Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 12:33 am GMT

PDB ID	:	6Y9E
Title	:	Crystal structure of putative ancestral haloalkane dehalogenase AncHLD2 (node 2)
Authors	:	Chaloupkova, R.; Damborsky, J.; Marek, M.
Deposited on	:	2020-03-09
Resolution	:	1.70 Å(reported)

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

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

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

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

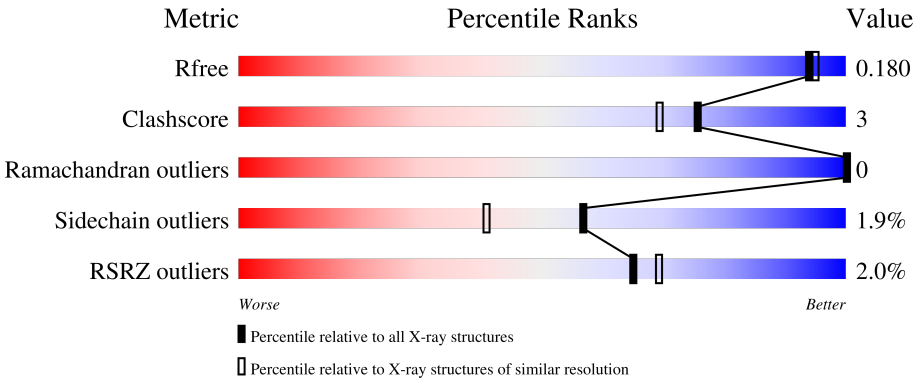
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	307	89% 6% 5%
1	B	307	87% 8% 5%
1	C	307	87% 8% 5%
1	D	307	88% 7% 5%
1	E	307	4% 86% 8% 7%

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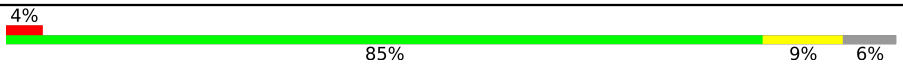
Mol	Chain	Length	Quality of chain
1	F	307	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15127 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.

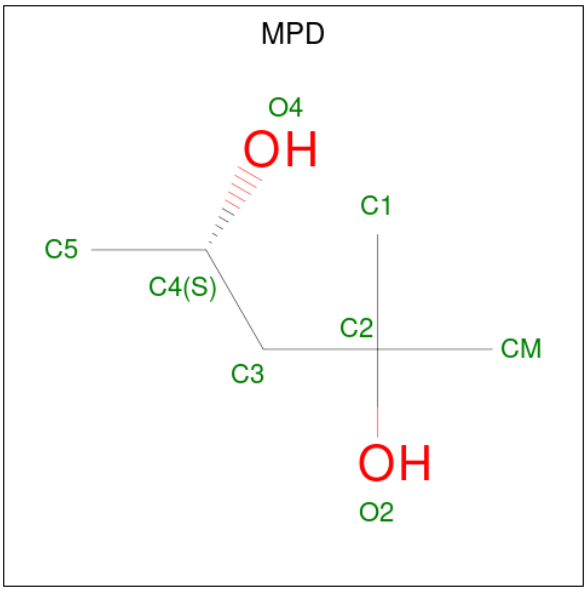
- Molecule 1 is a protein called Ancestral haloalkane dehalogenase AncHLD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2299	1477	402	412	8			
1	B	291	Total	C	N	O	S	11	2	0
			2317	1490	404	415	8			
1	C	291	Total	C	N	O	S	0	2	0
			2313	1484	404	417	8			
1	D	291	Total	C	N	O	S	0	6	0
			2348	1508	414	418	8			
1	E	287	Total	C	N	O	S	0	2	0
			2288	1473	400	407	8			
1	F	290	Total	C	N	O	S	0	1	0
			2304	1483	402	411	8			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

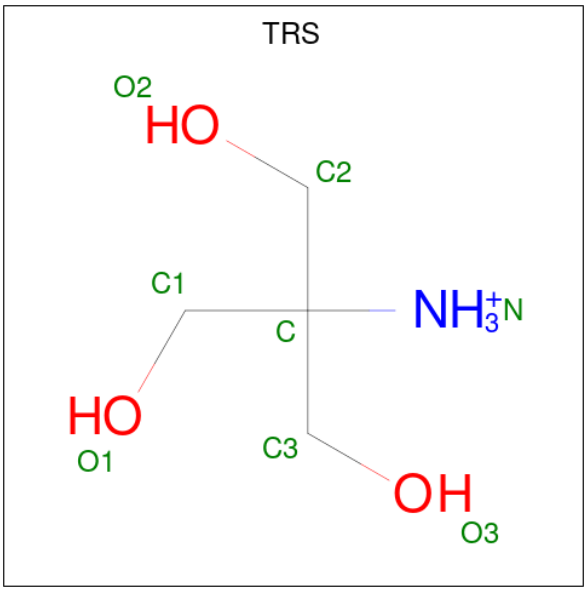
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	2	Total	Cl	0	0
			2	2		
2	C	2	Total	Cl	0	0
			2	2		
2	D	2	Total	Cl	0	0
			2	2		
2	E	2	Total	Cl	0	0
			2	2		
2	F	2	Total	Cl	0	0
			2	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$) (labeled as "Ligand of Interest" by depositor).



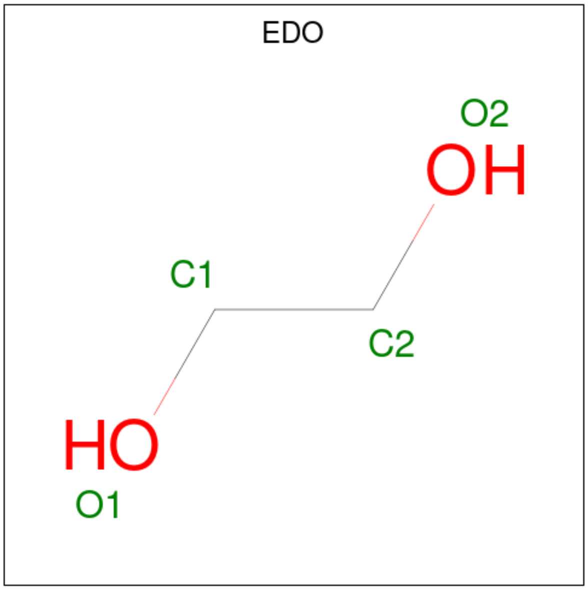
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	A	1	Total C N O 8 4 1 3	0	0
4	A	1	Total C N O 8 4 1 3	0	0
4	A	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0

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



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	196	Total O 196 196	0	0
6	B	204	Total O 206 206	0	2
6	C	185	Total O 185 185	0	0

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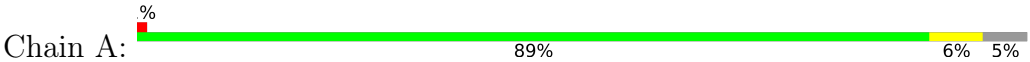
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	202	Total O 202 202	0	0
6	E	141	Total O 141 141	0	0
6	F	116	Total O 116 116	0	0

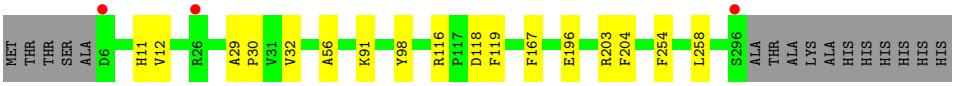
3 Residue-property plots (i)

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: Ancestral haloalkane dehalogenase AncHLD2

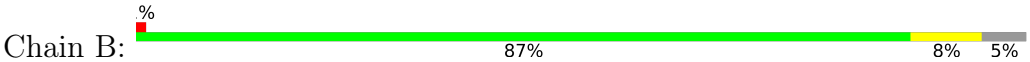
Chain A:

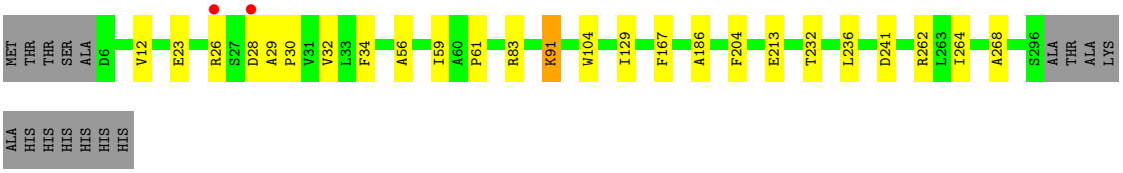




• Molecule 1: Ancestral haloalkane dehalogenase AncHLD2

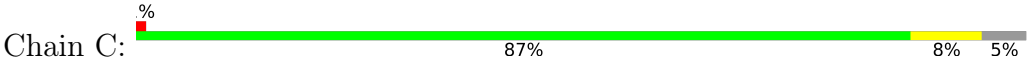
Chain B:

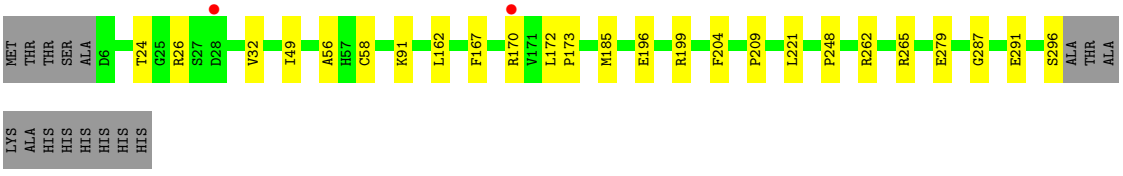




• Molecule 1: Ancestral haloalkane dehalogenase AncHLD2

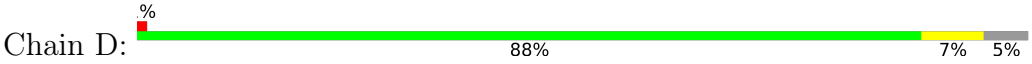
Chain C:





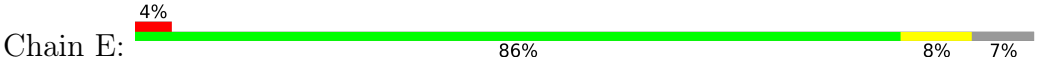
• Molecule 1: Ancestral haloalkane dehalogenase AncHLD2

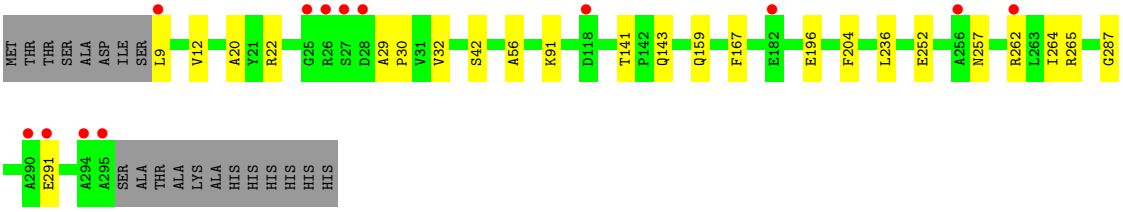
Chain D:



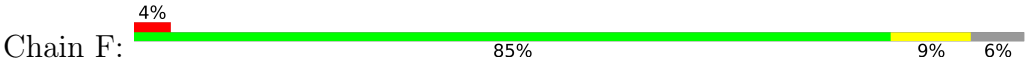
• Molecule 1: Ancestral haloalkane dehalogenase AncHLD2

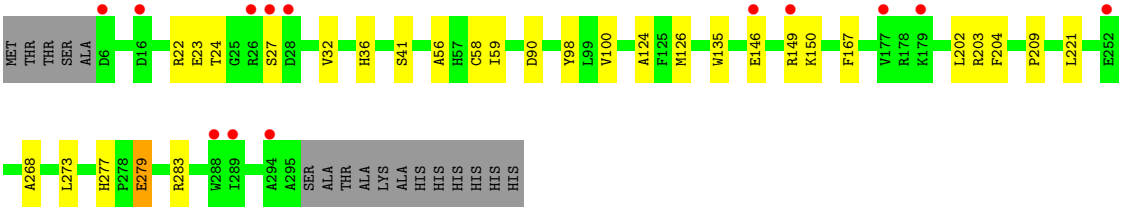
Chain E:





• Molecule 1: Ancestral haloalkane dehalogenase AncHLD2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.58Å 166.62Å 100.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.62 – 1.70 67.62 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.62-1.70) 99.8 (67.62-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.181 , 0.218 0.183 , 0.180	Depositor DCC
R_{free} test set	9800 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15127	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: CL, EDO, MPD, TRS

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	0.43	0/2365	0.57	0/3220
1	B	0.43	0/2384	0.57	0/3247
1	C	0.41	0/2379	0.55	0/3239
1	D	0.38	0/2415	0.55	0/3288
1	E	0.34	0/2355	0.51	0/3207
1	F	0.32	0/2371	0.49	0/3229
All	All	0.39	0/14269	0.54	0/19430

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	2299	0	2261	14	0
1	B	2317	0	2276	14	0
1	C	2313	0	2268	15	0
1	D	2348	0	2313	10	0
1	E	2288	0	2249	13	0
1	F	2304	0	2265	19	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
3	C	16	0	28	2	0
3	D	8	0	14	2	0
4	A	32	0	48	5	0
4	B	8	0	12	0	0
5	A	28	0	42	0	0
5	B	28	0	42	1	0
5	C	28	0	42	4	0
5	D	12	0	18	1	0
5	E	4	0	6	0	0
5	F	20	0	30	3	0
6	A	196	0	0	2	0
6	B	206	0	0	0	0
6	C	185	0	0	3	0
6	D	202	0	0	1	0
6	E	141	0	0	1	0
6	F	116	0	0	1	0
All	All	15127	0	13942	88	0

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

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ARG:HD3	5:F:405:EDO:H21	1.53	0.88
1:A:118:ASP:HA	4:A:406:TRS:H22	1.63	0.78
1:C:248:PRO:HB3	1:C:265:ARG:HH22	1.54	0.72
1:C:262:ARG:NH2	6:C:501:HOH:O	2.20	0.71
1:C:199:ARG:HG3	5:C:410:EDO:H11	1.73	0.69
1:D:9:LEU:HD12	5:D:404:EDO:H22	1.78	0.66
1:F:22:ARG:NH1	6:F:502:HOH:O	2.31	0.63
1:F:202:LEU:HG	5:F:405:EDO:H12	1.81	0.62
1:D:84:TYR:HE1	3:D:403:MPD:H12	1.64	0.62
1:A:12:VAL:CG2	1:A:91:LYS:HG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:HB2	5:B:411:EDO:H12	1.81	0.61
1:B:236:LEU:HD22	1:B:264:ILE:HD11	1.83	0.60
1:A:116:ARG:HD3	4:A:405:TRS:H11	1.87	0.57
1:C:24:THR:HG22	1:C:58:CYS:HB2	1.85	0.57
1:C:279:GLU:H	5:C:411:EDO:H21	1.69	0.56
1:C:24:THR:HG21	1:C:49:ILE:HG22	1.88	0.56
1:C:162:LEU:HD11	5:C:410:EDO:H12	1.88	0.56
1:D:32:VAL:HG22	1:D:98:TYR:HB2	1.88	0.56
1:A:11:HIS:ND1	6:A:502:HOH:O	2.29	0.55
1:C:32:VAL:HG23	1:C:56:ALA:HB1	1.90	0.53
1:F:146:GLU:O	1:F:150:LYS:HG3	2.08	0.53
1:F:135:TRP:CZ2	1:F:149:ARG:HD3	2.45	0.51
1:E:12:VAL:HG21	1:E:91:LYS:HG2	1.93	0.51
1:F:32:VAL:HG22	1:F:98:TYR:HB2	1.93	0.51
1:D:182:GLU:OE2	6:D:501:HOH:O	2.20	0.50
1:F:24:THR:HG22	1:F:58:CYS:HB2	1.92	0.50
1:A:196:GLU:OE2	4:A:407:TRS:O2	2.30	0.50
1:A:32:VAL:HG22	1:A:98:TYR:HB2	1.93	0.49
1:E:141:THR:HB	1:E:143:GLN:OE1	2.12	0.49
1:B:23:GLU:HG3	1:B:59:ILE:HD13	1.94	0.49
1:E:12:VAL:CG2	1:E:91:LYS:HG2	2.42	0.49
1:B:32:VAL:HG23	1:B:56:ALA:HB1	1.94	0.48
1:E:32:VAL:HG23	1:E:56:ALA:HB1	1.95	0.48
1:B:83:ARG:HD2	1:D:213:GLU:OE2	2.14	0.47
1:F:90:ASP:HB2	5:F:407:EDO:H11	1.95	0.47
1:A:12:VAL:HG22	1:A:91:LYS:HG2	1.95	0.47
1:C:172:LEU:HB3	1:C:173:PRO:HD3	1.97	0.47
1:E:252:GLU:OE2	1:E:265:ARG:NH2	2.48	0.46
3:C:404:MPD:H13	6:C:524:HOH:O	2.15	0.46
1:B:236:LEU:HD22	1:B:264:ILE:CD1	2.46	0.46
1:A:116:ARG:HH11	4:A:405:TRS:H11	1.81	0.46
1:F:135:TRP:CE2	1:F:149:ARG:HD3	2.50	0.46
1:C:279:GLU:HG3	5:C:411:EDO:H22	1.97	0.45
1:A:29:ALA:HB1	1:A:30:PRO:HD2	1.98	0.45
1:F:279:GLU:H	1:F:279:GLU:CD	2.18	0.45
1:A:32:VAL:HG23	1:A:56:ALA:HB1	1.98	0.45
1:B:26:ARG:HG3	1:B:29:ALA:HB2	1.98	0.45
1:F:268:ALA:O	1:F:277:HIS:NE2	2.44	0.45
1:B:29:ALA:HB1	1:B:30:PRO:HD2	1.98	0.44
1:C:196:GLU:H	1:C:196:GLU:CD	2.20	0.44
1:B:26:ARG:H	1:B:26:ARG:HG2	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:TRP:HA	1:D:129:ILE:HD12	1.98	0.44
1:C:209:PRO:HG3	1:C:221:LEU:HD12	2.00	0.44
1:D:172:LEU:HB3	1:D:173:PRO:HD3	2.00	0.44
1:E:22:ARG:NH1	1:E:42:SER:OG	2.46	0.43
1:F:32:VAL:HG23	1:F:56:ALA:HB1	1.99	0.43
1:B:241:ASP:O	1:B:268:ALA:HA	2.18	0.43
1:C:248:PRO:HB3	1:C:265:ARG:NH2	2.28	0.43
1:A:203:ARG:HA	1:A:203:ARG:HD2	1.78	0.43
4:A:406:TRS:H12	6:A:660:HOH:O	2.18	0.42
1:E:236:LEU:HG	1:E:264:ILE:HD11	2.01	0.42
1:B:213:GLU:OE2	3:B:403:MPD:H13	2.19	0.42
1:E:29:ALA:HB1	1:E:30:PRO:HD2	2.01	0.42
1:A:116:ARG:HG2	1:A:119:PHE:HB2	2.01	0.42
3:D:403:MPD:H52	3:D:403:MPD:H11	2.01	0.42
3:C:404:MPD:H12	6:C:627:HOH:O	2.19	0.42
1:E:236:LEU:HG	1:E:264:ILE:CD1	2.49	0.42
1:F:23:GLU:HG3	1:F:59:ILE:HD13	2.01	0.42
1:F:27:SER:O	1:F:27:SER:OG	2.31	0.42
1:F:279:GLU:O	1:F:283:ARG:HG3	2.20	0.42
1:E:196:GLU:H	1:E:196:GLU:CD	2.24	0.41
1:C:287:GLY:O	1:C:291:GLU:HG3	2.20	0.41
1:D:133:PRO:O	1:D:211:ALA:HA	2.20	0.41
1:D:32:VAL:HG23	1:D:56:ALA:HB1	2.03	0.41
1:F:36:HIS:CE1	1:F:41:SER:HA	2.56	0.41
1:B:12:VAL:CG2	1:B:91:LYS:HG2	2.50	0.41
1:B:34:PHE:O	1:B:61:PRO:HD2	2.19	0.41
1:E:287:GLY:O	1:E:291:GLU:HG2	2.21	0.41
1:A:254:PHE:CE2	1:A:258:LEU:HD11	2.56	0.41
1:E:9:LEU:HD12	6:E:558:HOH:O	2.21	0.41
1:F:100:VAL:HA	1:F:124:ALA:O	2.21	0.41
1:A:196:GLU:H	1:A:196:GLU:CD	2.24	0.41
1:E:9:LEU:HD11	1:E:20:ALA:HB1	2.03	0.41
1:F:209:PRO:HG3	1:F:221:LEU:HD12	2.02	0.40
1:C:173:PRO:HG3	1:C:185:MET:SD	2.61	0.40
1:D:23:GLU:HA	1:D:58:CYS:O	2.21	0.40
1:F:126:MET:HB2	1:F:273:LEU:HD12	2.03	0.40
1:B:104:TRP:HA	1:B:129:ILE:HD12	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	289/307 (94%)	277 (96%)	12 (4%)	0	100	100
1	B	291/307 (95%)	281 (97%)	10 (3%)	0	100	100
1	C	291/307 (95%)	282 (97%)	9 (3%)	0	100	100
1	D	295/307 (96%)	286 (97%)	9 (3%)	0	100	100
1	E	287/307 (94%)	275 (96%)	12 (4%)	0	100	100
1	F	289/307 (94%)	279 (96%)	10 (4%)	0	100	100
All	All	1742/1842 (95%)	1680 (96%)	62 (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	239/251 (95%)	237 (99%)	2 (1%)	81	74
1	B	241/251 (96%)	233 (97%)	8 (3%)	38	19
1	C	241/251 (96%)	235 (98%)	6 (2%)	47	29
1	D	244/251 (97%)	237 (97%)	7 (3%)	42	23
1	E	237/251 (94%)	231 (98%)	6 (2%)	47	29
1	F	239/251 (95%)	235 (98%)	4 (2%)	60	46
All	All	1441/1506 (96%)	1408 (98%)	33 (2%)	57	33

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	PHE
1	A	204	PHE
1	B	28	ASP
1	B	91	LYS
1	B	167	PHE
1	B	204[A]	PHE
1	B	204[B]	PHE
1	B	232[A]	THR
1	B	232[B]	THR
1	B	262	ARG
1	C	26	ARG
1	C	91	LYS
1	C	167	PHE
1	C	170	ARG
1	C	204	PHE
1	C	296	SER
1	D	26	ARG
1	D	143	GLN
1	D	166[A]	VAL
1	D	166[B]	VAL
1	D	167	PHE
1	D	204[A]	PHE
1	D	204[B]	PHE
1	E	159	GLN
1	E	167	PHE
1	E	204[A]	PHE
1	E	204[B]	PHE
1	E	257	ASN
1	E	262	ARG
1	F	167	PHE
1	F	204[A]	PHE
1	F	204[B]	PHE
1	F	279	GLU

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

Mol	Chain	Res	Type
1	B	257	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 12 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
5	EDO	D	406	-	3,3,3	0.47	0	2,2,2	0.62	0
5	EDO	A	413	-	3,3,3	0.47	0	2,2,2	0.46	0
5	EDO	C	411	-	3,3,3	0.51	0	2,2,2	0.61	0
5	EDO	C	408	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	C	405	-	3,3,3	0.42	0	2,2,2	0.69	0
5	EDO	B	411	-	3,3,3	0.54	0	2,2,2	0.73	0
4	TRS	A	407	-	7,7,7	0.14	0	9,9,9	0.22	0
5	EDO	D	404	-	3,3,3	0.45	0	2,2,2	0.62	0
5	EDO	E	403	-	3,3,3	0.47	0	2,2,2	0.54	0
5	EDO	A	408	-	3,3,3	0.48	0	2,2,2	0.45	0
3	MPD	A	403	-	7,7,7	0.23	0	9,10,10	0.50	0
5	EDO	D	405	-	3,3,3	0.45	0	2,2,2	0.44	0
5	EDO	C	407	-	3,3,3	0.46	0	2,2,2	0.54	0
5	EDO	C	409	-	3,3,3	0.47	0	2,2,2	0.37	0
3	MPD	D	403	-	7,7,7	1.06	1 (14%)	9,10,10	0.70	0
5	EDO	B	406	-	3,3,3	0.47	0	2,2,2	0.58	0
5	EDO	F	405	-	3,3,3	0.42	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	B	409	-	3,3,3	0.41	0	2,2,2	0.56	0
5	EDO	F	404	-	3,3,3	0.48	0	2,2,2	0.44	0
5	EDO	C	410	-	3,3,3	0.49	0	2,2,2	0.50	0
4	TRS	A	406	-	7,7,7	0.16	0	9,9,9	0.13	0
5	EDO	F	406	-	3,3,3	0.46	0	2,2,2	0.43	0
5	EDO	B	410	-	3,3,3	0.47	0	2,2,2	0.50	0
5	EDO	A	412	-	3,3,3	0.46	0	2,2,2	0.60	0
5	EDO	A	411	-	3,3,3	0.45	0	2,2,2	0.60	0
5	EDO	B	405	-	3,3,3	0.46	0	2,2,2	0.63	0
3	MPD	C	404	-	7,7,7	0.35	0	9,10,10	0.51	0
5	EDO	C	406	-	3,3,3	0.46	0	2,2,2	0.50	0
4	TRS	A	404	-	7,7,7	0.14	0	9,9,9	0.11	0
5	EDO	A	409	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	F	407	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	A	414	-	3,3,3	0.46	0	2,2,2	0.53	0
3	MPD	C	403	-	7,7,7	0.57	0	9,10,10	0.61	0
5	EDO	F	403	-	3,3,3	0.43	0	2,2,2	0.57	0
5	EDO	B	407	-	3,3,3	0.44	0	2,2,2	0.60	0
4	TRS	B	404	-	7,7,7	0.13	0	9,9,9	0.13	0
5	EDO	B	408	-	3,3,3	0.44	0	2,2,2	0.74	0
5	EDO	A	410	-	3,3,3	0.42	0	2,2,2	0.90	0
4	TRS	A	405	-	7,7,7	0.15	0	9,9,9	0.11	0
3	MPD	B	403	-	7,7,7	0.47	0	9,10,10	0.57	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
5	EDO	D	406	-	-	1/1/1/1	-
5	EDO	A	413	-	-	0/1/1/1	-
5	EDO	C	411	-	-	1/1/1/1	-
5	EDO	C	408	-	-	0/1/1/1	-
5	EDO	C	405	-	-	1/1/1/1	-
5	EDO	B	411	-	-	0/1/1/1	-
4	TRS	A	407	-	-	2/9/9/9	-
5	EDO	D	404	-	-	0/1/1/1	-
5	EDO	E	403	-	-	0/1/1/1	-
5	EDO	A	408	-	-	1/1/1/1	-
3	MPD	A	403	-	-	3/5/5/5	-
5	EDO	D	405	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	407	-	-	0/1/1/1	-
5	EDO	C	409	-	-	1/1/1/1	-
3	MPD	D	403	-	-	2/5/5/5	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	F	405	-	-	0/1/1/1	-
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	F	404	-	-	1/1/1/1	-
5	EDO	C	410	-	-	0/1/1/1	-
4	TRS	A	406	-	-	1/9/9/9	-
5	EDO	F	406	-	-	1/1/1/1	-
5	EDO	B	410	-	-	0/1/1/1	-
5	EDO	A	412	-	-	1/1/1/1	-
5	EDO	A	411	-	-	1/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
3	MPD	C	404	-	-	1/5/5/5	-
5	EDO	C	406	-	-	1/1/1/1	-
4	TRS	A	404	-	-	5/9/9/9	-
5	EDO	A	409	-	-	0/1/1/1	-
5	EDO	F	407	-	-	1/1/1/1	-
5	EDO	A	414	-	-	0/1/1/1	-
3	MPD	C	403	-	-	0/5/5/5	-
5	EDO	F	403	-	-	0/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
4	TRS	B	404	-	-	4/9/9/9	-
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	A	410	-	-	1/1/1/1	-
4	TRS	A	405	-	-	0/9/9/9	-
3	MPD	B	403	-	-	3/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	MPD	C3-C2	2.37	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	D	403	MPD	C2-C3-C4-O4
3	D	403	MPD	C2-C3-C4-C5
4	A	404	TRS	C1-C-C3-O3
4	A	404	TRS	C2-C-C3-O3
4	A	404	TRS	N-C-C3-O3
4	A	407	TRS	N-C-C1-O1
4	B	404	TRS	N-C-C1-O1
4	B	404	TRS	C1-C-C2-O2
4	B	404	TRS	N-C-C2-O2
5	A	411	EDO	O1-C1-C2-O2
5	B	406	EDO	O1-C1-C2-O2
5	F	404	EDO	O1-C1-C2-O2
4	A	407	TRS	C2-C-C1-O1
5	C	406	EDO	O1-C1-C2-O2
5	F	407	EDO	O1-C1-C2-O2
3	A	403	MPD	O2-C2-C3-C4
4	B	404	TRS	C3-C-C2-O2
5	C	411	EDO	O1-C1-C2-O2
5	F	406	EDO	O1-C1-C2-O2
3	A	403	MPD	C1-C2-C3-C4
3	A	403	MPD	CM-C2-C3-C4
5	A	408	EDO	O1-C1-C2-O2
5	C	405	EDO	O1-C1-C2-O2
5	D	405	EDO	O1-C1-C2-O2
5	B	409	EDO	O1-C1-C2-O2
5	C	409	EDO	O1-C1-C2-O2
4	A	404	TRS	C3-C-C2-O2
4	A	406	TRS	C2-C-C1-O1
3	B	403	MPD	O2-C2-C3-C4
5	A	410	EDO	O1-C1-C2-O2
5	A	412	EDO	O1-C1-C2-O2
5	B	405	EDO	O1-C1-C2-O2
5	D	406	EDO	O1-C1-C2-O2
4	A	404	TRS	N-C-C2-O2
3	B	403	MPD	C2-C3-C4-C5
3	C	404	MPD	C2-C3-C4-C5

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	411	EDO	2	0

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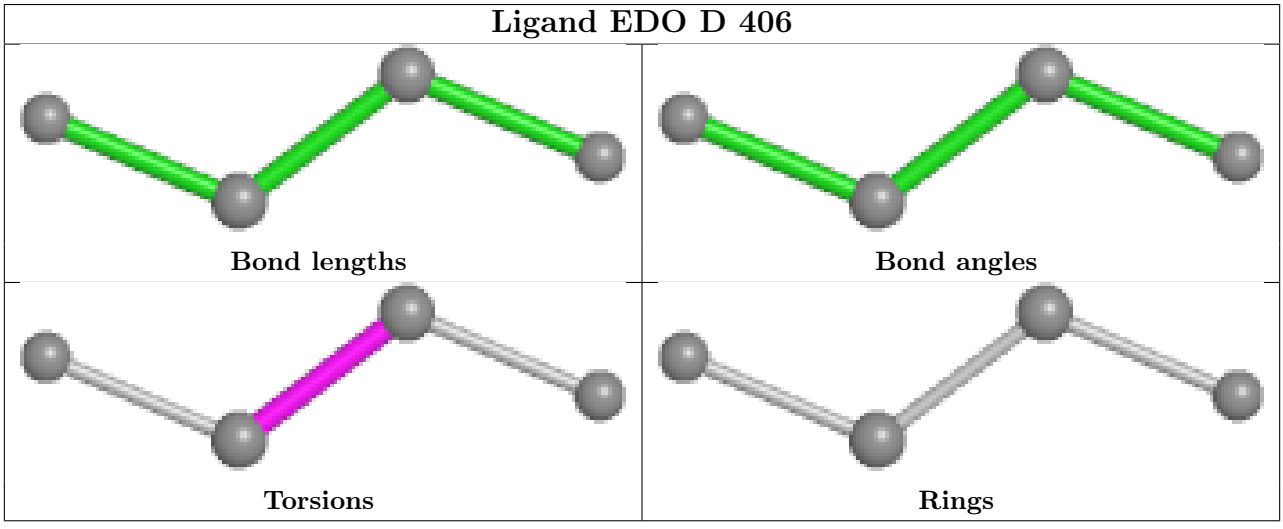
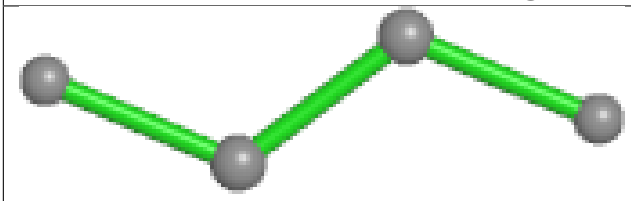
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	411	EDO	1	0
4	A	407	TRS	1	0
5	D	404	EDO	1	0
3	D	403	MPD	2	0
5	F	405	EDO	2	0
5	C	410	EDO	2	0
4	A	406	TRS	2	0
3	C	404	MPD	2	0
5	F	407	EDO	1	0
4	A	405	TRS	2	0
3	B	403	MPD	1	0

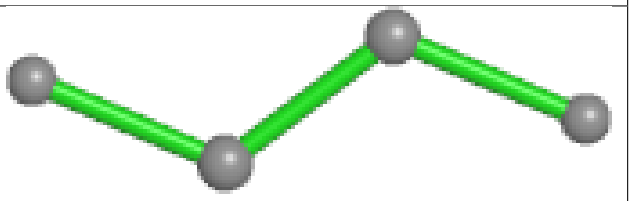
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



