wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 01:56 PM EDT

PDB ID	:	7KWN
Title	:	Dihydrodipicolinate synthase from C. jejuni with pyruvate bound to the active site in C2221 space group
Authors	:	Saran, S.; Sanders, D.A.R.
Deposited on	:	2020-12-01
Resolution	:	2.24 Å(reported)

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

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

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

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

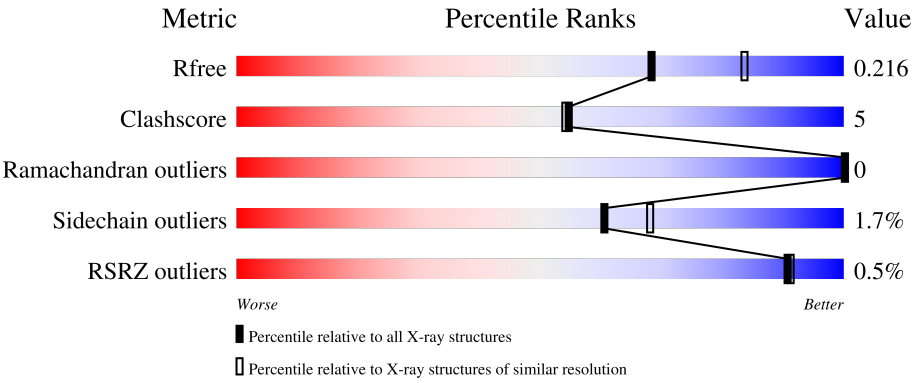
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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

Mol	Chain	Length	Quality of chain
1	A	310	87% 7% • 5%
1	B	310	% 85% 9% • 5%
1	C	310	87% 8% • 5%
1	D	310	% 87% 8% • •
1	E	310	85% 10% 5%

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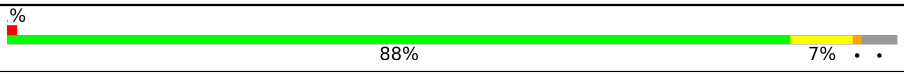
Mol	Chain	Length	Quality of chain
1	F	310	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	302	-	-	X	-
4	ACT	A	305	-	-	-	X
6	PEG	B	304	-	-	X	-
6	PEG	B	305	-	-	X	-
6	PEG	E	303	-	-	X	-
6	PEG	F	302	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14484 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
			2271	1444	377	437	13			
1	B	296	Total	C	N	O	S	0	0	0
			2265	1440	375	437	13			
1	C	296	Total	C	N	O	S	0	0	0
			2273	1446	377	437	13			
1	D	297	Total	C	N	O	S	0	0	0
			2276	1447	378	438	13			
1	E	296	Total	C	N	O	S	0	0	0
			2275	1447	378	437	13			
1	F	297	Total	C	N	O	S	0	0	0
			2281	1452	378	438	13			

There are 72 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
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
B	-7	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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

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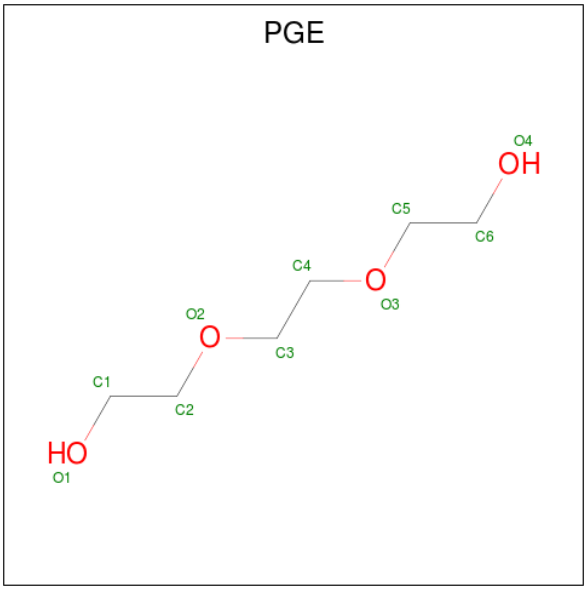
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP 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

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



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

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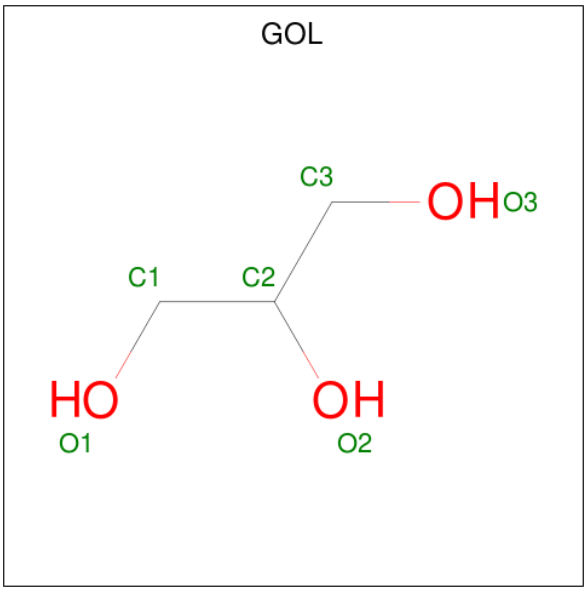
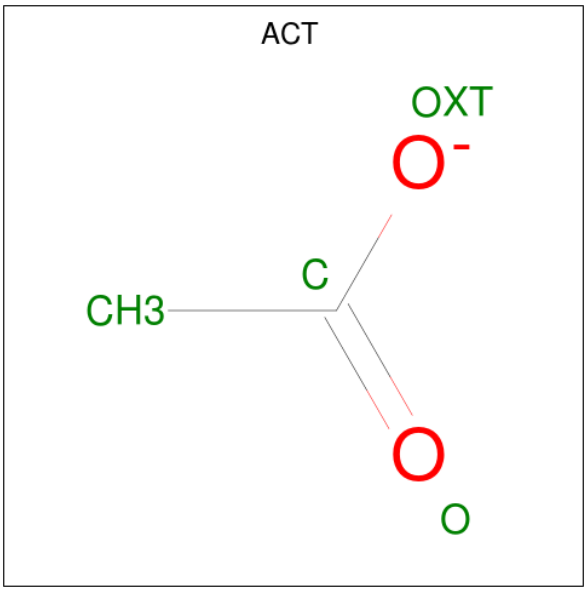
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 10 6 4	0	0
2	F	1	Total C O 10 6 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



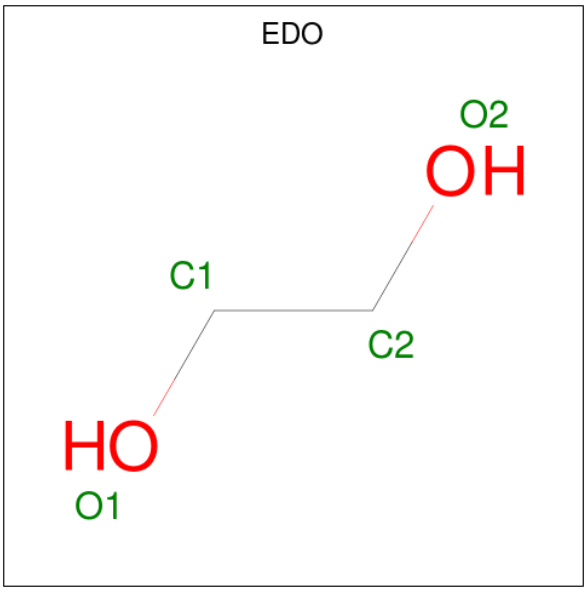
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

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



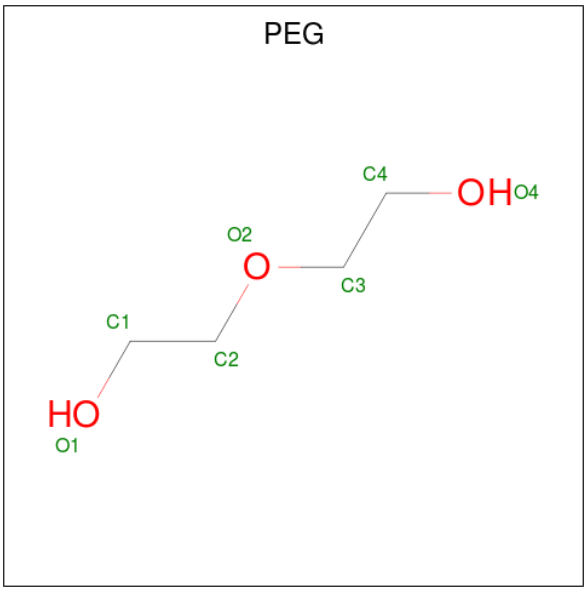
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Mg 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	120	Total O 120 120	0	0
8	B	114	Total O 114 114	0	0
8	C	113	Total O 113 113	0	0

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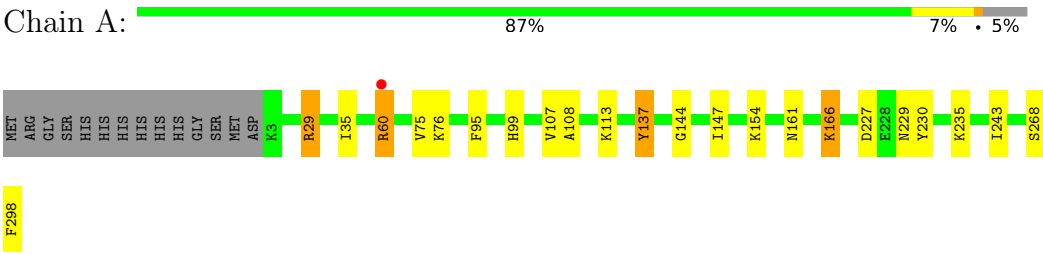
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	104	Total O 104 104	0	0
8	E	115	Total O 115 115	0	0
8	F	106	Total O 106 106	0	0

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.

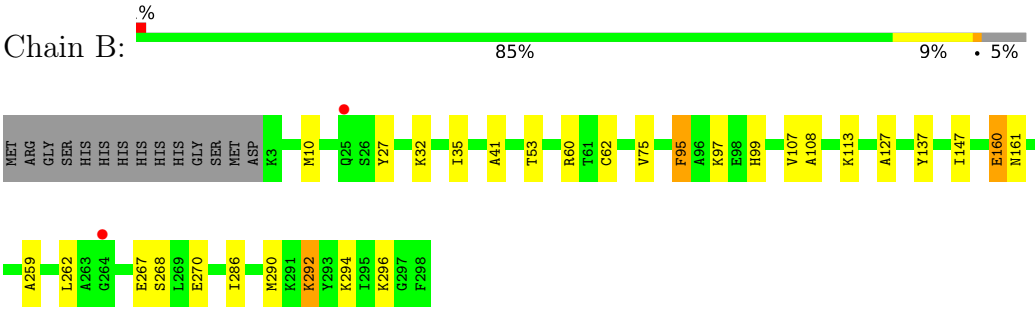
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A:



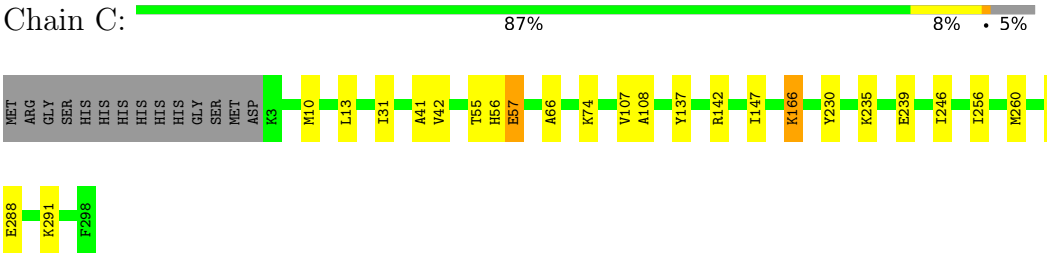
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:



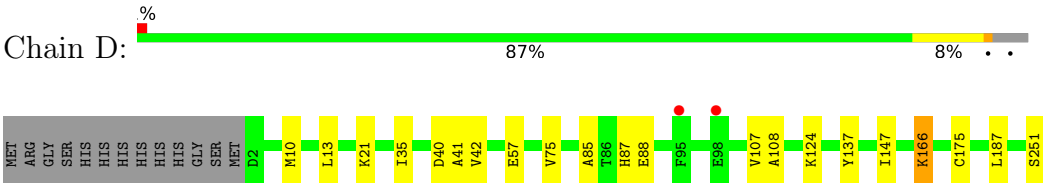
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

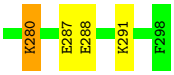
Chain C:



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

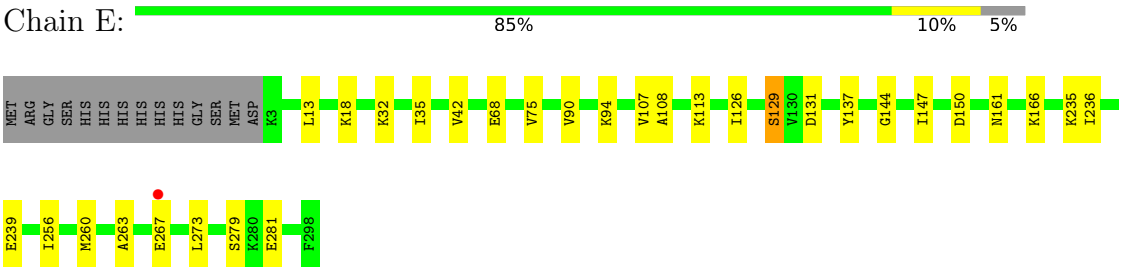
Chain D:





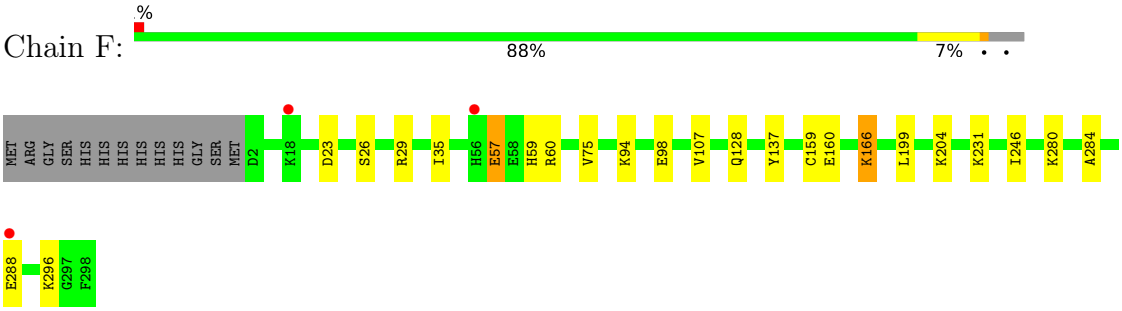
• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

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	83.99Å 230.19Å 200.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 2.24 49.30 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.89-2.24) 96.3 (49.30-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.177 , 0.216 0.181 , 0.216	Depositor DCC
R_{free} test set	4664 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14484	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.53	0/2295	0.57	0/3105
1	B	0.55	0/2289	0.55	0/3099
1	C	0.47	0/2297	0.54	0/3107
1	D	0.44	0/2300	0.53	0/3112
1	E	0.38	0/2299	0.53	0/3109
1	F	0.48	0/2305	0.51	0/3116
All	All	0.48	0/13785	0.54	0/18648

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	C	166	KPI	Mainchain
1	D	166	KPI	Mainchain
1	F	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	2271	0	2296	18	0
1	B	2265	0	2278	44	0
1	C	2273	0	2300	18	0
1	D	2276	0	2298	22	0
1	E	2275	0	2307	28	0
1	F	2281	0	2315	17	0
2	A	10	0	14	1	0
2	B	10	0	14	0	0
2	C	10	0	14	0	0
2	D	10	0	14	0	0
2	E	10	0	14	1	0
2	F	10	0	14	0	0
3	A	12	0	16	4	0
3	D	6	0	8	5	0
4	A	12	0	9	2	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
4	E	4	0	3	0	0
5	A	4	0	6	0	0
5	B	8	0	12	0	0
5	C	4	0	6	1	0
5	F	12	0	18	2	0
6	B	14	0	20	18	0
6	D	7	0	10	0	0
6	E	7	0	10	11	0
6	F	7	0	10	6	0
7	B	2	0	0	0	0
8	A	120	0	0	1	0
8	B	114	0	0	0	0
8	C	113	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	104	0	0	1	0
8	E	115	0	0	1	0
8	F	106	0	0	1	0
All	All	14484	0	14015	145	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 5.

The worst 5 of 145 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:LYS:HE3	6:E:303:PEG:C1	1.65	1.23
1:B:294:LYS:HE3	6:B:305:PEG:C2	1.75	1.16
1:B:286:ILE:HG22	1:B:290:MET:HE2	1.26	1.16
1:F:159:CYS:HA	6:F:302:PEG:H22	1.17	1.15
1:B:294:LYS:CE	6:B:305:PEG:H21	1.77	1.12

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%)	287 (98%)	6 (2%)	0	100	100
1	B	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	C	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	D	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	E	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	F	294/310 (95%)	287 (98%)	7 (2%)	0	100	100
All	All	1760/1860 (95%)	1721 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/260 (95%)	240 (98%)	6 (2%)	49	55
1	B	244/260 (94%)	236 (97%)	8 (3%)	38	43
1	C	246/260 (95%)	245 (100%)	1 (0%)	91	93
1	D	246/260 (95%)	243 (99%)	3 (1%)	71	78
1	E	247/260 (95%)	245 (99%)	2 (1%)	81	87
1	F	247/260 (95%)	242 (98%)	5 (2%)	55	62
All	All	1476/1560 (95%)	1451 (98%)	25 (2%)	60	68

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	57	GLU
1	D	280	LYS
1	F	280	LYS
1	D	57	GLU
1	E	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	D	25	GLN
1	E	4	ASN
1	E	161	ASN
1	F	56	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KPI	D	166	1	11,13,14	1.48	1 (9%)	10,15,17	3.19	5 (50%)
1	KPI	E	166	1	11,13,14	0.84	0	10,15,17	3.21	5 (50%)
1	KPI	A	166	1	11,13,14	1.49	1 (9%)	10,15,17	3.19	4 (40%)
1	KPI	C	166	1	11,13,14	2.16	3 (27%)	10,15,17	3.79	6 (60%)
1	KPI	B	166	1	11,13,14	2.19	3 (27%)	10,15,17	3.72	5 (50%)
1	KPI	F	166	1	11,13,14	1.47	1 (9%)	10,15,17	3.17	4 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	D	166	1	-	0/13/14/16	-
1	KPI	E	166	1	-	0/13/14/16	-
1	KPI	A	166	1	-	0/13/14/16	-
1	KPI	C	166	1	-	0/13/14/16	-
1	KPI	B	166	1	-	0/13/14/16	-
1	KPI	F	166	1	-	0/13/14/16	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	O2-CX2	5.15	1.36	1.22
1	C	166	KPI	O2-CX2	5.13	1.36	1.22
1	B	166	KPI	O-C	4.16	1.36	1.19
1	D	166	KPI	O-C	4.11	1.36	1.19
1	C	166	KPI	O-C	4.10	1.36	1.19

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	166	KPI	C1-CX1-CX2	-7.01	111.35	118.17
1	B	166	KPI	C1-CX1-CX2	-6.98	111.39	118.17
1	C	166	KPI	C1-CX1-CX2	-6.97	111.39	118.17
1	A	166	KPI	C1-CX1-CX2	-6.89	111.47	118.17
1	F	166	KPI	C1-CX1-CX2	-6.89	111.47	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	PGE	F	301	-	9,9,9	0.31	0	8,8,8	0.30	0
4	ACT	E	302	-	3,3,3	1.04	0	3,3,3	1.43	0
3	GOL	D	302	-	5,5,5	0.26	0	5,5,5	0.36	0
5	EDO	F	303	-	3,3,3	0.24	0	2,2,2	0.40	0
2	PGE	B	301	-	9,9,9	0.31	0	8,8,8	0.30	0
6	PEG	B	304	-	6,6,6	0.28	0	5,5,5	0.47	0
4	ACT	A	304	-	3,3,3	1.27	0	3,3,3	1.38	0
2	PGE	A	301	-	9,9,9	0.31	0	8,8,8	0.29	0
5	EDO	B	309	-	3,3,3	0.20	0	2,2,2	0.42	0
3	GOL	A	302	-	5,5,5	0.96	0	5,5,5	0.89	0
6	PEG	D	303	-	6,6,6	0.32	0	5,5,5	0.79	0
6	PEG	E	303	-	6,6,6	0.28	0	5,5,5	0.70	0
3	GOL	A	303	-	5,5,5	0.86	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	B	308	-	3,3,3	0.33	0	2,2,2	0.40	0
4	ACT	C	302	-	3,3,3	1.02	0	3,3,3	0.74	0
2	PGE	D	301	-	9,9,9	0.30	0	8,8,8	0.23	0
4	ACT	A	306	-	3,3,3	1.17	0	3,3,3	0.23	0
4	ACT	A	305	-	3,3,3	0.78	0	3,3,3	0.82	0
5	EDO	F	305	-	3,3,3	0.28	0	2,2,2	0.47	0
6	PEG	F	302	-	6,6,6	0.53	0	5,5,5	1.10	1 (20%)
2	PGE	E	301	-	9,9,9	0.30	0	8,8,8	0.24	0
5	EDO	F	304	-	3,3,3	0.33	0	2,2,2	0.50	0
5	EDO	A	307	-	3,3,3	0.37	0	2,2,2	0.55	0
4	ACT	B	302	-	3,3,3	1.35	0	3,3,3	1.52	0
4	ACT	B	303	-	3,3,3	0.82	0	3,3,3	0.65	0
5	EDO	C	303	-	3,3,3	0.30	0	2,2,2	0.63	0
6	PEG	B	305	-	6,6,6	0.44	0	5,5,5	0.34	0
2	PGE	C	301	-	9,9,9	0.31	0	8,8,8	0.24	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	PGE	F	301	-	-	6/7/7/7	-
3	GOL	D	302	-	-	2/4/4/4	-
5	EDO	F	303	-	-	1/1/1/1	-
2	PGE	B	301	-	-	0/7/7/7	-
6	PEG	B	304	-	-	1/4/4/4	-
2	PGE	A	301	-	-	3/7/7/7	-
5	EDO	B	309	-	-	1/1/1/1	-
3	GOL	A	302	-	-	2/4/4/4	-
6	PEG	D	303	-	-	2/4/4/4	-
6	PEG	E	303	-	-	3/4/4/4	-
3	GOL	A	303	-	-	4/4/4/4	-
5	EDO	B	308	-	-	1/1/1/1	-
2	PGE	D	301	-	-	3/7/7/7	-
5	EDO	F	305	-	-	1/1/1/1	-
6	PEG	F	302	-	-	2/4/4/4	-
2	PGE	E	301	-	-	3/7/7/7	-
5	EDO	F	304	-	-	0/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	303	-	-	1/1/1/1	-
6	PEG	B	305	-	-	3/4/4/4	-
2	PGE	C	301	-	-	1/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	302	PEG	O2-C3-C4	-2.01	101.25	110.07

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
3	A	303	GOL	C1-C2-C3-O3
3	A	303	GOL	O2-C2-C3-O3
6	D	303	PEG	O2-C3-C4-O4
6	B	305	PEG	O1-C1-C2-O2

There are no ring outliers.

