Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:53 PM EDT

PDB ID	:	7KEL
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H59K mutant with pyruvate bound in the active site
Authors	:	Saran, S.; Sanders, D.A.R.
Deposited on	:	2020-10-11
Resolution	:	2.10 Å(reported)

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

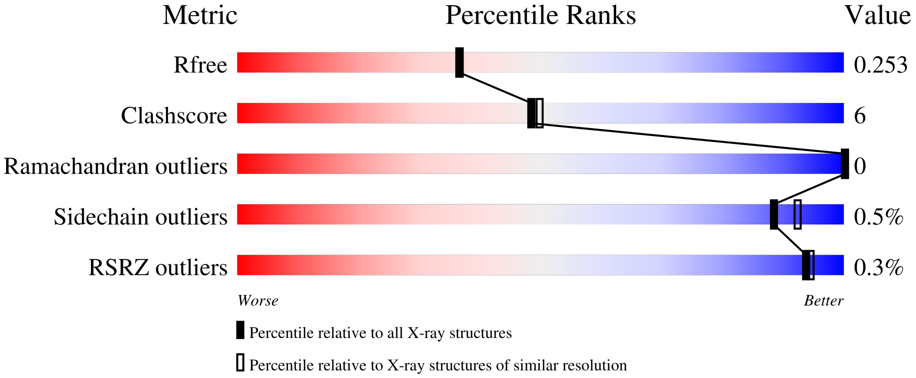
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance ⓘ

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

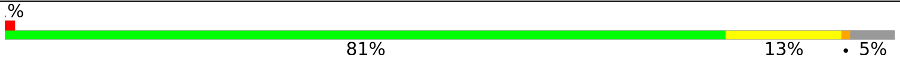
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	
1	B	310	
1	C	310	
1	D	310	
1	E	310	

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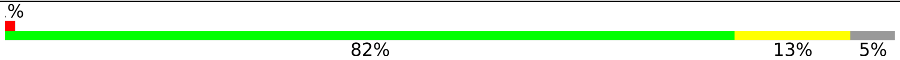
Mol	Chain	Length	Quality of chain
1	F	310	
1	G	310	
1	H	310	
1	I	310	
1	J	310	
1	K	310	
1	L	310	

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
3	ACT	L	303	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29356 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	295	2270	1444	376	437	13	0	0	0
1	B	296	2279	1450	378	438	13	0	0	0
1	C	296	2279	1450	378	438	13	0	0	0
1	D	295	2269	1444	376	436	13	0	0	0
1	E	295	2280	1450	379	438	13	0	1	0
1	F	296	2278	1450	378	437	13	0	0	0
1	G	296	2278	1450	378	437	13	1	0	0
1	H	296	2278	1450	378	437	13	0	0	0
1	I	296	2279	1450	378	438	13	0	0	0
1	J	294	2262	1440	374	435	13	0	0	0
1	K	296	2288	1456	381	438	13	0	1	0
1	L	296	2278	1450	378	437	13	0	0	0

There are 156 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
G	-11	MET	-	expression tag	UNP A0A2U0QMK8
G	-10	ARG	-	expression tag	UNP A0A2U0QMK8
G	-9	GLY	-	expression tag	UNP A0A2U0QMK8
G	-8	SER	-	expression tag	UNP A0A2U0QMK8
G	-7	HIS	-	expression tag	UNP A0A2U0QMK8
G	-6	HIS	-	expression tag	UNP A0A2U0QMK8
G	-5	HIS	-	expression tag	UNP A0A2U0QMK8
G	-4	HIS	-	expression tag	UNP A0A2U0QMK8
G	-3	HIS	-	expression tag	UNP A0A2U0QMK8
G	-2	HIS	-	expression tag	UNP A0A2U0QMK8
G	-1	GLY	-	expression tag	UNP A0A2U0QMK8

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

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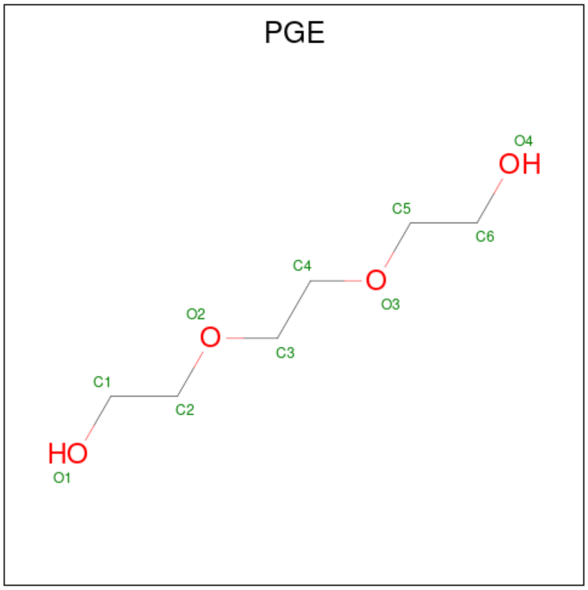
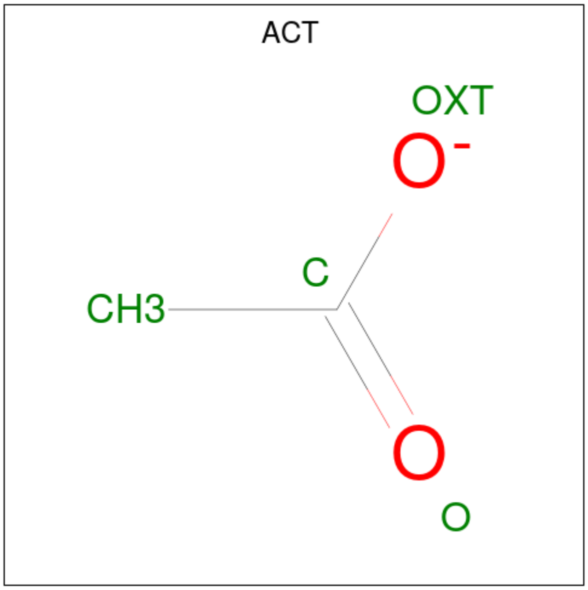
Chain	Residue	Modelled	Actual	Comment	Reference
K	-10	ARG	-	expression tag	UNP A0A2U0QMK8
K	-9	GLY	-	expression tag	UNP A0A2U0QMK8
K	-8	SER	-	expression tag	UNP A0A2U0QMK8
K	-7	HIS	-	expression tag	UNP A0A2U0QMK8
K	-6	HIS	-	expression tag	UNP A0A2U0QMK8
K	-5	HIS	-	expression tag	UNP A0A2U0QMK8
K	-4	HIS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

- Molecule 2 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
2	A	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0
2	E	1	Total C O 10 6 4	0	0
2	F	1	Total C O 10 6 4	0	0
2	I	1	Total C O 10 6 4	0	0
2	J	1	Total C O 10 6 4	0	0
2	K	1	Total C O 10 6 4	0	0
2	L	1	Total C O 10 6 4	0	0

- Molecule 3 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
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0

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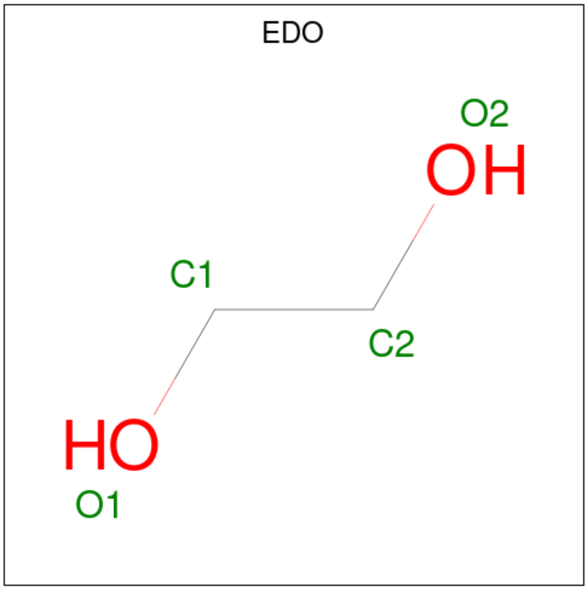
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 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
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

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

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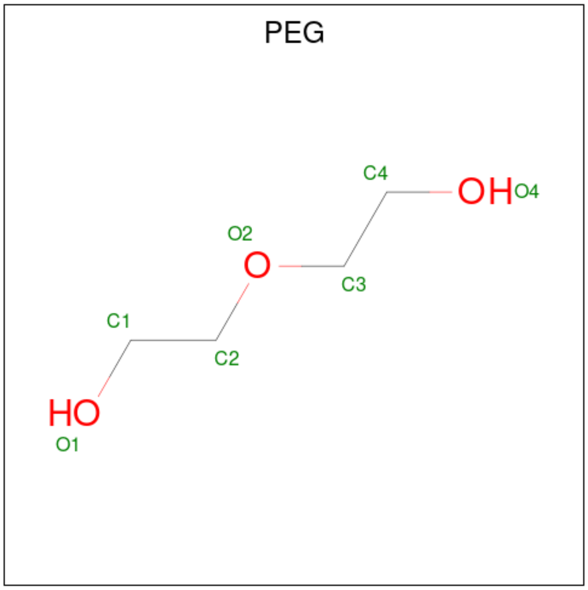
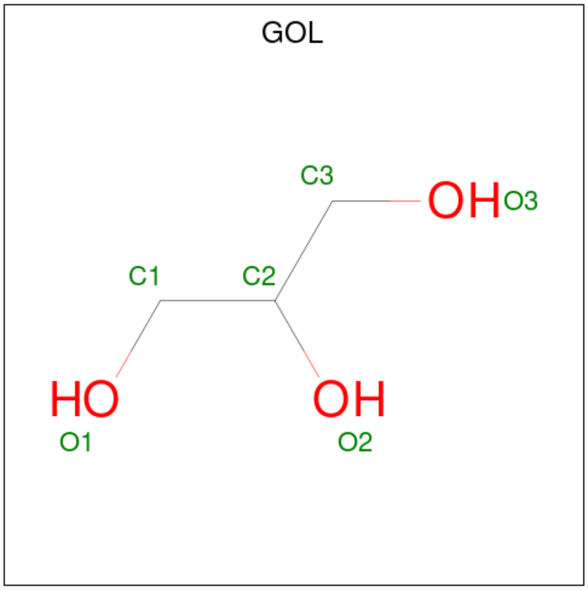
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 7 4 3	0	0
6	G	1	Total C O 7 4 3	0	0
6	H	1	Total C O 7 4 3	0	0
6	J	1	Total C O 7 4 3	0	0
6	L	1	Total C O 7 4 3	0	0
6	L	1	Total C O 7 4 3	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C O 6 3 3	0	0
7	I	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	137	Total O 137 137	0	0
8	B	123	Total O 123 123	0	0
8	C	123	Total O 123 123	0	0
8	D	144	Total O 144 144	0	0
8	E	146	Total O 146 146	0	0
8	F	139	Total O 139 139	0	0
8	G	130	Total O 130 130	0	0
8	H	126	Total O 126 126	0	0
8	I	131	Total O 131 131	0	0

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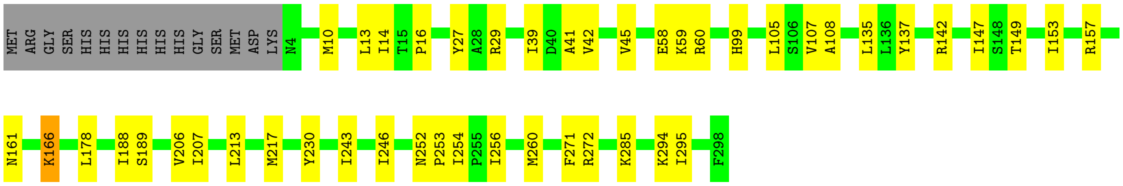
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	127	Total O 127 127	0	0
8	K	126	Total O 126 126	0	0
8	L	120	Total O 120 120	0	0

3 Residue-property plots

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

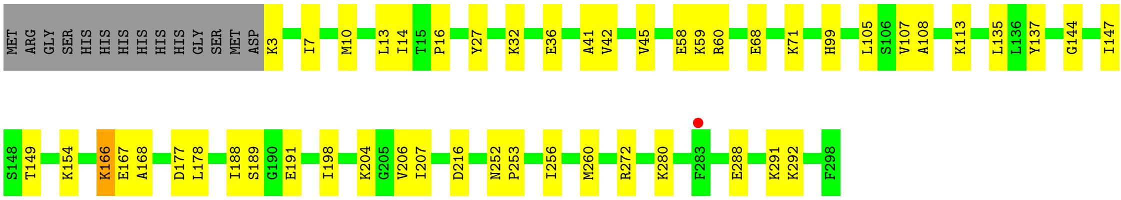
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A:



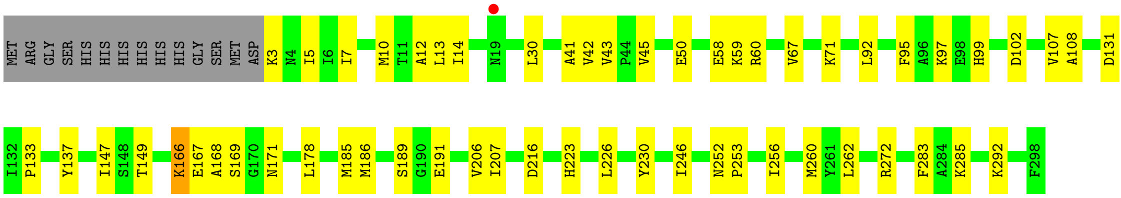
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:



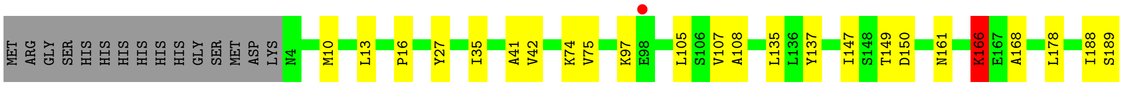
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

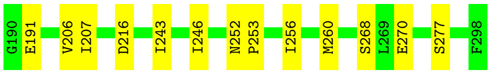
Chain C:



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

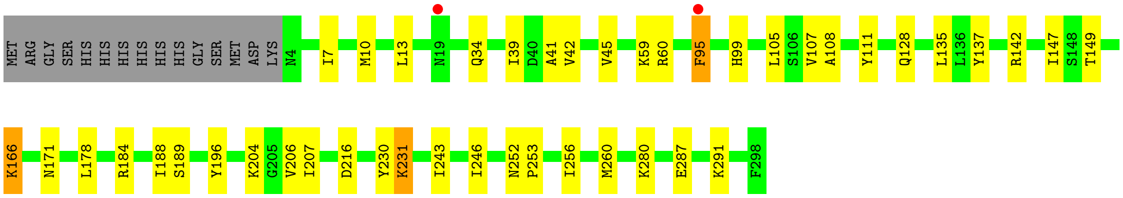
Chain D:





- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:

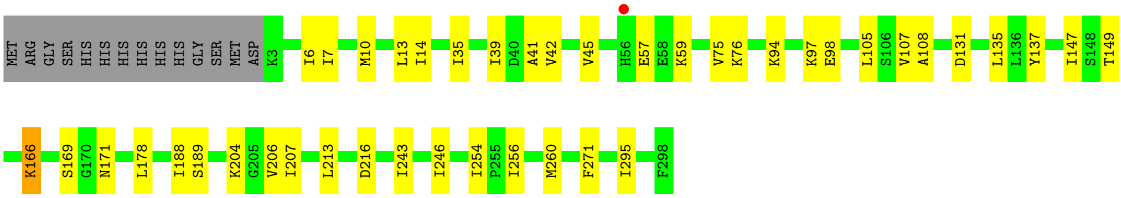


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F:

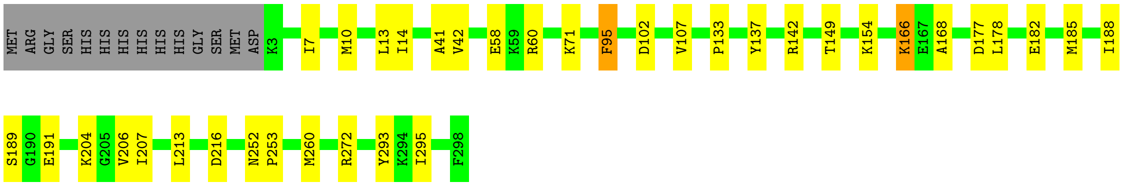
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain G:



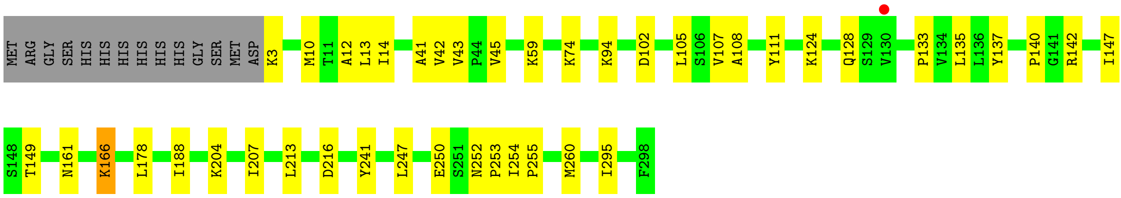
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain H:

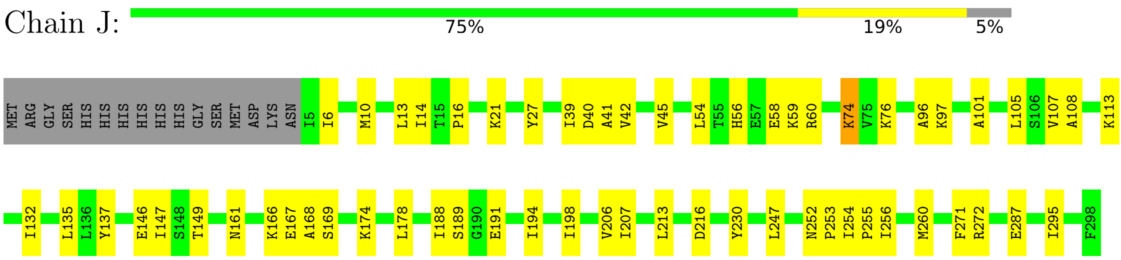


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

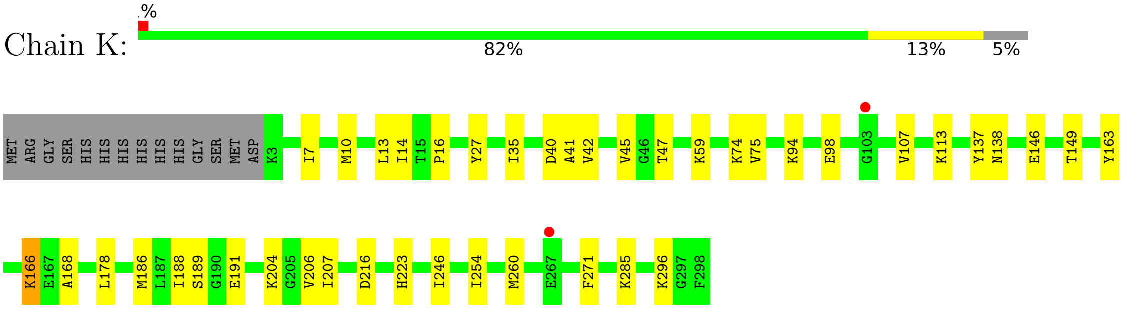
Chain I:



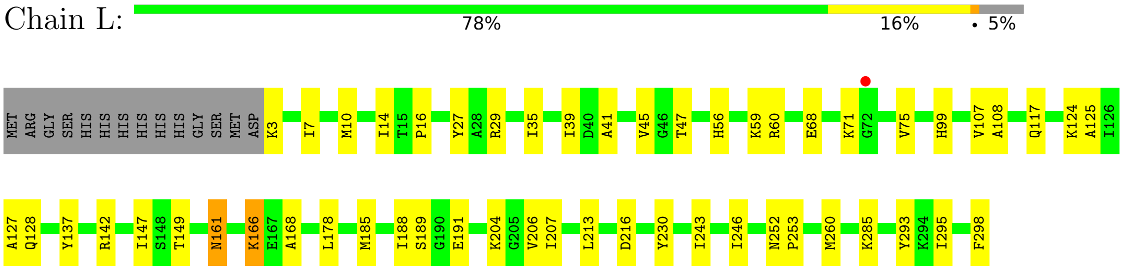
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



4 Data and refinement statistics (i)

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.88Å 201.44Å 113.66Å 90.00° 108.45° 90.00°	Depositor
Resolution (Å)	38.58 – 2.10 47.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.58-2.10) 99.7 (47.53-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.10Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.206 , 0.253 0.206 , 0.253	Depositor DCC
R_{free} test set	10225 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	29356	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: KPI, PGE, MG, ACT, GOL, PEG, 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	0.25	0/2293	0.45	0/3098
1	B	0.24	0/2302	0.44	0/3109
1	C	0.25	0/2302	0.43	0/3109
1	D	0.25	0/2292	0.43	0/3098
1	E	0.25	0/2304	0.44	0/3113
1	F	0.25	0/2301	0.44	0/3109
1	G	0.25	0/2301	0.43	0/3109
1	H	0.25	0/2301	0.44	0/3109
1	I	0.25	0/2302	0.44	0/3109
1	J	0.27	0/2285	0.46	0/3087
1	K	0.25	0/2312	0.44	0/3124
1	L	0.25	0/2301	0.44	0/3109
All	All	0.25	0/27596	0.44	0/37283

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	166	KPI	Mainchain

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	2270	0	2311	31	0
1	B	2279	0	2325	30	0
1	C	2279	0	2325	41	0
1	D	2269	0	2311	21	0
1	E	2280	0	2318	26	0
1	F	2278	0	2324	21	0
1	G	2278	0	2324	26	0
1	H	2278	0	2324	23	0
1	I	2279	0	2324	27	0
1	J	2262	0	2305	41	0
1	K	2288	0	2330	26	0
1	L	2278	0	2325	35	0
2	A	10	0	14	0	0
2	C	20	0	28	1	0
2	D	10	0	14	1	0
2	E	10	0	14	0	0
2	F	10	0	14	0	0
2	I	10	0	14	0	0
2	J	10	0	14	0	0
2	K	10	0	14	0	0
2	L	10	0	14	2	0
3	A	8	0	6	0	0
3	B	12	0	9	1	0
3	C	4	0	3	0	0
3	E	8	0	6	0	0
3	F	4	0	3	0	0
3	H	12	0	9	1	0
3	I	12	0	9	2	0
3	J	12	0	9	0	0
3	L	4	0	3	3	0
4	A	1	0	0	0	1
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	1
5	A	24	0	36	2	0
5	B	28	0	42	4	0
5	C	44	0	66	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	8	0	12	0	0
5	E	16	0	24	1	0
5	F	12	0	18	0	0
5	G	24	0	36	4	0
5	H	8	0	12	0	0
5	I	12	0	18	2	0
5	J	24	0	36	4	0
5	K	8	0	12	0	0
5	L	16	0	24	1	0
6	F	7	0	10	0	0
6	G	7	0	10	0	0
6	H	7	0	10	1	0
6	J	7	0	10	0	0
6	L	14	0	20	2	0
7	G	6	0	8	0	0
7	I	6	0	8	0	0
7	L	6	0	8	2	0
8	A	137	0	0	1	0
8	B	123	0	0	1	0
8	C	123	0	0	2	0
8	D	144	0	0	1	0
8	E	146	0	0	1	0
8	F	139	0	0	1	0
8	G	130	0	0	1	0
8	H	126	0	0	0	0
8	I	131	0	0	2	0
8	J	127	0	0	2	0
8	K	126	0	0	2	0
8	L	120	0	0	2	0
All	All	29356	0	28463	338	1

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 6.

All (338) 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:246:ILE:HG21	1:F:289:VAL:HG11	1.52	0.92
1:C:169:SER:H	5:C:311:EDO:H21	1.41	0.85
1:F:21:LYS:HZ2	1:F:22:VAL:H	1.32	0.78
1:K:107:VAL:HA	1:K:137:TYR:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.68	0.75
1:G:107:VAL:HA	1:G:137:TYR:HB3	1.69	0.74
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.70	0.73
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.71	0.73
1:J:107:VAL:HA	1:J:137:TYR:HB3	1.69	0.73
1:I:107:VAL:HA	1:I:137:TYR:HB3	1.71	0.73
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.70	0.72
1:L:107:VAL:HA	1:L:137:TYR:HB3	1.70	0.72
1:L:47:THR:HA	6:L:309:PEG:H41	1.72	0.71
1:H:107:VAL:HA	1:H:137:TYR:HB3	1.72	0.70
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.77	0.67
1:C:30:LEU:HB3	5:C:312:EDO:H11	1.76	0.67
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.75	0.67
1:L:3:LYS:N	7:L:302:GOL:HO1	1.94	0.66
1:A:142:ARG:HE	5:A:309:EDO:H21	1.61	0.65
1:J:189:SER:HB3	1:J:206:VAL:HG12	1.78	0.65
1:J:146:GLU:OE2	8:J:401:HOH:O	2.15	0.64
1:L:60:ARG:HB2	3:L:303:ACT:H3	1.80	0.62
1:E:189:SER:HB3	1:E:206:VAL:HG12	1.82	0.61
1:H:189:SER:HB3	1:H:206:VAL:HG12	1.83	0.61
1:D:189:SER:HB3	1:D:206:VAL:HG12	1.83	0.61
1:G:189:SER:HB3	1:G:206:VAL:HG12	1.83	0.60
1:K:10:MET:HG2	1:K:41:ALA:HB3	1.83	0.60
1:A:230:TYR:HD2	1:C:230:TYR:HD2	1.48	0.59
1:B:189:SER:HB3	1:B:206:VAL:HG12	1.84	0.59
1:C:189:SER:HB3	1:C:206:VAL:HG12	1.84	0.59
1:L:10:MET:HG2	1:L:41:ALA:HB3	1.84	0.59
1:A:246:ILE:HD11	1:A:285:LYS:HB3	1.84	0.59
1:J:174:LYS:HD2	8:J:401:HOH:O	2.03	0.59
1:F:189:SER:HB3	1:F:206:VAL:HG12	1.84	0.58
1:A:217:MET:SD	8:A:520:HOH:O	2.57	0.58
1:H:142:ARG:HG2	1:J:113:LYS:HD2	1.85	0.58
1:J:167:GLU:HB3	5:J:306:EDO:H12	1.85	0.58
1:E:45:VAL:HG11	1:E:59:LYS:HA	1.86	0.58
1:B:32:LYS:NZ	1:B:36:GLU:OE1	2.36	0.58
1:G:57:GLU:HB2	5:G:307:EDO:H21	1.84	0.57
1:I:3:LYS:N	8:I:406:HOH:O	2.36	0.57
1:I:45:VAL:HG11	1:I:59:LYS:HA	1.86	0.57
1:L:189:SER:HB3	1:L:206:VAL:HG12	1.85	0.57
1:B:3:LYS:N	8:B:402:HOH:O	2.36	0.57
1:B:108:ALA:HB2	1:B:147:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:ALA:HB2	1:G:147:ILE:HD11	1.87	0.57
1:K:246:ILE:HD11	1:K:285:LYS:HB3	1.87	0.57
1:I:142:ARG:HE	3:I:305:ACT:H1	1.69	0.57
1:D:35:ILE:HG12	1:D:75:VAL:HG21	1.86	0.57
1:B:198:ILE:HD11	5:B:305:EDO:H11	1.88	0.56
1:H:168:ALA:HA	1:H:191:GLU:HG3	1.86	0.56
1:D:97:LYS:NZ	8:D:408:HOH:O	2.38	0.56
1:C:223:HIS:CD2	1:D:74:LYS:HD2	2.41	0.56
1:F:10:MET:HG2	1:F:41:ALA:HB3	1.88	0.56
1:I:166:KPI:HDA	1:I:207:ILE:HD12	1.86	0.56
1:G:97:LYS:NZ	1:G:131:ASP:OD1	2.34	0.56
1:D:168:ALA:HA	1:D:191:GLU:HG3	1.88	0.56
1:C:95:PHE:O	1:C:99:HIS:ND1	2.30	0.55
1:F:29:ARG:NH1	8:F:406:HOH:O	2.38	0.55
1:C:168:ALA:HA	1:C:191:GLU:HG3	1.88	0.55
1:G:169:SER:H	5:G:303:EDO:H12	1.70	0.55
1:C:246:ILE:HD11	1:C:285:LYS:HB3	1.88	0.55
1:G:6:ILE:HG12	1:G:76:LYS:HD3	1.89	0.55
1:H:188:ILE:HG21	1:H:207:ILE:HG13	1.89	0.55
1:J:198:ILE:HD11	5:J:306:EDO:H11	1.89	0.55
1:K:189:SER:HB3	1:K:206:VAL:HG12	1.87	0.55
1:J:58:GLU:OE1	1:J:272:ARG:NH1	2.33	0.54
1:C:50:GLU:HA	5:C:308:EDO:H21	1.90	0.54
1:L:127:ALA:HB1	1:L:161:ASN:OD1	2.07	0.54
1:B:10:MET:HG2	1:B:41:ALA:HB3	1.90	0.54
1:H:14:ILE:HD13	1:H:260:MET:HG3	1.90	0.54
1:K:149:THR:HG23	1:K:178:LEU:HD23	1.89	0.54
1:C:171:ASN:HD21	2:C:302:PGE:H4	1.73	0.53
1:F:166:KPI:HDA	1:F:207:ILE:HD12	1.88	0.53
1:D:149:THR:HG23	1:D:178:LEU:HD23	1.90	0.53
1:B:58:GLU:OE2	1:B:272:ARG:NH2	2.32	0.53
1:A:108:ALA:HB2	1:A:147:ILE:HD11	1.90	0.53
1:C:167:GLU:HB3	5:C:311:EDO:H22	1.90	0.53
1:I:10:MET:HG2	1:I:41:ALA:HB3	1.91	0.53
1:J:54:LEU:O	1:J:59:LYS:NZ	2.41	0.53
1:B:167:GLU:HB3	5:B:305:EDO:H12	1.89	0.53
1:J:10:MET:HG2	1:J:41:ALA:HB3	1.90	0.53
1:H:154:LYS:HD2	6:H:306:PEG:H11	1.90	0.52
1:I:250:GLU:OE1	5:I:308:EDO:O1	2.27	0.52
1:C:10:MET:HG2	1:C:41:ALA:HB3	1.91	0.52
1:G:166:KPI:HDA	1:G:207:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HD11	1:C:42:VAL:HB	1.92	0.52
1:A:189:SER:HB3	1:A:206:VAL:HG12	1.91	0.52
1:E:60:ARG:HG3	1:E:99:HIS:CD2	2.44	0.52
1:A:149:THR:HG23	1:A:178:LEU:HD23	1.90	0.52
1:H:166:KPI:HDA	1:H:207:ILE:HD12	1.92	0.52
1:B:14:ILE:HD13	1:B:260:MET:HG3	1.92	0.52
1:G:35:ILE:HG12	1:G:75:VAL:HG21	1.92	0.52
1:D:13:LEU:HD11	1:D:42:VAL:HB	1.92	0.52
1:D:161:ASN:OD1	1:D:161:ASN:N	2.43	0.51
1:G:10:MET:HG2	1:G:41:ALA:HB3	1.92	0.51
1:E:108:ALA:HB2	1:E:147:ILE:HD11	1.93	0.51
1:I:13:LEU:HD11	1:I:42:VAL:HB	1.92	0.51
1:B:13:LEU:HD11	1:B:42:VAL:HB	1.92	0.51
1:K:40:ASP:OD1	1:K:74:LYS:NZ	2.38	0.51
1:H:213:LEU:HD11	1:H:295:ILE:HD13	1.92	0.51
1:I:108:ALA:HB2	1:I:147:ILE:HD11	1.93	0.51
1:J:45:VAL:HG11	1:J:59:LYS:HA	1.93	0.51
1:L:99:HIS:NE2	3:L:303:ACT:H2	2.26	0.51
1:J:16:PRO:HD2	1:J:27:TYR:HD1	1.76	0.51
1:L:149:THR:HG23	1:L:178:LEU:HD23	1.91	0.51
1:A:166:KPI:HDA	1:A:207:ILE:HD12	1.92	0.50
1:J:58:GLU:OE2	1:J:272:ARG:NH2	2.39	0.50
1:J:230:TYR:HD2	1:L:230:TYR:HD2	1.59	0.50
1:A:10:MET:HG2	1:A:41:ALA:HB3	1.94	0.50
1:I:188:ILE:HG21	1:I:207:ILE:HG13	1.93	0.50
1:J:14:ILE:HD13	1:J:260:MET:HG3	1.93	0.50
1:L:108:ALA:HB2	1:L:147:ILE:HD11	1.93	0.50
1:D:166:KPI:HDA	1:D:207:ILE:HD12	1.93	0.50
1:G:13:LEU:HD11	1:G:42:VAL:HB	1.93	0.50
1:K:166:KPI:HDA	1:K:207:ILE:HD12	1.92	0.50
1:K:113:LYS:NZ	8:K:413:HOH:O	2.45	0.50
1:J:6:ILE:HG12	1:J:76:LYS:HD2	1.94	0.50
1:K:40:ASP:OD2	1:K:223:HIS:NE2	2.37	0.50
1:K:163:TYR:O	1:K:186:MET:HG2	2.12	0.50
1:K:296:LYS:NZ	8:K:410:HOH:O	2.44	0.50
1:D:150:ASP:HB3	2:D:301:PGE:H1	1.94	0.49
1:K:14:ILE:HD13	1:K:260:MET:HG3	1.93	0.49
1:B:149:THR:HG23	1:B:178:LEU:HD23	1.93	0.49
1:L:166:KPI:HDA	1:L:207:ILE:HD12	1.93	0.49
1:L:246:ILE:HD11	1:L:285:LYS:HB3	1.92	0.49
1:L:3:LYS:N	7:L:302:GOL:HO2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:KPI:HDA	1:C:207:ILE:HD12	1.95	0.49
1:L:188:ILE:HG21	1:L:207:ILE:HG13	1.95	0.49
1:A:188:ILE:HG21	1:A:207:ILE:HG13	1.94	0.49
1:J:13:LEU:HD11	1:J:42:VAL:HB	1.95	0.49
1:C:60:ARG:HB3	1:C:95:PHE:CZ	2.47	0.49
1:C:97:LYS:NZ	1:C:131:ASP:OD1	2.39	0.49
1:D:108:ALA:HB2	1:D:147:ILE:HD11	1.95	0.48
1:H:10:MET:HG2	1:H:41:ALA:HB3	1.94	0.48
1:L:168:ALA:HA	1:L:191:GLU:HG3	1.94	0.48
1:C:149:THR:HG23	1:C:178:LEU:HD23	1.95	0.48
1:A:13:LEU:HD11	1:A:42:VAL:HB	1.95	0.48
1:C:5:ILE:HD12	1:C:186:MET:HE2	1.95	0.48
1:I:14:ILE:HD13	1:I:260:MET:HG3	1.94	0.48
1:J:40:ASP:OD1	1:J:74:LYS:NZ	2.45	0.48
1:A:45:VAL:HG11	1:A:59:LYS:HA	1.95	0.48
1:J:97:LYS:HA	1:J:132:ILE:HD13	1.96	0.48
1:J:194:ILE:HG21	2:L:301:PGE:H52	1.96	0.48
1:F:35:ILE:HG12	1:F:75:VAL:HG21	1.96	0.48
1:F:108:ALA:HB2	1:F:147:ILE:HD11	1.95	0.48
1:J:149:THR:HG23	1:J:178:LEU:HD23	1.95	0.48
1:K:13:LEU:HD11	1:K:42:VAL:HB	1.96	0.48
1:K:168:ALA:HA	1:K:191:GLU:HG3	1.94	0.48
1:A:230:TYR:CD2	1:C:230:TYR:HD2	2.29	0.48
1:A:60:ARG:HG3	1:A:99:HIS:NE2	2.28	0.48
1:E:188:ILE:HG21	1:E:207:ILE:HG13	1.96	0.48
1:G:149:THR:HG23	1:G:178:LEU:HD23	1.96	0.48
1:C:58:GLU:OE2	1:C:272:ARG:NH2	2.37	0.47
1:K:35:ILE:HG12	1:K:75:VAL:HG21	1.96	0.47
1:L:56:HIS:NE2	3:L:303:ACT:H1	2.29	0.47
1:C:252:ASN:ND2	1:C:253:PRO:HA	2.29	0.47
1:E:10:MET:HG2	1:E:41:ALA:HB3	1.95	0.47
1:G:105:LEU:HD13	1:G:135:LEU:HD23	1.95	0.47
1:I:124:LYS:NZ	1:I:128:GLN:OE1	2.40	0.47
1:L:213:LEU:HD11	1:L:295:ILE:HD13	1.96	0.47
1:C:99:HIS:O	5:C:316:EDO:O2	2.33	0.47
1:C:226:LEU:HD23	5:C:310:EDO:H12	1.96	0.47
1:I:161:ASN:OD1	1:I:161:ASN:N	2.40	0.47
1:L:35:ILE:HG12	1:L:75:VAL:HG21	1.96	0.47
1:A:14:ILE:HD13	1:A:260:MET:HG3	1.96	0.47
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.97	0.47
1:F:243:ILE:HA	1:F:246:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:45:VAL:HG11	1:L:59:LYS:HA	1.97	0.47
1:J:56:HIS:O	1:J:60:ARG:HG3	2.15	0.47
1:B:252:ASN:OD1	1:B:253:PRO:HA	2.14	0.47
1:K:45:VAL:HG11	1:K:59:LYS:HA	1.95	0.47
1:B:68:GLU:HA	1:B:71:LYS:HE2	1.97	0.47
1:H:252:ASN:HD22	3:H:303:ACT:C	2.28	0.47
1:A:16:PRO:HD2	1:A:27:TYR:HD1	1.80	0.46
1:B:45:VAL:HG11	1:B:59:LYS:HA	1.97	0.46
1:E:13:LEU:HD11	1:E:42:VAL:HB	1.97	0.46
1:A:142:ARG:NE	5:A:309:EDO:H21	2.27	0.46
1:I:111:TYR:HH	1:L:47:THR:HG1	1.63	0.46
1:C:108:ALA:HB2	1:C:147:ILE:HD11	1.98	0.46
5:I:308:EDO:H11	1:L:117:GLN:HB3	1.97	0.46
1:J:213:LEU:HD11	1:J:295:ILE:HD13	1.98	0.46
1:D:16:PRO:HD2	1:D:27:TYR:HD1	1.81	0.46
1:D:243:ILE:HA	1:D:246:ILE:HG22	1.98	0.46
1:G:256:ILE:O	1:G:260:MET:HG2	2.16	0.46
1:A:161:ASN:OD1	1:A:161:ASN:N	2.35	0.45
1:H:102:ASP:O	1:H:133:PRO:HD2	2.16	0.45
1:F:7:ILE:HB	1:F:204:LYS:O	2.16	0.45
1:L:142:ARG:HH21	5:L:304:EDO:H21	1.81	0.45
1:A:213:LEU:HD11	1:A:295:ILE:HD13	1.99	0.45
1:F:45:VAL:HG11	1:F:59:LYS:HA	1.98	0.45
1:K:163:TYR:HD2	1:K:186:MET:HG3	1.81	0.45
1:B:216:ASP:OD1	1:B:216:ASP:N	2.50	0.45
1:C:3:LYS:N	8:C:418:HOH:O	2.48	0.45
1:G:188:ILE:HG21	1:G:207:ILE:HG13	1.98	0.45
1:H:182:GLU:HB3	1:H:185:MET:HE3	1.99	0.45
1:I:149:THR:HG23	1:I:178:LEU:HD23	1.97	0.45
1:B:168:ALA:HA	1:B:191:GLU:HG3	1.98	0.45
1:C:13:LEU:HD22	5:C:312:EDO:H22	1.99	0.45
1:F:14:ILE:HD13	1:F:260:MET:HG3	1.98	0.45
1:F:216:ASP:OD1	1:F:216:ASP:N	2.50	0.45
1:J:194:ILE:HD13	2:L:301:PGE:H5	1.99	0.45
1:A:294:LYS:HA	1:A:294:LYS:HD3	1.60	0.45
1:B:60:ARG:HG3	1:B:99:HIS:NE2	2.32	0.45
1:G:45:VAL:HG11	1:G:59:LYS:HA	1.98	0.45
1:G:216:ASP:OD1	1:G:216:ASP:N	2.50	0.45
1:K:216:ASP:OD1	1:K:216:ASP:N	2.50	0.45
1:E:166:KPI:HDA	1:E:207:ILE:HD12	1.98	0.45
1:F:188:ILE:HG21	1:F:207:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:PRO:HB2	3:I:304:ACT:H1	1.99	0.45
1:J:254:ILE:HA	1:J:271:PHE:CE2	2.52	0.45
1:L:29:ARG:HG2	1:L:298:PHE:CE1	2.53	0.45
1:B:188:ILE:HG21	1:B:207:ILE:HG13	1.99	0.44
1:C:67:VAL:HA	5:C:315:EDO:H21	1.99	0.44
1:L:7:ILE:HB	1:L:204:LYS:O	2.16	0.44
1:D:188:ILE:HG21	1:D:207:ILE:HG13	1.98	0.44
1:H:252:ASN:OD1	1:H:253:PRO:HA	2.18	0.44
1:J:161:ASN:OD1	1:J:161:ASN:N	2.41	0.44
1:J:216:ASP:N	1:J:216:ASP:OD1	2.50	0.44
1:A:254:ILE:HA	1:A:271:PHE:CE2	2.53	0.44
1:E:7:ILE:HB	1:E:204:LYS:O	2.17	0.44
1:D:105:LEU:HD13	1:D:135:LEU:HD23	1.99	0.44
1:H:142:ARG:HG2	1:J:113:LYS:CD	2.47	0.44
1:K:7:ILE:HB	1:K:204:LYS:O	2.17	0.44
1:G:97:LYS:NZ	8:G:405:HOH:O	2.41	0.44
1:H:177:ASP:HB2	1:I:241:TYR:CZ	2.53	0.44
1:B:177:ASP:OD2	5:B:308:EDO:O2	2.27	0.44
1:G:254:ILE:HA	1:G:271:PHE:CE2	2.52	0.44
1:K:16:PRO:HD2	1:K:27:TYR:HD1	1.82	0.44
1:C:67:VAL:O	1:C:71:LYS:HG2	2.18	0.44
1:J:230:TYR:CD2	1:L:230:TYR:HD2	2.36	0.44
1:L:243:ILE:HB	1:L:293:TYR:CE1	2.53	0.44
1:A:230:TYR:HD2	1:C:230:TYR:CD2	2.33	0.43
1:C:216:ASP:N	1:C:216:ASP:OD1	2.51	0.43
1:J:105:LEU:HD13	1:J:135:LEU:HD23	2.00	0.43
1:E:142:ARG:NH2	1:E:252:ASN:HB3	2.34	0.43
1:G:14:ILE:HD13	1:G:260:MET:HG3	2.00	0.43
1:E:231:LYS:HB2	1:E:231:LYS:HE2	1.75	0.43
1:G:243:ILE:HA	1:G:246:ILE:HG22	1.99	0.43
1:G:94:LYS:O	1:G:98:GLU:HG2	2.18	0.43
1:K:186:MET:CE	1:K:204:LYS:HG3	2.48	0.43
1:A:252:ASN:OD1	1:A:253:PRO:HA	2.19	0.43
1:H:149:THR:HG23	1:H:178:LEU:HD23	1.99	0.43
1:A:153:ILE:HG22	1:A:157:ARG:HD2	2.00	0.43
1:G:213:LEU:HD11	1:G:295:ILE:HD13	2.01	0.43
1:I:252:ASN:OD1	1:I:253:PRO:HA	2.18	0.43
1:J:96:ALA:O	1:J:101:ALA:HB3	2.17	0.43
1:L:125:ALA:O	1:L:128:GLN:HG3	2.19	0.43
1:L:252:ASN:OD1	1:L:253:PRO:HA	2.19	0.43
1:C:45:VAL:HG11	1:C:59:LYS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:THR:HG23	1:E:178:LEU:HD23	2.01	0.43
1:I:102:ASP:O	1:I:133:PRO:HD2	2.18	0.43
1:J:247:LEU:HA	1:J:255:PRO:HB2	2.01	0.43
1:A:243:ILE:HA	1:A:246:ILE:HG22	2.01	0.43
1:C:12:ALA:HA	1:C:43:VAL:HB	2.01	0.43
1:G:171:ASN:H	5:G:303:EDO:H21	1.84	0.43
1:C:14:ILE:HD13	1:C:260:MET:HG3	2.00	0.43
1:E:196:TYR:OH	1:E:230:TYR:HB3	2.19	0.43
1:H:216:ASP:OD1	1:H:216:ASP:N	2.51	0.43
1:I:12:ALA:HA	1:I:43:VAL:HB	2.01	0.43
1:K:188:ILE:HG21	1:K:207:ILE:HG13	2.01	0.43
1:I:247:LEU:HA	1:I:255:PRO:HB2	2.01	0.42
1:A:105:LEU:HD11	1:A:137:TYR:HB2	2.02	0.42
1:J:287:GLU:HG3	5:J:310:EDO:H12	2.01	0.42
1:B:16:PRO:HD2	1:B:27:TYR:HD1	1.84	0.42
1:E:252:ASN:OD1	1:E:253:PRO:HA	2.18	0.42
1:E:256:ILE:O	1:E:260:MET:HG2	2.20	0.42
1:E:280:LYS:HA	1:E:280:LYS:HD2	1.59	0.42
1:F:21:LYS:NZ	1:F:22:VAL:H	2.11	0.42
1:H:60:ARG:HB2	1:H:95:PHE:HE1	1.84	0.42
1:L:178:LEU:HB3	1:L:185:MET:SD	2.59	0.42
1:J:108:ALA:HB2	1:J:147:ILE:HD11	2.01	0.42
1:J:252:ASN:OD1	1:J:253:PRO:HA	2.19	0.42
1:E:105:LEU:HD13	1:E:135:LEU:HD23	2.02	0.42
1:F:256:ILE:O	1:F:260:MET:HG2	2.19	0.42
1:I:213:LEU:HD11	1:I:295:ILE:HD13	2.02	0.42
1:I:216:ASP:OD1	1:I:216:ASP:N	2.51	0.42
1:J:188:ILE:HG21	1:J:207:ILE:HG13	2.02	0.42
1:L:14:ILE:HD13	1:L:260:MET:HG3	2.02	0.42
1:L:68:GLU:HB2	8:L:471:HOH:O	2.19	0.42
1:A:58:GLU:OE2	1:A:272:ARG:NH2	2.37	0.42
1:B:154:LYS:HD2	5:B:304:EDO:H11	2.01	0.42
1:B:256:ILE:O	1:B:260:MET:HG2	2.19	0.42
1:C:7:ILE:HG21	1:C:186:MET:CE	2.50	0.42
1:C:292:LYS:NZ	8:C:412:HOH:O	2.44	0.42
1:A:39:ILE:HD13	1:A:39:ILE:HA	1.97	0.42
1:D:216:ASP:N	1:D:216:ASP:OD1	2.53	0.42
1:F:142:ARG:NH2	1:F:252:ASN:HB3	2.35	0.42
1:H:7:ILE:HB	1:H:204:LYS:O	2.20	0.42
1:J:21:LYS:HA	1:J:21:LYS:HD3	1.84	0.42
1:D:252:ASN:OD1	1:D:253:PRO:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ARG:HB2	1:E:95:PHE:HE1	1.85	0.42
1:A:105:LEU:HD13	1:A:135:LEU:HD23	2.01	0.42
1:C:92:LEU:HA	1:C:95:PHE:HB3	2.02	0.42
1:E:34:GLN:OE1	1:E:39:ILE:HG13	2.20	0.41
1:E:111:TYR:HH	1:K:47:THR:HG1	1.57	0.41
1:E:171:ASN:HD21	5:E:309:EDO:H22	1.84	0.41
1:L:216:ASP:N	1:L:216:ASP:OD1	2.53	0.41
1:B:280:LYS:HA	1:B:280:LYS:HD3	1.79	0.41
1:H:71:LYS:HE2	1:H:71:LYS:HB3	1.83	0.41
1:K:94:LYS:O	1:K:98:GLU:HG2	2.20	0.41
1:E:287:GLU:HG2	1:E:291:LYS:NZ	2.35	0.41
1:F:254:ILE:HA	1:F:271:PHE:CE2	2.55	0.41
1:J:256:ILE:O	1:J:260:MET:HG2	2.20	0.41
1:F:140:PRO:HG3	1:F:146:GLU:OE2	2.21	0.41
1:C:14:ILE:HG12	5:C:312:EDO:H12	2.01	0.41
1:E:216:ASP:N	1:E:216:ASP:OD1	2.54	0.41
1:B:288:GLU:HA	1:B:291:LYS:HE3	2.03	0.41
1:D:256:ILE:O	1:D:260:MET:HG2	2.21	0.41
1:H:58:GLU:OE2	1:H:272:ARG:NH2	2.37	0.41
1:B:105:LEU:HD13	1:B:135:LEU:HD23	2.03	0.41
1:C:256:ILE:O	1:C:260:MET:HG2	2.21	0.41
1:C:262:LEU:HD21	1:C:283:PHE:CZ	2.55	0.41
1:K:138:ASN:HD21	1:K:146:GLU:HG3	1.86	0.41
1:K:254:ILE:HA	1:K:271:PHE:CE2	2.55	0.41
1:D:268:SER:OG	1:D:270:GLU:HG3	2.21	0.41
1:L:16:PRO:HD2	1:L:27:TYR:HD1	1.86	0.41
1:B:166:KPI:HDA	1:B:207:ILE:HD12	2.03	0.41
1:H:13:LEU:HD11	1:H:42:VAL:HB	2.02	0.41
1:I:105:LEU:HD13	1:I:135:LEU:HD23	2.02	0.41
6:L:309:PEG:H11	6:L:309:PEG:H32	1.89	0.41
1:B:7:ILE:HB	1:B:204:LYS:O	2.20	0.41
1:G:171:ASN:H	5:G:303:EDO:C2	2.34	0.41
1:J:168:ALA:HA	1:J:191:GLU:HG3	2.02	0.41
1:A:256:ILE:O	1:A:260:MET:HG2	2.21	0.40
1:B:292:LYS:HE3	3:B:303:ACT:O	2.21	0.40
1:C:102:ASP:O	1:C:133:PRO:HD2	2.21	0.40
1:I:204:LYS:NZ	8:I:410:HOH:O	2.47	0.40
1:J:169:SER:OG	5:J:306:EDO:O2	2.38	0.40
1:E:184:ARG:NH1	8:E:403:HOH:O	2.30	0.40
1:G:7:ILE:HB	1:G:204:LYS:O	2.20	0.40
1:L:124:LYS:NZ	8:L:416:HOH:O	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:NZ	1:B:144:GLY:O	2.38	0.40
1:E:243:ILE:HA	1:E:246:ILE:HG22	2.03	0.40
1:F:252:ASN:OD1	1:F:253:PRO:HA	2.21	0.40
1:I:94:LYS:HE2	1:I:94:LYS:HB3	1.94	0.40
1:I:254:ILE:HB	1:I:255:PRO:HD3	2.03	0.40
1:J:40:ASP:HA	1:J:74:LYS:NZ	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:304:MG:MG	4:E:305:MG:MG[1_455]	1.62	0.58

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	292/310 (94%)	285 (98%)	7 (2%)	0	100	100
1	B	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	C	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	D	292/310 (94%)	285 (98%)	7 (2%)	0	100	100
1	E	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	F	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	G	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	H	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	I	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	J	291/310 (94%)	284 (98%)	7 (2%)	0	100	100
1	K	294/310 (95%)	286 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
All	All	3513/3720 (94%)	3426 (98%)	87 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	247/260 (95%)	246 (100%)	1 (0%)	91	94
1	B	248/260 (95%)	248 (100%)	0	100	100
1	C	248/260 (95%)	247 (100%)	1 (0%)	91	94
1	D	247/260 (95%)	246 (100%)	1 (0%)	91	94
1	E	248/260 (95%)	245 (99%)	3 (1%)	71	77
1	F	248/260 (95%)	247 (100%)	1 (0%)	91	94
1	G	248/260 (95%)	247 (100%)	1 (0%)	91	94
1	H	248/260 (95%)	246 (99%)	2 (1%)	81	86
1	I	248/260 (95%)	247 (100%)	1 (0%)	91	94
1	J	246/260 (95%)	244 (99%)	2 (1%)	81	86
1	K	249/260 (96%)	249 (100%)	0	100	100
1	L	248/260 (95%)	245 (99%)	3 (1%)	71	77
All	All	2973/3120 (95%)	2957 (100%)	16 (0%)	88	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	C	185	MET
1	D	277	SER
1	E	95	PHE
1	E	128	GLN

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Mol	Chain	Res	Type
1	E	231	LYS
1	F	39	ILE
1	G	39	ILE
1	H	95	PHE
1	H	293	TYR
1	I	74	LYS
1	J	39	ILE
1	J	74	LYS
1	L	39	ILE
1	L	71	LYS
1	L	161	ASN

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

Mol	Chain	Res	Type
1	F	56	HIS
1	H	4	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 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	I	166	1	11,13,14	0.86	0	10,15,17	3.22	4 (40%)
1	KPI	A	166	1	11,13,14	1.83	2 (18%)	10,15,17	3.66	5 (50%)
1	KPI	C	166	1	11,13,14	1.83	2 (18%)	10,15,17	3.80	5 (50%)
1	KPI	D	166	1	11,13,14	2.20	3 (27%)	10,15,17	3.71	5 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	KPI	H	166	1	11,13,14	0.87	1 (9%)	10,15,17	3.20	5 (50%)
1	KPI	F	166	1	11,13,14	1.82	2 (18%)	10,15,17	3.57	5 (50%)
1	KPI	J	166	1	11,13,14	0.84	0	10,15,17	3.13	4 (40%)
1	KPI	L	166	1	11,13,14	1.84	2 (18%)	10,15,17	3.68	6 (60%)
1	KPI	B	166	1	11,13,14	1.82	2 (18%)	10,15,17	3.72	5 (50%)
1	KPI	E	166	1	11,13,14	0.89	0	10,15,17	3.19	4 (40%)
1	KPI	K	166	1	11,13,14	1.85	2 (18%)	10,15,17	3.68	6 (60%)
1	KPI	G	166	1	11,13,14	1.83	2 (18%)	10,15,17	3.70	5 (50%)

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	I	166	1	-	1/13/14/16	-
1	KPI	A	166	1	-	3/13/14/16	-
1	KPI	C	166	1	-	3/13/14/16	-
1	KPI	D	166	1	-	1/13/14/16	-
1	KPI	H	166	1	-	1/13/14/16	-
1	KPI	F	166	1	-	4/13/14/16	-
1	KPI	J	166	1	-	4/13/14/16	-
1	KPI	L	166	1	-	4/13/14/16	-
1	KPI	B	166	1	-	2/13/14/16	-
1	KPI	E	166	1	-	2/13/14/16	-
1	KPI	K	166	1	-	1/13/14/16	-
1	KPI	G	166	1	-	1/13/14/16	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	166	KPI	O2-CX2	5.23	1.36	1.22
1	L	166	KPI	O2-CX2	5.23	1.36	1.22
1	D	166	KPI	O2-CX2	5.23	1.36	1.22
1	C	166	KPI	O2-CX2	5.22	1.36	1.22
1	B	166	KPI	O2-CX2	5.21	1.36	1.22
1	A	166	KPI	O2-CX2	5.19	1.36	1.22
1	F	166	KPI	O2-CX2	5.17	1.36	1.22
1	G	166	KPI	O2-CX2	5.15	1.36	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	KPI	O-C	4.14	1.36	1.19
1	L	166	KPI	O1-CX2	-2.40	1.23	1.30
1	K	166	KPI	O1-CX2	-2.39	1.23	1.30
1	B	166	KPI	O1-CX2	-2.39	1.23	1.30
1	G	166	KPI	O1-CX2	-2.39	1.23	1.30
1	F	166	KPI	O1-CX2	-2.38	1.23	1.30
1	D	166	KPI	O1-CX2	-2.38	1.23	1.30
1	C	166	KPI	O1-CX2	-2.35	1.23	1.30
1	A	166	KPI	O1-CX2	-2.34	1.23	1.30
1	H	166	KPI	O1-CX2	2.05	1.36	1.30

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	166	KPI	C1-CX1-CX2	-7.99	110.40	118.17
1	K	166	KPI	C1-CX1-CX2	-7.71	110.67	118.17
1	L	166	KPI	C1-CX1-CX2	-7.68	110.70	118.17
1	D	166	KPI	C1-CX1-CX2	-7.66	110.72	118.17
1	G	166	KPI	C1-CX1-CX2	-7.58	110.80	118.17
1	B	166	KPI	C1-CX1-CX2	-7.51	110.87	118.17
1	A	166	KPI	C1-CX1-CX2	-7.45	110.92	118.17
1	H	166	KPI	C1-CX1-CX2	-7.30	111.07	118.17
1	I	166	KPI	C1-CX1-CX2	-7.26	111.11	118.17
1	J	166	KPI	C1-CX1-CX2	-7.10	111.27	118.17
1	F	166	KPI	C1-CX1-CX2	-7.05	111.31	118.17
1	E	166	KPI	C1-CX1-CX2	-6.79	111.56	118.17
1	B	166	KPI	O2-CX2-CX1	-5.56	114.28	121.38
1	E	166	KPI	O2-CX2-CX1	5.43	128.31	121.38
1	C	166	KPI	O2-CX2-CX1	-5.42	114.46	121.38
1	D	166	KPI	O2-CX2-CX1	-5.39	114.50	121.38
1	G	166	KPI	O1-CX2-CX1	5.35	127.97	116.35
1	A	166	KPI	O1-CX2-CX1	5.26	127.77	116.35
1	B	166	KPI	O1-CX2-CX1	5.22	127.69	116.35
1	F	166	KPI	O1-CX2-CX1	5.21	127.67	116.35
1	C	166	KPI	O1-CX2-CX1	5.21	127.66	116.35
1	D	166	KPI	O1-CX2-CX1	5.20	127.65	116.35
1	K	166	KPI	O1-CX2-CX1	5.18	127.61	116.35
1	A	166	KPI	O2-CX2-CX1	-5.18	114.77	121.38
1	L	166	KPI	O2-CX2-CX1	-5.11	114.85	121.38
1	L	166	KPI	O1-CX2-CX1	5.04	127.29	116.35
1	F	166	KPI	O2-CX2-CX1	-5.02	114.97	121.38
1	I	166	KPI	O2-CX2-CX1	5.01	127.77	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	166	KPI	O2-CX2-CX1	4.99	127.75	121.38
1	K	166	KPI	O2-CX2-CX1	-4.94	115.07	121.38
1	G	166	KPI	O2-CX2-CX1	-4.94	115.07	121.38
1	J	166	KPI	O2-CX2-CX1	4.85	127.57	121.38
1	F	166	KPI	C1-CX1-NZ	3.19	131.44	123.11
1	L	166	KPI	C1-CX1-NZ	3.09	131.19	123.11
1	B	166	KPI	C1-CX1-NZ	3.08	131.17	123.11
1	C	166	KPI	C1-CX1-NZ	3.06	131.10	123.11
1	J	166	KPI	C1-CX1-NZ	3.04	131.07	123.11
1	I	166	KPI	C1-CX1-NZ	3.02	131.01	123.11
1	D	166	KPI	C1-CX1-NZ	2.94	130.80	123.11
1	G	166	KPI	C1-CX1-NZ	2.93	130.77	123.11
1	G	166	KPI	O1-CX2-O2	-2.90	116.96	123.61
1	E	166	KPI	C1-CX1-NZ	2.89	130.67	123.11
1	A	166	KPI	C1-CX1-NZ	2.89	130.66	123.11
1	K	166	KPI	C1-CX1-NZ	2.87	130.62	123.11
1	E	166	KPI	O1-CX2-O2	-2.83	117.14	123.61
1	I	166	KPI	O1-CX2-O2	-2.77	117.27	123.61
1	K	166	KPI	O1-CX2-O2	-2.75	117.33	123.61
1	F	166	KPI	O1-CX2-O2	-2.73	117.36	123.61
1	H	166	KPI	C1-CX1-NZ	2.73	130.25	123.11
1	H	166	KPI	O1-CX2-O2	-2.70	117.42	123.61
1	A	166	KPI	O1-CX2-O2	-2.68	117.47	123.61
1	J	166	KPI	O1-CX2-O2	-2.61	117.63	123.61
1	D	166	KPI	O1-CX2-O2	-2.51	117.86	123.61
1	L	166	KPI	O1-CX2-O2	-2.51	117.86	123.61
1	C	166	KPI	O1-CX2-O2	-2.50	117.88	123.61
1	B	166	KPI	O1-CX2-O2	-2.44	118.03	123.61
1	L	166	KPI	CD-CE-NZ	2.14	114.55	110.66
1	H	166	KPI	CD-CE-NZ	2.11	114.49	110.66
1	K	166	KPI	CD-CE-NZ	2.03	114.35	110.66

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	KPI	C-CA-CB-CG
1	A	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	C1-CX1-NZ-CE
1	D	166	KPI	C-CA-CB-CG
1	E	166	KPI	C1-CX1-CX2-O1

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Mol	Chain	Res	Type	Atoms
1	E	166	KPI	C1-CX1-CX2-O2
1	F	166	KPI	C-CA-CB-CG
1	F	166	KPI	C1-CX1-NZ-CE
1	F	166	KPI	NZ-CX1-CX2-O1
1	J	166	KPI	C1-CX1-NZ-CE
1	J	166	KPI	CX2-CX1-NZ-CE
1	J	166	KPI	NZ-CX1-CX2-O1
1	L	166	KPI	C1-CX1-NZ-CE
1	L	166	KPI	CX2-CX1-NZ-CE
1	L	166	KPI	NZ-CX1-CX2-O1
1	L	166	KPI	NZ-CX1-CX2-O2
1	G	166	KPI	C1-CX1-NZ-CE
1	I	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	C-CA-CB-CG
1	H	166	KPI	C-CA-CB-CG
1	F	166	KPI	NZ-CX1-CX2-O2
1	J	166	KPI	NZ-CX1-CX2-O2
1	B	166	KPI	NZ-CX1-CX2-O1
1	C	166	KPI	NZ-CX1-CX2-O1
1	K	166	KPI	NZ-CX1-CX2-O1
1	A	166	KPI	N-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	166	KPI	1	0
1	A	166	KPI	1	0
1	C	166	KPI	1	0
1	D	166	KPI	1	0
1	H	166	KPI	1	0
1	F	166	KPI	1	0
1	L	166	KPI	1	0
1	B	166	KPI	1	0
1	E	166	KPI	1	0
1	K	166	KPI	1	0
1	G	166	KPI	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 100 ligands modelled in this entry, 6 are monoatomic - leaving 94 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	$\#\|Z\| > 2$
3	ACT	I	305	-	3,3,3	0.76	0	3,3,3	1.35	0
3	ACT	C	303	-	3,3,3	0.75	0	3,3,3	1.31	0
5	EDO	C	314	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	J	307	-	3,3,3	0.47	0	2,2,2	0.30	0
3	ACT	B	301	-	3,3,3	0.77	0	3,3,3	1.31	0
5	EDO	F	304	-	3,3,3	0.48	0	2,2,2	0.29	0
5	EDO	E	307	-	3,3,3	0.46	0	2,2,2	0.35	0
2	PGE	F	301	-	9,9,9	0.30	0	8,8,8	0.30	0
7	GOL	G	301	-	5,5,5	0.37	0	5,5,5	0.23	0
3	ACT	H	302	-	3,3,3	0.77	0	3,3,3	1.42	0
5	EDO	K	303	-	3,3,3	0.46	0	2,2,2	0.34	0
6	PEG	H	306	-	6,6,6	0.48	0	5,5,5	0.25	0
3	ACT	A	302	-	3,3,3	0.78	0	3,3,3	1.33	0
6	PEG	L	308	-	6,6,6	0.49	0	5,5,5	0.26	0
5	EDO	C	316	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	I	306	-	3,3,3	0.47	0	2,2,2	0.33	0
3	ACT	E	302	-	3,3,3	0.79	0	3,3,3	1.30	0
5	EDO	J	308	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	C	310	-	3,3,3	0.46	0	2,2,2	0.39	0
5	EDO	F	305	-	3,3,3	0.45	0	2,2,2	0.41	0
2	PGE	L	301	-	9,9,9	0.29	0	8,8,8	0.34	0
5	EDO	E	308	-	3,3,3	0.45	0	2,2,2	0.40	0
5	EDO	A	309	-	3,3,3	0.43	0	2,2,2	0.42	0
3	ACT	I	303	-	3,3,3	0.77	0	3,3,3	1.45	0
5	EDO	J	305	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	A	306	-	3,3,3	0.45	0	2,2,2	0.36	0
2	PGE	A	301	-	9,9,9	0.31	0	8,8,8	0.23	0
5	EDO	C	315	-	3,3,3	0.45	0	2,2,2	0.37	0
7	GOL	L	302	-	5,5,5	0.36	0	5,5,5	0.29	0
5	EDO	G	305	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	A	310	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	D	304	-	3,3,3	0.47	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	EDO	C	309	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	G	304	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	B	309	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	L	307	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	G	306	-	3,3,3	0.46	0	2,2,2	0.27	0
5	EDO	F	303	-	3,3,3	0.48	0	2,2,2	0.32	0
5	EDO	H	305	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	I	307	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	B	306	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	G	307	-	3,3,3	0.45	0	2,2,2	0.36	0
3	ACT	B	302	-	3,3,3	0.75	0	3,3,3	1.32	0
3	ACT	L	303	-	3,3,3	0.76	0	3,3,3	1.30	0
5	EDO	L	306	-	3,3,3	0.47	0	2,2,2	0.28	0
5	EDO	C	312	-	3,3,3	0.45	0	2,2,2	0.30	0
5	EDO	C	306	-	3,3,3	0.50	0	2,2,2	0.28	0
5	EDO	J	310	-	3,3,3	0.46	0	2,2,2	0.29	0
3	ACT	B	303	-	3,3,3	0.72	0	3,3,3	1.31	0
5	EDO	K	302	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	I	308	-	3,3,3	0.45	0	2,2,2	0.33	0
2	PGE	C	301	-	9,9,9	0.30	0	8,8,8	0.31	0
3	ACT	H	301	-	3,3,3	0.72	0	3,3,3	1.39	0
5	EDO	C	307	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	B	307	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	308	-	3,3,3	0.46	0	2,2,2	0.33	0
7	GOL	I	302	-	5,5,5	0.35	0	5,5,5	0.27	0
2	PGE	D	301	-	9,9,9	0.31	0	8,8,8	0.26	0
6	PEG	L	309	-	6,6,6	0.50	0	5,5,5	0.39	0
5	EDO	G	302	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	D	303	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	J	309	-	3,3,3	0.47	0	2,2,2	0.26	0
5	EDO	A	305	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	E	306	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	J	306	-	3,3,3	0.43	0	2,2,2	0.33	0
5	EDO	G	303	-	3,3,3	0.43	0	2,2,2	0.35	0
3	ACT	J	303	-	3,3,3	0.77	0	3,3,3	1.33	0
3	ACT	H	303	-	3,3,3	0.73	0	3,3,3	1.37	0
3	ACT	A	303	-	3,3,3	0.76	0	3,3,3	1.30	0
3	ACT	J	304	-	3,3,3	0.75	0	3,3,3	1.37	0
5	EDO	E	309	-	3,3,3	0.45	0	2,2,2	0.43	0
2	PGE	I	301	-	9,9,9	0.30	0	8,8,8	0.30	0
5	EDO	B	308	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	L	304	-	3,3,3	0.46	0	2,2,2	0.34	0
2	PGE	J	301	-	9,9,9	0.31	0	8,8,8	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	PGE	K	301	-	9,9,9	0.30	0	8,8,8	0.30	0
3	ACT	I	304	-	3,3,3	0.77	0	3,3,3	1.38	0
6	PEG	J	311	-	6,6,6	0.49	0	5,5,5	0.32	0
5	EDO	B	310	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	C	313	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	C	308	-	3,3,3	0.44	0	2,2,2	0.31	0
3	ACT	F	302	-	3,3,3	0.77	0	3,3,3	1.41	0
5	EDO	B	304	-	3,3,3	0.45	0	2,2,2	0.34	0
6	PEG	F	306	-	6,6,6	0.49	0	5,5,5	0.24	0
5	EDO	A	307	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	H	304	-	3,3,3	0.47	0	2,2,2	0.35	0
2	PGE	E	301	-	9,9,9	0.30	0	8,8,8	0.30	0
5	EDO	B	305	-	3,3,3	0.44	0	2,2,2	0.33	0
5	EDO	C	311	-	3,3,3	0.43	0	2,2,2	0.35	0
2	PGE	C	302	-	9,9,9	0.30	0	8,8,8	0.37	0
3	ACT	J	302	-	3,3,3	0.75	0	3,3,3	1.37	0
6	PEG	G	308	-	6,6,6	0.49	0	5,5,5	0.26	0
3	ACT	E	303	-	3,3,3	0.76	0	3,3,3	1.34	0
5	EDO	L	305	-	3,3,3	0.46	0	2,2,2	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	314	-	-	0/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	J	307	-	-	0/1/1/1	-
5	EDO	E	306	-	-	0/1/1/1	-
5	EDO	J	305	-	-	0/1/1/1	-
5	EDO	J	306	-	-	0/1/1/1	-
5	EDO	G	303	-	-	1/1/1/1	-
5	EDO	L	306	-	-	0/1/1/1	-
5	EDO	C	312	-	-	0/1/1/1	-
5	EDO	F	304	-	-	0/1/1/1	-
5	EDO	E	309	-	-	0/1/1/1	-
5	EDO	C	306	-	-	0/1/1/1	-
5	EDO	A	306	-	-	0/1/1/1	-
2	PGE	I	301	-	-	0/7/7/7	-
5	EDO	J	310	-	-	0/1/1/1	-
5	EDO	E	307	-	-	0/1/1/1	-
5	EDO	B	308	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	F	301	-	-	2/7/7/7	-
5	EDO	L	304	-	-	0/1/1/1	-
2	PGE	A	301	-	-	3/7/7/7	-
5	EDO	C	315	-	-	0/1/1/1	-
2	PGE	J	301	-	-	1/7/7/7	-
2	PGE	K	301	-	-	5/7/7/7	-
7	GOL	L	302	-	-	2/4/4/4	-
5	EDO	G	305	-	-	0/1/1/1	-
5	EDO	K	302	-	-	0/1/1/1	-
5	EDO	A	310	-	-	0/1/1/1	-
6	PEG	J	311	-	-	2/4/4/4	-
5	EDO	D	304	-	-	0/1/1/1	-
7	GOL	G	301	-	-	2/4/4/4	-
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	C	313	-	-	0/1/1/1	-
5	EDO	C	309	-	-	0/1/1/1	-
5	EDO	I	308	-	-	0/1/1/1	-
5	EDO	K	303	-	-	0/1/1/1	-
2	PGE	C	301	-	-	2/7/7/7	-
5	EDO	C	308	-	-	0/1/1/1	-
6	PEG	H	306	-	-	2/4/4/4	-
5	EDO	B	304	-	-	0/1/1/1	-
6	PEG	F	306	-	-	2/4/4/4	-
5	EDO	C	307	-	-	0/1/1/1	-
6	PEG	L	308	-	-	2/4/4/4	-
5	EDO	A	307	-	-	0/1/1/1	-
5	EDO	H	304	-	-	0/1/1/1	-
5	EDO	G	304	-	-	0/1/1/1	-
5	EDO	B	309	-	-	0/1/1/1	-
5	EDO	L	307	-	-	0/1/1/1	-
5	EDO	G	306	-	-	0/1/1/1	-
5	EDO	B	307	-	-	0/1/1/1	-
2	PGE	E	301	-	-	3/7/7/7	-
5	EDO	A	308	-	-	0/1/1/1	-
5	EDO	B	305	-	-	0/1/1/1	-
5	EDO	C	316	-	-	0/1/1/1	-
5	EDO	I	306	-	-	0/1/1/1	-
5	EDO	J	308	-	-	0/1/1/1	-
5	EDO	C	311	-	-	0/1/1/1	-
5	EDO	C	310	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	F	303	-	-	0/1/1/1	-
5	EDO	H	305	-	-	0/1/1/1	-
7	GOL	I	302	-	-	2/4/4/4	-
2	PGE	C	302	-	-	3/7/7/7	-
5	EDO	F	305	-	-	0/1/1/1	-
2	PGE	D	301	-	-	4/7/7/7	-
5	EDO	I	307	-	-	0/1/1/1	-
6	PEG	L	309	-	-	1/4/4/4	-
6	PEG	G	308	-	-	4/4/4/4	-
5	EDO	B	306	-	-	1/1/1/1	-
2	PGE	L	301	-	-	3/7/7/7	-
5	EDO	E	308	-	-	0/1/1/1	-
5	EDO	G	302	-	-	0/1/1/1	-
5	EDO	G	307	-	-	0/1/1/1	-
5	EDO	L	305	-	-	0/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	D	303	-	-	0/1/1/1	-
5	EDO	J	309	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	301	GOL	O1-C1-C2-C3
7	I	302	GOL	O1-C1-C2-O2
7	I	302	GOL	O1-C1-C2-C3
7	L	302	GOL	O1-C1-C2-C3
2	E	301	PGE	O2-C3-C4-O3
2	K	301	PGE	O2-C3-C4-O3
2	D	301	PGE	O2-C3-C4-O3
2	D	301	PGE	O1-C1-C2-O2
2	L	301	PGE	O1-C1-C2-O2
7	G	301	GOL	O1-C1-C2-O2
7	L	302	GOL	O1-C1-C2-O2
5	G	303	EDO	O1-C1-C2-O2
2	E	301	PGE	O3-C5-C6-O4
6	G	308	PEG	O2-C3-C4-O4
6	H	306	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	K	301	PGE	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
2	C	302	PGE	O1-C1-C2-O2
2	L	301	PGE	O3-C5-C6-O4
2	K	301	PGE	C1-C2-O2-C3
6	G	308	PEG	C1-C2-O2-C3
2	A	301	PGE	C1-C2-O2-C3
6	H	306	PEG	C1-C2-O2-C3
6	J	311	PEG	C1-C2-O2-C3
2	C	302	PGE	C6-C5-O3-C4
2	E	301	PGE	C1-C2-O2-C3
6	F	306	PEG	C4-C3-O2-C2
2	F	301	PGE	C1-C2-O2-C3
6	L	308	PEG	O1-C1-C2-O2
2	C	302	PGE	C4-C3-O2-C2
6	L	308	PEG	C1-C2-O2-C3
2	K	301	PGE	C3-C4-O3-C5
6	G	308	PEG	C4-C3-O2-C2
2	D	301	PGE	C6-C5-O3-C4
6	F	306	PEG	C1-C2-O2-C3
2	C	301	PGE	C4-C3-O2-C2
2	F	301	PGE	O2-C3-C4-O3
2	A	301	PGE	C3-C4-O3-C5
2	J	301	PGE	C1-C2-O2-C3
2	A	301	PGE	C6-C5-O3-C4
2	C	301	PGE	C1-C2-O2-C3
2	D	301	PGE	O3-C5-C6-O4
2	K	301	PGE	O3-C5-C6-O4
2	L	301	PGE	O2-C3-C4-O3
6	L	309	PEG	C1-C2-O2-C3
5	B	306	EDO	O1-C1-C2-O2
6	J	311	PEG	O2-C3-C4-O4
6	G	308	PEG	O1-C1-C2-O2

There are no ring outliers.