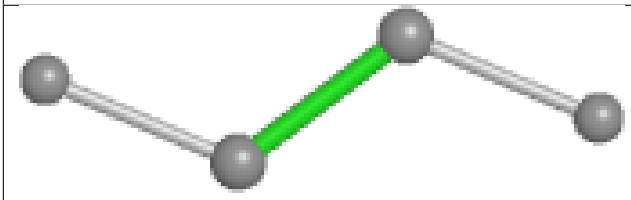
Ligand EDO A 413



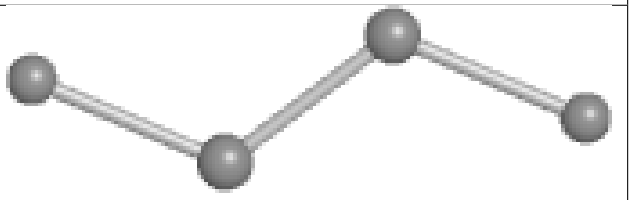
Bond lengths



Bond angles

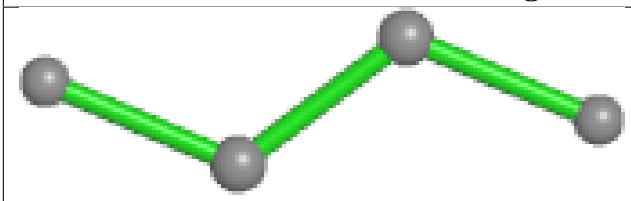


Torsions

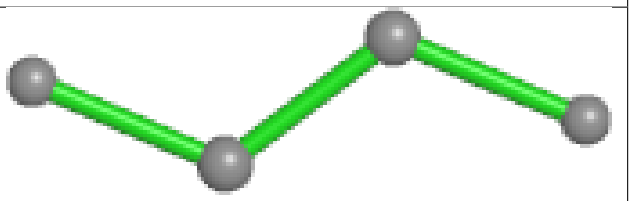


Rings

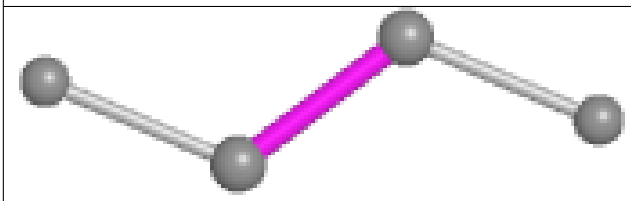
Ligand EDO C 411



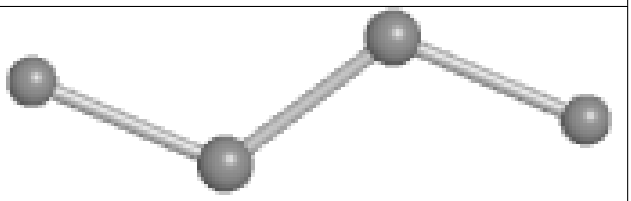
Bond lengths



Bond angles

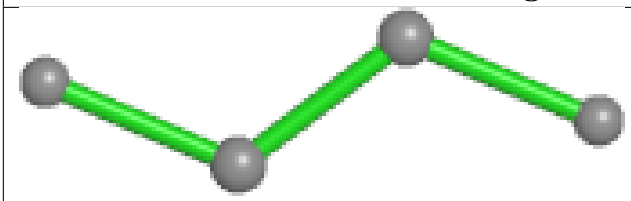


Torsions

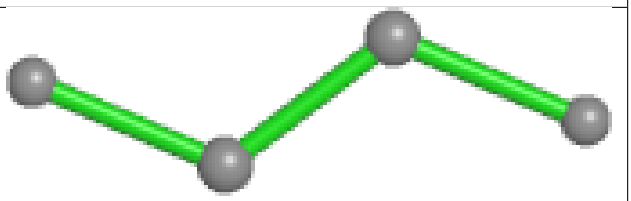


Rings

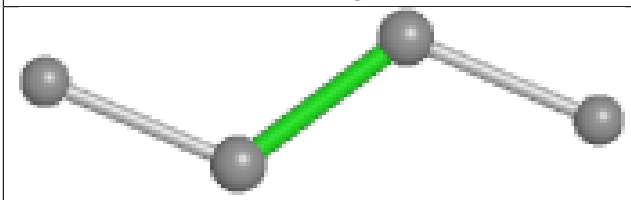
Ligand EDO C 408



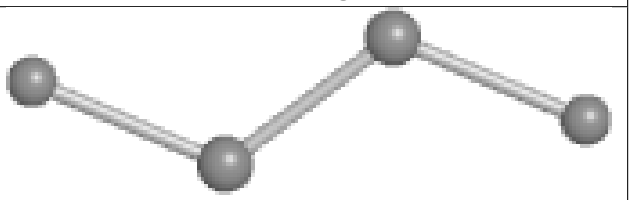
Bond lengths



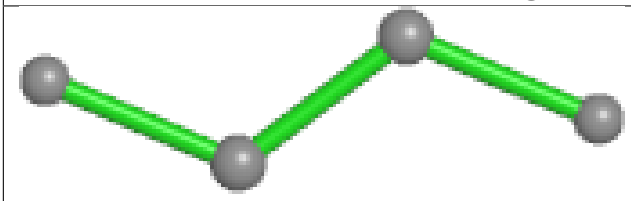
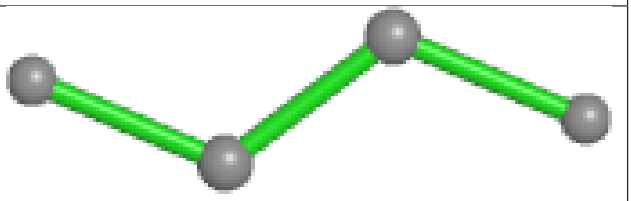
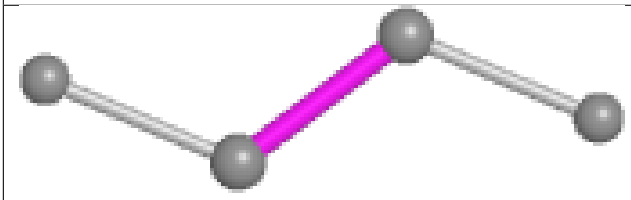
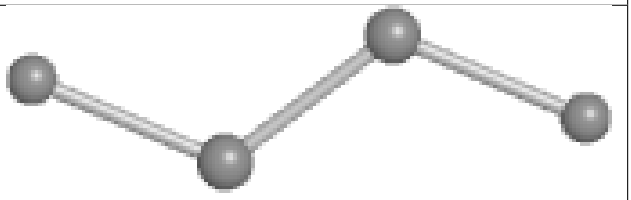
Bond angles

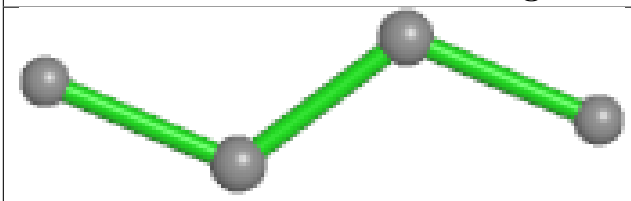
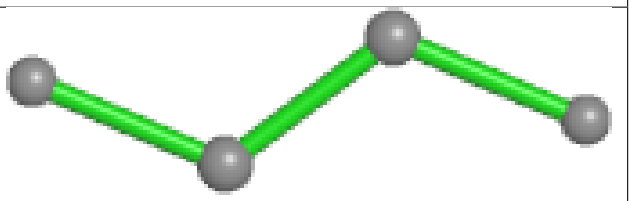
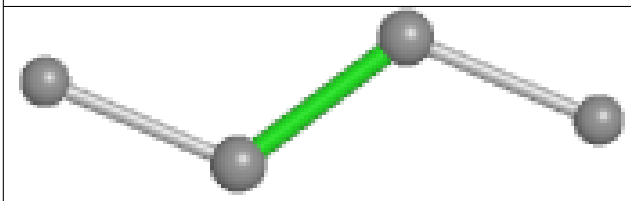
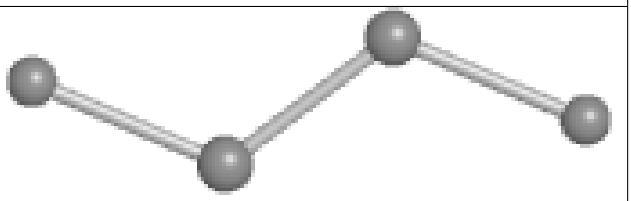


Torsions

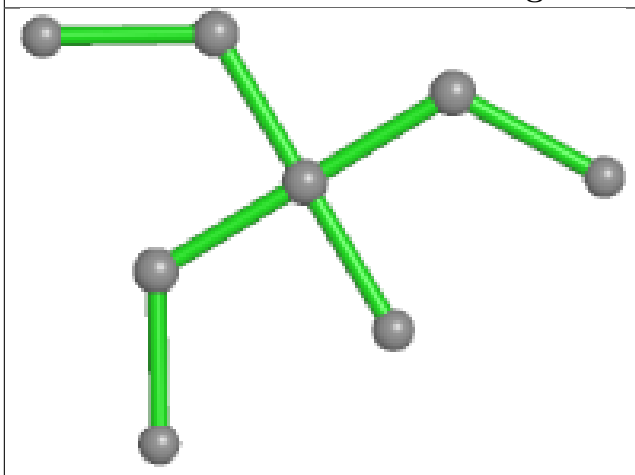


Rings

Ligand EDO C 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO B 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand TRS A 407



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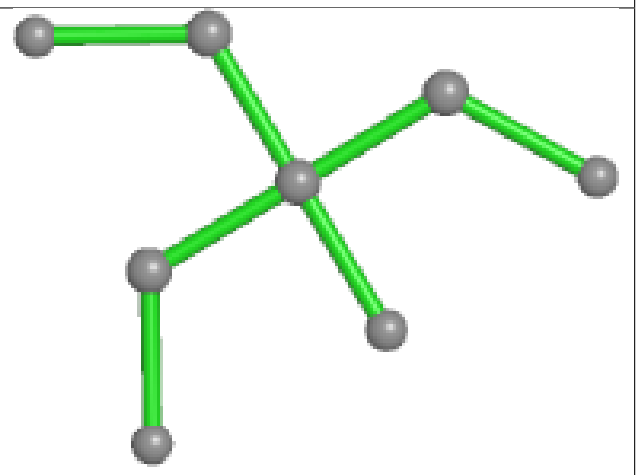
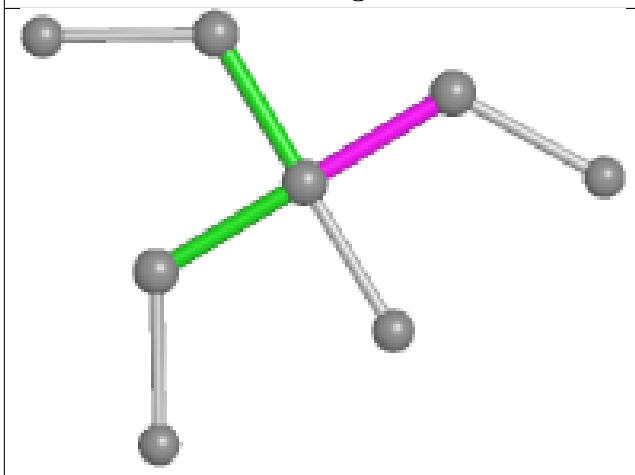


Bond angles



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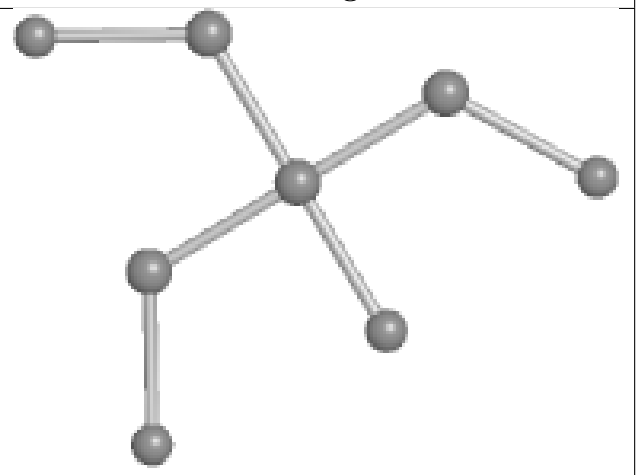
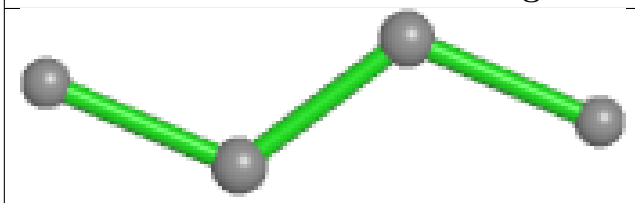


Rings

Ligand EDO D 404



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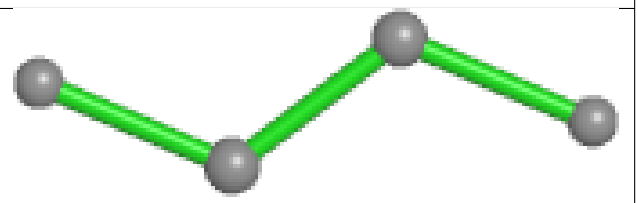

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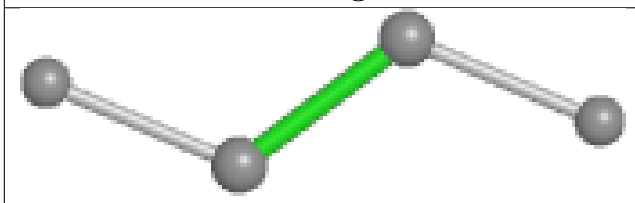

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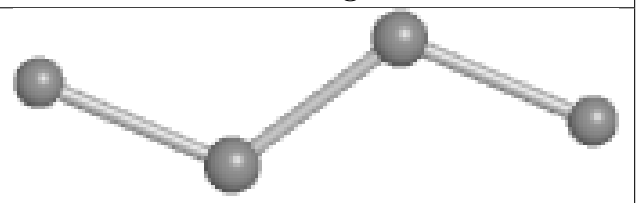
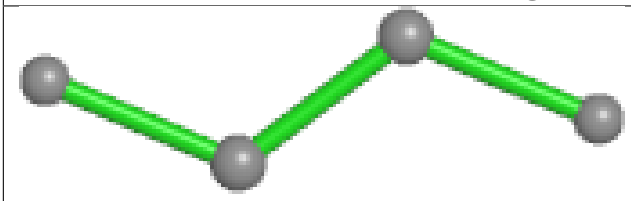
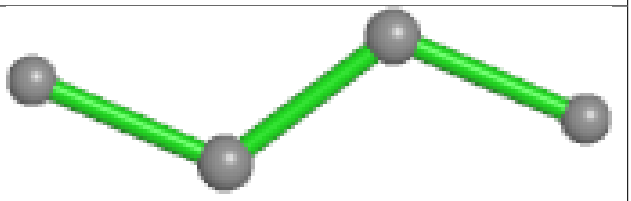
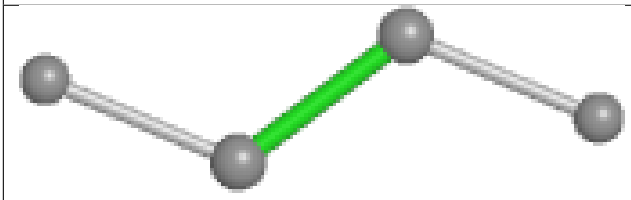
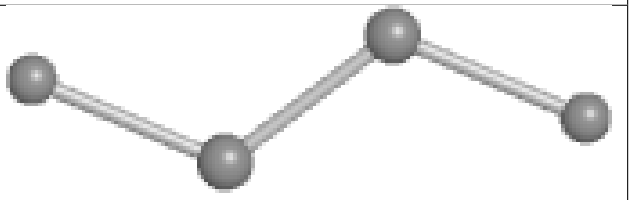
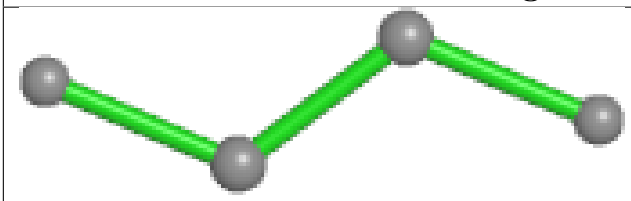
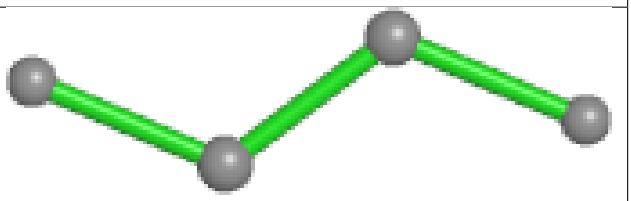
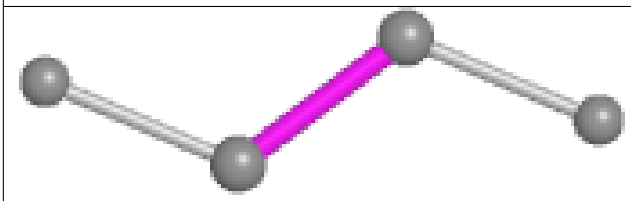
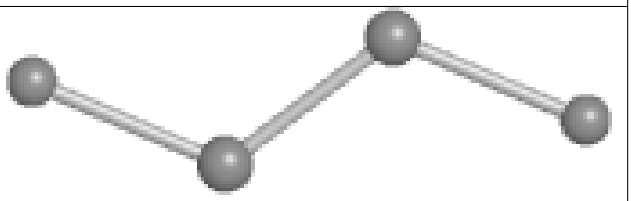
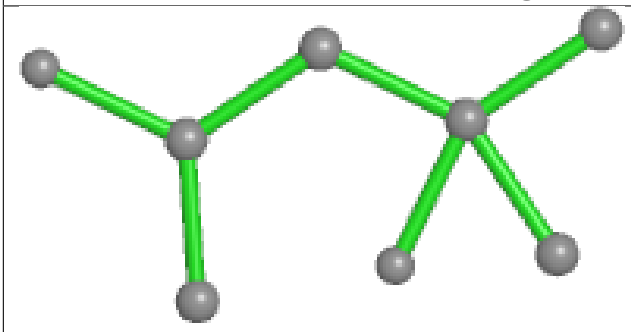


Rings

Ligand EDO E 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MPD A 403



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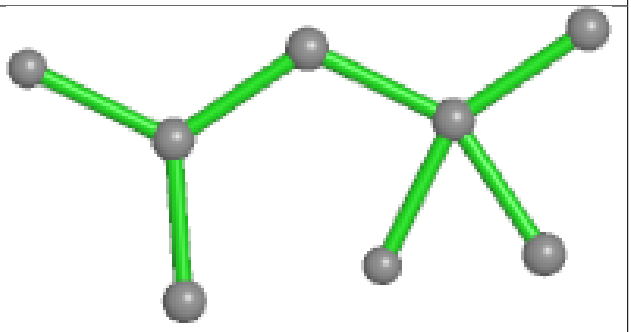
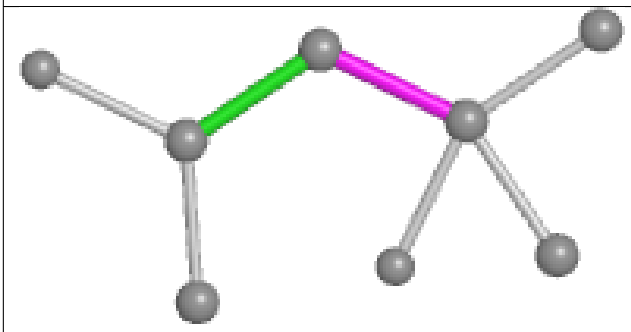


Bond angles



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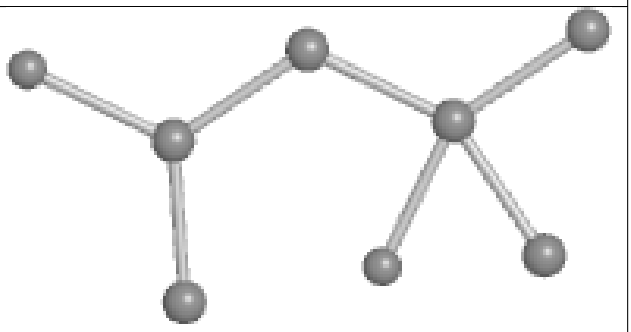
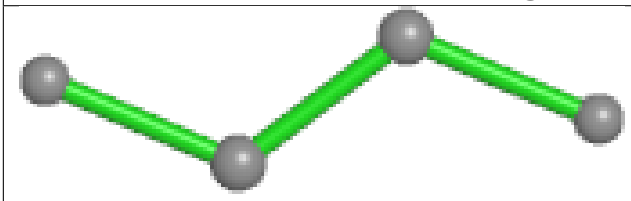


Rings

Ligand EDO D 405



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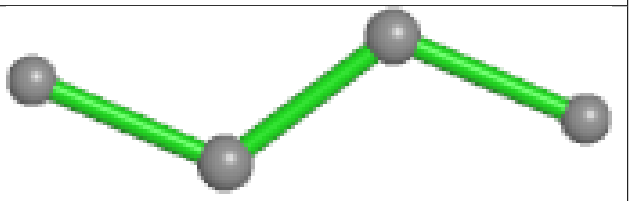
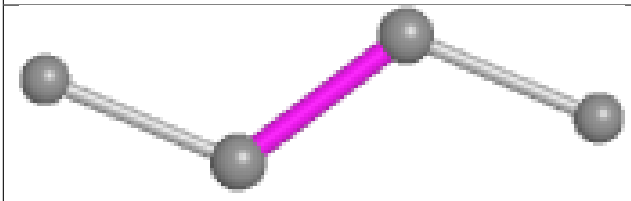
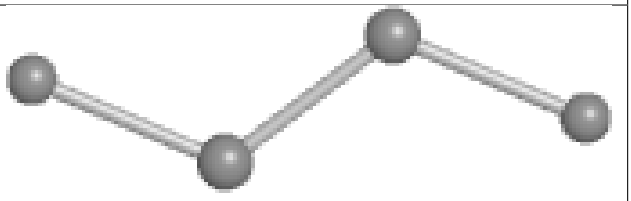


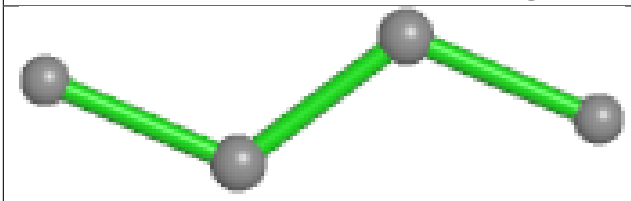
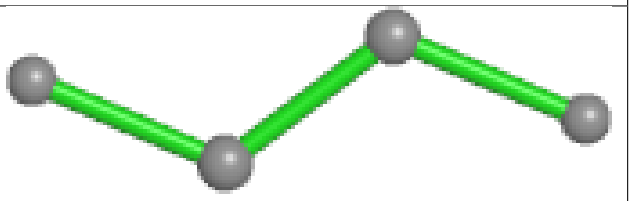
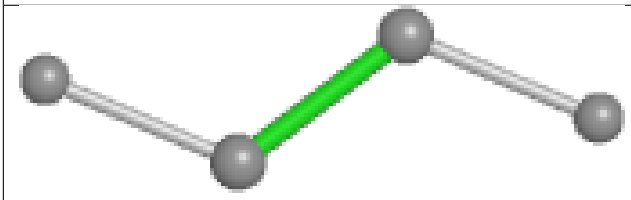
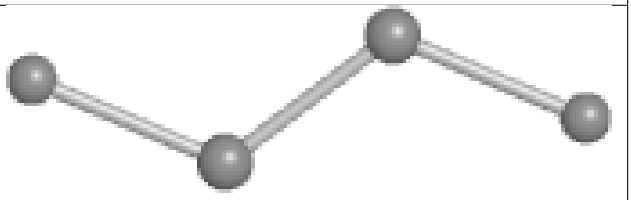
Bond angles

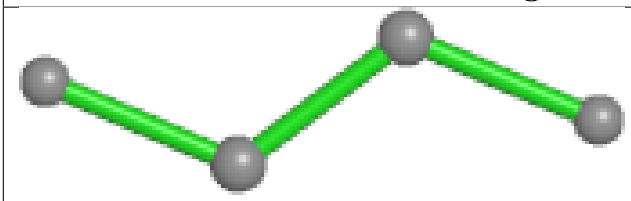
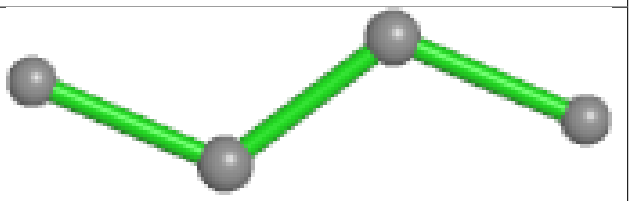
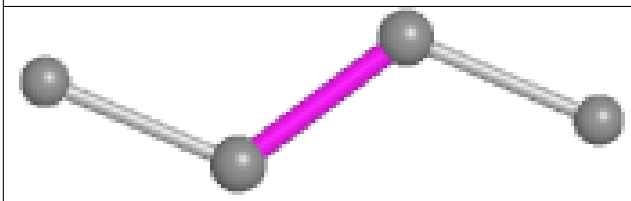
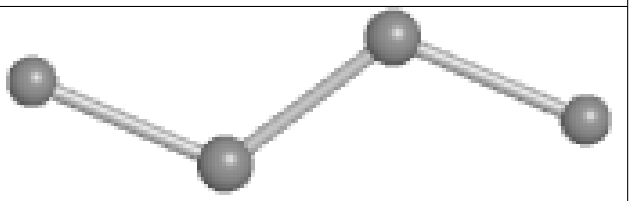


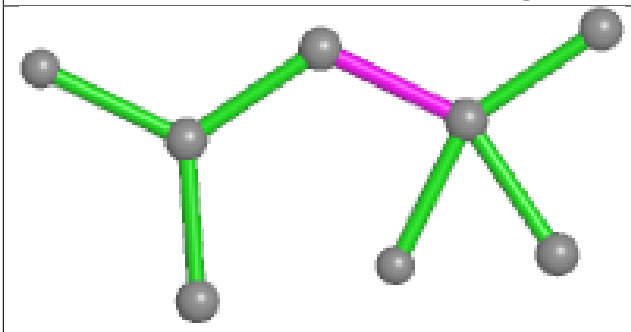
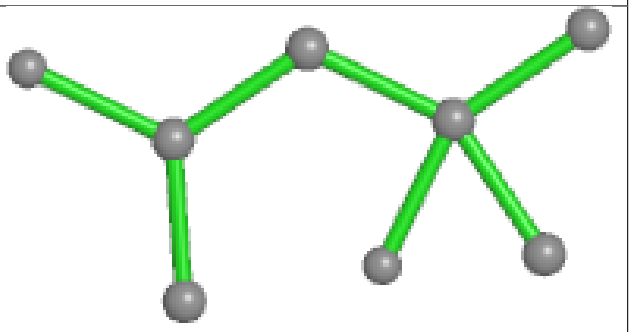
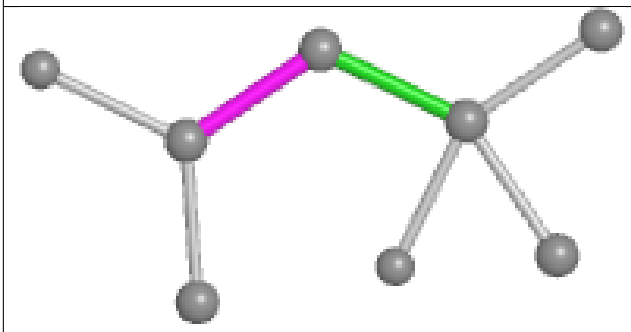
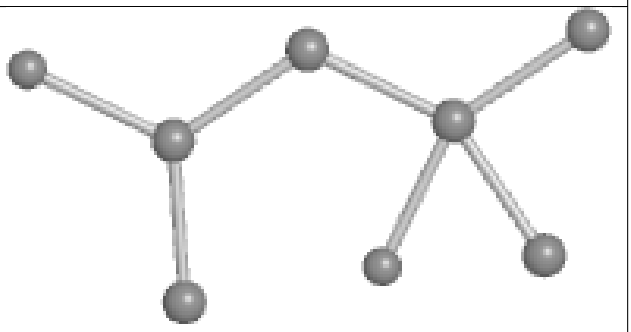
Torsions

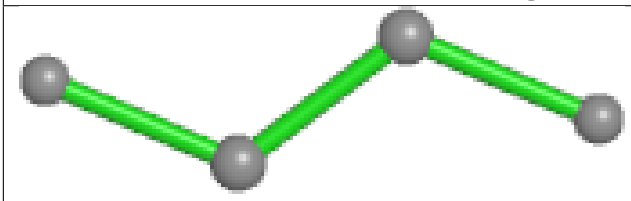
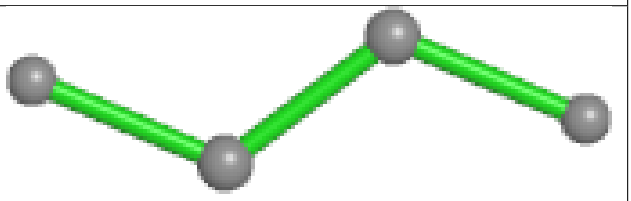
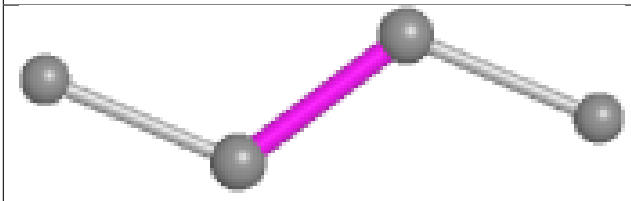
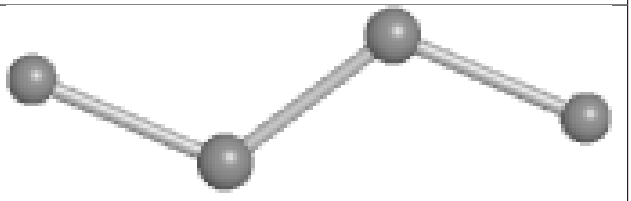


Rings

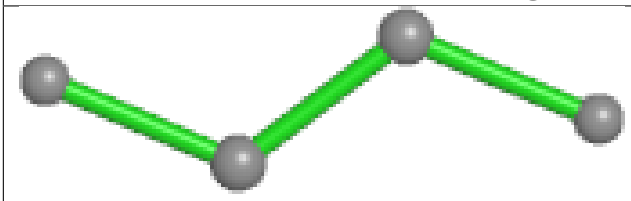
Ligand EDO C 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO C 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

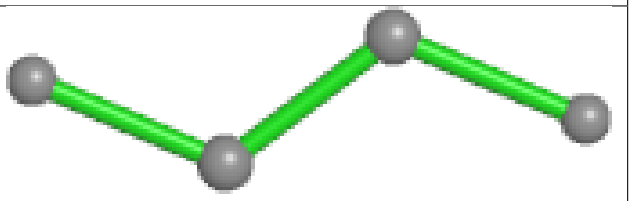
Ligand MPD D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO B 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

