Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:19 PM UTC

PDB ID	:	6EIU / pdb_00006eiu
Title	:	Crystal structure of KDM5B in complex with KDOPZ29a
Authors	:	Srikannathasan, V.; Newman, J.A.; Szykowska, A.; Wright, M.; Ruda, G.F.; Vazquez-Rodriguez, S.A.; Kupinska, K.; Strain-Damerell, C.; Burgess-Brown, N.A.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Oppermann, U.; Huber, K.; von Delft, F.
Deposited on	:	2017-09-19
Resolution	:	1.88 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 (1)) were used in the production of this report:

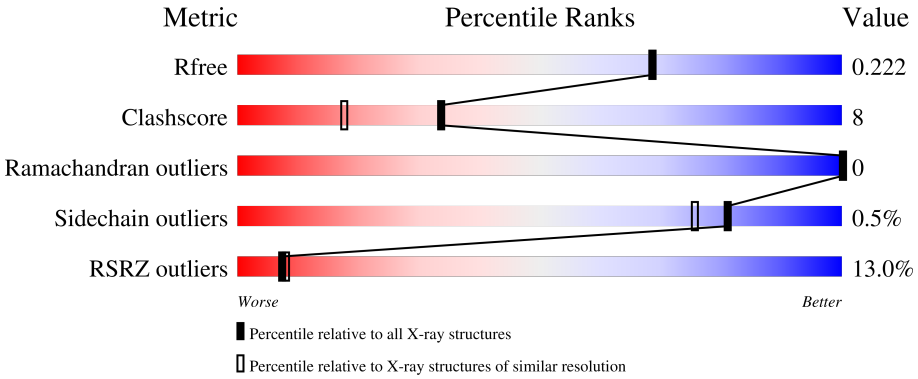
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	462	13% 88% 10% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	A	813	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3966 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 Lysine-specific demethylase 5B,Lysine-specific demethylase 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	6	0
			3613	2327	600	647	39			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP Q9UGL1
A	369	LEU	-	linker	UNP Q9UGL1
A	370	GLY	-	linker	UNP Q9UGL1
A	371	GLY	-	linker	UNP Q9UGL1
A	372	GLY	-	linker	UNP Q9UGL1
A	373	GLY	-	linker	UNP Q9UGL1

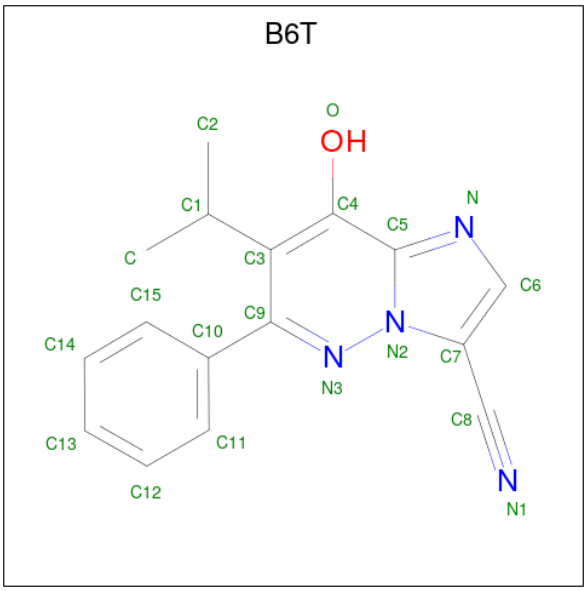
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

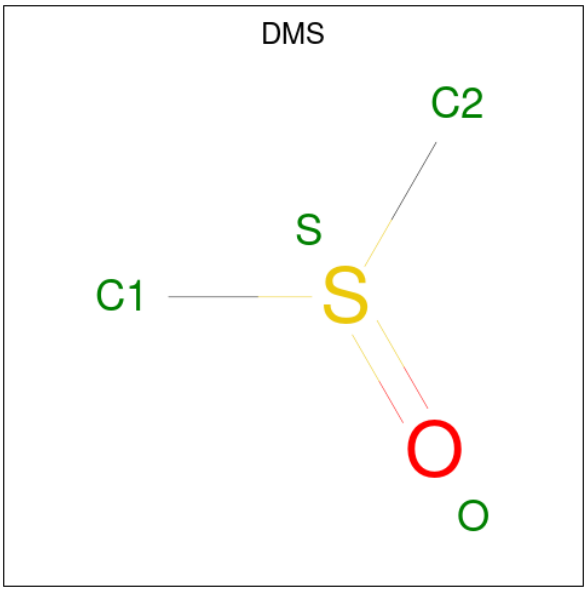
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is 8-oxidanyl-6-phenyl-7-propan-2-yl-imidazo[1,2-b]pyridazine-3-carbonitrile (CCD ID: B6T) (formula: $C_{16}H_{14}N_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	16	4	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS) (labeled as "Ligand of Interest" by depositor).



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

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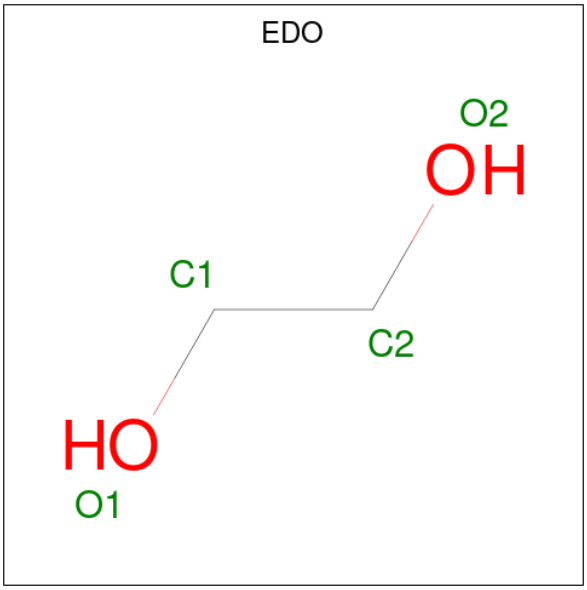
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

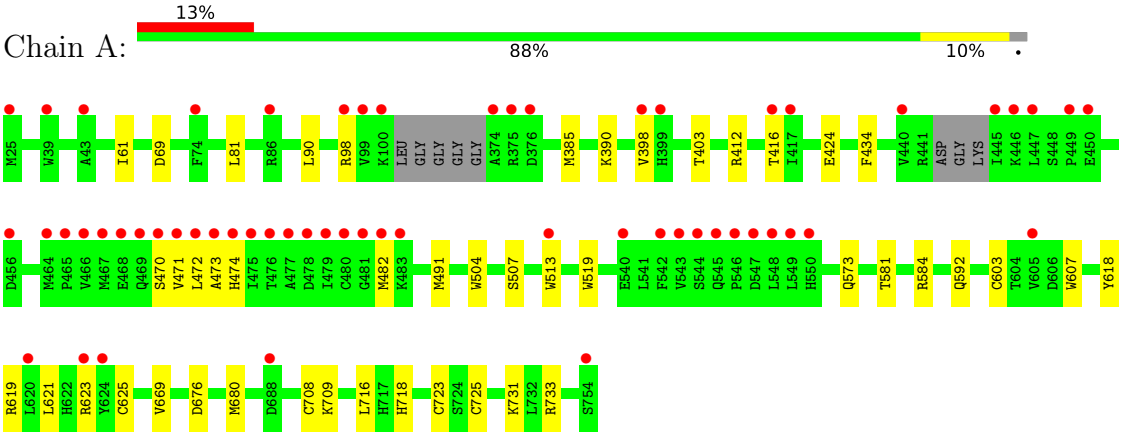
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	280	Total	O	0	0
			280	280		

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: Lysine-specific demethylase 5B,Lysine-specific demethylase 5B



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	143.38Å 143.38Å 153.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.38 – 1.88 65.38 – 1.88	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.38-1.88) 100.0 (65.38-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.83Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.221 0.198 , 0.222	Depositor DCC
R_{free} test set	4063 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ZN, MN, DMS, B6T

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	0.40	0/3721	0.51	0/5069

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	3613	0	3396	52	0
2	A	2	0	0	0	0
3	A	2	0	0	0	0
4	A	21	0	0	0	0
5	A	28	0	42	7	0
6	A	20	0	30	8	0
7	A	280	0	0	4	1
All	All	3966	0	3468	55	1

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 8.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:NH1	7:A:902:HOH:O	1.89	1.04
1:A:472:LEU:HD13	1:A:603:CYS:SG	2.04	0.97
1:A:470:SER:OG	7:A:901:HOH:O	1.82	0.95
1:A:472:LEU:CD1	1:A:603:CYS:SG	2.62	0.88
1:A:472:LEU:HD21	1:A:482:MET:HE2	1.63	0.79
1:A:680:MET:HE3	1:A:733:ARG:HD2	1.68	0.76
1:A:718:HIS:HE2	5:A:809:DMS:H13	1.52	0.73
1:A:385:MET:HE1	1:A:491:MET:HE2	1.69	0.73
1:A:424:GLU:O	1:A:491:MET:HE3	1.96	0.66
1:A:385:MET:HE1	1:A:491:MET:CE	2.27	0.63
1:A:472:LEU:HD11	1:A:603:CYS:SG	2.38	0.63
1:A:619:ARG:HA	6:A:813:EDO:H21	1.81	0.63
1:A:618:TYR:HB3	6:A:813:EDO:H12	1.80	0.62
1:A:472:LEU:HD13	1:A:603:CYS:CB	2.29	0.62
1:A:424:GLU:H	1:A:491:MET:HE3	1.65	0.60
1:A:472:LEU:HD13	1:A:603:CYS:HB2	1.84	0.60
1:A:390:LYS:HD3	1:A:398:VAL:HG13	1.81	0.60
1:A:98:ARG:CZ	7:A:902:HOH:O	2.41	0.58
1:A:412:ARG:O	1:A:416:THR:HG23	2.05	0.57
5:A:806:DMS:H13	5:A:807:DMS:H22	1.86	0.56
1:A:69:ASP:OD1	1:A:69:ASP:N	2.37	0.55
1:A:625:CYS:SG	6:A:813:EDO:H11	2.47	0.54
1:A:623:ARG:O	6:A:813:EDO:O2	2.24	0.53
1:A:618:TYR:CB	6:A:813:EDO:H12	2.39	0.52
1:A:424:GLU:C	1:A:491:MET:HE3	2.34	0.52
1:A:621:LEU:HD22	5:A:808:DMS:H12	1.92	0.52
1:A:61:ILE:HG22	1:A:581:THR:HG22	1.91	0.52
1:A:403:THR:HA	1:A:592:GLN:HE22	1.75	0.51
1:A:623:ARG:HG2	1:A:623:ARG:HH11	1.77	0.50
1:A:676:ASP:HB3	1:A:731:LYS:HG2	1.93	0.50
1:A:513:TRP:C	1:A:513:TRP:CD1	2.90	0.49
1:A:669:VAL:HG11	1:A:716:LEU:HG	1.93	0.49
1:A:519:TRP:HE1	1:A:573:GLN:NE2	2.11	0.49
1:A:424:GLU:CA	1:A:491:MET:HE3	2.43	0.49
1:A:708[B]:CYS:SG	1:A:709:LYS:HG2	2.52	0.48
1:A:424:GLU:N	1:A:491:MET:HE3	2.27	0.47
1:A:81[A]:LEU:HD22	1:A:434:PHE:HA	1.96	0.47
1:A:424:GLU:H	1:A:491:MET:CE	2.26	0.46
1:A:619:ARG:HA	6:A:813:EDO:C2	2.45	0.46
1:A:416:THR:O	7:A:903:HOH:O	2.20	0.46
1:A:504:TRP:CE2	1:A:584[A]:ARG:HD3	2.51	0.45
1:A:584[A]:ARG:O	1:A:584[A]:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:TYR:C	6:A:813:EDO:H21	2.42	0.45
1:A:618:TYR:CD1	5:A:808:DMS:H13	2.52	0.45
1:A:708[A]:CYS:SG	1:A:725:CYS:SG	3.13	0.44
5:A:806:DMS:H13	5:A:807:DMS:C2	2.48	0.43
1:A:385:MET:HE3	1:A:385:MET:HB3	1.92	0.43
1:A:603:CYS:HB3	1:A:607:TRP:CE3	2.53	0.43
1:A:507:SER:HB2	5:A:807:DMS:H13	2.01	0.42
1:A:471:VAL:C	1:A:473:ALA:H	2.27	0.42
1:A:482:MET:HE2	1:A:482:MET:HB3	1.90	0.42
1:A:676:ASP:OD2	1:A:731:LYS:NZ	2.53	0.41
1:A:709:LYS:HG3	1:A:723:CYS:HB3	2.03	0.41
1:A:680:MET:HE3	1:A:733:ARG:CD	2.46	0.40
5:A:811:DMS:H22	6:A:814:EDO:H12	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1126:HOH:O	7:A:1146:HOH:O[10_665]	2.07	0.13

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	453/462 (98%)	446 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	379/413 (92%)	376 (99%)	3 (1%)	73 68

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	474[A]	HIS
1	A	474[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	573	GLN
1	A	592	GLN
1	A	717	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
6	EDO	A	814	-	3,3,3	0.38	0	2,2,2	0.29	0
6	EDO	A	812	-	3,3,3	0.40	0	2,2,2	0.56	0
5	DMS	A	807	-	3,3,3	0.61	0	3,3,3	0.57	0
4	B6T	A	804	3	23,23,23	0.55	1 (4%)	23,33,33	0.66	0
5	DMS	A	808	-	3,3,3	0.73	0	3,3,3	0.29	0
6	EDO	A	816	-	3,3,3	0.56	0	2,2,2	0.14	0
6	EDO	A	815	-	3,3,3	0.41	0	2,2,2	0.54	0
5	DMS	A	806	-	3,3,3	0.67	0	3,3,3	0.54	0
5	DMS	A	809	-	3,3,3	0.69	0	3,3,3	0.53	0
5	DMS	A	805	-	3,3,3	0.78	0	3,3,3	0.29	0
5	DMS	A	811	-	3,3,3	0.67	0	3,3,3	0.56	0
6	EDO	A	813	-	3,3,3	0.36	0	2,2,2	0.39	0
5	DMS	A	810	-	3,3,3	0.66	0	3,3,3	0.63	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
6	EDO	A	814	-	-	0/1/1/1	-
6	EDO	A	812	-	-	0/1/1/1	-
4	B6T	A	804	3	-	0/8/10/10	0/3/3/3
6	EDO	A	816	-	-	0/1/1/1	-
6	EDO	A	815	-	-	0/1/1/1	-
6	EDO	A	813	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	B6T	C7-N2	2.15	1.39	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

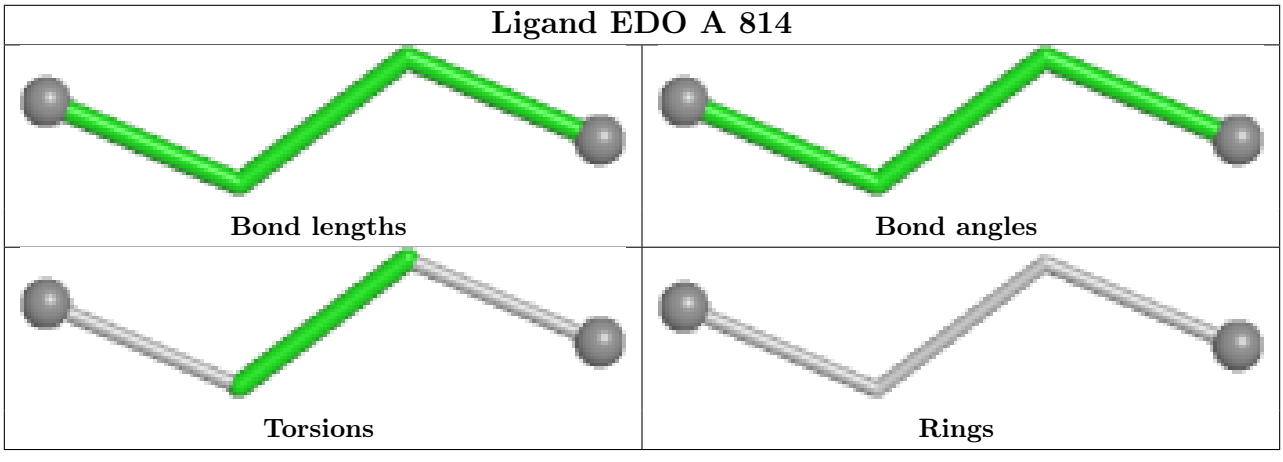
Mol	Chain	Res	Type	Atoms
6	A	813	EDO	O1-C1-C2-O2

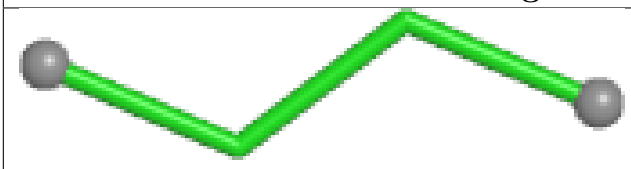
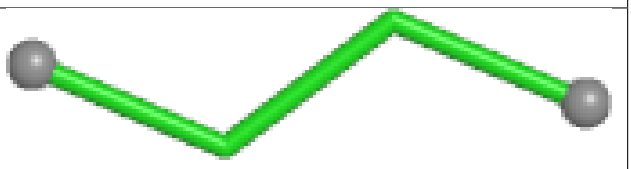
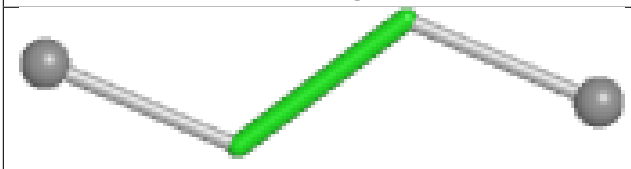
There are no ring outliers.