28 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	305	ACT	1	0
6	H	306	PEG	1	0
5	C	316	EDO	1	0
5	C	310	EDO	1	0

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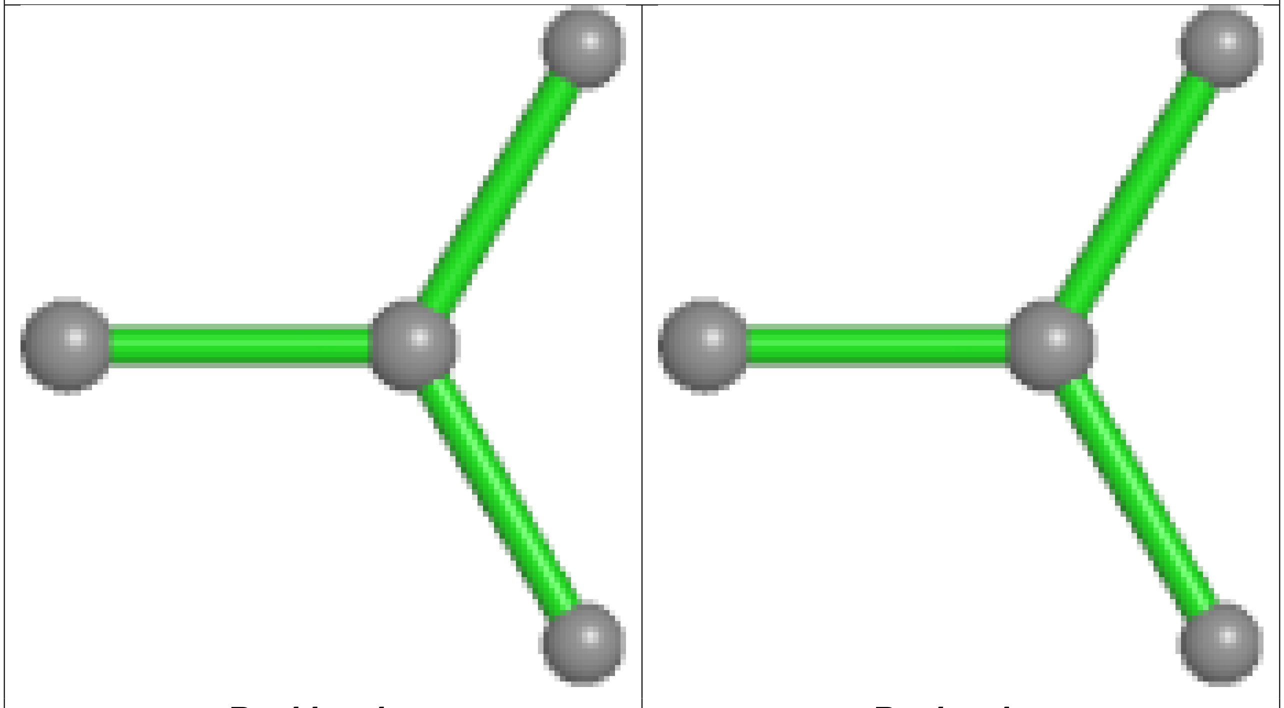
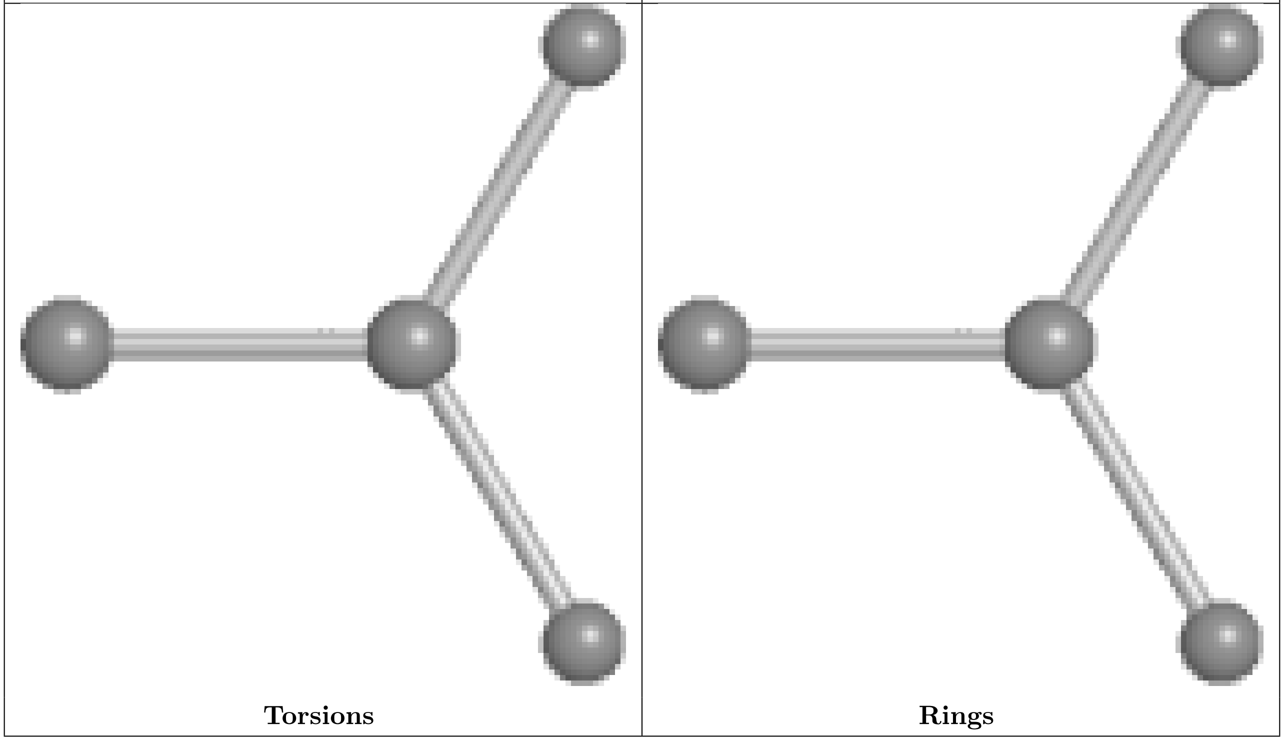
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	PGE	2	0
5	A	309	EDO	2	0
5	C	315	EDO	1	0
7	L	302	GOL	2	0
5	G	307	EDO	1	0
3	L	303	ACT	3	0
5	C	312	EDO	3	0
5	J	310	EDO	1	0
3	B	303	ACT	1	0
5	I	308	EDO	2	0
2	D	301	PGE	1	0
6	L	309	PEG	2	0
5	J	306	EDO	3	0
5	G	303	EDO	3	0
3	H	303	ACT	1	0
5	E	309	EDO	1	0
5	B	308	EDO	1	0
5	L	304	EDO	1	0
3	I	304	ACT	1	0
5	C	308	EDO	1	0
5	B	304	EDO	1	0
5	B	305	EDO	2	0
5	C	311	EDO	2	0
2	C	302	PGE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 I 305

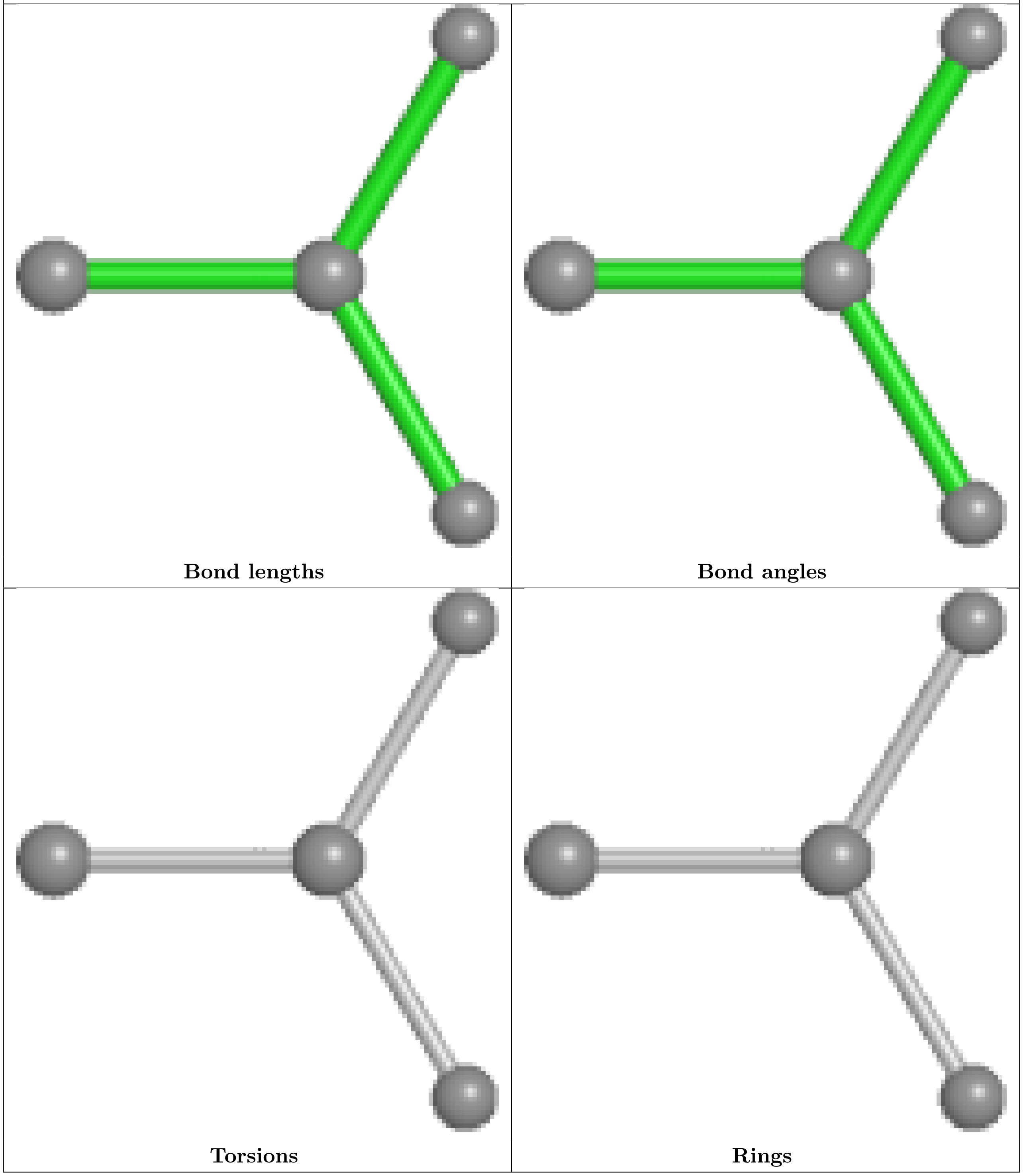


Bond lengths **Bond angles**



Torsions **Rings**

Ligand ACT C 303



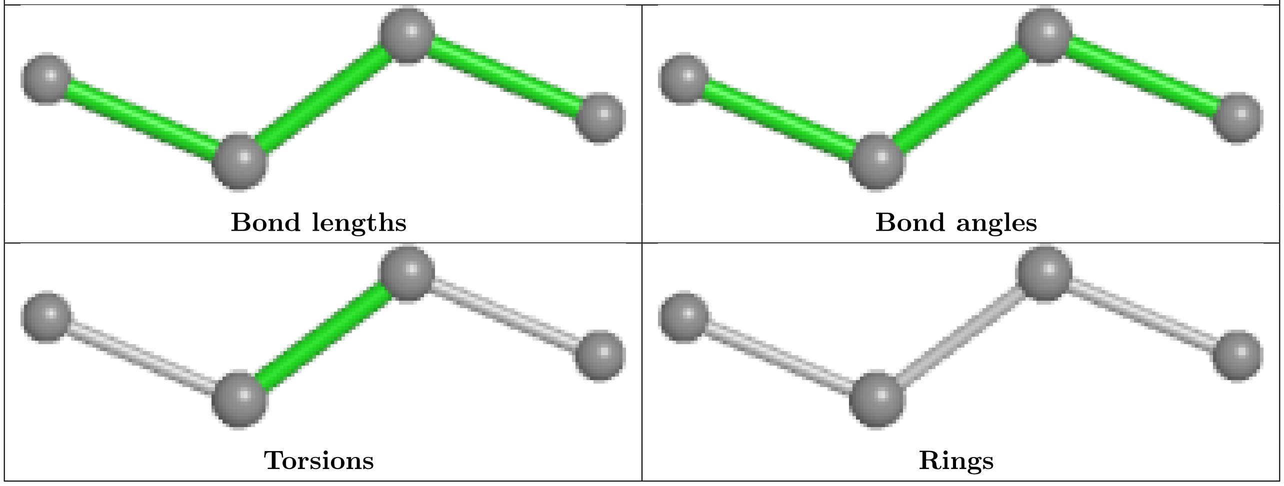
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 314



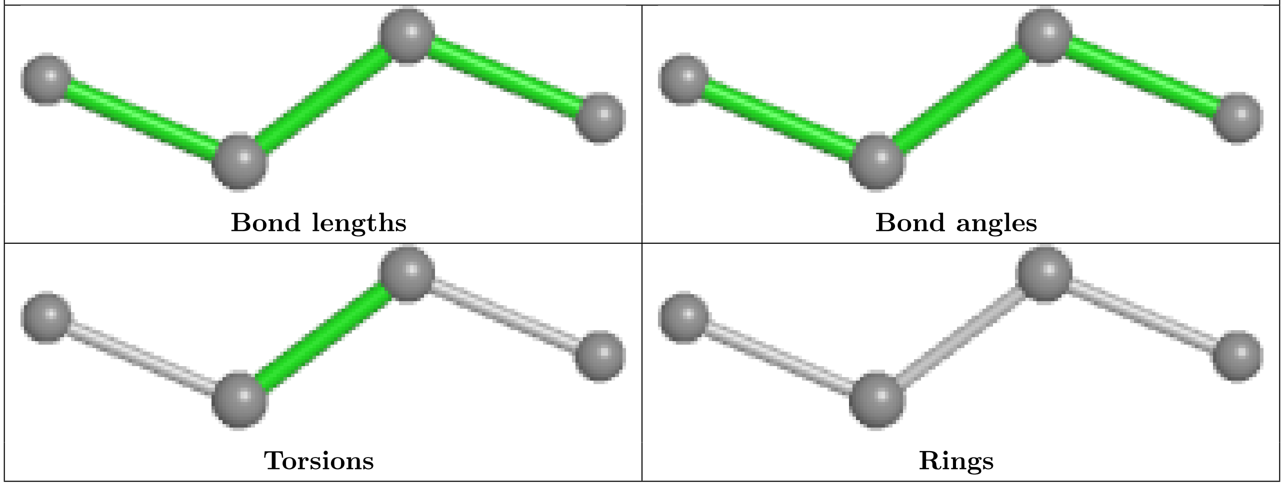
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO J 307



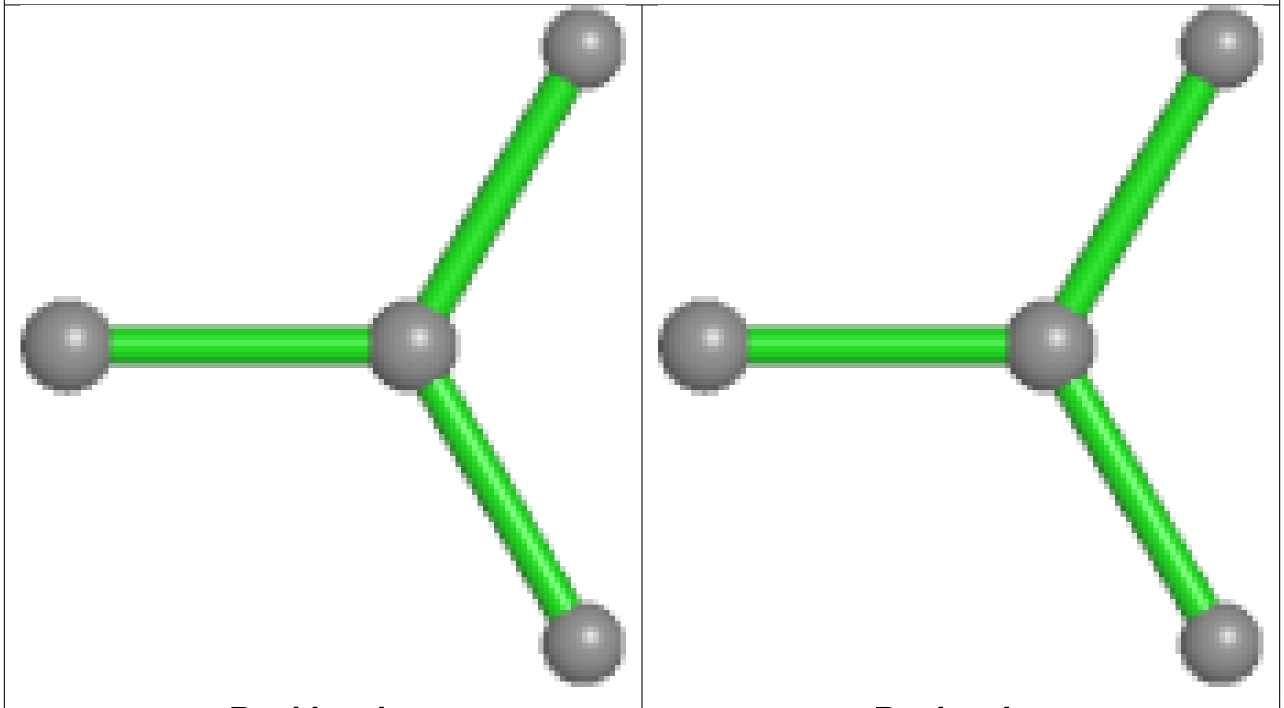
Bond lengths

Bond angles

Torsions

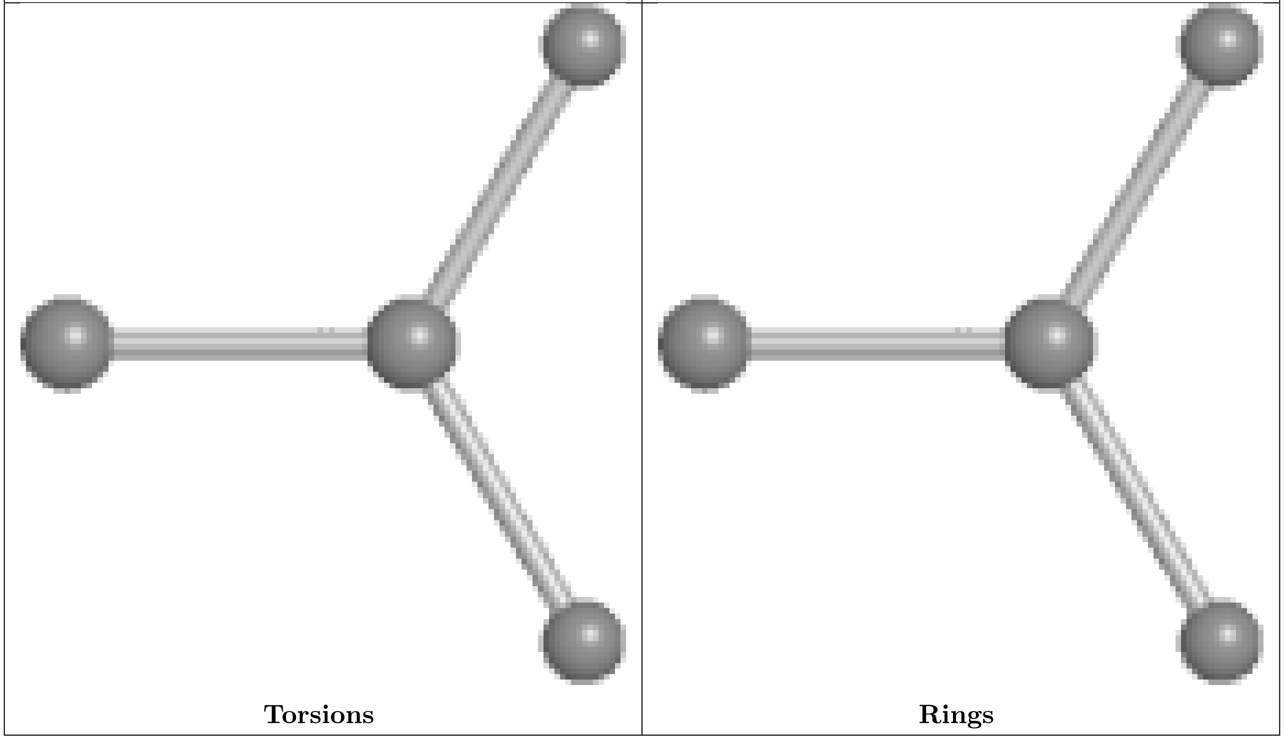
Rings

Ligand ACT B 301



Bond lengths

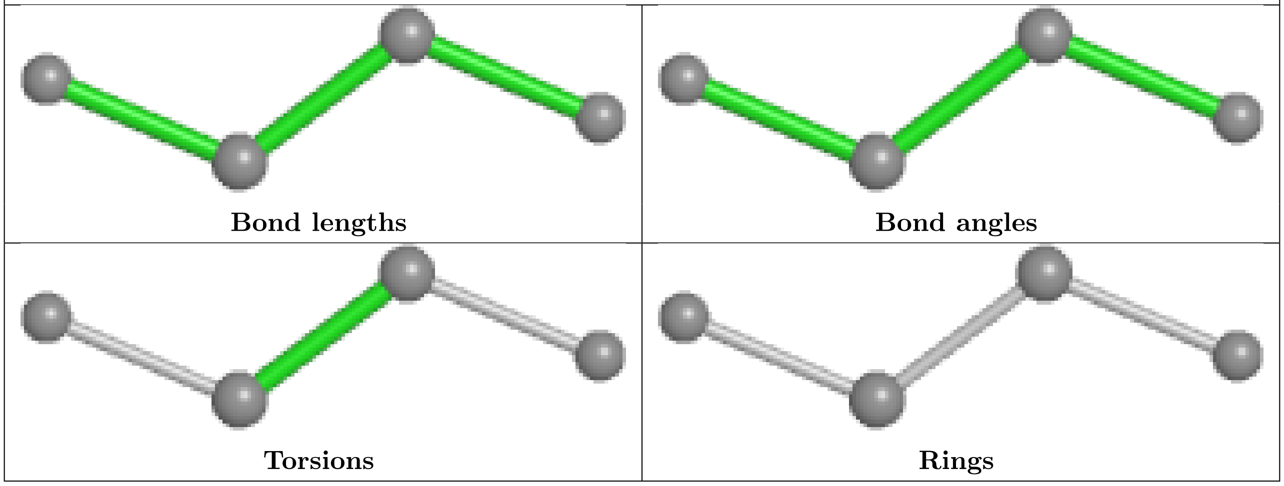
Bond angles



Torsions

Rings

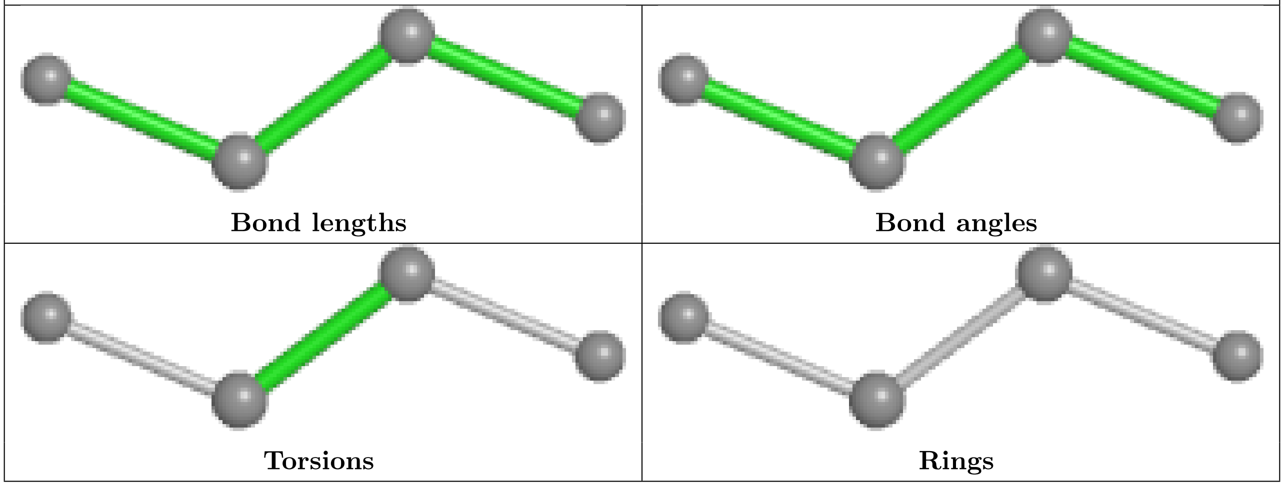
Ligand EDO F 304



Bond lengths Bond angles

Torsions Rings

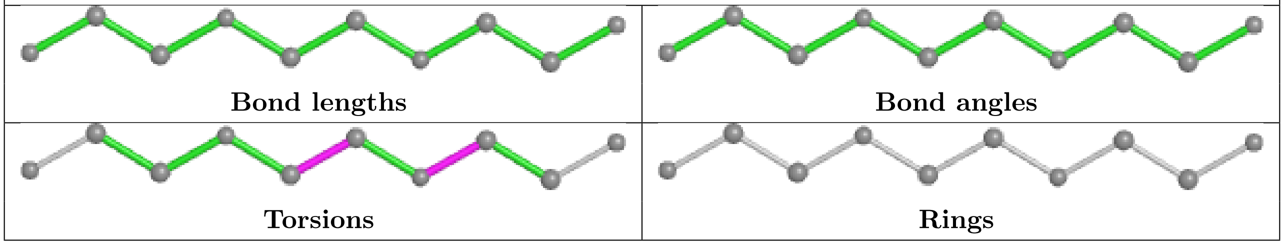
Ligand EDO E 307



Bond lengths Bond angles

Torsions Rings

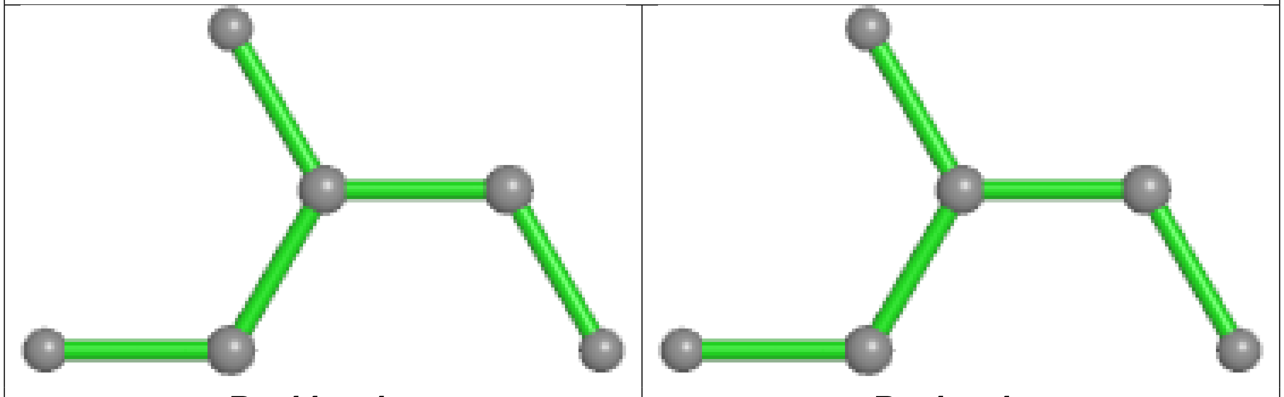
Ligand PGE F 301



Bond lengths Bond angles

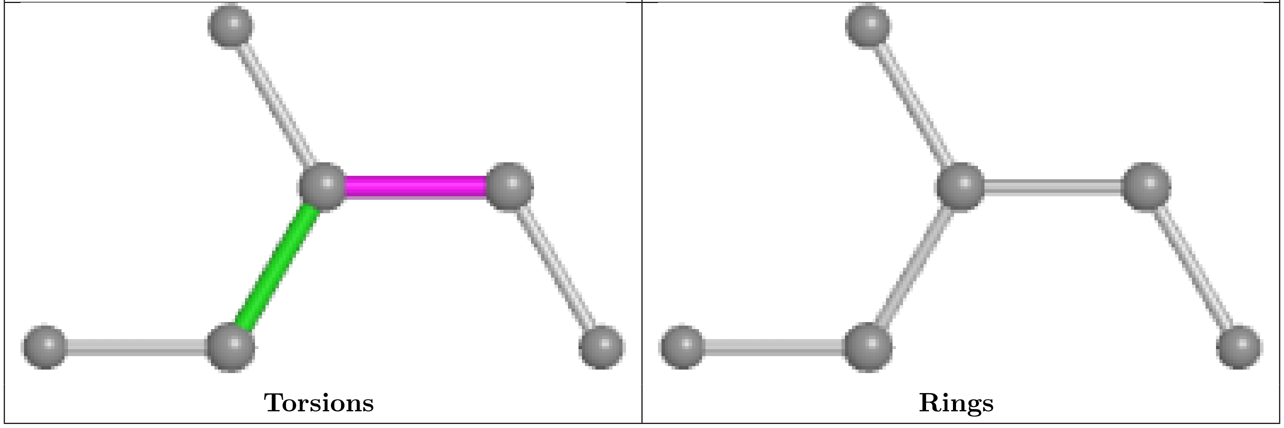
Torsions Rings

Ligand GOL G 301



Bond lengths

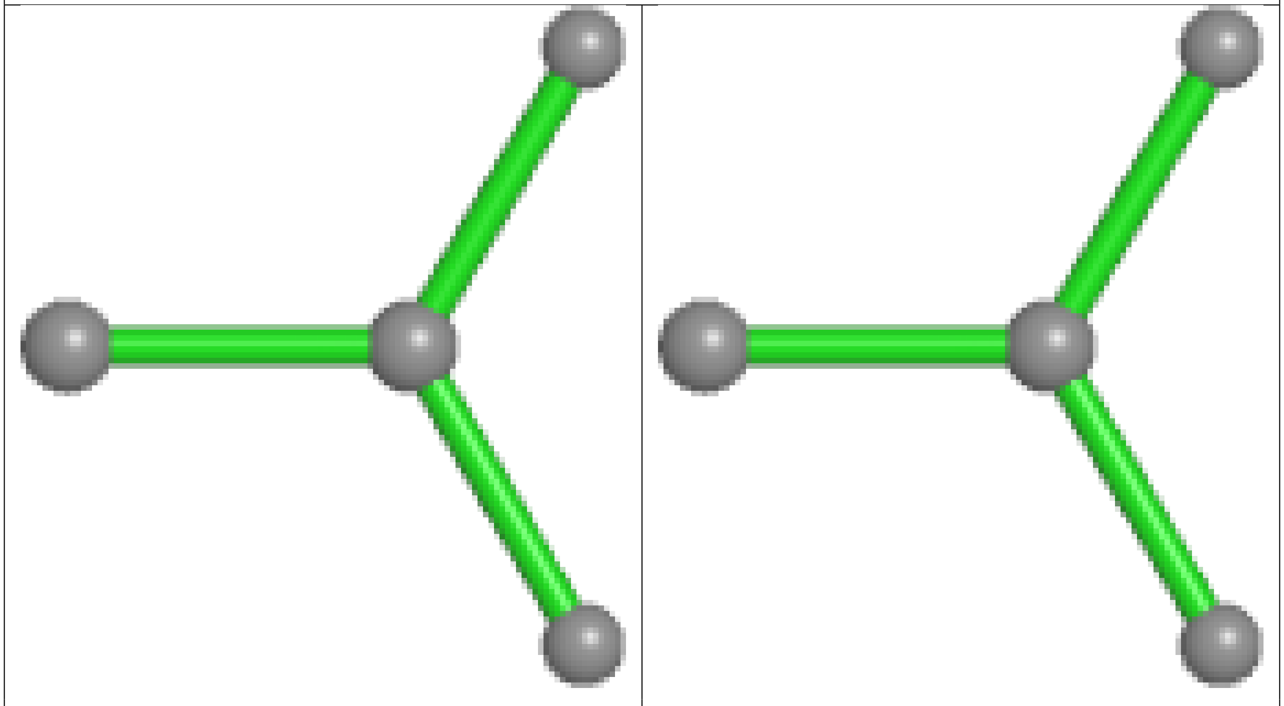
Bond angles



Torsions

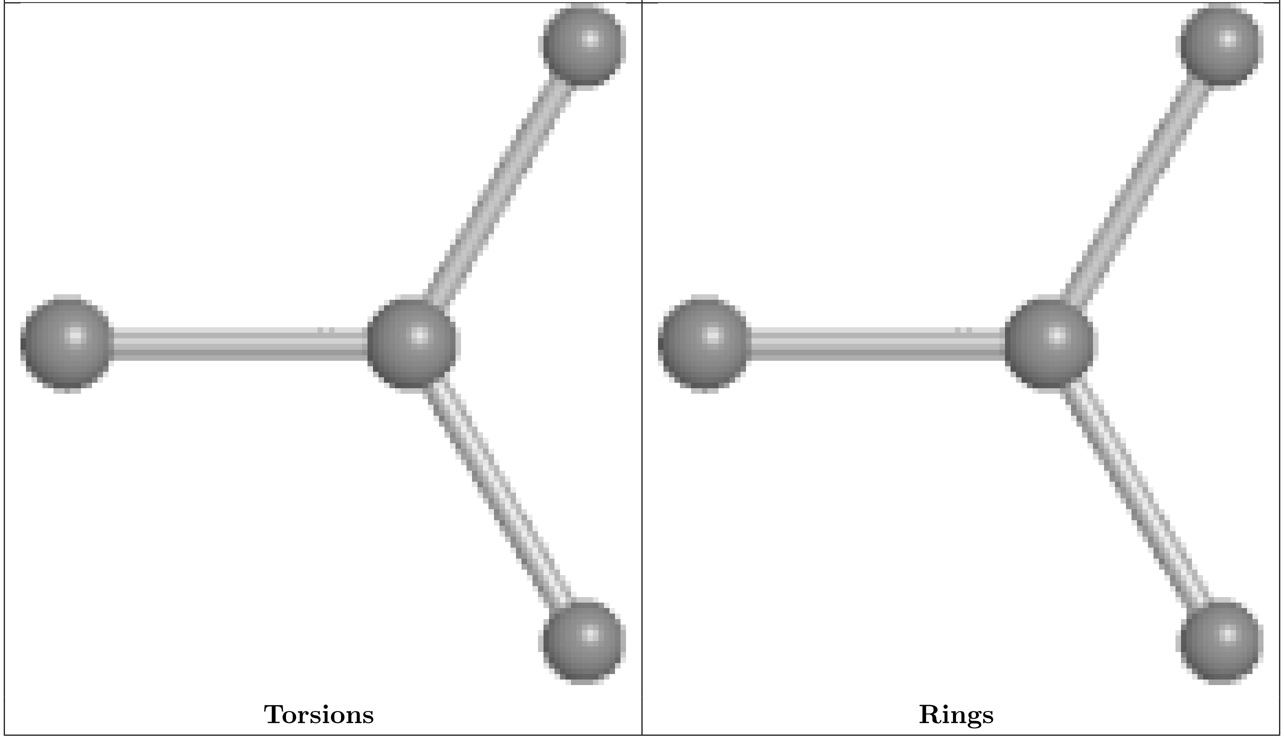
Rings

Ligand ACT H 302



Bond lengths

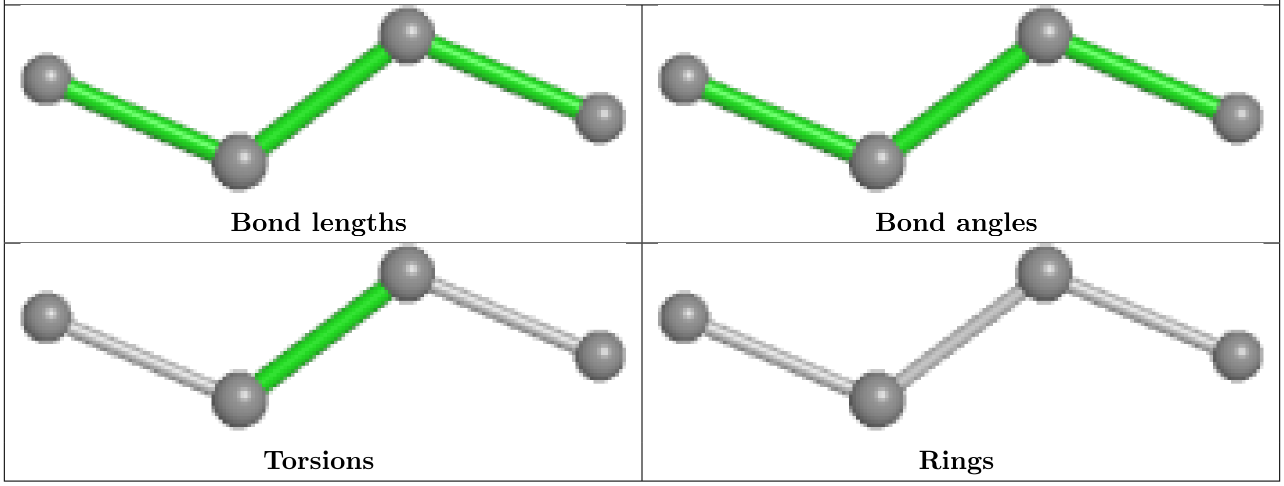
Bond angles



Torsions

Rings

Ligand EDO K 303



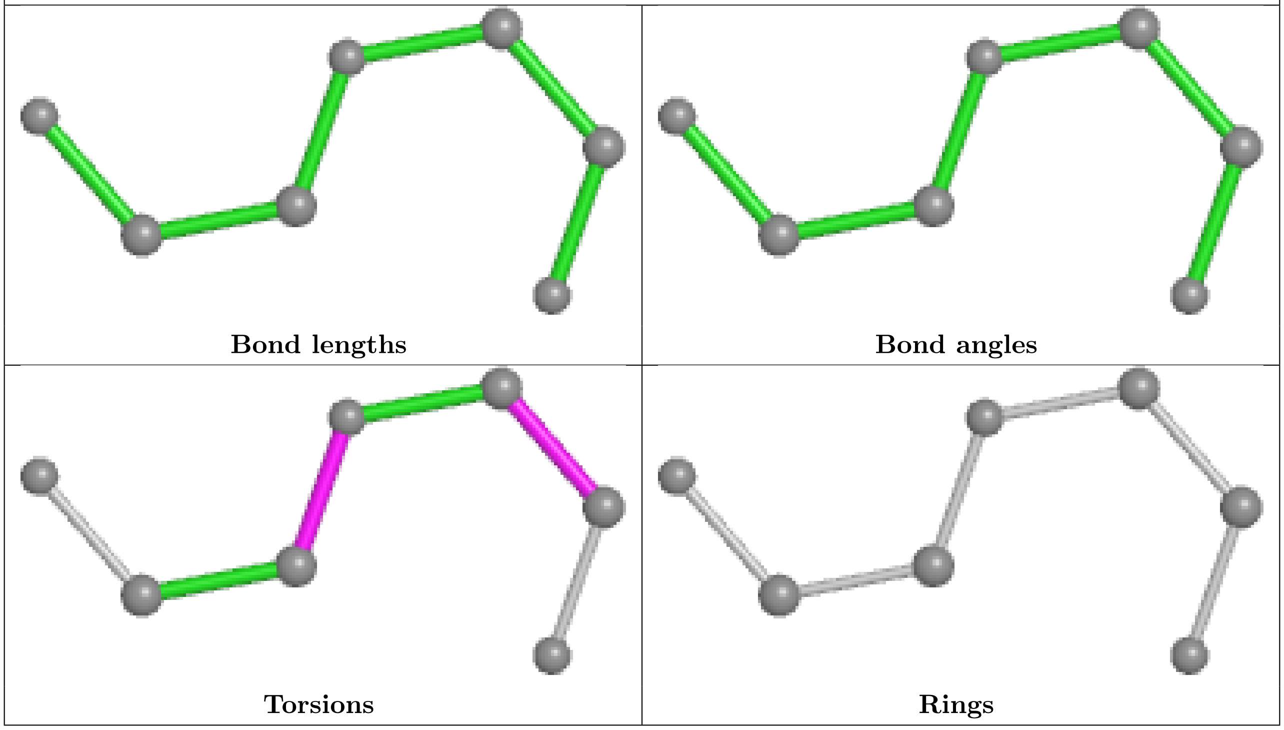
Bond lengths

Bond angles

Torsions

Rings

Ligand PEG H 306



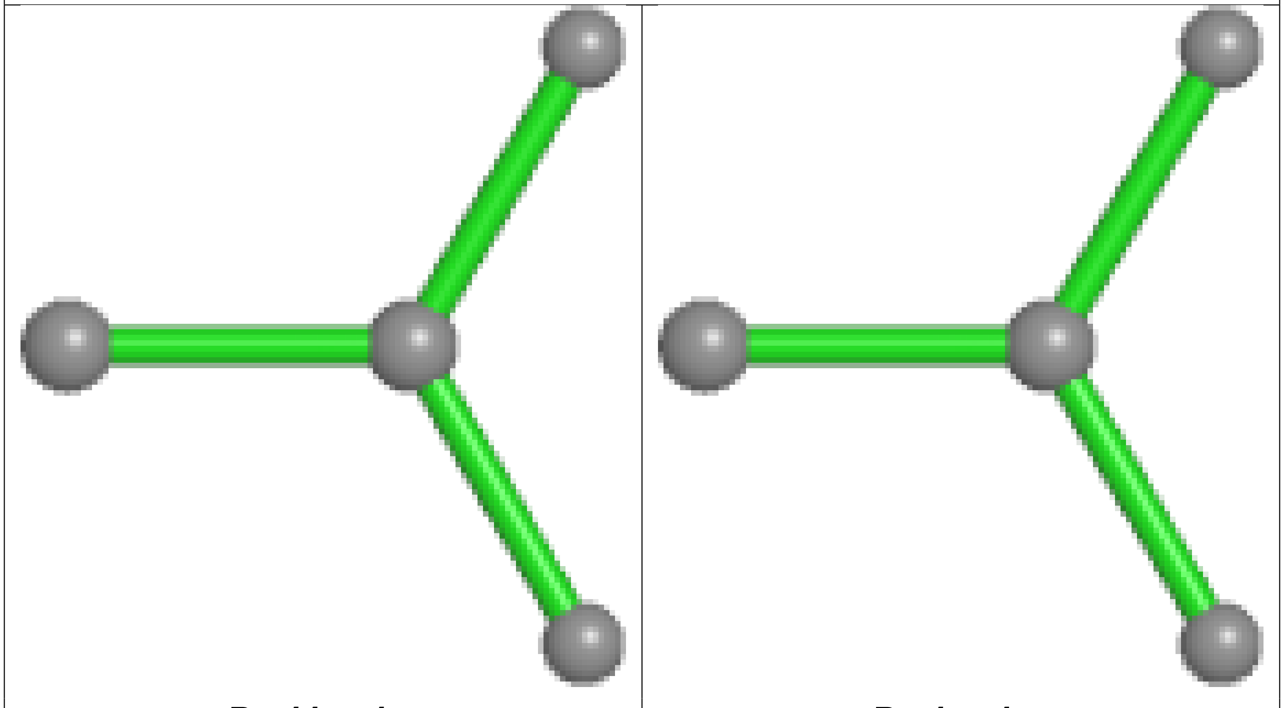
Bond lengths

Bond angles

Torsions

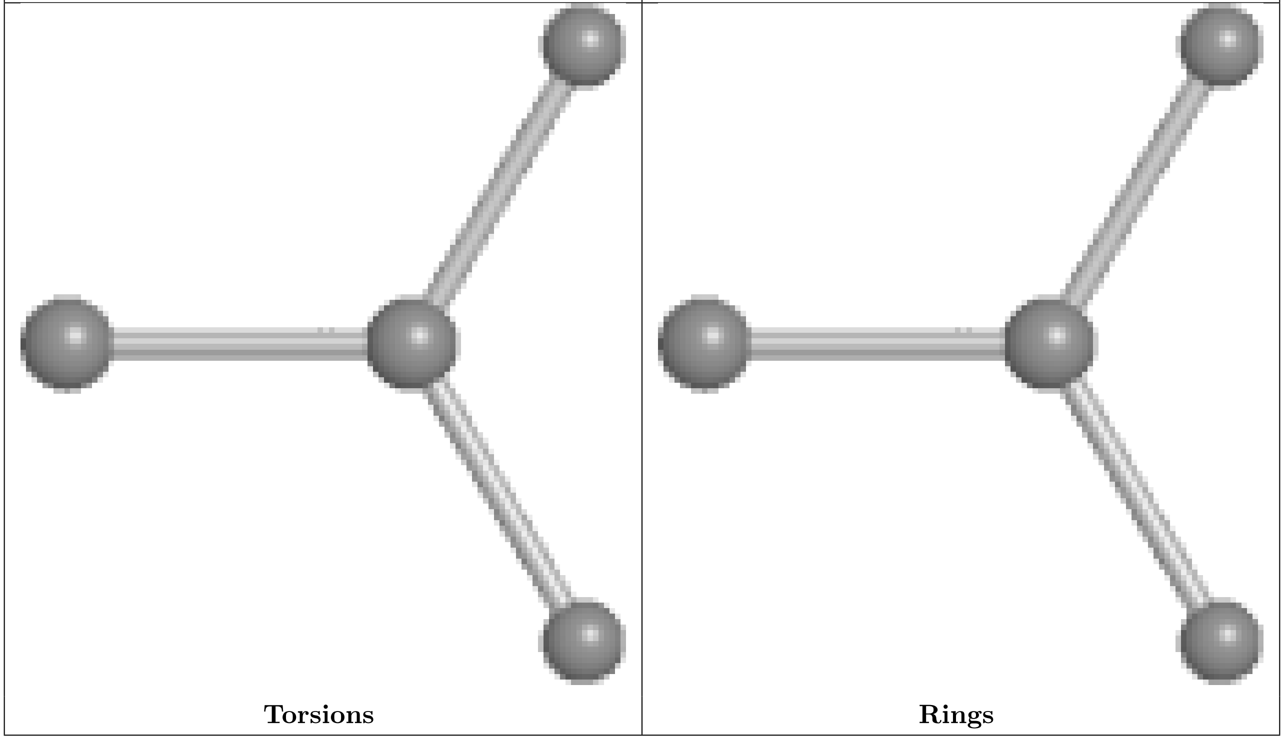
Rings

Ligand ACT A 302



Bond lengths

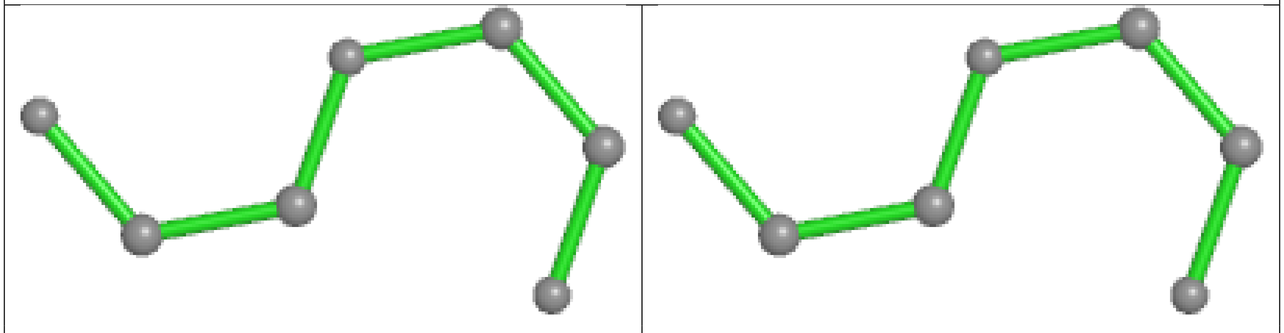
Bond angles



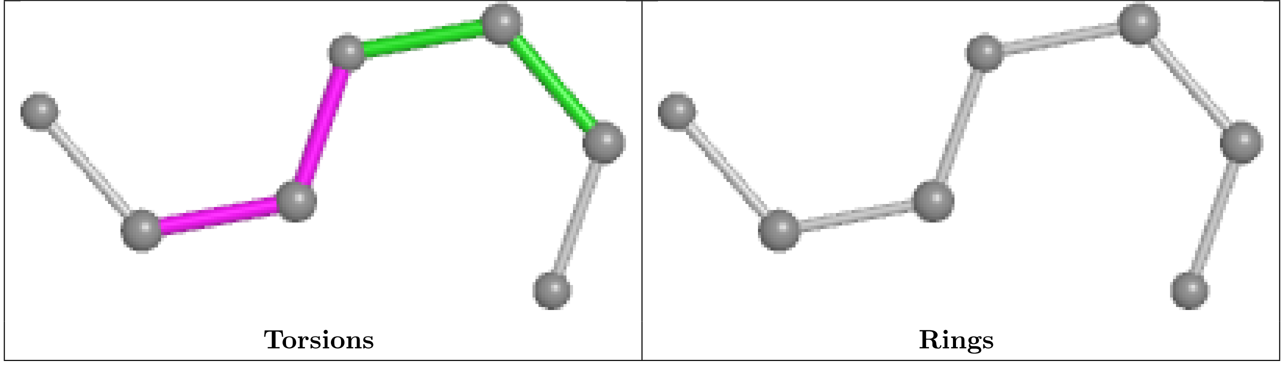
Torsions

Rings

Ligand PEG L 308

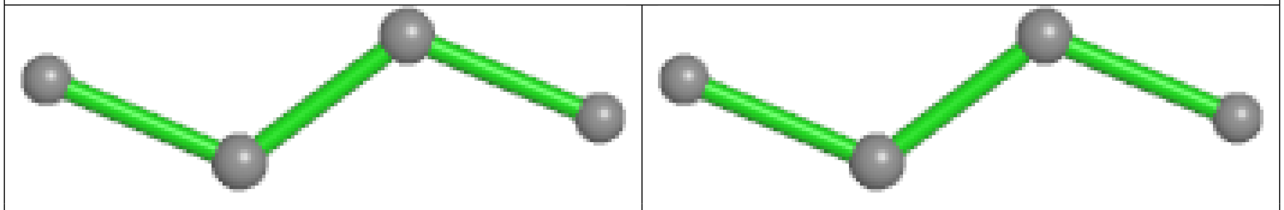


Bond lengths Bond angles

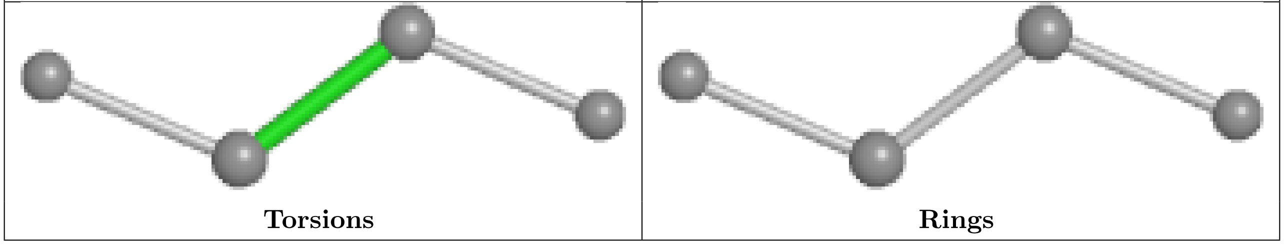


Torsions Rings

Ligand EDO C 316

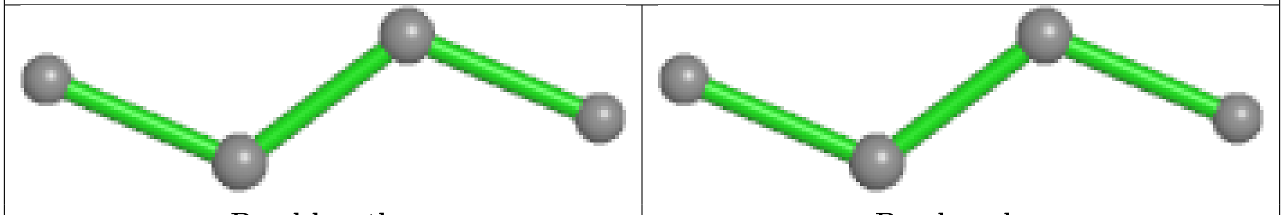


Bond lengths Bond angles



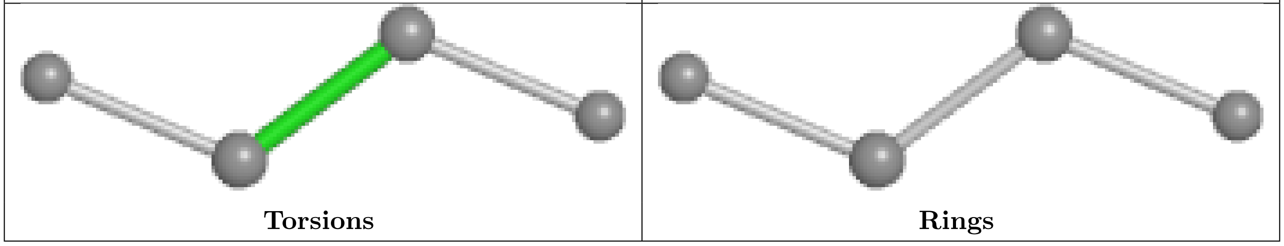
Torsions Rings

Ligand EDO I 306



Bond lengths

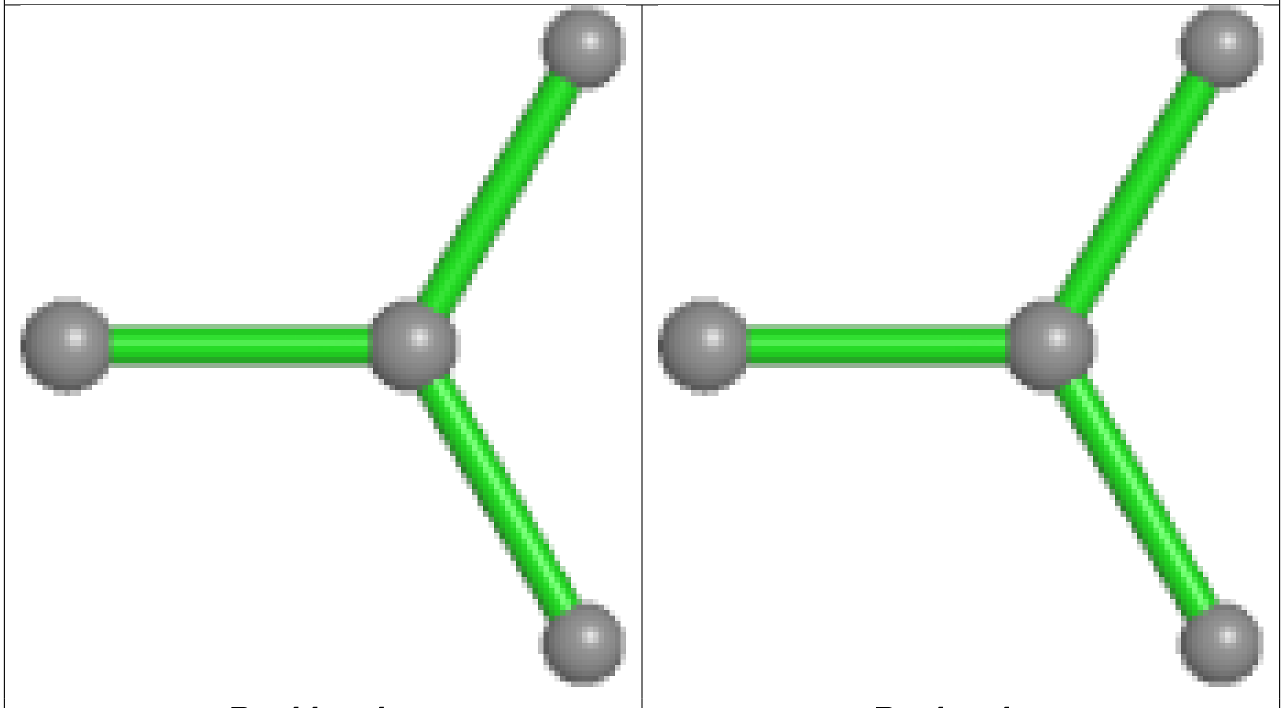
Bond angles



Torsions

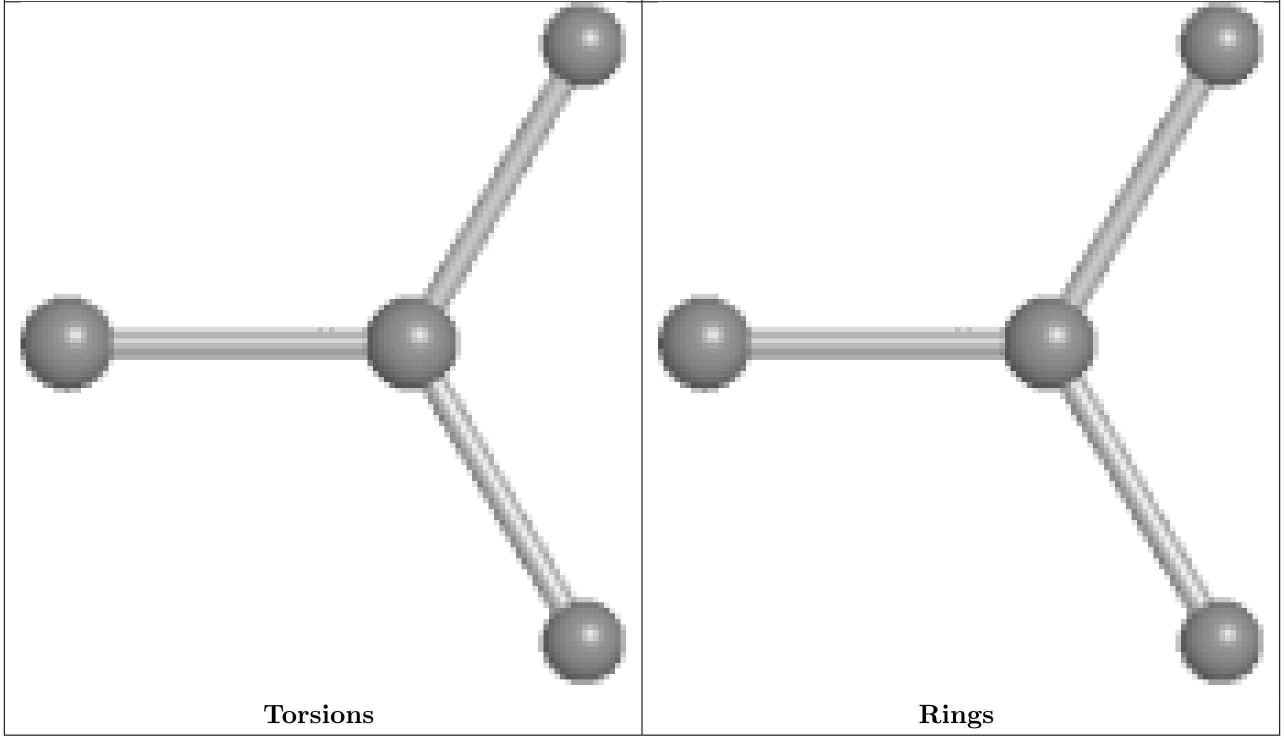
Rings

Ligand ACT E 302



Bond lengths

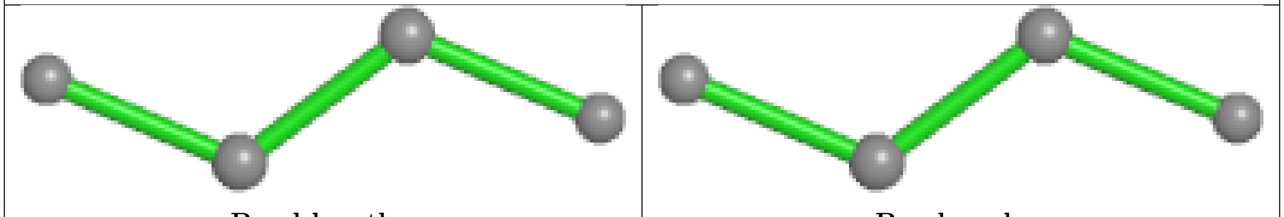
Bond angles



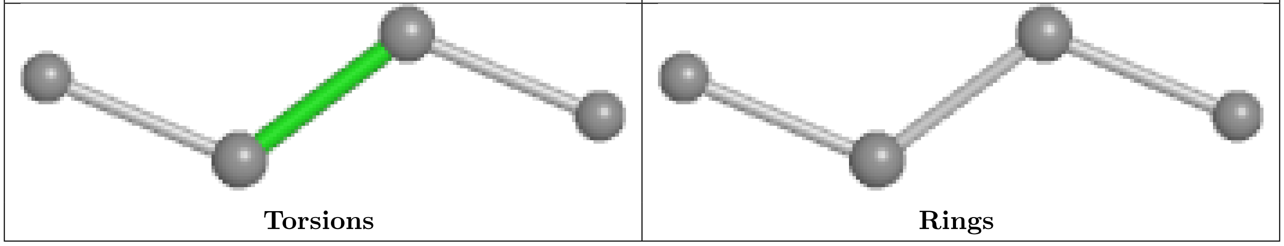
Torsions

Rings

Ligand EDO J 308

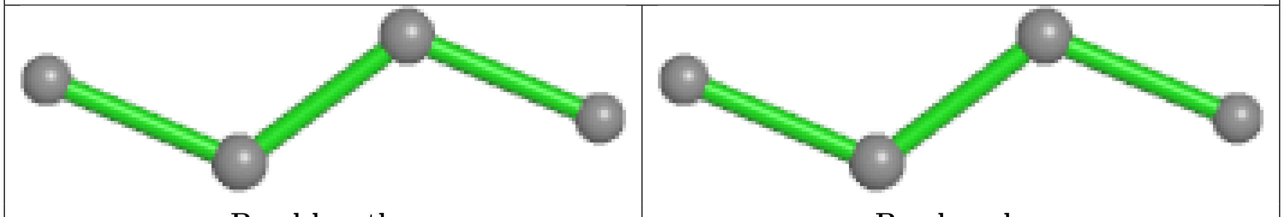


Bond lengths Bond angles

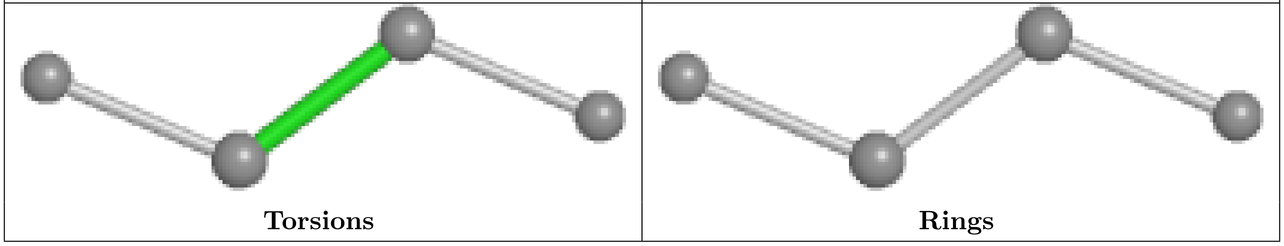


Torsions Rings

Ligand EDO C 310

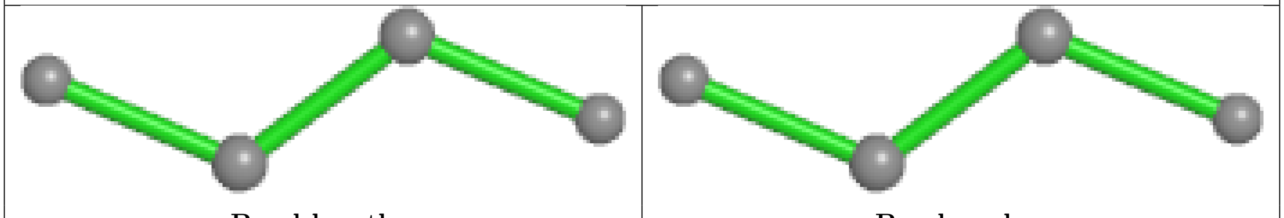


Bond lengths Bond angles

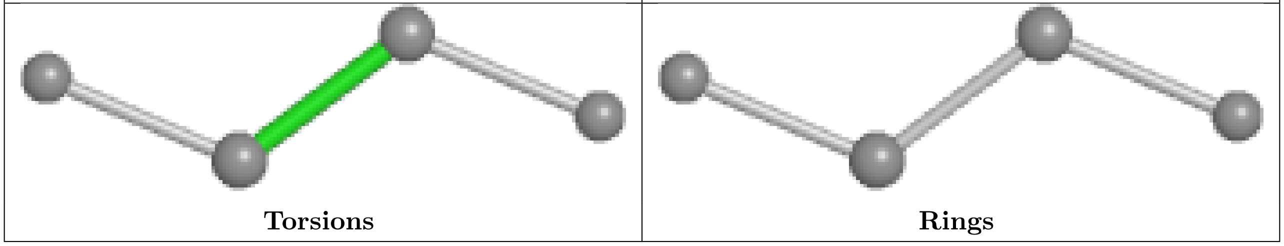


Torsions Rings

Ligand EDO F 305

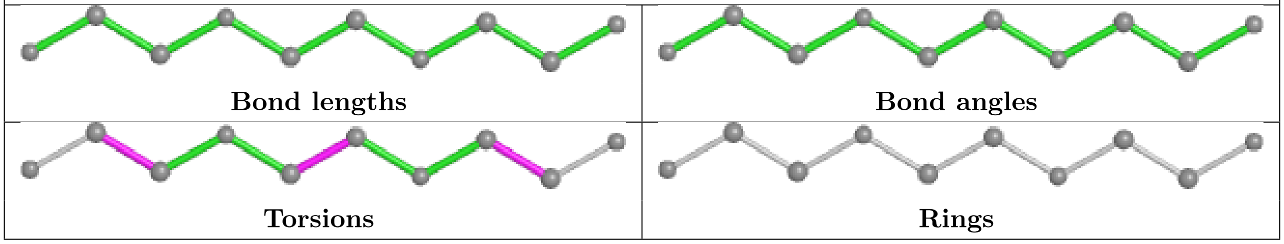


Bond lengths Bond angles



Torsions Rings

Ligand PGE L 301



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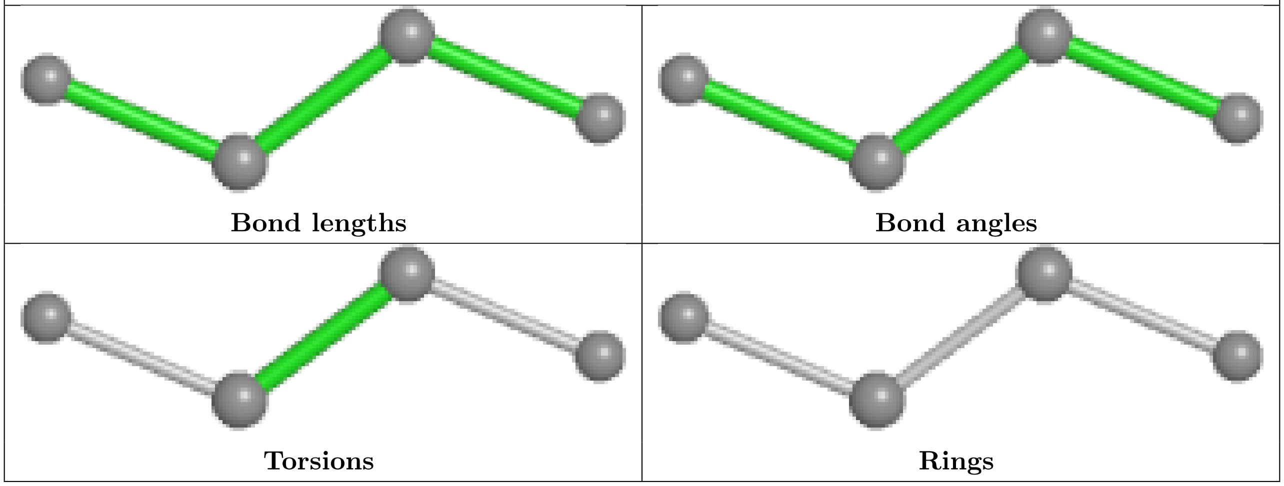
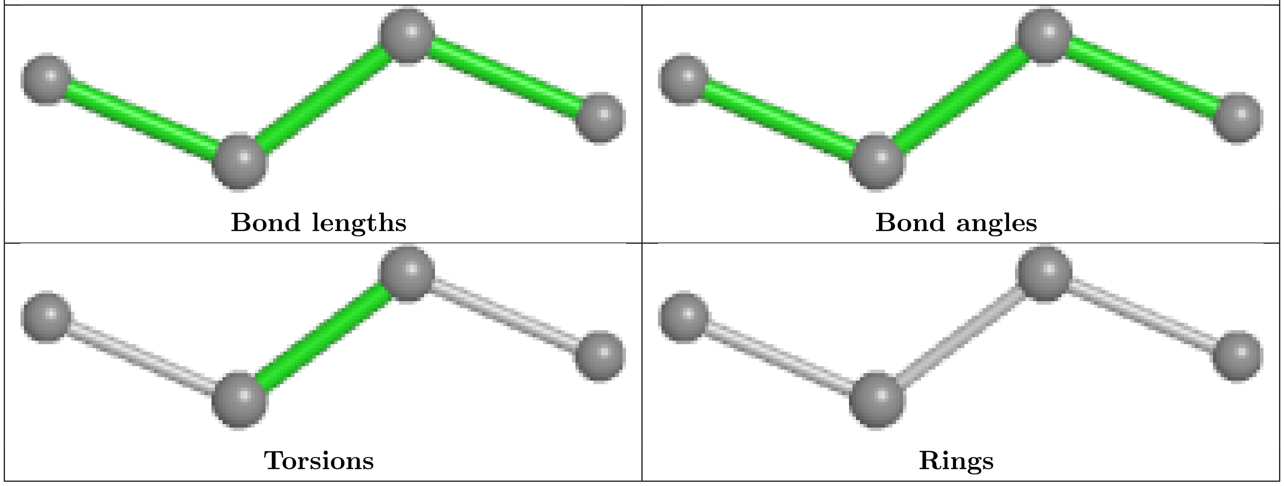
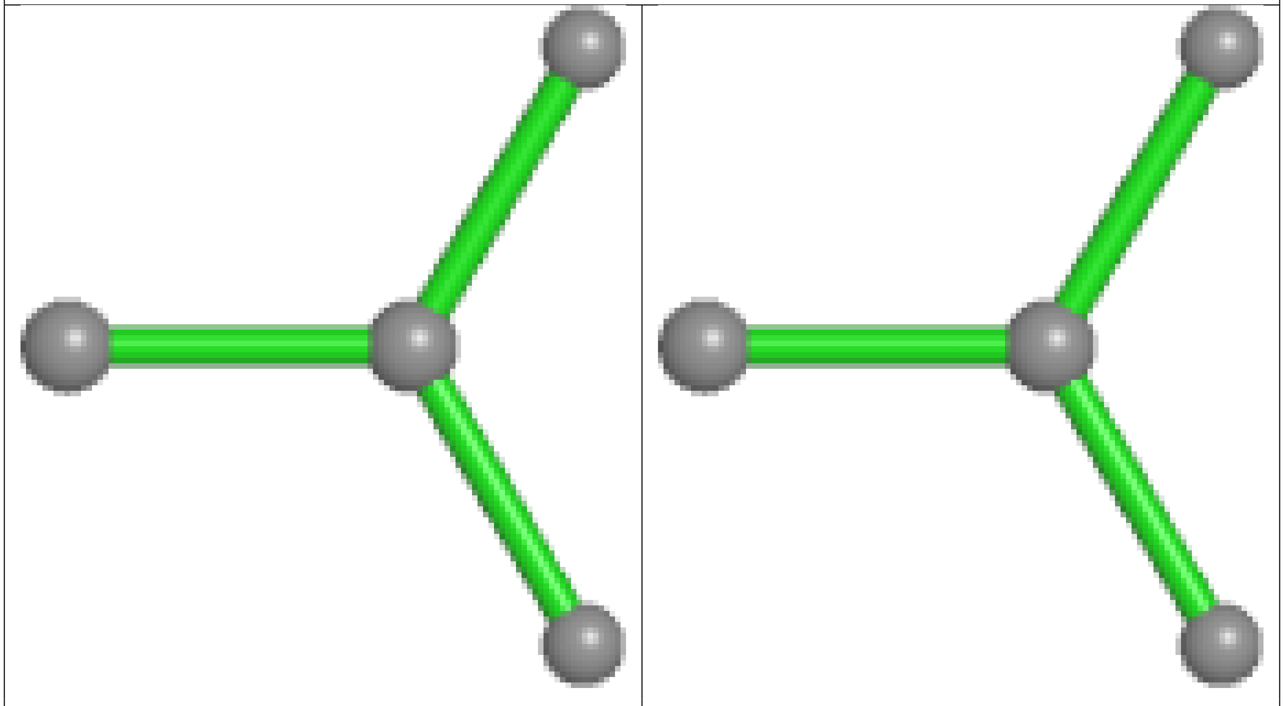


Ligand EDO A 309

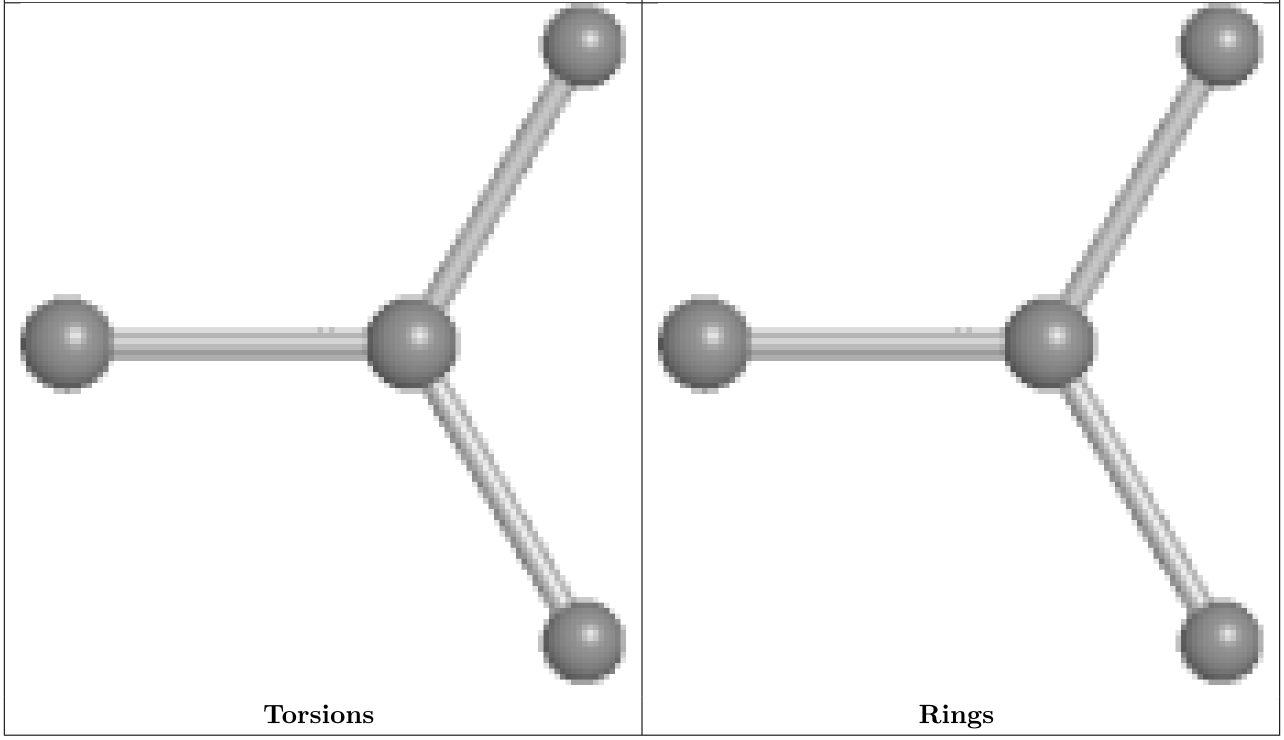


Ligand ACT I 303



Bond lengths

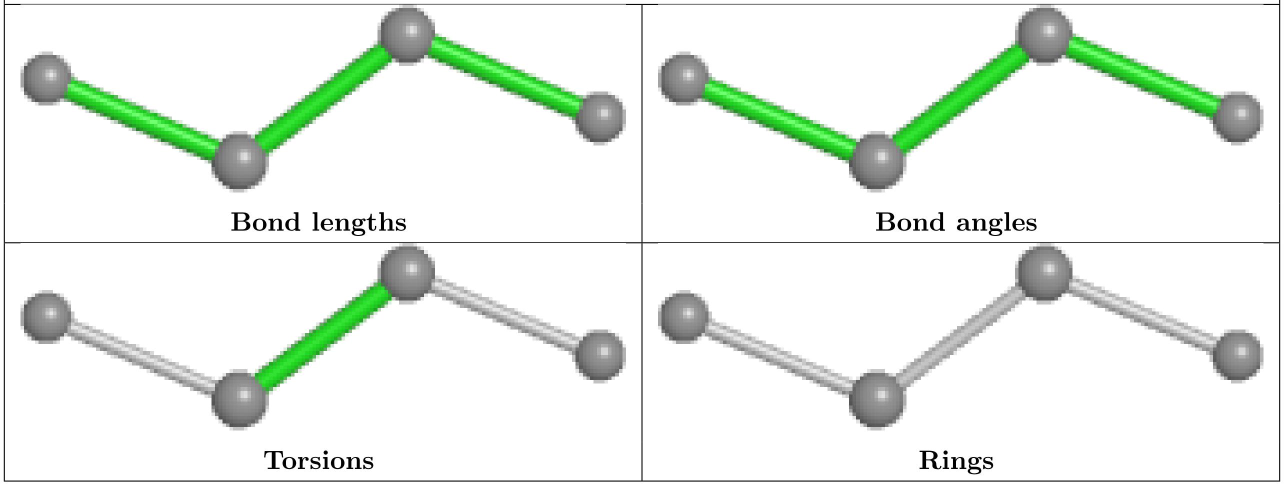
Bond angles



Torsions

Rings

Ligand EDO J 305



Bond lengths

Bond angles

Torsions

Rings

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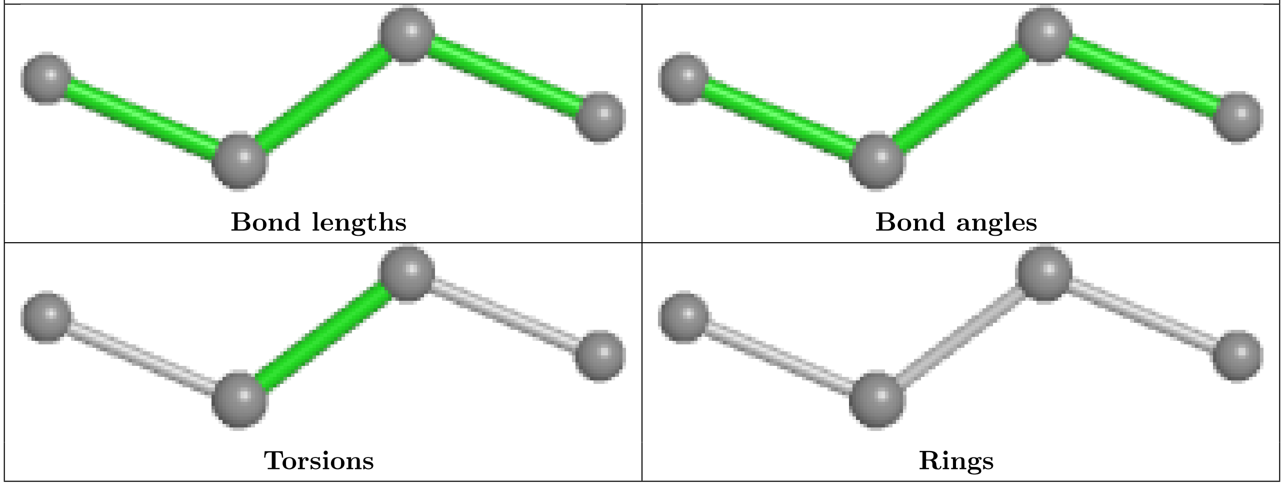