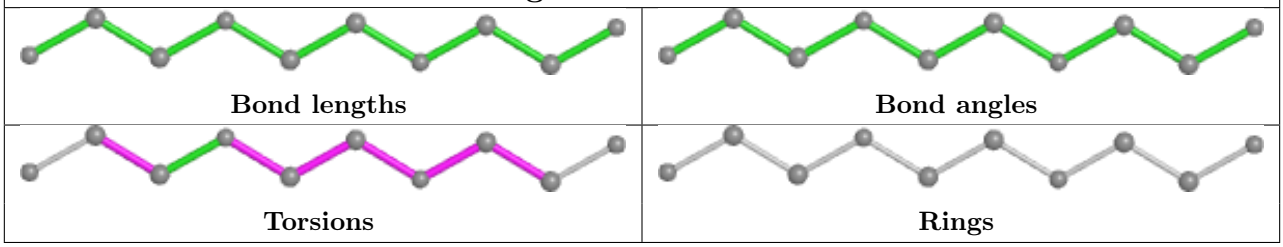
14 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	GOL	5	0
5	F	303	EDO	1	0
6	B	304	PEG	5	0
2	A	301	PGE	1	0
3	A	302	GOL	1	0
6	E	303	PEG	11	0
3	A	303	GOL	3	0
4	A	306	ACT	1	0
4	A	305	ACT	1	0
6	F	302	PEG	6	0
2	E	301	PGE	1	0
5	F	304	EDO	1	0
5	C	303	EDO	1	0
6	B	305	PEG	13	0

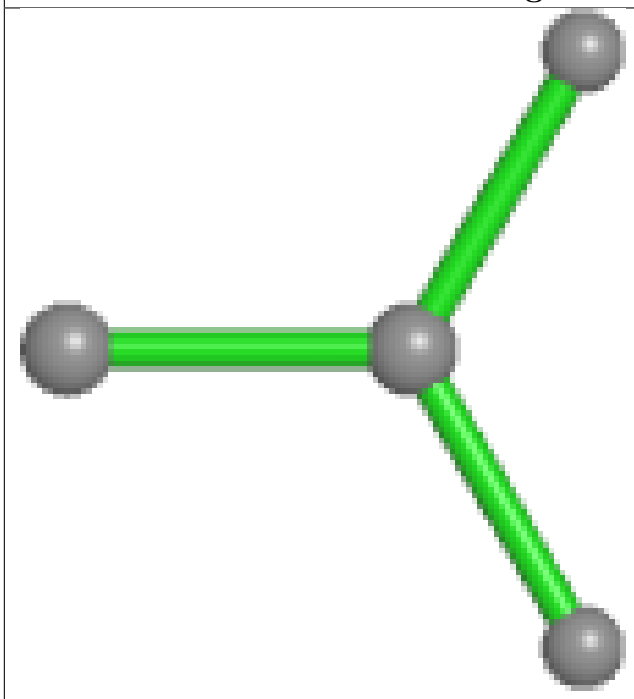
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

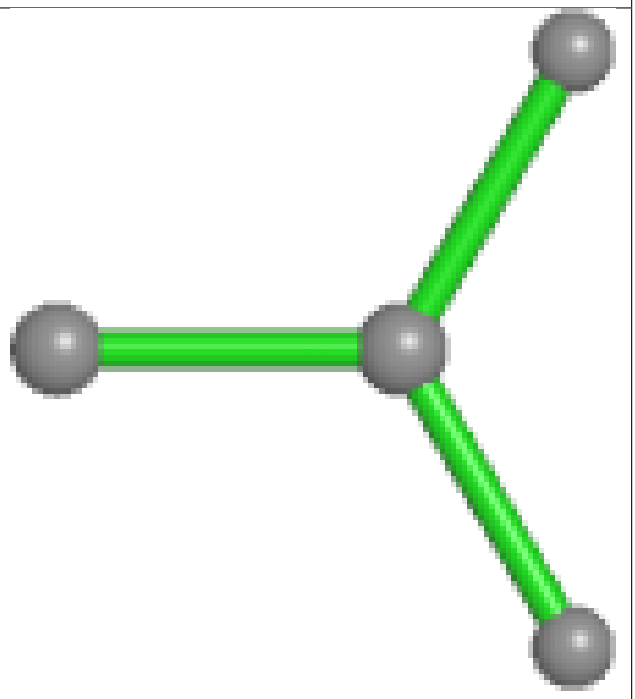
Ligand PGE F 301



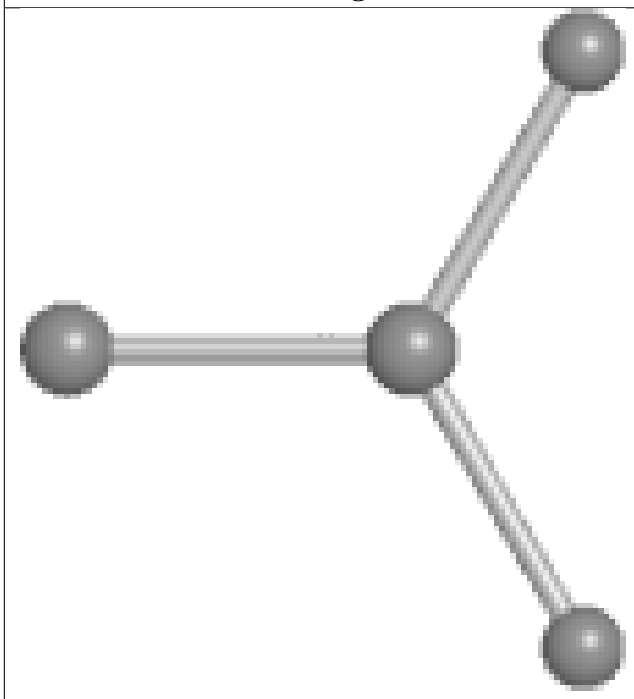
Ligand ACT E 302



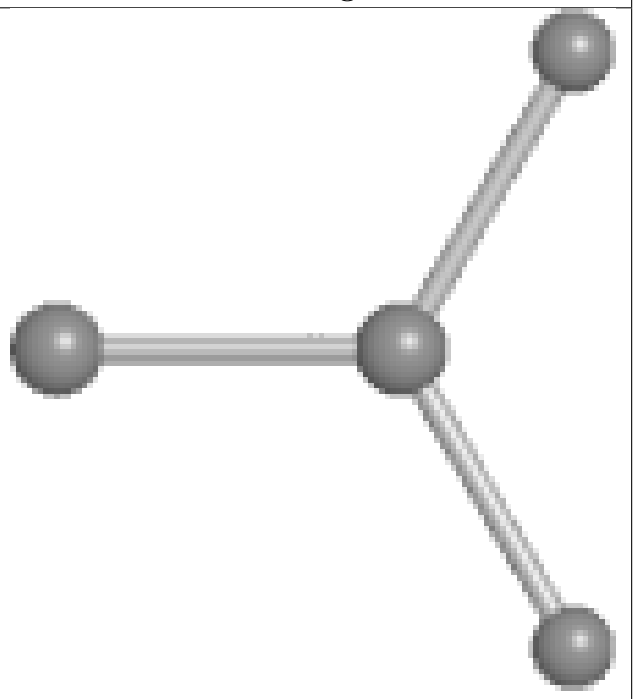
Bond lengths



Bond angles

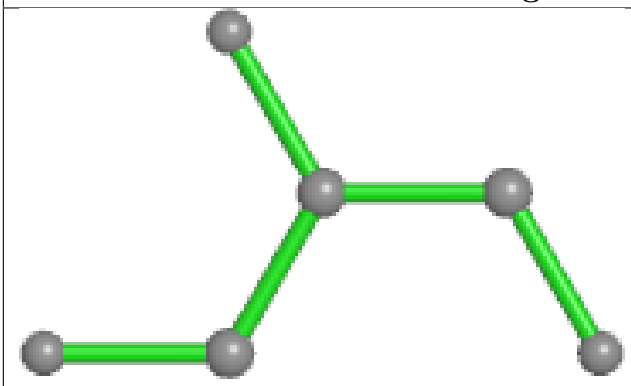


Torsions



Rings

Ligand GOL D 302



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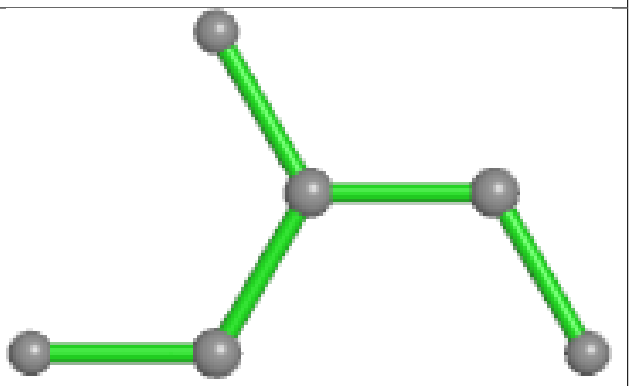

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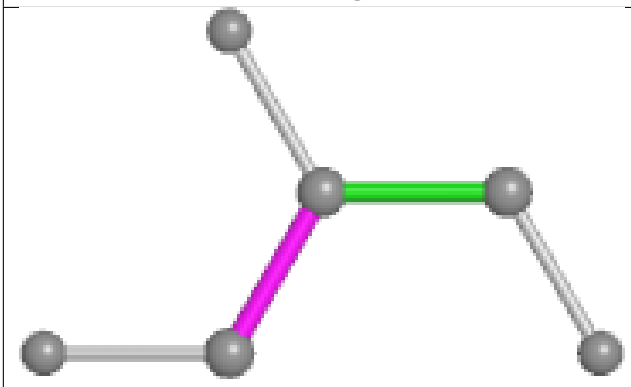

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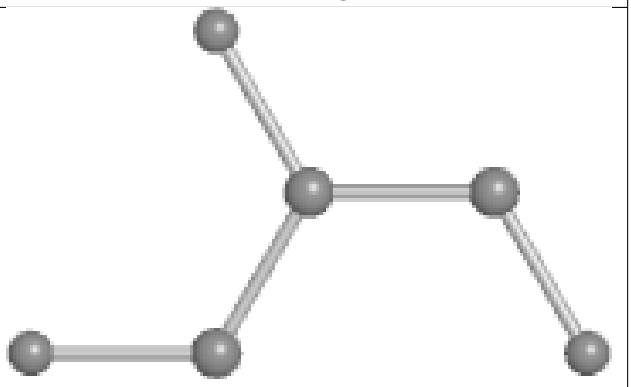
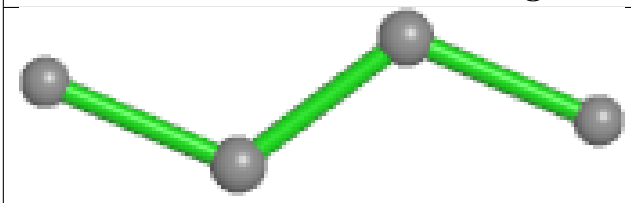


Rings

Ligand EDO F 303



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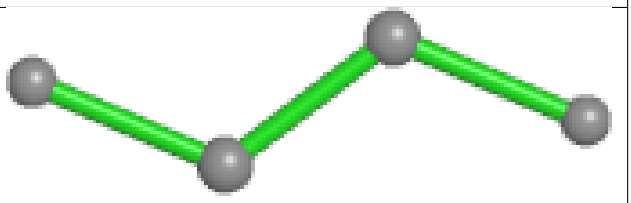
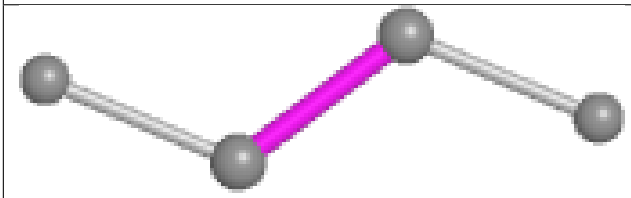
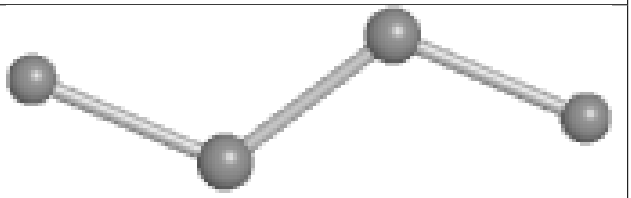


Bond angles



Torsions



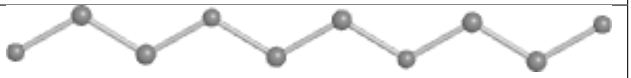
Rings

Ligand PGE B 301

Bond lengths

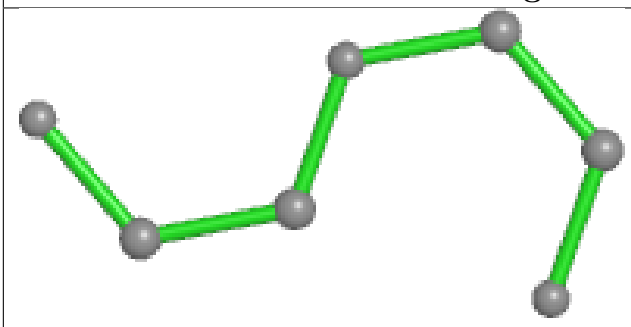
Bond angles

Torsions

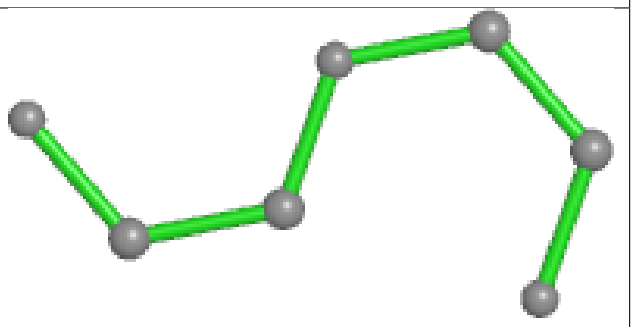


Rings

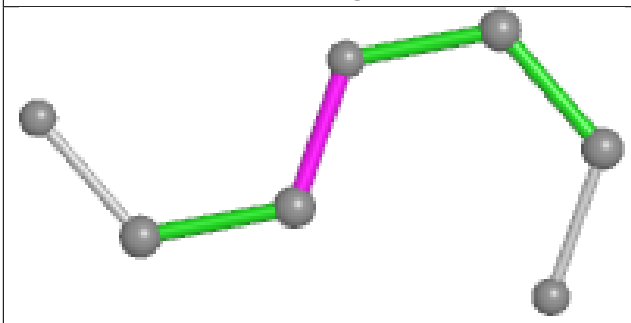
Ligand PEG B 304



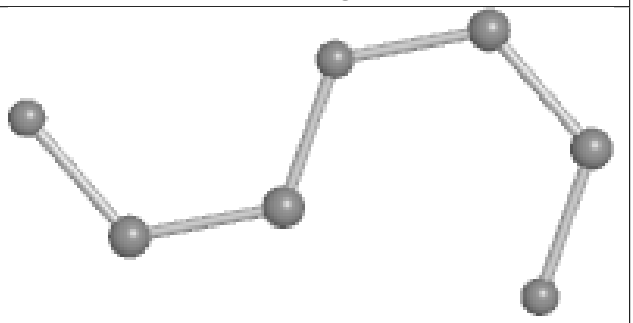
Bond lengths



Bond angles

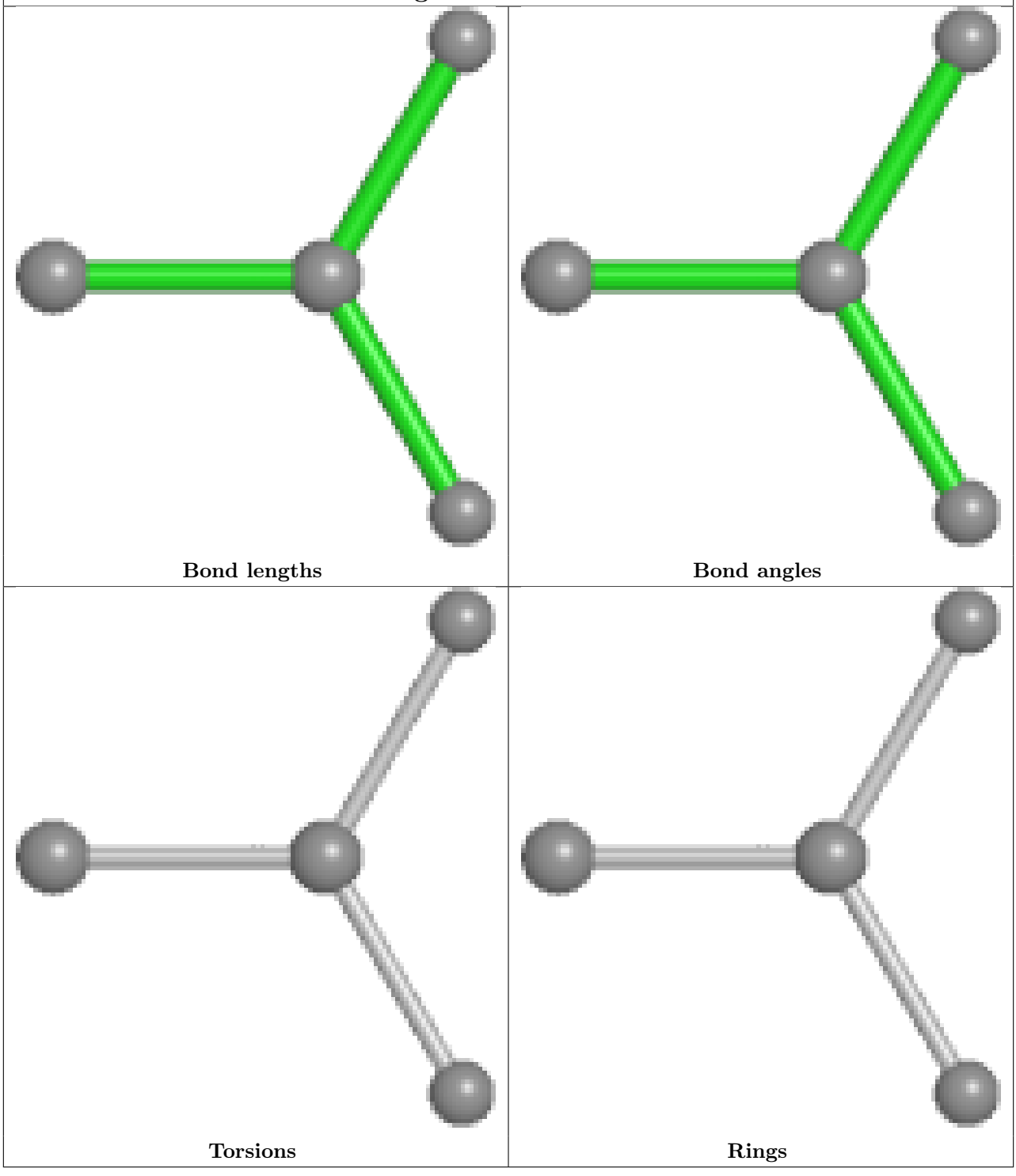


Torsions

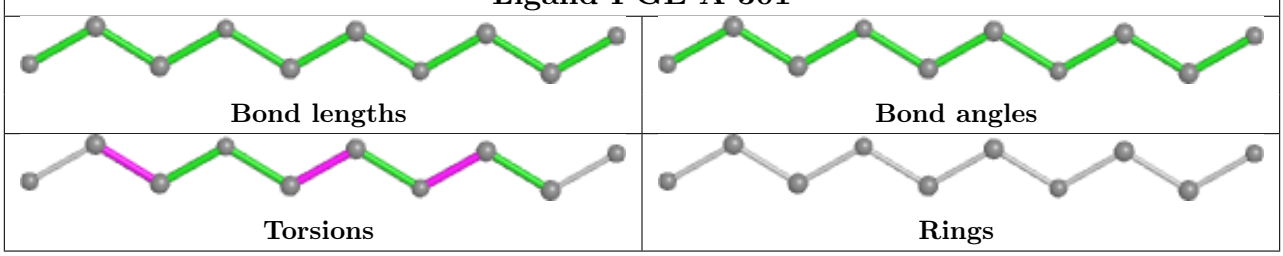


Rings

Ligand ACT A 304



Ligand PGE A 301



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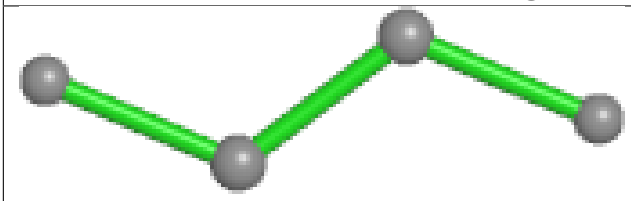
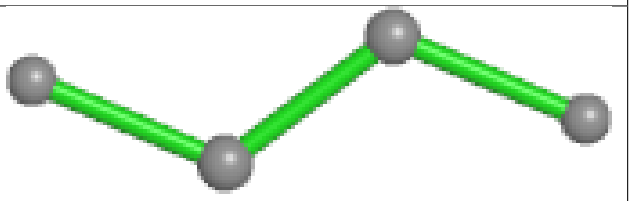
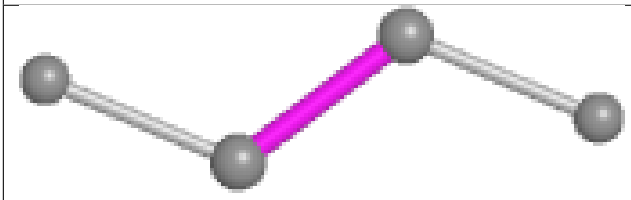


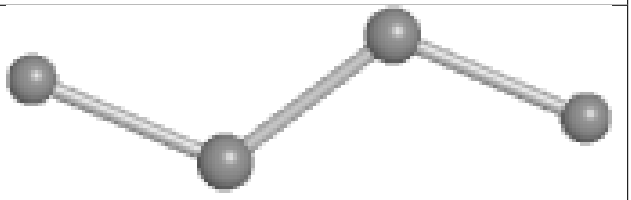
Bond lengths



Bond angles

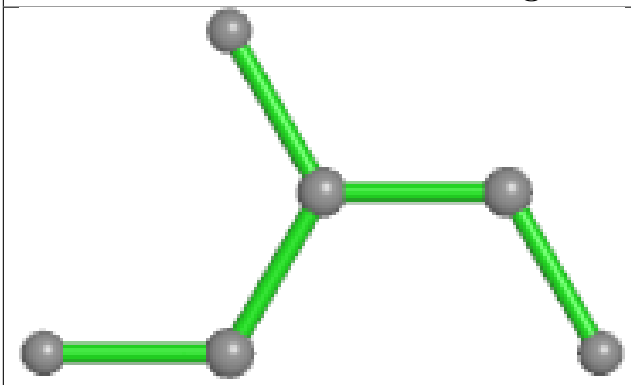


Torsions

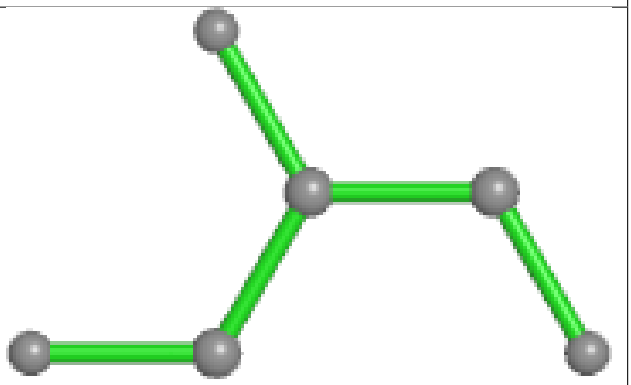


Rings

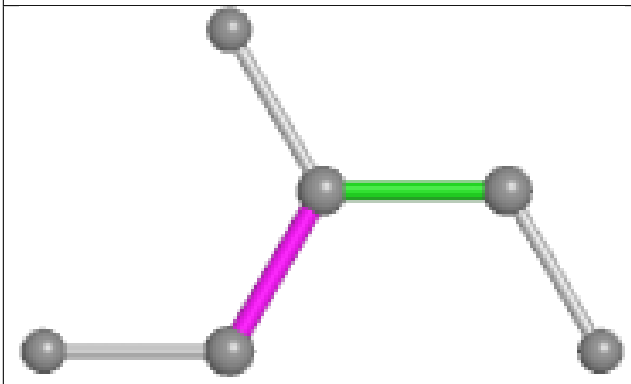
Ligand GOL A 302



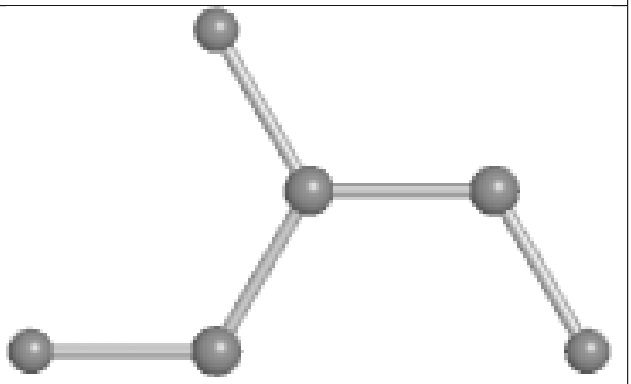
Bond lengths



Bond angles

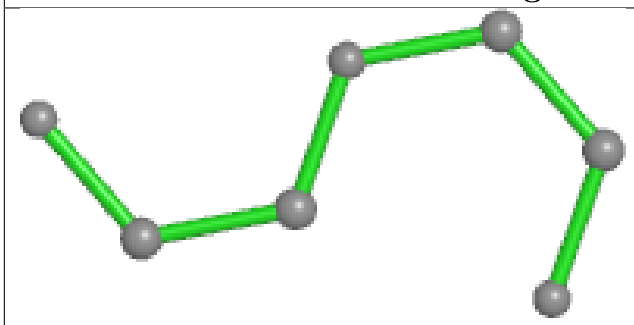


Torsions



Rings

Ligand PEG D 303



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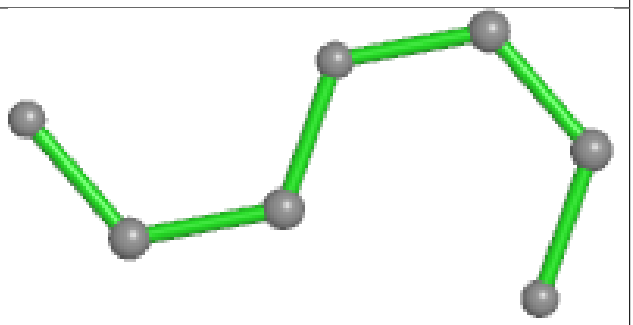
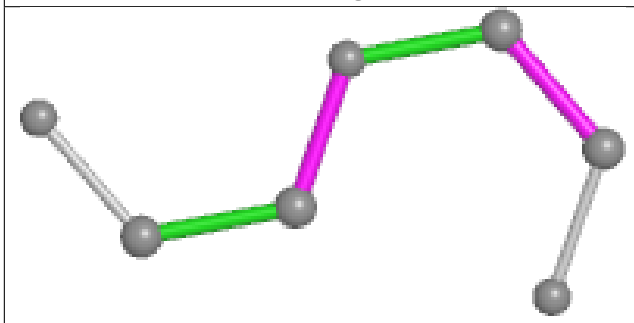
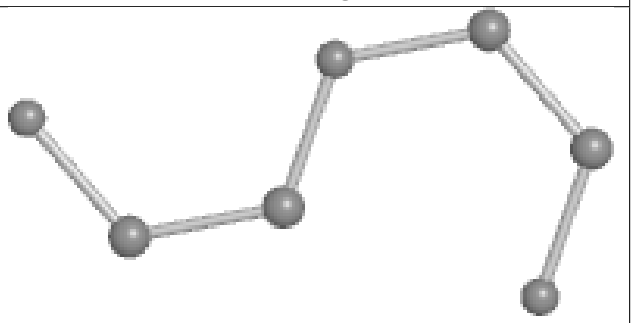