7 monomers are involved in 14 short contacts:

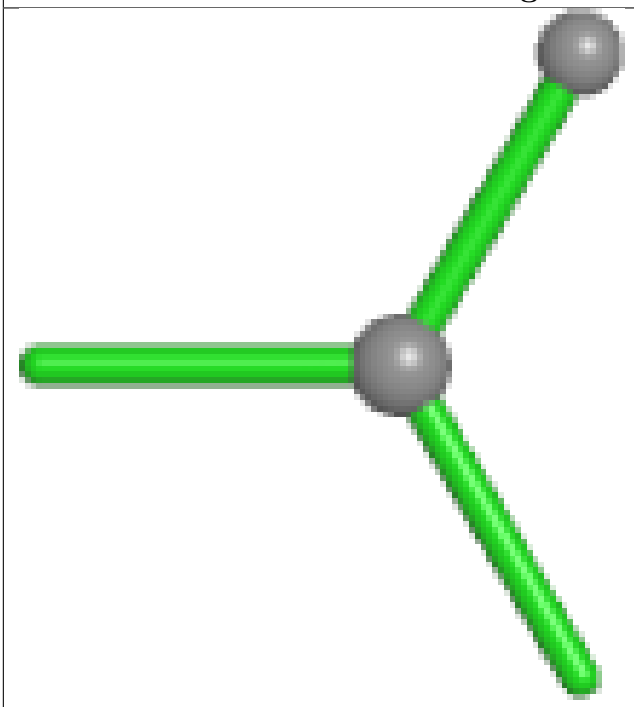
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	814	EDO	1	0
5	A	807	DMS	3	0
5	A	808	DMS	2	0
5	A	806	DMS	2	0
5	A	809	DMS	1	0
5	A	811	DMS	1	0
6	A	813	EDO	7	0

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.

