Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:53 PM EDT

PDB ID	:	7KNZ
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, E88A mutant with pyruvate bound in the active site and R,R-bislysine at the allosteric site
Authors	:	Saran, S.; Sanders, D.A.R.
Deposited on	:	2020-11-06
Resolution	:	2.28 Å(reported)

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

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

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

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

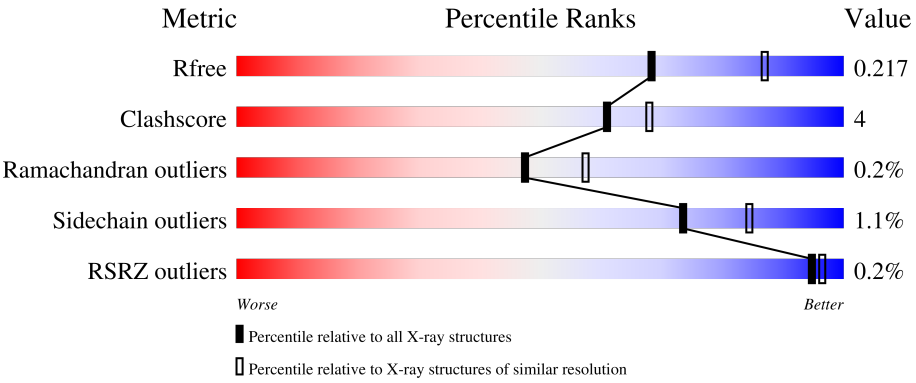
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	86% 9% 5%
1	B	310	88% 6% • 5%
1	C	310	88% 7% 5%
1	D	310	86% 9% 5%
1	E	310	85% 10% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	85% 11% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	E	303	-	-	-	X
4	PEG	A	306	-	-	-	X
4	PEG	E	305	-	-	X	-
4	PEG	F	304	-	-	X	-
6	EDO	C	306	-	-	X	-
8	GOL	F	308	-	X	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2253	1433	372	435	13			
1	B	296	Total	C	N	O	S	0	0	0
			2267	1443	376	435	13			
1	C	296	Total	C	N	O	S	0	0	0
			2267	1442	377	435	13			
1	D	296	Total	C	N	O	S	0	0	0
			2255	1435	372	435	13			
1	E	296	Total	C	N	O	S	0	0	0
			2265	1442	375	435	13			
1	F	296	Total	C	N	O	S	0	0	0
			2259	1437	374	435	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	88	ALA	GLU	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	88	ALA	GLU	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	88	ALA	GLU	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	88	ALA	GLU	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

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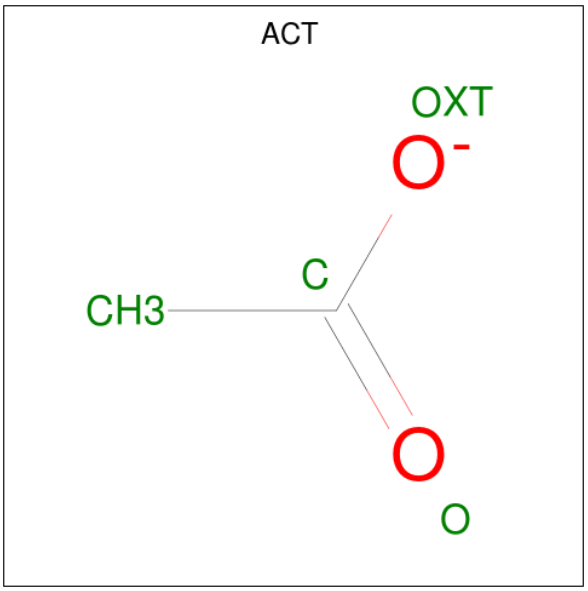
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	88	ALA	GLU	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	88	ALA	GLU	engineered mutation	UNP Q9PPB4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

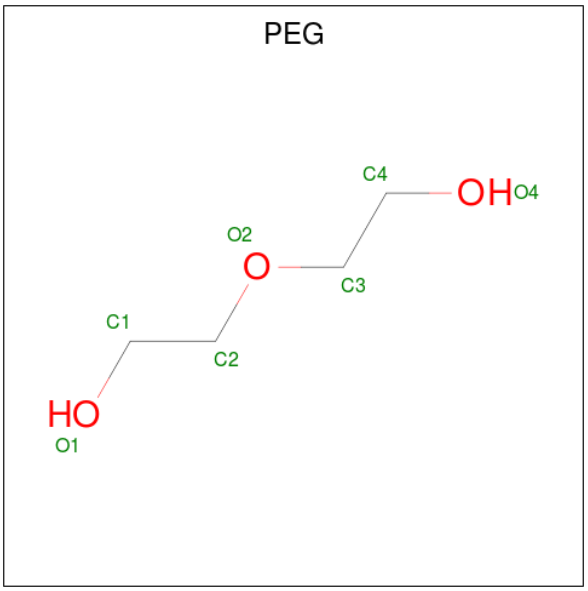
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



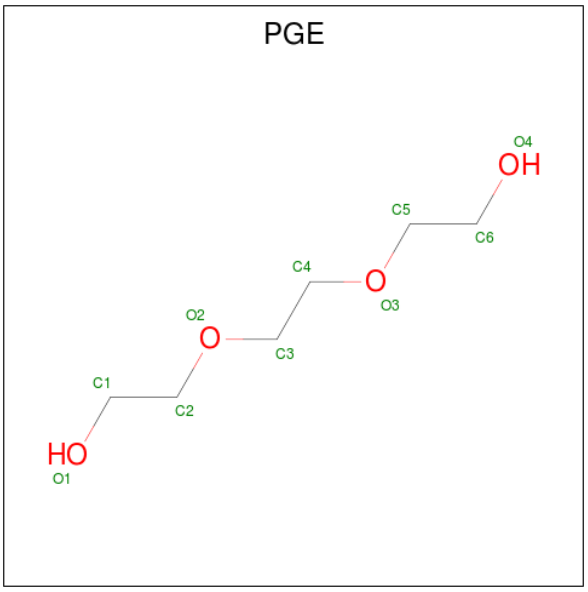
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



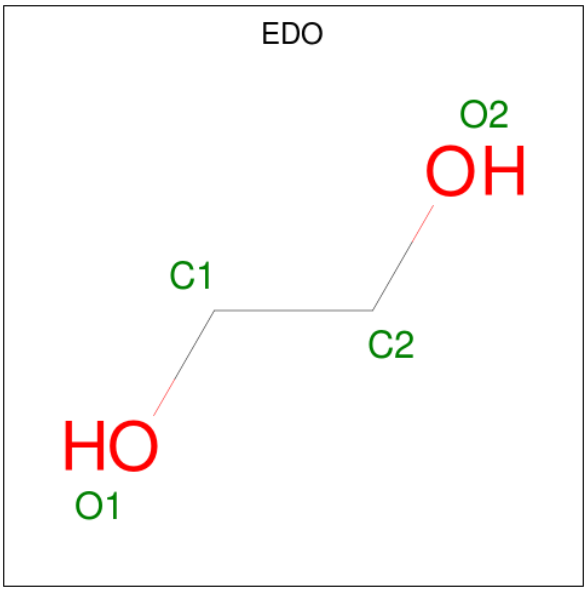
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 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
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0

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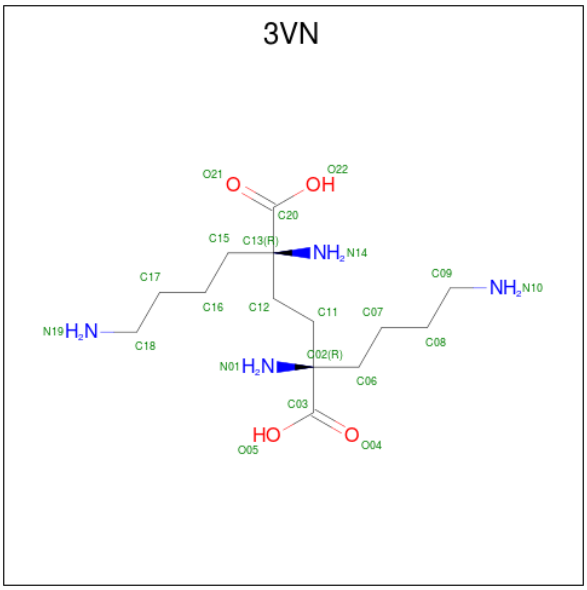
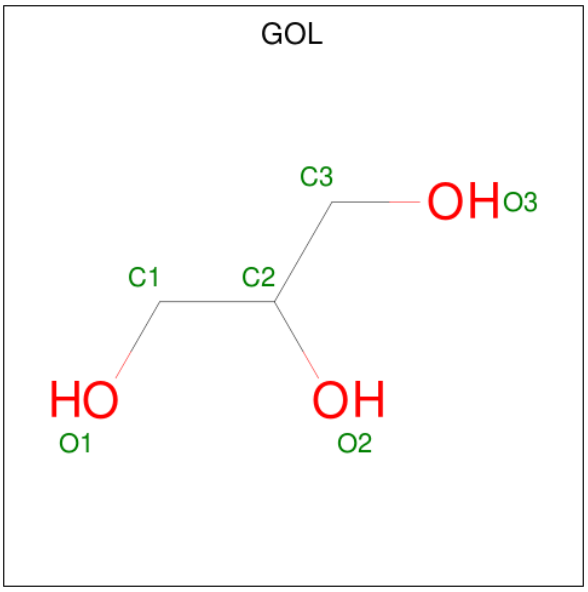
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 4 2 2	0	0

- Molecule 7 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (three-letter code: 3VN) (formula: $C_{14}H_{30}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is water.

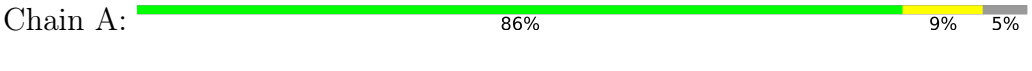
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	143	Total O 143 143	0	0
9	B	142	Total O 142 142	0	0
9	C	147	Total O 147 147	0	0
9	D	135	Total O 135 135	0	0
9	E	136	Total O 136 136	0	0
9	F	148	Total O 148 148	0	0

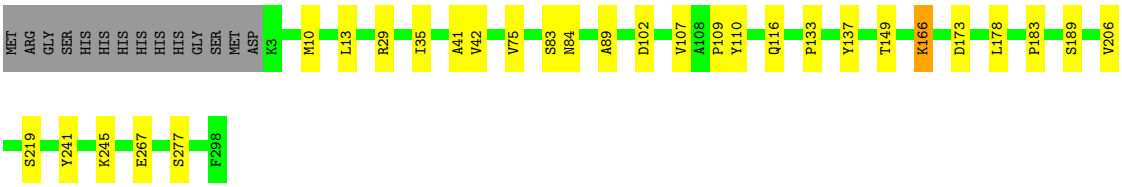
3 Residue-property plots (i)

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

• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

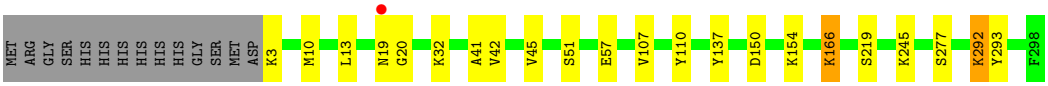
Chain A:





• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:

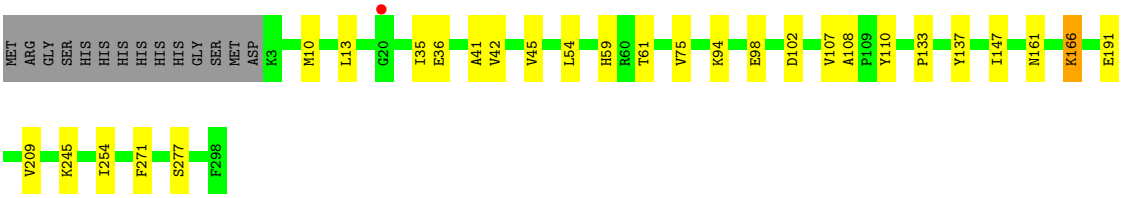


• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C:

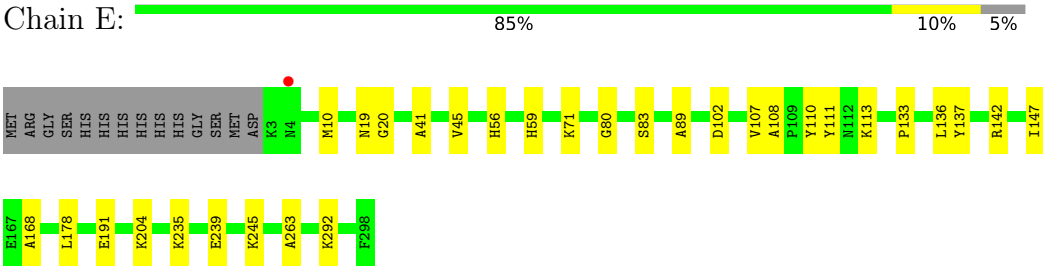
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D:



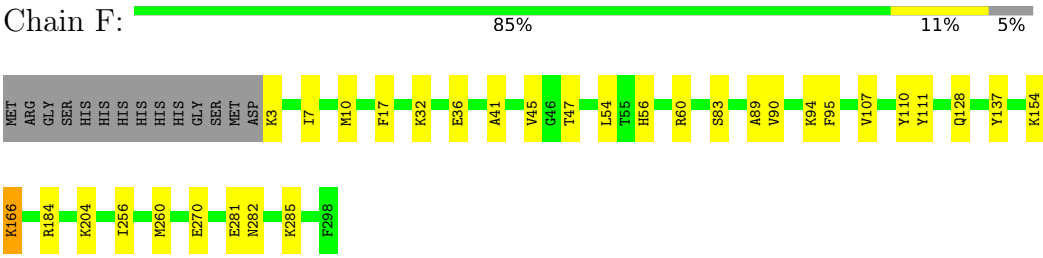
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:



• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.12Å 231.21Å 200.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.91 – 2.28 45.91 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.91-2.28) 92.9 (45.91-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.179 , 0.216 0.181 , 0.217	Depositor DCC
R_{free} test set	4499 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14744	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.31	0/2277	0.48	0/3086
1	B	0.27	0/2291	0.49	0/3100
1	C	0.35	0/2291	0.52	0/3100
1	D	0.48	0/2279	0.55	0/3087
1	E	0.37	0/2289	0.48	0/3098
1	F	0.37	0/2283	0.53	0/3092
All	All	0.37	0/13710	0.51	0/18563

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	A	0	1
1	B	0	1
1	D	0	1
1	E	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	KPI	Mainchain
1	B	166	KPI	Mainchain
1	D	166	KPI	Mainchain

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Mol	Chain	Res	Type	Group
1	E	166	KPI	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2253	0	2252	15	0
1	B	2267	0	2292	13	0
1	C	2267	0	2296	16	0
1	D	2255	0	2257	16	5
1	E	2265	0	2285	22	0
1	F	2259	0	2270	29	5
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	12	0	9	2	0
3	B	4	0	3	0	0
3	C	8	0	6	0	0
3	D	4	0	3	1	0
3	E	8	0	6	0	0
3	F	8	0	6	0	0
4	A	7	0	10	1	0
4	B	14	0	20	3	0
4	E	21	0	30	9	0
4	F	21	0	30	8	0
5	A	10	0	14	0	0
5	B	10	0	14	5	0
5	C	10	0	14	2	0
5	D	10	0	14	0	0
6	A	24	0	36	3	0
6	B	16	0	24	1	0
6	C	16	0	24	5	0
6	D	24	0	36	4	0
6	E	8	0	12	2	0
6	F	4	0	6	2	0
7	B	22	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	22	0	28	3	0
7	F	22	0	28	4	0
8	C	6	0	8	1	0
8	F	6	0	8	4	0
9	A	143	0	0	0	0
9	B	142	0	0	1	0
9	C	147	0	0	3	0
9	D	135	0	0	2	0
9	E	136	0	0	2	0
9	F	148	0	0	4	0
All	All	14744	0	14069	125	5

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

All (125) 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:159:CYS:HA	4:F:304:PEG:H21	1.54	0.89
4:E:305:PEG:H11	7:F:301:3VN:H14	1.67	0.76
4:E:305:PEG:H31	7:F:301:3VN:H2	1.56	0.71
1:C:154:LYS:NZ	9:C:401:HOH:O	2.23	0.70
1:F:90:VAL:HG21	6:F:307:EDO:H12	1.74	0.69
1:F:3:LYS:N	8:F:308:GOL:H31	2.08	0.69
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.74	0.69
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.74	0.68
3:A:303:ACT:H1	7:D:301:3VN:H2	1.58	0.68
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.76	0.68
1:C:56:HIS:HE2	6:C:306:EDO:H22	1.59	0.68
1:F:281:GLU:O	1:F:285:LYS:N	2.22	0.68
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.78	0.66
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.77	0.66
1:F:3:LYS:N	9:F:402:HOH:O	2.28	0.66
1:B:150:ASP:HB3	5:B:307:PGE:H22	1.76	0.66
1:F:154:LYS:HZ2	4:F:305:PEG:H12	1.62	0.65
1:A:116:GLN:H	6:A:313:EDO:H22	1.60	0.65
1:A:183:PRO:HB3	4:A:306:PEG:H11	1.79	0.64
7:B:301:3VN:H3	6:C:306:EDO:H21	1.80	0.64
1:C:124:LYS:NZ	9:C:405:HOH:O	2.30	0.64
8:F:308:GOL:H2	9:F:402:HOH:O	1.97	0.63
1:C:281:GLU:HG2	1:C:285:LYS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.82	0.62
1:F:128:GLN:HG2	4:F:304:PEG:H32	1.84	0.59
1:E:56:HIS:HE2	4:E:305:PEG:H22	1.67	0.59
1:A:29:ARG:HE	3:A:304:ACT:H1	1.69	0.58
1:B:57:GLU:HB3	4:B:305:PEG:H32	1.84	0.58
7:B:301:3VN:H30	6:C:306:EDO:H21	1.86	0.58
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.85	0.58
1:F:154:LYS:HZ3	4:F:305:PEG:H32	1.69	0.57
1:F:160:GLU:H	4:F:304:PEG:H12	1.69	0.57
8:C:310:GOL:O3	8:C:310:GOL:O1	2.16	0.57
1:A:10:MET:HG2	1:A:41:ALA:HB3	1.85	0.57
1:C:56:HIS:NE2	6:C:306:EDO:H22	2.20	0.57
6:A:312:EDO:H11	9:D:432:HOH:O	2.06	0.56
1:D:35:ILE:HG12	1:D:75:VAL:HG21	1.87	0.56
1:E:292:LYS:HD3	9:E:406:HOH:O	2.06	0.56
4:E:305:PEG:H11	7:F:301:3VN:C11	2.36	0.55
1:E:10:MET:HG2	1:E:41:ALA:HB3	1.90	0.53
1:E:204:LYS:HD2	4:E:306:PEG:H41	1.90	0.53
1:B:57:GLU:H	4:B:305:PEG:H12	1.73	0.53
1:E:168:ALA:HA	1:E:191:GLU:HG3	1.91	0.52
1:F:60:ARG:HB3	1:F:95:PHE:CZ	2.45	0.52
1:F:154:LYS:NZ	4:F:305:PEG:H12	2.25	0.52
1:F:32:LYS:O	1:F:36:GLU:HG3	2.10	0.51
1:E:56:HIS:HE2	4:E:305:PEG:C2	2.24	0.50
1:A:83:SER:HB3	1:A:89:ALA:HB2	1.94	0.50
1:C:94:LYS:O	1:C:98:GLU:HG3	2.12	0.50
1:D:45:VAL:HG13	1:D:54:LEU:HD12	1.93	0.50
1:E:149:THR:HG23	1:E:178:LEU:HD23	1.93	0.50
1:D:209:VAL:H	6:D:306:EDO:H11	1.76	0.49
1:D:61:THR:HG21	6:D:308:EDO:H12	1.93	0.49
1:E:239:GLU:HA	4:E:307:PEG:H21	1.95	0.49
1:D:191:GLU:HA	6:D:307:EDO:H12	1.93	0.49
7:D:301:3VN:N14	3:D:304:ACT:H2	2.27	0.49
1:F:282:ASN:HA	1:F:285:LYS:HB2	1.94	0.49
1:B:3:LYS:N	9:B:407:HOH:O	2.45	0.48
4:E:307:PEG:H31	6:E:309:EDO:H11	1.96	0.48
6:D:306:EDO:H12	9:D:468:HOH:O	2.14	0.48
1:A:189:SER:HB3	1:A:206:VAL:HG12	1.95	0.48
1:B:10:MET:HG2	1:B:41:ALA:HB3	1.95	0.48
1:D:245:LYS:HA	1:D:245:LYS:HD2	1.69	0.48
1:F:90:VAL:O	1:F:94:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HD11	1:B:42:VAL:HB	1.96	0.47
1:C:57:GLU:CD	9:C:404:HOH:O	2.54	0.47
1:A:35:ILE:HG12	1:A:75:VAL:HG21	1.97	0.47
1:D:161:ASN:OD1	1:D:161:ASN:N	2.46	0.47
1:F:56:HIS:HD1	1:F:60:ARG:HH22	1.62	0.47
1:C:108:ALA:HB2	1:C:147:ILE:HD11	1.98	0.46
1:A:13:LEU:HD11	1:A:42:VAL:HB	1.97	0.46
1:A:241:TYR:HB3	6:A:309:EDO:H11	1.96	0.46
1:B:154:LYS:NZ	5:B:307:PGE:H52	2.31	0.46
4:F:304:PEG:H22	4:F:304:PEG:H41	1.55	0.46
1:B:292:LYS:HE3	1:B:293:TYR:CZ	2.51	0.46
1:E:111:TYR:HH	1:F:47:THR:HG1	1.63	0.46
1:F:166:KPI:H1A	9:F:404:HOH:O	2.15	0.46
1:A:173:ASP:HB3	6:B:310:EDO:H21	1.98	0.45
1:C:10:MET:HA	1:C:41:ALA:O	2.17	0.45
1:C:295:ILE:HD12	6:C:309:EDO:H11	1.97	0.45
1:E:245:LYS:HA	1:E:245:LYS:HD2	1.70	0.45
1:C:245:LYS:HA	1:C:245:LYS:HD2	1.77	0.45
1:D:254:ILE:HA	1:D:271:PHE:CE2	2.52	0.45
1:D:45:VAL:HG11	1:D:59:HIS:CG	2.53	0.44
1:D:94:LYS:O	1:D:98:GLU:HG3	2.18	0.44
1:E:102:ASP:O	1:E:133:PRO:HD2	2.19	0.43
1:B:245:LYS:HA	1:B:245:LYS:HD2	1.76	0.43
1:D:108:ALA:HB2	1:D:147:ILE:HD11	2.01	0.43
5:C:305:PGE:H2	5:C:305:PGE:H42	1.85	0.43
1:F:160:GLU:H	4:F:304:PEG:C1	2.32	0.43
1:E:113:LYS:HA	9:E:435:HOH:O	2.19	0.43
1:A:102:ASP:O	1:A:133:PRO:HD2	2.19	0.42
1:D:54:LEU:O	7:D:301:3VN:H9	2.19	0.42
1:D:102:ASP:O	1:D:133:PRO:HD2	2.19	0.42
1:E:83:SER:OG	4:E:305:PEG:H12	2.19	0.42
1:C:74:LYS:HG2	1:E:263:ALA:O	2.19	0.42
6:F:307:EDO:H21	9:F:424:HOH:O	2.19	0.42
1:E:45:VAL:HG11	1:E:59:HIS:CG	2.55	0.42
1:F:3:LYS:N	8:F:308:GOL:C3	2.80	0.42
1:E:71:LYS:HA	6:E:308:EDO:H11	2.00	0.42
1:F:45:VAL:HG13	1:F:54:LEU:HD12	2.01	0.42
1:B:154:LYS:HZ3	5:B:307:PGE:H52	1.85	0.42
1:E:59:HIS:NE2	1:E:80:GLY:O	2.42	0.41
1:A:245:LYS:HA	1:A:245:LYS:HD2	1.76	0.41
1:E:108:ALA:HB2	1:E:147:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:LEU:O	7:F:301:3VN:H9	2.20	0.41
1:F:10:MET:HA	1:F:41:ALA:O	2.19	0.41
5:B:307:PGE:H52	5:B:307:PGE:H3	1.83	0.41
1:F:256:ILE:O	1:F:260:MET:HG2	2.20	0.41
1:A:149:THR:HG23	1:A:178:LEU:HD23	2.02	0.41
1:C:154:LYS:HD3	5:C:305:PGE:H22	2.01	0.41
1:F:17:PHE:HB2	1:F:270:GLU:HB3	2.02	0.41
1:B:45:VAL:HG12	1:B:51:SER:HB3	2.03	0.41
1:B:154:LYS:HD3	5:B:307:PGE:H3	2.02	0.41
1:E:83:SER:HB3	1:E:89:ALA:HB2	2.01	0.41
4:B:306:PEG:H22	4:B:306:PEG:H41	1.74	0.40
1:C:166:KPI:HDA	1:C:207:ILE:HD12	2.03	0.40
1:D:13:LEU:HD11	1:D:42:VAL:HB	2.02	0.40
1:F:7:ILE:HB	1:F:204:LYS:O	2.21	0.40
1:C:31:ILE:HD13	1:C:66:ALA:HA	2.02	0.40
1:E:142:ARG:O	1:F:111:TYR:HA	2.22	0.40
1:F:83:SER:HB3	1:F:89:ALA:HB2	2.02	0.40
1:E:136:LEU:O	1:E:166:KPI:N	2.54	0.40
1:A:84:ASN:HA	1:A:109:PRO:HB3	2.03	0.40
1:F:3:LYS:N	8:F:308:GOL:C2	2.85	0.40

All (5) 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)
1:D:36:GLU:OE2	1:F:184:ARG:NH1[3_555]	1.56	0.64
1:D:36:GLU:OE2	1:F:184:ARG:NH2[3_555]	1.56	0.64
1:D:36:GLU:OE2	1:F:184:ARG:CZ[3_555]	1.72	0.48
1:D:36:GLU:CD	1:F:184:ARG:NH1[3_555]	1.98	0.22
1:D:36:GLU:OE1	1:F:184:ARG:NH1[3_555]	2.03	0.17

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	B	293/310 (94%)	286 (98%)	5 (2%)	2 (1%)	22	25
1	C	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	D	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	E	293/310 (94%)	285 (97%)	6 (2%)	2 (1%)	22	25
1	F	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
All	All	1758/1860 (94%)	1722 (98%)	32 (2%)	4 (0%)	47	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLY
1	E	20	GLY
1	E	19	ASN
1	B	19	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/259 (93%)	236 (98%)	4 (2%)	60	74
1	B	244/259 (94%)	239 (98%)	5 (2%)	55	70
1	C	245/259 (95%)	243 (99%)	2 (1%)	81	90
1	D	240/259 (93%)	238 (99%)	2 (1%)	81	90
1	E	243/259 (94%)	241 (99%)	2 (1%)	81	90
1	F	242/259 (93%)	241 (100%)	1 (0%)	91	95
All	All	1454/1554 (94%)	1438 (99%)	16 (1%)	73	84

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

Mol	Chain	Res	Type
1	A	110	TYR
1	A	219	SER
1	A	267	GLU
1	A	277	SER
1	B	32	LYS
1	B	110	TYR
1	B	219	SER
1	B	277	SER
1	B	292	LYS
1	C	110	TYR
1	C	231	LYS
1	D	110	TYR
1	D	277	SER
1	E	110	TYR
1	E	235	LYS
1	F	110	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KPI	A	166	1	11,13,14	2.23	3 (27%)	10,15,17	3.69	6 (60%)
1	KPI	D	166	1	11,13,14	1.57	2 (18%)	10,15,17	3.39	5 (50%)
1	KPI	C	166	1	11,13,14	1.00	1 (9%)	10,15,17	2.75	5 (50%)
1	KPI	B	166	1	11,13,14	2.22	3 (27%)	10,15,17	3.90	6 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	KPI	E	166	1	11,13,14	2.22	3 (27%)	10,15,17	3.74	5 (50%)
1	KPI	F	166	1	11,13,14	0.94	1 (9%)	10,15,17	3.39	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	A	166	1	-	4/13/14/16	-
1	KPI	D	166	1	-	0/13/14/16	-
1	KPI	C	166	1	-	0/13/14/16	-
1	KPI	B	166	1	-	4/13/14/16	-
1	KPI	E	166	1	-	4/13/14/16	-
1	KPI	F	166	1	-	0/13/14/16	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	KPI	O2-CX2	5.38	1.36	1.22
1	E	166	KPI	O2-CX2	5.28	1.36	1.22
1	B	166	KPI	O2-CX2	5.24	1.36	1.22
1	B	166	KPI	O-C	4.22	1.36	1.19
1	D	166	KPI	O-C	4.21	1.36	1.19
1	E	166	KPI	O-C	4.14	1.36	1.19
1	A	166	KPI	O-C	4.09	1.36	1.19
1	E	166	KPI	O1-CX2	-2.38	1.23	1.30
1	B	166	KPI	O1-CX2	-2.25	1.24	1.30
1	A	166	KPI	O1-CX2	-2.25	1.24	1.30
1	C	166	KPI	O1-CX2	2.16	1.36	1.30
1	F	166	KPI	O1-CX2	2.10	1.36	1.30
1	D	166	KPI	O1-CX2	2.03	1.36	1.30

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	166	KPI	C1-CX1-CX2	-7.63	110.75	118.17
1	B	166	KPI	C1-CX1-CX2	-7.44	110.94	118.17
1	E	166	KPI	C1-CX1-CX2	-7.22	111.15	118.17
1	D	166	KPI	C1-CX1-CX2	-7.19	111.17	118.17
1	A	166	KPI	C1-CX1-CX2	-6.70	111.65	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	KPI	O2-CX2-CX1	-6.00	113.72	121.38
1	A	166	KPI	O2-CX2-CX1	-5.86	113.89	121.38
1	B	166	KPI	O1-CX2-CX1	5.66	128.63	116.35
1	D	166	KPI	O2-CX2-CX1	5.65	128.59	121.38
1	A	166	KPI	O1-CX2-CX1	5.60	128.51	116.35
1	E	166	KPI	O2-CX2-CX1	-5.58	114.26	121.38
1	C	166	KPI	C1-CX1-CX2	-5.50	112.82	118.17
1	E	166	KPI	O1-CX2-CX1	5.41	128.10	116.35
1	F	166	KPI	O2-CX2-CX1	5.15	127.95	121.38
1	C	166	KPI	O2-CX2-CX1	4.15	126.67	121.38
1	B	166	KPI	C1-CX1-NZ	3.48	132.22	123.11
1	D	166	KPI	C1-CX1-NZ	3.47	132.18	123.11
1	E	166	KPI	C1-CX1-NZ	3.45	132.14	123.11
1	F	166	KPI	C1-CX1-NZ	3.45	132.13	123.11
1	A	166	KPI	C1-CX1-NZ	3.23	131.56	123.11
1	C	166	KPI	C1-CX1-NZ	3.19	131.45	123.11
1	C	166	KPI	O1-CX2-O2	-2.87	117.04	123.61
1	D	166	KPI	O1-CX2-O2	-2.77	117.27	123.61
1	F	166	KPI	O1-CX2-O2	-2.72	117.39	123.61
1	B	166	KPI	CE-NZ-CX1	2.69	129.03	121.70
1	A	166	KPI	O1-CX2-O2	-2.64	117.58	123.61
1	E	166	KPI	O1-CX2-O2	-2.62	117.62	123.61
1	B	166	KPI	O1-CX2-O2	-2.62	117.62	123.61
1	C	166	KPI	CE-NZ-CX1	2.56	128.68	121.70
1	D	166	KPI	CE-NZ-CX1	2.56	128.67	121.70
1	F	166	KPI	CE-NZ-CX1	2.25	127.83	121.70
1	A	166	KPI	CE-NZ-CX1	2.17	127.62	121.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	KPI	NZ-CX1-CX2-O1
1	A	166	KPI	NZ-CX1-CX2-O2
1	A	166	KPI	C1-CX1-CX2-O2
1	B	166	KPI	NZ-CX1-CX2-O1
1	B	166	KPI	NZ-CX1-CX2-O2
1	B	166	KPI	C1-CX1-CX2-O2
1	E	166	KPI	NZ-CX1-CX2-O1
1	E	166	KPI	NZ-CX1-CX2-O2
1	E	166	KPI	C1-CX1-CX2-O2
1	A	166	KPI	C1-CX1-CX2-O1

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Mol	Chain	Res	Type	Atoms
1	B	166	KPI	C1-CX1-CX2-O1
1	E	166	KPI	C1-CX1-CX2-O1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 10 are monoatomic - leaving 52 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	$\#\|Z\| > 2$
6	EDO	C	306	-	3,3,3	0.50	0	2,2,2	0.16	0
8	GOL	C	310	-	5,5,5	0.85	0	5,5,5	1.00	0
3	ACT	A	305	-	3,3,3	1.31	0	3,3,3	1.37	0
5	PGE	A	307	-	9,9,9	0.29	0	8,8,8	0.33	0
6	EDO	D	310	-	3,3,3	0.48	0	2,2,2	0.32	0
3	ACT	D	304	-	3,3,3	1.13	0	3,3,3	1.56	0
6	EDO	C	307	-	3,3,3	0.48	0	2,2,2	0.19	0
3	ACT	F	303	-	3,3,3	1.37	1 (33%)	3,3,3	1.36	0
4	PEG	B	305	-	6,6,6	0.49	0	5,5,5	0.30	0
3	ACT	E	304	-	3,3,3	1.32	0	3,3,3	1.51	0
6	EDO	D	309	-	3,3,3	0.46	0	2,2,2	0.37	0
3	ACT	C	304	-	3,3,3	1.35	0	3,3,3	1.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	313	-	3,3,3	0.46	0	2,2,2	0.30	0
6	EDO	C	309	-	3,3,3	0.48	0	2,2,2	0.36	0
3	ACT	C	303	-	3,3,3	1.28	0	3,3,3	1.50	0
6	EDO	E	309	-	3,3,3	0.46	0	2,2,2	0.36	0
4	PEG	E	306	-	6,6,6	0.48	0	5,5,5	0.24	0
6	EDO	A	310	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	B	310	-	3,3,3	0.47	0	2,2,2	0.27	0
7	3VN	B	301	-	17,21,21	1.29	2 (11%)	18,28,28	1.65	4 (22%)
4	PEG	E	305	-	6,6,6	0.48	0	5,5,5	0.35	0
6	EDO	D	306	-	3,3,3	0.42	0	2,2,2	0.37	0
5	PGE	D	305	-	9,9,9	0.32	0	8,8,8	0.28	0
7	3VN	D	301	-	17,21,21	1.10	1 (5%)	18,28,28	1.92	7 (38%)
8	GOL	F	308	-	5,5,5	0.53	0	5,5,5	1.70	2 (40%)
6	EDO	D	307	-	3,3,3	0.44	0	2,2,2	0.41	0
6	EDO	A	308	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	D	311	-	3,3,3	0.39	0	2,2,2	0.45	0
6	EDO	B	311	-	3,3,3	0.47	0	2,2,2	0.31	0
4	PEG	B	306	-	6,6,6	0.47	0	5,5,5	0.26	0
3	ACT	A	304	-	3,3,3	1.24	0	3,3,3	1.54	0
3	ACT	F	302	-	3,3,3	1.10	0	3,3,3	1.58	0
4	PEG	F	304	-	6,6,6	0.51	0	5,5,5	0.49	0
6	EDO	A	312	-	3,3,3	0.46	0	2,2,2	0.36	0
4	PEG	E	307	-	6,6,6	0.50	0	5,5,5	0.25	0
6	EDO	B	309	-	3,3,3	0.47	0	2,2,2	0.34	0
4	PEG	A	306	-	6,6,6	0.46	0	5,5,5	0.48	0
6	EDO	F	307	-	3,3,3	0.47	0	2,2,2	0.24	0
6	EDO	A	311	-	3,3,3	0.46	0	2,2,2	0.38	0
3	ACT	A	303	-	3,3,3	1.25	0	3,3,3	1.54	0
6	EDO	D	308	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	B	308	-	3,3,3	0.47	0	2,2,2	0.25	0
5	PGE	B	307	-	9,9,9	0.31	0	8,8,8	0.33	0
4	PEG	F	306	-	6,6,6	0.48	0	5,5,5	0.28	0
5	PGE	C	305	-	9,9,9	0.31	0	8,8,8	0.30	0
6	EDO	E	308	-	3,3,3	0.42	0	2,2,2	0.43	0
7	3VN	F	301	-	17,21,21	1.19	1 (5%)	18,28,28	1.66	4 (22%)
3	ACT	E	303	-	3,3,3	1.35	1 (33%)	3,3,3	1.37	0
6	EDO	C	308	-	3,3,3	0.45	0	2,2,2	0.33	0
4	PEG	F	305	-	6,6,6	0.48	0	5,5,5	0.24	0
6	EDO	A	309	-	3,3,3	0.47	0	2,2,2	0.37	0
3	ACT	B	304	-	3,3,3	1.30	0	3,3,3	1.50	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
6	EDO	C	306	-	-	0/1/1/1	-
8	GOL	C	310	-	-	2/4/4/4	-
5	PGE	A	307	-	-	5/7/7/7	-
6	EDO	D	310	-	-	1/1/1/1	-
6	EDO	C	307	-	-	0/1/1/1	-
4	PEG	B	305	-	-	1/4/4/4	-
6	EDO	D	309	-	-	1/1/1/1	-
6	EDO	A	313	-	-	1/1/1/1	-
6	EDO	C	309	-	-	0/1/1/1	-
6	EDO	E	309	-	-	0/1/1/1	-
4	PEG	E	306	-	-	2/4/4/4	-
6	EDO	A	310	-	-	1/1/1/1	-
7	3VN	B	301	-	-	1/29/31/31	-
4	PEG	E	305	-	-	3/4/4/4	-
6	EDO	D	306	-	-	0/1/1/1	-
5	PGE	D	305	-	-	2/7/7/7	-
7	3VN	D	301	-	-	9/29/31/31	-
8	GOL	F	308	-	-	4/4/4/4	-
6	EDO	D	307	-	-	0/1/1/1	-
6	EDO	A	308	-	-	0/1/1/1	-
6	EDO	D	311	-	-	0/1/1/1	-
6	EDO	B	311	-	-	1/1/1/1	-
4	PEG	B	306	-	-	3/4/4/4	-
4	PEG	F	304	-	-	1/4/4/4	-
6	EDO	A	312	-	-	1/1/1/1	-
4	PEG	E	307	-	-	3/4/4/4	-
6	EDO	B	309	-	-	0/1/1/1	-
4	PEG	A	306	-	-	2/4/4/4	-
6	EDO	F	307	-	-	0/1/1/1	-
6	EDO	A	311	-	-	1/1/1/1	-
6	EDO	D	308	-	-	1/1/1/1	-
6	EDO	B	308	-	-	1/1/1/1	-
5	PGE	B	307	-	-	6/7/7/7	-
4	PEG	F	306	-	-	2/4/4/4	-
5	PGE	C	305	-	-	5/7/7/7	-
6	EDO	E	308	-	-	1/1/1/1	-
7	3VN	F	301	-	-	8/29/31/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	308	-	-	0/1/1/1	-
4	PEG	F	305	-	-	3/4/4/4	-
6	EDO	A	309	-	-	0/1/1/1	-
6	EDO	B	310	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	3VN	C06-C02	2.69	1.57	1.54
7	F	301	3VN	C06-C02	2.59	1.57	1.54
7	B	301	3VN	C11-C02	2.10	1.57	1.54
3	E	303	ACT	CH3-C	2.06	1.57	1.49
3	F	303	ACT	CH3-C	2.04	1.57	1.49
7	D	301	3VN	C06-C02	2.03	1.57	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	301	3VN	C07-C06-C02	-3.72	108.60	115.20
7	F	301	3VN	C11-C12-C13	-3.47	109.07	115.19
7	B	301	3VN	O05-C03-C02	3.22	122.36	113.70
7	F	301	3VN	O22-C20-C13	2.85	121.36	113.70
7	D	301	3VN	O22-C20-C13	2.82	121.28	113.70
7	B	301	3VN	O22-C20-C13	2.81	121.26	113.70
7	F	301	3VN	C16-C15-C13	-2.80	110.24	115.20
7	B	301	3VN	C16-C15-C13	-2.67	110.46	115.20
7	D	301	3VN	C11-C12-C13	-2.56	110.67	115.19
7	D	301	3VN	O05-C03-C02	2.54	120.54	113.70
7	D	301	3VN	C16-C15-C13	-2.40	110.94	115.20
8	F	308	GOL	O1-C1-C2	2.39	121.66	110.20
7	F	301	3VN	C07-C06-C02	-2.25	111.20	115.20
7	D	301	3VN	C06-C07-C08	-2.16	106.75	113.19
8	F	308	GOL	O2-C2-C3	-2.14	99.68	109.12
7	B	301	3VN	C07-C06-C02	-2.04	111.58	115.20
7	D	301	3VN	C12-C11-C02	-2.01	111.64	115.19

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	301	3VN	N14-C13-C20-O22

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Mol	Chain	Res	Type	Atoms
7	F	301	3VN	C11-C02-C03-O04
7	F	301	3VN	C11-C02-C03-O05
7	F	301	3VN	N14-C13-C20-O22
8	C	310	GOL	C1-C2-C3-O3
8	F	308	GOL	O1-C1-C2-C3
5	A	307	PGE	O2-C3-C4-O3
8	C	310	GOL	O2-C2-C3-O3
4	A	306	PEG	O2-C3-C4-O4
4	F	305	PEG	O1-C1-C2-O2
4	F	305	PEG	O2-C3-C4-O4
5	C	305	PGE	O3-C5-C6-O4
4	F	304	PEG	C4-C3-O2-C2
8	F	308	GOL	C1-C2-C3-O3
5	C	305	PGE	O2-C3-C4-O3
4	E	305	PEG	C1-C2-O2-C3
4	B	306	PEG	O1-C1-C2-O2
6	A	311	EDO	O1-C1-C2-O2
6	D	309	EDO	O1-C1-C2-O2
6	D	310	EDO	O1-C1-C2-O2
7	D	301	3VN	C02-C06-C07-C08
5	B	307	PGE	O3-C5-C6-O4
5	B	307	PGE	C3-C4-O3-C5
7	D	301	3VN	C11-C02-C06-C07
7	D	301	3VN	C06-C07-C08-C09
5	A	307	PGE	O3-C5-C6-O4
8	F	308	GOL	O2-C2-C3-O3
4	B	306	PEG	C4-C3-O2-C2
4	B	305	PEG	O2-C3-C4-O4
4	E	305	PEG	O2-C3-C4-O4
4	E	307	PEG	O2-C3-C4-O4
5	A	307	PGE	O1-C1-C2-O2
6	A	310	EDO	O1-C1-C2-O2
6	B	311	EDO	O1-C1-C2-O2
4	E	307	PEG	C4-C3-O2-C2
7	F	301	3VN	C15-C16-C17-C18
4	E	307	PEG	O1-C1-C2-O2
4	F	305	PEG	C1-C2-O2-C3
4	A	306	PEG	O1-C1-C2-O2
4	F	306	PEG	O2-C3-C4-O4
6	E	308	EDO	O1-C1-C2-O2
4	F	306	PEG	C4-C3-O2-C2
5	B	307	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
5	B	307	PGE	C1-C2-O2-C3
5	B	307	PGE	C4-C3-O2-C2
5	A	307	PGE	C4-C3-O2-C2
5	C	305	PGE	C6-C5-O3-C4
7	D	301	3VN	C12-C13-C20-O22
7	D	301	3VN	C15-C13-C20-O22
6	A	313	EDO	O1-C1-C2-O2
4	E	306	PEG	C1-C2-O2-C3
5	C	305	PGE	O1-C1-C2-O2
5	D	305	PGE	O1-C1-C2-O2
5	D	305	PGE	C1-C2-O2-C3
4	E	306	PEG	C4-C3-O2-C2
4	B	306	PEG	O2-C3-C4-O4
6	B	308	EDO	O1-C1-C2-O2
5	A	307	PGE	C6-C5-O3-C4
5	C	305	PGE	C4-C3-O2-C2
7	D	301	3VN	C16-C17-C18-N19
7	D	301	3VN	C03-C02-C06-C07
4	E	305	PEG	O1-C1-C2-O2
5	B	307	PGE	O2-C3-C4-O3
6	A	312	EDO	O1-C1-C2-O2
6	D	308	EDO	O1-C1-C2-O2
8	F	308	GOL	O1-C1-C2-O2
7	D	301	3VN	C15-C13-C20-O21
7	F	301	3VN	C06-C02-C03-O04
7	F	301	3VN	C06-C02-C03-O05
7	F	301	3VN	C12-C13-C20-O22
7	F	301	3VN	C15-C13-C20-O22
7	B	301	3VN	C16-C17-C18-N19

There are no ring outliers.

30 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	306	EDO	4	0
8	C	310	GOL	1	0
3	D	304	ACT	1	0
4	B	305	PEG	2	0
6	A	313	EDO	1	0
6	C	309	EDO	1	0
6	E	309	EDO	1	0
4	E	306	PEG	1	0

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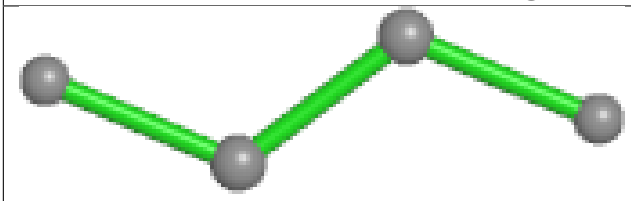
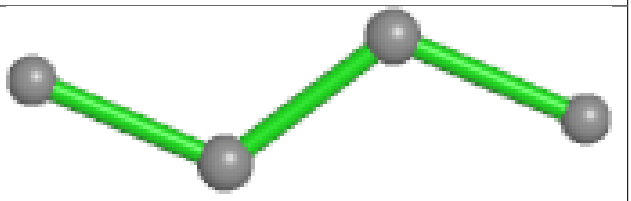
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	310	EDO	1	0
7	B	301	3VN	2	0
4	E	305	PEG	6	0
6	D	306	EDO	2	0
7	D	301	3VN	3	0
8	F	308	GOL	4	0
6	D	307	EDO	1	0
4	B	306	PEG	1	0
3	A	304	ACT	1	0
4	F	304	PEG	5	0
6	A	312	EDO	1	0
4	E	307	PEG	2	0
4	A	306	PEG	1	0
6	F	307	EDO	2	0
3	A	303	ACT	1	0
6	D	308	EDO	1	0
5	B	307	PGE	5	0
5	C	305	PGE	2	0
6	E	308	EDO	1	0
7	F	301	3VN	4	0
4	F	305	PEG	3	0
6	A	309	EDO	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.

