Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2025 – 02:52 PM JST

PDB ID	:	8XVR
Title	:	Crystal structure of inulosucrase from Lactobacillus reuteri 121 mutant R544W
Authors	:	Ni, D.; Hou, X.; Cheng, M.; Xu, W.; Rao, Y.; Mu, W.
Deposited on	:	2024-01-15
Resolution	:	2.44 Å(reported)

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

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

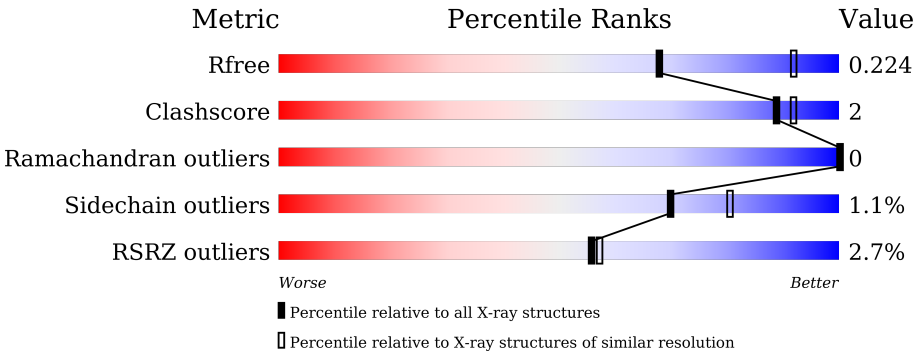
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.44 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	588	2% 85% · 12%
1	B	588	2% 84% 5% 11%
1	C	588	3% 84% 5% 11%
1	D	588	2% 85% · 12%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17513 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 Glycoside hydrolase family 68 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	1	0
			4058	2550	681	814	13			
1	B	524	Total	C	N	O	S	0	1	0
			4116	2586	692	825	13			
1	C	525	Total	C	N	O	S	0	1	0
			4129	2594	697	825	13			
1	D	517	Total	C	N	O	S	0	1	0
			4058	2548	681	816	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	initiating methionine	UNP A0A6N1ER42
A	300	PRO	LEU	conflict	UNP A0A6N1ER42
A	544	TRP	ARG	engineered mutation	UNP A0A6N1ER42
A	702	HIS	-	expression tag	UNP A0A6N1ER42
A	703	HIS	-	expression tag	UNP A0A6N1ER42
A	704	HIS	-	expression tag	UNP A0A6N1ER42
A	705	HIS	-	expression tag	UNP A0A6N1ER42
A	706	HIS	-	expression tag	UNP A0A6N1ER42
A	707	HIS	-	expression tag	UNP A0A6N1ER42
B	120	MET	-	initiating methionine	UNP A0A6N1ER42
B	300	PRO	LEU	conflict	UNP A0A6N1ER42
B	544	TRP	ARG	engineered mutation	UNP A0A6N1ER42
B	702	HIS	-	expression tag	UNP A0A6N1ER42
B	703	HIS	-	expression tag	UNP A0A6N1ER42
B	704	HIS	-	expression tag	UNP A0A6N1ER42
B	705	HIS	-	expression tag	UNP A0A6N1ER42
B	706	HIS	-	expression tag	UNP A0A6N1ER42
B	707	HIS	-	expression tag	UNP A0A6N1ER42
C	120	MET	-	initiating methionine	UNP A0A6N1ER42
C	300	PRO	LEU	conflict	UNP A0A6N1ER42
C	544	TRP	ARG	engineered mutation	UNP A0A6N1ER42

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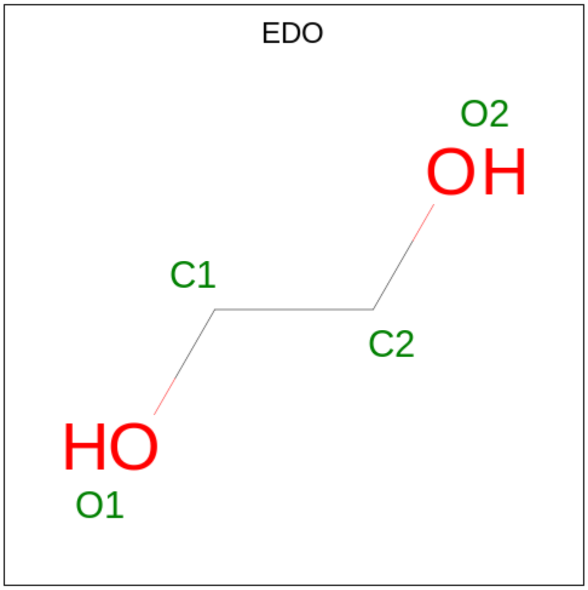
Chain	Residue	Modelled	Actual	Comment	Reference
C	702	HIS	-	expression tag	UNP A0A6N1ER42
C	703	HIS	-	expression tag	UNP A0A6N1ER42
C	704	HIS	-	expression tag	UNP A0A6N1ER42
C	705	HIS	-	expression tag	UNP A0A6N1ER42
C	706	HIS	-	expression tag	UNP A0A6N1ER42
C	707	HIS	-	expression tag	UNP A0A6N1ER42
D	120	MET	-	initiating methionine	UNP A0A6N1ER42
D	300	PRO	LEU	conflict	UNP A0A6N1ER42
D	544	TRP	ARG	engineered mutation	UNP A0A6N1ER42
D	702	HIS	-	expression tag	UNP A0A6N1ER42
D	703	HIS	-	expression tag	UNP A0A6N1ER42
D	704	HIS	-	expression tag	UNP A0A6N1ER42
D	705	HIS	-	expression tag	UNP A0A6N1ER42
D	706	HIS	-	expression tag	UNP A0A6N1ER42
D	707	HIS	-	expression tag	UNP A0A6N1ER42

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 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
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

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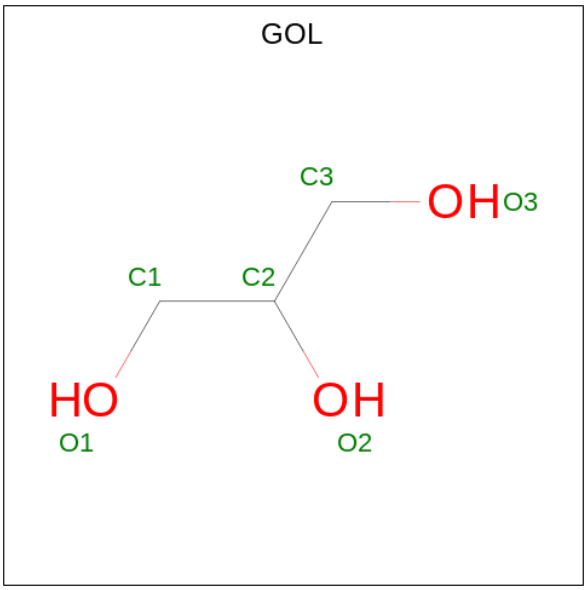
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

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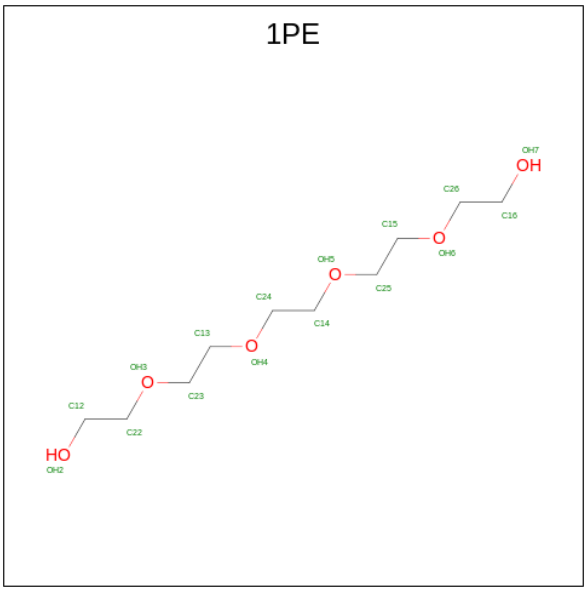
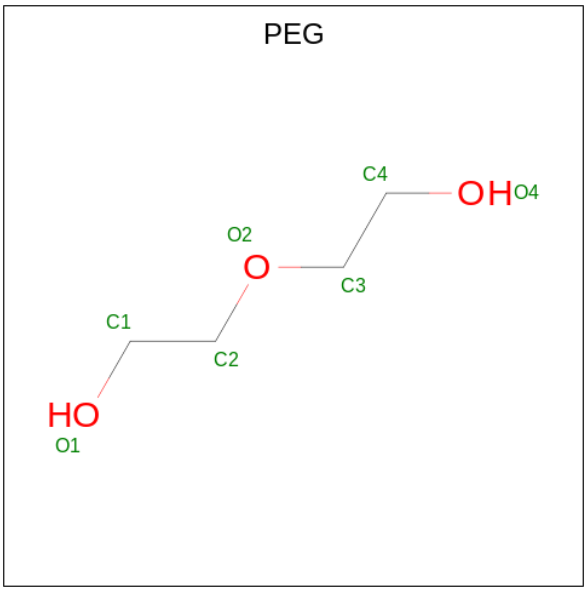
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 16 10 6	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	D	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

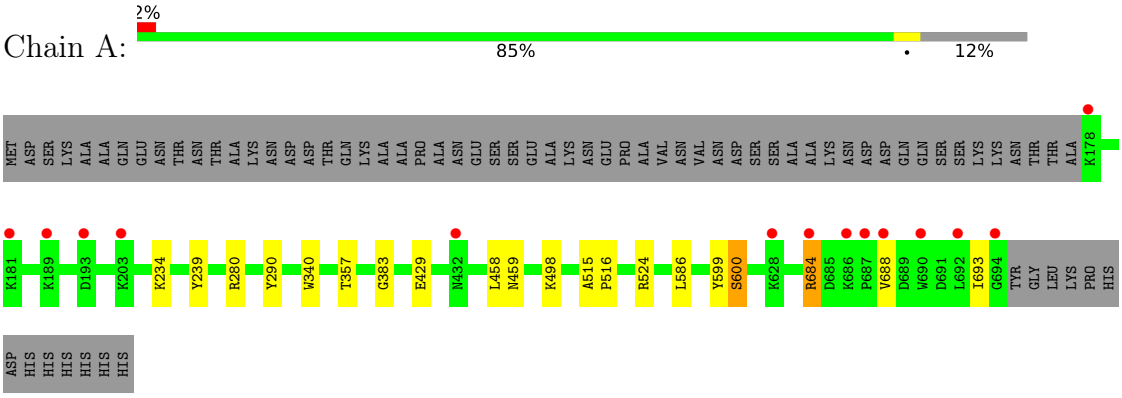
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	234	Total O 234 234	0	0
7	B	271	Total O 271 271	0	0
7	C	252	Total O 252 252	0	0
7	D	238	Total O 238 238	0	0

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.

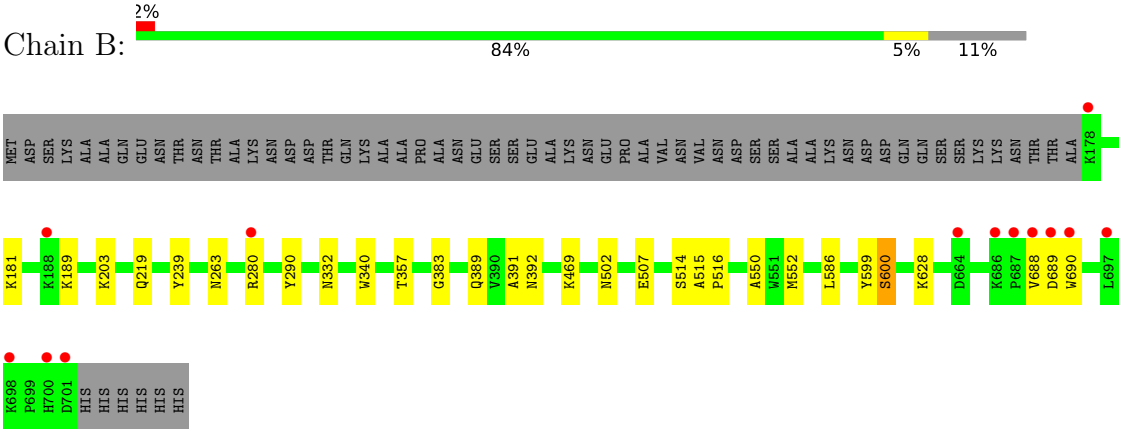
• Molecule 1: Glycoside hydrolase family 68 protein

Chain A:



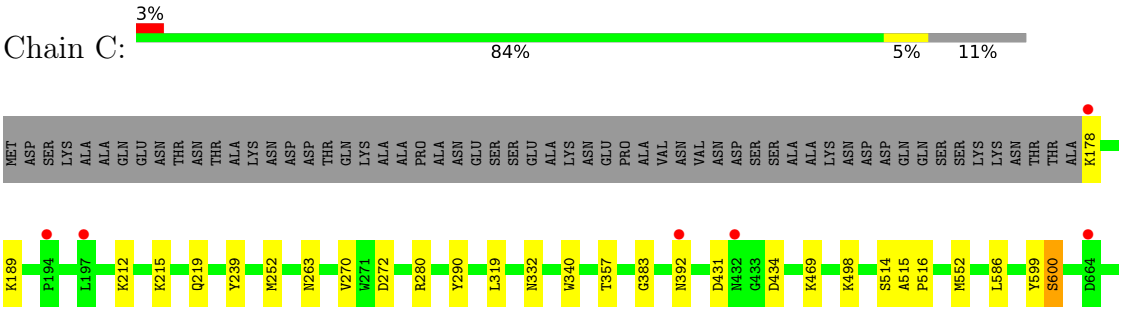
• Molecule 1: Glycoside hydrolase family 68 protein

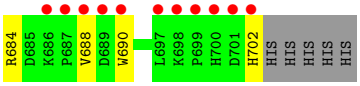
Chain B:



• Molecule 1: Glycoside hydrolase family 68 protein

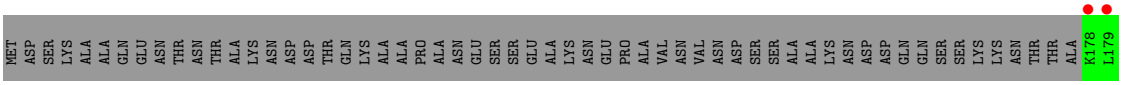
Chain C:

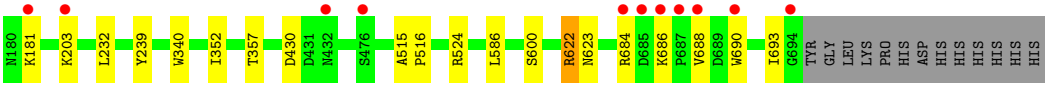




• Molecule 1: Glycoside hydrolase family 68 protein

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.57Å 132.08Å 121.78Å 90.00° 110.29° 90.00°	Depositor
Resolution (Å)	41.59 – 2.44 41.59 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.59-2.44) 98.3 (41.59-2.44)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.216 0.188 , 0.224	Depositor DCC
R_{free} test set	5048 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17513	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: EDO, CA, GOL, PEG, 1PE

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	0.63	0/4152	0.75	0/5660
1	B	0.67	0/4213	0.76	0/5743
1	C	0.67	0/4227	0.76	0/5761
1	D	0.63	0/4152	0.76	0/5660
All	All	0.65	0/16744	0.76	0/22824

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4058	0	3865	13	0
1	B	4116	0	3914	16	0
1	C	4129	0	3928	20	0
1	D	4058	0	3858	11	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	20	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	42	1	0
3	C	32	0	48	0	0
3	D	16	0	24	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	12	0	16	1	0
4	D	6	0	8	0	0
5	A	16	0	22	0	0
6	D	7	0	10	0	0
7	A	234	0	0	3	0
7	B	271	0	0	3	0
7	C	252	0	0	5	0
7	D	238	0	0	4	0
All	All	17513	0	15781	58	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 2.

All (58) 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:D:430:ASP:HB3	7:D:1022:HOH:O	1.61	1.00
1:C:392:ASN:HB3	7:C:905:HOH:O	1.71	0.89
1:C:252:MET:HG3	1:C:319:LEU:HD11	1.63	0.79
1:A:280:ARG:NH1	1:A:429:GLU:OE2	2.29	0.66
1:C:252:MET:HG3	1:C:319:LEU:CD1	2.28	0.64
1:D:686:LYS:NZ	7:D:901:HOH:O	2.32	0.62
1:C:688:VAL:HG13	7:C:1131:HOH:O	2.00	0.61
1:C:252:MET:HE3	1:C:270:VAL:HG11	1.83	0.59
1:C:280:ARG:NH1	1:C:431:ASP:OD1	2.35	0.59
1:C:280:ARG:HD3	7:C:1105:HOH:O	2.08	0.53
1:B:688:VAL:HG13	7:B:1074:HOH:O	2.09	0.52
1:A:684:ARG:NH2	1:C:498:LYS:HE2	2.24	0.52
1:D:524:ARG:NH1	7:D:908:HOH:O	2.44	0.51
1:B:392[A]:ASN:HD21	1:B:502:ASN:CG	2.13	0.51
1:A:239:TYR:O	1:A:586:LEU:HA	2.12	0.50
1:B:239:TYR:O	1:B:586:LEU:HA	2.11	0.50
1:A:498:LYS:HD3	7:A:1125:HOH:O	2.11	0.50
1:C:239:TYR:O	1:C:586:LEU:HA	2.12	0.50
1:D:239:TYR:O	1:D:586:LEU:HA	2.12	0.49
1:C:215:LYS:HE3	7:C:1139:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HE3	7:A:1105:HOH:O	2.14	0.48
1:C:272:ASP:OD2	4:C:811:GOL:H32	2.15	0.47
1:D:622:ARG:O	1:D:623:ASN:HB2	2.14	0.47
1:C:684:ARG:NH1	7:C:902:HOH:O	2.42	0.47
1:B:340:TRP:HB2	1:B:357:THR:HB	1.98	0.46
1:B:552:MET:HG2	1:B:690:TRP:HH2	1.81	0.45
1:A:340:TRP:HB2	1:A:357:THR:HB	1.97	0.45
1:C:552:MET:HG2	1:C:690:TRP:HH2	1.81	0.45
1:C:340:TRP:HB2	1:C:357:THR:HB	1.98	0.45
1:B:280:ARG:HD2	7:B:1117:HOH:O	2.17	0.45
1:B:507:GLU:OE2	1:D:690:TRP:NE1	2.45	0.45
1:D:340:TRP:HB2	1:D:357:THR:HB	1.99	0.44
1:C:290:TYR:OH	1:C:383:GLY:HA2	2.18	0.44
1:B:389:GLN:HE21	1:B:391:ALA:HB2	1.84	0.43
1:A:458[B]:LEU:HD23	1:A:459:ASN:N	2.33	0.43
1:A:290:TYR:OH	1:A:383:GLY:HA2	2.19	0.43
1:A:688:VAL:HG11	1:A:693:ILE:HD11	2.01	0.43
1:C:515:ALA:N	1:C:516:PRO:CD	2.82	0.43
1:D:688:VAL:HG11	1:D:693:ILE:HD11	2.01	0.42
1:A:524:ARG:NH1	7:A:909:HOH:O	2.51	0.42
1:B:219:GLN:HA	1:B:514:SER:O	2.20	0.42
1:B:290:TYR:OH	1:B:383:GLY:HA2	2.20	0.42
1:A:515:ALA:N	1:A:516:PRO:CD	2.82	0.41
1:B:263:ASN:ND2	1:B:332:ASN:OD1	2.51	0.41
1:B:688:VAL:HG12	1:B:689:ASP:N	2.35	0.41
1:C:219:GLN:HA	1:C:514:SER:O	2.20	0.41
1:D:352:ILE:HG13	7:D:962:HOH:O	2.20	0.41
1:C:434:ASP:OD1	1:C:498:LYS:NZ	2.54	0.41
1:B:550:ALA:HA	3:B:808:EDO:C2	2.51	0.41
1:C:263:ASN:ND2	1:C:332:ASN:OD1	2.49	0.41
1:D:515:ALA:N	1:D:516:PRO:CD	2.83	0.41
1:A:599:TYR:CG	1:A:600:SER:N	2.89	0.41
1:B:599:TYR:CG	1:B:600:SER:N	2.89	0.41
1:B:515:ALA:N	1:B:516:PRO:CD	2.83	0.41
1:C:599:TYR:CG	1:C:600:SER:N	2.89	0.40
1:B:280:ARG:HD2	7:B:1159:HOH:O	2.21	0.40
1:D:232:LEU:C	1:D:232:LEU:HD23	2.42	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	516/588 (88%)	496 (96%)	20 (4%)	0	100	100
1	B	523/588 (89%)	501 (96%)	22 (4%)	0	100	100
1	C	524/588 (89%)	504 (96%)	20 (4%)	0	100	100
1	D	516/588 (88%)	493 (96%)	23 (4%)	0	100	100
All	All	2079/2352 (88%)	1994 (96%)	85 (4%)	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	437/495 (88%)	435 (100%)	2 (0%)	86	92
1	B	443/495 (90%)	437 (99%)	6 (1%)	62	75
1	C	444/495 (90%)	438 (99%)	6 (1%)	62	75
1	D	437/495 (88%)	432 (99%)	5 (1%)	70	80
All	All	1761/1980 (89%)	1742 (99%)	19 (1%)	70	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	600	SER
1	A	684	ARG

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Mol	Chain	Res	Type
1	B	181	LYS
1	B	189	LYS
1	B	203	LYS
1	B	469	LYS
1	B	600	SER
1	B	628	LYS
1	C	178	LYS
1	C	189	LYS
1	C	212	LYS
1	C	469	LYS
1	C	600	SER
1	C	702	HIS
1	D	181	LYS
1	D	203	LYS
1	D	600	SER
1	D	622	ARG
1	D	684	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	219	GLN
1	A	226	GLN
1	A	261	GLN
1	A	382	ASN
1	B	195	ASN
1	B	288	ASN
1	B	382	ASN
1	C	195	ASN
1	C	283	GLN
1	C	288	ASN
1	C	382	ASN
1	D	185	ASN
1	D	195	ASN
1	D	219	GLN
1	D	226	GLN
1	D	261	GLN
1	D	532	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 8 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	805	-	3,3,3	0.45	0	2,2,2	0.72	0
3	EDO	A	804	-	3,3,3	0.63	0	2,2,2	0.45	0
3	EDO	B	806	-	3,3,3	0.58	0	2,2,2	0.21	0
3	EDO	D	805	-	3,3,3	0.58	0	2,2,2	0.41	0
4	GOL	D	807	-	5,5,5	0.89	0	5,5,5	1.02	0
3	EDO	C	808	-	3,3,3	0.40	0	2,2,2	0.54	0
3	EDO	C	806	-	3,3,3	0.60	0	2,2,2	0.09	0
3	EDO	A	806	-	3,3,3	0.55	0	2,2,2	0.51	0
3	EDO	D	806	-	3,3,3	0.56	0	2,2,2	0.53	0
4	GOL	A	808	-	5,5,5	0.97	0	5,5,5	0.93	0
3	EDO	B	808	-	3,3,3	0.35	0	2,2,2	0.57	0
3	EDO	B	809	-	3,3,3	0.73	0	2,2,2	0.21	0
4	GOL	C	811	-	5,5,5	0.75	0	5,5,5	1.07	1 (20%)
3	EDO	C	805	-	3,3,3	0.54	0	2,2,2	0.29	0
3	EDO	A	807	-	3,3,3	0.49	0	2,2,2	0.65	0
3	EDO	C	804	-	3,3,3	0.48	0	2,2,2	0.24	0
3	EDO	D	803	-	3,3,3	0.54	0	2,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	C	810	-	3,3,3	0.66	0	2,2,2	0.22	0
6	PEG	D	808	-	6,6,6	0.66	0	5,5,5	0.39	0
3	EDO	D	804	-	3,3,3	0.64	0	2,2,2	0.39	0
3	EDO	B	807	-	3,3,3	0.57	0	2,2,2	0.46	0
3	EDO	C	809	-	3,3,3	0.53	0	2,2,2	0.36	0
3	EDO	C	807	-	3,3,3	0.61	0	2,2,2	0.54	0
3	EDO	B	803	-	3,3,3	0.50	0	2,2,2	0.50	0
4	GOL	B	810	-	5,5,5	0.48	0	5,5,5	0.67	0
3	EDO	B	804	-	3,3,3	0.54	0	2,2,2	0.42	0
3	EDO	B	805	-	3,3,3	0.37	0	2,2,2	0.42	0
5	1PE	A	809	-	15,15,15	0.67	0	14,14,14	0.41	0
4	GOL	C	812	-	5,5,5	0.64	0	5,5,5	0.71	0
3	EDO	C	803	-	3,3,3	0.71	0	2,2,2	0.65	0
3	EDO	A	803	-	3,3,3	0.56	0	2,2,2	0.36	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
3	EDO	A	805	-	-	1/1/1/1	-
3	EDO	A	804	-	-	0/1/1/1	-
3	EDO	B	806	-	-	1/1/1/1	-
3	EDO	D	805	-	-	0/1/1/1	-
4	GOL	D	807	-	-	3/4/4/4	-
3	EDO	C	808	-	-	1/1/1/1	-
3	EDO	C	806	-	-	1/1/1/1	-
3	EDO	A	806	-	-	1/1/1/1	-
3	EDO	D	806	-	-	1/1/1/1	-
4	GOL	A	808	-	-	4/4/4/4	-
3	EDO	B	808	-	-	1/1/1/1	-
3	EDO	B	809	-	-	1/1/1/1	-
4	GOL	C	811	-	-	3/4/4/4	-
3	EDO	C	805	-	-	1/1/1/1	-
3	EDO	A	807	-	-	1/1/1/1	-
3	EDO	C	804	-	-	1/1/1/1	-
3	EDO	D	803	-	-	0/1/1/1	-
3	EDO	C	810	-	-	1/1/1/1	-
6	PEG	D	808	-	-	3/4/4/4	-
3	EDO	D	804	-	-	0/1/1/1	-
3	EDO	B	807	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	809	-	-	1/1/1/1	-
3	EDO	C	807	-	-	1/1/1/1	-
3	EDO	B	803	-	-	1/1/1/1	-
4	GOL	B	810	-	-	4/4/4/4	-
3	EDO	B	804	-	-	1/1/1/1	-
3	EDO	B	805	-	-	1/1/1/1	-
5	1PE	A	809	-	-	7/13/13/13	-
4	GOL	C	812	-	-	2/4/4/4	-
3	EDO	C	803	-	-	1/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	811	GOL	O2-C2-C1	2.02	118.01	109.12

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	803	EDO	O1-C1-C2-O2
4	A	808	GOL	O1-C1-C2-C3
4	B	810	GOL	O1-C1-C2-C3
4	B	810	GOL	C1-C2-C3-O3
4	C	811	GOL	O1-C1-C2-C3
4	C	811	GOL	C1-C2-C3-O3
4	C	812	GOL	C1-C2-C3-O3
5	A	809	1PE	OH5-C14-C24-OH4
4	D	807	GOL	O2-C2-C3-O3
5	A	809	1PE	OH7-C16-C26-OH6
6	D	808	PEG	O1-C1-C2-O2
4	A	808	GOL	C1-C2-C3-O3
4	D	807	GOL	O1-C1-C2-C3
4	D	807	GOL	C1-C2-C3-O3
4	B	810	GOL	O2-C2-C3-O3
4	C	812	GOL	O2-C2-C3-O3
3	B	803	EDO	O1-C1-C2-O2
3	B	808	EDO	O1-C1-C2-O2
3	C	807	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	809	EDO	O1-C1-C2-O2
6	D	808	PEG	O2-C3-C4-O4
4	A	808	GOL	O1-C1-C2-O2
4	B	810	GOL	O1-C1-C2-O2
3	A	805	EDO	O1-C1-C2-O2
3	B	805	EDO	O1-C1-C2-O2
3	B	806	EDO	O1-C1-C2-O2
3	C	810	EDO	O1-C1-C2-O2
3	D	806	EDO	O1-C1-C2-O2
5	A	809	1PE	C16-C26-OH6-C15
3	B	809	EDO	O1-C1-C2-O2
3	C	806	EDO	O1-C1-C2-O2
5	A	809	1PE	OH2-C12-C22-OH3
3	A	806	EDO	O1-C1-C2-O2
3	A	807	EDO	O1-C1-C2-O2
3	C	804	EDO	O1-C1-C2-O2
3	C	805	EDO	O1-C1-C2-O2
3	C	808	EDO	O1-C1-C2-O2
5	A	809	1PE	C15-C25-OH5-C14
5	A	809	1PE	C12-C22-OH3-C23
6	D	808	PEG	C4-C3-O2-C2
4	A	808	GOL	O2-C2-C3-O3
5	A	809	1PE	C14-C24-OH4-C13
3	B	804	EDO	O1-C1-C2-O2
4	C	811	GOL	O1-C1-C2-O2

There are no ring outliers.