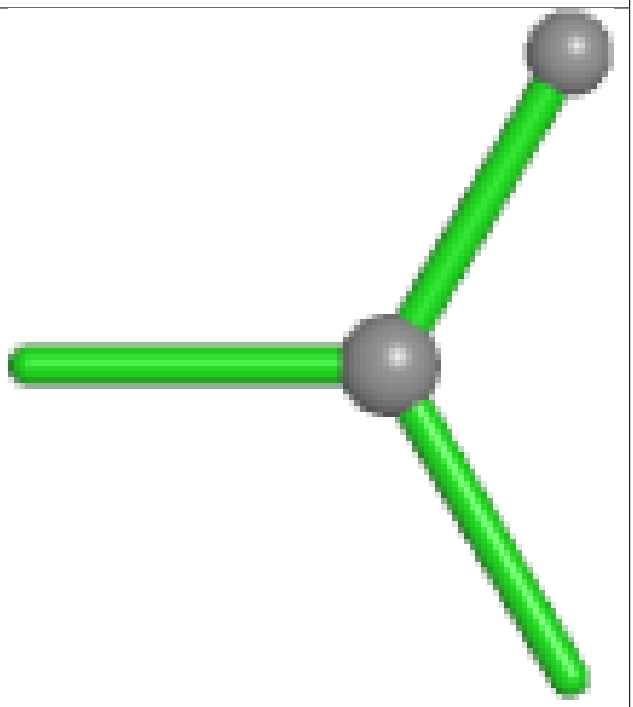


Ligand EDO A 812	
 Bond lengths	 Bond angles
 Torsions	Rings

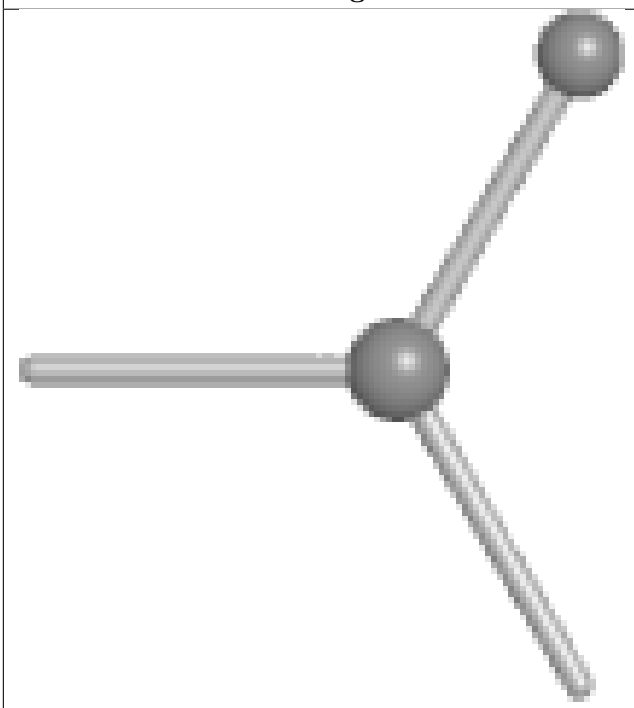
Ligand DMS A 807



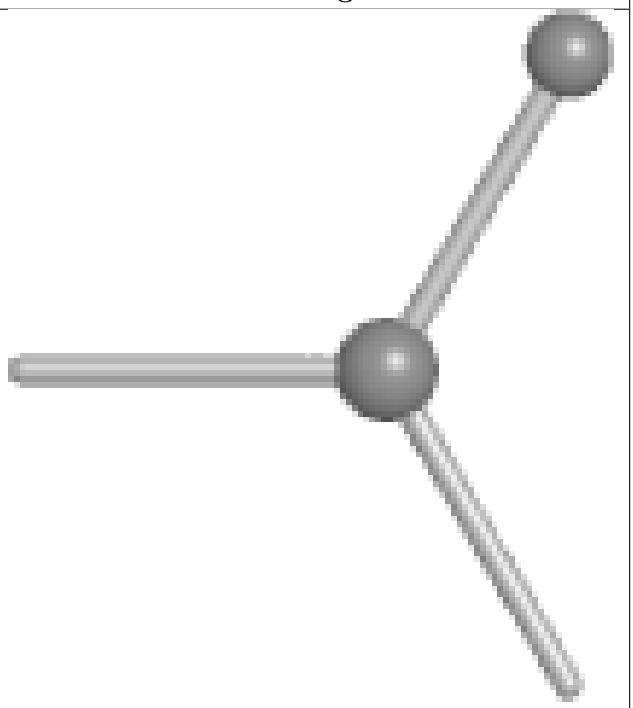
Bond lengths



Bond angles

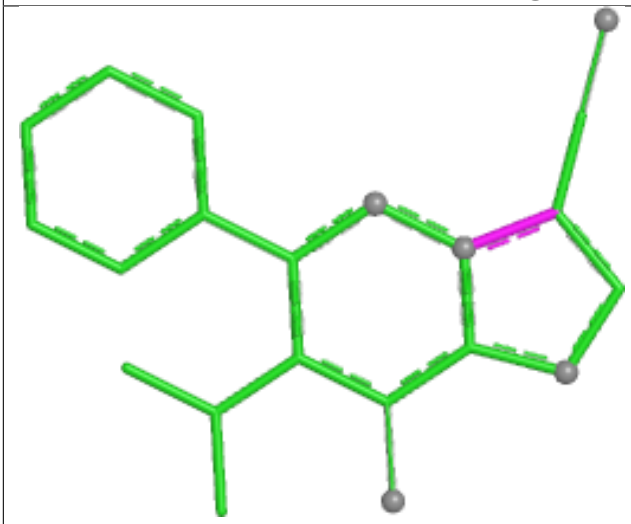


Torsions

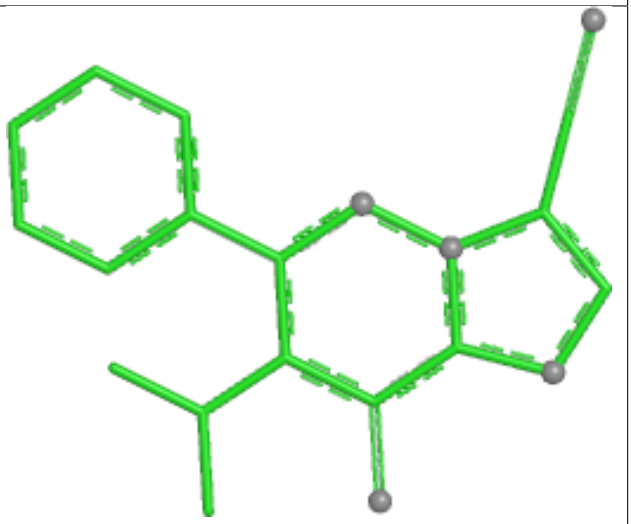


Rings

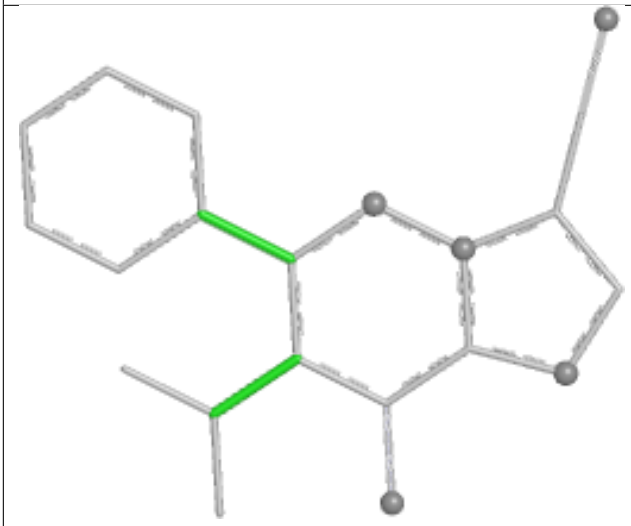
Ligand B6T A 804



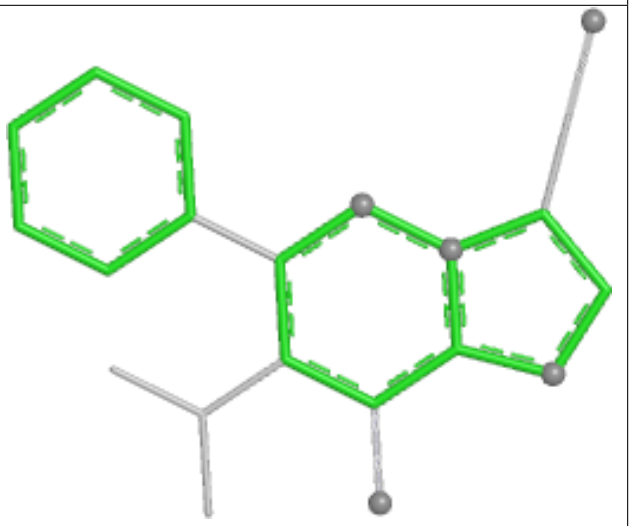
Bond lengths



Bond angles

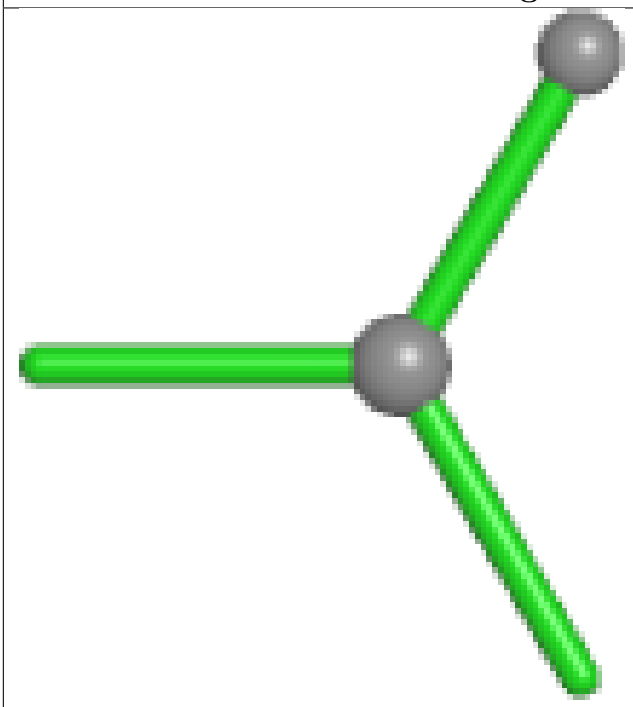


Torsions

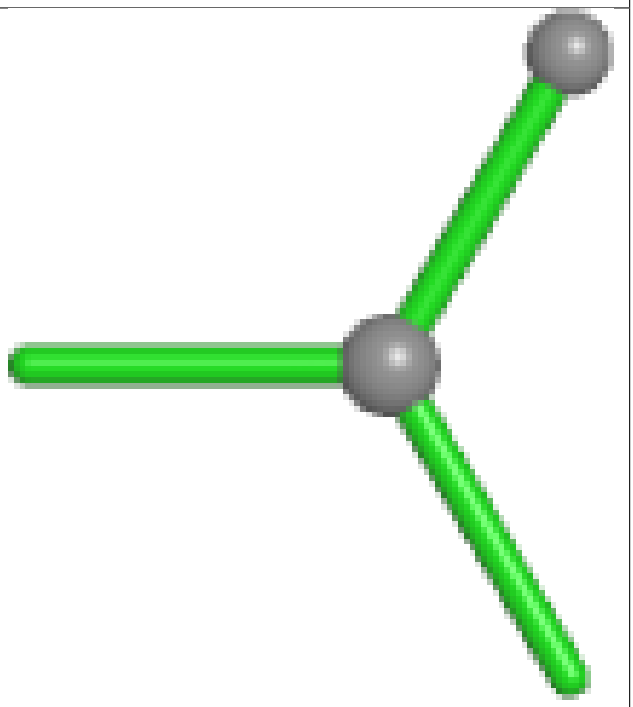


Rings

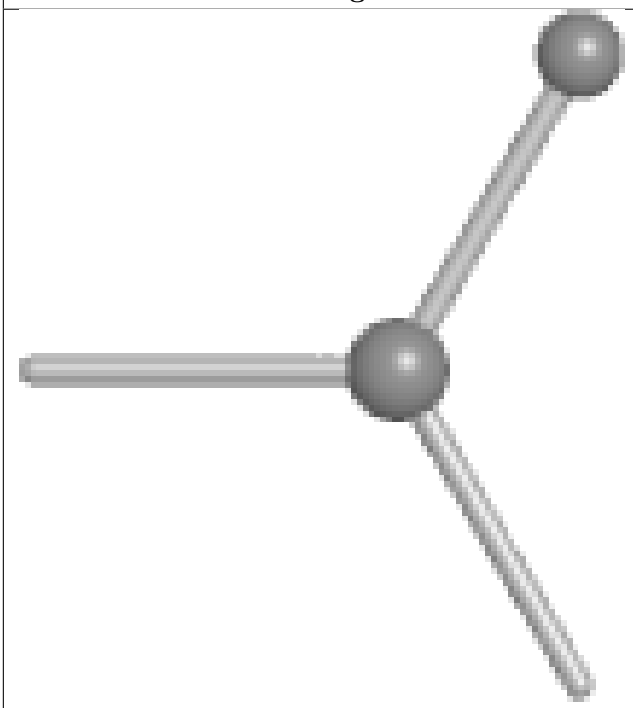
Ligand DMS A 808



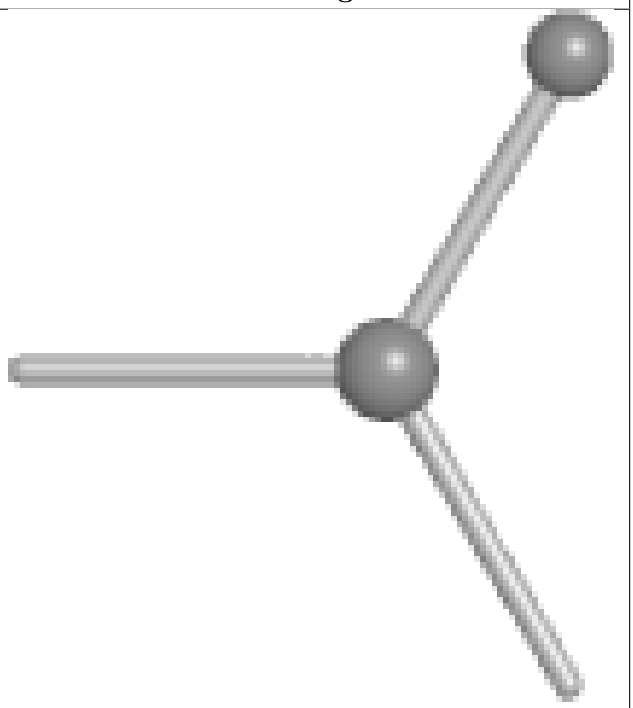
Bond lengths



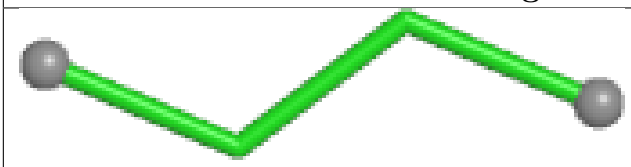
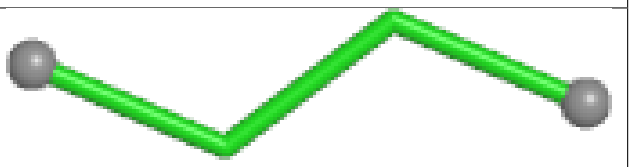
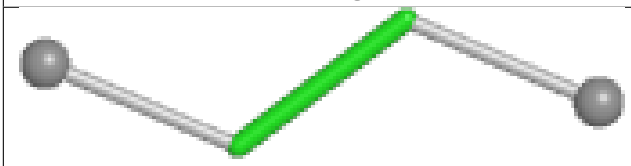
Bond angles

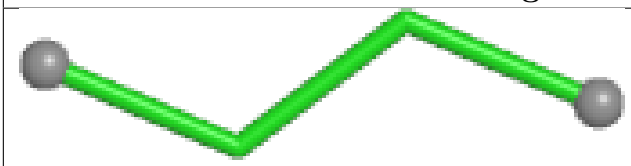
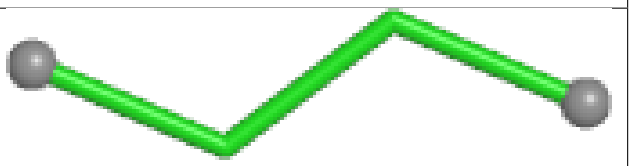
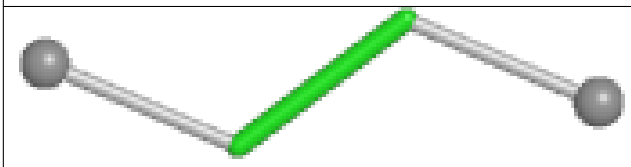


Torsions

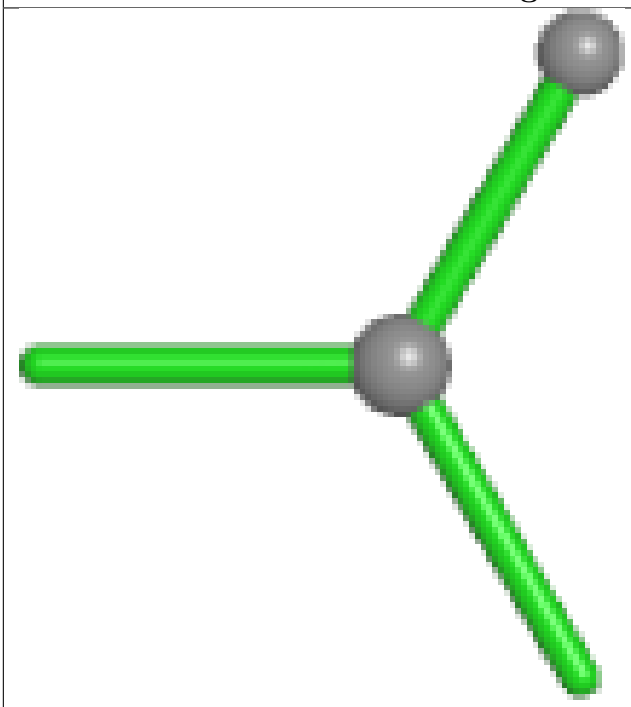


Rings

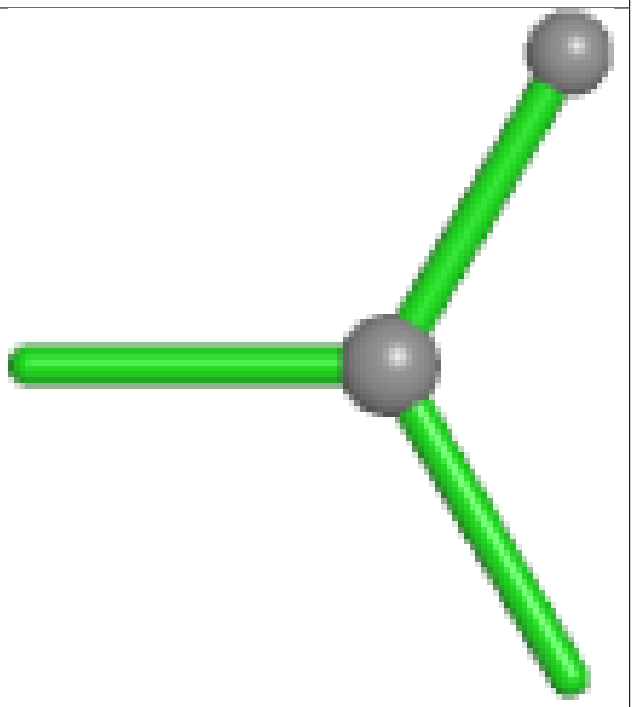
Ligand EDO A 816	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand EDO A 815	
 Bond lengths	 Bond angles
 Torsions	Rings

