WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:46 PM EDT

PDB ID	:	7KLT
Title	:	Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H59N mutant with pyruvate bound in the active site
Authors	:	Saran, S.; Sanders, D.A.R.
Deposited on	:	2020-11-01
Resolution	:	1.97 Å(reported)

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

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

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.97 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		0.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
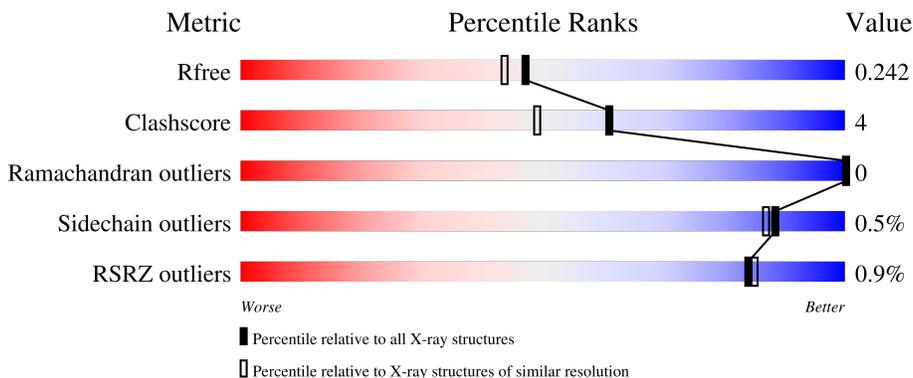
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	85% 10% 5%
1	B	310	87% 7% · 5%
1	C	310	89% 7% ·
1	D	310	90% 6% 5%
1	E	310	85% 11% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	3% 85% 10%

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
4	EDO	E	304	-	-	X	-
4	EDO	F	305	-	-	X	-
6	ACT	C	310	-	-	X	-
7	PEG	C	311	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14738 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 2288	C 1454	N 381	O 440	S 13	0	1	0
1	B	296	Total 2282	C 1450	N 379	O 440	S 13	0	1	0
1	C	297	Total 2290	C 1454	N 380	O 443	S 13	0	1	0
1	D	296	Total 2291	C 1455	N 381	O 442	S 13	0	3	0
1	E	296	Total 2288	C 1454	N 381	O 440	S 13	0	1	0
1	F	297	Total 2289	C 1454	N 379	O 443	S 13	0	1	0

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 (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).
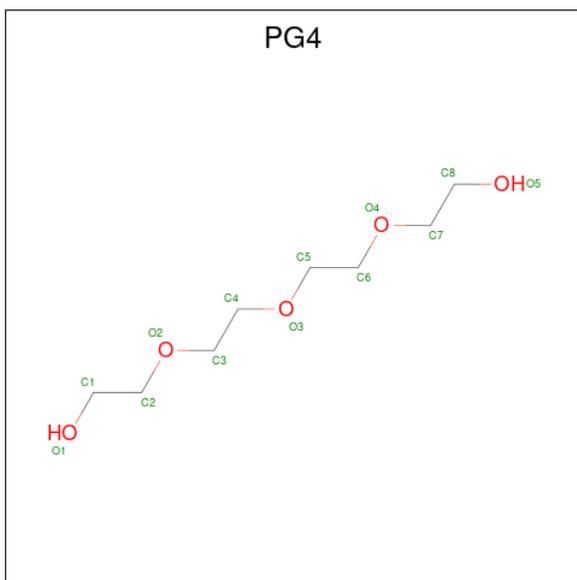
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		

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

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).
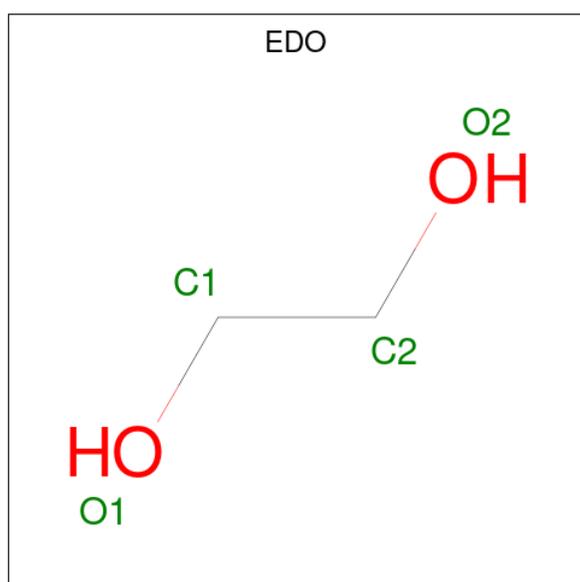
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).
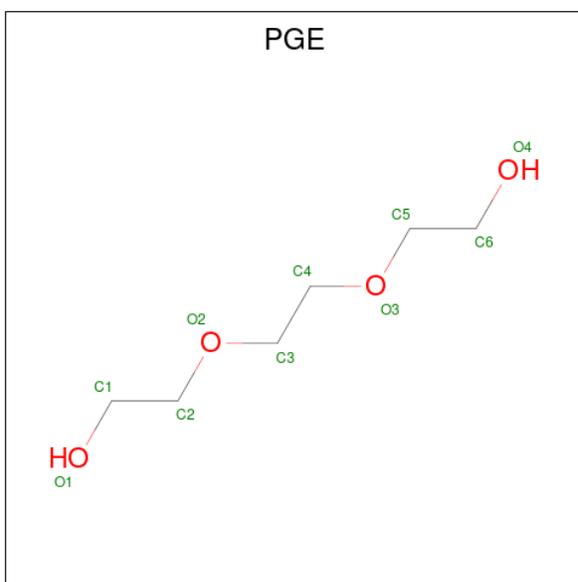
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 10	C 6	O 4	0	0
5	C	1	Total 10	C 6	O 4	0	0
5	D	1	Total 10	C 6	O 4	0	0
5	E	1	Total 10	C 6	O 4	0	0
5	F	1	Total 10	C 6	O 4	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).

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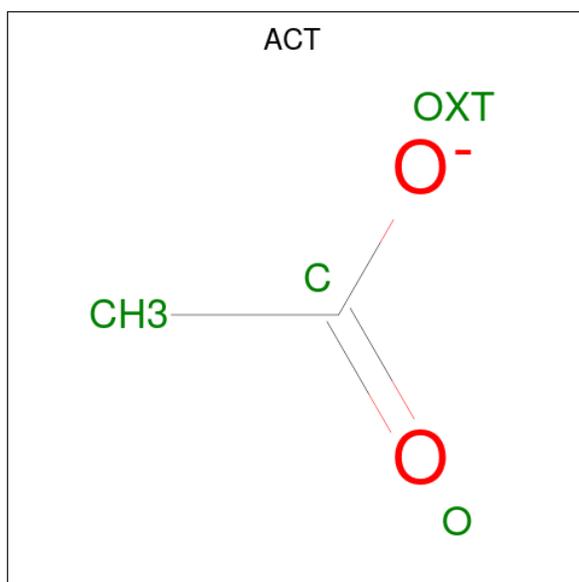
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).

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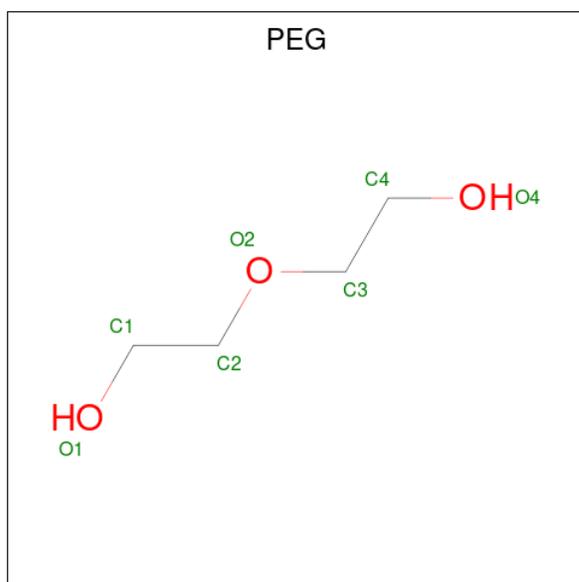
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 7	C 4	O 3	0	0
7	A	1	Total 7	C 4	O 3	0	0
7	C	1	Total 7	C 4	O 3	0	0
7	E	1	Total 7	C 4	O 3	0	0

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

GOL
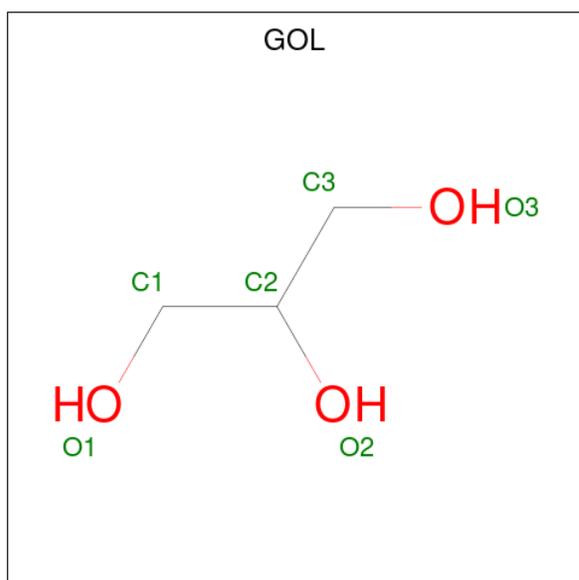
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 6	C 3	O 3	0	0
8	B	1	Total 6	C 3	O 3	0	0
8	B	1	Total 6	C 3	O 3	0	0
8	C	1	Total 6	C 3	O 3	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	122	Total 122	O 122	0	0
9	B	124	Total 124	O 124	0	0
9	C	123	Total 123	O 123	0	0
9	D	129	Total 129	O 129	0	0
9	E	91	Total 91	O 91	0	0
9	F	92	Total 92	O 92	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A:

%

85% 10% 5%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET ASP K3 I6 M10 P16 F17 K18 N19 Y27 G38 A41 R60 E68 K71 K74 V75 K76 F95 D102 V107 A108 A127 P133 Y137 R142 C145 E146 I147

N161 K166 E228 K235 E239 L240 Y241 K245 F248 N252 I256 M260 F298

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B:

87% 7% · 5%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET ASP K3 E24 K32 V45 R60 N84 F95 V107 A108 P109 L135 L136 Y137 C145 D150 K154 L155 F156 N161 I162 Y163 K166 R184 M185 K231 Y241 K245 E250

S268 L269 E270 F298

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C:

89% 7% ·

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET D2 K21 R29 R60 K74 E88 K94 F95 H99 V107 A108 T115 Q116 S129 Y137 R142 I147 K166 Y241 N252 P253 I254 P255 F298

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D:

90% 6% 5%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET ASP K3 G20 K32 E36 F95 A96 K97 V107 D131 Y137 R142 D150 K154 K166 I188 I207 D216 I254 P255 F271 K296 G297 F298

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:

85% 11% 5%

• 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	85.35Å 233.39Å 202.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.14 – 1.97 46.44 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.14-1.97) 99.8 (46.44-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.242 0.195 , 0.242	Depositor DCC
R_{free} test set	7106 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.7	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	14738	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, PGE, MG, PEG, EDO, PG4, GOL, 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	0.44	0/2312	0.57	0/3124
1	B	0.47	0/2306	0.56	0/3118
1	C	0.40	0/2317	0.55	0/3131
1	D	0.40	0/2326	0.53	0/3144
1	E	0.39	0/2312	0.52	0/3124
1	F	0.37	0/2316	0.54	0/3131
All	All	0.41	0/13889	0.54	0/18772

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	KPI	Mainchain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2288	0	2324	24	0
1	B	2282	0	2305	25	0
1	C	2290	0	2324	19	0
1	D	2291	0	2323	15	0
1	E	2288	0	2324	24	0
1	F	2289	0	2323	25	0
2	A	13	0	18	0	0
2	B	13	0	18	4	0
2	C	13	0	18	0	0
2	D	13	0	18	3	0
2	E	13	0	18	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	12	0	18	0	0
4	B	28	0	42	6	0
4	C	20	0	30	3	0
4	D	16	0	24	4	0
4	E	16	0	24	5	0
4	F	12	0	18	5	0
5	A	10	0	14	5	0
5	C	10	0	14	2	0
5	D	10	0	14	1	0
5	E	10	0	14	0	0
5	F	10	0	14	1	0
6	A	12	0	9	0	0
6	B	8	0	6	1	0
6	C	4	0	3	3	0
6	D	8	0	6	0	0
6	E	4	0	3	1	0
6	F	12	0	9	0	0
7	A	14	0	20	1	0
7	C	7	0	10	4	0
7	E	7	0	10	0	0
8	A	6	0	8	0	0
8	B	12	0	16	0	0
8	C	6	0	8	0	0
9	A	122	0	0	2	0
9	B	124	0	0	1	0
9	C	123	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	129	0	0	0	0
9	E	91	0	0	1	0
9	F	92	0	0	0	0
All	All	14738	0	14347	127	0

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

All (127) 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:A:228:GLU:OE2	1:B:231:LYS:HE2	1.50	1.12
1:A:142:ARG:HH21	5:A:308:PGE:H4	1.32	0.93
1:B:154:LYS:HZ2	2:B:301:PG4:H41	1.33	0.92
1:F:167:GLU:HB3	4:F:305:EDO:H21	1.50	0.91
1:B:145:CYS:HB2	4:B:303:EDO:H11	1.68	0.74
1:E:142:ARG:HH21	6:E:309:ACT:H1	1.52	0.74
1:C:142:ARG:HE	6:C:310:ACT:H3	1.54	0.72
1:B:24:GLU:H	4:B:309:EDO:H11	1.59	0.68
1:C:29:ARG:NH1	9:C:401:HOH:O	2.22	0.67
1:A:228:GLU:OE2	1:B:231:LYS:CE	2.38	0.67
1:D:20:GLY:HA2	4:D:302:EDO:H22	1.75	0.67
1:F:35:ILE:HG12	1:F:75:VAL:HG21	1.77	0.67
1:E:171:ASN:H	4:E:304:EDO:H11	1.61	0.66
1:C:142:ARG:NE	6:C:310:ACT:H3	2.11	0.65
1:B:150:ASP:HB3	2:B:301:PG4:H51	1.80	0.64
1:C:115:THR:HA	7:C:311:PEG:H32	1.81	0.63
1:A:142:ARG:NH2	5:A:308:PGE:H4	2.09	0.63
1:D:32:LYS:HG3	5:D:306:PGE:H42	1.79	0.63
1:F:198:ILE:HD11	4:F:305:EDO:H12	1.81	0.62
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.82	0.62
1:C:2:ASP:N	9:C:403:HOH:O	2.33	0.61
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.83	0.61
1:E:169:SER:H	4:E:304:EDO:H12	1.66	0.61
1:F:18:LYS:NZ	1:F:21:LYS:HE3	2.15	0.61
1:C:94:LYS:HE3	1:C:129:SER:HB2	1.84	0.60
1:C:116:GLN:HG2	7:C:311:PEG:H41	1.83	0.59
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.83	0.59
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.85	0.58
1:A:38:GLY:HA2	7:A:312:PEG:H11	1.87	0.57
1:F:194:ILE:HD11	4:F:305:EDO:H11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HE3	1:A:239:GLU:OE2	2.05	0.55
1:D:97:LYS:NZ	1:D:131:ASP:OD1	2.38	0.55
1:B:24:GLU:HB2	4:B:309:EDO:H22	1.89	0.55
1:B:154:LYS:HZ2	2:B:301:PG4:H21	1.72	0.55
1:D:154:LYS:HE3	2:D:301:PG4:H52	1.90	0.54
1:A:74:LYS:HE2	9:A:516:HOH:O	2.08	0.53
1:D:32:LYS:NZ	1:D:36[B]:GLU:OE2	2.42	0.53
1:F:18:LYS:HD2	1:F:18:LYS:O	2.09	0.52
1:E:111:TYR:HH	1:F:47:THR:HG1	1.56	0.52
1:B:161:ASN:OD1	1:B:161:ASN:N	2.41	0.51
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.92	0.51
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.92	0.51
1:D:150:ASP:HB3	2:D:301:PG4:H51	1.91	0.51
1:E:231:LYS:HG3	1:E:232:GLU:N	2.25	0.51
1:F:169:SER:H	4:F:305:EDO:H22	1.76	0.51
5:C:309:PGE:H3	1:E:294:LYS:NZ	2.25	0.51
1:B:250:GLU:HG2	4:B:306:EDO:H22	1.93	0.50
1:E:111:TYR:OH	1:F:47:THR:OG1	2.30	0.50
1:D:188:ILE:HG21	1:D:207:ILE:HG13	1.94	0.50
1:A:108:ALA:HB2	1:A:147:ILE:HD11	1.94	0.50
1:A:248:PHE:CE2	5:A:308:PGE:H42	2.46	0.50
1:B:154:LYS:NZ	2:B:301:PG4:H21	2.27	0.50
1:A:10:MET:HG2	1:A:41:ALA:HB3	1.94	0.50
1:F:120:TYR:CG	5:F:306:PGE:H22	2.47	0.49
1:E:97:LYS:HE3	1:E:131:ASP:OD1	2.13	0.49
1:F:18:LYS:HZ3	1:F:21:LYS:HE3	1.78	0.48
1:F:241:TYR:CE2	1:F:245:LYS:HG3	2.47	0.48
1:A:248:PHE:CD2	5:A:308:PGE:H42	2.47	0.48
1:B:32:LYS:HG2	4:B:305:EDO:H12	1.95	0.48
1:C:74:LYS:NZ	1:E:264:GLY:O	2.39	0.48
1:C:252:ASN:ND2	1:C:253:PRO:HA	2.27	0.48
1:E:198:ILE:HD11	4:E:304:EDO:H22	1.93	0.48
4:C:306:EDO:H21	9:C:417:HOH:O	2.12	0.48
1:D:20:GLY:HA2	4:D:302:EDO:C2	2.43	0.48
1:F:281:GLU:O	1:F:285:LYS:HG3	2.14	0.48
1:B:241:TYR:CE2	1:B:245:LYS:HG3	2.49	0.48
1:E:59:ASN:ND2	9:E:404:HOH:O	2.43	0.48
1:C:116:GLN:HE21	7:C:311:PEG:H41	1.80	0.47
9:A:403:HOH:O	1:B:231:LYS:HE3	2.14	0.47
1:C:241:TYR:HB3	4:C:304:EDO:H22	1.96	0.47
1:E:171:ASN:H	4:E:304:EDO:C1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ASN:ND2	1:E:253:PRO:HA	2.30	0.46
1:B:45:VAL:O	6:B:310:ACT:H1	2.15	0.46
1:B:135:LEU:HD13	1:B:163:TYR:CZ	2.50	0.46
1:C:108:ALA:HB2	1:C:147:ILE:HD11	1.96	0.46
1:B:184:ARG:HG3	1:B:184:ARG:HH11	1.80	0.46
1:F:10:MET:HG2	1:F:41:ALA:HB3	1.98	0.46
1:F:18:LYS:HZ2	1:F:21:LYS:HE3	1.80	0.46
1:C:254:ILE:HB	1:C:255:PRO:HD3	1.97	0.46
1:F:188:ILE:HG21	1:F:207:ILE:HG13	1.98	0.46
1:A:6:ILE:HG12	1:A:76:LYS:HD3	1.98	0.46
1:B:60:ARG:HG3	1:B:95:PHE:HZ	1.80	0.45
1:D:271:PHE:O	4:D:302:EDO:H11	2.17	0.45
1:E:13:LEU:HD11	1:E:42:VAL:HB	1.98	0.45
1:A:68:GLU:O	1:A:71:LYS:HG2	2.17	0.45
1:F:256:ILE:O	1:F:260:MET:HG2	2.17	0.45
1:A:137:TYR:CD1	1:A:166:KPI:HD	2.51	0.45
1:F:243:ILE:HB	1:F:293:TYR:CE1	2.52	0.45
1:D:254:ILE:HB	1:D:255:PRO:HD3	1.98	0.45
1:C:60:ARG:HG3	1:C:99:HIS:CD2	2.52	0.44
1:C:88:GLU:HG3	4:C:308:EDO:H22	1.99	0.44
1:D:216:ASP:OD1	1:D:216:ASP:N	2.51	0.44
1:B:24:GLU:H	4:B:309:EDO:C1	2.28	0.44
1:E:84:ASN:HA	1:E:109:PRO:HB3	2.00	0.44
1:B:60:ARG:HB2	1:B:95:PHE:CZ	2.52	0.44
1:A:16:PRO:HD2	1:A:27:TYR:HD1	1.83	0.44
1:A:102:ASP:O	1:A:133:PRO:HD2	2.17	0.44
1:A:256:ILE:O	1:A:260:MET:HG2	2.18	0.44
1:F:135:LEU:HD13	1:F:163:TYR:CZ	2.52	0.44
5:C:309:PGE:H3	1:E:294:LYS:HZ3	1.82	0.44
1:D:142:ARG:NH2	4:D:304:EDO:H22	2.33	0.44
1:E:246:ILE:HD11	1:E:285:LYS:HB3	1.99	0.43
1:C:116:GLN:HB2	7:C:311:PEG:H12	1.99	0.43
1:A:60:ARG:HB2	1:A:95:PHE:CZ	2.53	0.43
1:A:68:GLU:HA	1:A:71:LYS:HD2	2.01	0.43
1:A:252:ASN:HD22	5:A:308:PGE:H12	1.83	0.43
1:F:169:SER:OG	4:F:305:EDO:H22	2.18	0.43
1:A:127:ALA:O	1:A:161:ASN:ND2	2.51	0.43
1:D:154:LYS:NZ	2:D:301:PG4:H41	2.34	0.43
1:E:149:THR:HG23	1:E:178:LEU:HD23	2.00	0.43
1:F:254:ILE:HB	1:F:255:PRO:HD3	2.01	0.42
1:B:231:LYS:HD2	1:B:231:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PHE:CE1	1:B:185:MET:HA	2.54	0.42
1:A:71:LYS:HB2	1:A:71:LYS:HE3	1.87	0.42
1:C:252:ASN:OD1	6:C:310:ACT:H1	2.20	0.42
1:E:245:LYS:HD2	1:E:245:LYS:HA	1.90	0.42
1:B:84:ASN:HA	1:B:109:PRO:HB3	2.02	0.41
1:F:102:ASP:O	1:F:133:PRO:HD2	2.19	0.41
1:C:60:ARG:HG3	1:C:99:HIS:NE2	2.35	0.41
1:E:262:LEU:HD21	1:E:283:PHE:CZ	2.56	0.41
1:F:269:LEU:C	1:F:269:LEU:HD13	2.40	0.41
1:A:241:TYR:CE2	1:A:245:LYS:HG3	2.55	0.41
1:B:270:GLU:OE2	9:B:401:HOH:O	2.21	0.41
1:D:296:LYS:HA	1:D:296:LYS:HD2	1.95	0.41
1:E:213:LEU:HD11	1:E:295:ILE:HD13	2.03	0.40
1:E:167:GLU:HB3	4:E:304:EDO:H21	2.04	0.40
1:E:114:PRO:HB3	1:F:274:PRO:HB2	2.04	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	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	B	294/310 (95%)	287 (98%)	7 (2%)	0	100	100
1	C	295/310 (95%)	290 (98%)	5 (2%)	0	100	100
1	D	296/310 (96%)	288 (97%)	8 (3%)	0	100	100
1	E	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	F	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
All	All	1767/1860 (95%)	1729 (98%)	38 (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	249/260 (96%)	249 (100%)	0	100	100
1	B	247/260 (95%)	245 (99%)	2 (1%)	81	80
1	C	250/260 (96%)	249 (100%)	1 (0%)	91	90
1	D	251/260 (96%)	251 (100%)	0	100	100
1	E	249/260 (96%)	248 (100%)	1 (0%)	91	90
1	F	250/260 (96%)	247 (99%)	3 (1%)	71	67
All	All	1496/1560 (96%)	1489 (100%)	7 (0%)	88	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	231	LYS
1	B	268	SER
1	C	21	LYS
1	E	56	HIS
1	F	18	LYS
1	F	21	LYS
1	F	25	GLN

