wwPDB X-ray Structure Validation Summary Report (i)

Mar 6, 2026 – 07:07 PM UTC

PDB ID	:	7UTC / pdb_00007utc
Title	:	Crystal structure of secondary alcohol dehydrogenases from the Thermoanaerobacter ethanolicus with NADP and transition-state analogue inhibitor DMSO
Authors	:	Dinh, T.; Phillips, R.
Deposited on	:	2022-04-26
Resolution	:	1.85 Å(reported)

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

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

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

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

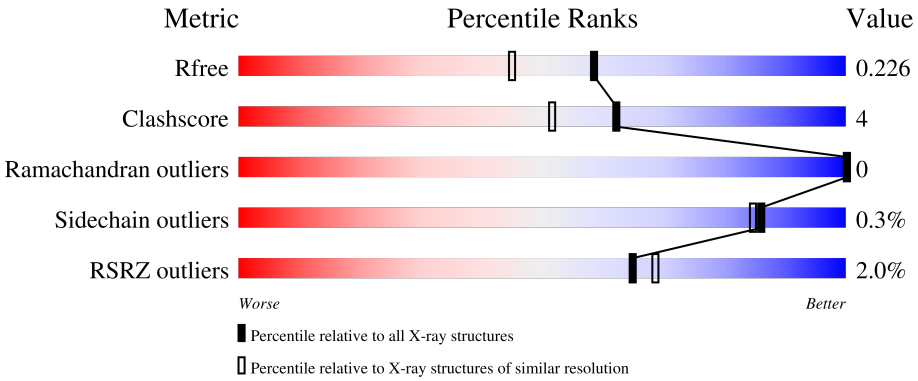
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	352	4% 89% 11%
1	B	352	2% 92% 8%
1	C	352	% 89% 11%
1	D	352	% 90% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11438 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 Secondary-alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2642	1693	455	476	18			
1	B	352	Total	C	N	O	S	0	1	0
			2647	1697	455	476	19			
1	C	352	Total	C	N	O	S	0	5	0
			2670	1716	457	479	18			
1	D	352	Total	C	N	O	S	0	2	0
			2651	1702	455	476	18			

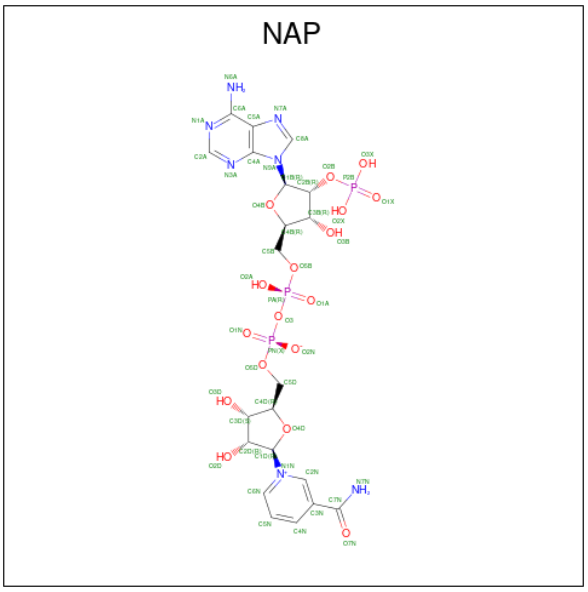
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	ALA	CYS	engineered mutation	UNP P14941
B	295	ALA	CYS	engineered mutation	UNP P14941
C	295	ALA	CYS	engineered mutation	UNP P14941
D	295	ALA	CYS	engineered mutation	UNP P14941

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

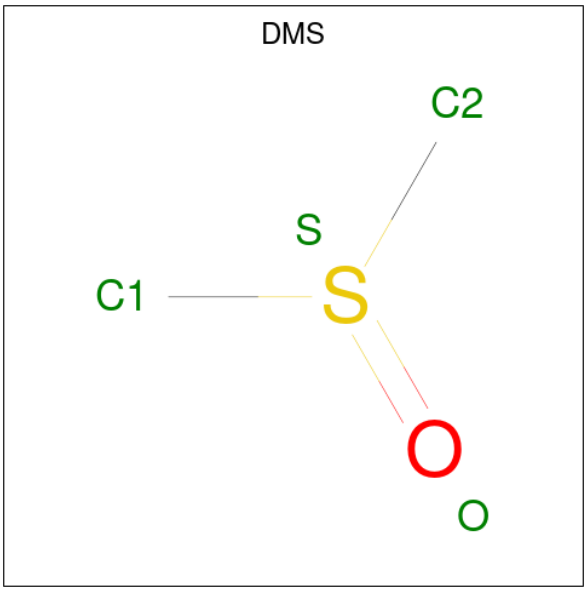
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 5 is water.

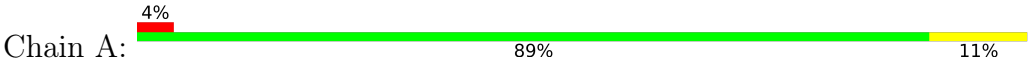
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	1
			62	62		
5	B	101	Total	O	0	1
			101	101		
5	C	158	Total	O	0	0
			158	158		
5	D	171	Total	O	0	6
			171	171		

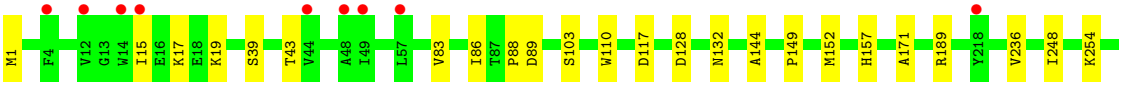
3 Residue-property plots (i)

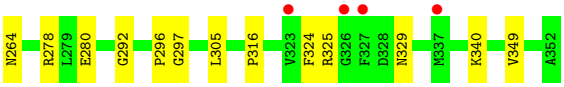
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Secondary-alcohol dehydrogenase

Chain A:

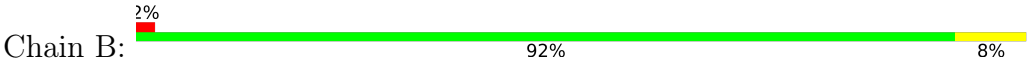


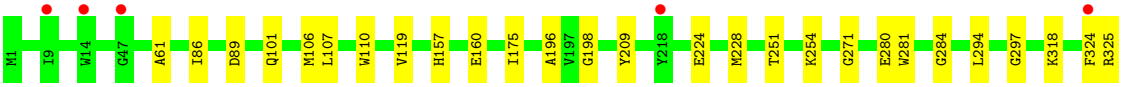


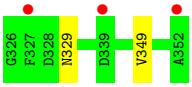


• Molecule 1: Secondary-alcohol dehydrogenase

Chain B:

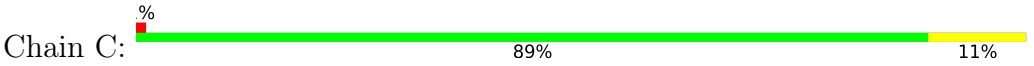


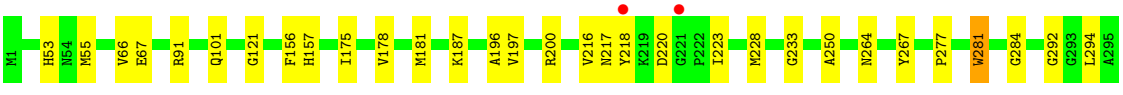




• Molecule 1: Secondary-alcohol dehydrogenase

Chain C:

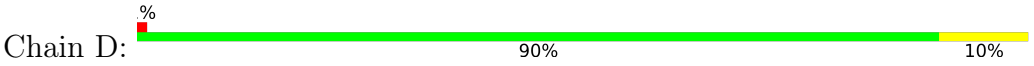


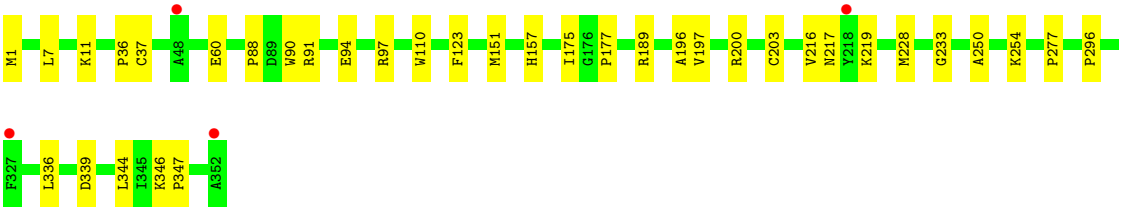




• Molecule 1: Secondary-alcohol dehydrogenase

Chain D:




M1
L7
K11
P36
C37
A48
E60
P88
D89
W90
R91
E94
R97
W110
F123
M151
H157
I175
G176
P177
R189
A196
V197
R200
C203
V216
N217
Y218
K219
M228
G233
A250
K254
P277
P296

F327
L336
D339
L344
I345
K346
P347
A352

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.71Å 125.33Å 137.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.26 – 1.85 67.26 – 1.85	Depositor EDS
% Data completeness (in resolution range)	57.0 (67.26-1.85) 57.2 (67.26-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.178 , 0.227 0.179 , 0.226	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11438	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.95% 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: ZN, NAP, DMS

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	0.17	0/2700	0.35	0/3653
1	B	0.18	0/2708	0.35	0/3663
1	C	0.22	0/2740	0.42	0/3707
1	D	0.22	0/2715	0.42	0/3674
All	All	0.20	0/10863	0.39	0/14697

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	2642	0	2689	26	0
1	B	2647	0	2698	18	0
1	C	2670	0	2736	25	0
1	D	2651	0	2709	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	24	1	0
3	C	48	0	24	3	0
3	D	48	0	24	1	0
4	A	36	0	54	4	0
4	B	32	0	48	0	0
4	C	36	0	54	1	0
4	D	36	0	54	2	0
5	A	62	0	0	0	0
5	B	101	0	0	1	0
5	C	158	0	0	2	1
5	D	171	0	0	1	1
All	All	11438	0	11138	90	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 4.

The worst 5 of 90 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:B:86:ILE:HB	1:B:297:GLY:HA3	1.79	0.63
1:A:325:ARG:O	1:A:329:ASN:ND2	2.33	0.61
1:A:254:LYS:HG2	1:A:280:GLU:HG2	1.84	0.59
1:A:86:ILE:HB	1:A:297:GLY:HA3	1.84	0.58
1:A:17:LYS:NZ	1:A:117:ASP:OD1	2.38	0.56

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)
5:C:648:HOH:O	5:D:950:HOH:O[1_455]	2.19	0.01

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	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
1	B	351/352 (100%)	336 (96%)	15 (4%)	0	100	100
1	C	355/352 (101%)	342 (96%)	13 (4%)	0	100	100
1	D	352/352 (100%)	334 (95%)	18 (5%)	0	100	100
All	All	1408/1408 (100%)	1349 (96%)	59 (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	273/273 (100%)	273 (100%)	0	100	100
1	B	274/273 (100%)	274 (100%)	0	100	100
1	C	278/273 (102%)	277 (100%)	1 (0%)	84	82
1	D	275/273 (101%)	272 (99%)	3 (1%)	65	57
All	All	1100/1092 (101%)	1096 (100%)	4 (0%)	86	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	281	TRP
1	D	336[A]	LEU
1	D	336[B]	LEU
1	D	339	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	114	ASN
1	D	329	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 4 are monoatomic - leaving 39 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	A	409	-	3,3,3	0.68	0	3,3,3	0.70	0
3	NAP	D	803	-	50,52,52	4.18	20 (40%)	71,80,80	1.93	18 (25%)
4	DMS	D	809	-	3,3,3	0.69	0	3,3,3	0.70	0
4	DMS	A	410	-	3,3,3	0.67	0	3,3,3	0.64	0
4	DMS	A	408	-	3,3,3	0.64	0	3,3,3	0.66	0
4	DMS	C	409	-	3,3,3	0.71	0	3,3,3	0.85	0
4	DMS	B	404	2	3,3,3	0.67	0	3,3,3	0.68	0
4	DMS	D	804	-	3,3,3	0.66	0	3,3,3	0.53	0
4	DMS	C	411	-	3,3,3	0.69	0	3,3,3	0.67	0
4	DMS	D	806	2	3,3,3	0.64	0	3,3,3	0.73	0
4	DMS	A	407	-	3,3,3	0.70	0	3,3,3	0.80	0
4	DMS	B	405	-	3,3,3	0.66	0	3,3,3	0.75	0
4	DMS	A	406	-	3,3,3	0.68	0	3,3,3	0.53	0
4	DMS	D	808	-	3,3,3	0.67	0	3,3,3	0.54	0
3	NAP	A	402	-	50,52,52	4.18	20 (40%)	71,80,80	1.83	15 (21%)
4	DMS	D	805	-	3,3,3	0.63	0	3,3,3	0.29	0
4	DMS	C	404	-	3,3,3	0.70	0	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	A	404	-	3,3,3	0.67	0	3,3,3	0.56	0
4	DMS	C	410	-	3,3,3	0.69	0	3,3,3	0.64	0
4	DMS	D	807	-	3,3,3	0.69	0	3,3,3	0.87	0
4	DMS	B	407	-	3,3,3	0.69	0	3,3,3	0.69	0
4	DMS	A	405	2	3,3,3	0.66	0	3,3,3	0.72	0
3	NAP	B	402	-	50,52,52	4.20	20 (40%)	71,80,80	1.85	16 (22%)
4	DMS	A	403	-	3,3,3	0.69	0	3,3,3	0.54	0
4	DMS	D	811	-	3,3,3	0.70	0	3,3,3	0.59	0
4	DMS	B	409	-	3,3,3	0.71	0	3,3,3	0.60	0
4	DMS	A	411	-	3,3,3	0.68	0	3,3,3	0.63	0
4	DMS	D	801	-	3,3,3	0.68	0	3,3,3	0.67	0
4	DMS	B	403	-	3,3,3	0.64	0	3,3,3	0.64	0
4	DMS	D	810	-	3,3,3	0.69	0	3,3,3	0.69	0
4	DMS	C	405	-	3,3,3	0.68	0	3,3,3	0.70	0
4	DMS	C	403	2	3,3,3	0.62	0	3,3,3	0.58	0
4	DMS	B	410	-	3,3,3	0.69	0	3,3,3	0.63	0
4	DMS	B	408	-	3,3,3	0.65	0	3,3,3	0.79	0
4	DMS	C	408	-	3,3,3	0.70	0	3,3,3	0.75	0
4	DMS	B	406	-	3,3,3	0.68	0	3,3,3	0.63	0
4	DMS	C	406	-	3,3,3	0.66	0	3,3,3	0.46	0
3	NAP	C	402	-	50,52,52	4.21	20 (40%)	71,80,80	1.86	14 (19%)
4	DMS	C	407	-	3,3,3	0.66	0	3,3,3	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	C	402	-	-	14/35/67/67	0/5/5/5
3	NAP	B	402	-	-	10/35/67/67	0/5/5/5
3	NAP	A	402	-	-	4/35/67/67	0/5/5/5
3	NAP	D	803	-	-	15/35/67/67	0/5/5/5

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAP	O4D-C1D	16.47	1.62	1.40
3	A	402	NAP	O4D-C1D	16.12	1.62	1.40
3	C	402	NAP	O4D-C1D	15.78	1.61	1.40
3	D	803	NAP	O4D-C1D	15.67	1.61	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	803	NAP	C7N-N7N	9.90	1.51	1.33

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	NAP	N3A-C2A-N1A	-5.87	119.69	128.58
3	A	402	NAP	N3A-C2A-N1A	-5.86	119.71	128.58
3	D	803	NAP	N3A-C2A-N1A	-5.84	119.75	128.58
3	B	402	NAP	N3A-C2A-N1A	-5.60	120.11	128.58
3	D	803	NAP	N6A-C6A-N1A	-5.24	106.71	118.38

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAP	O4D-C1D-N1N-C2N
3	A	402	NAP	O4D-C1D-N1N-C6N
3	A	402	NAP	C2D-C1D-N1N-C2N
3	A	402	NAP	C2D-C1D-N1N-C6N
3	B	402	NAP	O4D-C1D-N1N-C2N

There are no ring outliers.

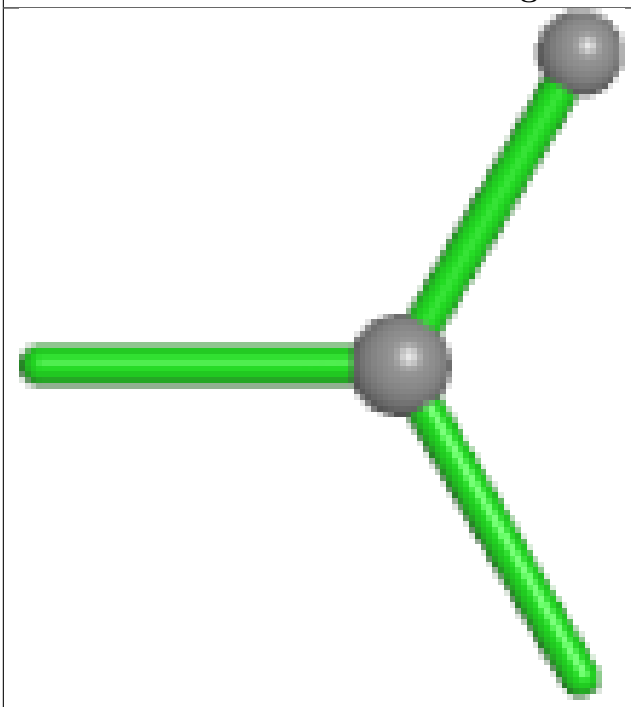
10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	803	NAP	1	0
4	A	410	DMS	1	0
4	A	408	DMS	1	0
4	C	409	DMS	1	0
4	D	806	DMS	1	0
3	A	402	NAP	2	0
4	D	805	DMS	1	0
4	A	405	DMS	2	0
3	B	402	NAP	1	0
3	C	402	NAP	3	0

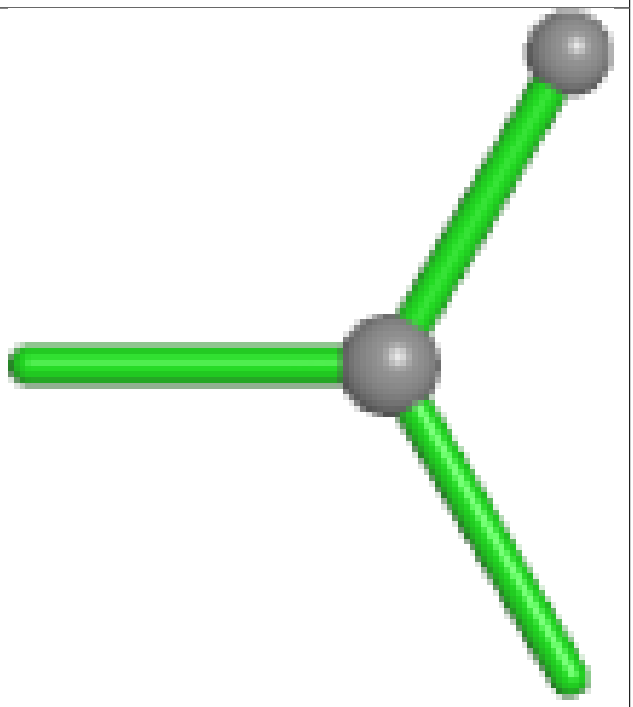
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

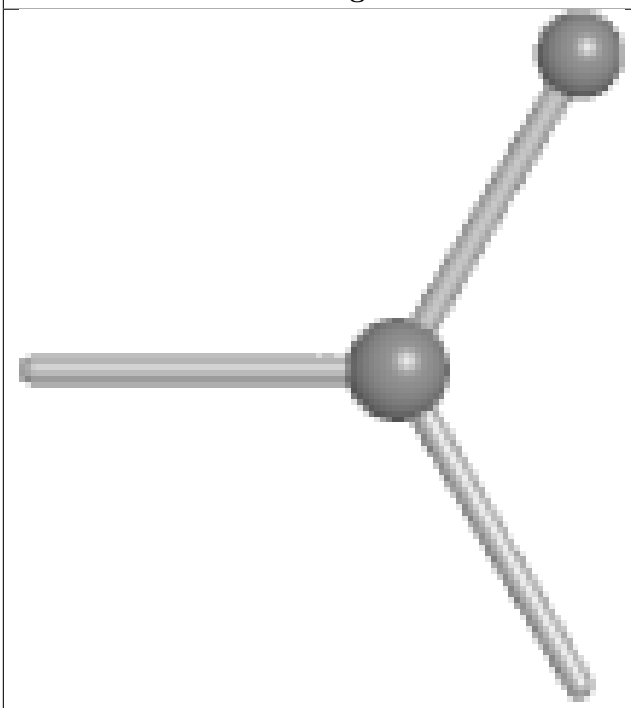
Ligand DMS A 409



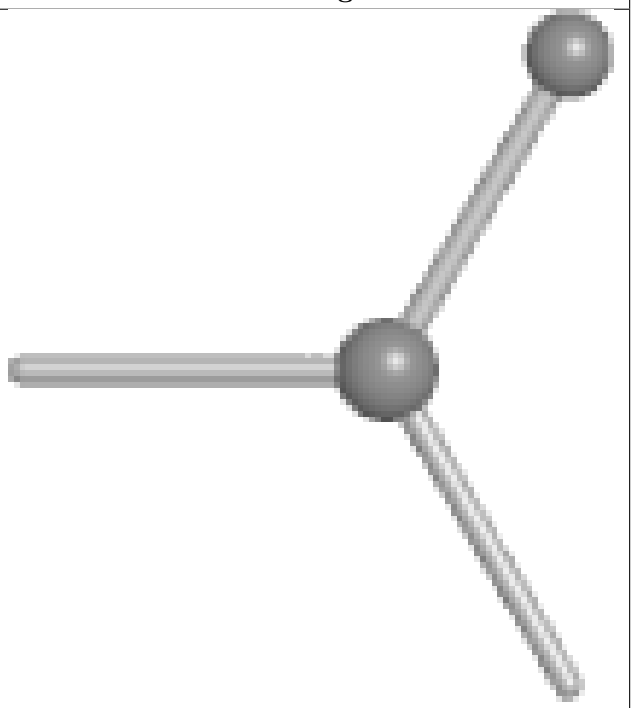
Bond lengths



Bond angles

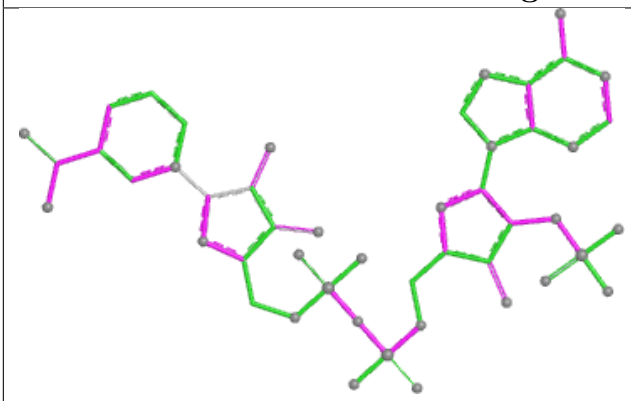


Torsions

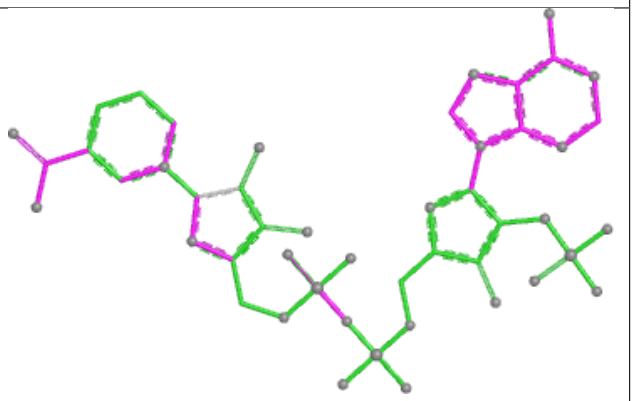


Rings

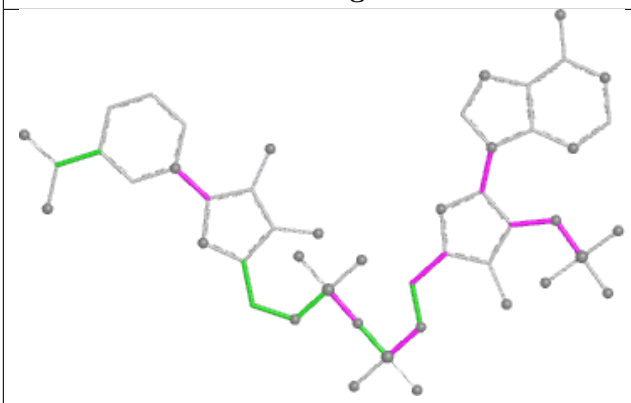
Ligand NAP D 803



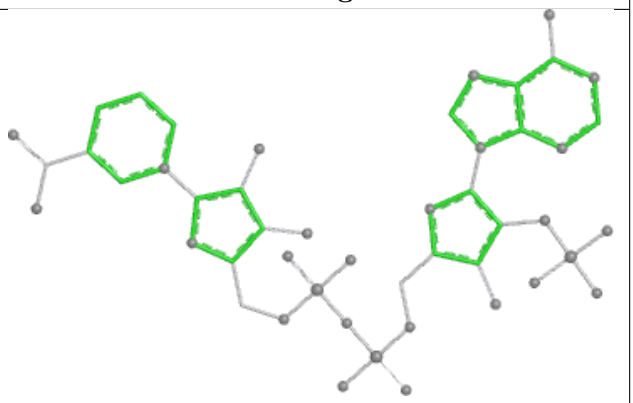
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Bond angles

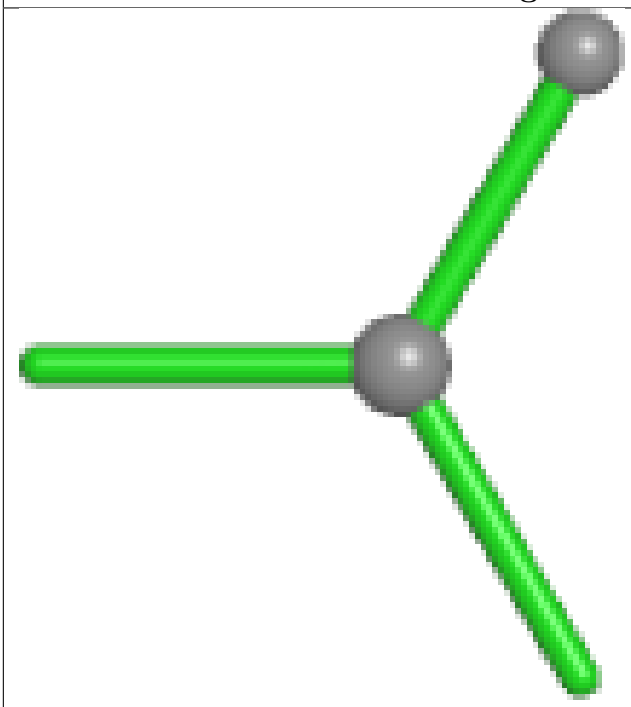


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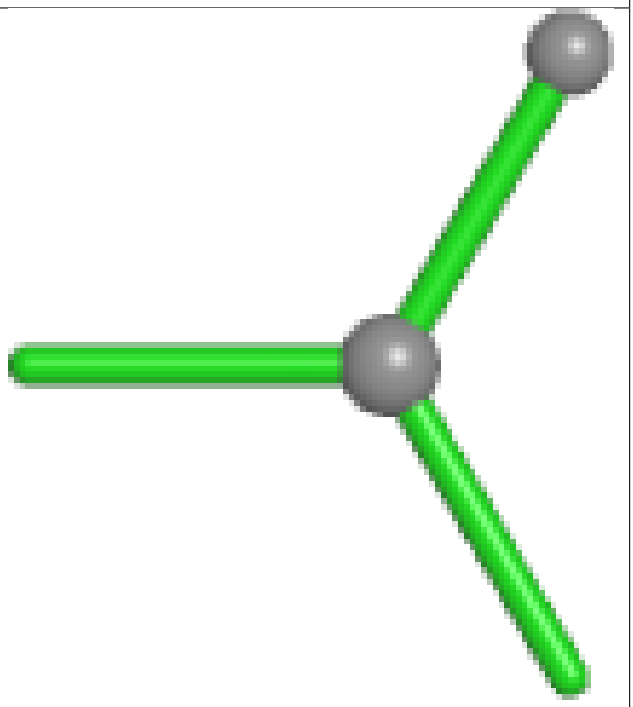


Rings

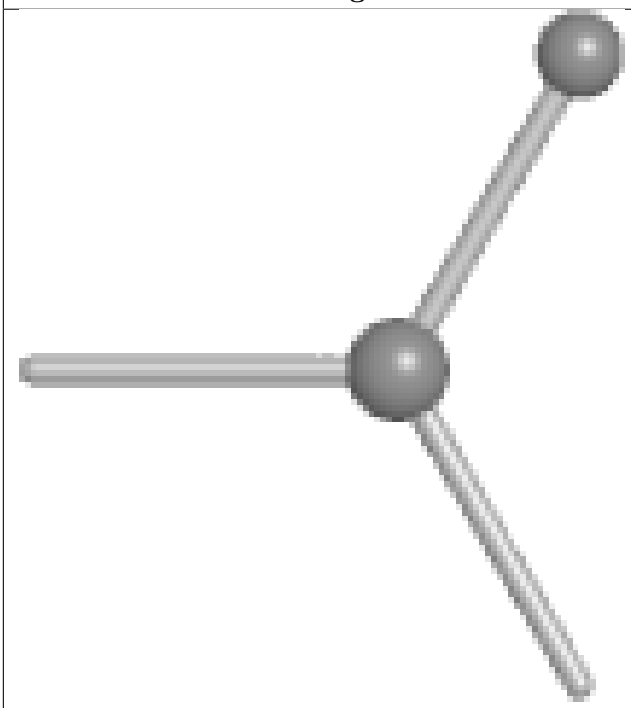
Ligand DMS D 809



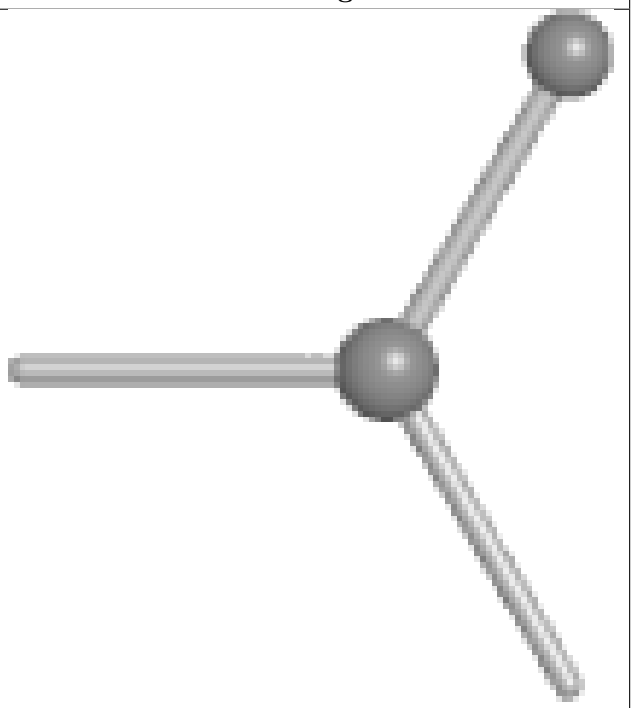
Bond lengths



Bond angles

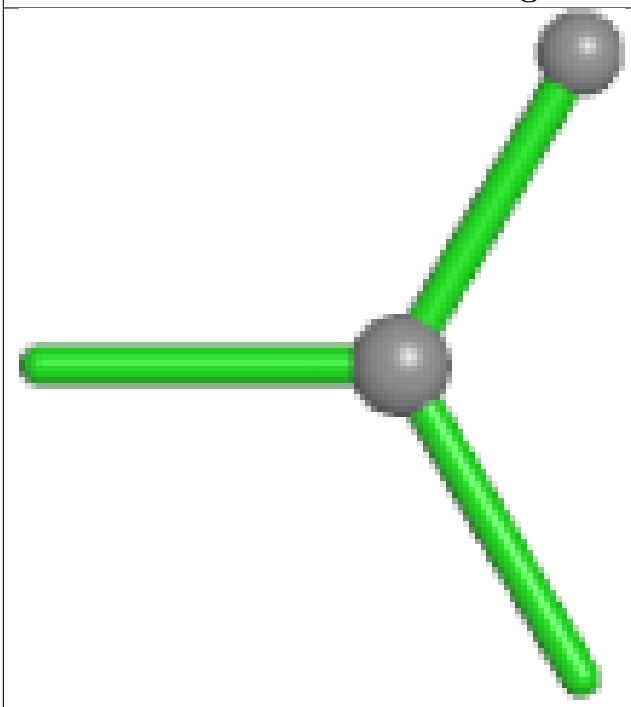


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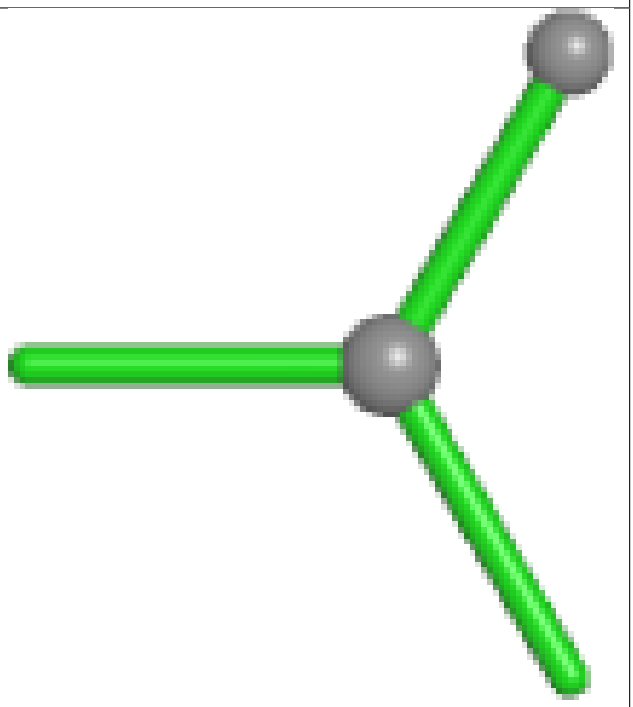


Rings

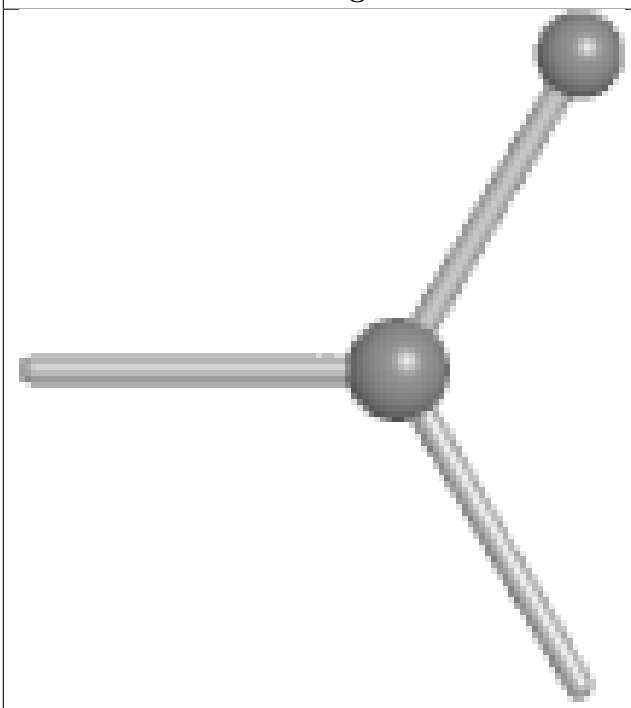
Ligand DMS A 410



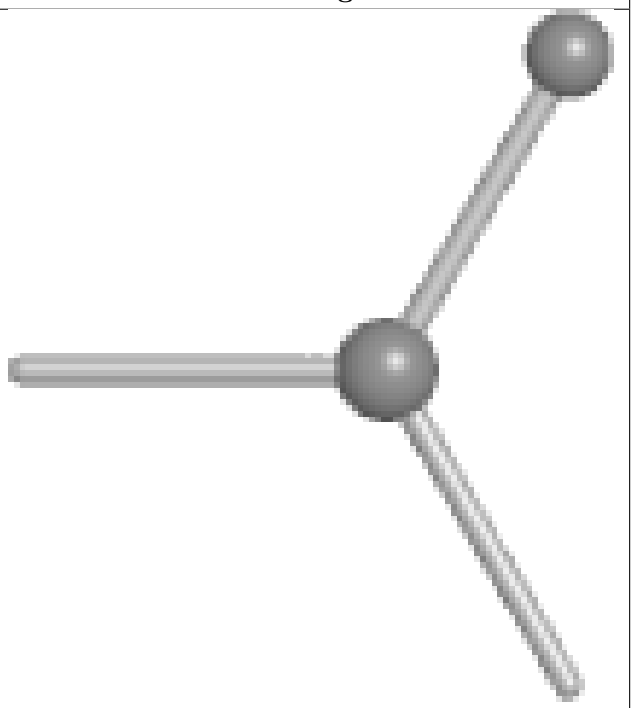
Bond lengths



Bond angles

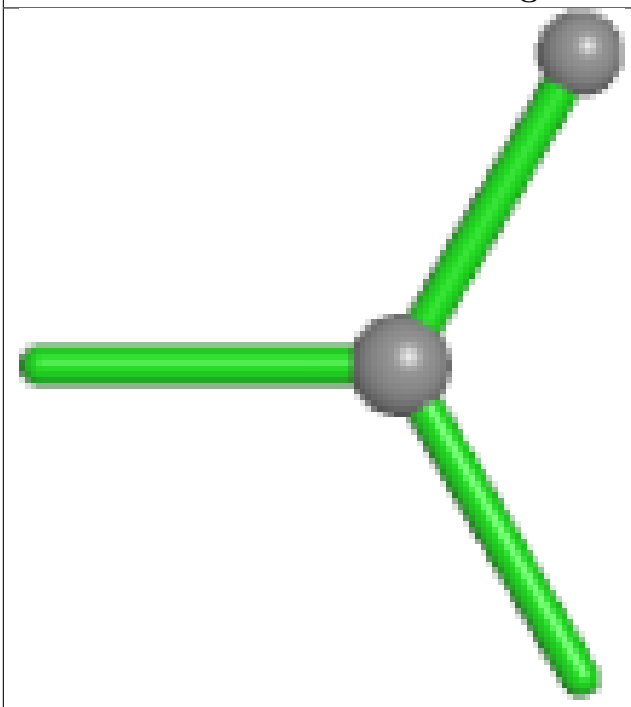


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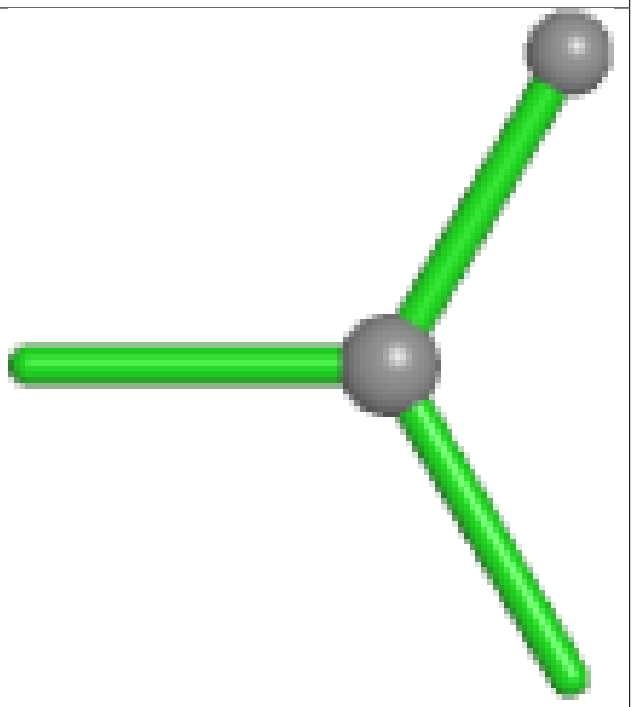


Rings

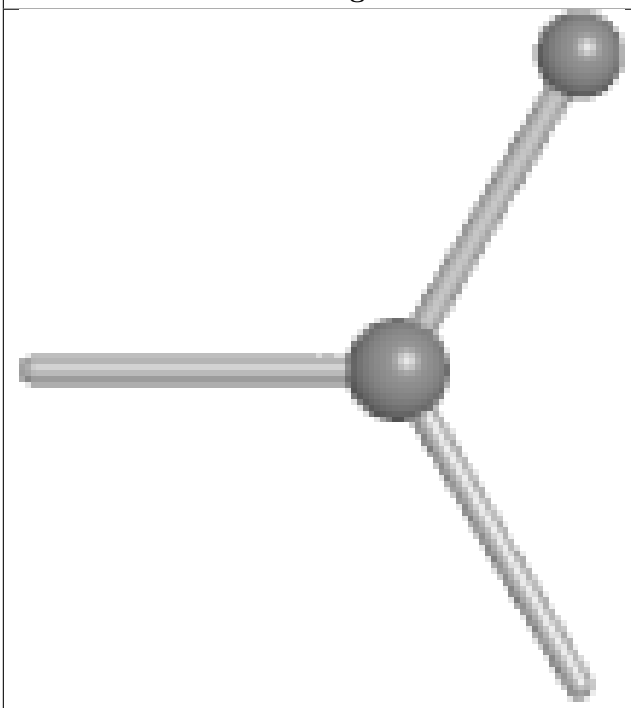
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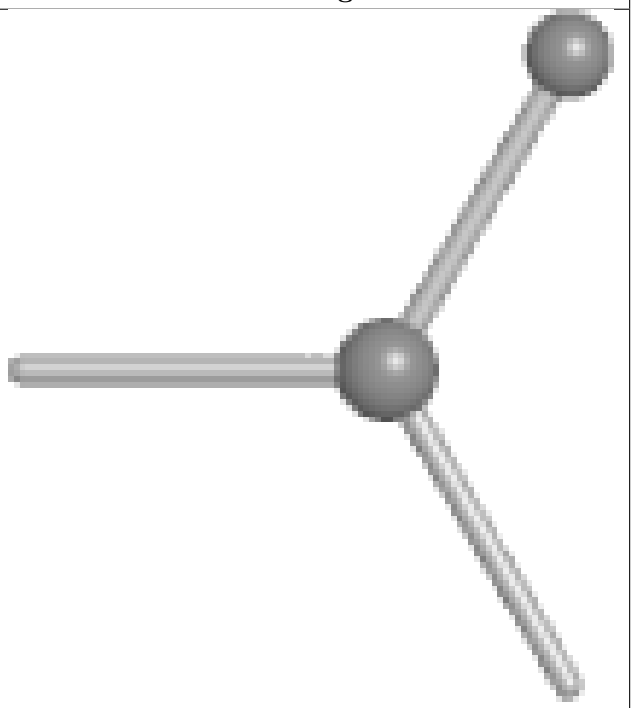
Bond lengths



Bond angles

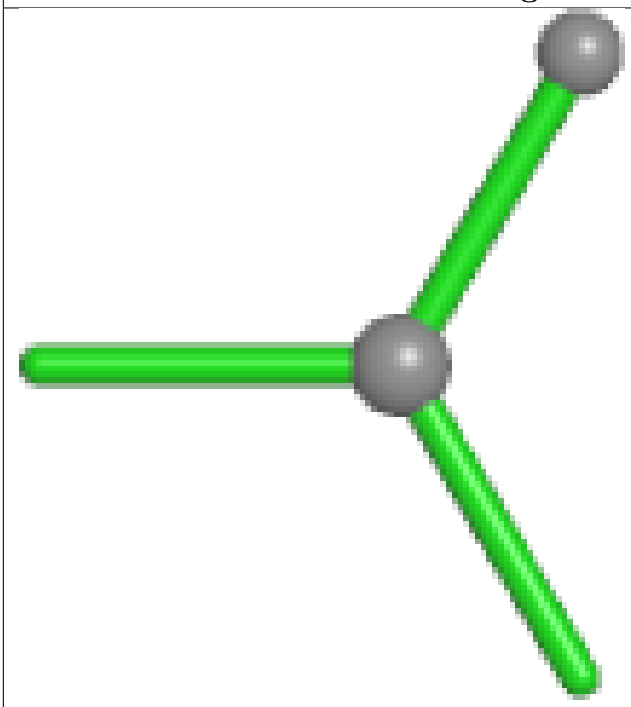


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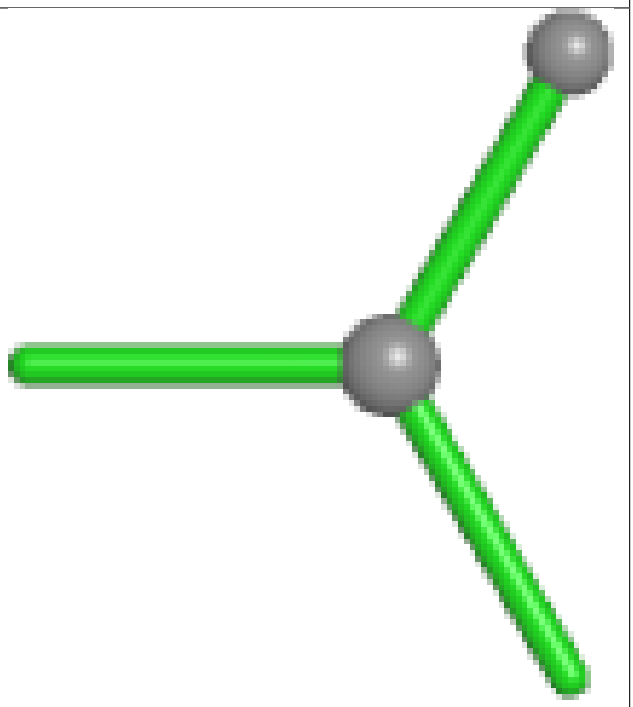