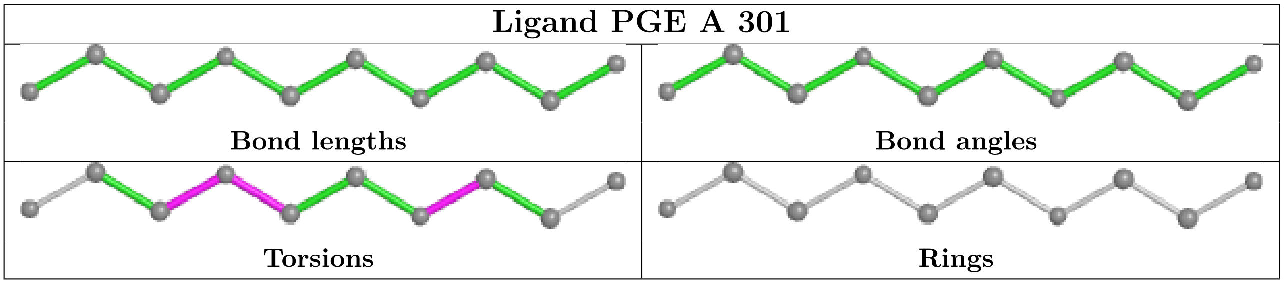
Bond lengths

Bond angles

Torsions

Rings

Ligand PGE A 301



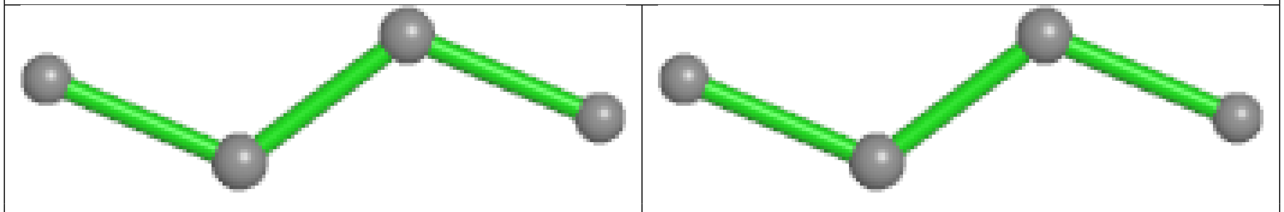
Bond lengths

Bond angles

Torsions

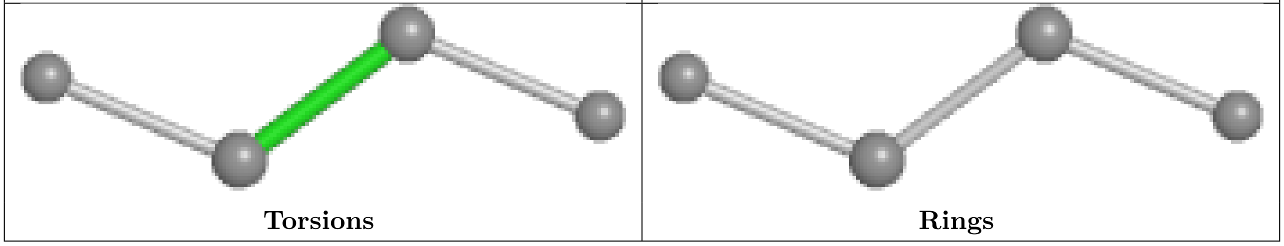
Rings

Ligand EDO C 315



Bond lengths

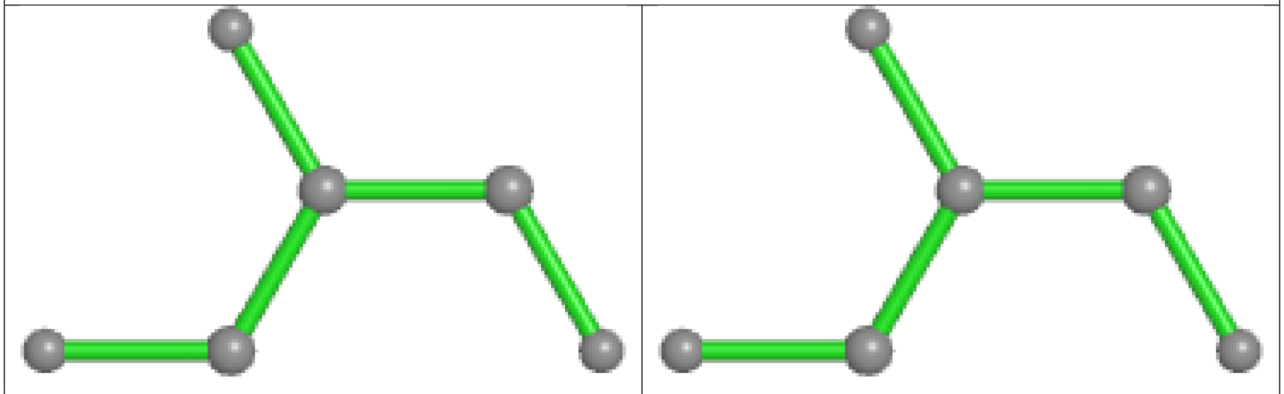
Bond angles



Torsions

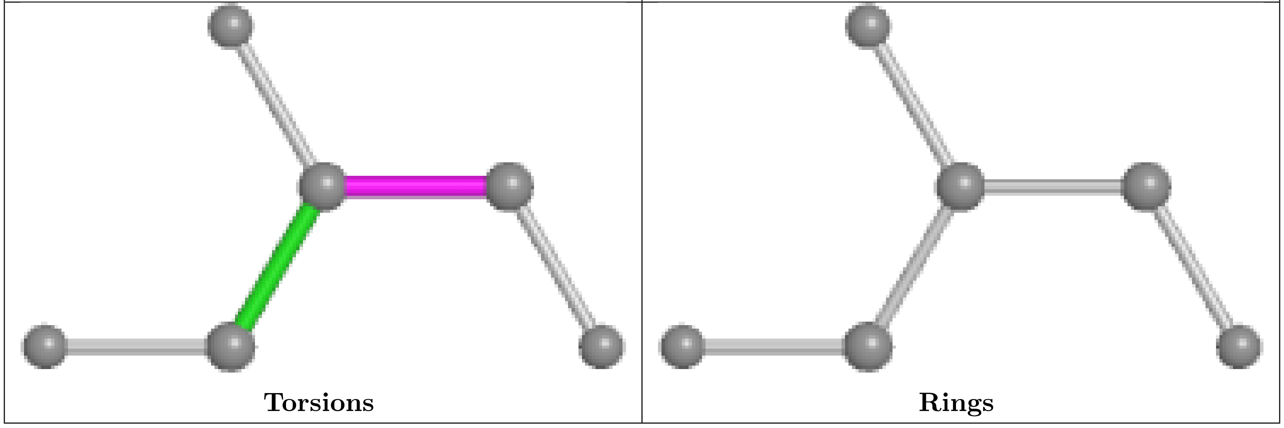
Rings

Ligand GOL L 302



Bond lengths

Bond angles



Torsions

Rings

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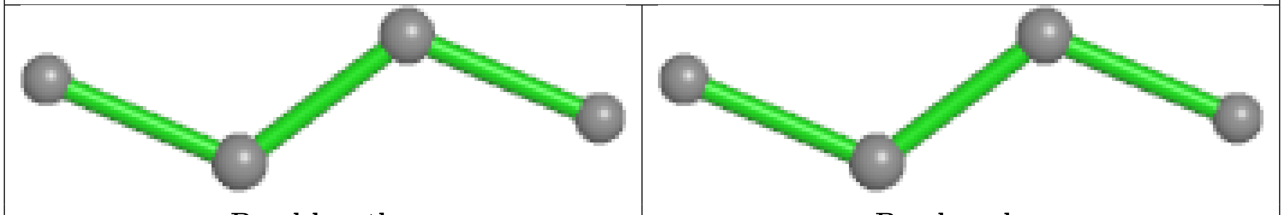
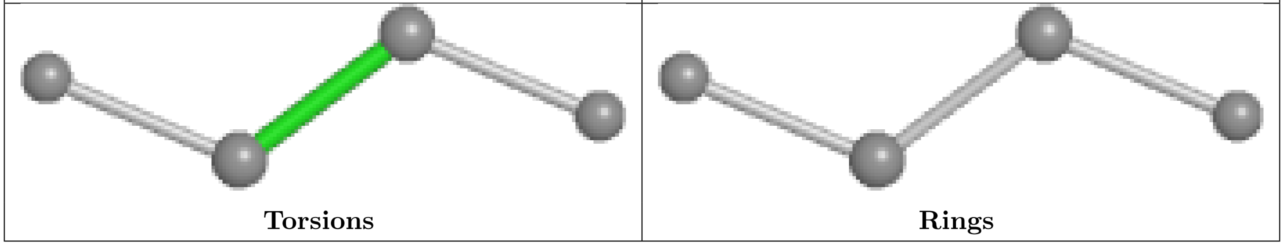


Bond lengths

Bond angles



Torsions

Rings

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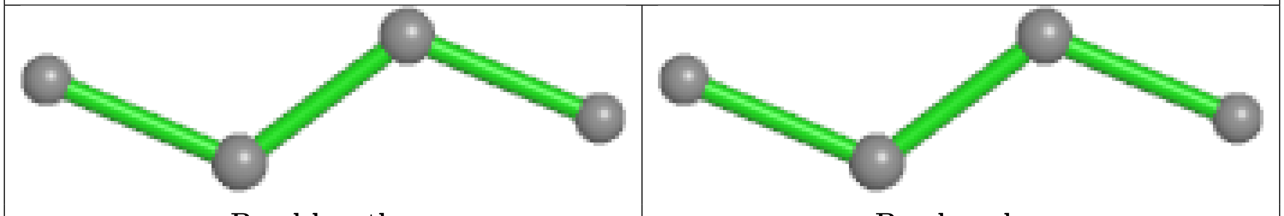
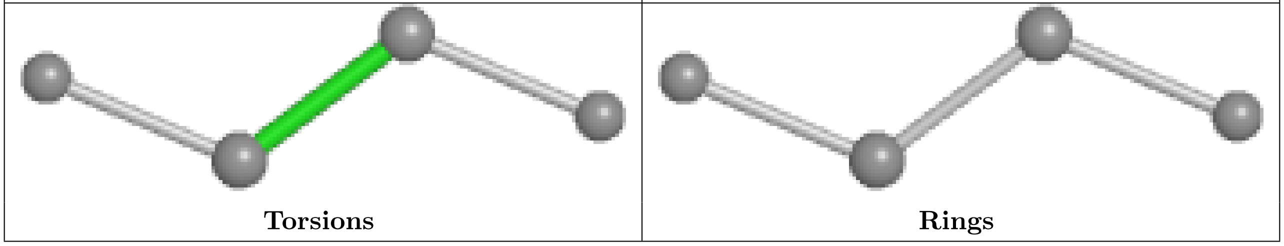


Bond lengths

Bond angles



Torsions

Rings

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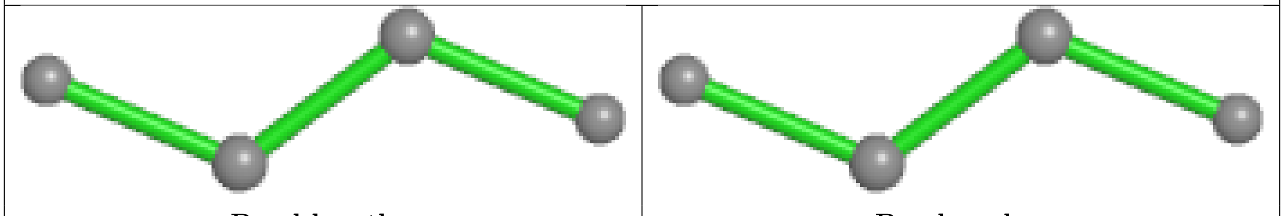
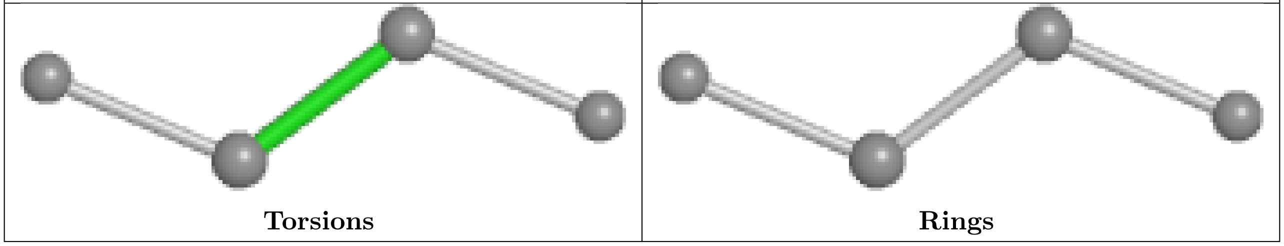


Bond lengths

Bond angles



Torsions

Rings

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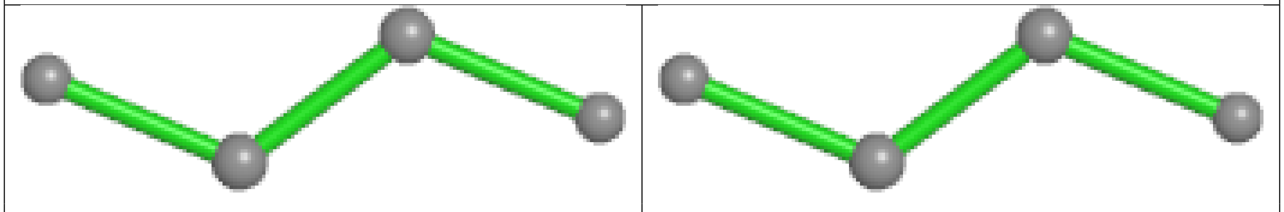
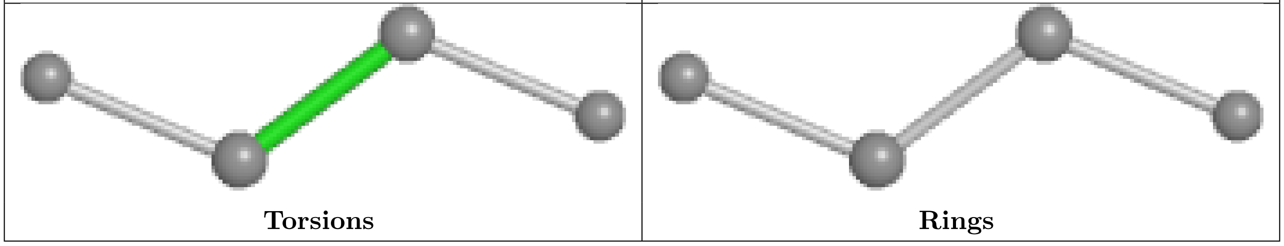


Bond lengths

Bond angles



Torsions

Rings

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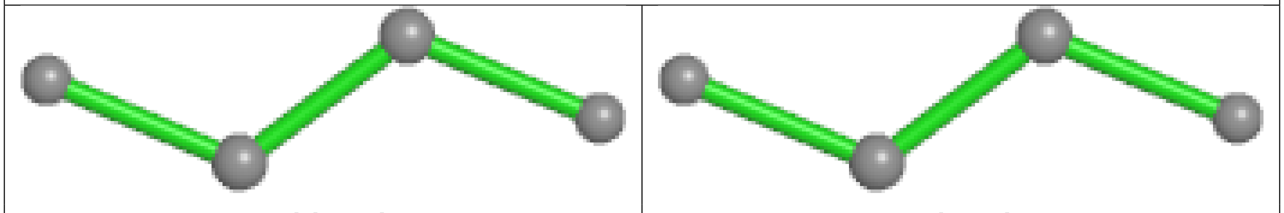
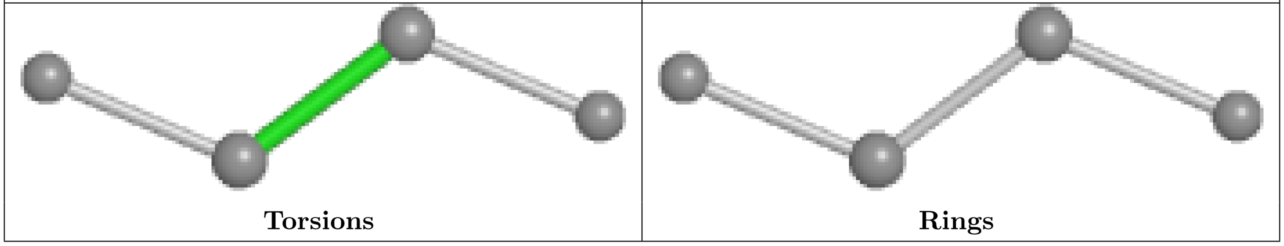


Bond lengths

Bond angles



Torsions

Rings

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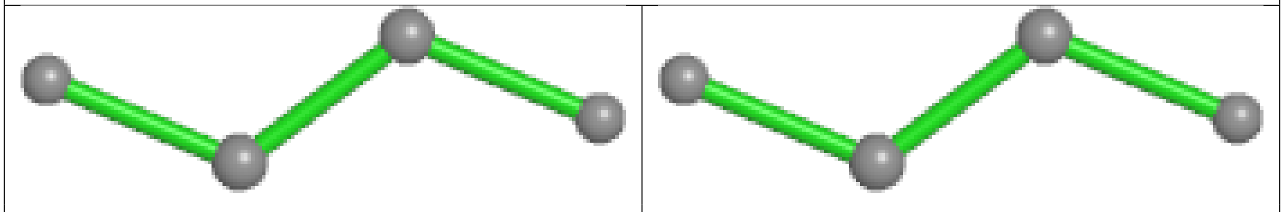
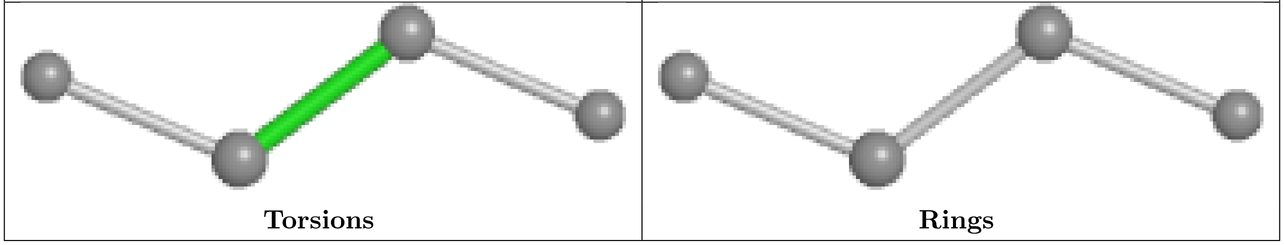


Bond lengths

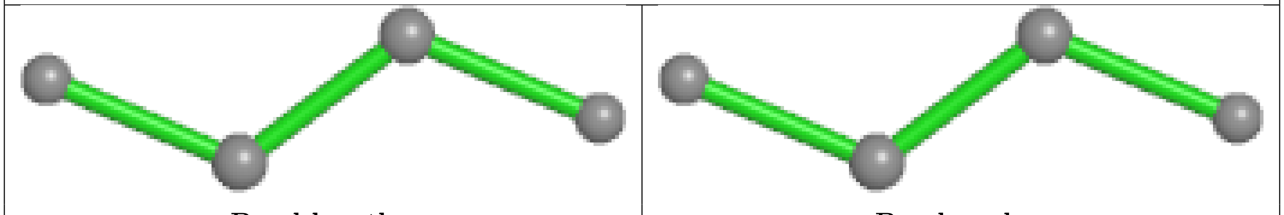
Bond angles



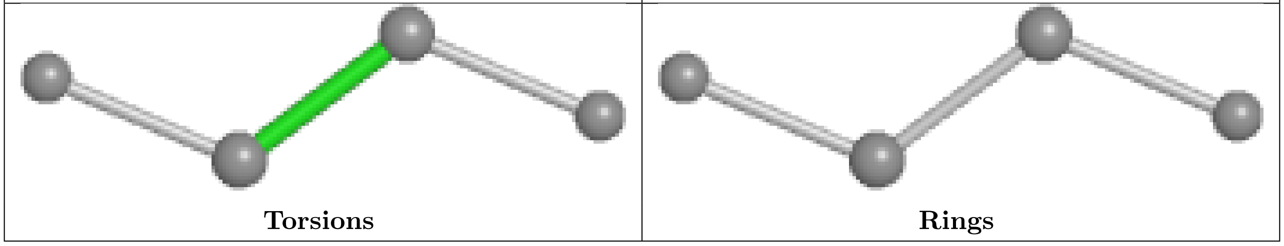
Torsions

Rings

Ligand EDO L 307

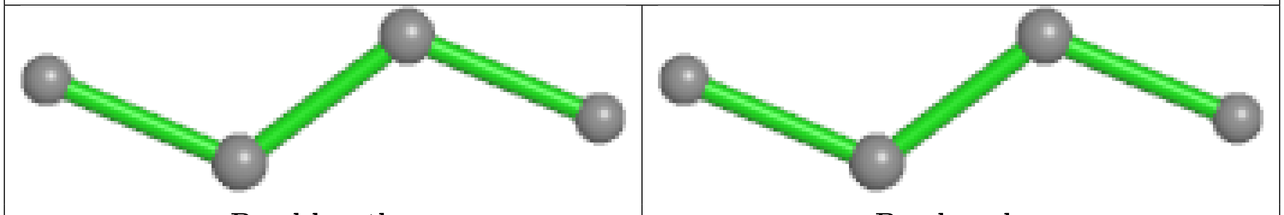


Bond lengths Bond angles

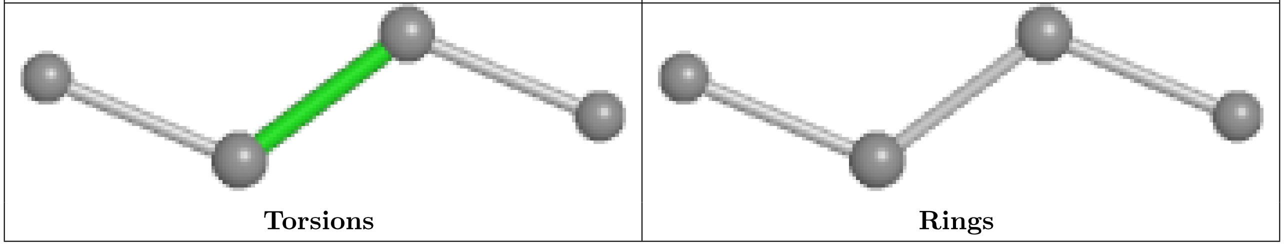


Torsions Rings

Ligand EDO G 306

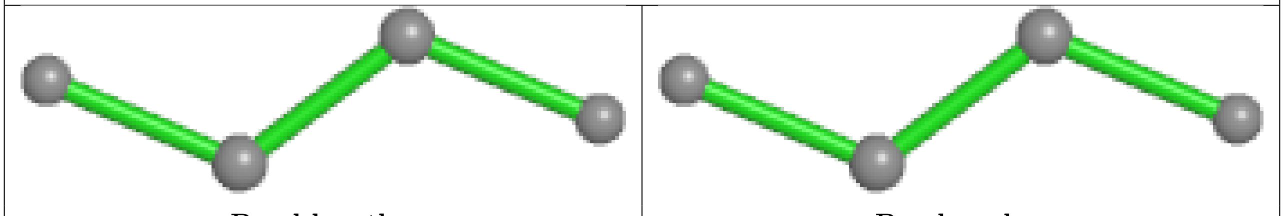


Bond lengths Bond angles

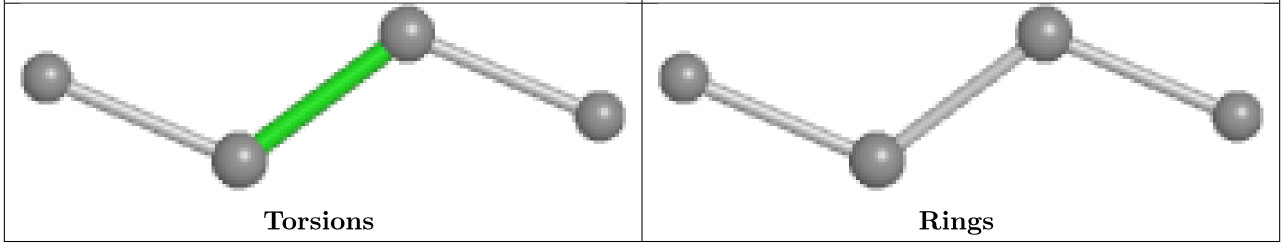


Torsions Rings

Ligand EDO F 303

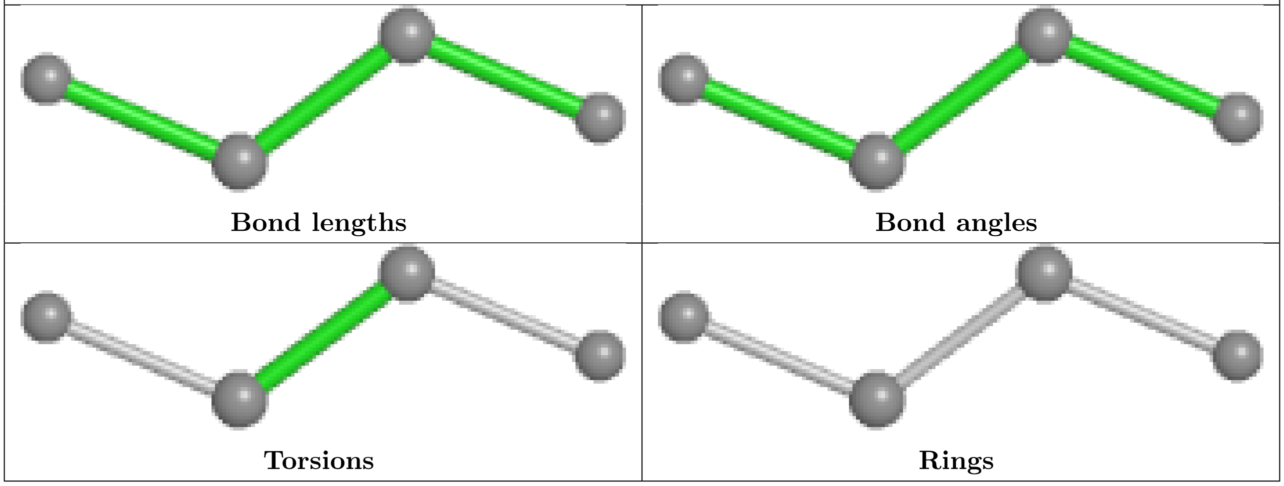


Bond lengths Bond angles



Torsions Rings

Ligand EDO H 305



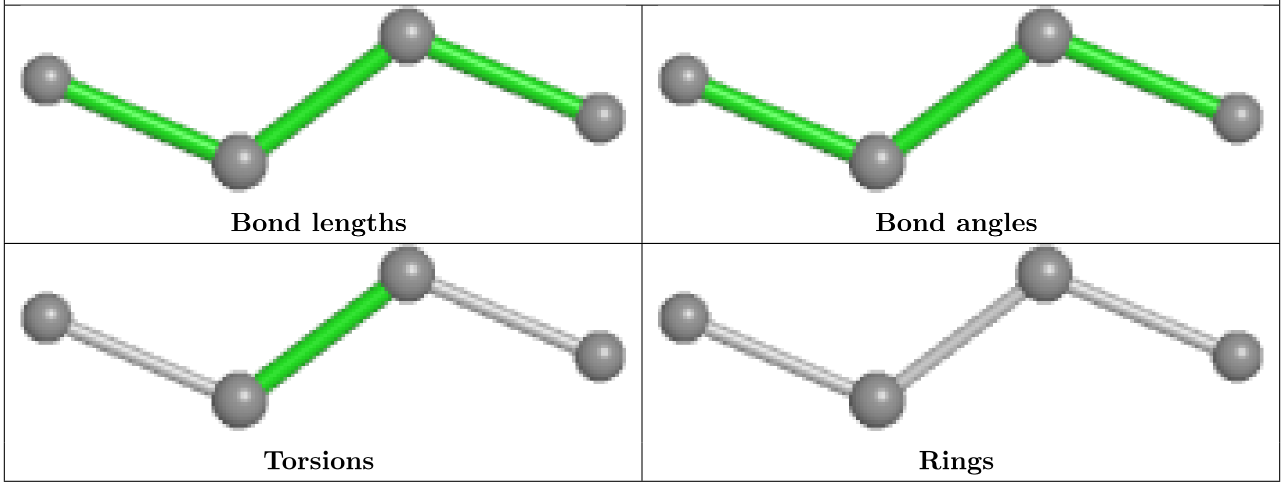
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO I 307



Bond lengths

Bond angles

Torsions

Rings

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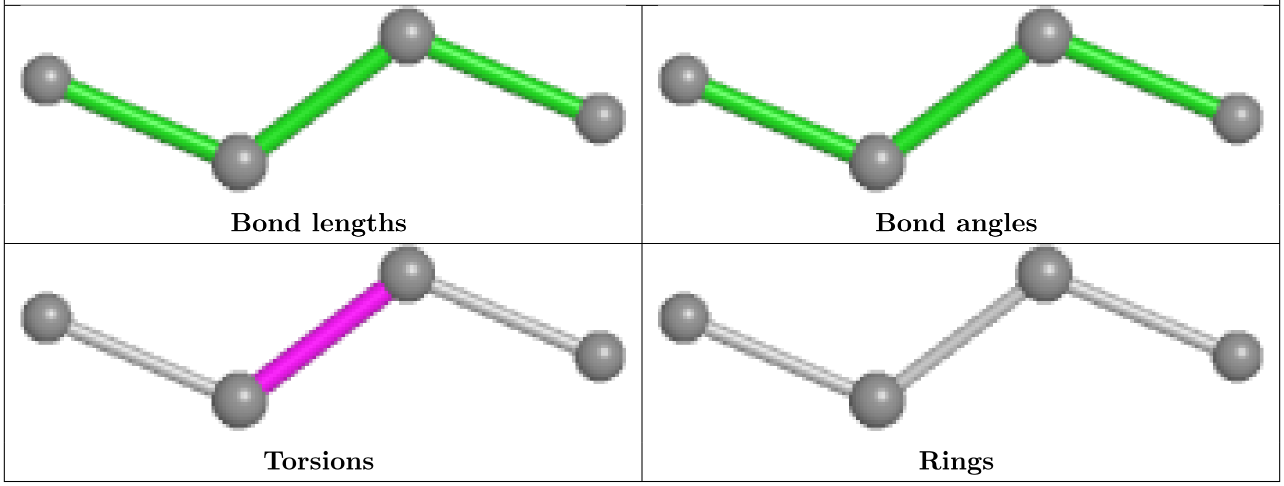

Bond lengths

Bond angles

Torsions

Rings

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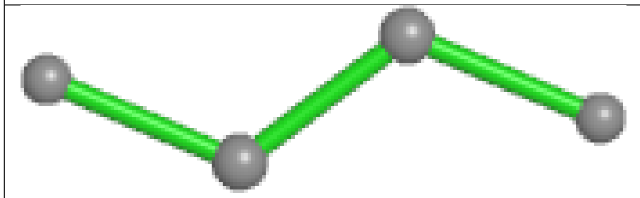
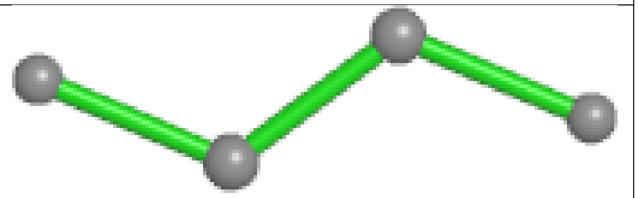
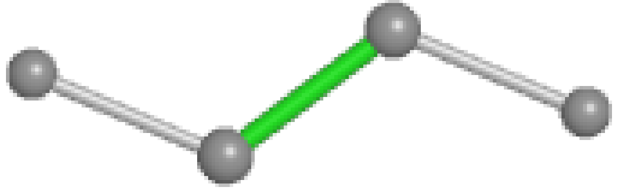


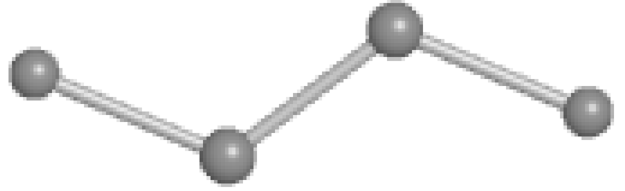
Bond lengths



Bond angles

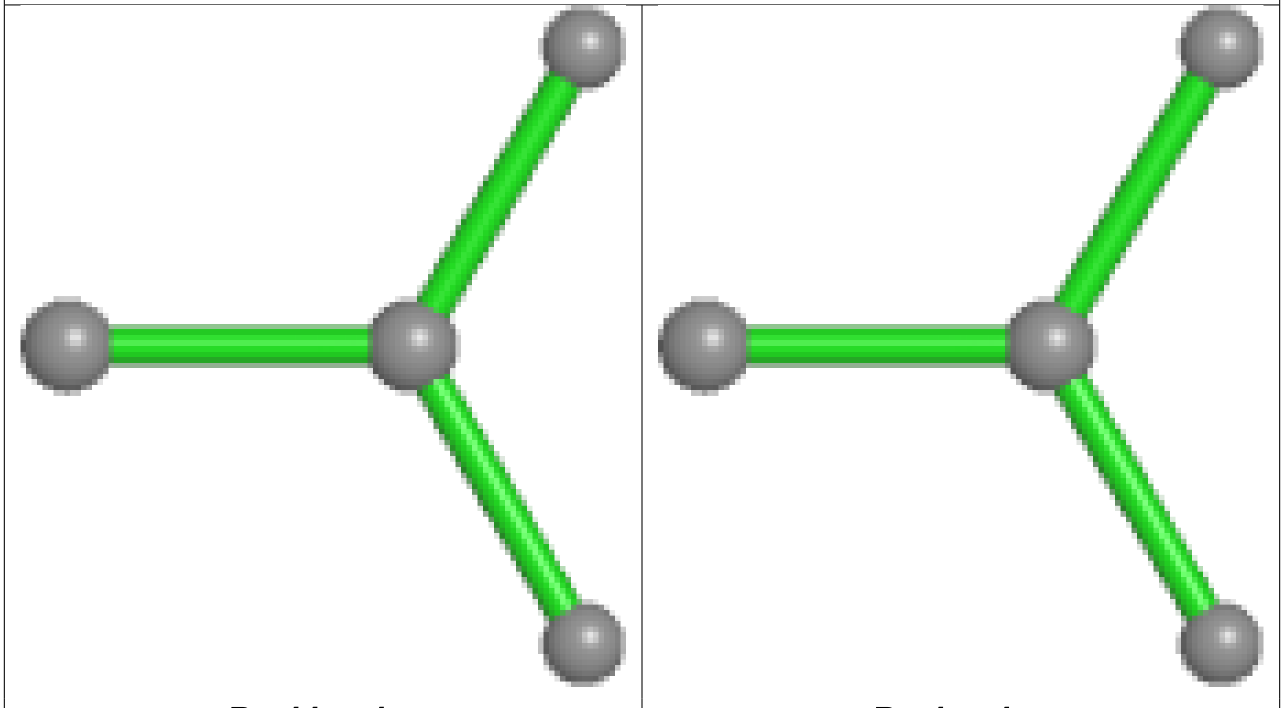


Torsions



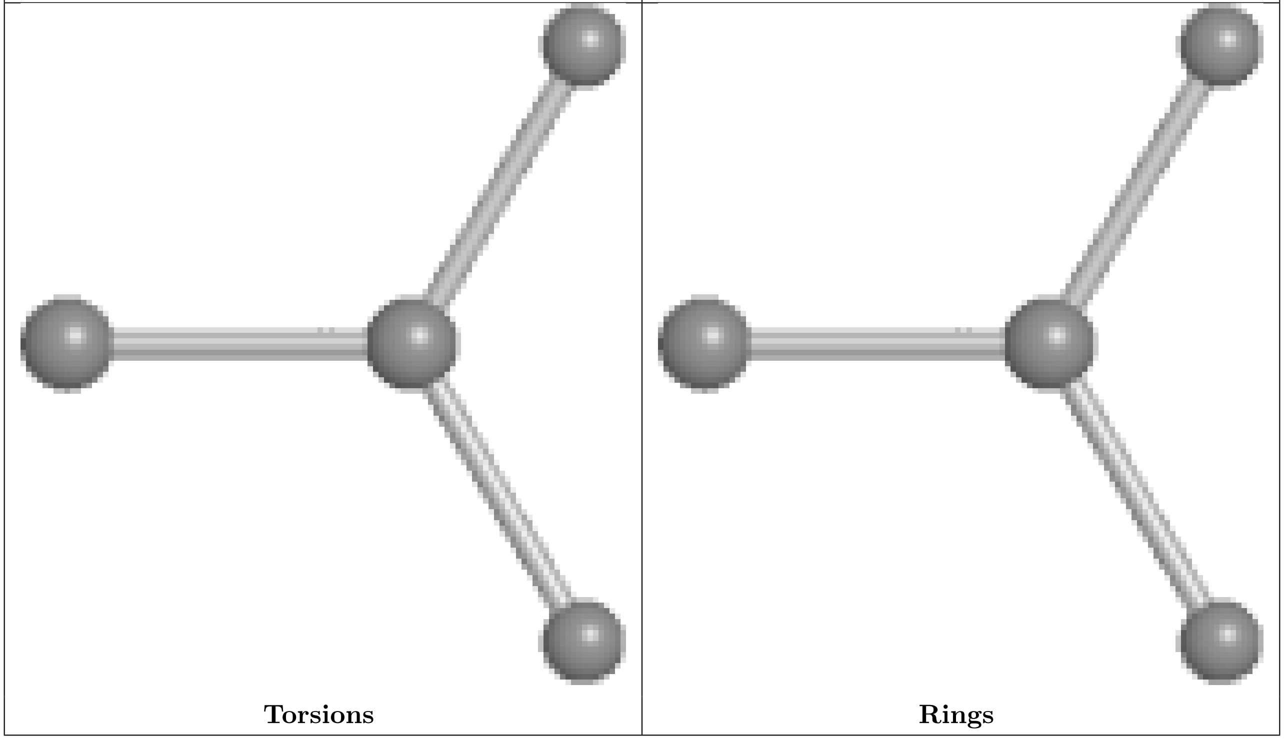
Rings

Ligand ACT B 302



Bond lengths

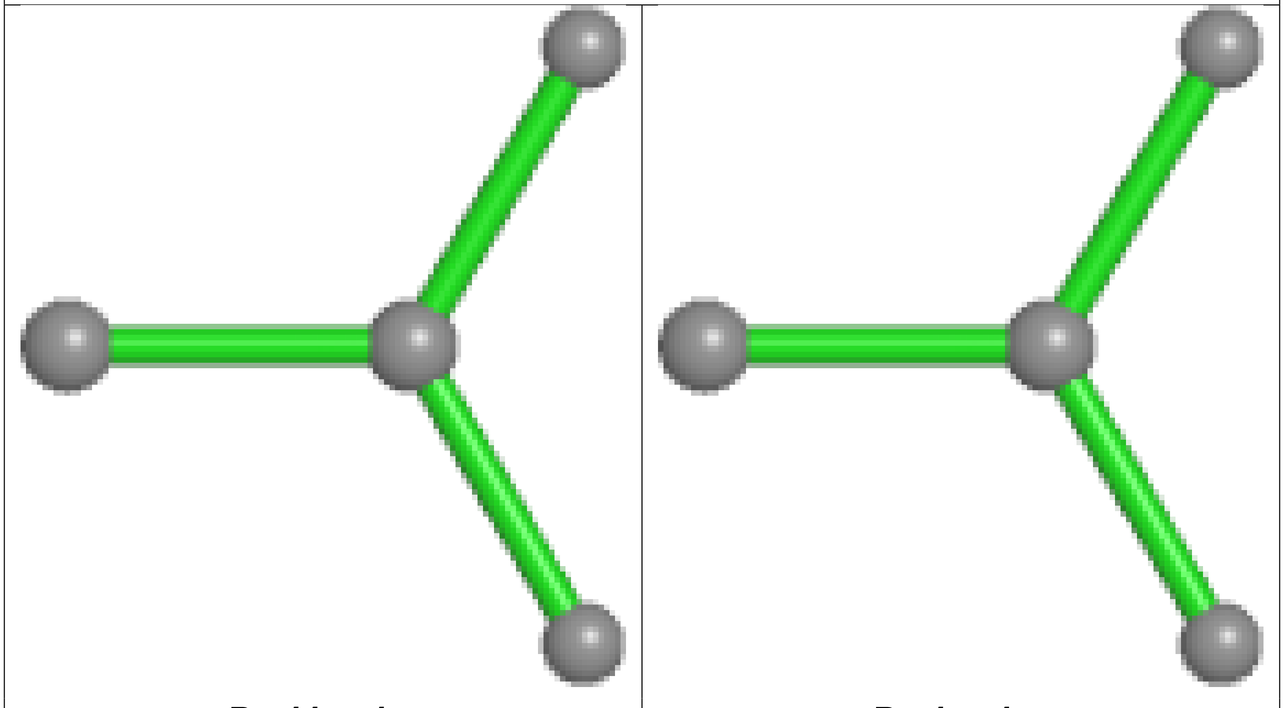
Bond angles



Torsions

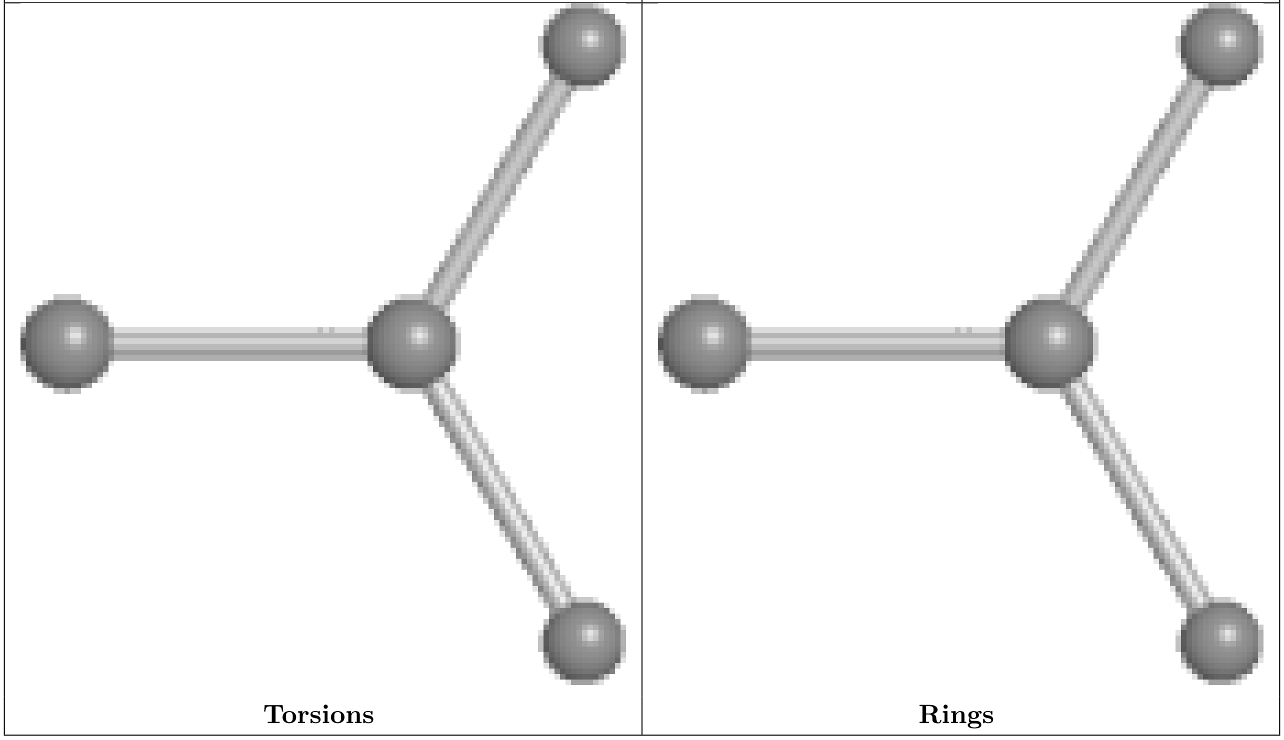
Rings

Ligand ACT L 303



Bond lengths

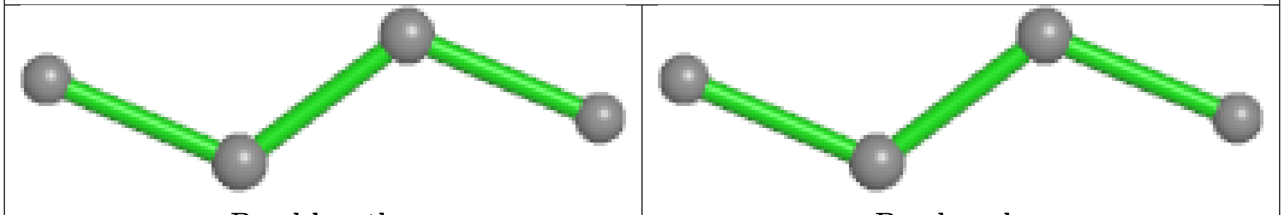
Bond angles



Torsions

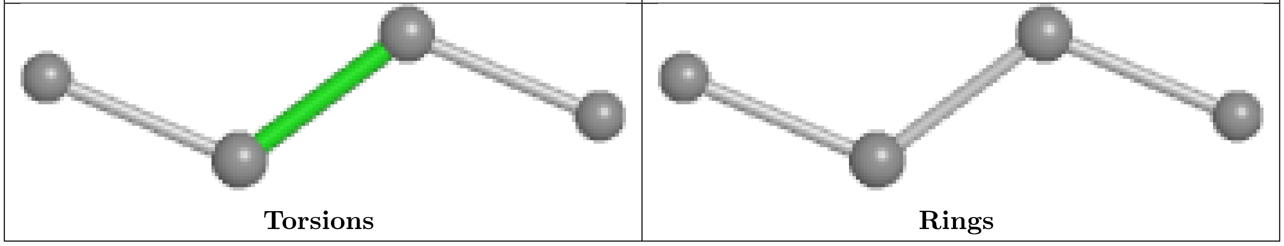
Rings

Ligand EDO L 306



Bond lengths

Bond angles



Torsions

Rings

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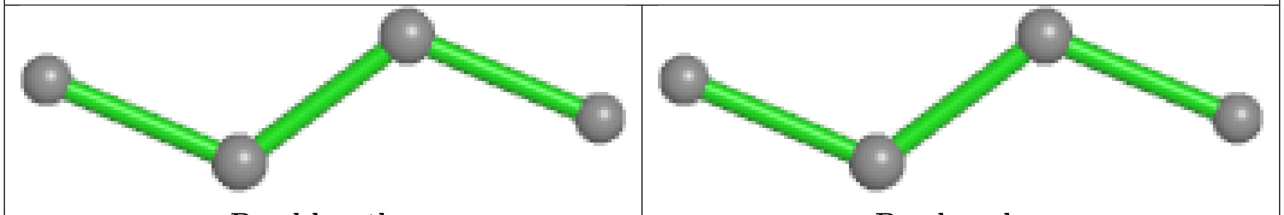
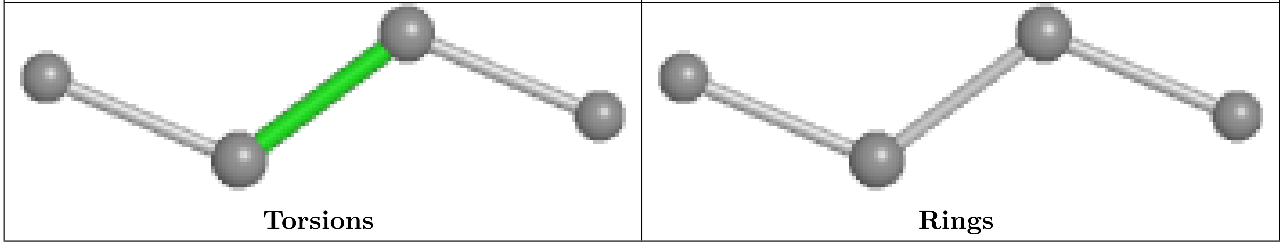


Bond lengths

Bond angles



Torsions

Rings

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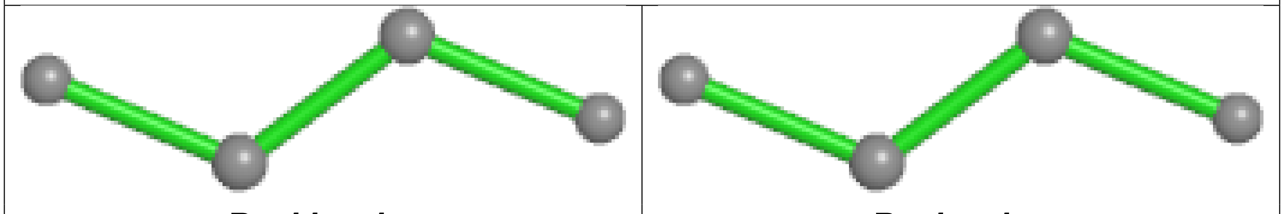
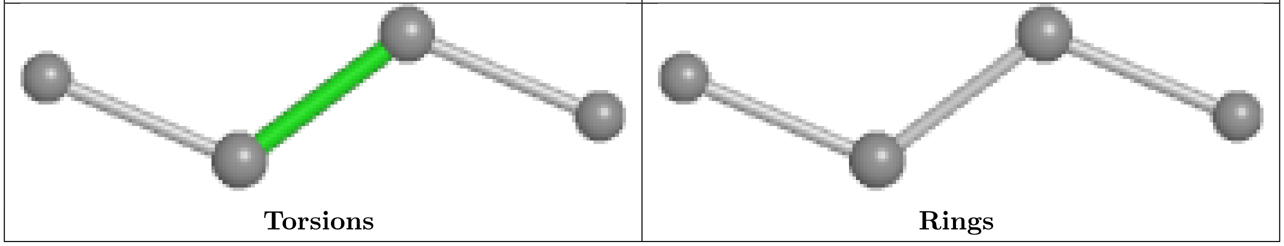


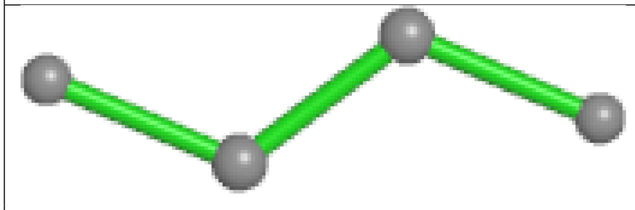
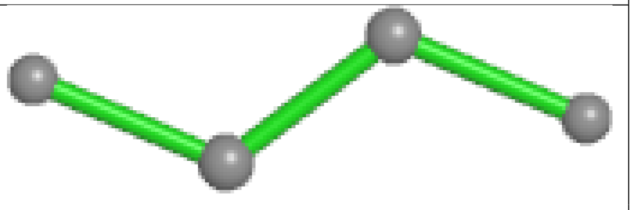
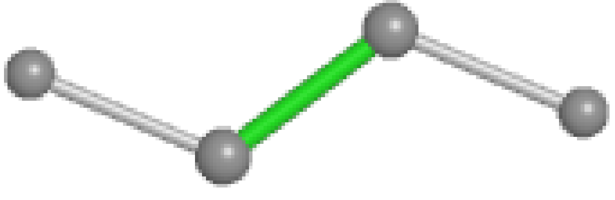
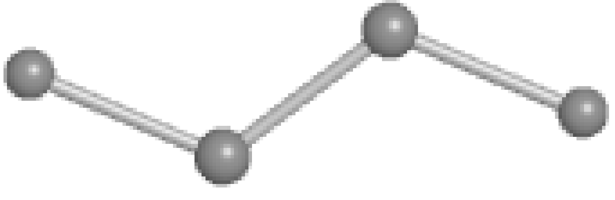
Bond lengths

Bond angles

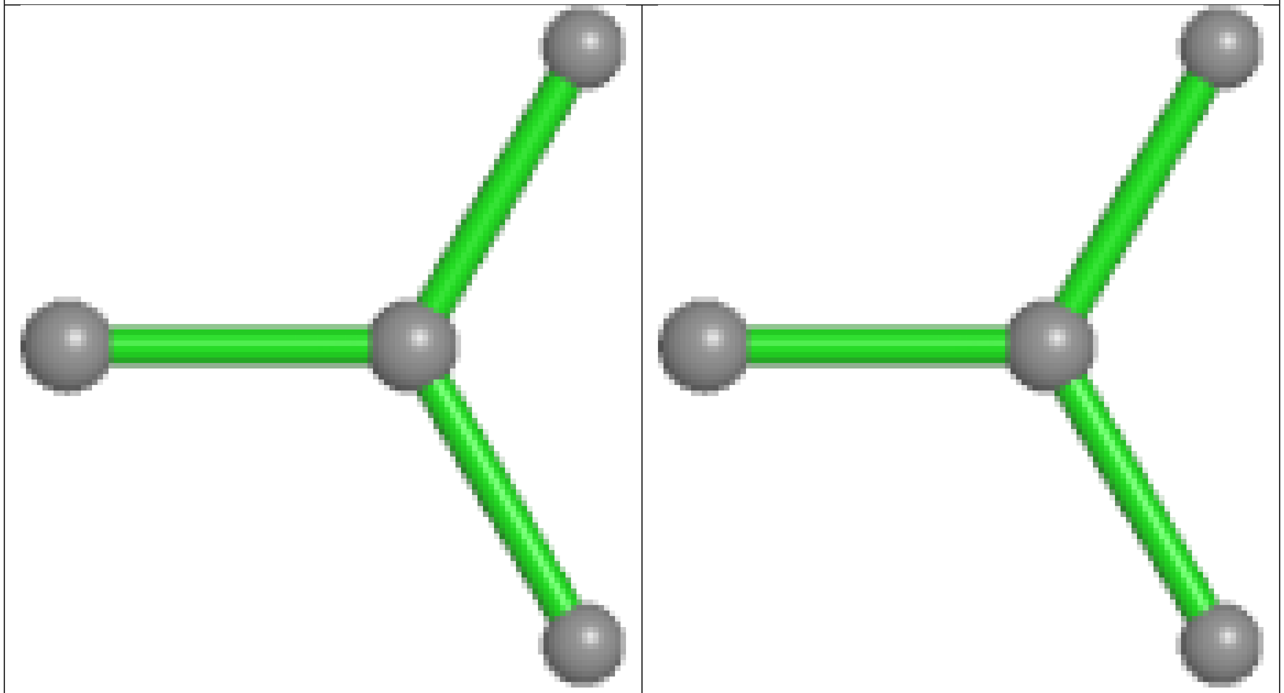


Torsions

Rings

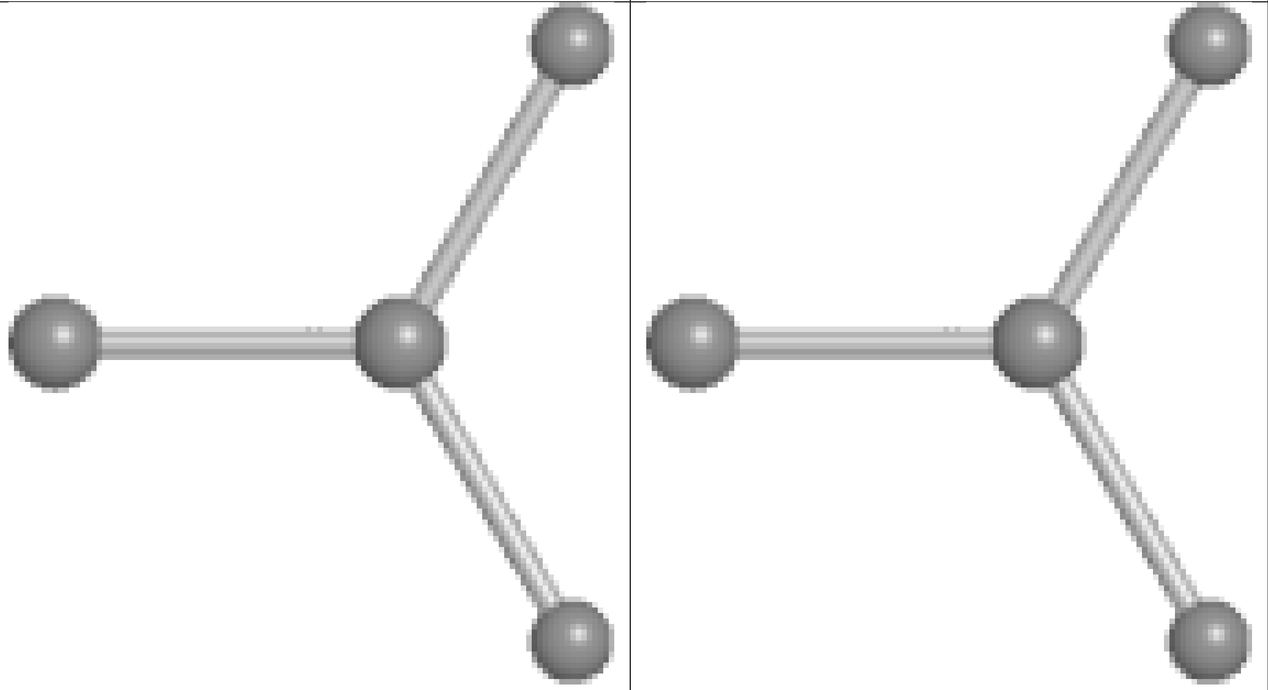
Ligand EDO J 310	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand ACT B 303



Bond lengths

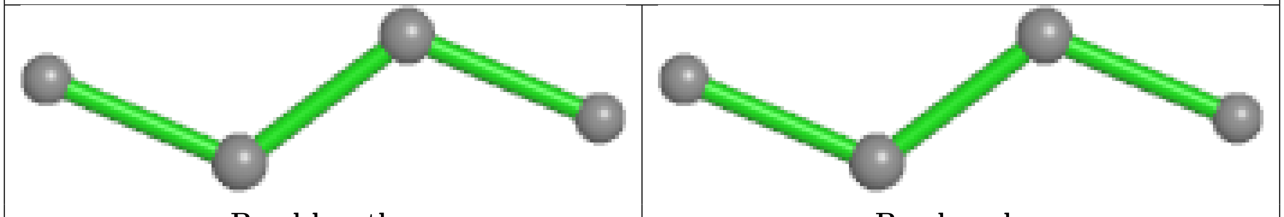
Bond angles



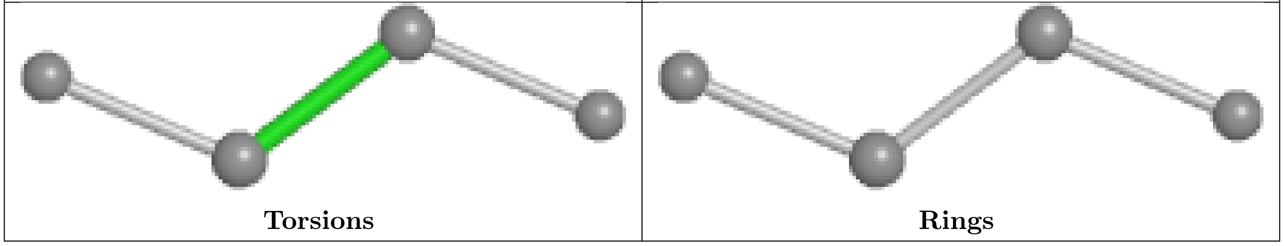
Torsions

Rings

Ligand EDO K 302

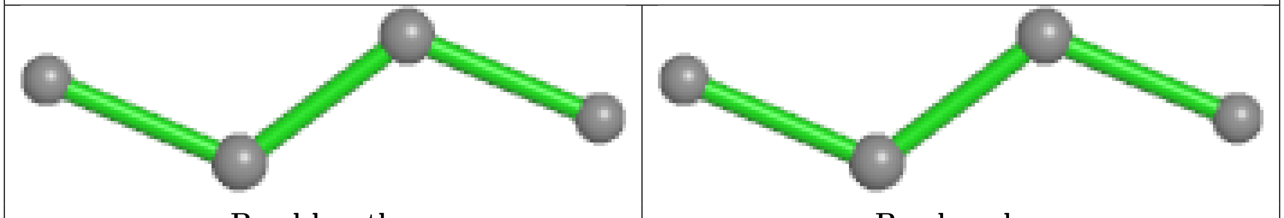


Bond lengths Bond angles

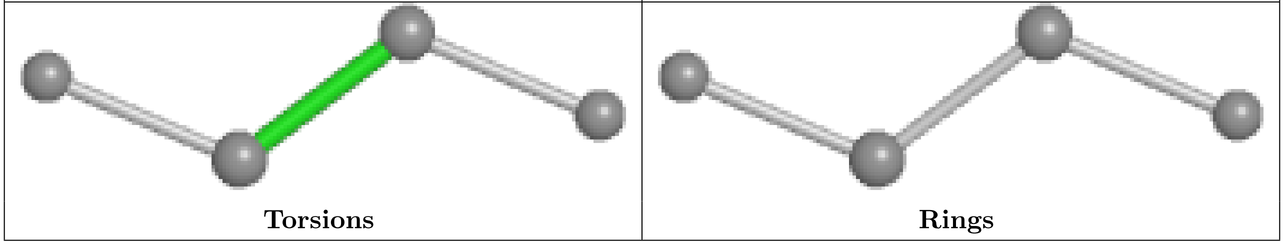


Torsions Rings

Ligand EDO I 308

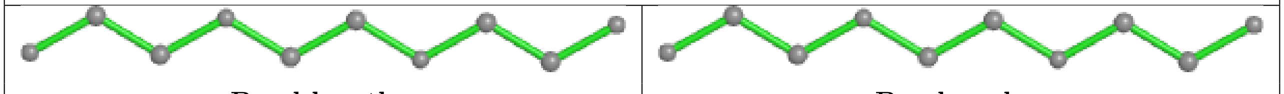


Bond lengths Bond angles

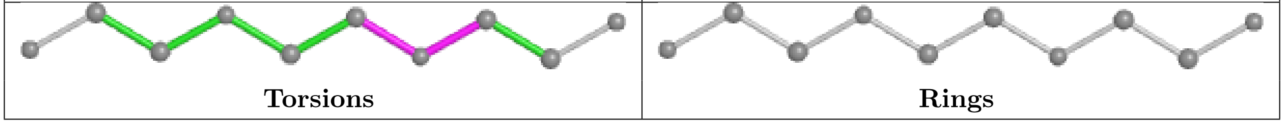


Torsions Rings

Ligand PGE C 301

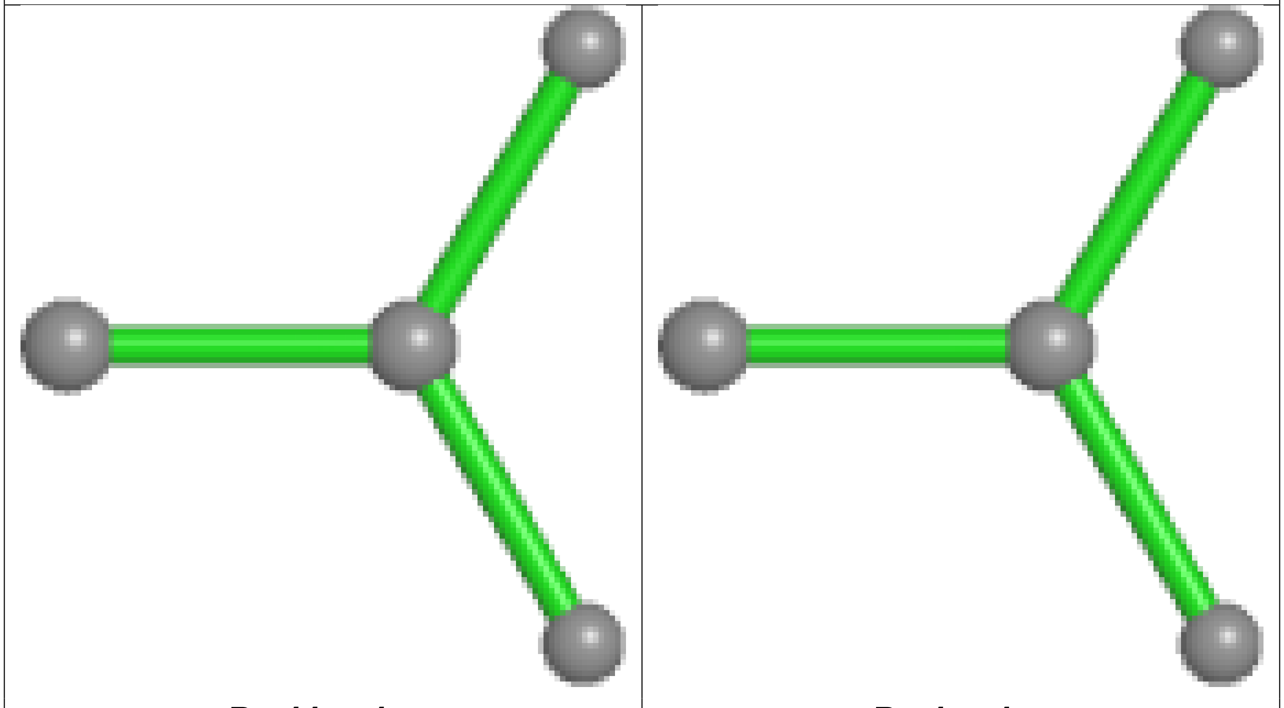


Bond lengths Bond angles



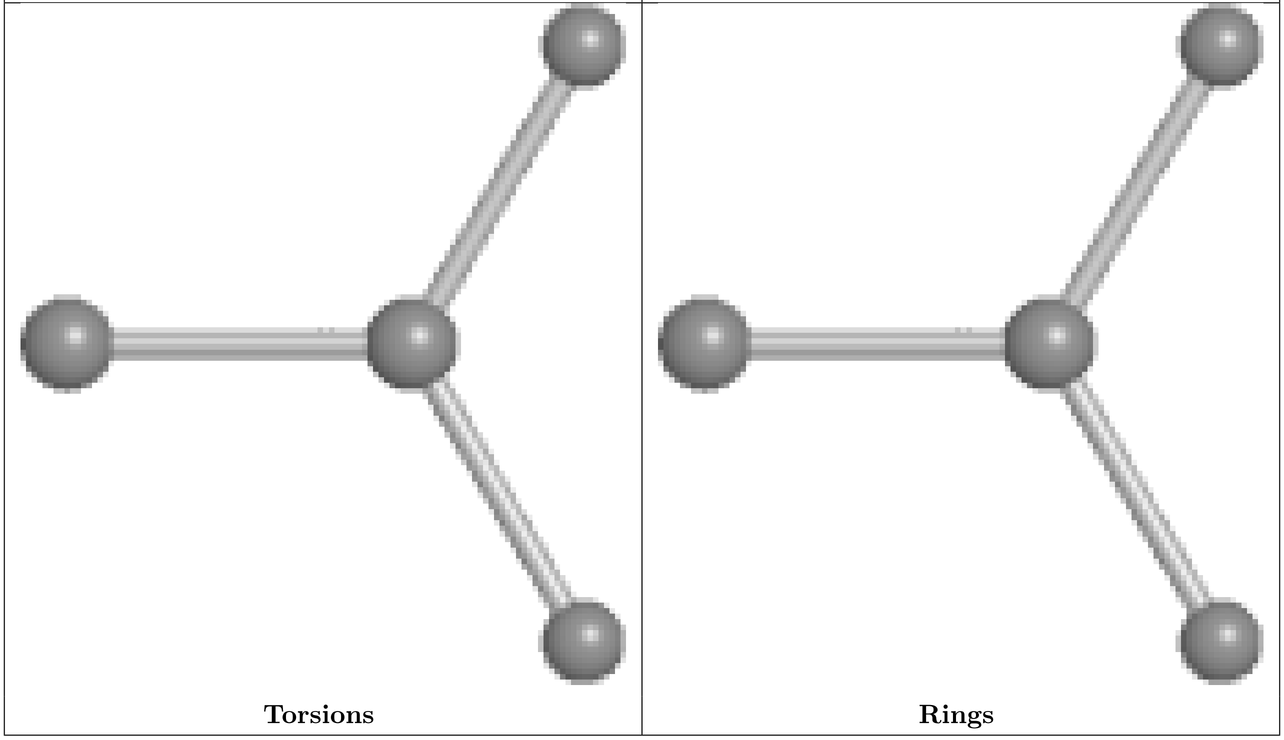
Torsions Rings

Ligand ACT H 301



Bond lengths

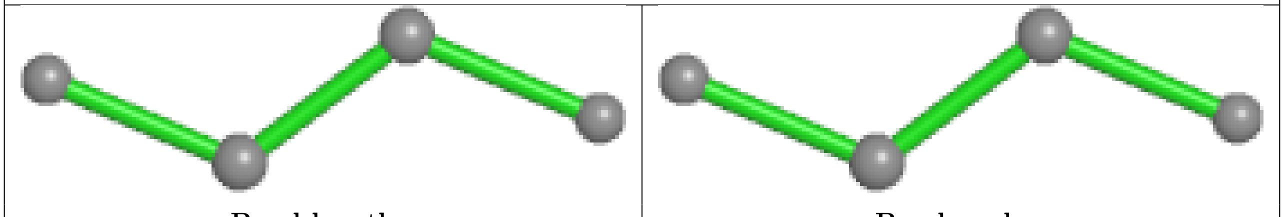
Bond angles

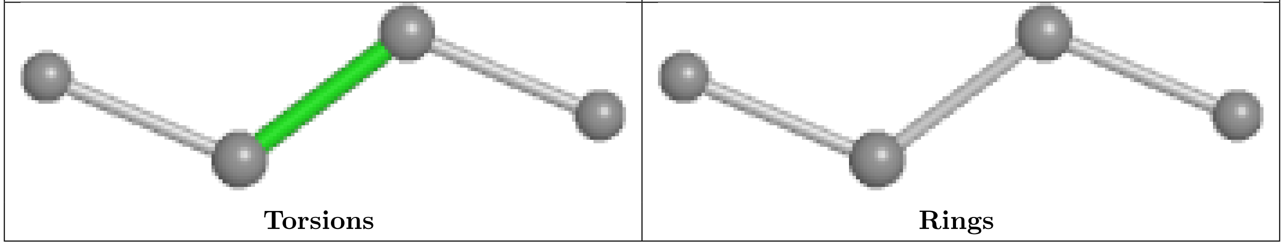


Torsions

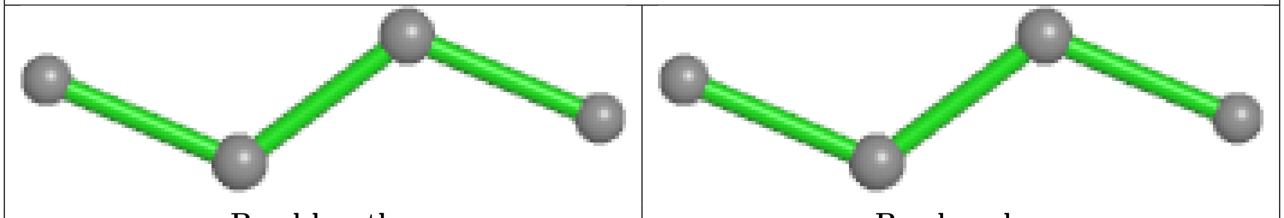
Rings

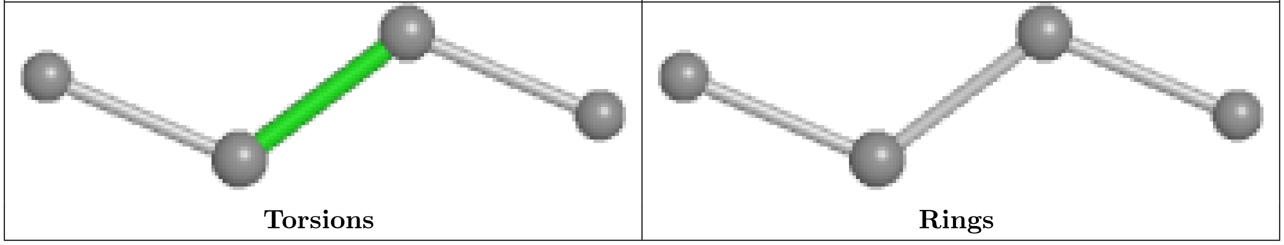
Ligand EDO C 307


Bond lengths Bond angles

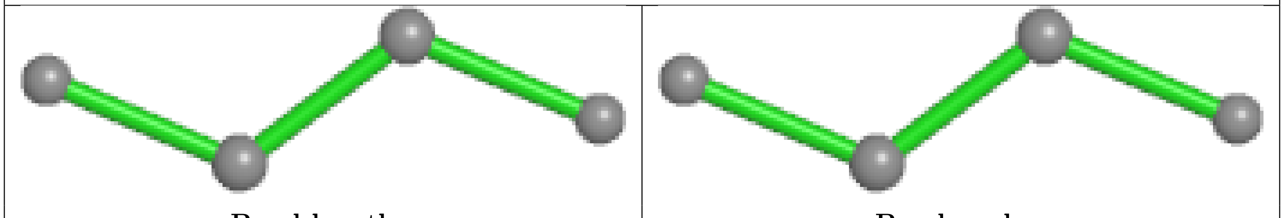

Torsions Rings

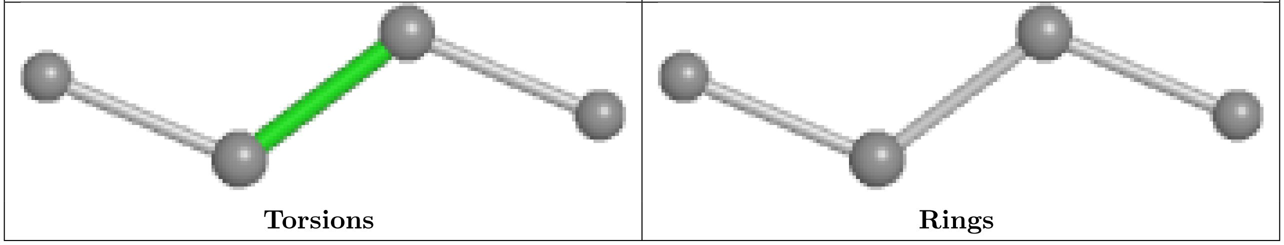
Ligand EDO B 307


Bond lengths Bond angles

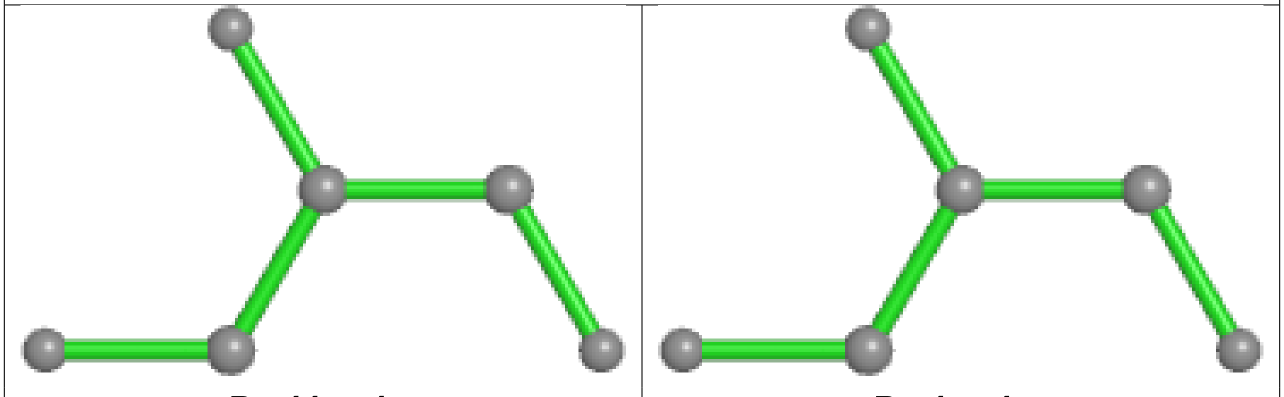

Torsions Rings

Ligand EDO A 308


Bond lengths Bond angles

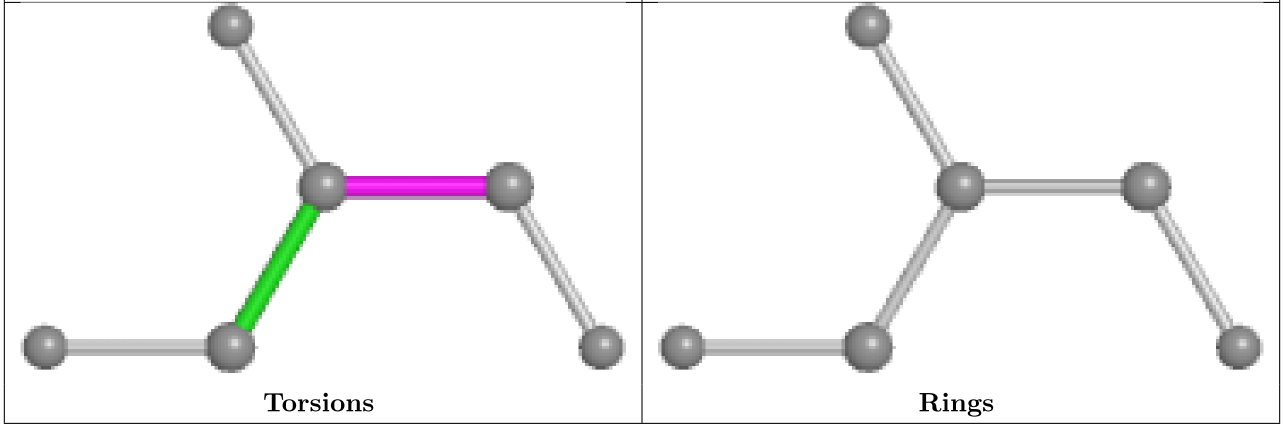

Torsions Rings

Ligand GOL I 302



Bond lengths

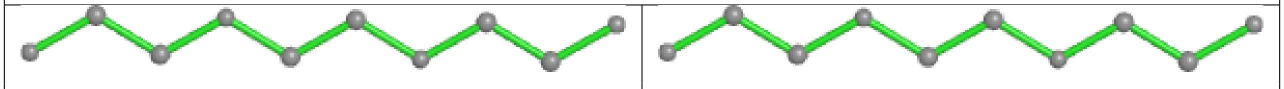
Bond angles



Torsions

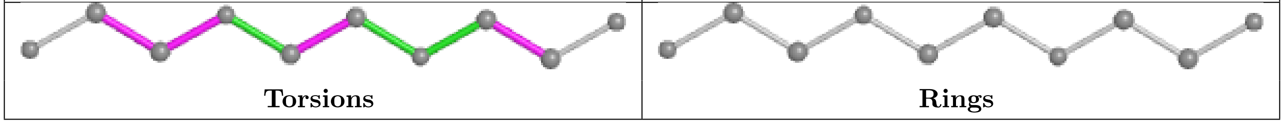
Rings

Ligand PGE D 301



Bond lengths

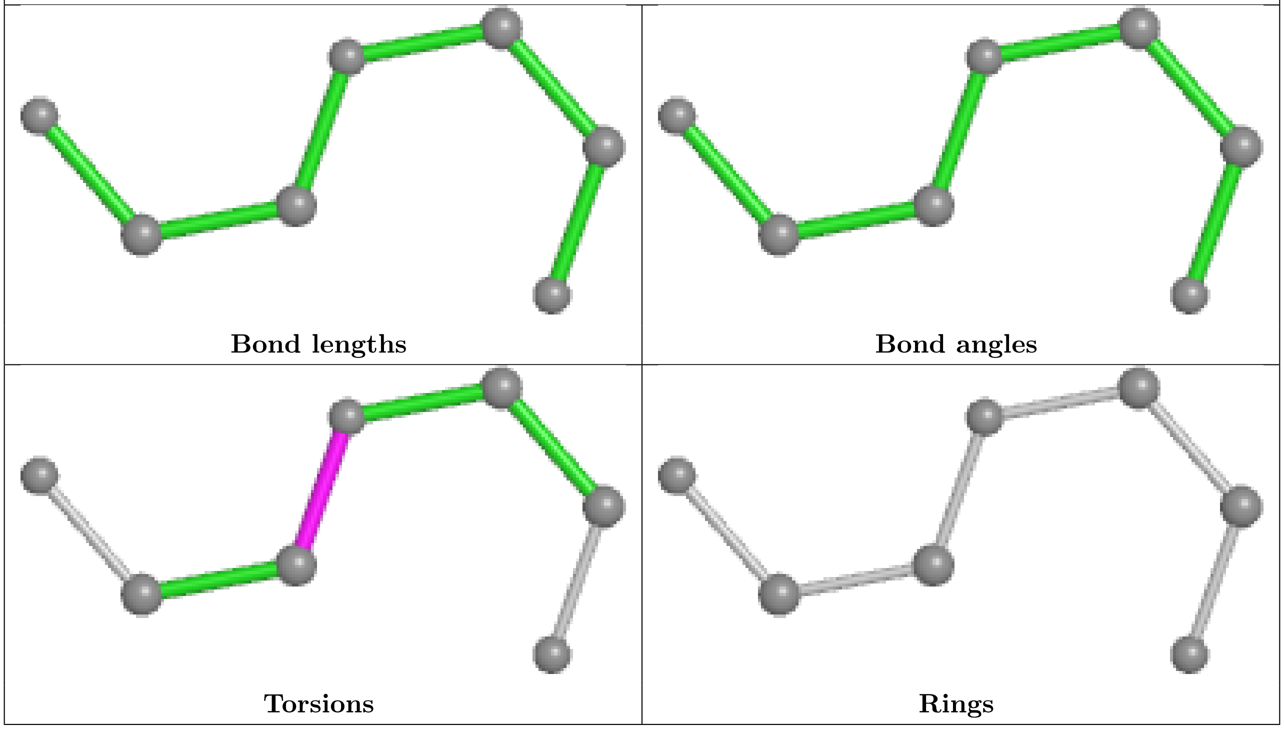
Bond angles



Torsions

Rings

Ligand PEG L 309



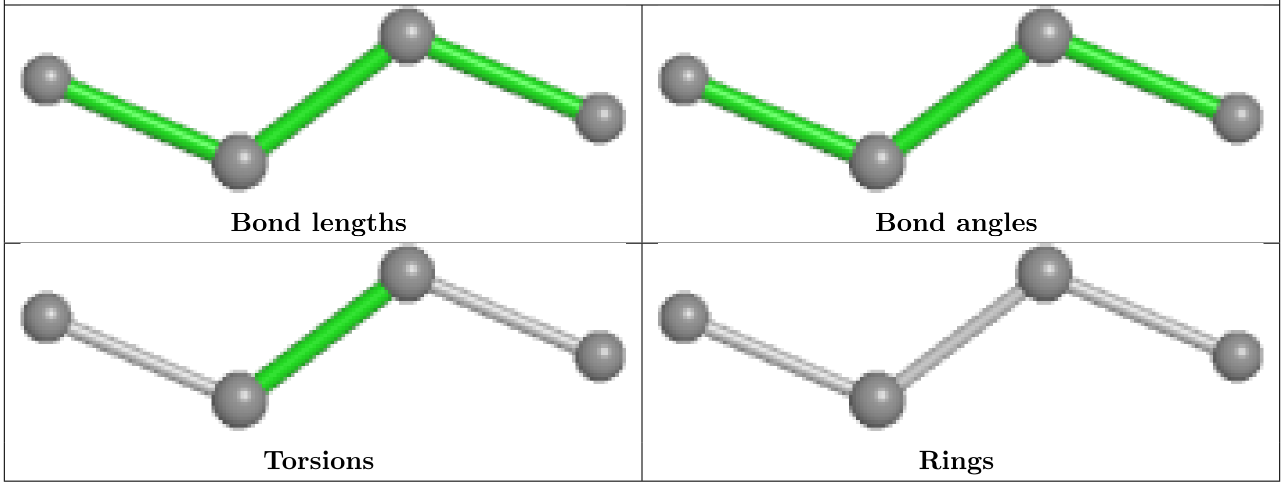
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO G 302



