Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 01:37 pm GMT

PDB ID	:	8BLL
Title	:	Structure of RutB
Authors	:	Rajendran, C.
Deposited on	:	2022-11-09
Resolution	:	1.54 Å(reported)

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

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

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

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

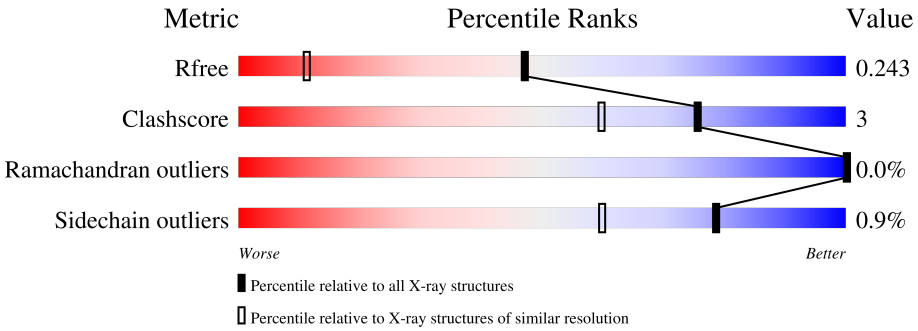
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.54 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)

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%

Mol	Chain	Length	Quality of chain
1	A	230	90% 7% ·
1	B	230	92% · ·
1	C	230	92% · ·
1	D	230	90% 6% ·
1	E	230	90% 5% · ·
1	F	230	91% · · ·
1	G	230	90% 6% ·

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Mol	Chain	Length	Quality of chain
1	H	230	92%
1	I	230	90% 5%
1	J	230	90% 6%
1	K	230	93%
1	L	230	91% 5%
1	M	230	89% 7%
1	N	230	92%
1	O	230	90% 7%
1	P	230	89% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	C	301	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 57341 atoms, of which 26479 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.

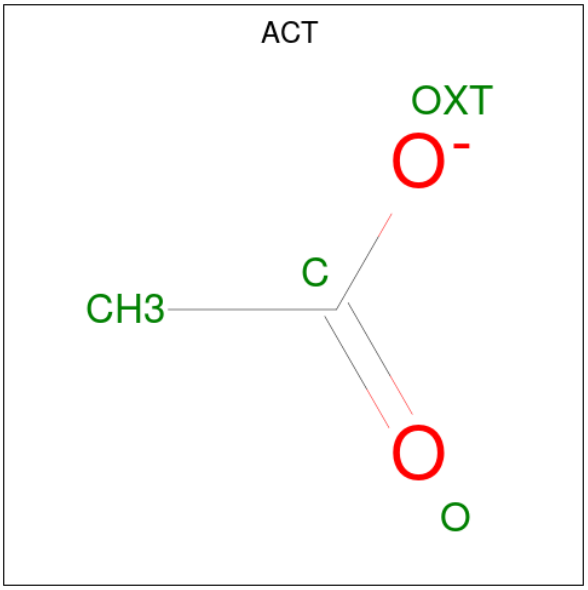
- Molecule 1 is a protein called Ureidoacrylate amidohydrolase RutB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	B	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	C	222	Total	C	H	N	O	S	0	0	0
			3359	1104	1644	285	322	4			
1	D	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	E	222	Total	C	H	N	O	S	0	0	0
			3359	1104	1644	285	322	4			
1	F	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	G	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	H	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	I	222	Total	C	H	N	O	S	0	0	0
			3356	1104	1641	285	322	4			
1	J	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	K	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	L	222	Total	C	H	N	O	S	0	0	0
			3369	1104	1654	285	322	4			
1	M	222	Total	C	H	N	O	S	0	0	0
			3344	1099	1639	282	320	4			
1	N	222	Total	C	H	N	O	S	0	0	0
			3354	1101	1643	284	322	4			
1	O	222	Total	C	H	N	O	S	0	0	0
			3358	1104	1643	285	322	4			
1	P	222	Total	C	H	N	O	S	0	0	0
			3352	1101	1643	282	322	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	conflict	UNP C9QZ65
B	166	SER	CYS	conflict	UNP C9QZ65
C	166	SER	CYS	conflict	UNP C9QZ65
D	166	SER	CYS	conflict	UNP C9QZ65
E	166	SER	CYS	conflict	UNP C9QZ65
F	166	SER	CYS	conflict	UNP C9QZ65
G	166	SER	CYS	conflict	UNP C9QZ65
H	166	SER	CYS	conflict	UNP C9QZ65
I	166	SER	CYS	conflict	UNP C9QZ65
J	166	SER	CYS	conflict	UNP C9QZ65
K	166	SER	CYS	conflict	UNP C9QZ65
L	166	SER	CYS	conflict	UNP C9QZ65
M	166	SER	CYS	conflict	UNP C9QZ65
N	166	SER	CYS	conflict	UNP C9QZ65
O	166	SER	CYS	conflict	UNP C9QZ65
P	166	SER	CYS	conflict	UNP C9QZ65

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 7 2 3 2	0	0
2	A	1	Total C H O 7 2 3 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		
2	C	1	Total	C	H	O	0	0
			7	2	3	2		
2	C	1	Total	C	H	O	0	0
			7	2	3	2		
2	D	1	Total	C	H	O	0	0
			7	2	3	2		
2	D	1	Total	C	H	O	0	0
			7	2	3	2		
2	E	1	Total	C	H	O	0	0
			7	2	3	2		
2	E	1	Total	C	H	O	0	0
			7	2	3	2		
2	F	1	Total	C	H	O	0	0
			7	2	3	2		
2	F	1	Total	C	H	O	0	0
			7	2	3	2		
2	G	1	Total	C	H	O	0	0
			7	2	3	2		
2	G	1	Total	C	H	O	0	0
			7	2	3	2		
2	H	1	Total	C	H	O	0	0
			7	2	3	2		
2	H	1	Total	C	H	O	0	0
			7	2	3	2		
2	I	1	Total	C	H	O	0	0
			7	2	3	2		
2	I	1	Total	C	H	O	0	0
			7	2	3	2		
2	J	1	Total	C	H	O	0	0
			7	2	3	2		
2	J	1	Total	C	H	O	0	0
			7	2	3	2		
2	K	1	Total	C	H	O	0	0
			7	2	3	2		
2	K	1	Total	C	H	O	0	0
			7	2	3	2		
2	L	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total	C	H	O	0	0
			7	2	3	2		
2	M	1	Total	C	H	O	0	0
			7	2	3	2		
2	M	1	Total	C	H	O	0	0
			7	2	3	2		
2	N	1	Total	C	H	O	0	0
			7	2	3	2		
2	N	1	Total	C	H	O	0	0
			7	2	3	2		
2	O	1	Total	C	H	O	0	0
			7	2	3	2		
2	O	1	Total	C	H	O	0	0
			7	2	3	2		
2	P	1	Total	C	H	O	0	0
			7	2	3	2		
2	P	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	238	Total	O	0	0
			238	238		
3	B	252	Total	O	0	0
			252	252		
3	C	233	Total	O	0	0
			233	233		
3	D	255	Total	O	0	0
			255	255		
3	E	239	Total	O	0	0
			239	239		
3	F	228	Total	O	0	0
			228	228		
3	G	233	Total	O	0	0
			233	233		
3	H	210	Total	O	0	0
			210	210		
3	I	173	Total	O	0	0
			173	173		
3	J	246	Total	O	0	0
			246	246		

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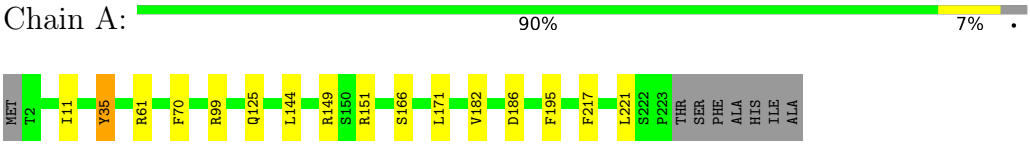
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	189	Total O 189 189	0	0
3	L	208	Total O 208 208	0	0
3	M	148	Total O 148 148	0	0
3	N	155	Total O 155 155	0	0
3	O	168	Total O 168 168	0	0
3	P	139	Total O 139 139	0	0

3 Residue-property plots (i)

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

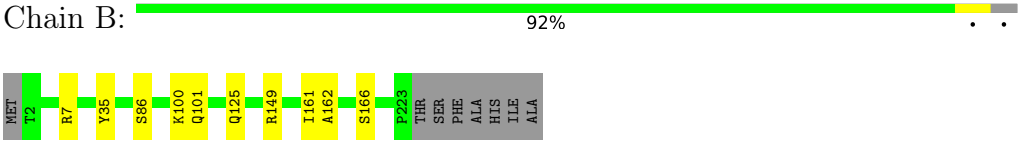
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain A:



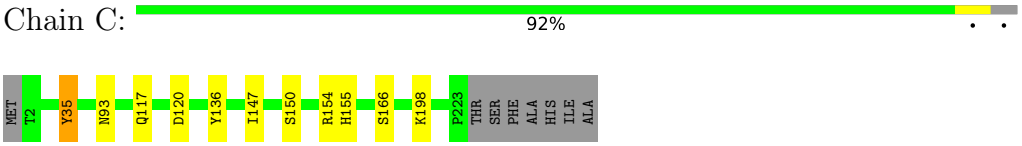
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain B:



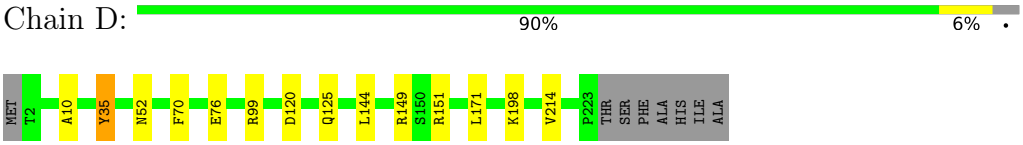
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain C:



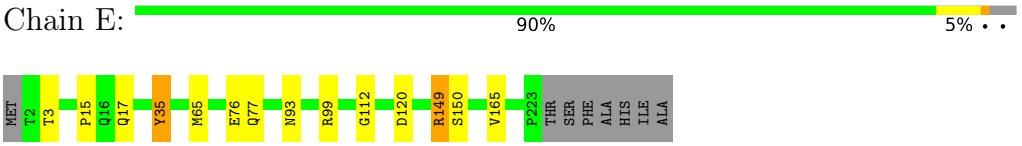
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain D:



• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain E:

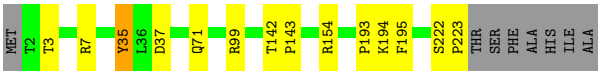


• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain F:

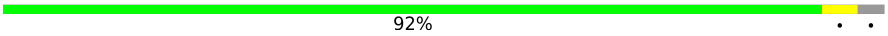
• Molecule 1: Ureidoacrylate amidohydrolase RutB

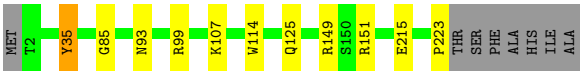
Chain G:



• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain H:



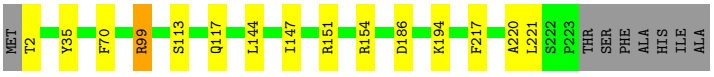


• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain I:

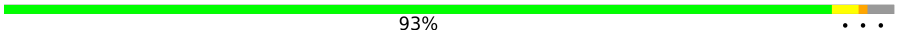
• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain J:



• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain K:



• Molecule 1: Ureidoacrylate amidohydrolase RutB

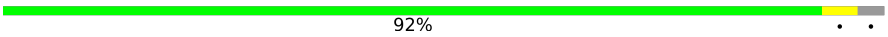
Chain L:

• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain M:

• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain N:

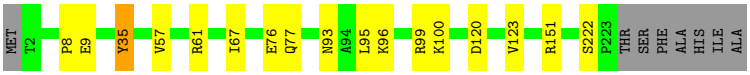


• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain O:

• Molecule 1: Ureidoacrylate amidohydrolase RutB

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.46Å 108.61Å 124.34Å 85.66° 83.22° 74.34°	Depositor
Resolution (Å)	47.00 – 1.54 47.71 – 1.54	Depositor EDS
% Data completeness (in resolution range)	83.7 (47.00-1.54) 85.5 (47.71-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.18rc2_3793	Depositor
R, R_{free}	0.207 , 0.243 0.207 , 0.243	Depositor DCC
R_{free} test set	21901 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	57341	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.99% 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: ACT

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	0.53	0/1760	0.70	1/2401 (0.0%)
1	B	0.53	0/1760	0.68	0/2401
1	C	0.53	0/1760	0.69	0/2401
1	D	0.56	0/1760	0.70	0/2401
1	E	0.52	0/1760	0.68	1/2401 (0.0%)
1	F	0.52	0/1760	0.66	0/2401
1	G	0.54	0/1760	0.68	0/2401
1	H	0.51	0/1760	0.66	0/2401
1	I	0.50	0/1760	0.64	1/2401 (0.0%)
1	J	0.53	0/1760	0.70	2/2401 (0.1%)
1	K	0.48	0/1760	0.62	0/2401
1	L	0.49	0/1760	0.66	0/2401
1	M	0.46	0/1750	0.63	0/2389
1	N	0.47	0/1756	0.62	0/2397
1	O	0.49	0/1760	0.64	0/2401
1	P	0.48	0/1754	0.62	0/2394
All	All	0.51	0/28140	0.66	5/38393 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	186	ASP	CB-CG-OD1	6.37	124.03	118.30
1	E	149	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	I	99	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	J	99	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	186	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1715	1654	1675	12	0
1	B	1715	1654	1675	8	0
1	C	1715	1644	1675	14	0
1	D	1715	1654	1675	14	0
1	E	1715	1644	1675	13	0
1	F	1715	1654	1675	10	0
1	G	1715	1654	1675	15	0
1	H	1715	1654	1675	11	0
1	I	1715	1641	1675	9	0
1	J	1715	1654	1675	10	0
1	K	1715	1654	1675	7	0
1	L	1715	1654	1675	11	0
1	M	1705	1639	1660	10	0
1	N	1711	1643	1664	8	0
1	O	1715	1643	1675	11	0
1	P	1709	1643	1664	13	0
2	A	8	6	6	1	0
2	B	8	6	6	1	0
2	C	8	6	6	2	0
2	D	8	6	6	0	0
2	E	8	6	6	0	0
2	F	8	6	6	0	0
2	G	8	6	6	0	0
2	H	8	6	6	1	0
2	I	8	6	6	0	0
2	J	8	6	6	0	0
2	K	8	6	6	0	0
2	L	8	6	6	0	0
2	M	8	6	6	0	0
2	N	8	6	6	0	0
2	O	8	6	6	0	0
2	P	8	6	6	0	0
3	A	238	0	0	5	2
3	B	252	0	0	2	0
3	C	233	0	0	7	1
3	D	255	0	0	8	0
3	E	239	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	228	0	0	3	1
3	G	233	0	0	7	0
3	H	210	0	0	10	2
3	I	173	0	0	5	0
3	J	246	0	0	4	3
3	K	189	0	0	4	2
3	L	208	0	0	7	0
3	M	148	0	0	2	0
3	N	155	0	0	4	0
3	O	168	0	0	4	1
3	P	139	0	0	8	0
All	All	30862	26479	26859	170	6

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

All (170) 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:H:215:GLU:OE2	3:H:401:HOH:O	1.58	1.20
1:H:151:ARG:NH2	3:H:402:HOH:O	1.96	0.97
1:E:149:ARG:NH2	3:E:401:HOH:O	1.98	0.96
1:E:3:THR:HG23	1:G:3:THR:H	1.30	0.94
1:A:125:GLN:NE2	3:A:401:HOH:O	2.00	0.93
1:B:166:SER:OG	2:B:302:ACT:H1	1.71	0.90
1:D:149:ARG:NH2	3:D:401:HOH:O	2.06	0.89
1:A:151:ARG:NH2	3:A:402:HOH:O	2.07	0.87
1:A:166:SER:OG	2:A:301:ACT:H1	1.75	0.87
1:C:147:ILE:O	3:C:401:HOH:O	1.94	0.86
1:D:151:ARG:NH2	3:D:405:HOH:O	2.13	0.81
1:H:223:PRO:O	3:H:403:HOH:O	1.98	0.80
1:I:223:PRO:O	3:I:401:HOH:O	2.00	0.79
1:B:7:ARG:NH1	3:B:401:HOH:O	2.15	0.79
1:E:112:GLY:O	3:E:402:HOH:O	2.01	0.79
1:L:117:GLN:NE2	3:L:403:HOH:O	2.15	0.78
1:O:185:GLU:OE2	3:O:401:HOH:O	2.02	0.76
1:E:120:ASP:OD1	3:E:403:HOH:O	2.03	0.76
1:K:16:GLN:OE1	3:K:401:HOH:O	2.06	0.73
1:C:154:ARG:NH1	3:C:402:HOH:O	2.12	0.73
1:D:10:ALA:O	3:D:402:HOH:O	2.08	0.72
1:I:154:ARG:NH1	3:I:403:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:OD1	3:D:403:HOH:O	2.08	0.71
1:G:71:GLN:OE1	3:G:401:HOH:O	2.07	0.71
1:H:125:GLN:NE2	3:H:404:HOH:O	2.00	0.70
1:O:126:PRO:O	3:O:402:HOH:O	2.09	0.70
1:F:3:THR:OG1	3:F:401:HOH:O	2.08	0.69
1:A:149:ARG:NH2	3:A:404:HOH:O	2.23	0.69
1:M:151:ARG:NH2	3:M:401:HOH:O	2.25	0.68
1:D:76:GLU:OE2	3:D:404:HOH:O	2.10	0.68
1:P:151:ARG:NH2	3:P:403:HOH:O	2.26	0.68
1:O:154:ARG:NH1	3:O:404:HOH:O	2.28	0.67
1:E:3:THR:HG23	1:G:3:THR:N	2.08	0.67
1:K:120:ASP:OD1	3:K:402:HOH:O	2.13	0.66
1:L:76:GLU:OE2	3:L:401:HOH:O	2.13	0.66
1:L:120:ASP:OD1	3:L:402:HOH:O	2.15	0.65
1:H:114:TRP:N	3:H:409:HOH:O	2.31	0.64
1:I:149:ARG:HG2	1:I:149:ARG:HH11	1.62	0.64
1:C:147:ILE:HA	3:C:401:HOH:O	1.99	0.62
1:B:100:LYS:NZ	1:B:101:GLN:OE1	2.33	0.61
1:J:151:ARG:NH2	3:J:405:HOH:O	2.33	0.61
1:L:76:GLU:OE1	3:L:404:HOH:O	2.16	0.61
1:E:17:GLN:OE1	3:E:404:HOH:O	2.16	0.61
1:N:198:LYS:NZ	3:N:406:HOH:O	2.34	0.60
1:P:120:ASP:O	3:P:401:HOH:O	2.17	0.60
1:G:99:ARG:NH2	3:G:403:HOH:O	2.33	0.59
1:N:15:PRO:O	1:N:65:MET:HG2	2.02	0.59
1:J:99:ARG:NH2	3:J:406:HOH:O	2.33	0.59
1:N:155:HIS:ND1	3:N:404:HOH:O	2.32	0.59
1:F:99:ARG:NH2	3:F:405:HOH:O	2.33	0.57
1:P:9:GLU:OE2	3:P:402:HOH:O	2.17	0.57
1:K:100:LYS:NZ	3:K:404:HOH:O	2.37	0.57
1:G:154:ARG:NH1	3:G:405:HOH:O	2.38	0.57
2:H:301:ACT:H2	3:H:511:HOH:O	2.06	0.55
1:A:99:ARG:NH2	3:A:406:HOH:O	2.32	0.55
1:C:150:SER:HB2	3:C:401:HOH:O	2.07	0.55
1:O:100:LYS:N	1:O:100:LYS:HD3	2.22	0.54
1:J:70:PHE:HZ	1:J:144:LEU:HD22	1.73	0.54
1:I:42:ASP:O	3:I:402:HOH:O	2.18	0.53
1:H:99:ARG:NH2	3:H:413:HOH:O	2.40	0.53
1:A:61:ARG:HG3	3:A:414:HOH:O	2.08	0.52
1:L:151:ARG:NH2	3:L:412:HOH:O	2.43	0.52
1:P:77:GLN:NE2	3:P:412:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:401:HOH:O	1:F:149:ARG:NE	2.43	0.52
1:A:195:PHE:CD2	1:C:198:LYS:HE3	2.46	0.51
1:H:35:TYR:OH	1:H:93:ASN:HB2	2.10	0.51
1:K:15:PRO:O	1:K:65:MET:HG3	2.10	0.51
1:B:100:LYS:HG3	1:B:101:GLN:HG3	1.92	0.51
1:K:117:GLN:HG3	3:K:497:HOH:O	2.11	0.51
1:F:52:ASN:HB3	1:F:214:VAL:HG21	1.93	0.51
1:O:50:ILE:HD13	1:O:119:VAL:HG21	1.93	0.51
1:G:222:SER:OG	1:G:223:PRO:HD3	2.11	0.50
1:I:99:ARG:NH2	3:I:409:HOH:O	2.39	0.50
1:I:2:THR:CG2	1:I:220:ALA:O	2.59	0.50
1:N:113:SER:O	1:N:117:GLN:HG3	2.13	0.49
1:P:123:VAL:N	3:P:407:HOH:O	2.34	0.49
1:C:120:ASP:OD2	3:C:403:HOH:O	2.19	0.49
1:P:57:VAL:HG13	1:P:67:ILE:HD13	1.96	0.48
1:J:113:SER:O	1:J:117:GLN:HG3	2.13	0.47
1:C:35:TYR:OH	1:C:93:ASN:HB2	2.14	0.47
1:A:11:ILE:HD11	1:A:182:VAL:HG21	1.96	0.47
1:O:160:GLY:O	1:O:188:THR:HA	2.15	0.47
1:P:61:ARG:HB2	1:P:67:ILE:HD11	1.95	0.47
1:B:149:ARG:HD3	1:D:149:ARG:CZ	2.45	0.47
1:M:54:GLN:HG3	1:M:122:LEU:HD21	1.95	0.47
1:M:101:GLN:HB3	1:M:103:GLN:NE2	2.30	0.47
1:E:3:THR:CG2	1:G:3:THR:H	2.15	0.47
1:M:217:PHE:CZ	1:M:221:LEU:HD11	2.50	0.47
1:E:35:TYR:C	1:E:35:TYR:CD1	2.88	0.47
1:E:76:GLU:OE1	1:E:77:GLN:OE1	2.34	0.46
1:G:7:ARG:NH1	3:G:410:HOH:O	2.44	0.46
1:G:154:ARG:NH1	3:G:412:HOH:O	2.46	0.46
1:H:107:LYS:HE2	3:H:459:HOH:O	2.15	0.46
1:L:17:GLN:OE1	3:L:405:HOH:O	2.20	0.46
1:D:99:ARG:NH2	3:D:415:HOH:O	2.43	0.46
1:I:52:ASN:HB3	1:I:214:VAL:HG21	1.98	0.45
1:F:217:PHE:CZ	1:F:221:LEU:HD11	2.51	0.45
1:C:136:TYR:HD1	2:C:301:ACT:H2	1.82	0.45
1:C:166:SER:OG	2:C:301:ACT:CH3	2.64	0.45
1:D:70:PHE:HZ	1:D:144:LEU:HD22	1.81	0.45
1:P:95:LEU:O	1:P:99:ARG:HG3	2.15	0.45
1:L:35:TYR:CD1	1:L:35:TYR:C	2.90	0.45
1:N:222:SER:OG	1:N:223:PRO:HD3	2.16	0.45
1:D:52:ASN:HB3	1:D:214:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:TYR:OH	1:O:93:ASN:HB2	2.17	0.45
1:F:61:ARG:HB2	1:F:67:ILE:HD11	1.99	0.44
1:H:149:ARG:NE	3:H:410:HOH:O	2.32	0.44
1:F:35:TYR:CD1	1:F:35:TYR:C	2.91	0.44
1:J:2:THR:HG23	1:J:220:ALA:O	2.18	0.44
1:J:70:PHE:CZ	1:J:144:LEU:HD22	2.52	0.44
1:M:35:TYR:C	1:M:35:TYR:CD1	2.90	0.44
1:P:96:LYS:HG3	3:P:421:HOH:O	2.17	0.44
1:J:151:ARG:NH2	3:J:401:HOH:O	2.22	0.44
1:D:35:TYR:CD1	1:D:35:TYR:C	2.91	0.44
1:E:15:PRO:O	1:E:65:MET:HG2	2.18	0.44
1:A:217:PHE:CZ	1:A:221:LEU:HD11	2.54	0.43
1:H:151:ARG:NH2	3:H:411:HOH:O	2.34	0.43
1:P:35:TYR:CD1	1:P:35:TYR:C	2.91	0.43
1:C:198:LYS:HB3	1:C:198:LYS:HE2	1.70	0.43
1:M:74:TRP:HB3	1:M:80:GLU:HB2	2.00	0.43
1:G:142:THR:HB	1:G:143:PRO:HD2	2.00	0.43
1:G:193:PRO:HG2	1:G:195:PHE:CE2	2.54	0.43
1:A:35:TYR:C	1:A:35:TYR:CD1	2.91	0.43
1:F:45:THR:O	1:F:45:THR:OG1	2.31	0.43
3:I:566:HOH:O	1:J:147:ILE:HD11	2.19	0.43
1:L:217:PHE:CZ	1:L:221:LEU:HD11	2.54	0.43
1:E:99:ARG:NH1	3:E:415:HOH:O	2.48	0.43
1:P:35:TYR:OH	1:P:93:ASN:HB2	2.19	0.42
1:K:142:THR:HB	1:K:143:PRO:HD2	2.01	0.42
1:O:105:GLN:NE2	3:O:406:HOH:O	2.38	0.42
1:C:35:TYR:C	1:C:35:TYR:CD1	2.92	0.42
1:P:8:PRO:HB3	3:P:524:HOH:O	2.19	0.42
1:A:70:PHE:HZ	1:A:144:LEU:HD22	1.84	0.42
1:B:86:SER:HB2	1:E:150:SER:OG	2.19	0.42
1:C:117:GLN:NE2	3:C:412:HOH:O	2.52	0.42
1:C:155:HIS:NE2	3:C:404:HOH:O	2.36	0.42
1:D:171:LEU:O	1:D:171:LEU:HD23	2.19	0.42
1:J:154:ARG:NH1	3:J:414:HOH:O	2.51	0.42
1:M:61:ARG:HG3	3:M:455:HOH:O	2.19	0.42
1:B:161:ILE:HA	1:B:162:ALA:HA	1.83	0.42
1:D:198:LYS:NZ	3:D:419:HOH:O	2.46	0.42
1:P:99:ARG:NH2	3:P:421:HOH:O	2.53	0.42
1:B:125:GLN:NE2	3:B:402:HOH:O	2.32	0.41
1:N:154:ARG:NH1	3:N:415:HOH:O	2.52	0.41
1:G:35:TYR:CD1	1:G:35:TYR:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:SER:HB3	1:L:223:PRO:HD3	2.01	0.41
1:M:131:LEU:HD23	1:M:131:LEU:HA	1.96	0.41
1:E:35:TYR:OH	1:E:93:ASN:HB2	2.21	0.41
1:N:151:ARG:NH2	3:N:417:HOH:O	2.53	0.41
1:J:217:PHE:CZ	1:J:221:LEU:HD11	2.56	0.41
1:O:35:TYR:C	1:O:35:TYR:CD1	2.94	0.41
1:I:35:TYR:OH	1:I:93:ASN:HB2	2.21	0.41
1:K:35:TYR:CD1	1:K:35:TYR:C	2.93	0.41
1:D:125:GLN:NE2	3:D:406:HOH:O	2.21	0.41
1:F:2:THR:N	3:F:416:HOH:O	2.53	0.41
1:G:154:ARG:NH2	1:H:85:GLY:O	2.54	0.41
1:I:15:PRO:O	1:I:65:MET:HG2	2.21	0.41
1:M:76:GLU:HG3	1:M:110:ALA:HB1	2.03	0.41
1:N:35:TYR:CD1	1:N:35:TYR:C	2.94	0.41
1:O:95:LEU:HD23	1:O:98:MET:CE	2.51	0.41
1:M:222:SER:OG	1:M:223:PRO:HD3	2.21	0.41
1:O:34:GLY:O	1:O:38:LEU:HD23	2.21	0.41
1:C:154:ARG:HE	1:C:154:ARG:HB3	1.69	0.40
1:D:171:LEU:HD23	1:D:171:LEU:C	2.41	0.40
1:G:194:LYS:NZ	3:G:419:HOH:O	2.54	0.40
1:L:61:ARG:HG3	1:L:61:ARG:HH11	1.86	0.40
1:L:149:ARG:HD2	3:L:428:HOH:O	2.22	0.40
1:A:171:LEU:HD23	1:A:171:LEU:C	2.42	0.40
1:F:61:ARG:CB	1:F:67:ILE:HD11	2.52	0.40
1:G:37:ASP:O	3:G:402:HOH:O	2.22	0.40

