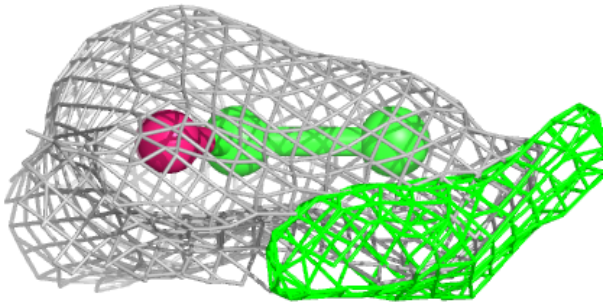


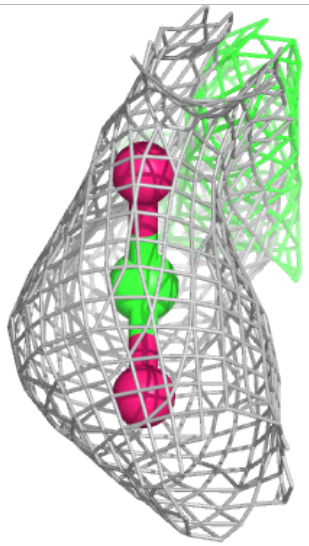


Electron density around ACT C 312:

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

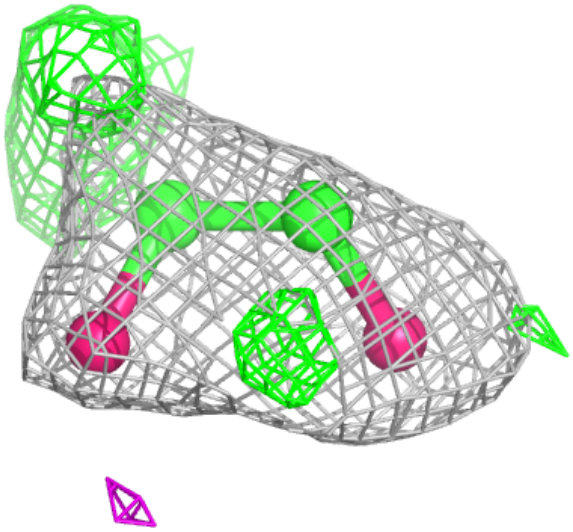


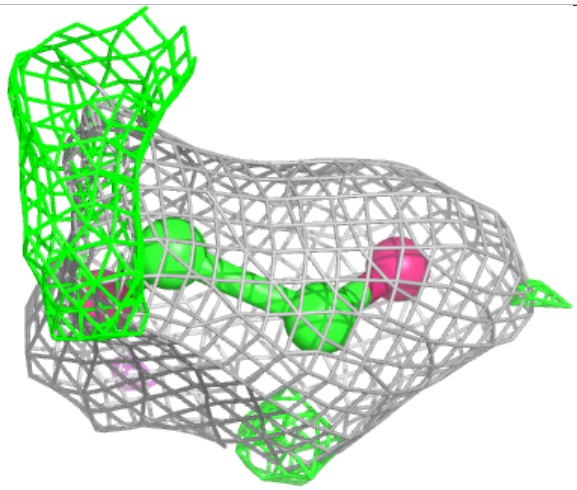


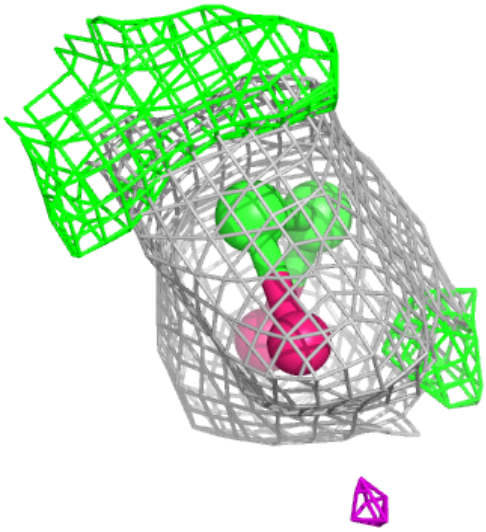


Electron density around EDO C 305:

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

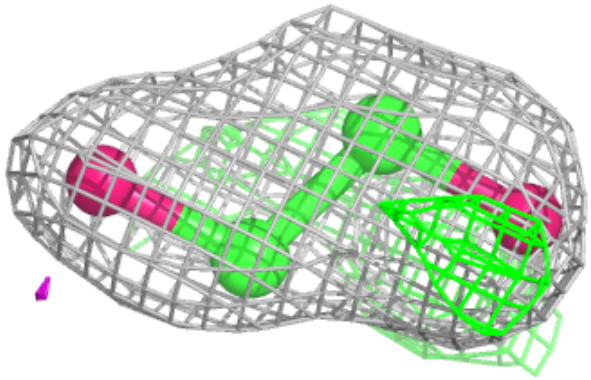


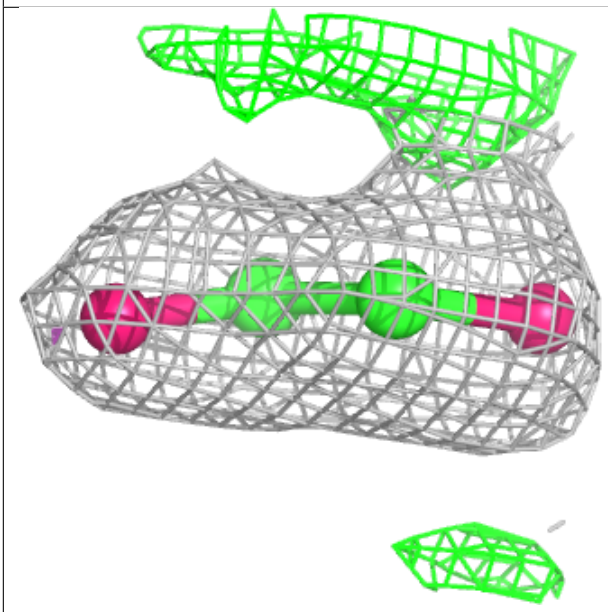


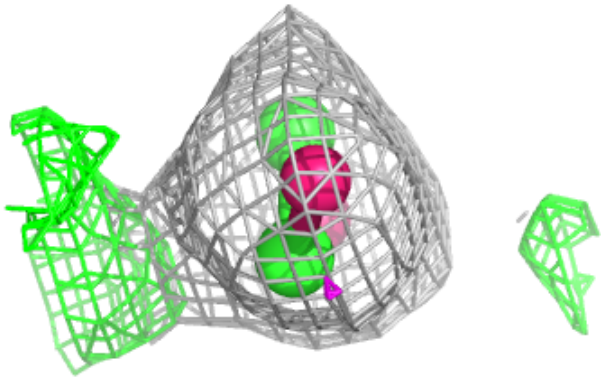


Electron density around EDO E 306:

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

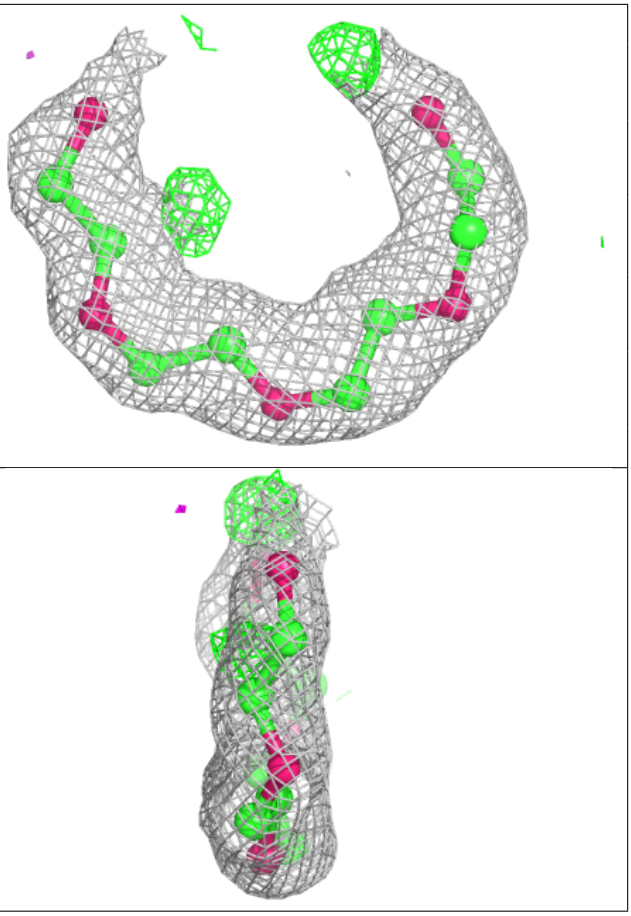






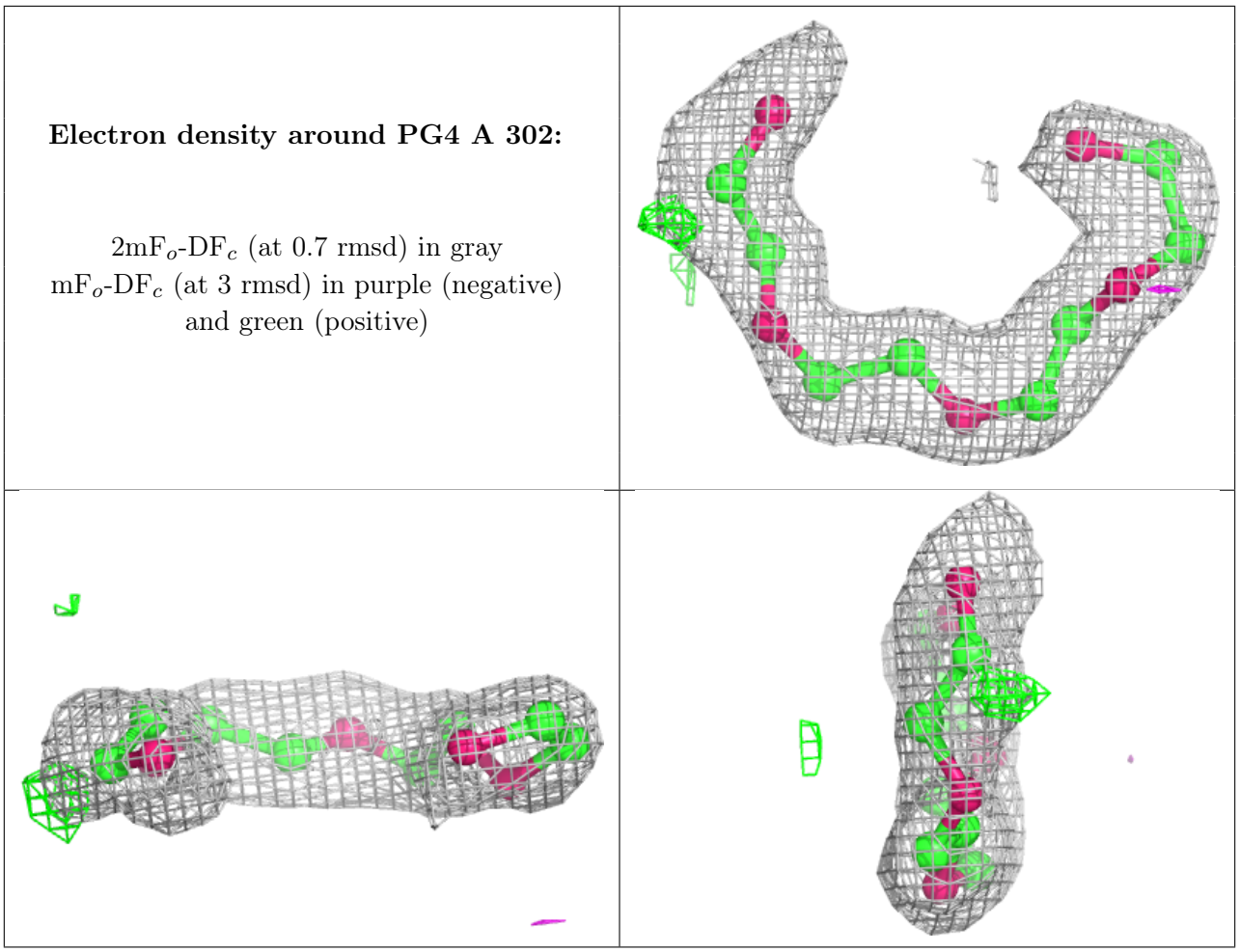
Electron density around PG4 C 302:

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



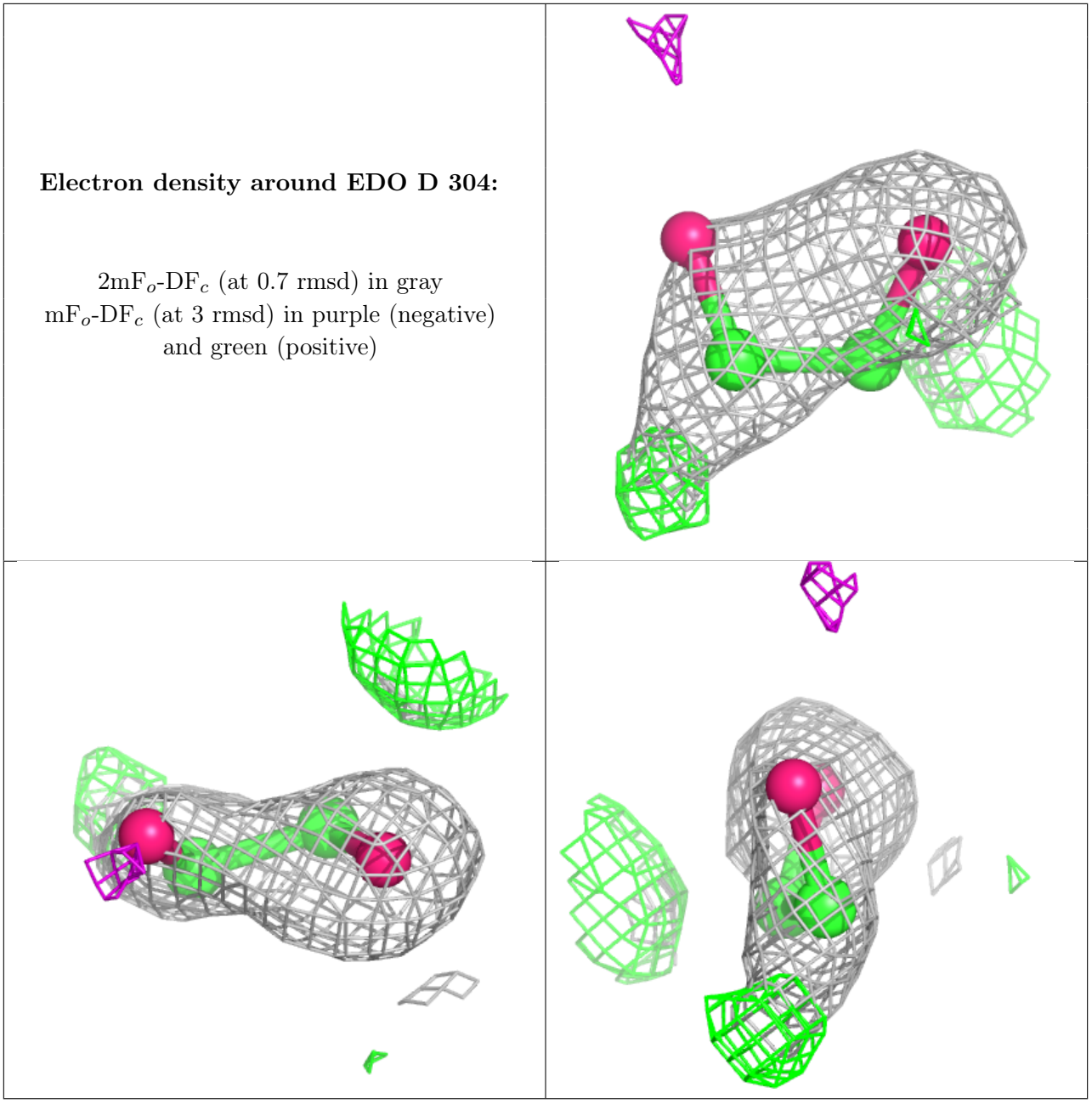
Electron density around PG4 A 302:

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



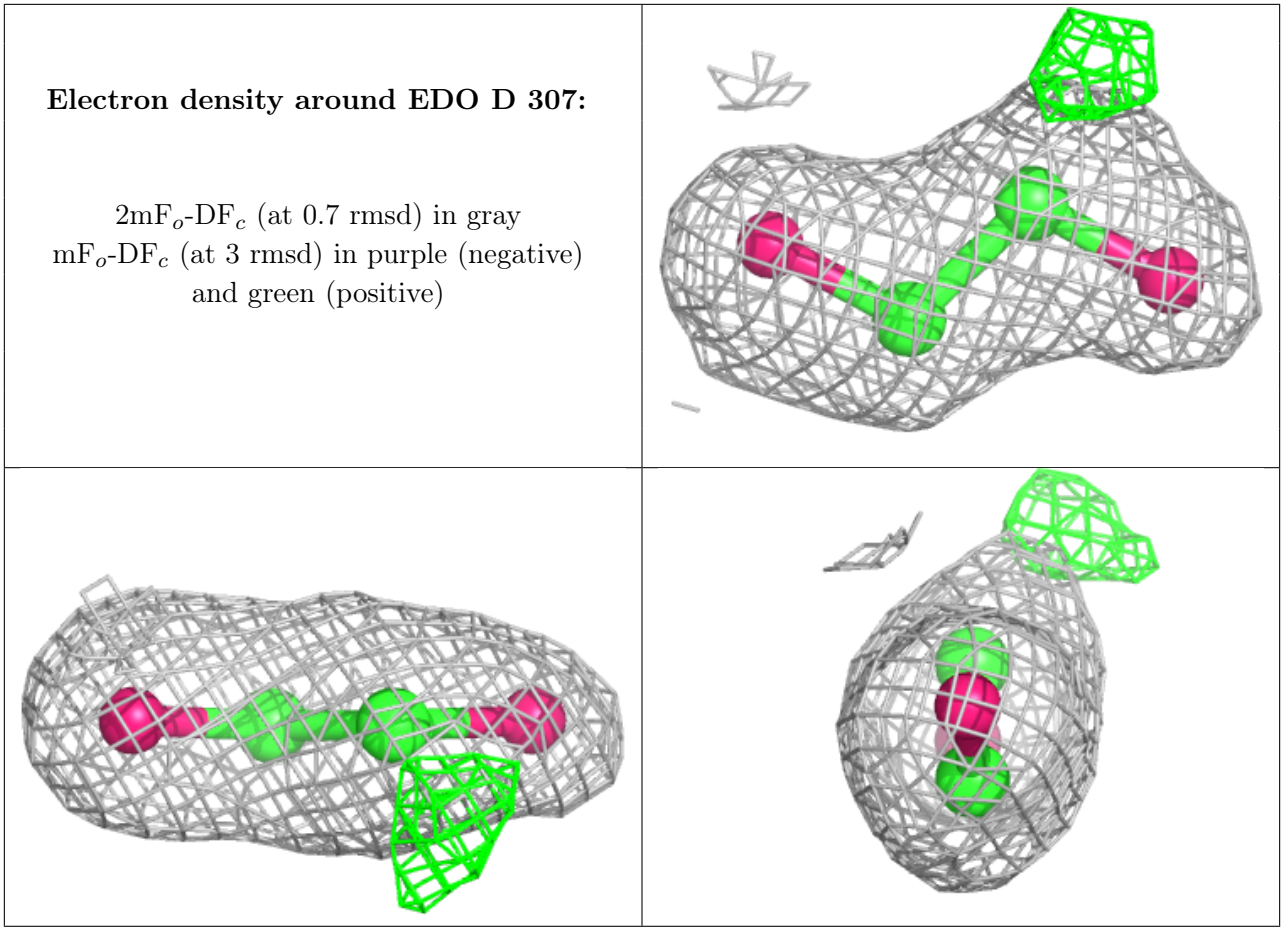
Electron density around EDO D 304:

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



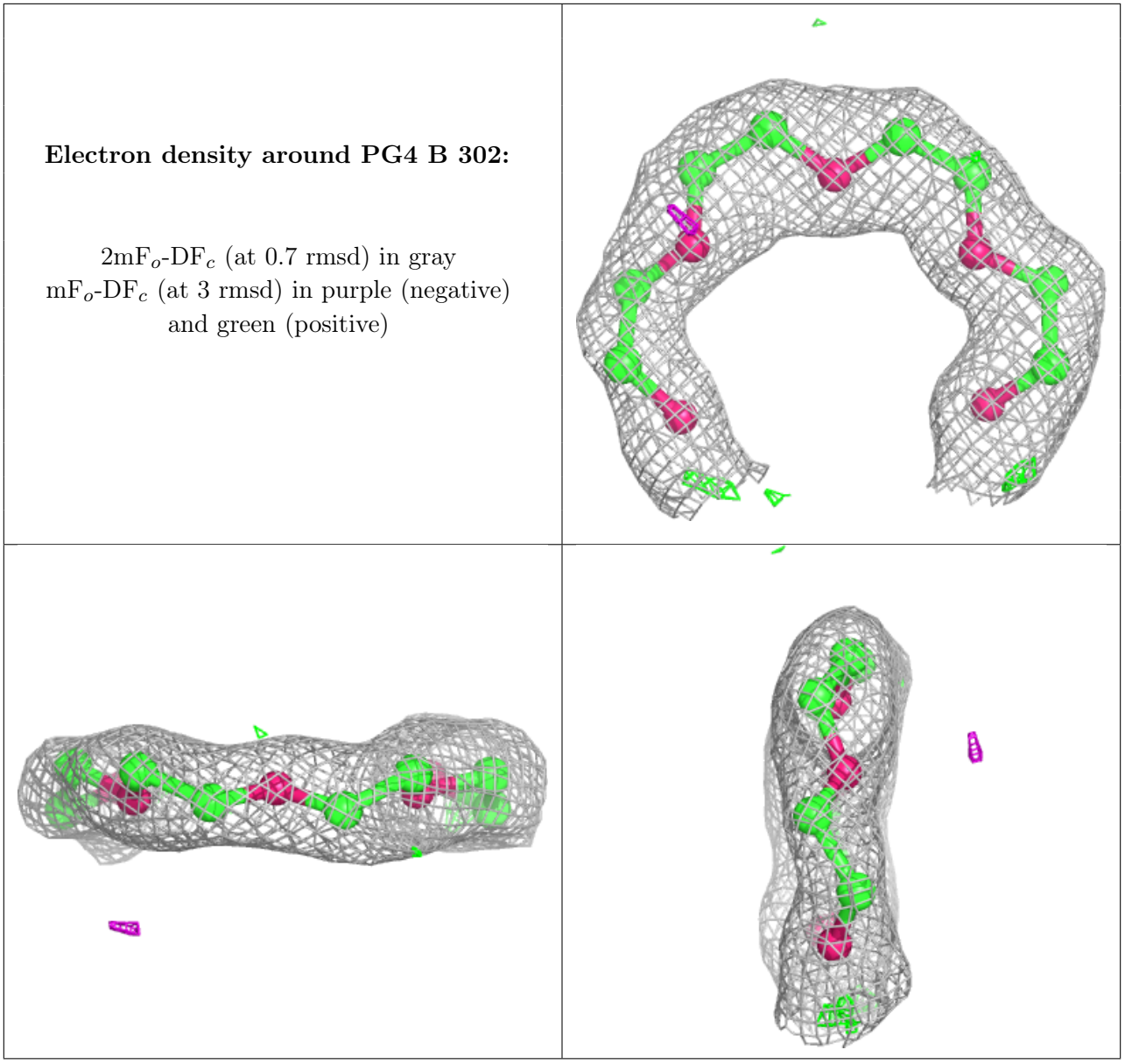
Electron density around EDO D 307:

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



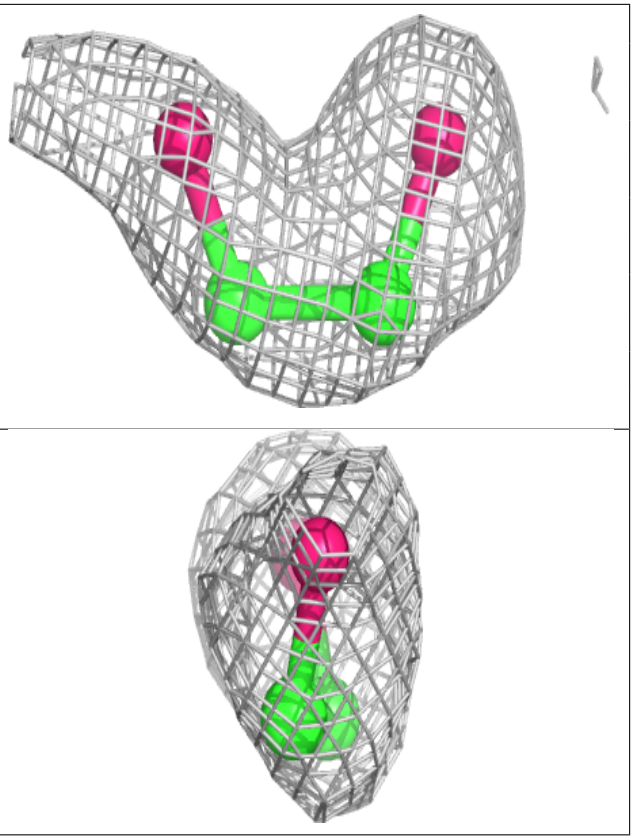
Electron density around PG4 B 302:

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



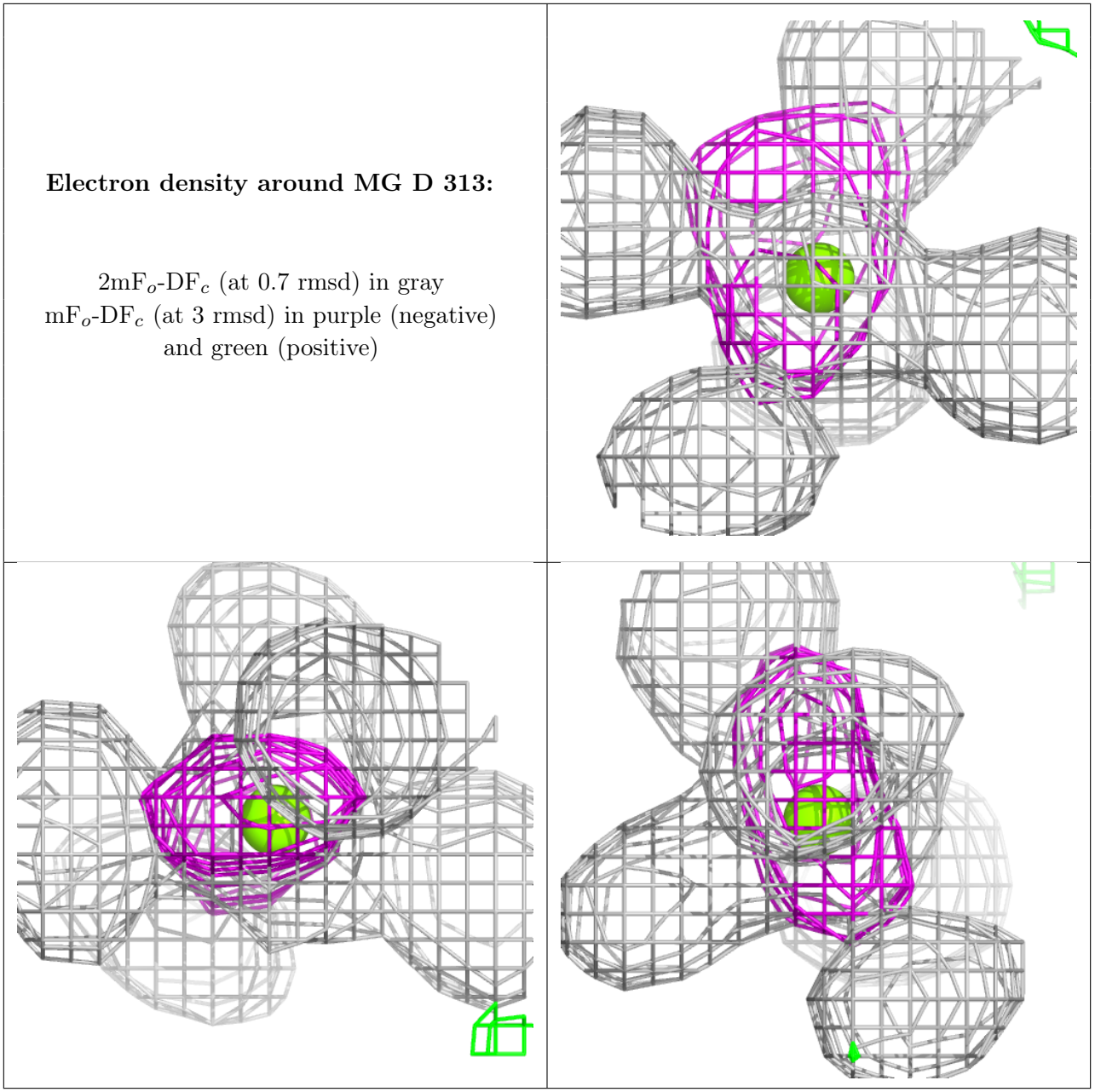
Electron density around EDO B 305:

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



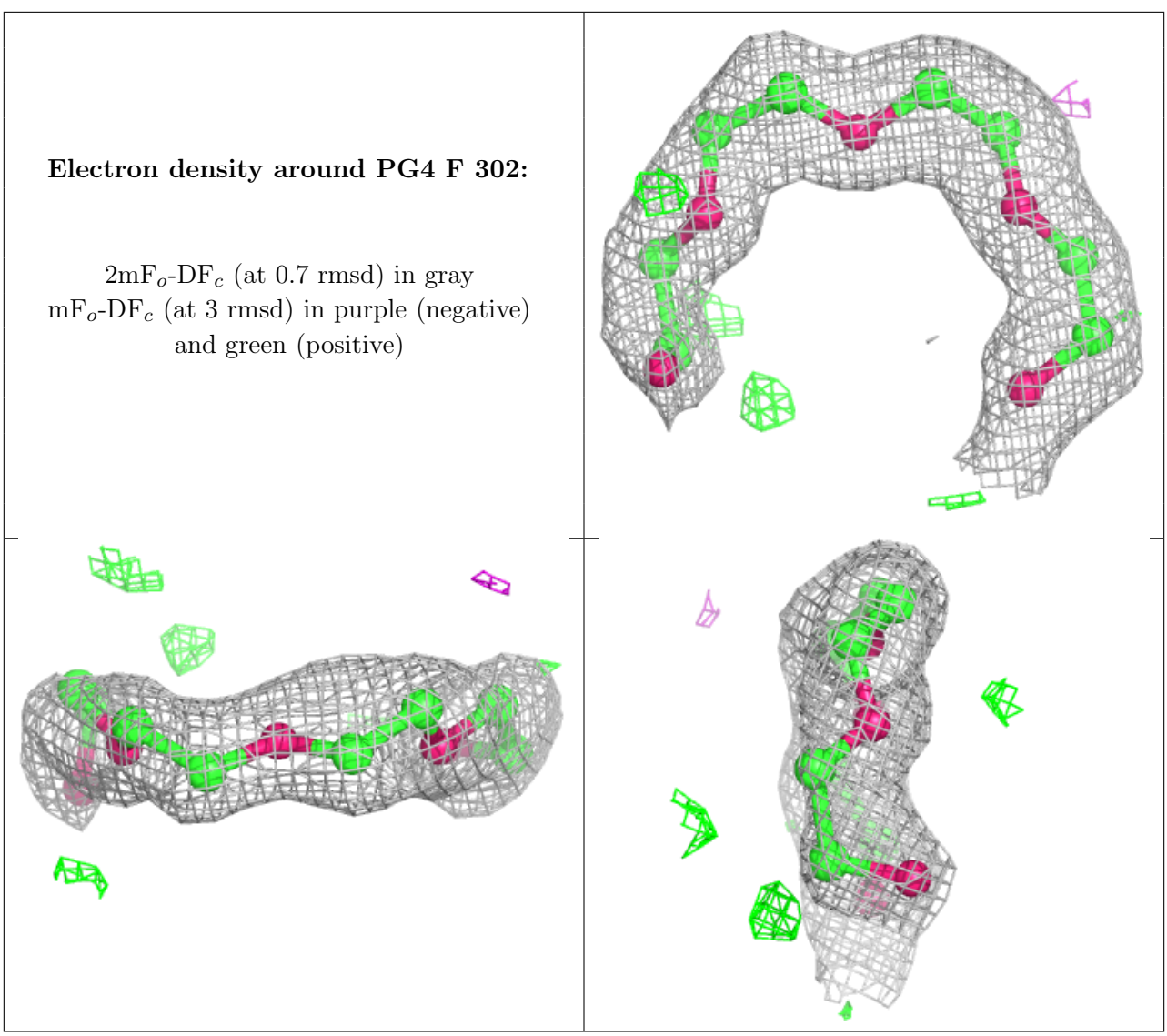
Electron density around MG D 313:

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



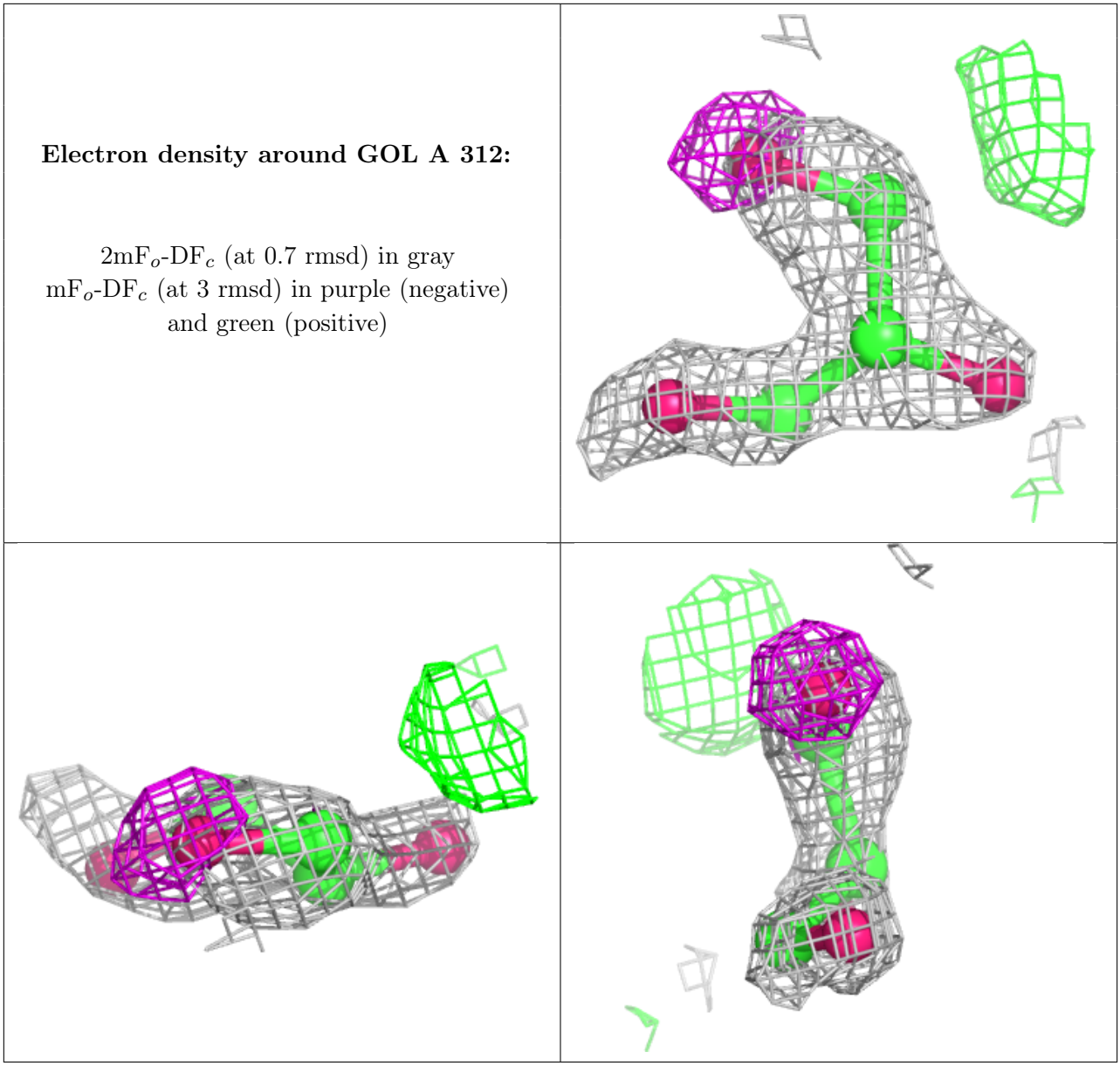
Electron density around PG4 F 302:

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



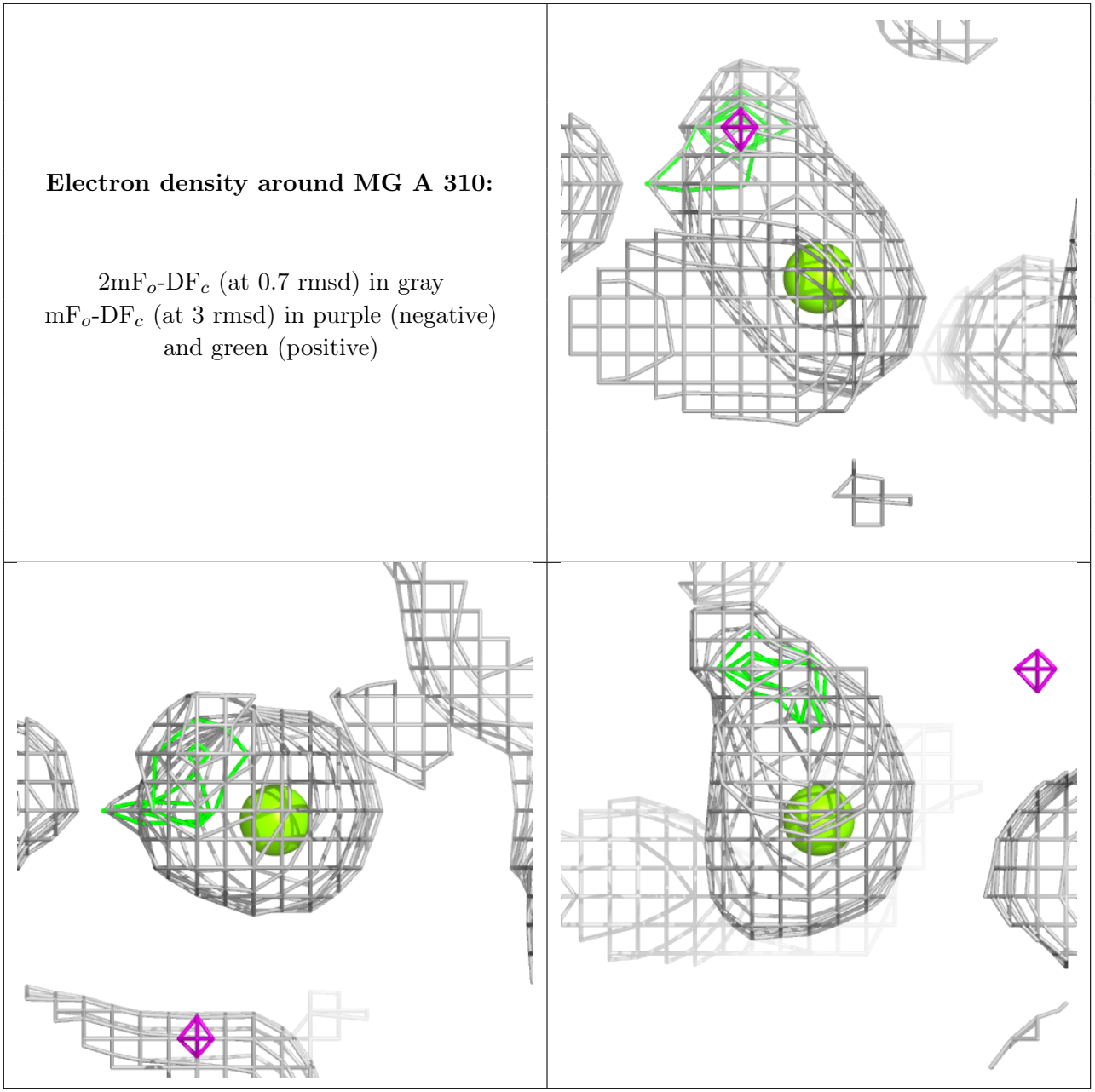
Electron density around GOL A 312:

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



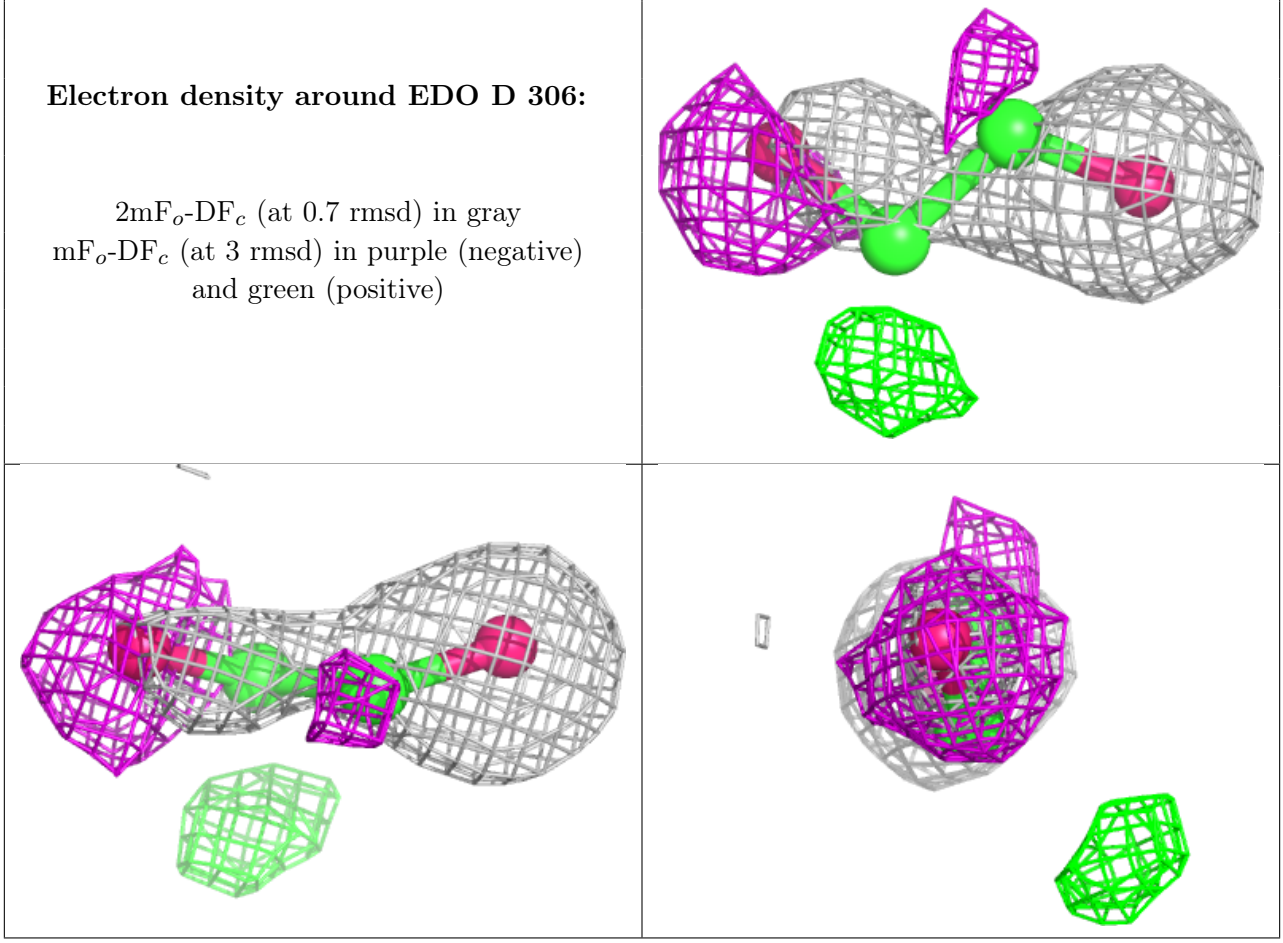
Electron density around MG A 310:

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



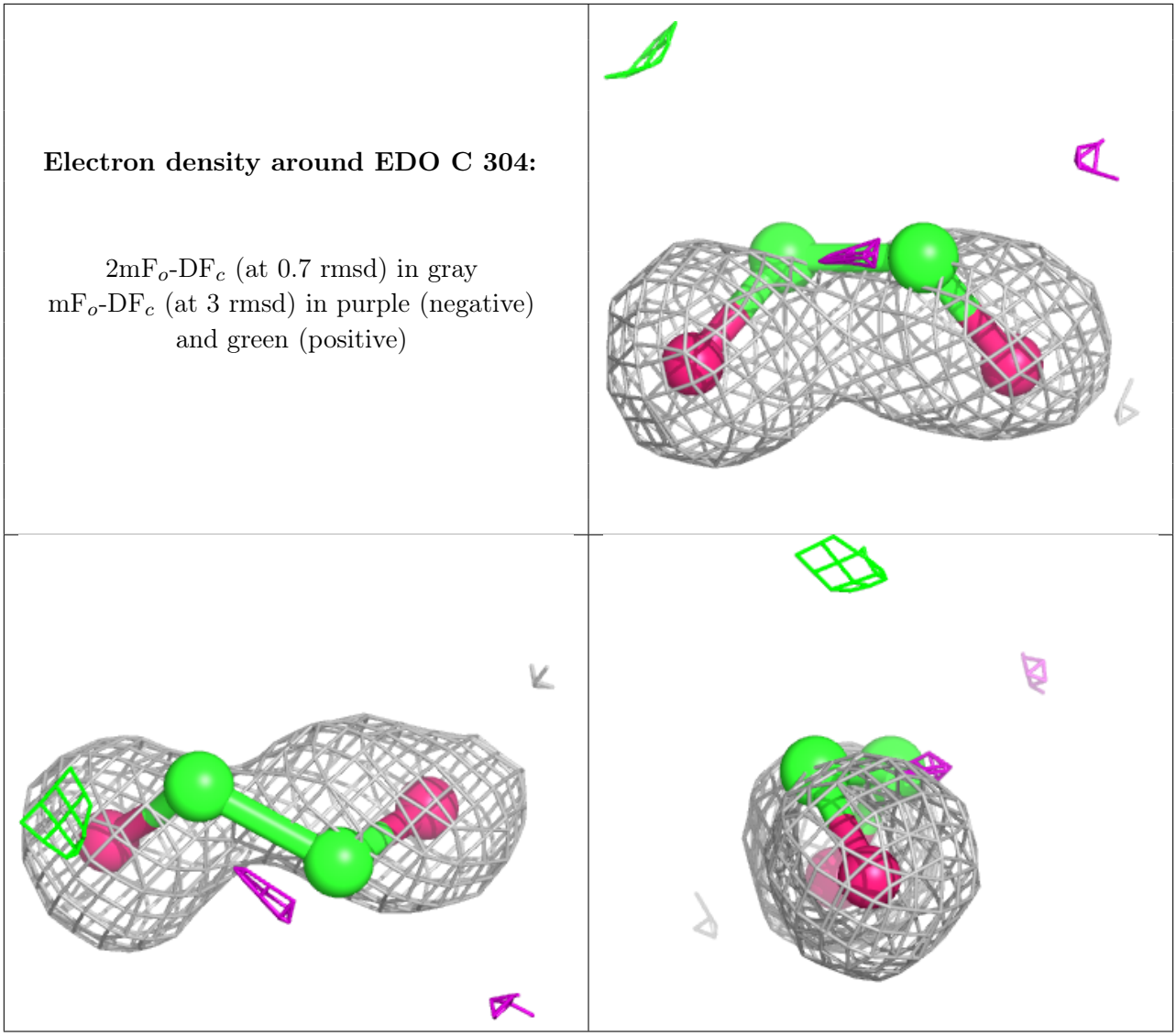
Electron density around EDO D 306:

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



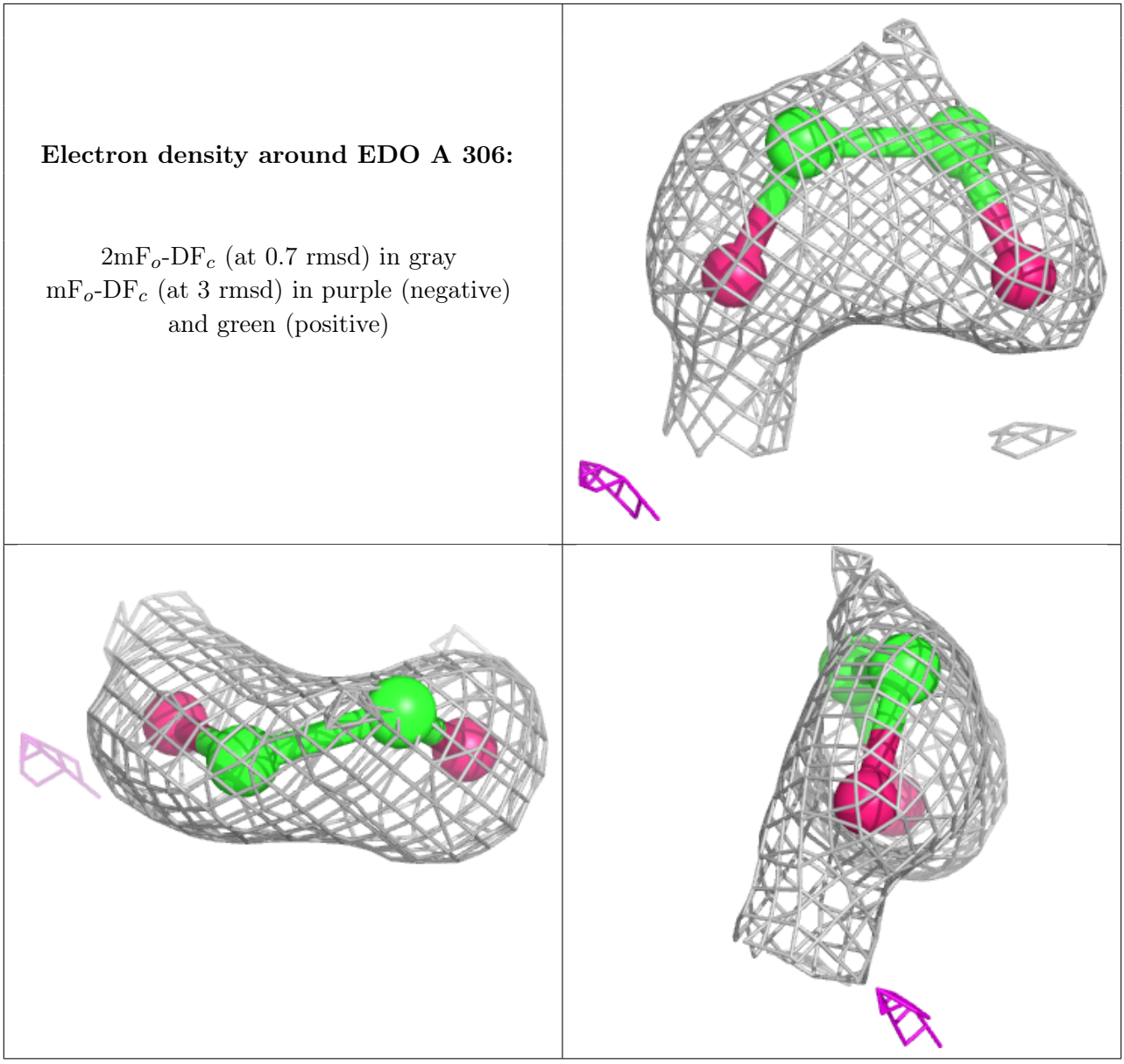
Electron density around EDO C 304:

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



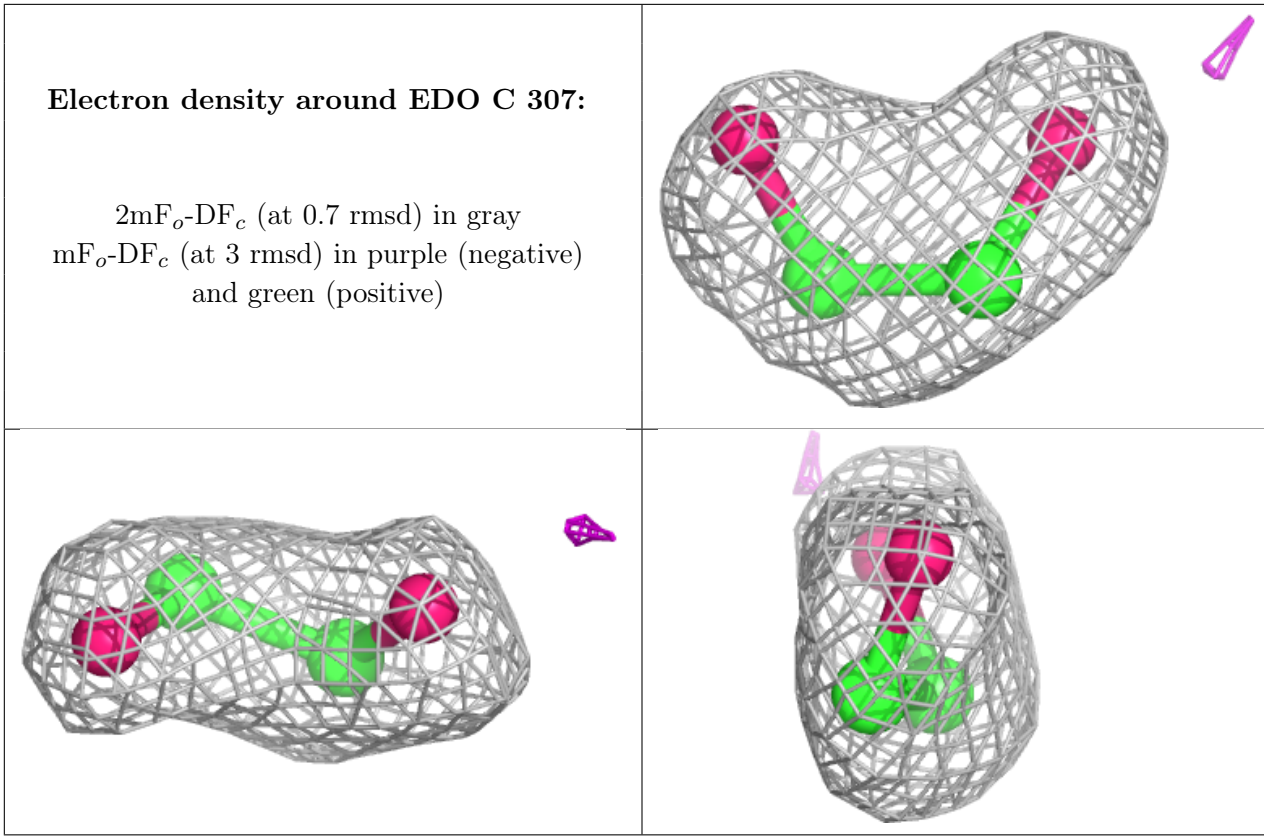
Electron density around EDO A 306:

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



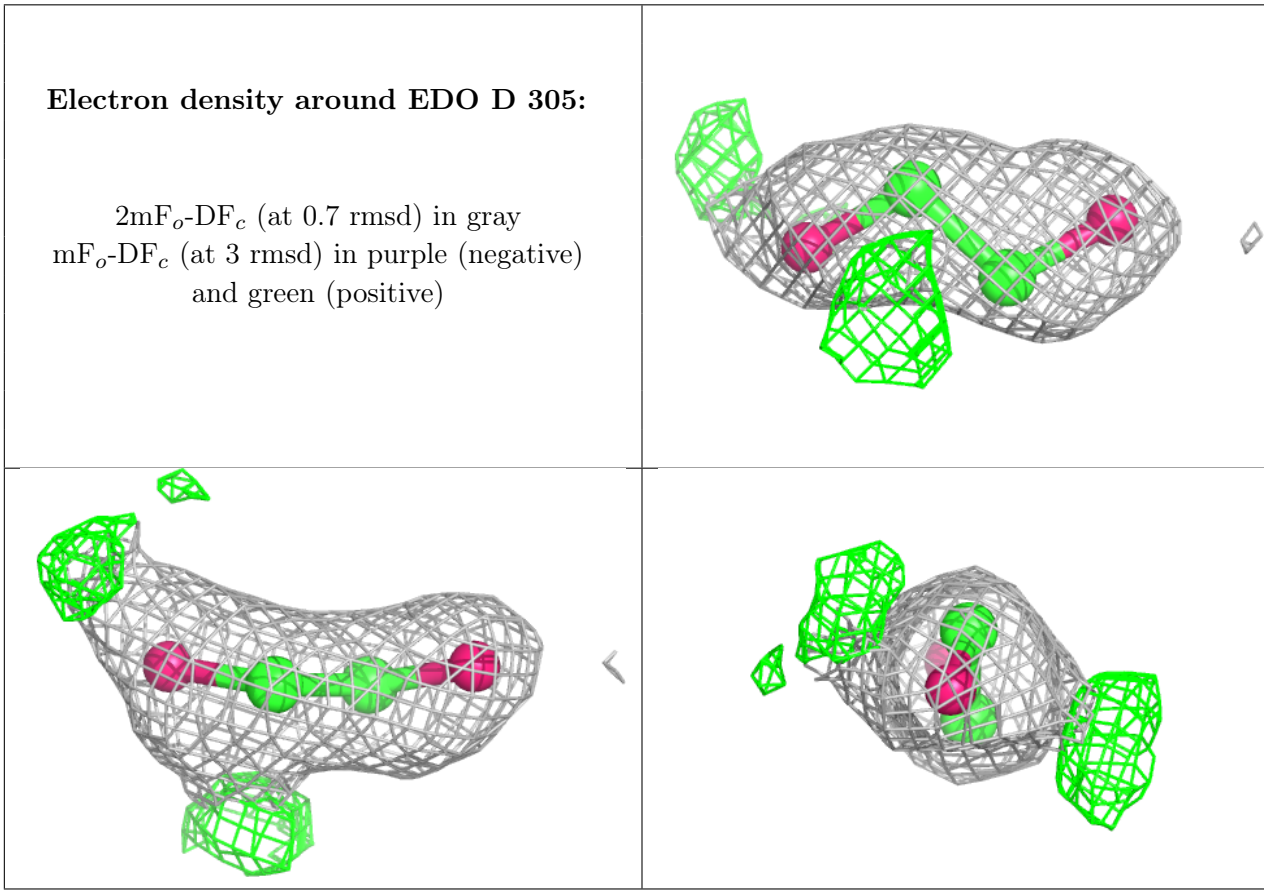
Electron density around EDO C 307:

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



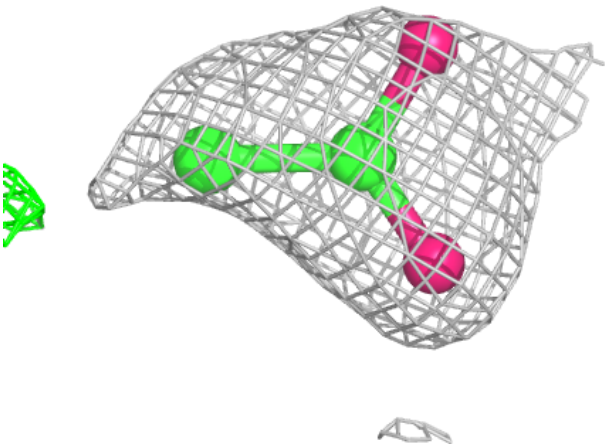
Electron density around EDO D 305:

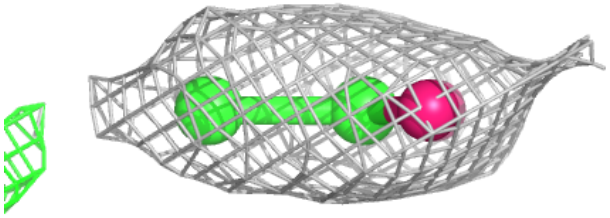
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

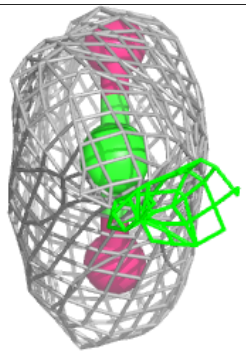


Electron density around ACT B 306:

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

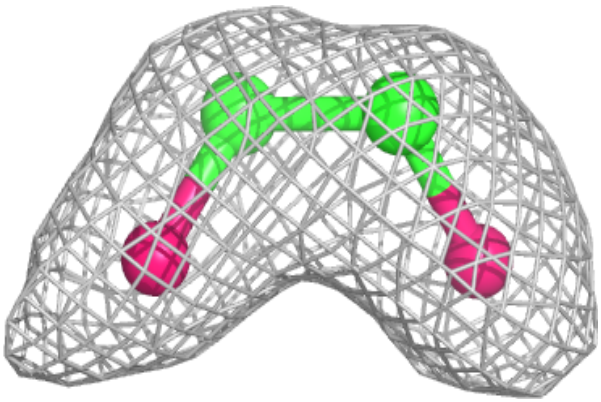


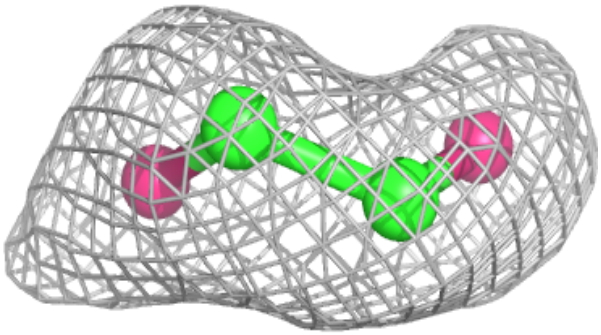


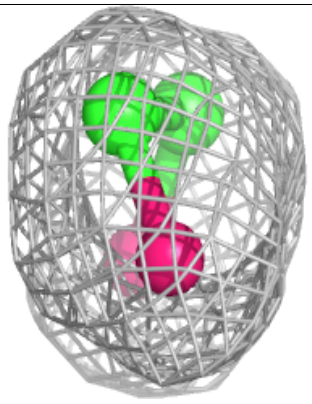


Electron density around EDO A 303:

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

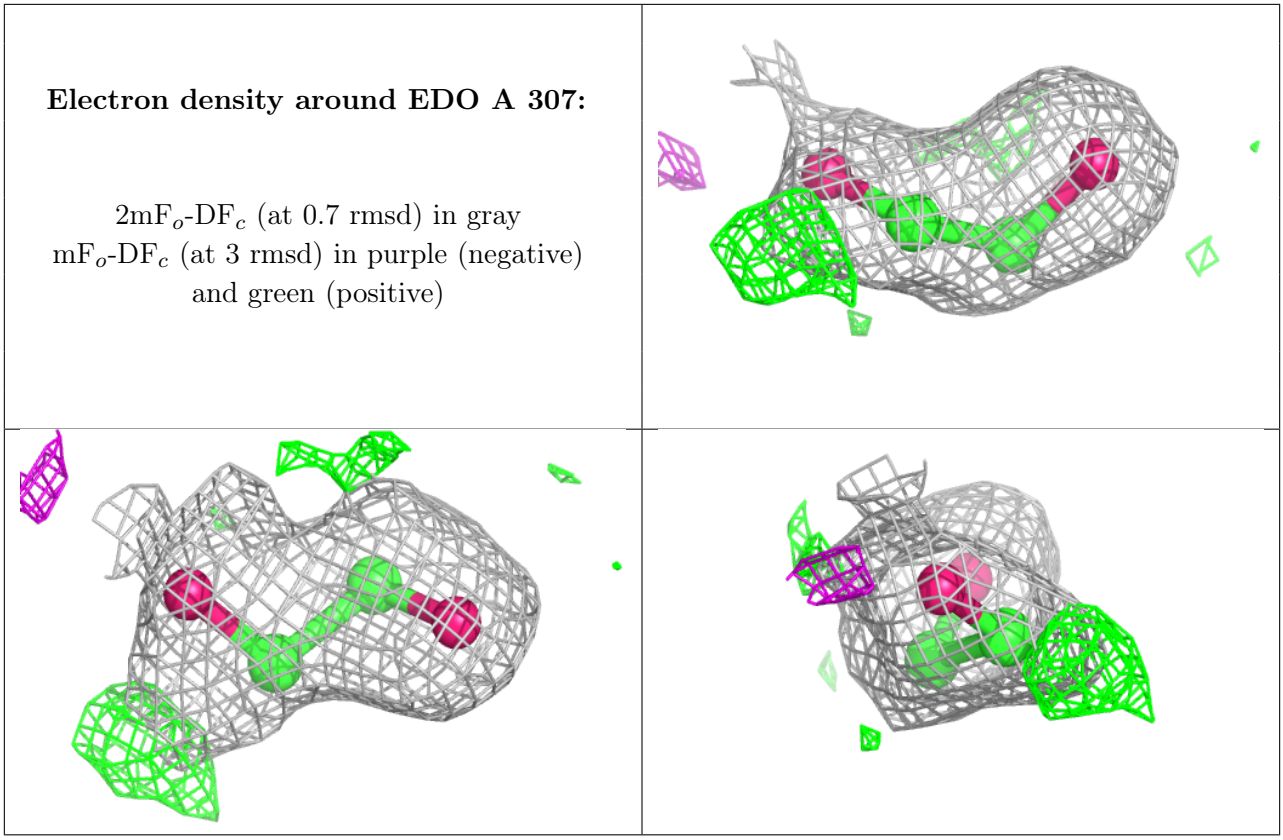






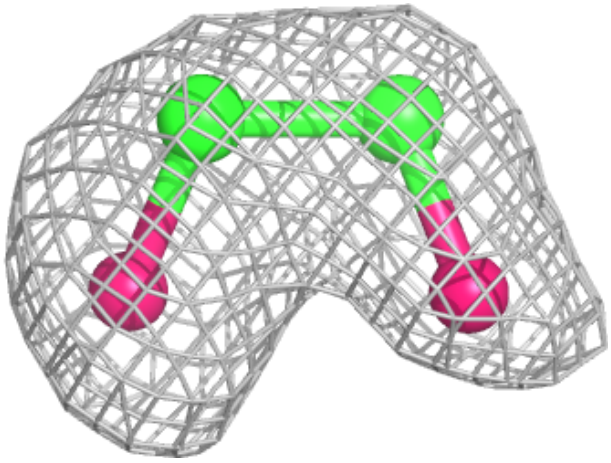
Electron density around EDO A 307:

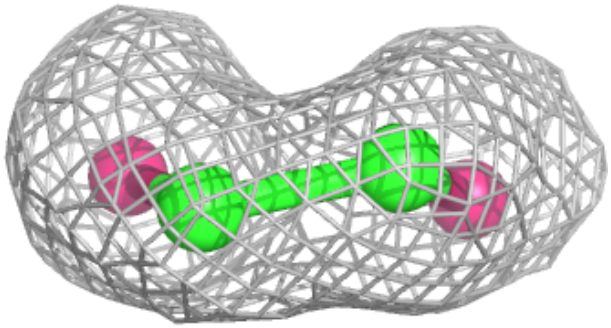
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

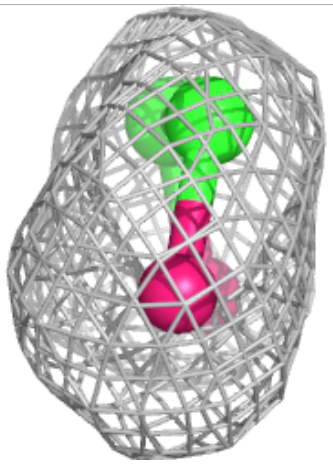


Electron density around EDO A 305:

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

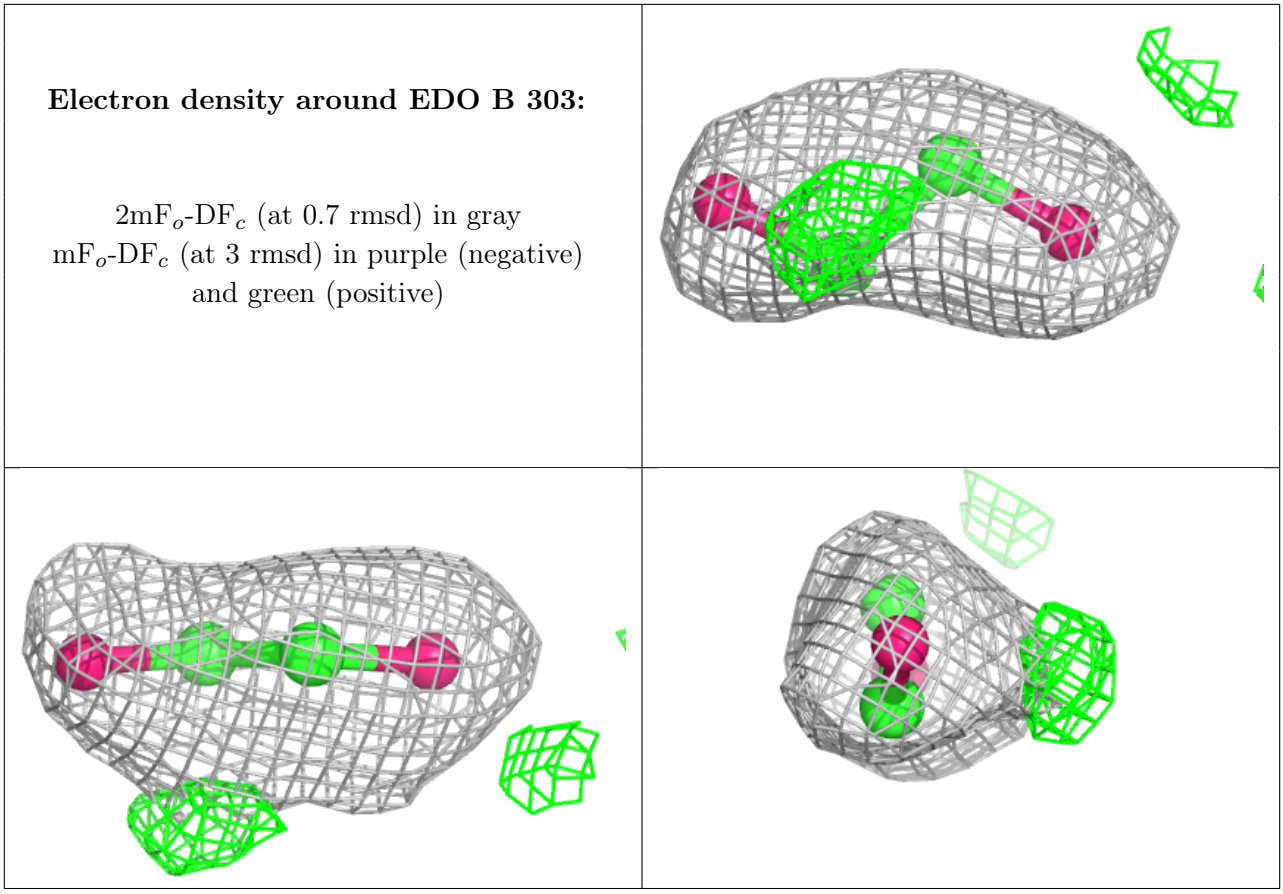






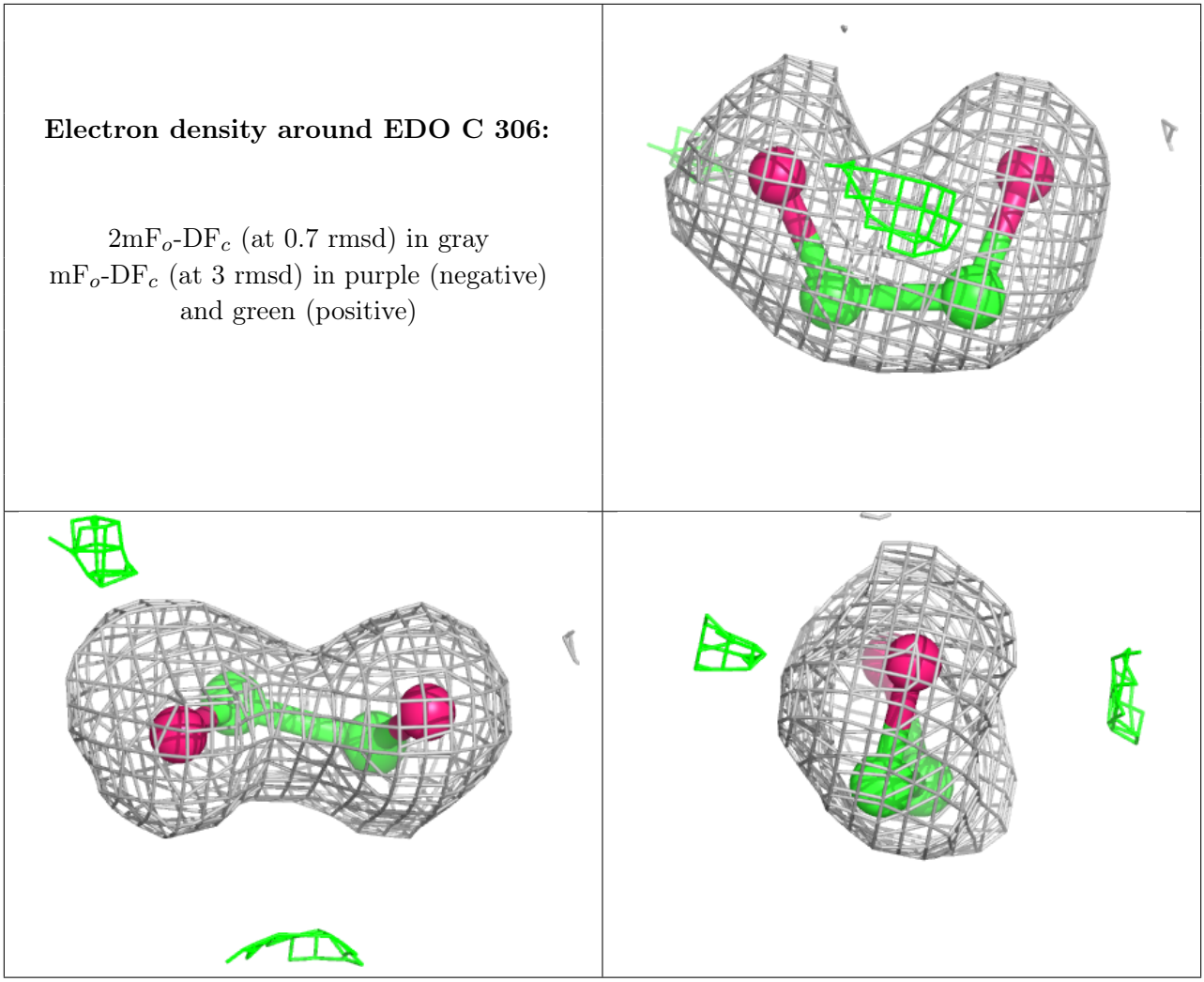
Electron density around EDO B 303:

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



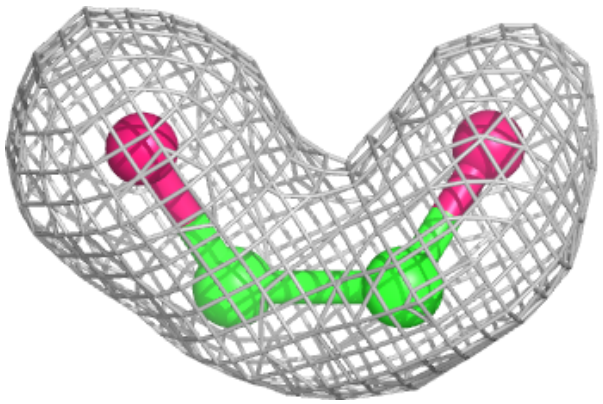
Electron density around EDO C 306:

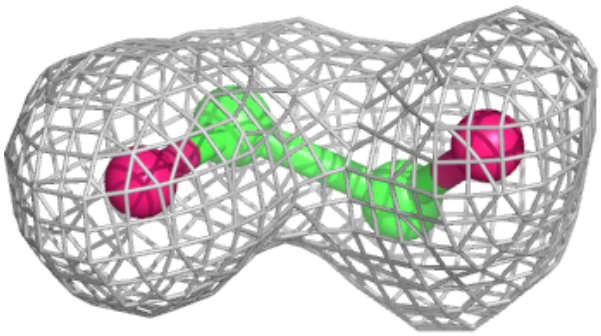
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

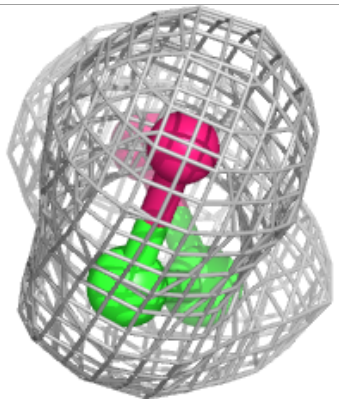


Electron density around EDO D 303:

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

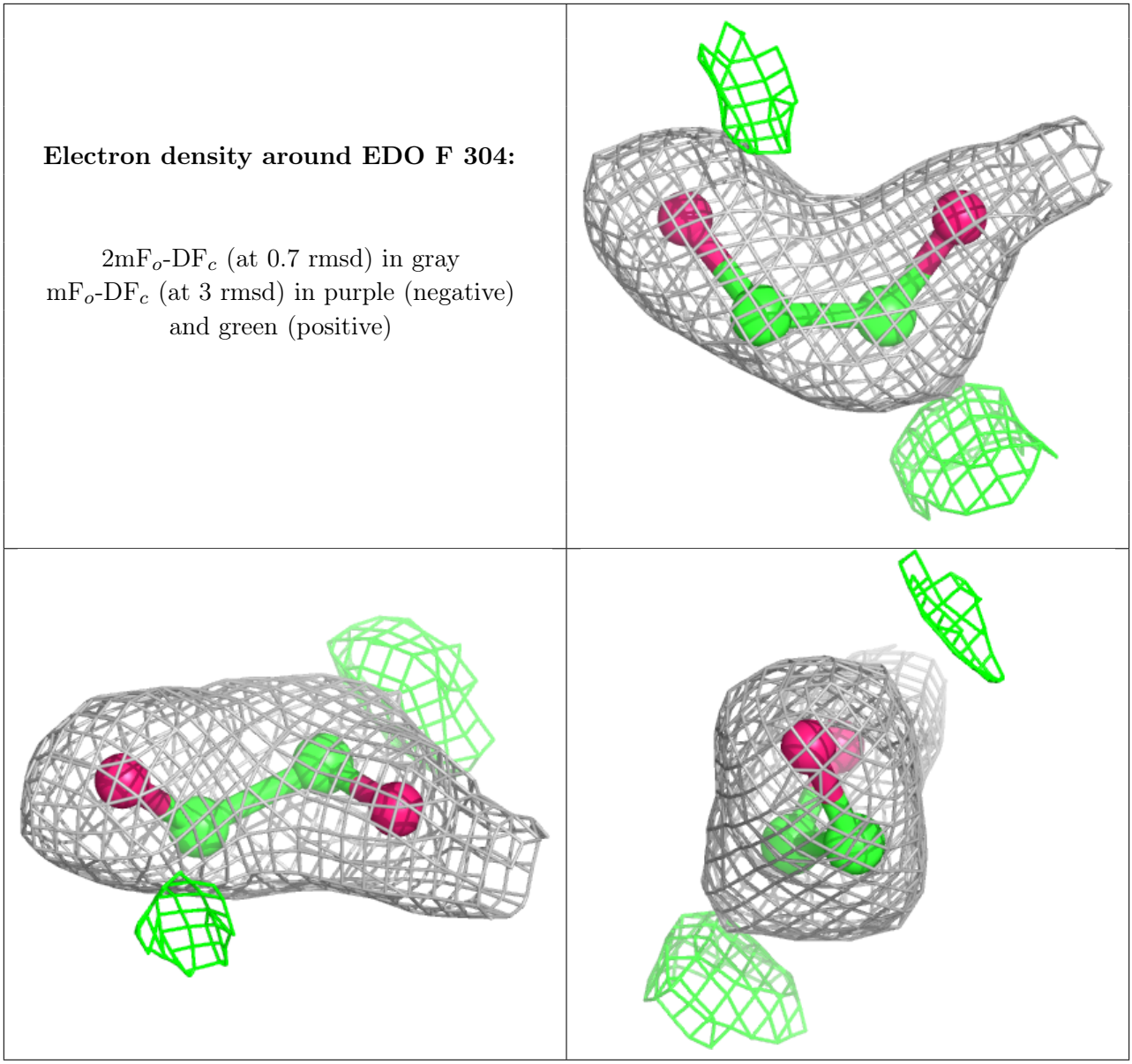






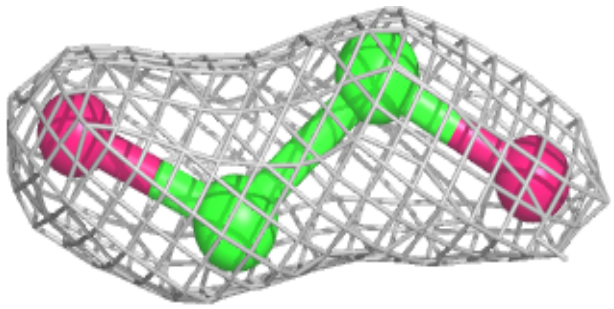
Electron density around EDO F 304:

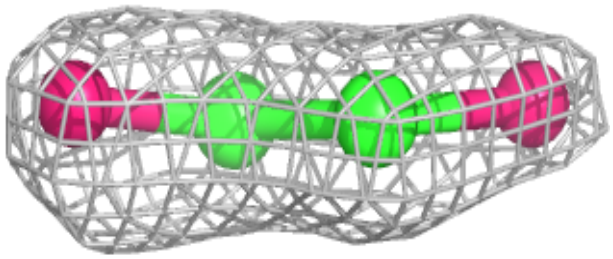
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

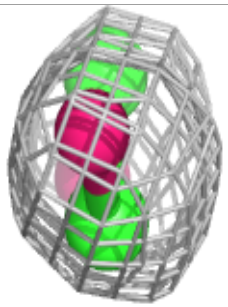


Electron density around EDO F 306:

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

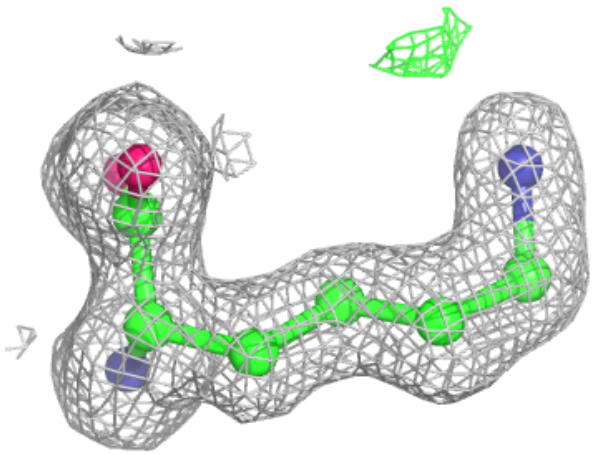


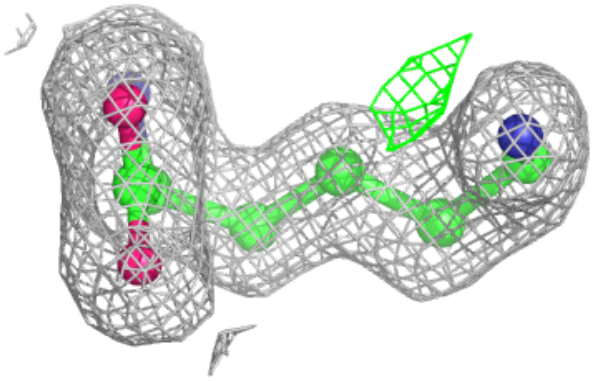


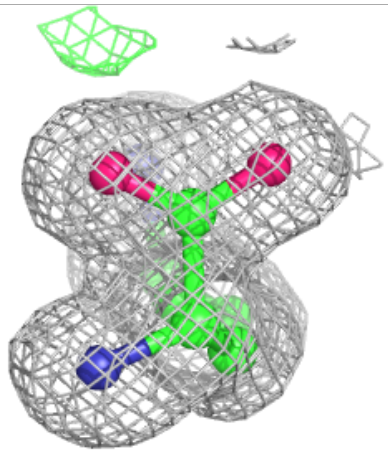


Electron density around LYS A 301:

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

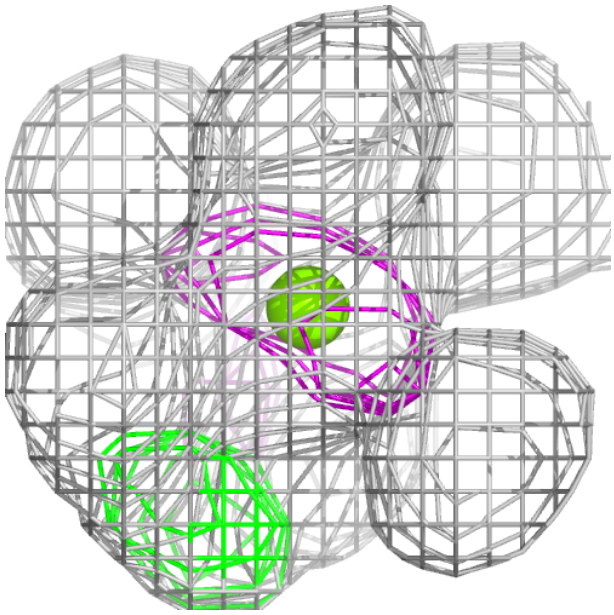


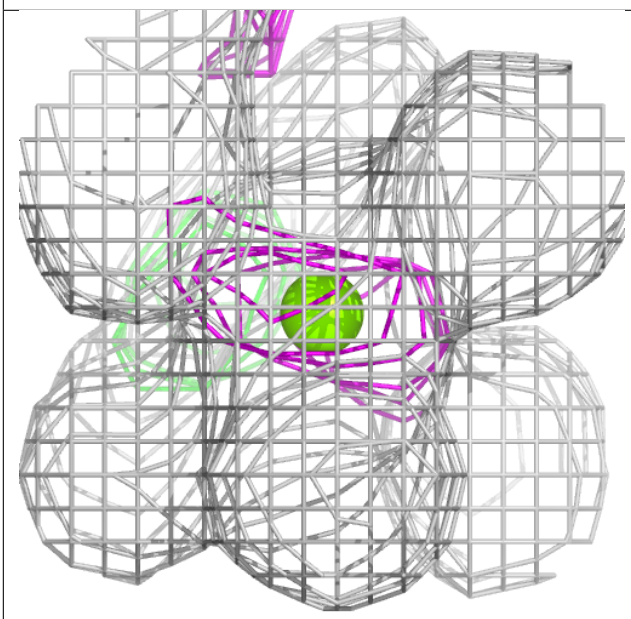


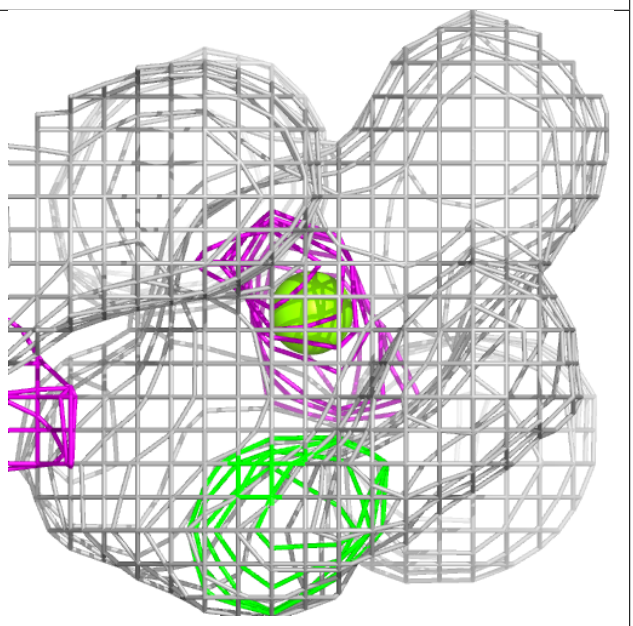


Electron density around MG B 310:

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

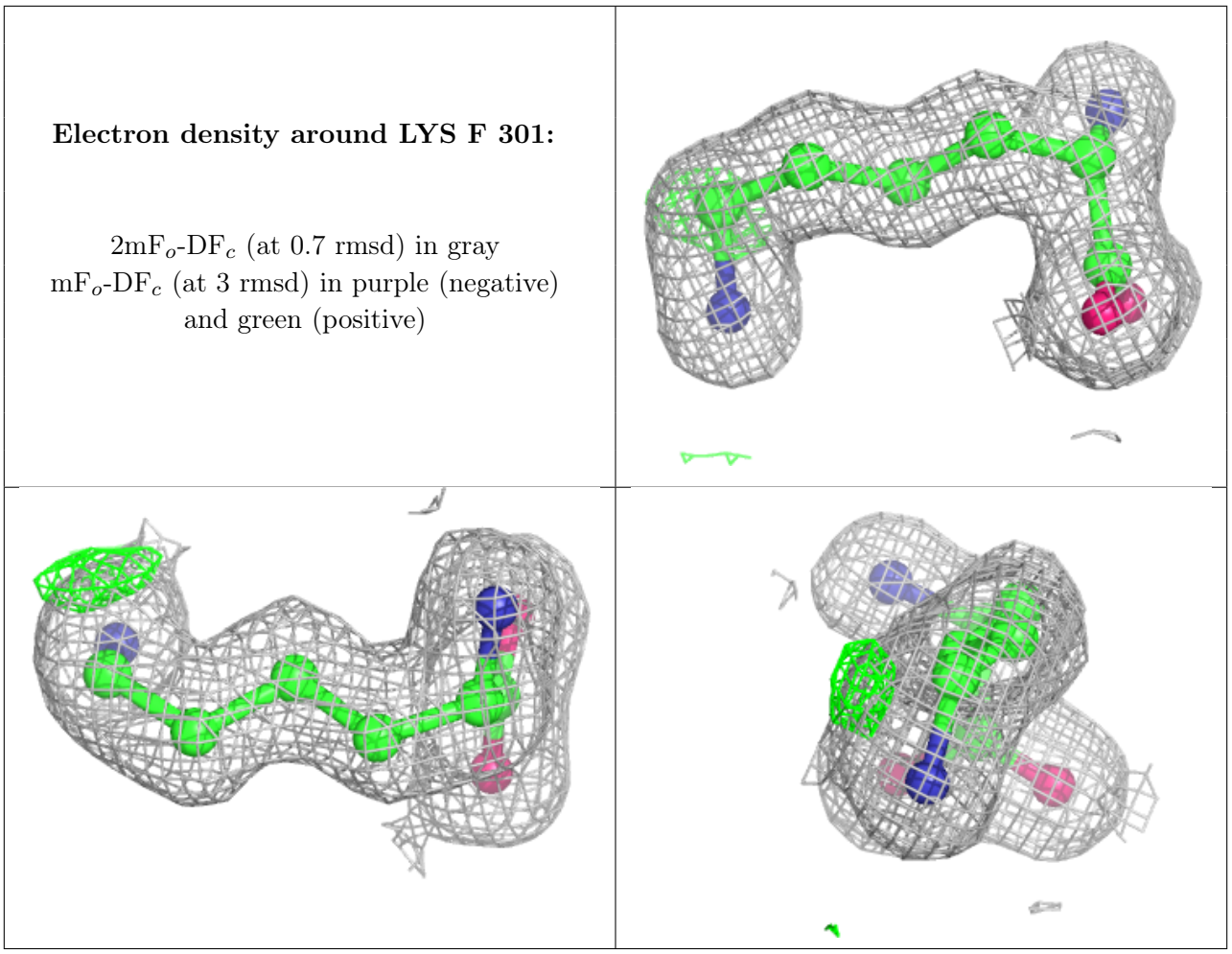






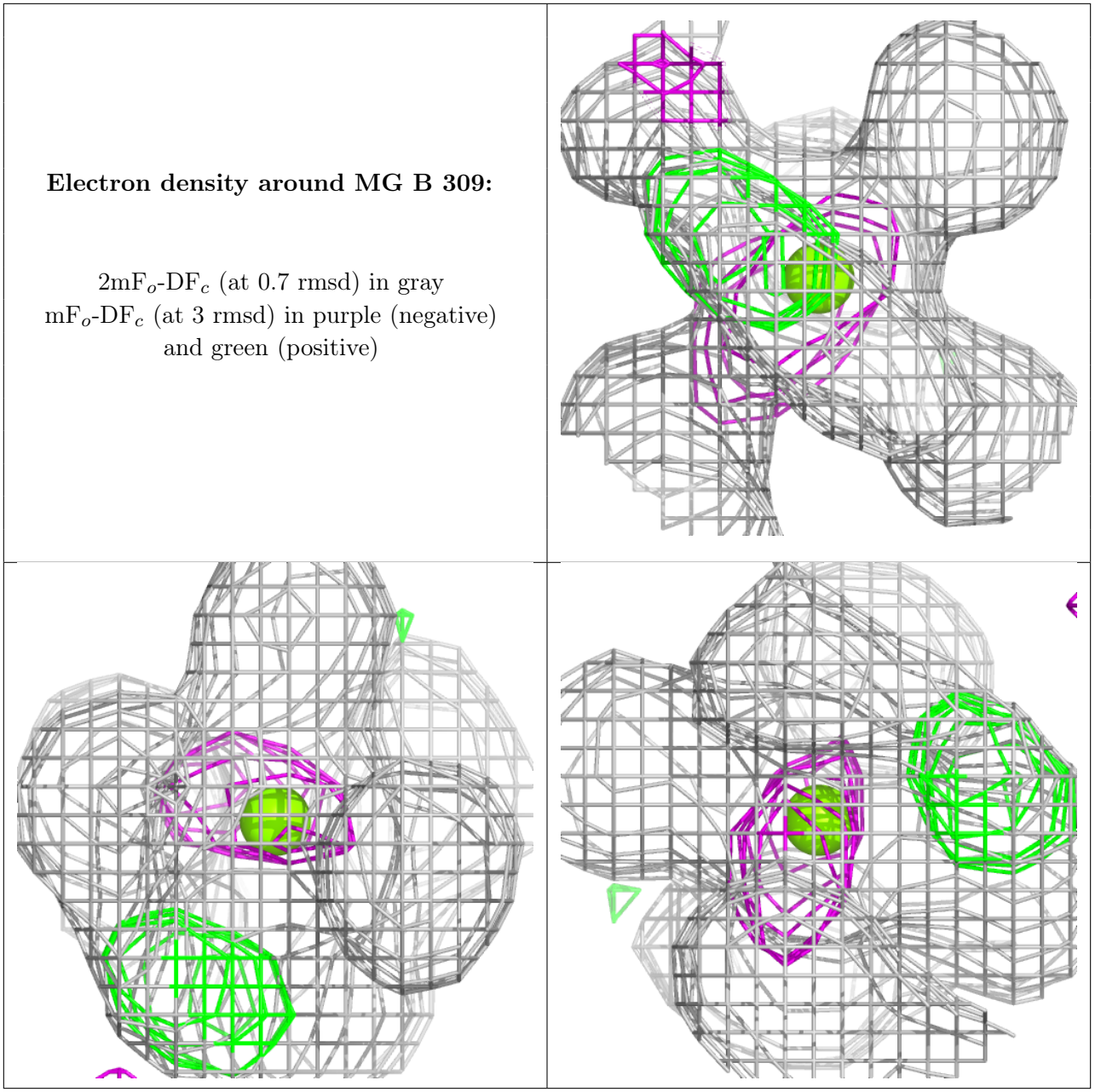
Electron density around LYS F 301:

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



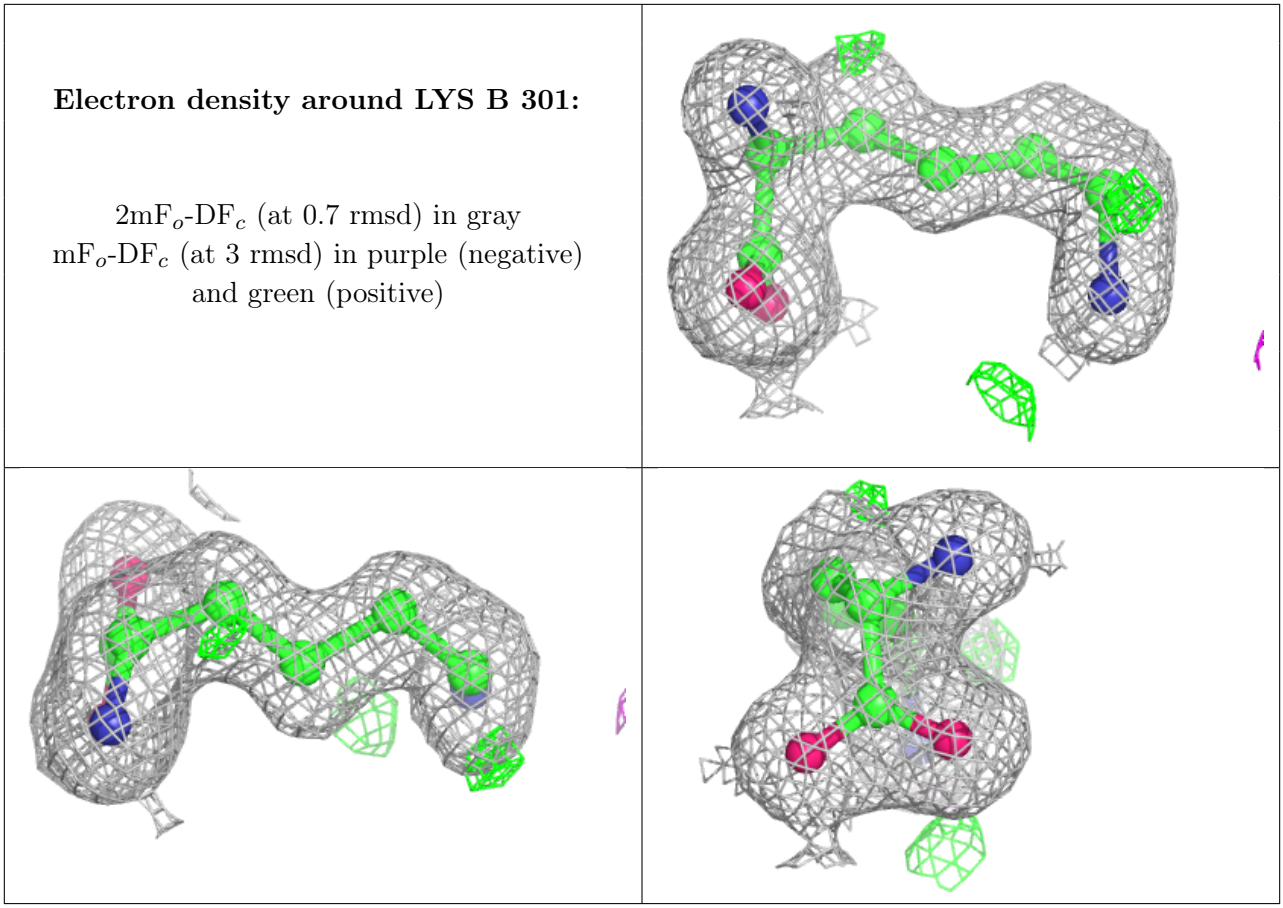
Electron density around MG B 309:

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



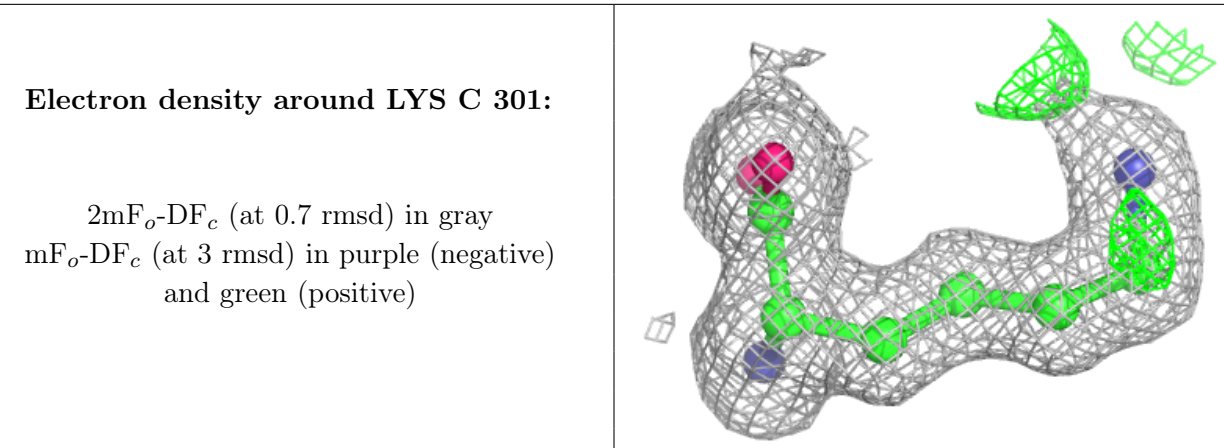
Electron density around LYS B 301:

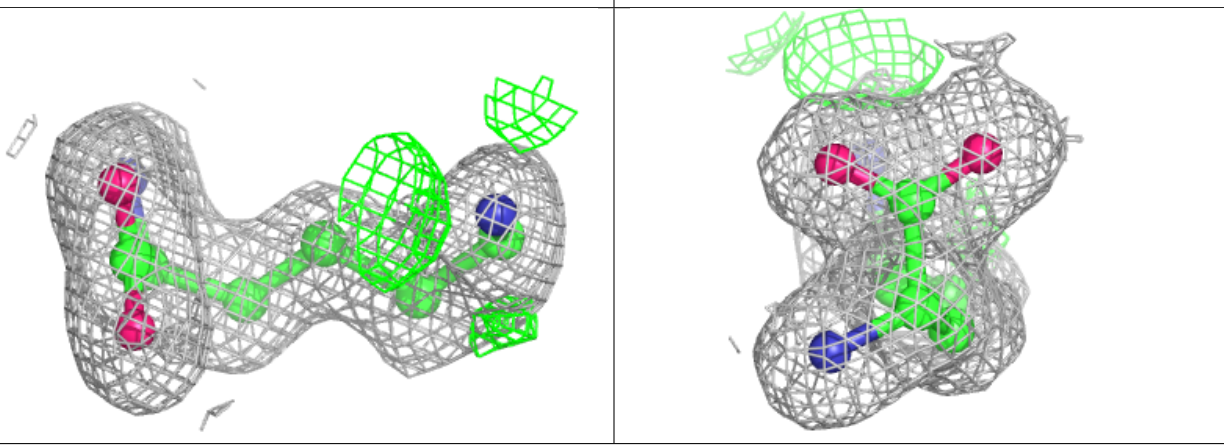
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LYS C 301:

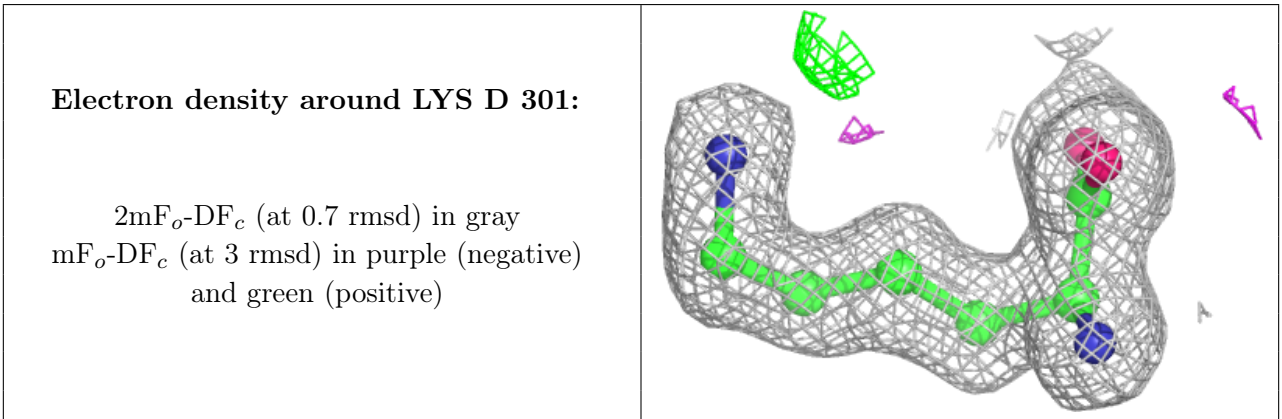
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

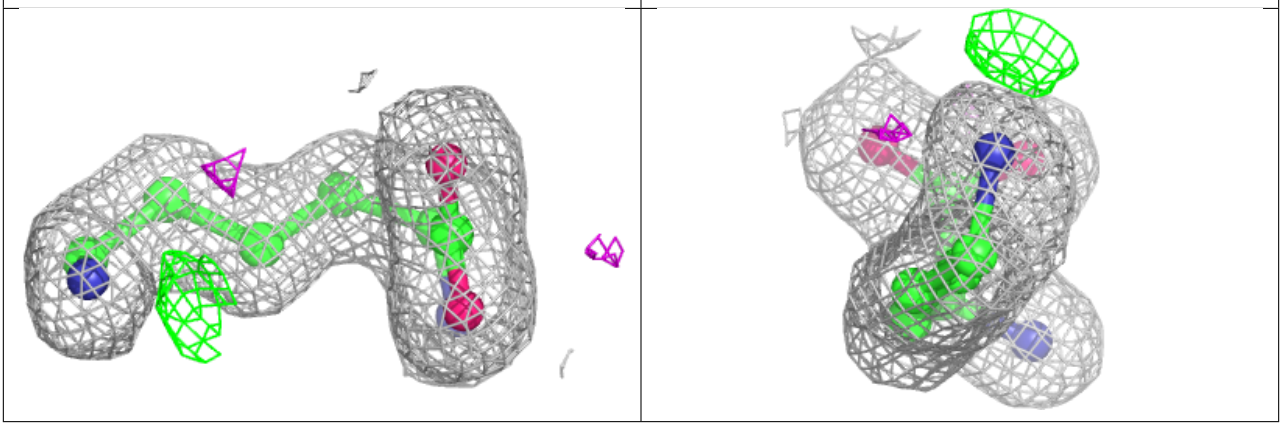




Electron density around LYS D 301:

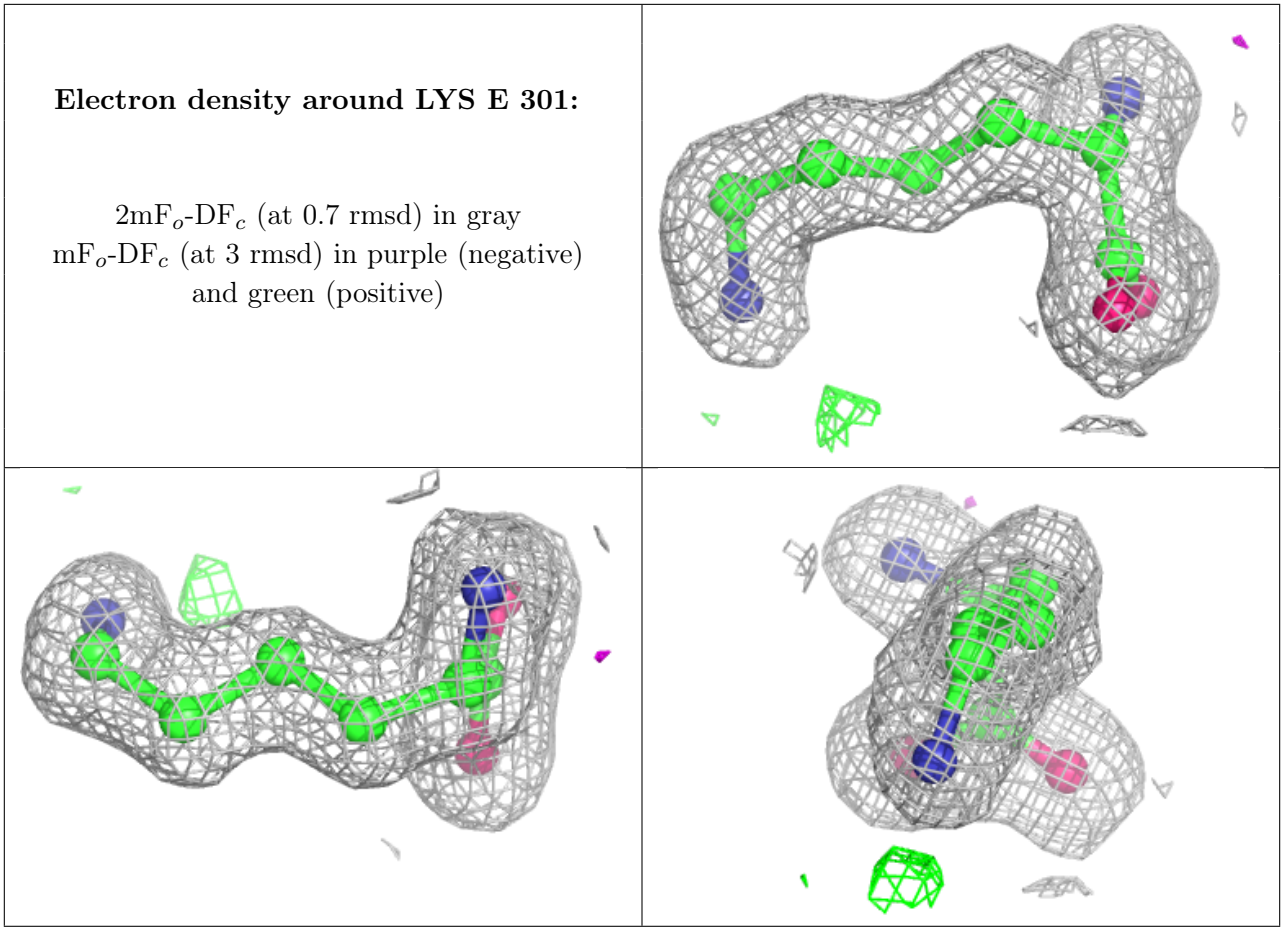
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





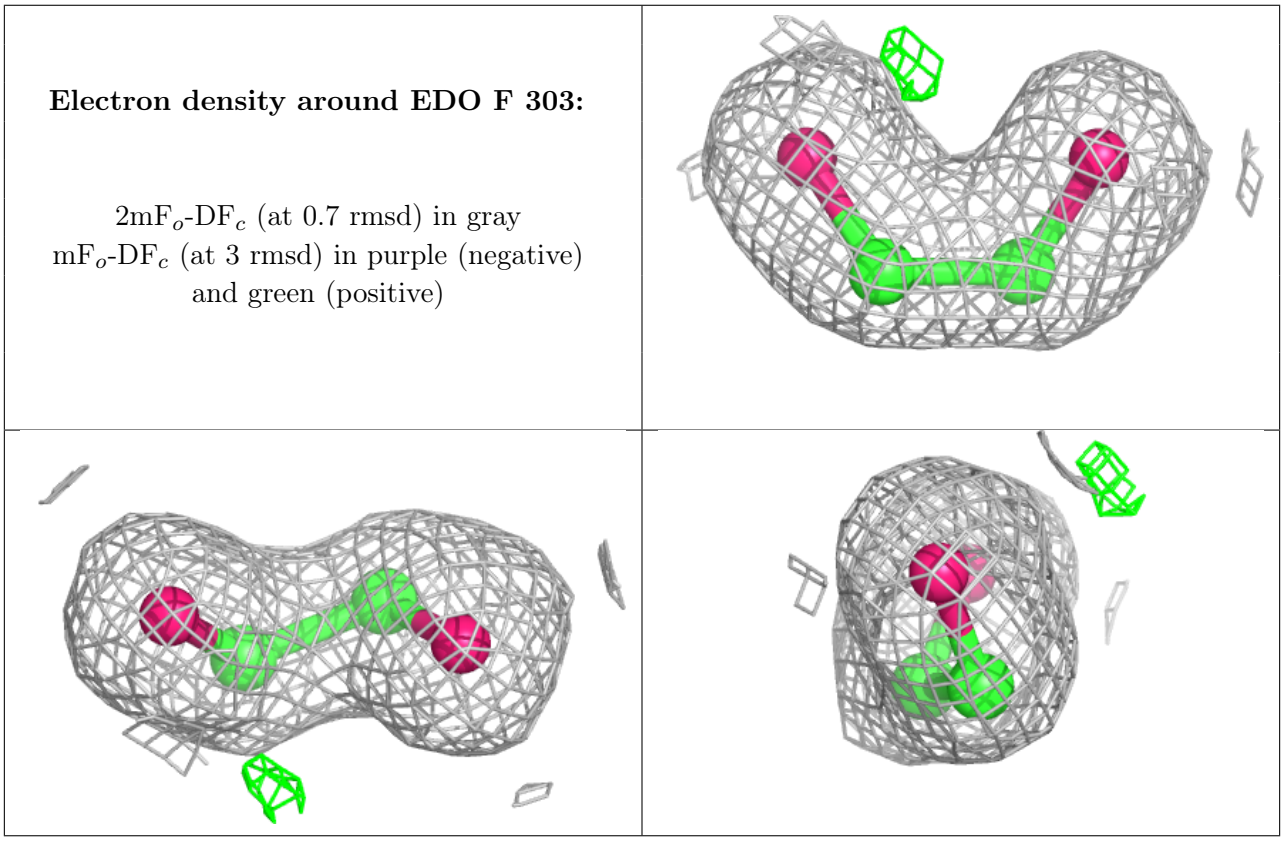
Electron density around LYS E 301:

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



Electron density around EDO 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)



6.5 Other polymers (i)

There are no such residues in this entry.