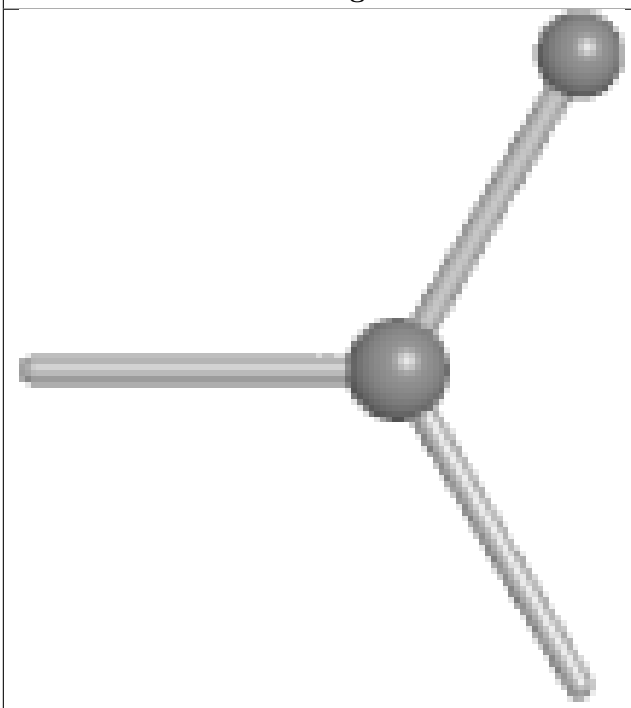
Ligand DMS A 806



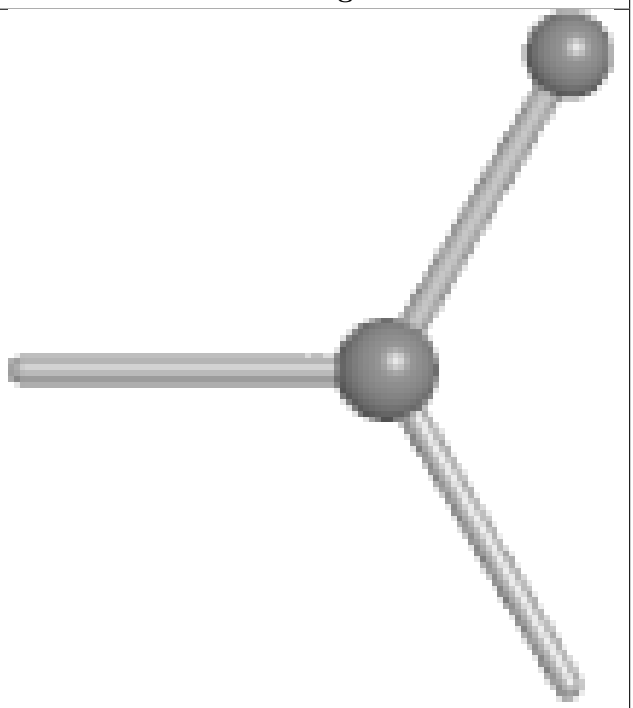
Bond lengths



Bond angles

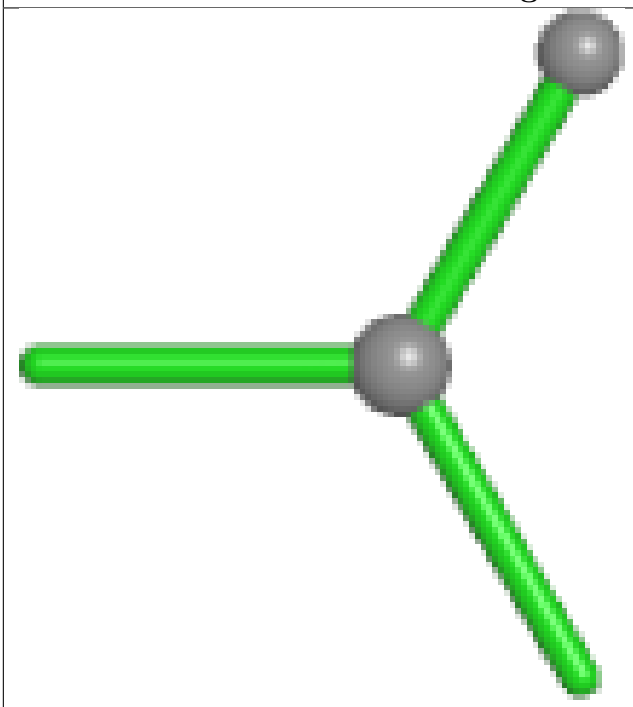


Torsions

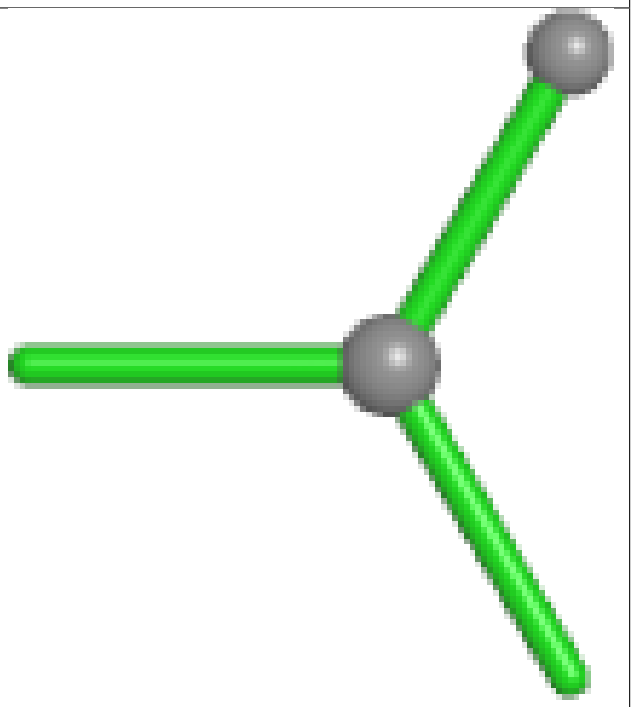


Rings

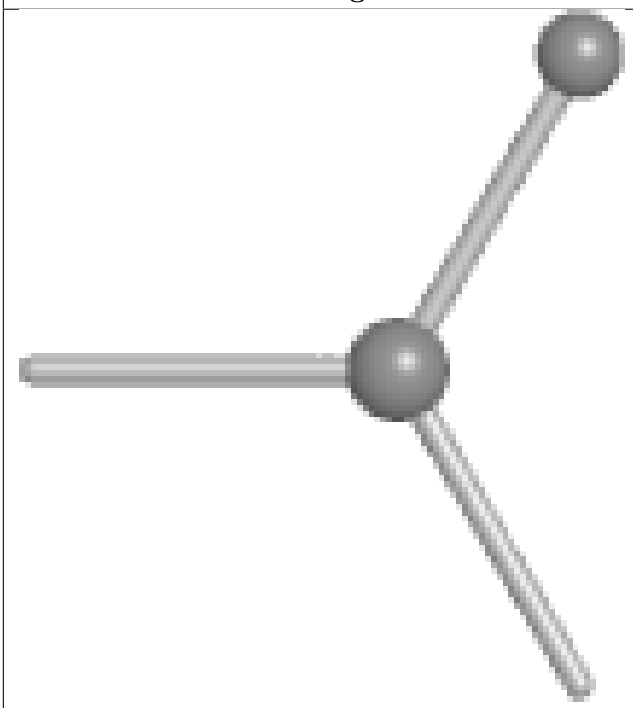
Ligand DMS A 809



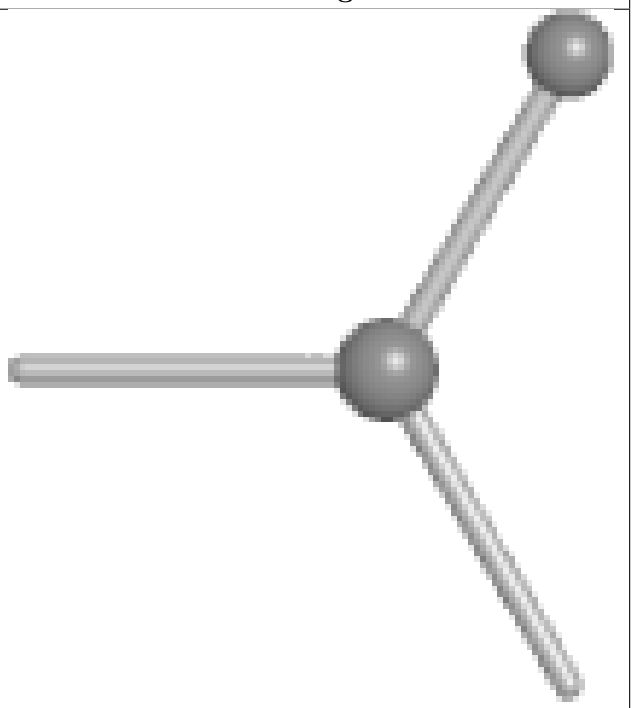
Bond lengths



Bond angles

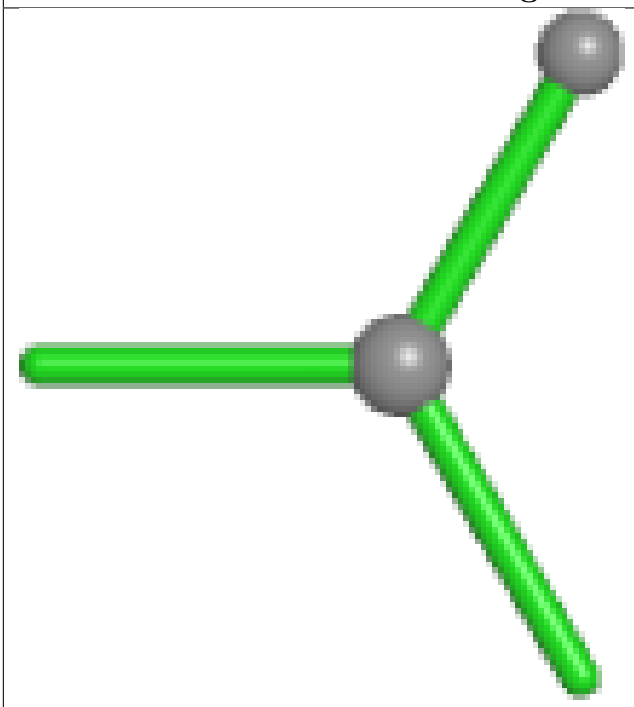


Torsions

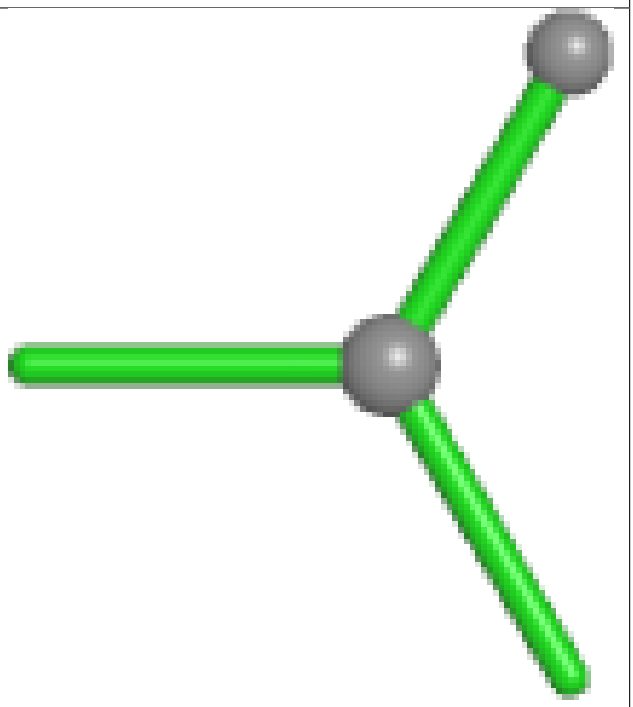


Rings

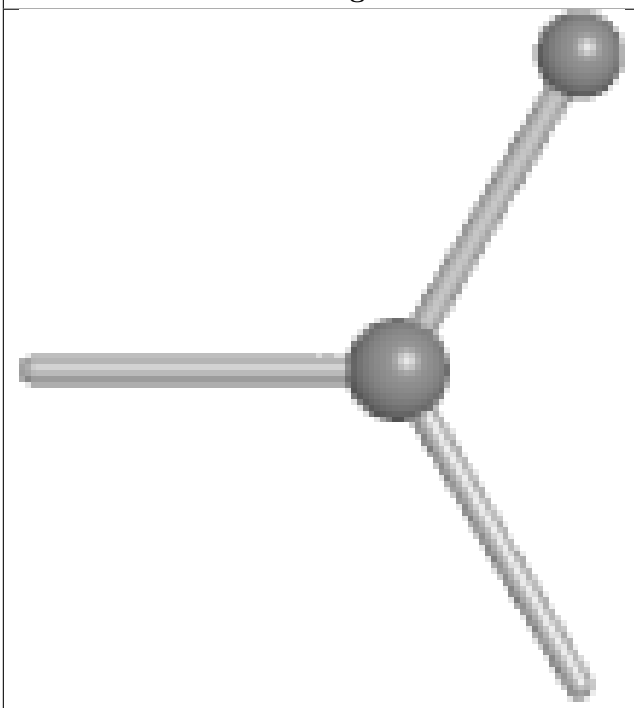
Ligand DMS A 805



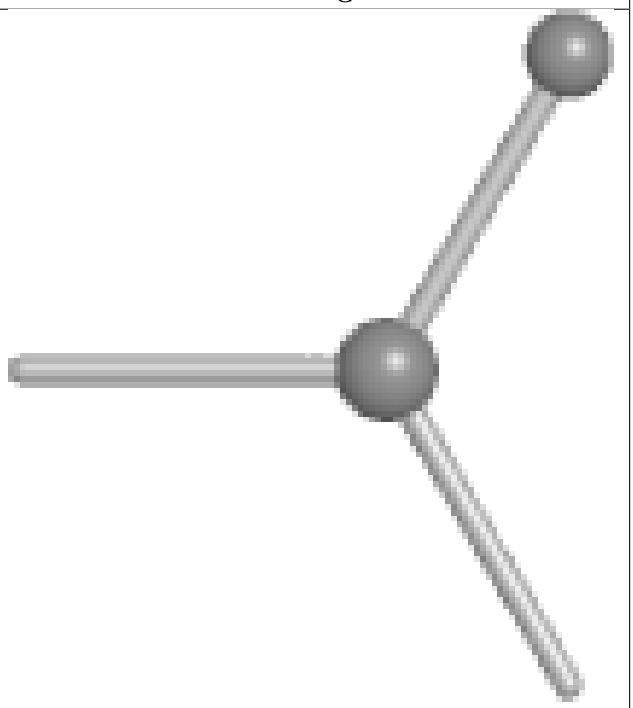
Bond lengths



Bond angles

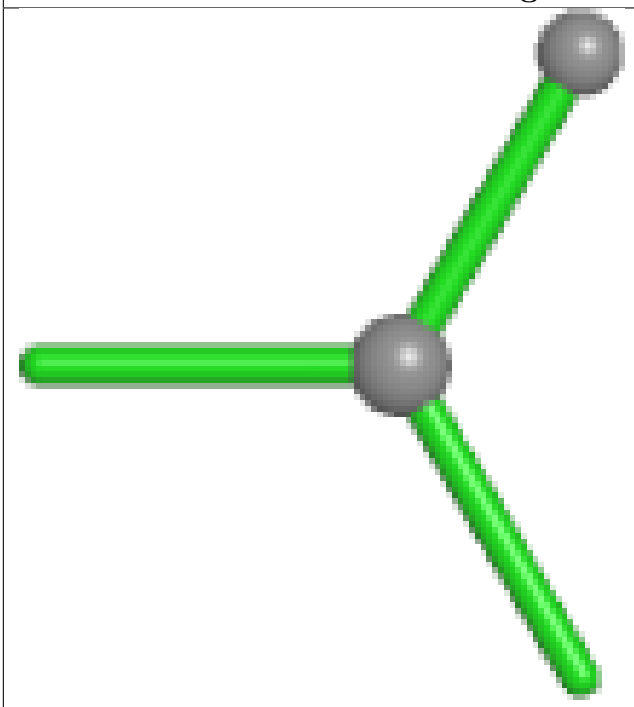


Torsions

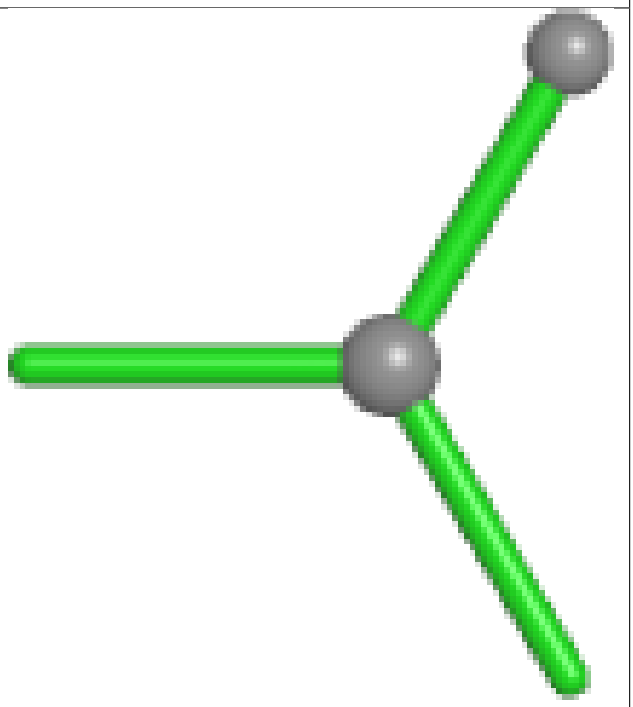


Rings

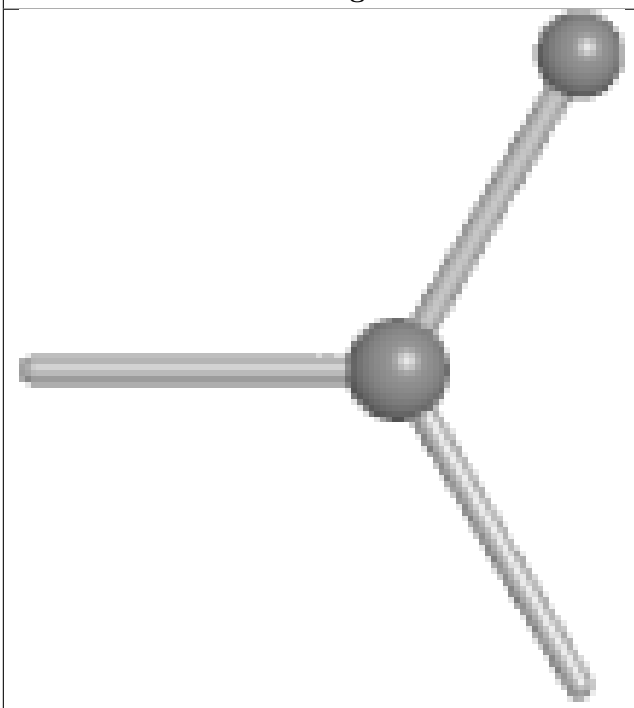
Ligand DMS A 811



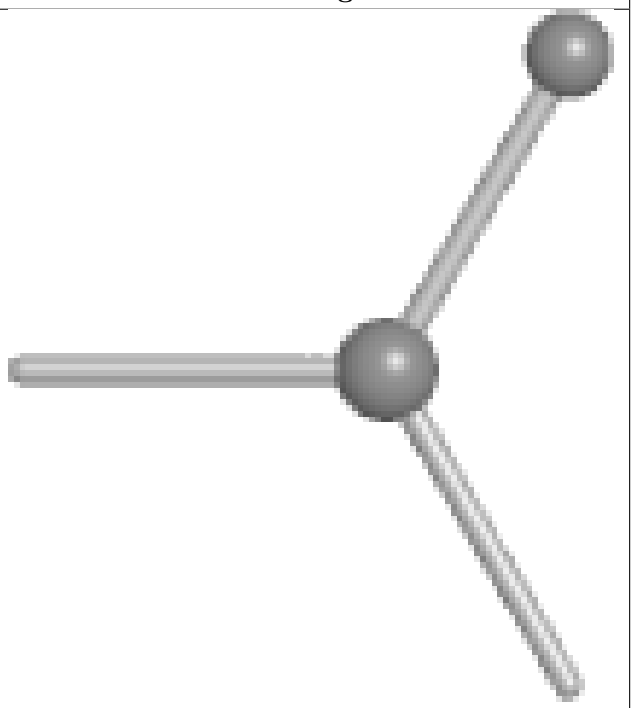
Bond lengths



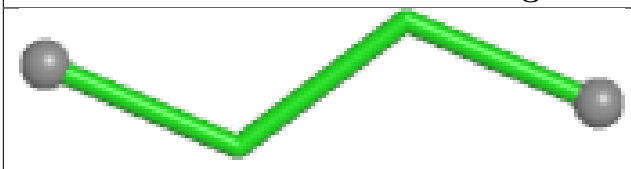
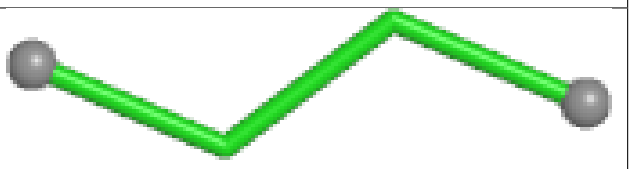
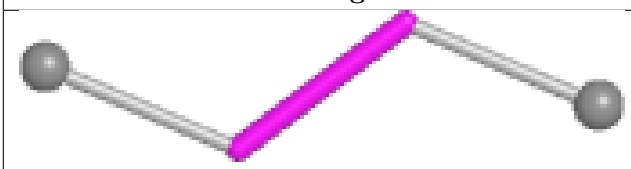
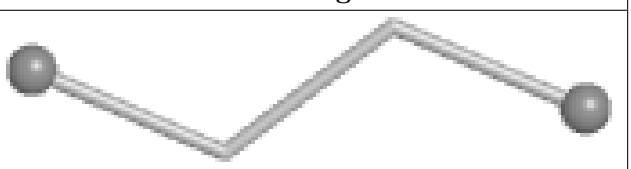
Bond angles