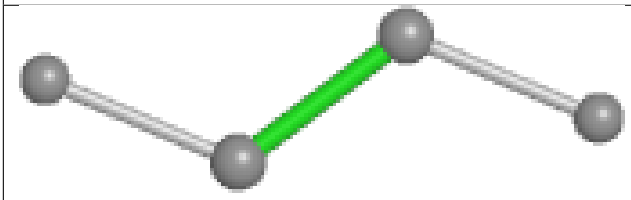
Ligand EDO C 306



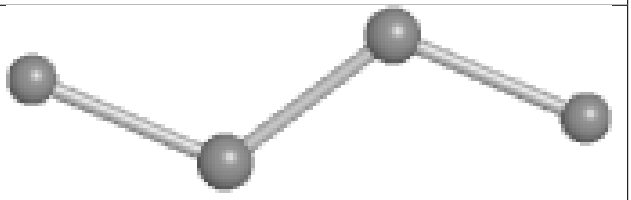
Bond lengths



Bond angles

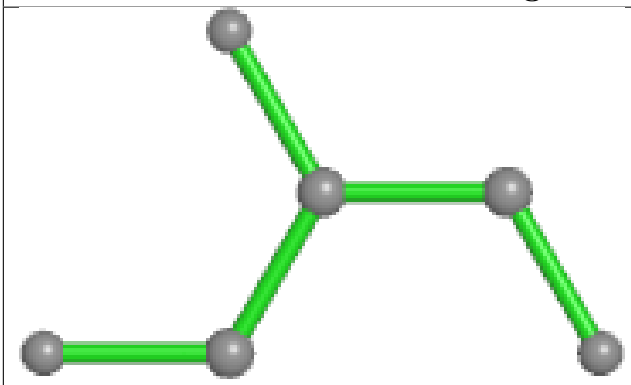


Torsions

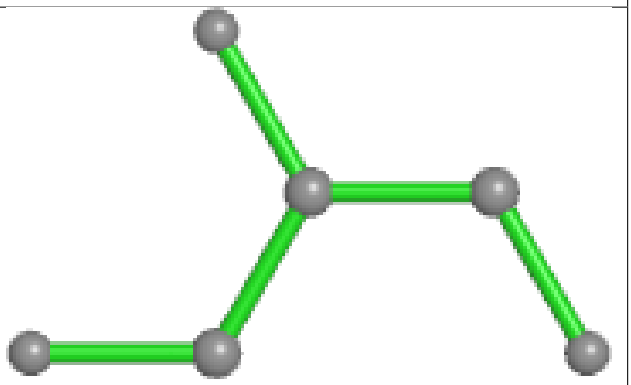


Rings

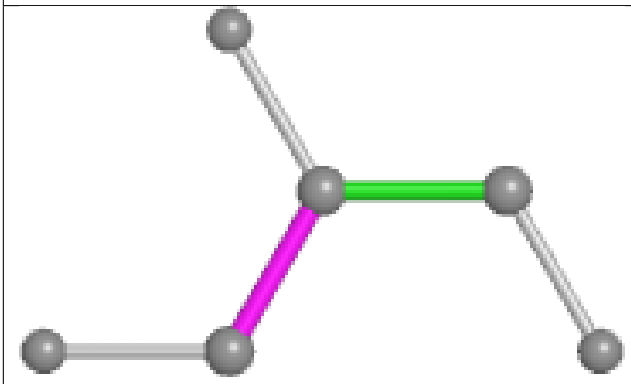
Ligand GOL C 310



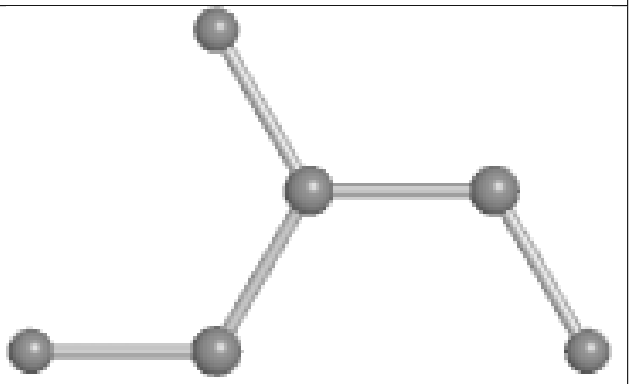
Bond lengths



Bond angles

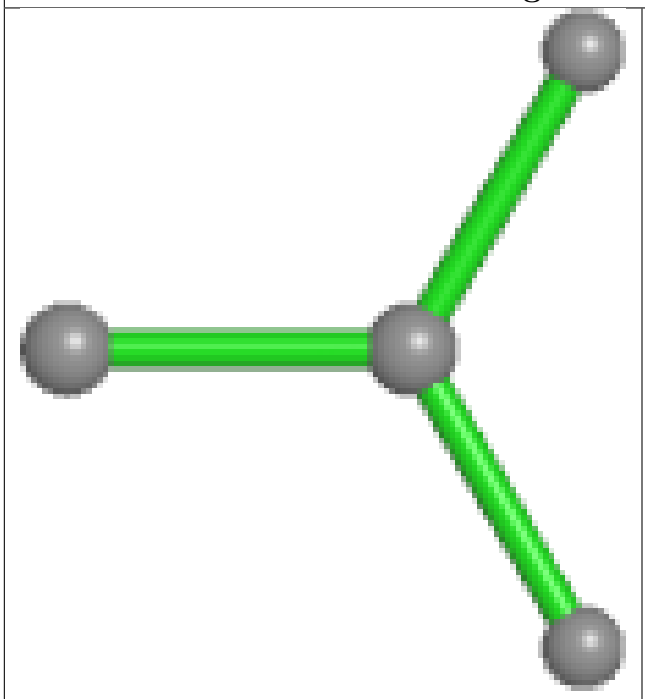


Torsions

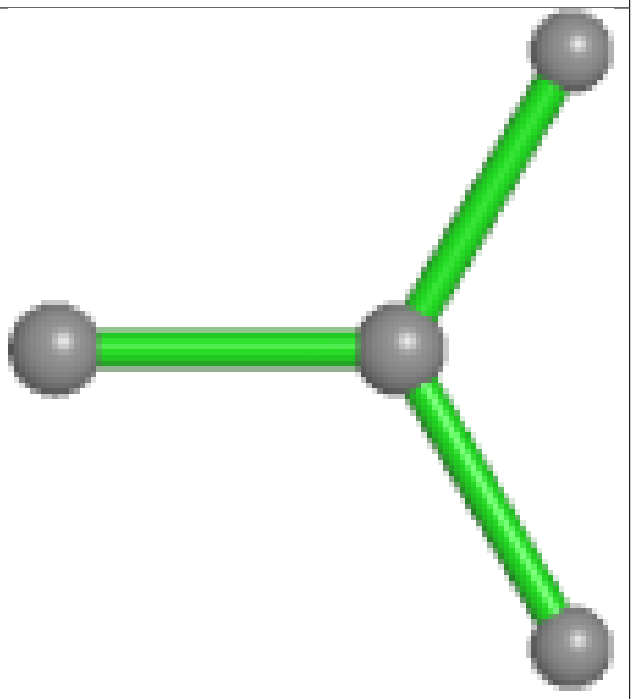


Rings

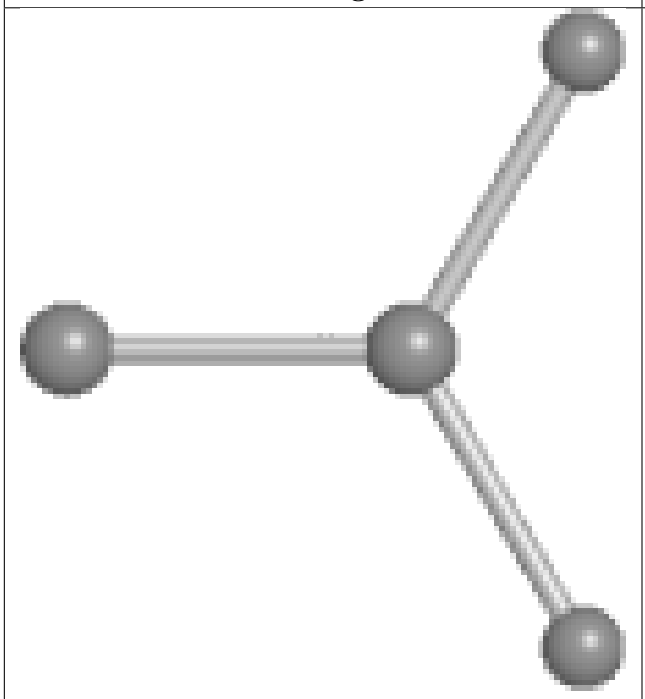
Ligand ACT A 305



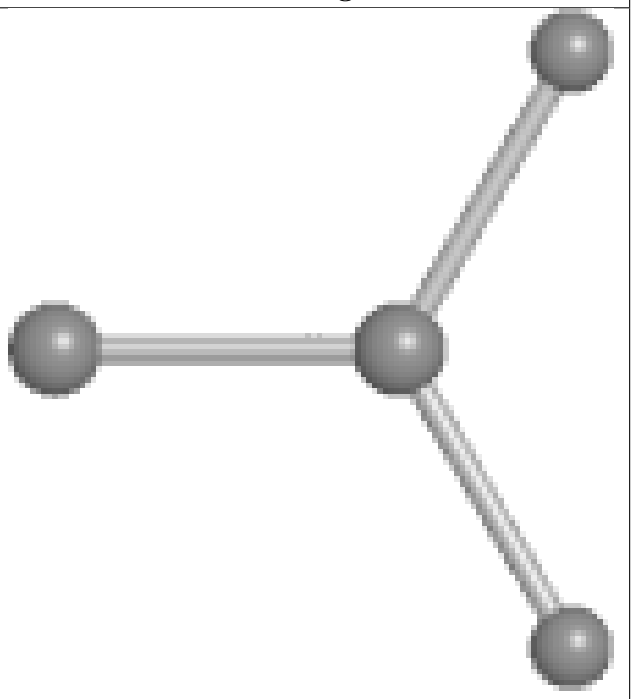
Bond lengths



Bond angles



Torsions

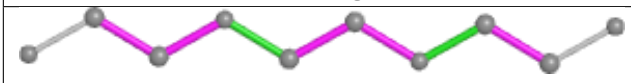


Rings

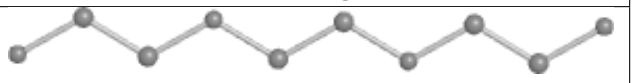
Ligand PGE A 307

Bond lengths

Bond angles

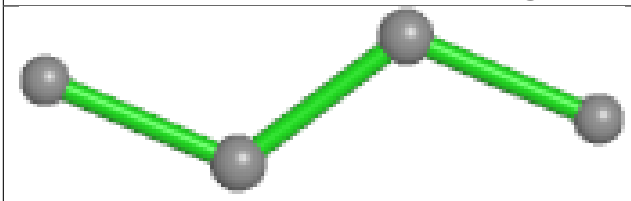


Torsions

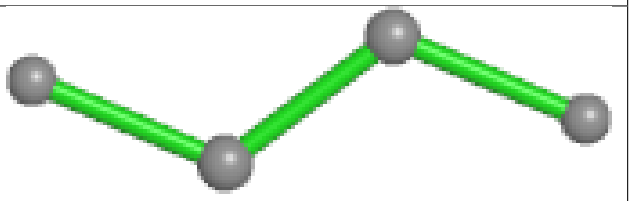


Rings

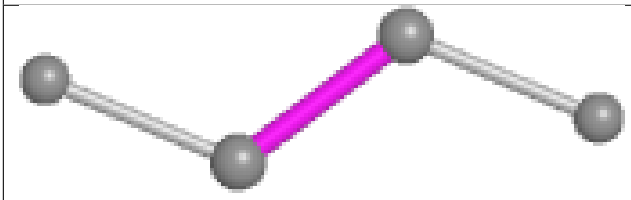
Ligand EDO D 310



Bond lengths



Bond angles



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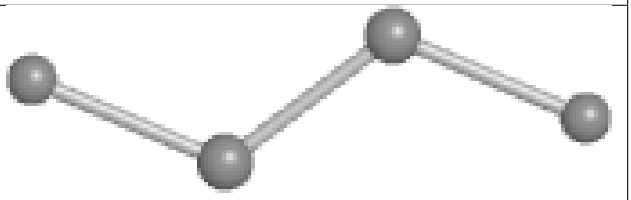
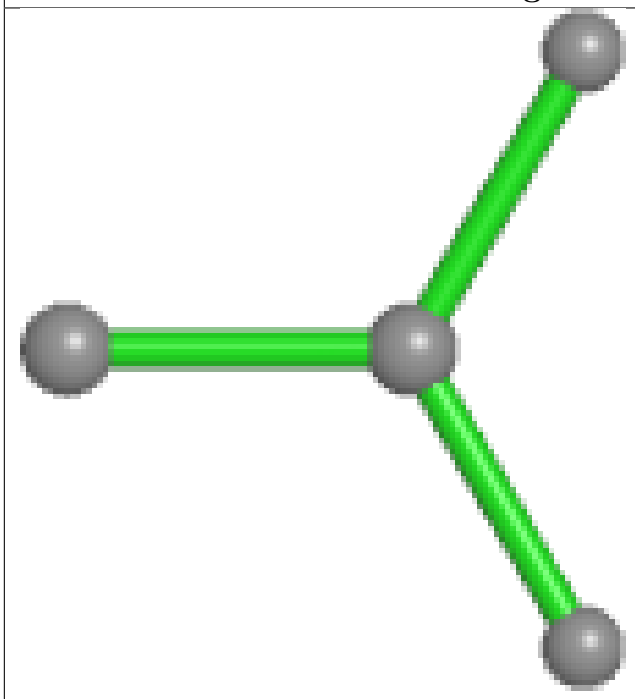
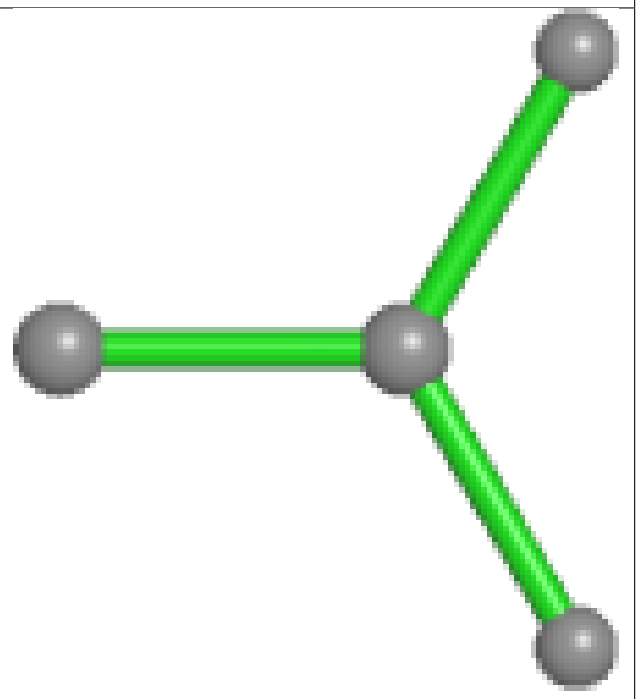


Rings

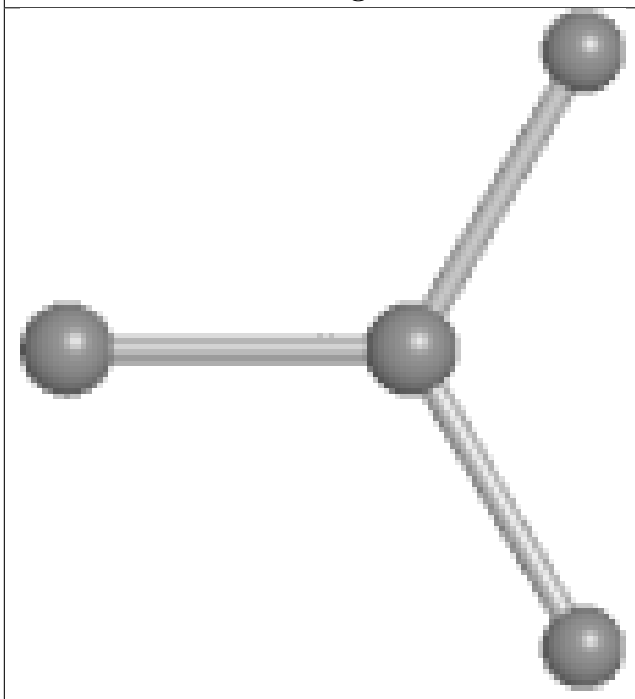
Ligand ACT D 304



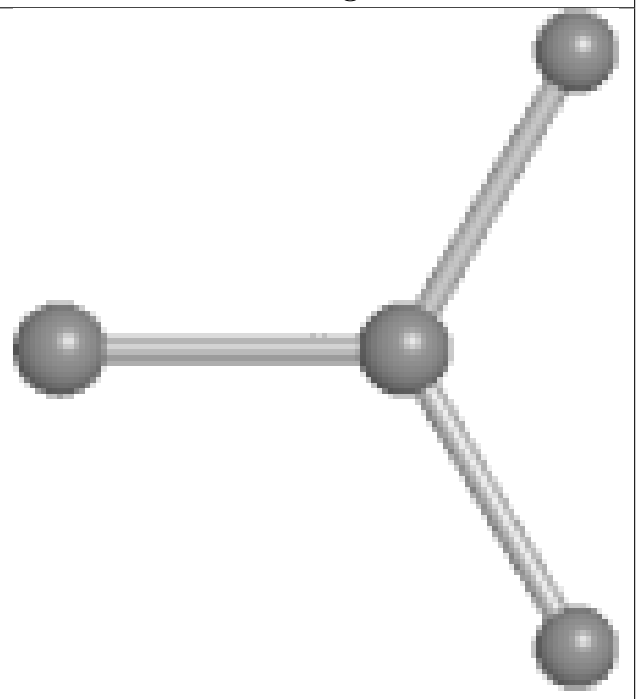
Bond lengths



Bond angles

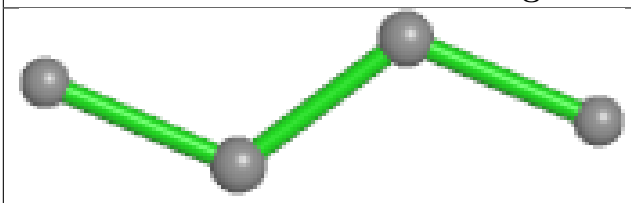


Torsions



Rings

Ligand EDO C 307



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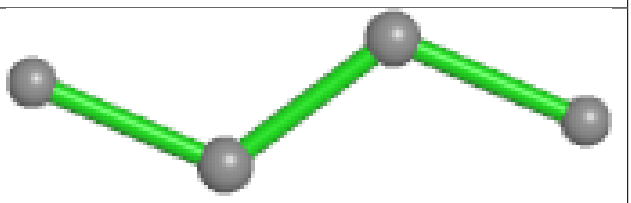
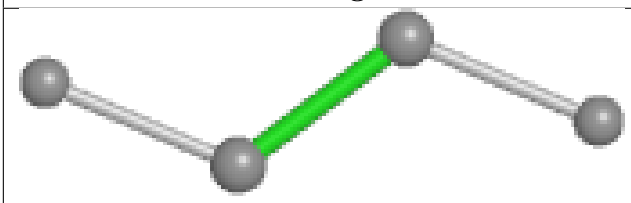


Bond angles



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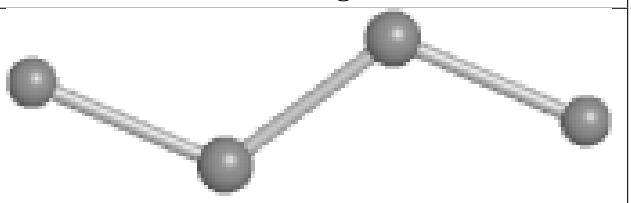
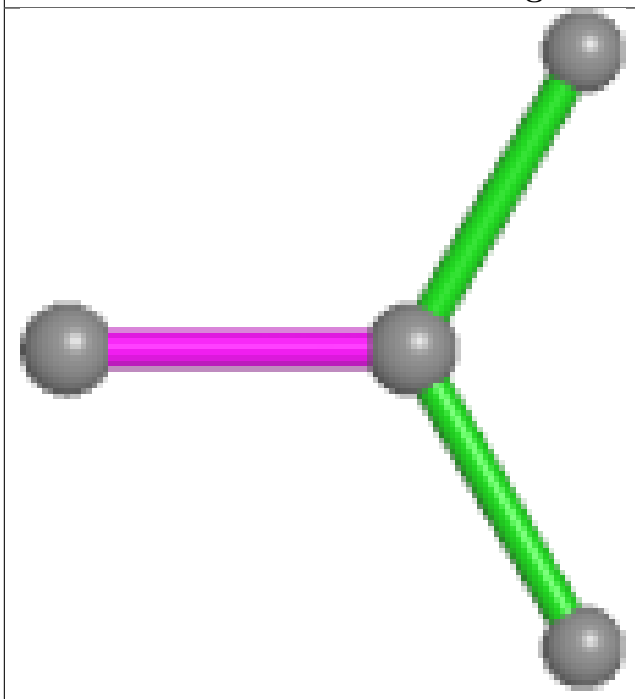
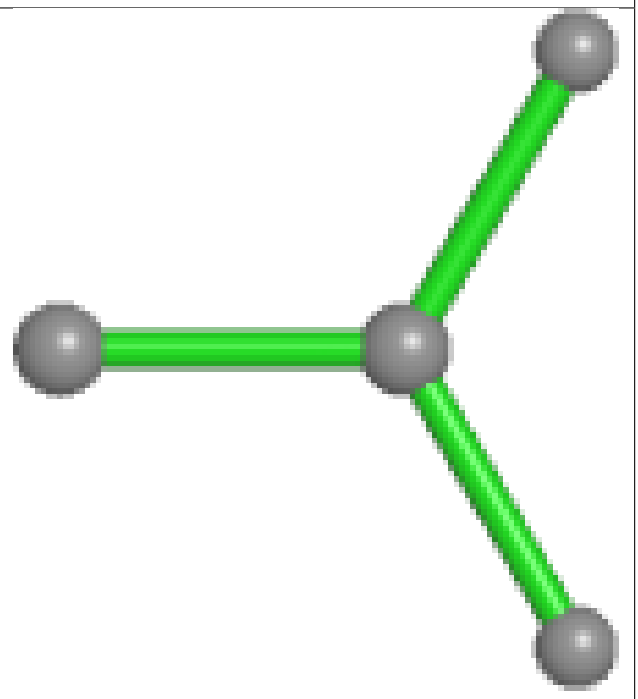


Rings

Ligand ACT F 303



Bond lengths



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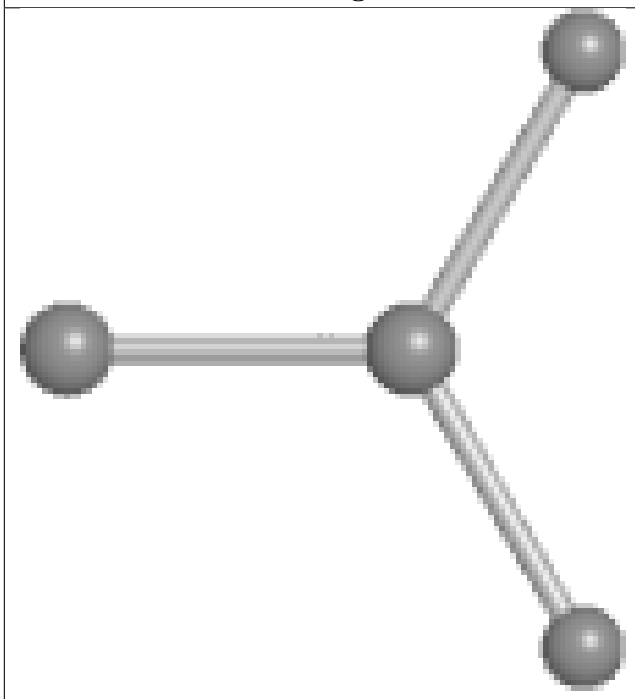
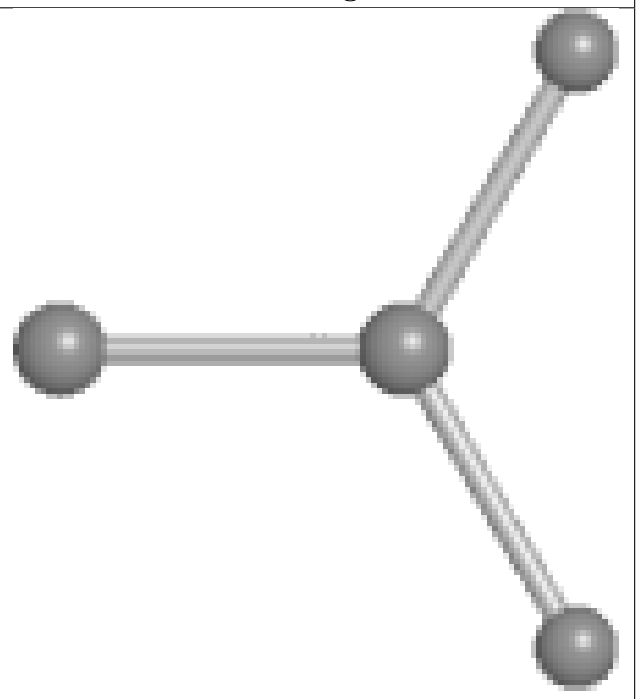
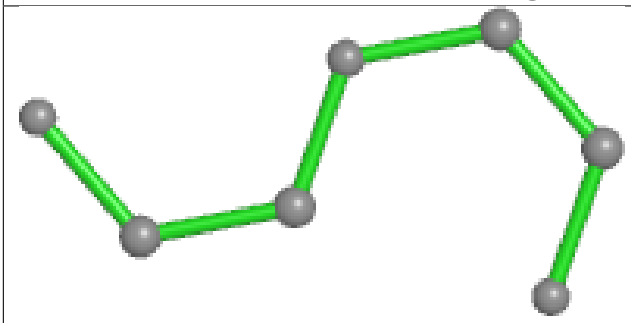


Torsions

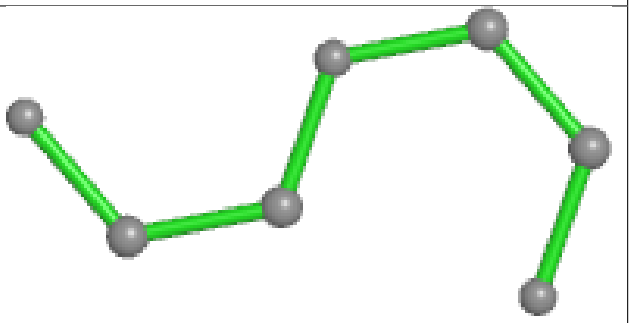


Rings

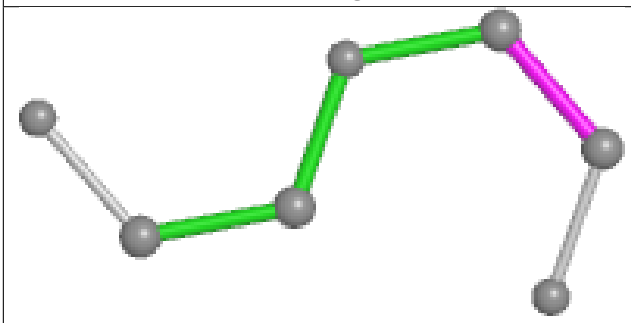
Ligand PEG B 305



Bond lengths



Bond angles



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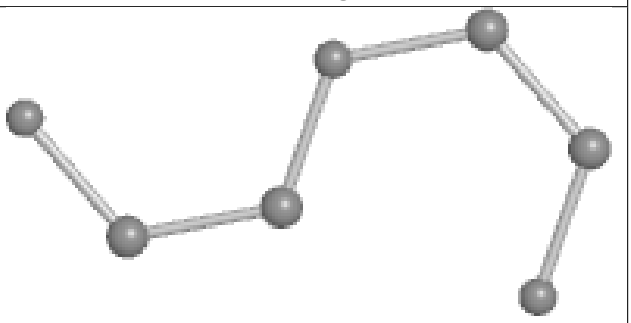
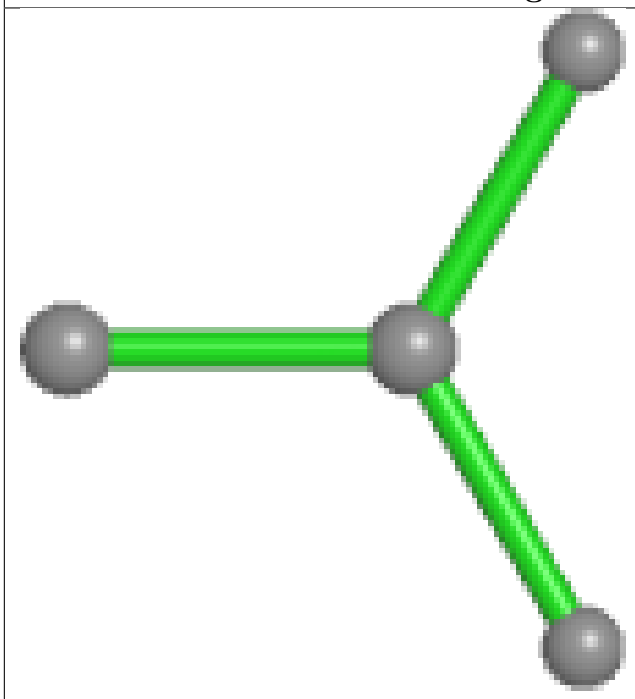


Rings

Ligand ACT E 304



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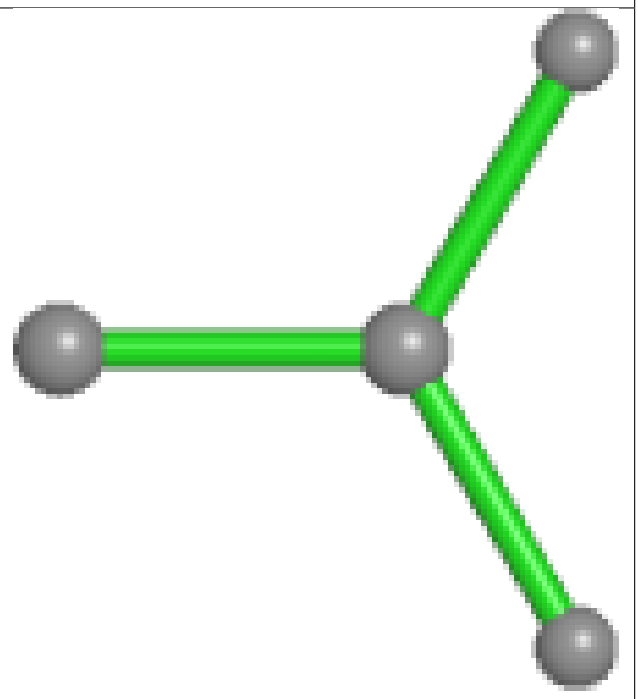
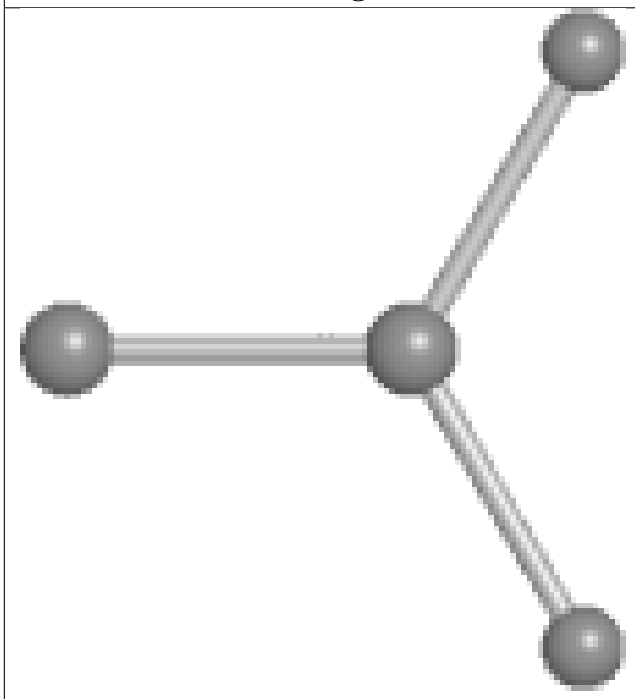
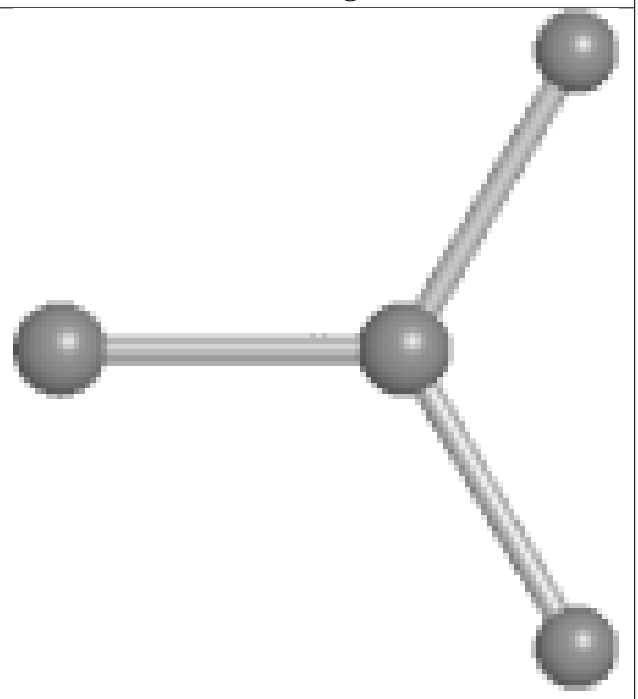


Bond angles

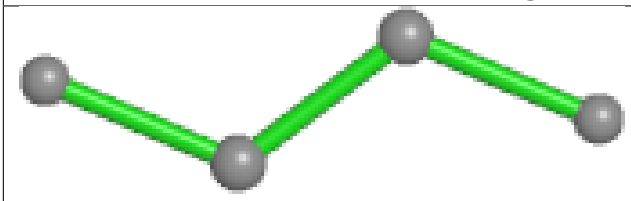


Torsions

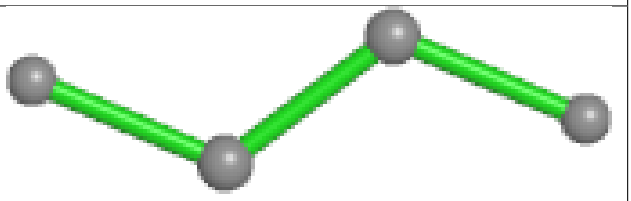


Rings

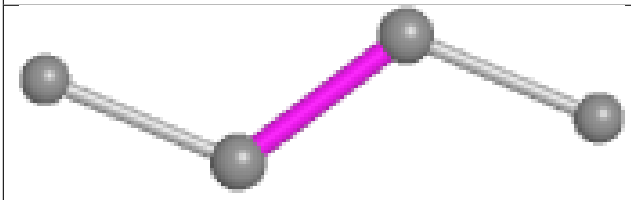
Ligand EDO D 309



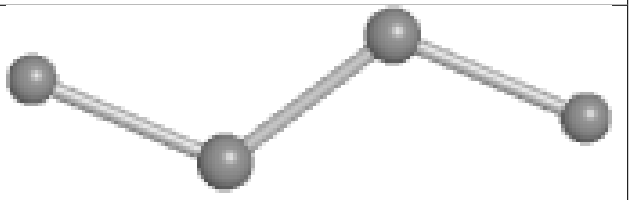
Bond lengths



Bond angles

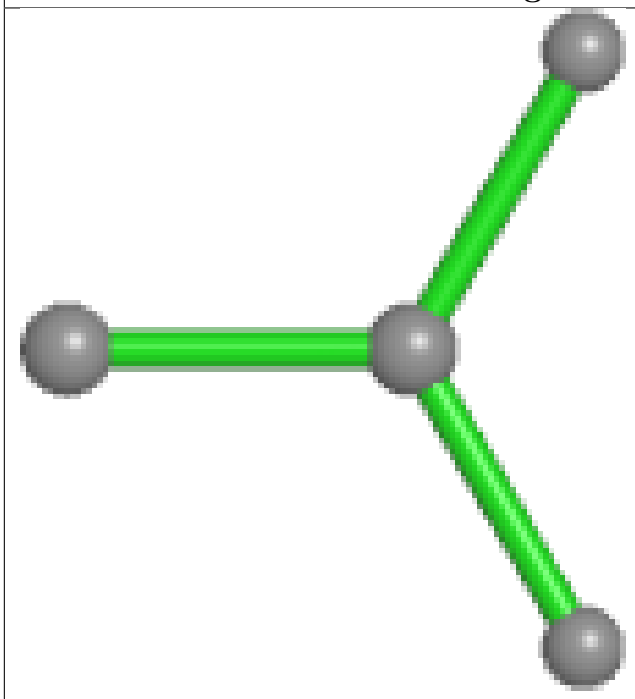


Torsions

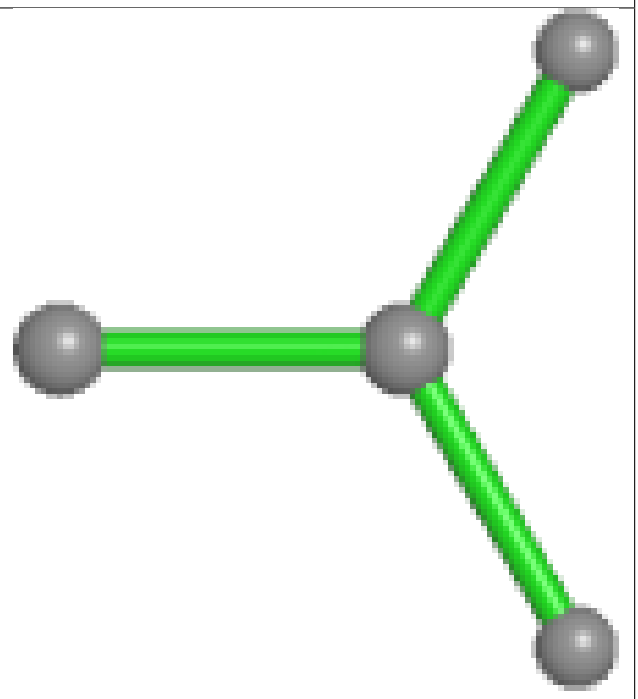


Rings

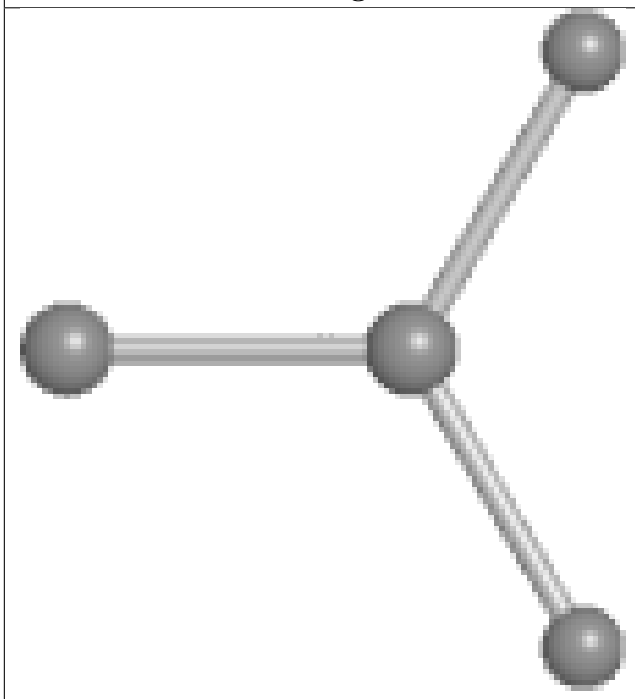
Ligand ACT C 304



Bond lengths



Bond angles



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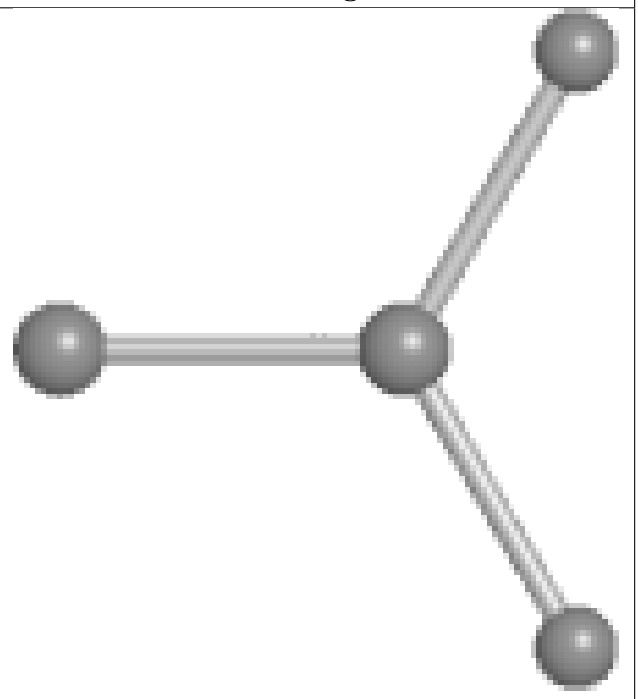
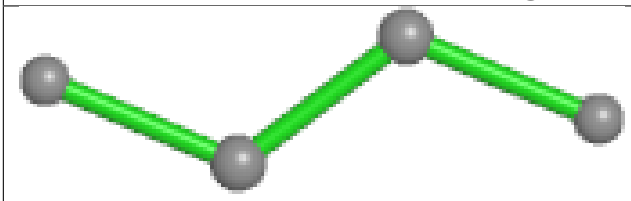
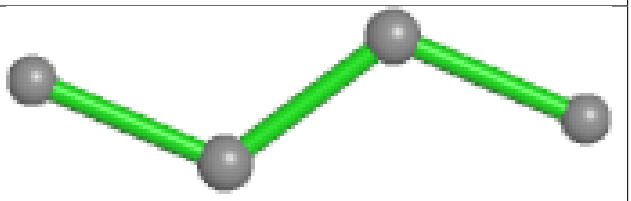
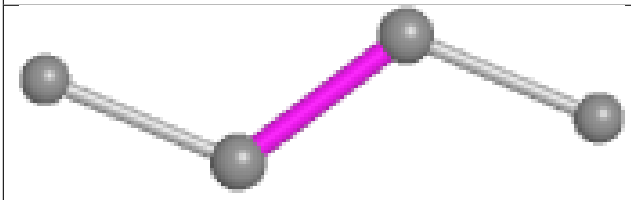
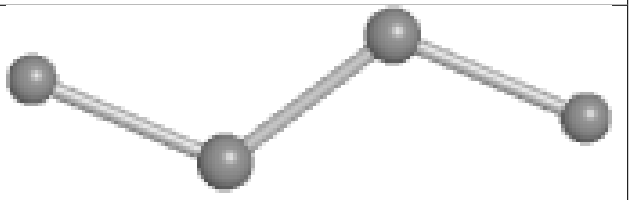
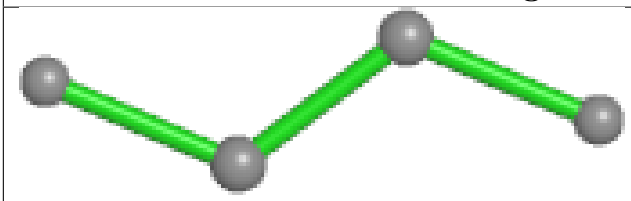
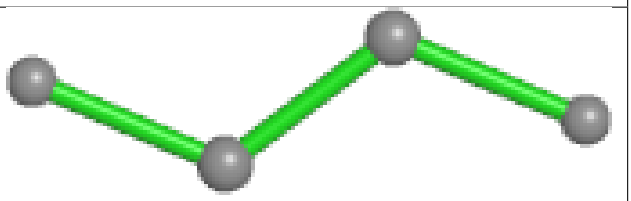
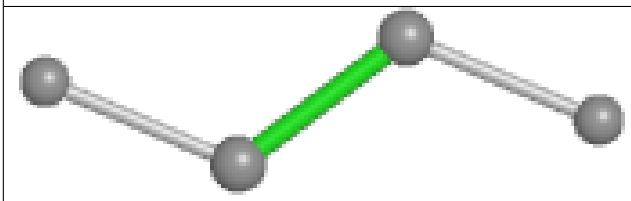
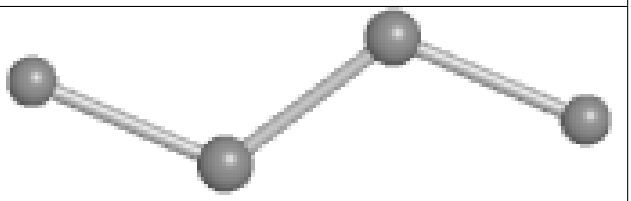
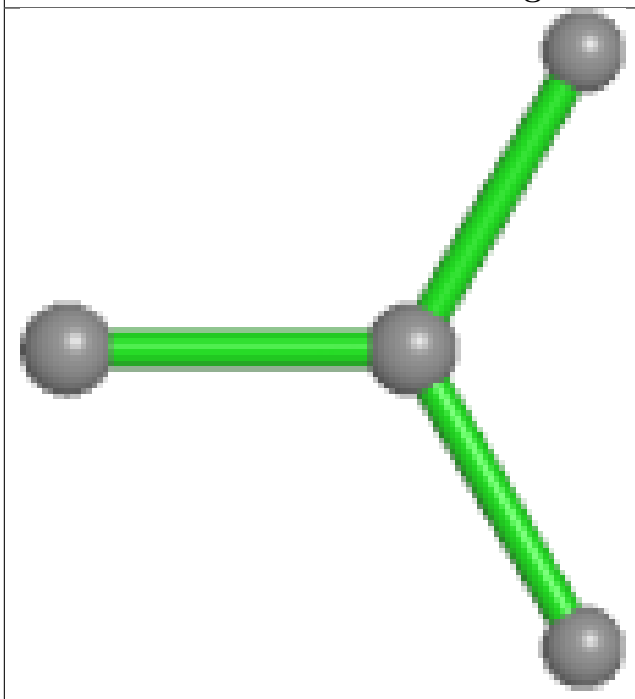


