Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 06:33 PM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

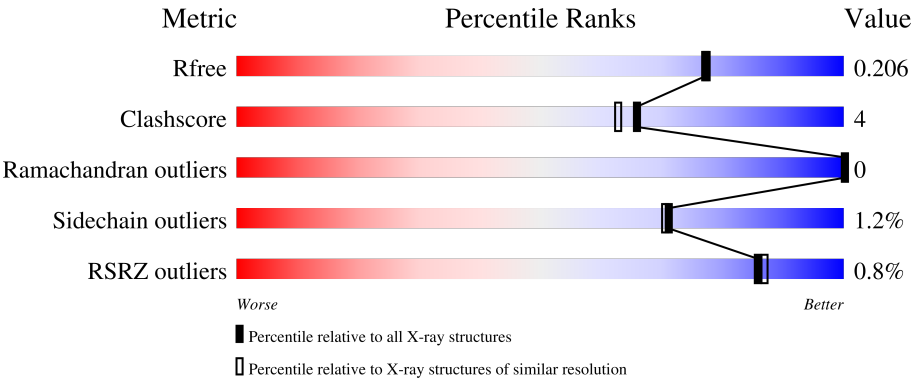
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.89 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	310	87% 7% • 5%
1	B	310	86% 8% • 5%
1	C	310	86% 8% • 5%
1	D	310	87% 7% • 5%
1	E	310	85% 10% 5%

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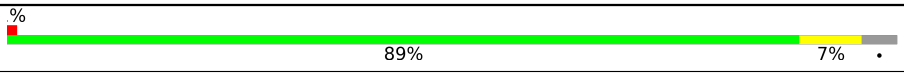
Mol	Chain	Length	Quality of chain
1	F	310	

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

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

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2279	1450	378	438	13			
1	B	296	Total	C	N	O	S	0	2	0
			2283	1451	378	441	13			
1	C	296	Total	C	N	O	S	0	1	0
			2281	1451	378	439	13			
1	D	296	Total	C	N	O	S	0	0	0
			2277	1449	377	438	13			
1	E	296	Total	C	N	O	S	0	2	0
			2281	1450	377	441	13			
1	F	297	Total	C	N	O	S	0	1	0
			2290	1455	379	443	13			

There are 78 discrepancies between the modelled and reference sequences:

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

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

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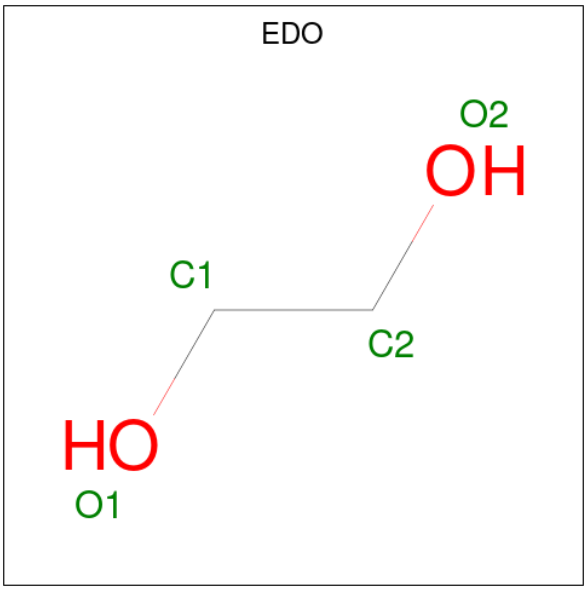
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP A0A2U0QMK8
E	-3	HIS	-	expression tag	UNP A0A2U0QMK8
E	-2	HIS	-	expression tag	UNP A0A2U0QMK8
E	-1	GLY	-	expression tag	UNP A0A2U0QMK8
E	0	SER	-	expression tag	UNP A0A2U0QMK8
E	59	LYS	HIS	engineered mutation	UNP A0A2U0QMK8
F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

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



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

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

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

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

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

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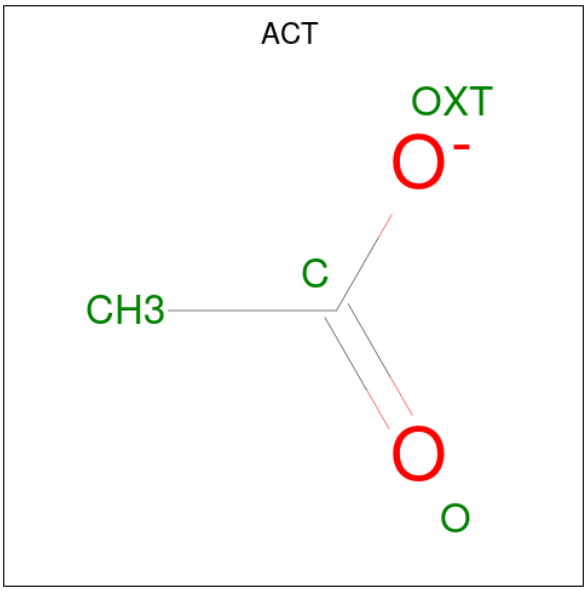
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	3	Total Mg 3 3	0	0
3	E	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0

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



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

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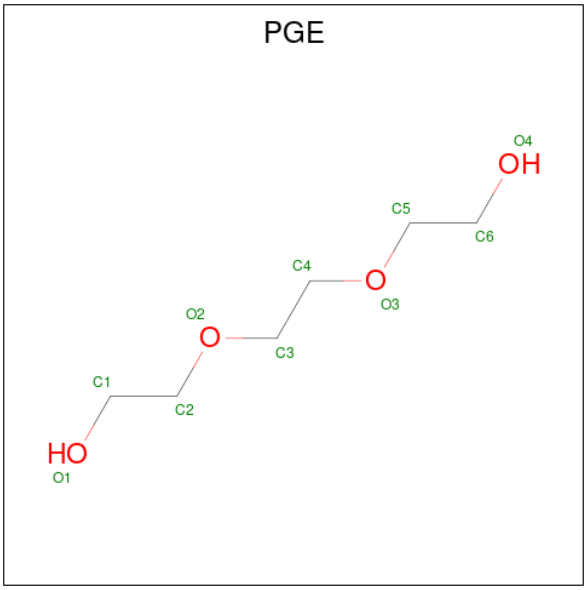
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 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
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0

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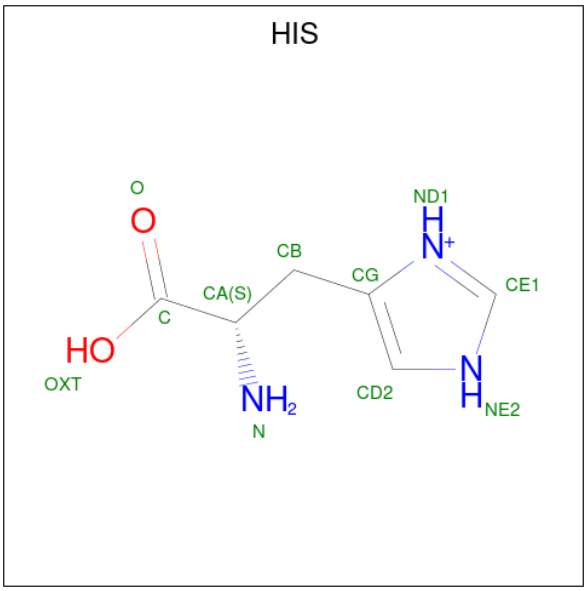
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0

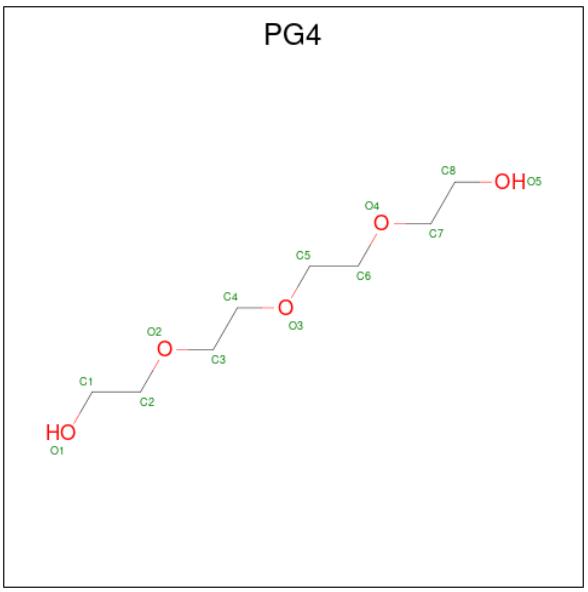
- Molecule 6 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



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

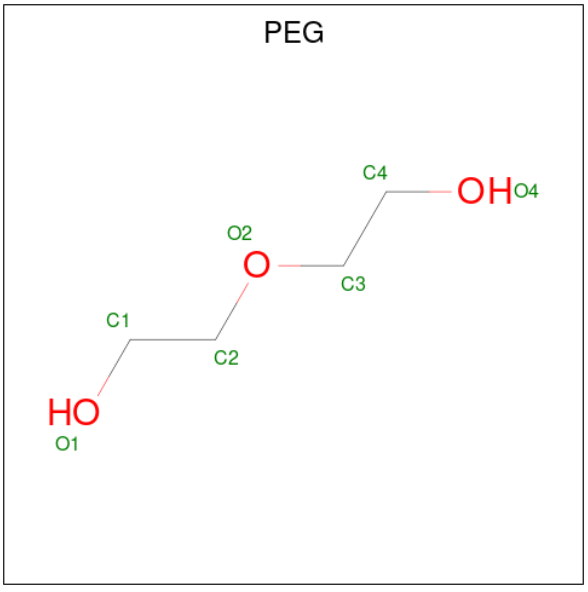
- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$)

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



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

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



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

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

- Molecule 9 is water.

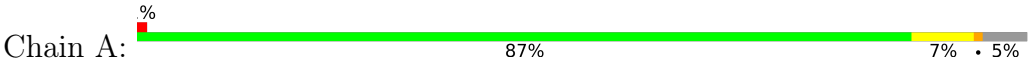
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	136	Total O 136 136	0	0
9	B	126	Total O 126 126	0	0
9	C	128	Total O 128 128	0	0
9	D	128	Total O 128 128	0	0
9	E	110	Total O 110 110	0	0
9	F	133	Total O 133 133	0	0

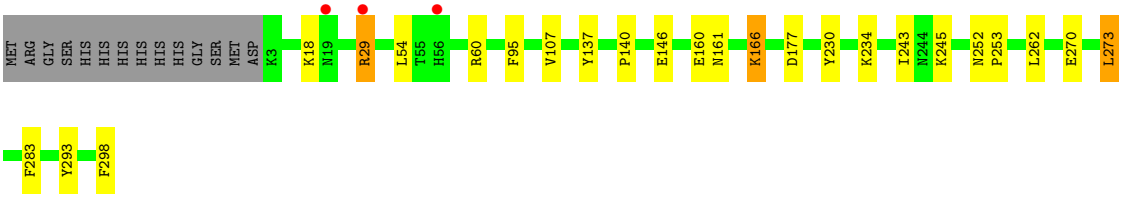
3 Residue-property plots (i)

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

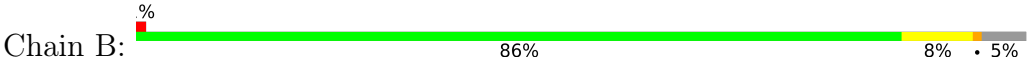
Chain A:

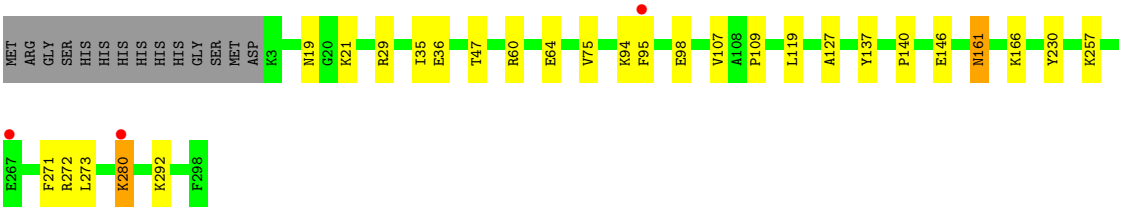




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

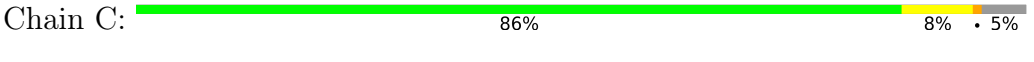
Chain B:

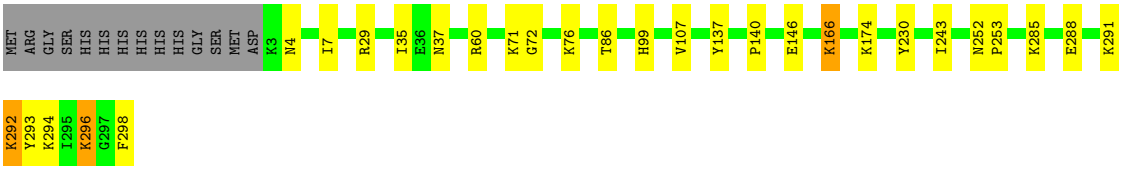




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

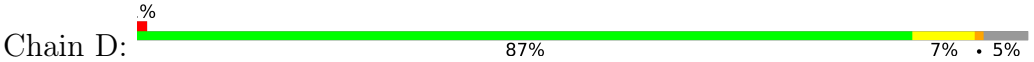
Chain C:

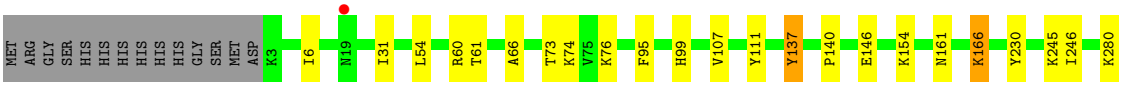




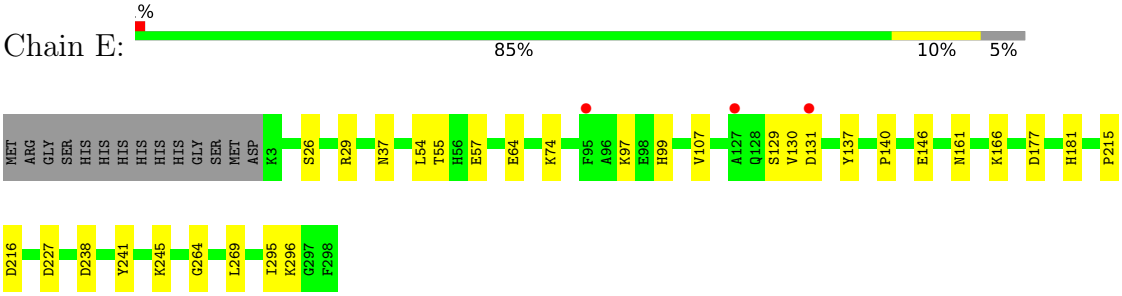
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D:

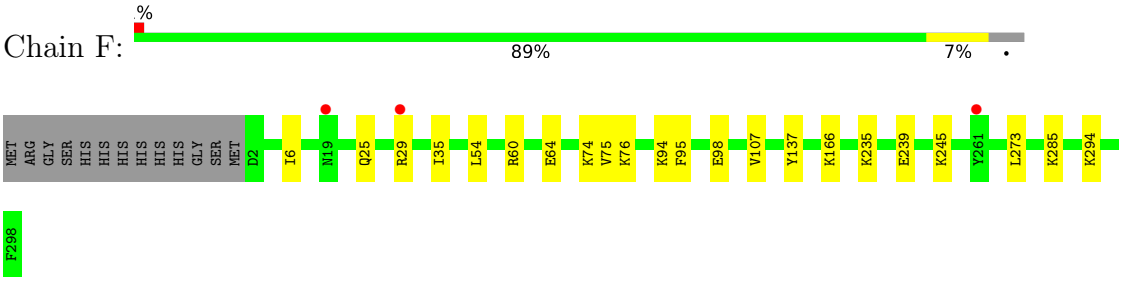




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	84.78Å 230.74Å 202.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 1.89 49.63 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.63-1.89) 98.8 (49.63-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.207 0.170 , 0.206	Depositor DCC
R_{free} test set	7806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.8	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	0.96	EDS
Total number of atoms	14872	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

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

[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: ACT, KPI, MG, PG4, PEG, PGE, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.86	2/2302 (0.1%)	0.81	1/3109 (0.0%)
1	B	0.80	0/2316	0.75	0/3129
1	C	0.81	0/2308	0.73	0/3117
1	D	0.76	0/2300	0.77	0/3107
1	E	0.80	0/2315	0.80	3/3127 (0.1%)
1	F	0.78	0/2318	0.71	0/3131
All	All	0.80	2/13859 (0.0%)	0.76	4/18720 (0.0%)

All (2) bond length outliers are listed below:

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

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

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

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

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

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:LEU:H	2:F:302:EDO:H12	1.24	0.98
1:E:29:ARG:HE	2:E:307:EDO:H12	1.32	0.93
1:E:26:SER:HA	2:E:307:EDO:H11	1.52	0.92
1:F:25:GLN:HB3	1:F:29:ARG:NH1	1.93	0.84
1:E:177:ASP:OD1	8:E:316:PEG:H21	1.79	0.82
1:B:273:LEU:H	2:B:304:EDO:H22	1.47	0.79
1:E:29:ARG:HE	2:E:307:EDO:C1	1.98	0.76
1:C:288:GLU:HA	1:C:291:LYS:HE2	1.68	0.74
1:A:234:LYS:HD3	2:B:301:EDO:H21	1.69	0.72
1:B:94:LYS:O	1:B:98:GLU:HG2	1.89	0.72
1:B:272:ARG:HG3	2:B:304:EDO:H21	1.72	0.70
1:C:4:ASN:HB3	2:C:304:EDO:H12	1.74	0.70
1:B:127:ALA:O	1:B:161[A]:ASN:ND2	2.25	0.69
1:B:140:PRO:HG3	1:B:146[B]:GLU:OE1	1.94	0.67
1:E:29:ARG:NE	2:E:307:EDO:H12	2.07	0.67
1:E:26:SER:CA	2:E:307:EDO:H11	2.25	0.66
1:B:273:LEU:H	2:B:304:EDO:C2	2.10	0.65
1:E:140:PRO:HG3	1:E:146[A]:GLU:OE1	1.98	0.64
1:C:7:ILE:H	2:C:302:EDO:H21	1.63	0.62
1:D:73:THR:O	1:D:74:LYS:HB2	1.98	0.62
1:E:130:VAL:O	1:E:161:ASN:ND2	2.33	0.61
1:B:60:ARG:HB2	1:B:95:PHE:HZ	1.65	0.61
1:C:7:ILE:O	2:C:302:EDO:H21	2.01	0.61
1:D:140:PRO:HG3	1:D:146:GLU:OE1	2.00	0.60
1:E:55:THR:OG1	1:E:57:GLU:HG2	2.01	0.60
1:C:292:LYS:HD2	9:C:494:HOH:O	2.00	0.60
1:C:174:LYS:HA	2:C:305:EDO:H21	1.85	0.59
1:C:7:ILE:H	2:C:302:EDO:C2	2.16	0.58
1:E:181:HIS:CE1	8:E:316:PEG:H21	2.38	0.58
1:E:97:LYS:NZ	1:E:131:ASP:OD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:LEU:O	6:F:309:HIS:HE1	1.88	0.57
1:B:47:THR:OG1	1:D:111:TYR:OH	2.23	0.57
1:C:35:ILE:HG22	2:E:306:EDO:H21	1.87	0.57
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.87	0.56
1:E:29:ARG:HH21	2:E:307:EDO:H12	1.70	0.55
1:A:273:LEU:HB3	1:C:86:THR:OG1	2.06	0.55
1:A:60:ARG:HB2	1:A:95:PHE:HZ	1.72	0.55
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.88	0.54
1:D:60:ARG:HG3	1:D:99:HIS:CE1	2.44	0.53
1:B:273:LEU:N	2:B:304:EDO:H22	2.20	0.53
1:A:29:ARG:HH21	1:A:298:PHE:HB2	1.72	0.53
1:D:154:LYS:HD2	5:D:316:PGE:H32	1.91	0.53
1:D:61:THR:HG23	2:D:309:EDO:H21	1.89	0.53
1:C:29:ARG:HG2	1:C:298:PHE:CE1	2.44	0.53
1:C:166:KPI:H1B	4:C:308:ACT:H2	1.90	0.52
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.90	0.52
1:A:230:TYR:HD2	1:B:230:TYR:HD2	1.58	0.52
1:F:60:ARG:NH2	1:F:64:GLU:OE2	2.43	0.52
1:F:235:LYS:HE3	1:F:239:GLU:OE2	2.10	0.52
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.91	0.51
1:A:54:LEU:O	6:A:317:HIS:HE1	1.94	0.51
1:F:60:ARG:HB2	1:F:95:PHE:HZ	1.75	0.50
1:F:94:LYS:O	1:F:98:GLU:HG2	2.12	0.50
1:D:297:GLY:HA2	8:D:320:PEG:H31	1.92	0.50
1:C:230:TYR:CD2	1:D:230:TYR:HD2	2.30	0.50
1:A:262:LEU:HD21	1:A:283:PHE:CE1	2.48	0.49
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.93	0.49
1:D:6:ILE:HG12	1:D:76:LYS:HD2	1.95	0.48
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.95	0.48
1:B:36:GLU:OE1	2:B:302:EDO:O2	2.31	0.47
1:A:29:ARG:HH21	1:A:298:PHE:CB	2.27	0.47
1:B:60:ARG:NH2	1:B:64:GLU:OE2	2.48	0.47
1:C:243:ILE:HB	1:C:293:TYR:CE2	2.50	0.47
1:B:273:LEU:HB2	2:B:304:EDO:H22	1.97	0.47
1:E:74:LYS:HD2	1:E:74:LYS:N	2.30	0.46
1:A:177:ASP:OD1	4:A:314:ACT:H2	2.14	0.46
1:E:264:GLY:O	5:E:314:PGE:H22	2.16	0.46
1:B:257:LYS:HD3	1:B:271:PHE:CE2	2.50	0.46
1:A:166:KPI:H1B	4:A:313:ACT:H3	1.98	0.46
2:E:306:EDO:H12	9:E:463:HOH:O	2.14	0.46
1:D:166:KPI:H1B	4:D:313:ACT:H3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ILE:HD13	1:D:66:ALA:HA	1.97	0.46
1:B:60:ARG:HB2	1:B:95:PHE:CZ	2.47	0.45
1:D:54:LEU:O	6:D:321:HIS:HE1	1.99	0.45
1:E:245:LYS:HA	1:E:245:LYS:HD2	1.68	0.45
1:C:72:GLY:C	1:E:295:ILE:HD12	2.36	0.45
1:A:252:ASN:OD1	1:A:253:PRO:HA	2.16	0.45
1:C:294:LYS:HA	1:C:294:LYS:HD3	1.73	0.45
1:C:60:ARG:HG3	1:C:99:HIS:CE1	2.51	0.44
1:C:140:PRO:HG3	1:C:146:GLU:OE1	2.17	0.44
1:A:243:ILE:HB	1:A:293:TYR:CE2	2.53	0.44
1:B:19:ASN:O	1:B:21:LYS:HE2	2.18	0.43
1:F:35:ILE:HG12	1:F:75:VAL:HG21	2.00	0.43
1:B:109:PRO:HD2	1:B:119:LEU:CD2	2.49	0.43
1:E:181:HIS:CE1	8:E:316:PEG:C2	3.01	0.43
1:E:54:LEU:O	6:E:317:HIS:HE1	2.02	0.43
1:E:269:LEU:HD12	1:E:269:LEU:HA	1.82	0.43
1:C:285:LYS:HA	1:C:285:LYS:HD2	1.76	0.42
1:F:25:GLN:HB3	1:F:29:ARG:HH11	1.81	0.42
1:E:29:ARG:NH2	2:E:307:EDO:H12	2.32	0.42
1:E:238:ASP:O	2:E:304:EDO:H11	2.19	0.42
1:E:131:ASP:HA	1:E:161:ASN:HD21	1.84	0.42
1:A:140:PRO:HG3	1:A:146:GLU:OE1	2.20	0.42
1:A:230:TYR:HD2	1:B:230:TYR:CD2	2.37	0.42
1:B:280:LYS:HD2	1:B:280:LYS:HA	1.83	0.42
8:E:316:PEG:H31	8:E:316:PEG:H11	1.70	0.42
1:C:252:ASN:OD1	1:C:253:PRO:HA	2.19	0.42
1:F:245:LYS:HD2	1:F:245:LYS:HA	1.82	0.42
1:A:245:LYS:HD2	1:A:245:LYS:HA	1.85	0.41
1:E:241:TYR:CE2	1:E:245:LYS:HG3	2.55	0.41
1:C:76:LYS:HD3	2:C:306:EDO:O1	2.20	0.41
1:B:35:ILE:HG12	1:B:75:VAL:HG21	2.02	0.41
1:D:161:ASN:OD1	1:D:161:ASN:N	2.40	0.41
1:D:60:ARG:HB2	1:D:95:PHE:HZ	1.85	0.41
1:D:246:ILE:HD12	1:D:246:ILE:HA	1.95	0.41
1:E:64:GLU:OE1	1:E:99:HIS:HD2	2.03	0.41
1:C:37:ASN:OD1	1:C:296:LYS:HE2	2.21	0.41
1:C:76:LYS:HZ2	2:C:302:EDO:H11	1.86	0.41
1:F:6:ILE:HG12	1:F:76:LYS:HD3	2.03	0.40
1:D:54:LEU:O	6:D:321:HIS:CE1	2.75	0.40
1:C:71:LYS:NZ	2:C:303:EDO:H11	2.36	0.40
1:D:245:LYS:HD2	1:D:245:LYS:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ASN:OD1	1:E:296:LYS:HD3	2.21	0.40
8:D:320:PEG:H22	8:D:320:PEG:H41	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	B	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
1	C	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	D	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	E	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
1	F	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
All	All	1765/1860 (95%)	1728 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/260 (95%)	244 (98%)	4 (2%)	62	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	249/260 (96%)	244 (98%)	5 (2%)	55 51
1	C	249/260 (96%)	247 (99%)	2 (1%)	81 82
1	D	247/260 (95%)	244 (99%)	3 (1%)	71 70
1	E	249/260 (96%)	247 (99%)	2 (1%)	81 82
1	F	250/260 (96%)	247 (99%)	3 (1%)	71 70
All	All	1492/1560 (96%)	1473 (99%)	19 (1%)	71 68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	29	ARG
1	A	160	GLU
1	A	161	ASN
1	B	29	ARG
1	B	161[A]	ASN
1	B	161[B]	ASN
1	B	280	LYS
1	B	292	LYS
1	C	292	LYS
1	C	296	LYS
1	D	137	TYR
1	D	280	LYS
1	D	292	LYS
1	E	129	SER
1	E	227	ASP
1	F	74	LYS
1	F	285	LYS
1	F	294	LYS

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

Mol	Chain	Res	Type
1	E	128	GLN

5.3.3 RNA

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

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	O2-CX2	5.22	1.36	1.22
1	C	166	KPI	O2-CX2	4.70	1.35	1.22
1	C	166	KPI	CX2-CX1	3.36	1.53	1.49
1	F	166	KPI	O-C	3.13	1.32	1.19
1	B	166	KPI	CX2-CX1	2.87	1.53	1.49
1	D	166	KPI	O1-CX2	2.35	1.37	1.30
1	F	166	KPI	O1-CX2	2.31	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	O1-CX2	-2.17	1.24	1.30
1	A	166	KPI	CX2-CX1	2.11	1.52	1.49
1	B	166	KPI	CA-N	-2.05	1.41	1.48
1	B	166	KPI	O1-CX2	-2.01	1.24	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	KPI	C1-CX1-CX2	-10.38	108.08	118.17
1	D	166	KPI	C1-CX1-CX2	-8.19	110.20	118.17
1	F	166	KPI	C1-CX1-CX2	-7.36	111.01	118.17
1	C	166	KPI	C1-CX1-CX2	-7.33	111.04	118.17
1	B	166	KPI	C1-CX1-CX2	-7.21	111.16	118.17
1	E	166	KPI	C1-CX1-CX2	-6.97	111.39	118.17
1	E	166	KPI	O2-CX2-CX1	6.87	130.15	121.38
1	C	166	KPI	O2-CX2-CX1	-5.46	114.40	121.38
1	A	166	KPI	O2-CX2-CX1	5.26	128.09	121.38
1	F	166	KPI	O2-CX2-CX1	5.22	128.04	121.38
1	C	166	KPI	O1-CX2-CX1	5.15	127.54	116.35
1	B	166	KPI	O1-CX2-CX1	5.14	127.51	116.35
1	B	166	KPI	O2-CX2-CX1	-4.35	115.82	121.38
1	D	166	KPI	O2-CX2-CX1	3.71	126.12	121.38
1	E	166	KPI	O1-CX2-O2	-3.42	115.79	123.61
1	A	166	KPI	O1-CX2-O2	-3.15	116.40	123.61
1	B	166	KPI	O1-CX2-O2	-3.03	116.67	123.61
1	F	166	KPI	O1-CX2-O2	-2.96	116.84	123.61
1	A	166	KPI	C1-CX1-NZ	2.58	129.86	123.11
1	D	166	KPI	C1-CX1-NZ	2.56	129.80	123.11
1	F	166	KPI	C1-CX1-NZ	2.55	129.77	123.11
1	D	166	KPI	O1-CX2-O2	-2.52	117.84	123.61
1	C	166	KPI	O1-CX2-O2	-2.42	118.06	123.61
1	B	166	KPI	C1-CX1-NZ	2.25	129.00	123.11
1	A	166	KPI	CE-NZ-CX1	2.24	127.80	121.70
1	B	166	KPI	CD-CE-NZ	2.03	114.35	110.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	E	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	C1-CX1-NZ-CE
1	F	166	KPI	C1-CX1-NZ-CE

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 87 ligands modelled in this entry, 14 are monoatomic - leaving 73 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	F	308	-	3,3,3	2.28	1 (33%)	3,3,3	1.37	0
2	EDO	E	302	-	3,3,3	0.44	0	2,2,2	0.28	0
2	EDO	D	305	-	3,3,3	0.48	0	2,2,2	0.07	0
2	EDO	C	304	-	3,3,3	0.51	0	2,2,2	0.22	0
2	EDO	A	306	-	3,3,3	0.63	0	2,2,2	0.50	0
2	EDO	D	309	-	3,3,3	0.41	0	2,2,2	0.71	0
2	EDO	E	307	-	3,3,3	0.23	0	2,2,2	0.63	0
8	PEG	D	319	-	6,6,6	0.47	0	5,5,5	0.58	0
2	EDO	A	307	-	3,3,3	0.65	0	2,2,2	0.13	0
2	EDO	F	301	-	3,3,3	0.64	0	2,2,2	0.38	0
8	PEG	D	318	-	6,6,6	0.45	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	D	308	-	3,3,3	0.52	0	2,2,2	0.27	0
2	EDO	B	301	-	3,3,3	0.72	0	2,2,2	0.31	0
4	ACT	B	308	-	3,3,3	1.72	1 (33%)	3,3,3	1.20	0
2	EDO	F	303	-	3,3,3	0.56	0	2,2,2	0.15	0
4	ACT	B	310	-	3,3,3	1.28	0	3,3,3	1.33	0
2	EDO	D	306	-	3,3,3	0.57	0	2,2,2	0.37	0
4	ACT	D	314	-	3,3,3	1.46	1 (33%)	3,3,3	1.70	1 (33%)
2	EDO	E	305	-	3,3,3	0.29	0	2,2,2	0.44	0
4	ACT	A	313	-	3,3,3	1.27	1 (33%)	3,3,3	1.53	1 (33%)
2	EDO	A	304	-	3,3,3	0.46	0	2,2,2	0.25	0
2	EDO	C	306	-	3,3,3	0.62	0	2,2,2	0.61	0
2	EDO	A	301	-	3,3,3	0.63	0	2,2,2	0.59	0
2	EDO	B	303	-	3,3,3	0.83	0	2,2,2	0.46	0
6	HIS	F	309	-	6,11,11	0.94	1 (16%)	7,14,14	1.51	3 (42%)
4	ACT	F	306	-	3,3,3	1.63	1 (33%)	3,3,3	1.42	0
5	PGE	A	316	-	9,9,9	0.39	0	8,8,8	0.38	0
2	EDO	C	301	-	3,3,3	0.56	0	2,2,2	0.17	0
2	EDO	E	304	-	3,3,3	0.64	0	2,2,2	0.19	0
2	EDO	F	302	-	3,3,3	0.55	0	2,2,2	0.43	0
2	EDO	B	302	-	3,3,3	0.40	0	2,2,2	0.80	0
4	ACT	A	314	-	3,3,3	2.09	1 (33%)	3,3,3	1.22	0
4	ACT	F	307	-	3,3,3	1.98	1 (33%)	3,3,3	1.20	0
5	PGE	C	309	-	9,9,9	0.32	0	8,8,8	0.46	0
6	HIS	C	310	-	6,11,11	1.26	1 (16%)	7,14,14	1.70	3 (42%)
8	PEG	E	315	-	6,6,6	0.53	0	5,5,5	0.34	0
8	PEG	E	316	-	6,6,6	0.37	0	5,5,5	1.87	2 (40%)
2	EDO	B	305	-	3,3,3	0.35	0	2,2,2	0.79	0
2	EDO	E	306	-	3,3,3	0.36	0	2,2,2	0.42	0
7	PG4	D	317	-	12,12,12	1.09	1 (8%)	11,11,11	1.56	3 (27%)
6	HIS	A	317	-	6,11,11	0.81	0	7,14,14	1.43	2 (28%)
6	HIS	B	313	-	6,11,11	0.96	0	7,14,14	1.59	3 (42%)
2	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.55	0
4	ACT	B	309	-	3,3,3	1.60	1 (33%)	3,3,3	1.37	0
6	HIS	E	317	-	6,11,11	0.84	0	7,14,14	1.54	1 (14%)
4	ACT	E	310	-	3,3,3	1.80	1 (33%)	3,3,3	1.28	0
2	EDO	A	303	-	3,3,3	0.69	0	2,2,2	0.58	0
2	EDO	B	304	3	3,3,3	0.50	0	2,2,2	0.50	0
2	EDO	D	303	-	3,3,3	0.60	0	2,2,2	0.33	0
2	EDO	F	304	-	3,3,3	0.42	0	2,2,2	0.76	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	E	302	-	-	1/1/1/1	-
2	EDO	D	305	-	-	1/1/1/1	-
2	EDO	C	304	-	-	0/1/1/1	-
2	EDO	A	306	-	-	0/1/1/1	-
2	EDO	D	309	-	-	1/1/1/1	-
2	EDO	E	307	-	-	1/1/1/1	-
8	PEG	D	319	-	-	1/4/4/4	-
2	EDO	A	307	-	-	0/1/1/1	-
2	EDO	F	301	-	-	0/1/1/1	-
8	PEG	D	318	-	-	4/4/4/4	-
2	EDO	D	308	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	F	303	-	-	0/1/1/1	-
2	EDO	D	306	-	-	0/1/1/1	-
2	EDO	E	305	-	-	0/1/1/1	-
2	EDO	A	304	-	-	0/1/1/1	-
2	EDO	C	306	-	-	0/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
6	HIS	F	309	-	-	1/8/8/8	0/1/1/1
5	PGE	A	316	-	-	1/7/7/7	-
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	E	304	-	-	0/1/1/1	-
2	EDO	F	302	-	-	1/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
6	HIS	C	310	-	-	3/8/8/8	0/1/1/1
5	PGE	C	309	-	-	0/7/7/7	-
8	PEG	E	315	-	-	2/4/4/4	-
8	PEG	E	316	-	-	4/4/4/4	-
2	EDO	B	305	-	-	0/1/1/1	-
2	EDO	E	306	-	-	1/1/1/1	-
7	PG4	D	317	-	-	3/10/10/10	-
6	HIS	A	317	-	-	2/8/8/8	0/1/1/1
6	HIS	B	313	-	-	1/8/8/8	0/1/1/1
2	EDO	C	303	-	-	1/1/1/1	-
6	HIS	E	317	-	-	1/8/8/8	0/1/1/1
2	EDO	A	303	-	-	0/1/1/1	-
2	EDO	B	304	3	-	0/1/1/1	-
2	EDO	D	303	-	-	0/1/1/1	-
2	EDO	F	304	-	-	1/1/1/1	-
6	HIS	D	321	-	-	1/8/8/8	0/1/1/1
2	EDO	A	305	-	-	0/1/1/1	-
5	PGE	B	312	-	-	3/7/7/7	-
5	PGE	D	316	-	-	2/7/7/7	-
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	D	301	-	-	0/1/1/1	-
2	EDO	D	302	-	-	0/1/1/1	-
5	PGE	E	313	-	-	3/7/7/7	-
2	EDO	E	303	-	-	1/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
5	PGE	B	311	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	E	314	-	-	2/7/7/7	-
2	EDO	C	305	-	-	0/1/1/1	-
2	EDO	E	301	-	-	0/1/1/1	-
2	EDO	D	307	-	-	1/1/1/1	-
5	PGE	E	312	-	-	0/7/7/7	-
8	PEG	D	320	-	-	2/4/4/4	-
2	EDO	D	304	-	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	308	ACT	CH3-C	3.78	1.65	1.49
4	A	315	ACT	CH3-C	3.28	1.62	1.49
4	A	314	ACT	CH3-C	3.26	1.62	1.49
4	E	310	ACT	CH3-C	2.86	1.61	1.49
6	C	310	HIS	OXT-C	-2.74	1.21	1.30
4	B	308	ACT	CH3-C	2.70	1.60	1.49
4	F	307	ACT	CH3-C	2.68	1.60	1.49
4	E	311	ACT	CH3-C	2.61	1.60	1.49
4	D	313	ACT	CH3-C	2.46	1.59	1.49
4	F	306	ACT	CH3-C	2.42	1.59	1.49
4	D	315	ACT	CH3-C	2.25	1.58	1.49
4	B	309	ACT	CH3-C	2.19	1.58	1.49
4	D	314	ACT	CH3-C	2.19	1.58	1.49
4	A	313	ACT	CH3-C	2.11	1.58	1.49
6	F	309	HIS	OXT-C	-2.11	1.23	1.30
7	D	317	PG4	O4-C6	2.03	1.50	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	310	HIS	OXT-C-O	-3.11	117.03	124.09
7	D	317	PG4	C5-O3-C4	3.09	126.69	113.29
6	E	317	HIS	OXT-C-O	-2.93	117.44	124.09
8	E	316	PEG	O2-C3-C4	-2.92	97.22	110.07
6	D	321	HIS	OXT-C-O	-2.81	117.70	124.09
7	D	317	PG4	O4-C6-C5	2.71	122.63	110.39
7	D	317	PG4	C7-O4-C6	2.69	124.93	113.29
6	B	313	HIS	OXT-C-O	-2.58	118.24	124.09
6	F	309	HIS	OXT-C-O	-2.54	118.32	124.09
6	B	313	HIS	OXT-C-CA	2.37	121.45	113.38
8	E	316	PEG	O4-C4-C3	-2.28	98.56	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	314	ACT	O-C-CH3	-2.24	113.61	122.33
6	C	310	HIS	CD2-NE2-CE1	2.12	109.08	105.78
6	C	310	HIS	OXT-C-CA	2.11	120.58	113.38
6	A	317	HIS	OXT-C-O	-2.09	119.34	124.09
6	F	309	HIS	OXT-C-CA	2.08	120.47	113.38
4	A	313	ACT	O-C-CH3	-2.03	114.42	122.33
6	D	321	HIS	CD2-NE2-CE1	2.03	108.95	105.78
6	B	313	HIS	CD2-NE2-CE1	2.01	108.92	105.78
6	A	317	HIS	CD2-NE2-CE1	2.01	108.91	105.78
6	F	309	HIS	CD2-NE2-CE1	2.00	108.90	105.78

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	317	HIS	CA-CB-CG-ND1
6	C	310	HIS	CA-CB-CG-ND1
6	D	321	HIS	CA-CB-CG-ND1
6	E	317	HIS	CA-CB-CG-ND1
6	F	309	HIS	CA-CB-CG-ND1
8	E	316	PEG	C1-C2-O2-C3
5	E	313	PGE	O3-C5-C6-O4
5	B	312	PGE	O1-C1-C2-O2
5	E	314	PGE	O1-C1-C2-O2
5	B	311	PGE	O3-C5-C6-O4
8	E	315	PEG	O1-C1-C2-O2
5	A	316	PGE	O3-C5-C6-O4
8	E	316	PEG	O2-C3-C4-O4
2	E	307	EDO	O1-C1-C2-O2
8	D	319	PEG	C1-C2-O2-C3
5	B	311	PGE	O2-C3-C4-O3
5	E	314	PGE	O3-C5-C6-O4
7	D	317	PG4	O4-C7-C8-O5
8	D	318	PEG	O1-C1-C2-O2
8	D	320	PEG	O2-C3-C4-O4
5	B	312	PGE	C4-C3-O2-C2
2	E	302	EDO	O1-C1-C2-O2
8	D	318	PEG	C1-C2-O2-C3
8	E	316	PEG	C4-C3-O2-C2
5	E	313	PGE	C1-C2-O2-C3
5	D	316	PGE	C3-C4-O3-C5
5	D	316	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
8	E	316	PEG	O1-C1-C2-O2
2	E	306	EDO	O1-C1-C2-O2
6	C	310	HIS	N-CA-CB-CG
8	D	318	PEG	O2-C3-C4-O4
2	A	302	EDO	O1-C1-C2-O2
2	C	303	EDO	O1-C1-C2-O2
2	F	304	EDO	O1-C1-C2-O2
5	E	313	PGE	C3-C4-O3-C5
5	B	312	PGE	C6-C5-O3-C4
7	D	317	PG4	C5-C6-O4-C7
7	D	317	PG4	C3-C4-O3-C5
6	B	313	HIS	O-C-CA-N
8	D	320	PEG	C4-C3-O2-C2
2	C	302	EDO	O1-C1-C2-O2
2	D	309	EDO	O1-C1-C2-O2
6	C	310	HIS	C-CA-CB-CG
8	E	315	PEG	C1-C2-O2-C3
2	A	301	EDO	O1-C1-C2-O2
2	D	305	EDO	O1-C1-C2-O2
2	E	303	EDO	O1-C1-C2-O2
2	F	302	EDO	O1-C1-C2-O2
6	A	317	HIS	CA-CB-CG-CD2
2	D	307	EDO	O1-C1-C2-O2
8	D	318	PEG	C4-C3-O2-C2

There are no ring outliers.

25 monomers are involved in 44 short contacts:

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

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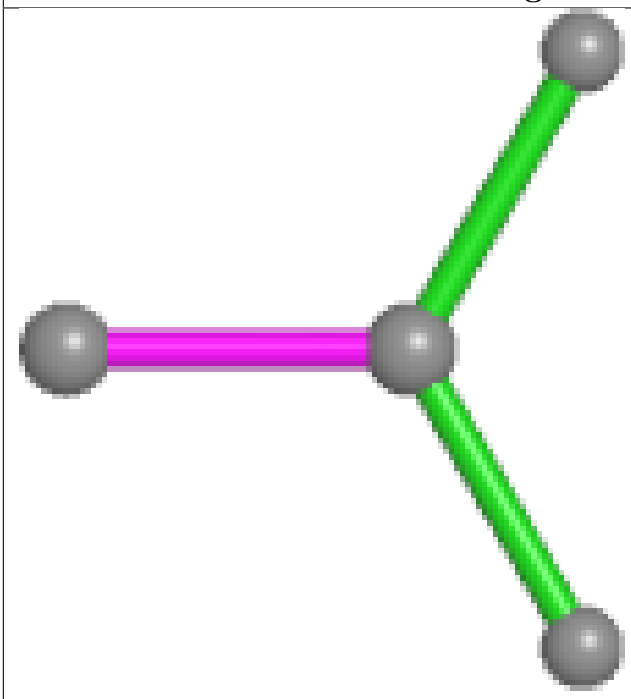
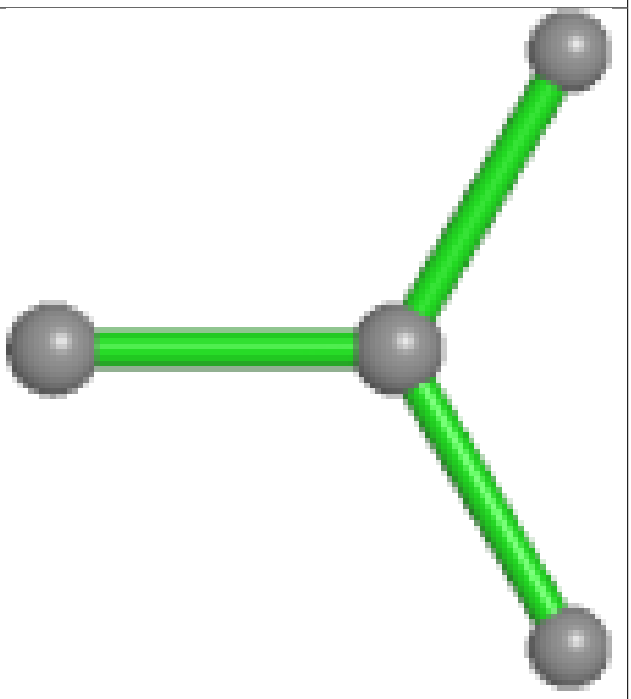
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	317	HIS	1	0
2	C	303	EDO	1	0
6	E	317	HIS	1	0
2	B	304	EDO	5	0
6	D	321	HIS	2	0
5	D	316	PGE	1	0
2	C	302	EDO	4	0
4	D	313	ACT	1	0
5	E	314	PGE	1	0
2	C	305	EDO	1	0
4	C	308	ACT	1	0
8	D	320	PEG	2	0

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

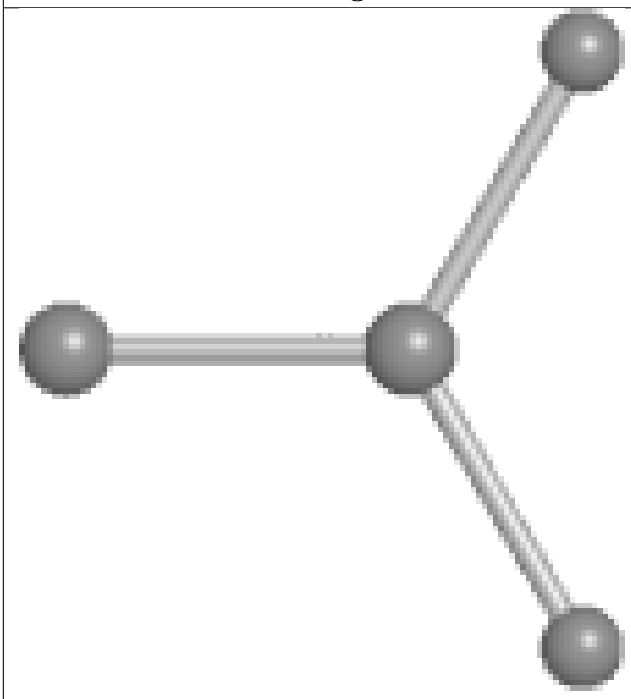
Ligand ACT F 308



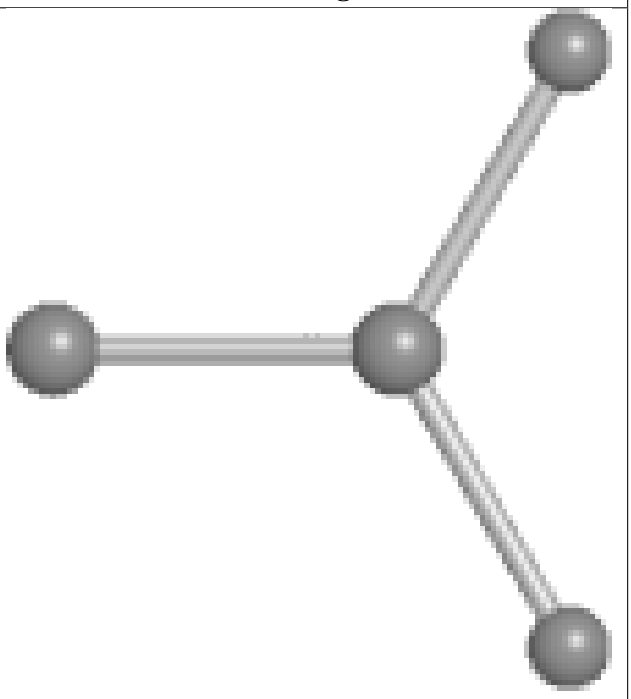
Bond lengths



Bond angles

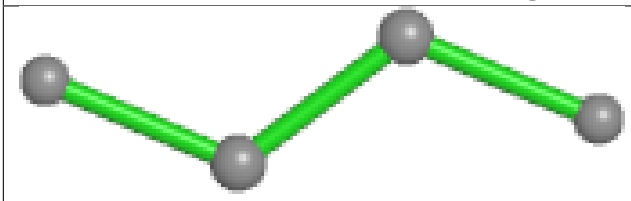


Torsions



Rings

Ligand EDO E 302



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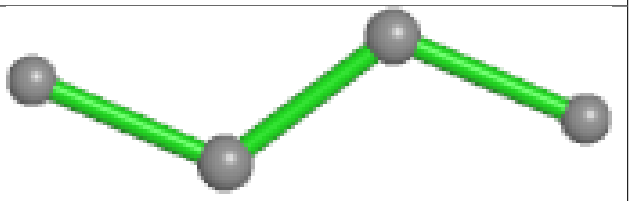
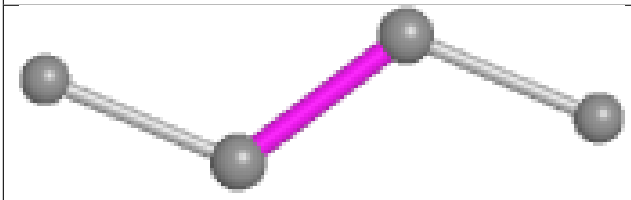
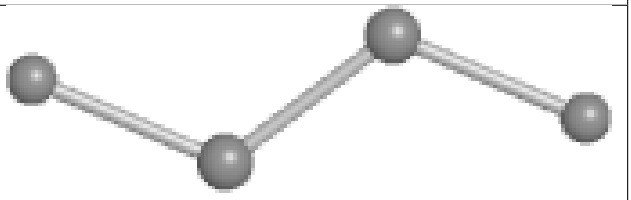


Bond angles

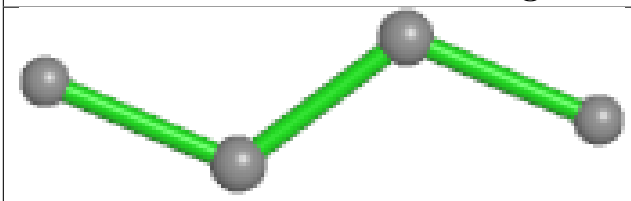


Torsions

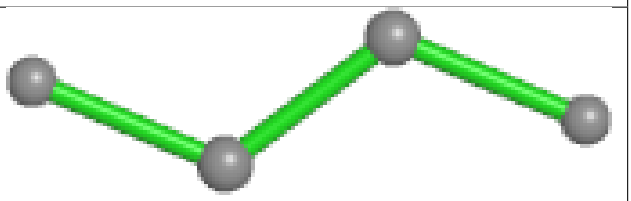


Rings

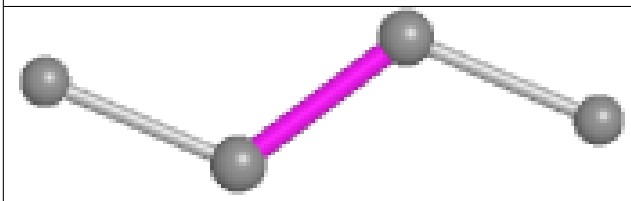
Ligand EDO D 305



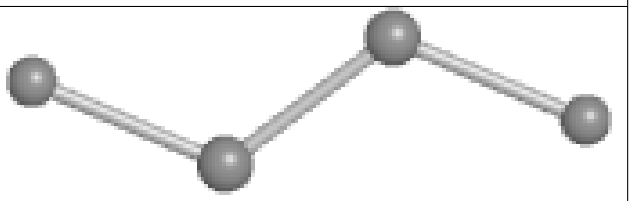
Bond lengths



Bond angles

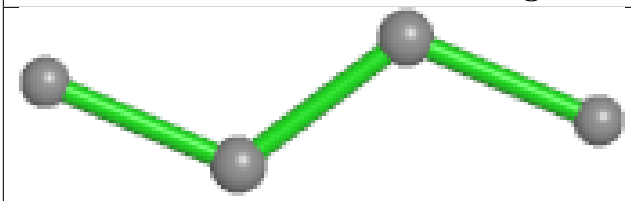


Torsions

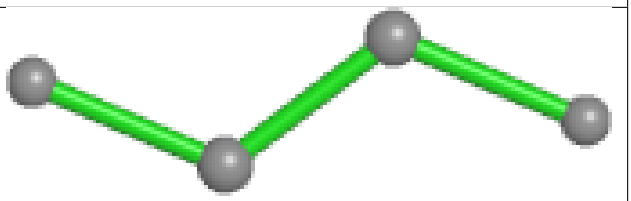


Rings

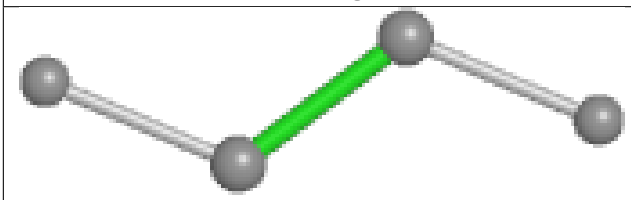
Ligand EDO C 304



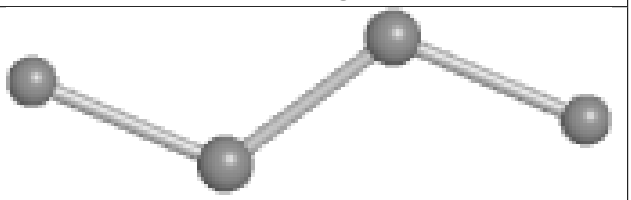
Bond lengths



Bond angles

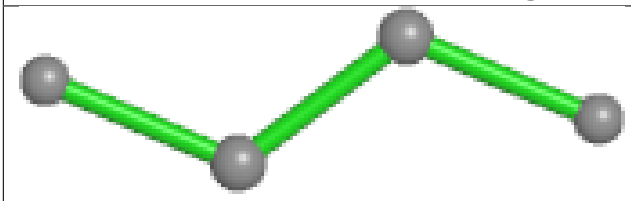


Torsions



Rings

Ligand EDO A 306



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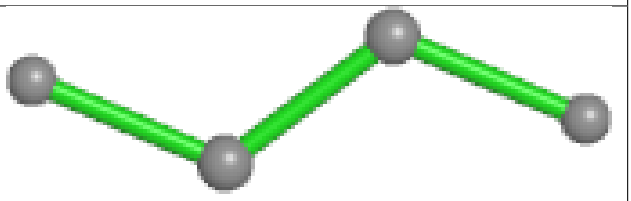

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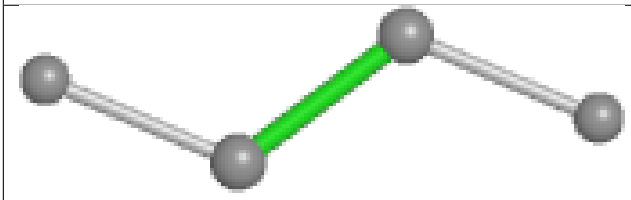

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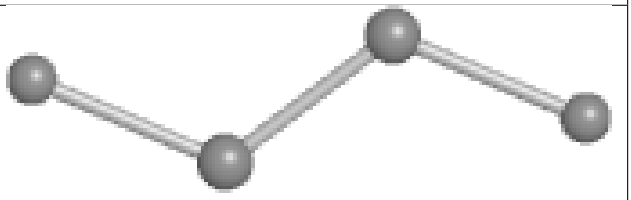
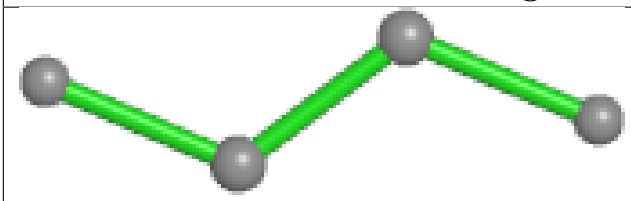


Rings

Ligand EDO D 309



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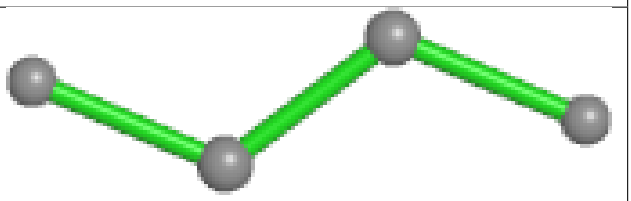

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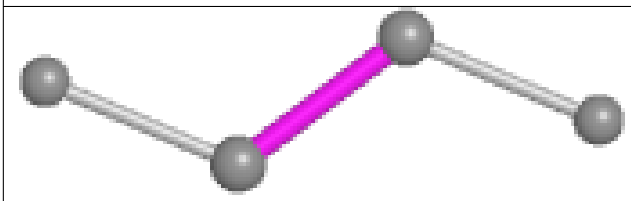

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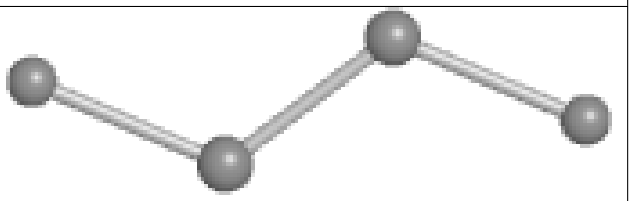
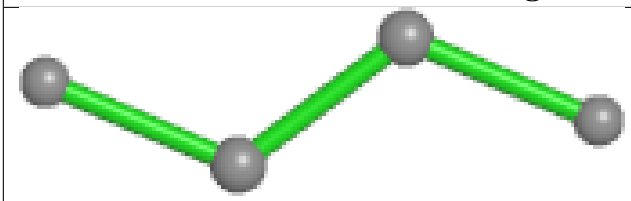


Rings

Ligand EDO E 307



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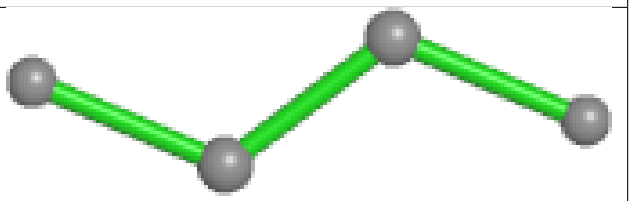

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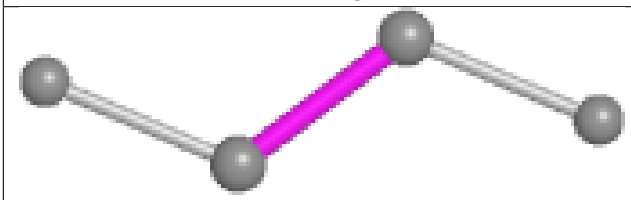

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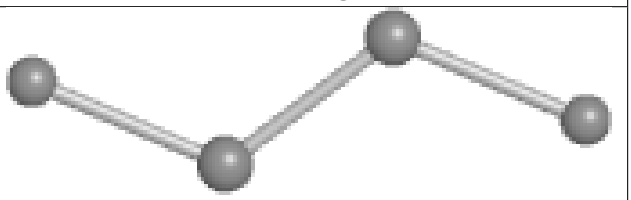
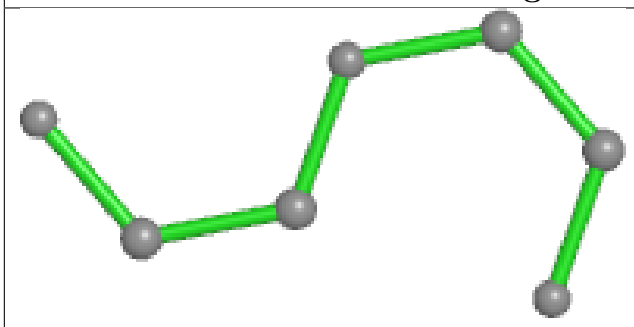


Rings

Ligand PEG D 319



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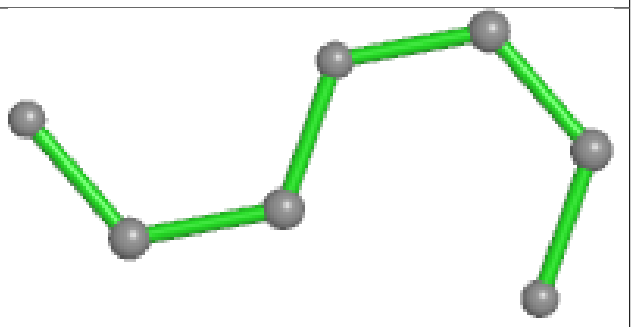

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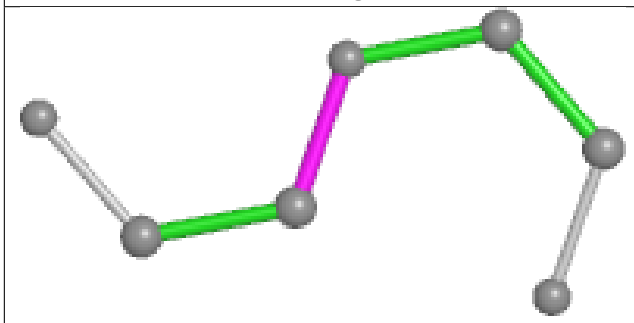

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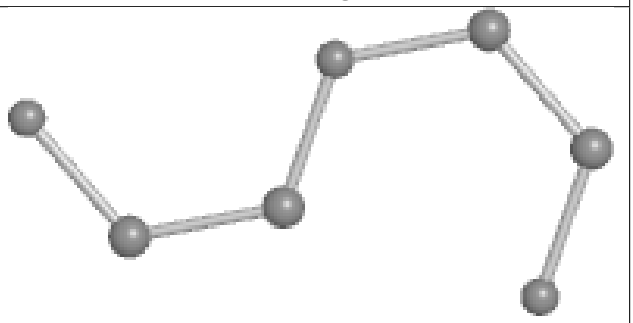
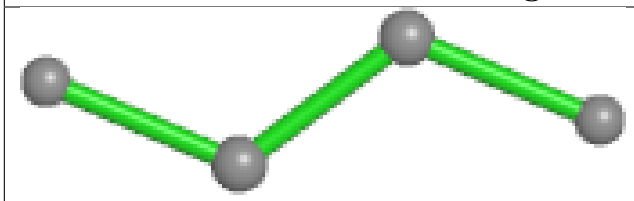
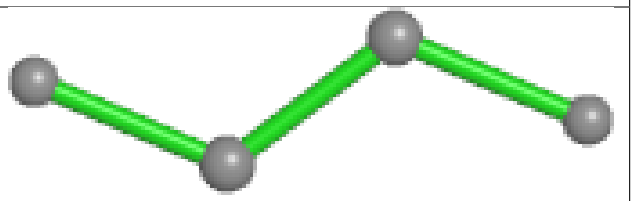


Rings

Ligand EDO A 307



Bond lengths



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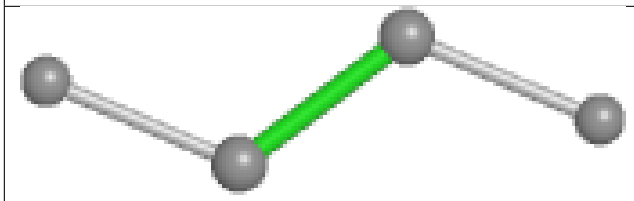

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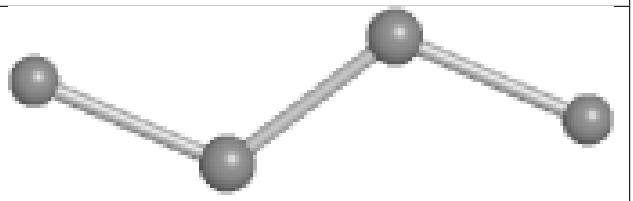
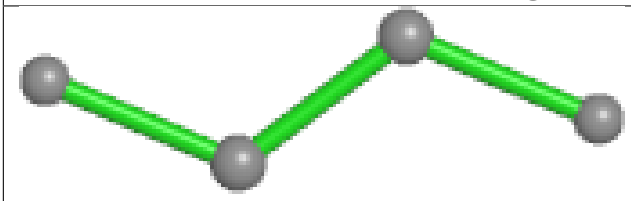