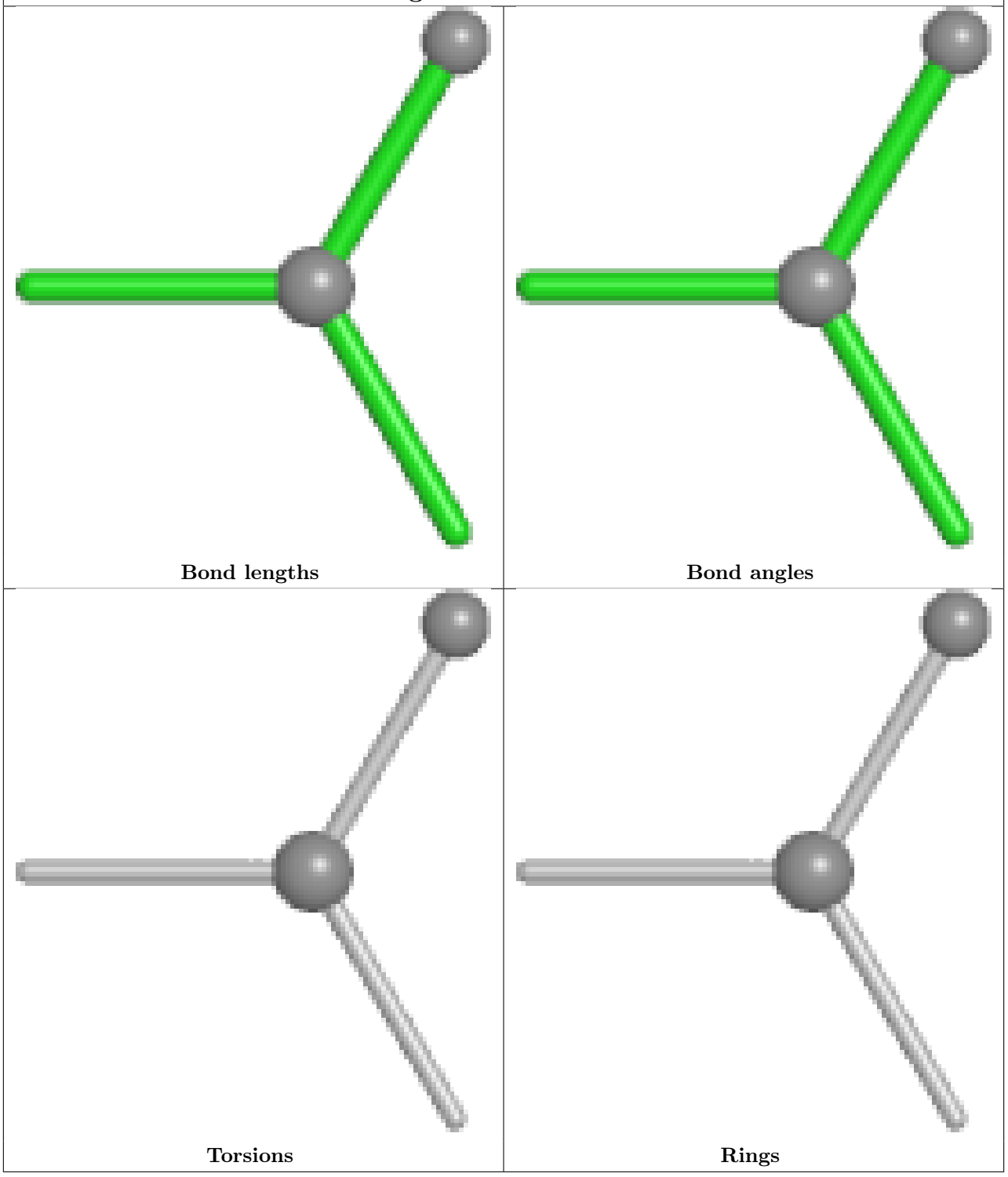
Torsions



Rings

Ligand EDO A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DMS A 810



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	454/462 (98%)	0.73	59 (12%)	7 8	15, 39, 76, 114	5 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	481	GLY	8.4
1	A	513	TRP	7.5
1	A	398	VAL	7.4
1	A	466	VAL	6.9
1	A	374	ALA	6.7
1	A	74	PHE	6.4
1	A	473	ALA	6.4
1	A	479	ILE	6.3
1	A	475	ILE	6.2
1	A	548	LEU	6.1
1	A	472	LEU	6.1
1	A	39	TRP	6.0
1	A	480	CYS	5.8
1	A	546	PRO	5.7
1	A	474[A]	HIS	5.7
1	A	476	THR	5.6
1	A	417	ILE	5.6
1	A	547	ASP	5.5
1	A	464	MET	5.2
1	A	399	HIS	5.0
1	A	468	GLU	4.9
1	A	445	ILE	4.7
1	A	375	ARG	4.6
1	A	478	ASP	4.6
1	A	482	MET	4.3
1	A	550	HIS	4.3
1	A	544	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	477	ALA	4.2
1	A	465	PRO	4.1
1	A	549	LEU	4.1
1	A	471	VAL	4.0
1	A	100	LYS	3.9
1	A	99	VAL	3.8
1	A	754	SER	3.7
1	A	545	GLN	3.6
1	A	483	LYS	3.4
1	A	543	VAL	3.4
1	A	446	LYS	3.3
1	A	467	MET	3.1
1	A	447	LEU	3.1
1	A	376	ASP	3.0
1	A	43	ALA	3.0
1	A	469	GLN	2.9
1	A	620	LEU	2.8
1	A	540	GLU	2.7
1	A	450	GLU	2.7
1	A	624	TYR	2.7
1	A	470	SER	2.7
1	A	98	ARG	2.6
1	A	623	ARG	2.5
1	A	25	MET	2.5
1	A	440	VAL	2.5
1	A	86[A]	ARG	2.5
1	A	449	PRO	2.3
1	A	456	ASP	2.3
1	A	688	ASP	2.1
1	A	416	THR	2.1
1	A	605	VAL	2.0
1	A	542	PHE	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 oligosaccharides in this entry.

6.4 Ligands (i)

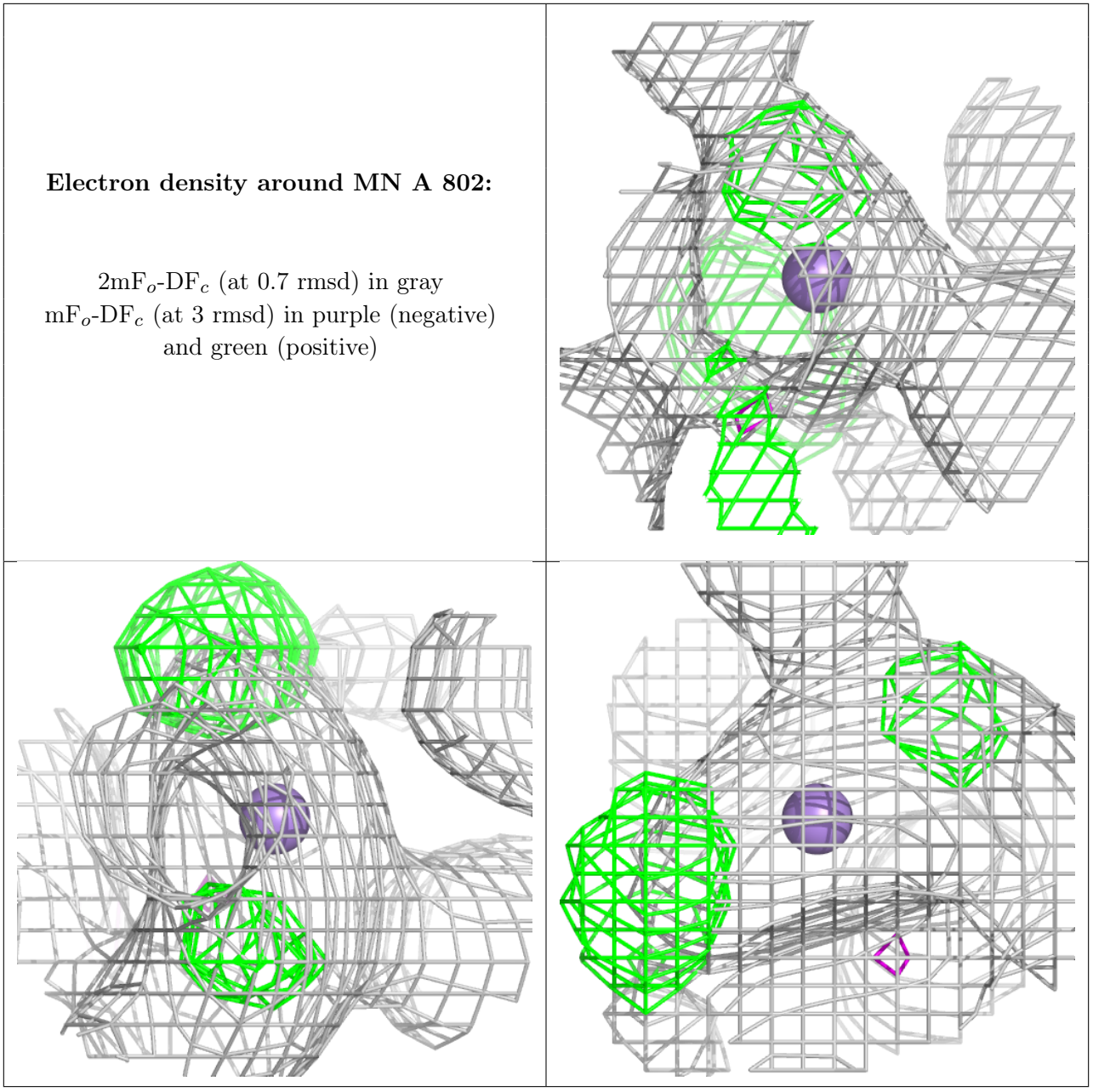
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	A	802	1/1	0.86	0.15	58,58,58,58	1
5	DMS	A	807	4/4	0.87	0.23	45,45,61,63	0
5	DMS	A	809	4/4	0.88	0.20	49,65,66,67	0
5	DMS	A	808	4/4	0.89	0.22	38,52,54,60	0
5	DMS	A	810	4/4	0.90	0.21	75,77,77,81	0
6	EDO	A	815	4/4	0.90	0.21	47,64,69,70	0
5	DMS	A	811	4/4	0.91	0.21	64,68,73,75	0
6	EDO	A	812	4/4	0.91	0.22	47,55,58,59	0
6	EDO	A	813	4/4	0.91	0.23	35,39,49,50	0
5	DMS	A	806	4/4	0.91	0.21	82,83,87,87	0
6	EDO	A	814	4/4	0.93	0.16	40,45,47,51	0
6	EDO	A	816	4/4	0.93	0.18	37,43,47,47	0
4	B6T	A	804	21/21	0.97	0.07	25,29,39,43	0
2	ZN	A	817	1/1	0.97	0.07	45,45,45,45	1
5	DMS	A	805	4/4	0.99	0.09	34,37,38,40	0
3	MN	A	803	1/1	1.00	0.03	26,26,26,26	0
2	ZN	A	801	1/1	1.00	0.03	31,31,31,31	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.

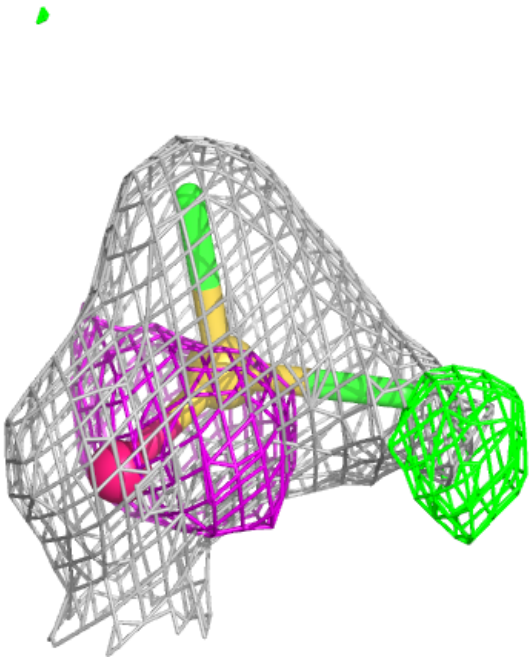
Electron density around MN A 802:

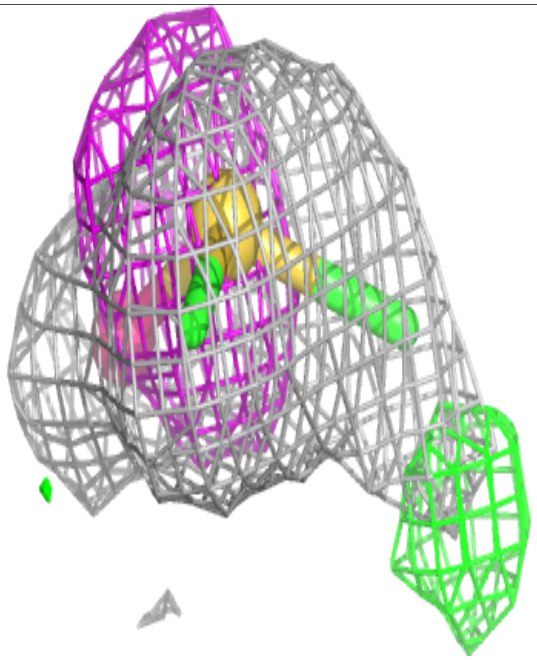
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

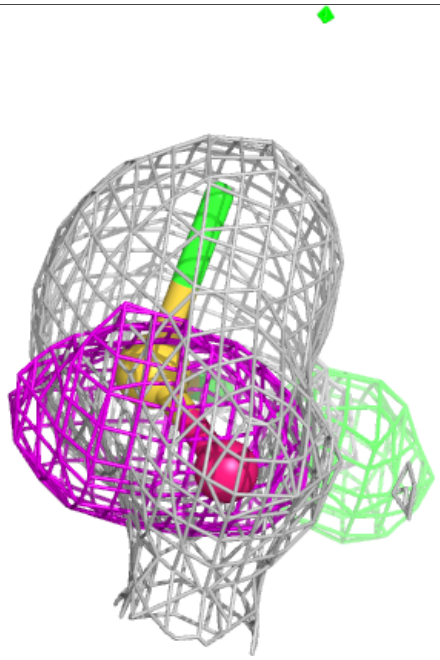


Electron density around DMS A 807:

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

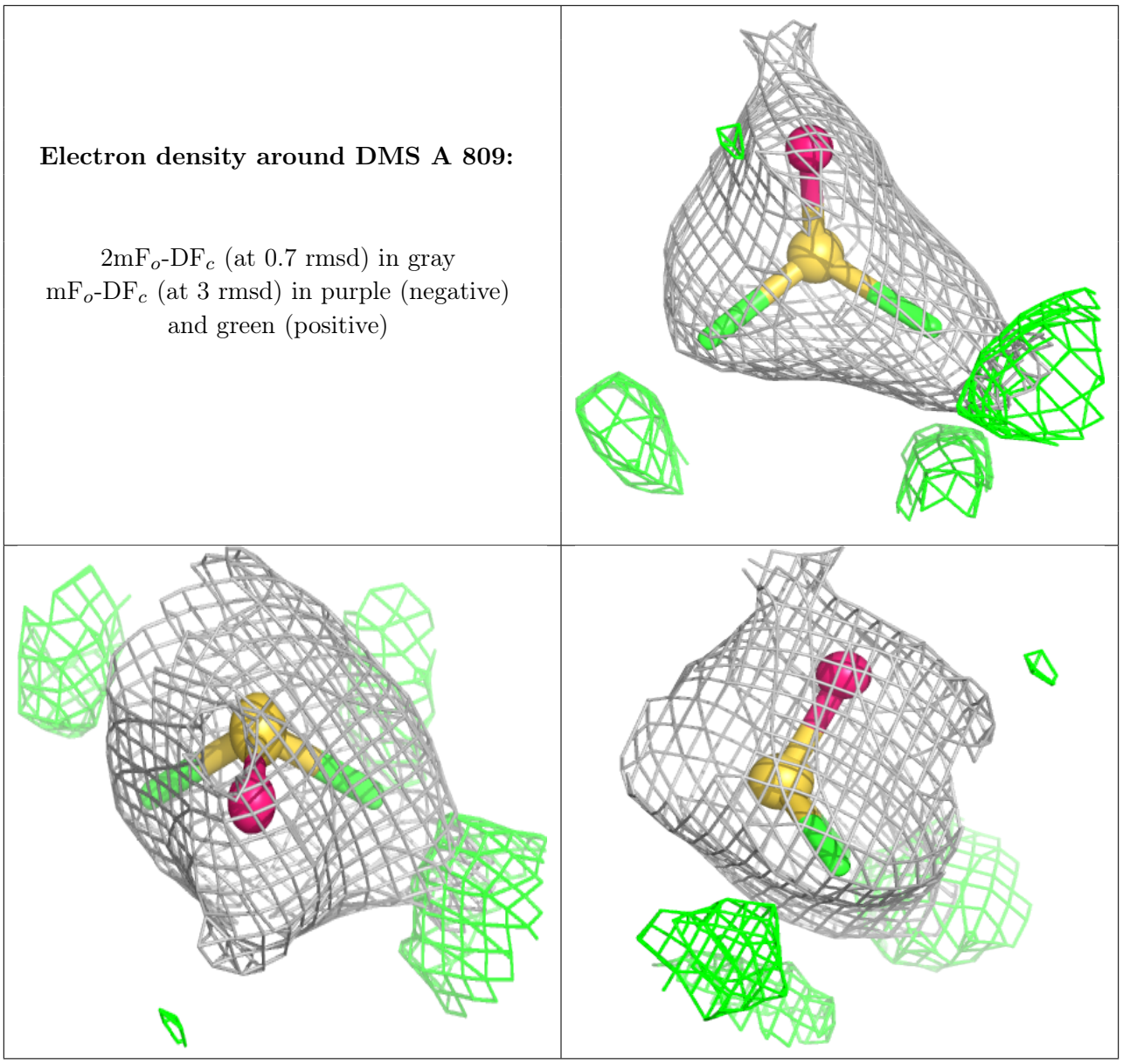






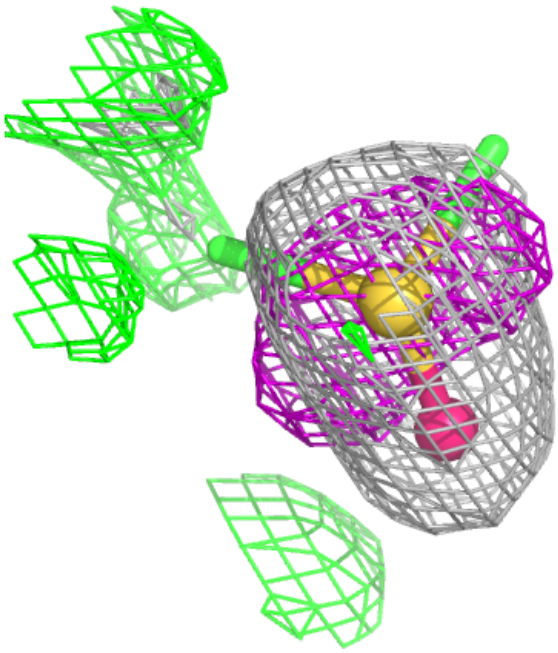
Electron density around DMS A 809:

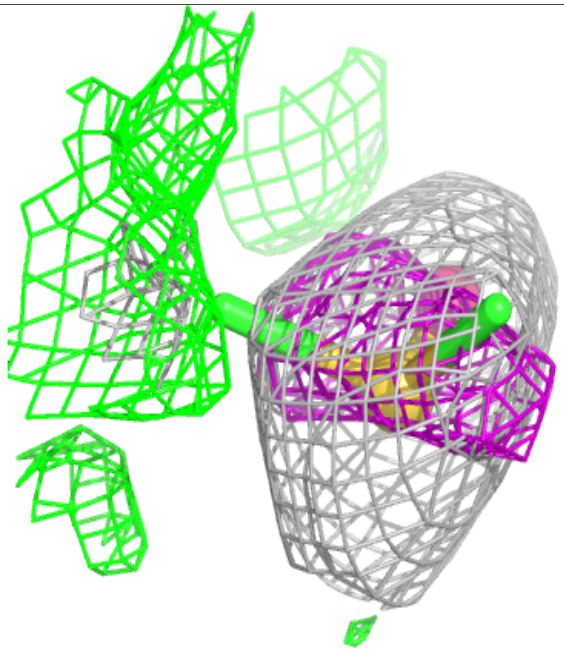
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

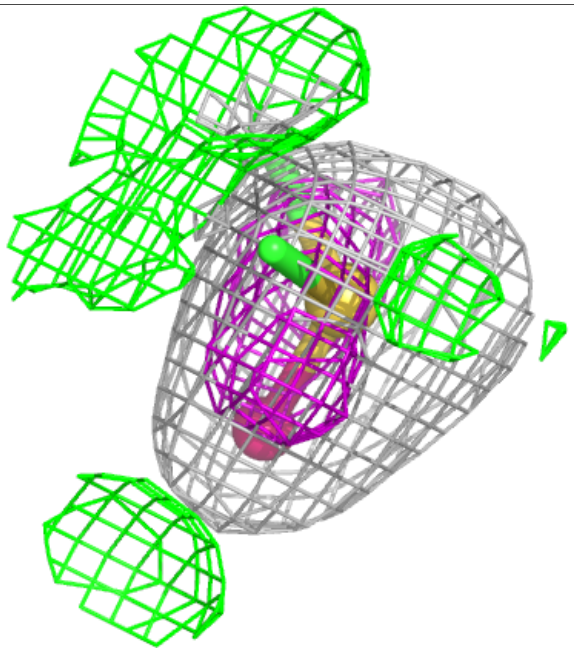


Electron density around DMS A 808:

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

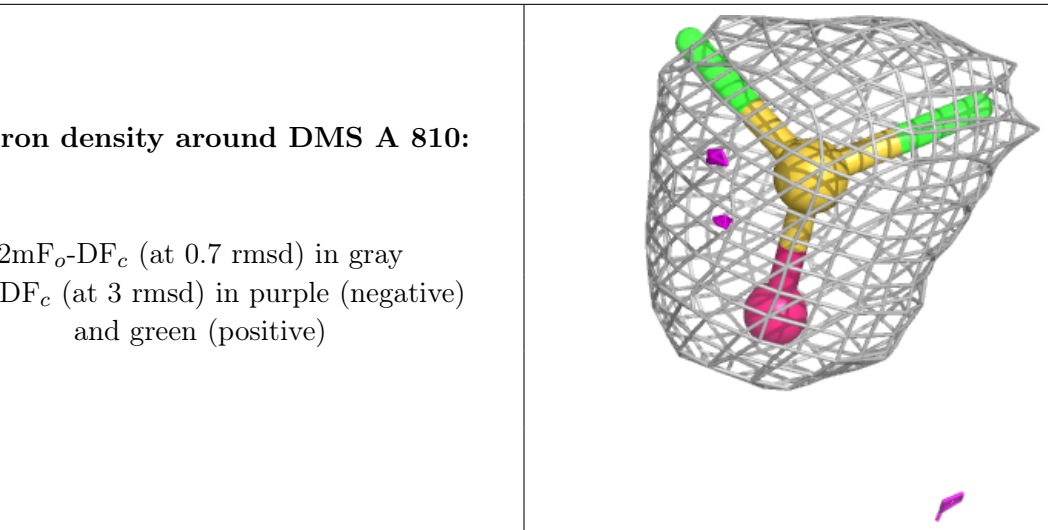


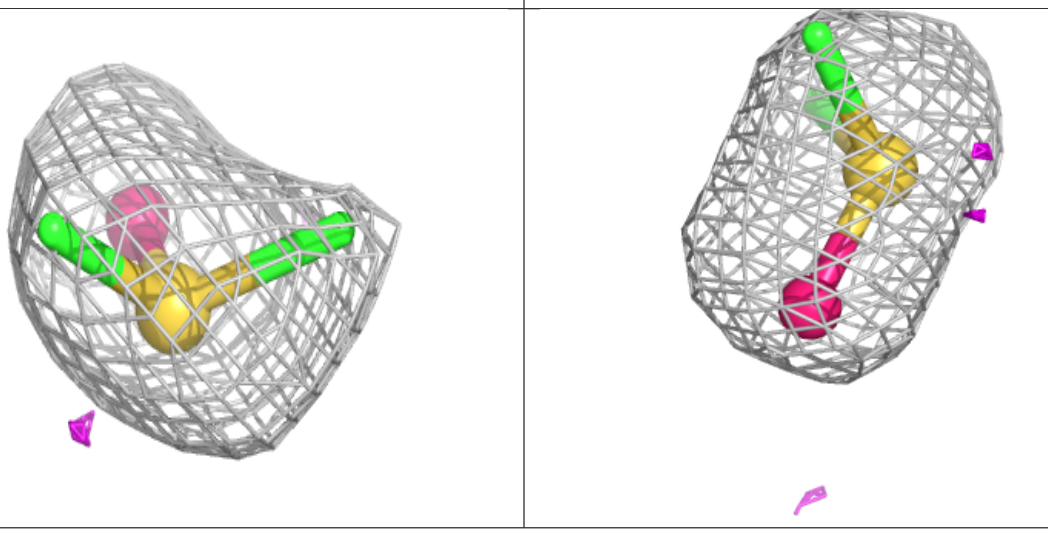




Electron density around DMS A 810:

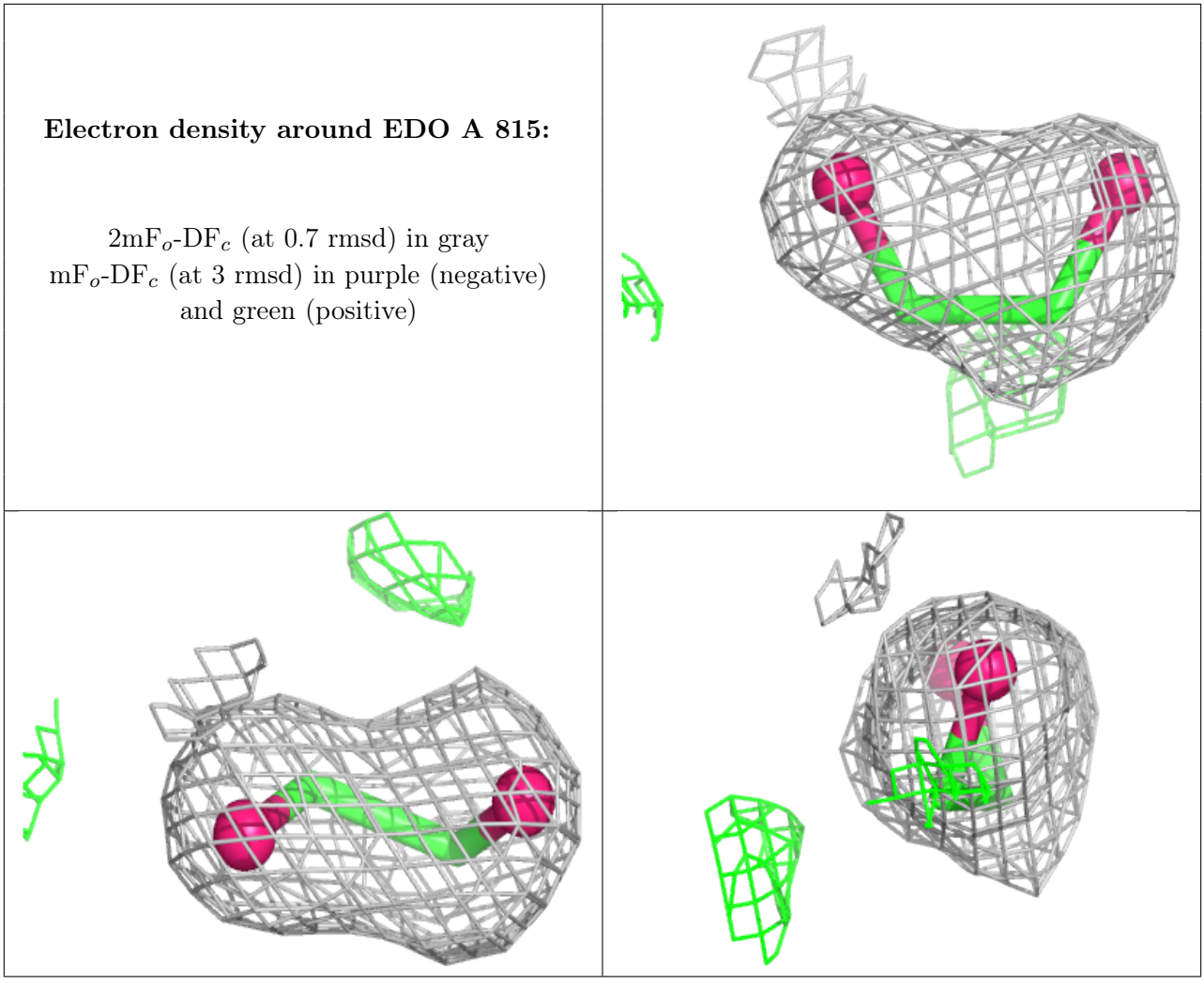
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