Rings

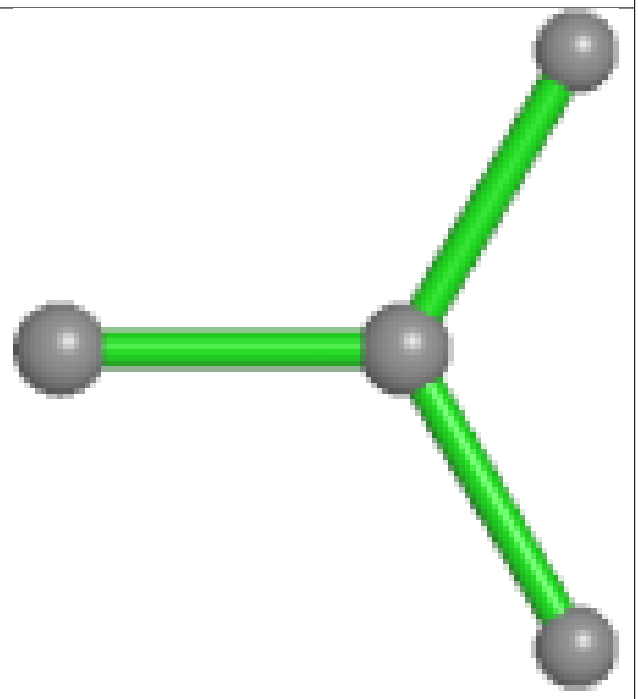
Ligand EDO A 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO C 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

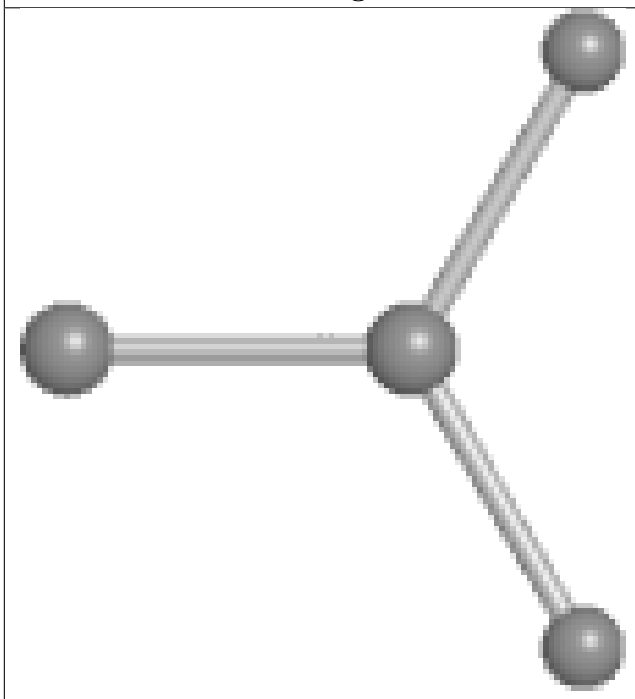
Ligand ACT C 303



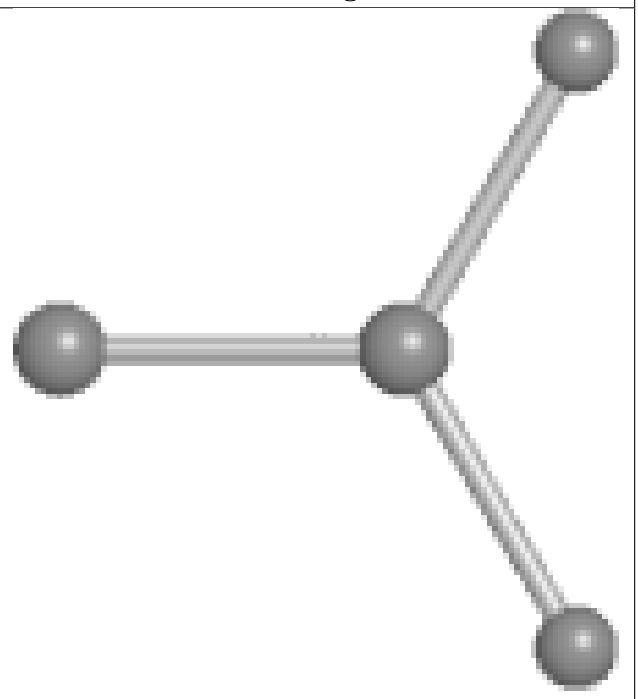
Bond lengths



Bond angles

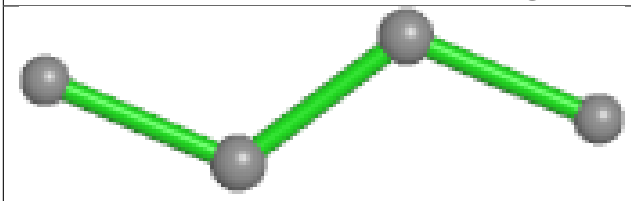


Torsions

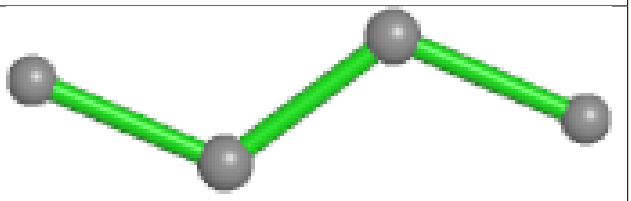


Rings

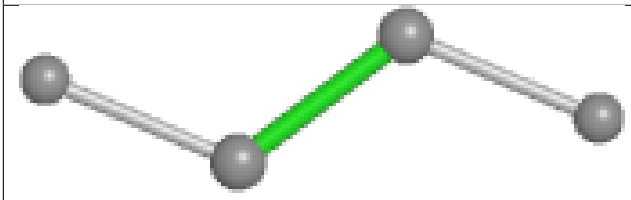
Ligand EDO E 309



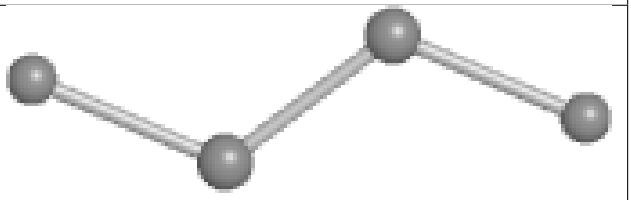
Bond lengths



Bond angles

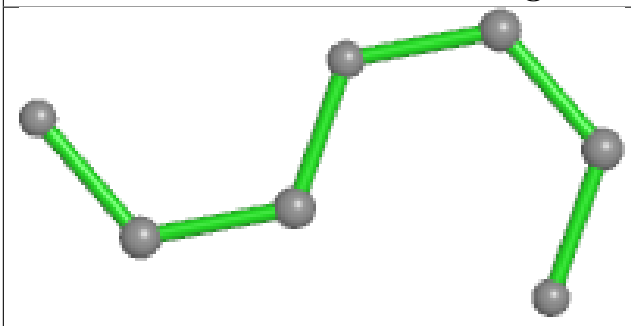


Torsions

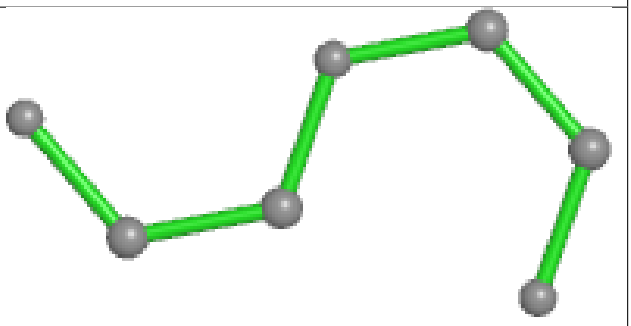


Rings

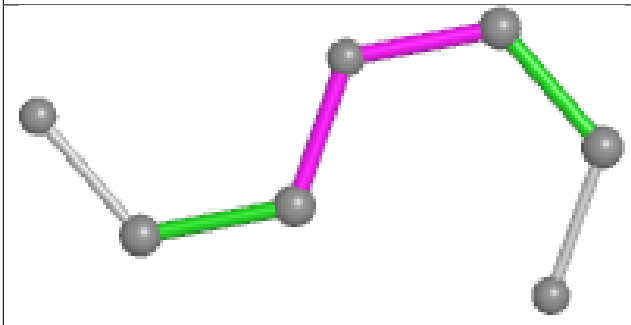
Ligand PEG E 306



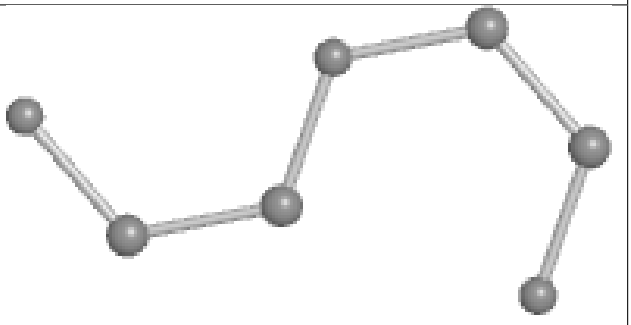
Bond lengths



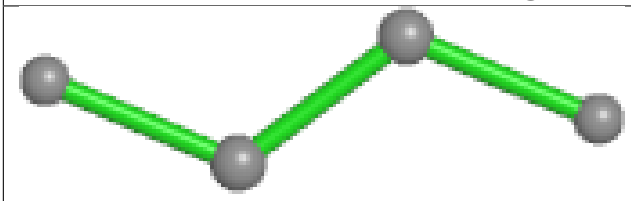
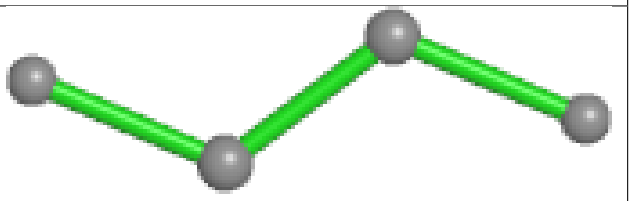
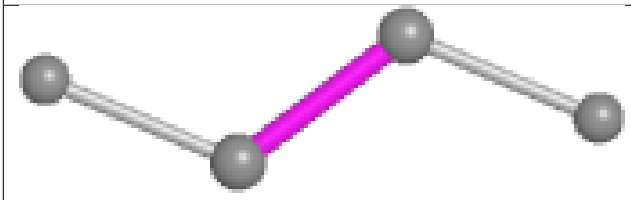
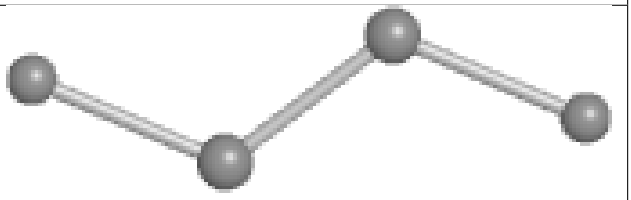
Bond angles

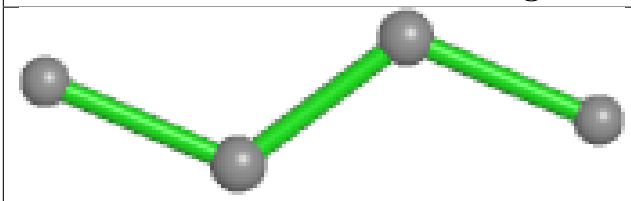
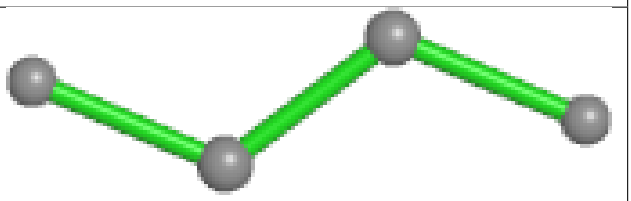
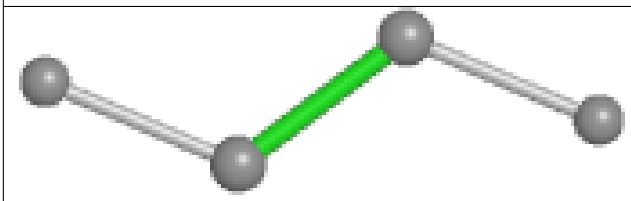
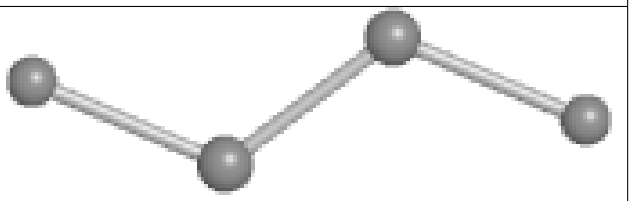


Torsions

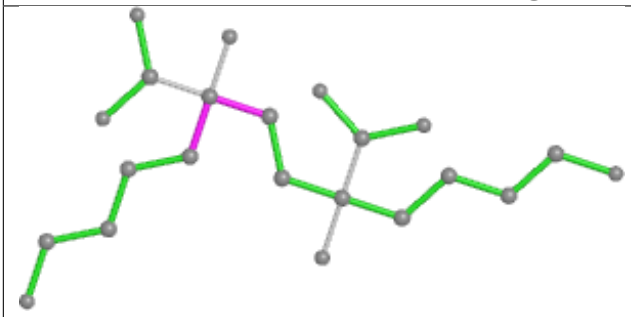


Rings

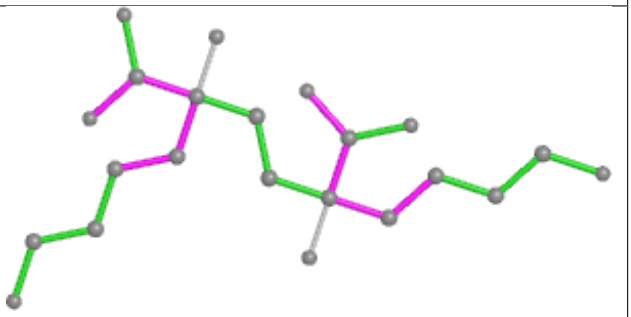
Ligand EDO A 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO B 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