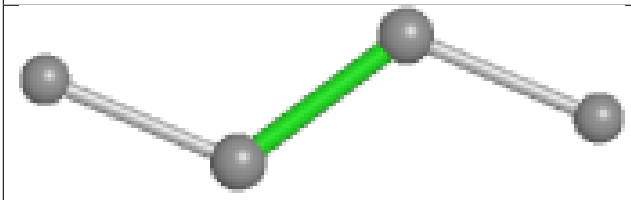
Ligand EDO F 405



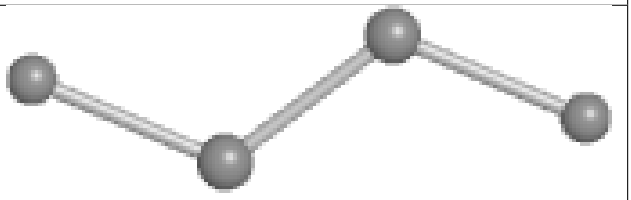
Bond lengths



Bond angles

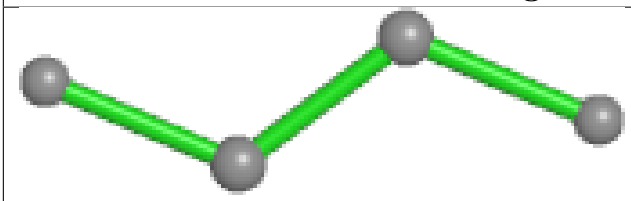


Torsions

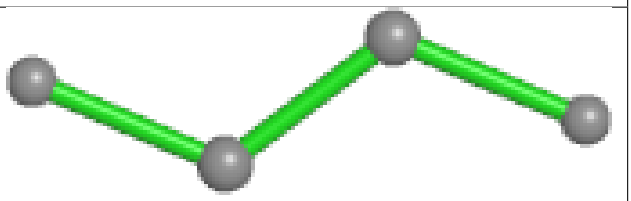


Rings

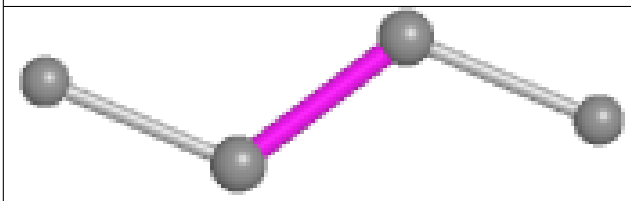
Ligand EDO B 409



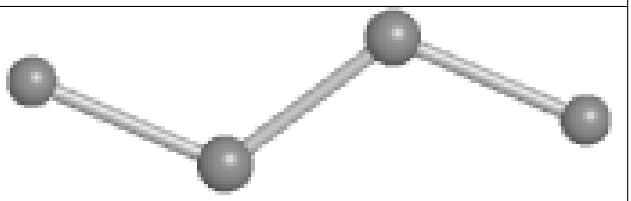
Bond lengths



Bond angles

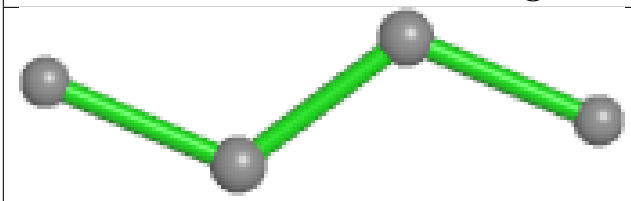


Torsions

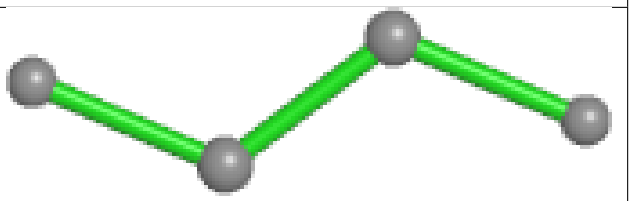


Rings

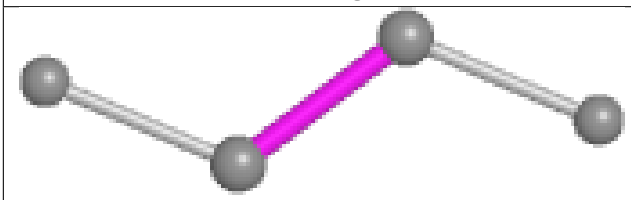
Ligand EDO F 404



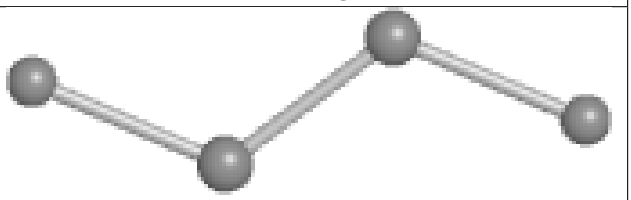
Bond lengths



Bond angles

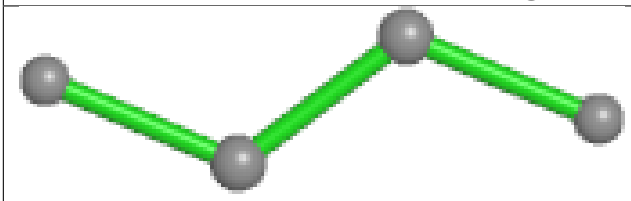


Torsions

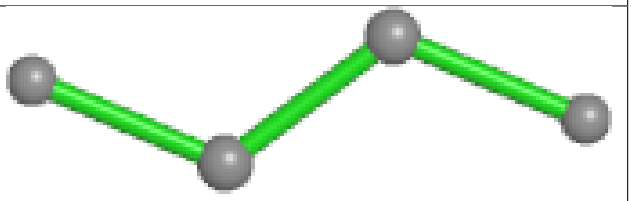


Rings

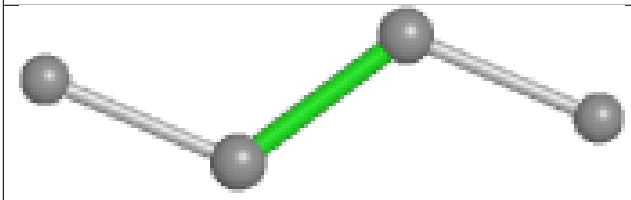
Ligand EDO C 410



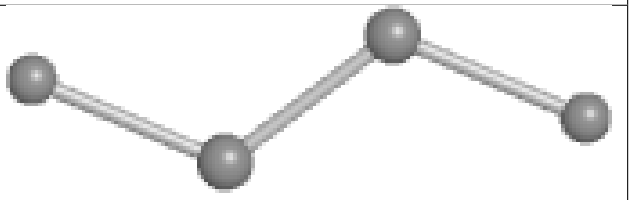
Bond lengths



Bond angles

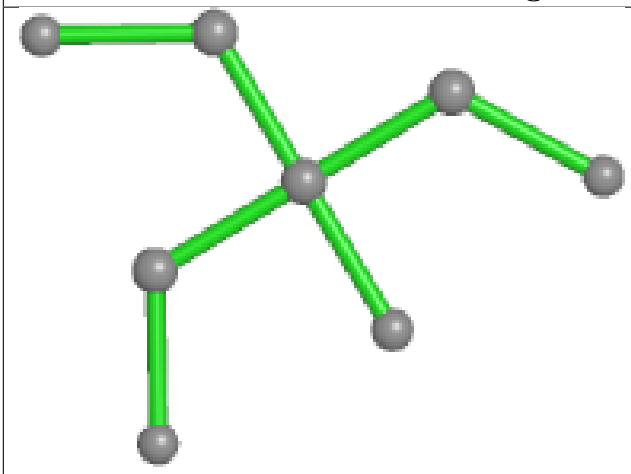


Torsions

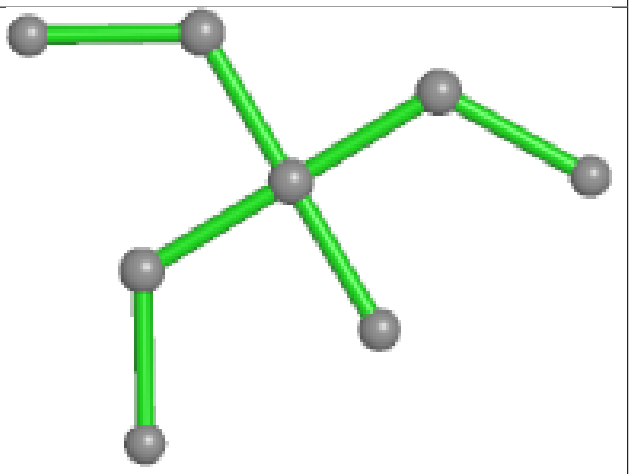


Rings

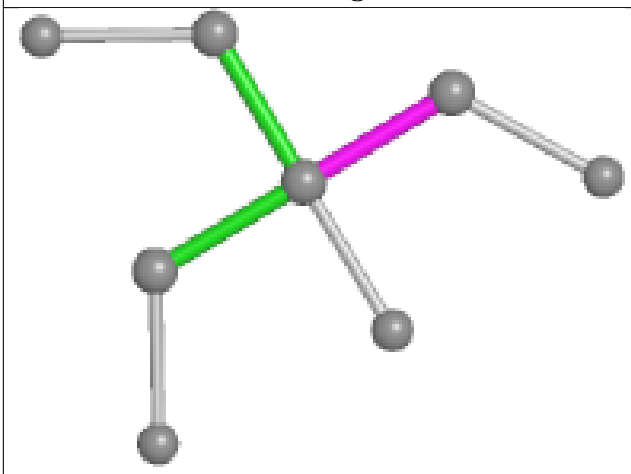
Ligand TRS A 406



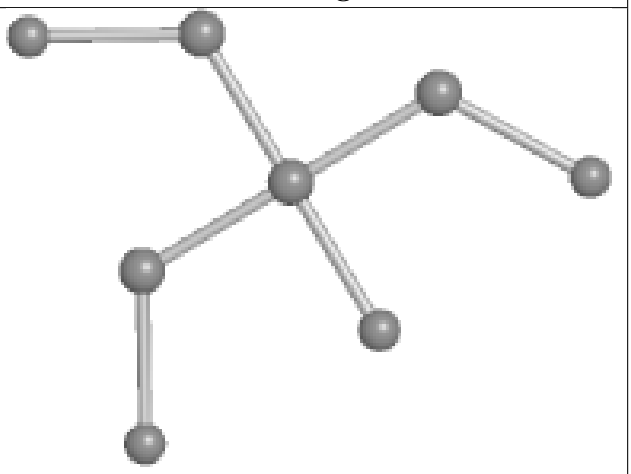
Bond lengths



Bond angles

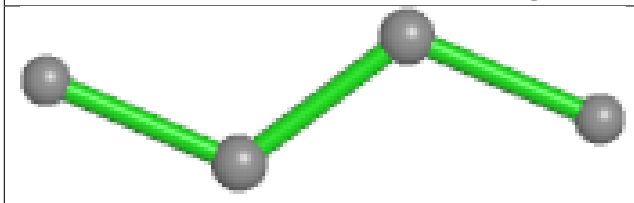


Torsions

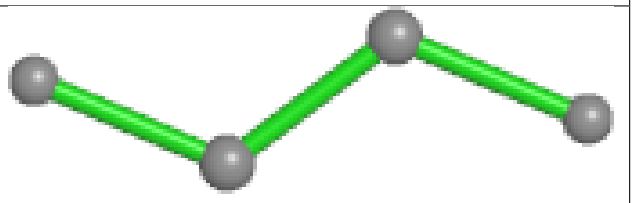


Rings

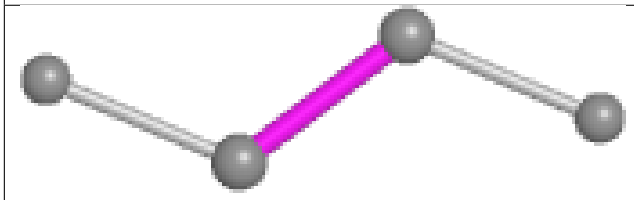
Ligand EDO F 406



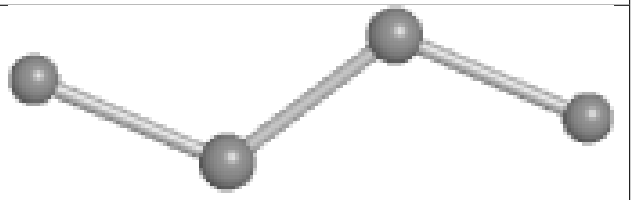
Bond lengths



Bond angles

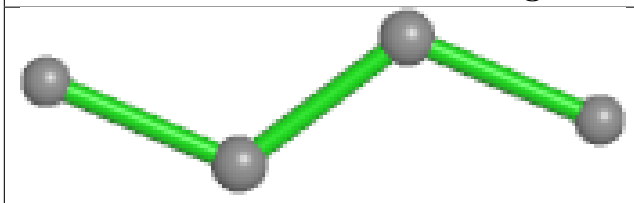


Torsions

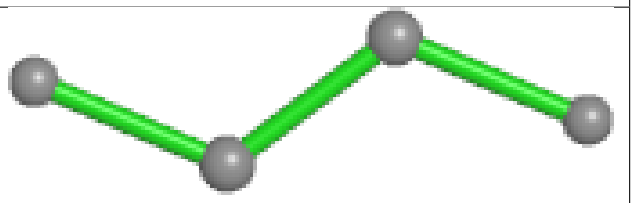


Rings

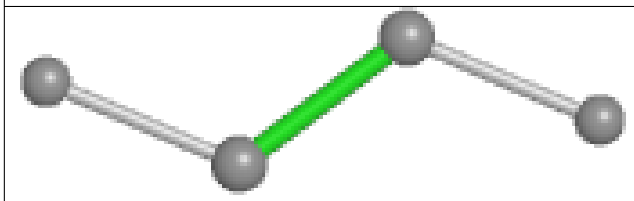
Ligand EDO B 410



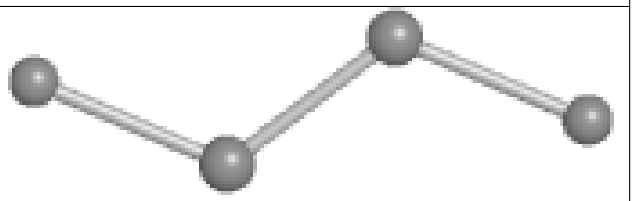
Bond lengths



Bond angles

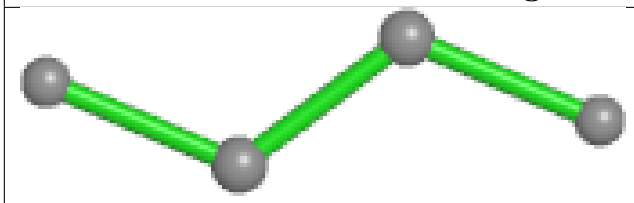


Torsions

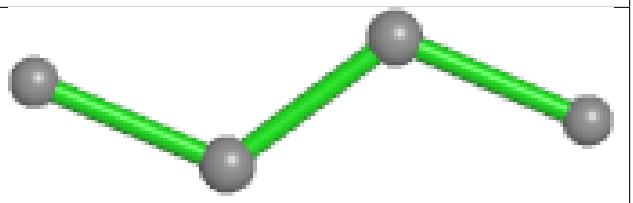


Rings

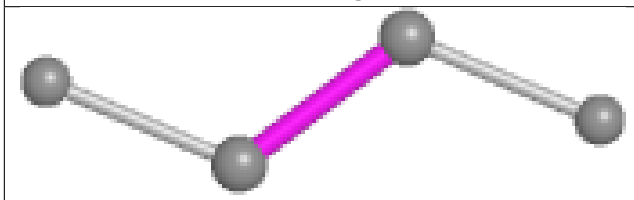
Ligand EDO A 412



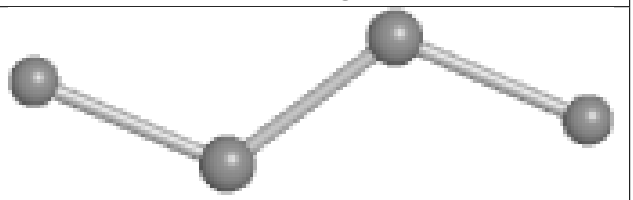
Bond lengths



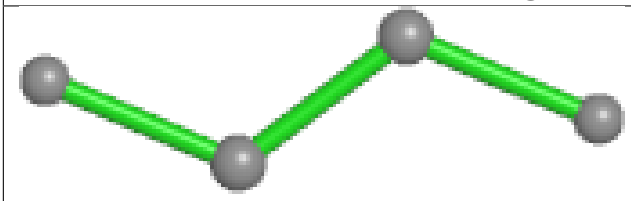
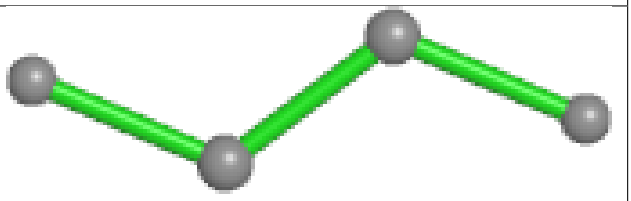
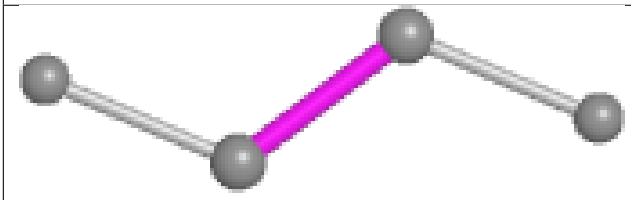
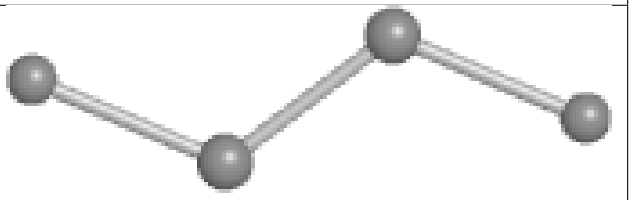
Bond angles

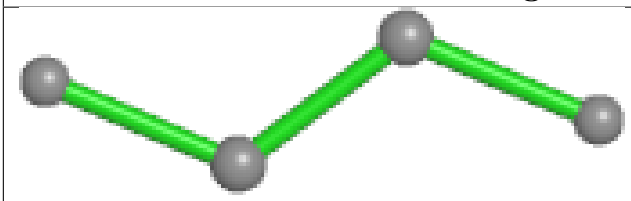
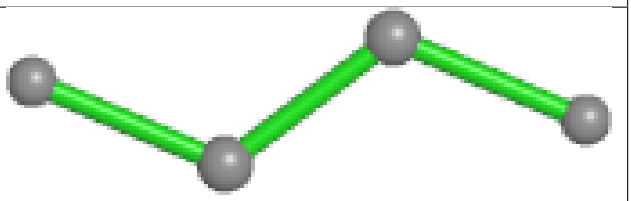
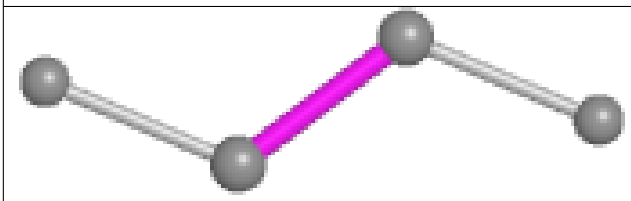
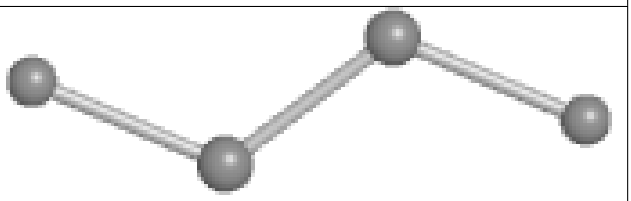


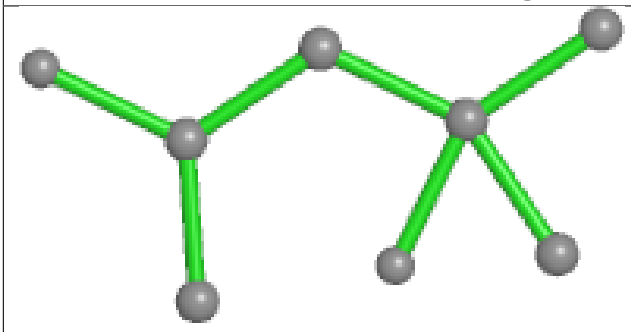
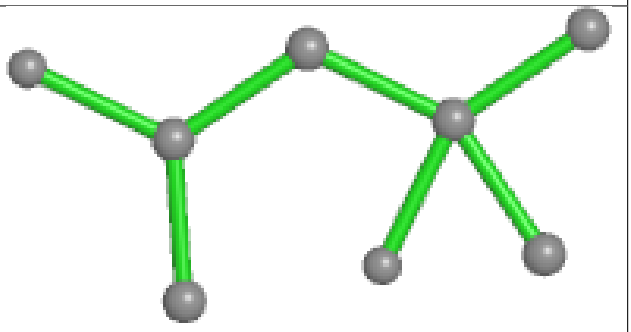
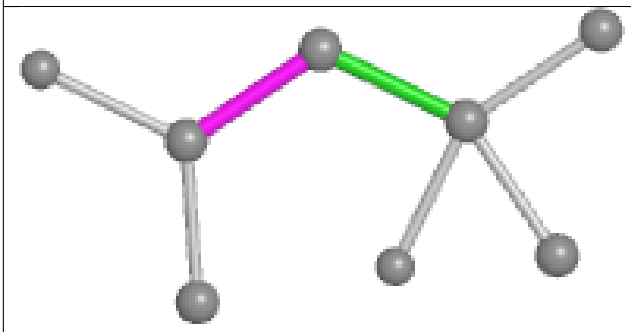
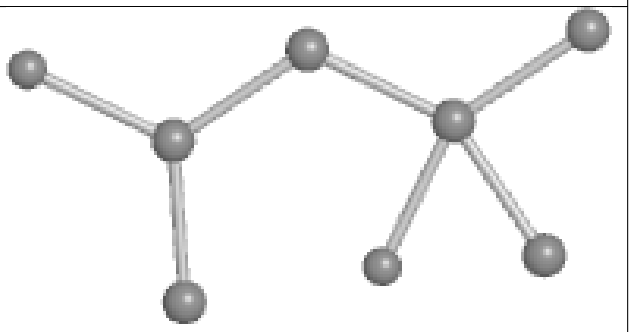
Torsions

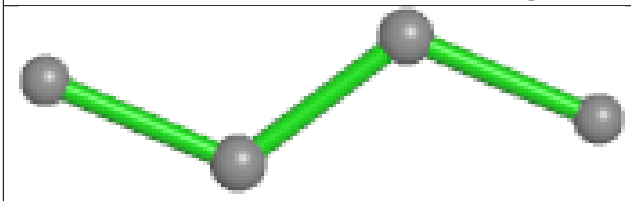
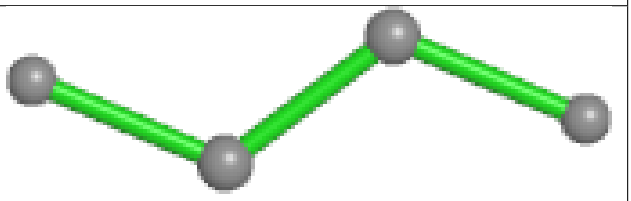
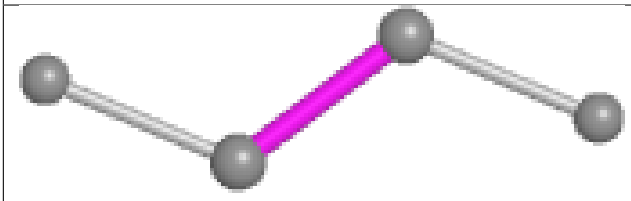
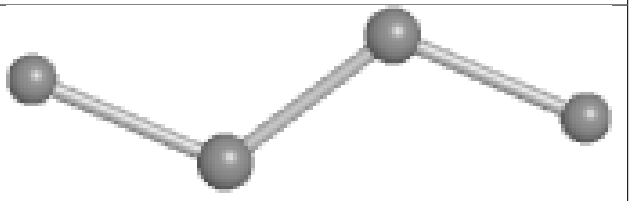


Rings

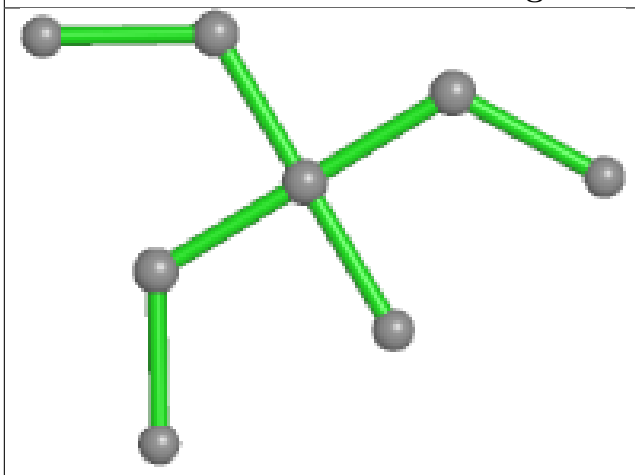
Ligand EDO A 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO B 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

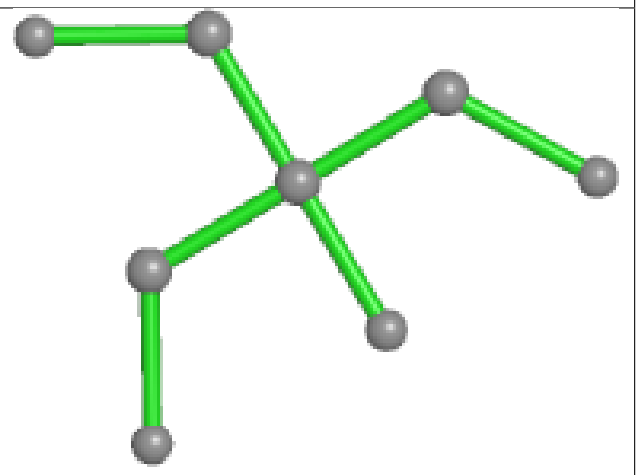
Ligand MPD C 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO C 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

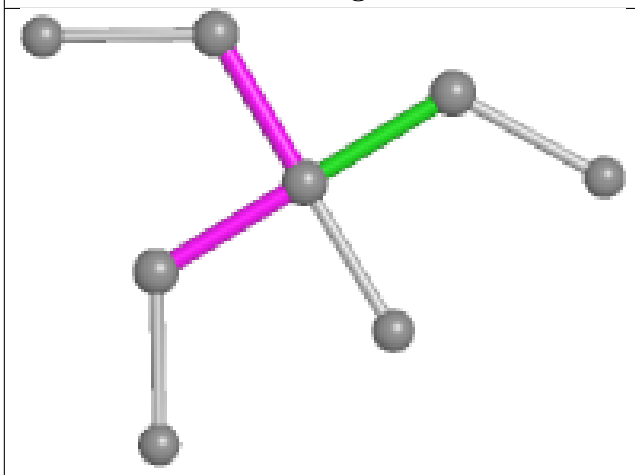
Ligand TRS A 404



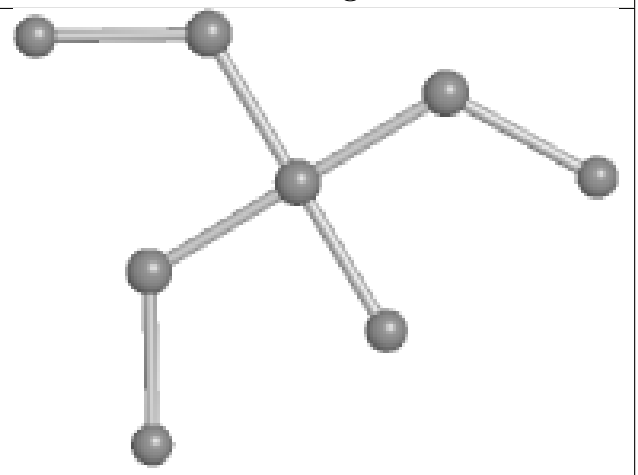
Bond lengths



Bond angles

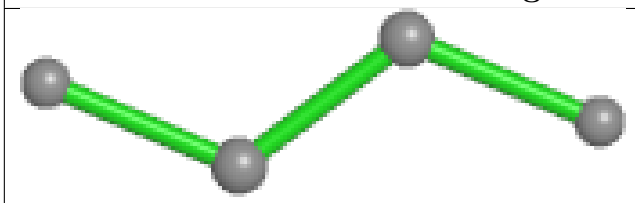


Torsions

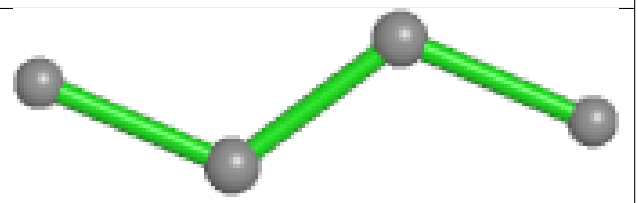


Rings

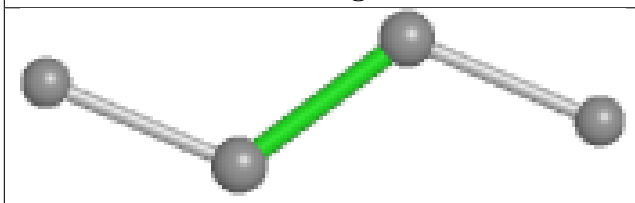
Ligand EDO A 409



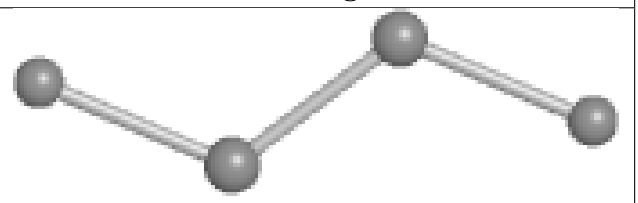
Bond lengths



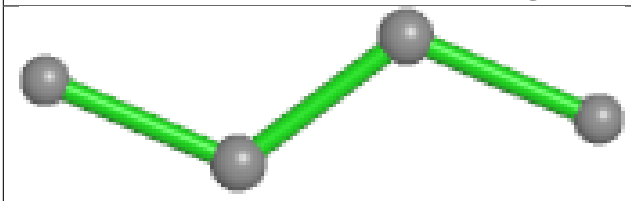
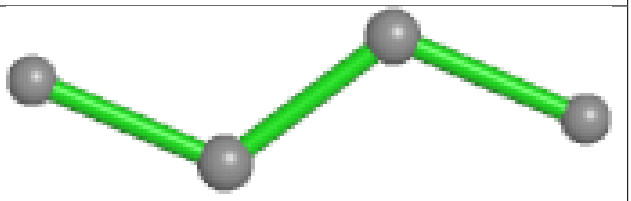
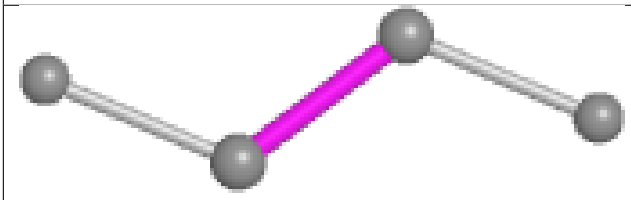
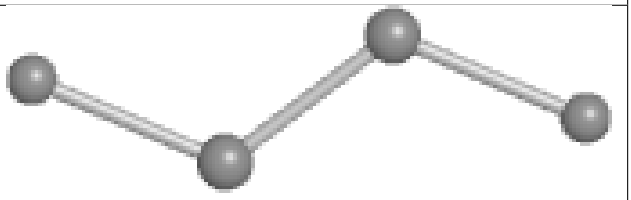
Bond angles

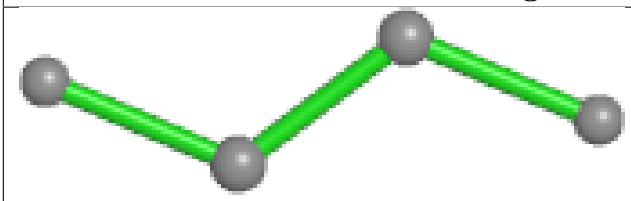
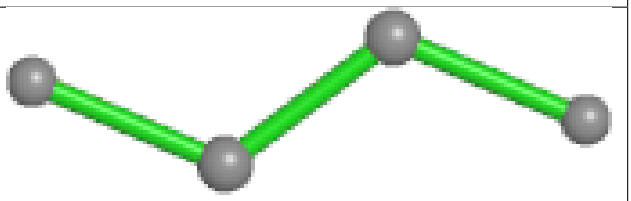
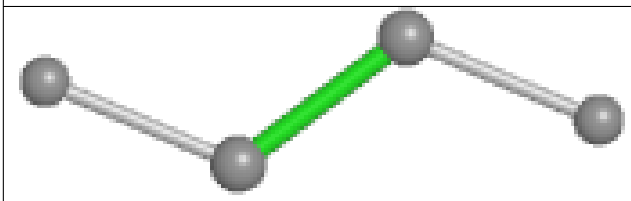
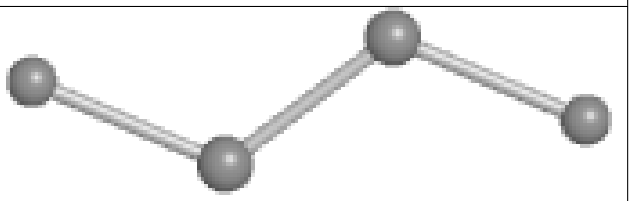


Torsions

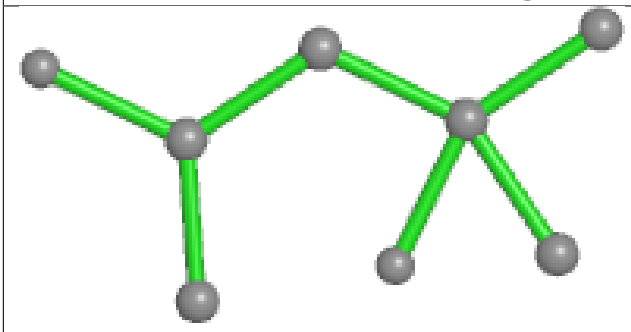


Rings

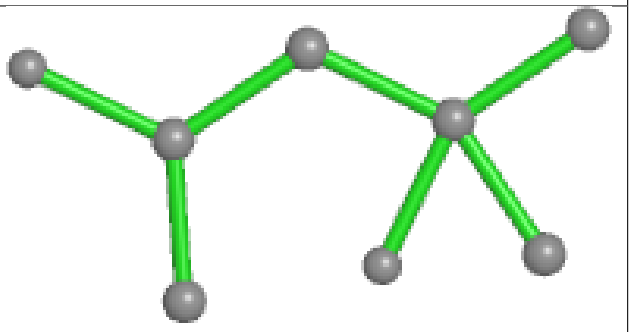
Ligand EDO F 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand EDO A 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

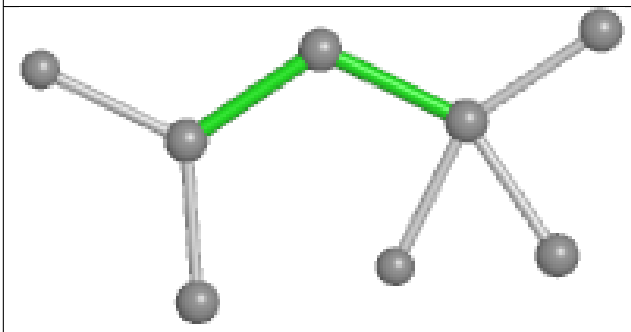
Ligand MPD C 403



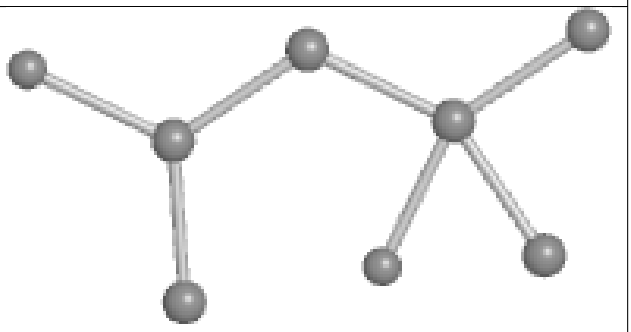
Bond lengths



Bond angles

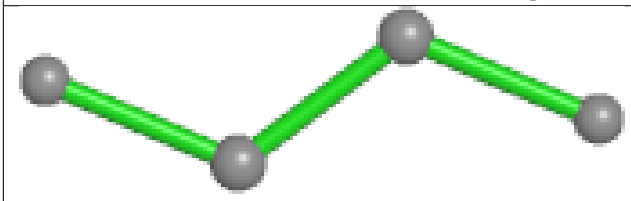


Torsions

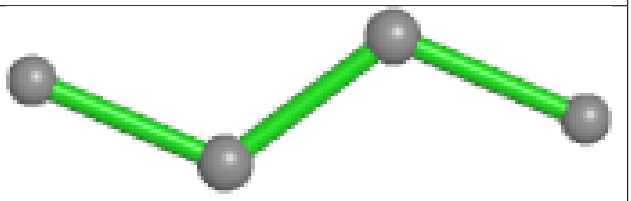


Rings

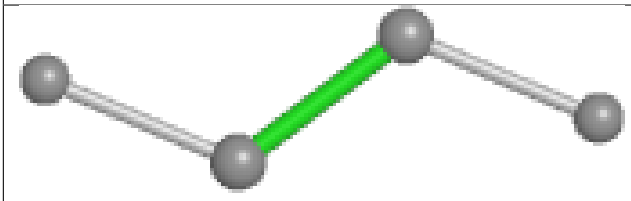
Ligand EDO F 403



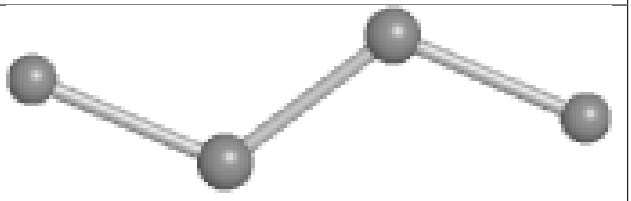
Bond lengths



Bond angles

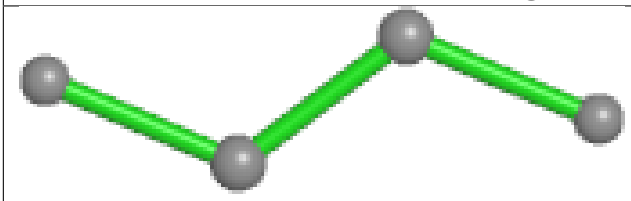


Torsions

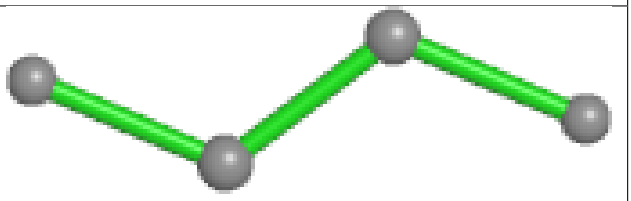


Rings

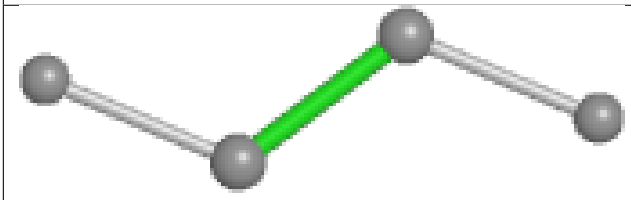
Ligand EDO B 407



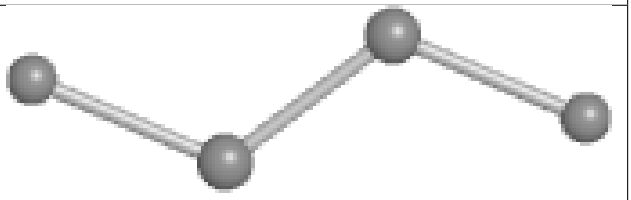
Bond lengths



Bond angles

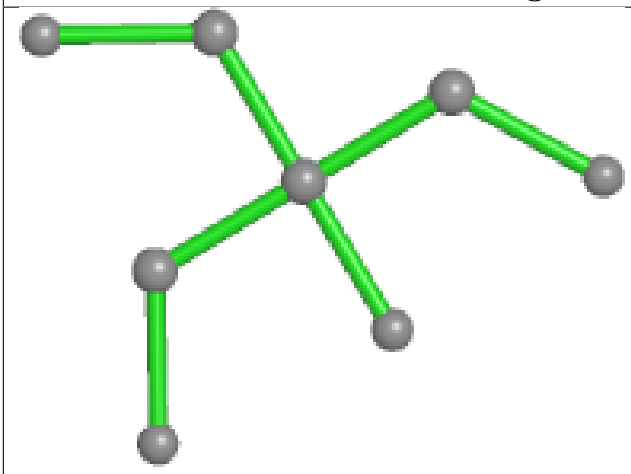


Torsions

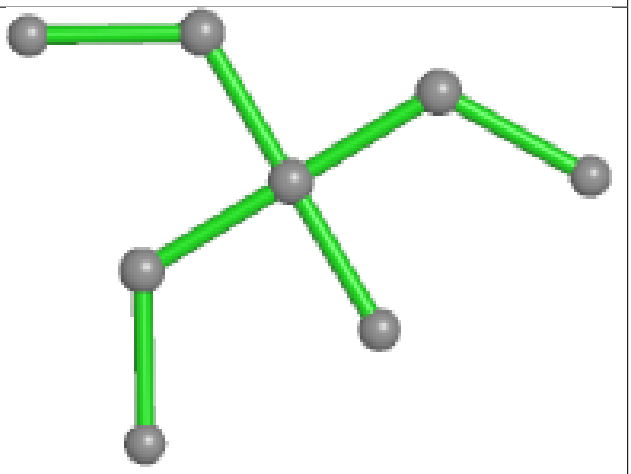


Rings

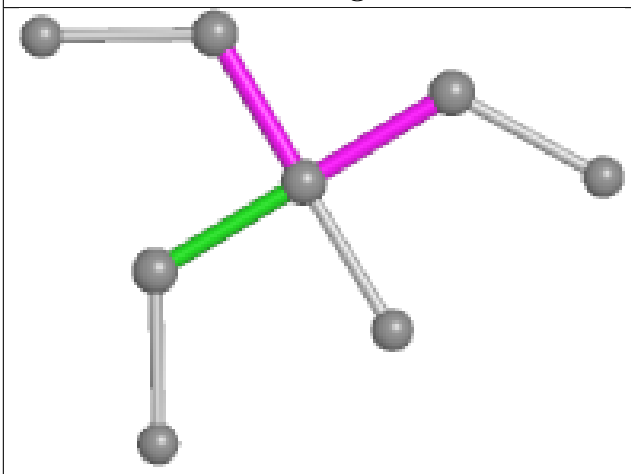
Ligand TRS B 404



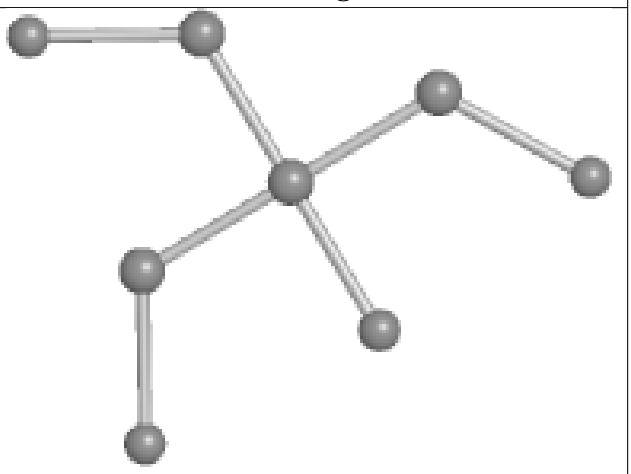
Bond lengths



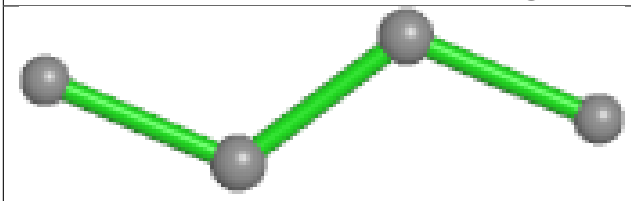
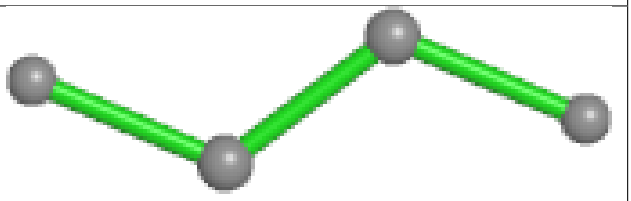
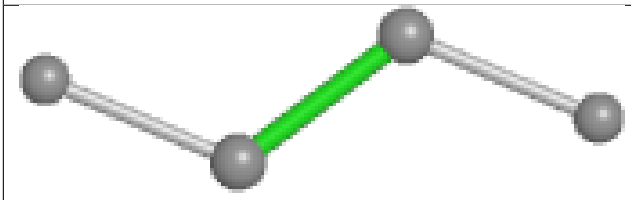
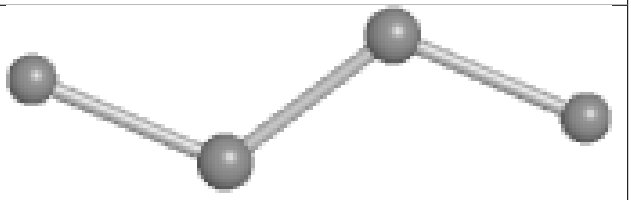
Bond angles