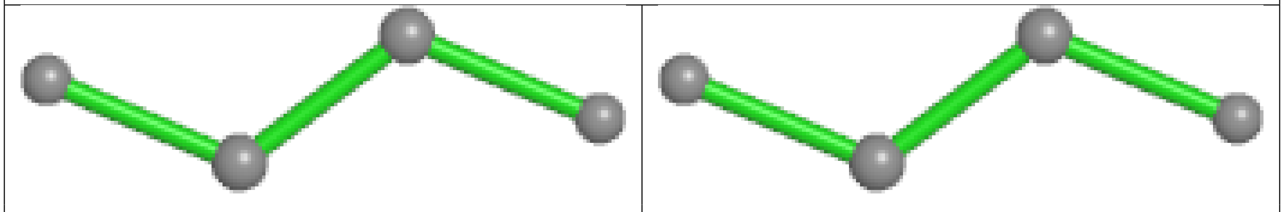
Bond lengths

Bond angles

Torsions

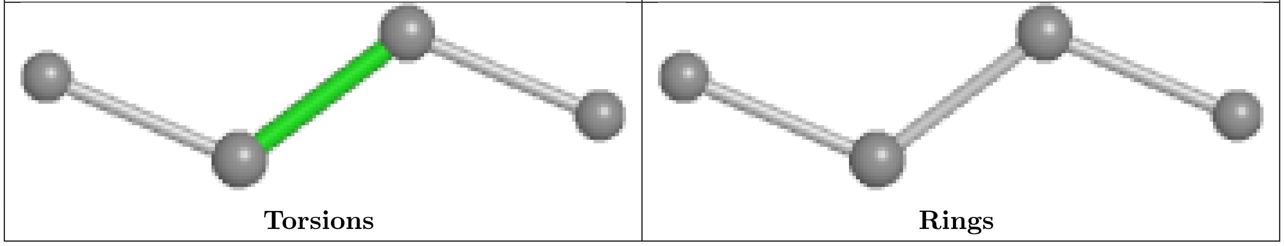
Rings

Ligand EDO D 303



Bond lengths

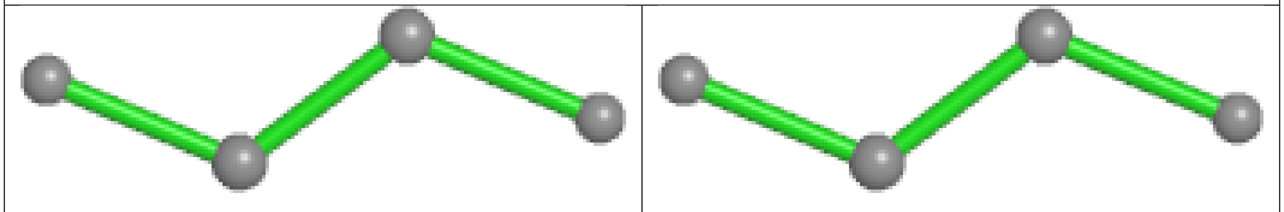
Bond angles



Torsions

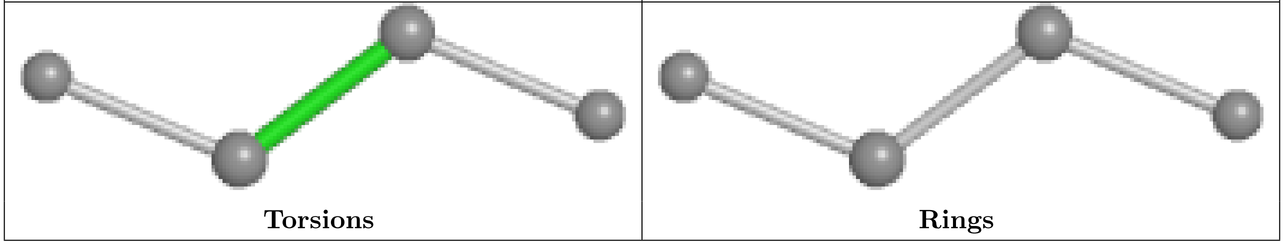
Rings

Ligand EDO J 309



Bond lengths

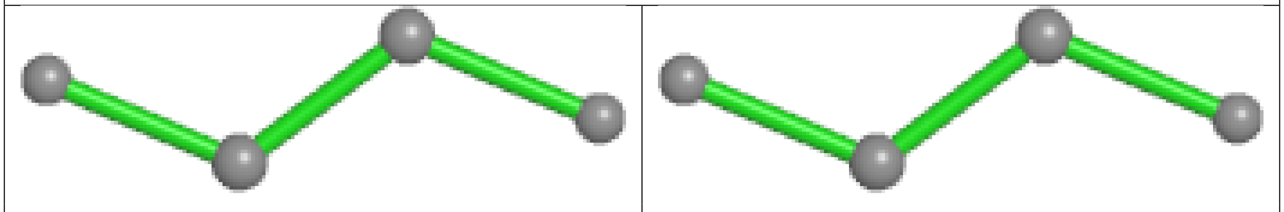
Bond angles



Torsions

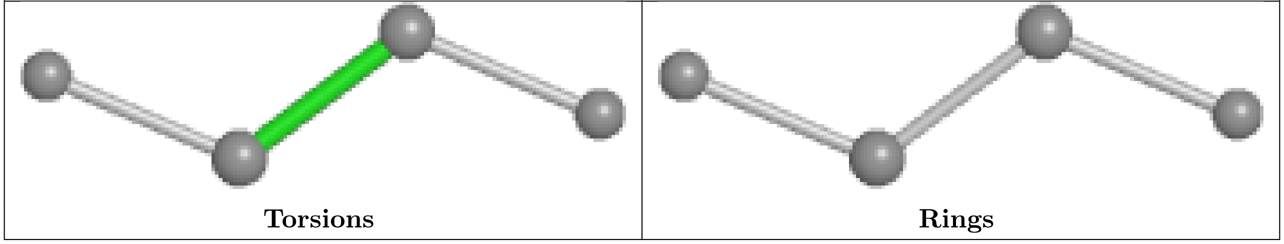
Rings

Ligand EDO A 305



Bond lengths

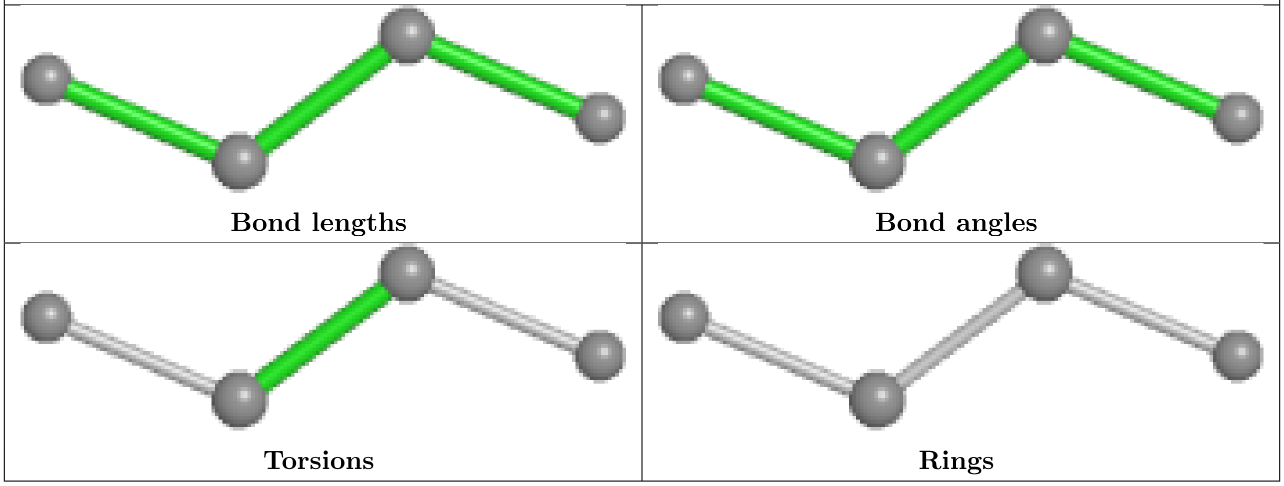
Bond angles



Torsions

Rings

Ligand EDO E 306



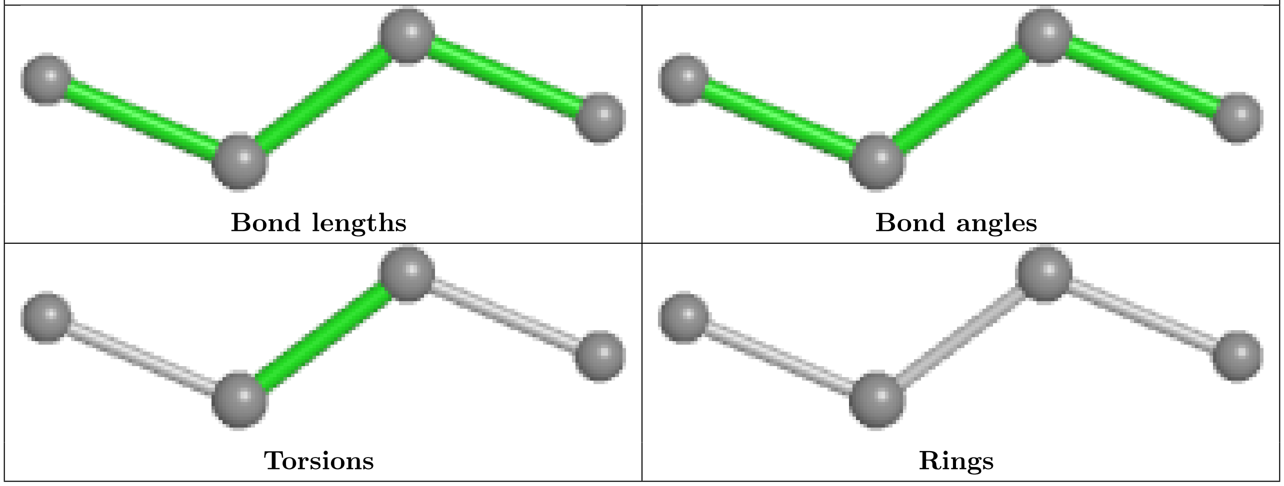
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO J 306



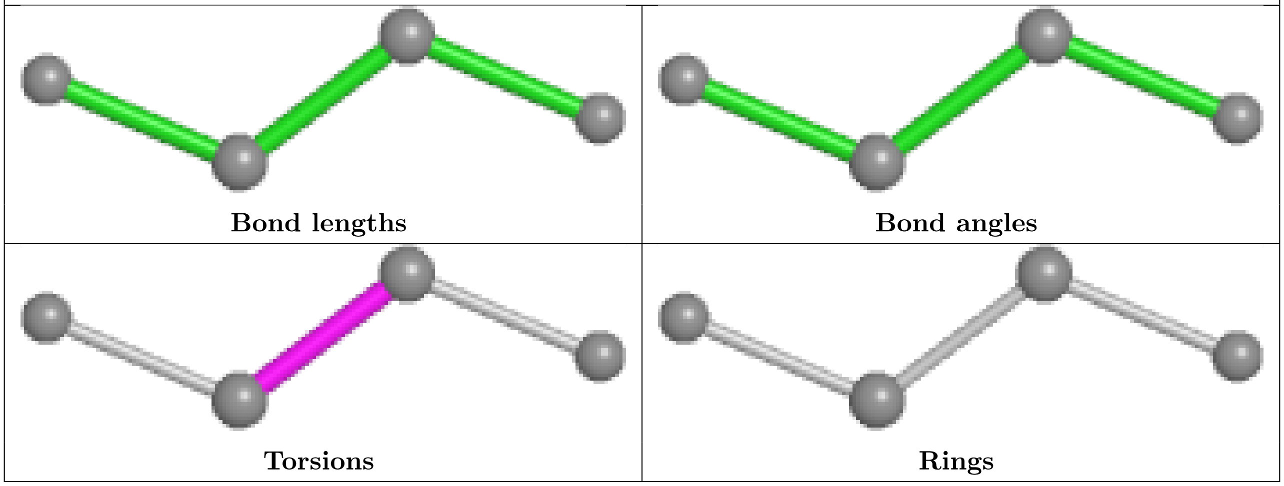
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO G 303



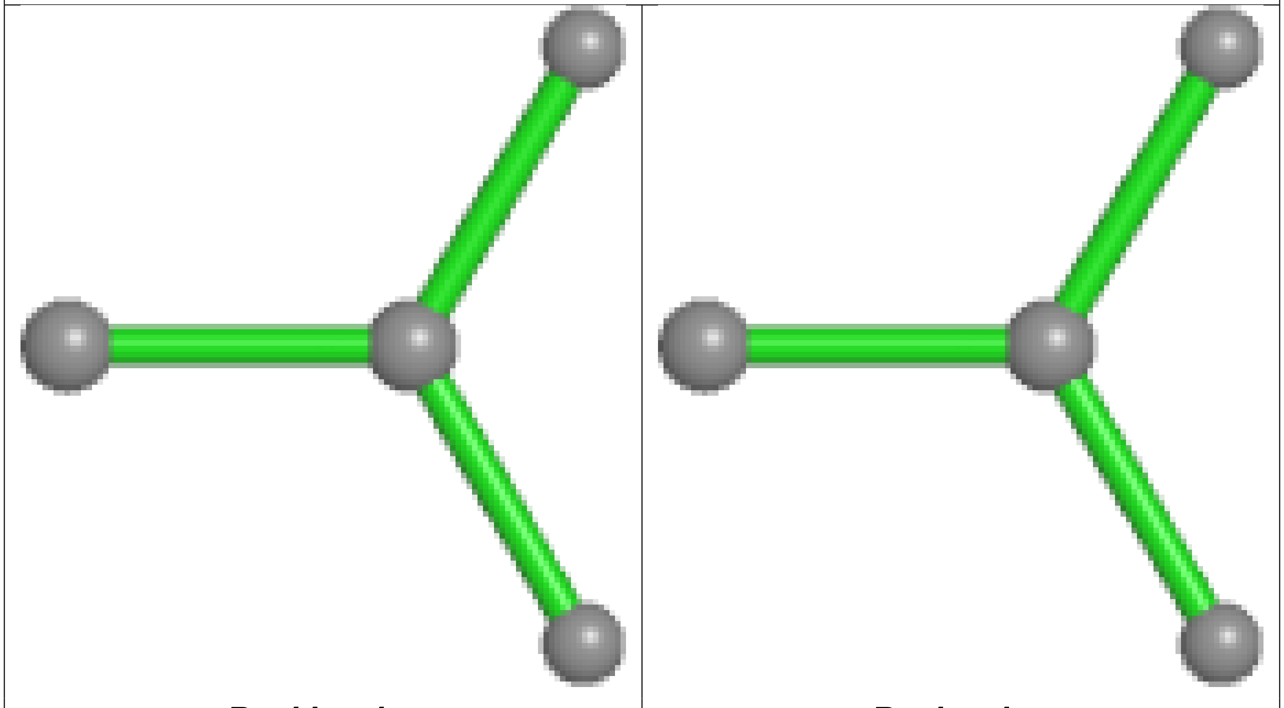
Bond lengths

Bond angles

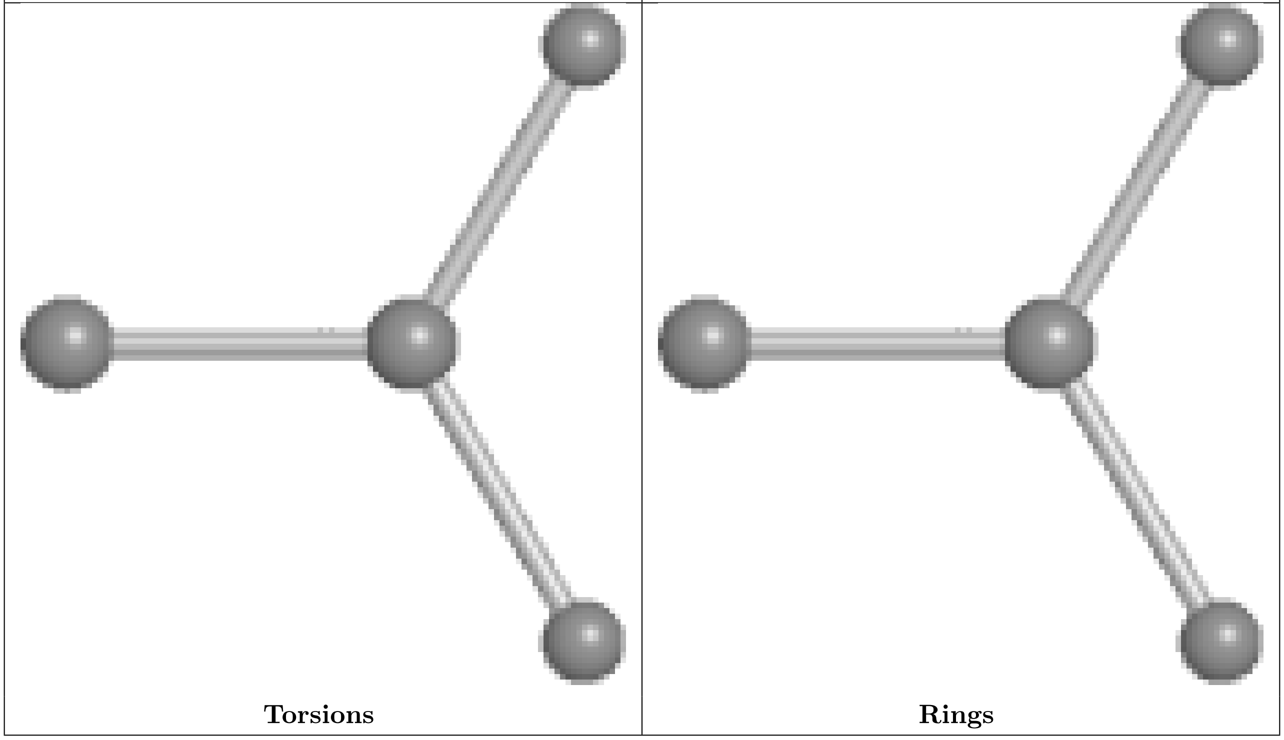
Torsions

Rings

Ligand ACT J 303

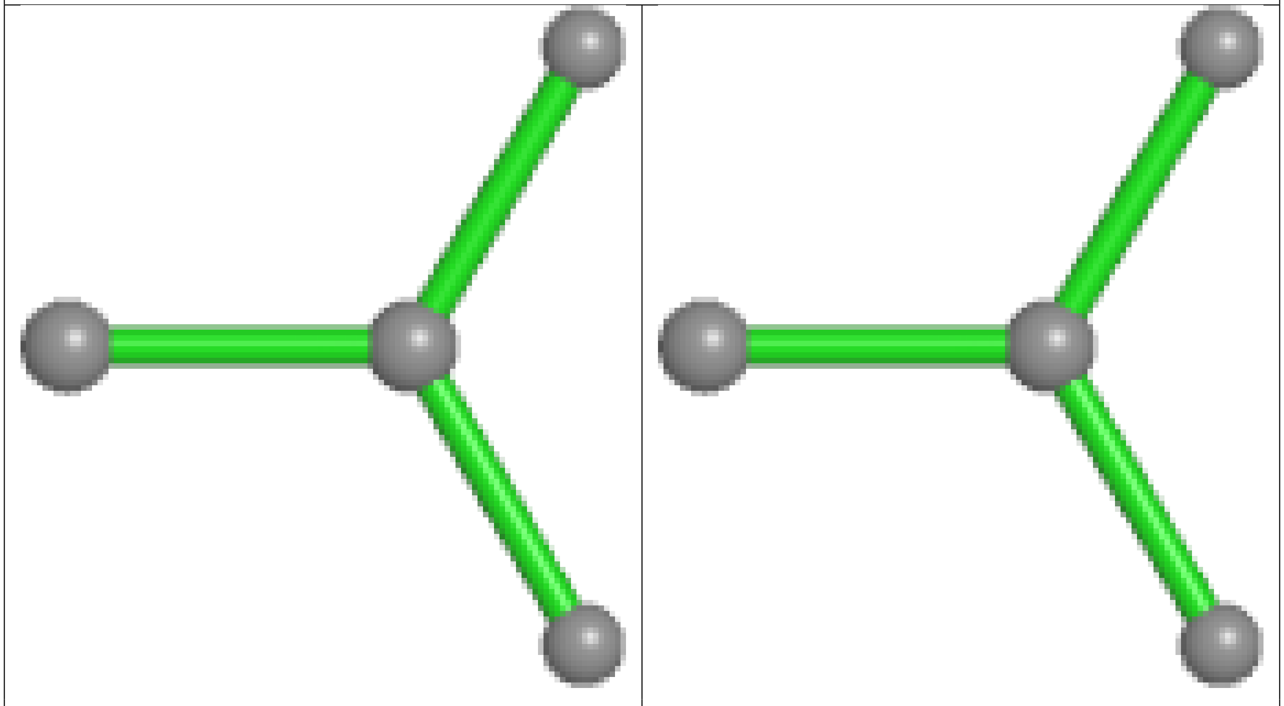


Bond lengths **Bond angles**



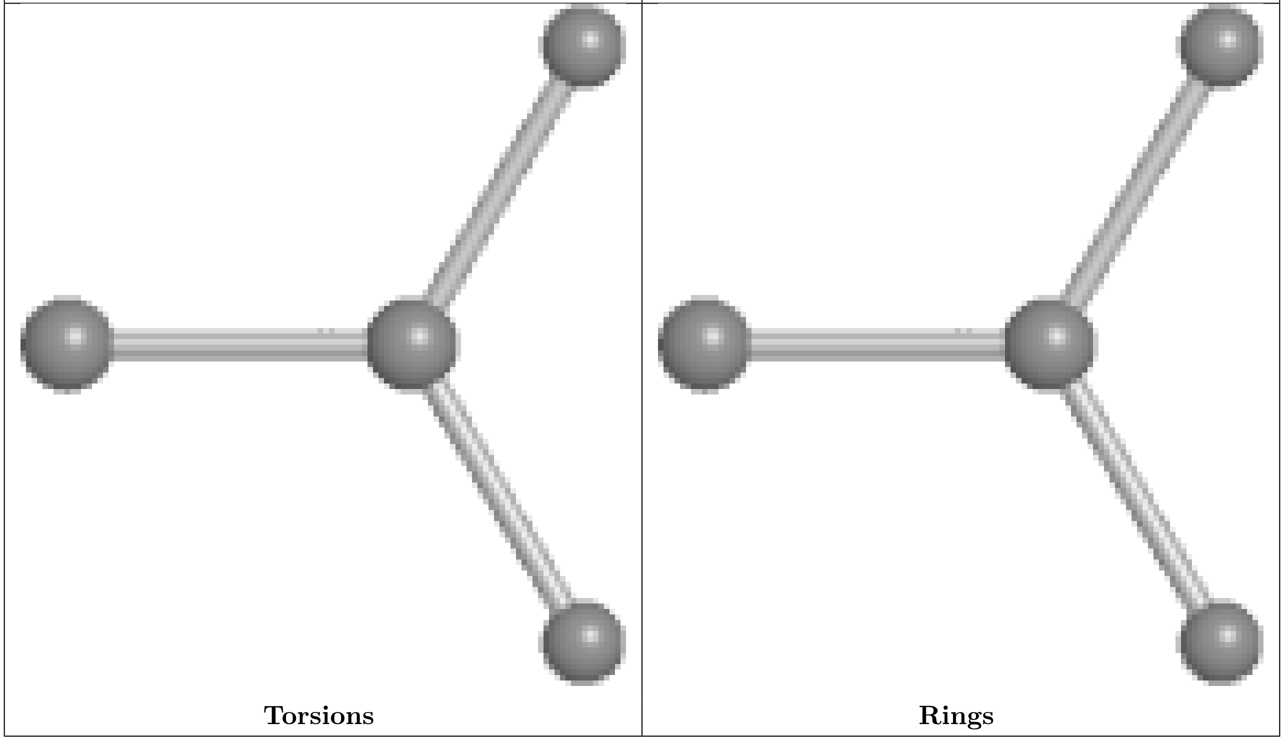
Torsions **Rings**

Ligand ACT H 303



Bond lengths

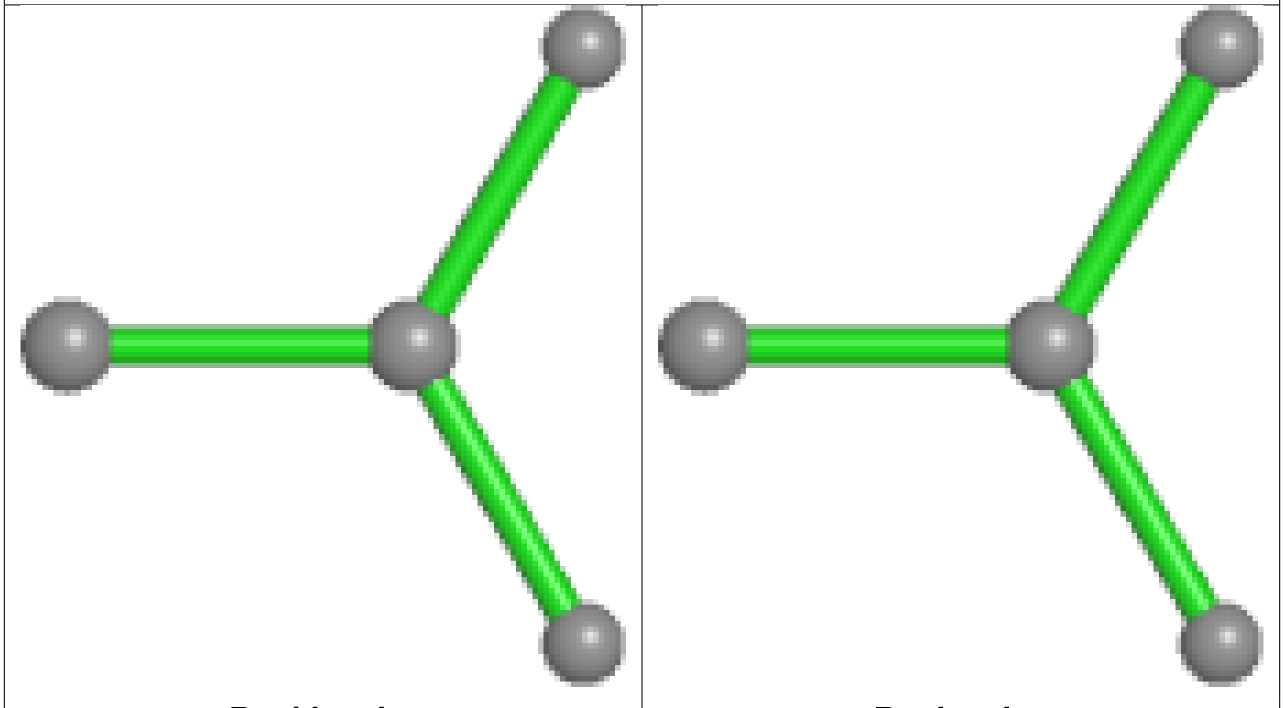
Bond angles



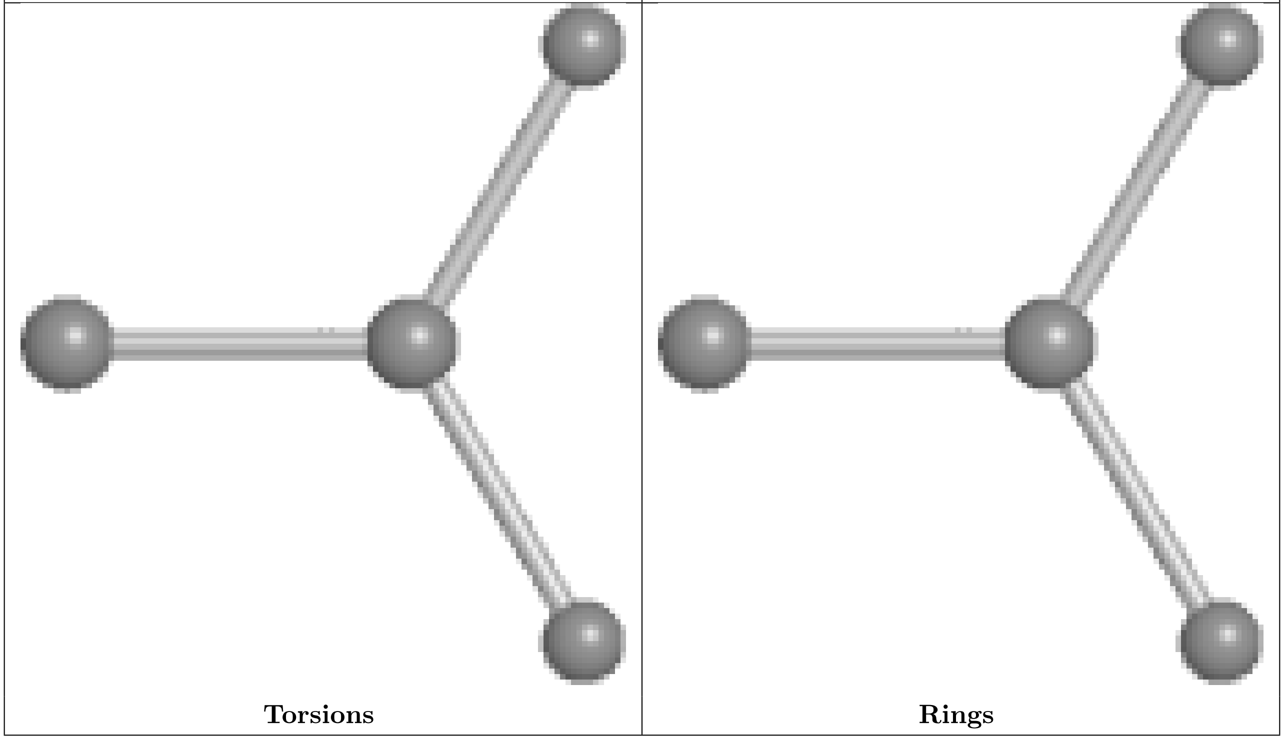
Torsions

Rings

Ligand ACT A 303

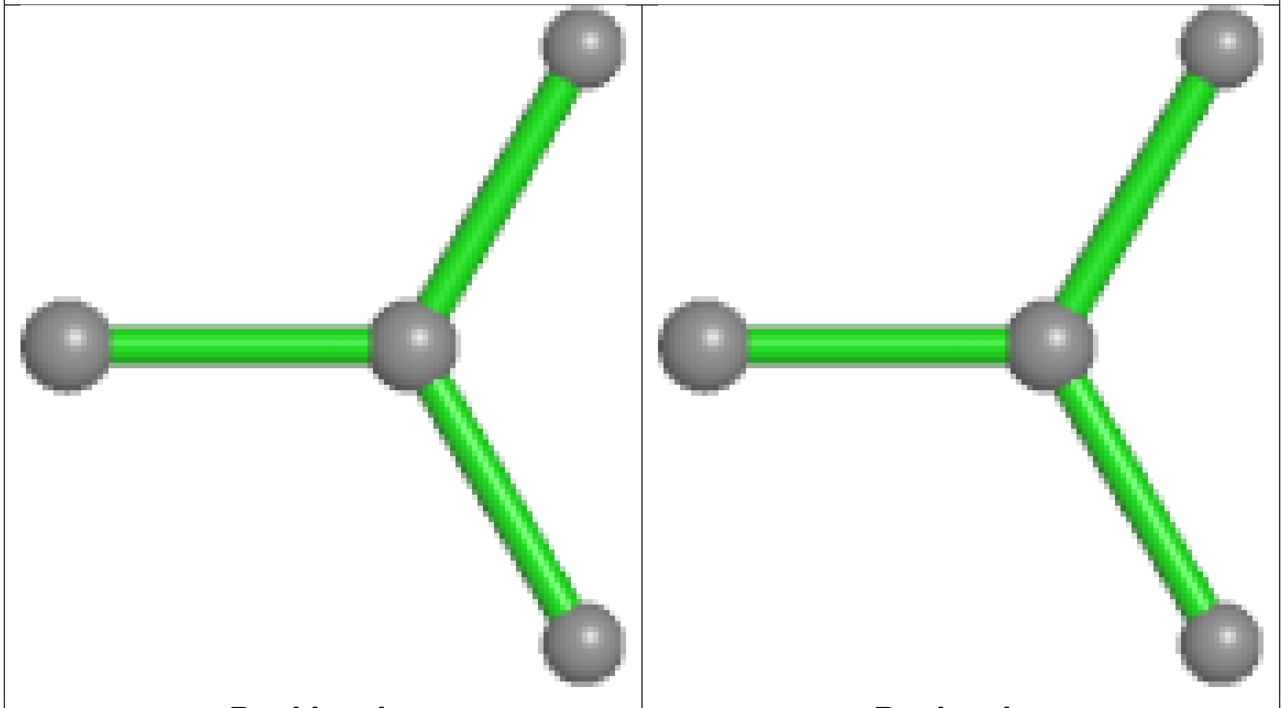


Bond lengths Bond angles

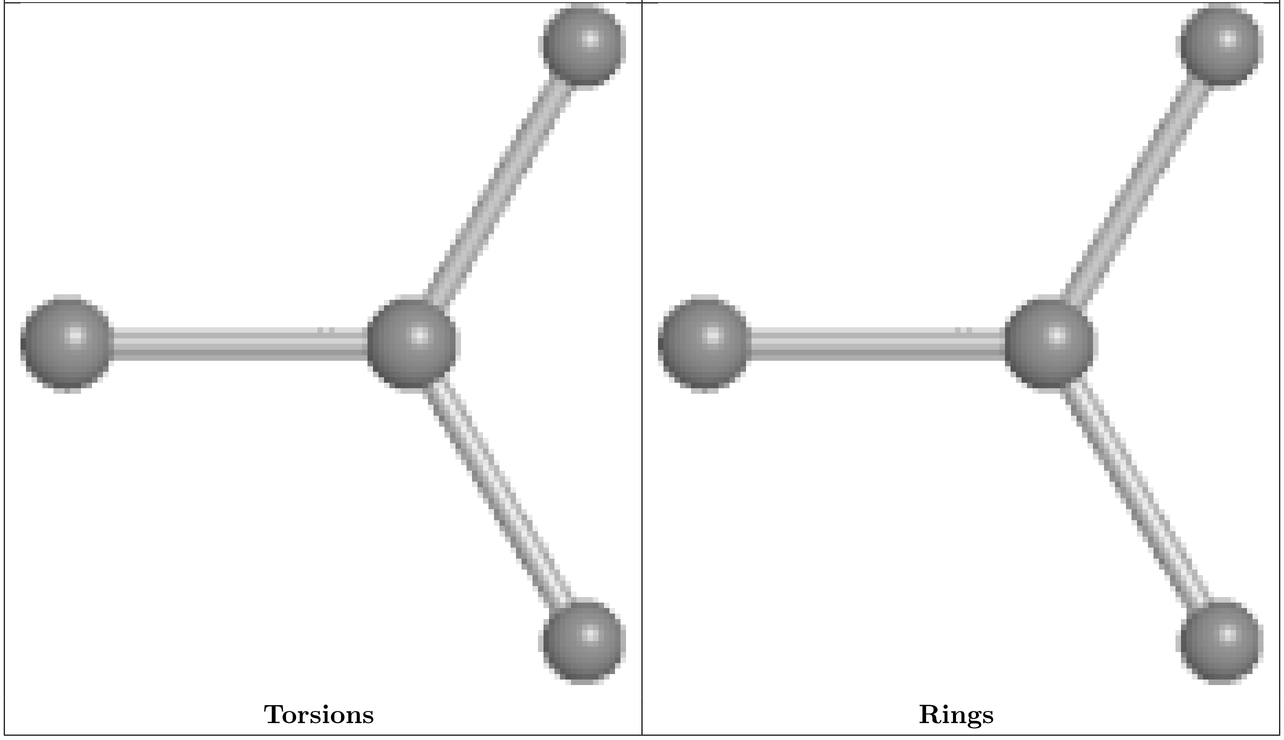


Torsions Rings

Ligand ACT J 304

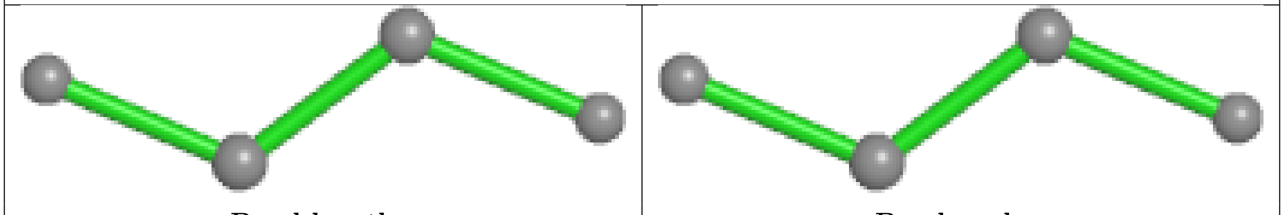


Bond lengths **Bond angles**

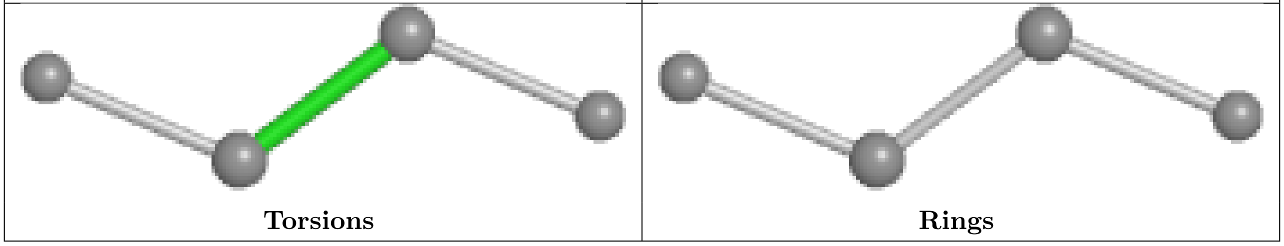


Torsions **Rings**

Ligand EDO E 309

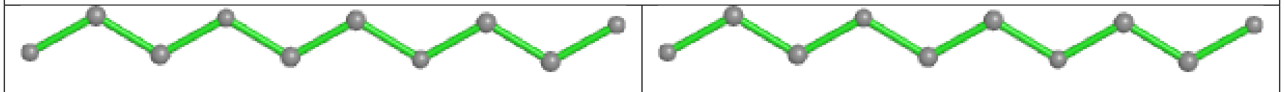


Bond lengths Bond angles

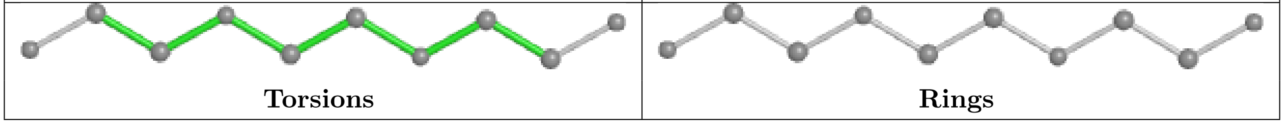


Torsions Rings

Ligand PGE I 301

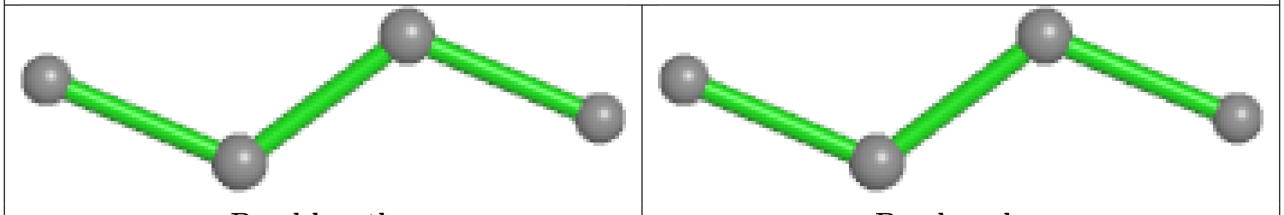


Bond lengths Bond angles

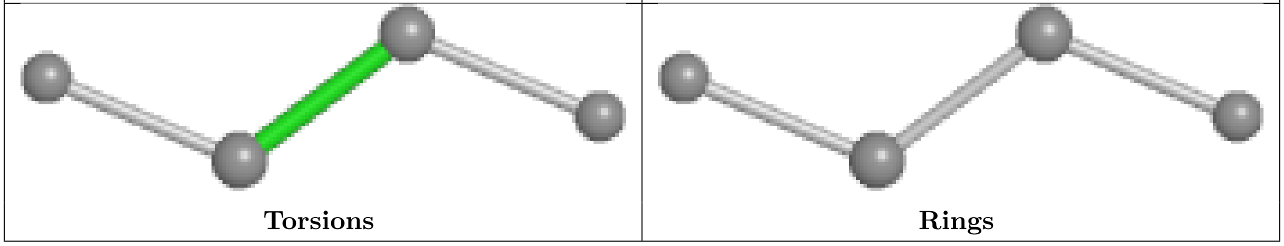


Torsions Rings

Ligand EDO B 308

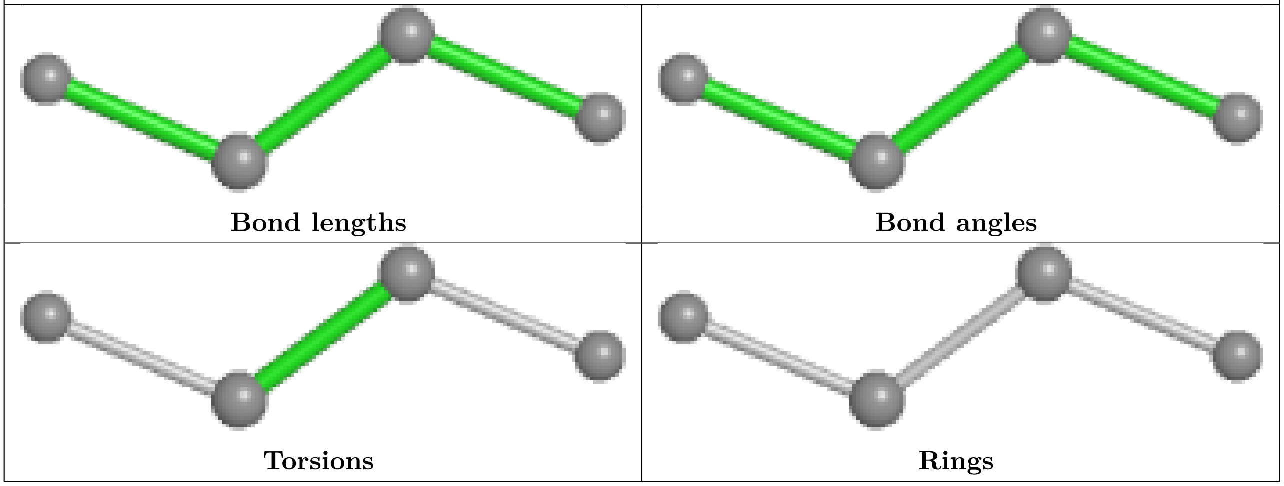


Bond lengths Bond angles



Torsions Rings

Ligand EDO L 304



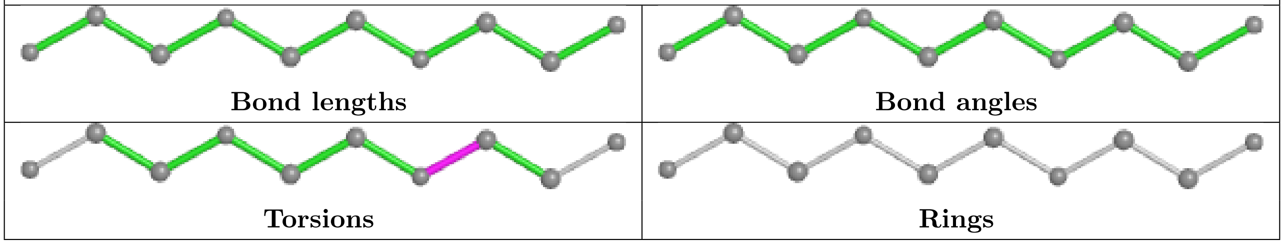
Bond lengths

Bond angles

Torsions

Rings

Ligand PGE J 301



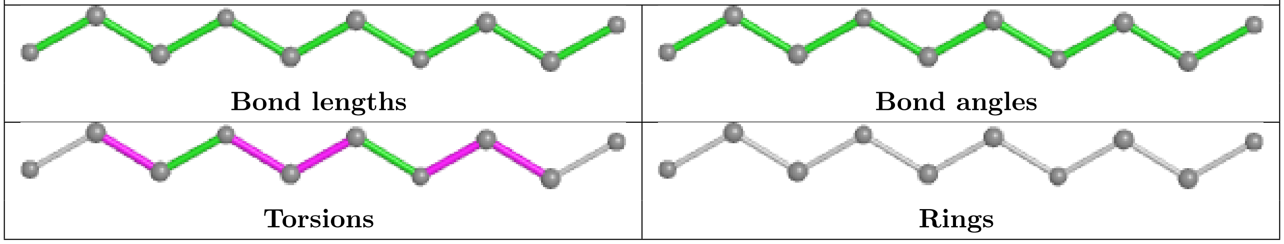
Bond lengths

Bond angles

Torsions

Rings

Ligand PGE K 301



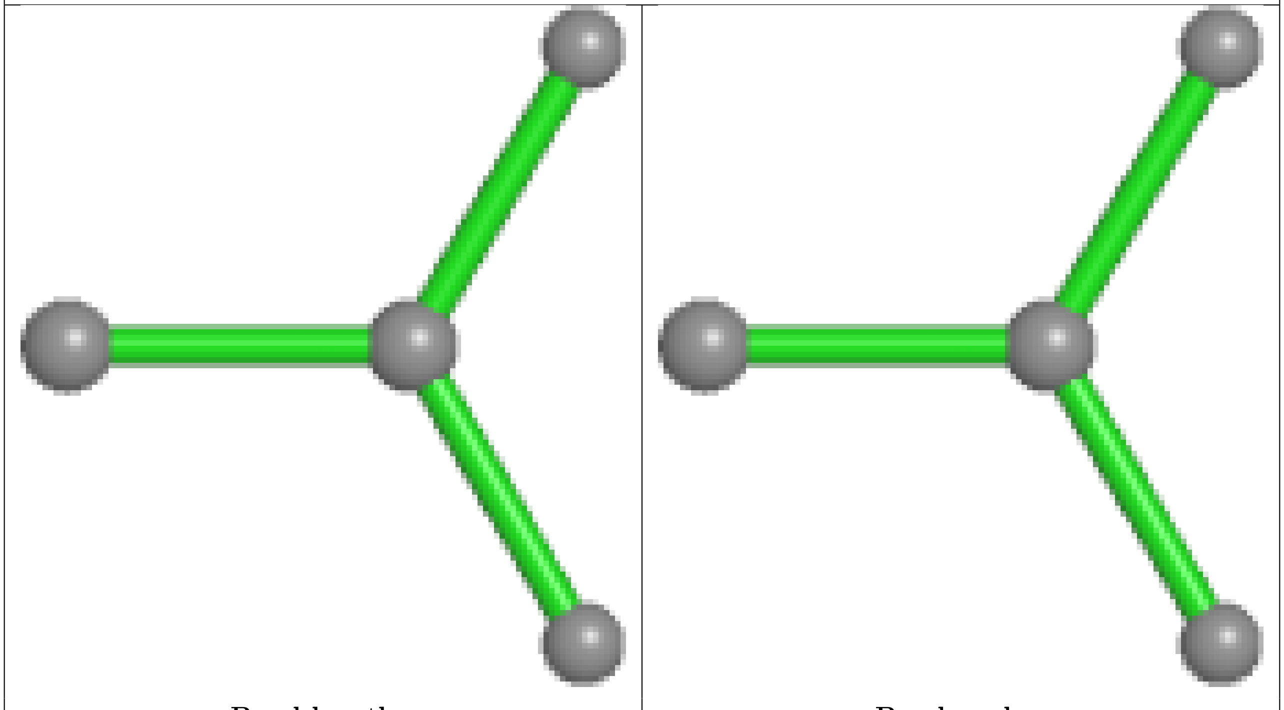
Bond lengths

Bond angles

Torsions

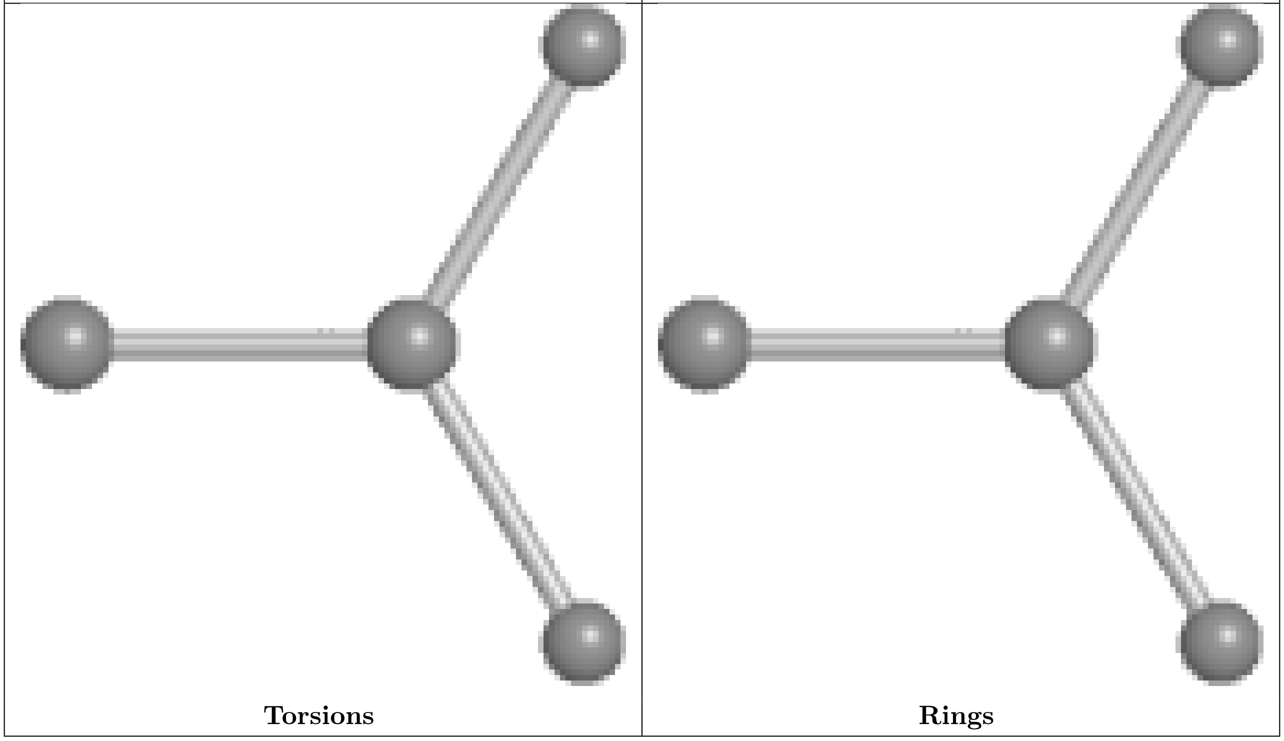
Rings

Ligand ACT I 304



Bond lengths

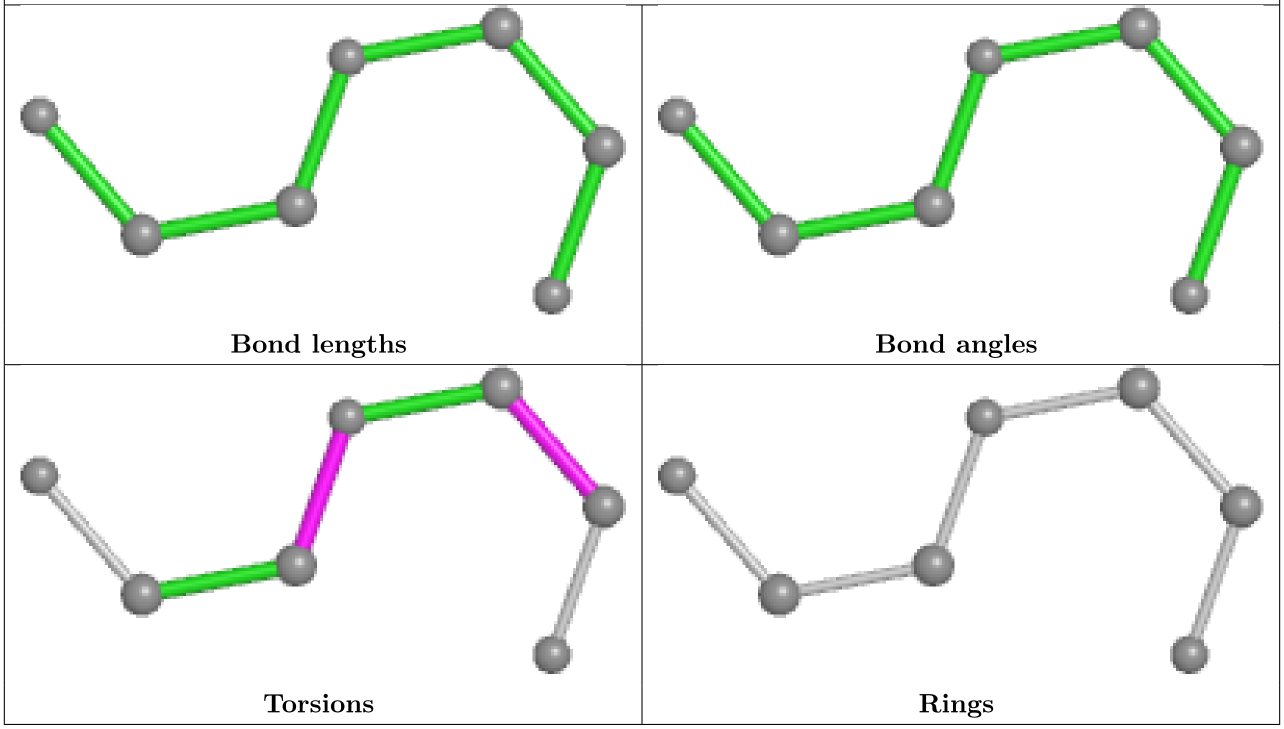
Bond angles



Torsions

Rings

Ligand PEG J 311



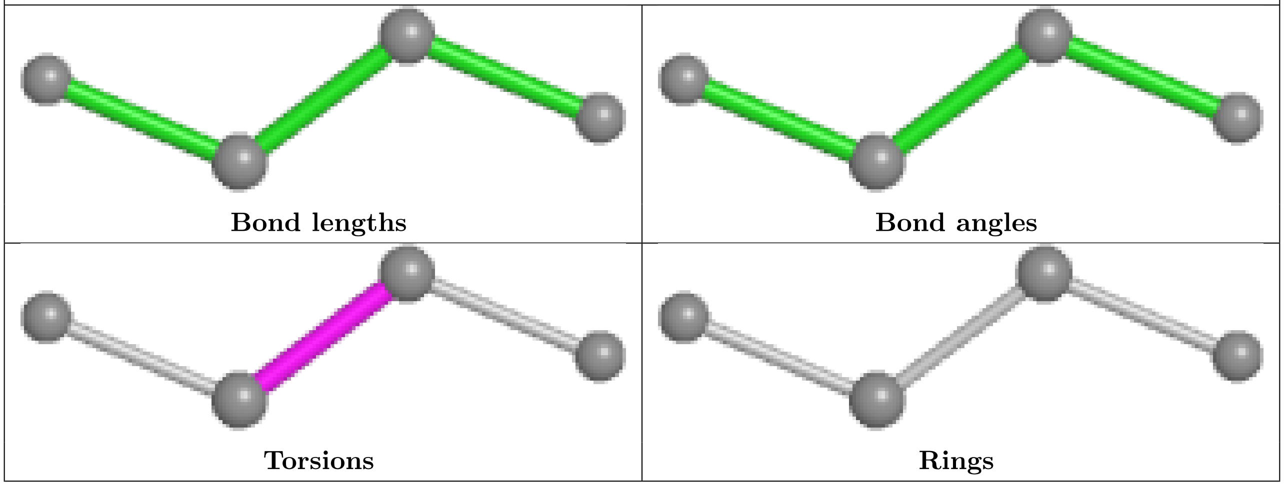
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 310