All (6) 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)
3:A:557:HOH:O	3:H:558:HOH:O[1_655]	2.02	0.18
3:C:620:HOH:O	3:F:593:HOH:O[1_465]	2.03	0.17
3:J:577:HOH:O	3:K:457:HOH:O[1_556]	2.08	0.12
3:A:437:HOH:O	3:H:421:HOH:O[1_655]	2.14	0.06
3:J:577:HOH:O	3:K:566:HOH:O[1_556]	2.18	0.02
3:J:542:HOH:O	3:O:537:HOH:O[1_456]	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	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	B	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	C	220/230 (96%)	214 (97%)	6 (3%)	0	100	100
1	D	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	E	220/230 (96%)	213 (97%)	6 (3%)	1 (0%)	29	9
1	F	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	G	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	H	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	I	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
1	J	220/230 (96%)	214 (97%)	6 (3%)	0	100	100
1	K	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
1	L	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	M	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	N	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
1	O	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
1	P	220/230 (96%)	217 (99%)	3 (1%)	0	100	100
All	All	3520/3680 (96%)	3443 (98%)	76 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	165	VAL

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	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	B	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	C	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	D	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	E	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	F	181/188 (96%)	179 (99%)	2 (1%)	73	51
1	G	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	H	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	I	181/188 (96%)	178 (98%)	3 (2%)	60	31
1	J	181/188 (96%)	179 (99%)	2 (1%)	73	51
1	K	181/188 (96%)	179 (99%)	2 (1%)	73	51
1	L	181/188 (96%)	180 (99%)	1 (1%)	86	72
1	M	179/188 (95%)	177 (99%)	2 (1%)	73	51
1	N	180/188 (96%)	179 (99%)	1 (1%)	86	72
1	O	181/188 (96%)	179 (99%)	2 (1%)	73	51
1	P	180/188 (96%)	176 (98%)	4 (2%)	52	21
All	All	2892/3008 (96%)	2866 (99%)	26 (1%)	78	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TYR
1	B	35	TYR
1	C	35	TYR
1	D	35	TYR
1	E	35	TYR
1	F	35	TYR
1	F	45	THR
1	G	35	TYR
1	H	35	TYR
1	I	2	THR
1	I	35	TYR
1	I	222	SER

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Mol	Chain	Res	Type
1	J	35	TYR
1	J	194	LYS
1	K	35	TYR
1	K	65	MET
1	L	35	TYR
1	M	35	TYR
1	M	194	LYS
1	N	35	TYR
1	O	16	GLN
1	O	35	TYR
1	P	35	TYR
1	P	76	GLU
1	P	100	LYS
1	P	222	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	117	GLN
1	H	17	GLN
1	J	117	GLN
1	L	117	GLN
1	M	16	GLN
1	N	117	GLN
1	P	77	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	N	302	-	3,3,3	0.99	0	3,3,3	1.50	0
2	ACT	D	301	-	3,3,3	1.06	0	3,3,3	1.29	0
2	ACT	K	301	-	3,3,3	0.77	0	3,3,3	1.32	0
2	ACT	H	301	-	3,3,3	1.24	1 (33%)	3,3,3	1.30	0
2	ACT	C	301	-	3,3,3	1.46	1 (33%)	3,3,3	1.51	0
2	ACT	P	302	-	3,3,3	0.82	0	3,3,3	1.69	2 (66%)
2	ACT	I	302	-	3,3,3	1.39	0	3,3,3	1.30	0
2	ACT	D	302	-	3,3,3	0.84	0	3,3,3	1.53	0
2	ACT	A	301	-	3,3,3	1.39	0	3,3,3	1.89	2 (66%)
2	ACT	F	301	-	3,3,3	0.91	0	3,3,3	1.54	0
2	ACT	L	301	-	3,3,3	1.08	0	3,3,3	1.10	0
2	ACT	M	302	-	3,3,3	0.76	0	3,3,3	1.69	1 (33%)
2	ACT	B	302	-	3,3,3	1.23	0	3,3,3	1.49	1 (33%)
2	ACT	F	302	-	3,3,3	0.98	0	3,3,3	1.38	0
2	ACT	I	301	-	3,3,3	1.04	0	3,3,3	1.48	0
2	ACT	P	301	-	3,3,3	1.19	0	3,3,3	1.69	2 (66%)
2	ACT	A	302	-	3,3,3	0.60	0	3,3,3	1.33	0
2	ACT	G	302	-	3,3,3	0.78	0	3,3,3	1.54	0
2	ACT	K	302	-	3,3,3	1.03	0	3,3,3	1.61	0
2	ACT	J	302	-	3,3,3	0.59	0	3,3,3	1.43	0
2	ACT	L	302	-	3,3,3	1.13	0	3,3,3	1.33	0
2	ACT	M	301	-	3,3,3	0.88	0	3,3,3	1.48	1 (33%)
2	ACT	E	302	-	3,3,3	0.79	0	3,3,3	1.72	2 (66%)
2	ACT	B	301	-	3,3,3	0.89	0	3,3,3	1.40	0
2	ACT	N	301	-	3,3,3	1.10	0	3,3,3	1.80	2 (66%)
2	ACT	O	301	-	3,3,3	0.75	0	3,3,3	1.79	2 (66%)
2	ACT	G	301	-	3,3,3	1.04	0	3,3,3	1.64	1 (33%)
2	ACT	E	301	-	3,3,3	1.18	0	3,3,3	1.69	1 (33%)
2	ACT	O	302	-	3,3,3	1.38	0	3,3,3	1.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ACT	H	302	-	3,3,3	1.11	0	3,3,3	1.62	1 (33%)
2	ACT	J	301	-	3,3,3	0.45	0	3,3,3	1.87	2 (66%)
2	ACT	C	302	-	3,3,3	1.19	0	3,3,3	1.54	1 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ACT	CH3-C	-2.35	1.39	1.49
2	H	301	ACT	O-C	2.07	1.31	1.22

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ACT	OXT-C-O	2.55	131.44	122.05
2	N	301	ACT	O-C-CH3	-2.32	113.30	122.33
2	J	301	ACT	O-C-CH3	-2.30	113.39	122.33
2	J	301	ACT	OXT-C-O	2.28	130.47	122.05
2	O	301	ACT	OXT-C-O	2.22	130.22	122.05
2	G	301	ACT	O-C-CH3	-2.20	113.78	122.33
2	O	301	ACT	O-C-CH3	-2.17	113.89	122.33
2	E	301	ACT	O-C-CH3	-2.16	113.93	122.33
2	M	301	ACT	OXT-C-O	2.15	129.99	122.05
2	M	302	ACT	O-C-CH3	-2.15	113.97	122.33
2	P	302	ACT	OXT-C-O	2.13	129.90	122.05
2	P	301	ACT	OXT-C-O	2.12	129.88	122.05
2	E	302	ACT	OXT-C-O	2.11	129.85	122.05
2	C	302	ACT	OXT-C-O	2.11	129.82	122.05
2	B	302	ACT	OXT-C-O	2.10	129.79	122.05
2	E	302	ACT	O-C-CH3	-2.10	114.17	122.33
2	A	301	ACT	O-C-CH3	-2.04	114.38	122.33
2	H	302	ACT	O-C-CH3	-2.03	114.42	122.33
2	P	302	ACT	O-C-CH3	-2.01	114.49	122.33
2	N	301	ACT	OXT-C-O	2.01	129.47	122.05
2	P	301	ACT	O-C-CH3	-2.01	114.50	122.33

There are no chirality outliers.

There are no torsion outliers.

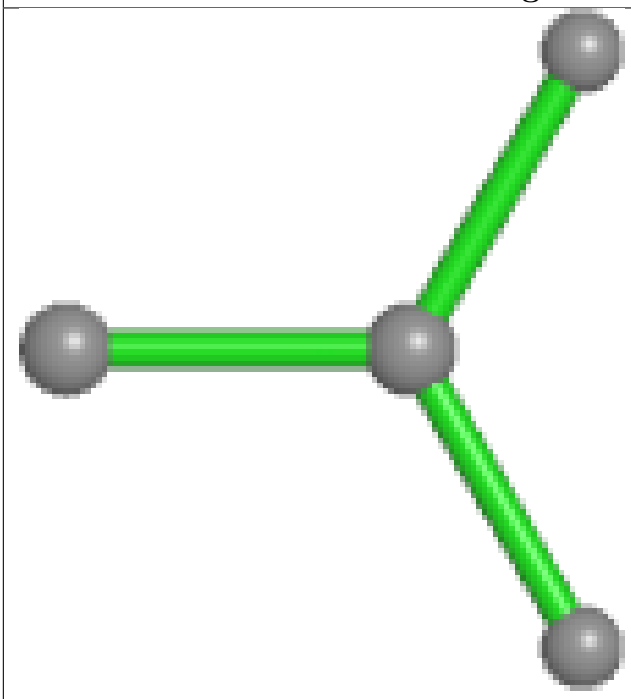
There are no ring outliers.

4 monomers are involved in 5 short contacts:

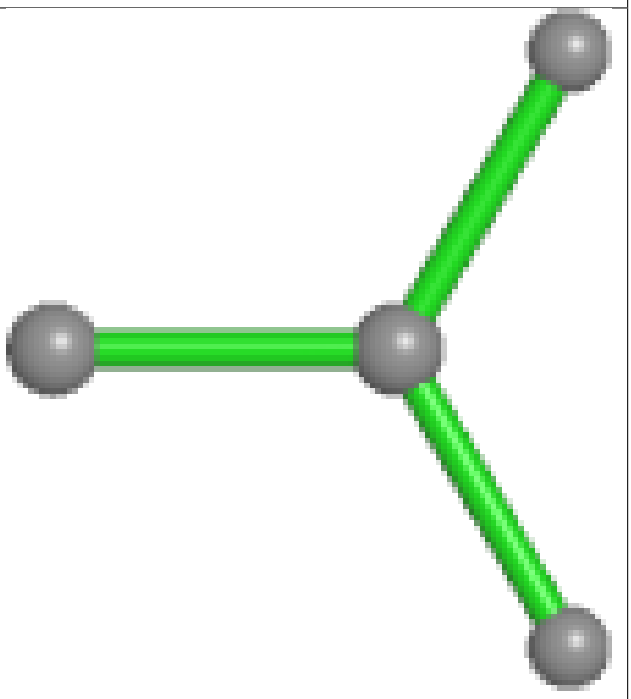
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	ACT	1	0
2	C	301	ACT	2	0
2	A	301	ACT	1	0
2	B	302	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

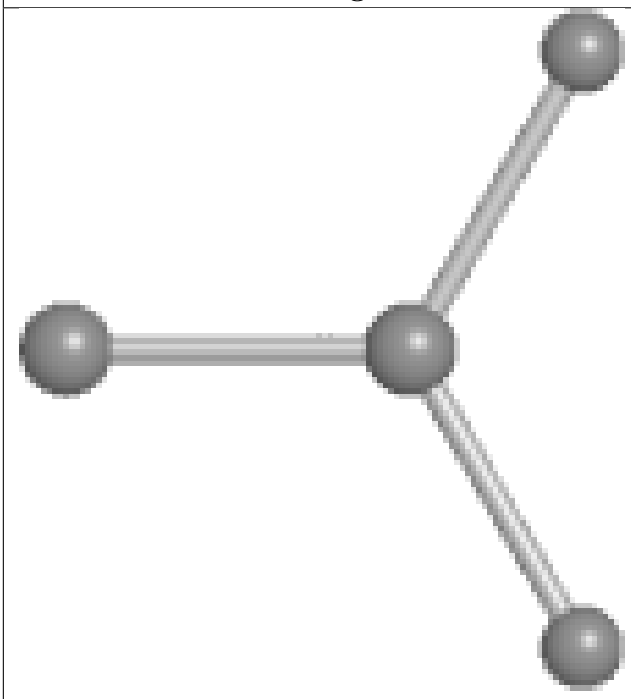
Ligand ACT N 302



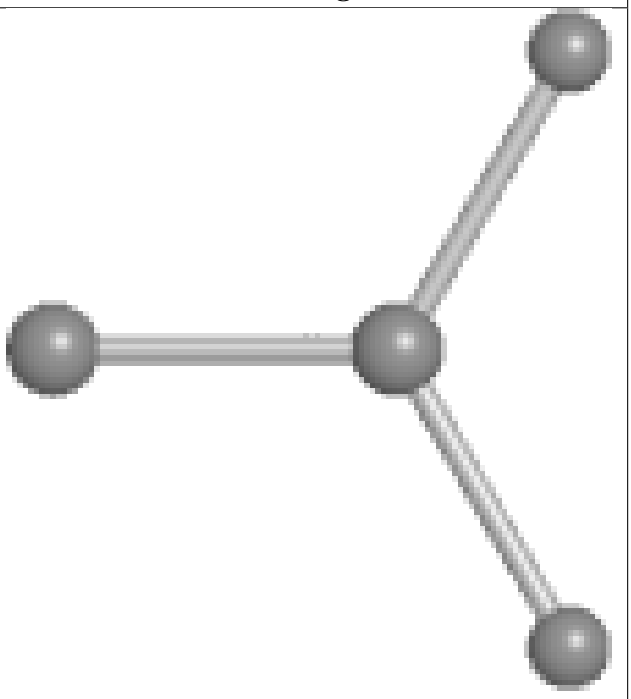
Bond lengths



Bond angles

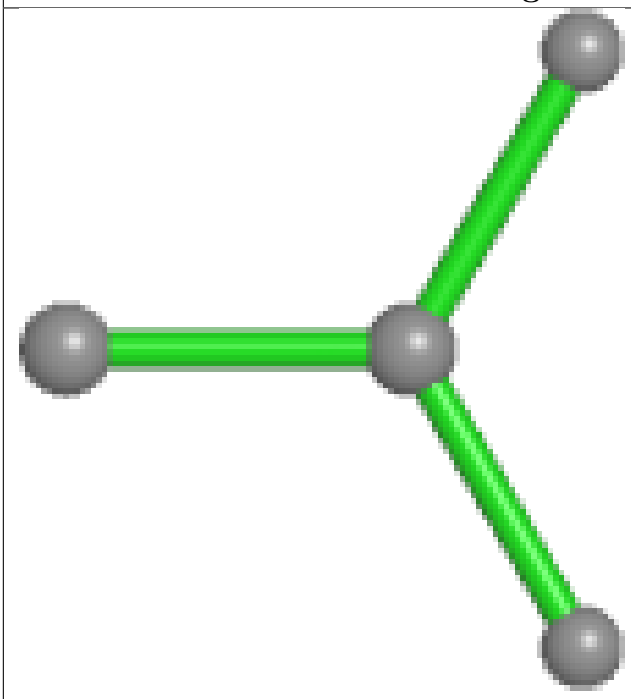


Torsions



Rings

Ligand ACT D 301



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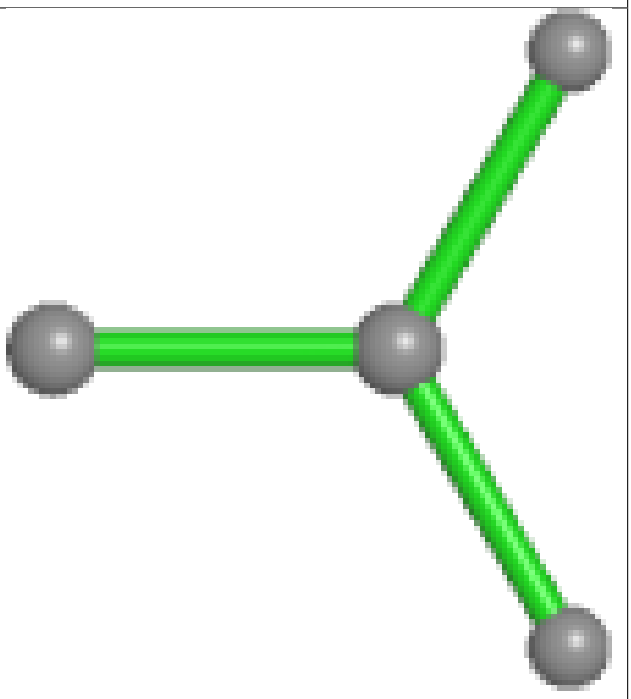
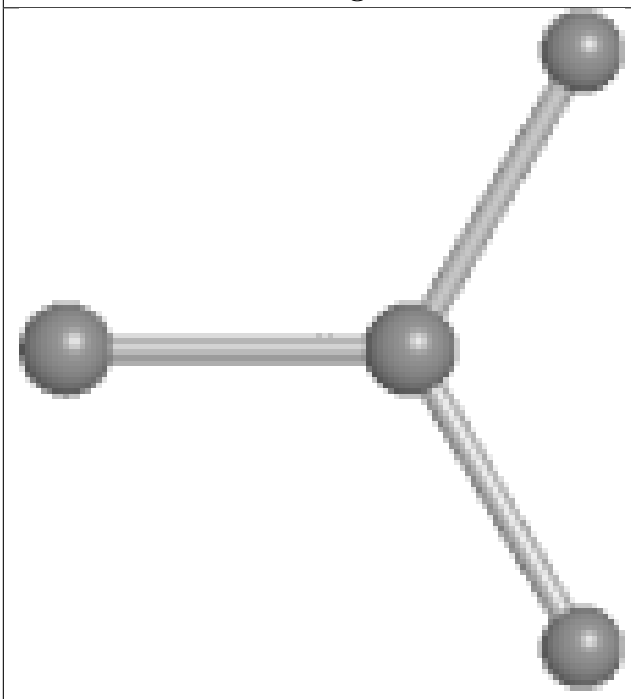


Bond angles



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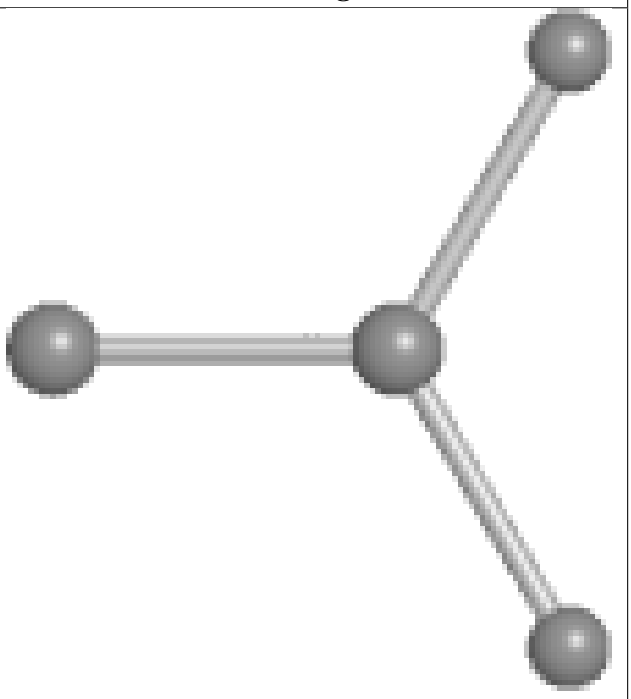
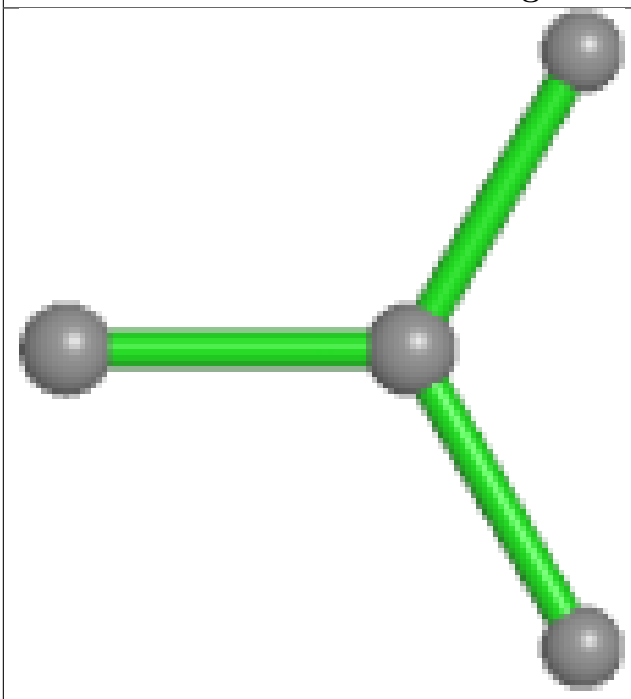


Rings

Ligand ACT K 301



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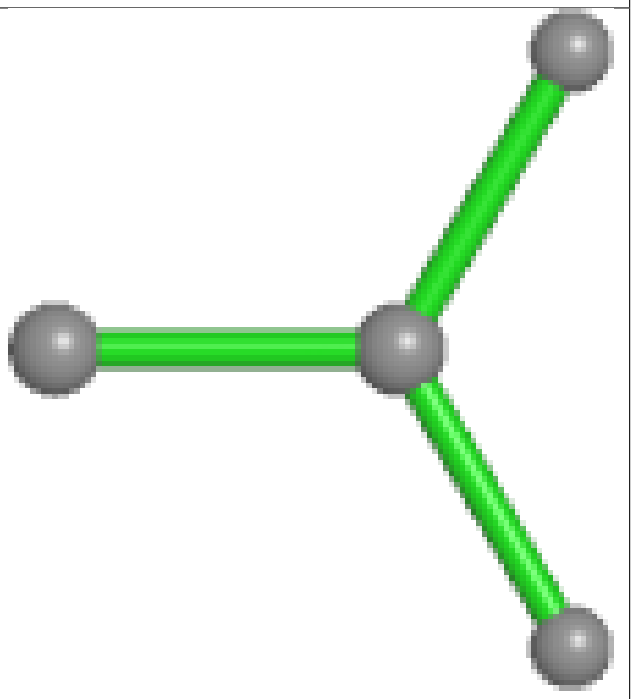

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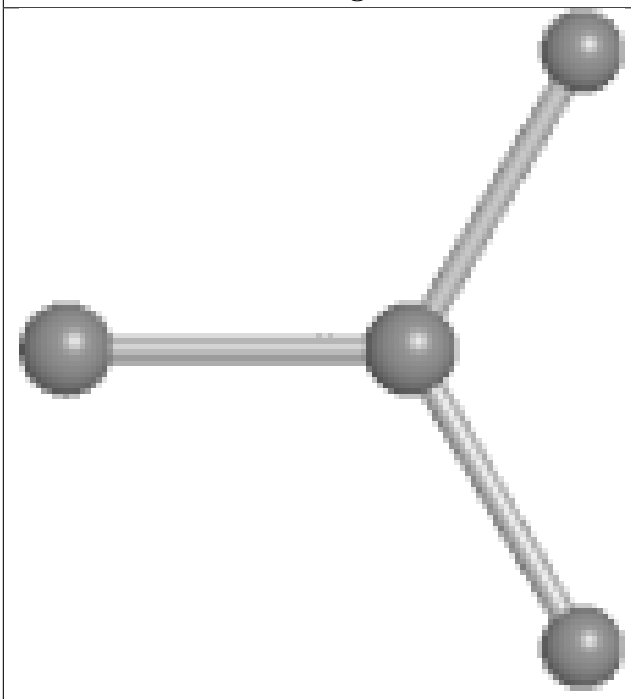