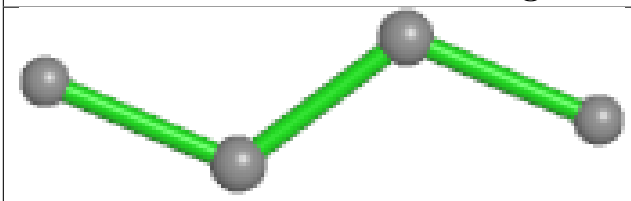
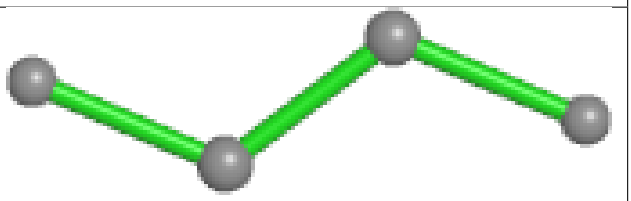
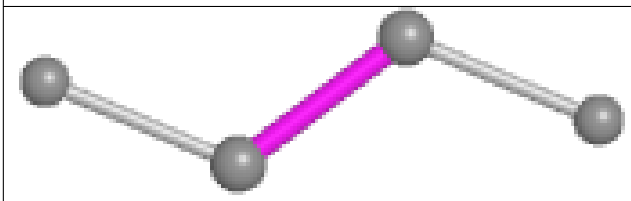
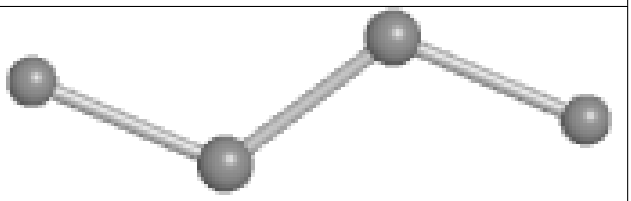


Torsions

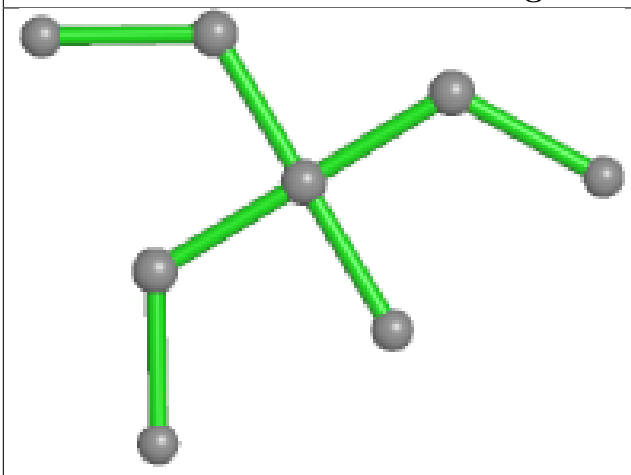


Rings

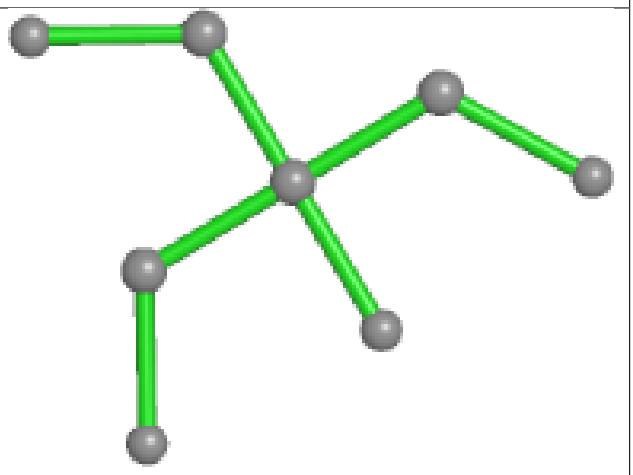
Ligand EDO B 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EDO A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

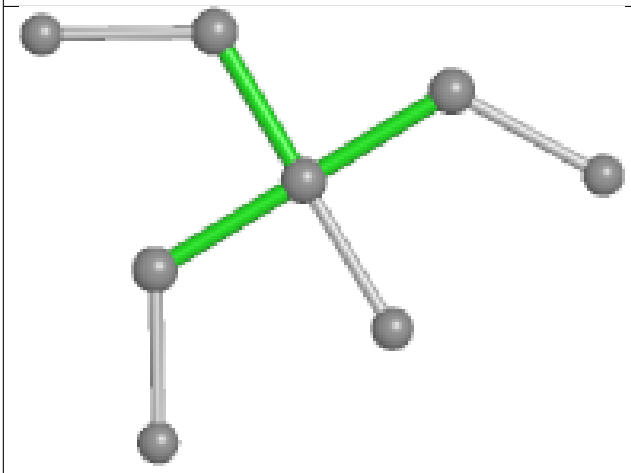
Ligand TRS A 405



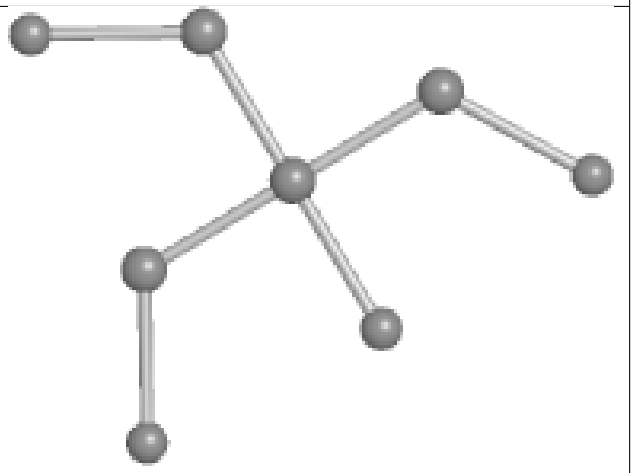
Bond lengths



Bond angles

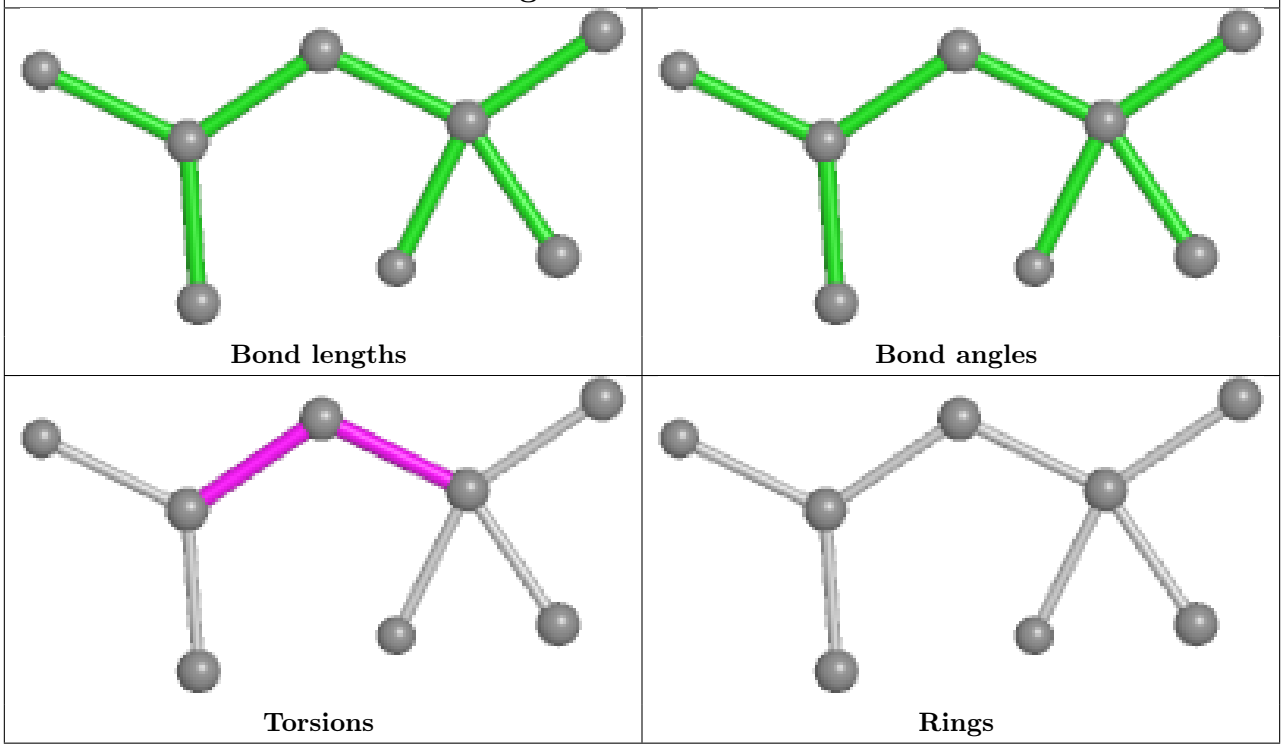


Torsions



Rings

Ligand MPD B 403



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	291/307 (94%)	-0.02	3 (1%)	82	85	15, 23, 40, 66	0
1	B	291/307 (94%)	-0.03	2 (0%)	87	90	15, 22, 38, 60	0
1	C	291/307 (94%)	-0.04	2 (0%)	87	90	17, 25, 39, 58	0
1	D	291/307 (94%)	-0.02	2 (0%)	87	90	16, 24, 38, 62	0
1	E	287/307 (93%)	0.22	13 (4%)	33	37	21, 32, 51, 73	0
1	F	290/307 (94%)	0.35	13 (4%)	33	37	22, 35, 54, 70	0
All	All	1741/1842 (94%)	0.08	35 (2%)	65	69	15, 26, 46, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	26	ARG	6.8
1	D	297	ALA	6.1
1	E	28	ASP	4.2
1	A	26	ARG	4.1
1	F	28	ASP	4.1
1	F	26	ARG	4.0
1	E	295	ALA	3.8
1	E	294	ALA	3.8
1	F	294	ALA	3.7
1	F	289	ILE	3.4
1	A	6	ASP	3.2
1	B	28	ASP	2.8
1	F	179	LYS	2.7
1	E	291	GLU	2.7
1	D	296	SER	2.7
1	E	27	SER	2.7
1	E	290	ALA	2.6
1	C	170	ARG	2.5
1	F	252	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	262	ARG	2.5
1	E	9	LEU	2.5
1	F	27	SER	2.5
1	A	296	SER	2.4
1	E	118	ASP	2.4
1	F	16	ASP	2.3
1	F	288	TRP	2.3
1	B	26	ARG	2.2
1	E	25	GLY	2.1
1	E	256	ALA	2.1
1	E	182	GLU	2.1
1	C	28	ASP	2.1
1	F	149	ARG	2.0
1	F	177	VAL	2.0
1	F	146	GLU	2.0
1	F	6	ASP	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
5	EDO	F	404	4/4	0.53	0.16	51,57,58,59	0
5	EDO	C	408	4/4	0.67	0.24	45,46,49,51	0
5	EDO	F	406	4/4	0.67	0.16	55,56,56,56	0
5	EDO	D	405	4/4	0.68	0.14	50,50,51,54	0
5	EDO	B	406	4/4	0.70	0.15	40,42,49,50	0
5	EDO	A	409	4/4	0.71	0.20	36,38,42,48	0
5	EDO	C	406	4/4	0.74	0.14	52,53,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	F	407	4/4	0.74	0.31	40,44,48,50	0
5	EDO	A	414	4/4	0.75	0.11	51,55,55,56	0
4	TRS	A	407	8/8	0.77	0.24	34,40,46,50	0
4	TRS	A	405	8/8	0.78	0.18	38,48,49,49	0
5	EDO	B	410	4/4	0.78	0.12	48,49,50,59	0
5	EDO	B	409	4/4	0.79	0.14	28,36,38,40	0
4	TRS	B	404	8/8	0.79	0.31	35,41,47,52	0
5	EDO	A	411	4/4	0.80	0.12	43,45,49,54	0
5	EDO	C	407	4/4	0.80	0.23	37,41,45,50	0
5	EDO	F	403	4/4	0.80	0.12	53,54,56,59	0
3	MPD	C	403	8/8	0.81	0.17	29,35,39,42	0
5	EDO	C	409	4/4	0.81	0.21	48,51,56,60	0
5	EDO	C	405	4/4	0.81	0.15	40,40,43,54	0
5	EDO	D	406	4/4	0.81	0.11	43,46,51,52	0
4	TRS	A	406	8/8	0.83	0.27	26,43,47,53	0
3	MPD	D	403	8/8	0.83	0.21	34,35,40,43	0
5	EDO	B	411	4/4	0.84	0.26	26,30,31,35	0
3	MPD	B	403	8/8	0.85	0.24	41,47,49,52	0
5	EDO	D	404	4/4	0.85	0.29	34,36,38,43	0
5	EDO	B	408	4/4	0.85	0.18	35,37,42,44	0
5	EDO	B	405	4/4	0.85	0.11	33,41,42,45	0
5	EDO	A	408	4/4	0.86	0.18	36,36,39,46	0
5	EDO	E	403	4/4	0.86	0.10	41,51,55,63	0
5	EDO	C	410	4/4	0.86	0.15	40,40,43,43	0
5	EDO	C	411	4/4	0.87	0.30	28,29,35,49	0
5	EDO	A	412	4/4	0.87	0.23	40,44,45,46	0
5	EDO	A	410	4/4	0.87	0.11	37,43,47,52	0
5	EDO	A	413	4/4	0.88	0.20	35,37,38,46	0
4	TRS	A	404	8/8	0.89	0.17	31,45,47,50	0
5	EDO	F	405	4/4	0.89	0.36	32,40,45,46	0
3	MPD	A	403	8/8	0.90	0.22	34,42,45,48	0
5	EDO	B	407	4/4	0.90	0.26	34,45,48,55	0
3	MPD	C	404	8/8	0.91	0.12	39,46,54,59	0
2	CL	F	402	1/1	0.97	0.06	33,33,33,33	0
2	CL	E	402	1/1	0.98	0.08	30,30,30,30	0
2	CL	D	402	1/1	0.98	0.09	22,22,22,22	0
2	CL	E	401	1/1	0.98	0.09	24,24,24,24	0
2	CL	C	401	1/1	0.99	0.11	20,20,20,20	0
2	CL	C	402	1/1	0.99	0.08	24,24,24,24	0
2	CL	F	401	1/1	0.99	0.08	27,27,27,27	0
2	CL	A	402	1/1	0.99	0.08	17,17,17,17	0
2	CL	A	401	1/1	1.00	0.08	16,16,16,16	0

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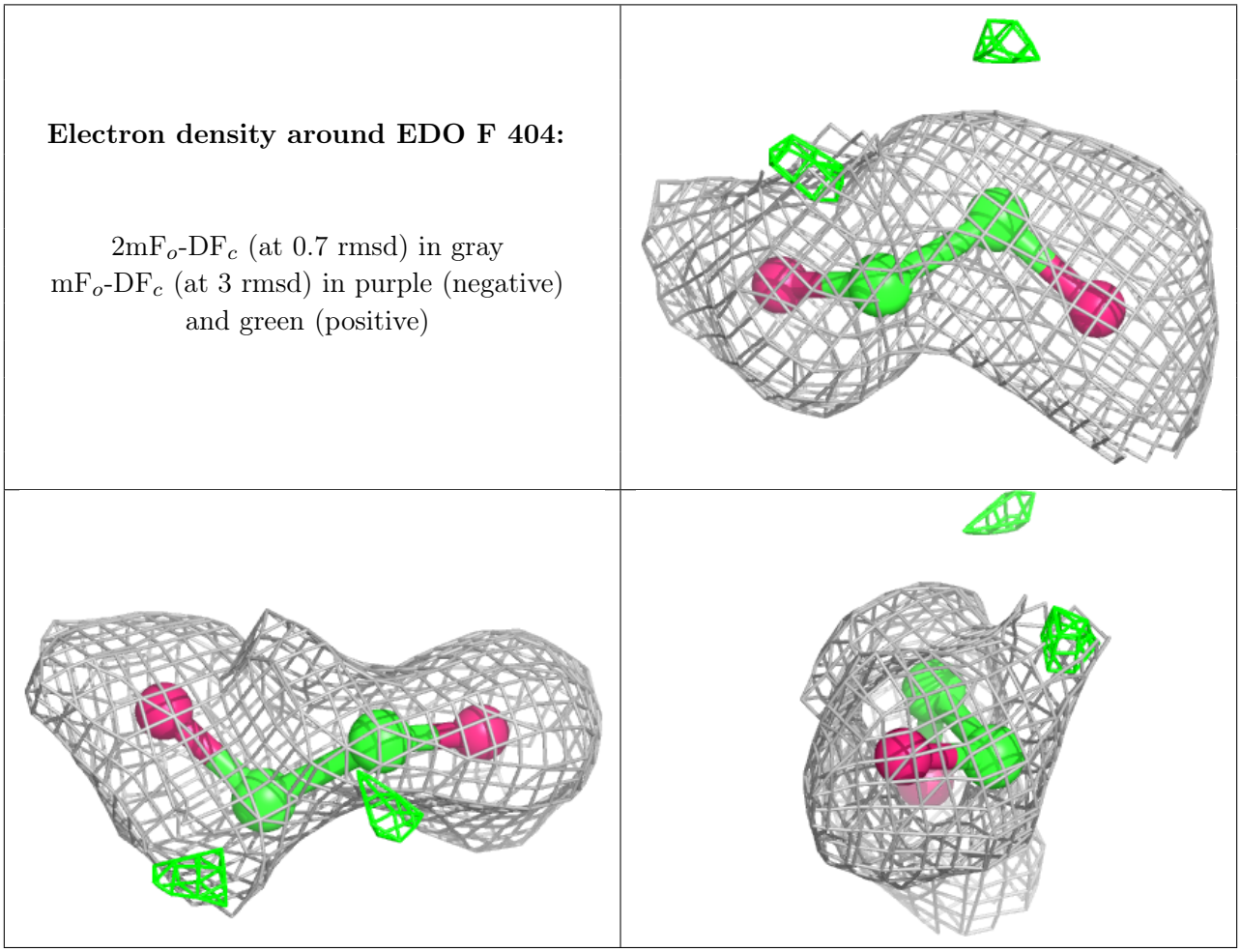
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	B	401	1/1	1.00	0.09	18,18,18,18	0
2	CL	D	401	1/1	1.00	0.10	23,23,23,23	0
2	CL	B	402	1/1	1.00	0.11	16,16,16,16	0

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.

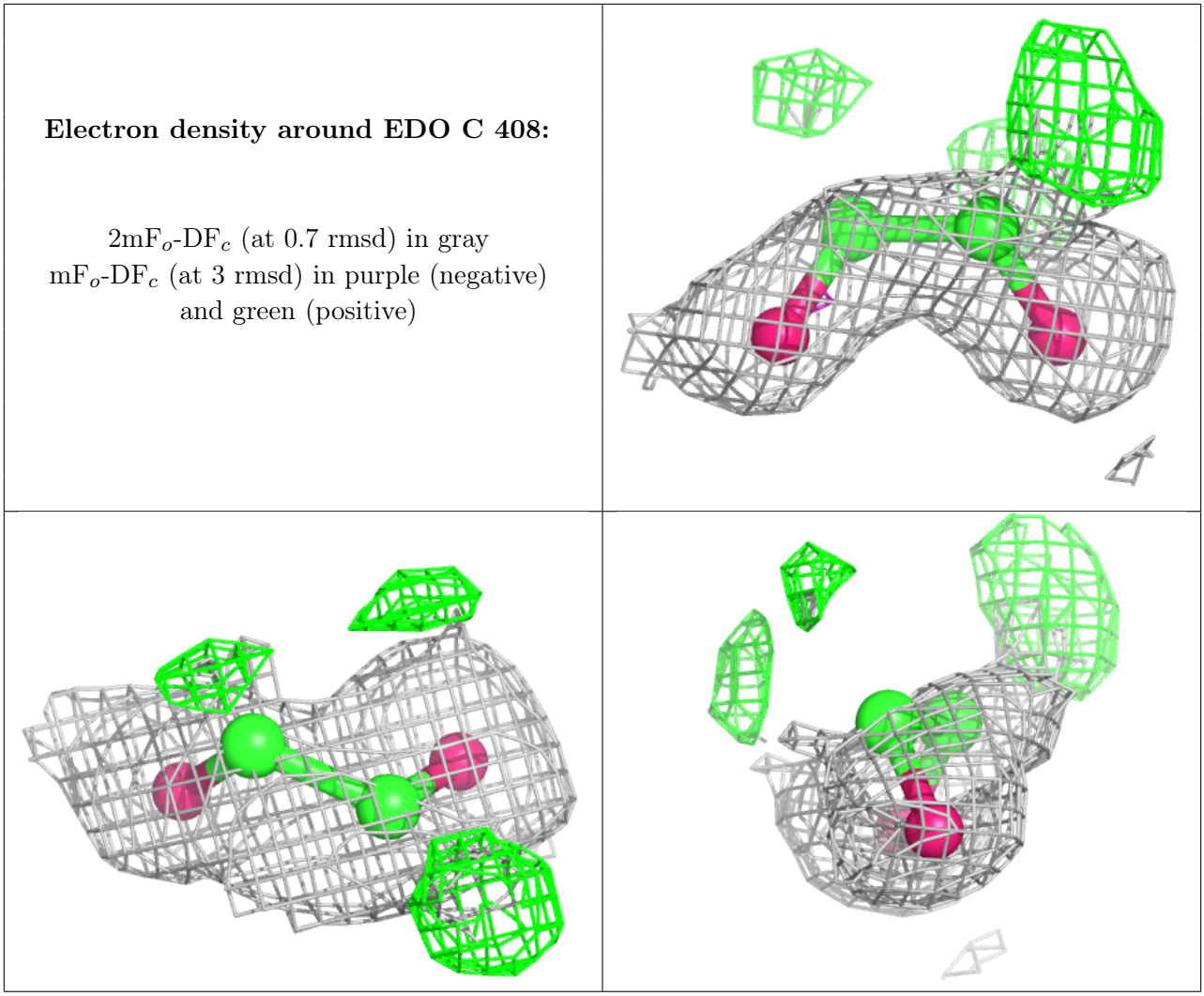
Electron density around EDO F 404:

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



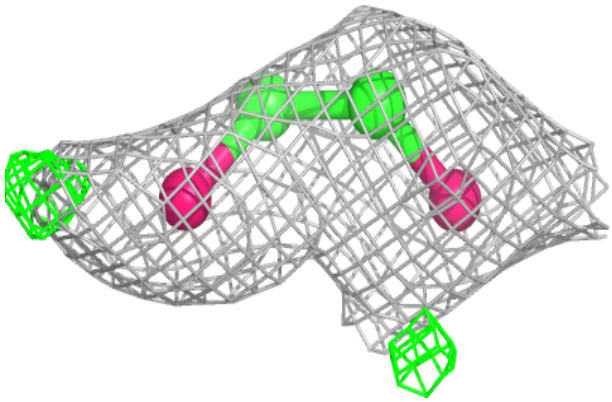
Electron density around EDO C 408:

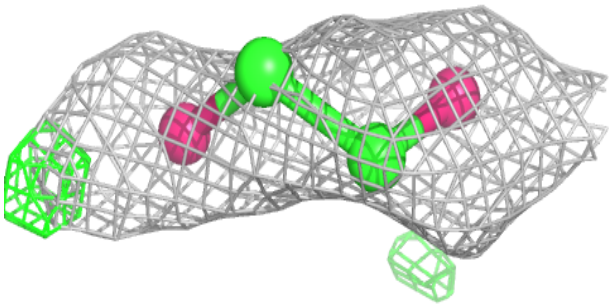
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

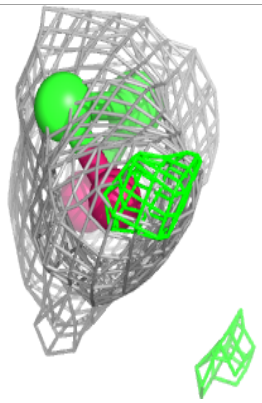


Electron density around EDO F 406:

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

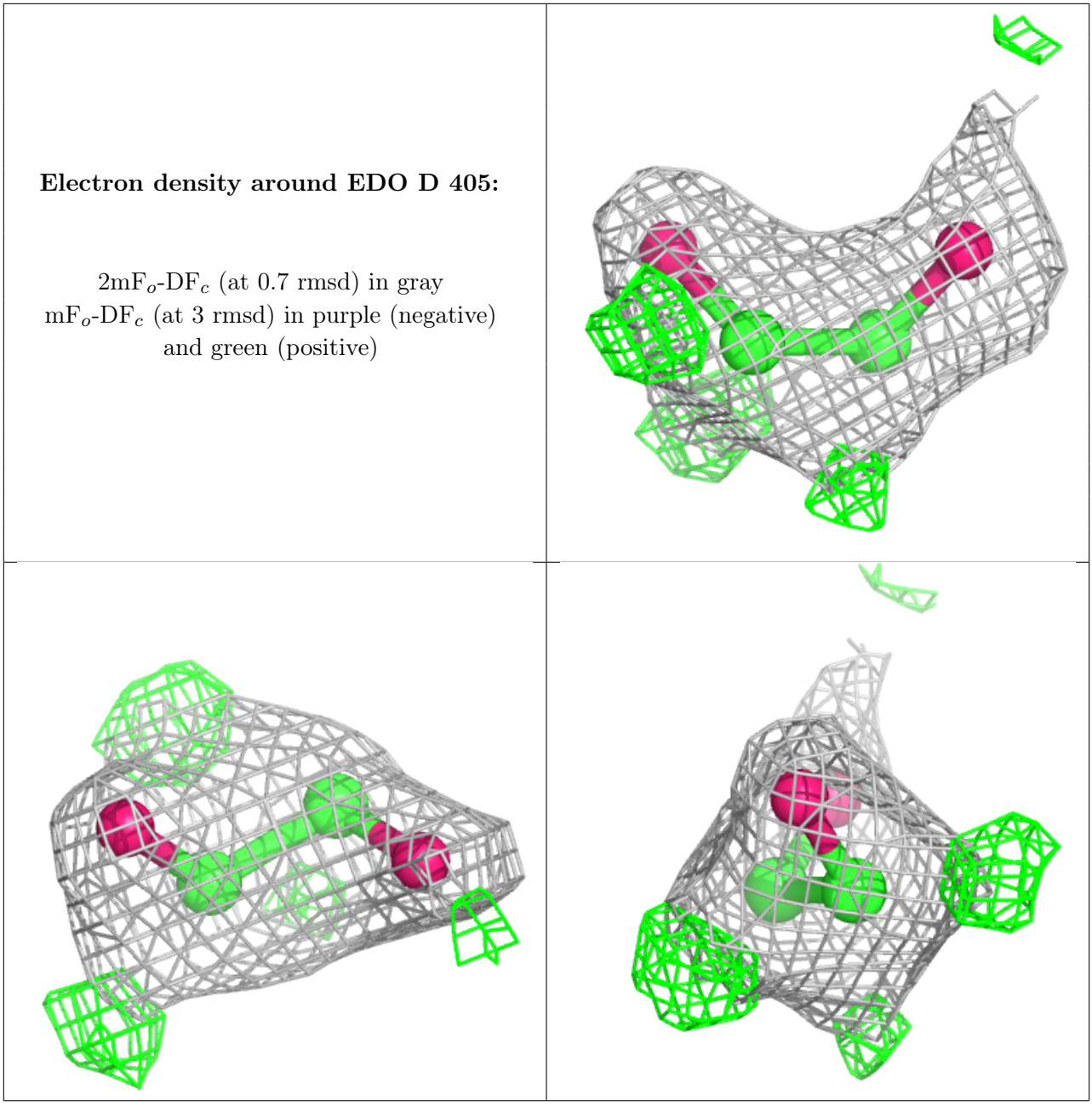






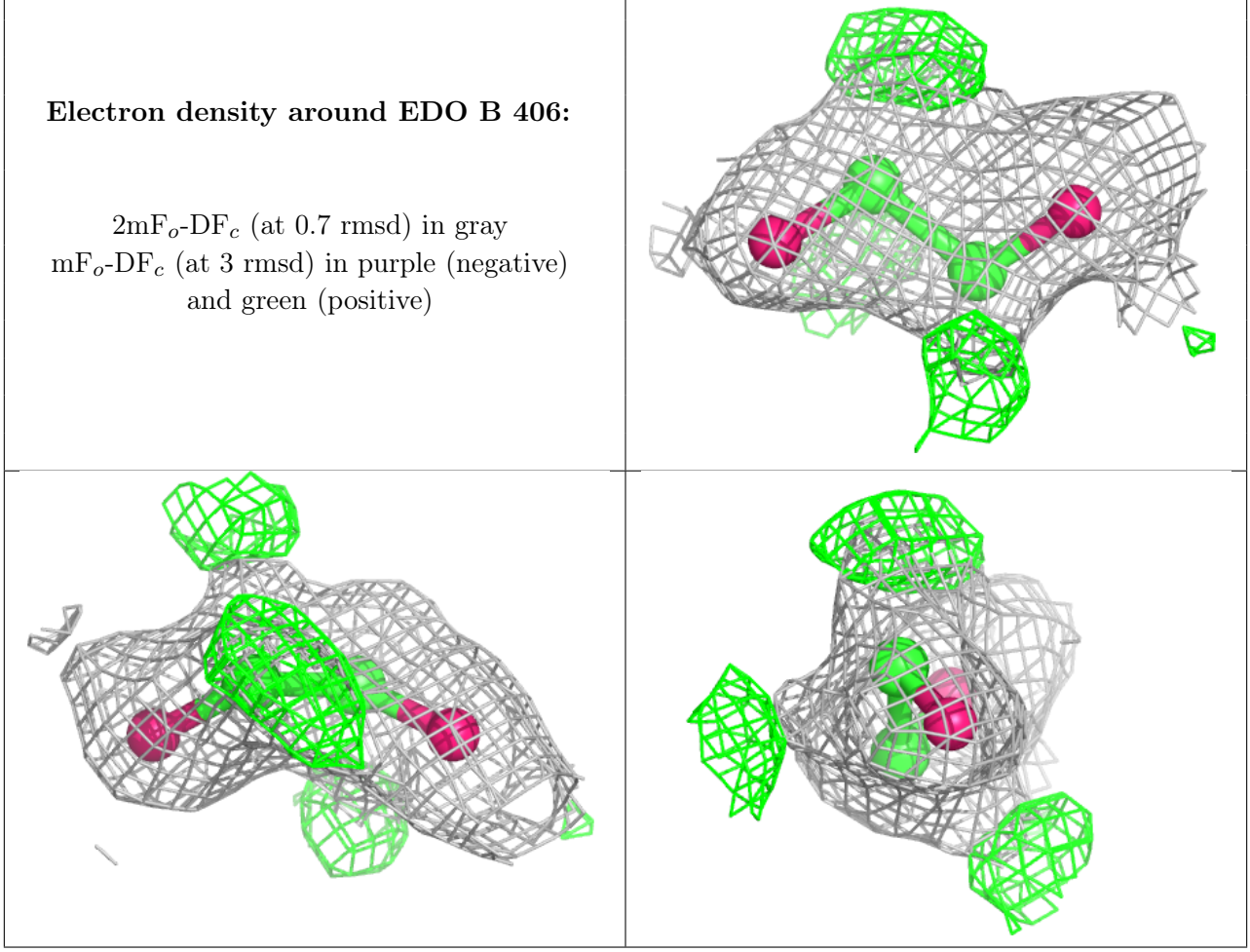
Electron density around EDO D 405:

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



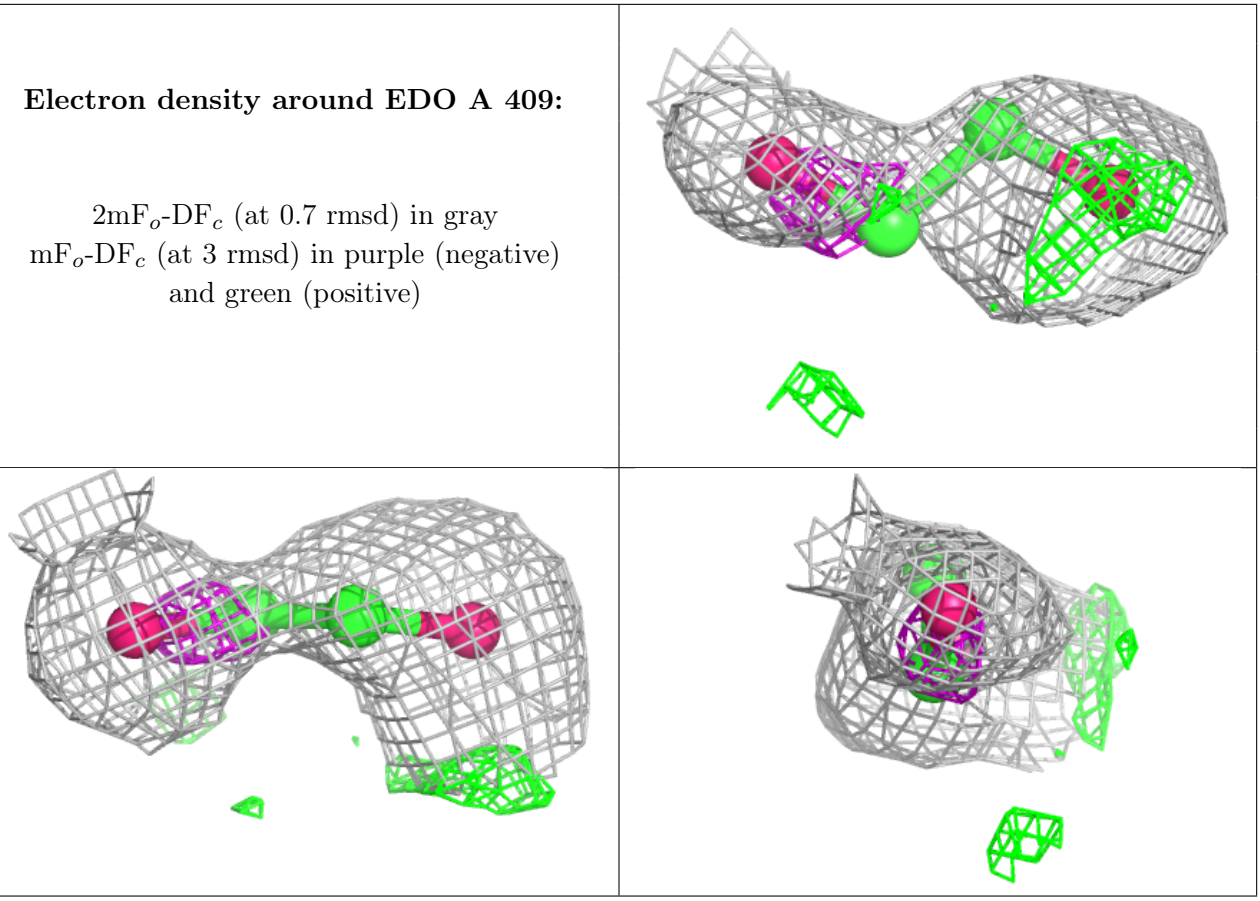
Electron density around EDO B 406:

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



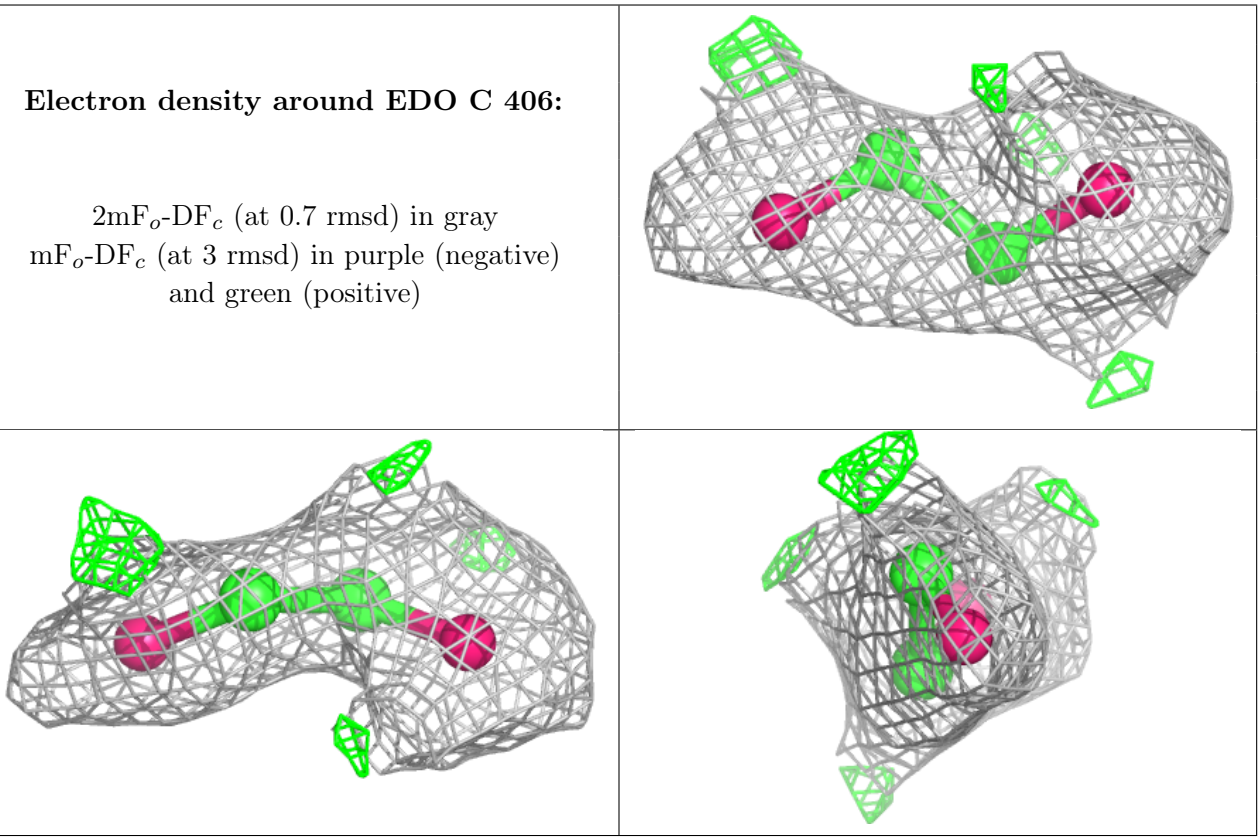
Electron density around EDO A 409:

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



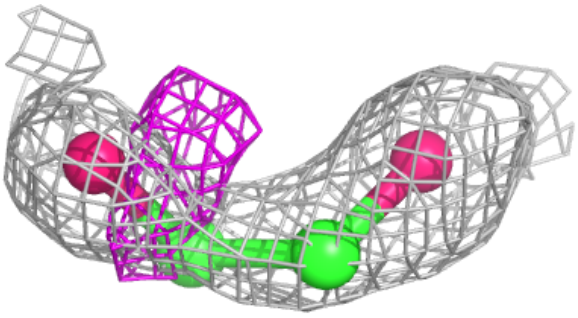
Electron density around EDO C 406:

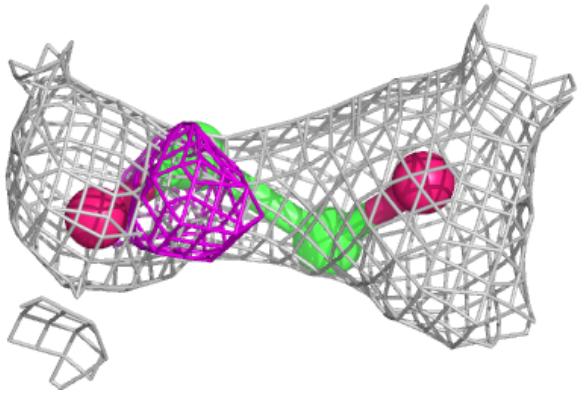
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

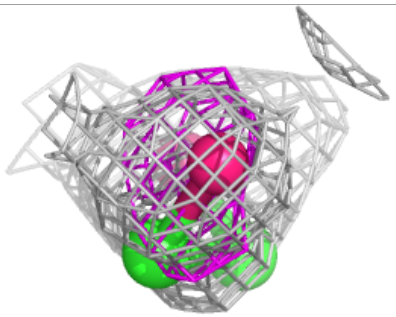


Electron density around EDO F 407:

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

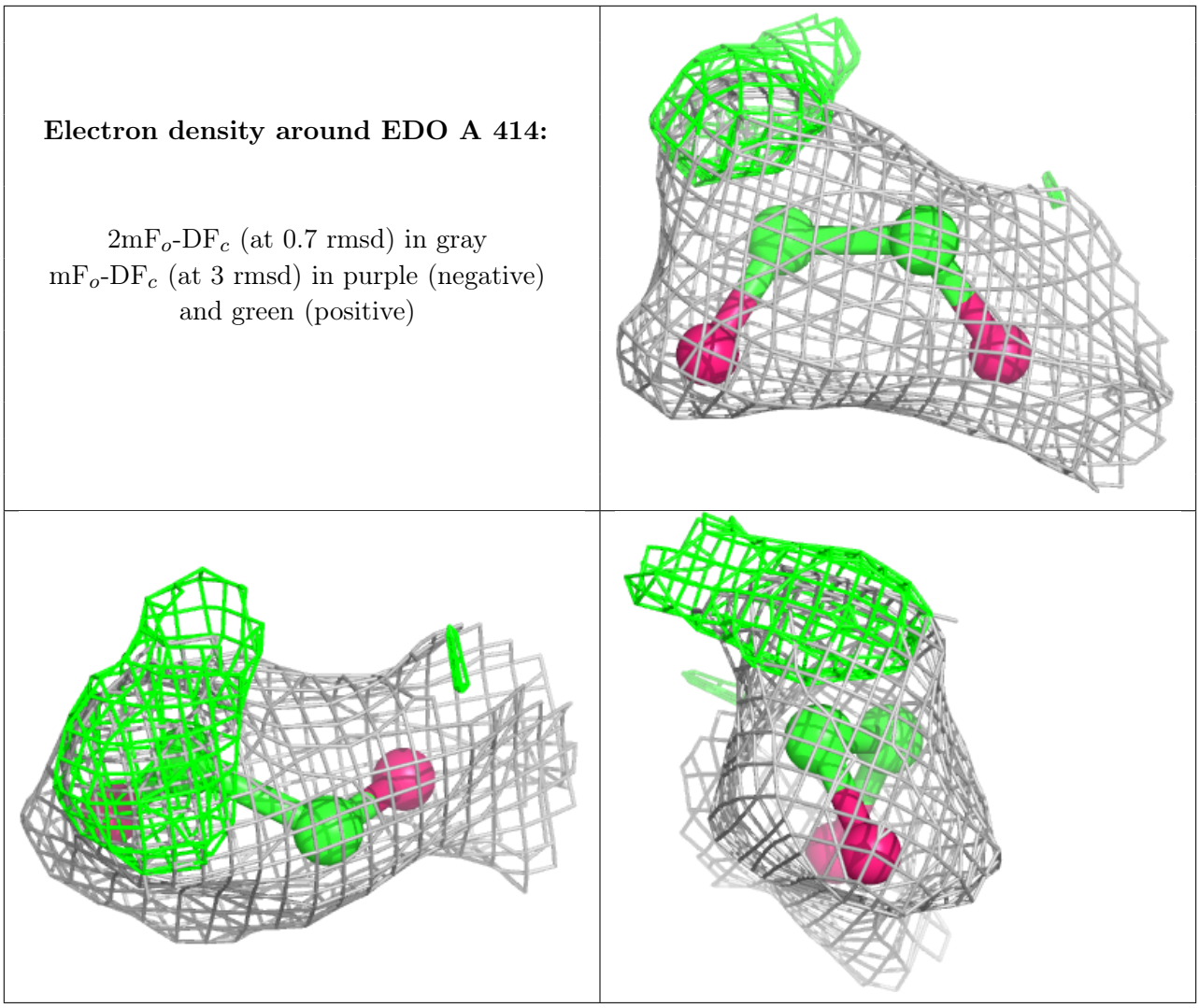






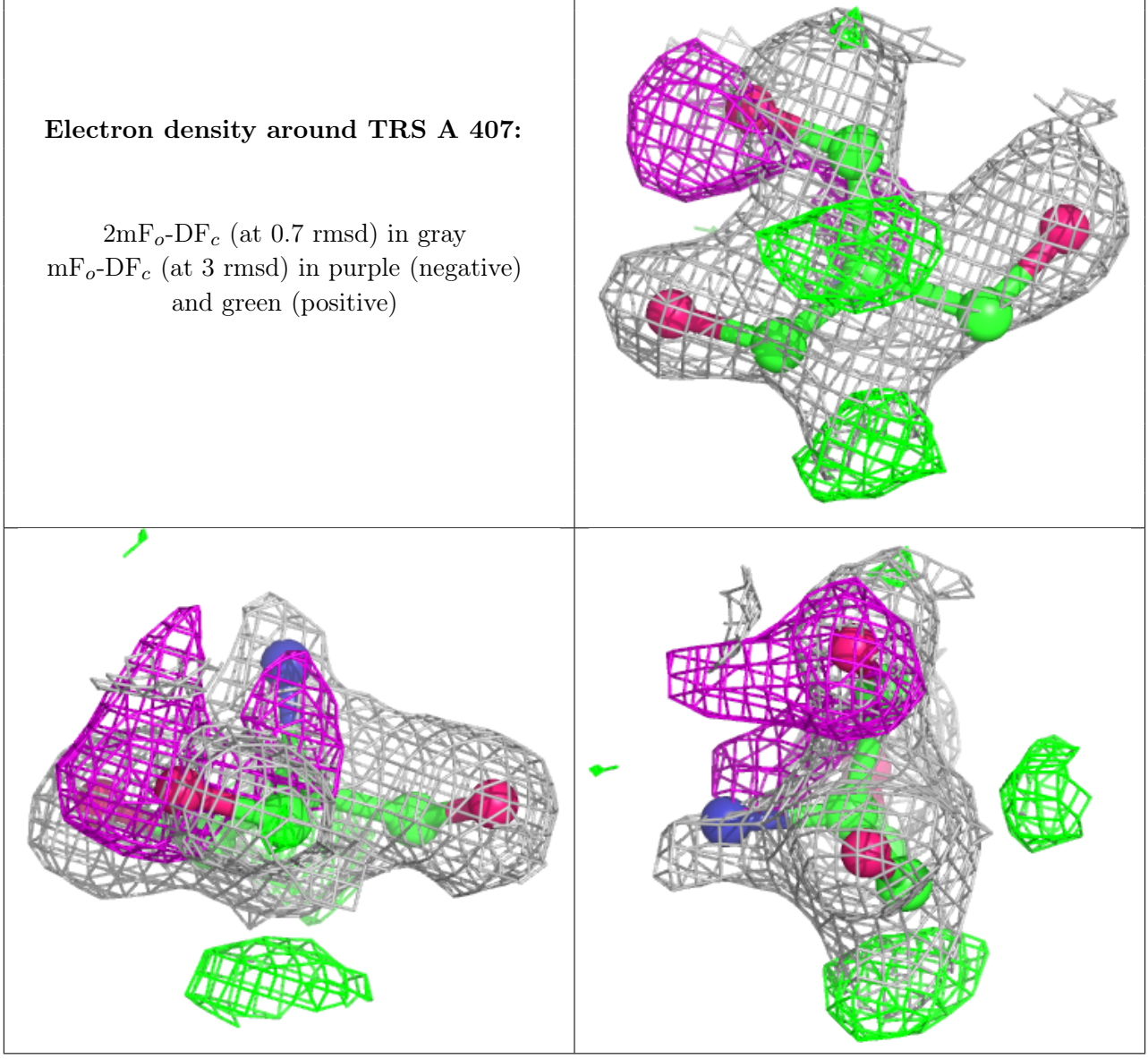
Electron density around EDO A 414:

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



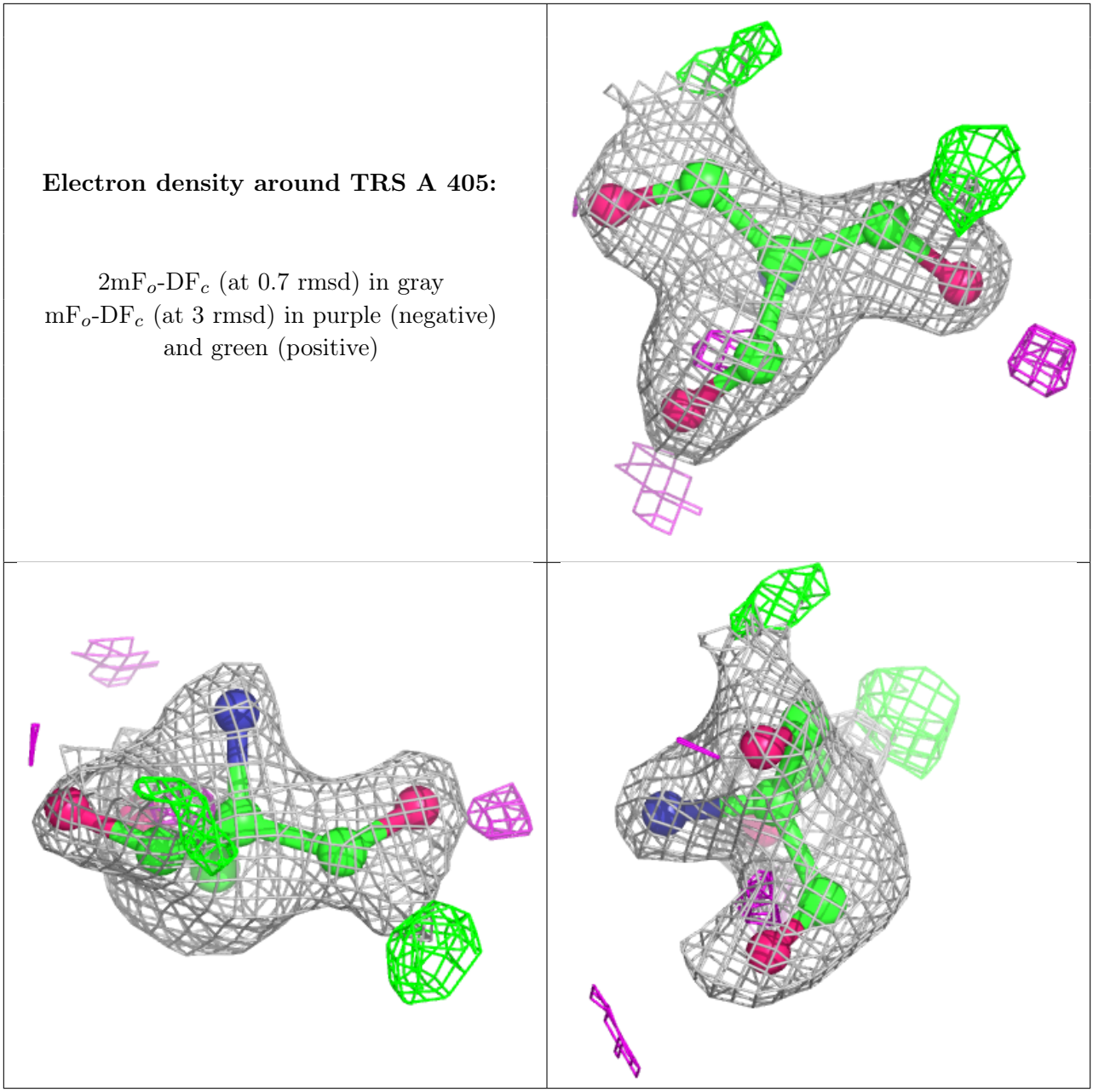
Electron density around TRS A 407:

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



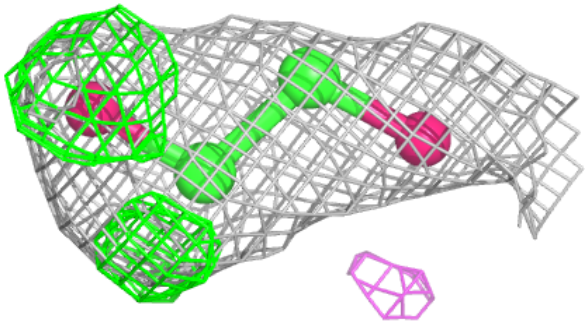
Electron density around TRS A 405:

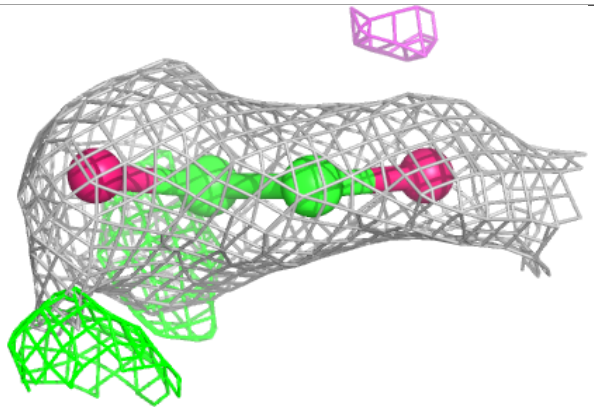
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

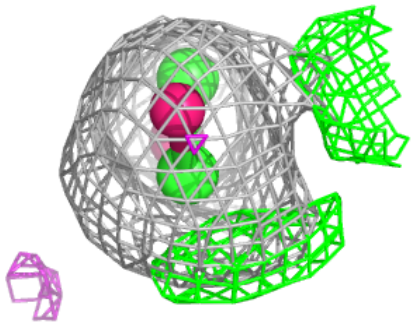


Electron density around EDO B 410:

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

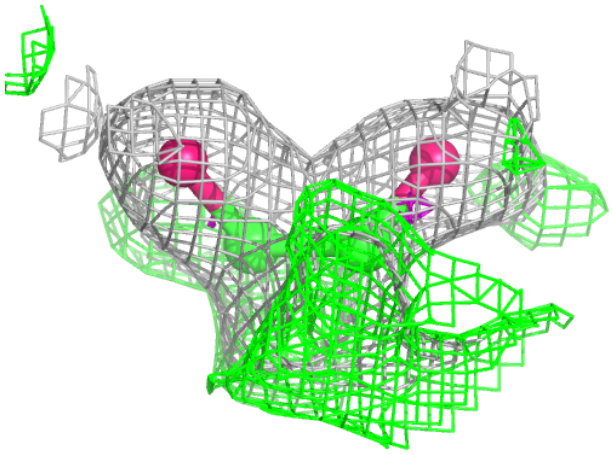


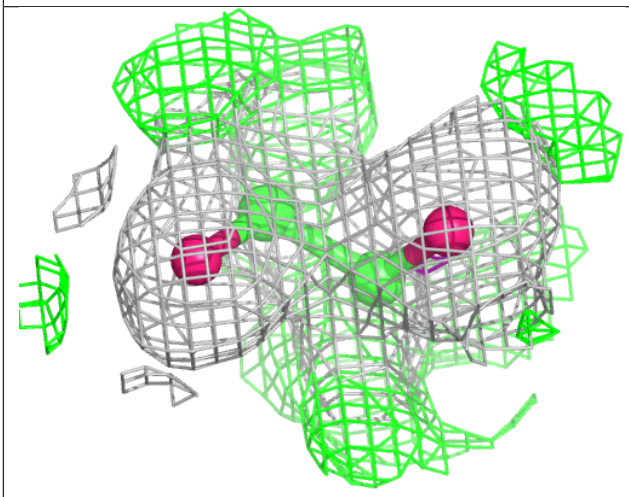


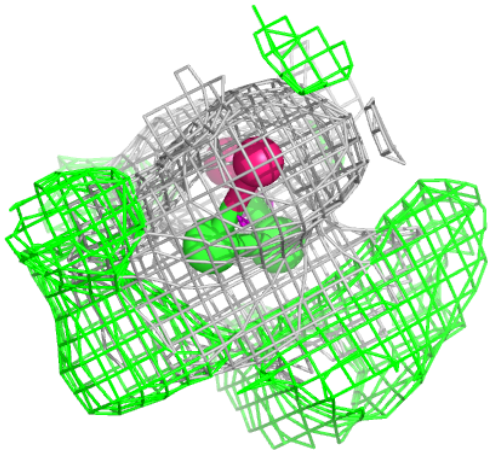


Electron density around EDO B 409:

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

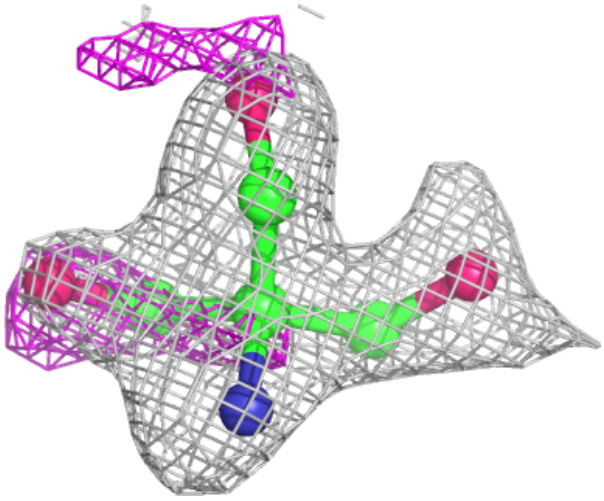


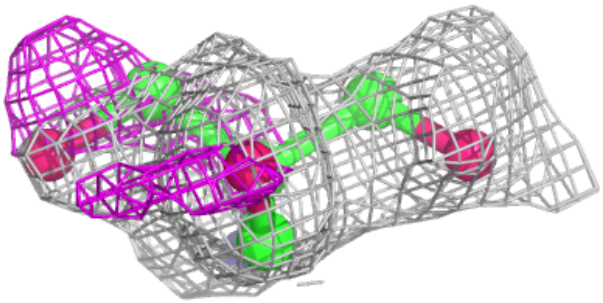


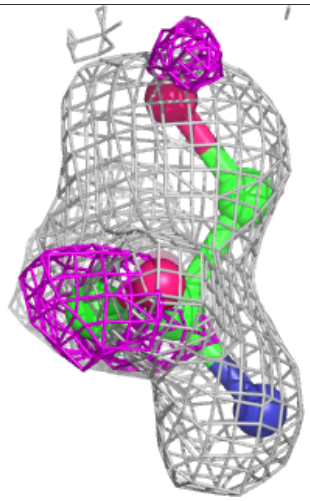


Electron density around TRS B 404:

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

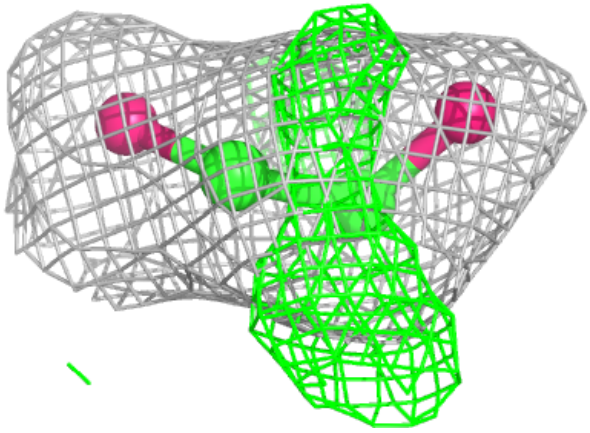


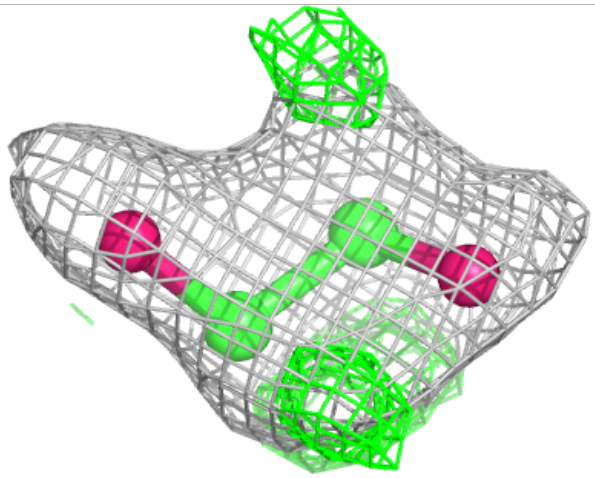


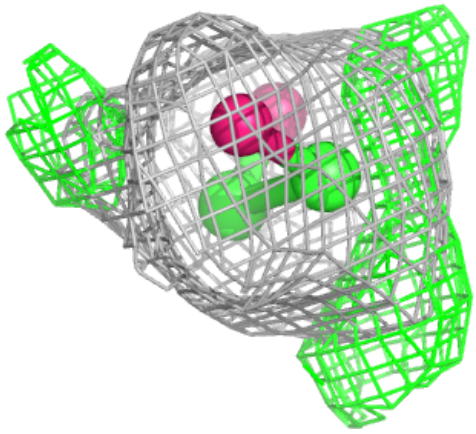


Electron density around EDO A 411:

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

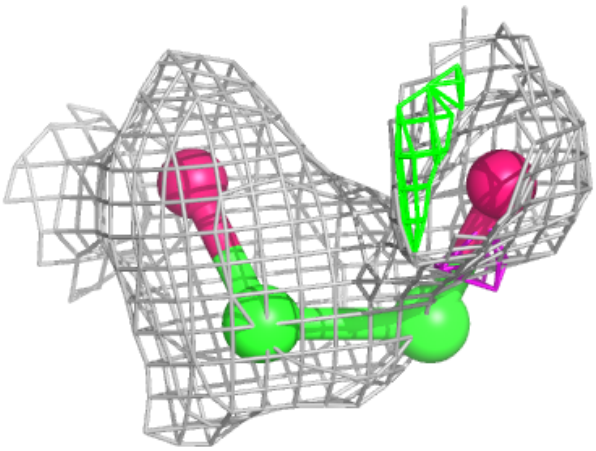


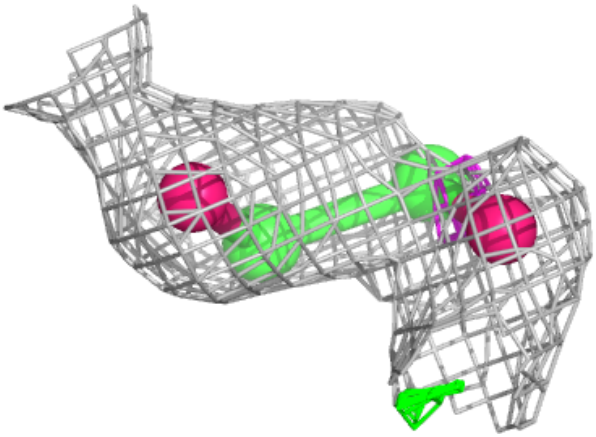


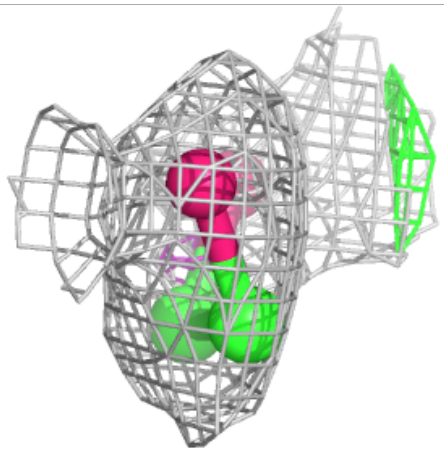


Electron density around EDO C 407:

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

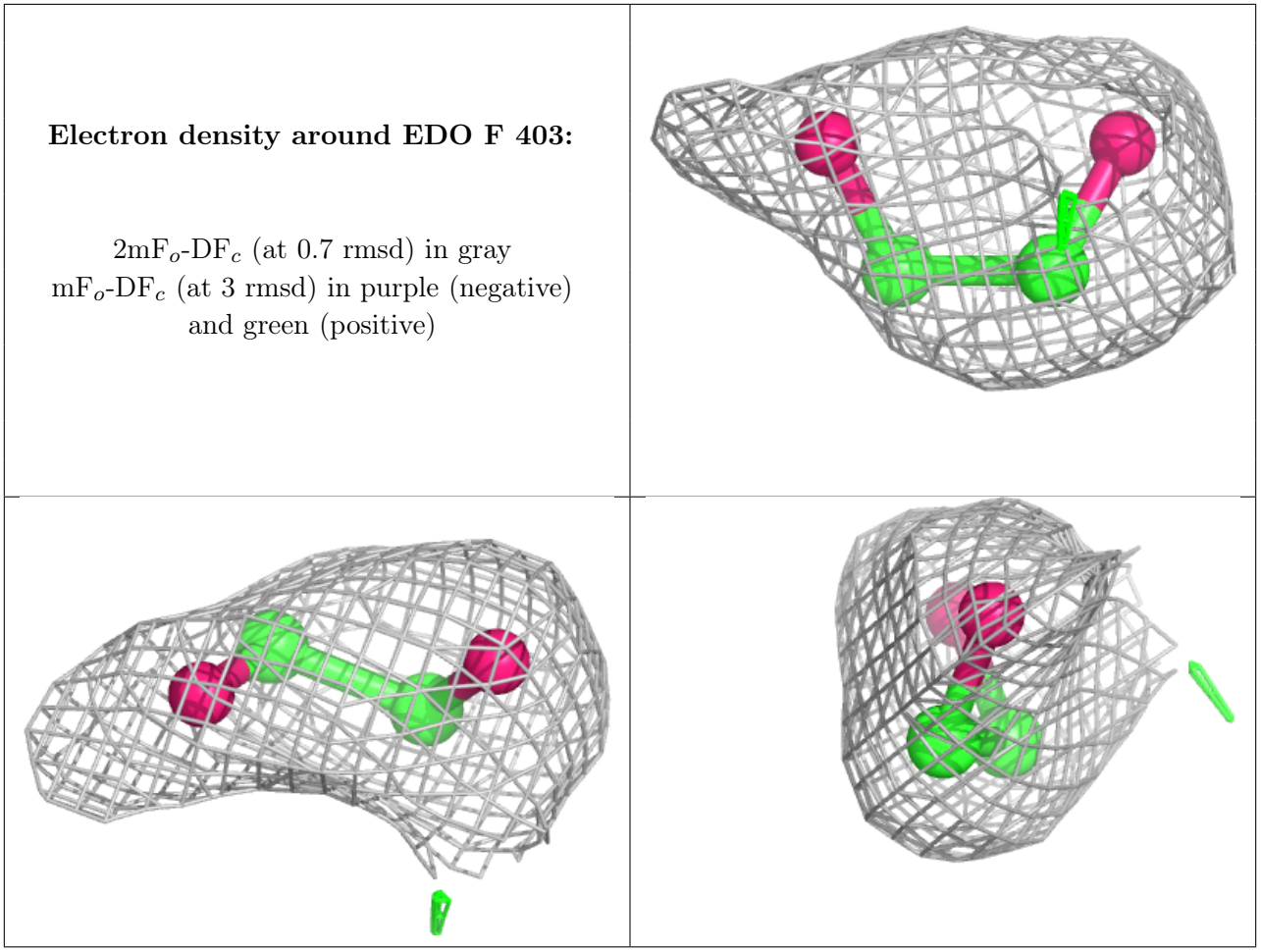






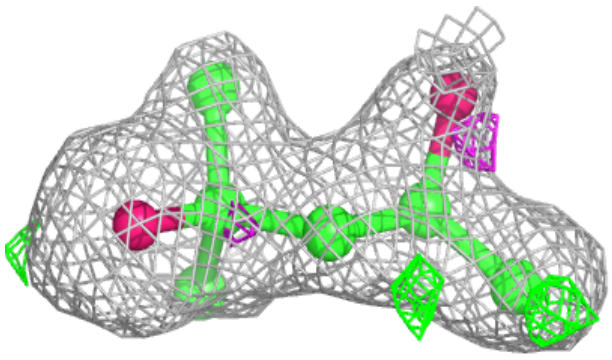
Electron density around EDO F 403:

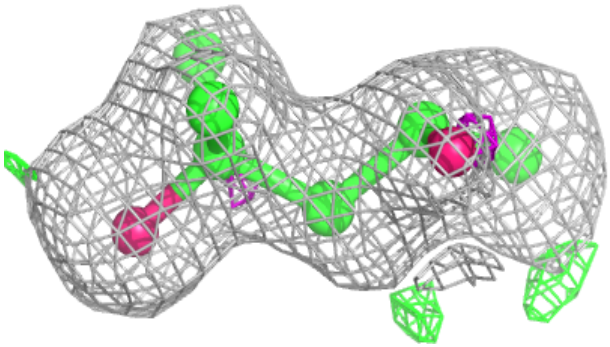
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

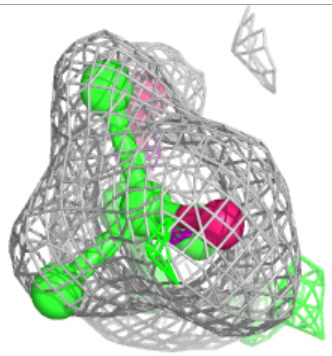


Electron density around MPD C 403:

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

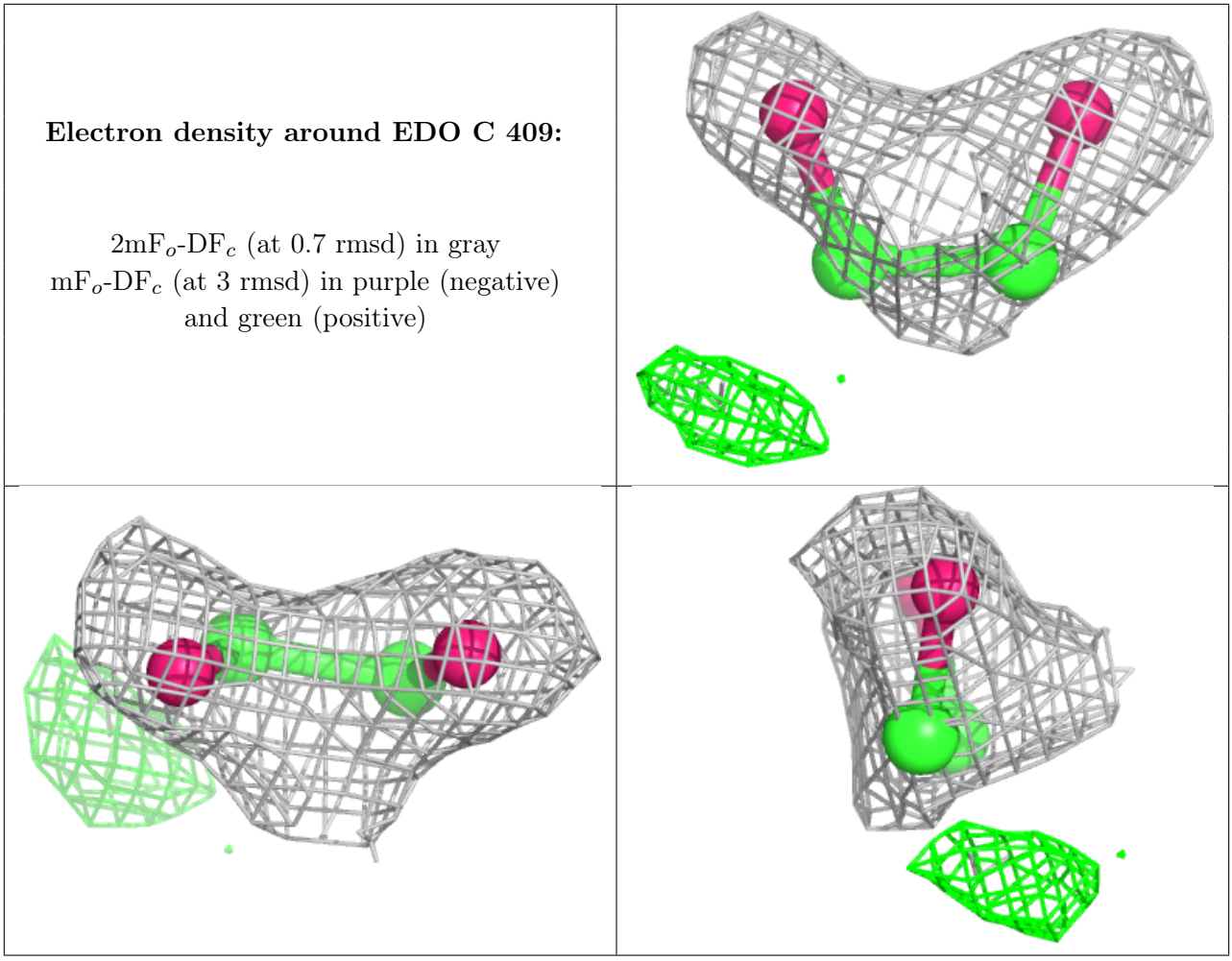






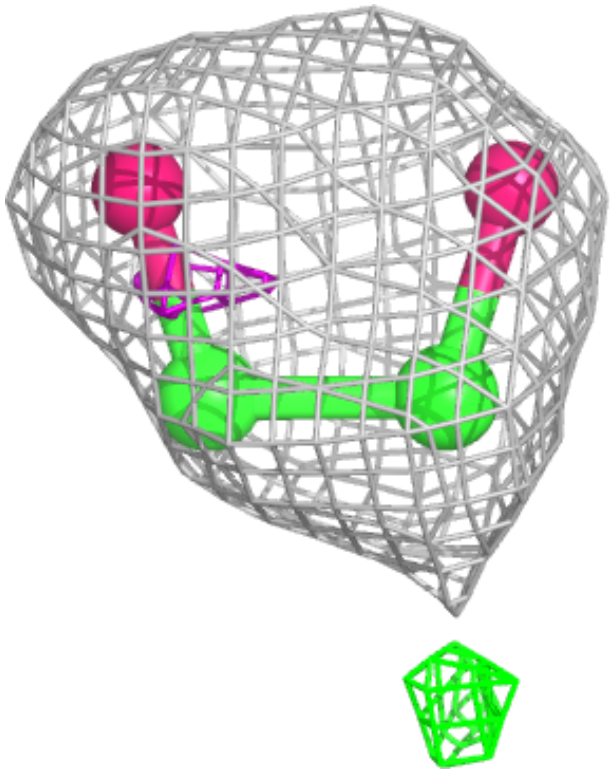
Electron density around EDO C 409:

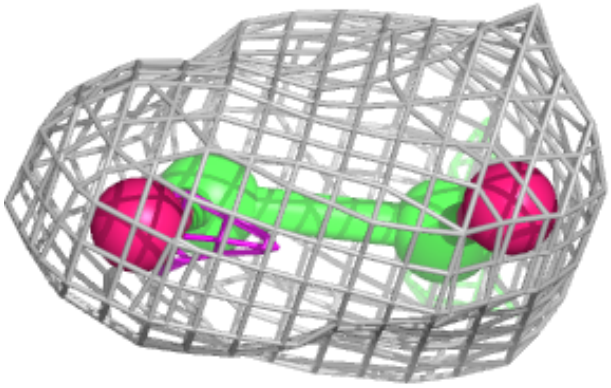
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

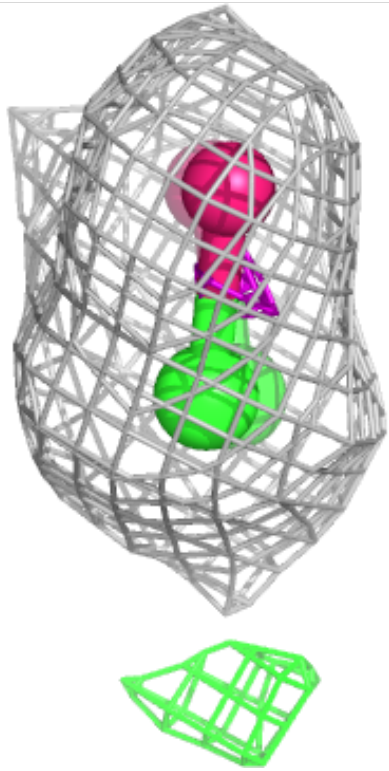


Electron density around EDO C 405:

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

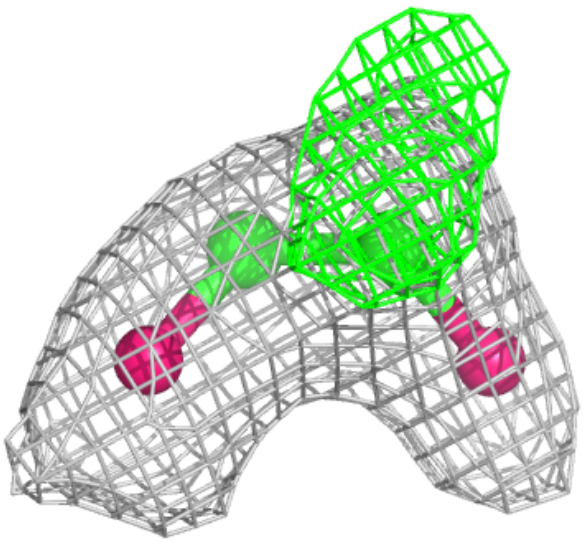


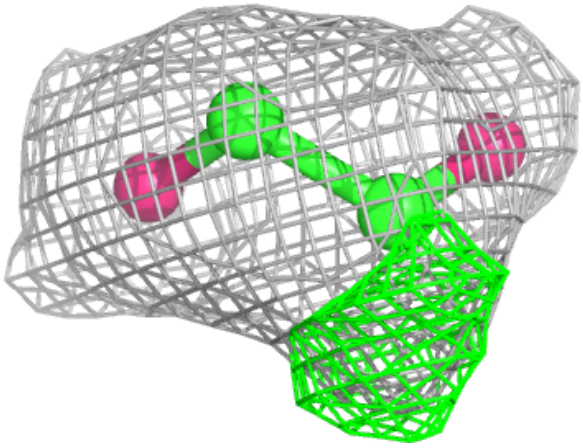


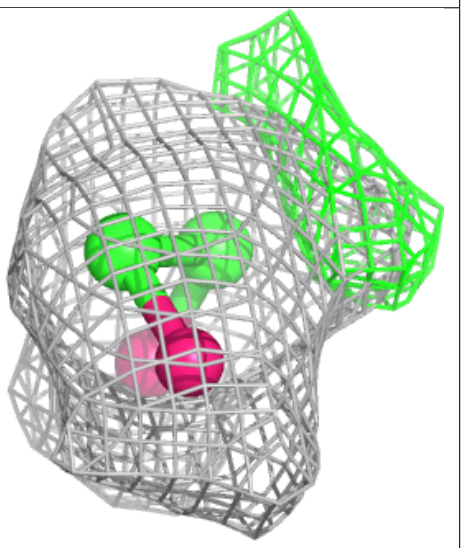


Electron density around EDO D 406:

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

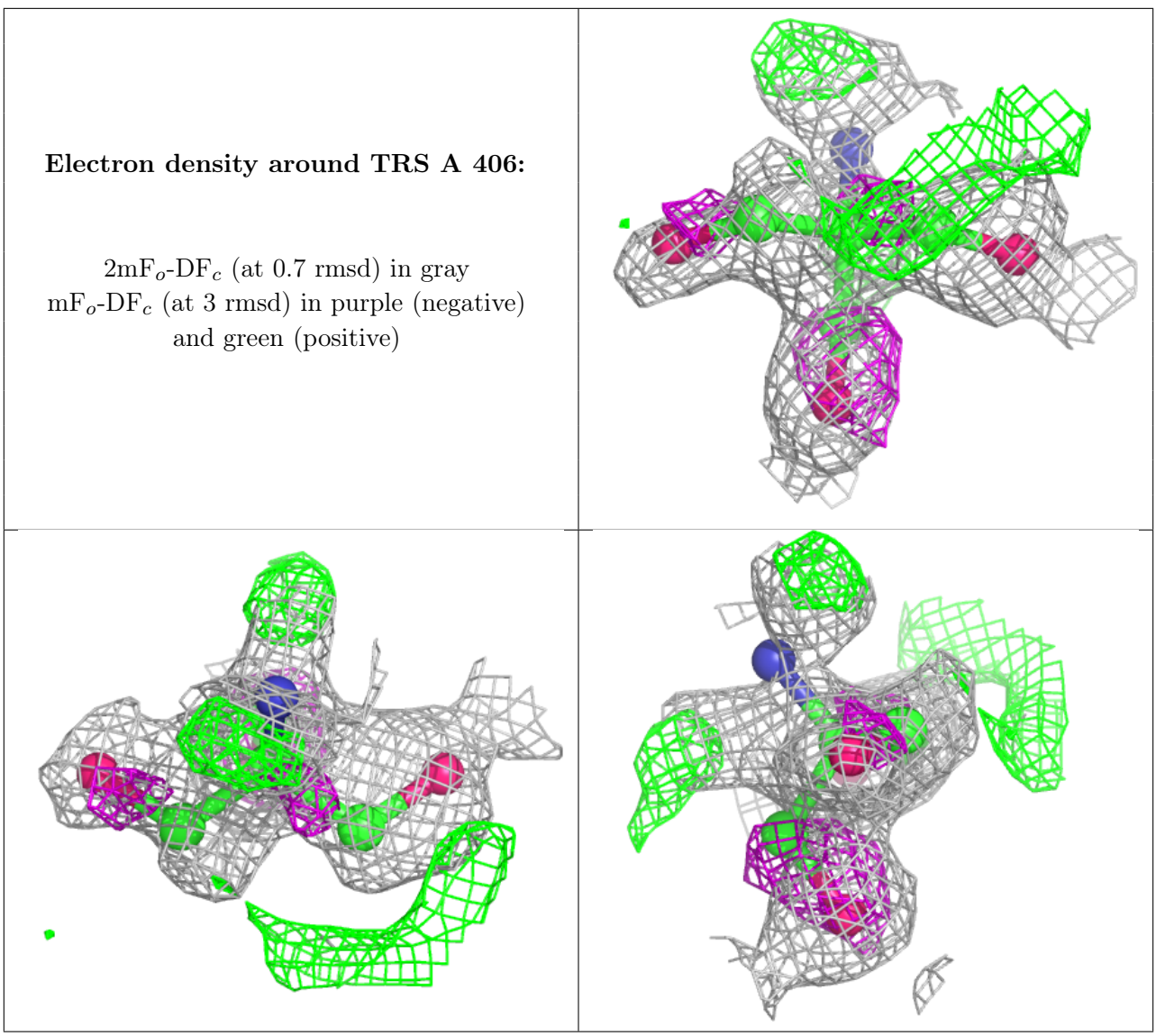






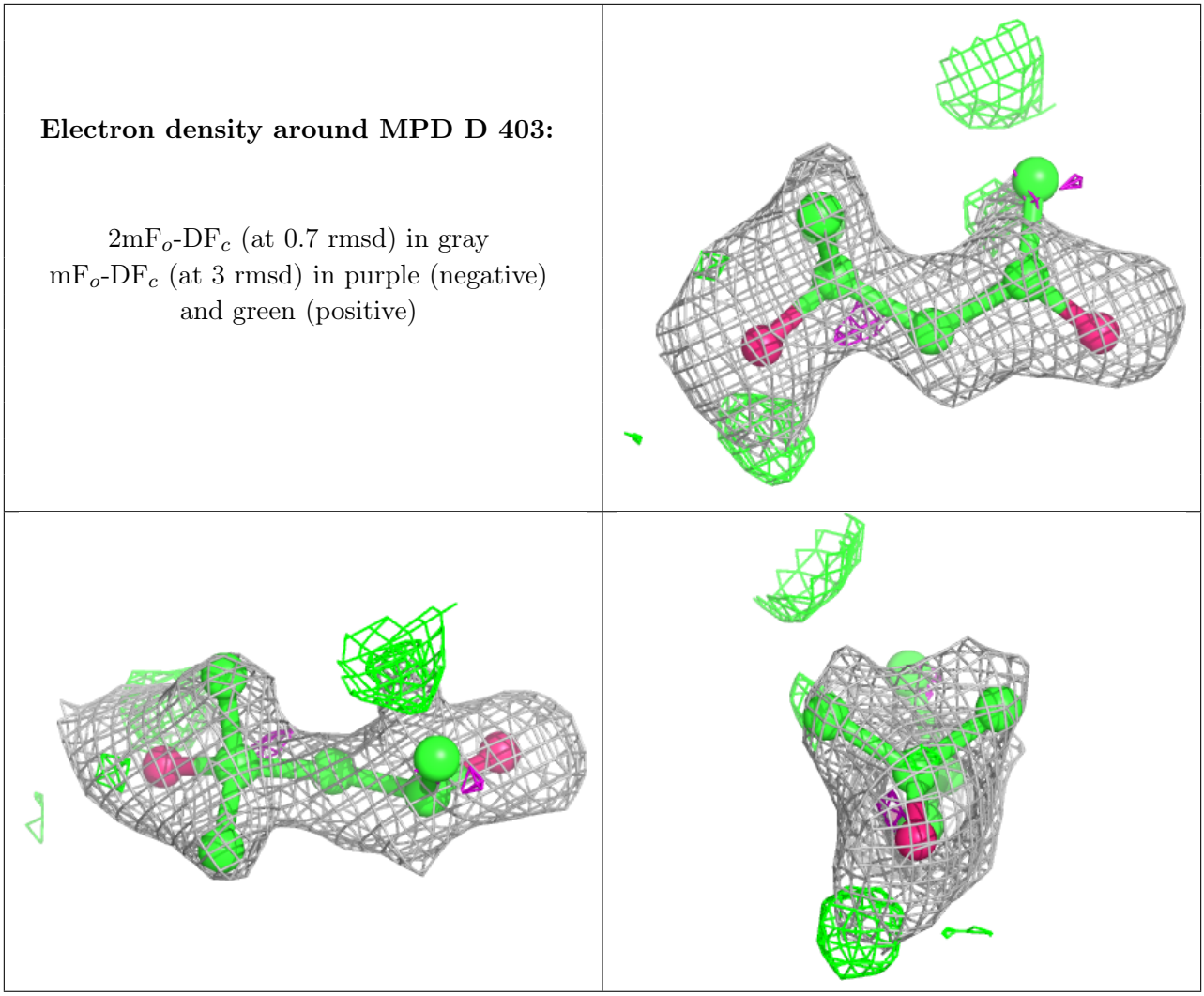
Electron density around TRS A 406:

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



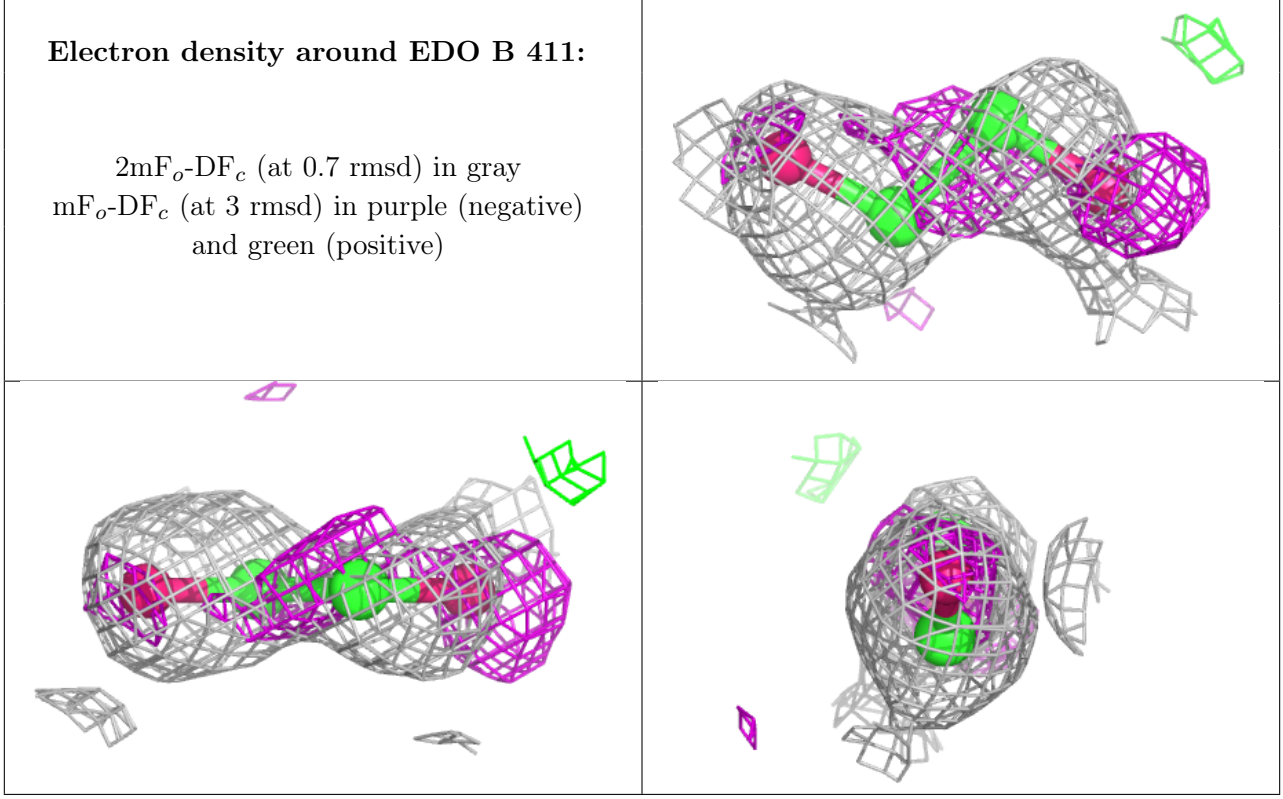
Electron density around MPD D 403:

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



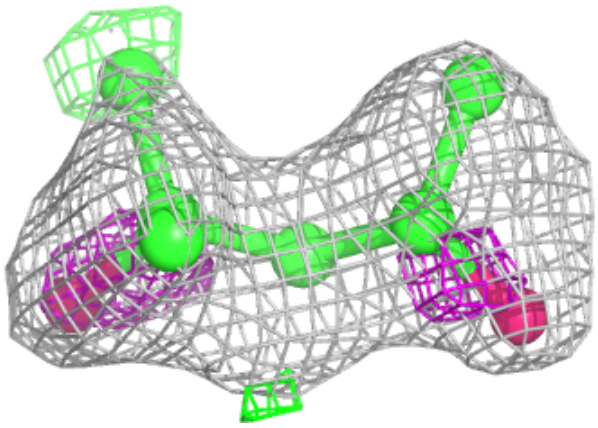
Electron density around EDO B 411:

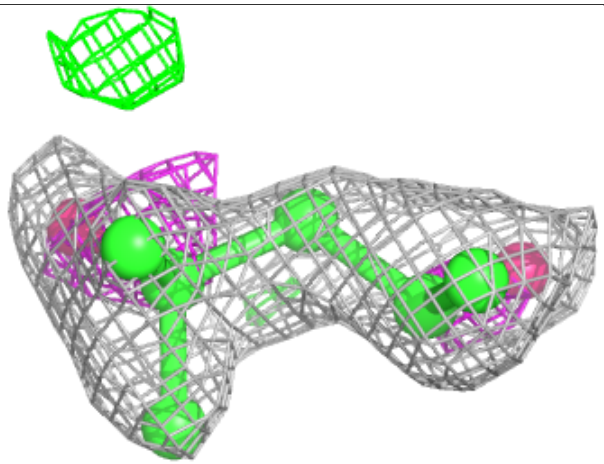
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

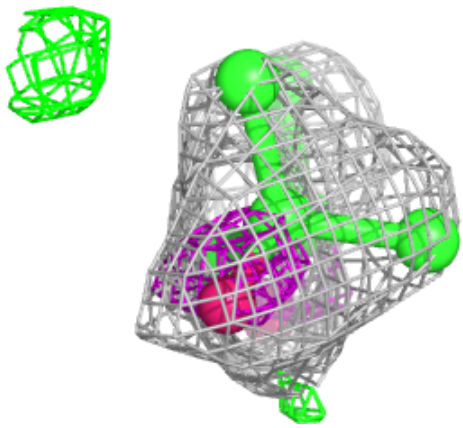


Electron density around MPD B 403:

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

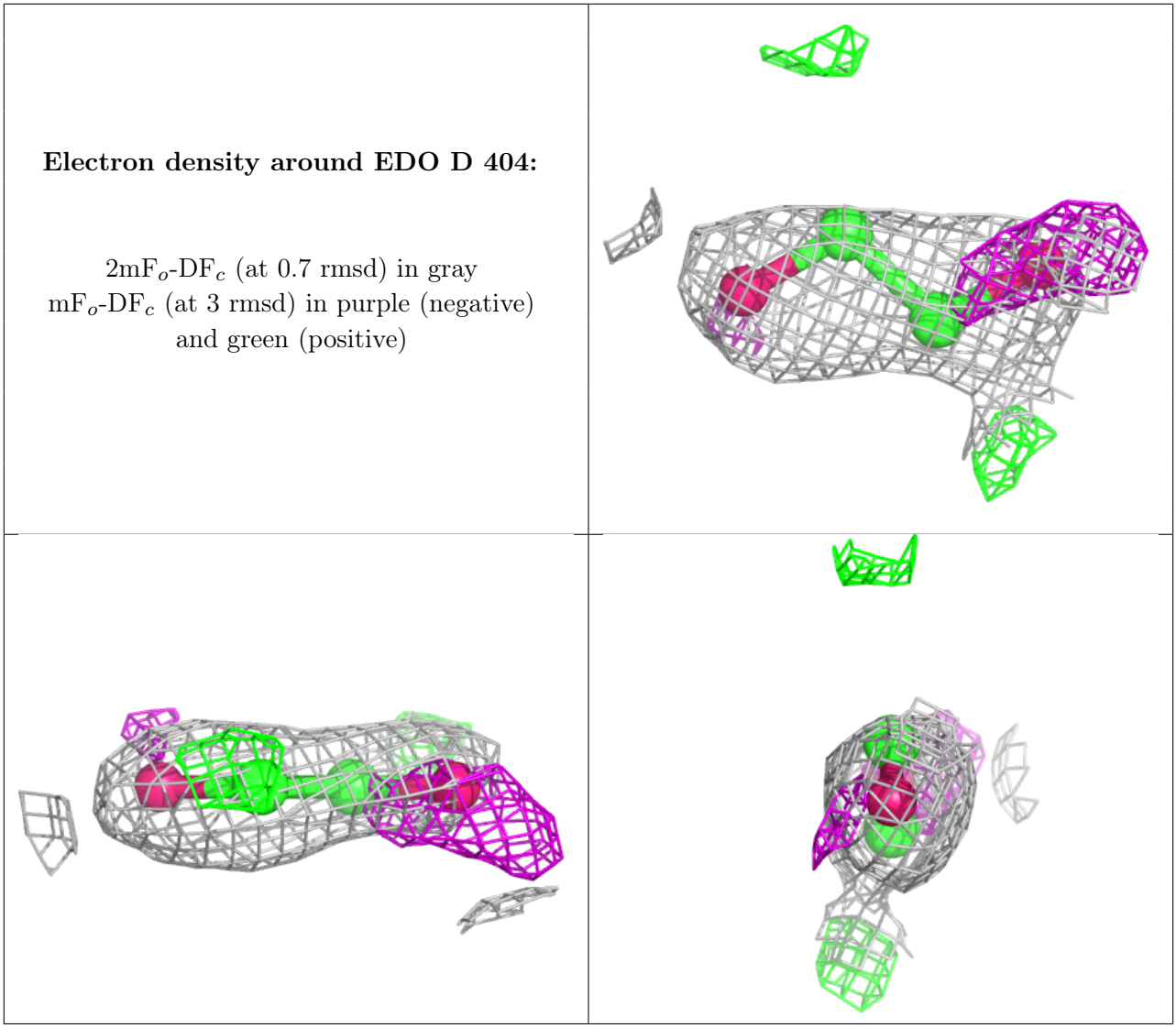






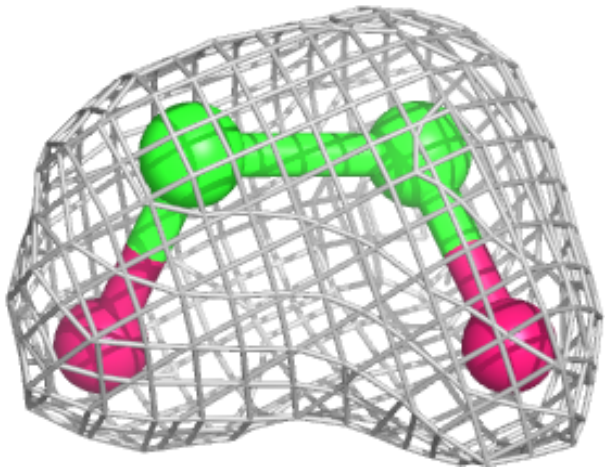
Electron density around EDO D 404:

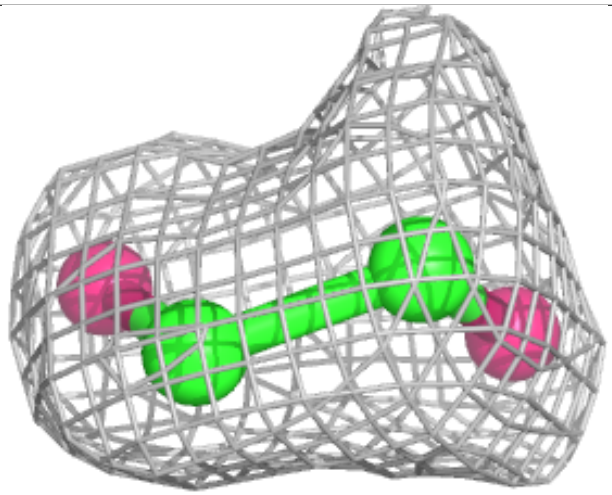
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

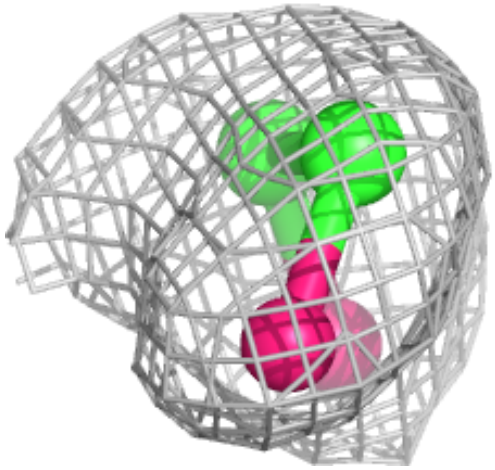


Electron density around EDO B 408:

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

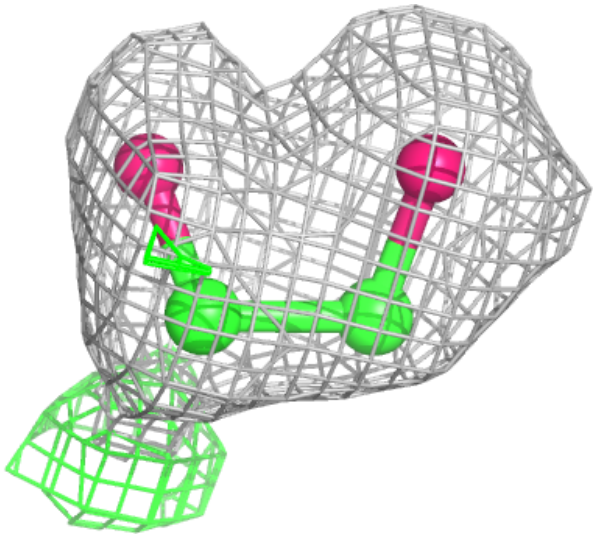


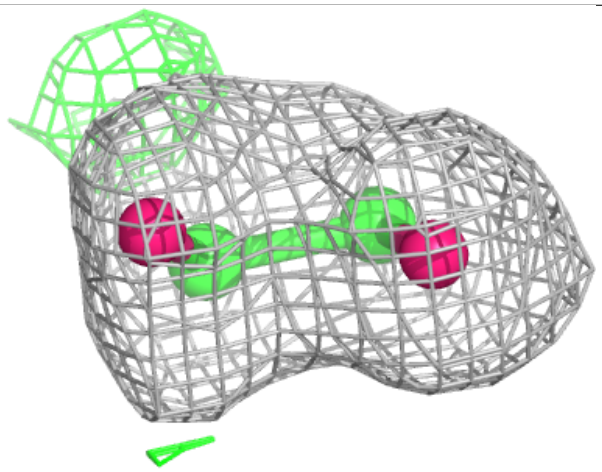


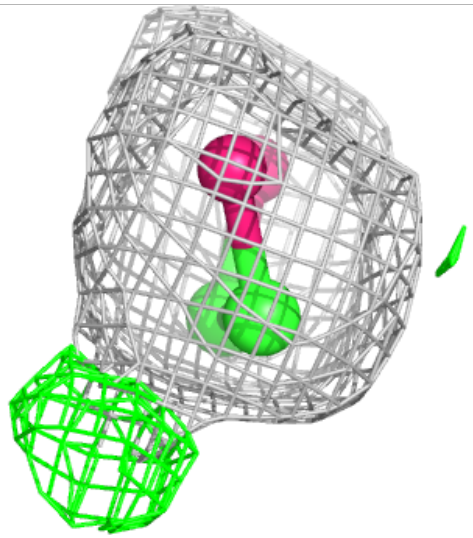


Electron density around EDO B 405:

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

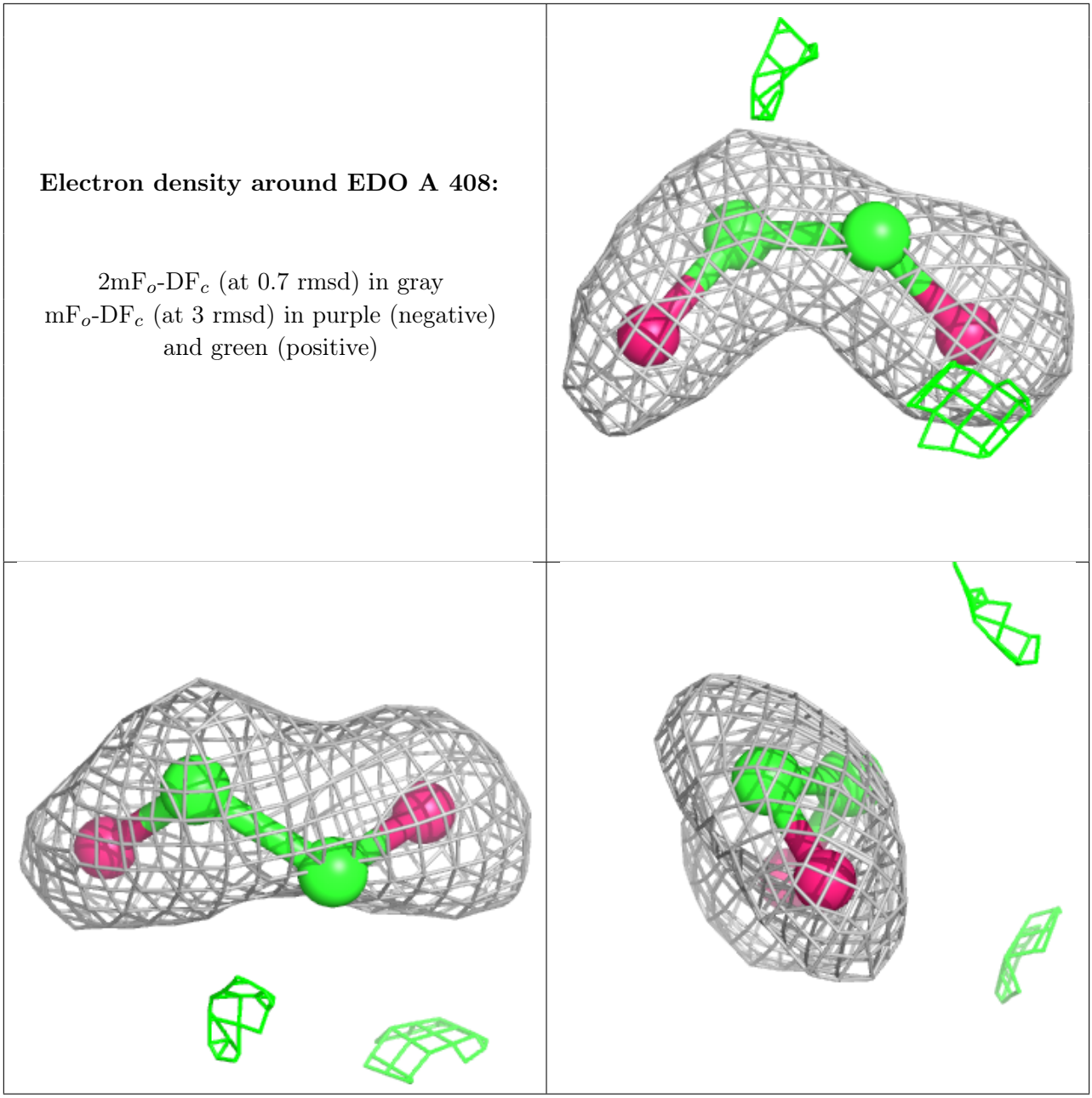






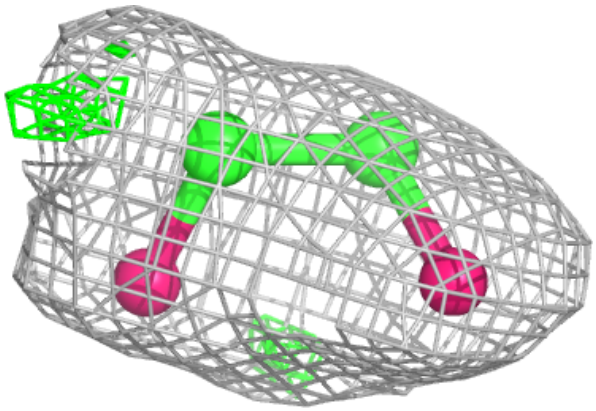
Electron density around EDO A 408:

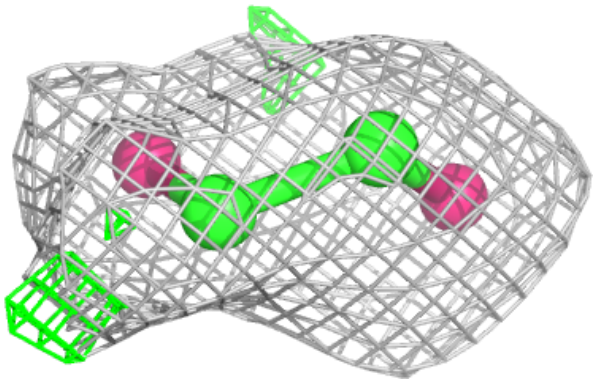
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