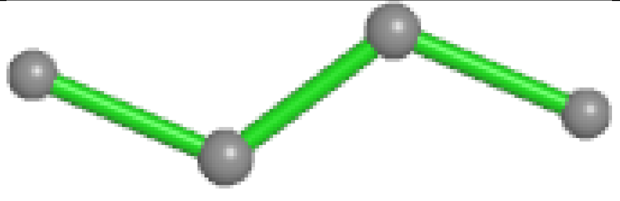
Bond lengths

Bond angles

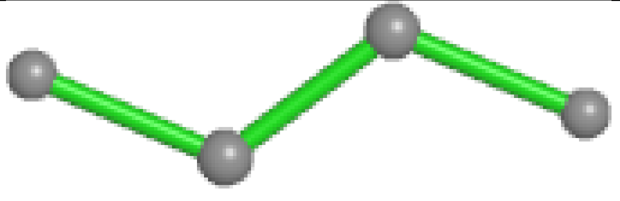
Torsions

Rings

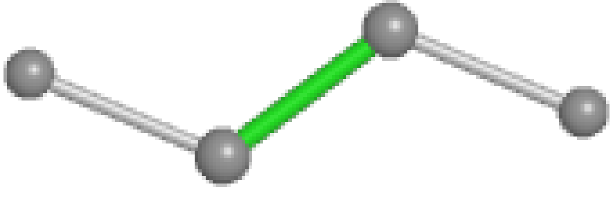
Ligand EDO C 313



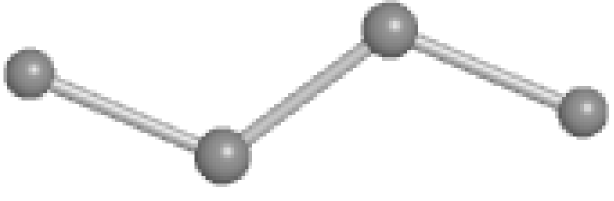
Bond lengths



Bond angles

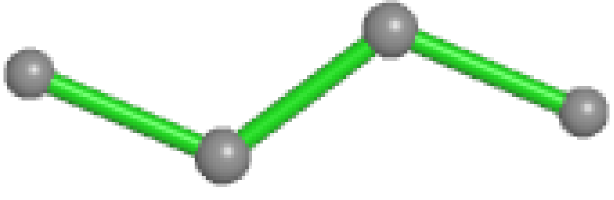


Torsions

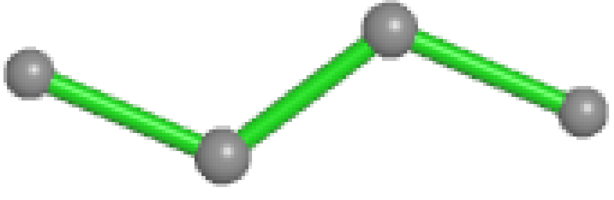


Rings

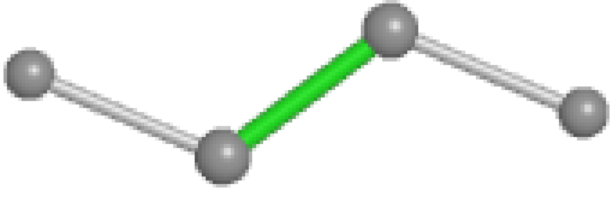
Ligand EDO C 308



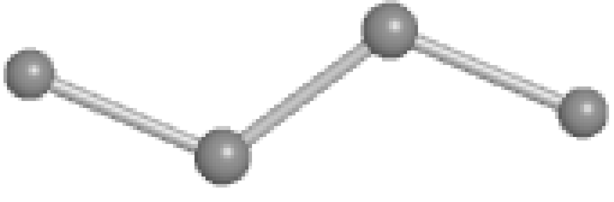
Bond lengths



Bond angles

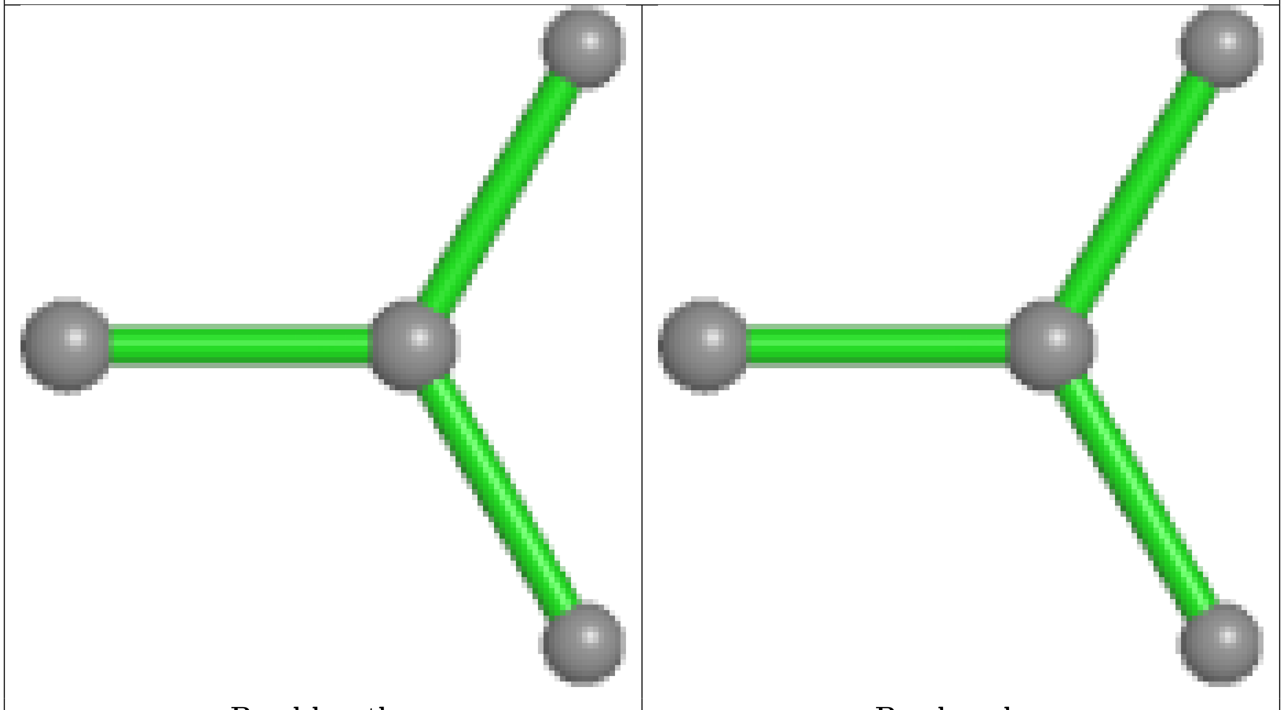


Torsions

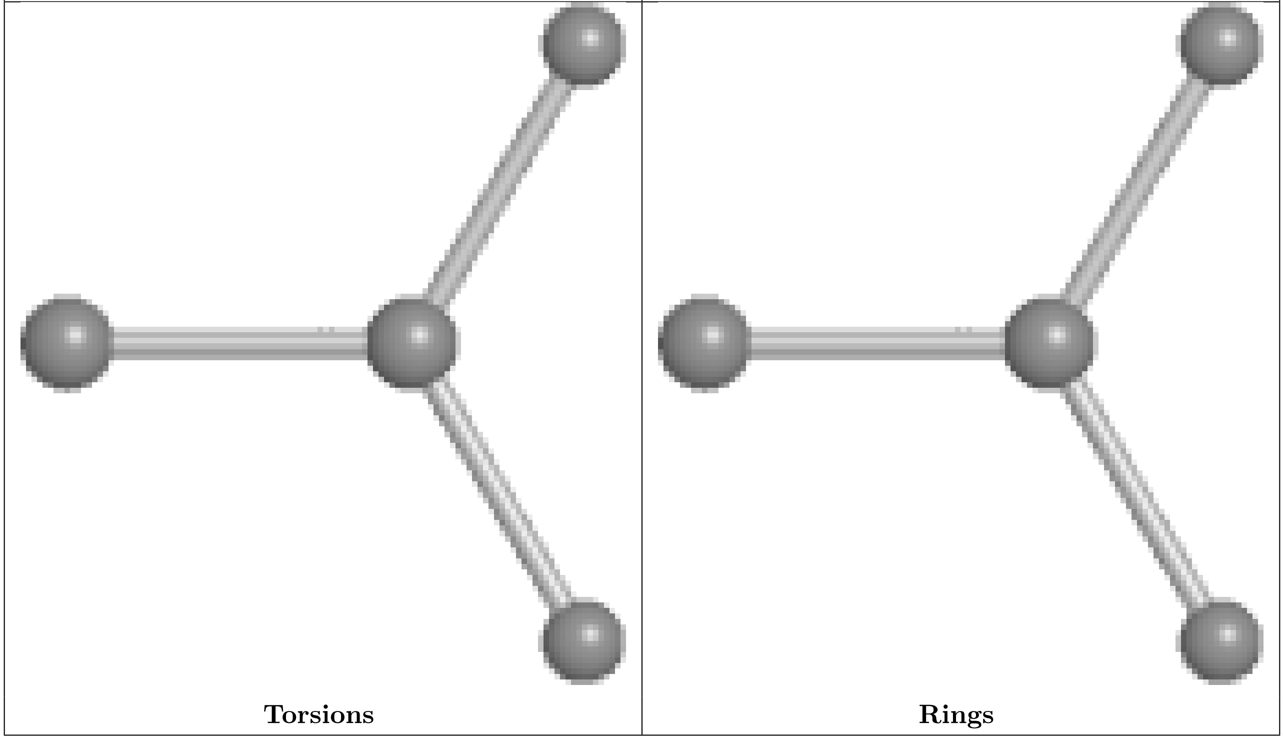


Rings

Ligand ACT F 302

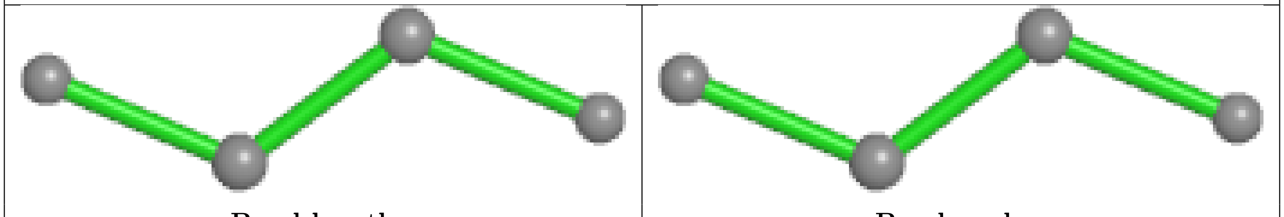


Bond lengths **Bond angles**



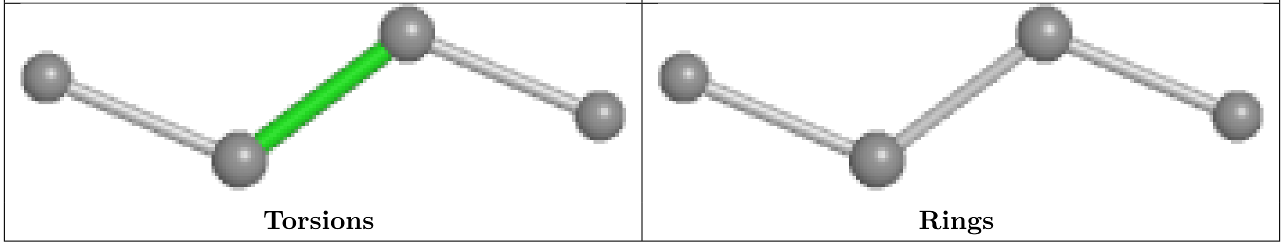
Torsions **Rings**

Ligand EDO B 304



Bond lengths

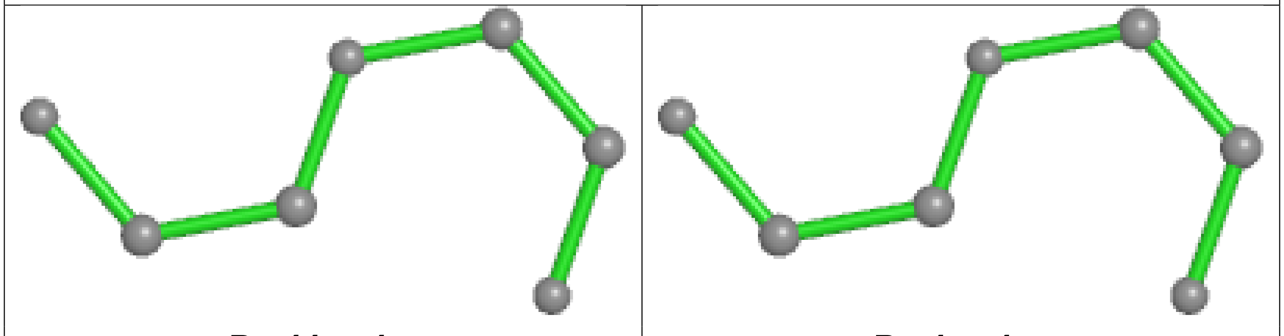
Bond angles



Torsions

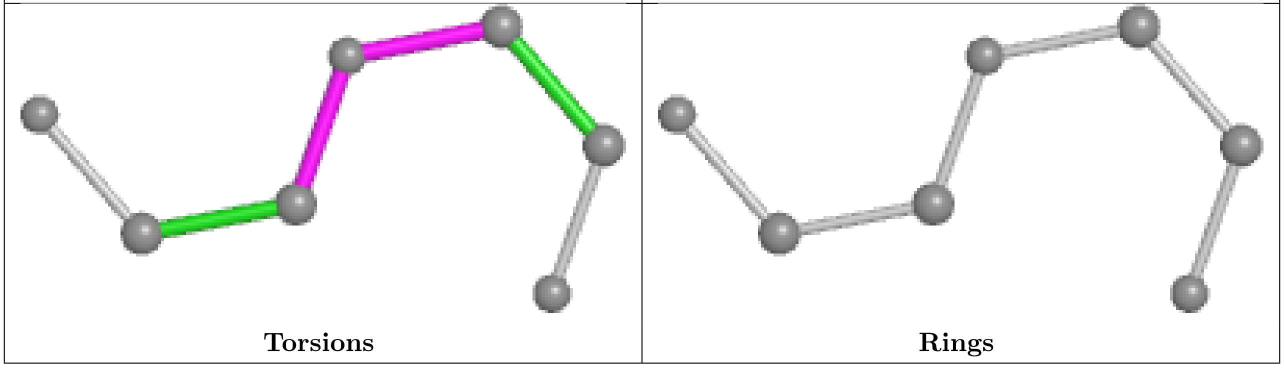
Rings

Ligand PEG F 306



Bond lengths

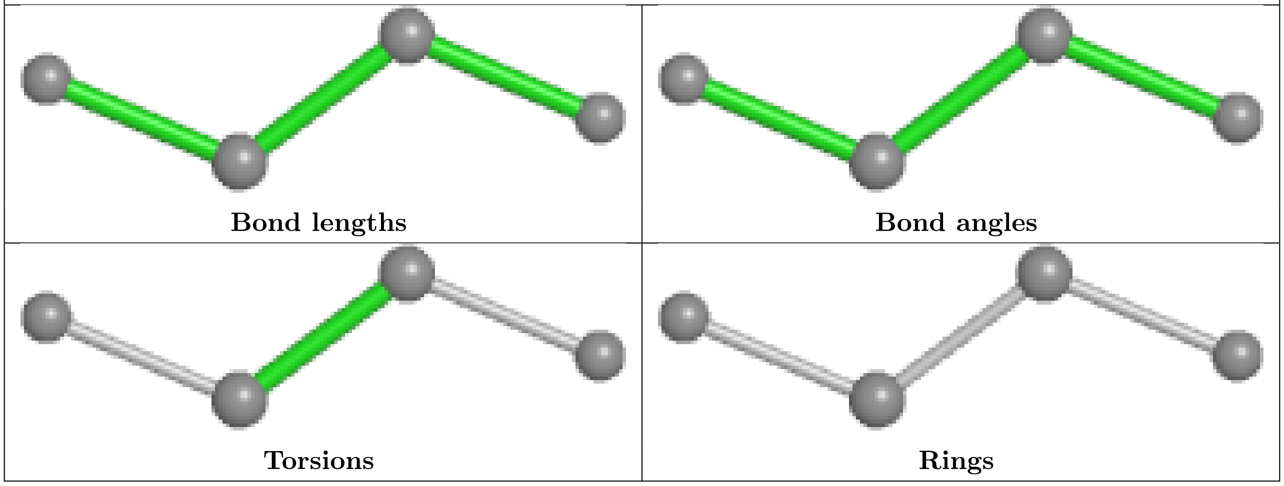
Bond angles



Torsions

Rings

Ligand EDO A 307



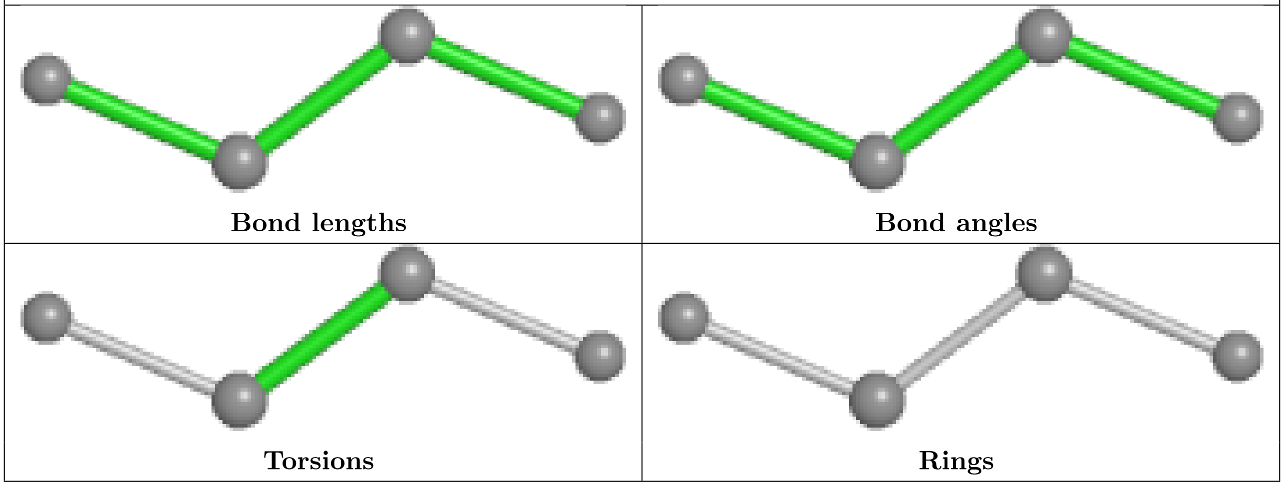
Bond lengths

Bond angles

Torsions

Rings

Ligand EDO H 304



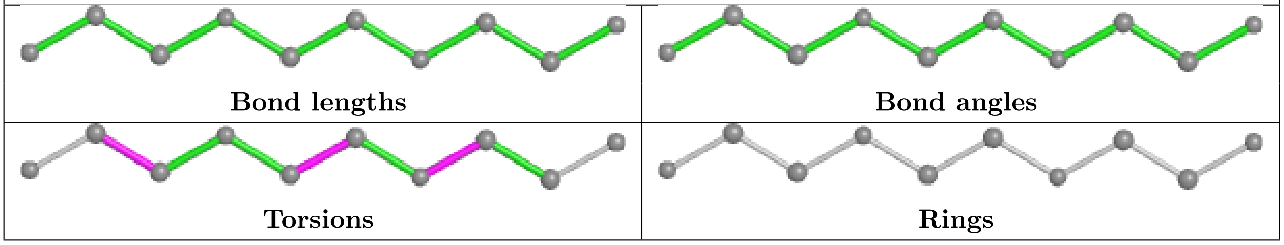
Bond lengths

Bond angles

Torsions

Rings

Ligand PGE E 301



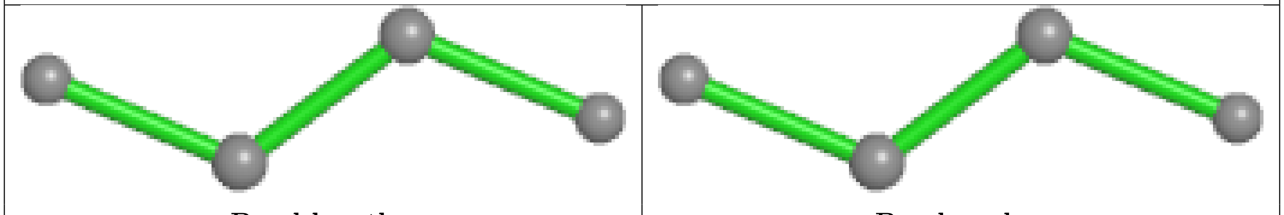
Bond lengths

Bond angles

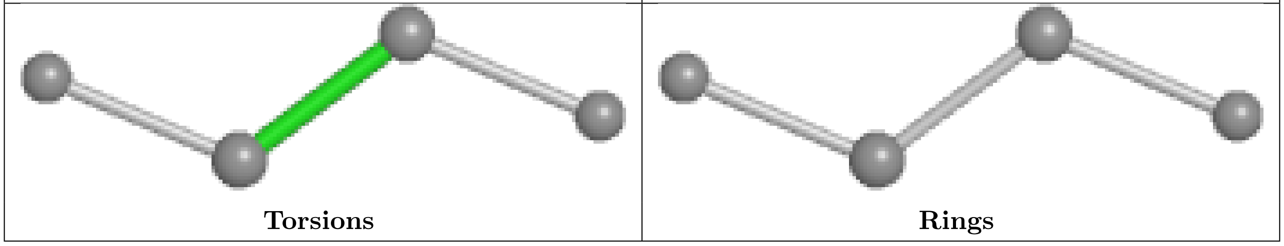
Torsions

Rings

Ligand EDO B 305

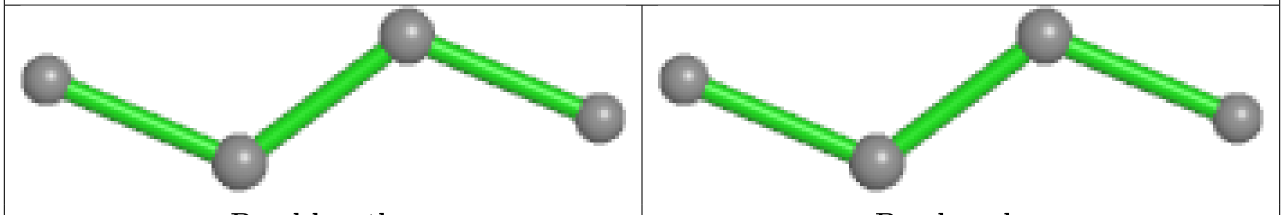


Bond lengths Bond angles

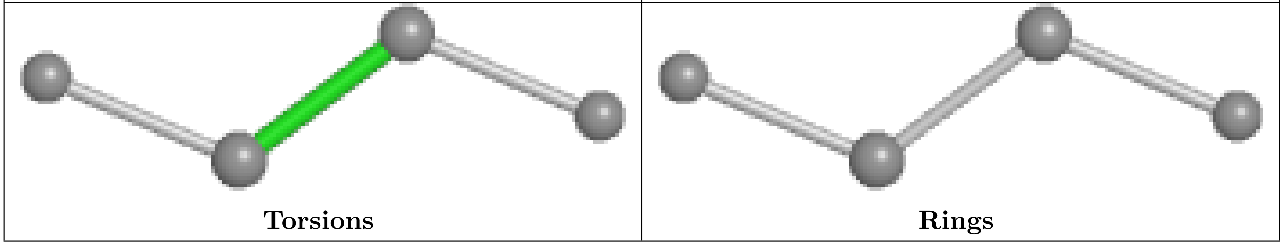


Torsions Rings

Ligand EDO C 311

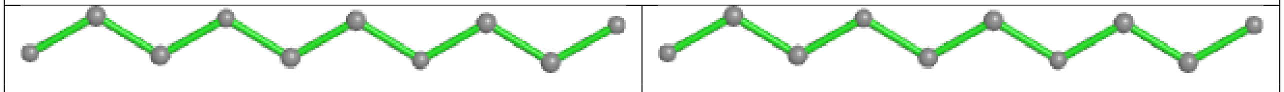


Bond lengths Bond angles

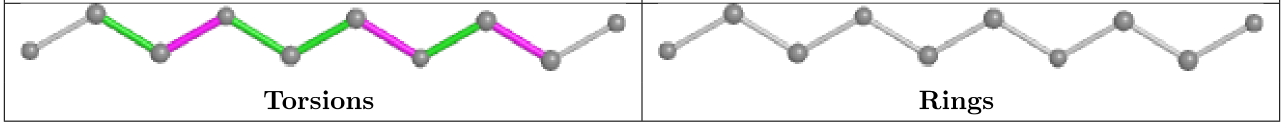


Torsions Rings

Ligand PGE C 302

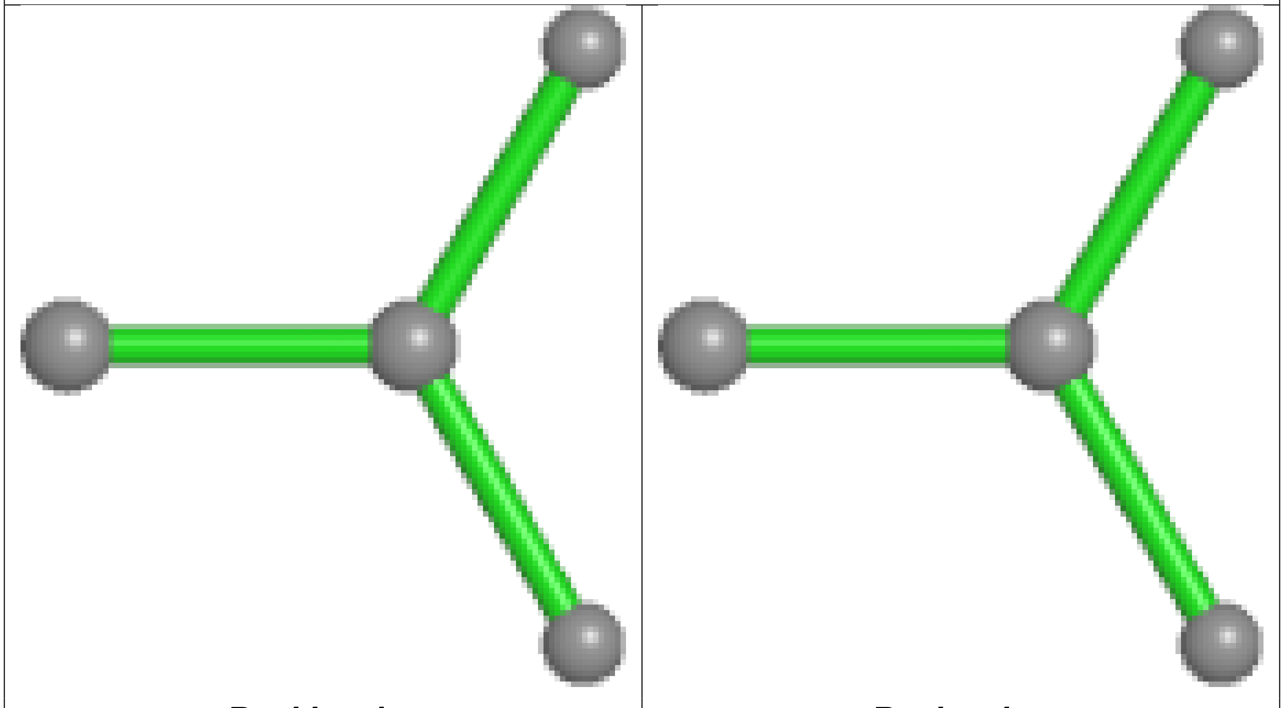


Bond lengths Bond angles



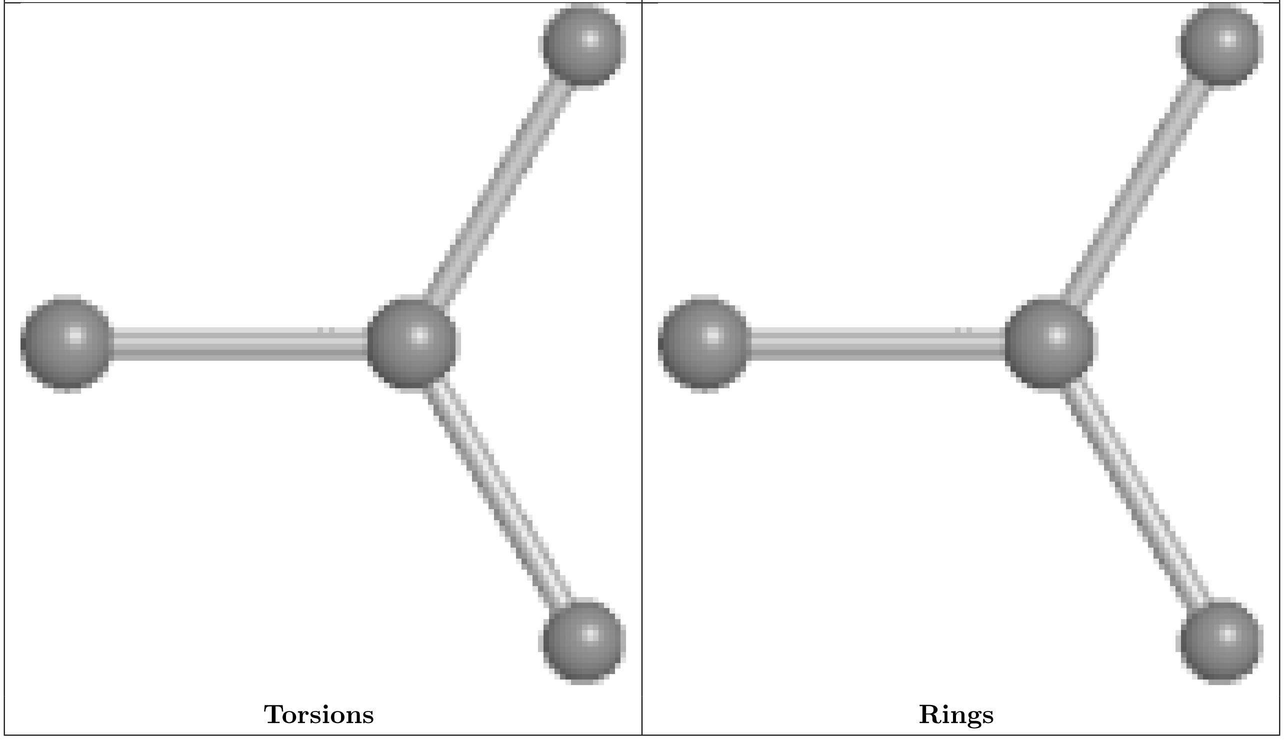
Torsions Rings

Ligand ACT J 302



Bond lengths

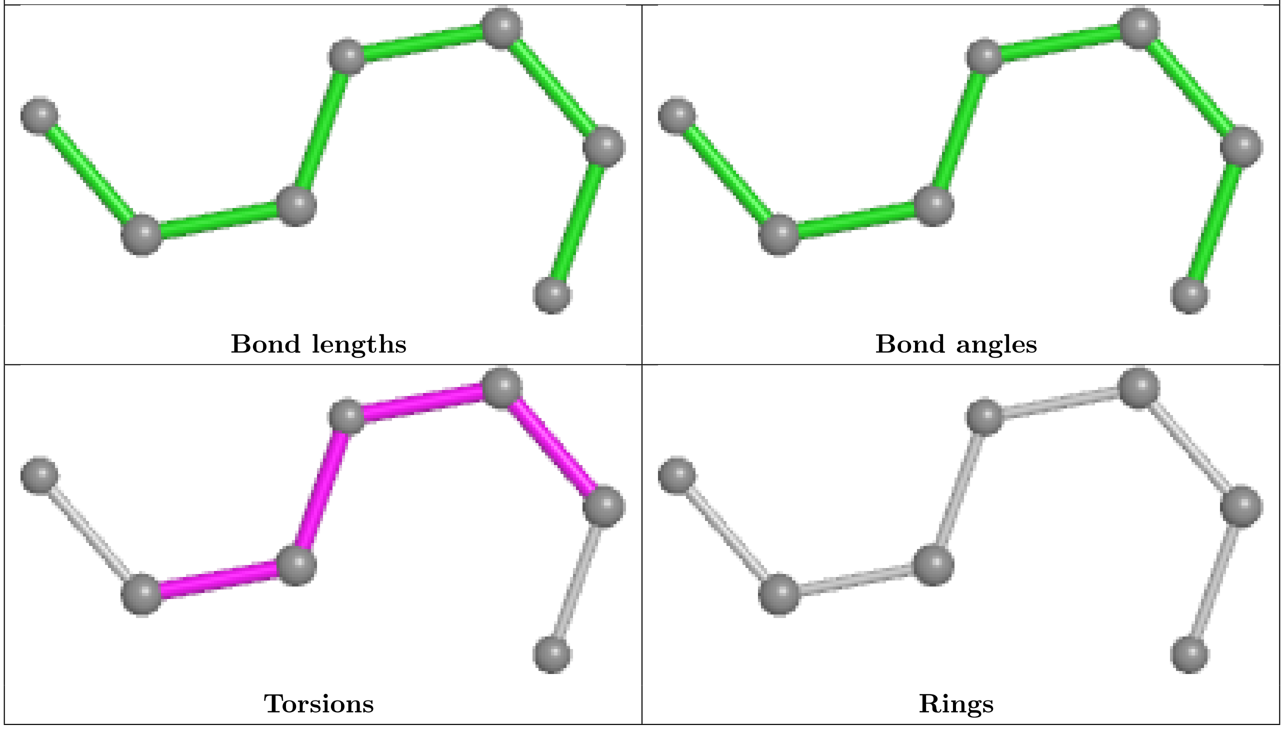
Bond angles



Torsions

Rings

Ligand PEG G 308



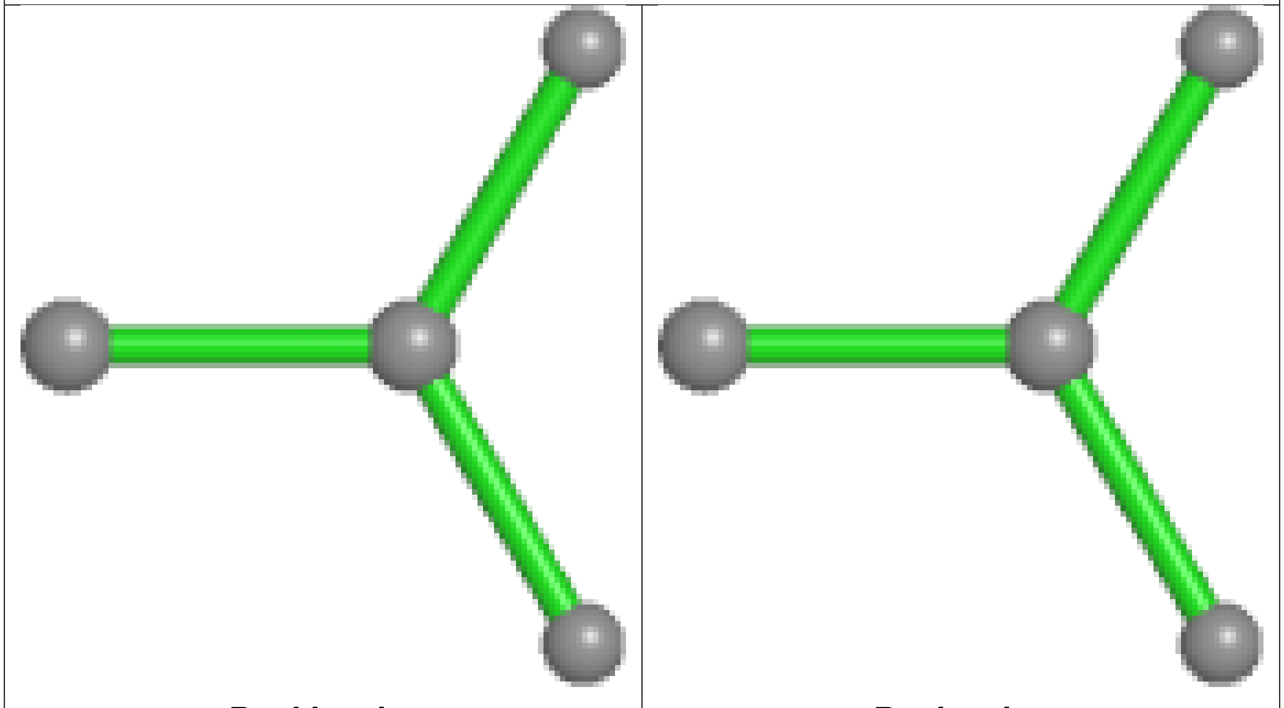
Bond lengths

Bond angles

Torsions

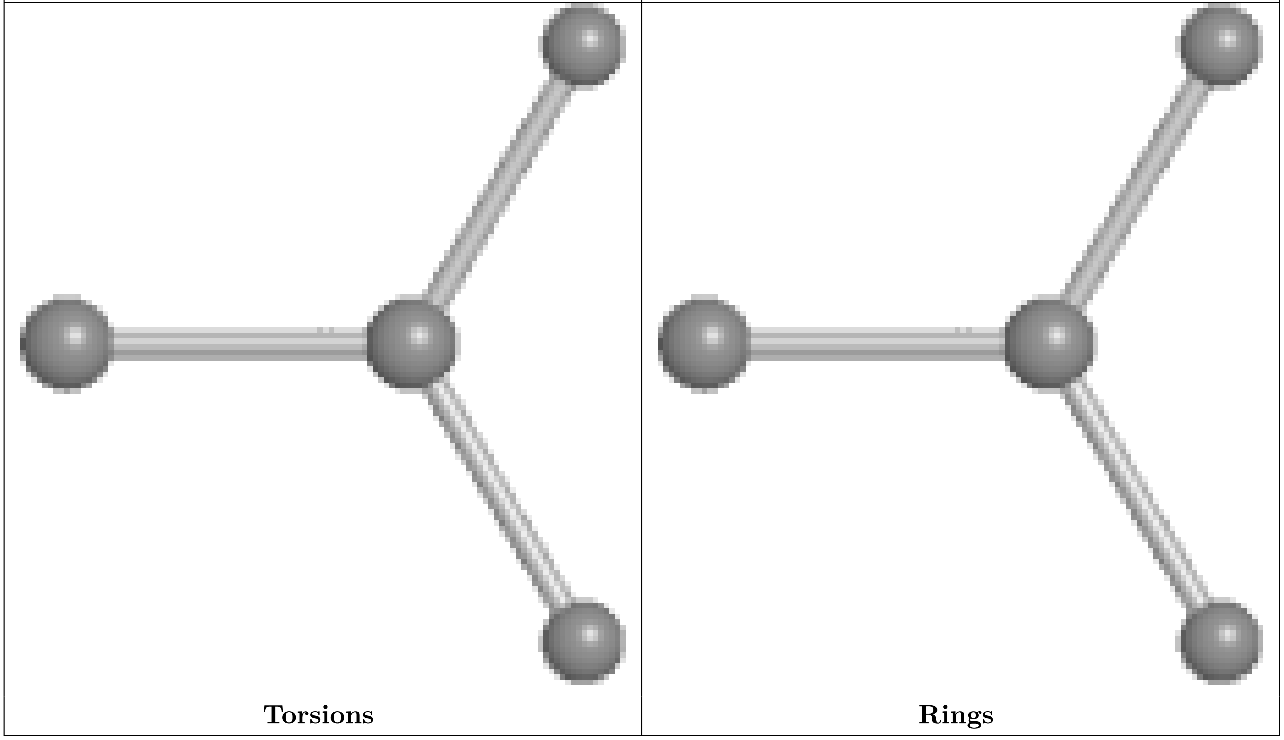
Rings

Ligand ACT E 303



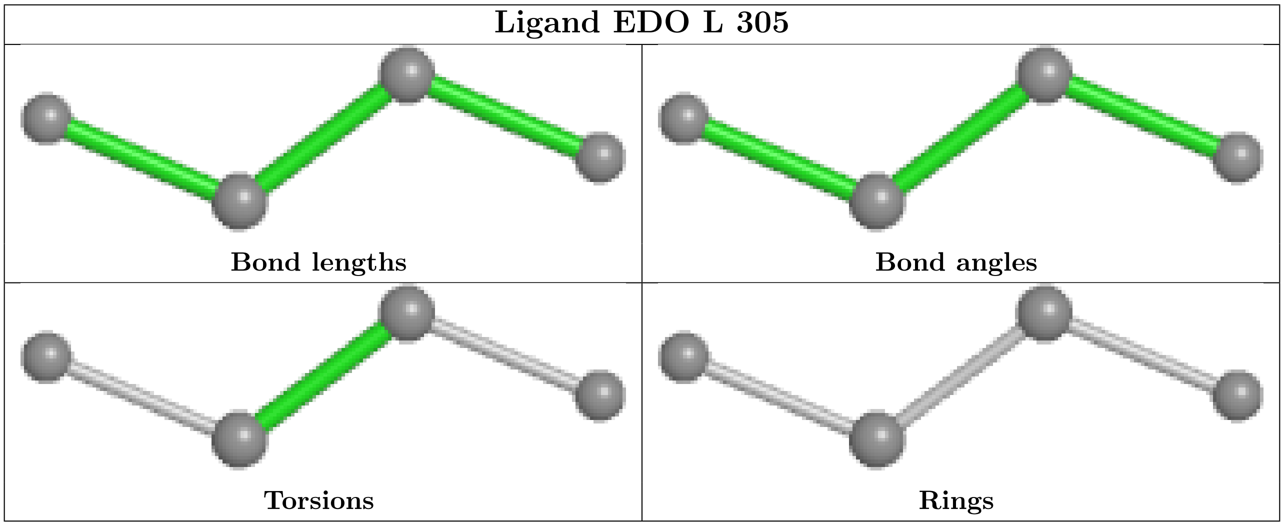
Bond lengths

Bond angles



Torsions

Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	294/310 (94%)	-0.01	0	100	100	16, 25, 37, 49	0
1	B	295/310 (95%)	-0.00	1 (0%)	94	94	19, 25, 35, 42	0
1	C	295/310 (95%)	-0.02	1 (0%)	94	94	19, 26, 38, 48	0
1	D	294/310 (94%)	-0.08	1 (0%)	94	94	16, 24, 39, 47	0
1	E	294/310 (94%)	-0.07	2 (0%)	87	89	17, 24, 39, 47	0
1	F	295/310 (95%)	0.05	0	100	100	21, 28, 40, 46	0
1	G	295/310 (95%)	0.08	1 (0%)	94	94	19, 26, 38, 48	0
1	H	295/310 (95%)	0.02	0	100	100	19, 26, 40, 48	0
1	I	295/310 (95%)	-0.06	1 (0%)	94	94	19, 26, 41, 51	0
1	J	293/310 (94%)	-0.02	0	100	100	18, 26, 39, 55	0
1	K	295/310 (95%)	0.17	2 (0%)	87	89	19, 28, 39, 47	0
1	L	295/310 (95%)	0.07	1 (0%)	94	94	19, 27, 40, 49	0
All	All	3535/3720 (95%)	0.01	10 (0%)	94	94	16, 26, 39, 55	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	72	GLY	3.5
1	B	283	PHE	2.9
1	I	130	VAL	2.7
1	C	19	ASN	2.7
1	K	267	GLU	2.5
1	E	95	PHE	2.3
1	E	19	ASN	2.3
1	K	103	GLY	2.2
1	D	98	GLU	2.1
1	G	56	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	J	166	14/15	0.91	0.15	17,23,28,29	3
1	KPI	E	166	14/15	0.92	0.15	18,20,26,27	3
1	KPI	H	166	14/15	0.92	0.15	19,24,30,32	2
1	KPI	C	166	14/15	0.92	0.14	19,24,31,33	2
1	KPI	D	166	14/15	0.93	0.13	14,19,22,24	2
1	KPI	F	166	14/15	0.93	0.14	21,27,32,33	2
1	KPI	K	166	14/15	0.93	0.16	21,25,28,30	2
1	KPI	I	166	14/15	0.95	0.12	18,24,28,32	3
1	KPI	L	166	14/15	0.95	0.12	16,21,26,28	2
1	KPI	G	166	14/15	0.96	0.13	20,22,27,27	3
1	KPI	A	166	14/15	0.96	0.14	17,24,35,35	3
1	KPI	B	166	14/15	0.96	0.13	17,21,25,27	3

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	EDO	C	313	4/4	0.66	0.21	37,41,45,45	0
5	EDO	L	306	4/4	0.76	0.24	31,37,37,43	0
7	GOL	G	301	6/6	0.76	0.13	40,45,47,48	0
7	GOL	I	302	6/6	0.76	0.16	39,45,47,51	0
7	GOL	L	302	6/6	0.78	0.21	38,45,50,53	0
2	PGE	K	301	10/10	0.79	0.20	35,40,48,55	0
5	EDO	G	305	4/4	0.80	0.21	27,29,34,43	0
2	PGE	C	302	10/10	0.80	0.23	28,37,44,49	0
5	EDO	L	307	4/4	0.80	0.18	38,41,44,45	0
5	EDO	H	304	4/4	0.81	0.20	33,35,49,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	E	307	4/4	0.81	0.23	35,47,47,56	0
3	ACT	F	302	4/4	0.82	0.26	41,42,44,49	0
3	ACT	I	303	4/4	0.82	0.22	25,30,32,37	0
3	ACT	L	303	4/4	0.82	0.22	45,47,51,55	0
5	EDO	A	309	4/4	0.82	0.23	34,39,42,45	0
5	EDO	J	309	4/4	0.82	0.33	27,32,42,42	0
6	PEG	L	308	7/7	0.84	0.17	31,42,48,51	0
5	EDO	E	309	4/4	0.84	0.29	26,38,40,43	0
5	EDO	F	303	4/4	0.85	0.17	38,38,38,39	0
5	EDO	B	306	4/4	0.85	0.19	21,29,31,41	0
2	PGE	L	301	10/10	0.85	0.22	25,37,43,44	0
6	PEG	J	311	7/7	0.85	0.20	32,40,44,45	0
5	EDO	G	304	4/4	0.86	0.20	32,35,37,37	0
3	ACT	C	303	4/4	0.86	0.18	30,33,40,42	0
3	ACT	B	301	4/4	0.86	0.19	33,38,39,45	0
3	ACT	H	301	4/4	0.86	0.23	28,32,33,41	0
5	EDO	L	305	4/4	0.86	0.26	31,35,39,39	0
3	ACT	H	302	4/4	0.86	0.18	30,31,36,37	0
3	ACT	A	302	4/4	0.87	0.14	45,49,49,50	0
3	ACT	B	302	4/4	0.87	0.22	28,38,38,46	0
5	EDO	J	306	4/4	0.87	0.20	28,31,32,33	0
5	EDO	A	306	4/4	0.87	0.28	28,32,34,39	0
5	EDO	G	302	4/4	0.87	0.15	31,34,39,45	0
5	EDO	E	306	4/4	0.87	0.19	30,34,34,40	0
4	MG	E	305	1/1	0.88	0.10	47,47,47,47	0
3	ACT	A	303	4/4	0.88	0.21	27,36,37,45	0
6	PEG	F	306	7/7	0.88	0.21	36,40,43,48	0
5	EDO	G	306	4/4	0.88	0.14	29,34,39,40	0
2	PGE	D	301	10/10	0.88	0.15	28,36,48,56	0
2	PGE	A	301	10/10	0.88	0.11	35,38,46,48	0
5	EDO	B	308	4/4	0.88	0.14	37,38,38,41	0
5	EDO	B	309	4/4	0.88	0.18	36,36,37,40	0
6	PEG	L	309	7/7	0.89	0.37	13,28,41,52	0
6	PEG	G	308	7/7	0.89	0.14	32,34,37,42	0
5	EDO	B	310	4/4	0.89	0.19	37,38,39,42	0
5	EDO	L	304	4/4	0.89	0.18	27,31,35,49	0
5	EDO	B	305	4/4	0.90	0.20	22,28,29,33	0
5	EDO	G	303	4/4	0.90	0.17	24,27,29,30	0
4	MG	A	304	1/1	0.90	0.07	44,44,44,44	0
5	EDO	C	306	4/4	0.90	0.17	25,27,34,35	0
3	ACT	B	303	4/4	0.90	0.18	26,27,34,39	0
5	EDO	F	305	4/4	0.90	0.17	34,35,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	H	305	4/4	0.90	0.28	28,29,33,36	0
5	EDO	C	316	4/4	0.91	0.18	34,36,42,49	0
2	PGE	I	301	10/10	0.91	0.15	29,33,40,40	0
5	EDO	I	308	4/4	0.91	0.22	27,30,33,41	0
5	EDO	J	305	4/4	0.91	0.12	31,34,39,39	0
5	EDO	C	314	4/4	0.91	0.13	30,37,38,39	0
5	EDO	E	308	4/4	0.91	0.24	29,33,38,47	0
5	EDO	F	304	4/4	0.92	0.13	32,35,38,43	0
5	EDO	K	302	4/4	0.92	0.14	24,32,32,36	0
5	EDO	A	307	4/4	0.92	0.21	29,30,32,36	0
5	EDO	C	307	4/4	0.92	0.15	25,29,32,42	0
2	PGE	F	301	10/10	0.92	0.12	33,38,42,44	0
5	EDO	A	310	4/4	0.92	0.14	38,40,40,46	0
4	MG	C	304	1/1	0.92	0.08	33,33,33,33	0
3	ACT	J	304	4/4	0.93	0.22	31,35,38,46	0
5	EDO	C	308	4/4	0.93	0.24	21,26,26,29	0
5	EDO	C	310	4/4	0.93	0.11	30,32,34,35	0
5	EDO	I	307	4/4	0.93	0.32	27,33,34,35	0
2	PGE	E	301	10/10	0.93	0.10	24,32,37,44	0
3	ACT	E	303	4/4	0.93	0.18	32,40,42,43	0
5	EDO	A	308	4/4	0.93	0.10	32,34,34,41	0
5	EDO	D	304	4/4	0.93	0.16	24,26,26,38	0
3	ACT	I	304	4/4	0.93	0.19	27,28,39,44	0
5	EDO	K	303	4/4	0.93	0.12	36,40,42,49	0
4	MG	C	305	1/1	0.93	0.17	42,42,42,42	0
5	EDO	I	306	4/4	0.94	0.18	27,30,32,34	0
6	PEG	H	306	7/7	0.94	0.10	35,37,42,43	0
2	PGE	J	301	10/10	0.94	0.13	33,36,37,47	0
5	EDO	B	304	4/4	0.94	0.15	27,30,35,37	0
5	EDO	B	307	4/4	0.94	0.12	33,35,38,38	0
5	EDO	C	309	4/4	0.94	0.11	32,34,35,42	0
5	EDO	J	308	4/4	0.94	0.14	25,29,29,33	0
5	EDO	D	303	4/4	0.94	0.14	23,30,32,34	0
2	PGE	C	301	10/10	0.95	0.09	30,33,40,43	0
5	EDO	C	311	4/4	0.95	0.17	26,26,28,32	0
5	EDO	J	310	4/4	0.95	0.12	26,31,34,38	0
5	EDO	C	312	4/4	0.95	0.35	25,26,28,29	0
3	ACT	I	305	4/4	0.95	0.11	29,34,40,45	0
3	ACT	J	303	4/4	0.95	0.10	33,34,35,35	0
5	EDO	C	315	4/4	0.95	0.28	32,33,35,38	0
5	EDO	A	305	4/4	0.95	0.14	24,35,38,40	0
5	EDO	J	307	4/4	0.95	0.21	25,29,30,34	0

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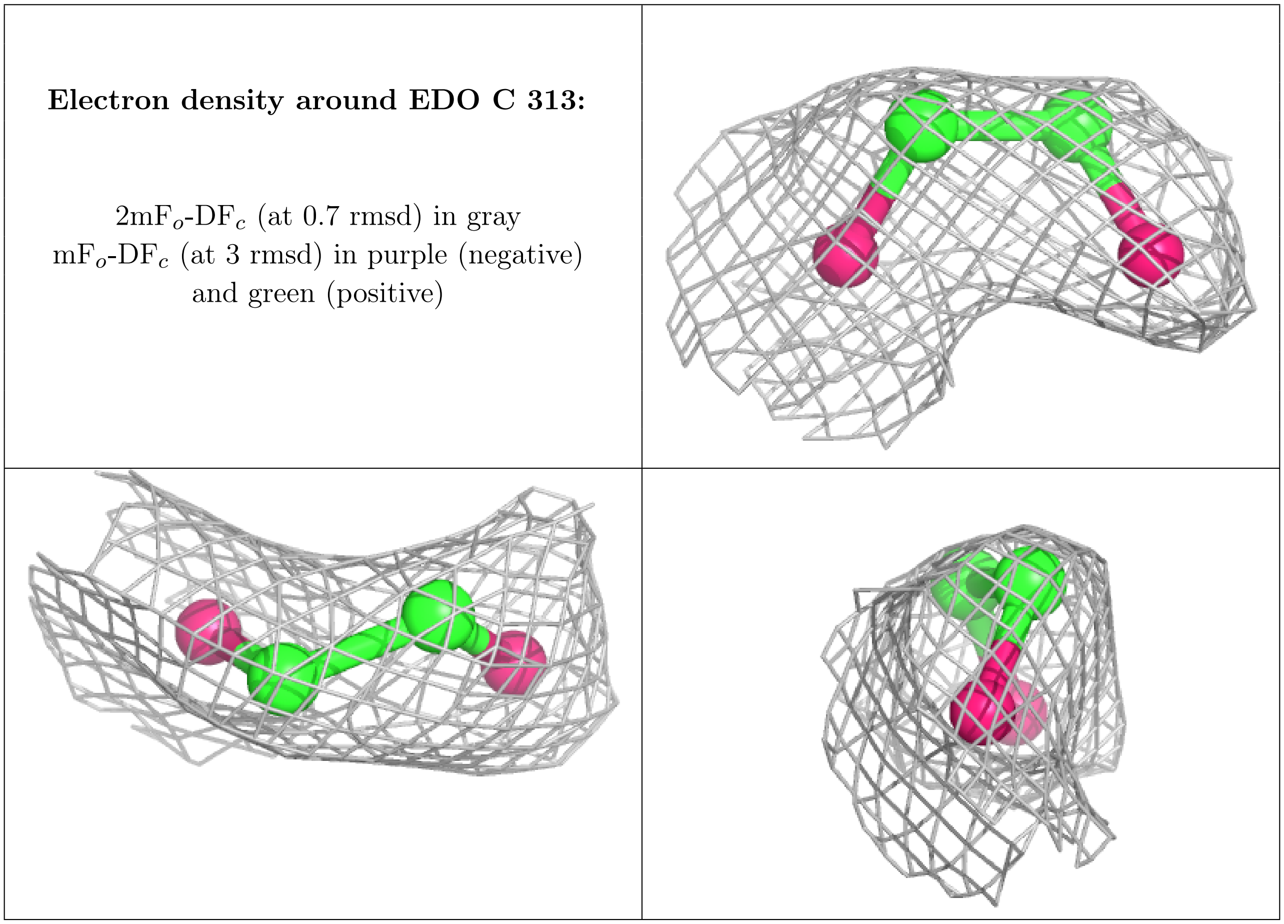
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	ACT	E	302	4/4	0.96	0.11	29,32,38,39	0
3	ACT	J	302	4/4	0.96	0.13	25,35,35,44	0
4	MG	D	302	1/1	0.96	0.05	31,31,31,31	0
5	EDO	G	307	4/4	0.96	0.23	36,41,41,50	0
4	MG	E	304	1/1	0.96	0.08	39,39,39,39	0
3	ACT	H	303	4/4	0.96	0.12	29,29,29,39	0

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.

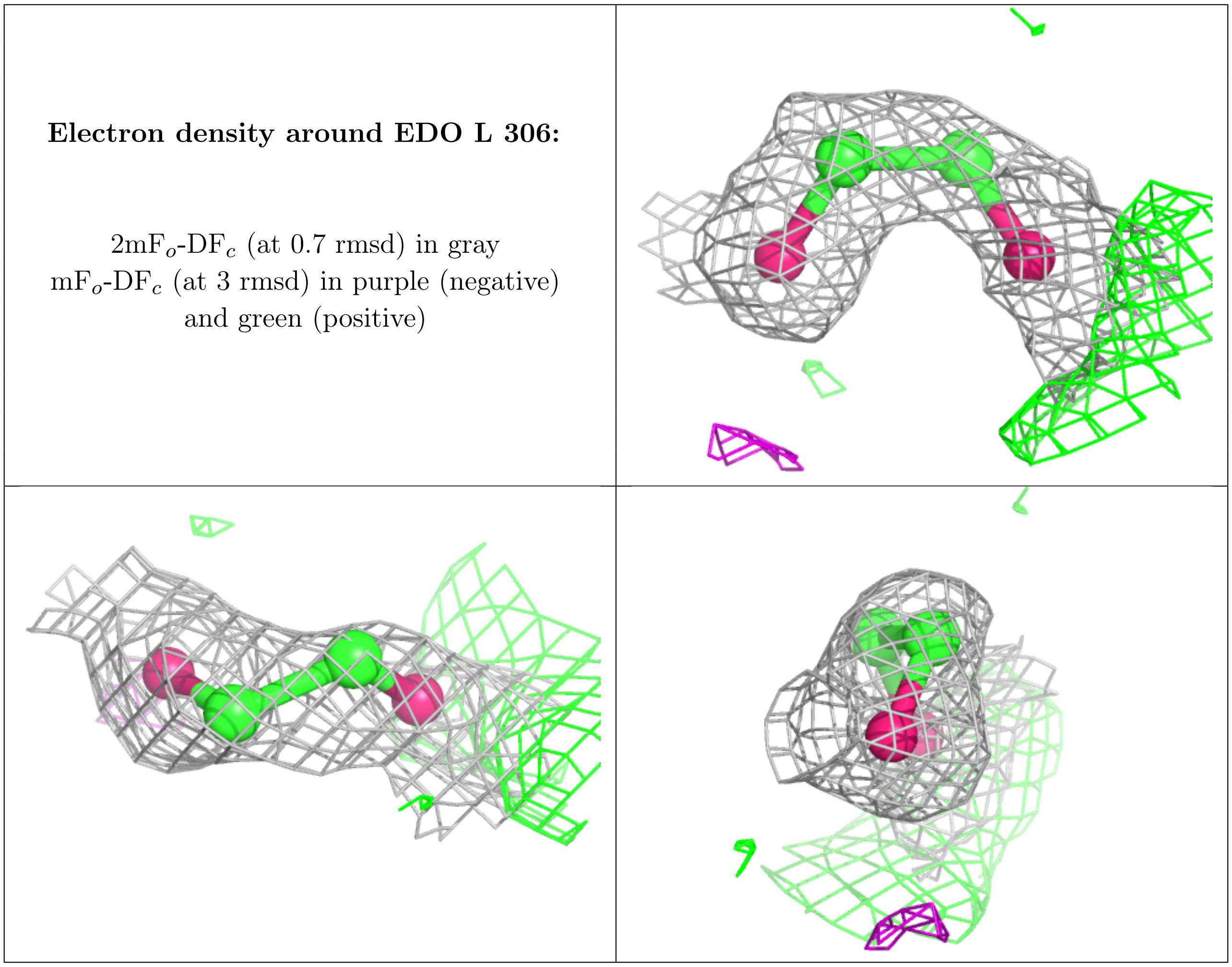


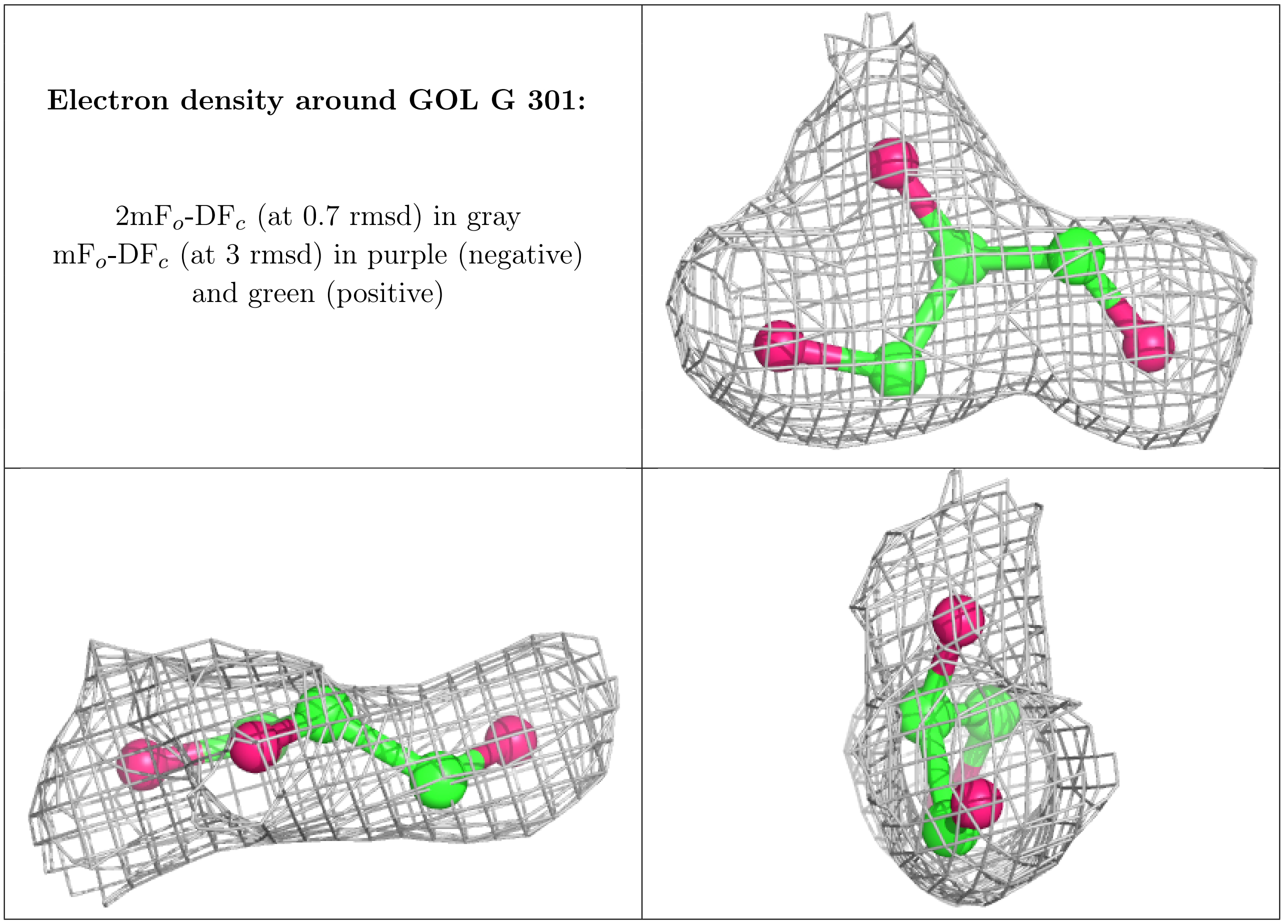
Electron density around EDO C 313:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around EDO L 306:

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



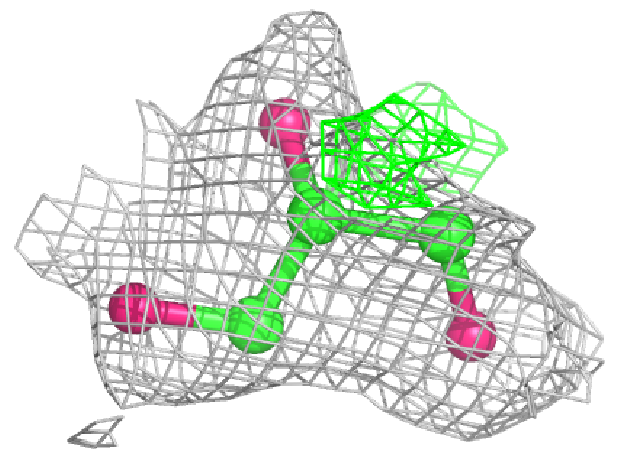


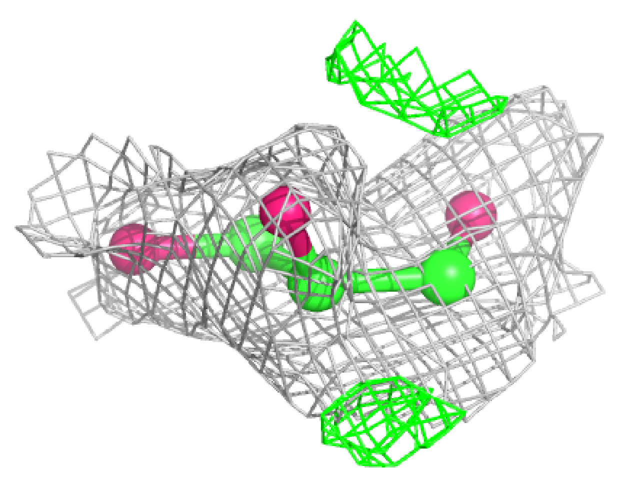
Electron density around GOL G 301:

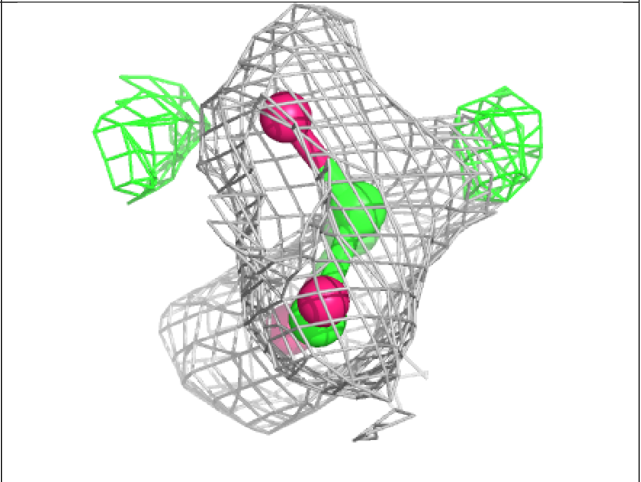
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GOL I 302:

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

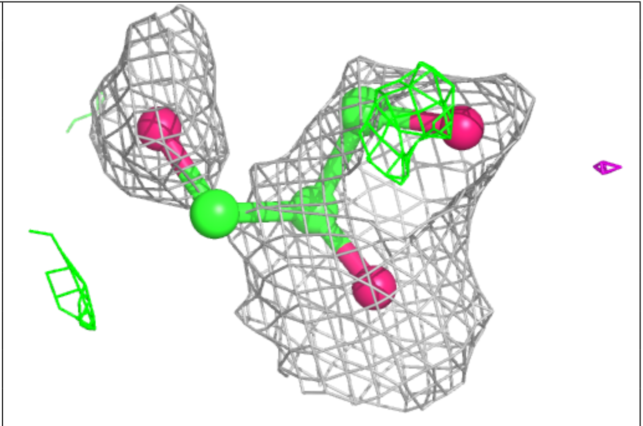


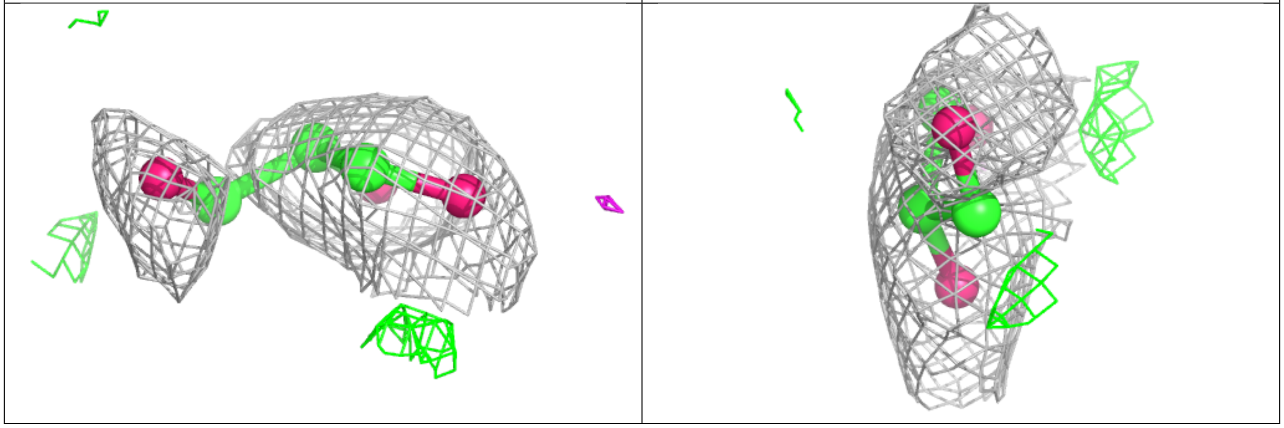




Electron density around GOL L 302:

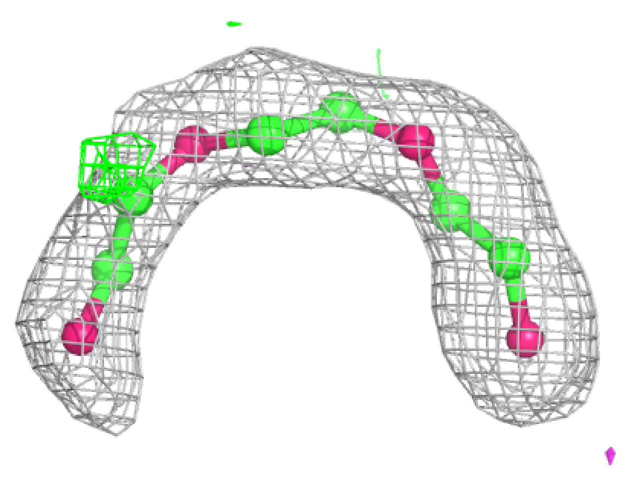
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

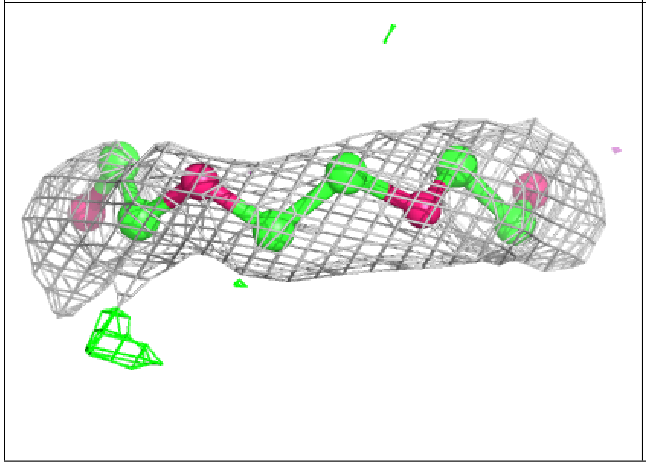


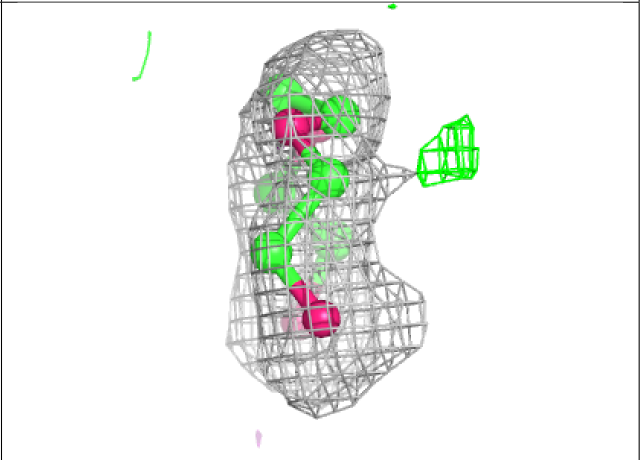


Electron density around PGE K 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

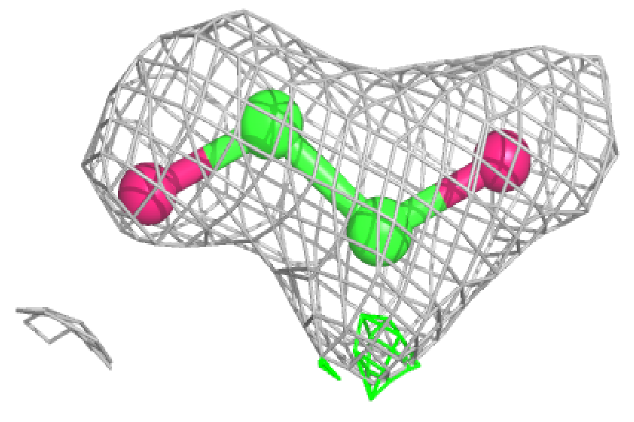


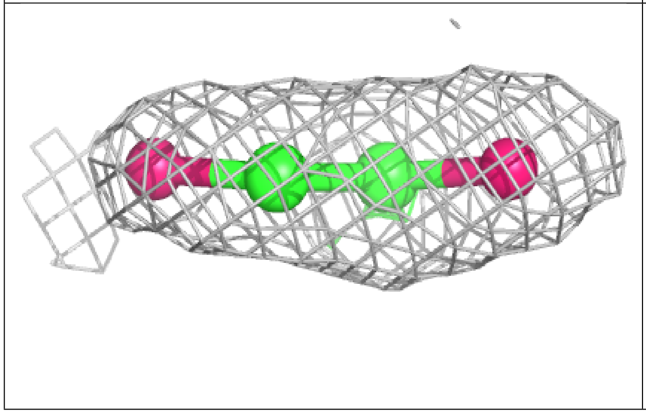


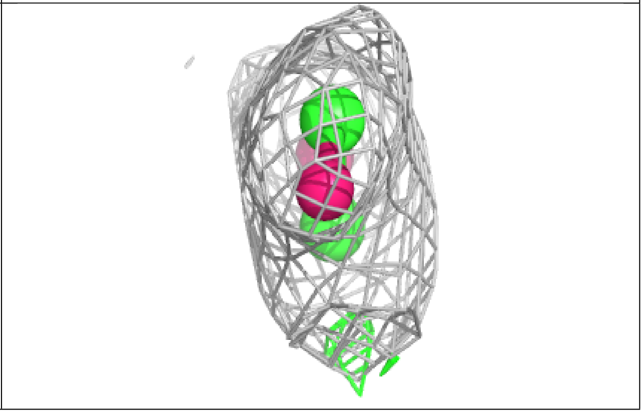


Electron density around EDO G 305:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

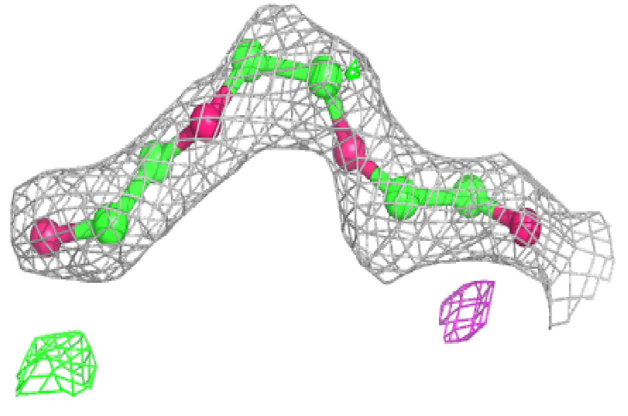


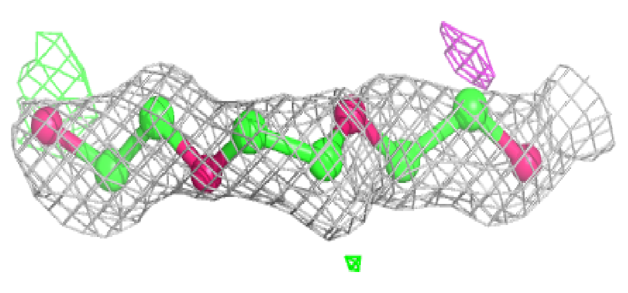


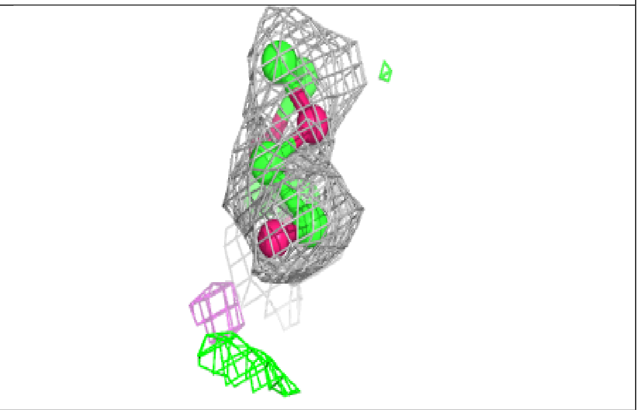


Electron density around PGE C 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

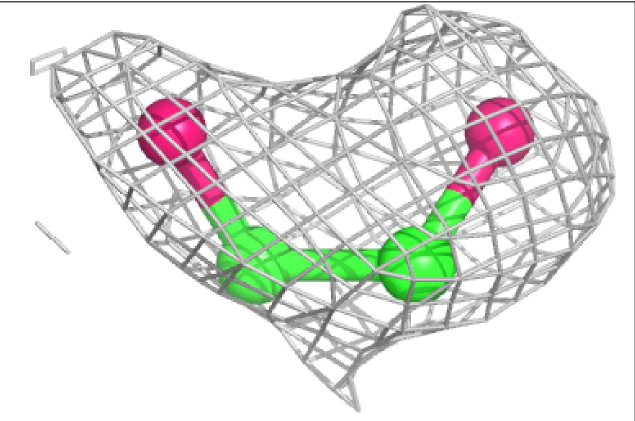


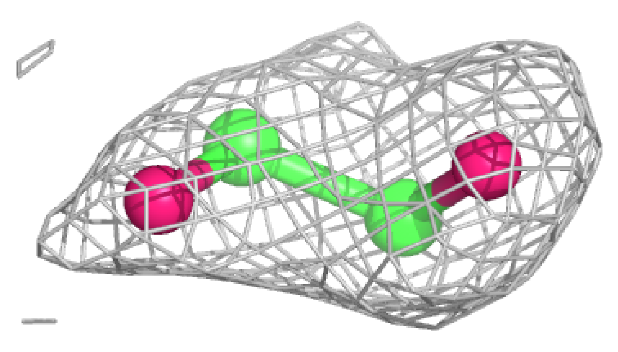


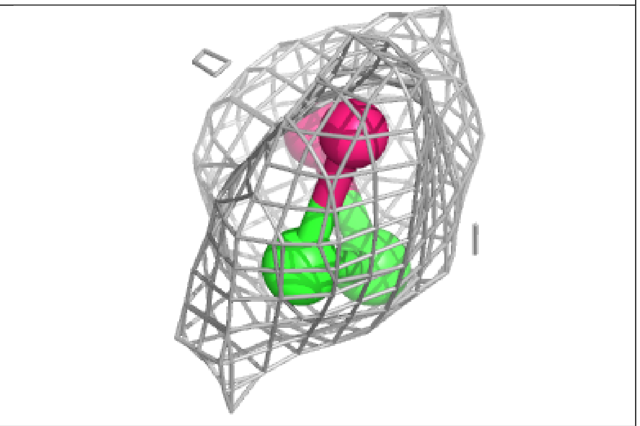


Electron density around EDO L 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

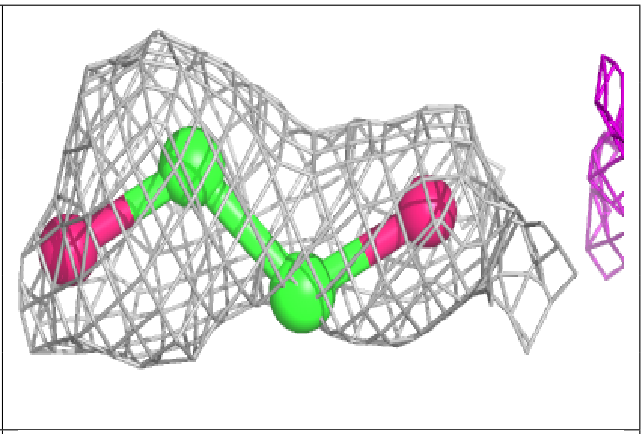


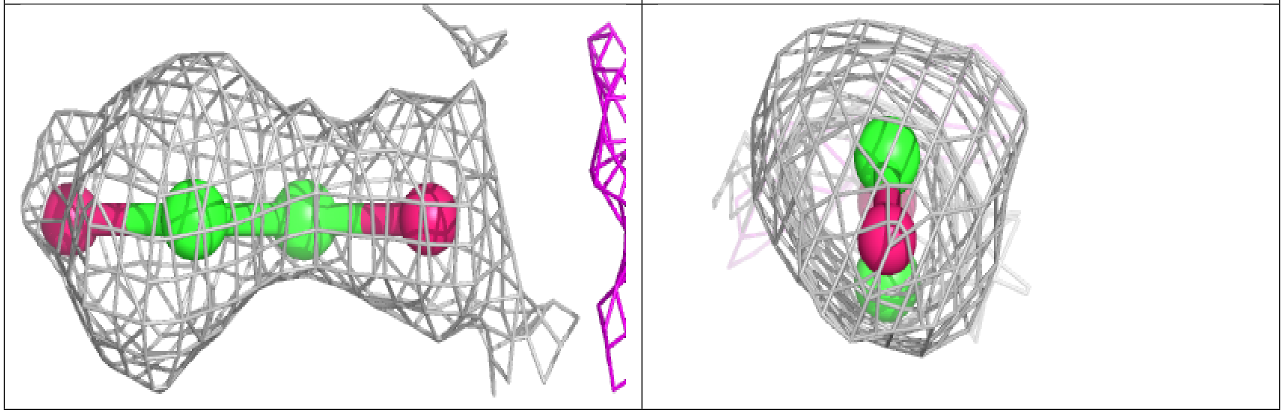




Electron density around EDO H 304:

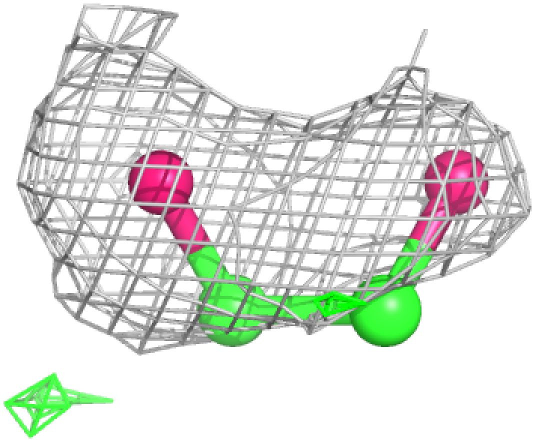
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

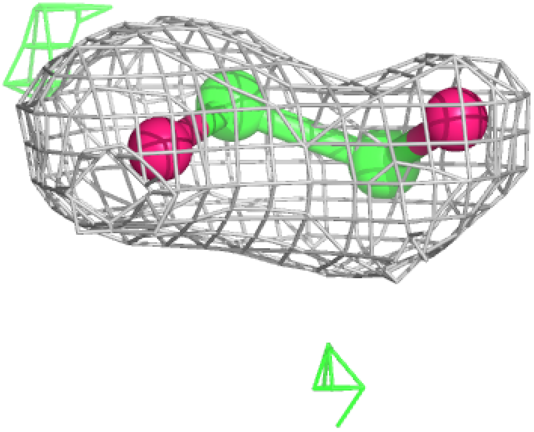


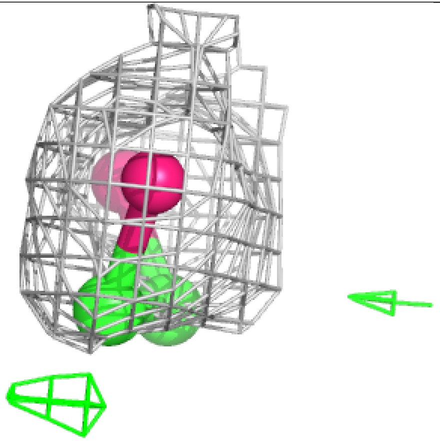


Electron density around EDO E 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

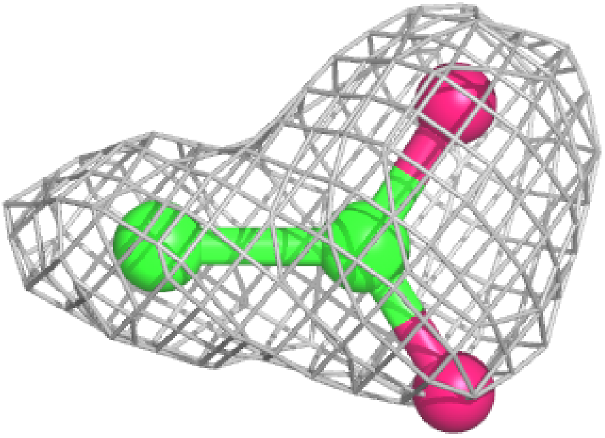


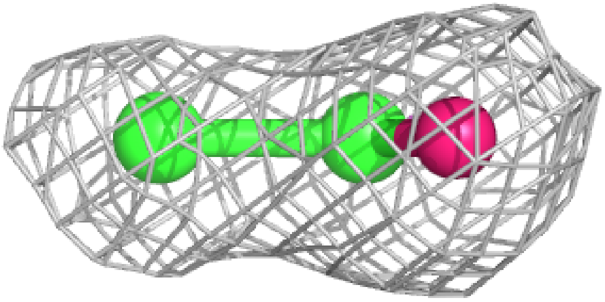


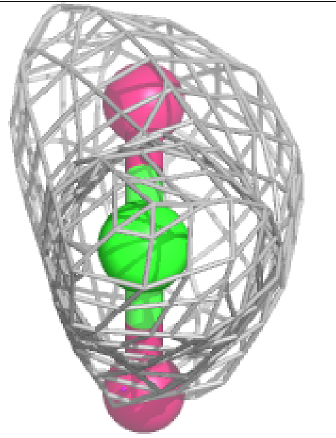


Electron density around ACT F 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

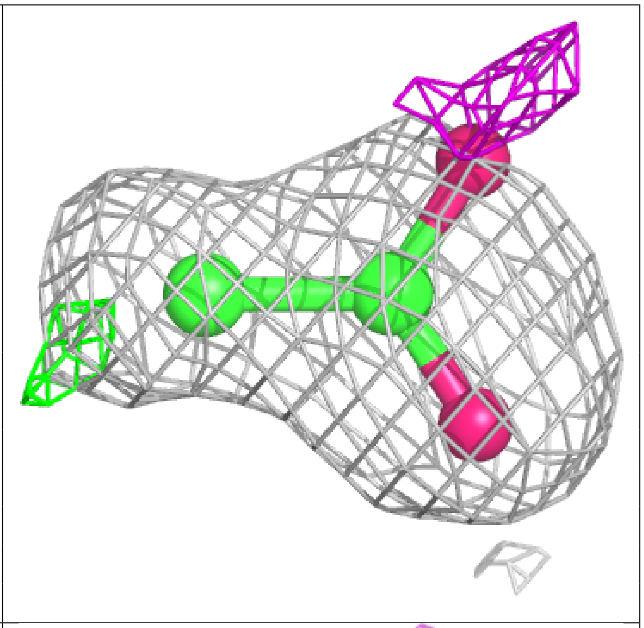


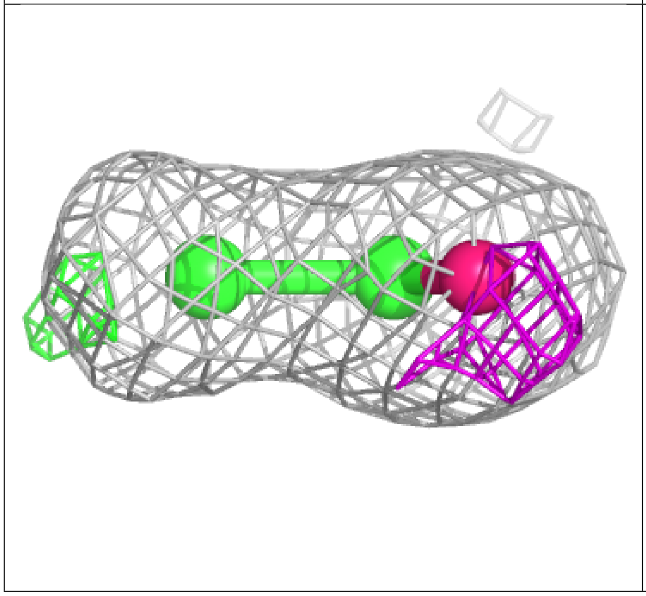


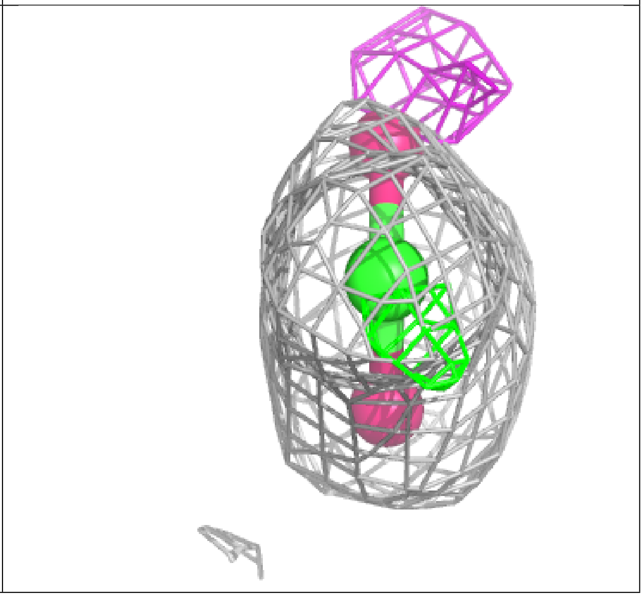


Electron density around ACT I 303:

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

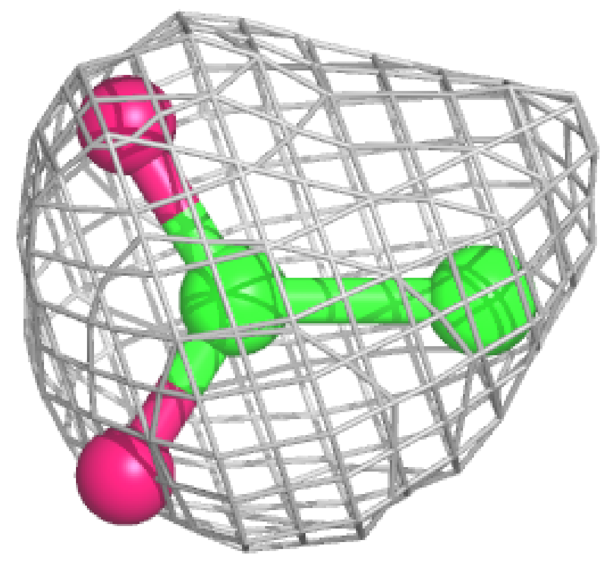


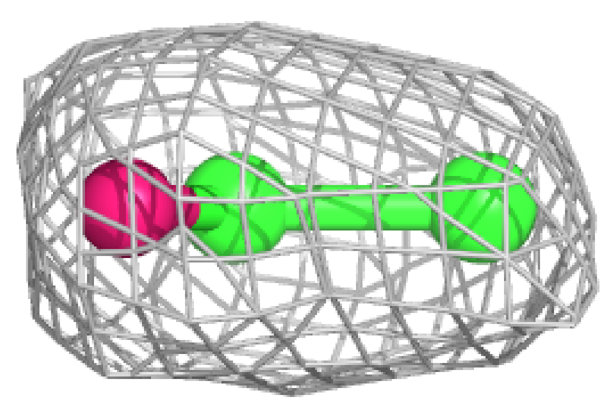


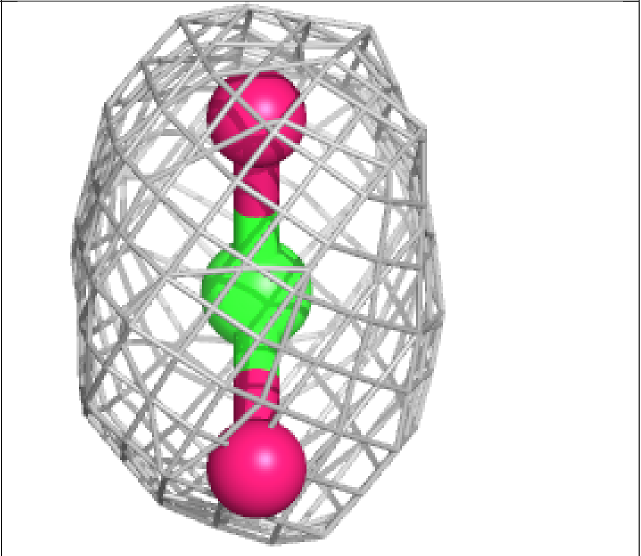


Electron density around ACT L 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

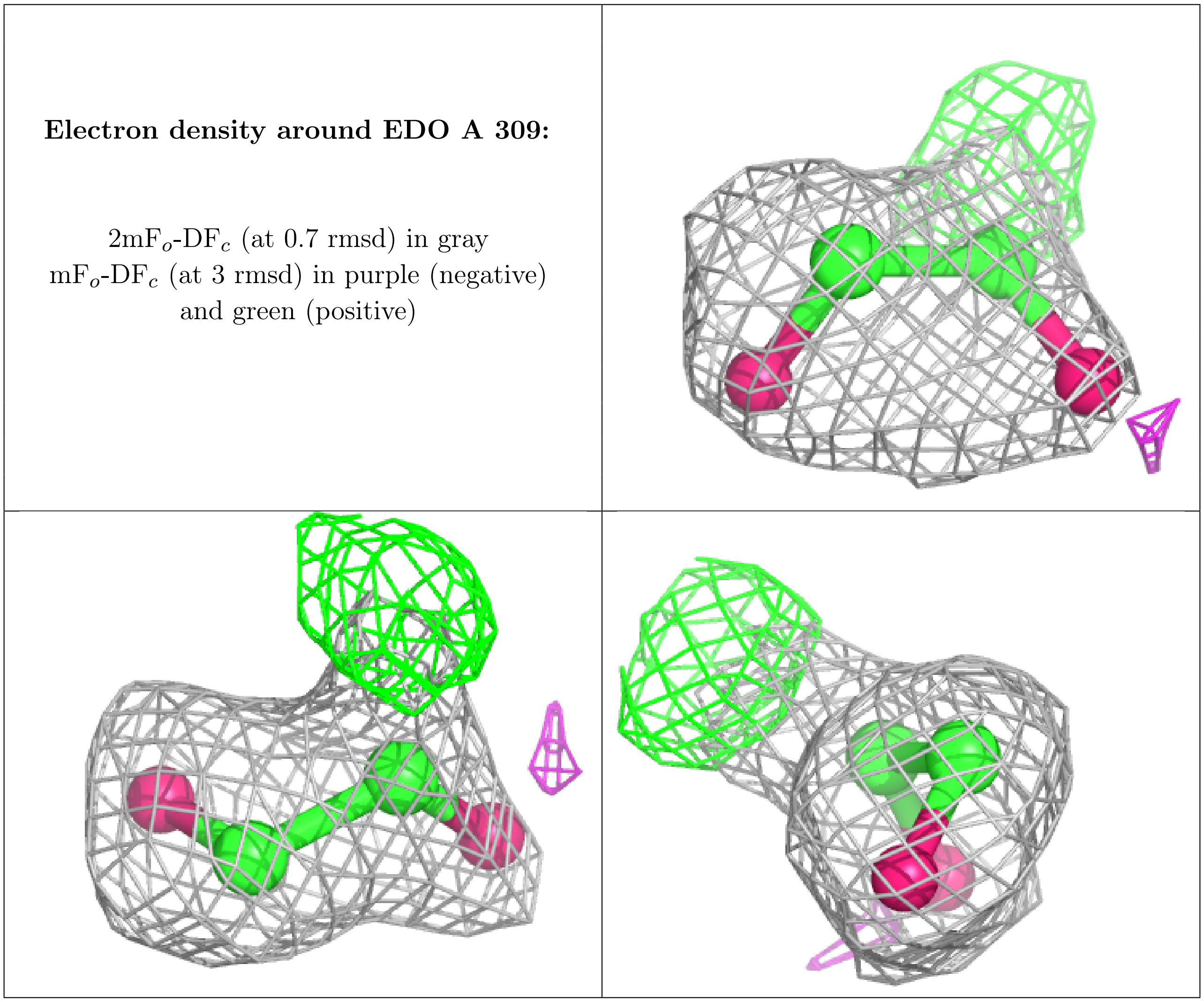






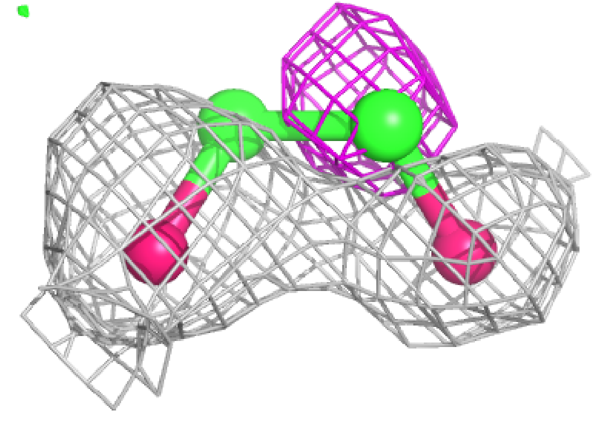
Electron density around EDO A 309:

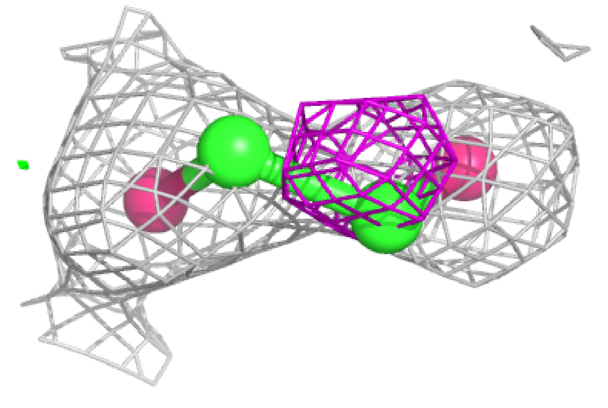
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

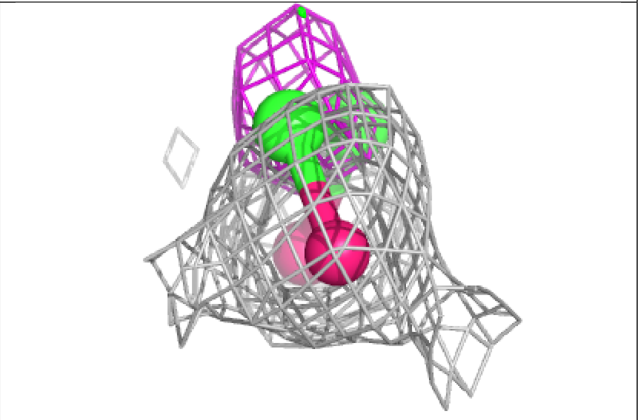


Electron density around EDO J 309:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

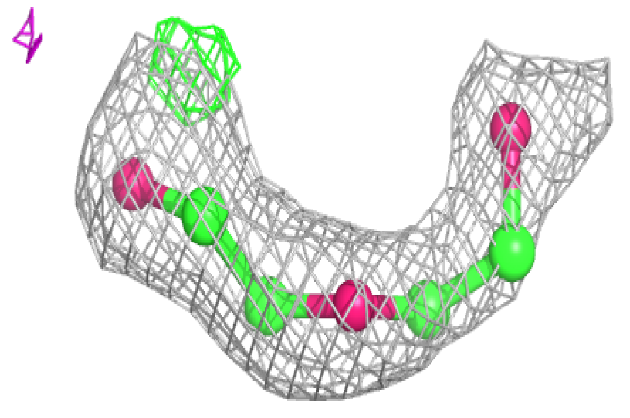


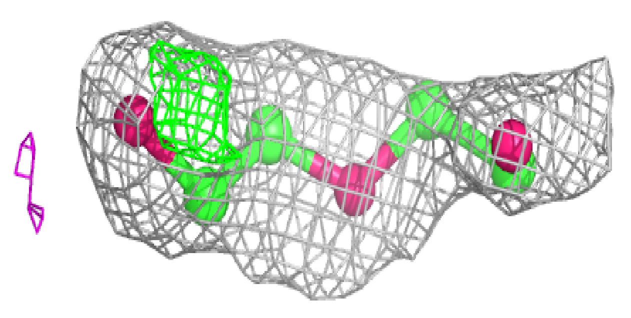


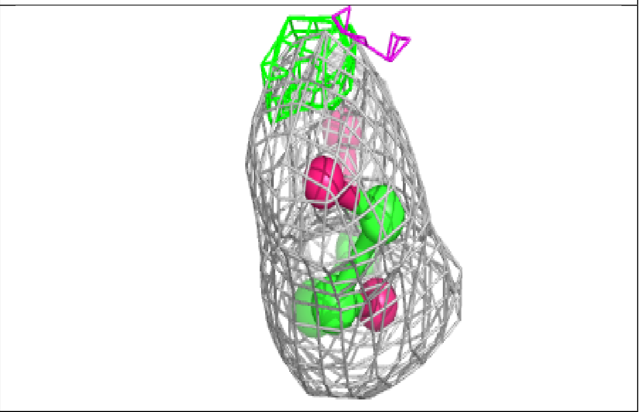


Electron density around PEG L 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

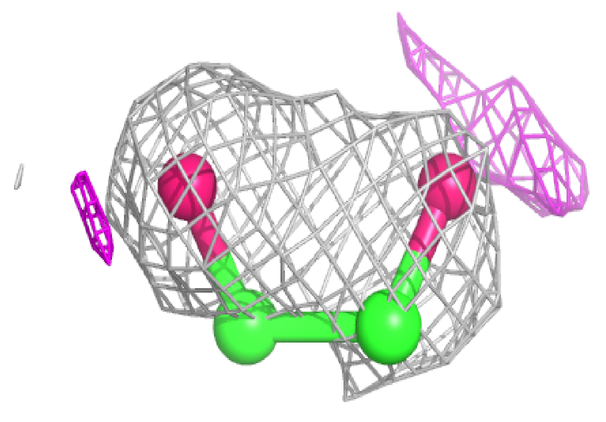


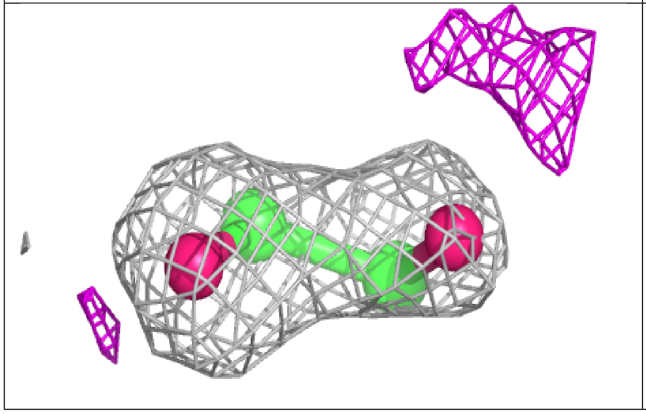


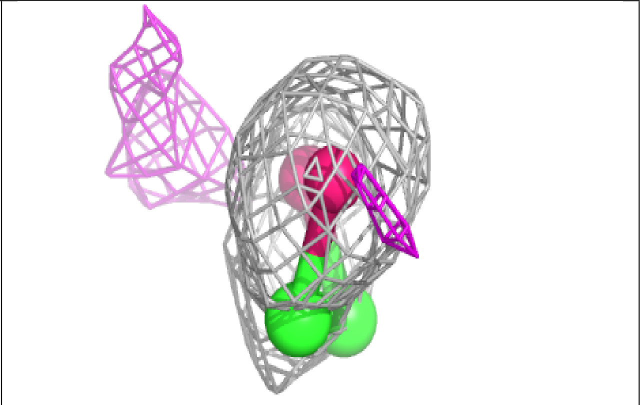


Electron density around EDO E 309:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

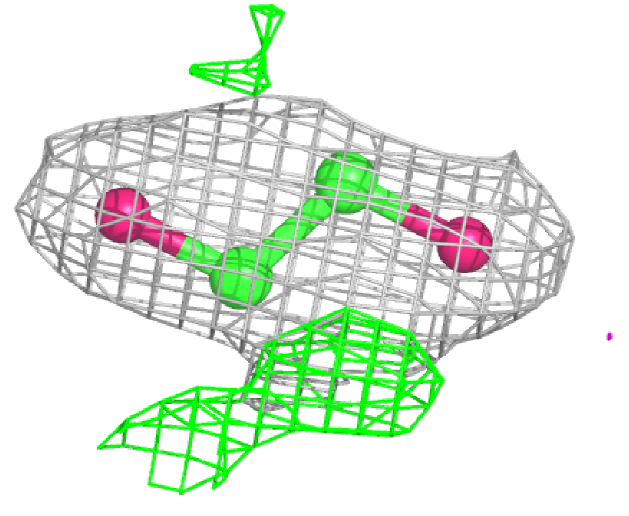


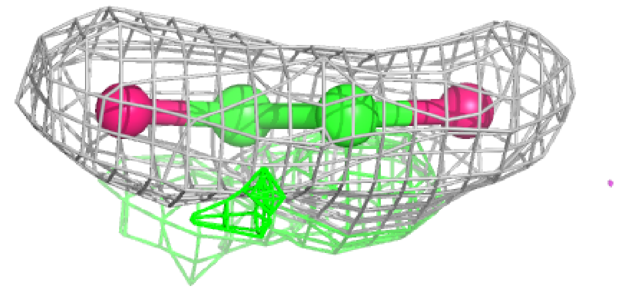


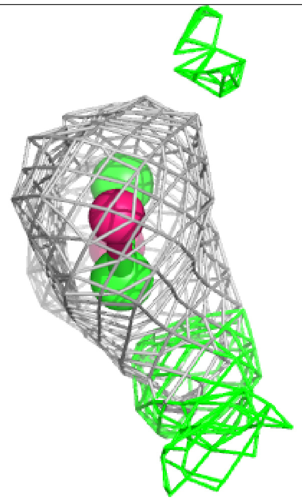


Electron density around EDO F 303:

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

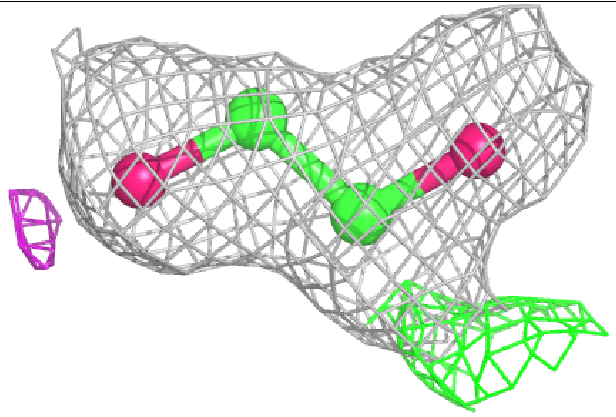


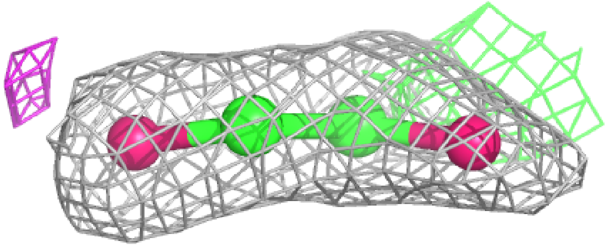


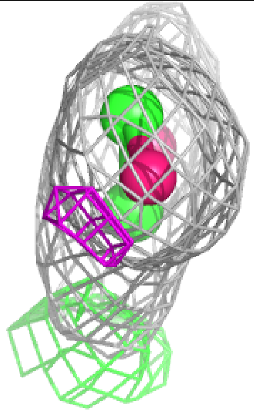


Electron density around EDO B 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

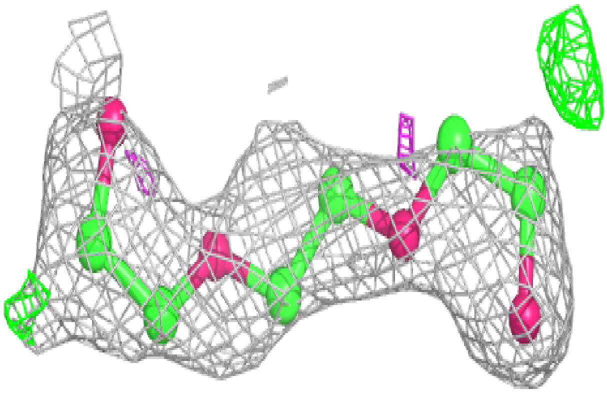


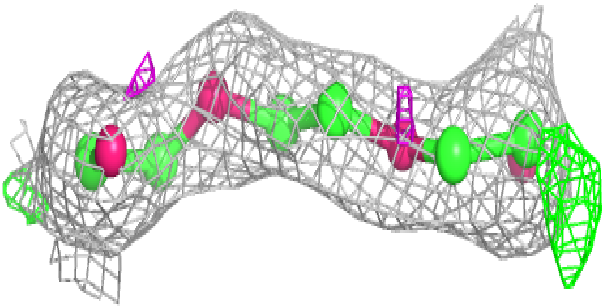


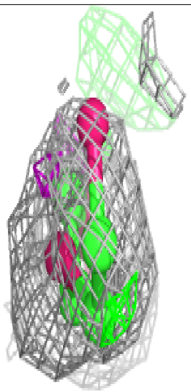


Electron density around PGE L 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

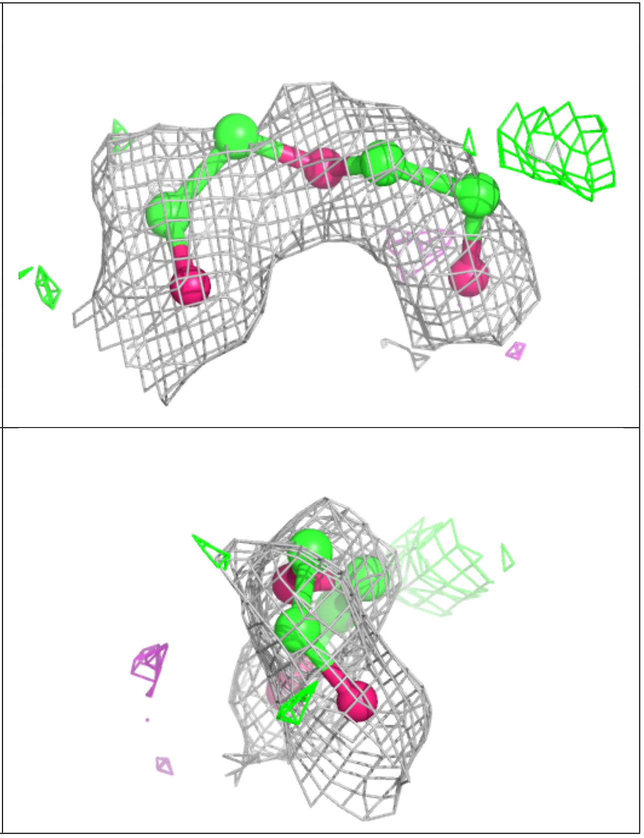






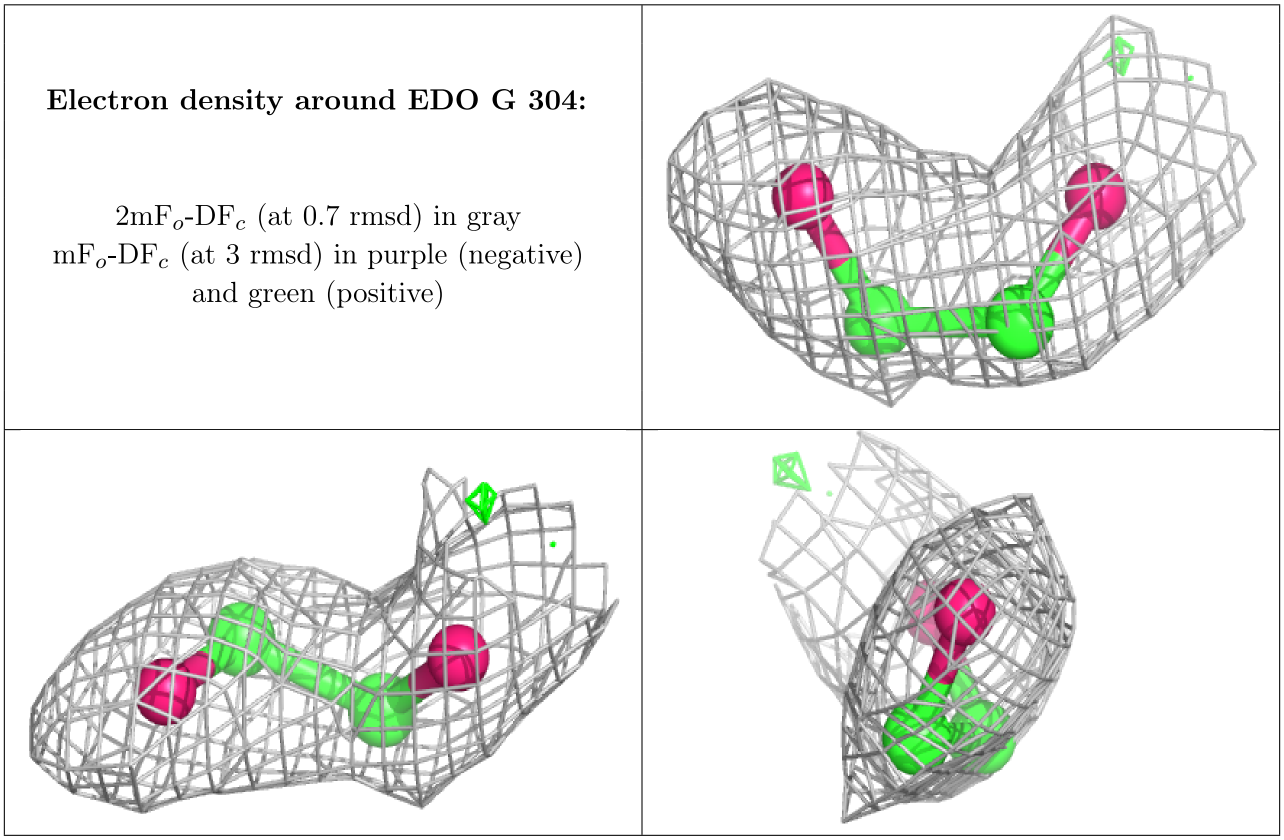
Electron density around PEG J 311:

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



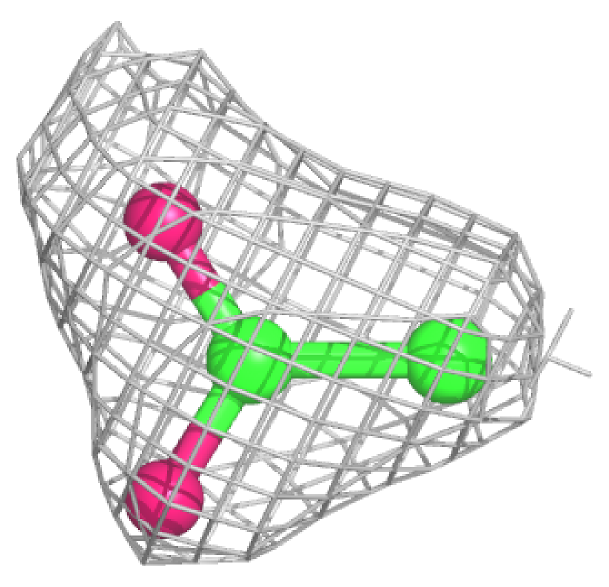
Electron density around EDO G 304:

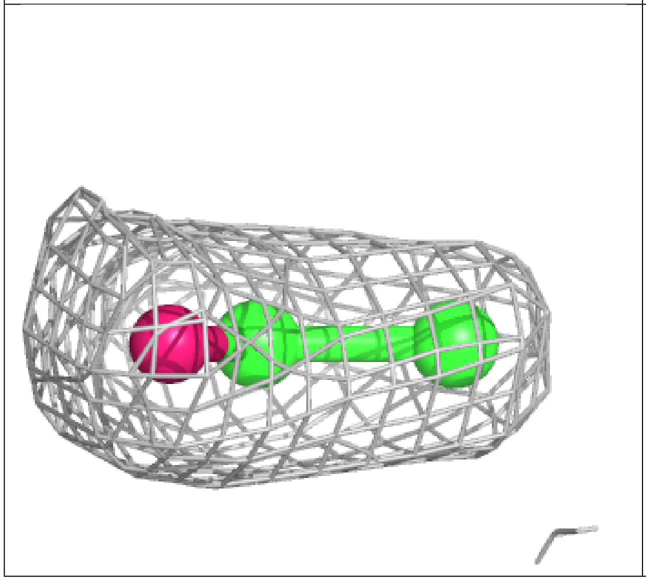
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

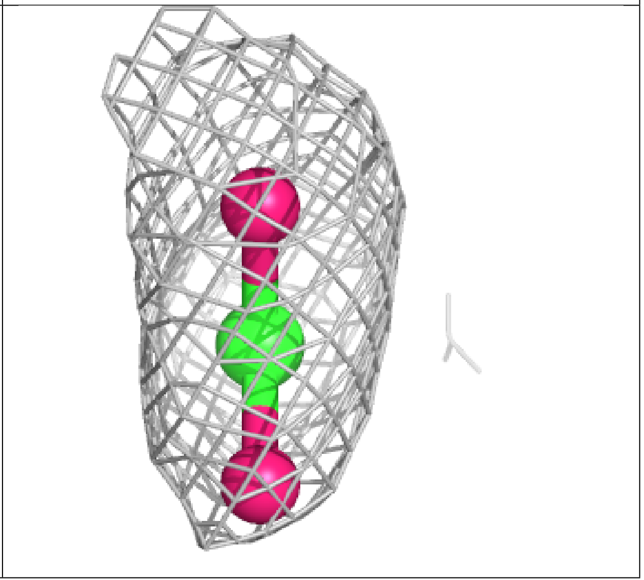


Electron density around ACT C 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

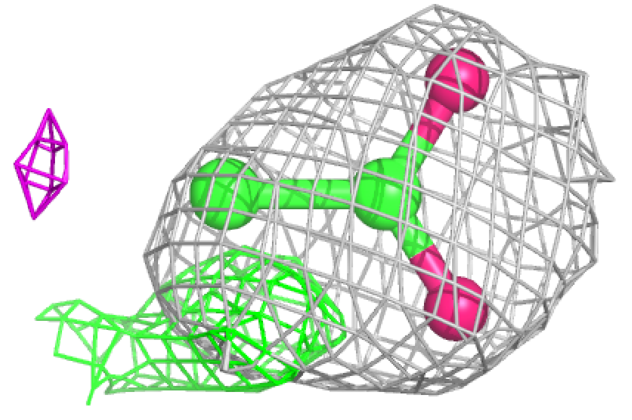


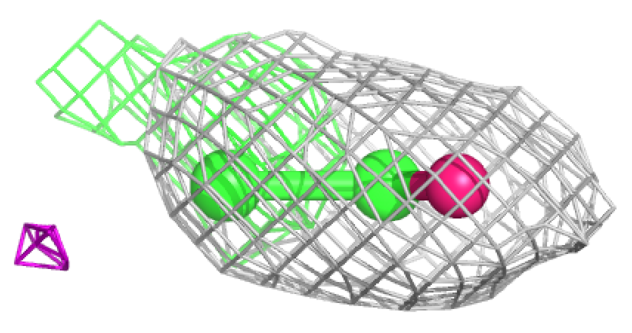


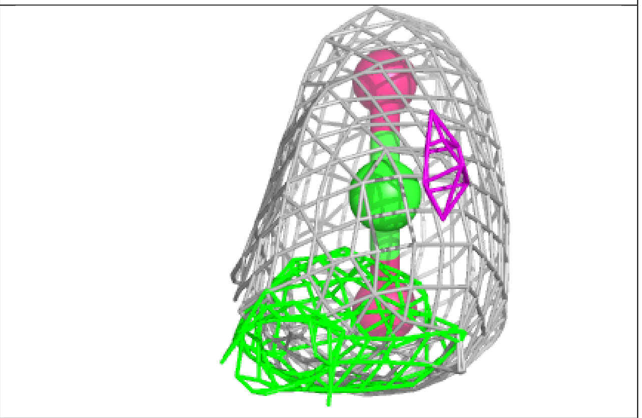


Electron density around ACT B 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

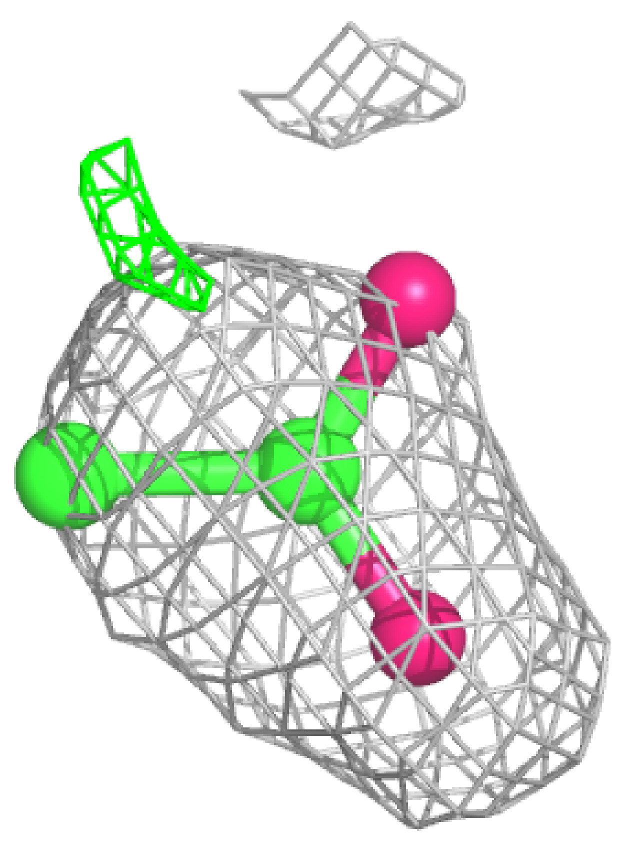


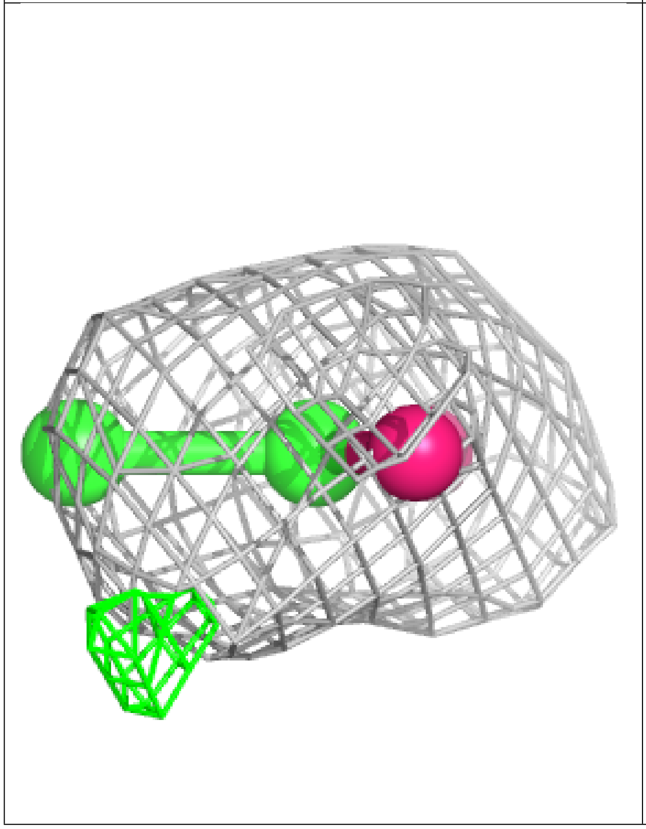


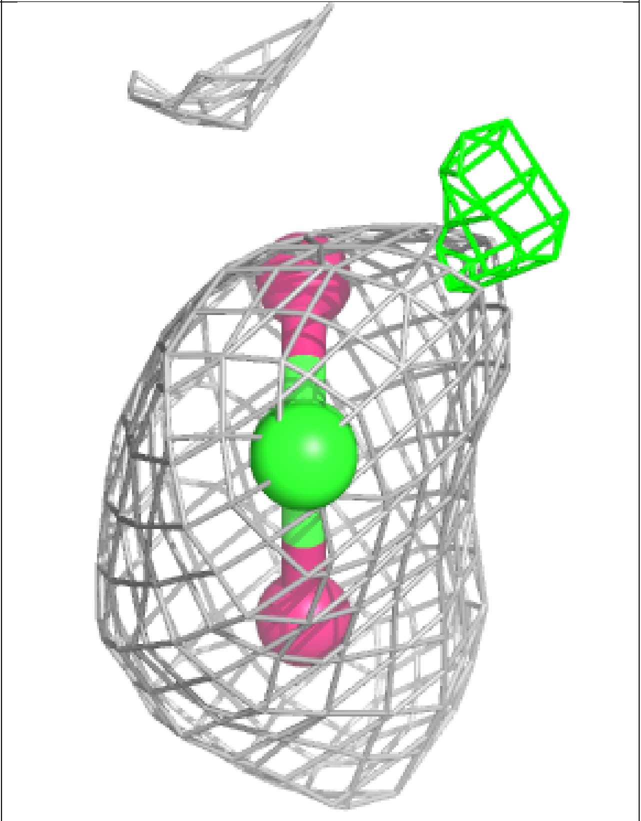


Electron density around ACT H 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

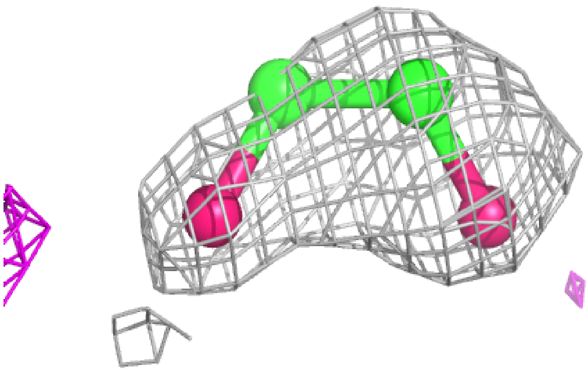


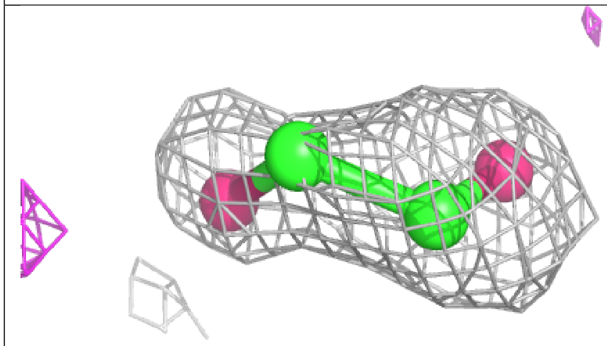


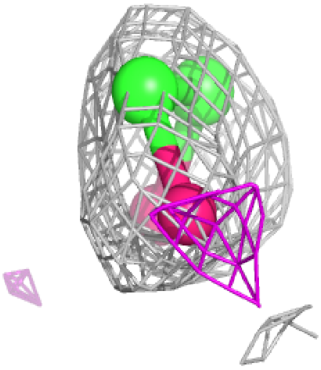


Electron density around EDO L 305:

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

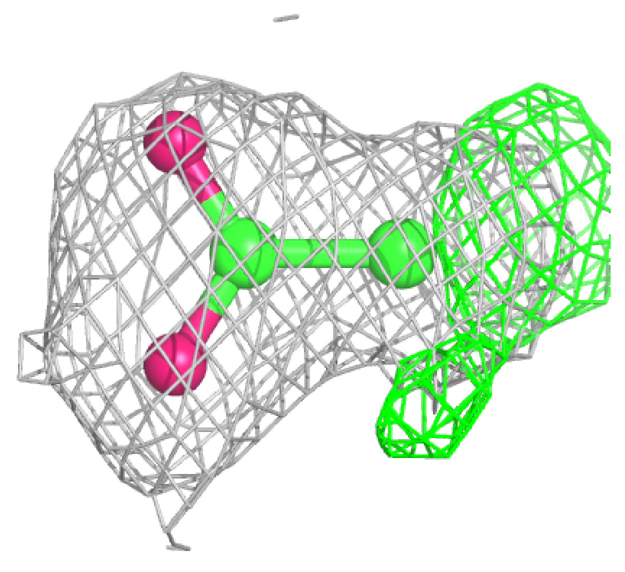


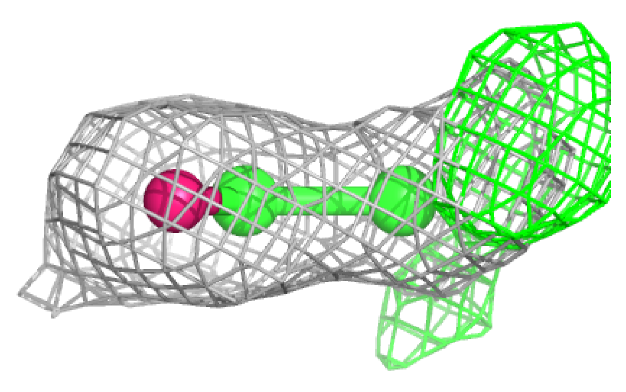


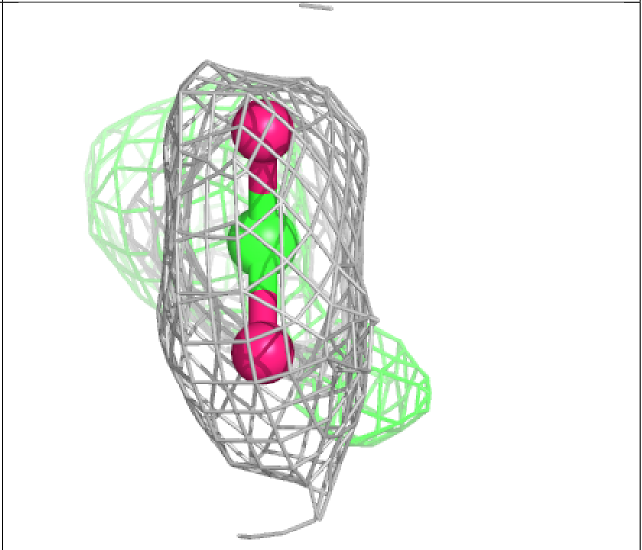


Electron density around ACT H 302:

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

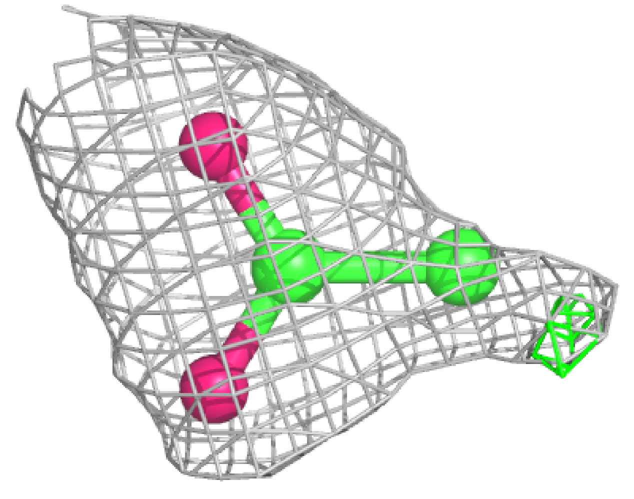


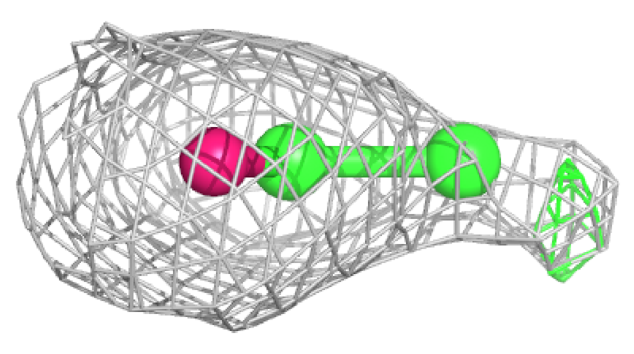


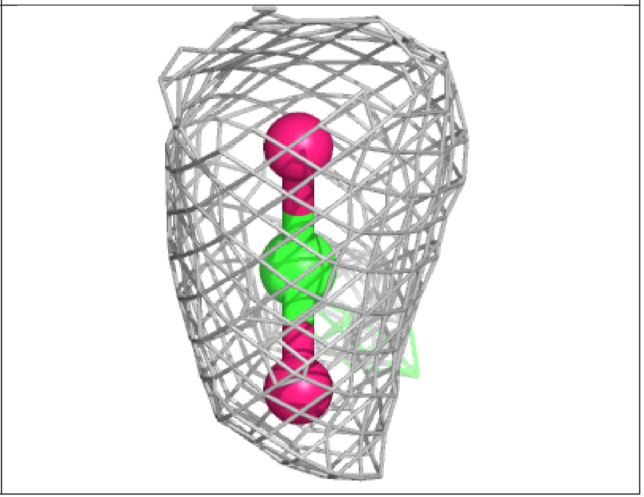


Electron density around ACT A 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

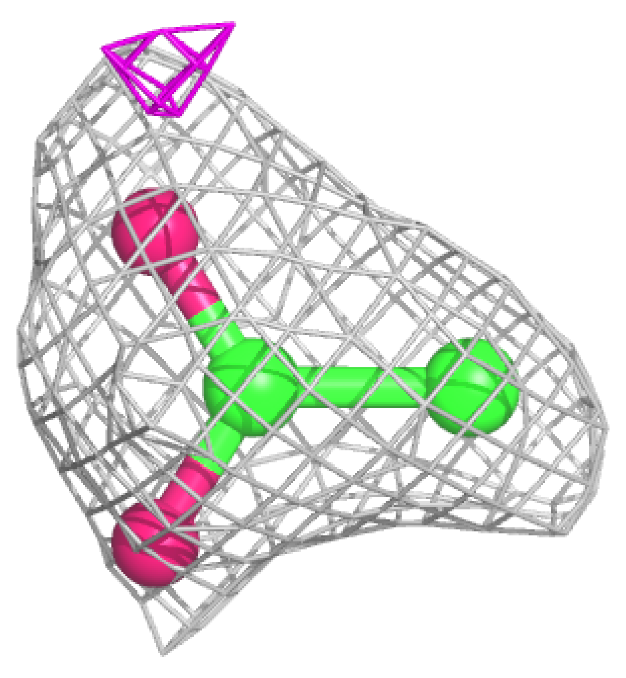


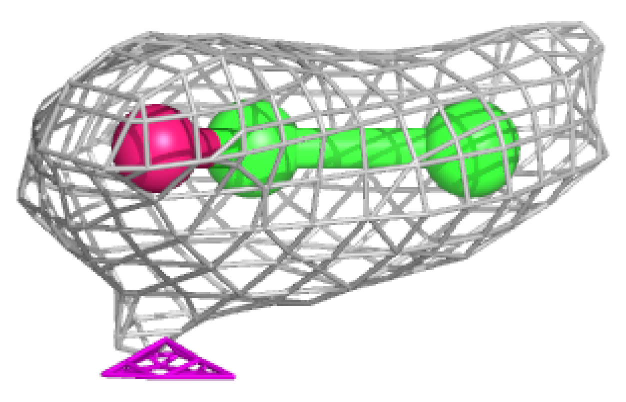


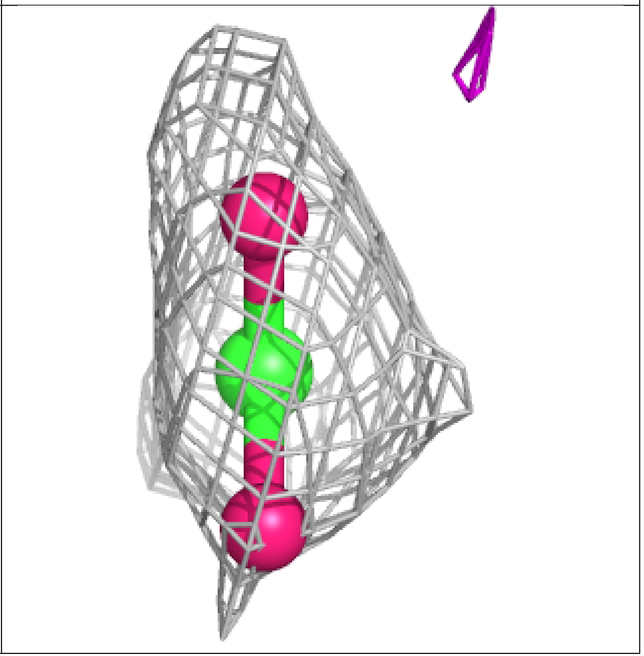


Electron density around ACT B 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

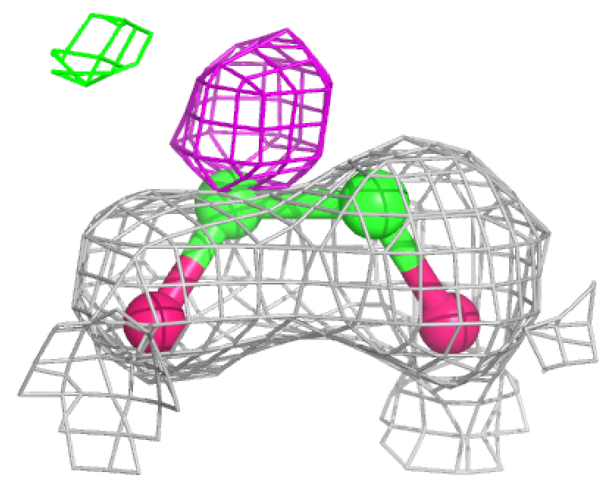


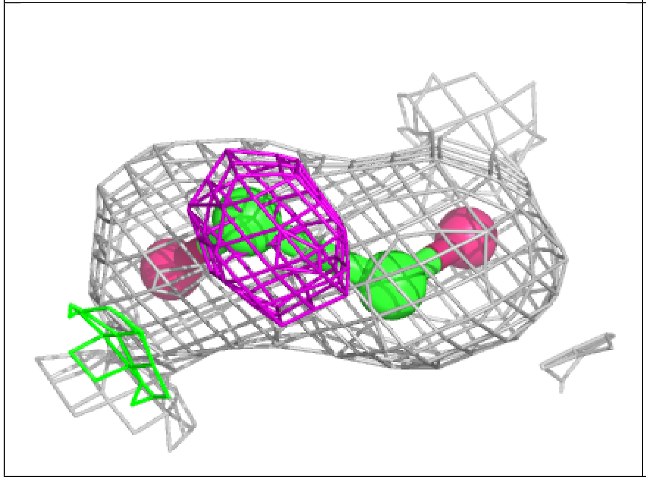


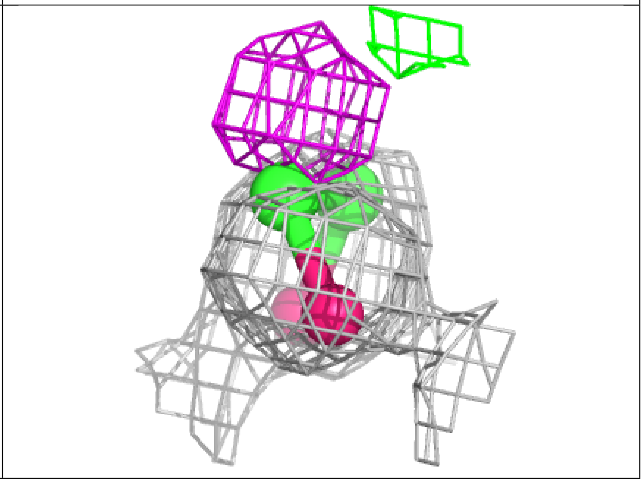


Electron density around EDO J 306:

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

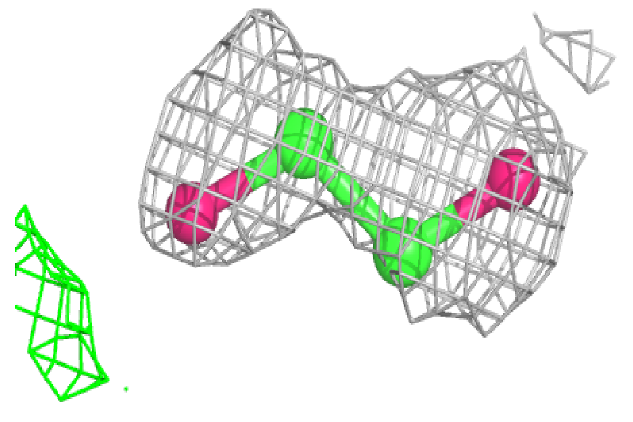


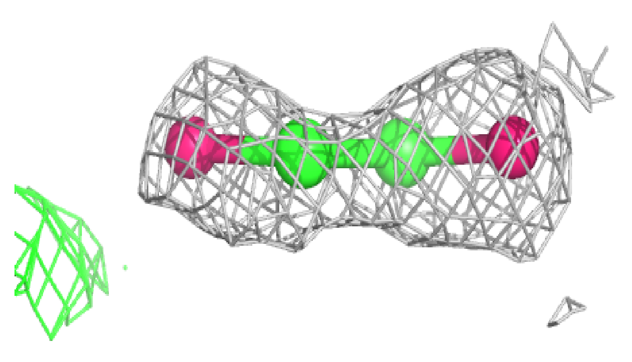


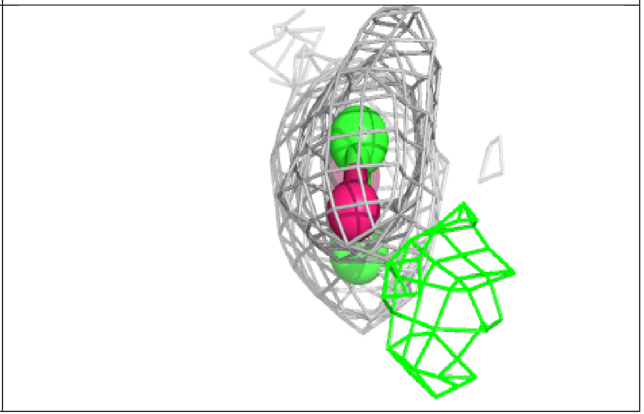


Electron density around EDO A 306:

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

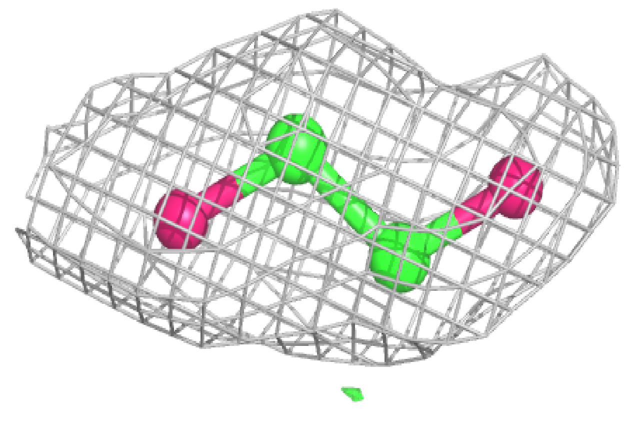


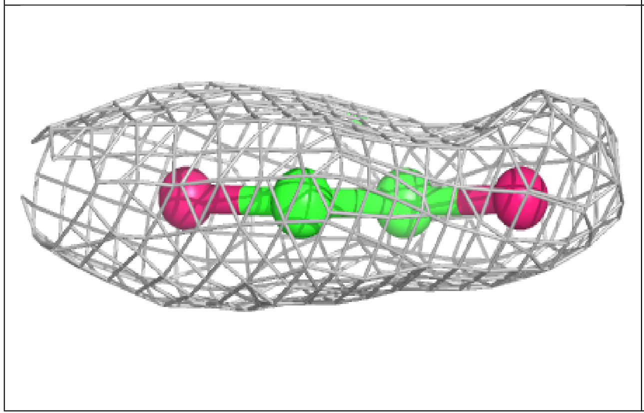


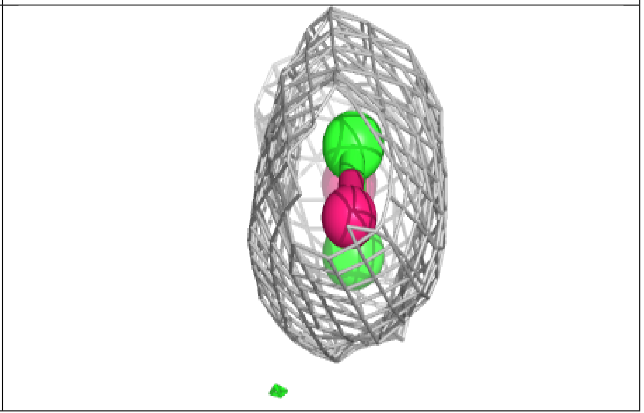


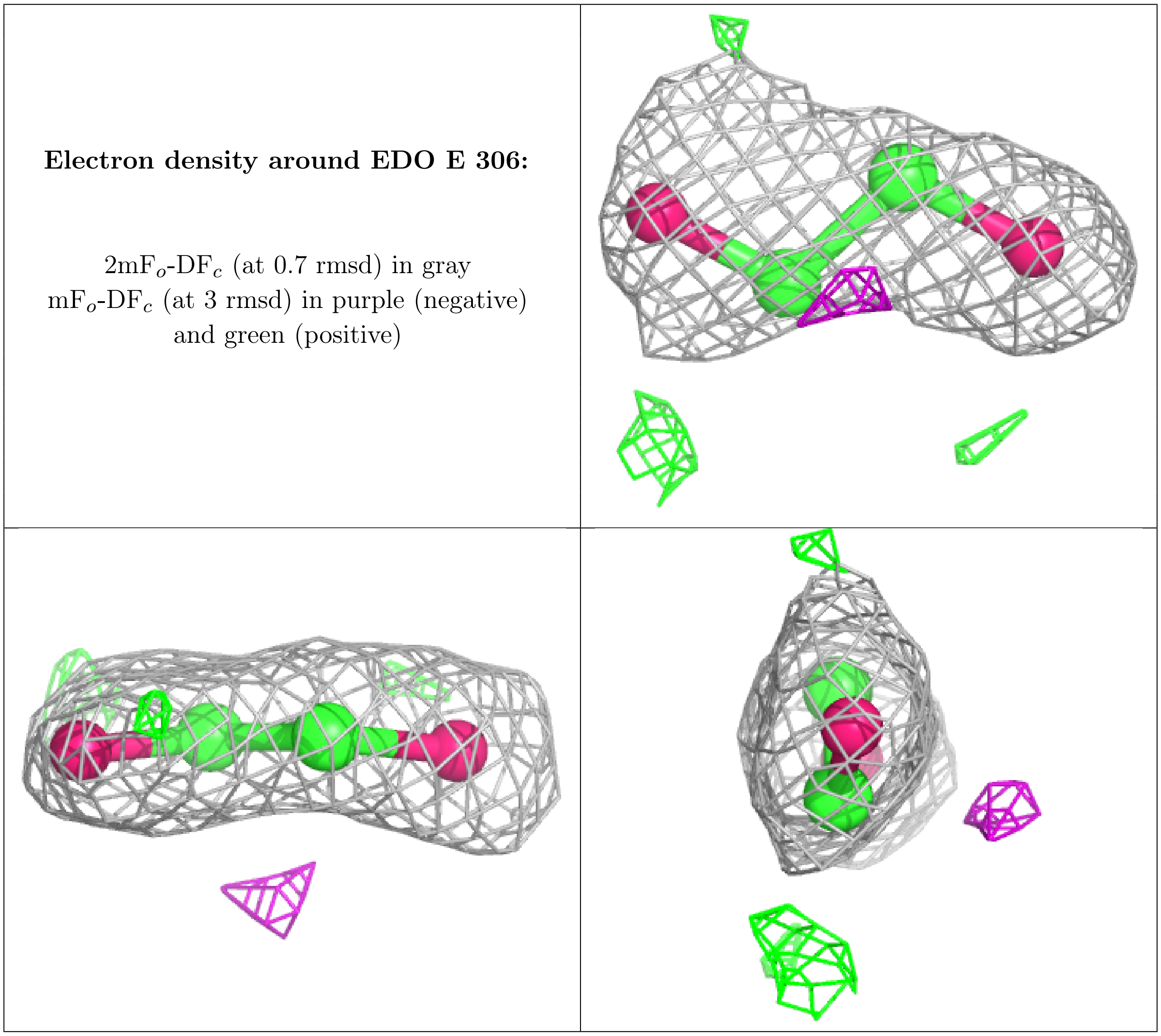
Electron density around EDO G 302:

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



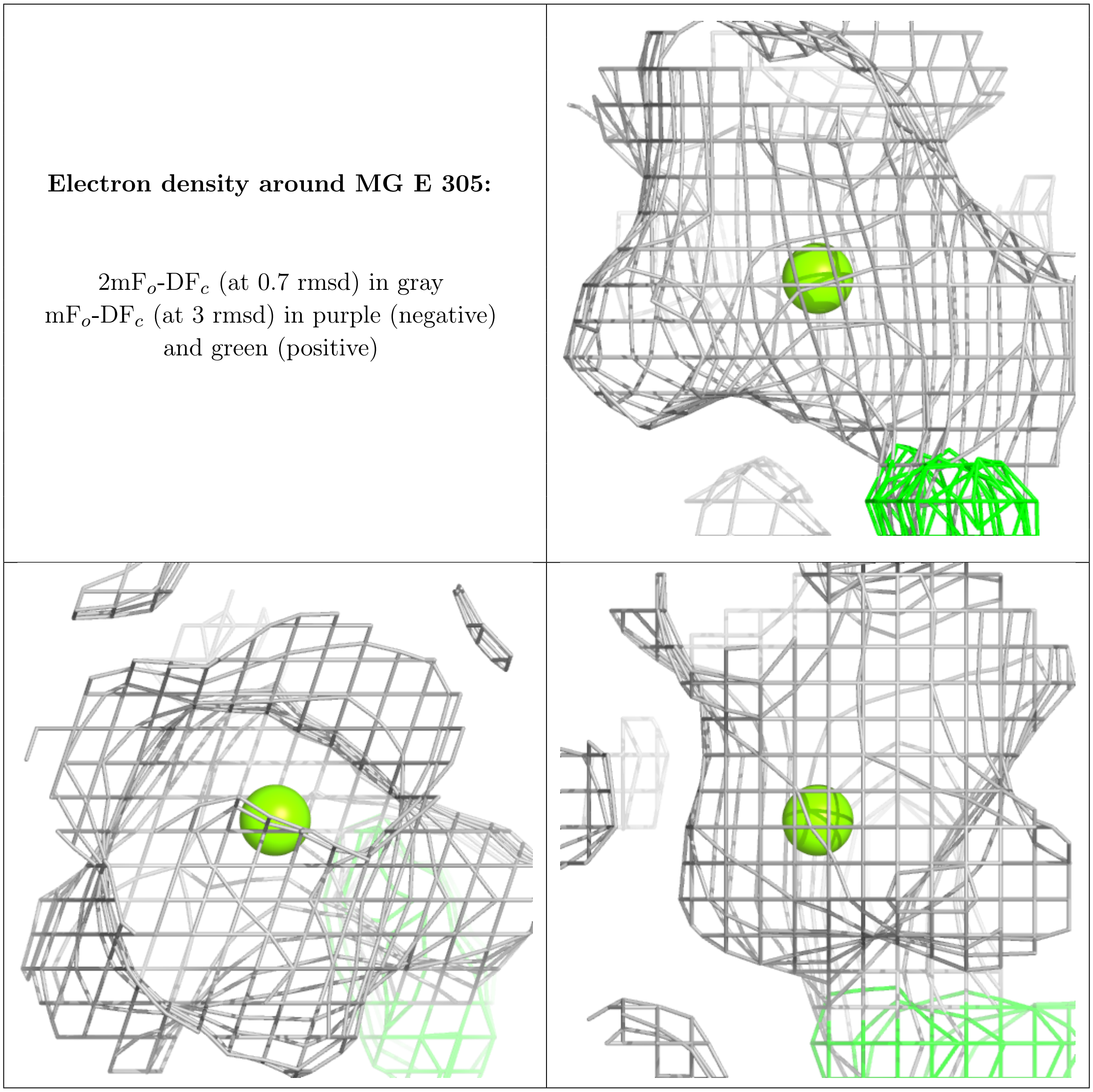






Electron density around EDO E 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

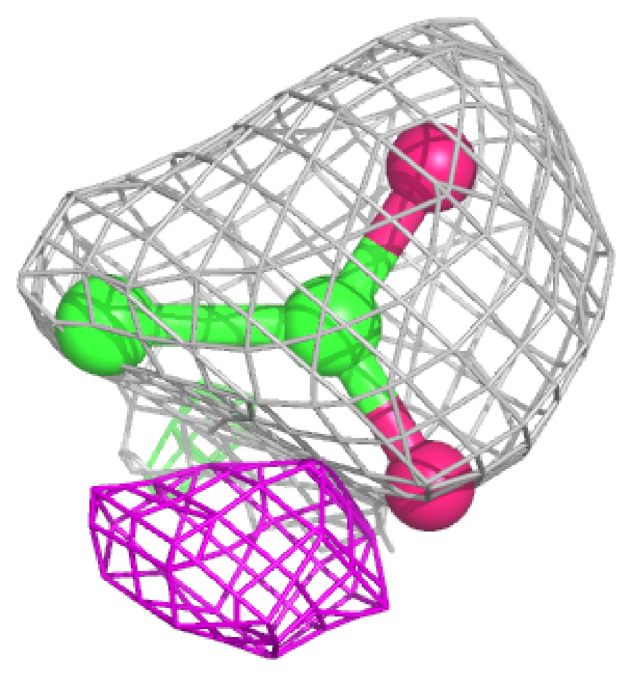


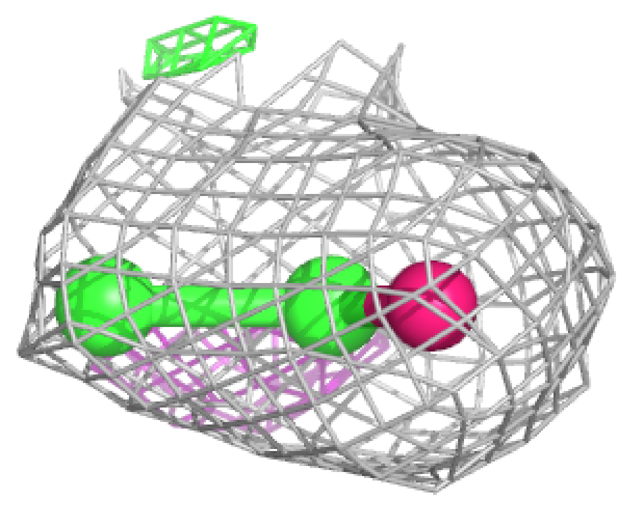
Electron density around MG E 305:

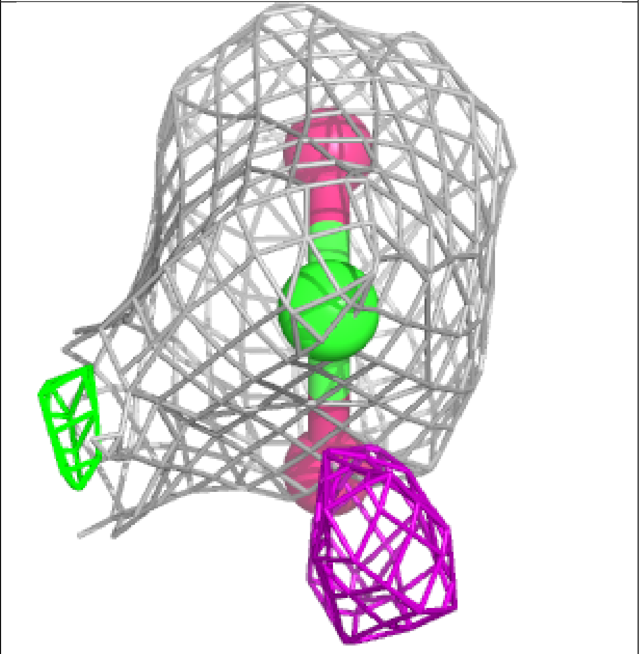
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ACT 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)

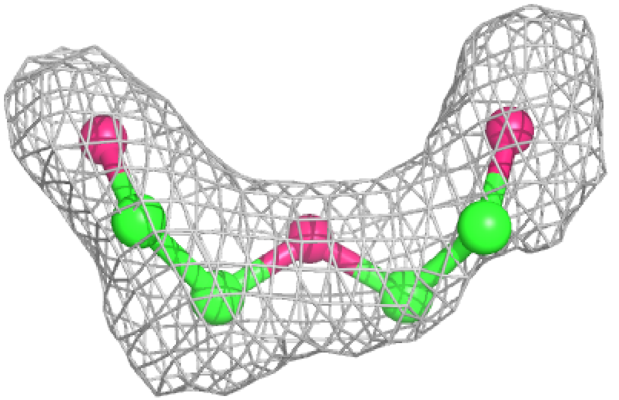


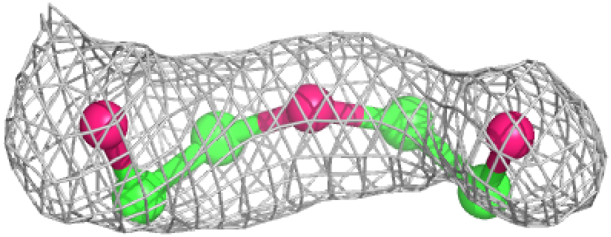


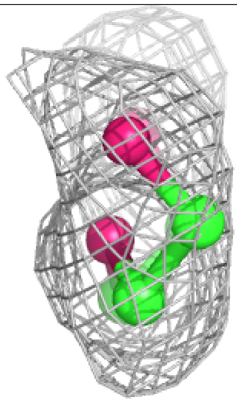


Electron density around PEG F 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

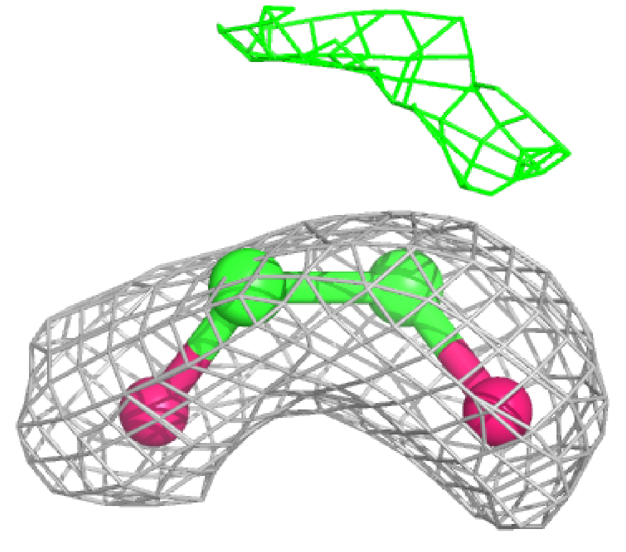


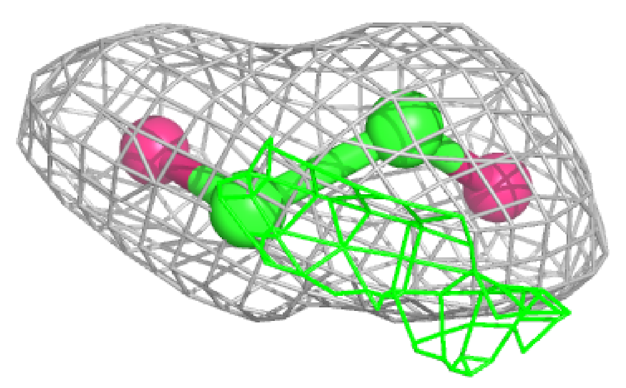


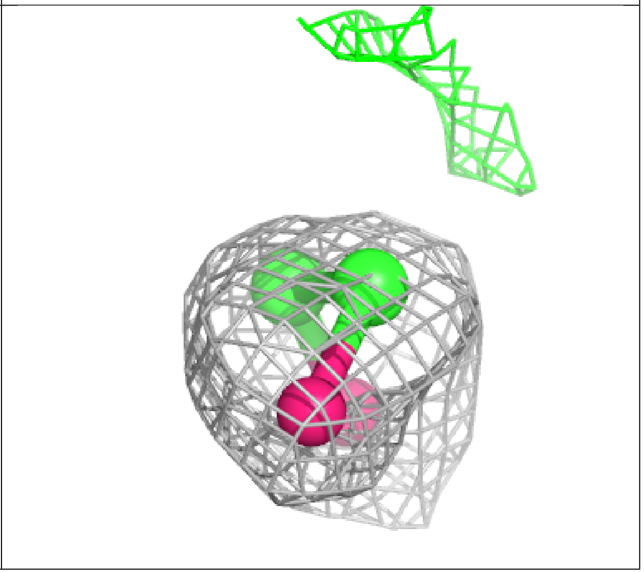


Electron density around EDO G 306:

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

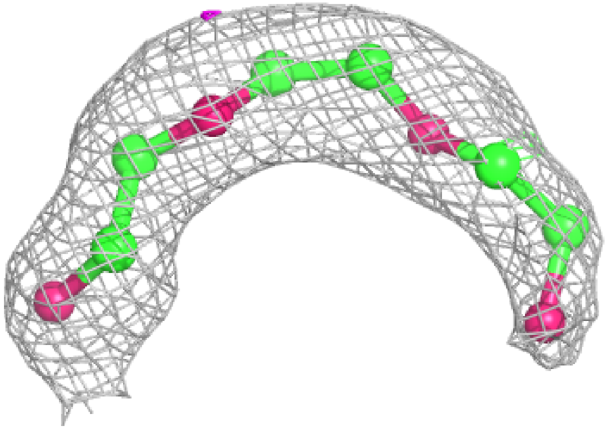


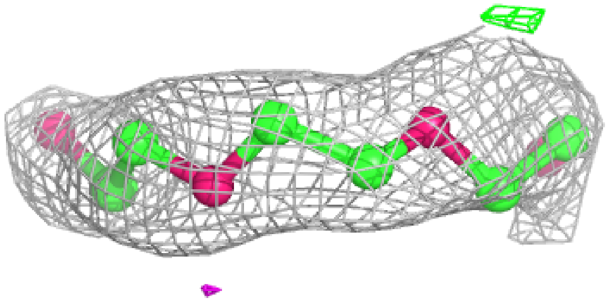


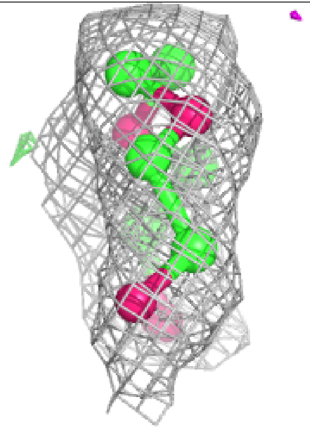


Electron density around PGE D 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

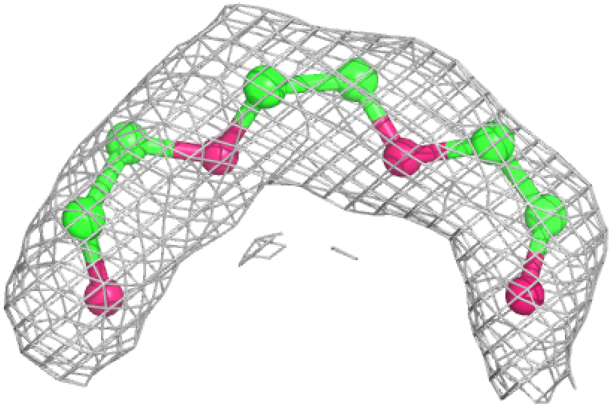


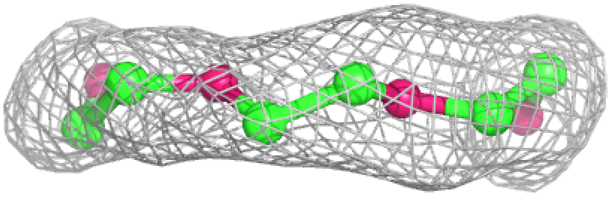


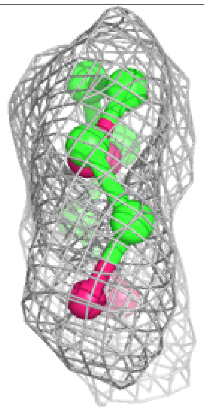


Electron density around PGE A 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

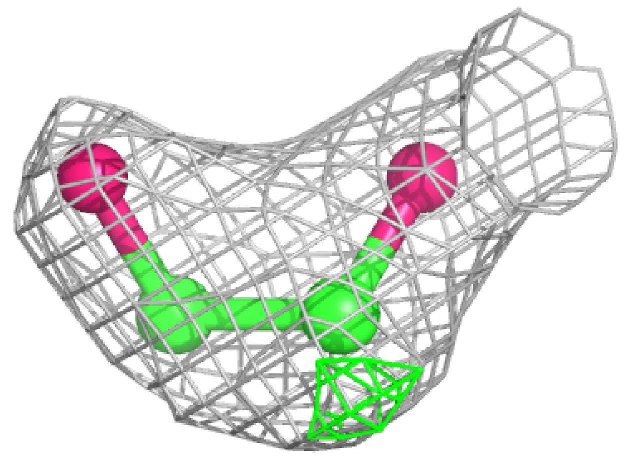


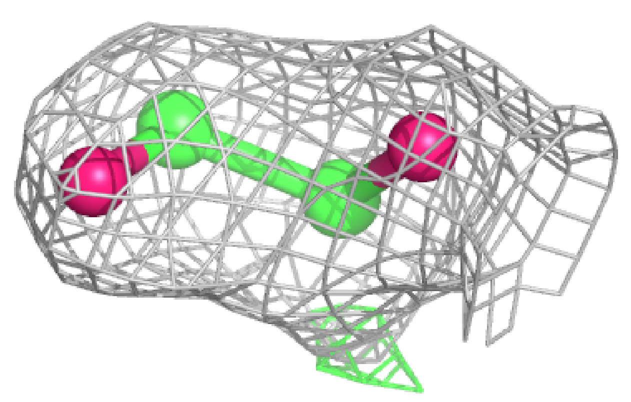


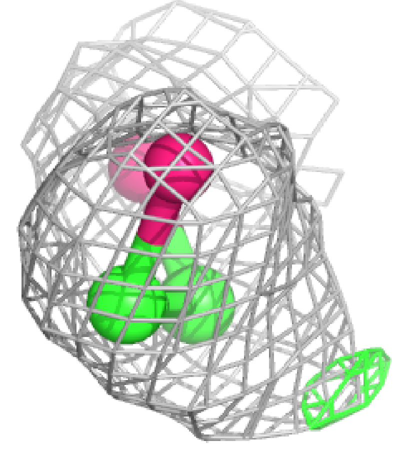


Electron density around EDO B 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

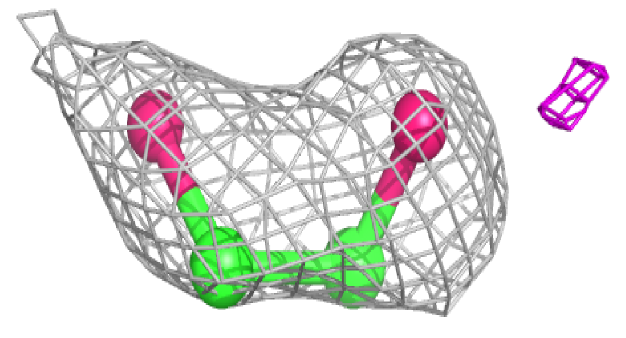


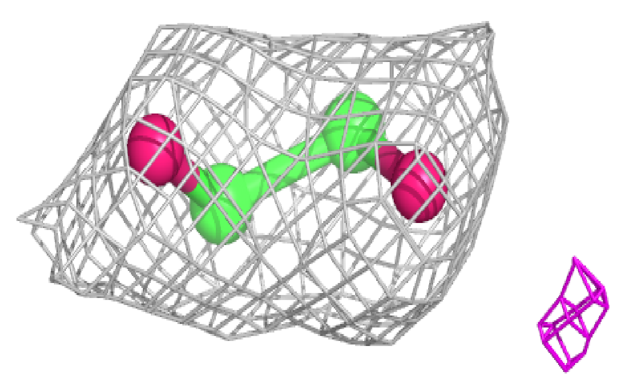


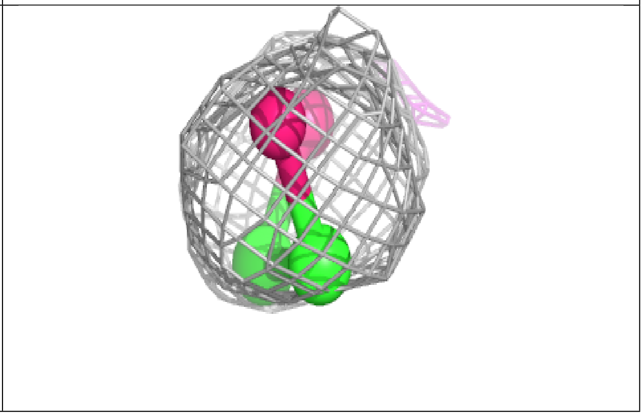


Electron density around EDO B 309:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

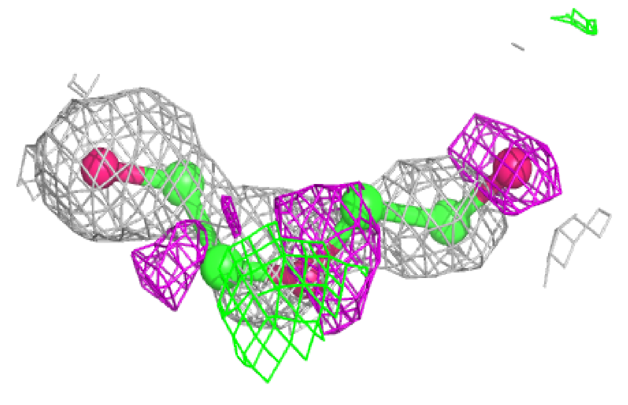


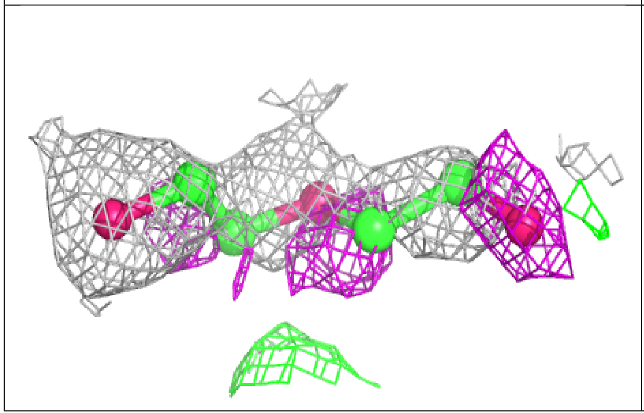


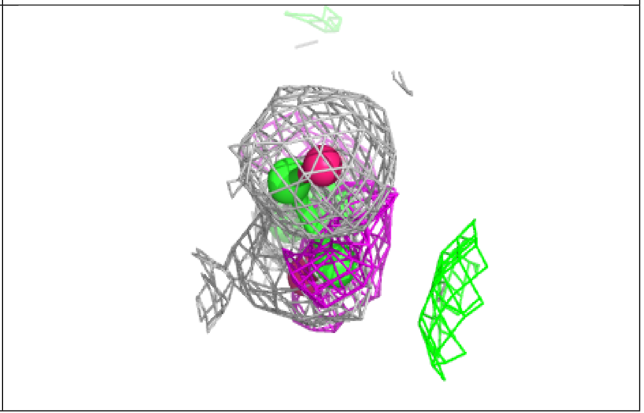


Electron density around PEG L 309:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

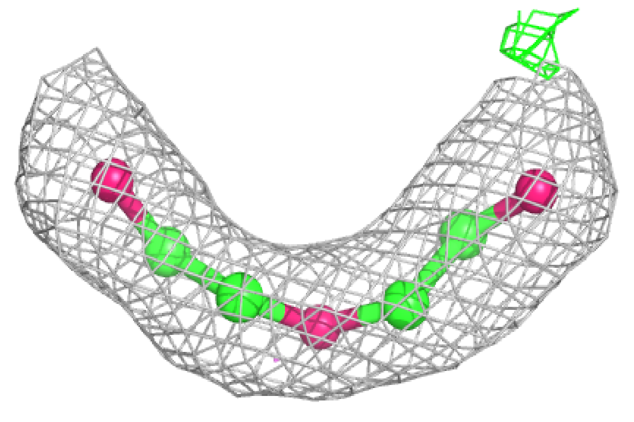


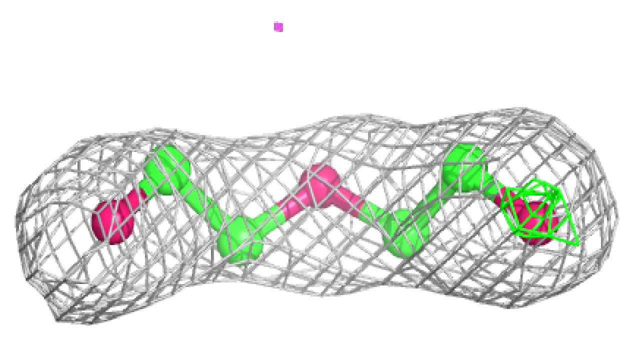


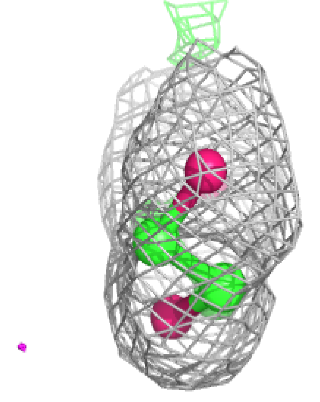


Electron density around PEG G 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