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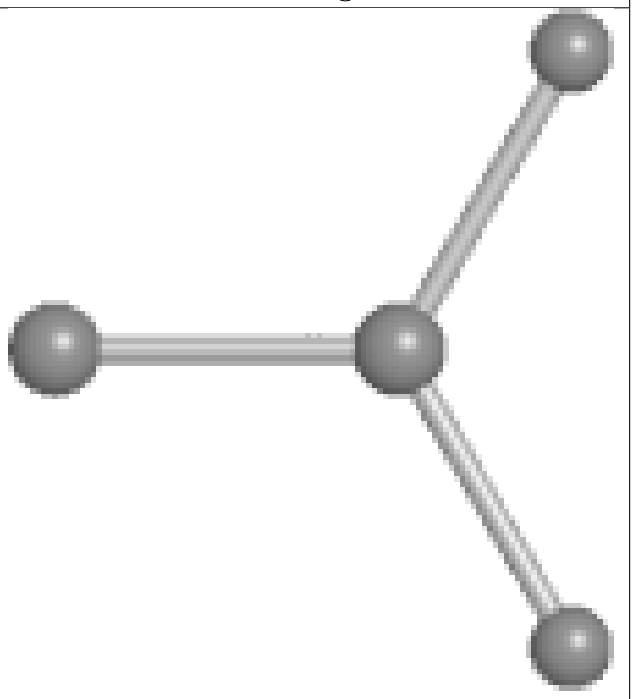
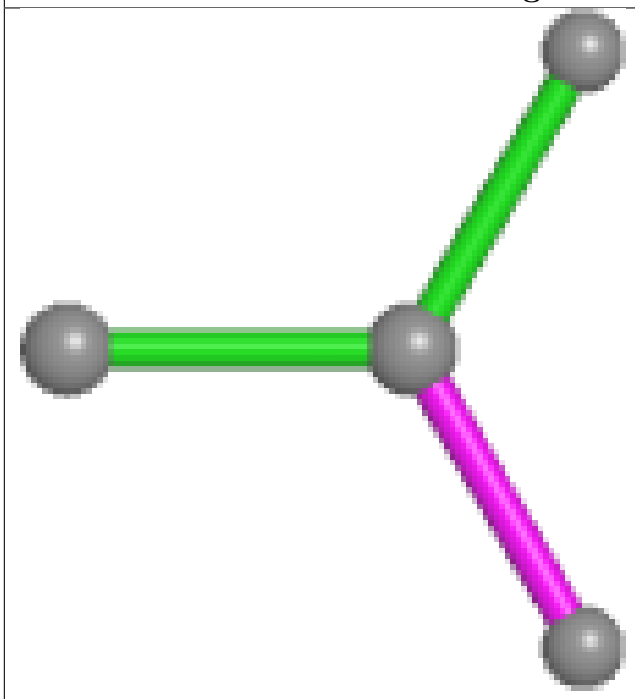


Rings

Ligand ACT H 301



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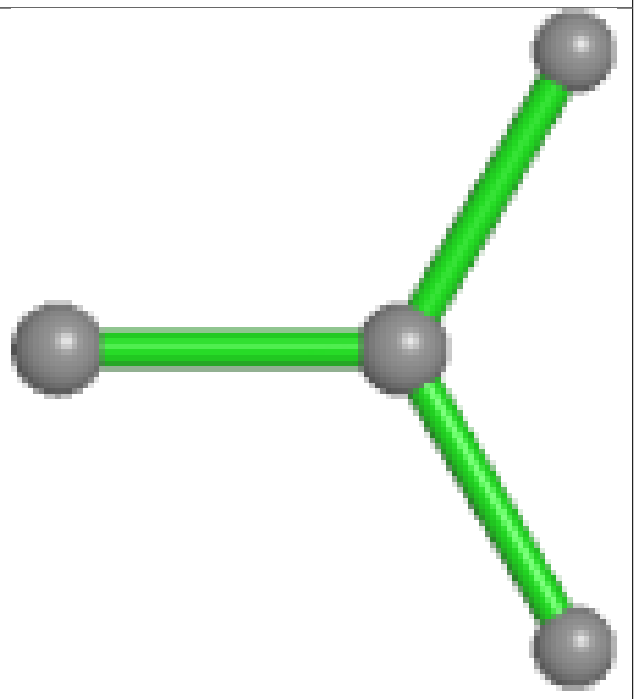
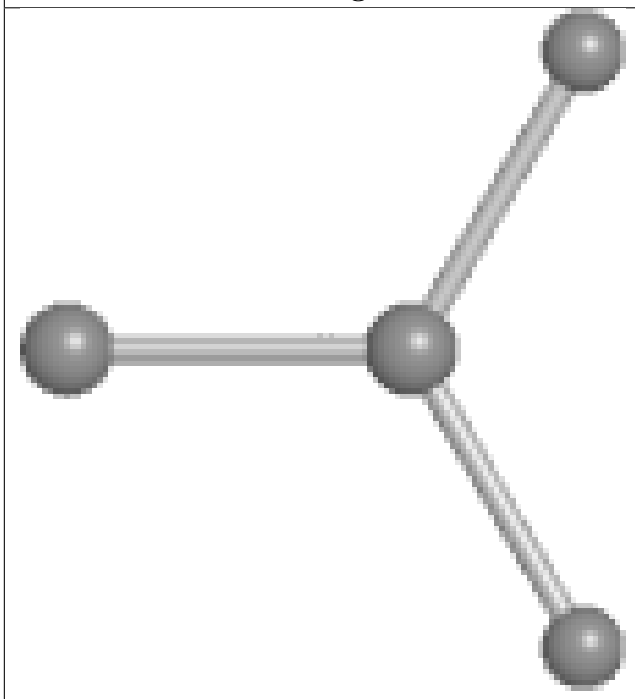


Bond angles



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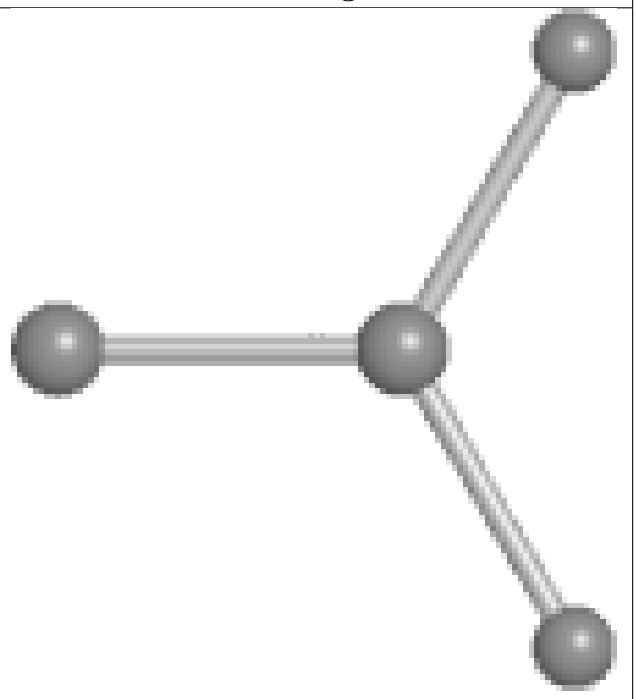
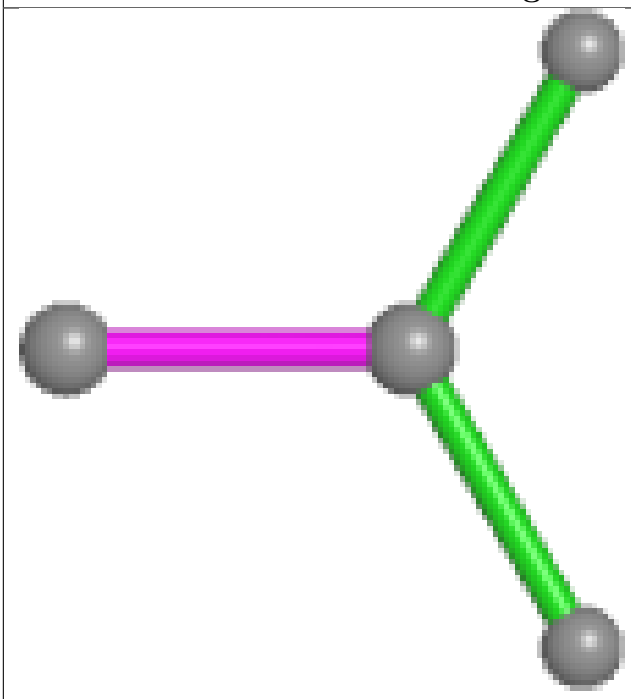


Rings

Ligand ACT C 301



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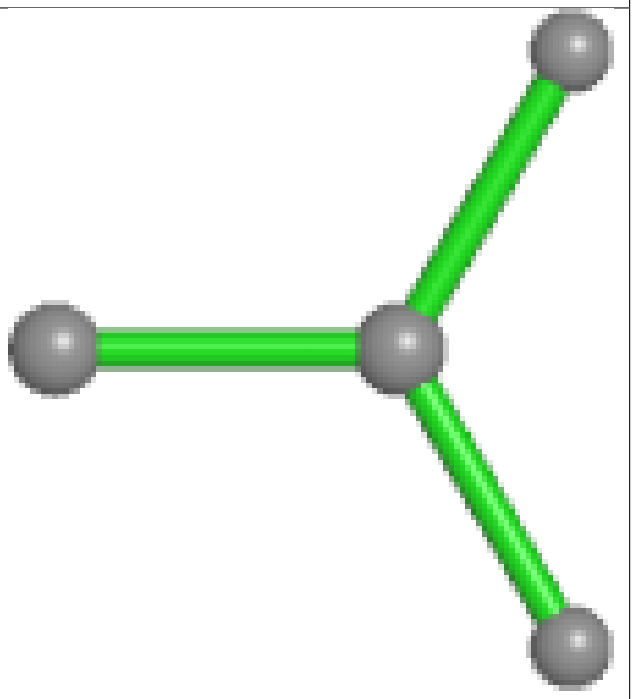
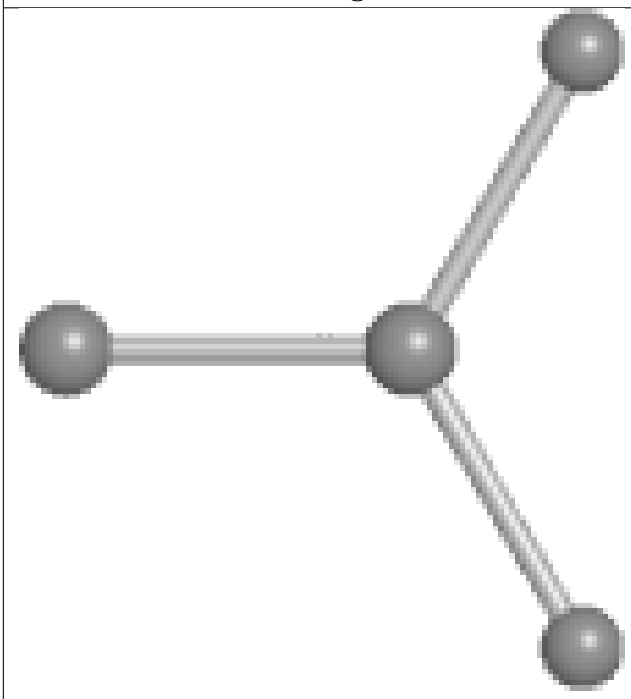


Bond angles



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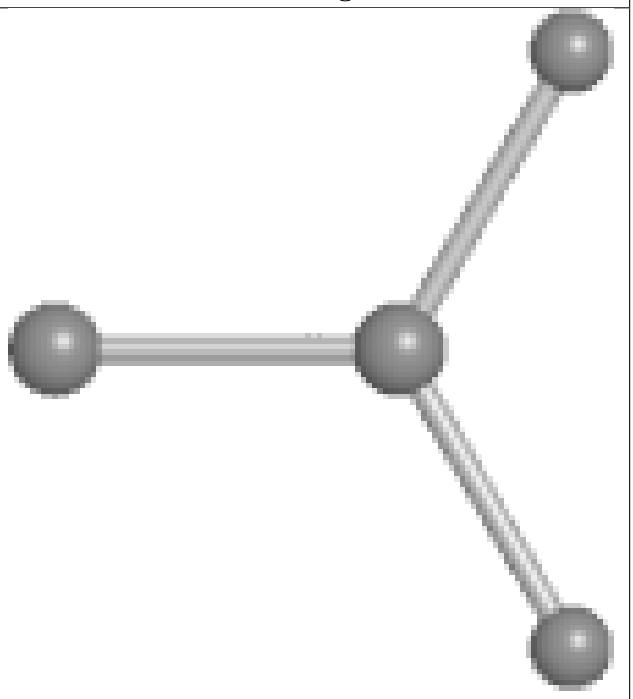
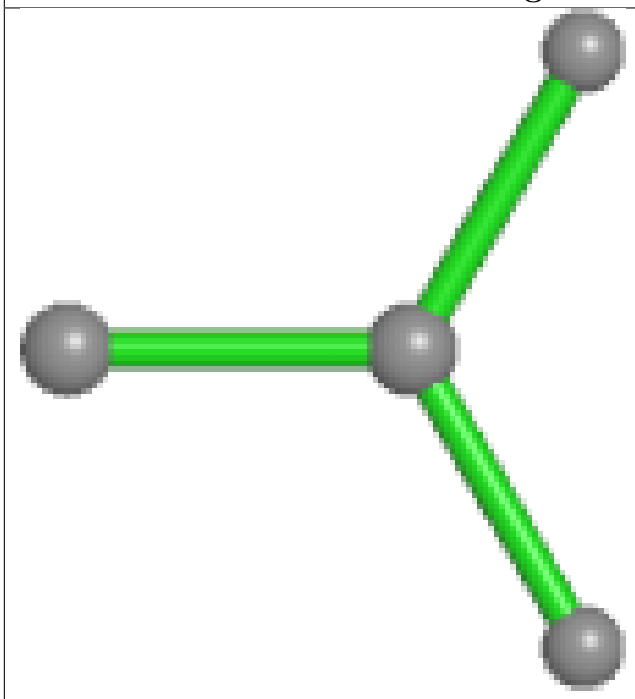


Rings

Ligand ACT P 302



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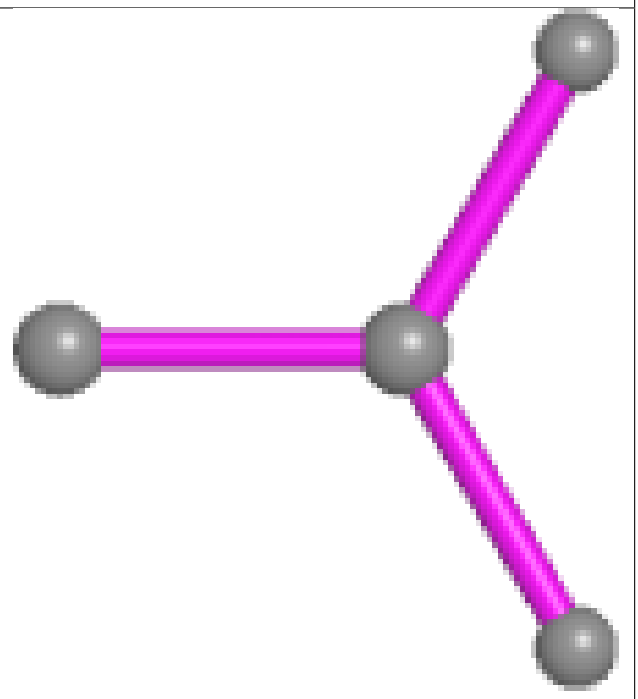

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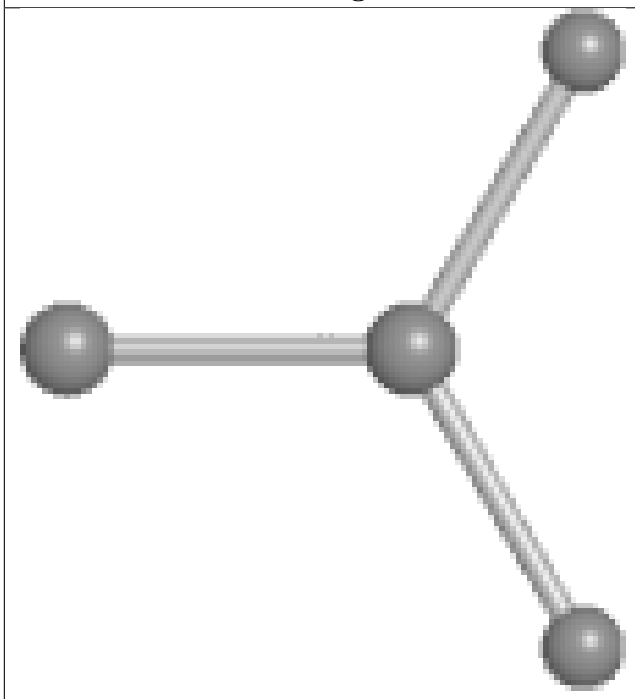

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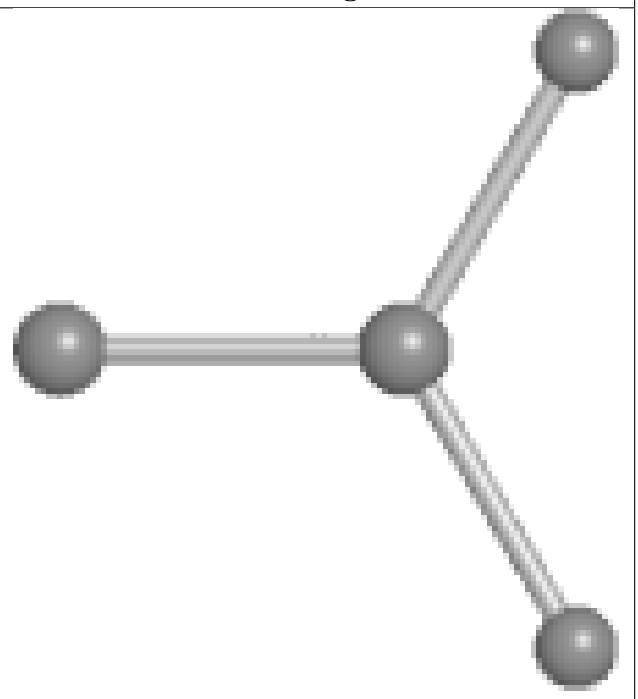
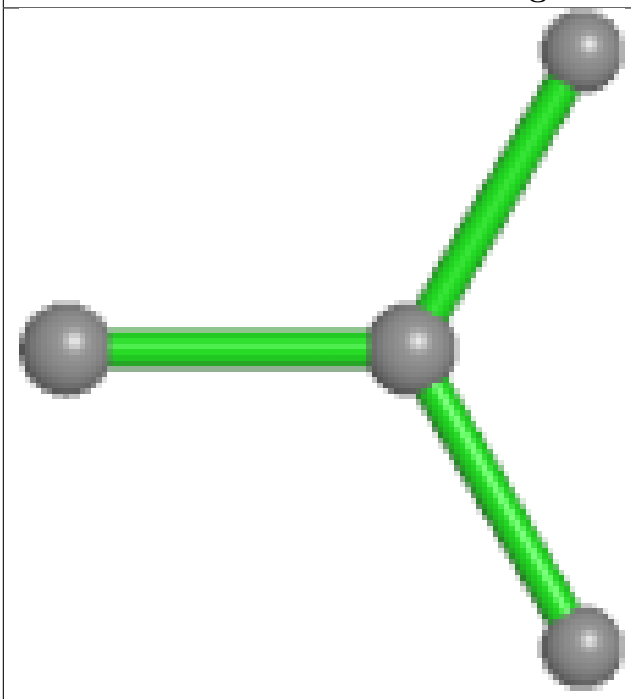


Rings

Ligand ACT I 302



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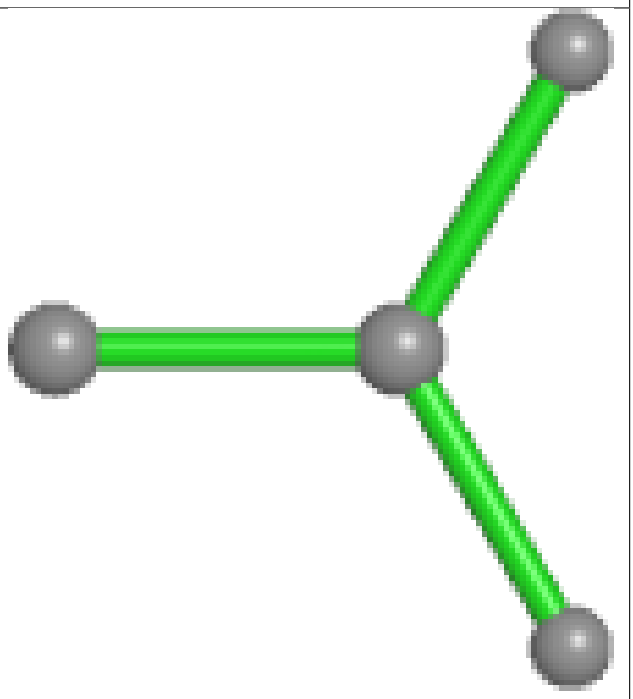
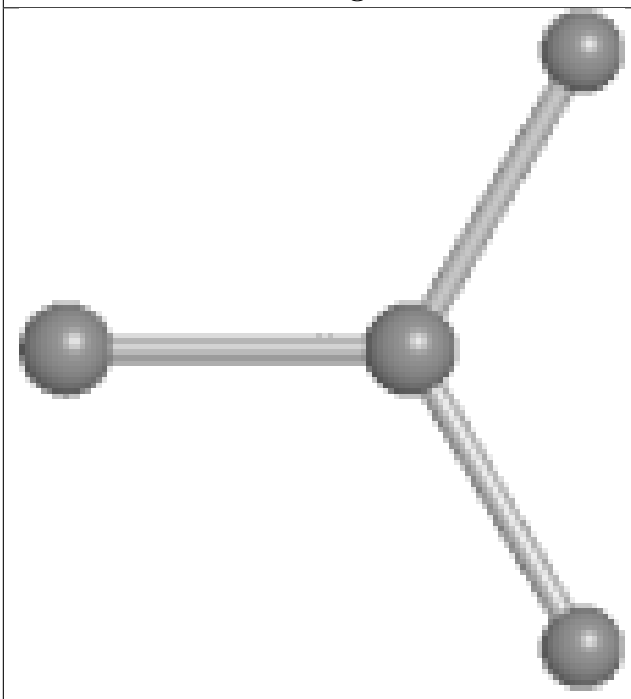


Bond angles



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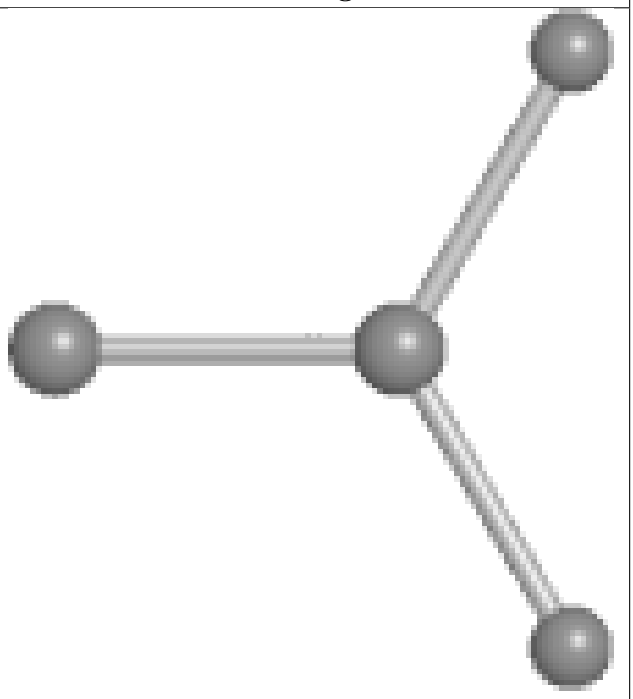
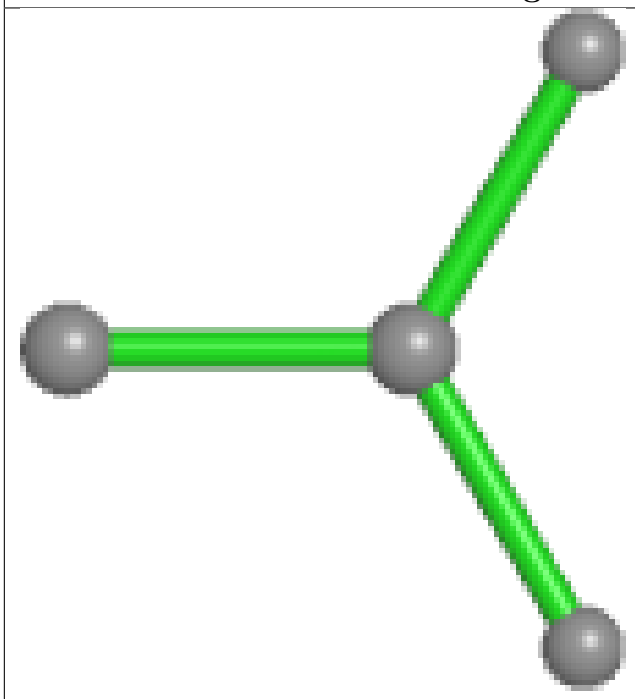