Rings

Ligand EDO F 301



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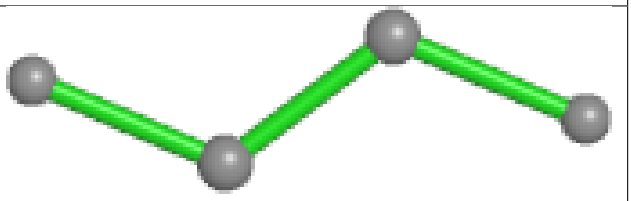
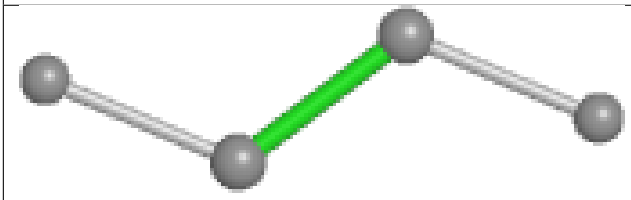


Bond angles



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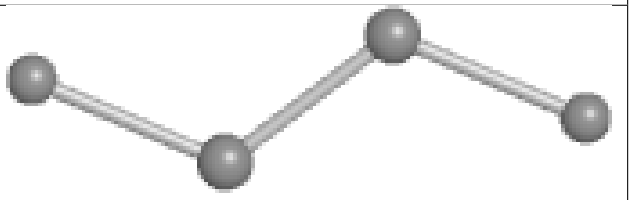
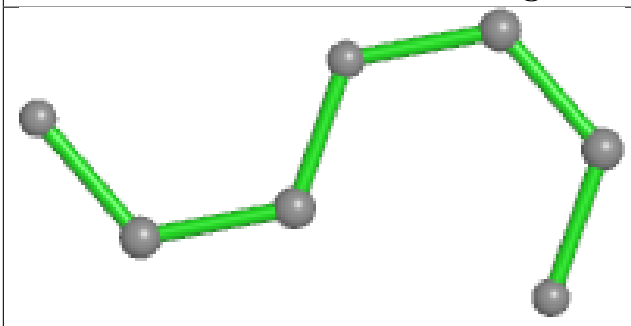


Rings

Ligand PEG D 318



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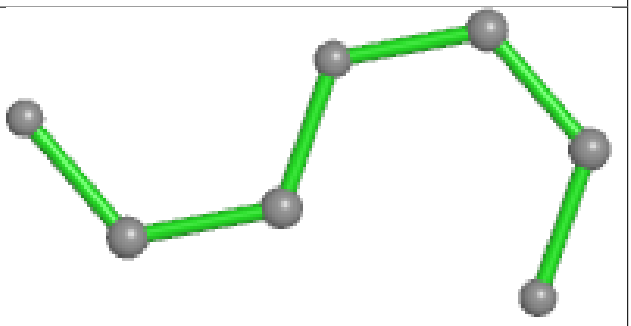
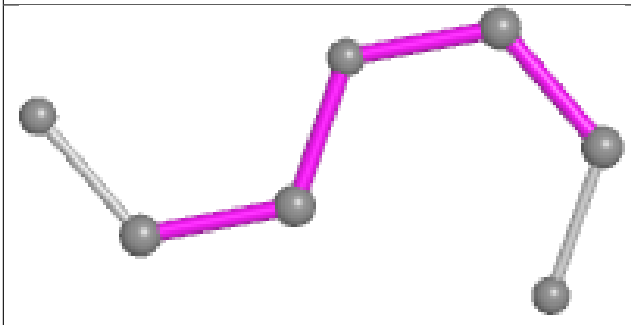


Bond angles



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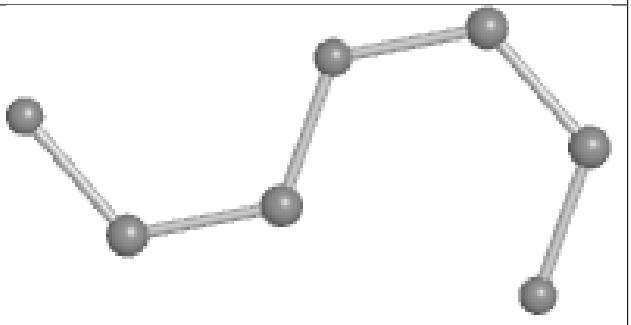
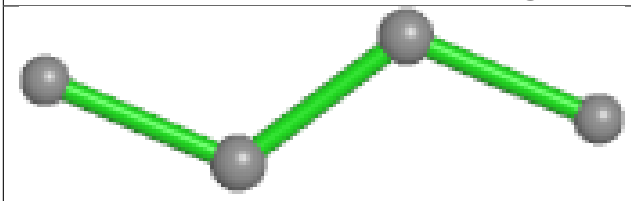
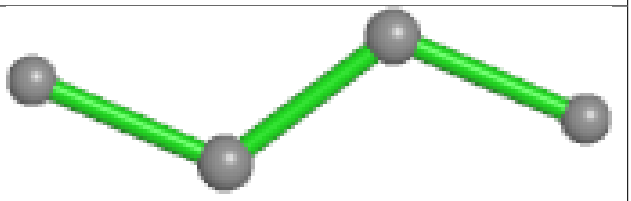
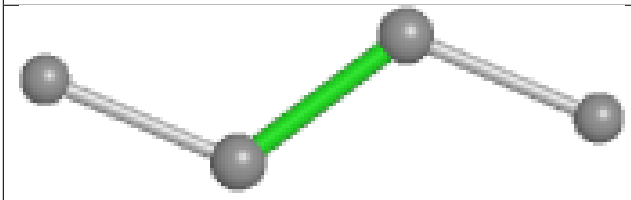
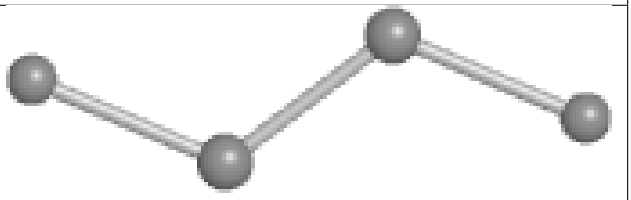
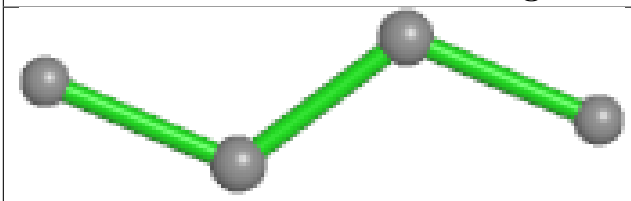
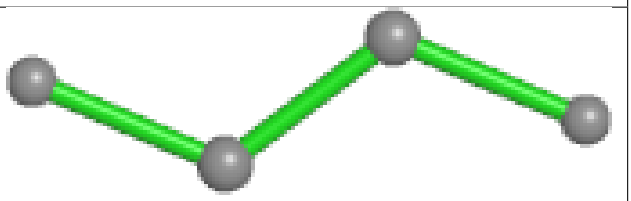
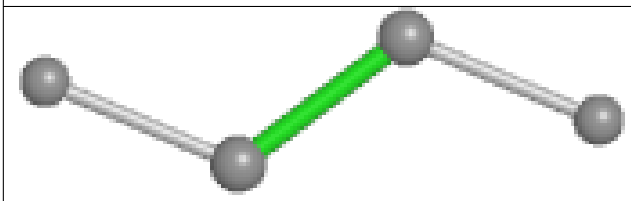
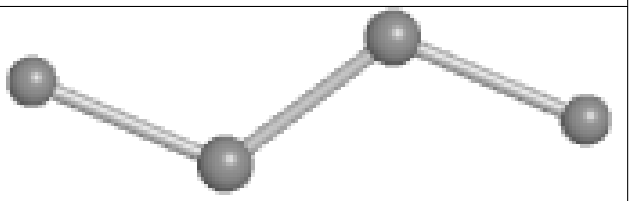
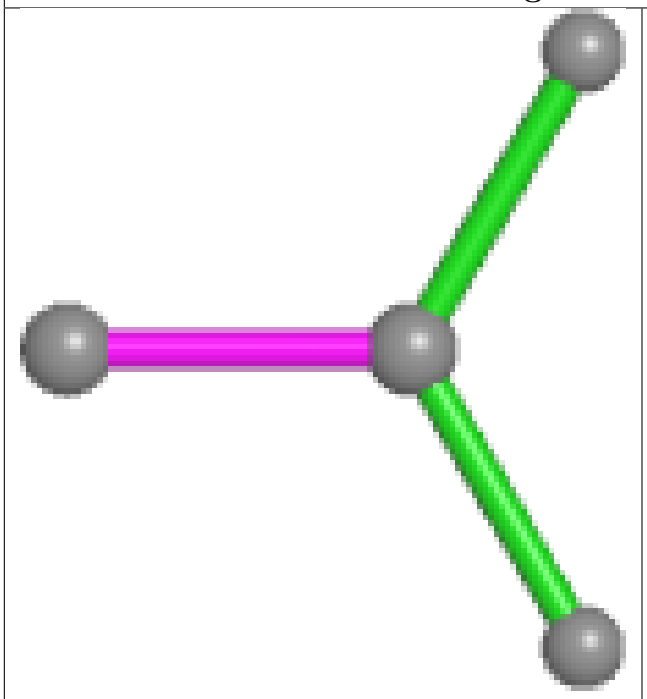


Rings

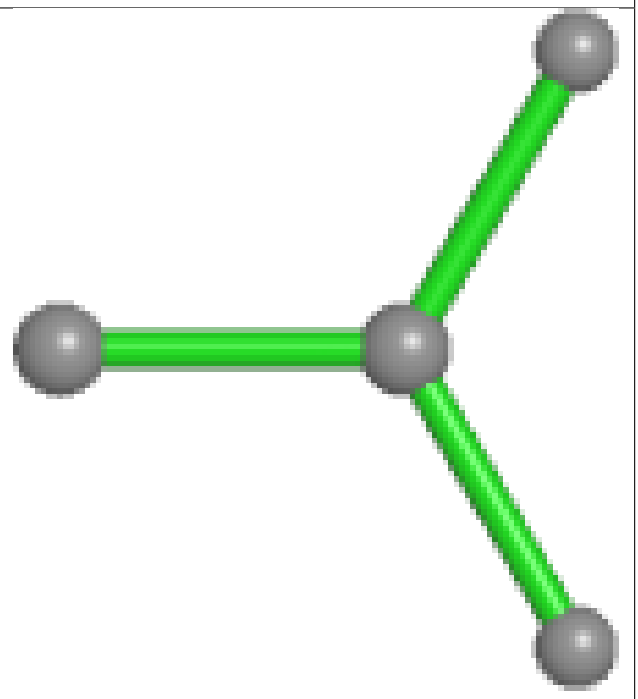
Ligand EDO D 308	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand EDO B 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

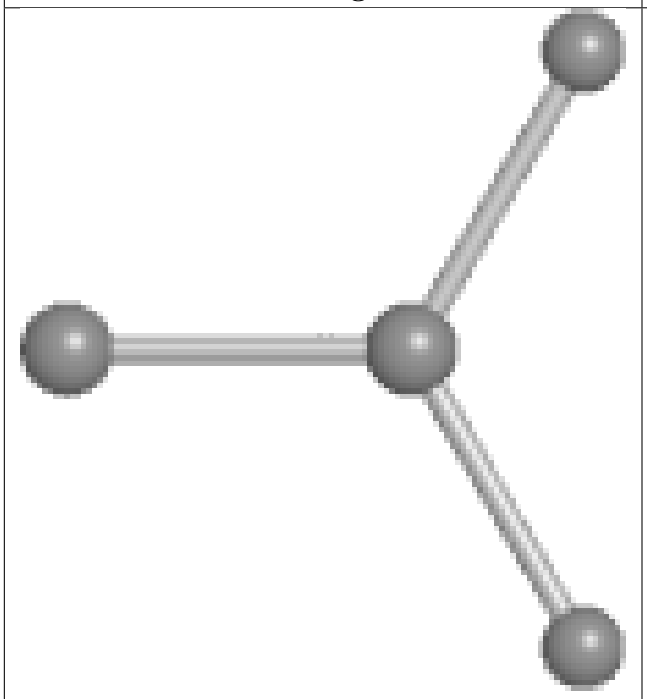
Ligand ACT B 308



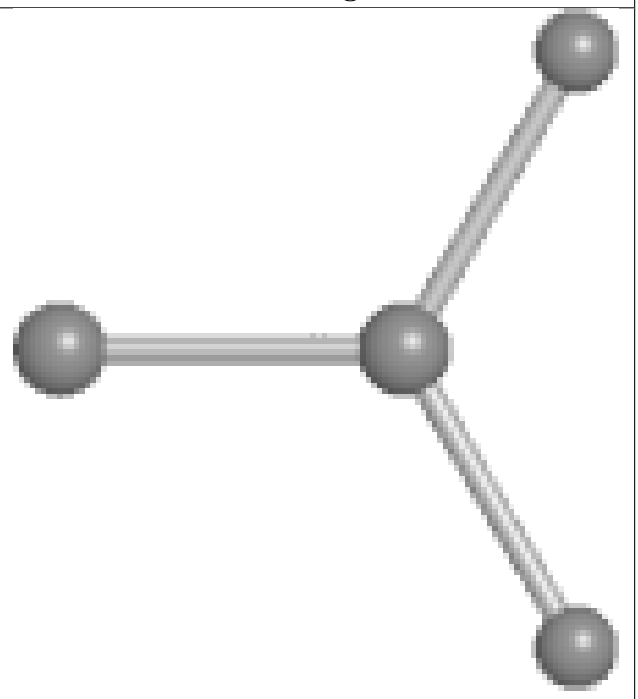
Bond lengths



Bond angles

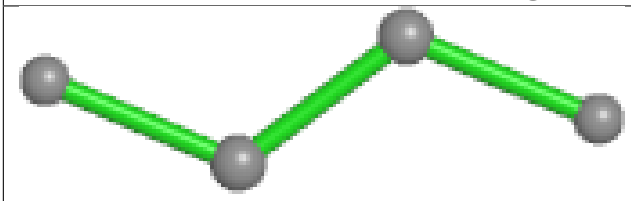


Torsions



Rings

Ligand EDO F 303



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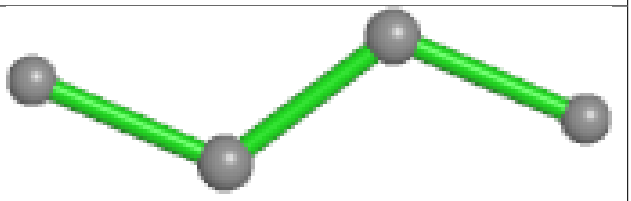
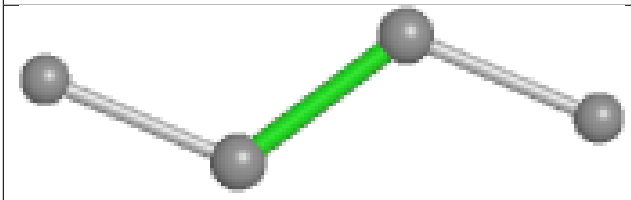
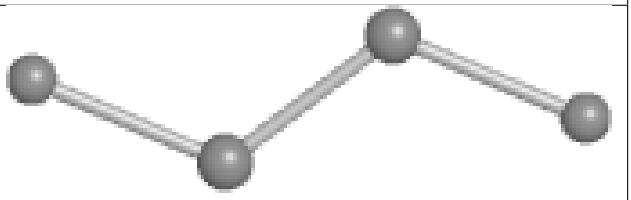


Bond angles

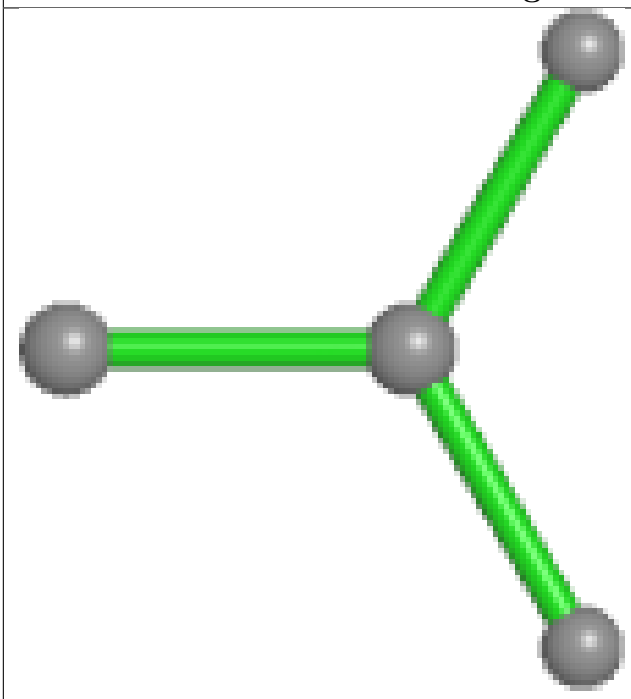


Torsions

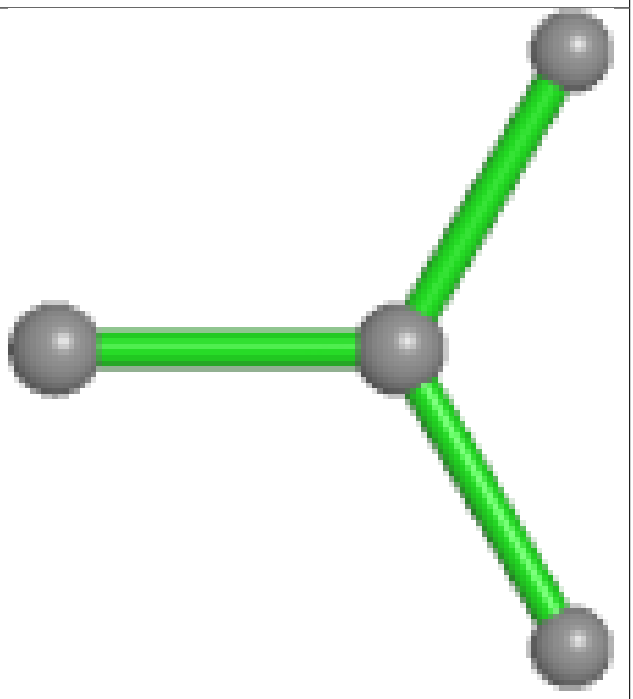


Rings

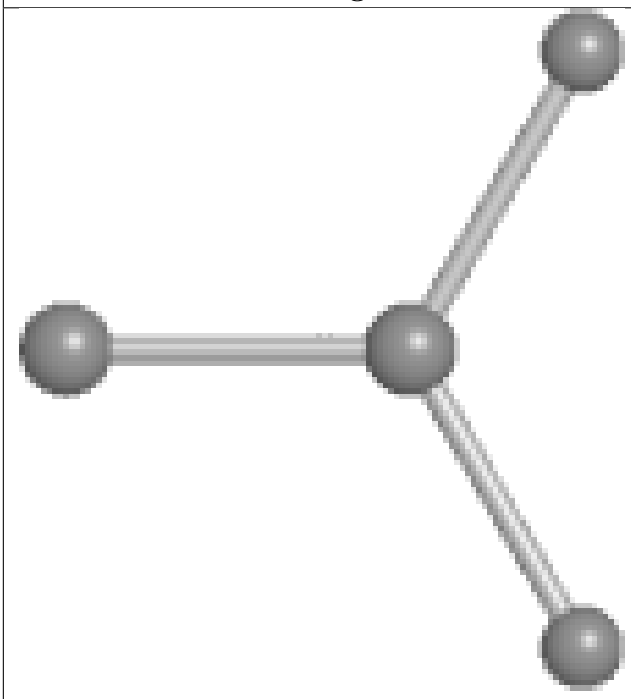
Ligand ACT B 310



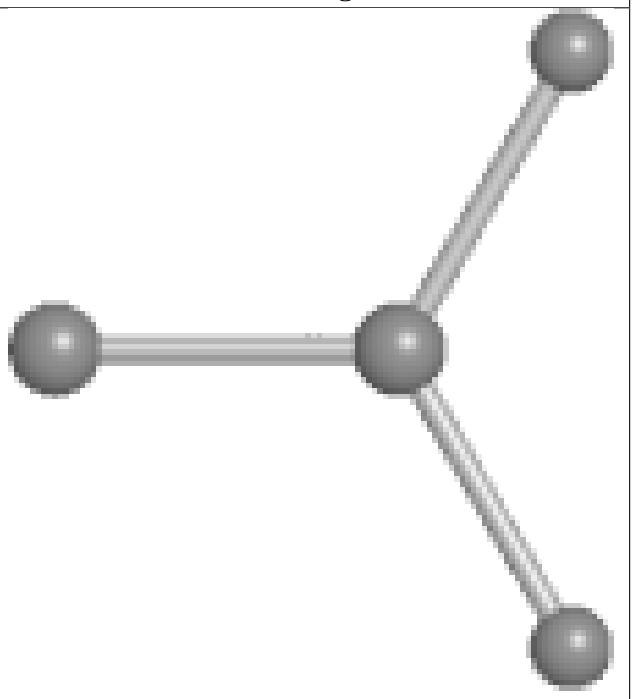
Bond lengths



Bond angles

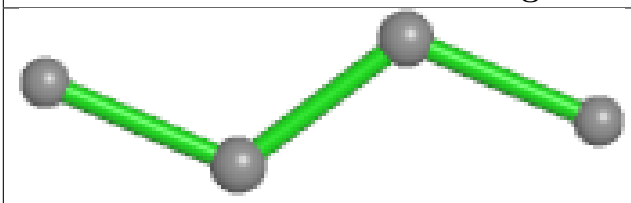


Torsions



Rings

Ligand EDO D 306



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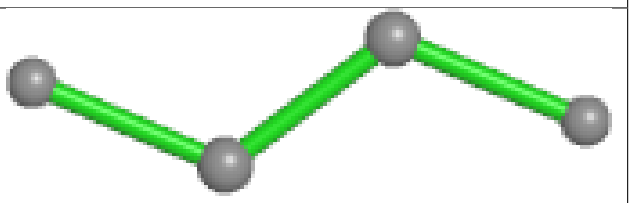
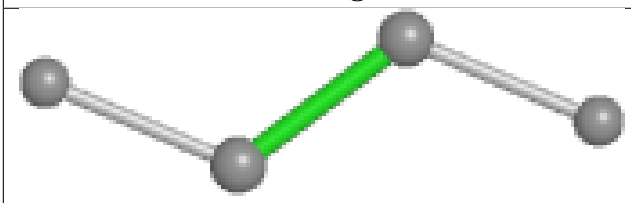


Bond angles



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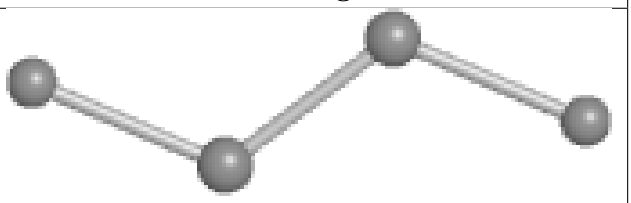
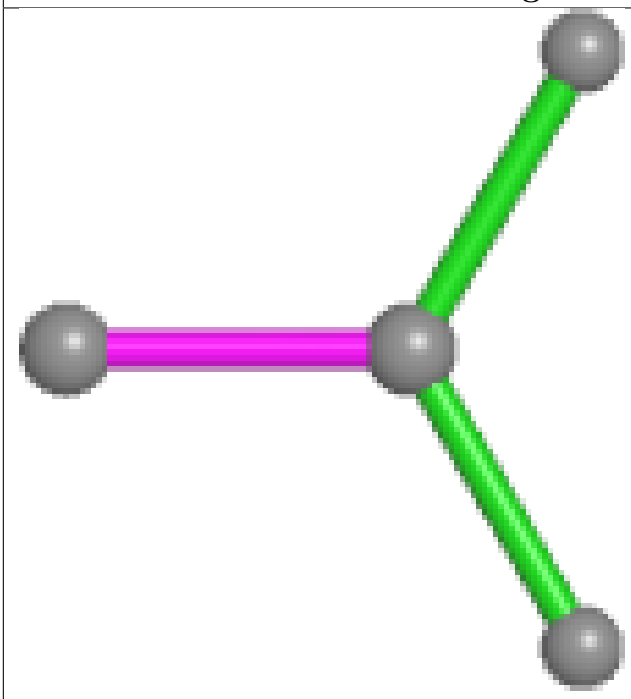


Rings

Ligand ACT D 314



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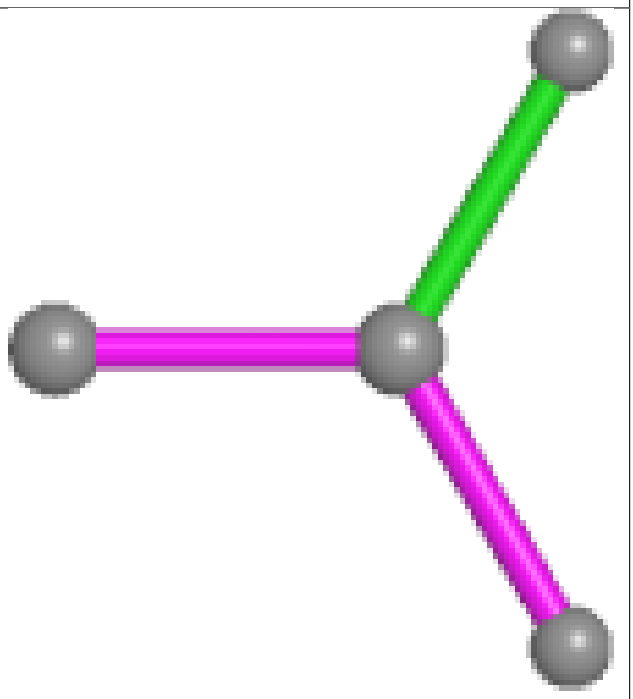
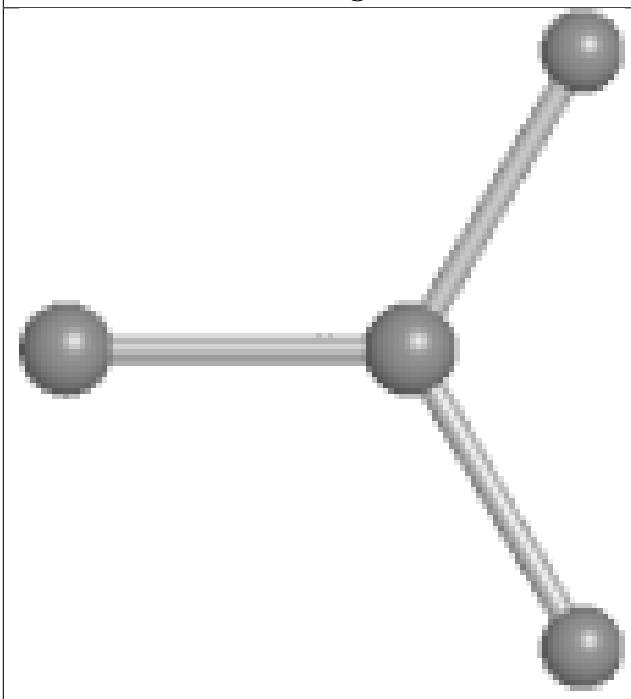


Bond angles



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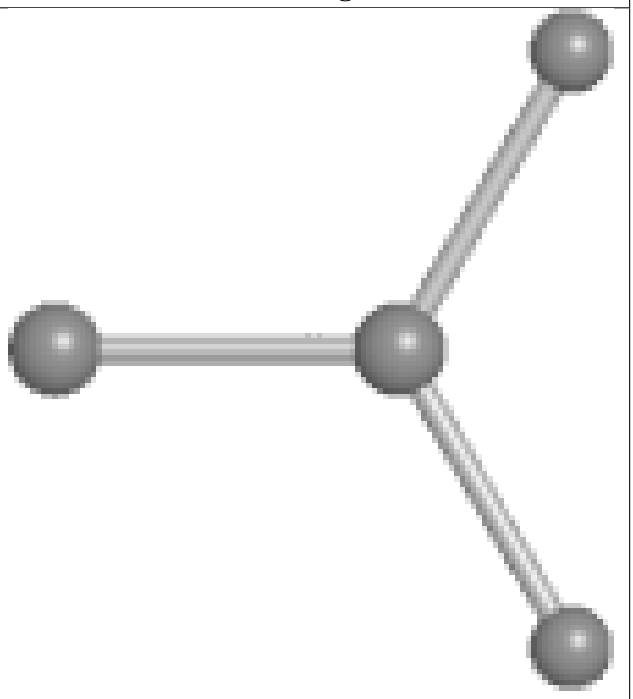
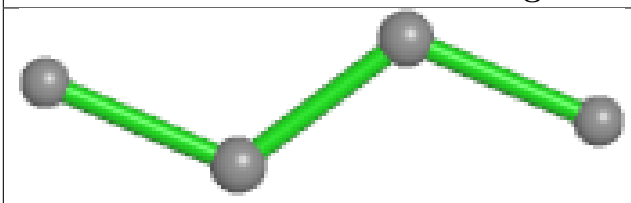
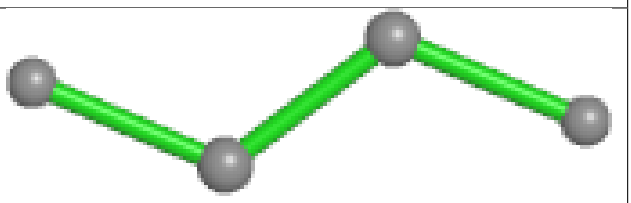


Rings

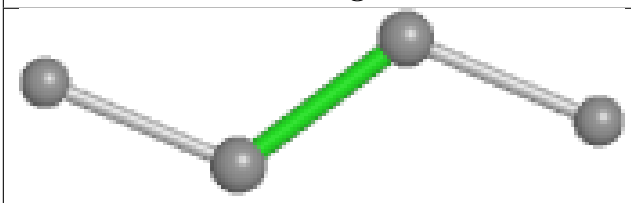
Ligand EDO E 305



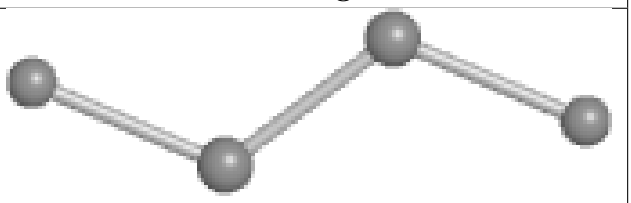
Bond lengths



Bond angles

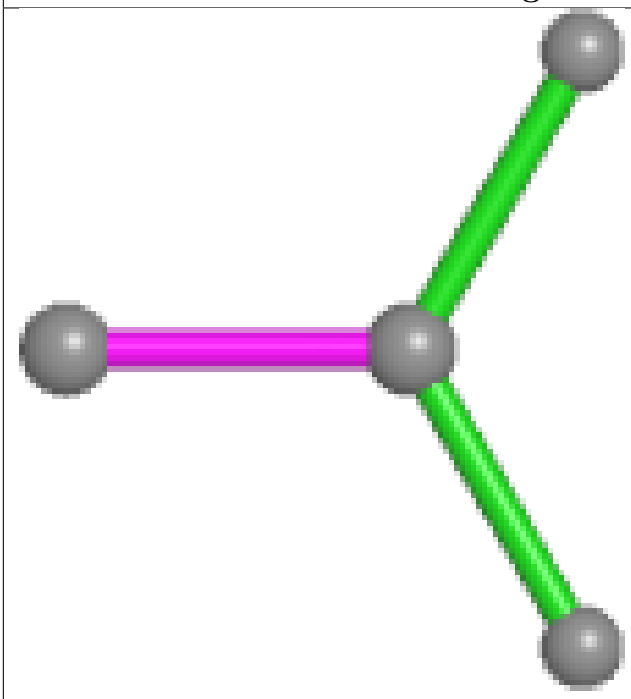


Torsions



Rings

Ligand ACT A 313



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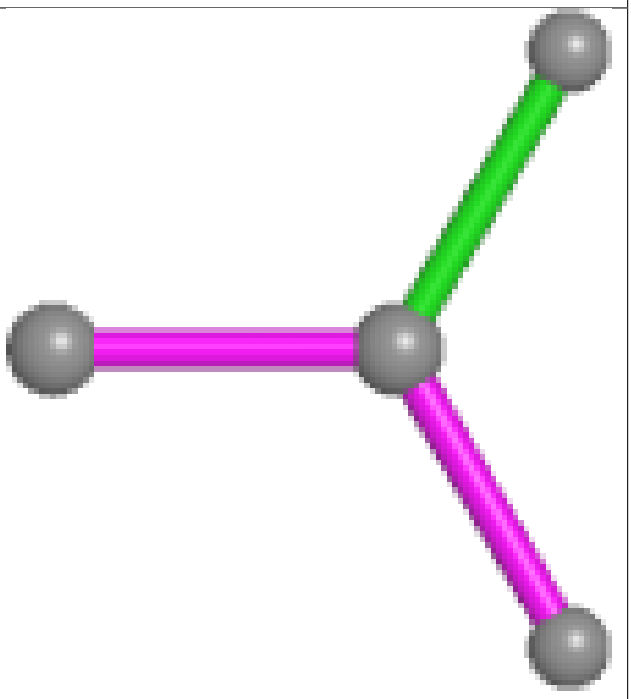
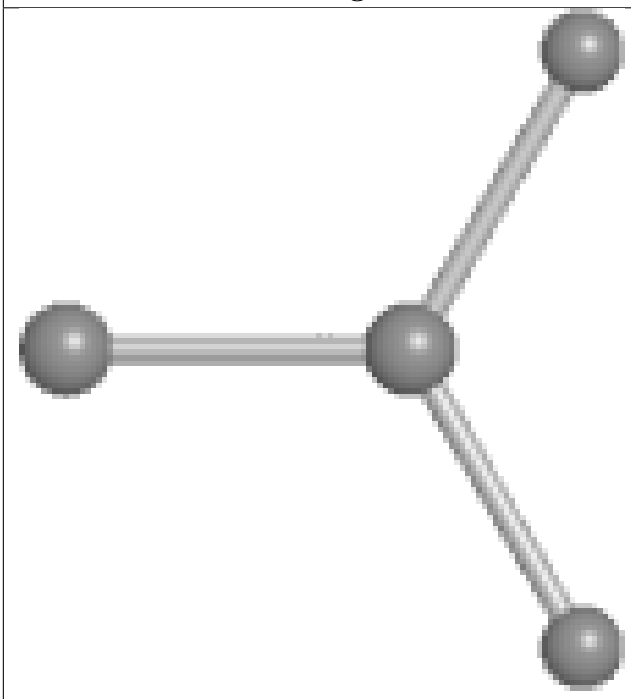
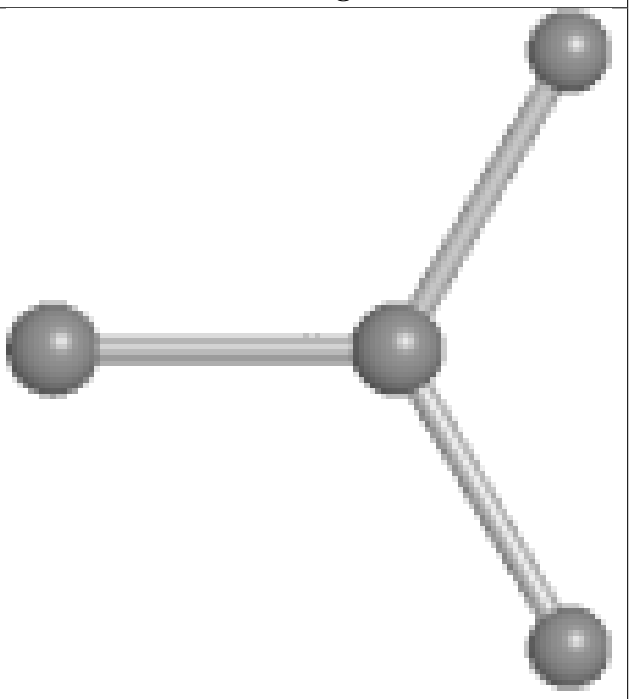


Bond angles

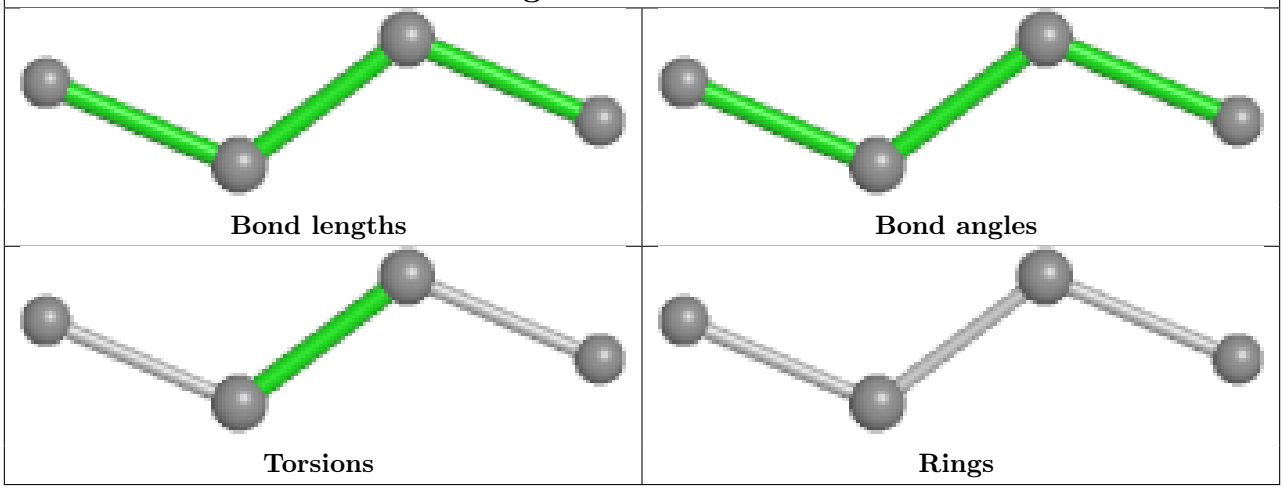


Torsions

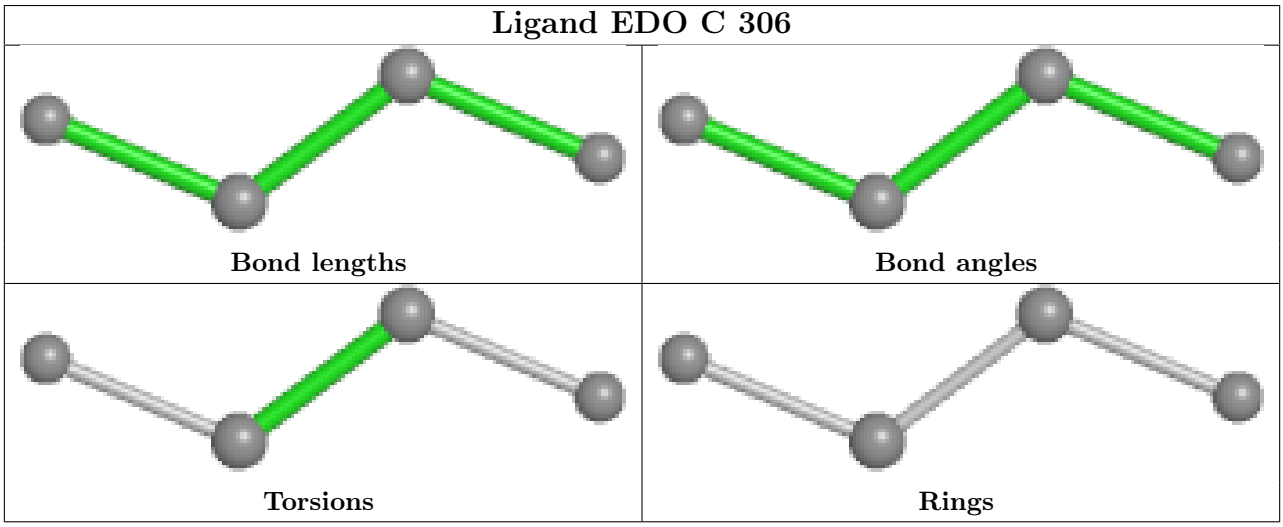


Rings

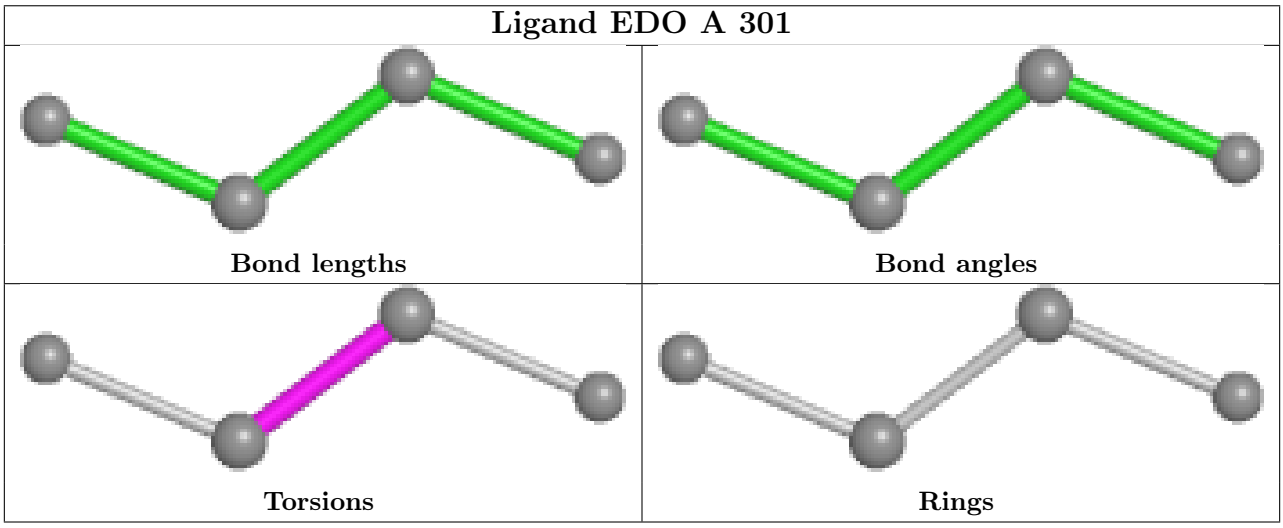
Ligand EDO A 304



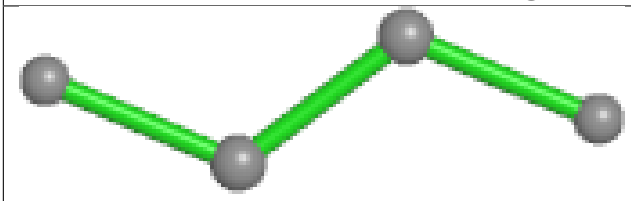
Ligand EDO C 306



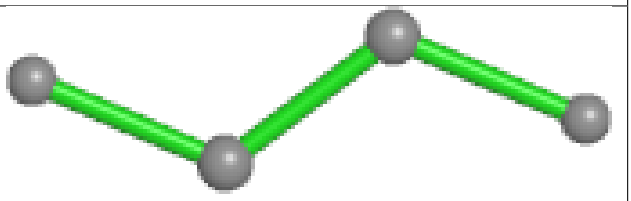
Ligand EDO A 301



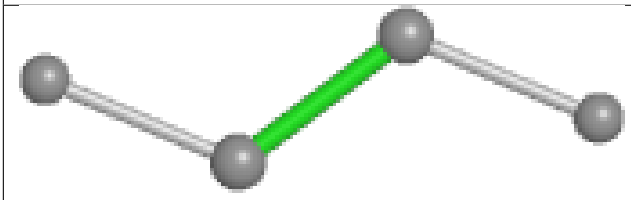
Ligand EDO B 303



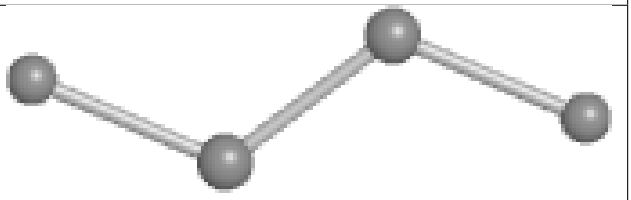
Bond lengths



Bond angles

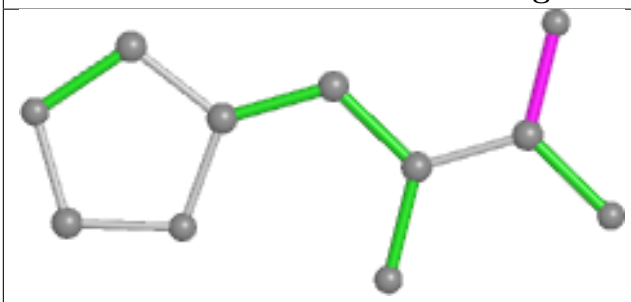


Torsions

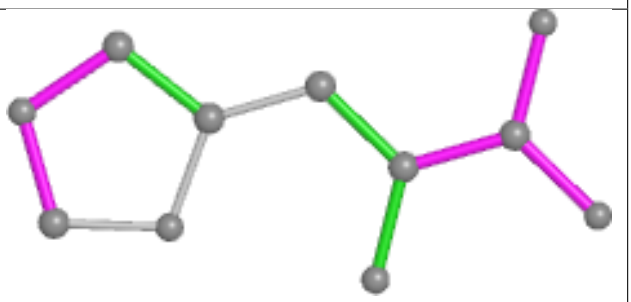


Rings

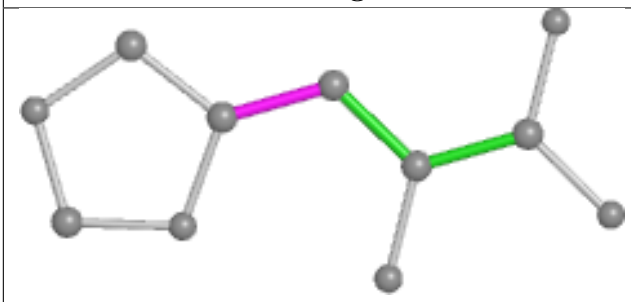
Ligand HIS F 309



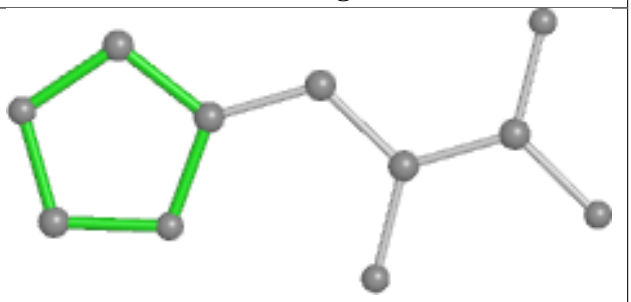
Bond lengths



Bond angles

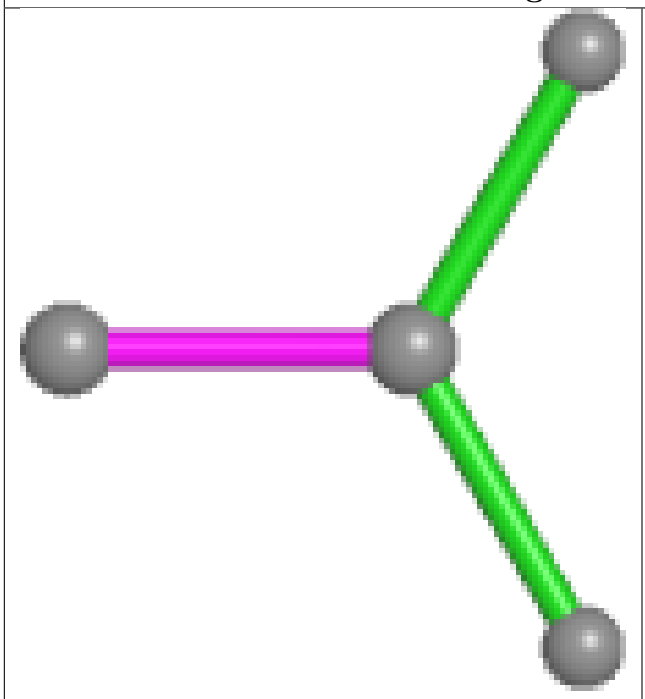


Torsions

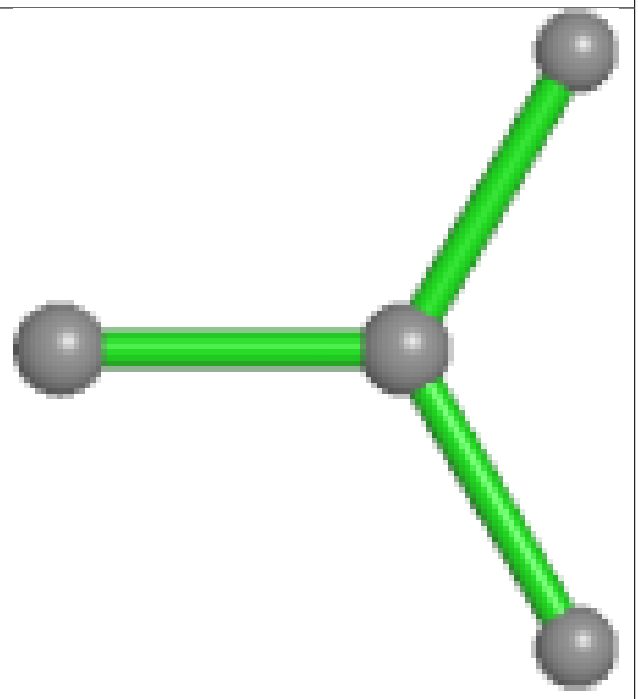


Rings

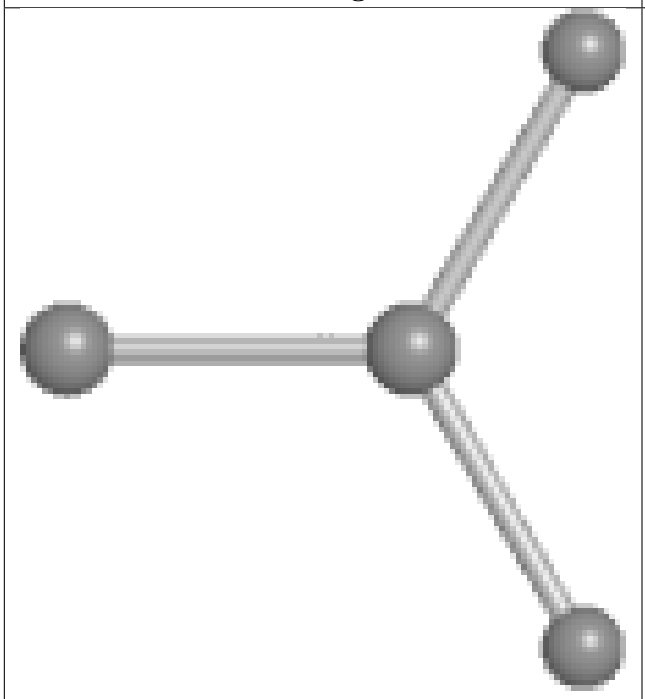
Ligand ACT F 306



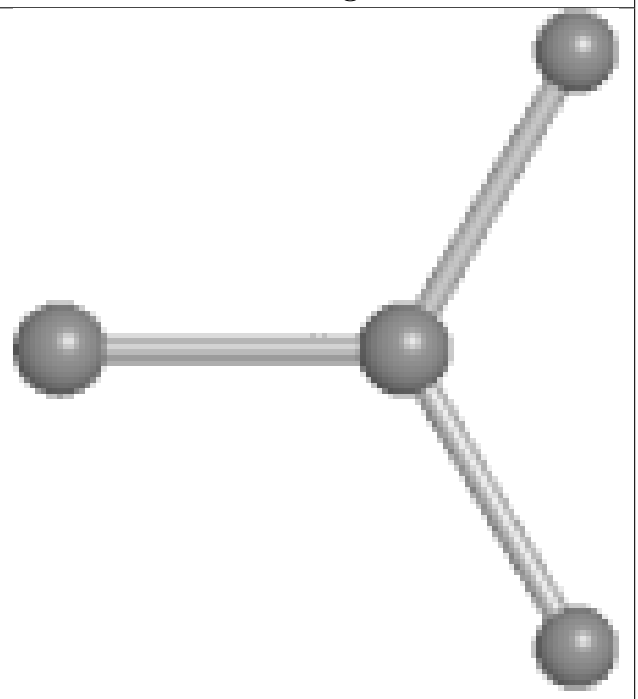
Bond lengths



Bond angles

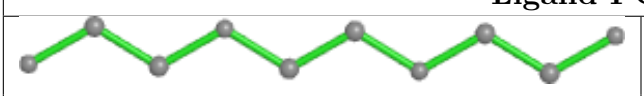


Torsions

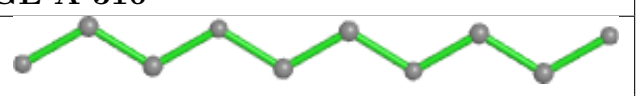


Rings

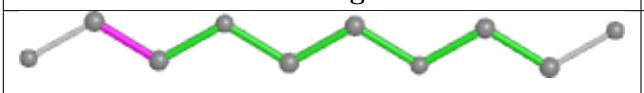
Ligand PGE A 316



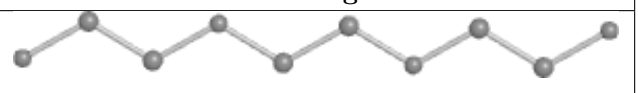
Bond lengths



Bond angles

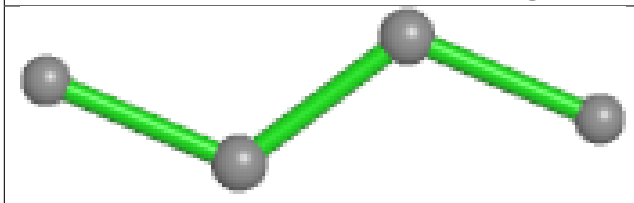


Torsions



Rings

Ligand EDO C 301



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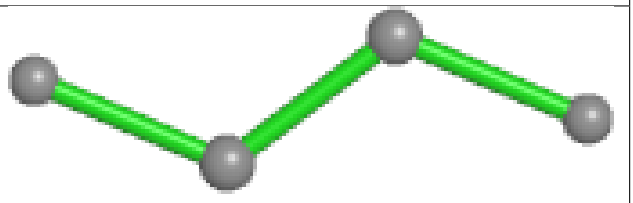
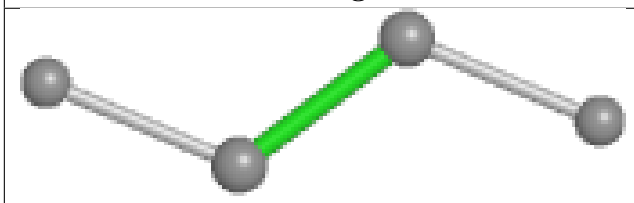
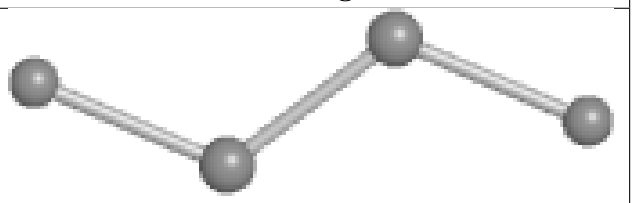


Bond angles

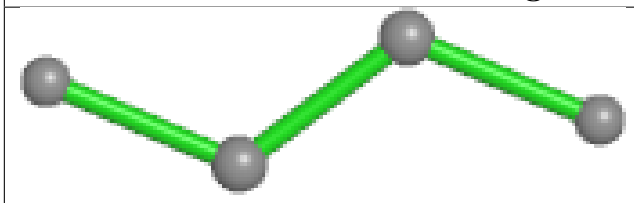


Torsions

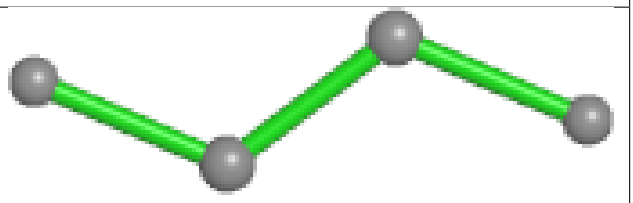


Rings

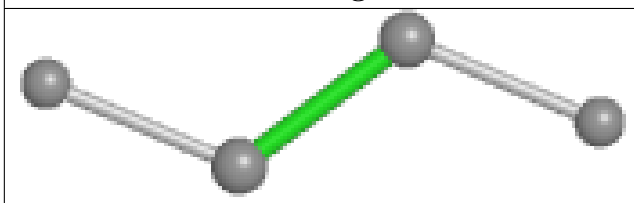
Ligand EDO E 304



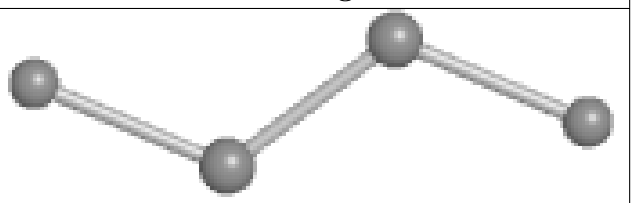
Bond lengths



Bond angles

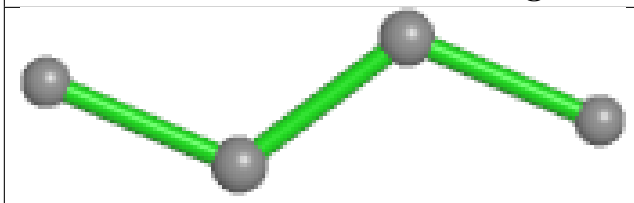


Torsions

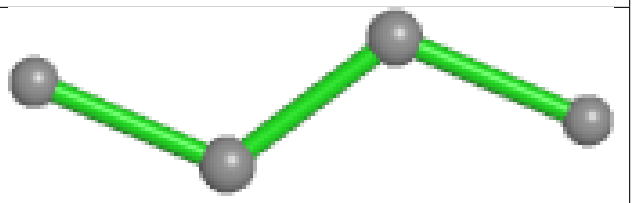


Rings

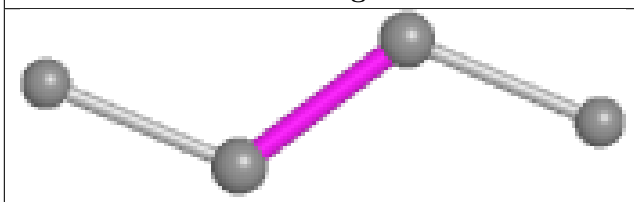
Ligand EDO F 302



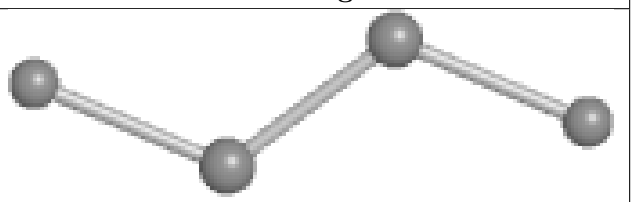
Bond lengths



Bond angles

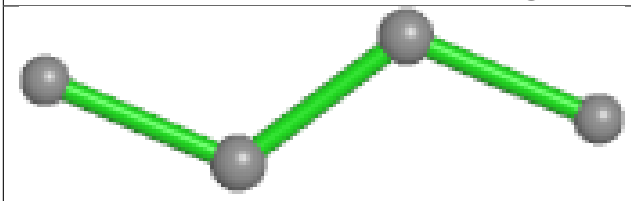


Torsions



Rings

Ligand EDO B 302



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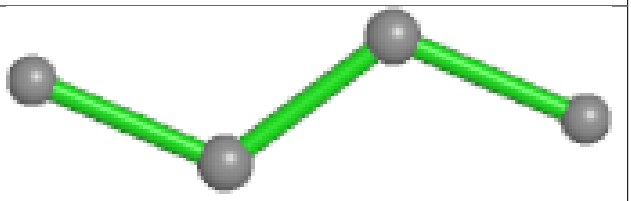
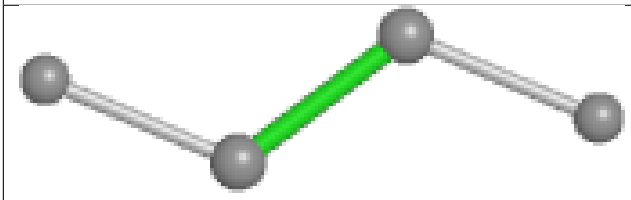
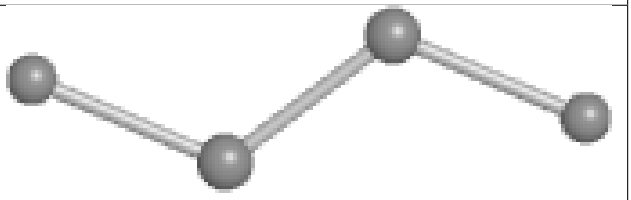