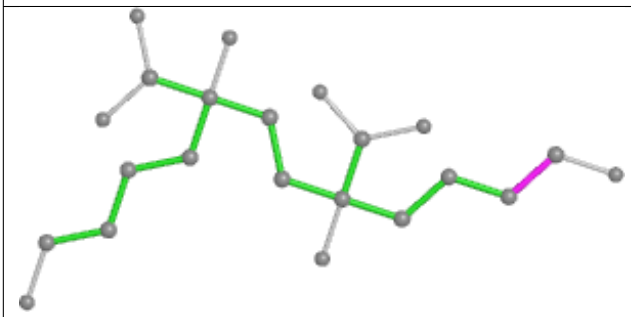
Ligand 3VN B 301



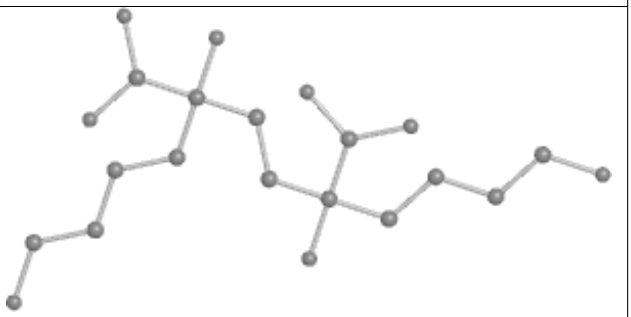
Bond lengths



Bond angles

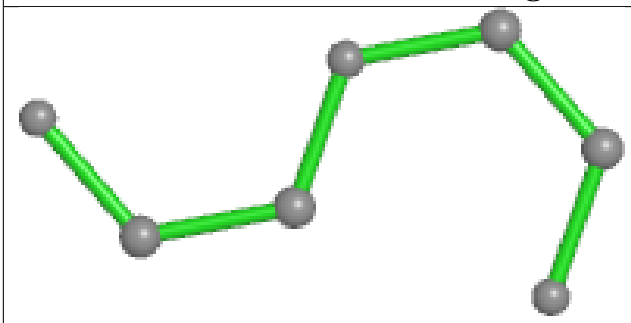


Torsions

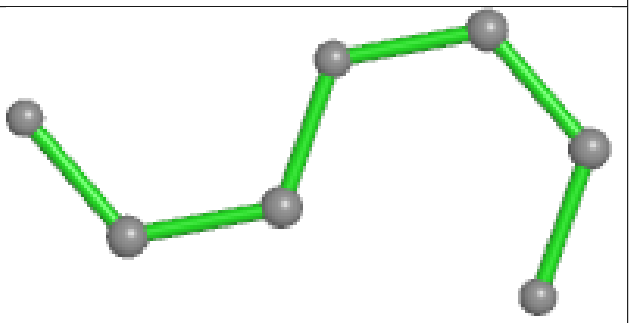


Rings

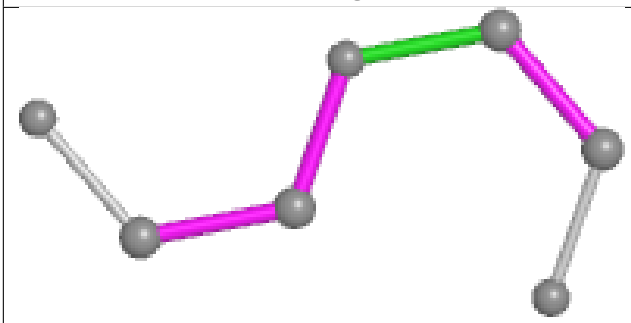
Ligand PEG E 305



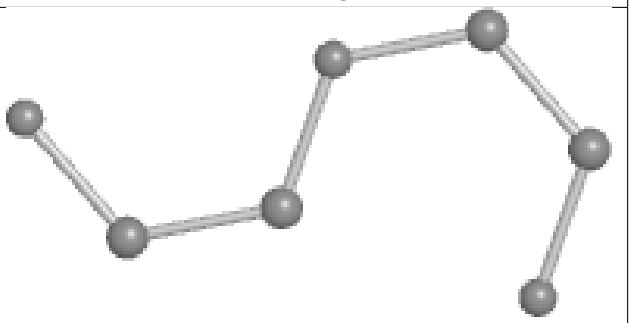
Bond lengths



Bond angles

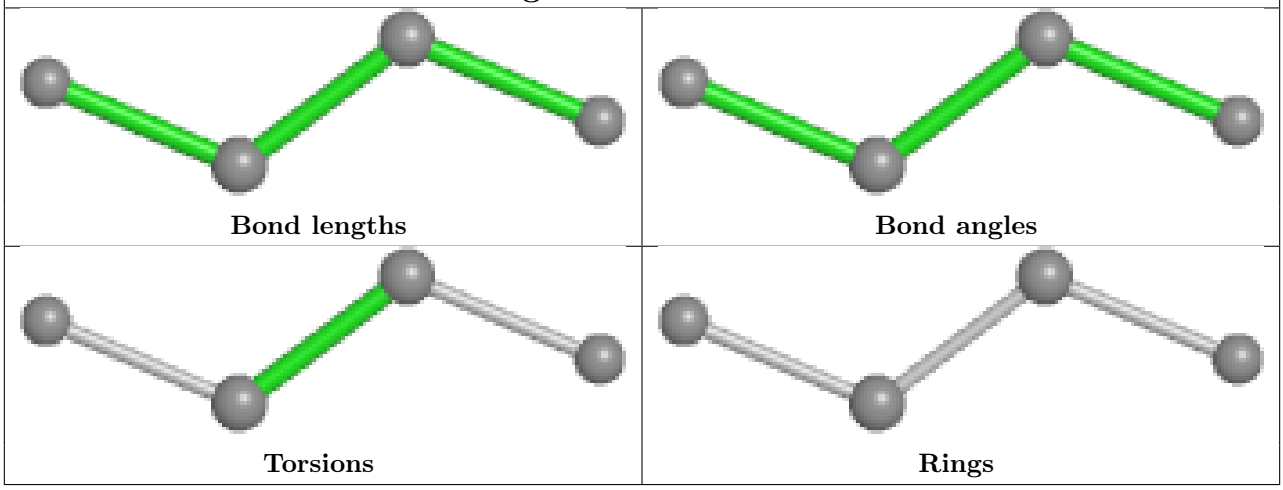


Torsions

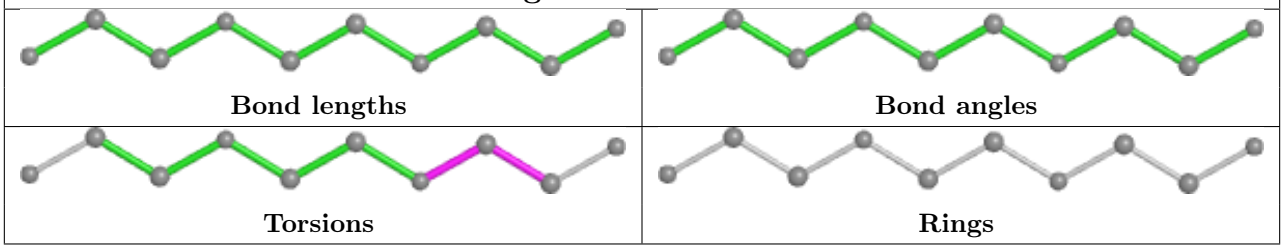


Rings

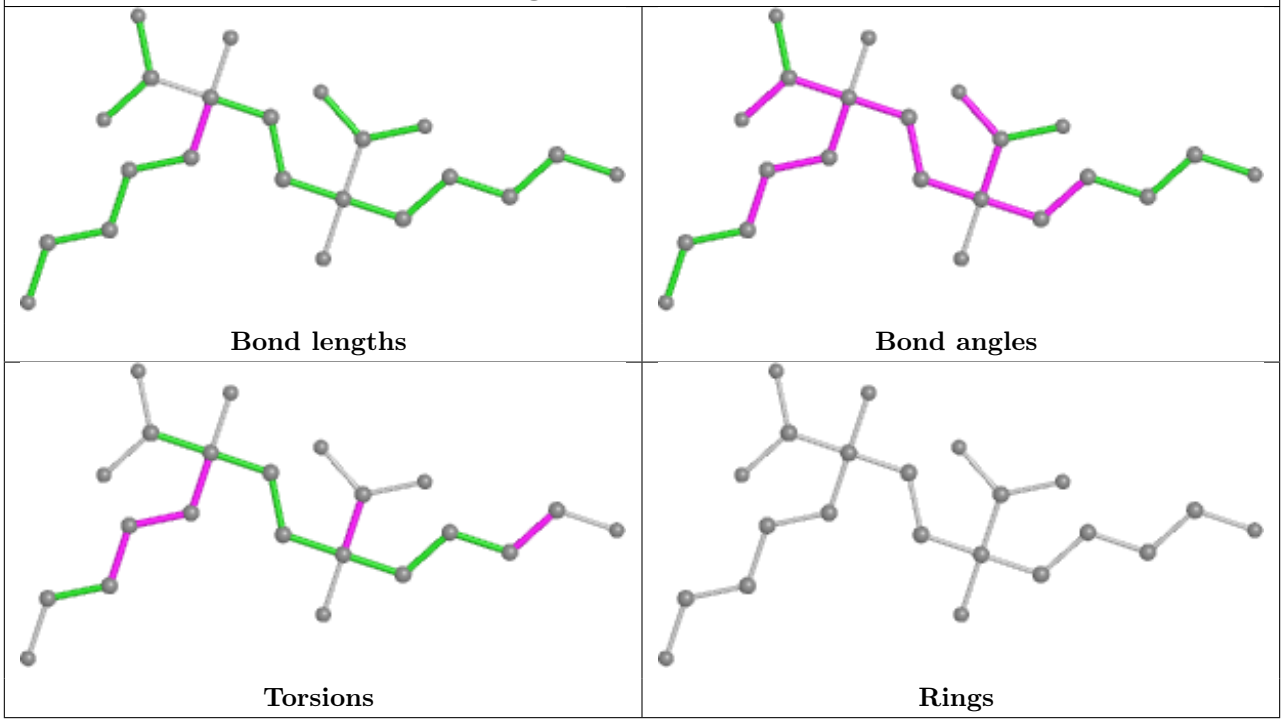
Ligand EDO D 306



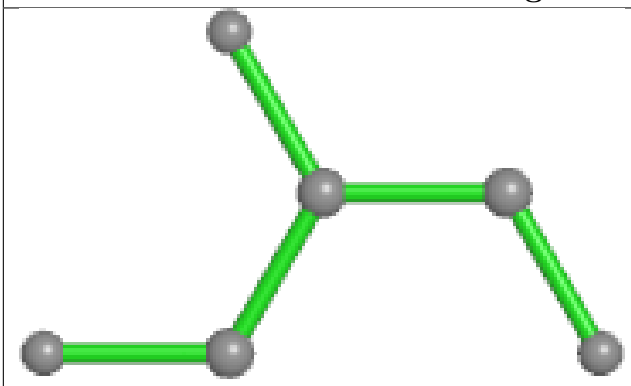
Ligand PGE D 305



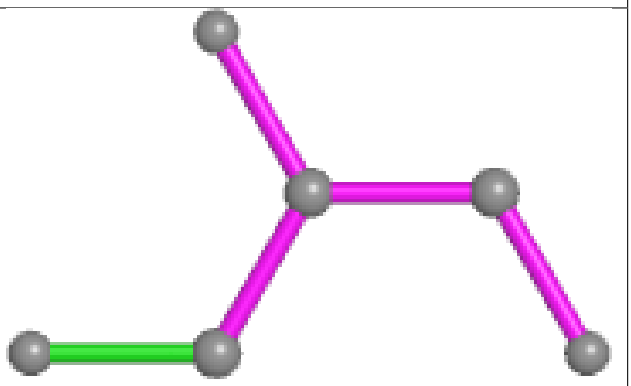
Ligand 3VN D 301



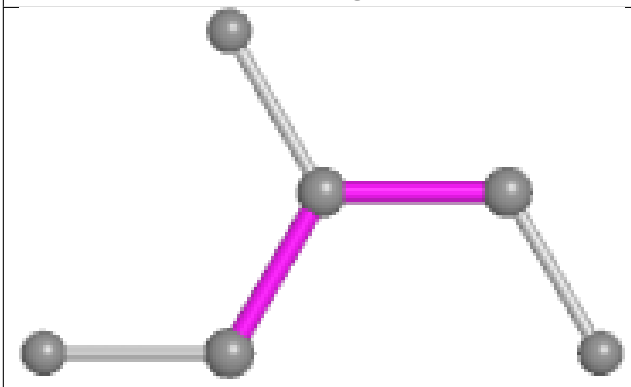
Ligand GOL F 308



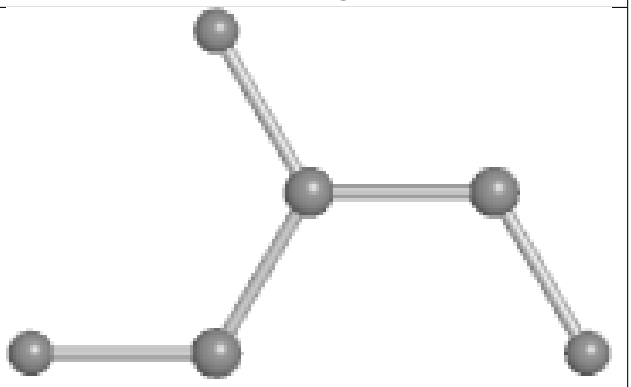
Bond lengths



Bond angles

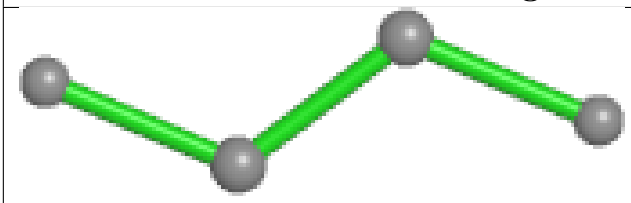


Torsions

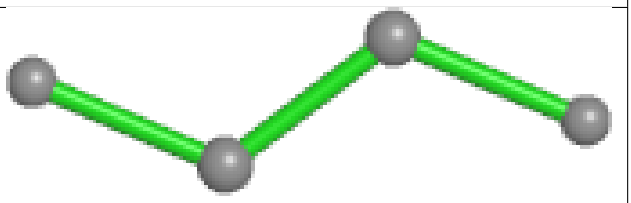


Rings

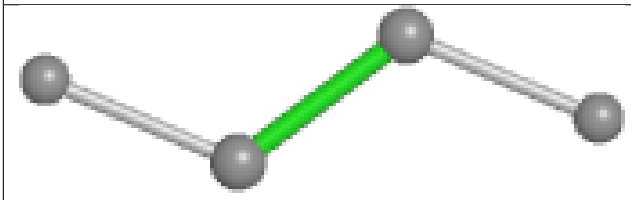
Ligand EDO D 307



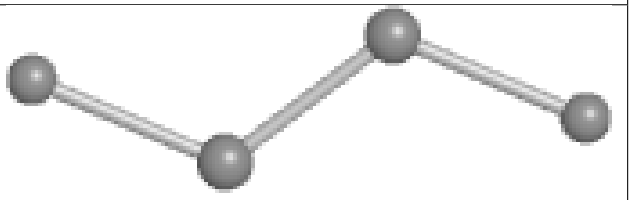
Bond lengths



Bond angles

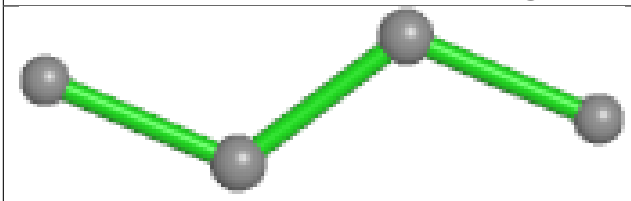


Torsions

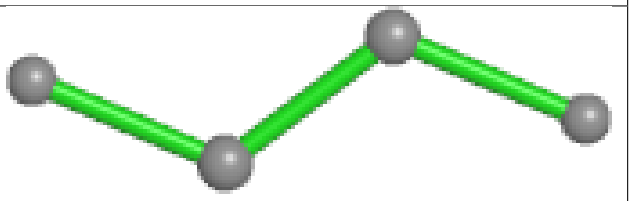


Rings

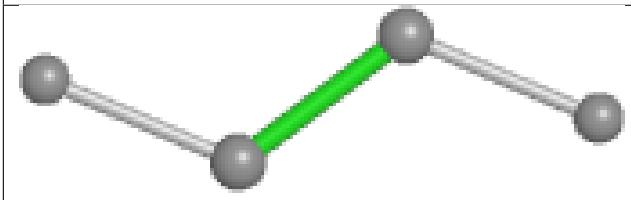
Ligand EDO A 308



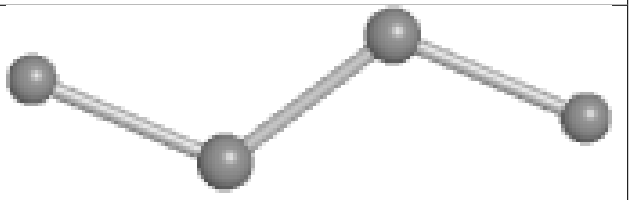
Bond lengths



Bond angles

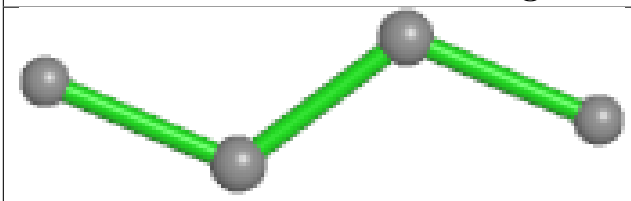


Torsions

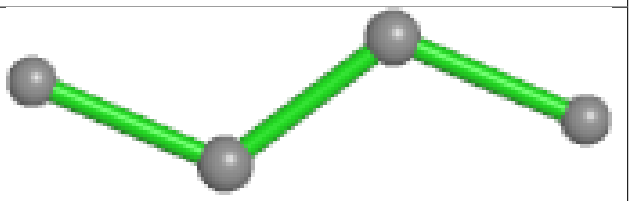


Rings

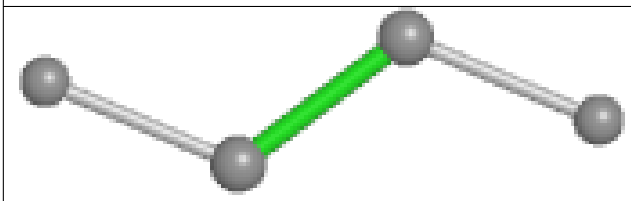
Ligand EDO D 311



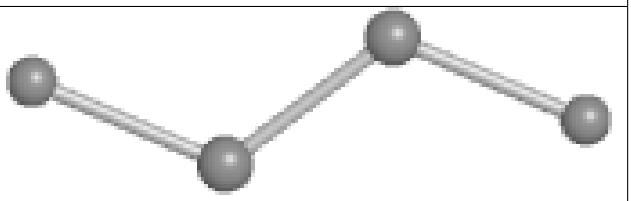
Bond lengths



Bond angles

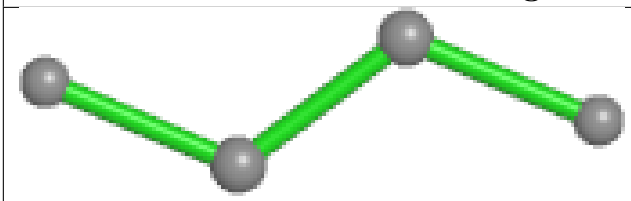


Torsions

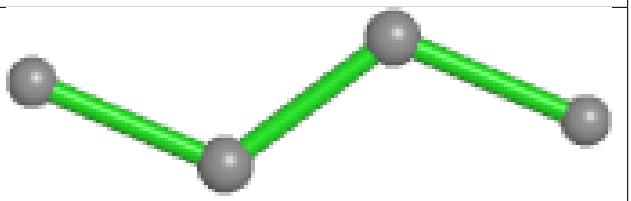


Rings

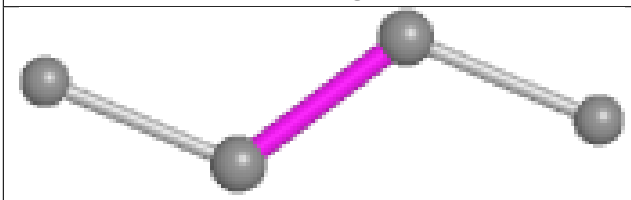
Ligand EDO B 311



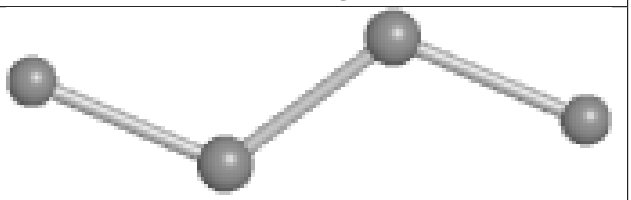
Bond lengths



Bond angles

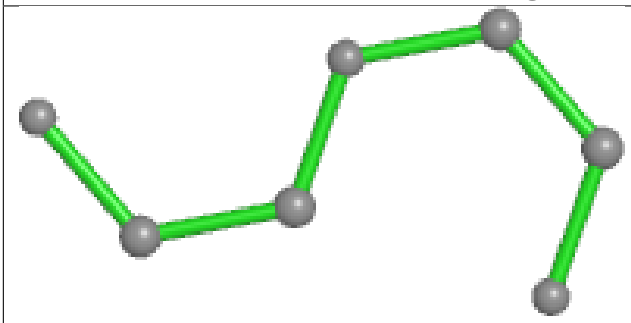


Torsions

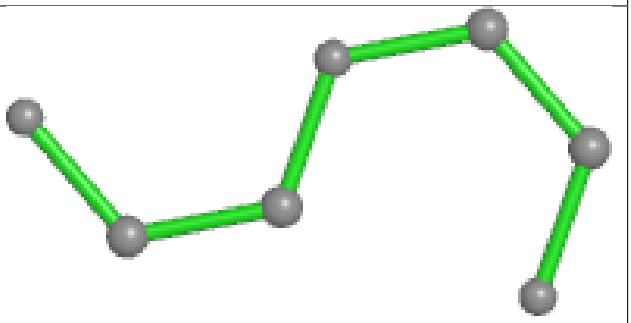


Rings

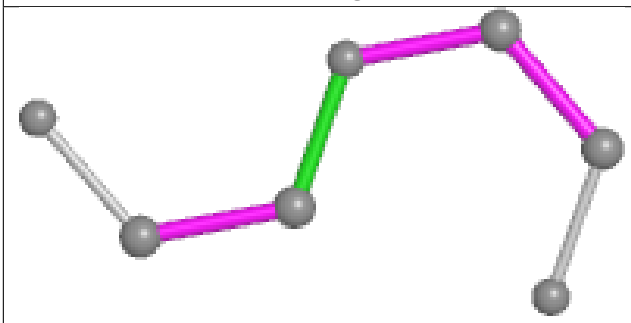
Ligand PEG B 306



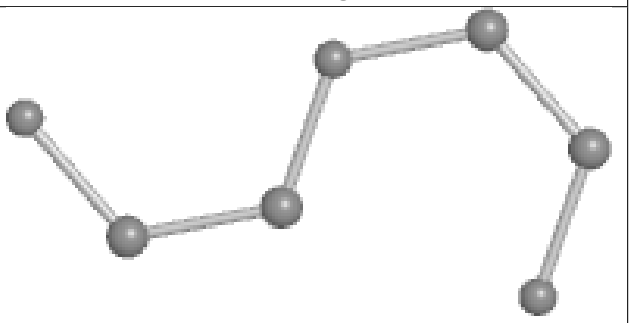
Bond lengths



Bond angles

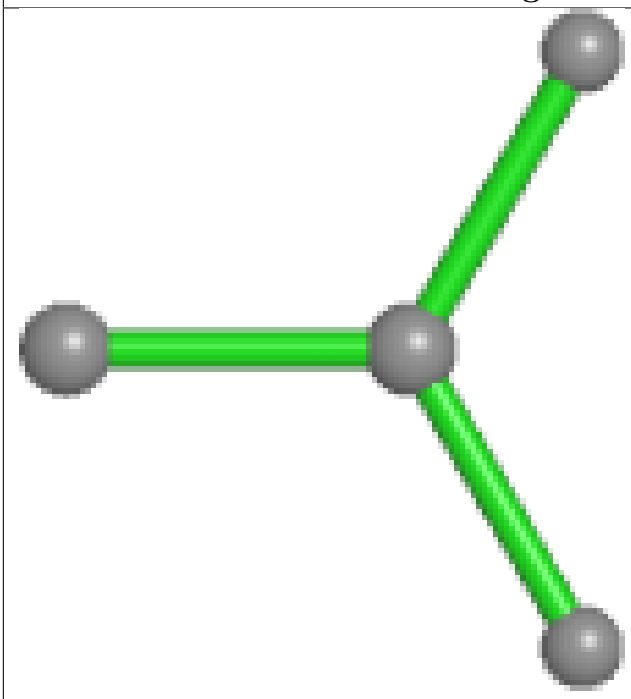


Torsions

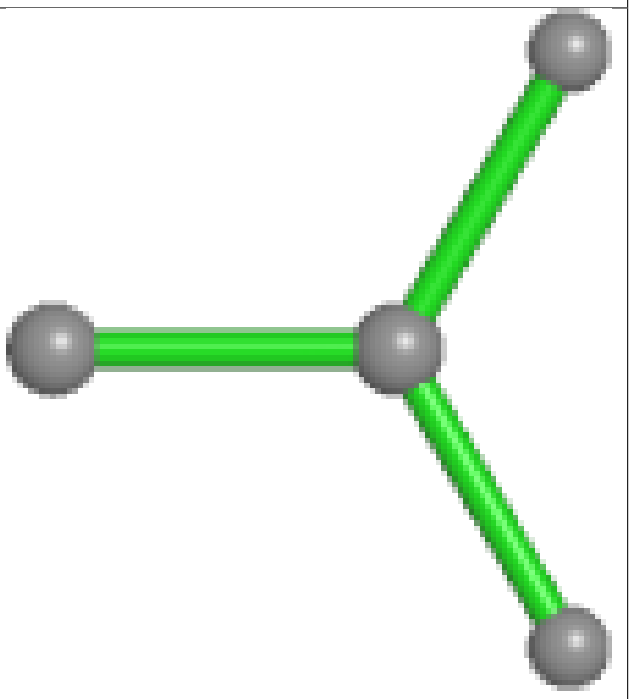


Rings

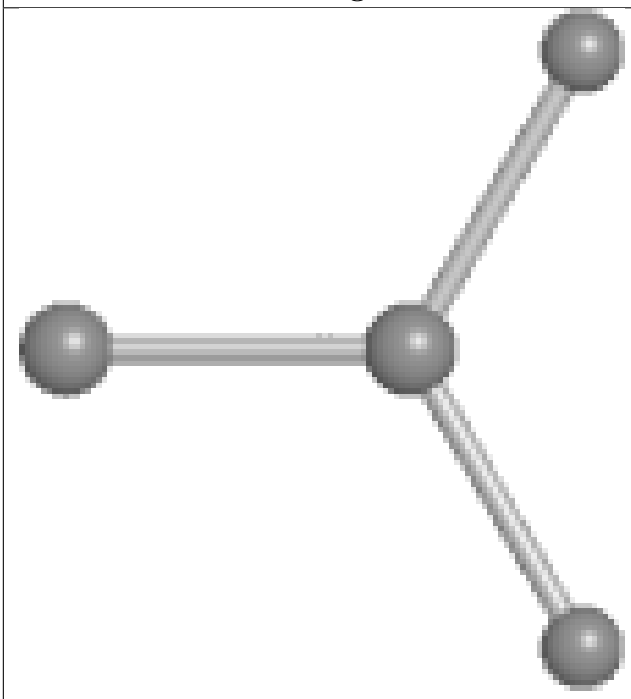
Ligand ACT A 304



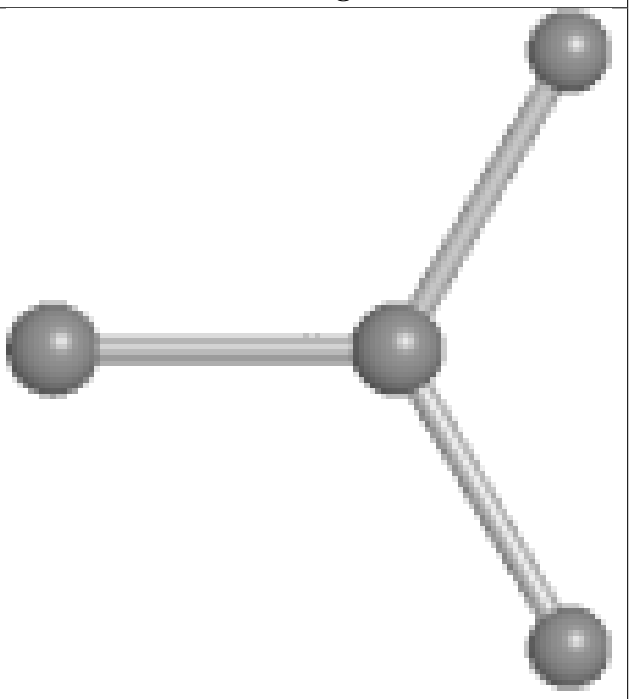
Bond lengths



Bond angles

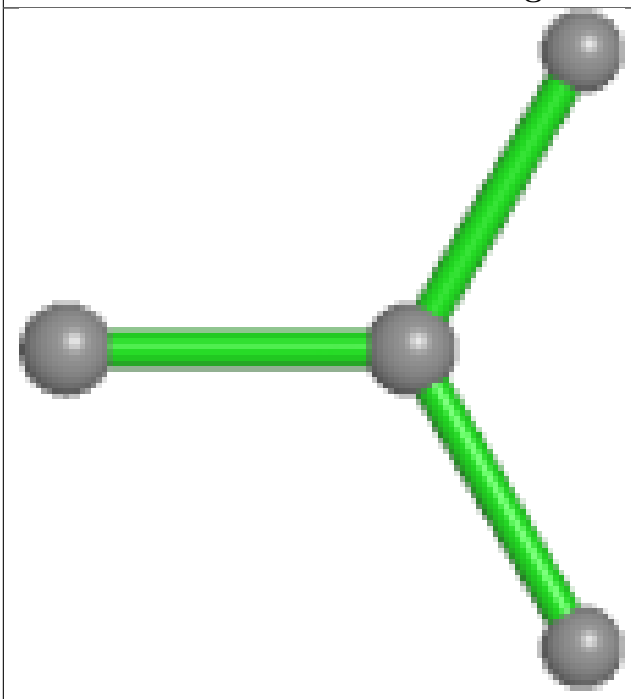


Torsions

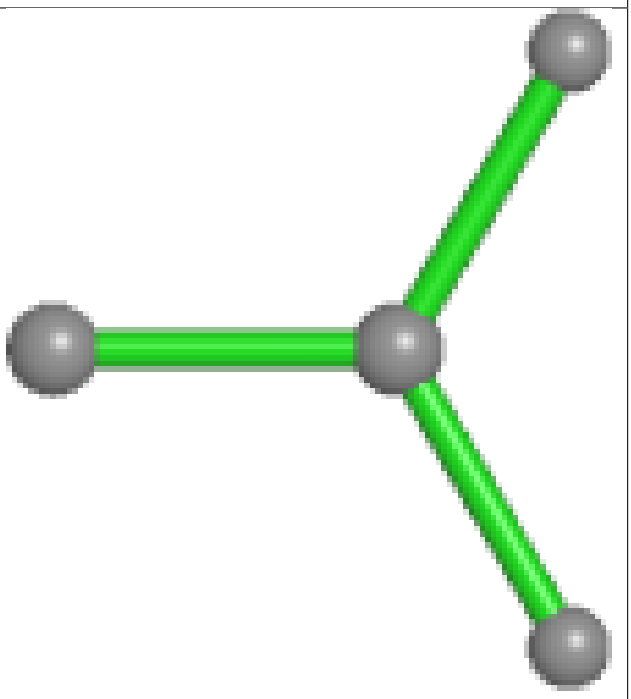


Rings

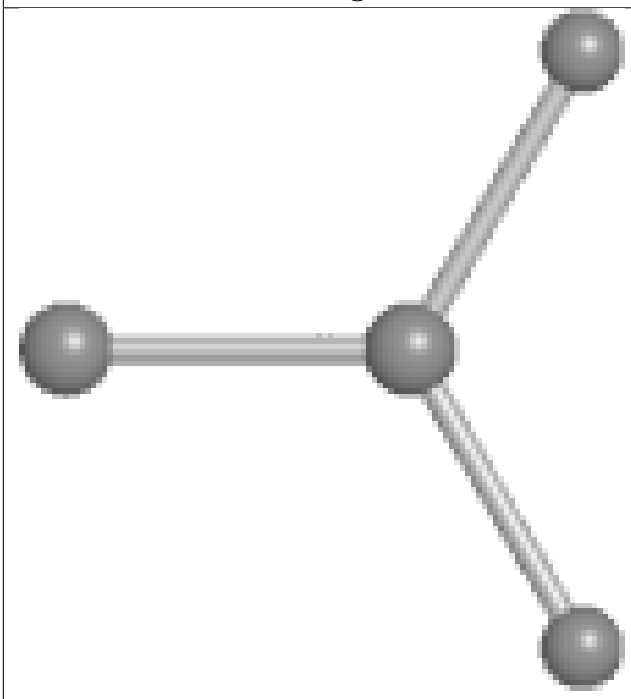
Ligand ACT F 302



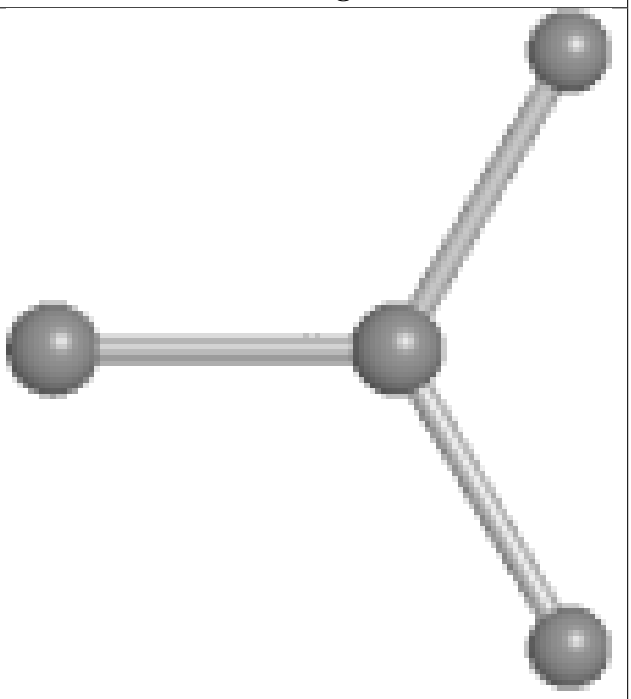
Bond lengths



Bond angles

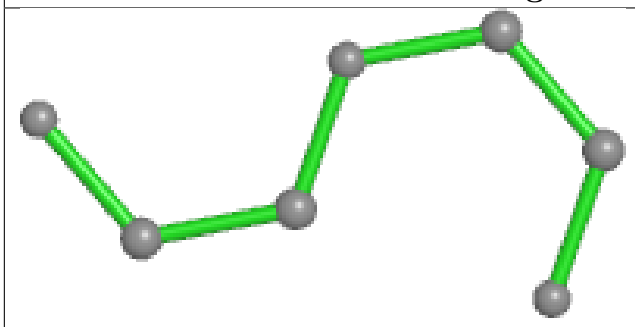


Torsions

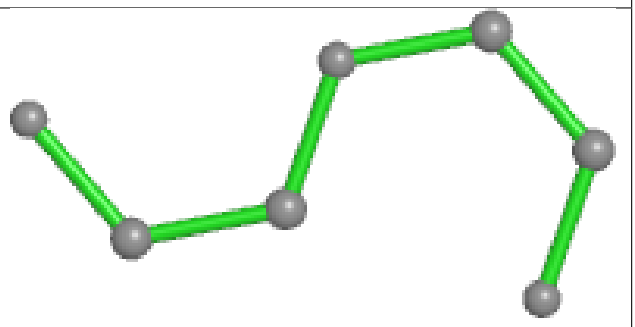


Rings

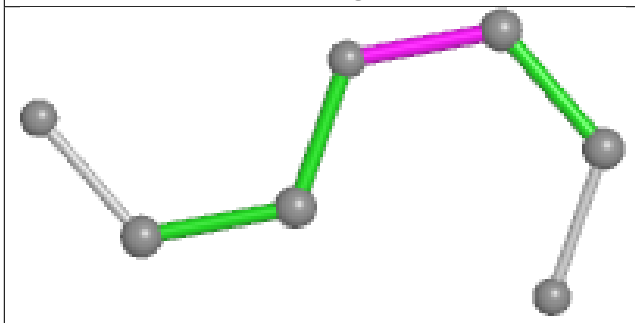
Ligand PEG F 304



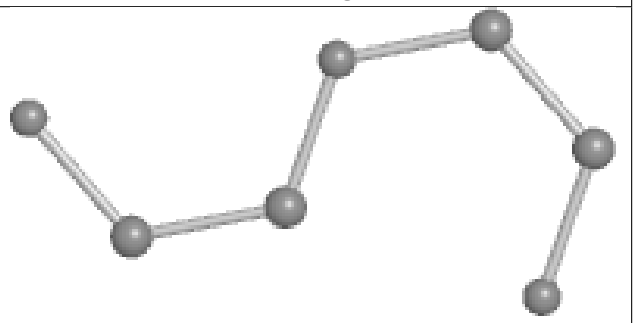
Bond lengths



Bond angles

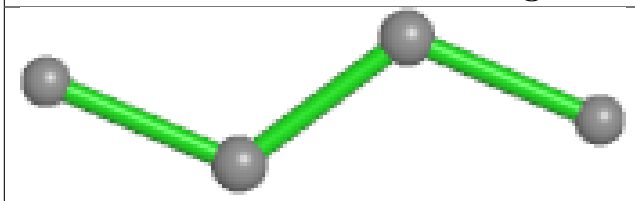


Torsions

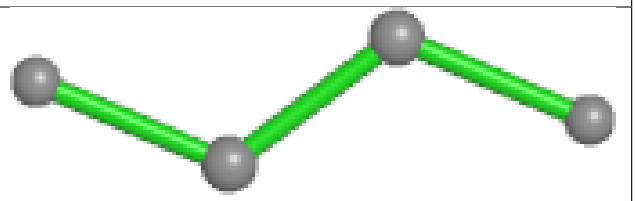


Rings

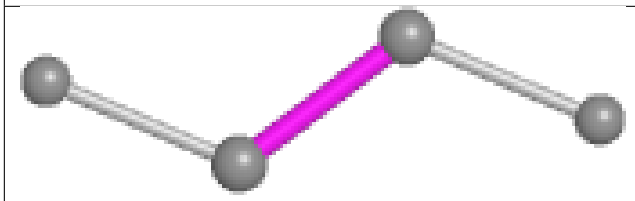
Ligand EDO A 312



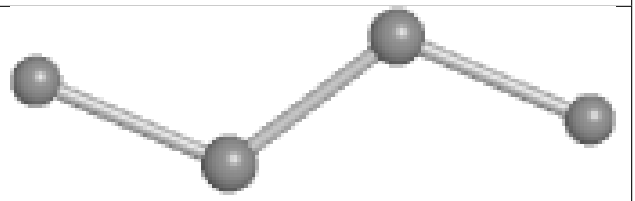
Bond lengths



Bond angles

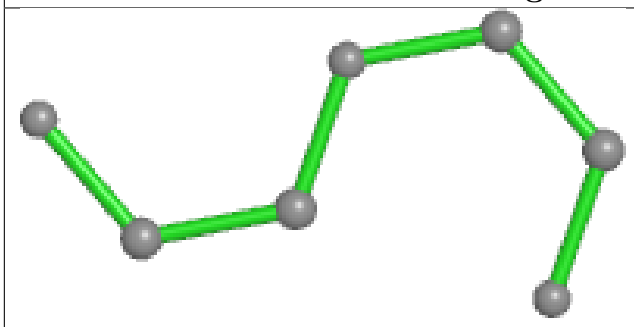


Torsions



Rings

Ligand PEG E 307



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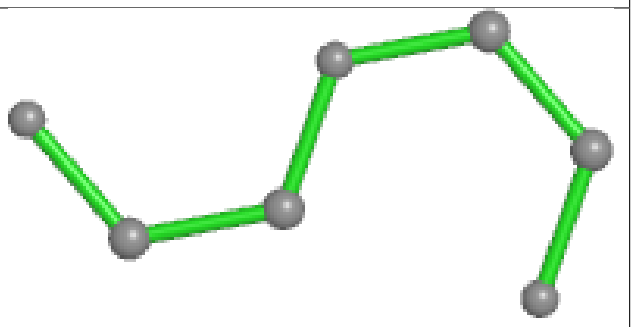
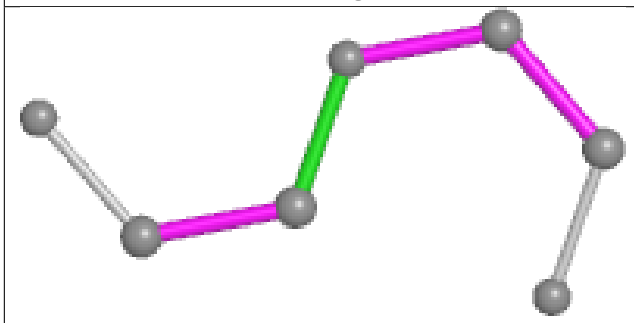


Bond angles



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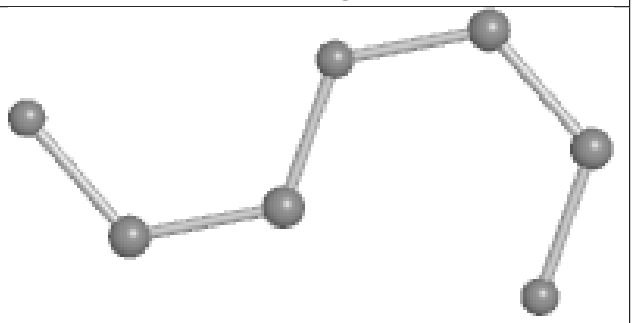
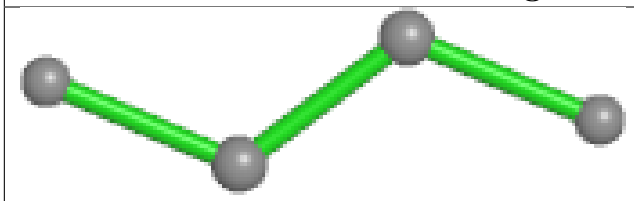


Rings

Ligand EDO B 309



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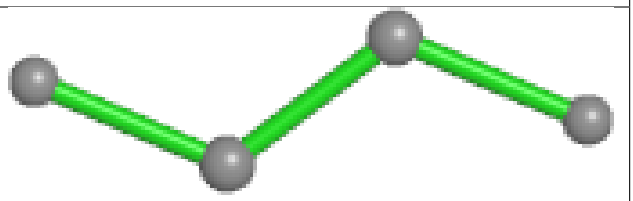

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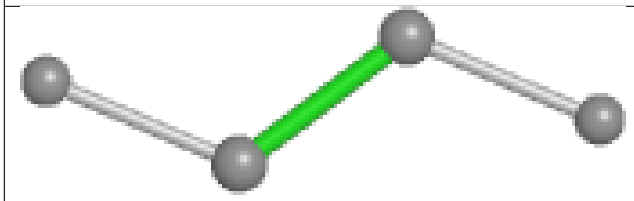

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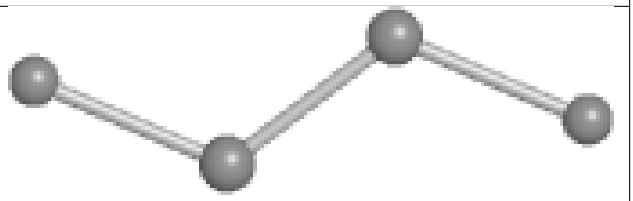
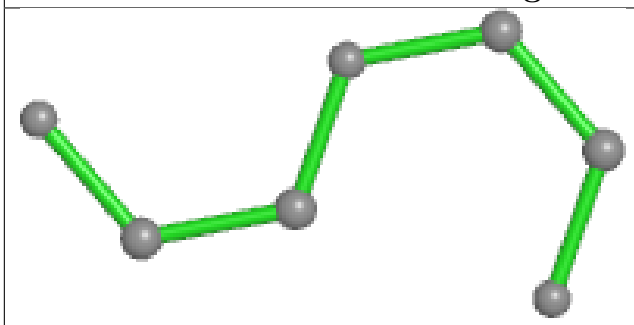


Rings

Ligand PEG A 306



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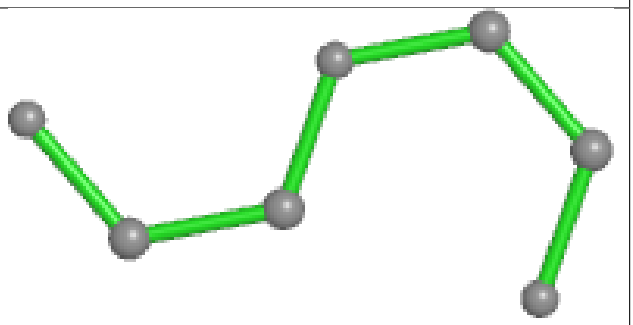
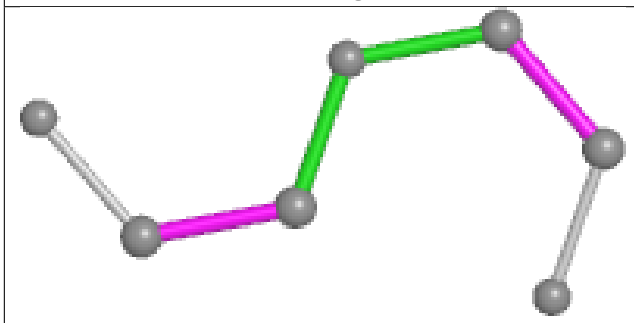


Bond angles



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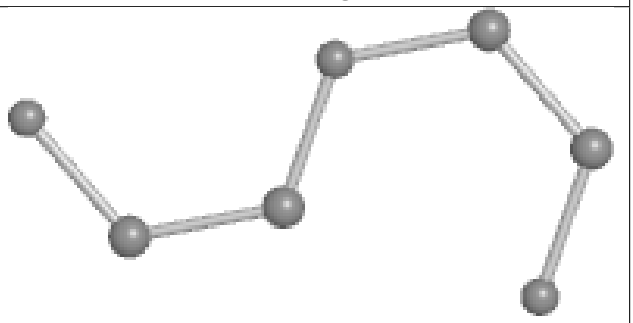
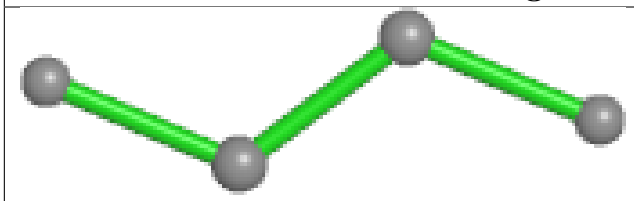


Rings

Ligand EDO F 307



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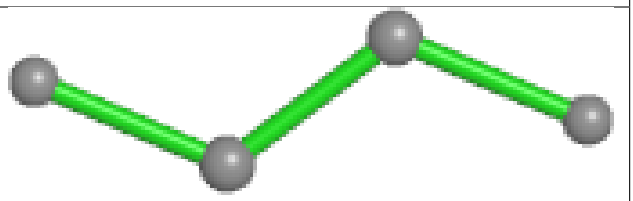
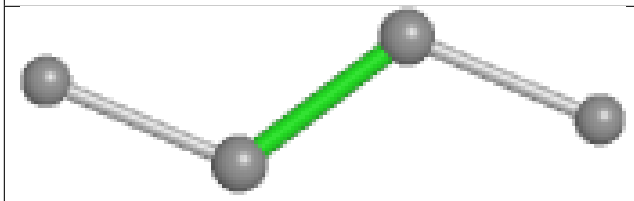


Bond angles



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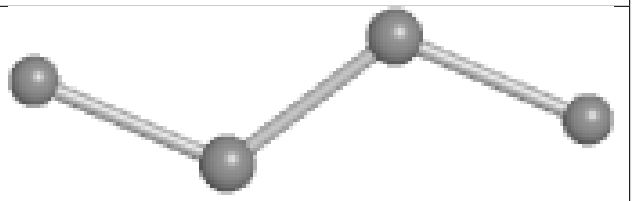
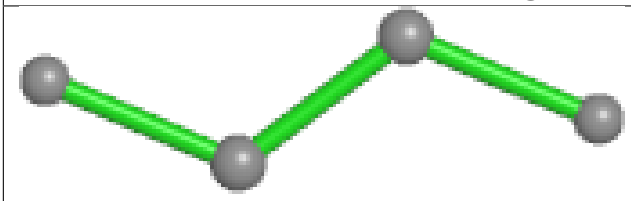


Rings

Ligand EDO A 311



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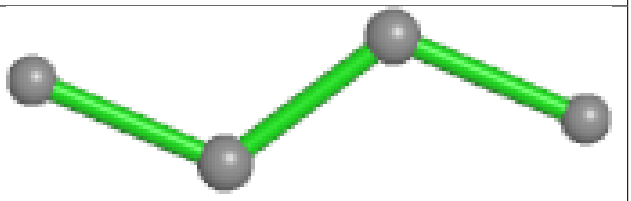
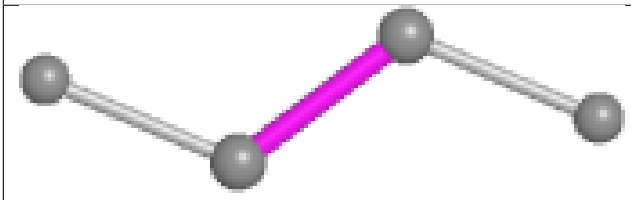


Bond angles



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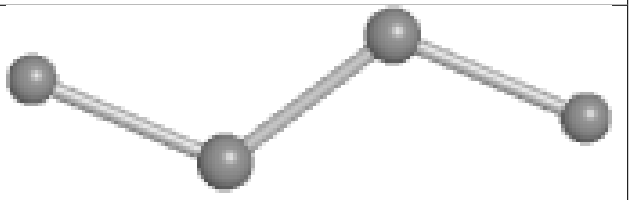
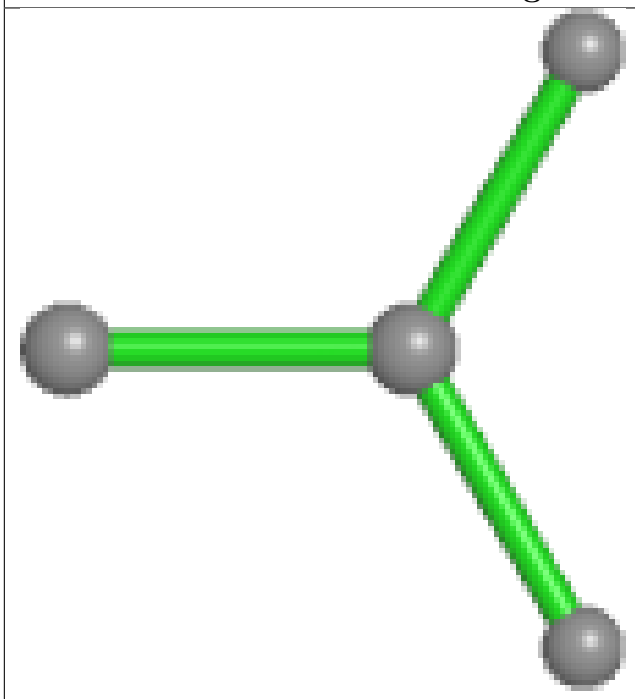


Rings

Ligand ACT A 303



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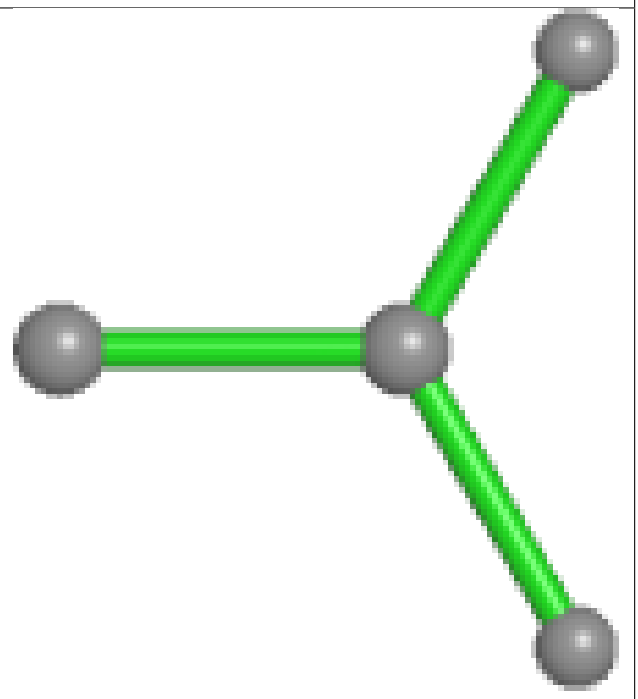
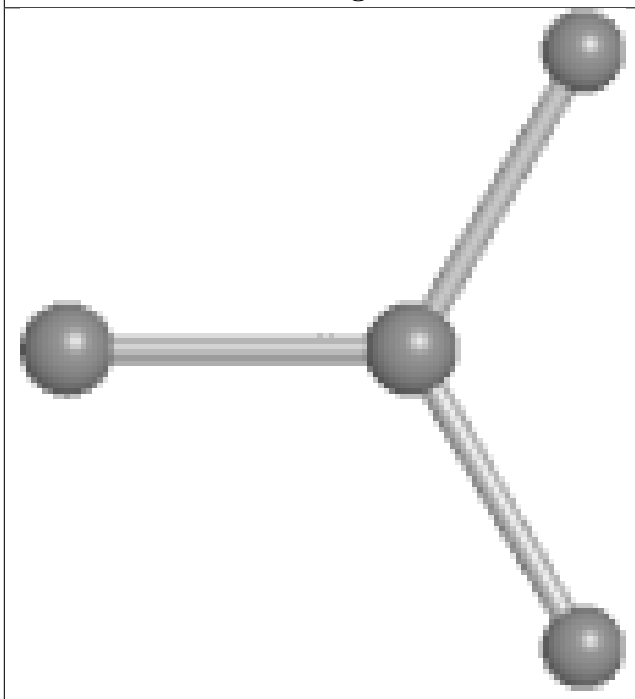


Bond angles



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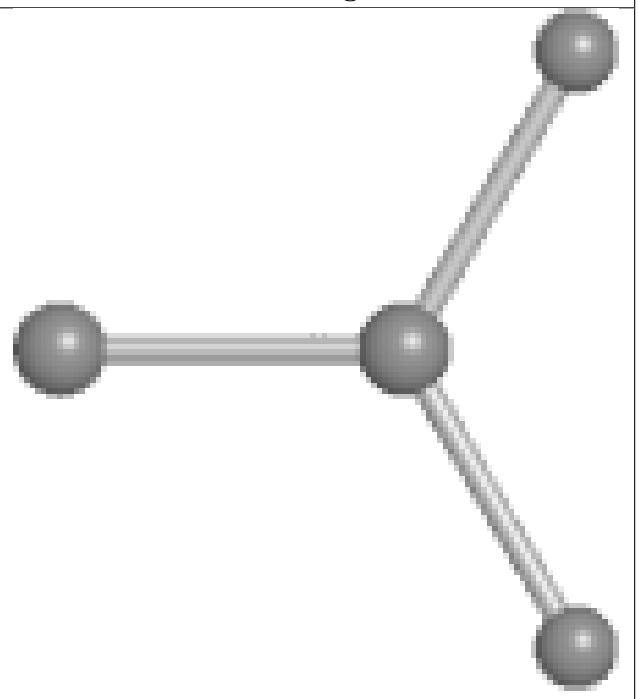
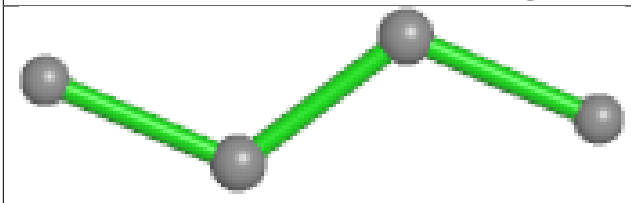
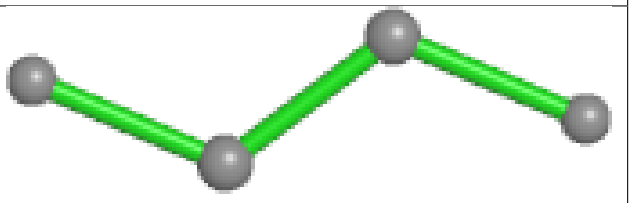


Rings

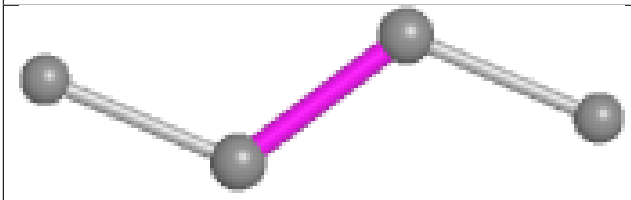
Ligand EDO D 308



Bond lengths



Bond angles



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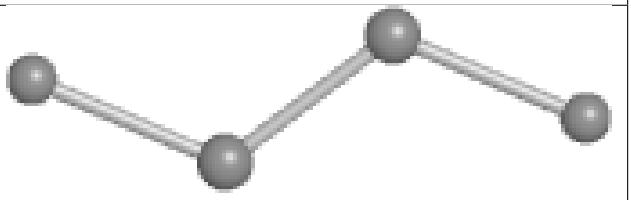
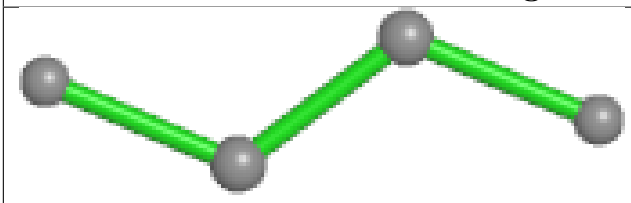
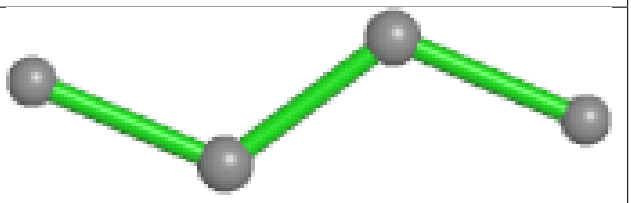


Rings

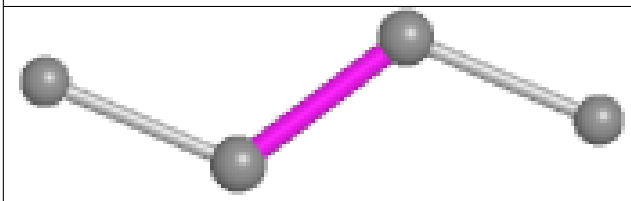
Ligand EDO B 308



Bond lengths



Bond angles



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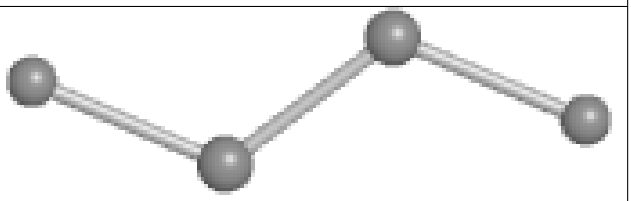


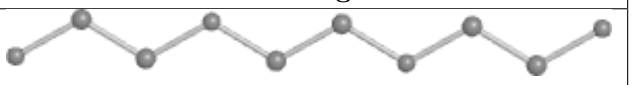
Rings

Ligand PGE B 307

Bond lengths

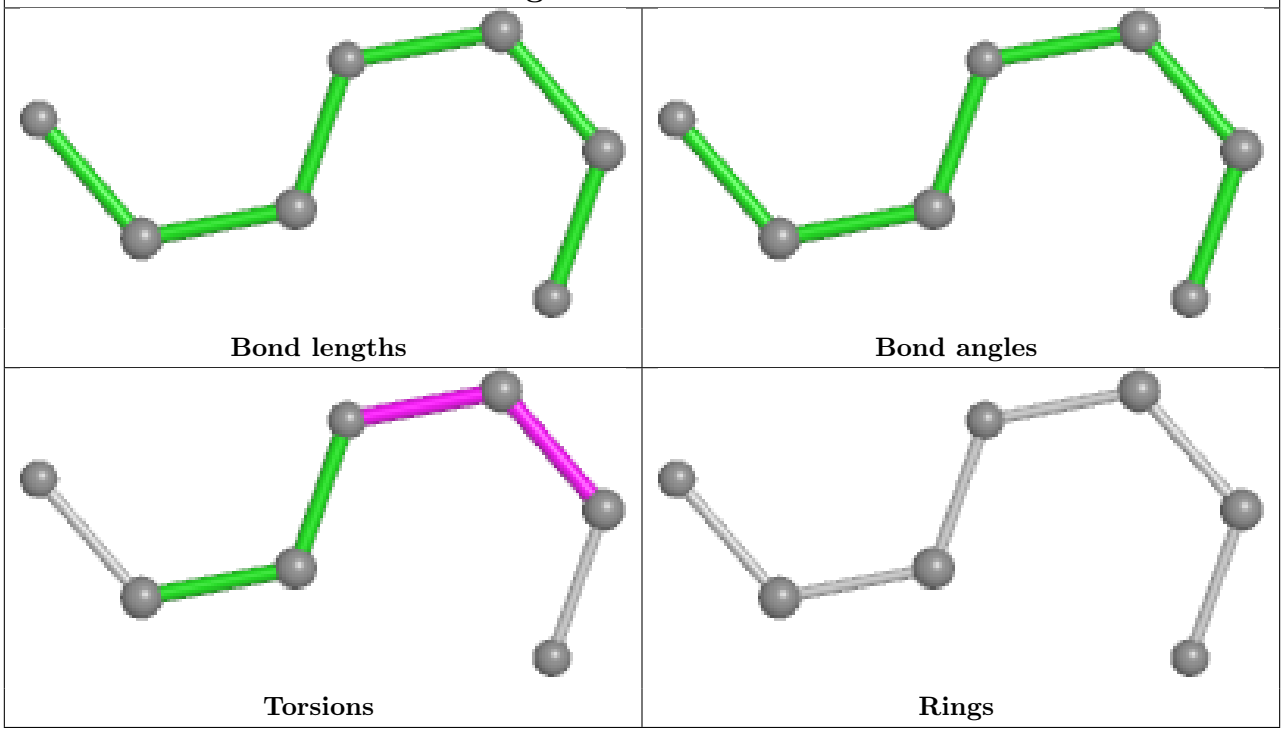
Bond angles

Torsions

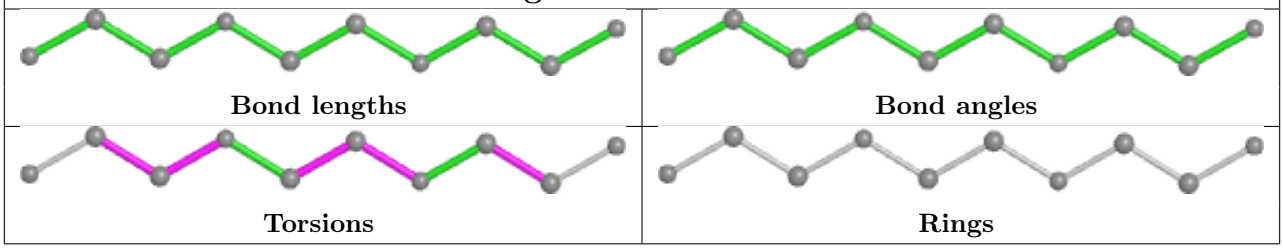


Rings

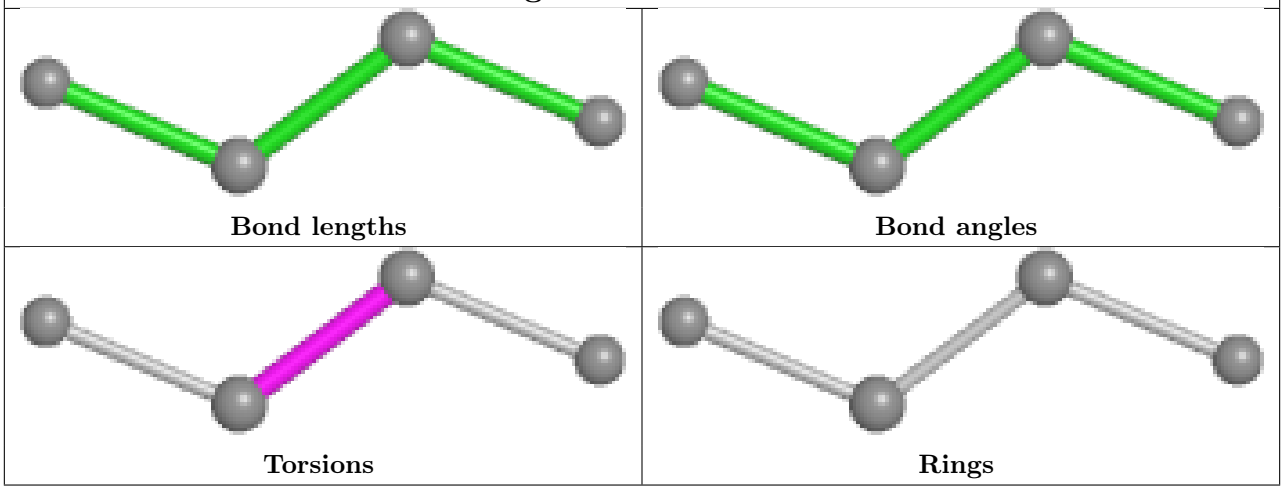
Ligand PEG F 306



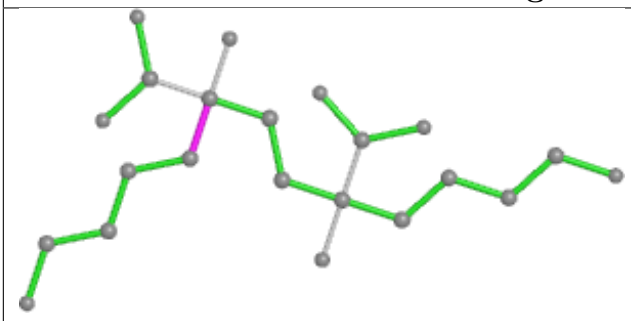
Ligand PGE C 305



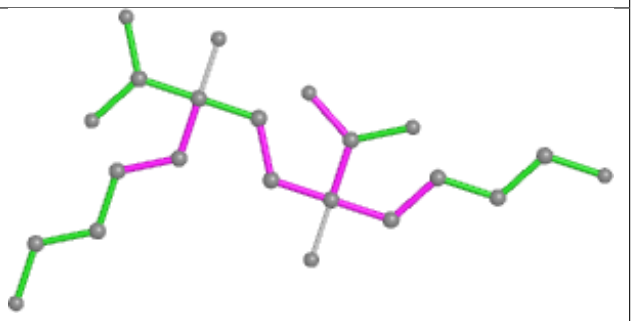
Ligand EDO E 308



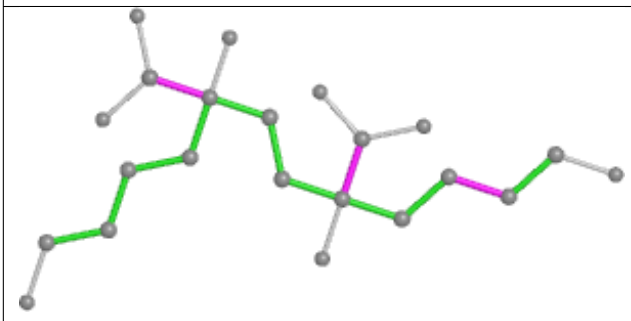
Ligand 3VN F 301



Bond lengths



Bond angles



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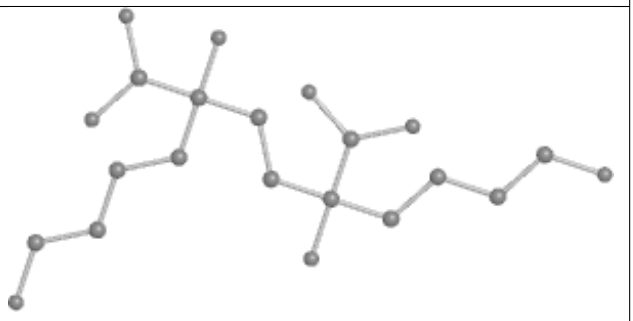
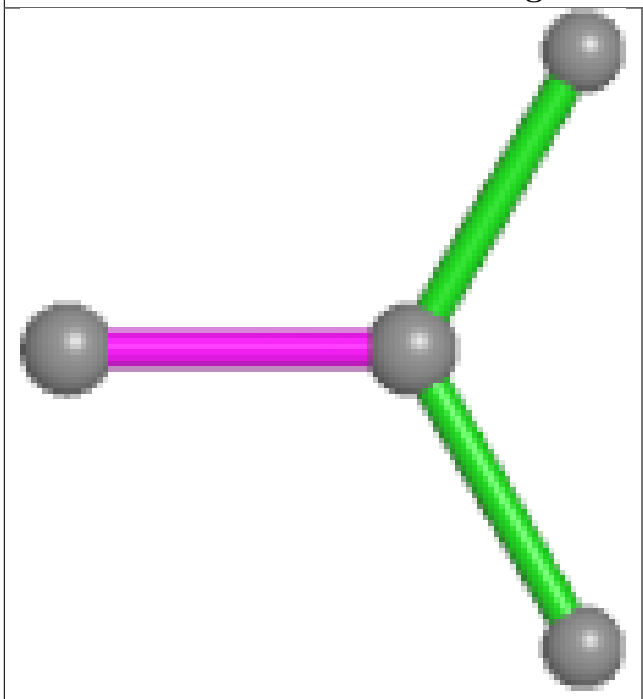


Rings

Ligand ACT E 303



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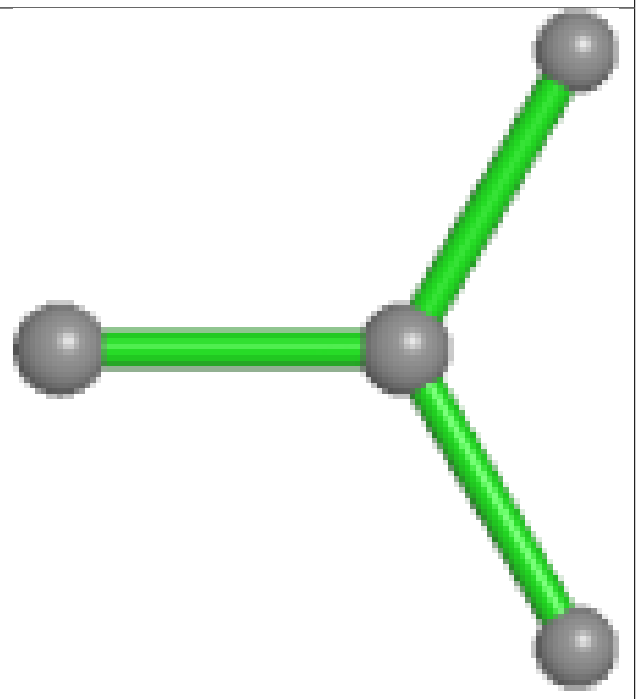
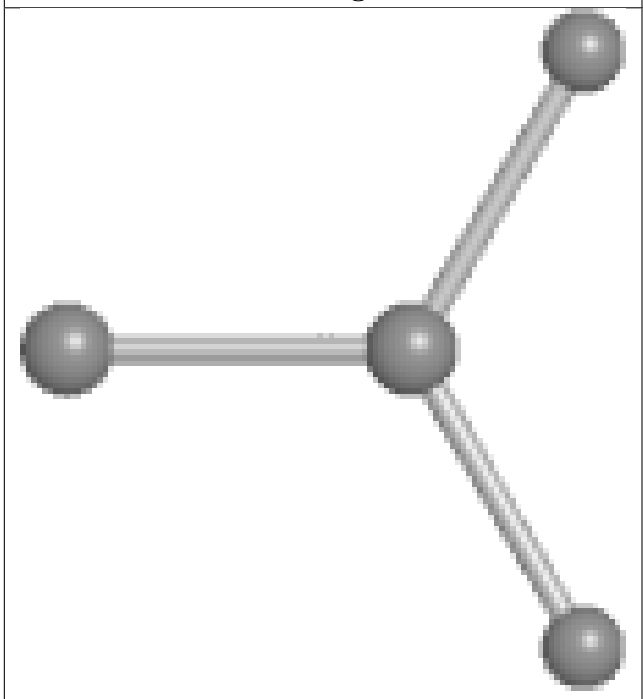


Bond angles



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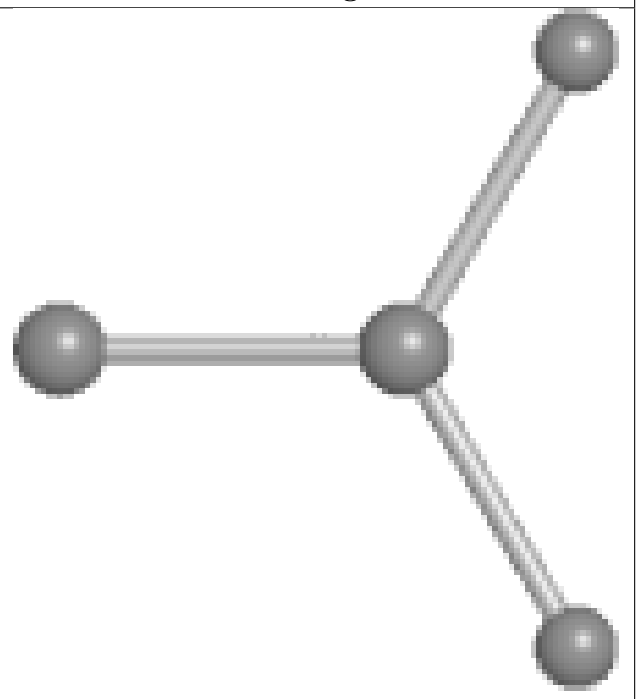
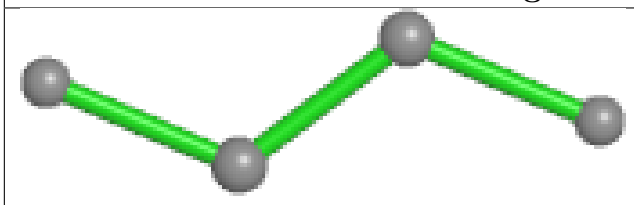


Rings

Ligand EDO C 308



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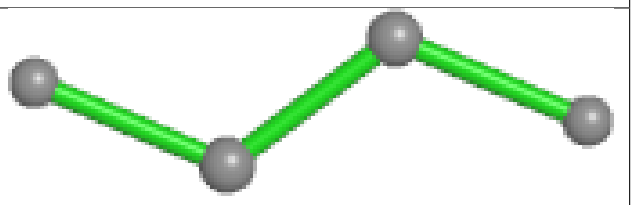
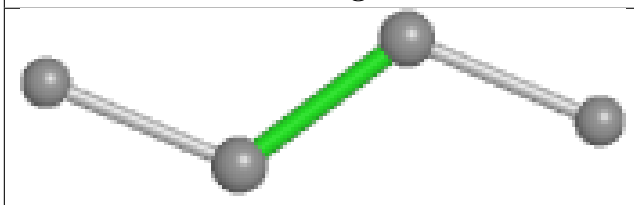