Rings

Ligand ACT D 302



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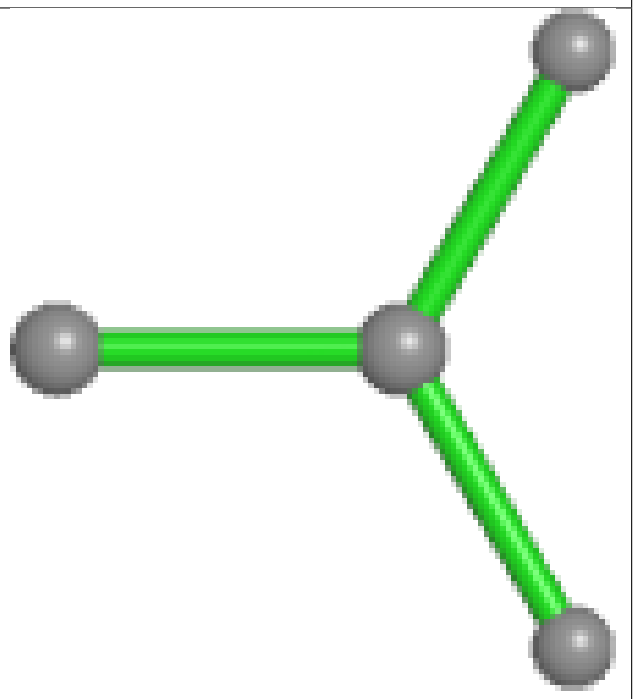

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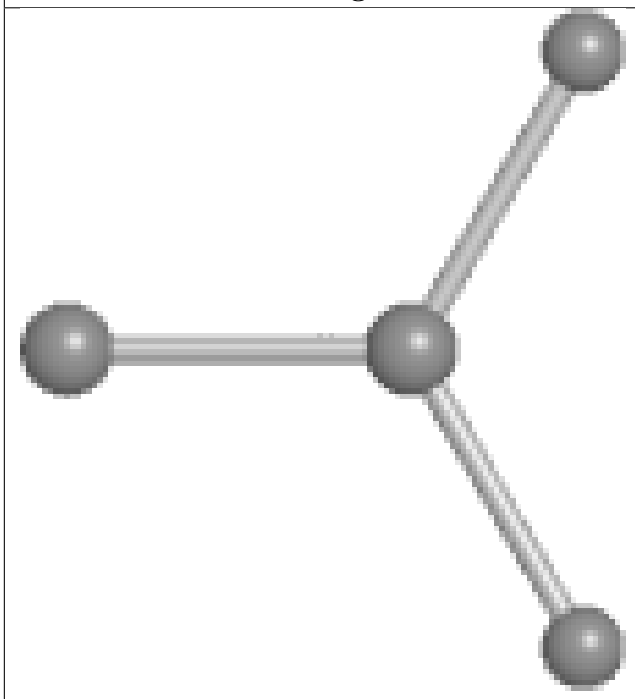

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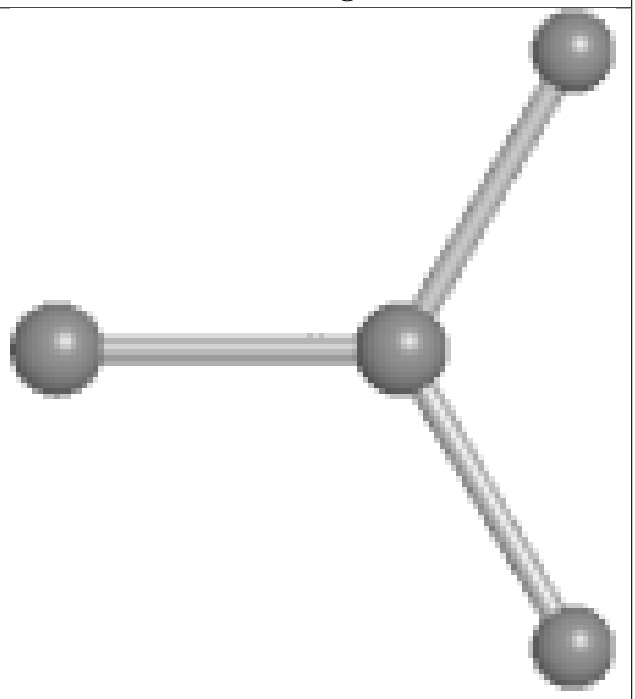
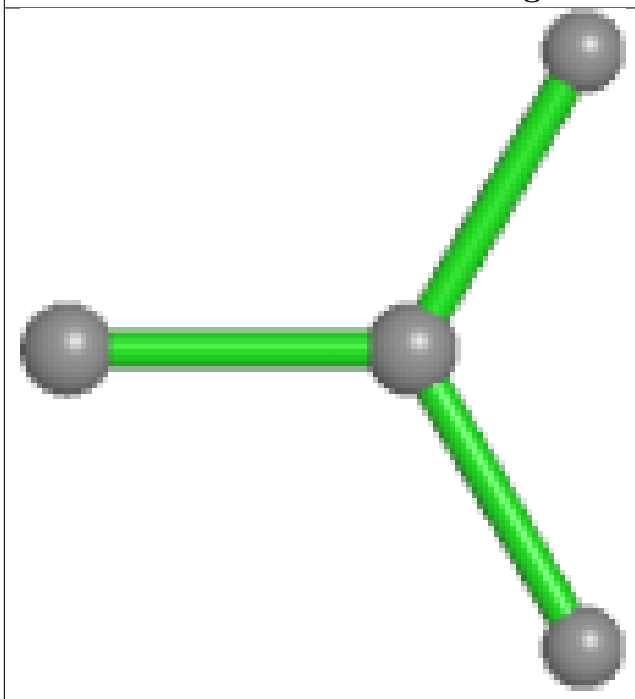
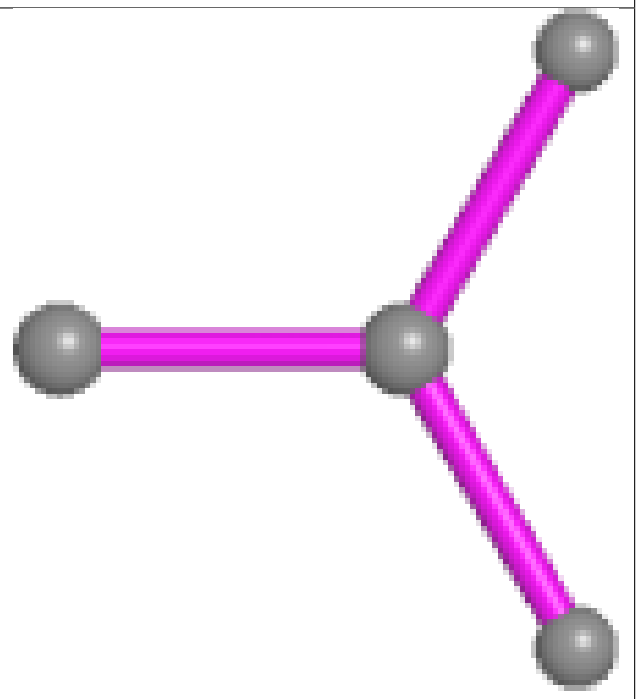


Rings

Ligand ACT A 301



Bond lengths



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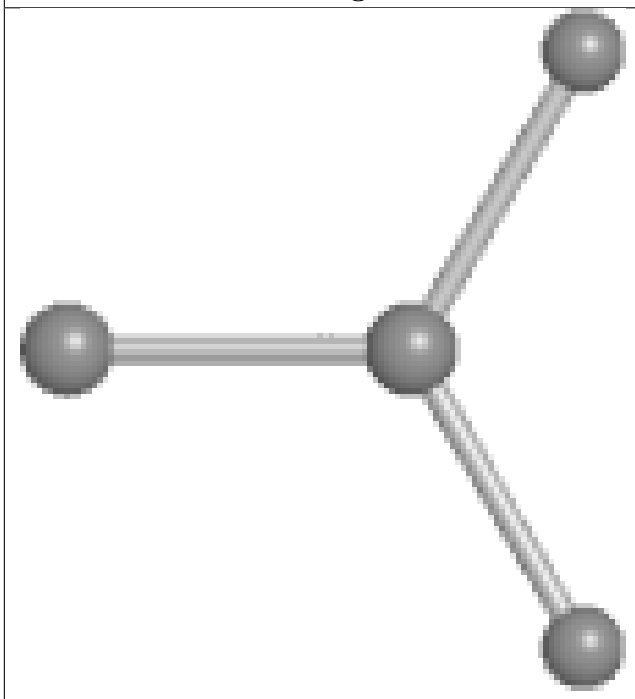

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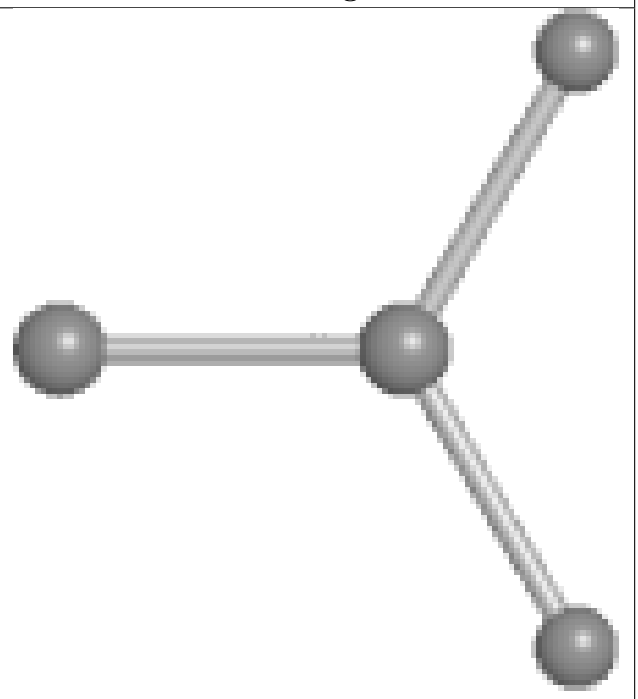
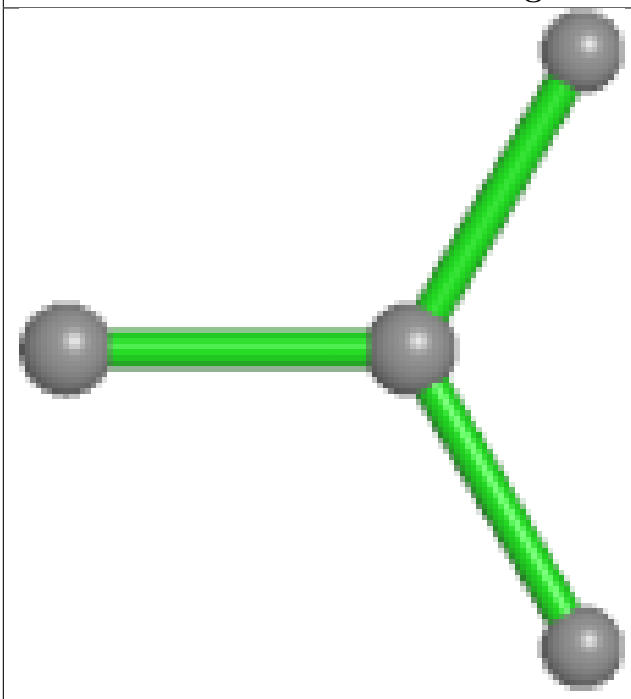


Rings

Ligand ACT F 301



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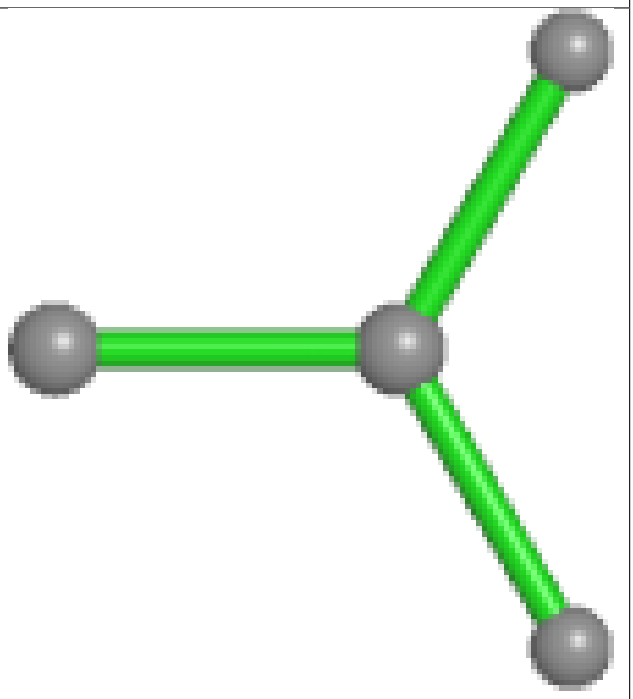

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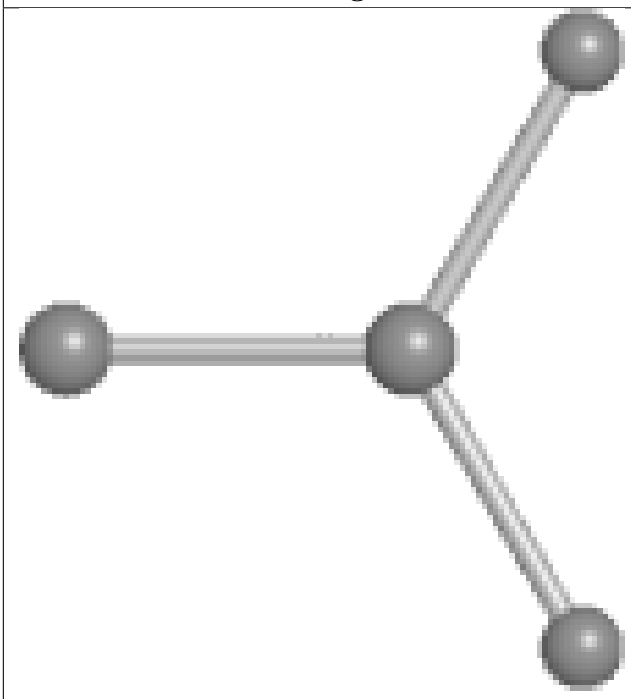

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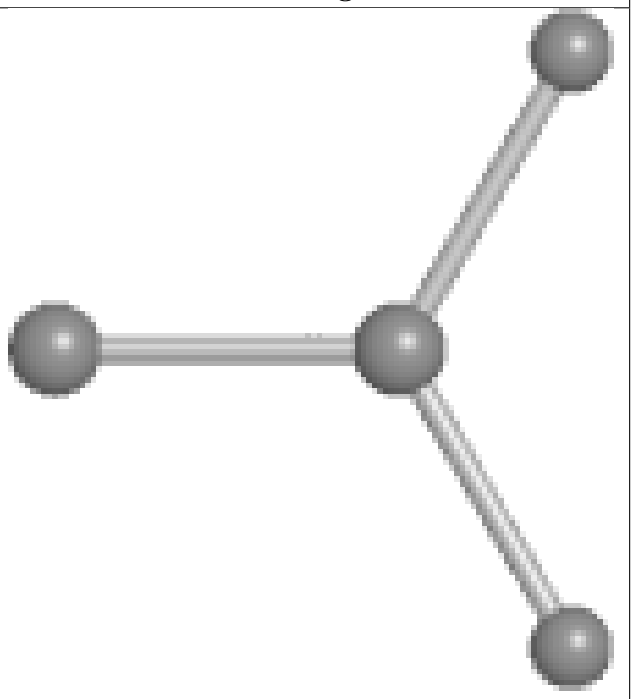
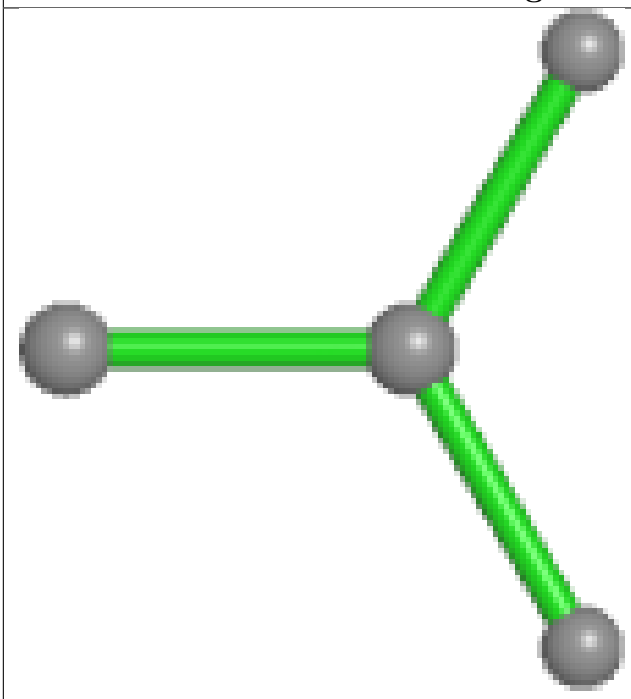


Rings

Ligand ACT L 301



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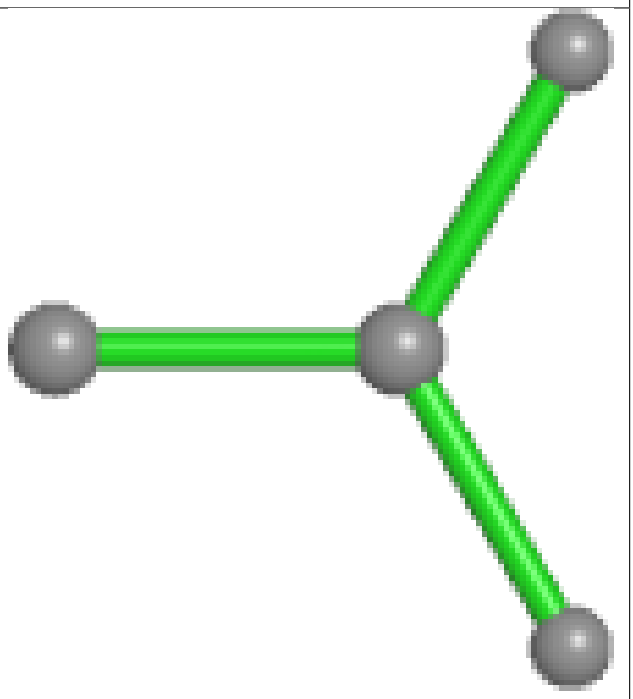
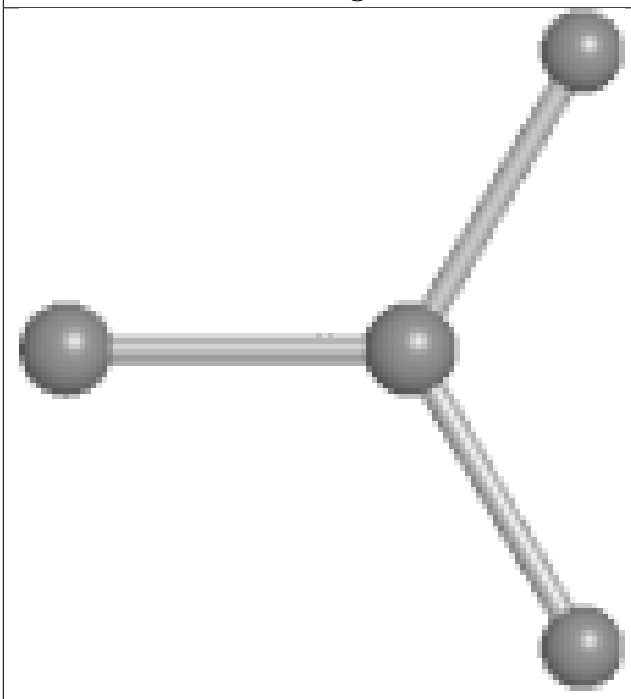
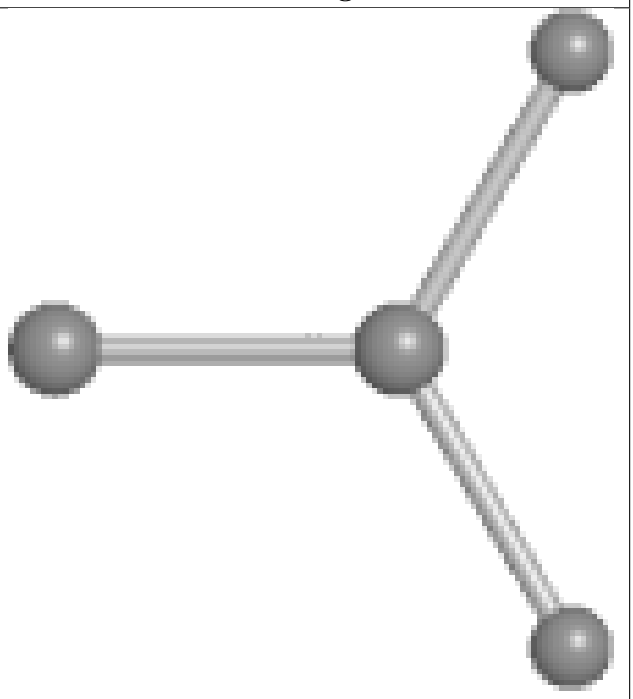


Bond angles

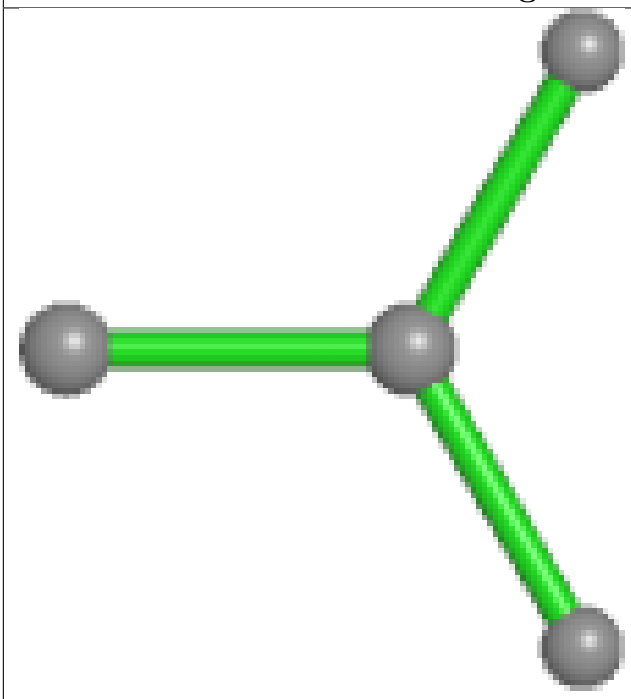


Torsions



Rings

Ligand ACT M 302



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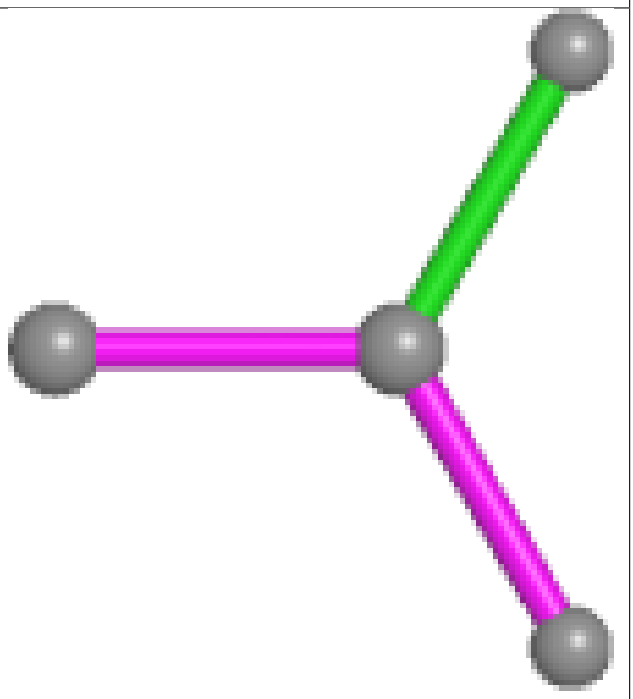

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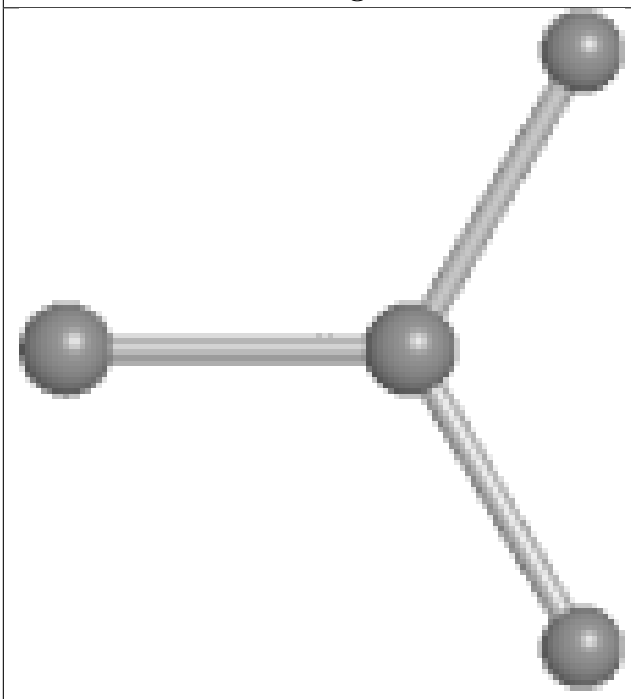