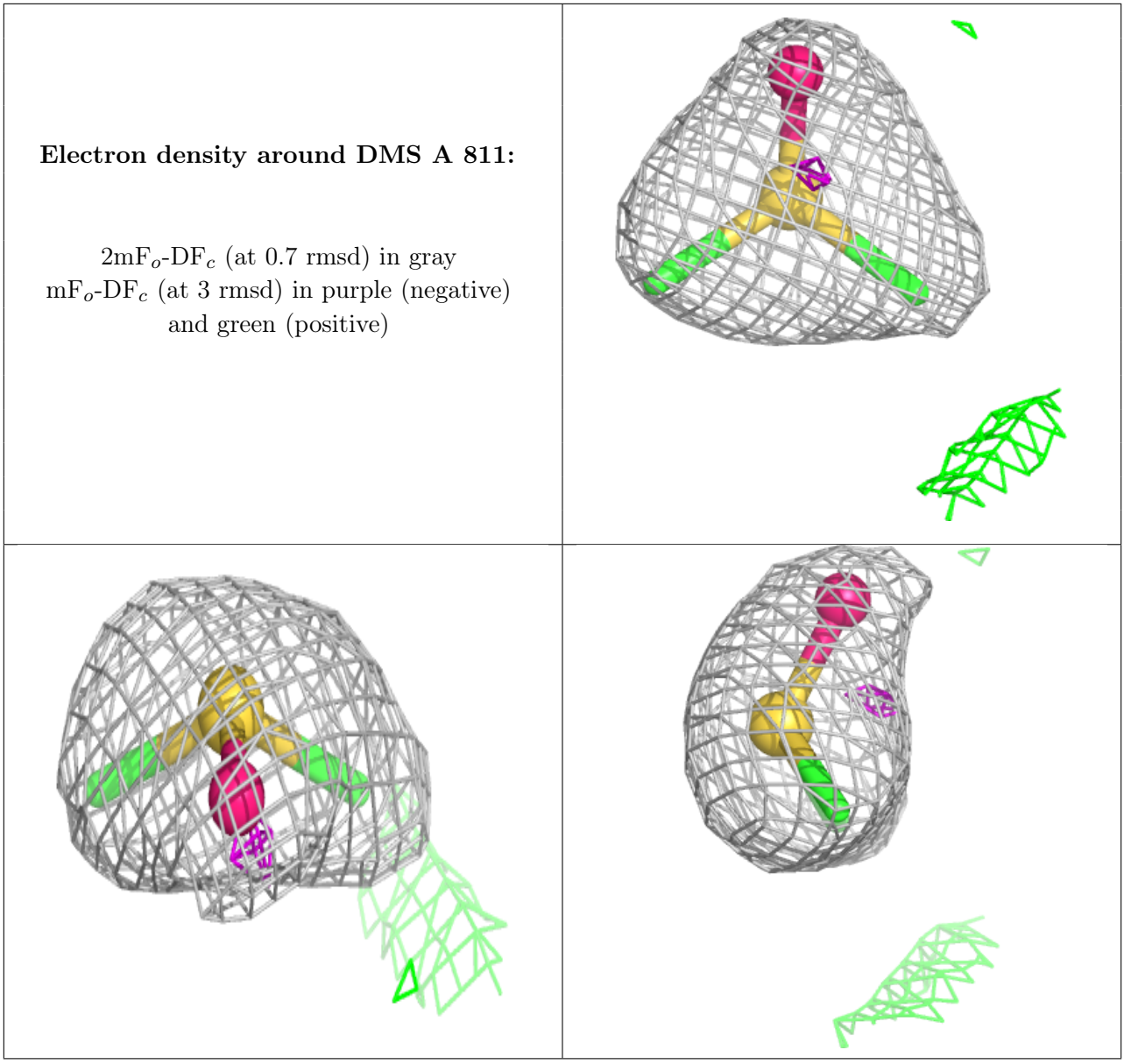
Electron density around EDO A 815:

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



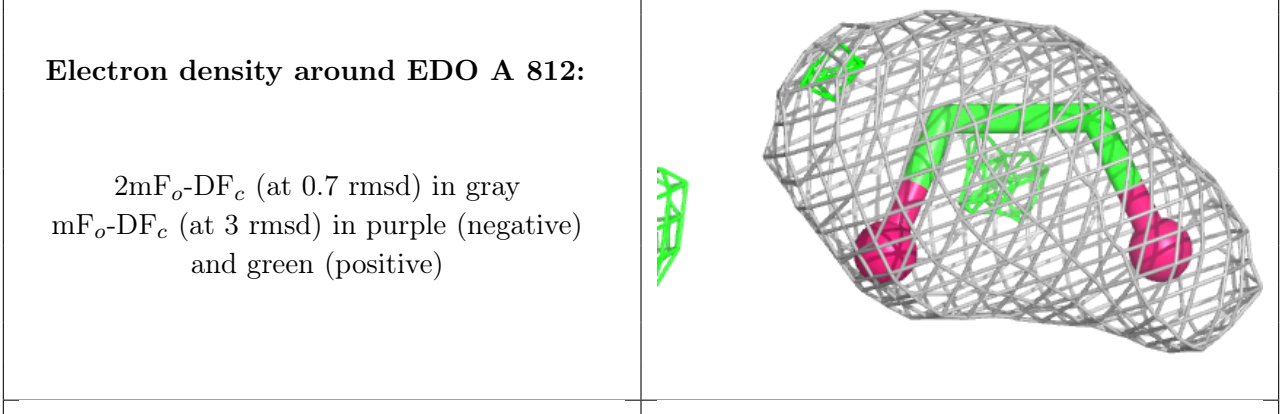
Electron density around DMS A 811:

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



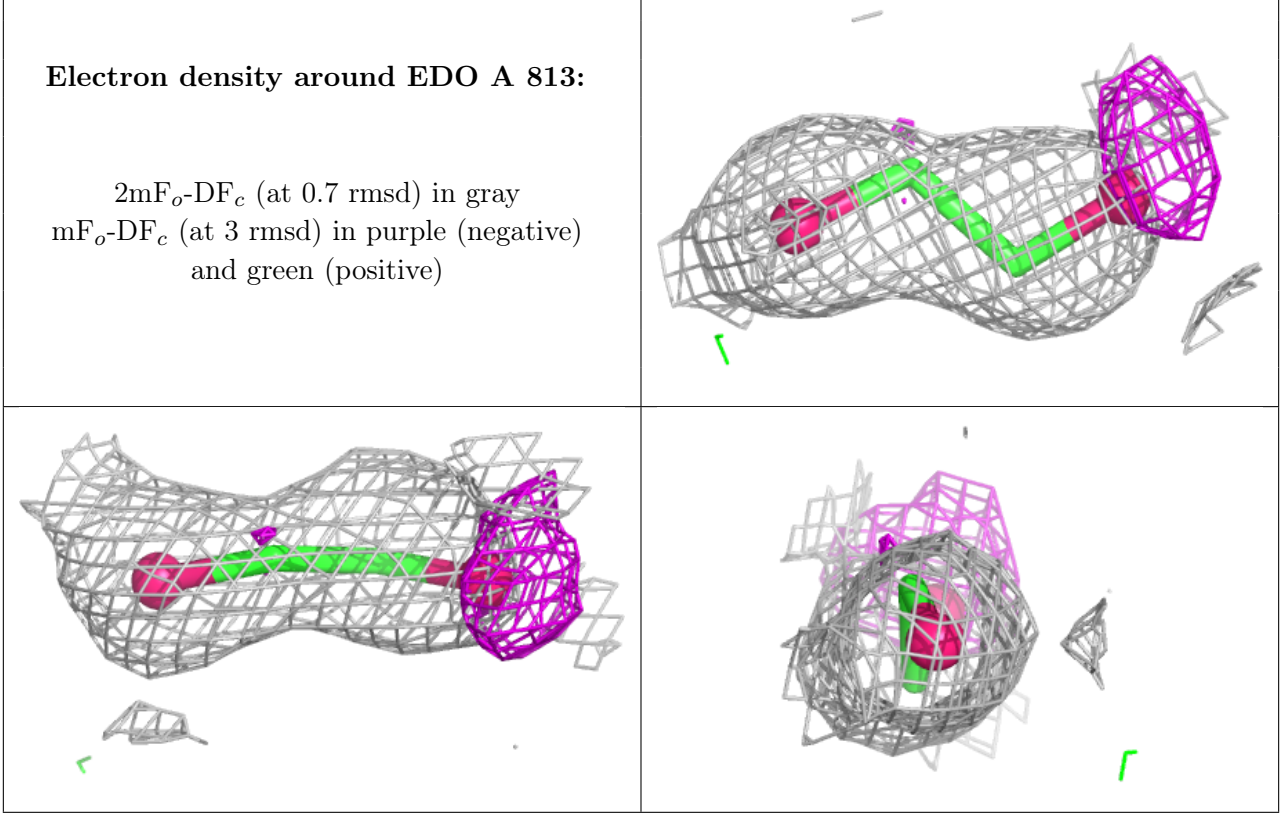
Electron density around EDO A 812:

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



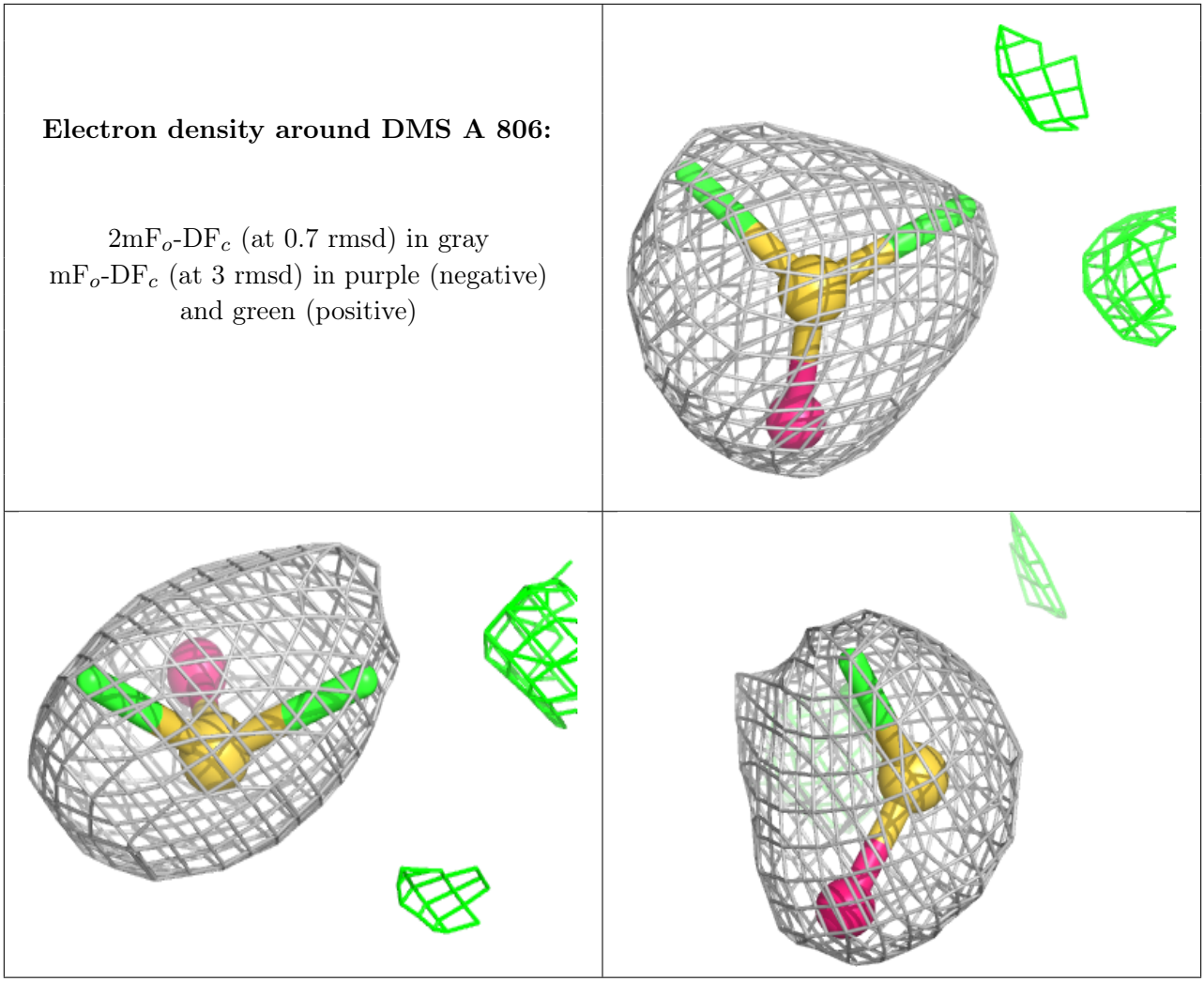
Electron density around EDO A 813:

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



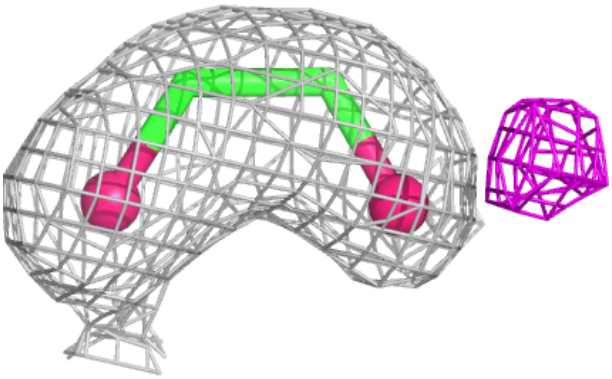
Electron density around DMS A 806:

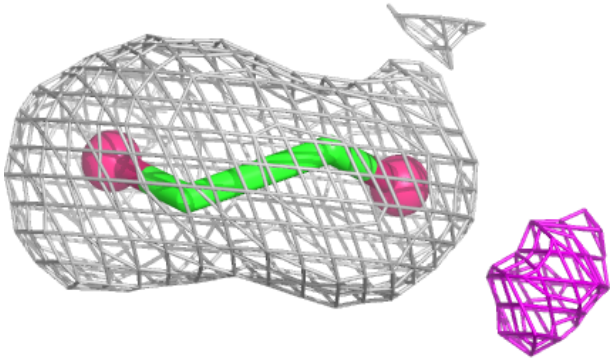
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

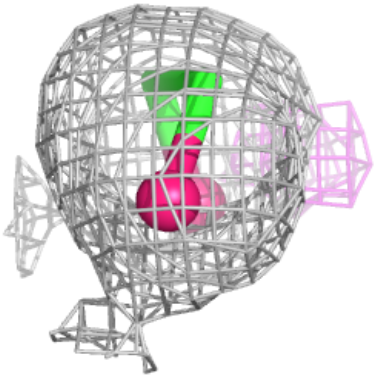


Electron density around EDO A 814:

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

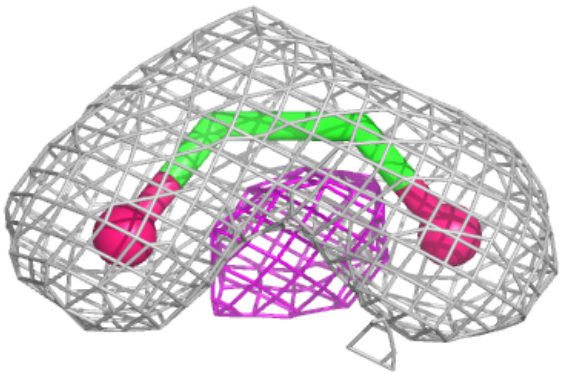


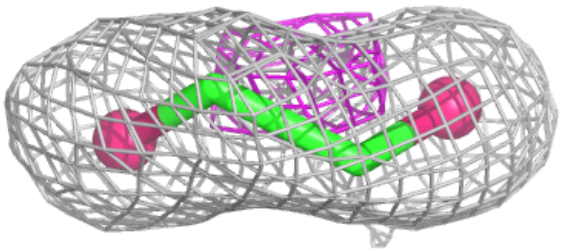


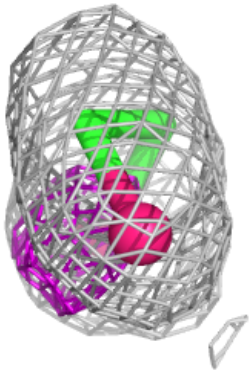


Electron density around EDO A 816:

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

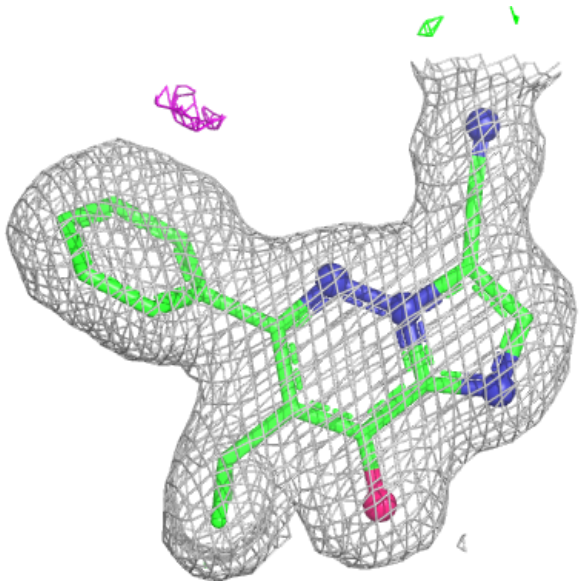


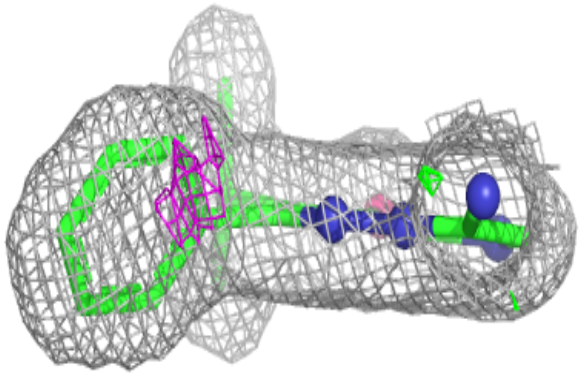


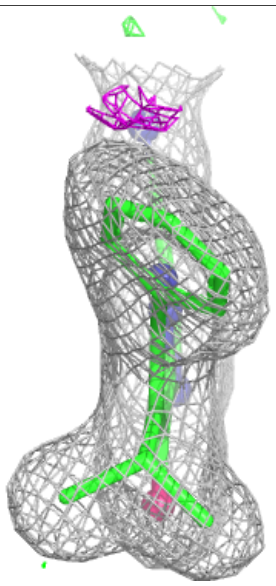


Electron density around B6T A 804:

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

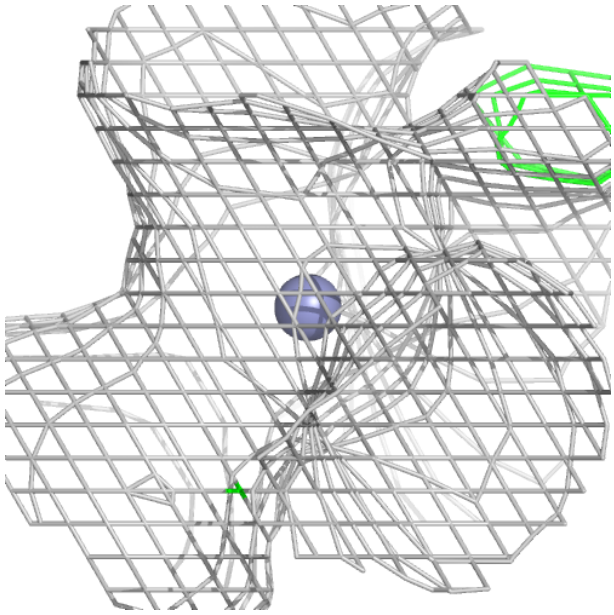


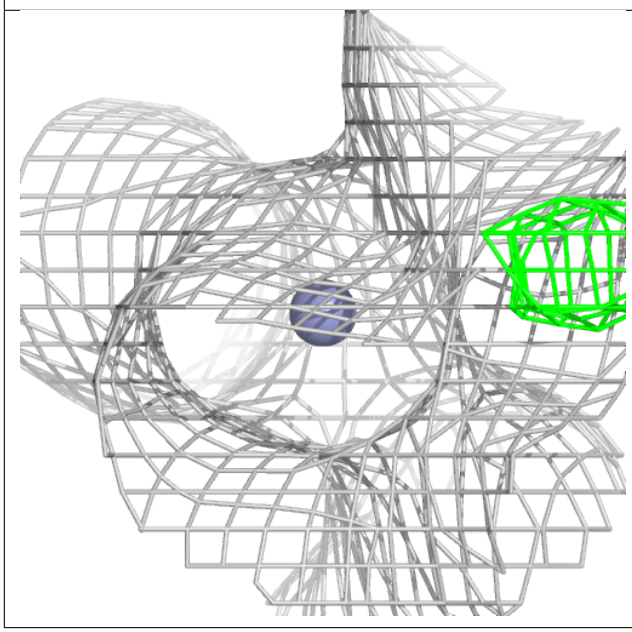


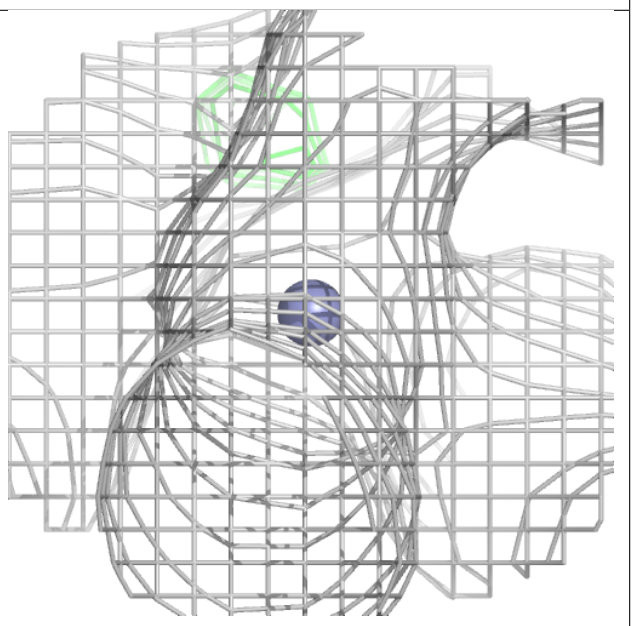


Electron density around ZN A 817:

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

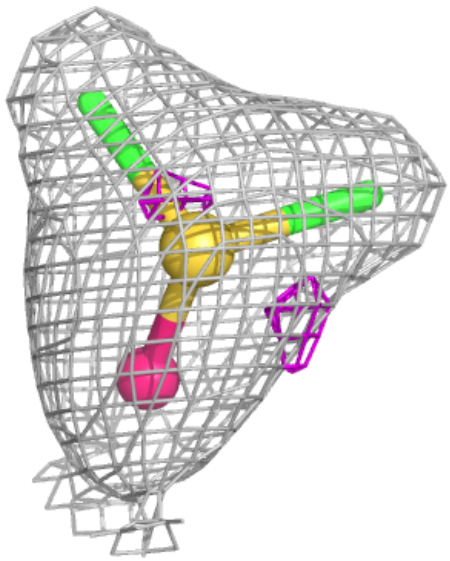


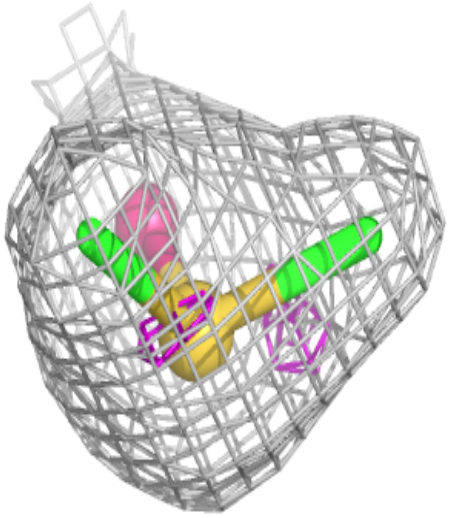


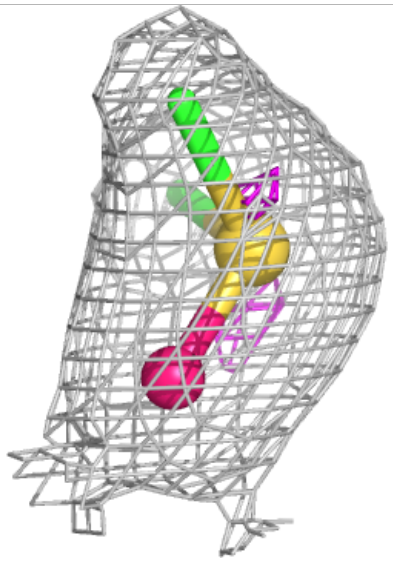


Electron density around DMS A 805:

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

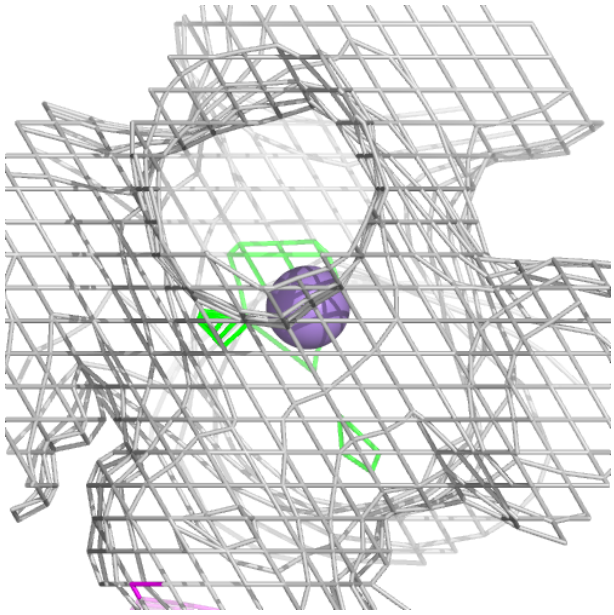


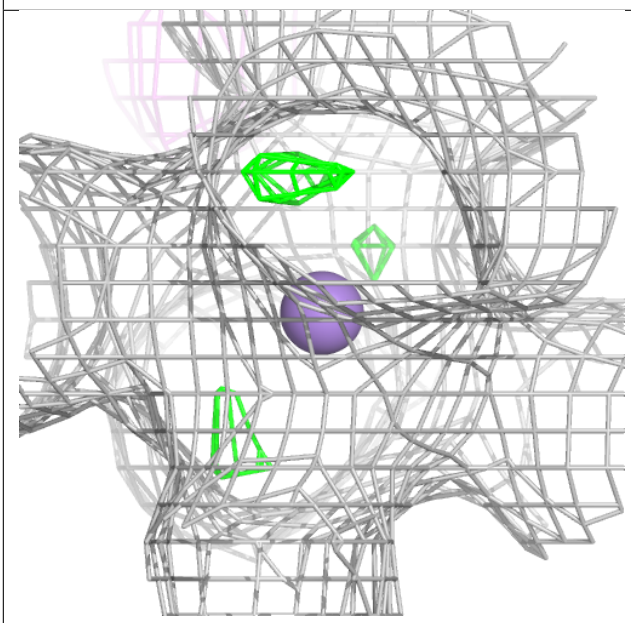


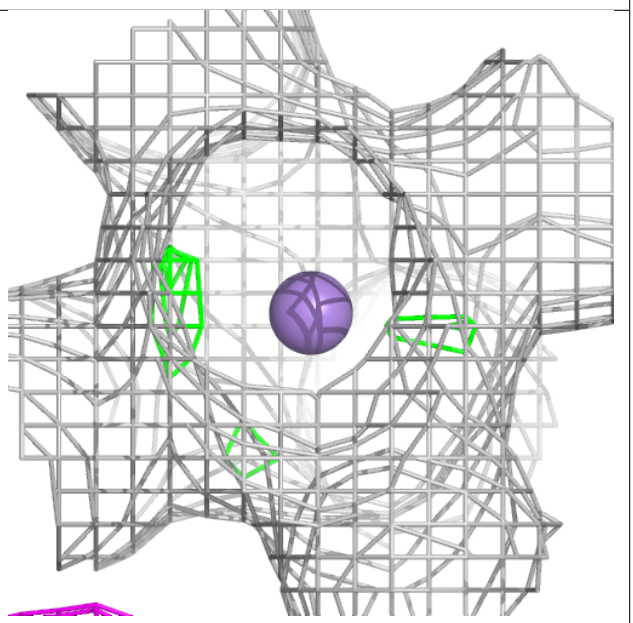


Electron density around MN A 803:

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

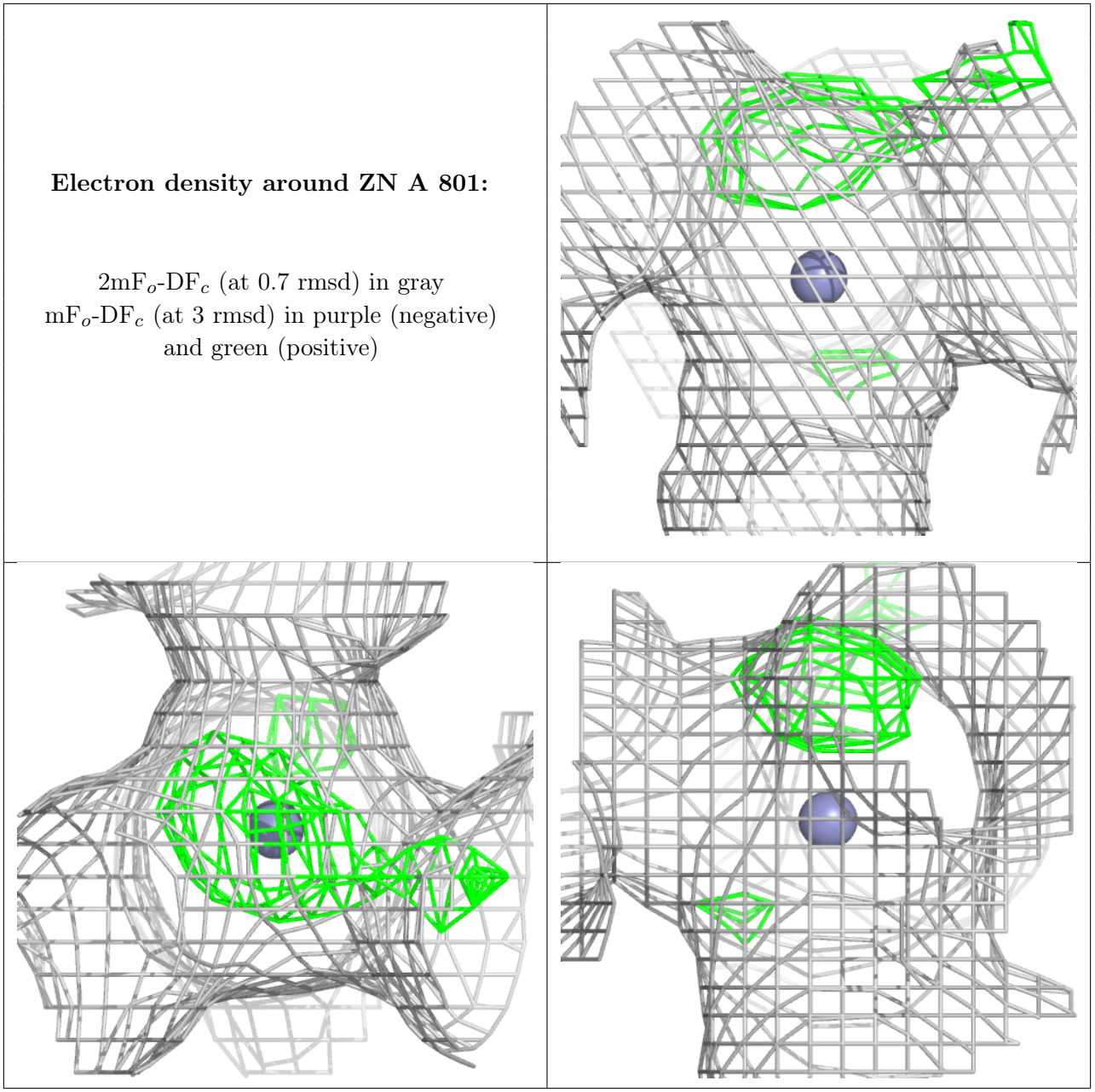






Electron density around ZN A 801:

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



6.5 Other polymers

There are no such residues in this entry.