Bond angles

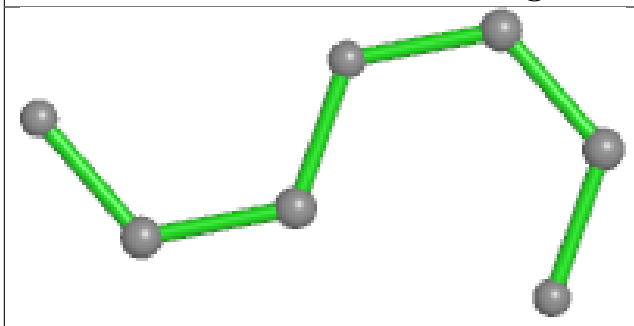


Torsions

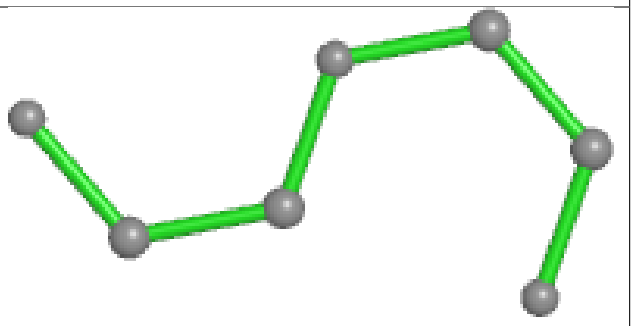


Rings

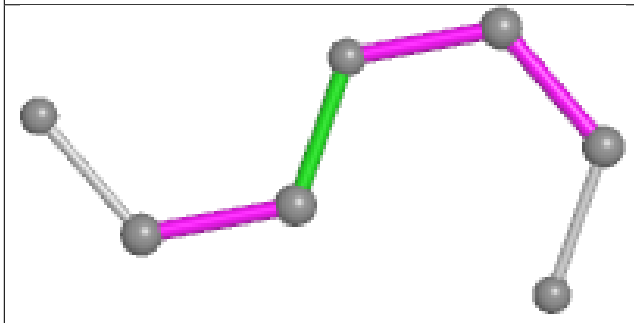
Ligand PEG E 303



Bond lengths



Bond angles



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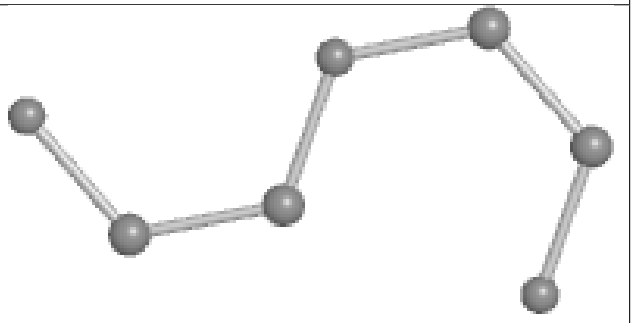
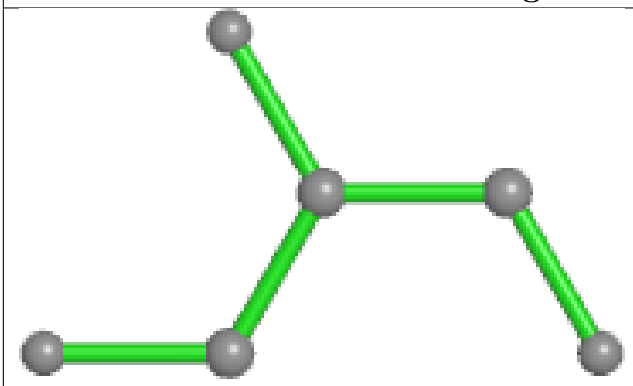


Rings

Ligand GOL A 303



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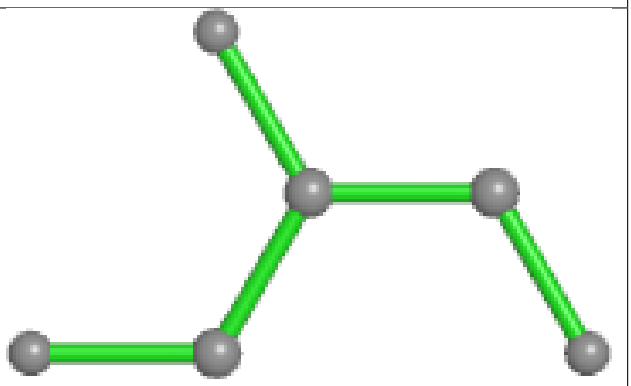
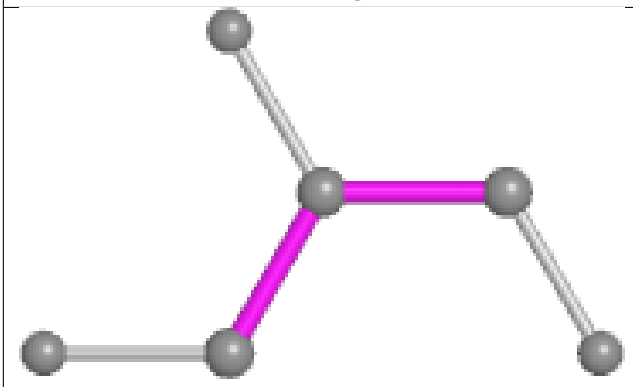


Bond angles



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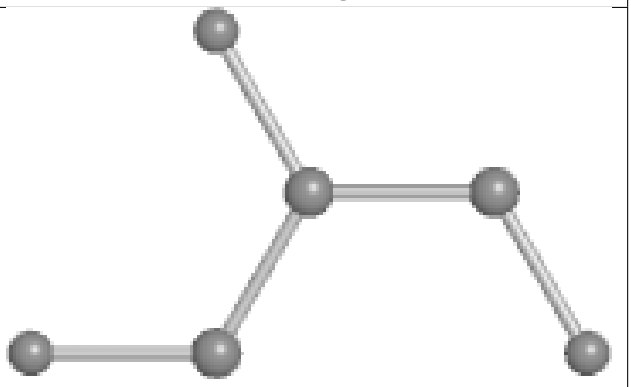
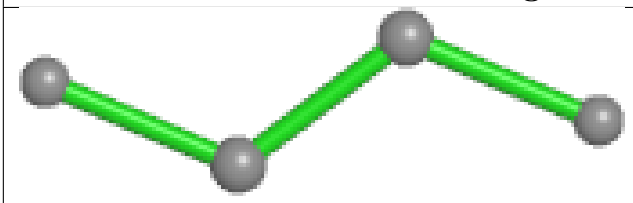


Rings

Ligand EDO B 308



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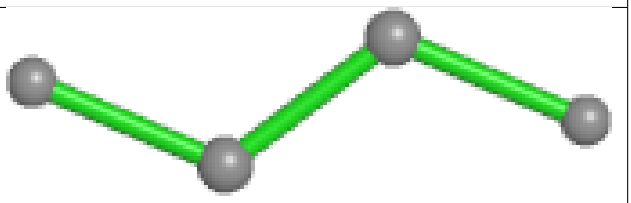
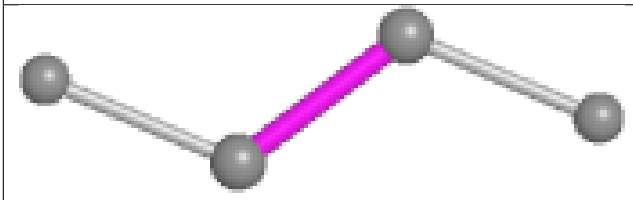


Bond angles



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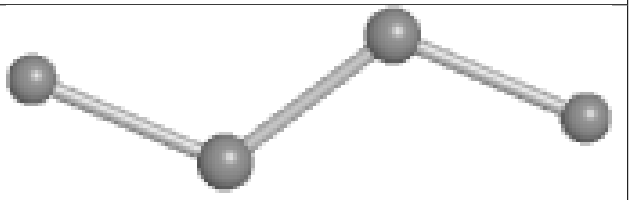
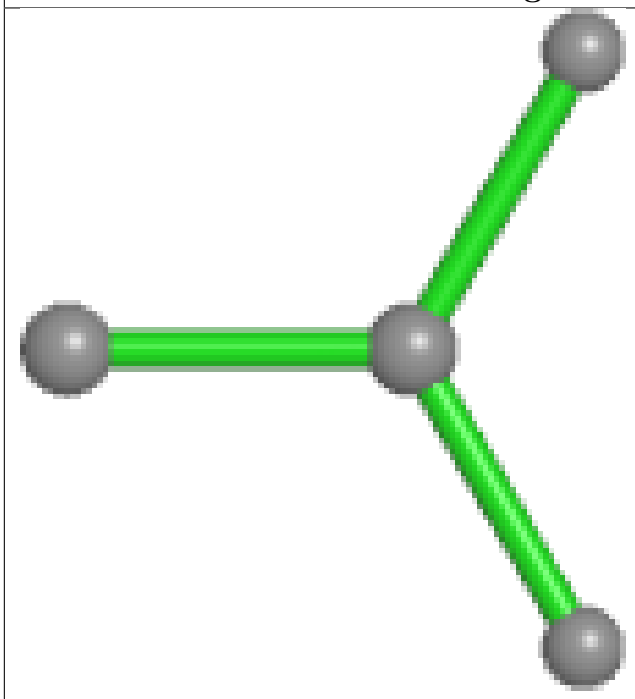
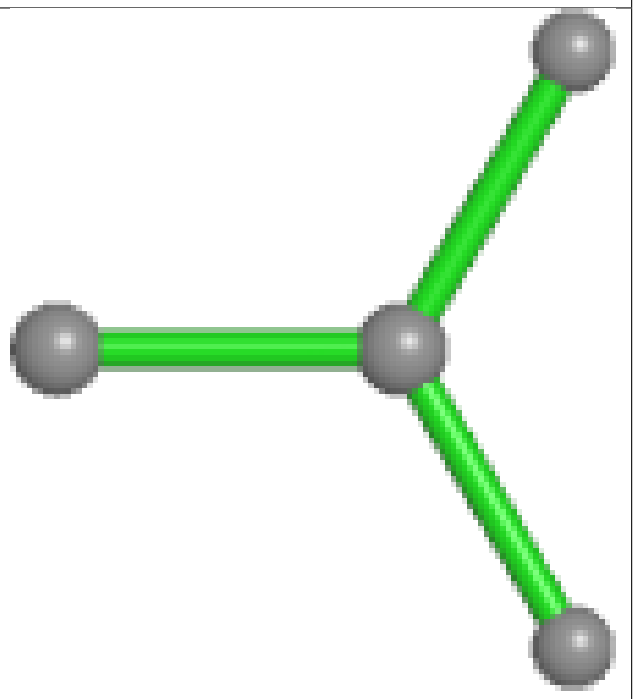


Rings

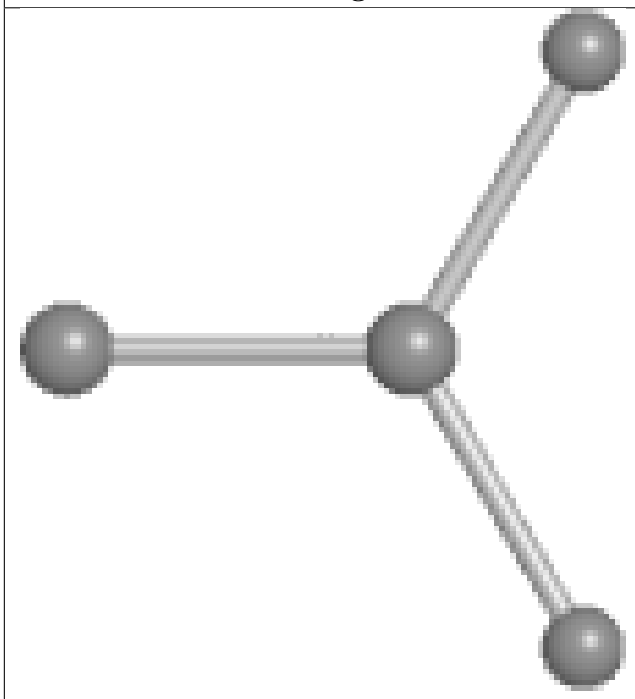
Ligand ACT C 302



Bond lengths



Bond angles



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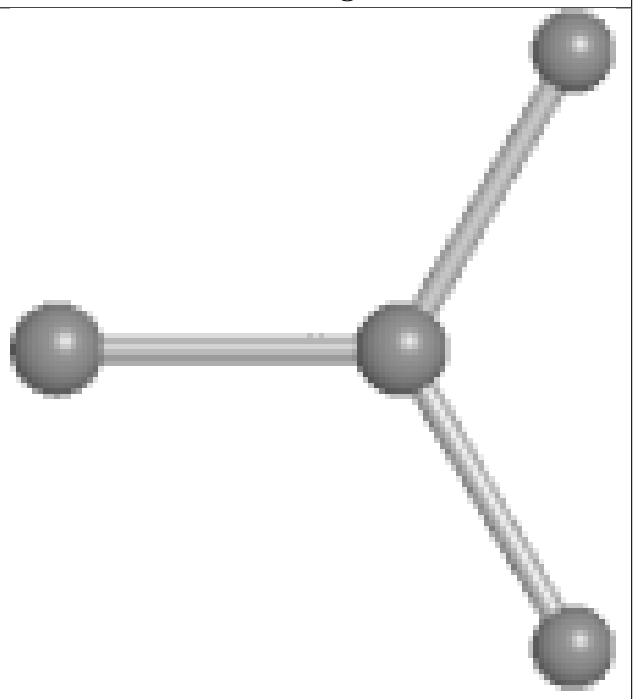
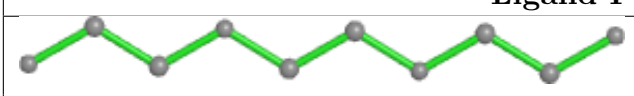


Rings

Ligand PGE D 301



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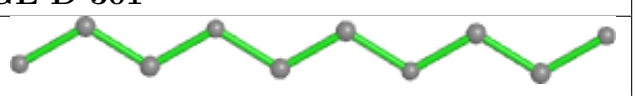
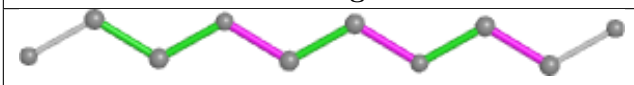


Bond angles



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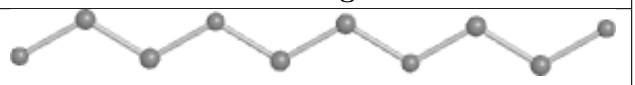
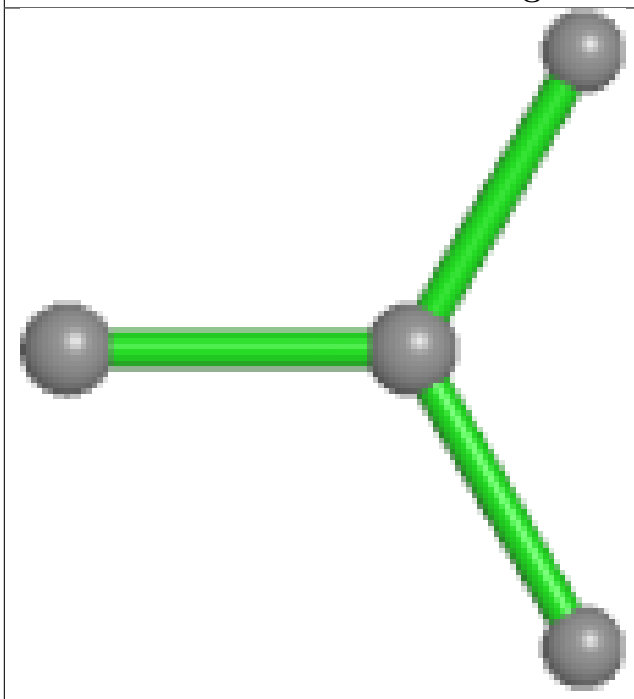


Rings

Ligand ACT A 306



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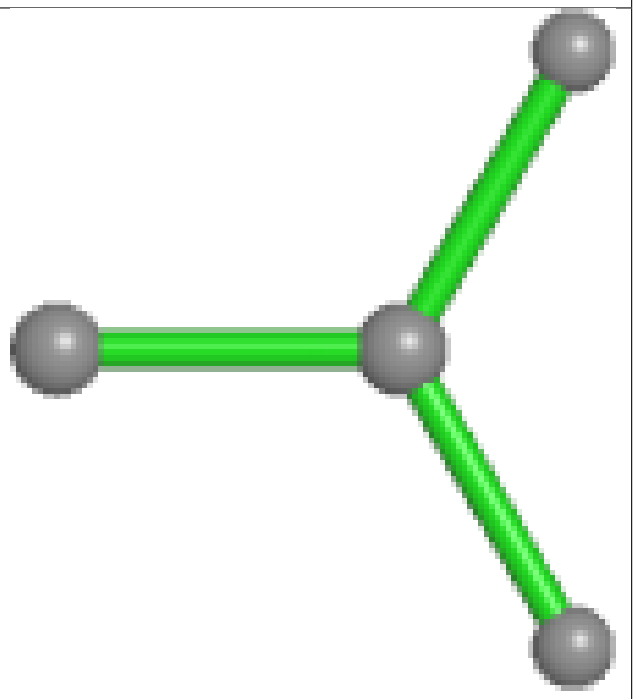
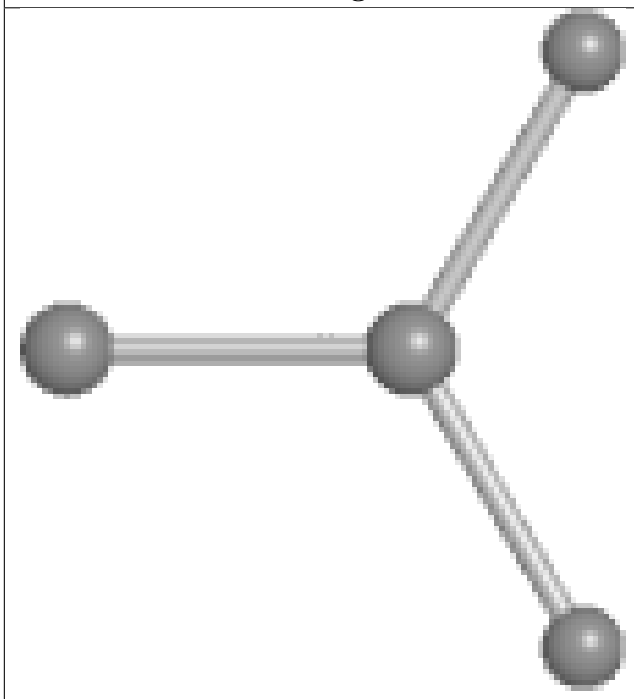
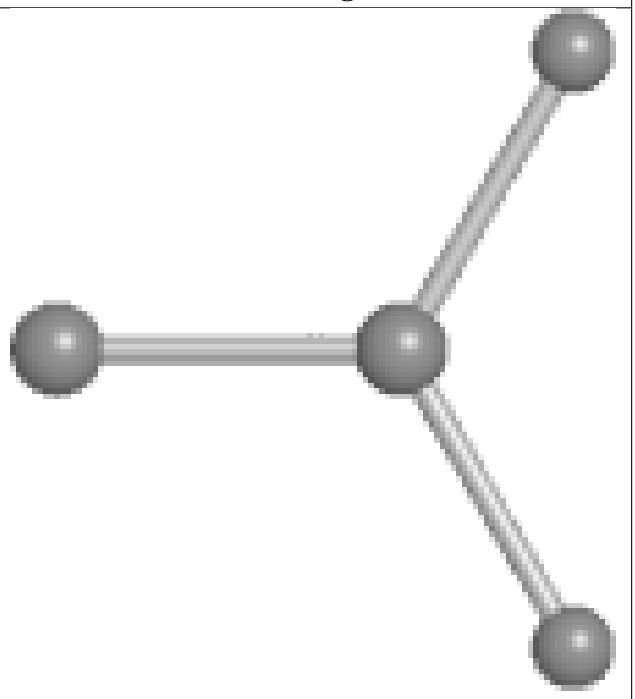