Rings

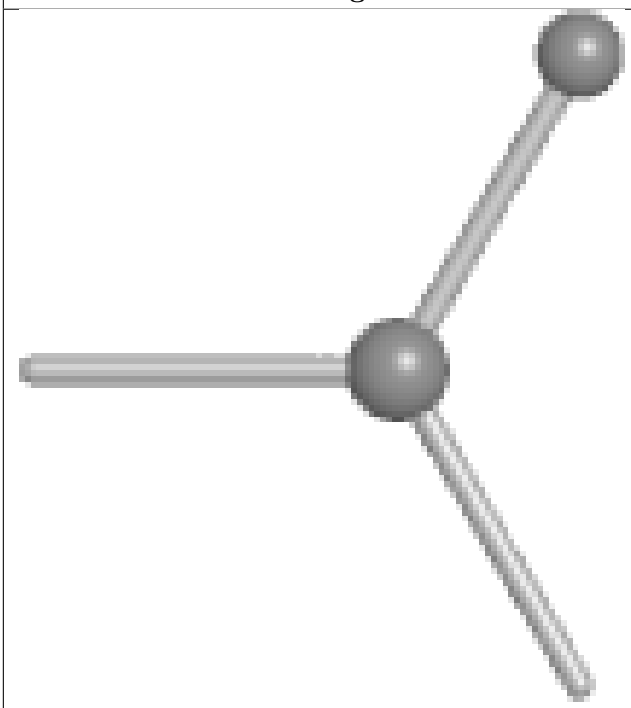
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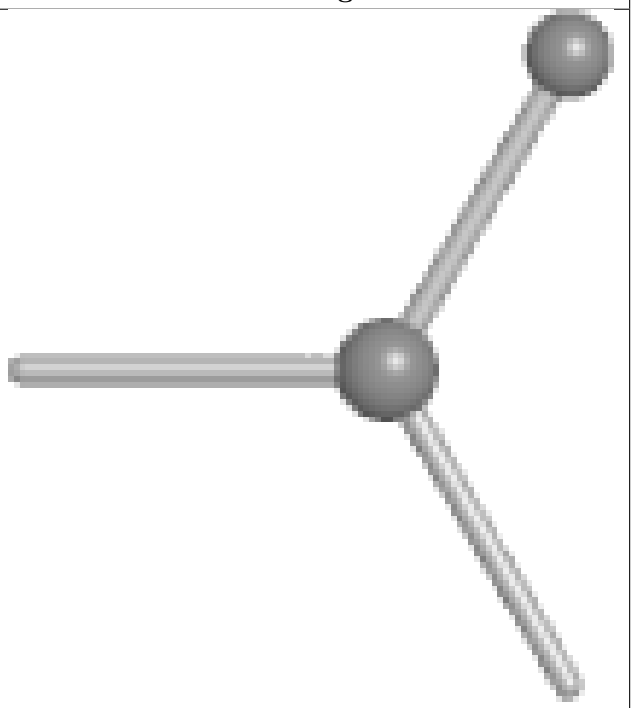
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Bond angles

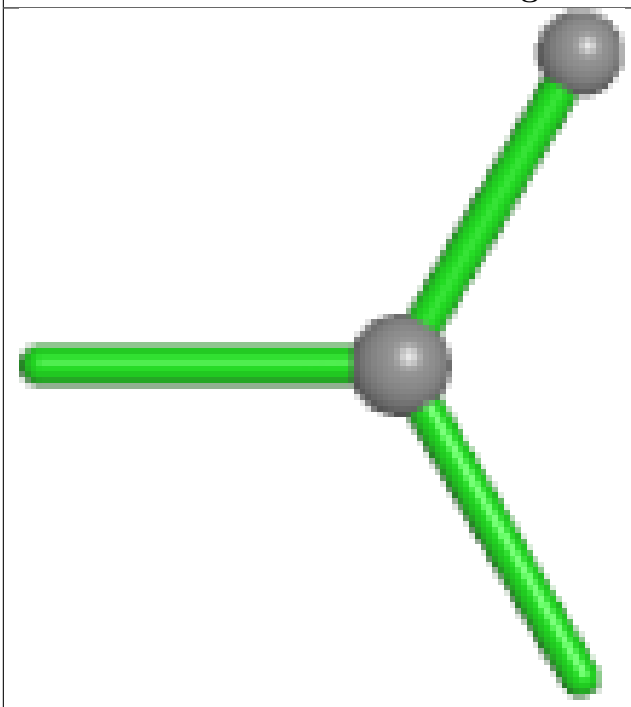


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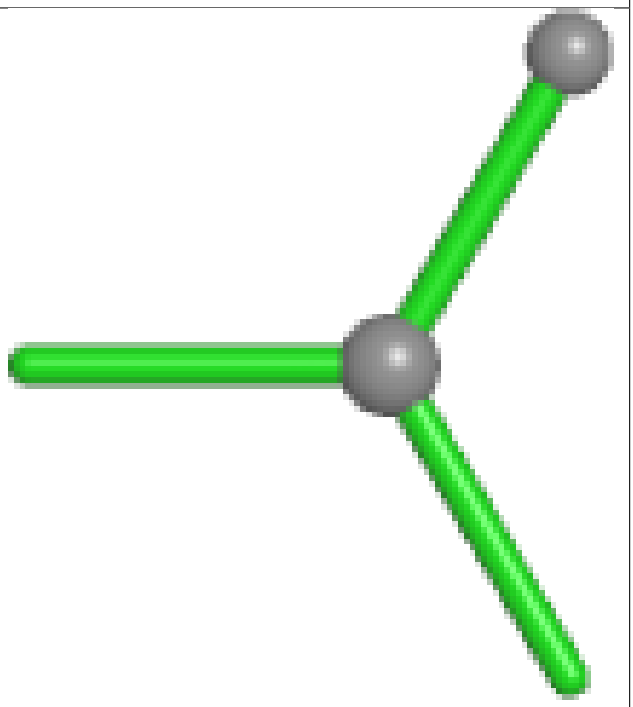


Rings

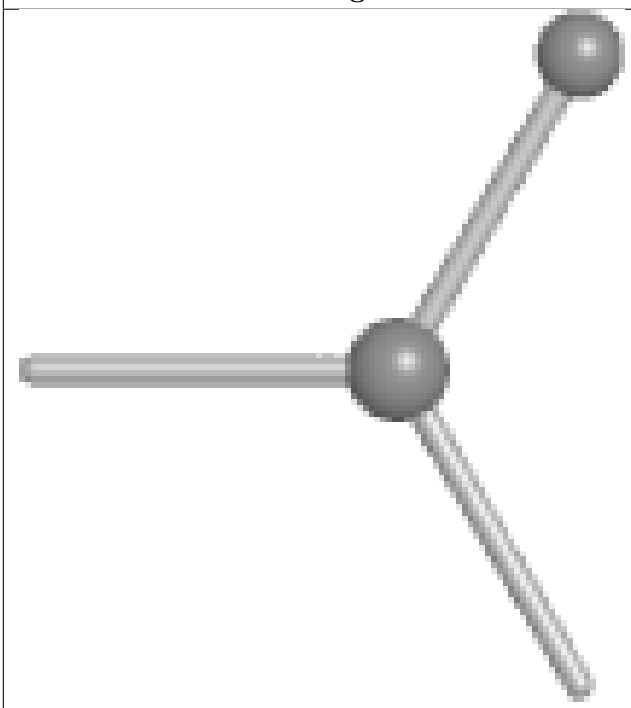
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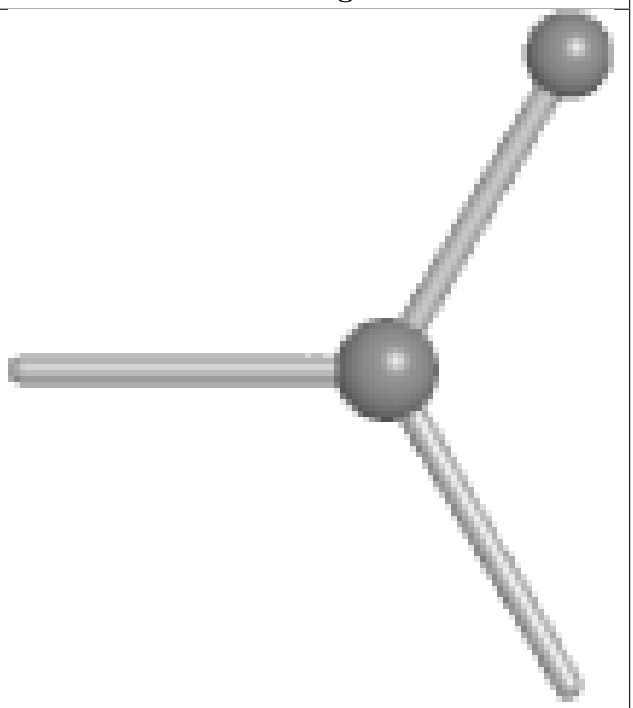
Bond lengths



Bond angles

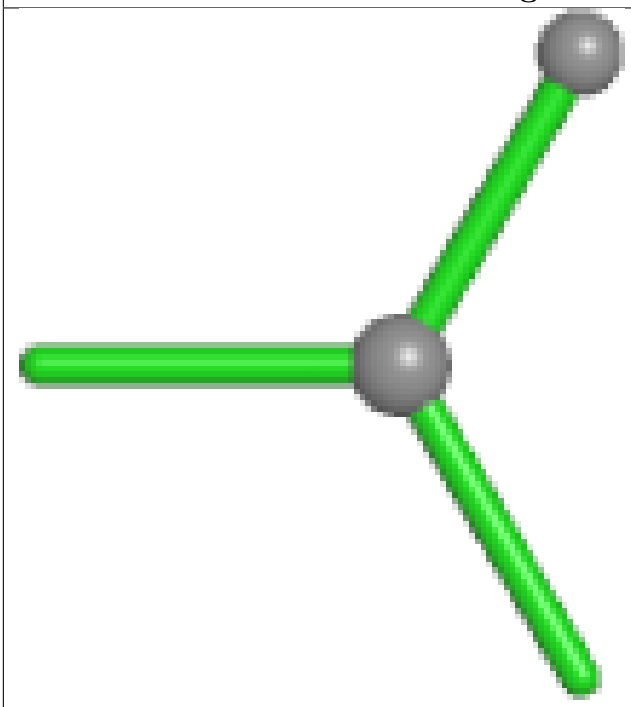


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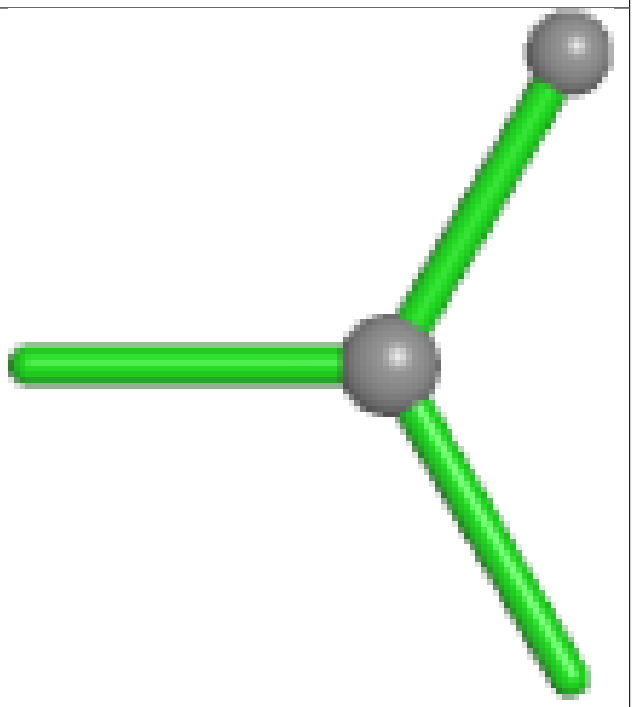


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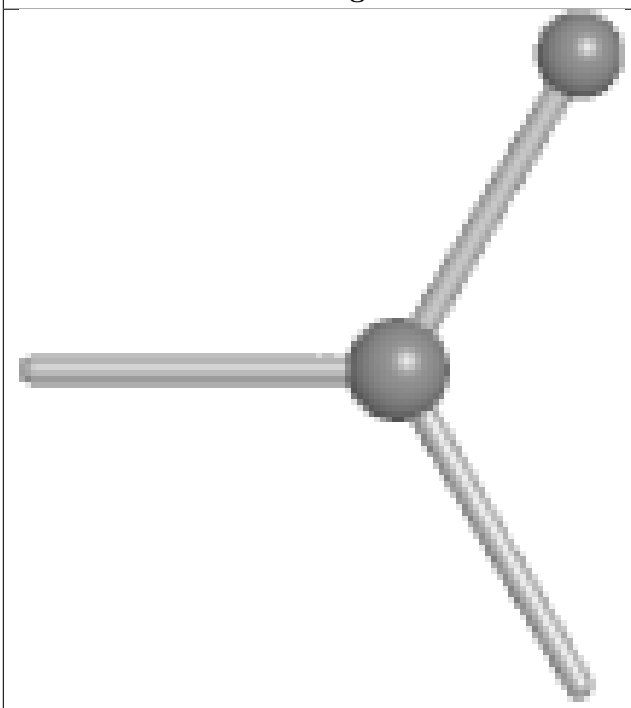
Ligand DMS D 804



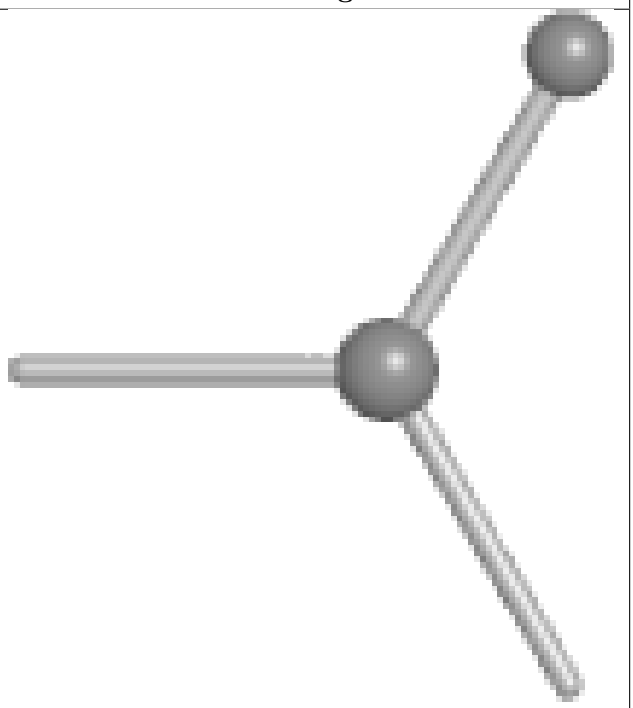
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Bond angles

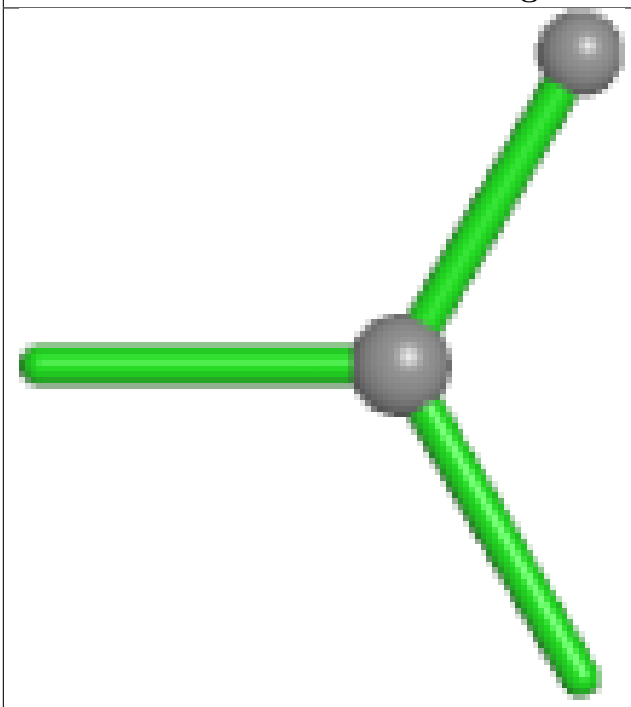


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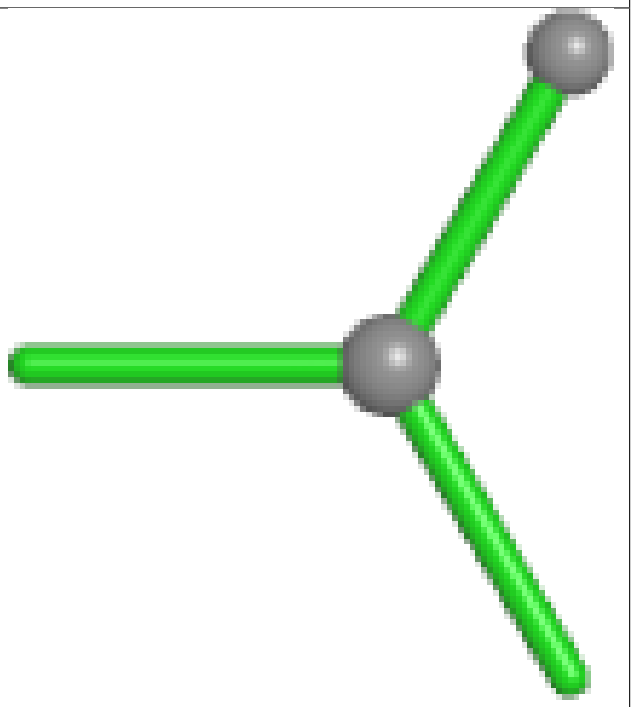


Rings

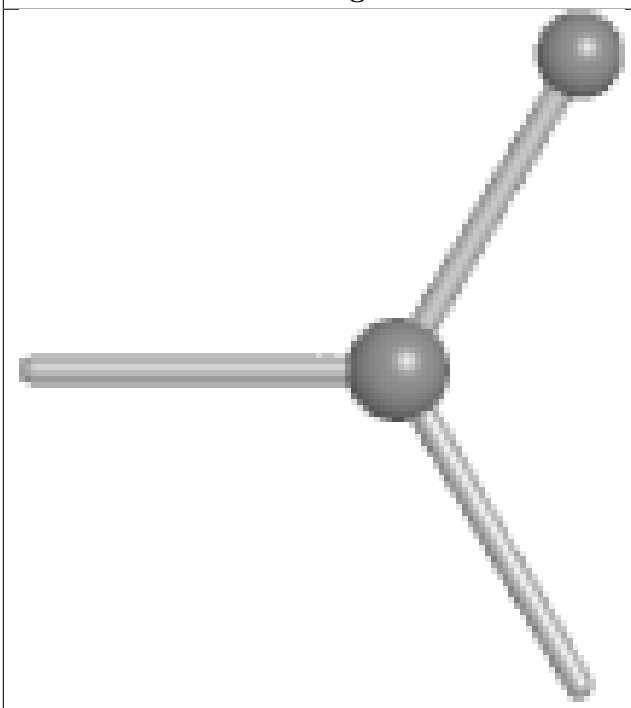
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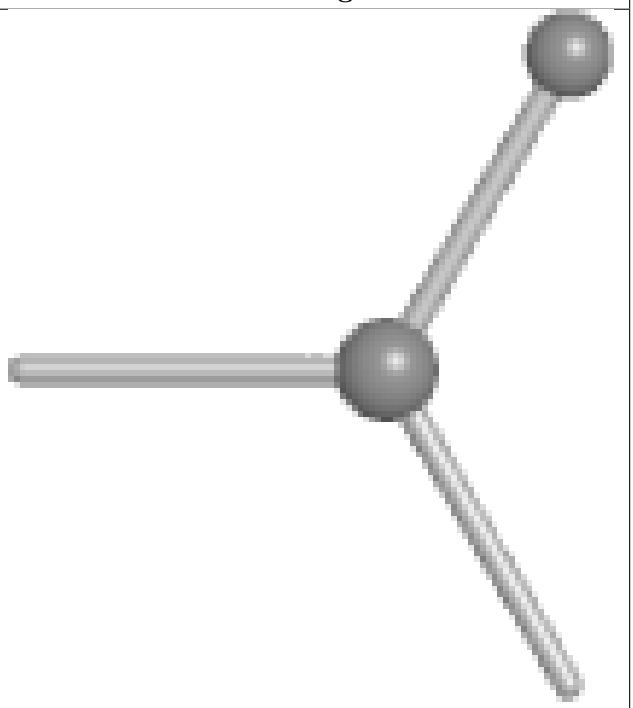
Bond lengths



Bond angles

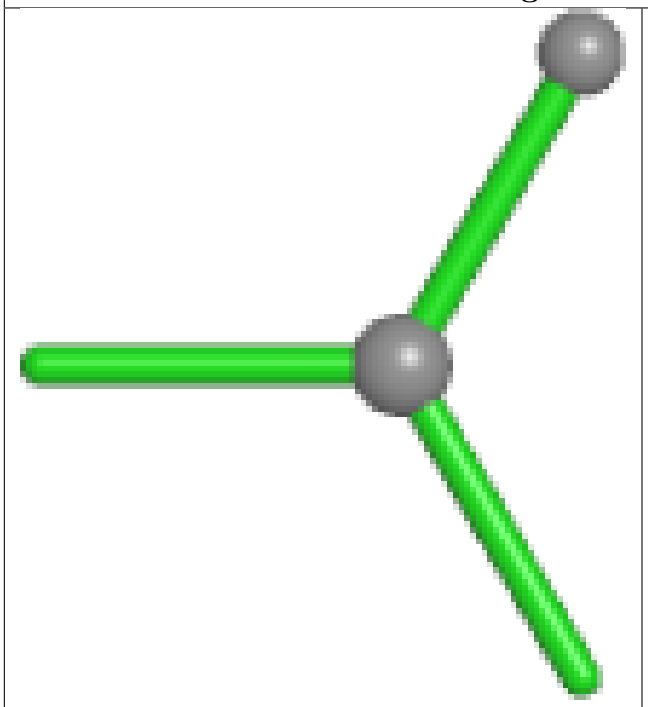


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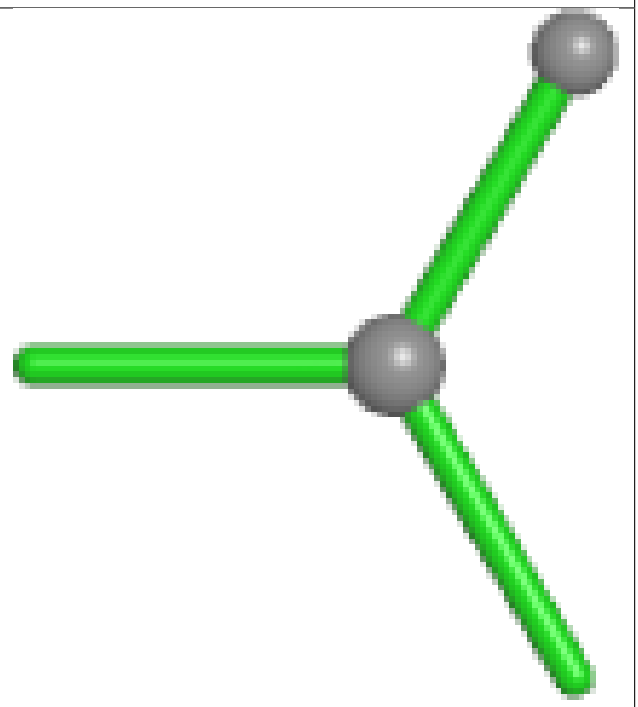


Rings

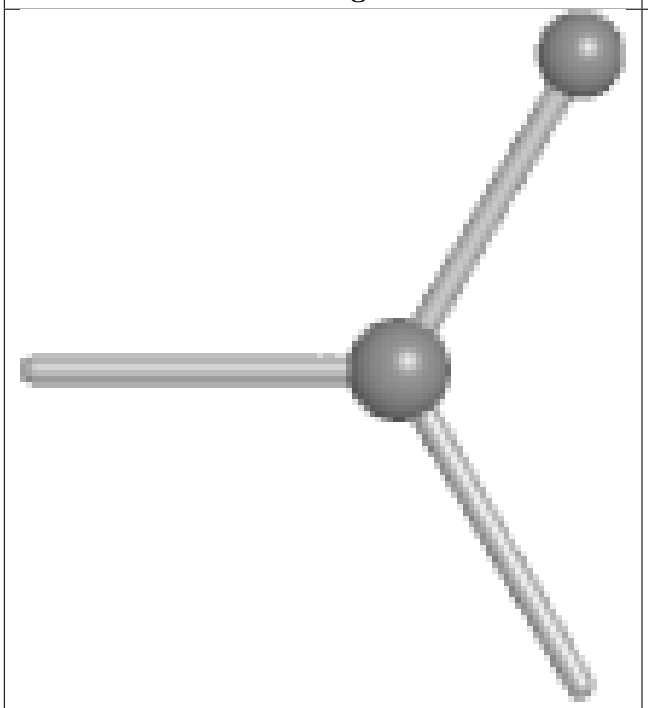
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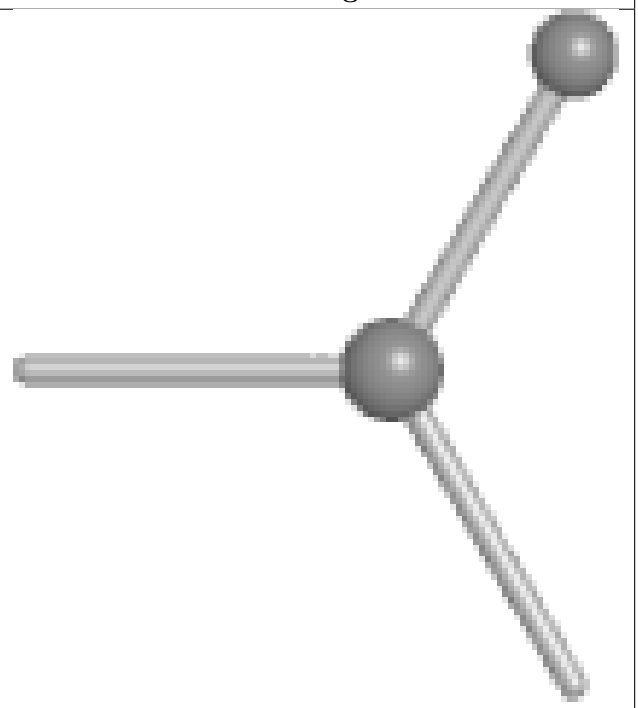
Bond lengths



Bond angles

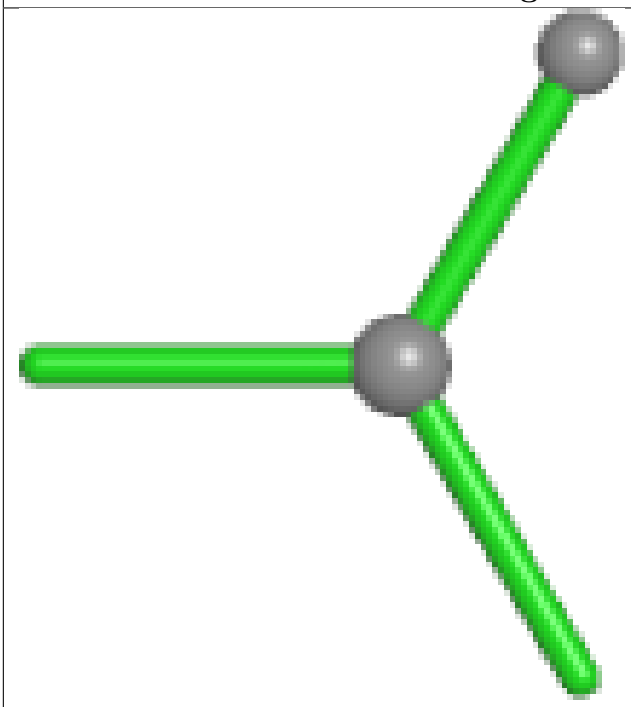


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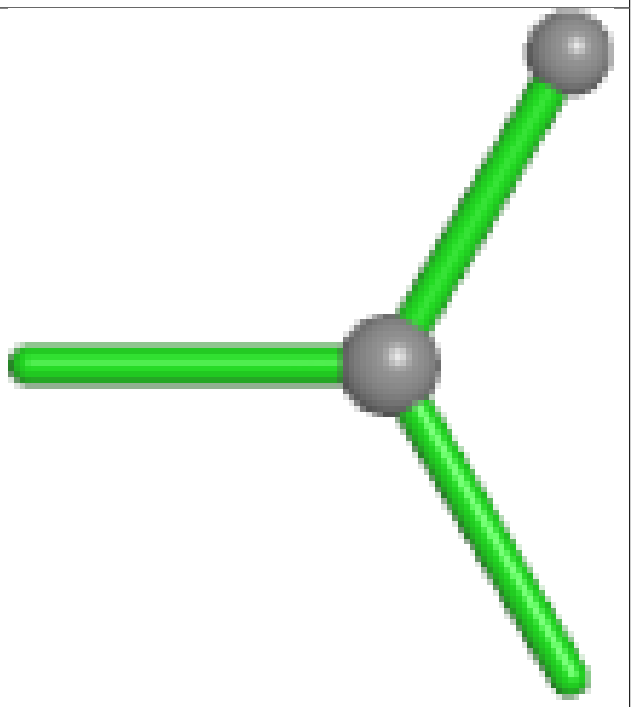


Rings

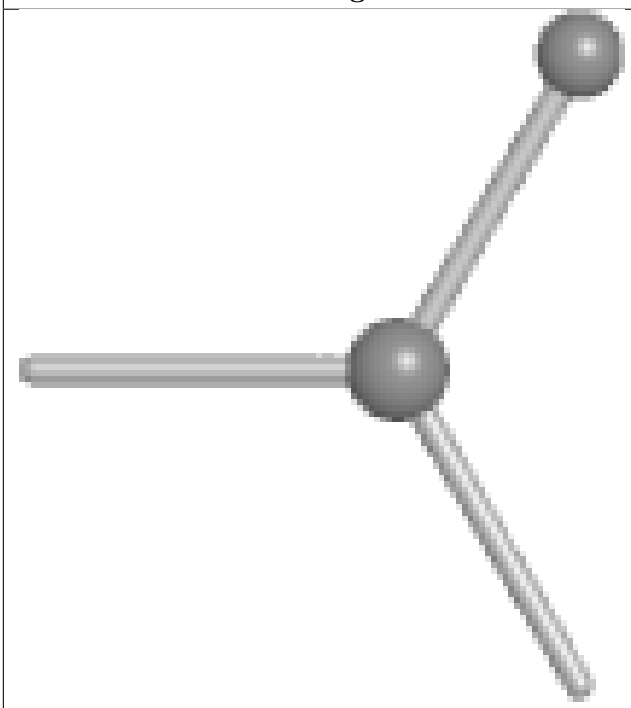
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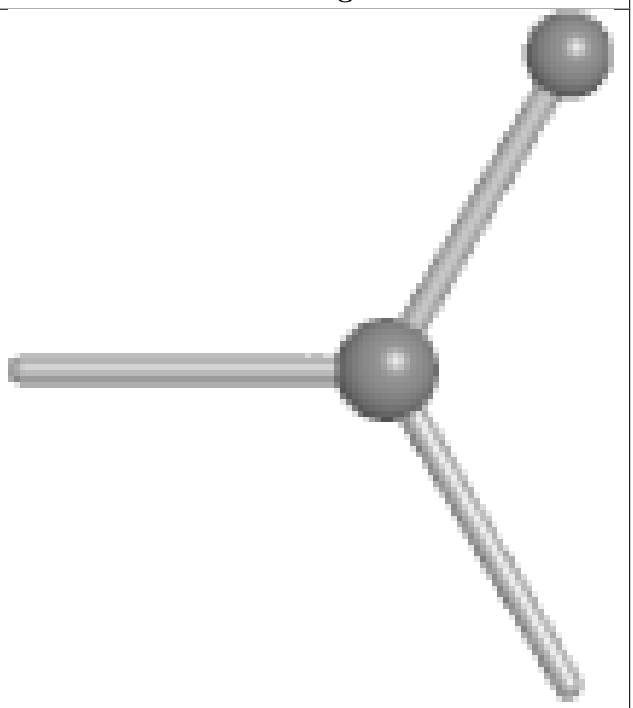
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Bond angles

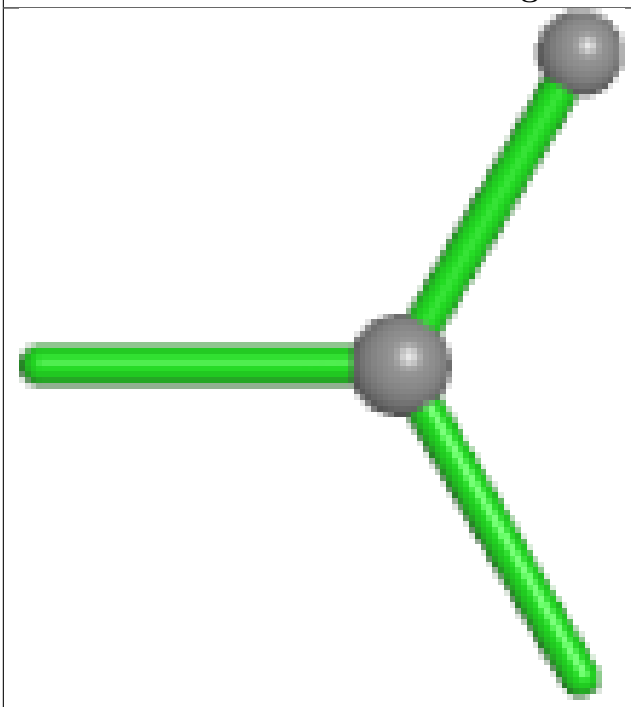


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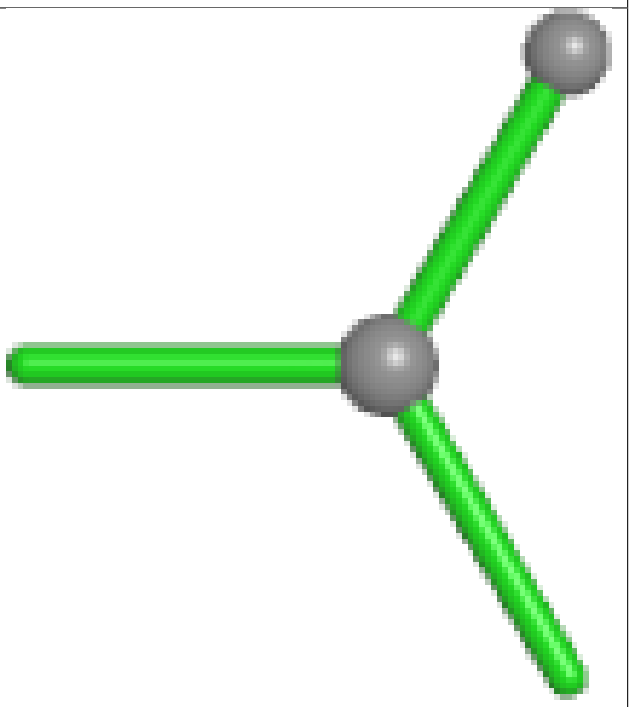


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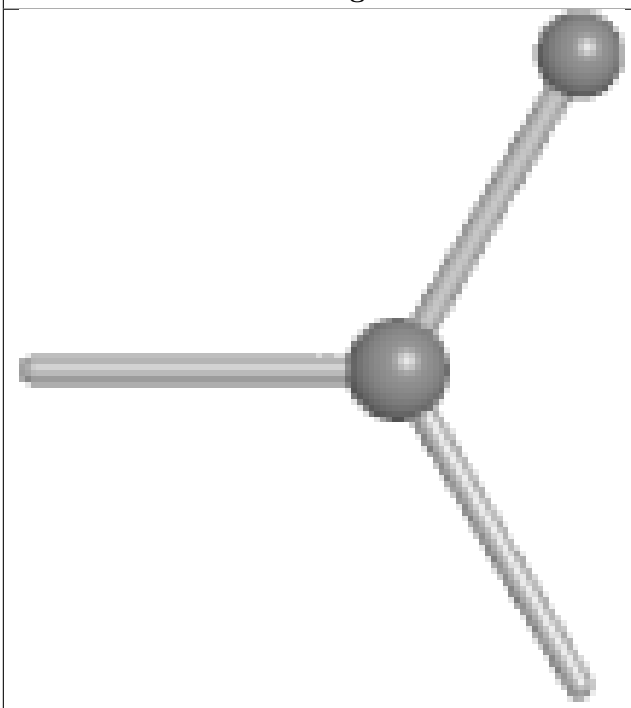
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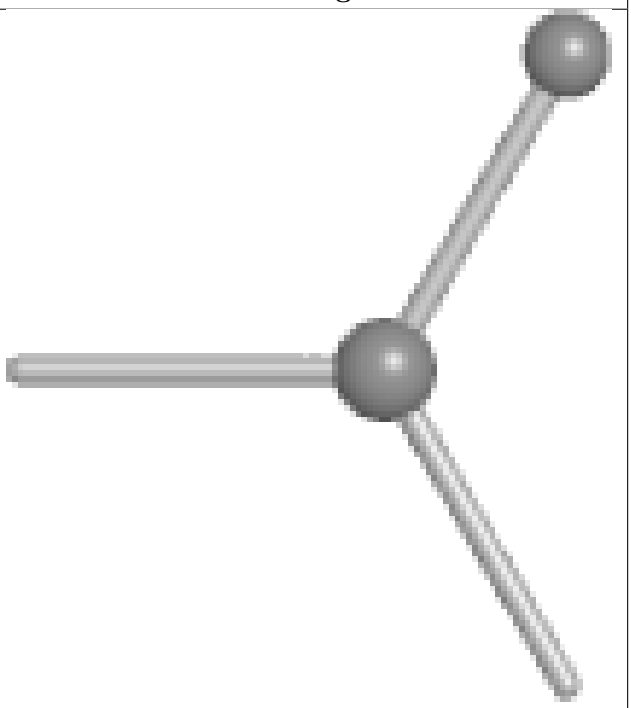
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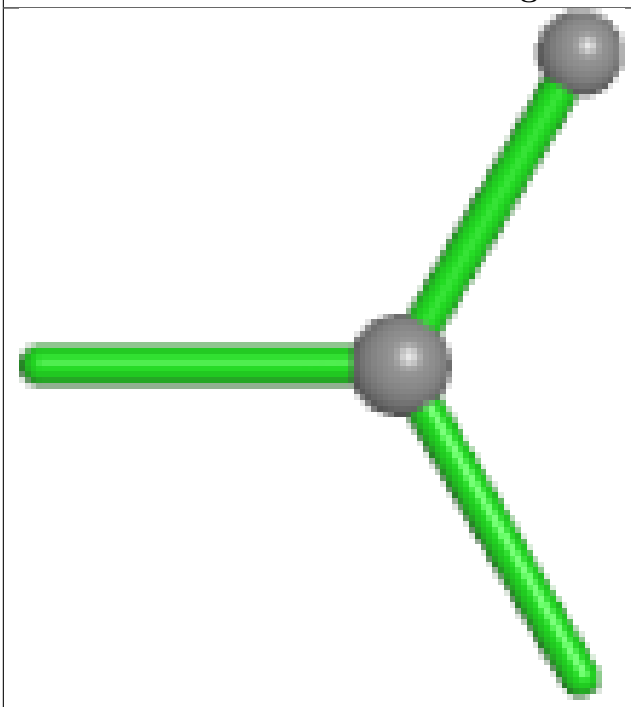


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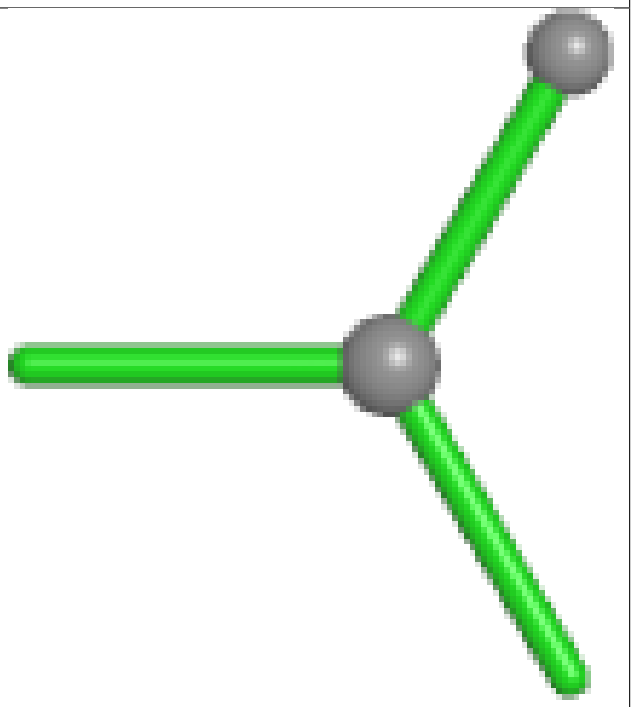


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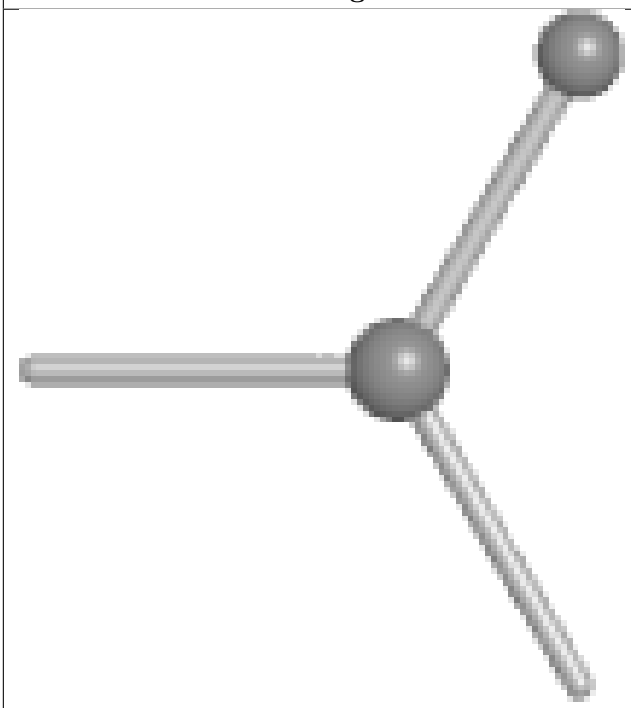
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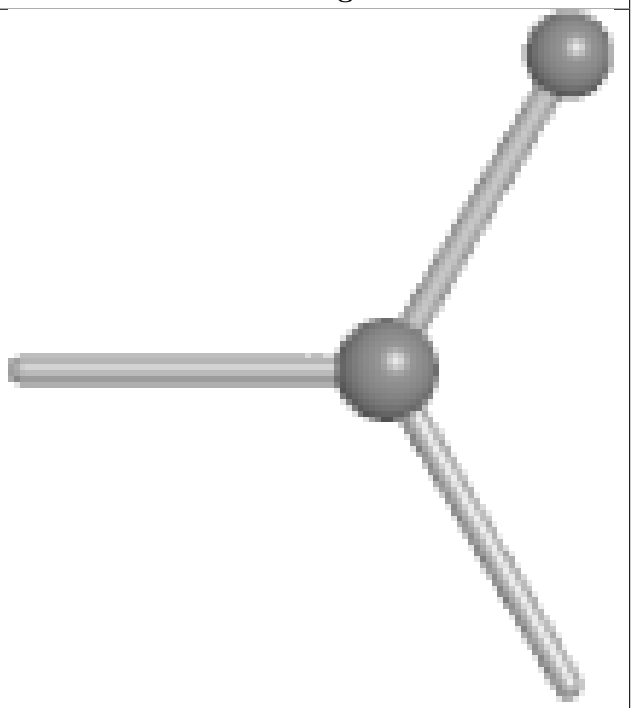
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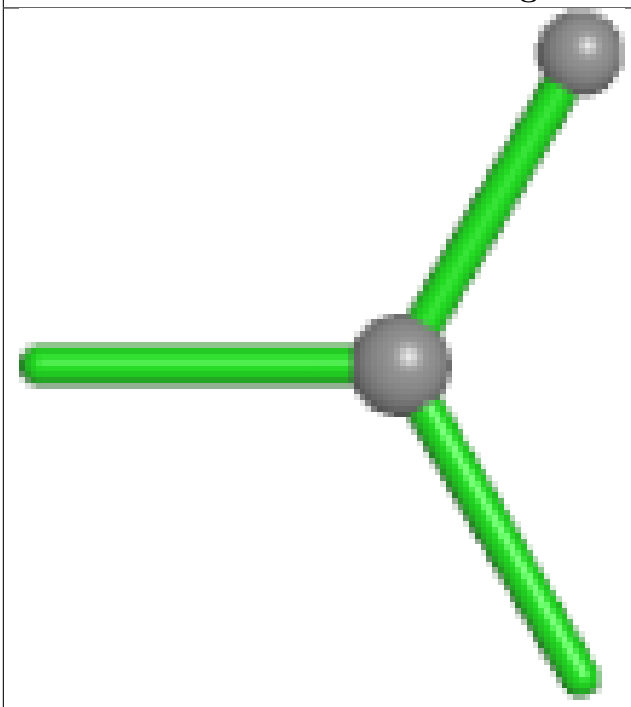


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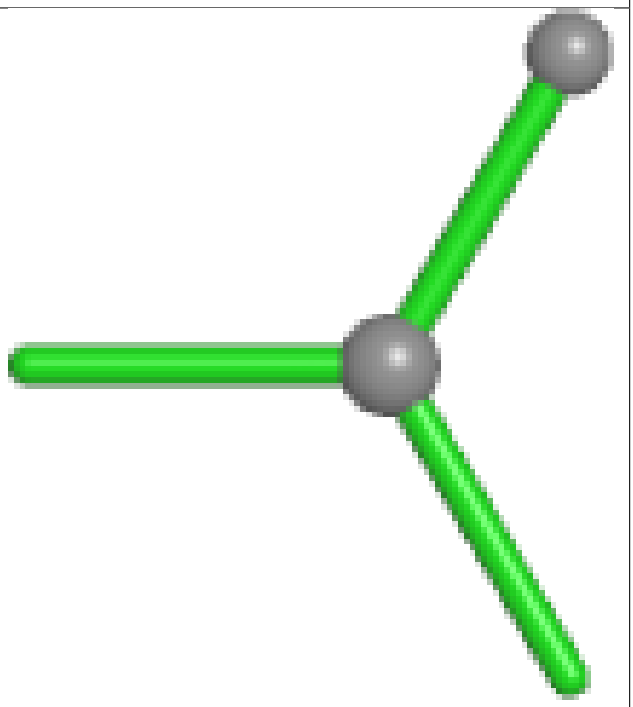


