Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:59 PM UTC

PDB ID	:	7KM1 / pdb_00007km1
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H59N mutant with pyruvate bound in the active site and R,R-bislysine bound at the allosteric site
Authors	:	Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.
Deposited on	:	2020-11-02
Resolution	:	1.84 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:

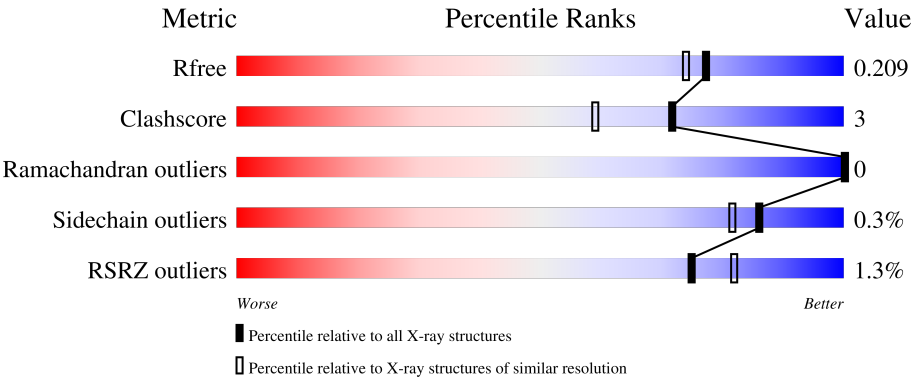
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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

Mol	Chain	Length	Quality of chain
1	A	310	87% 8% 5%
1	B	310	% 89% 5% • 5%
1	C	310	% 91% • 5%
1	D	310	2% 90% 5% 5%

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Mol	Chain	Length	Quality of chain
1	E	310	2% 90% 5% 5%
1	F	310	2% 88% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	F	301	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14728 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
			2278	1448	378	439	13			
1	B	296	Total	C	N	O	S	0	1	0
			2281	1449	379	440	13			
1	C	296	Total	C	N	O	S	0	0	0
			2278	1448	378	439	13			
1	D	296	Total	C	N	O	S	0	2	0
			2285	1451	379	442	13			
1	E	296	Total	C	N	O	S	0	0	0
			2278	1448	378	439	13			
1	F	297	Total	C	N	O	S	0	1	0
			2291	1454	383	441	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	59	ASN	HIS	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

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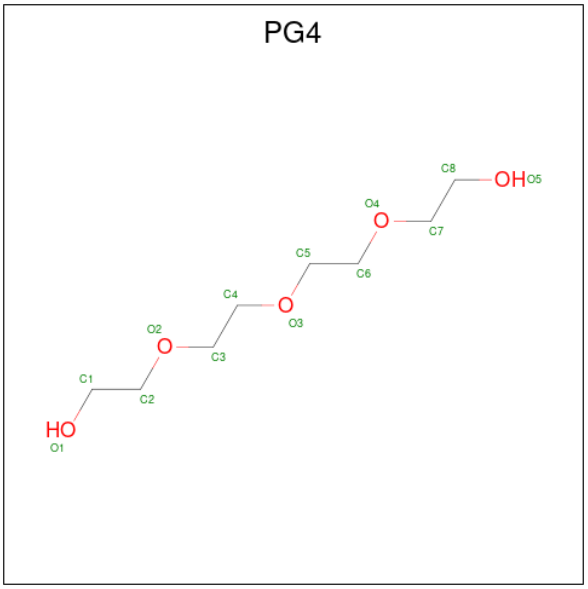
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	59	ASN	HIS	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	59	ASN	HIS	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	59	ASN	HIS	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	59	ASN	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	59	ASN	HIS	engineered mutation	UNP Q9PPB4

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



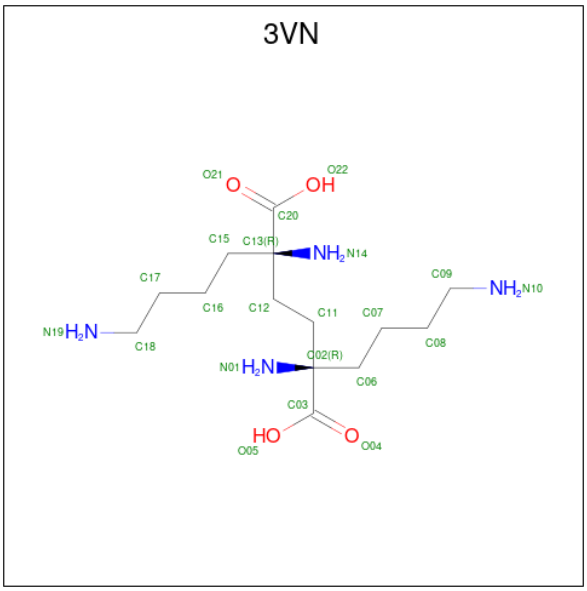
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0

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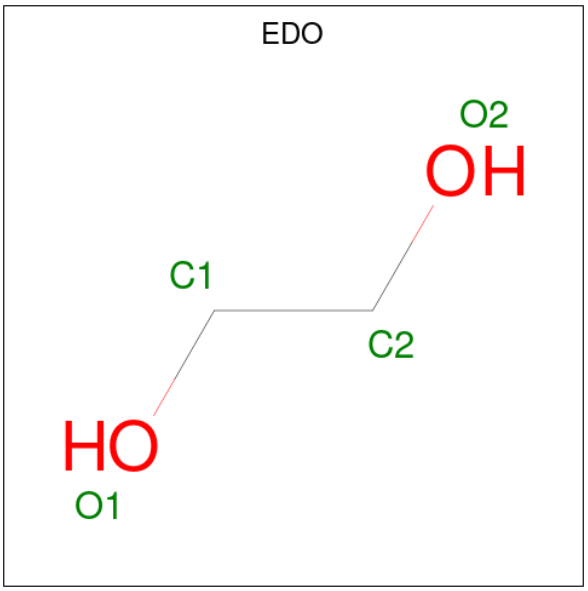
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0
2	C	1	Total C O 13 8 5	0	0
2	E	1	Total C O 13 8 5	0	0
2	F	1	Total C O 13 8 5	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 22 14 4 4	0	0
3	C	1	Total C N O 22 14 4 4	0	0
3	F	1	Total C N O 22 14 4 4	0	0

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



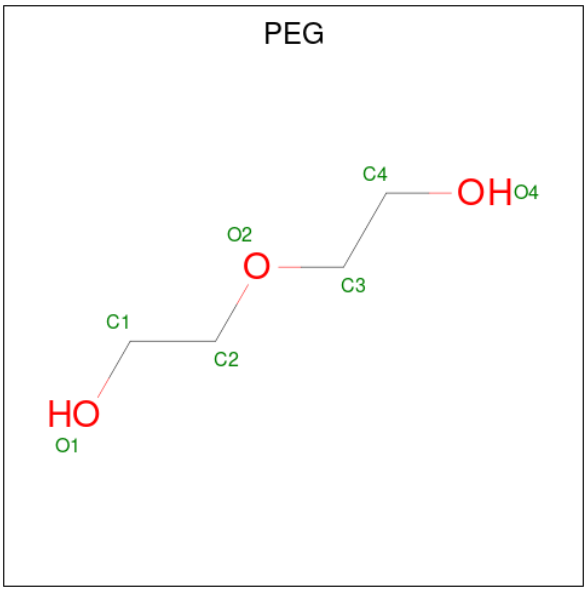
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



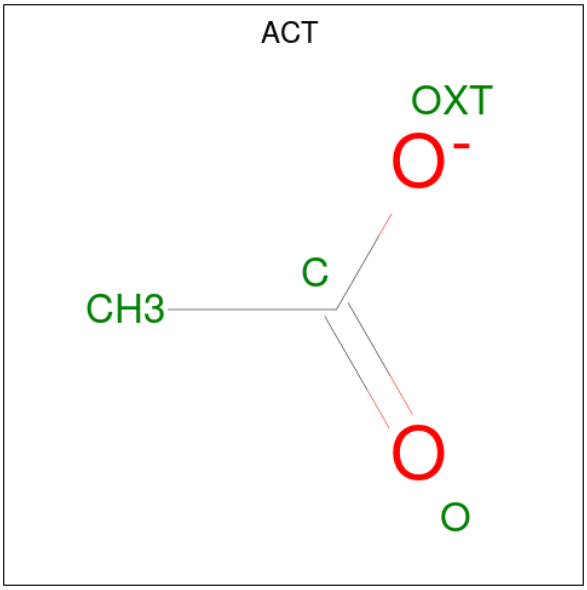
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

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

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



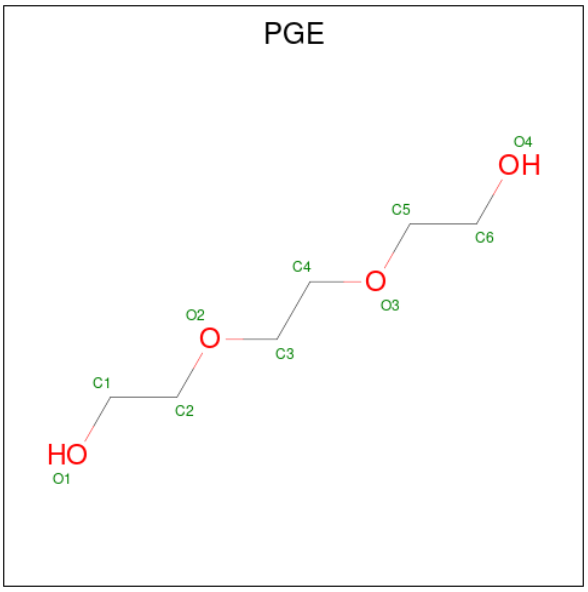
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0

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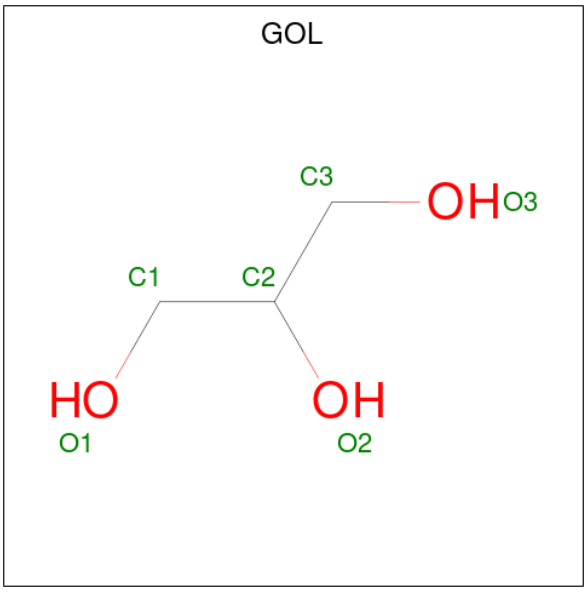
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

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



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

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



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

- Molecule 10 is water.

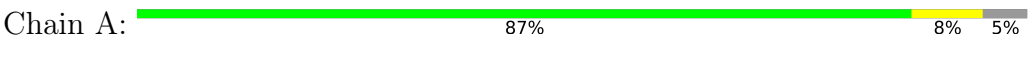
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	127	Total O 127 127	0	0
10	B	111	Total O 111 111	0	0
10	C	115	Total O 115 115	0	0
10	D	114	Total O 114 114	0	0
10	E	96	Total O 96 96	0	0
10	F	124	Total O 124 124	0	0

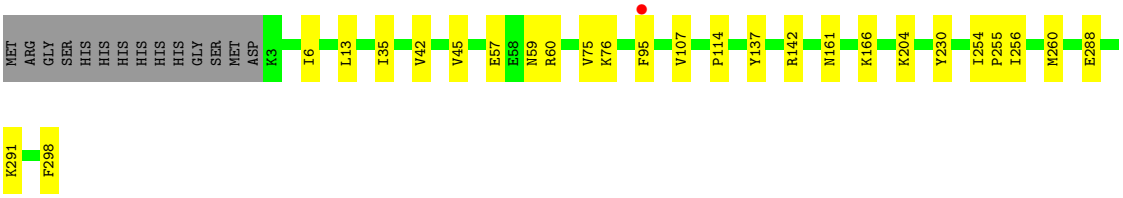
3 Residue-property plots (i)

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

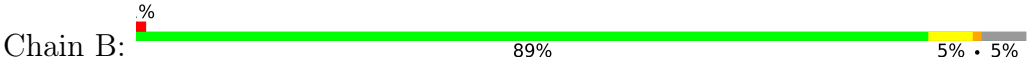
Chain A:

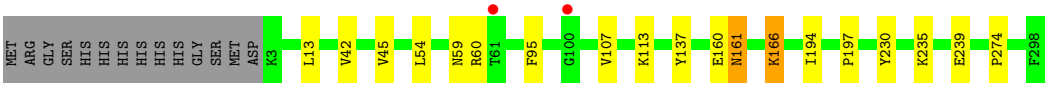




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

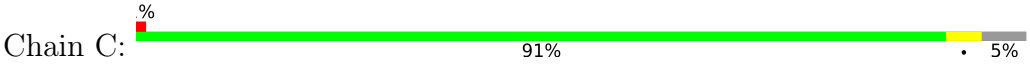
Chain B:

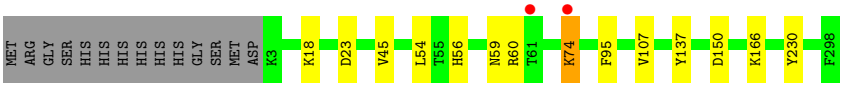




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

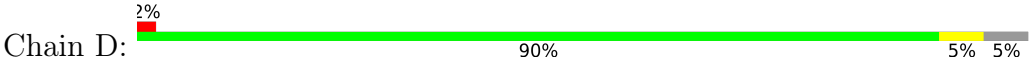
Chain C:

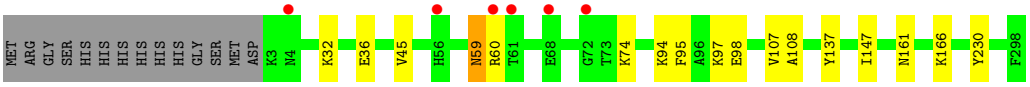




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

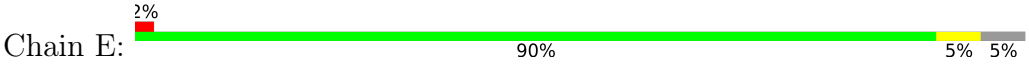
Chain D:

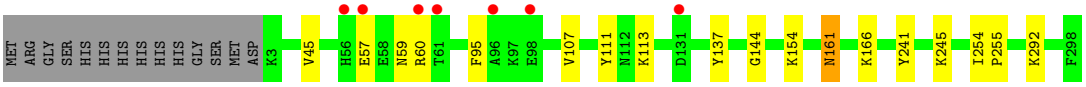




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:

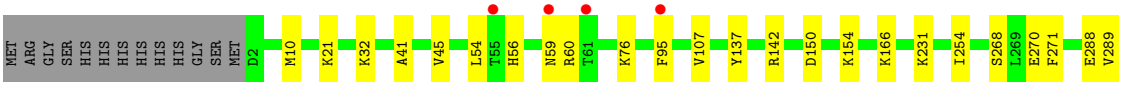




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

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	85.01Å 230.45Å 200.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 1.84 49.56 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.56-1.84) 98.6 (49.56-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.84Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.181 , 0.211 (Not available) , 0.209	Depositor DCC
R_{free} test set	8382 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14728	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.17	0/2301	0.42	0/3109
1	B	0.34	0/2309	0.43	0/3120
1	C	0.26	0/2301	0.43	0/3109
1	D	0.31	0/2318	0.45	0/3132
1	E	0.20	0/2301	0.45	1/3109 (0.0%)
1	F	0.27	1/2319 (0.0%)	0.43	1/3134 (0.0%)
All	All	0.27	1/13849 (0.0%)	0.43	2/18713 (0.0%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	289	VAL	C-O	-5.26	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	57	GLU	CB-CA-C	-5.03	102.98	110.88
1	F	21	LYS	CG-CD-CE	-5.03	99.73	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	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	2278	0	2318	23	0
1	B	2281	0	2320	15	0
1	C	2278	0	2318	13	0
1	D	2285	0	2318	16	0
1	E	2278	0	2318	12	0
1	F	2291	0	2331	22	0
2	A	26	0	36	2	0
2	C	13	0	18	0	0
2	E	13	0	18	1	0
2	F	13	0	18	7	0
3	A	22	0	28	2	0
3	C	22	0	28	0	0
3	F	22	0	28	0	0
4	A	8	0	12	3	0
4	B	24	0	36	0	0
4	C	12	0	18	0	0
4	D	8	0	12	0	0
4	E	12	0	18	0	0
4	F	8	0	12	2	0
5	A	21	0	30	1	0
5	C	7	0	10	0	0
5	D	7	0	10	0	0
5	E	7	0	10	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	8	0	6	0	0
7	B	4	0	3	0	0
7	C	4	0	3	0	0
7	D	4	0	3	0	0
7	E	8	0	6	1	0
7	F	8	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	10	0	14	0	0
8	C	20	0	28	1	0
8	D	10	0	14	0	0
8	E	10	0	14	0	0
9	E	6	0	8	0	0
9	F	6	0	8	1	0
10	A	127	0	0	0	0
10	B	111	0	0	0	0
10	C	115	0	0	0	0
10	D	114	0	0	1	0
10	E	96	0	0	0	0
10	F	124	0	0	0	0
All	All	14728	0	14378	95	0

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

All (95) 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:C:74:LYS:HZ3	1:C:74:LYS:H	1.18	0.91
1:D:94:LYS:O	1:D:98:GLU:HG2	1.74	0.88
1:F:154:LYS:HZ2	2:F:301:PG4:H32	1.50	0.76
1:F:154:LYS:HZ2	2:F:301:PG4:H11	1.52	0.74
1:D:74:LYS:HA	1:D:74:LYS:HE2	1.71	0.72
1:D:161[B]:ASN:ND2	10:D:401:HOH:O	2.27	0.67
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.82	0.61
1:D:45:VAL:HG21	1:D:59:ASN:ND2	2.16	0.60
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.84	0.60
2:A:302:PG4:HO5	4:A:305:EDO:HO2	1.47	0.60
1:F:32:LYS:NZ	4:F:304:EDO:O2	2.34	0.60
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.83	0.59
1:A:288:GLU:HA	1:A:291:LYS:HE2	1.83	0.59
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.84	0.58
1:E:113:LYS:HE2	1:F:142[A]:ARG:HD3	1.85	0.58
1:E:154:LYS:HD2	2:E:301:PG4:H31	1.85	0.58
1:A:142:ARG:HD3	1:B:113:LYS:HE2	1.85	0.57
1:E:60:ARG:HB3	1:E:95:PHE:CZ	2.40	0.56
1:A:45:VAL:HG21	1:A:59:ASN:OD1	2.06	0.56
1:F:150:ASP:HB3	2:F:301:PG4:H12	1.88	0.56
1:F:154:LYS:HZ3	2:F:301:PG4:H51	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.88	0.55
1:D:32:LYS:O	1:D:36[B]:GLU:HG2	2.05	0.55
1:F:76:LYS:HD2	4:F:303:EDO:H22	1.89	0.55
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.89	0.55
1:B:161:ASN:OD1	1:B:161:ASN:N	2.40	0.55
1:C:74:LYS:H	1:C:74:LYS:NZ	1.98	0.55
1:B:60:ARG:HB3	1:B:95:PHE:CZ	2.42	0.54
1:E:113:LYS:NZ	1:E:144:GLY:O	2.38	0.53
1:F:154:LYS:NZ	2:F:301:PG4:H11	2.24	0.53
1:D:97:LYS:HD3	1:D:97:LYS:C	2.34	0.53
1:F:142[B]:ARG:HE	7:F:306:ACT:C	2.22	0.52
1:A:59:ASN:HD22	3:A:303:3VN:H26	1.55	0.52
1:E:161:ASN:OD1	1:E:161:ASN:N	2.36	0.52
1:F:60:ARG:HB3	1:F:95:PHE:CZ	2.45	0.51
1:D:60:ARG:HB3	1:D:95:PHE:CZ	2.45	0.51
9:F:307:GOL:O1	9:F:307:GOL:O3	2.23	0.51
1:B:230:TYR:HD2	1:C:230:TYR:HD2	1.58	0.51
1:A:60:ARG:HB3	1:A:95:PHE:CZ	2.46	0.50
1:A:204:LYS:NZ	4:A:305:EDO:O2	2.44	0.50
1:F:154:LYS:NZ	2:F:301:PG4:H32	2.24	0.50
1:F:45:VAL:HG13	1:F:54:LEU:HD12	1.94	0.50
1:B:45:VAL:HG13	1:B:54:LEU:HD12	1.94	0.49
1:A:204:LYS:HE3	2:A:302:PG4:H32	1.94	0.49
1:C:60:ARG:HB3	1:C:95:PHE:CZ	2.47	0.49
1:B:13:LEU:HD11	1:B:42:VAL:HB	1.94	0.49
1:A:161:ASN:OD1	1:A:161:ASN:N	2.42	0.48
1:A:57:GLU:CB	1:A:60:ARG:HH11	2.27	0.48
1:D:32:LYS:O	1:D:36[A]:GLU:HG3	2.13	0.48
1:A:57:GLU:HB2	1:A:60:ARG:HH11	1.79	0.47
1:F:60:ARG:HD3	1:F:95:PHE:CD2	2.50	0.47
1:C:56:HIS:O	1:C:60:ARG:HG3	2.15	0.47
1:A:57:GLU:HG3	1:A:60:ARG:NH1	2.31	0.46
1:A:142:ARG:CD	1:B:113:LYS:HE2	2.46	0.46
1:F:231:LYS:HD3	1:F:231:LYS:HA	1.73	0.46
1:F:45:VAL:HG11	1:F:59:ASN:CG	2.41	0.45
1:B:160:GLU:H	1:B:160:GLU:CD	2.24	0.45
1:D:59:ASN:HD22	1:D:59:ASN:C	2.25	0.45
1:A:57:GLU:HA	1:A:60:ARG:HE	1.80	0.45
1:F:56:HIS:O	1:F:60:ARG:HG3	2.17	0.45
1:E:45:VAL:HG11	1:E:59:ASN:CG	2.41	0.44
1:D:97:LYS:C	1:D:97:LYS:CD	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG12	1:A:75:VAL:HG21	1.98	0.44
1:D:60:ARG:HG2	1:D:95:PHE:CD1	2.53	0.43
1:A:230:TYR:CD2	1:D:230:TYR:HD2	2.36	0.43
1:A:254:ILE:HB	1:A:255:PRO:HD3	2.01	0.43
1:C:60:ARG:HD3	1:C:95:PHE:CD2	2.54	0.43
1:F:268:SER:OG	1:F:270:GLU:HG3	2.18	0.43
1:A:298:PHE:OXT	5:A:306:PEG:H11	2.18	0.43
3:A:303:3VN:H5	4:A:304:EDO:H21	2.00	0.43
1:A:288:GLU:OE1	1:A:291:LYS:NZ	2.34	0.43
1:A:256:ILE:O	1:A:260:MET:HG2	2.19	0.43
1:E:111:TYR:O	1:F:142[A]:ARG:HD2	2.18	0.43
1:B:230:TYR:HD2	1:C:230:TYR:CD2	2.37	0.42
1:B:235:LYS:HE3	1:B:239:GLU:OE2	2.19	0.42
1:E:292:LYS:HD3	7:E:308:ACT:H2	2.01	0.42
1:B:59:ASN:C	1:B:59:ASN:HD22	2.28	0.42
1:A:6:ILE:HG12	1:A:76:LYS:HD3	2.01	0.42
1:B:230:TYR:CD2	1:C:230:TYR:HD2	2.35	0.42
1:E:254:ILE:HB	1:E:255:PRO:HD3	2.02	0.42
1:B:194:ILE:C	1:B:197:PRO:HD2	2.45	0.42
1:F:154:LYS:NZ	2:F:301:PG4:H51	2.33	0.42
1:C:18:LYS:HD3	1:C:23:ASP:OD2	2.19	0.42
1:A:114:PRO:HB3	1:B:274:PRO:HB2	2.02	0.41
1:C:45:VAL:HG13	1:C:54:LEU:HD12	2.02	0.41
1:F:10:MET:HG2	1:F:41:ALA:HB3	2.01	0.41
1:C:59:ASN:HD22	1:C:59:ASN:C	2.27	0.41
1:A:13:LEU:HD11	1:A:42:VAL:HB	2.03	0.41
1:F:254:ILE:HA	1:F:271:PHE:CE2	2.56	0.41
1:E:45:VAL:O	1:E:45:VAL:HG12	2.20	0.41
1:C:150:ASP:HB3	8:C:303:PGE:H2	2.04	0.40
1:D:97:LYS:HD3	1:D:97:LYS:O	2.22	0.40
1:D:108:ALA:HB2	1:D:147:ILE:HD11	2.04	0.40
1:E:241:TYR:CE2	1:E:245:LYS:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	B	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
1	C	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	D	295/310 (95%)	289 (98%)	6 (2%)	0	100	100
1	E	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	F	295/310 (95%)	291 (99%)	4 (1%)	0	100	100
All	All	1763/1860 (95%)	1733 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/260 (95%)	248 (100%)	0	100	100
1	B	249/260 (96%)	248 (100%)	1 (0%)	84	78
1	C	248/260 (95%)	247 (100%)	1 (0%)	84	78
1	D	250/260 (96%)	249 (100%)	1 (0%)	84	78
1	E	248/260 (95%)	247 (100%)	1 (0%)	84	78
1	F	250/260 (96%)	249 (100%)	1 (0%)	84	78
All	All	1493/1560 (96%)	1488 (100%)	5 (0%)	86	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	161	ASN
1	C	74	LYS
1	D	59	ASN

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Mol	Chain	Res	Type
1	E	161	ASN
1	F	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	C	37	ASN
1	C	229	ASN
1	E	59	ASN
1	E	99	HIS
1	E	201	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	C	166	1	11,13,14	0.91	1 (9%)	9,15,17	3.78	4 (44%)
1	KPI	A	166	1	11,13,14	0.96	1 (9%)	9,15,17	3.30	3 (33%)
1	KPI	B	166	1	11,13,14	2.32	3 (27%)	9,15,17	3.91	5 (55%)
1	KPI	E	166	1	11,13,14	1.92	2 (18%)	9,15,17	3.93	4 (44%)
1	KPI	F	166	1	11,13,14	2.30	3 (27%)	9,15,17	3.92	5 (55%)
1	KPI	D	166	1	11,13,14	1.95	2 (18%)	9,15,17	3.97	4 (44%)

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	C	166	1	-	1/13/14/16	-
1	KPI	A	166	1	-	0/13/14/16	-
1	KPI	B	166	1	-	2/13/14/16	-
1	KPI	E	166	1	-	2/13/14/16	-
1	KPI	F	166	1	-	0/13/14/16	-
1	KPI	D	166	1	-	0/13/14/16	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	KPI	O2-CX2	5.62	1.36	1.22
1	D	166	KPI	O2-CX2	5.56	1.36	1.22
1	B	166	KPI	O2-CX2	5.53	1.36	1.22
1	E	166	KPI	O2-CX2	5.51	1.36	1.22
1	B	166	KPI	O-C	4.31	1.36	1.20
1	F	166	KPI	O-C	4.18	1.35	1.20
1	D	166	KPI	O1-CX2	-2.45	1.23	1.30
1	E	166	KPI	O1-CX2	-2.43	1.24	1.30
1	B	166	KPI	O1-CX2	-2.42	1.24	1.30
1	F	166	KPI	O1-CX2	-2.32	1.24	1.30
1	A	166	KPI	O1-CX2	2.13	1.36	1.30
1	C	166	KPI	O1-CX2	2.05	1.36	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	166	KPI	C1-CX1-CX2	-8.53	110.07	118.11
1	D	166	KPI	C1-CX1-CX2	-8.12	110.46	118.11
1	F	166	KPI	C1-CX1-CX2	-7.44	111.10	118.11
1	E	166	KPI	C1-CX1-CX2	-7.29	111.24	118.11
1	B	166	KPI	C1-CX1-CX2	-7.15	111.37	118.11
1	A	166	KPI	C1-CX1-CX2	-7.00	111.51	118.11
1	E	166	KPI	O2-CX2-CX1	-6.11	113.88	121.35
1	F	166	KPI	O2-CX2-CX1	-5.82	114.23	121.35
1	B	166	KPI	O1-CX2-CX1	5.82	128.90	116.50
1	C	166	KPI	O2-CX2-CX1	5.77	128.39	121.35
1	B	166	KPI	O2-CX2-CX1	-5.73	114.34	121.35
1	E	166	KPI	O1-CX2-CX1	5.67	128.59	116.50
1	A	166	KPI	O2-CX2-CX1	5.59	128.17	121.35
1	F	166	KPI	O1-CX2-CX1	5.57	128.36	116.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	166	KPI	O2-CX2-CX1	-5.41	114.73	121.35
1	D	166	KPI	O1-CX2-CX1	5.38	127.97	116.50
1	A	166	KPI	O1-CX2-O2	-3.15	116.41	123.90
1	B	166	KPI	O1-CX2-O2	-3.00	116.76	123.90
1	C	166	KPI	O1-CX2-O2	-2.82	117.18	123.90
1	D	166	KPI	O1-CX2-O2	-2.78	117.29	123.90
1	C	166	KPI	CD-CE-NZ	2.74	115.52	110.67
1	F	166	KPI	O1-CX2-O2	-2.73	117.40	123.90
1	E	166	KPI	O1-CX2-O2	-2.68	117.53	123.90
1	B	166	KPI	CD-CE-NZ	2.42	114.96	110.67
1	F	166	KPI	CD-CE-NZ	2.36	114.85	110.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	C-CA-CB-CG
1	E	166	KPI	NZ-CX1-CX2-O2
1	E	166	KPI	NZ-CX1-CX2-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 7 are monoatomic - leaving 48 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	$\#\|Z\|>2$
2	PG4	C	301	-	12,12,12	0.53	0	11,11,11	0.26	0
4	EDO	B	302	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	B	304	-	3,3,3	0.42	0	2,2,2	0.39	0
5	PEG	A	306	-	6,6,6	0.48	0	5,5,5	0.24	0
5	PEG	E	306	-	6,6,6	0.50	0	5,5,5	0.25	0
3	3VN	C	302	-	17,21,21	0.86	0	18,28,28	1.49	3 (16%)
4	EDO	D	303	-	3,3,3	0.43	0	2,2,2	0.38	0
7	ACT	A	312	-	3,3,3	0.77	0	3,3,3	1.43	0
7	ACT	A	311	-	3,3,3	0.81	0	3,3,3	1.37	0
7	ACT	F	306	-	3,3,3	0.81	0	3,3,3	1.35	0
9	GOL	F	307	-	5,5,5	0.38	0	5,5,5	0.33	0
5	PEG	A	307	-	6,6,6	0.51	0	5,5,5	0.29	0
4	EDO	C	306	-	3,3,3	0.42	0	2,2,2	0.40	0
7	ACT	D	307	-	3,3,3	0.80	0	3,3,3	1.38	0
4	EDO	B	305	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	E	303	-	3,3,3	0.45	0	2,2,2	0.32	0
2	PG4	F	301	-	12,12,12	0.52	0	11,11,11	0.27	0
4	EDO	C	307	-	3,3,3	0.44	0	2,2,2	0.30	0
4	EDO	E	305	-	3,3,3	0.43	0	2,2,2	0.34	0
7	ACT	E	308	-	3,3,3	0.81	0	3,3,3	1.32	0
7	ACT	F	305	-	3,3,3	0.79	0	3,3,3	1.38	0
2	PG4	A	301	-	12,12,12	0.53	0	11,11,11	0.24	0
7	ACT	B	310	-	3,3,3	0.83	0	3,3,3	1.32	0
4	EDO	B	306	-	3,3,3	0.46	0	2,2,2	0.37	0
3	3VN	A	303	-	17,21,21	0.85	0	18,28,28	1.38	3 (16%)
4	EDO	C	305	-	3,3,3	0.43	0	2,2,2	0.36	0
7	ACT	E	307	-	3,3,3	0.83	0	3,3,3	1.26	0
8	PGE	E	302	-	9,9,9	0.32	0	8,8,8	0.30	0
5	PEG	C	308	-	6,6,6	0.47	0	5,5,5	0.24	0
4	EDO	F	303	-	3,3,3	0.45	0	2,2,2	0.38	0
8	PGE	B	301	-	9,9,9	0.32	0	8,8,8	0.24	0
4	EDO	F	304	-	3,3,3	0.42	0	2,2,2	0.38	0
5	PEG	D	304	-	6,6,6	0.50	0	5,5,5	0.25	0
9	GOL	E	309	-	5,5,5	0.34	0	5,5,5	0.37	0
8	PGE	C	303	-	9,9,9	0.33	0	8,8,8	0.19	0
2	PG4	A	302	-	12,12,12	0.53	0	11,11,11	0.23	0
4	EDO	A	305	-	3,3,3	0.44	0	2,2,2	0.42	0
5	PEG	A	308	-	6,6,6	0.50	0	5,5,5	0.29	0
4	EDO	B	307	-	3,3,3	0.44	0	2,2,2	0.41	0
2	PG4	E	301	-	12,12,12	0.53	0	11,11,11	0.22	0
8	PGE	C	304	-	9,9,9	0.31	0	8,8,8	0.36	0
8	PGE	D	301	-	9,9,9	0.30	0	8,8,8	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	ACT	C	310	-	3,3,3	0.83	0	3,3,3	1.36	0
4	EDO	E	304	-	3,3,3	0.43	0	2,2,2	0.37	0
3	3VN	F	302	-	17,21,21	0.87	0	18,28,28	1.46	4 (22%)
4	EDO	D	302	-	3,3,3	0.43	0	2,2,2	0.28	0
4	EDO	B	303	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	A	304	-	3,3,3	0.41	0	2,2,2	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	C	301	-	-	6/10/10/10	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	B	304	-	-	0/1/1/1	-
5	PEG	A	306	-	-	2/4/4/4	-
5	PEG	E	306	-	-	0/4/4/4	-
3	3VN	C	302	-	-	5/31/31/31	-
4	EDO	D	303	-	-	0/1/1/1	-
9	GOL	F	307	-	-	2/4/4/4	-
5	PEG	A	307	-	-	1/4/4/4	-
4	EDO	C	306	-	-	0/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
2	PG4	F	301	-	-	3/10/10/10	-
4	EDO	C	307	-	-	0/1/1/1	-
4	EDO	E	305	-	-	1/1/1/1	-
2	PG4	A	301	-	-	1/10/10/10	-
4	EDO	B	306	-	-	0/1/1/1	-
3	3VN	A	303	-	-	9/31/31/31	-
4	EDO	C	305	-	-	1/1/1/1	-
8	PGE	E	302	-	-	4/7/7/7	-
5	PEG	C	308	-	-	1/4/4/4	-
4	EDO	F	303	-	-	1/1/1/1	-
8	PGE	B	301	-	-	1/7/7/7	-
4	EDO	F	304	-	-	0/1/1/1	-
5	PEG	D	304	-	-	2/4/4/4	-
9	GOL	E	309	-	-	2/4/4/4	-
8	PGE	C	303	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	A	302	-	-	5/10/10/10	-
4	EDO	A	305	-	-	0/1/1/1	-
5	PEG	A	308	-	-	2/4/4/4	-
4	EDO	B	307	-	-	0/1/1/1	-
2	PG4	E	301	-	-	4/10/10/10	-
8	PGE	C	304	-	-	2/7/7/7	-
8	PGE	D	301	-	-	2/7/7/7	-
4	EDO	E	304	-	-	1/1/1/1	-
3	3VN	F	302	-	-	13/31/31/31	-
4	EDO	D	302	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	303	3VN	C07-C06-C02	-3.07	109.72	115.16
3	F	302	3VN	C07-C06-C02	-2.97	109.90	115.16
3	C	302	3VN	O22-C20-C13	2.93	121.50	113.69
3	C	302	3VN	C07-C06-C02	-2.93	109.97	115.16
3	F	302	3VN	O22-C20-C13	2.38	120.05	113.69
3	F	302	3VN	O05-C03-C02	2.32	119.87	113.69
3	F	302	3VN	C16-C15-C13	-2.25	111.17	115.16
3	A	303	3VN	C16-C15-C13	-2.18	111.30	115.16
3	A	303	3VN	O05-C03-C02	2.09	119.28	113.69
3	C	302	3VN	O05-C03-C02	2.09	119.27	113.69

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	3VN	C12-C13-C20-O21
3	F	302	3VN	C11-C02-C03-O04
3	F	302	3VN	C11-C02-C03-O05
3	F	302	3VN	C12-C13-C20-O21
3	F	302	3VN	C12-C13-C20-O22
9	E	309	GOL	O1-C1-C2-C3
9	F	307	GOL	O1-C1-C2-O2
9	F	307	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	302	PG4	O2-C3-C4-O3
2	E	301	PG4	O2-C3-C4-O3
8	C	304	PGE	O3-C5-C6-O4
2	A	302	PG4	O3-C5-C6-O4
5	A	308	PEG	O2-C3-C4-O4
4	E	305	EDO	O1-C1-C2-O2
8	E	302	PGE	O3-C5-C6-O4
2	E	301	PG4	O1-C1-C2-O2
9	E	309	GOL	O1-C1-C2-O2
8	C	304	PGE	O2-C3-C4-O3
8	E	302	PGE	O2-C3-C4-O3
2	C	301	PG4	C5-C6-O4-C7
8	C	303	PGE	O3-C5-C6-O4
5	A	307	PEG	C1-C2-O2-C3
8	C	303	PGE	O2-C3-C4-O3
2	A	302	PG4	C6-C5-O3-C4
2	E	301	PG4	C8-C7-O4-C6
2	C	301	PG4	C4-C3-O2-C2
2	C	301	PG4	C3-C4-O3-C5
3	A	303	3VN	C07-C08-C09-N10
2	F	301	PG4	O1-C1-C2-O2
3	F	302	3VN	C06-C07-C08-C09
3	A	303	3VN	C11-C02-C03-O04
3	A	303	3VN	C11-C02-C03-O05
3	A	303	3VN	C12-C13-C20-O22
3	C	302	3VN	C06-C02-C03-O05
3	C	302	3VN	C11-C02-C03-O04
3	C	302	3VN	C11-C02-C03-O05
3	F	302	3VN	C06-C02-C03-O04
3	F	302	3VN	C15-C13-C20-O21
2	A	302	PG4	O1-C1-C2-O2
2	E	301	PG4	O3-C5-C6-O4
5	A	306	PEG	C1-C2-O2-C3
8	D	301	PGE	C3-C4-O3-C5
8	E	302	PGE	O1-C1-C2-O2
8	C	303	PGE	O1-C1-C2-O2
8	E	302	PGE	C1-C2-O2-C3
2	A	301	PG4	C1-C2-O2-C3
4	C	305	EDO	O1-C1-C2-O2
3	F	302	3VN	C07-C08-C09-N10
2	C	301	PG4	C6-C5-O3-C4
5	A	306	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	C	302	3VN	C07-C08-C09-N10
2	A	302	PG4	C5-C6-O4-C7
8	B	301	PGE	C1-C2-O2-C3
2	C	301	PG4	C1-C2-O2-C3
5	C	308	PEG	C1-C2-O2-C3
3	F	302	3VN	N01-C02-C03-O04
3	F	302	3VN	N14-C13-C20-O21
4	F	303	EDO	O1-C1-C2-O2
2	F	301	PG4	C5-C6-O4-C7
4	E	304	EDO	O1-C1-C2-O2
5	A	308	PEG	O1-C1-C2-O2
5	D	304	PEG	C1-C2-O2-C3
3	F	302	3VN	C16-C17-C18-N19
8	D	301	PGE	C6-C5-O3-C4
2	C	301	PG4	O2-C3-C4-O3
3	A	303	3VN	C06-C02-C03-O04
3	A	303	3VN	C06-C02-C03-O05
3	A	303	3VN	C15-C13-C20-O21
3	A	303	3VN	C15-C13-C20-O22
3	C	302	3VN	C06-C02-C03-O04
3	F	302	3VN	C06-C02-C03-O05
3	F	302	3VN	C15-C13-C20-O22
5	D	304	PEG	O1-C1-C2-O2
2	F	301	PG4	C8-C7-O4-C6

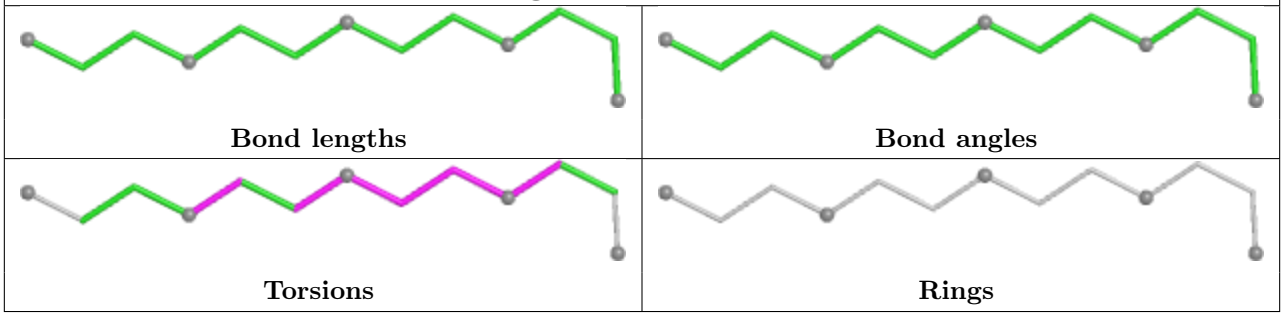
There are no ring outliers.