Bond angles



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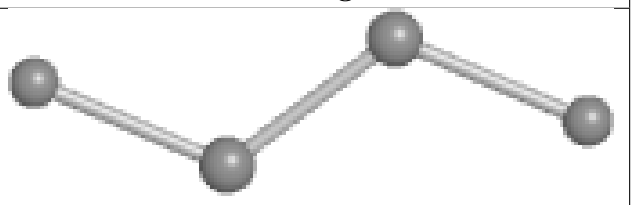
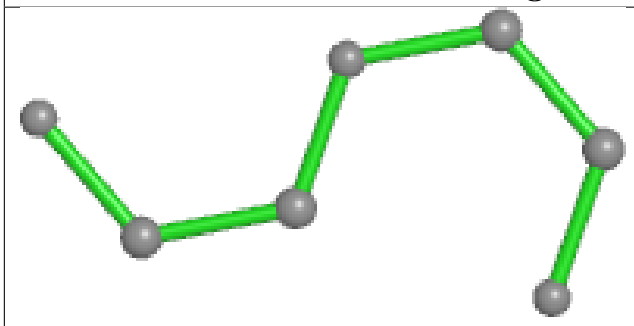
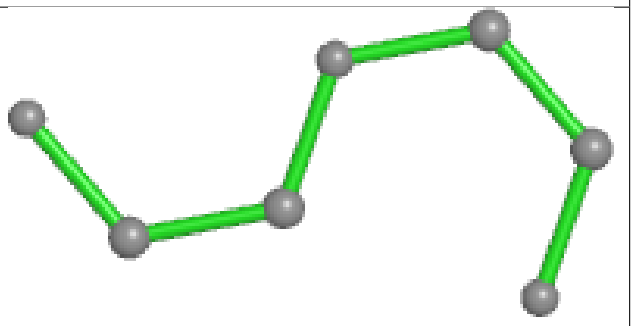


Rings

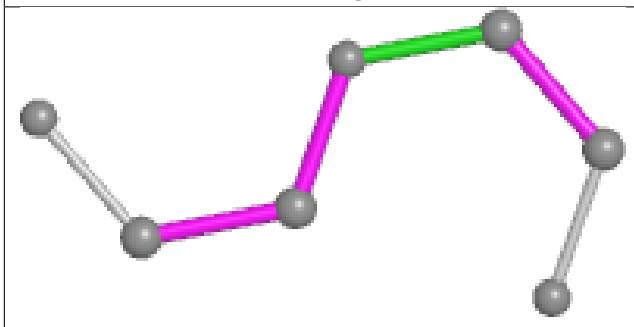
Ligand PEG F 305



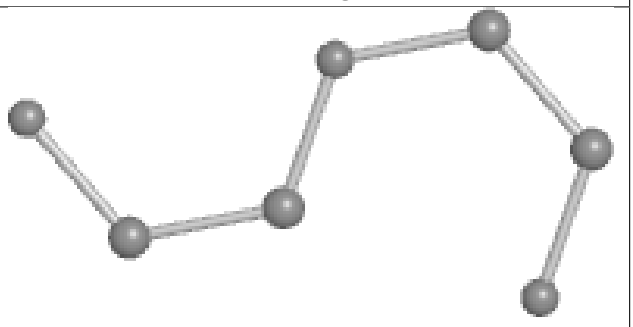
Bond lengths



Bond angles

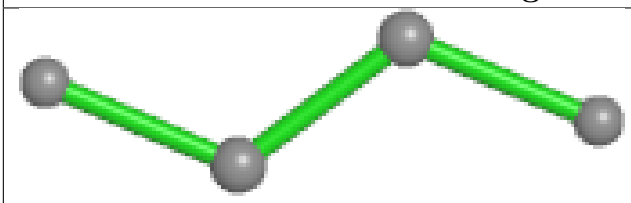


Torsions

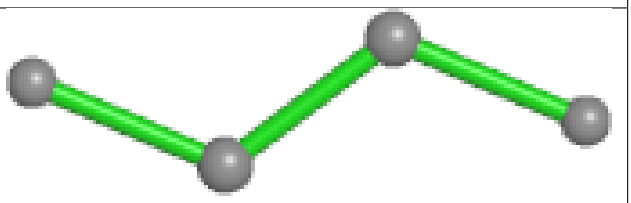


Rings

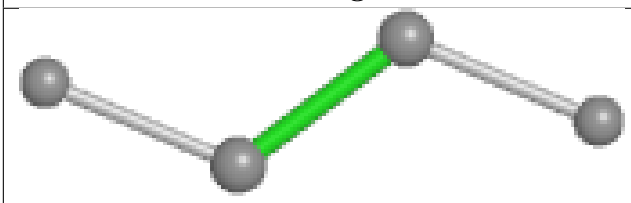
Ligand EDO A 309



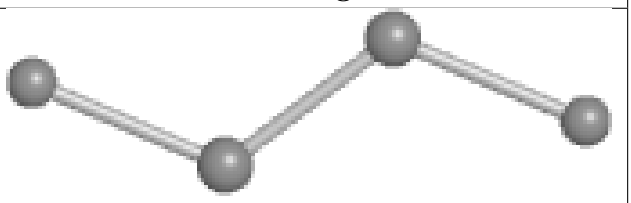
Bond lengths



Bond angles

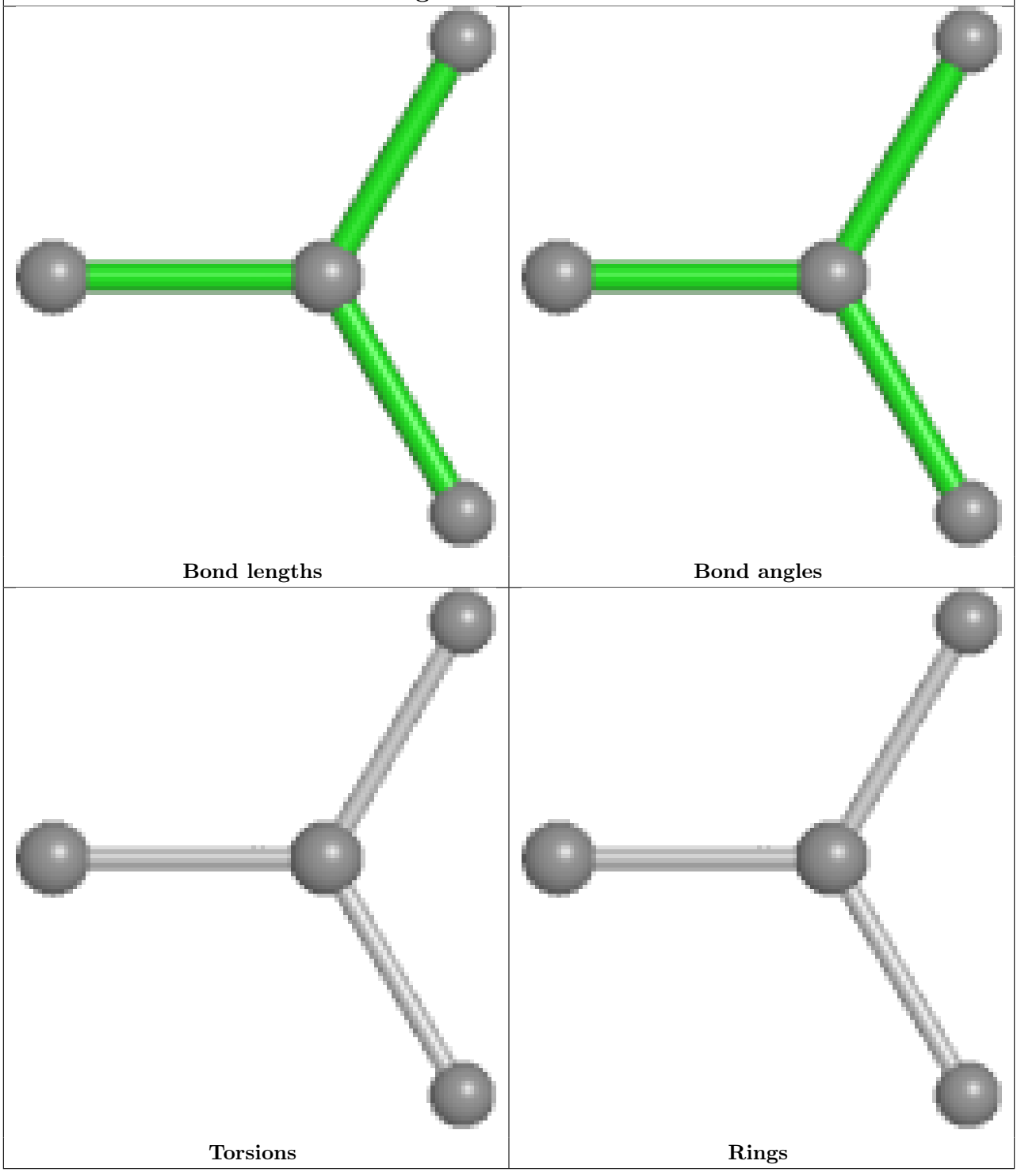


Torsions



Rings

Ligand ACT B 304



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	295/310 (95%)	-0.33	0 100 100	22, 28, 40, 54	0
1	B	295/310 (95%)	-0.39	1 (0%) 94 95	22, 28, 40, 52	0
1	C	295/310 (95%)	-0.26	1 (0%) 94 95	22, 29, 43, 52	0
1	D	295/310 (95%)	-0.23	1 (0%) 94 95	22, 29, 42, 54	0
1	E	295/310 (95%)	-0.30	1 (0%) 94 95	24, 31, 44, 57	0
1	F	295/310 (95%)	-0.24	0 100 100	23, 31, 44, 59	0
All	All	1770/1860 (95%)	-0.29	4 (0%) 95 96	22, 29, 42, 59	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	ASN	2.4
1	D	20	GLY	2.3
1	E	4	ASN	2.1
1	C	281	GLU	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	A	166	14/15	0.81	0.22	18,24,43,47	0
1	KPI	D	166	14/15	0.81	0.17	23,27,39,42	0
1	KPI	B	166	14/15	0.83	0.17	22,25,39,45	0
1	KPI	C	166	14/15	0.84	0.19	22,24,39,40	0
1	KPI	F	166	14/15	0.86	0.17	23,29,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	E	166	14/15	0.87	0.16	24,29,44,47	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	E	303	4/4	0.51	0.48	42,48,55,62	0
2	MG	D	302	1/1	0.56	0.14	41,41,41,41	0
3	ACT	E	304	4/4	0.65	0.23	30,44,46,50	0
8	GOL	C	310	6/6	0.71	0.19	42,49,52,54	0
6	EDO	B	309	4/4	0.74	0.22	41,42,46,52	0
3	ACT	A	305	4/4	0.75	0.29	42,52,58,60	0
6	EDO	C	309	4/4	0.76	0.33	40,43,44,53	0
4	PEG	F	306	7/7	0.76	0.29	51,54,55,59	0
6	EDO	A	310	4/4	0.77	0.27	39,45,46,54	0
8	GOL	F	308	6/6	0.77	0.26	20,20,20,20	0
4	PEG	B	305	7/7	0.78	0.39	40,48,54,56	0
4	PEG	A	306	7/7	0.79	0.48	38,39,47,48	0
3	ACT	A	304	4/4	0.79	0.30	43,51,53,60	0
6	EDO	C	306	4/4	0.80	0.21	29,31,35,43	0
6	EDO	F	307	4/4	0.80	0.30	33,36,36,44	0
2	MG	A	301	1/1	0.81	0.13	35,35,35,35	0
4	PEG	E	307	7/7	0.82	0.29	34,40,44,50	0
3	ACT	F	302	4/4	0.82	0.24	26,32,36,48	0
6	EDO	E	308	4/4	0.82	0.33	42,44,45,48	0
6	EDO	C	308	4/4	0.83	0.45	45,48,49,50	0
6	EDO	B	310	4/4	0.83	0.25	39,43,44,46	0
6	EDO	A	308	4/4	0.84	0.26	46,49,50,52	0
4	PEG	E	306	7/7	0.84	0.17	41,44,52,54	0
6	EDO	D	310	4/4	0.84	0.14	40,40,47,50	0
3	ACT	C	303	4/4	0.84	0.16	39,51,55,57	0
4	PEG	F	305	7/7	0.84	0.16	36,43,45,51	0
2	MG	C	302	1/1	0.84	0.14	56,56,56,56	0

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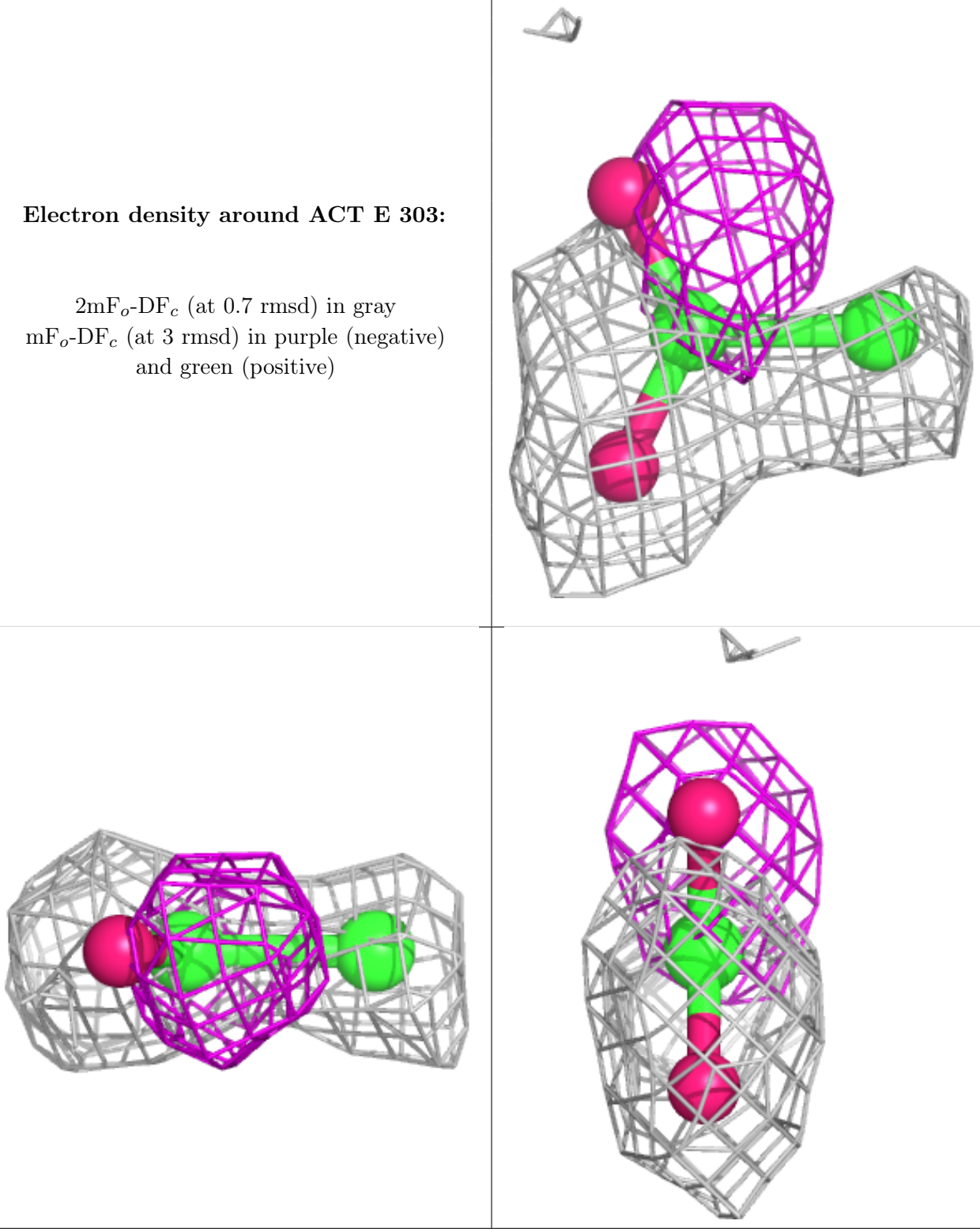
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	C	307	4/4	0.84	0.37	42,43,43,45	0
3	ACT	B	304	4/4	0.85	0.13	45,45,53,54	0
3	ACT	F	303	4/4	0.85	0.20	40,44,44,51	0
6	EDO	E	309	4/4	0.85	0.32	41,42,44,51	0
6	EDO	D	306	4/4	0.86	0.36	31,31,33,41	0
5	PGE	D	305	10/10	0.86	0.17	33,38,44,48	0
6	EDO	D	311	4/4	0.86	0.23	36,39,40,41	0
6	EDO	B	311	4/4	0.86	0.37	50,50,56,61	0
6	EDO	D	309	4/4	0.87	0.27	41,42,46,53	0
5	PGE	C	305	10/10	0.87	0.20	30,38,46,57	0
3	ACT	D	304	4/4	0.87	0.18	24,37,41,49	0
4	PEG	E	305	7/7	0.87	0.24	29,32,39,42	0
2	MG	B	303	1/1	0.88	0.20	38,38,38,38	0
4	PEG	B	306	7/7	0.88	0.12	37,43,48,49	0
6	EDO	A	313	4/4	0.88	0.28	32,35,38,41	0
6	EDO	B	308	4/4	0.88	0.21	33,37,42,52	0
2	MG	D	303	1/1	0.88	0.21	51,51,51,51	0
2	MG	E	301	1/1	0.89	0.10	48,48,48,48	0
5	PGE	B	307	10/10	0.89	0.18	38,43,48,52	0
3	ACT	A	303	4/4	0.89	0.19	25,34,36,40	0
3	ACT	C	304	4/4	0.89	0.13	33,43,45,52	0
6	EDO	D	308	4/4	0.90	0.16	38,43,43,48	0
7	3VN	D	301	22/22	0.91	0.14	24,28,33,39	0
6	EDO	D	307	4/4	0.91	0.19	27,29,35,43	0
6	EDO	A	311	4/4	0.91	0.34	43,44,45,54	0
6	EDO	A	312	4/4	0.92	0.34	34,39,39,42	0
2	MG	A	302	1/1	0.93	0.14	45,45,45,45	0
2	MG	E	302	1/1	0.93	0.12	52,52,52,52	0
2	MG	B	302	1/1	0.93	0.05	33,33,33,33	0
5	PGE	A	307	10/10	0.93	0.19	34,41,44,48	0
4	PEG	F	304	7/7	0.94	0.17	26,33,37,39	0
7	3VN	F	301	22/22	0.95	0.13	26,30,32,34	0
7	3VN	B	301	22/22	0.95	0.13	24,28,31,34	0
6	EDO	A	309	4/4	0.95	0.14	30,33,33,36	0
2	MG	C	301	1/1	0.96	0.11	38,38,38,38	0

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

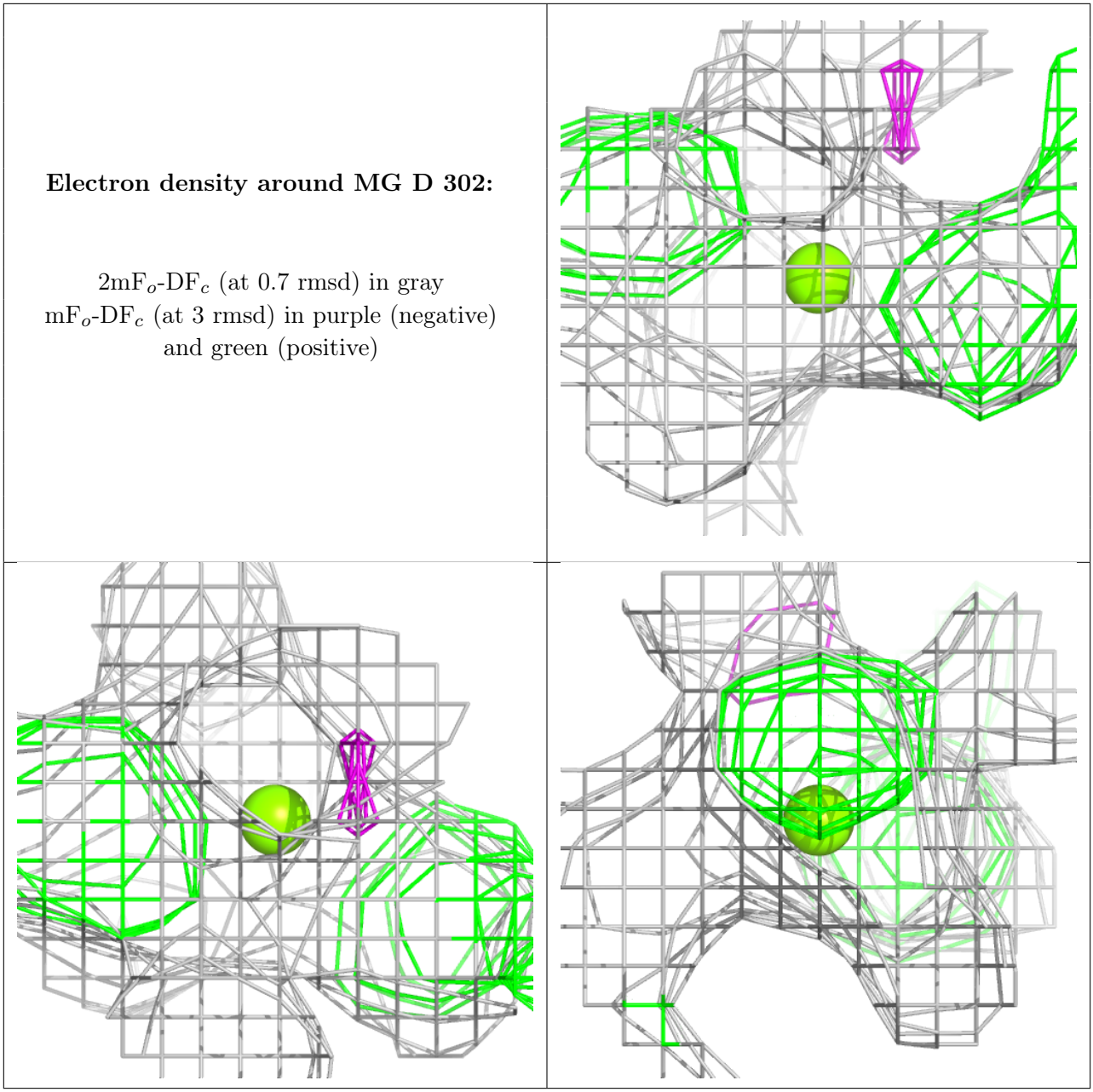
Electron density around ACT E 303:

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



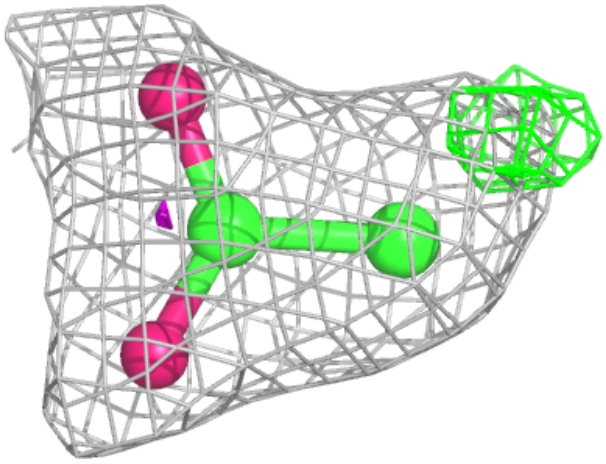
Electron density around MG D 302:

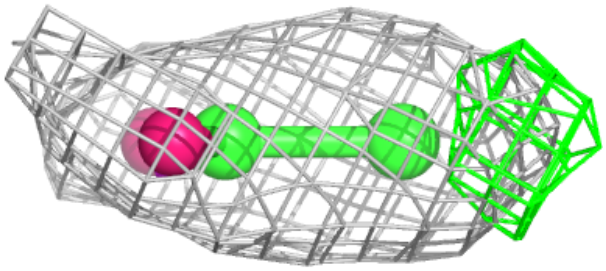
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

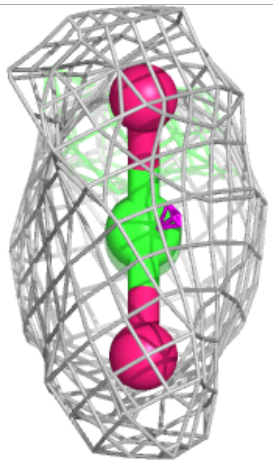


Electron density around ACT E 304:

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

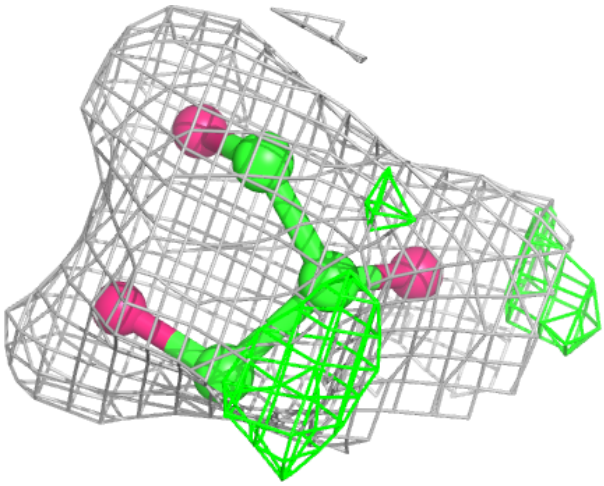


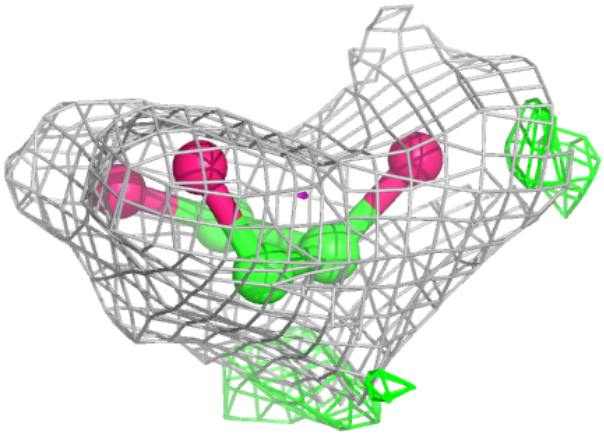


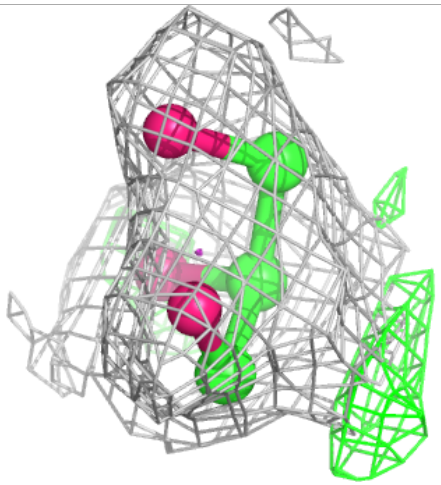


Electron density around GOL C 310:

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

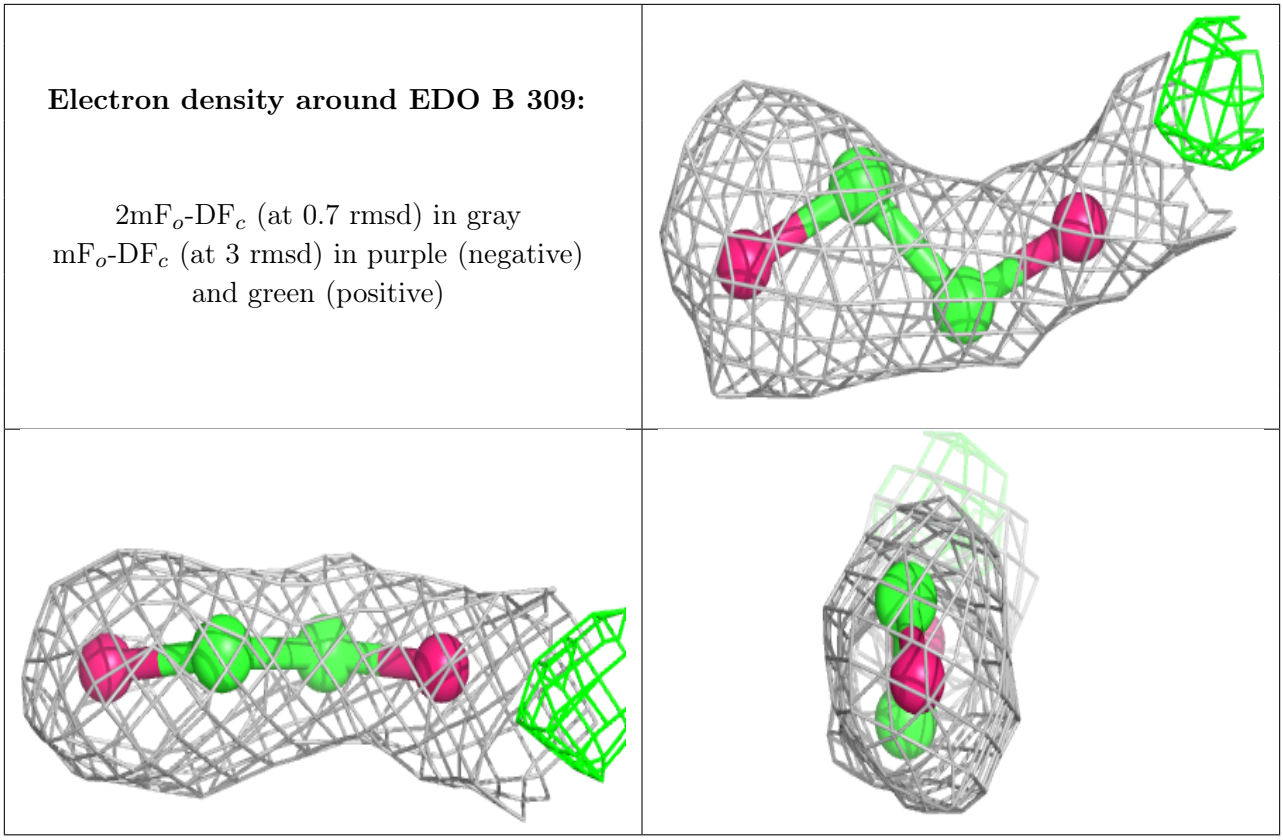






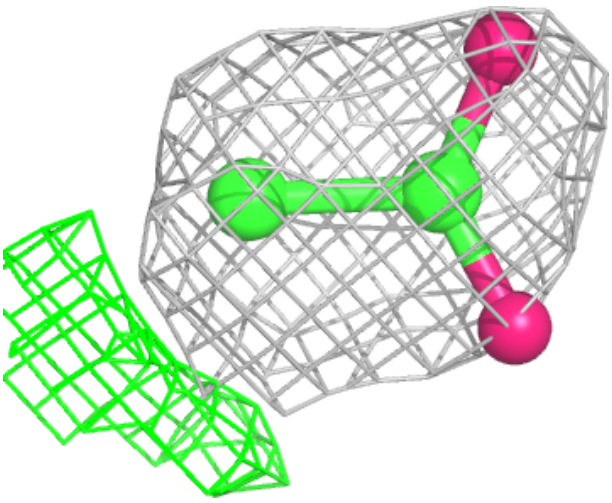
Electron density around EDO B 309:

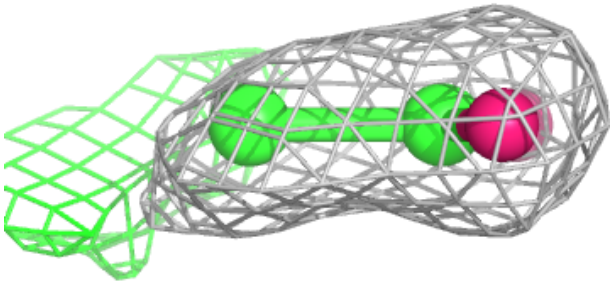
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

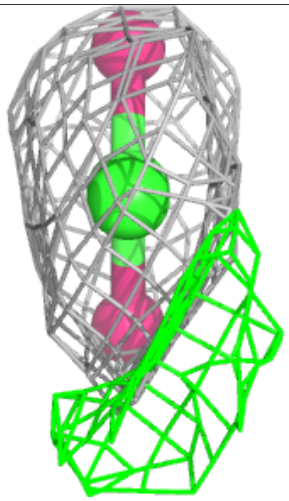


Electron density around ACT A 305:

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

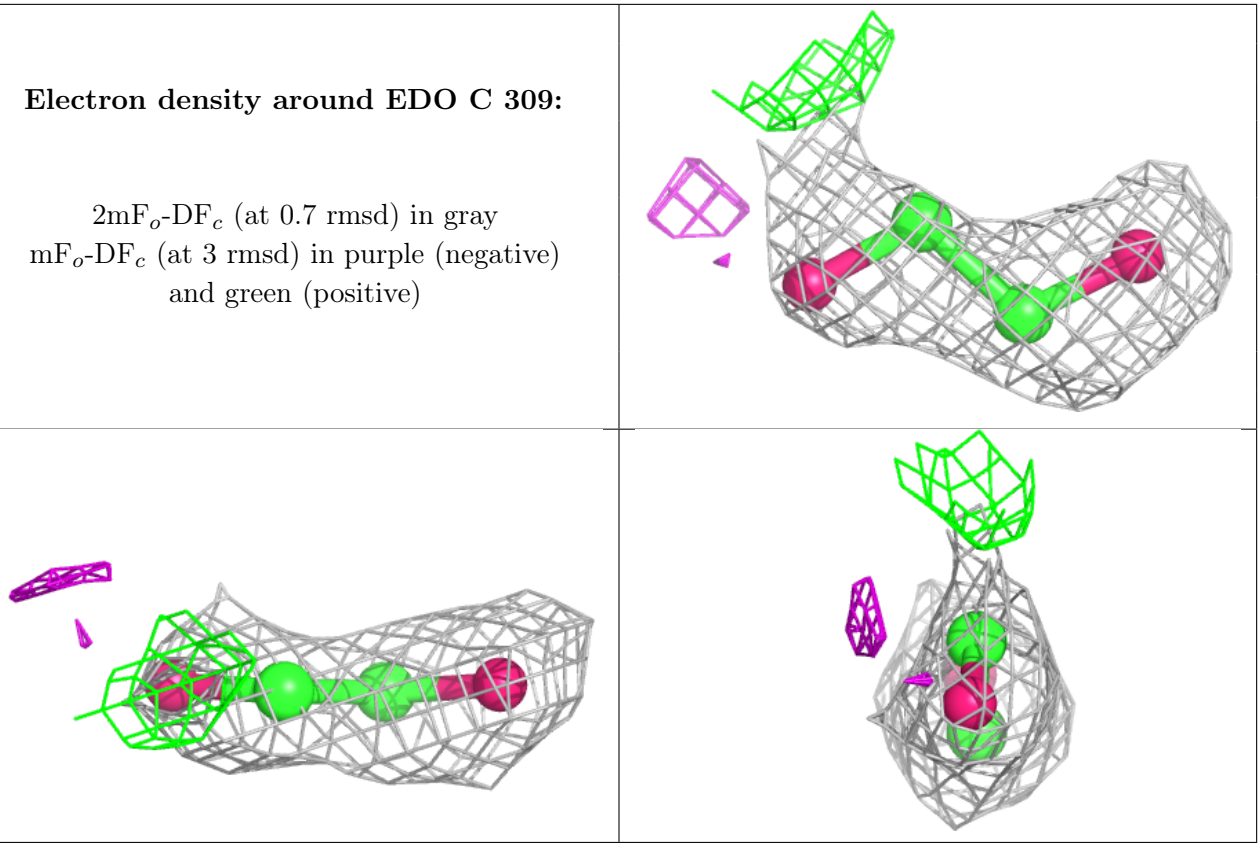






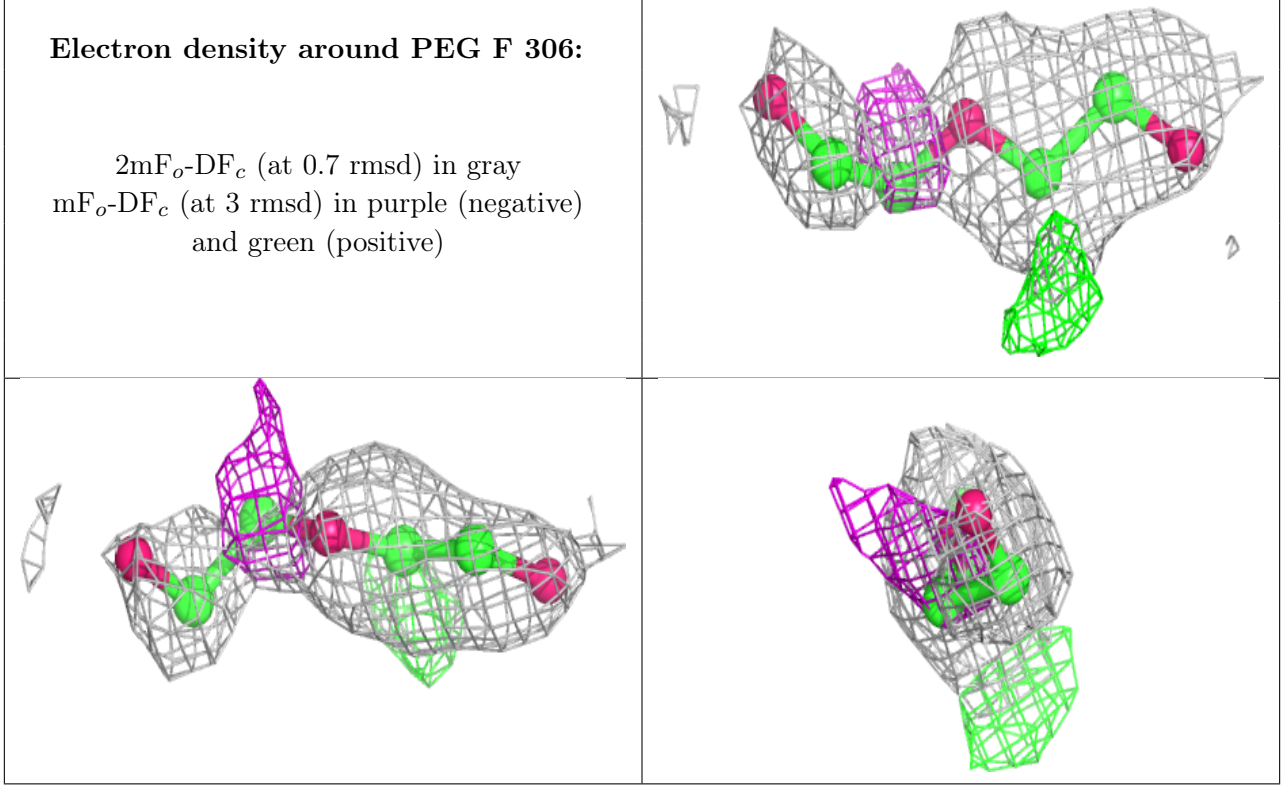
Electron density around EDO C 309:

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



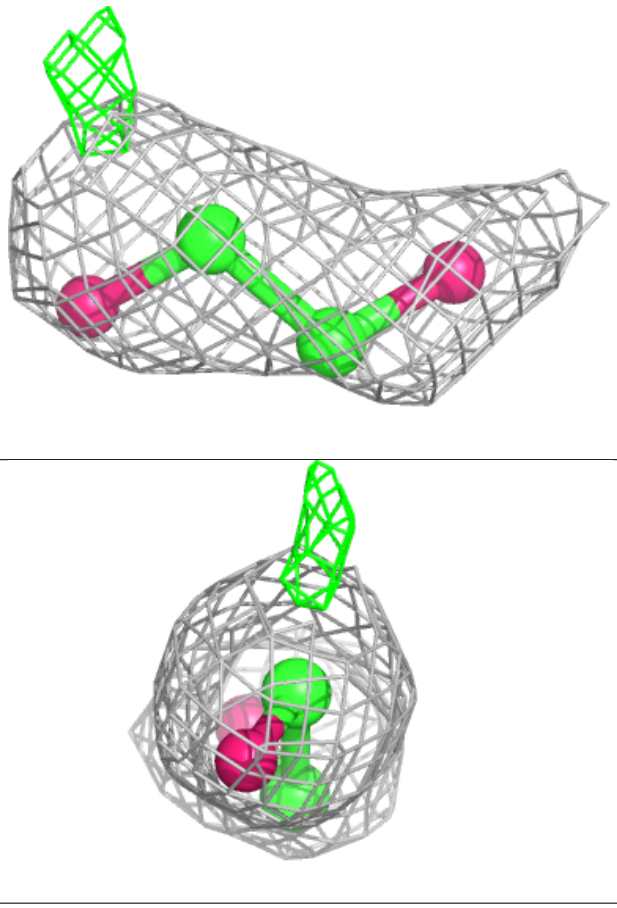
Electron density around PEG F 306:

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



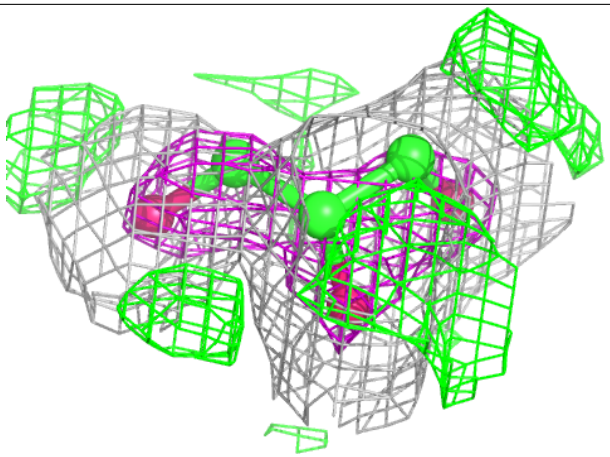
Electron density around EDO A 310:

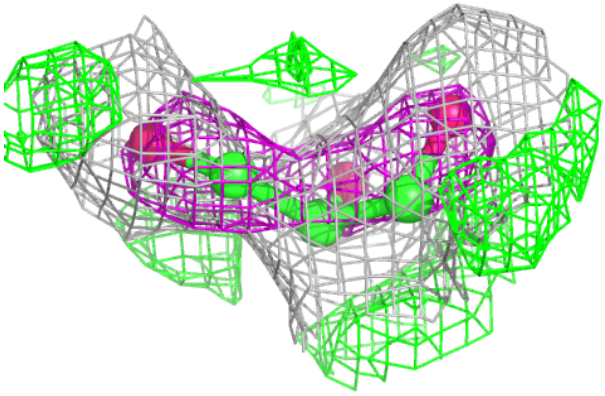
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

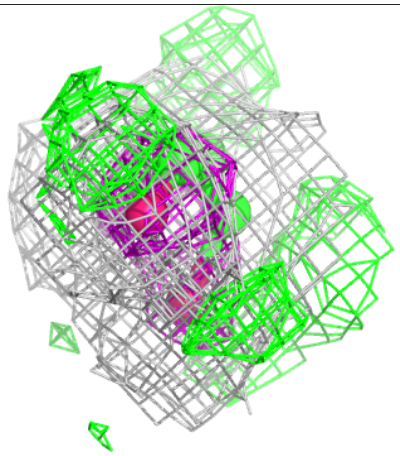


Electron density around GOL F 308:

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

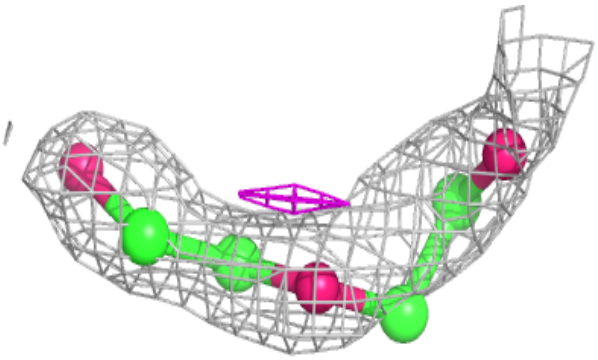


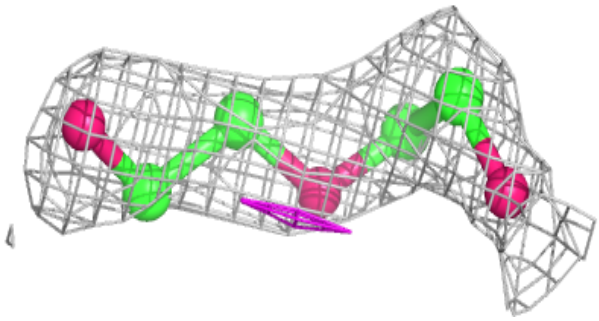


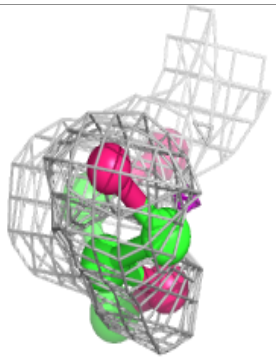


Electron density around PEG B 305:

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

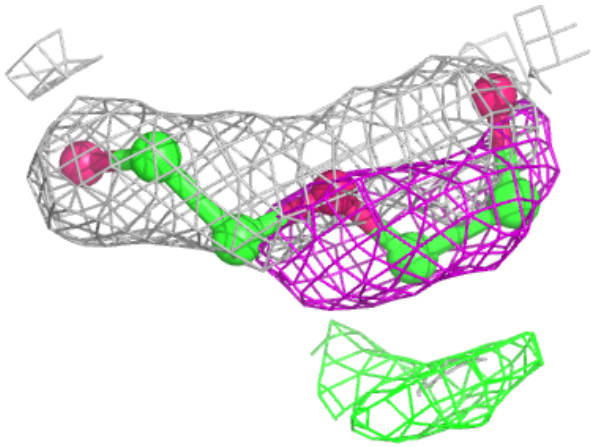


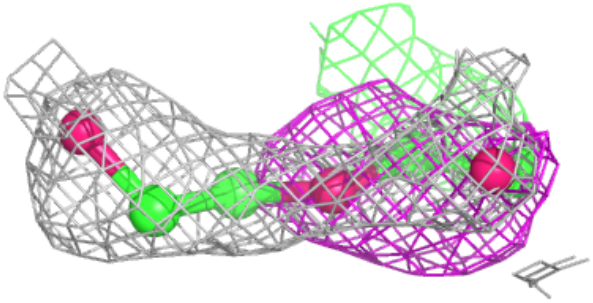


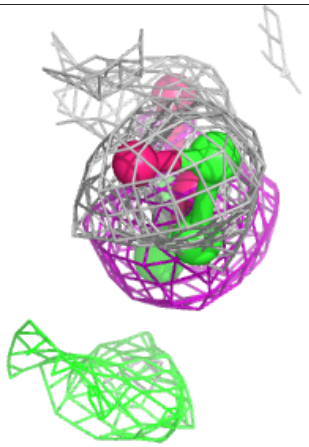


Electron density around PEG A 306:

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

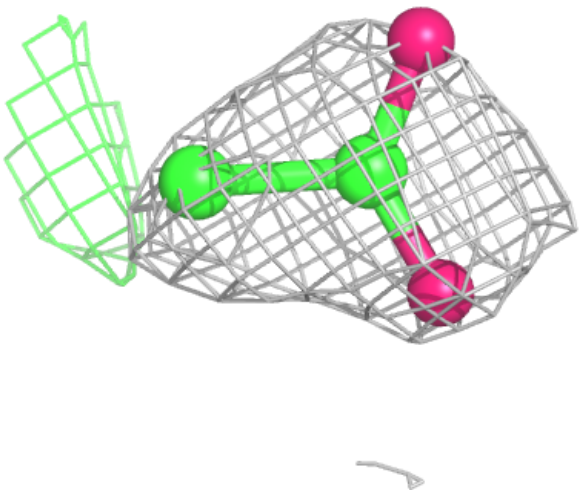


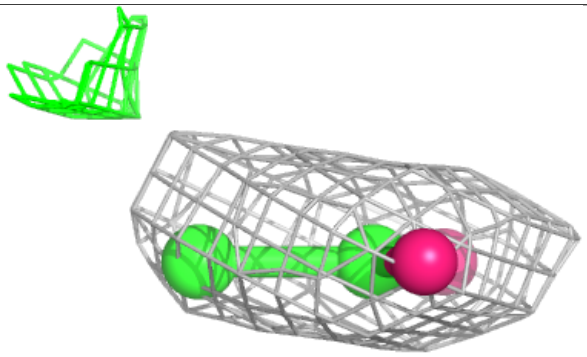


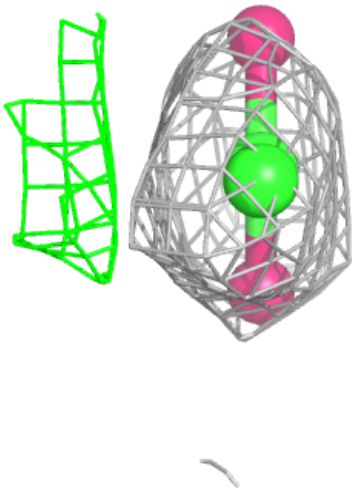


Electron density around ACT A 304:

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

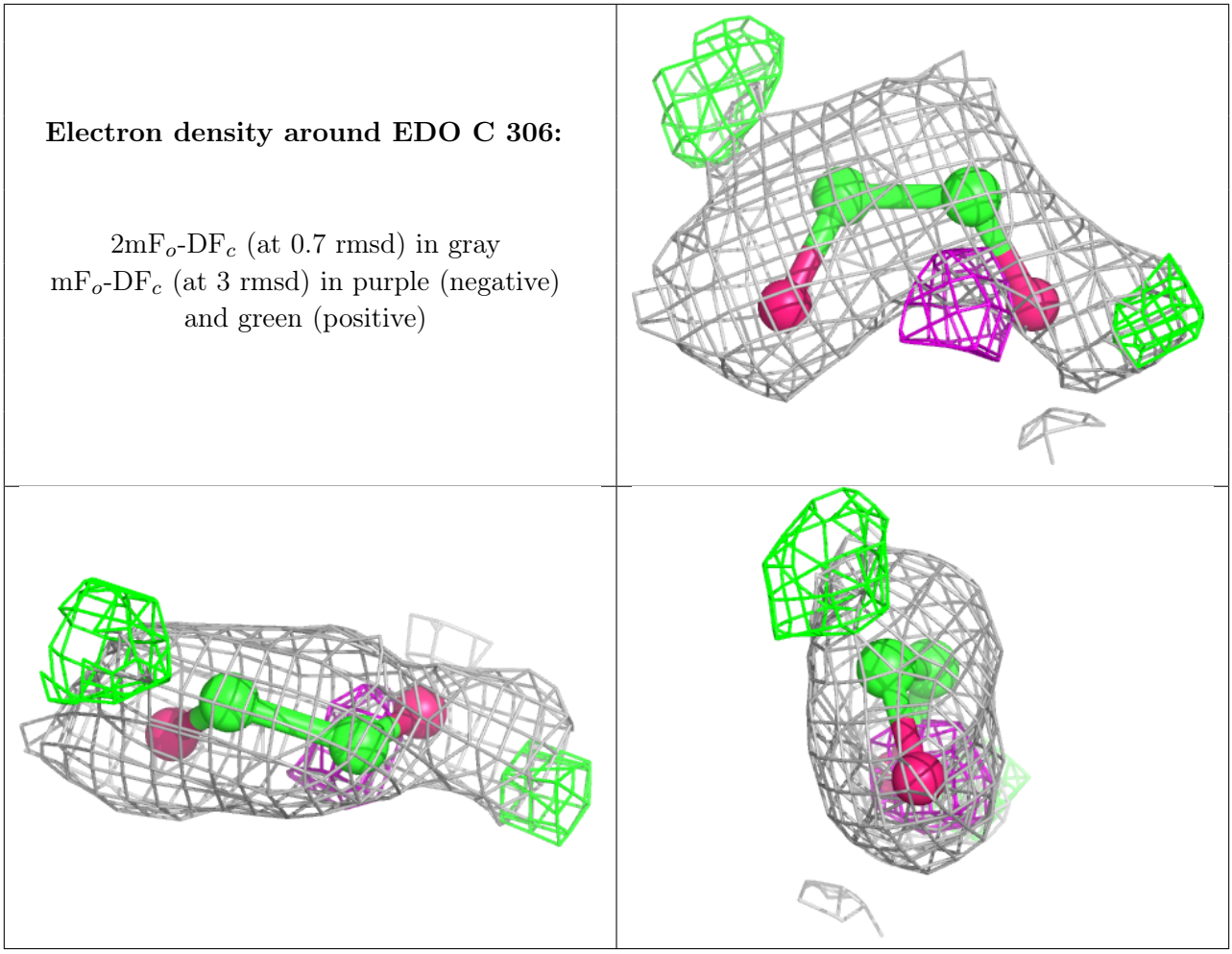






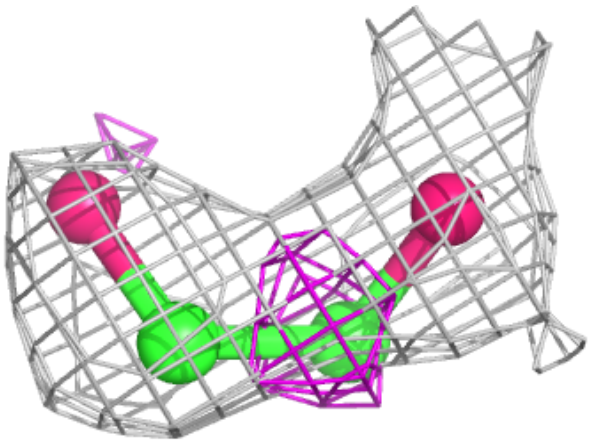
Electron density around EDO C 306:

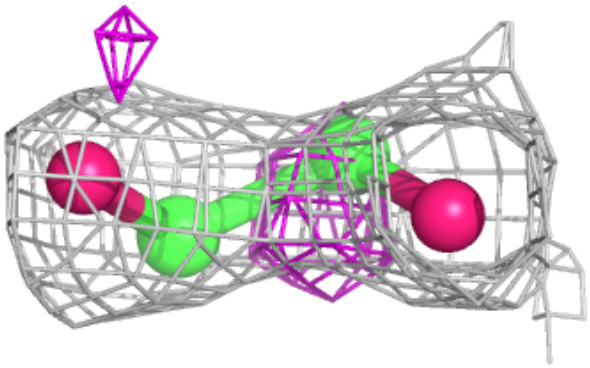
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

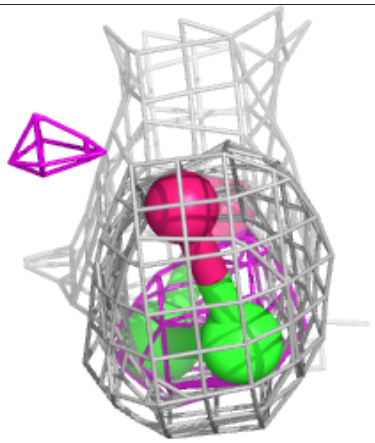


Electron density around EDO F 307:

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

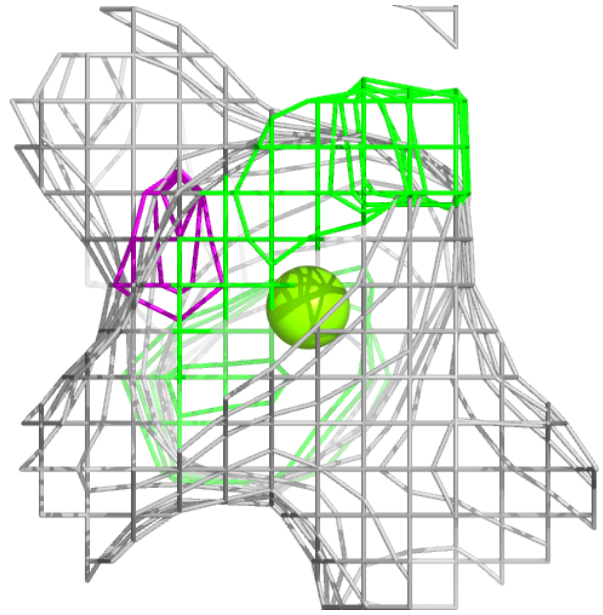


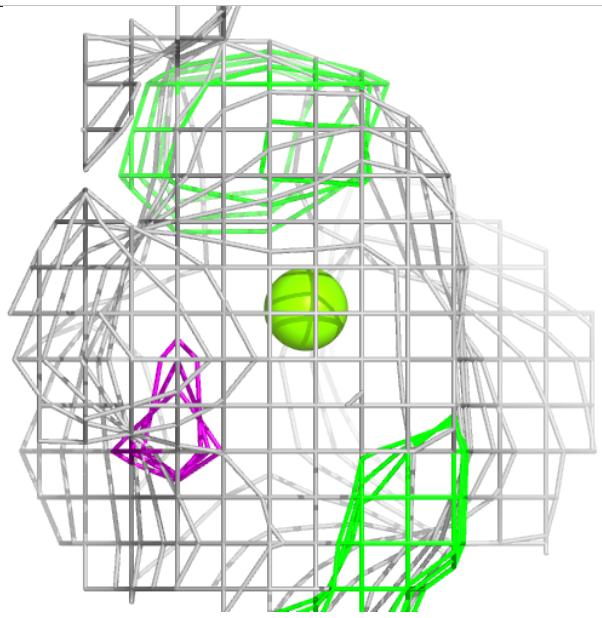


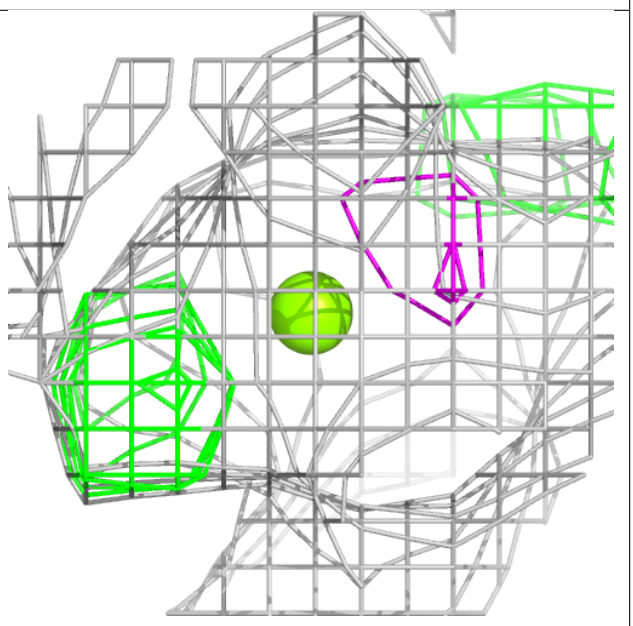


Electron density around MG A 301:

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

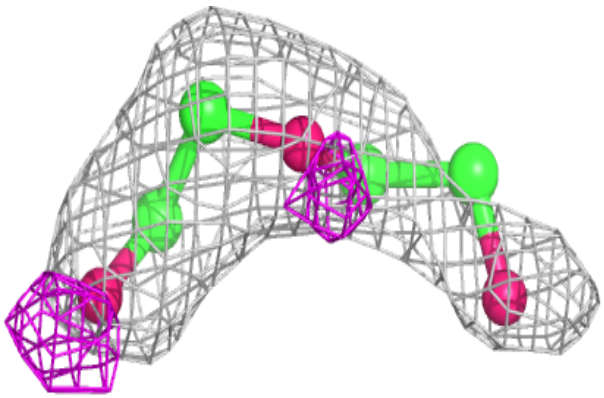


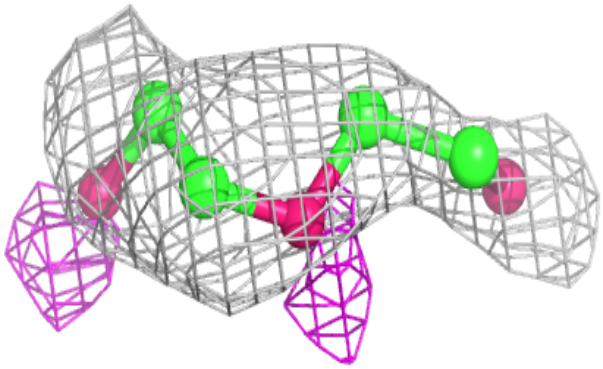


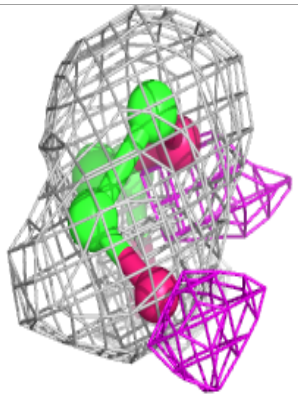


Electron density around PEG E 307:

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

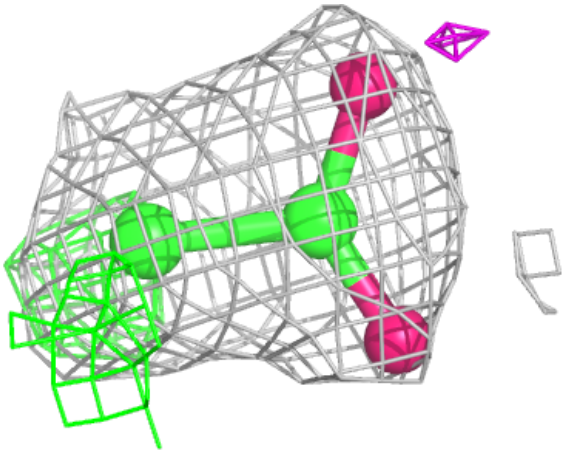


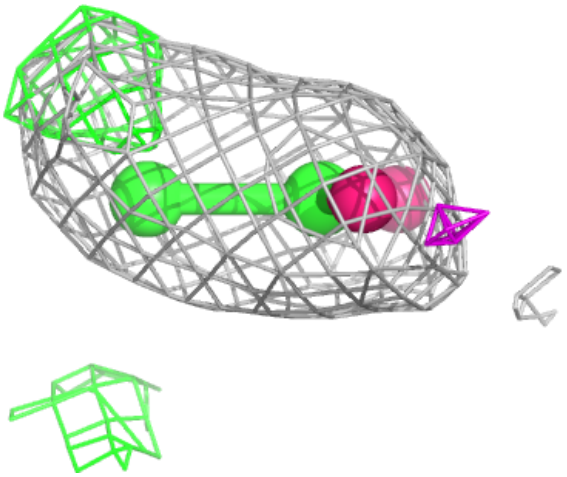


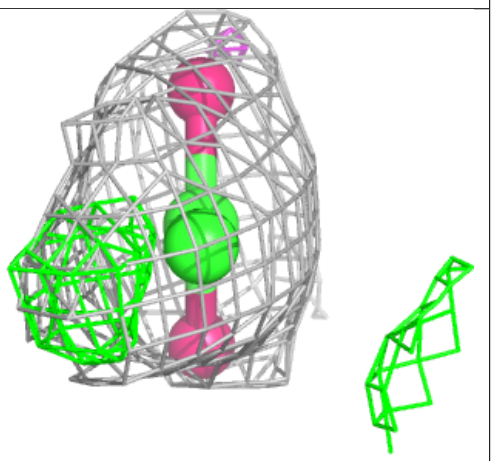


Electron density around ACT F 302:

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

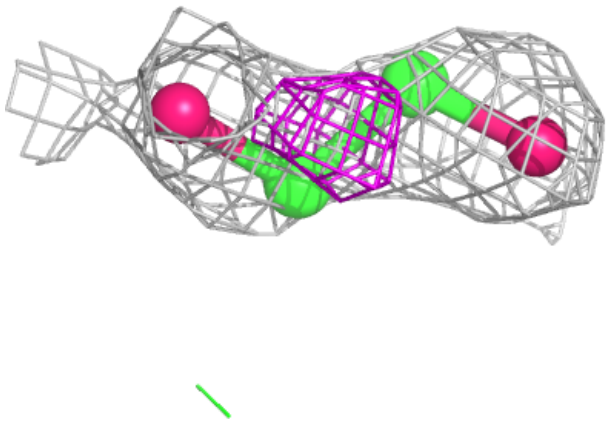


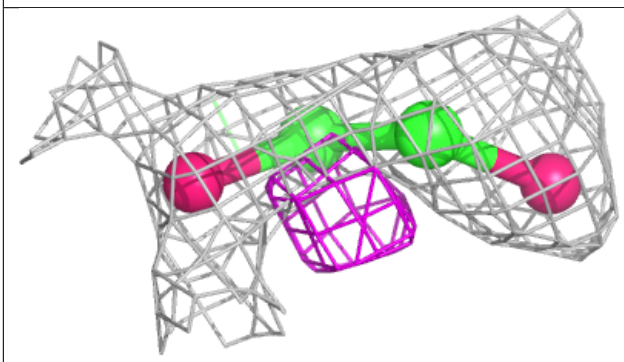


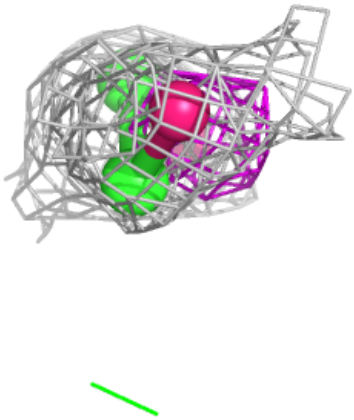


Electron density around EDO E 308:

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

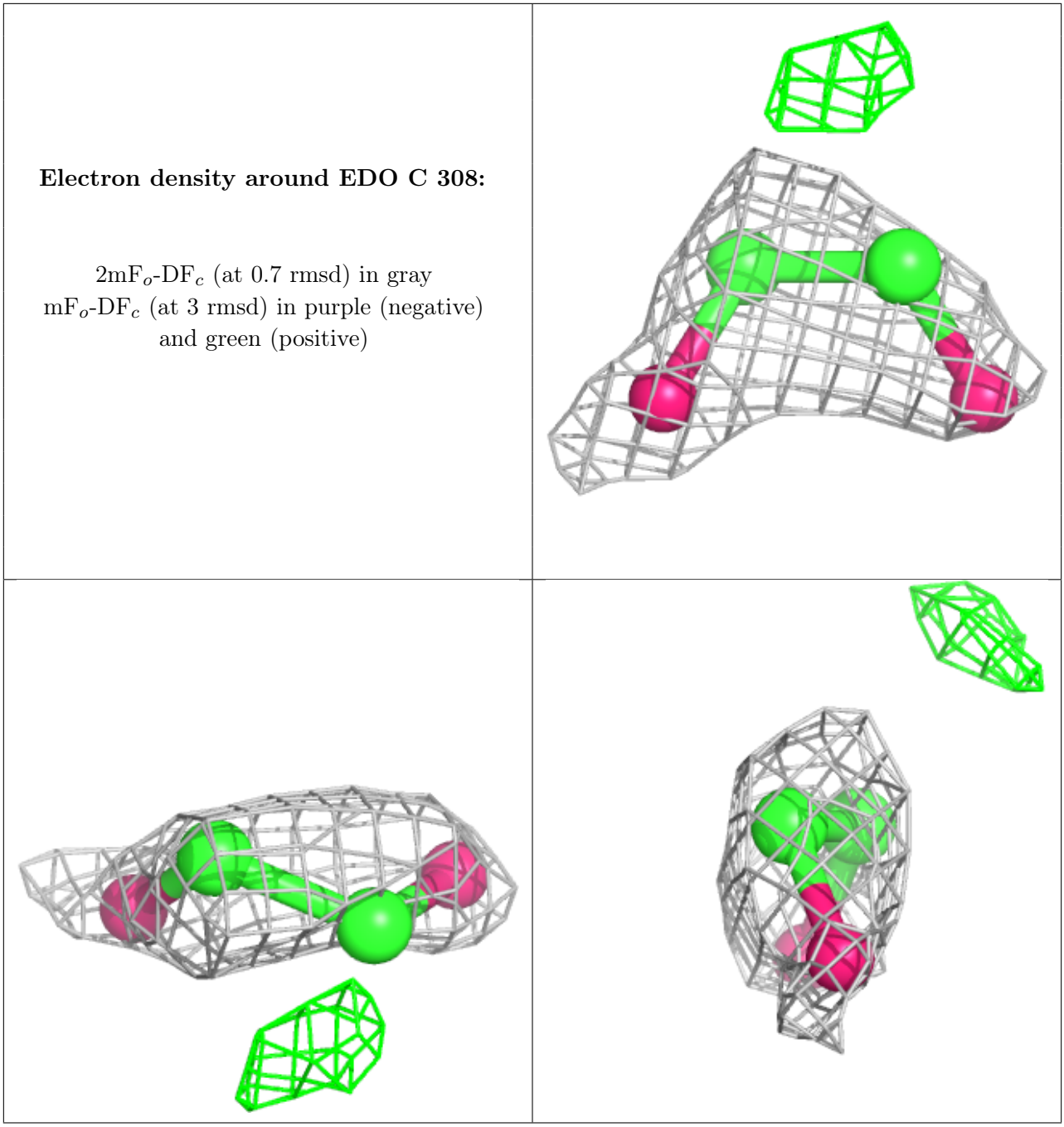






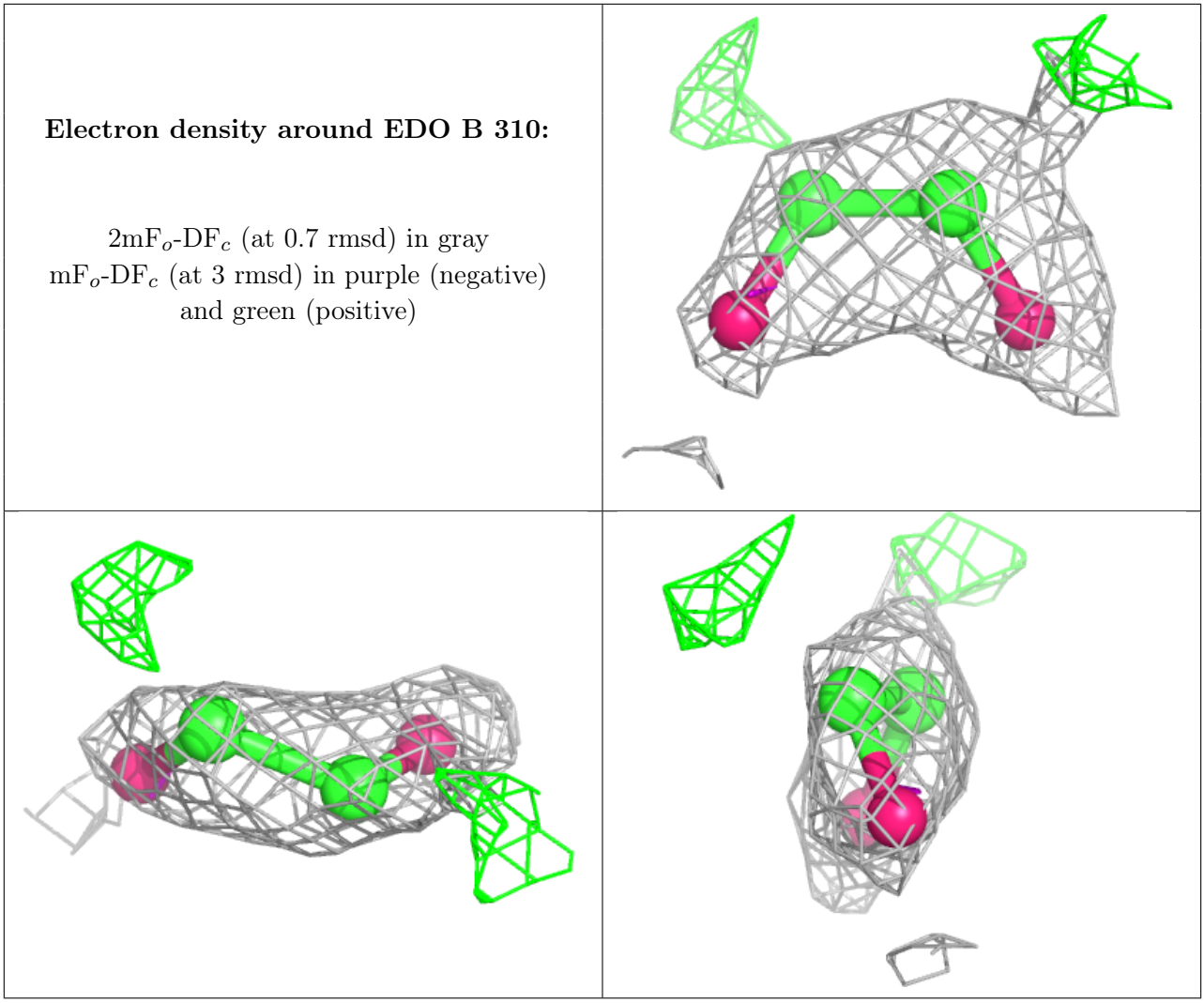
Electron density around EDO C 308:

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



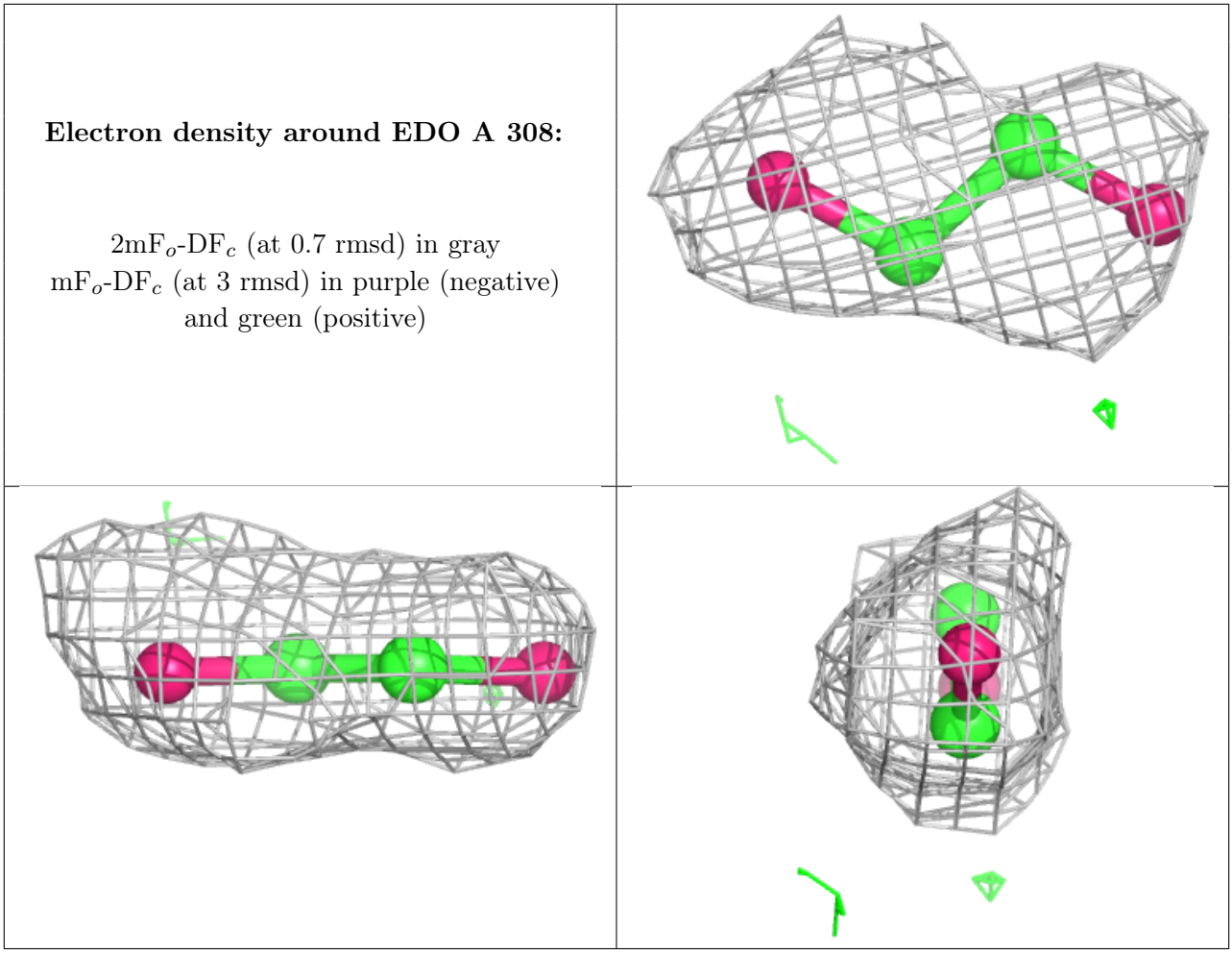
Electron density around EDO B 310:

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



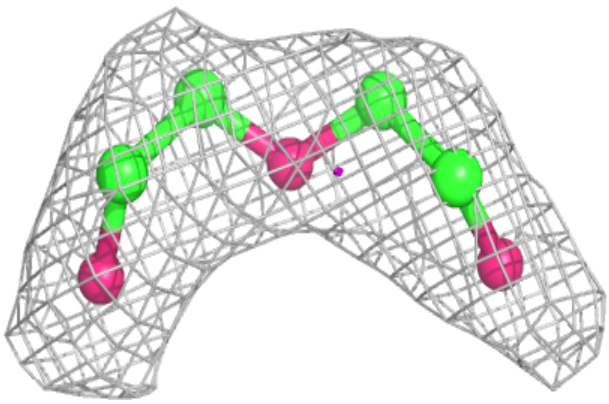
Electron density around EDO A 308:

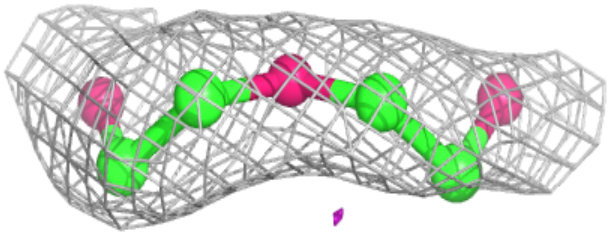
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

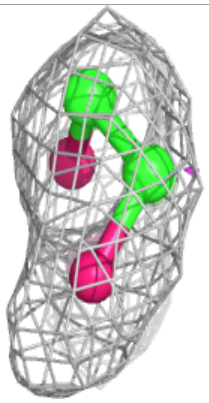


Electron density around PEG E 306:

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

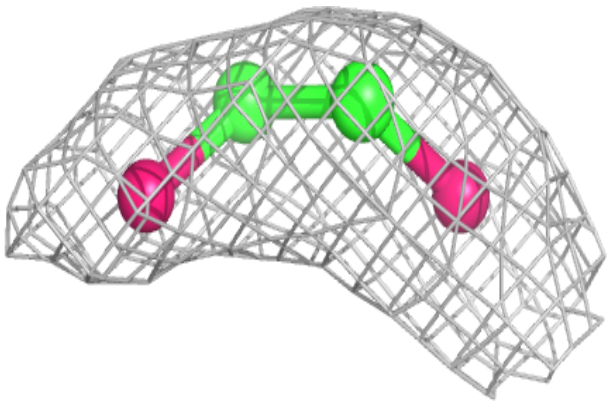


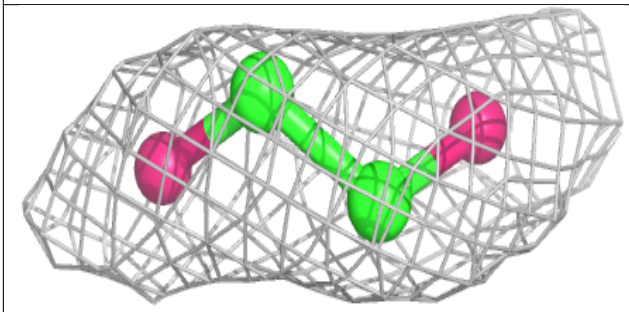


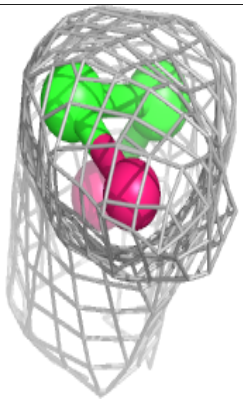


Electron density around EDO D 310:

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

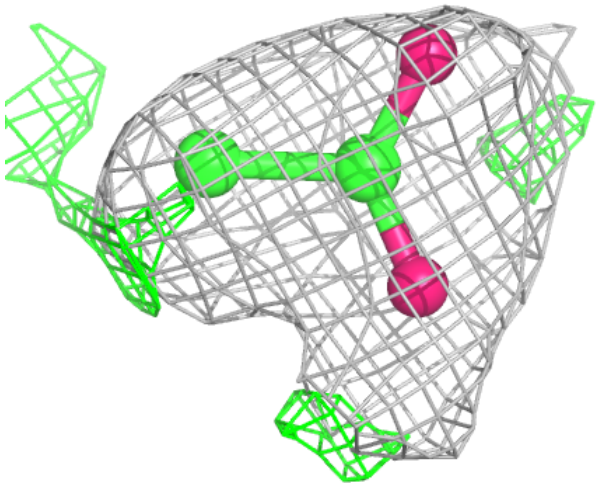


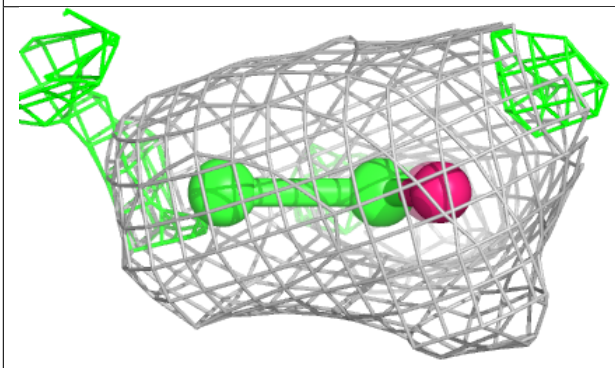


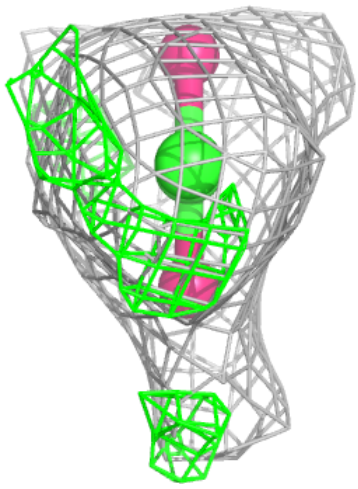


Electron density around ACT C 303:

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

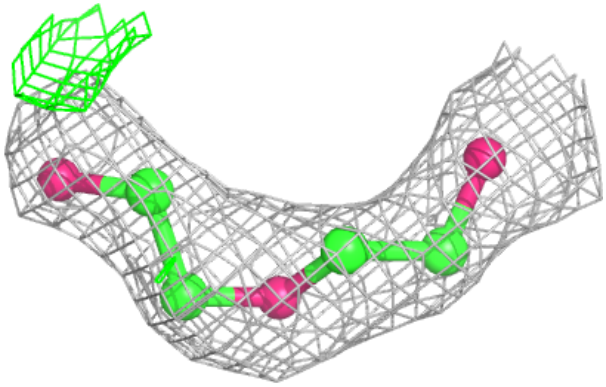


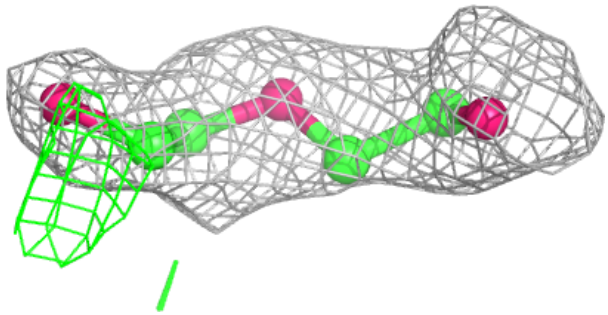


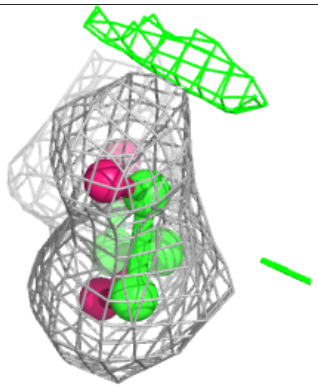


Electron density around PEG F 305:

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

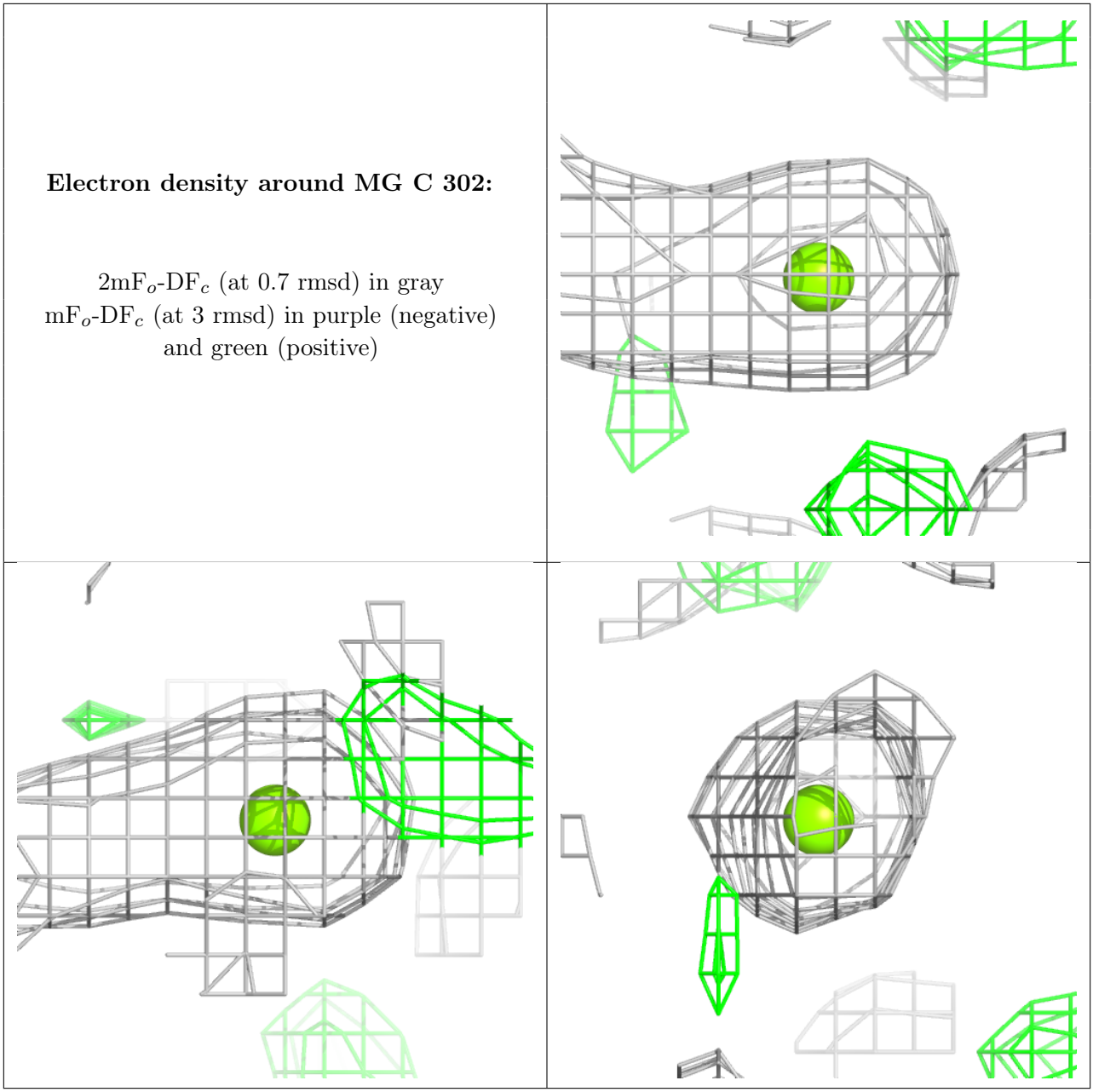






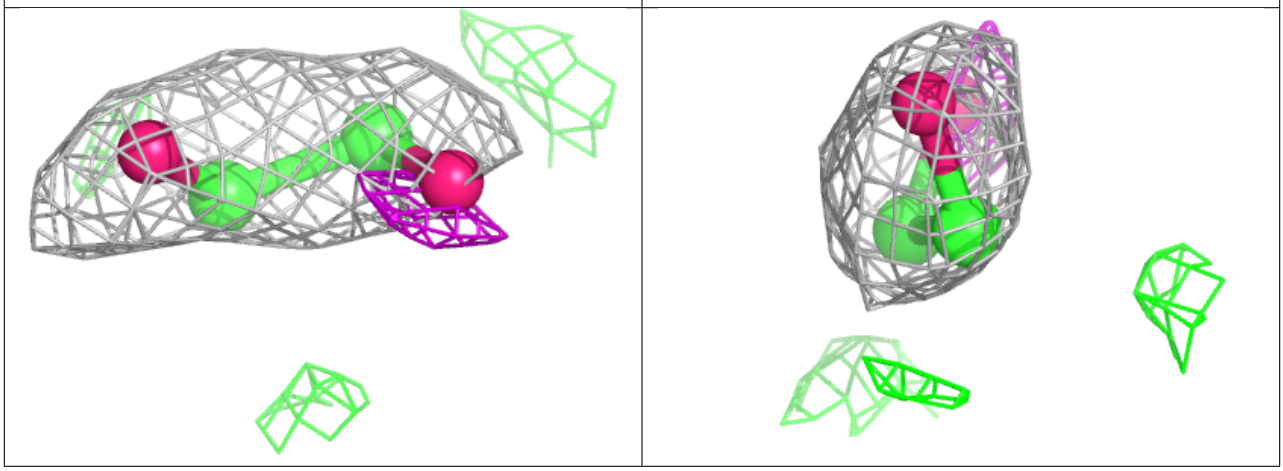
Electron density around MG C 302:

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



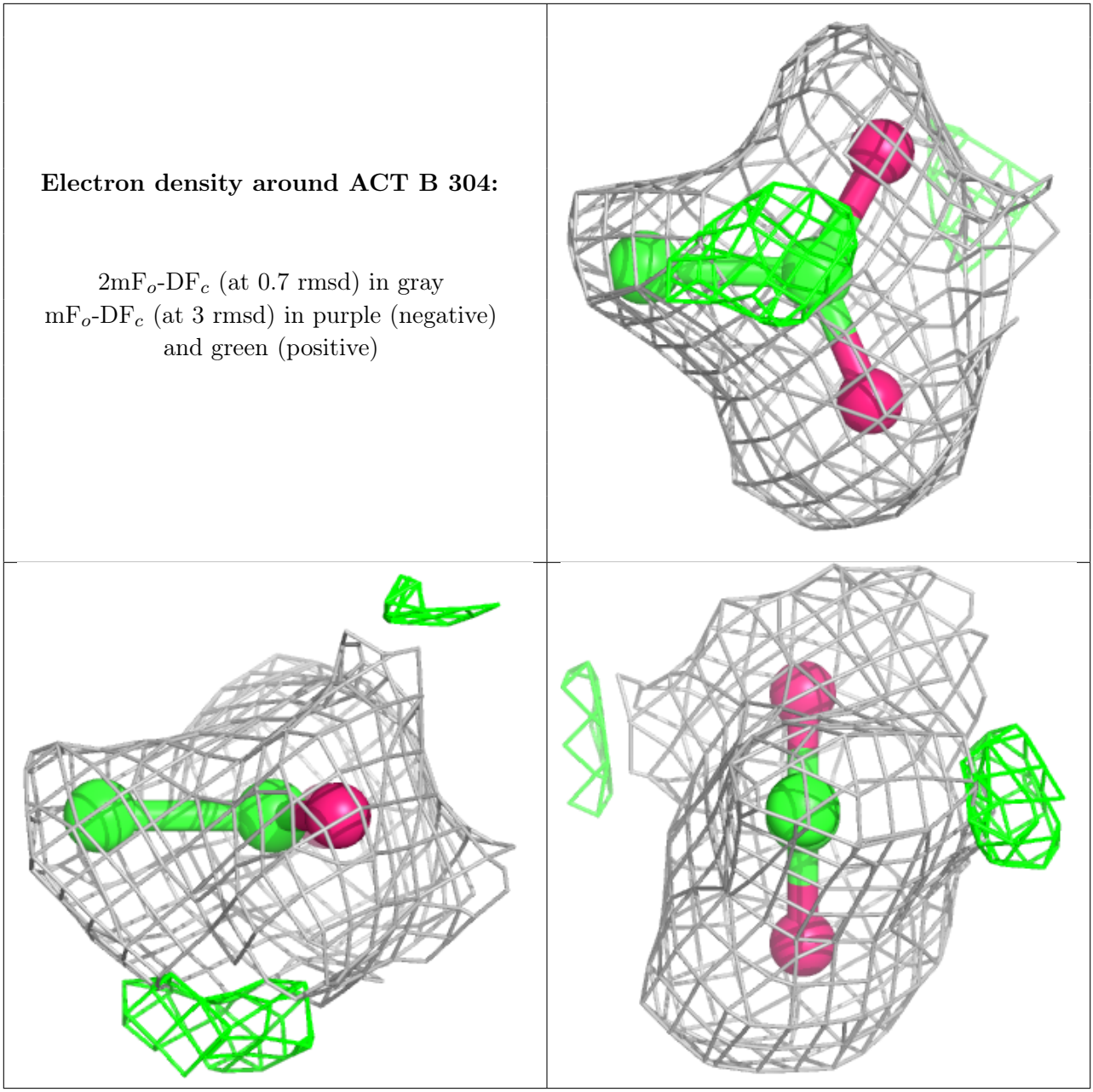
Electron density around EDO C 307:

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



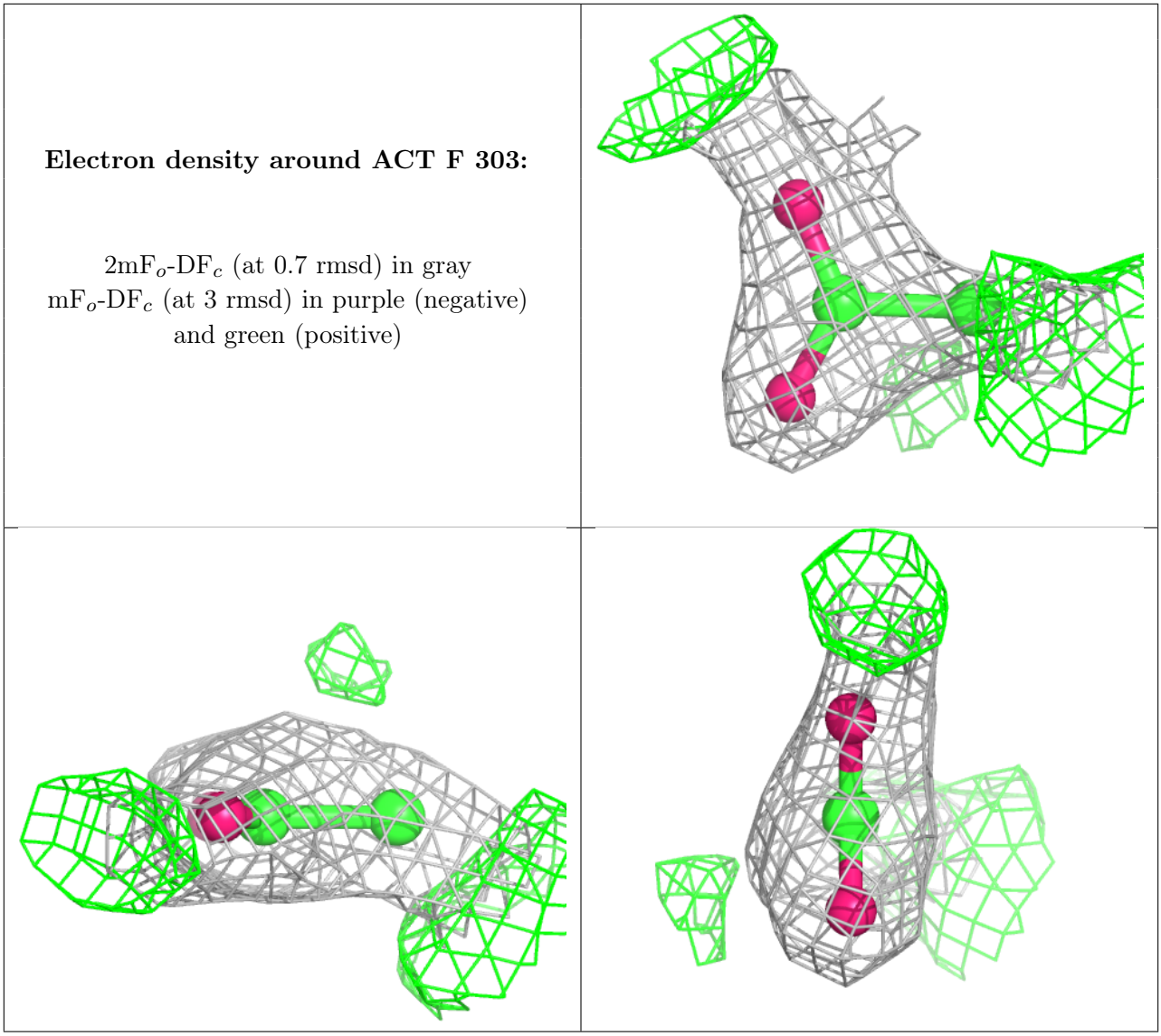
Electron density around ACT B 304:

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



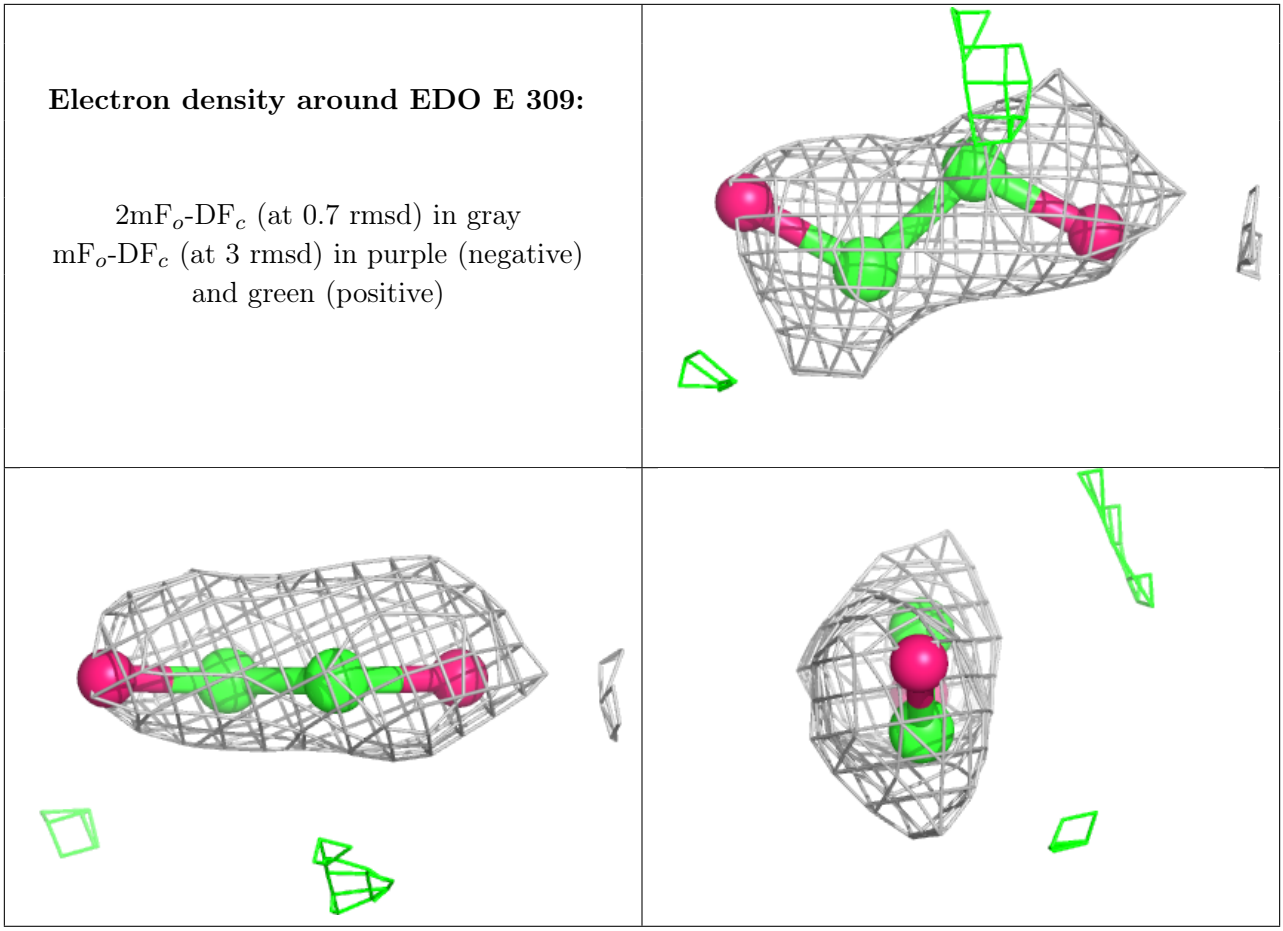
Electron density around ACT F 303:

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



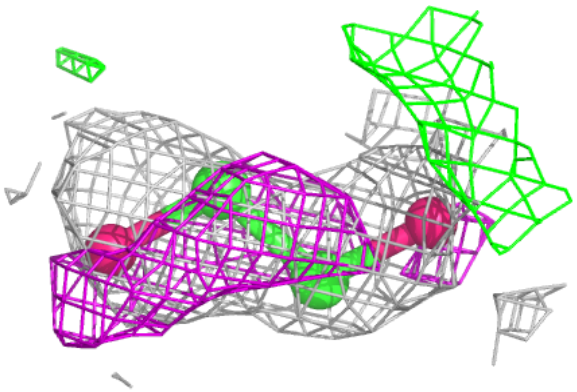
Electron density around EDO E 309:

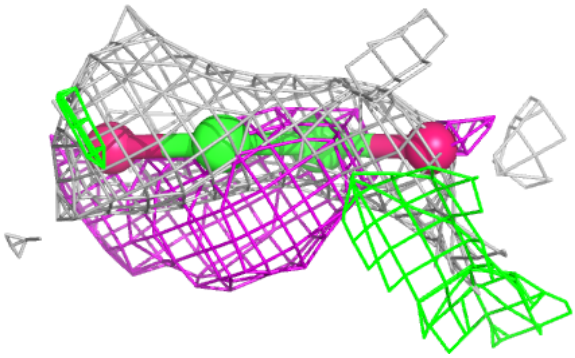
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

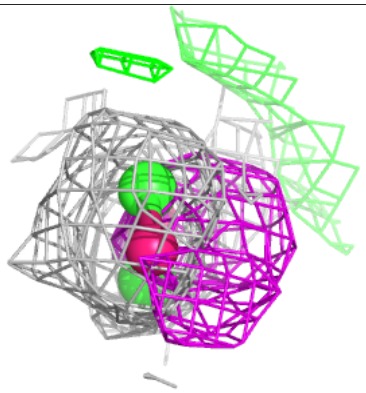


Electron density around EDO D 306:

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

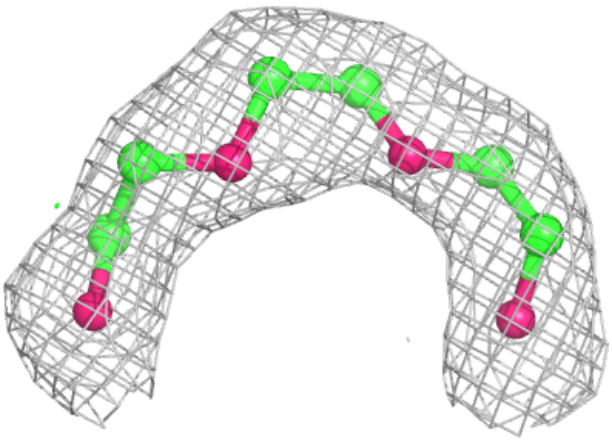


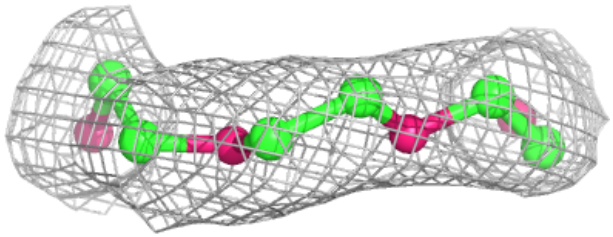


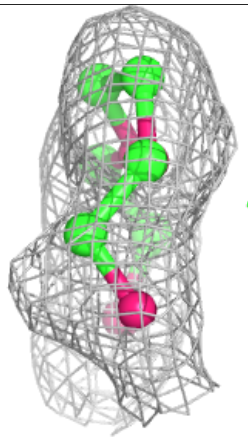


Electron density around PGE D 305:

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

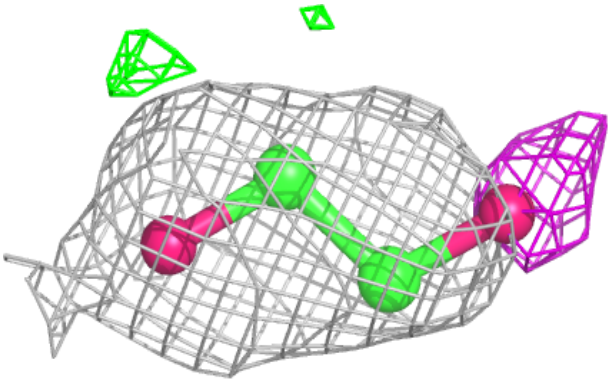


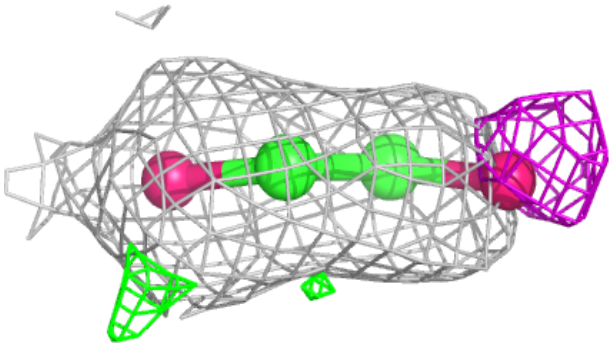


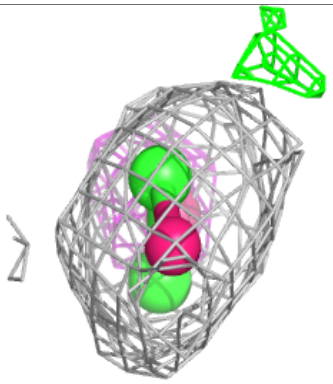


Electron density around EDO D 311:

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

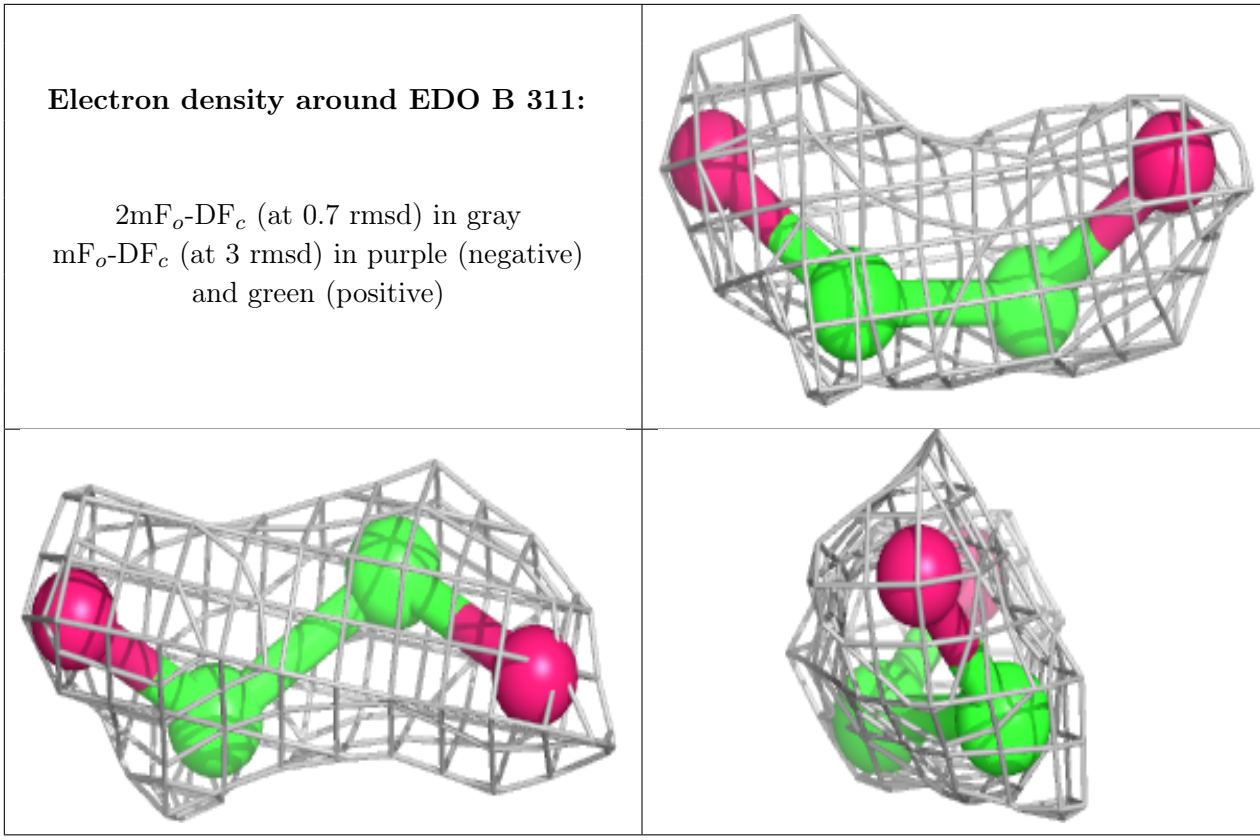






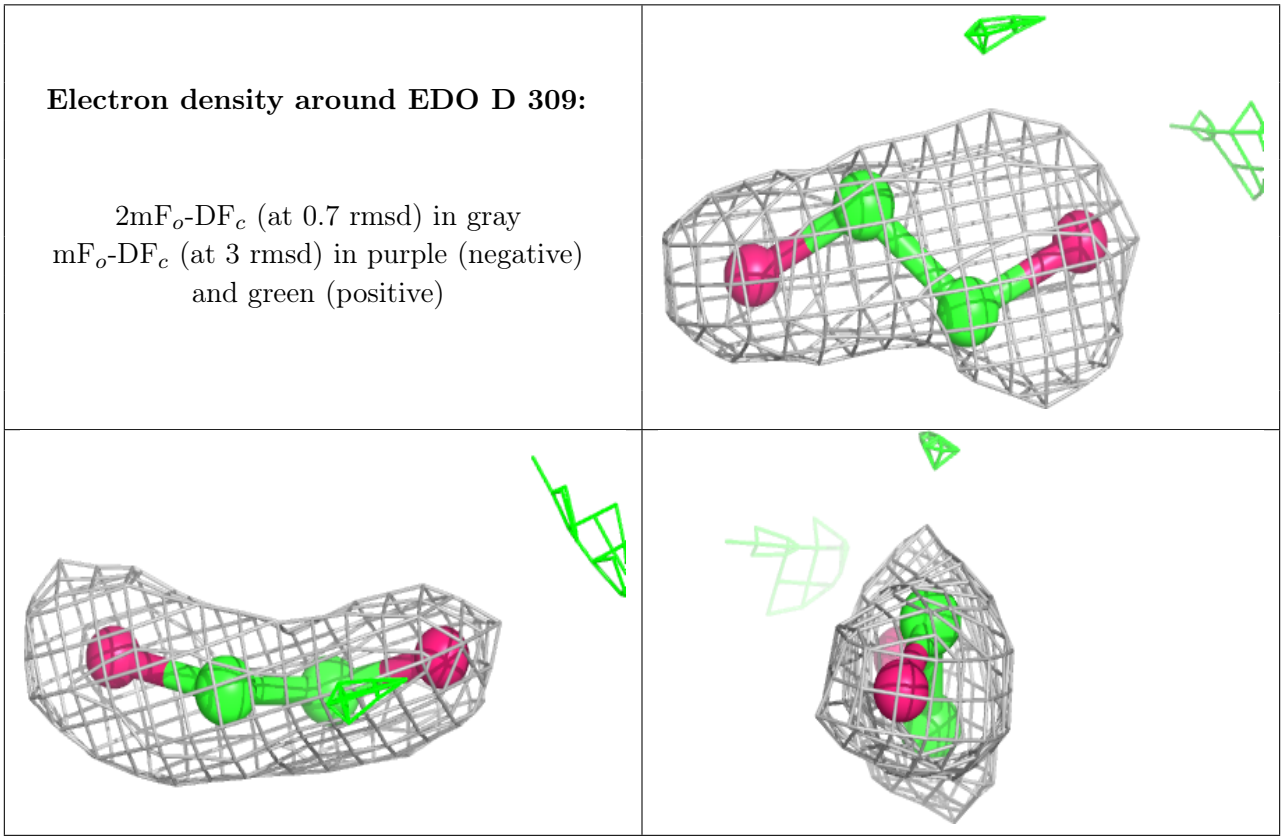
Electron density around EDO B 311:

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



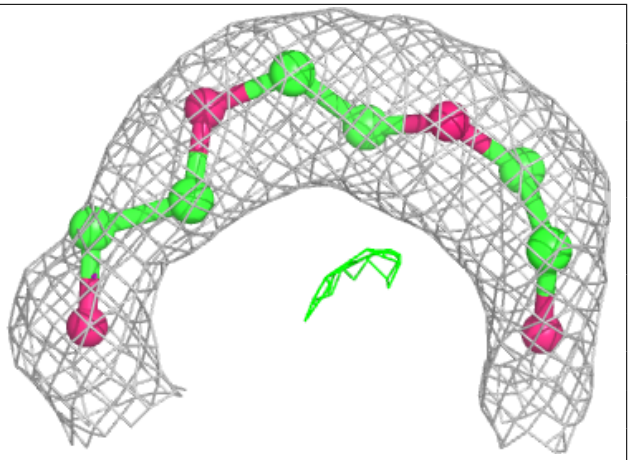
Electron density around EDO D 309:

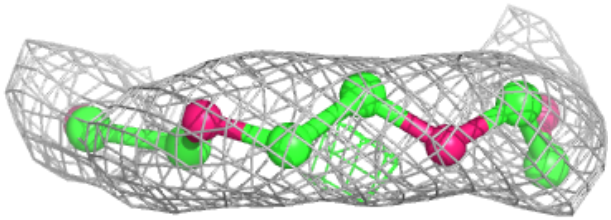
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

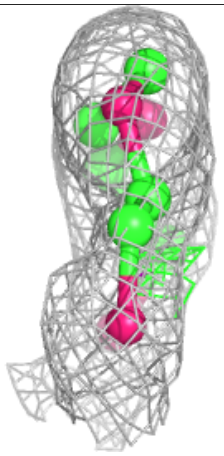


Electron density around PGE C 305:

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

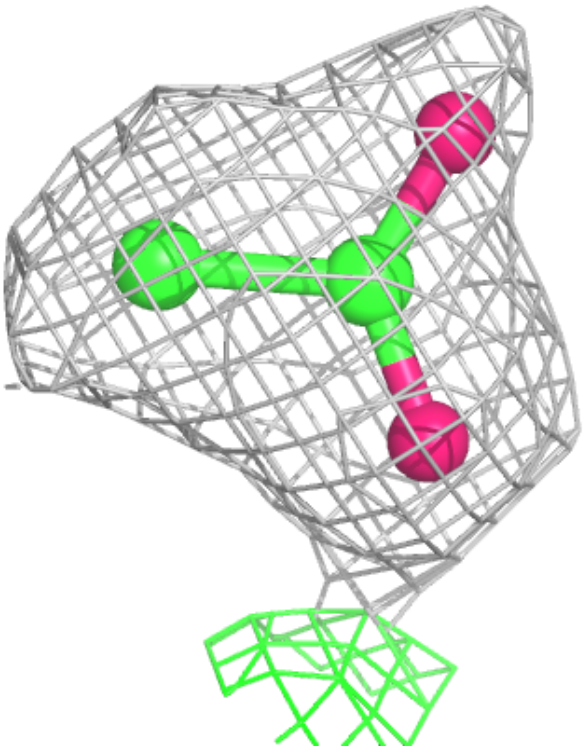


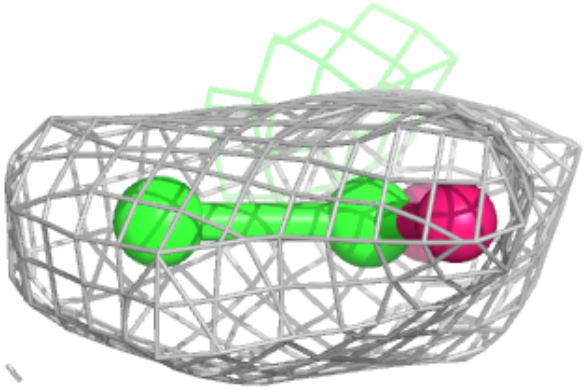


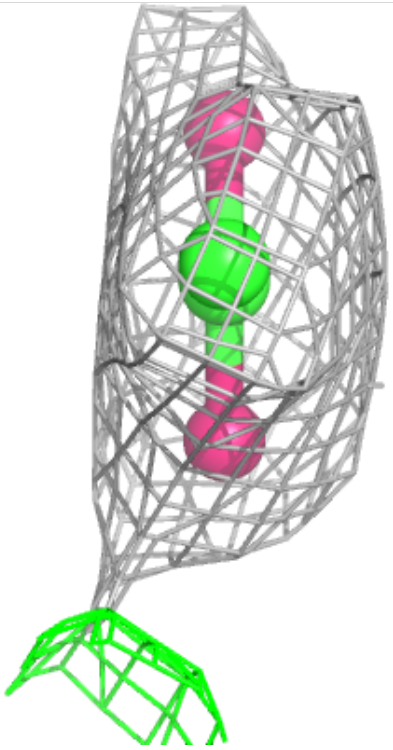


Electron density around ACT D 304:

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

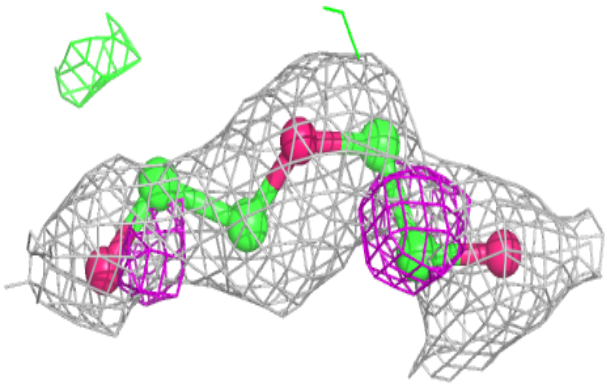


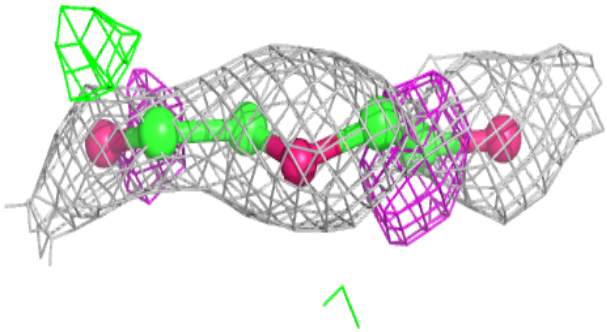


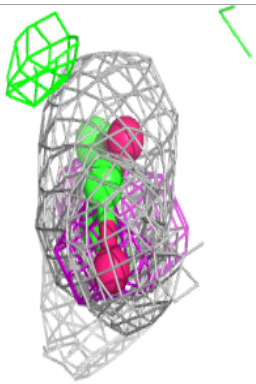


Electron density around PEG E 305:

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

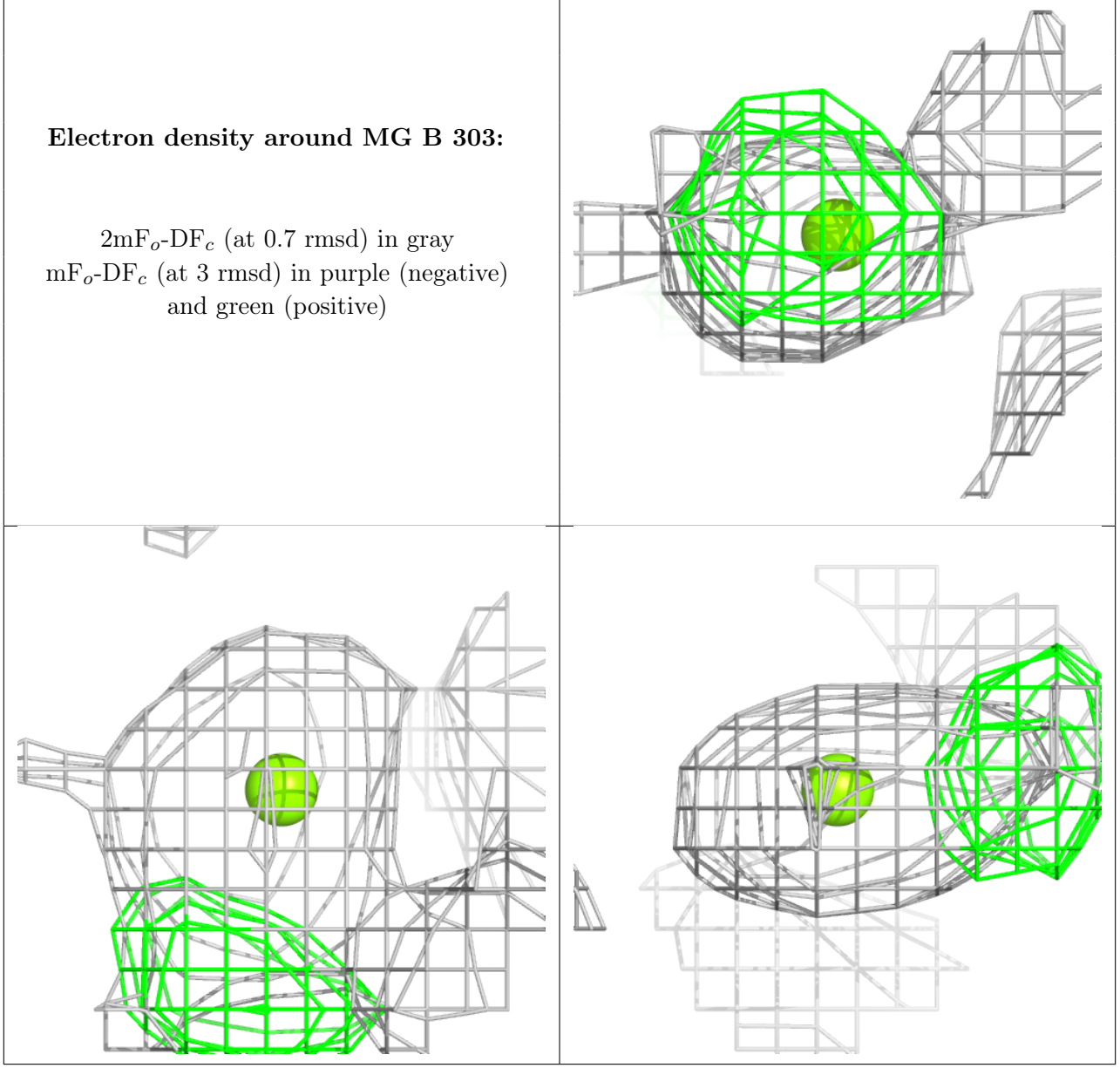






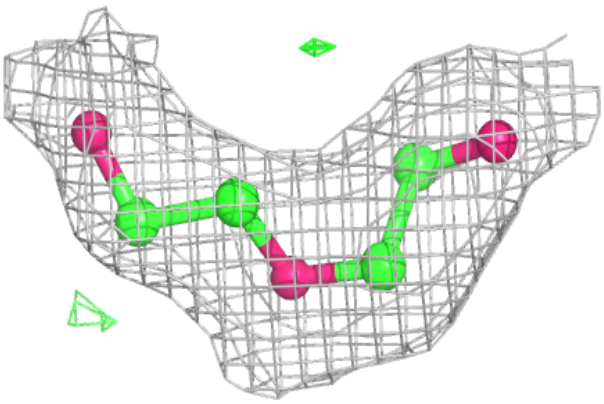
Electron density around MG B 303:

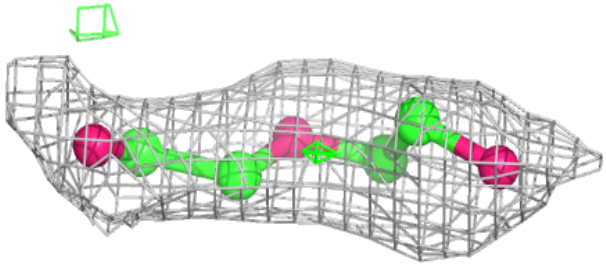
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

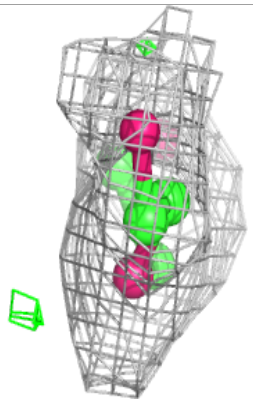


Electron density around PEG B 306:

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

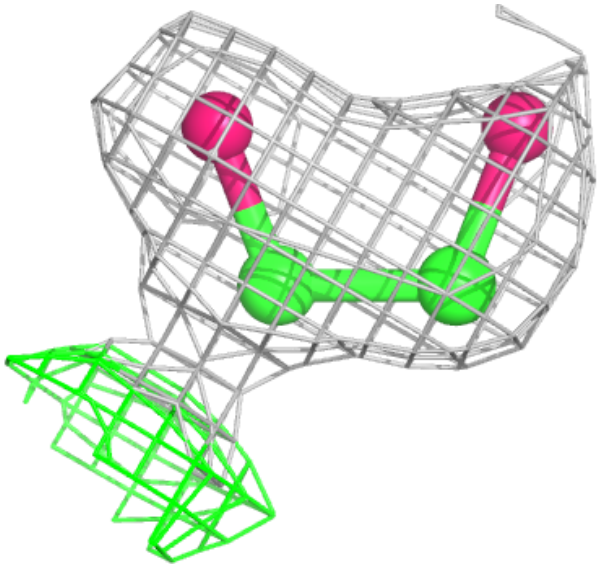


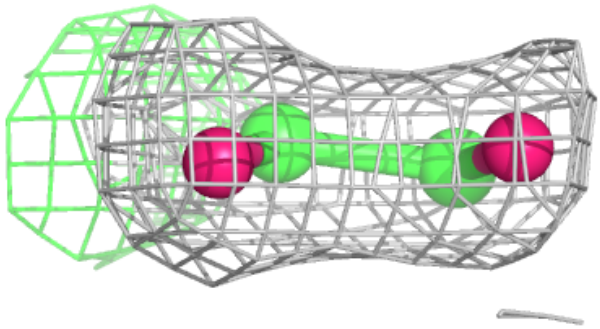


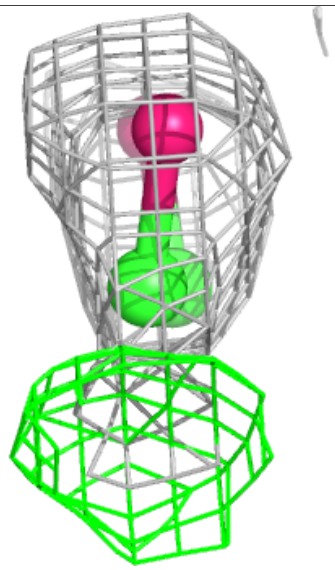


Electron density around EDO A 313:

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

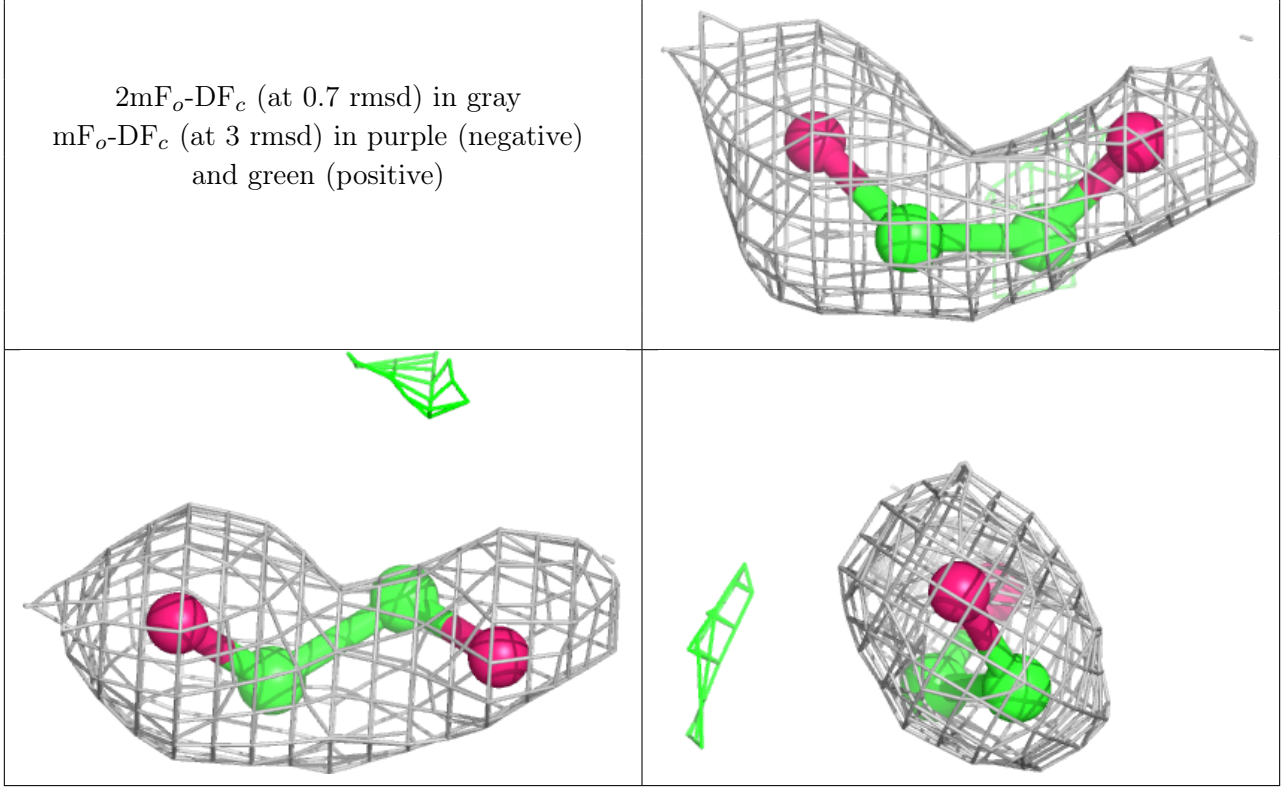






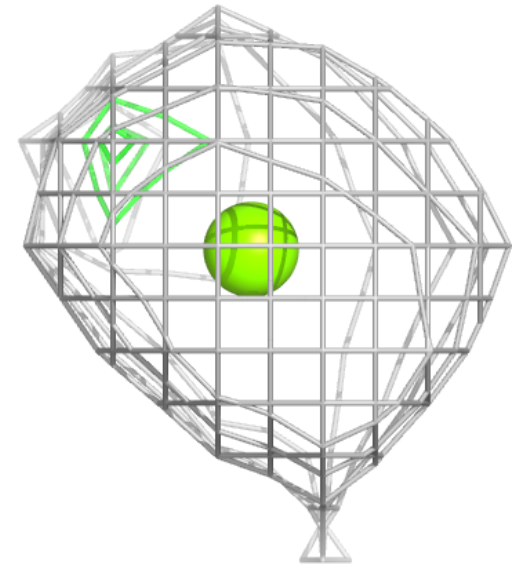
Electron density around EDO B 308:

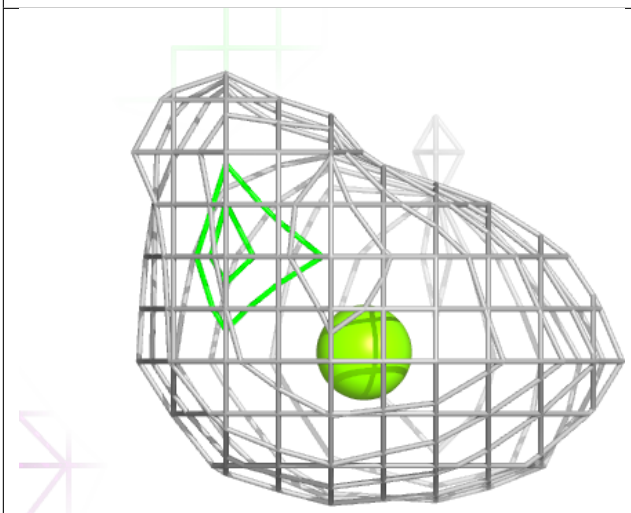
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

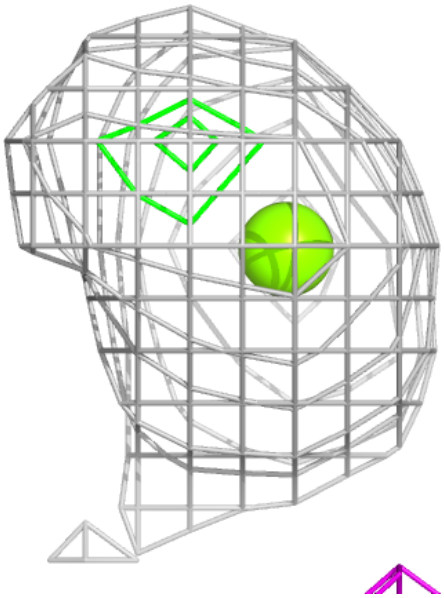


Electron density around MG D 303:

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

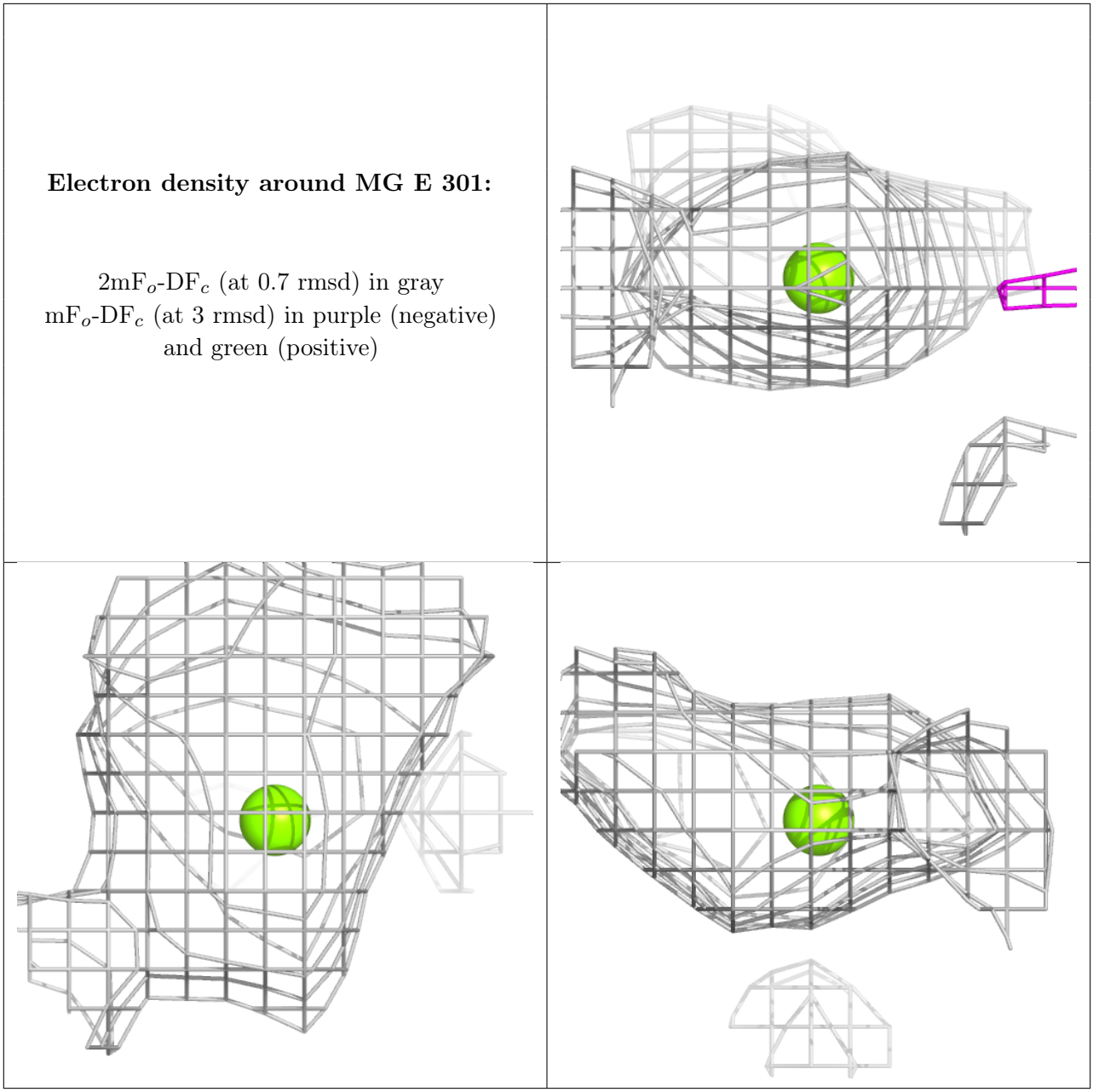






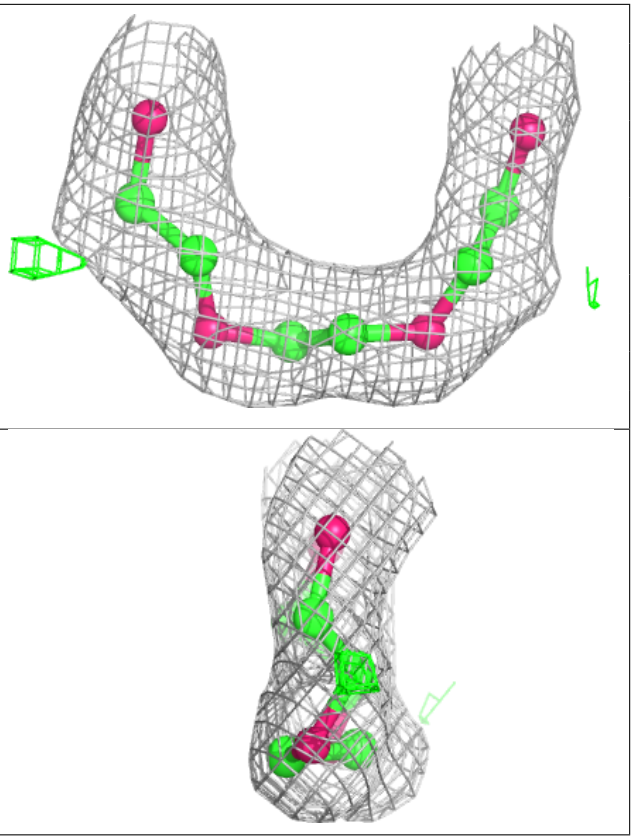
Electron density around MG E 301:

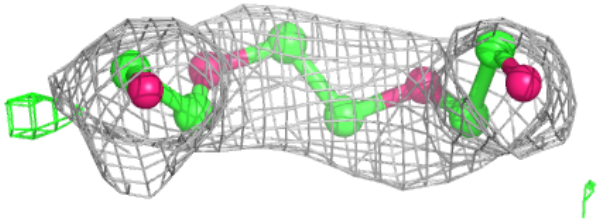
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PGE B 307:

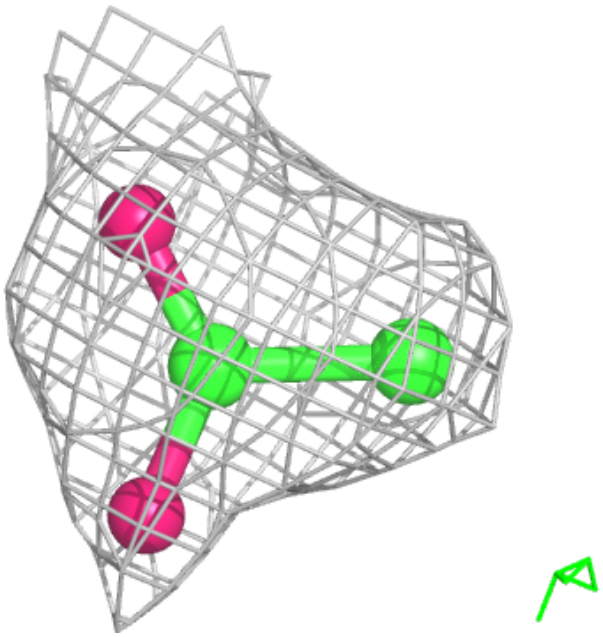
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

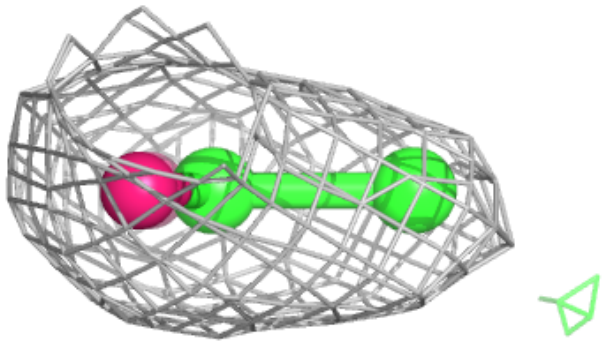


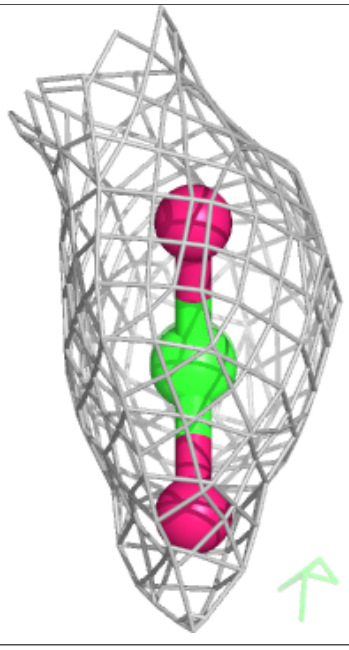


Electron density around ACT A 303:

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

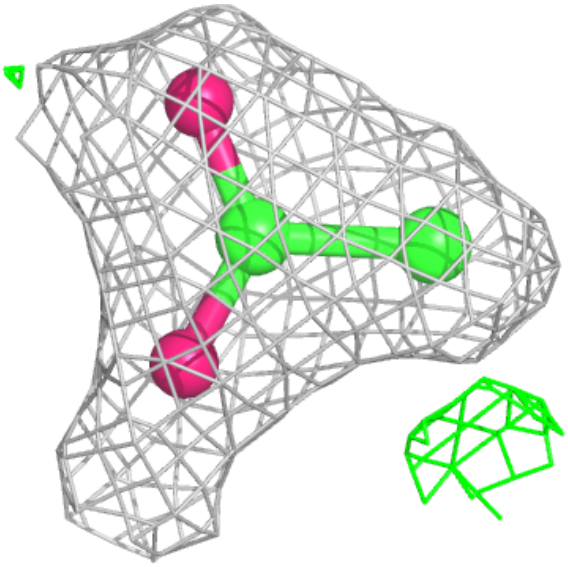


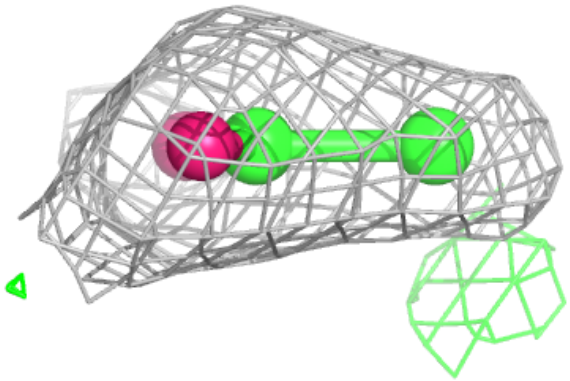


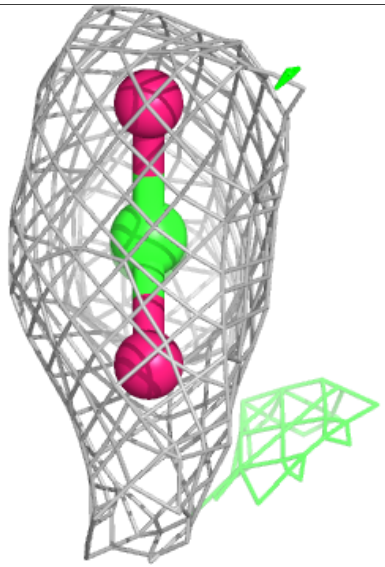


Electron density around ACT C 304:

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

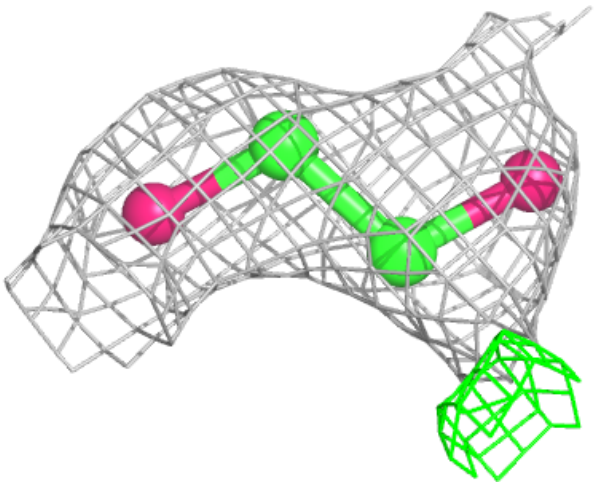


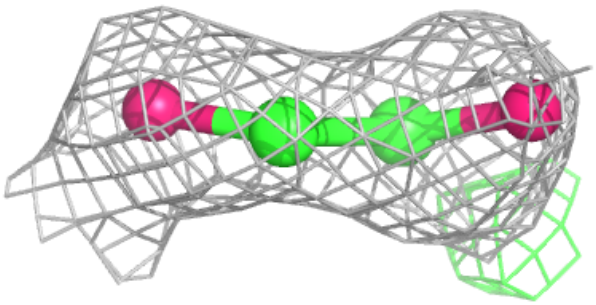


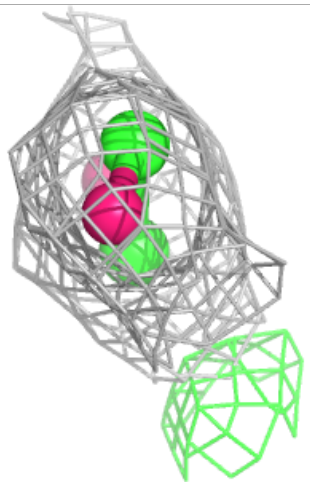


Electron density around EDO D 308:

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

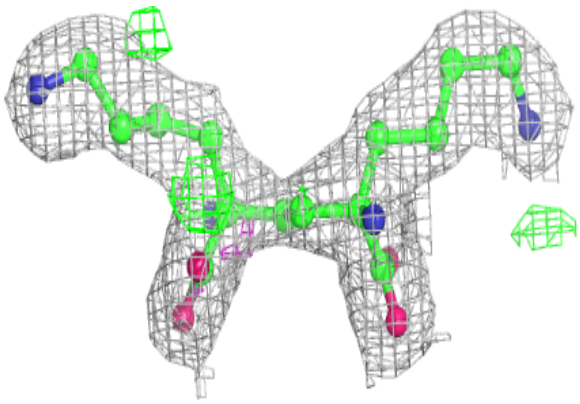


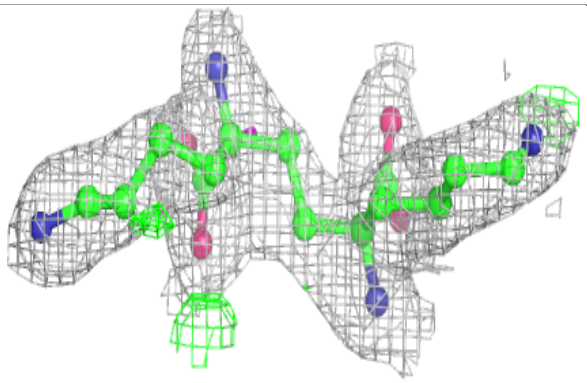


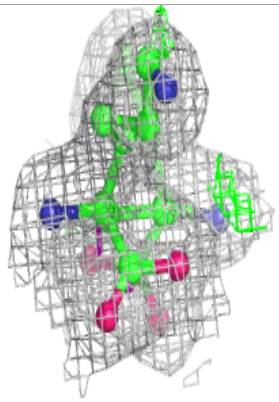


Electron density around 3VN D 301:

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

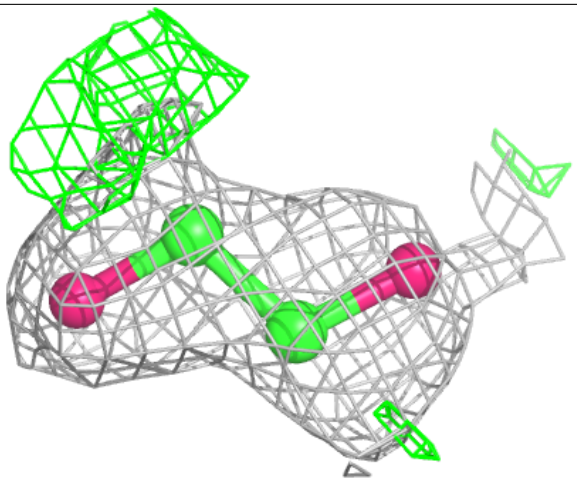


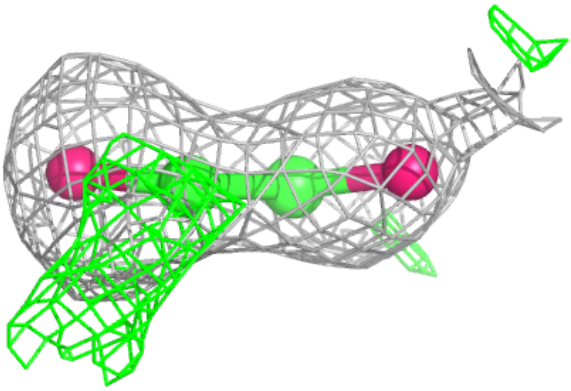


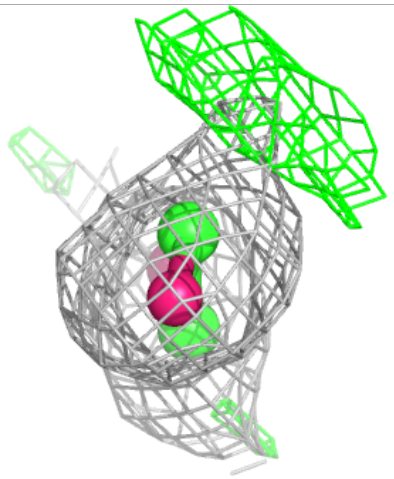


Electron density around EDO D 307:

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

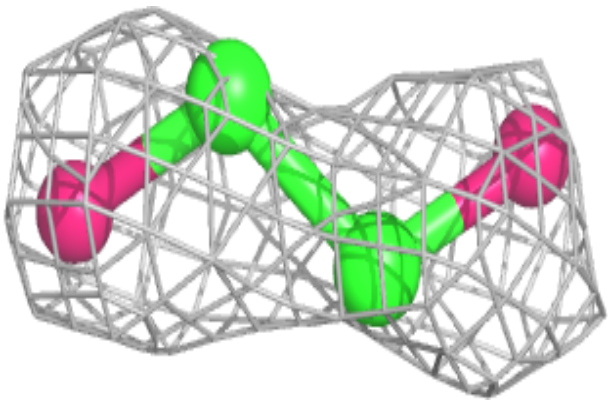


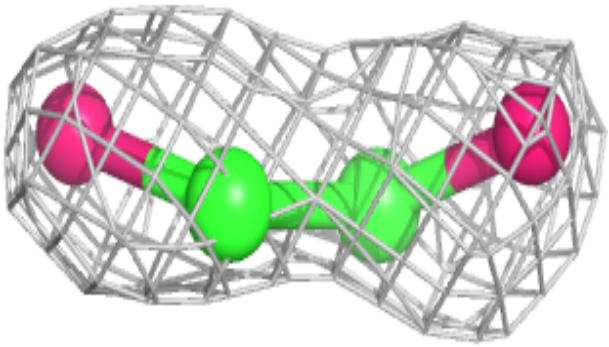


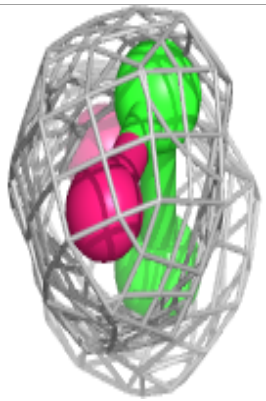


Electron density around EDO A 311:

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

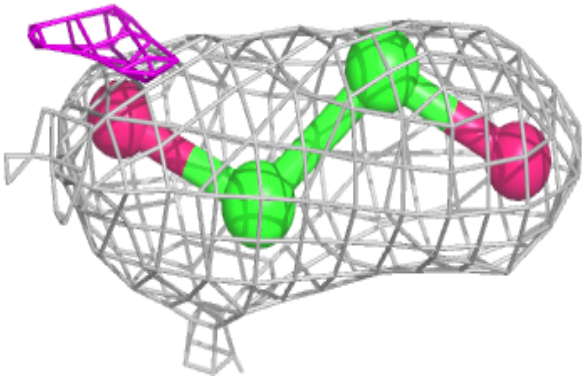


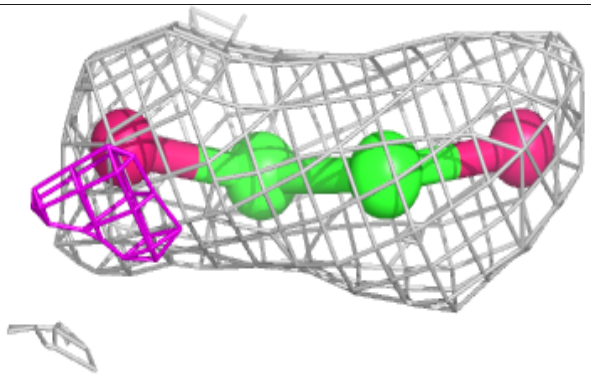


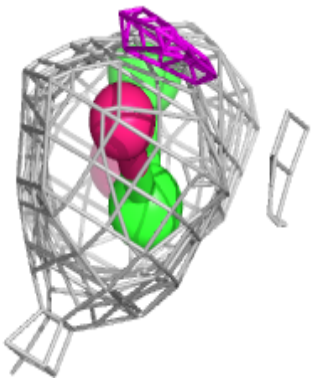


Electron density around EDO A 312:

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

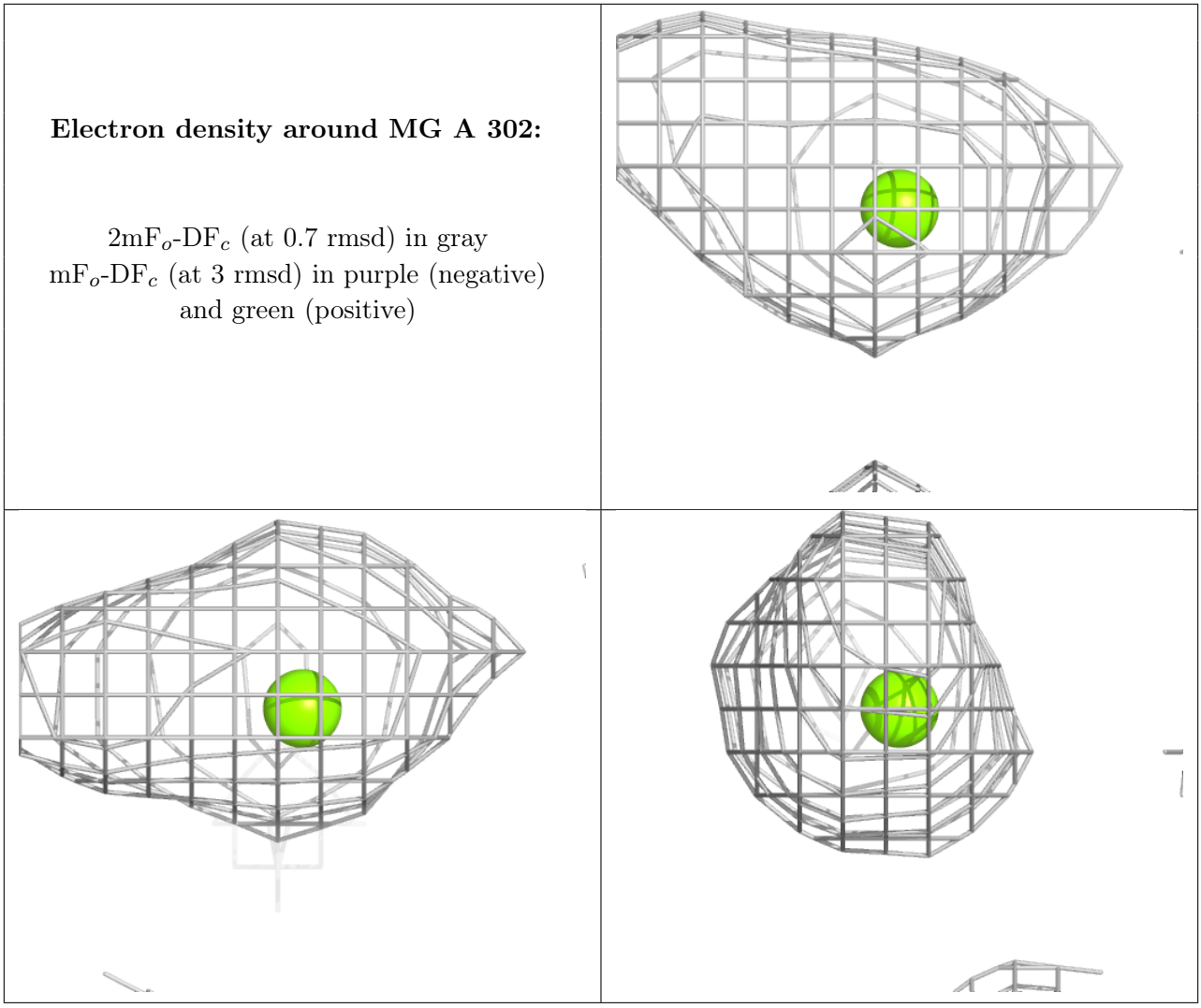






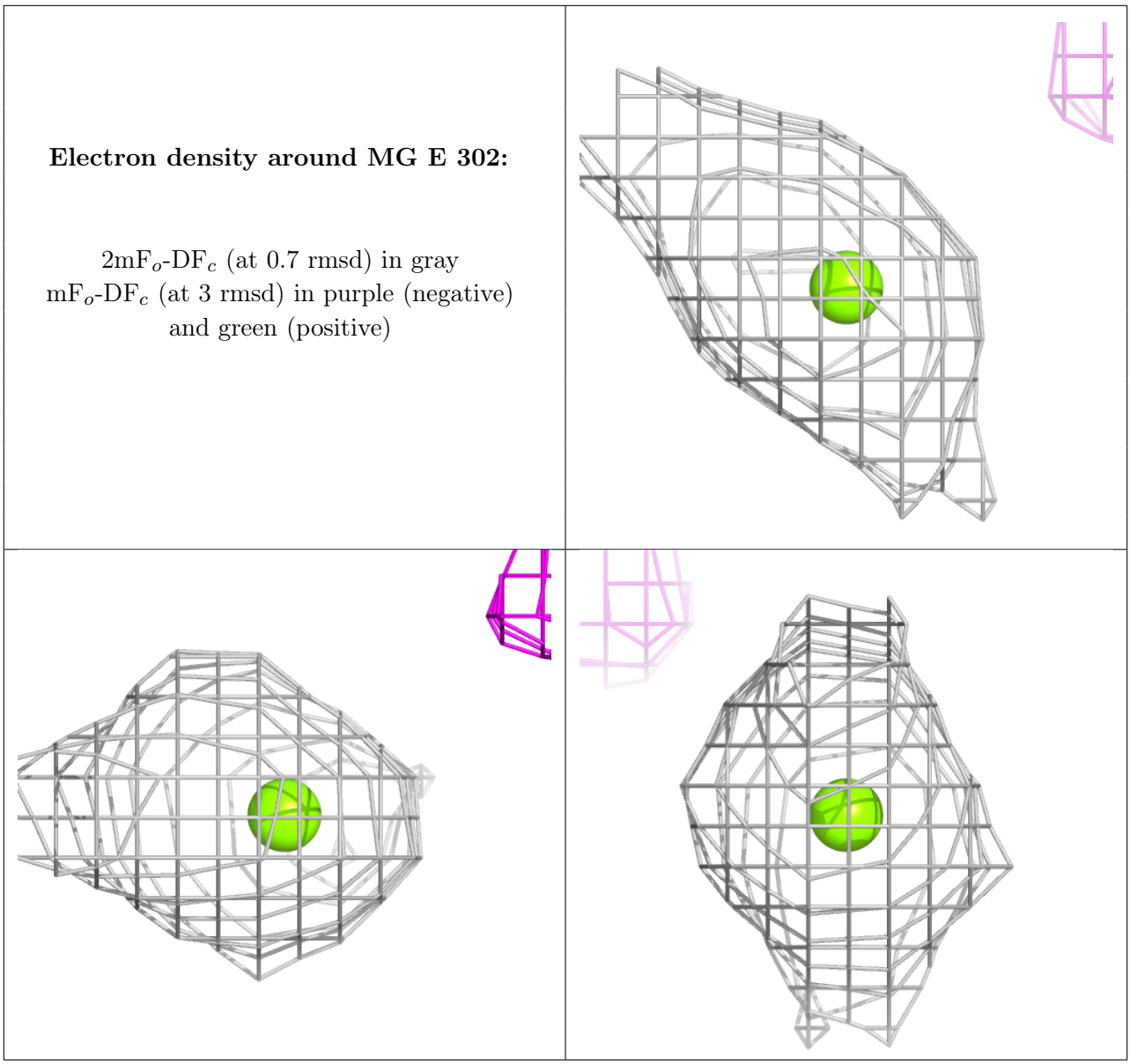
Electron density around MG A 302:

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



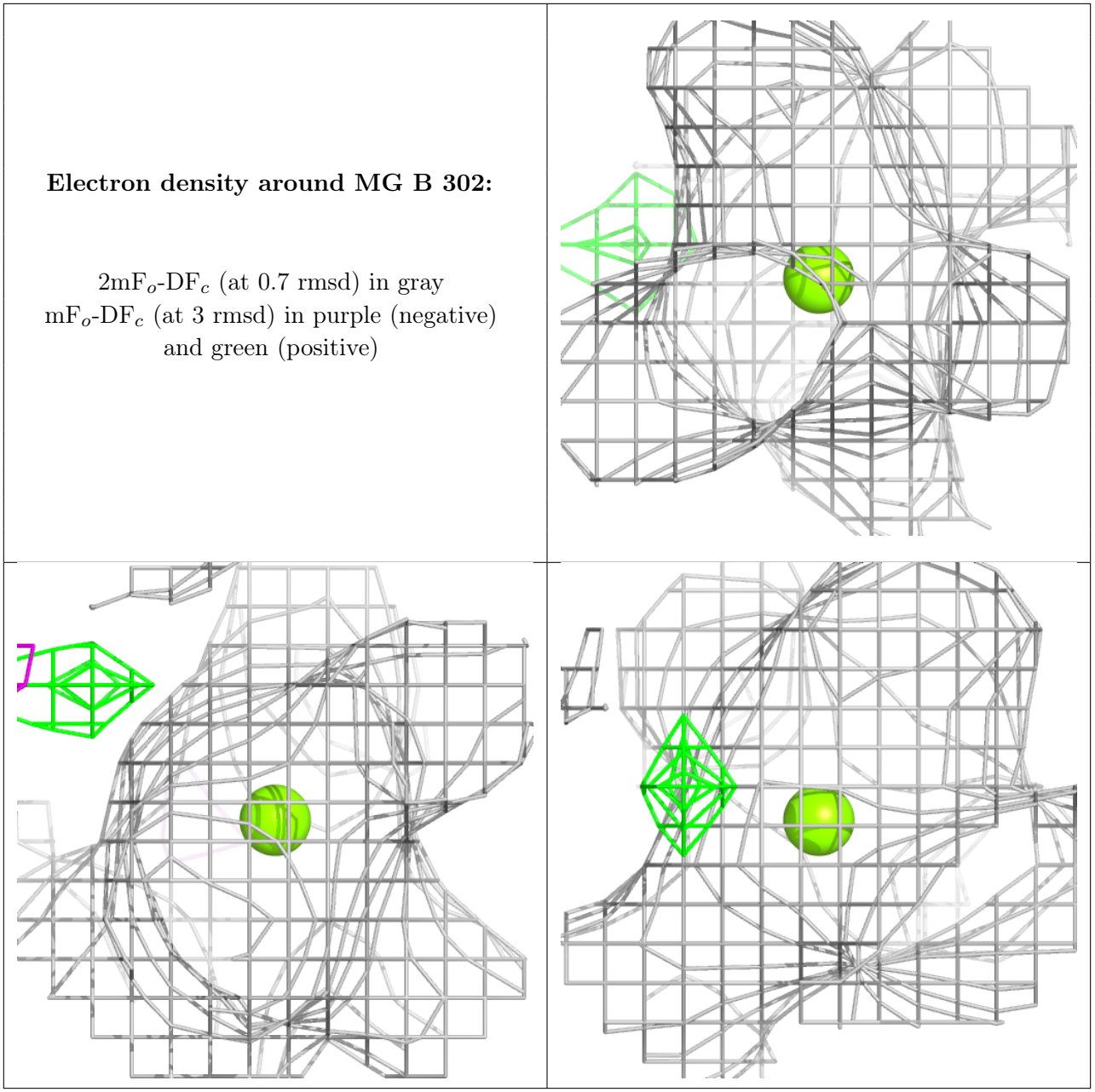
Electron density around MG E 302:

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



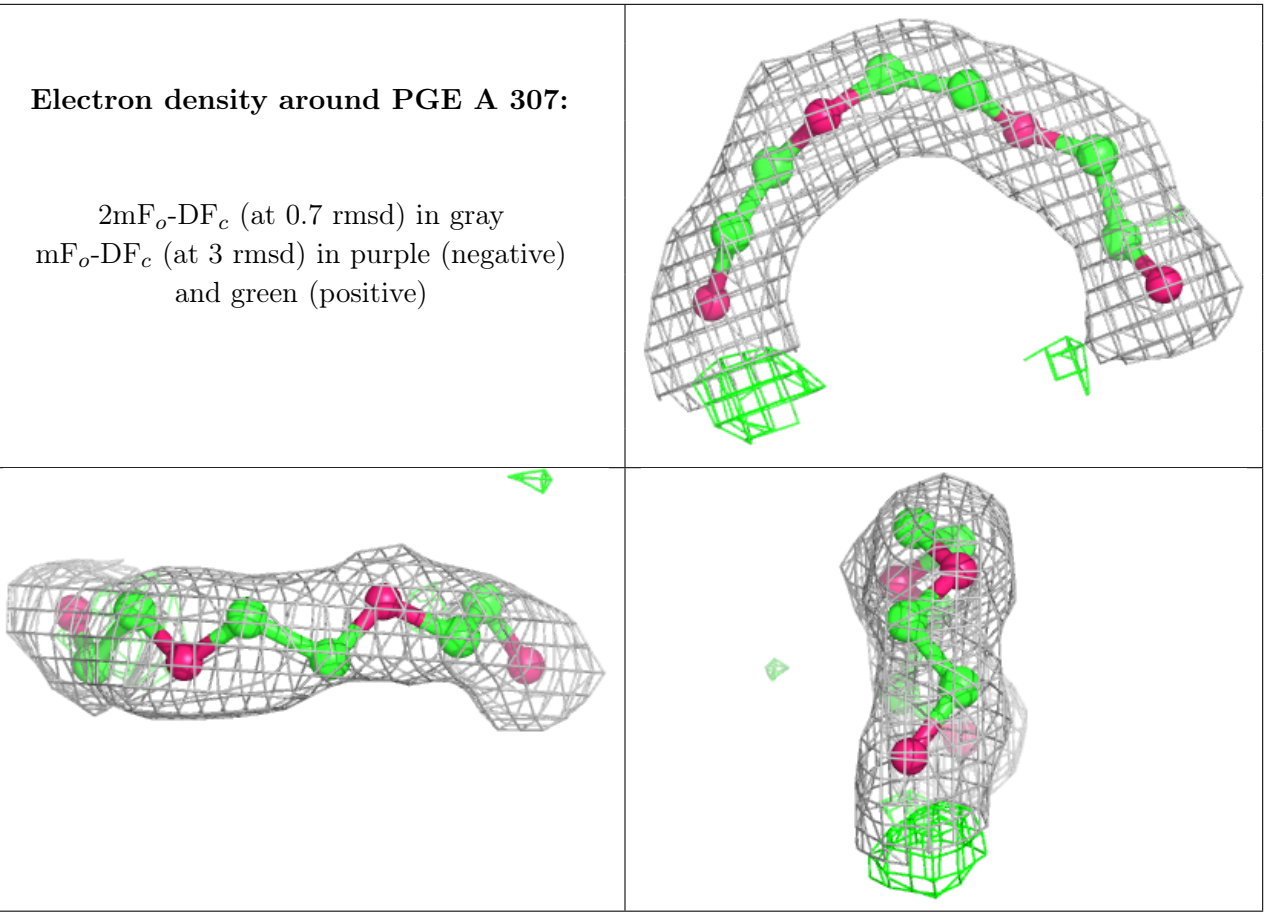
Electron density around MG B 302:

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



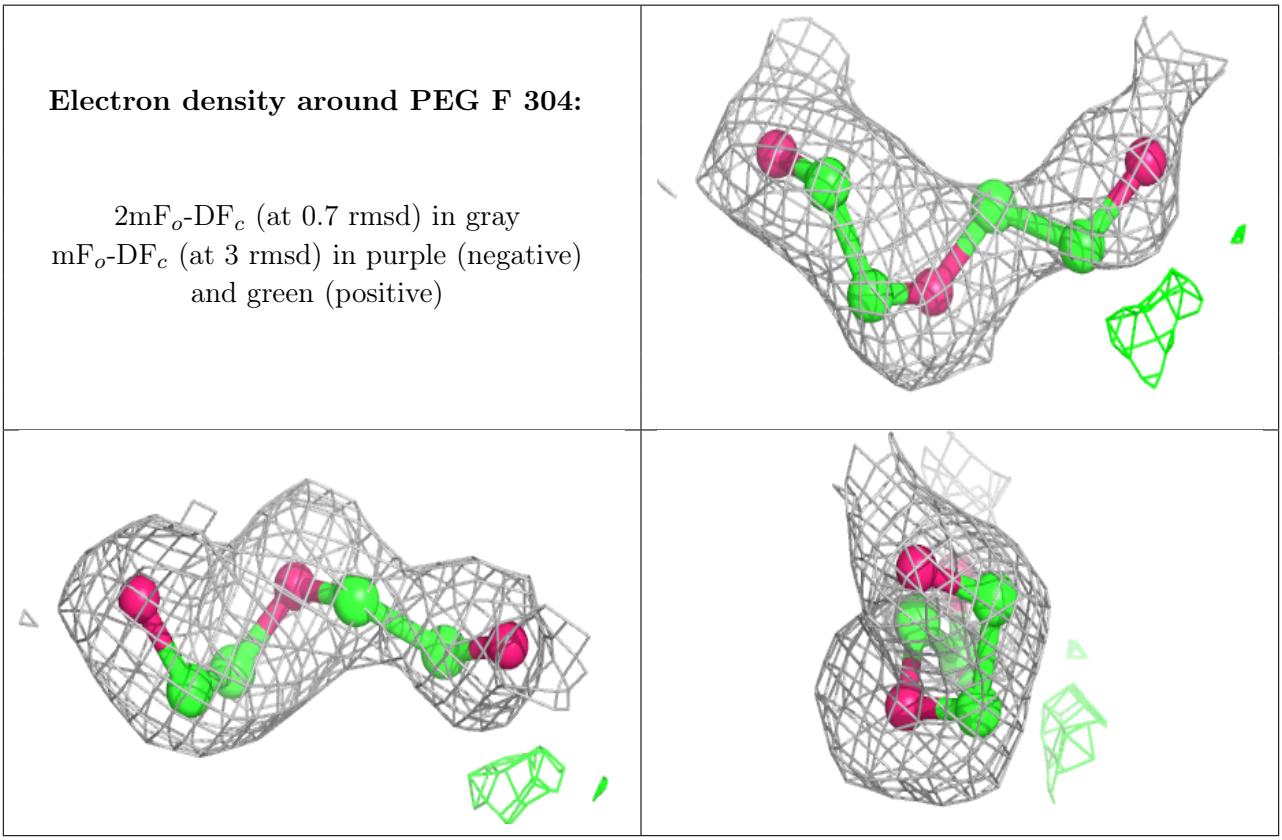
Electron density around PGE A 307:

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



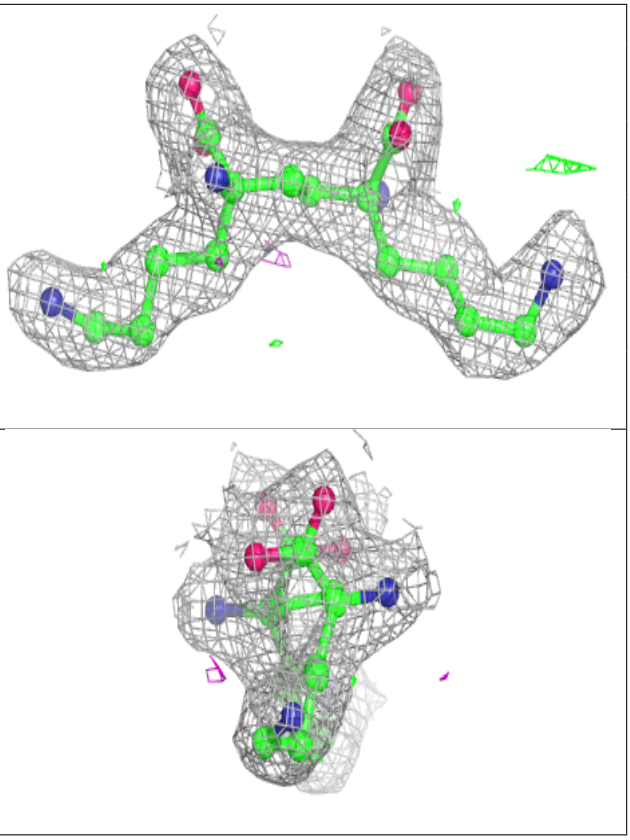
Electron density around PEG F 304:

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



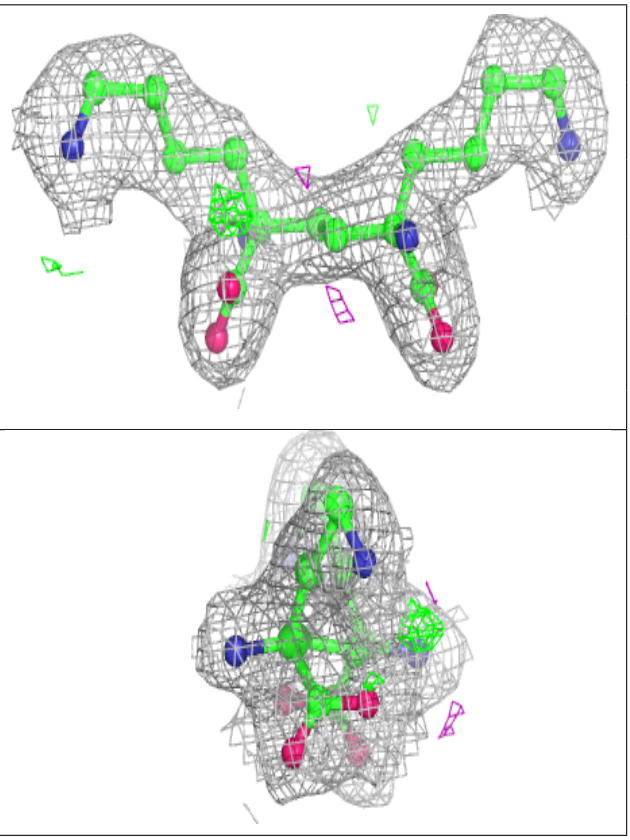
Electron density around 3VN F 301:

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



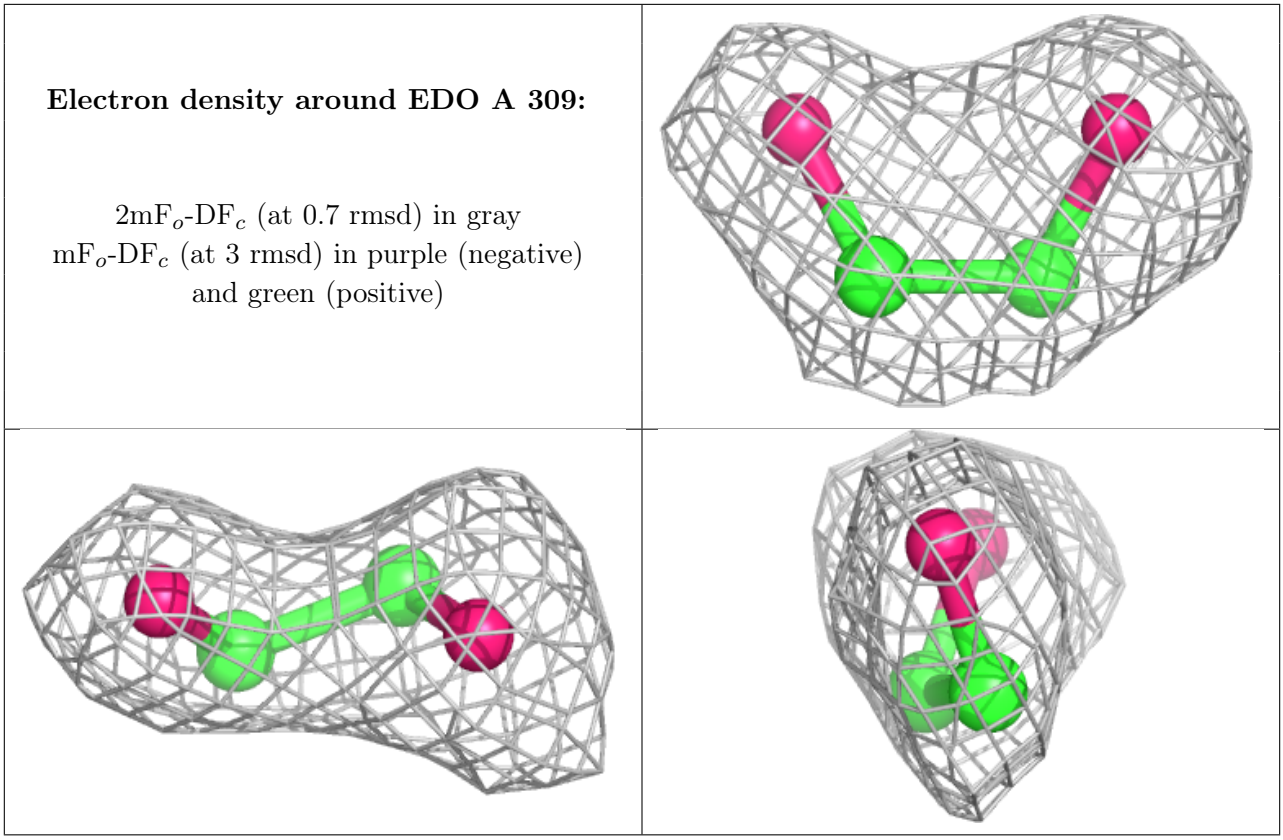
Electron density around 3VN B 301:

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



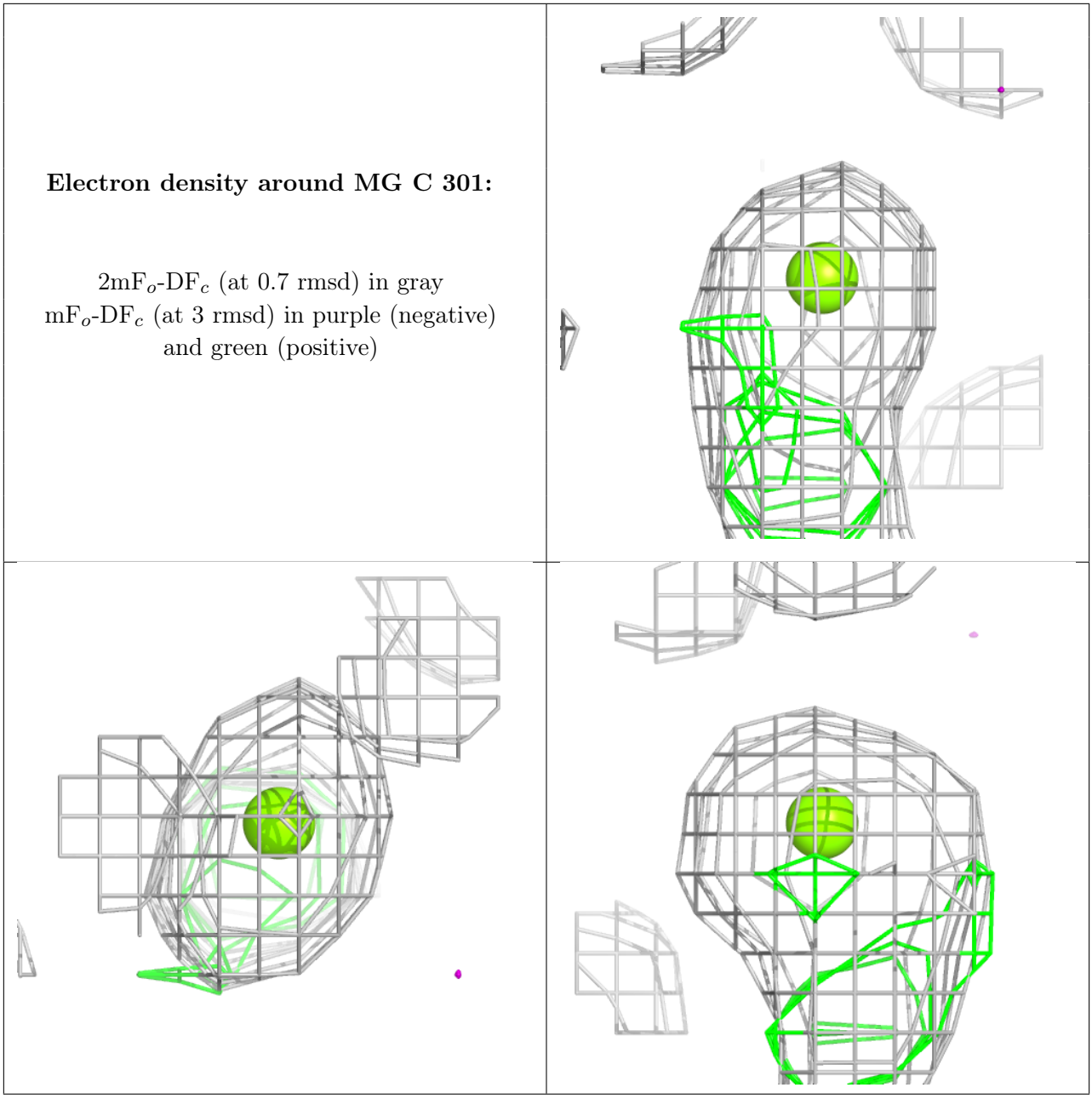
Electron density around EDO A 309:

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



Electron density around MG C 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.