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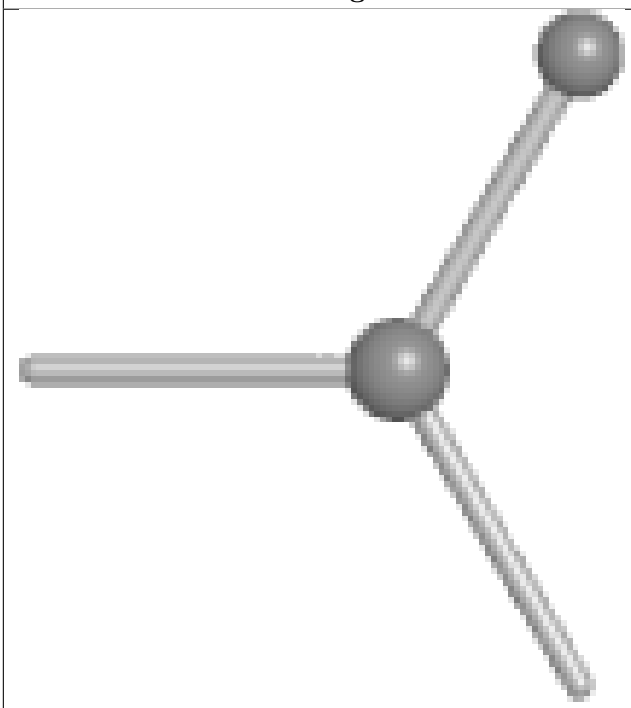
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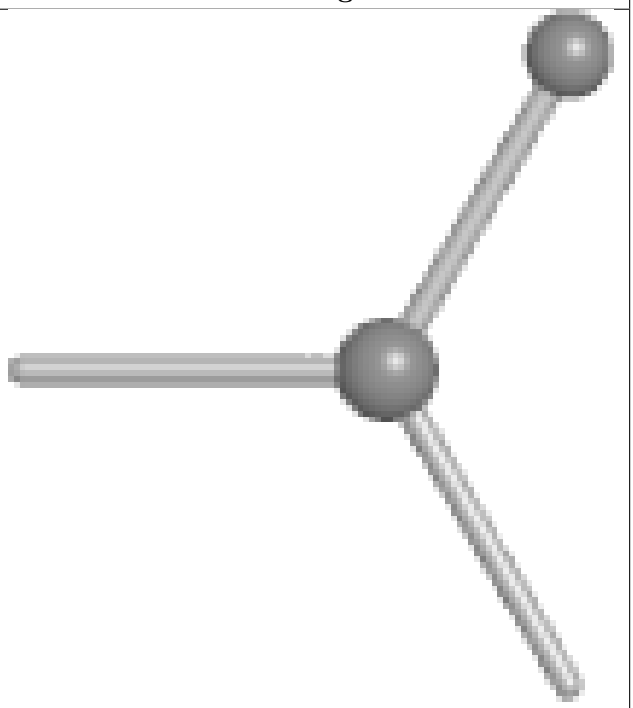
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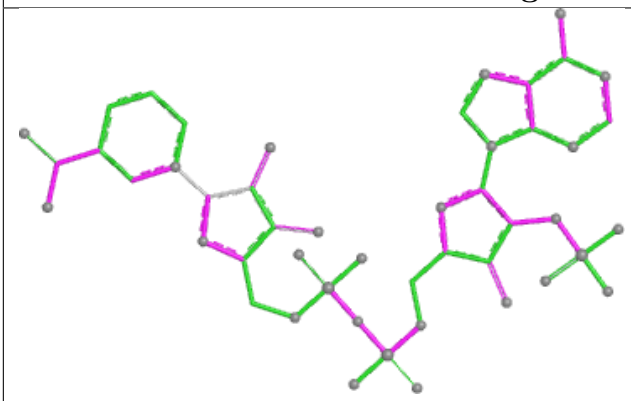


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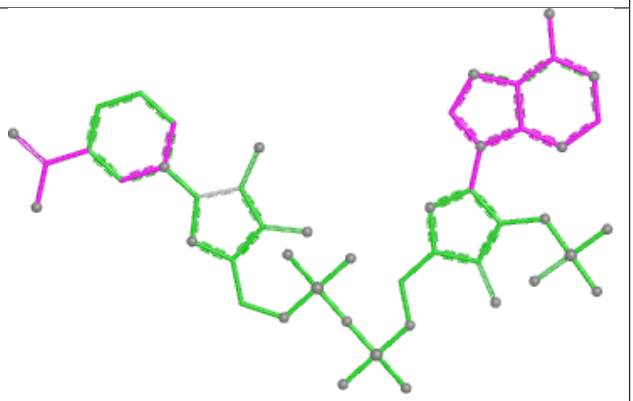


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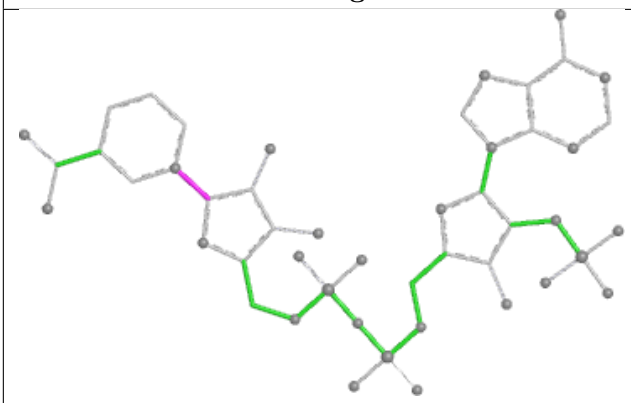
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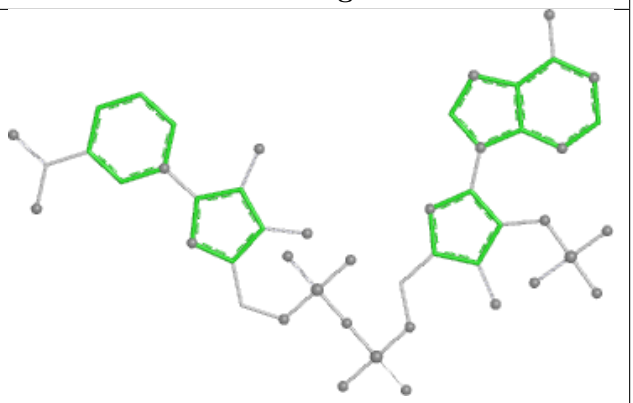
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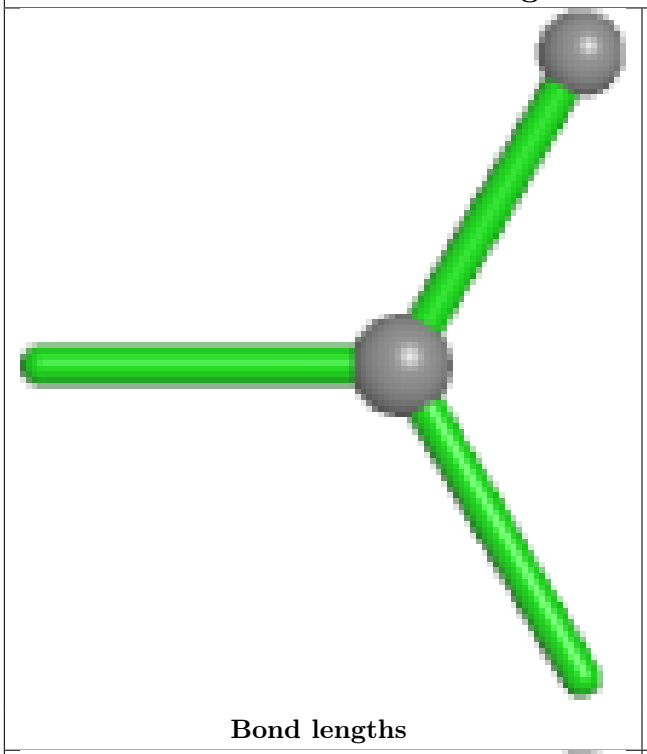


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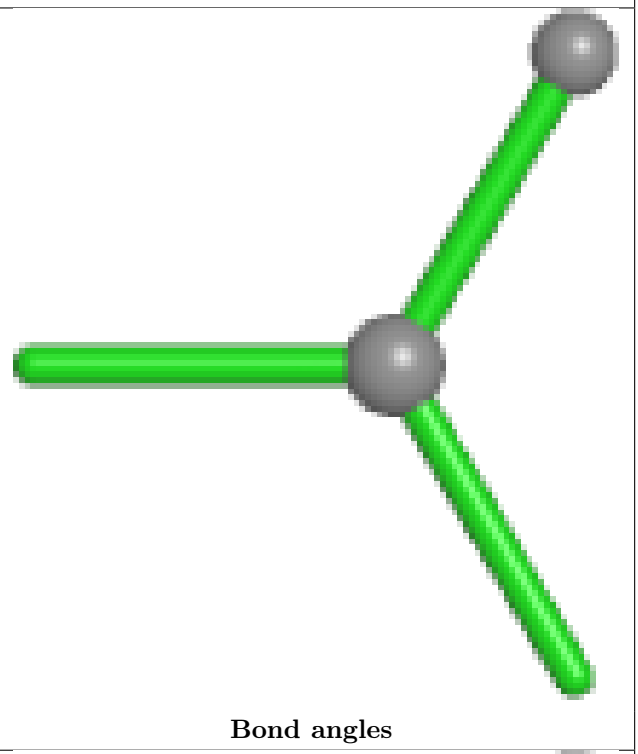


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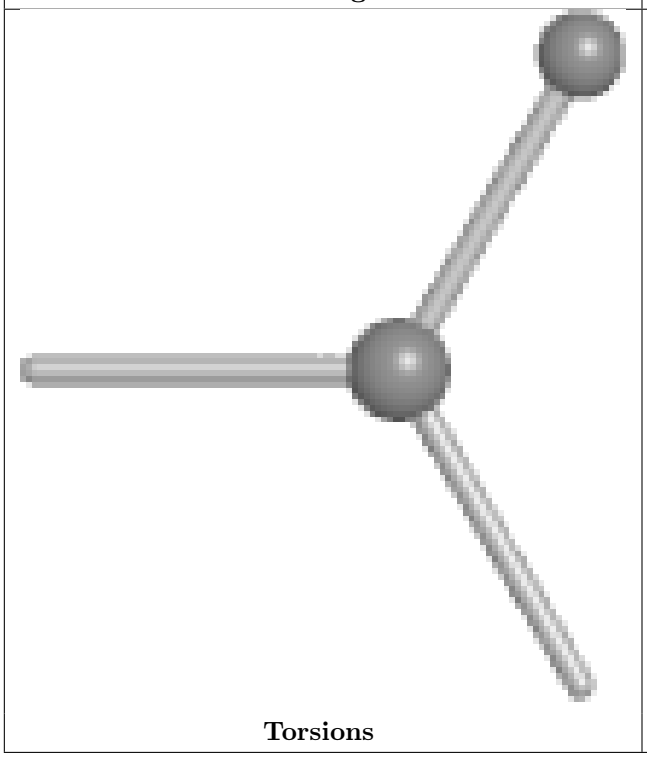
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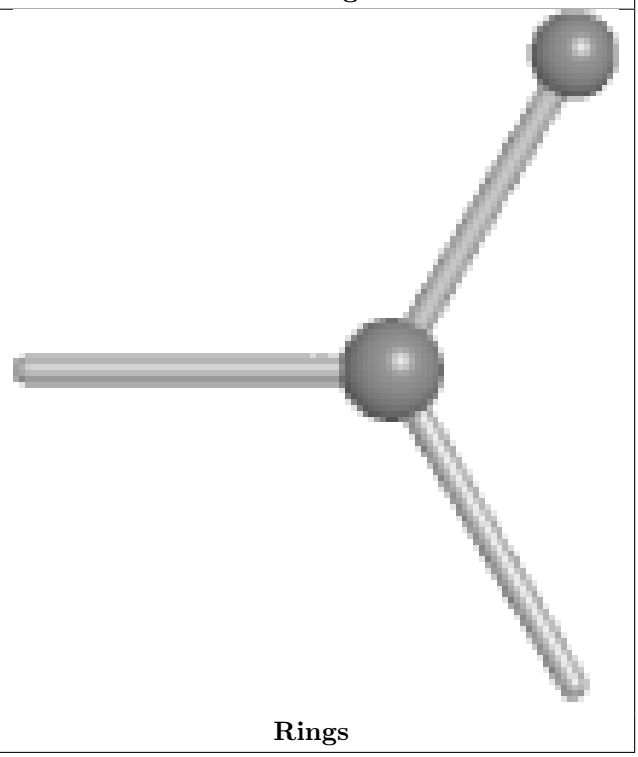
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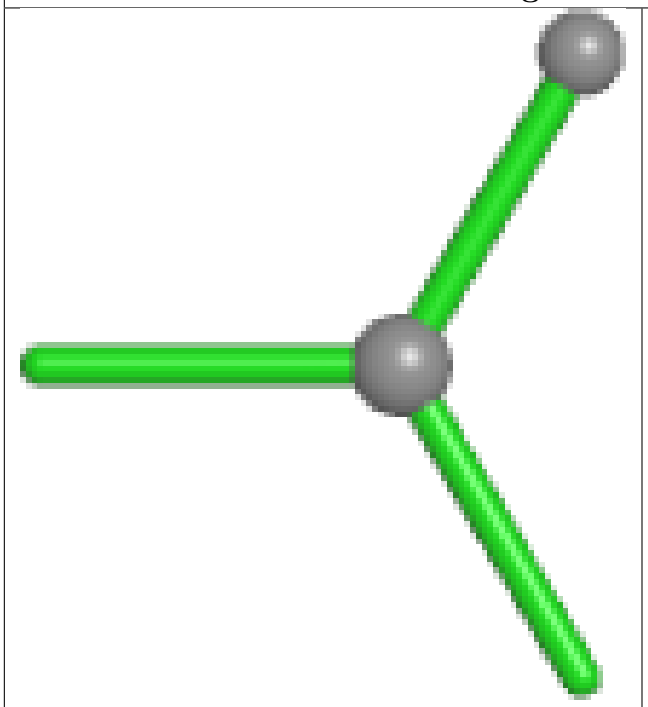


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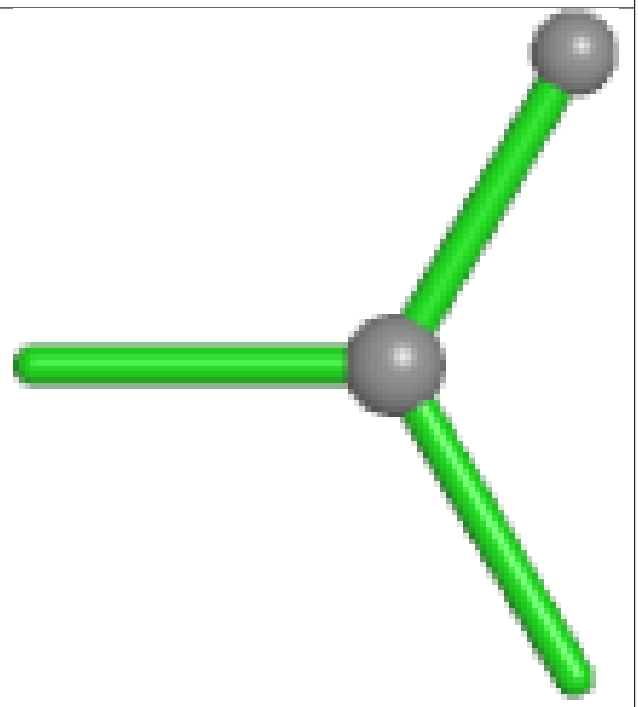


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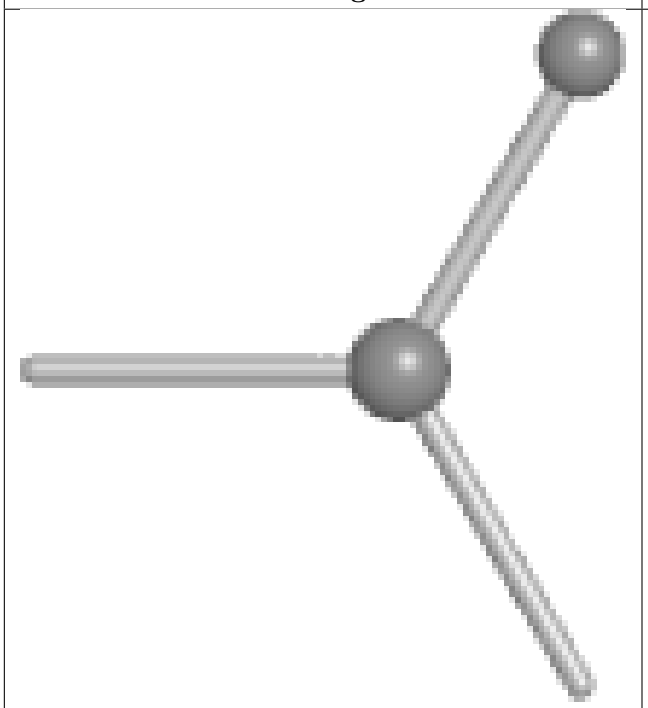
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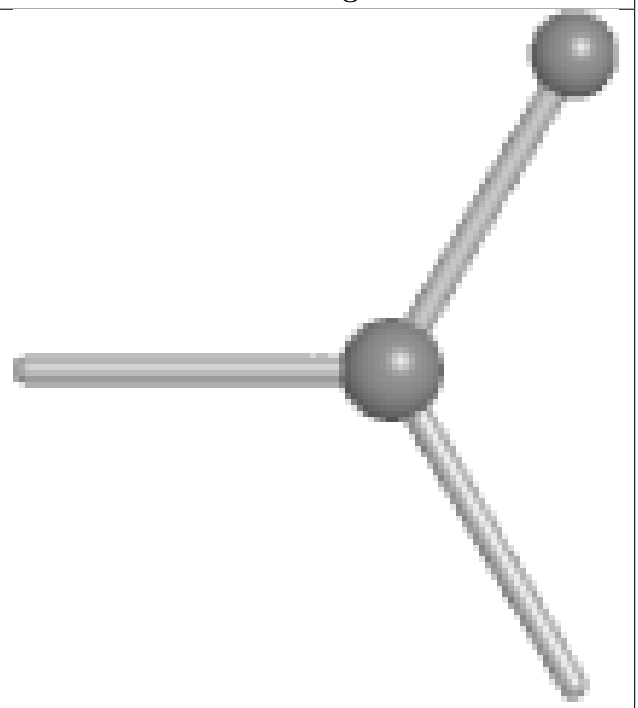
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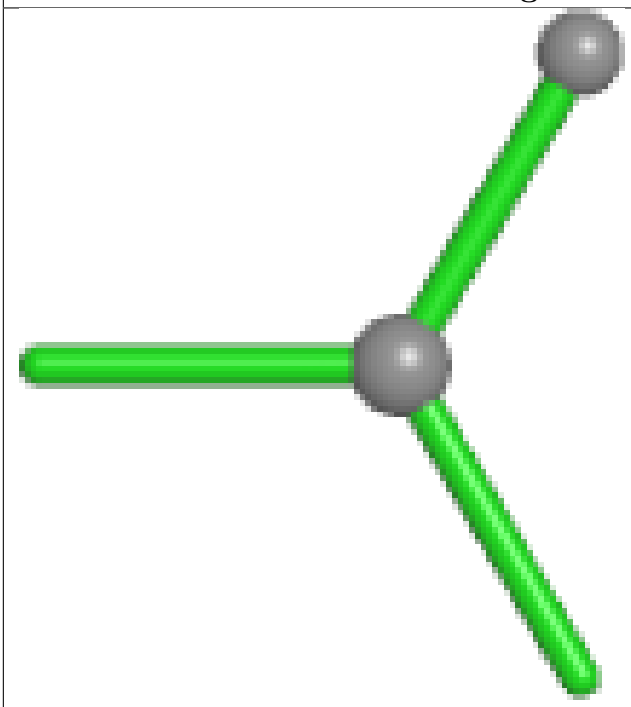


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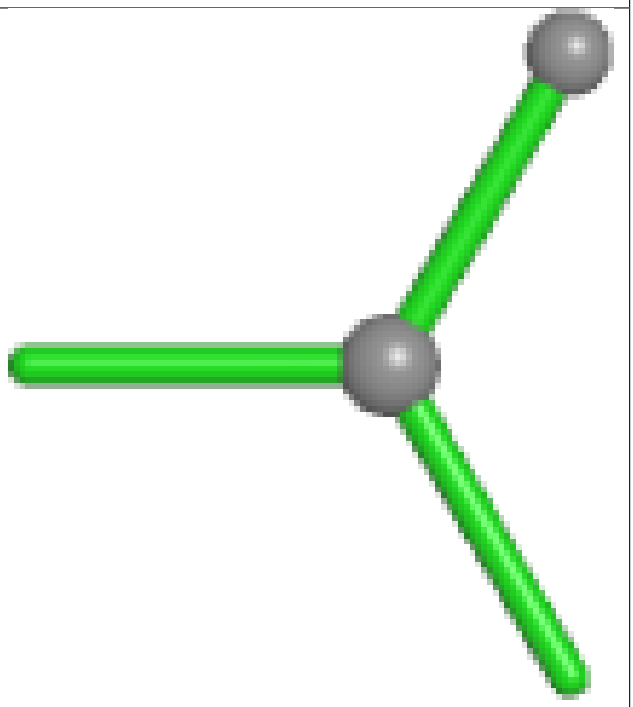


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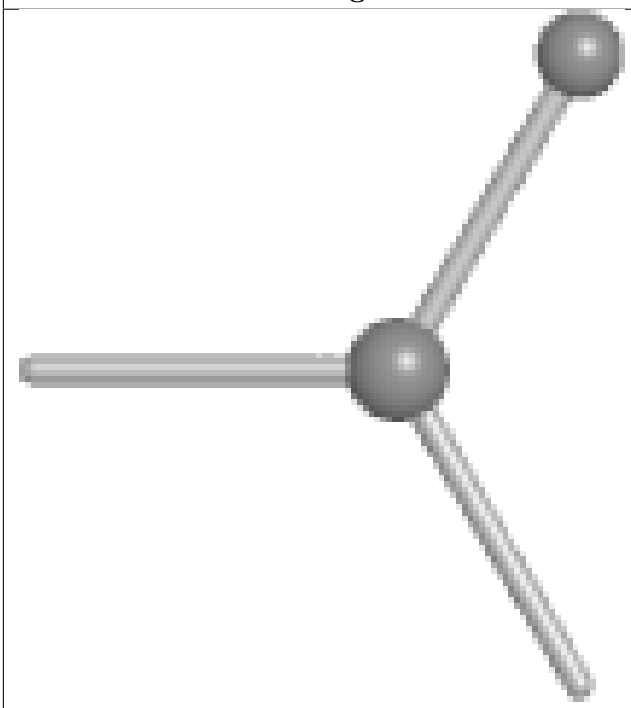
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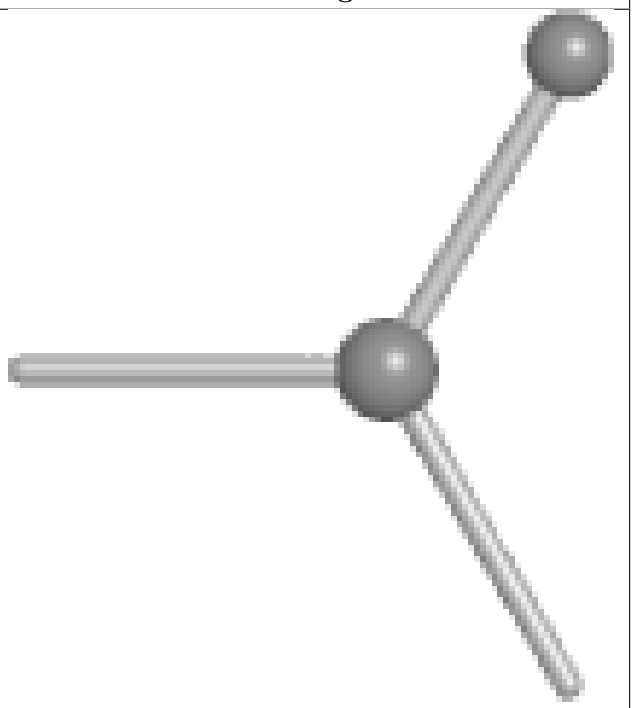
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Bond angles

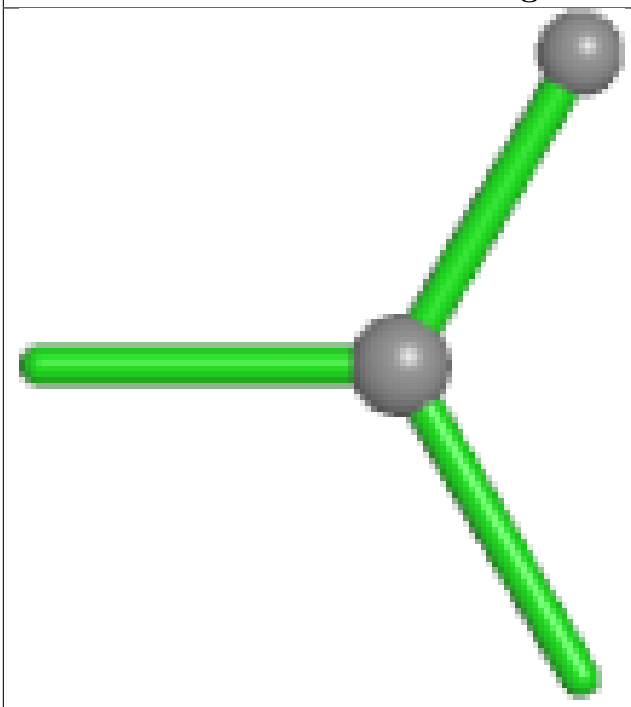


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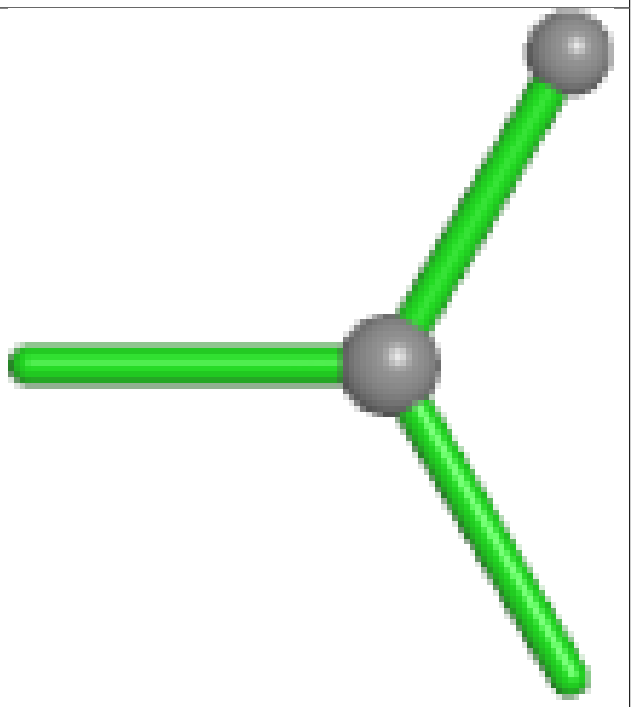


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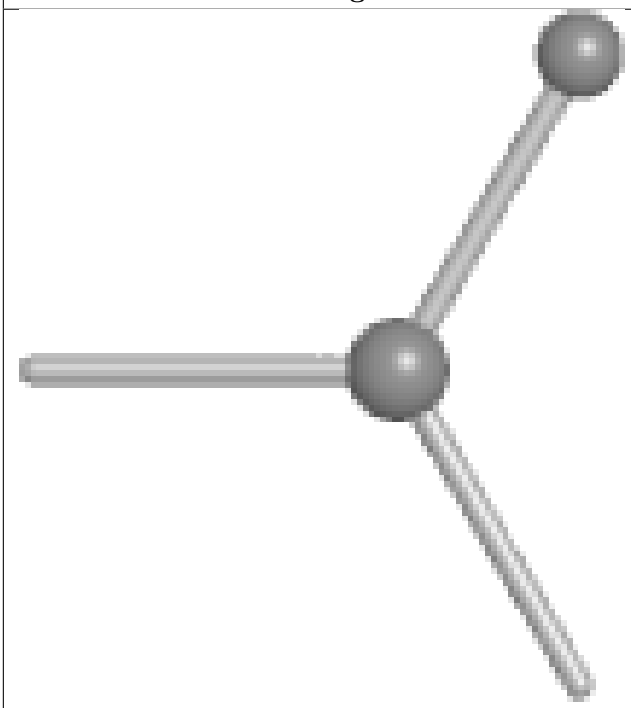
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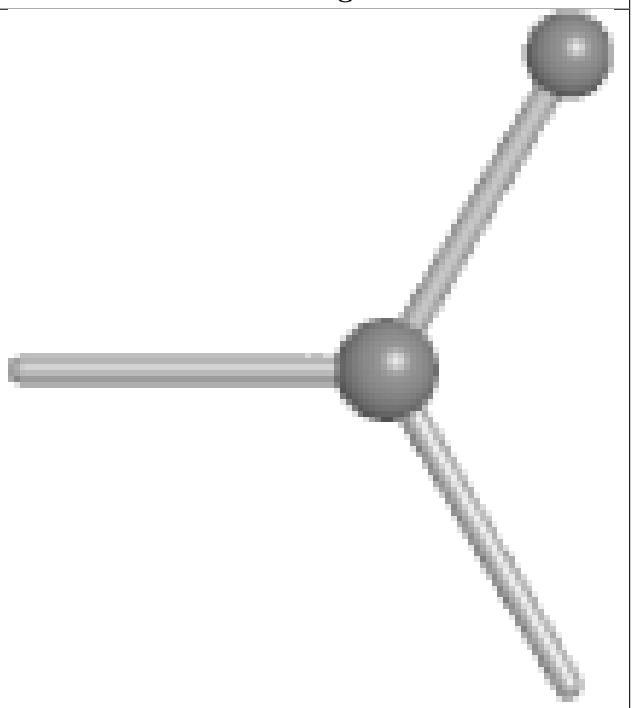
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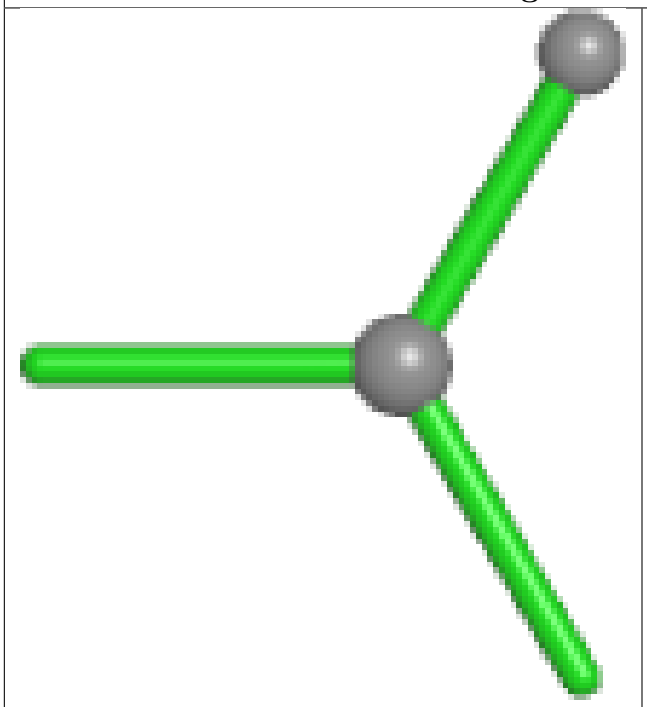


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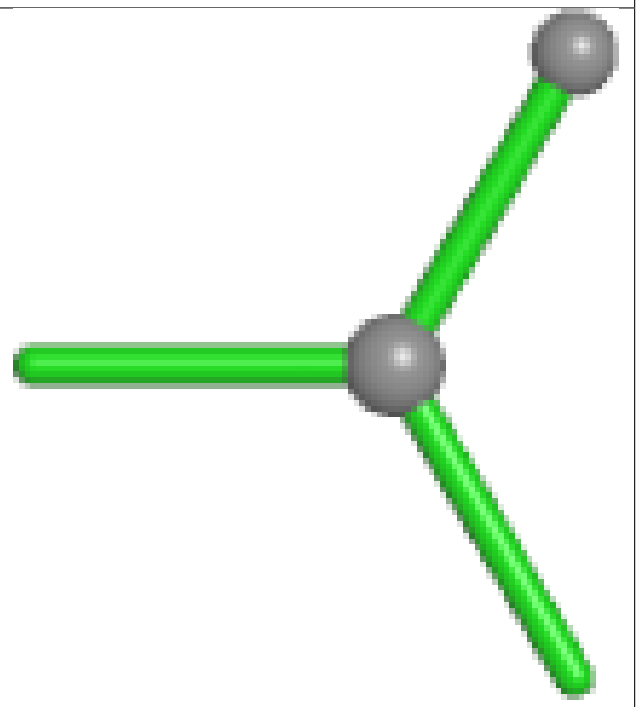


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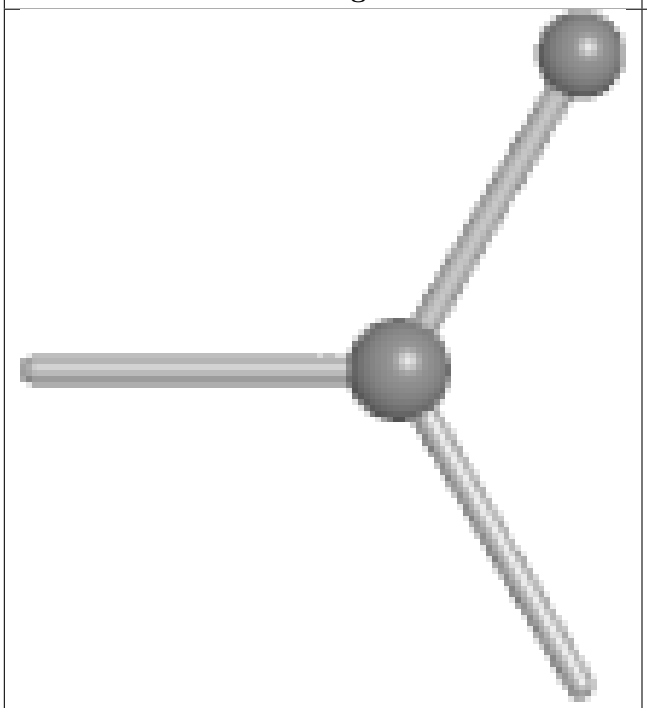
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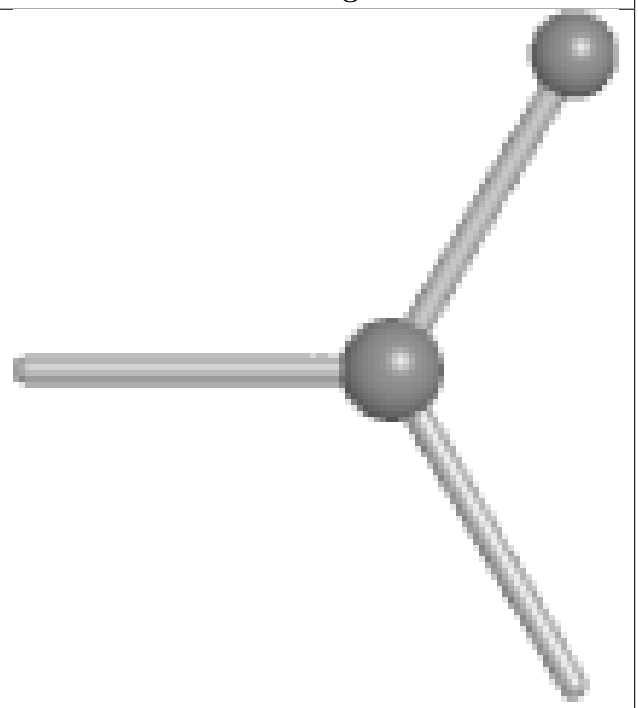
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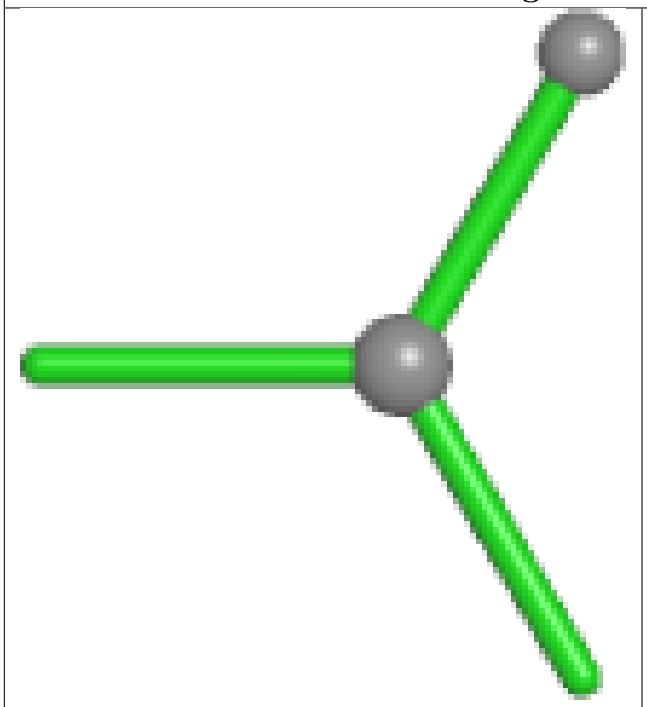


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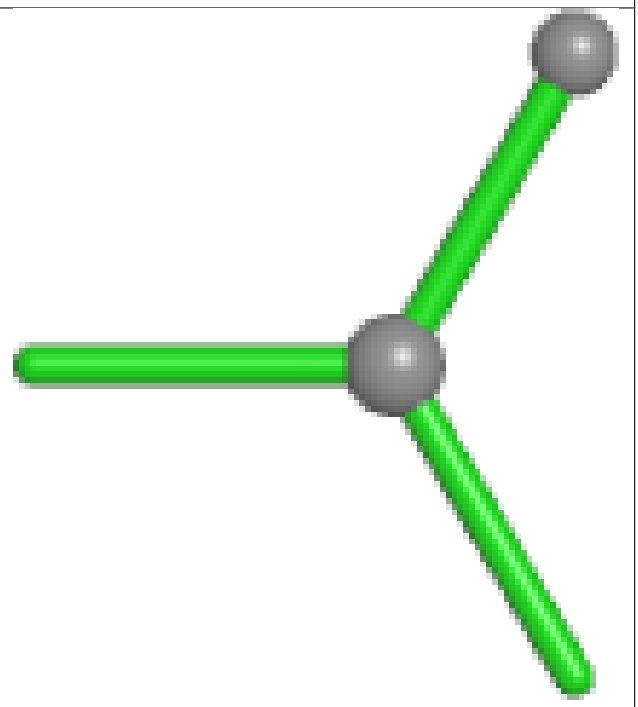


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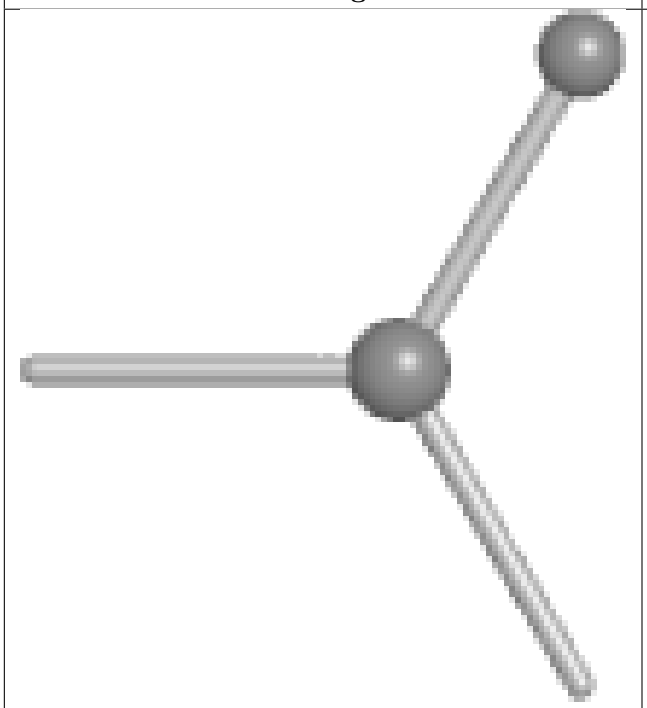
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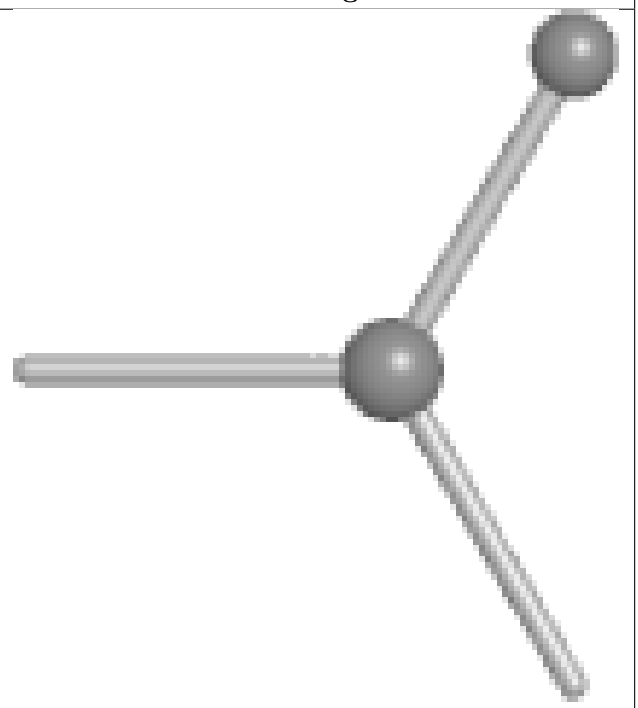
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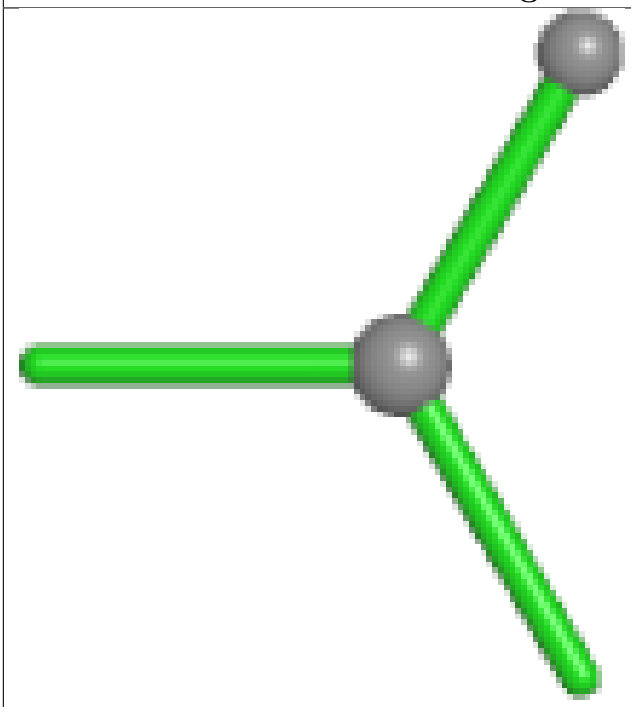


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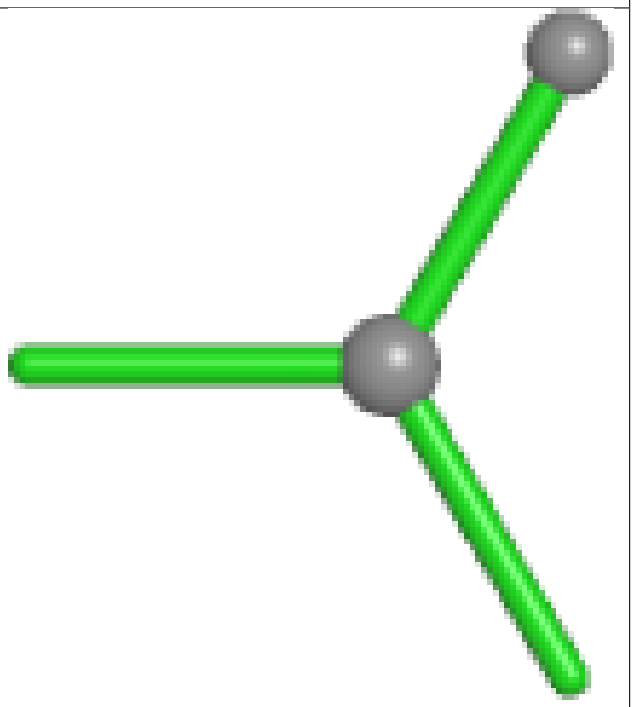


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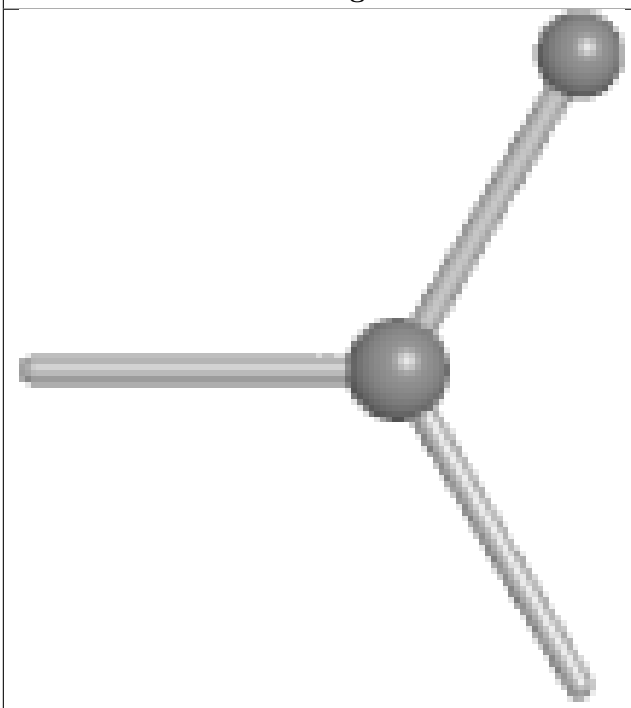
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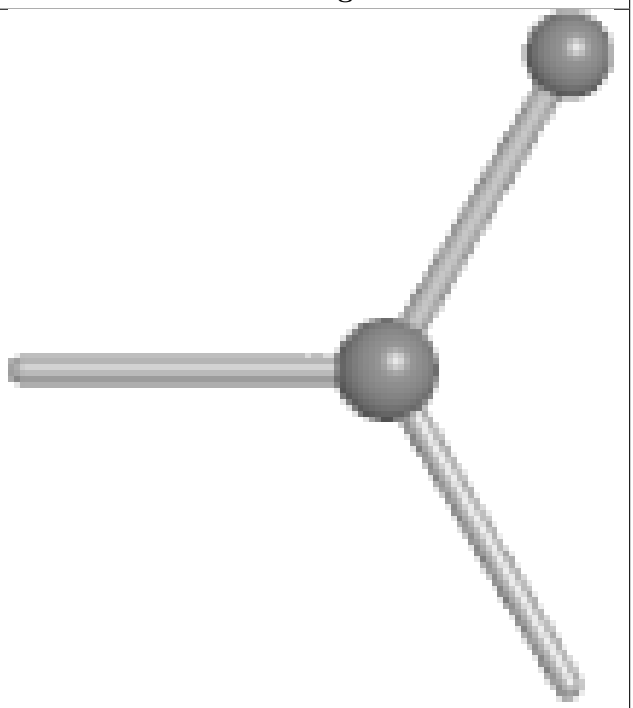
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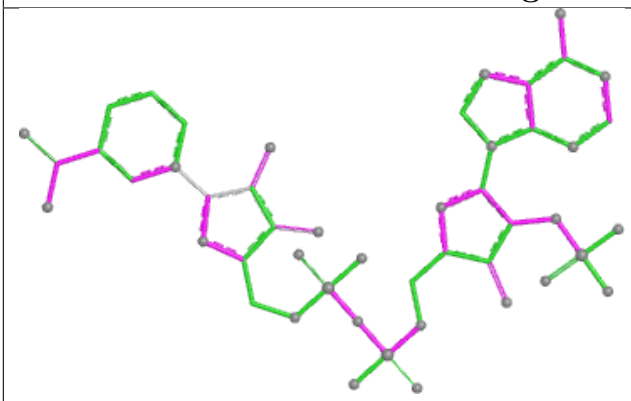