13 monomers are involved in 20 short contacts:

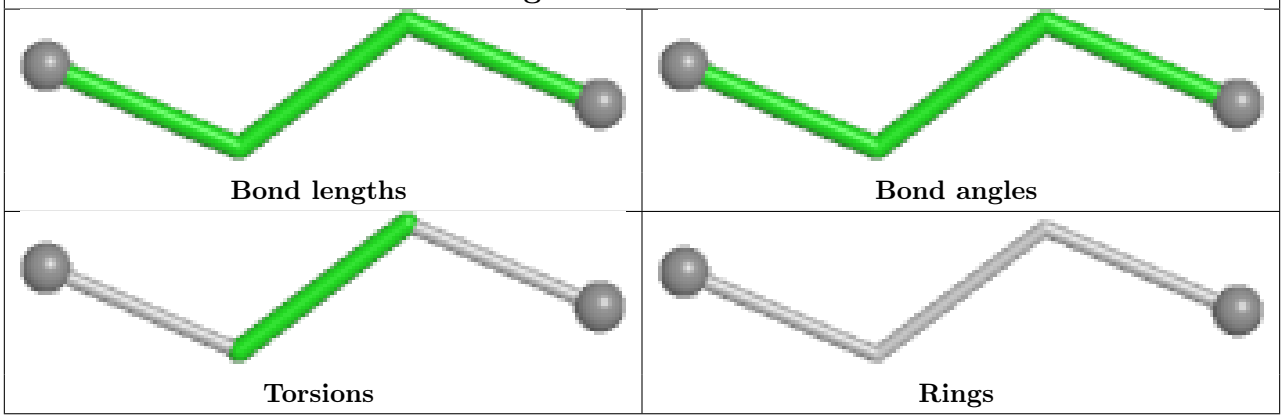
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	306	PEG	1	0
7	F	306	ACT	1	0
9	F	307	GOL	1	0
2	F	301	PG4	7	0
7	E	308	ACT	1	0
3	A	303	3VN	2	0
4	F	303	EDO	1	0
4	F	304	EDO	1	0
8	C	303	PGE	1	0
2	A	302	PG4	2	0
4	A	305	EDO	2	0
2	E	301	PG4	1	0
4	A	304	EDO	1	0

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.

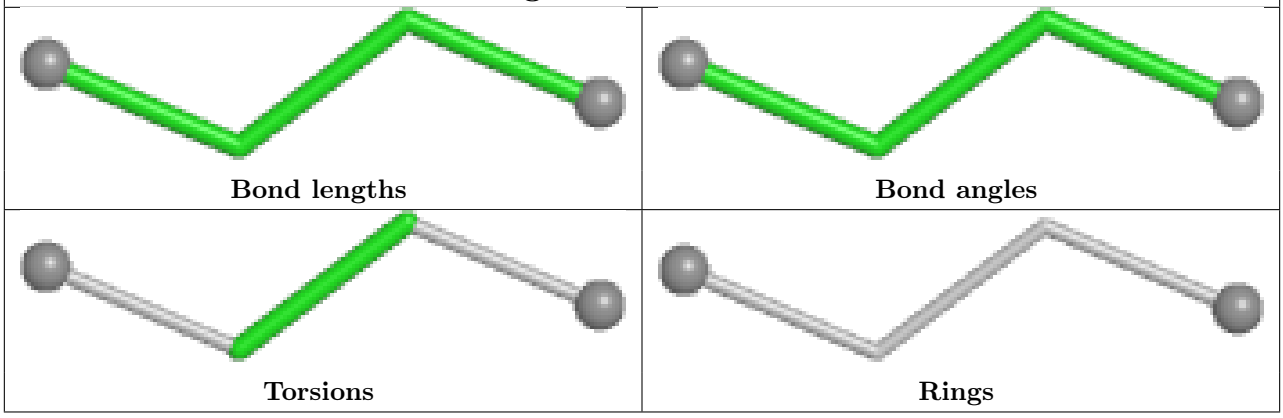
Ligand PG4 C 301



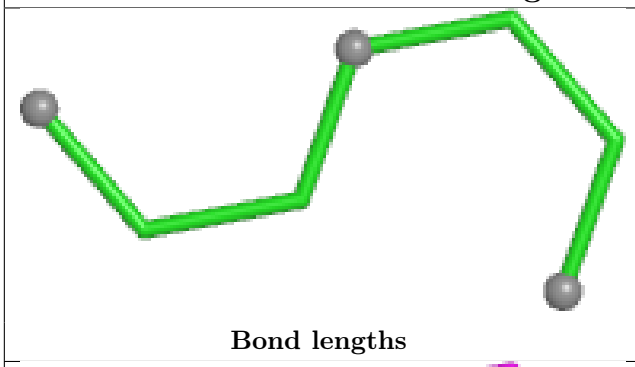
Ligand EDO B 302



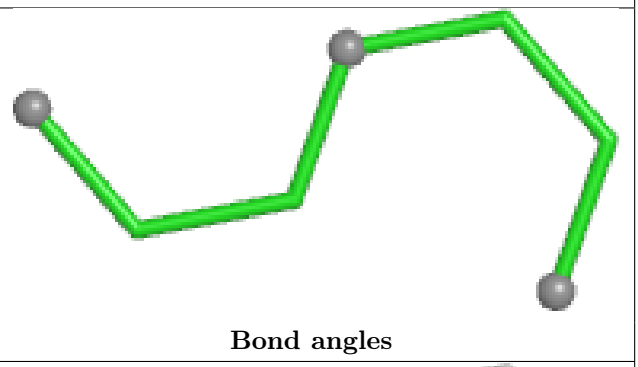
Ligand EDO B 304



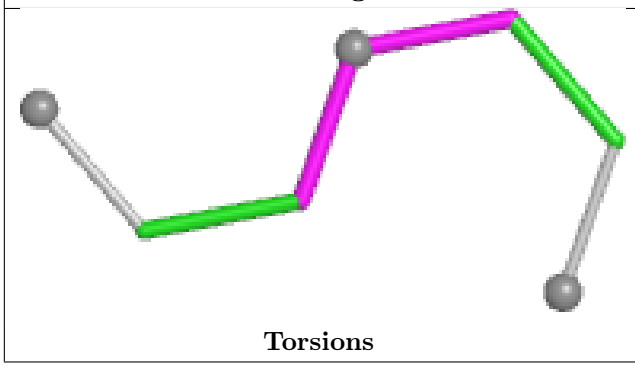
Ligand PEG A 306



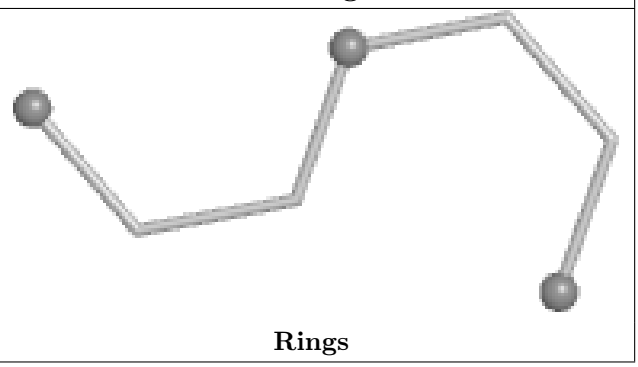
Bond lengths



Bond angles

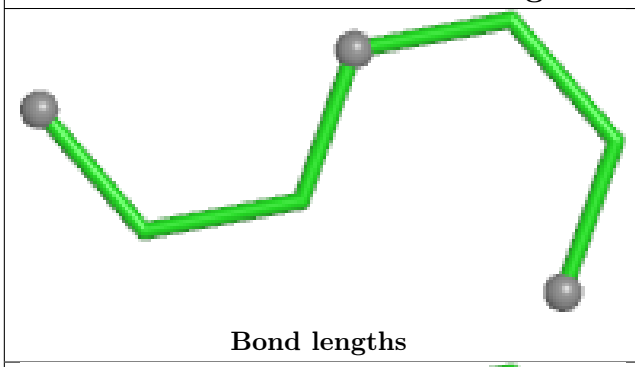


Torsions

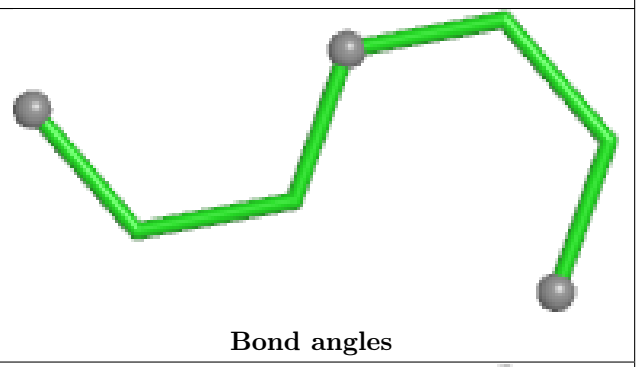


Rings

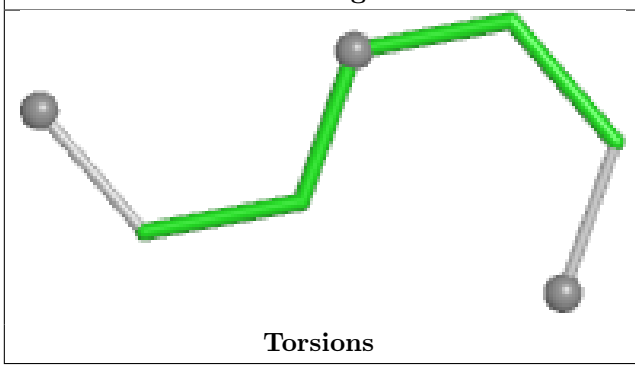
Ligand PEG E 306



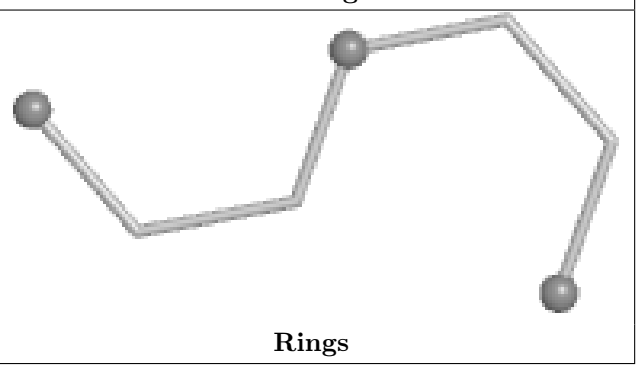
Bond lengths



Bond angles

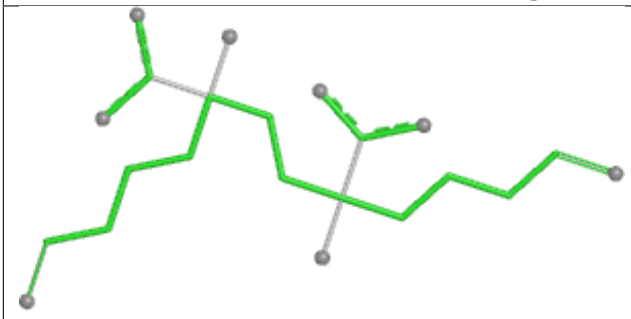


Torsions

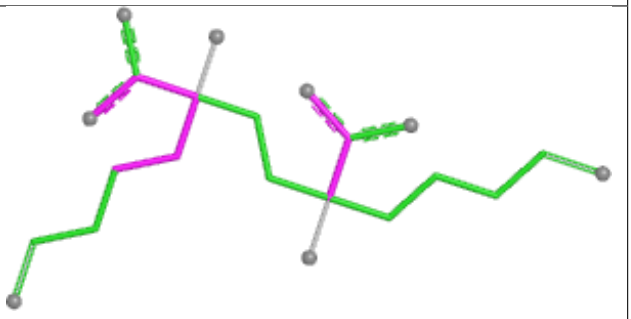


Rings

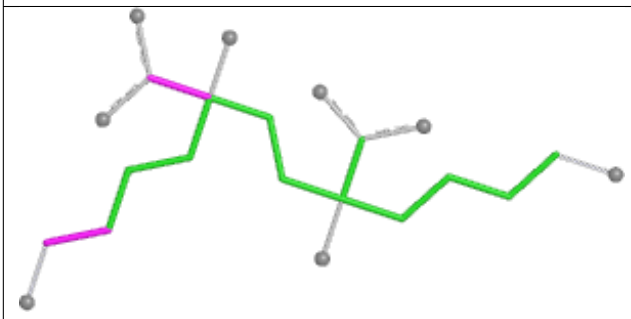
Ligand 3VN C 302



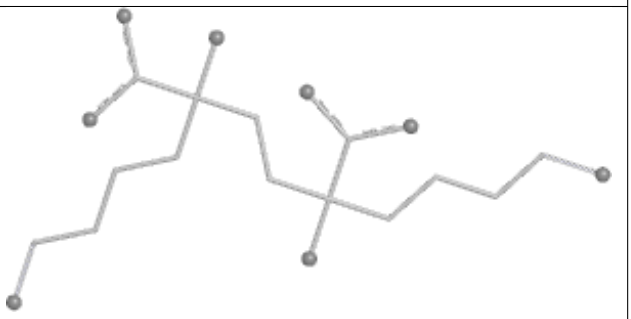
Bond lengths



Bond angles

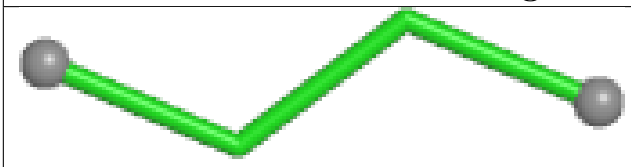


Torsions

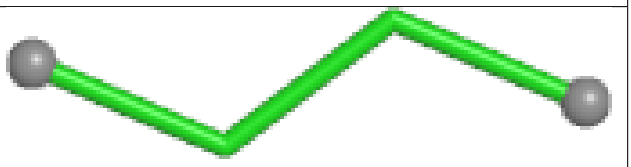


Rings

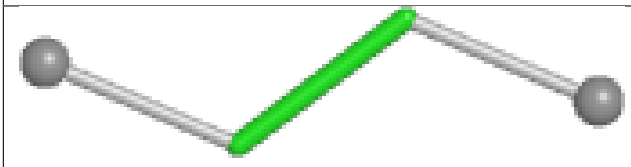
Ligand EDO D 303



Bond lengths



Bond angles

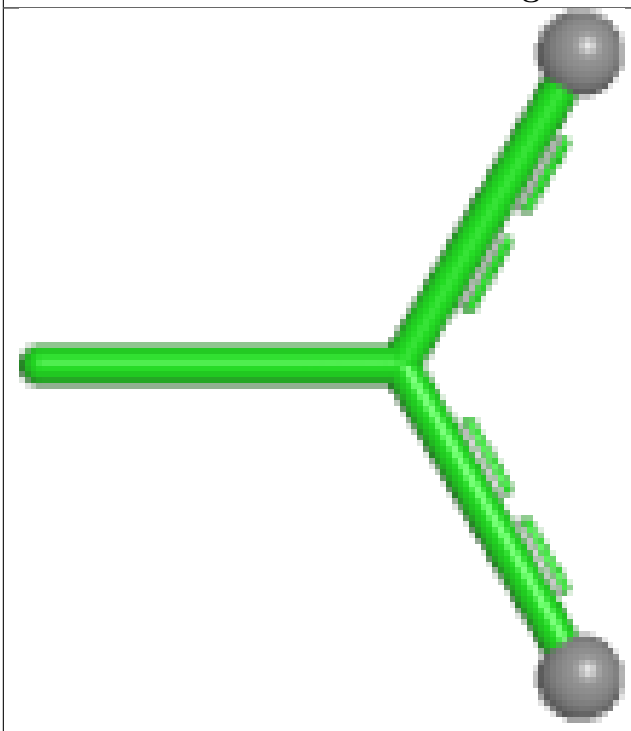


Torsions

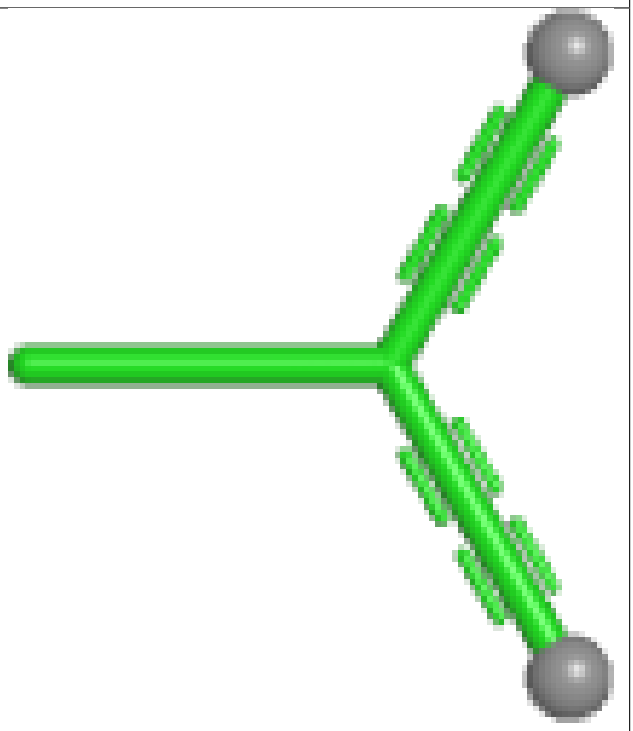


Rings

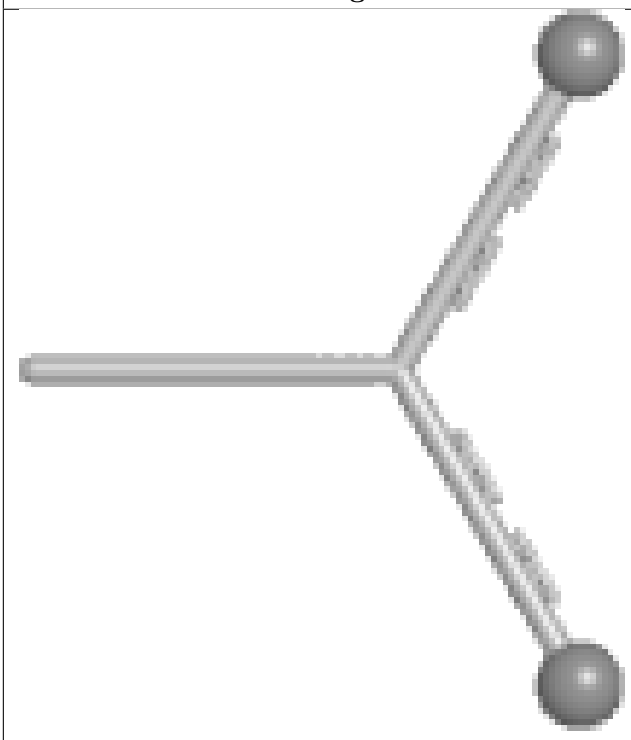
Ligand ACT A 312



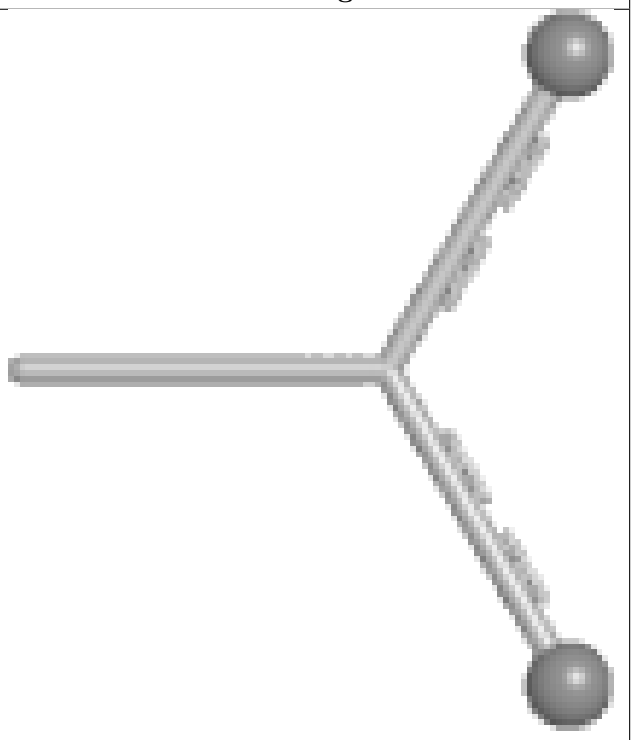
Bond lengths



Bond angles

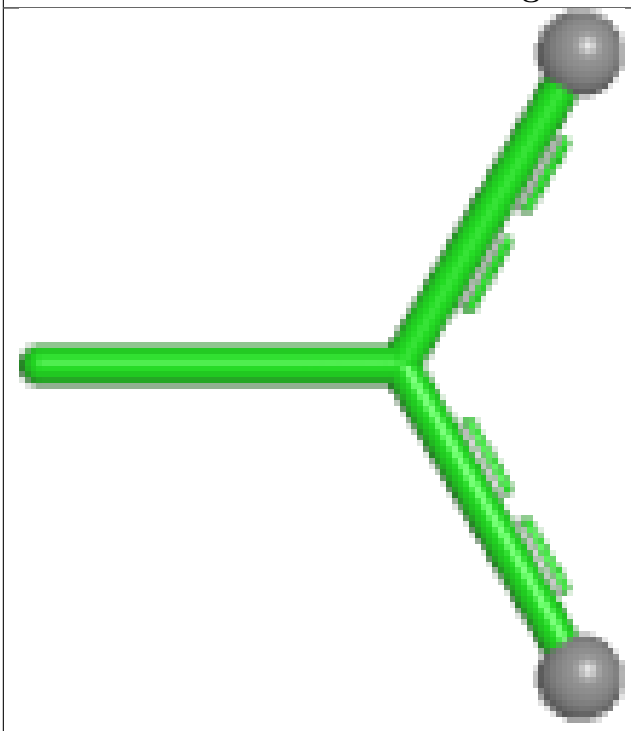


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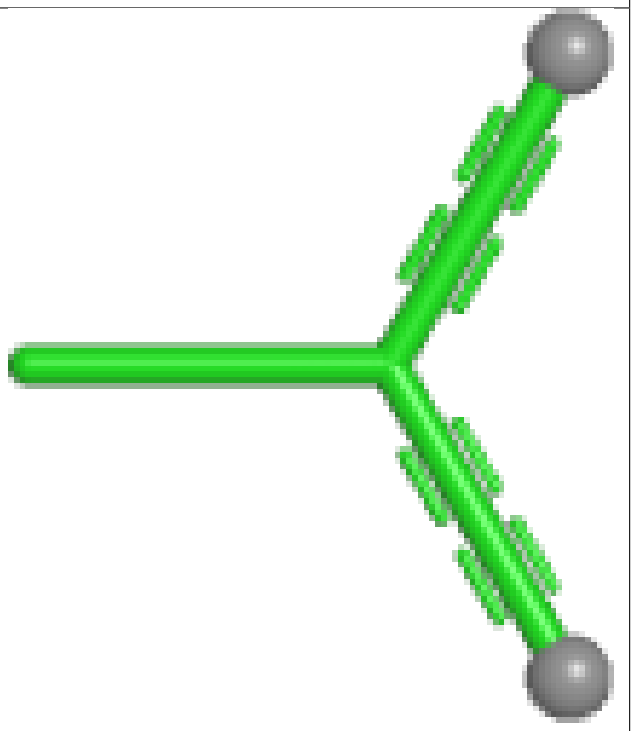


Rings

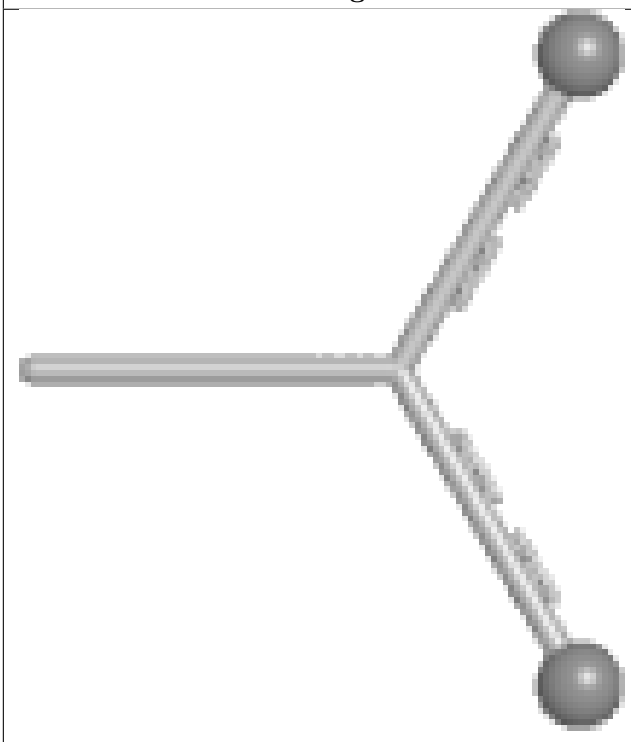
Ligand ACT A 311



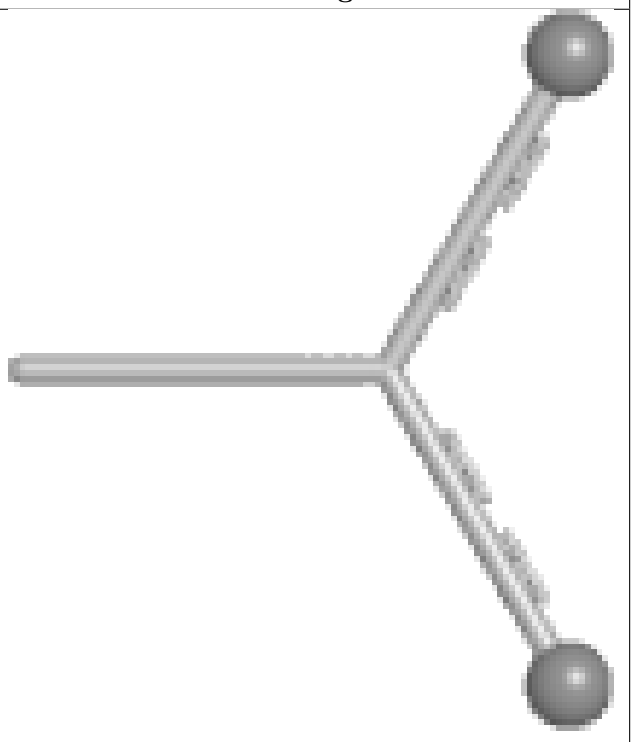
Bond lengths



Bond angles

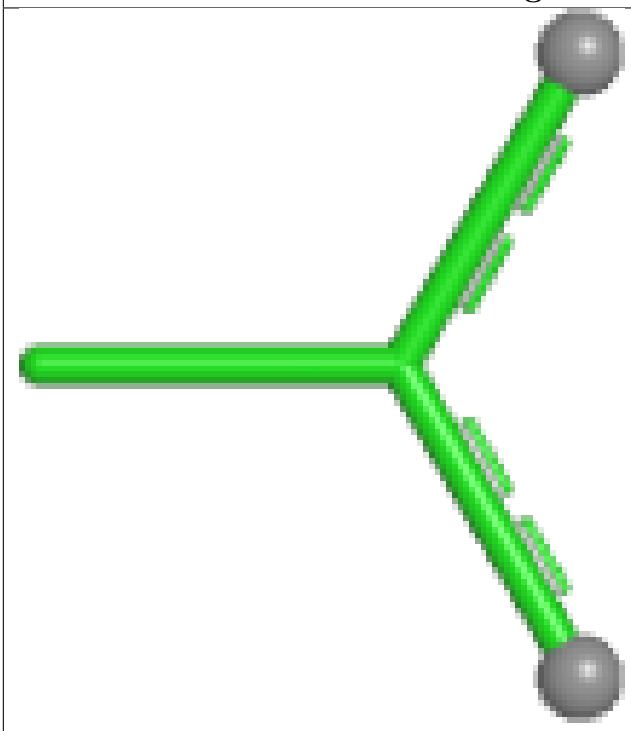


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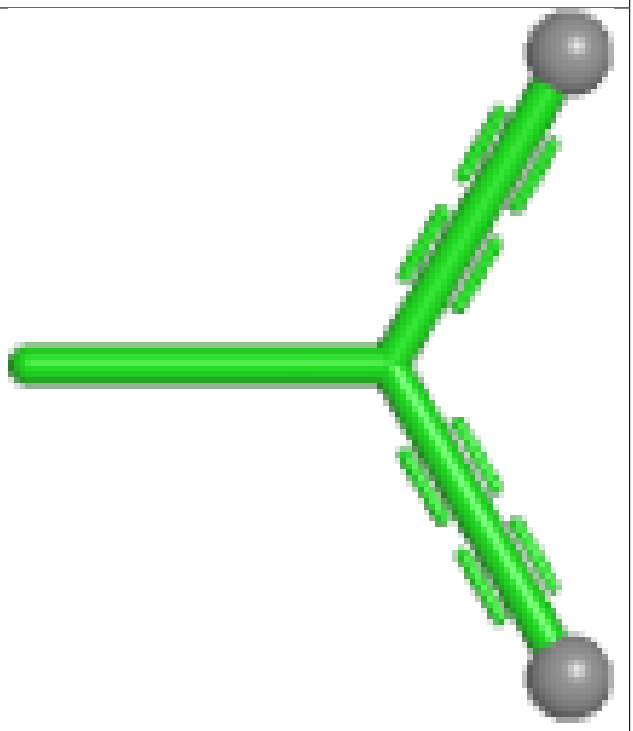


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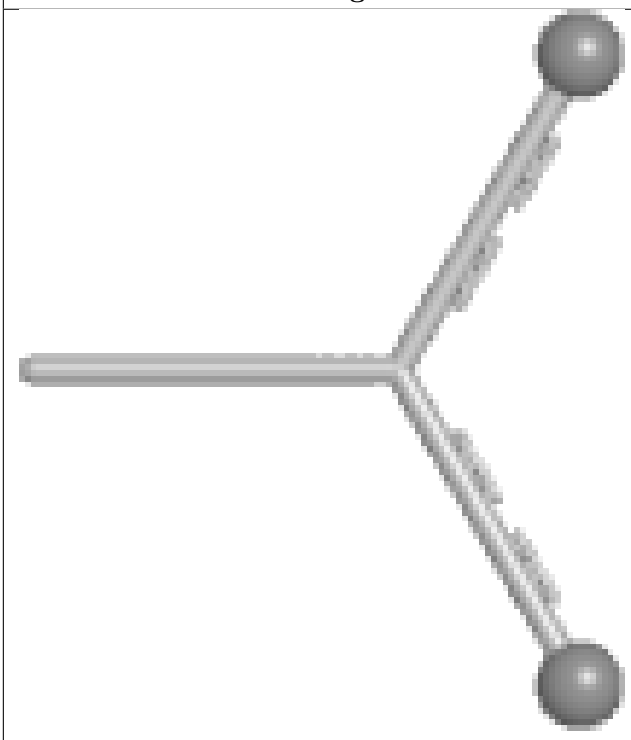
Ligand ACT F 306



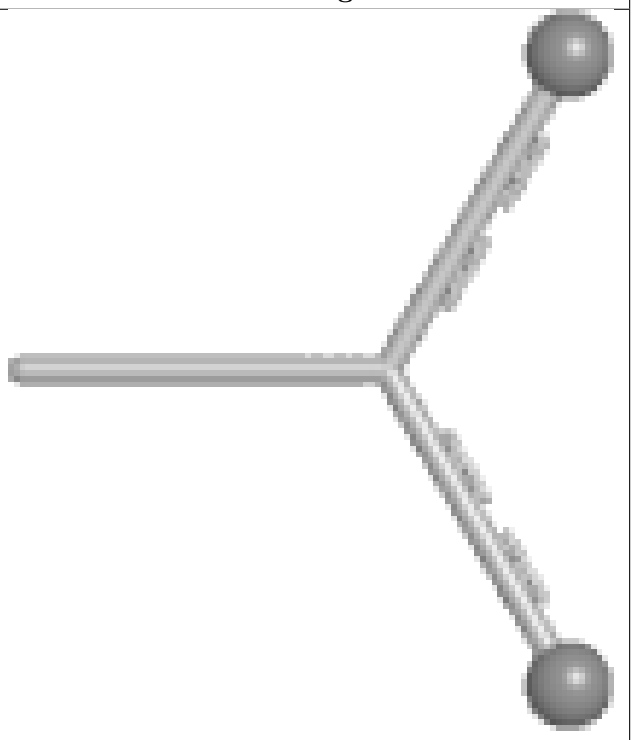
Bond lengths



Bond angles

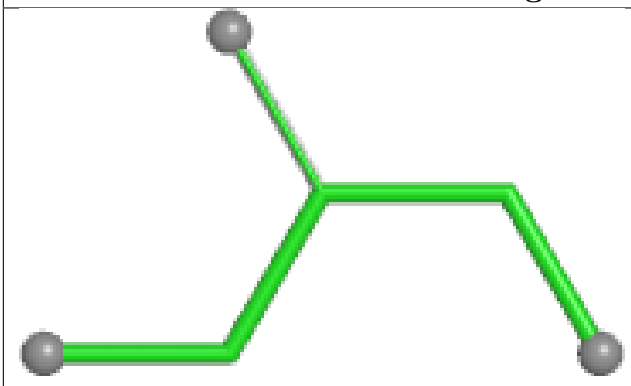


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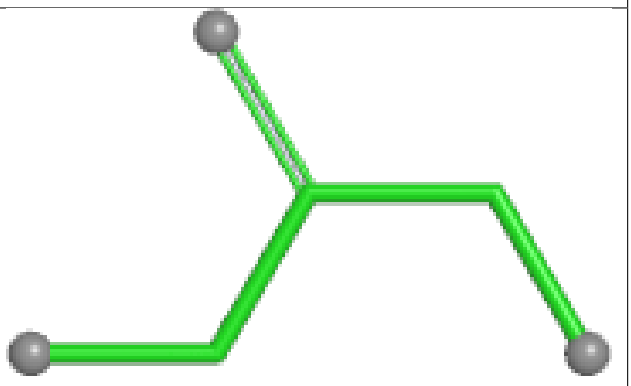


Rings

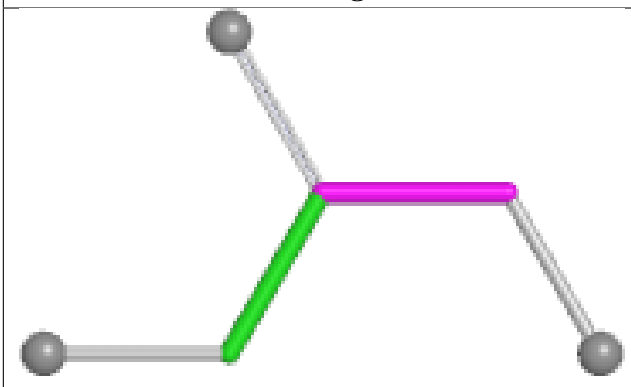
Ligand GOL F 307



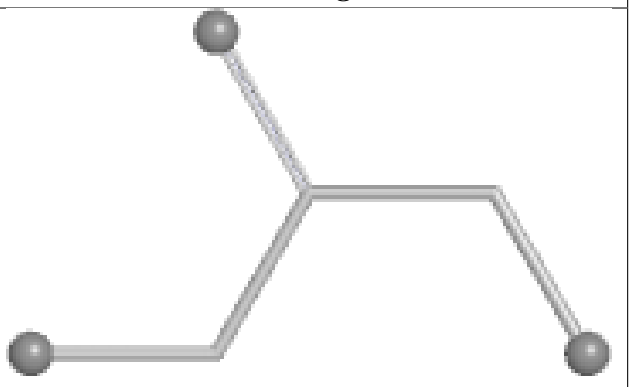
Bond lengths



Bond angles

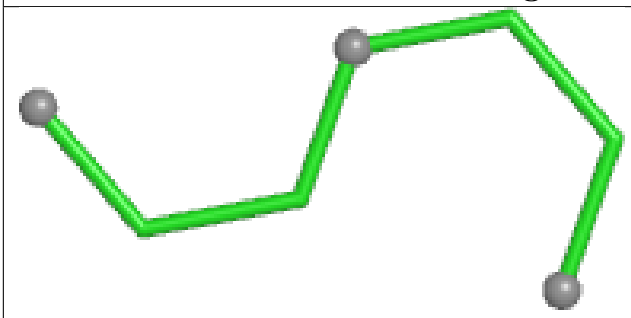


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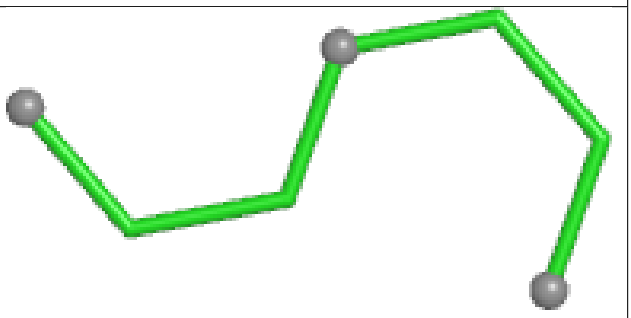


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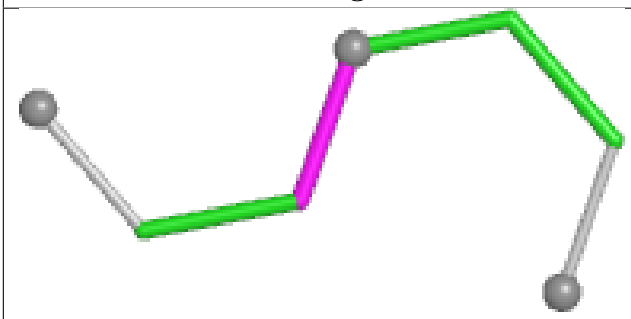
Ligand PEG A 307