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

Mol	Chain	Res	Type
1	F	19	ASN

5.3.3 RNA (i)

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	1.88	2 (18%)	10,15,17	3.94	5 (50%)
1	KPI	A	166	1	11,13,14	0.94	0	10,15,17	3.85	4 (40%)
1	KPI	D	166	1	11,13,14	1.13	2 (18%)	10,15,17	3.08	4 (40%)
1	KPI	E	166	1	11,13,14	0.97	0	10,15,17	3.30	4 (40%)
1	KPI	B	166	1	11,13,14	2.17	3 (27%)	10,15,17	4.15	6 (60%)
1	KPI	F	166	1	11,13,14	0.94	0	10,15,17	3.79	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	C	166	1	-	1/13/14/16	-
1	KPI	A	166	1	-	0/13/14/16	-
1	KPI	D	166	1	-	1/13/14/16	-
1	KPI	E	166	1	-	0/13/14/16	-
1	KPI	B	166	1	-	0/13/14/16	-
1	KPI	F	166	1	-	1/13/14/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	O2-CX2	4.92	1.35	1.22
1	C	166	KPI	O2-CX2	4.83	1.35	1.22
1	B	166	KPI	O-C	4.25	1.36	1.19
1	C	166	KPI	CX2-CX1	2.30	1.52	1.49
1	D	166	KPI	O1-CX2	2.13	1.36	1.30
1	B	166	KPI	O1-CX2	-2.08	1.24	1.30
1	D	166	KPI	CB-CA	2.05	1.56	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	KPI	C1-CX1-CX2	-9.63	108.81	118.17
1	B	166	KPI	C1-CX1-CX2	-8.56	109.85	118.17
1	F	166	KPI	C1-CX1-CX2	-8.55	109.86	118.17
1	C	166	KPI	C1-CX1-CX2	-8.33	110.07	118.17
1	D	166	KPI	C1-CX1-CX2	-7.28	111.09	118.17
1	E	166	KPI	C1-CX1-CX2	-6.61	111.74	118.17
1	F	166	KPI	O2-CX2-CX1	6.50	129.68	121.38
1	E	166	KPI	O2-CX2-CX1	6.11	129.17	121.38
1	B	166	KPI	O2-CX2-CX1	-5.98	113.74	121.38
1	B	166	KPI	O1-CX2-CX1	5.90	129.15	116.35
1	C	166	KPI	O2-CX2-CX1	-5.68	114.12	121.38
1	C	166	KPI	O1-CX2-CX1	5.46	128.21	116.35
1	A	166	KPI	O2-CX2-CX1	5.24	128.06	121.38
1	D	166	KPI	O2-CX2-CX1	4.48	127.10	121.38
1	E	166	KPI	O1-CX2-O2	-3.52	115.55	123.61
1	B	166	KPI	C1-CX1-NZ	3.24	131.60	123.11
1	A	166	KPI	C1-CX1-NZ	3.07	131.14	123.11
1	C	166	KPI	C1-CX1-NZ	2.98	130.89	123.11
1	A	166	KPI	O1-CX2-O2	-2.92	116.92	123.61
1	F	166	KPI	O1-CX2-O2	-2.91	116.96	123.61
1	F	166	KPI	C1-CX1-NZ	2.88	130.63	123.11
1	D	166	KPI	C1-CX1-NZ	2.87	130.62	123.11
1	B	166	KPI	O1-CX2-O2	-2.84	117.11	123.61
1	E	166	KPI	C1-CX1-NZ	2.81	130.46	123.11
1	D	166	KPI	O1-CX2-O2	-2.76	117.30	123.61
1	C	166	KPI	O1-CX2-O2	-2.59	117.67	123.61
1	B	166	KPI	CD-CE-NZ	2.05	114.38	110.66

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	166	KPI	C1-CX1-NZ-CE
1	D	166	KPI	CG-CD-CE-NZ
1	C	166	KPI	C1-CX1-NZ-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 10 are monoatomic - leaving 56 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	D	303	-	3,3,3	0.37	0	2,2,2	0.78	0
4	EDO	A	306	-	3,3,3	0.50	0	2,2,2	0.41	0
2	PG4	D	301	-	12,12,12	0.47	0	11,11,11	0.44	0
6	ACT	A	310	-	3,3,3	1.42	1 (33%)	3,3,3	1.37	0
4	EDO	F	303	-	3,3,3	0.51	0	2,2,2	0.29	0
4	EDO	A	307	-	3,3,3	0.48	0	2,2,2	0.53	0
4	EDO	E	305	-	3,3,3	0.52	0	2,2,2	0.28	0
6	ACT	A	309	-	3,3,3	1.74	1 (33%)	3,3,3	1.16	0
6	ACT	D	308	-	3,3,3	1.45	1 (33%)	3,3,3	1.18	0
8	GOL	B	312	-	5,5,5	0.90	0	5,5,5	0.87	0
6	ACT	B	310	-	3,3,3	1.31	0	3,3,3	1.49	0
5	PGE	A	308	-	9,9,9	0.41	0	8,8,8	0.57	0
4	EDO	B	305	-	3,3,3	0.53	0	2,2,2	0.14	0
4	EDO	B	303	-	3,3,3	0.54	0	2,2,2	0.26	0
4	EDO	C	306	-	3,3,3	0.39	0	2,2,2	0.47	0
4	EDO	C	308	-	3,3,3	0.45	0	2,2,2	0.29	0
4	EDO	A	305	-	3,3,3	0.45	0	2,2,2	0.28	0
8	GOL	A	314	-	5,5,5	0.65	0	5,5,5	1.05	0
4	EDO	B	306	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	B	308	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	D	305	-	3,3,3	0.46	0	2,2,2	0.53	0
6	ACT	C	310	-	3,3,3	0.86	0	3,3,3	1.53	1 (33%)
7	PEG	E	310	-	6,6,6	0.50	0	5,5,5	0.30	0
5	PGE	F	306	-	9,9,9	0.33	0	8,8,8	0.41	0
4	EDO	B	309	-	3,3,3	0.47	0	2,2,2	0.34	0
2	PG4	E	301	-	12,12,12	0.54	0	11,11,11	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	EDO	C	304	-	3,3,3	0.51	0	2,2,2	0.20	0
2	PG4	C	301	-	12,12,12	0.51	0	11,11,11	0.39	0
4	EDO	E	304	-	3,3,3	0.31	0	2,2,2	0.34	0
8	GOL	C	312	-	5,5,5	0.68	0	5,5,5	1.09	1 (20%)
2	PG4	B	301	-	12,12,12	0.49	0	11,11,11	0.51	0
6	ACT	F	309	-	3,3,3	1.32	0	3,3,3	1.42	0
7	PEG	C	311	-	6,6,6	0.52	0	5,5,5	0.33	0
5	PGE	C	309	-	9,9,9	0.33	0	8,8,8	0.37	0
7	PEG	A	312	-	6,6,6	0.46	0	5,5,5	0.30	0
4	EDO	B	307	-	3,3,3	0.47	0	2,2,2	0.36	0
6	ACT	B	311	-	3,3,3	1.44	1 (33%)	3,3,3	1.52	0
4	EDO	F	305	-	3,3,3	0.32	0	2,2,2	0.31	0
4	EDO	D	304	-	3,3,3	0.39	0	2,2,2	0.43	0
6	ACT	F	307	-	3,3,3	1.39	1 (33%)	3,3,3	1.12	0
4	EDO	E	306	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	C	305	-	3,3,3	0.39	0	2,2,2	0.61	0
4	EDO	D	302	-	3,3,3	0.42	0	2,2,2	0.37	0
2	PG4	A	301	-	12,12,12	0.50	0	11,11,11	0.26	0
6	ACT	E	309	-	3,3,3	0.94	0	3,3,3	1.55	1 (33%)
8	GOL	B	313	-	5,5,5	0.82	0	5,5,5	0.82	0
7	PEG	A	313	-	6,6,6	0.47	0	5,5,5	0.44	0
5	PGE	E	308	-	9,9,9	0.36	0	8,8,8	0.28	0
4	EDO	F	304	-	3,3,3	0.39	0	2,2,2	0.59	0
5	PGE	D	306	-	9,9,9	0.33	0	8,8,8	0.35	0
4	EDO	E	307	-	3,3,3	0.46	0	2,2,2	0.44	0
6	ACT	D	307	-	3,3,3	1.38	0	3,3,3	1.26	0
6	ACT	A	311	-	3,3,3	1.26	0	3,3,3	1.53	0
4	EDO	C	307	-	3,3,3	0.43	0	2,2,2	0.35	0
6	ACT	F	308	-	3,3,3	1.53	1 (33%)	3,3,3	1.19	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
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	A	306	-	-	0/1/1/1	-
2	PG4	D	301	-	-	8/10/10/10	-
4	EDO	F	303	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	307	-	-	1/1/1/1	-
4	EDO	E	305	-	-	1/1/1/1	-
8	GOL	B	312	-	-	0/4/4/4	-
5	PGE	A	308	-	-	5/7/7/7	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	C	308	-	-	1/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
8	GOL	A	314	-	-	2/4/4/4	-
4	EDO	B	306	-	-	0/1/1/1	-
4	EDO	B	308	-	-	1/1/1/1	-
4	EDO	D	305	-	-	0/1/1/1	-
7	PEG	E	310	-	-	2/4/4/4	-
5	PGE	F	306	-	-	5/7/7/7	-
4	EDO	B	309	-	-	1/1/1/1	-
2	PG4	E	301	-	-	2/10/10/10	-
4	EDO	C	304	-	-	0/1/1/1	-
2	PG4	C	301	-	-	6/10/10/10	-
4	EDO	E	304	-	-	1/1/1/1	-
8	GOL	C	312	-	-	2/4/4/4	-
2	PG4	B	301	-	-	7/10/10/10	-
7	PEG	C	311	-	-	2/4/4/4	-
5	PGE	C	309	-	-	5/7/7/7	-
7	PEG	A	312	-	-	2/4/4/4	-
4	EDO	B	307	-	-	1/1/1/1	-
4	EDO	F	305	-	-	0/1/1/1	-
4	EDO	D	304	-	-	0/1/1/1	-
4	EDO	E	306	-	-	0/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	C	305	-	-	0/1/1/1	-
4	EDO	D	302	-	-	0/1/1/1	-
2	PG4	A	301	-	-	1/10/10/10	-
8	GOL	B	313	-	-	2/4/4/4	-
7	PEG	A	313	-	-	3/4/4/4	-
5	PGE	E	308	-	-	2/7/7/7	-
4	EDO	F	304	-	-	0/1/1/1	-
5	PGE	D	306	-	-	4/7/7/7	-
4	EDO	E	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	307	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	309	ACT	CH3-C	2.60	1.60	1.49
6	F	308	ACT	CH3-C	2.22	1.58	1.49
6	B	311	ACT	CH3-C	2.21	1.58	1.49
6	D	308	ACT	CH3-C	2.17	1.58	1.49
6	A	310	ACT	CH3-C	2.11	1.58	1.49
6	F	307	ACT	CH3-C	2.06	1.57	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	309	ACT	OXT-C-O	2.13	129.91	122.05
6	C	310	ACT	OXT-C-O	2.07	129.67	122.05
8	C	312	GOL	C3-C2-C1	-2.02	103.83	111.70

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	314	GOL	O1-C1-C2-C3
5	A	308	PGE	C3-C4-O3-C5
2	B	301	PG4	C4-C3-O2-C2
5	C	309	PGE	O2-C3-C4-O3
2	B	301	PG4	O3-C5-C6-O4
5	F	306	PGE	O2-C3-C4-O3
2	C	301	PG4	O2-C3-C4-O3
8	C	312	GOL	O1-C1-C2-O2
7	C	311	PEG	O2-C3-C4-O4
5	A	308	PGE	O2-C3-C4-O3
2	D	301	PG4	O3-C5-C6-O4
2	C	301	PG4	O1-C1-C2-O2
7	A	313	PEG	O1-C1-C2-O2
7	C	311	PEG	O1-C1-C2-O2
8	B	313	GOL	O1-C1-C2-C3
8	C	312	GOL	O1-C1-C2-C3
2	C	301	PG4	C1-C2-O2-C3
8	A	314	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	B	313	GOL	O1-C1-C2-O2
5	C	309	PGE	O3-C5-C6-O4
4	B	307	EDO	O1-C1-C2-O2
2	D	301	PG4	O1-C1-C2-O2
5	A	308	PGE	O1-C1-C2-O2
7	E	310	PEG	O1-C1-C2-O2
2	E	301	PG4	O2-C3-C4-O3
4	B	304	EDO	O1-C1-C2-O2
4	C	308	EDO	O1-C1-C2-O2
5	F	306	PGE	C1-C2-O2-C3
2	B	301	PG4	O4-C7-C8-O5
5	F	306	PGE	O1-C1-C2-O2
2	B	301	PG4	C5-C6-O4-C7
5	E	308	PGE	C4-C3-O2-C2
2	C	301	PG4	C3-C4-O3-C5
7	E	310	PEG	C1-C2-O2-C3
5	D	306	PGE	O2-C3-C4-O3
2	C	301	PG4	C5-C6-O4-C7
2	E	301	PG4	C8-C7-O4-C6
2	D	301	PG4	C4-C3-O2-C2
5	A	308	PGE	C1-C2-O2-C3
5	C	309	PGE	O1-C1-C2-O2
5	F	306	PGE	O3-C5-C6-O4
5	C	309	PGE	C6-C5-O3-C4
5	A	308	PGE	O3-C5-C6-O4
5	D	306	PGE	O1-C1-C2-O2
2	D	301	PG4	C8-C7-O4-C6
7	A	313	PEG	C1-C2-O2-C3
5	D	306	PGE	C6-C5-O3-C4
2	D	301	PG4	C1-C2-O2-C3
7	A	312	PEG	C1-C2-O2-C3
2	D	301	PG4	C3-C4-O3-C5
4	A	307	EDO	O1-C1-C2-O2
4	C	306	EDO	O1-C1-C2-O2
2	B	301	PG4	C1-C2-O2-C3
2	C	301	PG4	C4-C3-O2-C2
5	F	306	PGE	C3-C4-O3-C5
2	D	301	PG4	C6-C5-O3-C4
5	C	309	PGE	C3-C4-O3-C5
2	B	301	PG4	C3-C4-O3-C5
7	A	313	PEG	O2-C3-C4-O4
5	D	306	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
7	A	312	PEG	O2-C3-C4-O4
2	D	301	PG4	O2-C3-C4-O3
4	B	308	EDO	O1-C1-C2-O2
4	B	309	EDO	O1-C1-C2-O2
4	C	307	EDO	O1-C1-C2-O2
4	E	304	EDO	O1-C1-C2-O2
2	A	301	PG4	C4-C3-O2-C2
4	E	305	EDO	O1-C1-C2-O2
2	B	301	PG4	O2-C3-C4-O3
5	E	308	PGE	O3-C5-C6-O4

There are no ring outliers.

22 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	PG4	3	0
6	B	310	ACT	1	0
5	A	308	PGE	5	0
4	B	305	EDO	1	0
4	B	303	EDO	1	0
4	C	306	EDO	1	0
4	C	308	EDO	1	0
4	B	306	EDO	1	0
6	C	310	ACT	3	0
5	F	306	PGE	1	0
4	B	309	EDO	3	0
4	C	304	EDO	1	0
4	E	304	EDO	5	0
2	B	301	PG4	4	0
7	C	311	PEG	4	0
5	C	309	PGE	2	0
7	A	312	PEG	1	0
4	F	305	EDO	5	0
4	D	304	EDO	1	0
4	D	302	EDO	3	0
6	E	309	ACT	1	0
5	D	306	PGE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand EDO D 303

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 306

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT A 310

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO F 303

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 307

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO E 305

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT A 309

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT D 308

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 312

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT B 310

Bond lengths

Bond angles

Torsions

Rings

Ligand PGE A 308

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 305

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 306

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 308

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 305

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 314

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 306

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 308

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 305

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT C 310

Bond lengths

Bond angles

Torsions

Rings

Ligand PEG E 310

Bond lengths

Bond angles

Torsions

Rings

Ligand PGE F 306

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 309

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 304

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO E 304

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL C 312

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT F 309

Bond lengths

Bond angles

Torsions

Rings

Ligand PEG C 311	
Bond lengths	Bond angles
Torsions	Rings

Ligand PGE C 309	
Bond lengths	Bond angles
Torsions	Rings

Ligand PEG A 312

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 307

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT B 311

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO F 305

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 304

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT F 307

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO E 306

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 304

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 305

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PG4 A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACT E 309

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 313

Bond lengths

Bond angles

Torsions

Rings

Ligand PEG A 313

Bond lengths

Bond angles

Torsions

Rings

Ligand PGE E 308

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO F 304

Bond lengths

Bond angles

Torsions

Rings

Ligand PGE D 306

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO E 307

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT D 307

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT A 311

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 307

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT F 308

Bond lengths

Bond angles

Torsions

Rings

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, 95th 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%)	0.08	3 (1%)	82	83	24, 30, 45, 51	0
1	B	295/310 (95%)	0.01	0	100	100	23, 30, 44, 51	0
1	C	296/310 (95%)	0.11	1 (0%)	94	94	24, 32, 45, 59	0
1	D	295/310 (95%)	0.04	1 (0%)	94	94	24, 31, 46, 54	0
1	E	295/310 (95%)	0.13	1 (0%)	94	94	27, 35, 50, 60	0
1	F	296/310 (95%)	0.32	10 (3%)	45	48	26, 36, 52, 60	0
All	All	1772/1860 (95%)	0.12	16 (0%)	84	85	23, 33, 48, 60	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	LYS	3.4
1	E	95	PHE	3.3
1	F	298	PHE	2.8
1	C	95	PHE	2.6
1	F	35	ILE	2.5
1	F	19	ASN	2.5
1	F	283	PHE	2.4
1	D	95	PHE	2.4
1	F	294	LYS	2.4
1	F	39	ILE	2.3
1	F	267	GLU	2.2
1	F	72	GLY	2.1
1	F	266	ILE	2.1
1	F	230	TYR	2.0
1	A	19	ASN	2.0
1	A	145	CYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	KPI	E	166	14/15	0.92	0.11	28,33,41,41	0
1	KPI	B	166	14/15	0.94	0.11	22,25,34,35	0
1	KPI	C	166	14/15	0.95	0.14	24,28,33,33	0
1	KPI	F	166	14/15	0.95	0.14	25,32,37,39	0
1	KPI	A	166	14/15	0.96	0.10	24,28,33,38	0
1	KPI	D	166	14/15	0.96	0.11	26,29,35,36	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	302	1/1	0.73	0.21	49,49,49,49	0
3	MG	A	302	1/1	0.76	0.14	57,57,57,57	0
6	ACT	A	309	4/4	0.76	0.20	35,38,39,41	0
5	PGE	A	308	10/10	0.77	0.21	34,42,47,51	0
5	PGE	E	308	10/10	0.77	0.20	49,54,60,60	0
2	PG4	D	301	13/13	0.77	0.18	37,48,59,59	0
6	ACT	F	307	4/4	0.79	0.23	28,42,43,49	0
6	ACT	A	310	4/4	0.80	0.20	41,50,50,57	0
6	ACT	B	311	4/4	0.81	0.21	40,42,48,49	0
7	PEG	A	313	7/7	0.81	0.21	48,50,55,56	0
4	EDO	B	303	4/4	0.82	0.28	34,39,40,44	0
8	GOL	B	313	6/6	0.82	0.15	43,46,49,50	0
3	MG	B	302	1/1	0.83	0.07	36,36,36,36	0
5	PGE	C	309	10/10	0.83	0.20	40,47,51,54	0
4	EDO	B	308	4/4	0.83	0.21	42,47,47,58	0
2	PG4	E	301	13/13	0.84	0.22	44,47,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	306	4/4	0.85	0.17	45,47,48,51	0
4	EDO	B	309	4/4	0.85	0.28	37,46,49,57	0
7	PEG	C	311	7/7	0.85	0.34	29,37,47,52	0
4	EDO	D	302	4/4	0.85	0.38	37,45,46,49	0
8	GOL	C	312	6/6	0.85	0.18	41,48,49,59	0
3	MG	F	302	1/1	0.86	0.28	48,48,48,48	0
7	PEG	E	310	7/7	0.86	0.15	47,50,53,56	0
3	MG	E	303	1/1	0.87	0.17	52,52,52,52	0
6	ACT	F	308	4/4	0.87	0.24	52,54,54,63	0
4	EDO	B	305	4/4	0.87	0.13	50,50,52,56	0
4	EDO	B	307	4/4	0.87	0.14	40,47,48,49	0
4	EDO	A	307	4/4	0.87	0.31	36,46,46,49	0
6	ACT	D	308	4/4	0.87	0.17	39,40,43,46	0
6	ACT	E	309	4/4	0.87	0.22	34,47,47,54	0
4	EDO	D	303	4/4	0.88	0.18	35,40,40,43	0
5	PGE	D	306	10/10	0.88	0.21	45,52,57,63	0
6	ACT	B	310	4/4	0.88	0.25	38,40,49,49	0
8	GOL	A	314	6/6	0.88	0.11	43,47,51,58	0
8	GOL	B	312	6/6	0.88	0.20	29,41,51,57	0
2	PG4	B	301	13/13	0.88	0.14	36,43,54,59	0
7	PEG	A	312	7/7	0.88	0.14	40,43,45,50	0
4	EDO	F	304	4/4	0.89	0.37	31,39,42,42	0
4	EDO	C	308	4/4	0.89	0.18	44,45,49,60	0
4	EDO	E	307	4/4	0.89	0.19	50,50,54,59	0
6	ACT	C	310	4/4	0.89	0.21	38,45,46,51	0
6	ACT	A	311	4/4	0.90	0.27	39,43,51,62	0
5	PGE	F	306	10/10	0.90	0.15	40,46,53,54	0
2	PG4	A	301	13/13	0.90	0.14	37,43,51,52	0
4	EDO	B	306	4/4	0.90	0.27	39,39,41,50	0
2	PG4	C	301	13/13	0.91	0.20	36,42,52,57	0
3	MG	F	301	1/1	0.92	0.07	45,45,45,45	0
4	EDO	C	306	4/4	0.92	0.29	35,41,42,47	0
4	EDO	C	307	4/4	0.92	0.12	43,44,46,49	0
4	EDO	D	305	4/4	0.92	0.14	39,40,42,44	0
4	EDO	E	304	4/4	0.92	0.32	34,35,37,39	0
6	ACT	D	307	4/4	0.93	0.14	41,48,53,53	0
3	MG	A	304	1/1	0.94	0.06	36,36,36,36	0
4	EDO	E	305	4/4	0.94	0.19	34,40,44,45	0
4	EDO	D	304	4/4	0.95	0.18	29,36,40,57	0
4	EDO	A	305	4/4	0.95	0.09	40,47,52,55	0
4	EDO	C	304	4/4	0.95	0.14	35,37,39,48	0
4	EDO	C	305	4/4	0.95	0.28	36,39,40,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	E	306	4/4	0.95	0.16	32,39,41,45	0
6	ACT	F	309	4/4	0.95	0.11	44,44,50,53	0
3	MG	A	303	1/1	0.95	0.11	37,37,37,37	0
4	EDO	F	305	4/4	0.96	0.19	33,34,34,36	0
4	EDO	B	304	4/4	0.96	0.12	38,45,46,51	0
4	EDO	F	303	4/4	0.97	0.10	28,31,33,35	0
3	MG	E	302	1/1	0.97	0.12	37,37,37,37	0
3	MG	C	303	1/1	0.98	0.22	49,49,49,49	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 MG C 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
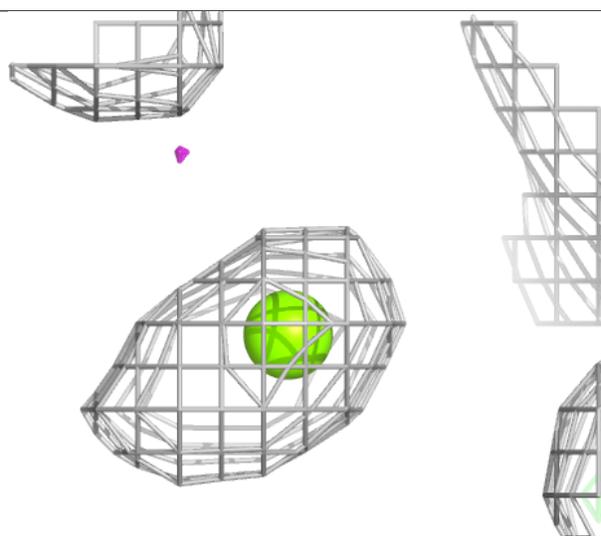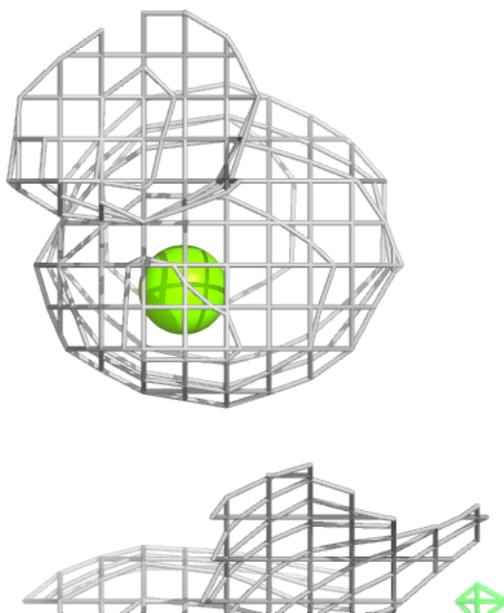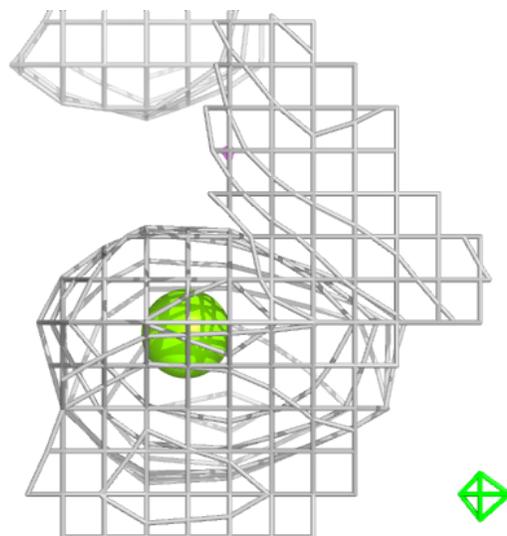
Electron density around MG A 302:

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

Electron density around ACT 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 PGE A 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
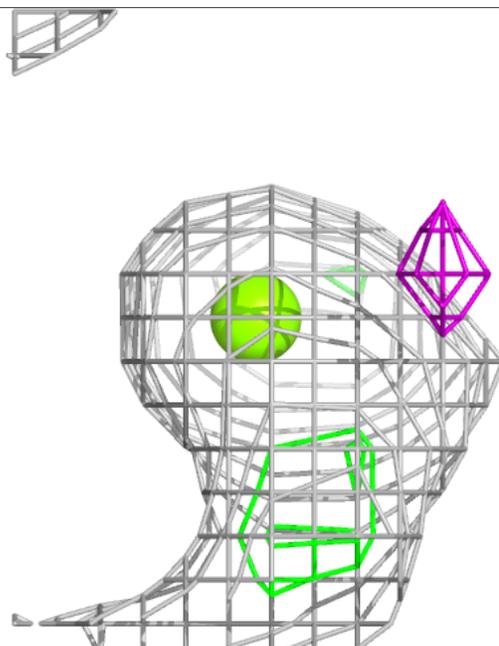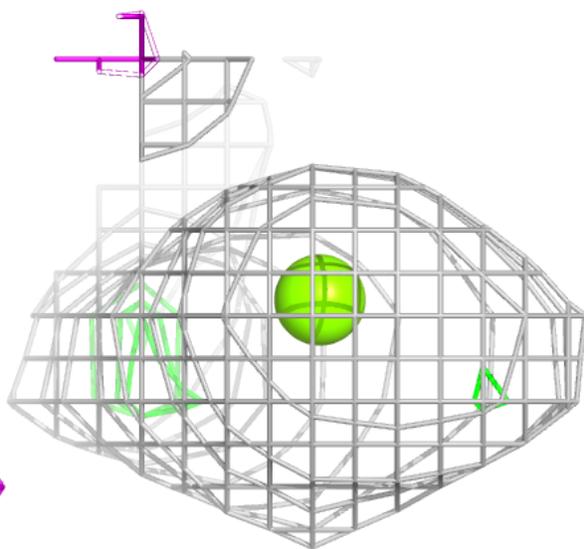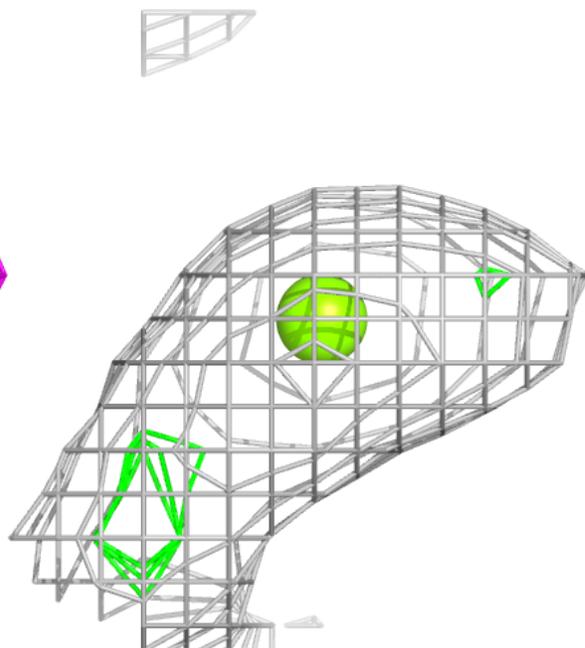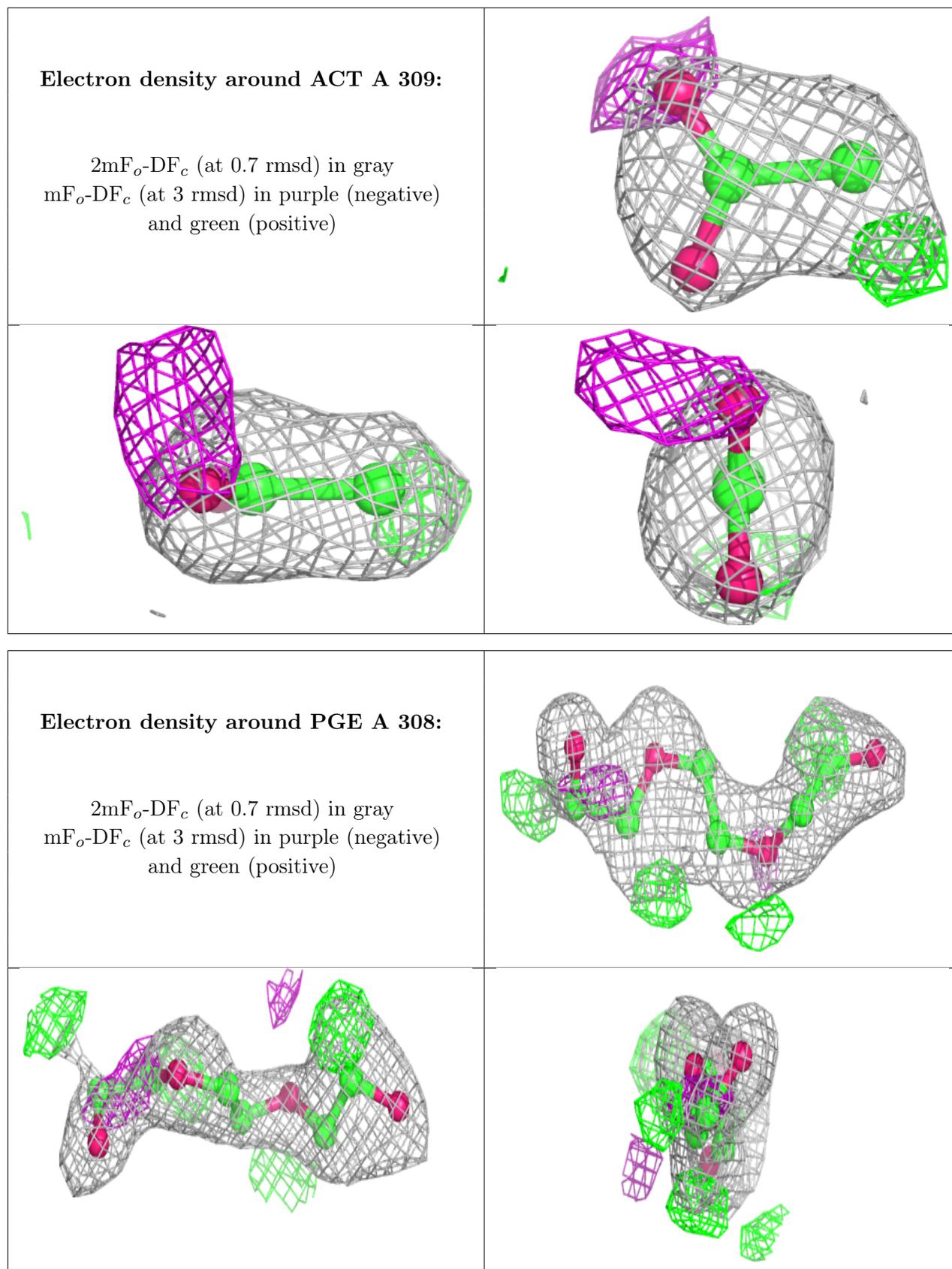
Electron density around PGE E 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
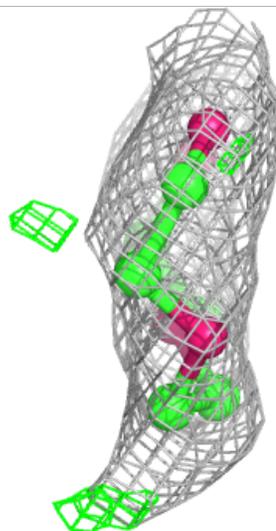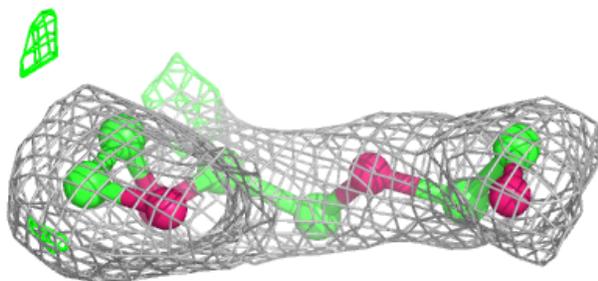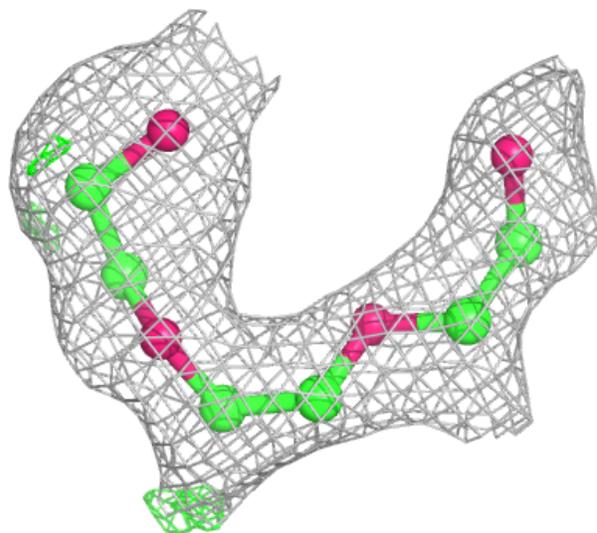
Electron density around PG4 D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
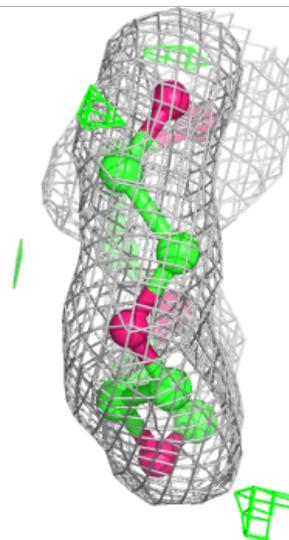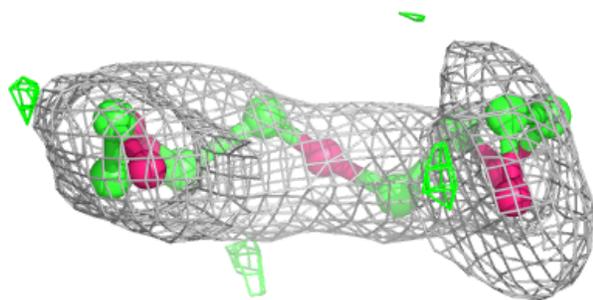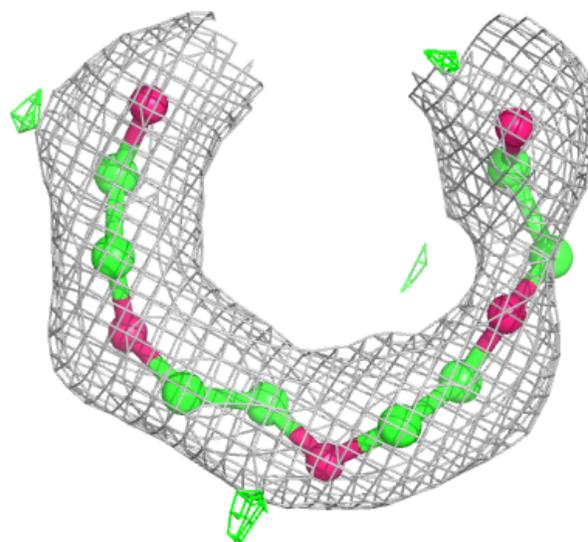
Electron density around ACT F 307:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
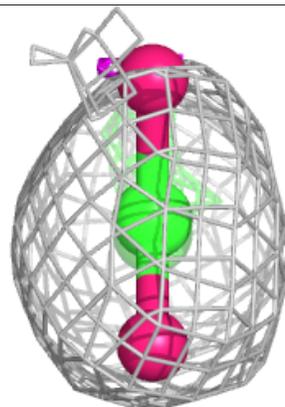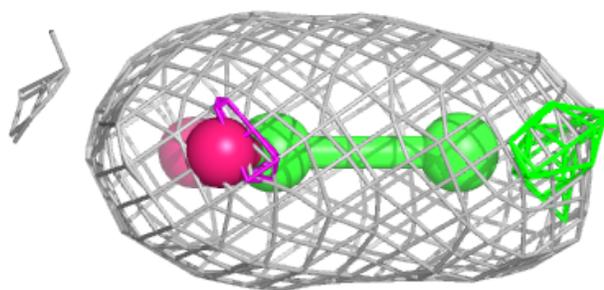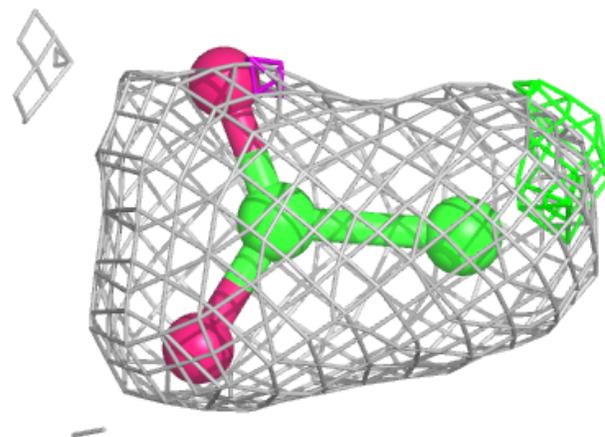
Electron density around ACT A 310:

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

Electron density around ACT B 311:

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

Electron density around PEG A 313:

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

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)
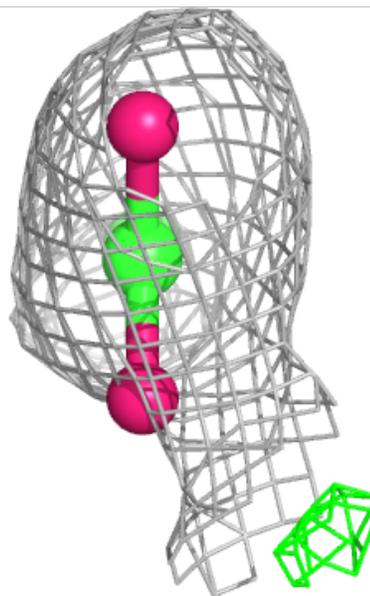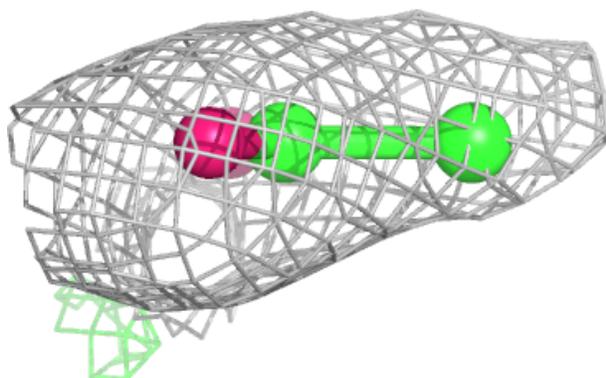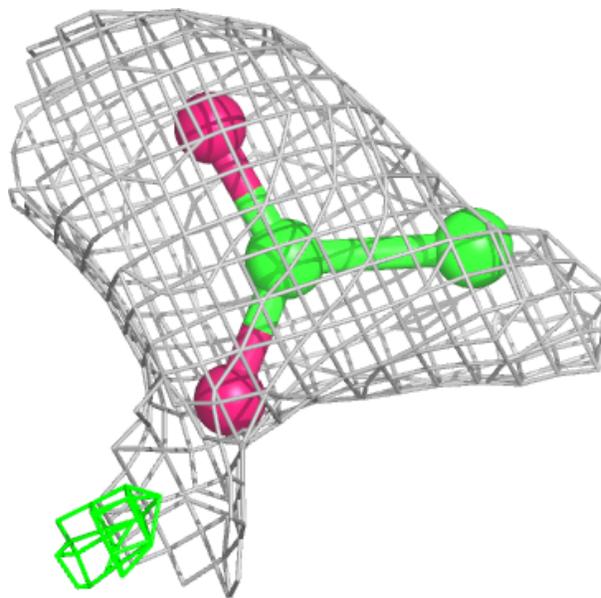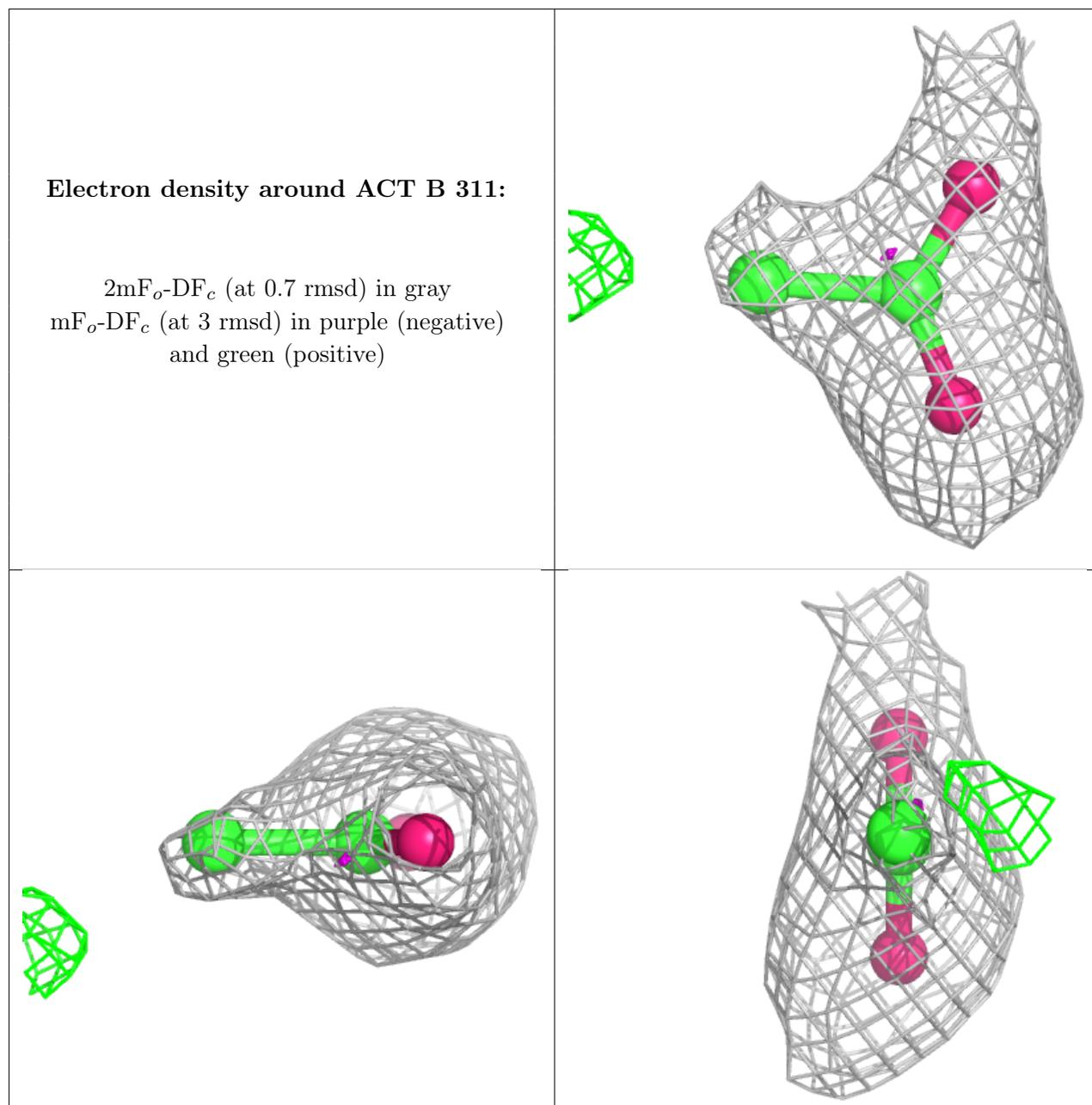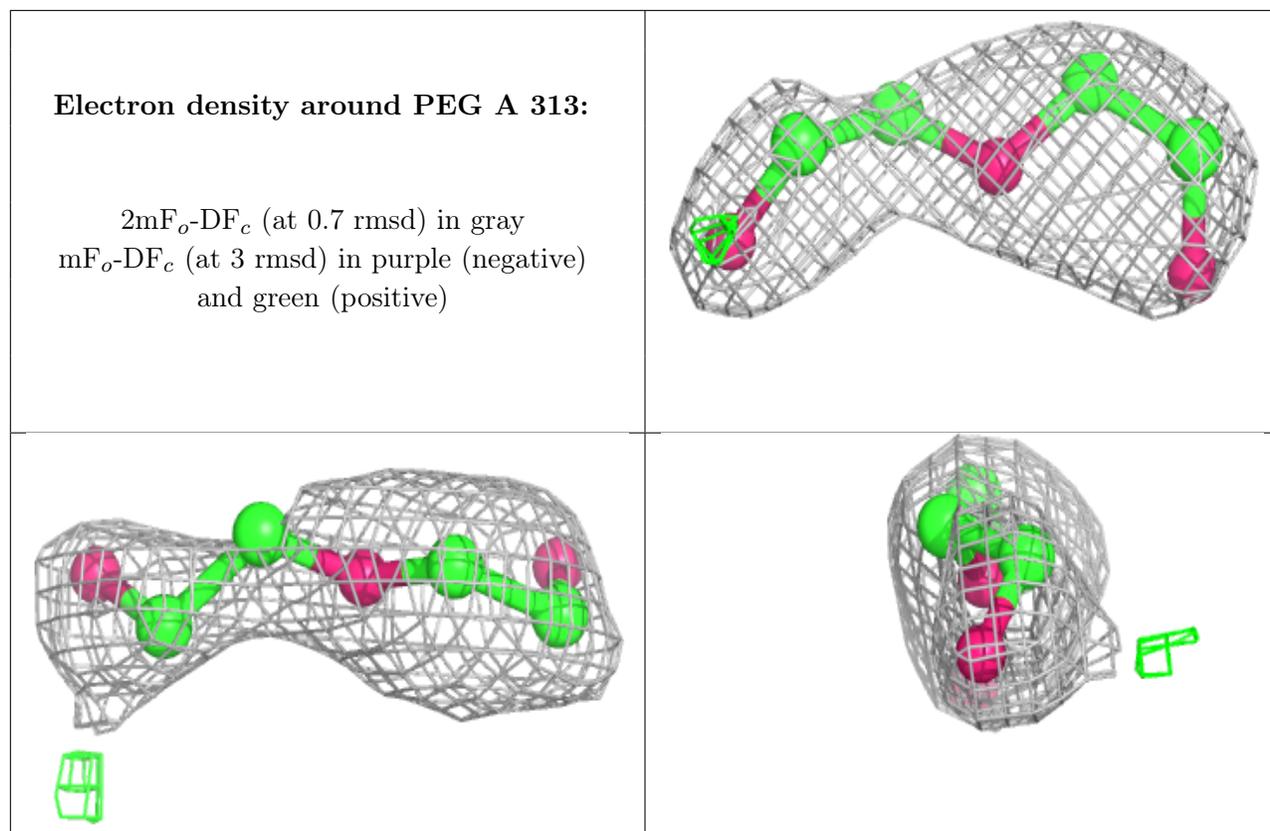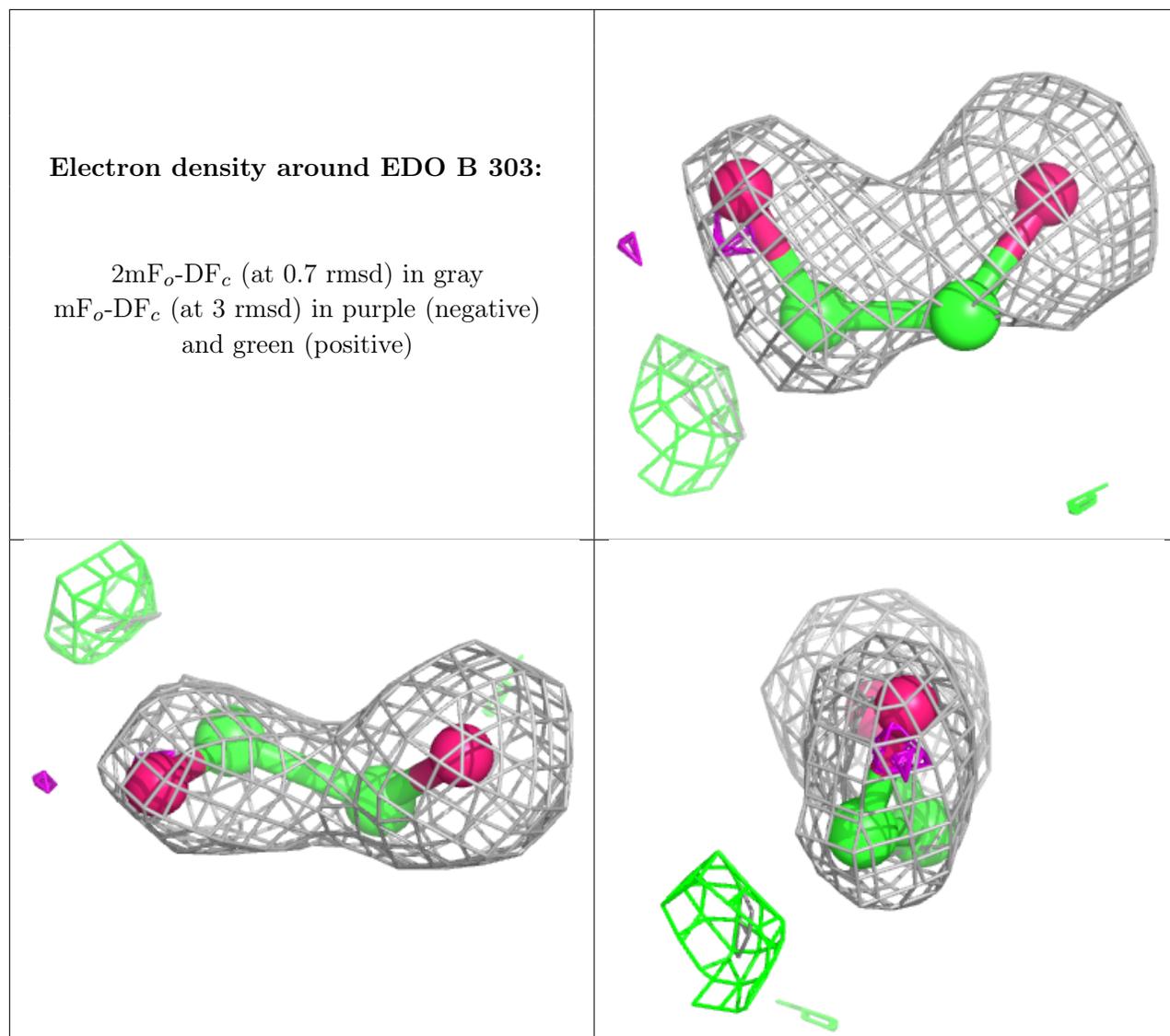
Electron density around GOL B 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
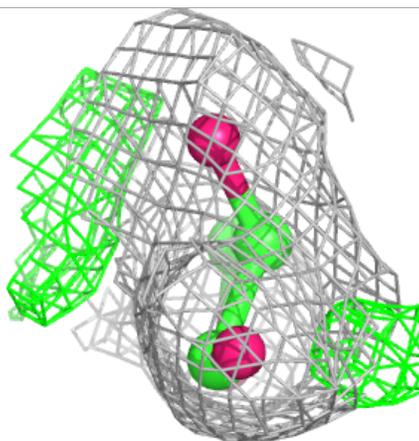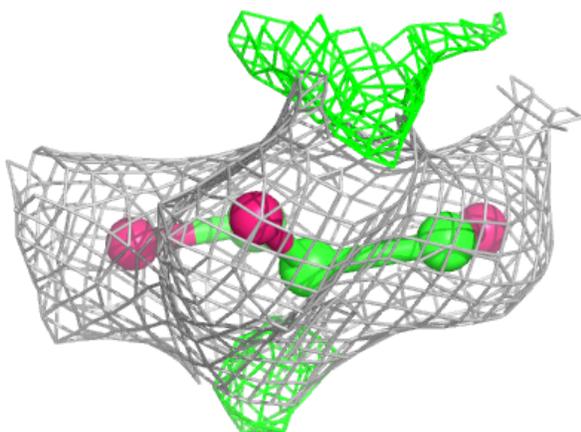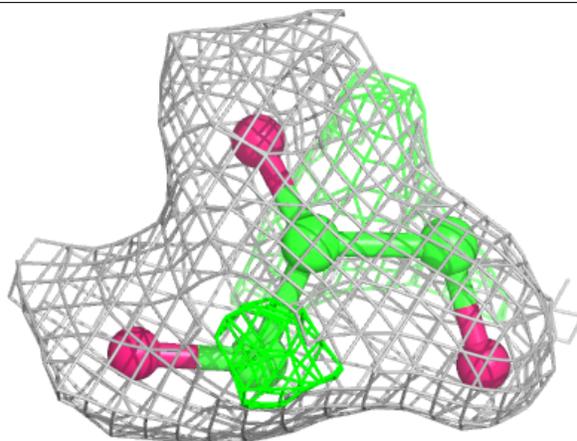
Electron density around MG B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
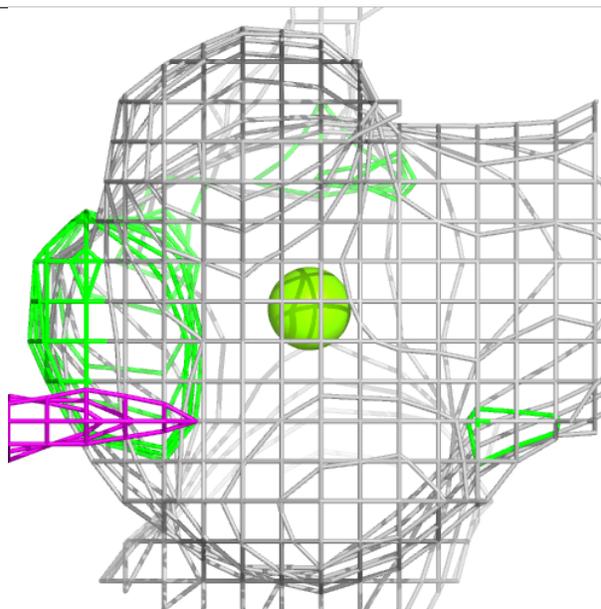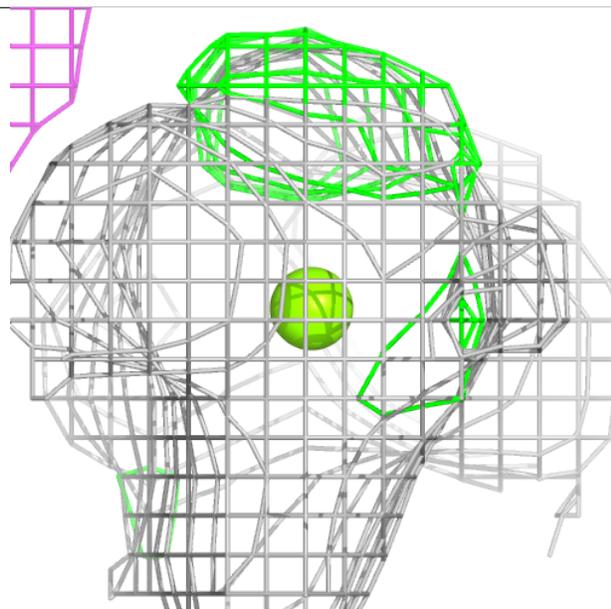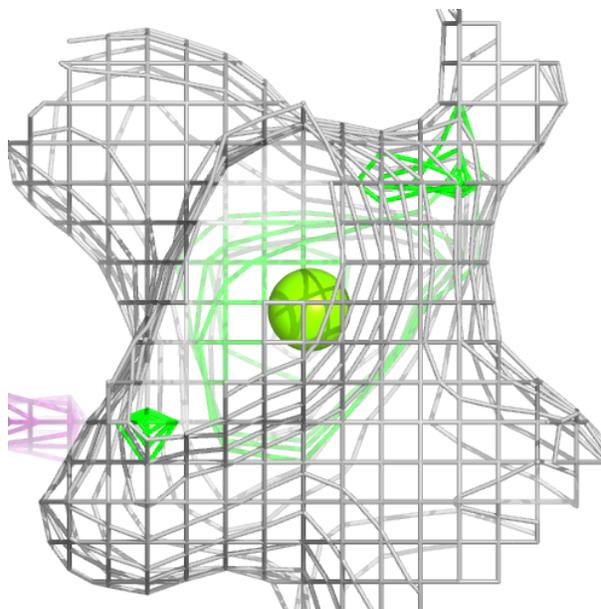
Electron density around PGE C 309:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
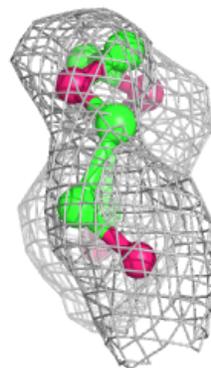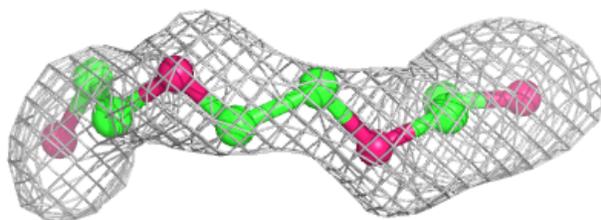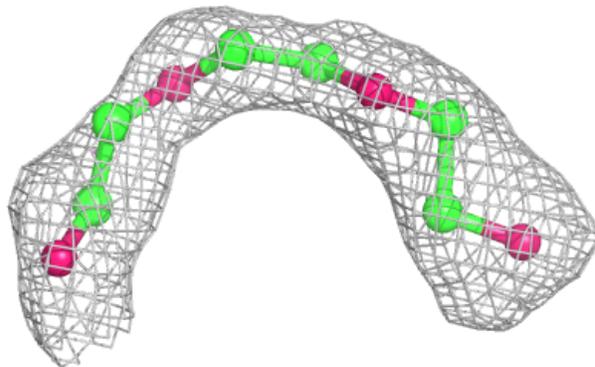
Electron density around EDO B 308:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
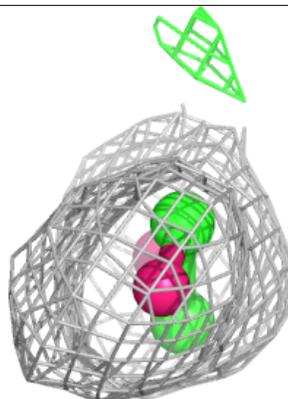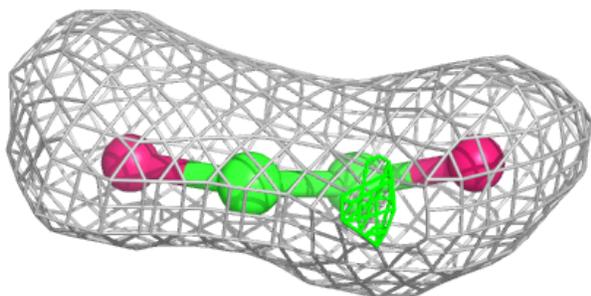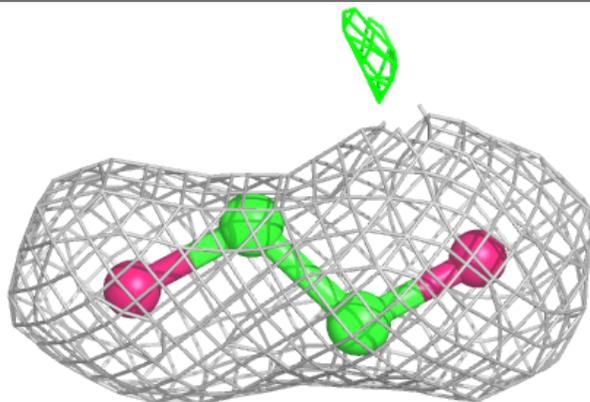
Electron density around PG4 E 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
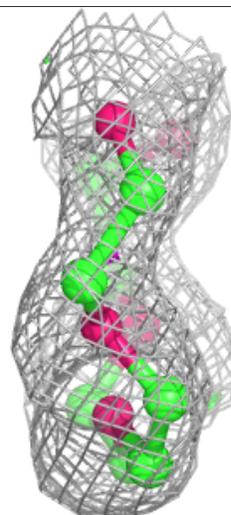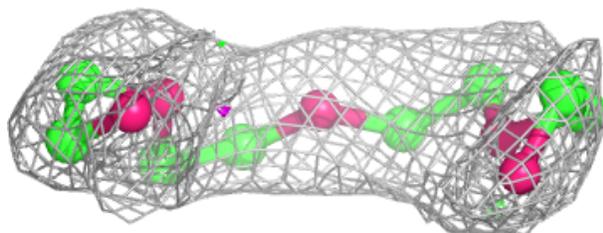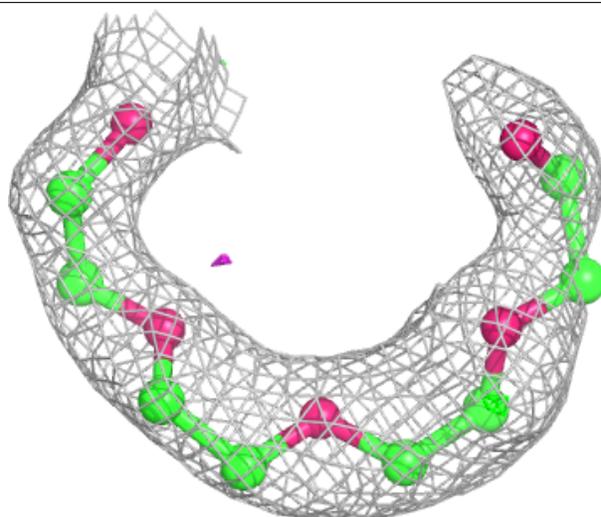
Electron density around EDO A 306:

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

Electron density around EDO 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 C 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
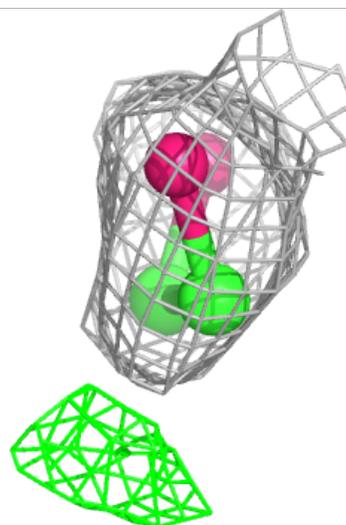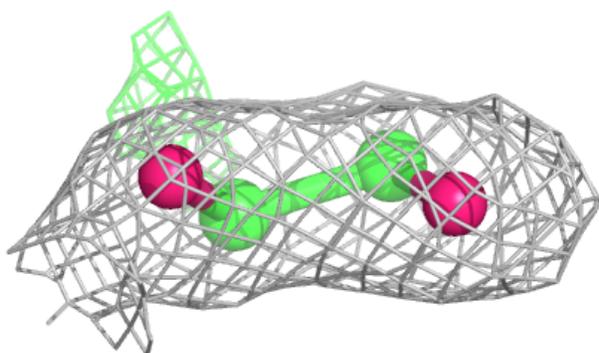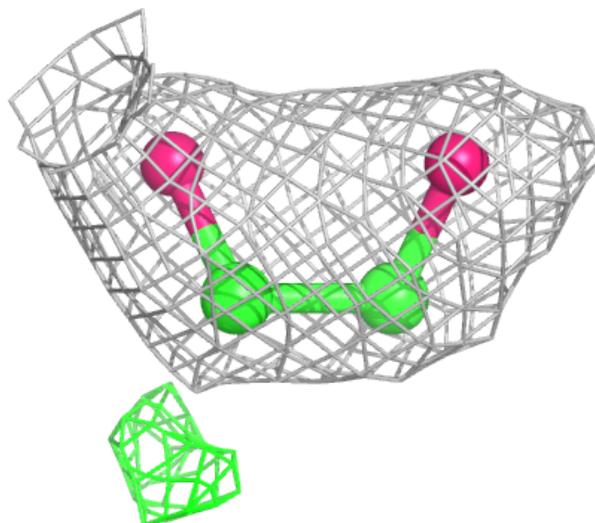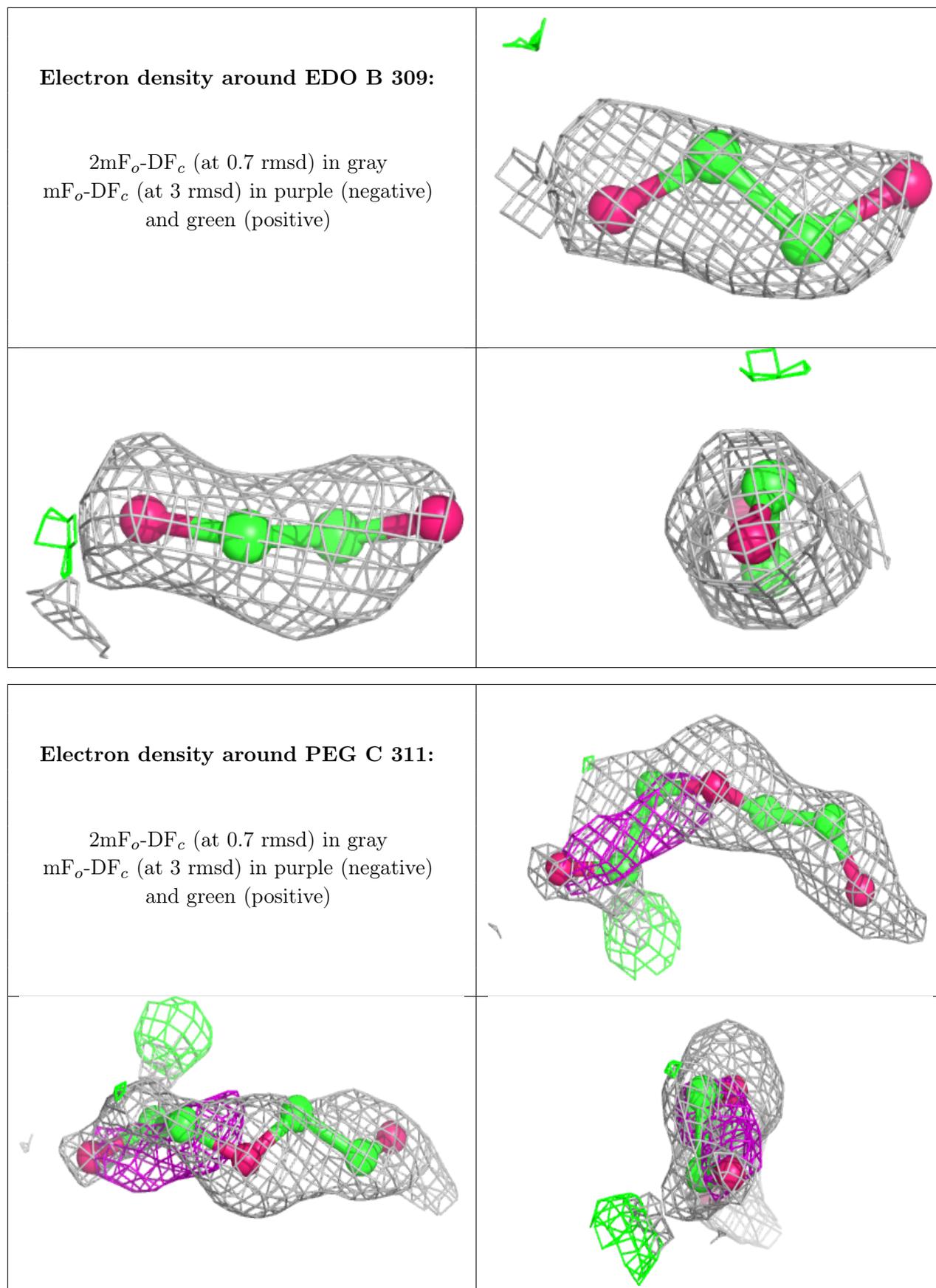
Electron density around EDO D 302:

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

Electron density around GOL C 312:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
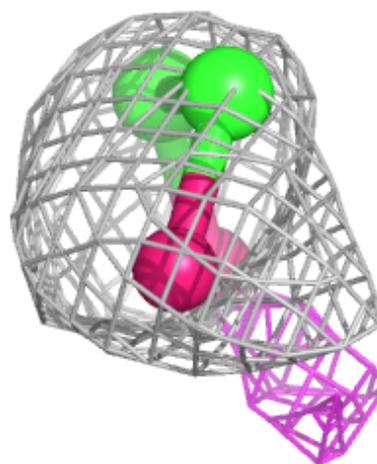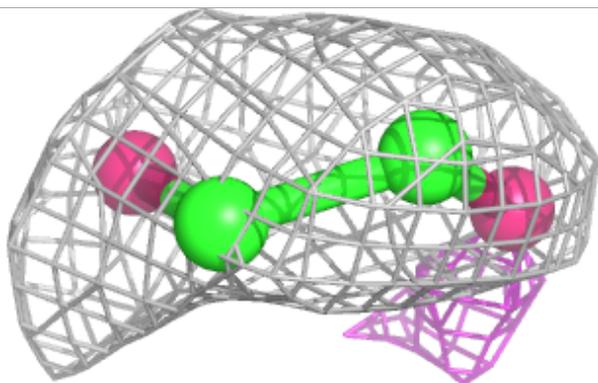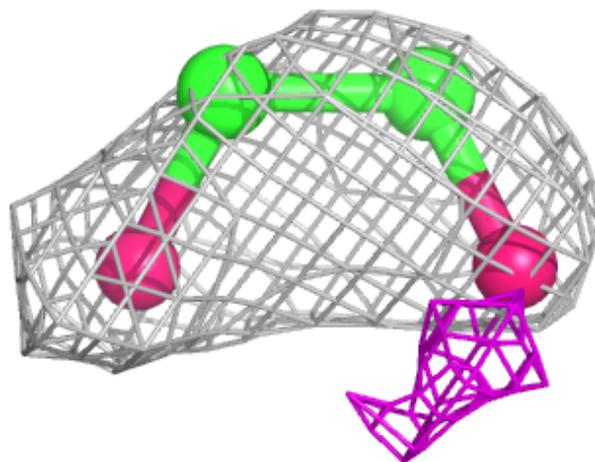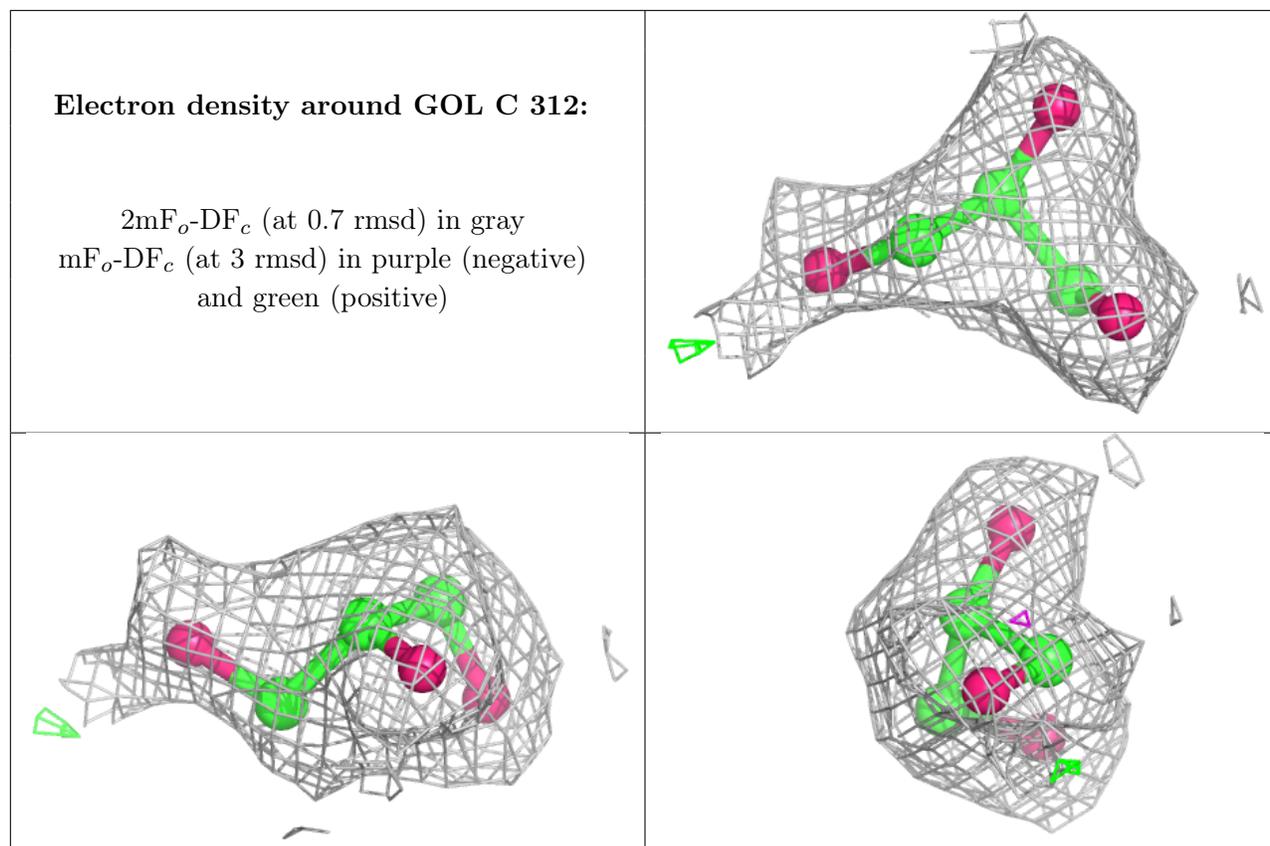
Electron density around MG F 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
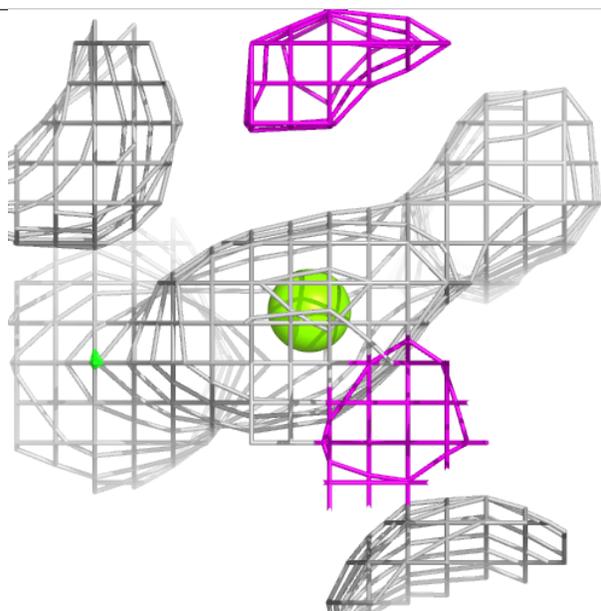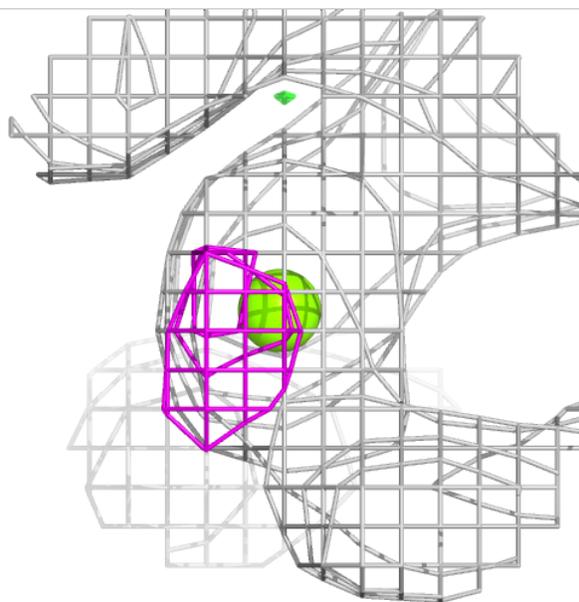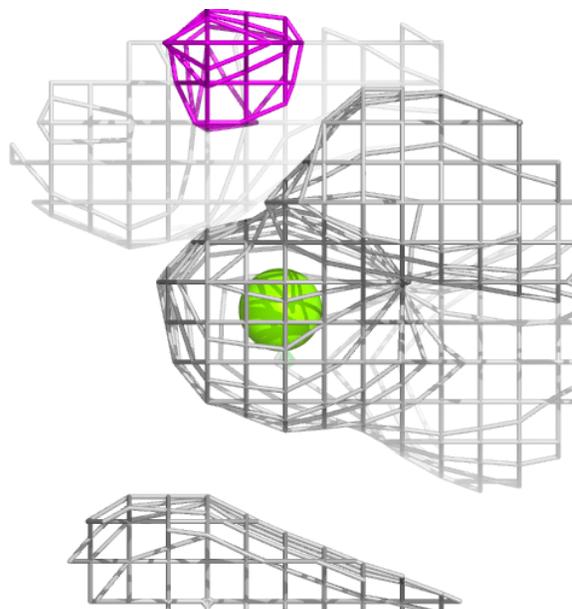
Electron density around PEG E 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
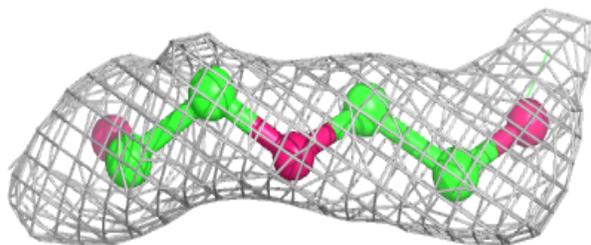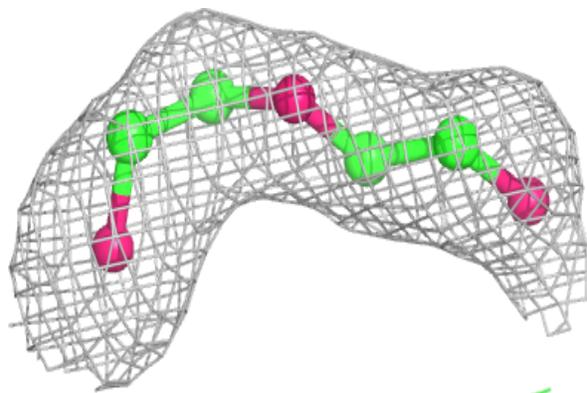
Electron density around MG E 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
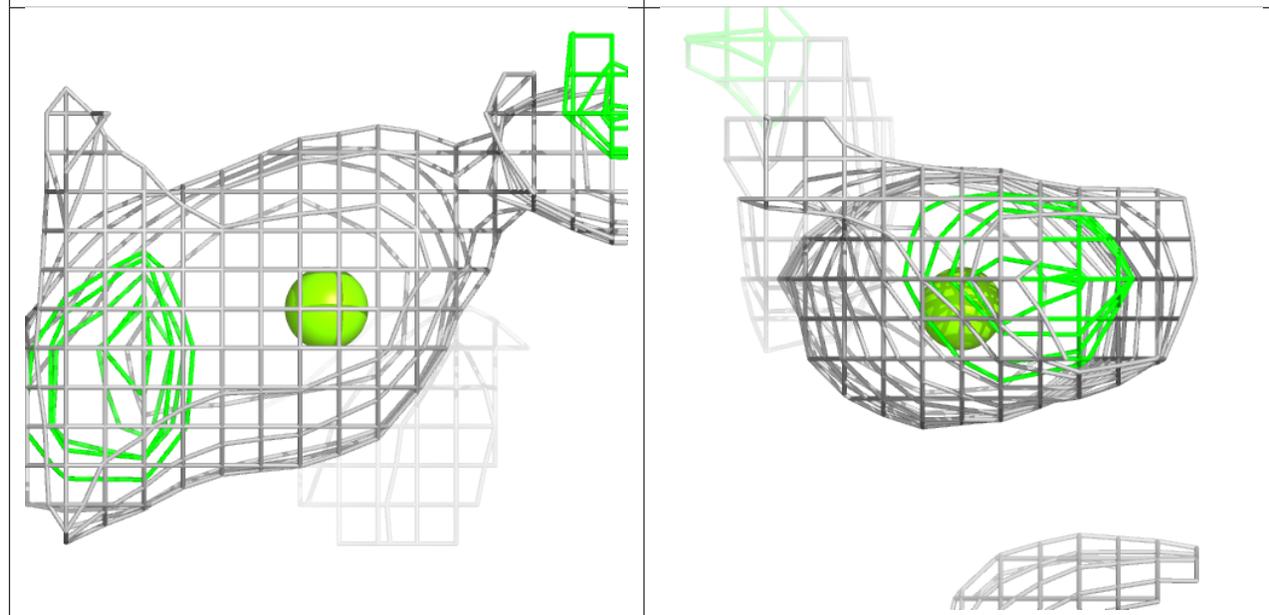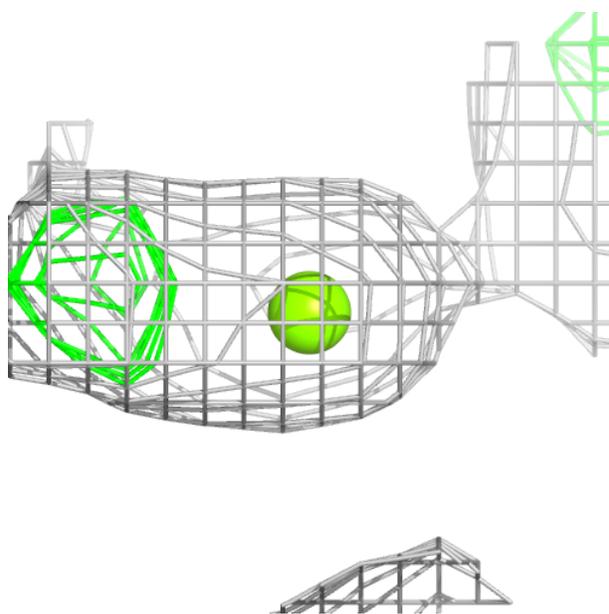
Electron density around ACT F 308:

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

Electron density around 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 B 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
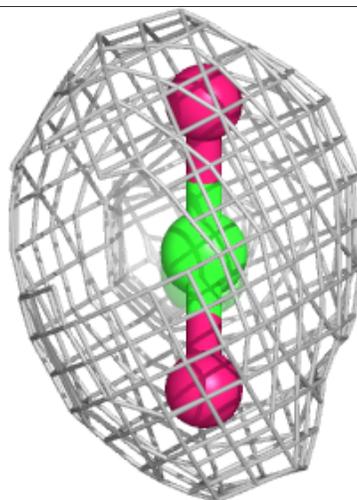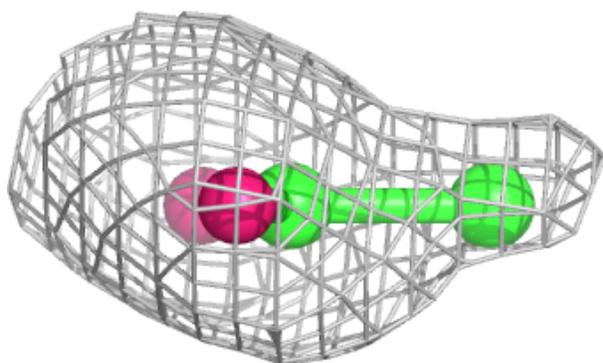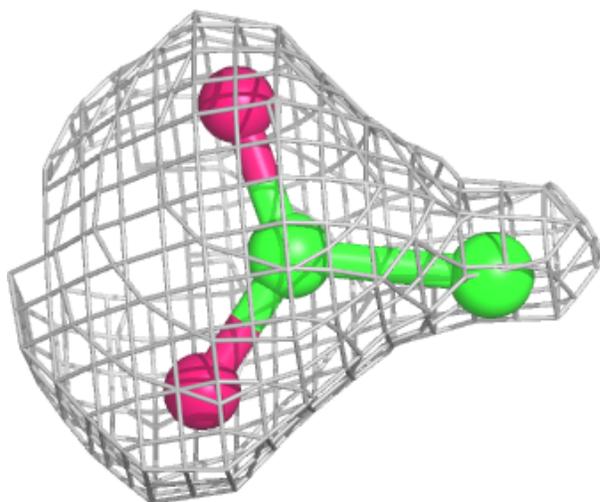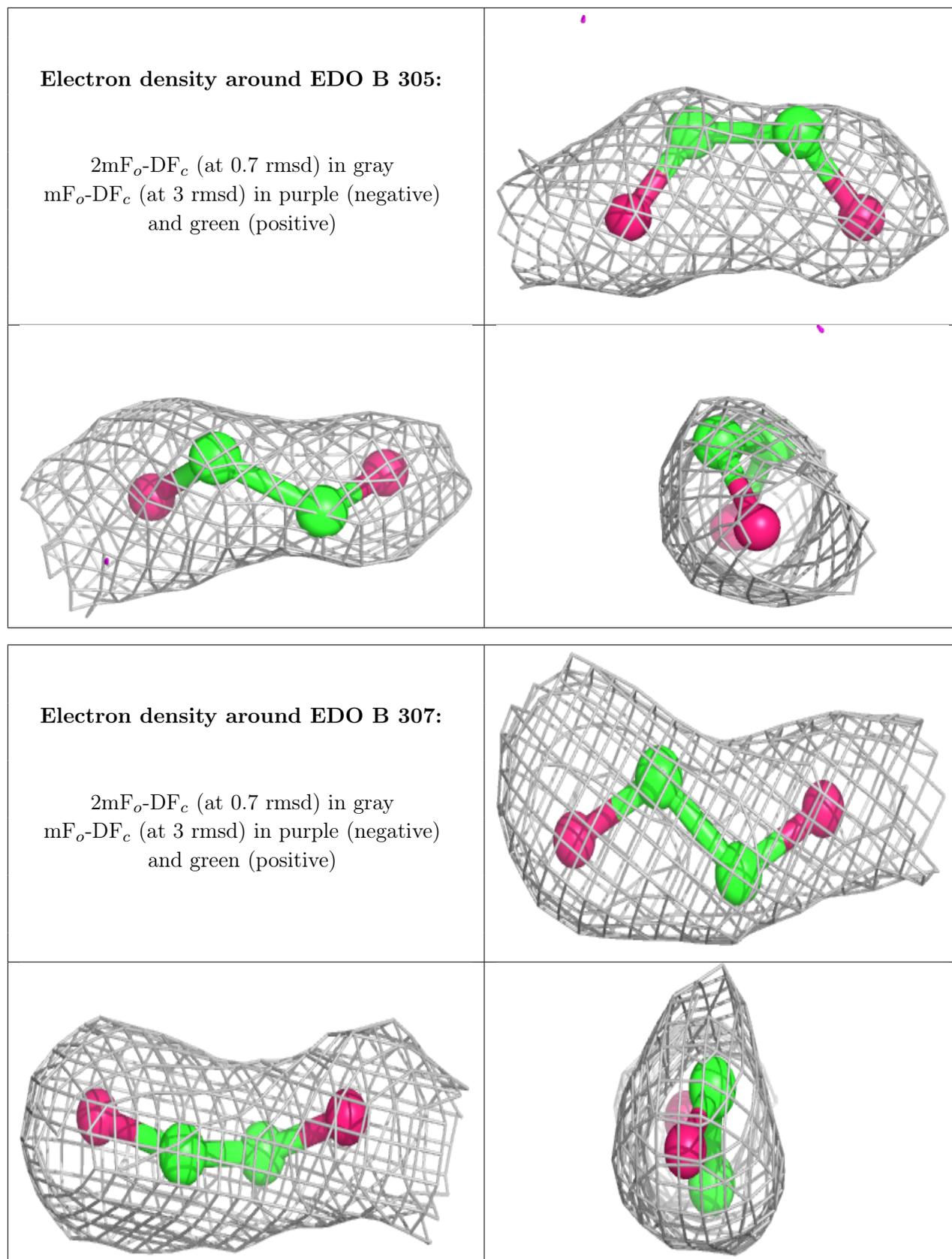
Electron density around EDO A 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
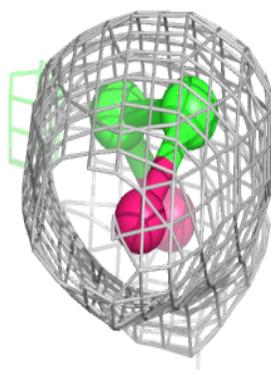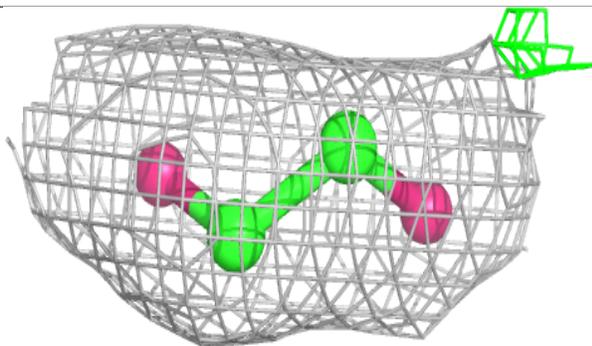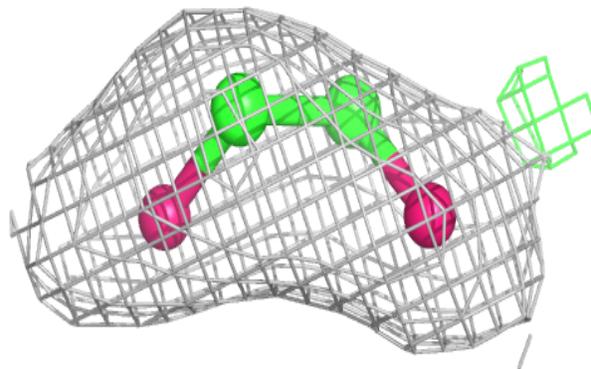
Electron density around ACT D 308:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
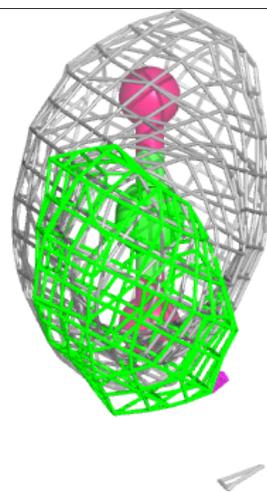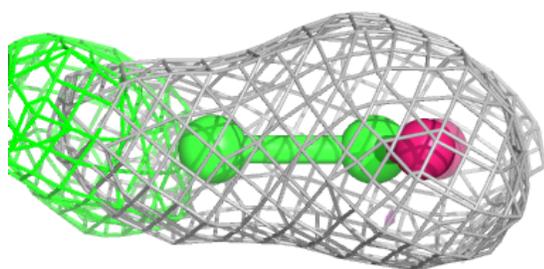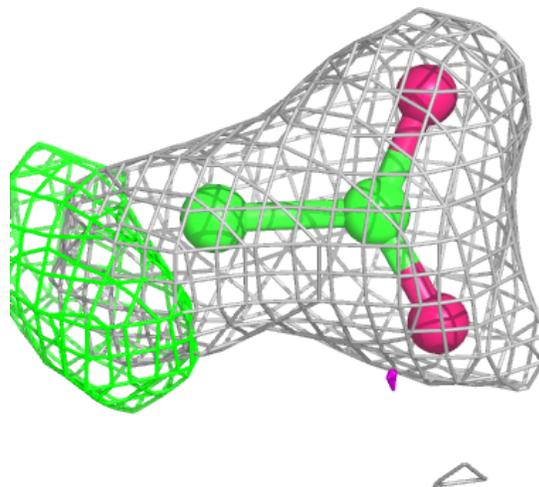
Electron density around ACT E 309:

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

Electron density around EDO D 303:

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

Electron density around PGE D 306:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
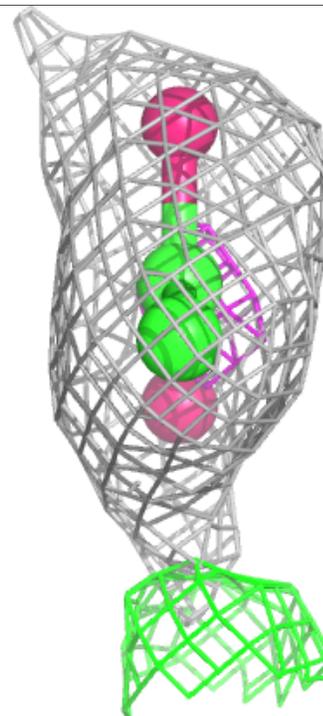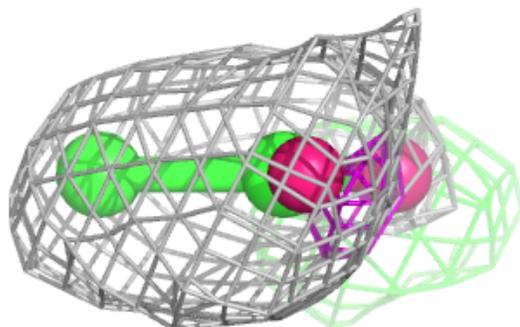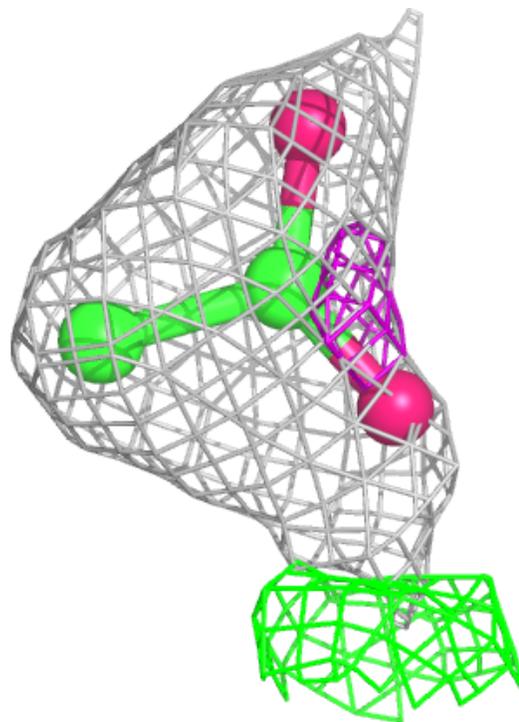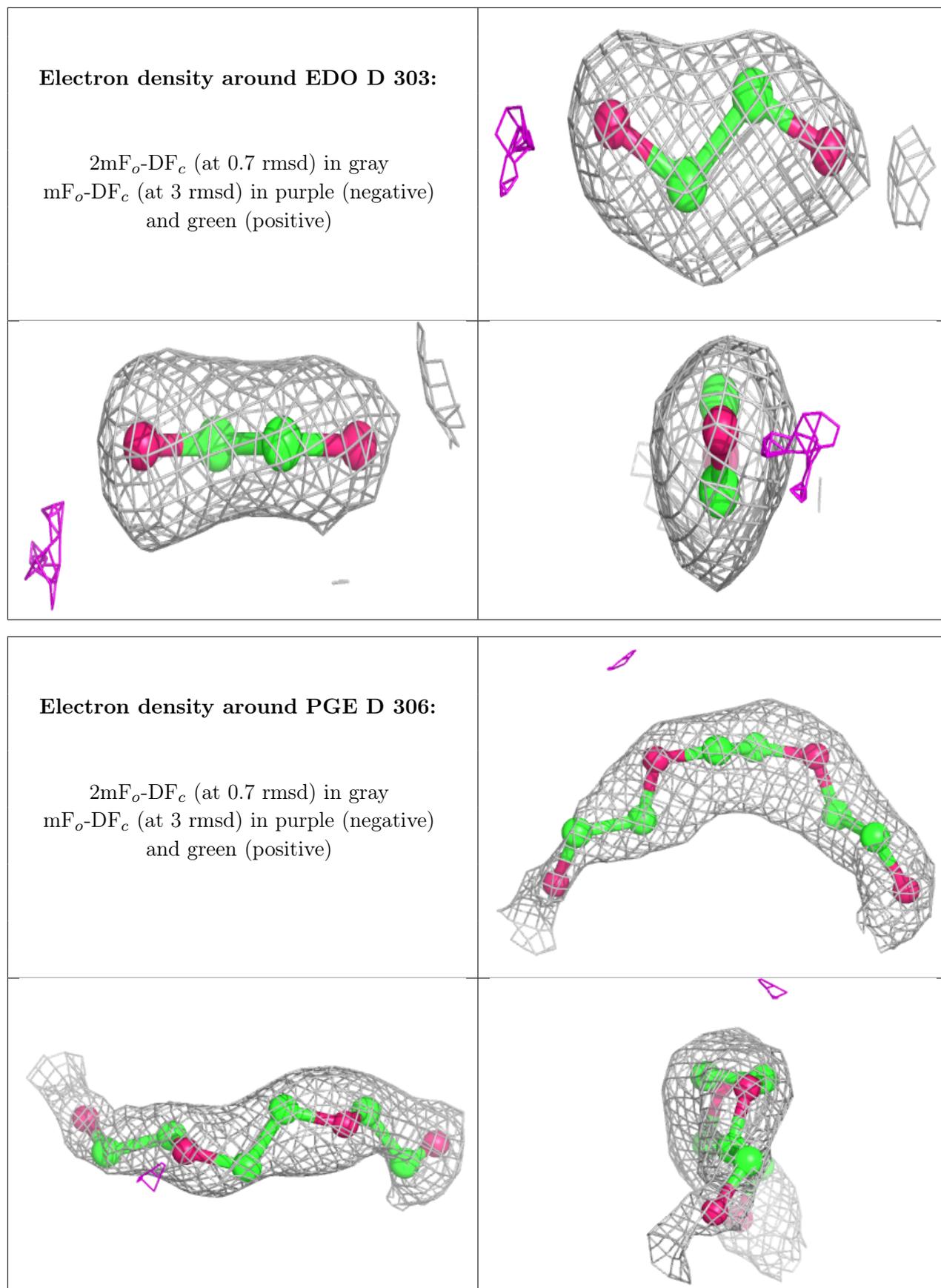
Electron density around ACT B 310:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
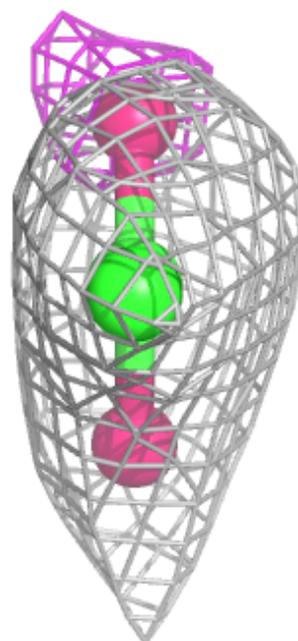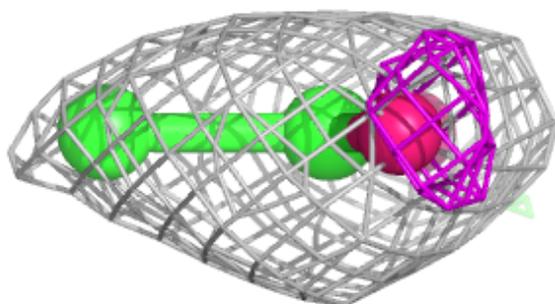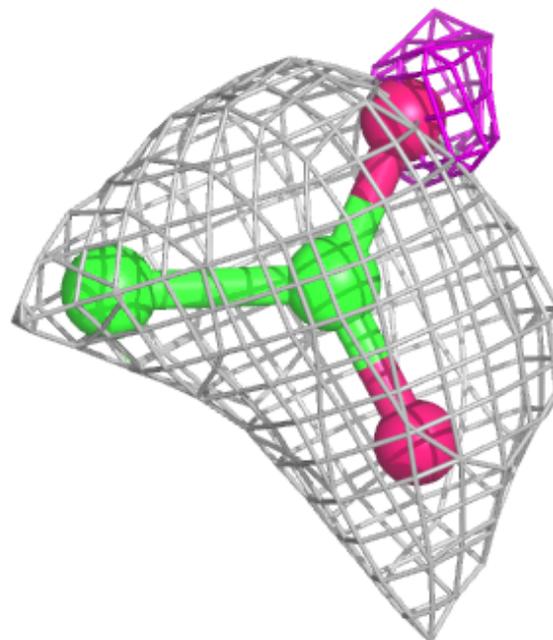
Electron density around GOL A 314:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
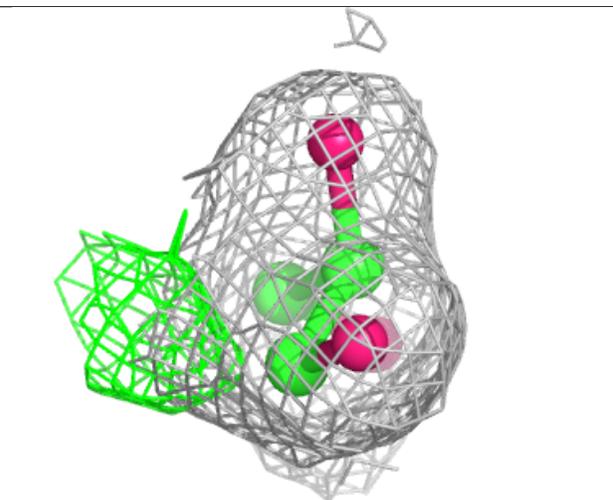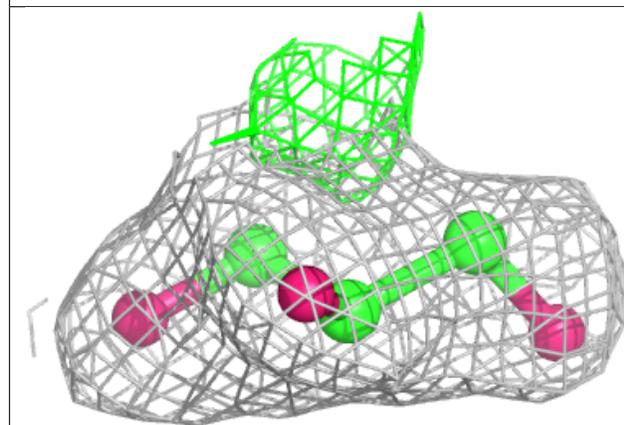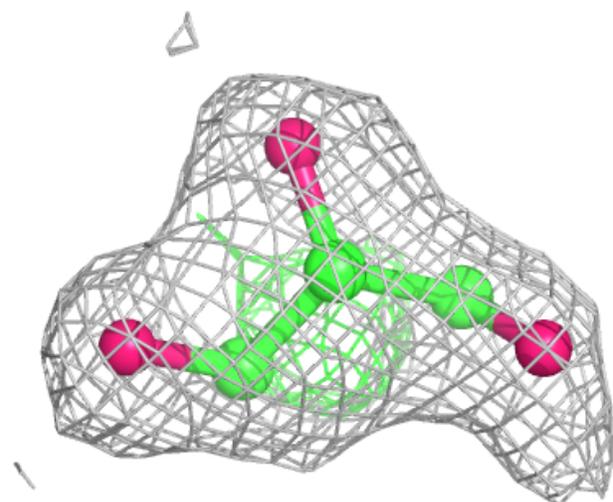
Electron density around GOL B 312:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
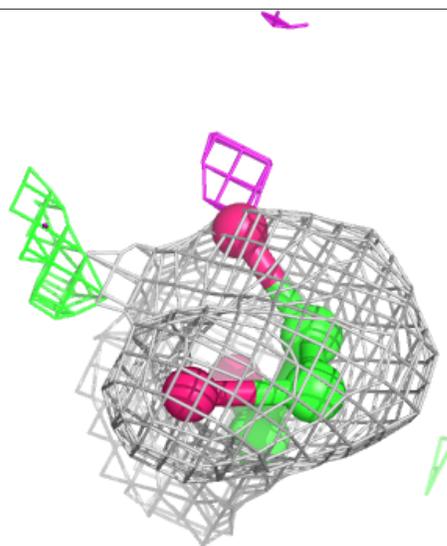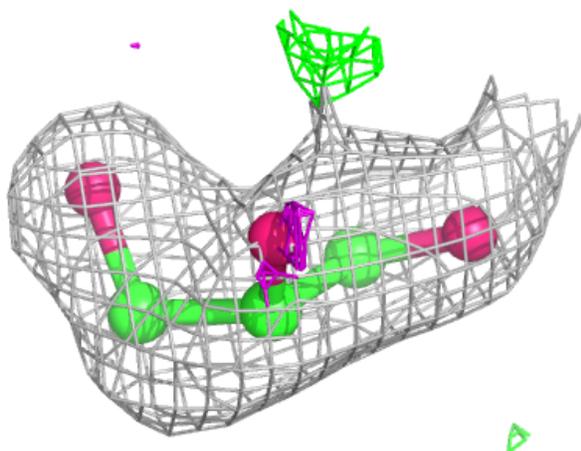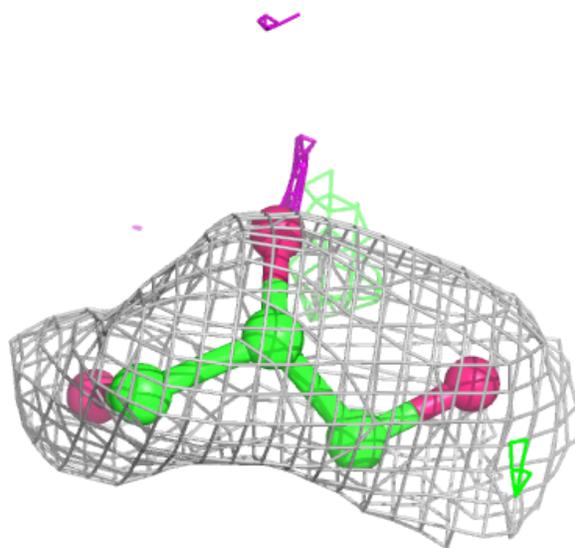
Electron density around PG4 B 301:

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

Electron density around PEG A 312:

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

Electron density around EDO F 304:

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

**Electron density around EDO C 308:**

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

Electron density around EDO E 307:

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

Electron density around ACT 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)
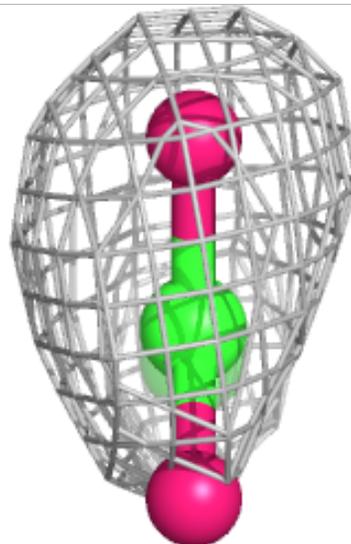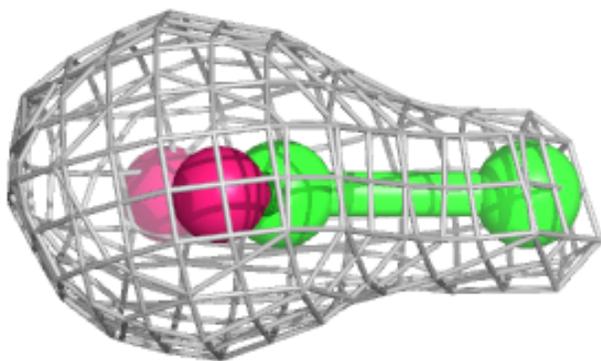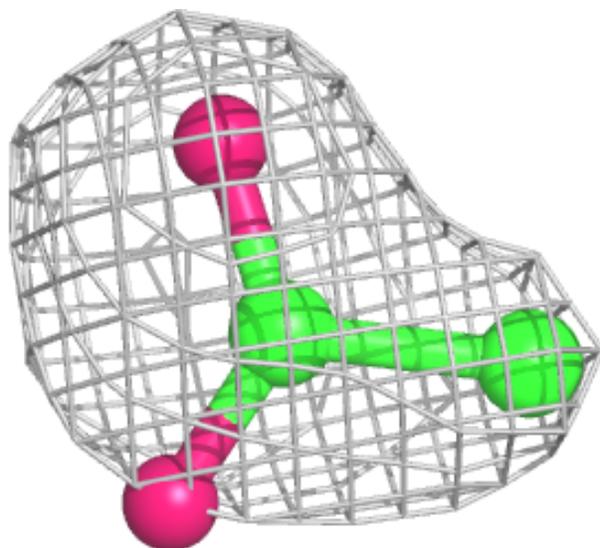
Electron density around PGE F 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
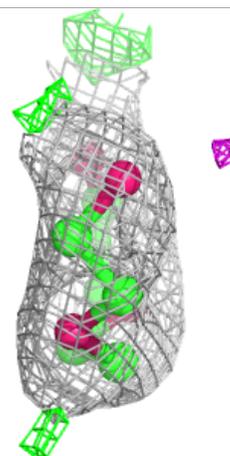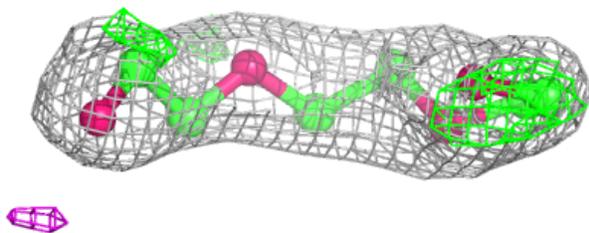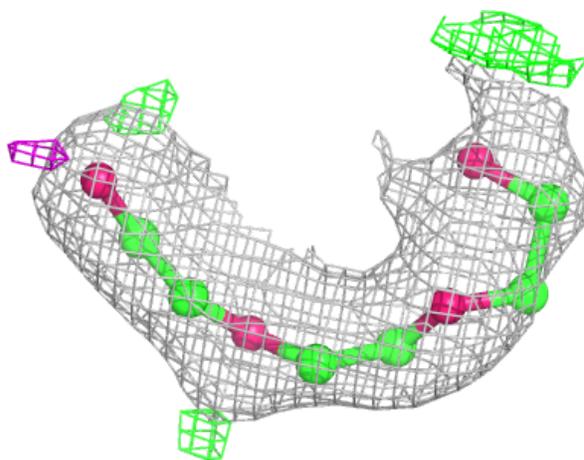
Electron density around PG4 A 301:

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 EDO B 306:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
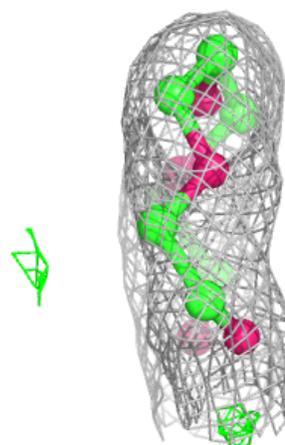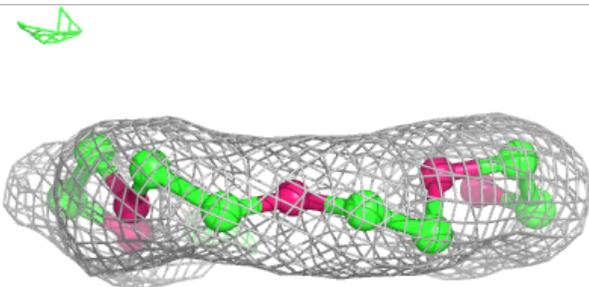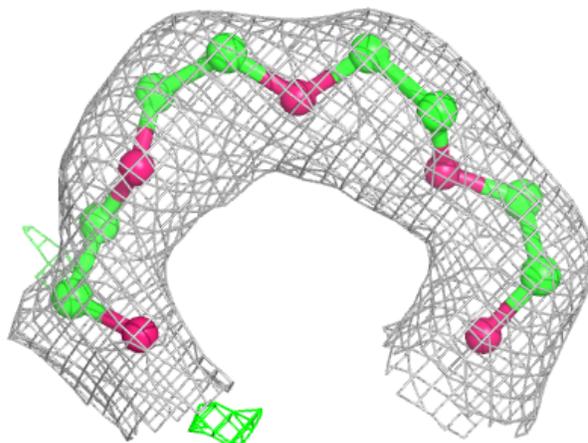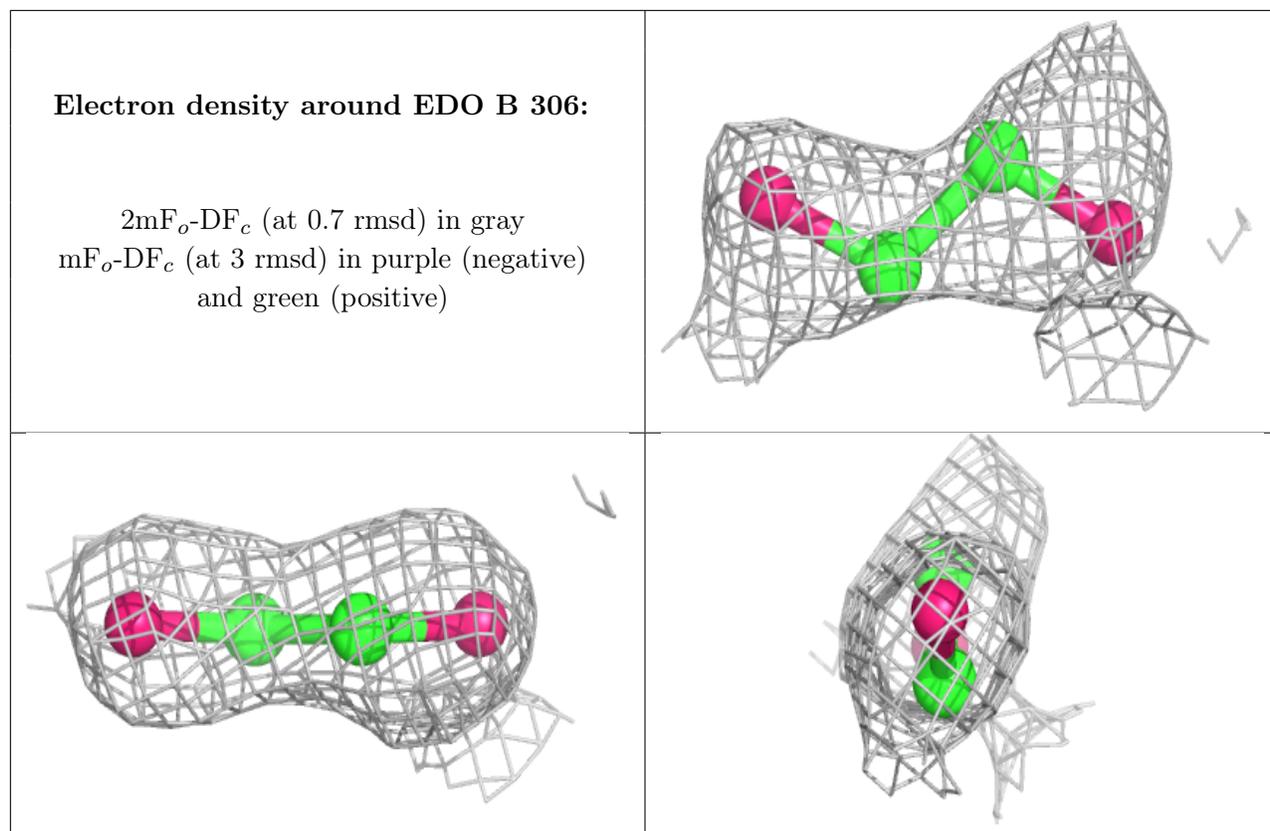
Electron density around PG4 C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
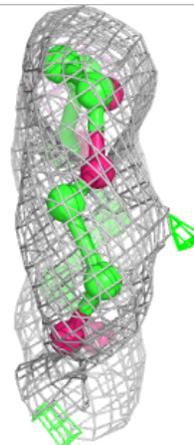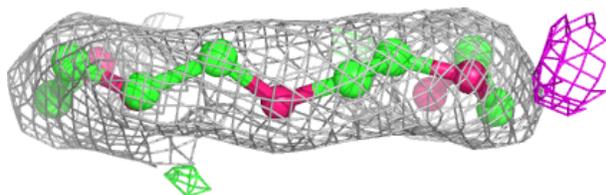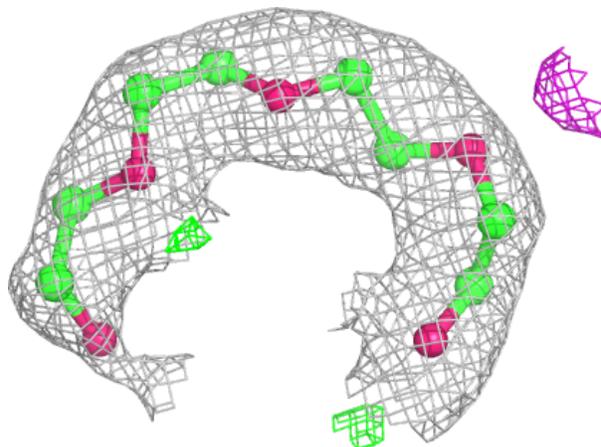
Electron density around MG F 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
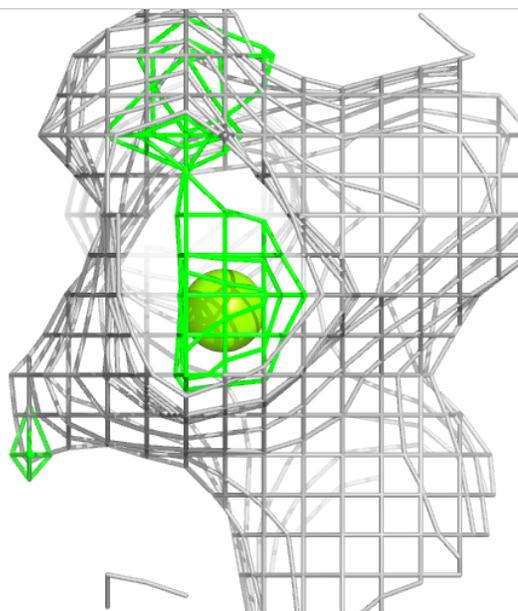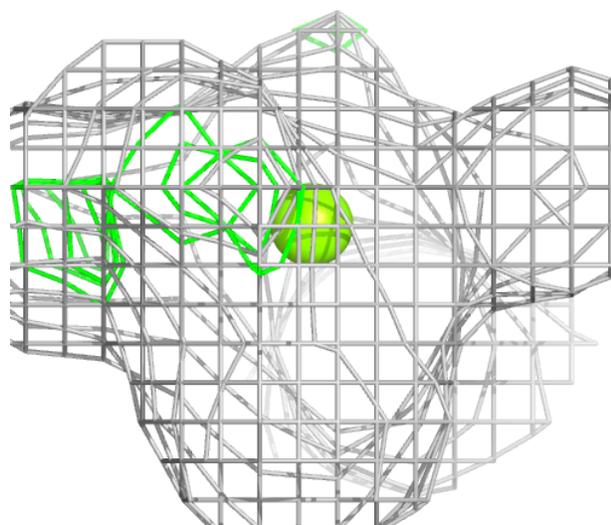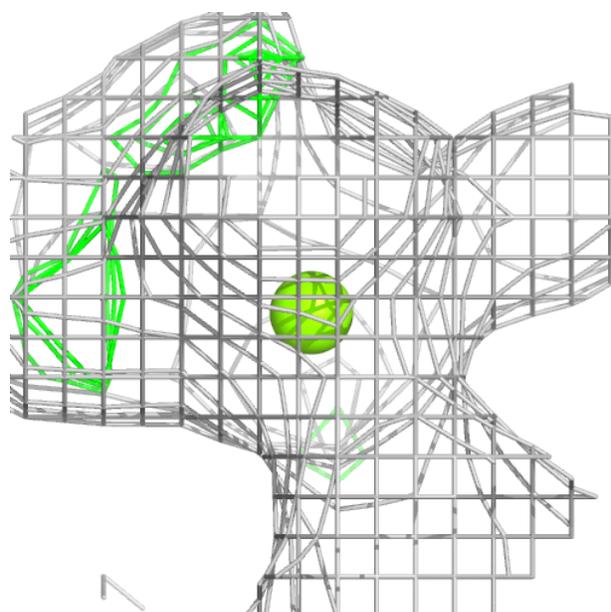
Electron density around EDO C 306:

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

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 D 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
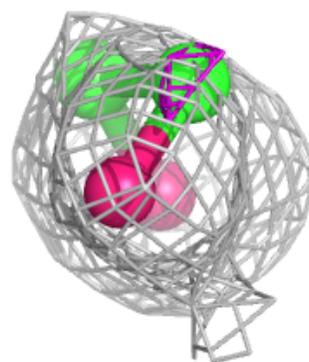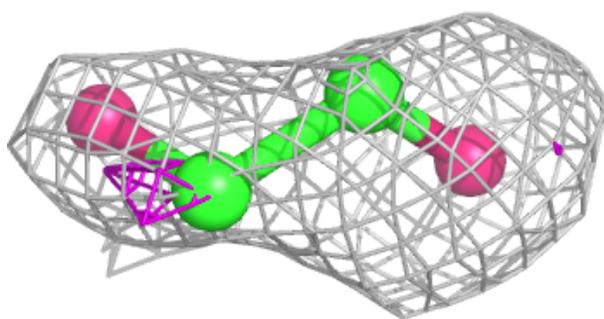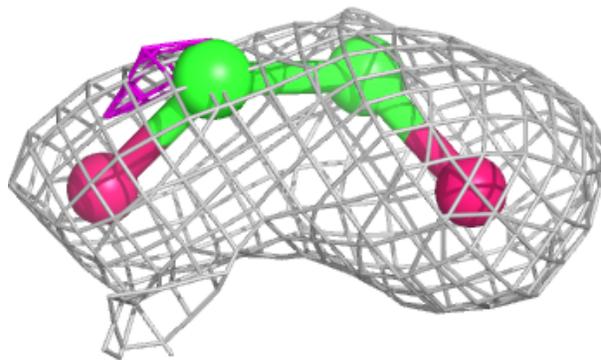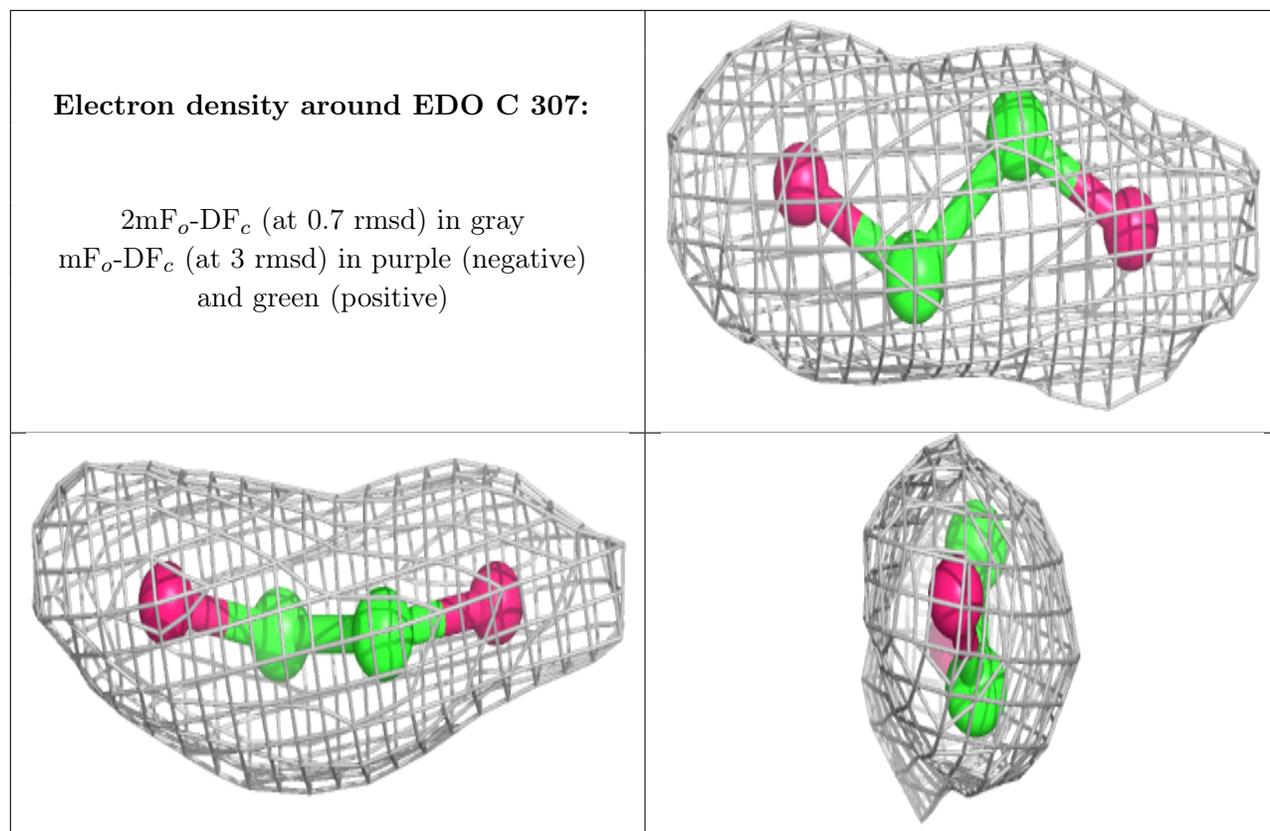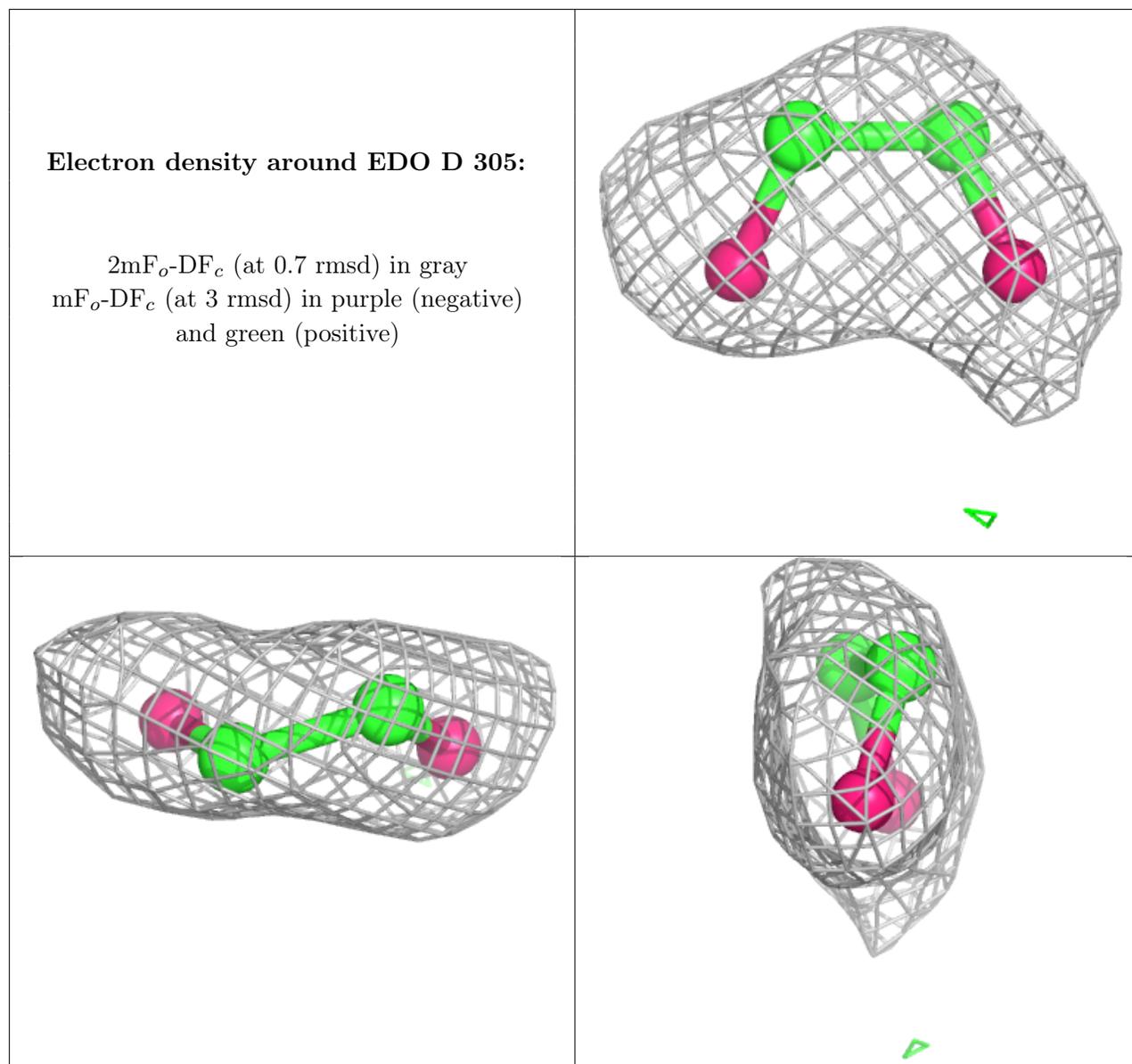
Electron density around EDO E 304:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
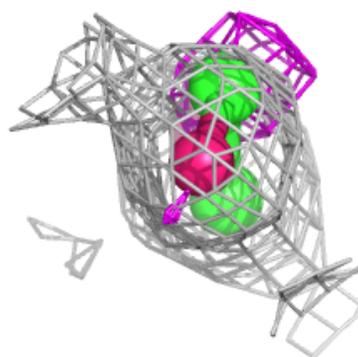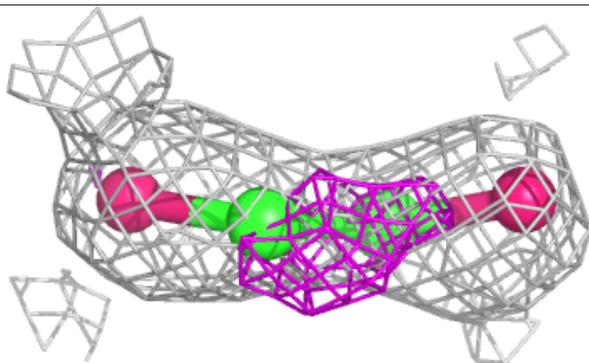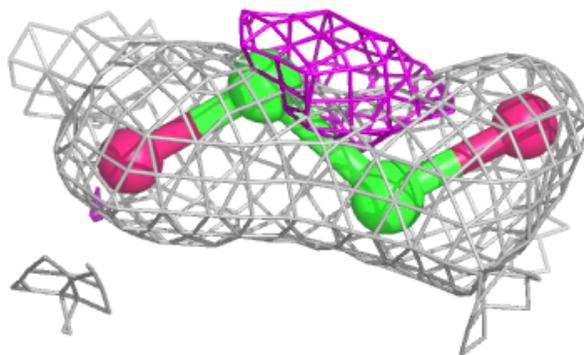
Electron density around ACT D 307:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
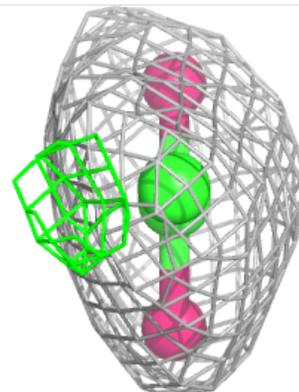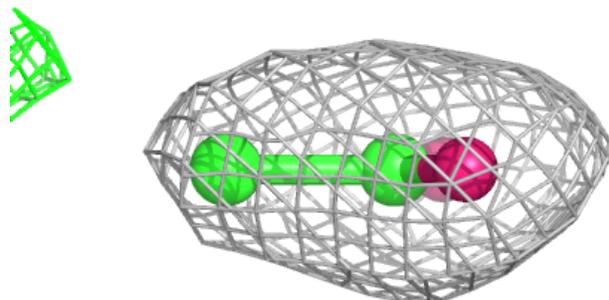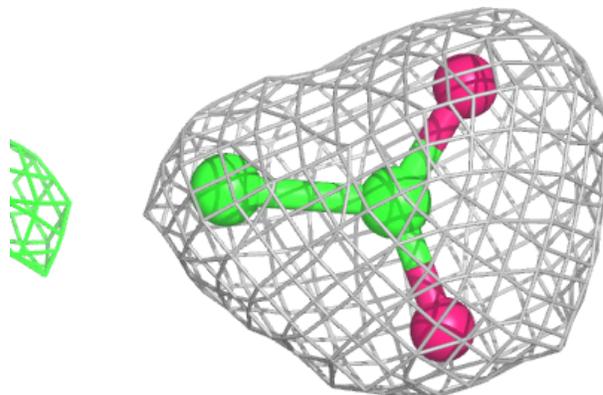
Electron density around MG A 304:

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

Electron density around EDO 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 D 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
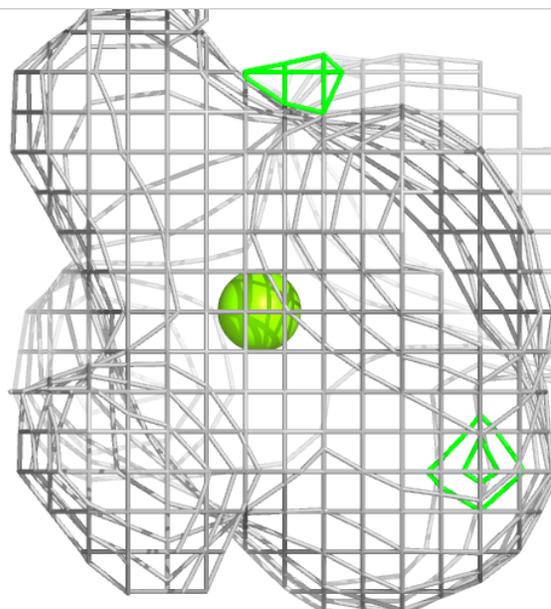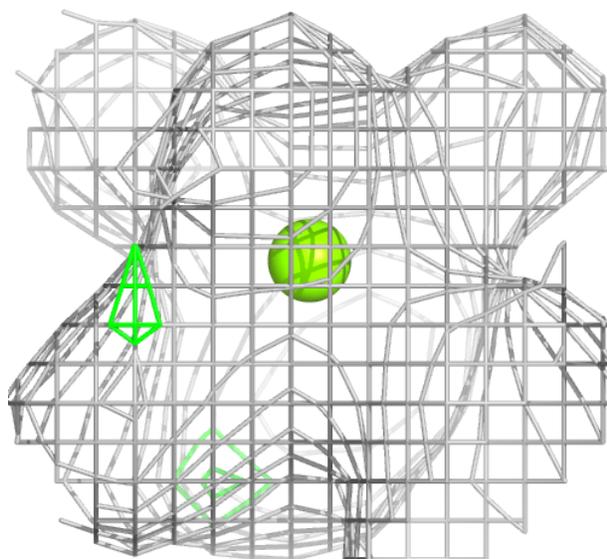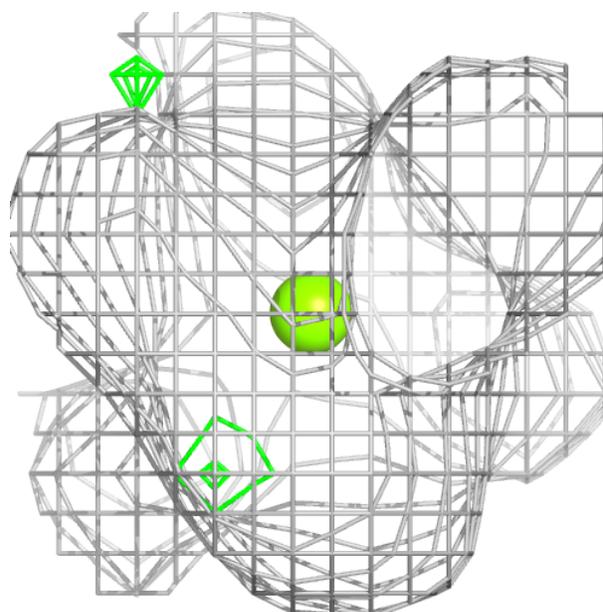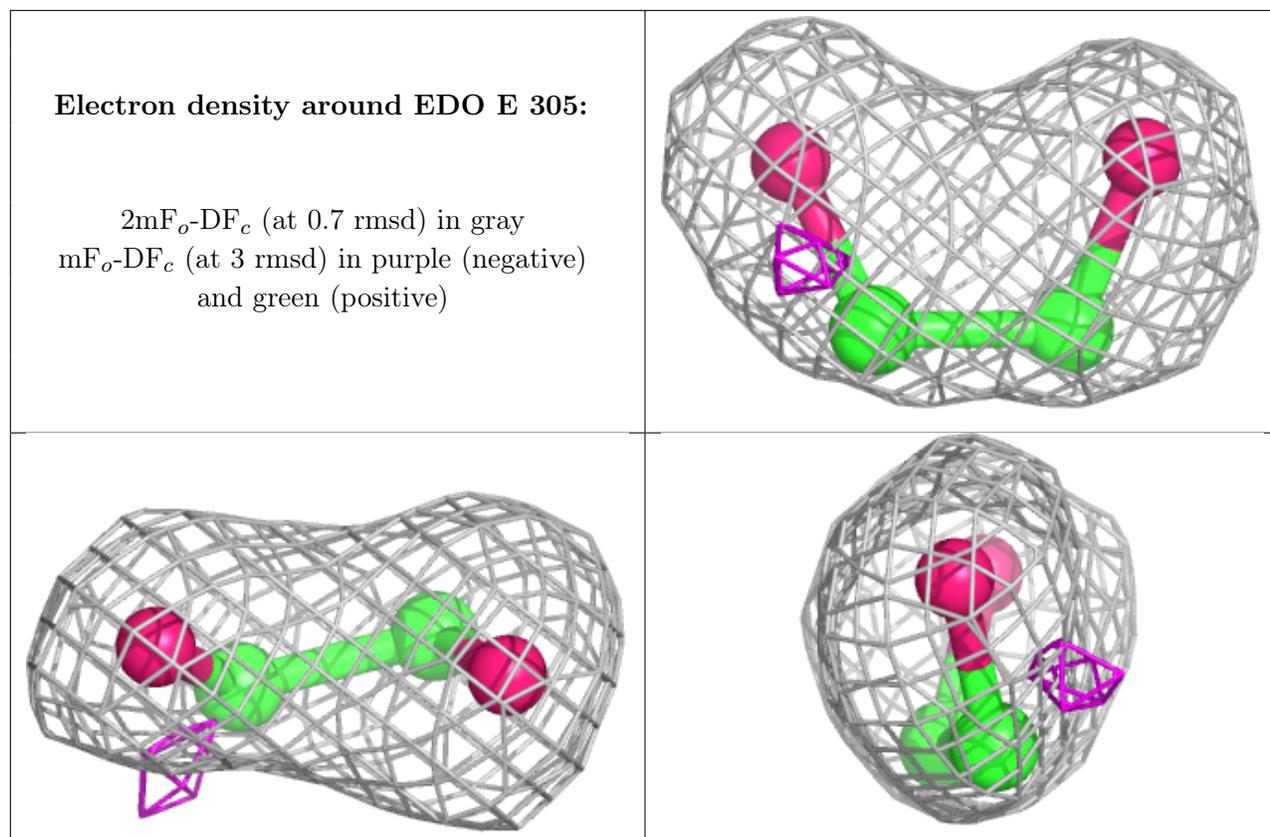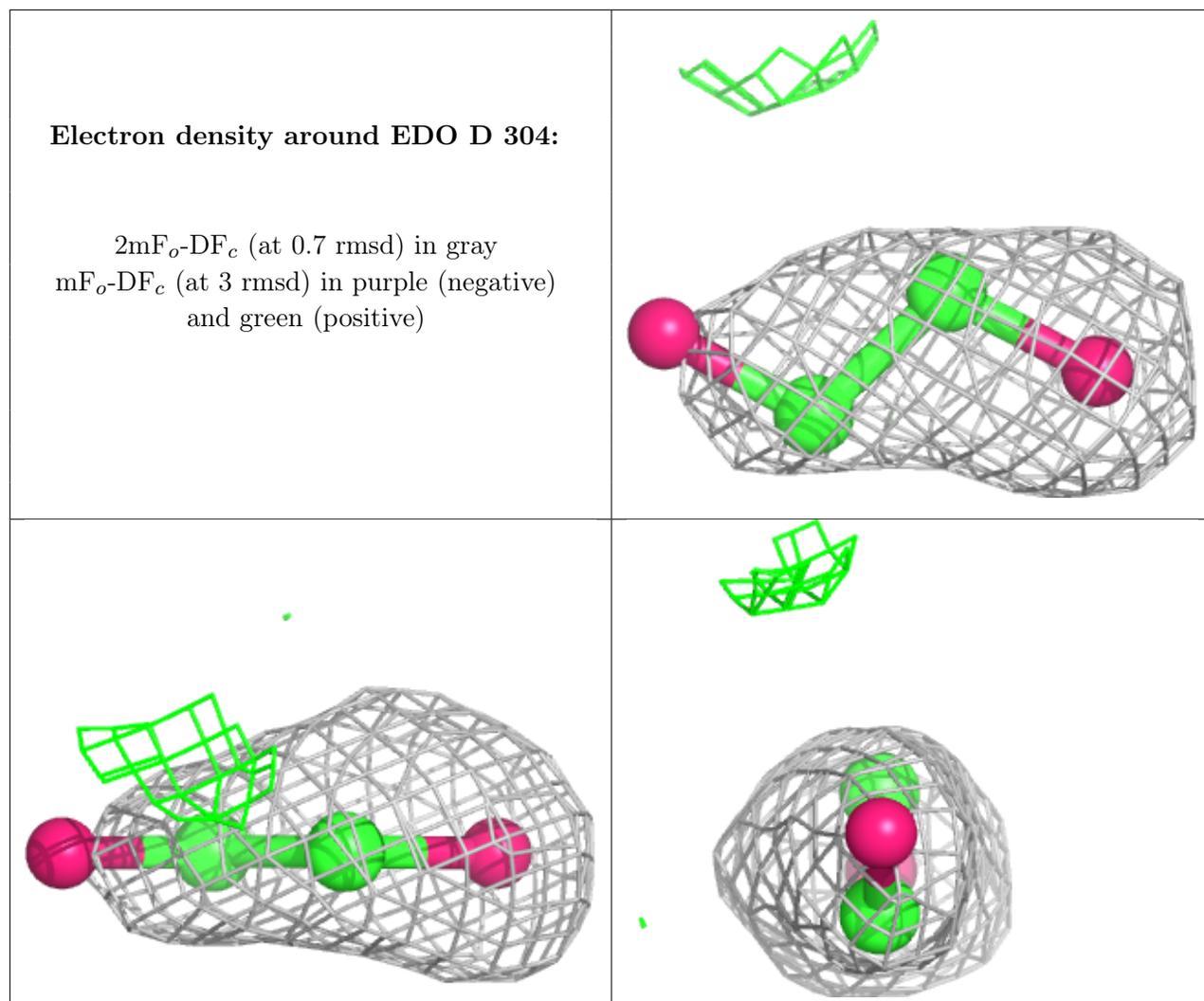
Electron density around EDO A 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
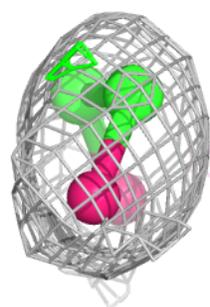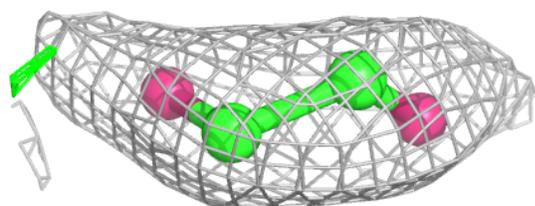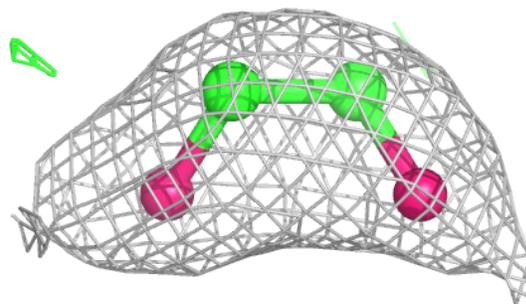
Electron density around EDO C 304:

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

Electron density around EDO C 305:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
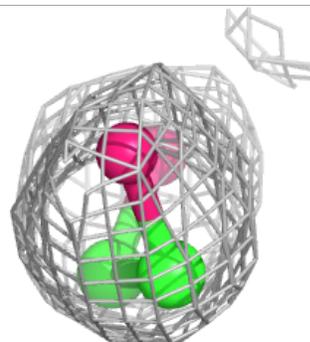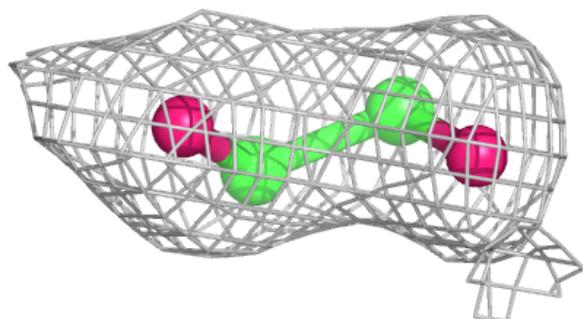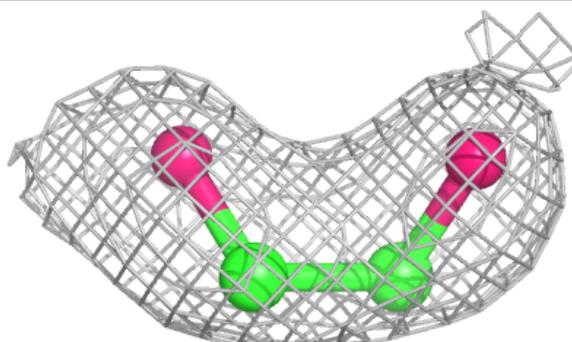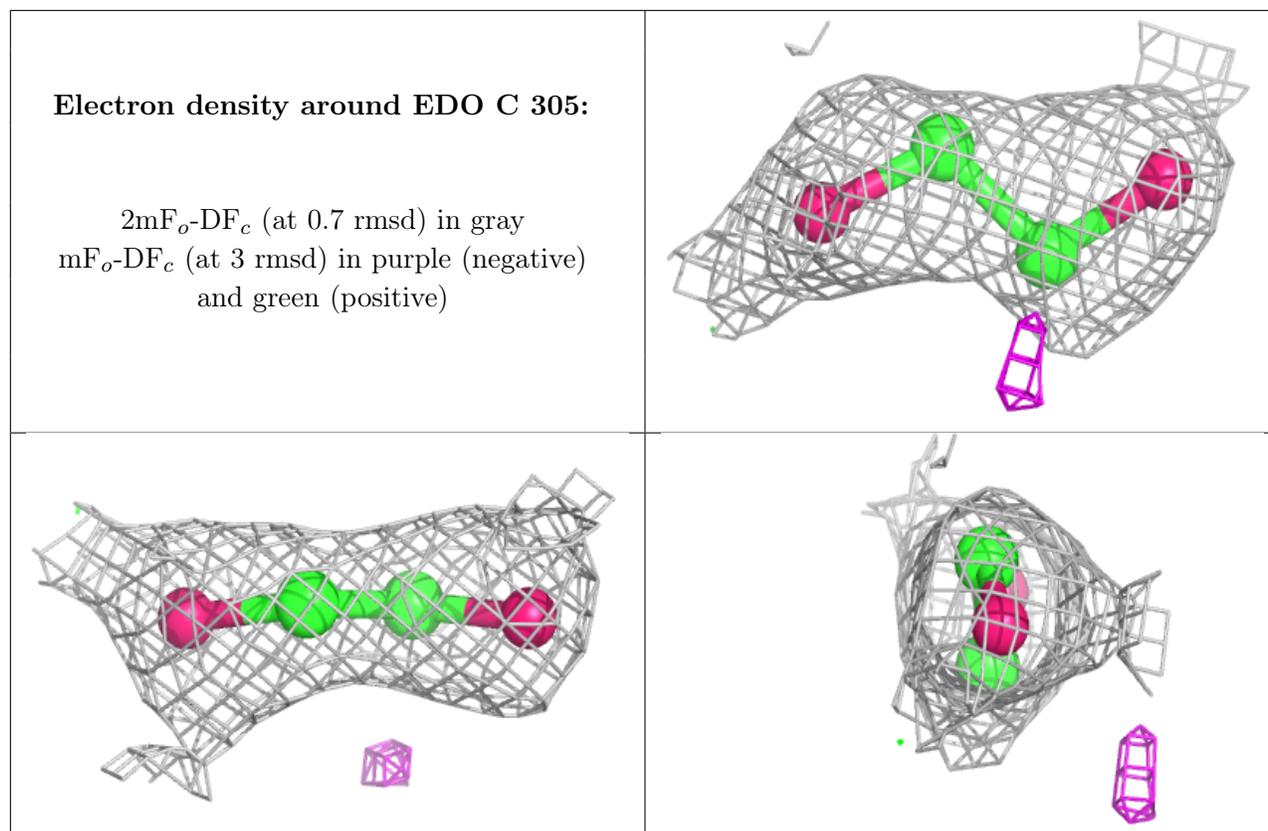
Electron density around EDO E 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
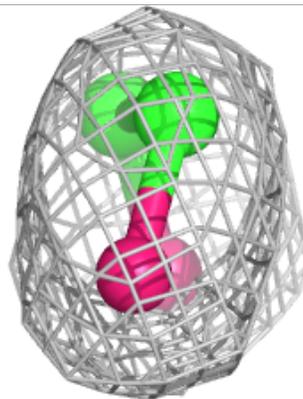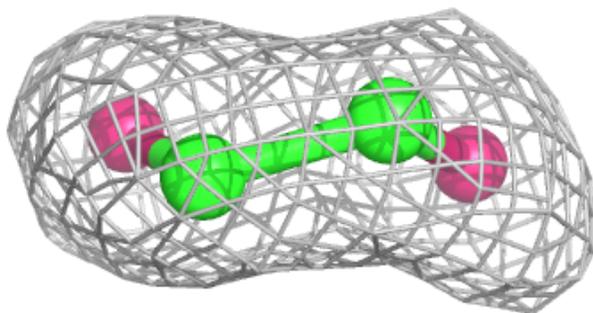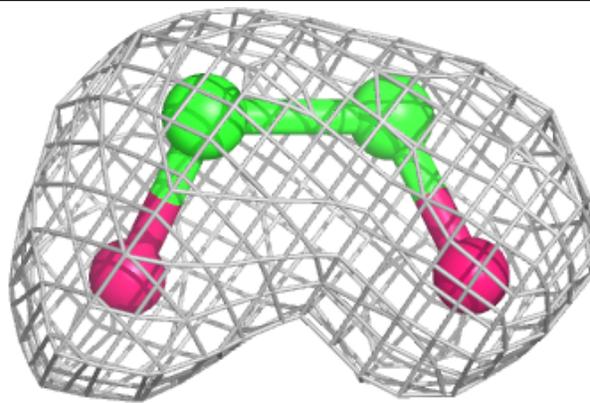
Electron density around ACT F 309:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
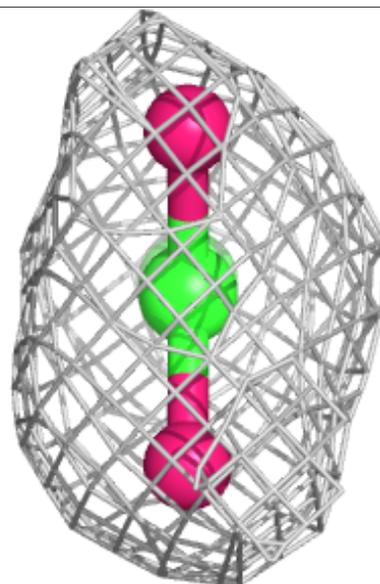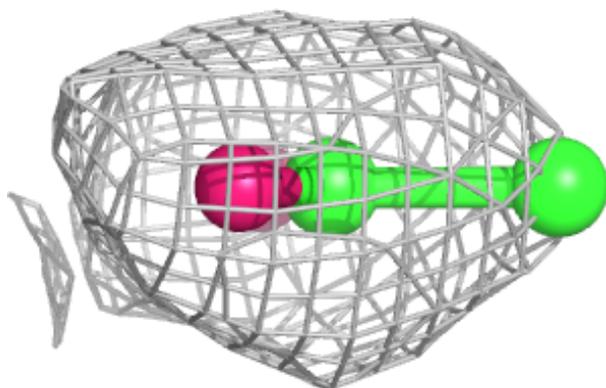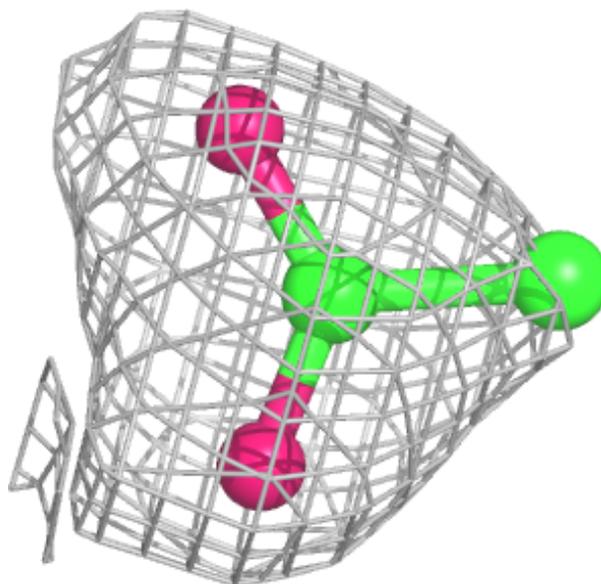
Electron density around MG A 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
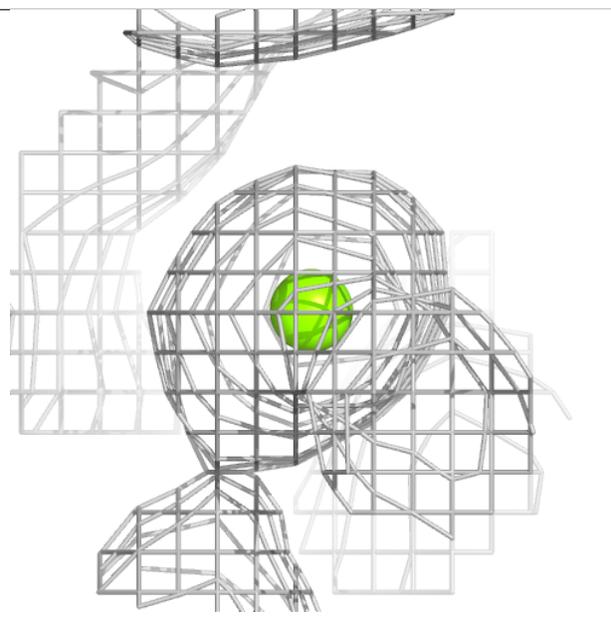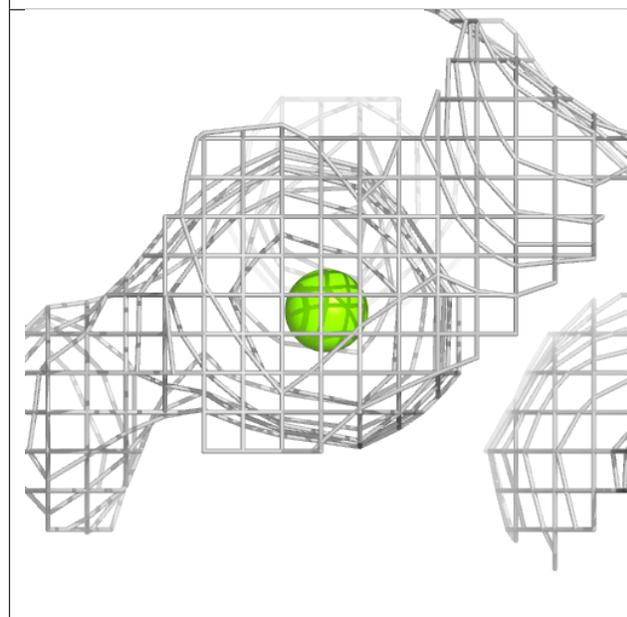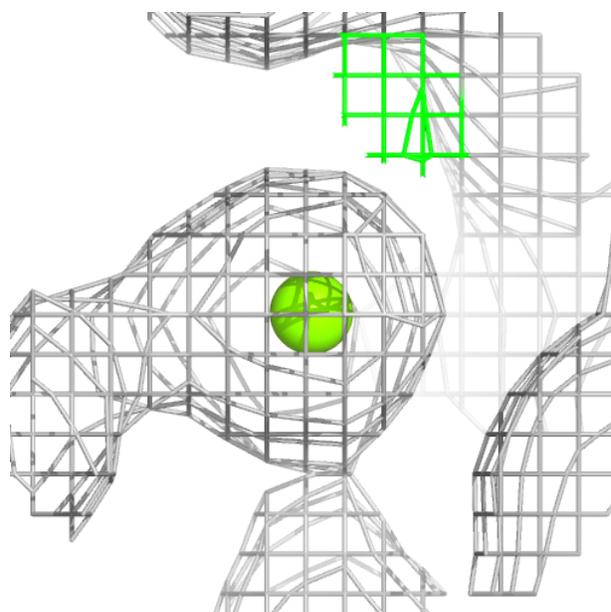
Electron density around EDO F 305:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
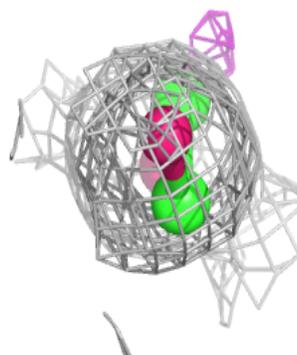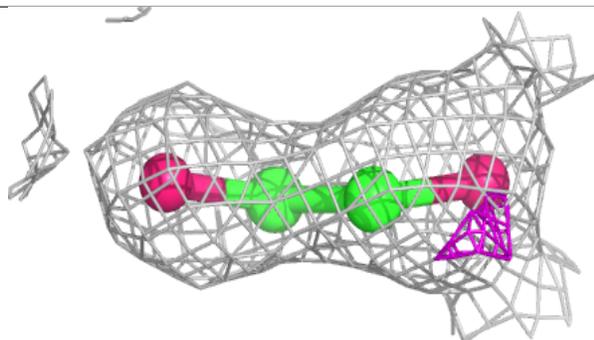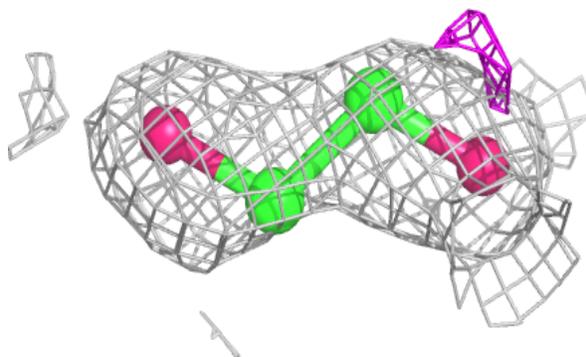
Electron density around EDO B 304:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
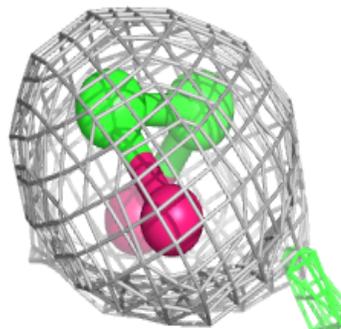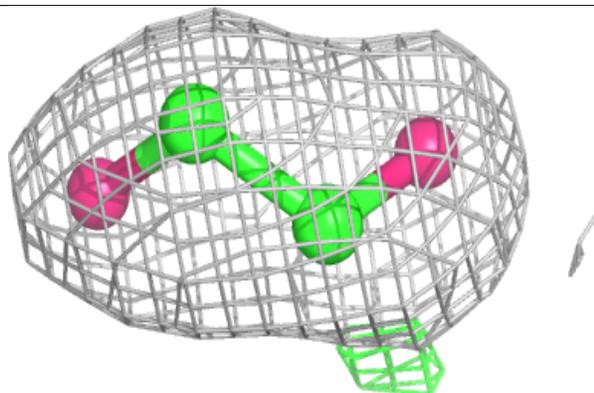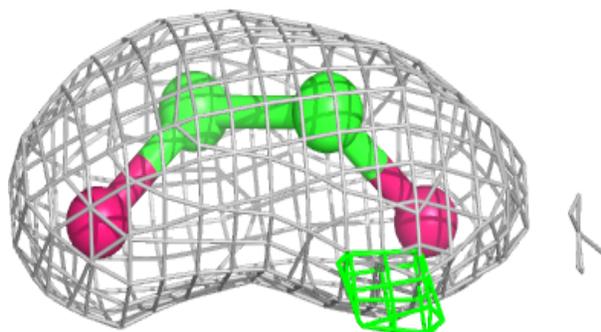
Electron density around EDO F 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
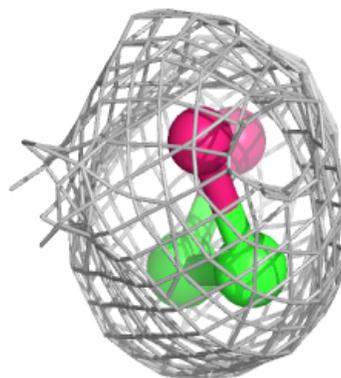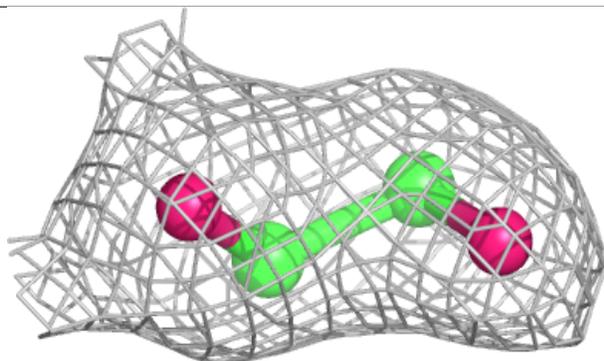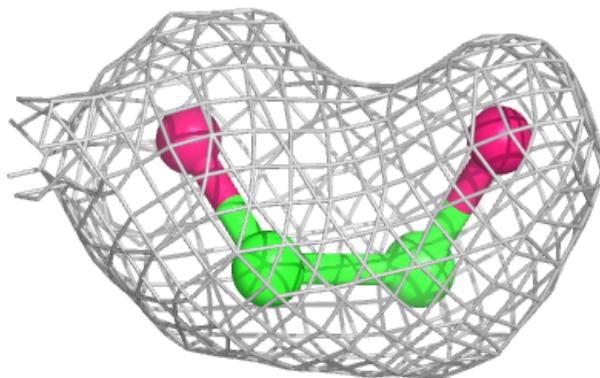
Electron density around MG E 302:

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

Electron density around MG 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.