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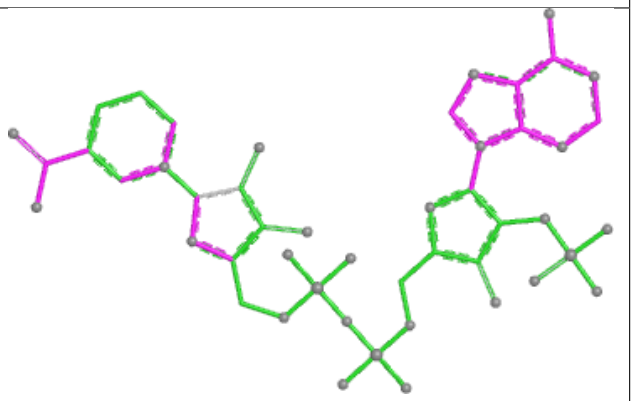


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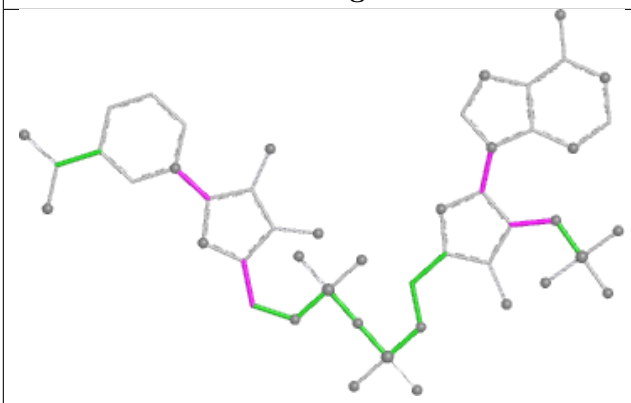
Ligand NAP B 402



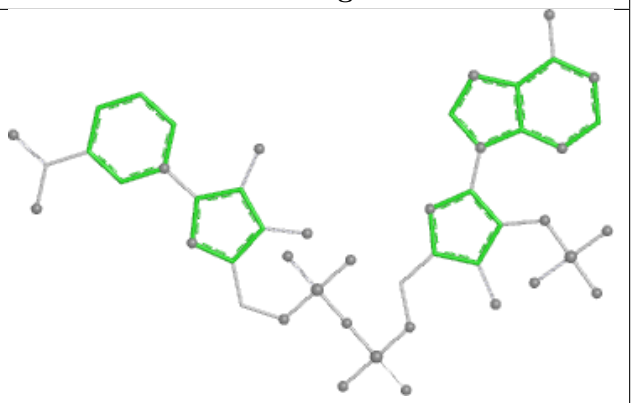
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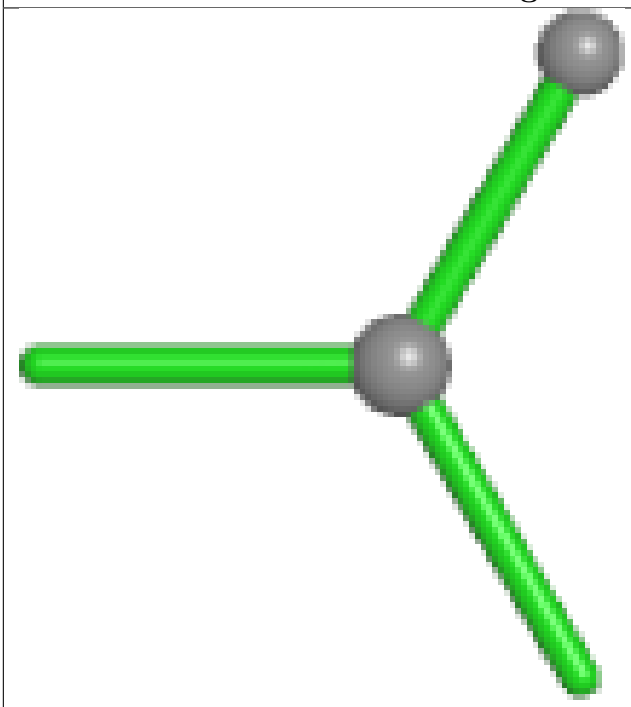


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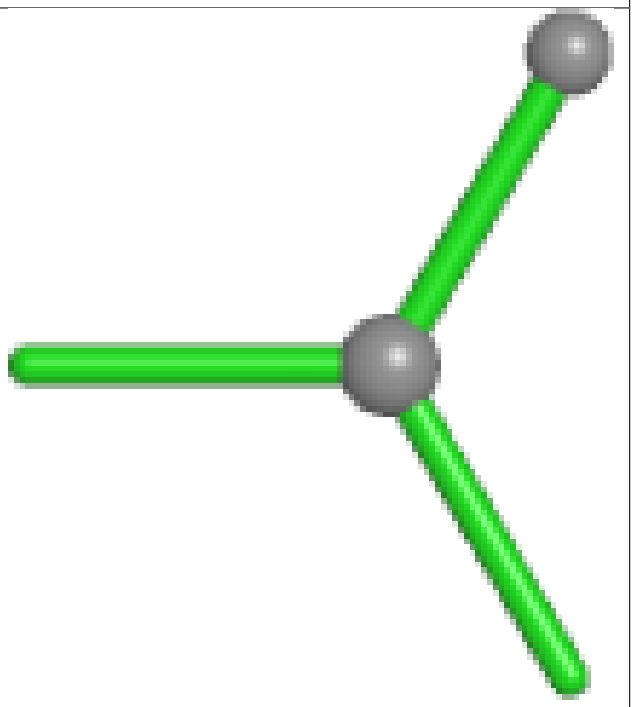


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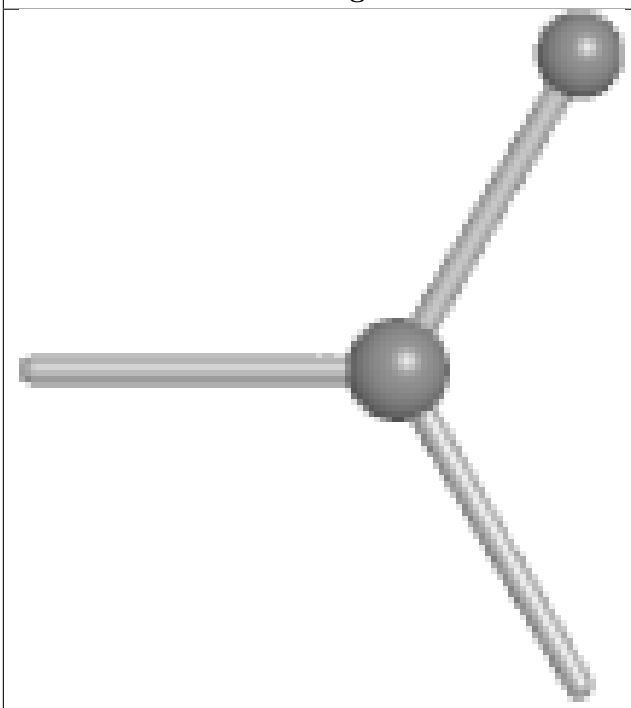
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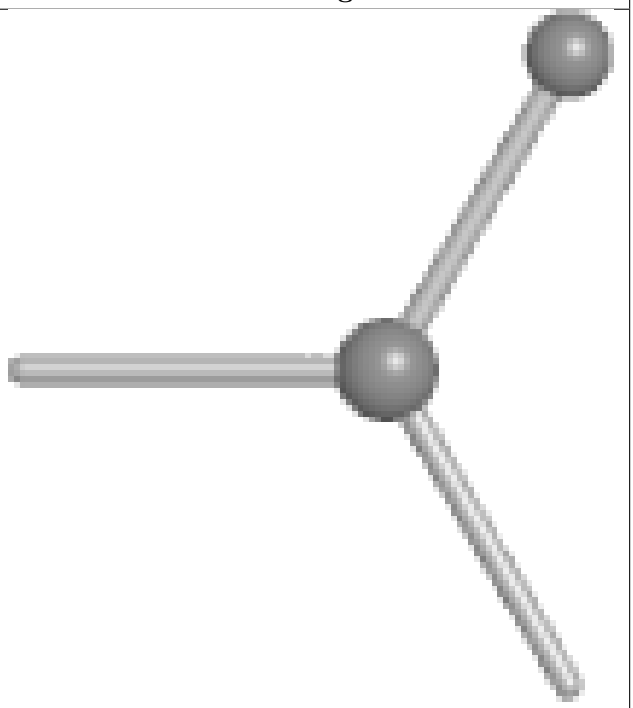
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Bond angles

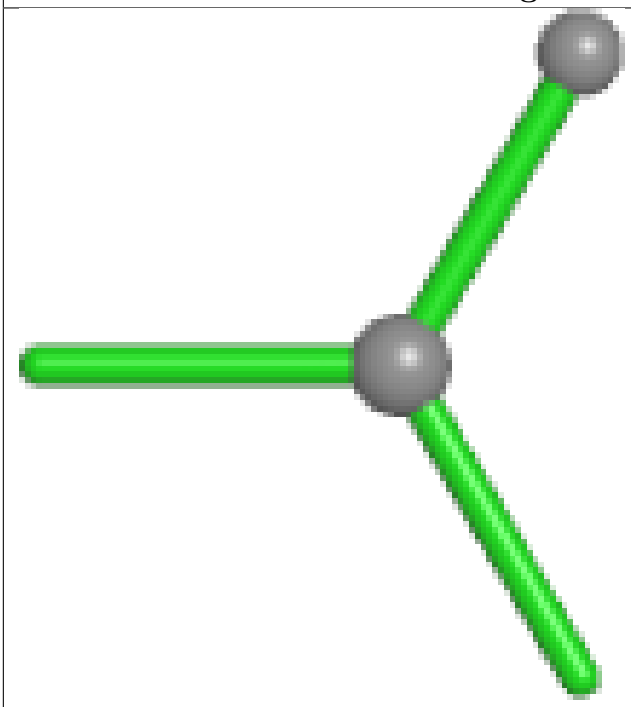


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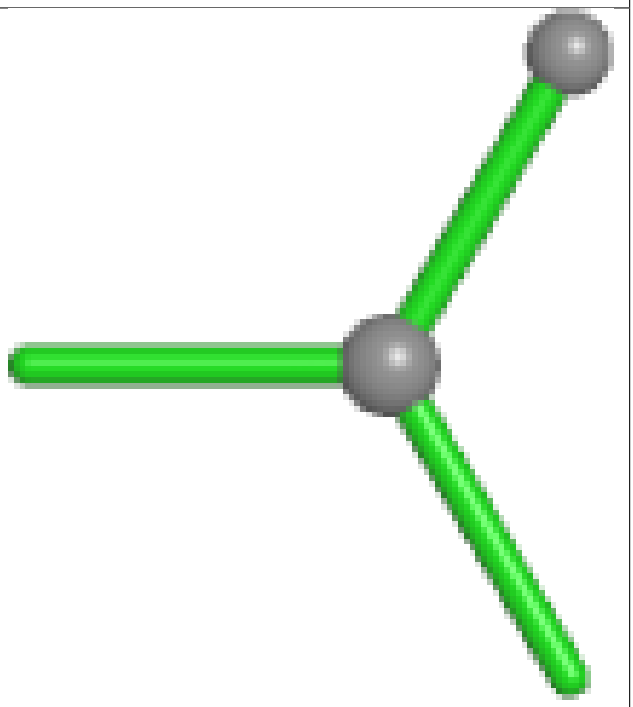


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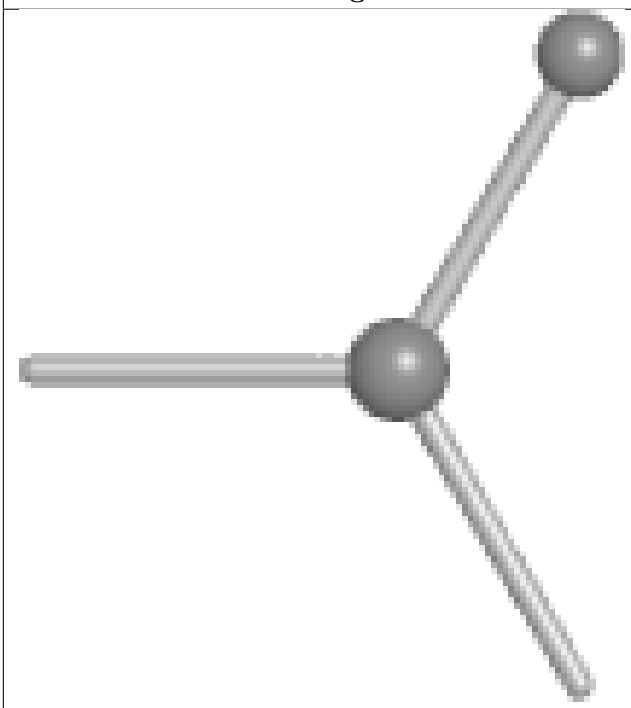
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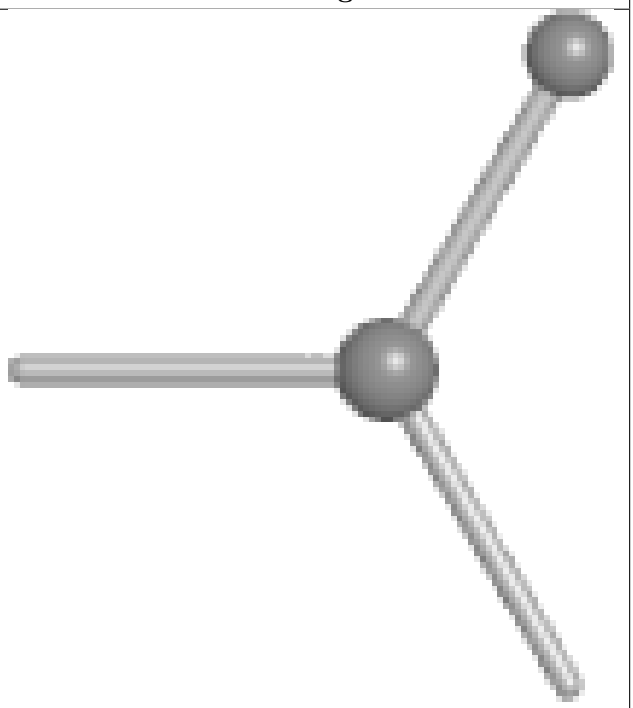
Bond lengths



Bond angles

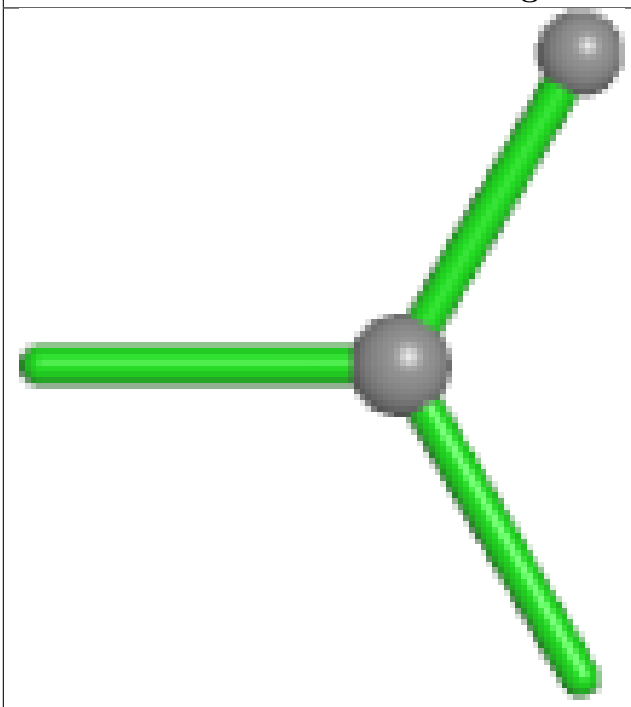


Torsions

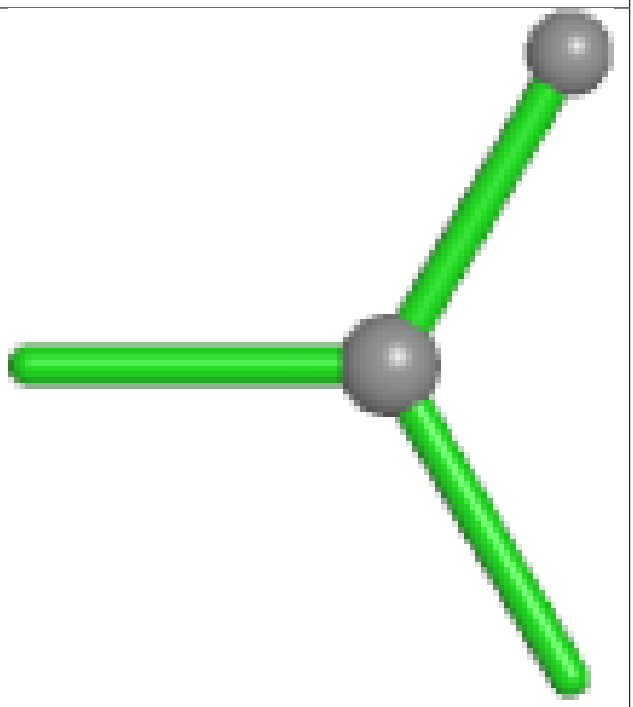


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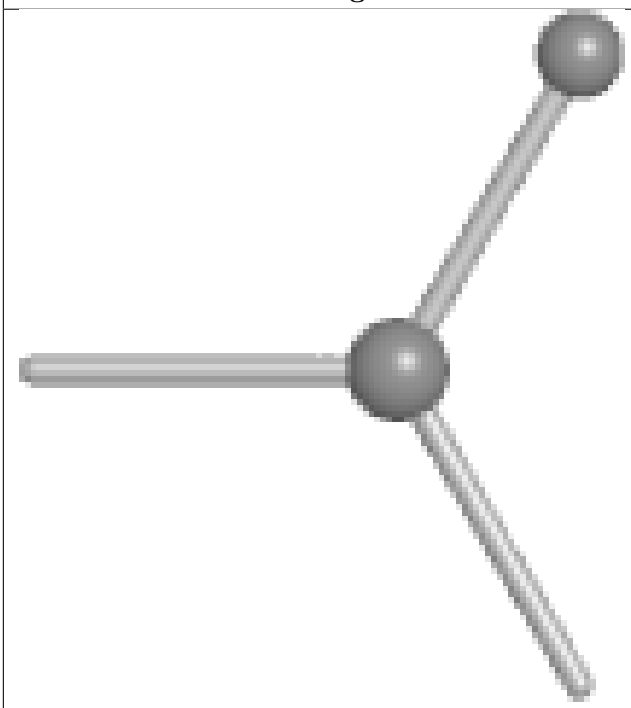
Ligand DMS B 409



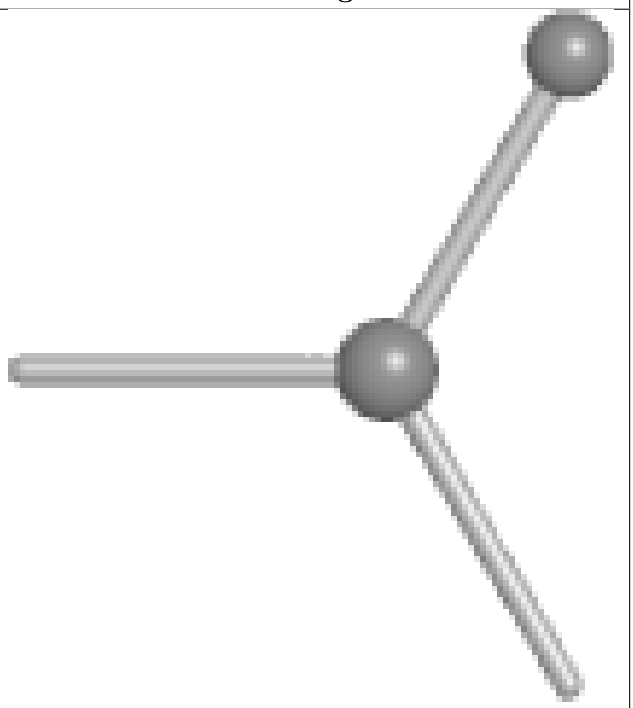
Bond lengths



Bond angles

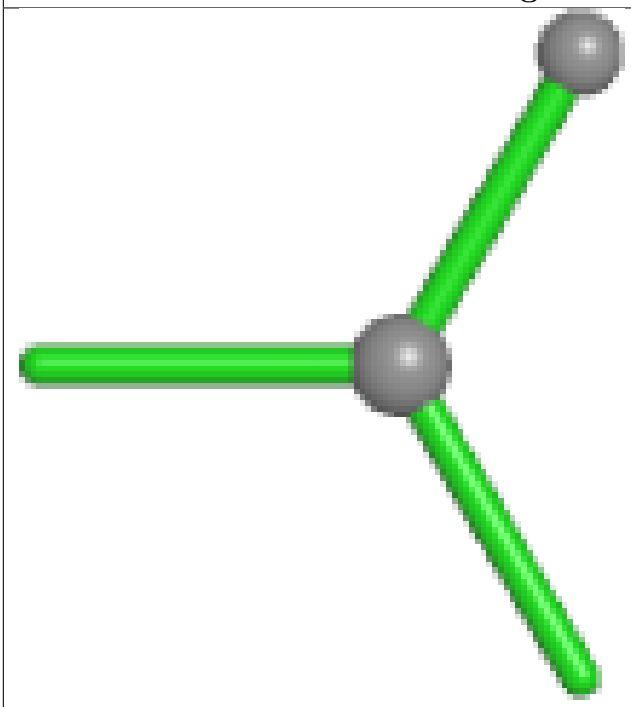


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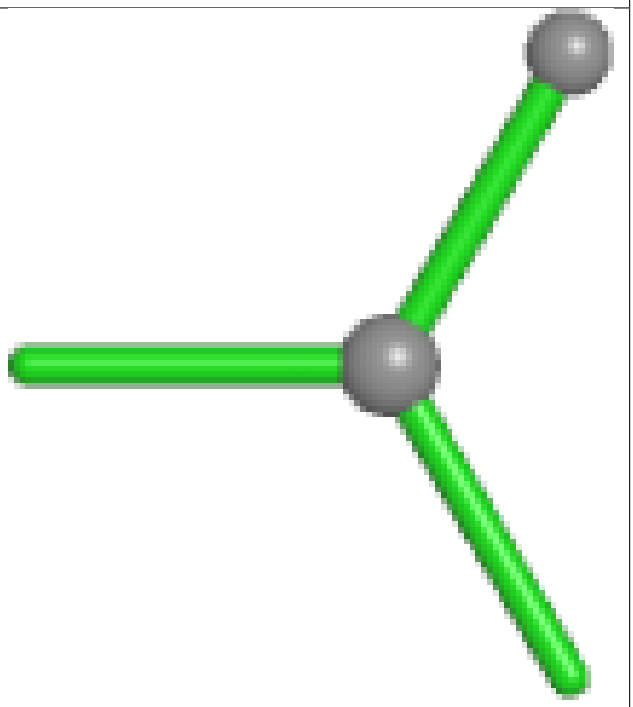


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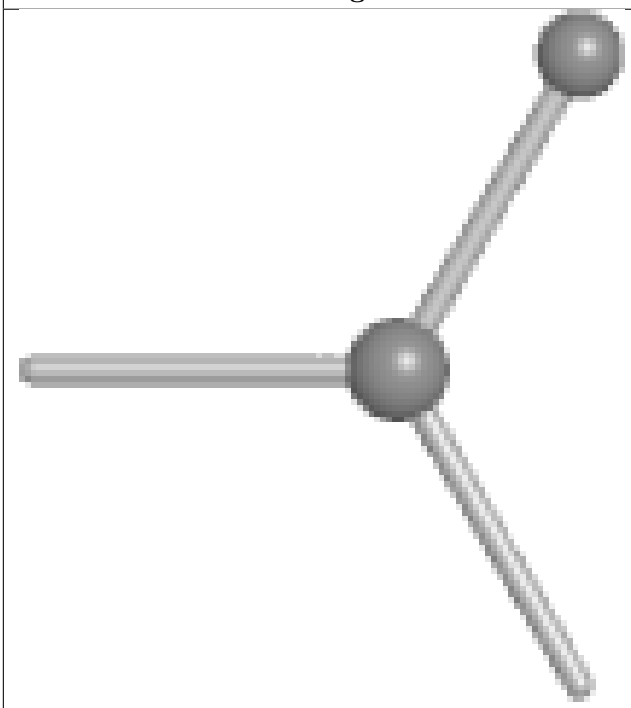
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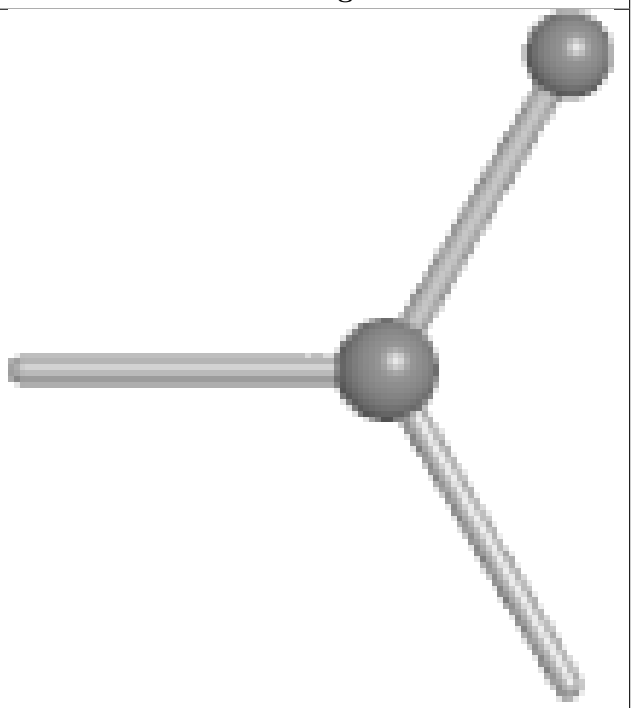
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Bond angles

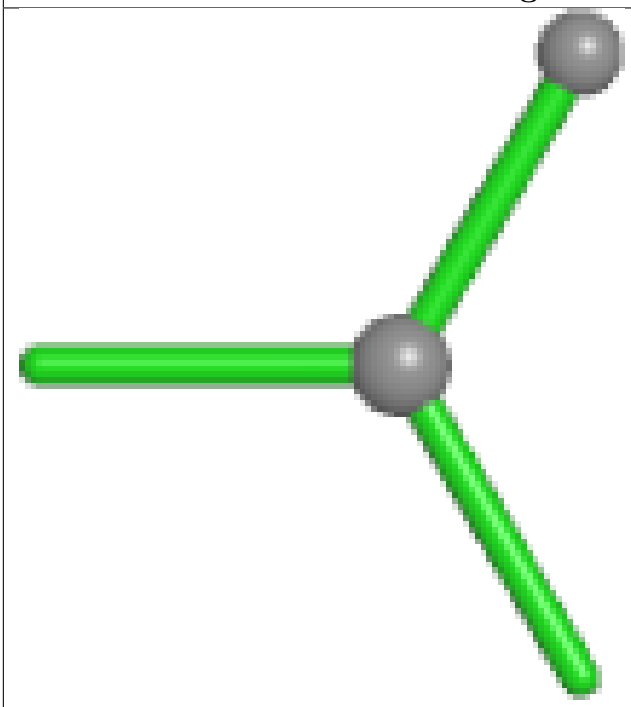


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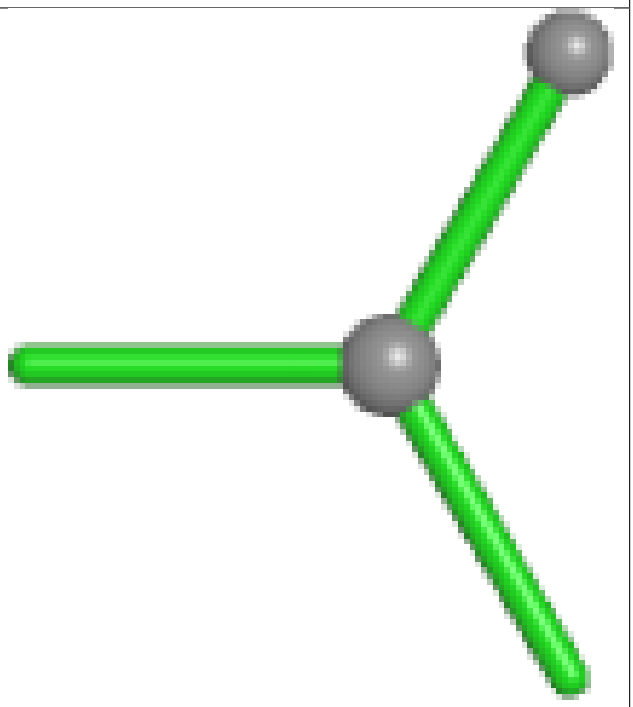


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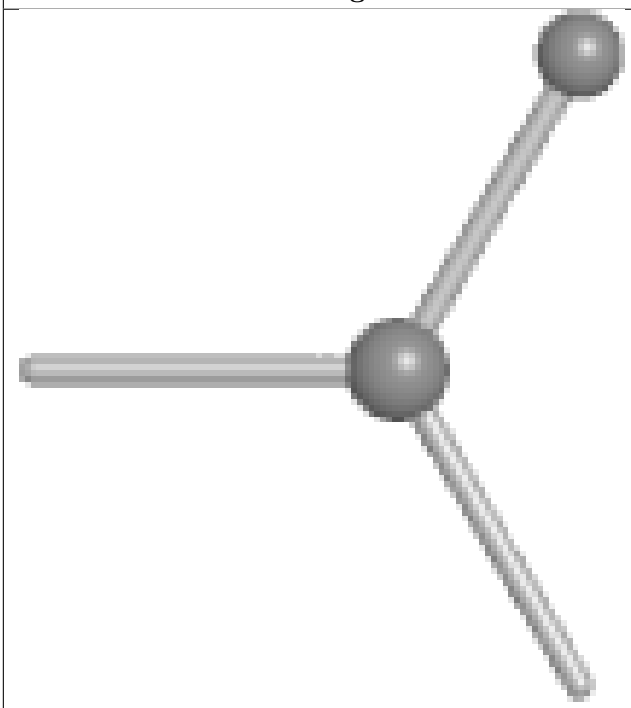
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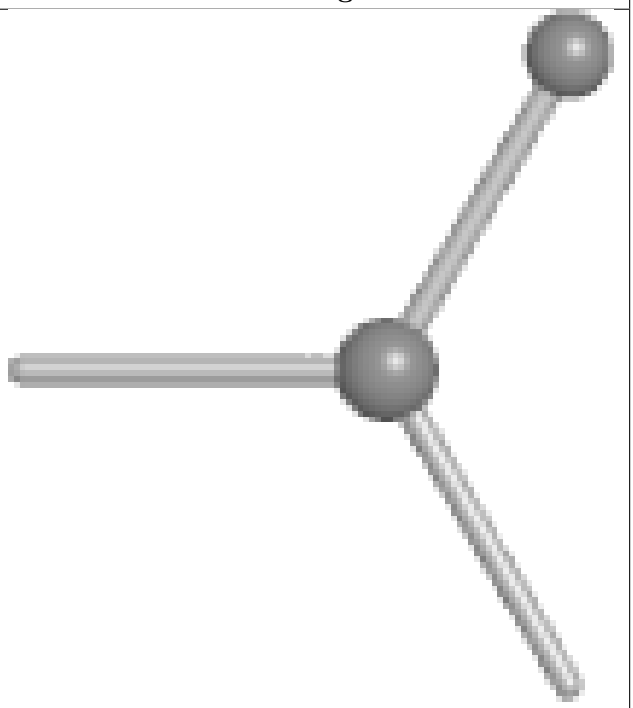
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Bond angles

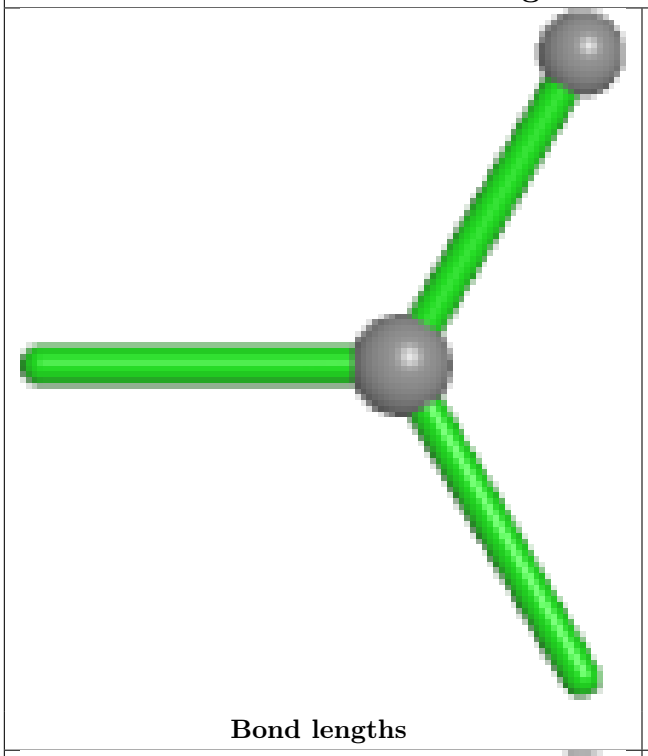


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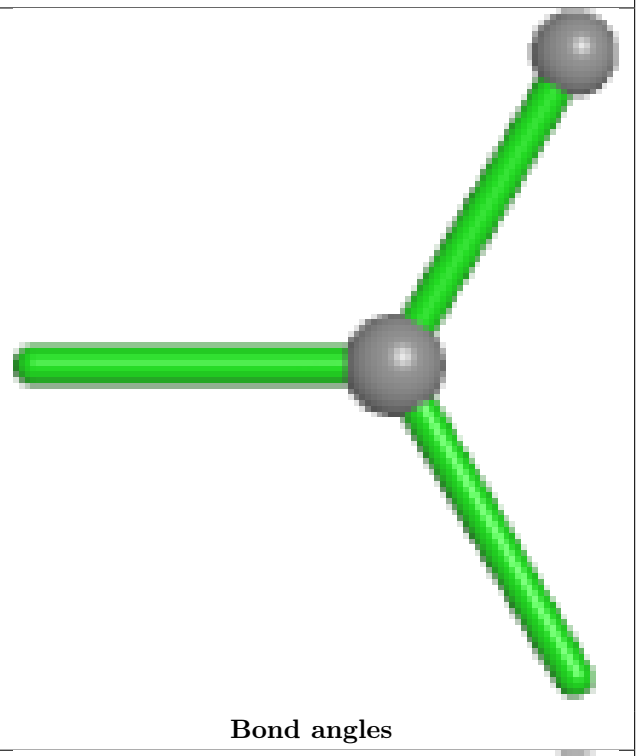


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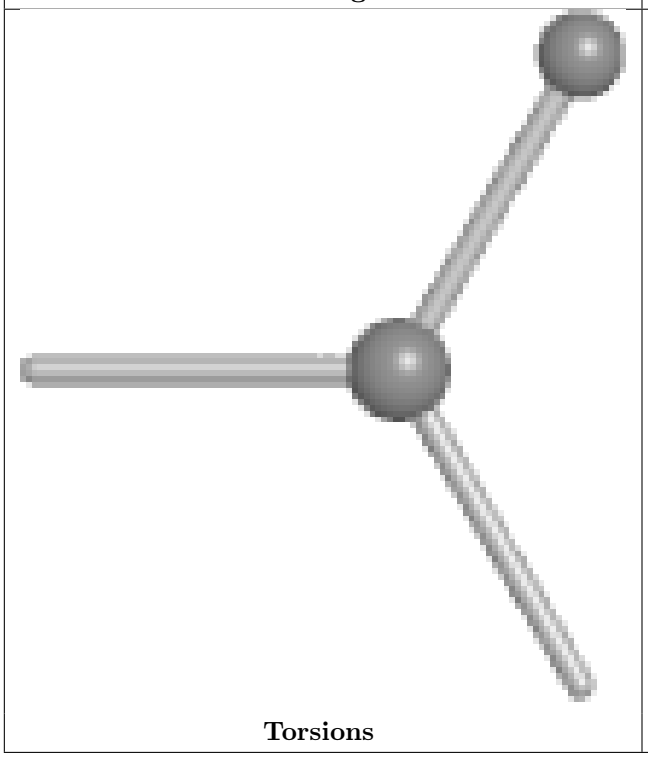
Ligand DMS B 403



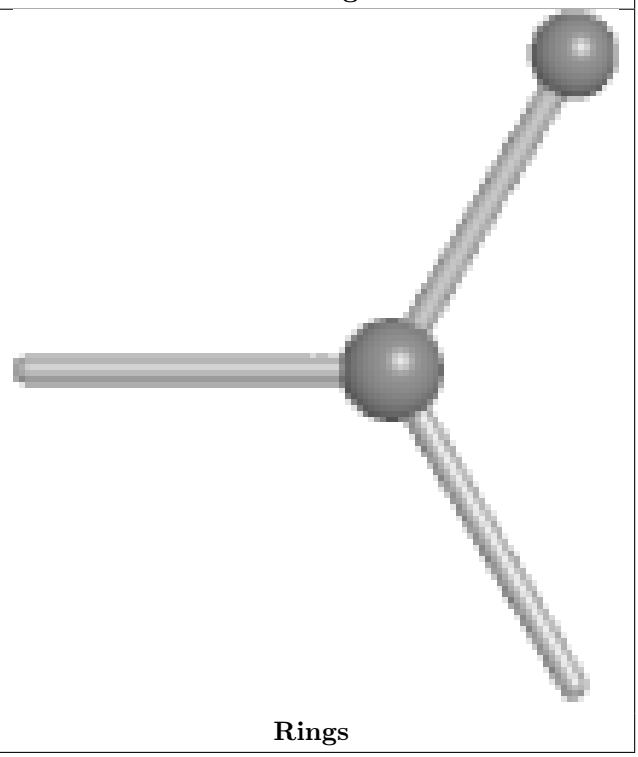
Bond lengths



Bond angles

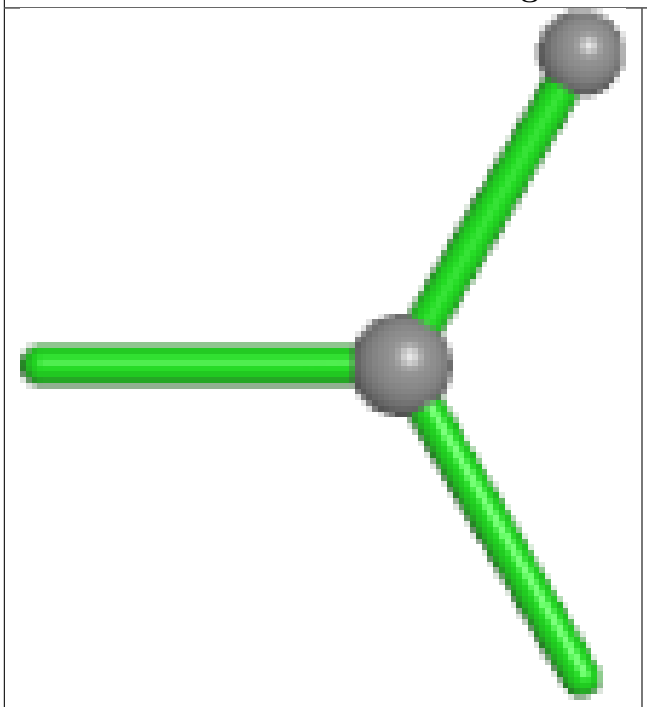


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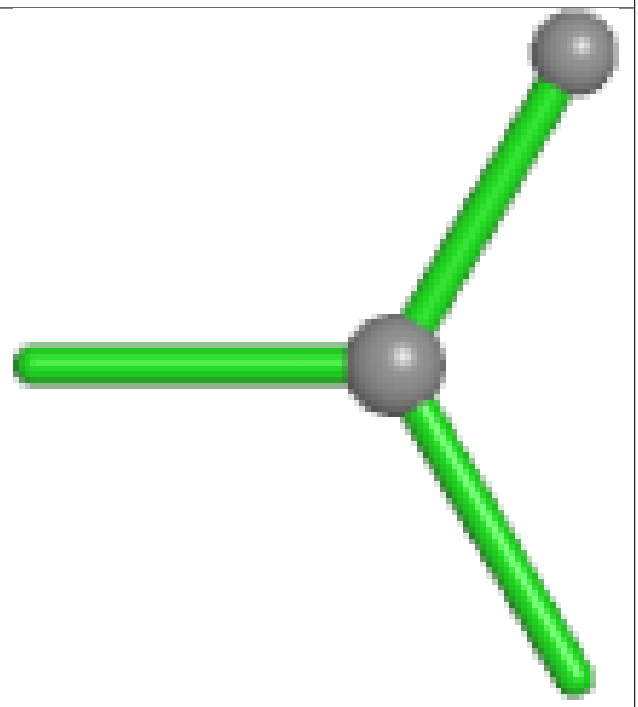


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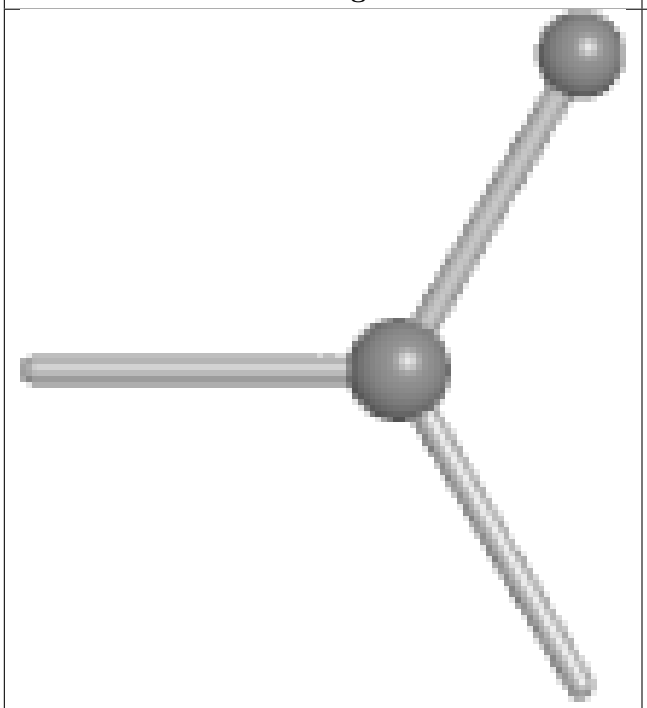
Ligand DMS D 810



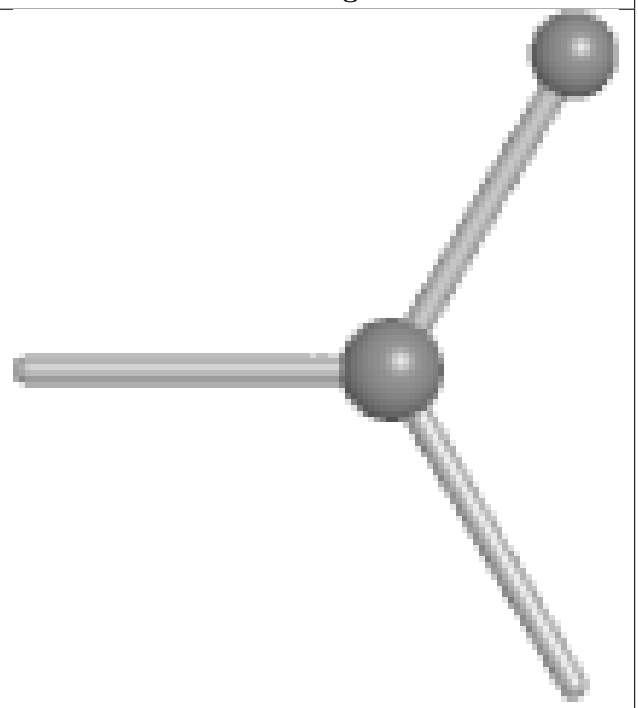
Bond lengths



Bond angles

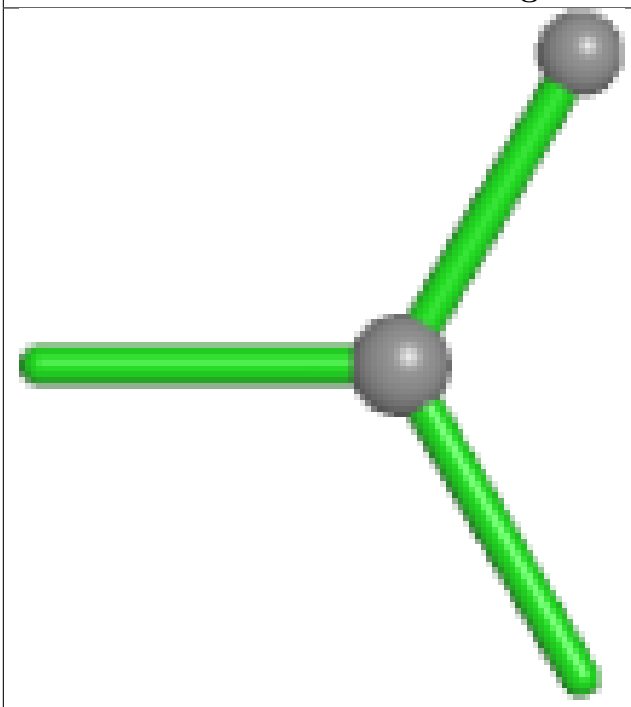


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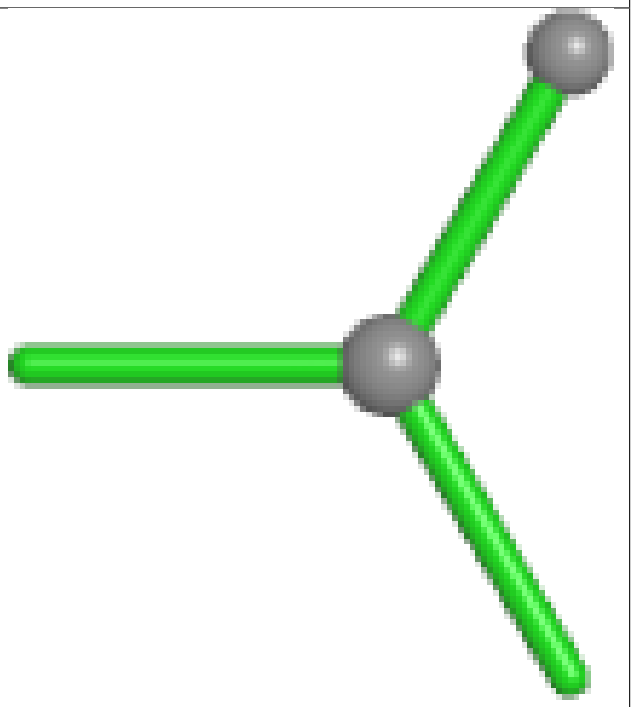