Bond angles

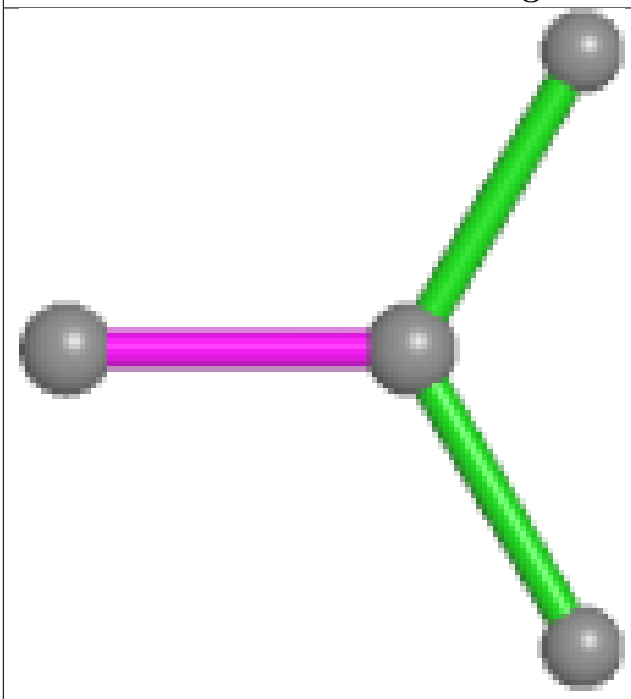


Torsions

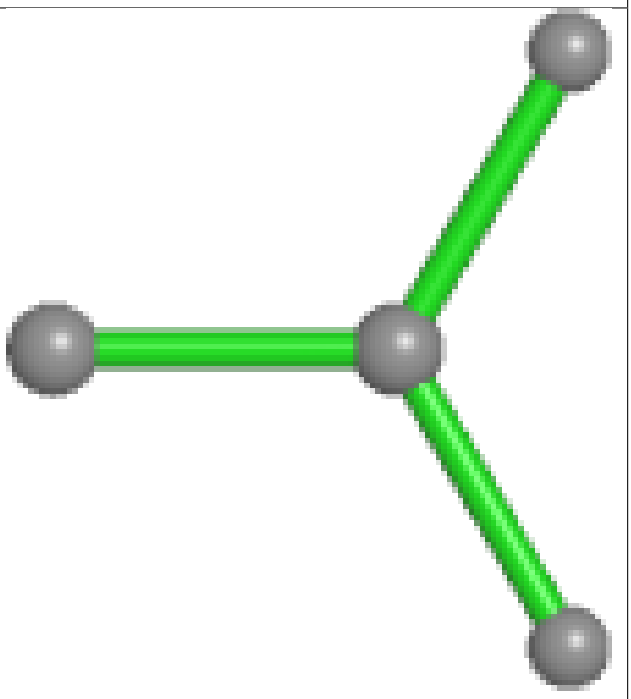


Rings

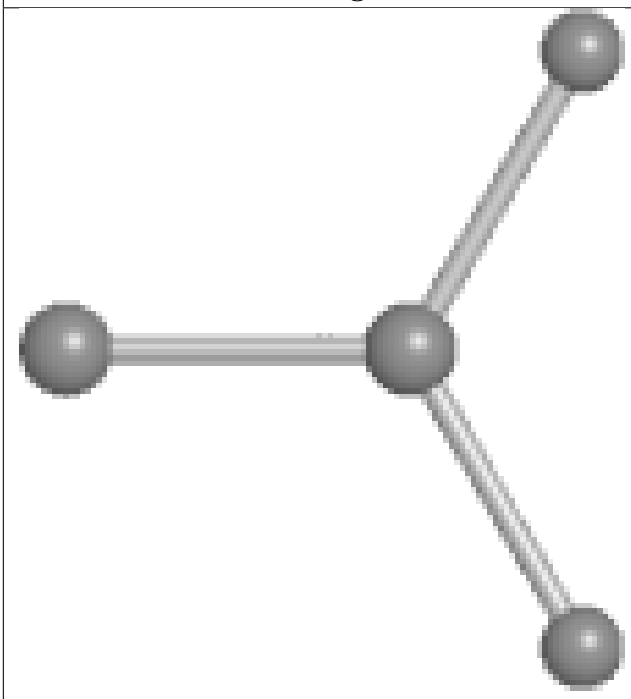
Ligand ACT A 314



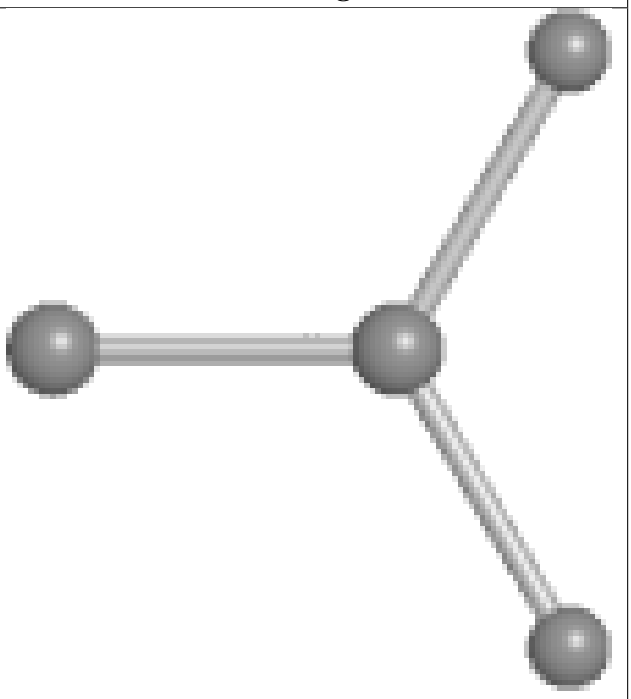
Bond lengths



Bond angles

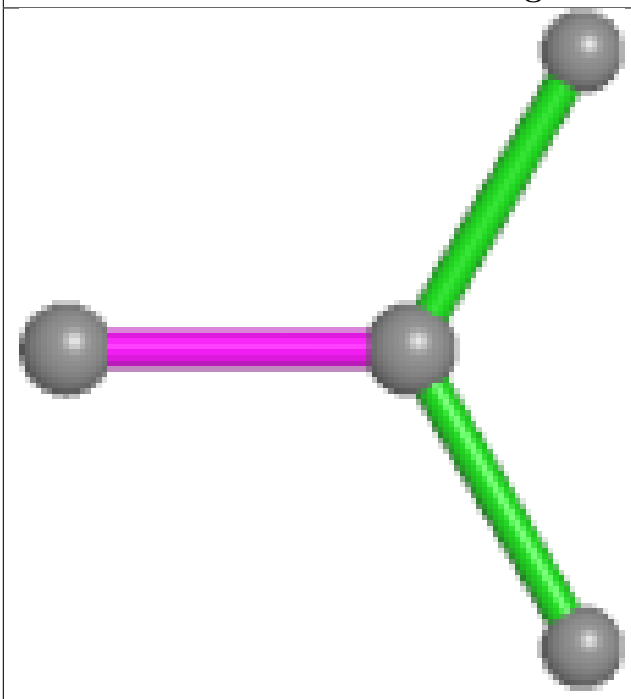


Torsions

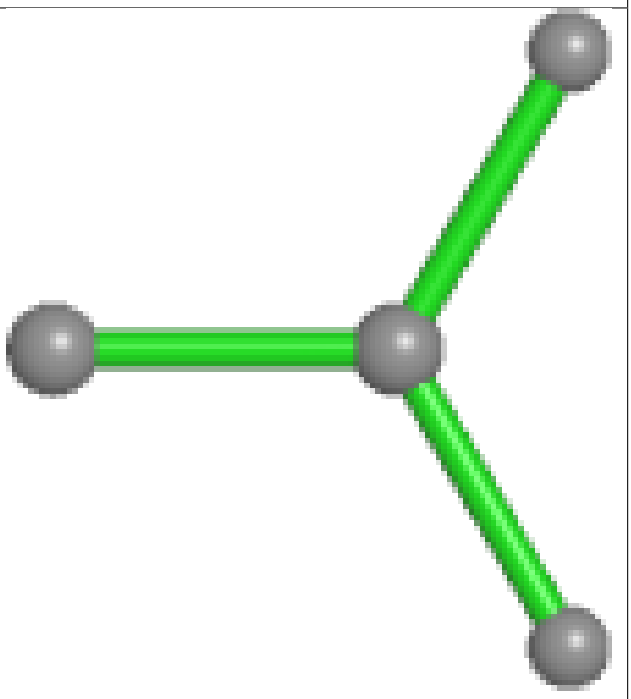


Rings

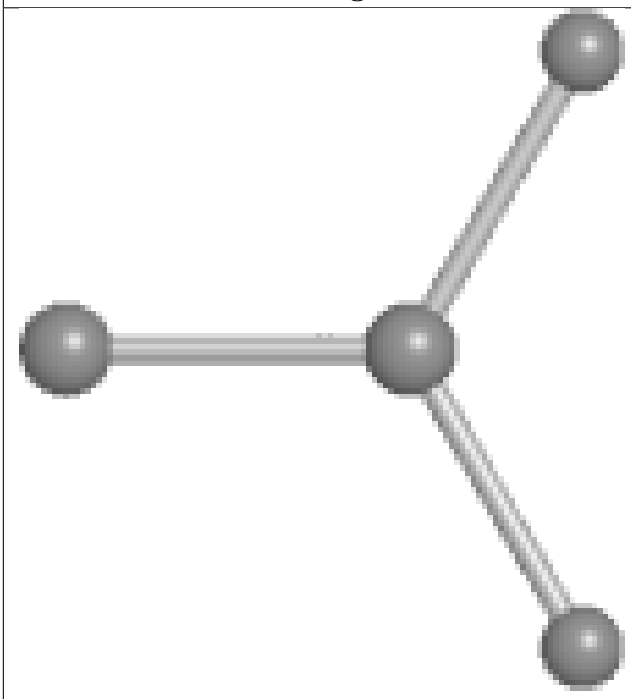
Ligand ACT F 307



Bond lengths



Bond angles



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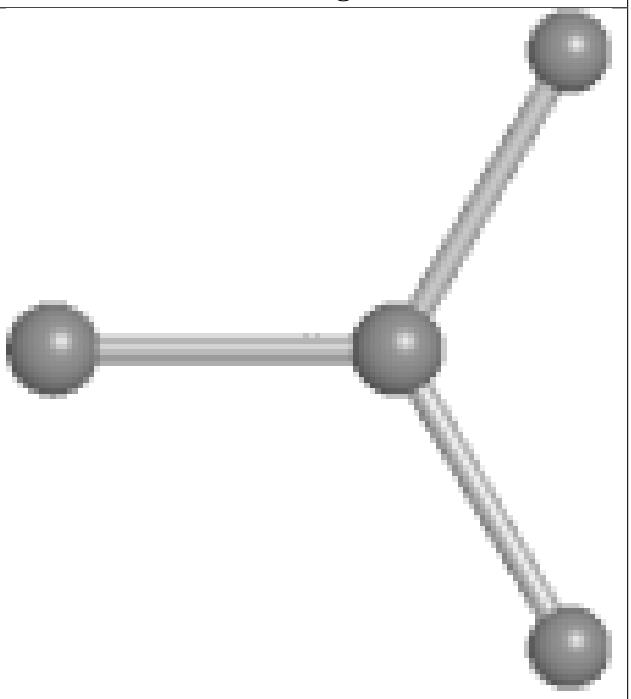
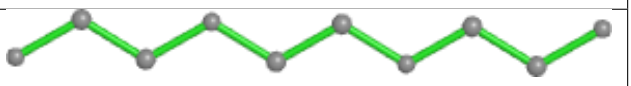


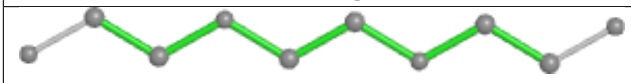
Rings

Ligand PGE C 309

Bond lengths



Bond angles



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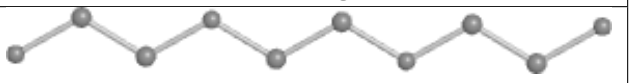
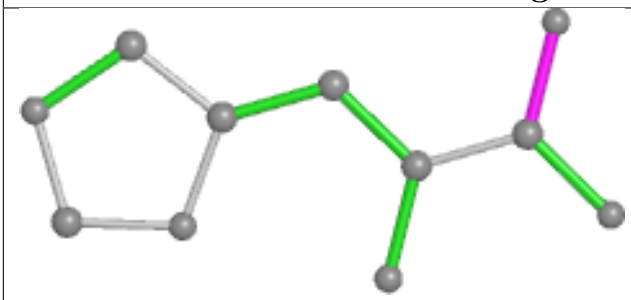


Rings

Ligand HIS C 310



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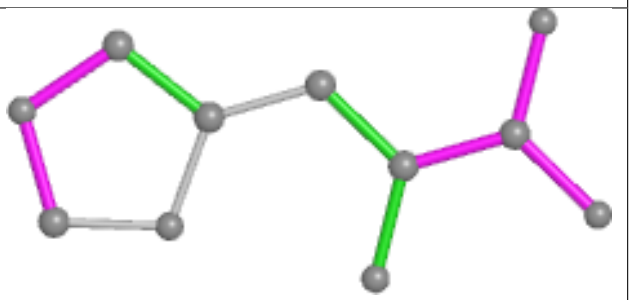
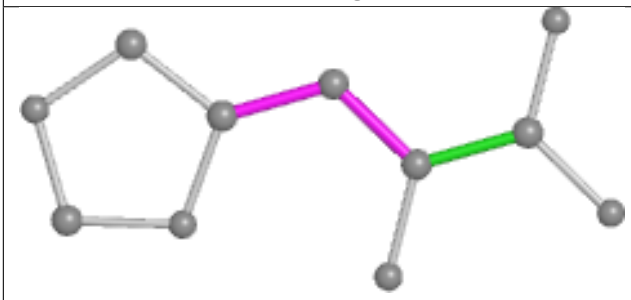


Bond angles



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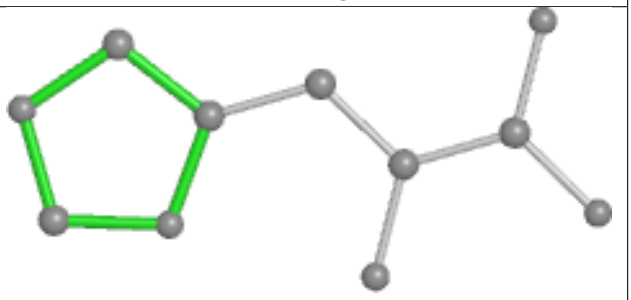
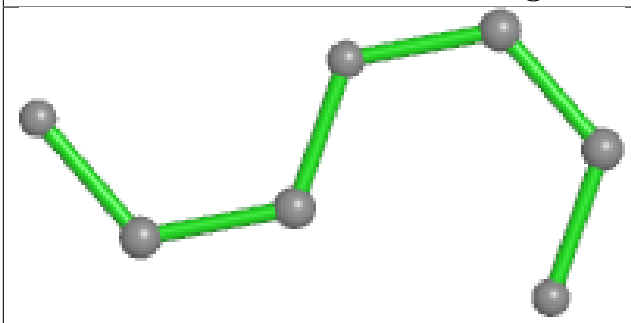
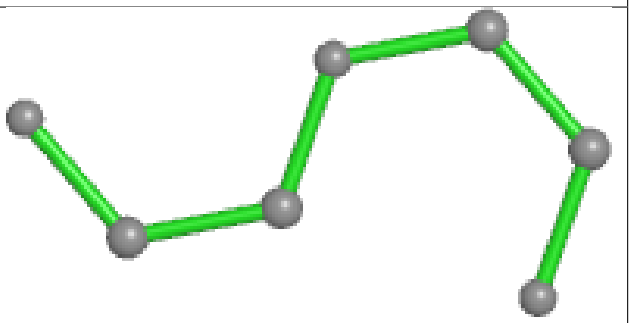


Rings

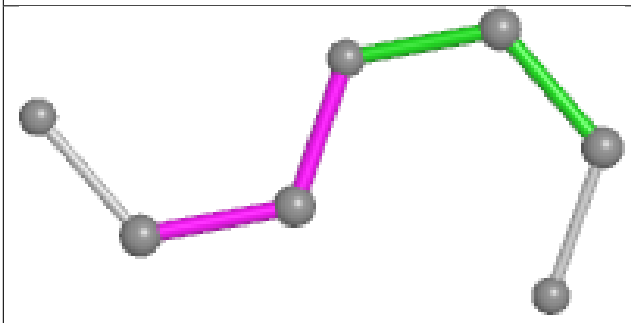
Ligand PEG E 315



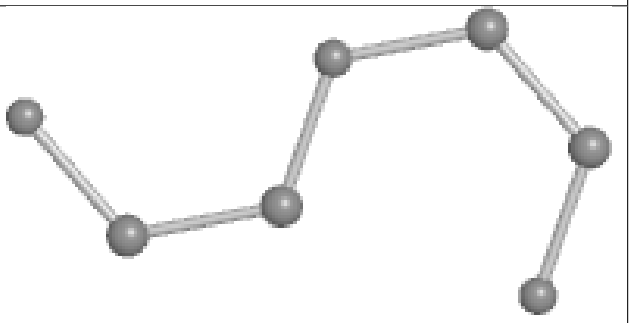
Bond lengths



Bond angles

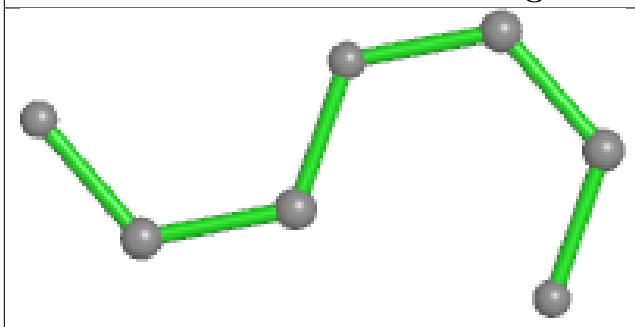


Torsions



Rings

Ligand PEG E 316



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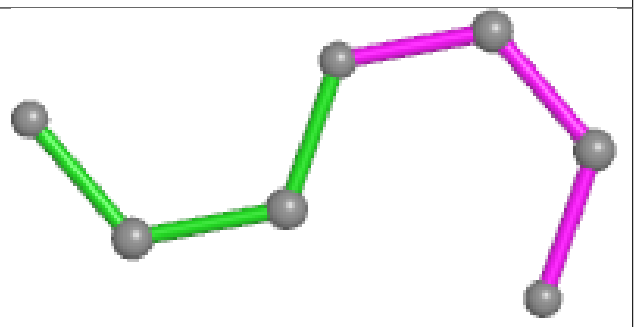
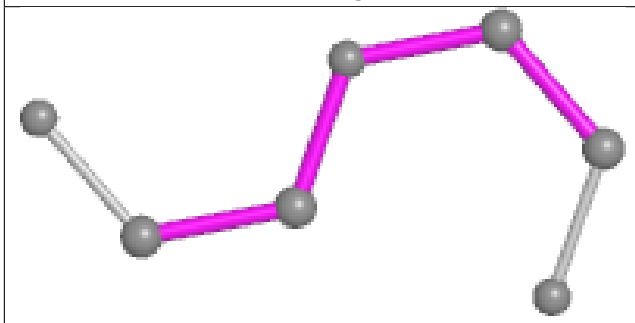
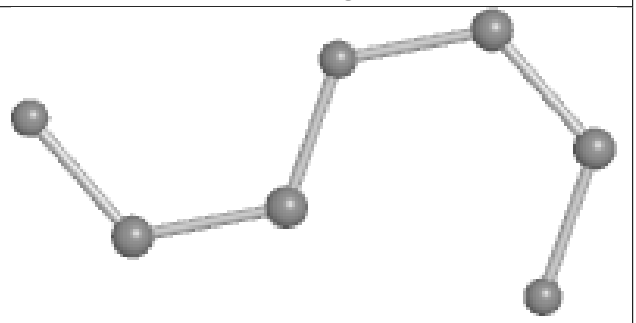


Bond angles

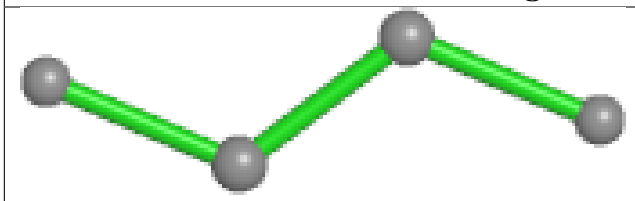


Torsions



Rings

Ligand EDO B 305



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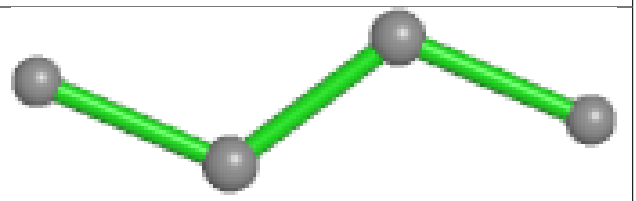
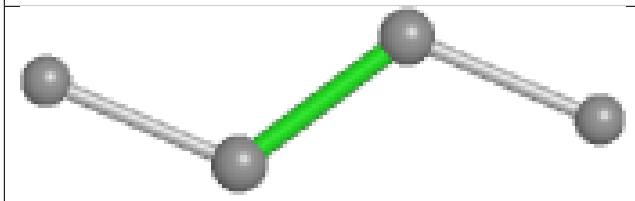
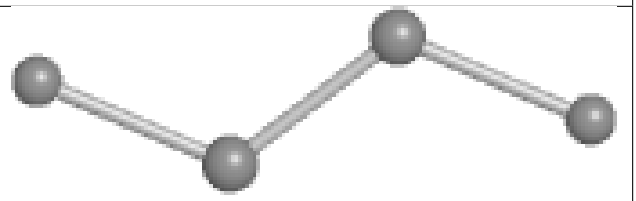


Bond angles

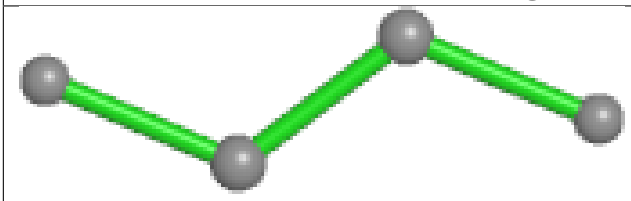


Torsions

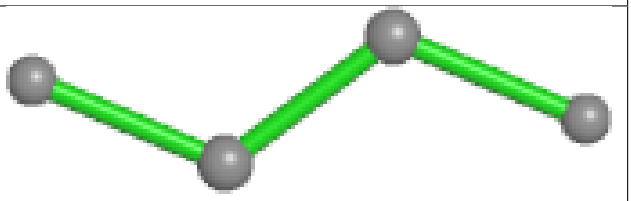


Rings

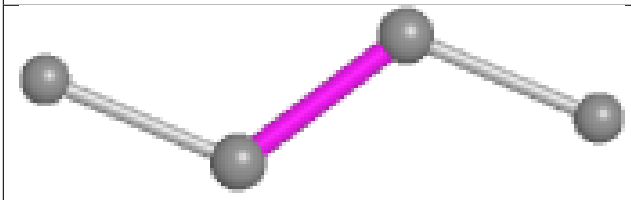
Ligand EDO E 306



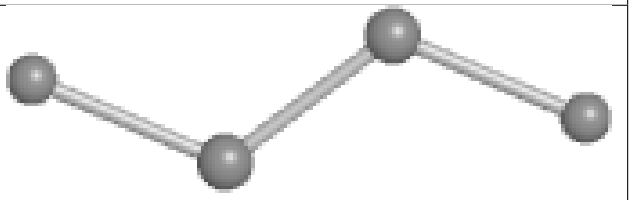
Bond lengths



Bond angles

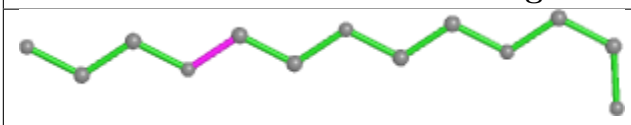


Torsions



Rings

Ligand PG4 D 317



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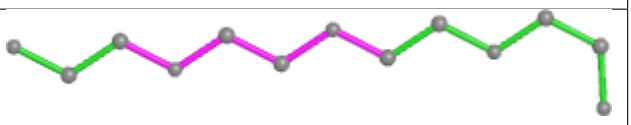
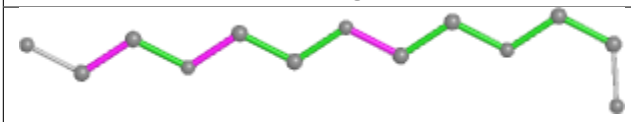


Bond angles



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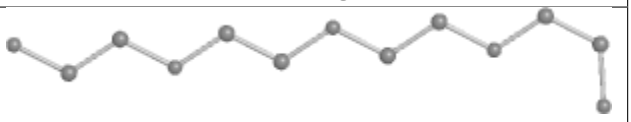
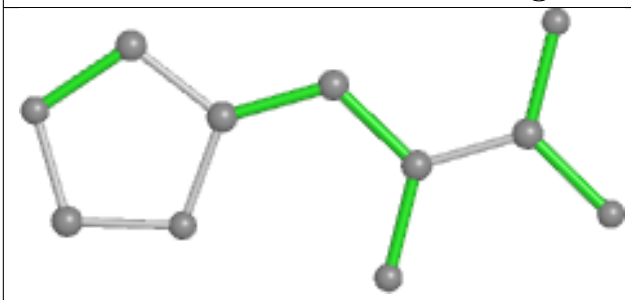


Rings

Ligand HIS A 317



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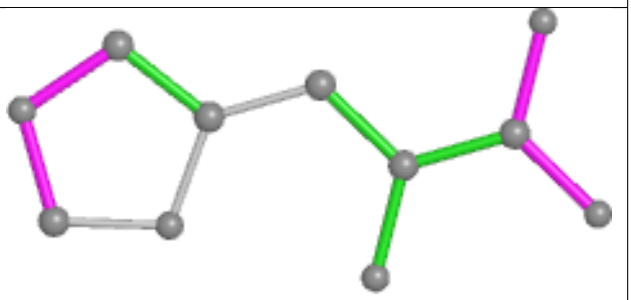
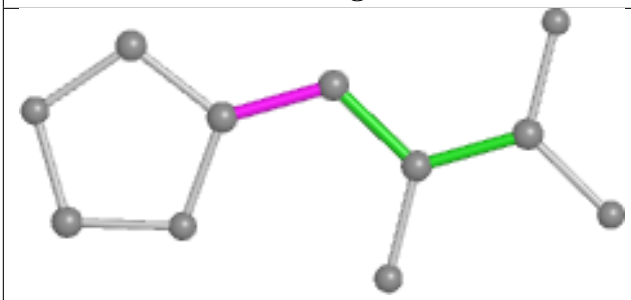
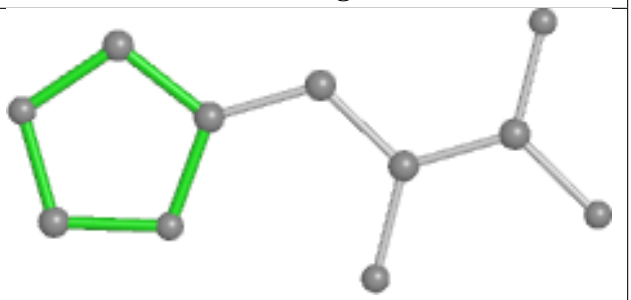


Bond angles

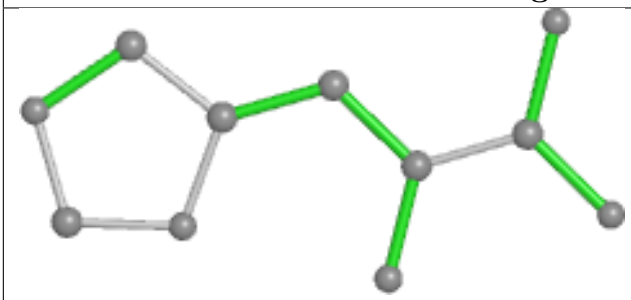


Torsions

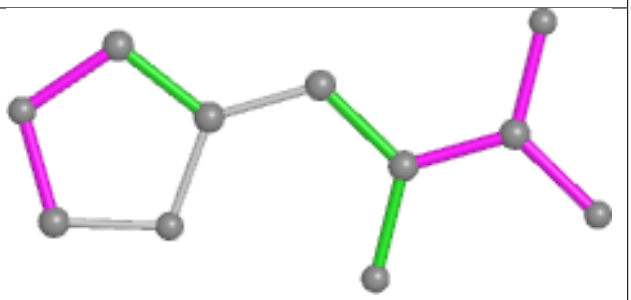


Rings

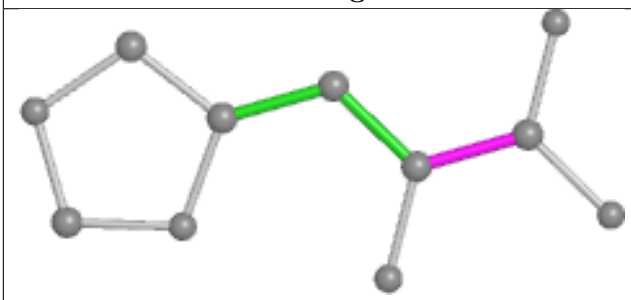
Ligand HIS B 313



Bond lengths



Bond angles



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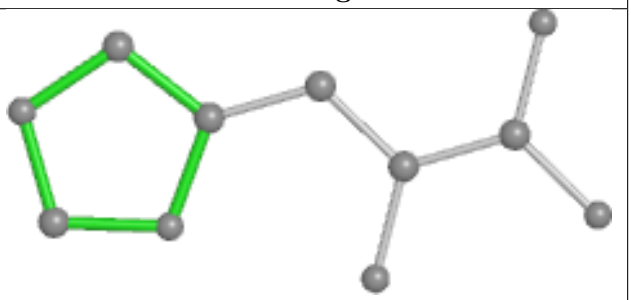
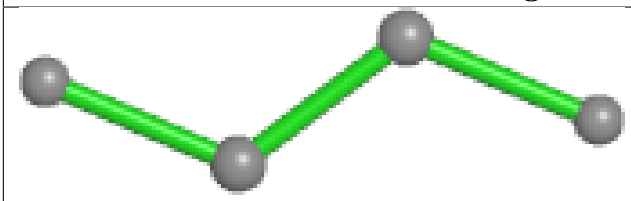
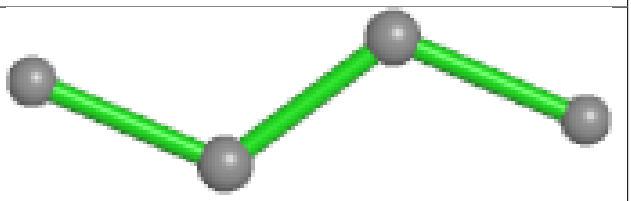


Rings

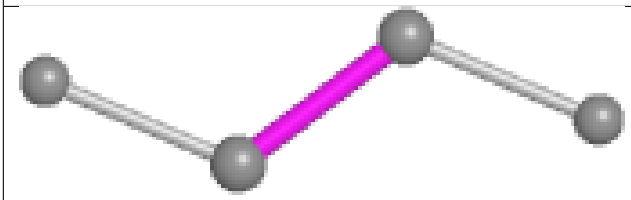
Ligand EDO C 303



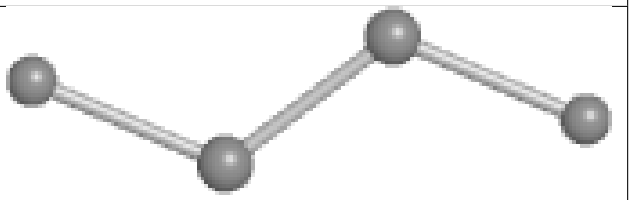
Bond lengths



Bond angles

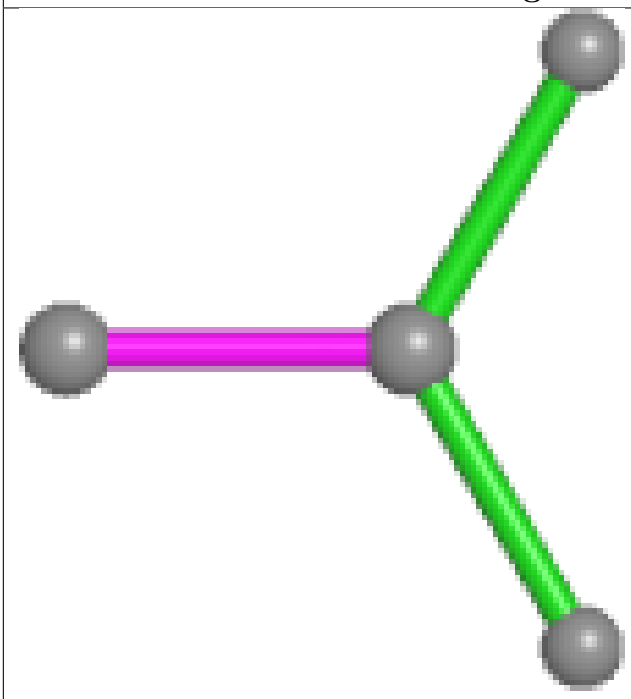


Torsions

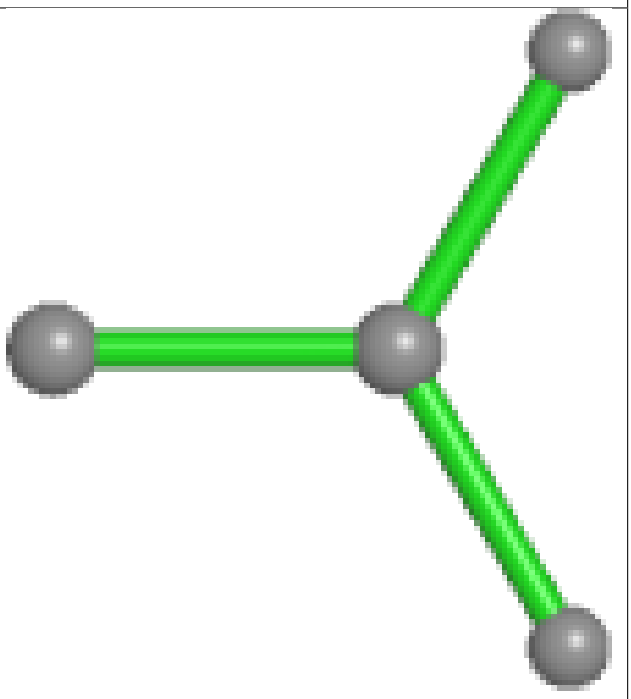


Rings

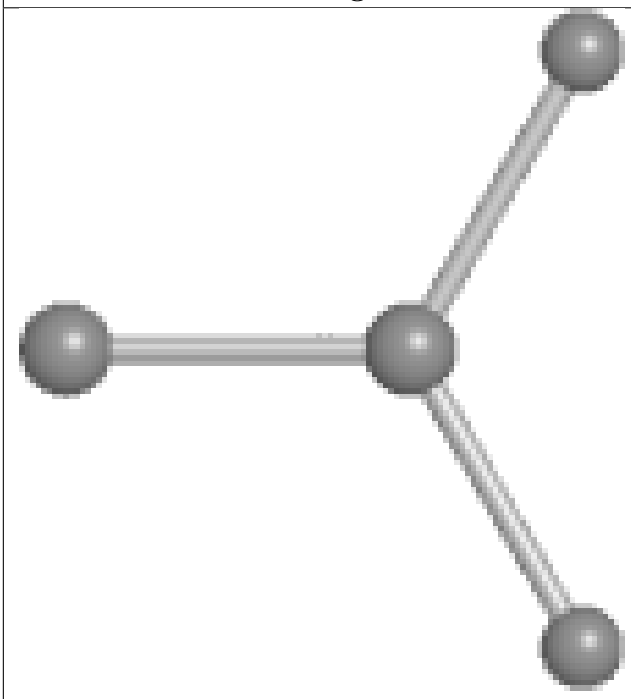
Ligand ACT B 309



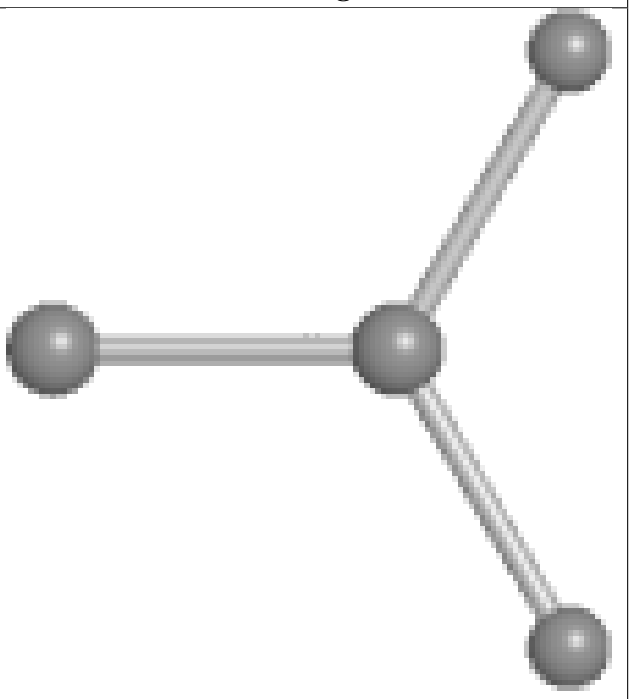
Bond lengths



Bond angles

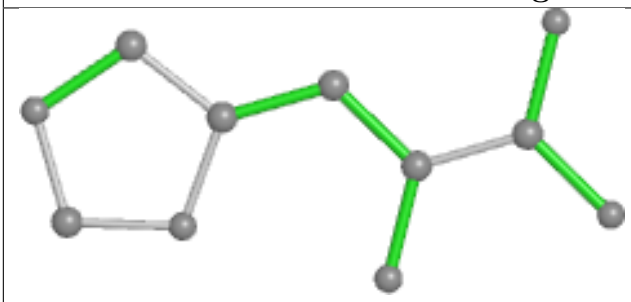


Torsions

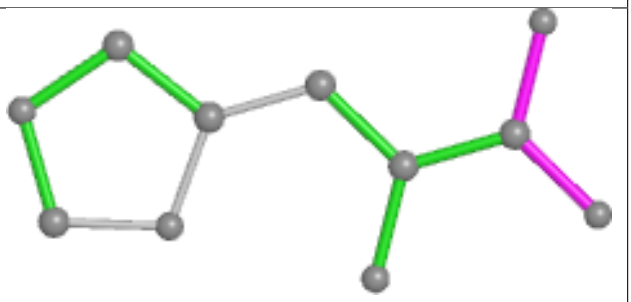


Rings

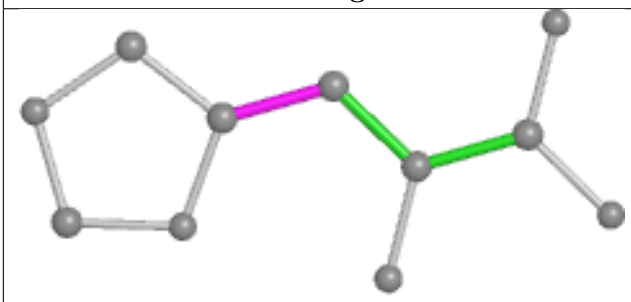
Ligand HIS E 317



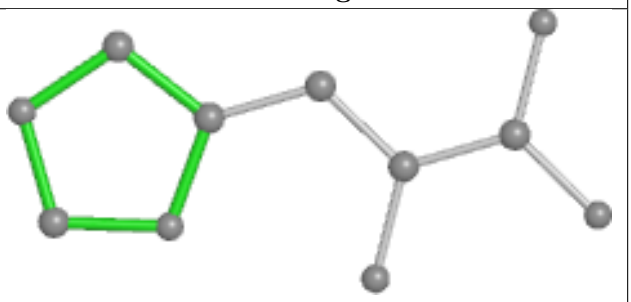
Bond lengths



Bond angles

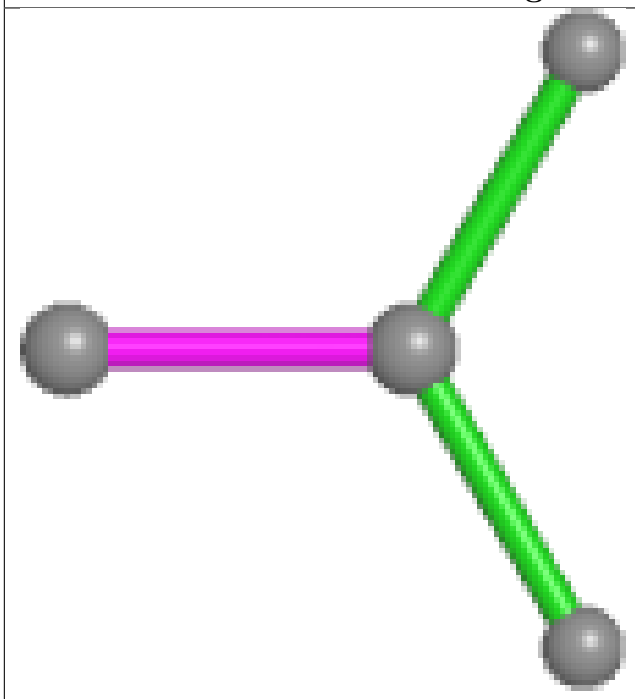


Torsions

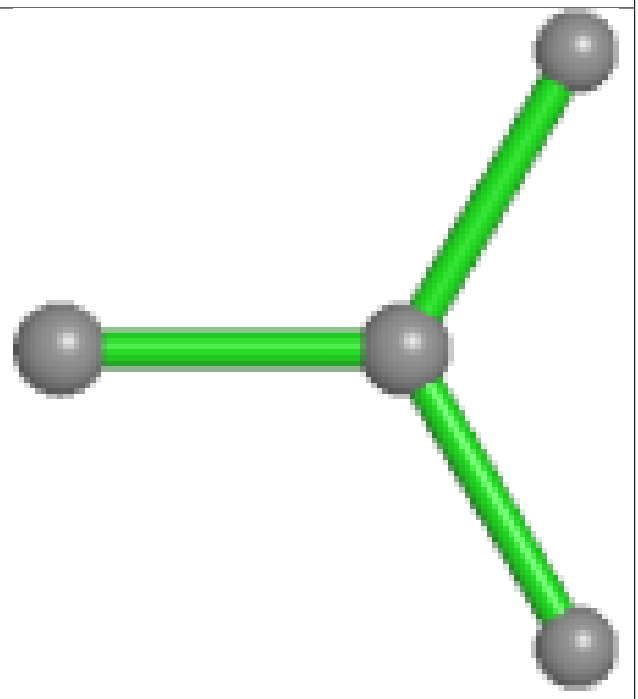


Rings

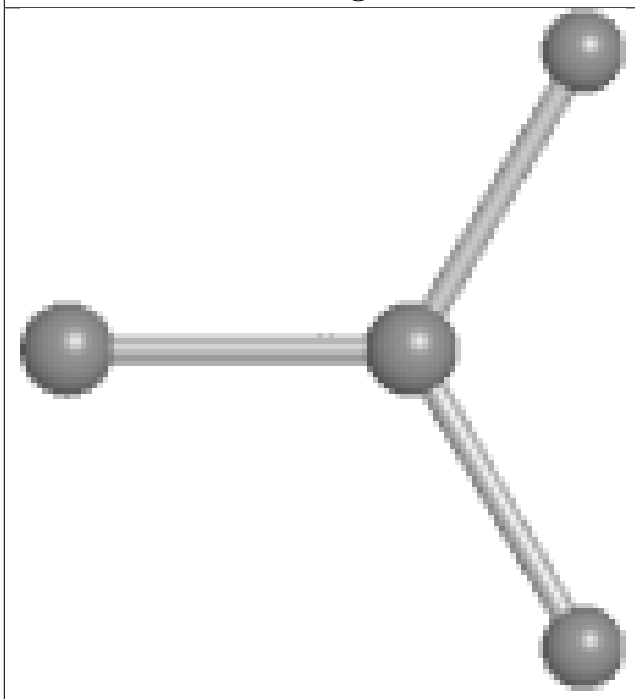
Ligand ACT E 310



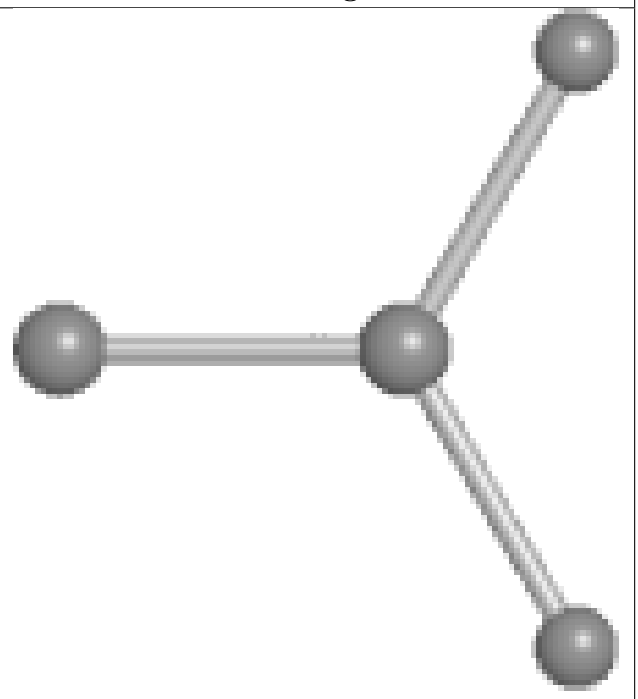
Bond lengths



Bond angles

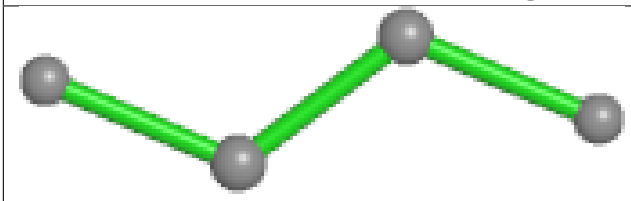


Torsions

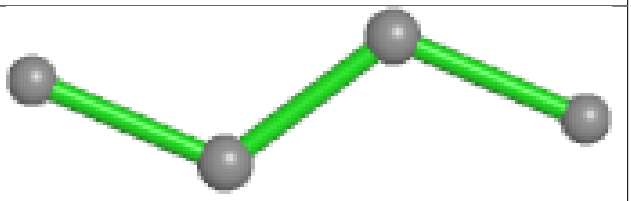


Rings

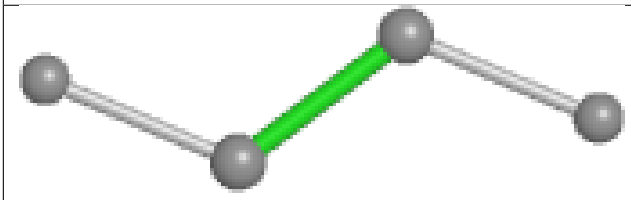
Ligand EDO A 303



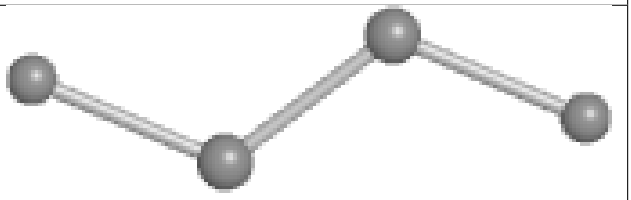
Bond lengths



Bond angles

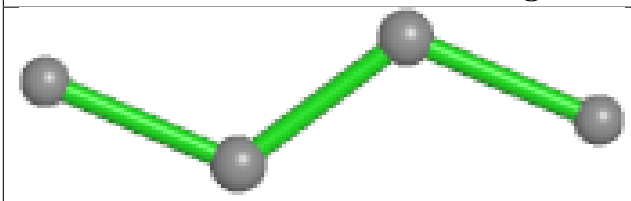


Torsions

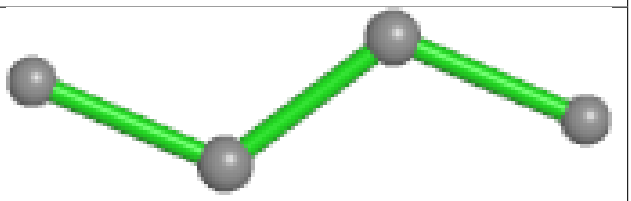


Rings

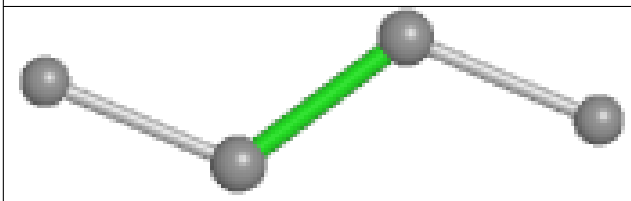
Ligand EDO B 304



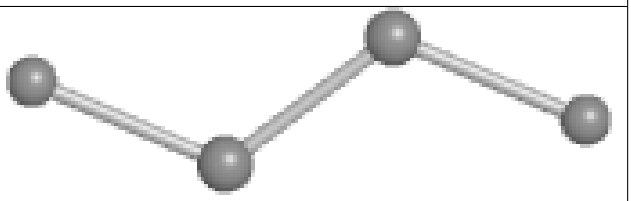
Bond lengths



Bond angles

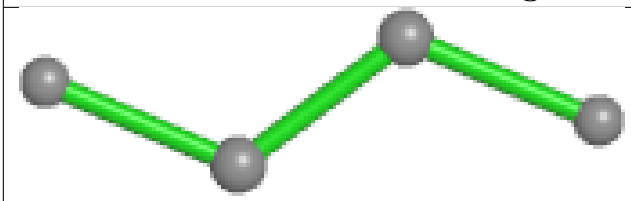


Torsions

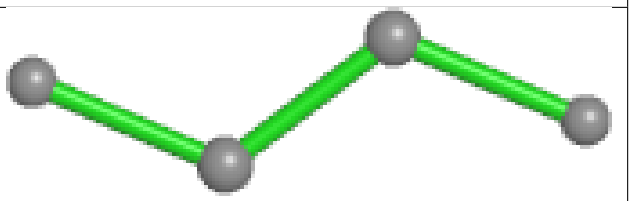


Rings

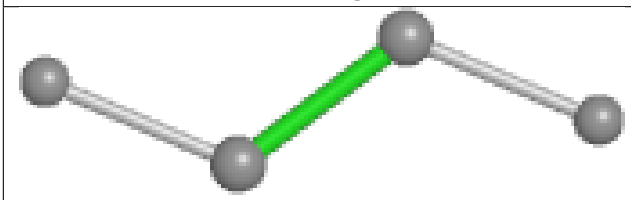
Ligand EDO D 303



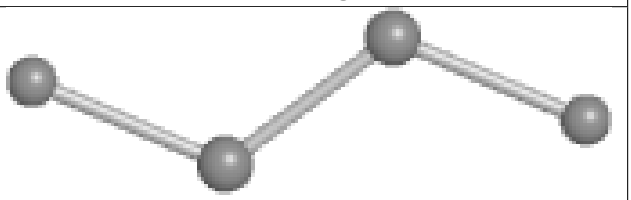
Bond lengths



Bond angles

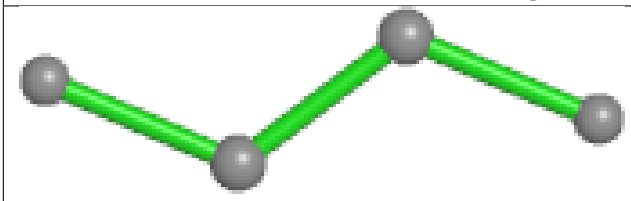


Torsions

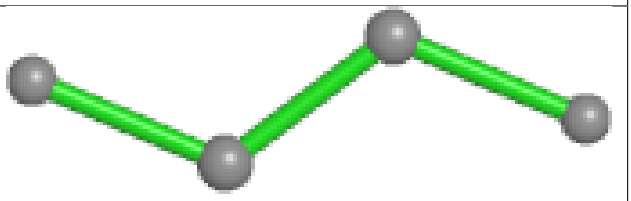


Rings

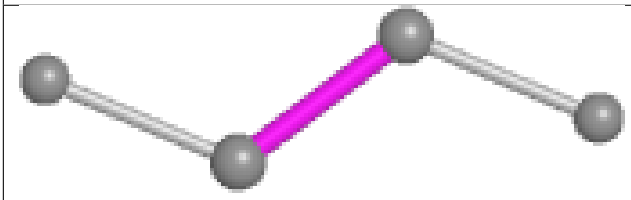
Ligand EDO F 304



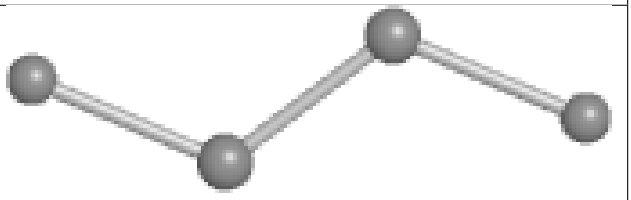
Bond lengths



Bond angles

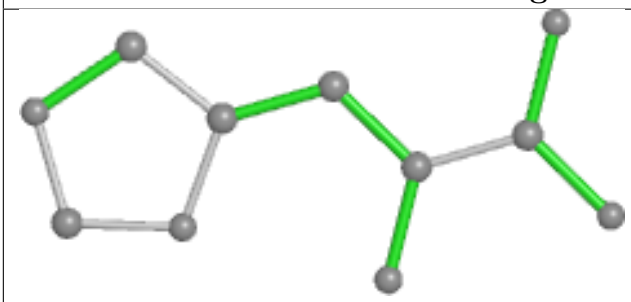


Torsions

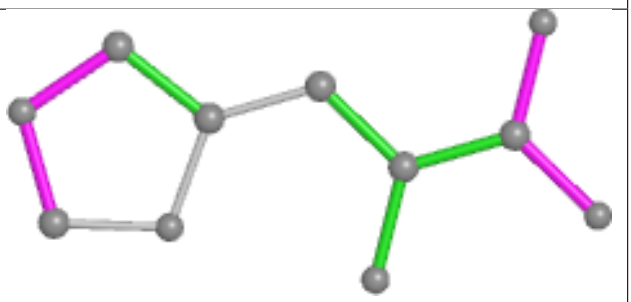


Rings

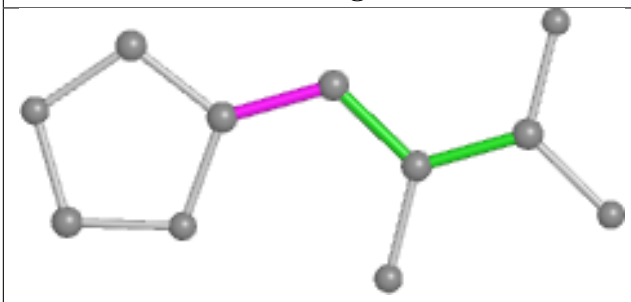
Ligand HIS D 321



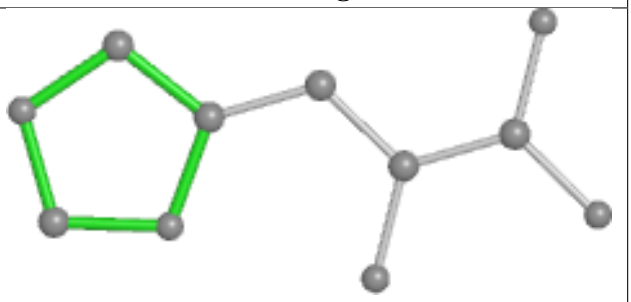
Bond lengths



Bond angles

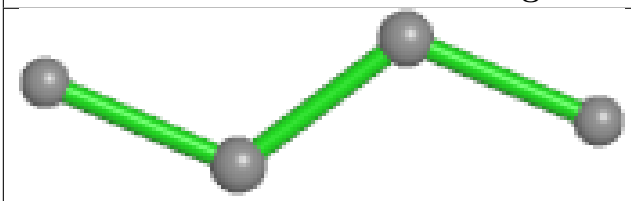


Torsions

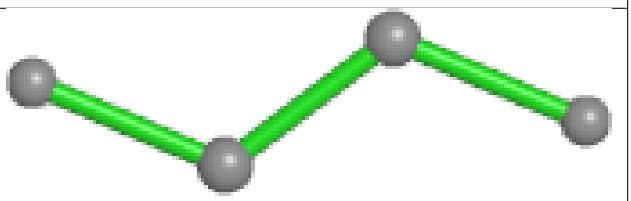


Rings

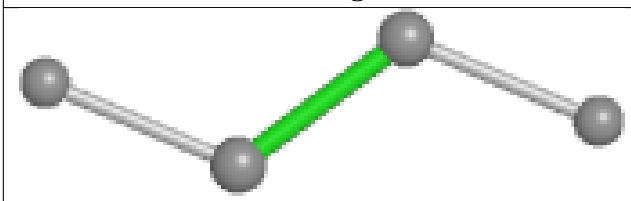
Ligand EDO A 305



Bond lengths



Bond angles



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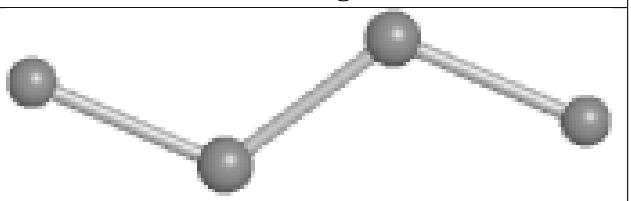
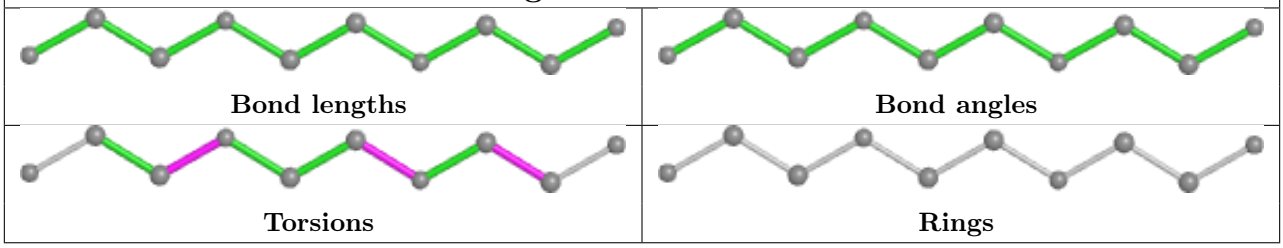
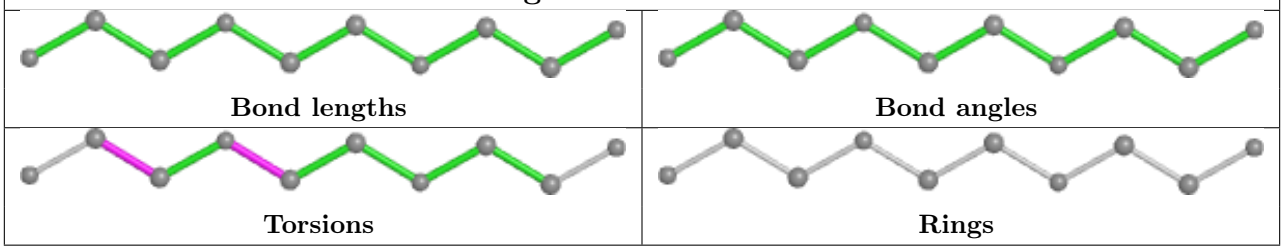


Rings

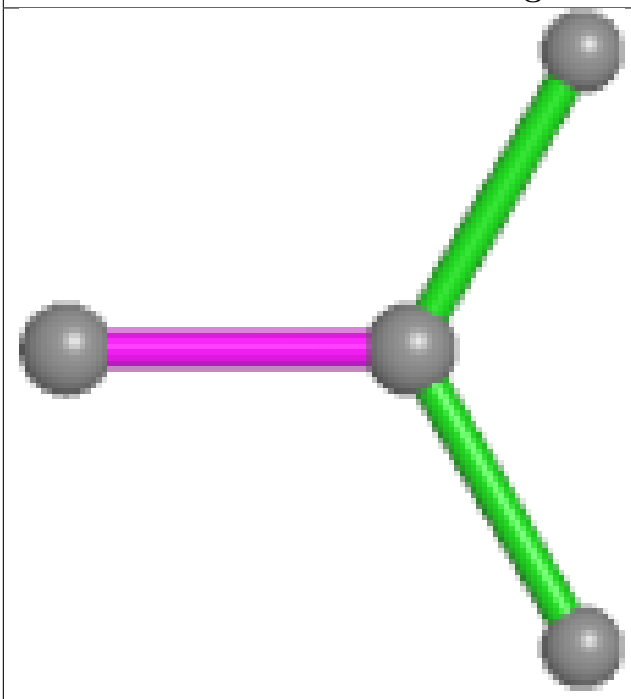
Ligand PGE B 312



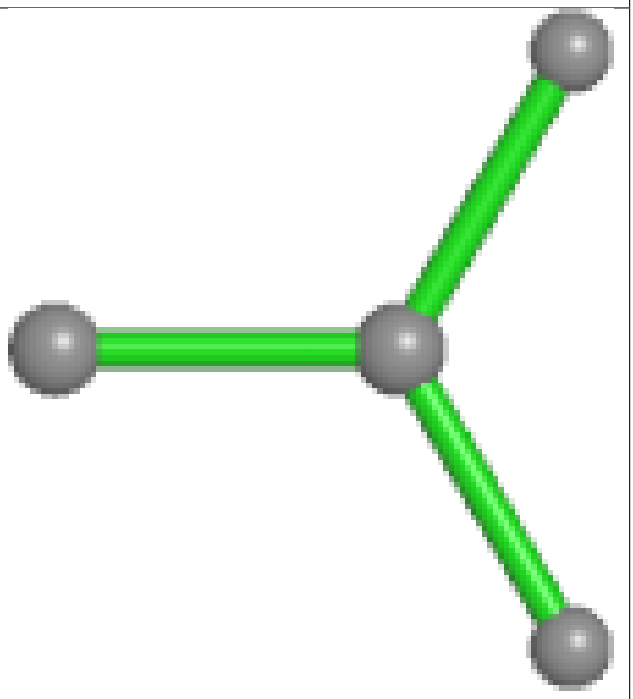
Ligand PGE D 316



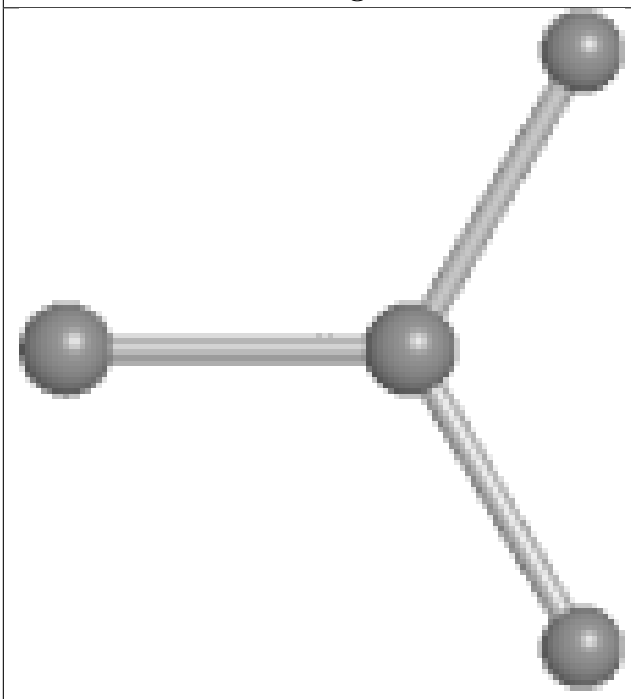
Ligand ACT E 311



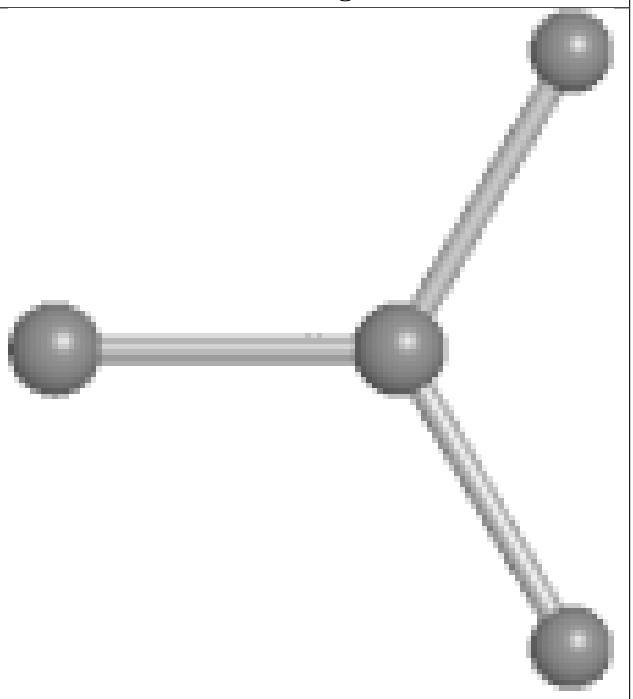
Bond lengths



Bond angles

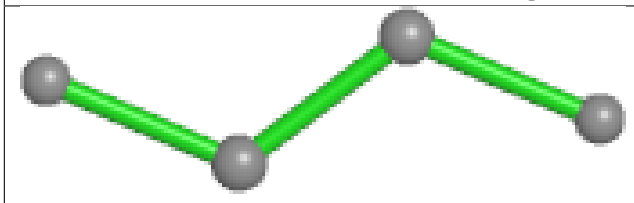


Torsions



Rings

Ligand EDO A 302



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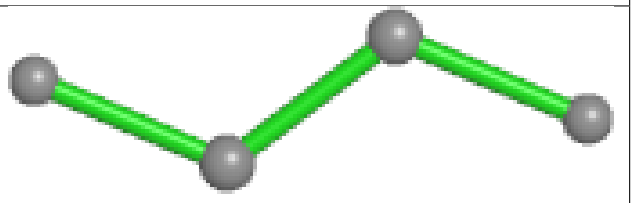
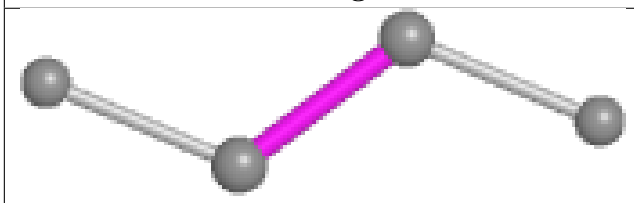
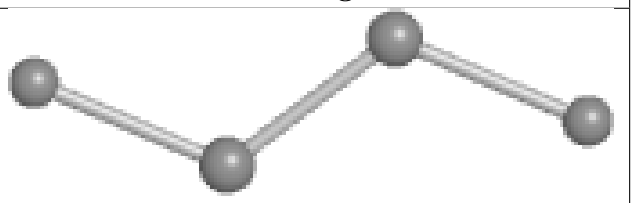