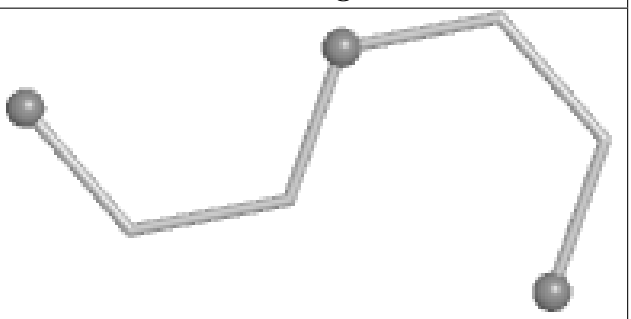
Bond lengths



Bond angles

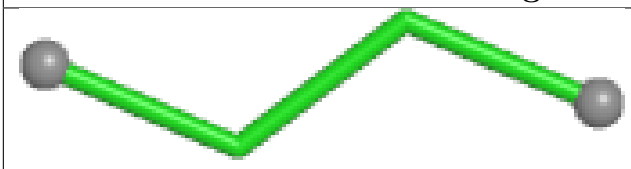


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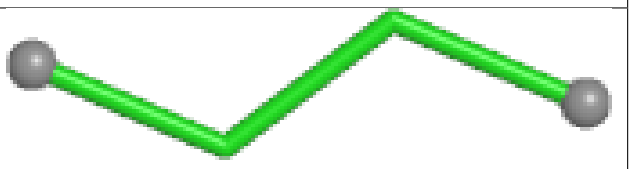


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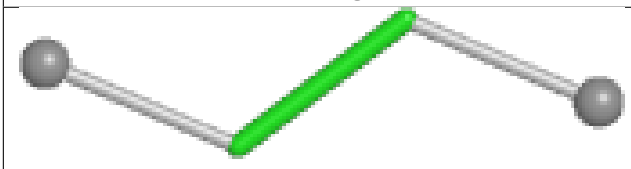
Ligand EDO C 306



Bond lengths



Bond angles

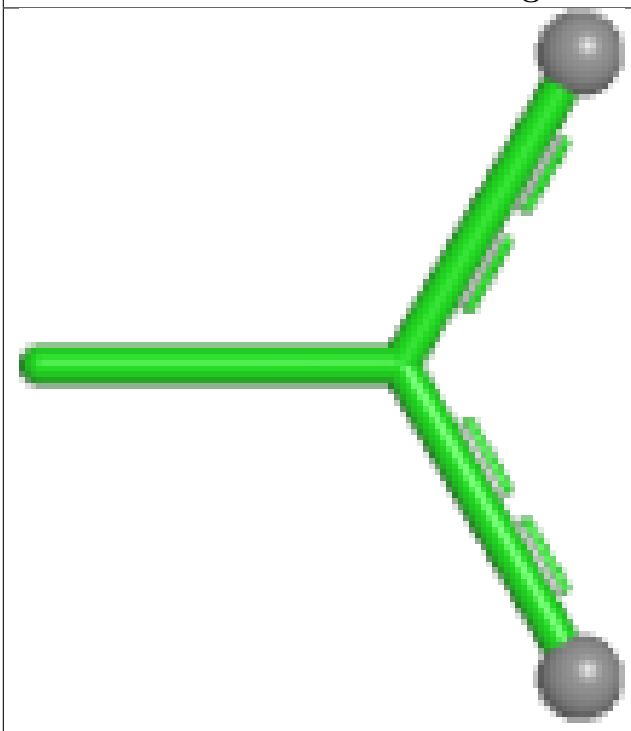


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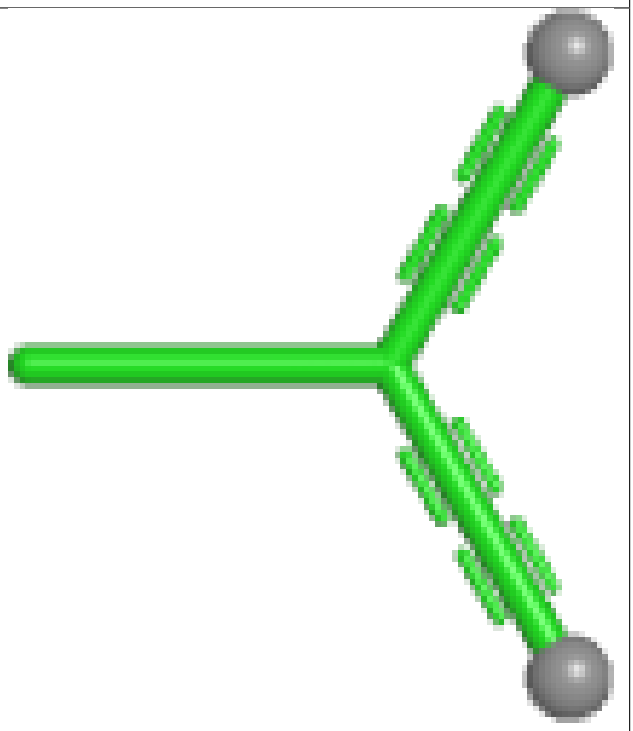


Rings

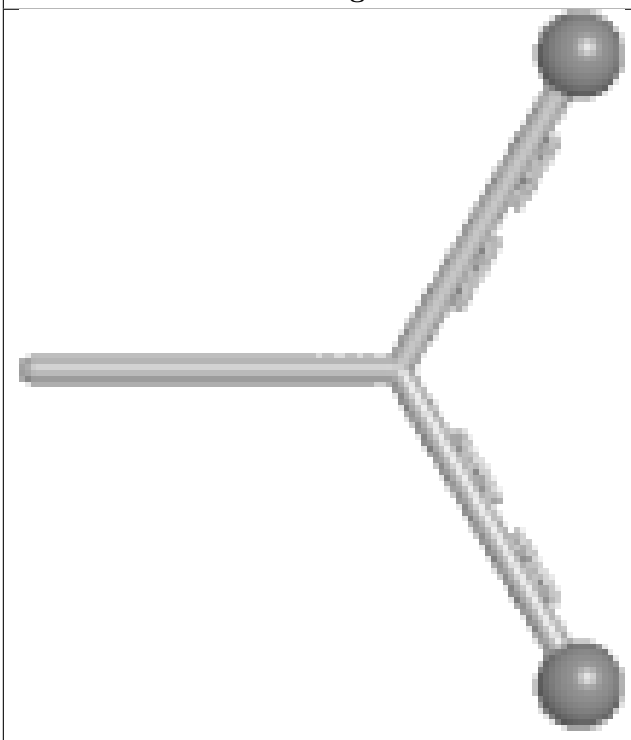
Ligand ACT D 307



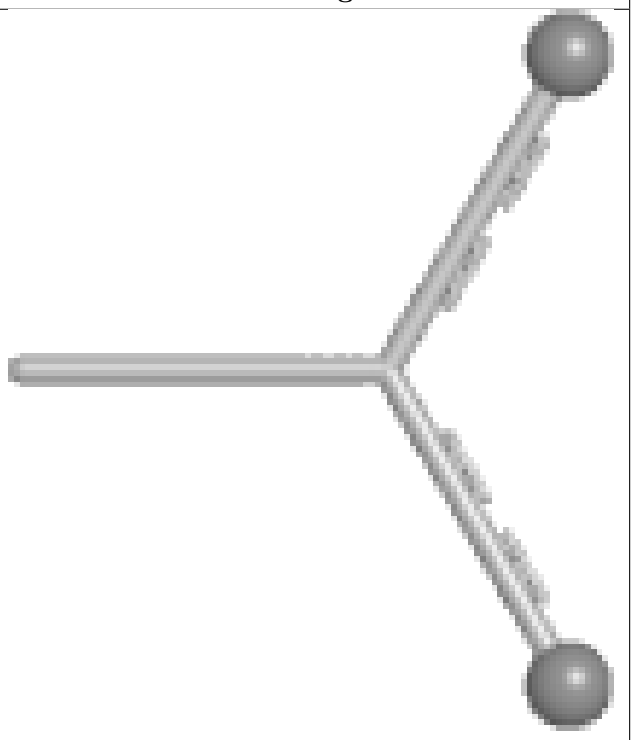
Bond lengths



Bond angles

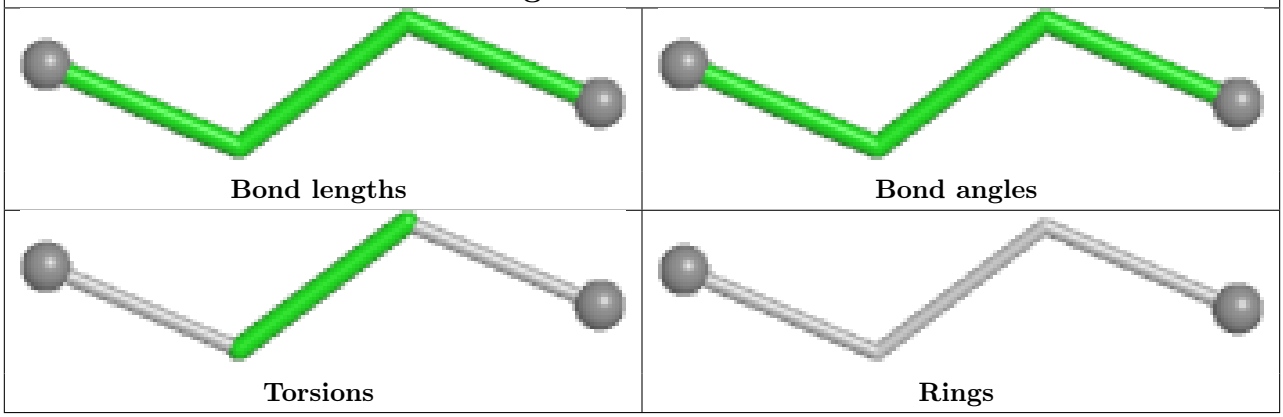


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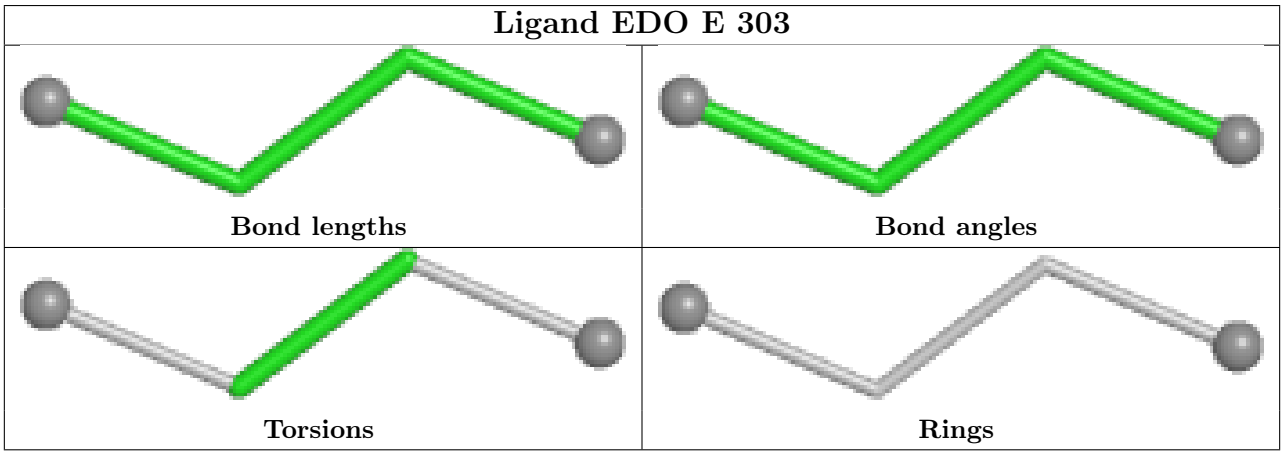


Rings

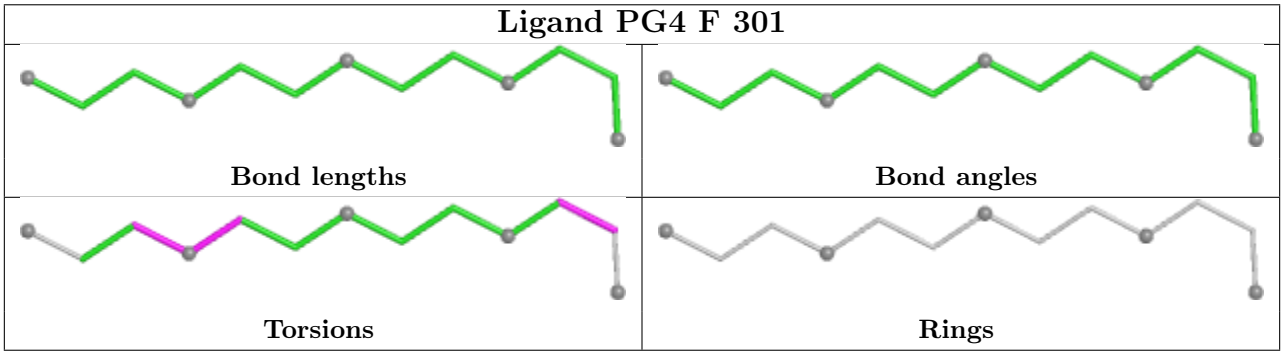
Ligand EDO B 305



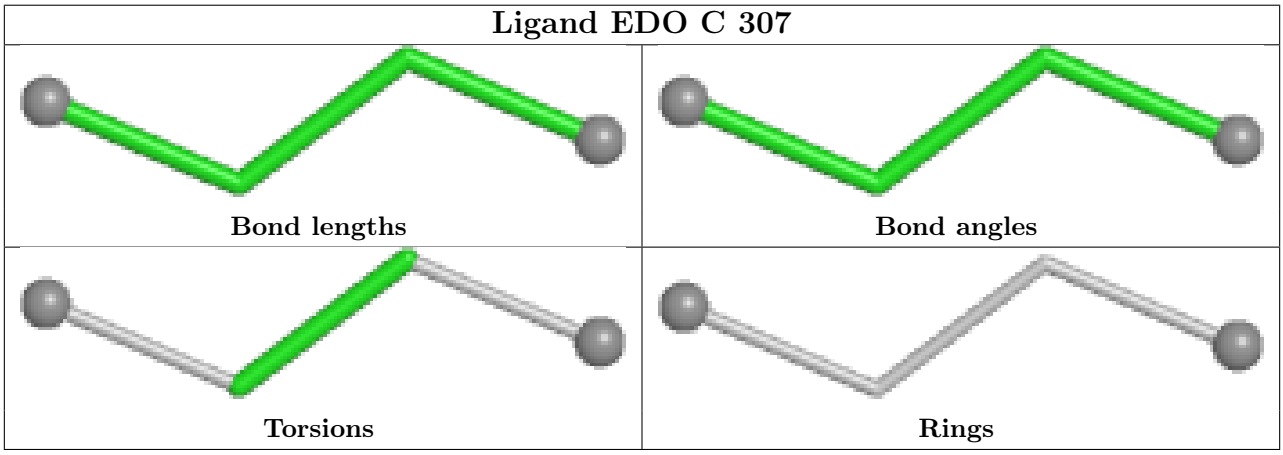
Ligand EDO E 303



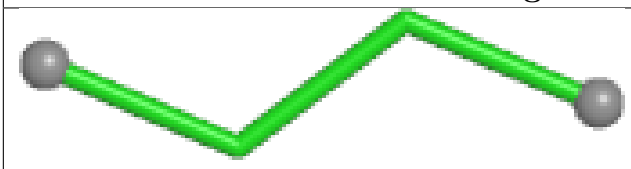
Ligand PG4 F 301



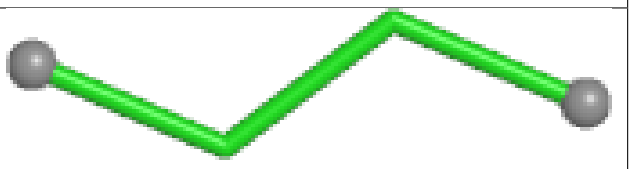
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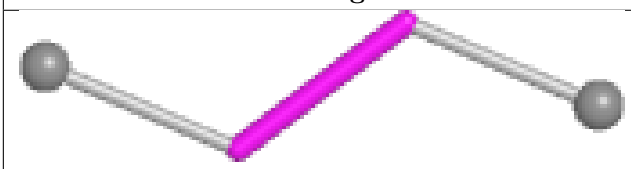
Ligand EDO E 305



Bond lengths



Bond angles

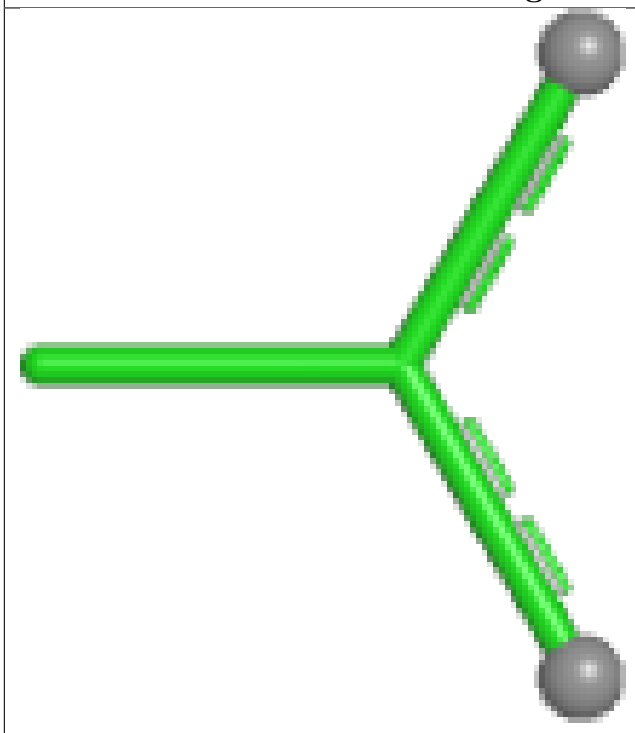


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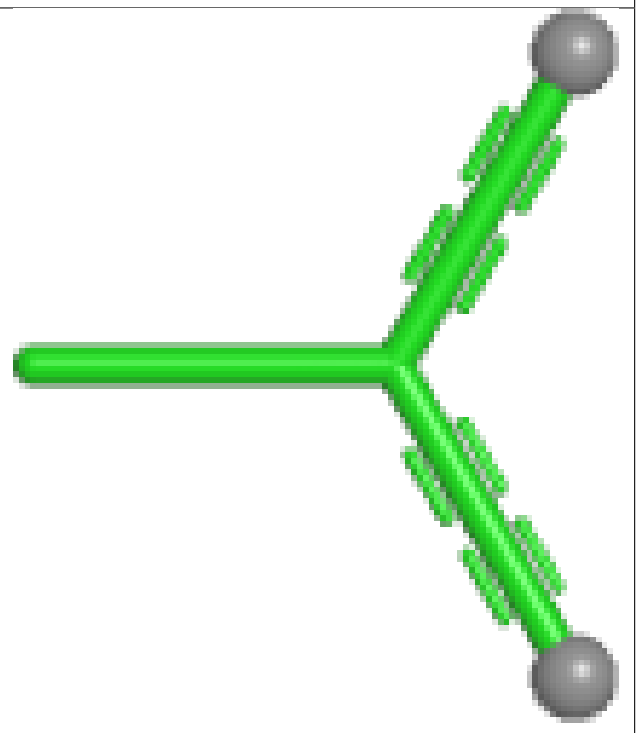


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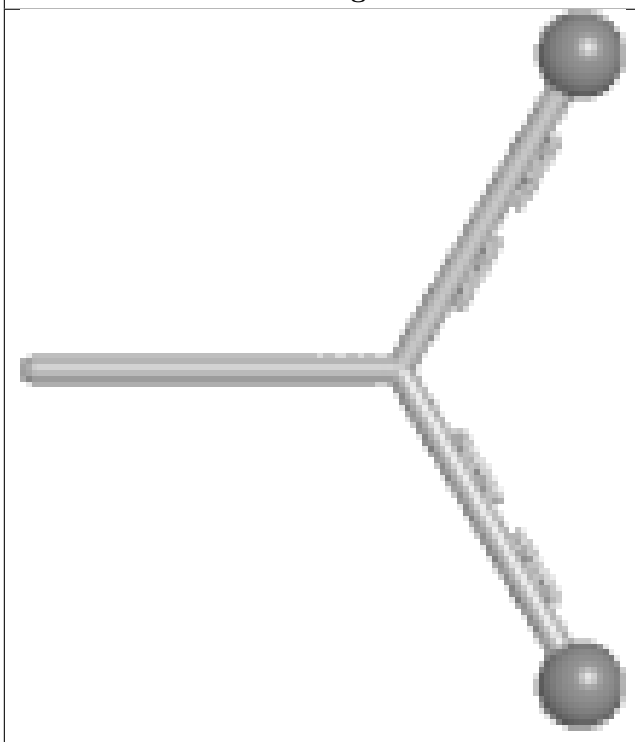
Ligand ACT E 308



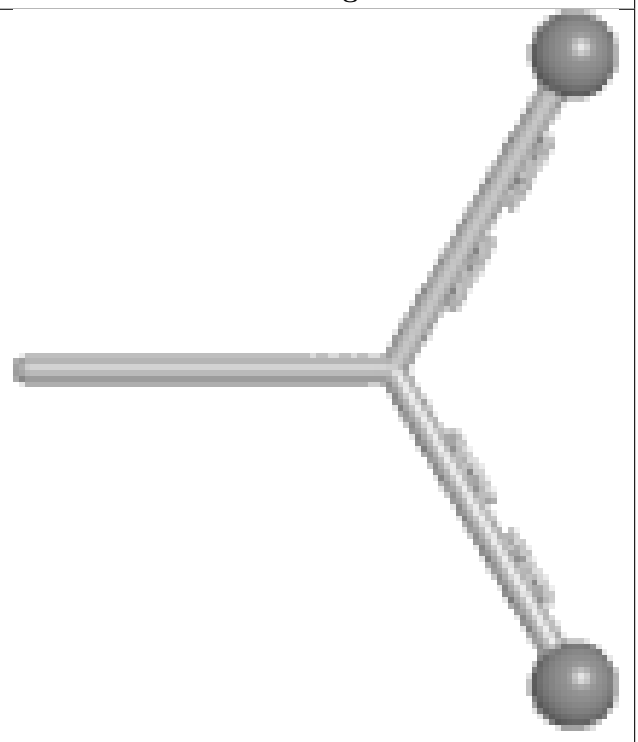
Bond lengths



Bond angles

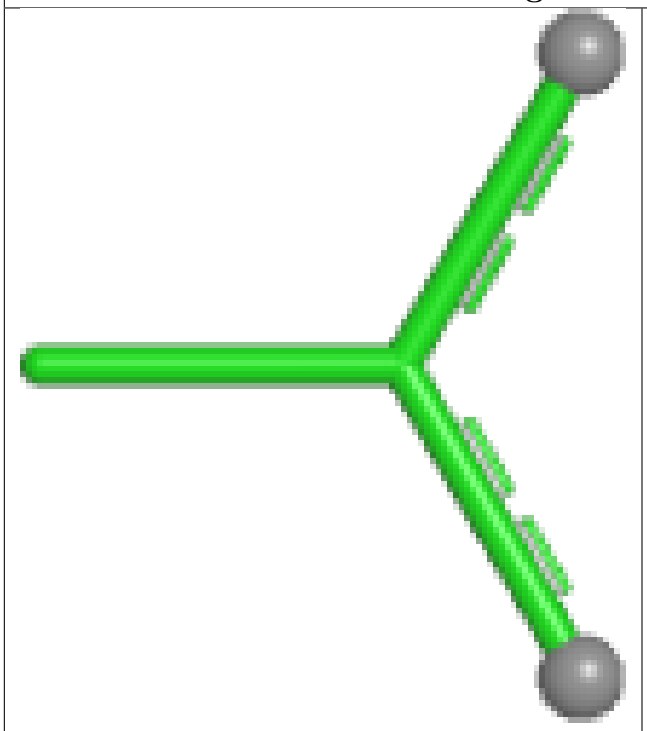


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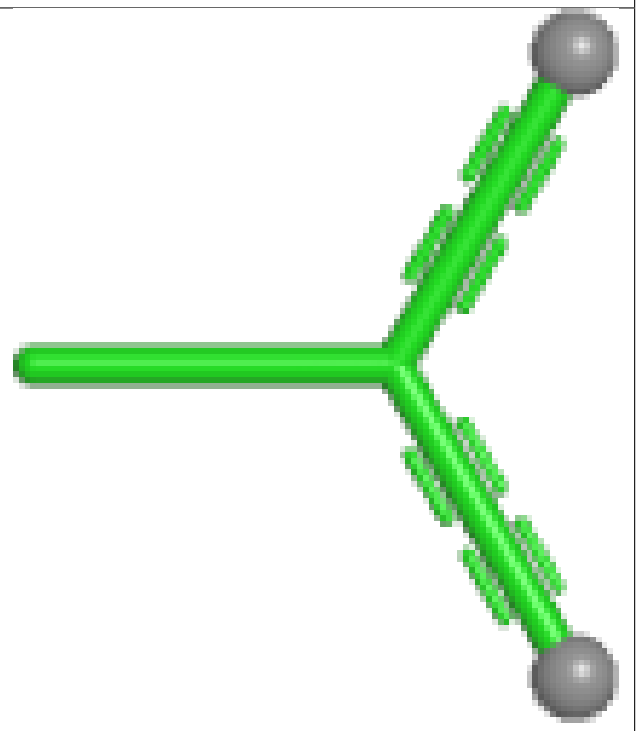


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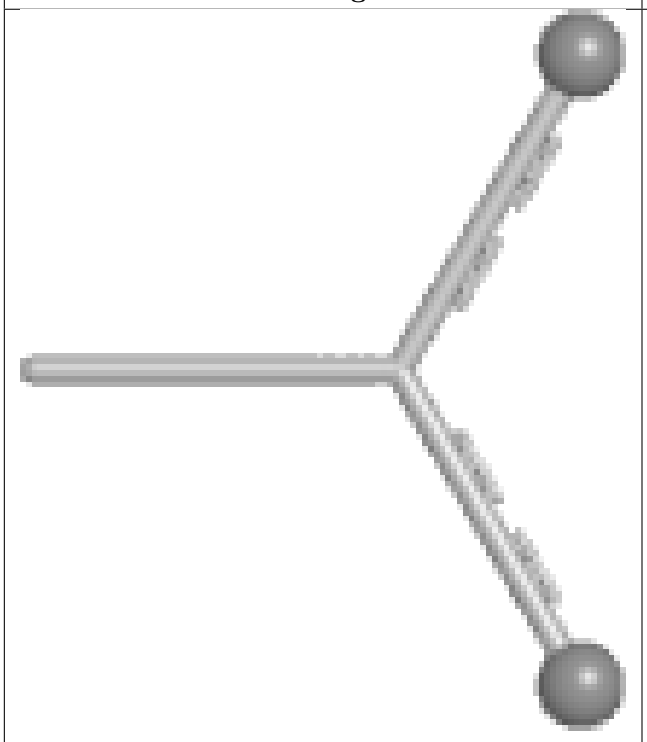
Ligand ACT F 305



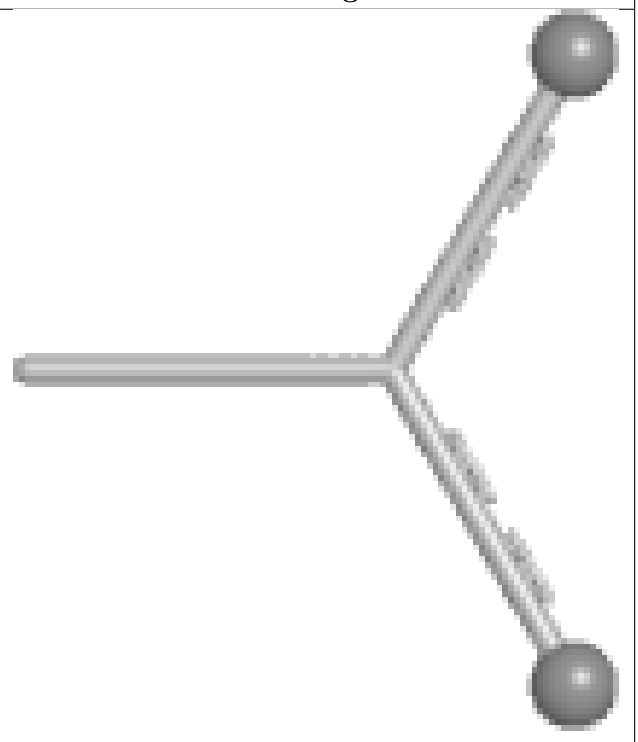
Bond lengths



Bond angles

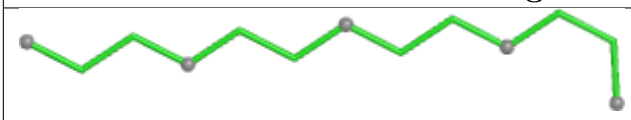


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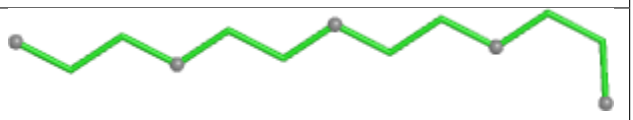


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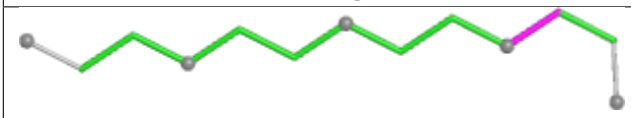
Ligand PG4 A 301



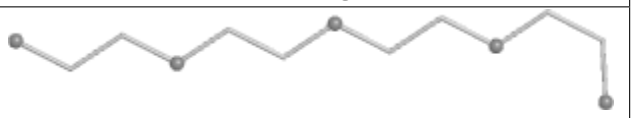
Bond lengths



Bond angles

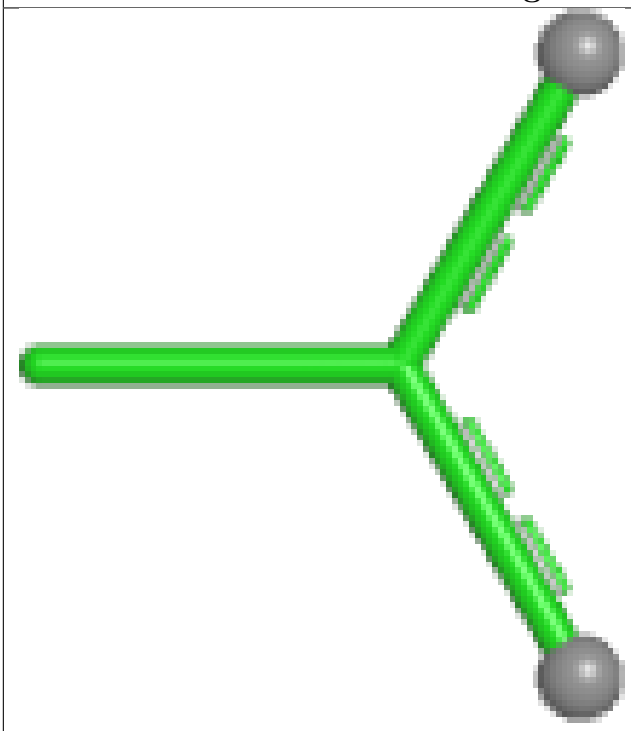


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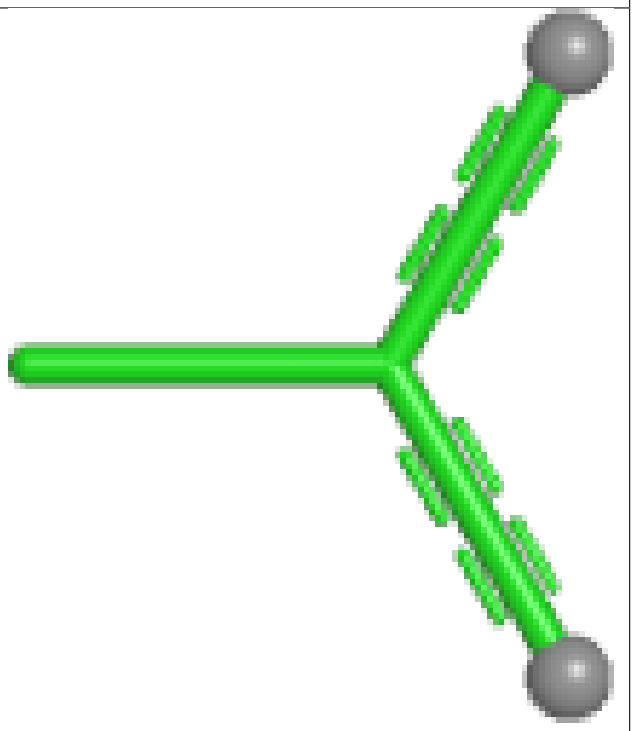


Rings

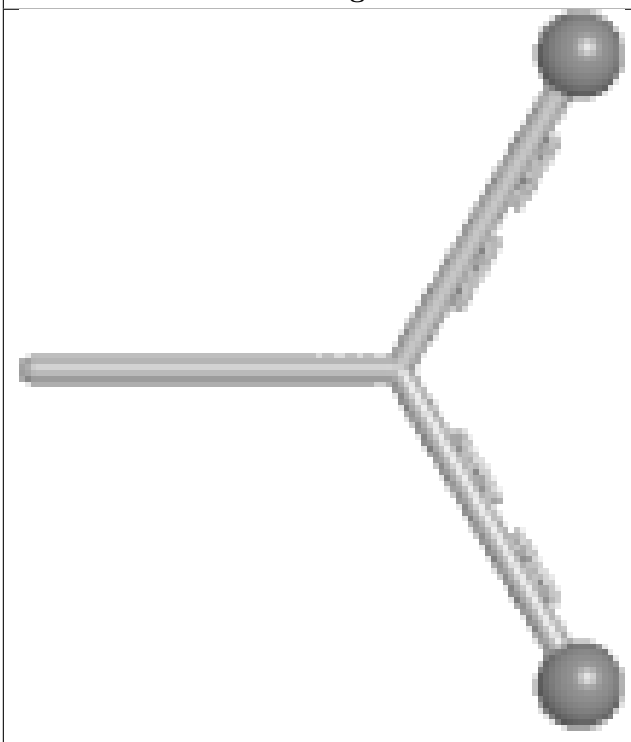
Ligand ACT B 310



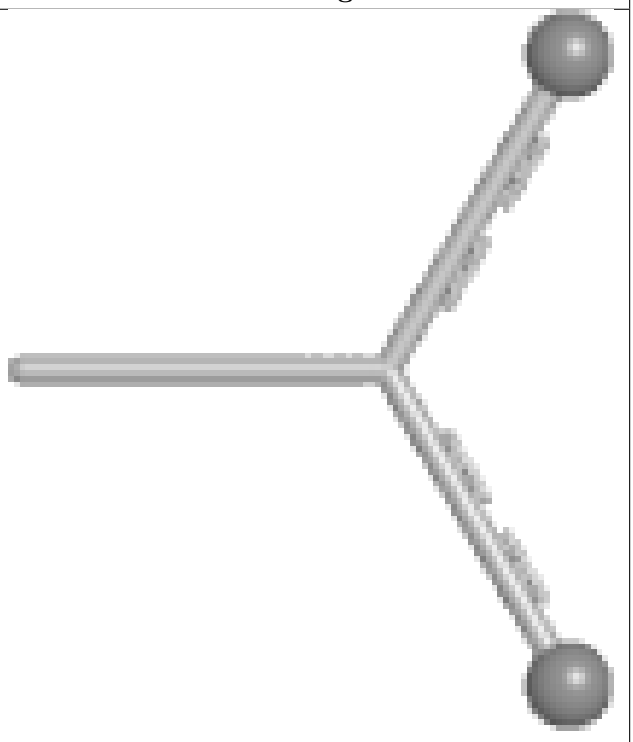
Bond lengths



Bond angles

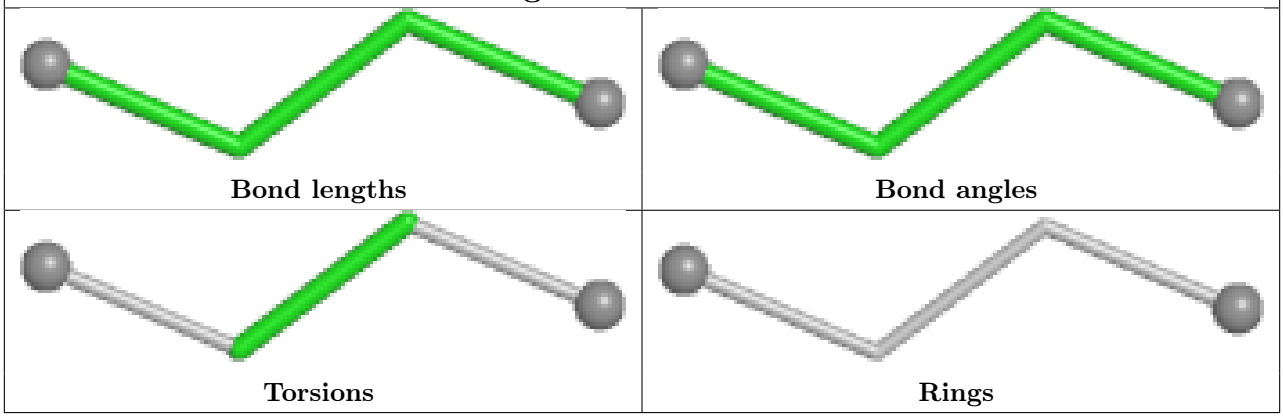


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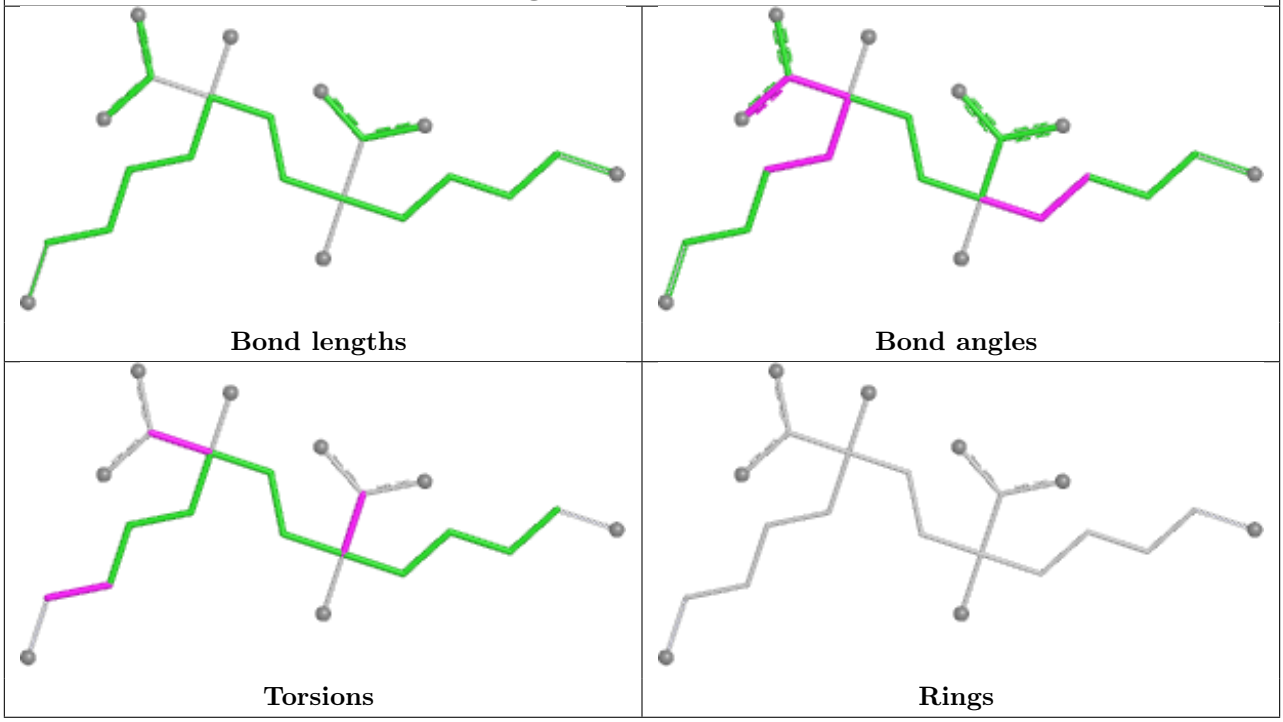