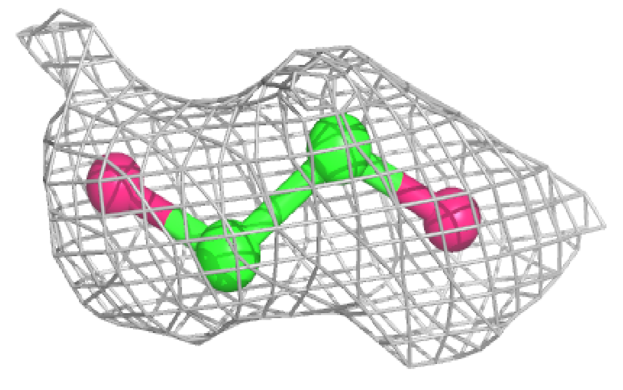


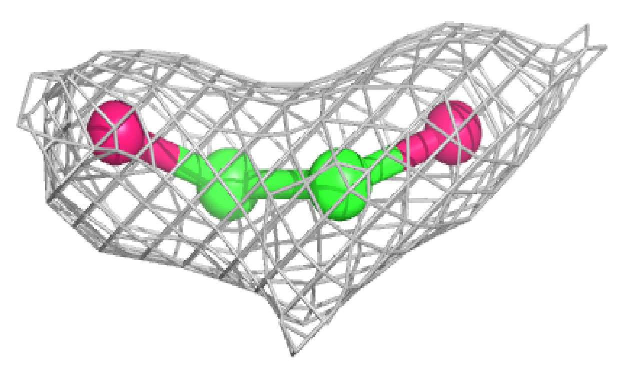


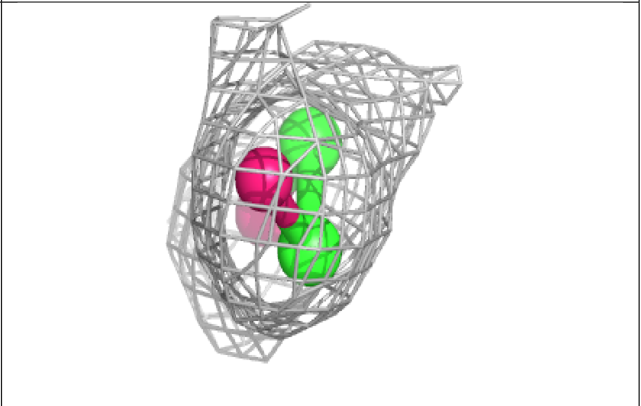


Electron density around EDO B 310:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

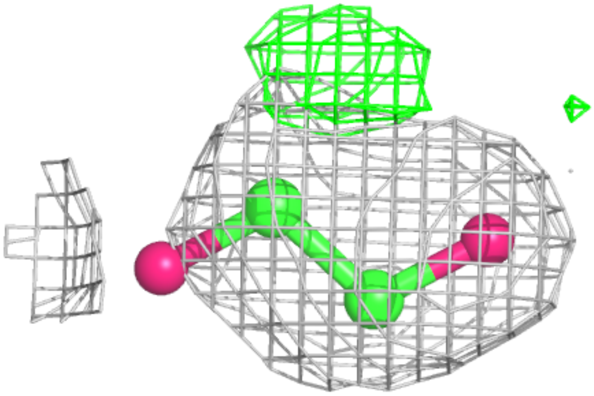


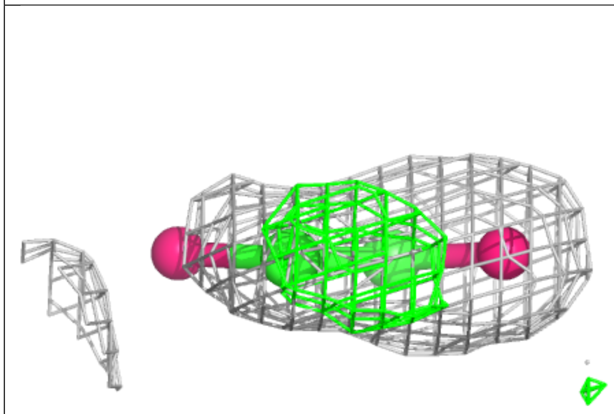


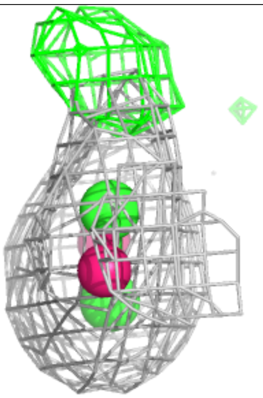


Electron density around EDO L 304:

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

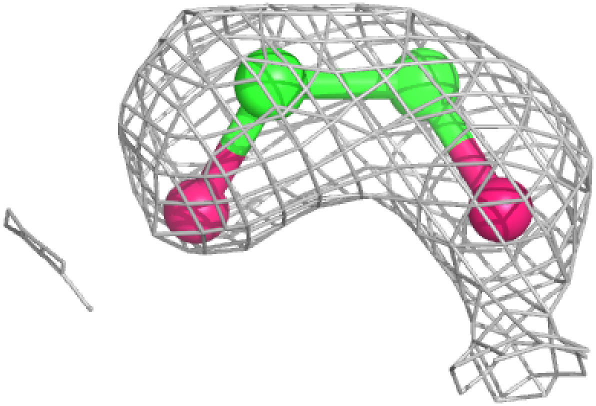


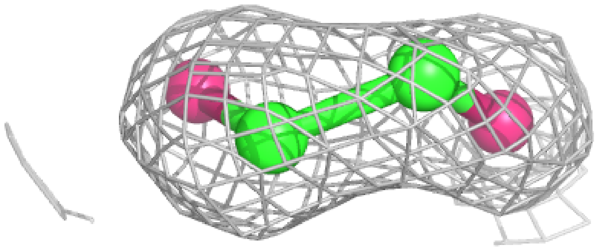


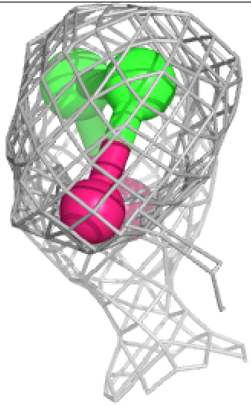


Electron density around EDO B 305:

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

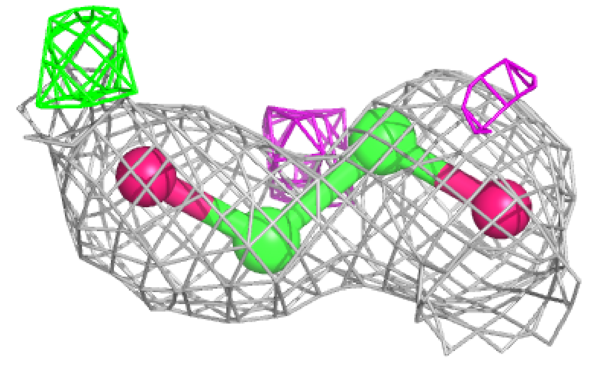


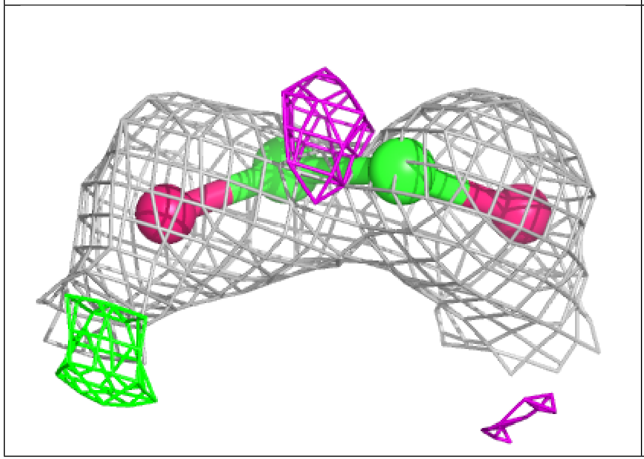


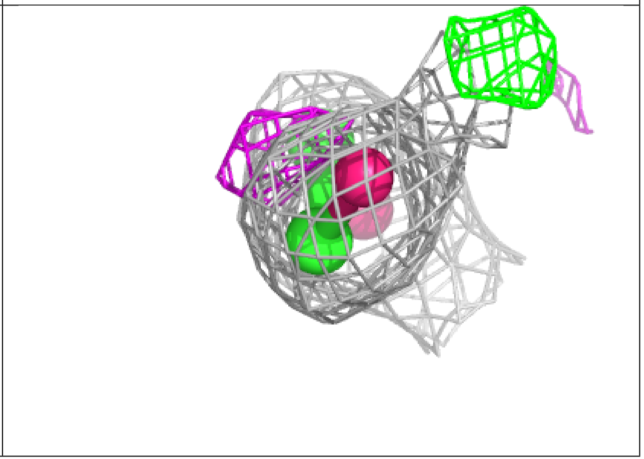


Electron density around EDO G 303:

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

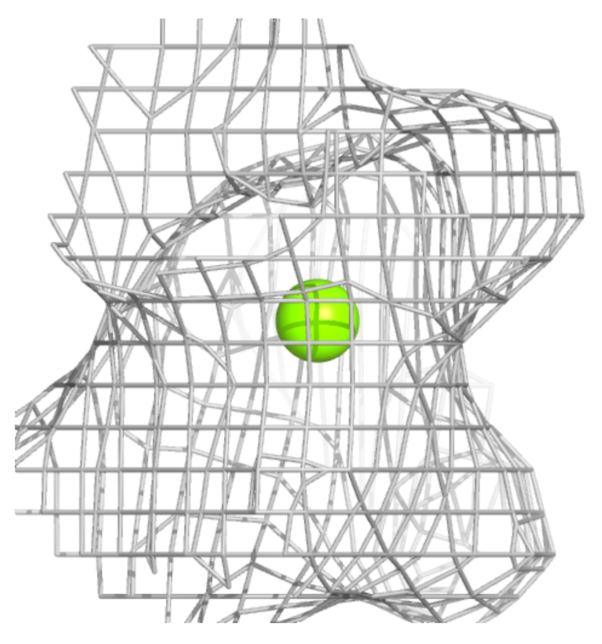


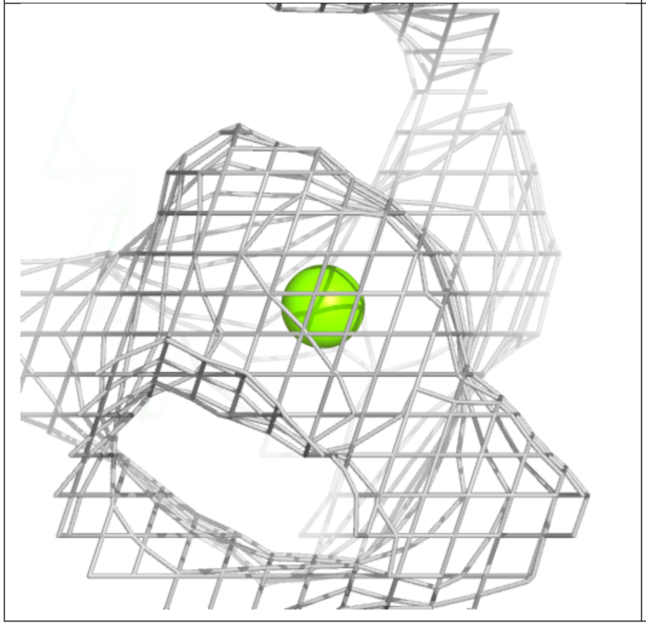


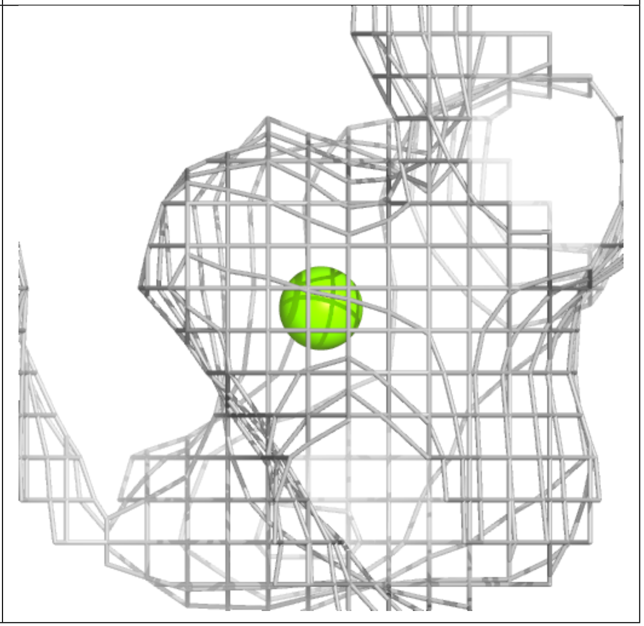


Electron density around MG A 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

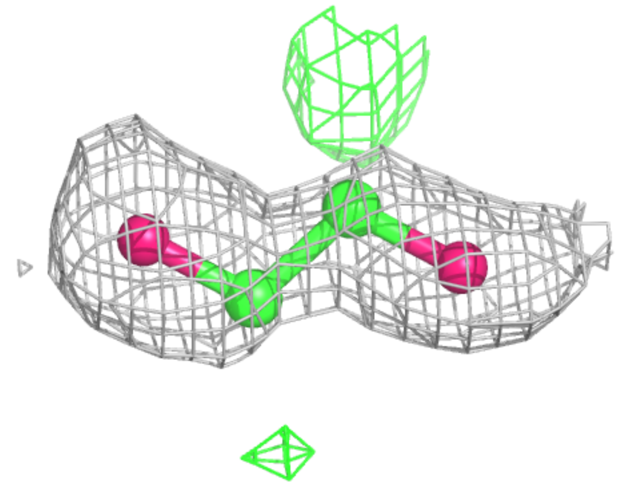


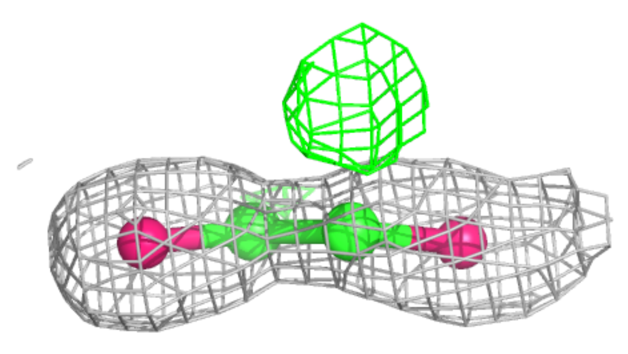


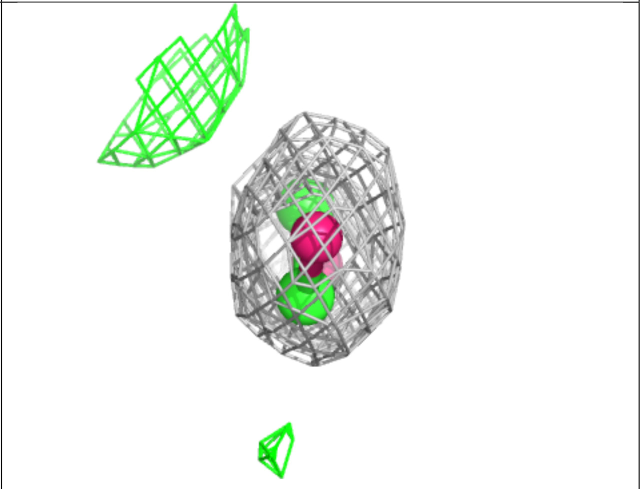


Electron density around EDO C 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

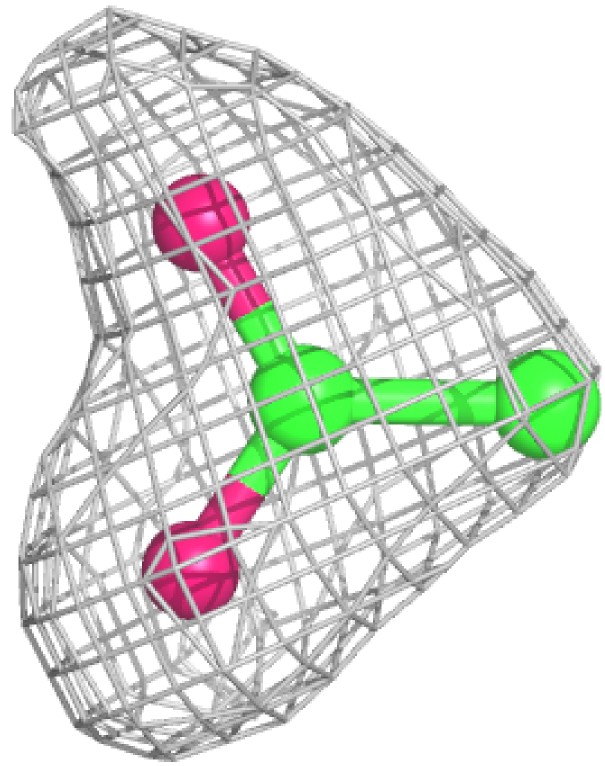


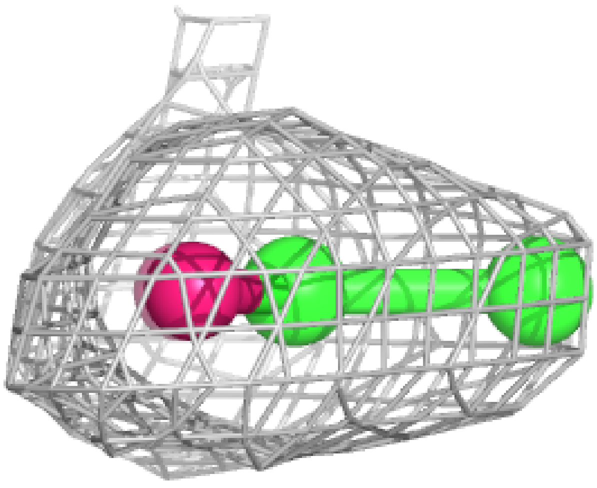


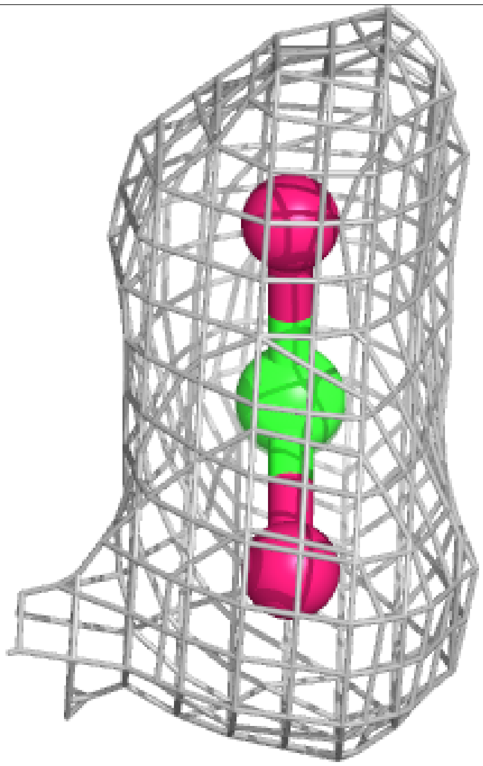


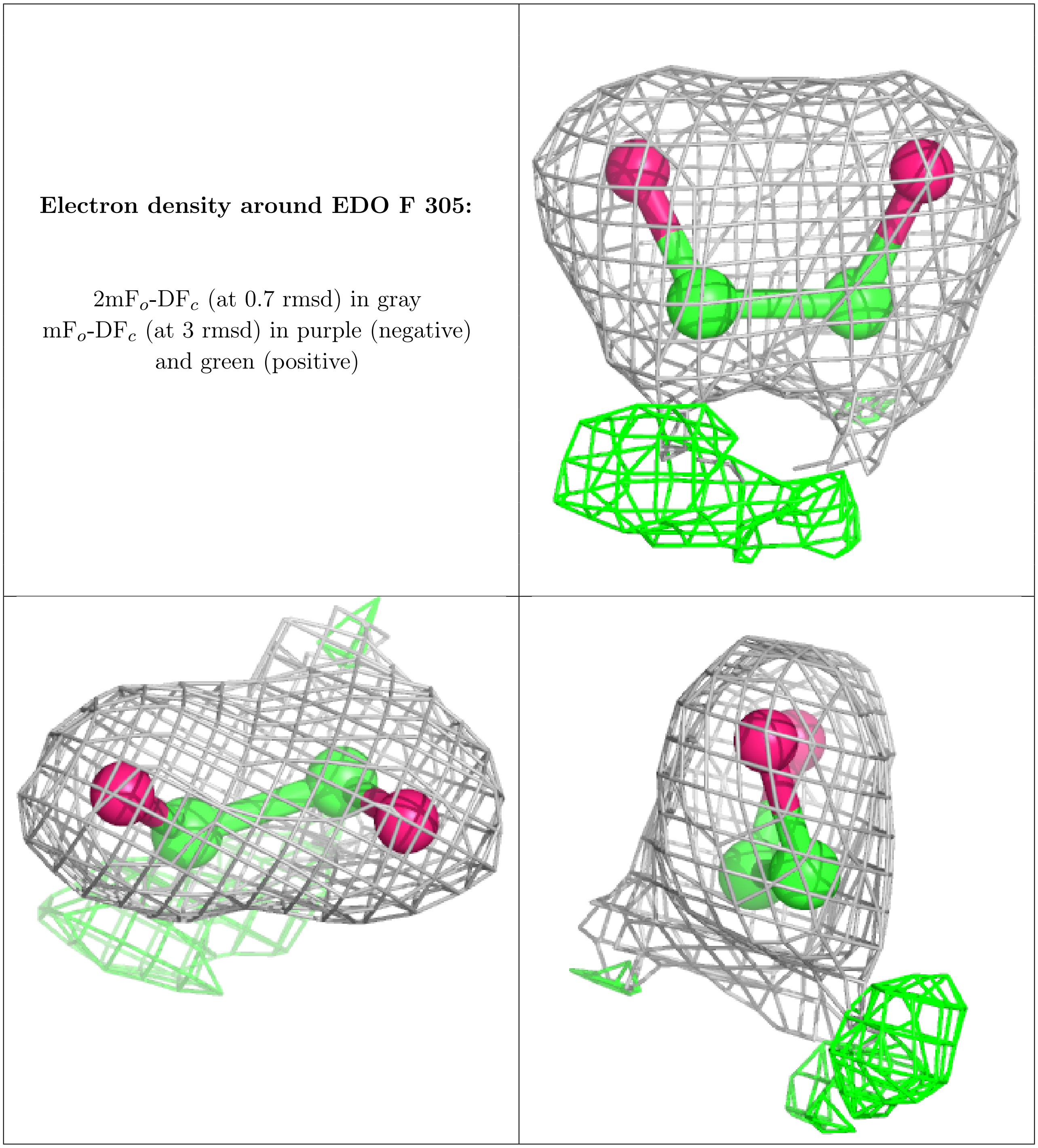
Electron density around ACT B 303:

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







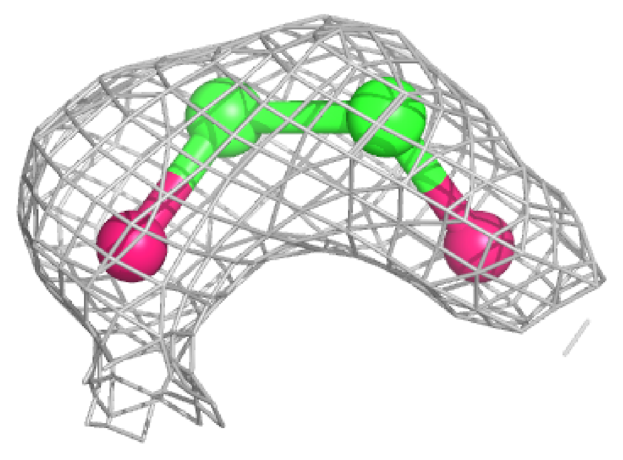


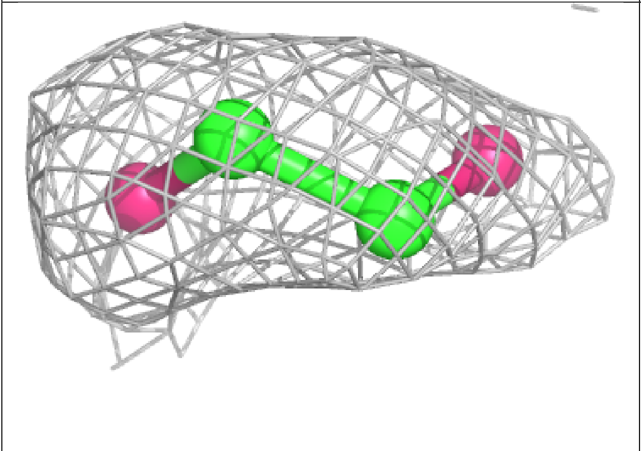
Electron density around EDO F 305:

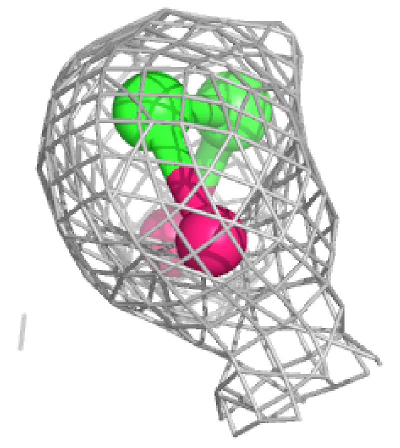
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around EDO H 305:

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

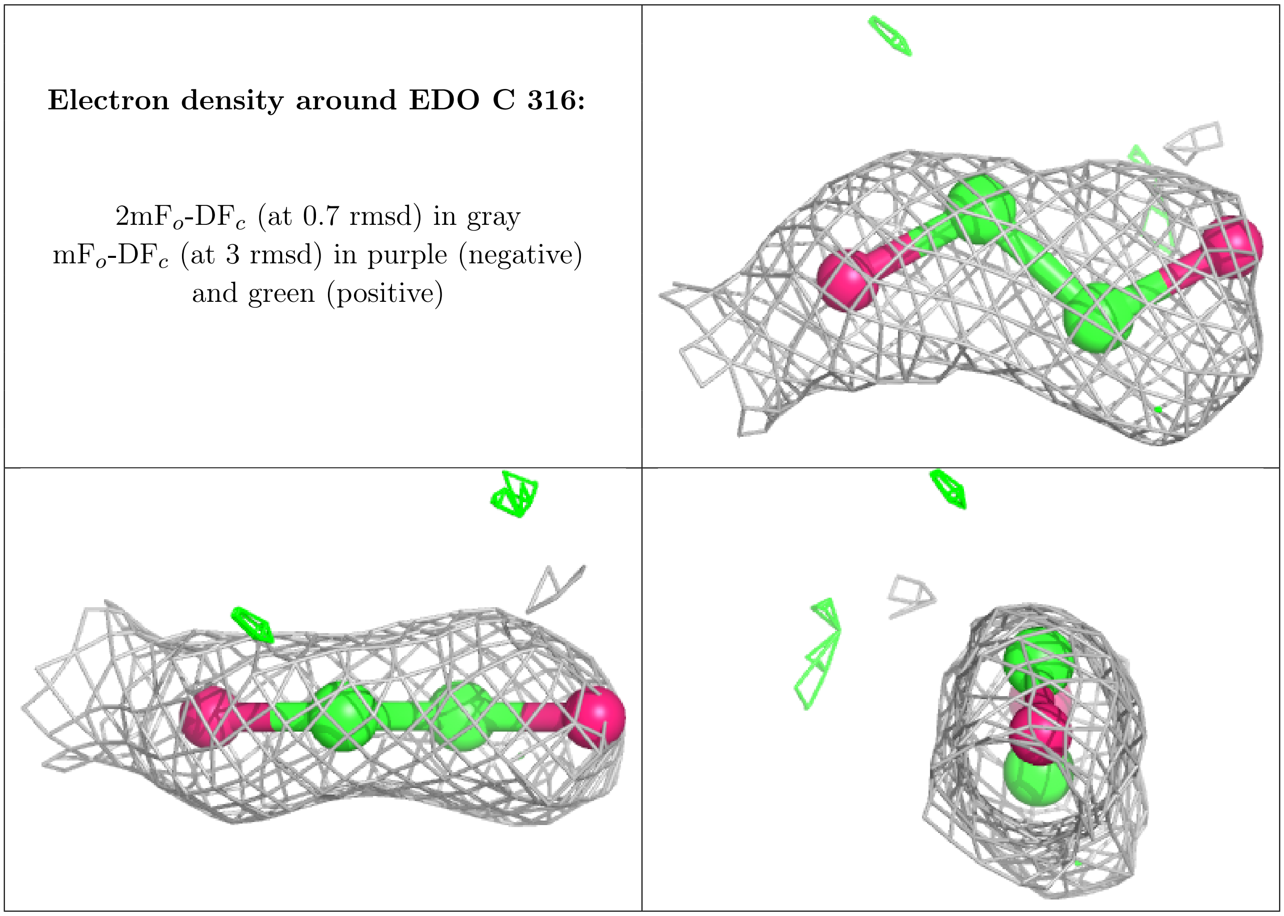






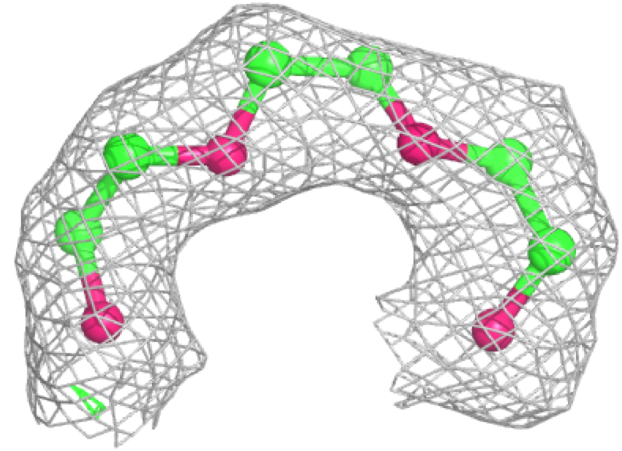
Electron density around EDO C 316:

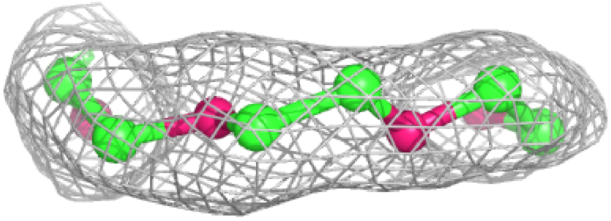
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

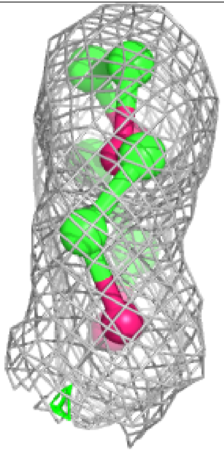


Electron density around PGE I 301:

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

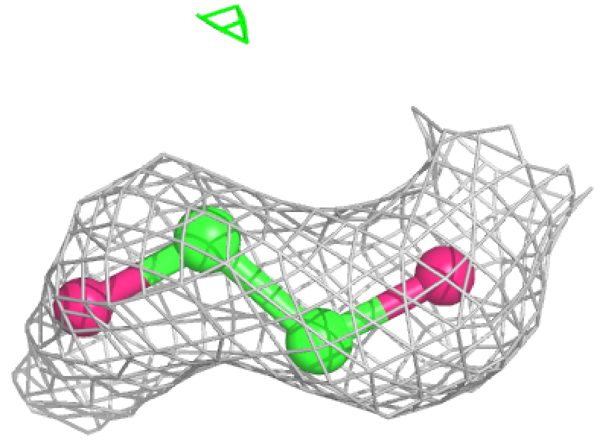


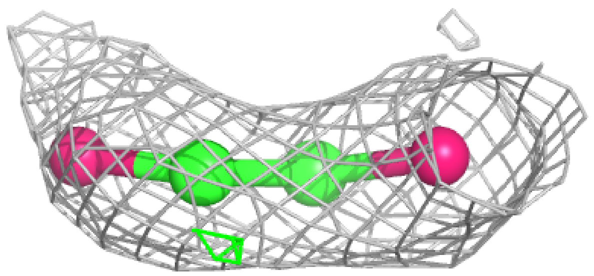


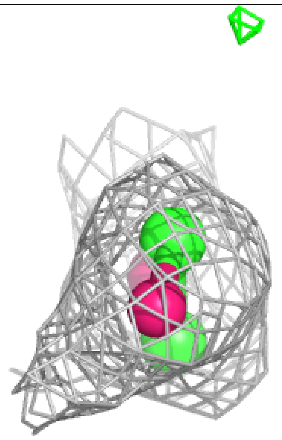


Electron density around EDO I 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

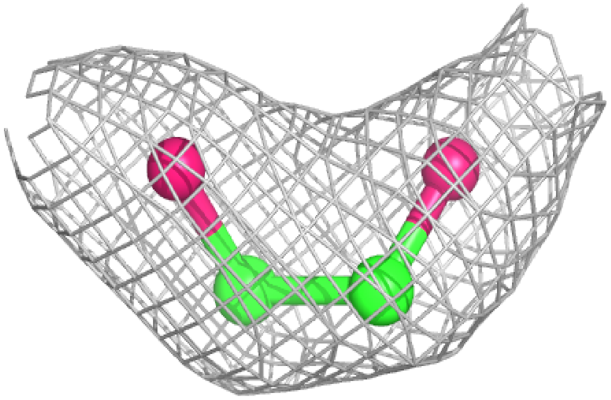


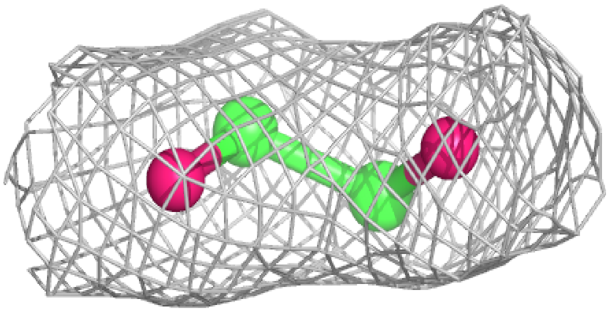


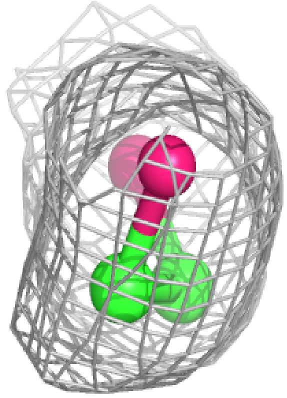


Electron density around EDO J 305:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

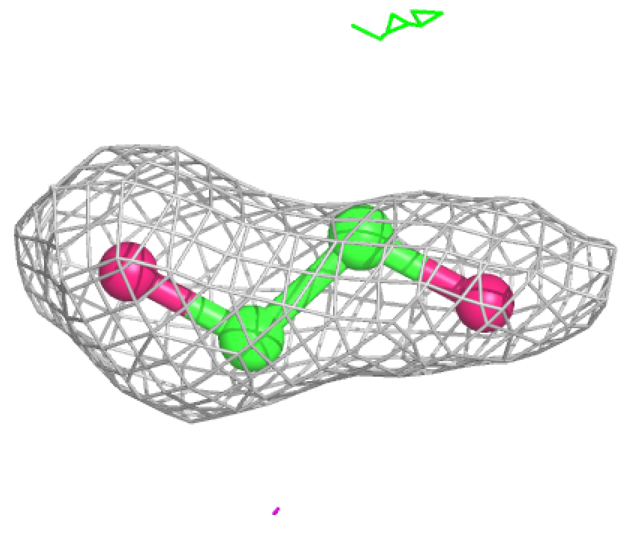


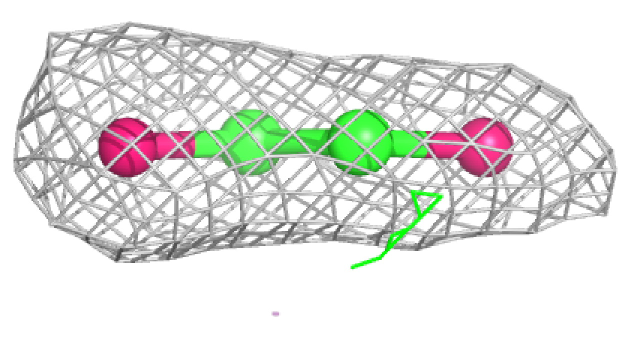


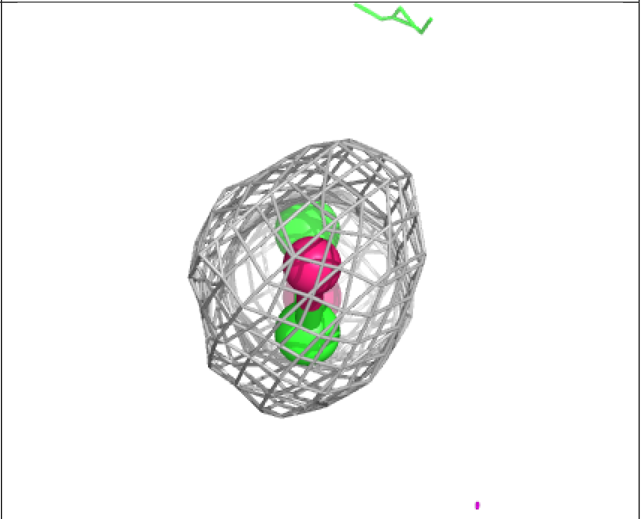


Electron density around EDO C 314:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

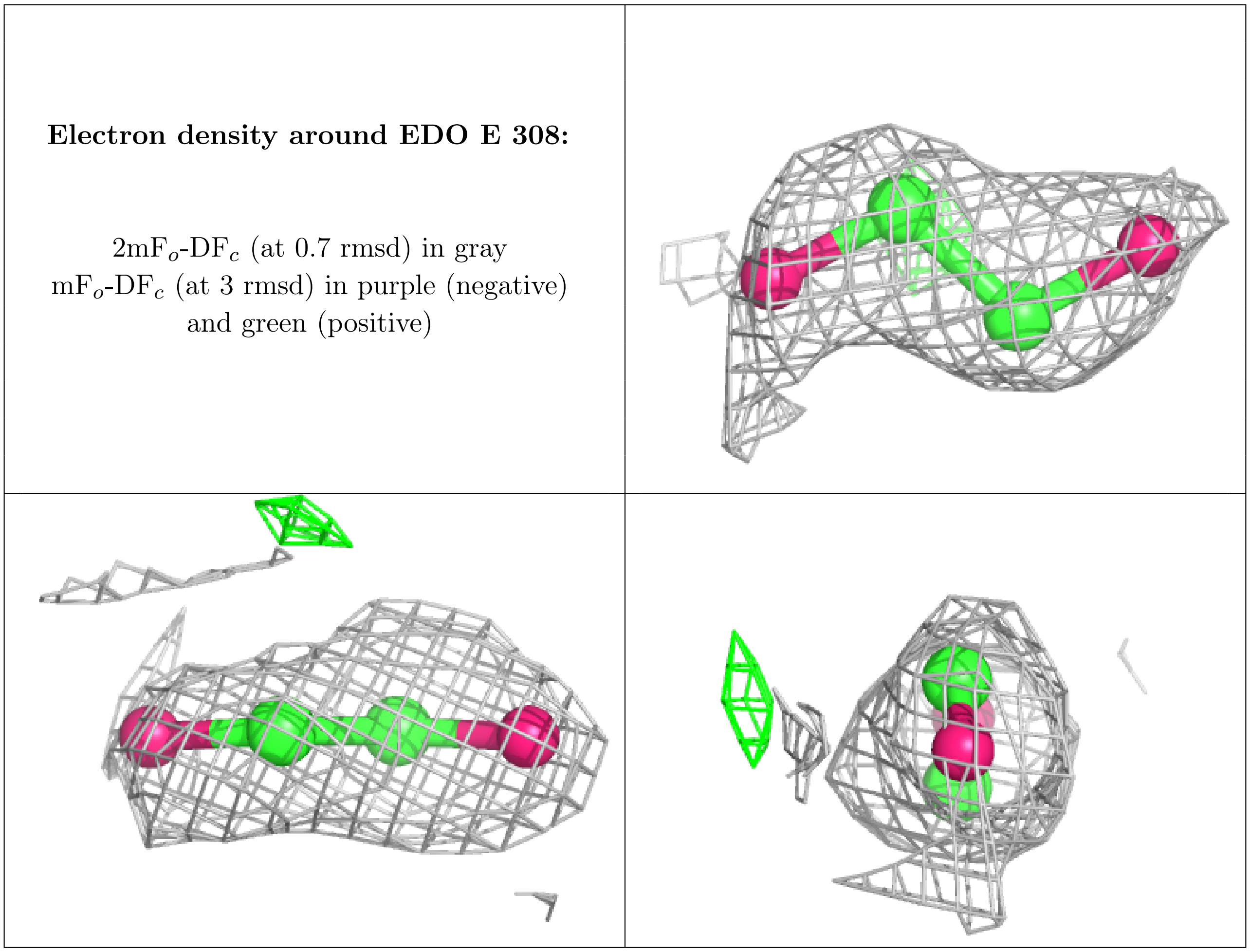






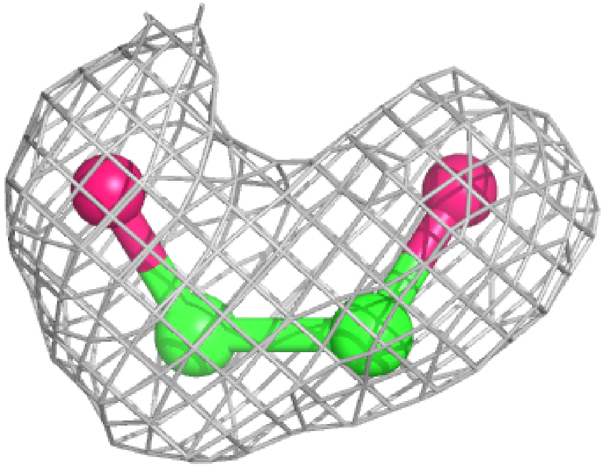
Electron density around EDO E 308:

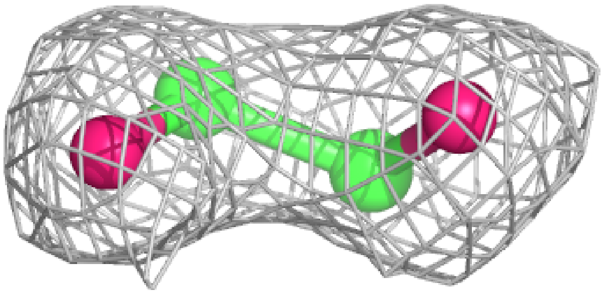
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

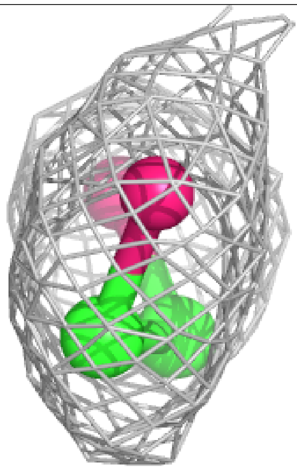


Electron density around EDO F 304:

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

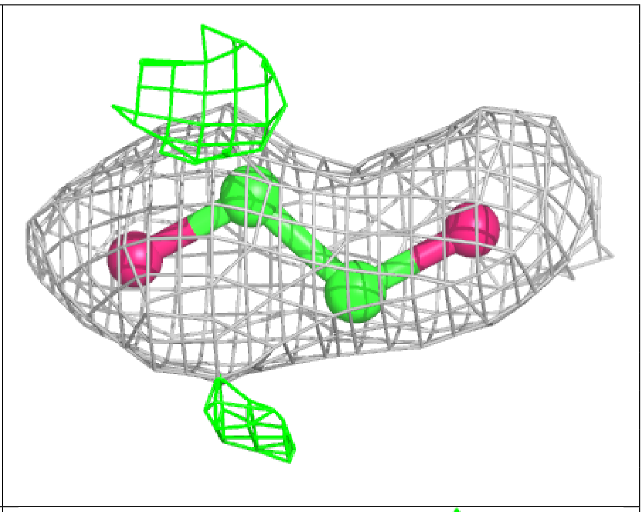


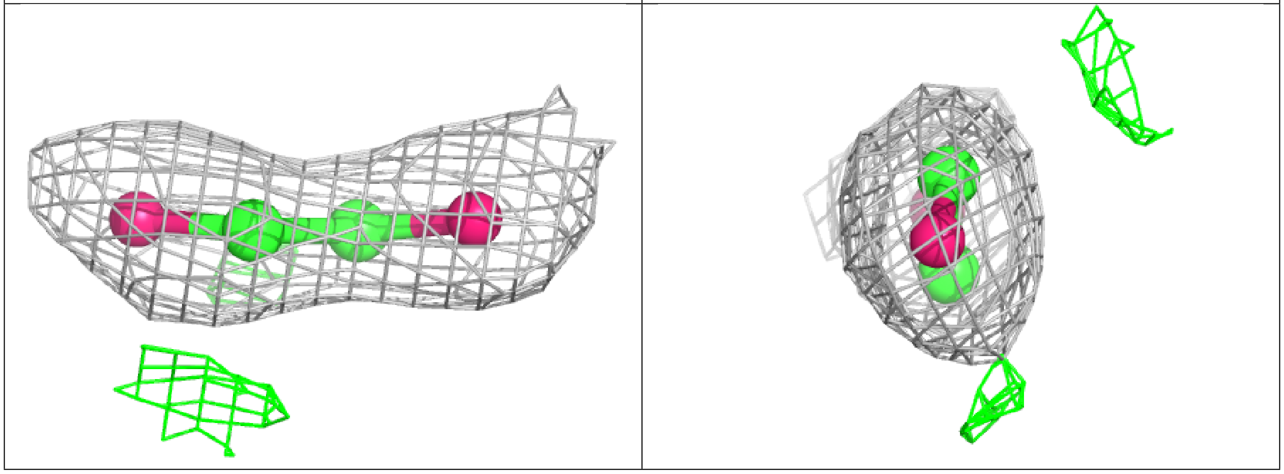




Electron density around EDO K 302:

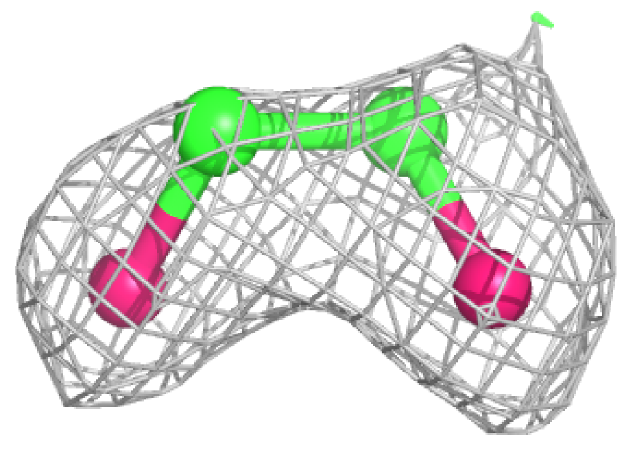
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

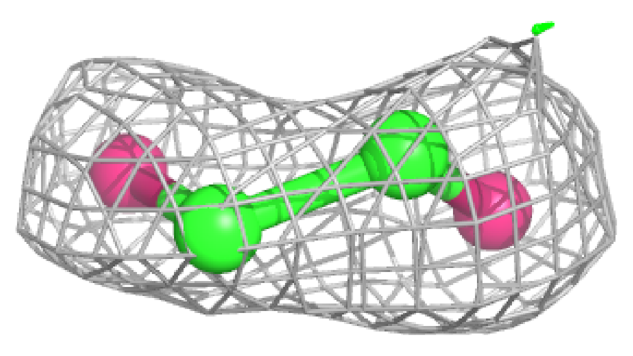


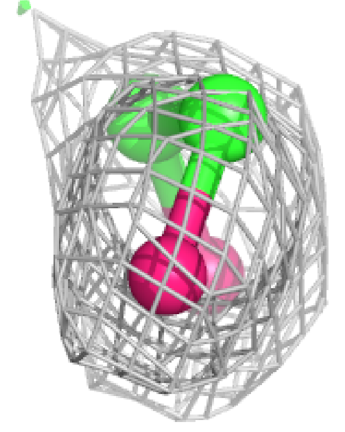


Electron density around EDO A 307:

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

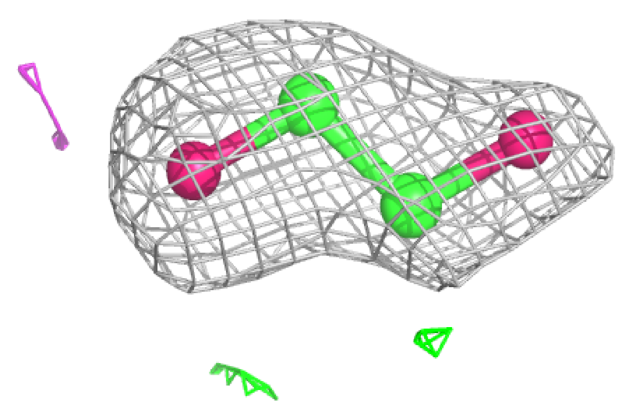


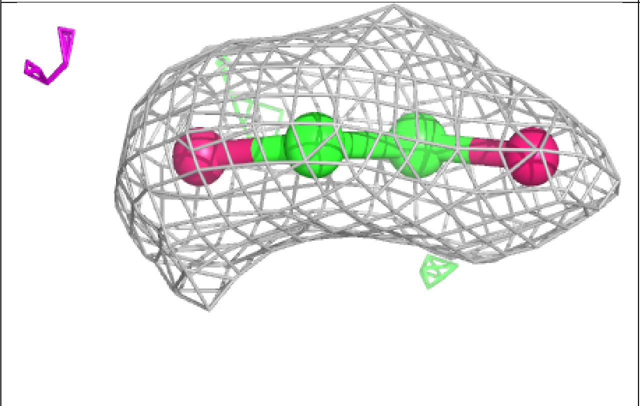


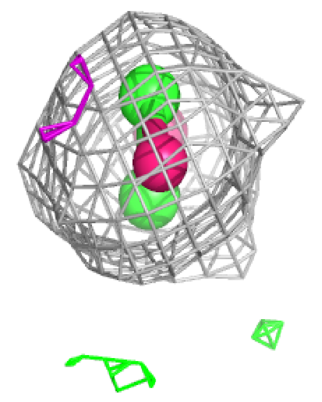


Electron density around EDO C 307:

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

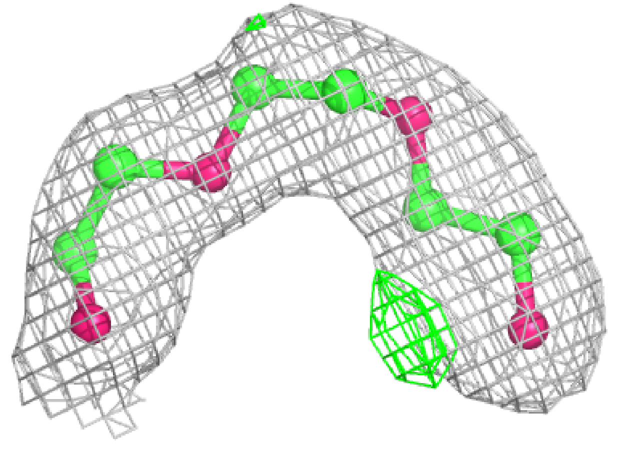


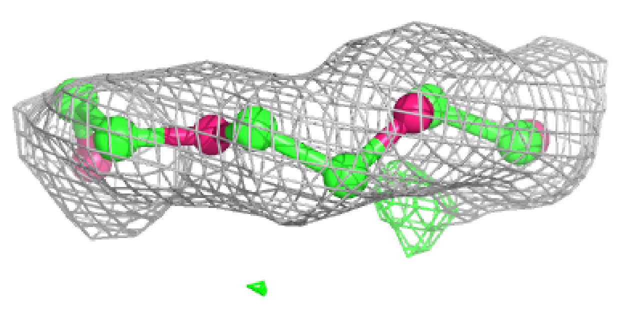


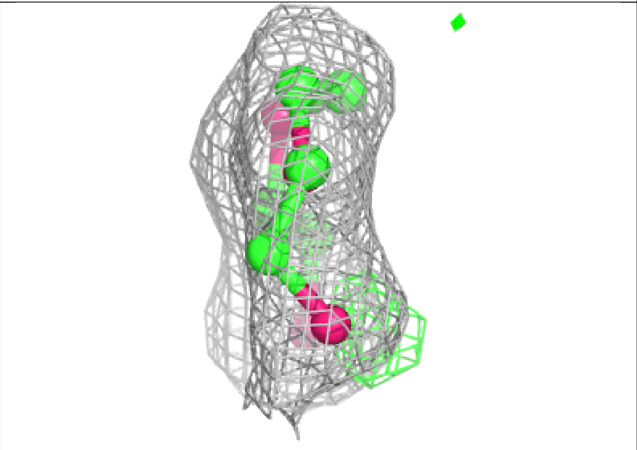


Electron density around PGE F 301:

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

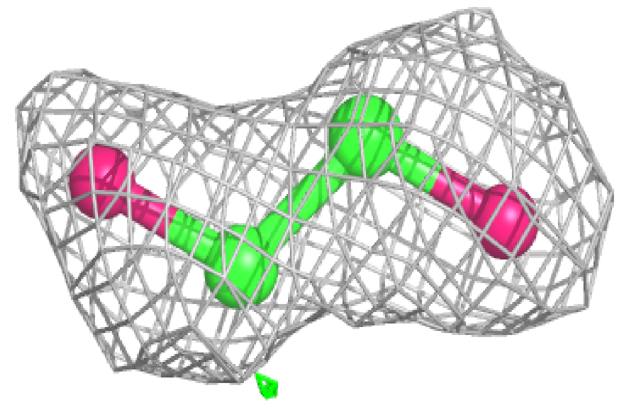


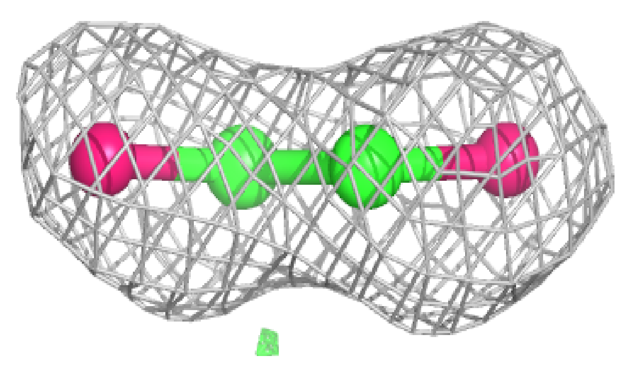


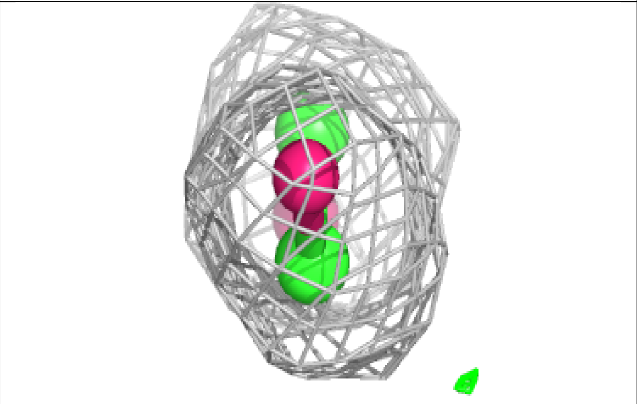


Electron density around EDO A 310:

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

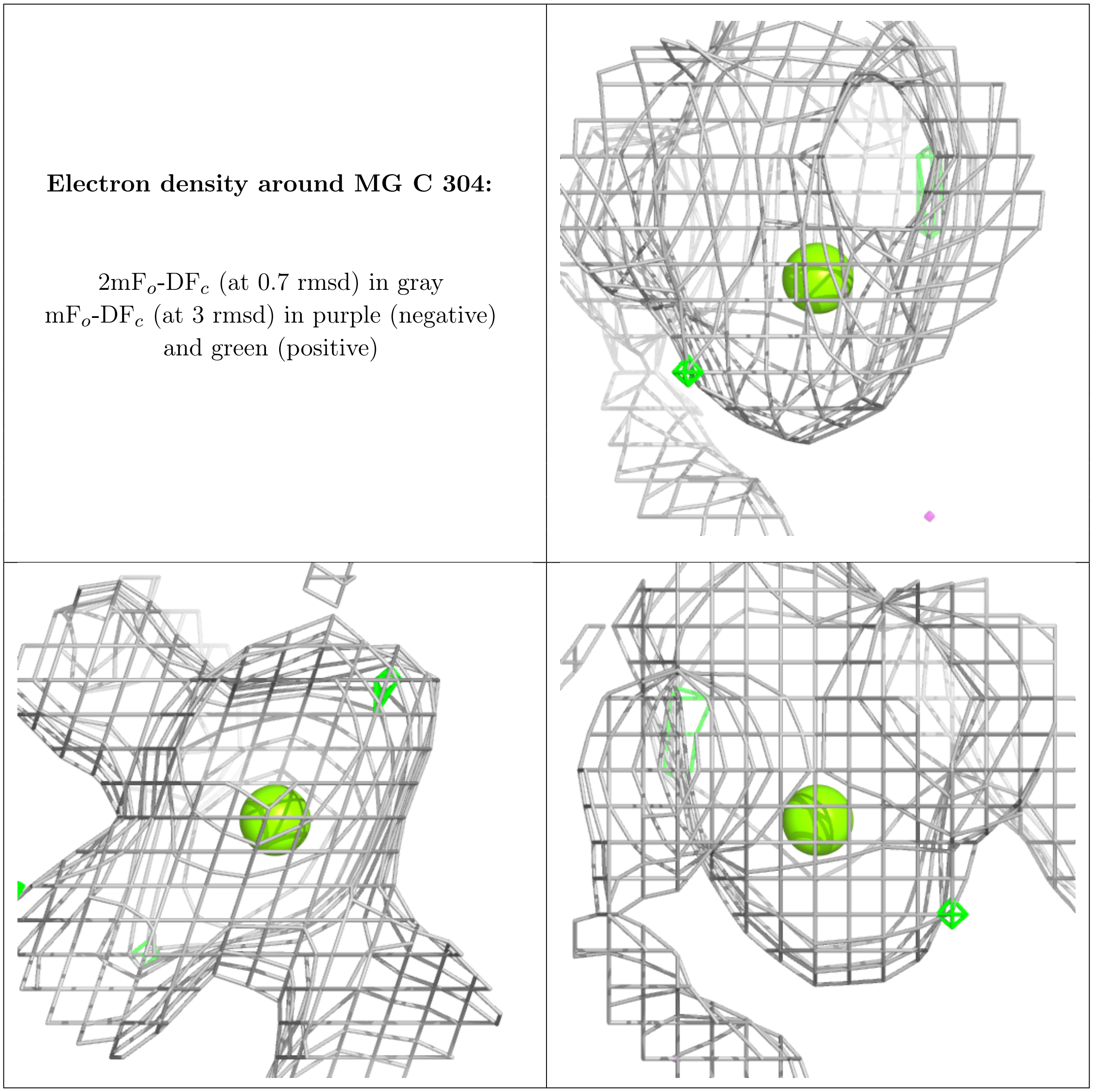






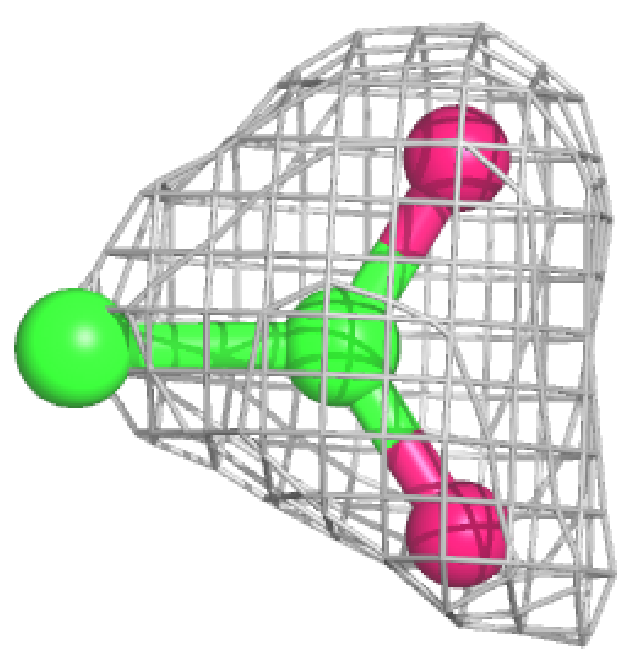
Electron density around MG C 304:

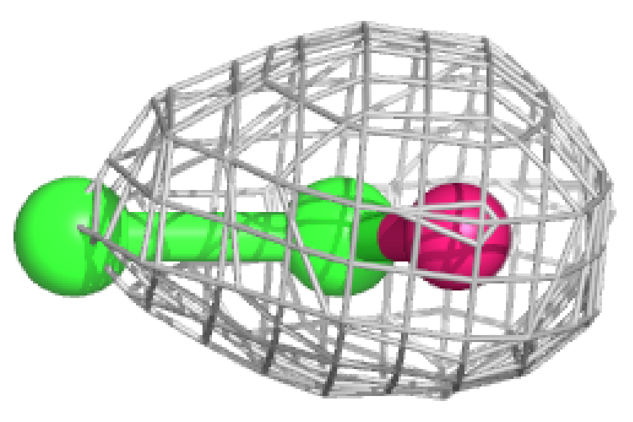
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

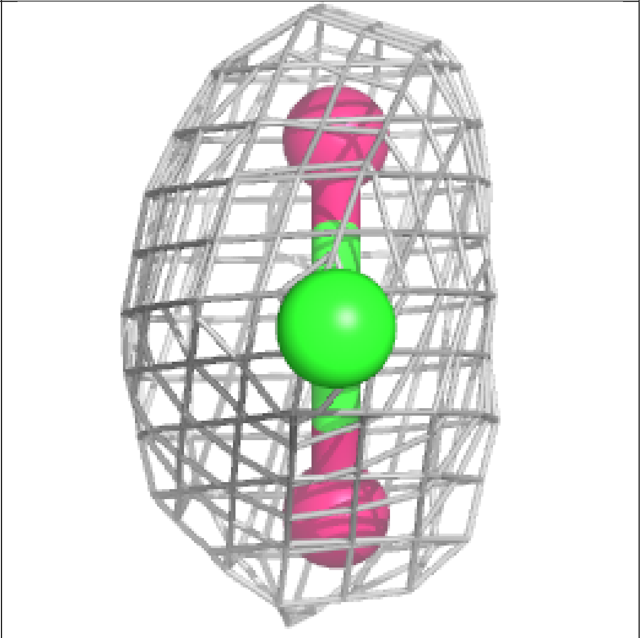


Electron density around ACT J 304:

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

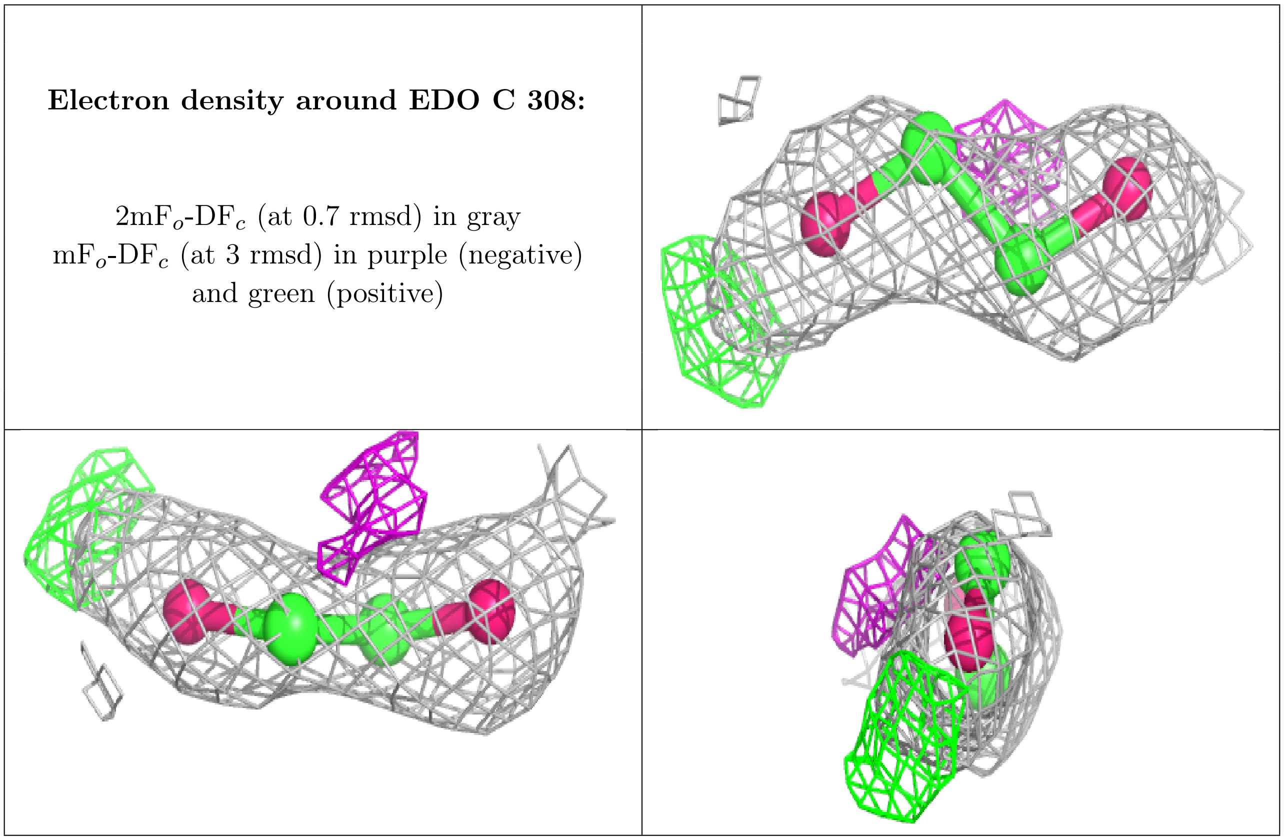


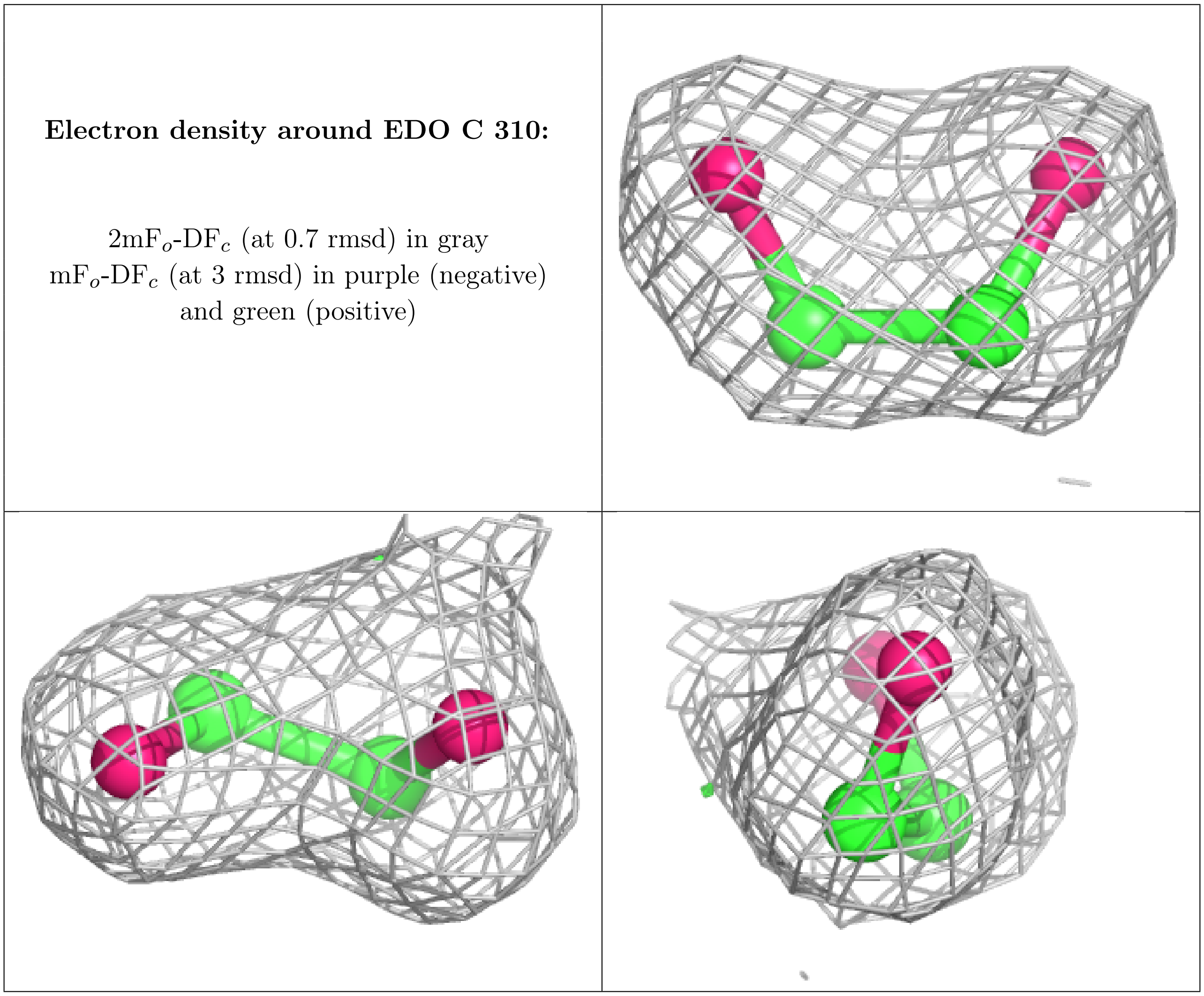




Electron density around EDO C 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



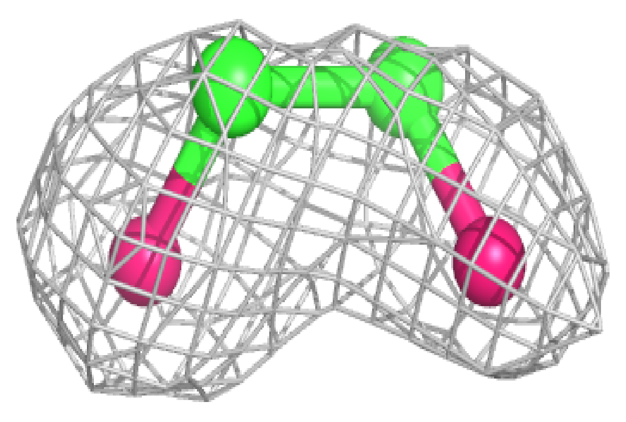


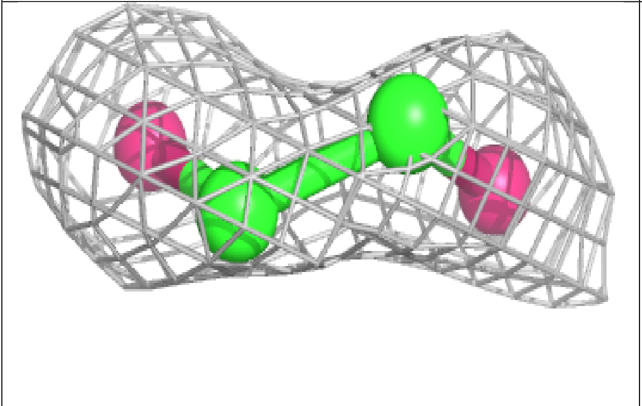
Electron density around EDO C 310:

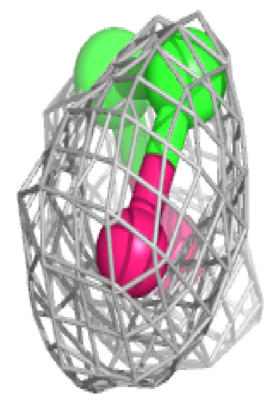
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around EDO I 307:

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

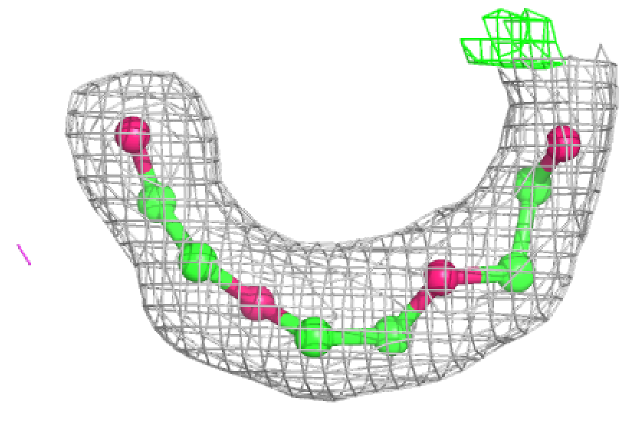


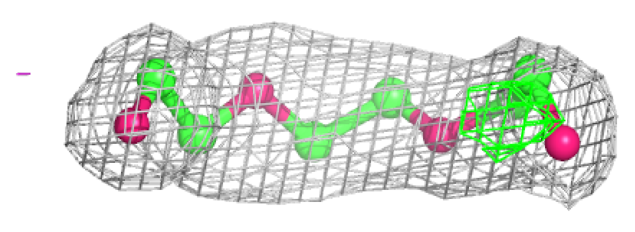


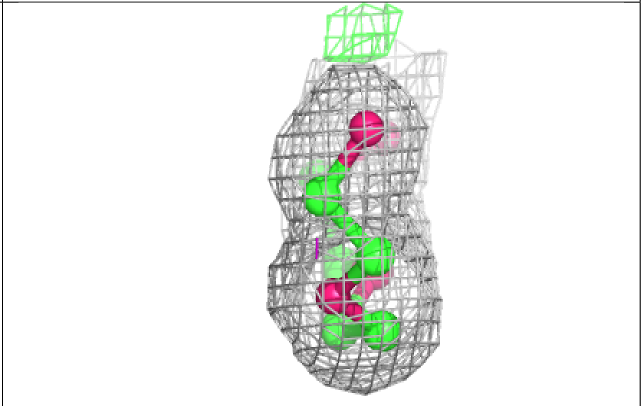


Electron density around PGE E 301:

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

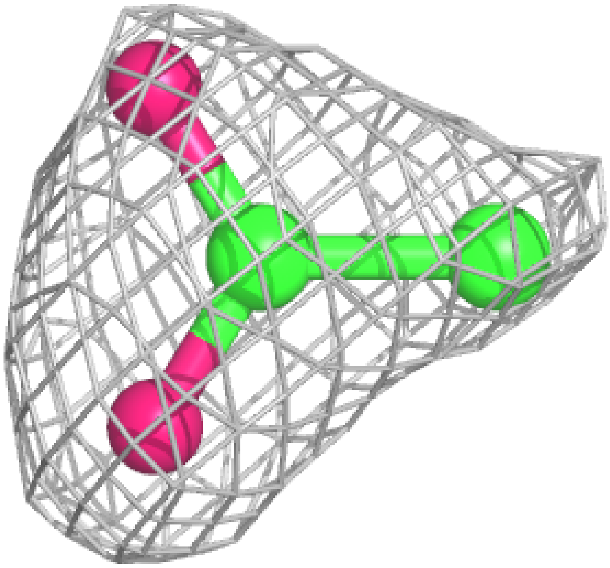


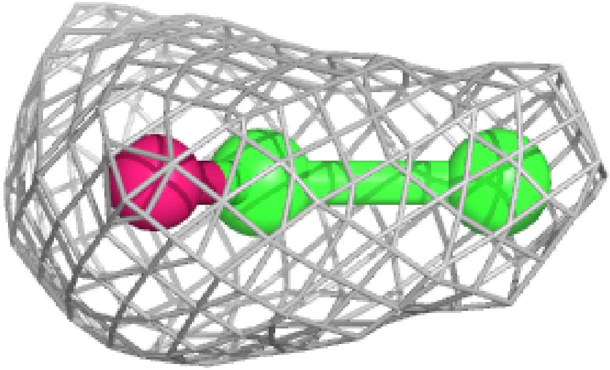


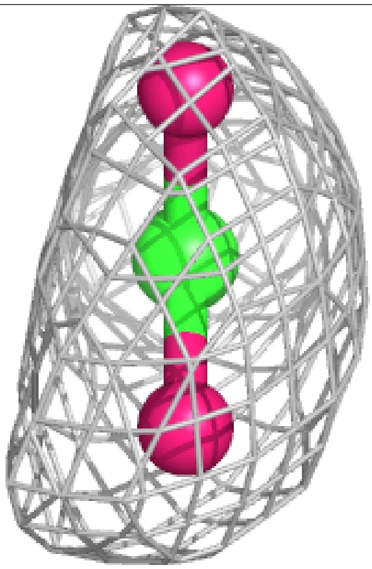


Electron density around ACT E 303:

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

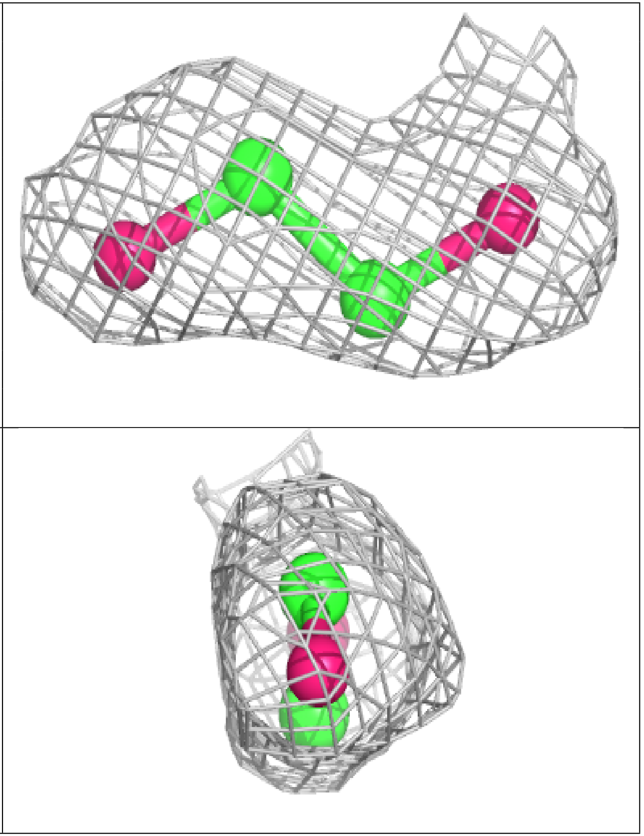






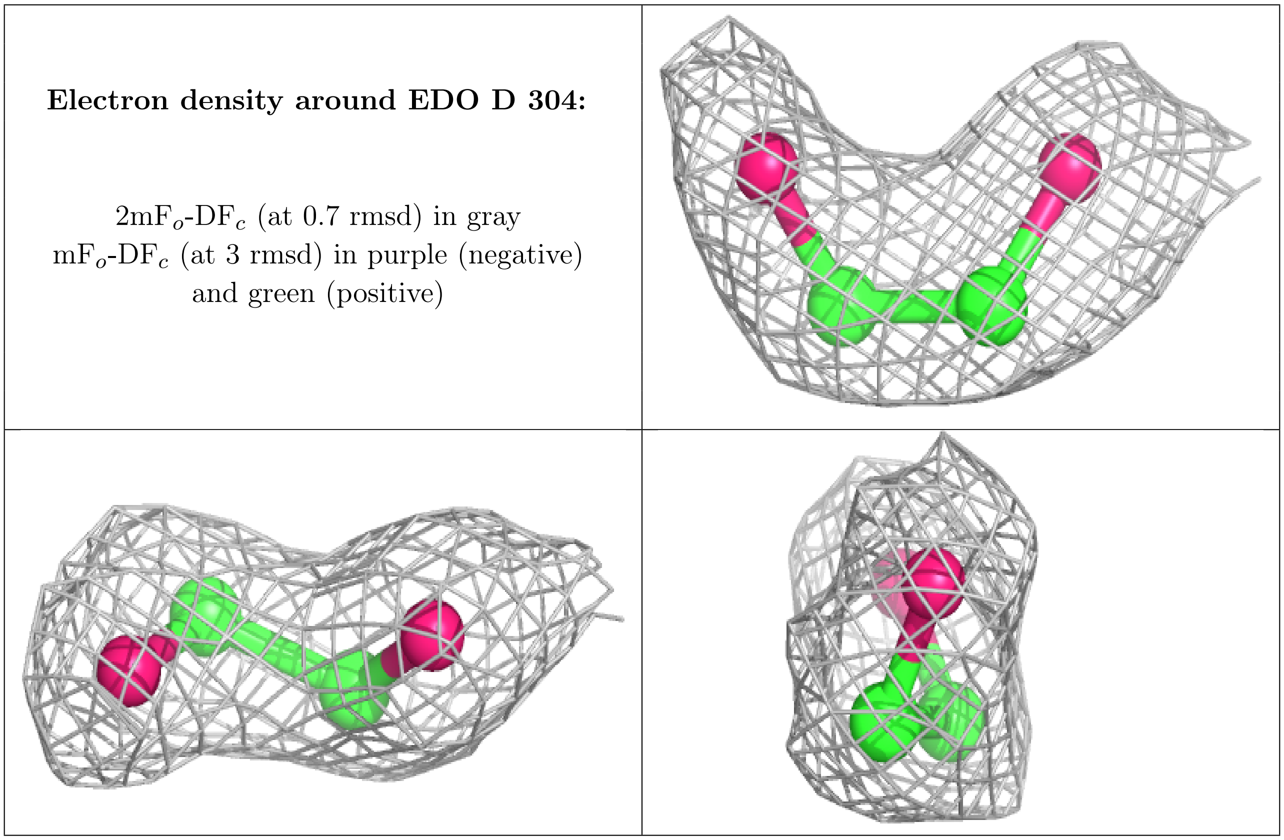
Electron density around EDO A 308:

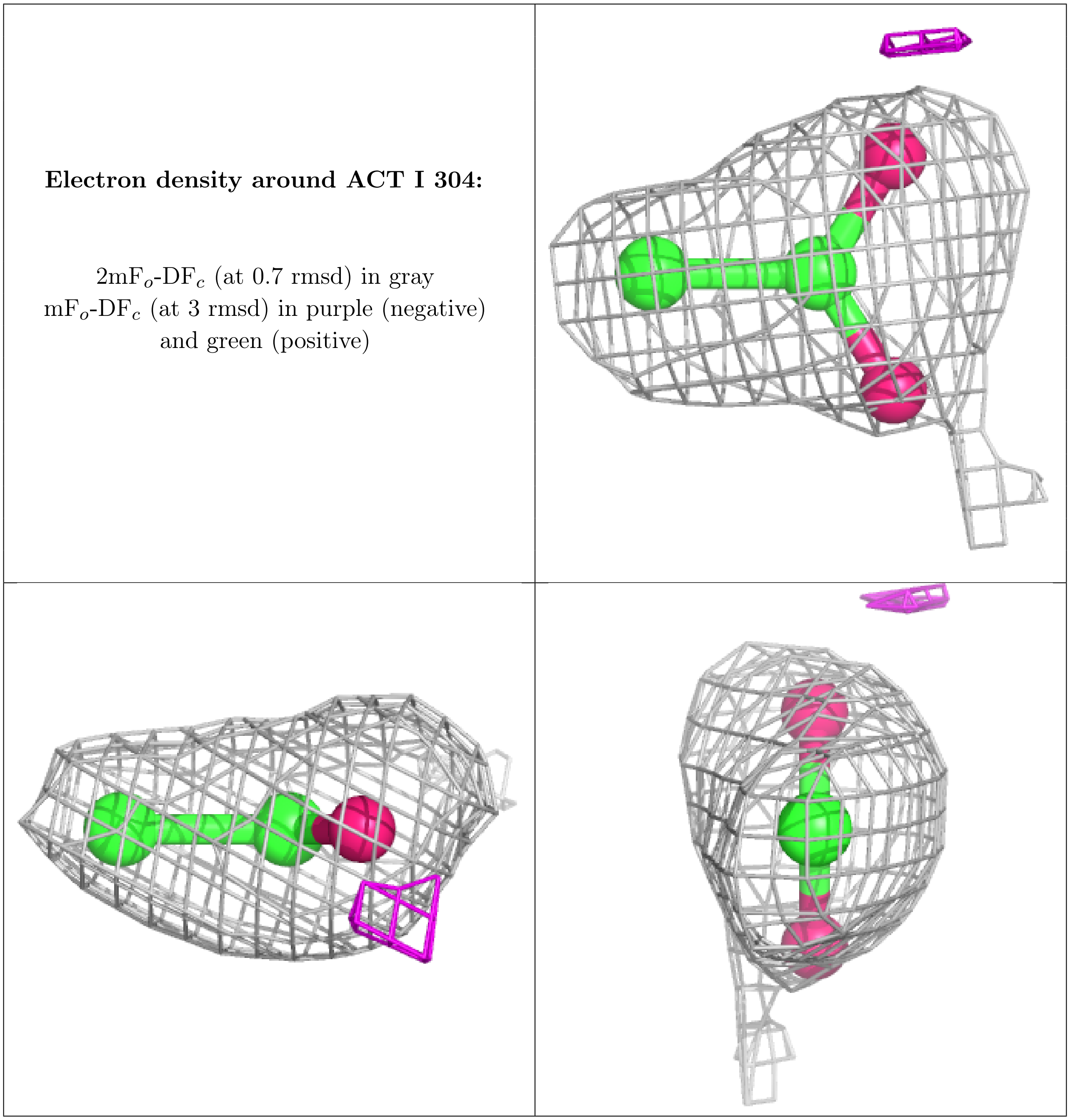
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)



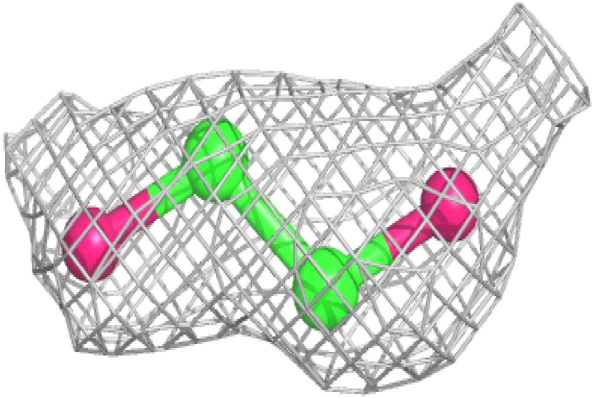


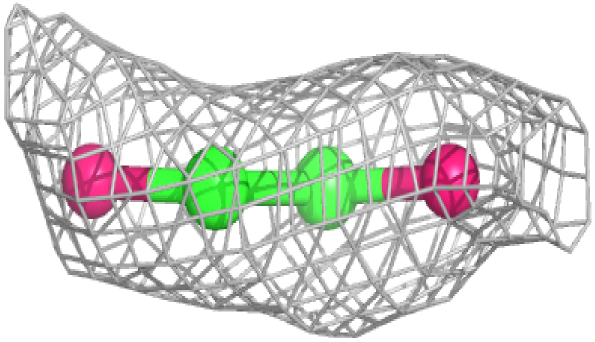
Electron density around ACT I 304:

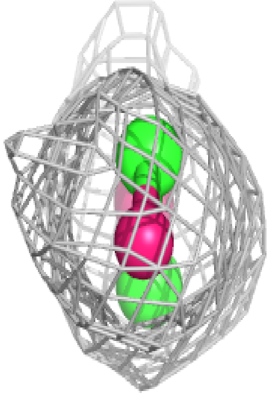
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around EDO K 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

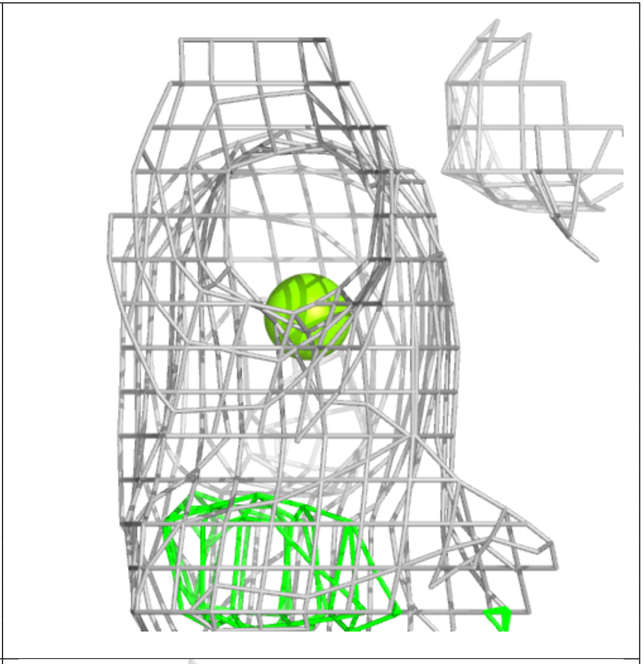


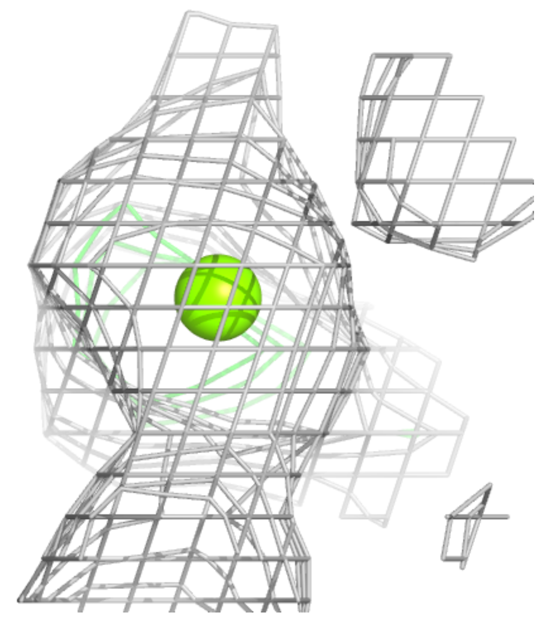


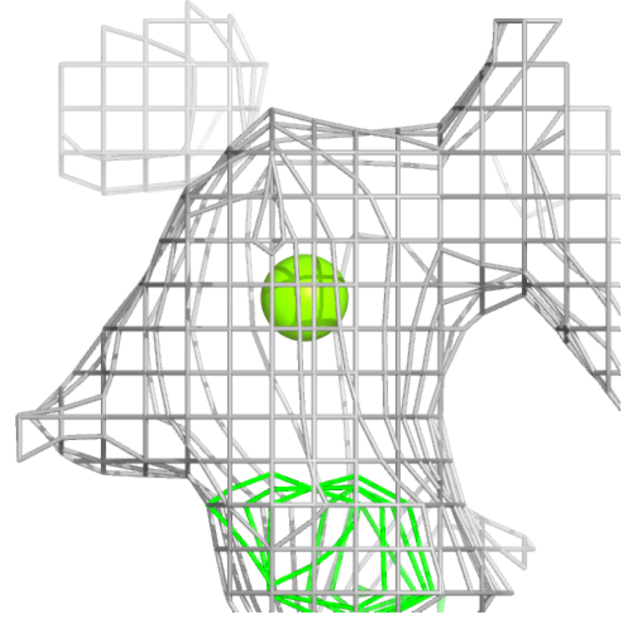


Electron density around MG C 305:

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

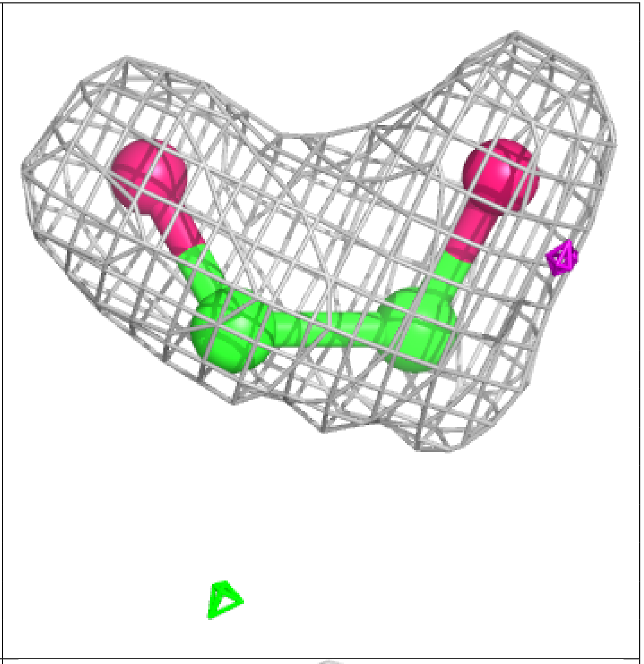


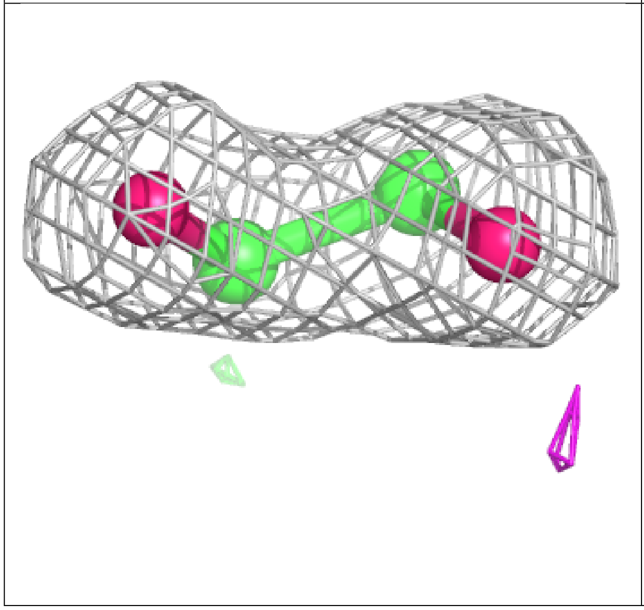


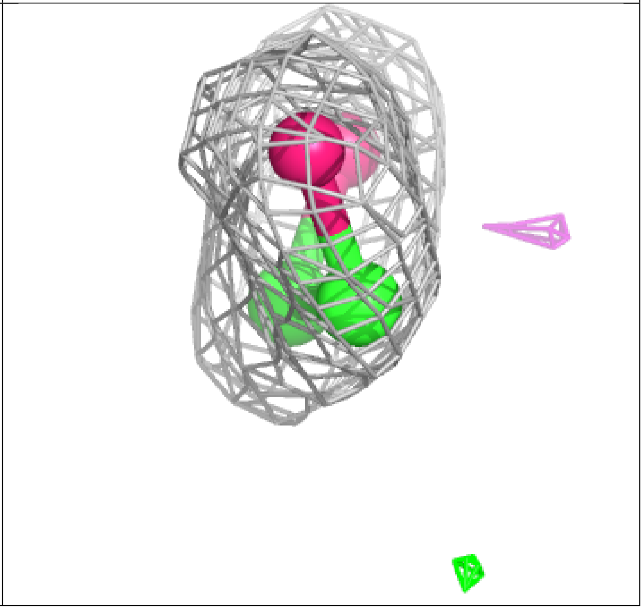


Electron density around EDO I 306:

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

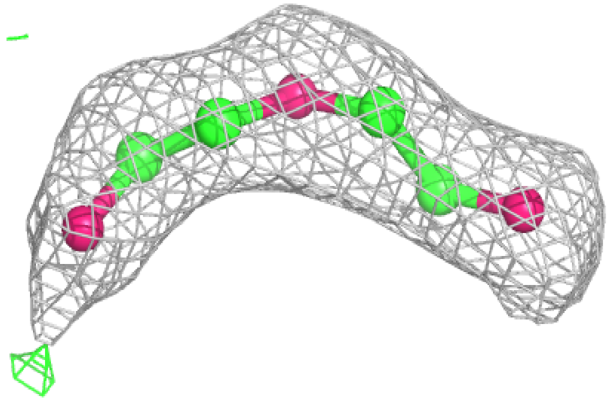


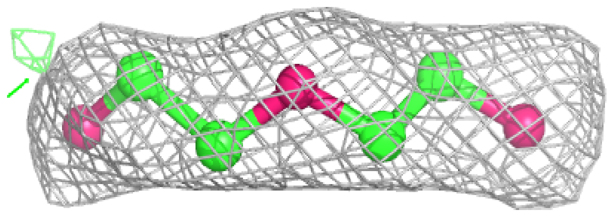


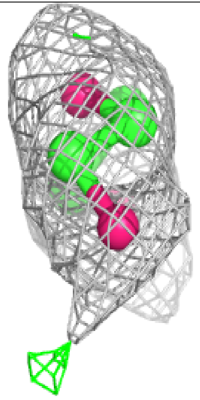


Electron density around PEG H 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

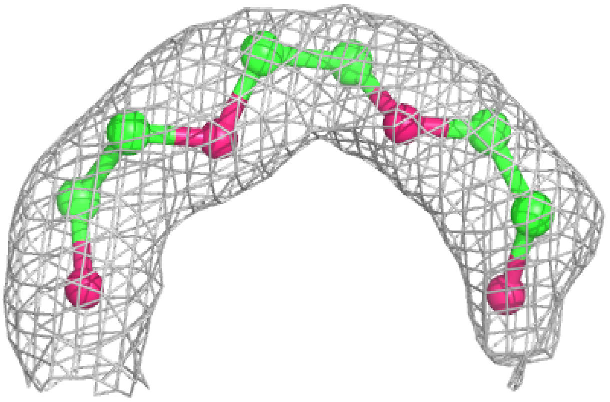


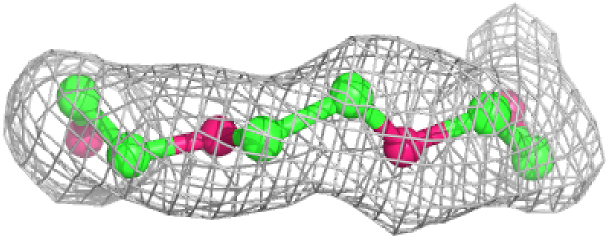


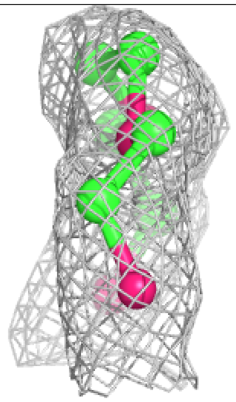


Electron density around PGE J 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

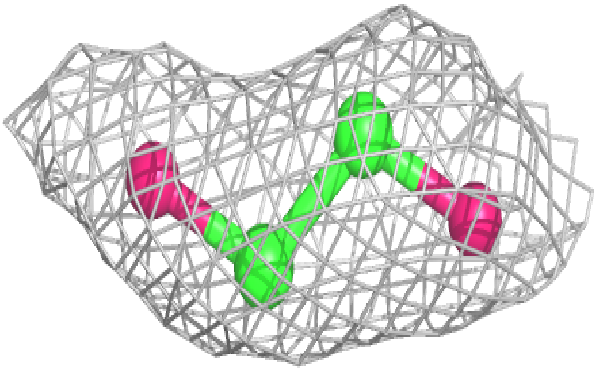


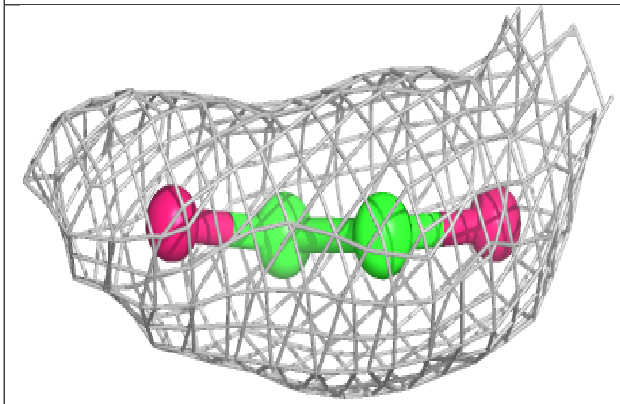


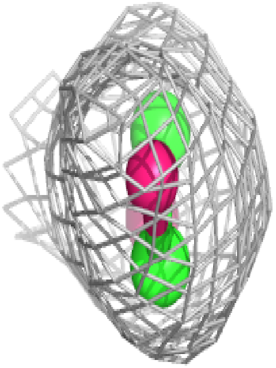


Electron density around EDO B 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

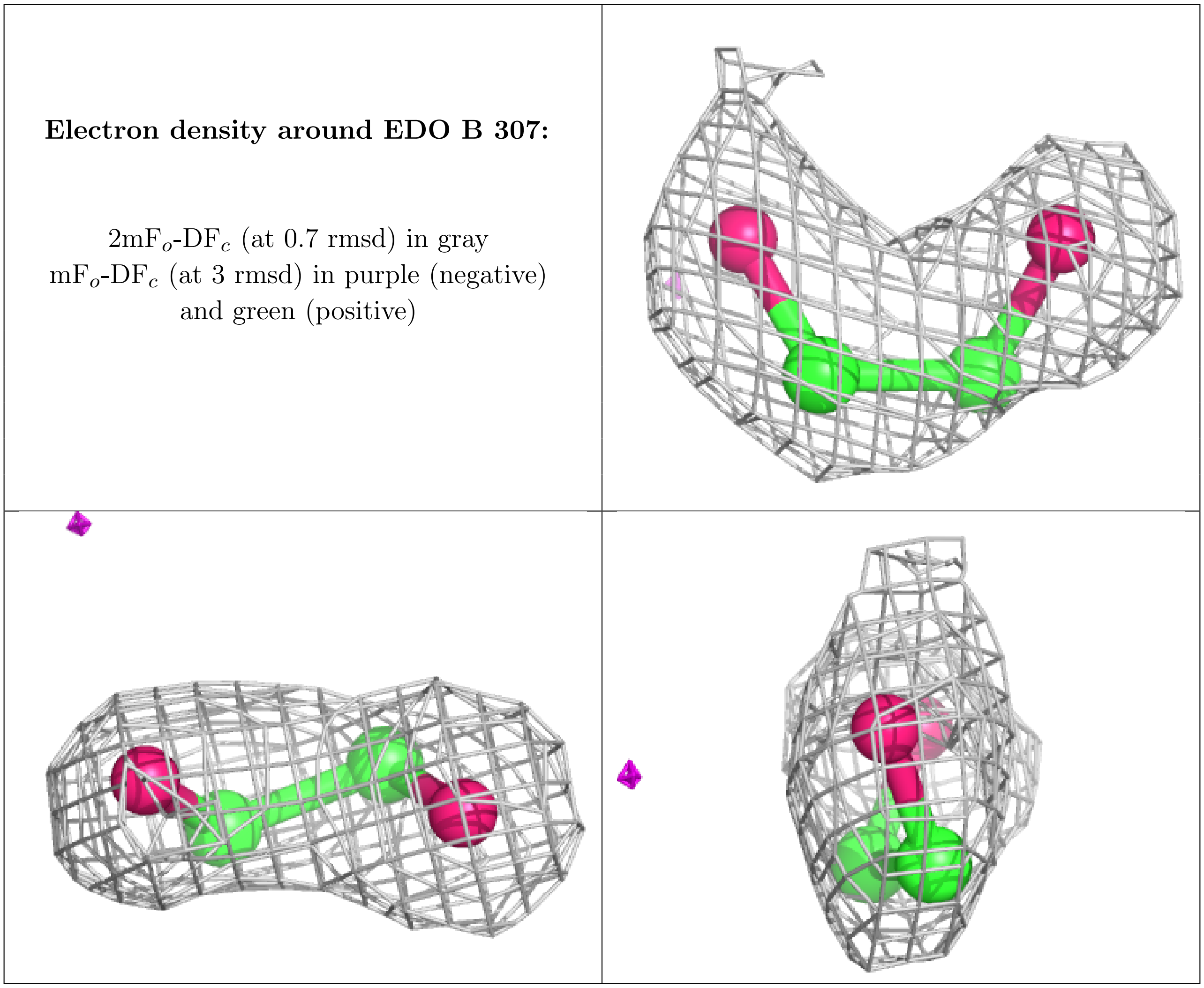






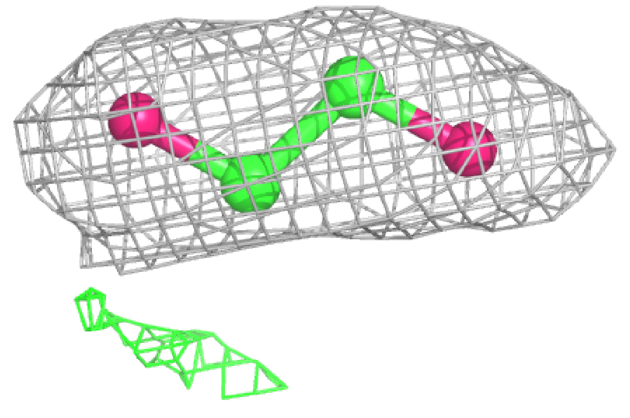
Electron density around EDO B 307:

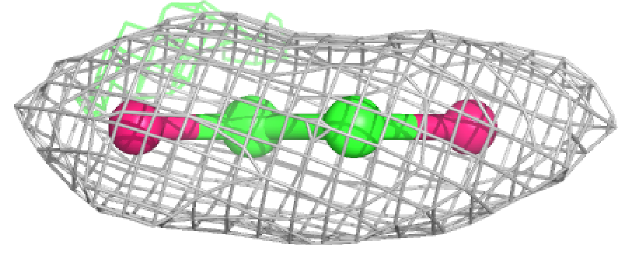
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

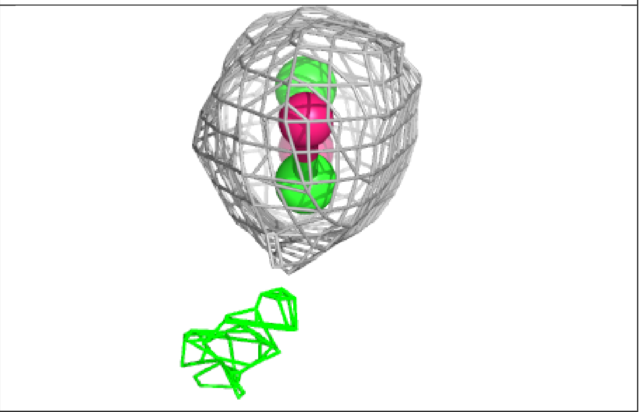


Electron density around EDO C 309:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

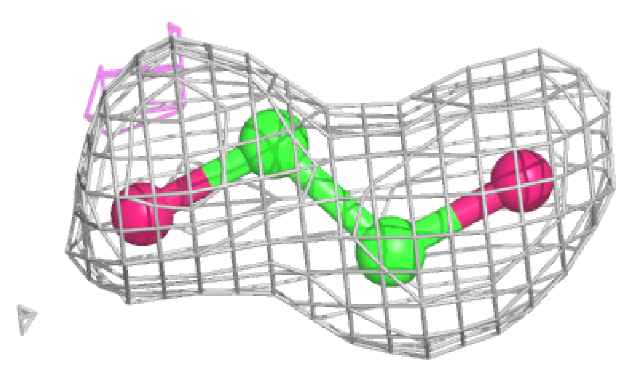


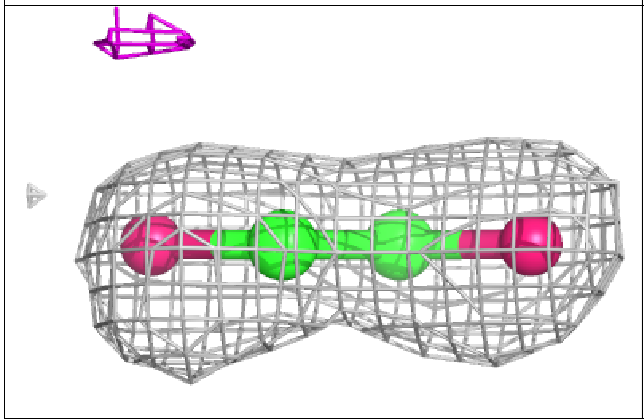


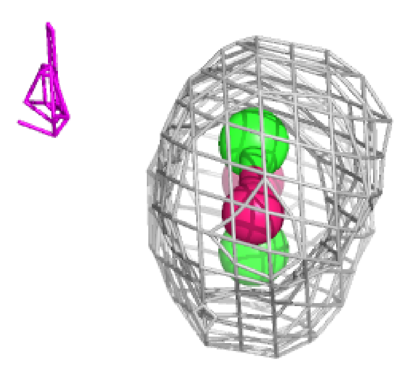


Electron density around EDO J 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

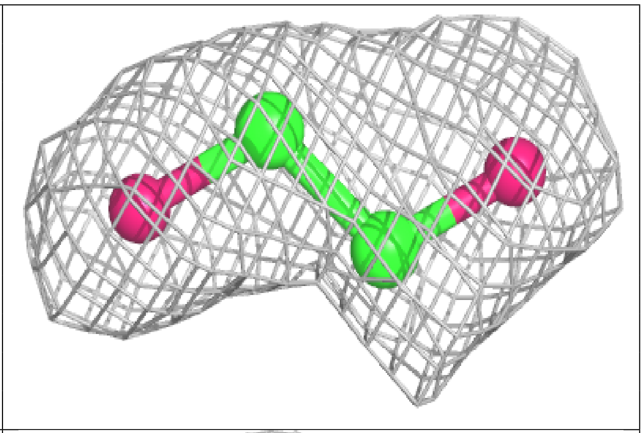


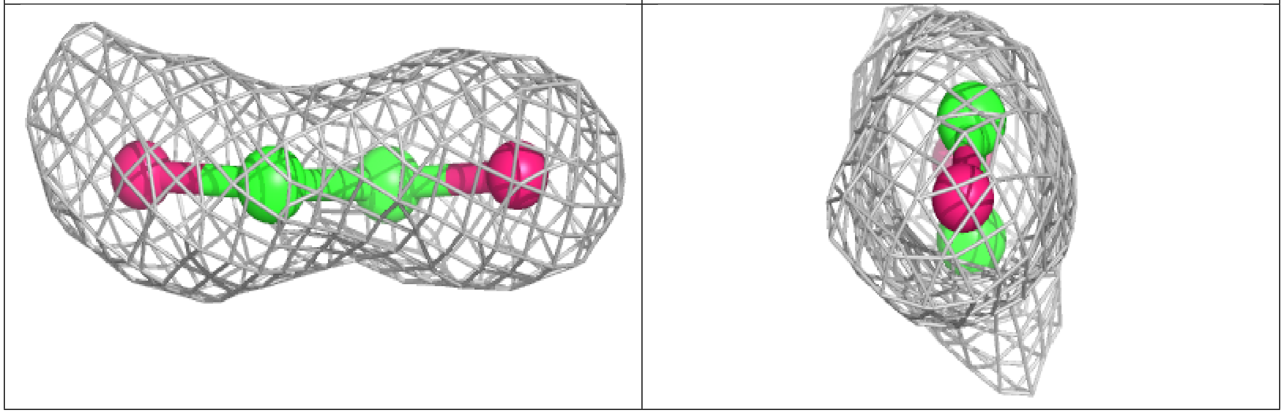




Electron density around EDO D 303:

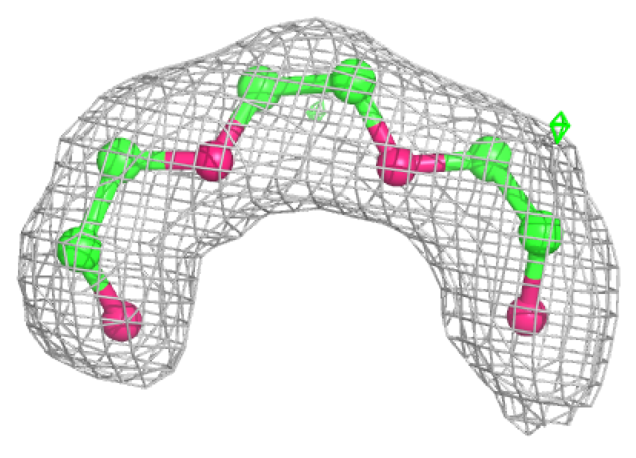
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

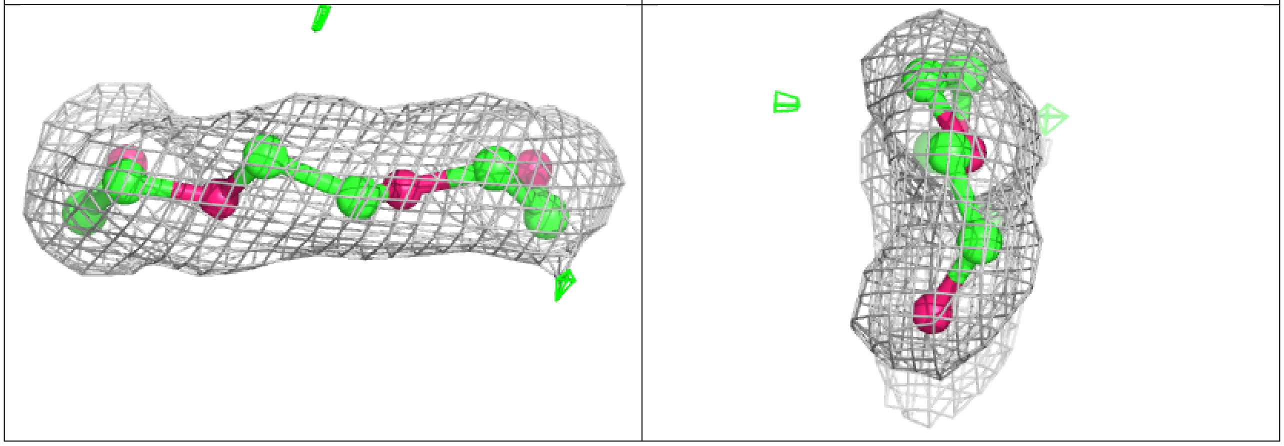




Electron density around PGE C 301:

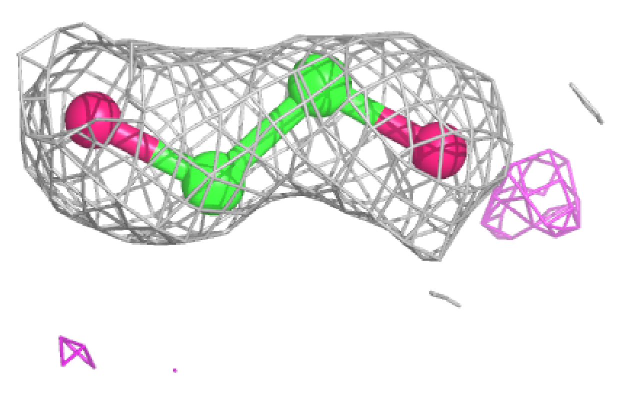
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

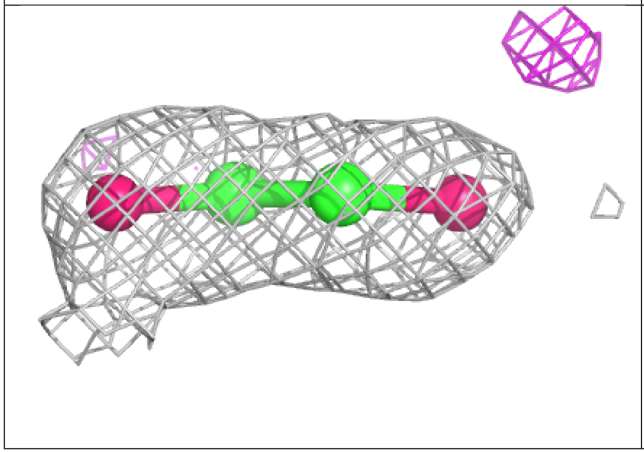


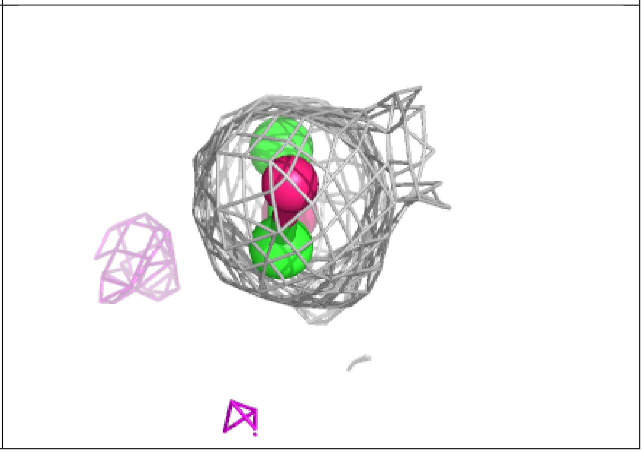


Electron density around EDO C 311:

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

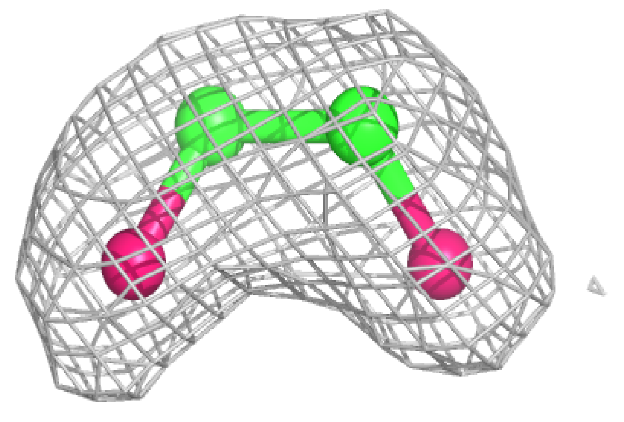


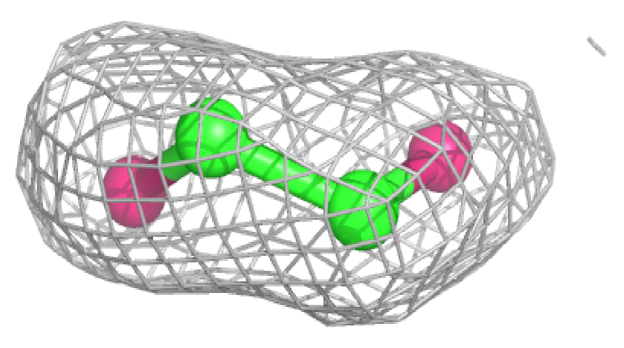


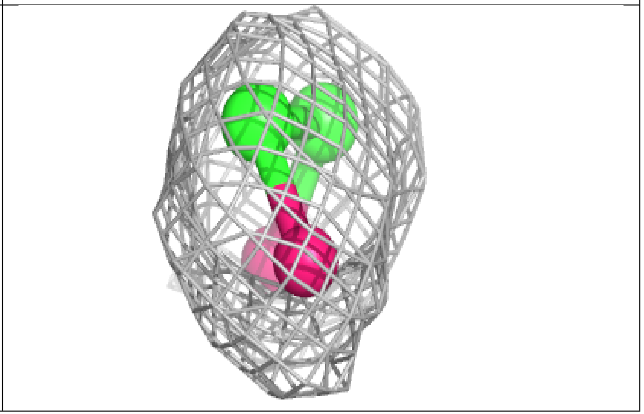


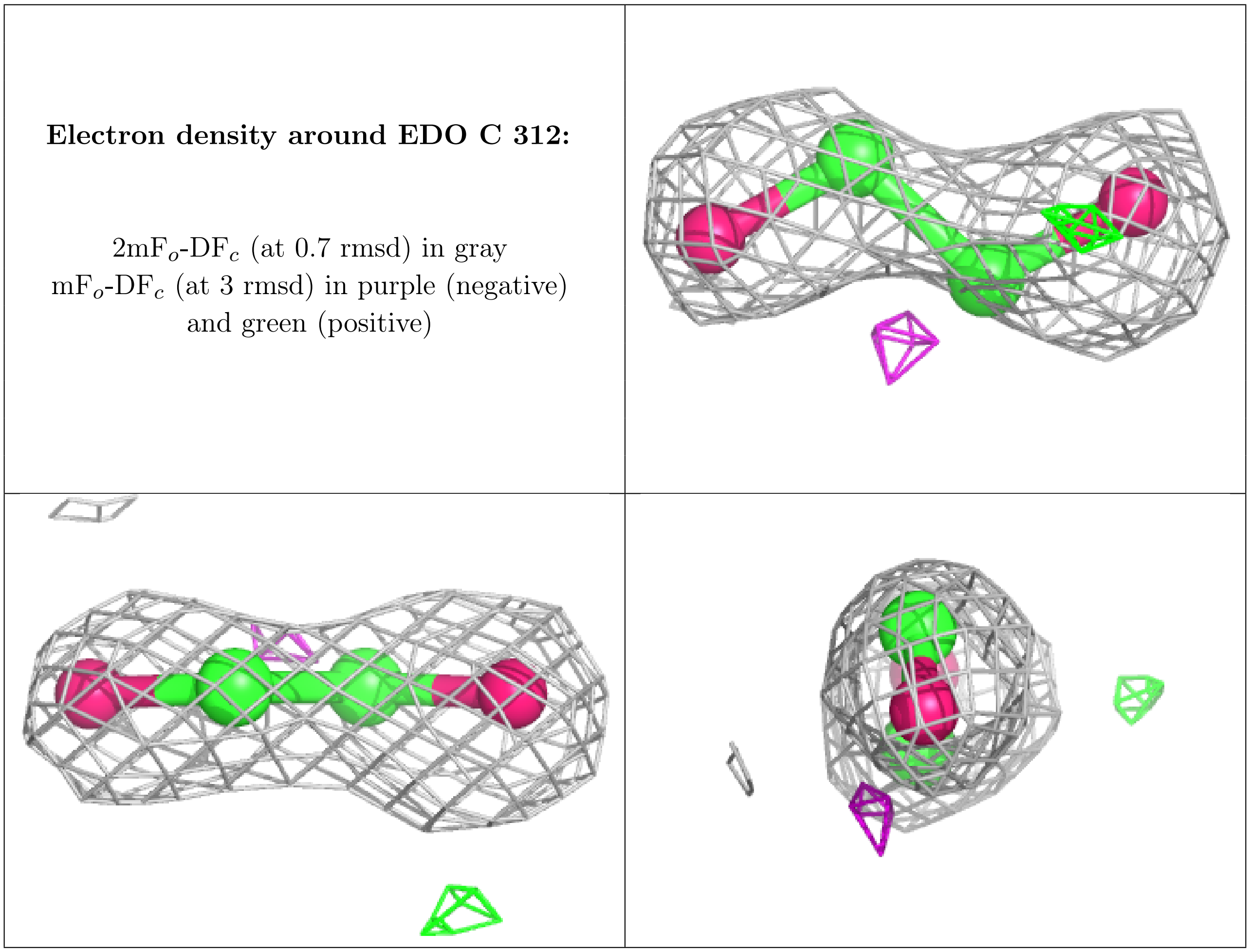
Electron density around EDO J 310:

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







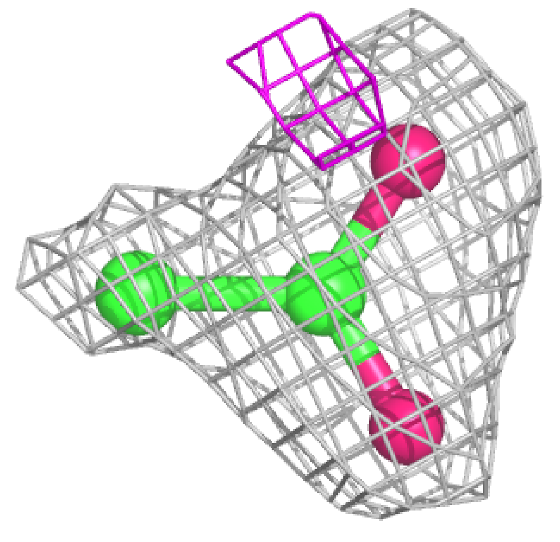


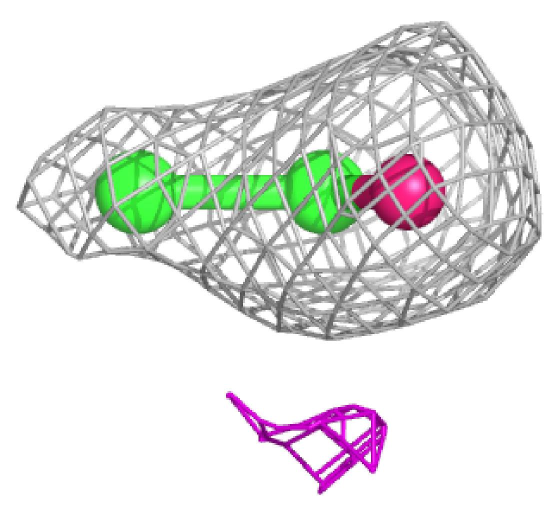
Electron density around EDO C 312:

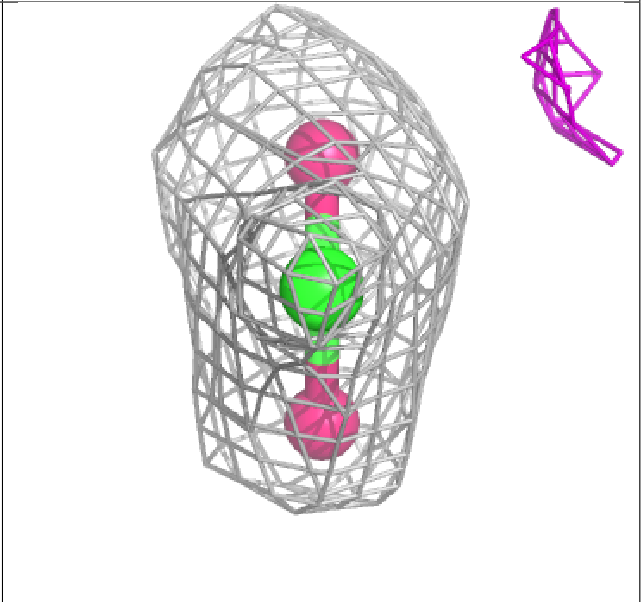
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ACT I 305:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

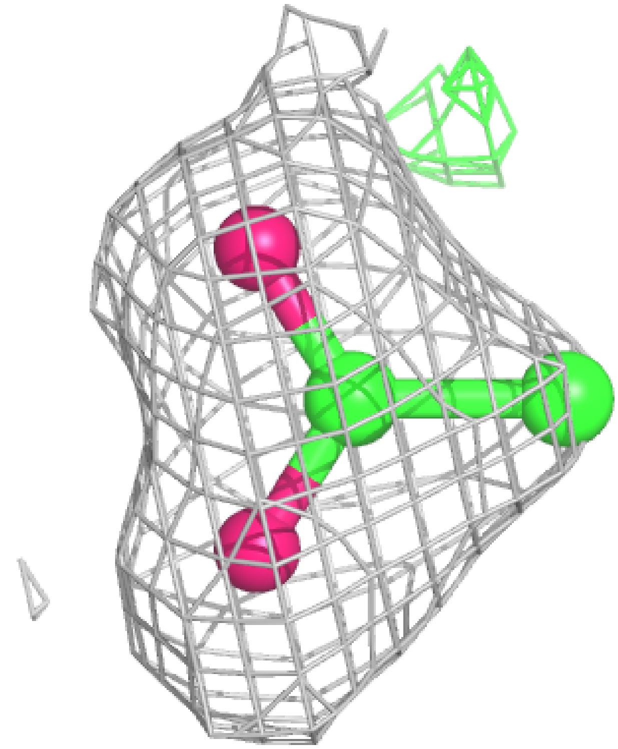


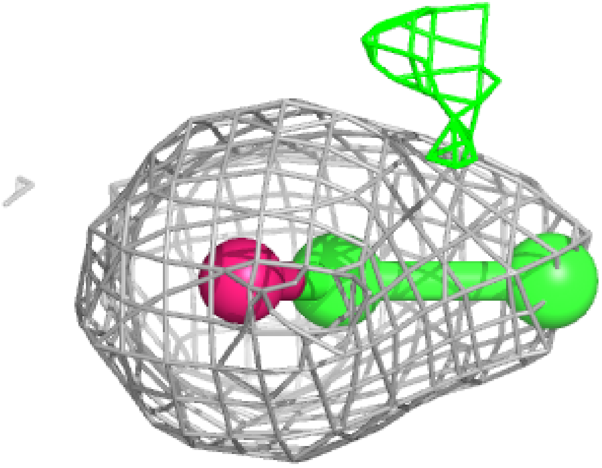


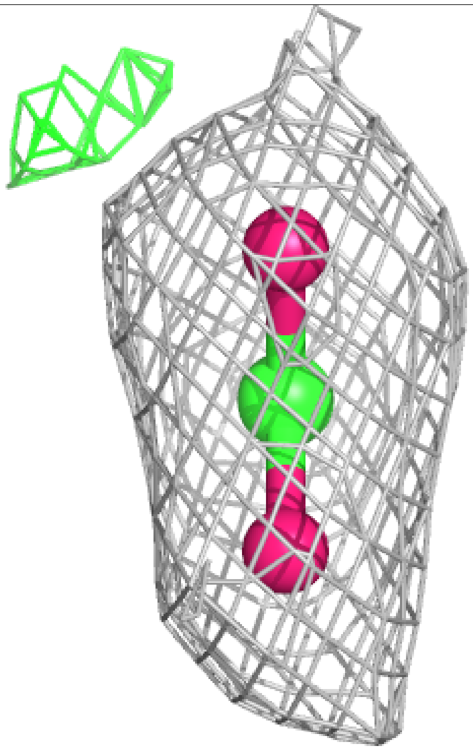


Electron density around ACT J 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

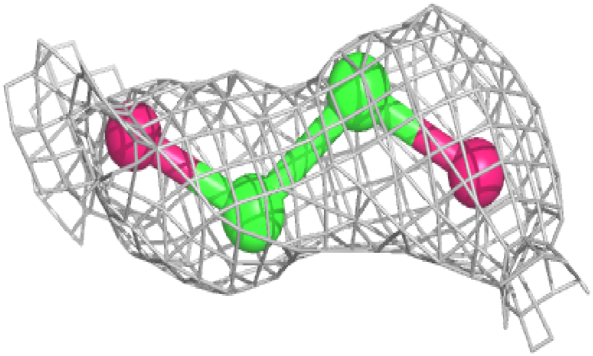


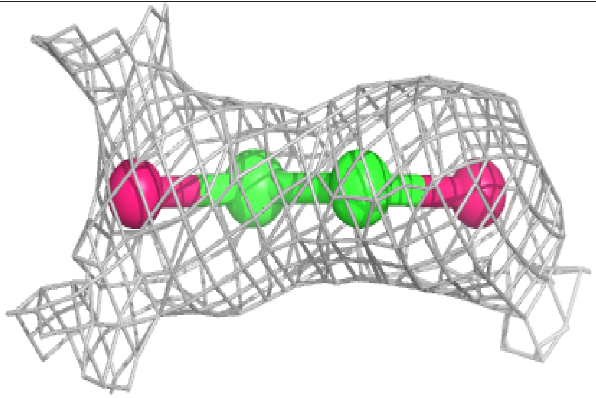


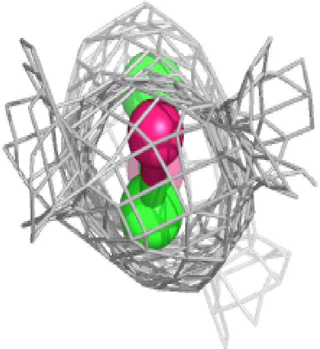


Electron density around EDO C 315:

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

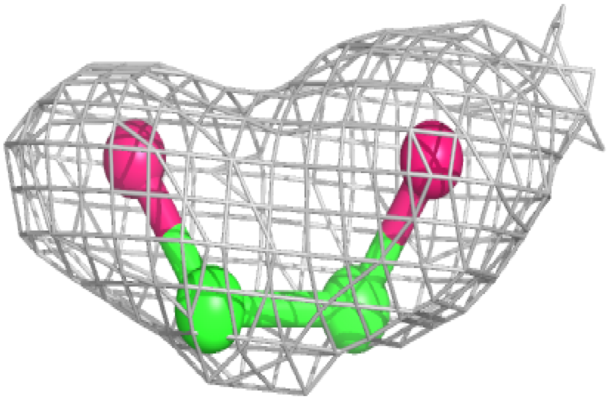


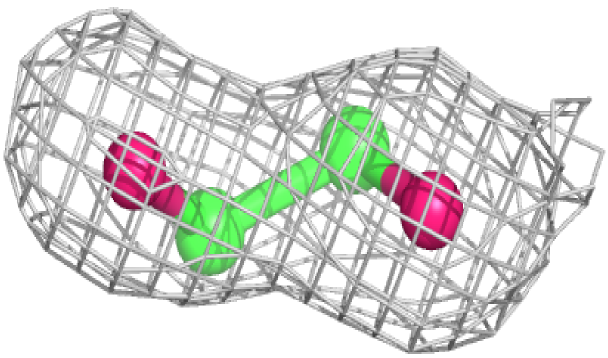


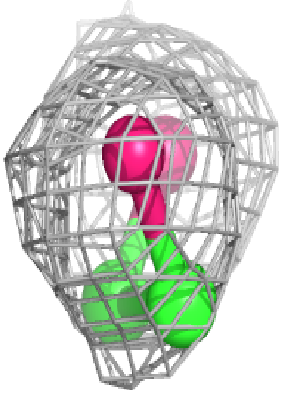


Electron density around EDO A 305:

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

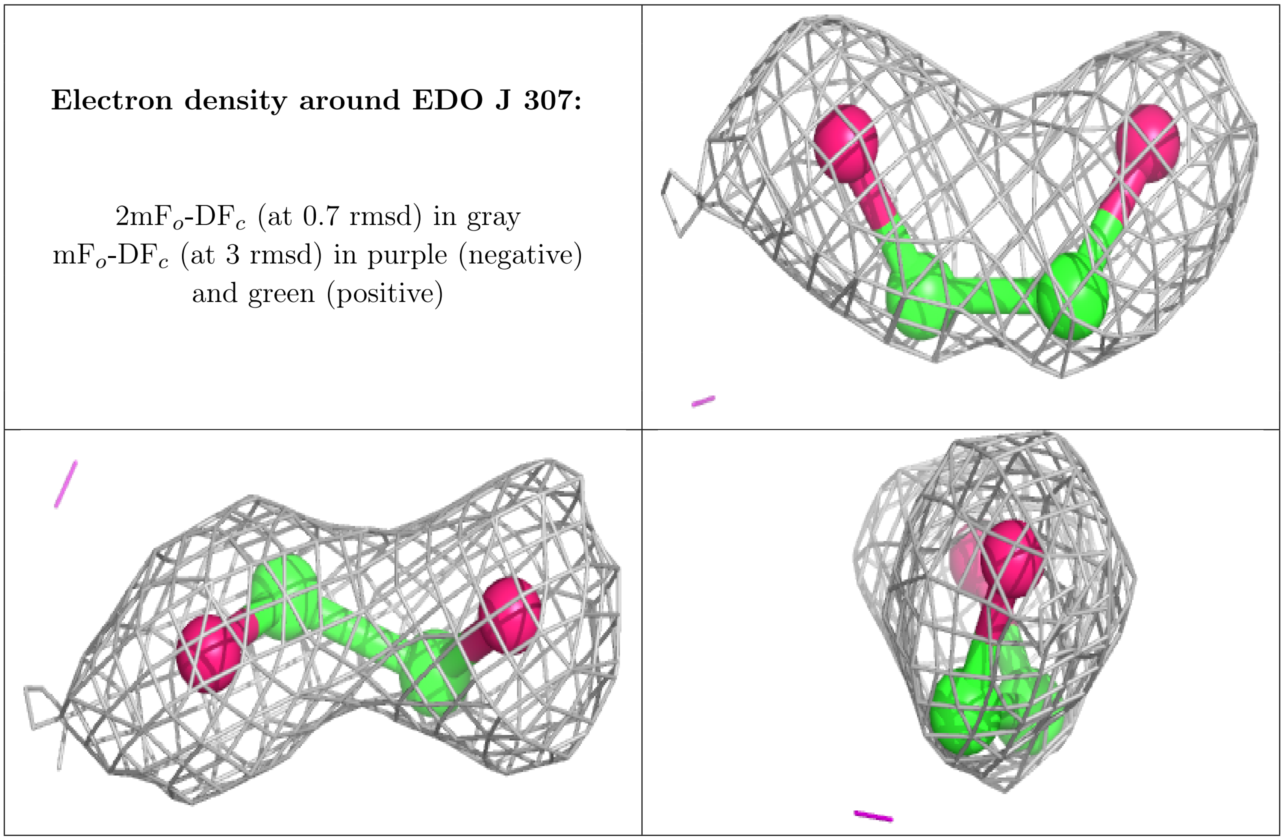






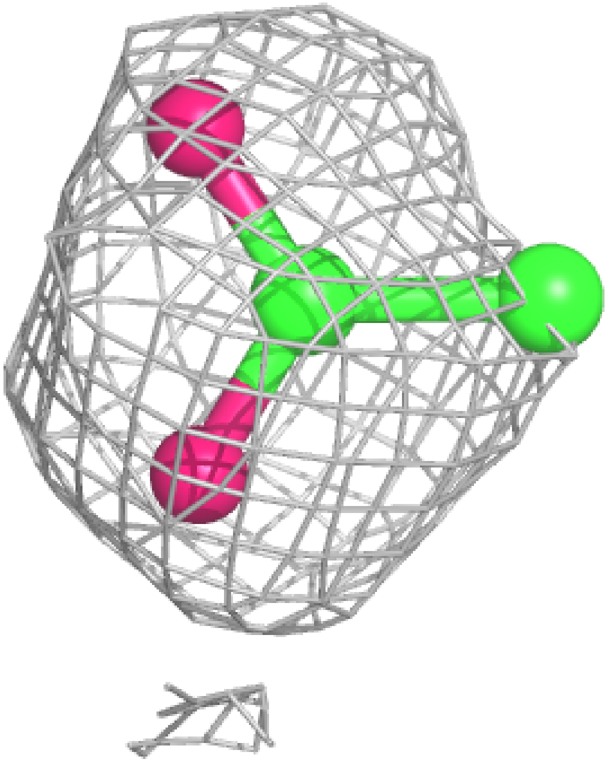
Electron density around EDO J 307:

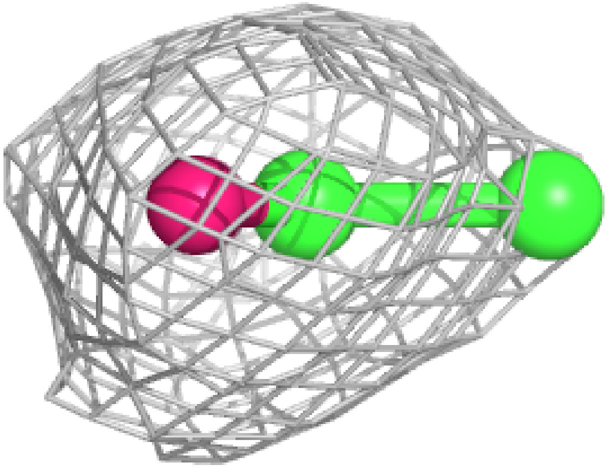
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

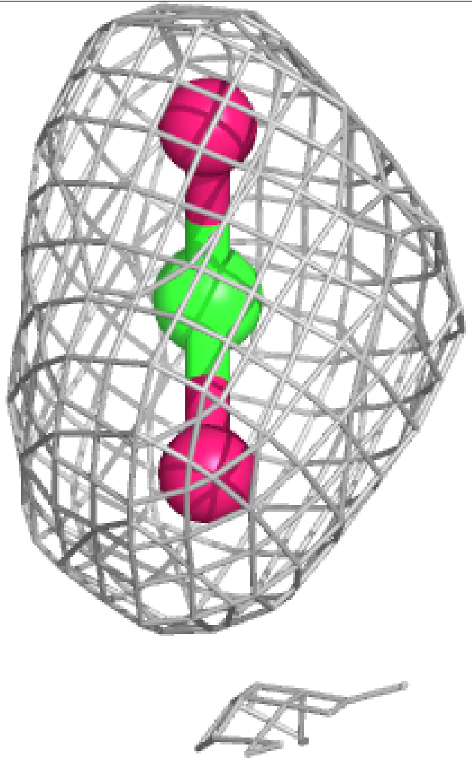


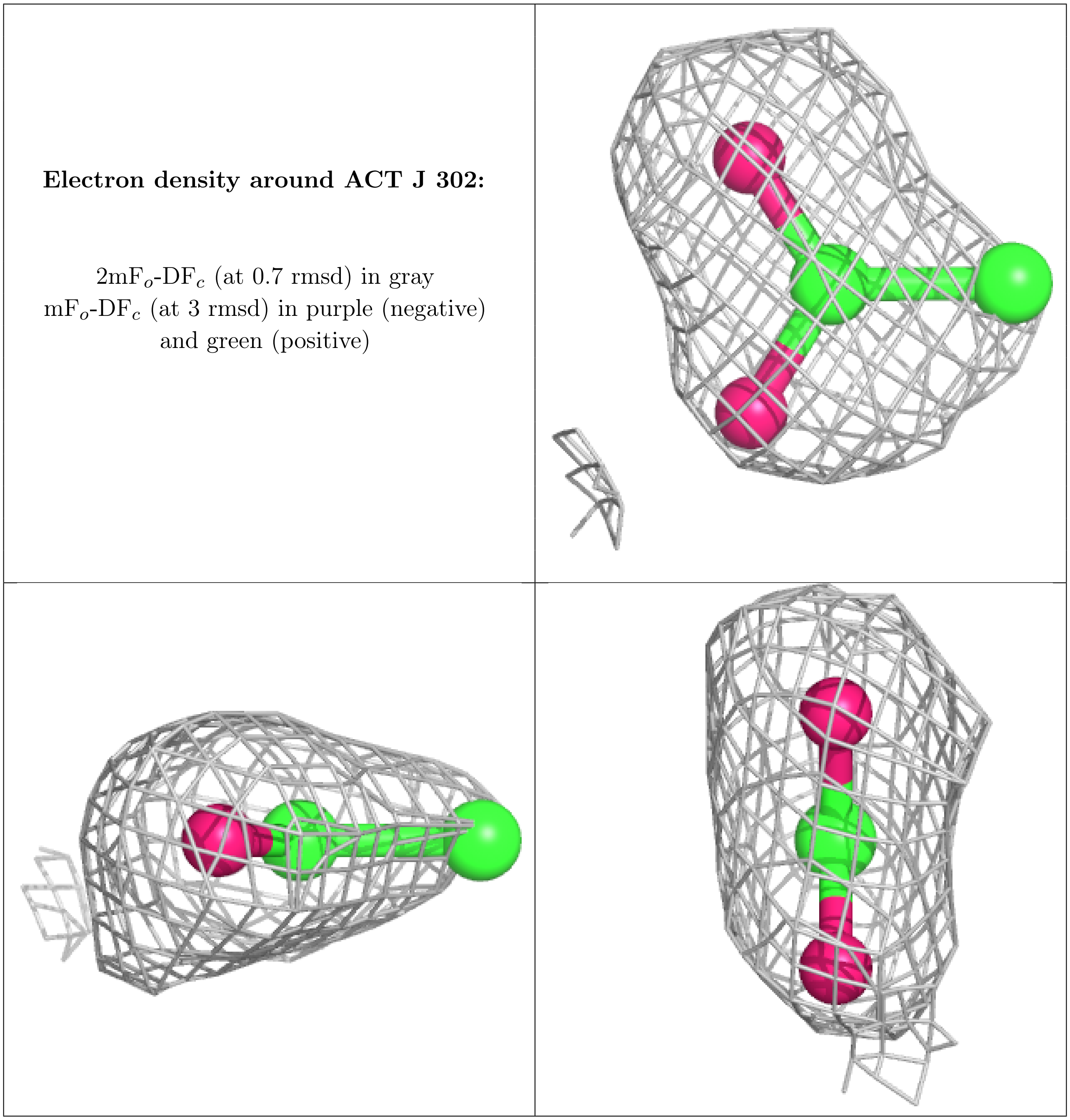
Electron density around ACT E 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







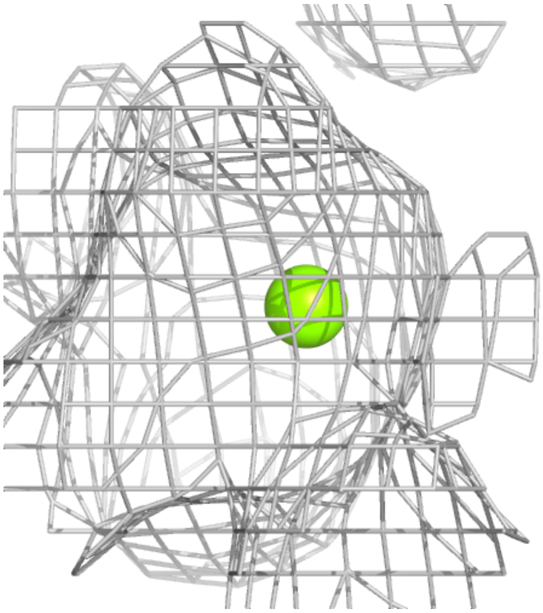


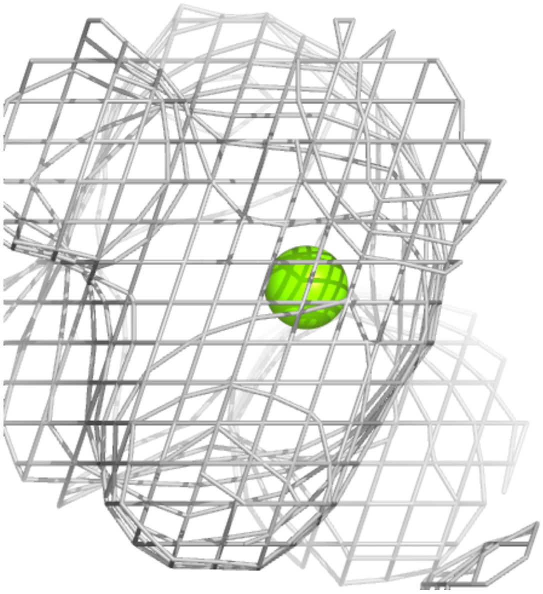
Electron density around ACT J 302:

$2mF_o$-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 D 302:

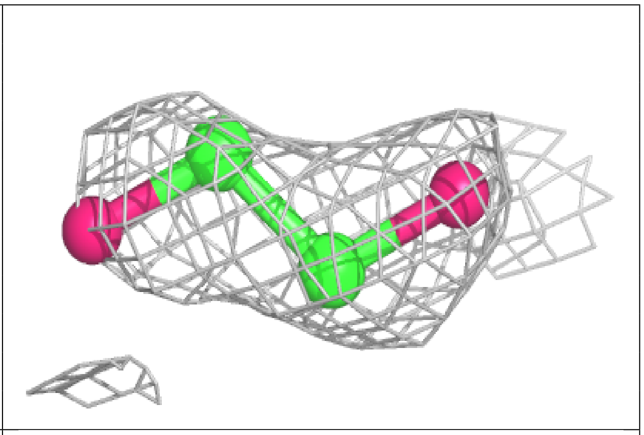
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

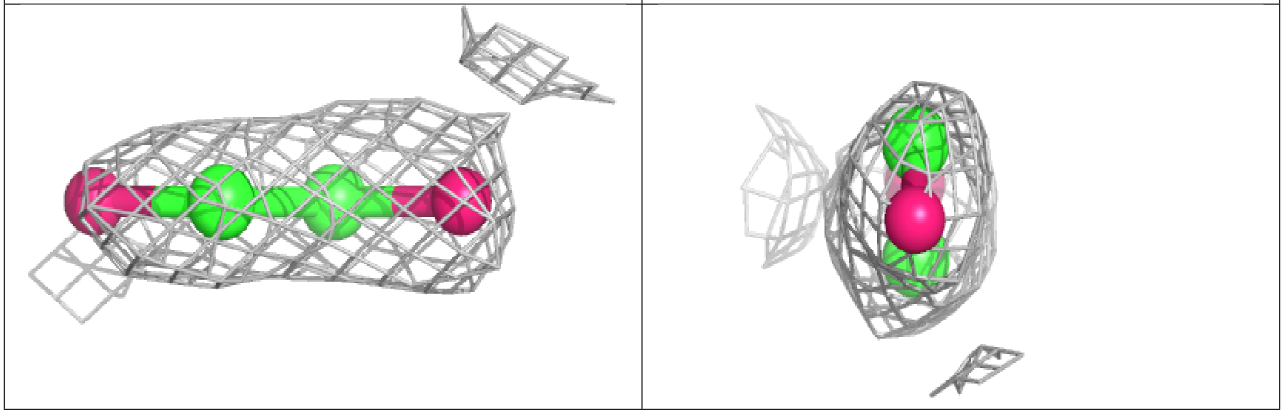




Electron density around EDO G 307:

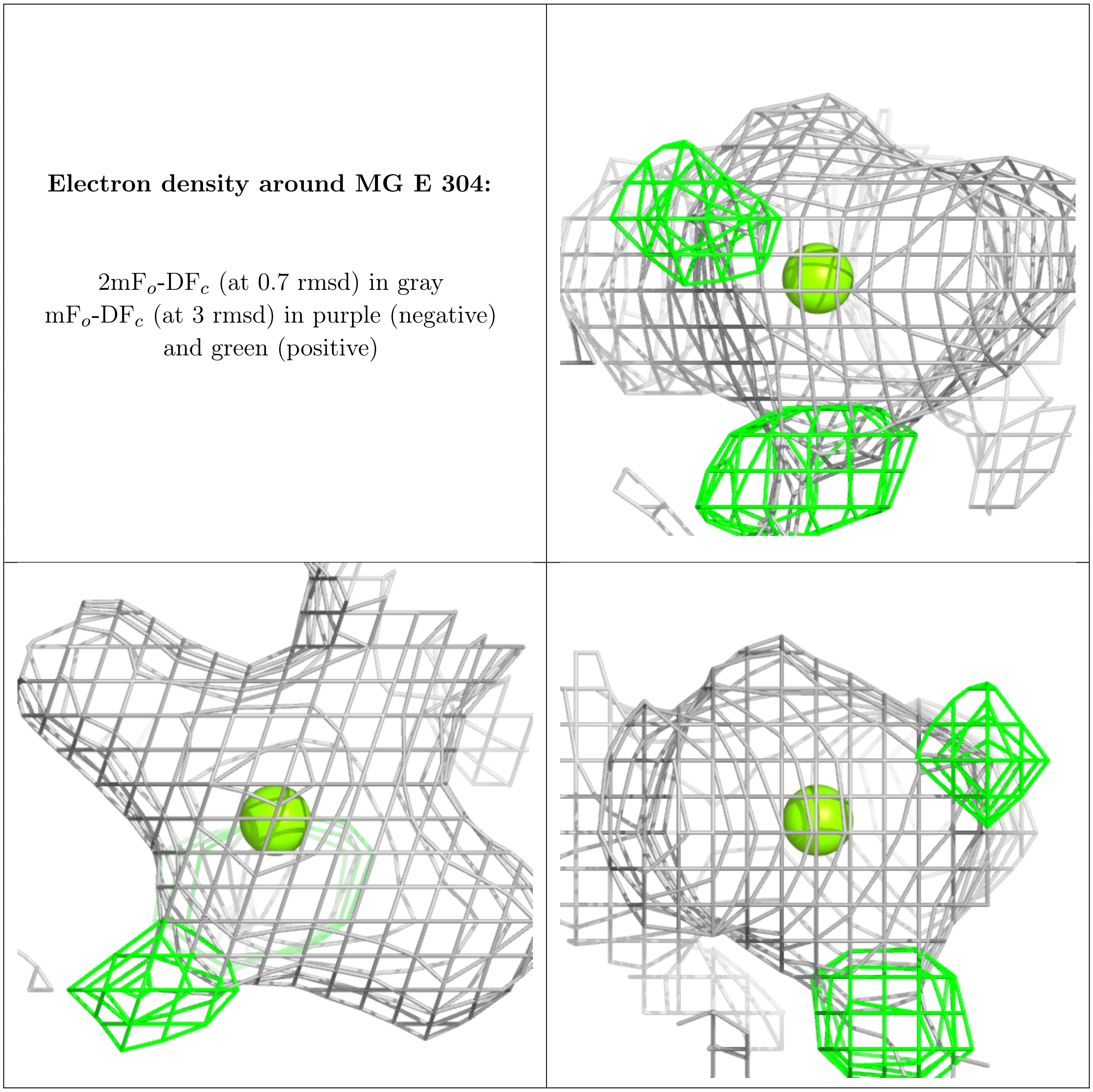
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





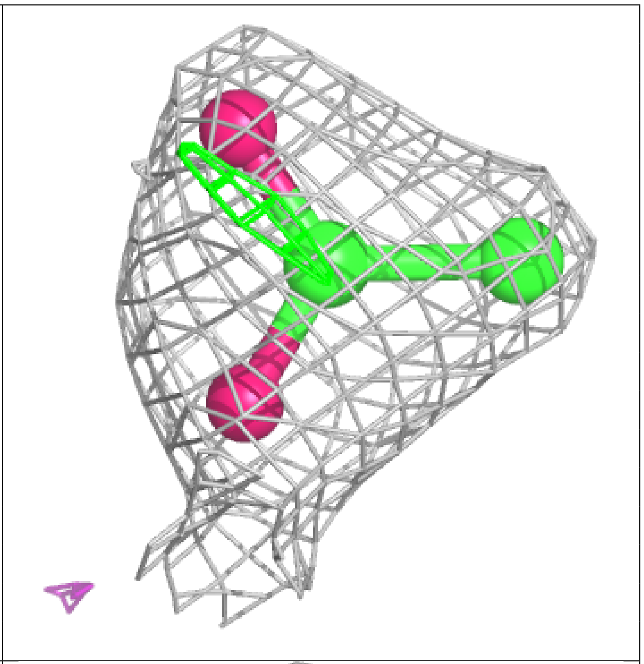
Electron density around MG E 304:

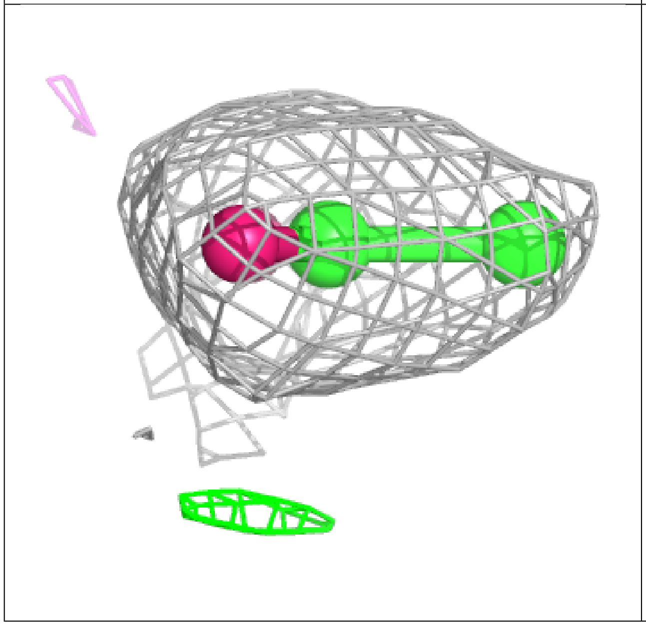
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

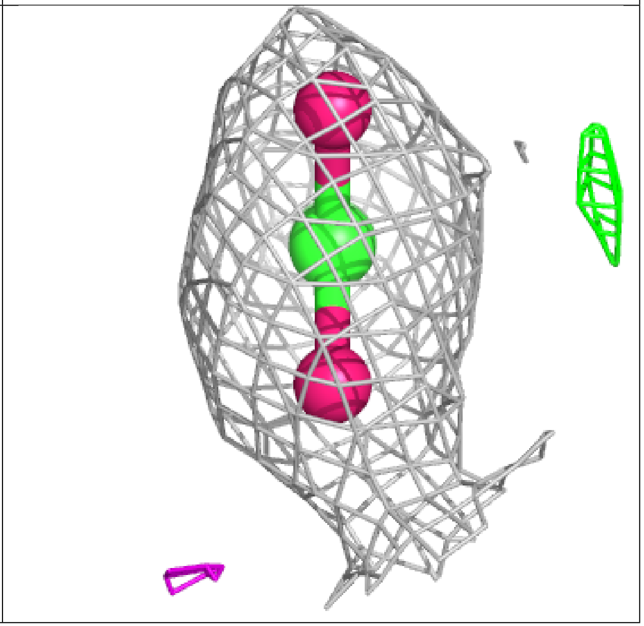


Electron density around ACT H 303:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.