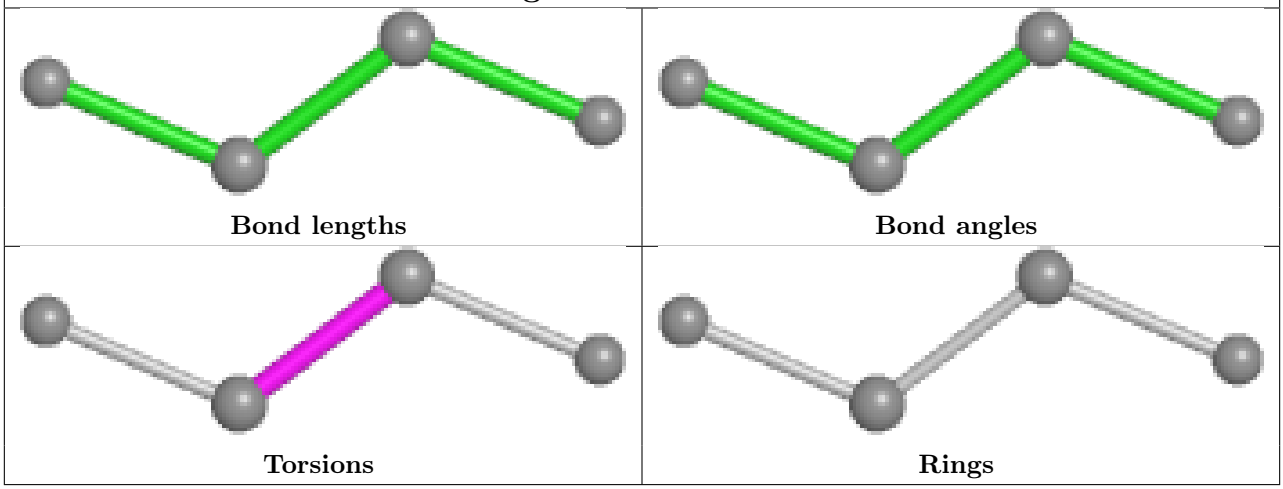
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	808	EDO	1	0
4	C	811	GOL	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 A 805



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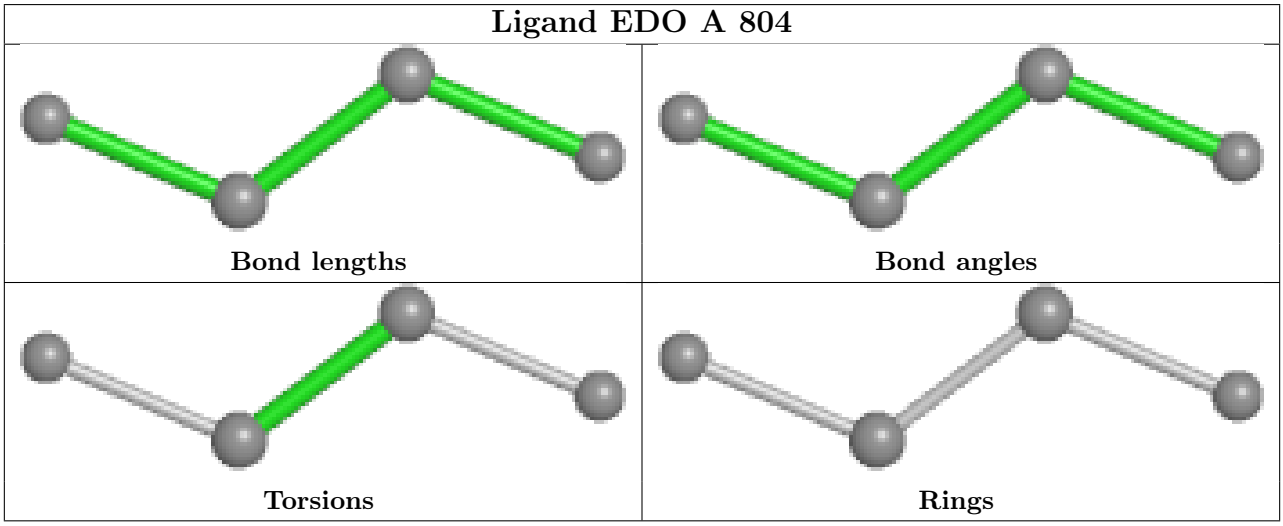
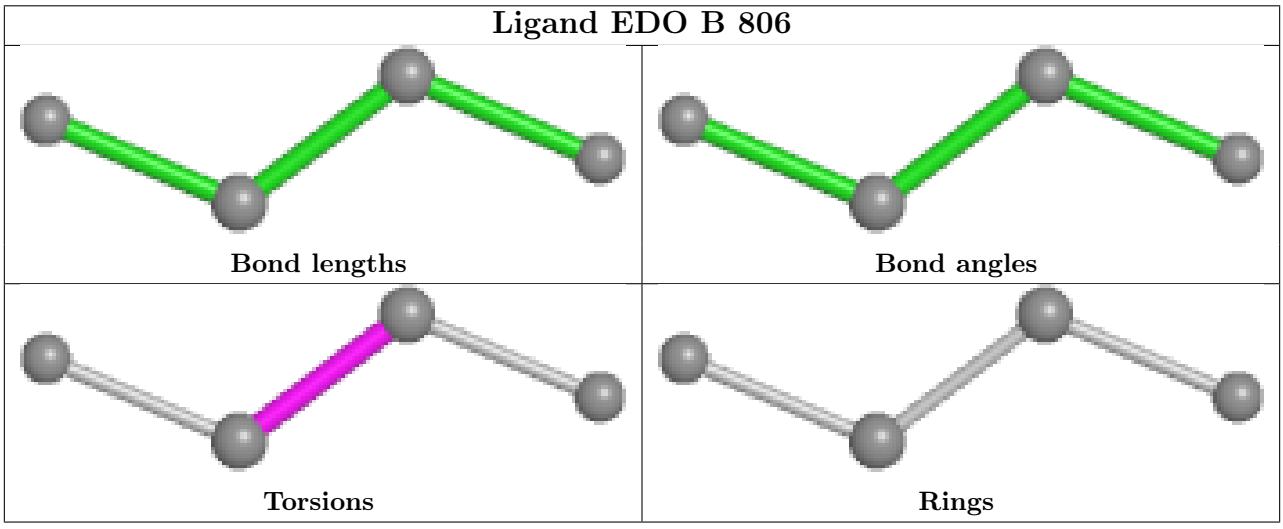


Ligand EDO B 806



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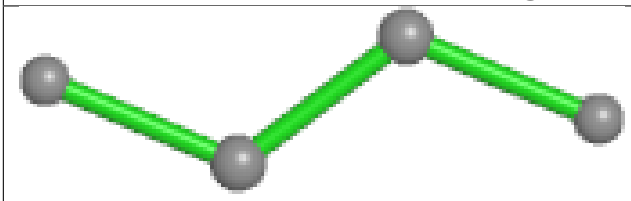
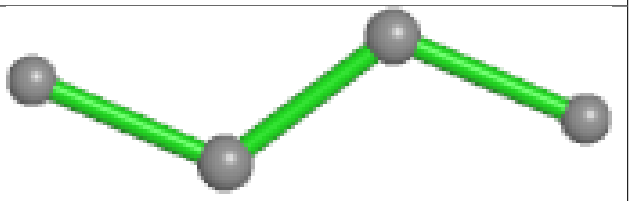
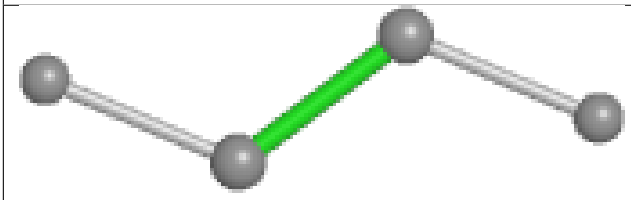


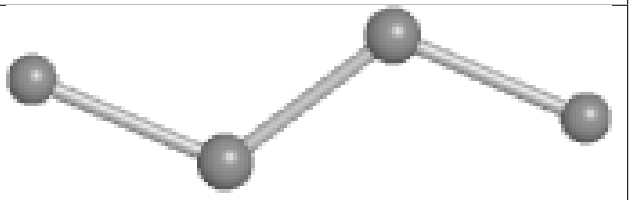
Bond lengths



Bond angles

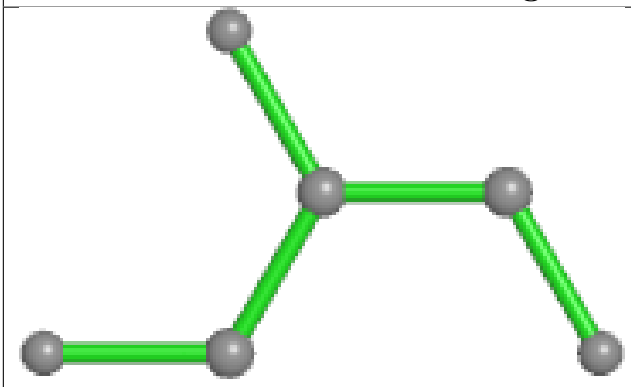


Torsions

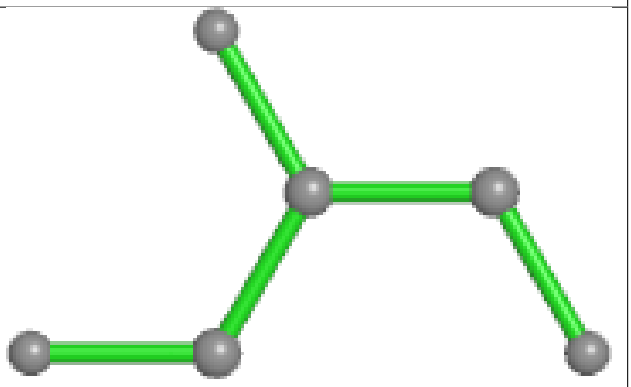


Rings

Ligand GOL D 807



Bond lengths



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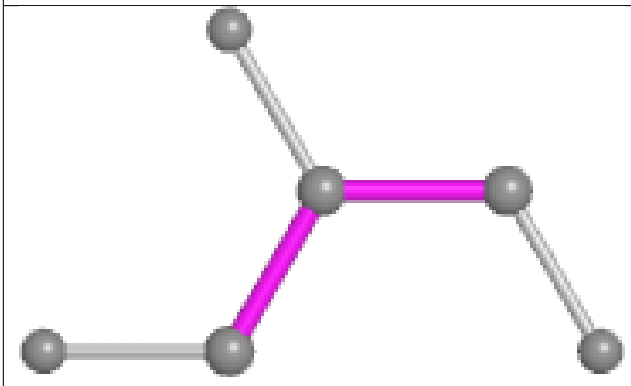

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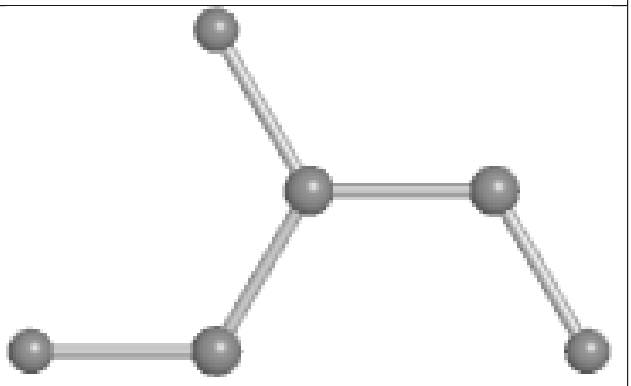
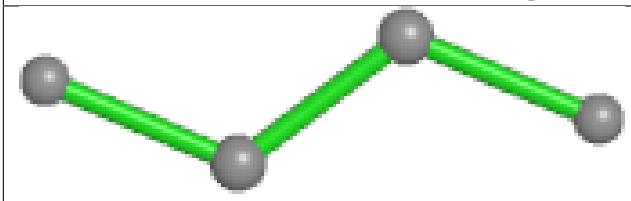
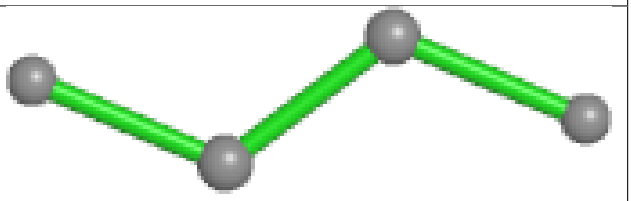


Rings

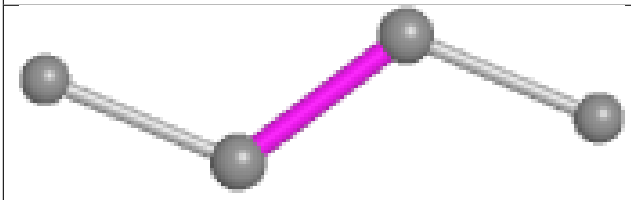
Ligand EDO C 808



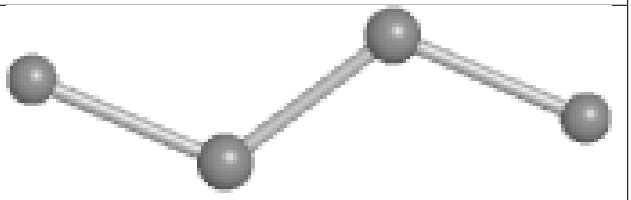
Bond lengths



Bond angles

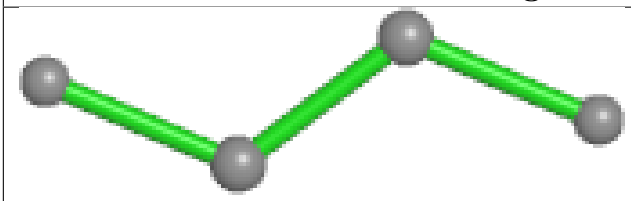


Torsions

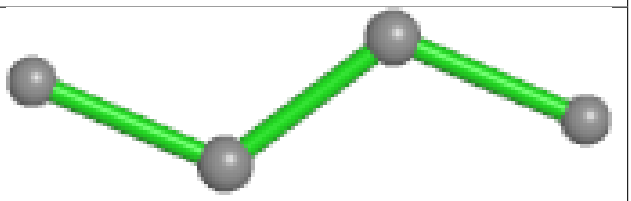


Rings

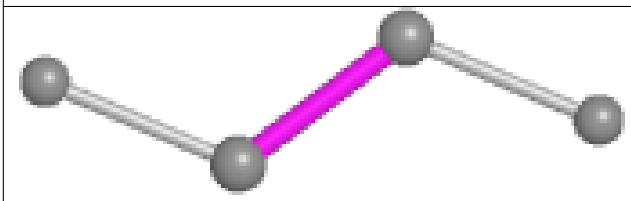
Ligand EDO C 806



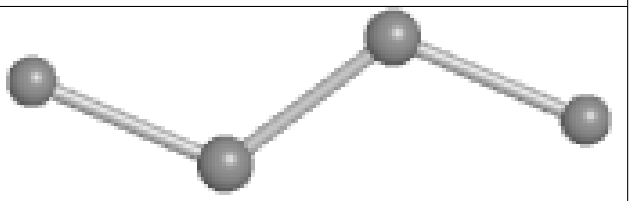
Bond lengths



Bond angles

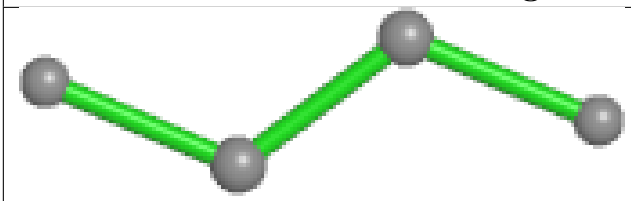


Torsions

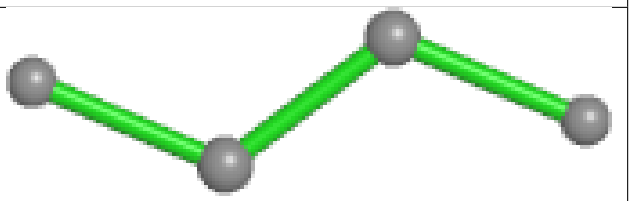


Rings

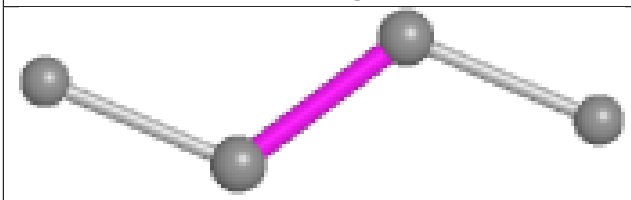
Ligand EDO A 806



Bond lengths



Bond angles



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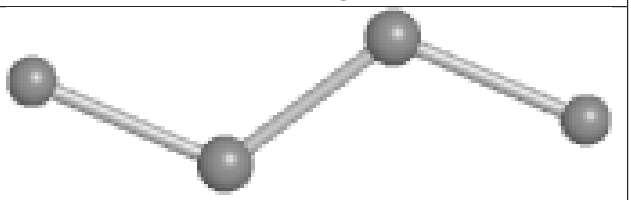
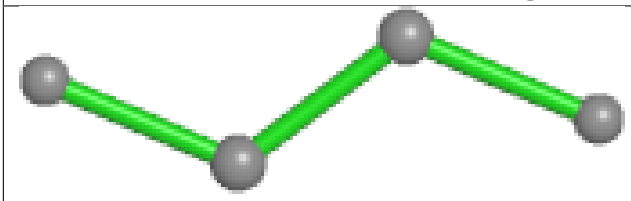
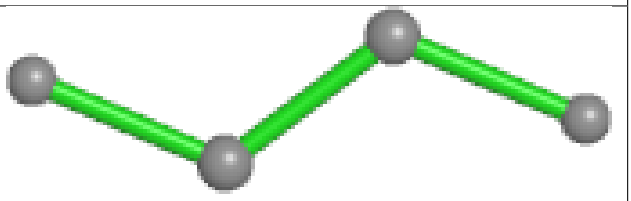


Rings

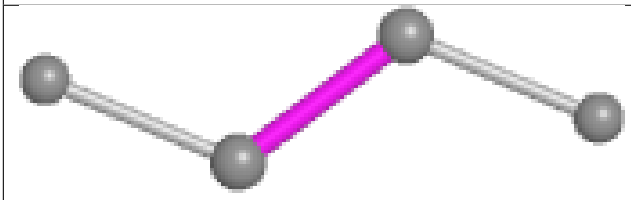
Ligand EDO D 806



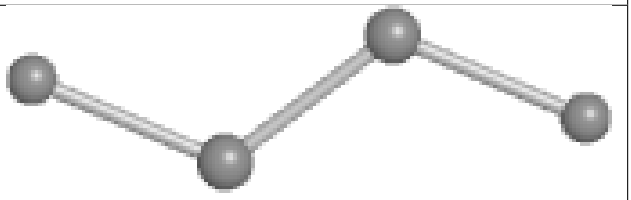
Bond lengths



Bond angles

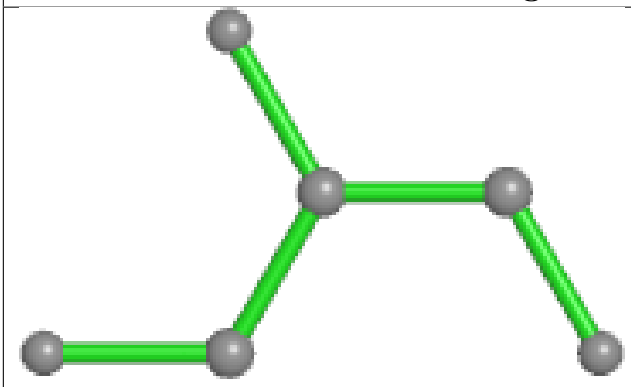


Torsions



Rings

Ligand GOL A 808



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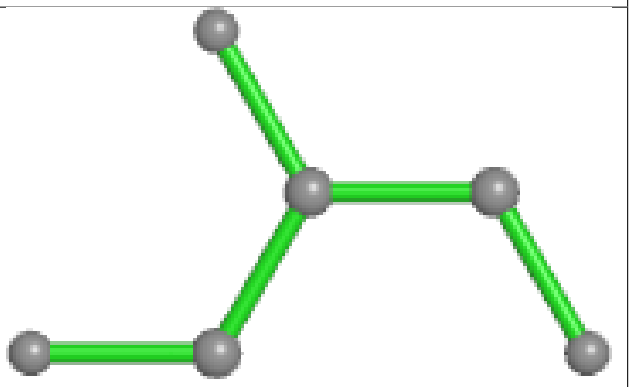
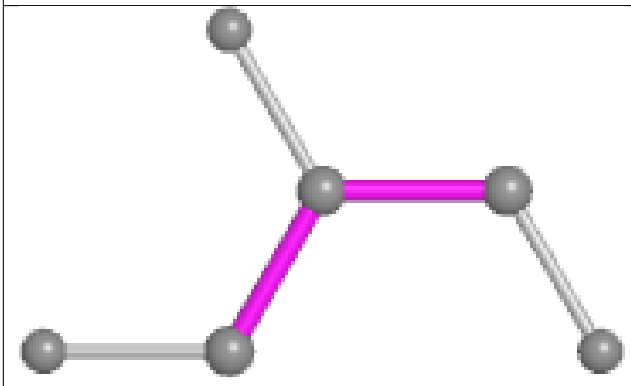


Bond angles



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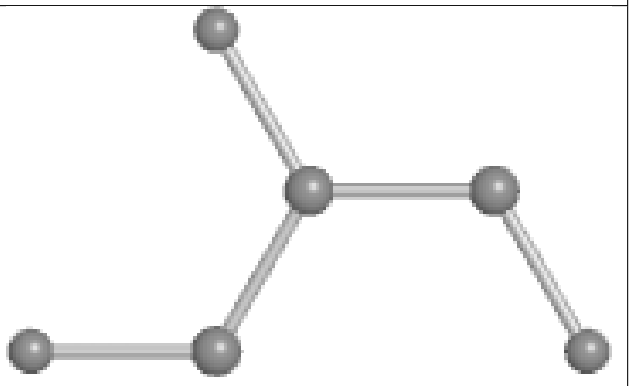
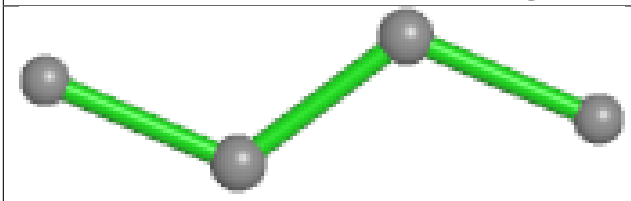
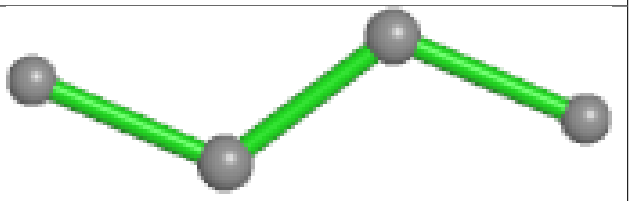
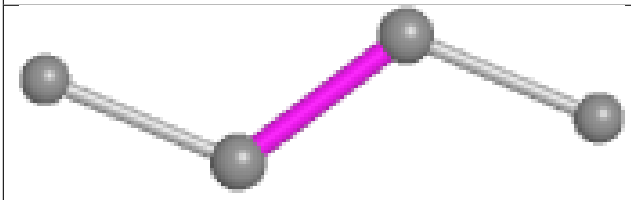
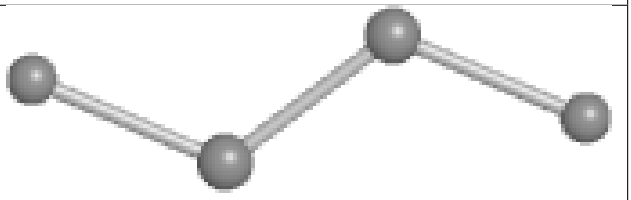


Rings

Ligand EDO B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

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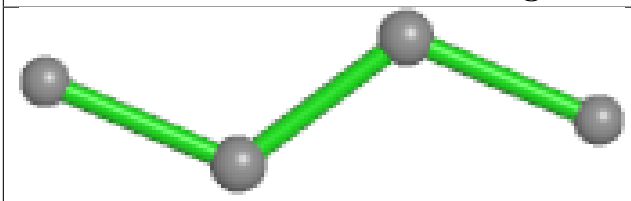
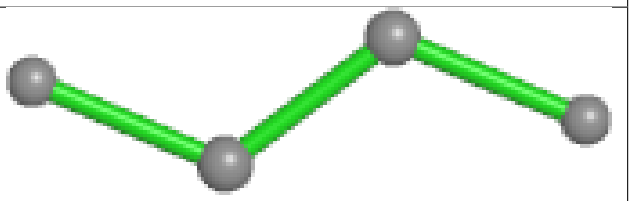
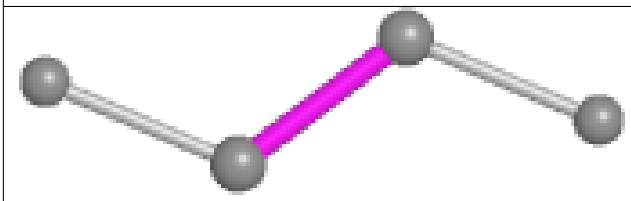
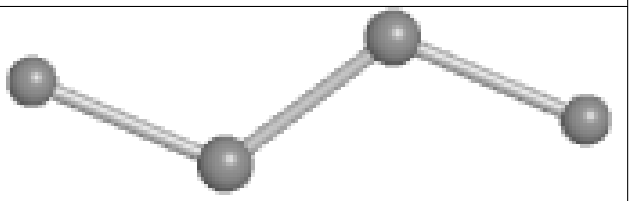
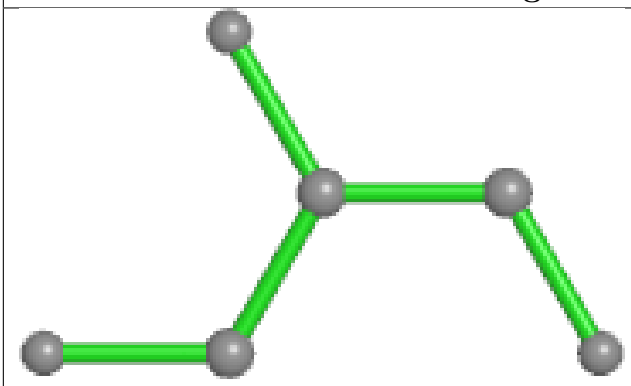
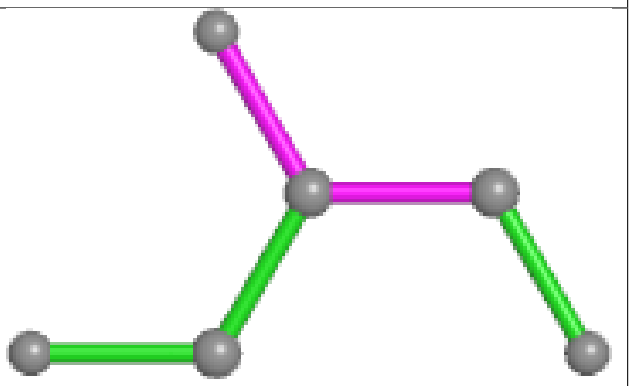
	