Rings

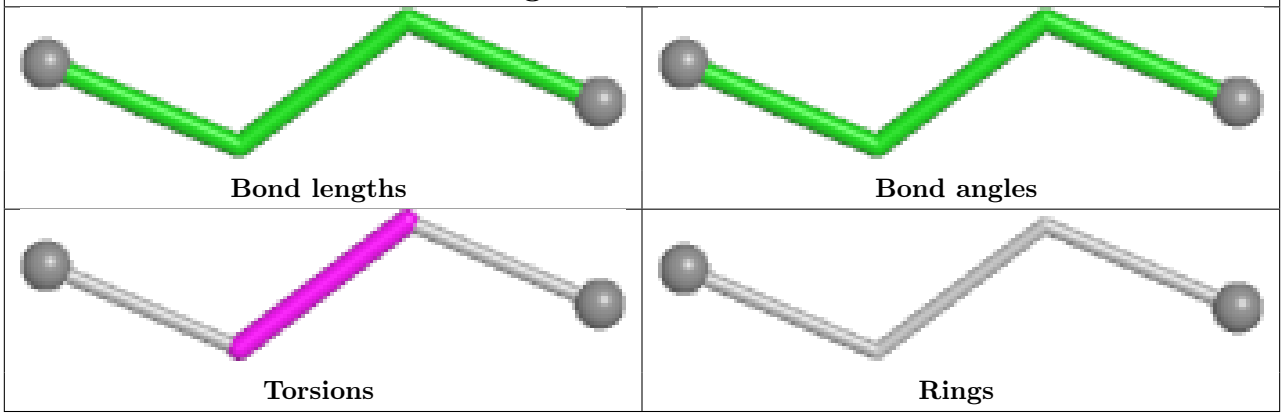
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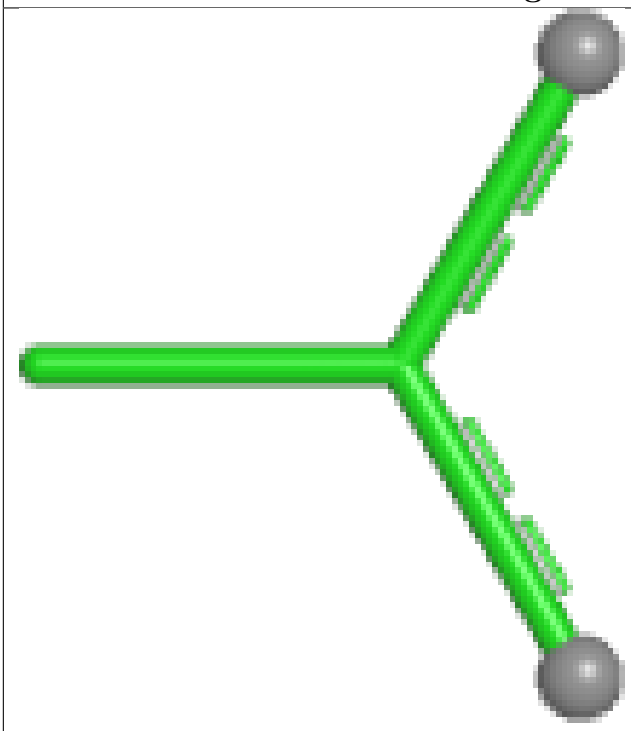
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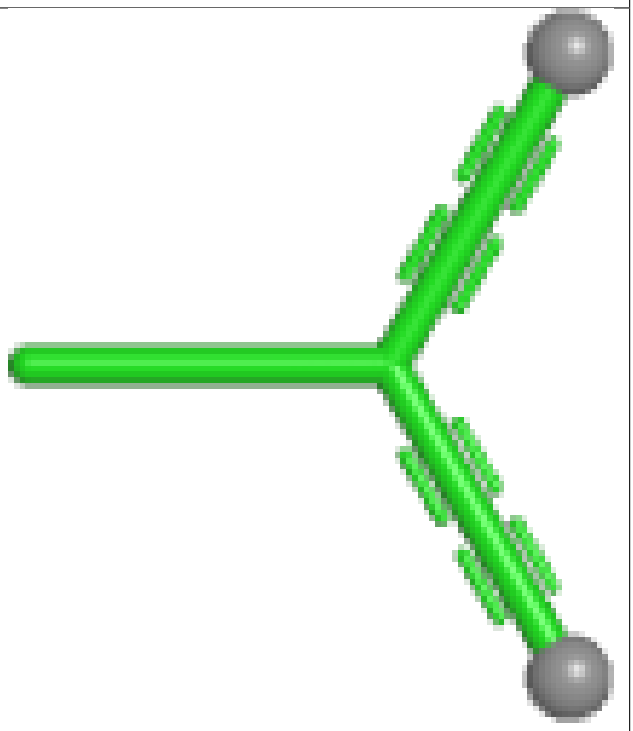
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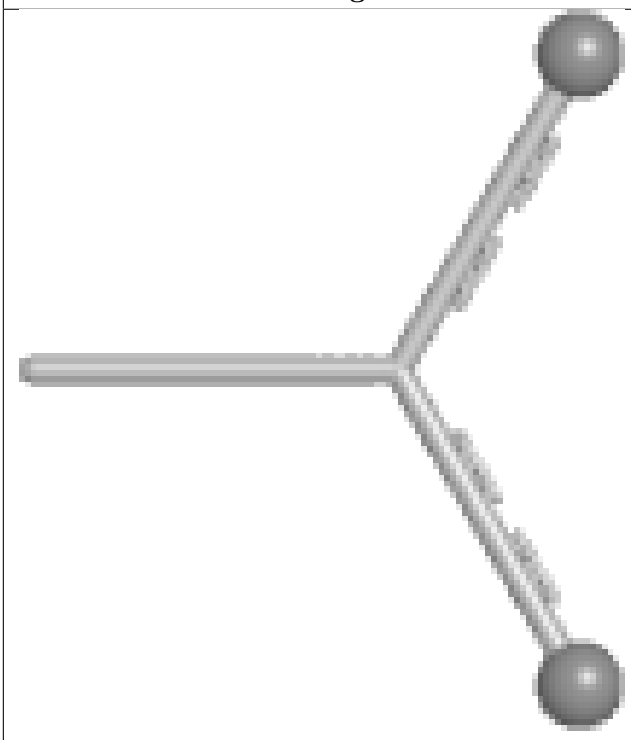
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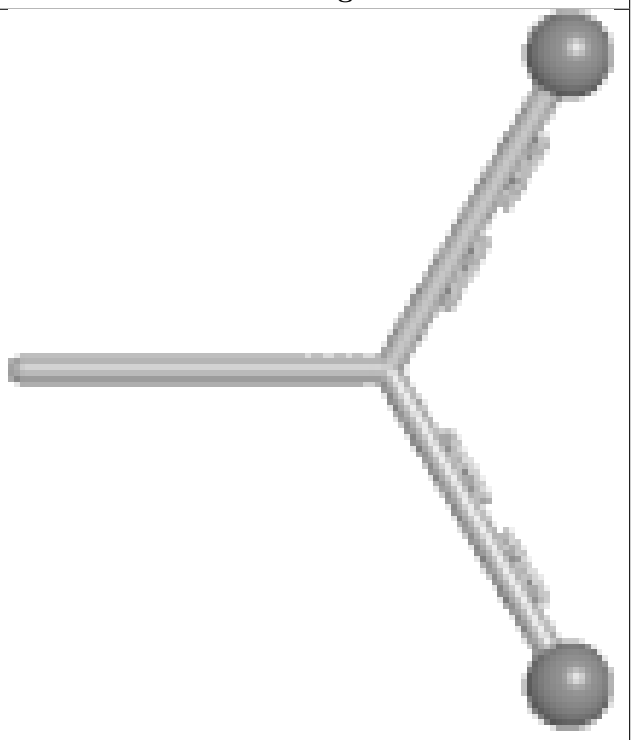
Bond lengths



Bond angles

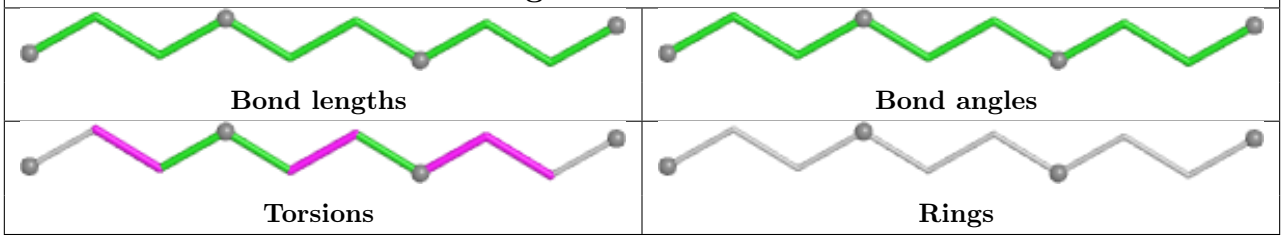


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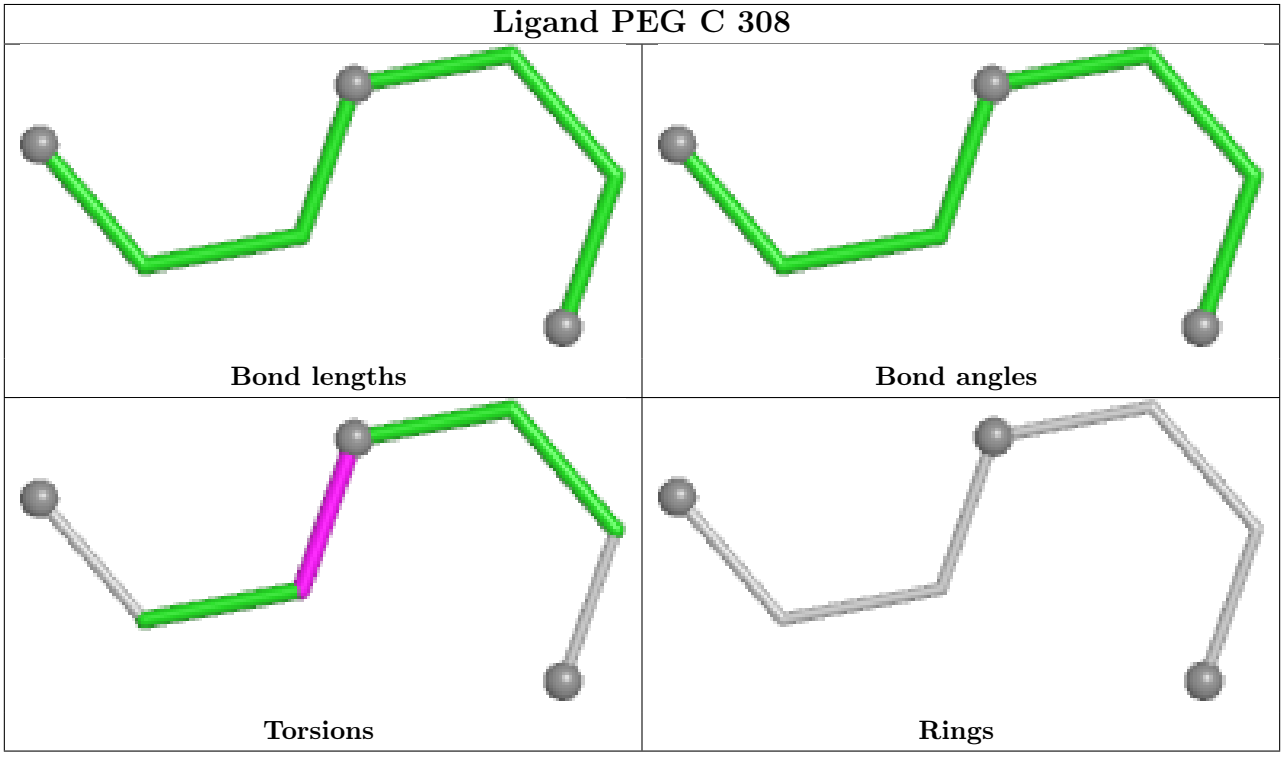


Rings

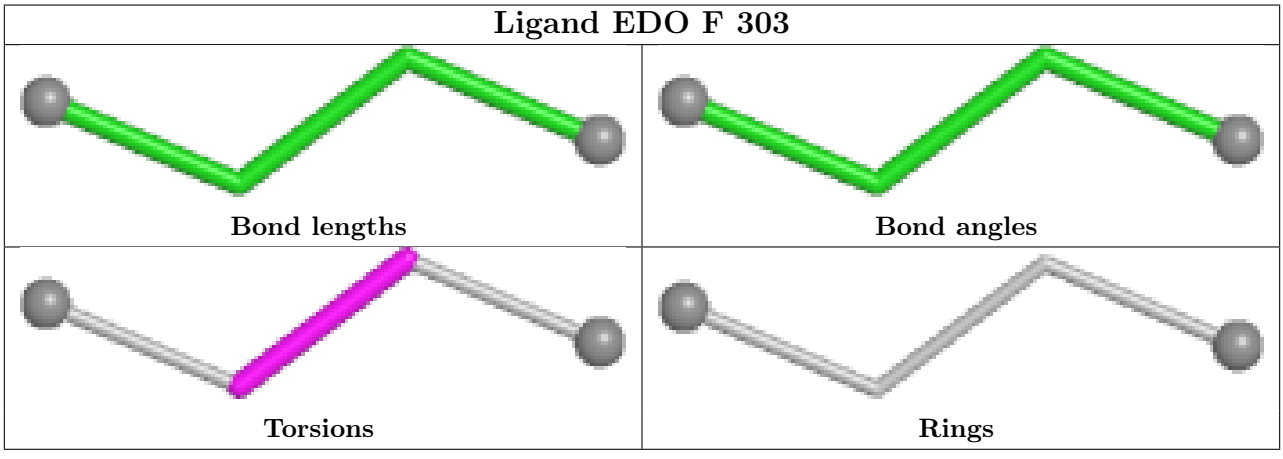
Ligand PGE E 302



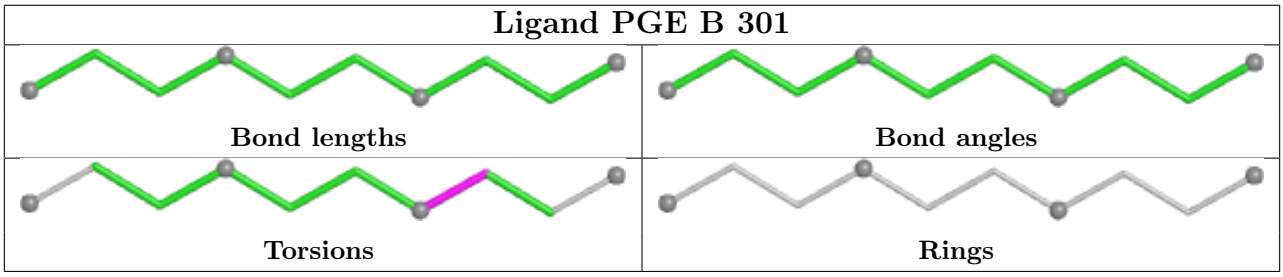
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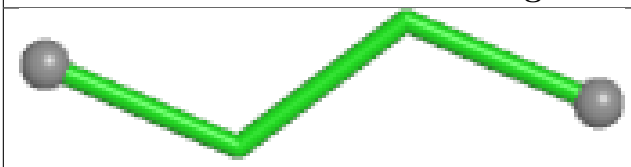
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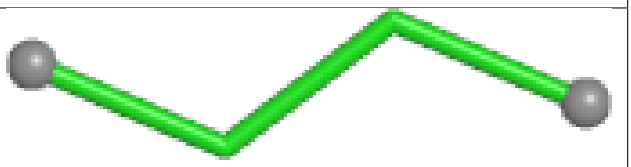
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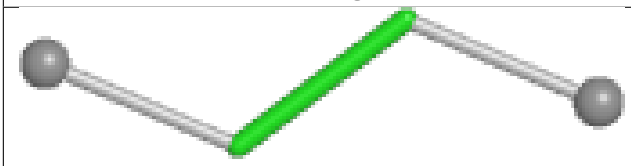
Ligand EDO F 304



Bond lengths



Bond angles

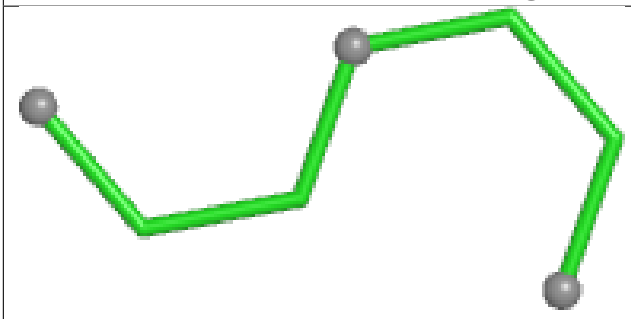


Torsions

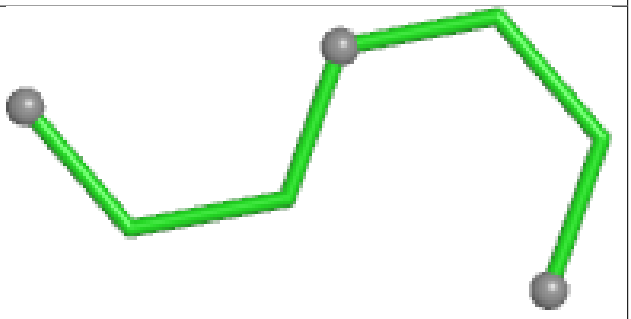


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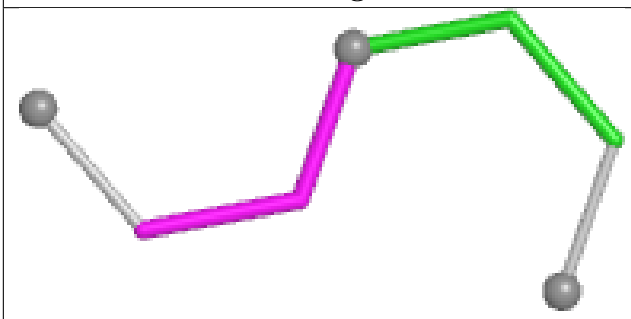
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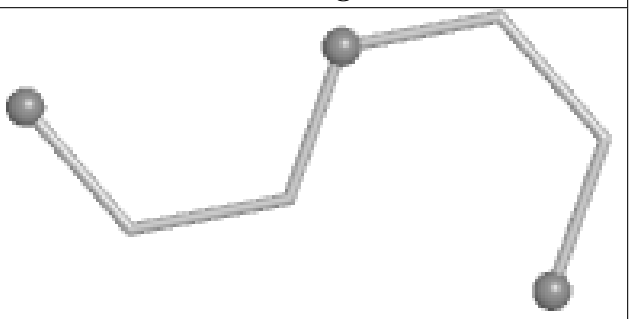
Bond lengths



Bond angles

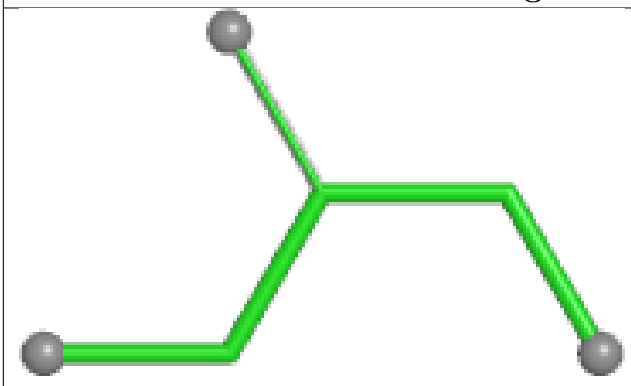


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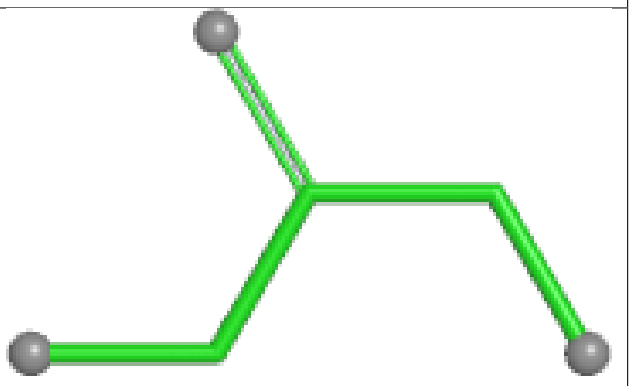


Rings

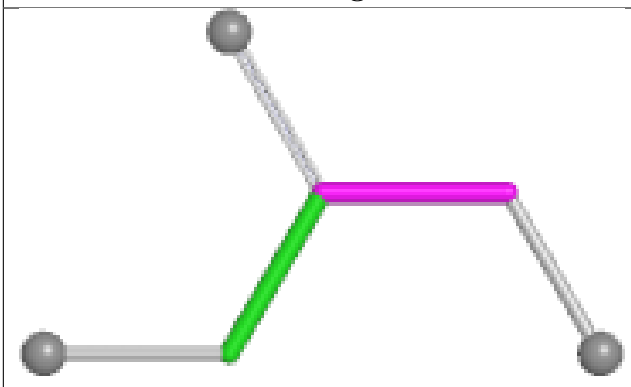
Ligand GOL E 309



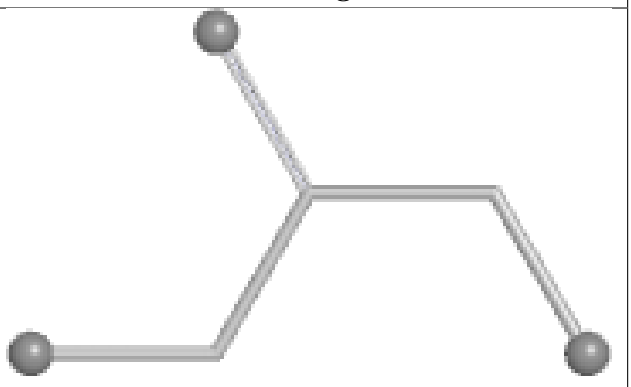
Bond lengths



Bond angles



Torsions

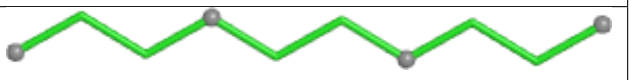


Rings

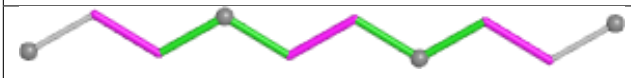
Ligand PGE C 303



Bond lengths



Bond angles

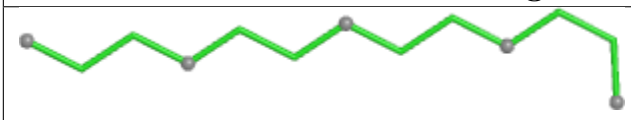


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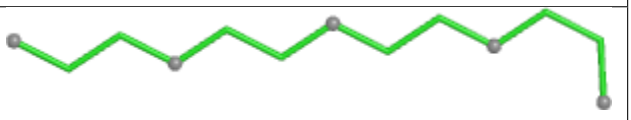


Rings

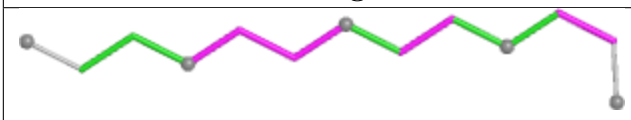
Ligand PG4 A 302



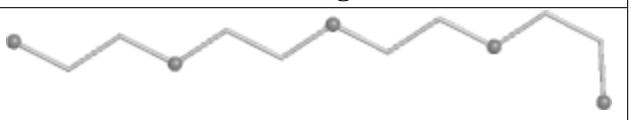
Bond lengths



Bond angles

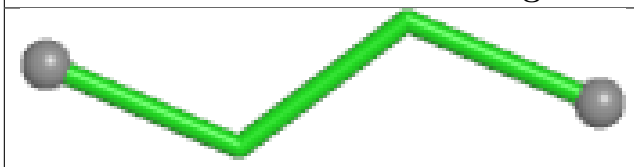


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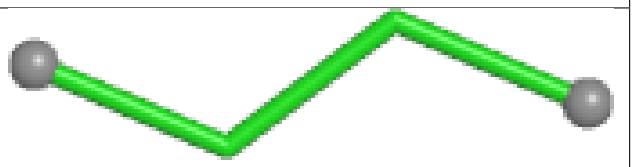


Rings

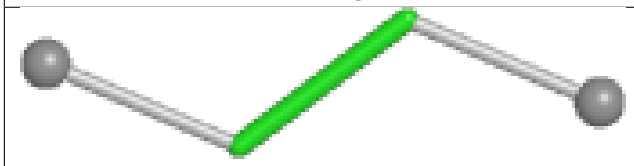
Ligand EDO A 305



Bond lengths



Bond angles

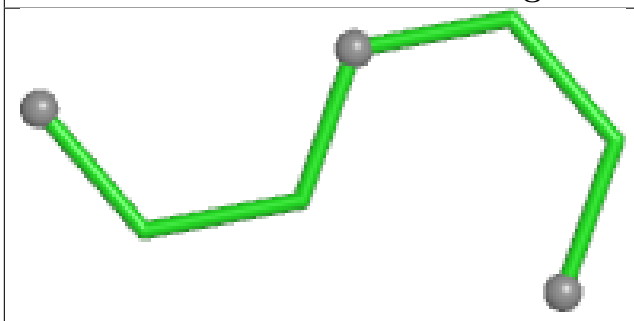


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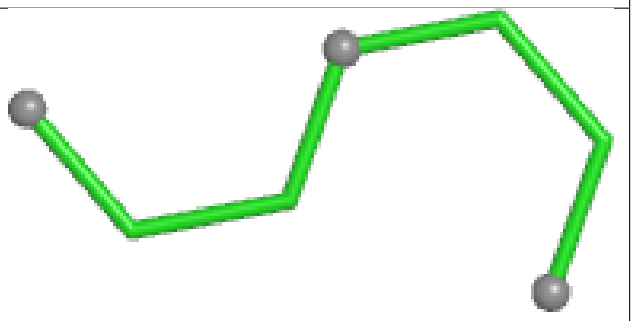


Rings

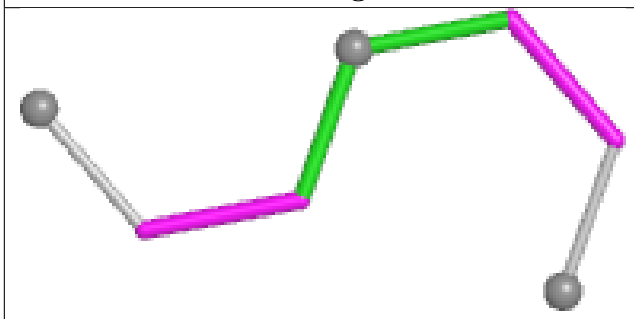
Ligand PEG A 308



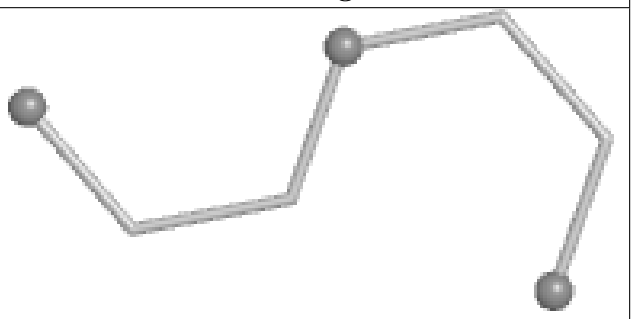
Bond lengths



Bond angles

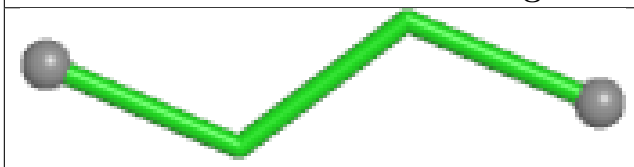


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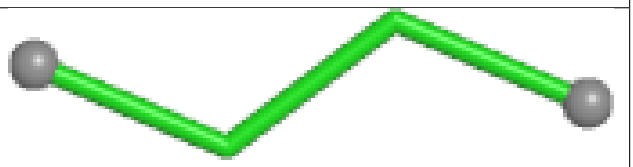


Rings

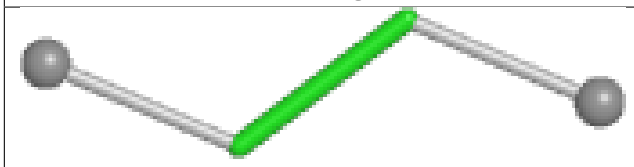
Ligand EDO B 307



Bond lengths



Bond angles

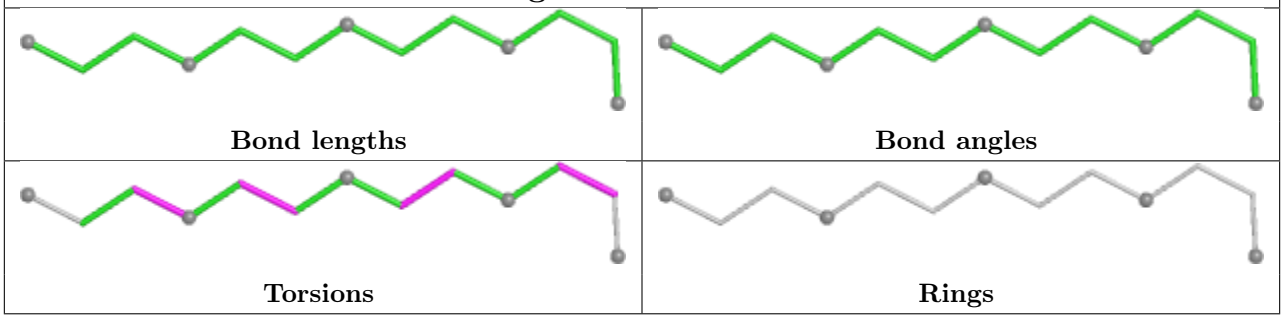


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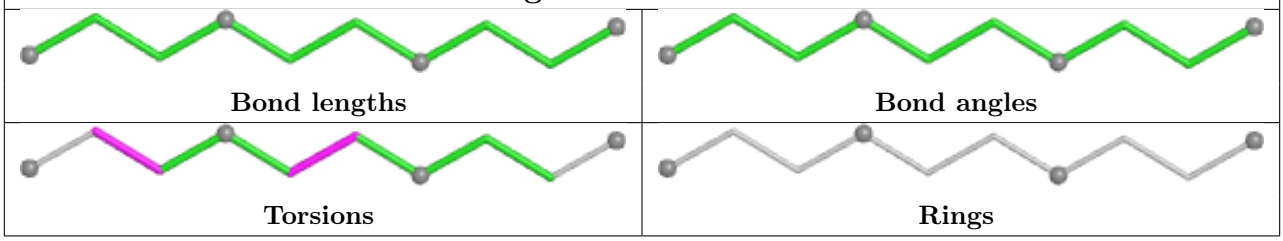


Rings

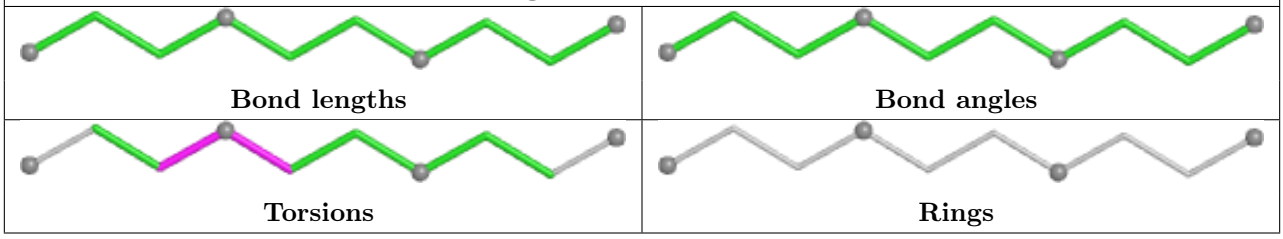
Ligand PG4 E 301



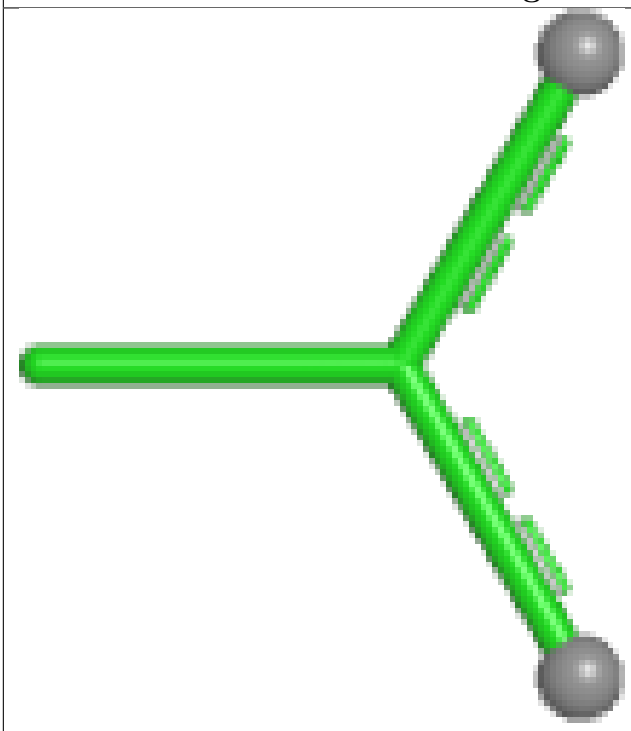
Ligand PGE C 304



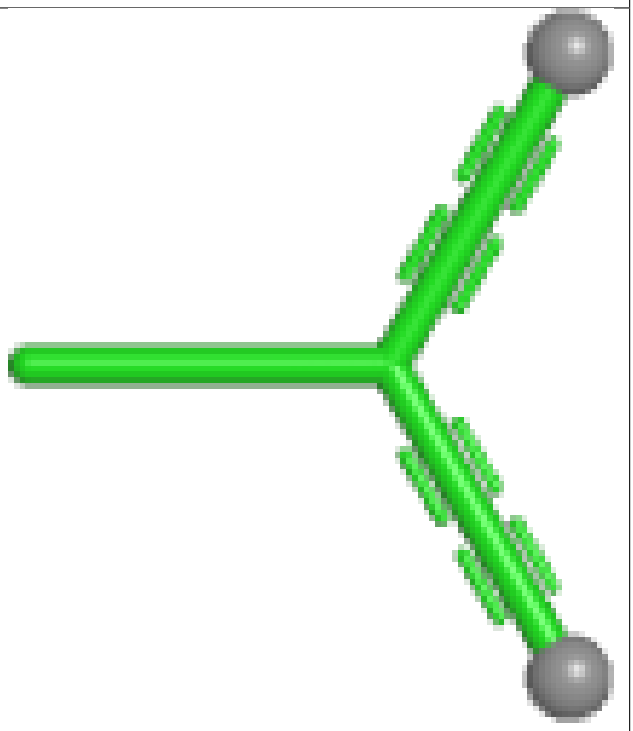
Ligand PGE D 301



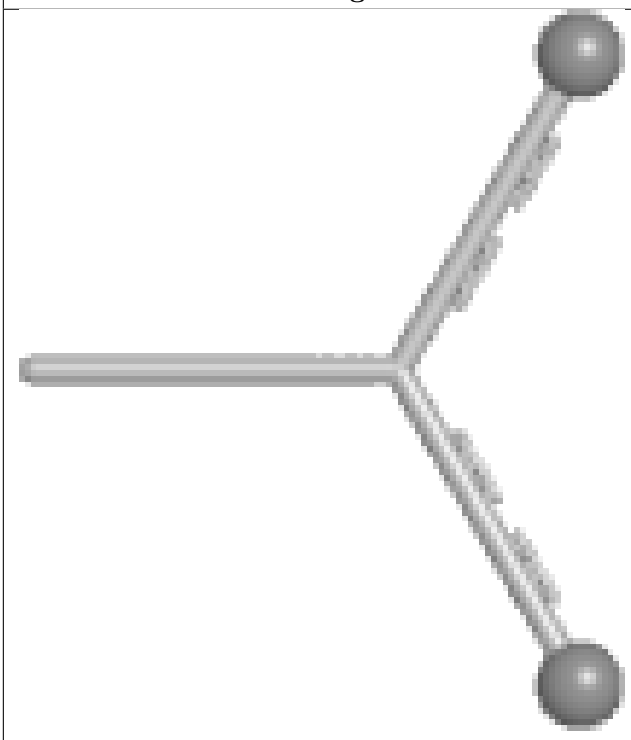
Ligand ACT C 310



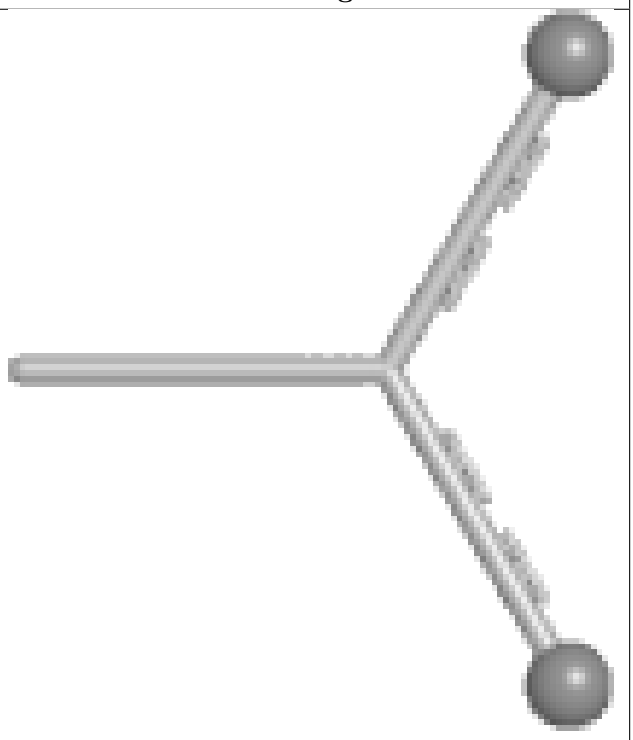
Bond lengths



Bond angles

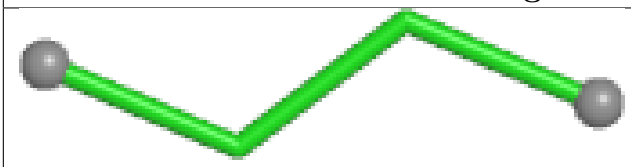


Torsions

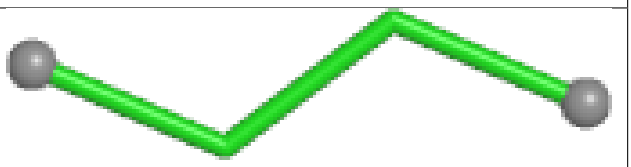


Rings

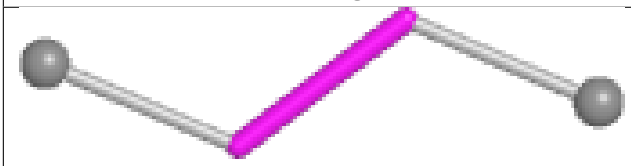
Ligand EDO E 304



Bond lengths



Bond angles

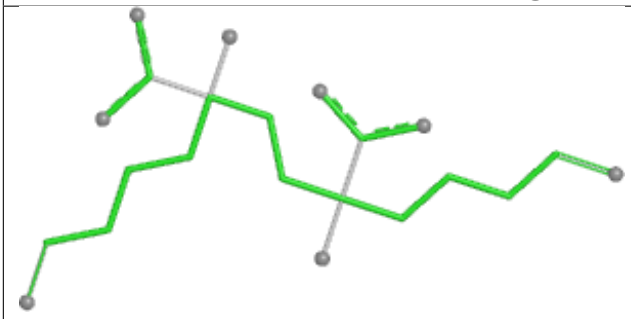


Torsions

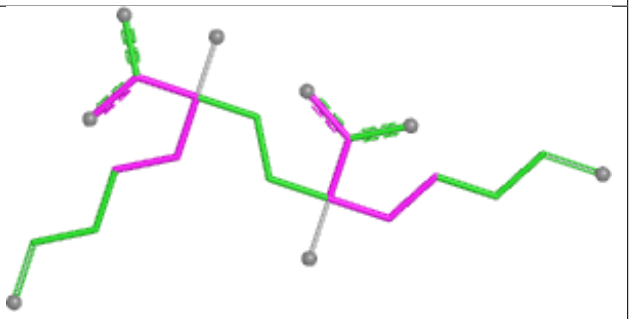


Rings

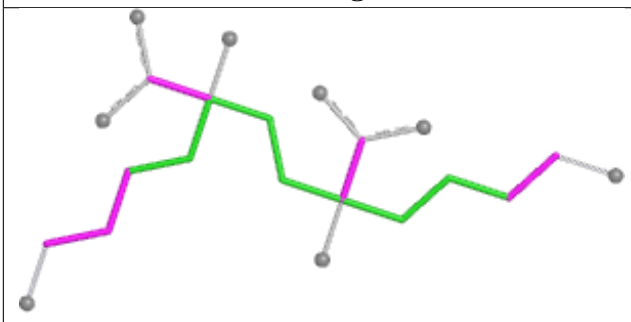
Ligand 3VN F 302



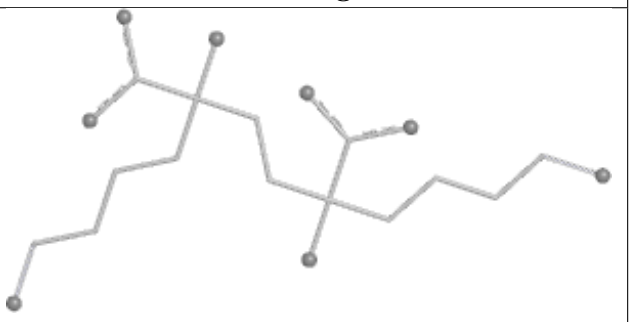
Bond lengths



Bond angles

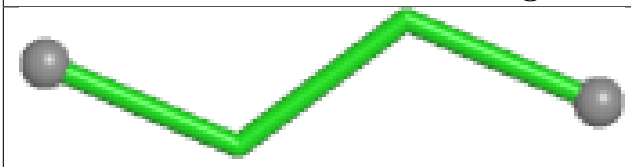


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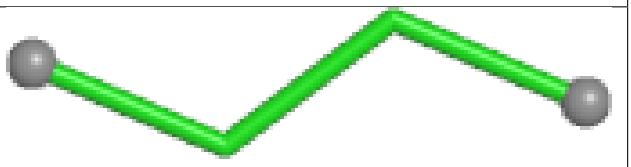