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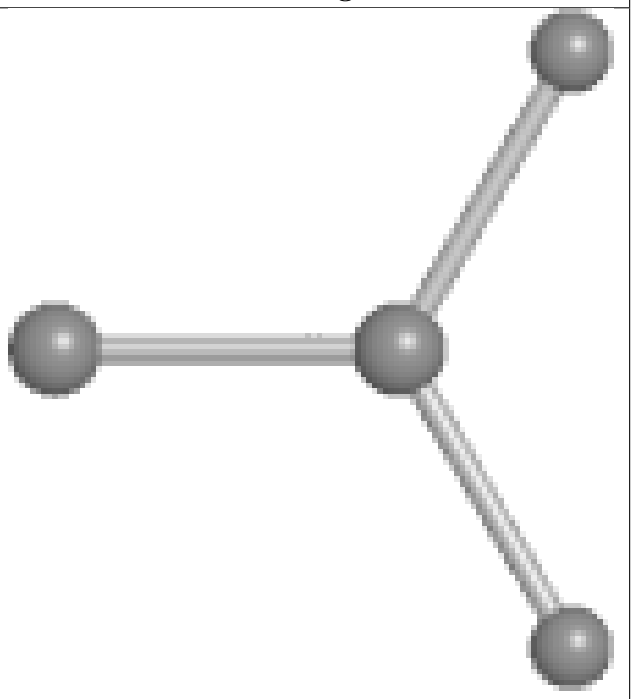
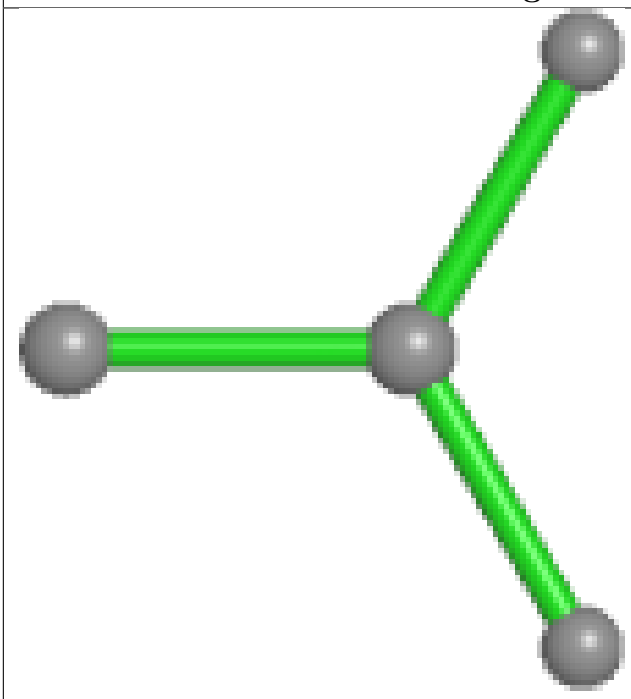


Rings

Ligand ACT B 302



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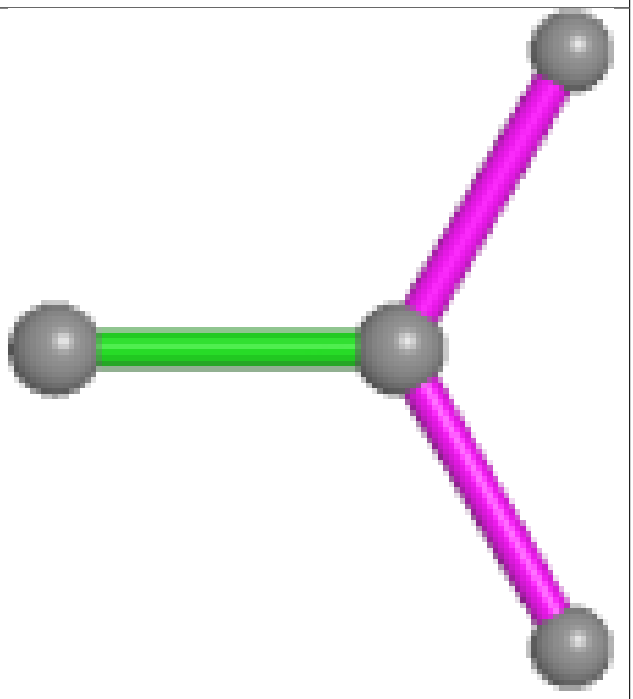

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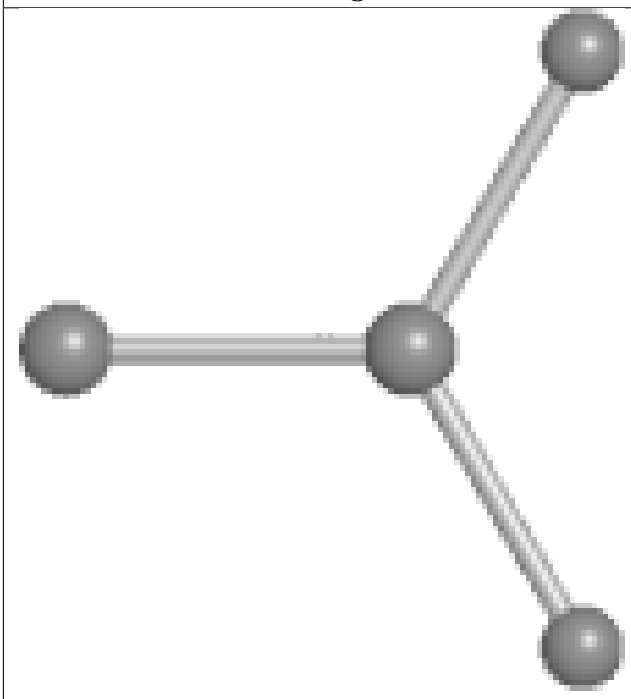

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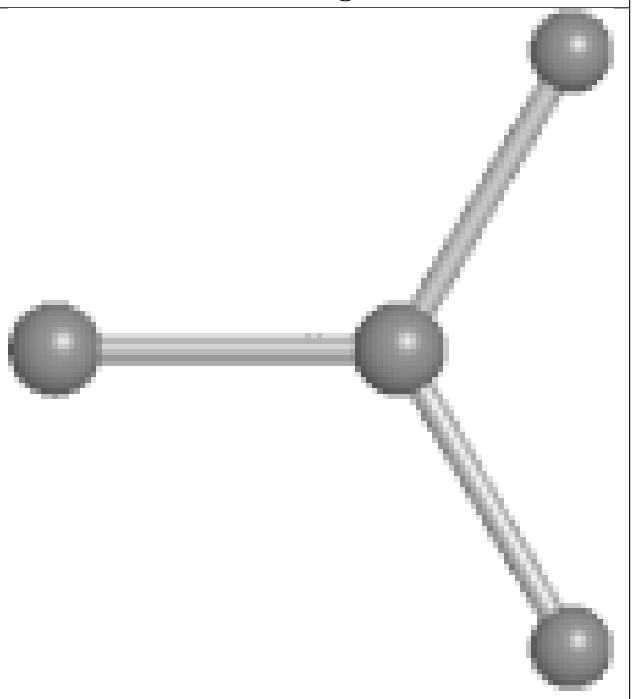
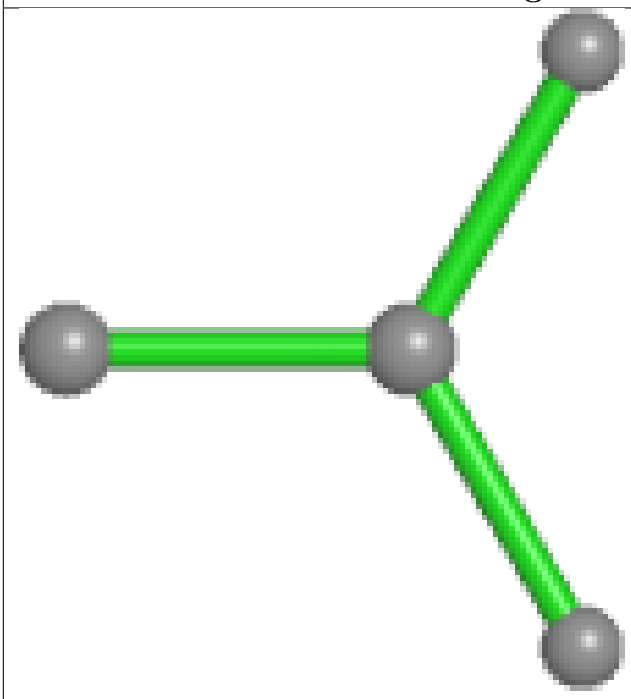


Rings

Ligand ACT F 302



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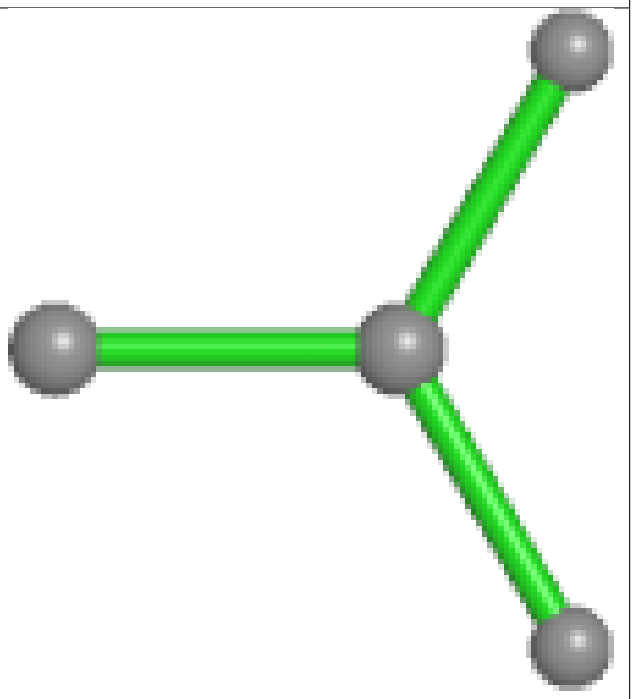
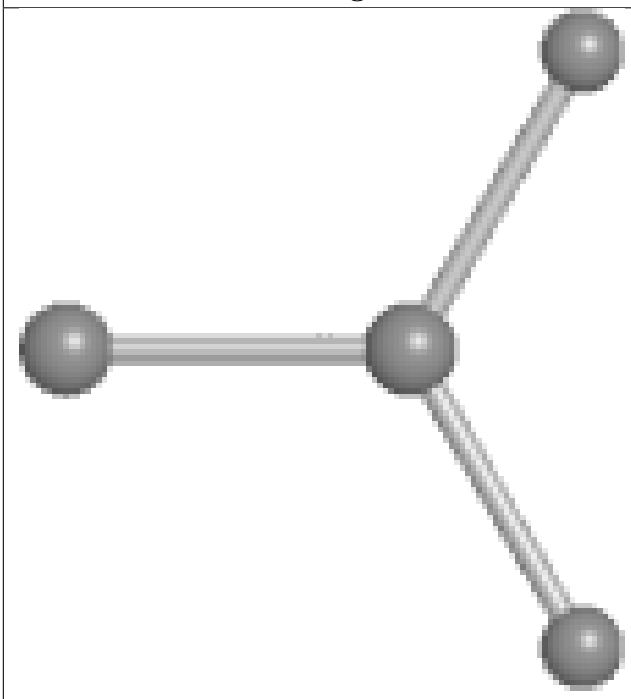


Bond angles



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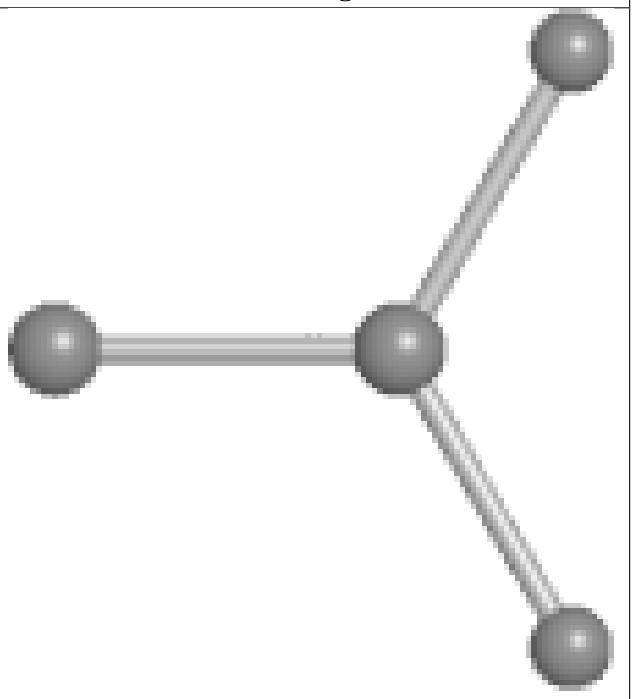
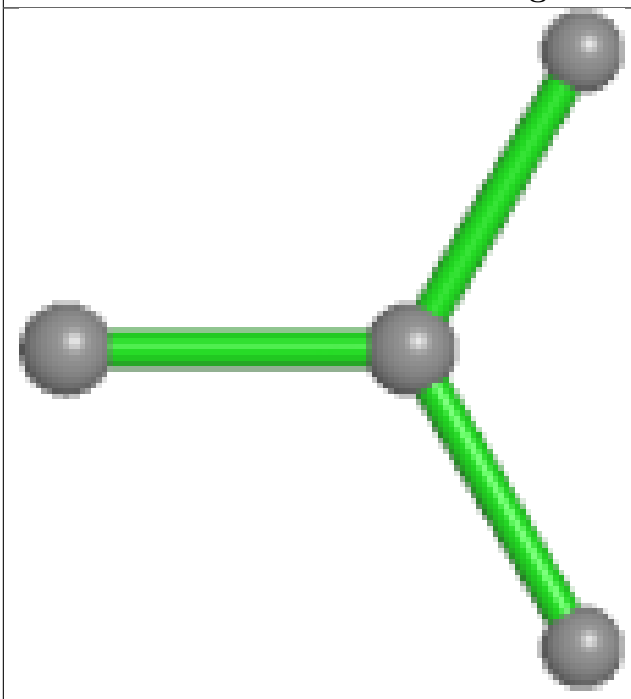


Rings

Ligand ACT I 301



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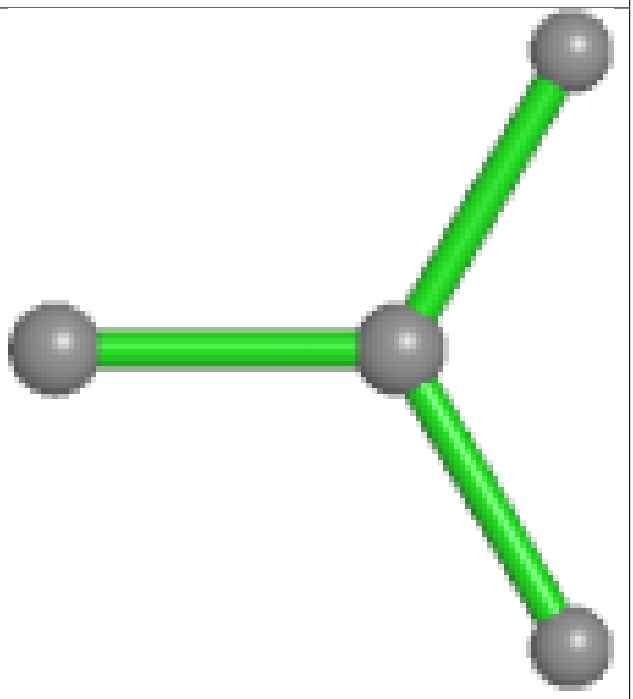

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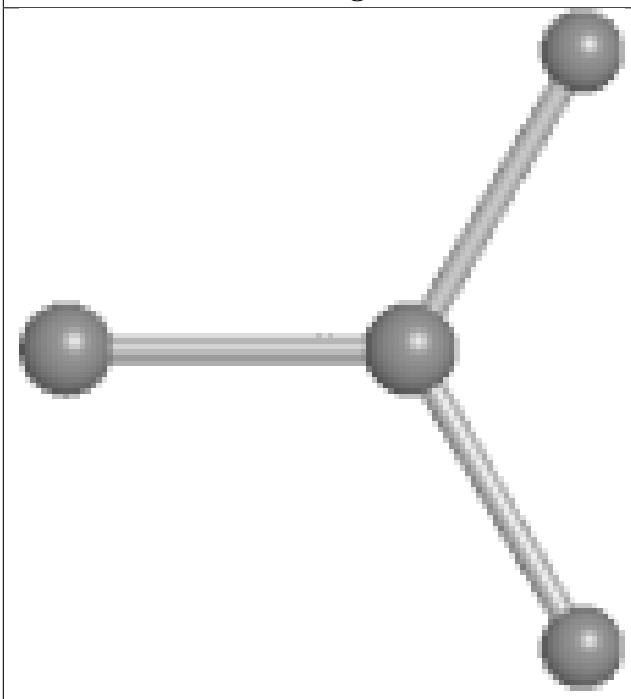

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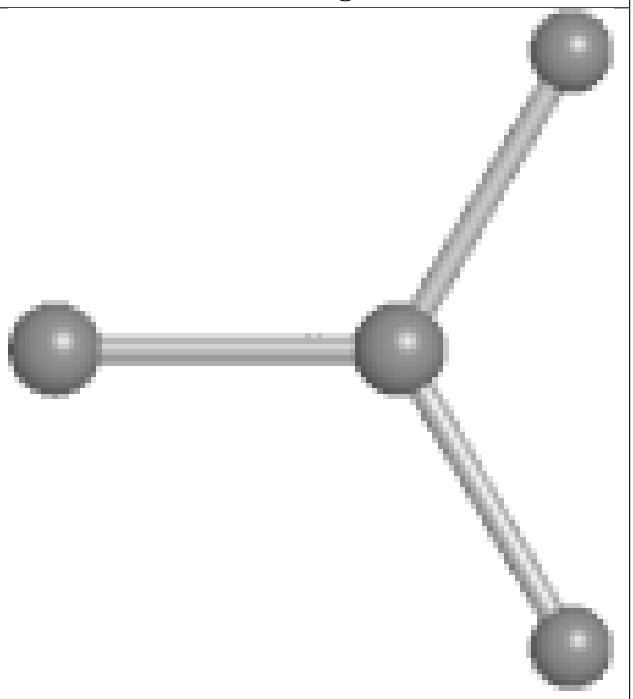
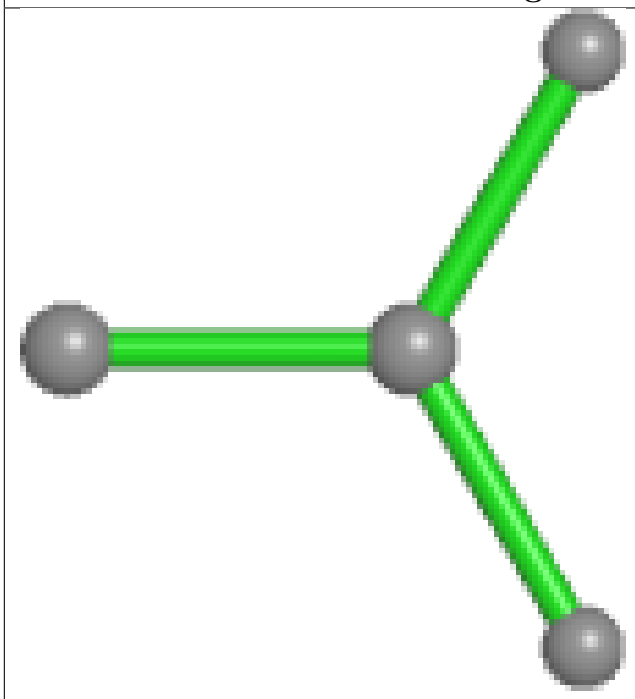


Rings

Ligand ACT P 301



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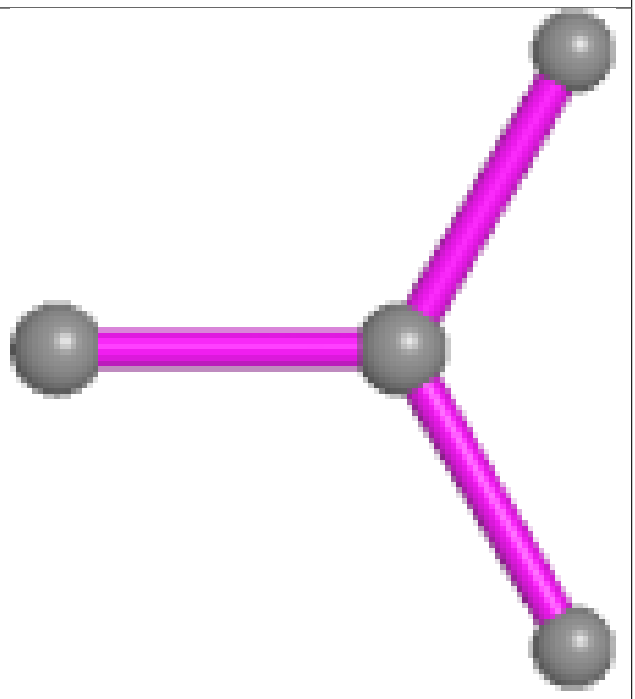

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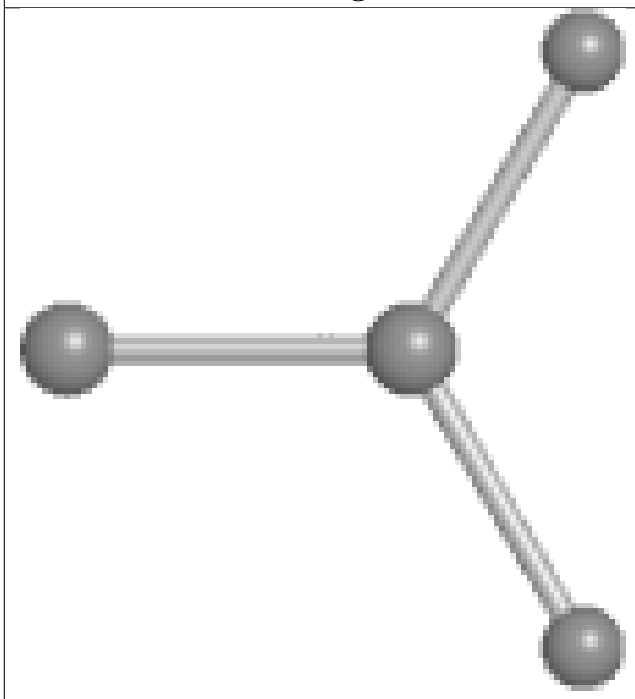

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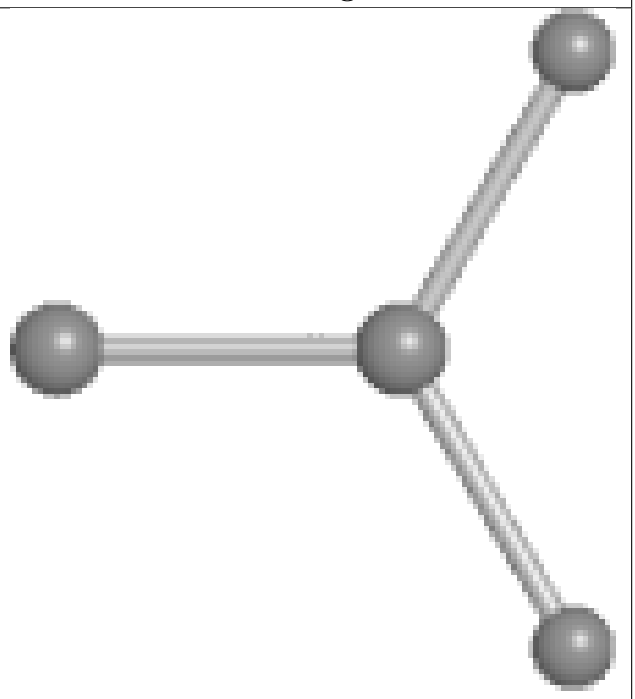
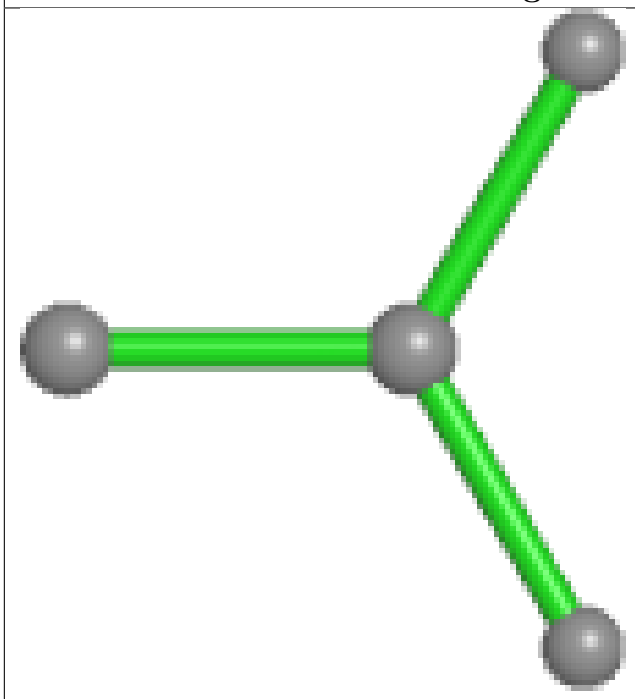