Bond lengths	Bond angles
	
Torsions	Rings

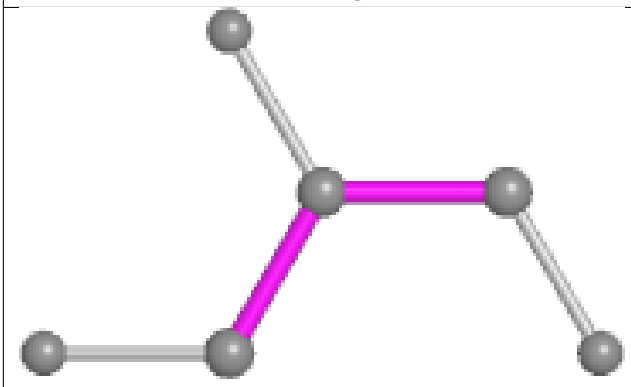
Ligand GOL C 811



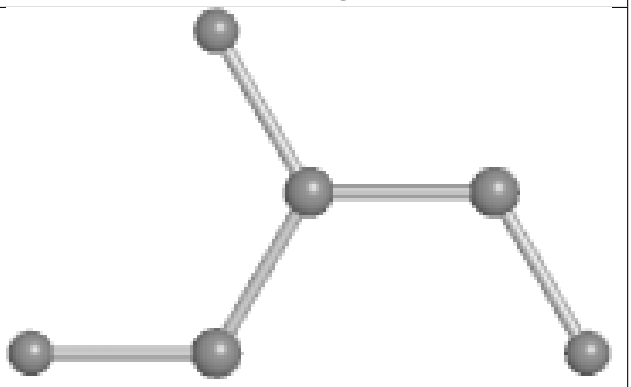
Bond lengths



Bond angles

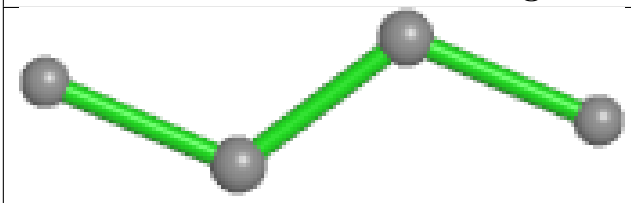


Torsions

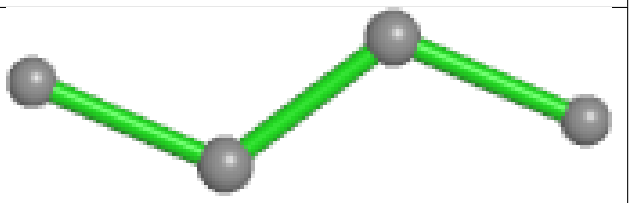


Rings

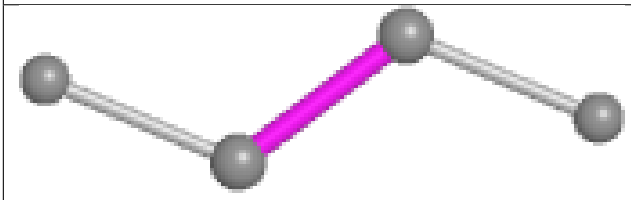
Ligand EDO C 805



Bond lengths



Bond angles



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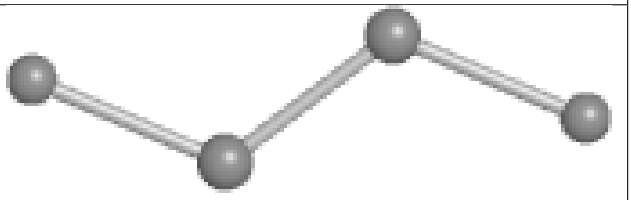
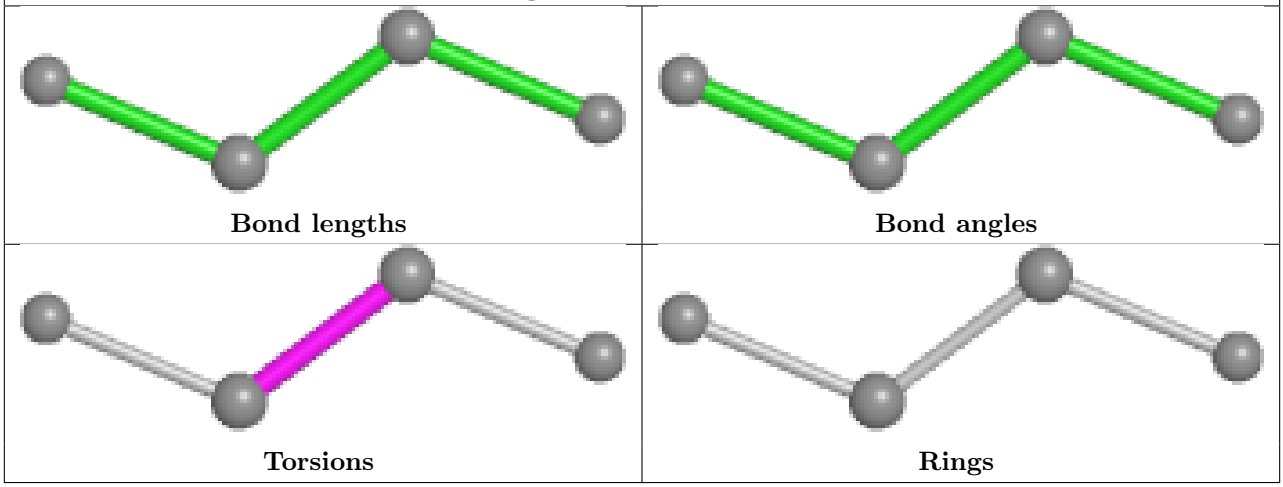
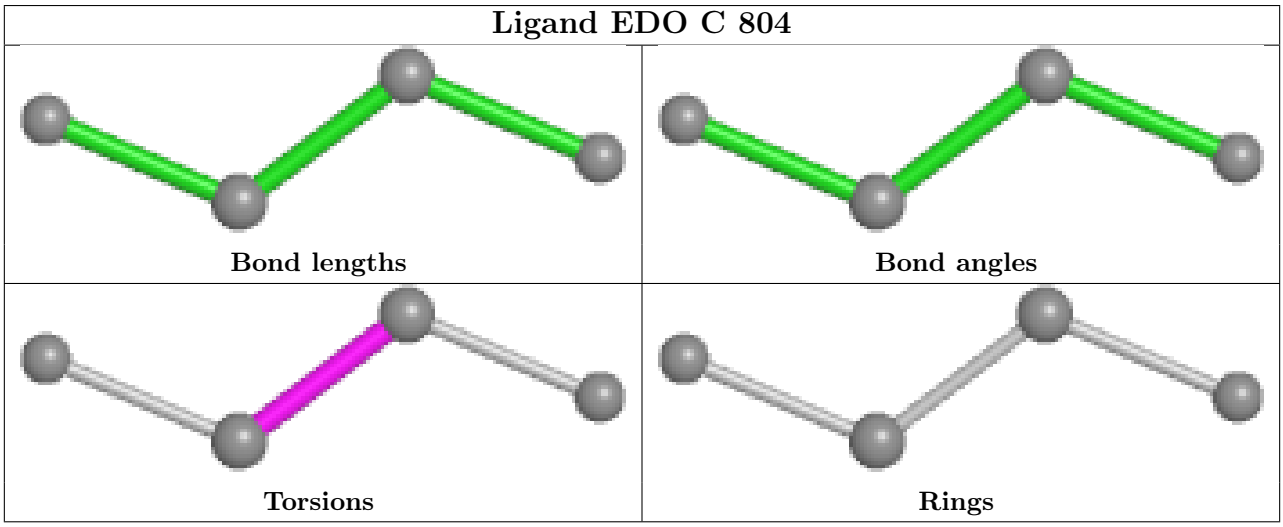


Rings

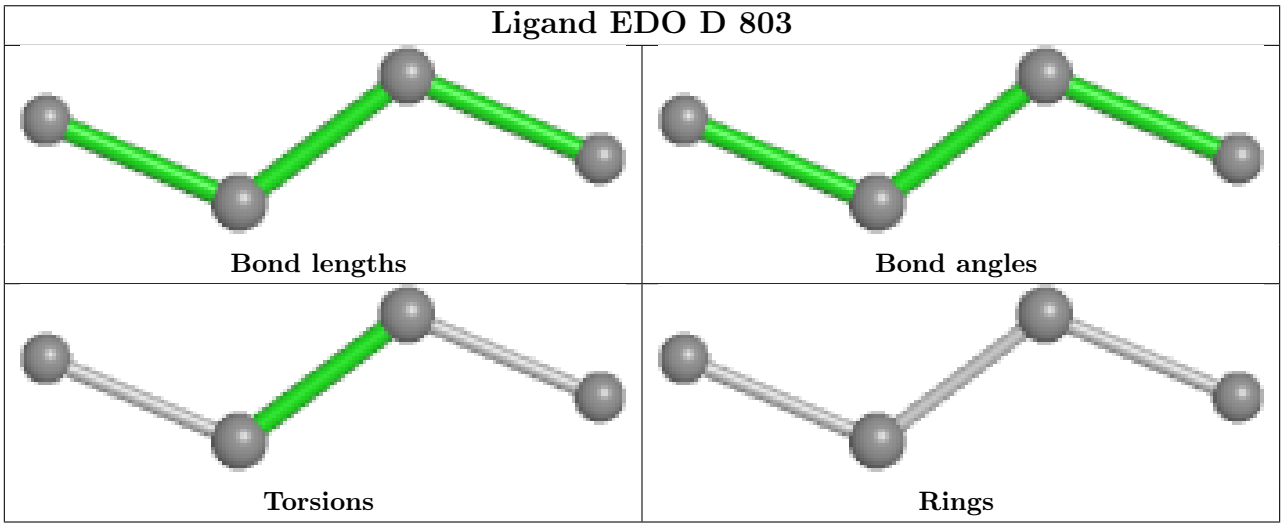
Ligand EDO A 807



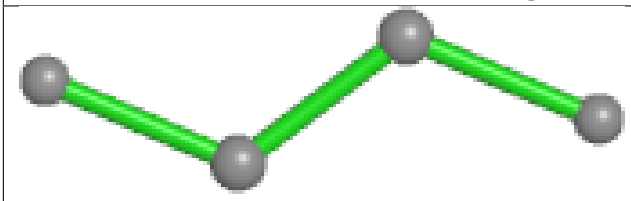
Ligand EDO C 804



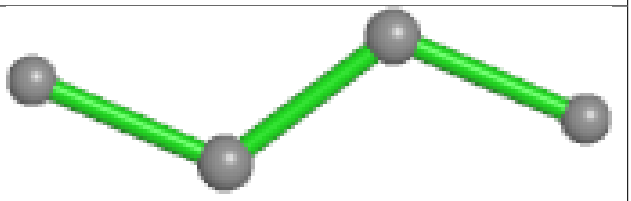
Ligand EDO D 803



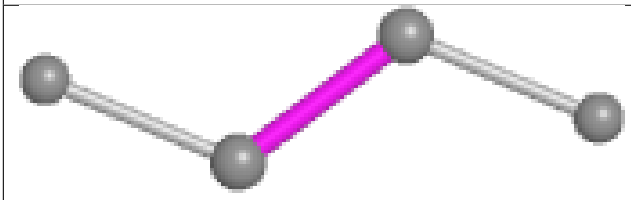
Ligand EDO C 810



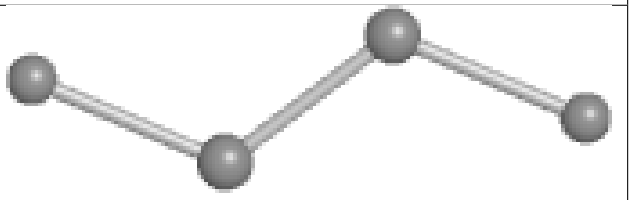
Bond lengths



Bond angles

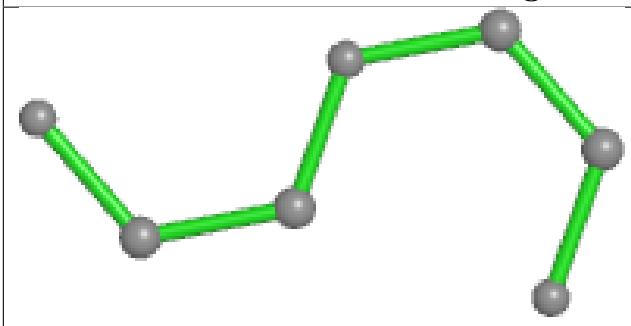


Torsions

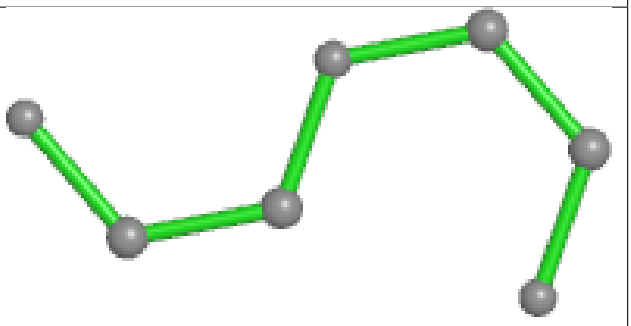


Rings

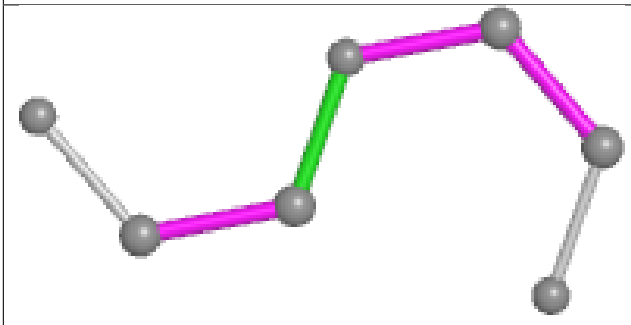
Ligand PEG D 808



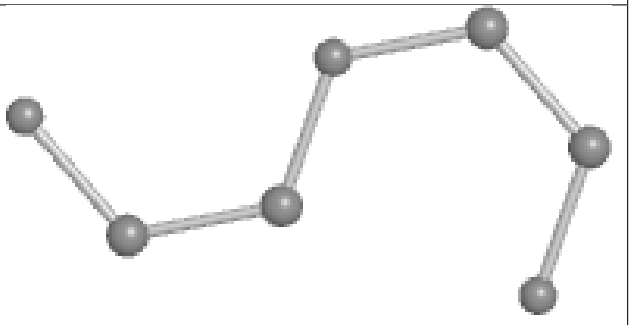
Bond lengths



Bond angles

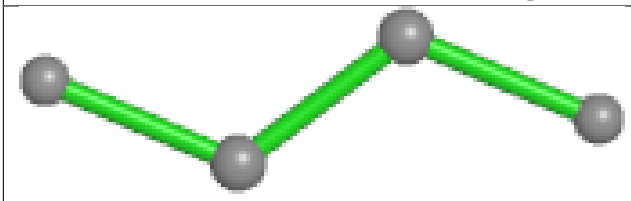


Torsions

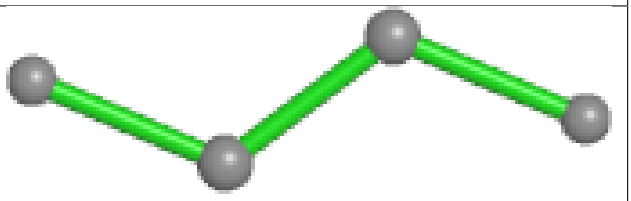


Rings

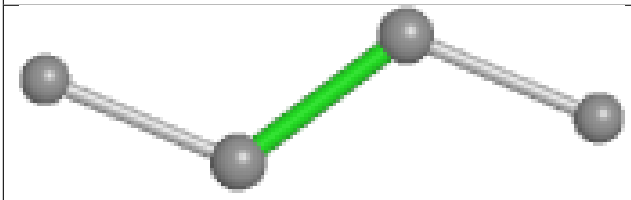
Ligand EDO D 804



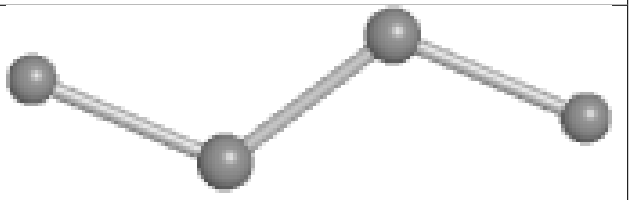
Bond lengths



Bond angles

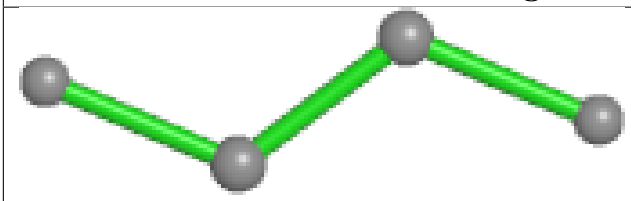


Torsions



Rings

Ligand EDO B 807



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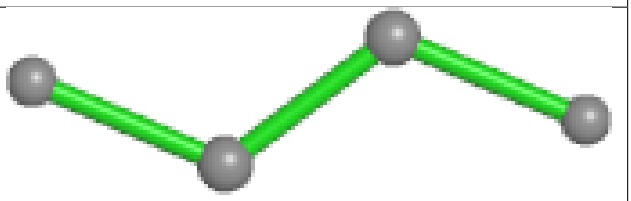
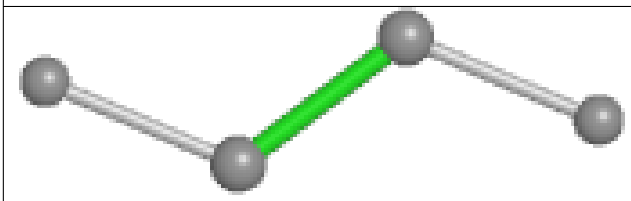
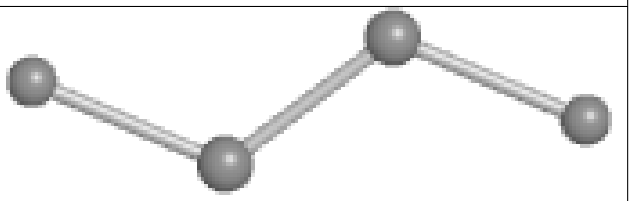


Bond angles

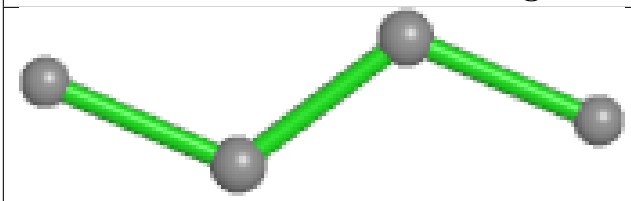


Torsions

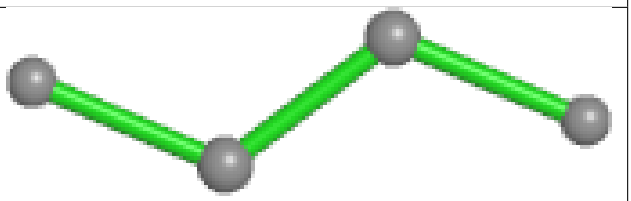


Rings

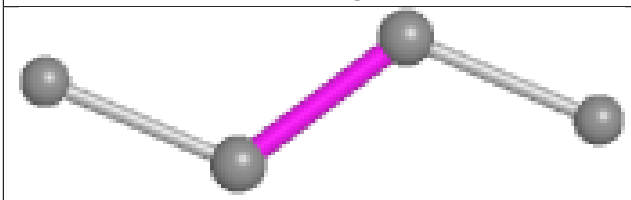
Ligand EDO C 809



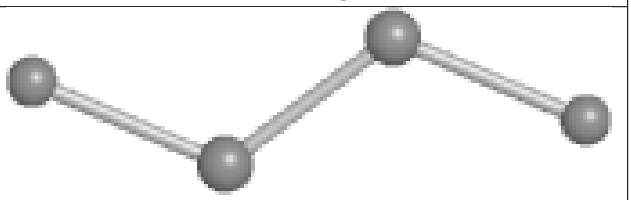
Bond lengths



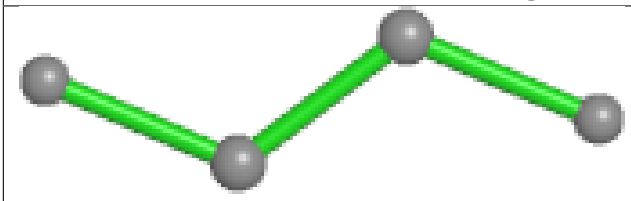
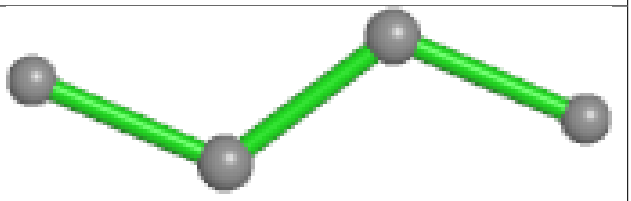
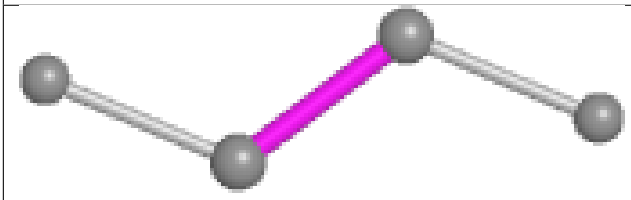
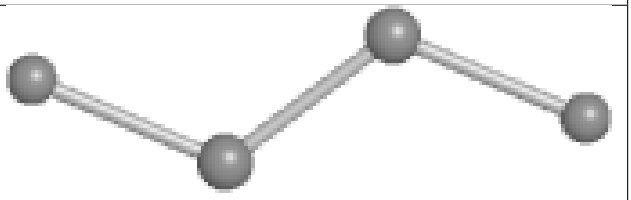
Bond angles

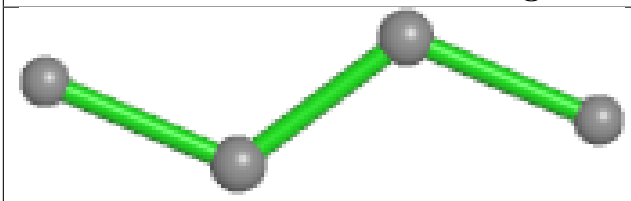
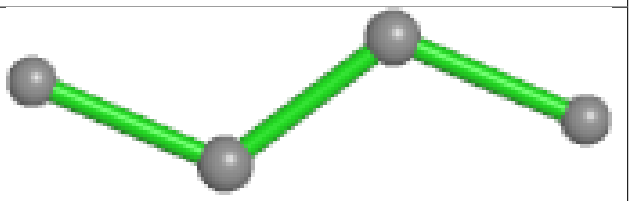
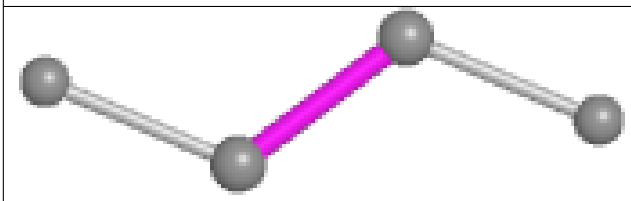
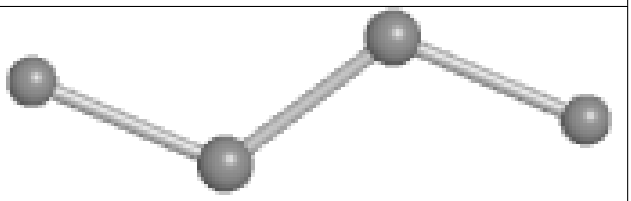


Torsions

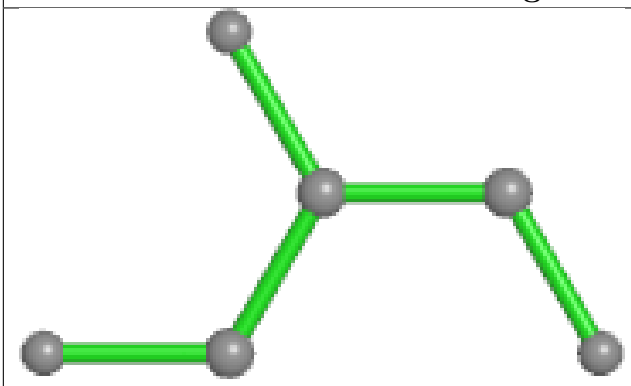


Rings

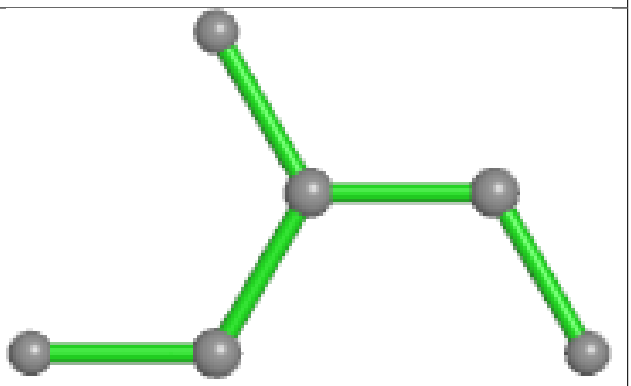
Ligand EDO C 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO B 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