Rings

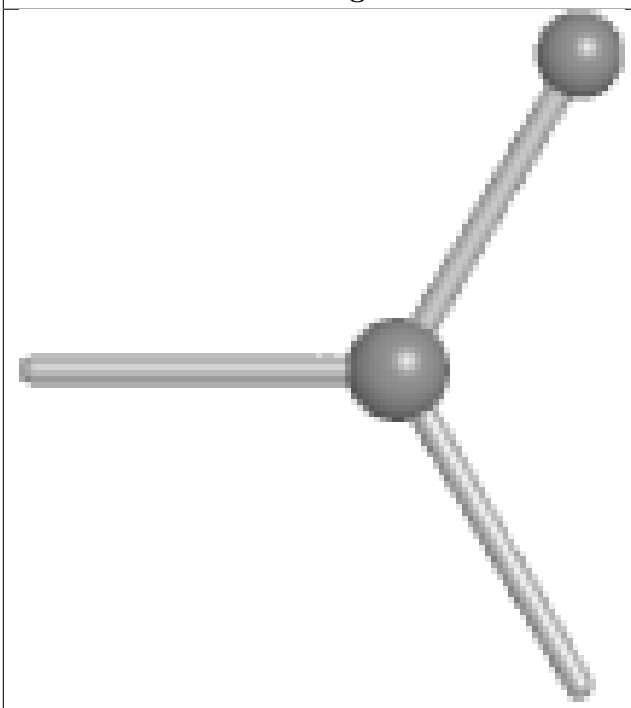
Ligand DMS C 405



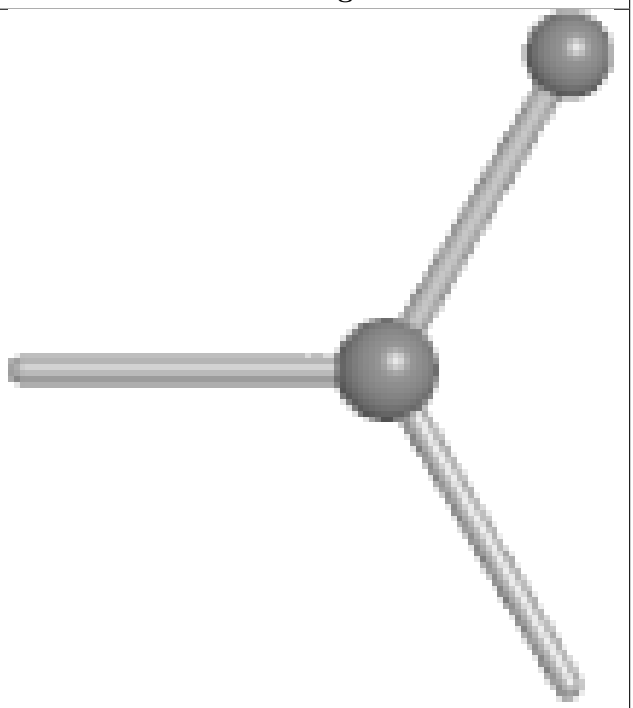
Bond lengths



Bond angles

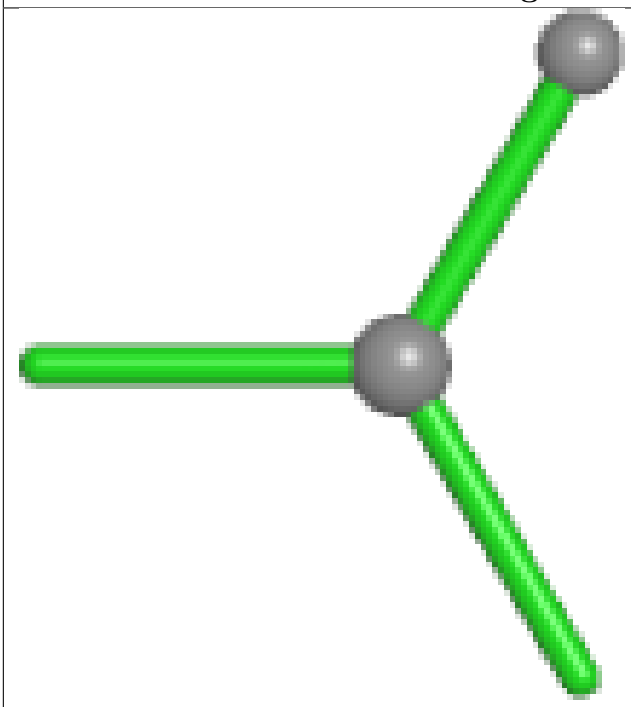


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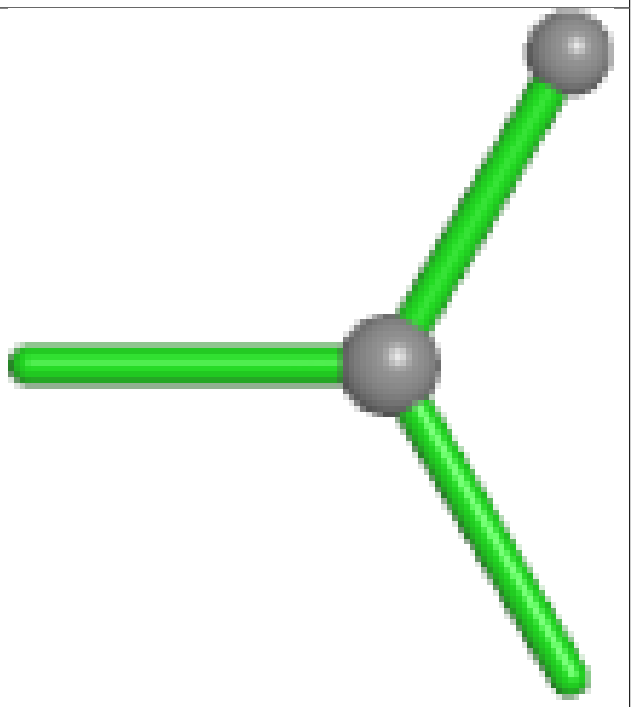


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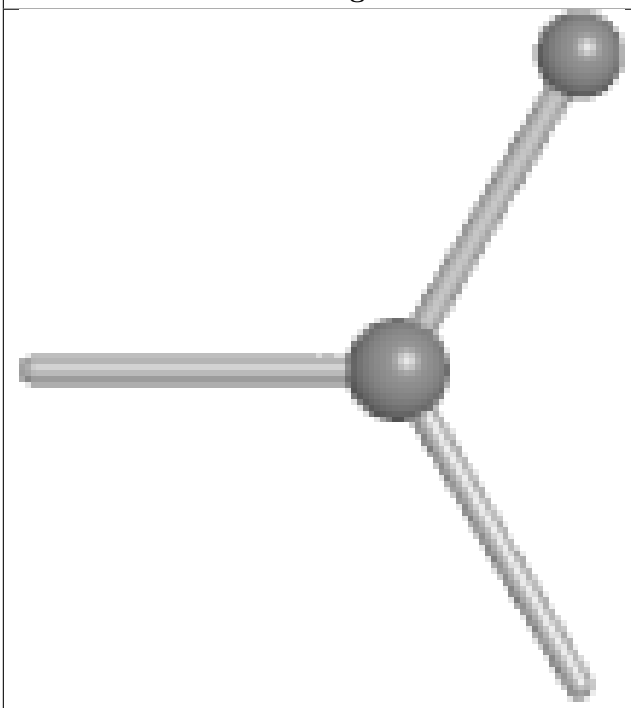
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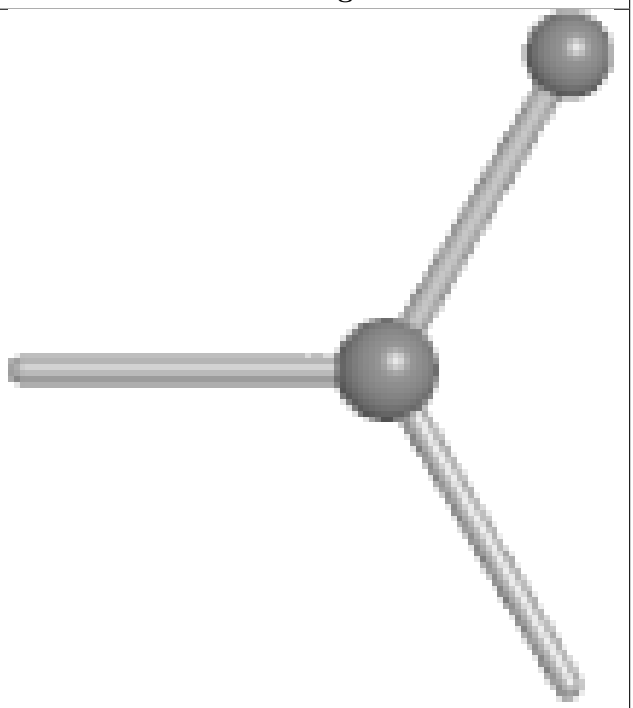
Bond lengths



Bond angles

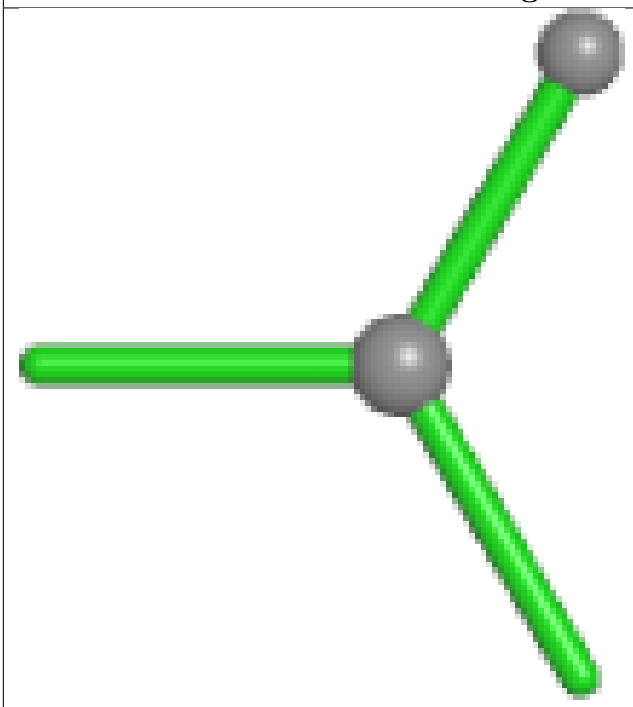


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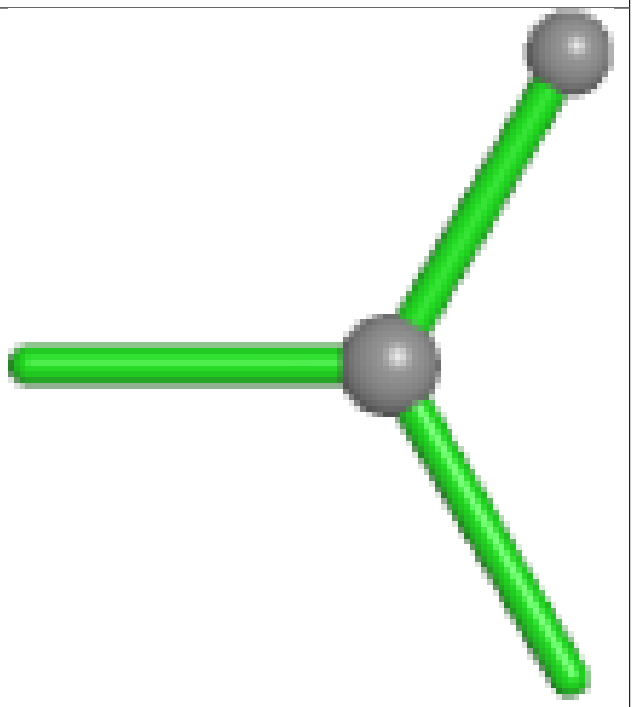


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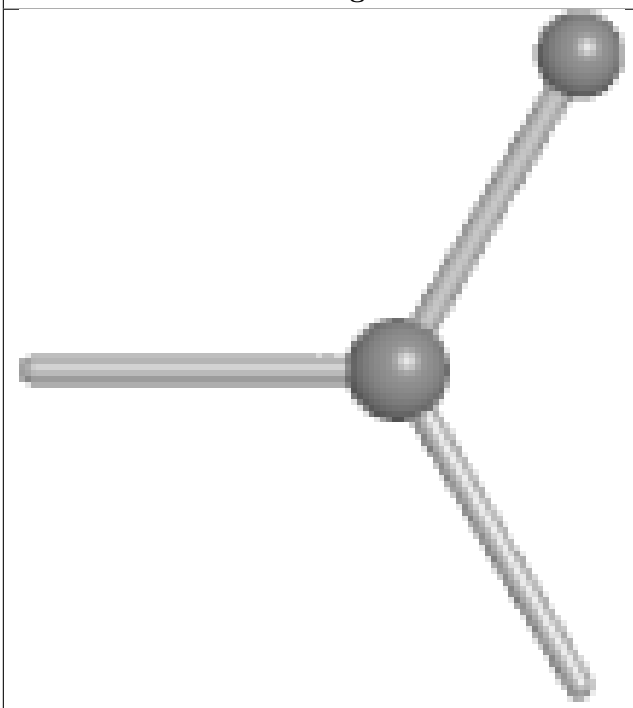
Ligand DMS B 410



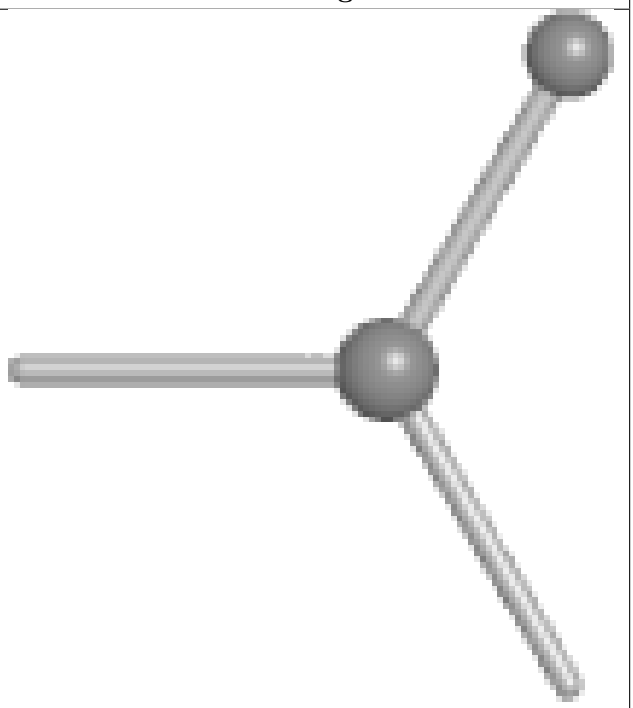
Bond lengths



Bond angles

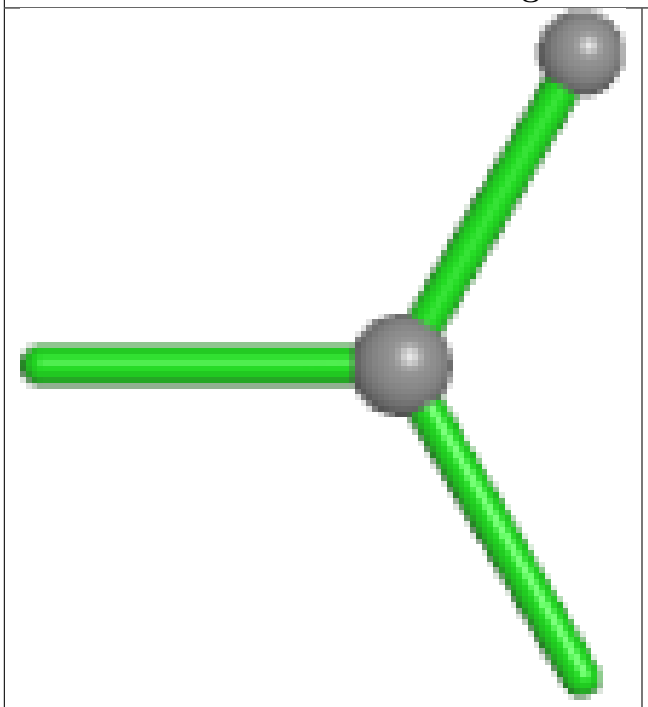


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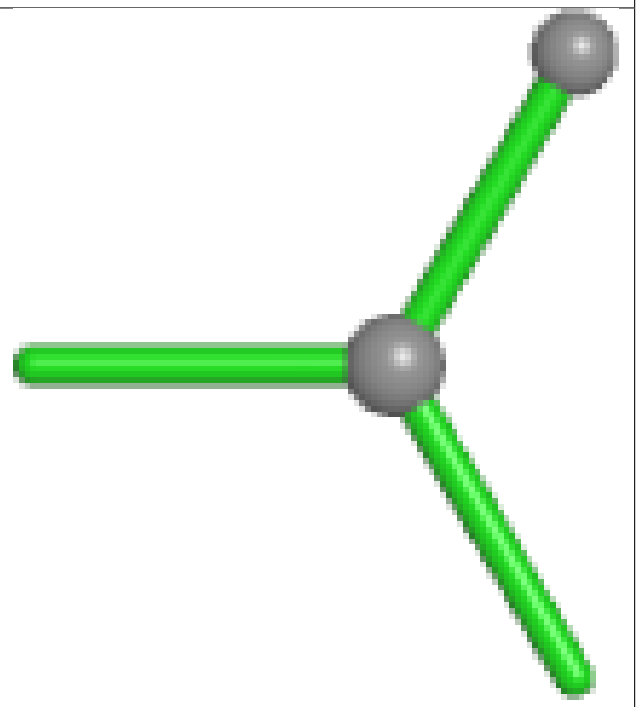


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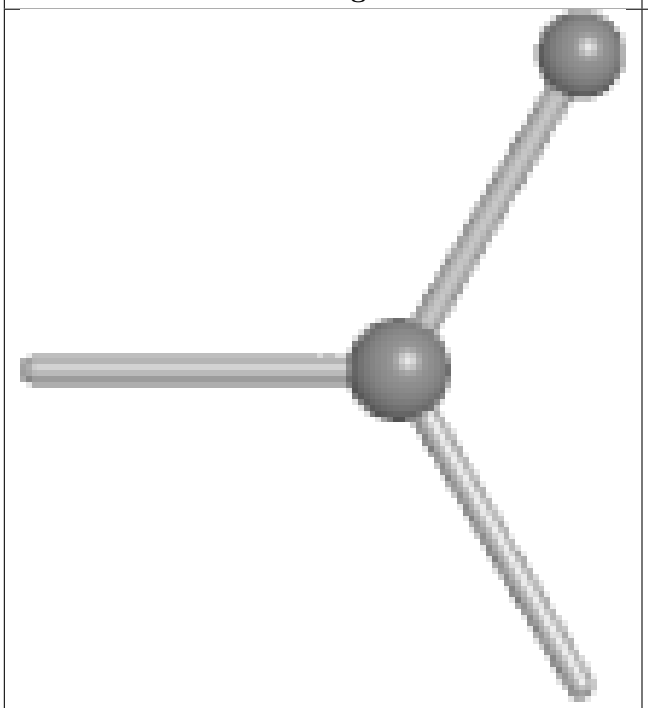
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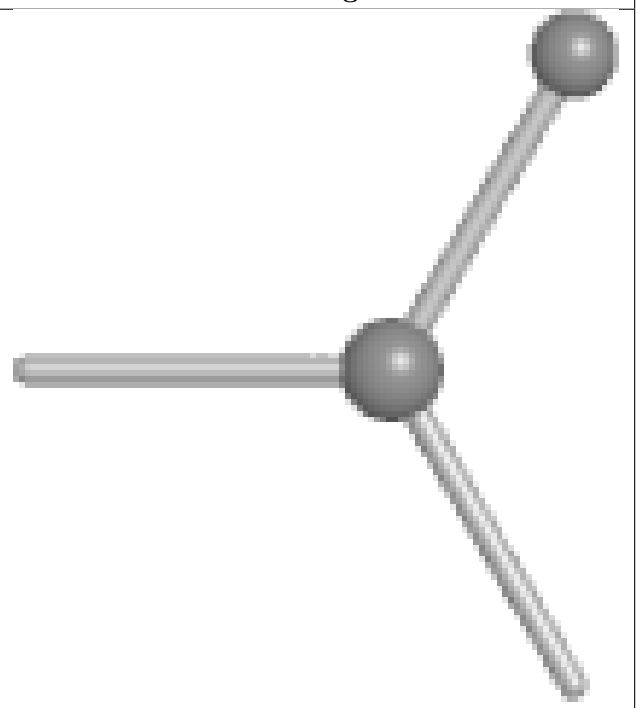
Bond lengths



Bond angles

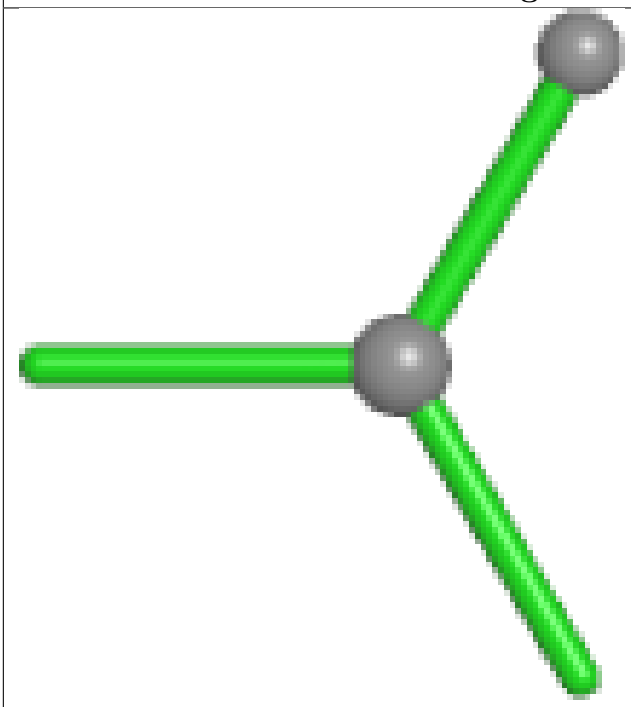


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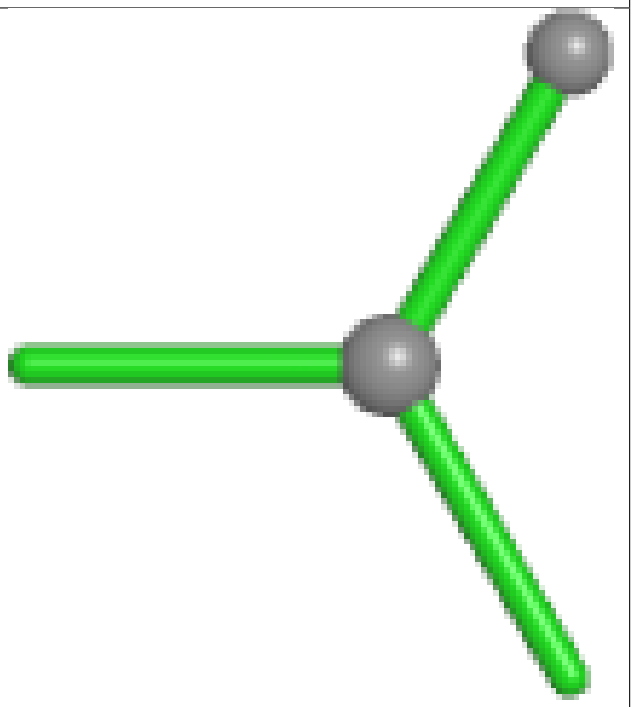


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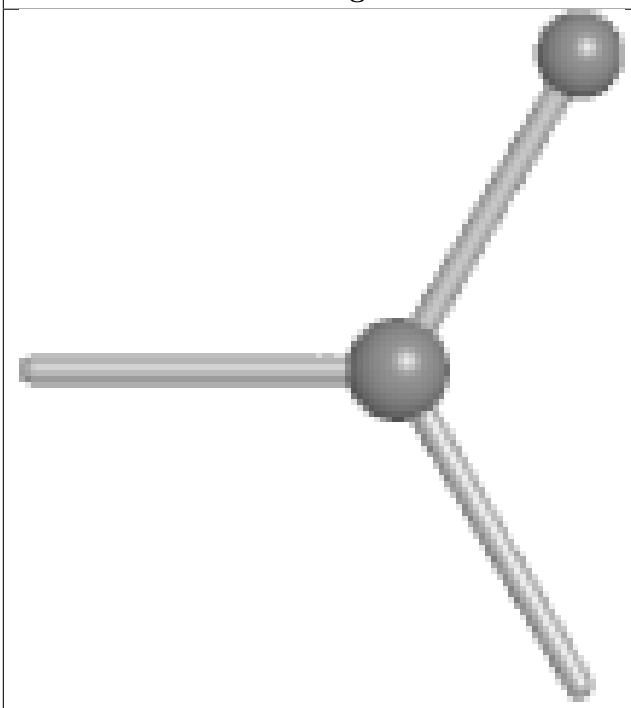
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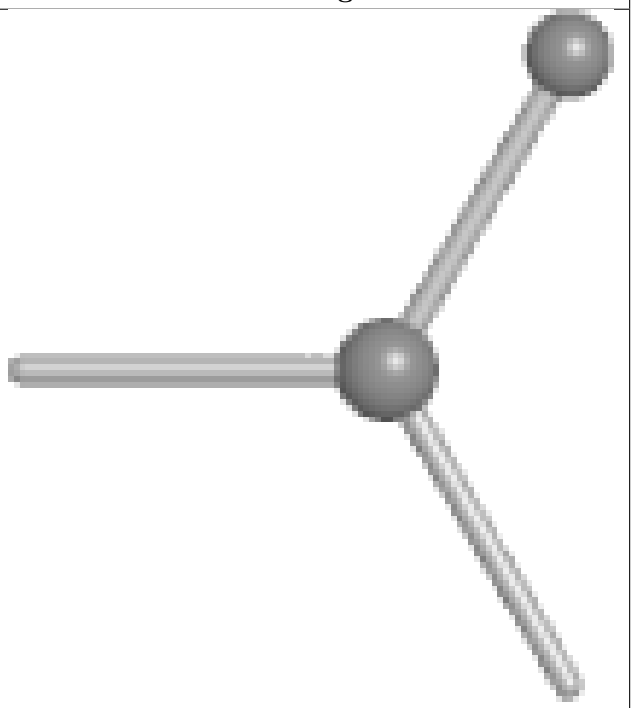
Bond lengths



Bond angles

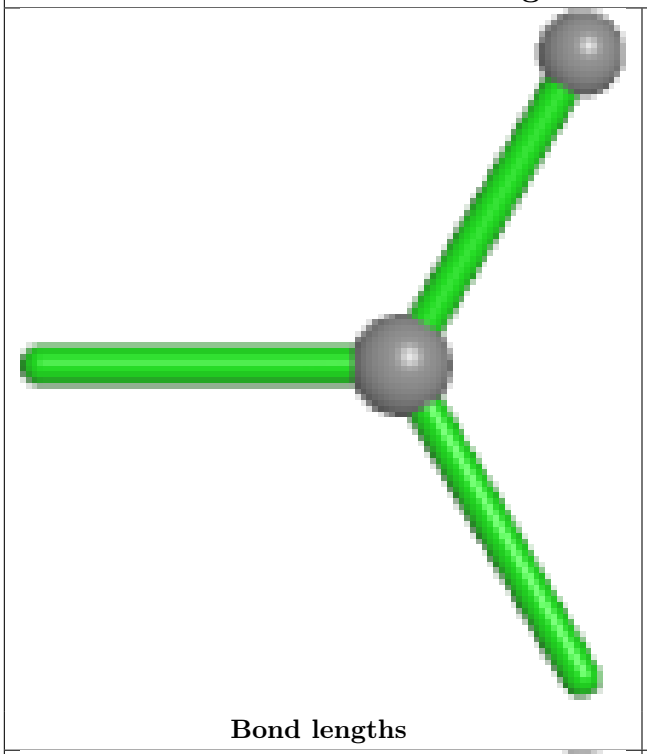


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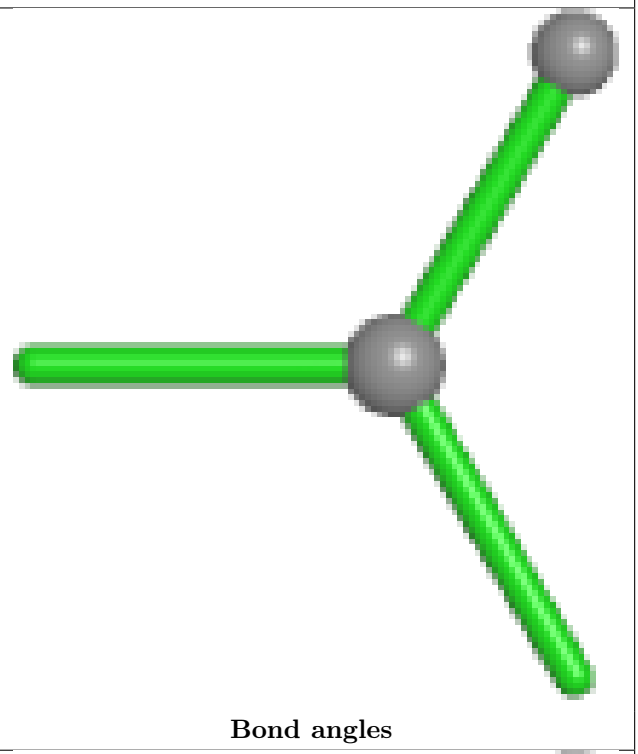


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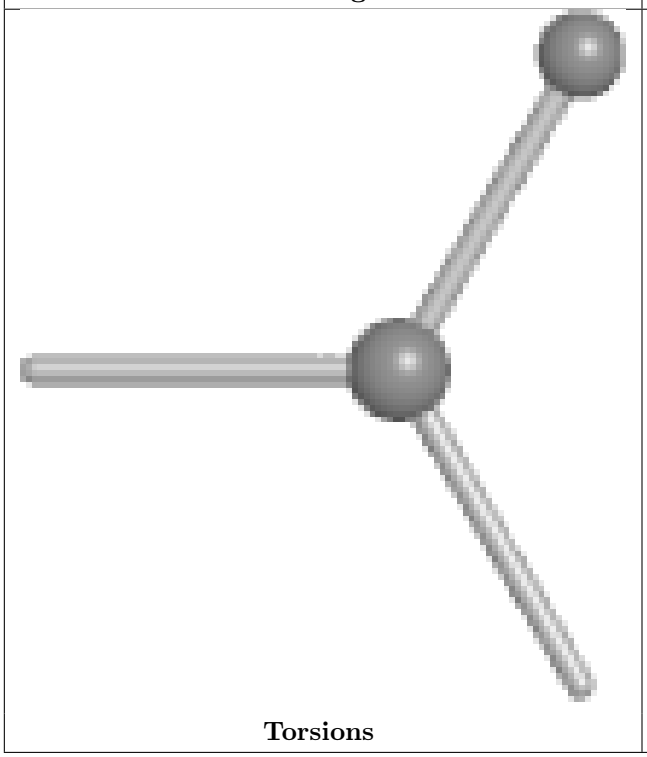
Ligand DMS B 406



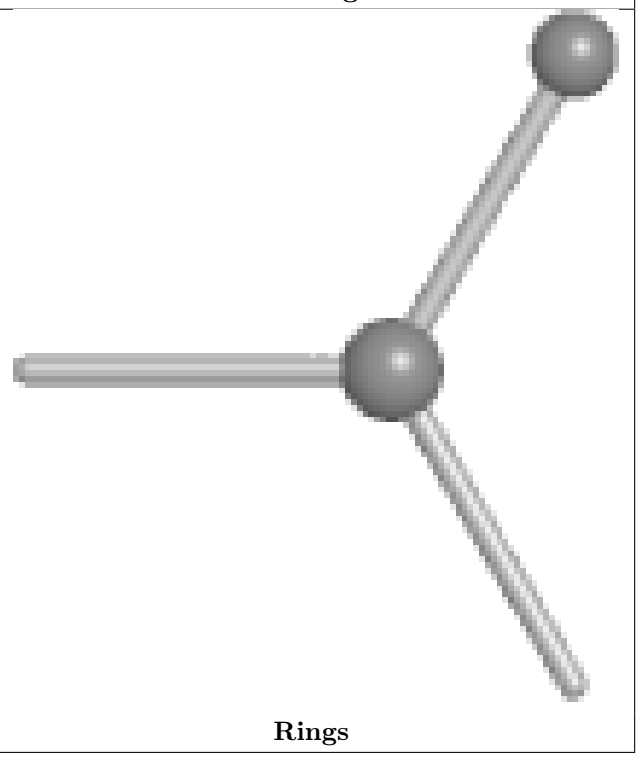
Bond lengths



Bond angles

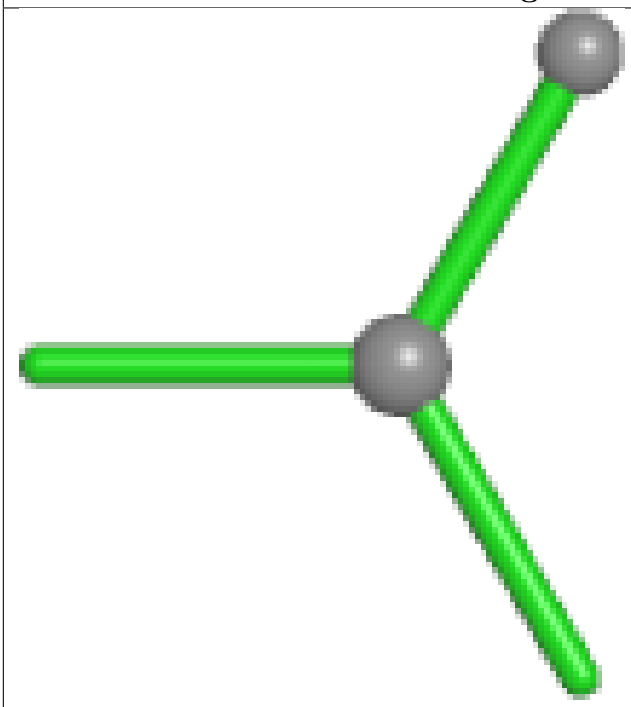


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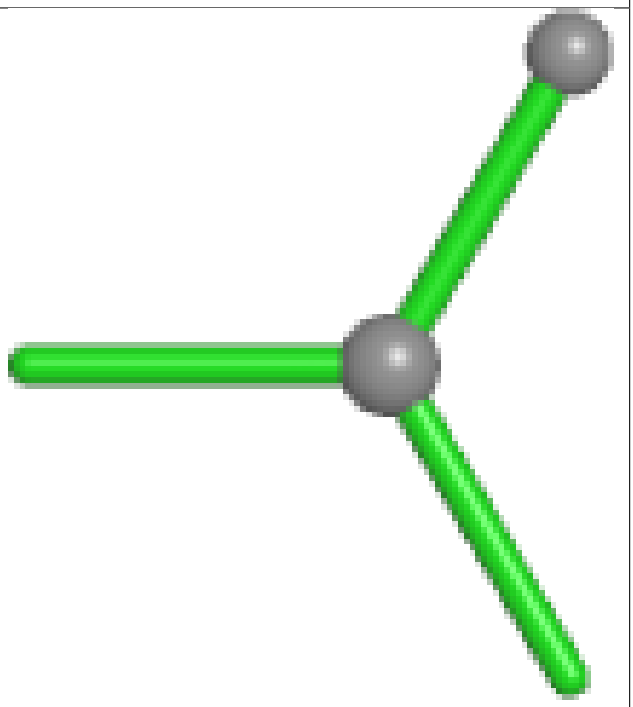


Rings

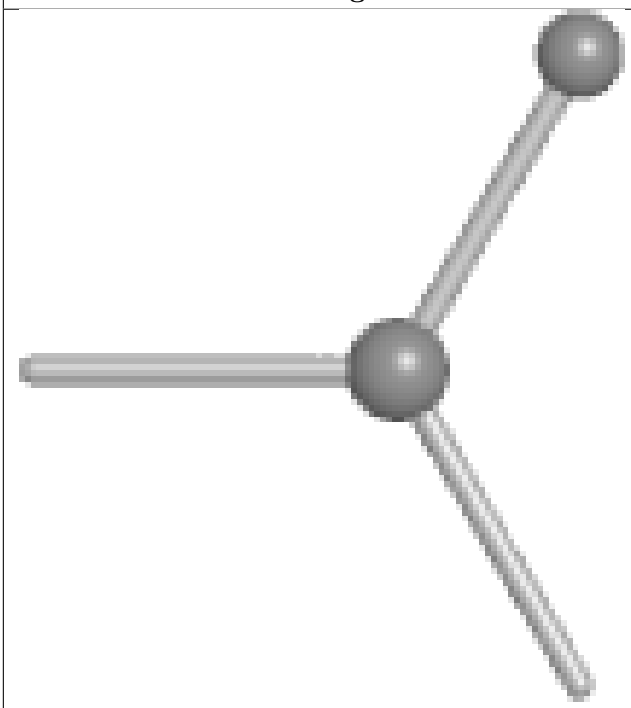
Ligand DMS C 406



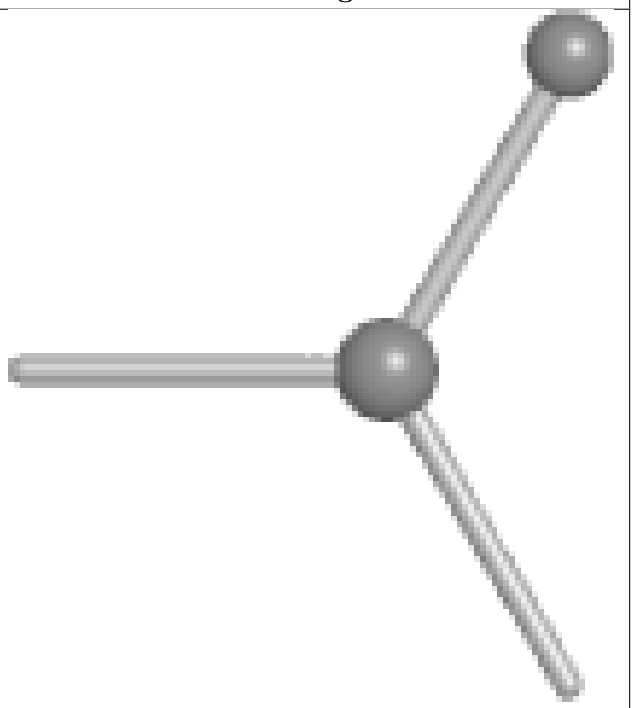
Bond lengths



Bond angles

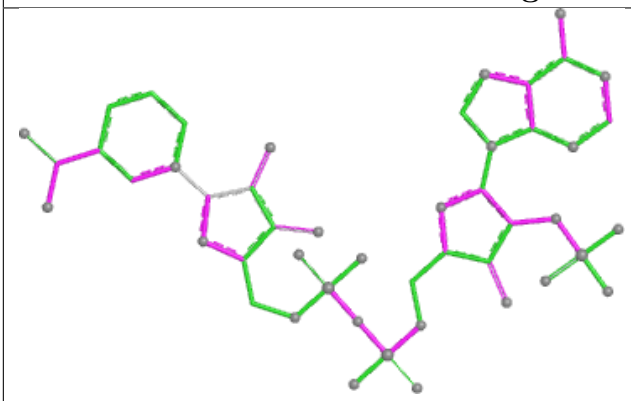


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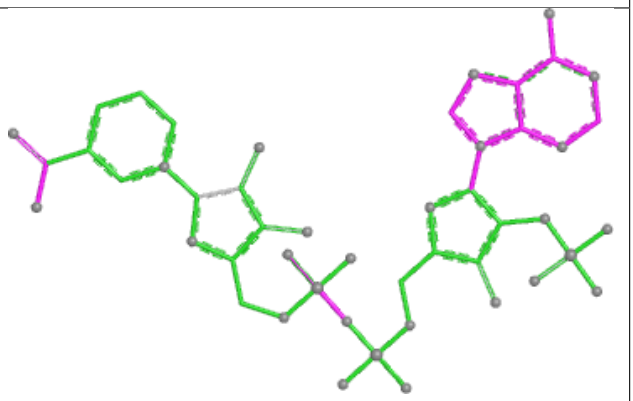


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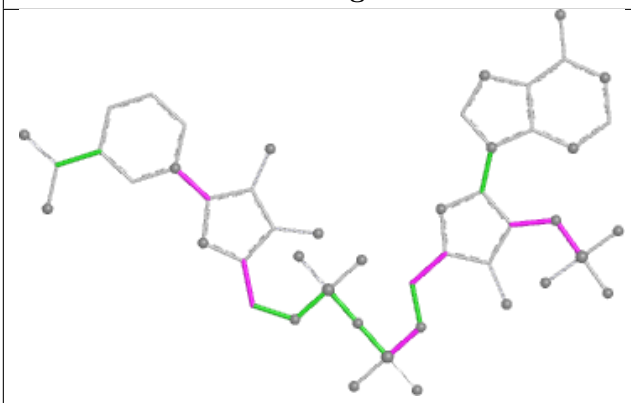
Ligand NAP C 402



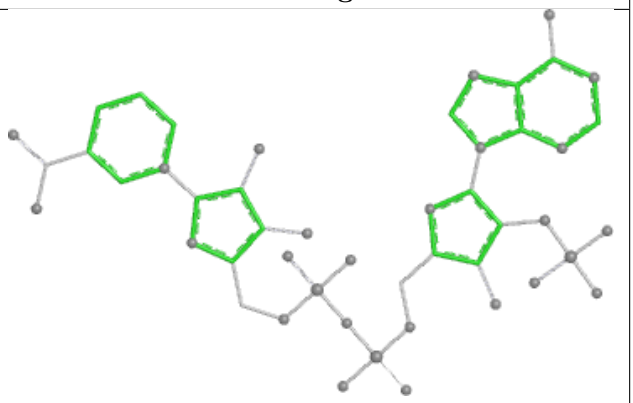
Bond lengths



Bond angles

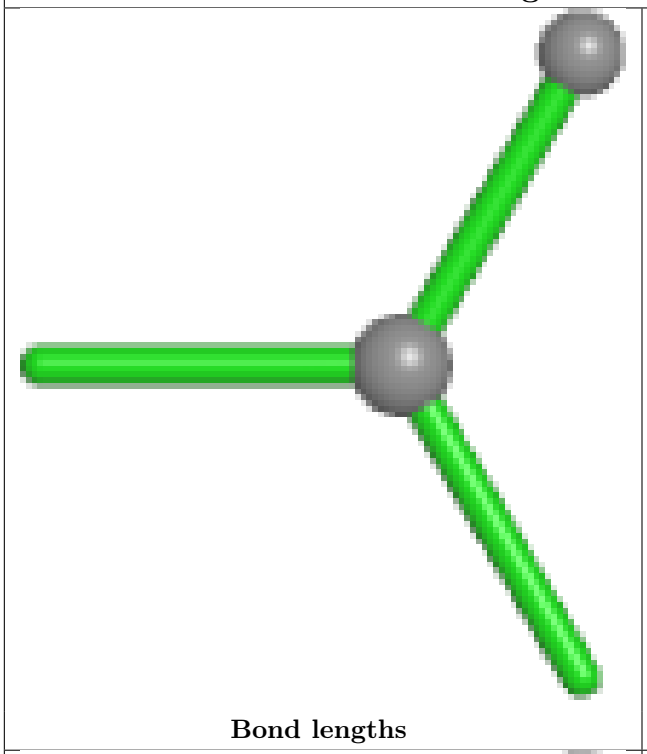


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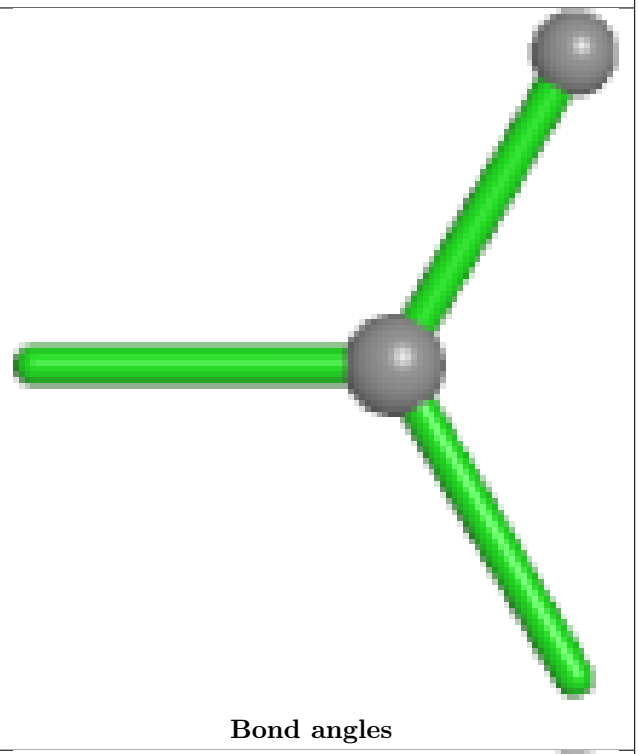