Bond angles

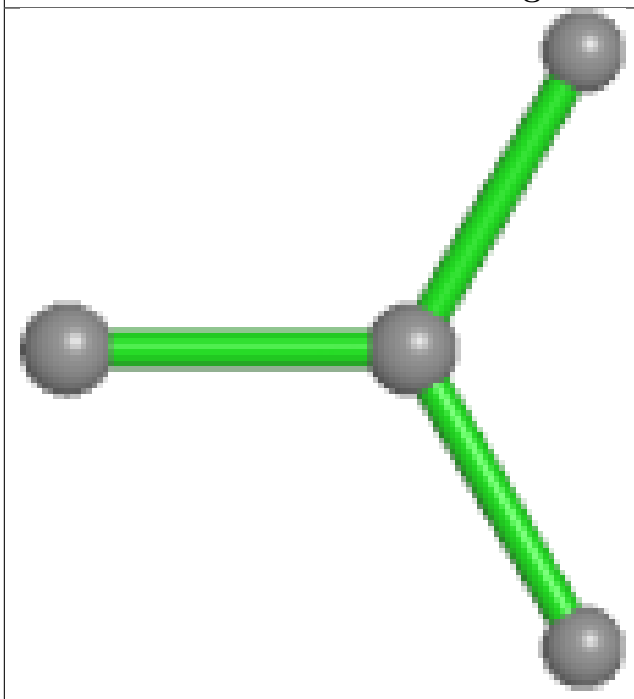


Torsions

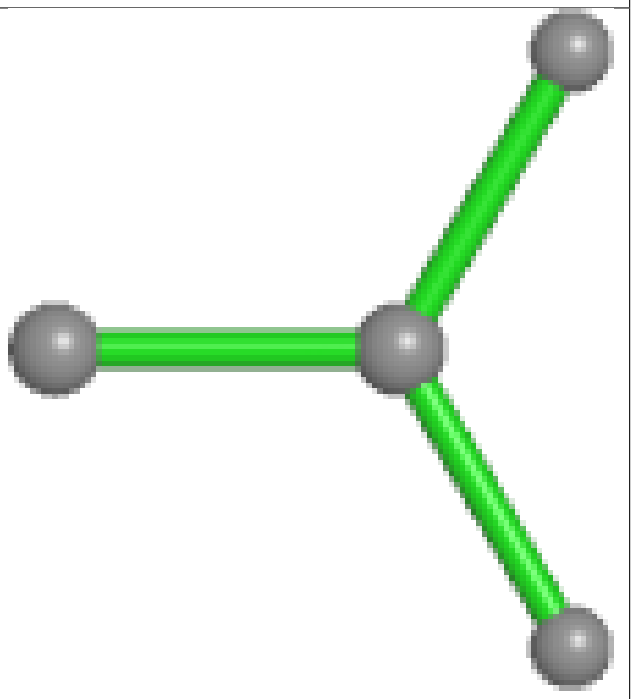


Rings

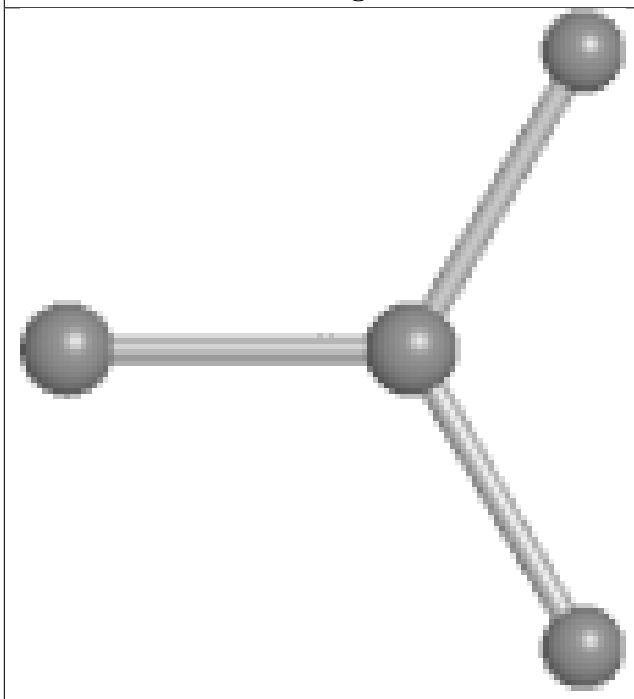
Ligand ACT A 305



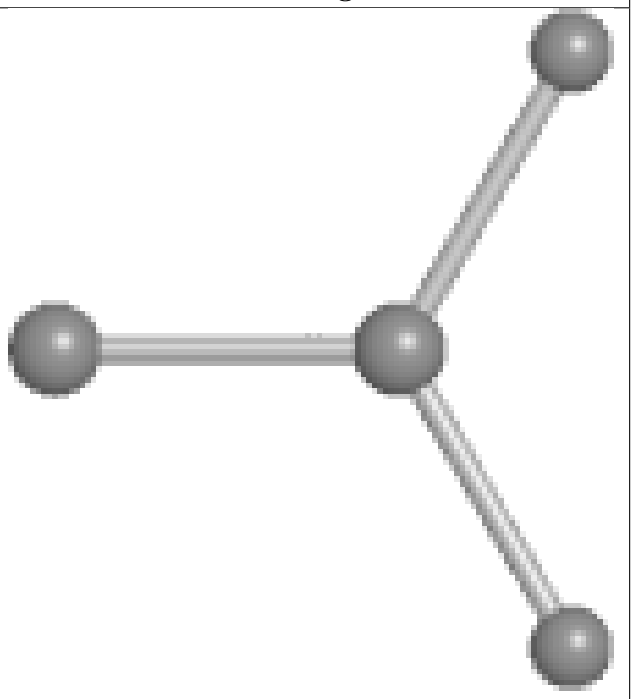
Bond lengths



Bond angles

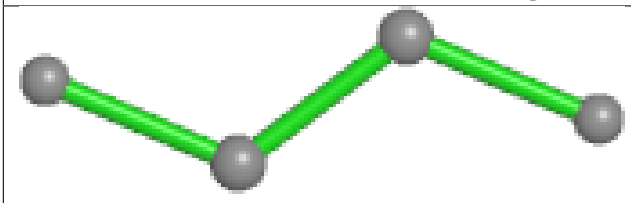


Torsions

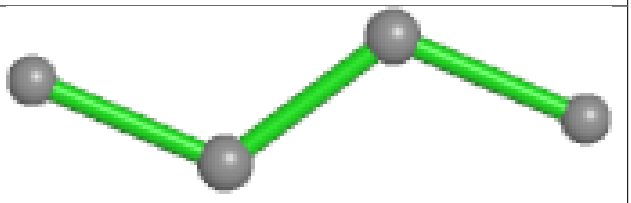


Rings

Ligand EDO F 305



Bond lengths



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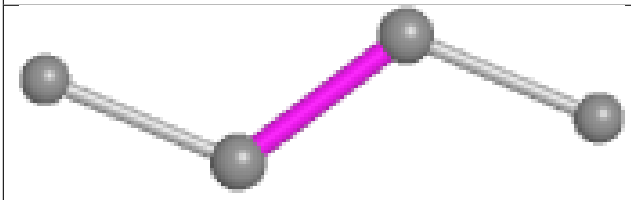

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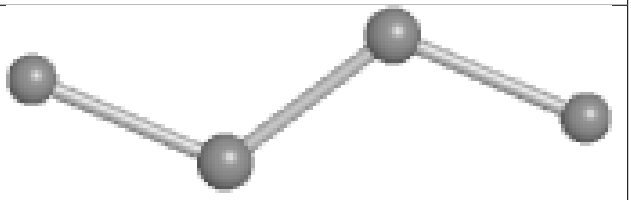
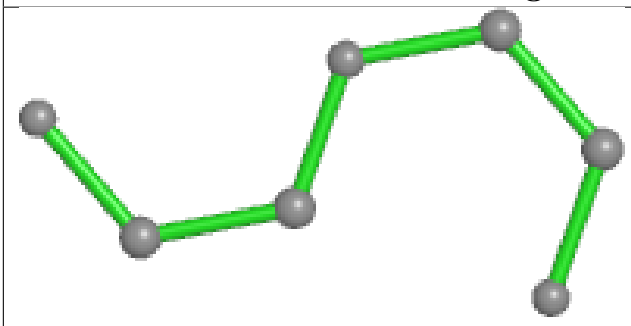


Rings

Ligand PEG F 302



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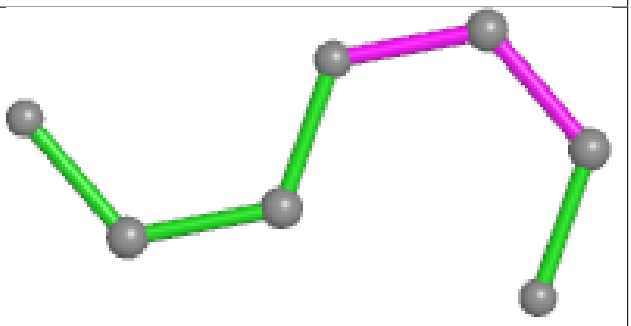
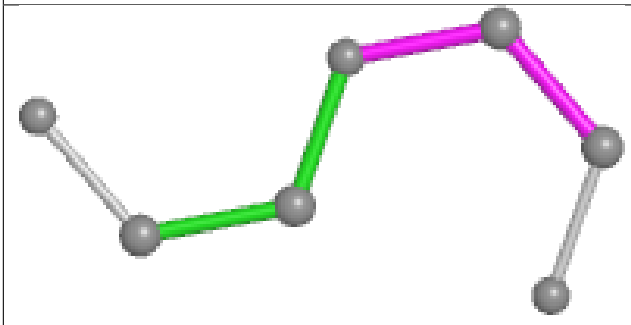


Bond angles



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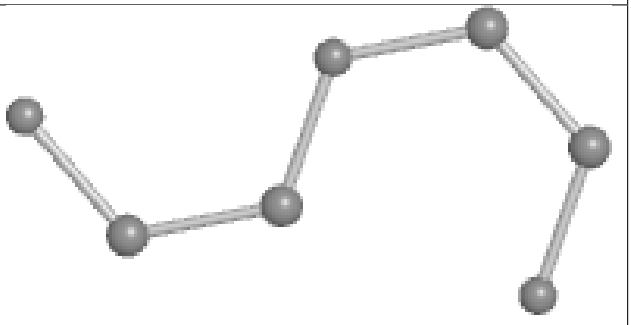
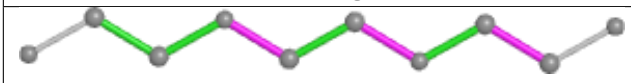


Rings

Ligand PGE E 301

Bond lengths

Bond angles



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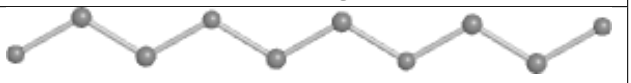
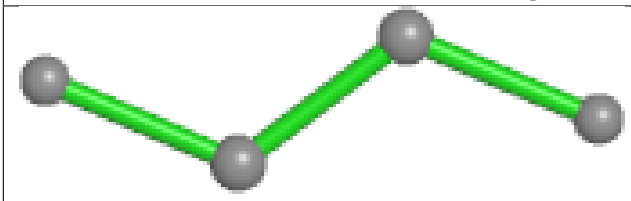
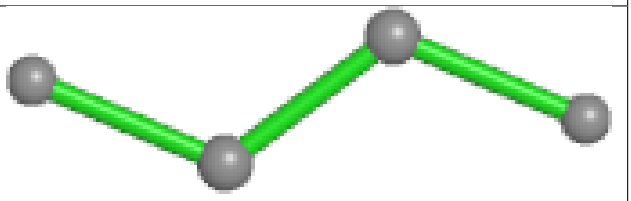
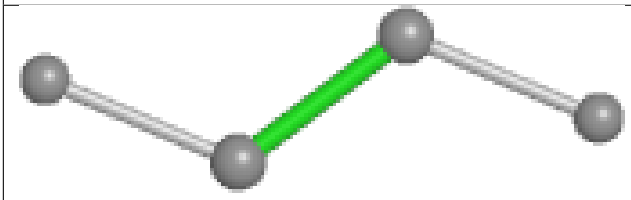
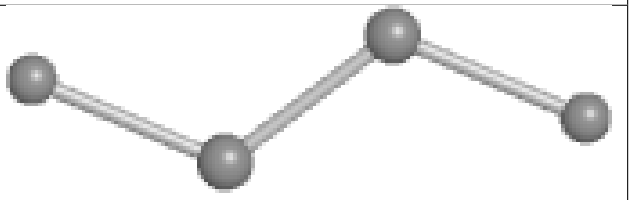
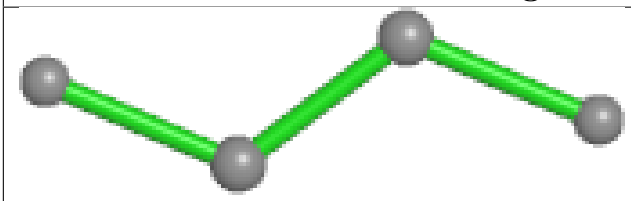
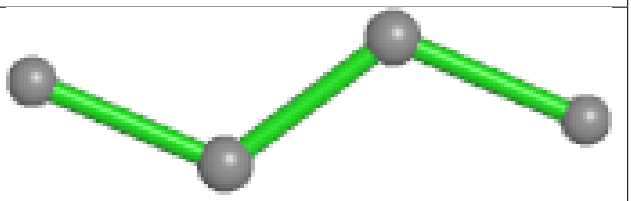
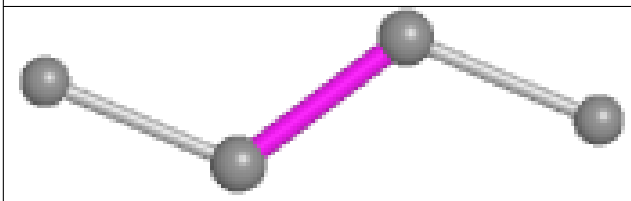
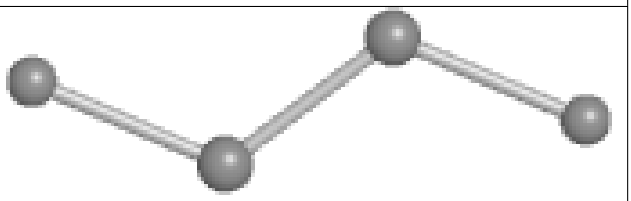
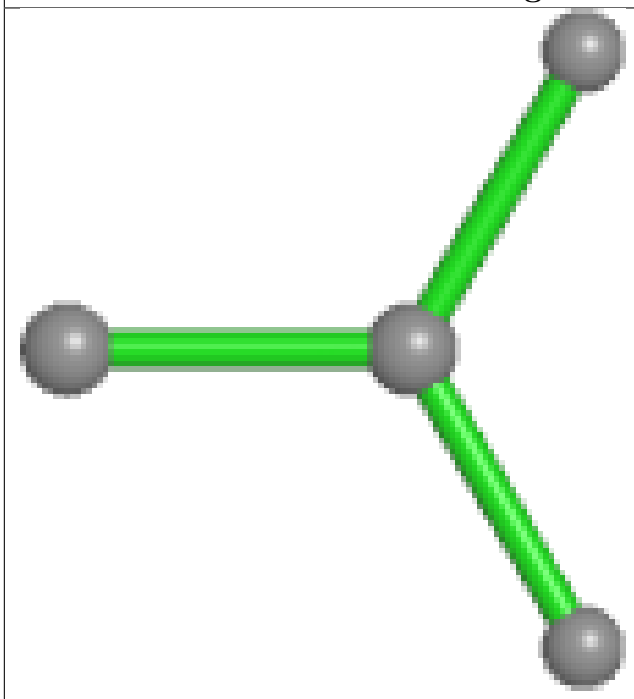


Rings

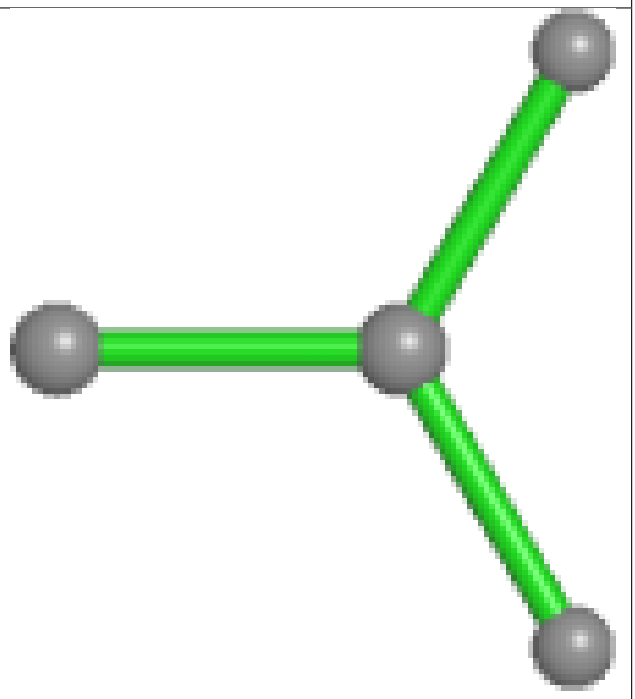
Ligand EDO F 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO A 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