Rings

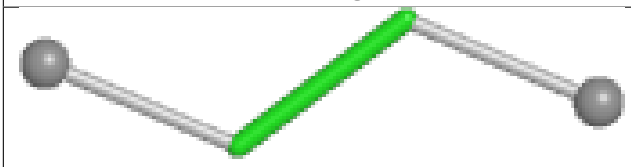
Ligand EDO D 302



Bond lengths



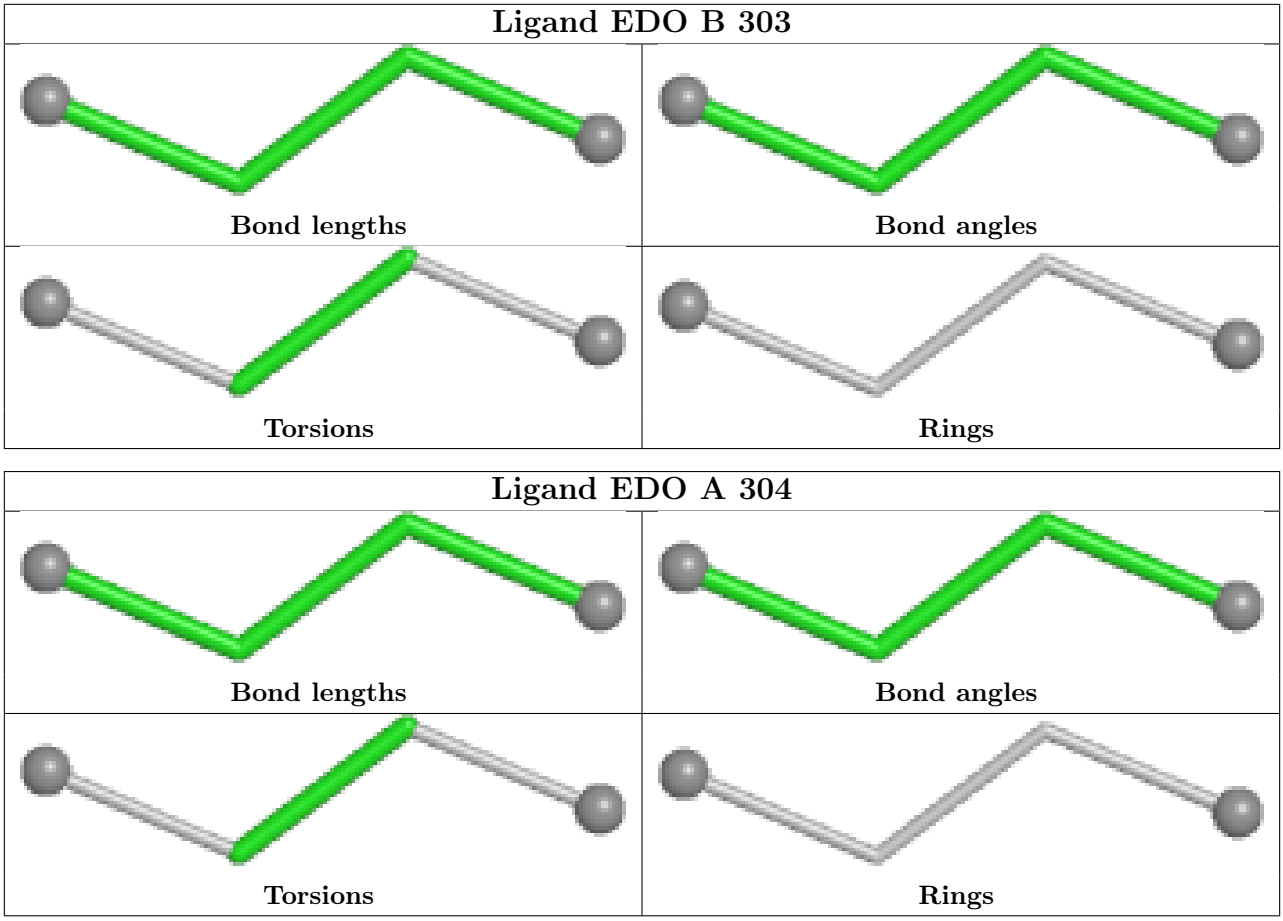
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	295/310 (95%)	-0.03	1 (0%)	90	94	23, 29, 45, 56	0
1	B	295/310 (95%)	-0.02	2 (0%)	84	90	20, 28, 44, 55	1 (0%)
1	C	295/310 (95%)	0.08	2 (0%)	84	90	23, 30, 48, 57	0
1	D	295/310 (95%)	0.18	6 (2%)	65	72	23, 30, 48, 65	2 (0%)
1	E	295/310 (95%)	0.14	7 (2%)	59	66	23, 31, 48, 62	0
1	F	296/310 (95%)	0.14	5 (1%)	69	77	17, 31, 53, 61	1 (0%)
All	All	1771/1860 (95%)	0.08	23 (1%)	75	82	17, 30, 48, 65	4 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	59	ASN	3.5
1	D	72	GLY	3.3
1	F	61	THR	3.0
1	E	61	THR	2.8
1	B	61	THR	2.8
1	D	61	THR	2.7
1	E	57	GLU	2.6
1	F	95	PHE	2.5
1	F	298	PHE	2.4
1	E	96	ALA	2.4
1	E	131	ASP	2.3
1	E	60	ARG	2.3
1	A	95	PHE	2.3
1	C	61	THR	2.3
1	D	56	HIS	2.2
1	D	4	ASN	2.1
1	E	98	GLU	2.1
1	D	60	ARG	2.1
1	C	74	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	68	GLU	2.1
1	F	55	THR	2.0
1	B	100	GLY	2.0
1	E	56	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	A	166	14/15	0.93	0.09	22,26,32,35	0
1	KPI	C	166	14/15	0.94	0.08	20,24,37,39	0
1	KPI	D	166	14/15	0.94	0.08	21,27,34,34	0
1	KPI	E	166	14/15	0.94	0.07	24,28,36,36	0
1	KPI	B	166	14/15	0.95	0.07	20,26,33,33	0
1	KPI	F	166	14/15	0.95	0.07	21,27,38,40	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	C	308	7/7	0.65	0.19	44,46,52,57	0
9	GOL	E	309	6/6	0.68	0.17	48,54,56,61	0
7	ACT	F	305	4/4	0.69	0.20	47,50,57,60	0
7	ACT	F	306	4/4	0.70	0.20	40,47,54,57	0
7	ACT	E	308	4/4	0.70	0.17	41,48,57,59	0
7	ACT	B	310	4/4	0.78	0.18	35,47,49,59	0
7	ACT	C	310	4/4	0.78	0.16	38,43,49,55	0
7	ACT	A	311	4/4	0.79	0.14	45,50,50,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	A	307	7/7	0.80	0.15	50,55,55,57	0
7	ACT	E	307	4/4	0.80	0.17	39,45,49,55	0
2	PG4	A	302	13/13	0.82	0.15	44,55,60,63	0
8	PGE	C	304	10/10	0.82	0.16	49,54,60,61	0
8	PGE	E	302	10/10	0.82	0.14	46,54,61,62	0
4	EDO	F	303	4/4	0.82	0.19	34,42,44,55	0
4	EDO	C	305	4/4	0.83	0.13	42,43,49,60	0
4	EDO	B	304	4/4	0.83	0.18	38,41,45,53	0
5	PEG	A	306	7/7	0.83	0.13	46,47,56,61	0
9	GOL	F	307	6/6	0.83	0.13	49,53,60,60	0
6	MG	D	305	1/1	0.84	0.12	52,52,52,52	0
5	PEG	A	308	7/7	0.84	0.14	48,49,54,55	0
7	ACT	A	312	4/4	0.85	0.17	40,46,50,51	0
2	PG4	F	301	13/13	0.86	0.13	36,43,56,57	0
5	PEG	D	304	7/7	0.87	0.13	46,52,56,61	0
7	ACT	D	307	4/4	0.87	0.13	41,46,47,48	0
6	MG	B	308	1/1	0.88	0.12	49,49,49,49	0
8	PGE	C	303	10/10	0.88	0.14	31,41,51,59	0
4	EDO	C	306	4/4	0.88	0.12	33,34,45,46	0
4	EDO	E	303	4/4	0.88	0.12	44,48,48,60	0
2	PG4	C	301	13/13	0.88	0.11	41,49,57,58	0
4	EDO	A	304	4/4	0.88	0.23	33,39,40,56	0
4	EDO	A	305	4/4	0.89	0.14	32,37,45,49	0
4	EDO	E	305	4/4	0.89	0.13	45,47,47,51	0
4	EDO	F	304	4/4	0.90	0.12	50,56,57,61	0
2	PG4	A	301	13/13	0.90	0.10	34,38,55,61	0
3	3VN	C	302	22/22	0.90	0.10	27,31,38,43	0
5	PEG	E	306	7/7	0.90	0.10	41,49,53,61	0
4	EDO	B	302	4/4	0.91	0.13	29,36,48,50	0
6	MG	A	310	1/1	0.91	0.21	61,61,61,61	0
4	EDO	E	304	4/4	0.92	0.12	35,40,42,44	0
4	EDO	B	303	4/4	0.92	0.10	40,47,49,59	0
6	MG	C	309	1/1	0.92	0.06	30,30,30,30	0
2	PG4	E	301	13/13	0.92	0.12	40,46,54,56	0
4	EDO	C	307	4/4	0.92	0.10	47,48,49,53	0
4	EDO	B	306	4/4	0.92	0.12	31,33,38,48	0
3	3VN	A	303	22/22	0.93	0.09	21,28,37,41	0
4	EDO	B	307	4/4	0.94	0.10	37,40,46,50	0
8	PGE	D	301	10/10	0.94	0.10	36,41,44,49	0
6	MG	D	306	1/1	0.94	0.07	35,35,35,35	0
8	PGE	B	301	10/10	0.94	0.08	35,42,48,56	0
3	3VN	F	302	22/22	0.94	0.08	26,29,43,45	0

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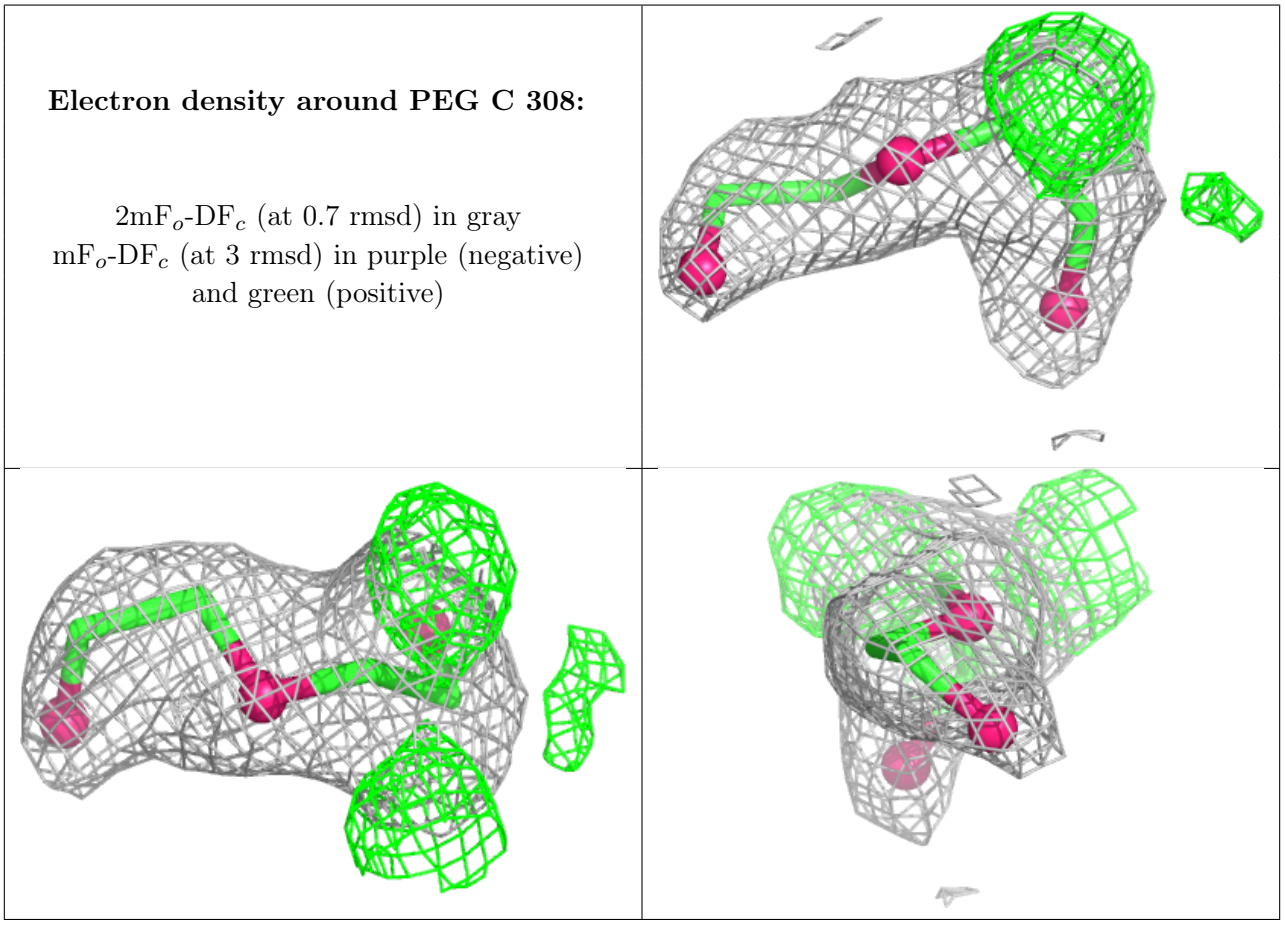
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	D	303	4/4	0.95	0.09	30,36,38,41	0
4	EDO	B	305	4/4	0.96	0.07	32,36,37,49	0
4	EDO	D	302	4/4	0.96	0.08	28,28,31,31	0
6	MG	A	309	1/1	0.96	0.05	51,51,51,51	0
6	MG	B	309	1/1	0.97	0.06	30,30,30,30	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.

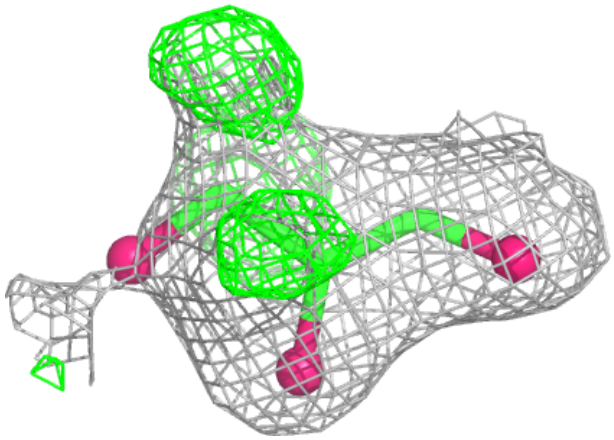
Electron density around PEG C 308:

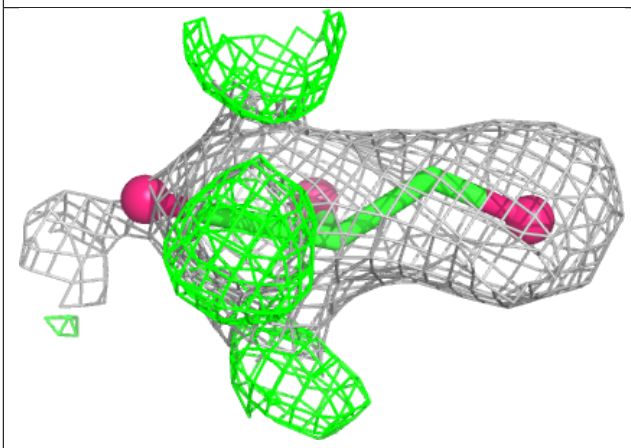
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

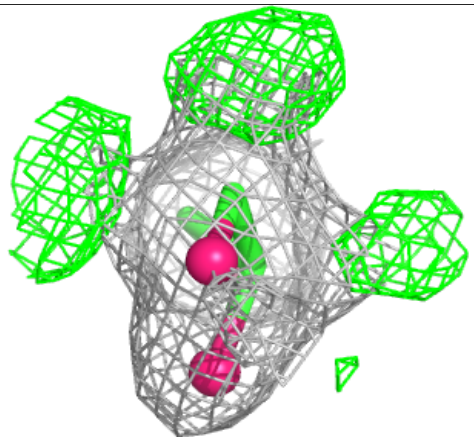


Electron density around GOL E 309:

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

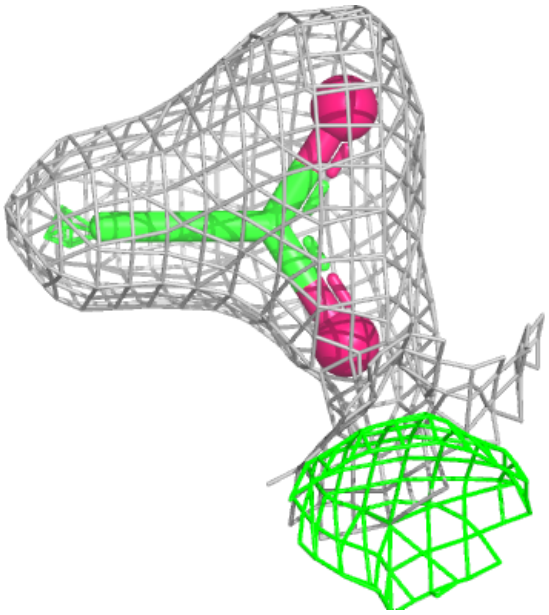


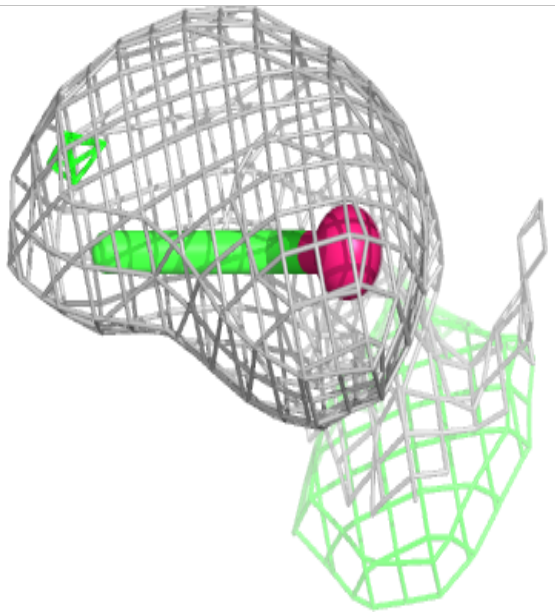


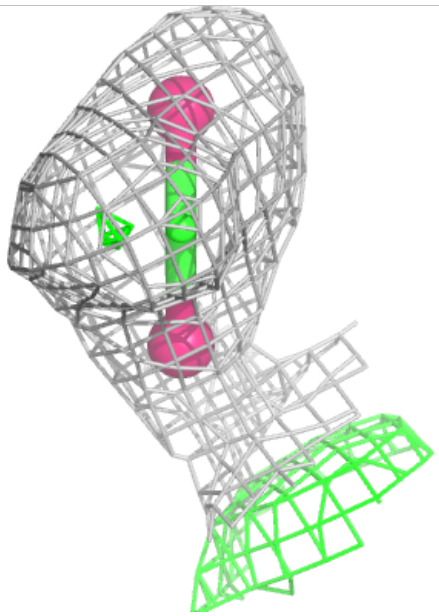


Electron density around ACT F 305:

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

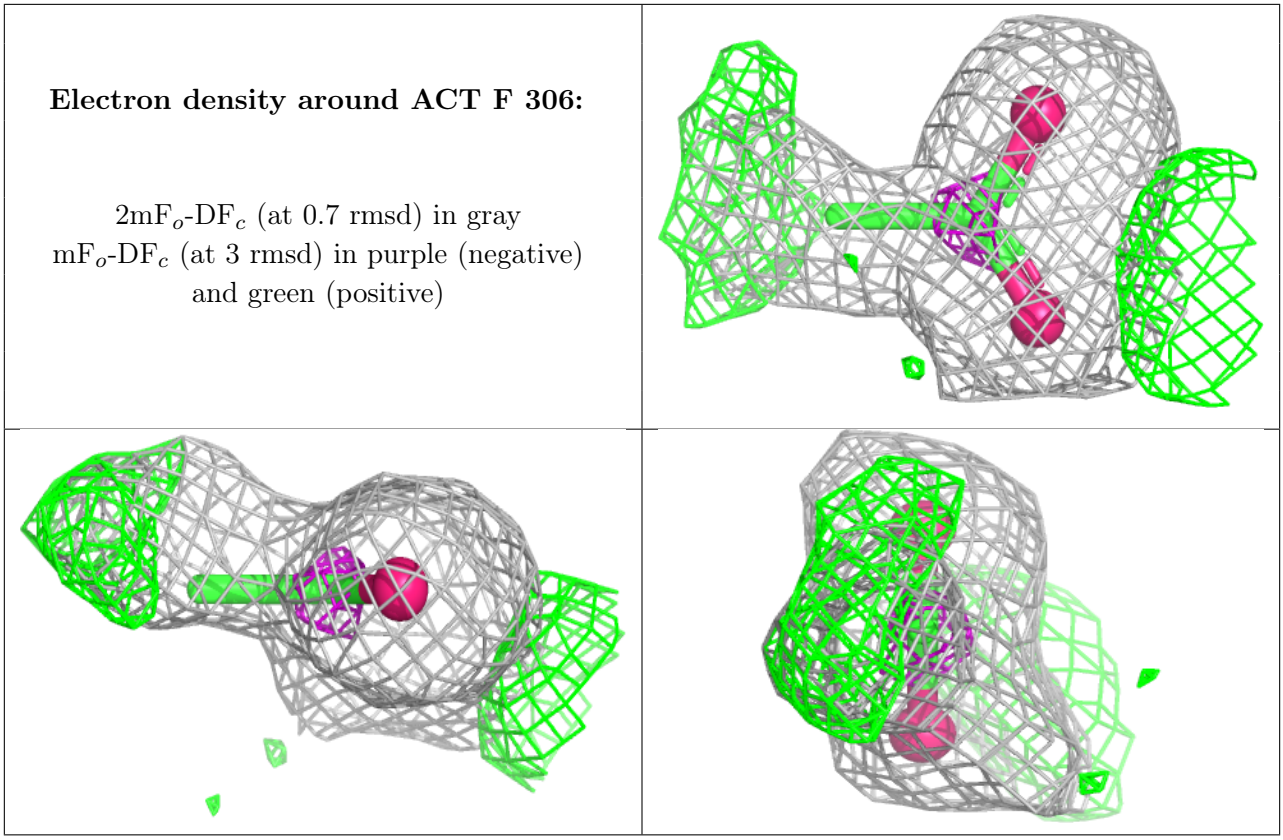






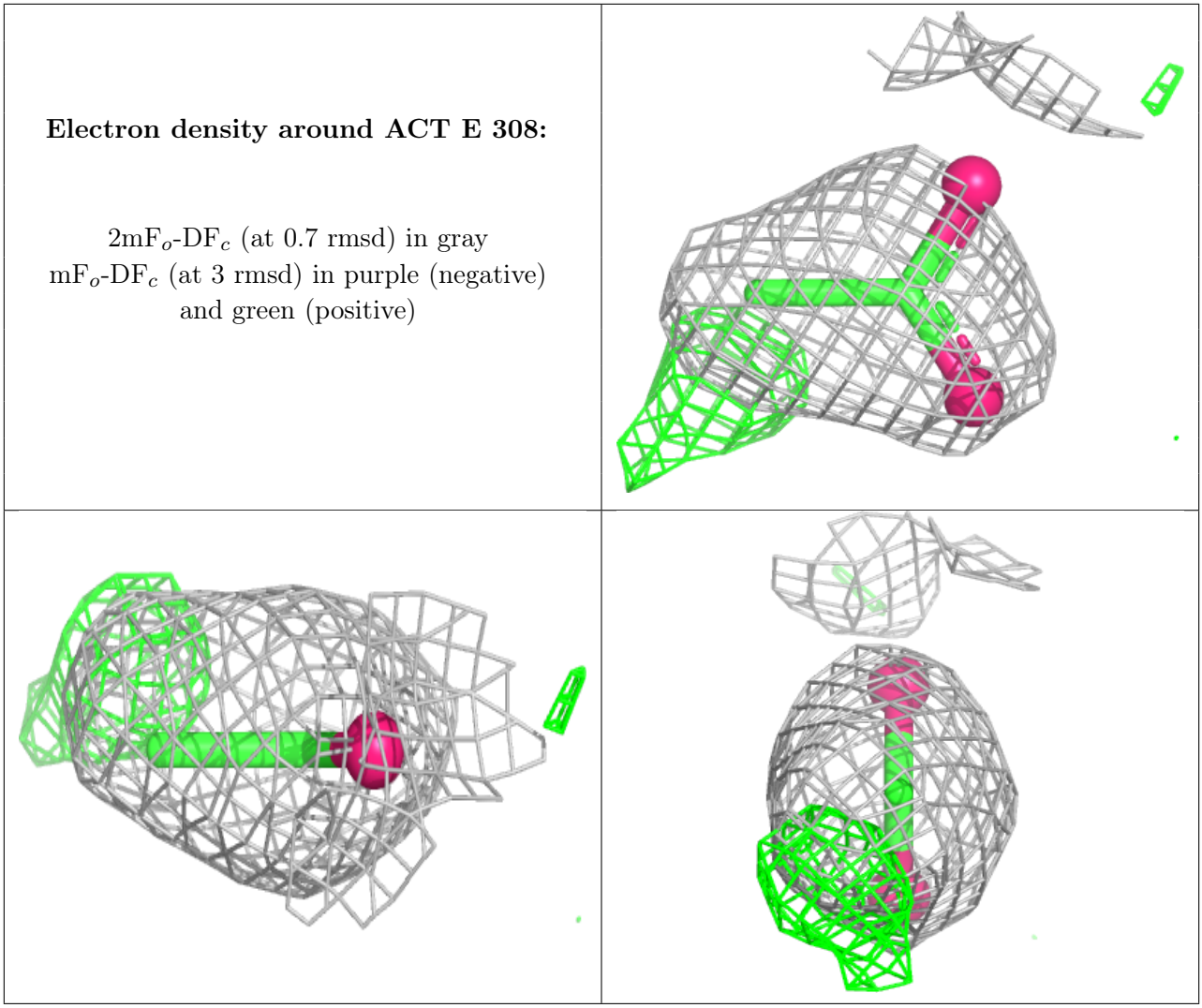
Electron density around ACT F 306:

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



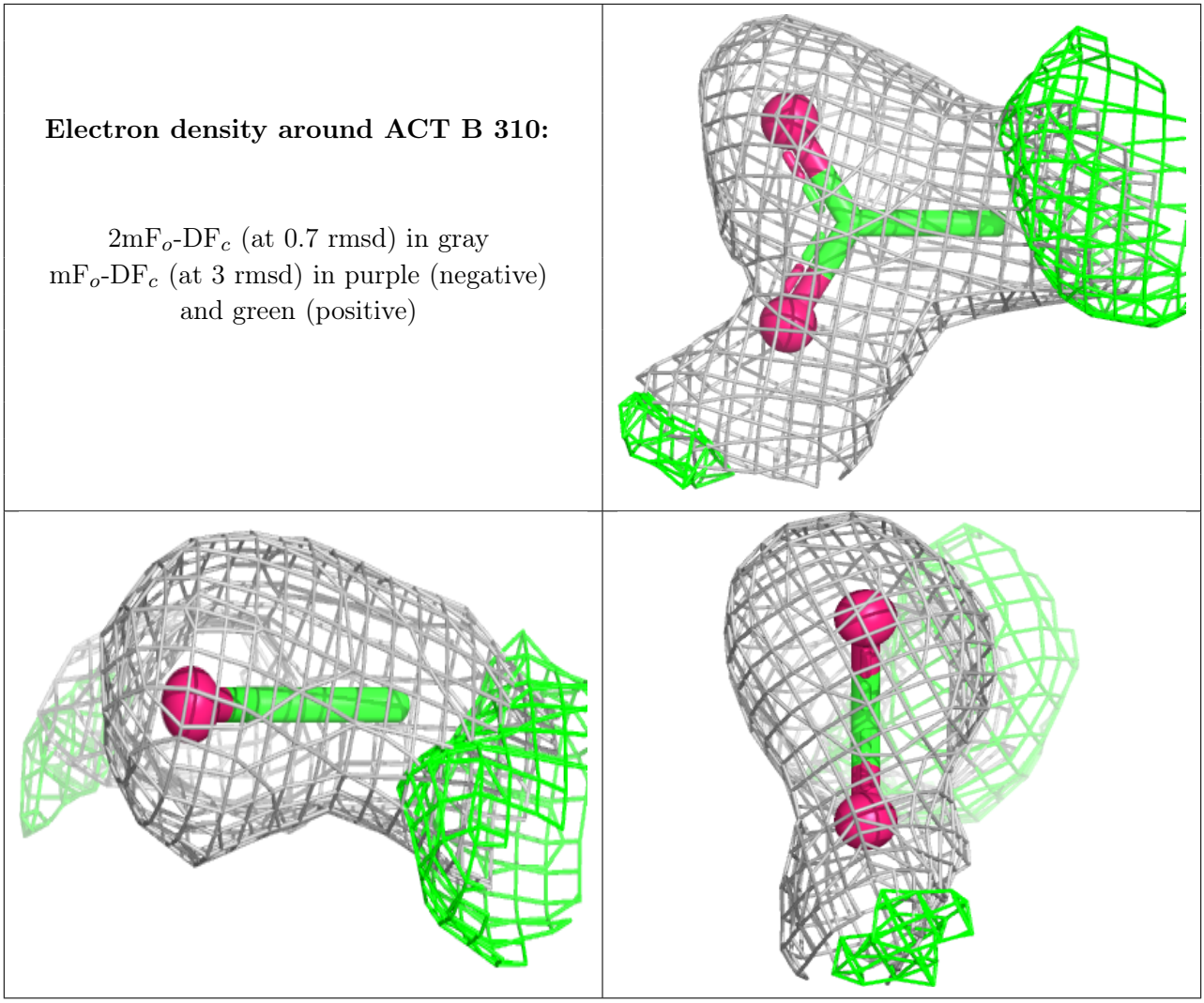
Electron density around ACT E 308:

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



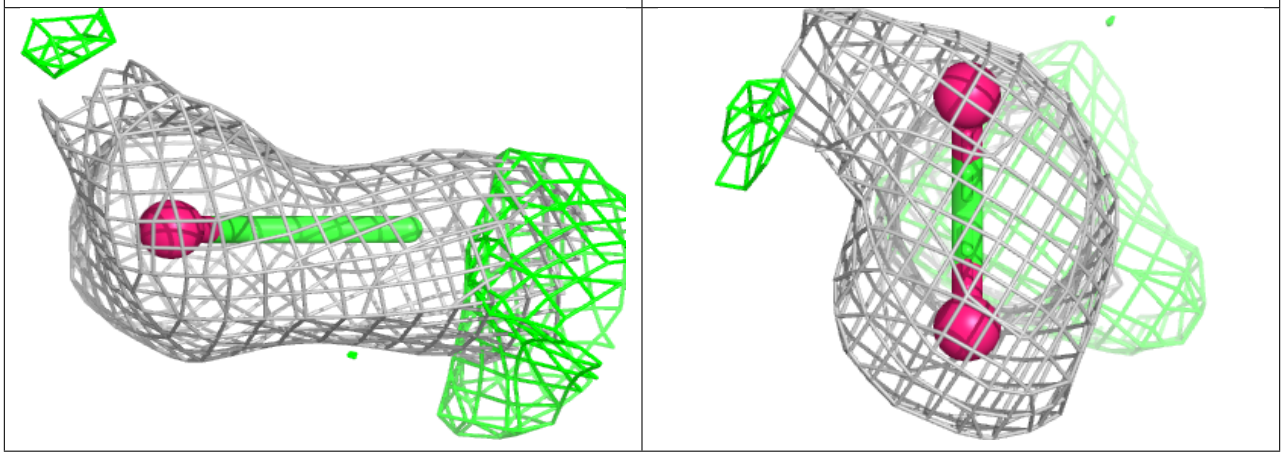
Electron density around ACT B 310:

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



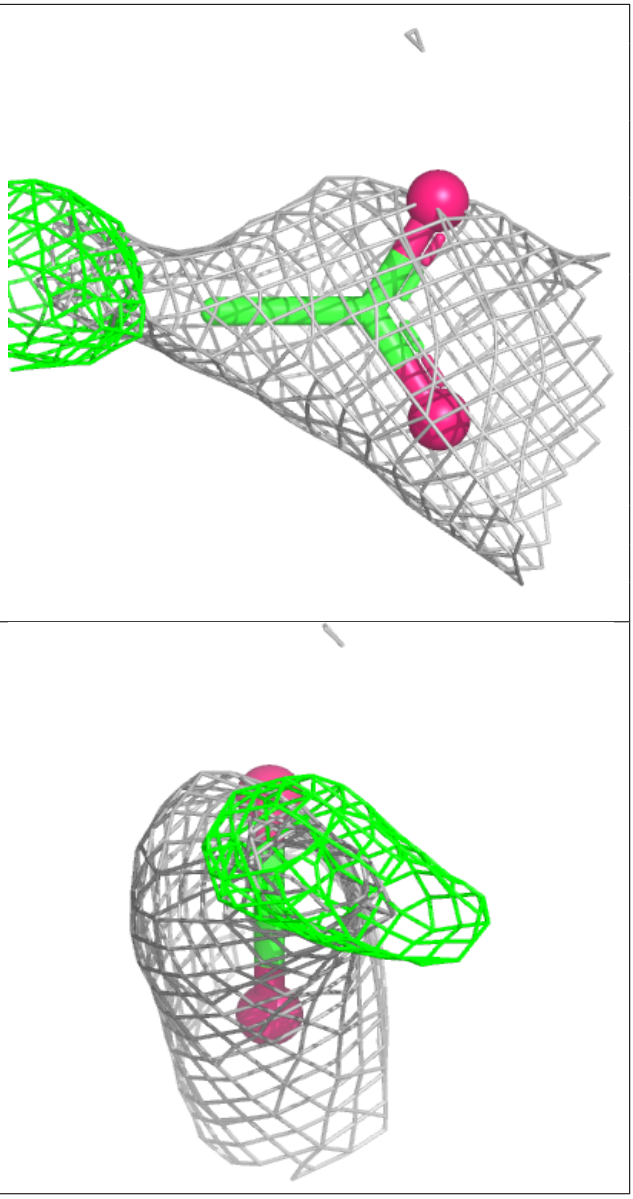
Electron density around ACT C 310:

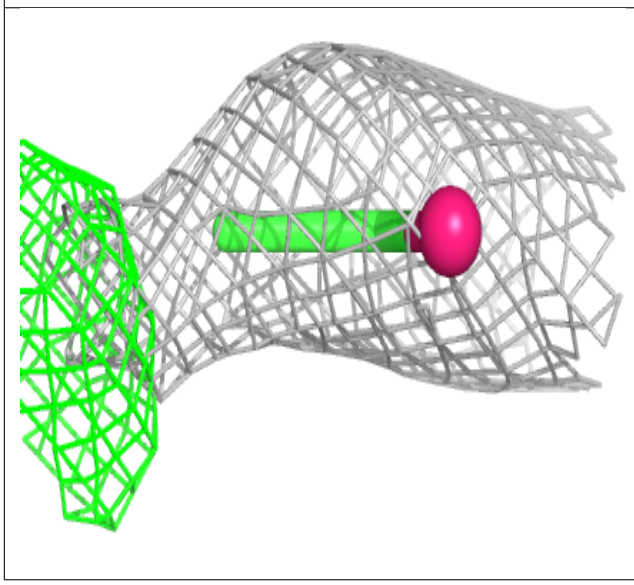
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ACT A 311:

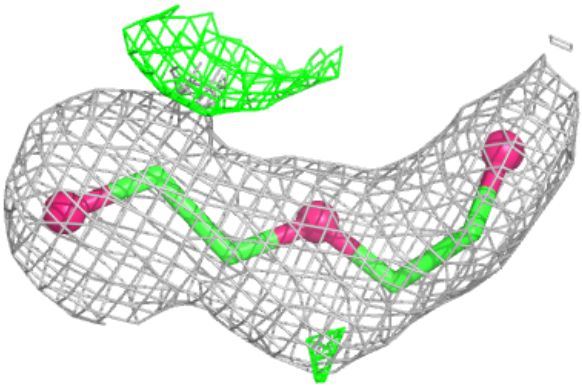
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

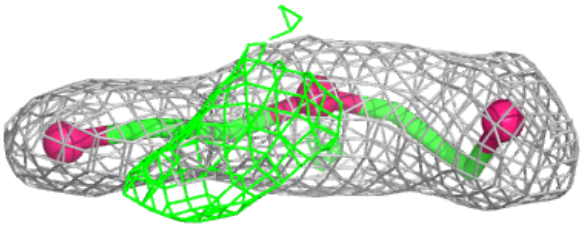


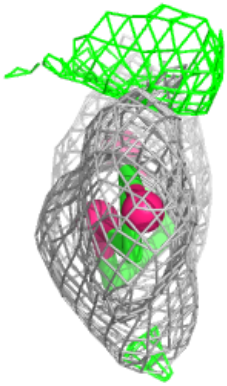


Electron density around PEG A 307:

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

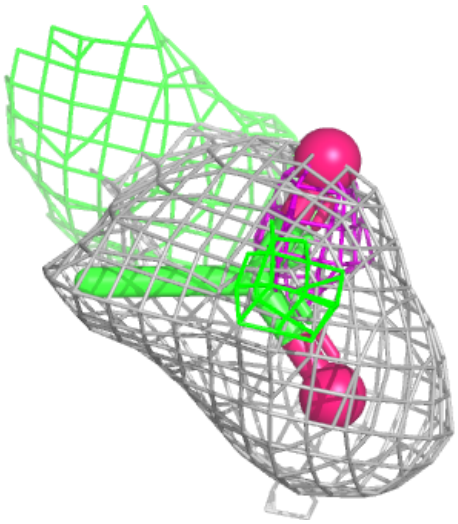


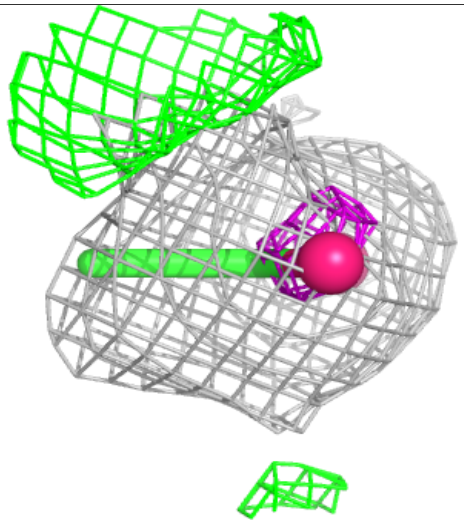


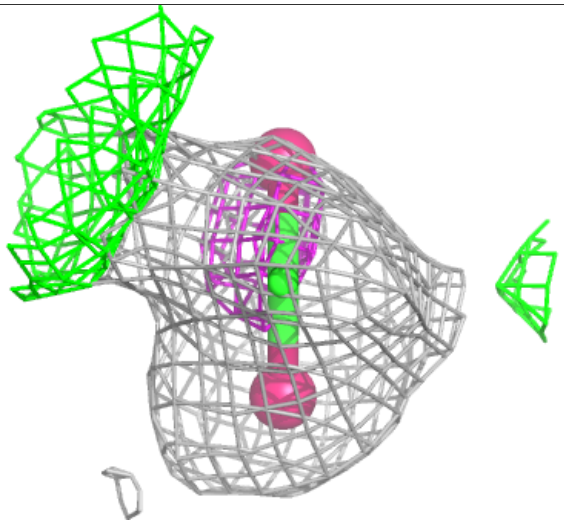


Electron density around ACT E 307:

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

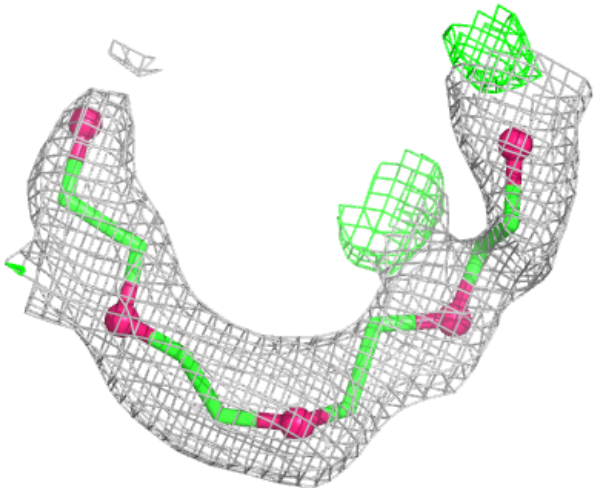


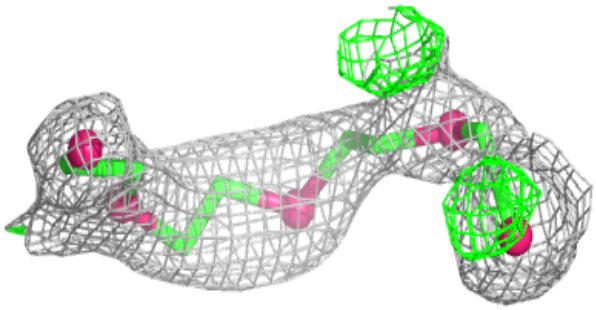


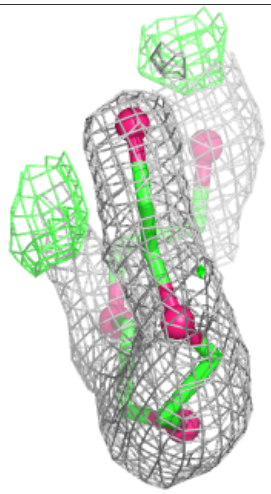


Electron density around PG4 A 302:

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

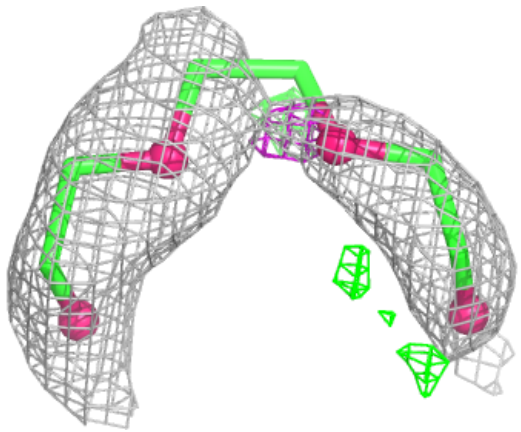


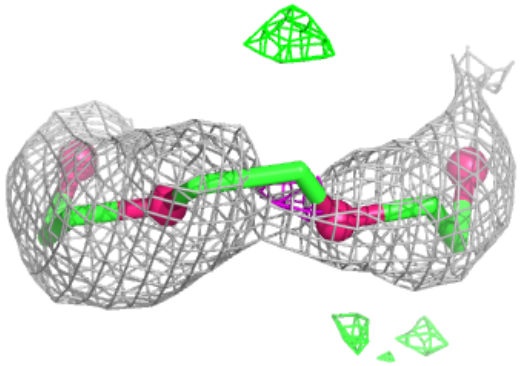


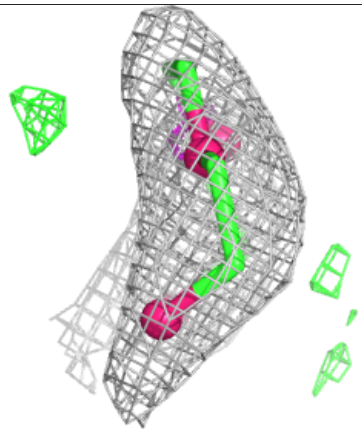


Electron density around PGE C 304:

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

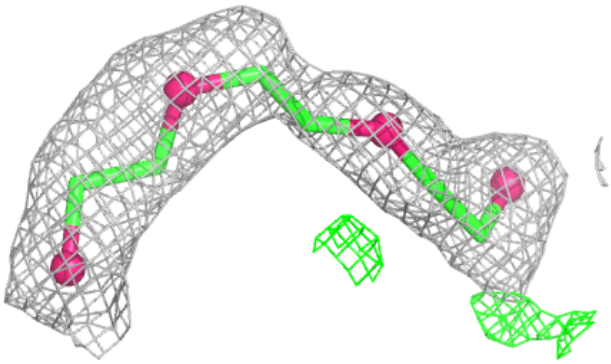


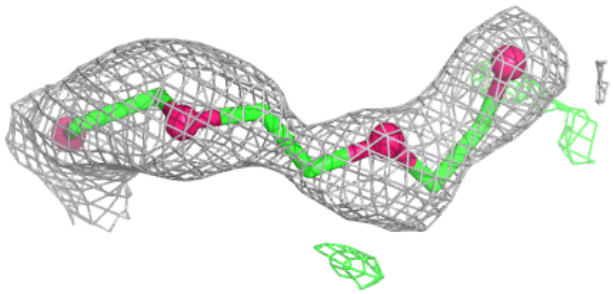


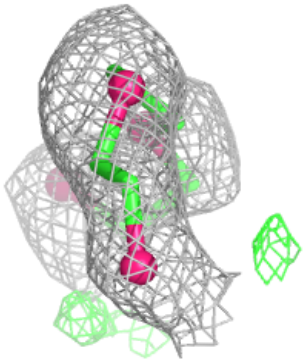


Electron density around PGE E 302:

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

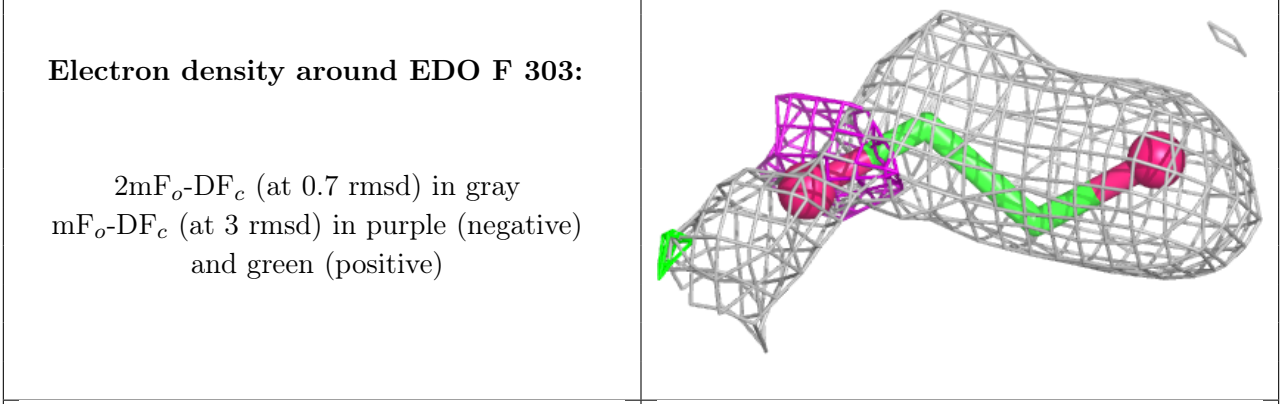






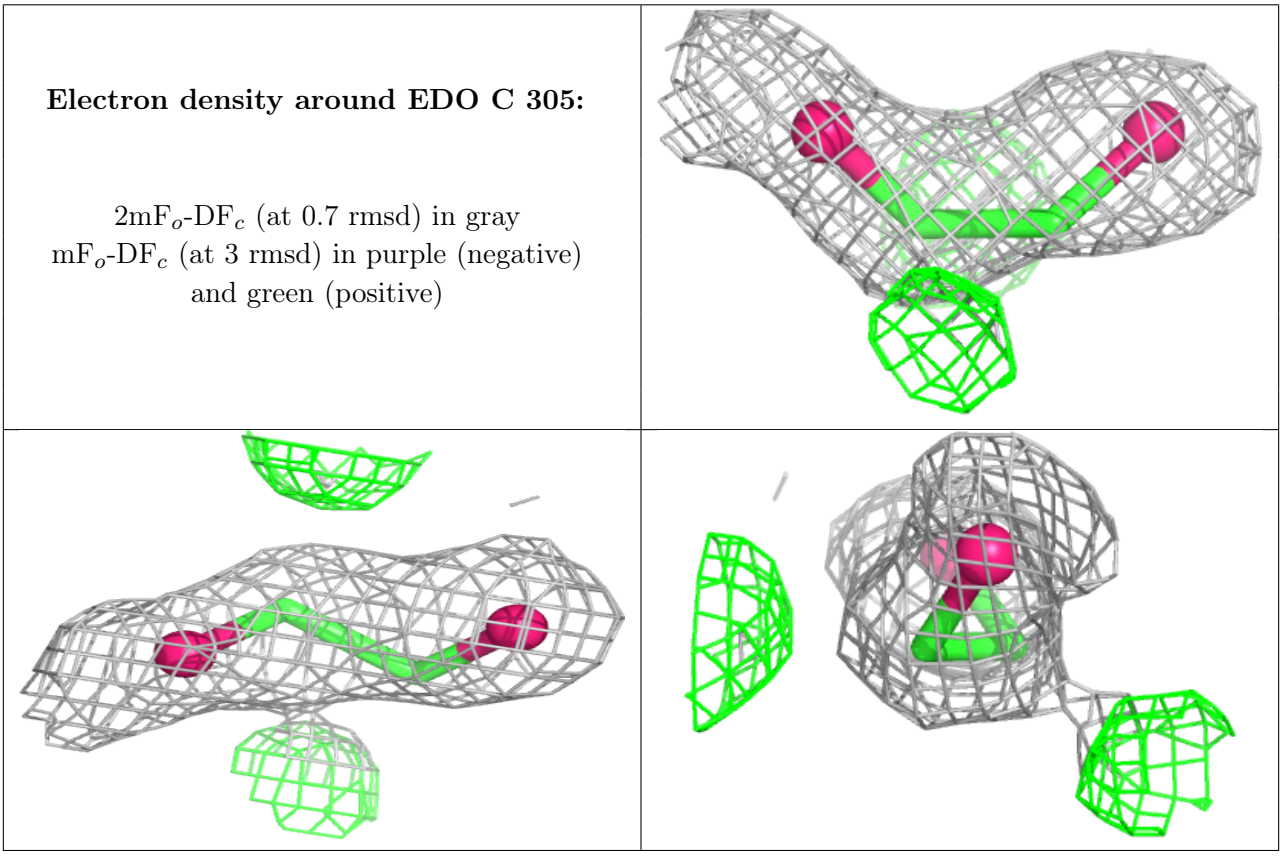
Electron density around EDO F 303:

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



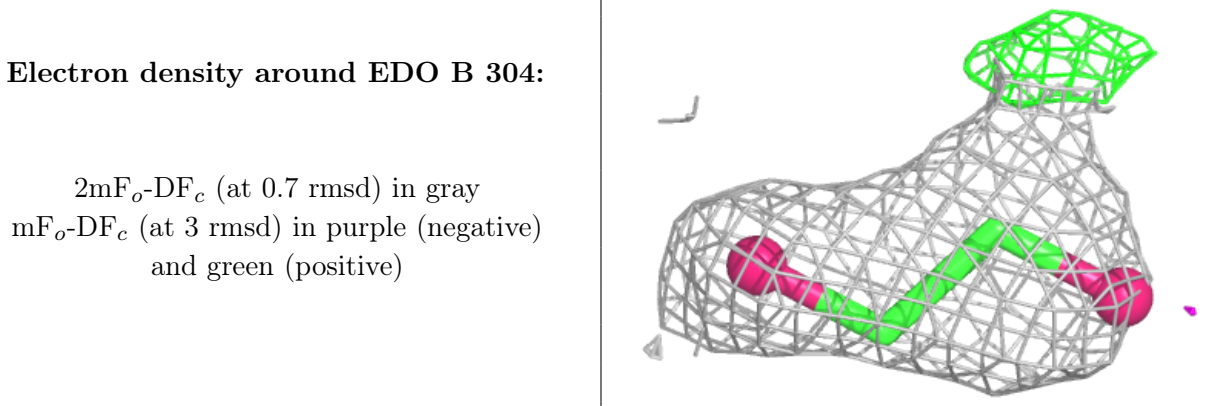
Electron density around EDO C 305:

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



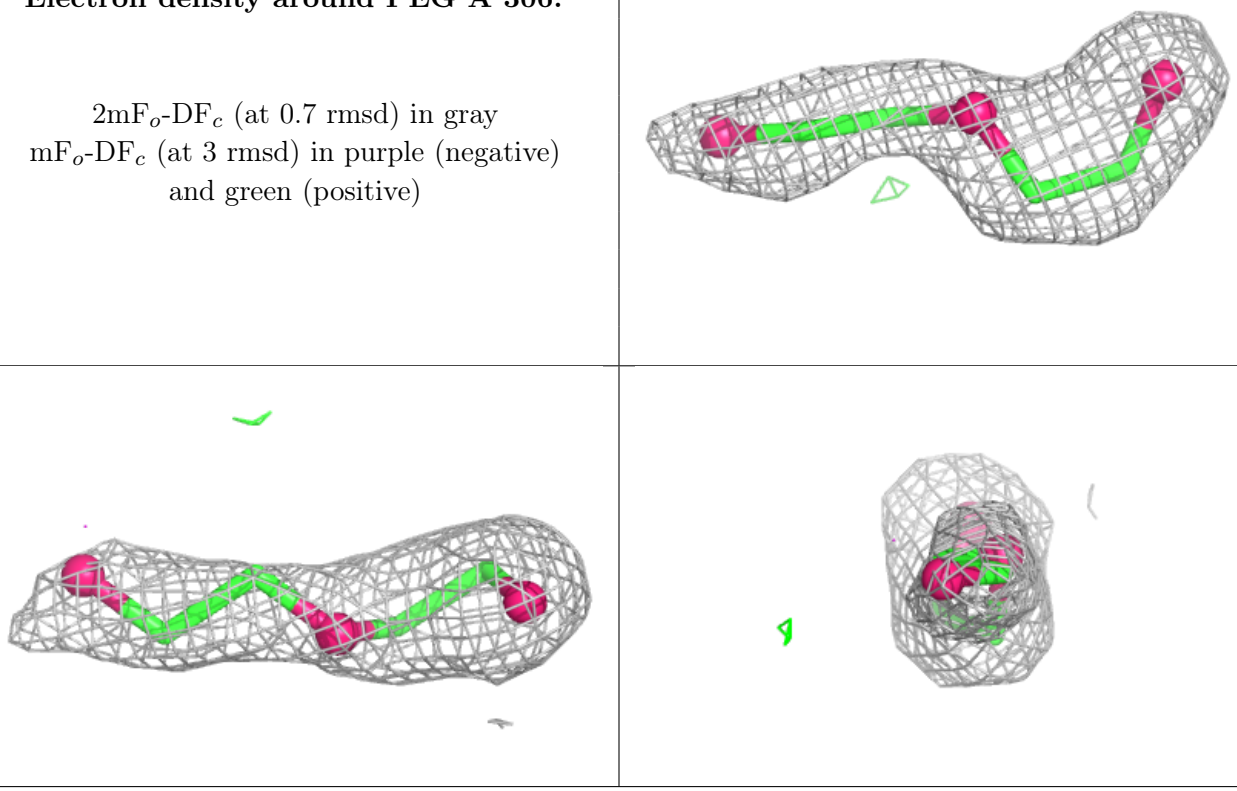
Electron density around EDO B 304:

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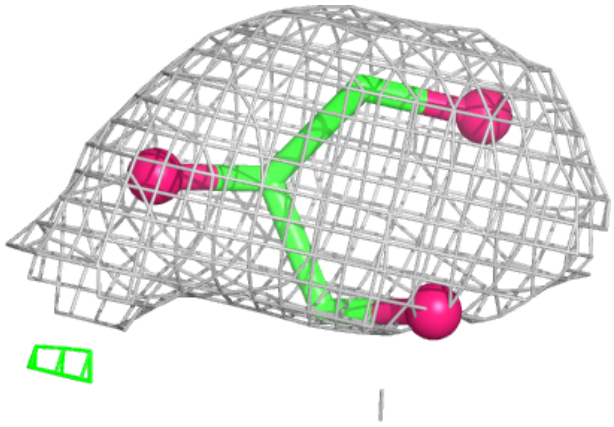
Electron density around PEG A 306:

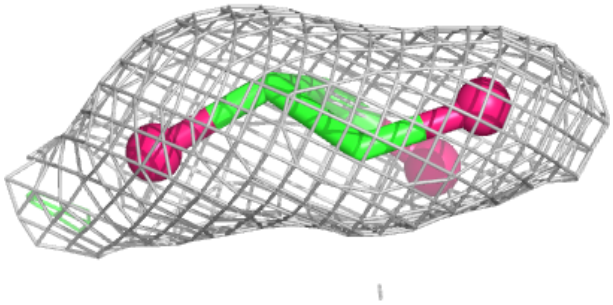
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

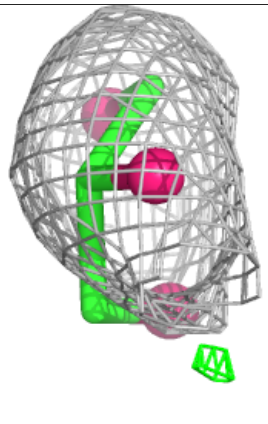


Electron density around GOL F 307:

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

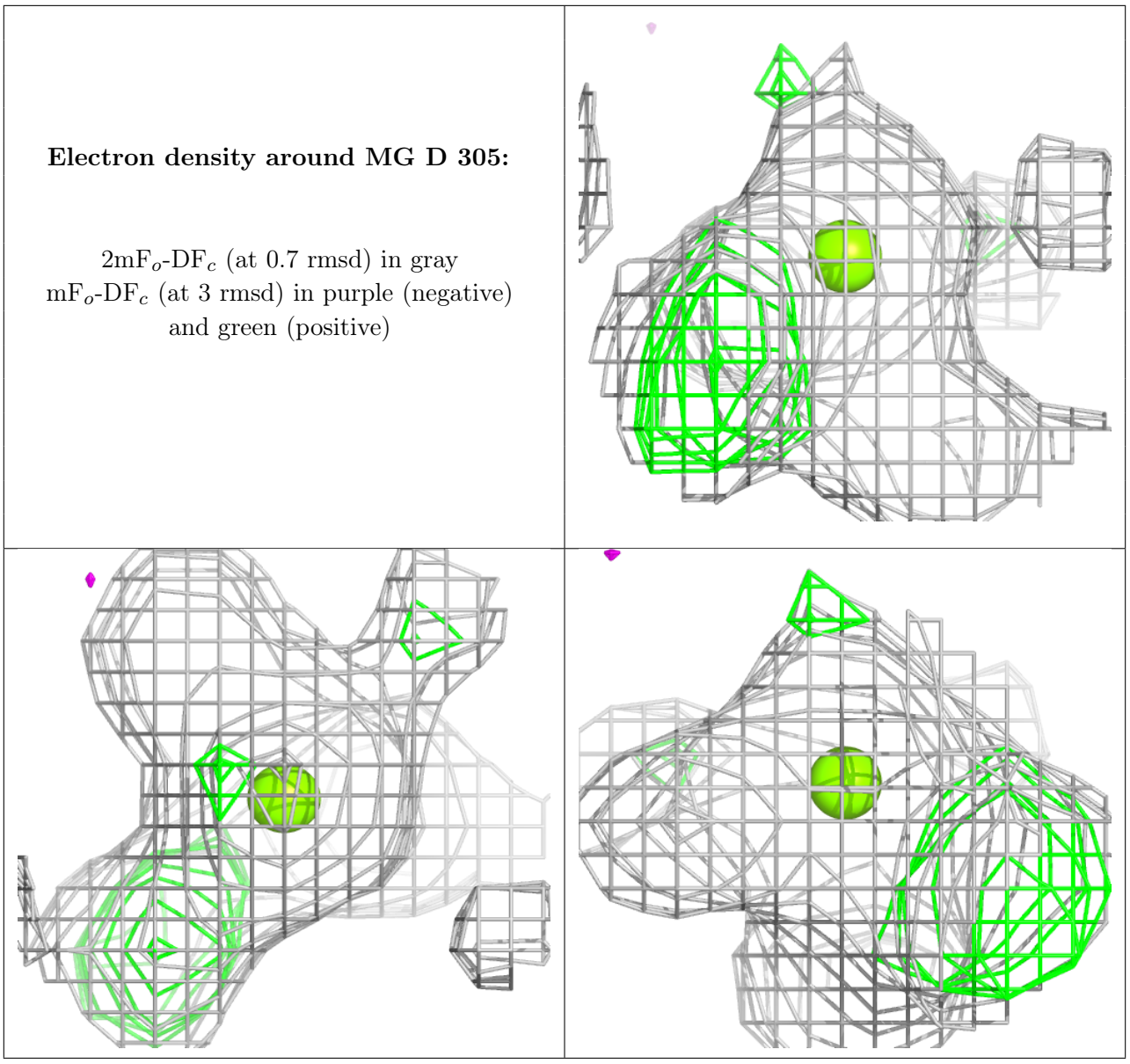






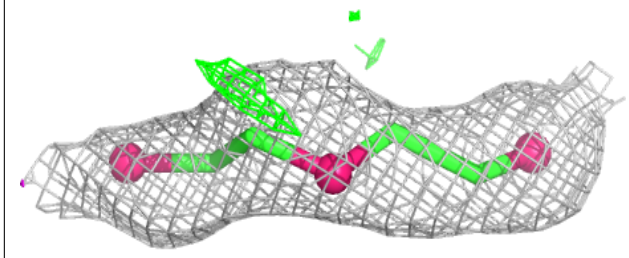
Electron density around MG D 305:

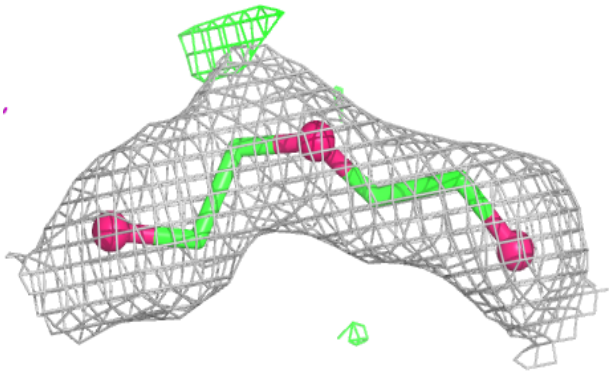
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

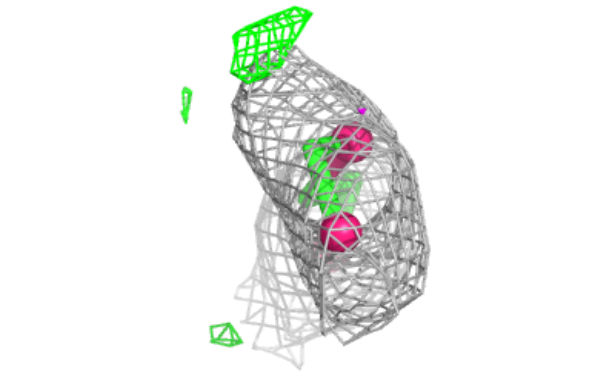


Electron density around PEG A 308:

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

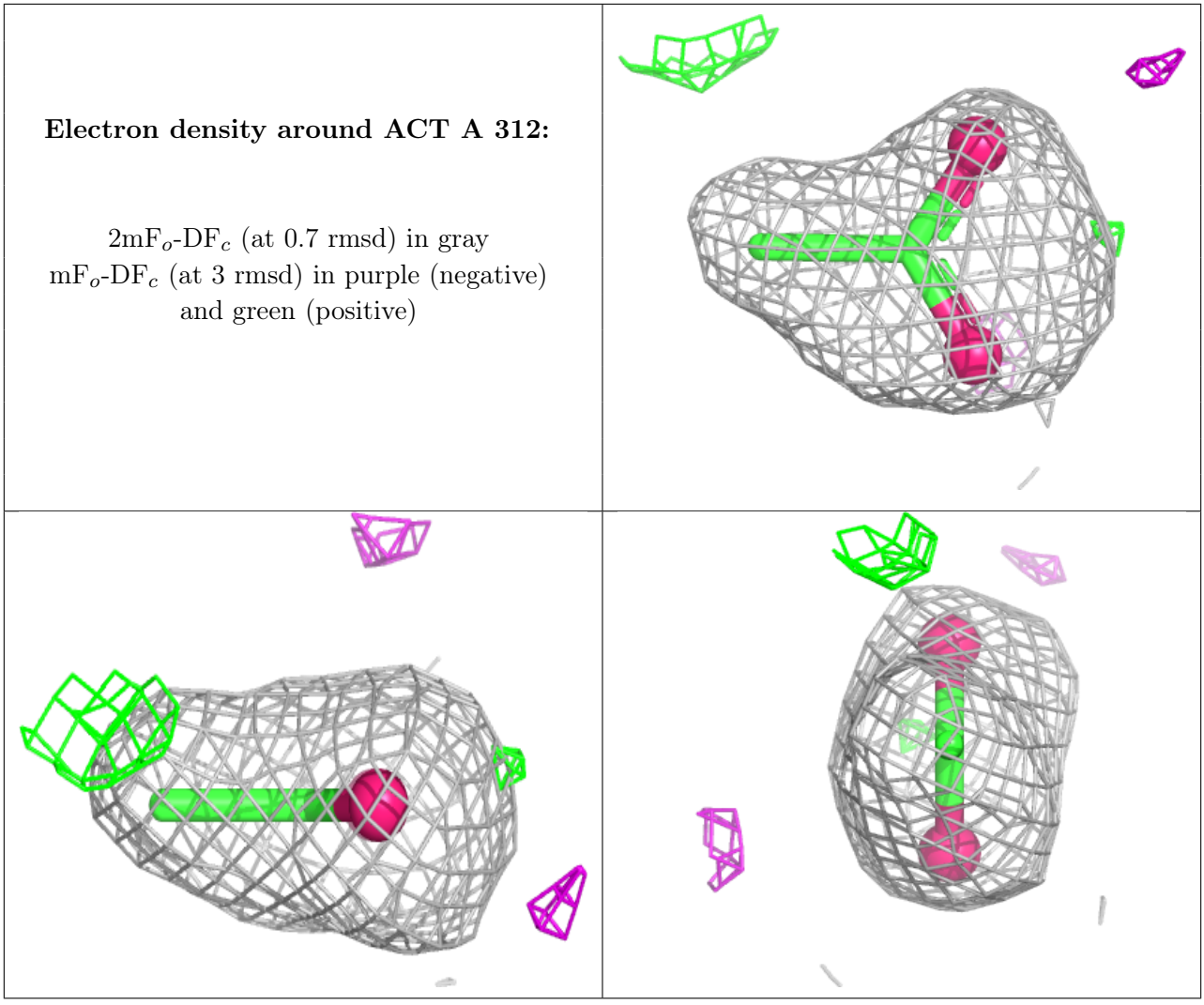






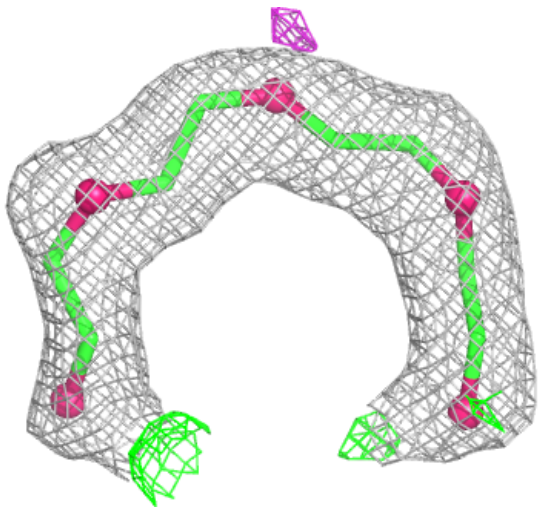
Electron density around ACT A 312:

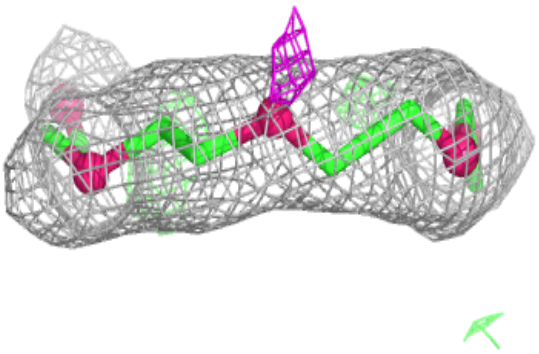
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

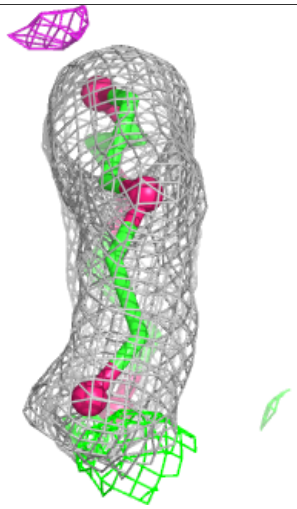


Electron density around PG4 F 301:

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

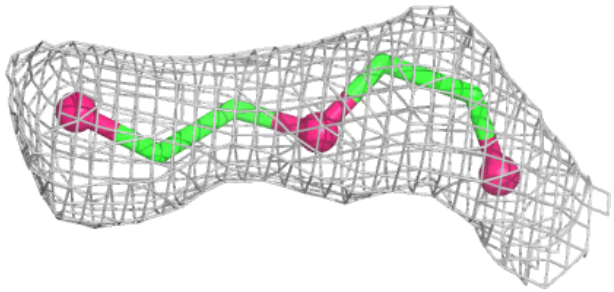


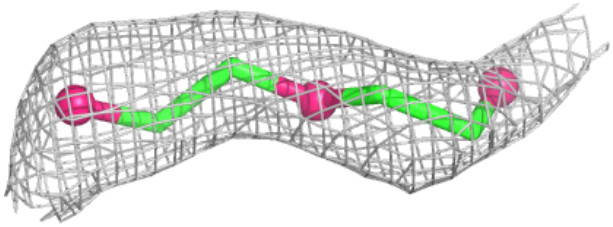


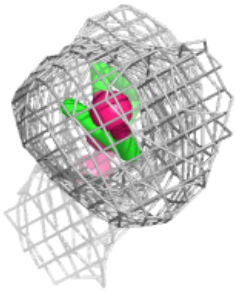


Electron density around PEG D 304:

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

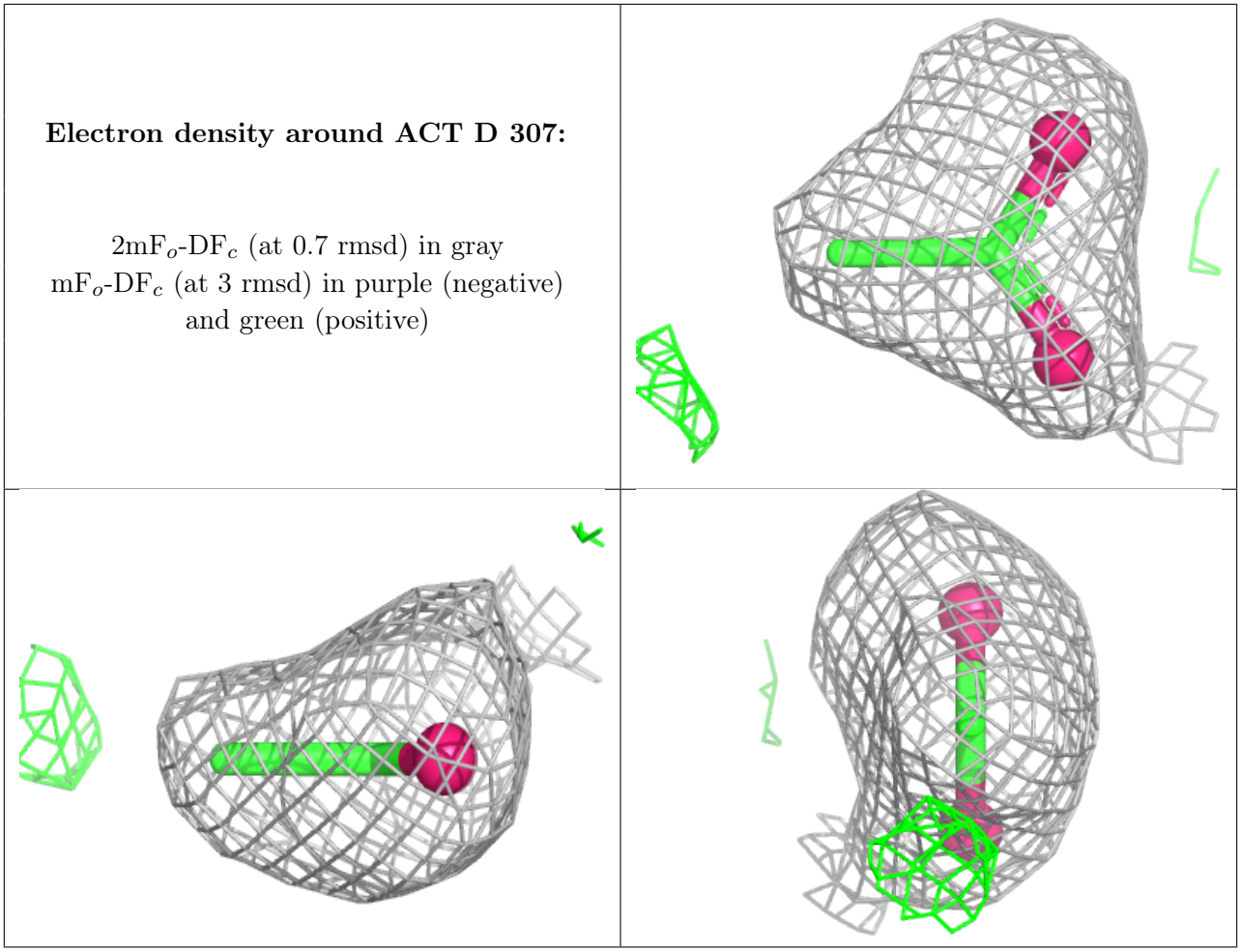






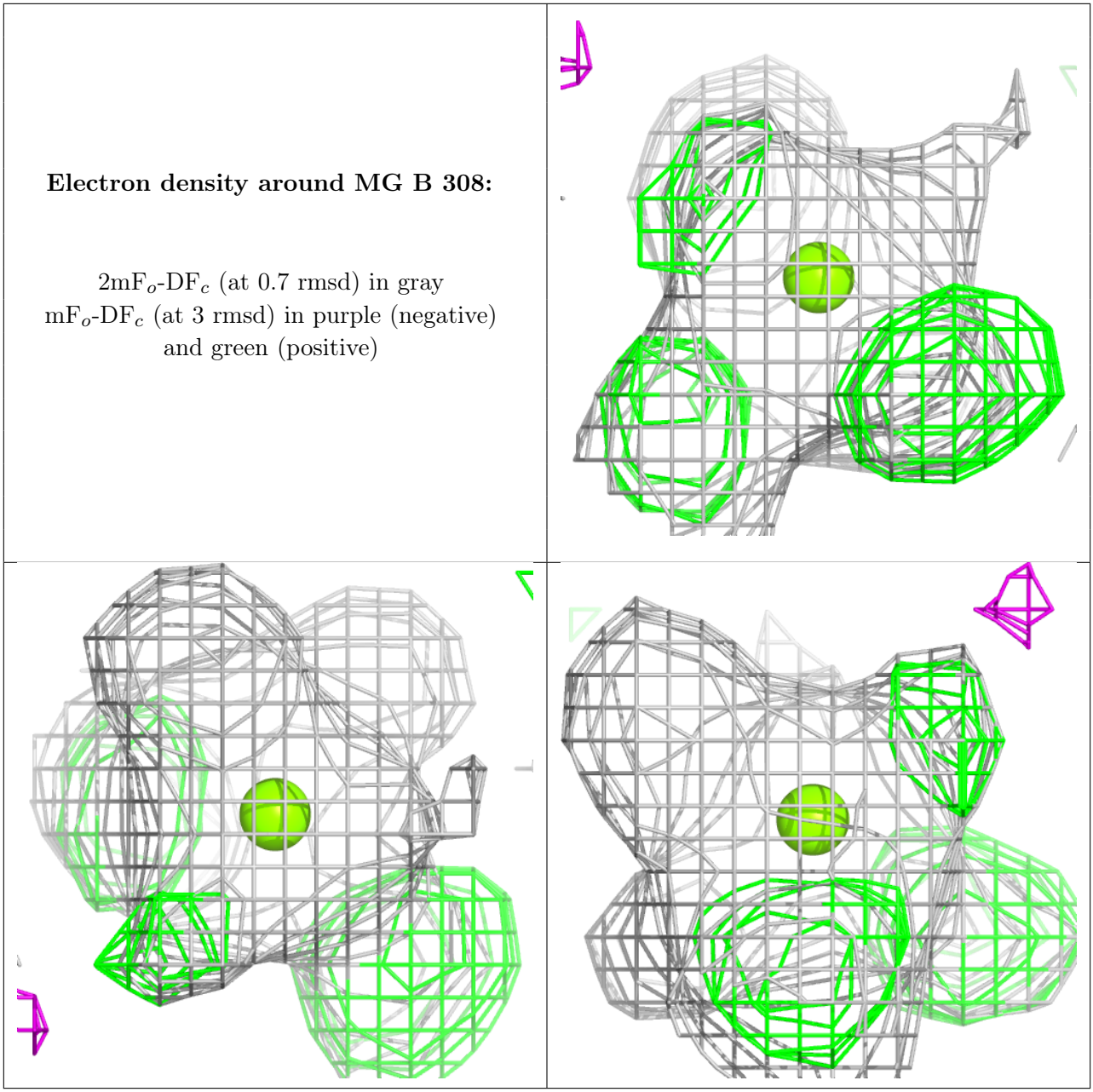
Electron density around ACT D 307:

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



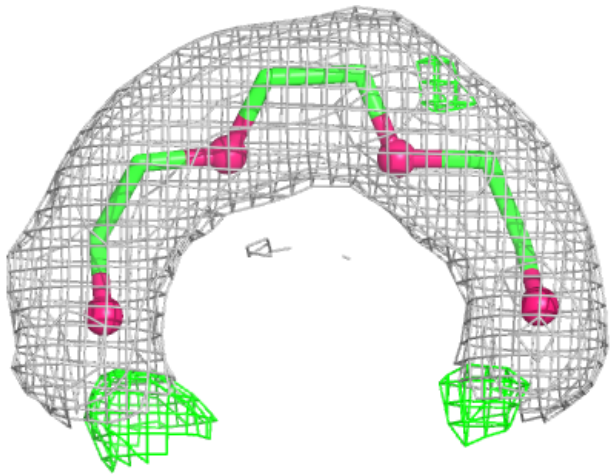
Electron density around MG B 308:

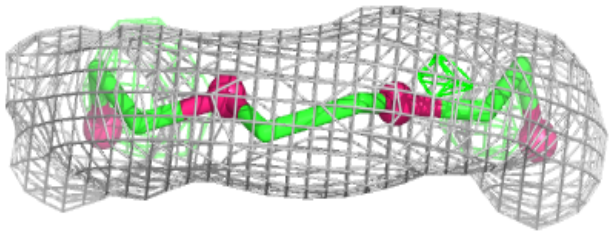
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

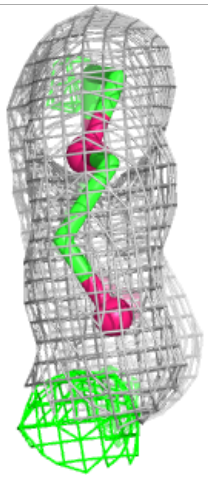


Electron density around PGE C 303:

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

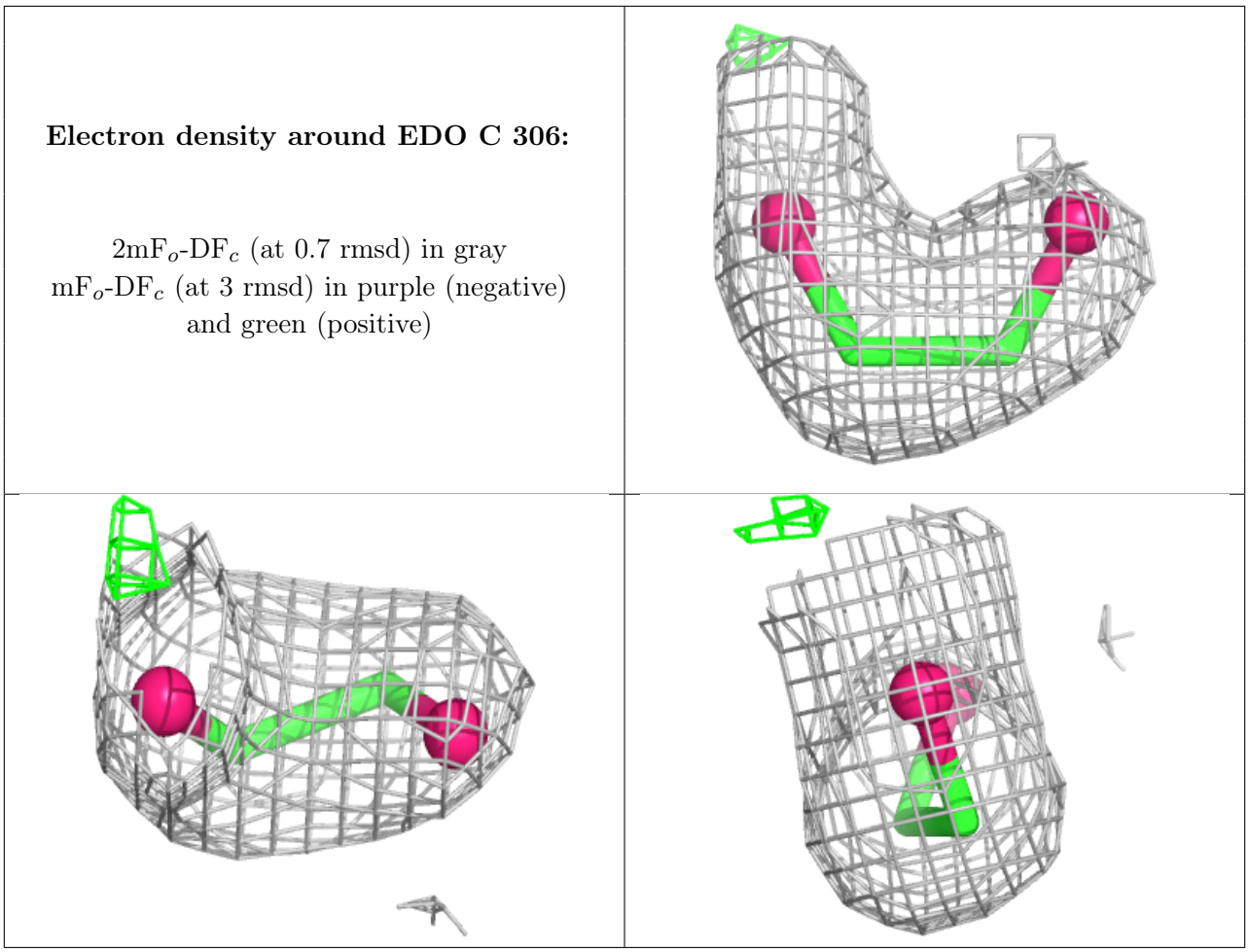






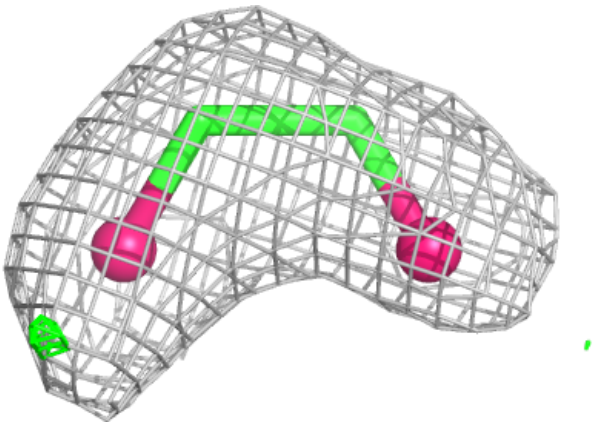
Electron density around EDO C 306:

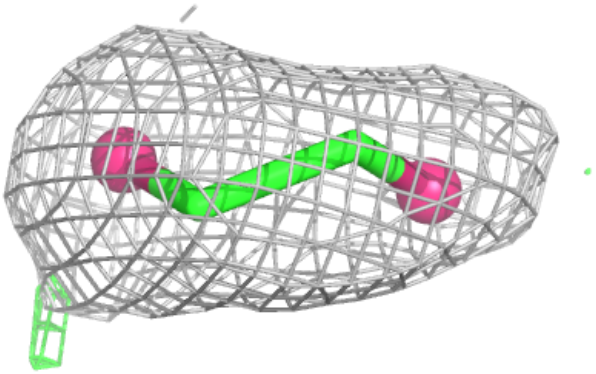
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

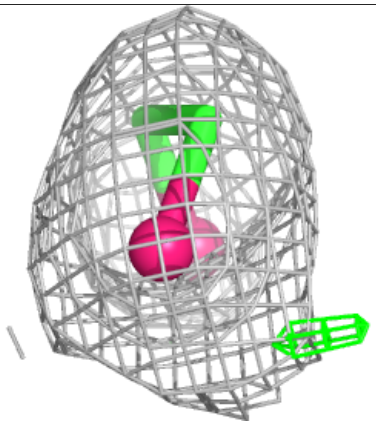


Electron density around EDO E 303:

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

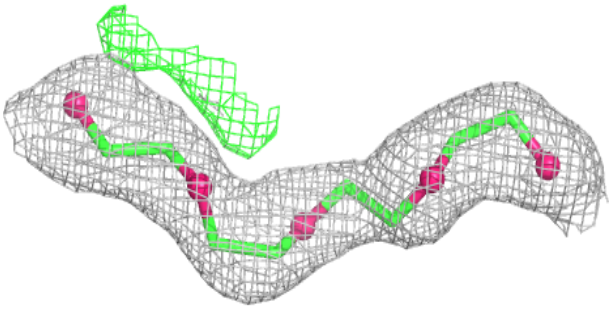


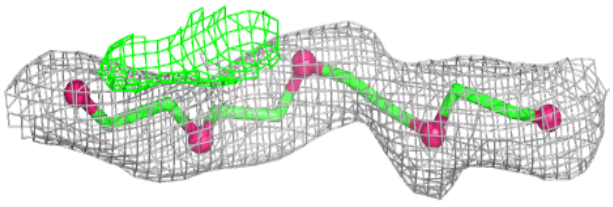


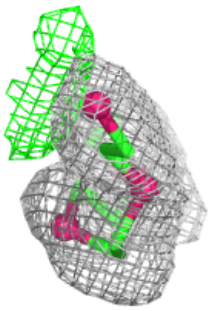


Electron density around PG4 C 301:

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

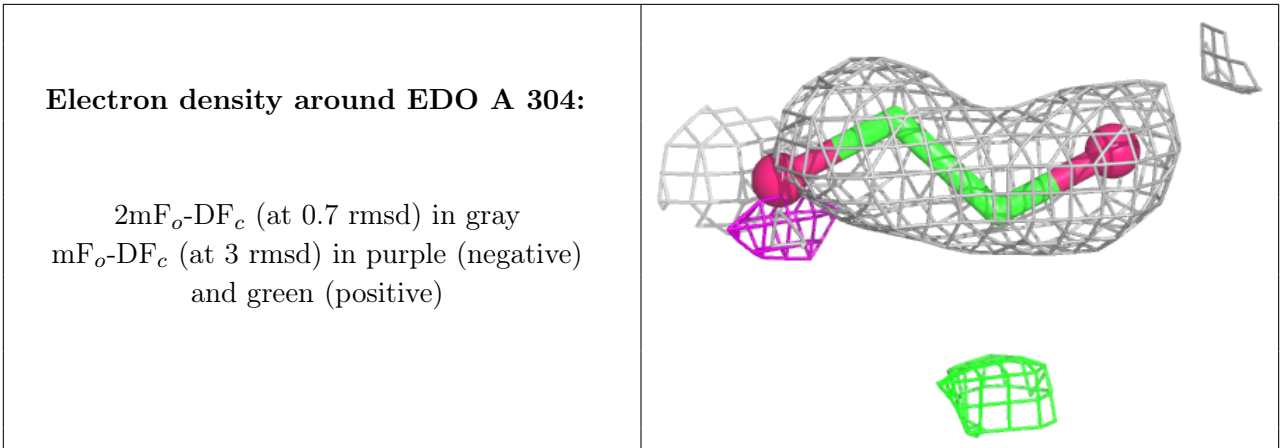


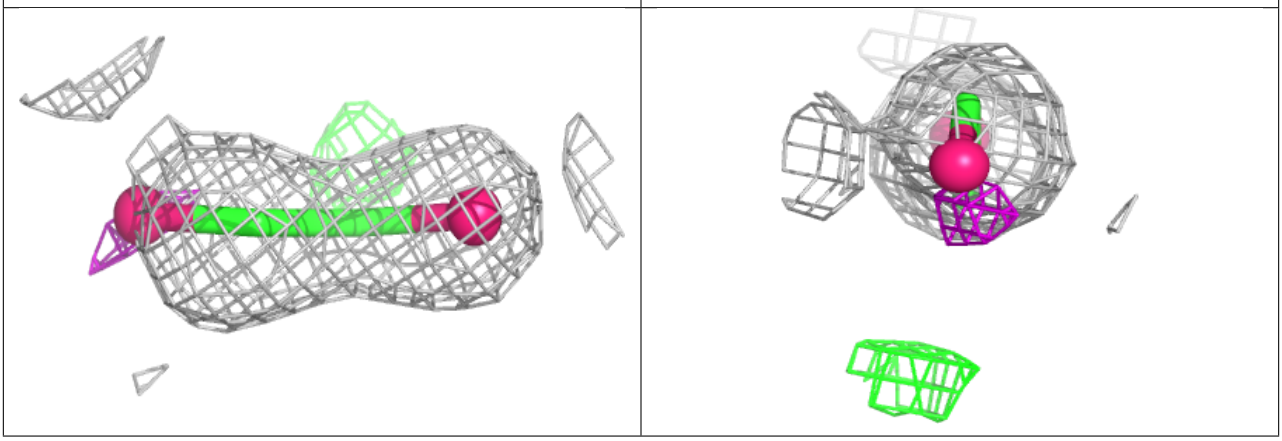




Electron density around EDO A 304:

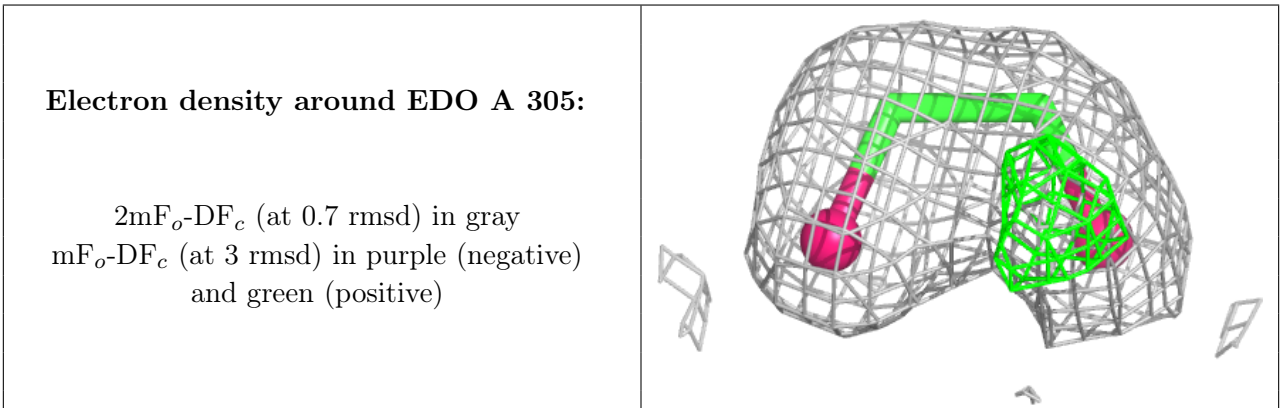
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

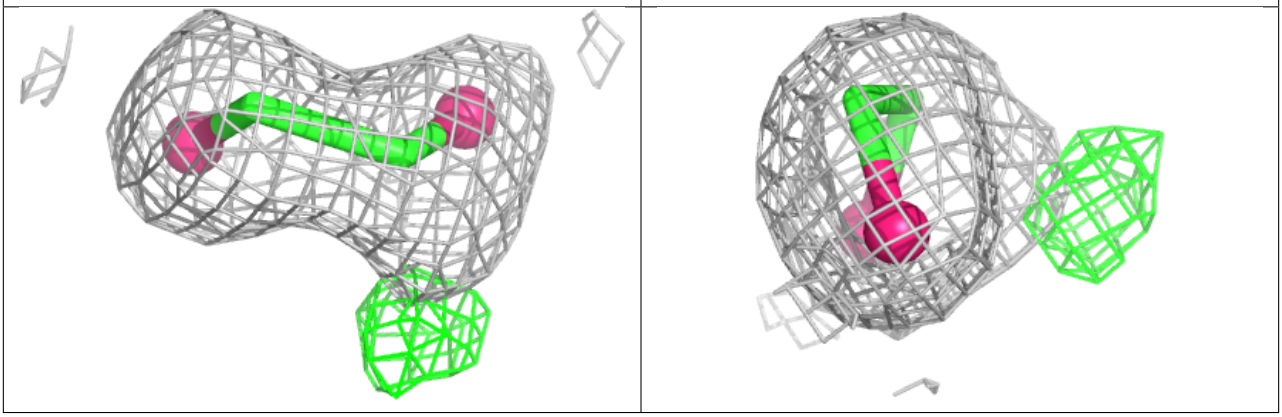




Electron density around EDO A 305:

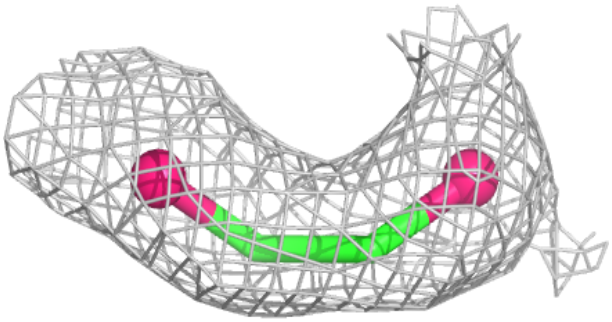
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

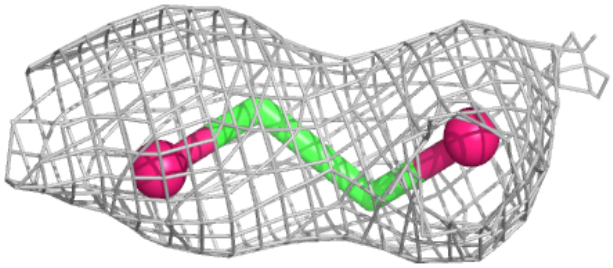


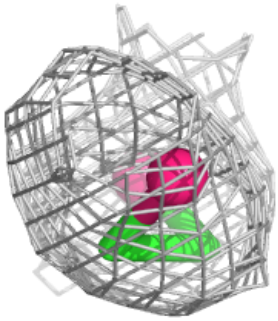


Electron density around EDO E 305:

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

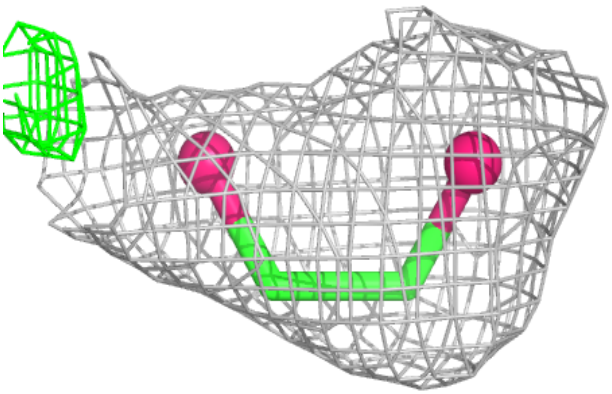


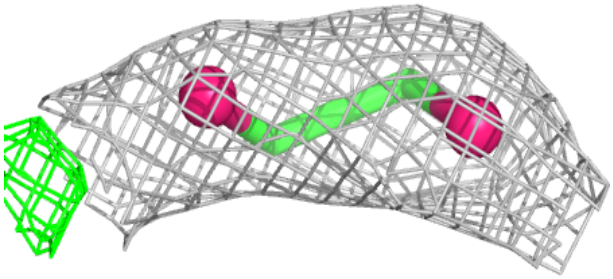


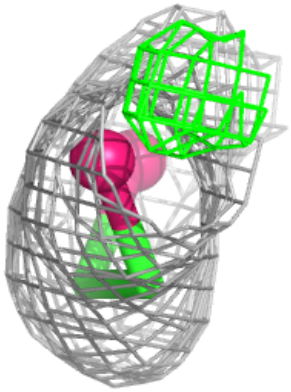


Electron density around EDO F 304:

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

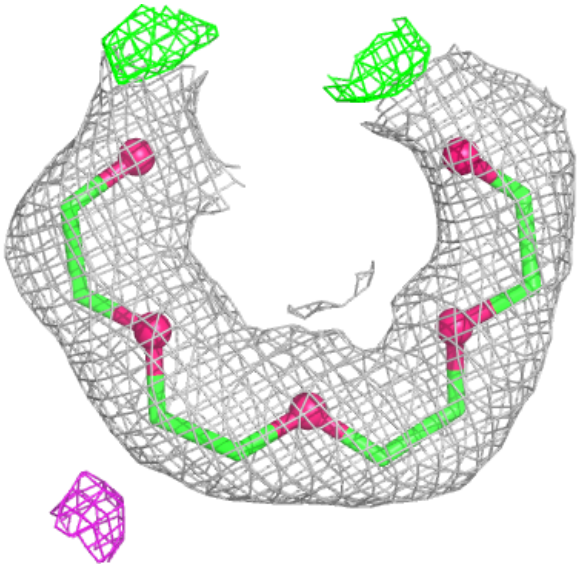


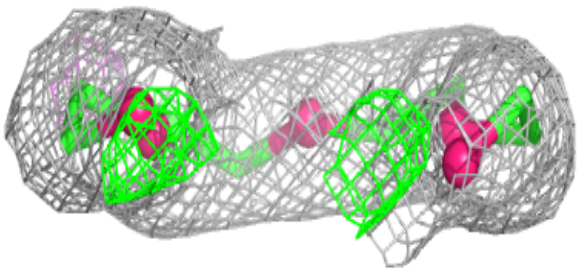


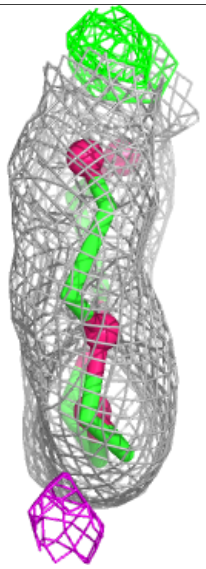


Electron density around PG4 A 301:

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

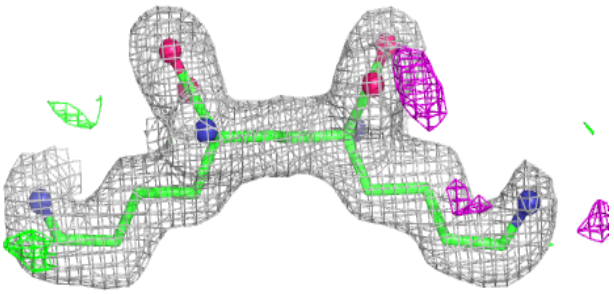


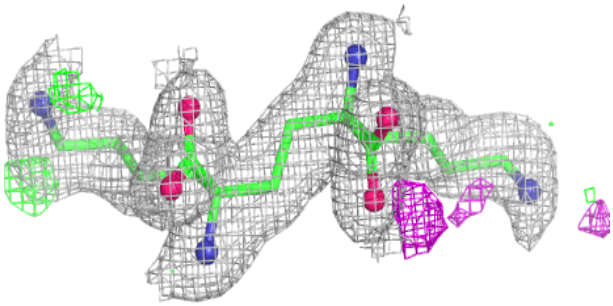


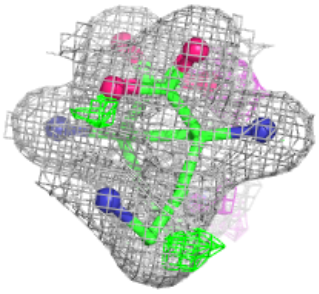


Electron density around 3VN C 302:

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

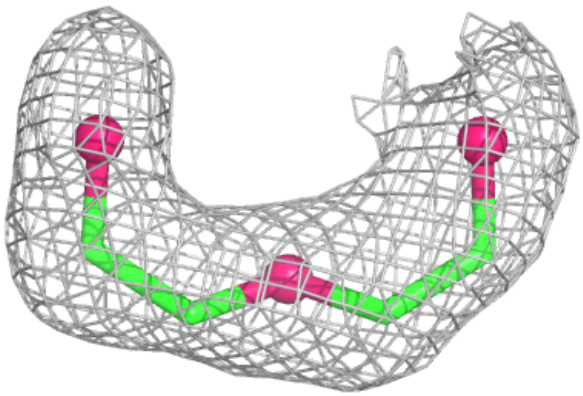


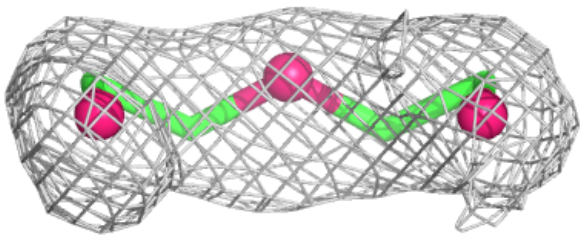


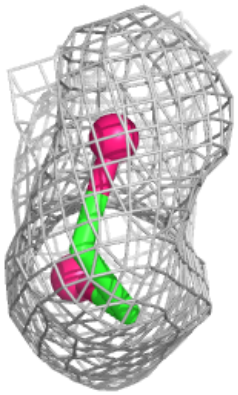


Electron density around PEG E 306:

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

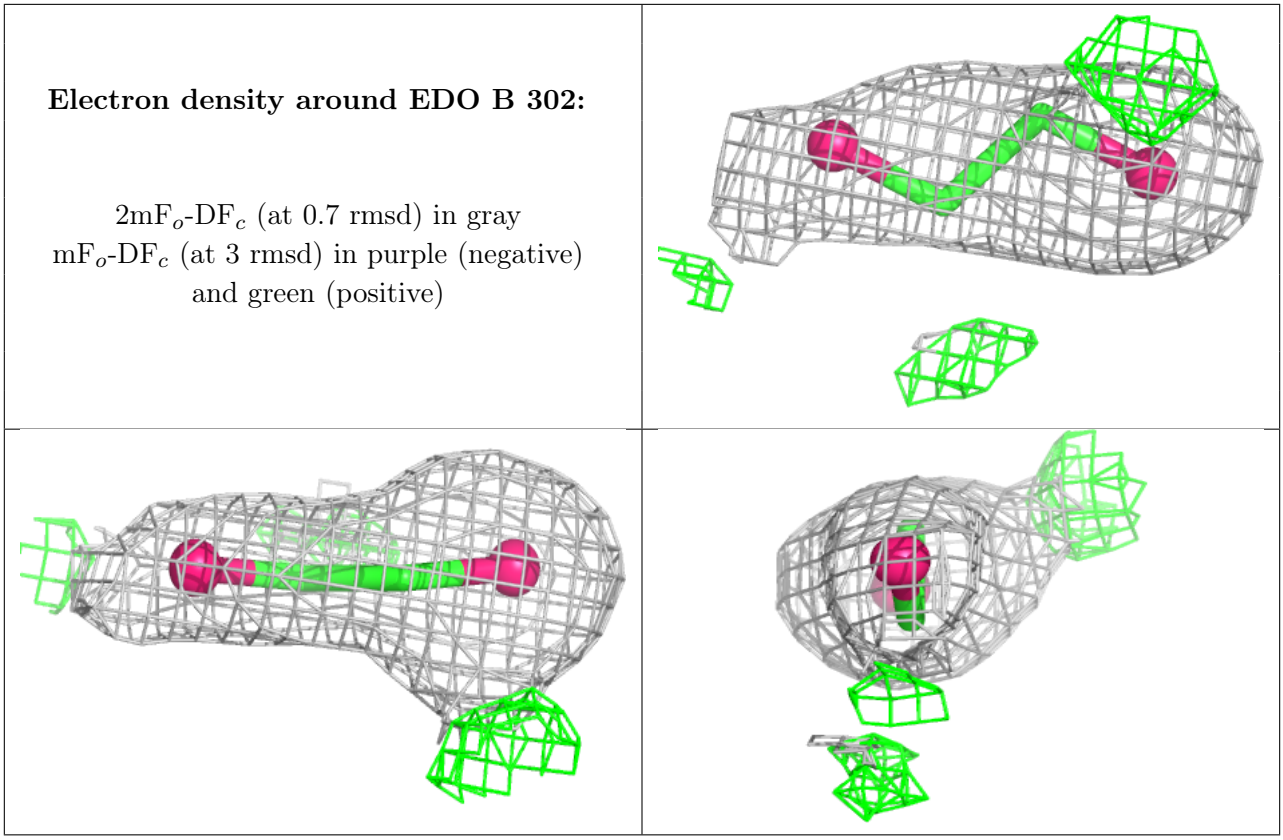






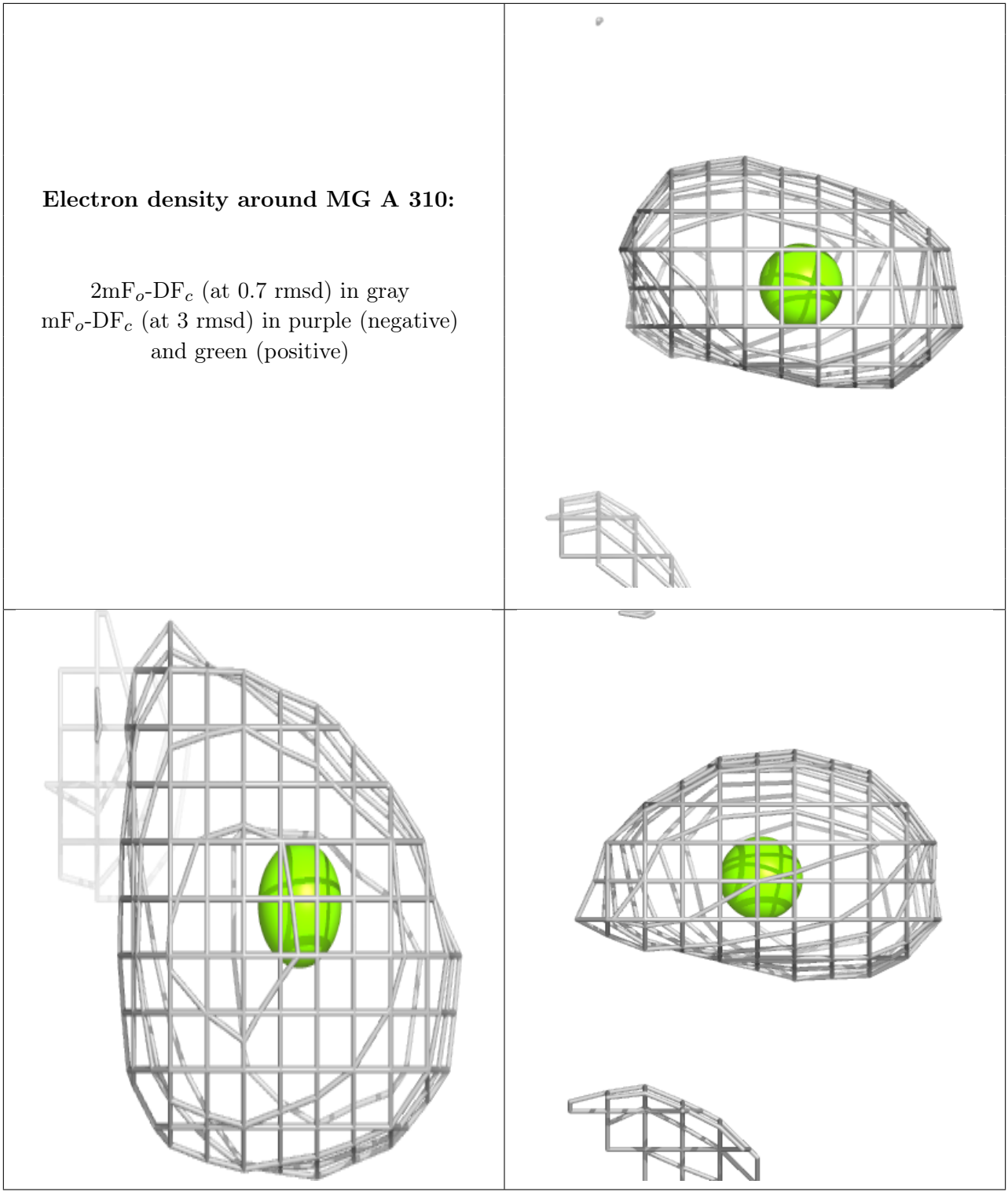
Electron density around EDO B 302:

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



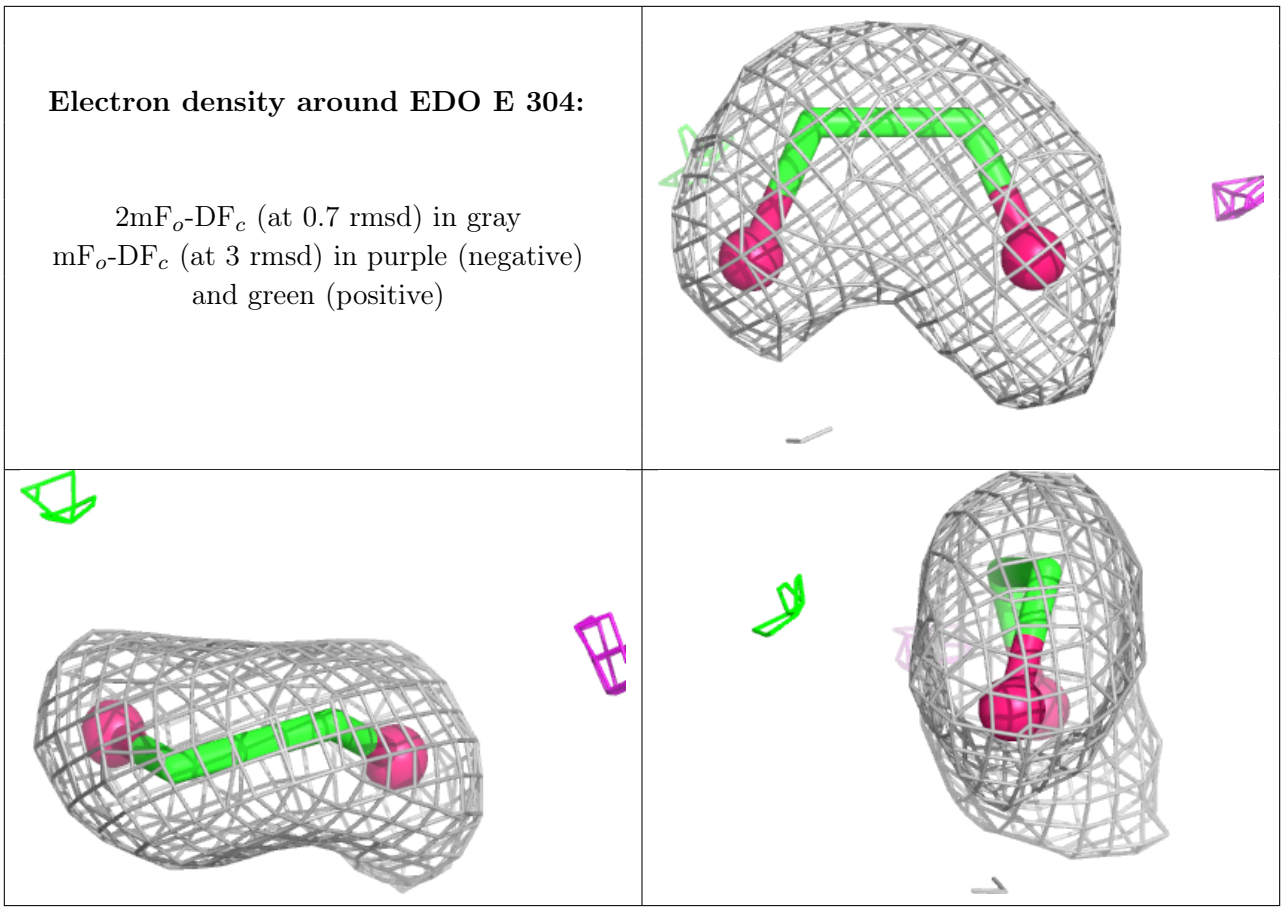
Electron density around MG A 310:

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



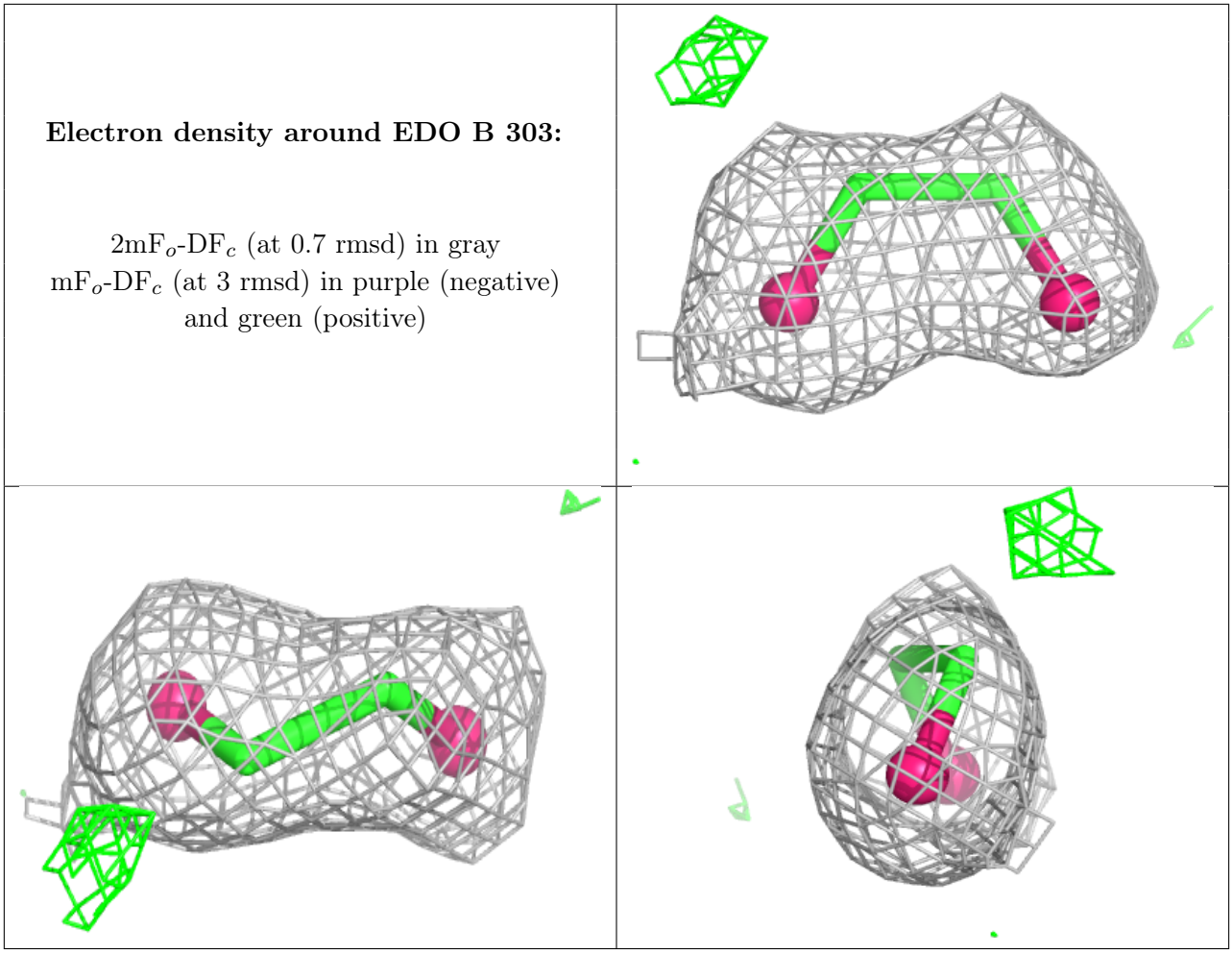
Electron density around EDO E 304:

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



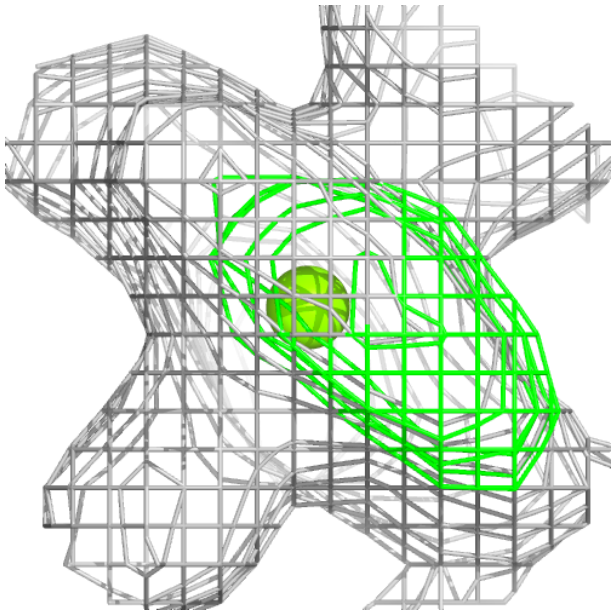
Electron density around EDO B 303:

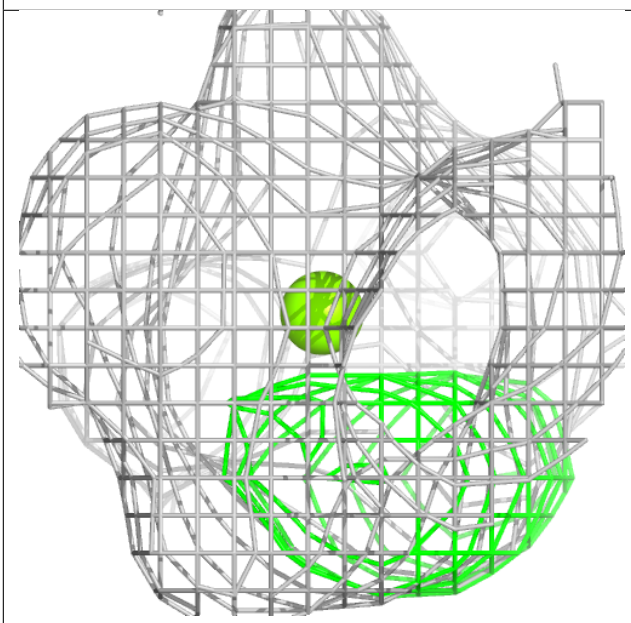
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

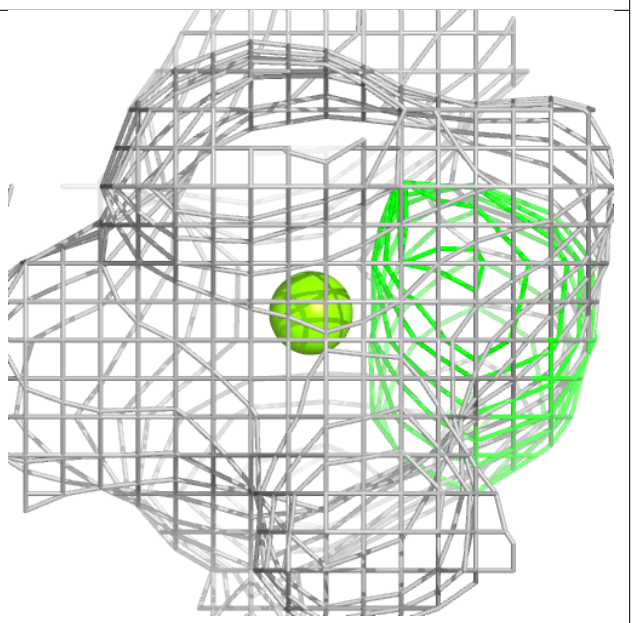


Electron density around MG C 309:

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

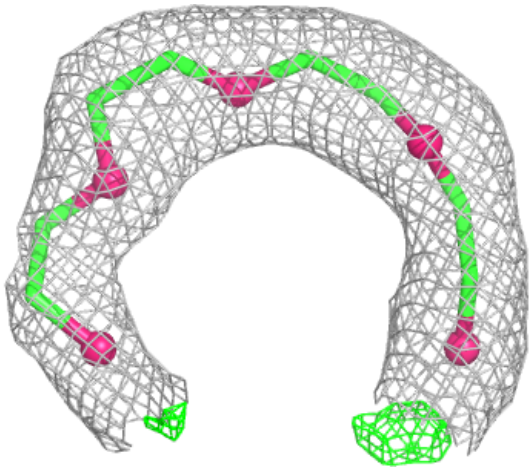


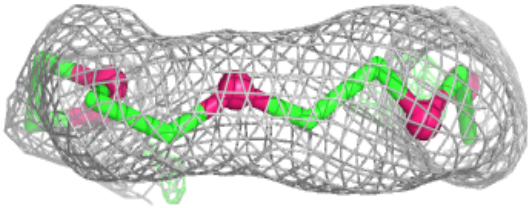


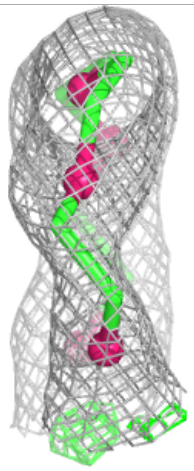


Electron density around PG4 E 301:

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

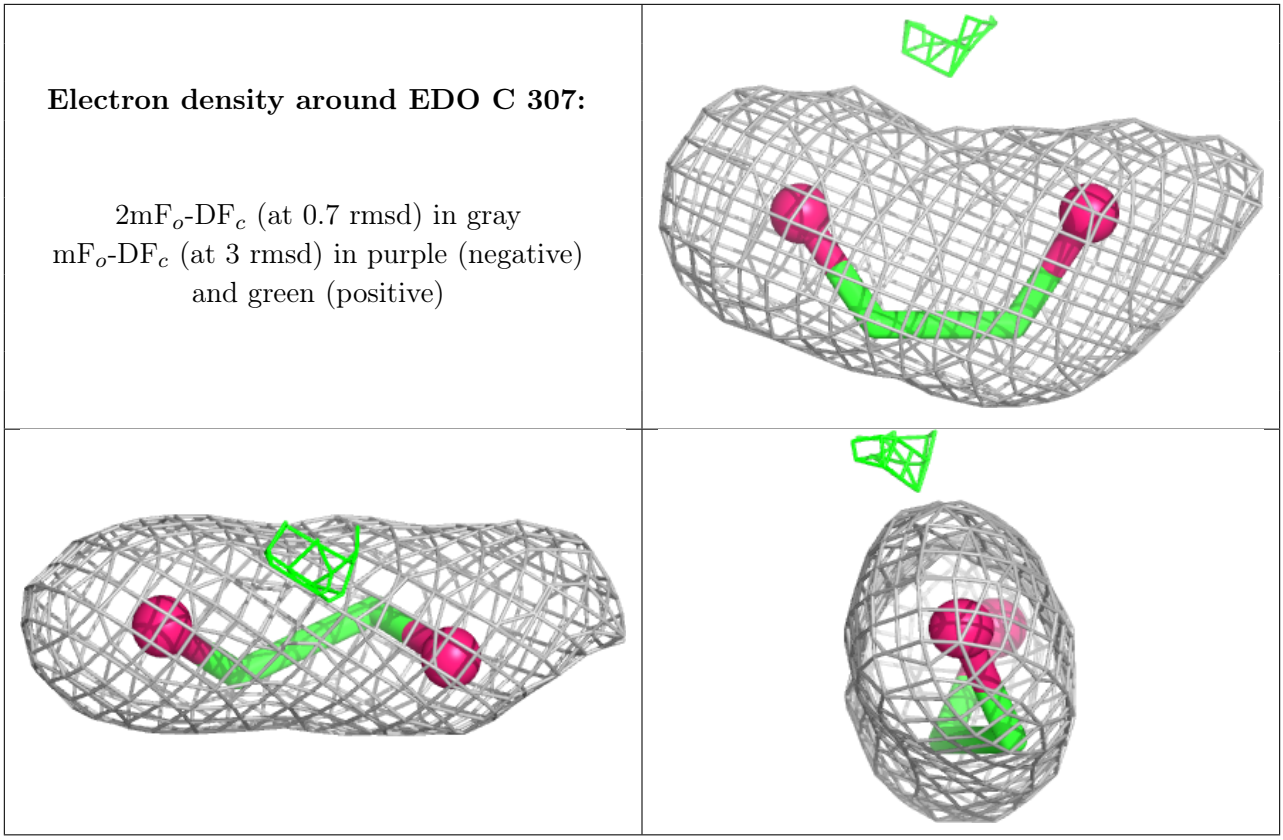






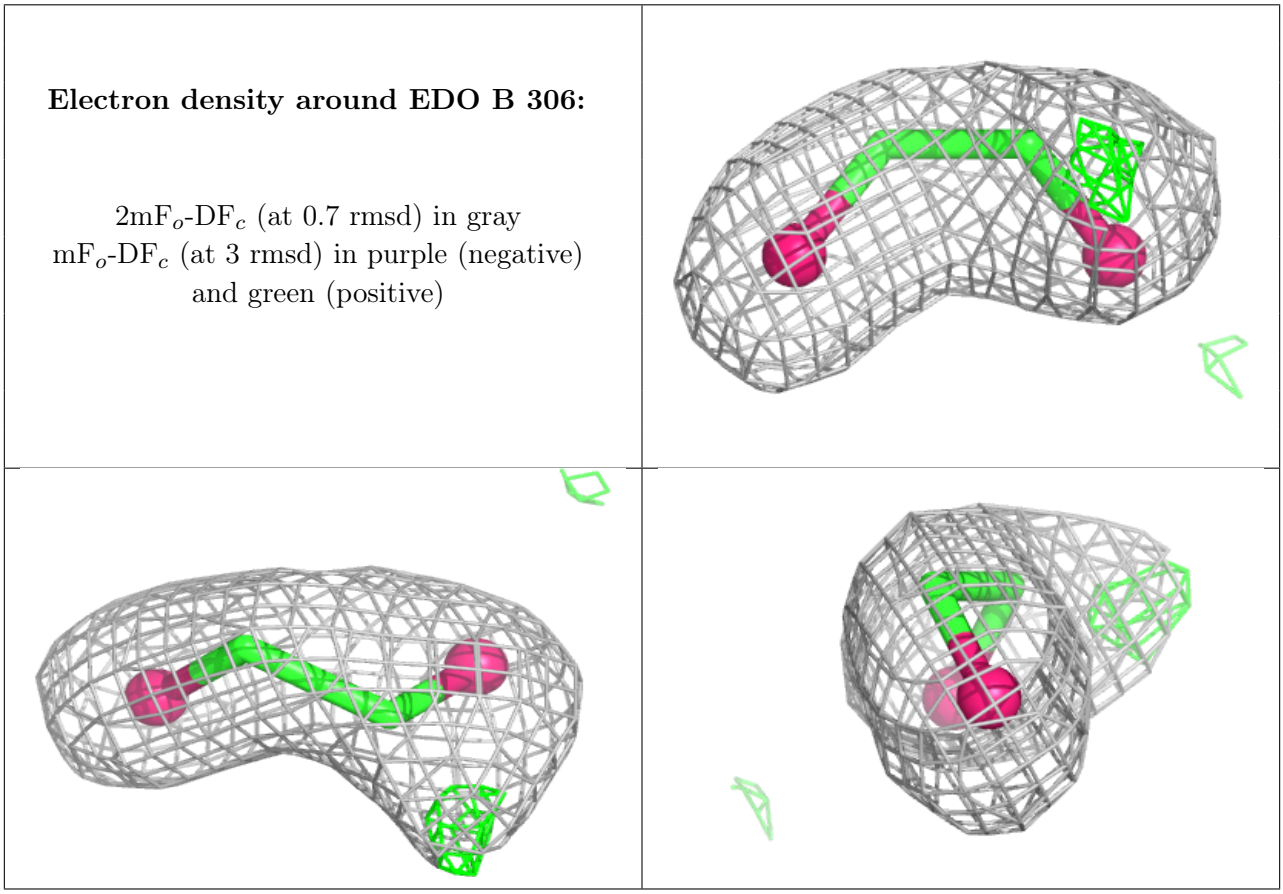
Electron density around EDO C 307:

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



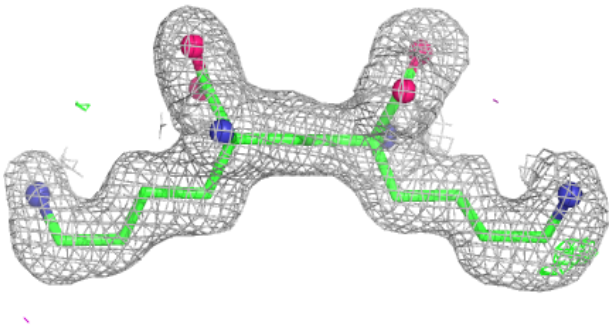
Electron density around EDO B 306:

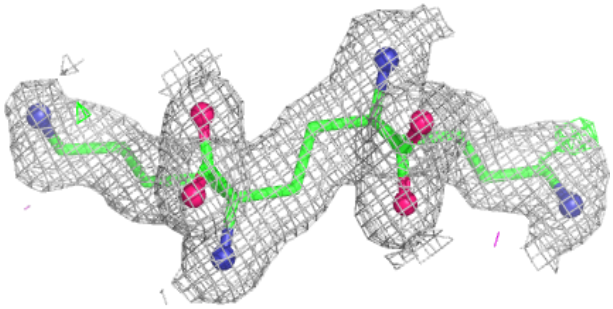
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

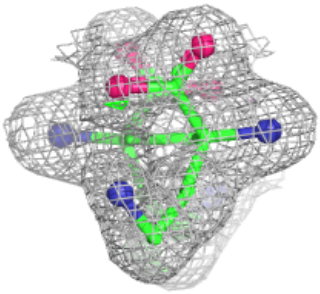


Electron density around 3VN A 303:

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

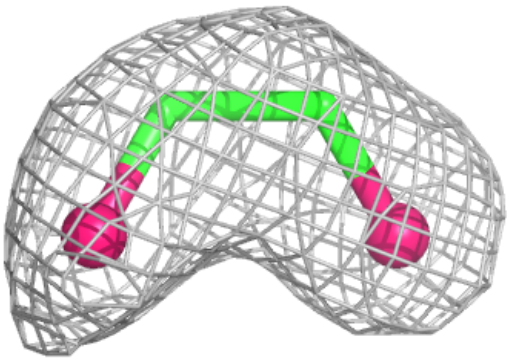


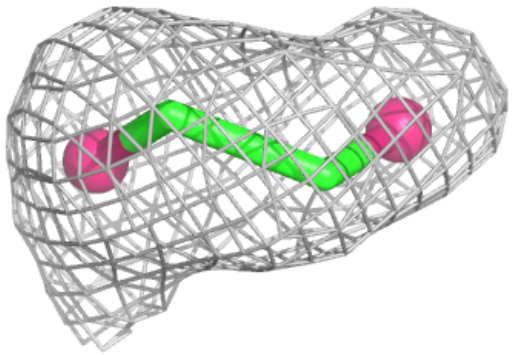


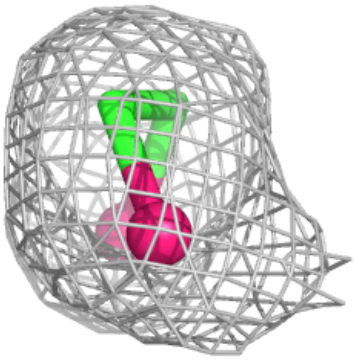


Electron density around EDO B 307:

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

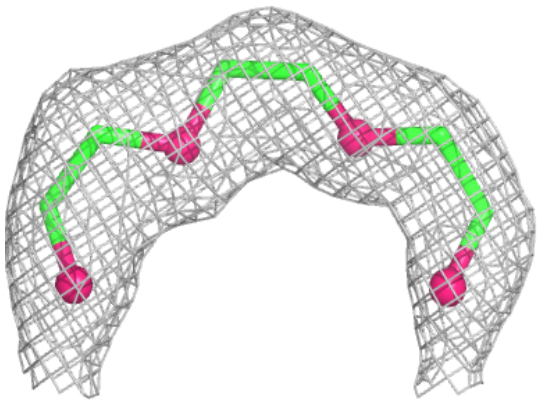


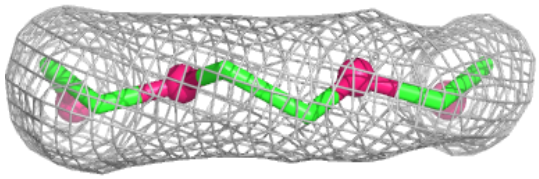


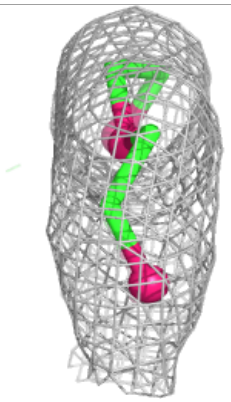


Electron density around PGE D 301:

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

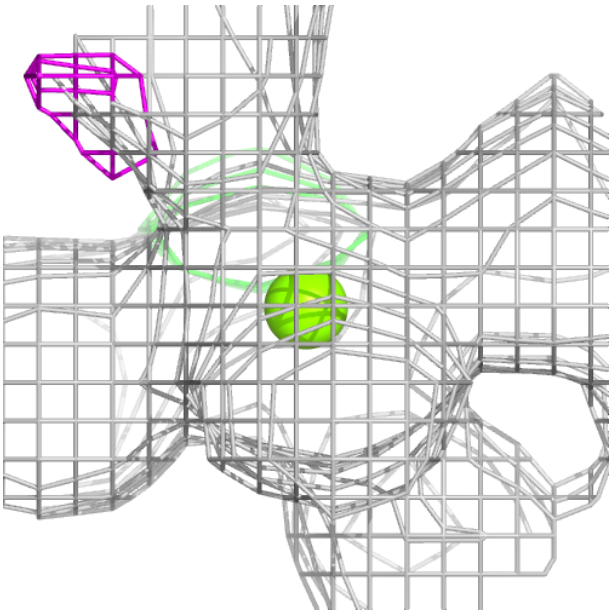


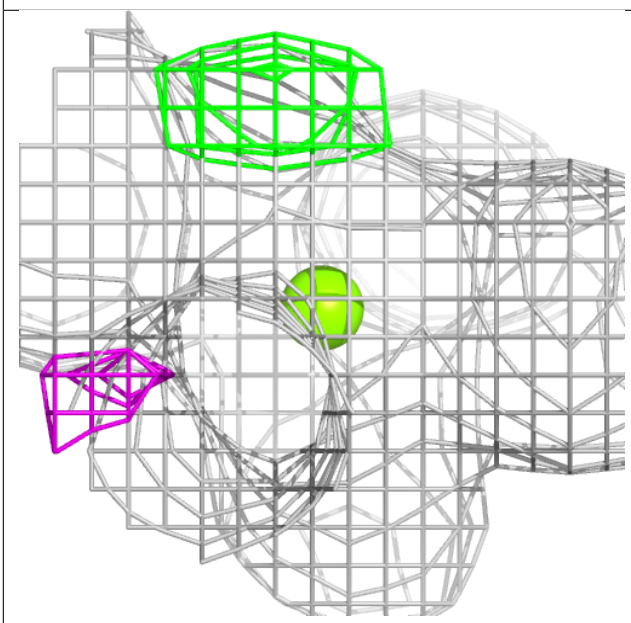


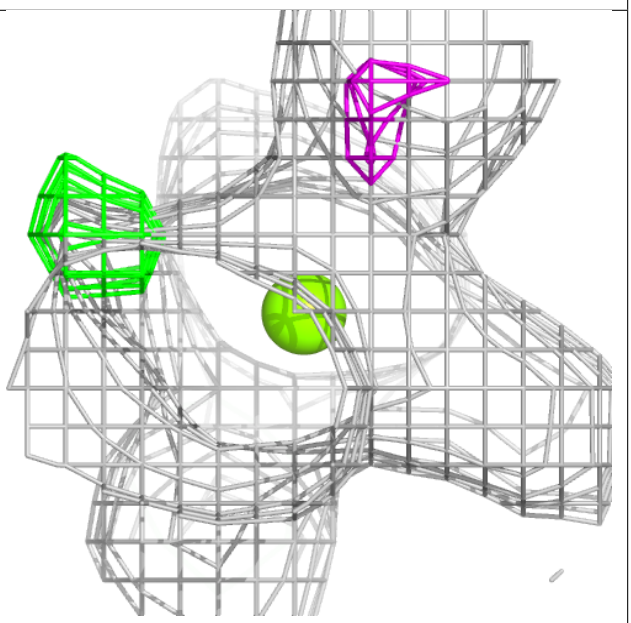


Electron density around MG D 306:

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

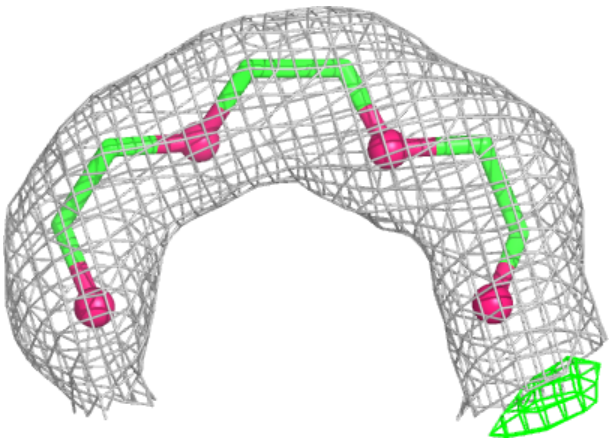


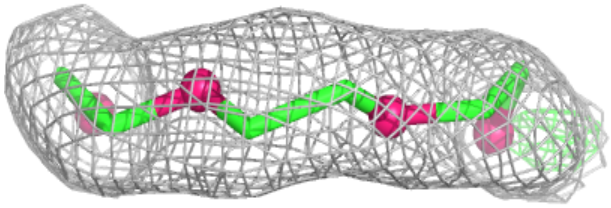


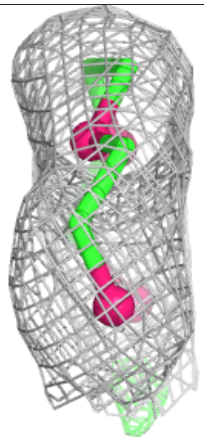


Electron density around PGE B 301:

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

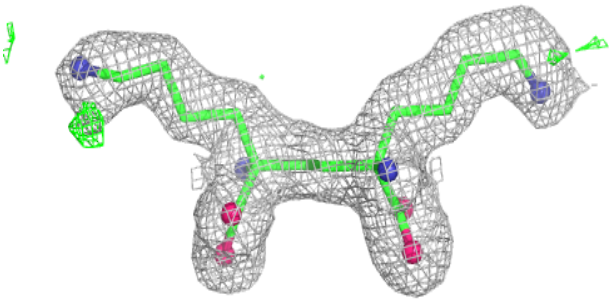


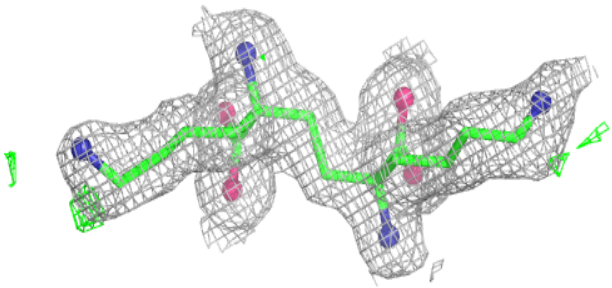


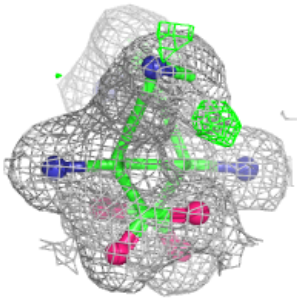


Electron density around 3VN F 302:

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

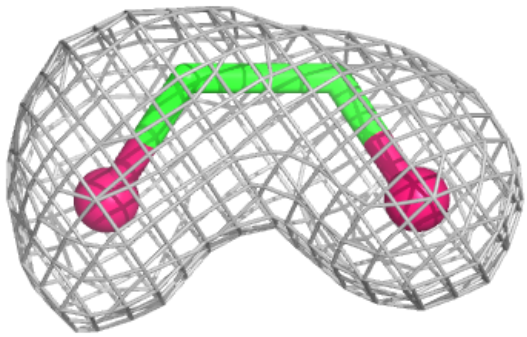


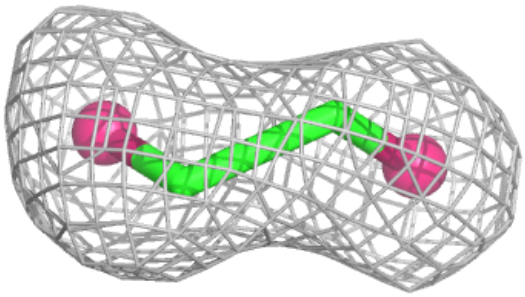


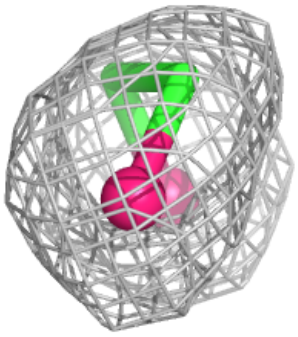


Electron density around EDO D 303:

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

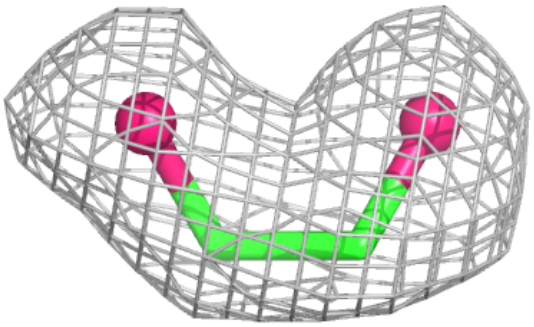


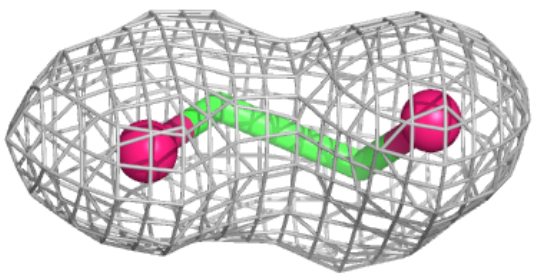


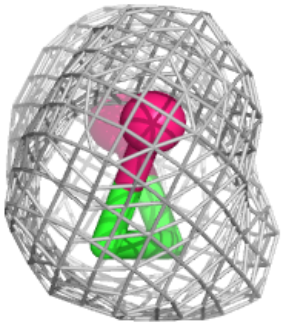


Electron density around EDO B 305:

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

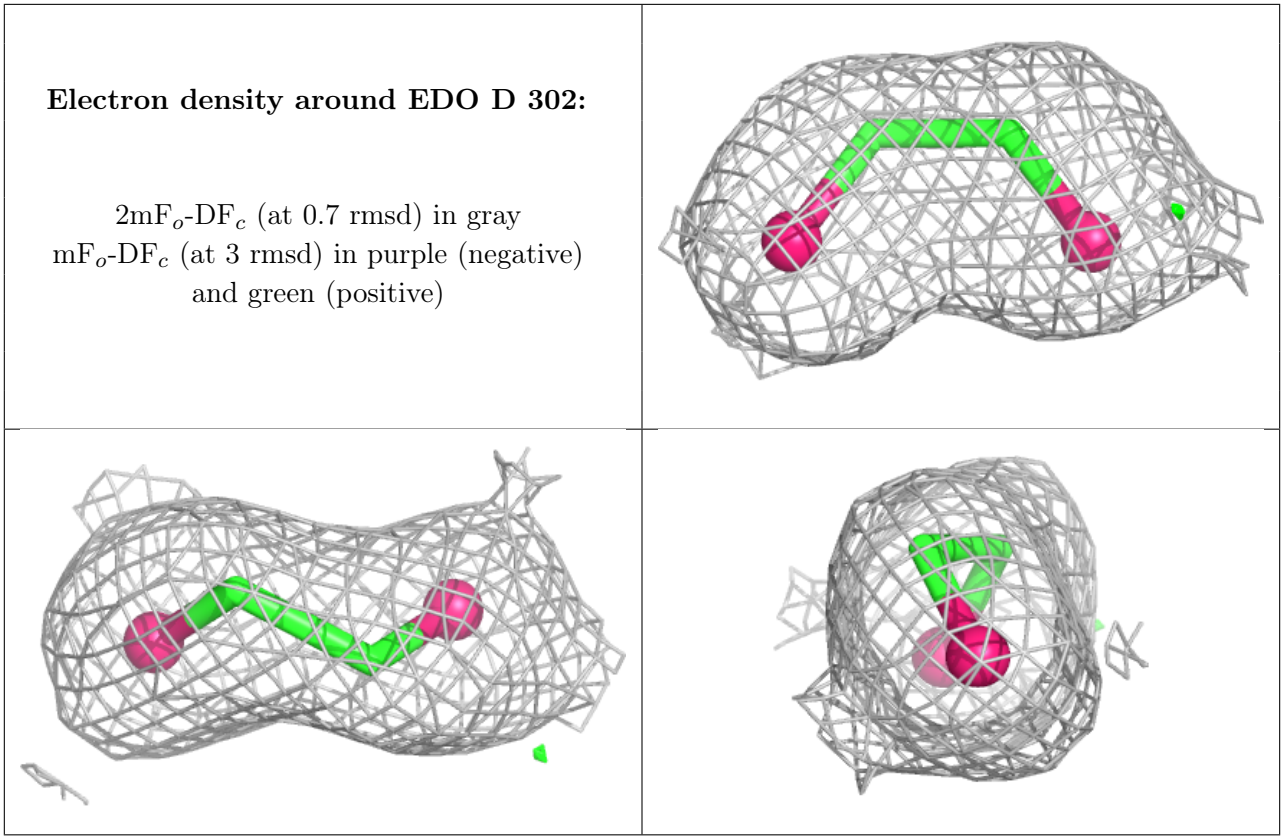






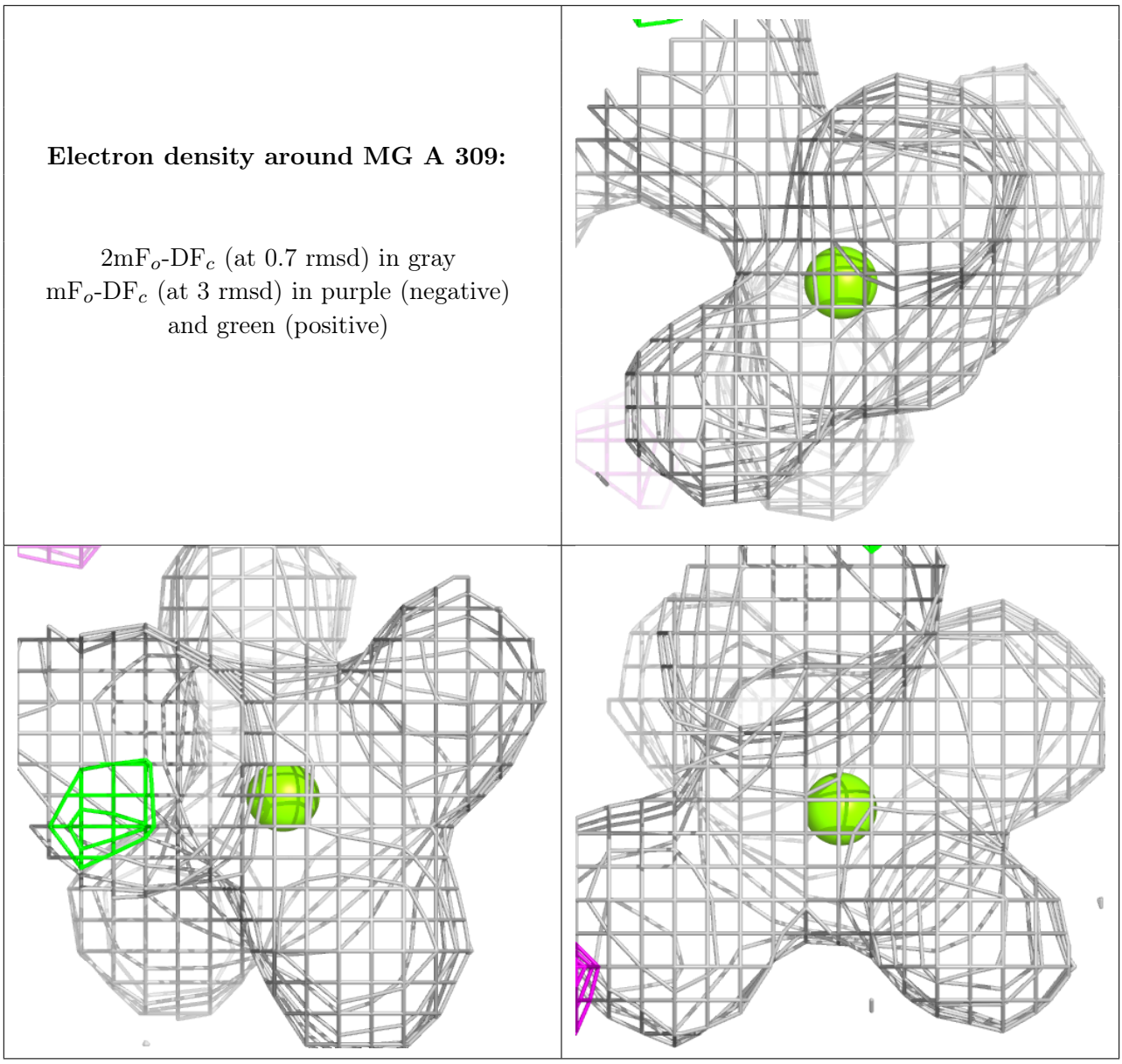
Electron density around EDO D 302:

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



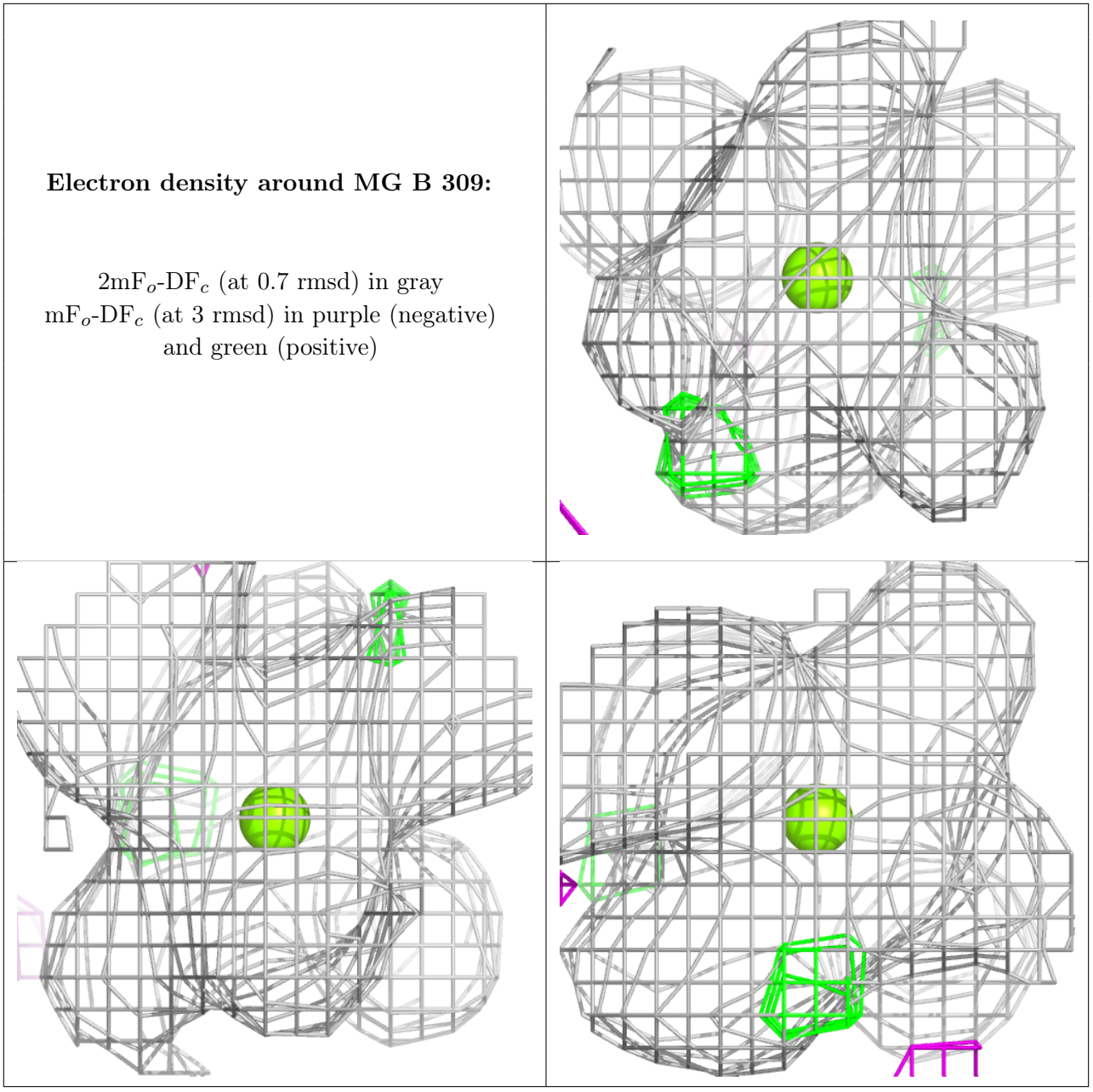
Electron density around MG A 309:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.