Rings

Ligand ACT A 302



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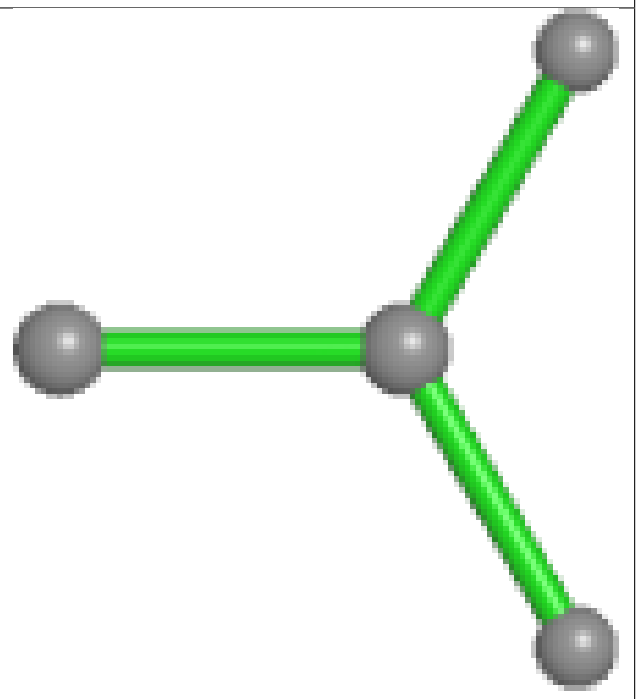

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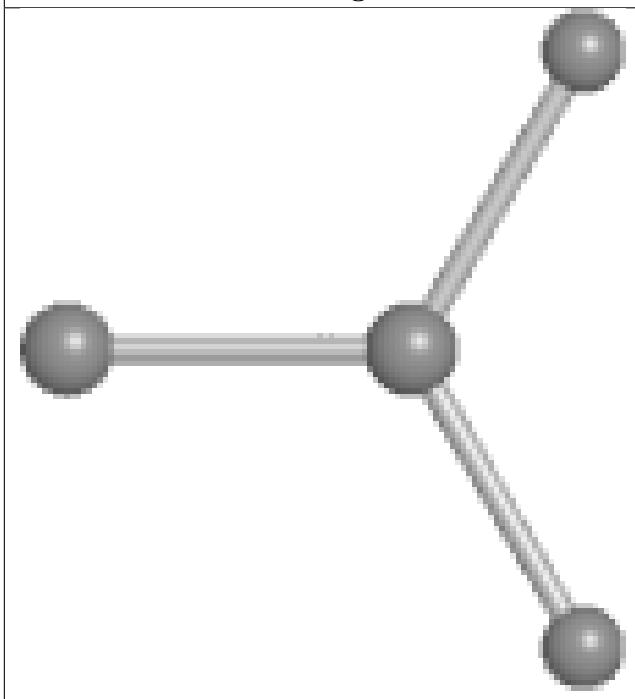

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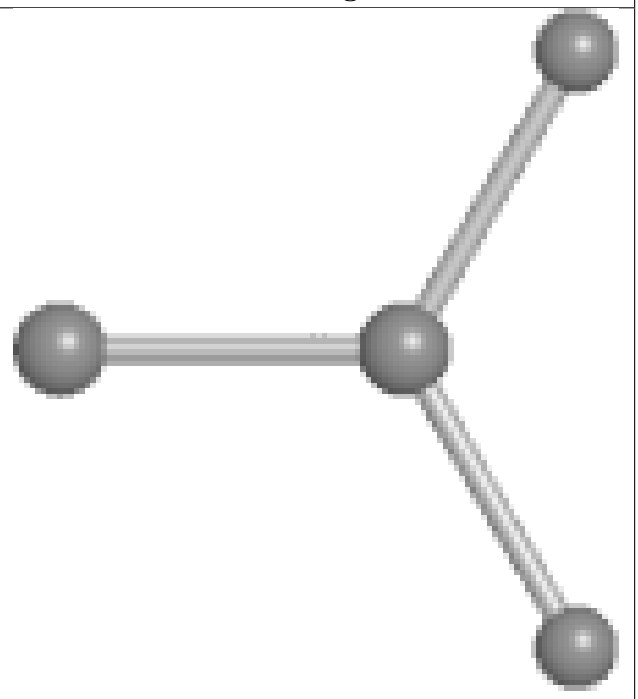
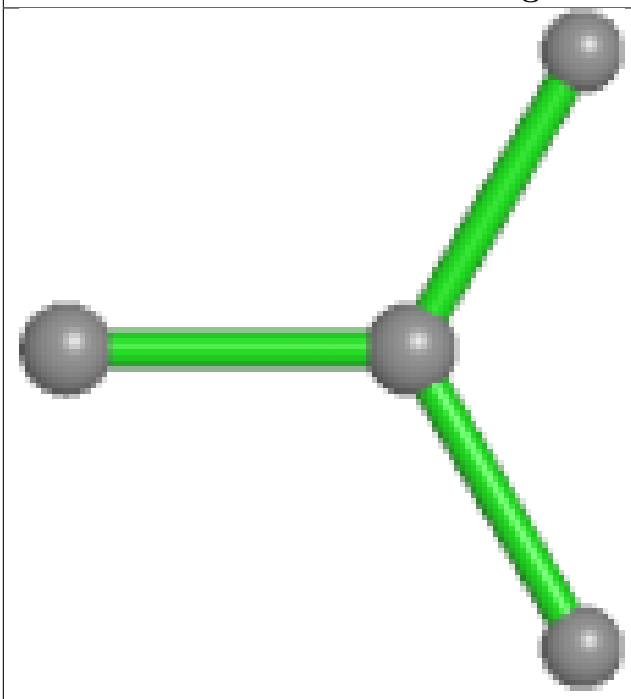


Rings

Ligand ACT G 302



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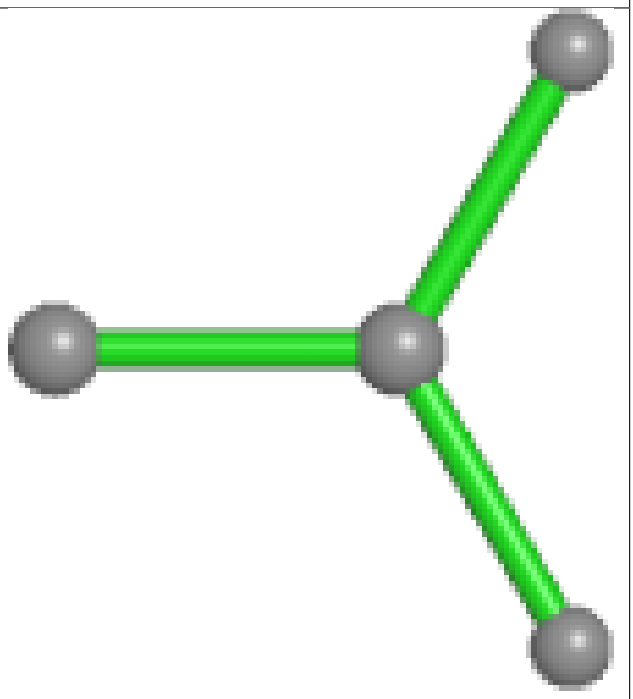

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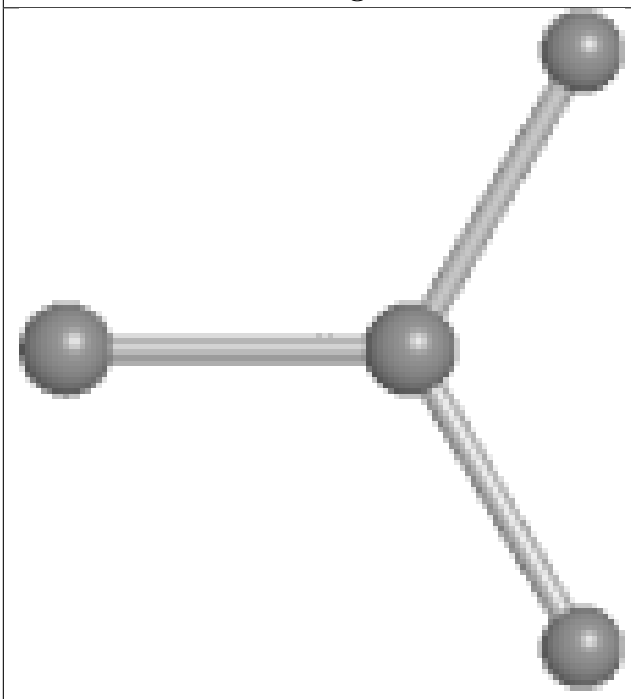

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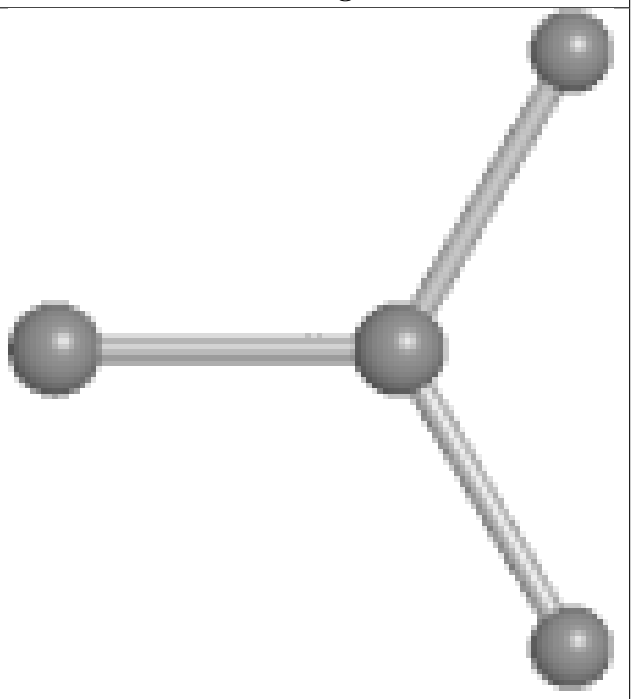
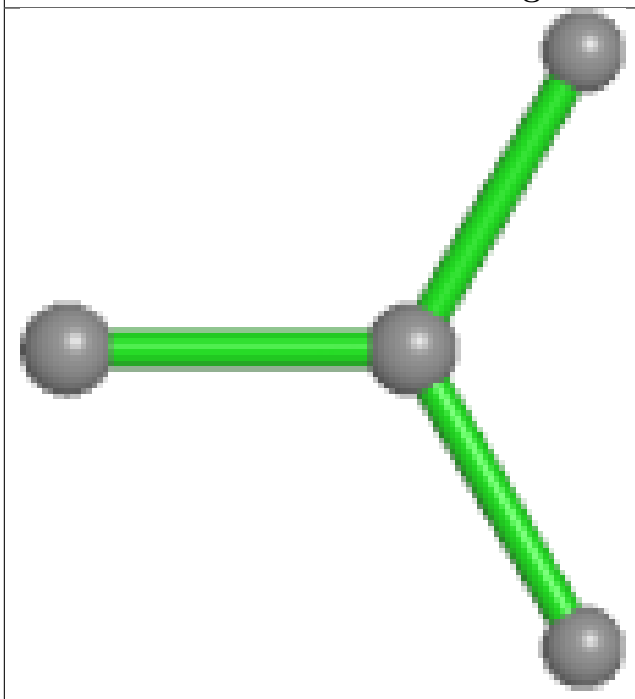


Rings

Ligand ACT K 302



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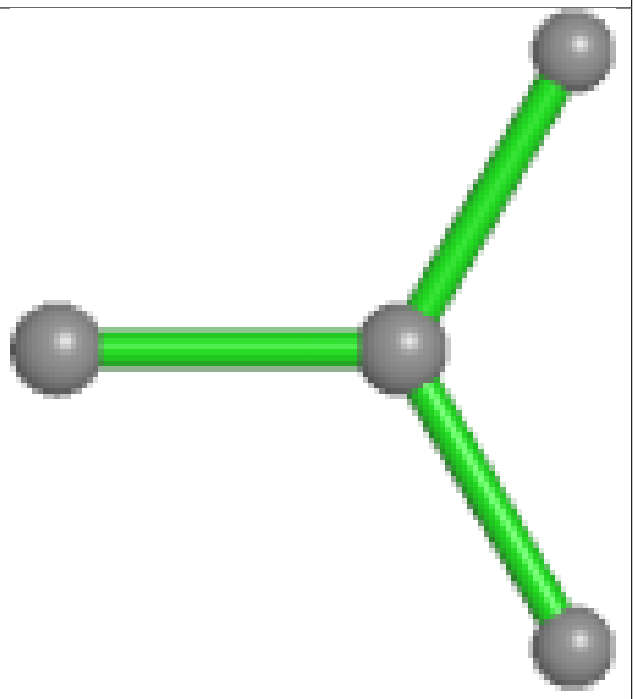

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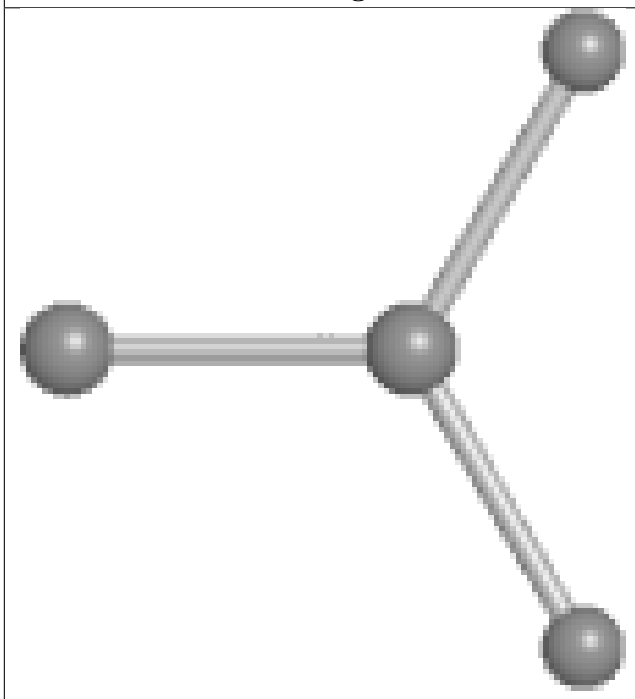

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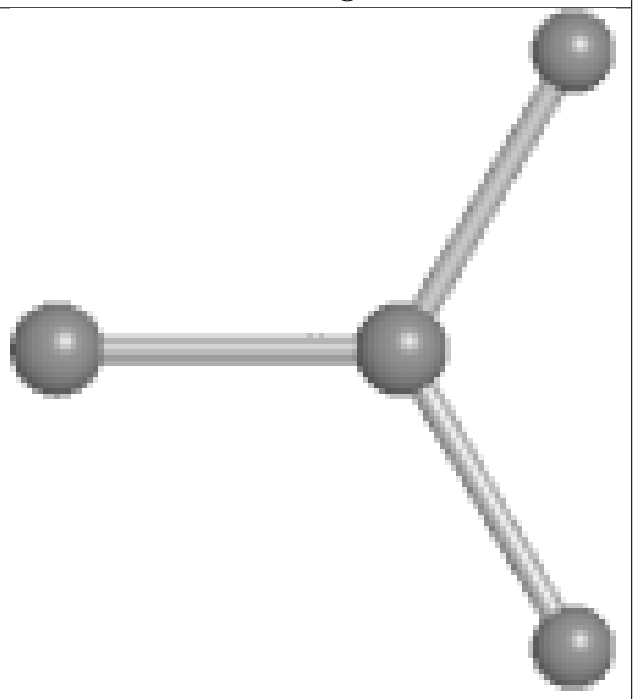
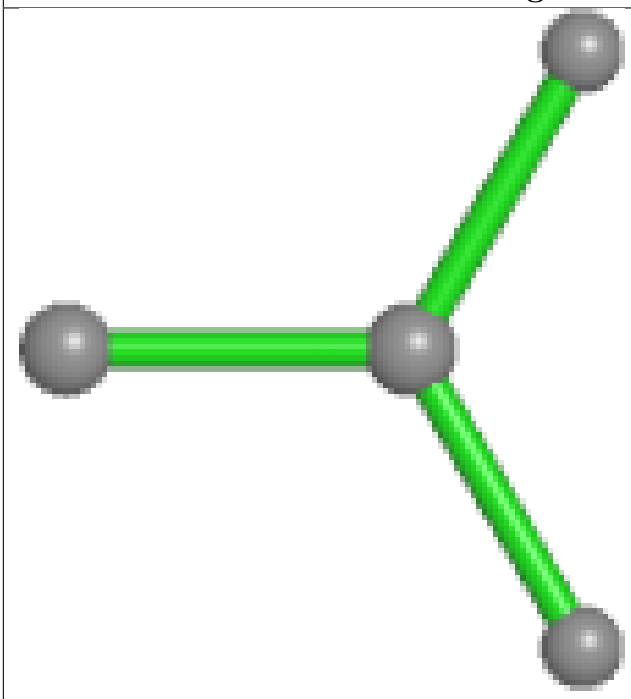


Rings

Ligand ACT J 302



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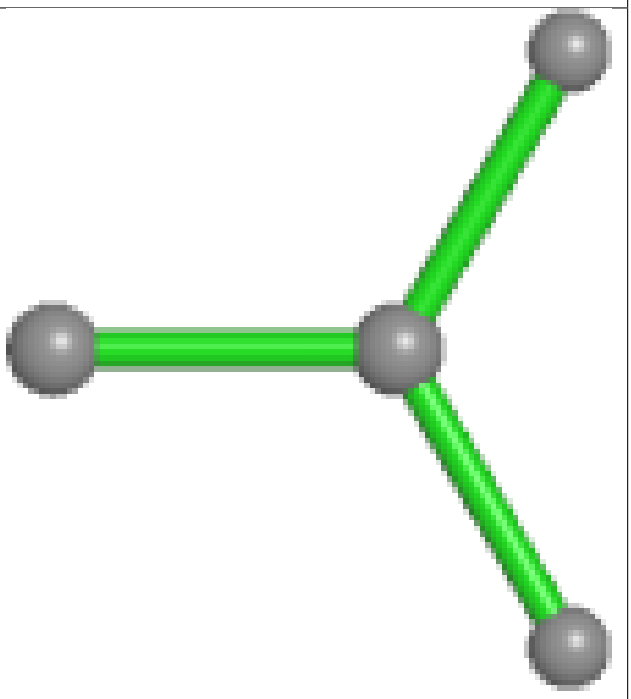

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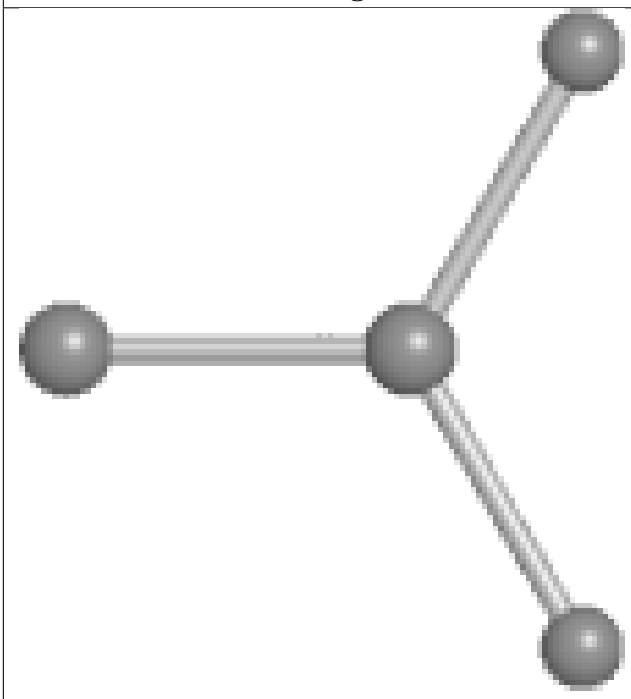

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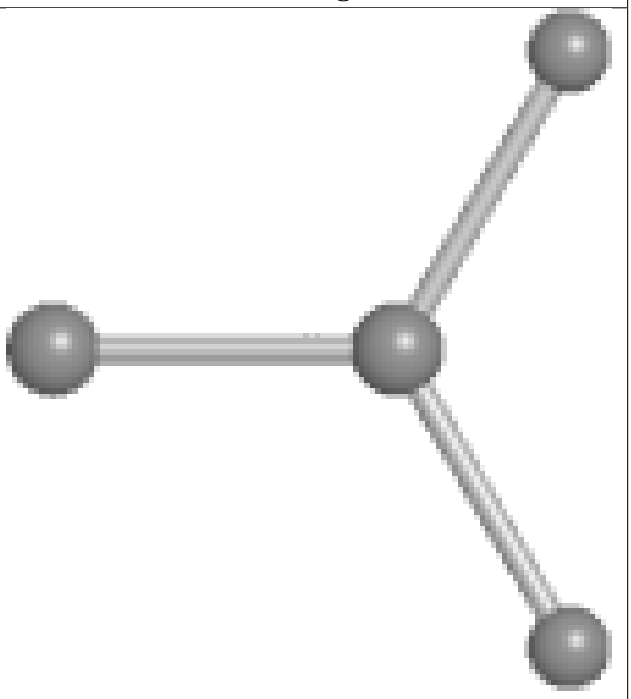
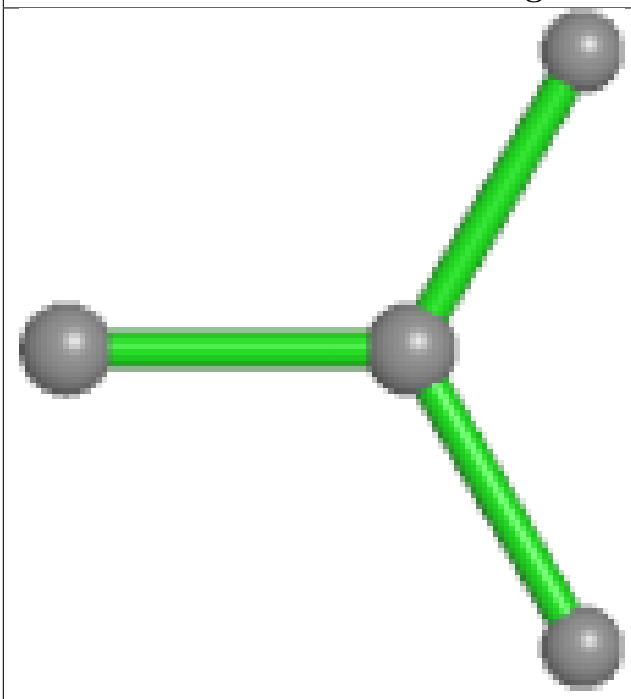


Rings

Ligand ACT L 302



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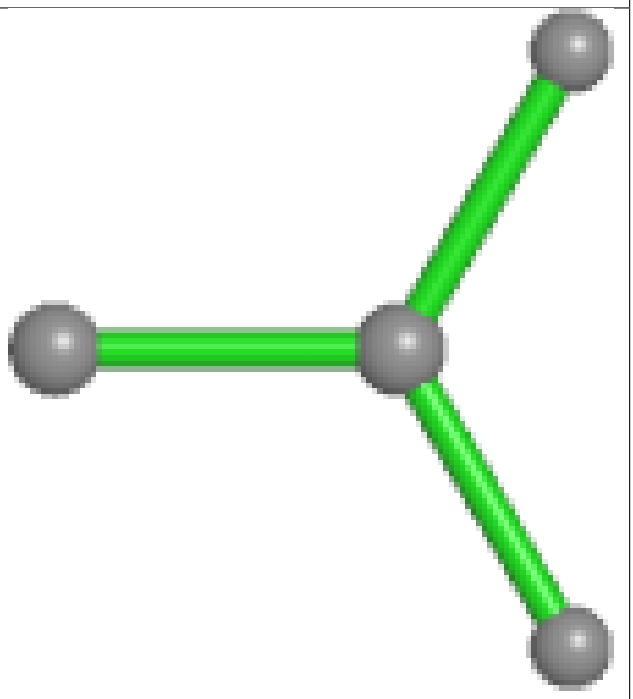

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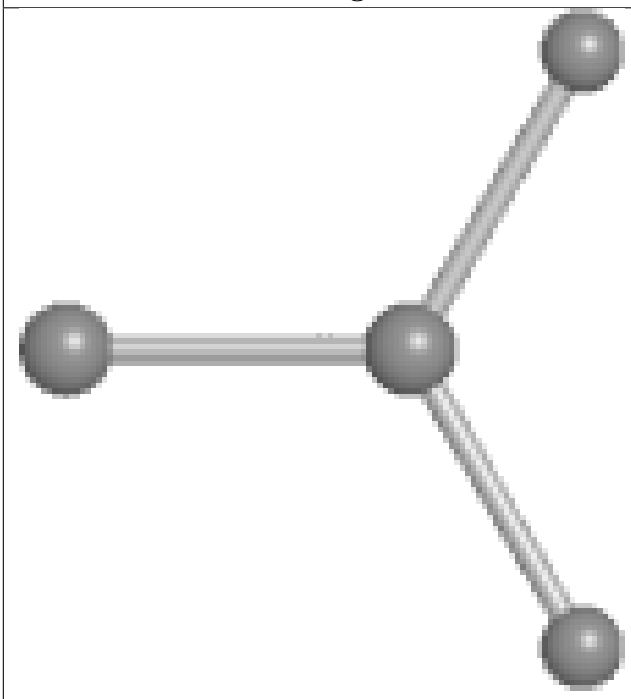