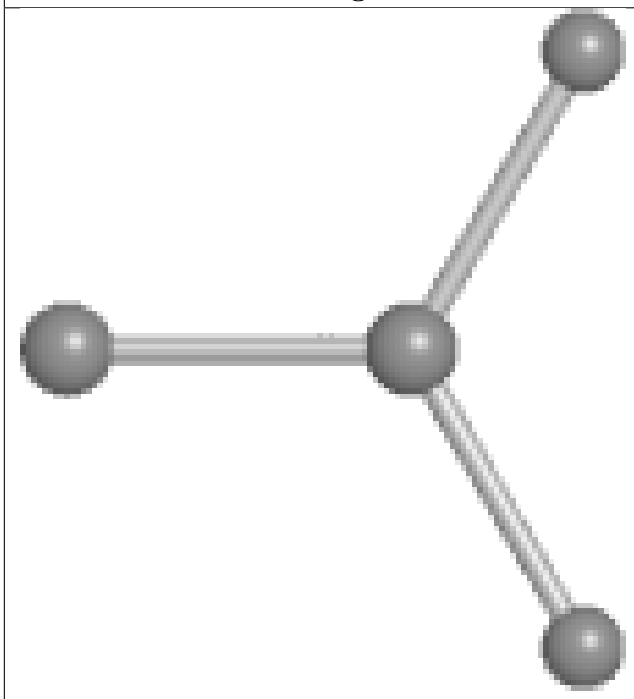
Ligand ACT B 302



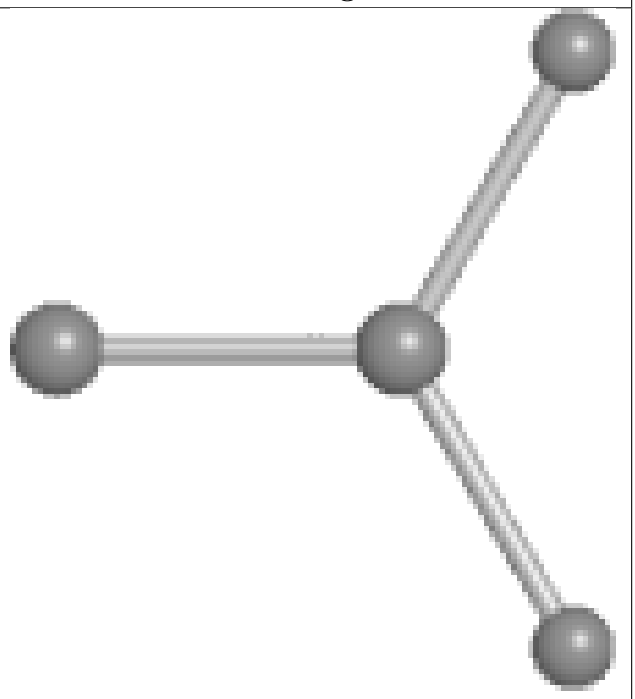
Bond lengths



Bond angles

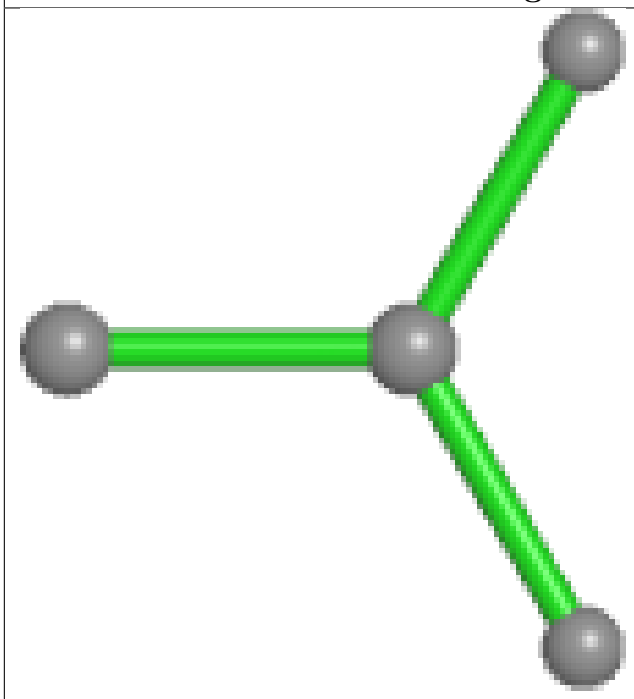


Torsions

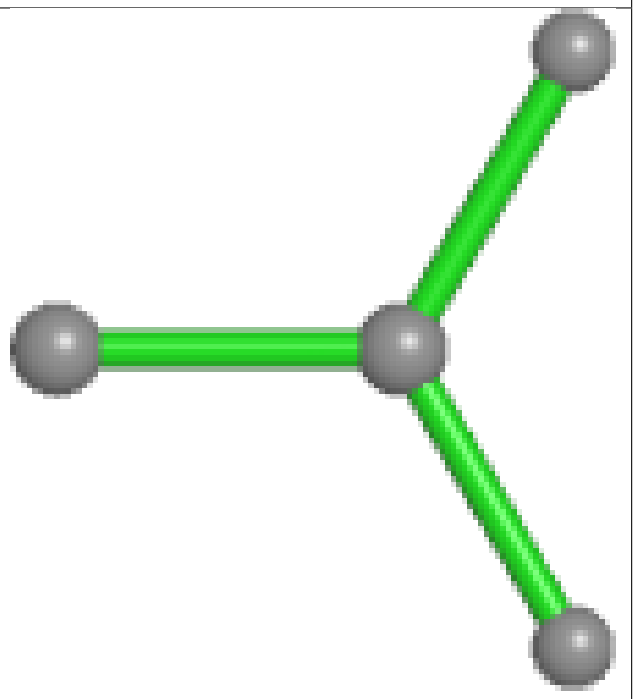


Rings

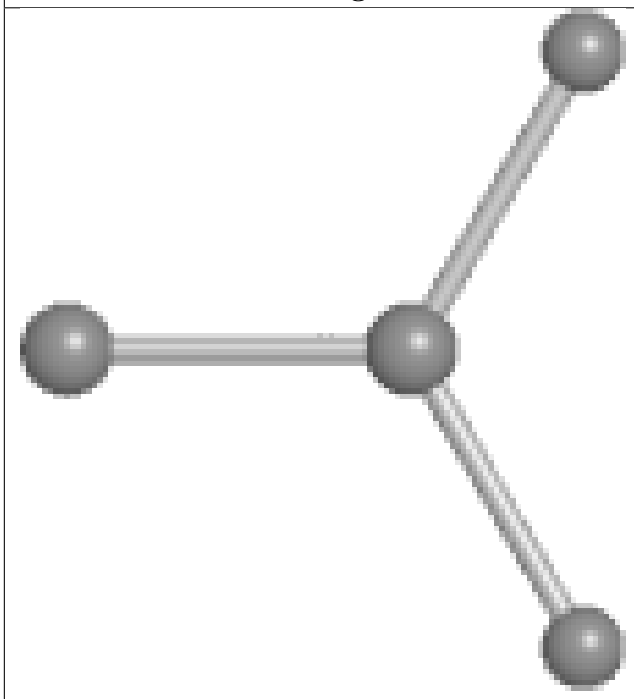
Ligand ACT B 303



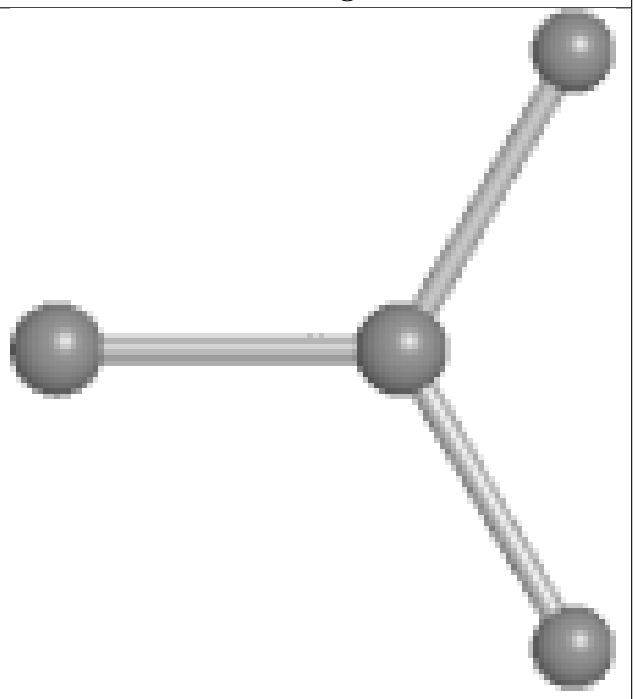
Bond lengths



Bond angles

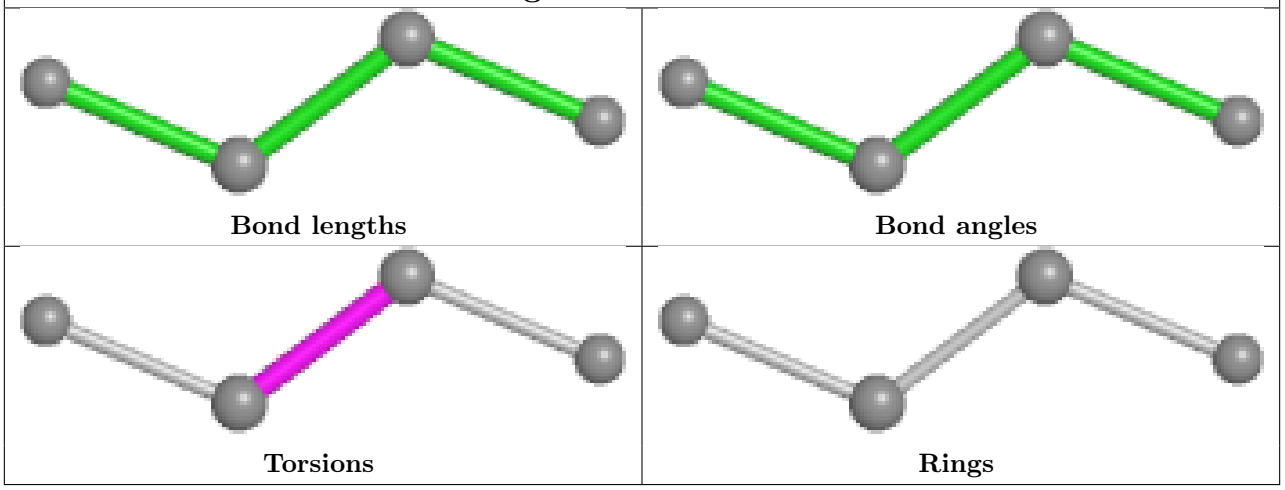


Torsions

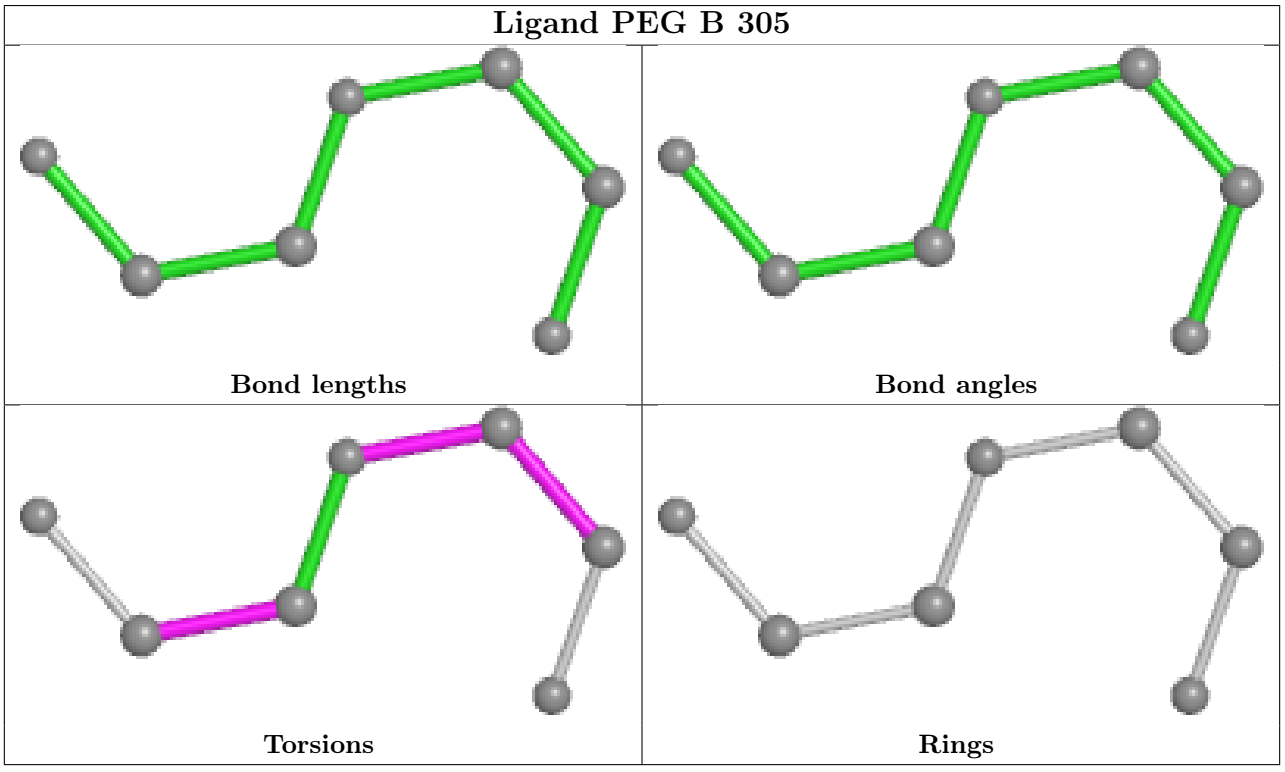


Rings

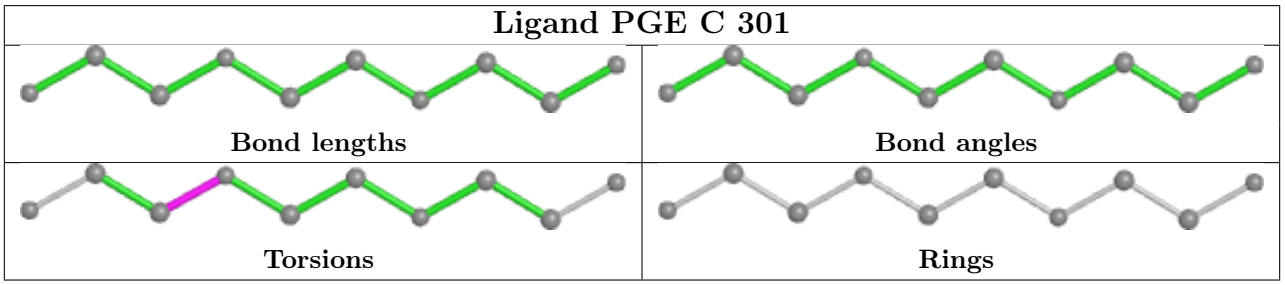
Ligand EDO C 303



Ligand PEG B 305



Ligand PGE C 301



5.7 Other polymers

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%)	-0.44	1 (0%)	94	94	22, 32, 53, 67	0
1	B	295/310 (95%)	-0.36	2 (0%)	87	87	22, 32, 53, 74	0
1	C	295/310 (95%)	-0.40	0	100	100	24, 32, 51, 67	0
1	D	296/310 (95%)	-0.32	2 (0%)	87	87	25, 35, 52, 67	0
1	E	295/310 (95%)	-0.40	1 (0%)	94	94	25, 35, 54, 71	0
1	F	296/310 (95%)	-0.39	3 (1%)	82	83	25, 35, 57, 77	0
All	All	1772/1860 (95%)	-0.38	9 (0%)	91	91	22, 34, 54, 77	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	95	PHE	2.6
1	F	288	GLU	2.6
1	B	25	GLN	2.6
1	A	60	ARG	2.5
1	D	98	GLU	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	C	166	14/15	0.95	0.14	23,28,32,35	0
1	KPI	D	166	14/15	0.95	0.15	29,33,35,36	0
1	KPI	E	166	14/15	0.96	0.13	25,32,37,37	0
1	KPI	B	166	14/15	0.97	0.13	21,25,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KPI	A	166	14/15	0.97	0.13	24,29,33,33	0
1	KPI	F	166	14/15	0.97	0.12	22,29,41,41	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	A	305	4/4	0.61	0.53	20,20,20,20	0
3	GOL	A	302	6/6	0.70	0.29	46,50,54,54	0
3	GOL	D	302	6/6	0.73	0.33	20,20,20,20	0
4	ACT	A	306	4/4	0.73	0.35	20,20,20,20	0
5	EDO	A	307	4/4	0.74	0.35	20,20,20,20	0
6	PEG	B	305	7/7	0.76	0.38	20,20,20,20	0
5	EDO	B	309	4/4	0.80	0.24	20,20,20,20	0
6	PEG	D	303	7/7	0.81	0.32	20,20,20,20	0
2	PGE	E	301	10/10	0.83	0.15	49,52,59,62	0
4	ACT	C	302	4/4	0.84	0.37	20,20,20,20	0
4	ACT	E	302	4/4	0.84	0.31	20,20,20,20	0
5	EDO	F	303	4/4	0.85	0.34	20,20,20,20	0
7	MG	B	307	1/1	0.85	0.11	30,30,30,30	0
4	ACT	A	304	4/4	0.86	0.17	68,68,69,70	0
4	ACT	B	302	4/4	0.86	0.15	54,55,56,56	0
2	PGE	F	301	10/10	0.87	0.16	55,59,71,72	0
2	PGE	A	301	10/10	0.88	0.16	46,50,63,64	0
5	EDO	B	308	4/4	0.89	0.23	20,20,20,20	0
2	PGE	C	301	10/10	0.89	0.14	39,45,49,52	0
6	PEG	F	302	7/7	0.89	0.36	20,20,20,20	0
7	MG	B	306	1/1	0.89	0.15	30,30,30,30	0
3	GOL	A	303	6/6	0.89	0.22	51,54,56,57	0
6	PEG	B	304	7/7	0.90	0.44	20,20,20,20	0
4	ACT	B	303	4/4	0.90	0.27	20,20,20,20	0
5	EDO	C	303	4/4	0.91	0.32	20,20,20,20	0
5	EDO	F	304	4/4	0.91	0.39	20,20,20,20	0

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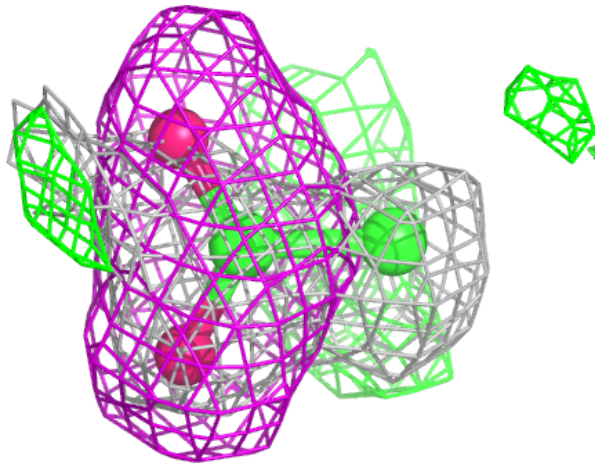
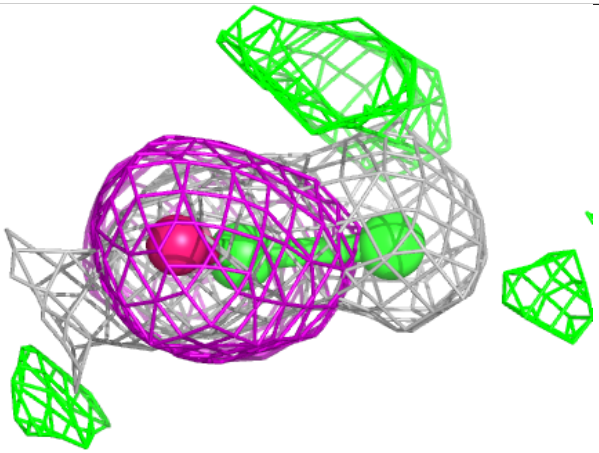
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	E	303	7/7	0.93	0.29	20,20,20,20	0
2	PGE	D	301	10/10	0.94	0.10	45,50,57,59	0
5	EDO	F	305	4/4	0.94	0.30	20,20,20,20	0
2	PGE	B	301	10/10	0.94	0.14	42,43,48,51	0

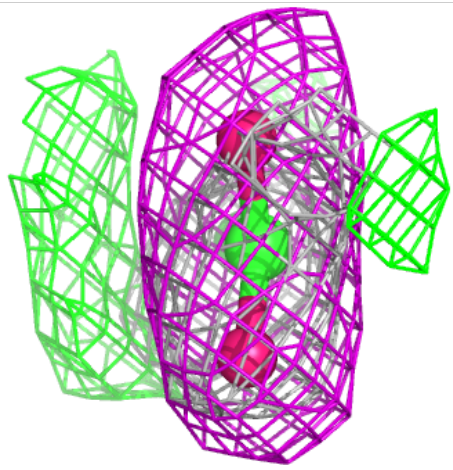
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACT 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)

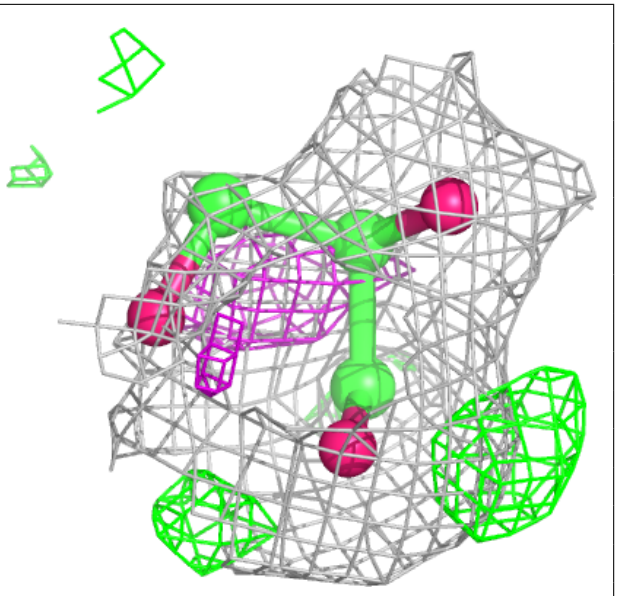


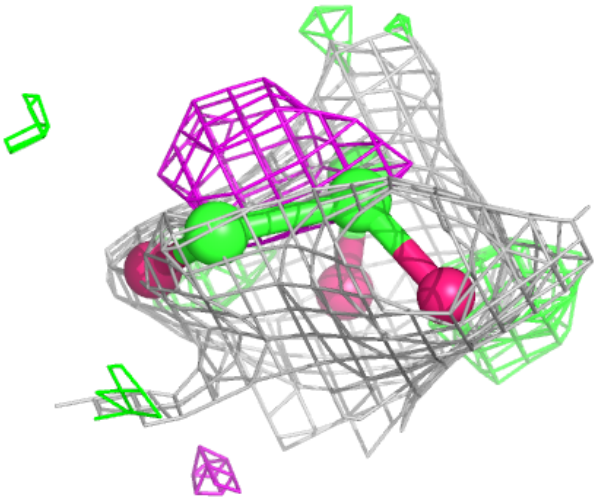


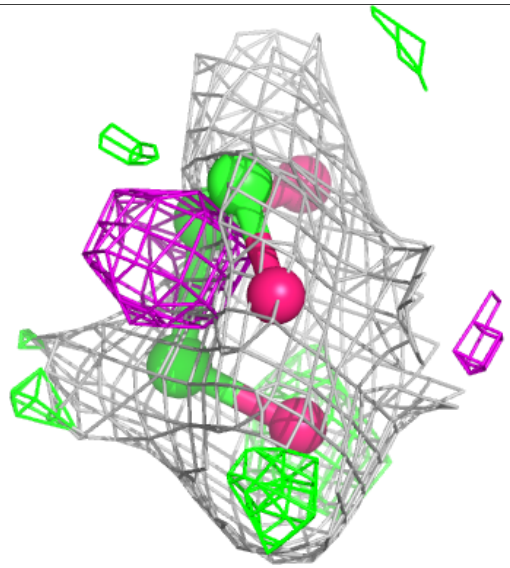


Electron density around GOL A 302:

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

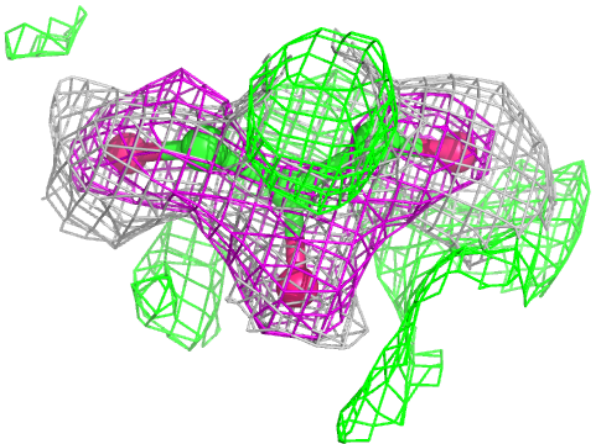


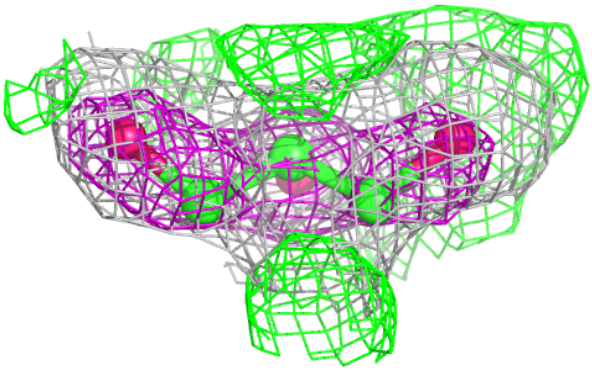


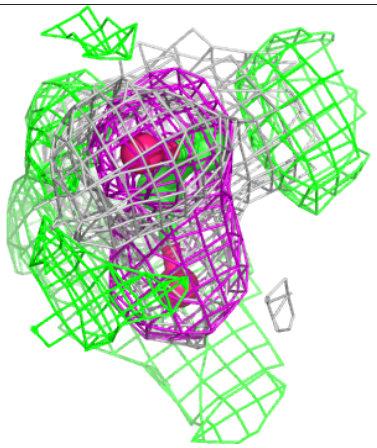


Electron density around GOL D 302:

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

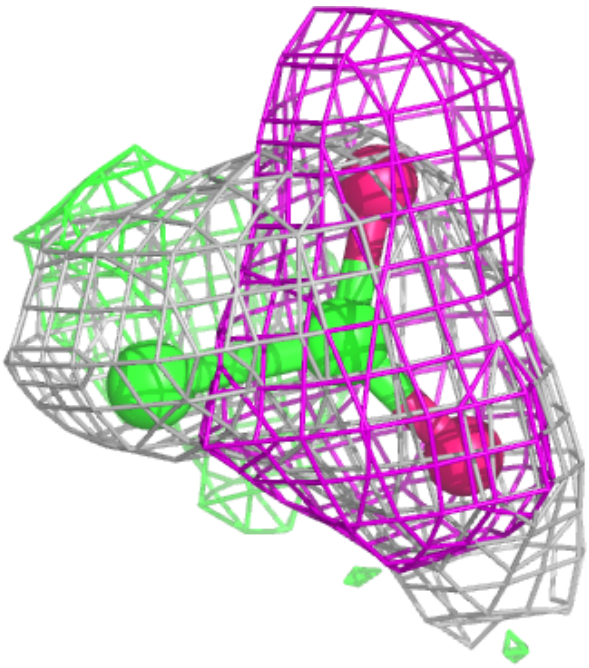


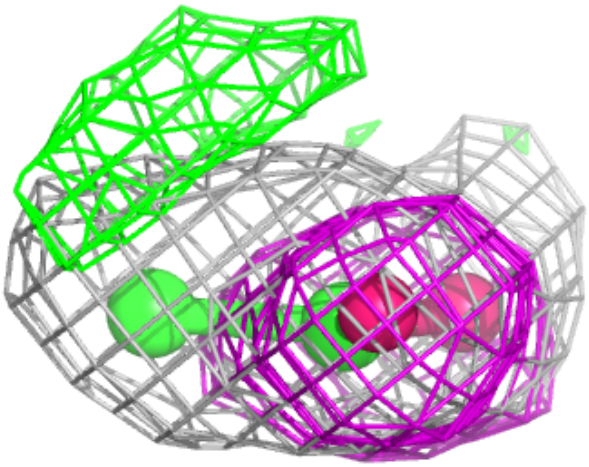


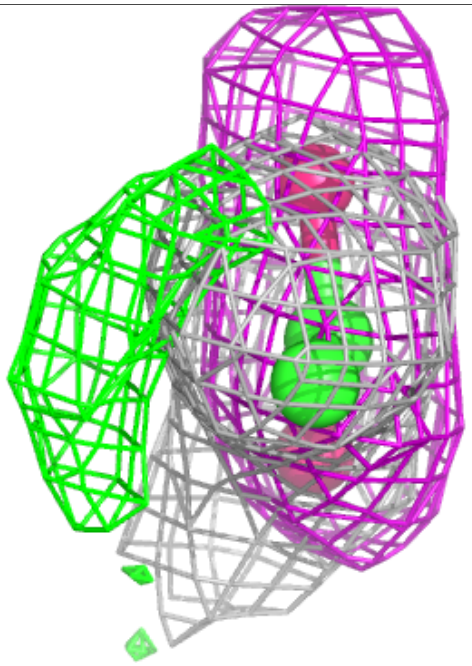


Electron density around ACT A 306:

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

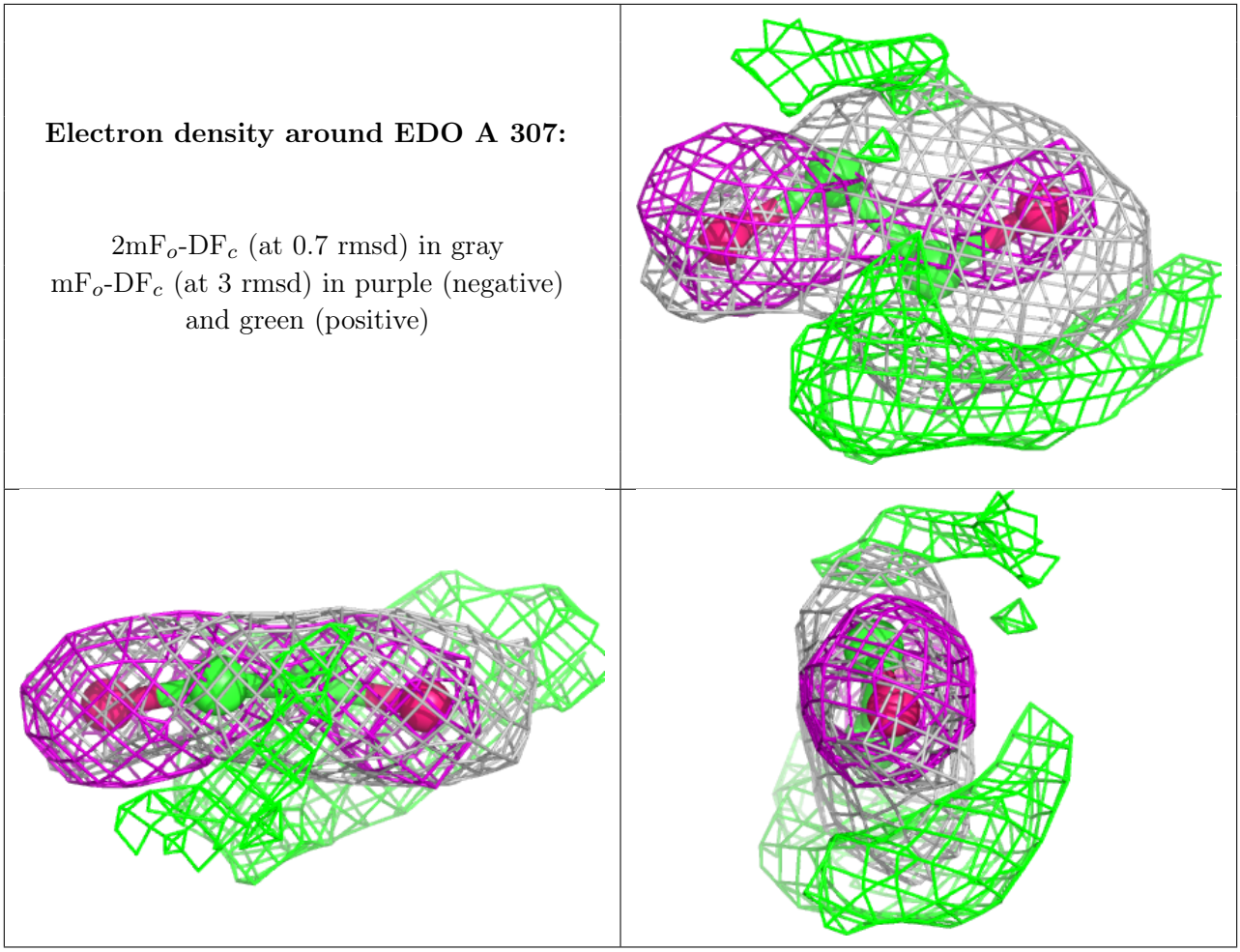






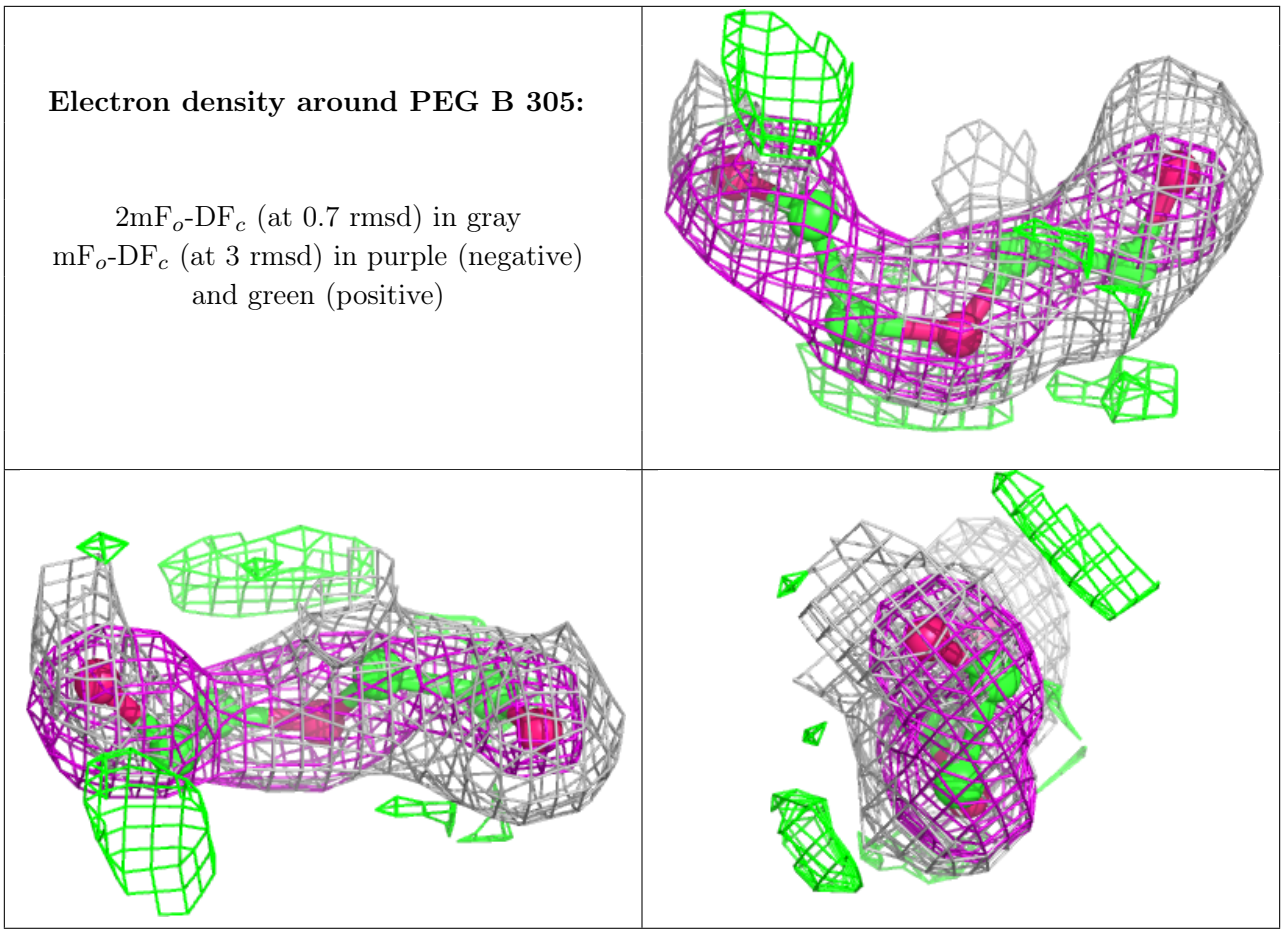
Electron density around EDO A 307:

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



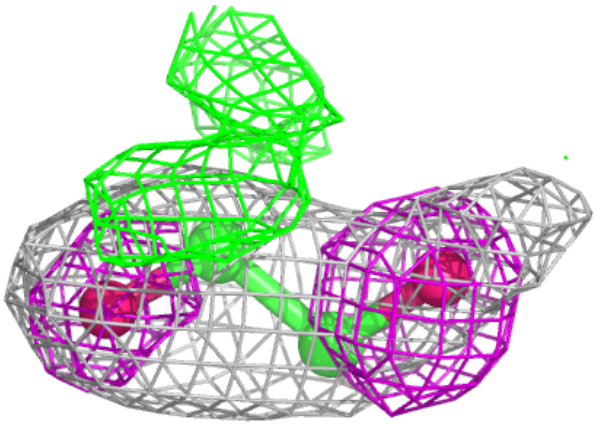
Electron density around PEG B 305:

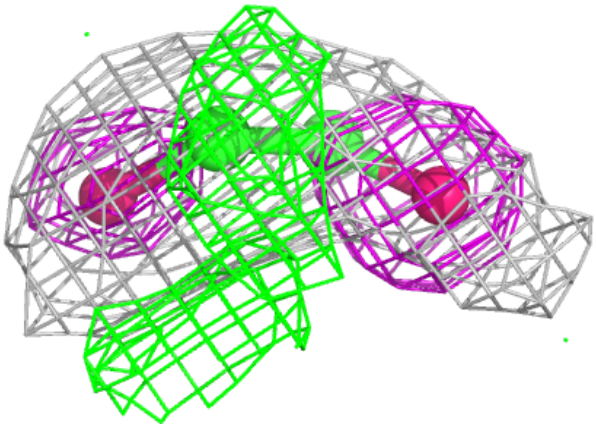
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

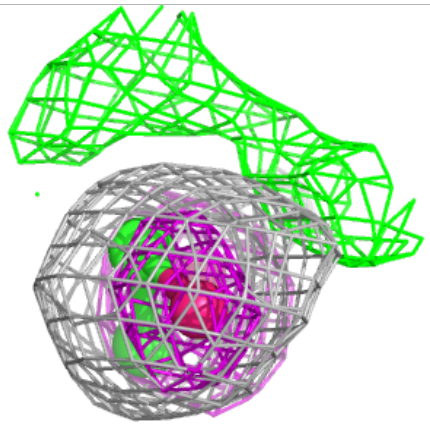


Electron density around EDO B 309:

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

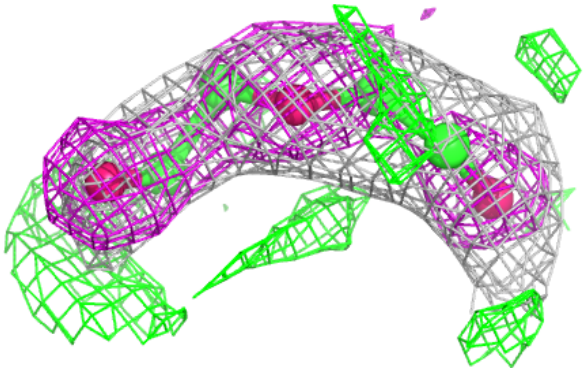


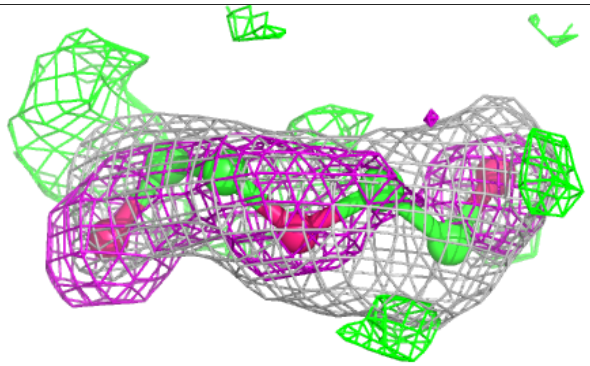


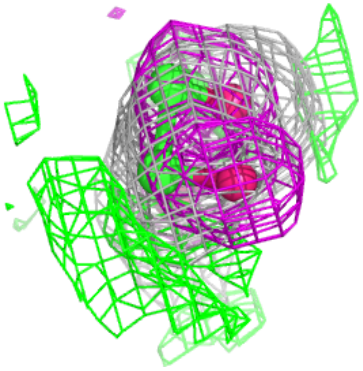


Electron density around PEG D 303:

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

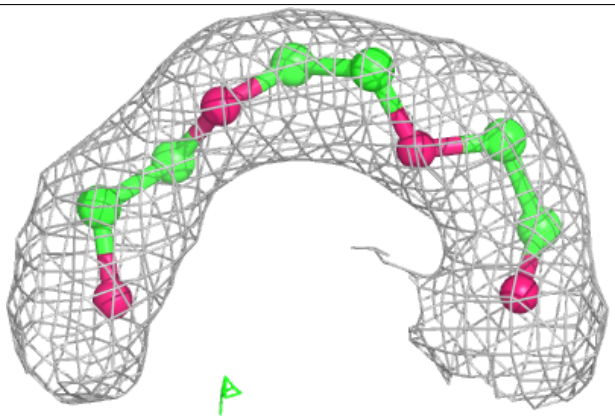


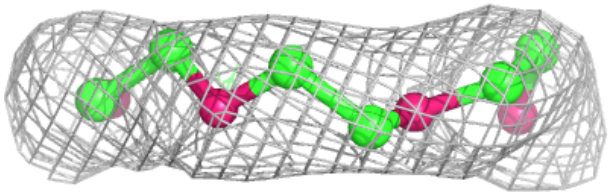


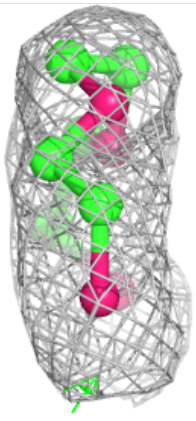


Electron density around PGE E 301:

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

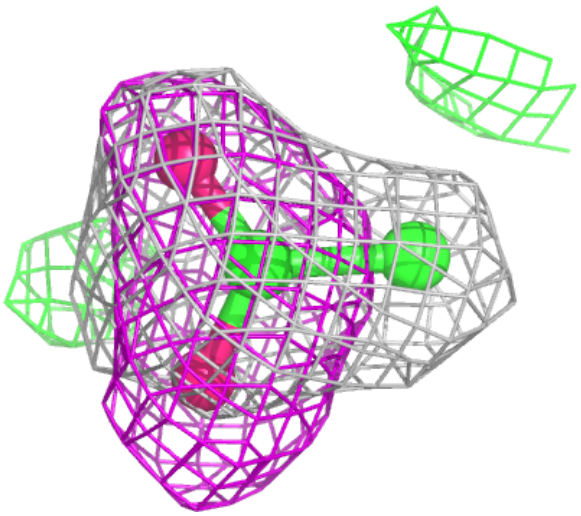


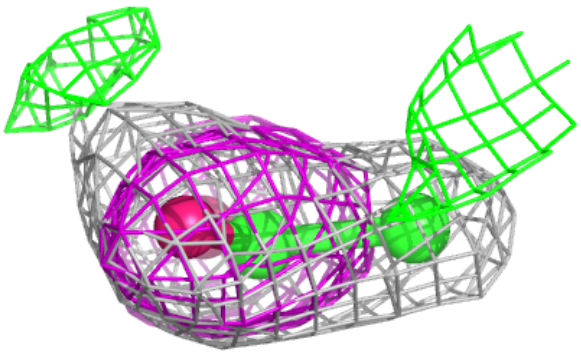


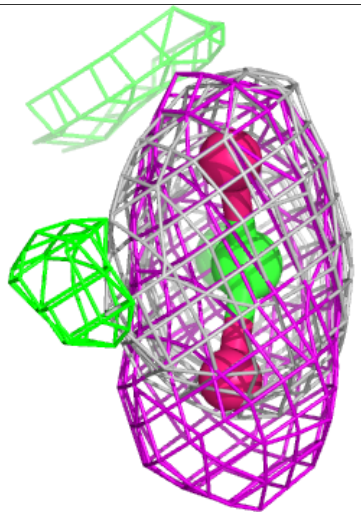


Electron density around ACT C 302:

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

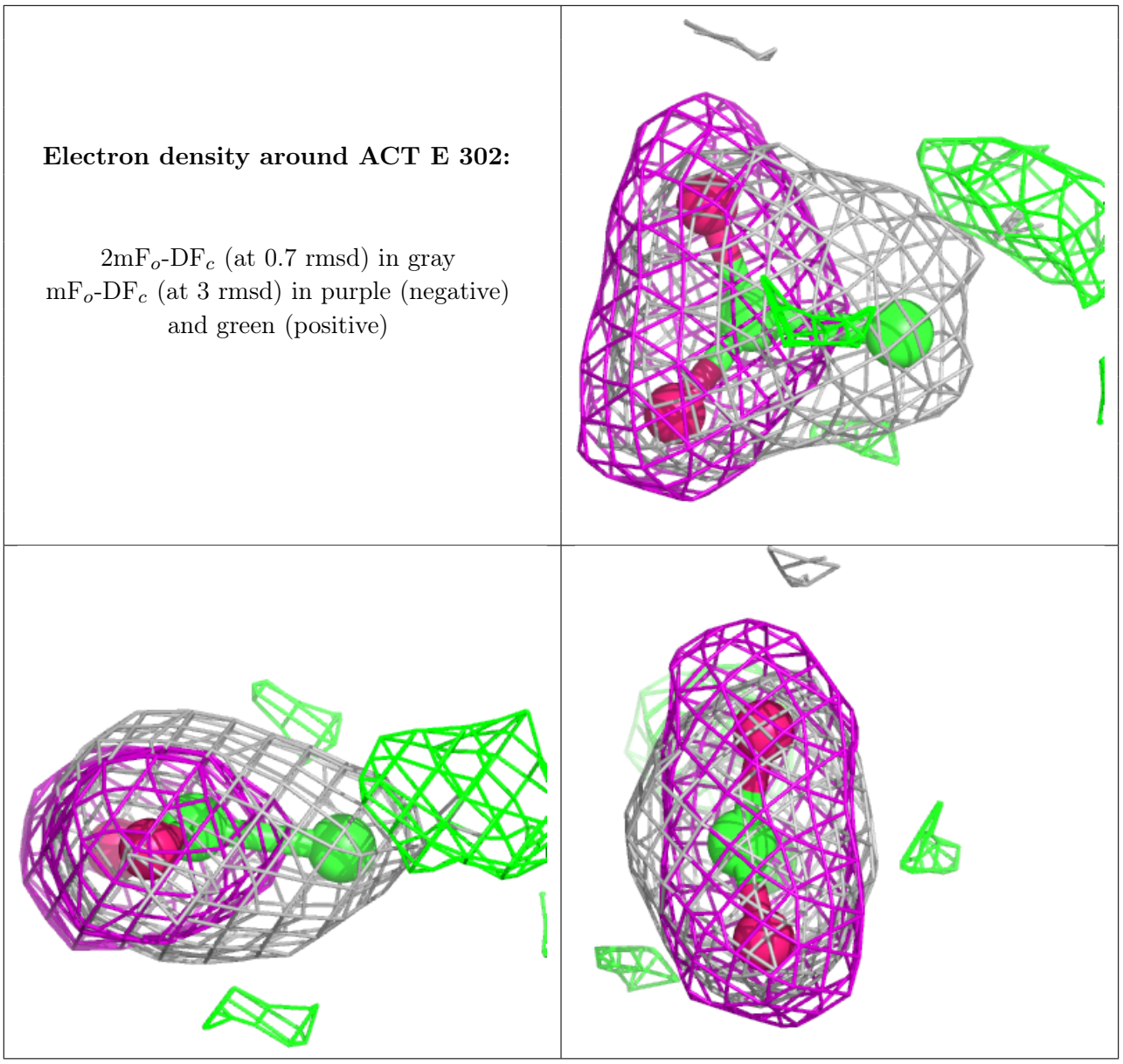






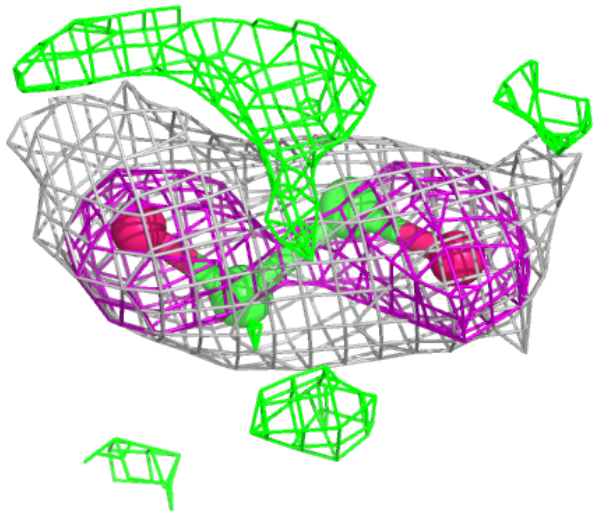
Electron density around ACT E 302:

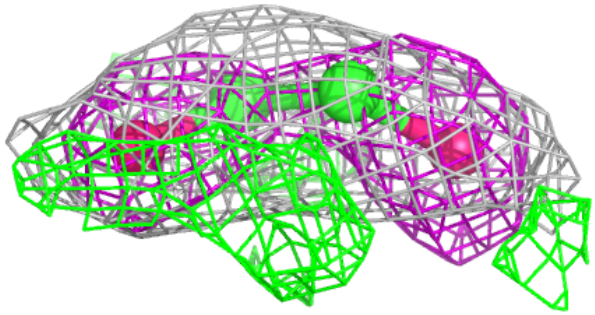
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

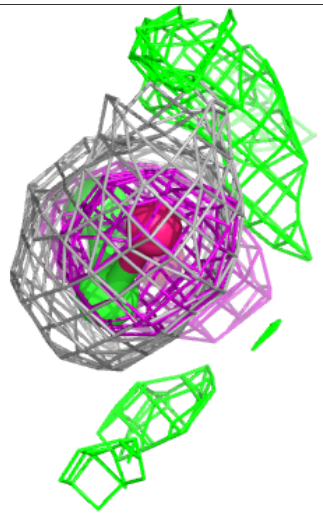


Electron density around EDO F 303:

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

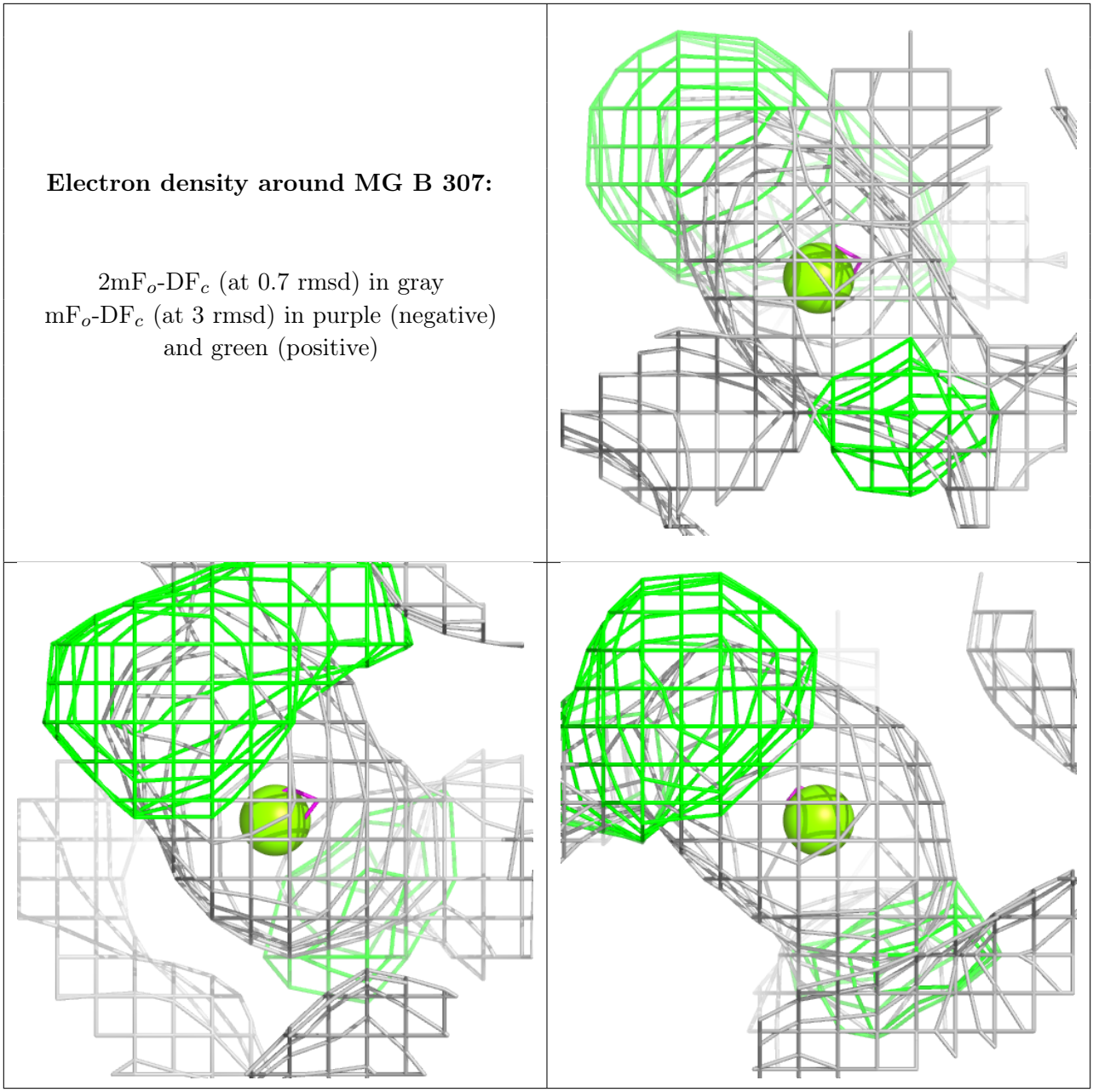






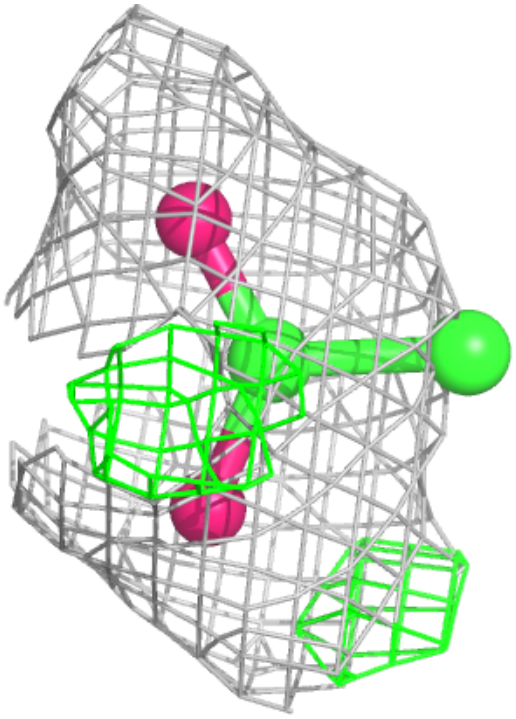
Electron density around MG B 307:

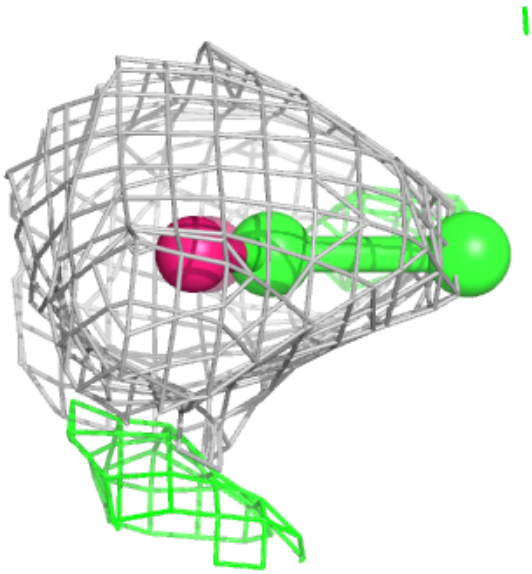
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ACT A 304:

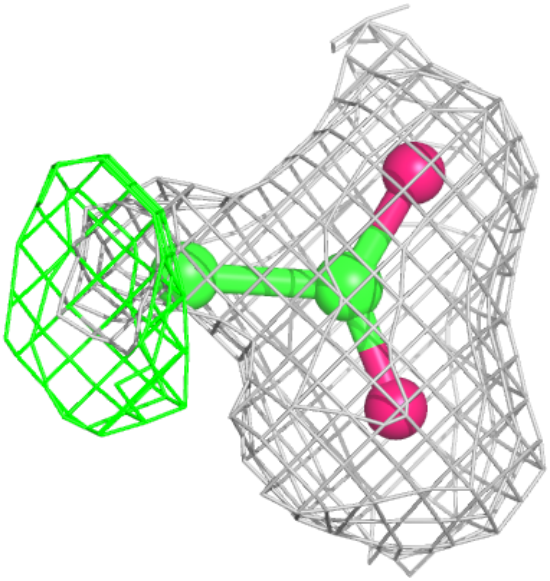
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

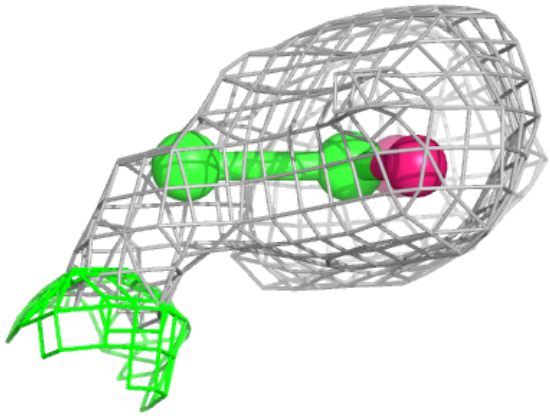


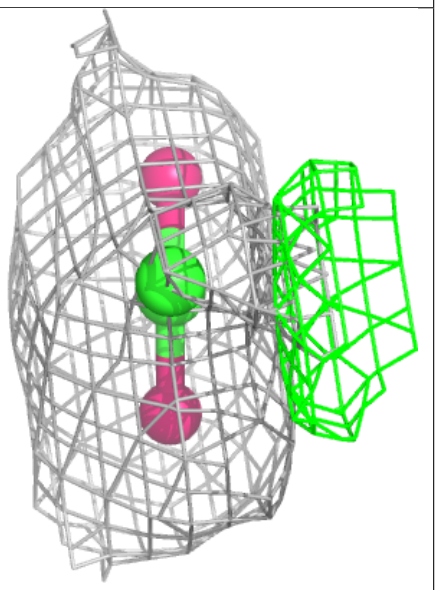


Electron density around ACT B 302:

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

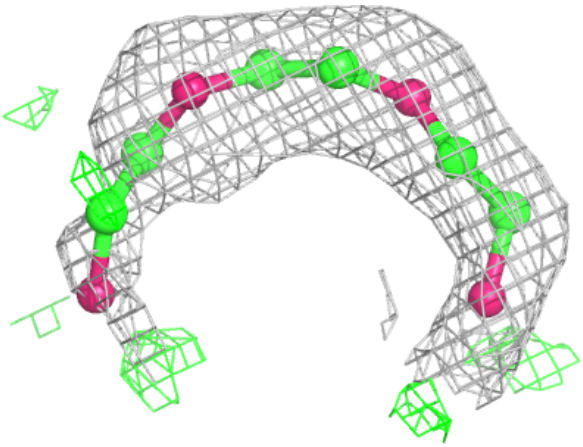


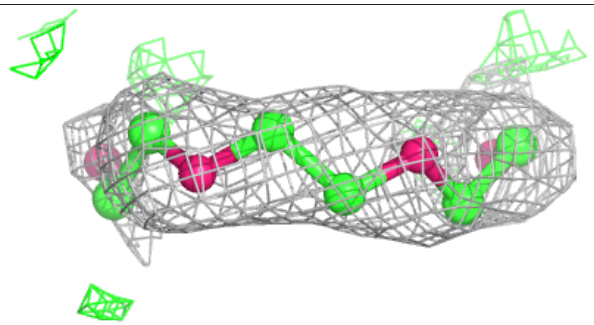


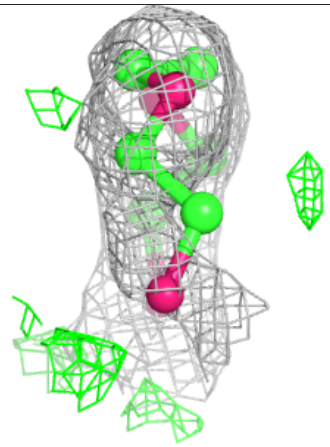


Electron density around PGE F 301:

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

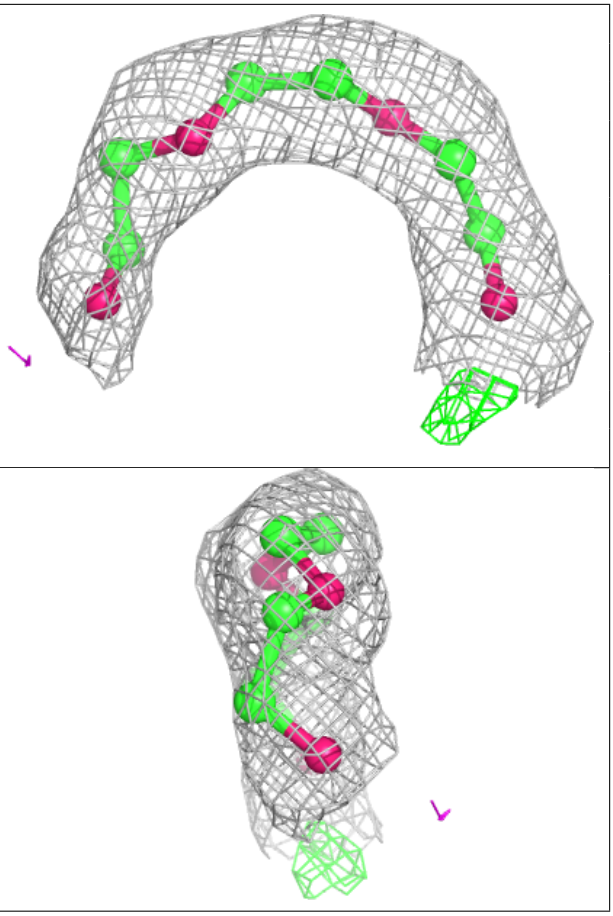


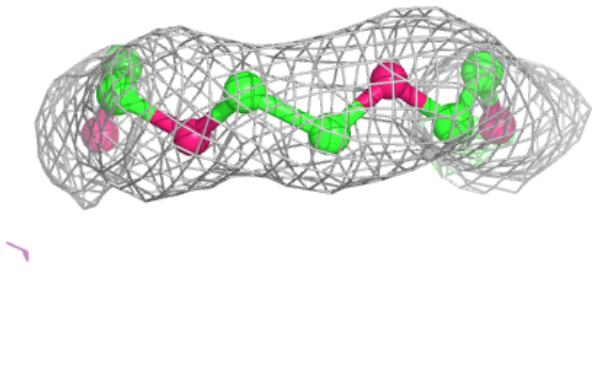




Electron density around PGE A 301:

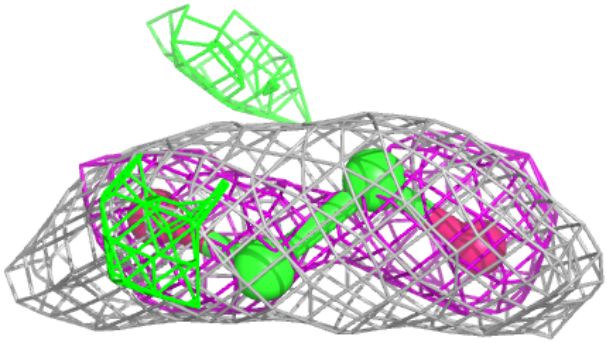
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

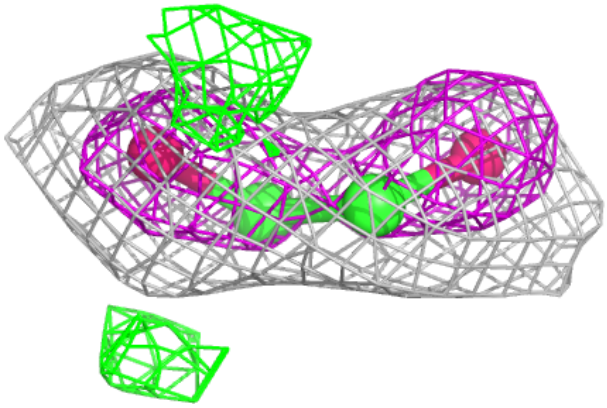


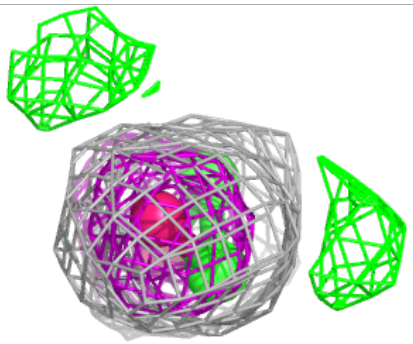


Electron density around EDO B 308:

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

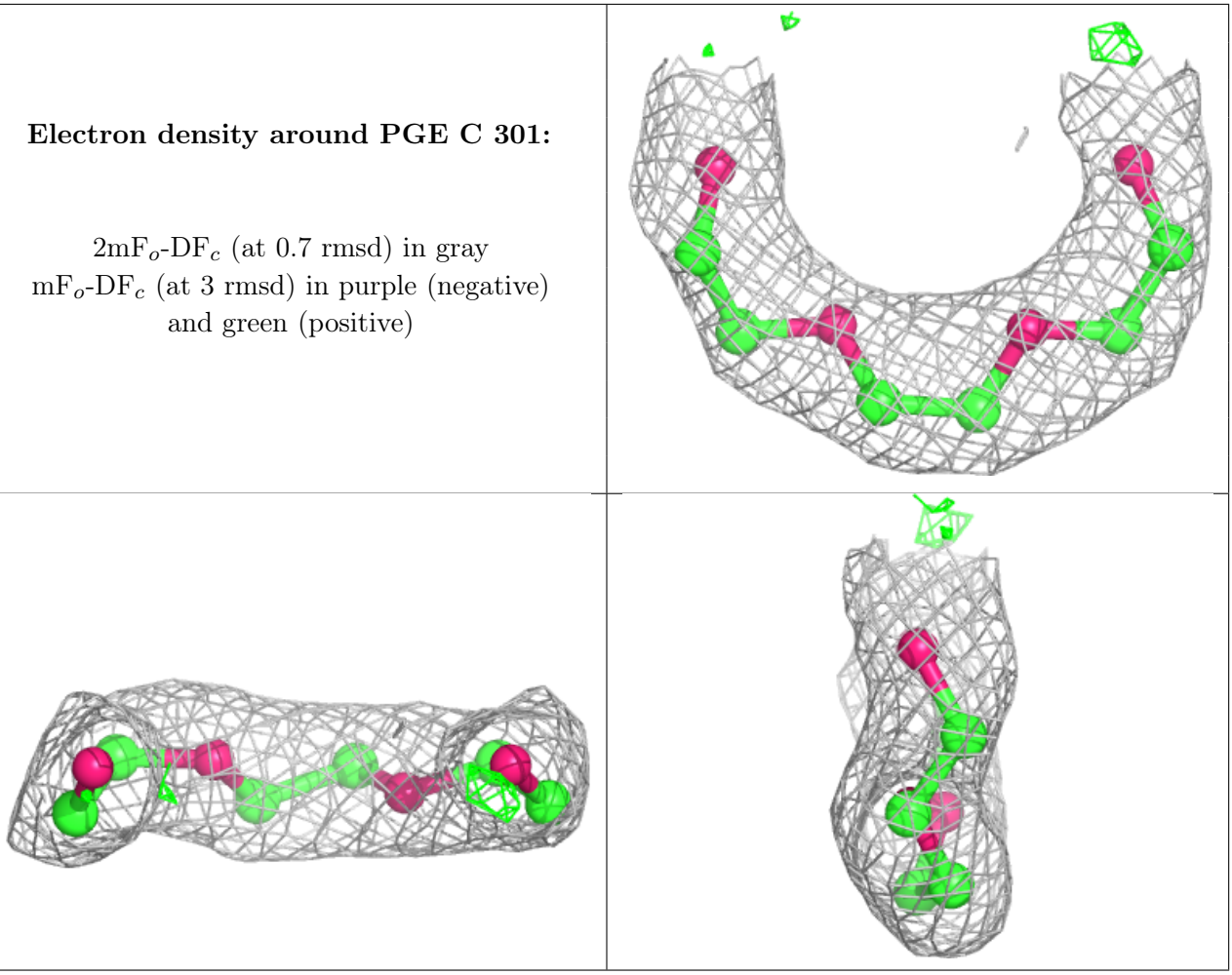






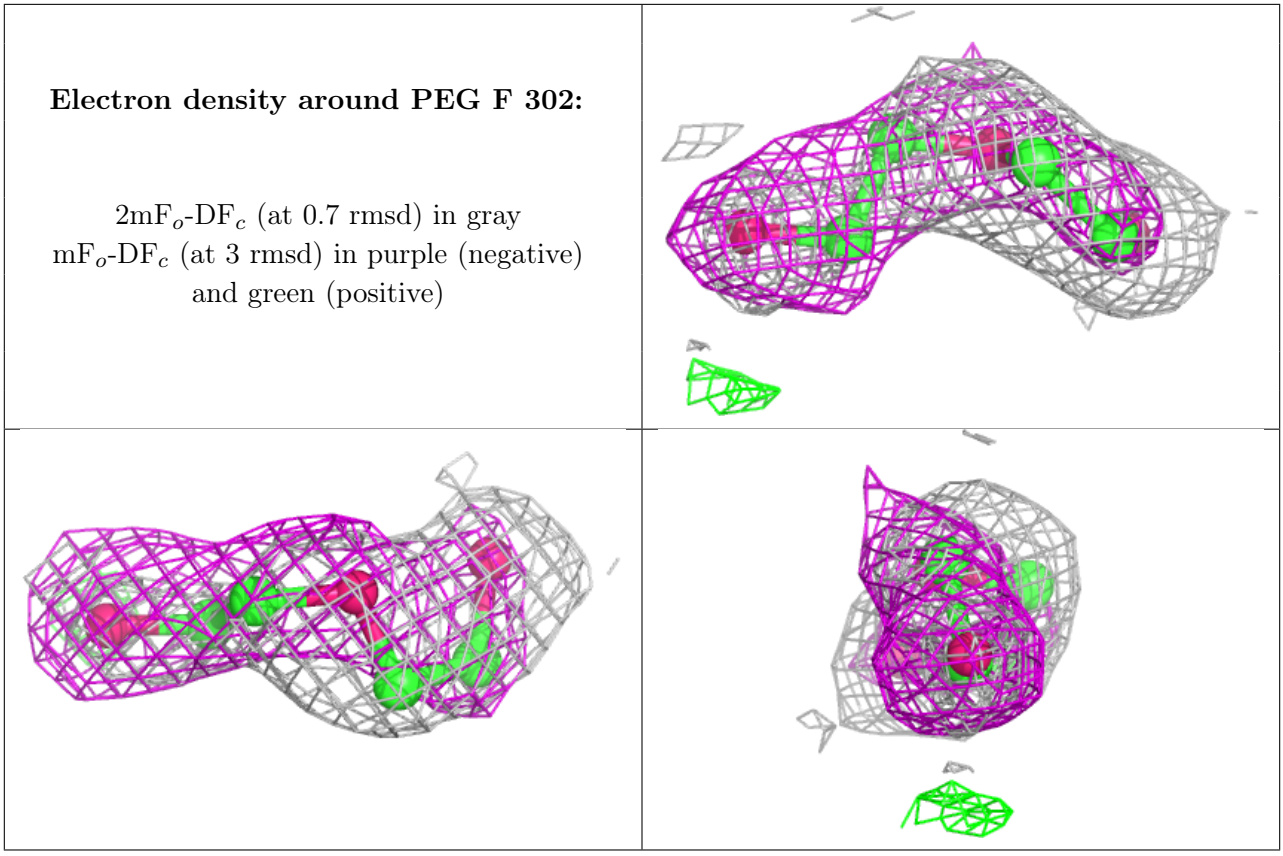
Electron density around PGE C 301:

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



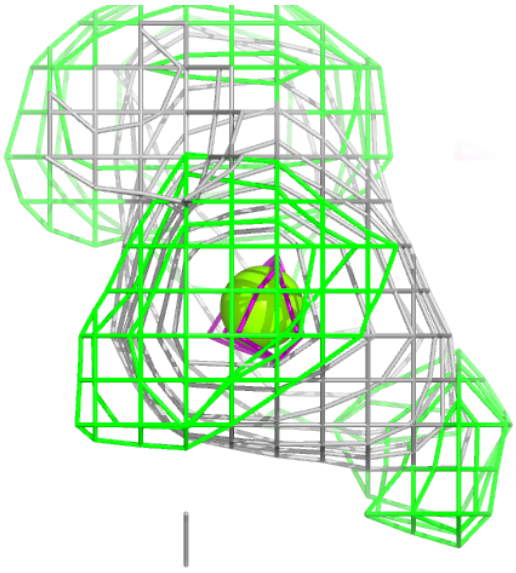
Electron density around PEG F 302:

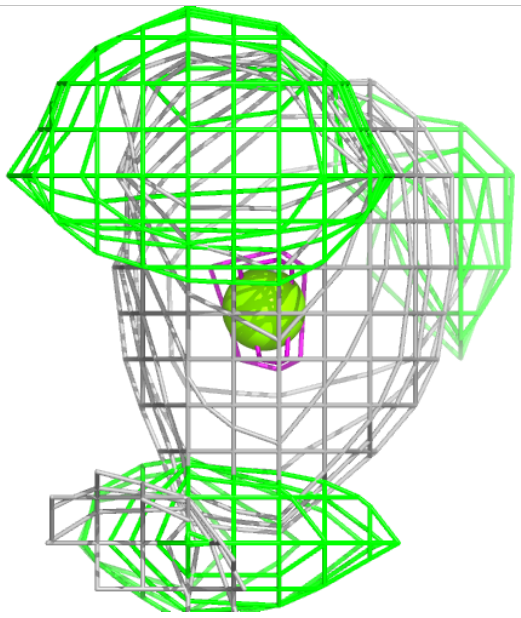
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

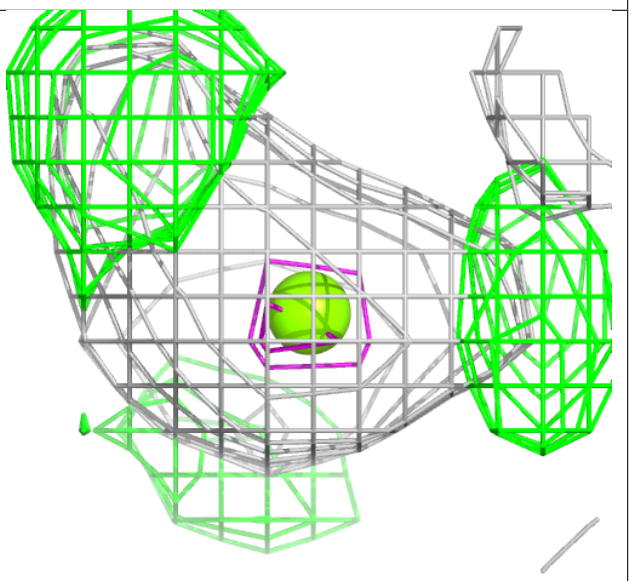


Electron density around MG B 306:

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

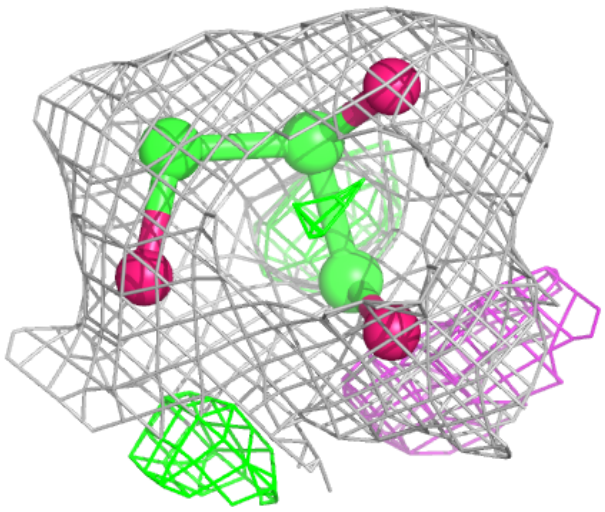


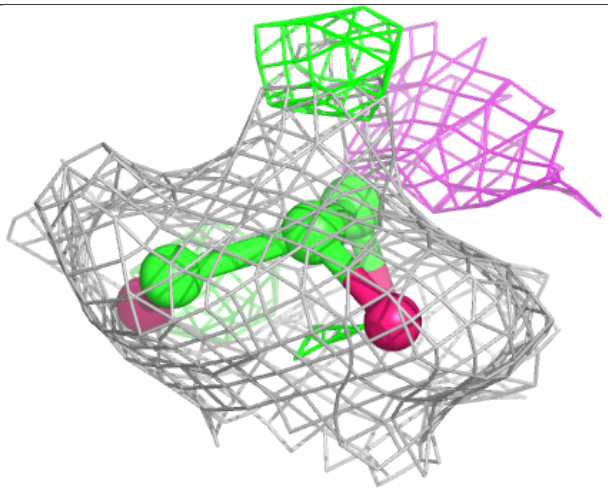


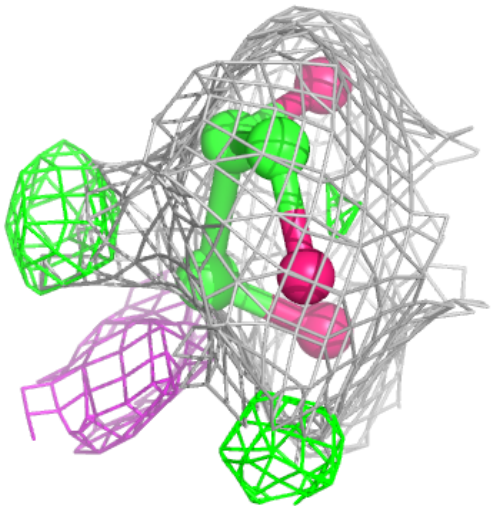


Electron density around GOL A 303:

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

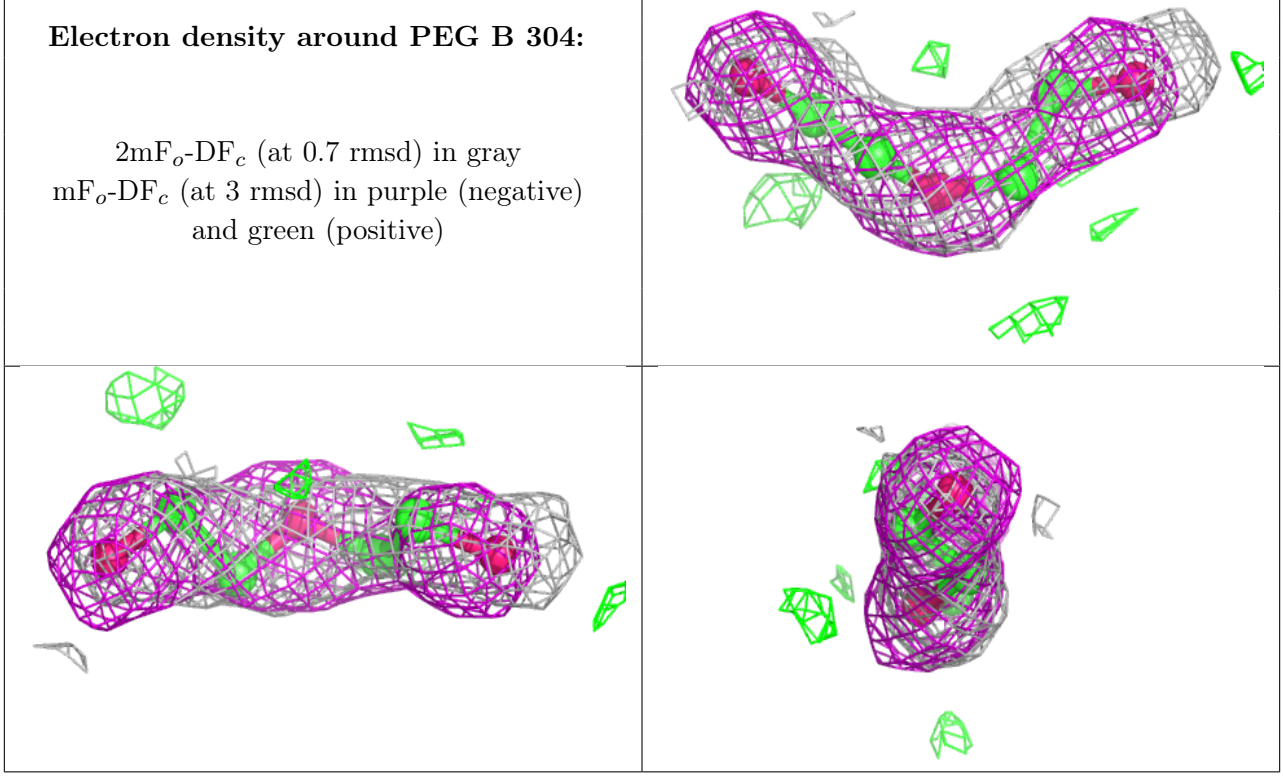






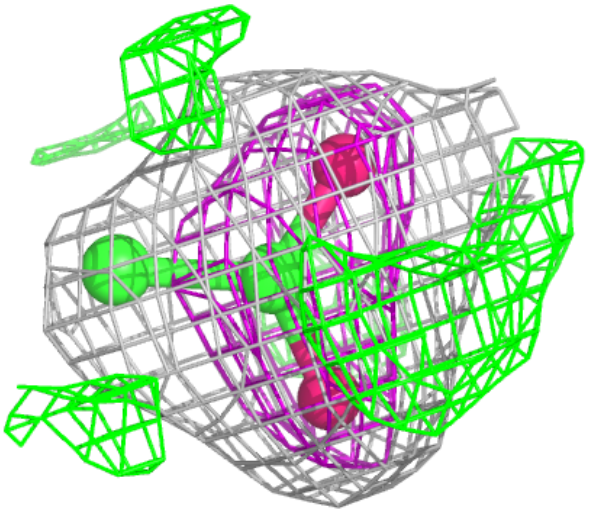
Electron density around PEG B 304:

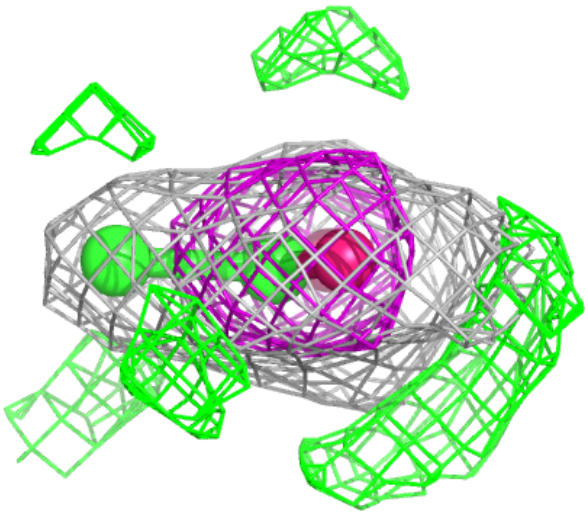
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

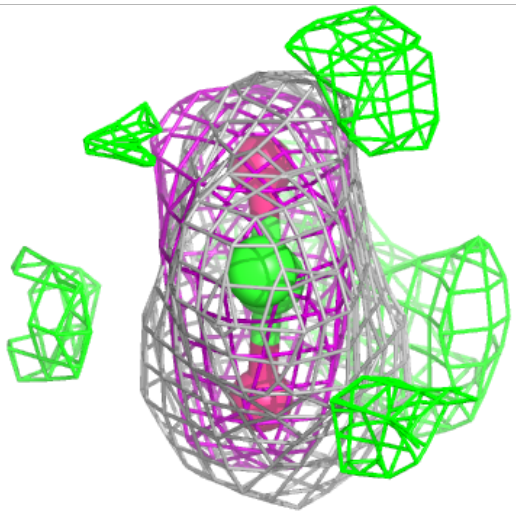


Electron density around ACT B 303:

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

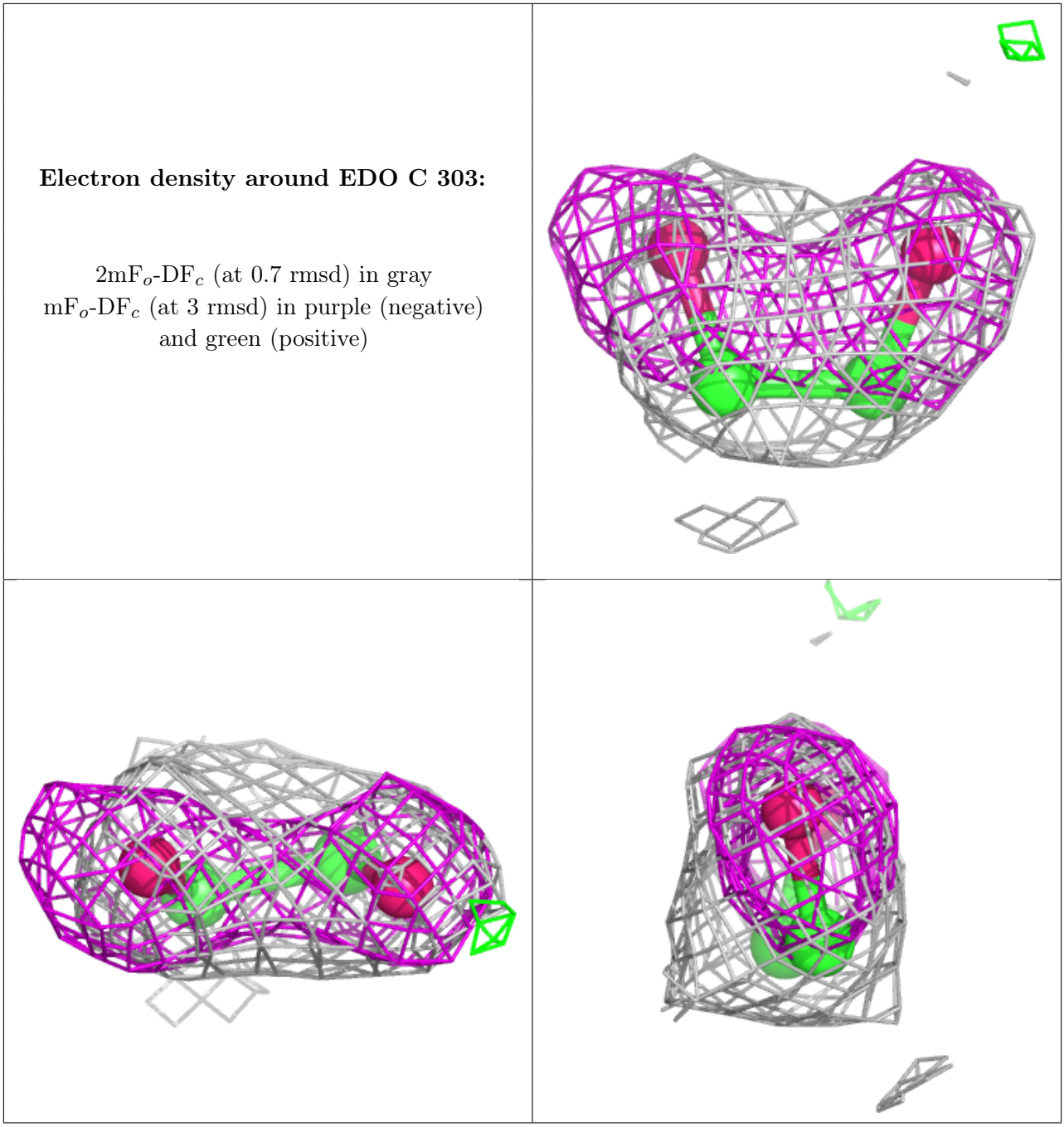






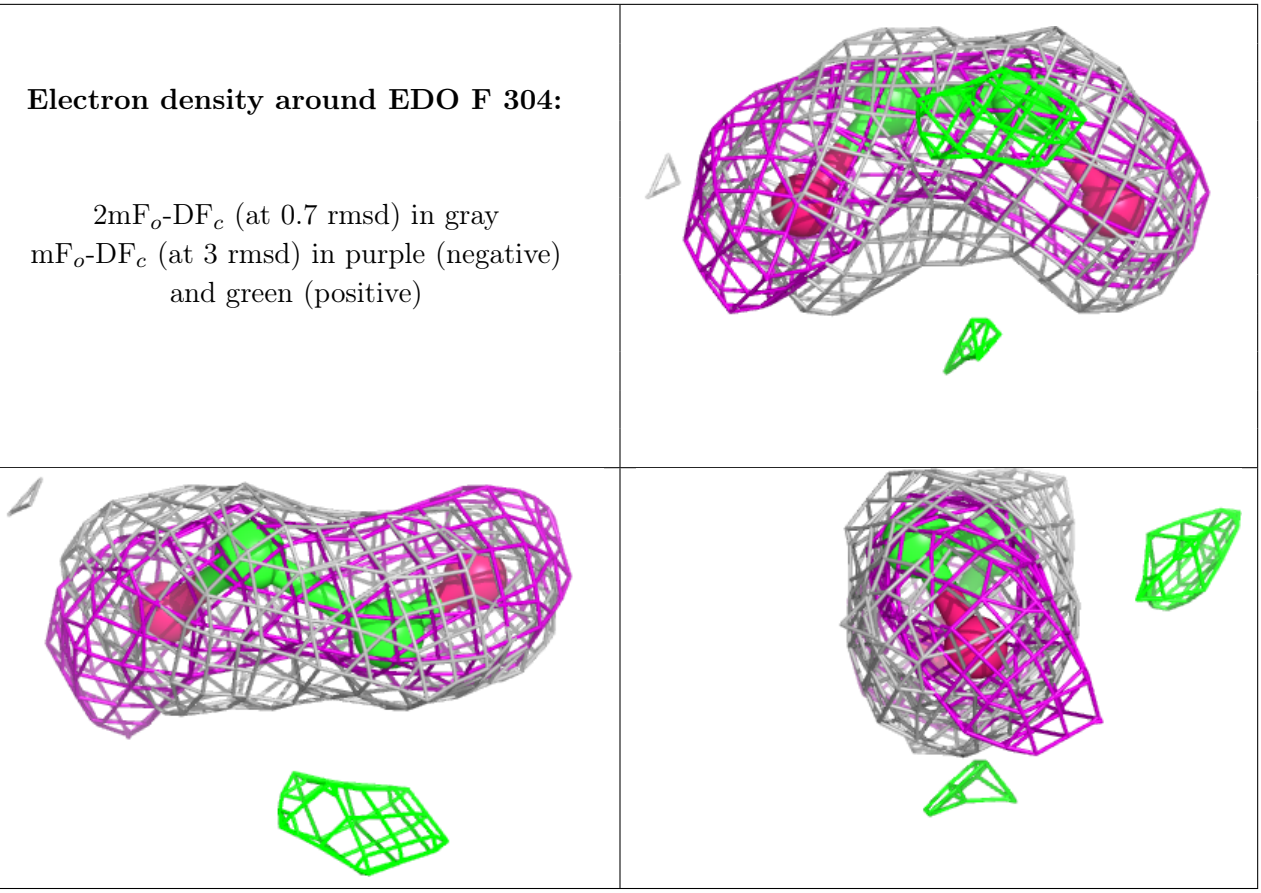
Electron density around EDO C 303:

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



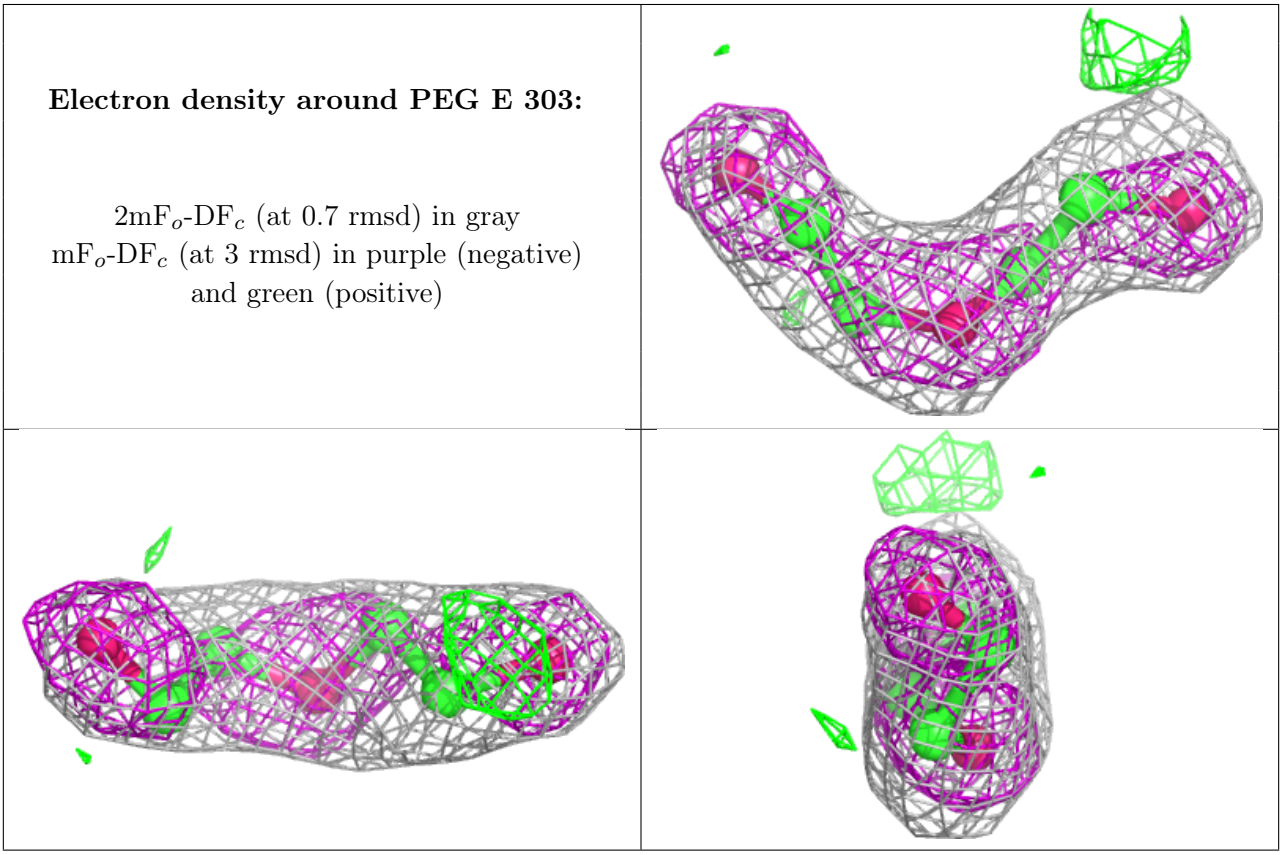
Electron density around EDO F 304:

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



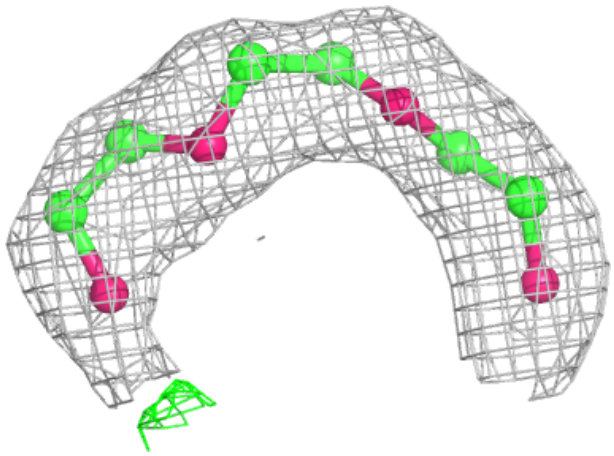
Electron density around PEG E 303:

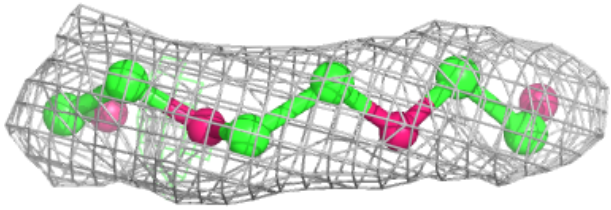
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

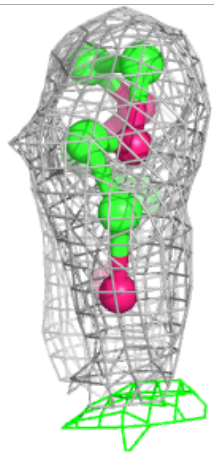


Electron density around PGE D 301:

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

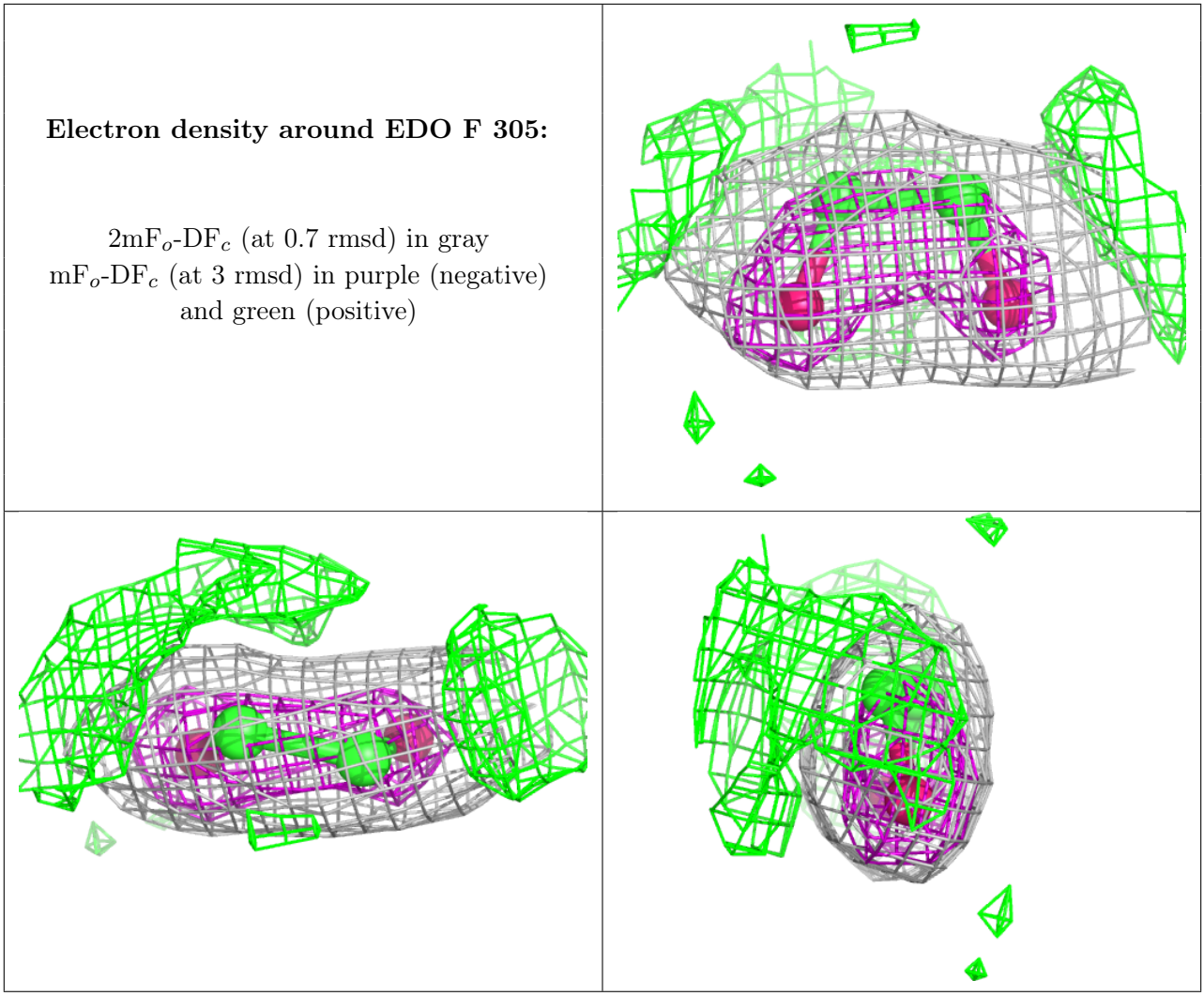






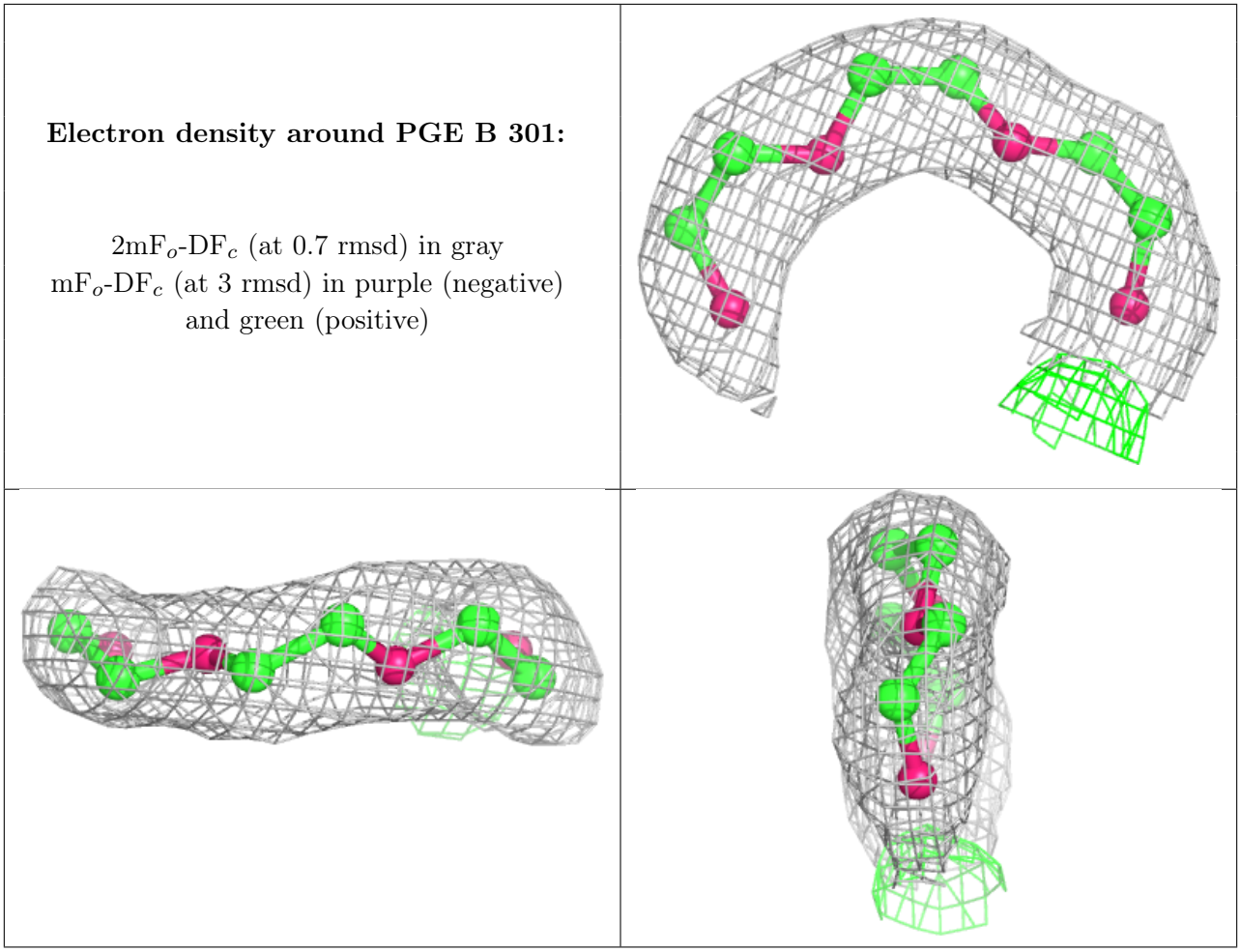
Electron density around EDO F 305:

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



Electron density around 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)



6.5 Other polymers (i)

There are no such residues in this entry.