Bond angles

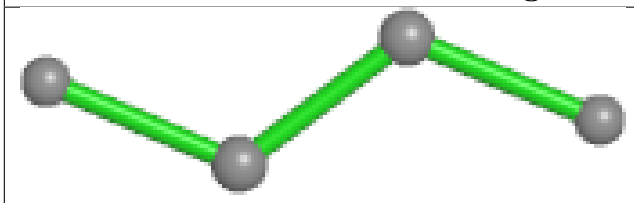


Torsions

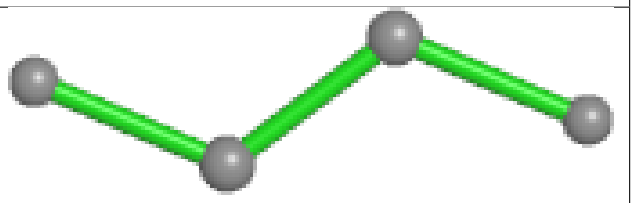


Rings

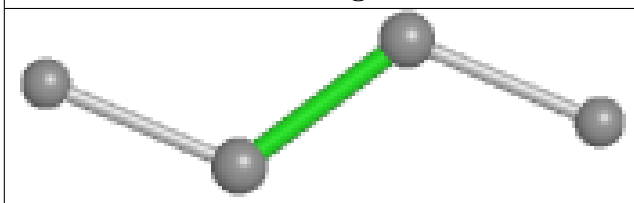
Ligand EDO D 301



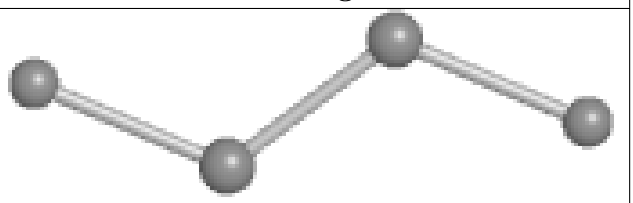
Bond lengths



Bond angles

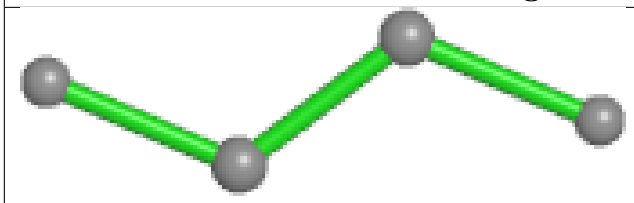


Torsions



Rings

Ligand EDO D 302



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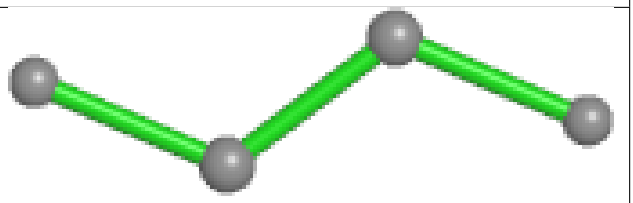
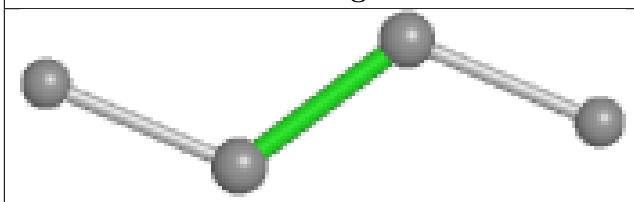
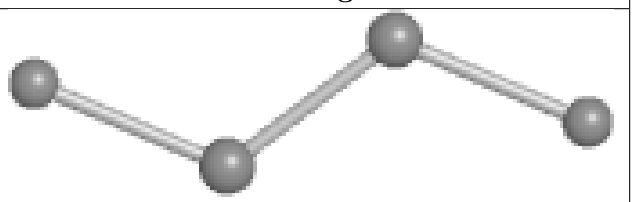


Bond angles

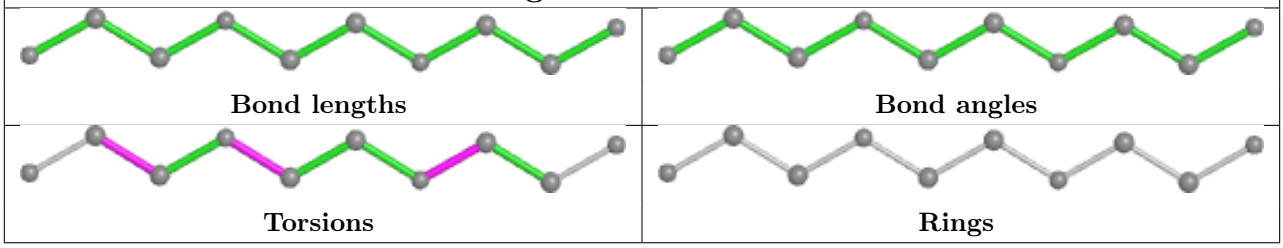


Torsions

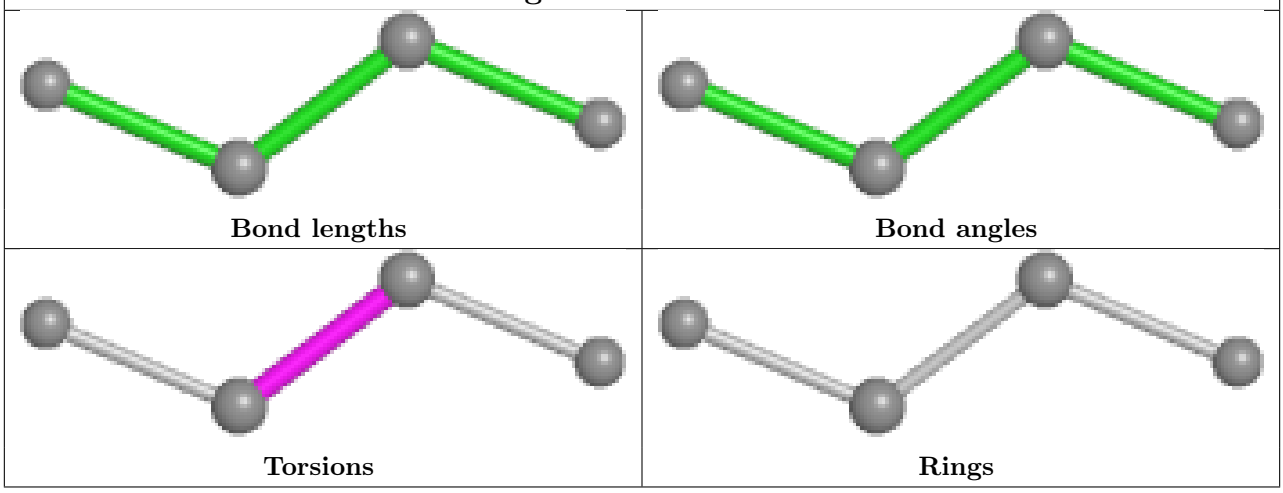


Rings

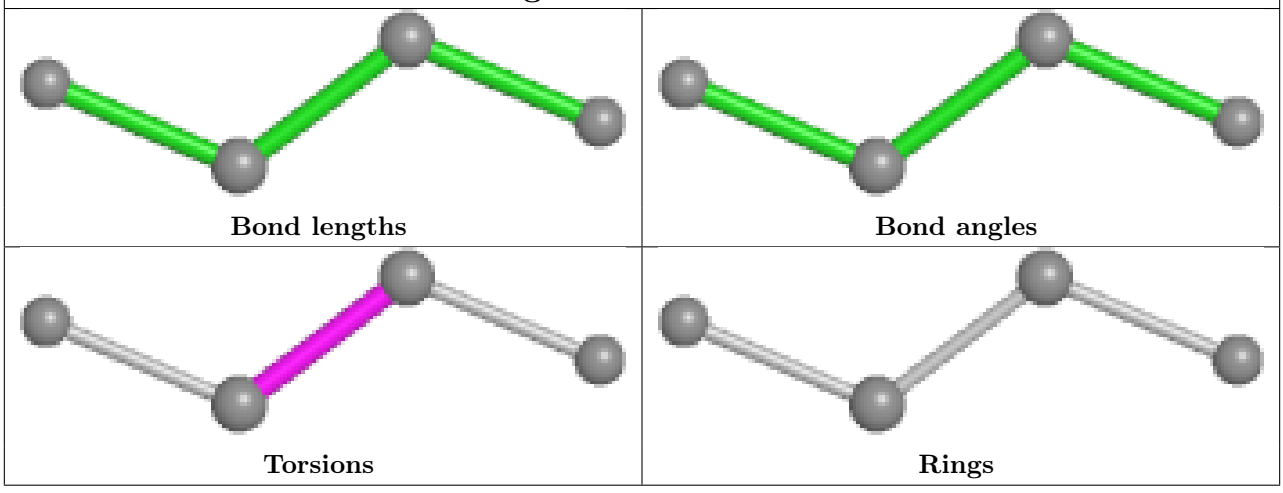
Ligand PGE E 313



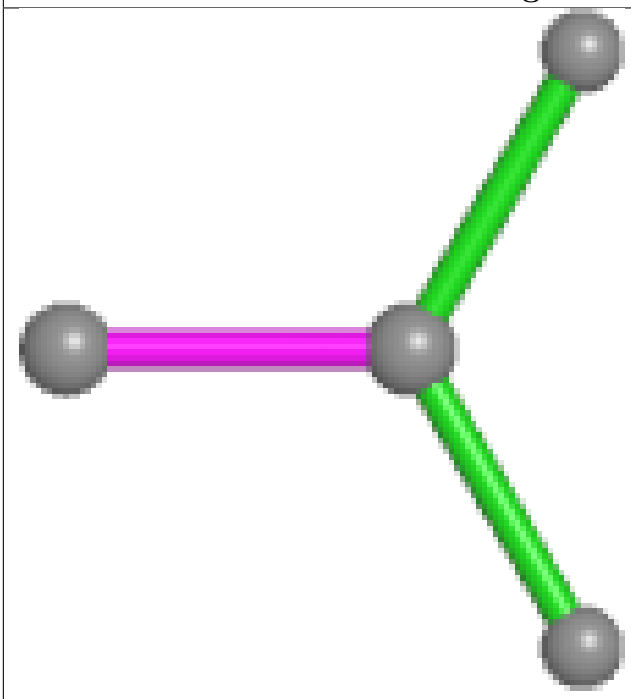
Ligand EDO E 303



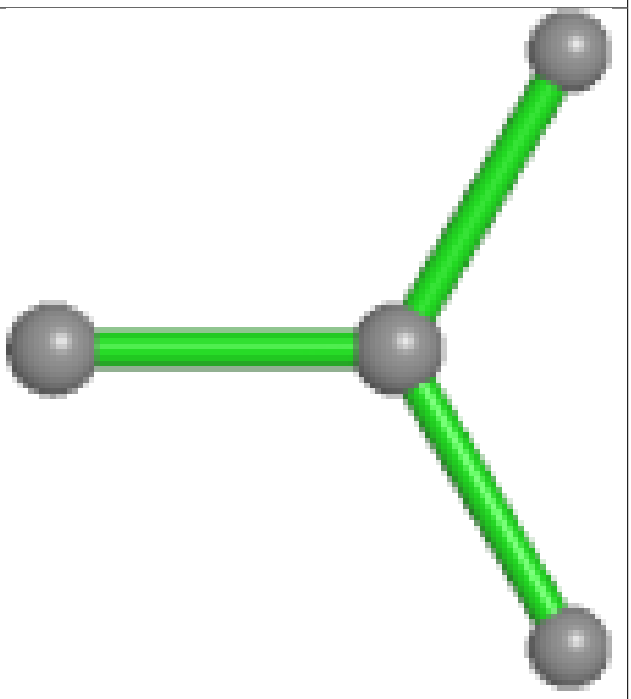
Ligand EDO C 302



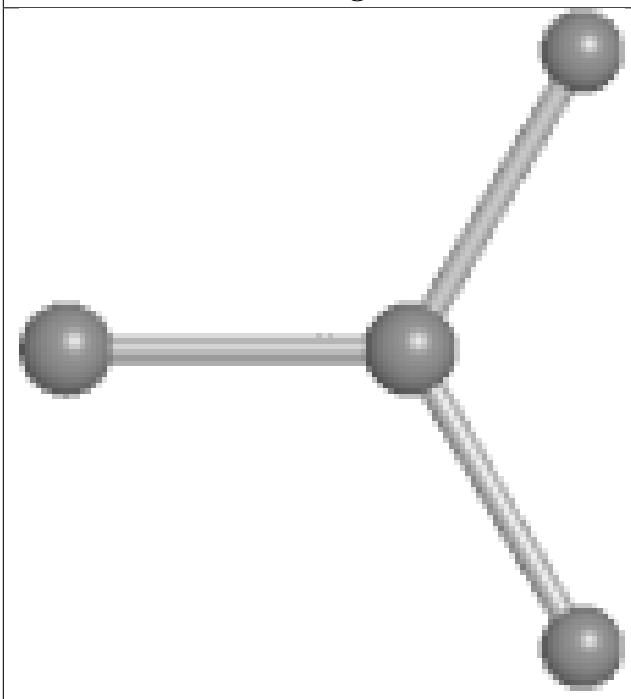
Ligand ACT D 313



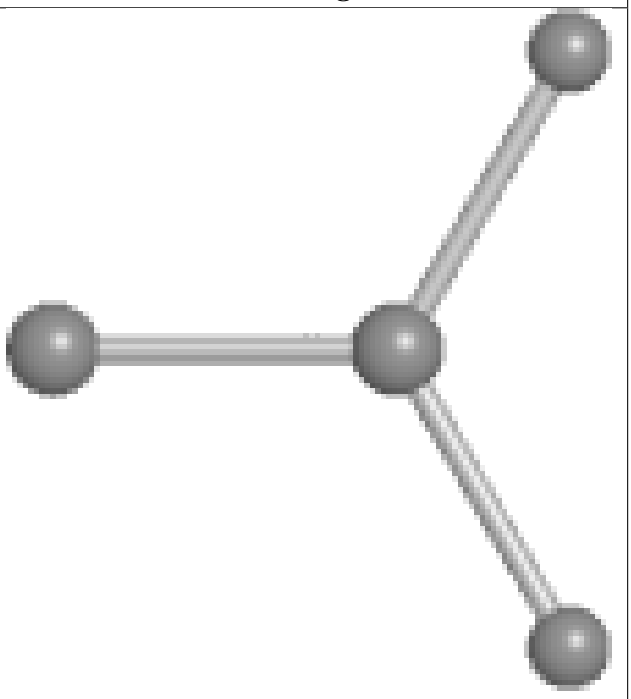
Bond lengths



Bond angles



Torsions

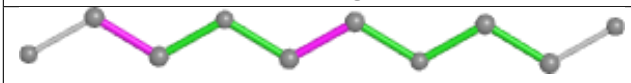


Rings

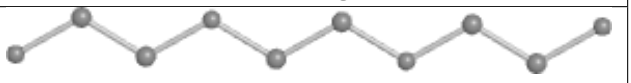
Ligand PGE B 311

Bond lengths

Bond angles



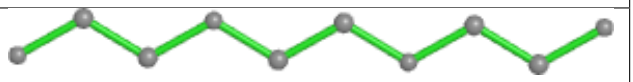
Torsions



Rings

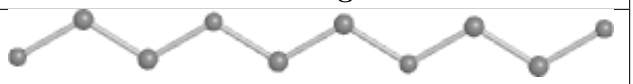
Ligand PGE E 314

Bond lengths



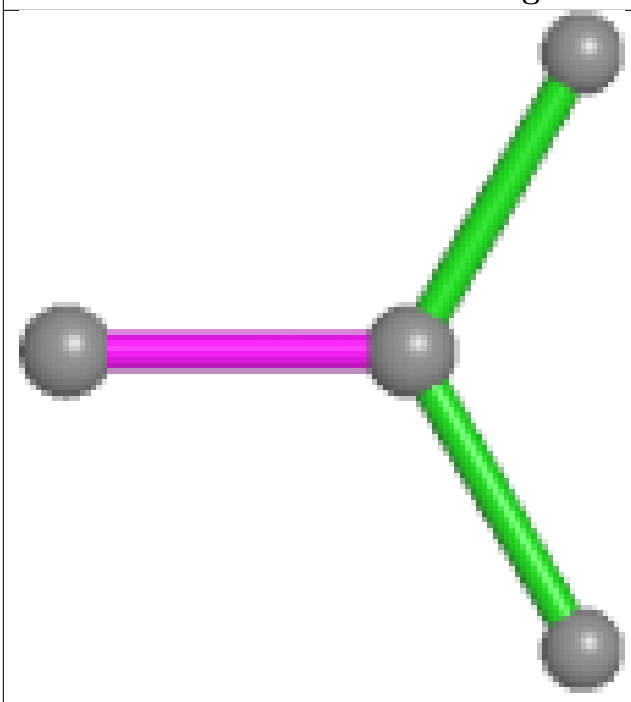
Bond angles

Torsions

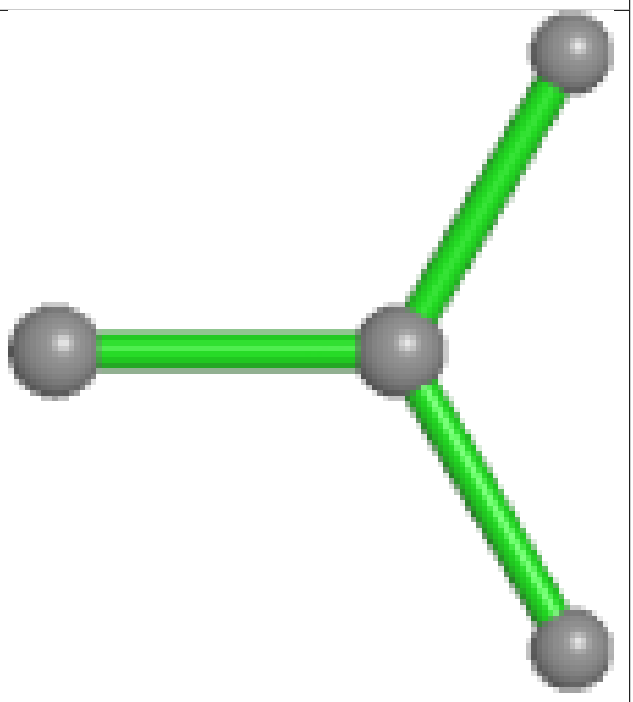


Rings

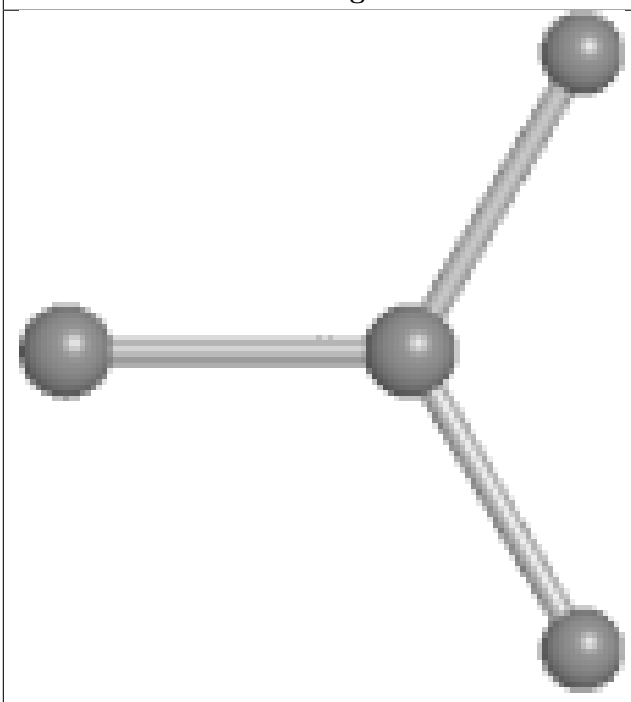
Ligand ACT D 315



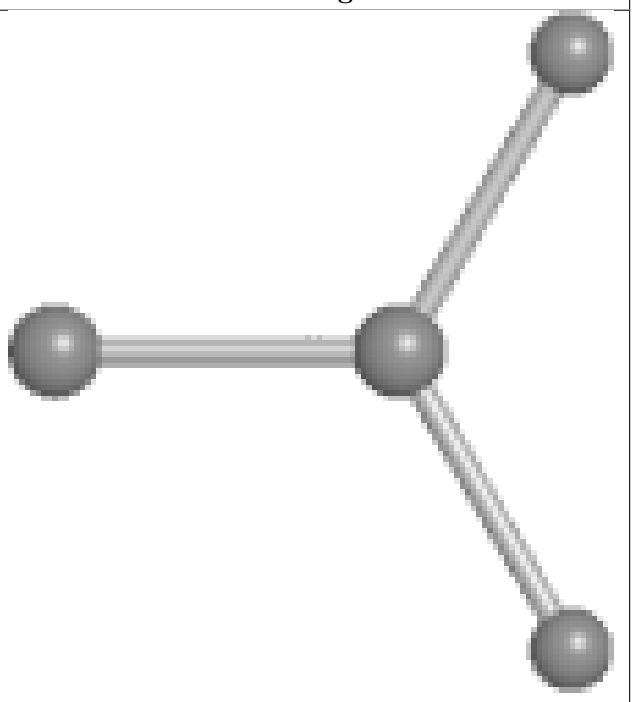
Bond lengths



Bond angles

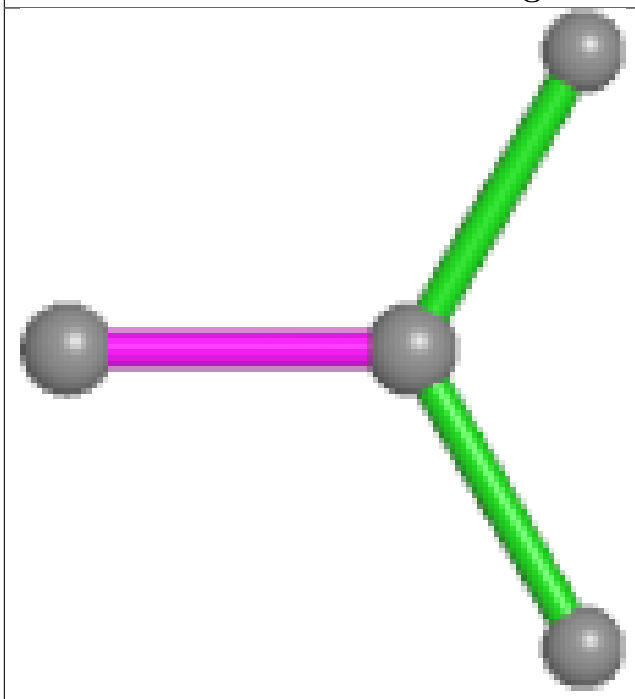


Torsions

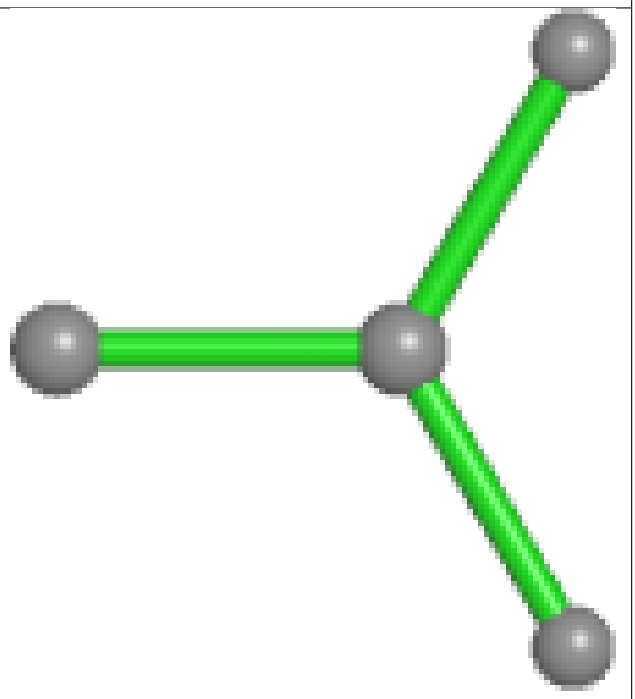


Rings

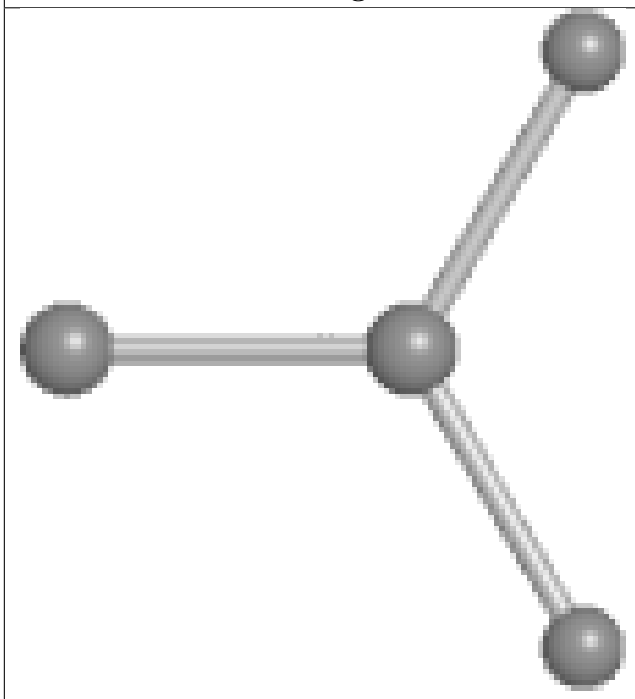
Ligand ACT A 315



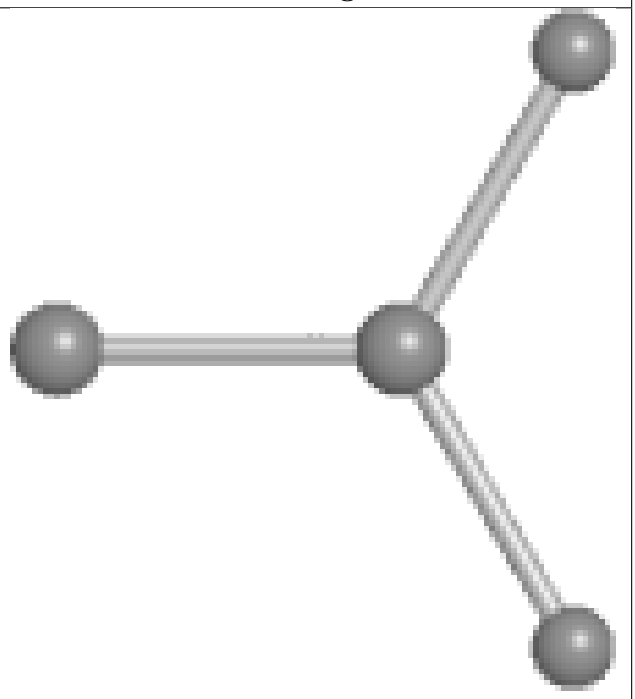
Bond lengths



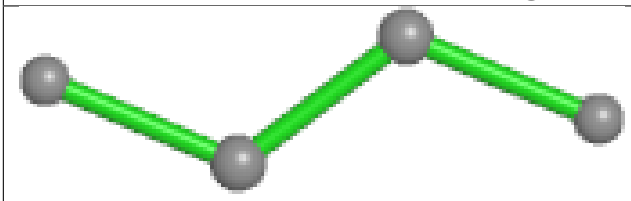
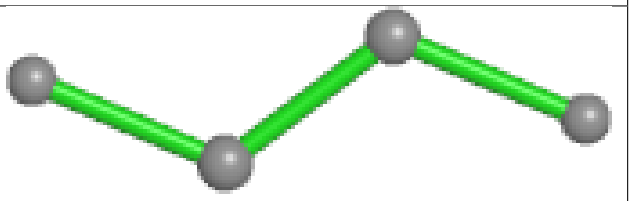
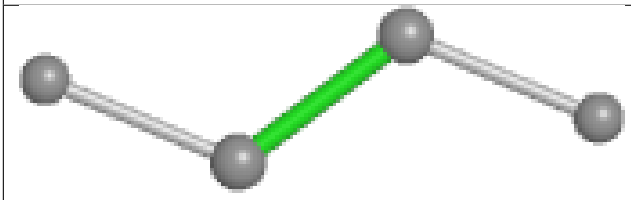
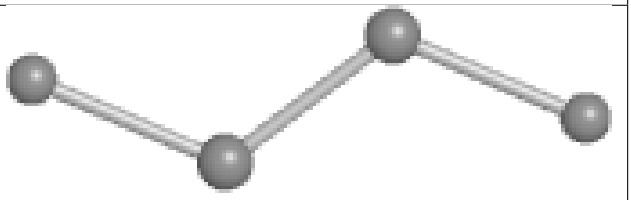
Bond angles

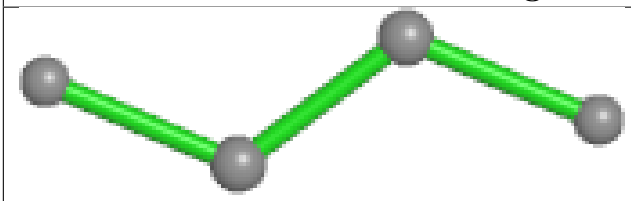
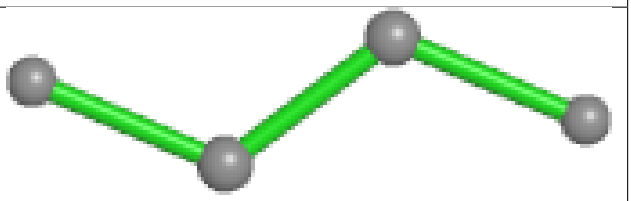
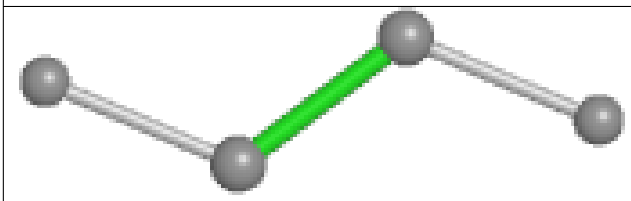
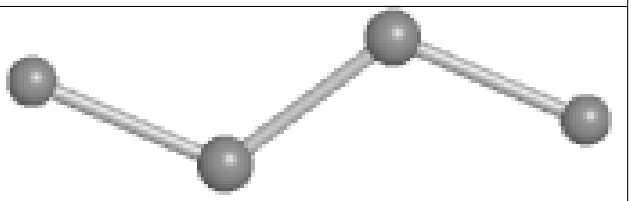


Torsions

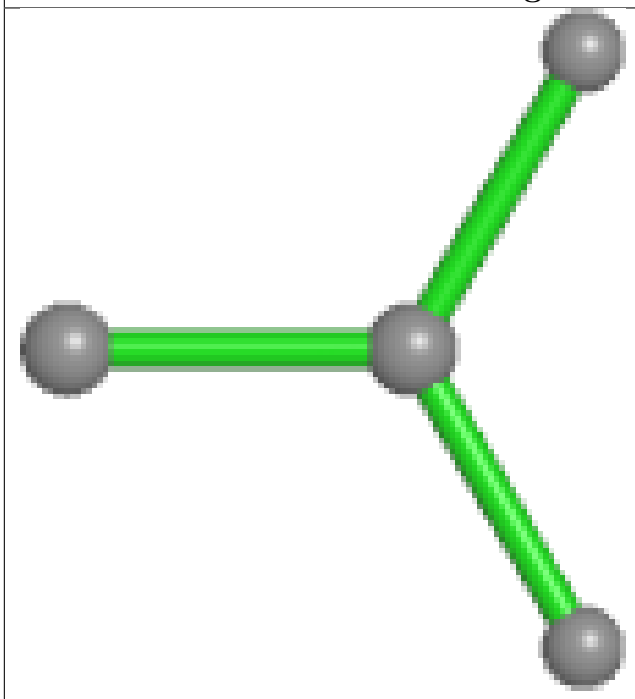


Rings

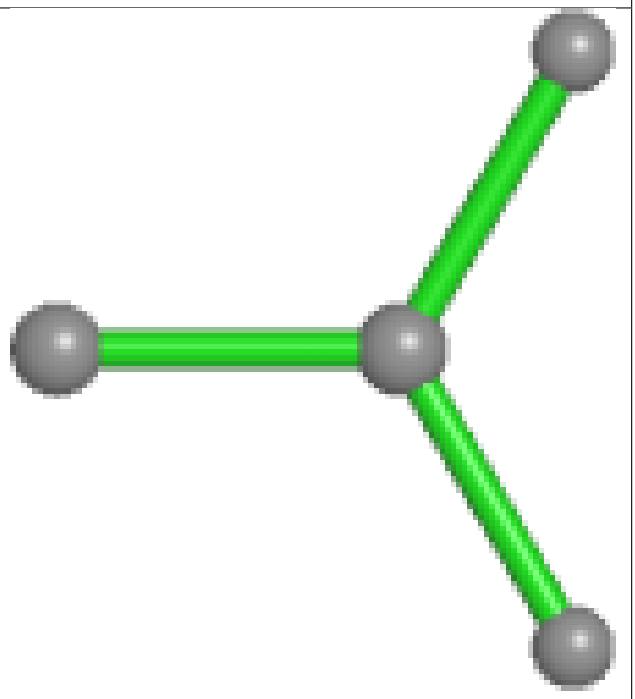
Ligand EDO C 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO E 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

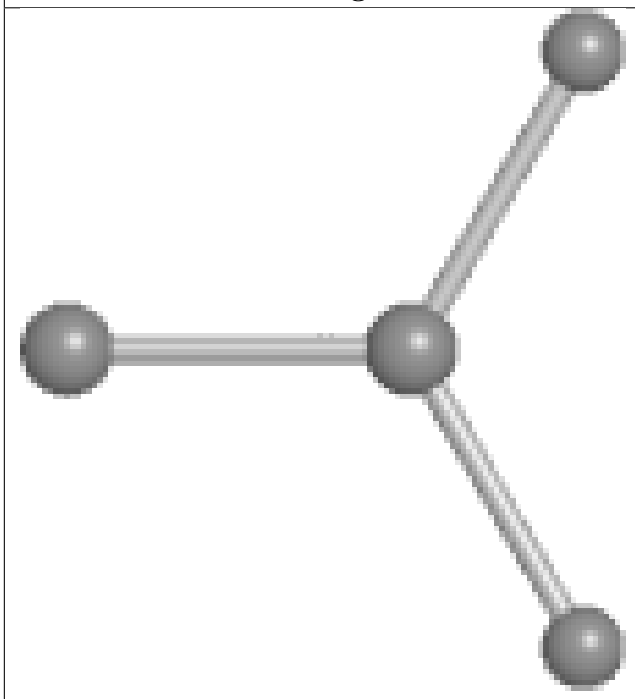
Ligand ACT C 308



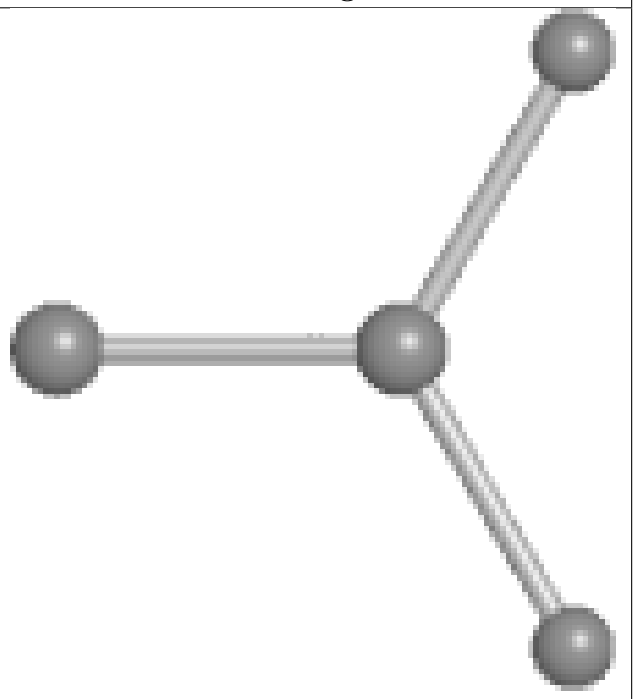
Bond lengths



Bond angles

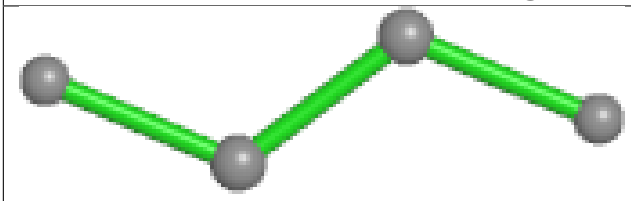


Torsions

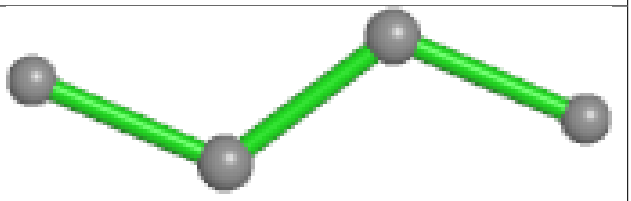


Rings

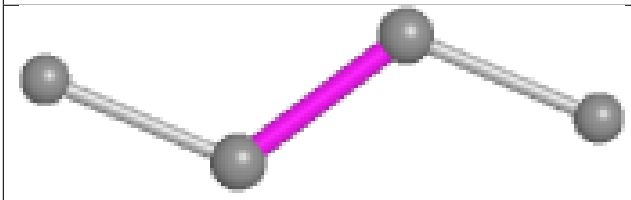
Ligand EDO D 307



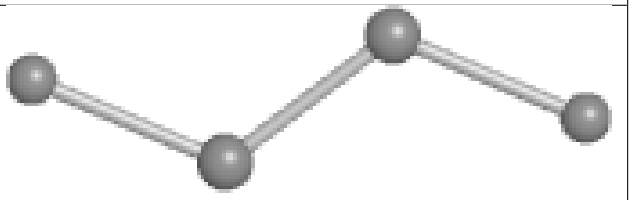
Bond lengths



Bond angles

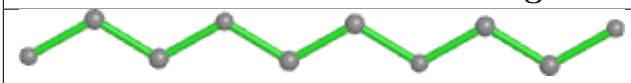


Torsions



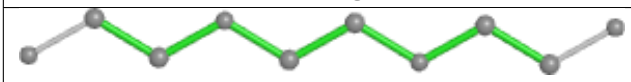
Rings

Ligand PGE E 312

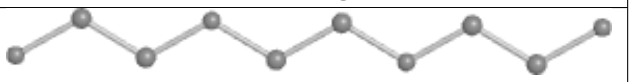


Bond lengths

Bond angles

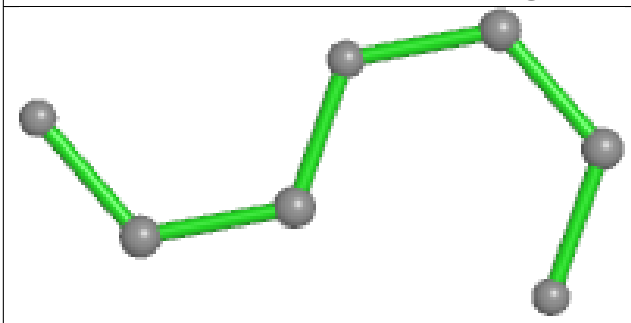


Torsions

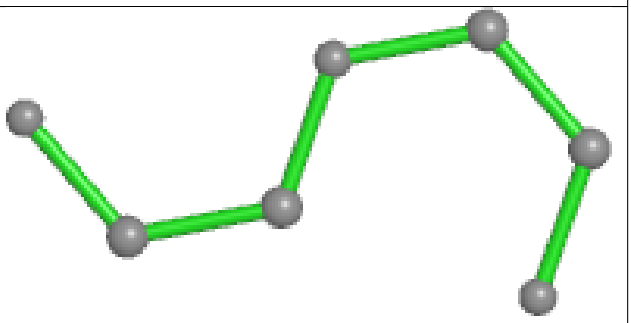


Rings

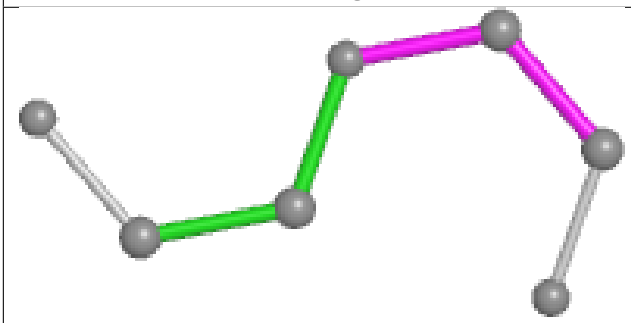
Ligand PEG D 320



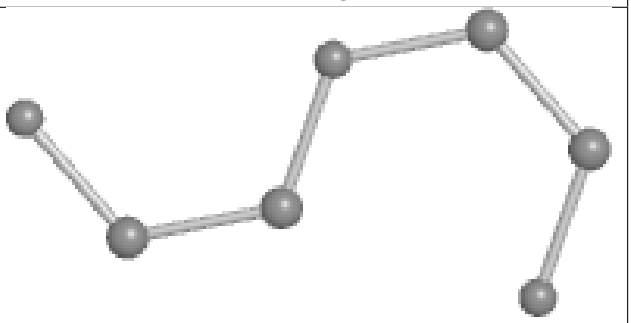
Bond lengths



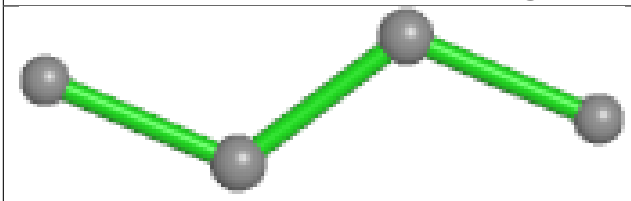
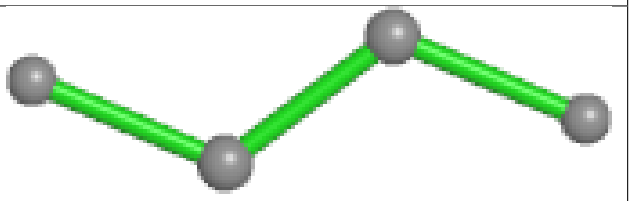
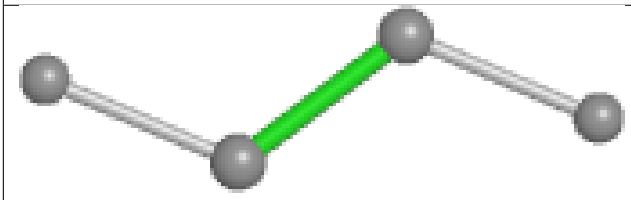
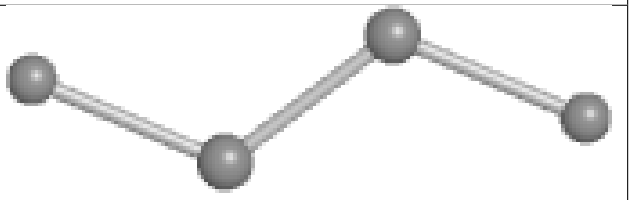
Bond angles



Torsions



Rings

Ligand EDO D 304	
 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%)	-0.02	3 (1%) 82 84	19, 25, 42, 54	0
1	B	295/310 (95%)	0.07	3 (1%) 82 84	19, 27, 45, 58	0
1	C	295/310 (95%)	0.09	0 100 100	20, 27, 44, 54	0
1	D	295/310 (95%)	0.10	2 (0%) 87 88	20, 27, 44, 51	0
1	E	295/310 (95%)	-0.04	3 (1%) 82 84	19, 28, 45, 59	0
1	F	296/310 (95%)	0.06	3 (1%) 82 84	19, 28, 47, 56	0
All	All	1771/1860 (95%)	0.04	14 (0%) 86 87	19, 27, 45, 59	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ASN	3.3
1	B	267	GLU	2.9
1	F	29	ARG	2.9
1	E	131	ASP	2.7
1	F	261	TYR	2.7
1	F	19	ASN	2.6
1	B	280	LYS	2.4
1	E	95	PHE	2.3
1	D	19	ASN	2.2
1	A	29	ARG	2.2
1	A	56	HIS	2.2
1	E	127	ALA	2.1
1	B	95	PHE	2.1
1	D	292	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	F	166	14/15	0.93	0.13	19,25,31,31	0
1	KPI	E	166	14/15	0.94	0.10	23,24,28,28	0
1	KPI	C	166	14/15	0.95	0.15	15,24,28,29	0
1	KPI	D	166	14/15	0.96	0.12	20,25,29,32	0
1	KPI	B	166	14/15	0.96	0.11	16,21,30,31	0
1	KPI	A	166	14/15	0.96	0.11	18,21,28,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	EDO	A	307	4/4	0.24	0.36	63,66,66,69	0
4	ACT	A	314	4/4	0.69	0.21	37,38,50,59	0
4	ACT	D	314	4/4	0.69	0.17	49,51,53,54	0
8	PEG	D	318	7/7	0.70	0.32	45,46,55,59	0
4	ACT	E	311	4/4	0.75	0.29	36,42,45,55	0
4	ACT	D	315	4/4	0.77	0.19	38,49,51,53	0
3	MG	A	312	1/1	0.78	0.12	56,56,56,56	0
3	MG	E	308	1/1	0.80	0.15	59,59,59,59	0
4	ACT	F	308	4/4	0.80	0.18	42,44,48,53	0
5	PGE	E	314	10/10	0.80	0.40	20,20,20,20	0
2	EDO	B	303	4/4	0.80	0.25	35,36,48,54	0
5	PGE	B	312	10/10	0.81	0.17	44,50,56,58	0
8	PEG	E	316	7/7	0.81	0.42	20,20,20,20	0
2	EDO	D	308	4/4	0.82	0.25	43,45,48,49	0
4	ACT	A	315	4/4	0.83	0.19	32,35,40,46	0
2	EDO	F	302	4/4	0.83	0.20	27,43,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PEG	D	319	7/7	0.83	0.15	39,47,52,55	0
2	EDO	C	303	4/4	0.83	0.15	51,54,58,59	0
3	MG	A	311	1/1	0.84	0.40	54,54,54,54	0
4	ACT	B	308	4/4	0.84	0.25	37,38,39,44	0
4	ACT	D	313	4/4	0.84	0.22	35,39,42,44	0
4	ACT	E	310	4/4	0.85	0.16	31,36,38,40	0
5	PGE	E	313	10/10	0.86	0.14	41,44,50,58	0
2	EDO	A	305	4/4	0.86	0.13	39,43,50,53	0
3	MG	F	305	1/1	0.86	0.23	54,54,54,54	0
2	EDO	B	304	4/4	0.86	0.20	29,34,45,48	0
8	PEG	D	320	7/7	0.86	0.47	20,20,20,20	0
2	EDO	E	306	4/4	0.86	0.35	20,20,20,20	0
7	PG4	D	317	13/13	0.87	0.14	32,45,49,56	0
3	MG	D	311	1/1	0.87	0.09	41,41,41,41	0
2	EDO	C	305	4/4	0.87	0.20	32,33,37,44	0
3	MG	E	309	1/1	0.87	0.29	54,54,54,54	0
2	EDO	B	302	4/4	0.87	0.12	39,44,48,50	0
2	EDO	B	301	4/4	0.88	0.12	38,41,42,45	0
4	ACT	B	309	4/4	0.88	0.11	41,47,49,49	0
2	EDO	E	302	4/4	0.89	0.16	36,41,42,57	0
2	EDO	C	304	4/4	0.89	0.14	45,47,48,59	0
2	EDO	E	307	4/4	0.89	0.37	20,20,20,20	0
4	ACT	A	313	4/4	0.89	0.15	34,40,40,47	0
2	EDO	C	301	4/4	0.89	0.12	43,46,48,51	0
3	MG	A	308	1/1	0.89	0.24	47,47,47,47	0
6	HIS	B	313	11/11	0.89	0.13	27,33,39,41	0
3	MG	A	309	1/1	0.89	0.18	57,57,57,57	0
2	EDO	D	304	4/4	0.89	0.19	35,40,45,54	0
2	EDO	D	306	4/4	0.89	0.11	39,41,49,50	0
3	MG	D	310	1/1	0.89	0.14	41,41,41,41	0
2	EDO	A	306	4/4	0.89	0.10	34,37,42,45	0
4	ACT	F	307	4/4	0.90	0.13	38,39,47,48	0
3	MG	C	307	1/1	0.90	0.25	52,52,52,52	0
5	PGE	B	311	10/10	0.90	0.12	31,34,44,45	0
2	EDO	E	301	4/4	0.90	0.10	34,34,36,42	0
5	PGE	D	316	10/10	0.91	0.12	37,39,44,54	0
2	EDO	D	305	4/4	0.91	0.10	39,39,49,52	0
2	EDO	E	305	4/4	0.91	0.35	20,20,20,20	0
2	EDO	B	305	4/4	0.91	0.14	39,41,42,50	0
6	HIS	C	310	11/11	0.91	0.15	24,30,37,37	0
6	HIS	D	321	11/11	0.91	0.12	27,31,37,38	0
6	HIS	E	317	11/11	0.91	0.12	27,32,35,36	0

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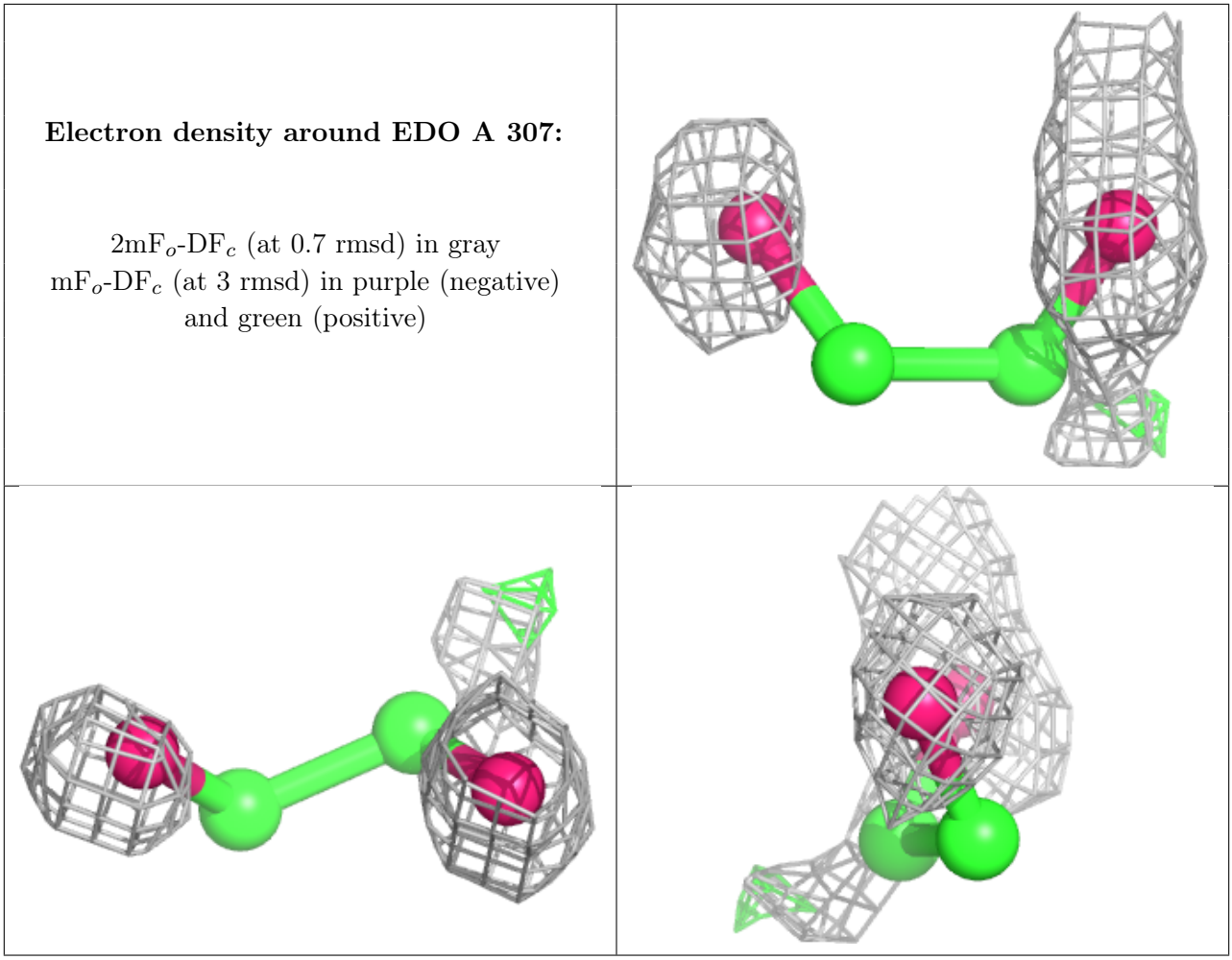
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	F	306	4/4	0.91	0.17	38,38,44,48	0
2	EDO	C	306	4/4	0.91	0.34	33,40,43,51	0
4	ACT	B	310	4/4	0.91	0.11	46,51,54,56	0
3	MG	B	307	1/1	0.91	0.15	42,42,42,42	0
8	PEG	E	315	7/7	0.91	0.12	36,45,54,55	0
2	EDO	A	303	4/4	0.91	0.11	33,37,44,46	0
2	EDO	F	303	4/4	0.92	0.16	33,39,40,50	0
2	EDO	A	301	4/4	0.92	0.12	25,29,32,39	0
2	EDO	E	304	4/4	0.92	0.12	29,30,36,43	0
4	ACT	C	308	4/4	0.92	0.21	34,36,40,45	0
5	PGE	A	316	10/10	0.92	0.10	31,38,45,47	0
2	EDO	D	303	4/4	0.93	0.13	41,42,42,52	0
6	HIS	A	317	11/11	0.93	0.14	26,31,38,39	0
5	PGE	E	312	10/10	0.93	0.17	37,41,46,53	0
5	PGE	C	309	10/10	0.93	0.09	32,37,41,57	0
2	EDO	E	303	4/4	0.94	0.11	41,41,41,49	0
3	MG	A	310	1/1	0.94	0.08	33,33,33,33	0
2	EDO	D	309	4/4	0.94	0.11	42,43,47,47	0
2	EDO	D	307	4/4	0.94	0.14	31,35,40,51	0
2	EDO	D	301	4/4	0.94	0.13	27,35,40,45	0
2	EDO	A	304	4/4	0.95	0.08	41,42,52,56	0
2	EDO	D	302	4/4	0.96	0.11	28,28,29,35	0
2	EDO	C	302	4/4	0.96	0.17	30,31,38,39	0
2	EDO	F	304	4/4	0.96	0.17	29,35,43,51	0
6	HIS	F	309	11/11	0.96	0.12	29,34,39,43	0
2	EDO	A	302	4/4	0.96	0.20	31,42,43,49	0
3	MG	B	306	1/1	0.97	0.10	28,28,28,28	0
2	EDO	F	301	4/4	0.98	0.15	22,25,26,31	0
3	MG	D	312	1/1	0.99	0.10	39,39,39,39	0

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

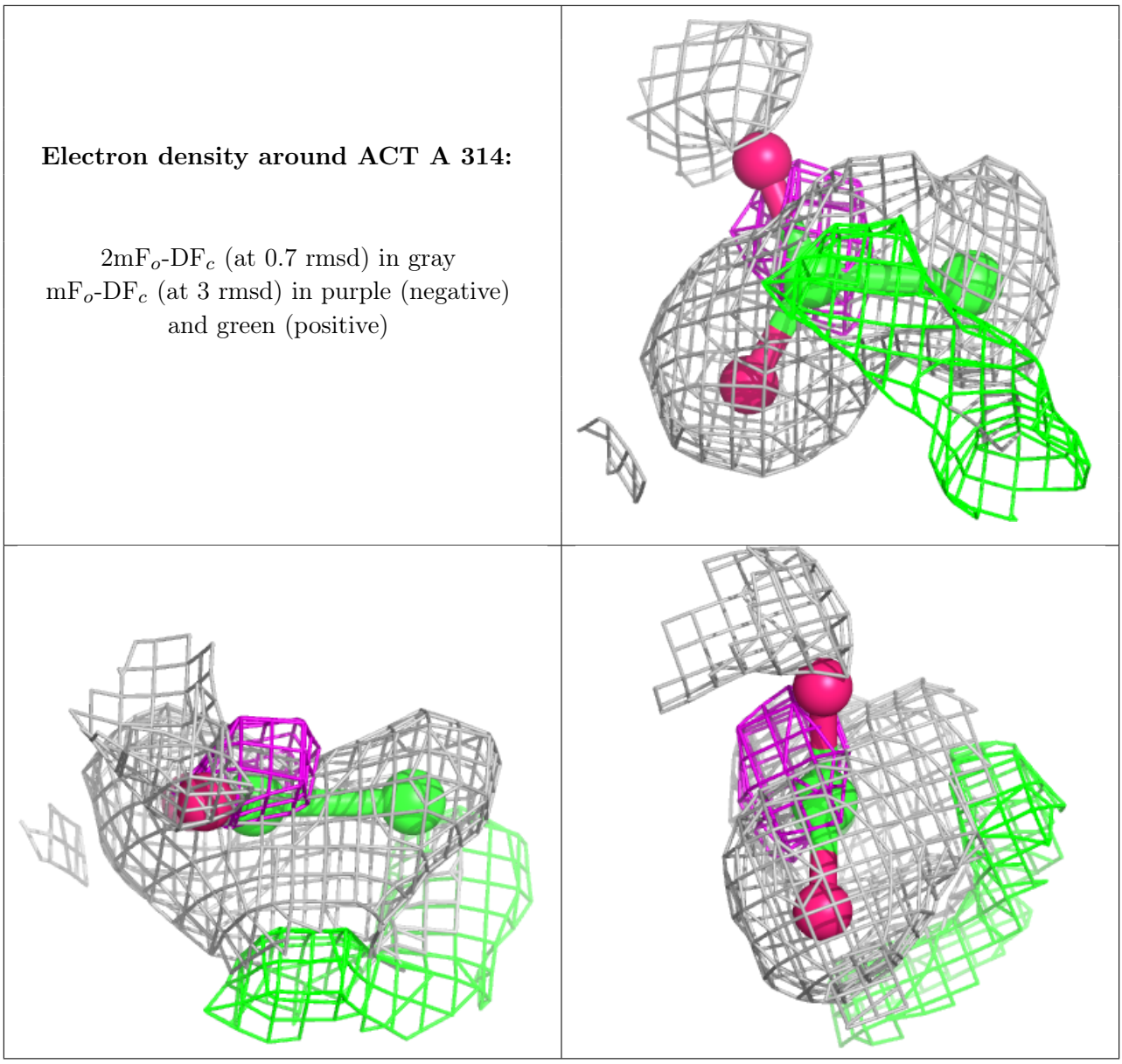
Electron density around EDO A 307:

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



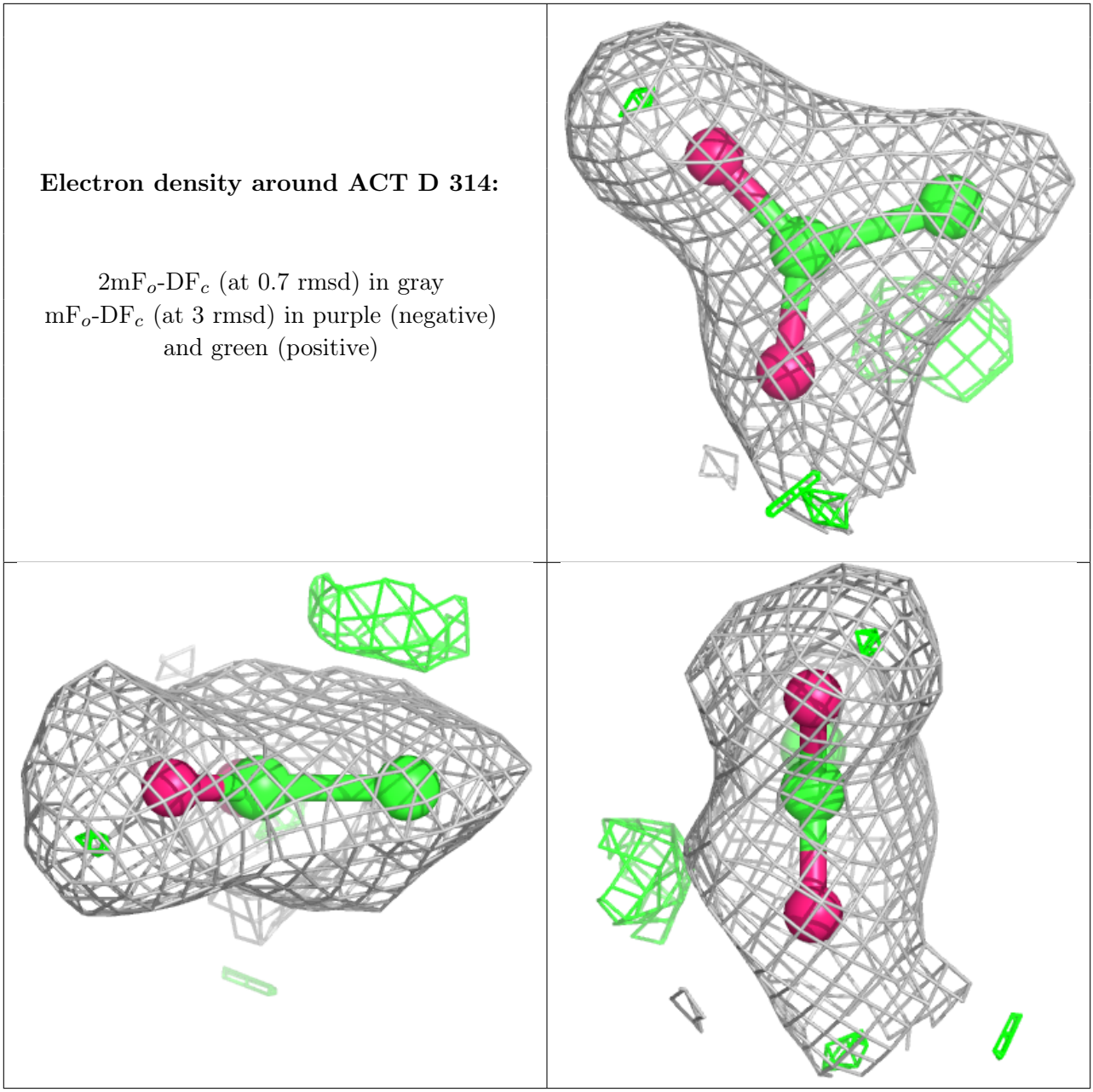
Electron density around ACT A 314:

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



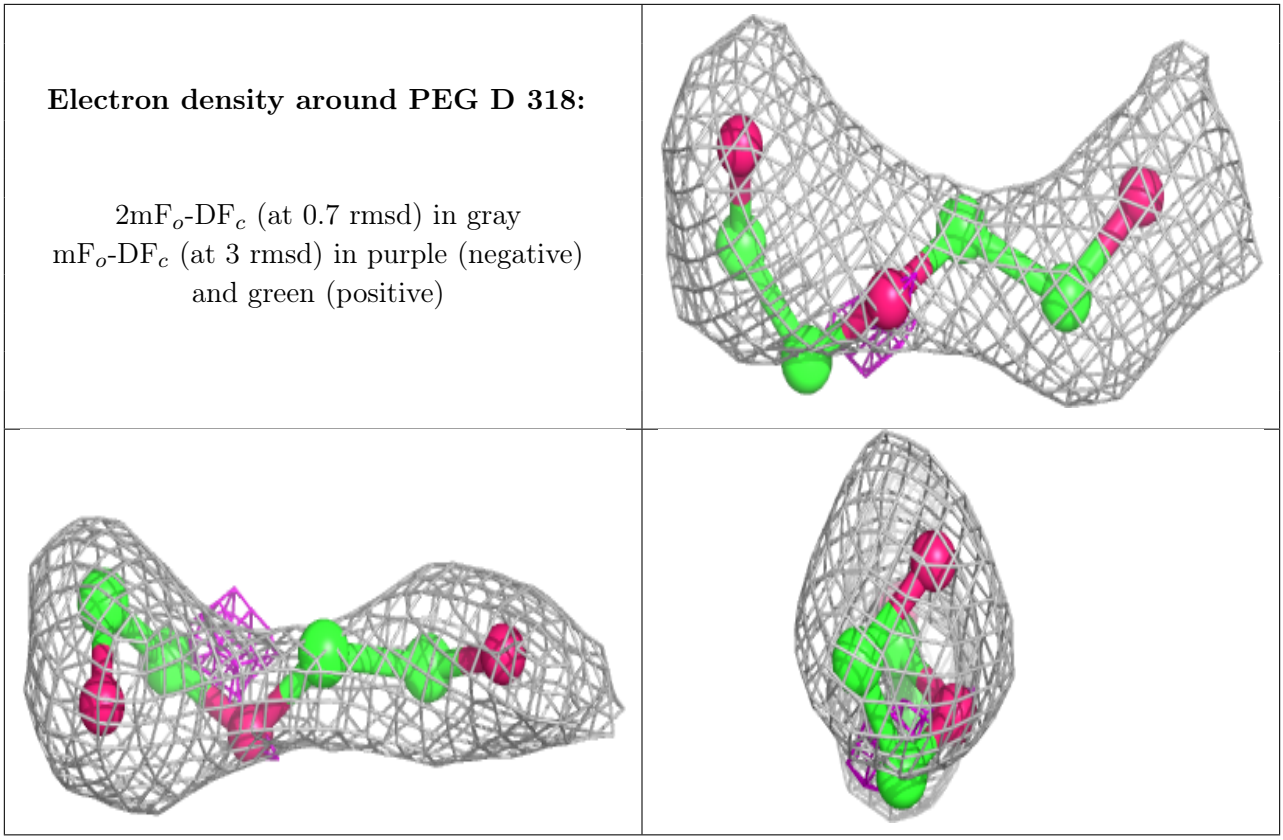
Electron density around ACT D 314:

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



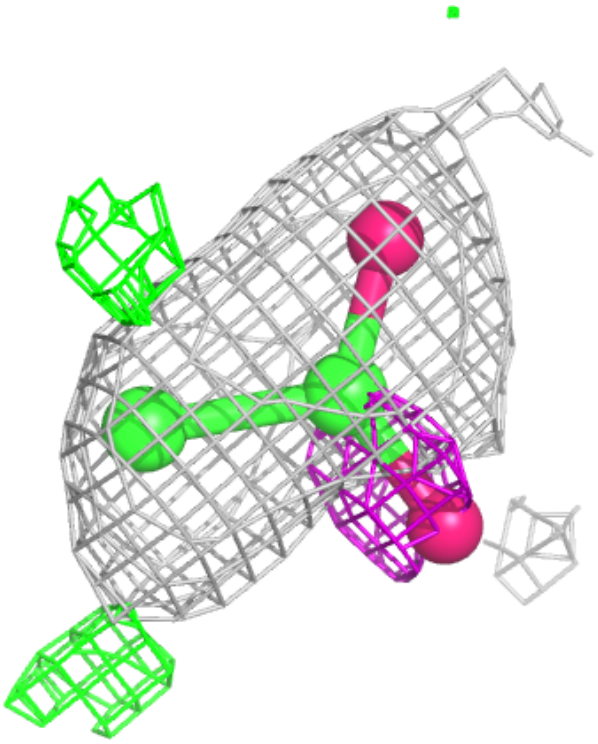
Electron density around PEG D 318:

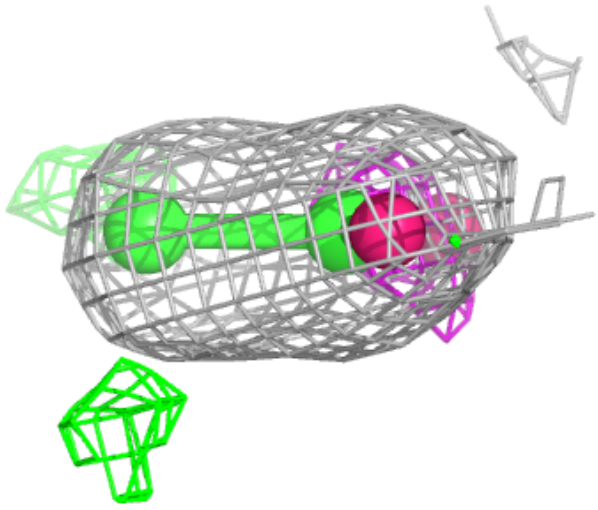
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

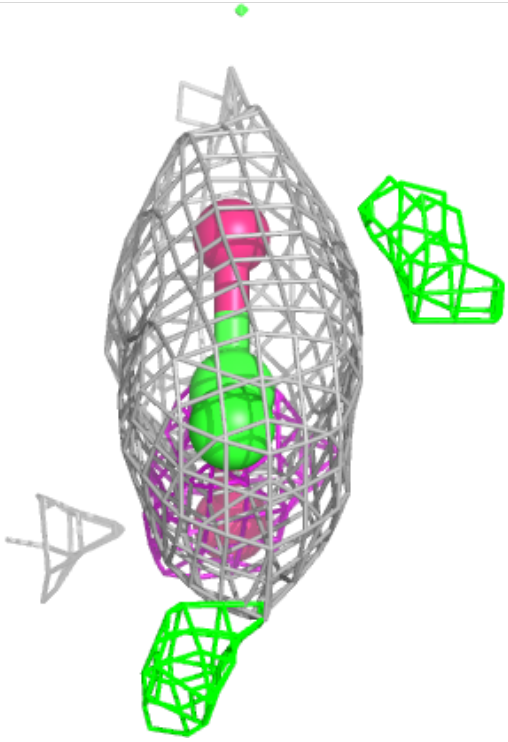


Electron density around ACT E 311:

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

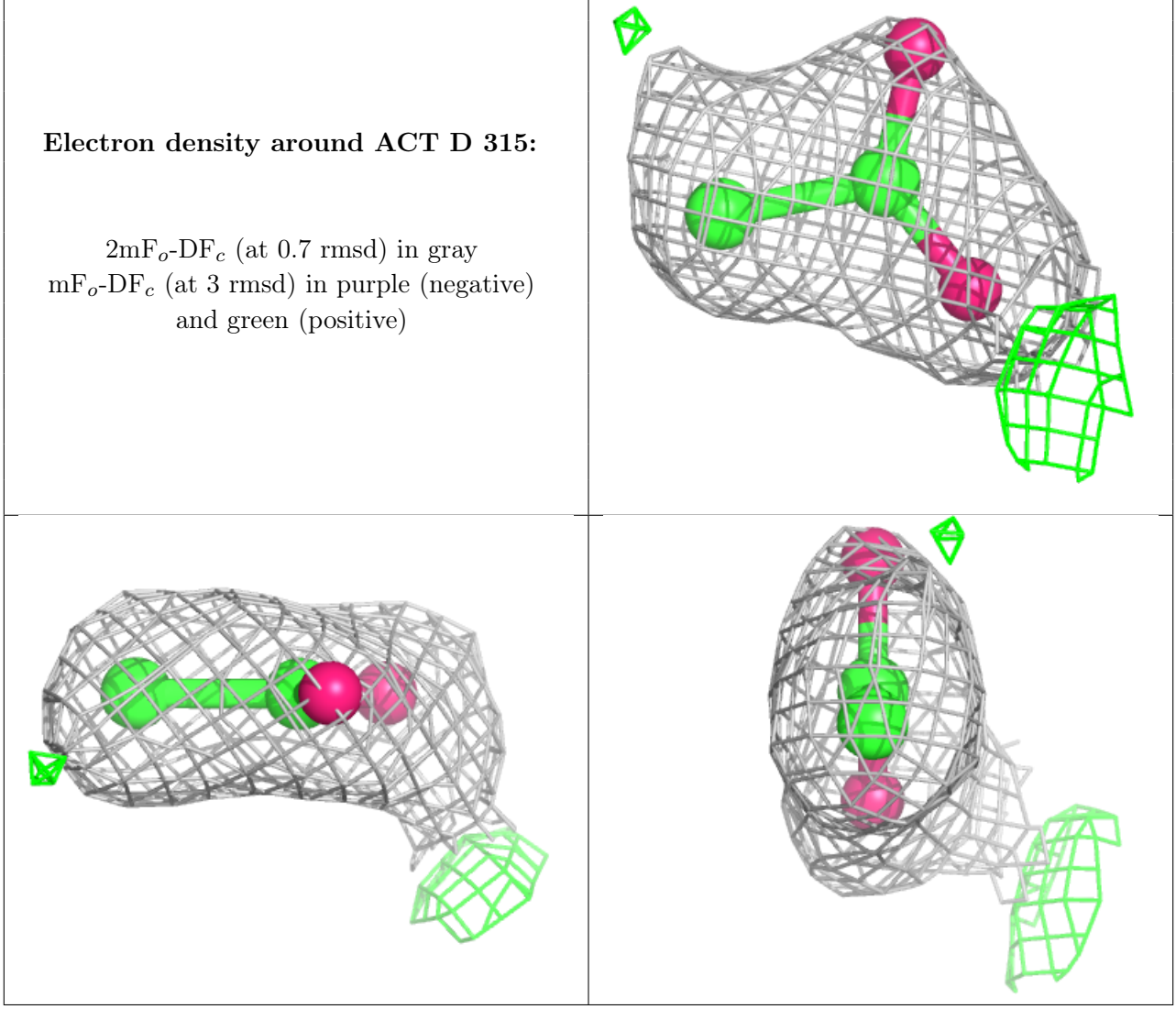






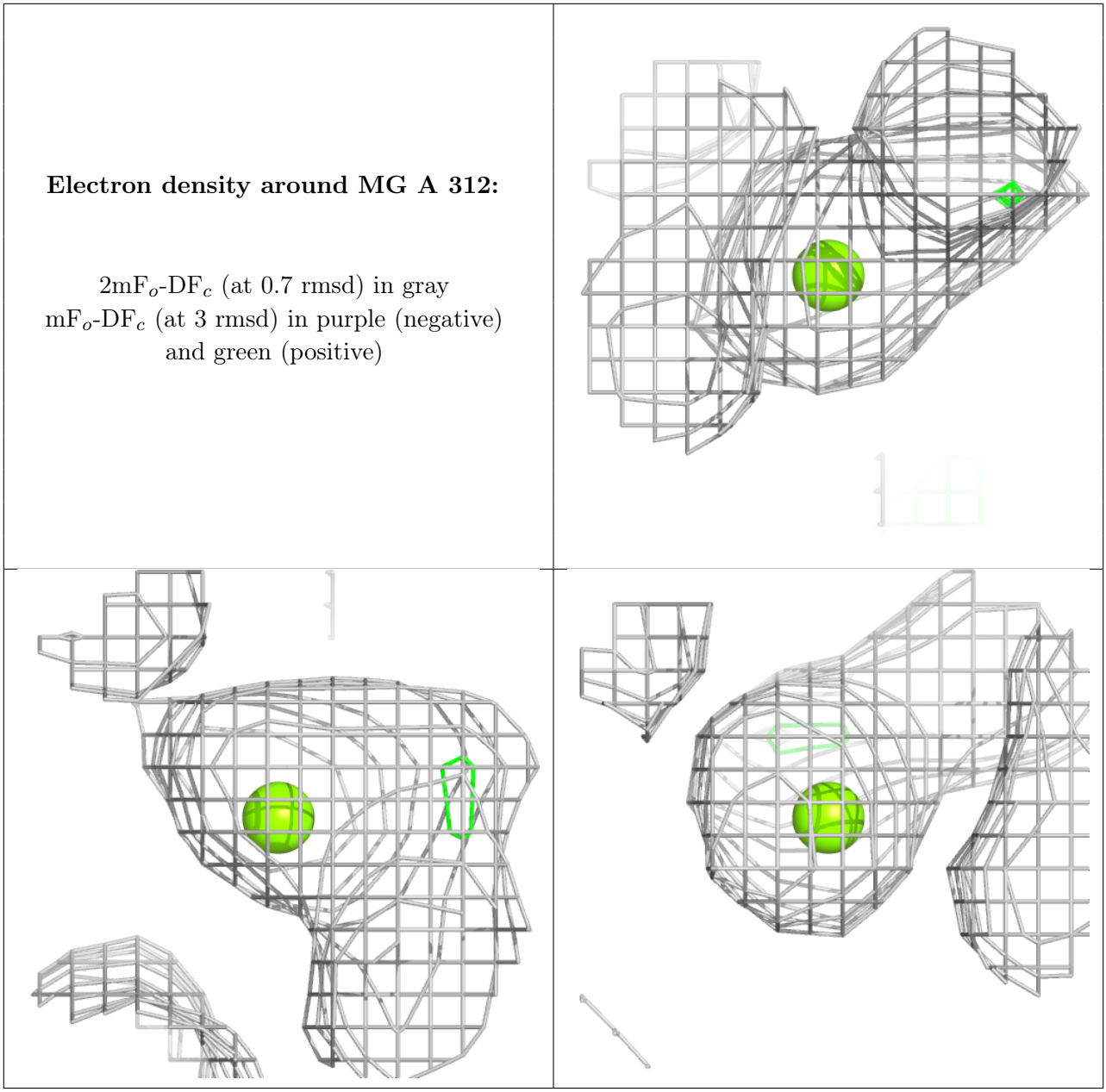
Electron density around ACT D 315:

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



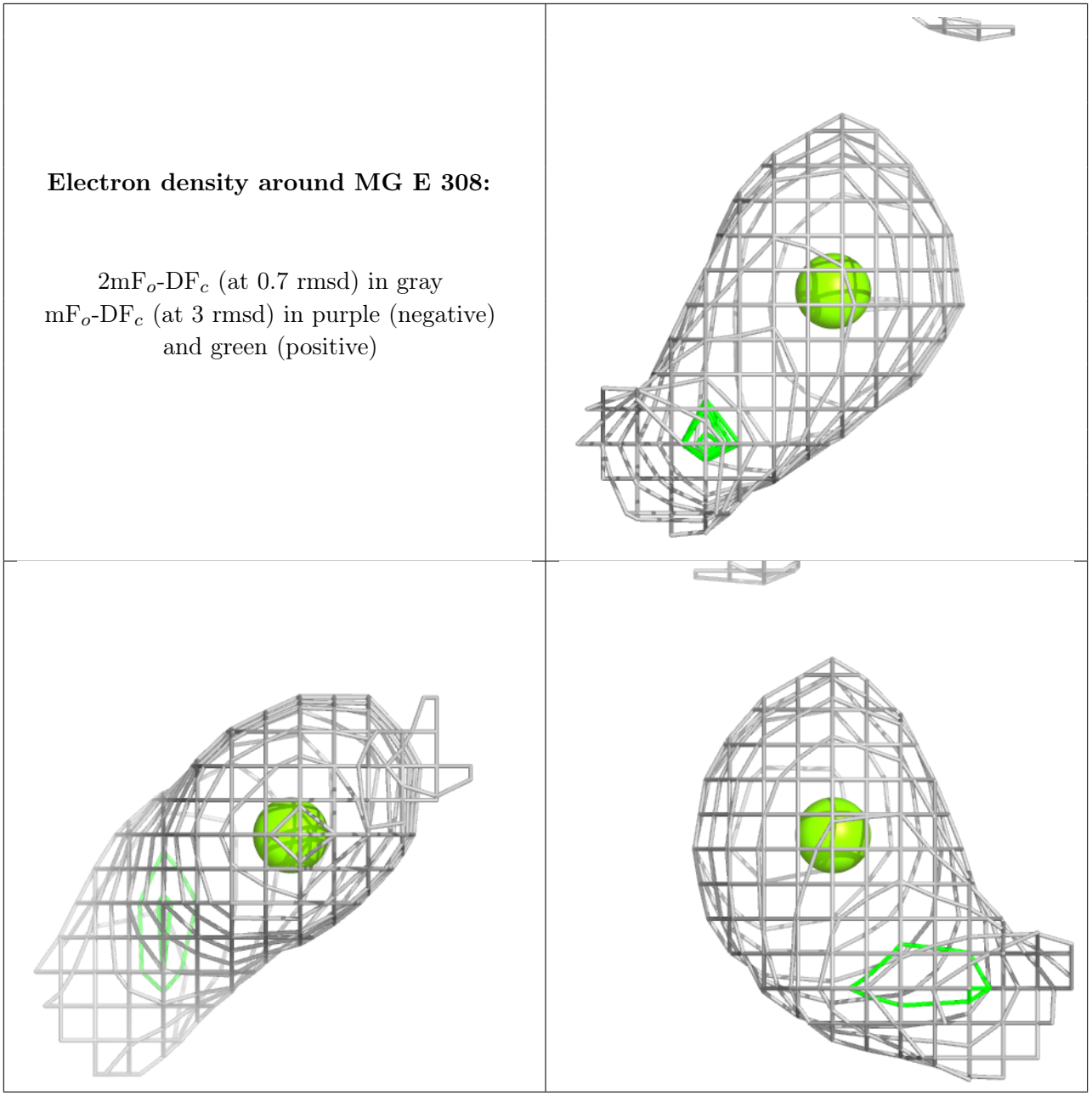
Electron density around MG A 312:

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



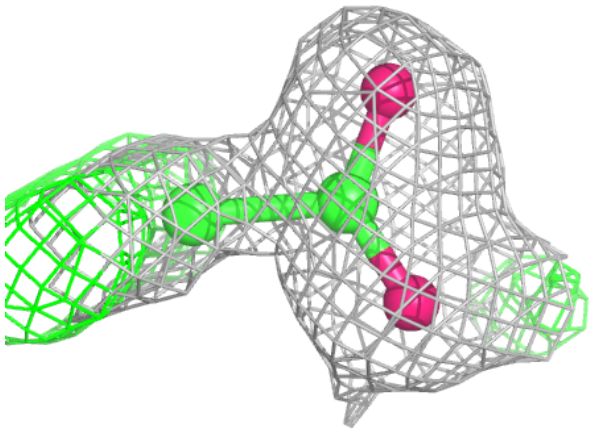
Electron density around MG E 308:

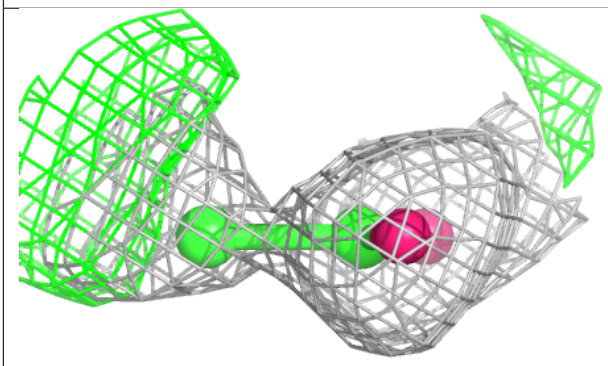
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

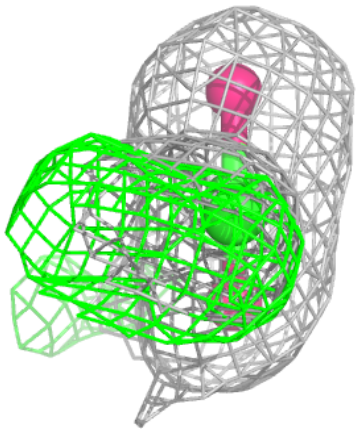


Electron density around ACT F 308:

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

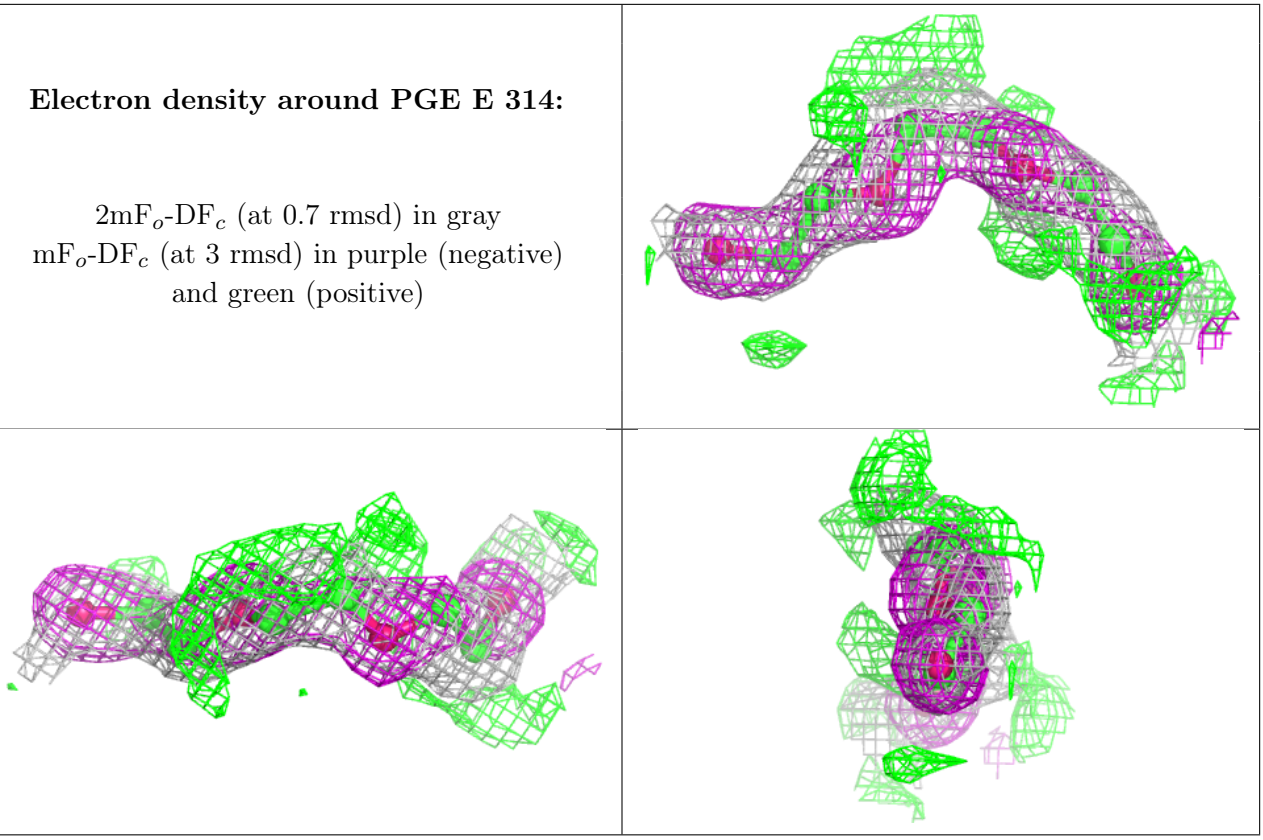






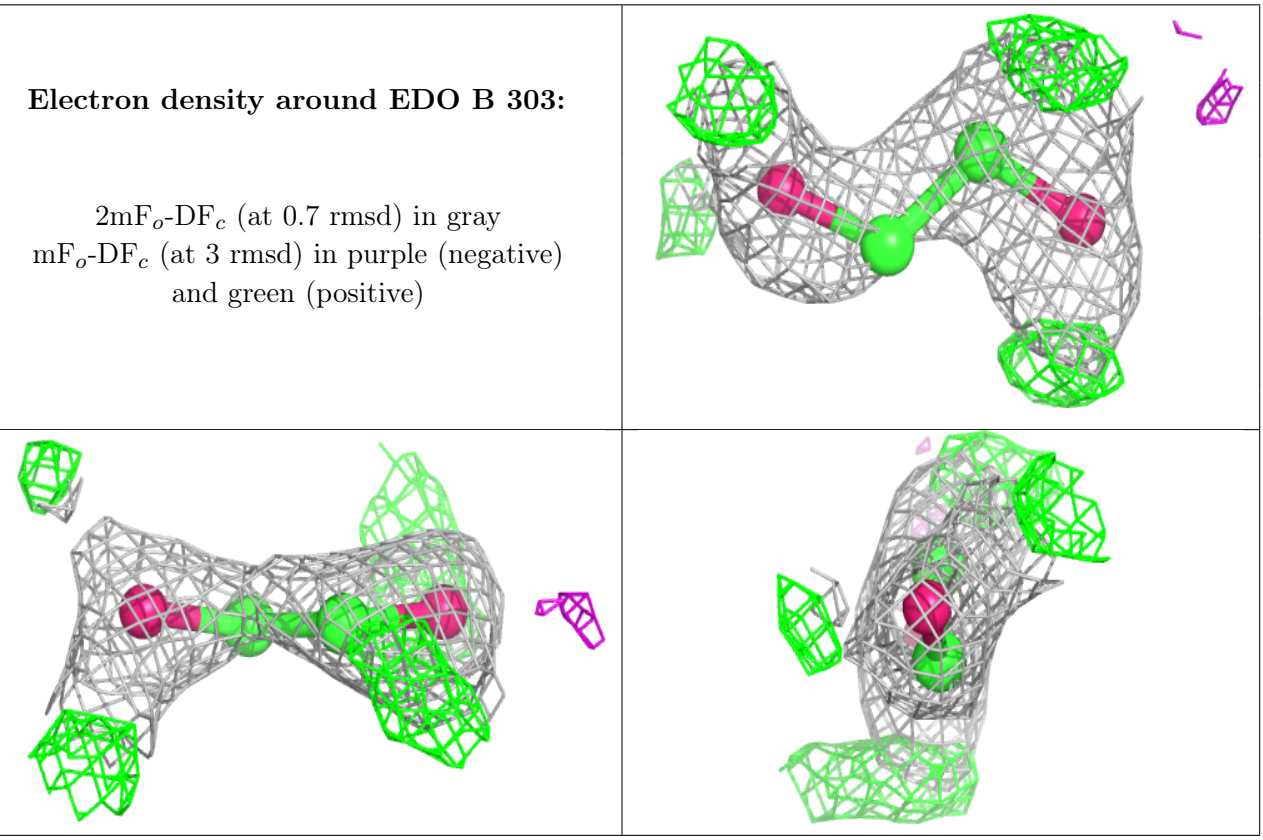
Electron density around PGE E 314:

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



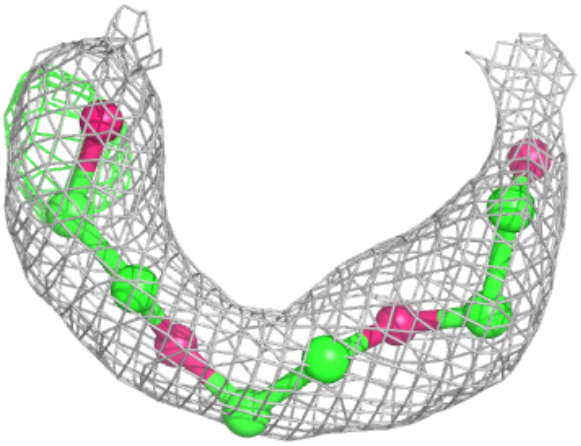
Electron density around EDO B 303:

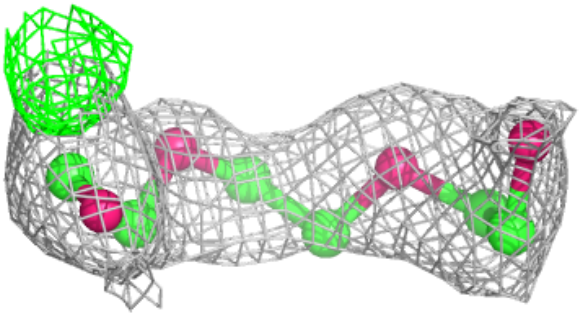
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

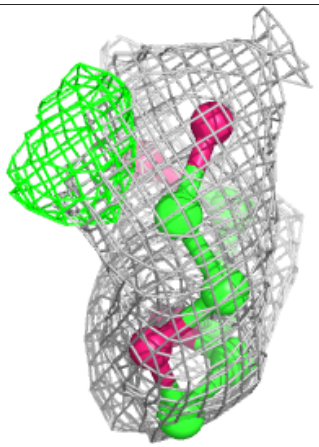


Electron density around PGE B 312:

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

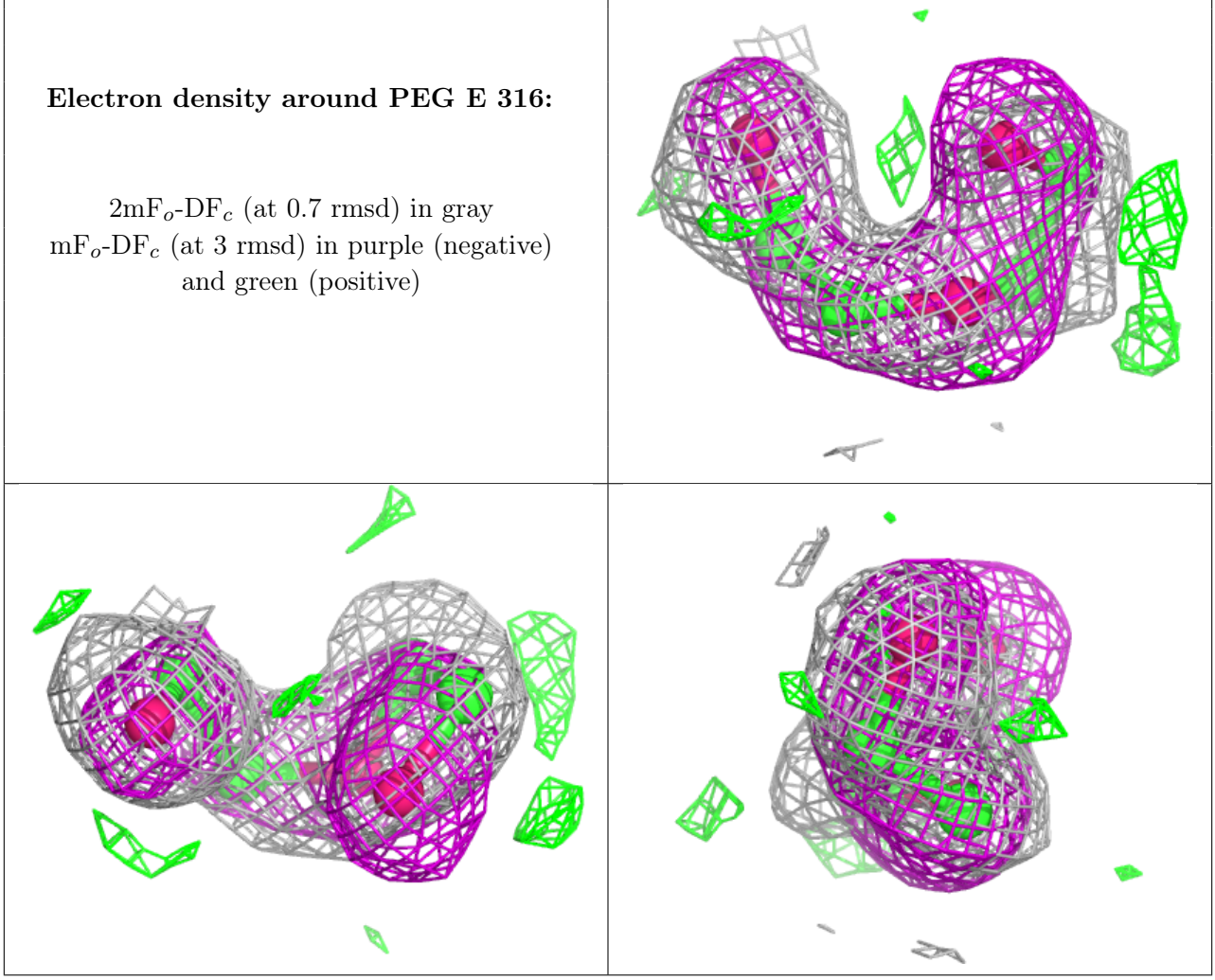






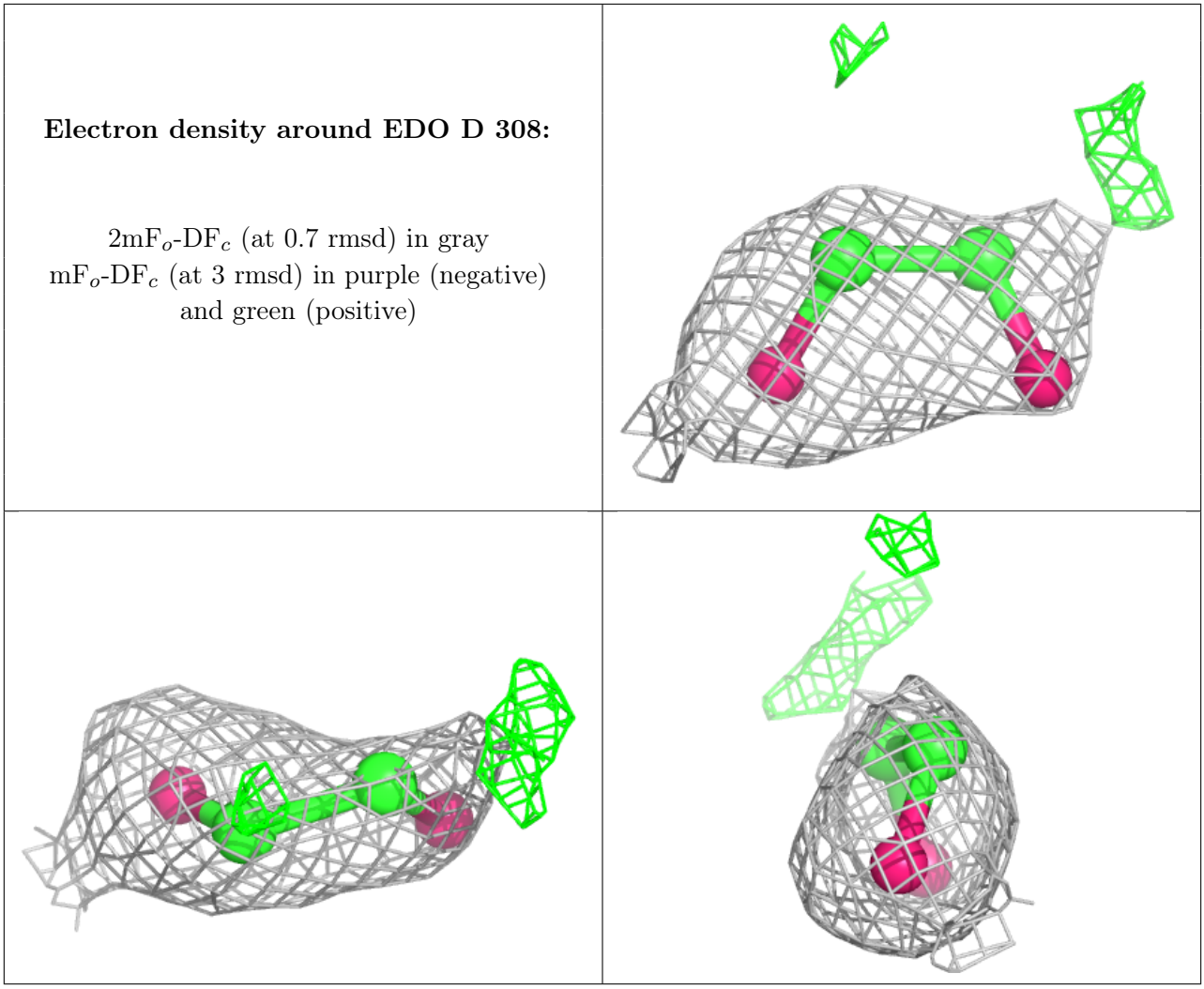
Electron density around PEG E 316:

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



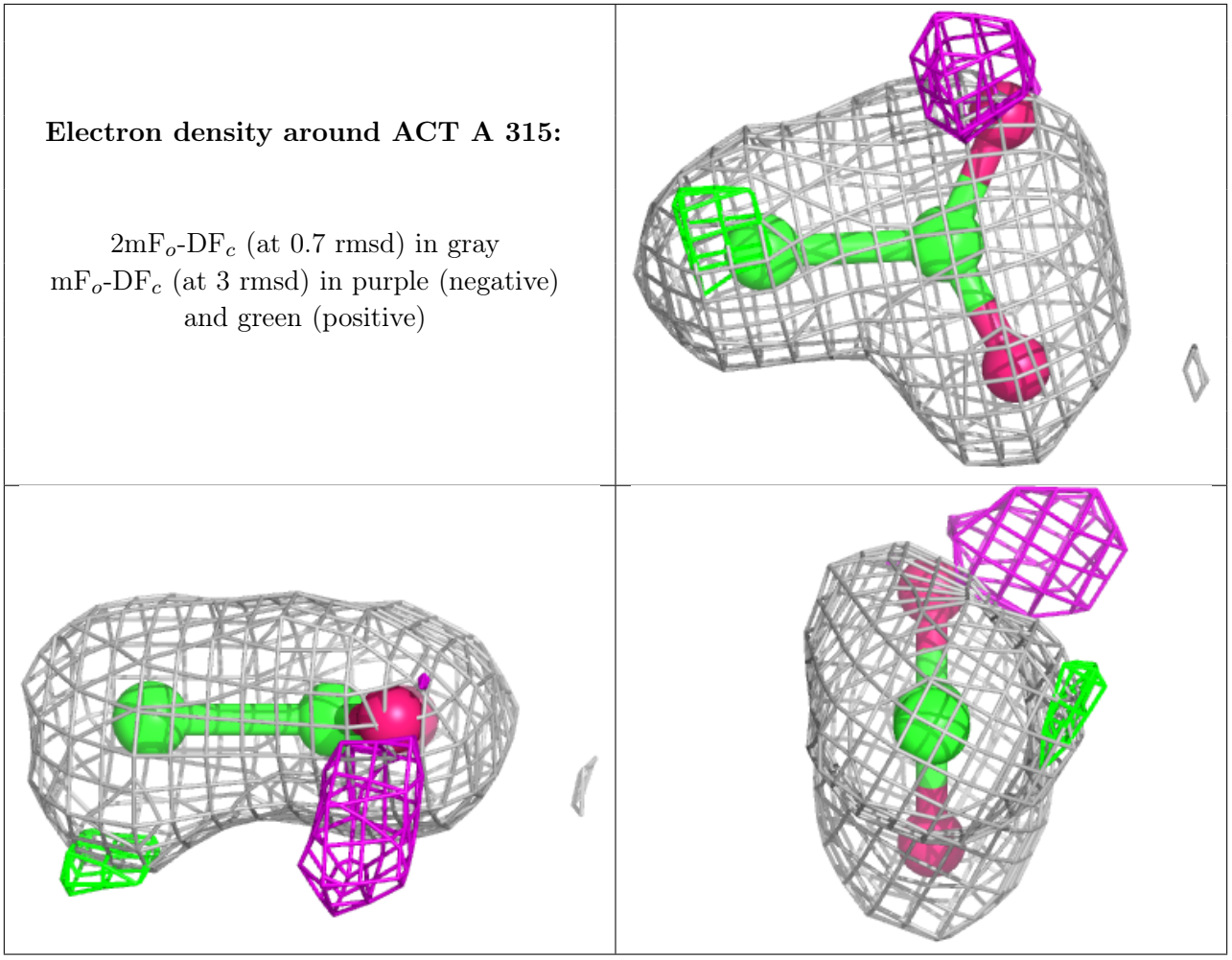
Electron density around EDO D 308:

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



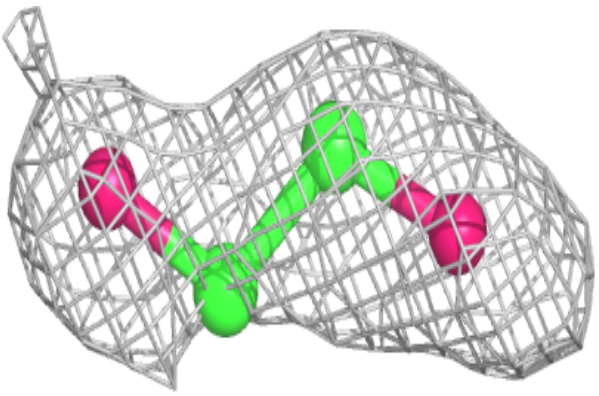
Electron density around ACT A 315:

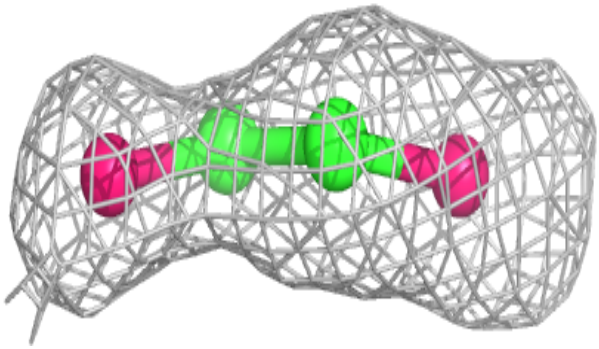
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

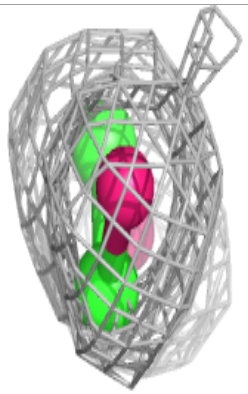


Electron density around EDO F 302:

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

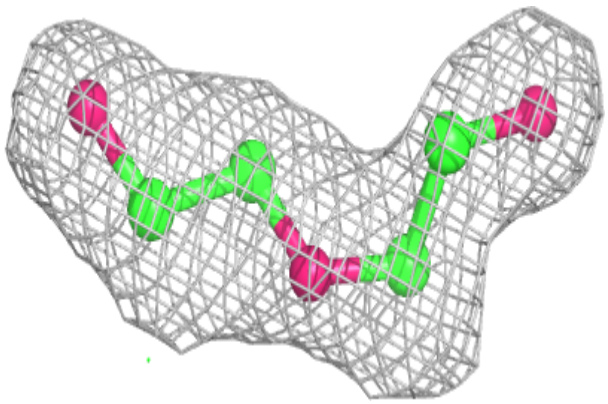


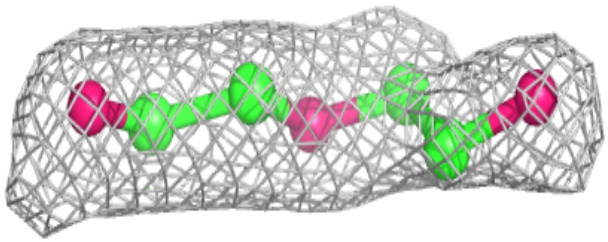


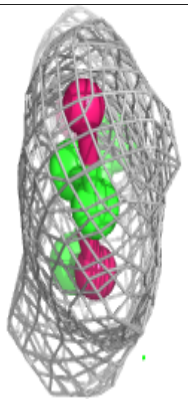


Electron density around PEG D 319:

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

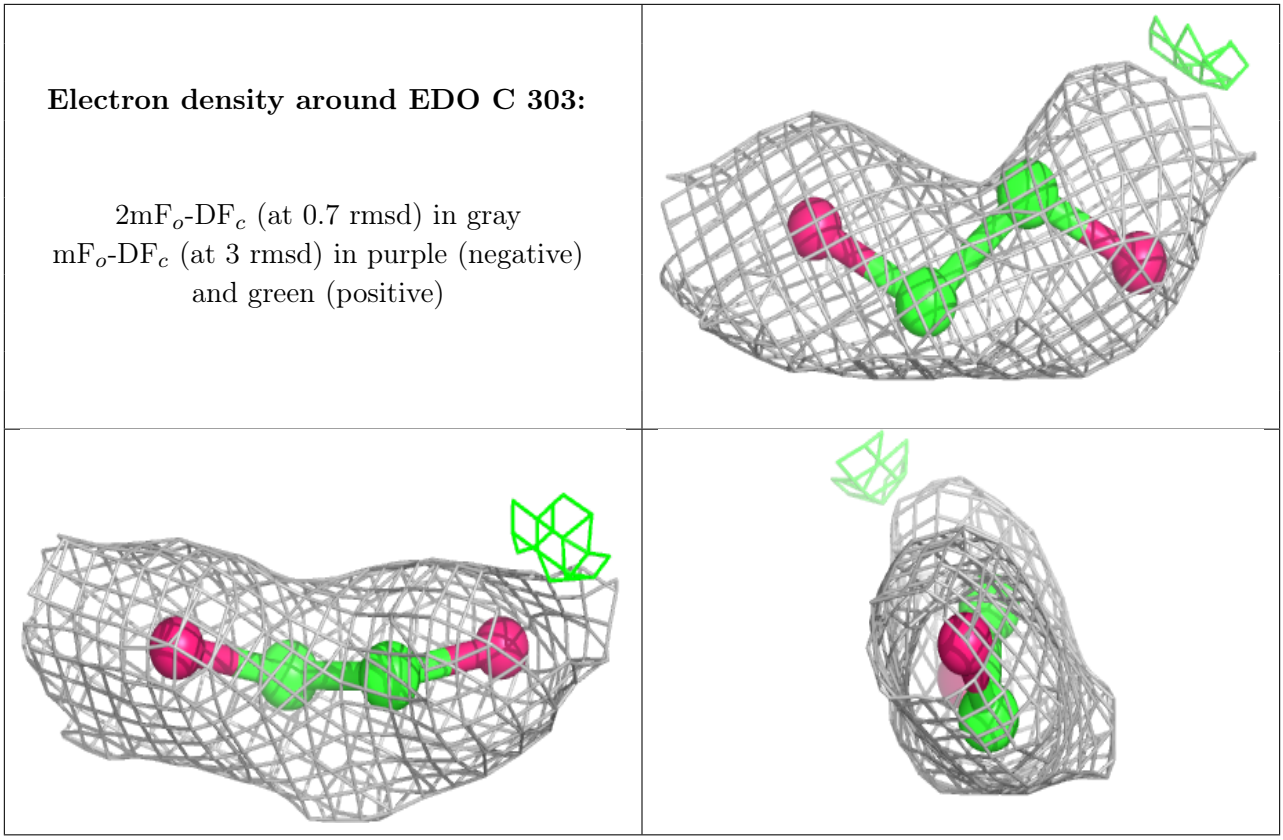






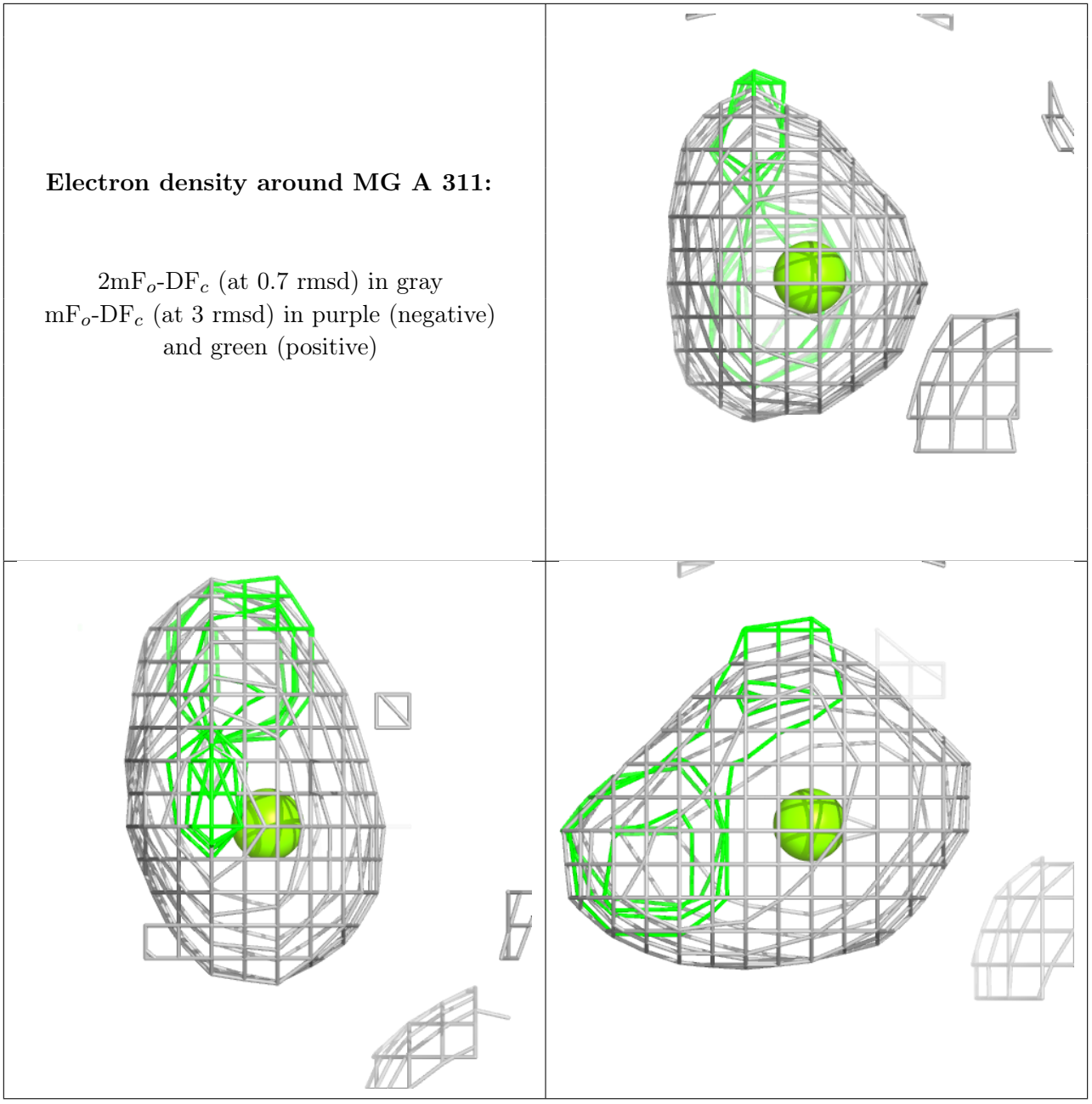
Electron density around EDO C 303:

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



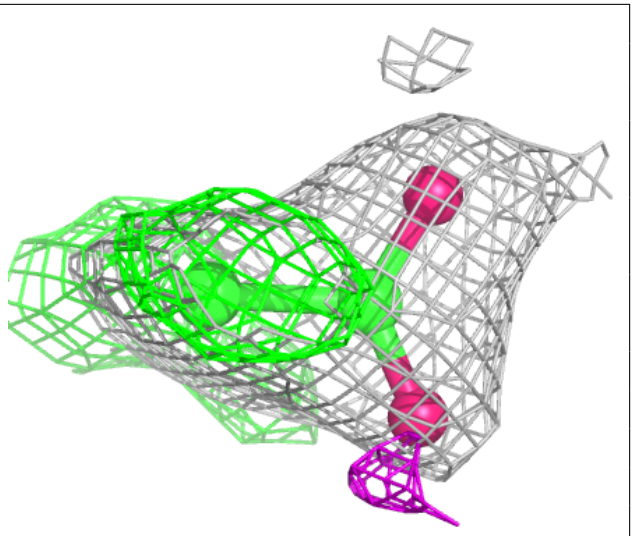
Electron density around MG A 311:

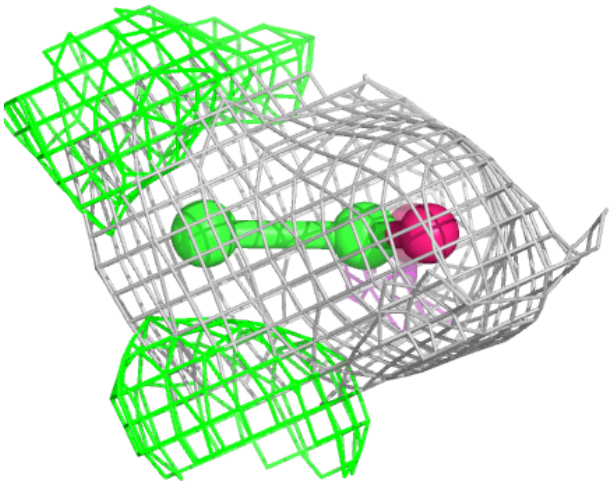
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

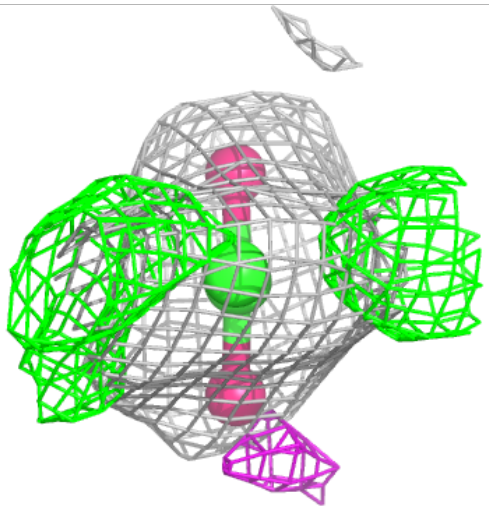


Electron density around ACT B 308:

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

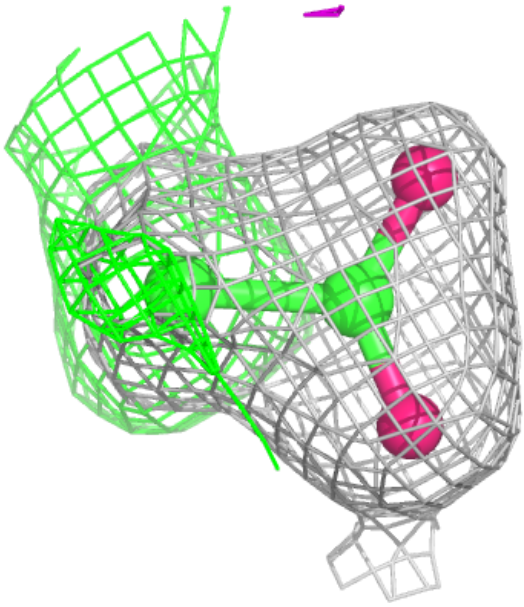


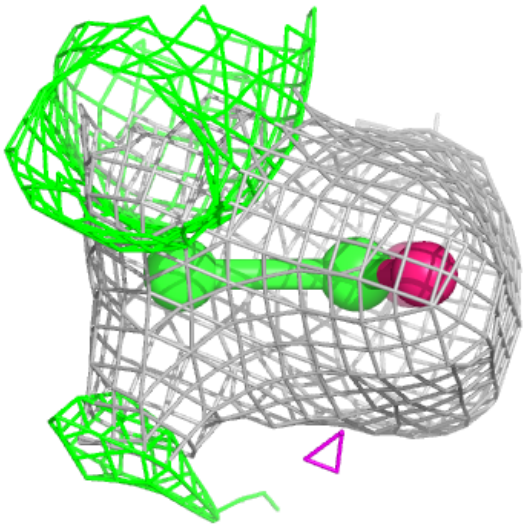


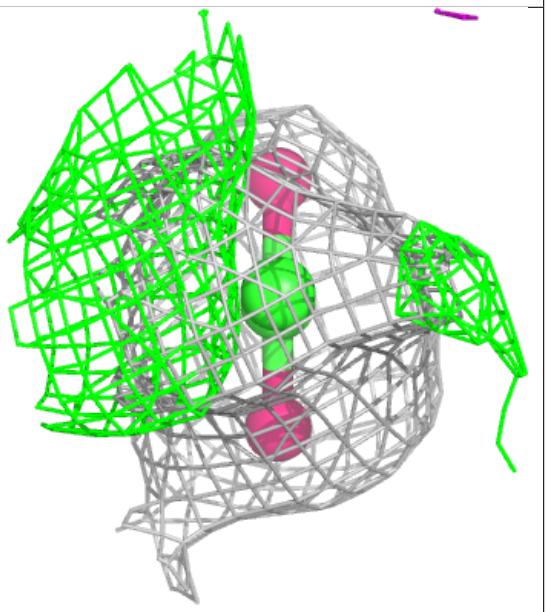


Electron density around ACT D 313:

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

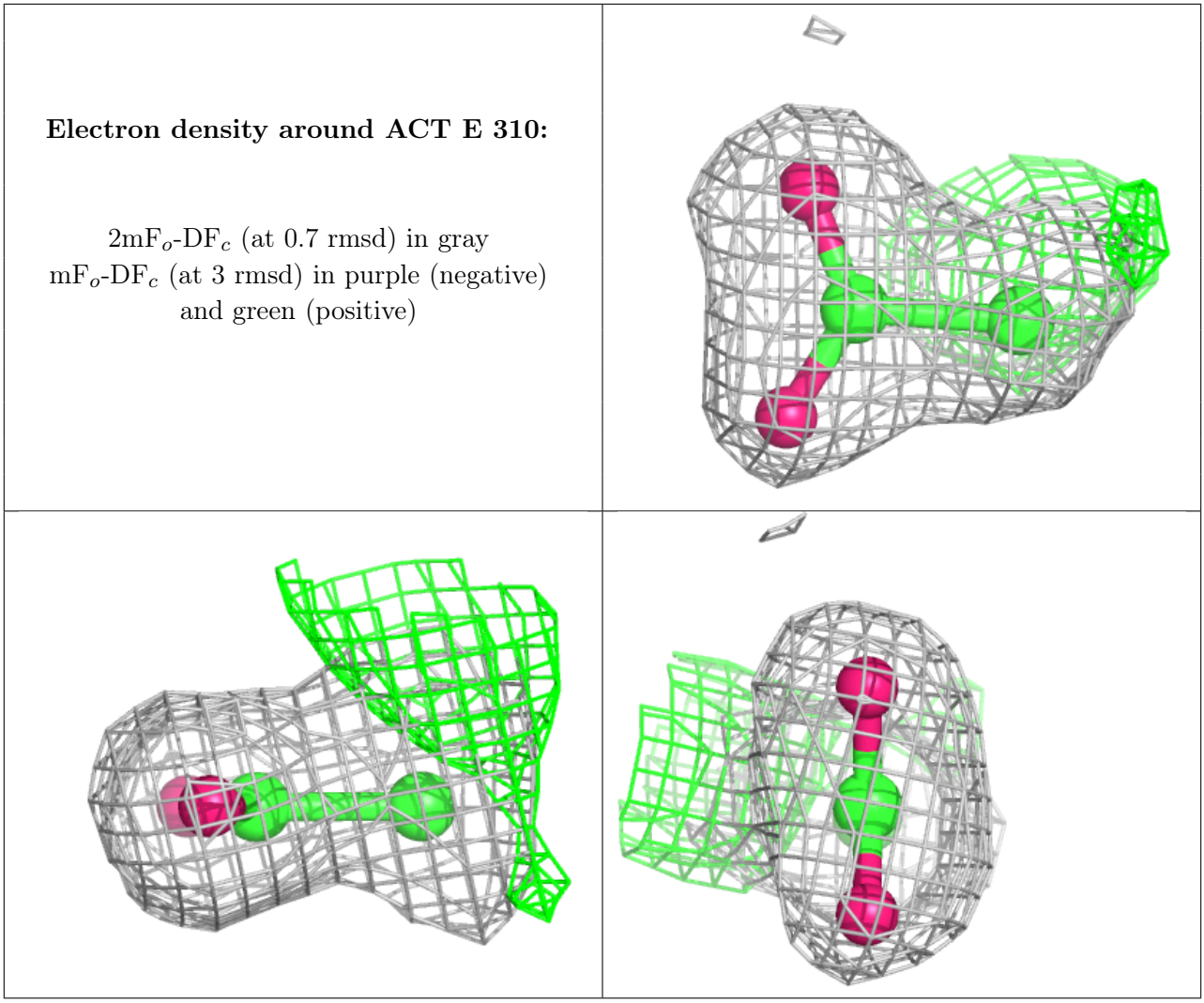






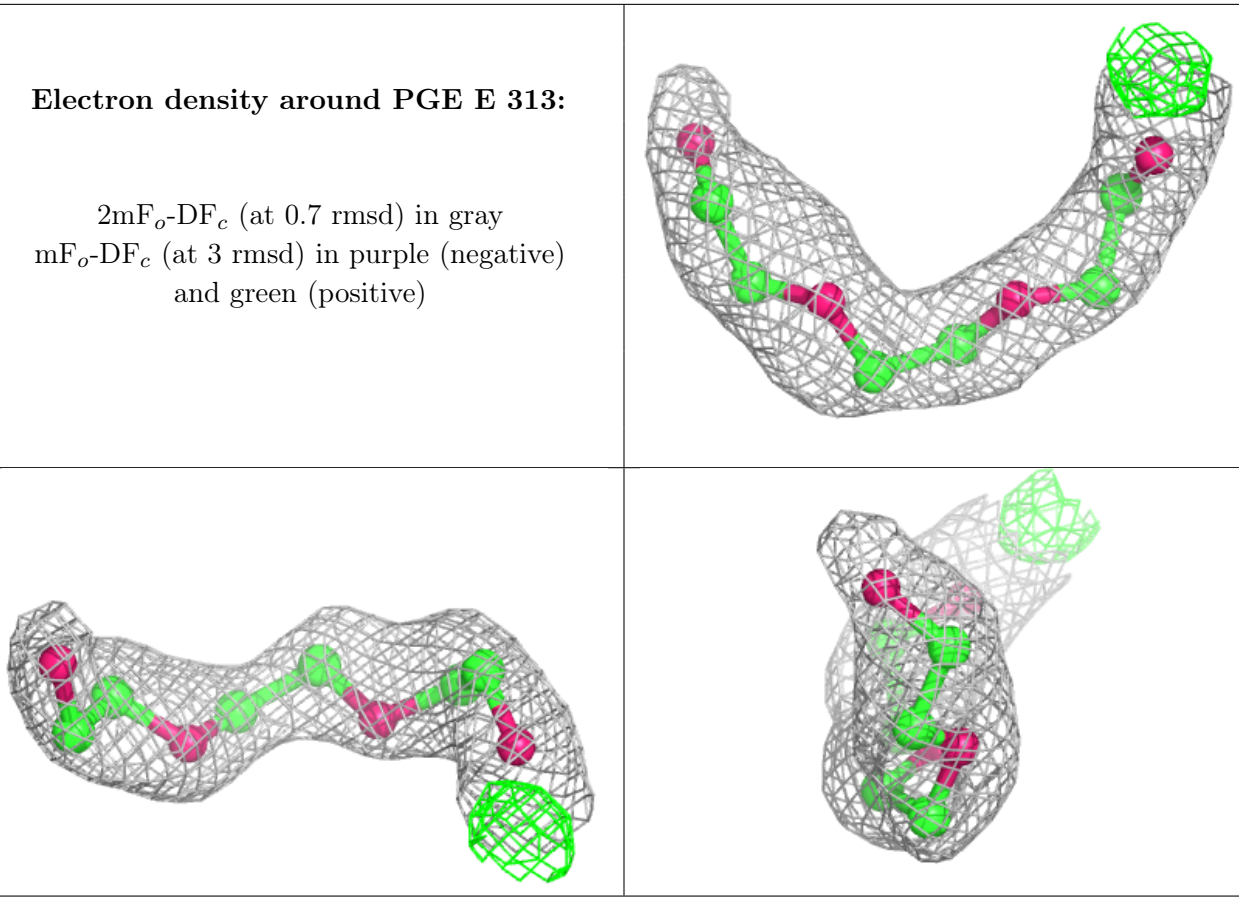
Electron density around ACT E 310:

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



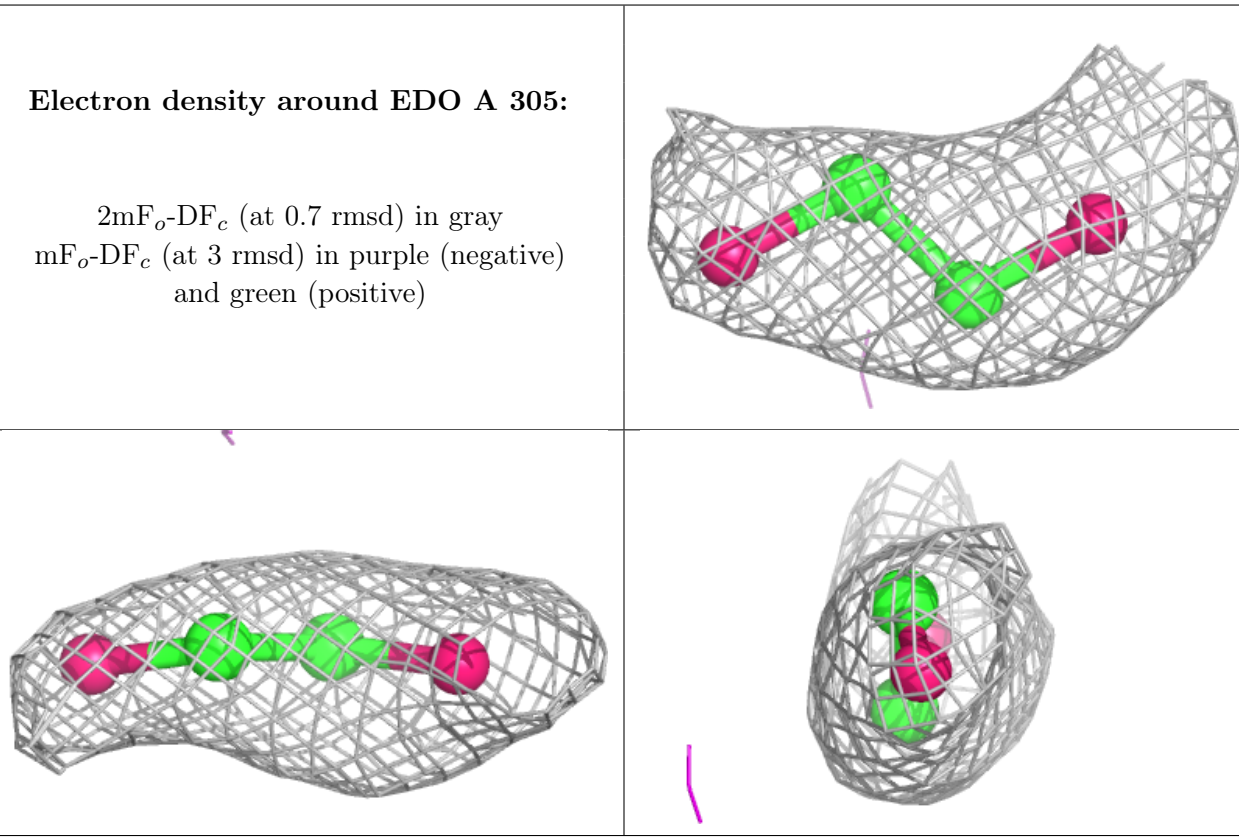
Electron density around PGE E 313:

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



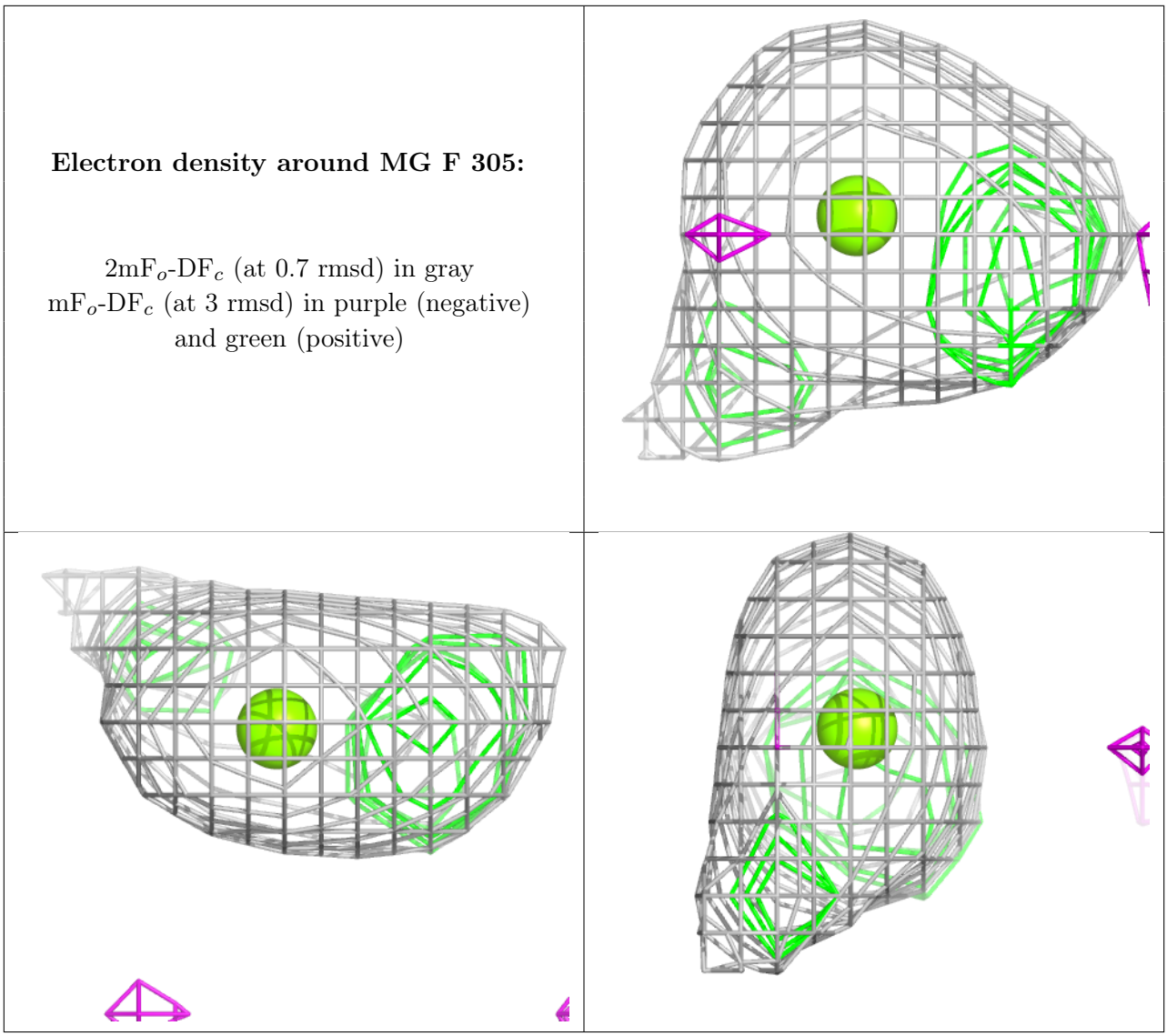
Electron density around EDO A 305:

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



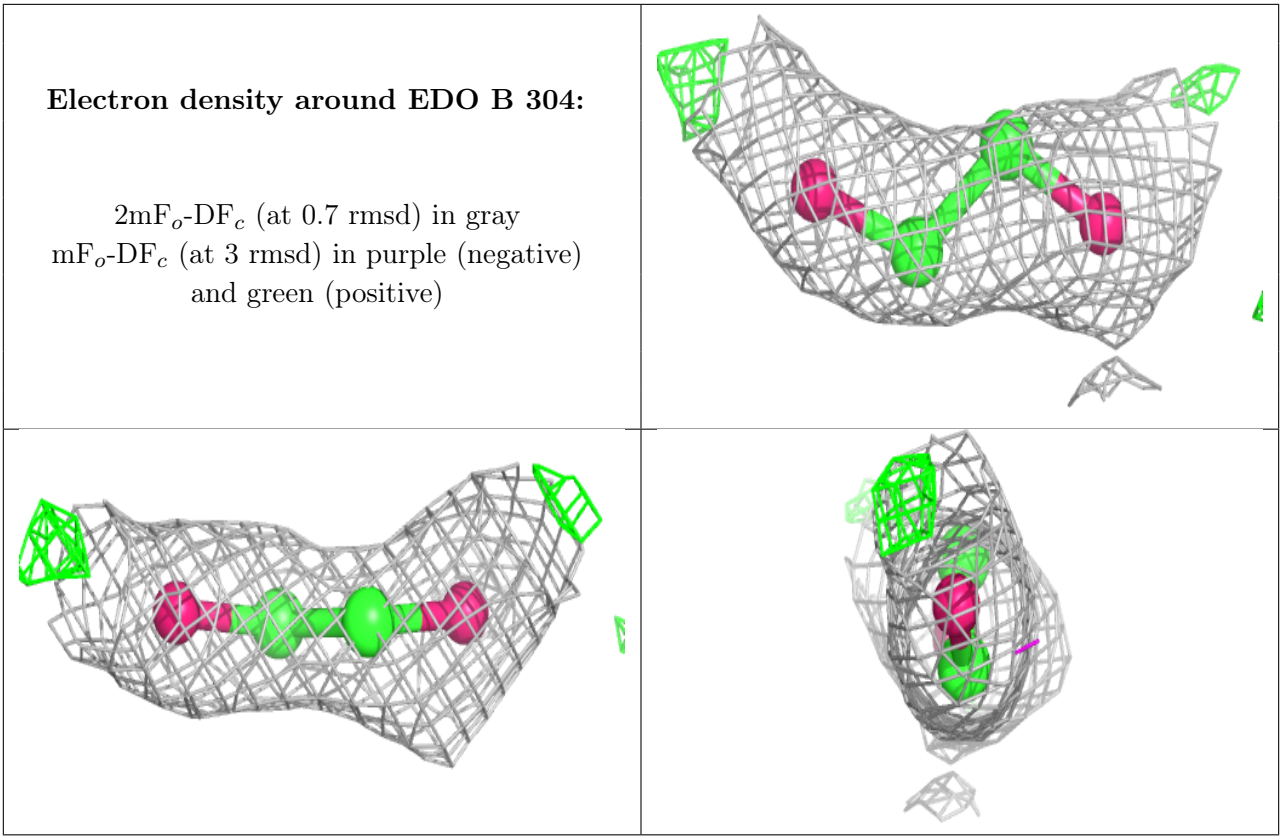
Electron density around MG F 305:

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



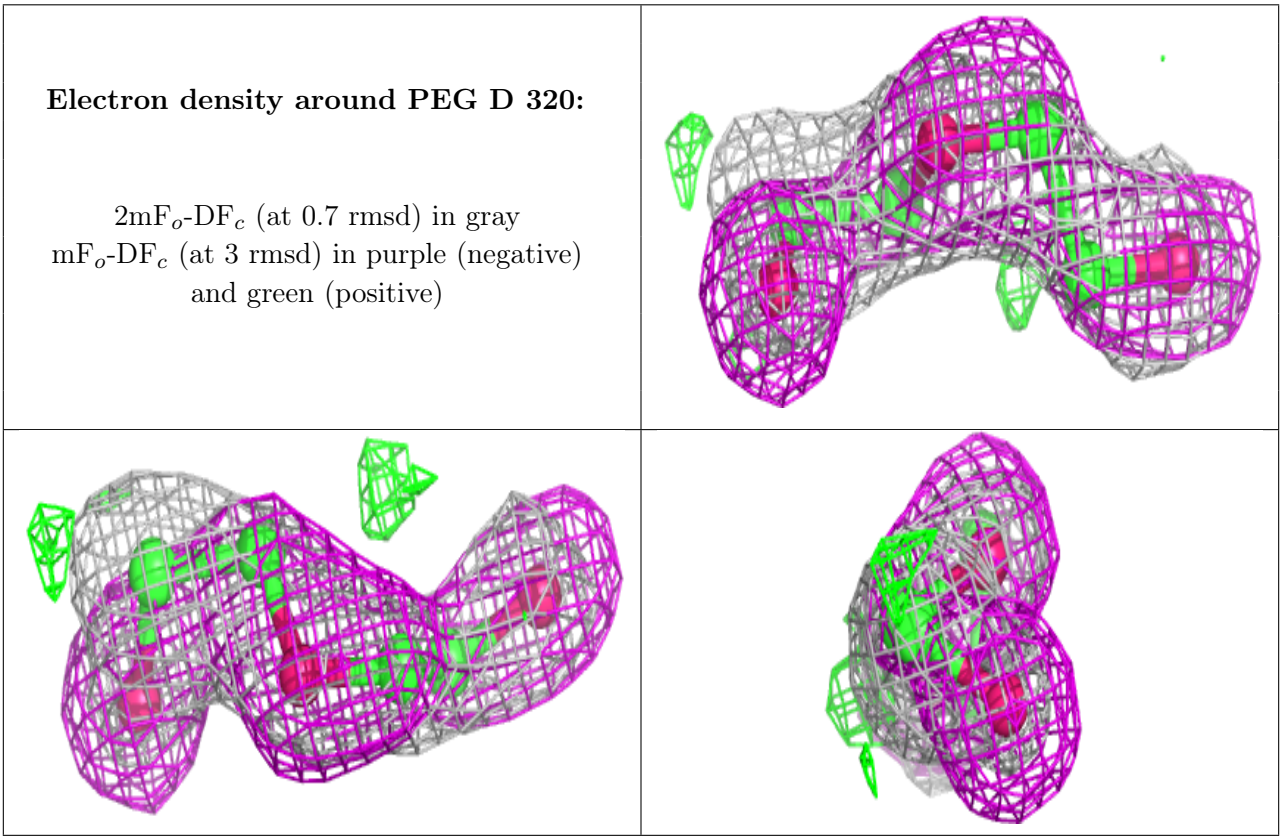
Electron density around EDO B 304:

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



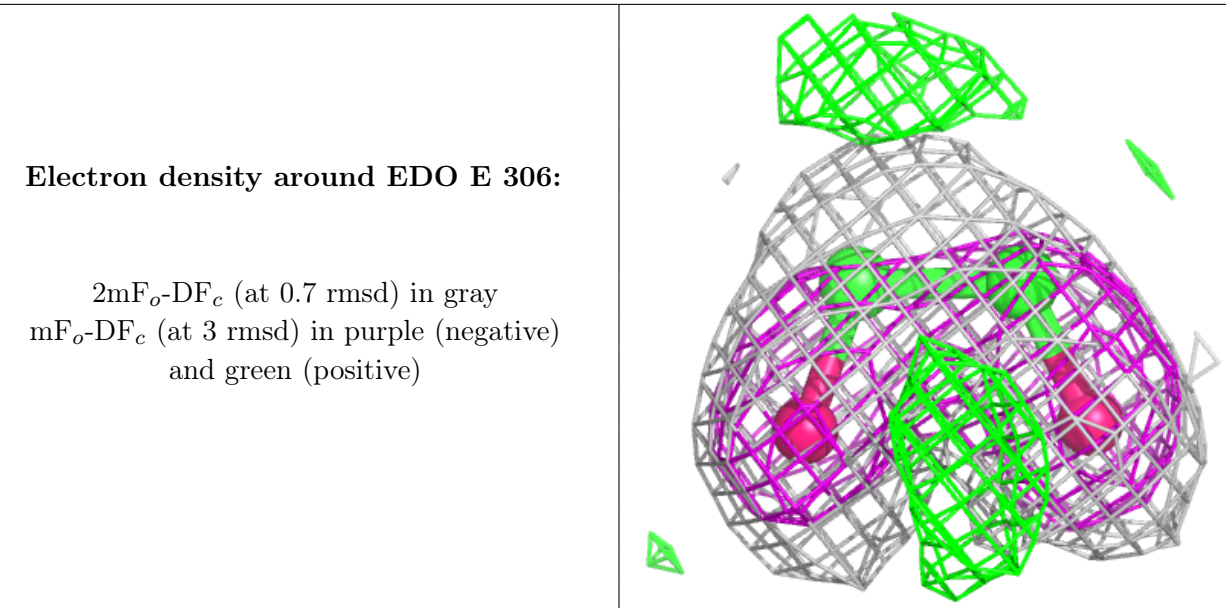
Electron density around PEG D 320:

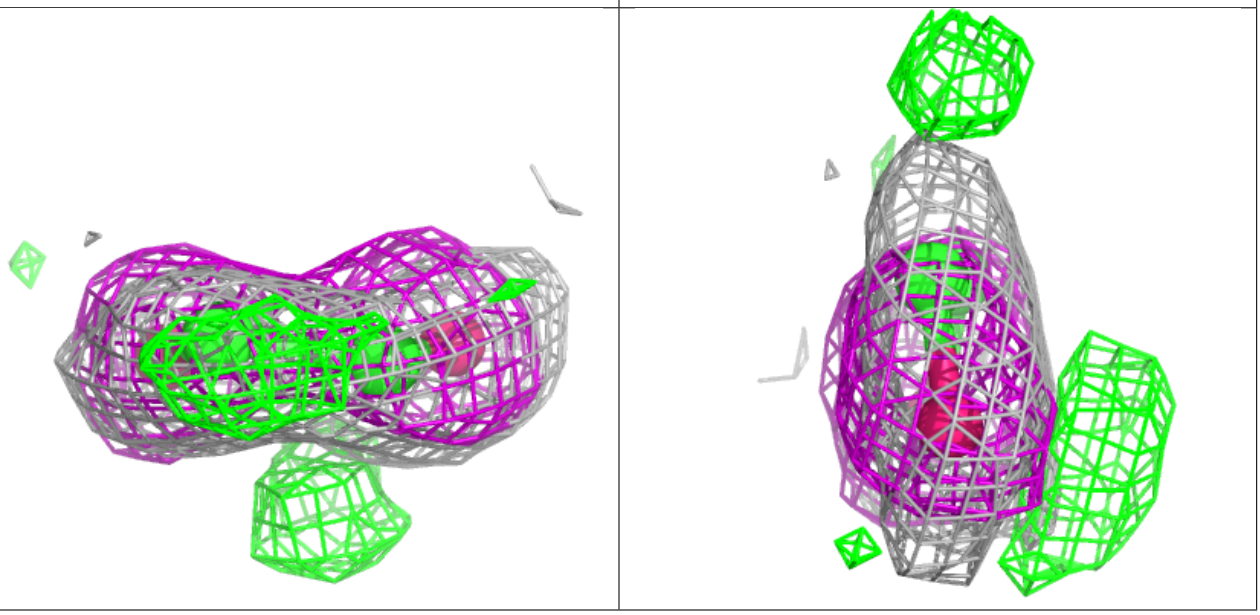
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around EDO E 306:

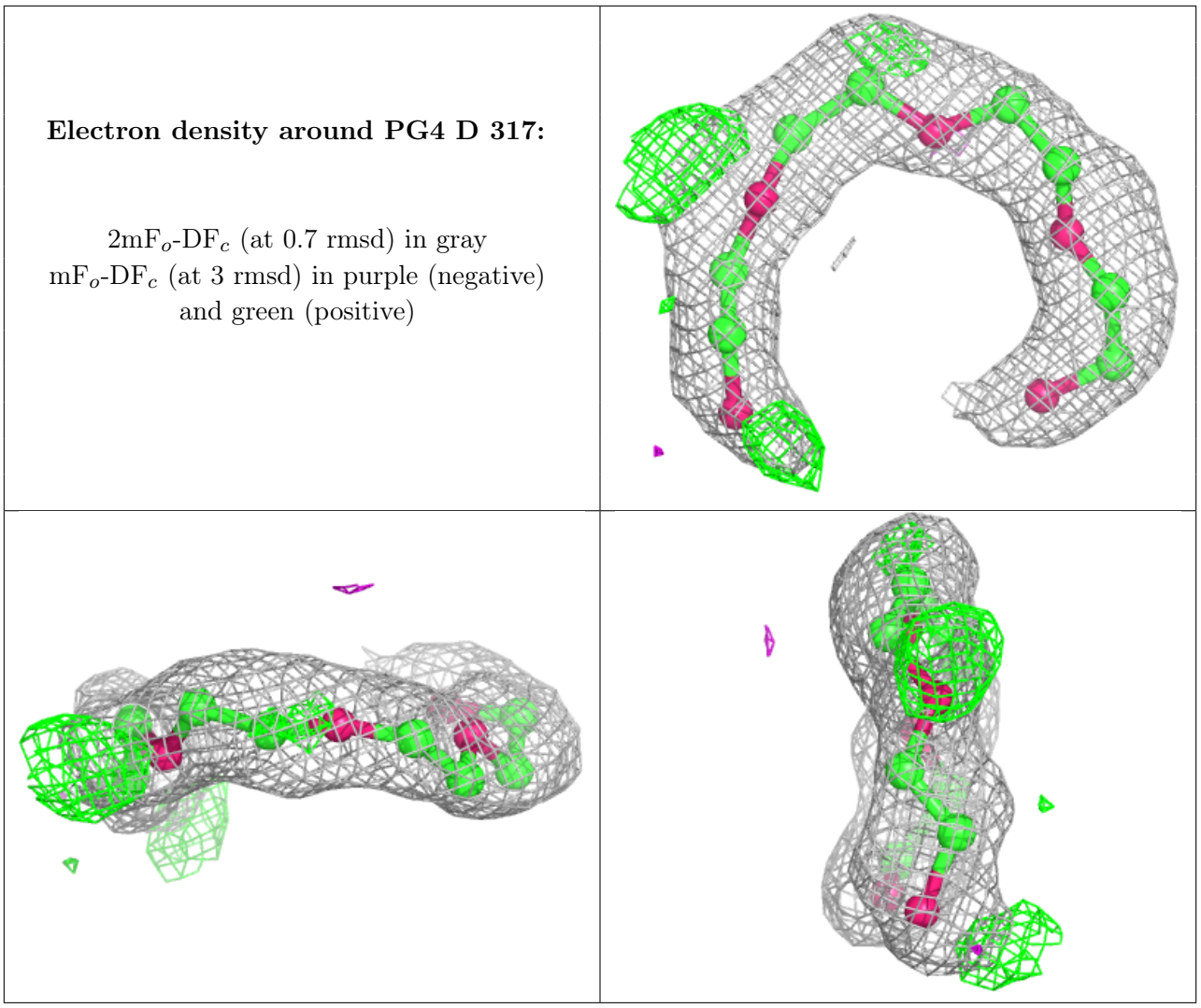
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





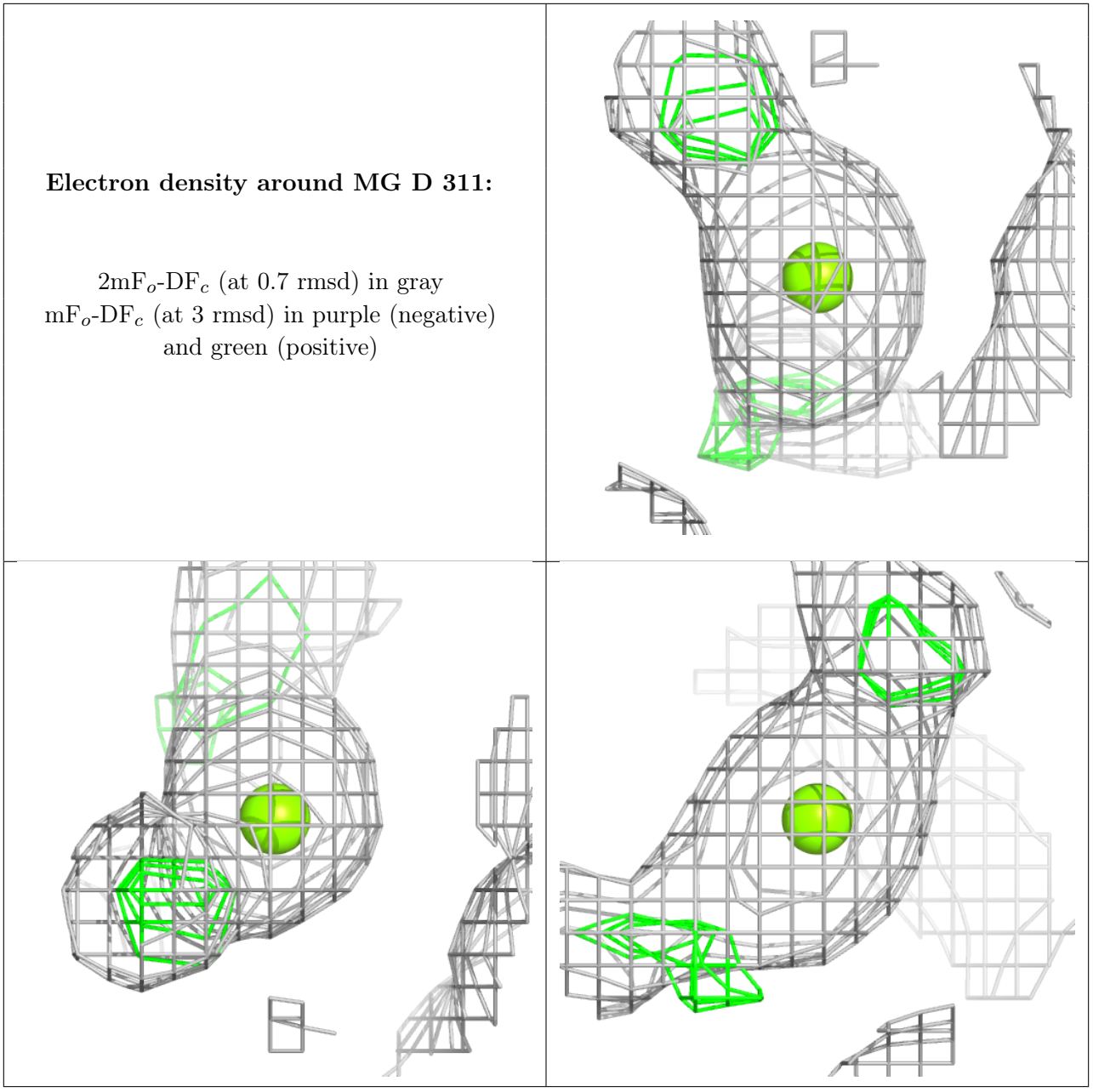
Electron density around PG4 D 317:

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



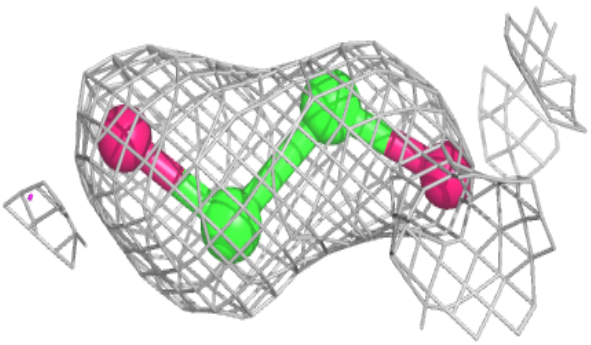
Electron density around MG D 311:

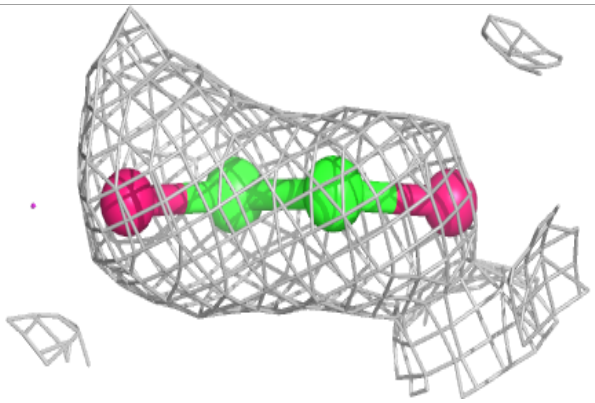
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

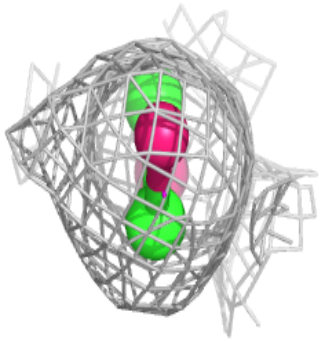


Electron density around EDO C 305:

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

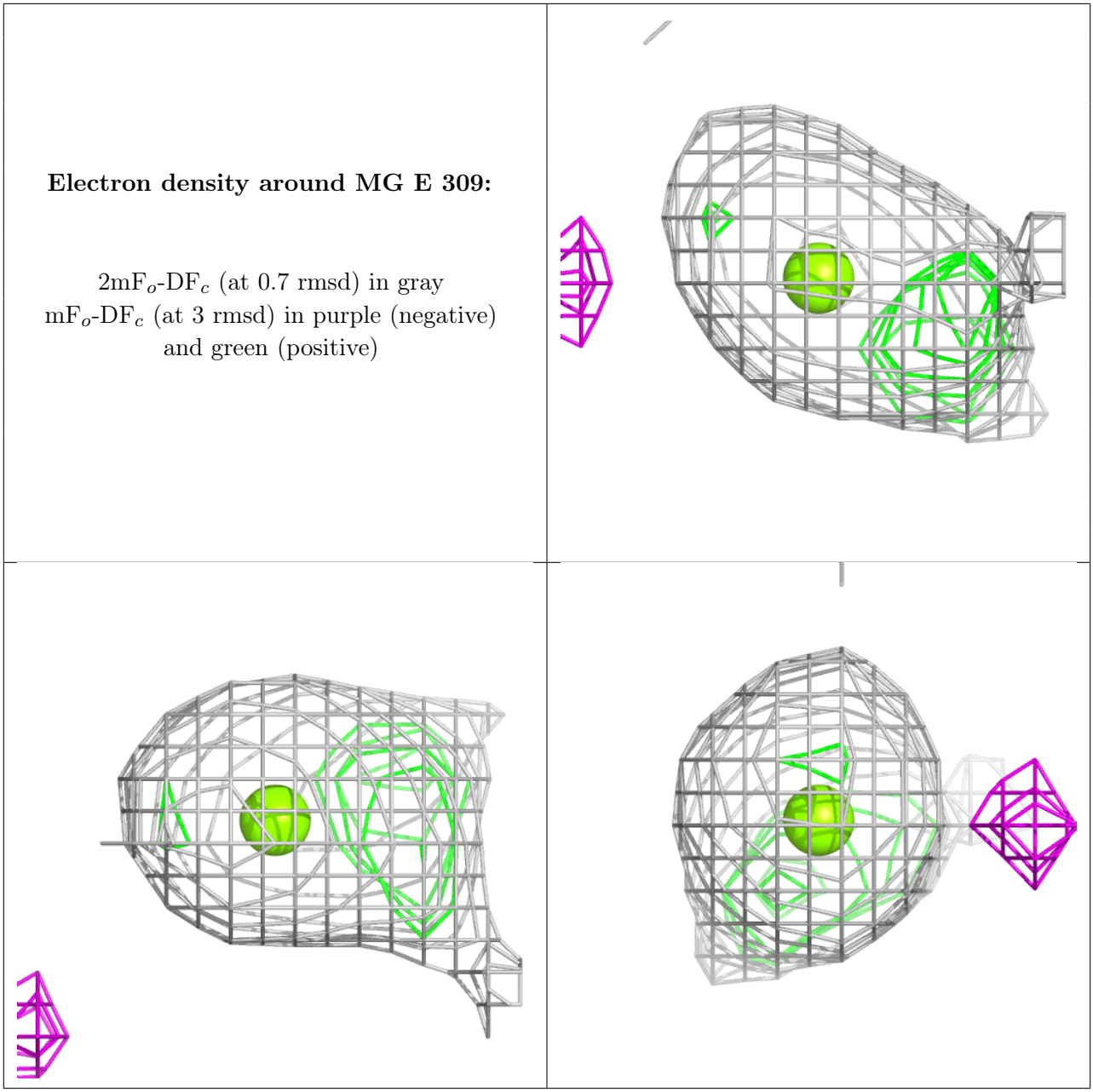






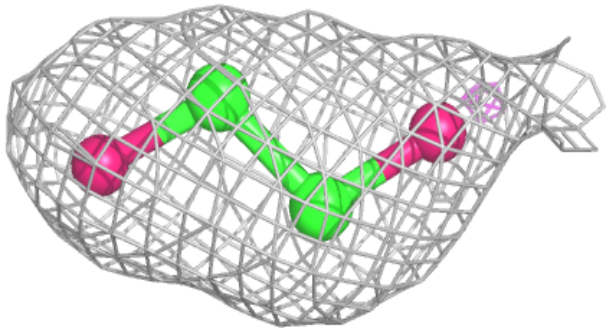
Electron density around MG E 309:

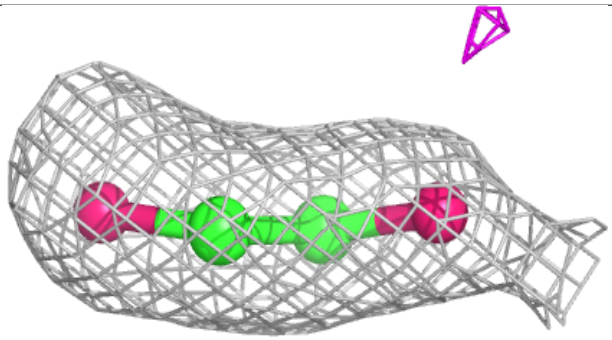
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

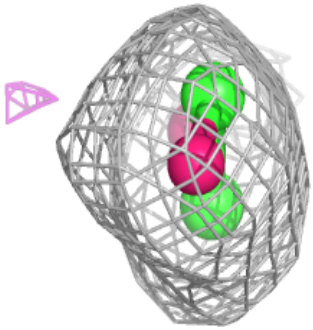


Electron density around EDO B 302:

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

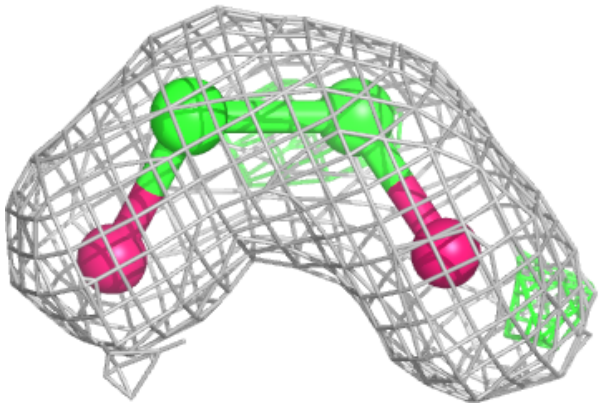


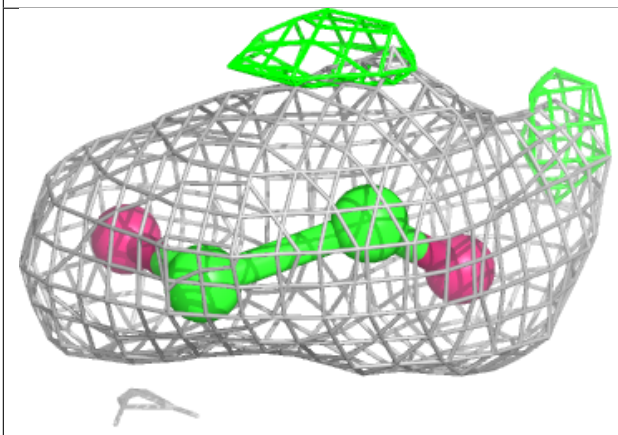


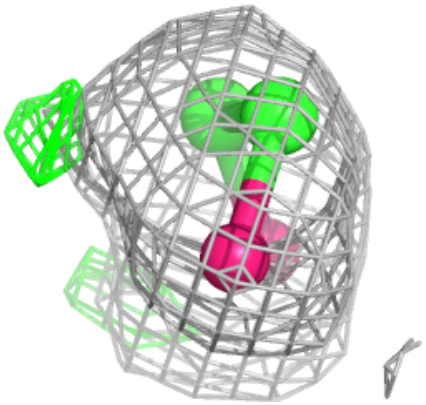


Electron density around EDO B 301:

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

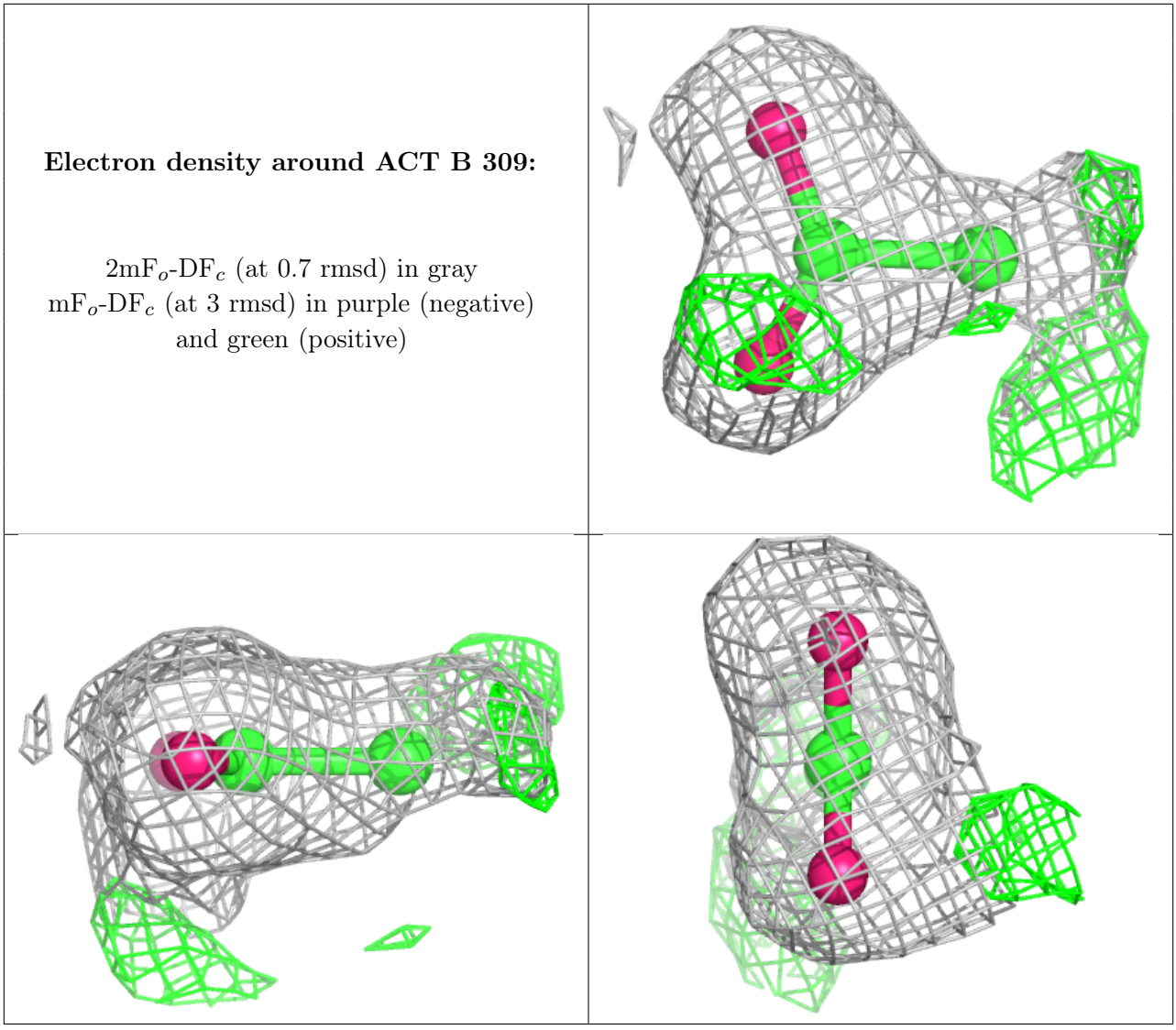






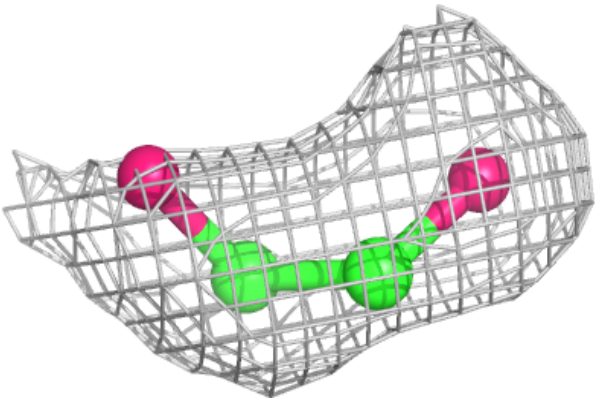
Electron density around ACT B 309:

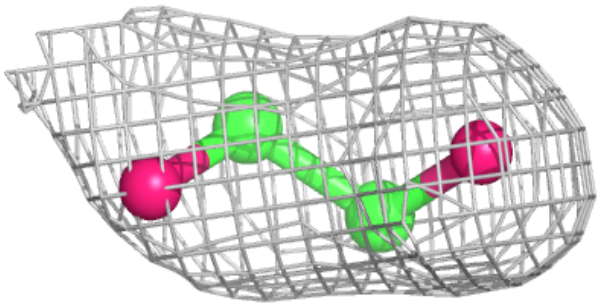
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

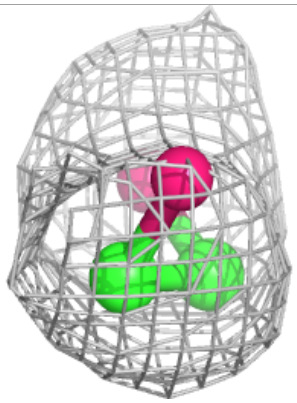


Electron density around EDO E 302:

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

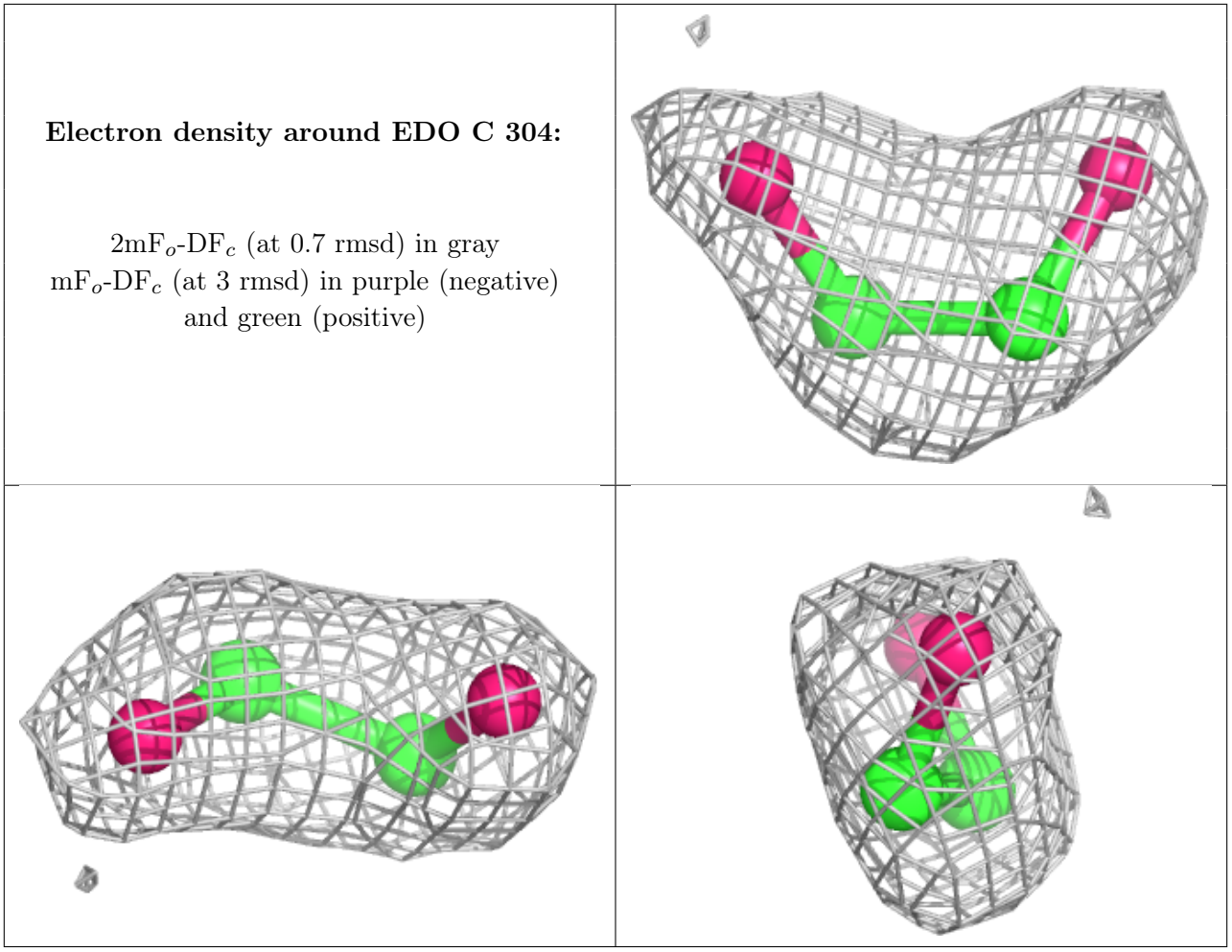






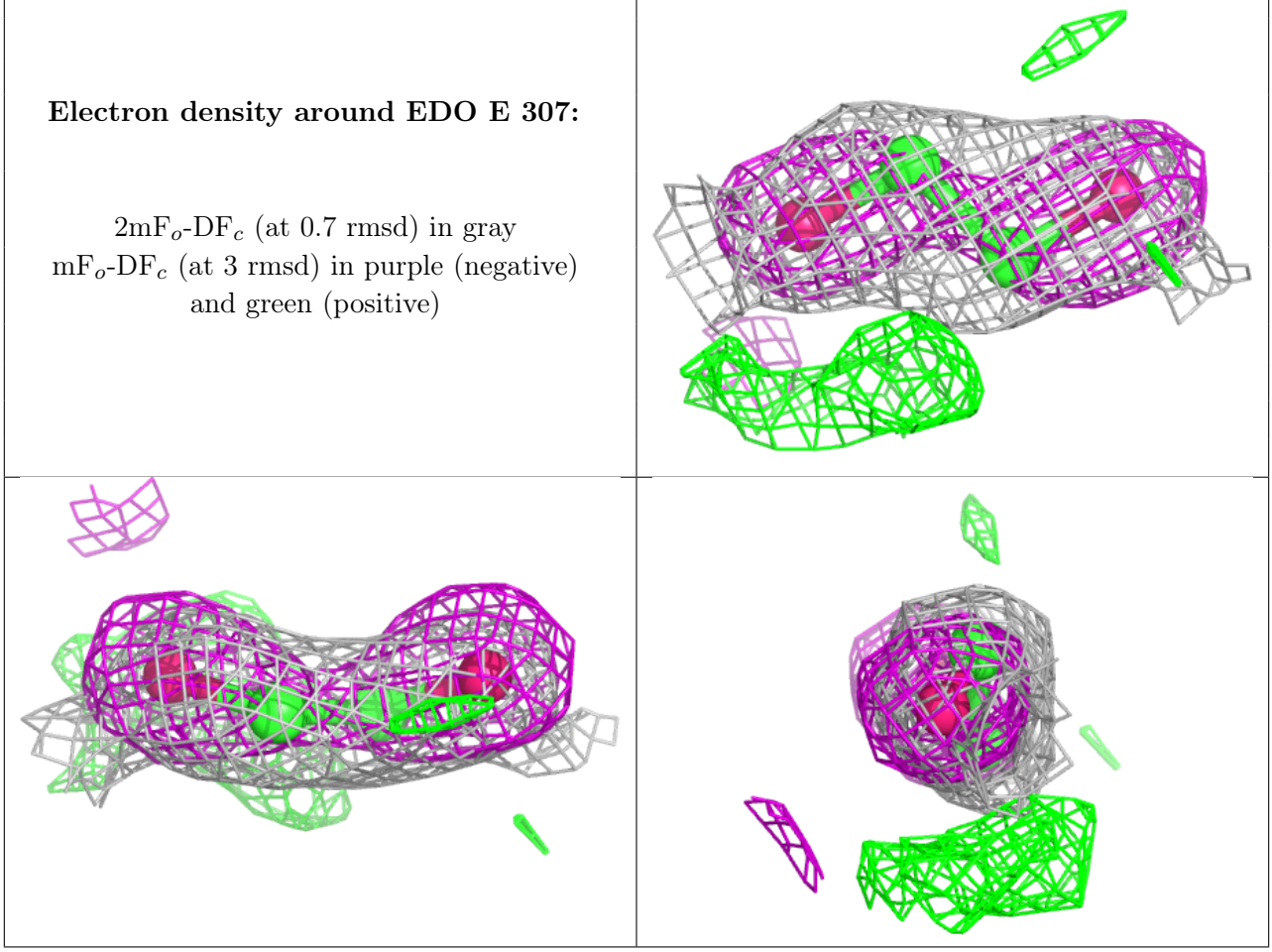
Electron density around EDO C 304:

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



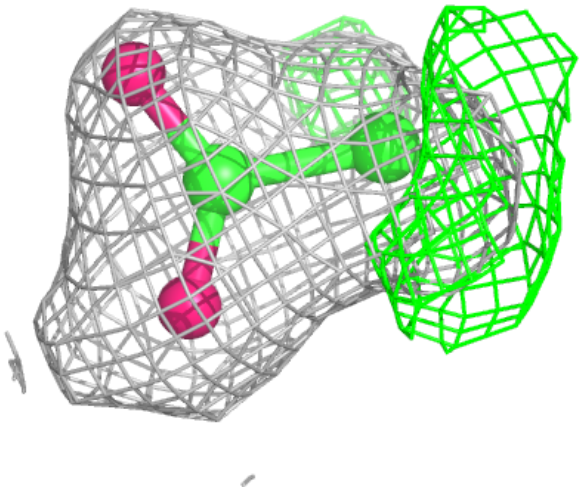
Electron density around EDO E 307:

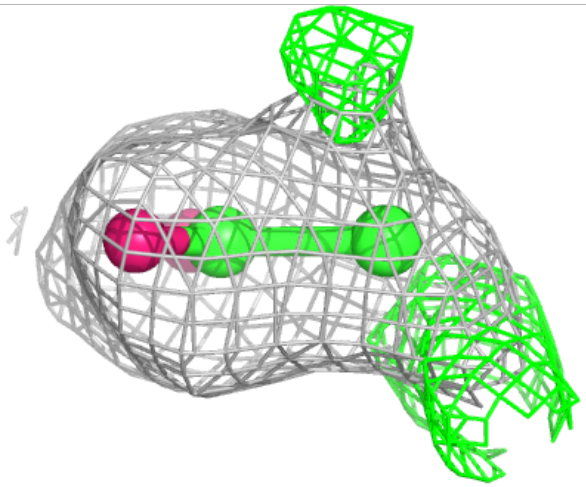
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

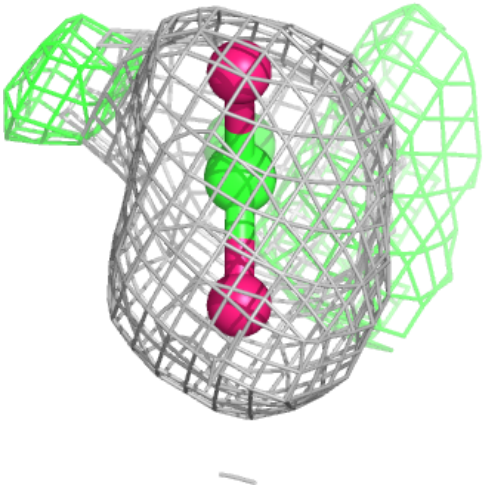


Electron density around ACT A 313:

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

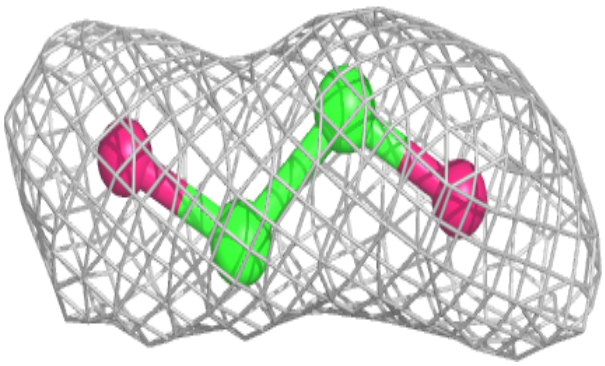


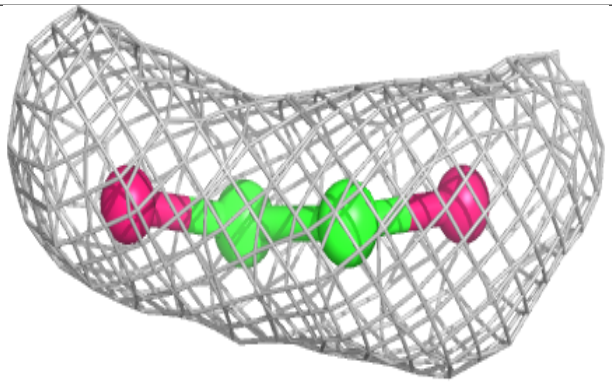


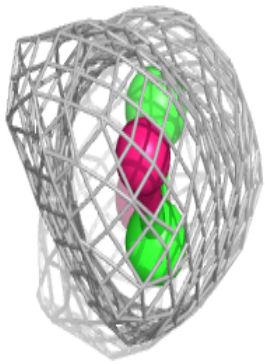


Electron density around EDO C 301:

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

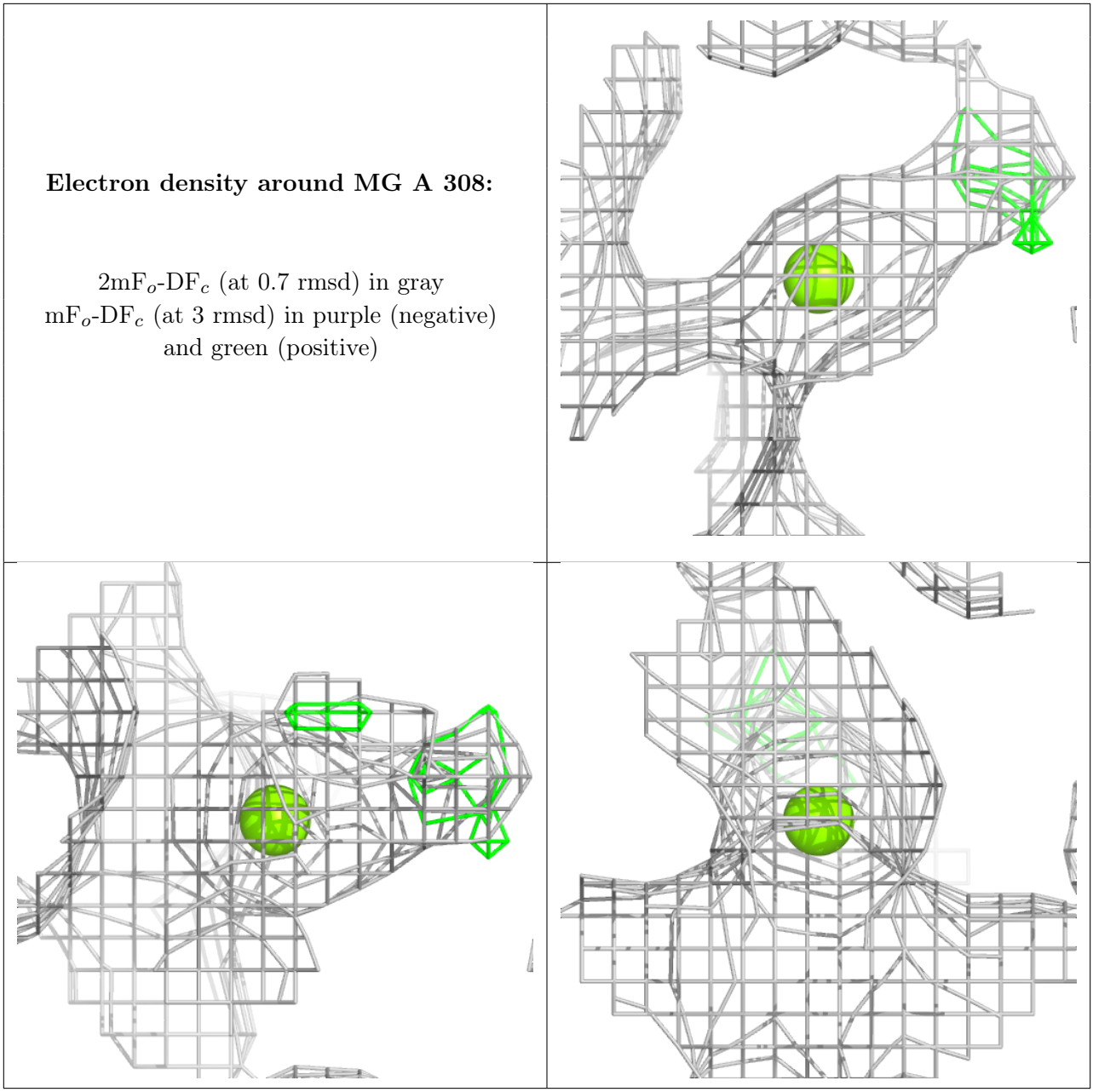






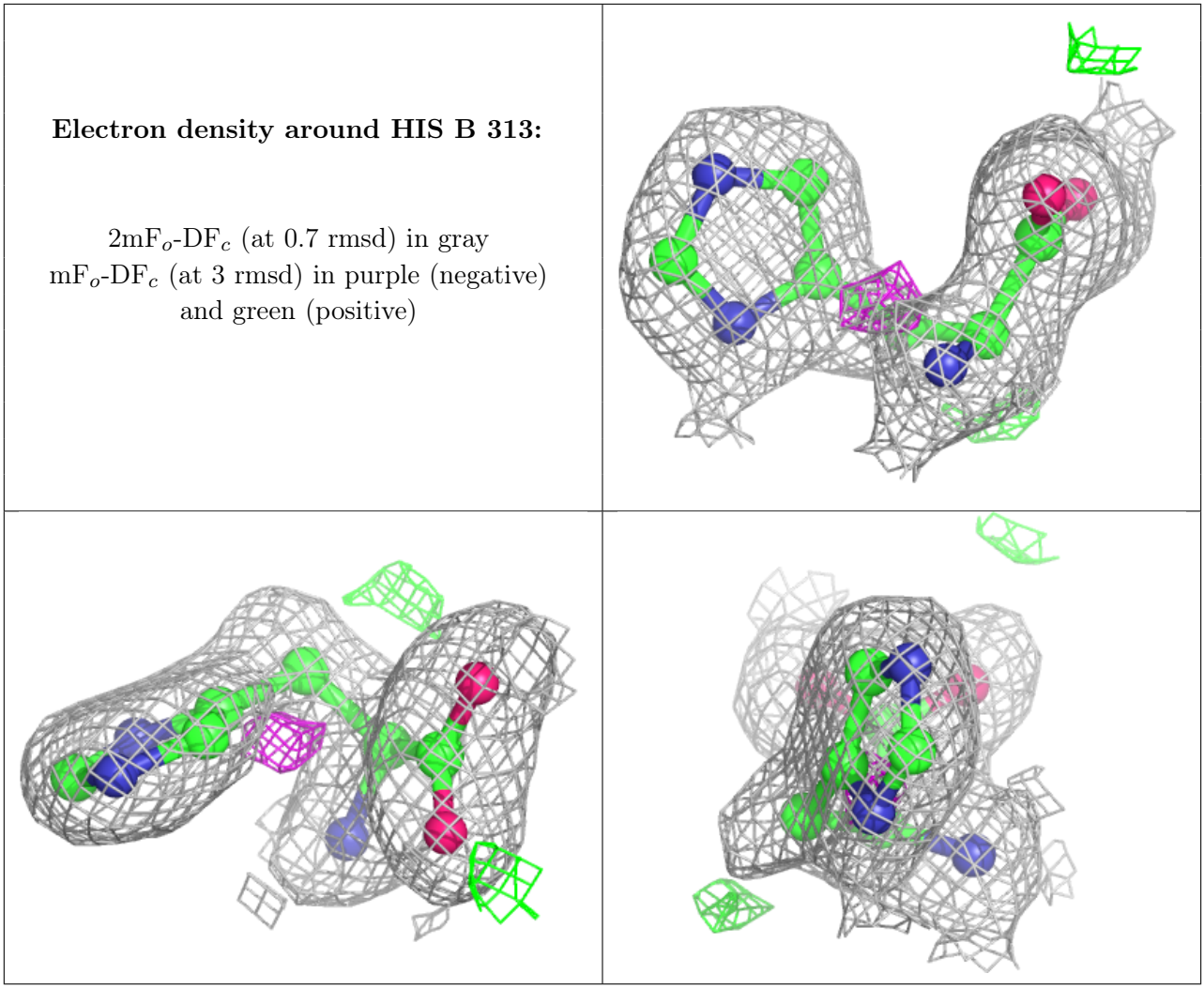
Electron density around MG A 308:

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



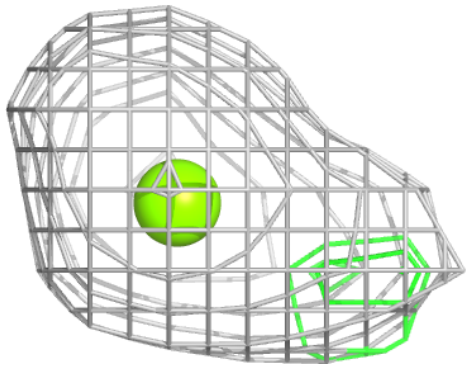
Electron density around HIS B 313:

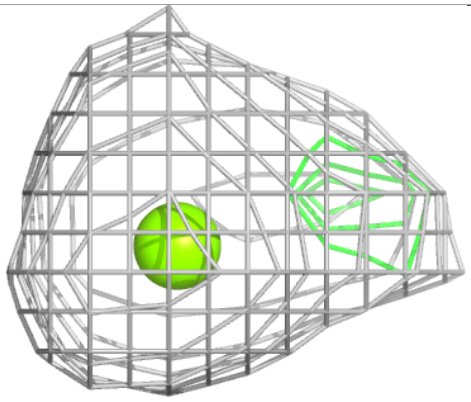
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

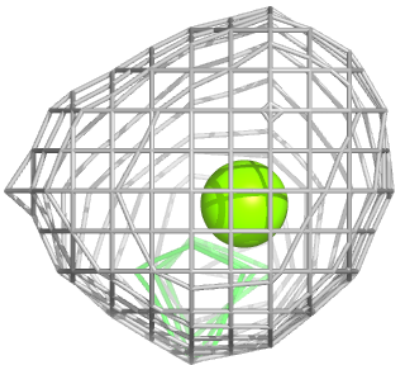


Electron density around MG A 309:

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

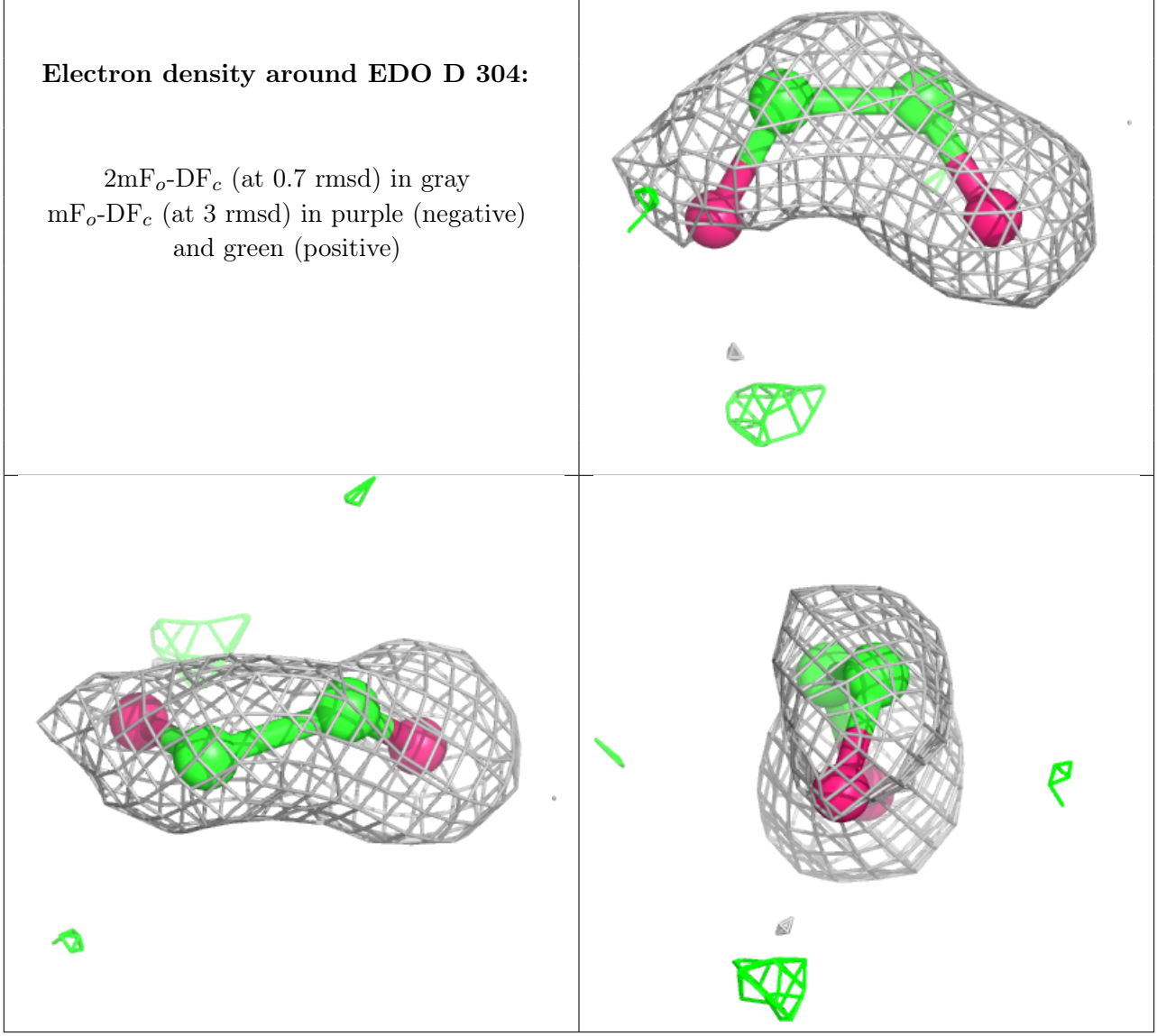






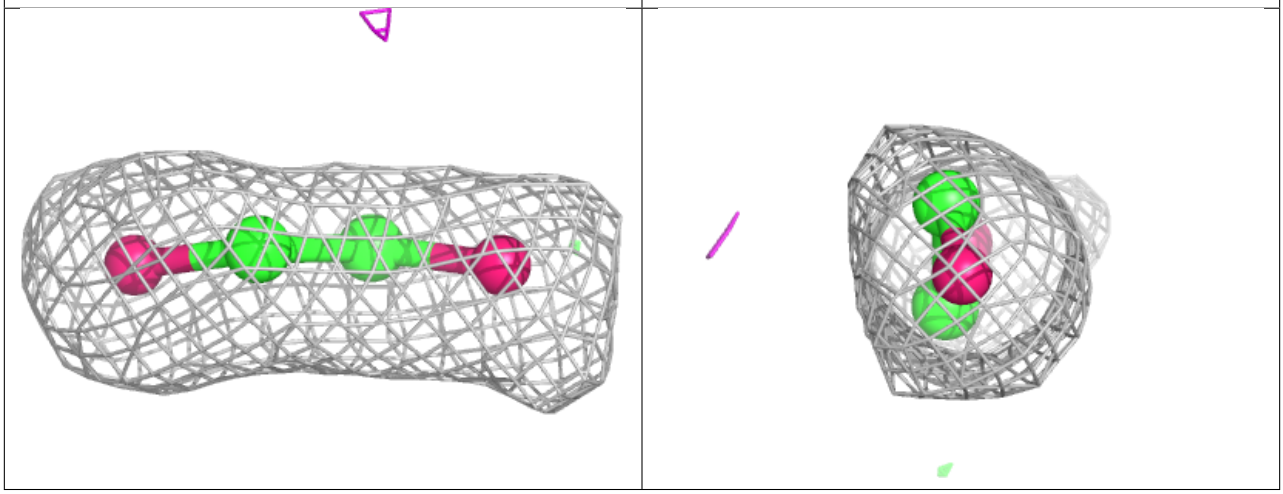
Electron density around EDO D 304:

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



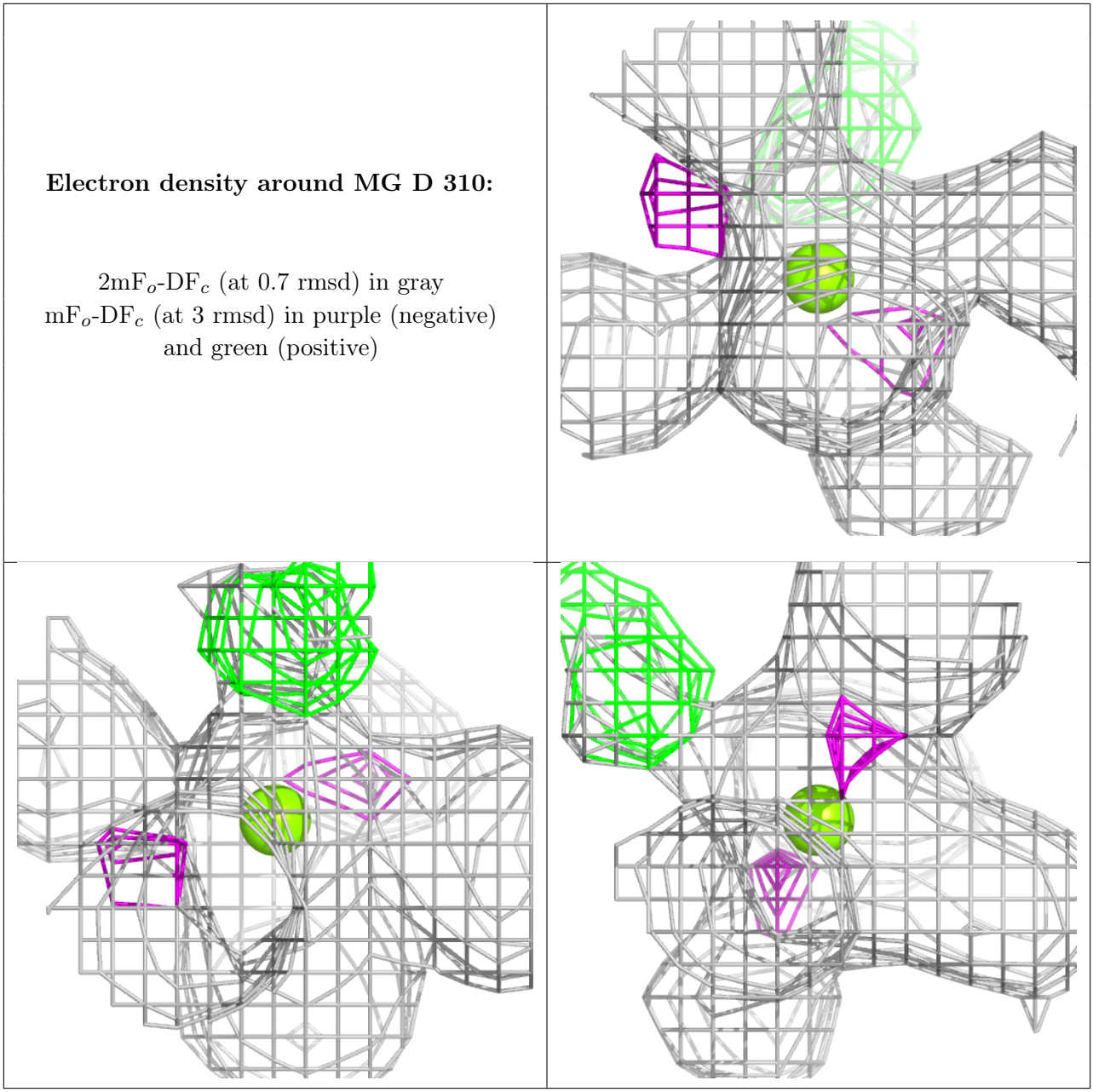
Electron density around EDO D 306:

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



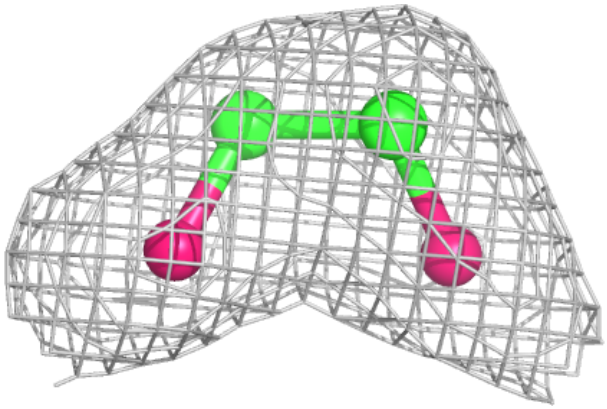
Electron density around MG D 310:

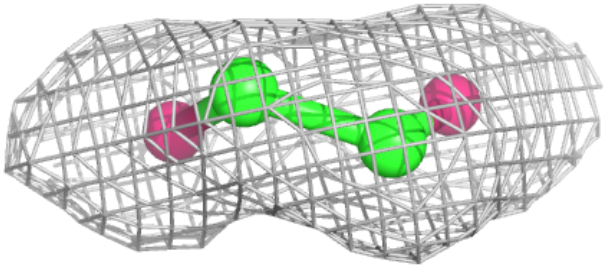
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

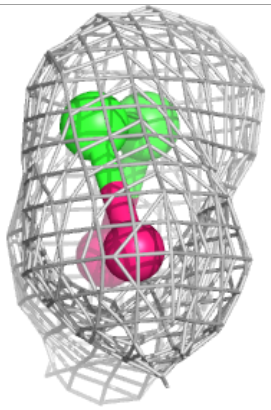


Electron density around EDO A 306:

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

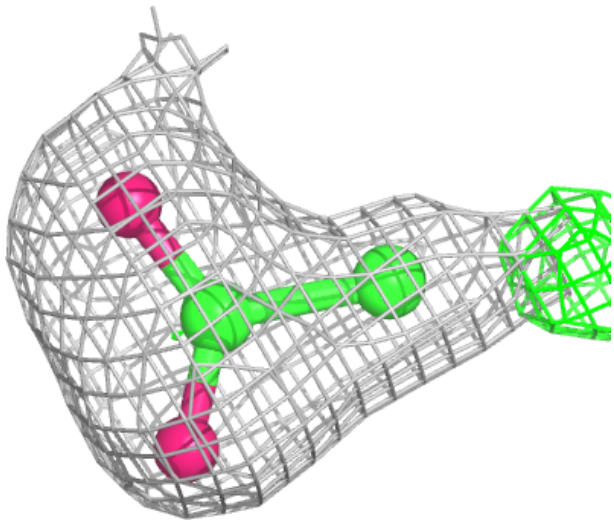


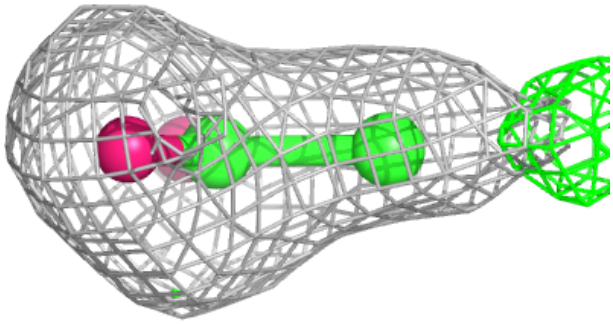


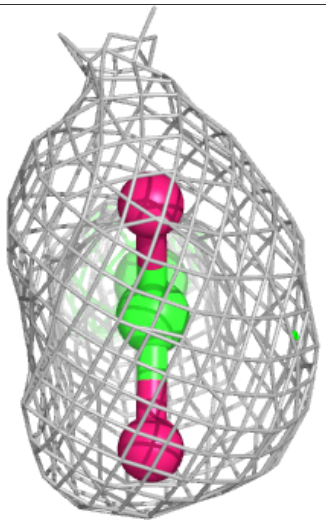


Electron density around ACT F 307:

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

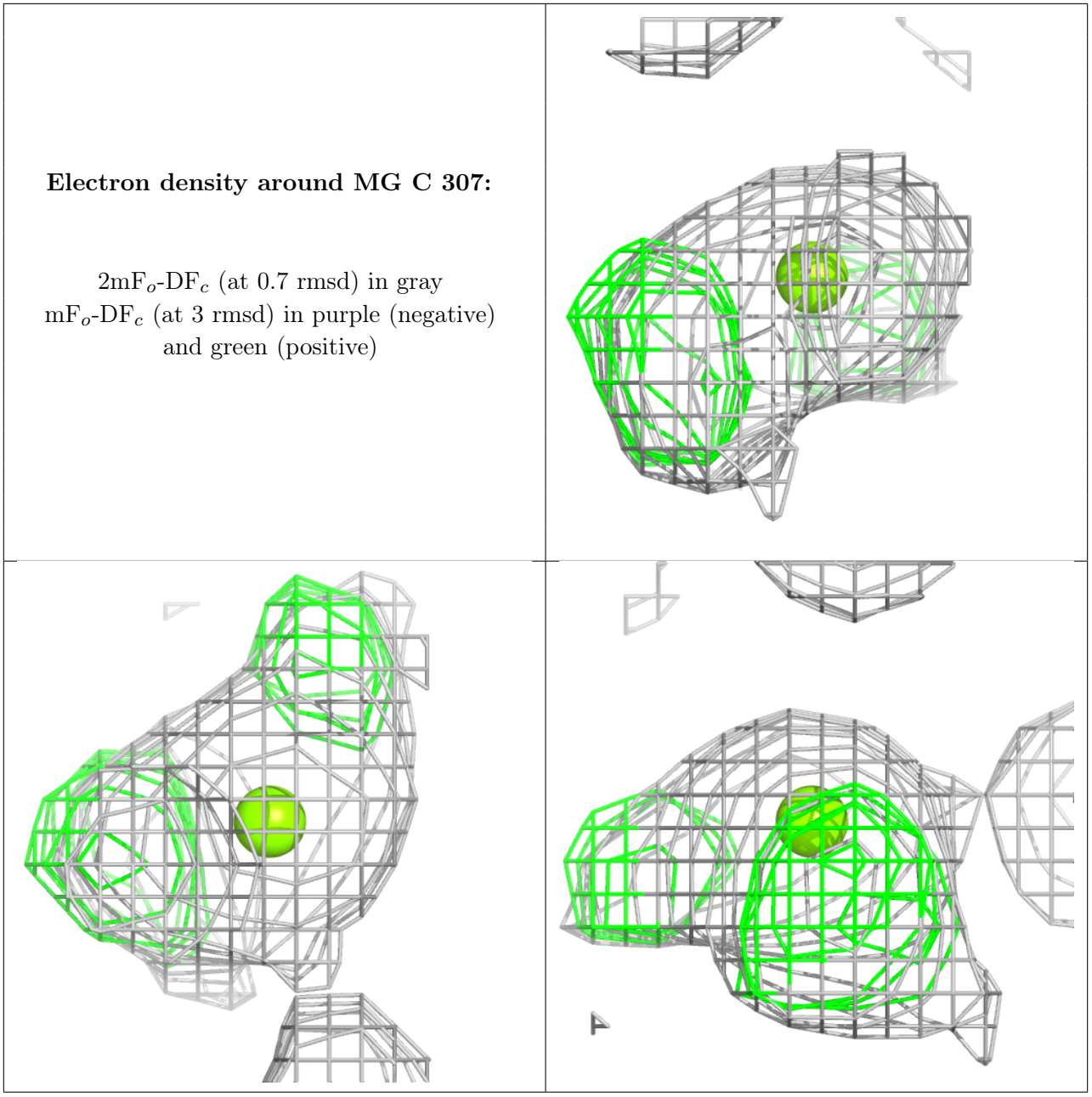






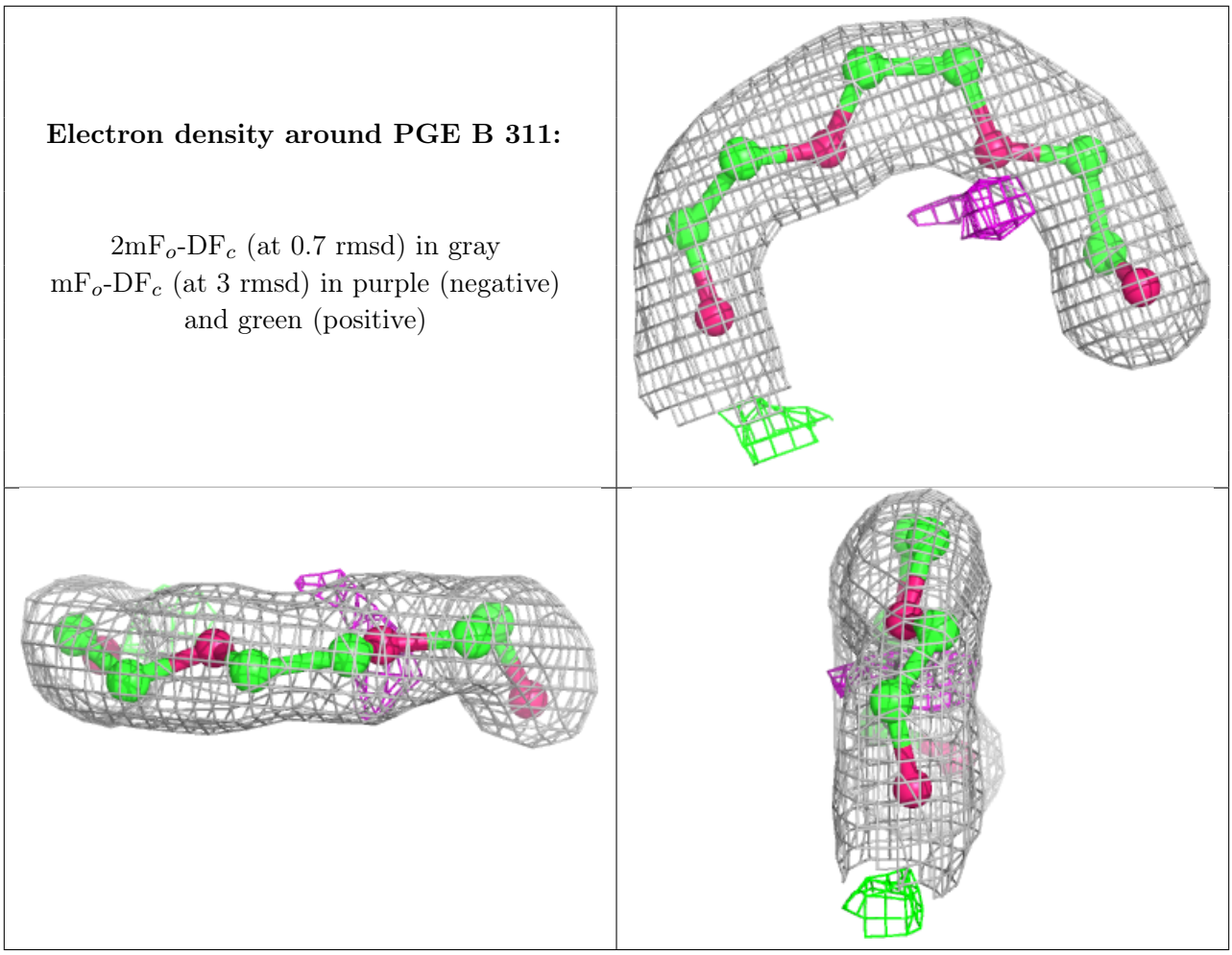
Electron density around MG C 307:

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



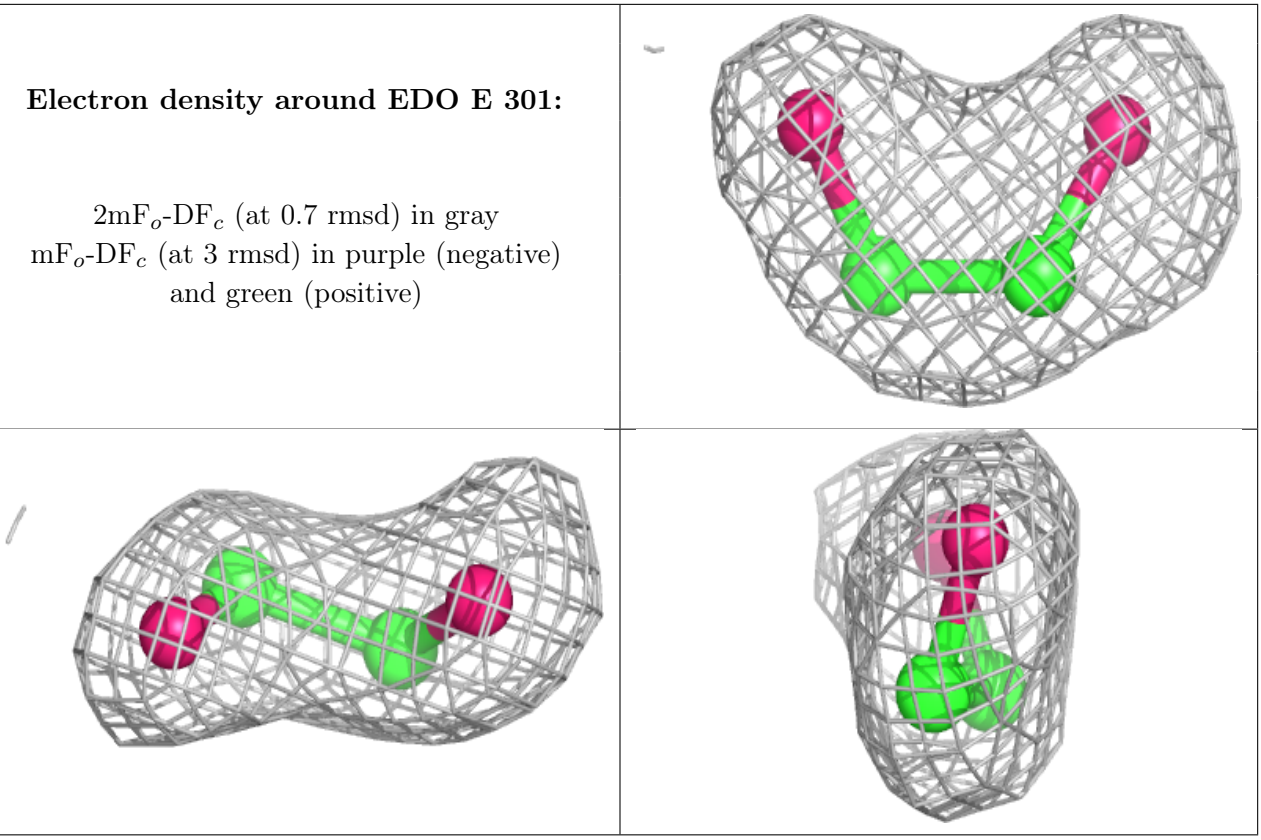
Electron density around PGE B 311:

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



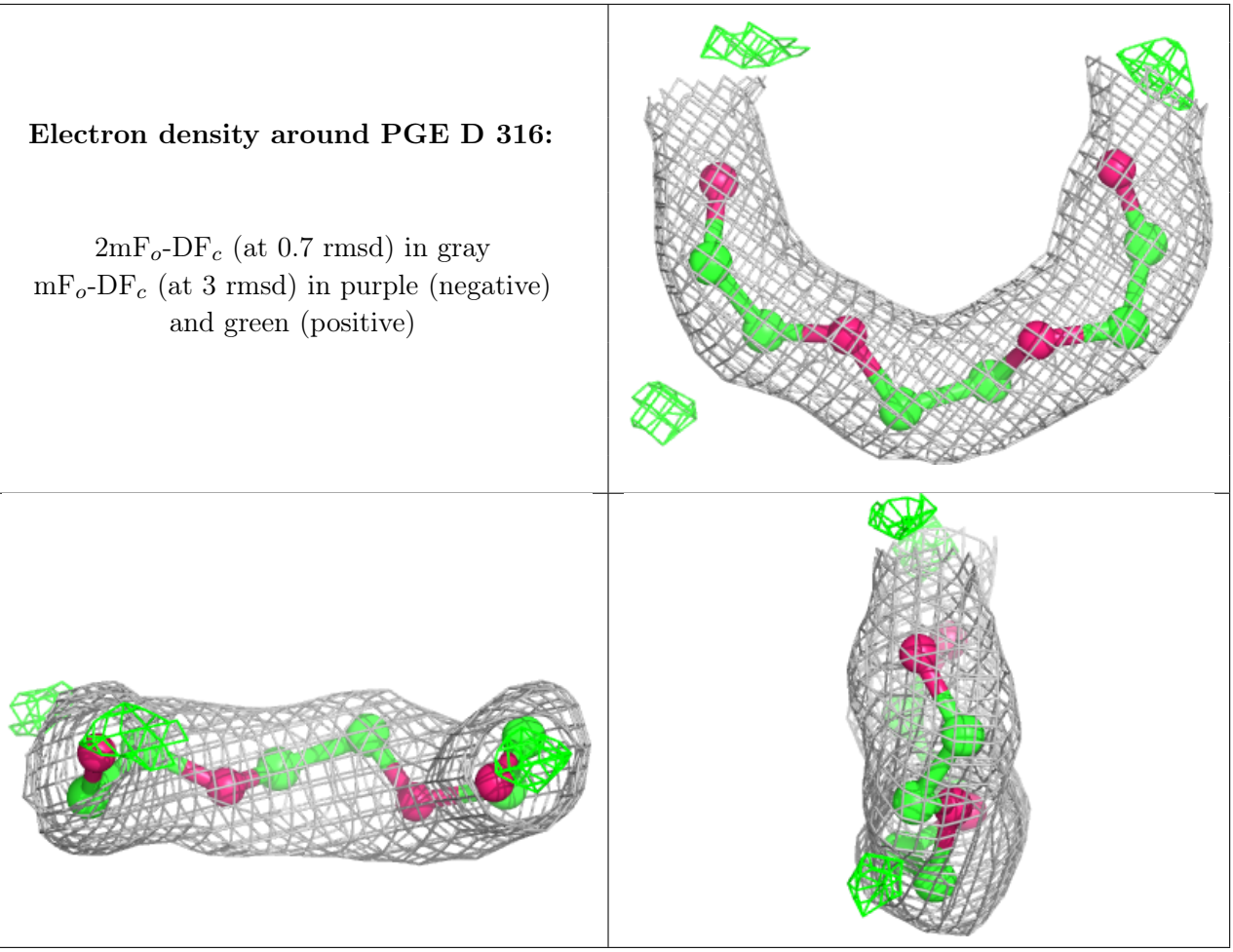
Electron density around EDO E 301:

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



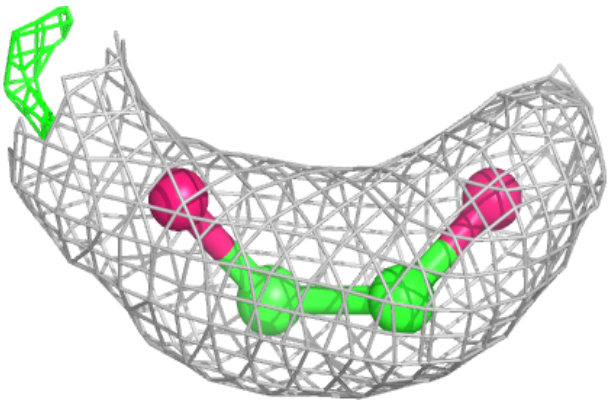
Electron density around PGE D 316:

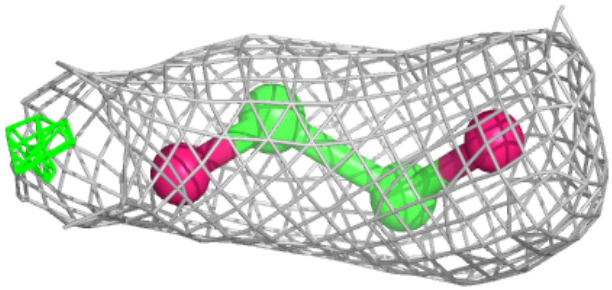
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

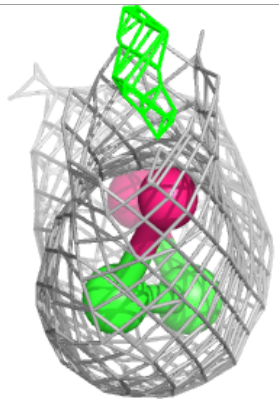


Electron density around EDO D 305:

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

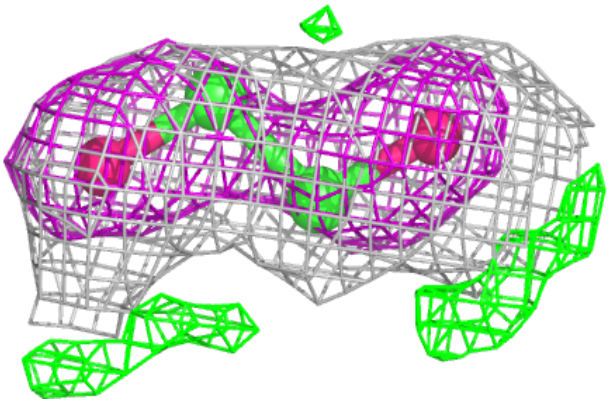


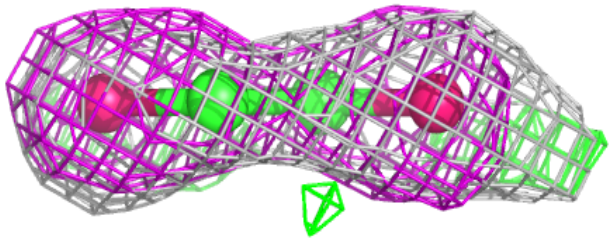


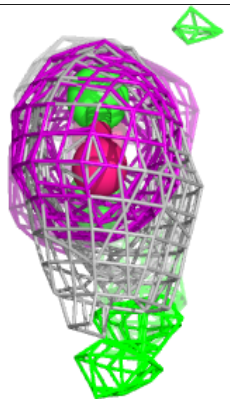


Electron density around EDO E 305:

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

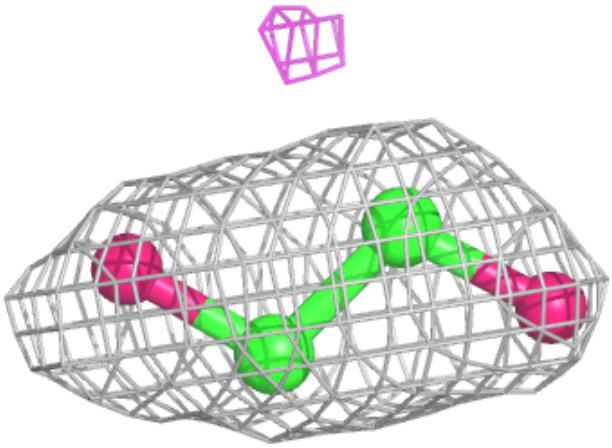


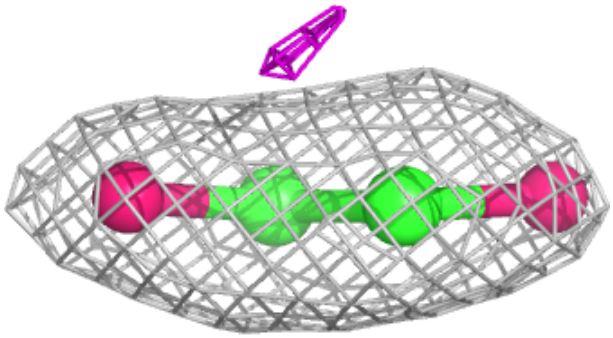


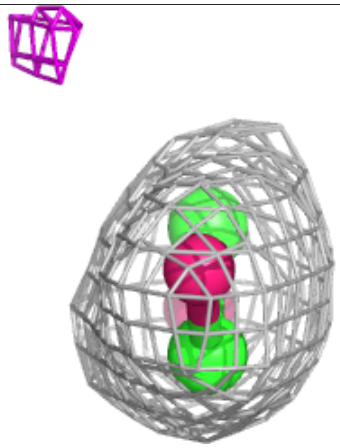


Electron density around EDO B 305:

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

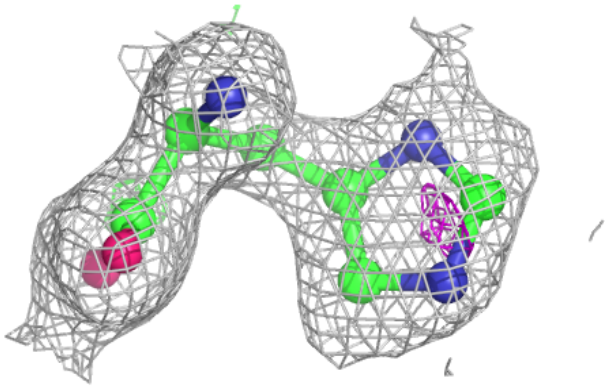


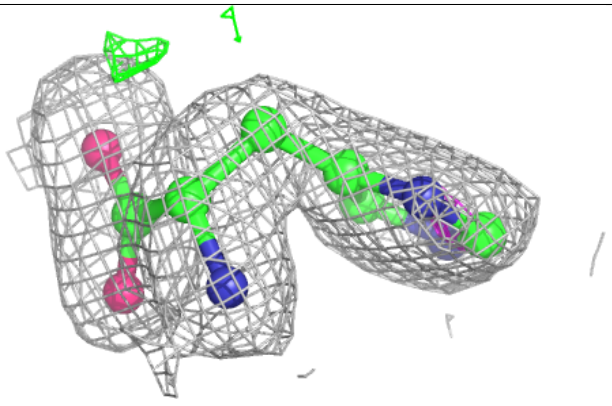


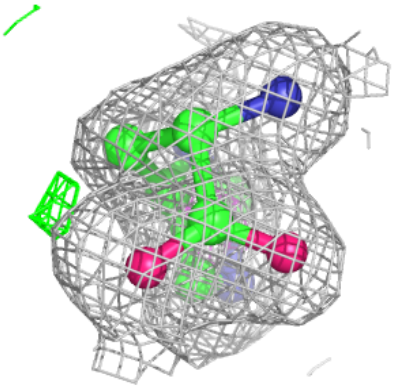


Electron density around HIS C 310:

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

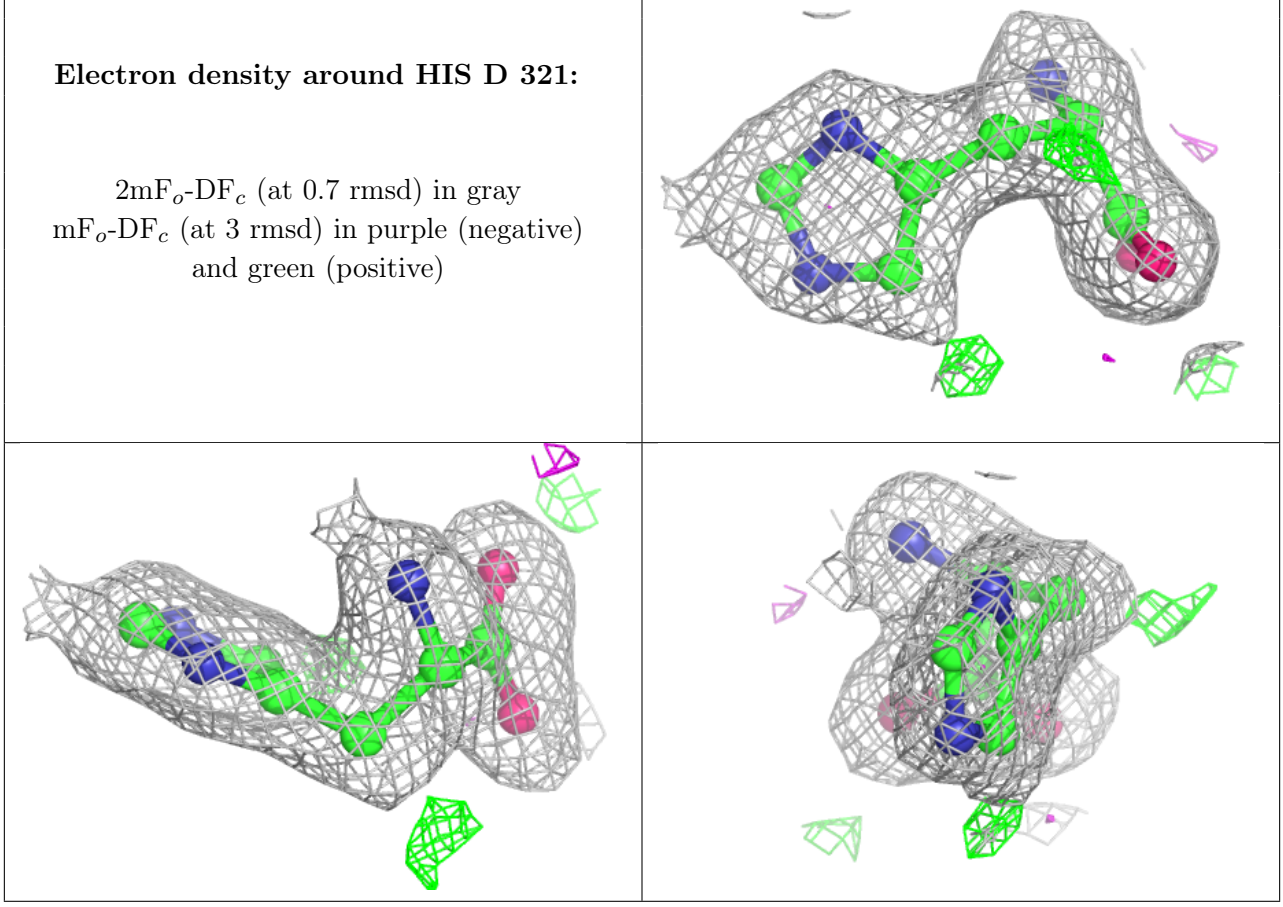






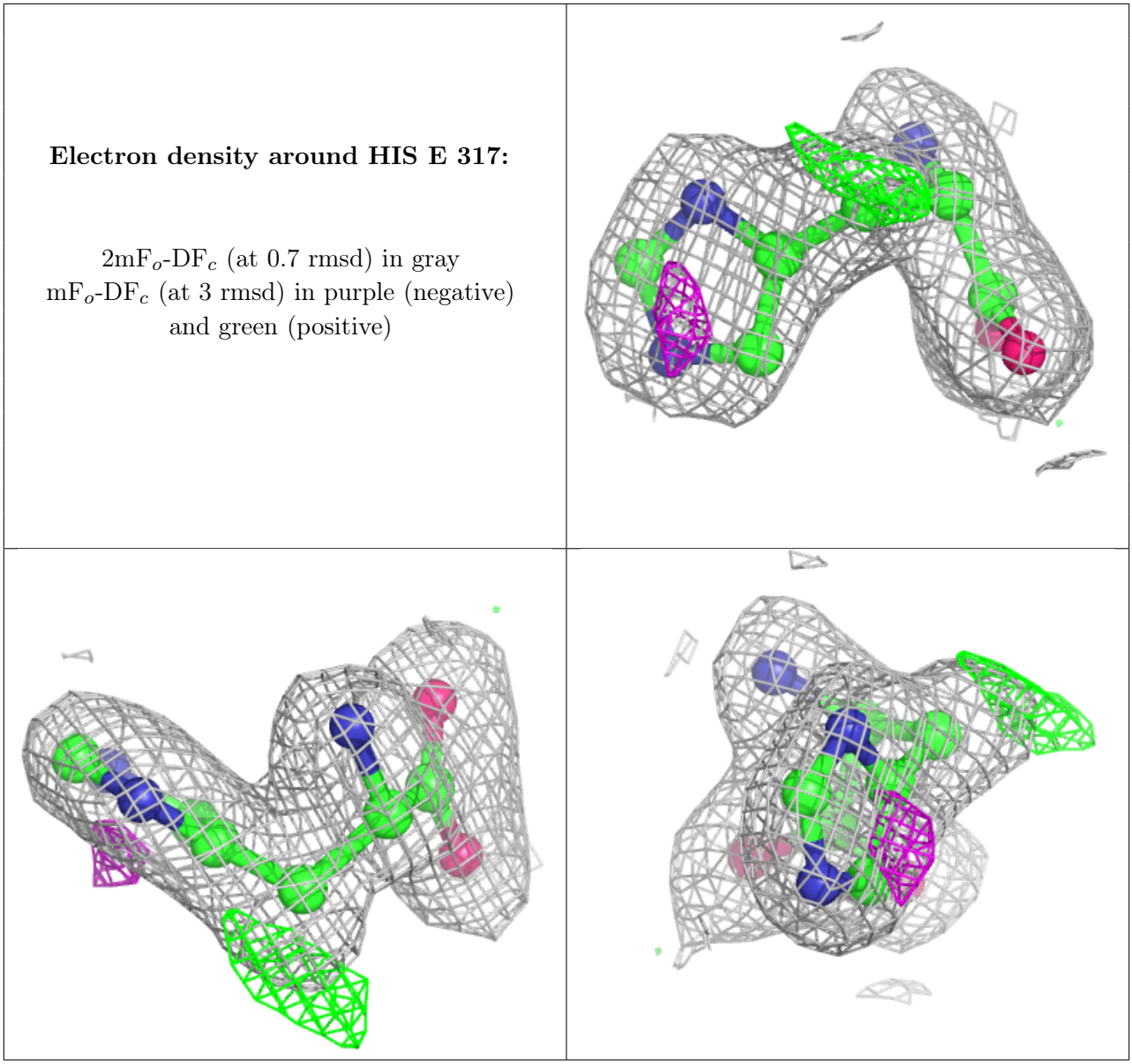
Electron density around HIS D 321:

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



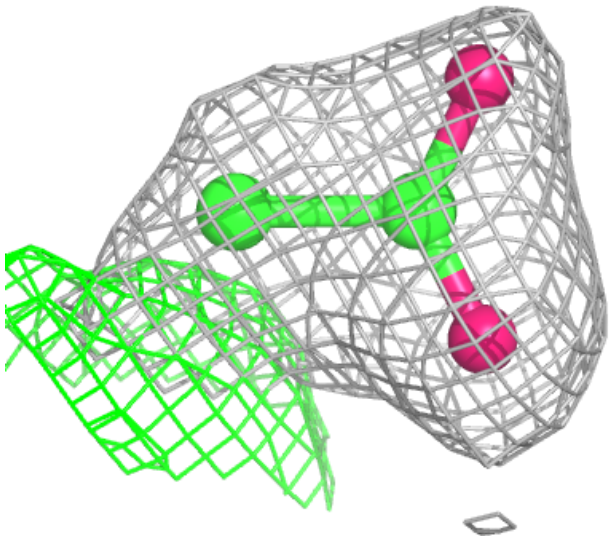
Electron density around HIS E 317:

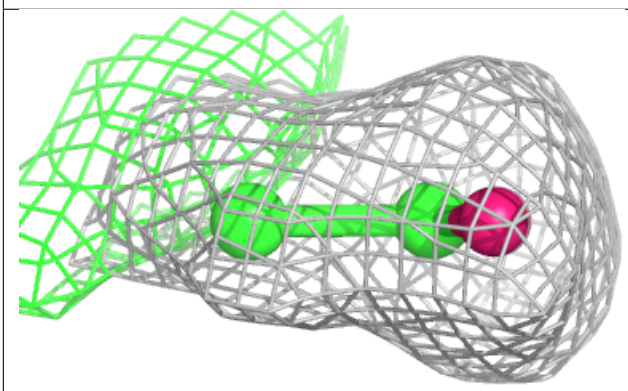
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

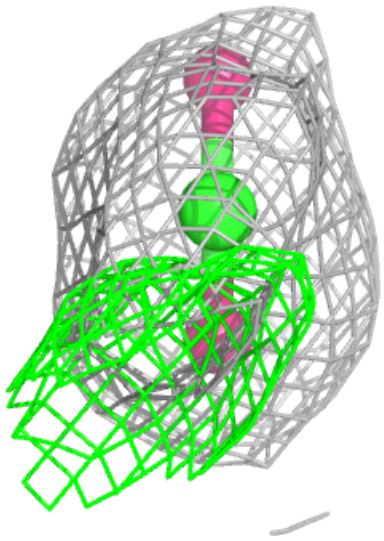


Electron density around ACT F 306:

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

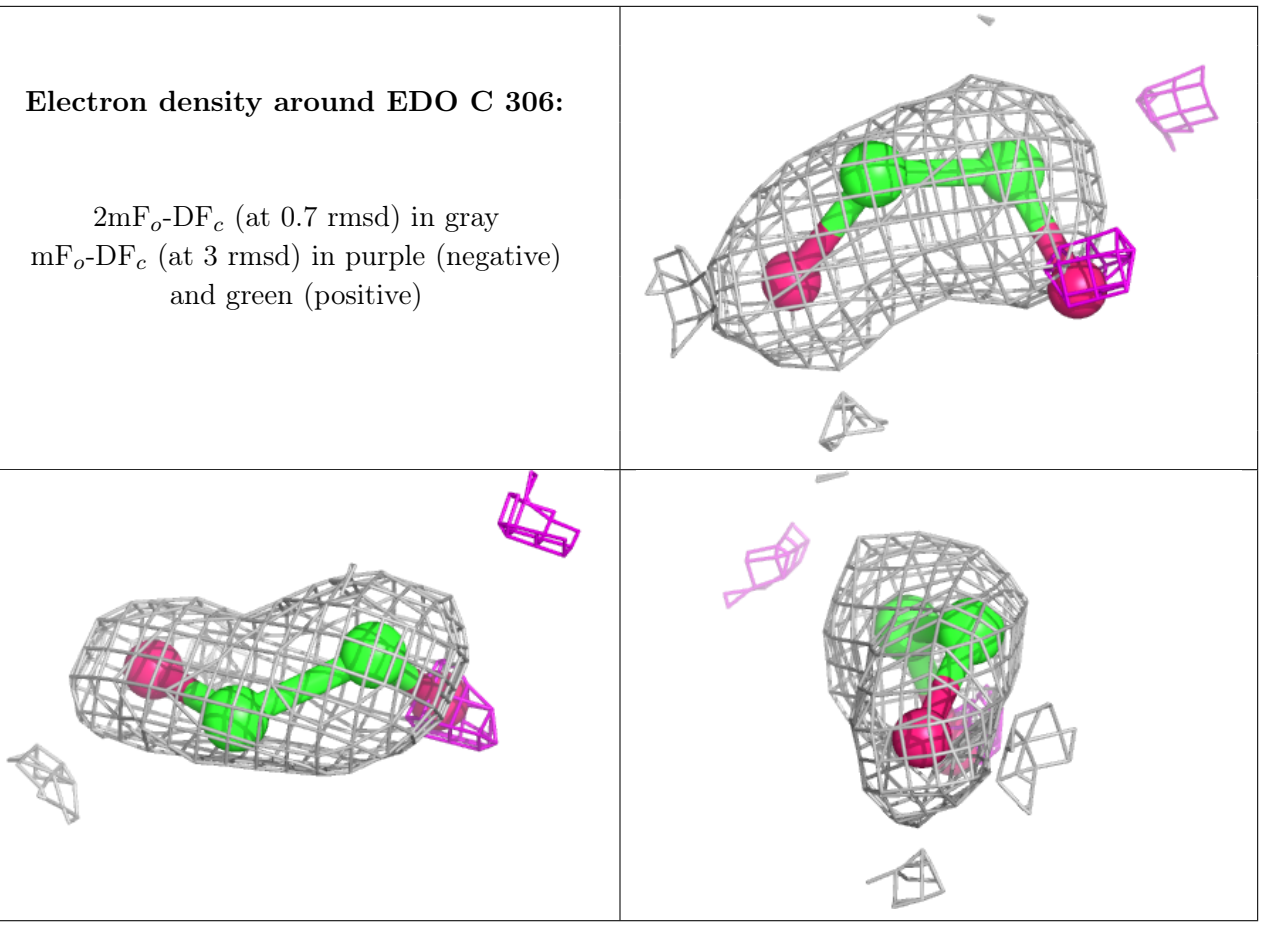






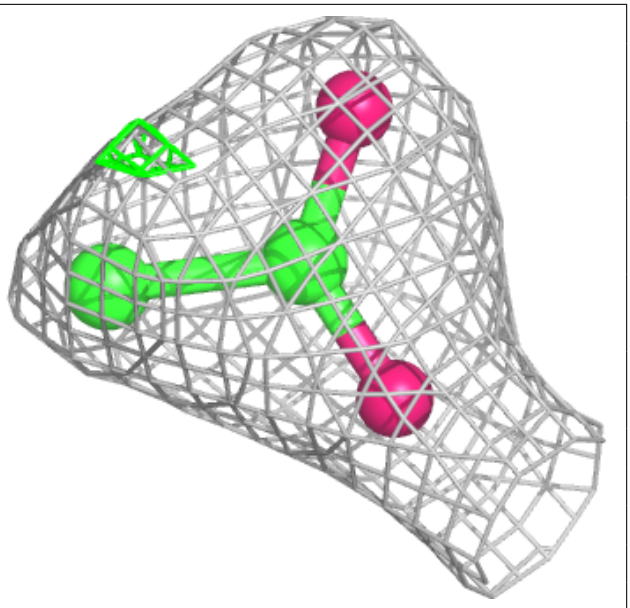
Electron density around EDO C 306:

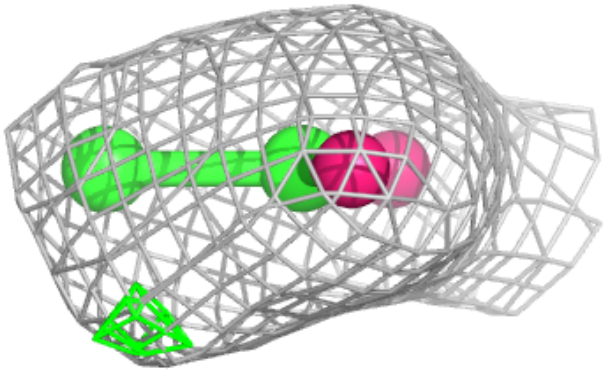
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

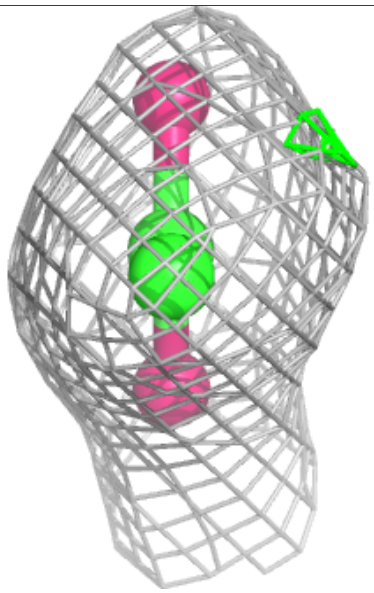


Electron density around ACT B 310:

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

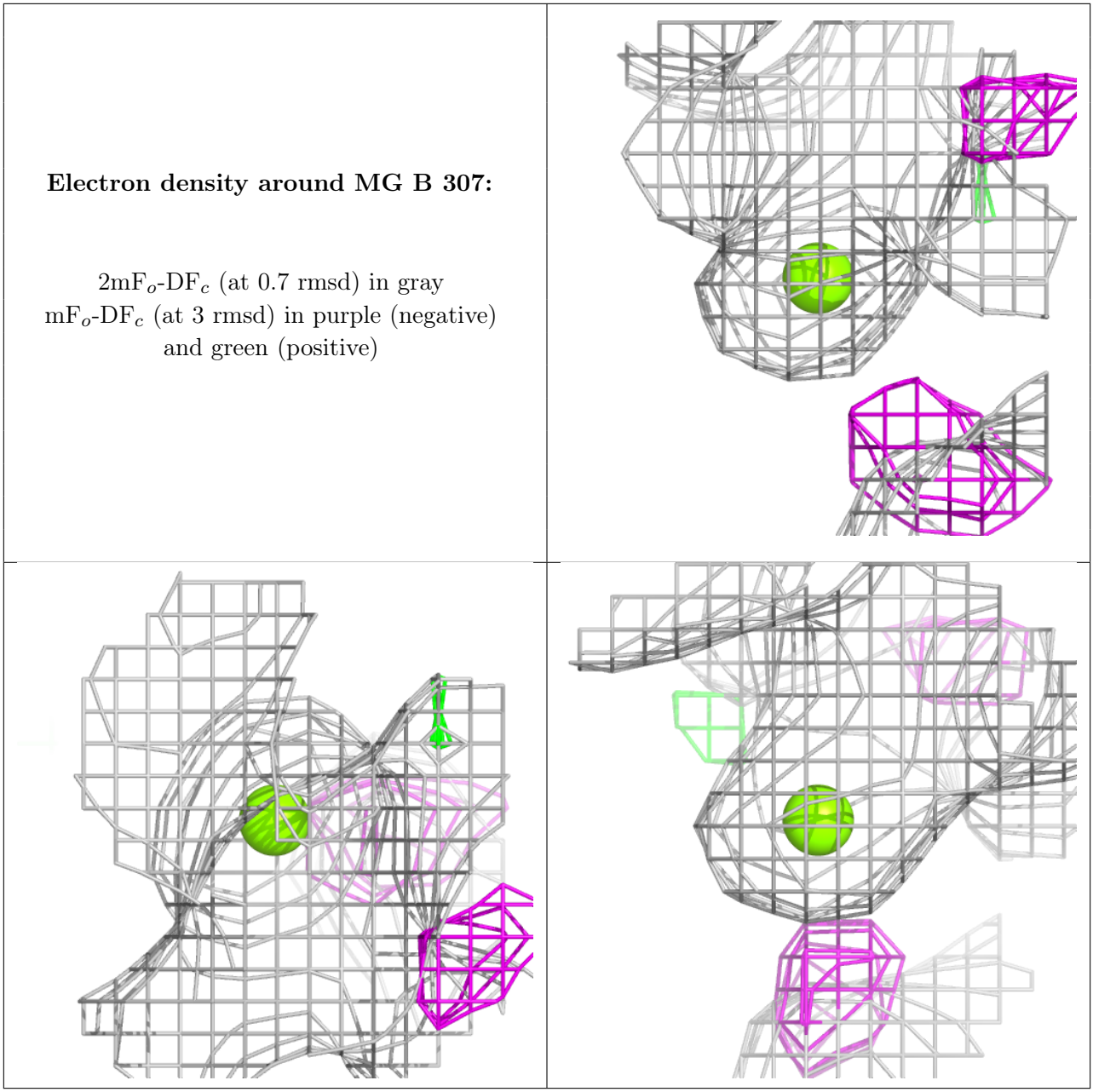






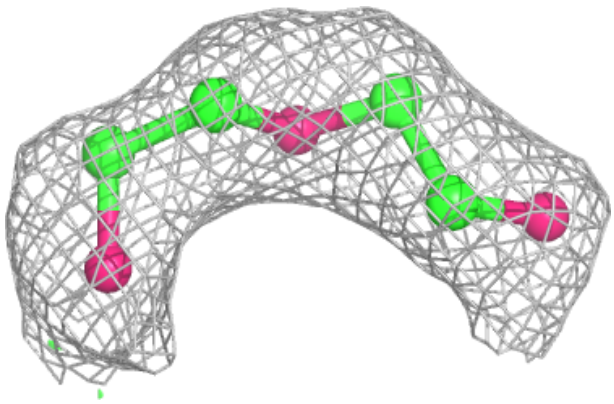
Electron density around MG B 307:

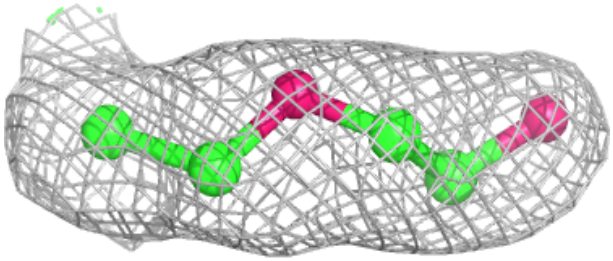
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

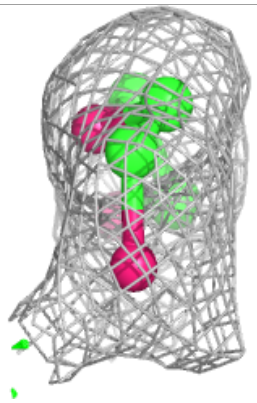


Electron density around PEG E 315:

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

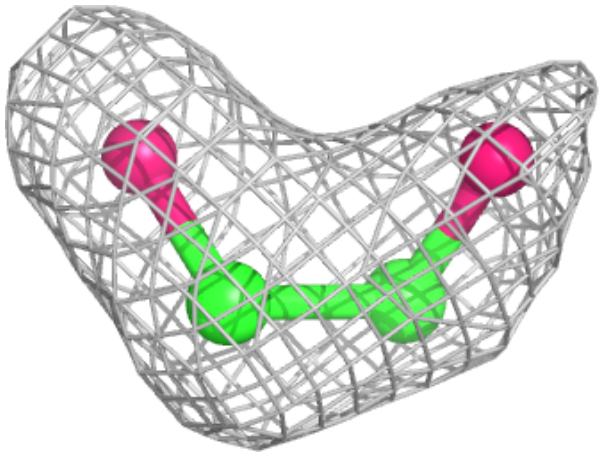


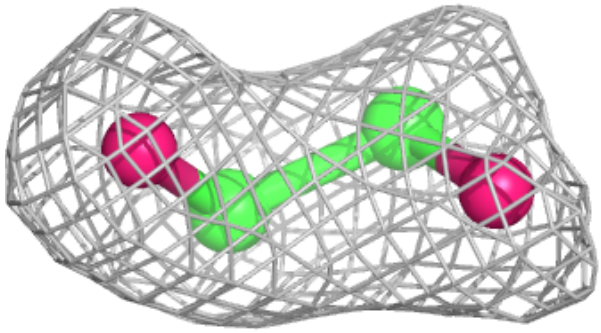


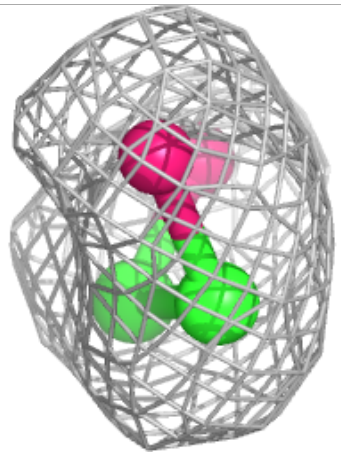


Electron density around EDO A 303:

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

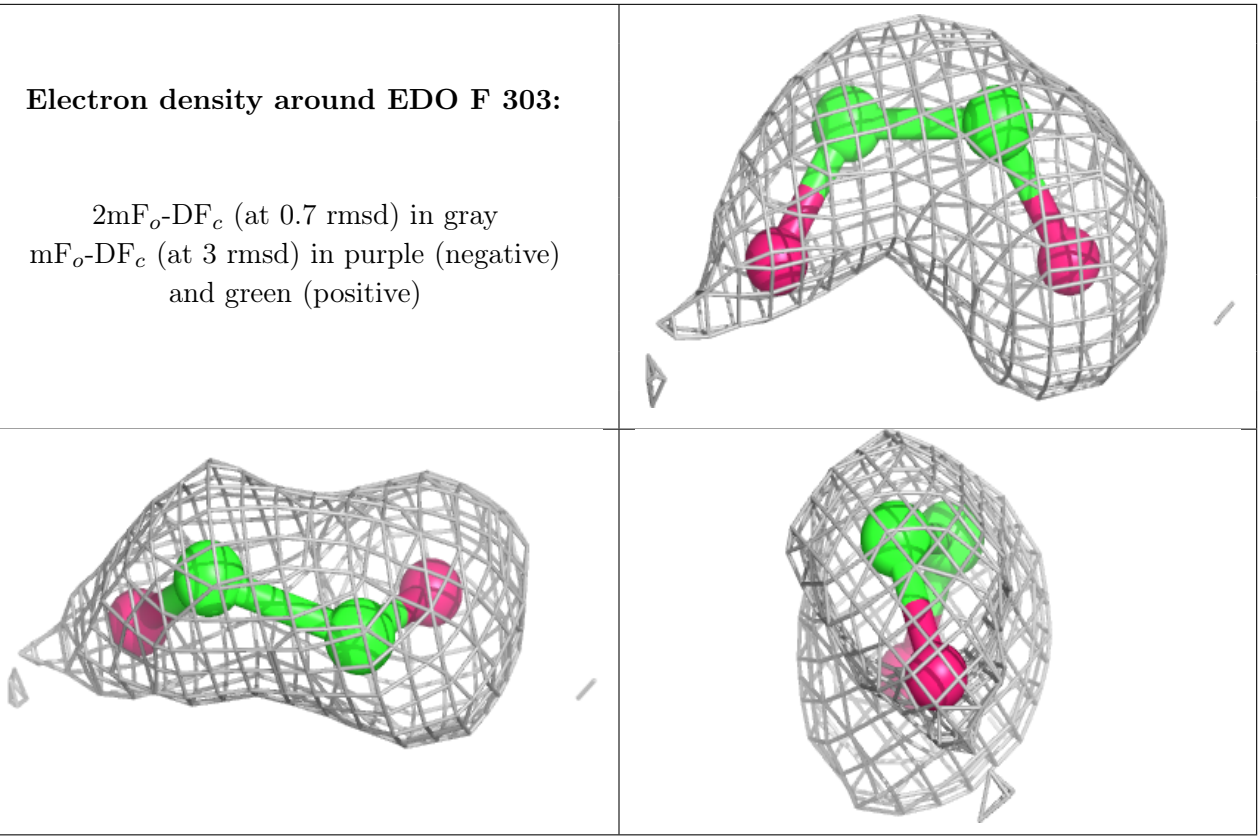






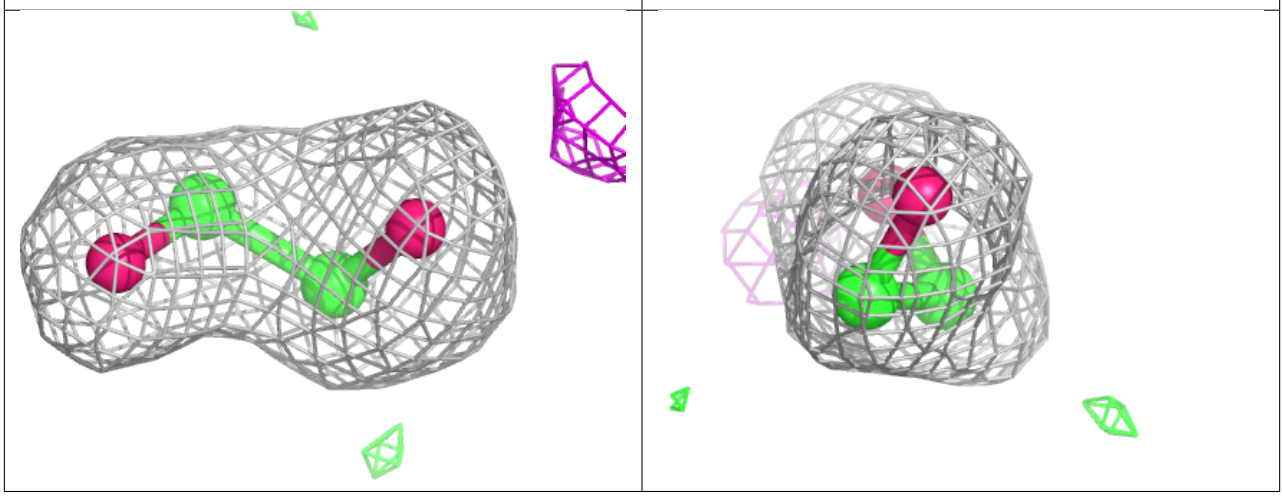
Electron density around EDO F 303:

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



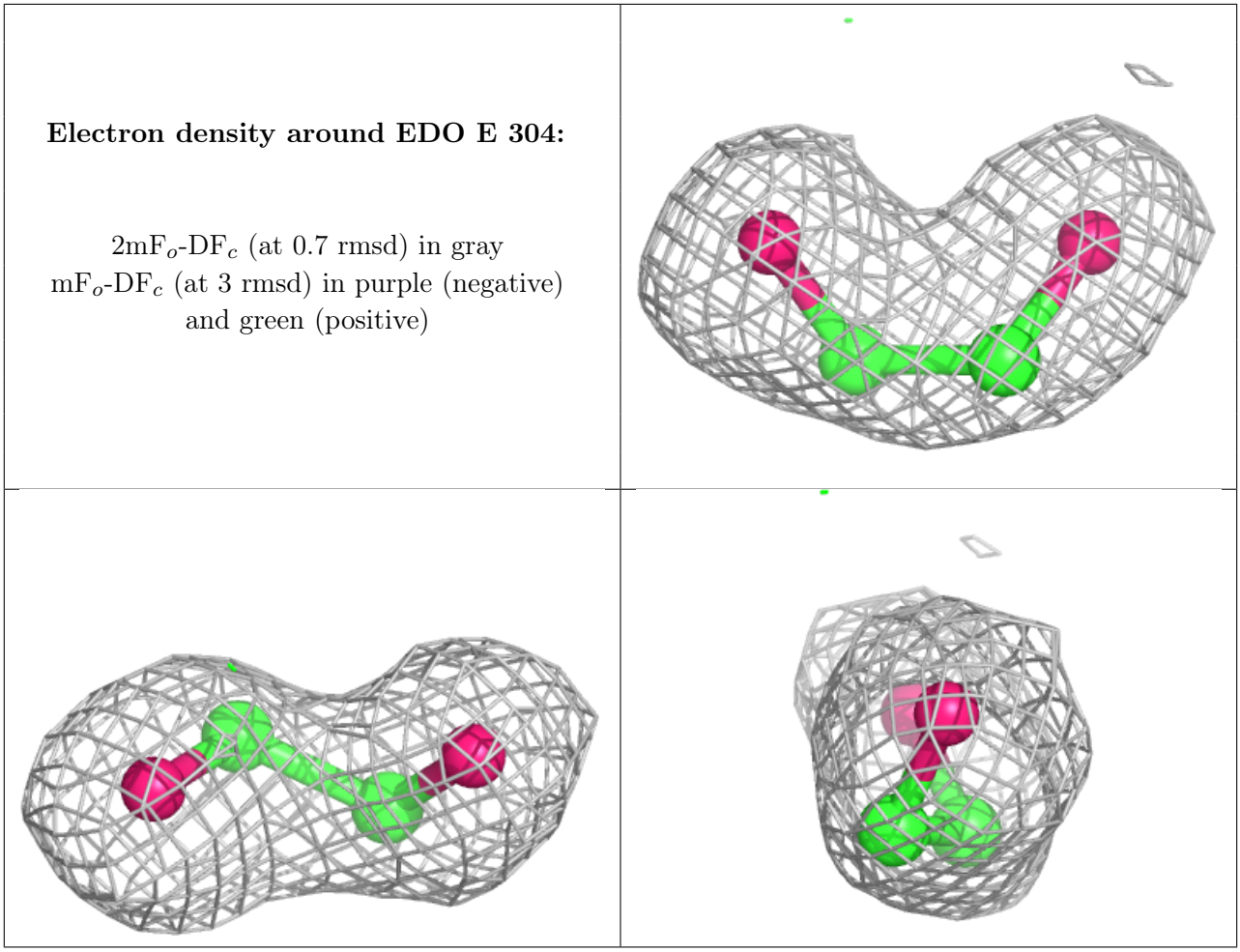
Electron density around EDO A 301:

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



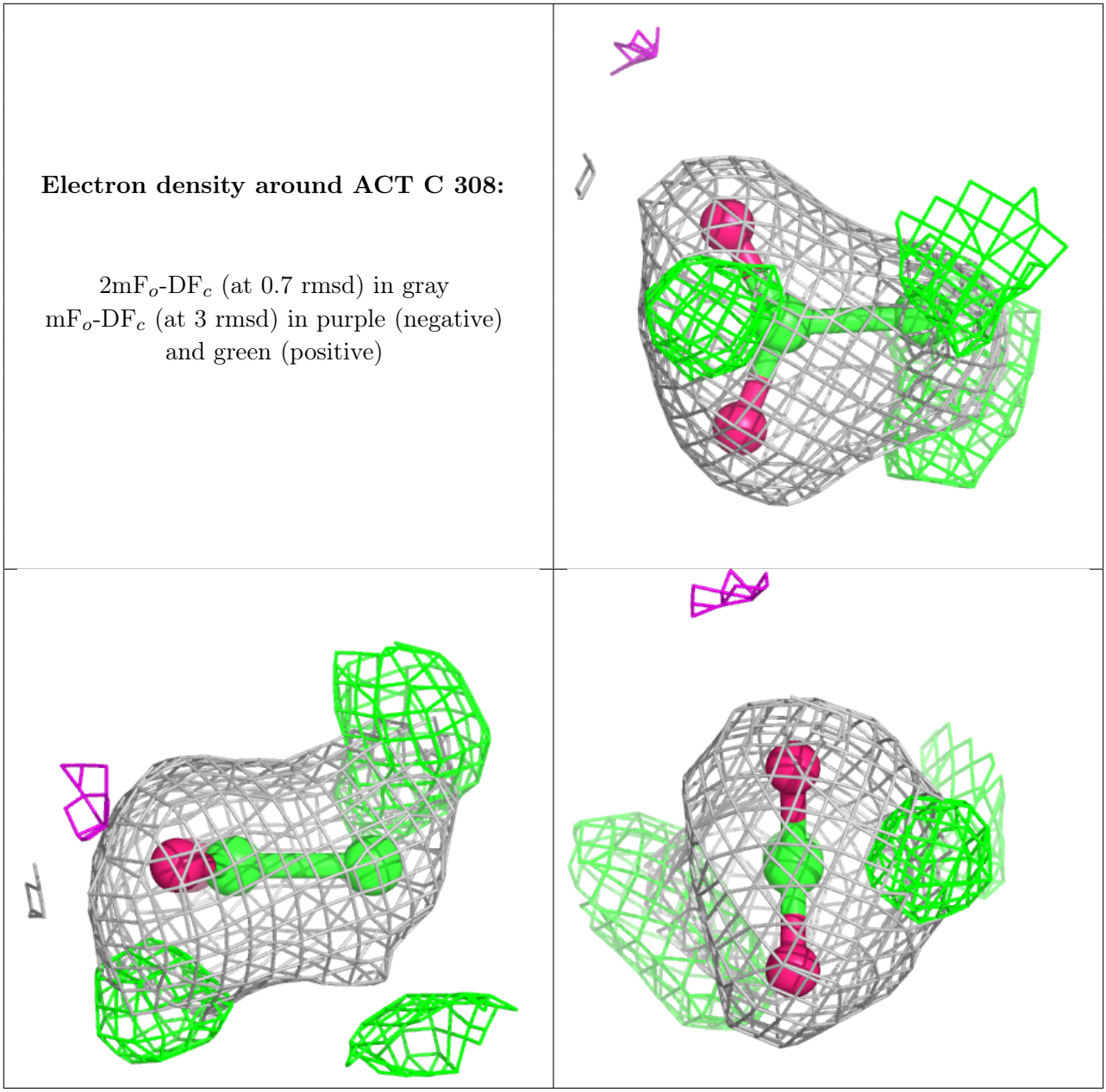
Electron density around EDO E 304:

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



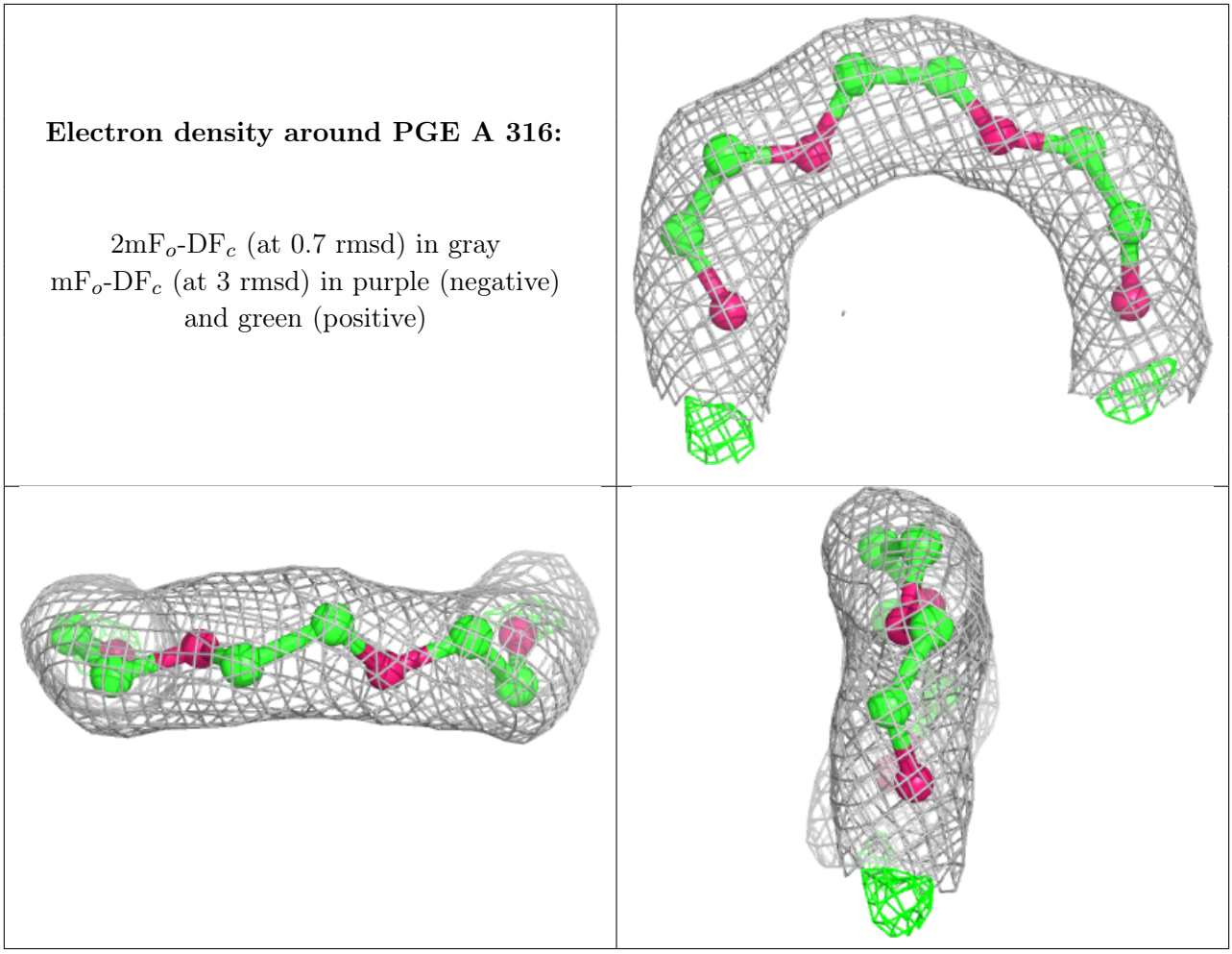
Electron density around ACT C 308:

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



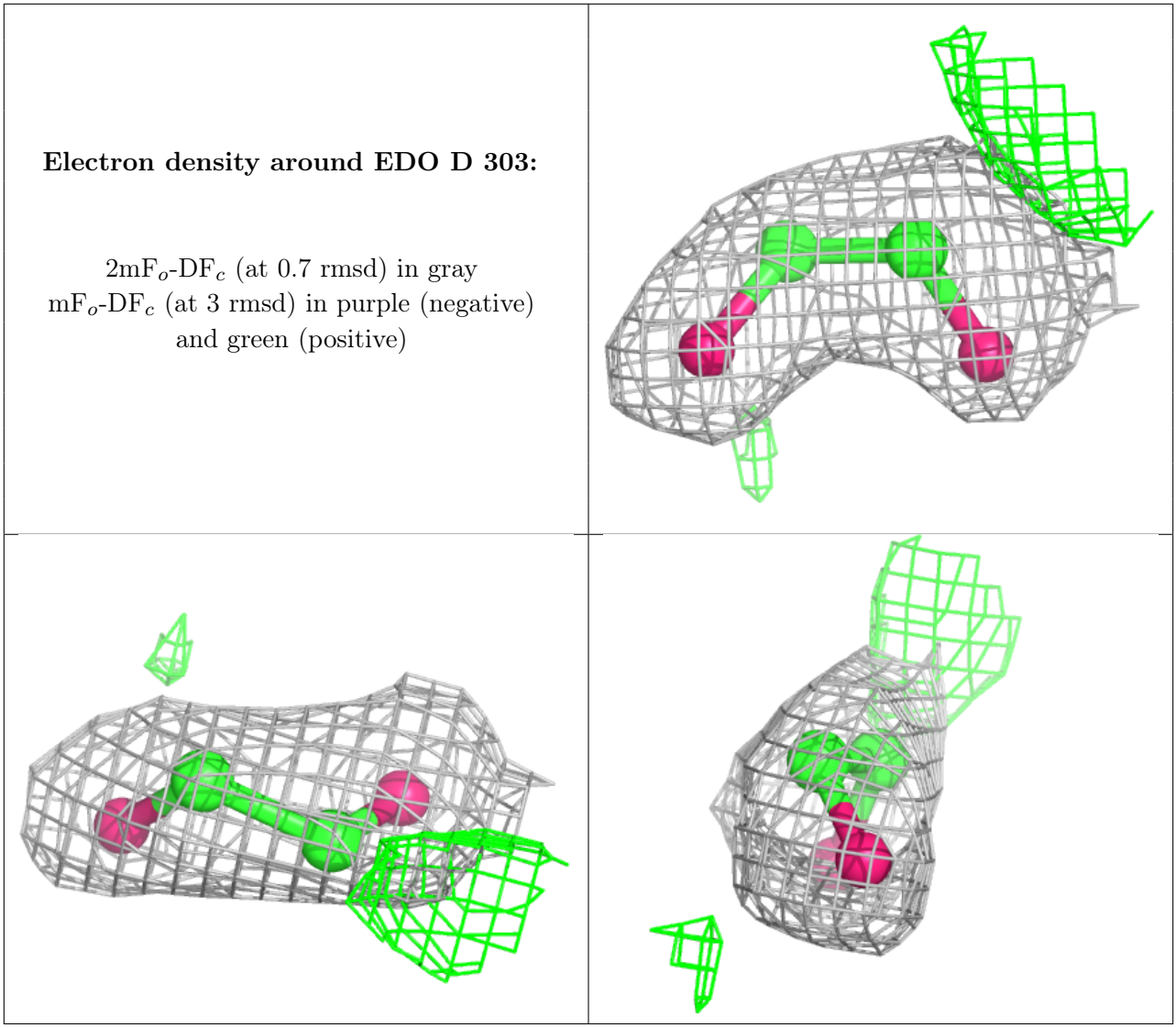
Electron density around PGE A 316:

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



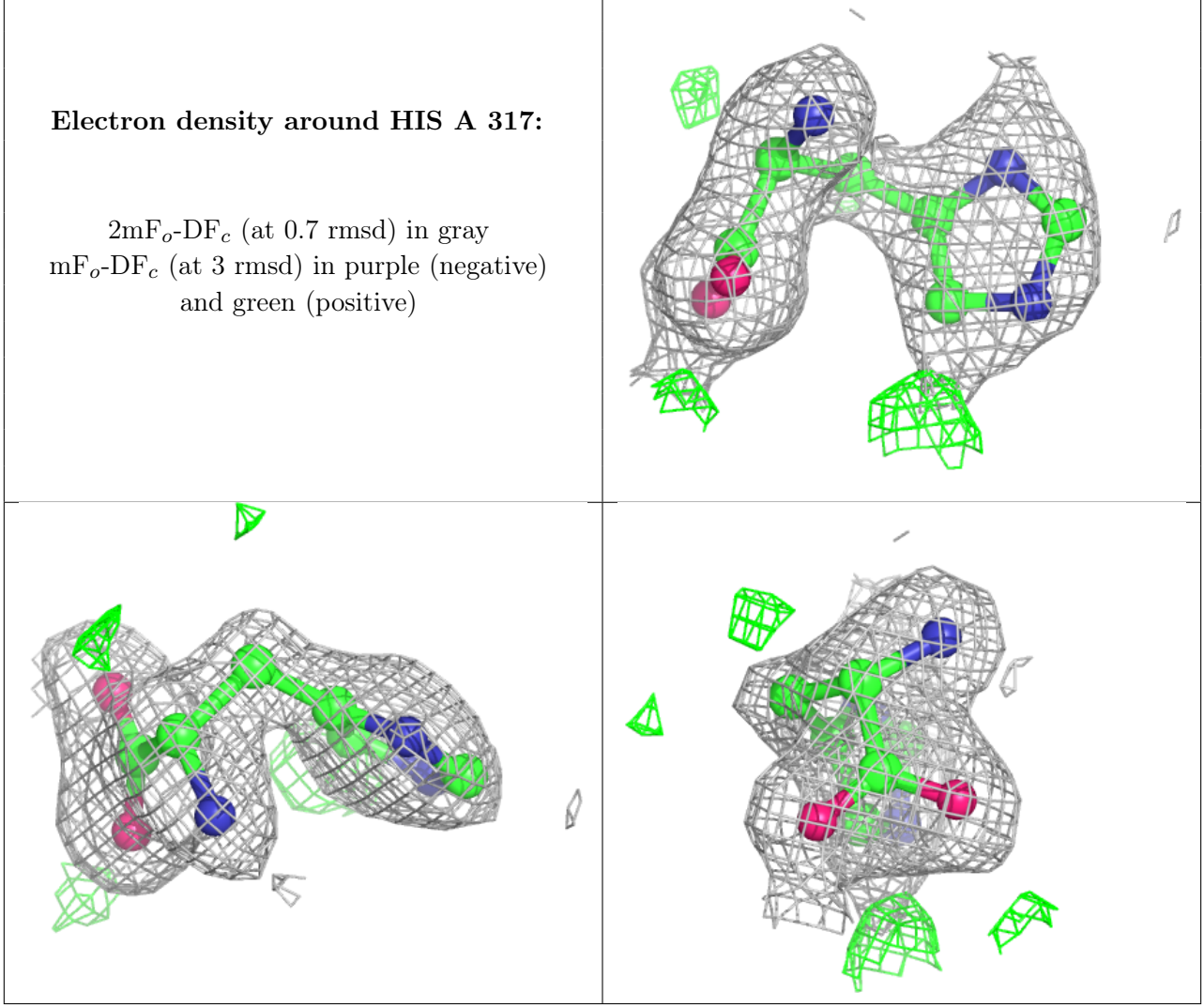
Electron density around EDO D 303:

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



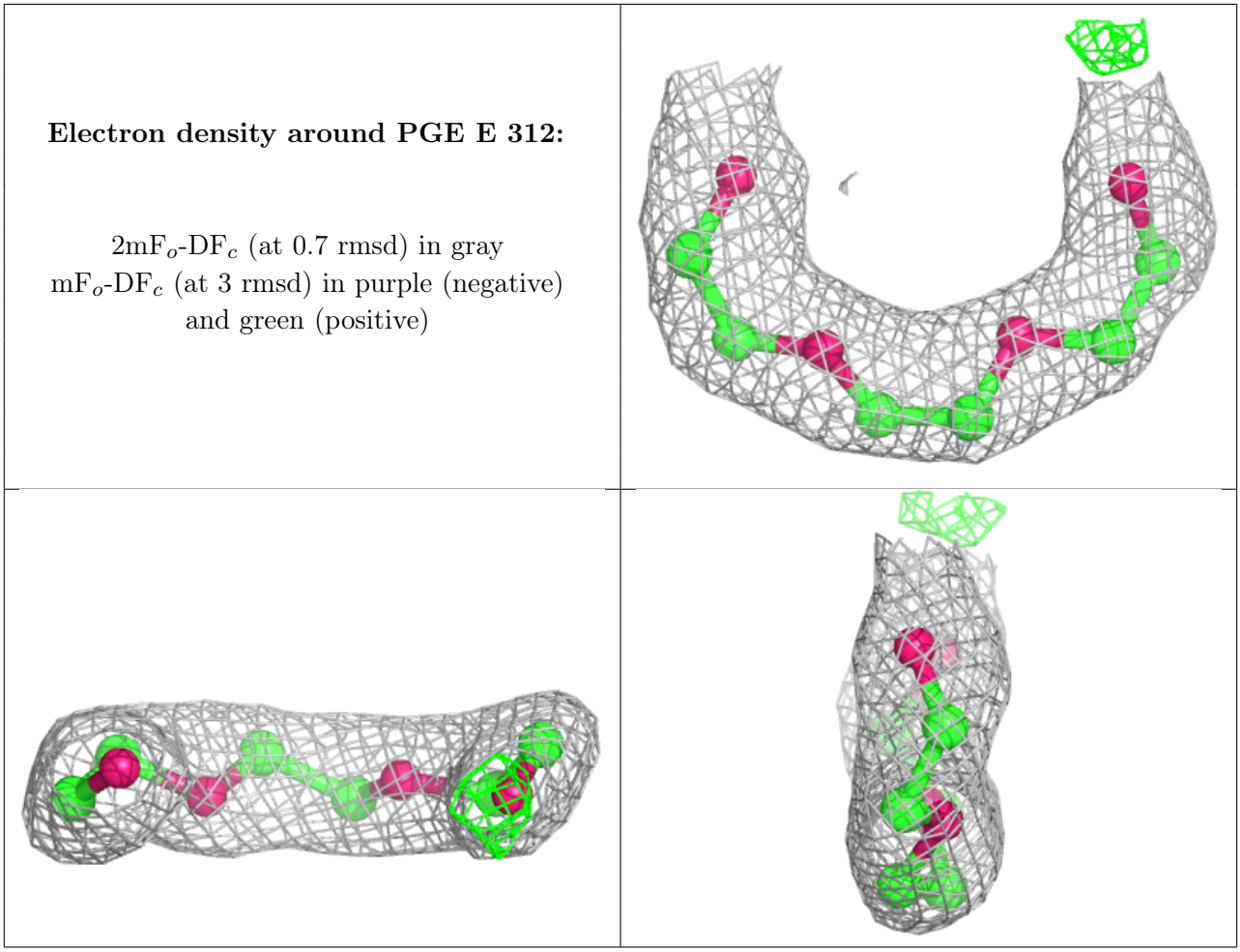
Electron density around HIS A 317:

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



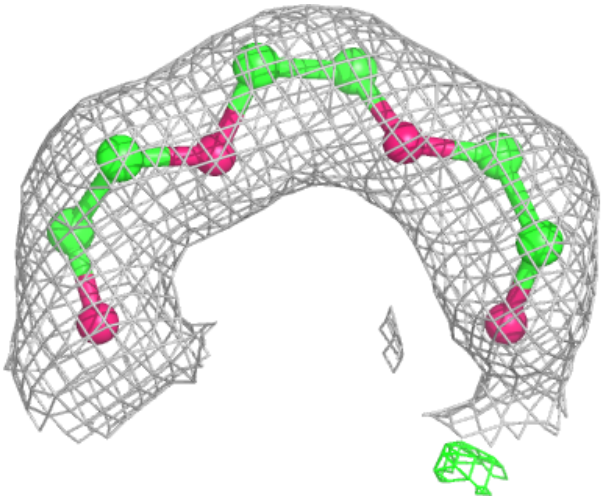
Electron density around PGE E 312:

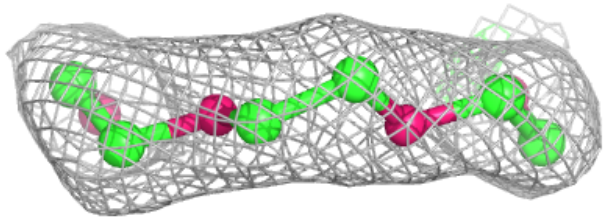
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

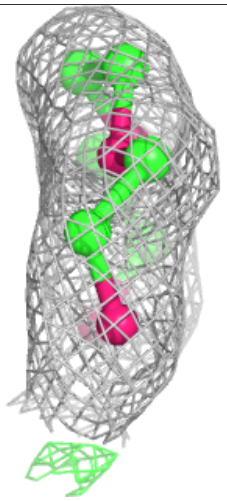


Electron density around PGE C 309:

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

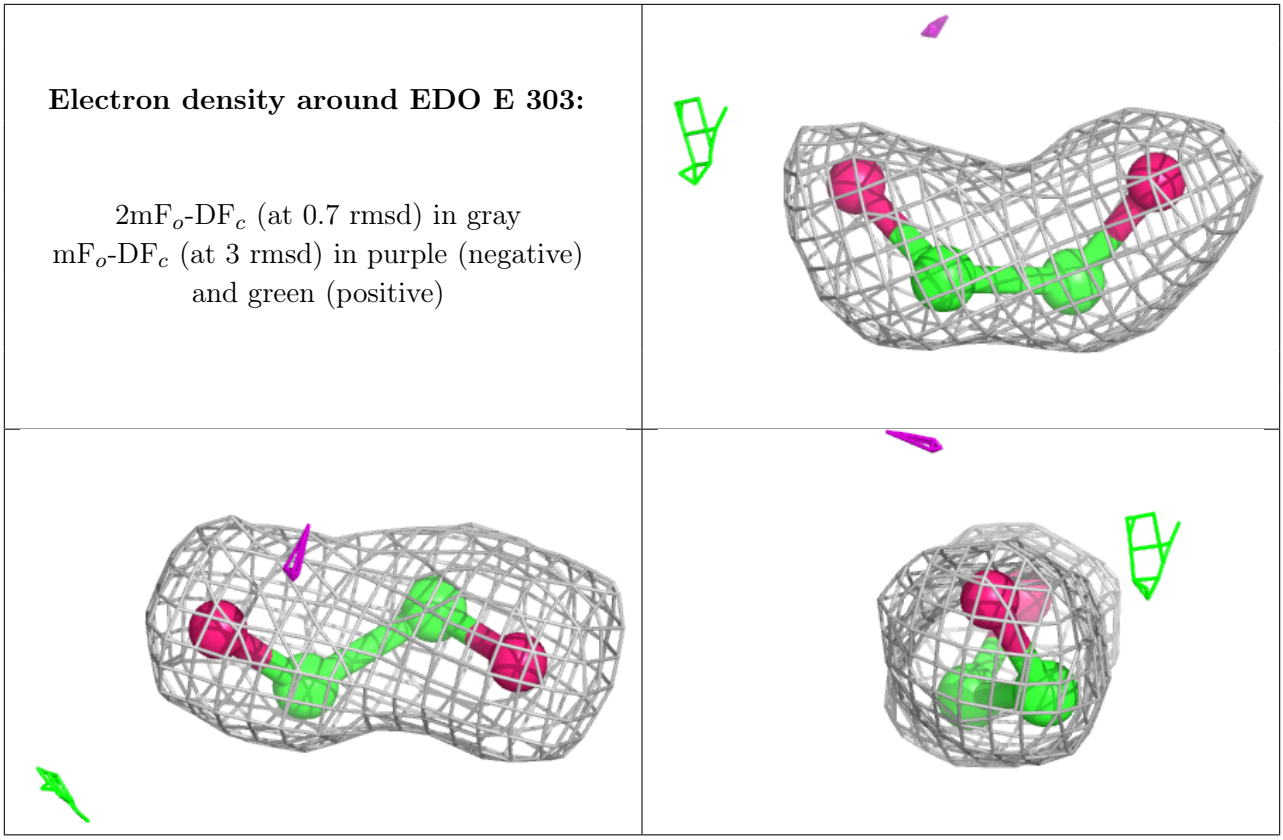






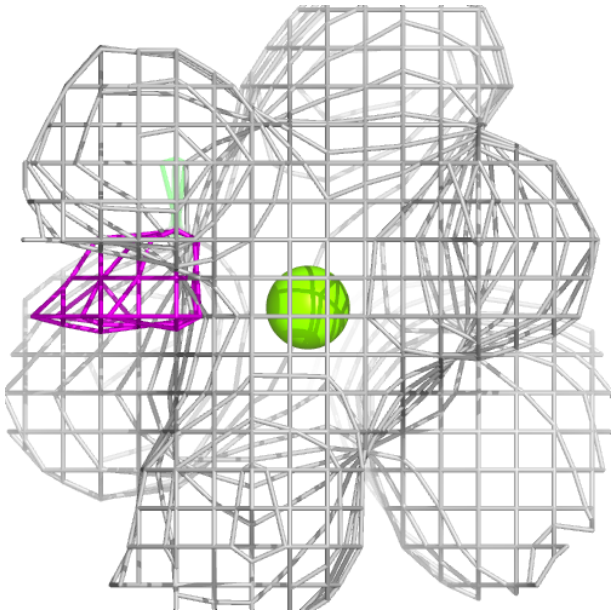
Electron density around EDO E 303:

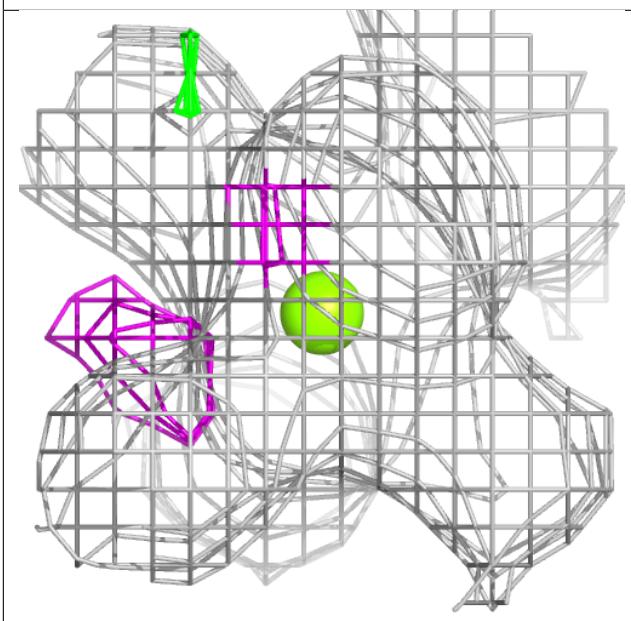
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

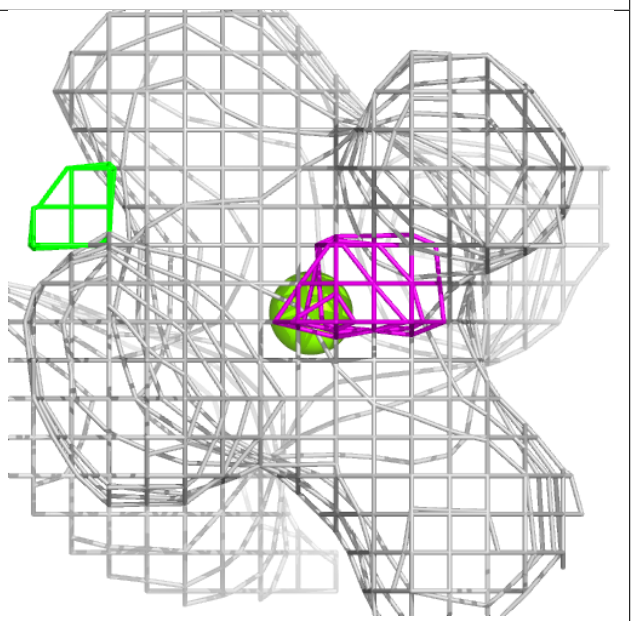


Electron density around MG A 310:

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

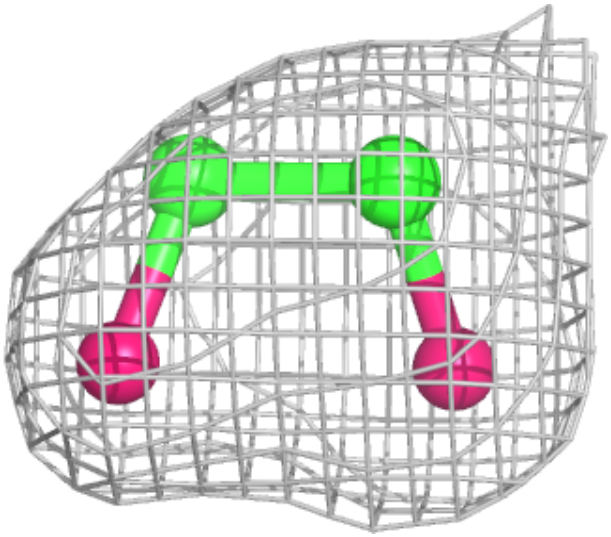


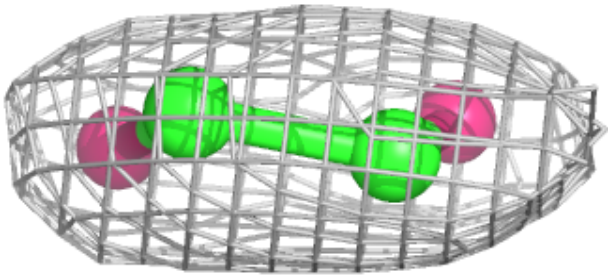


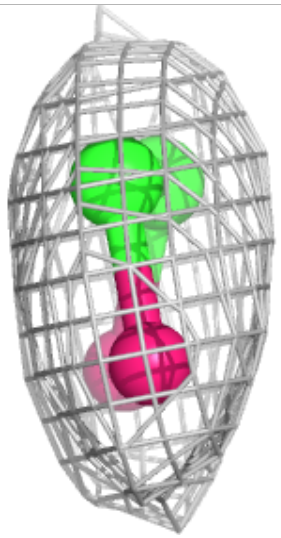


Electron density around EDO D 309:

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

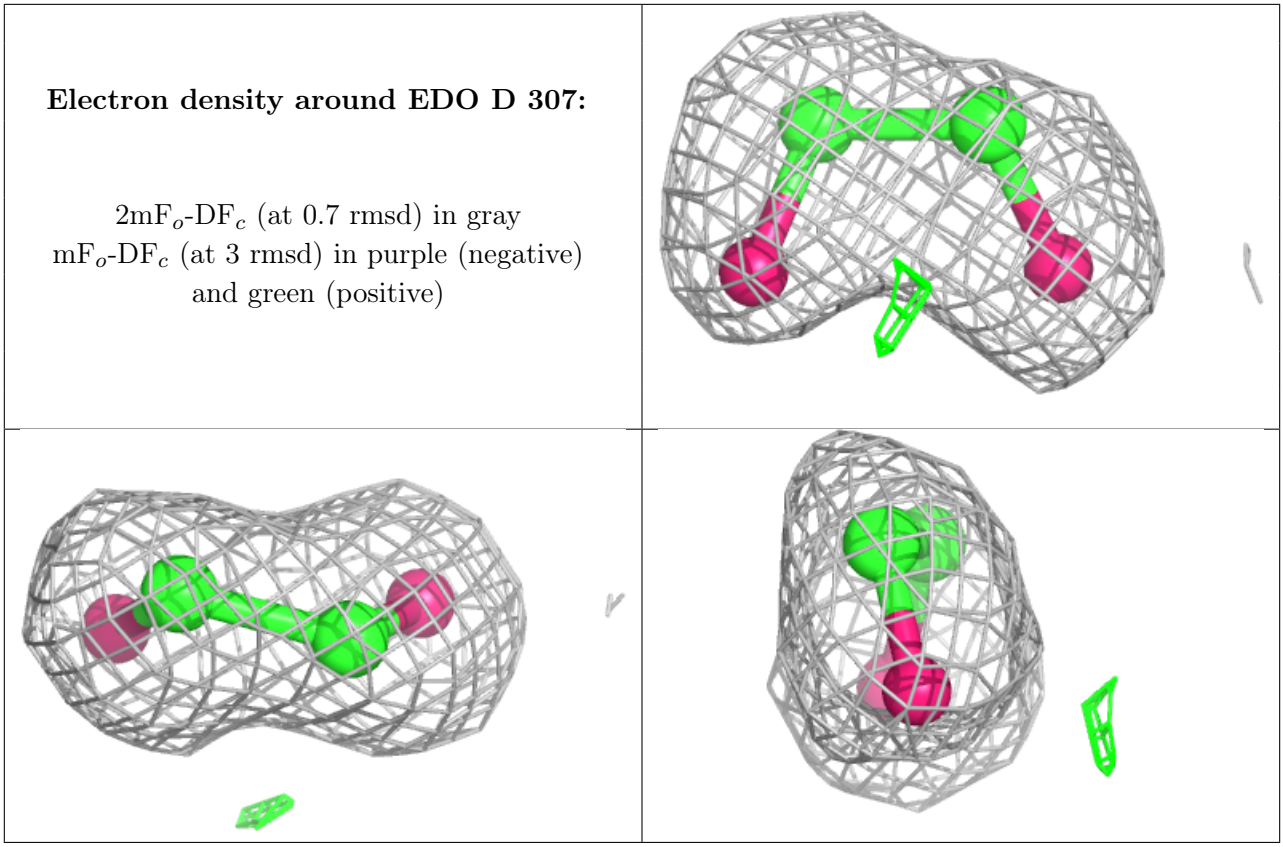






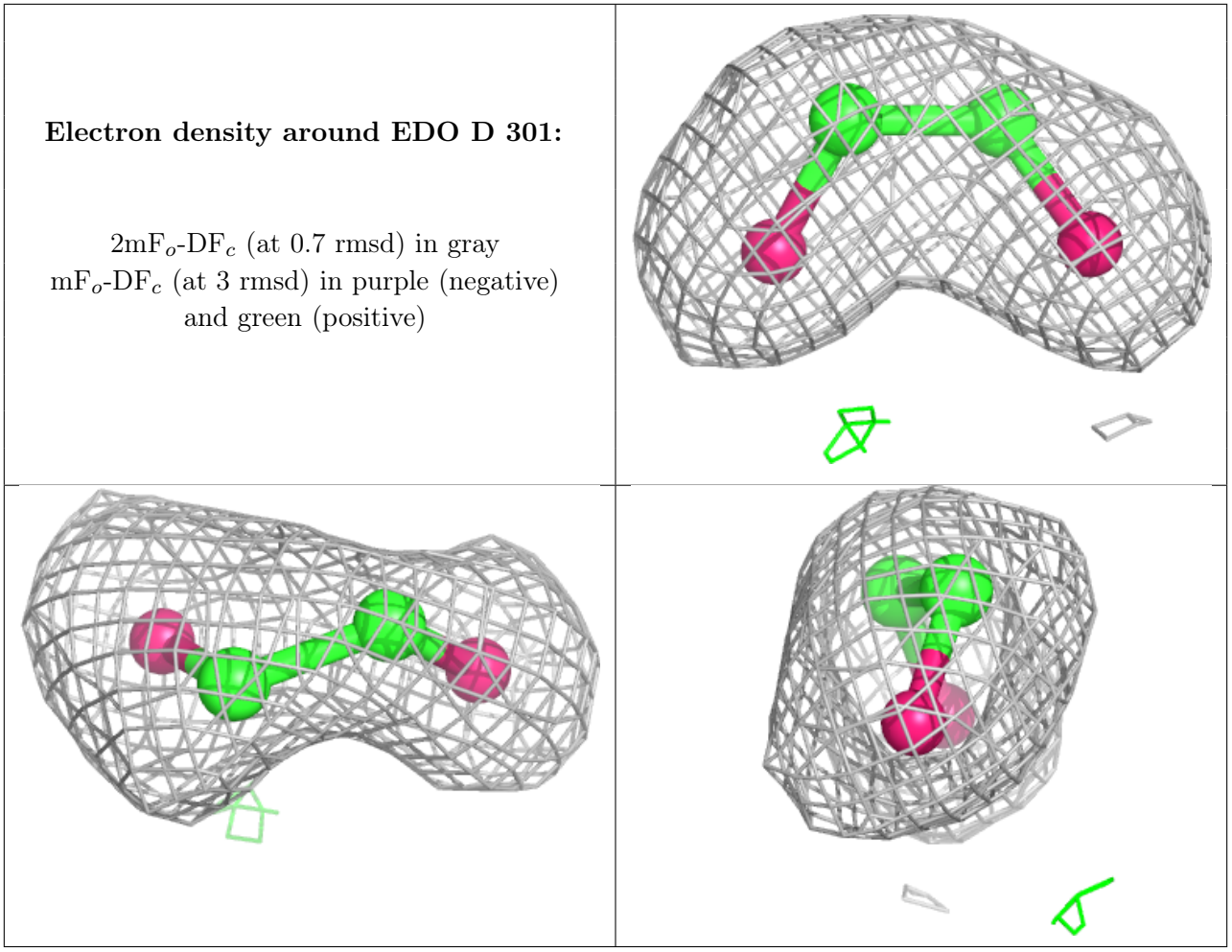
Electron density around EDO D 307:

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



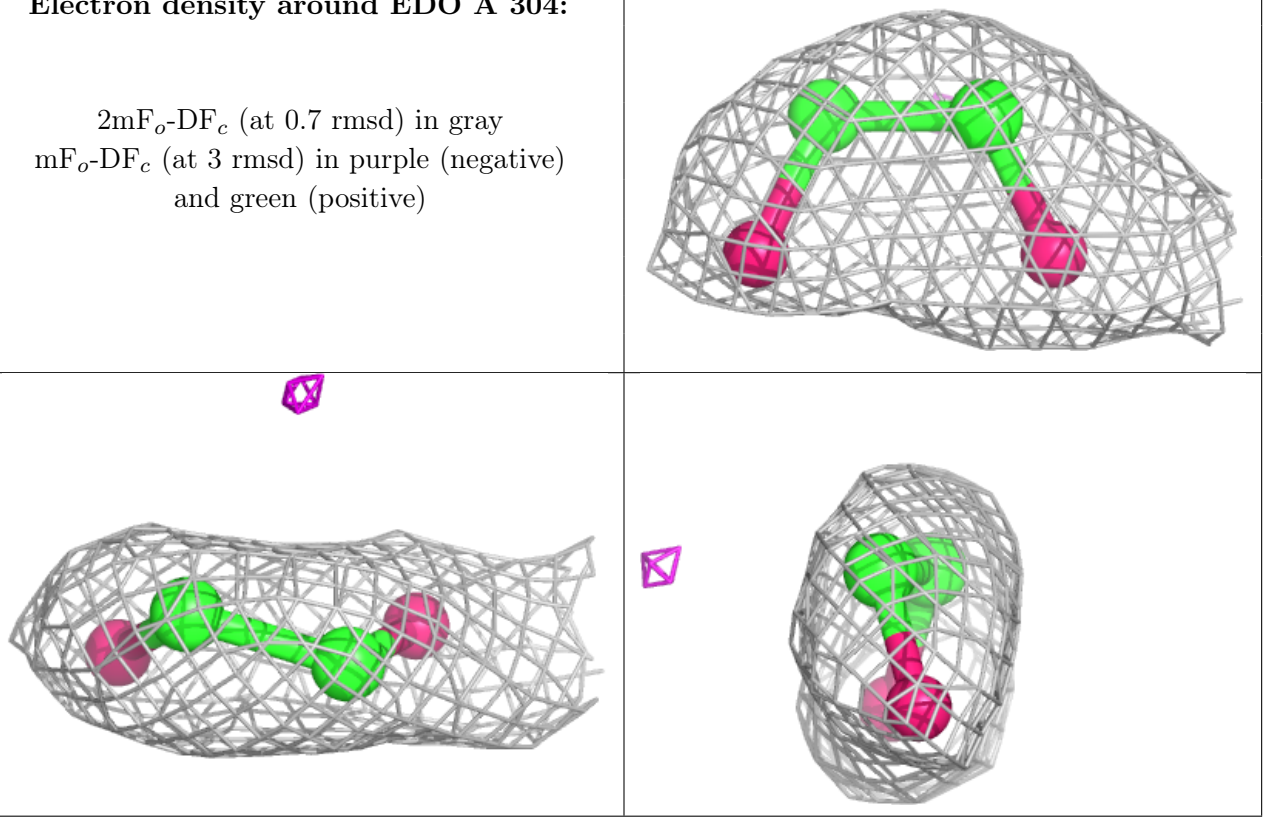
Electron density around EDO D 301:

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



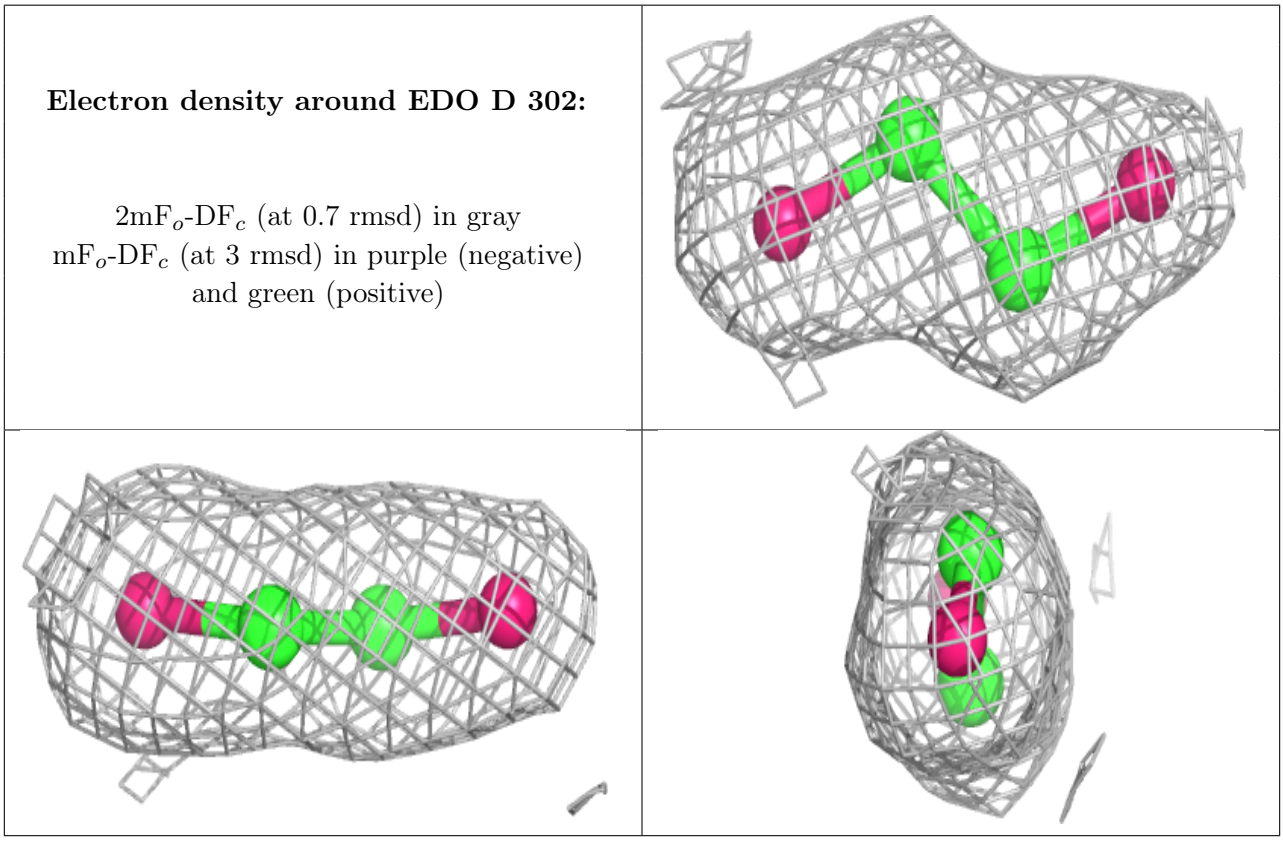
Electron density around EDO A 304:

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



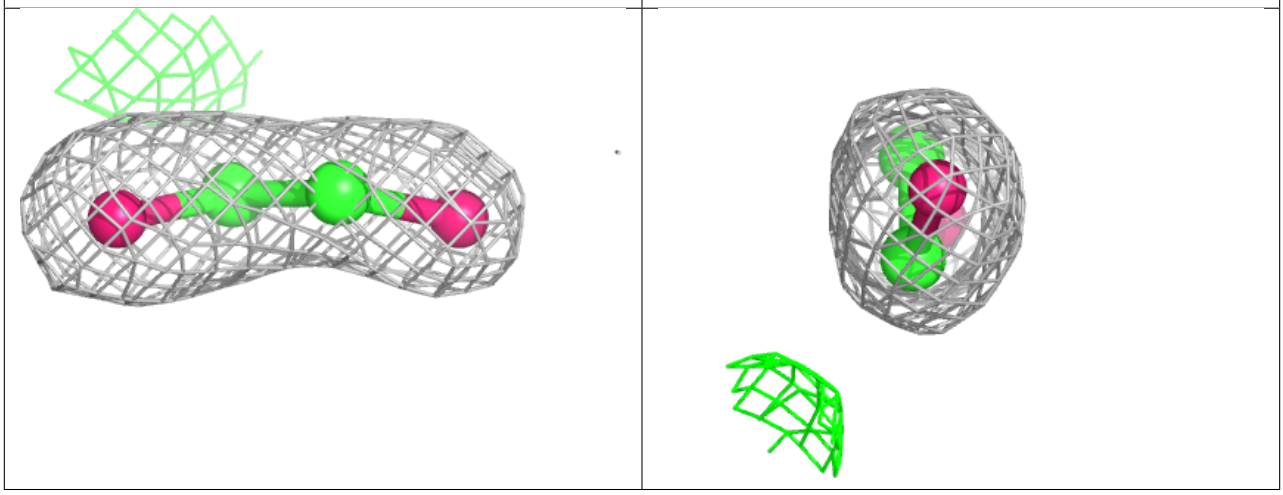
Electron density around EDO D 302:

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



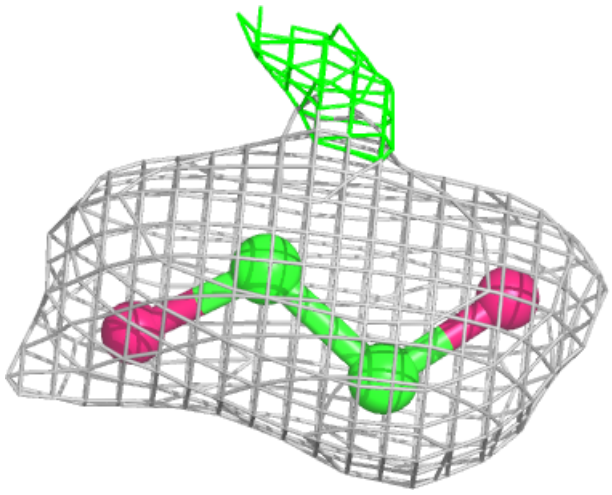
Electron density around EDO C 302:

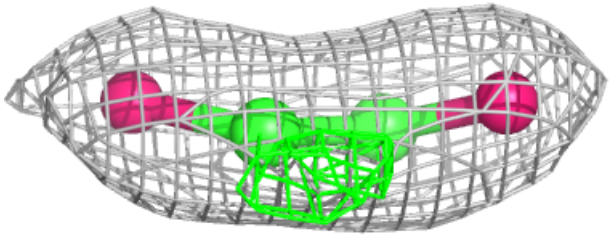
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

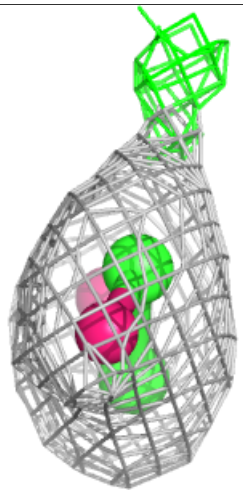


Electron density around EDO F 304:

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

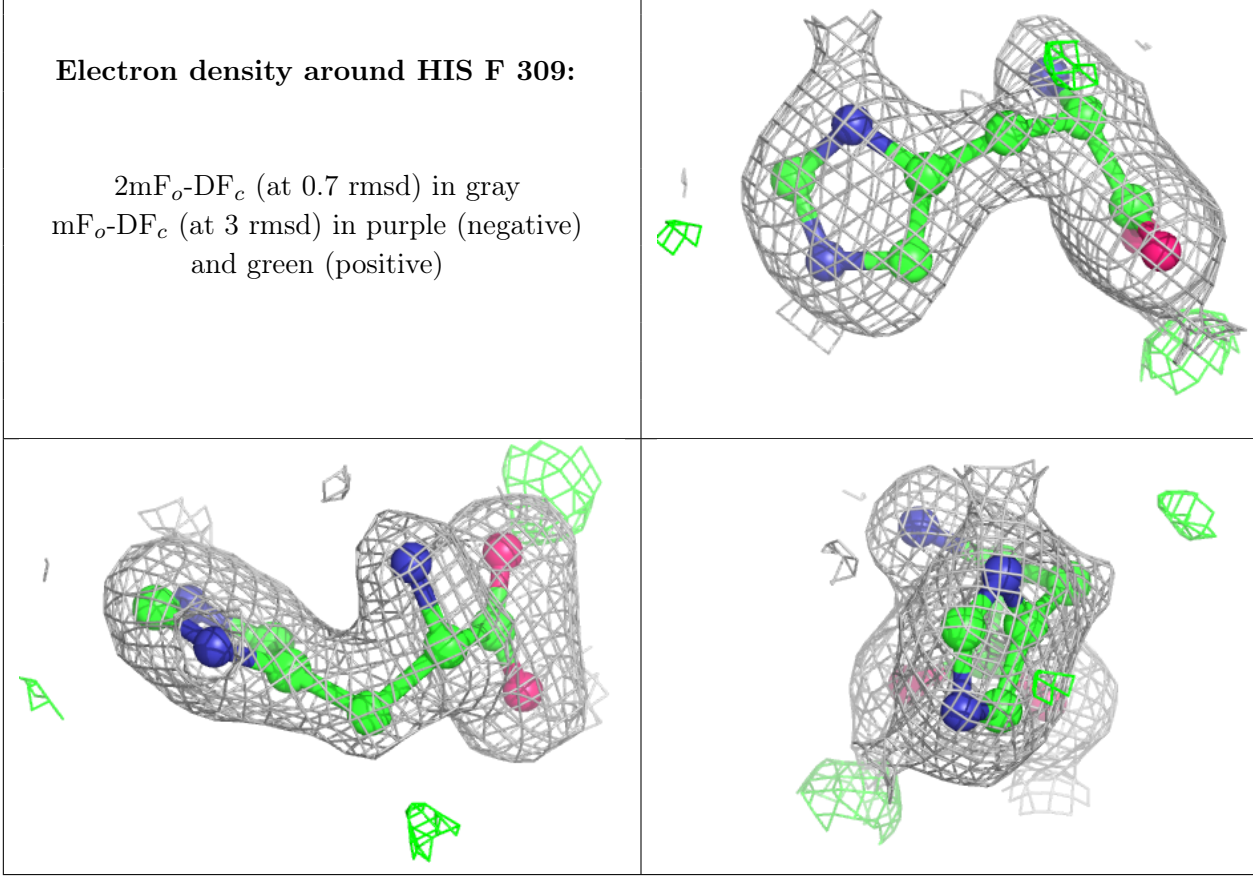






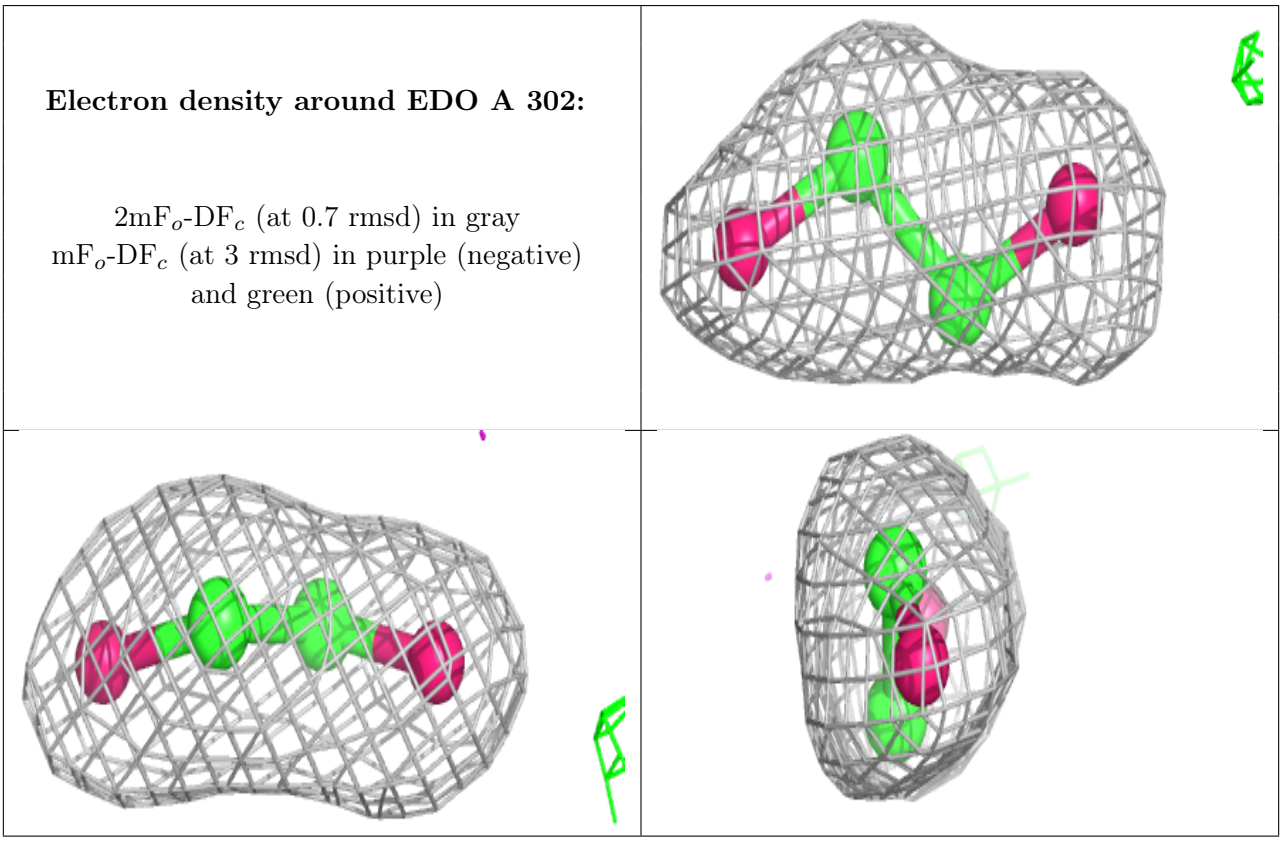
Electron density around HIS F 309:

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



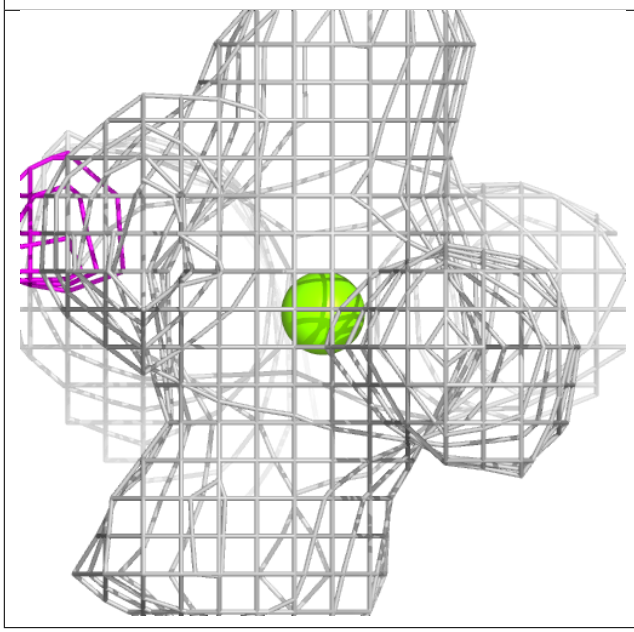
Electron density around EDO A 302:

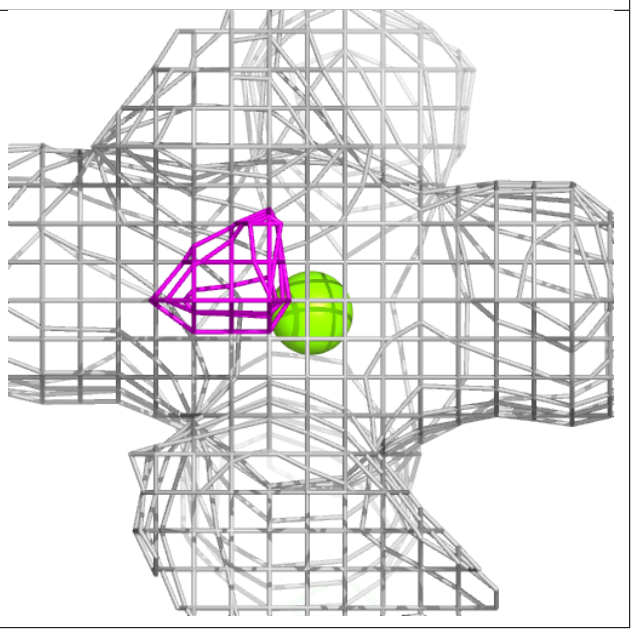
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MG B 306:

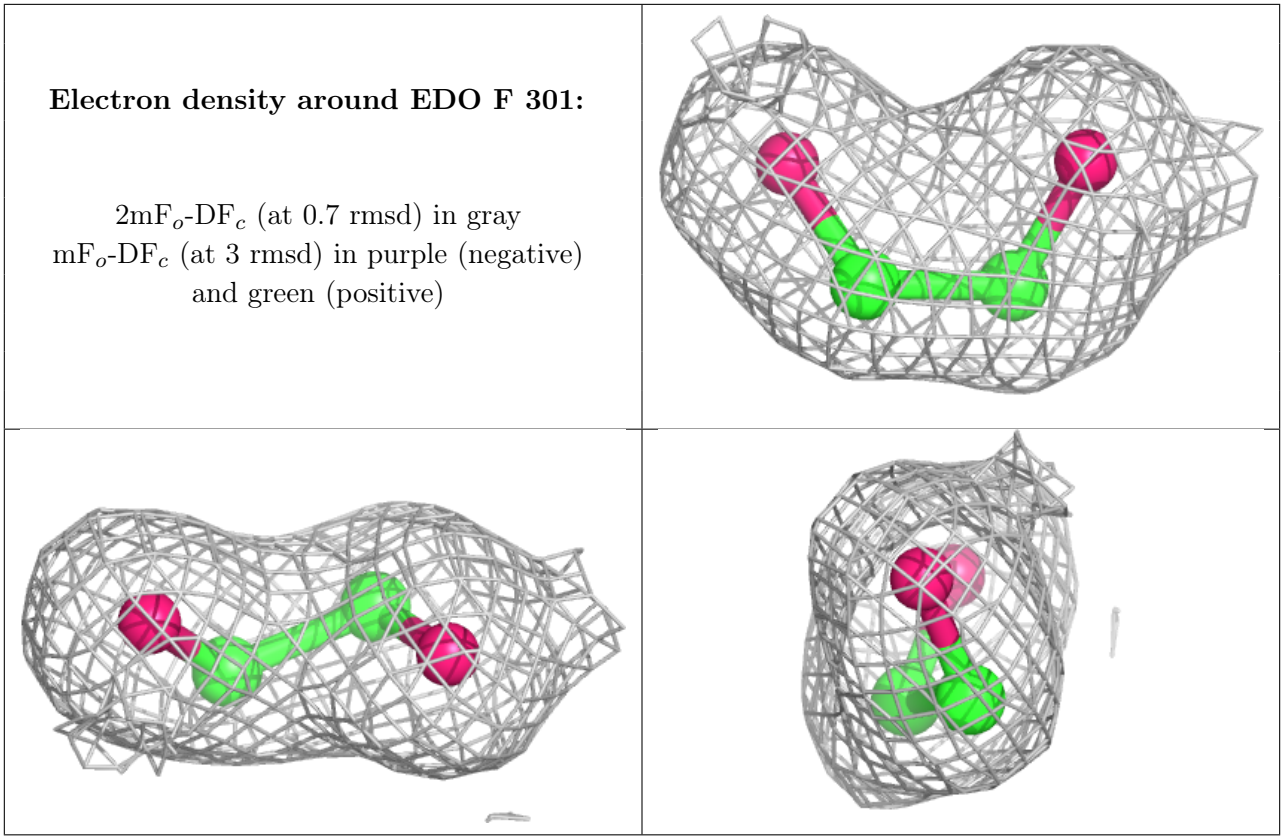
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





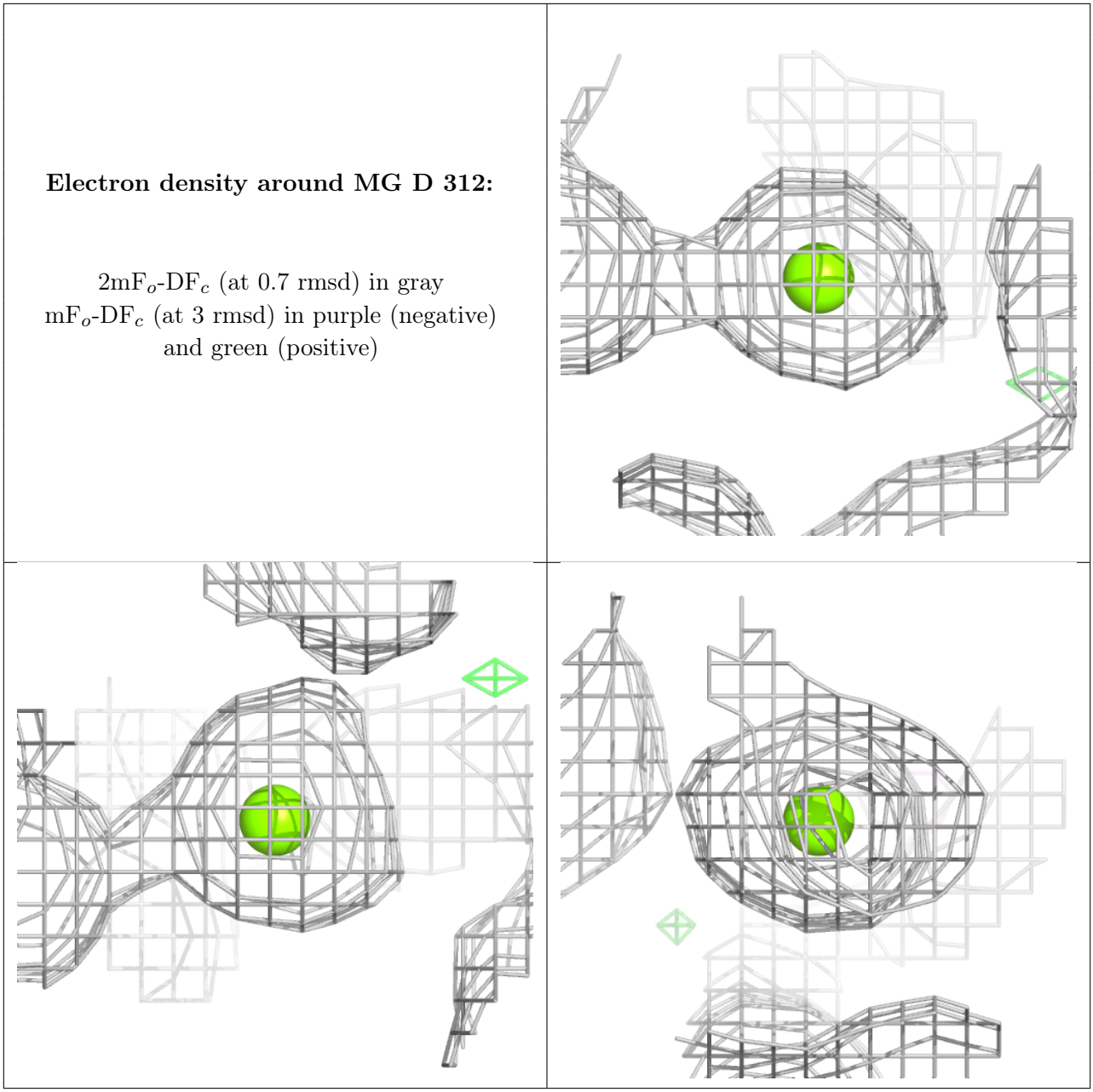
Electron density around EDO F 301:

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



Electron density around MG 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)



6.5 Other polymers

There are no such residues in this entry.