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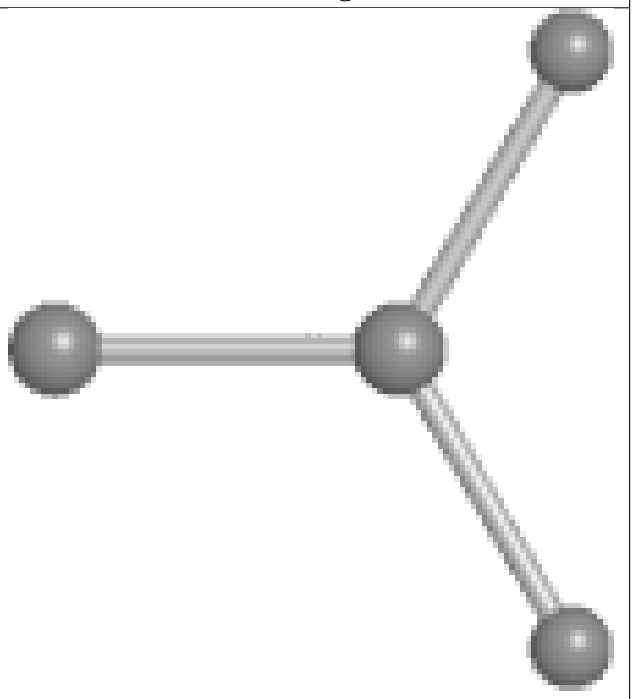
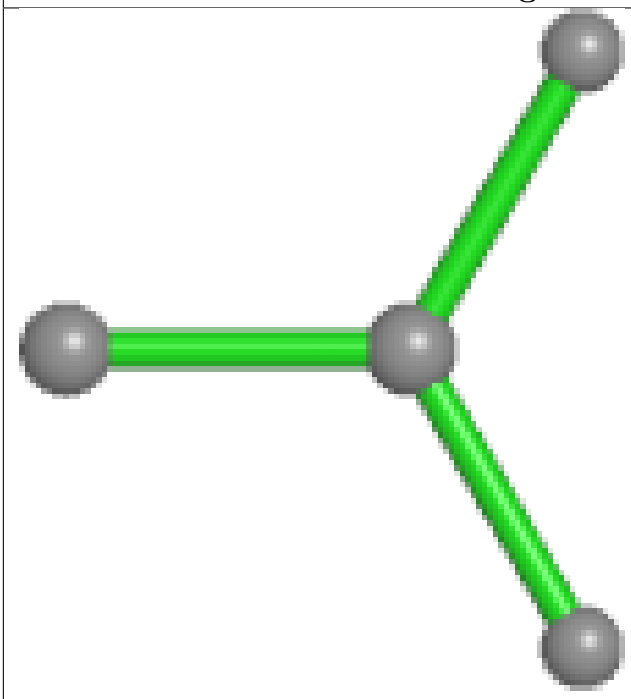


Rings

Ligand ACT M 301



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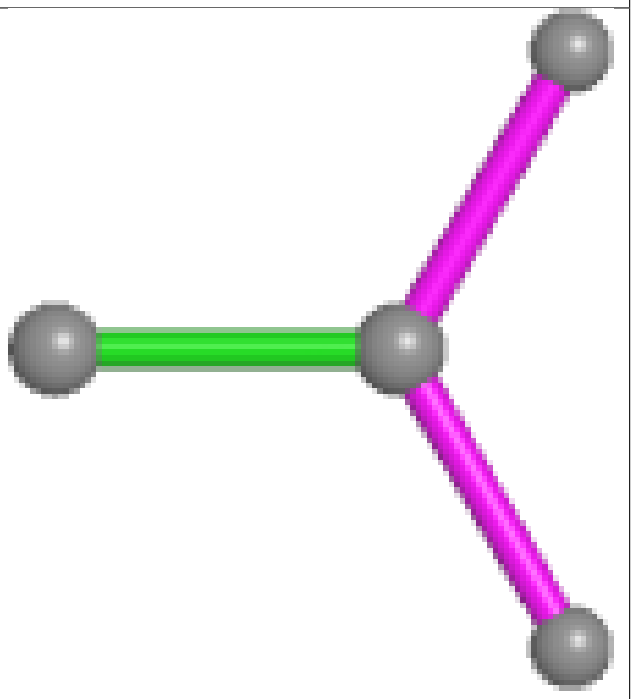

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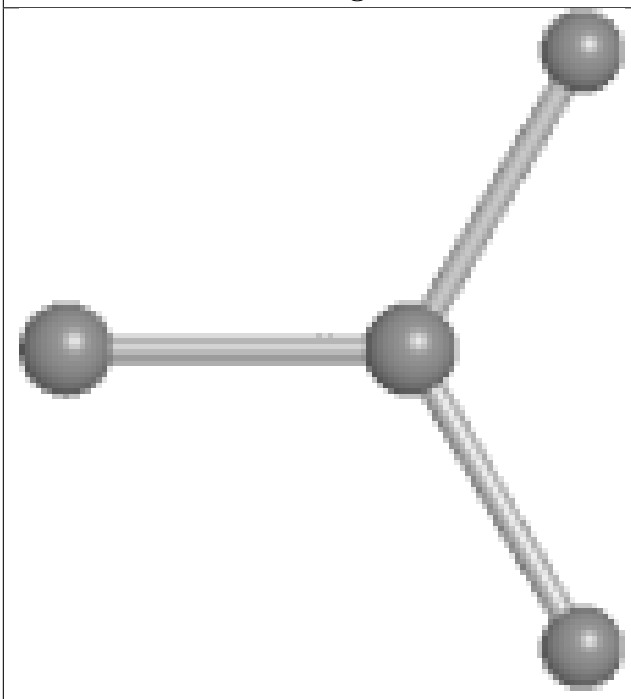

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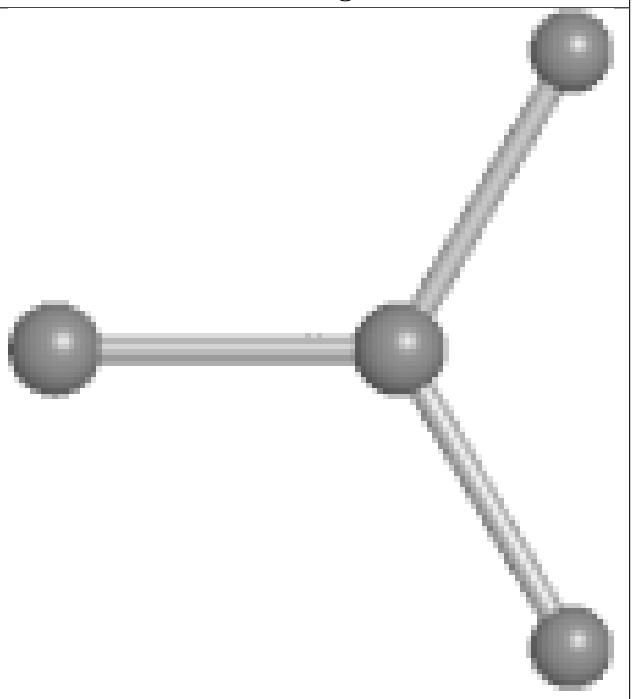
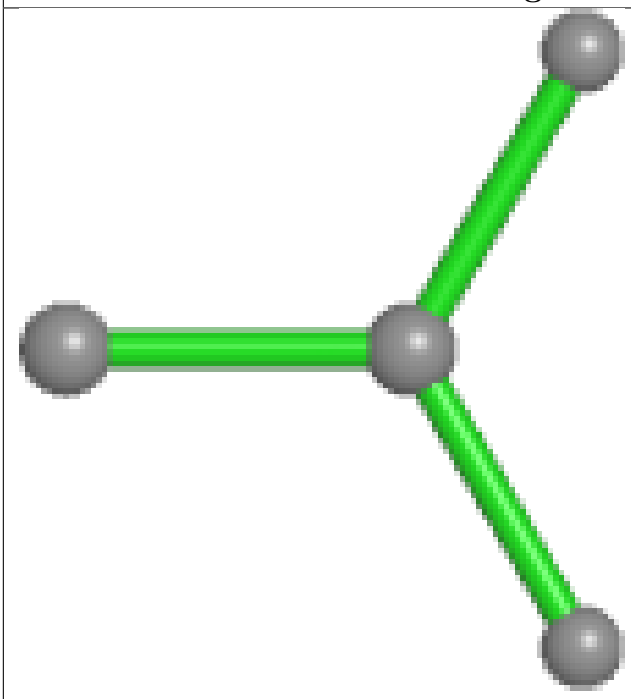


Rings

Ligand ACT E 302



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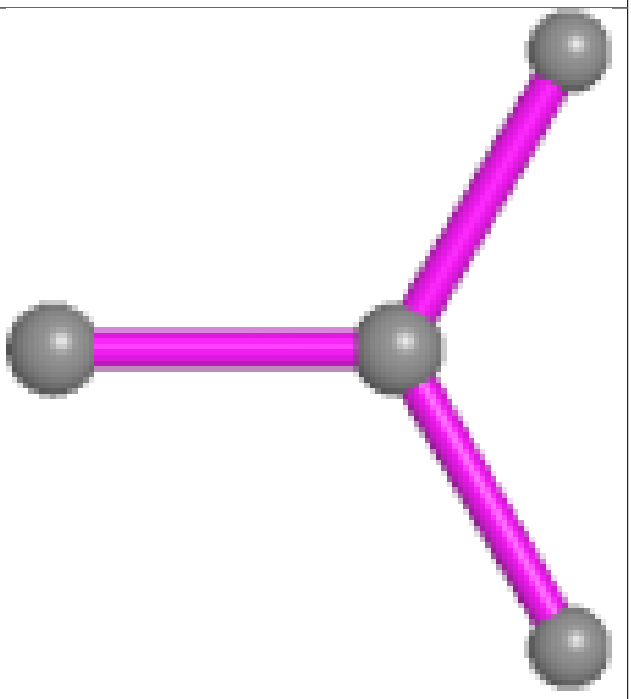

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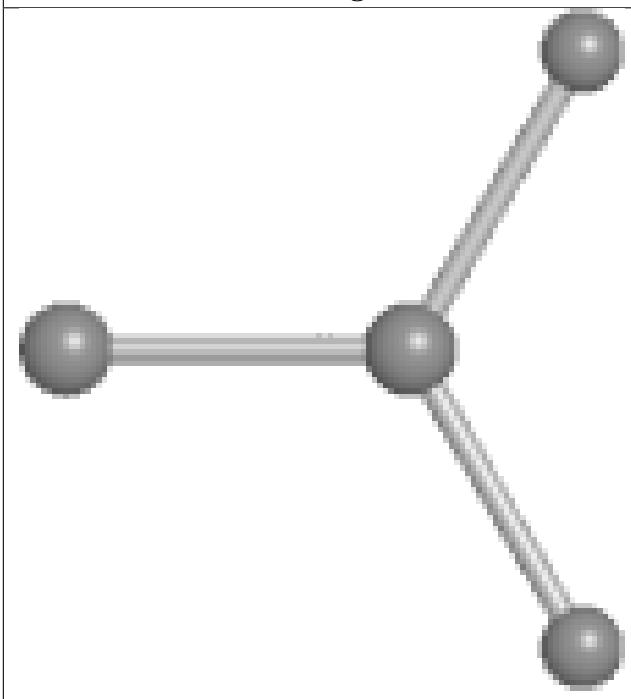

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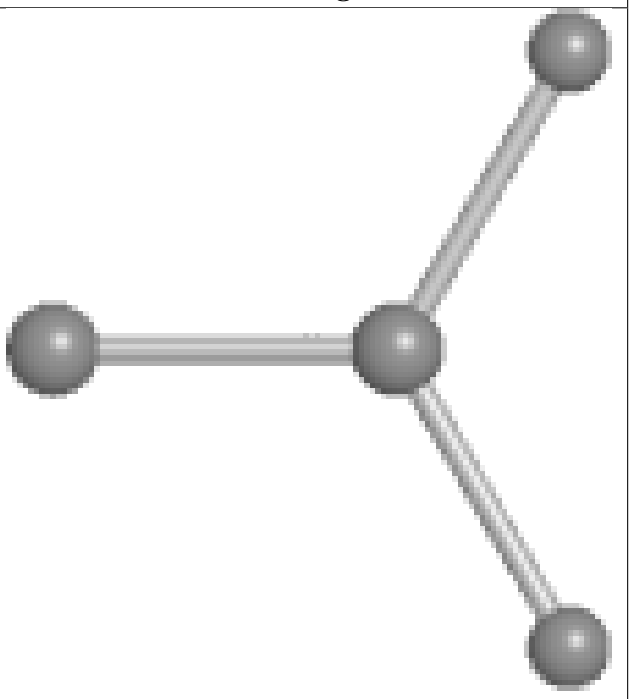
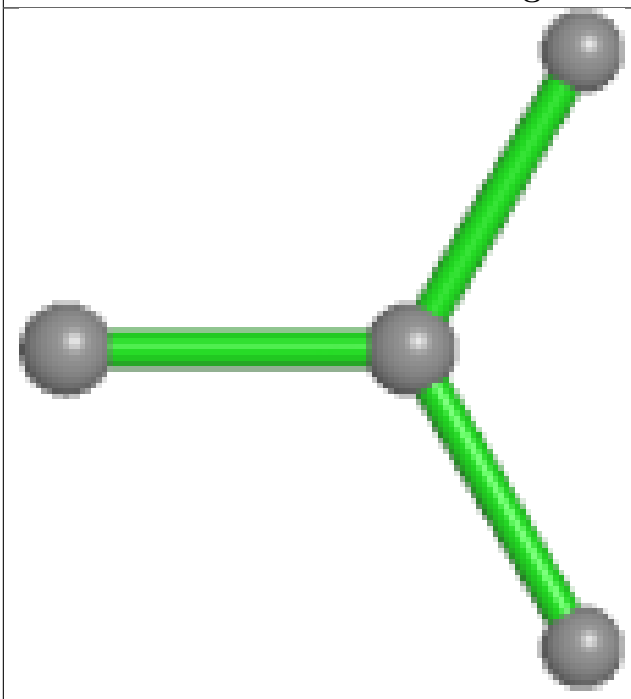
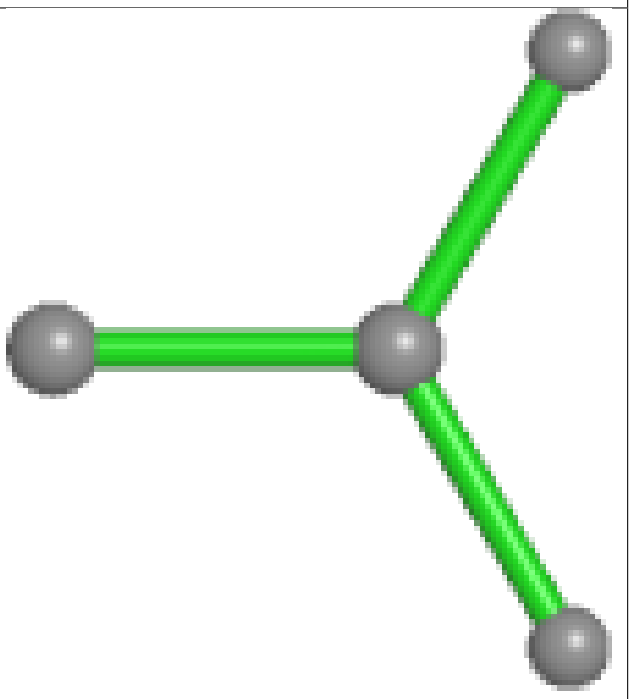


Rings

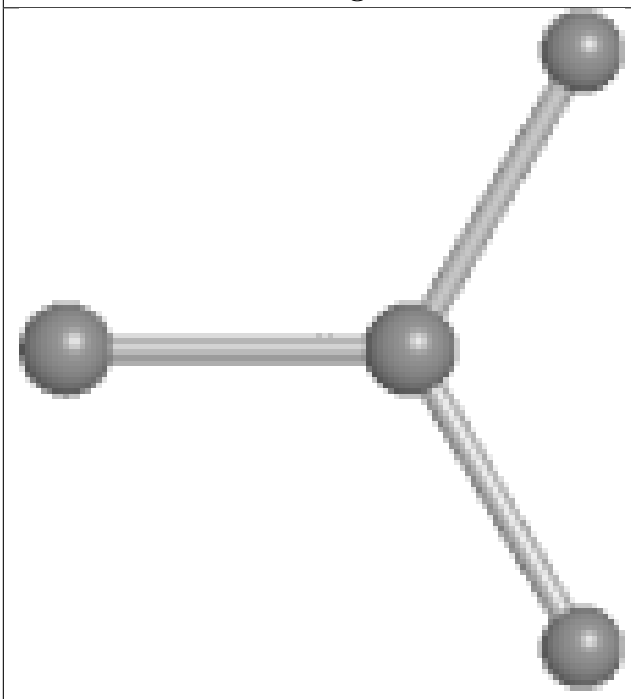
Ligand ACT B 301



Bond lengths



Bond angles



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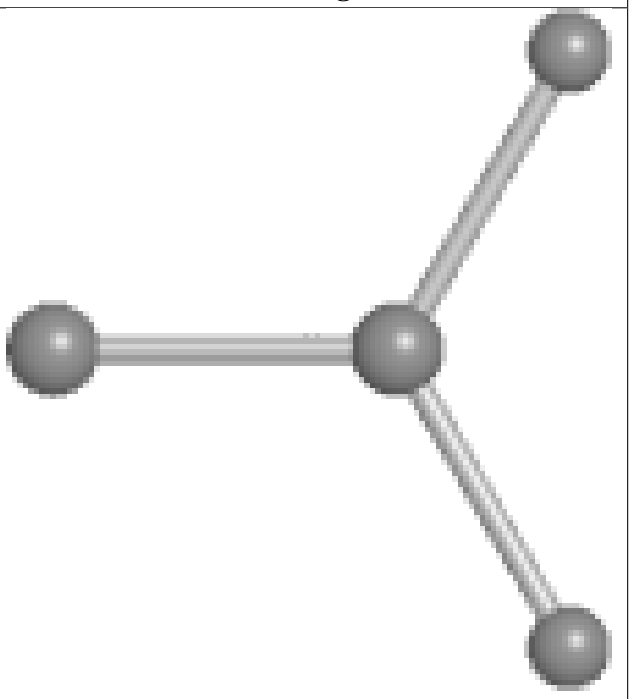
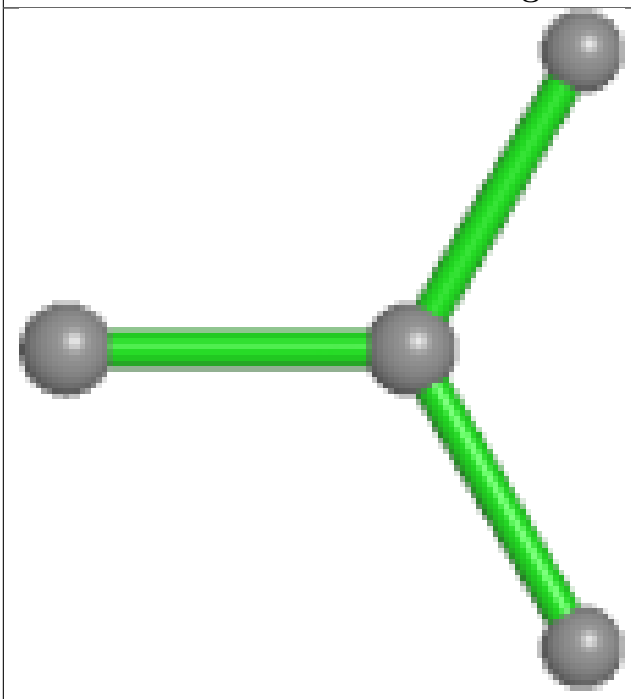


Rings

Ligand ACT N 301



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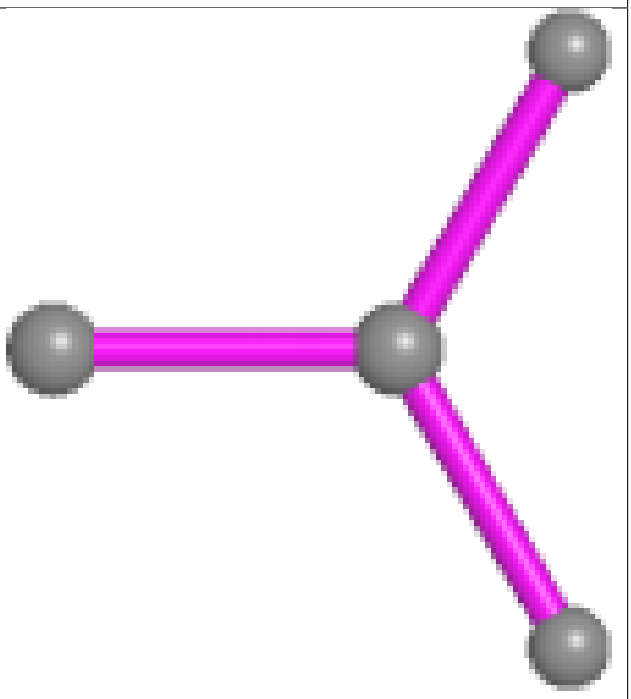
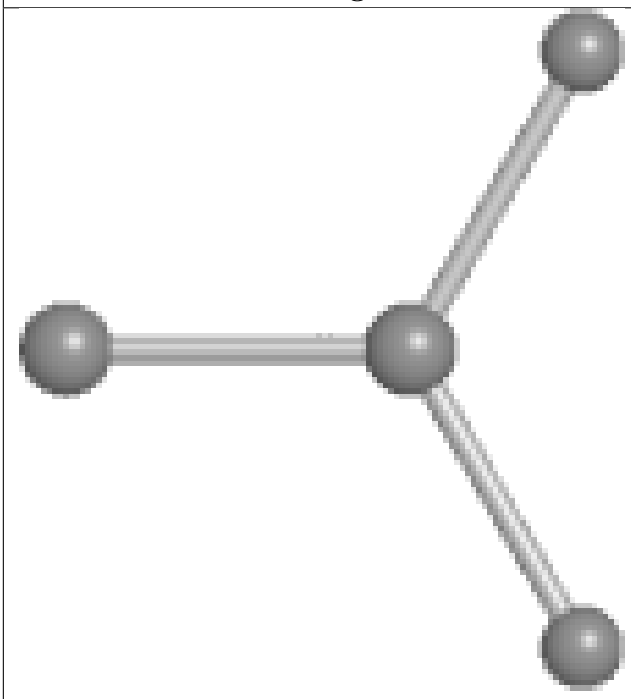


Bond angles



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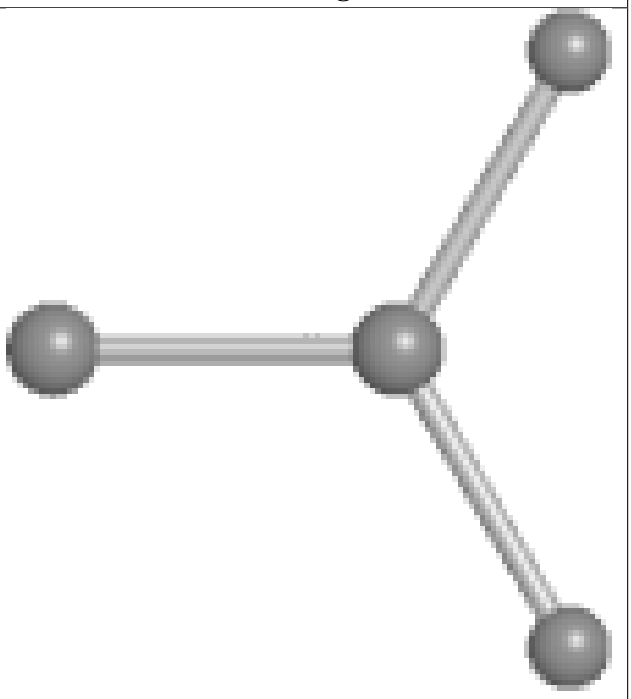
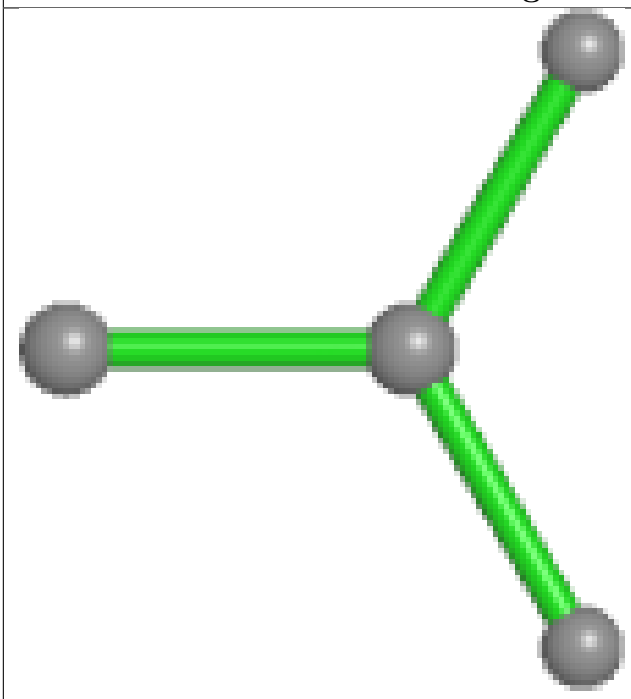
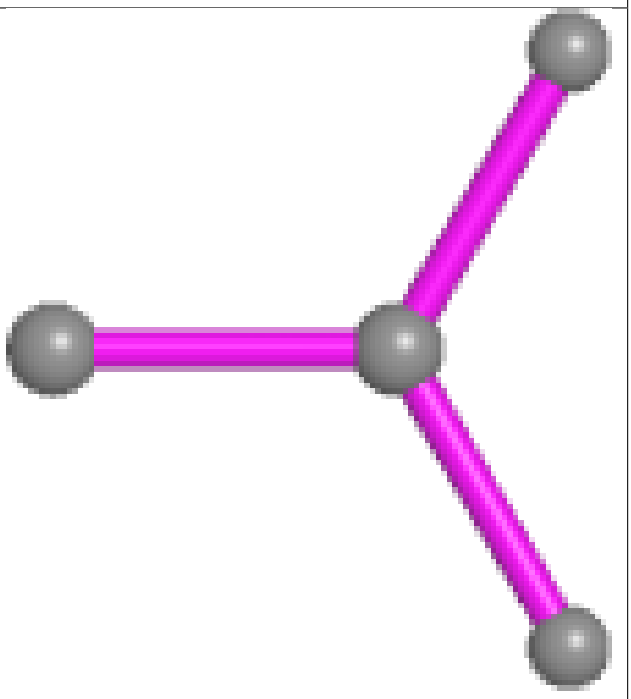