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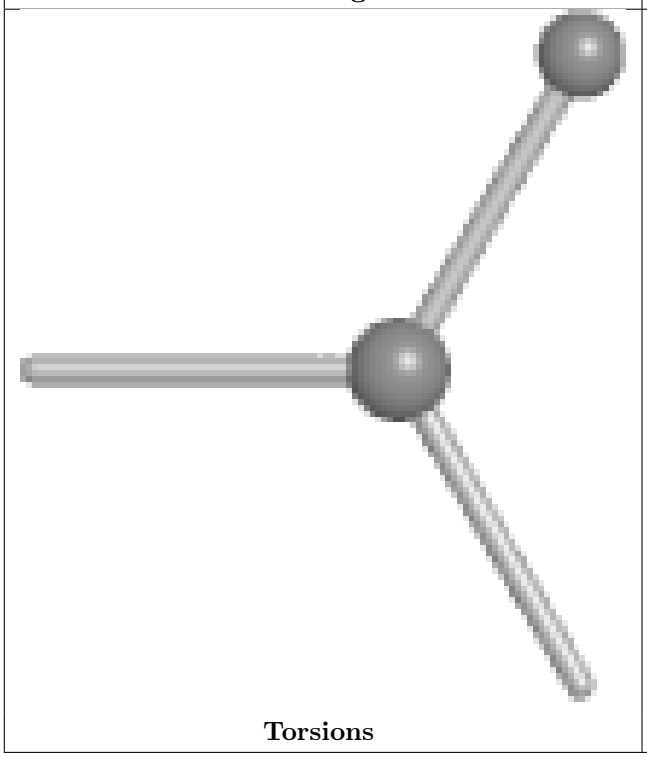
Ligand DMS C 407



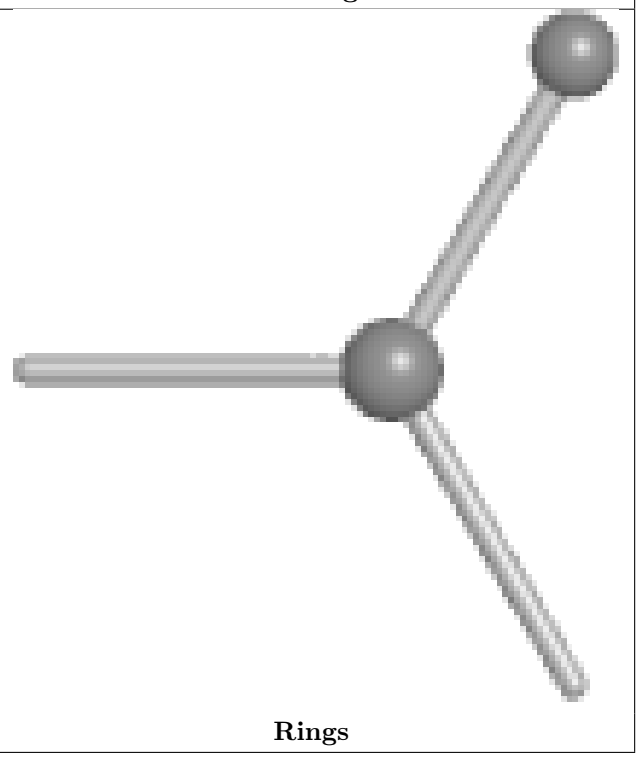
Bond lengths



Bond angles



Torsions



Rings

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	352/352 (100%)	0.31	13 (3%)	45	49	27, 52, 93, 114	0
1	B	352/352 (100%)	0.15	8 (2%)	61	64	19, 47, 81, 123	1 (0%)
1	C	352/352 (100%)	-0.43	3 (0%)	81	84	16, 33, 53, 87	5 (1%)
1	D	352/352 (100%)	-0.43	4 (1%)	78	81	18, 33, 57, 84	2 (0%)
All	All	1408/1408 (100%)	-0.10	28 (1%)	65	68	16, 40, 81, 123	8 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	ALA	3.5
1	D	352	ALA	3.5
1	B	327	PHE	3.1
1	A	48	ALA	3.0
1	A	49	ILE	3.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

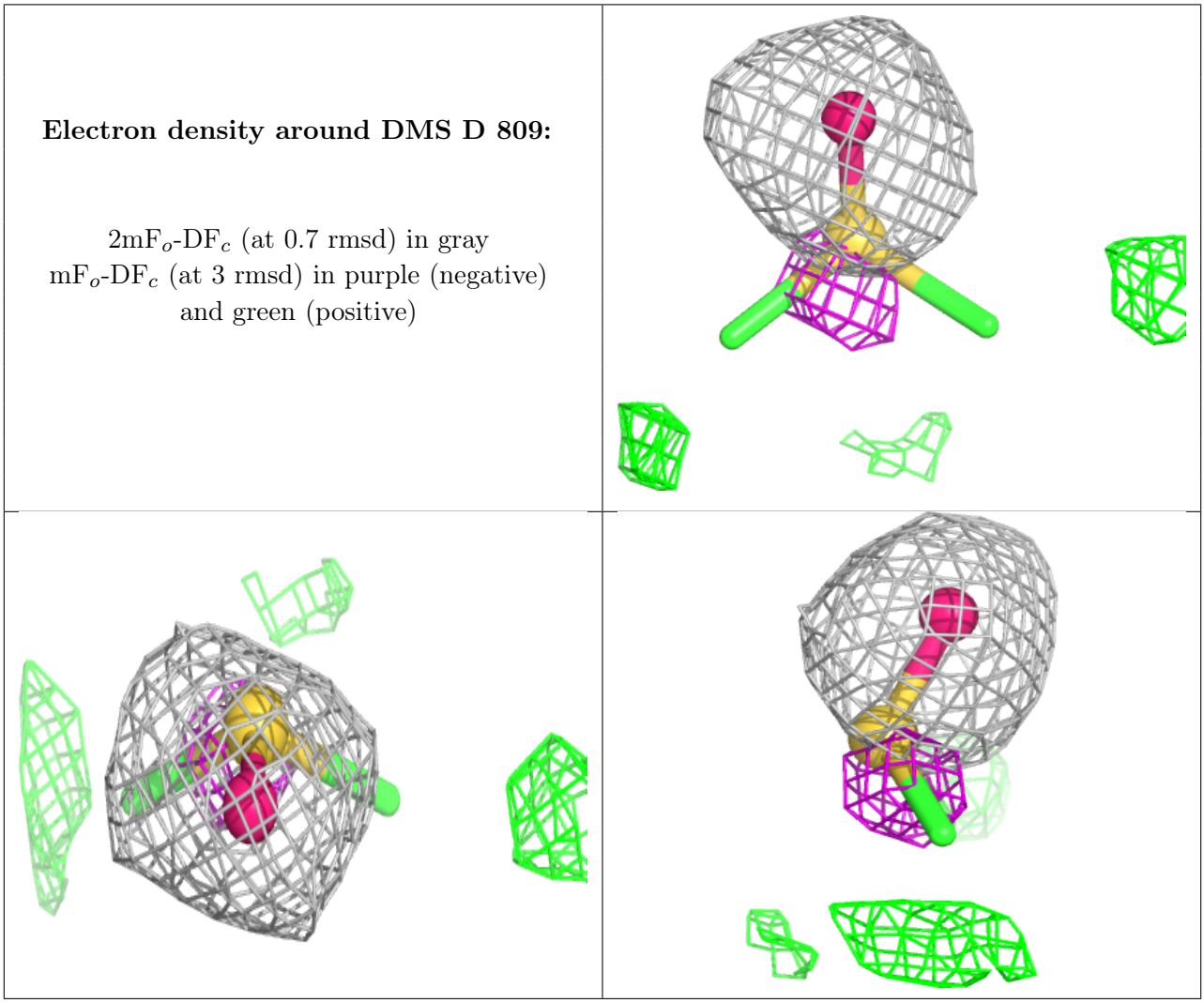
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	DMS	D	809	4/4	0.70	0.23	46,74,87,104	0
3	NAP	A	402	48/48	0.74	0.15	45,69,88,97	48
4	DMS	D	810	4/4	0.75	0.18	67,71,78,92	0
4	DMS	C	408	4/4	0.76	0.18	35,43,70,70	4
4	DMS	A	410	4/4	0.81	0.14	41,54,60,80	0
3	NAP	B	402	48/48	0.81	0.14	42,63,77,84	48
4	DMS	C	407	4/4	0.82	0.16	39,42,56,66	4
4	DMS	C	409	4/4	0.82	0.14	32,54,63,93	0
4	DMS	C	411	4/4	0.85	0.15	46,53,65,102	0
4	DMS	D	801	4/4	0.85	0.15	54,59,59,82	0
4	DMS	A	408	4/4	0.85	0.17	82,82,84,85	0
4	DMS	A	409	4/4	0.85	0.15	55,59,62,83	0
4	DMS	B	409	4/4	0.87	0.11	46,47,61,71	0
4	DMS	A	406	4/4	0.87	0.13	49,62,67,83	0
4	DMS	D	807	4/4	0.87	0.13	41,49,55,63	0
3	NAP	C	402	48/48	0.87	0.12	16,44,65,72	48
4	DMS	B	407	4/4	0.87	0.13	49,52,53,79	0
4	DMS	A	407	4/4	0.88	0.13	51,51,63,65	0
3	NAP	D	803	48/48	0.88	0.12	21,43,60,67	48
4	DMS	C	410	4/4	0.89	0.15	48,65,72,78	0
4	DMS	B	410	4/4	0.89	0.14	55,65,72,82	0
4	DMS	B	406	4/4	0.90	0.12	42,52,55,78	0
4	DMS	D	808	4/4	0.90	0.12	49,52,66,79	0
4	DMS	B	404	4/4	0.91	0.14	40,44,52,58	4
4	DMS	B	405	4/4	0.91	0.12	36,48,49,61	0
4	DMS	B	408	4/4	0.91	0.10	43,44,46,60	0
4	DMS	A	404	4/4	0.92	0.11	40,48,59,67	0
4	DMS	A	405	4/4	0.92	0.15	54,56,62,74	4
4	DMS	A	411	4/4	0.93	0.12	52,58,66,66	0
4	DMS	C	405	4/4	0.94	0.10	38,39,46,67	0
4	DMS	D	811	4/4	0.94	0.10	40,44,45,54	0
4	DMS	C	404	4/4	0.96	0.11	41,43,47,52	0
4	DMS	A	403	4/4	0.96	0.09	37,39,40,48	4
4	DMS	C	406	4/4	0.96	0.09	40,51,59,59	0
4	DMS	D	805	4/4	0.96	0.11	38,43,49,52	0
4	DMS	D	806	4/4	0.96	0.08	27,35,36,44	4
4	DMS	B	403	4/4	0.97	0.07	27,40,46,48	0
4	DMS	C	403	4/4	0.97	0.07	32,36,37,43	4
4	DMS	D	804	4/4	0.98	0.07	34,37,46,46	0
2	ZN	A	401	1/1	0.98	0.04	62,62,62,62	1
2	ZN	B	401	1/1	0.99	0.03	43,43,43,43	1
2	ZN	D	802	1/1	1.00	0.02	31,31,31,31	1
2	ZN	C	401	1/1	1.00	0.04	28,28,28,28	1

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.

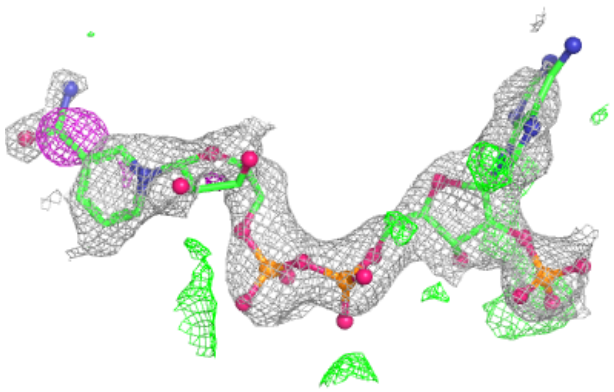
Electron density around DMS D 809:

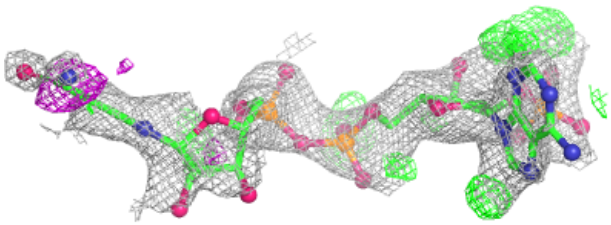
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

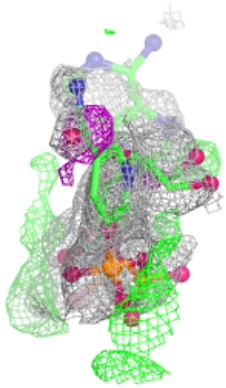


Electron density around NAP A 402:

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

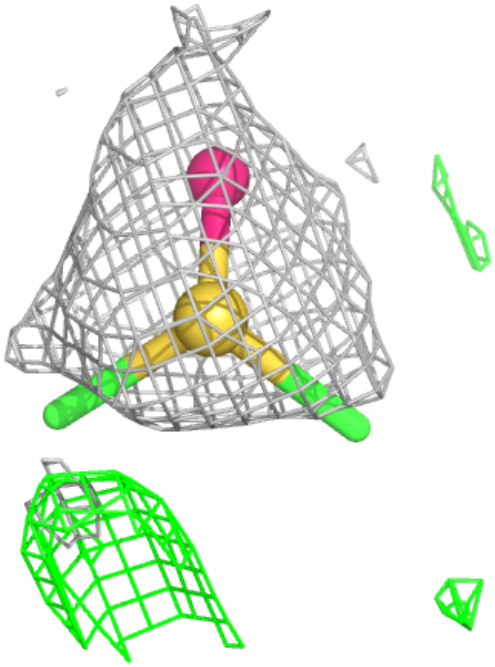


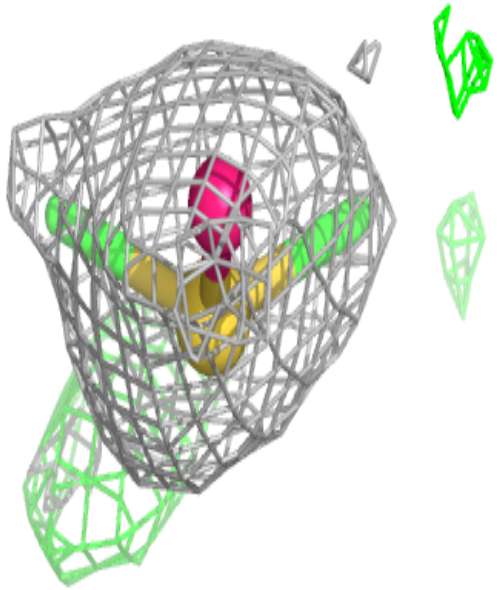


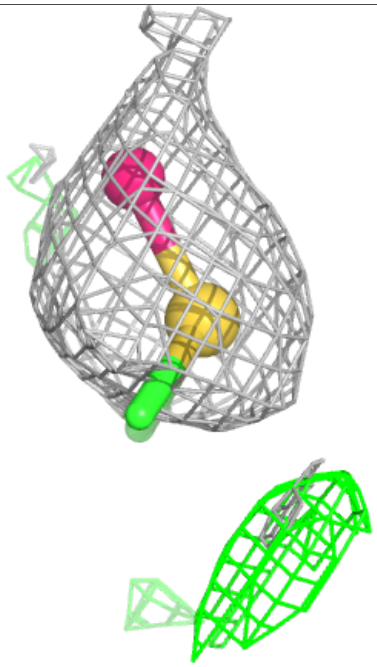


Electron density around DMS D 810:

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

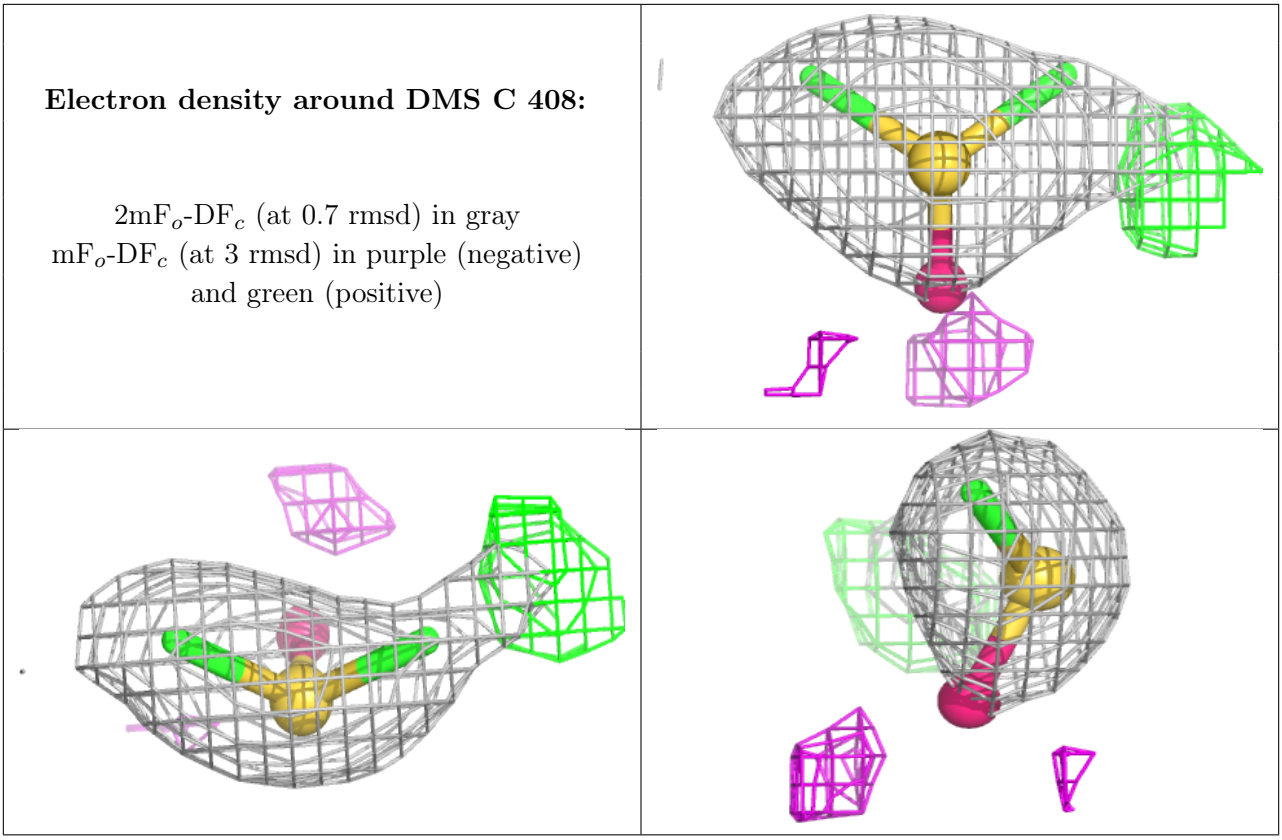






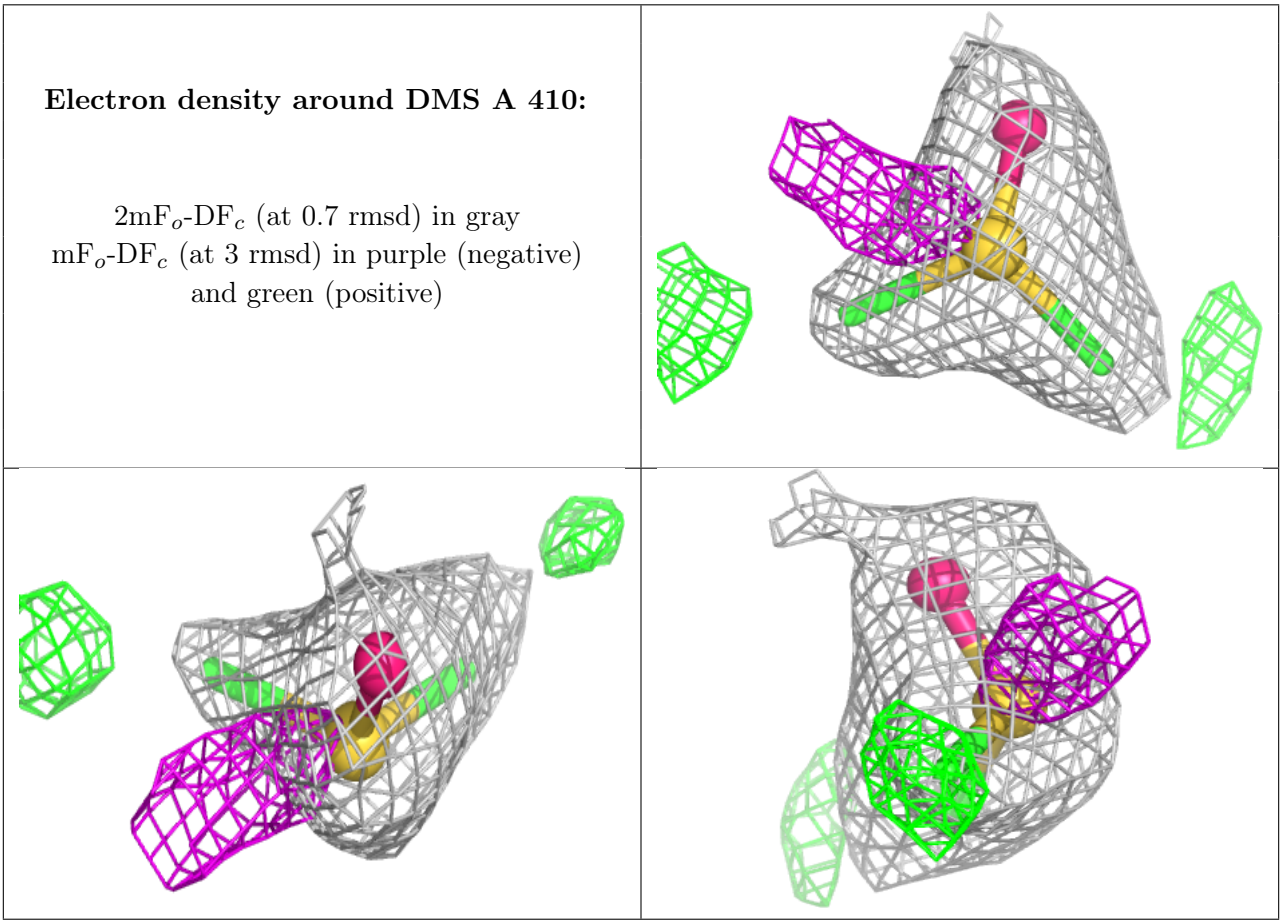
Electron density around DMS C 408:

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



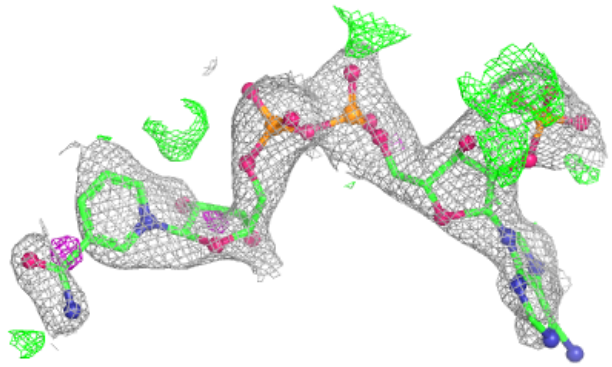
Electron density around DMS A 410:

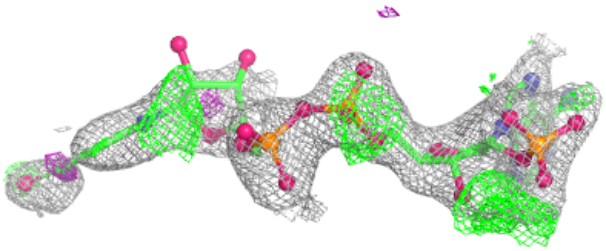
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

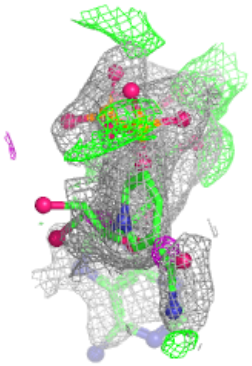


Electron density around NAP B 402:

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

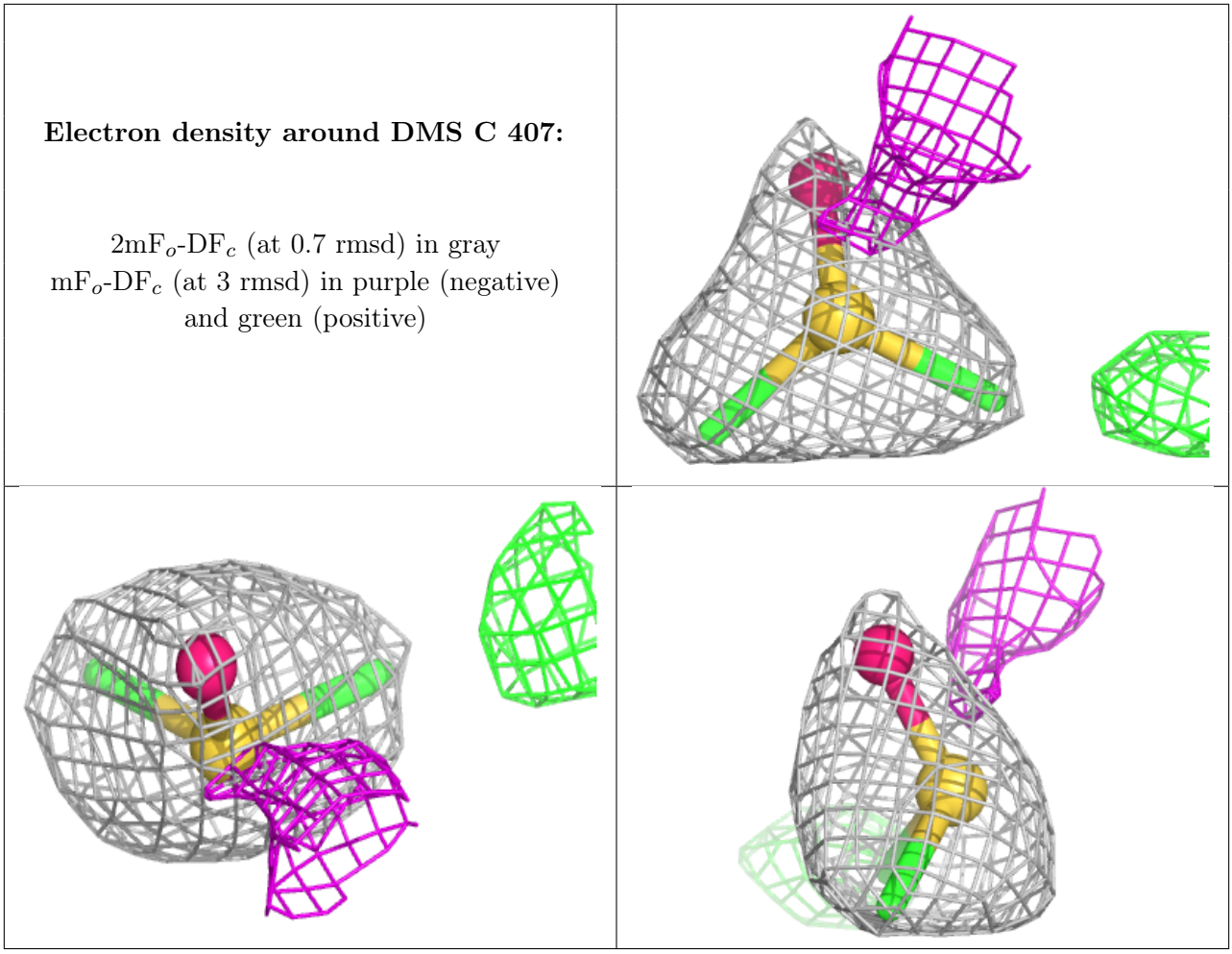






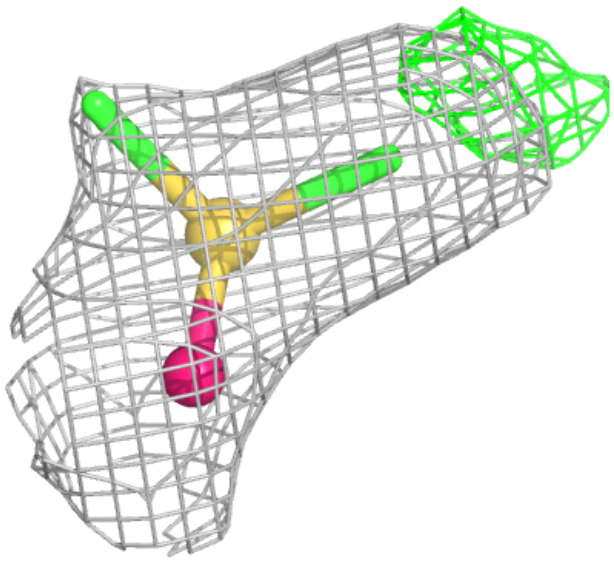
Electron density around DMS C 407:

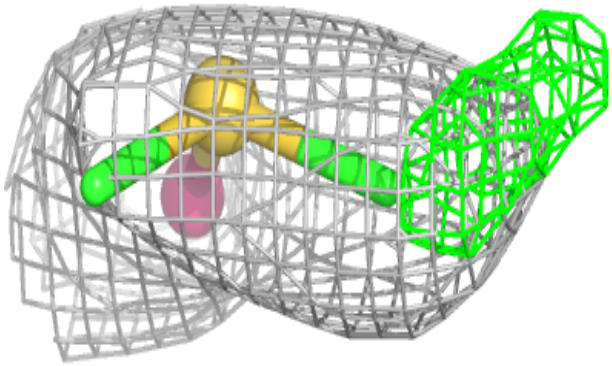
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

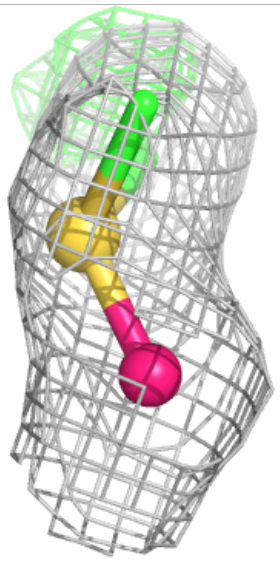


Electron density around DMS C 409:

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

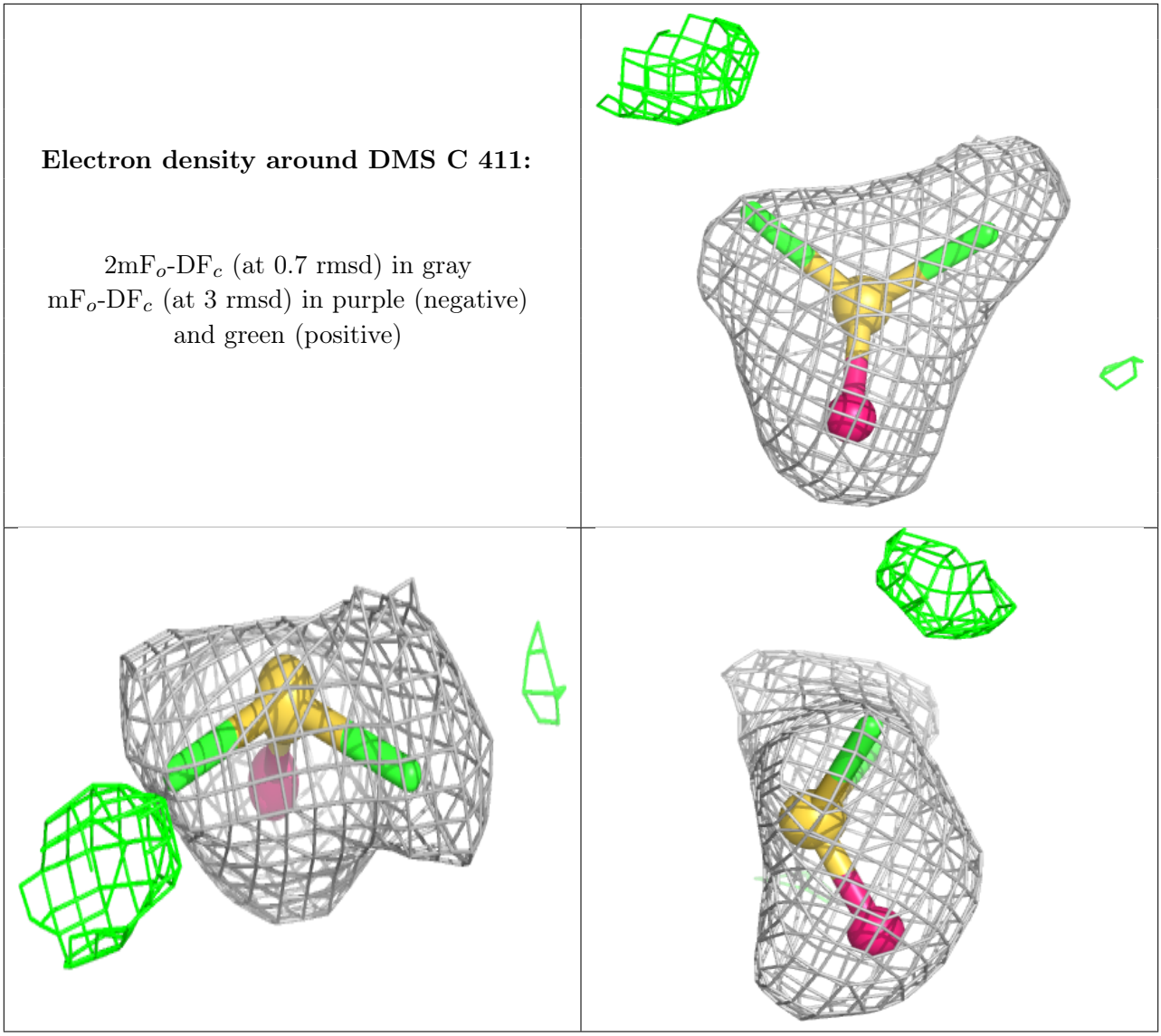






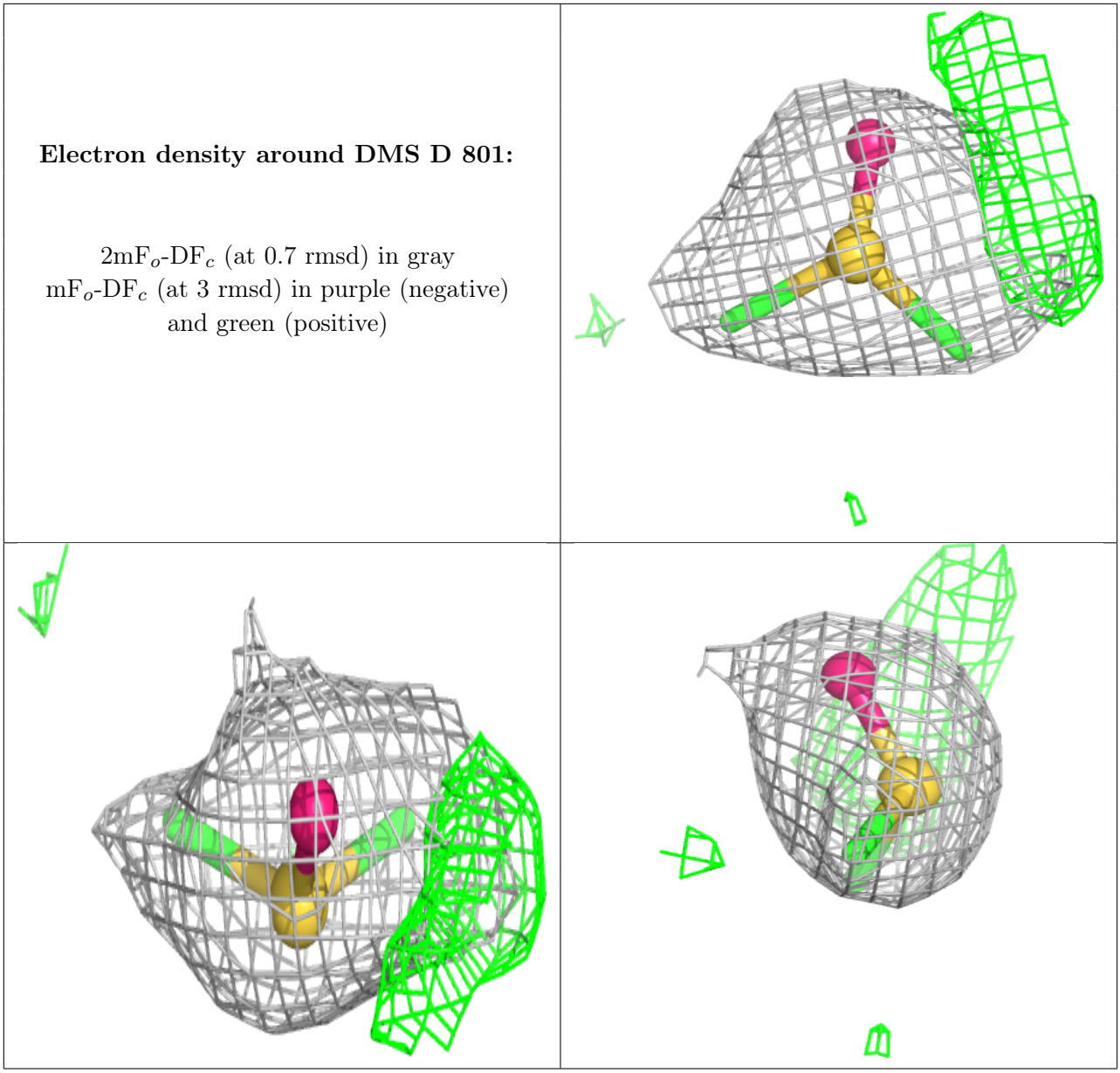
Electron density around DMS C 411:

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



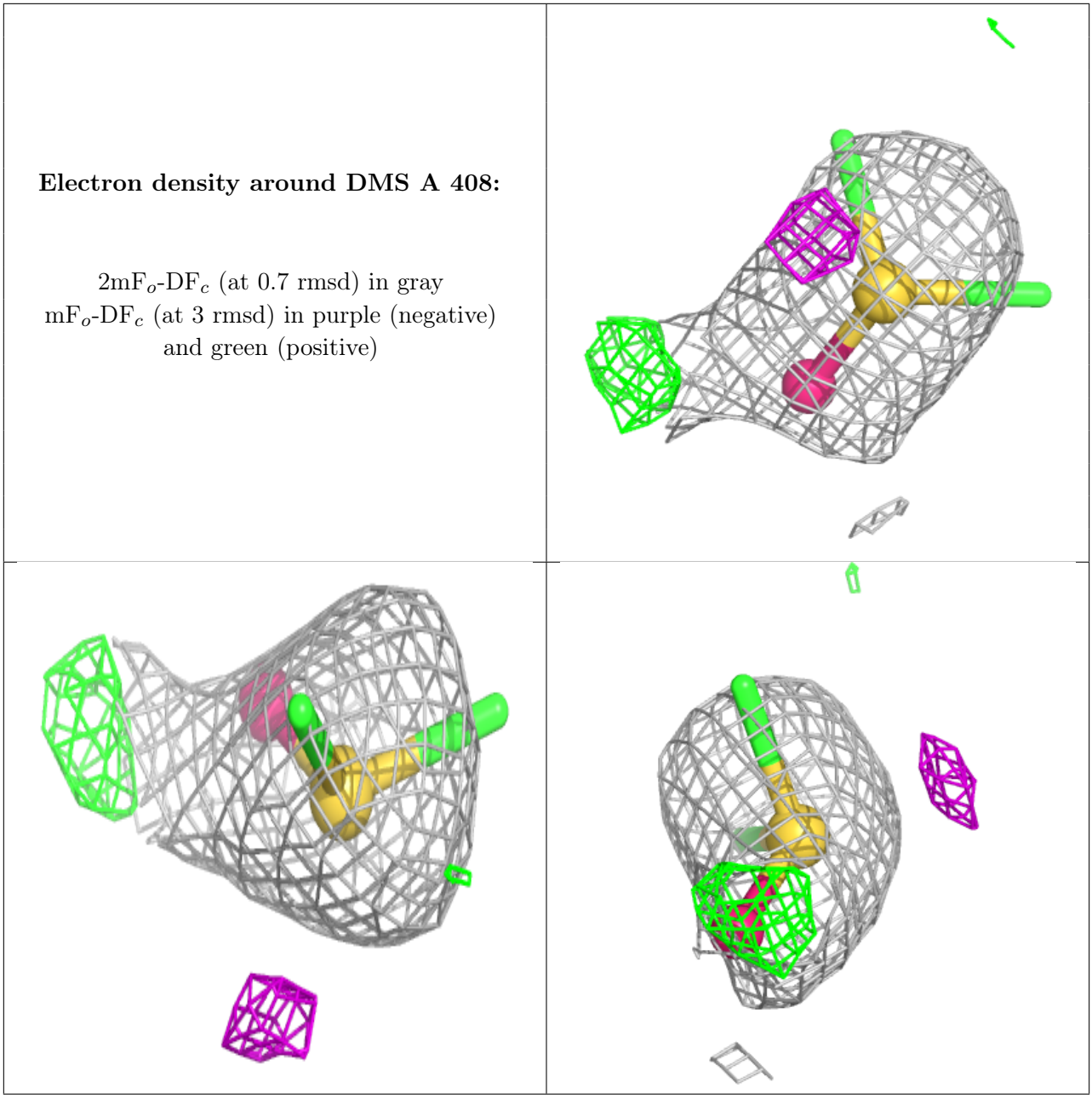
Electron density around DMS D 801:

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



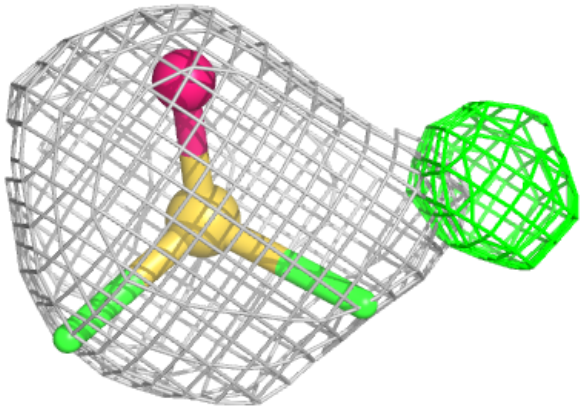
Electron density around DMS A 408:

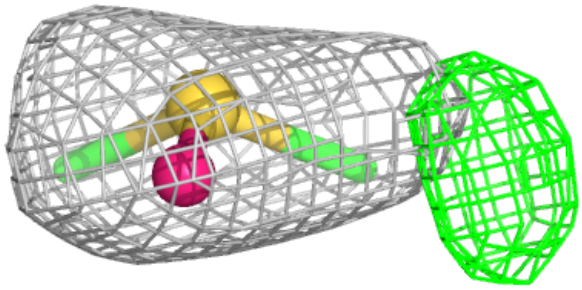
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

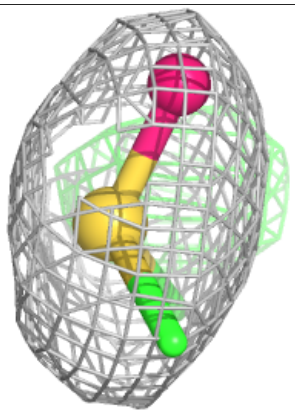


Electron density around DMS A 409:

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

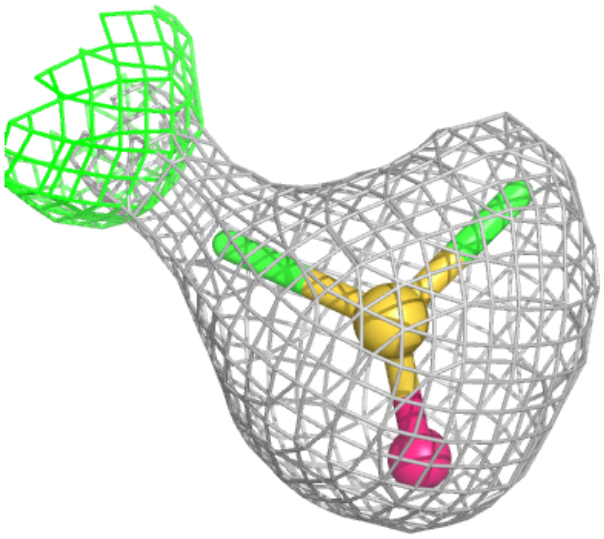


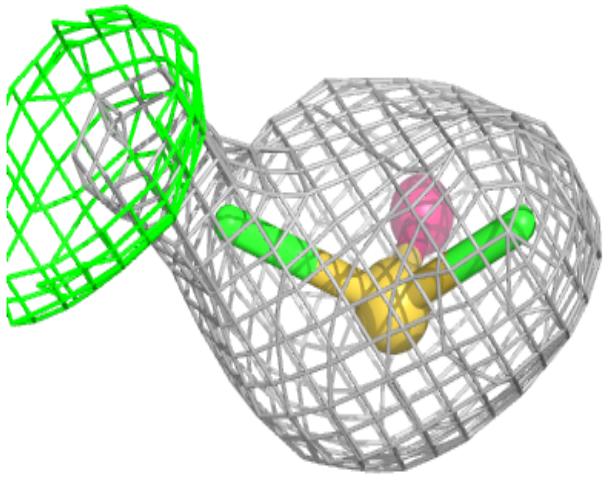


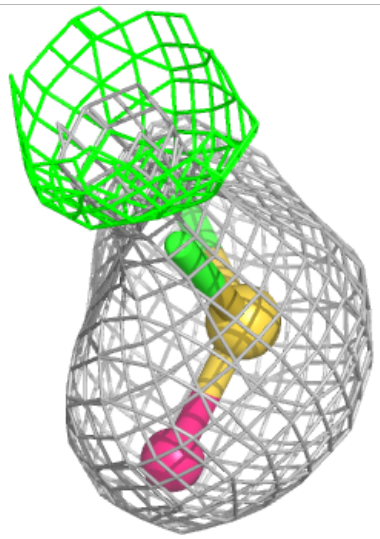


Electron density around DMS B 409:

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

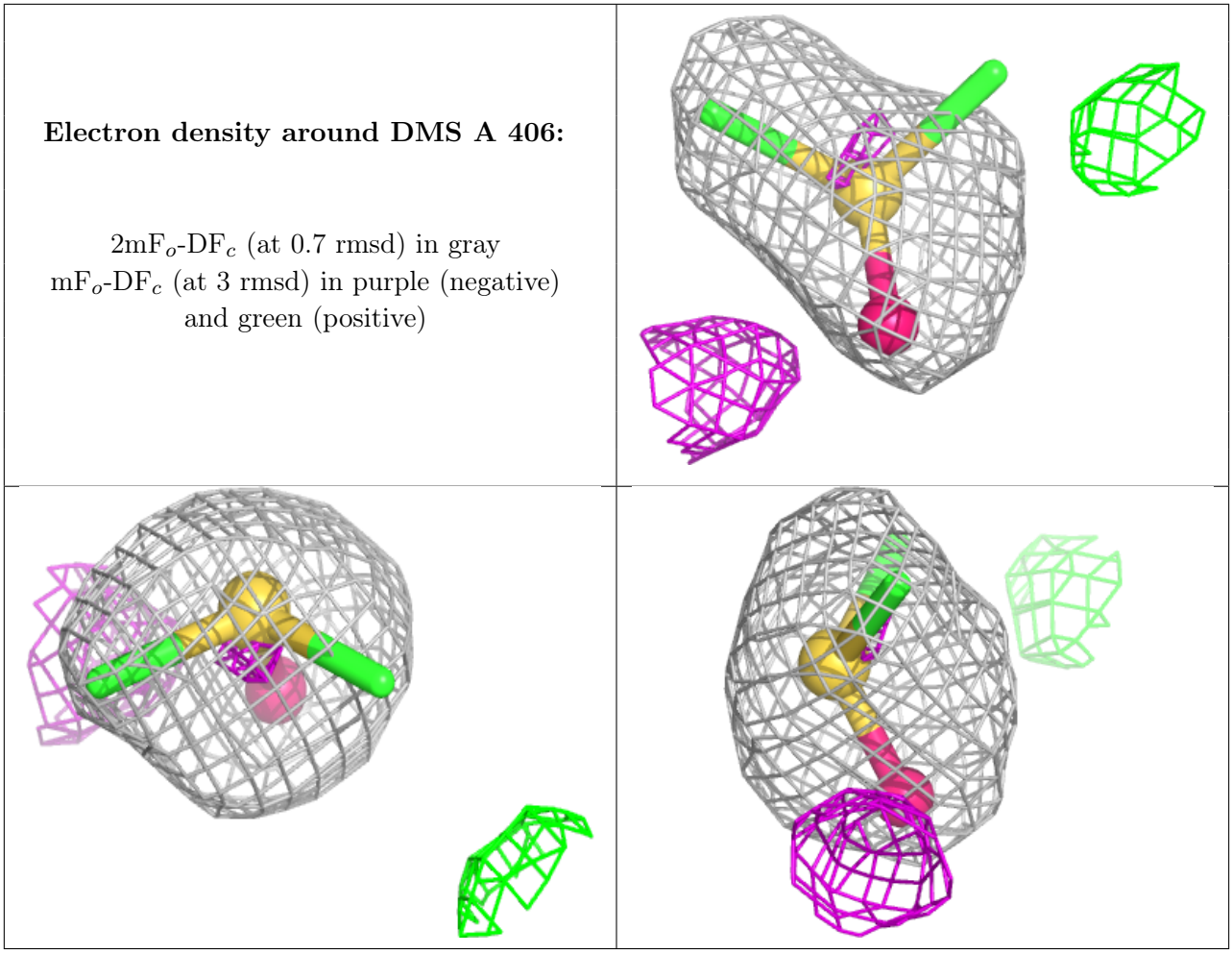






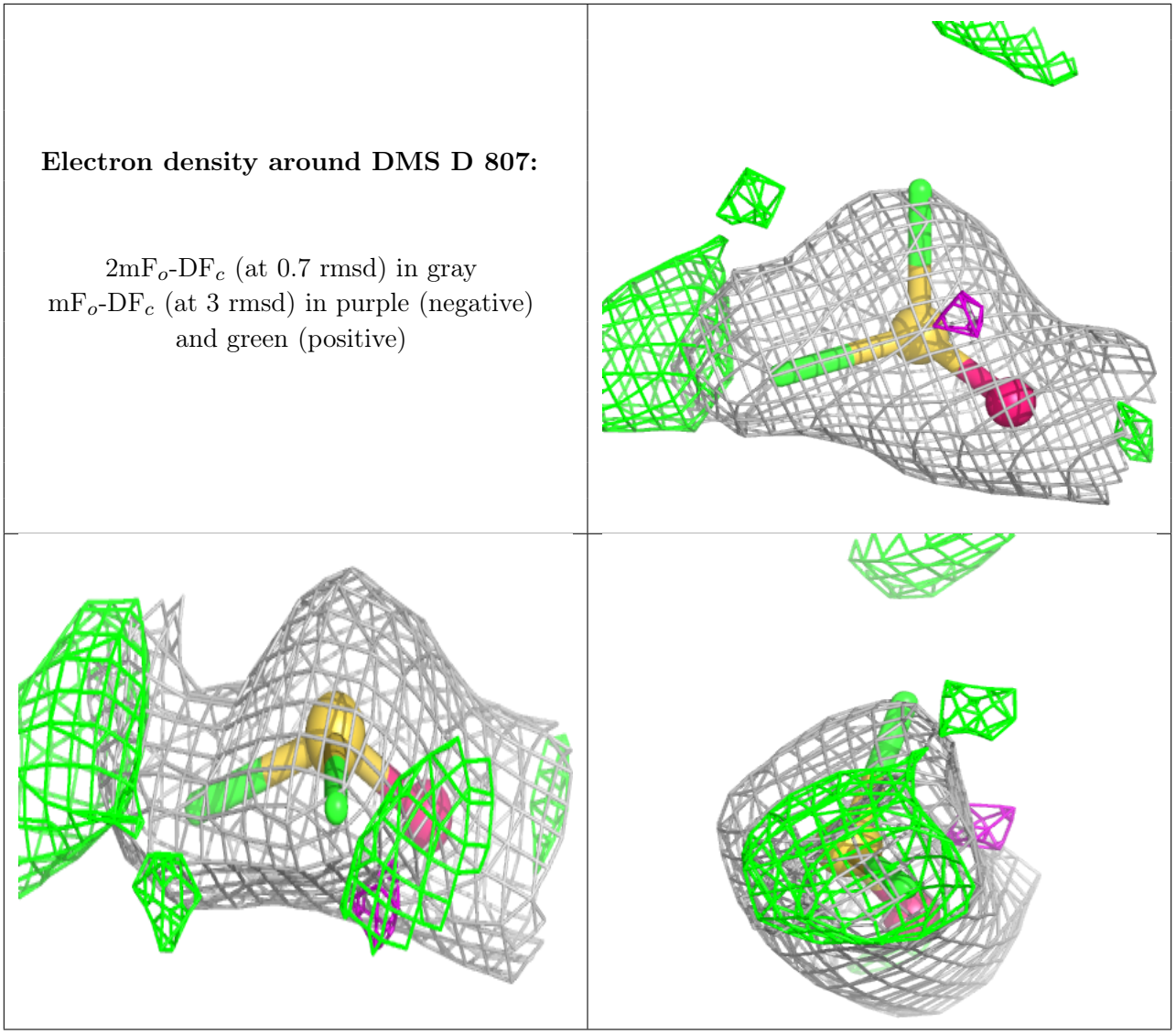
Electron density around DMS A 406:

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



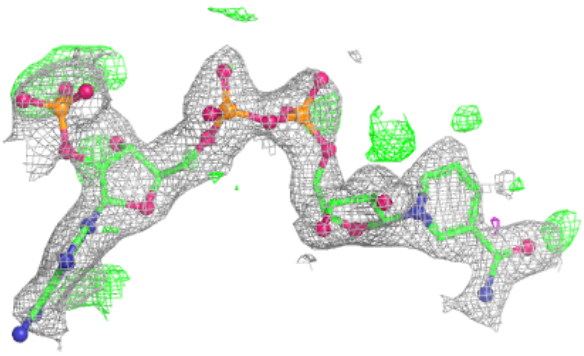
Electron density around DMS D 807:

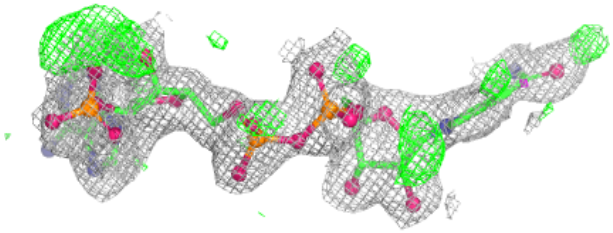
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAP 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)

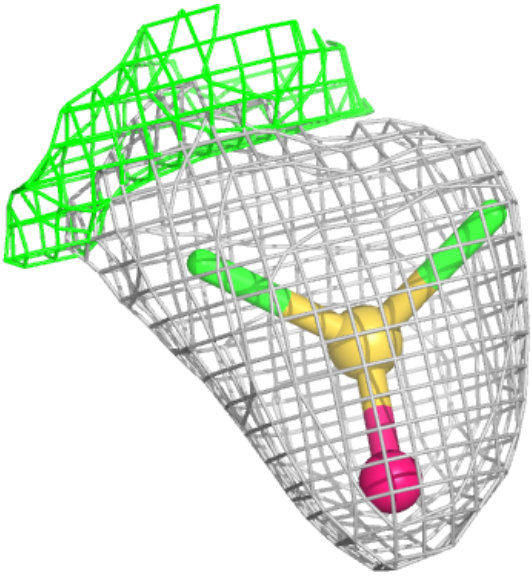


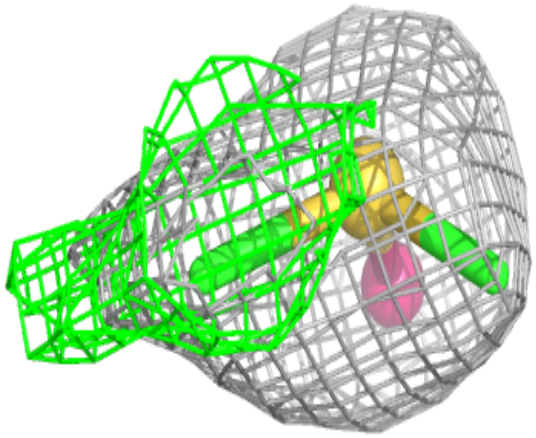


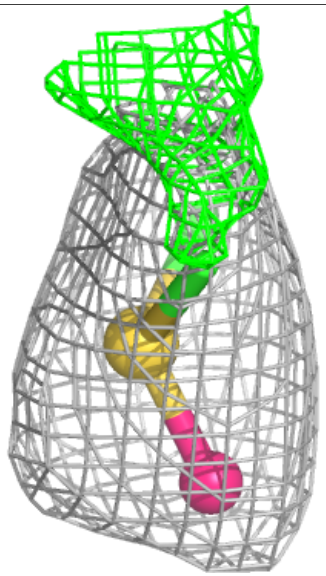


Electron density around DMS B 407:

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

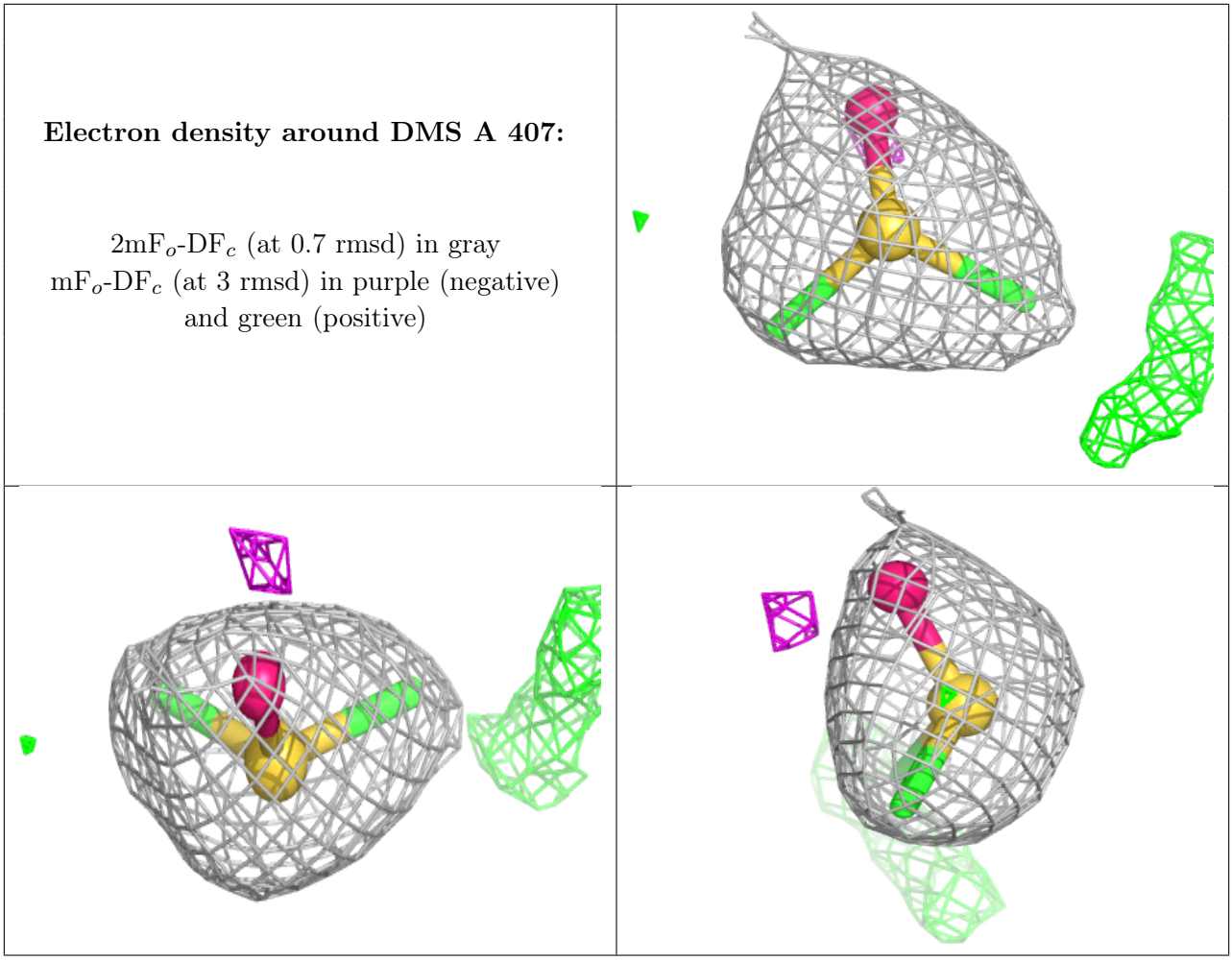






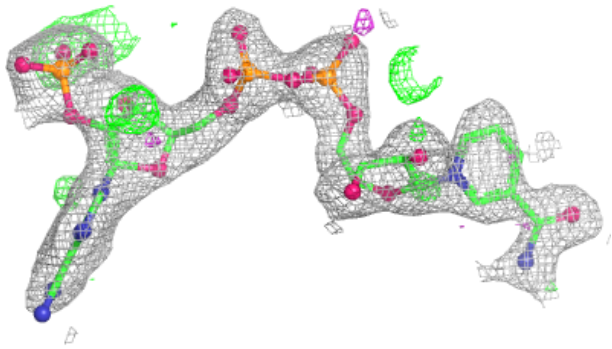
Electron density around DMS A 407:

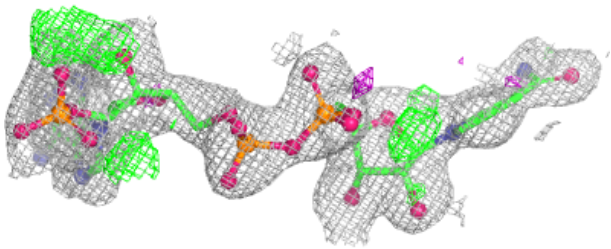
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

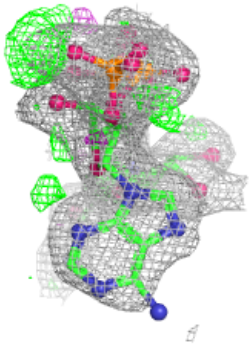


Electron density around NAP D 803:

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

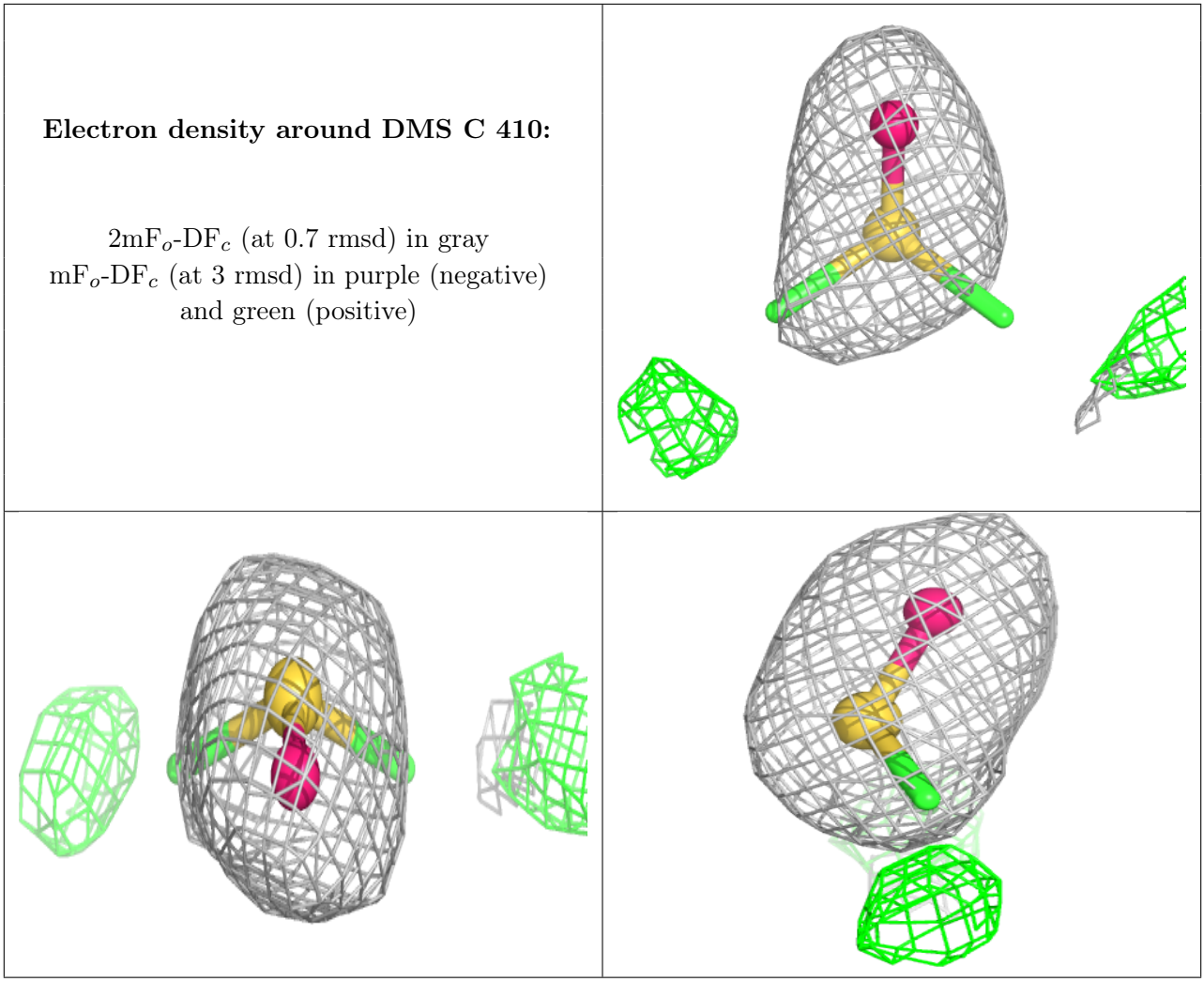






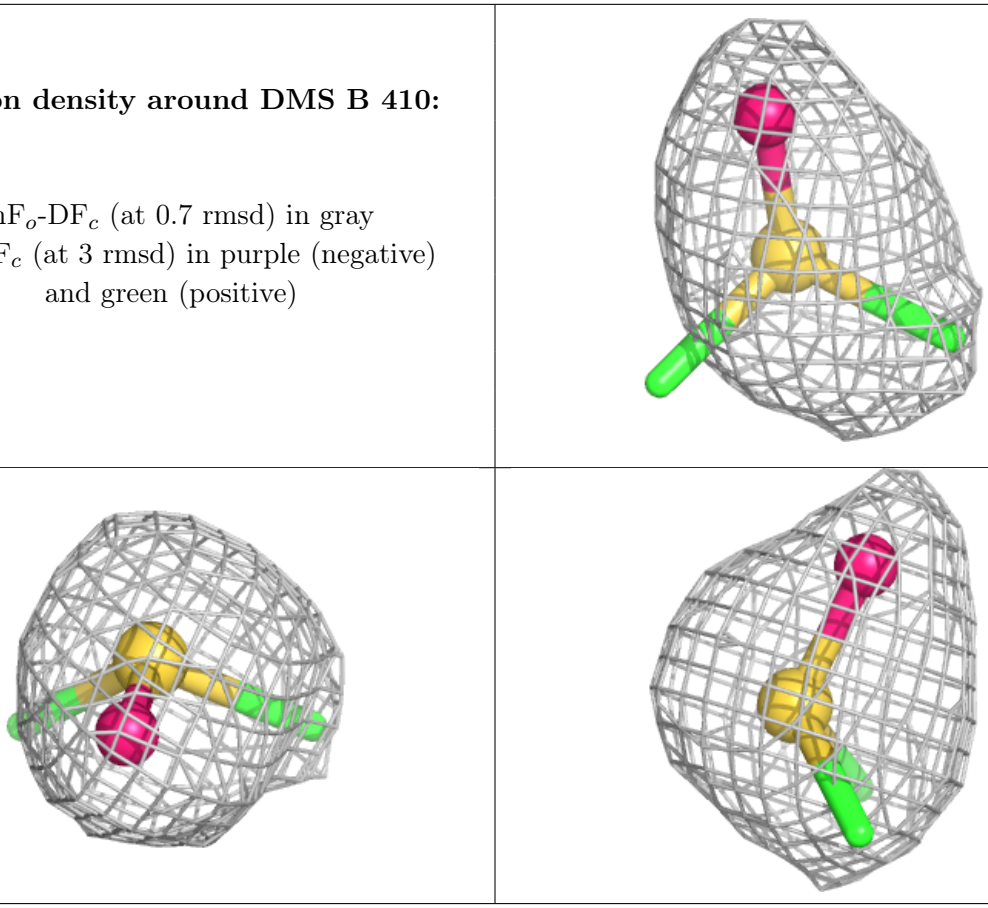
Electron density around DMS C 410:

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



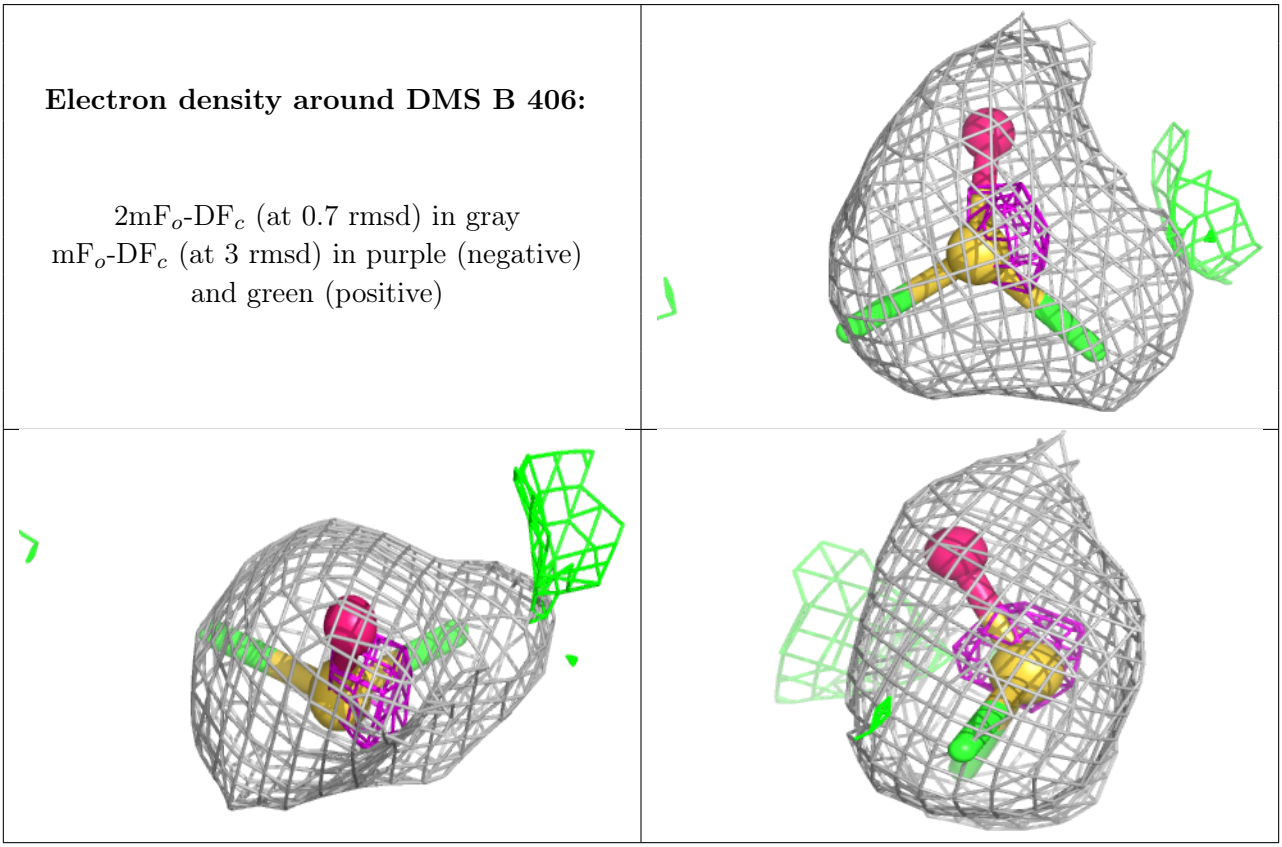
Electron density around DMS B 410:

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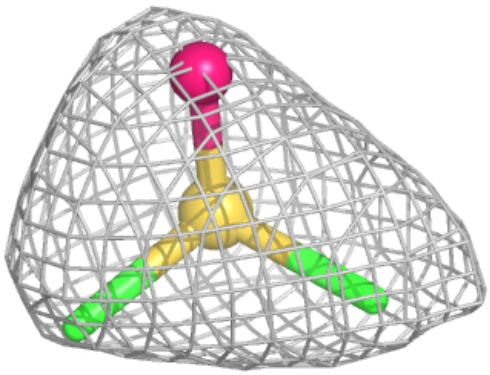
Electron density around DMS B 406:

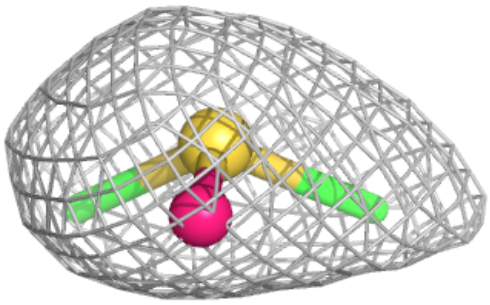
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

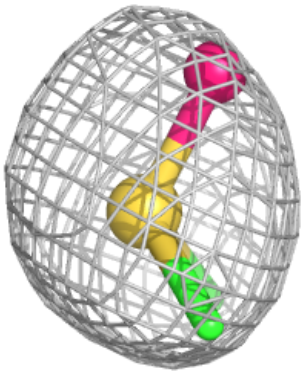


Electron density around DMS D 808:

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

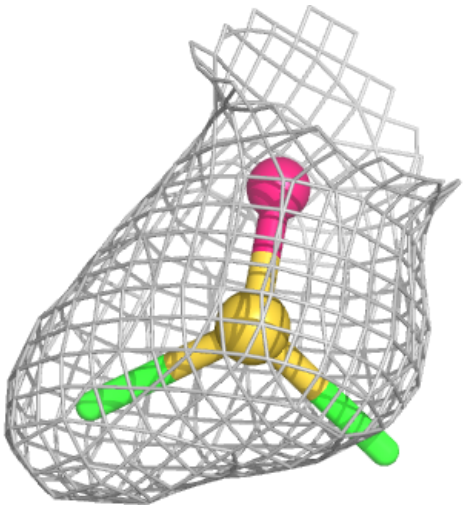


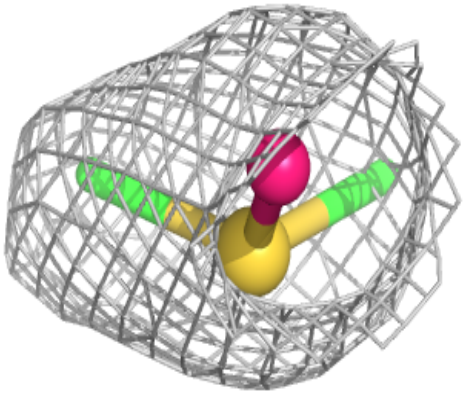


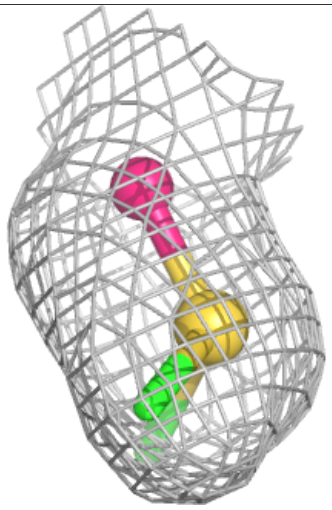


Electron density around DMS B 404:

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

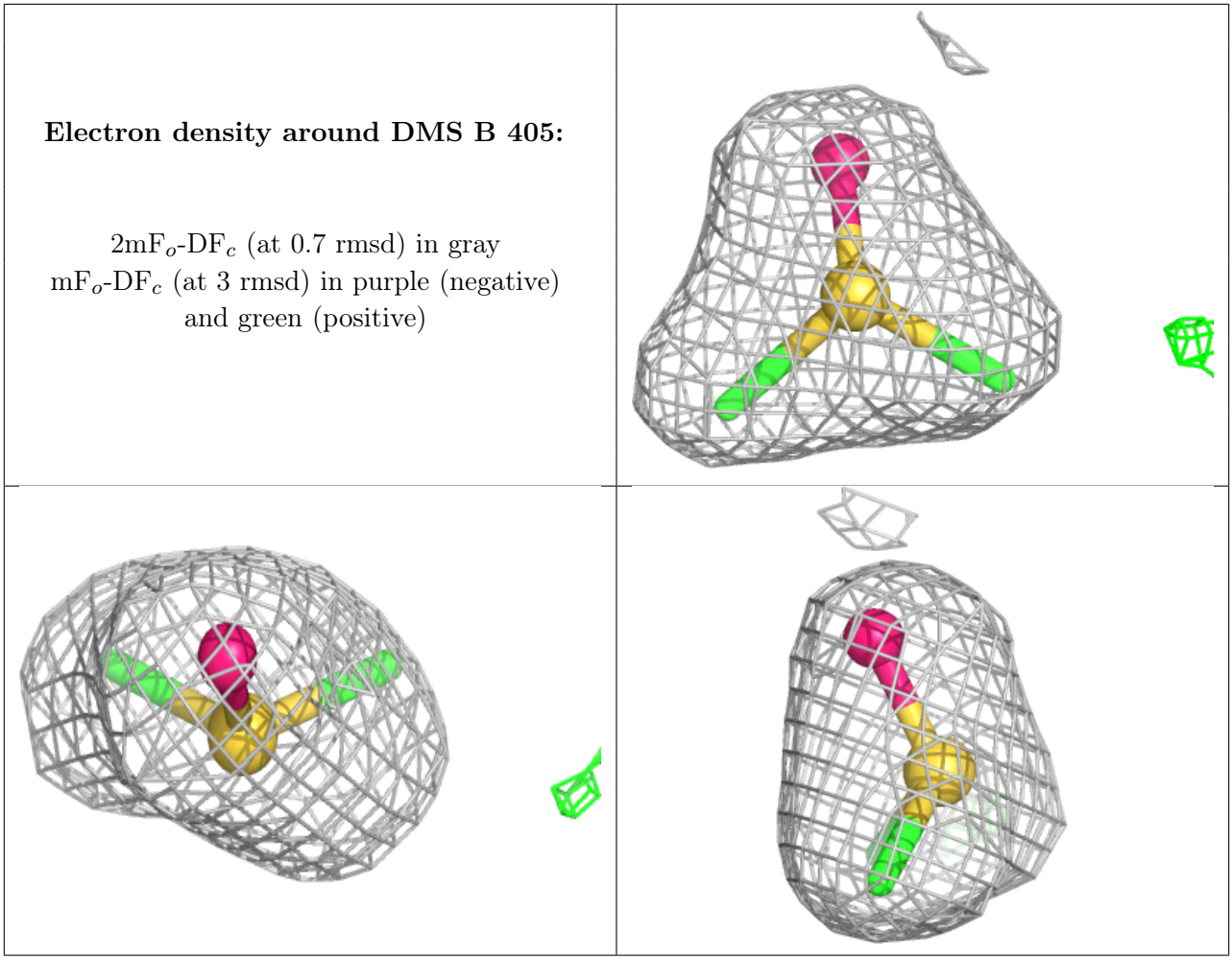






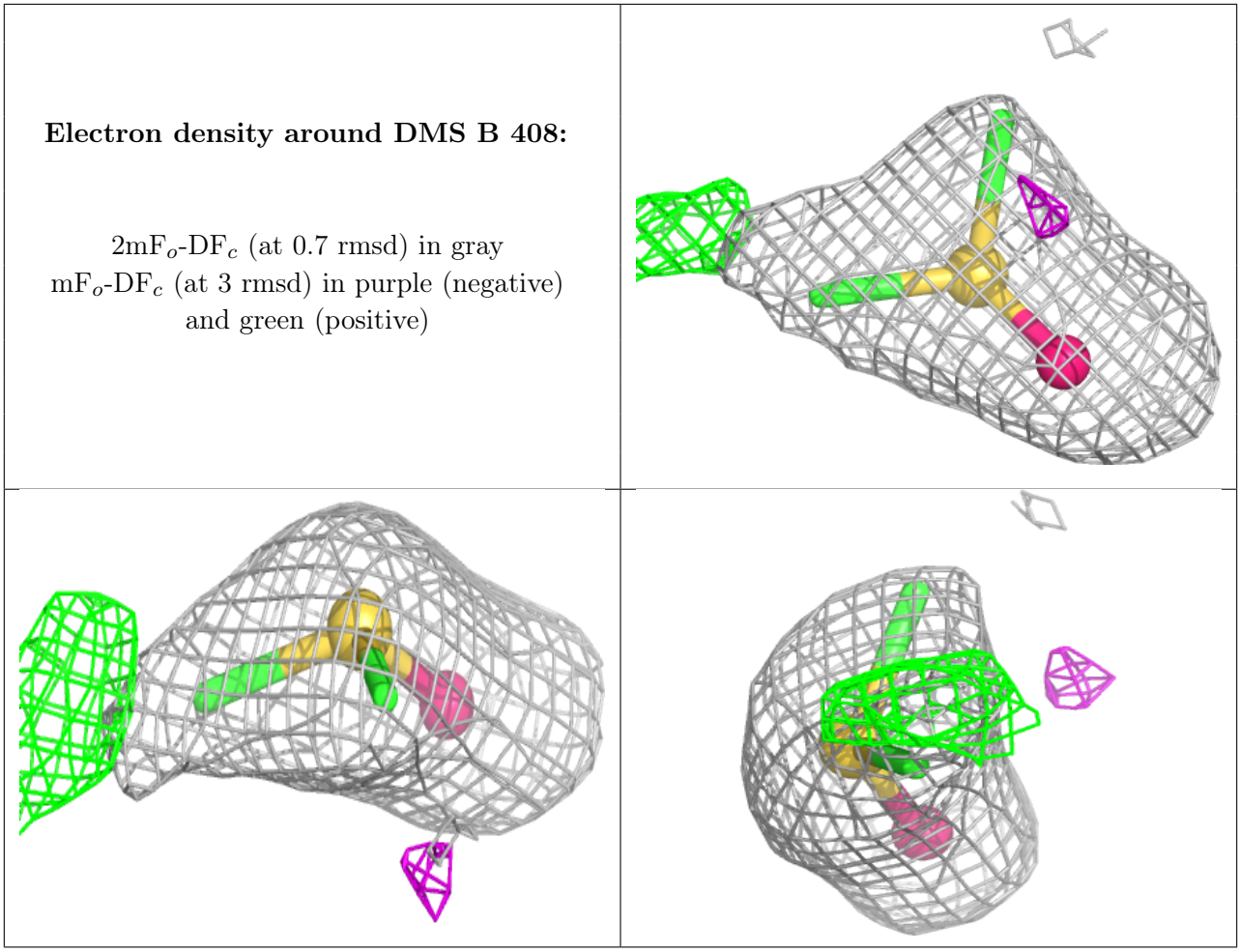
Electron density around DMS B 405:

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



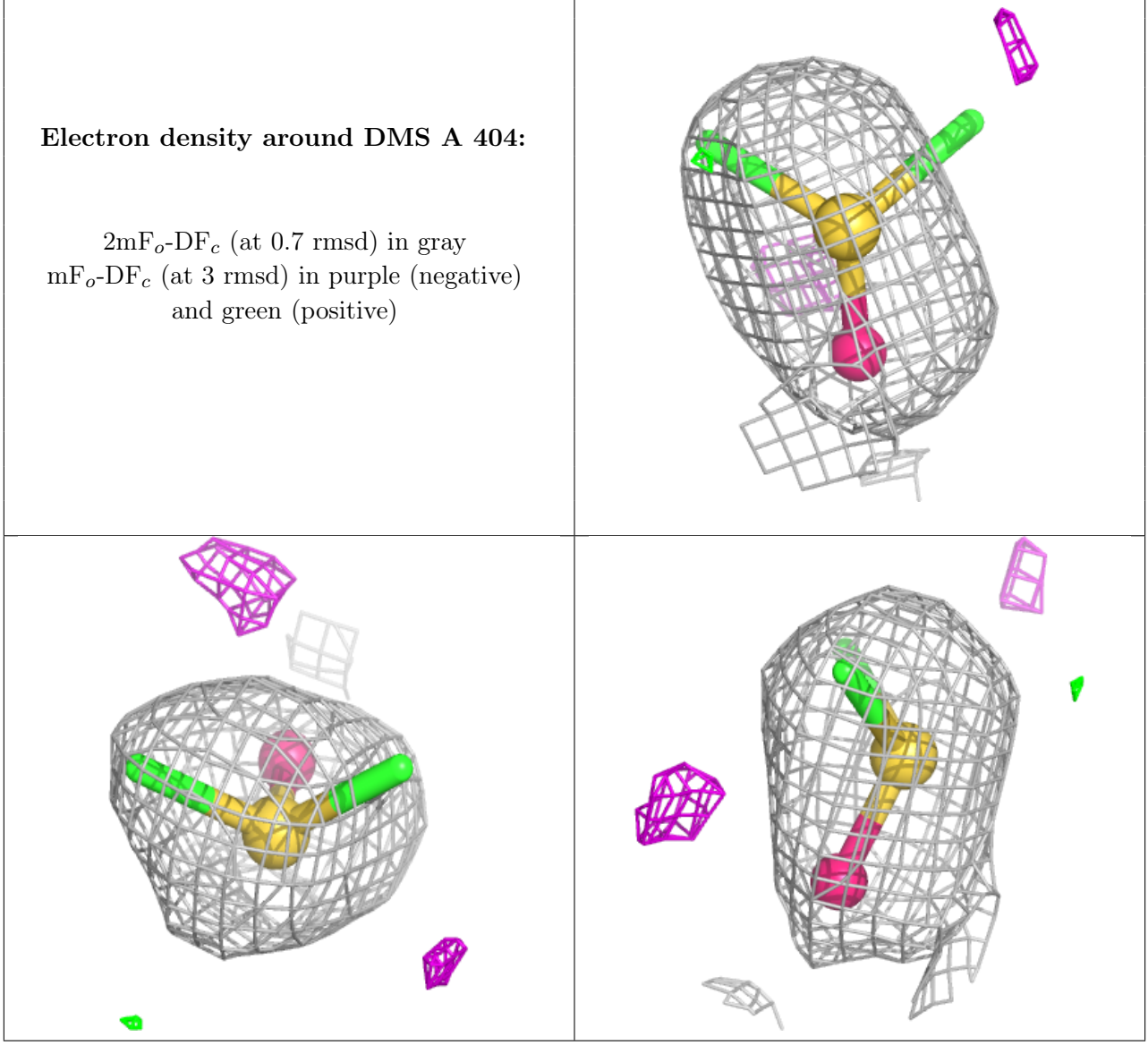
Electron density around DMS B 408:

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



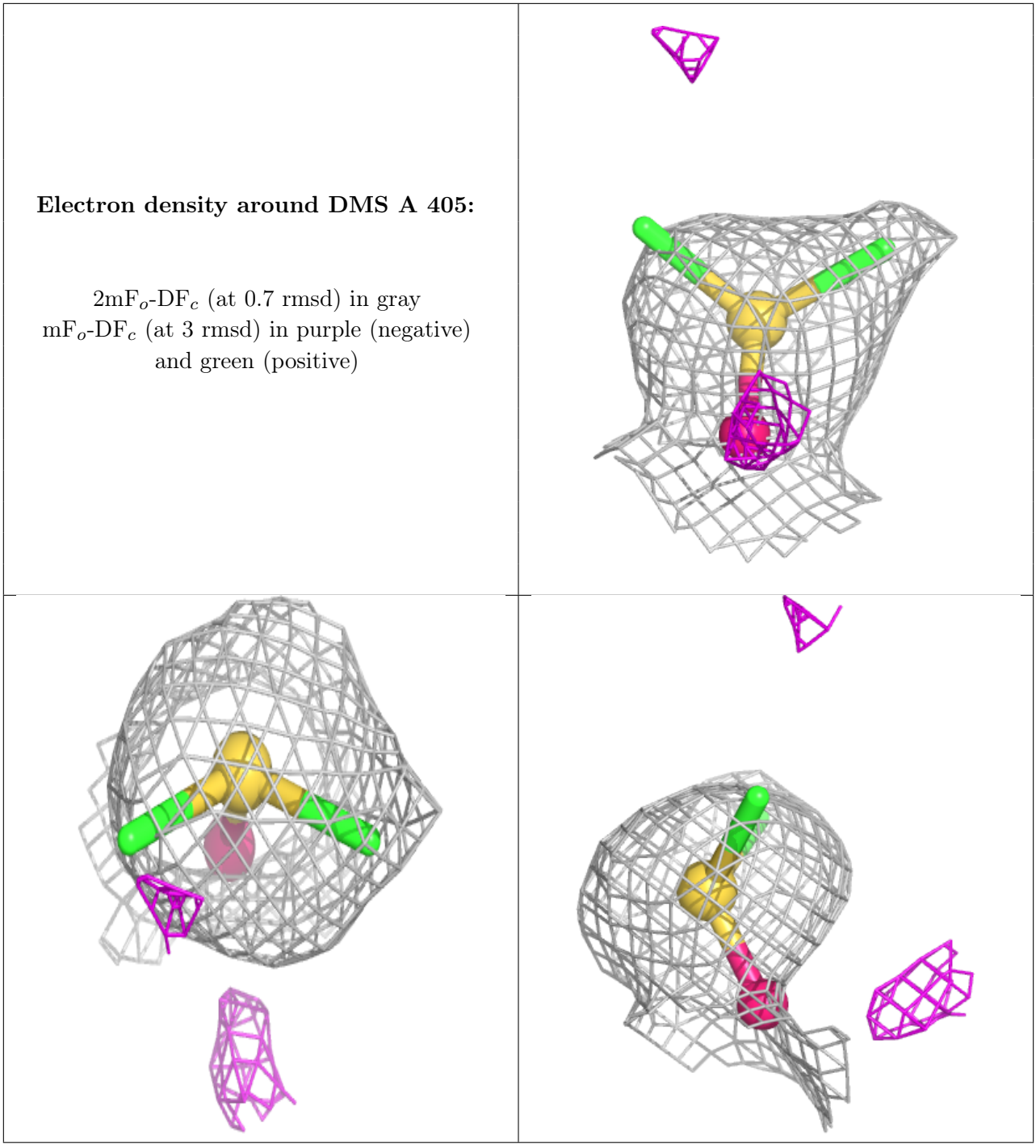
Electron density around DMS A 404:

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



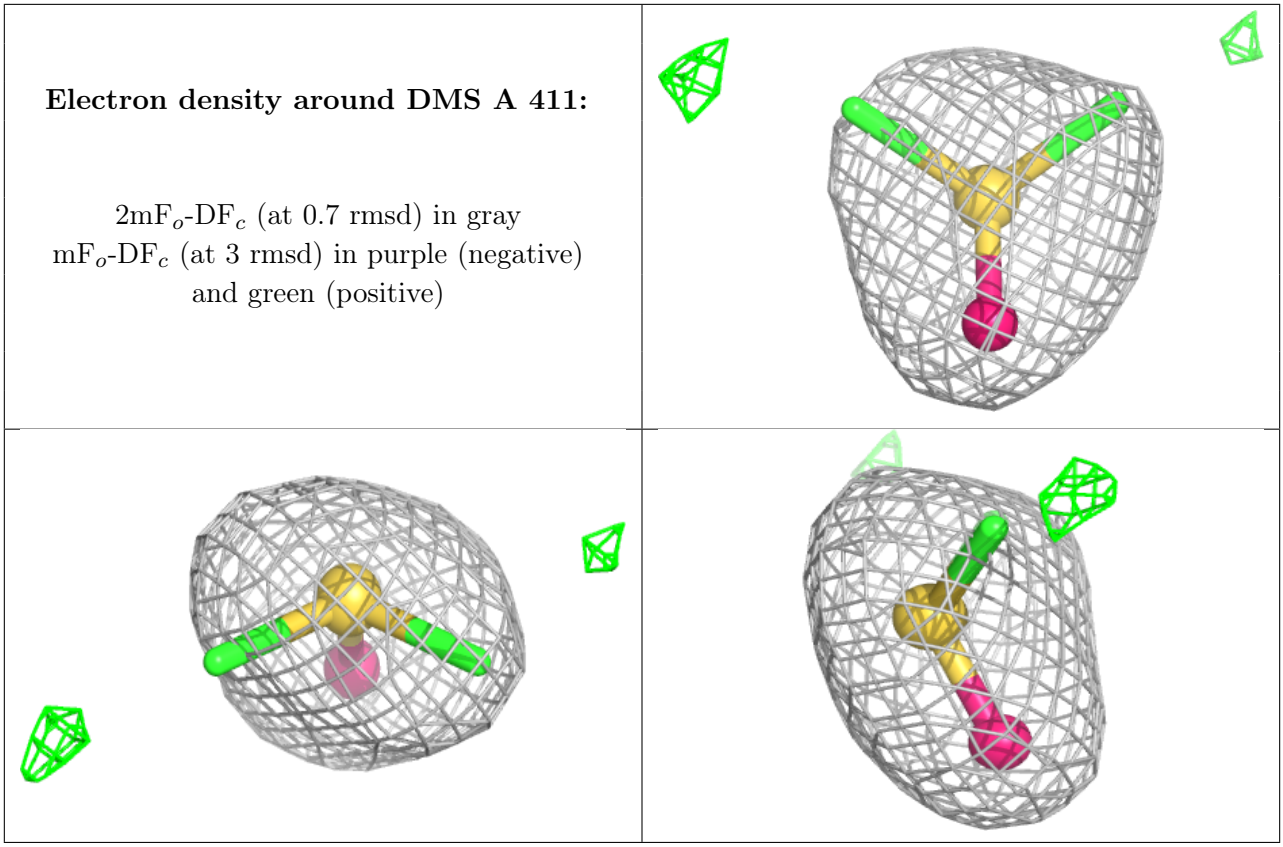
Electron density around DMS A 405:

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



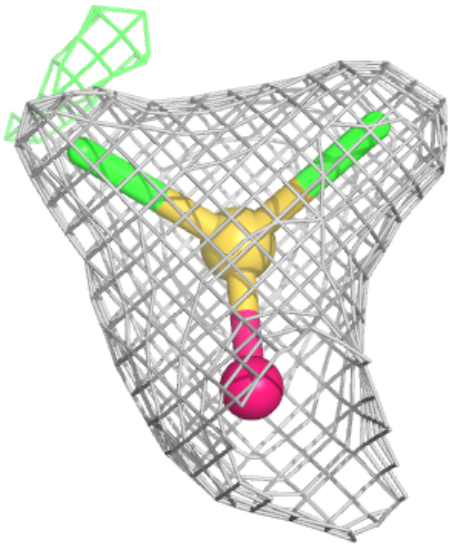
Electron density around DMS A 411:

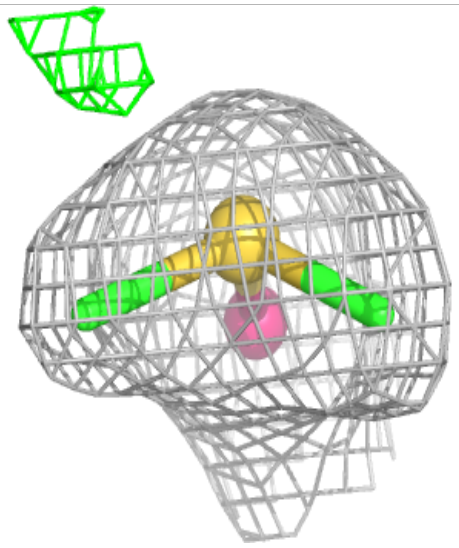
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

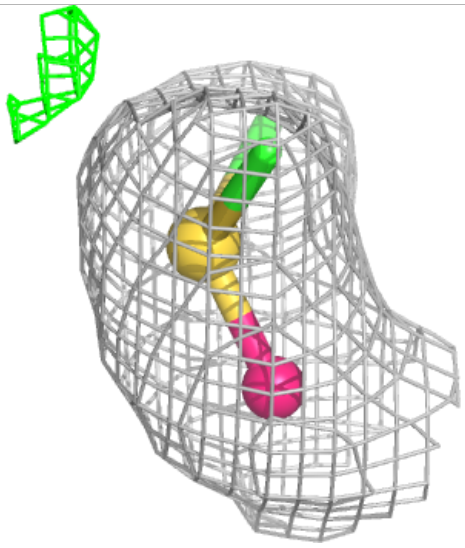


Electron density around DMS C 405:

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

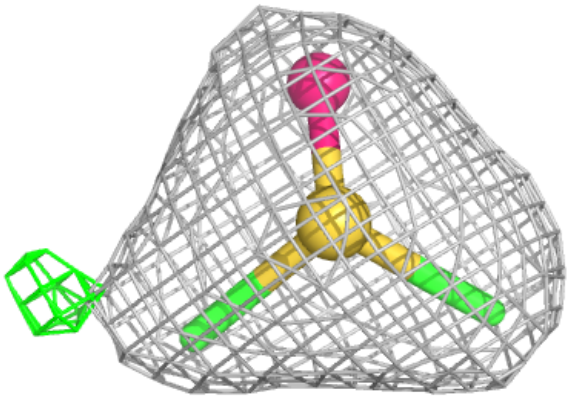


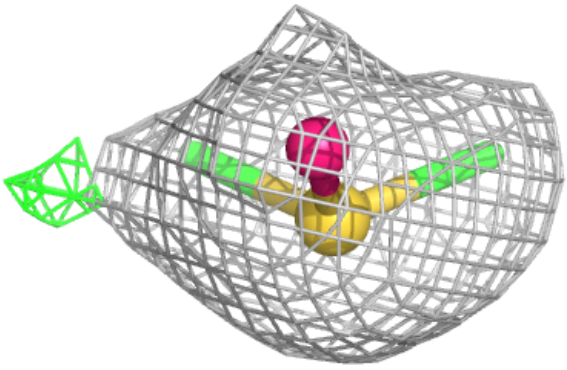


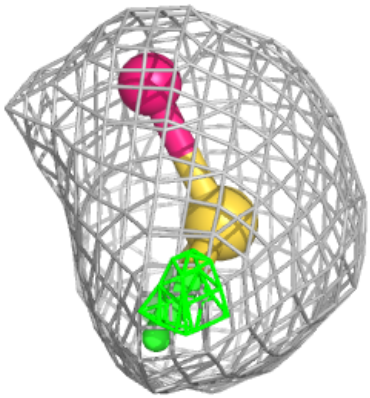


Electron density around DMS D 811:

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

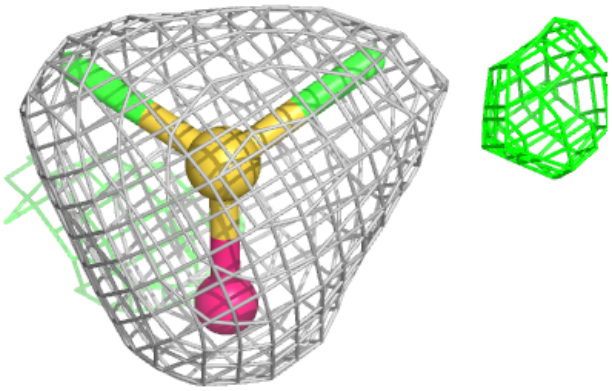


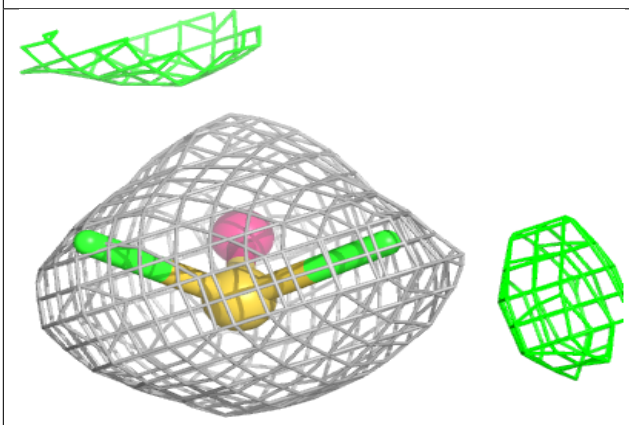


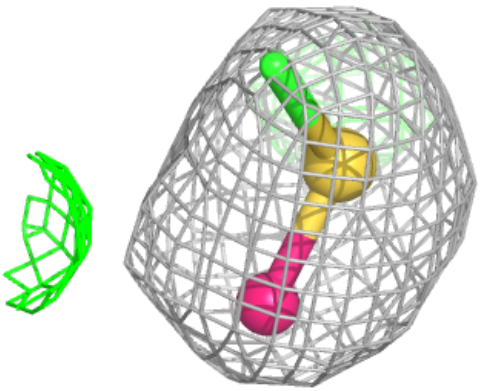


Electron density around DMS C 404:

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

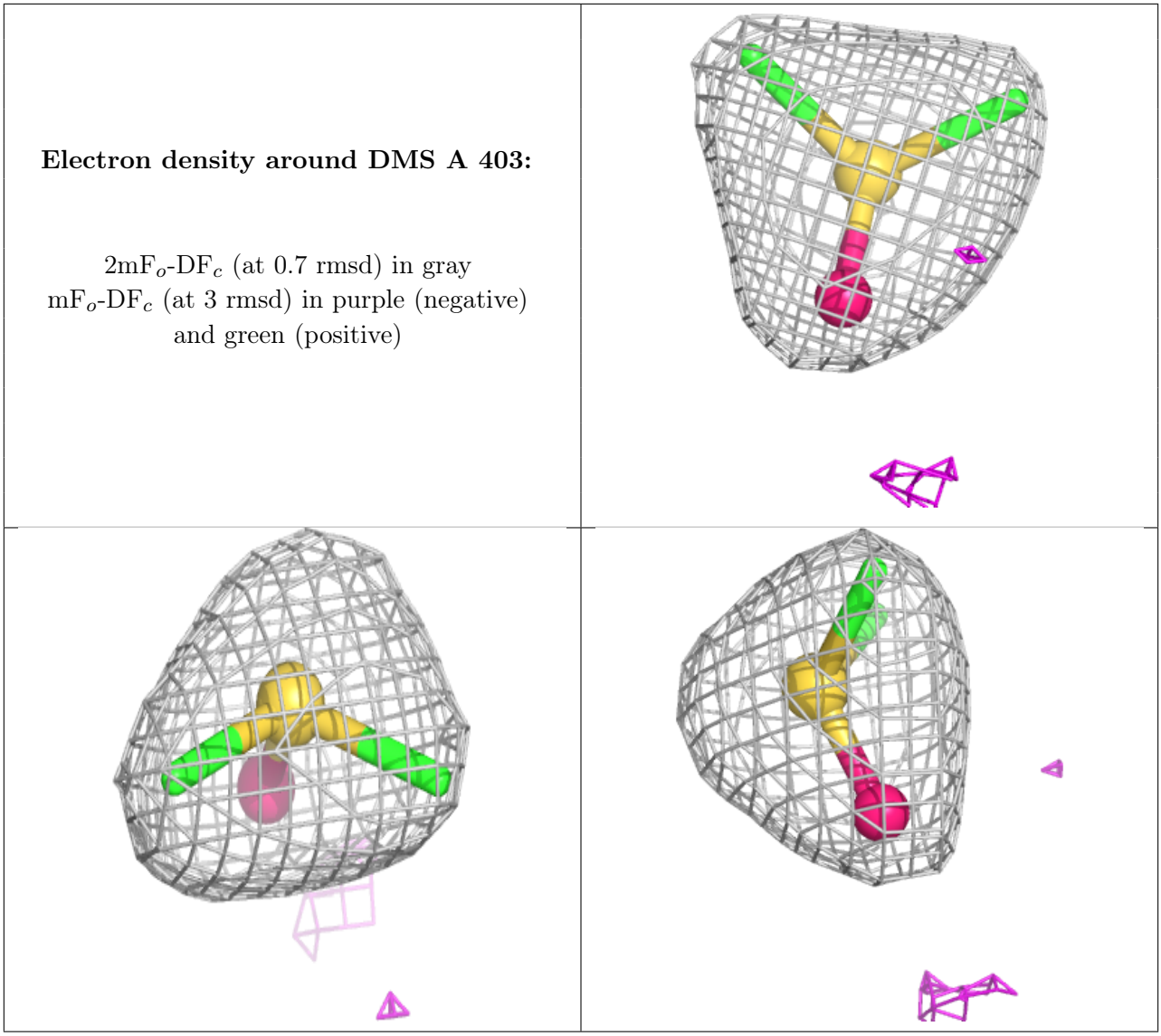






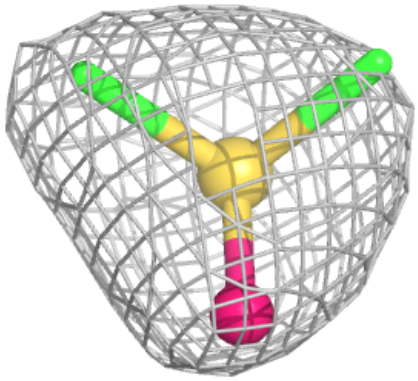
Electron density around DMS A 403:

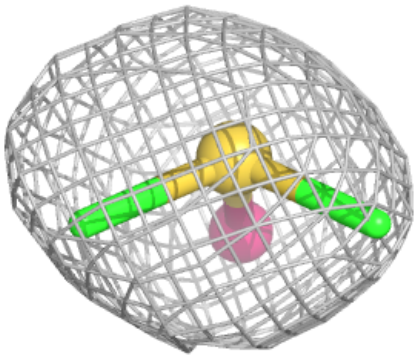
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

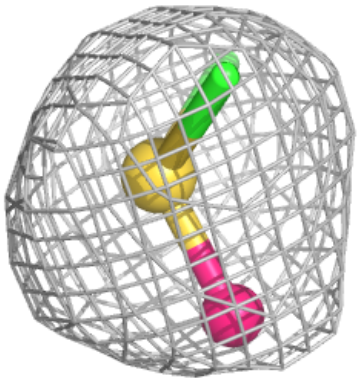


Electron density around DMS C 406:

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

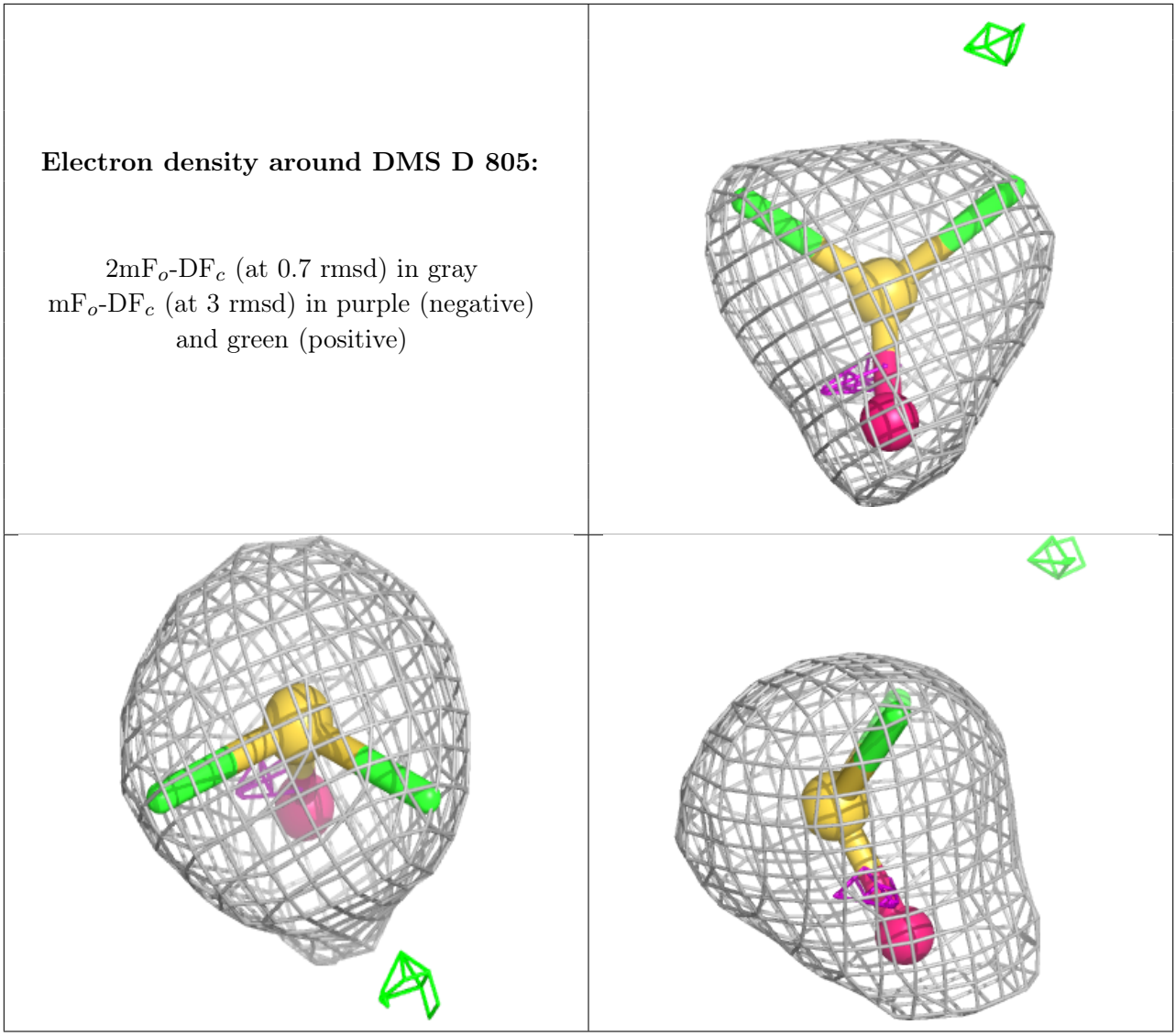






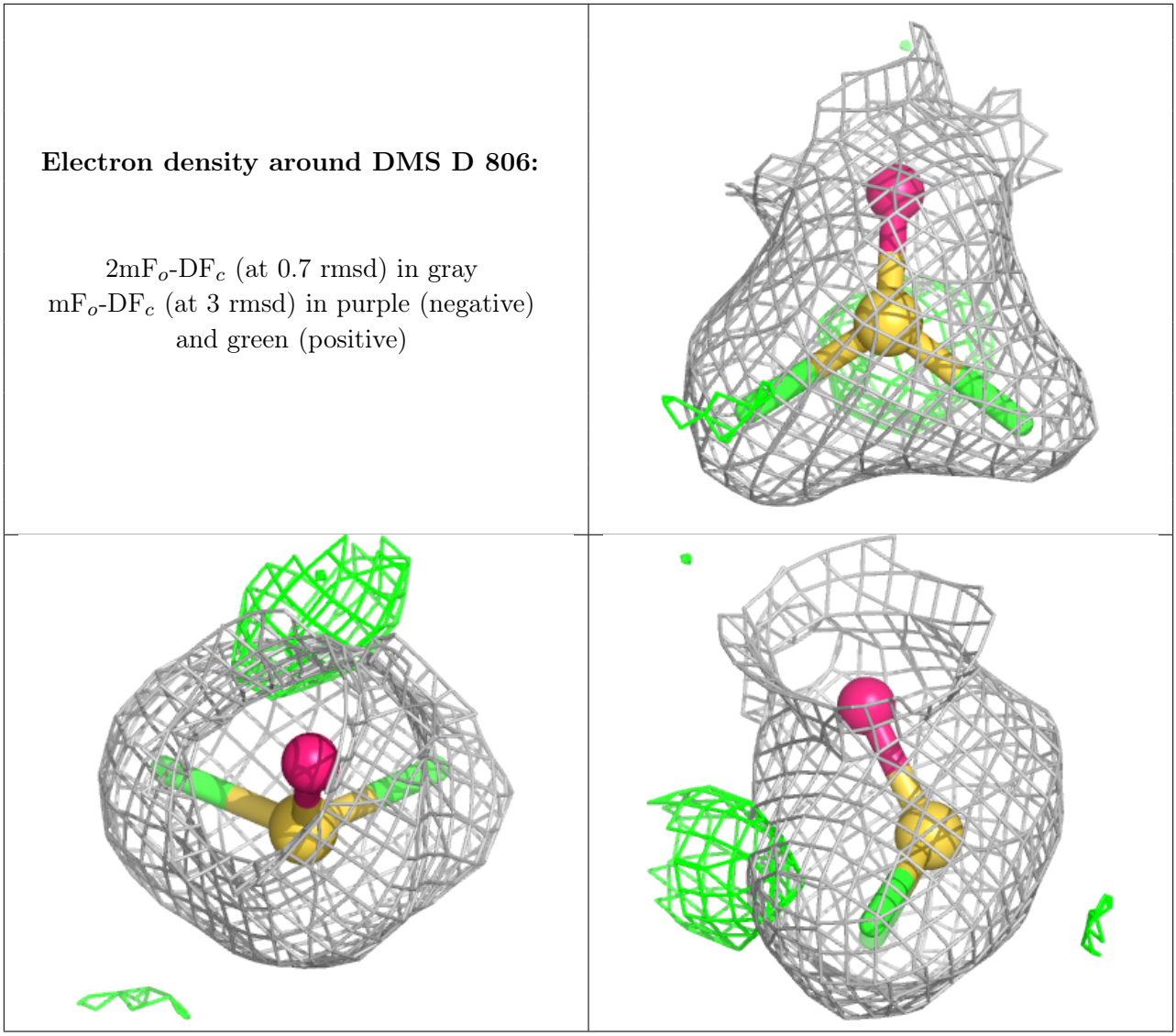
Electron density around DMS D 805:

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



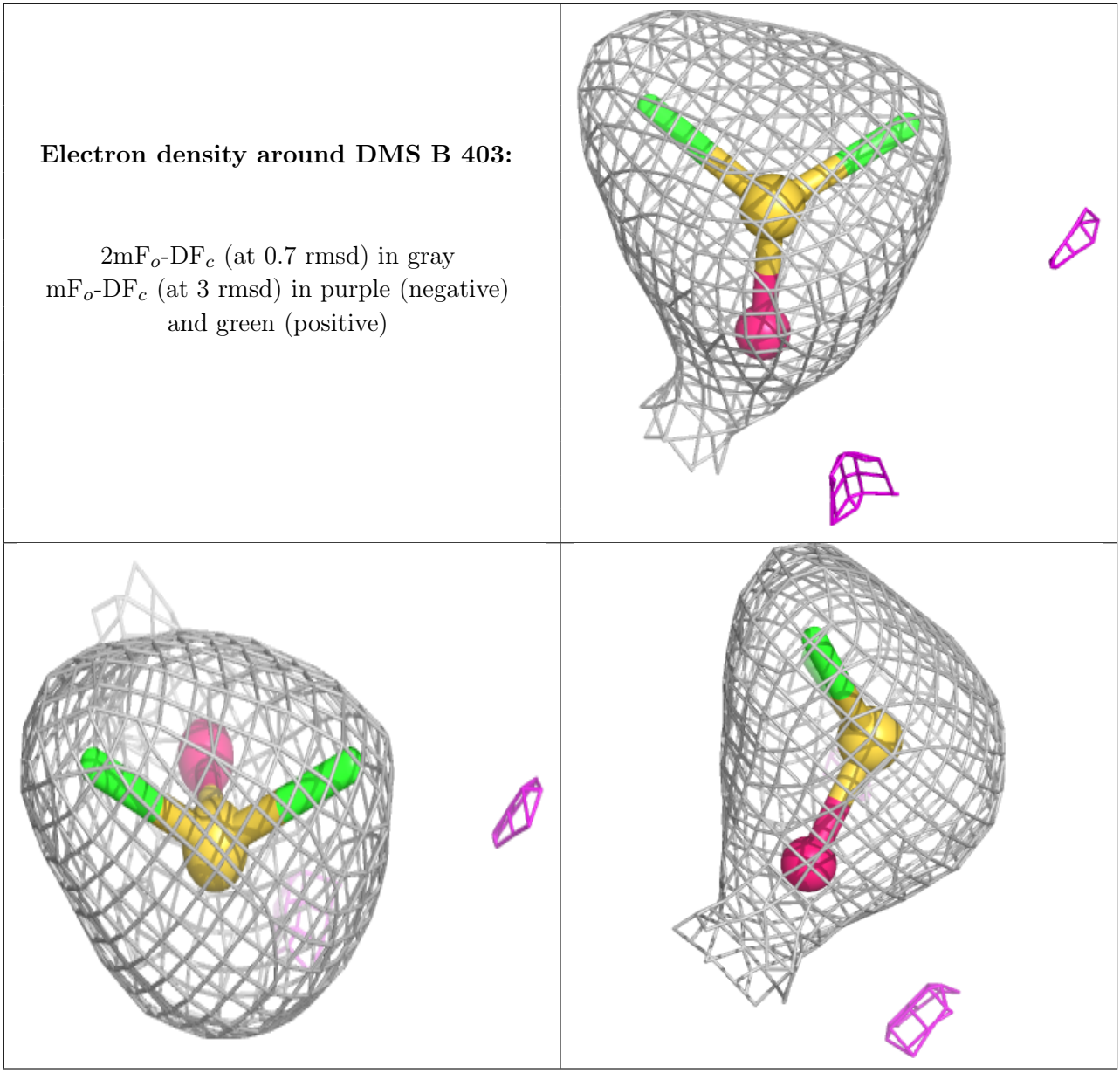
Electron density around DMS D 806:

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



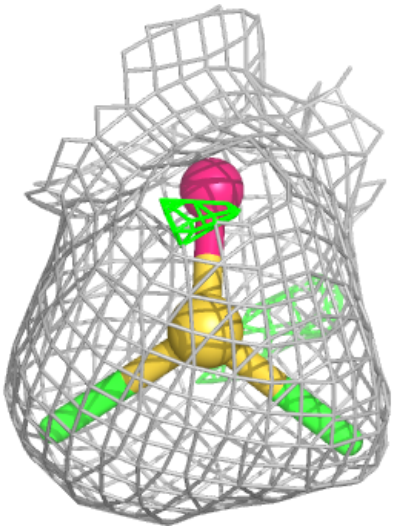
Electron density around DMS B 403:

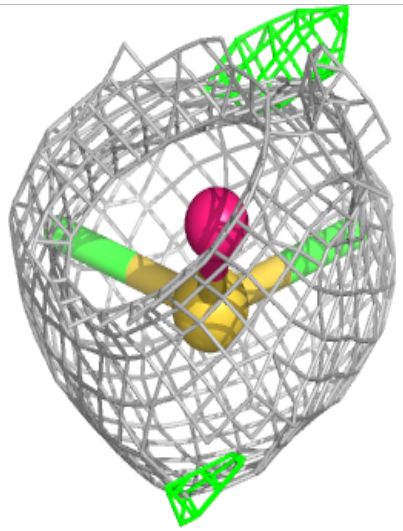
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

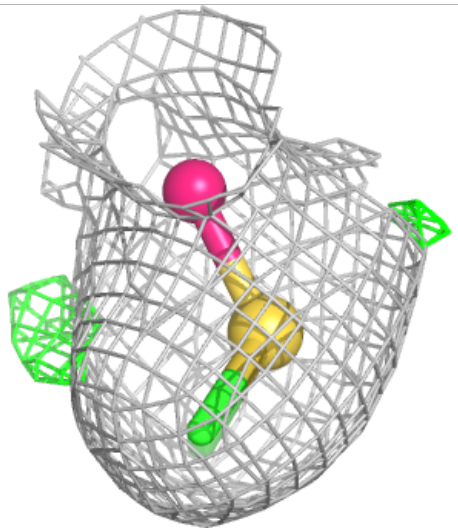


Electron density around DMS C 403:

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

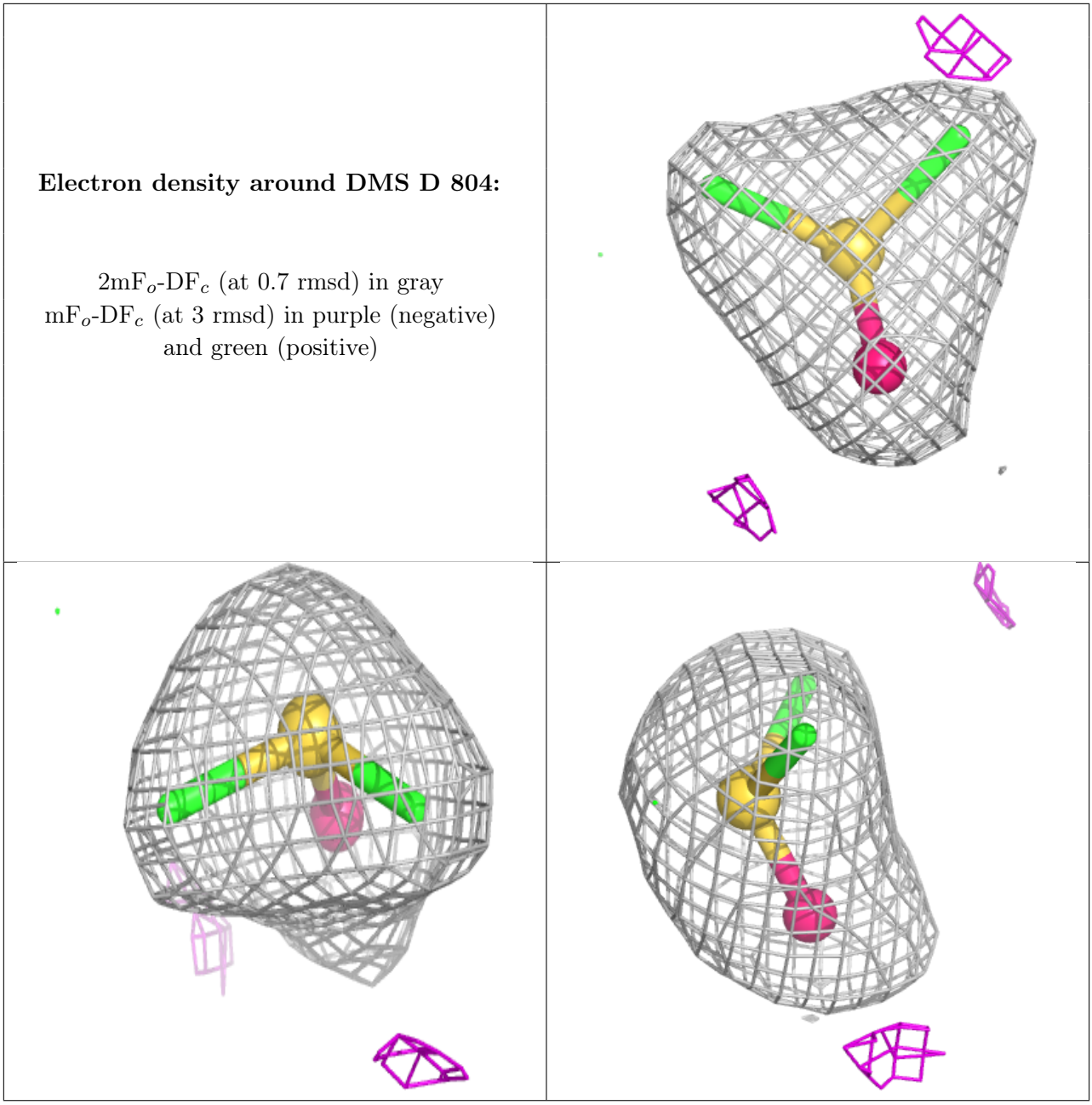






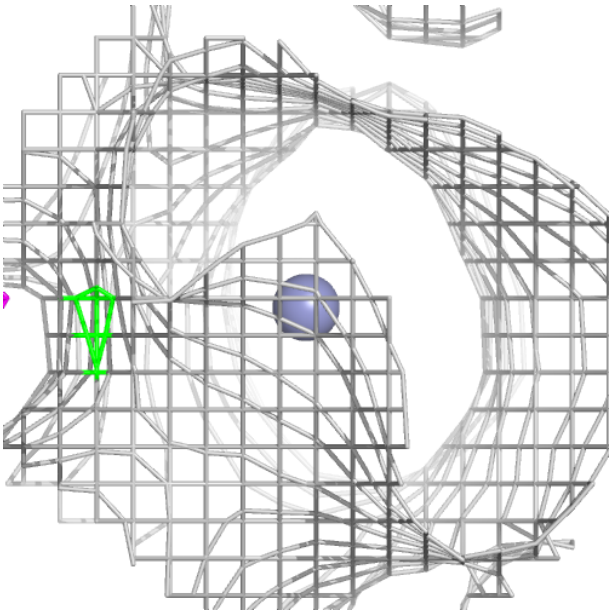
Electron density around DMS D 804:

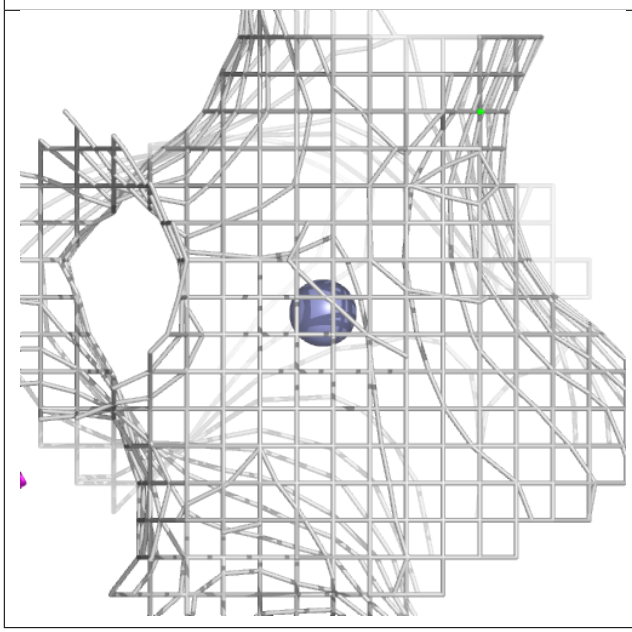
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

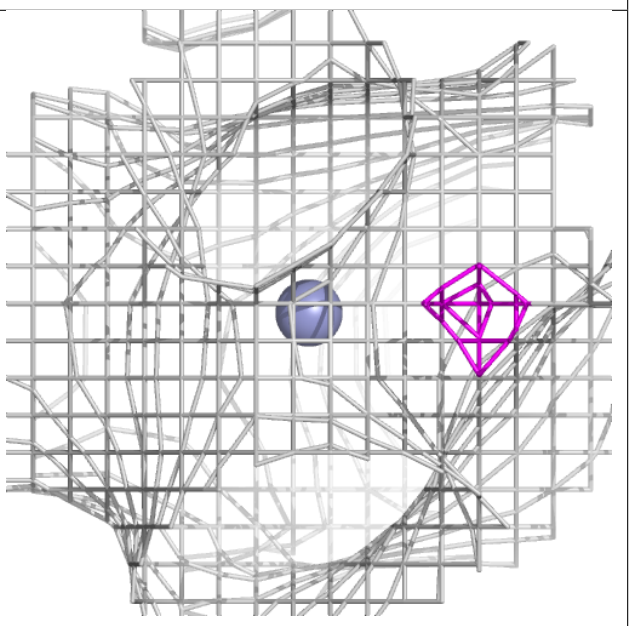


Electron density around ZN A 401:

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

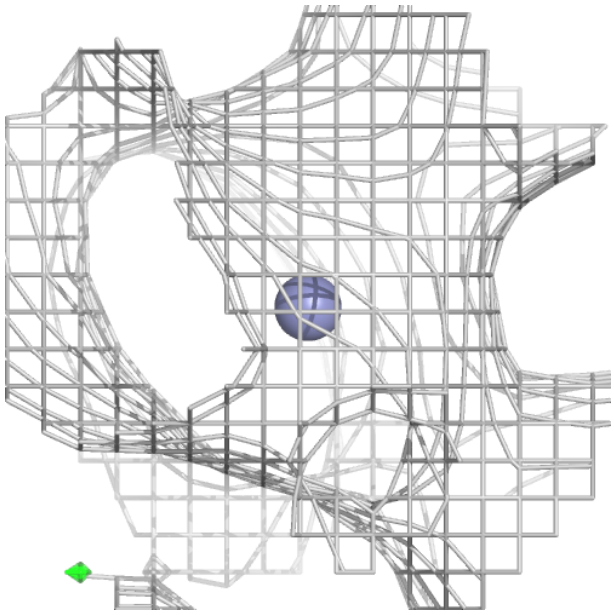


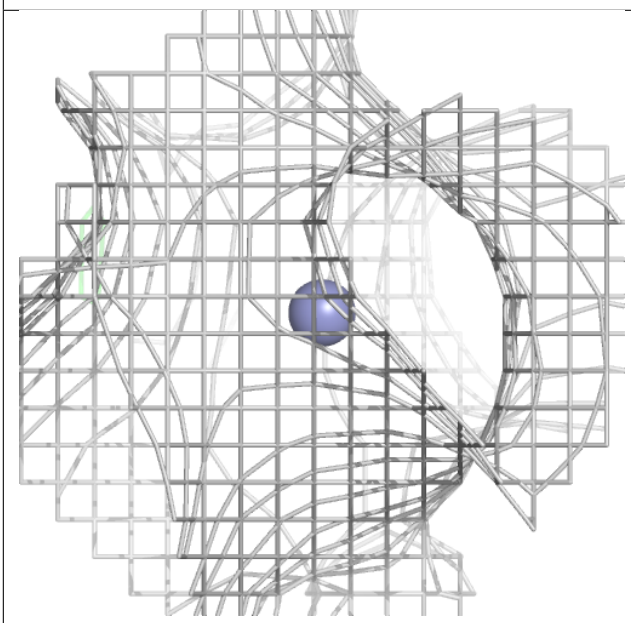


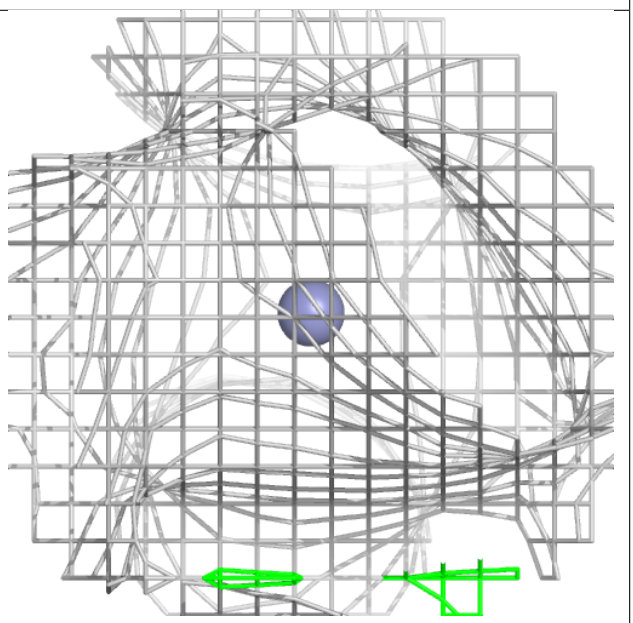


Electron density around ZN B 401:

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

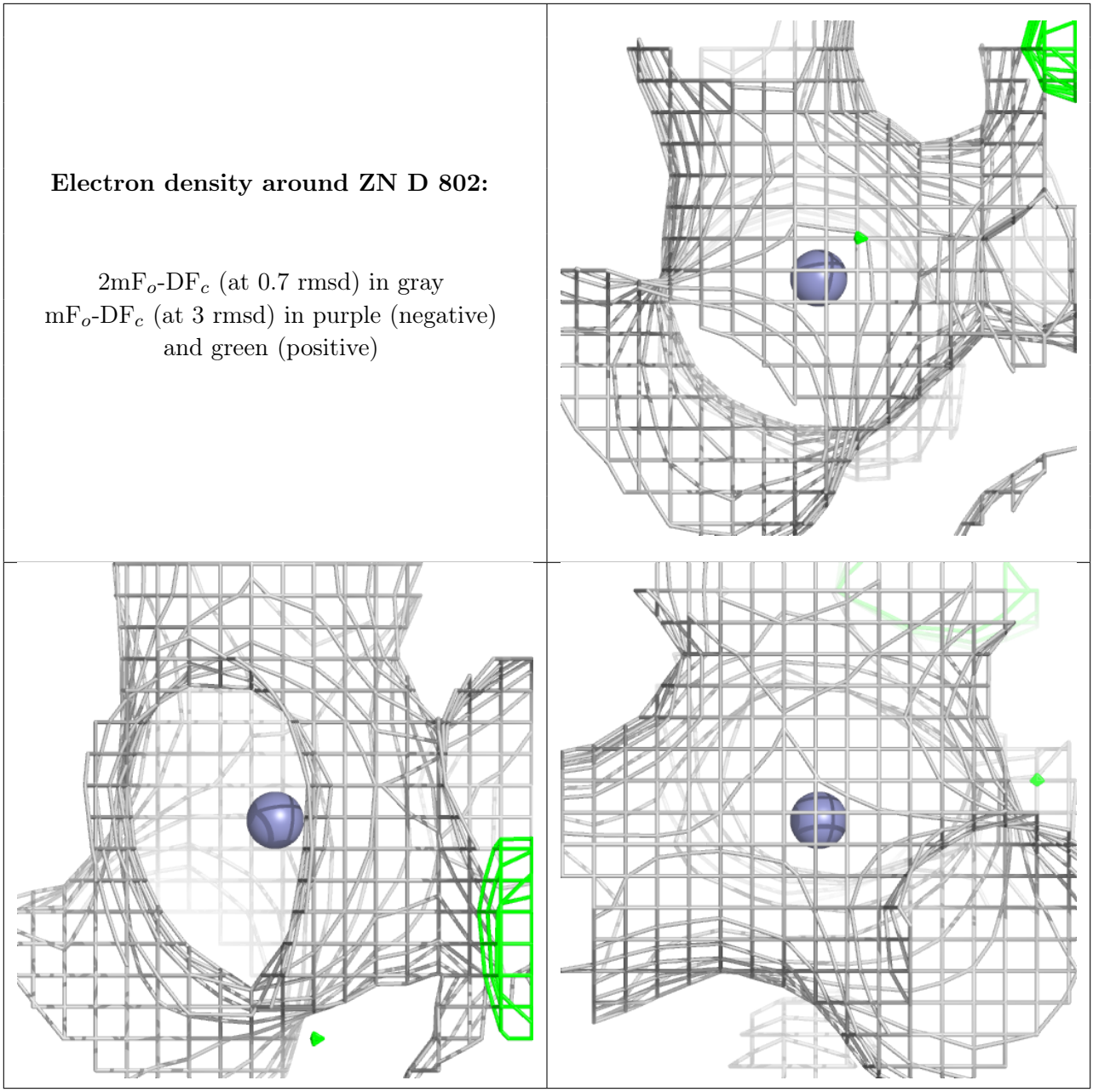






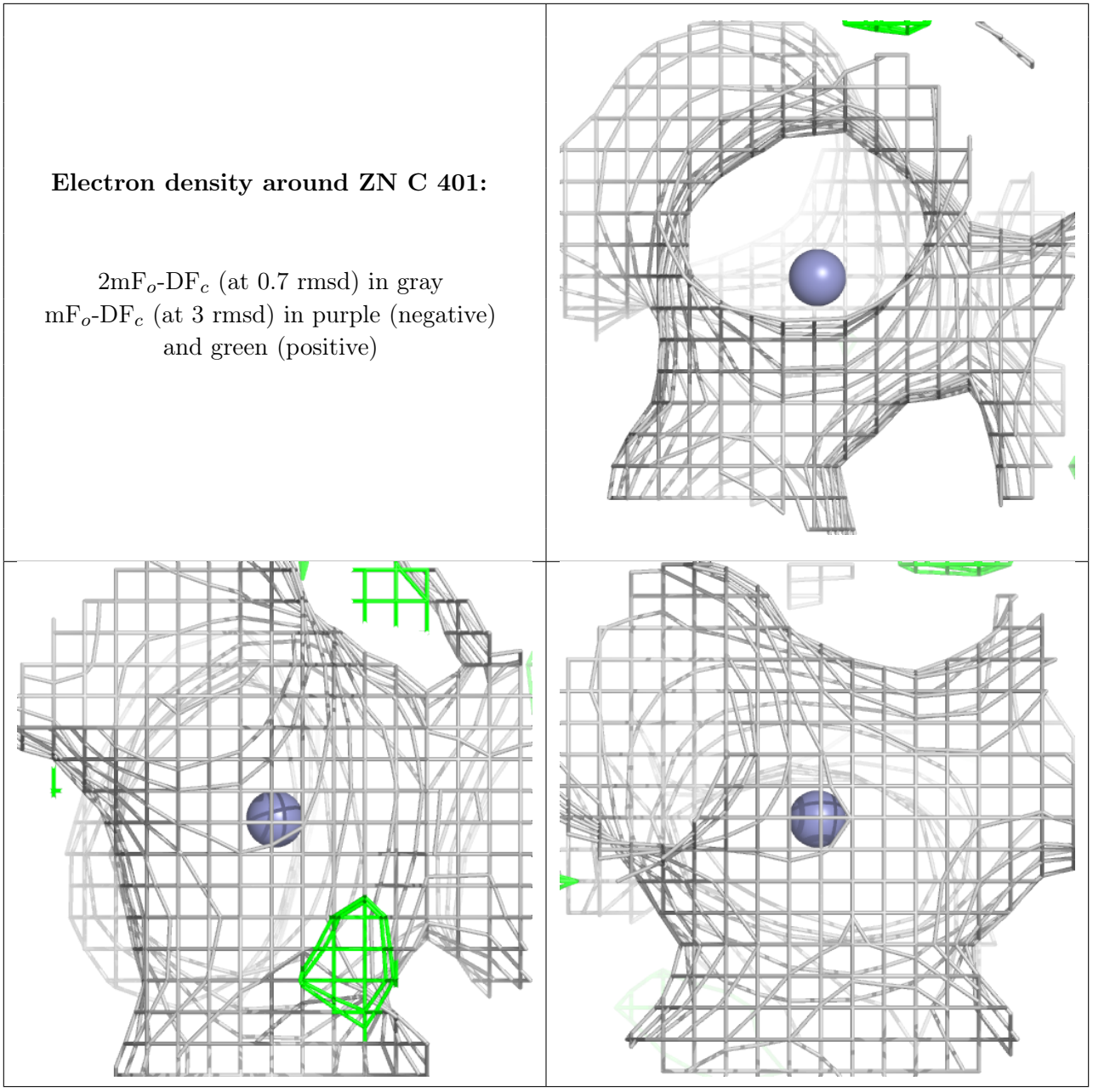
Electron density around ZN D 802:

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



Electron density around ZN 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)



6.5 Other polymers

There are no such residues in this entry.