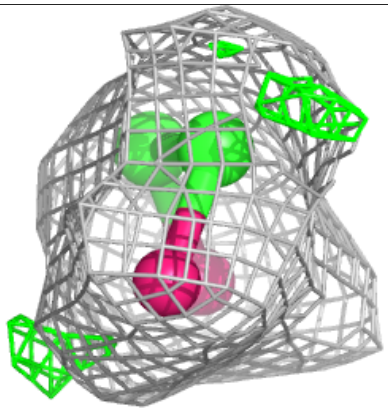


Electron density around EDO E 403:

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

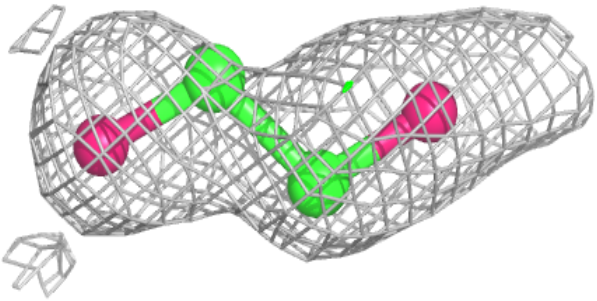


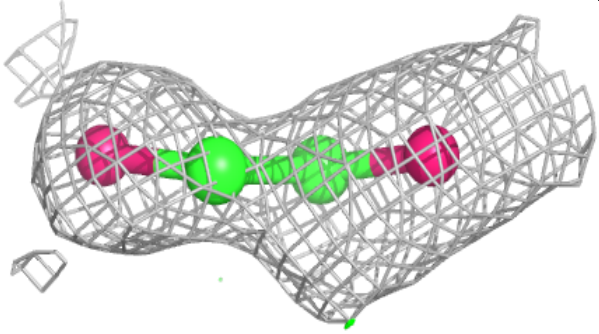


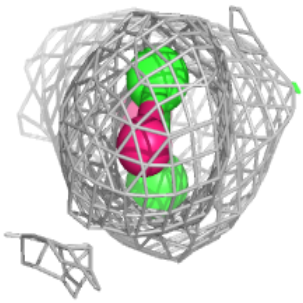


Electron density around EDO C 410:

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

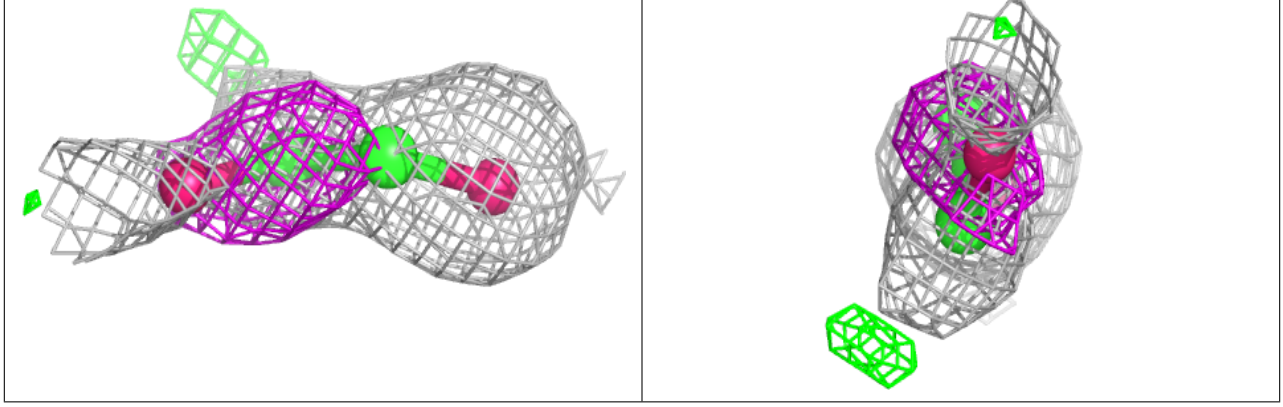






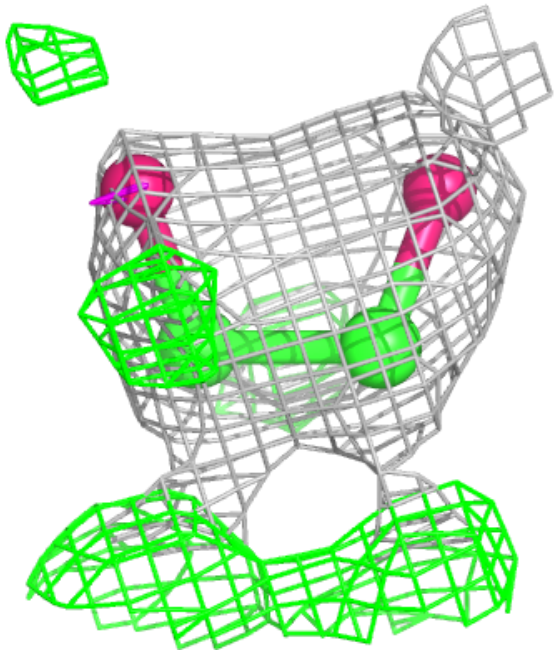
Electron density around EDO C 411:

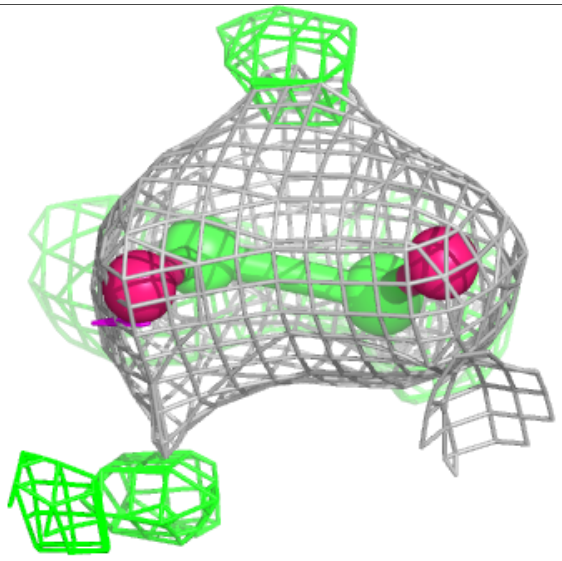
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

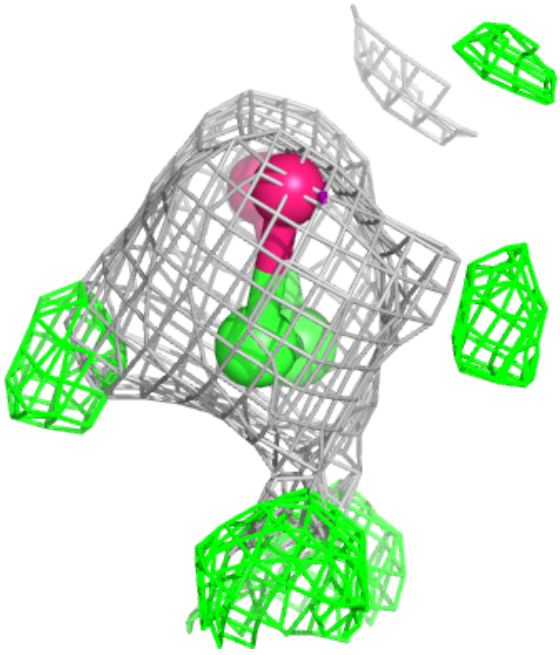


Electron density around EDO A 412:

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

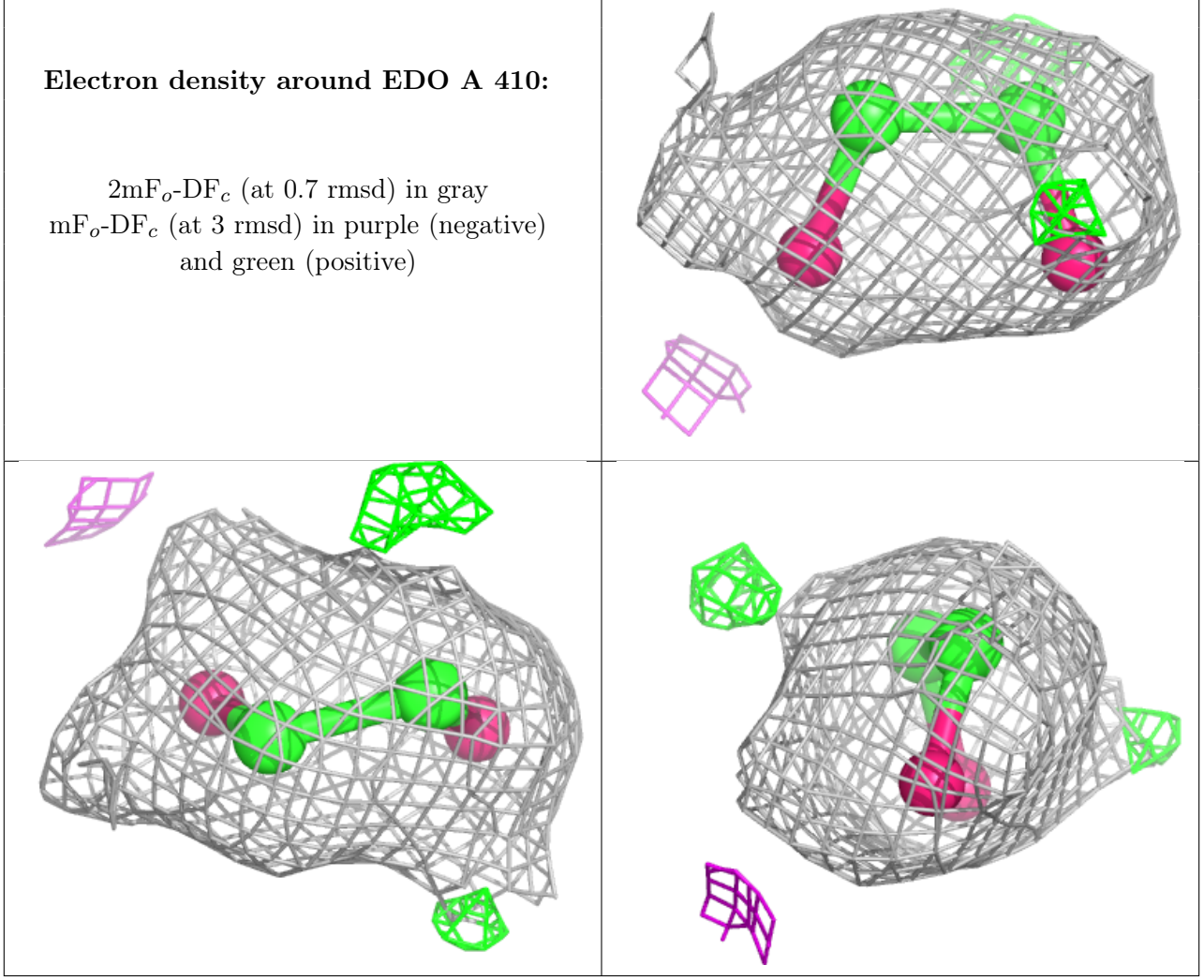






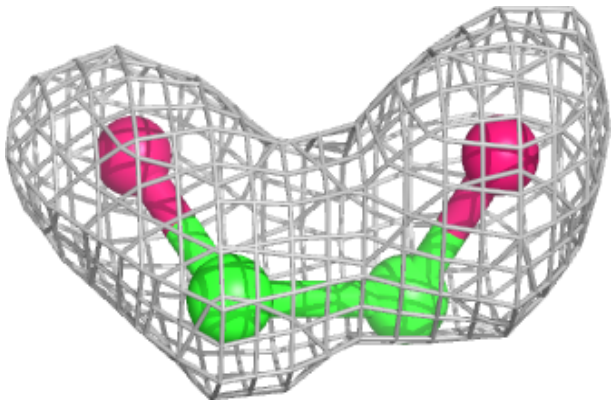
Electron density around EDO A 410:

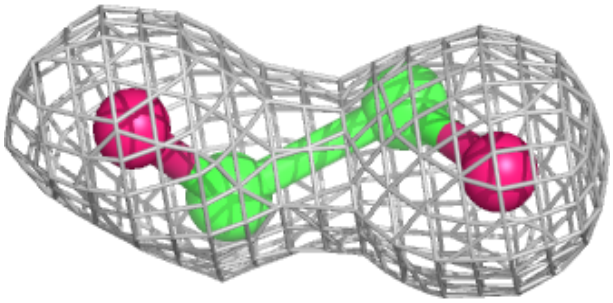
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

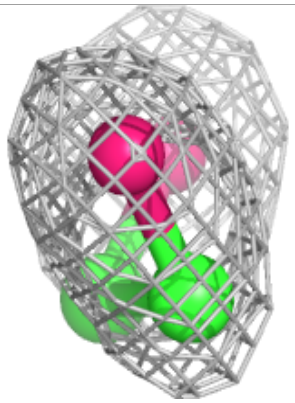


Electron density around EDO A 413:

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

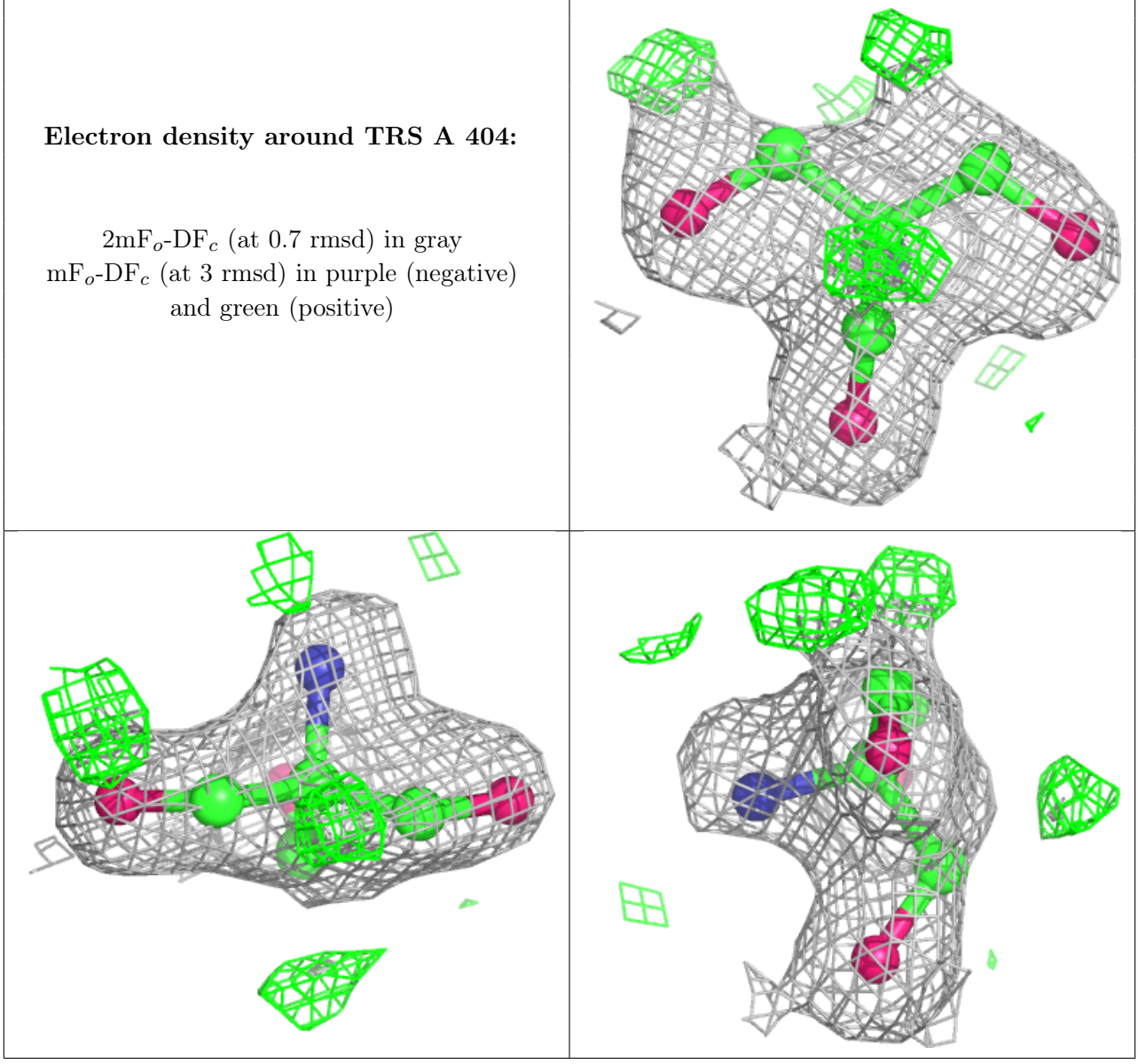






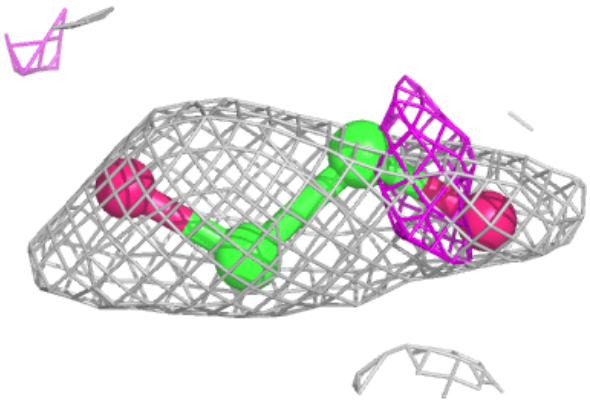
Electron density around TRS A 404:

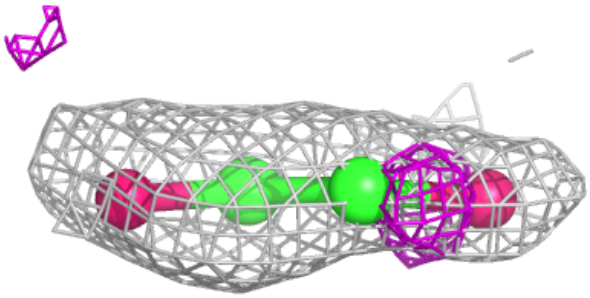
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

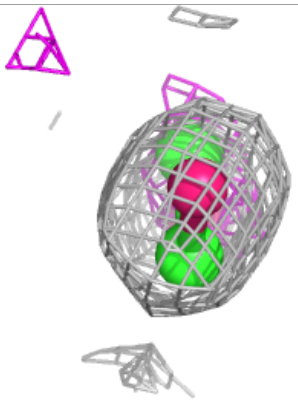


Electron density around EDO F 405:

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

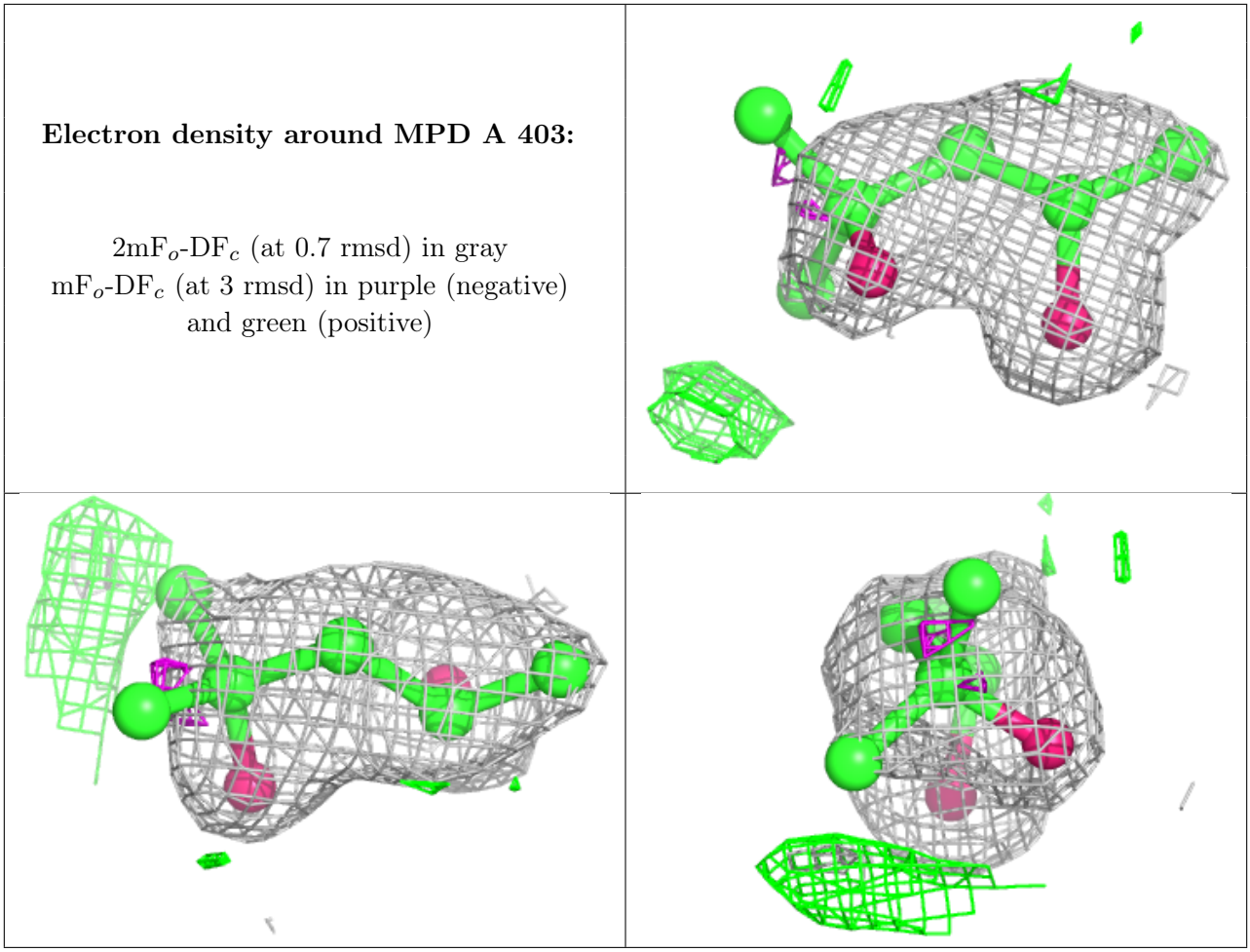






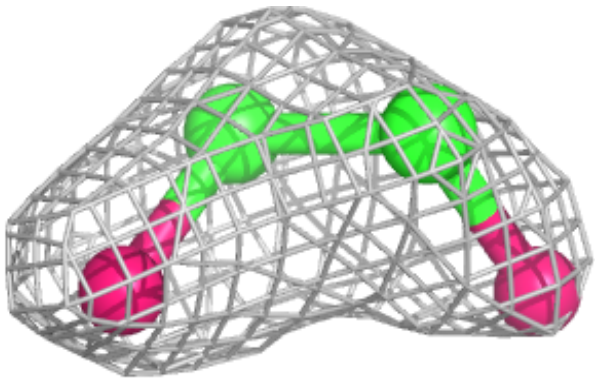
Electron density around MPD A 403:

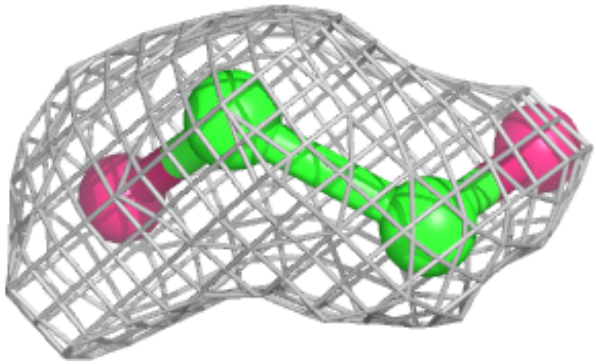
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

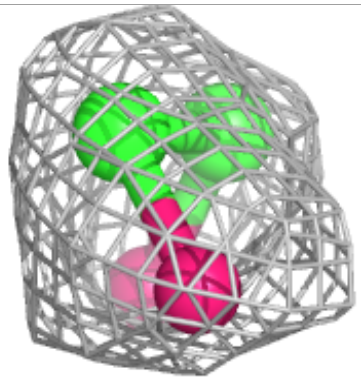


Electron density around EDO B 407:

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

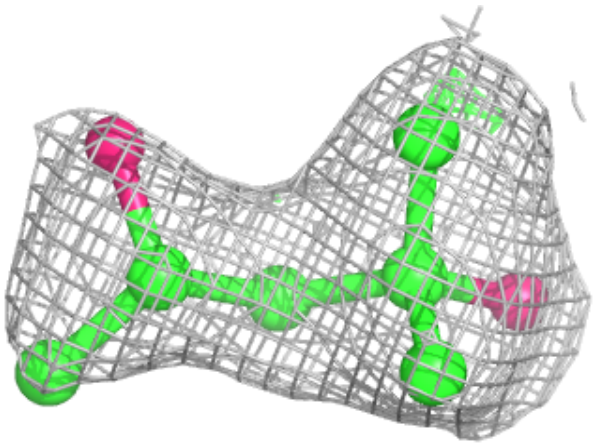


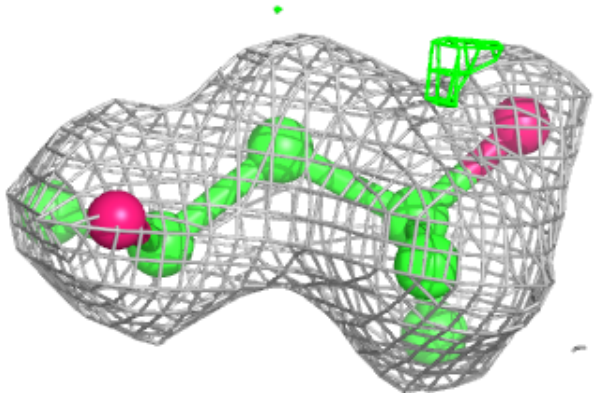


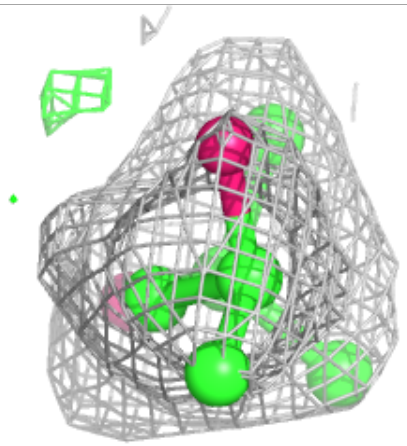


Electron density around MPD C 404:

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

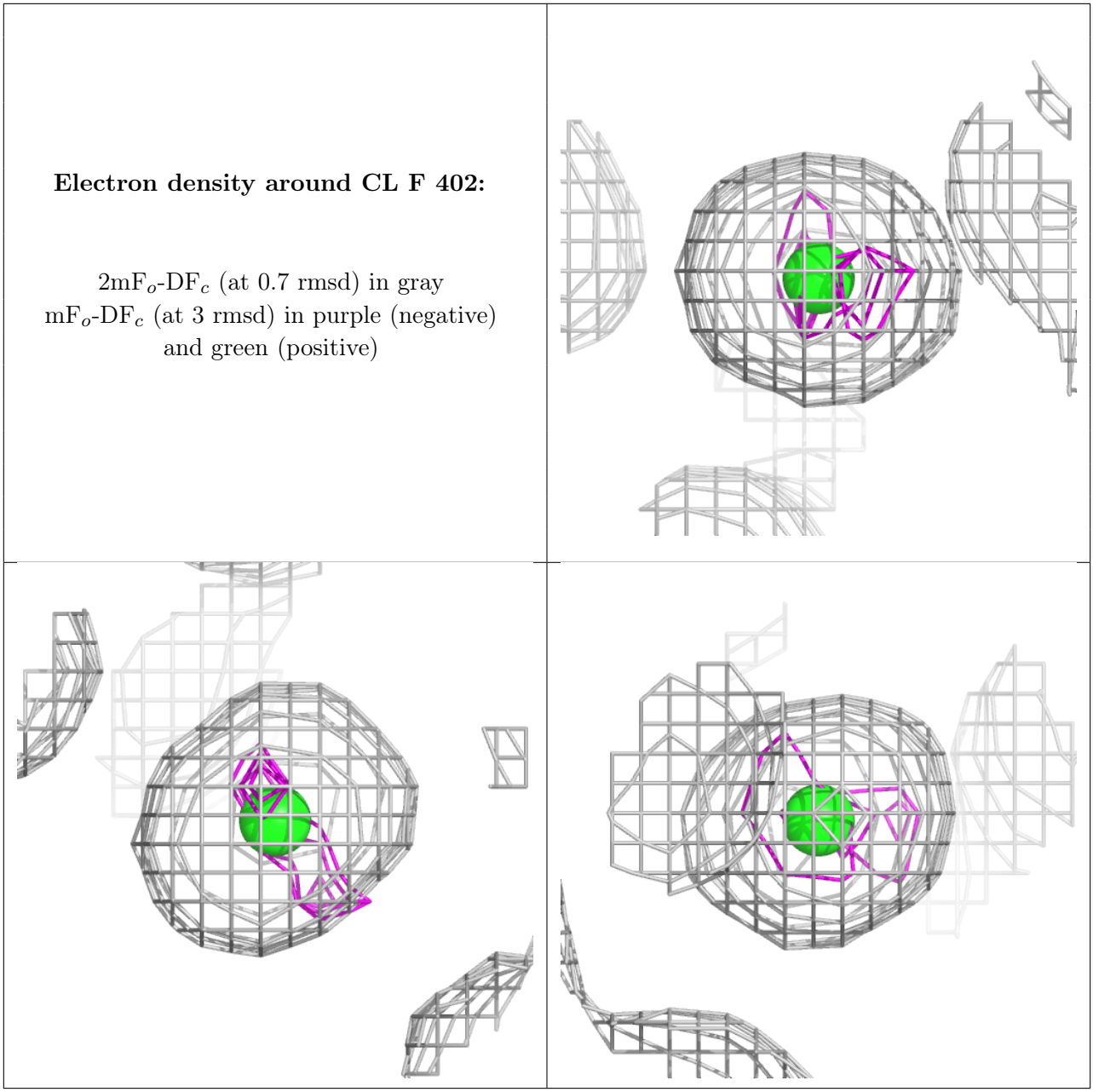






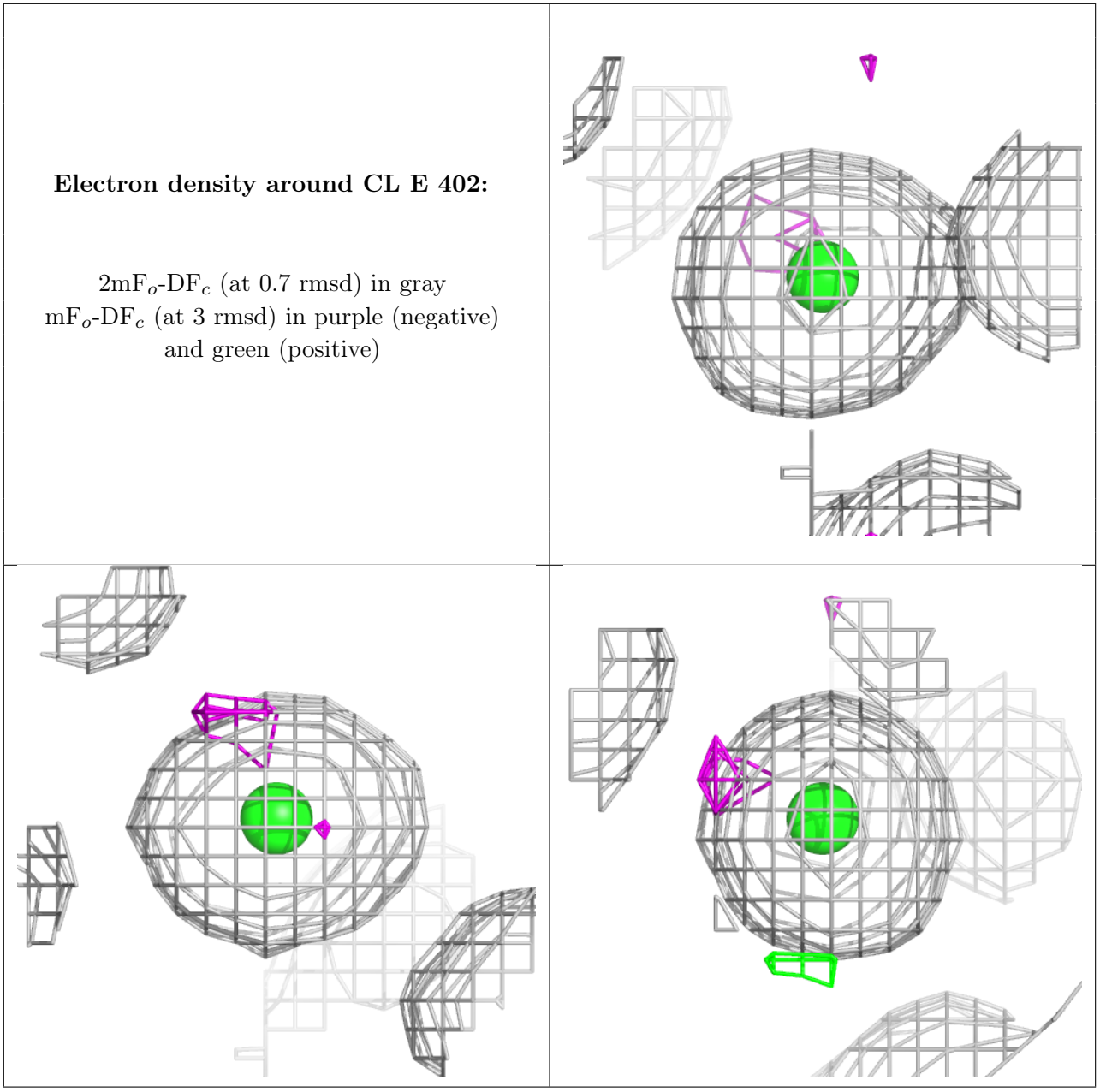
Electron density around CL F 402:

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



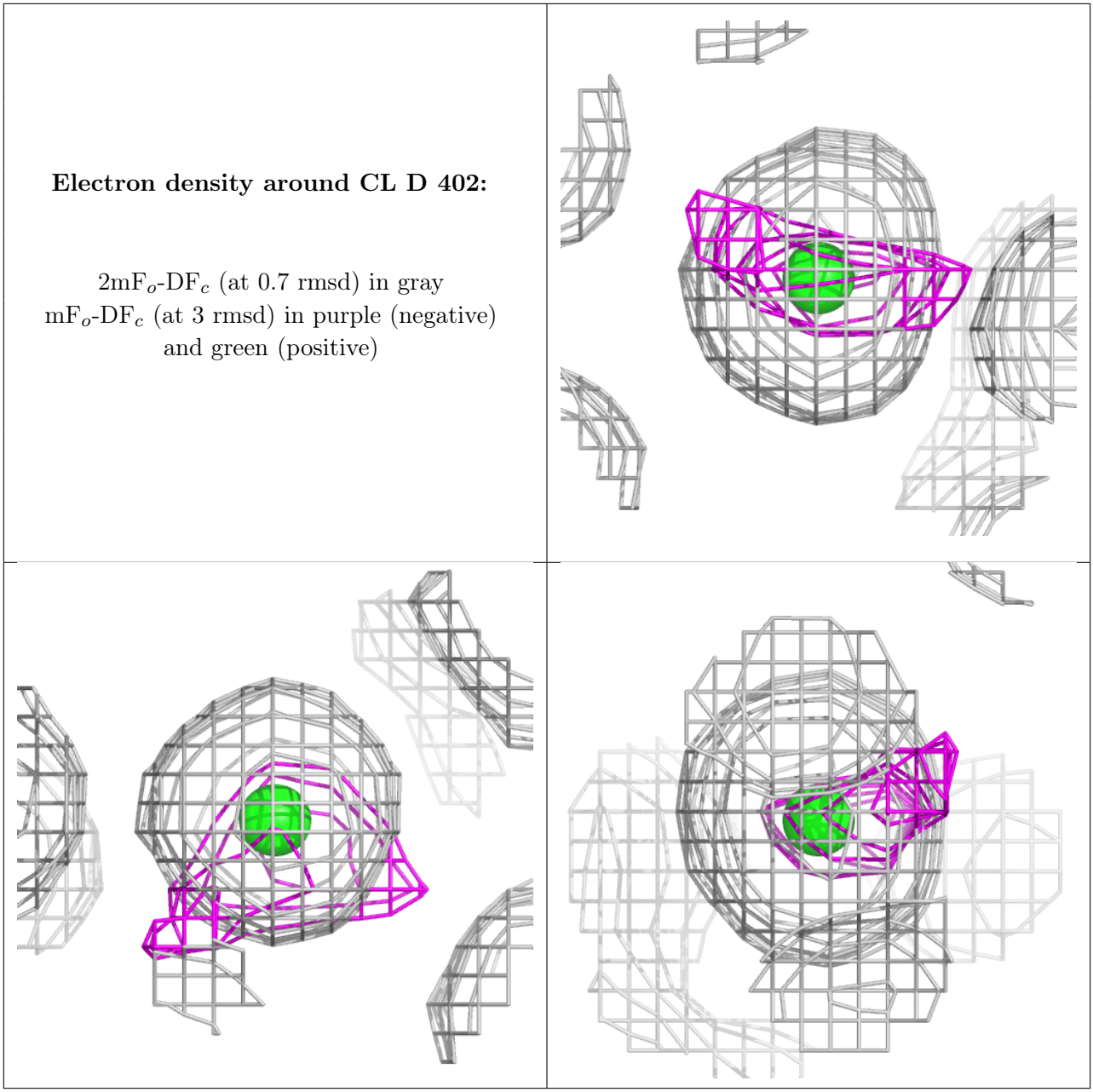
Electron density around CL E 402:

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



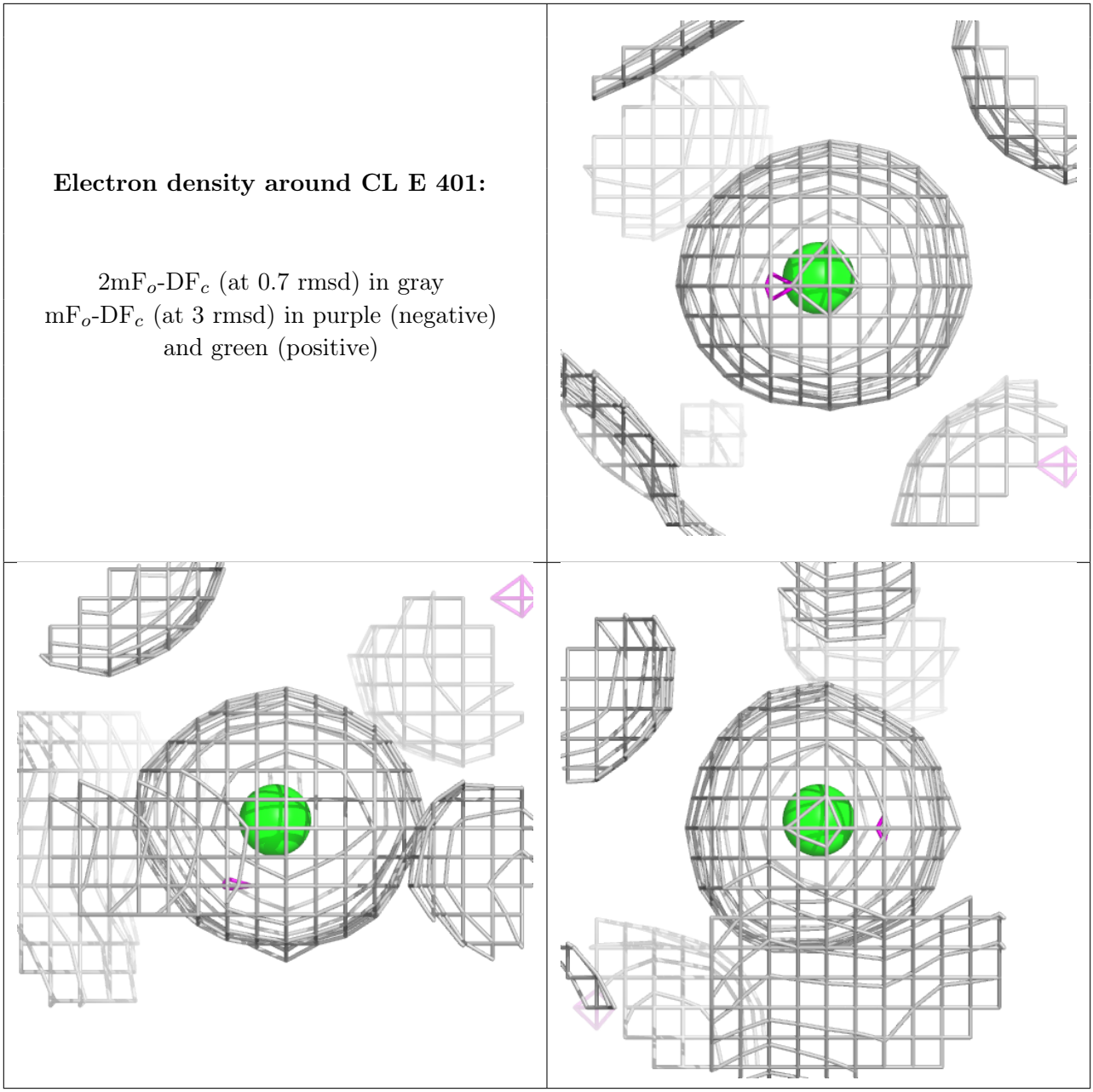
Electron density around CL D 402:

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



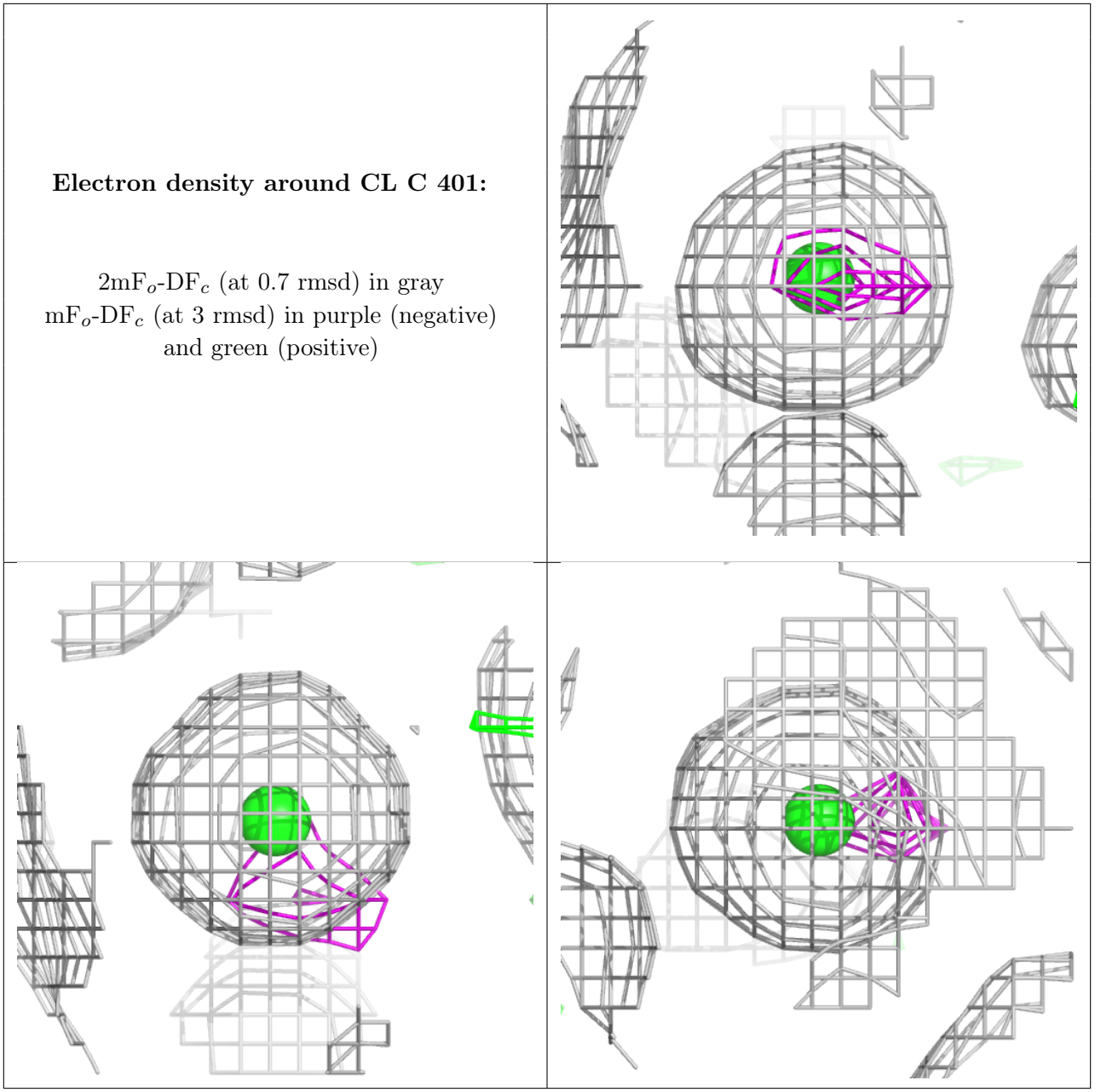
Electron density around CL E 401:

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



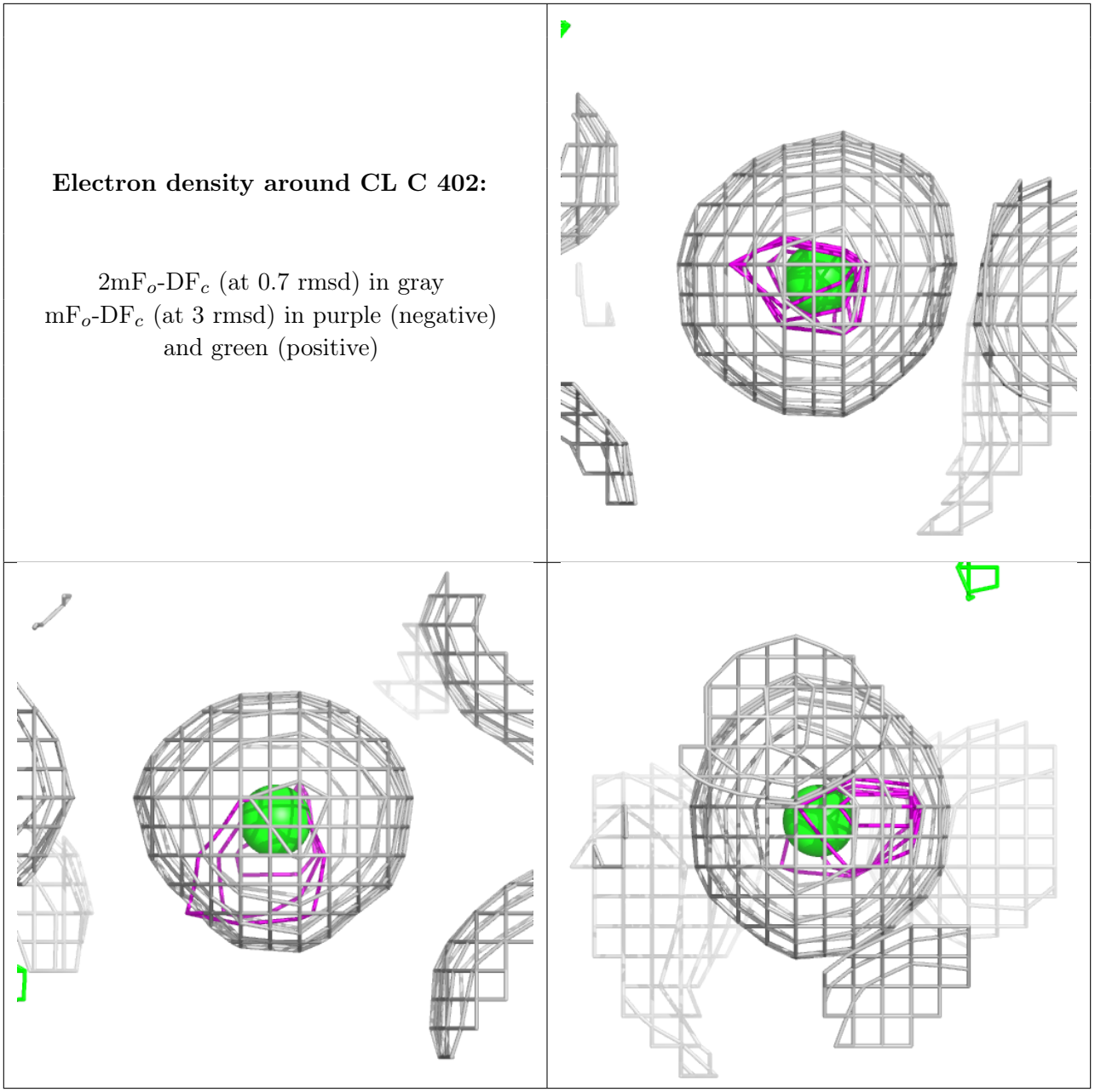
Electron density around CL C 401:

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



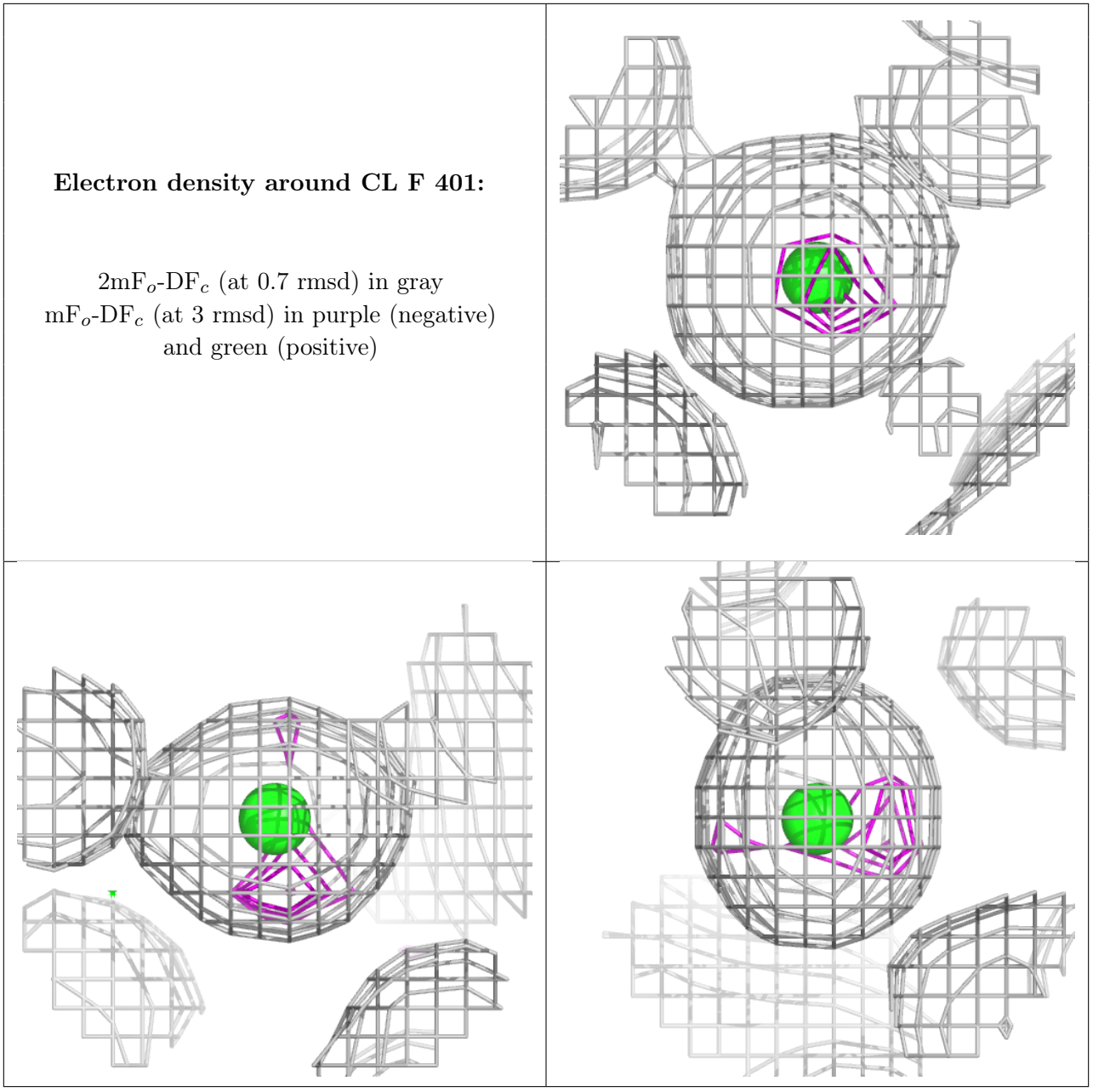
Electron density around CL C 402:

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



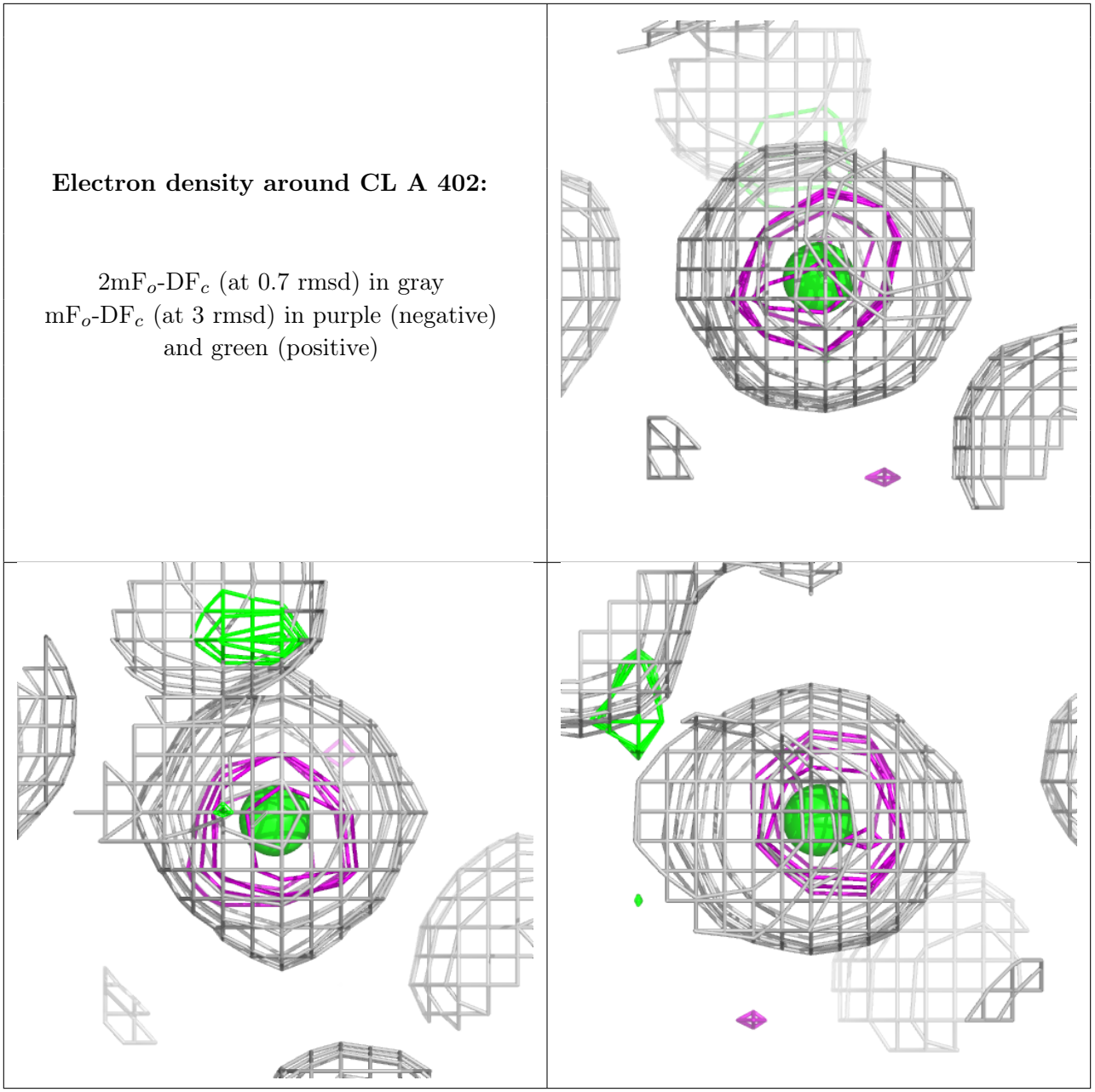
Electron density around CL F 401:

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



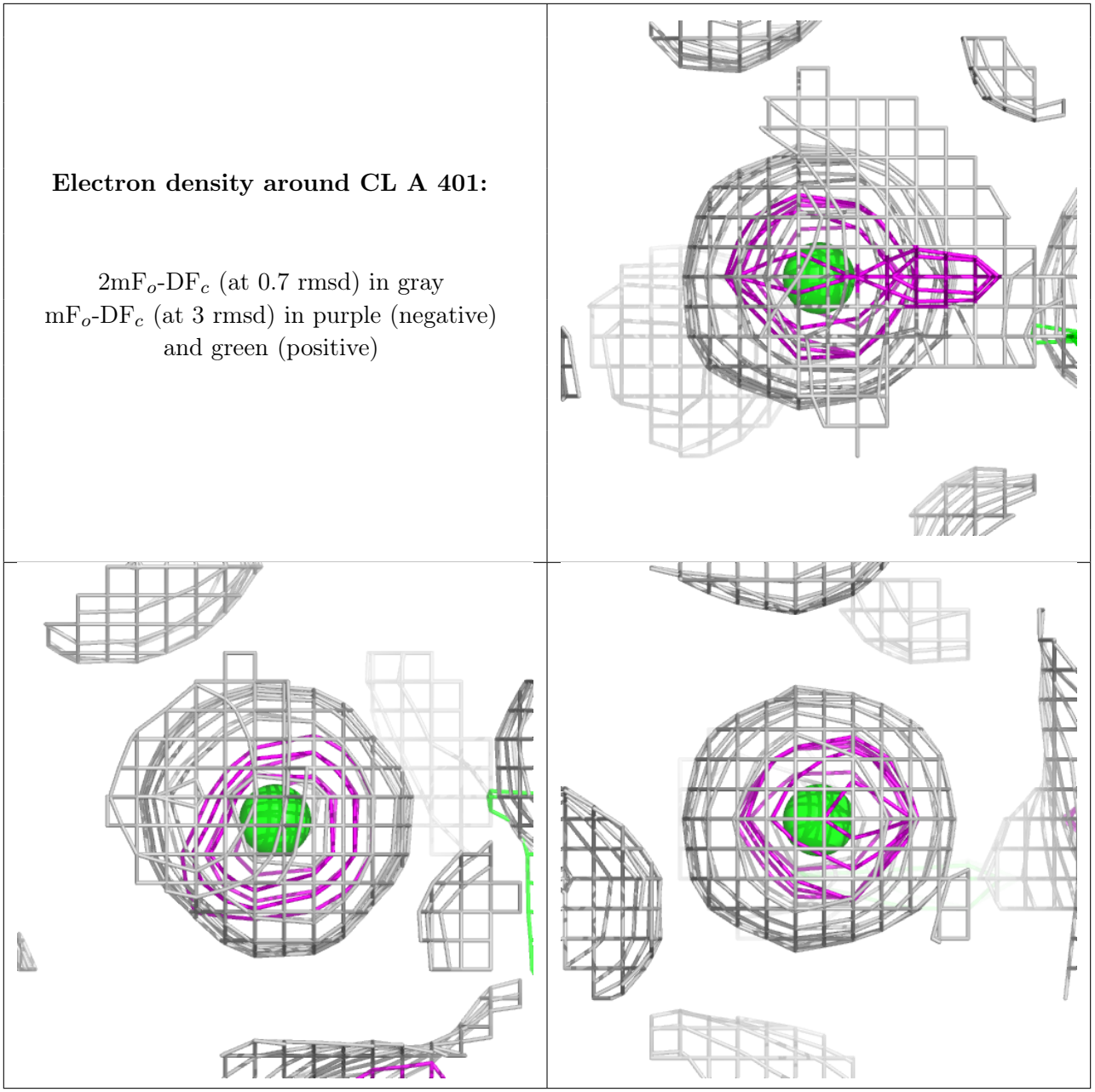
Electron density around CL A 402:

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



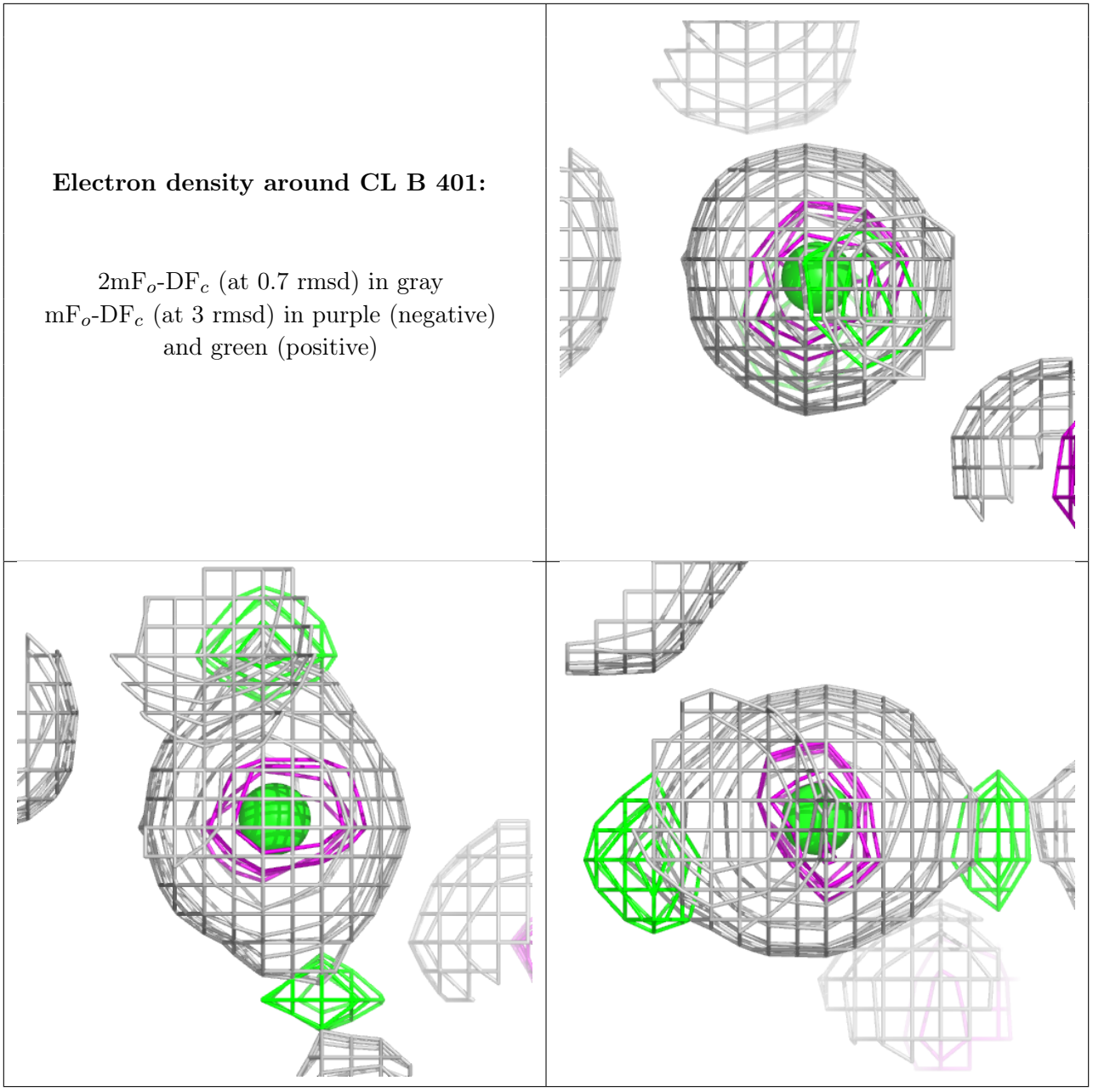
Electron density around CL A 401:

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



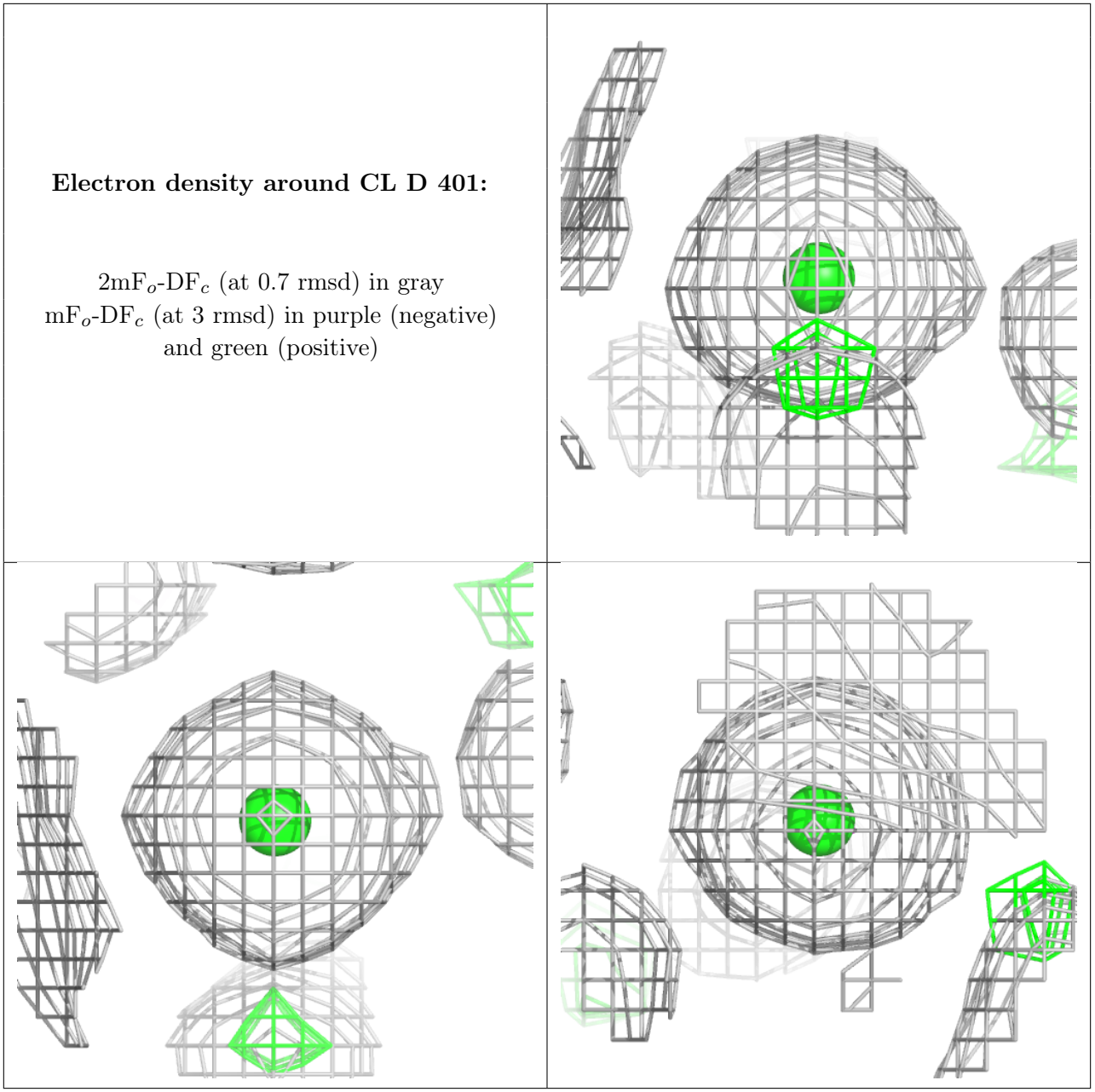
Electron density around CL B 401:

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



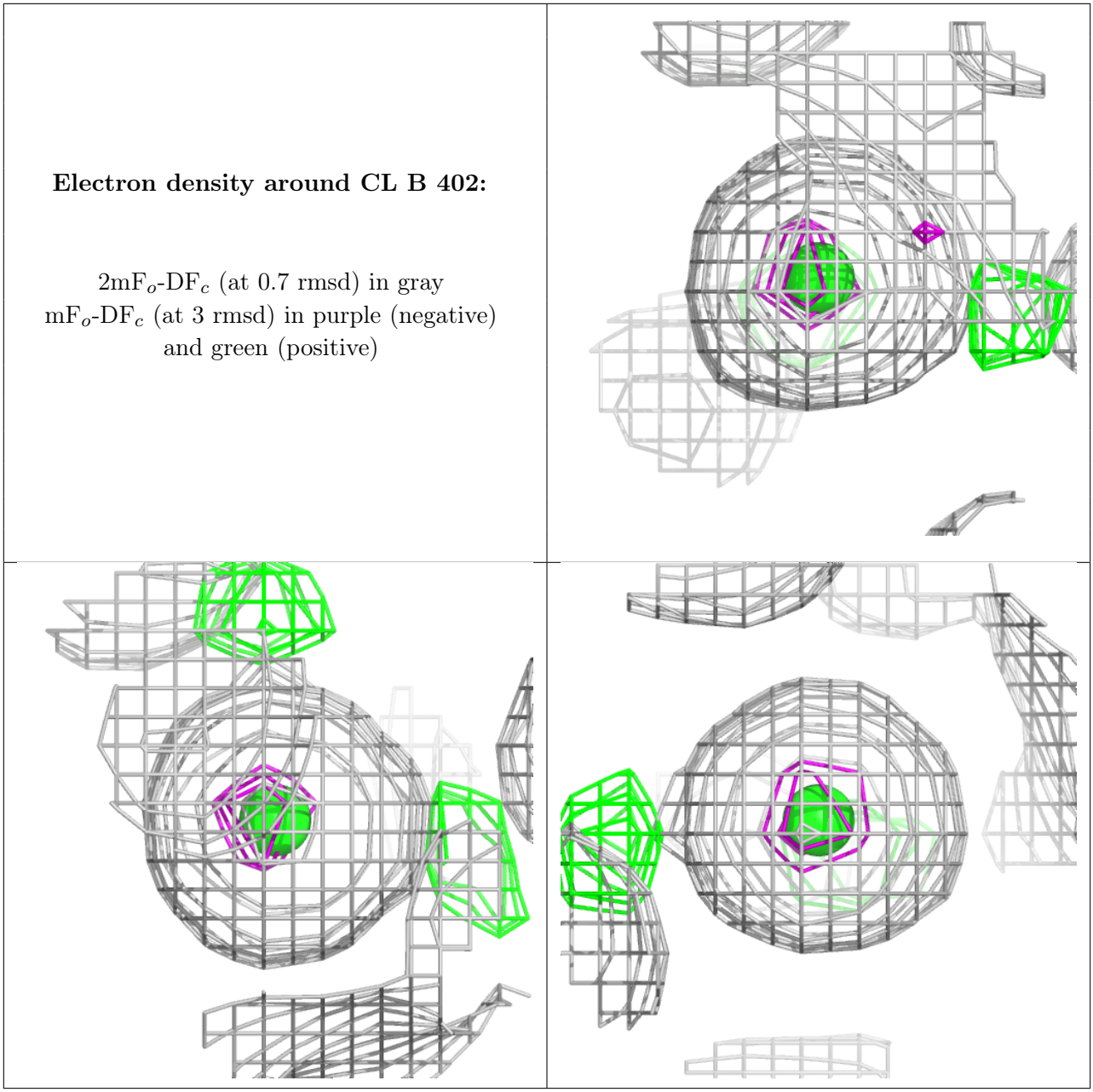
Electron density around CL D 401:

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



Electron density around CL B 402:

$2mF_o$-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.