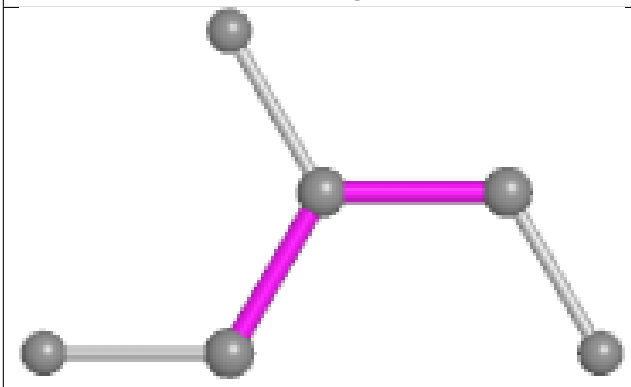
Ligand GOL B 810



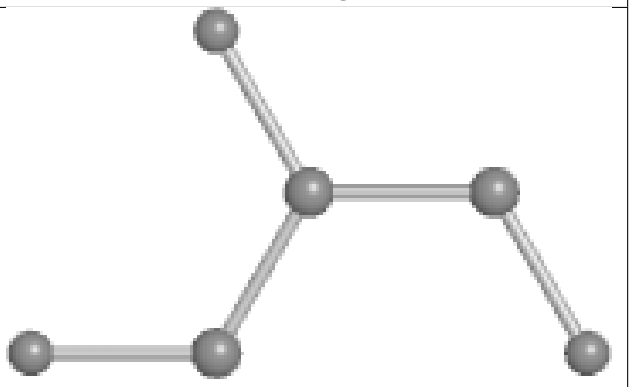
Bond lengths



Bond angles

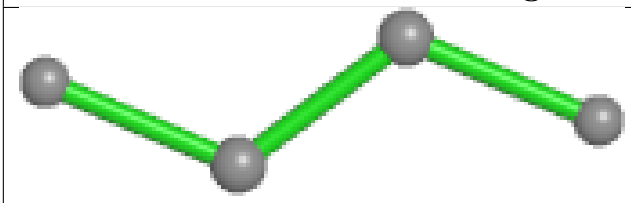


Torsions

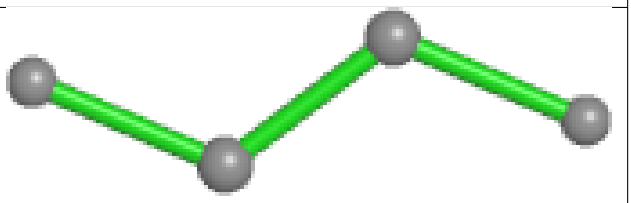


Rings

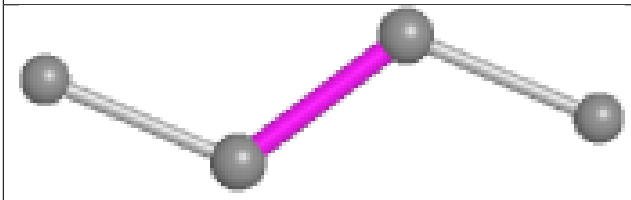
Ligand EDO B 804



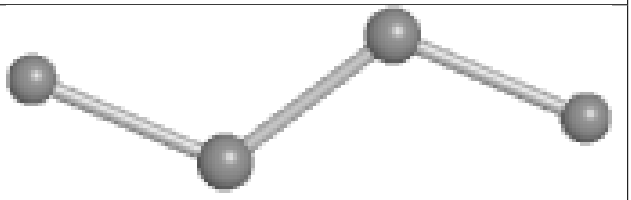
Bond lengths



Bond angles

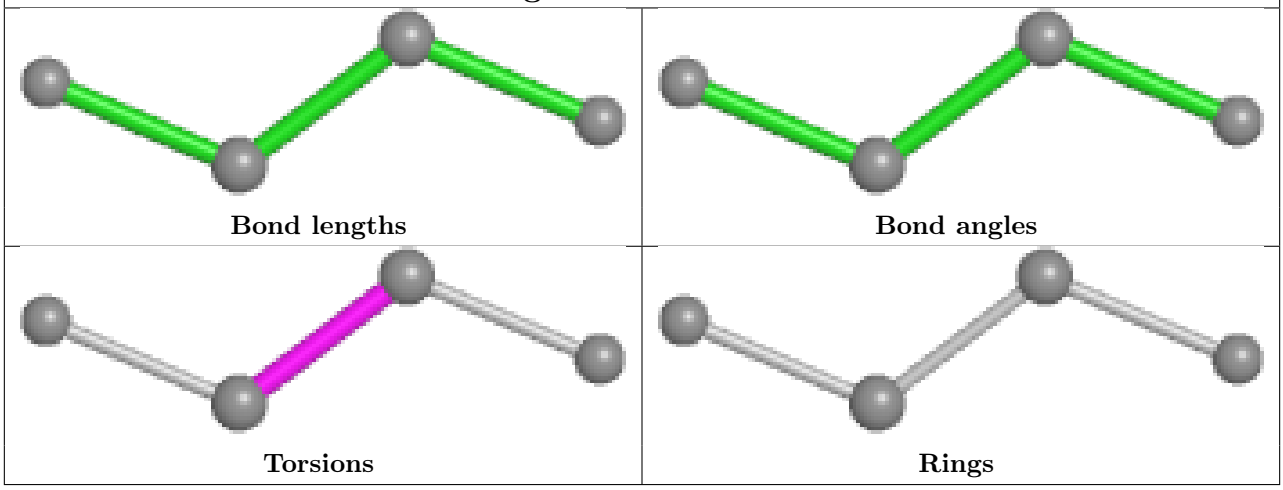


Torsions

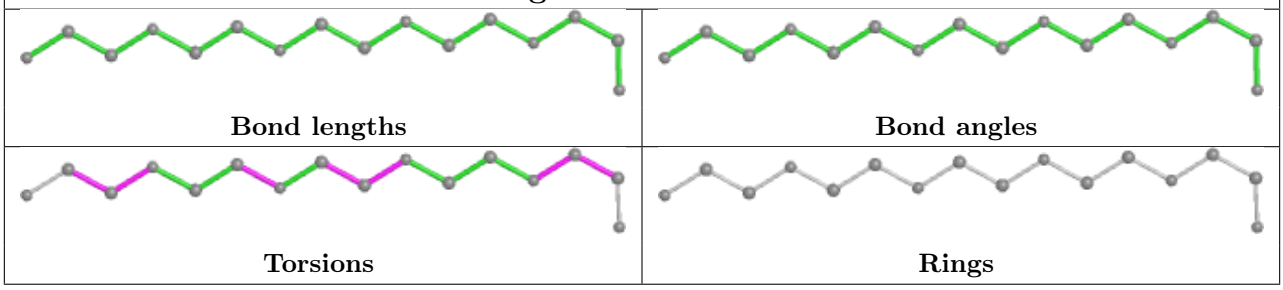


Rings

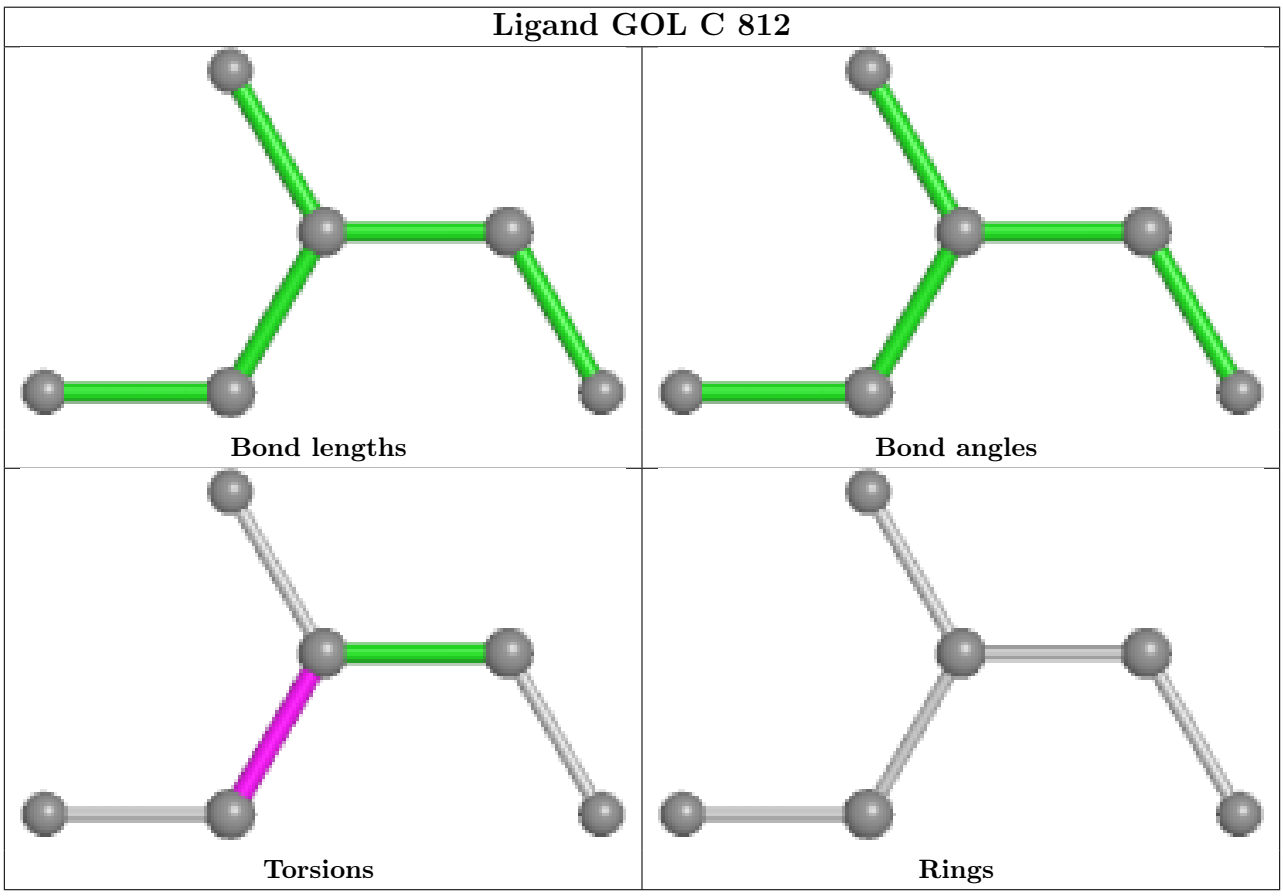
Ligand EDO B 805

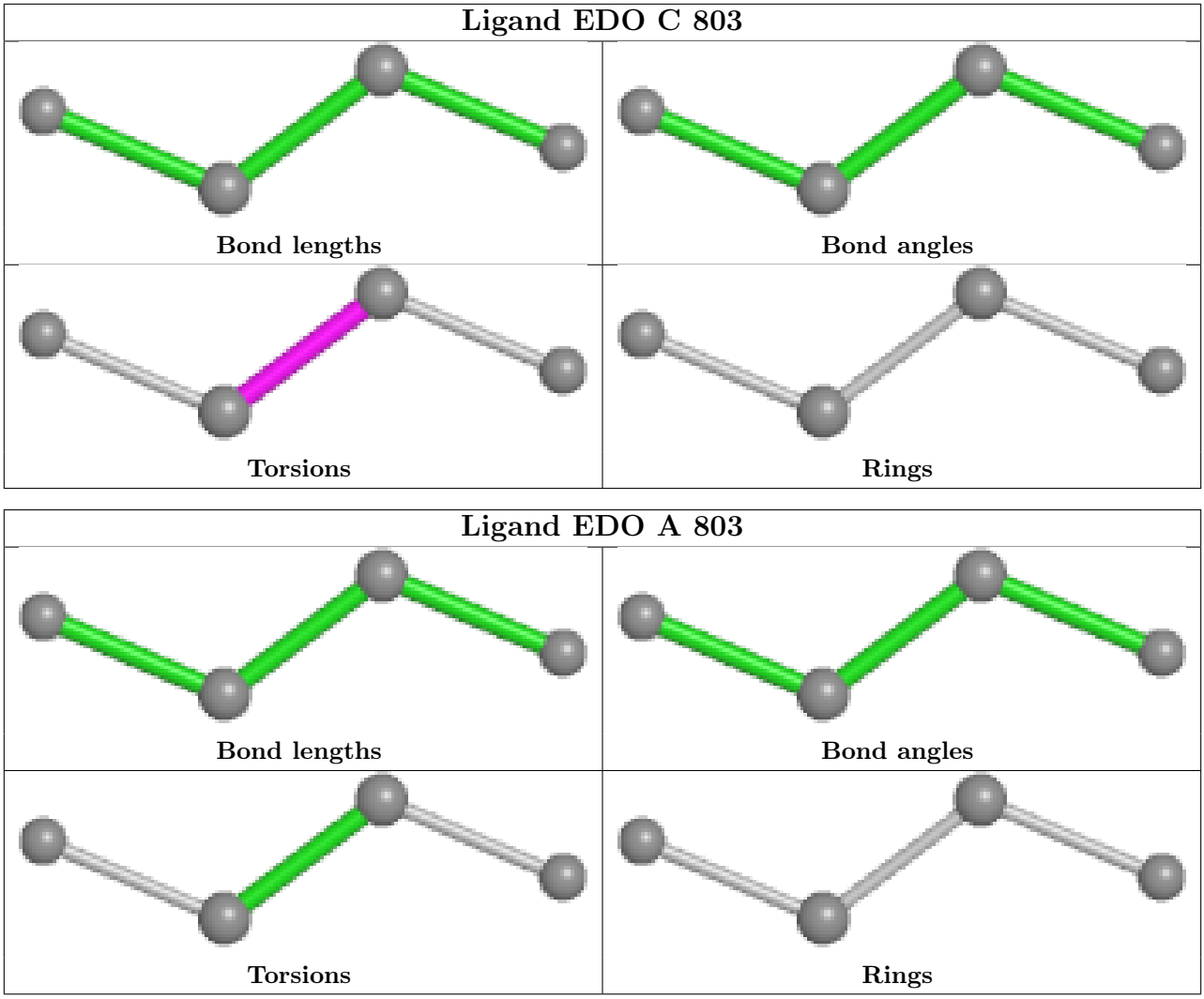


Ligand 1PE A 809



Ligand GOL C 812





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	517/588 (87%)	-0.16	14 (2%)	56	57	13, 20, 51, 71	1 (0%)
1	B	524/588 (89%)	-0.24	13 (2%)	58	60	10, 17, 46, 68	1 (0%)
1	C	525/588 (89%)	-0.20	17 (3%)	50	51	9, 18, 47, 67	1 (0%)
1	D	517/588 (87%)	-0.12	13 (2%)	58	60	10, 21, 52, 74	1 (0%)
All	All	2083/2352 (88%)	-0.18	57 (2%)	56	57	9, 19, 49, 74	4 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	702	HIS	6.0
1	C	687	PRO	4.6
1	C	689	ASP	4.4
1	B	689	ASP	4.2
1	A	432	ASN	4.1
1	C	700	HIS	4.0
1	C	688	VAL	4.0
1	D	178	LYS	3.9
1	D	687	PRO	3.7
1	A	690	TRP	3.7
1	B	687	PRO	3.6
1	C	698	LYS	3.6
1	A	687	PRO	3.6
1	B	700	HIS	3.6
1	D	690	TRP	3.4
1	C	178	LYS	3.2
1	B	688	VAL	3.2
1	D	688	VAL	3.2
1	D	684	ARG	3.1
1	B	280	ARG	3.0
1	C	699	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	203	LYS	2.9
1	B	701	ASP	2.9
1	A	178	LYS	2.9
1	B	690	TRP	2.9
1	A	694	GLY	2.8
1	D	686	LYS	2.8
1	B	698	LYS	2.8
1	C	392	ASN	2.8
1	C	432	ASN	2.8
1	C	701	ASP	2.7
1	A	686	LYS	2.6
1	A	688	VAL	2.6
1	D	203	LYS	2.6
1	C	697	LEU	2.5
1	B	664	ASP	2.5
1	B	697	LEU	2.5
1	D	694	GLY	2.5
1	B	686	LYS	2.5
1	B	178	LYS	2.5
1	A	181	LYS	2.4
1	A	684	ARG	2.4
1	D	476	SER	2.4
1	C	690	TRP	2.4
1	C	194	PRO	2.3
1	C	197	LEU	2.3
1	A	692	LEU	2.2
1	D	432	ASN	2.2
1	A	189	LYS	2.2
1	D	685	ASP	2.2
1	A	193	ASP	2.1
1	C	664	ASP	2.1
1	C	686	LYS	2.1
1	A	628	LYS	2.1
1	D	179	LEU	2.1
1	B	188	LYS	2.1
1	D	181	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
3	EDO	B	809	4/4	0.79	0.19	42,43,44,44	0
3	EDO	C	810	4/4	0.80	0.19	43,44,45,45	0
3	EDO	D	806	4/4	0.80	0.17	45,47,47,48	0
3	EDO	C	806	4/4	0.81	0.18	40,44,44,45	0
3	EDO	C	804	4/4	0.82	0.17	43,46,46,49	0
3	EDO	C	809	4/4	0.82	0.18	46,52,53,53	0
3	EDO	C	808	4/4	0.83	0.15	41,41,43,44	0
3	EDO	A	806	4/4	0.83	0.17	39,44,46,46	0
4	GOL	B	810	6/6	0.83	0.14	29,36,37,41	0
3	EDO	B	803	4/4	0.84	0.16	29,31,32,33	0
3	EDO	B	808	4/4	0.84	0.15	42,44,45,45	0
3	EDO	C	805	4/4	0.84	0.19	44,46,50,53	0
5	1PE	A	809	16/16	0.84	0.15	39,47,49,50	0
4	GOL	D	807	6/6	0.85	0.14	27,30,33,34	0
3	EDO	C	803	4/4	0.85	0.15	33,33,33,34	0
3	EDO	A	805	4/4	0.86	0.11	26,30,30,32	0
3	EDO	C	807	4/4	0.86	0.16	33,34,35,36	0
3	EDO	A	804	4/4	0.86	0.13	28,29,32,34	0
3	EDO	A	807	4/4	0.87	0.19	40,42,44,45	0
3	EDO	B	807	4/4	0.87	0.17	29,34,36,36	0
3	EDO	D	804	4/4	0.87	0.15	34,34,36,39	0
3	EDO	D	805	4/4	0.87	0.13	37,37,39,40	0
3	EDO	B	804	4/4	0.88	0.14	37,40,41,42	0
4	GOL	C	812	6/6	0.88	0.11	28,34,36,37	0
3	EDO	B	806	4/4	0.88	0.14	34,37,37,37	0
4	GOL	A	808	6/6	0.88	0.13	25,28,31,34	0
6	PEG	D	808	7/7	0.88	0.14	42,44,48,49	0
3	EDO	D	803	4/4	0.89	0.12	28,29,30,31	0
4	GOL	C	811	6/6	0.89	0.12	28,34,36,39	0
3	EDO	A	803	4/4	0.90	0.11	18,21,22,22	0
3	EDO	B	805	4/4	0.91	0.13	38,41,42,46	0
2	CA	D	801	1/1	0.98	0.04	19,19,19,19	0

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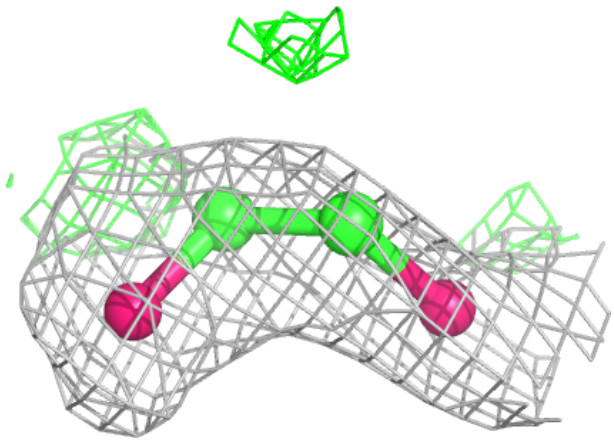
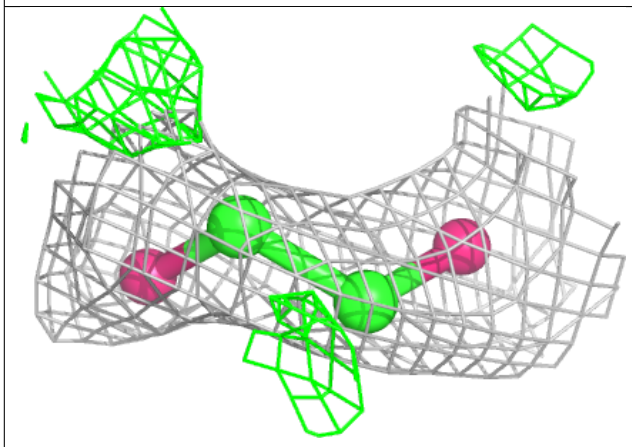
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	801	1/1	0.98	0.05	17,17,17,17	0
2	CA	B	802	1/1	0.98	0.04	14,14,14,14	0
2	CA	C	802	1/1	0.98	0.04	14,14,14,14	0
2	CA	D	802	1/1	0.99	0.02	17,17,17,17	0
2	CA	C	801	1/1	0.99	0.03	16,16,16,16	0
2	CA	B	801	1/1	0.99	0.03	16,16,16,16	0
2	CA	A	802	1/1	0.99	0.03	17,17,17,17	0

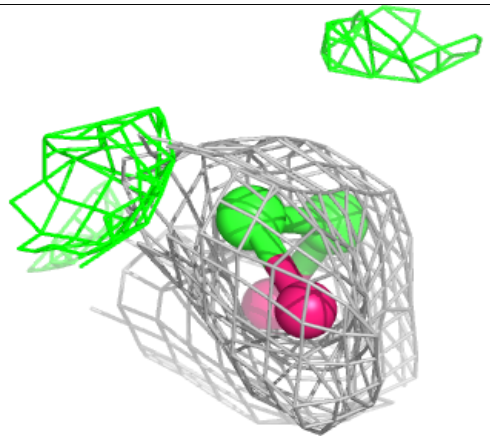
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO B 809:

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

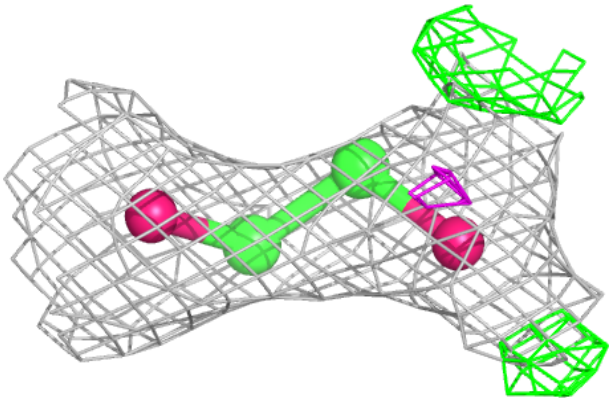


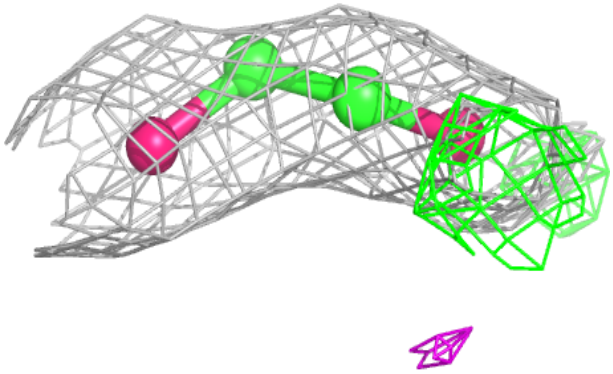


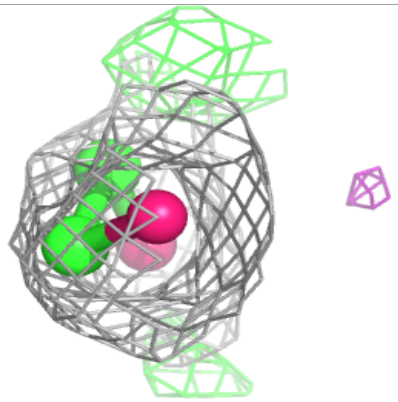


Electron density around EDO C 810:

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

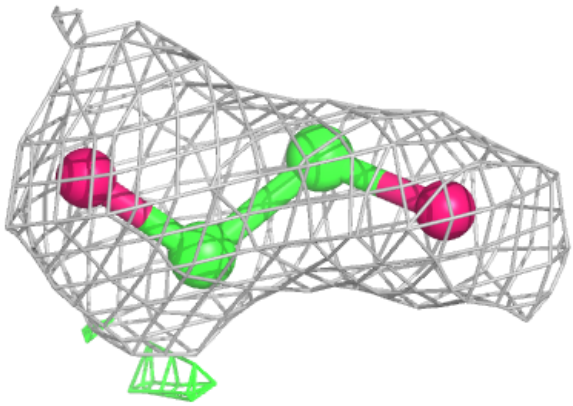


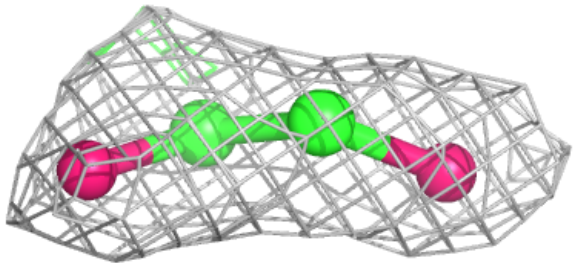


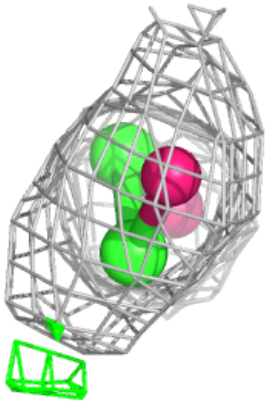


Electron density around EDO D 806:

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

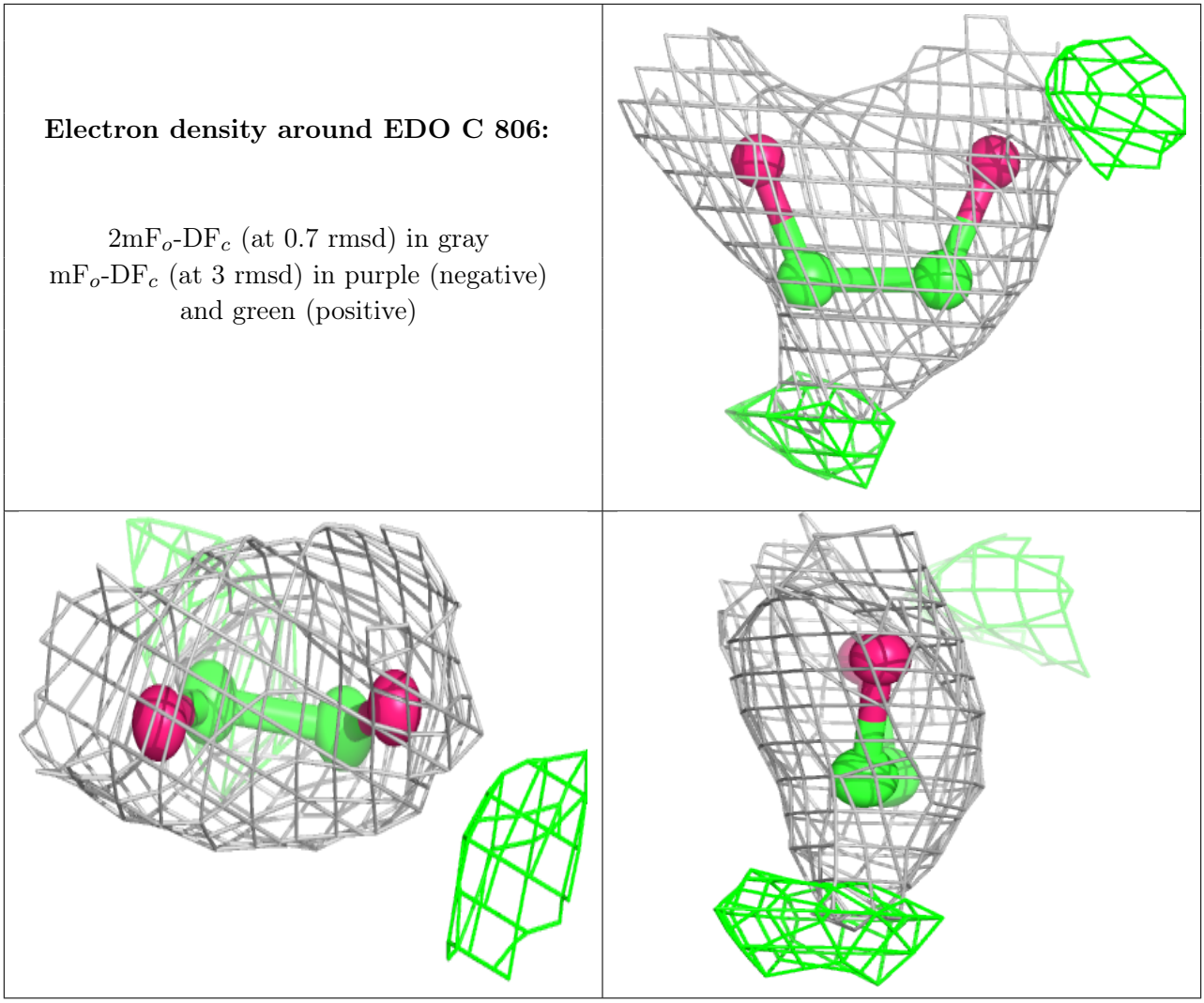






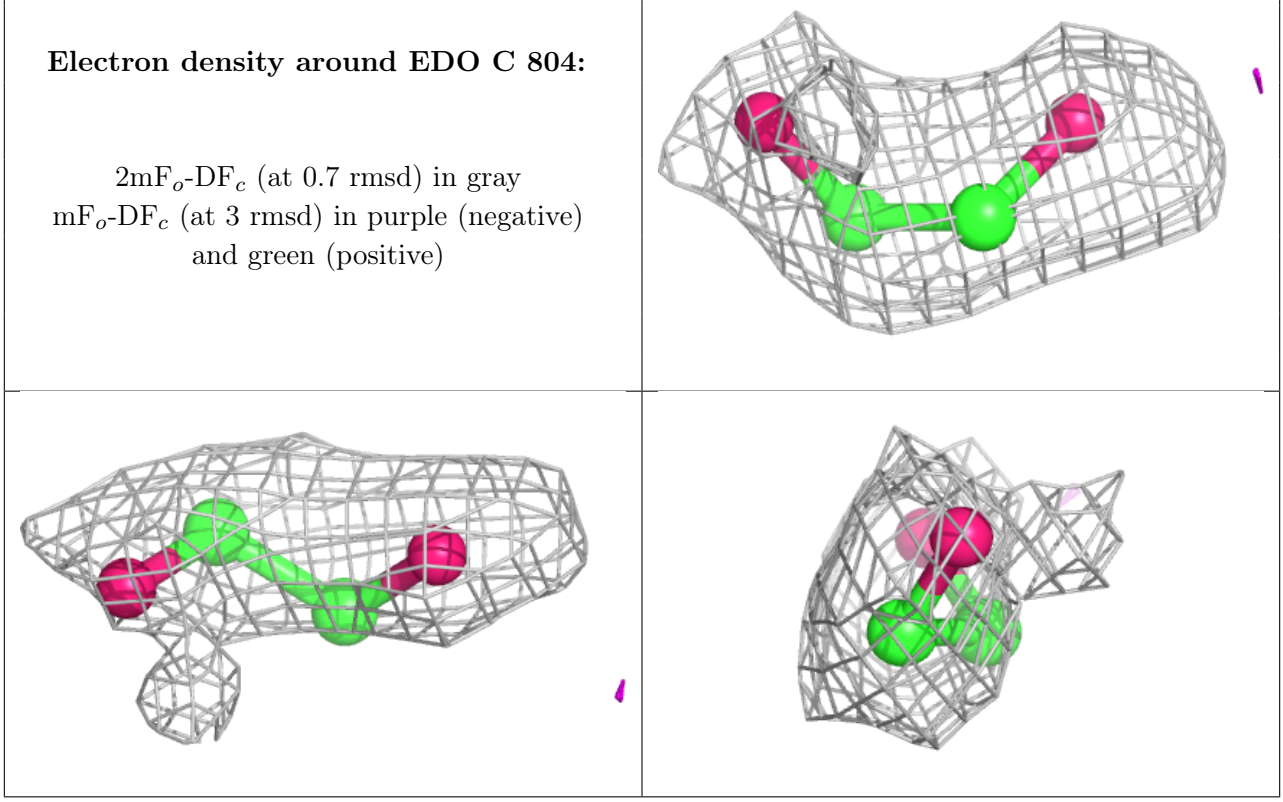
Electron density around EDO C 806:

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



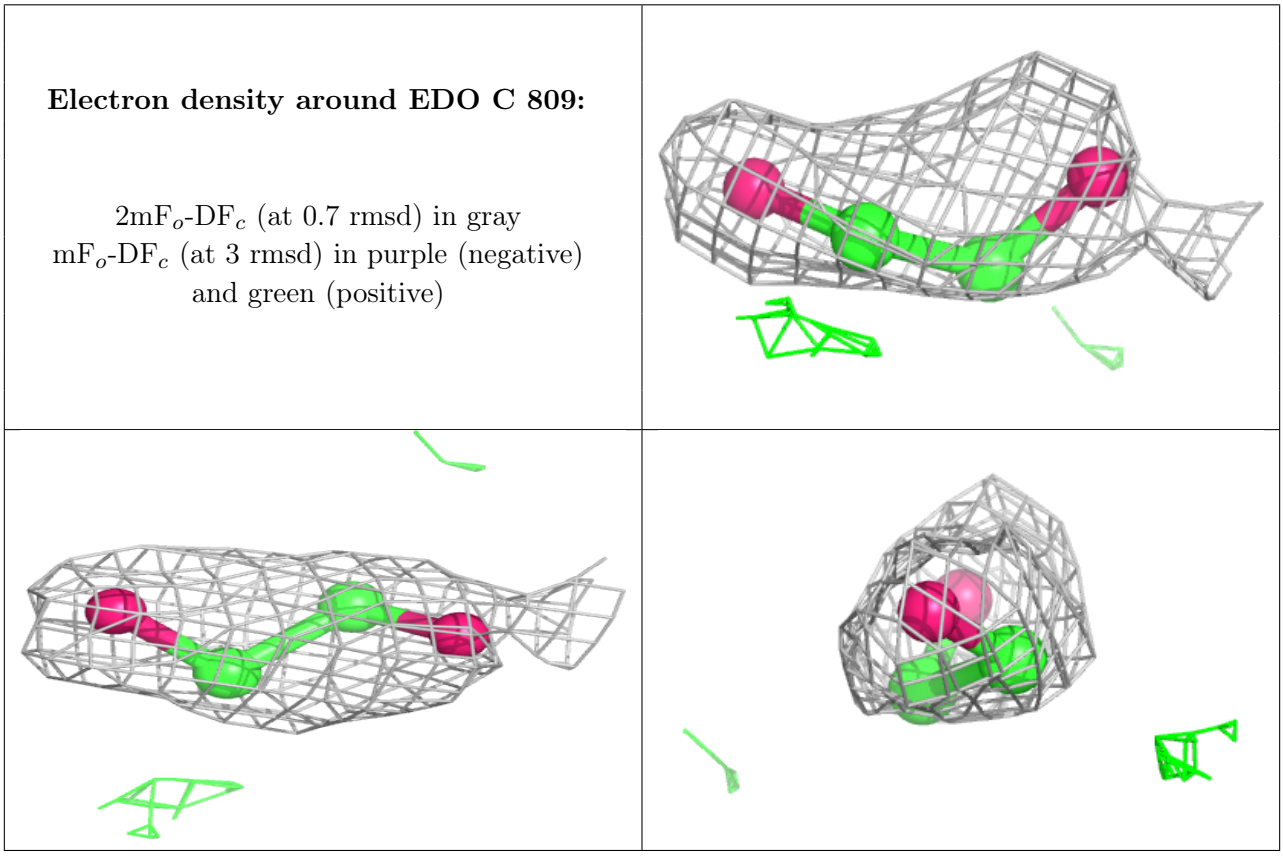
Electron density around EDO C 804:

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



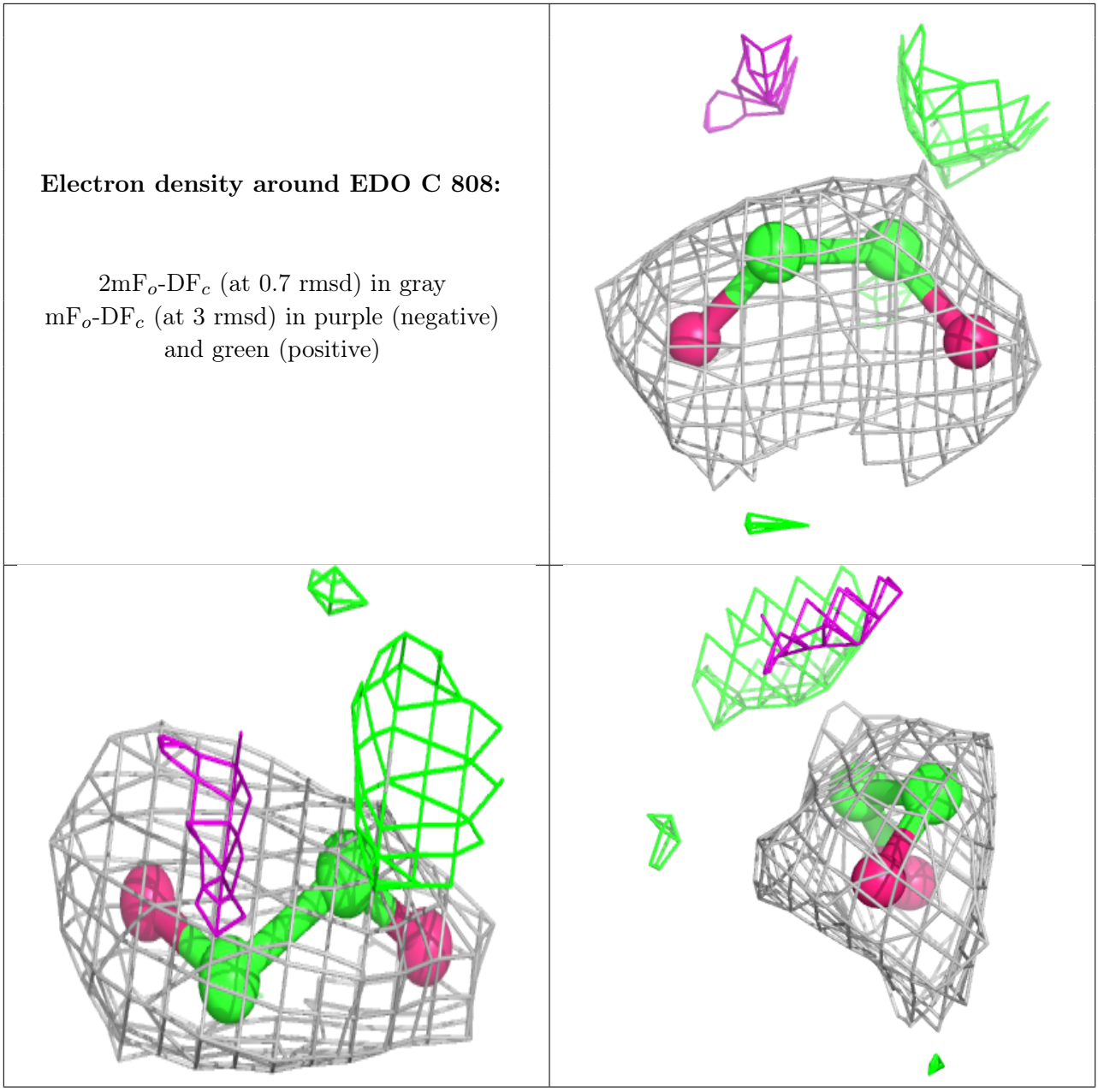
Electron density around EDO C 809:

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



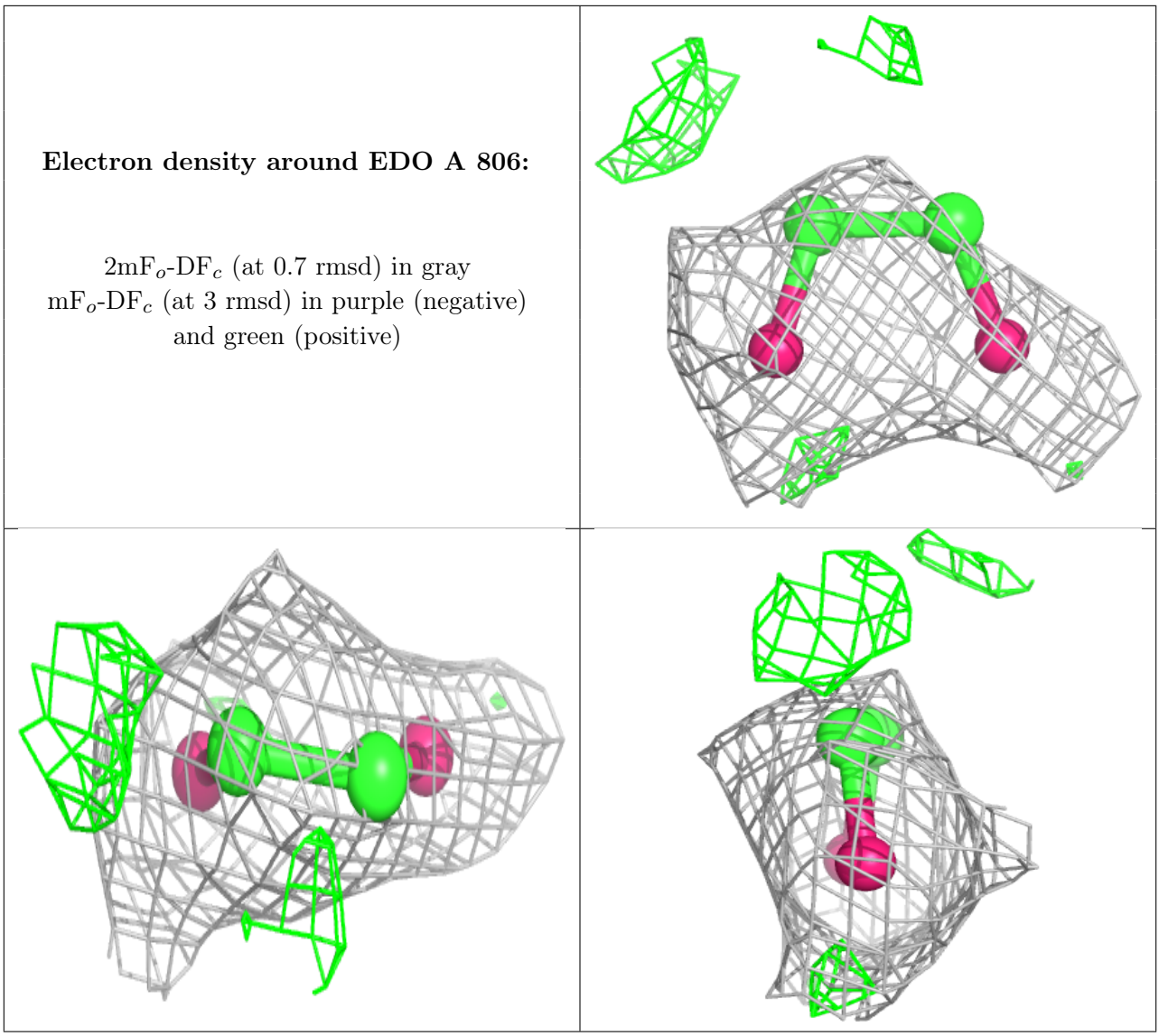
Electron density around EDO C 808:

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



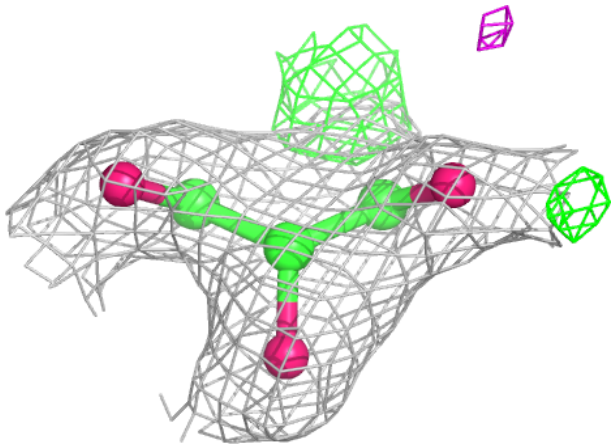
Electron density around EDO A 806:

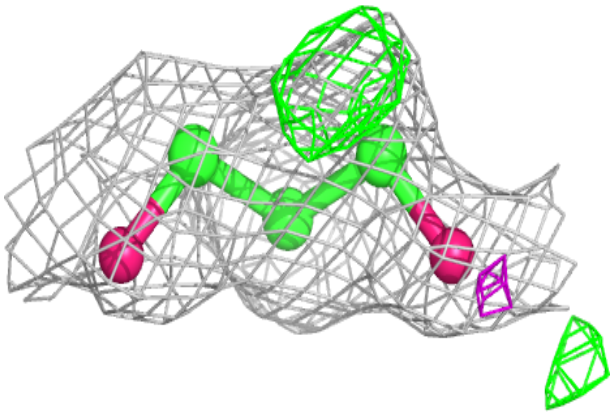
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

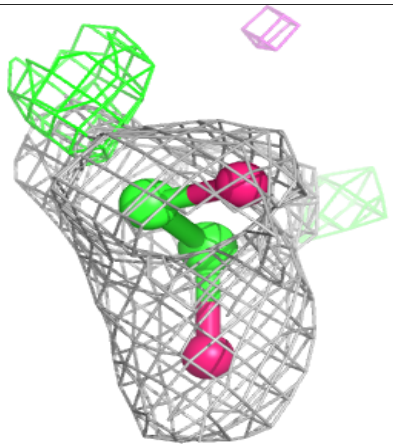


Electron density around GOL B 810:

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

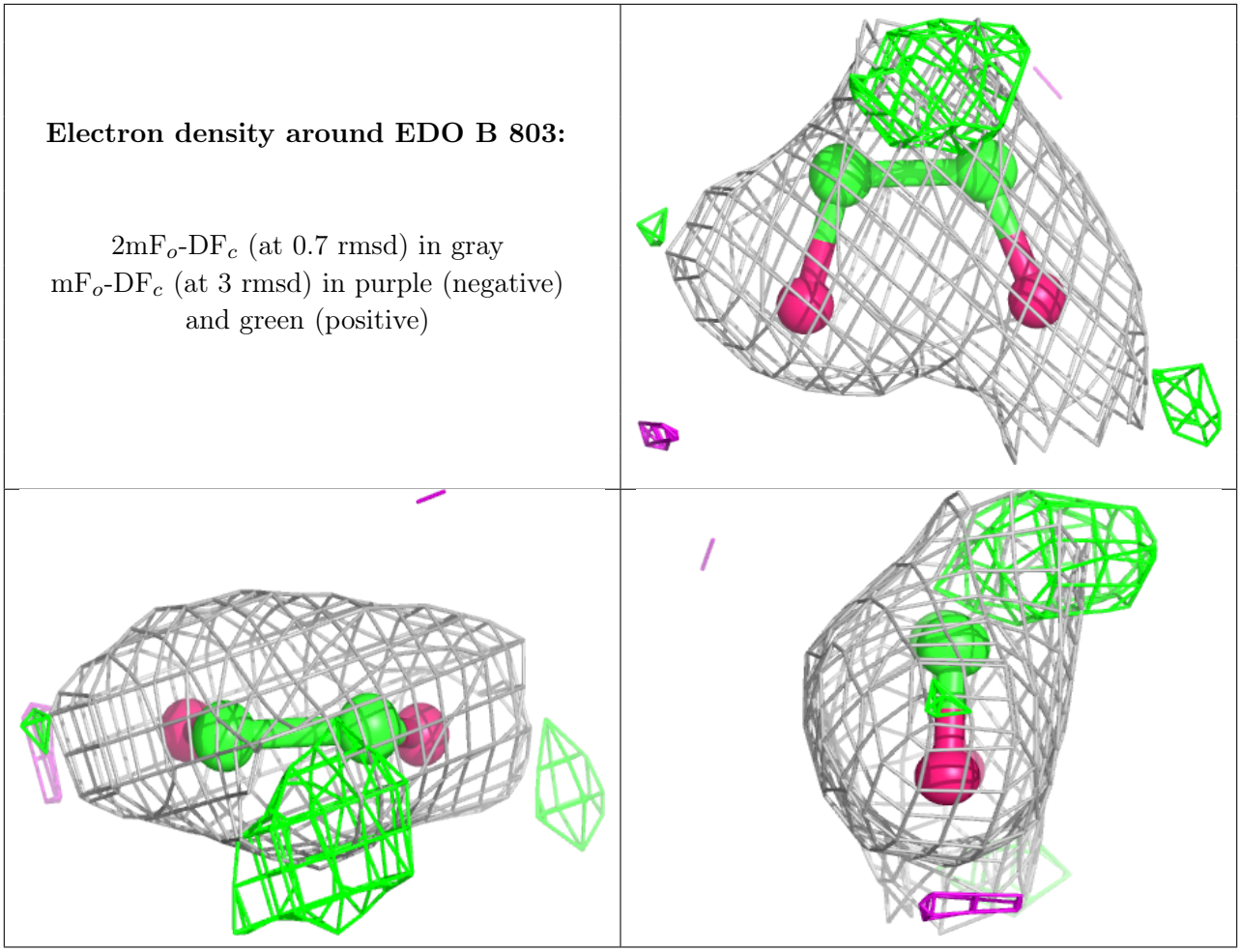






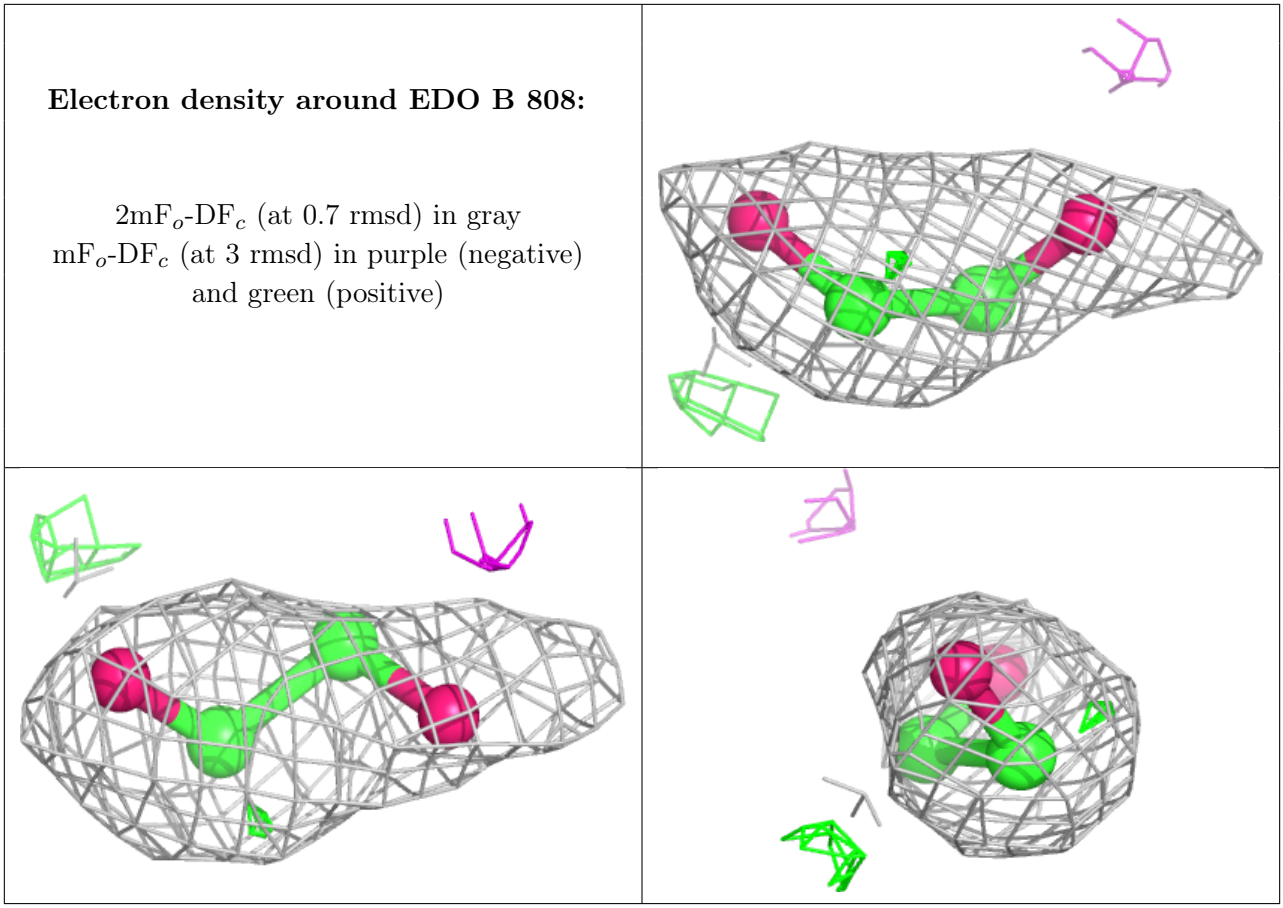
Electron density around EDO B 803:

$2mF_o$-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 808:

$2mF_o$-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 805:

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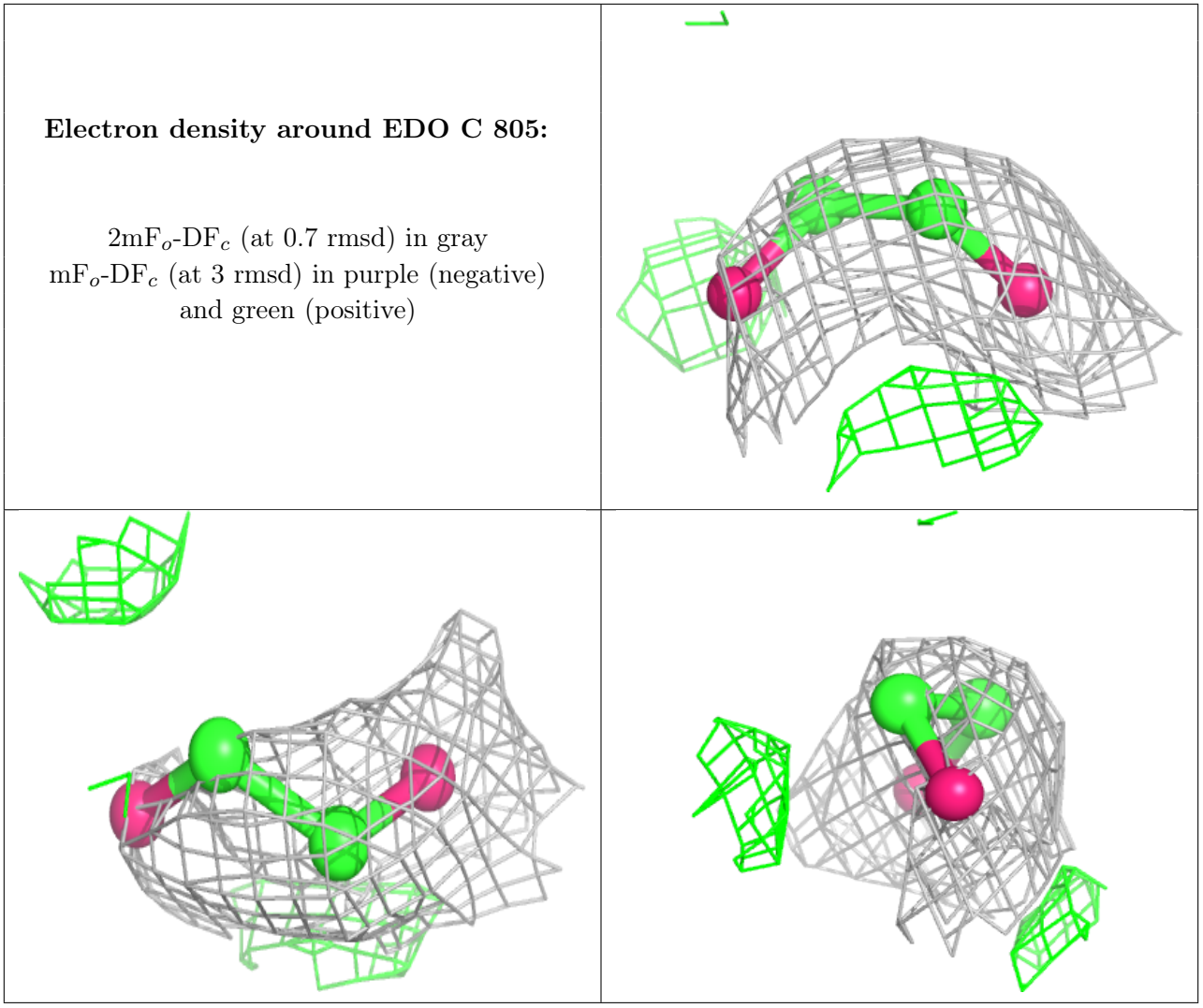
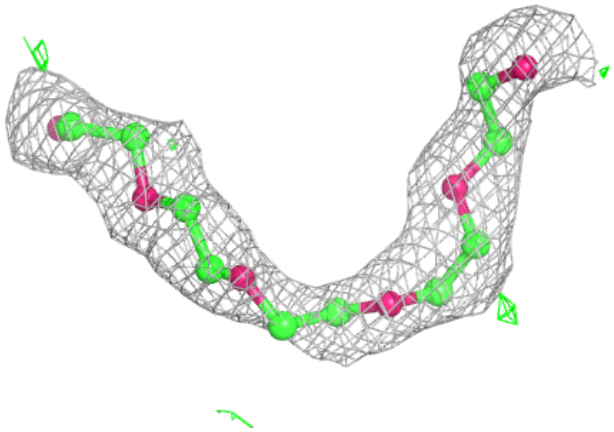
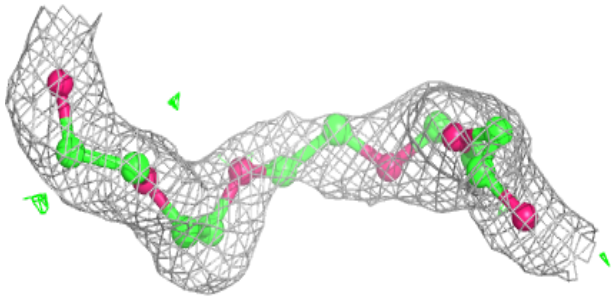
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

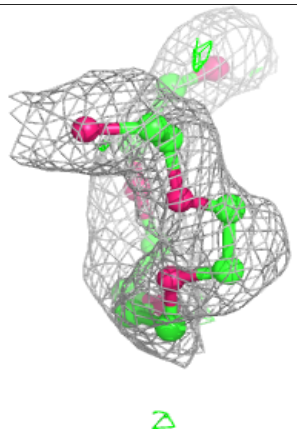


Electron density around 1PE A 809:

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

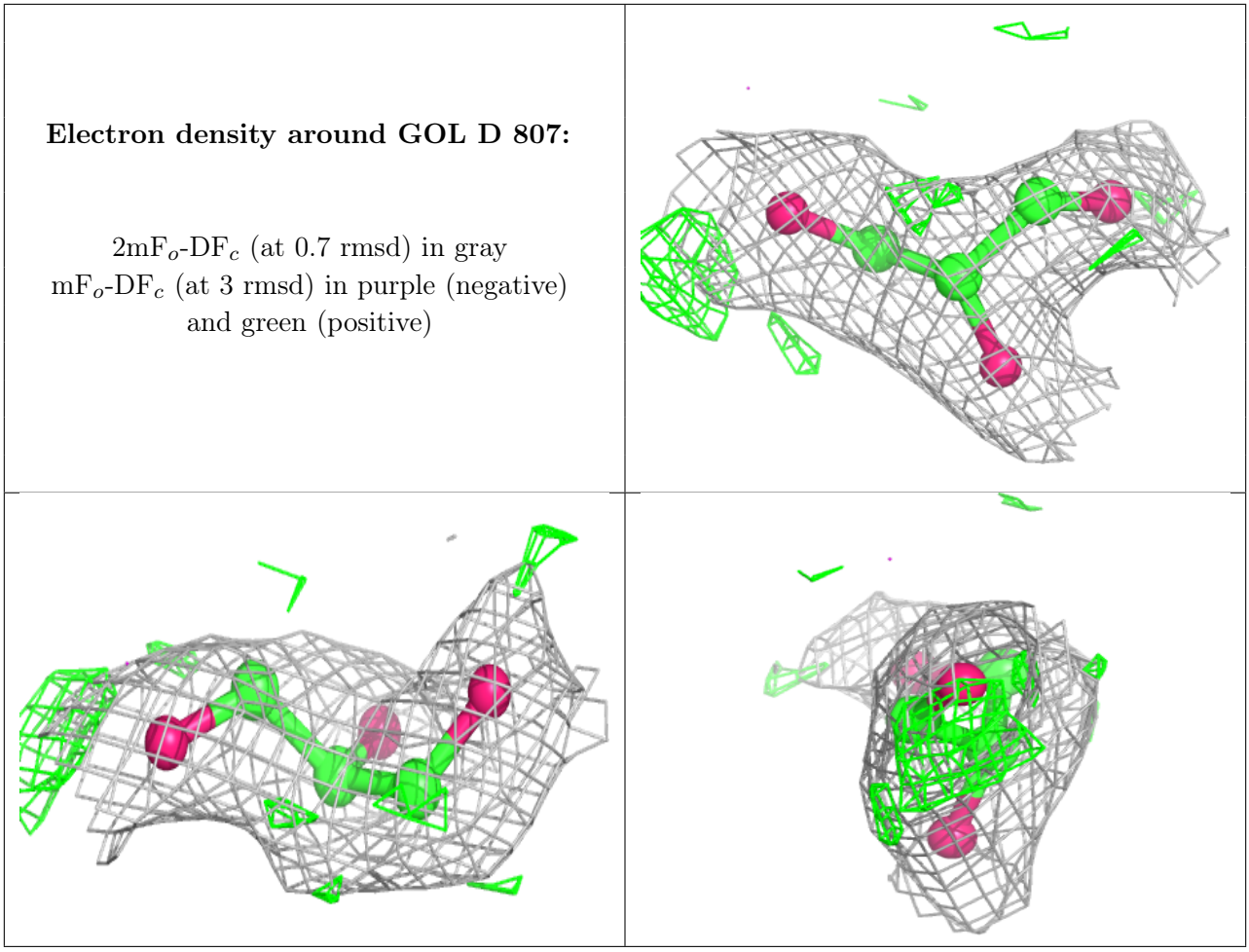






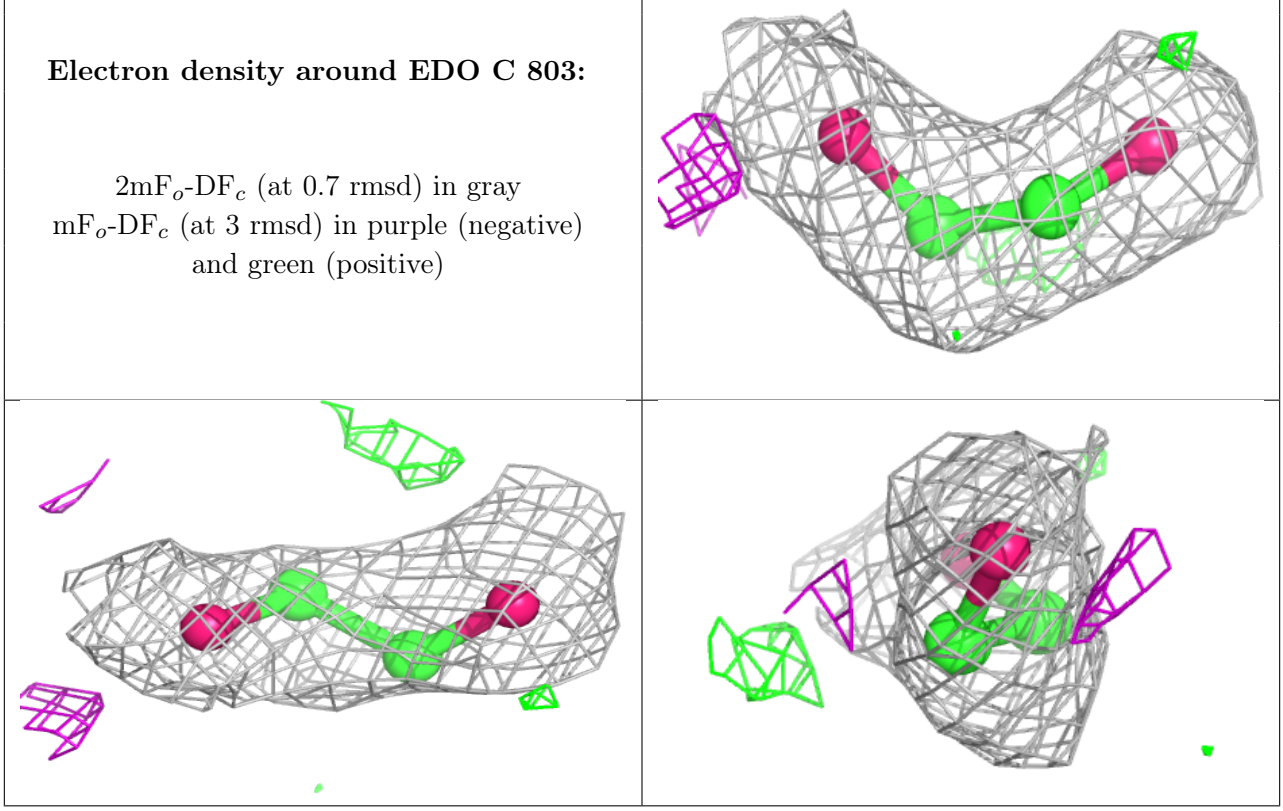
Electron density around GOL D 807:

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



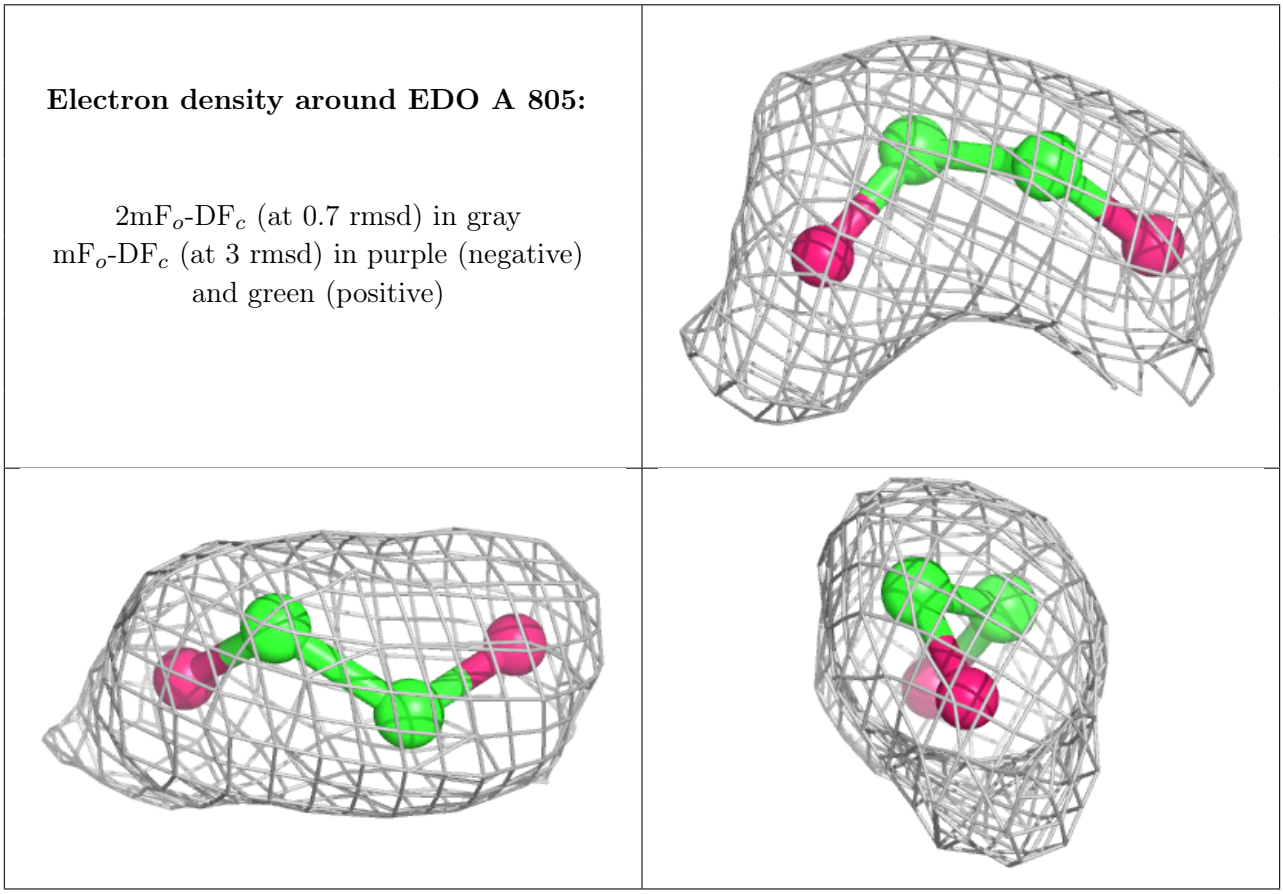
Electron density around EDO C 803:

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



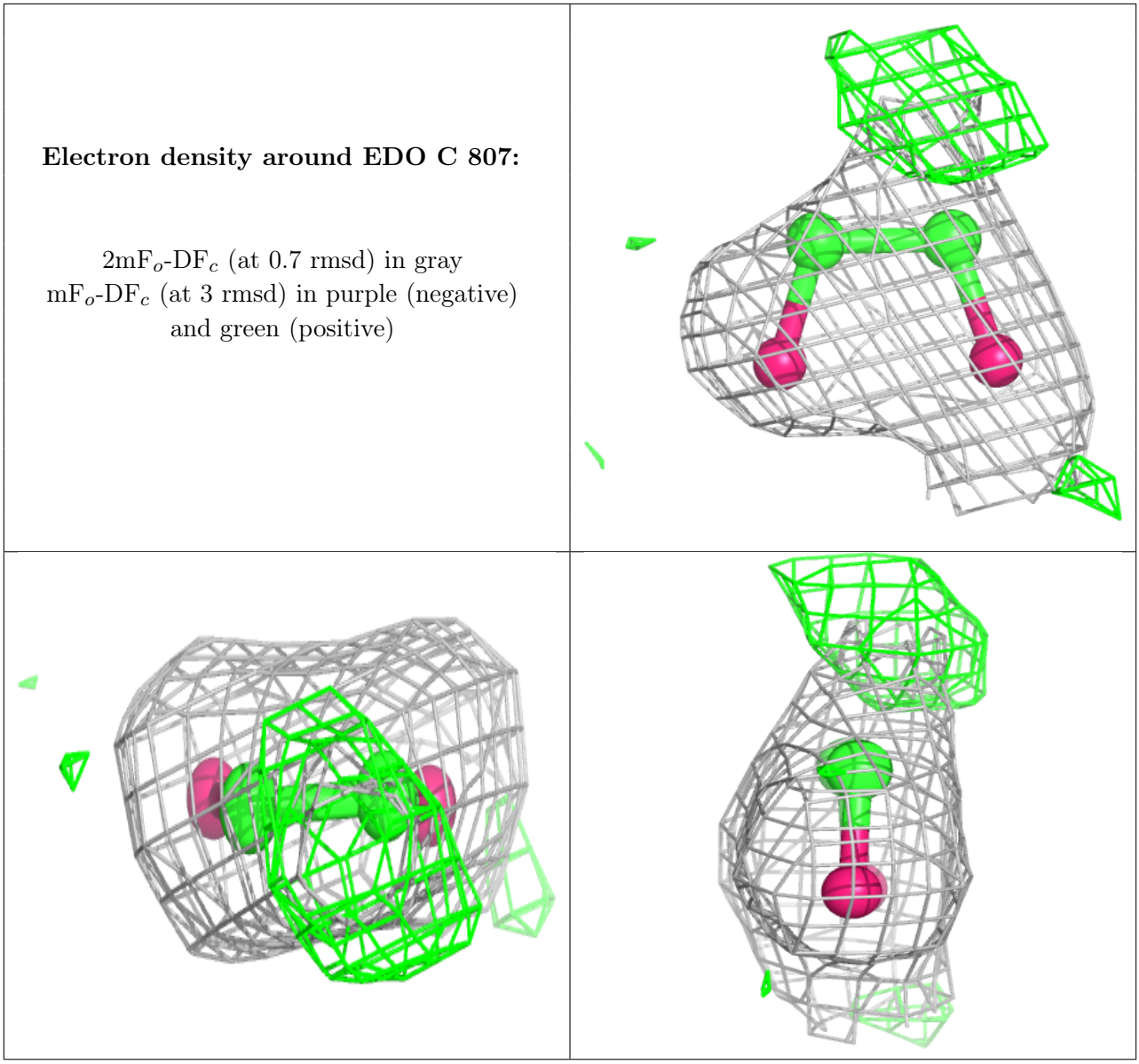
Electron density around EDO A 805:

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



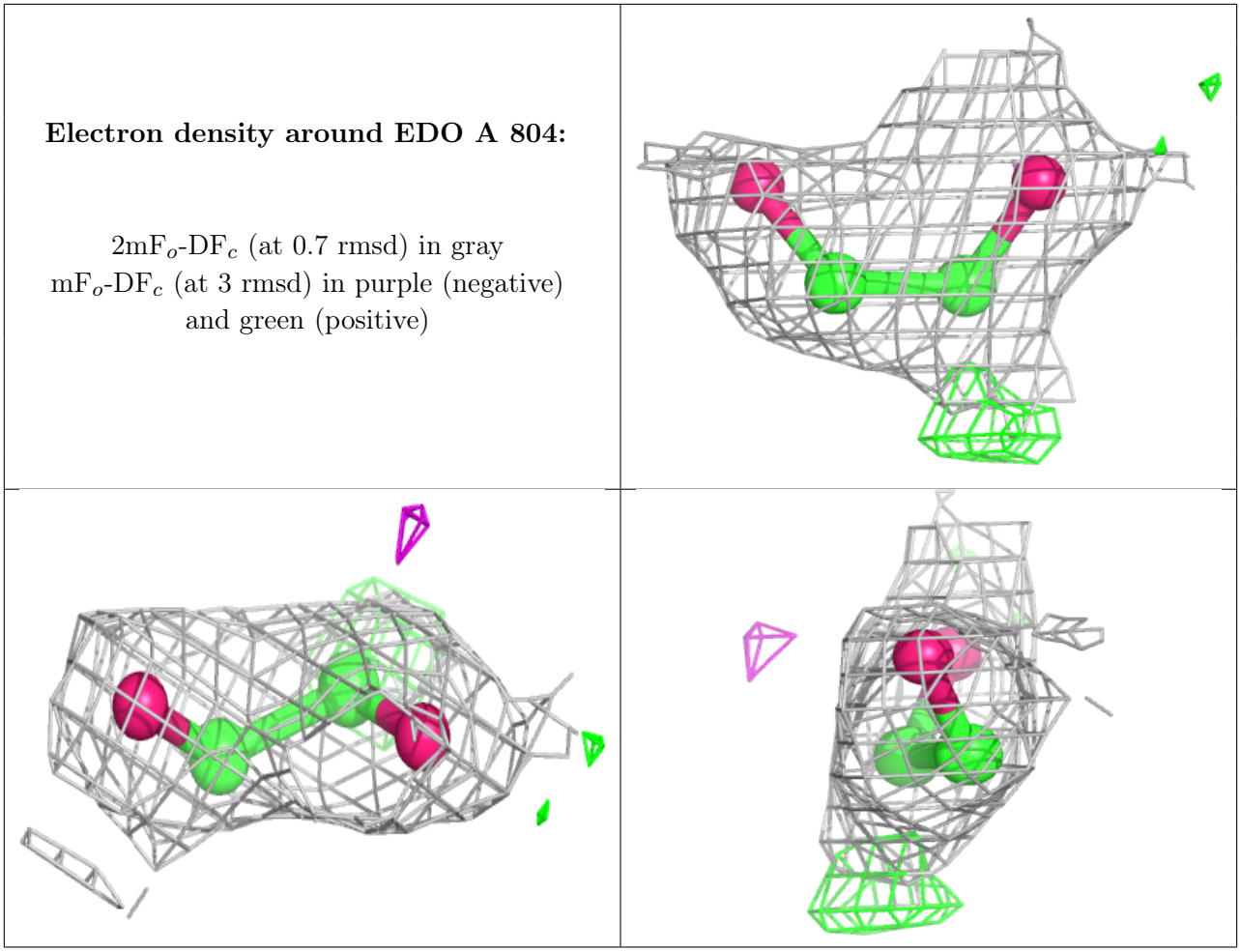
Electron density around EDO C 807:

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



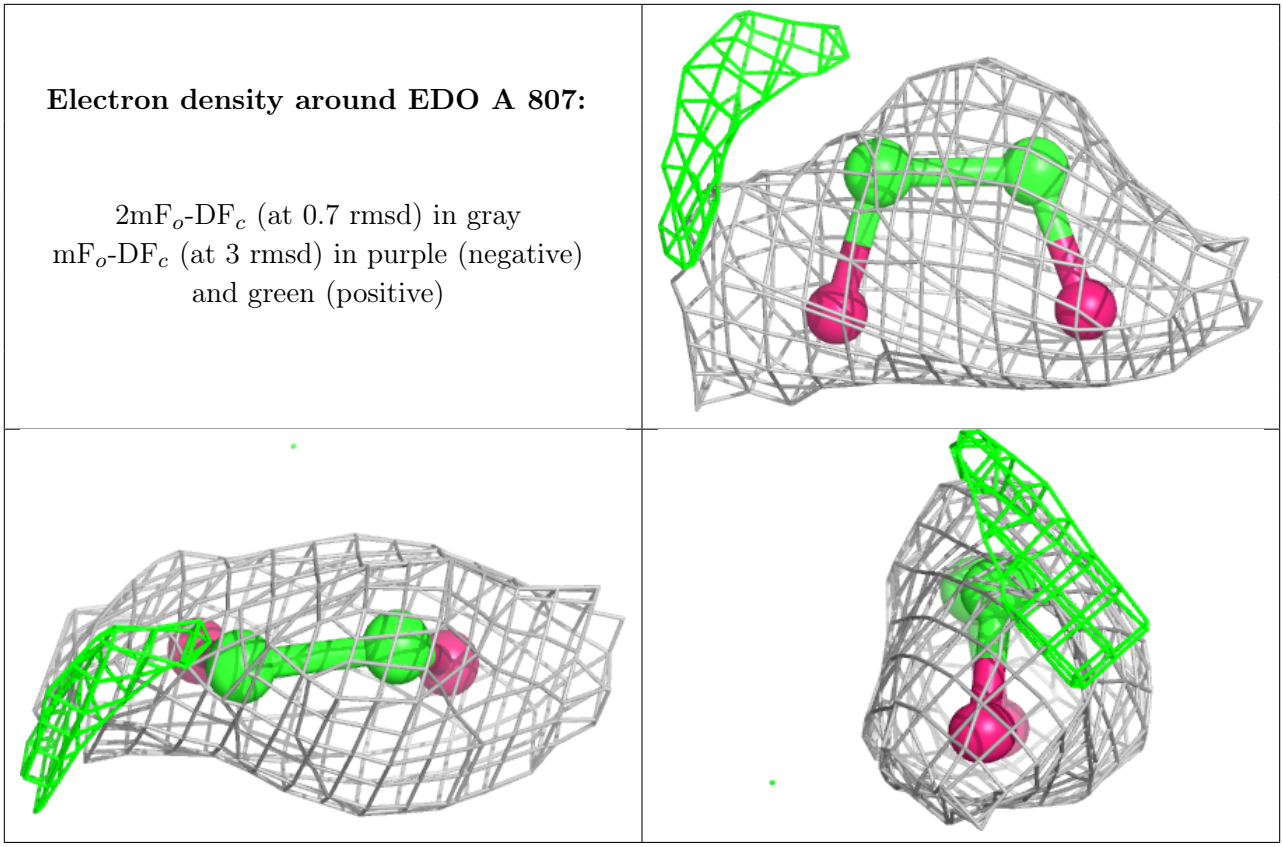
Electron density around EDO A 804:

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



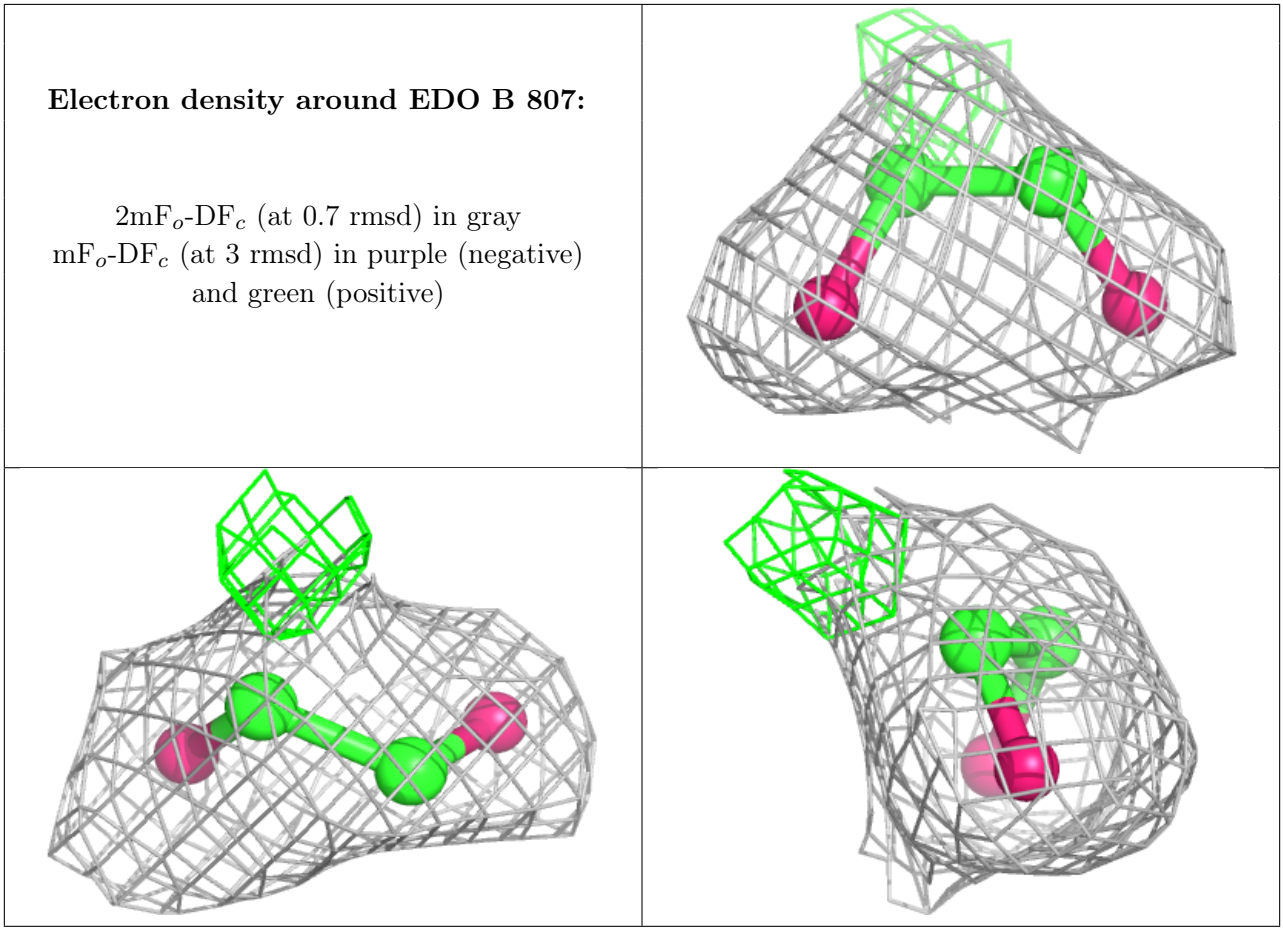
Electron density around EDO A 807:

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



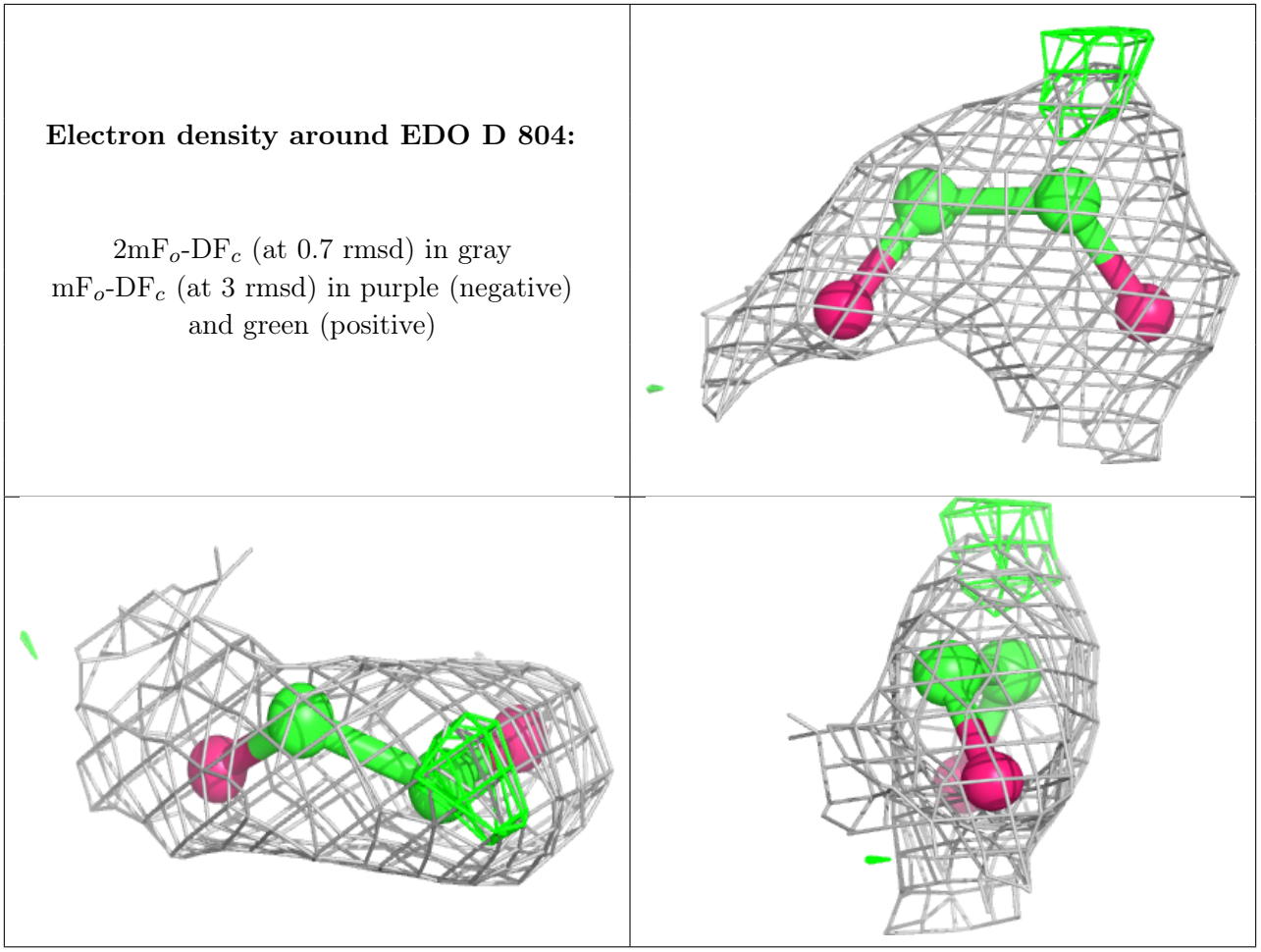
Electron density around EDO B 807:

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



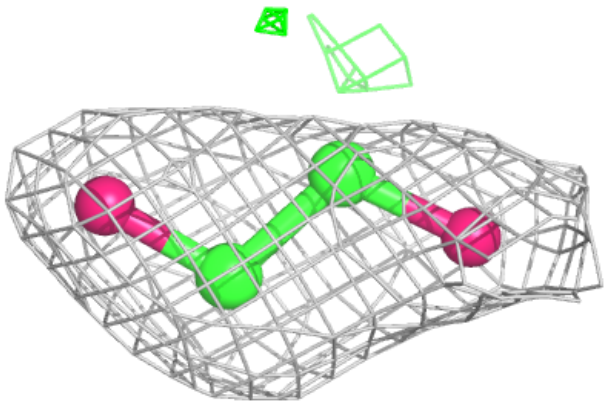
Electron density around EDO D 804:

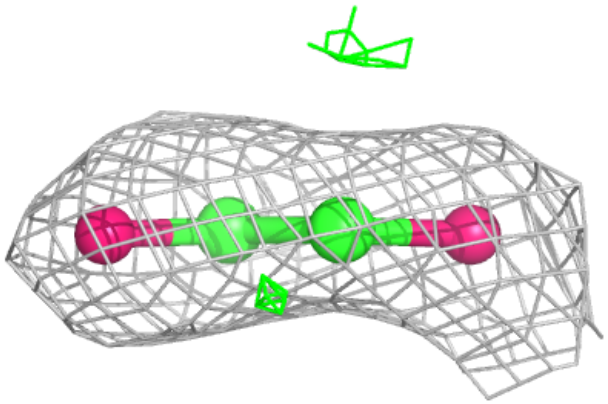
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

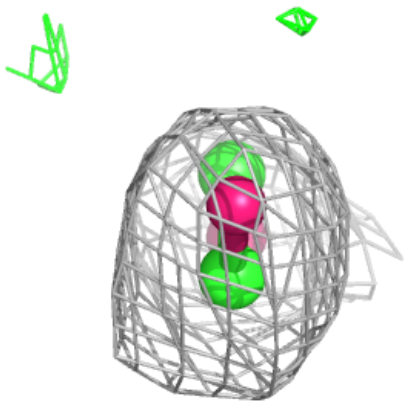


Electron density around EDO D 805:

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

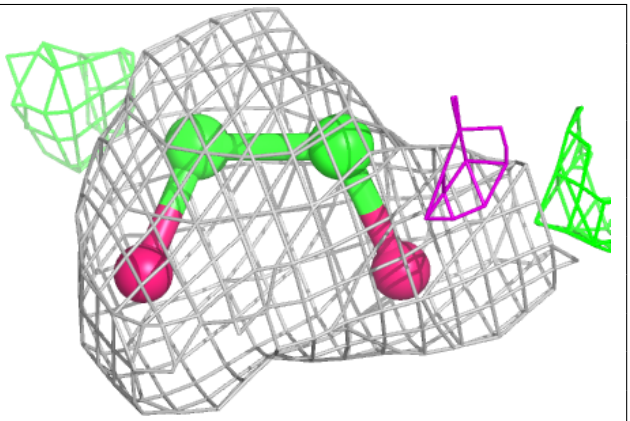


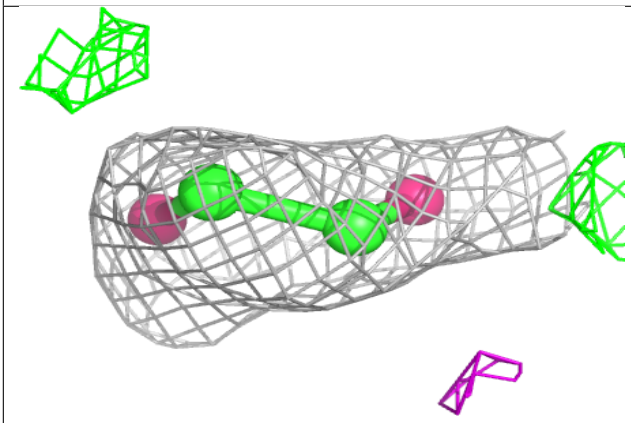


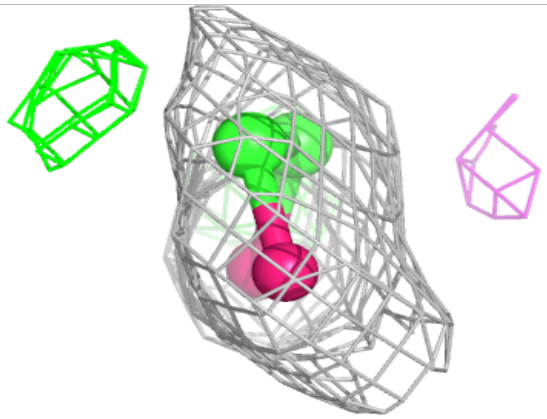


Electron density around EDO B 804:

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

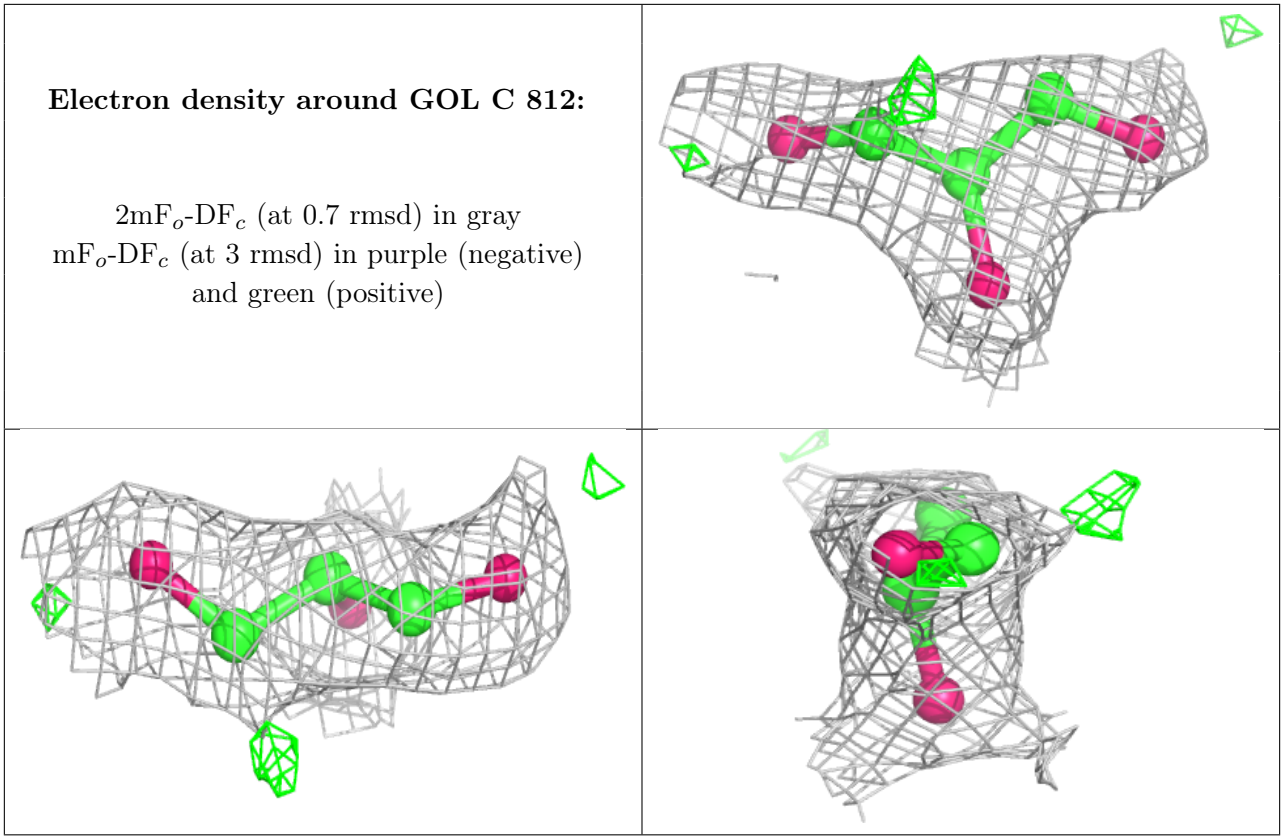






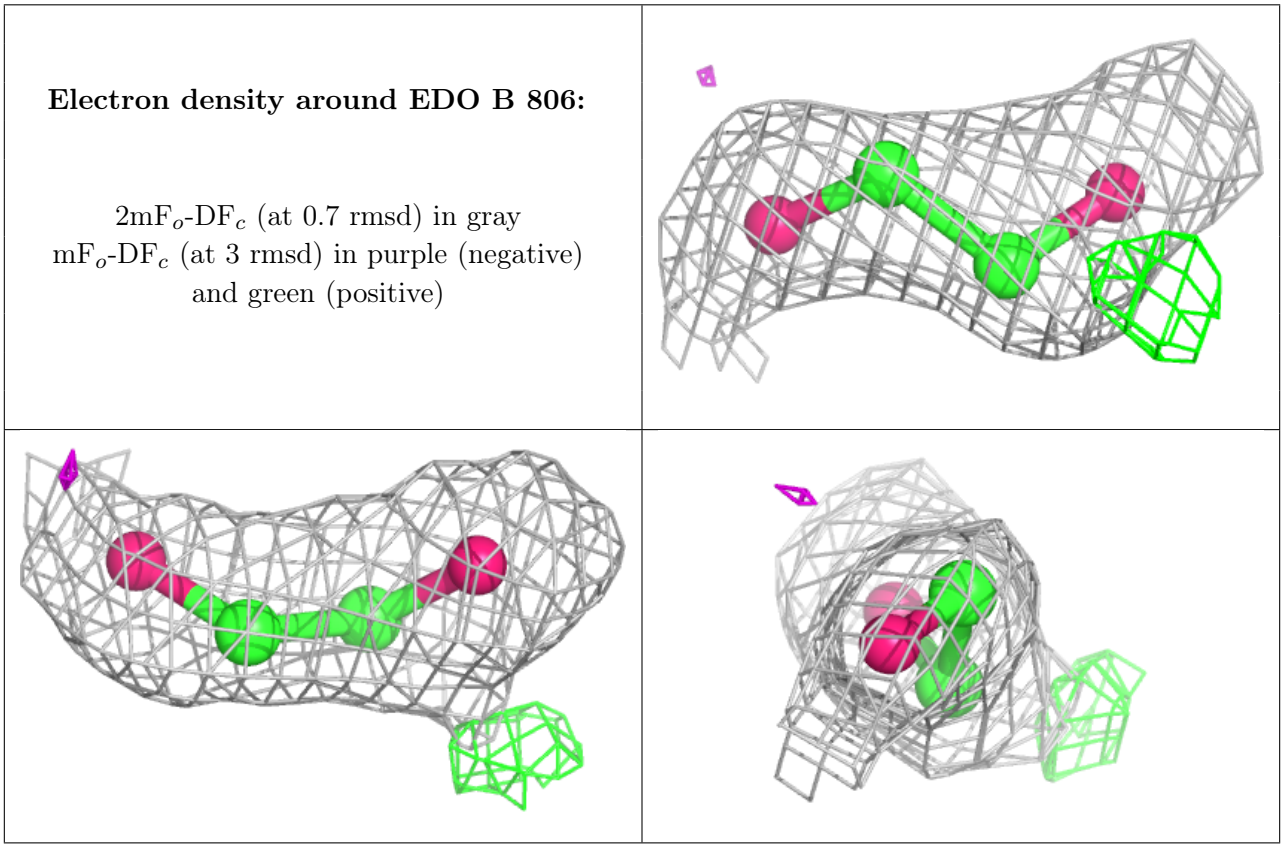
Electron density around GOL C 812:

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



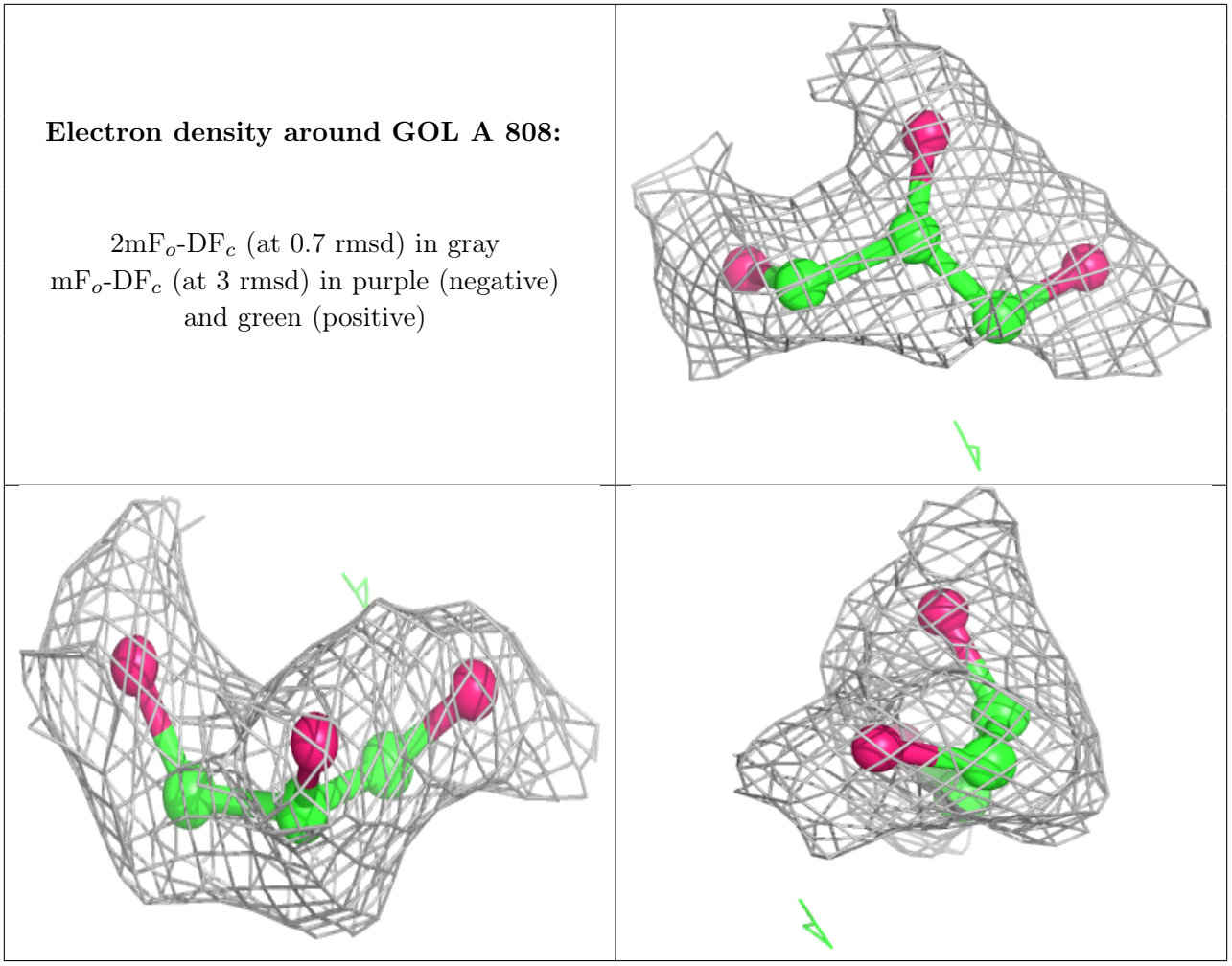
Electron density around EDO B 806:

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



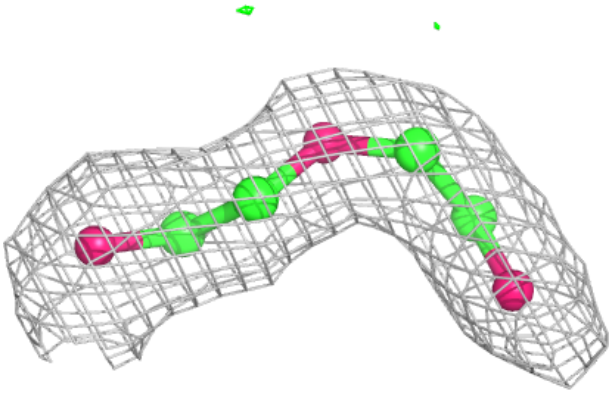
Electron density around GOL A 808:

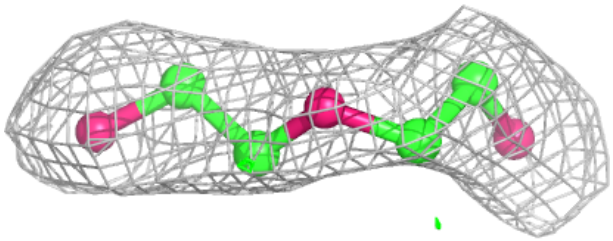
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

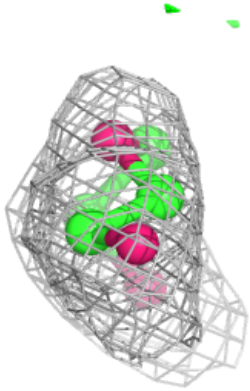


Electron density around PEG D 808:

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

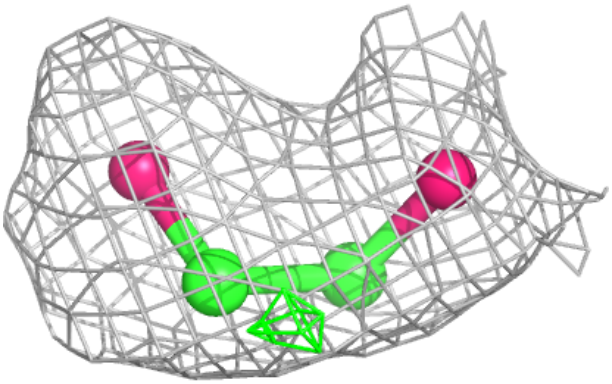


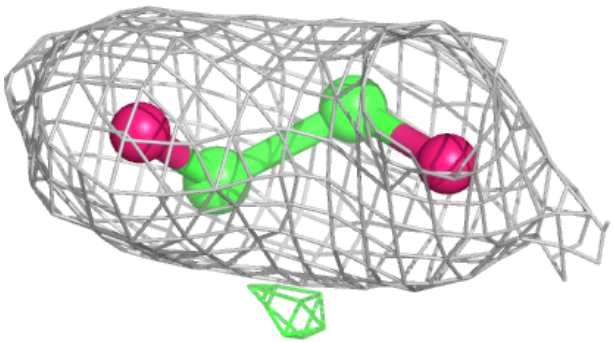


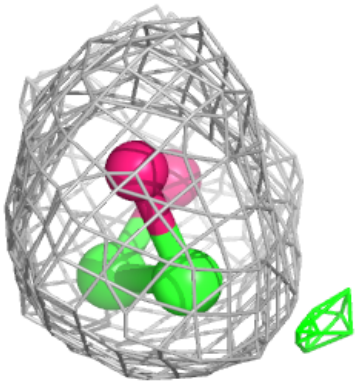


Electron density around EDO D 803:

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

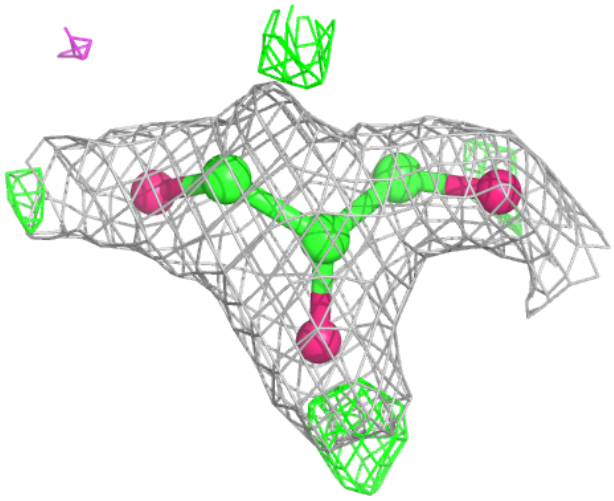


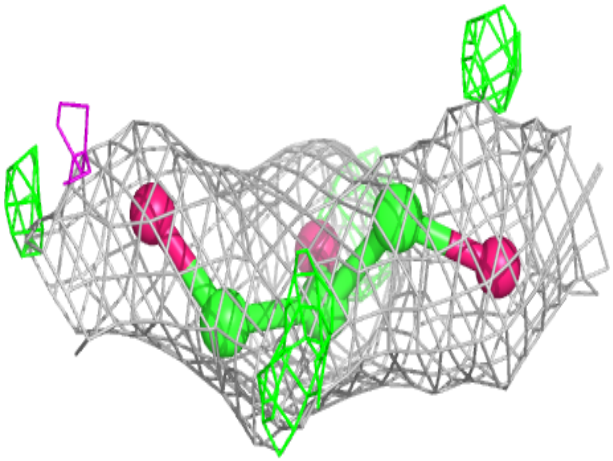


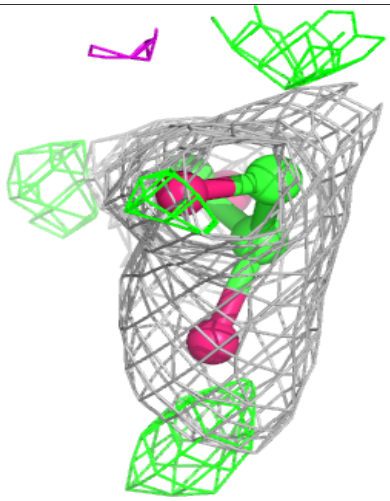


Electron density around GOL C 811:

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

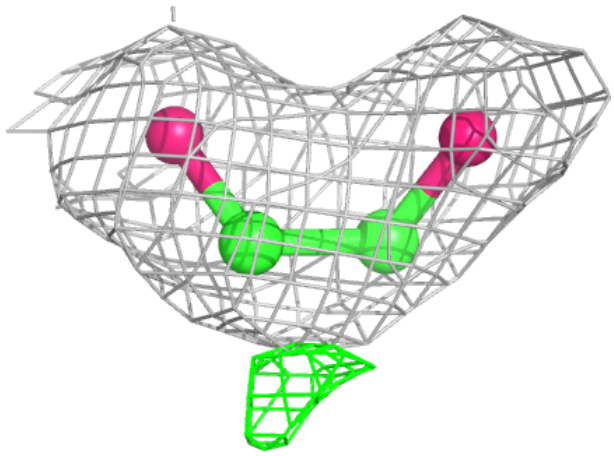


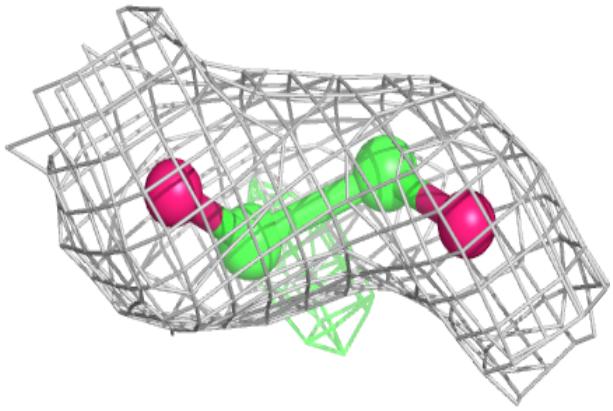


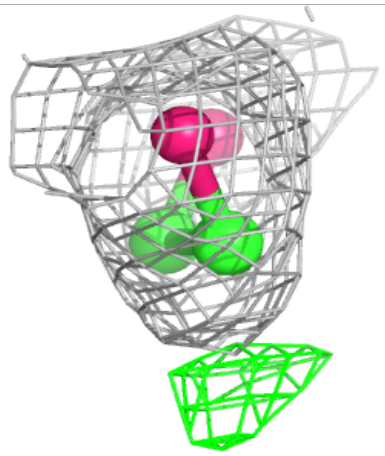


Electron density around EDO A 803:

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

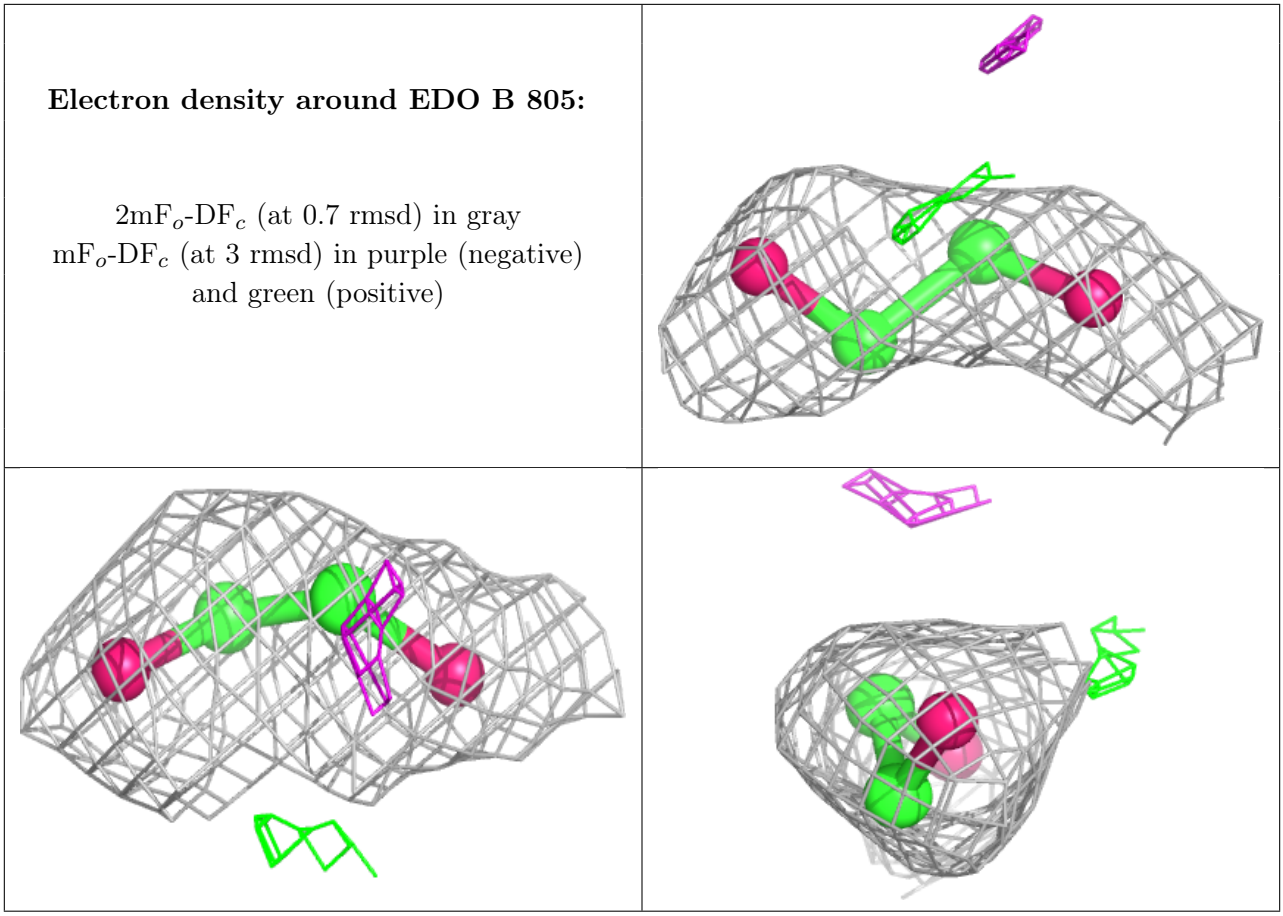






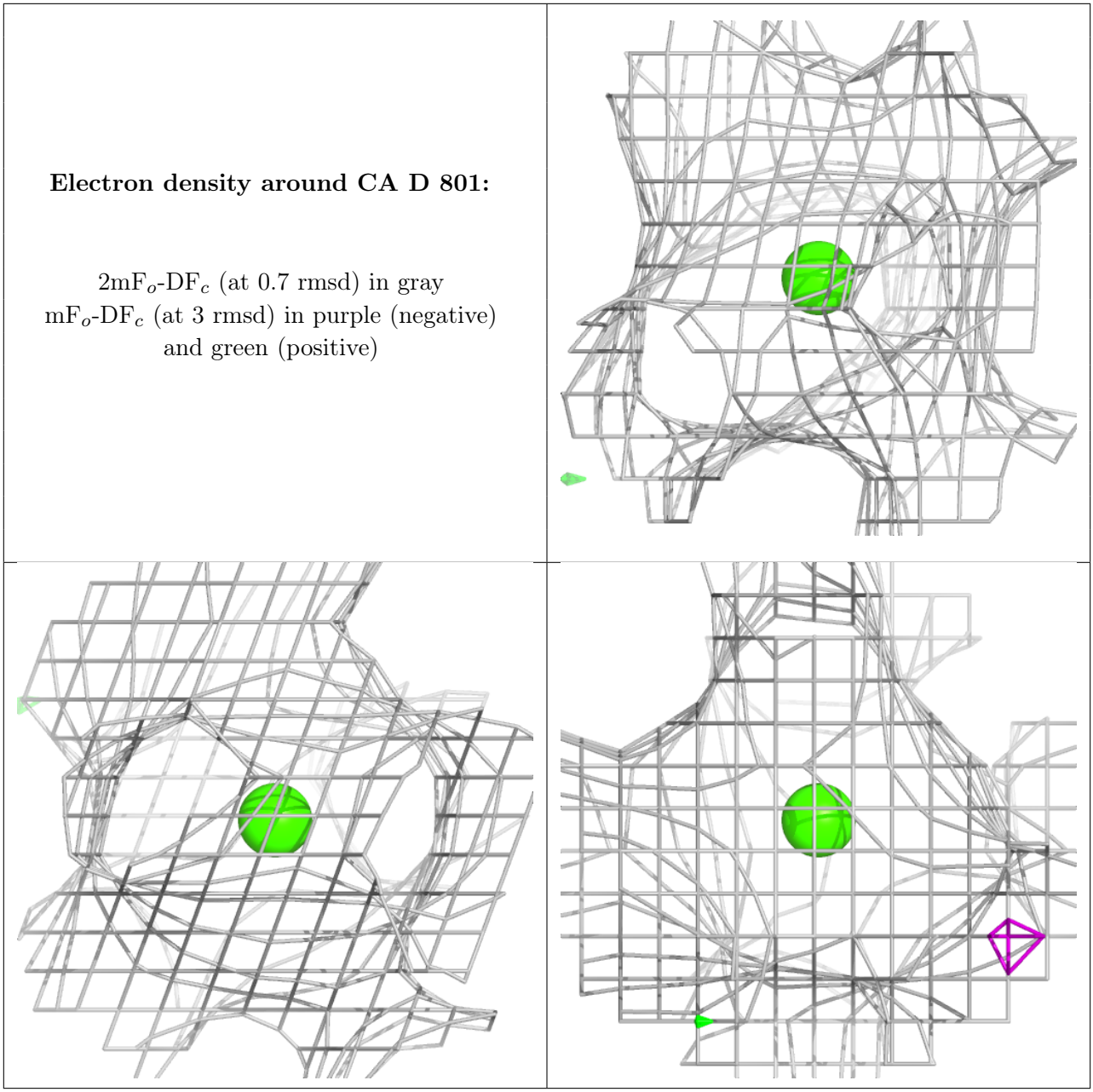
Electron density around EDO B 805:

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



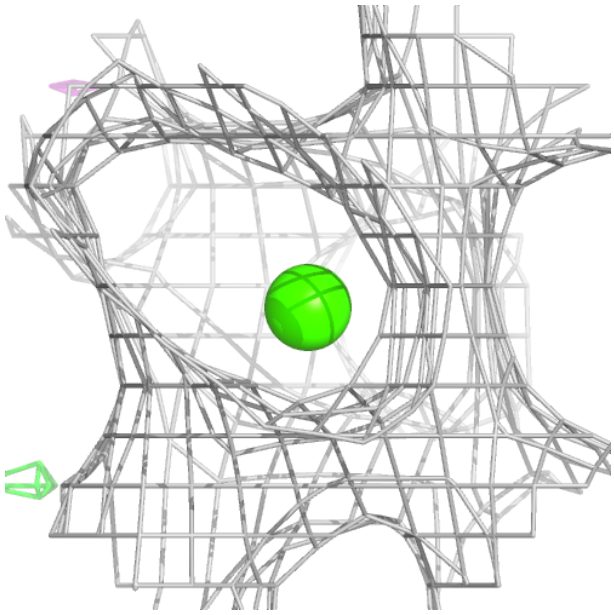
Electron density around CA D 801:

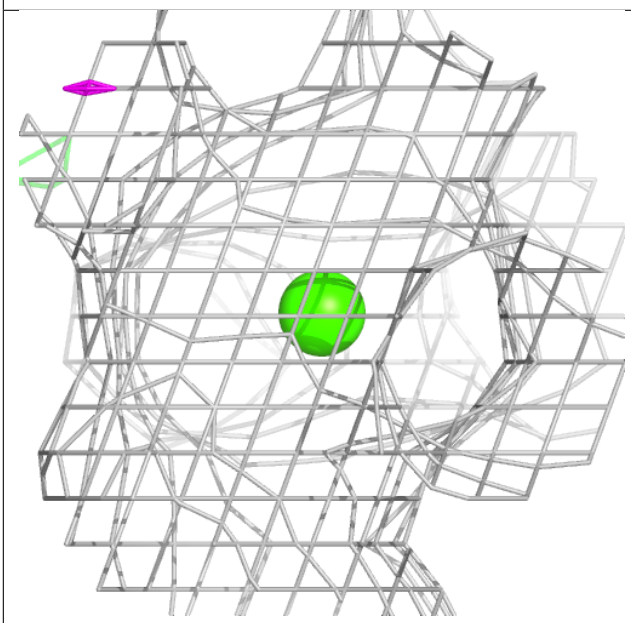
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

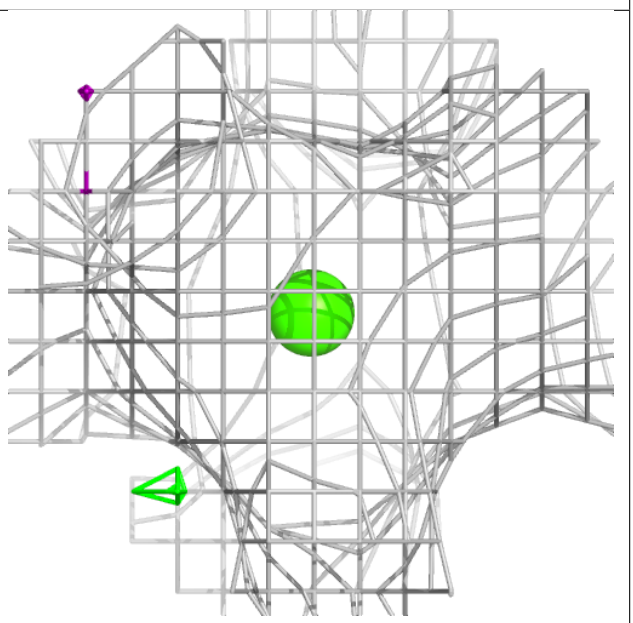


Electron density around CA A 801:

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

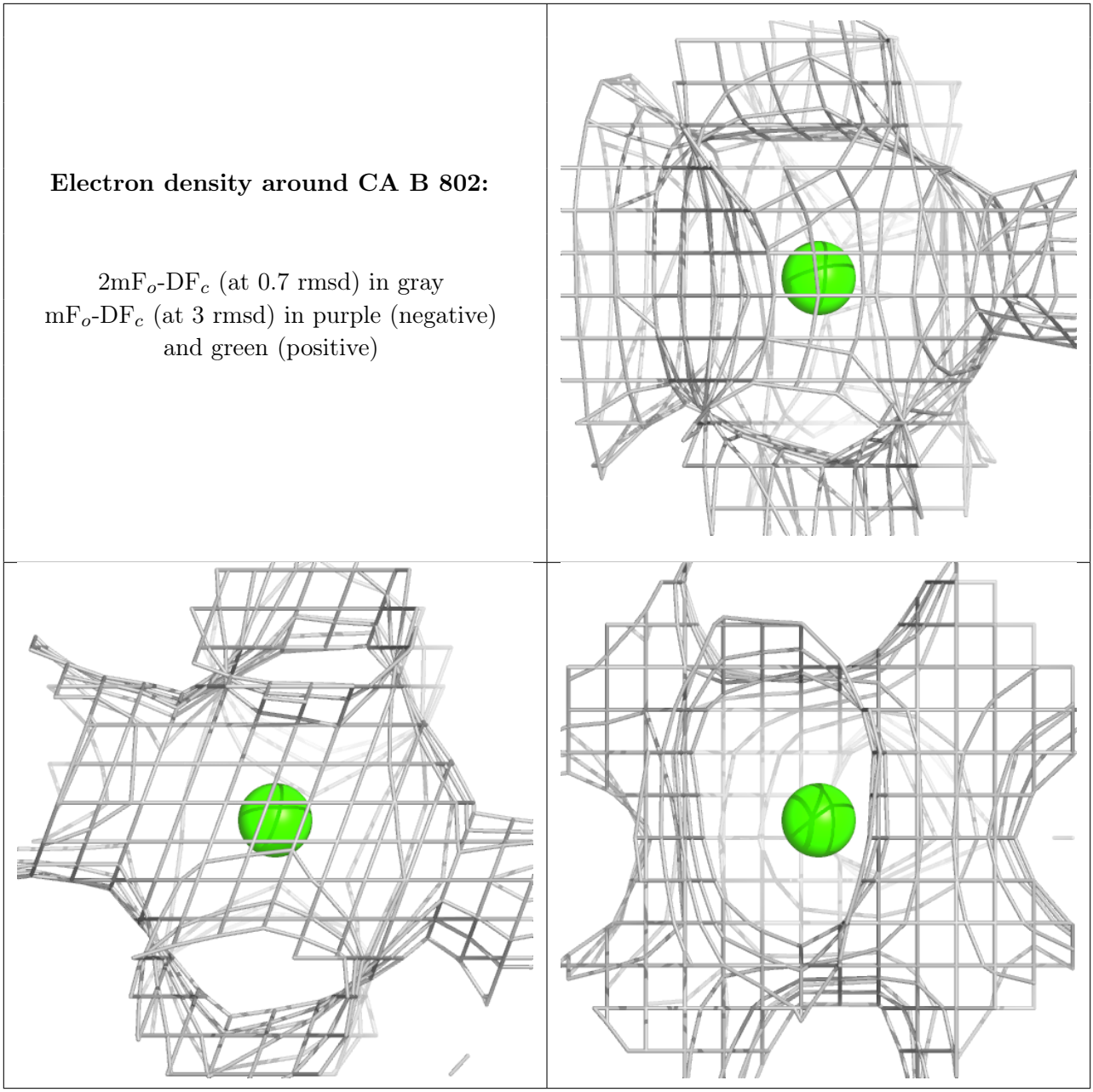






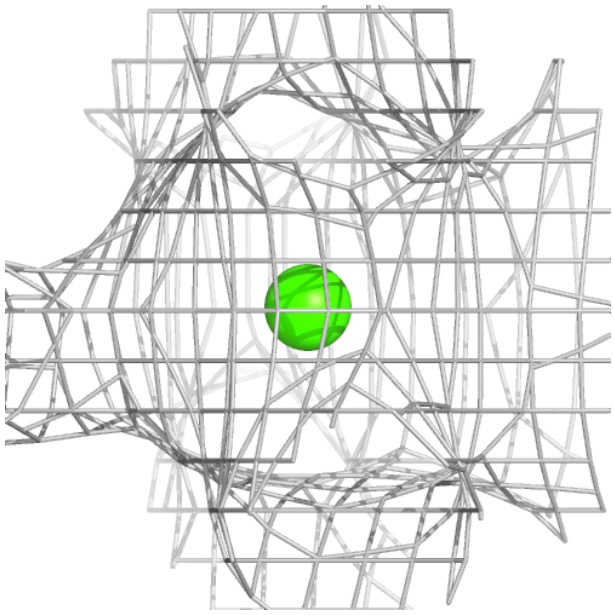
Electron density around CA B 802:

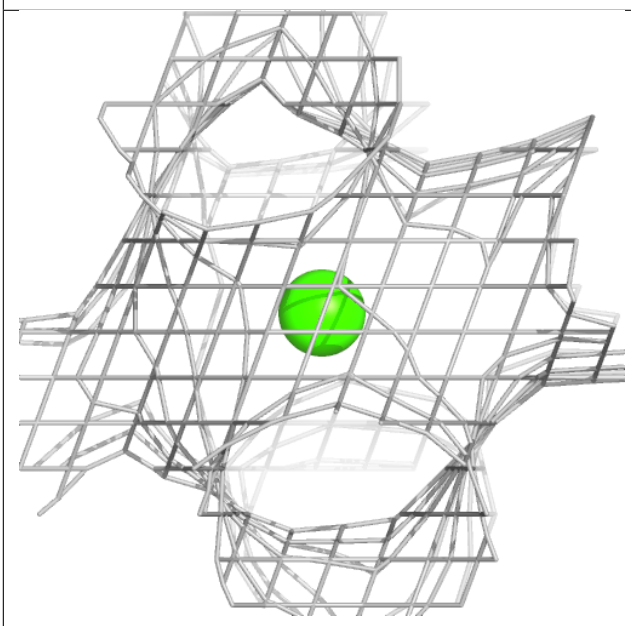
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CA C 802:

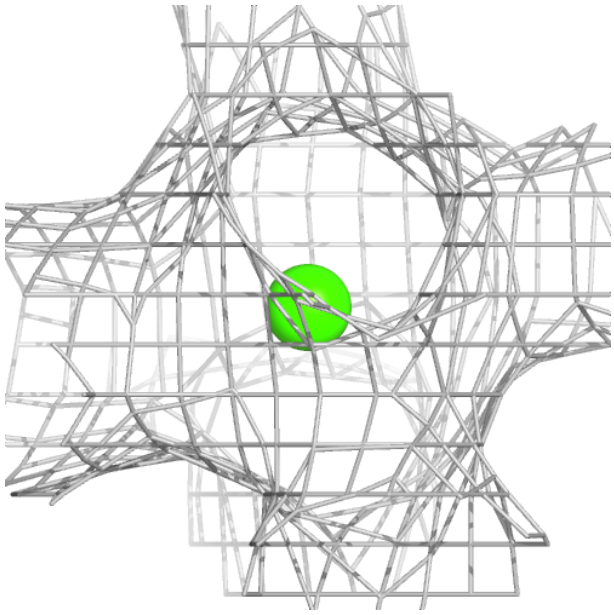
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

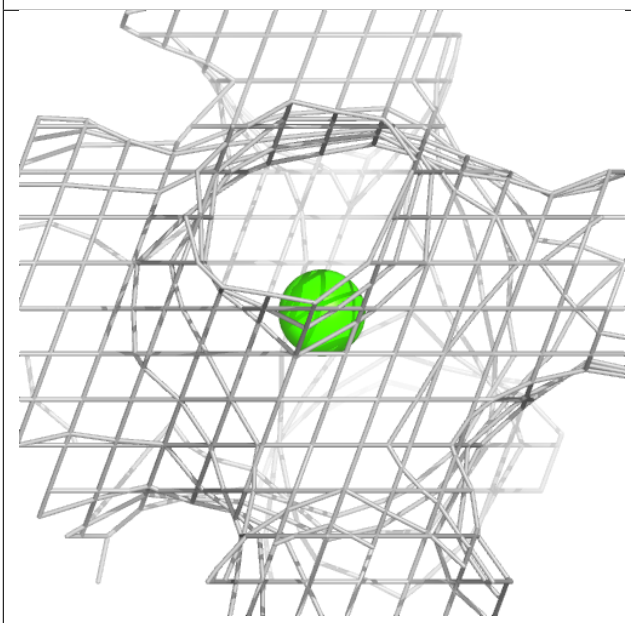


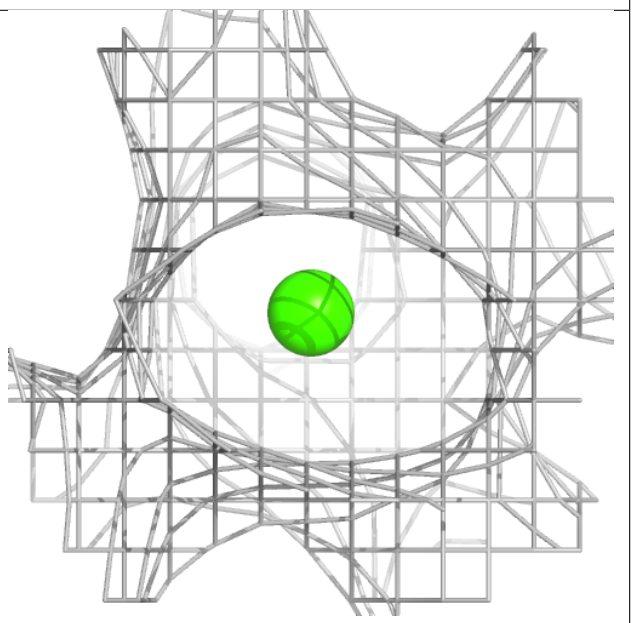


Electron density around CA D 802:

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

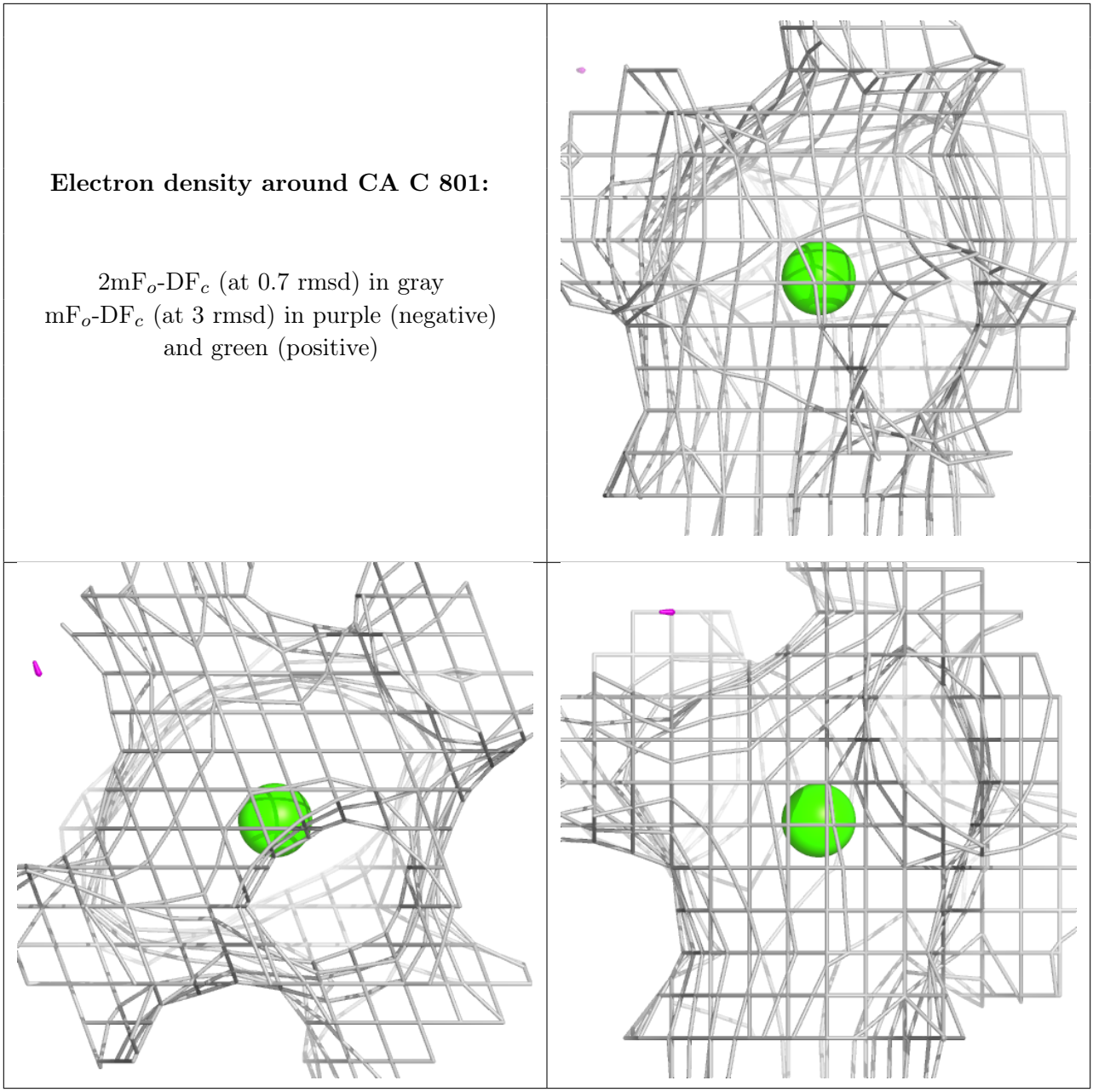






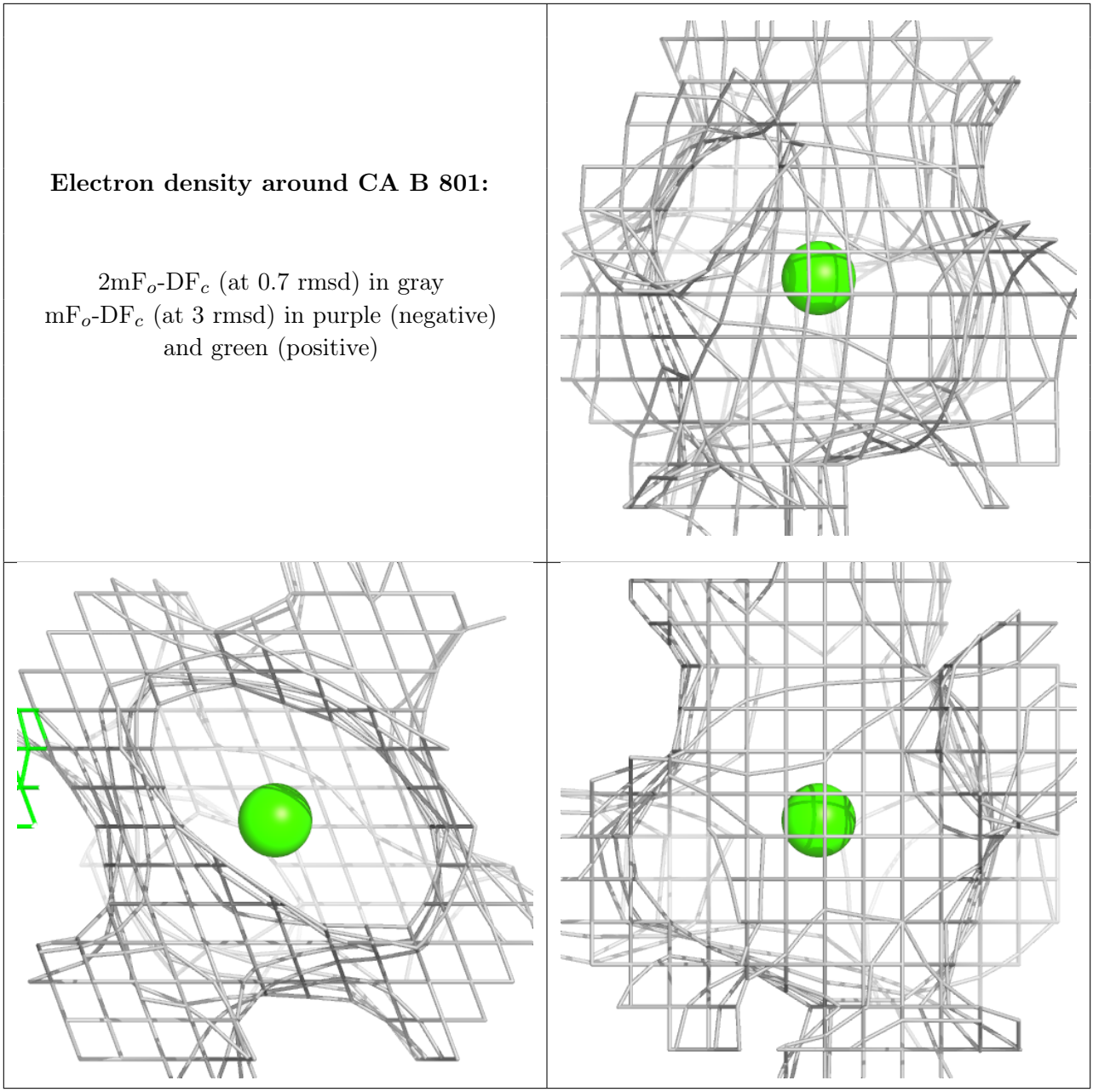
Electron density around CA C 801:

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



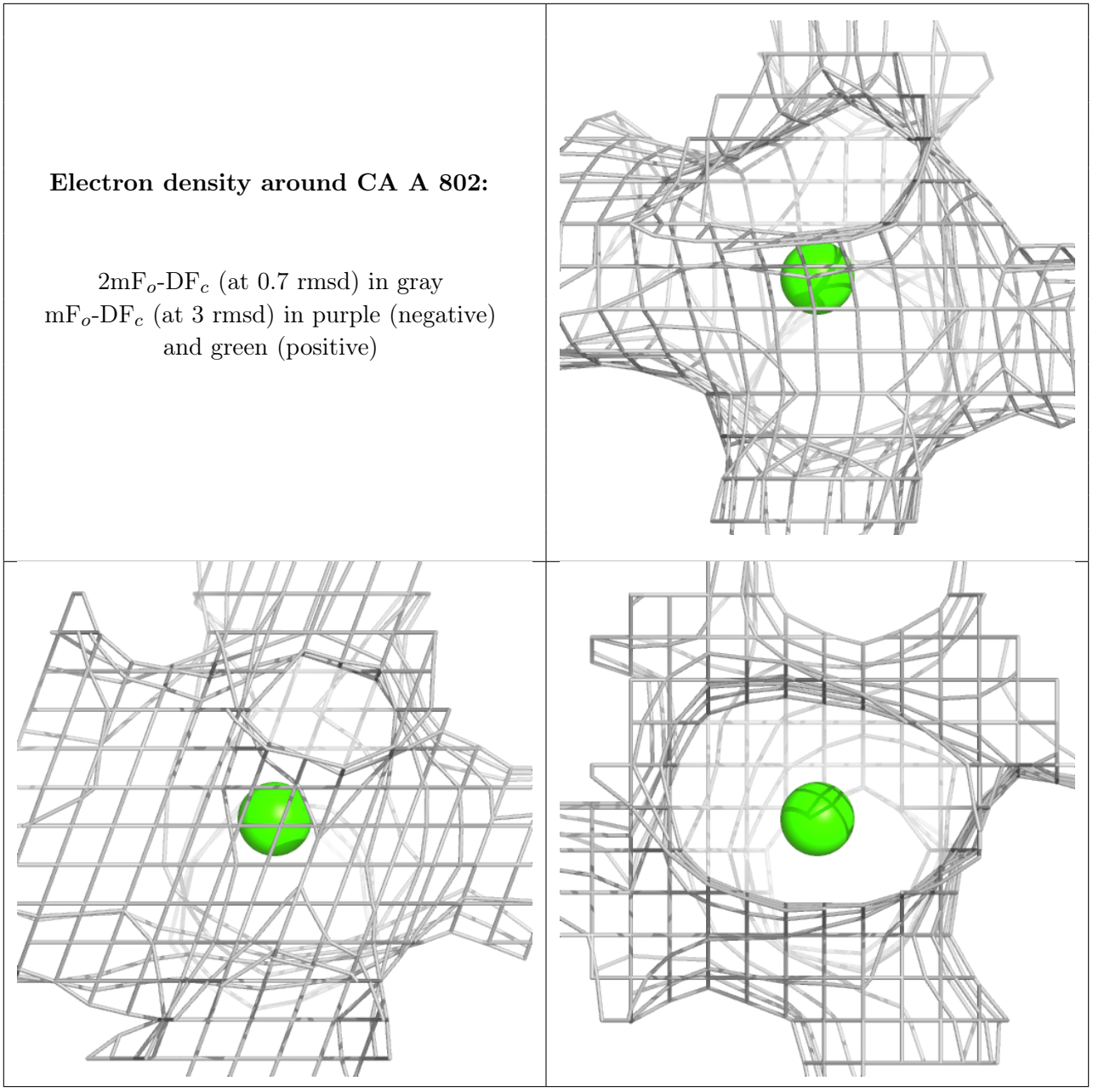
Electron density around CA B 801:

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



Electron density around CA A 802:

$2mF_o$-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.