Rings

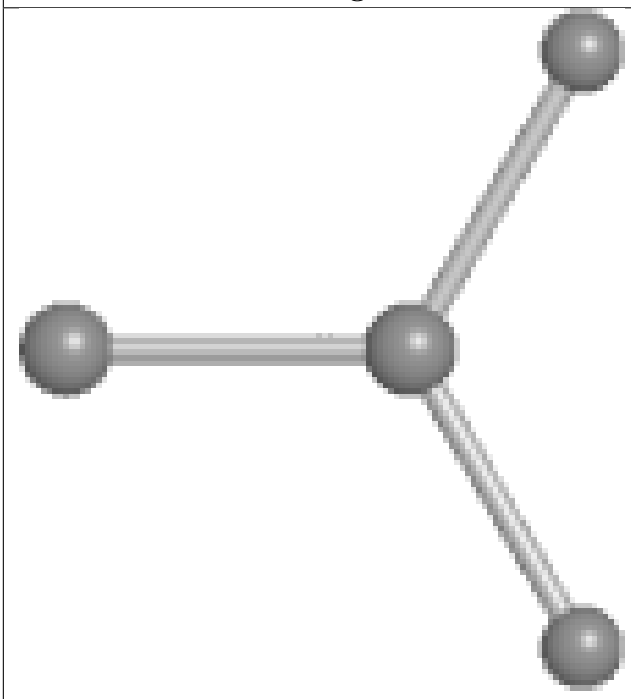
Ligand ACT O 301



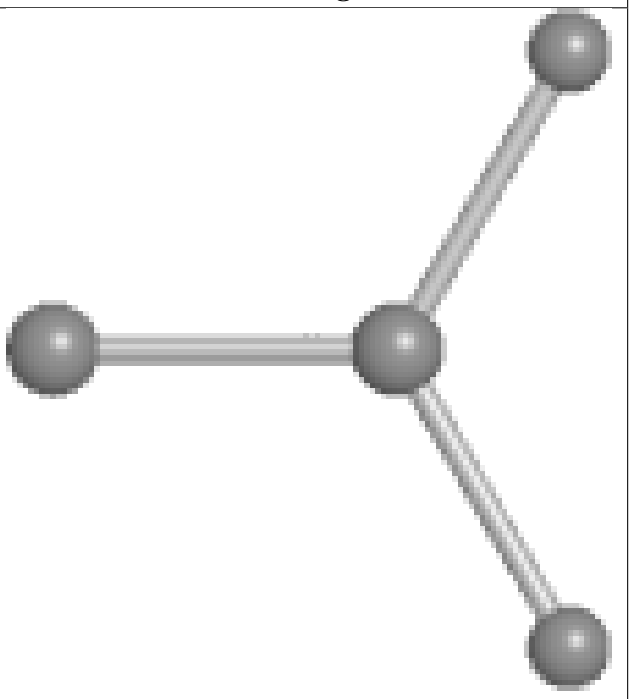
Bond lengths



Bond angles

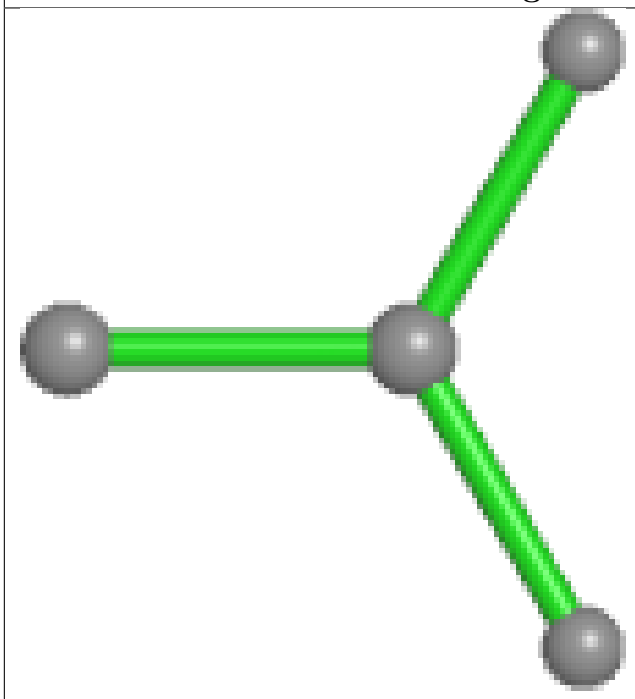


Torsions

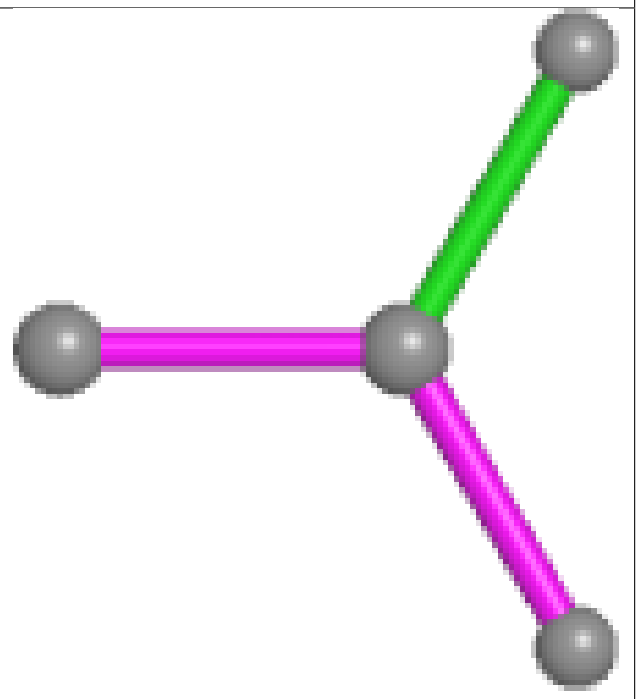


Rings

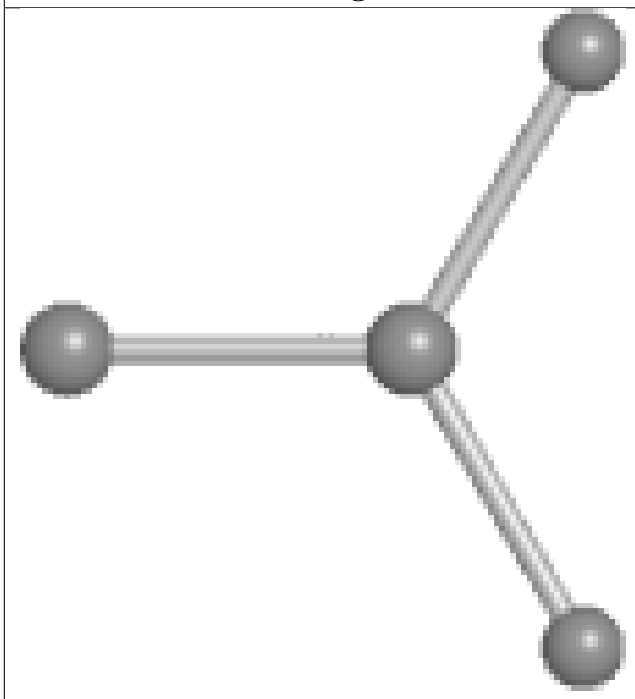
Ligand ACT G 301



Bond lengths



Bond angles



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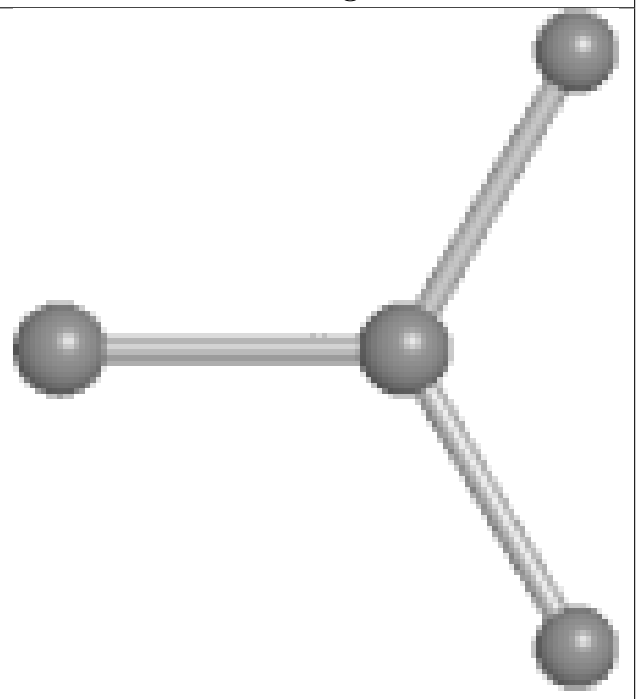
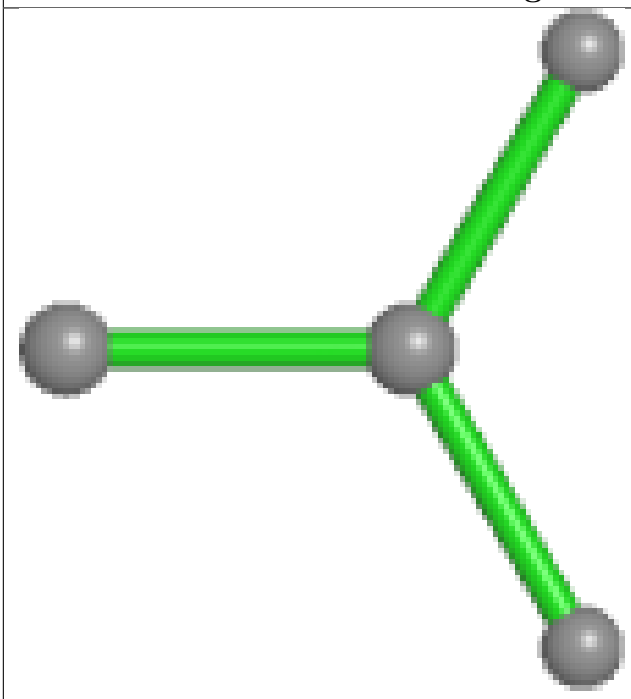
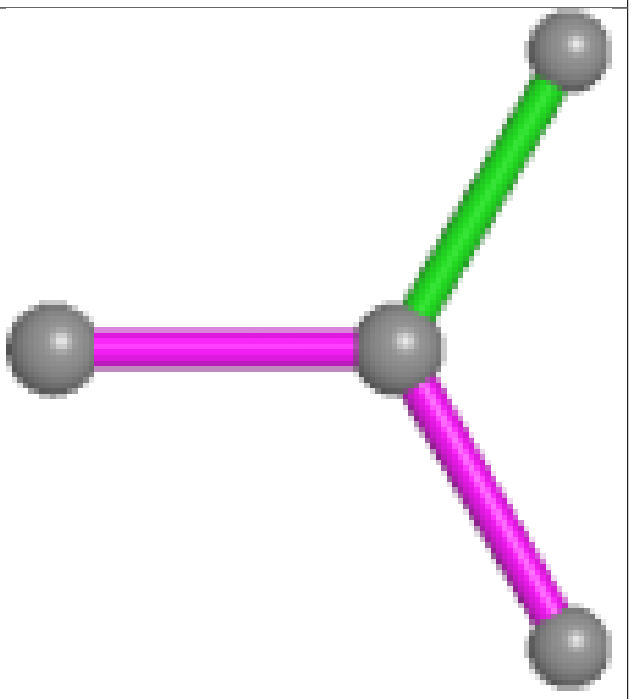


Rings

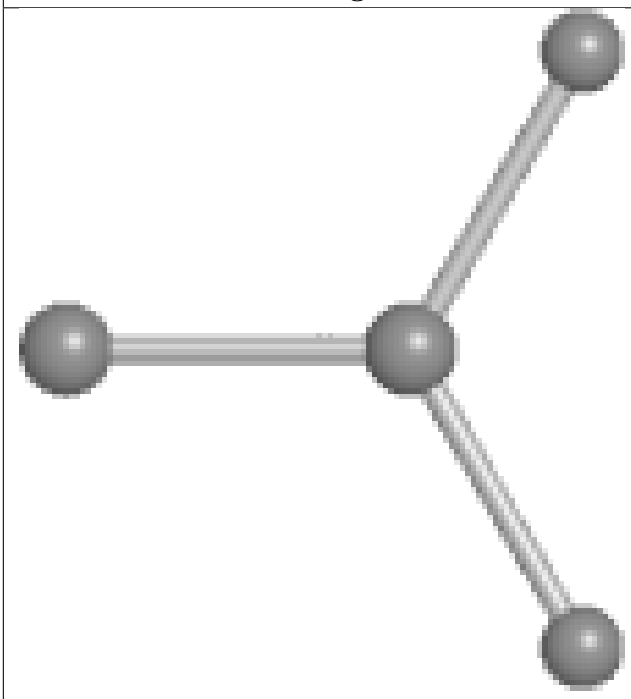
Ligand ACT E 301



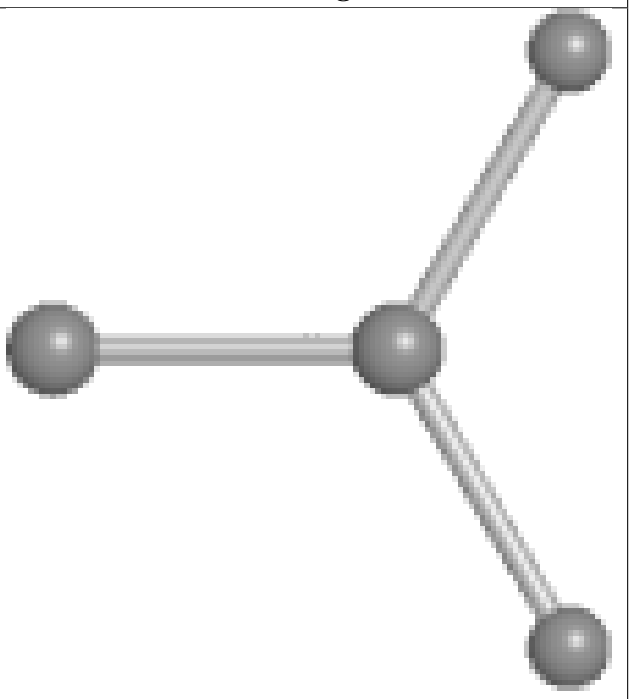
Bond lengths



Bond angles

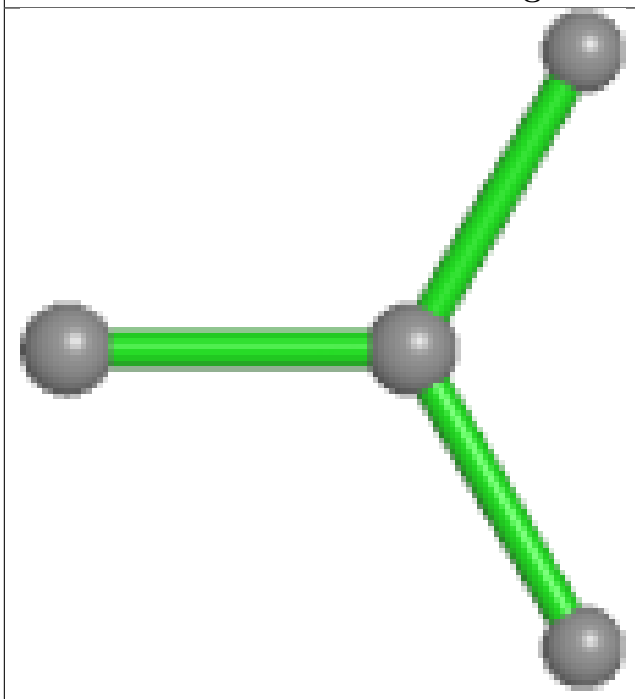


Torsions

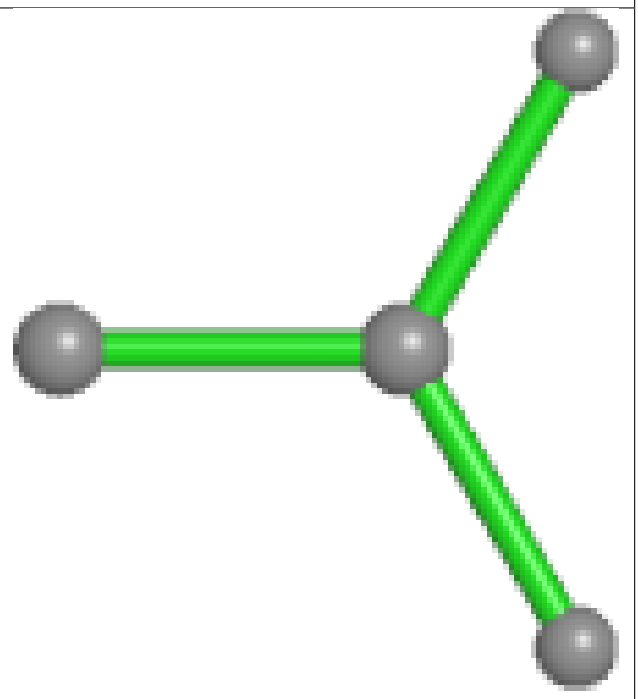


Rings

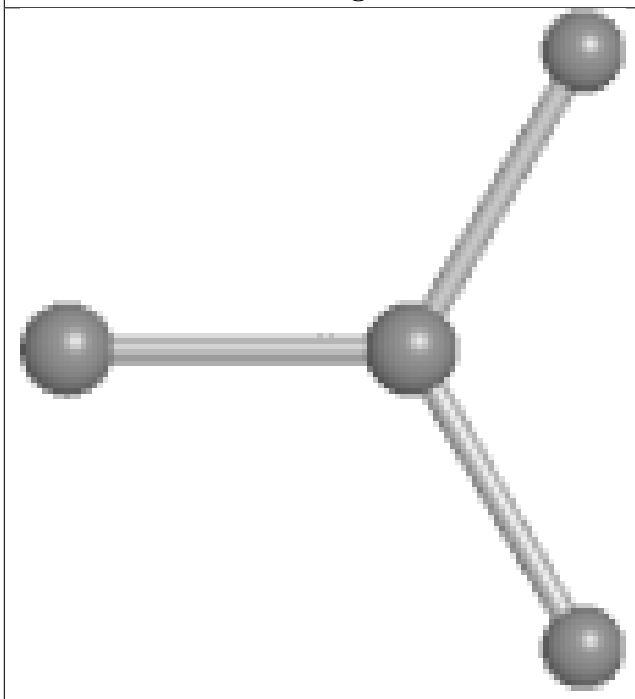
Ligand ACT O 302



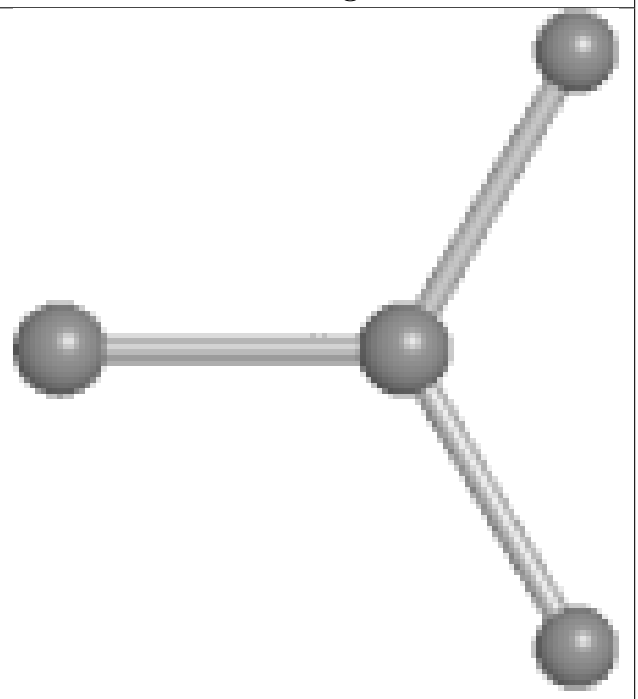
Bond lengths



Bond angles

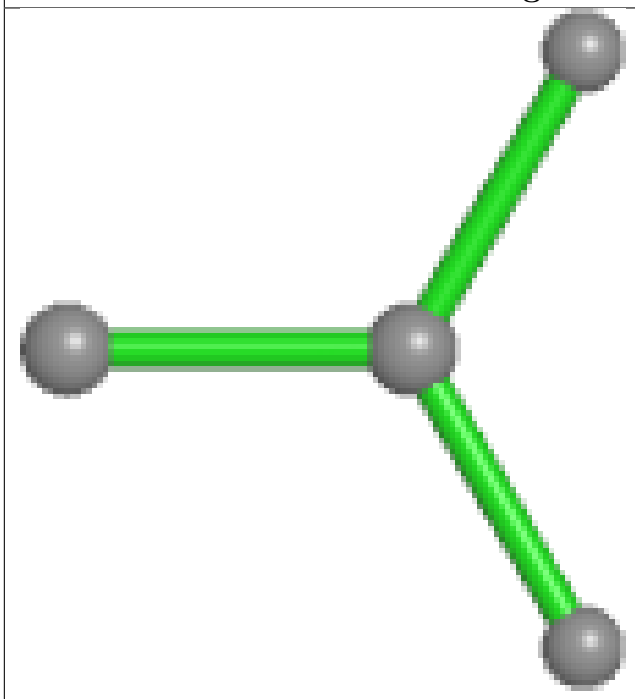


Torsions

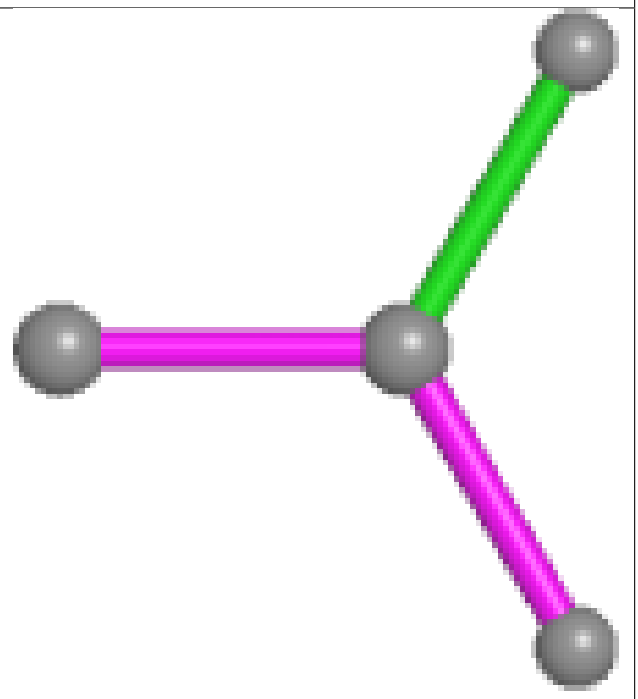


Rings

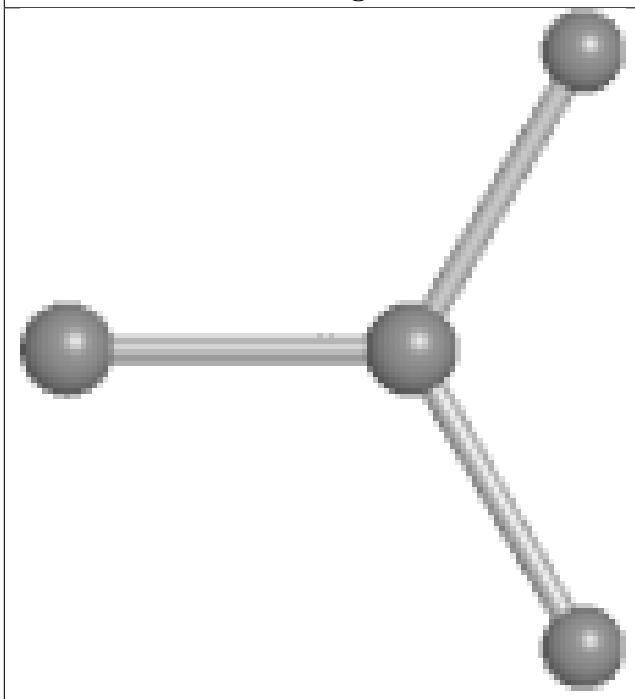
Ligand ACT H 302



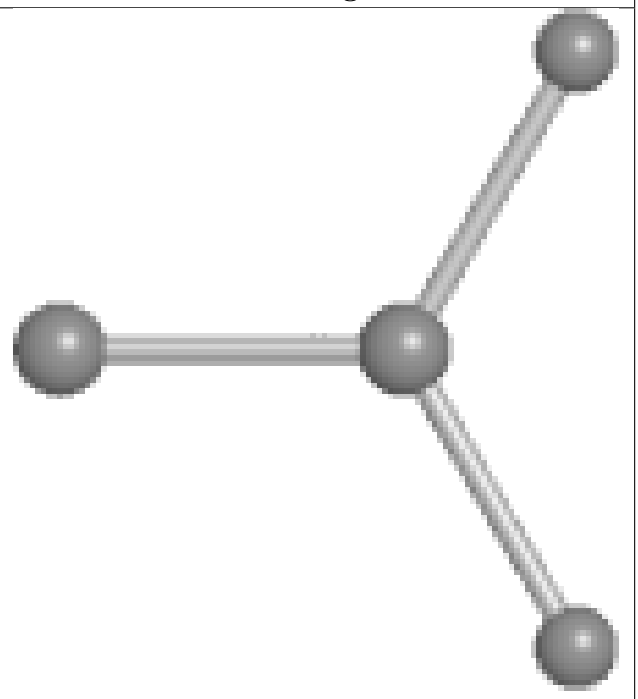
Bond lengths



Bond angles

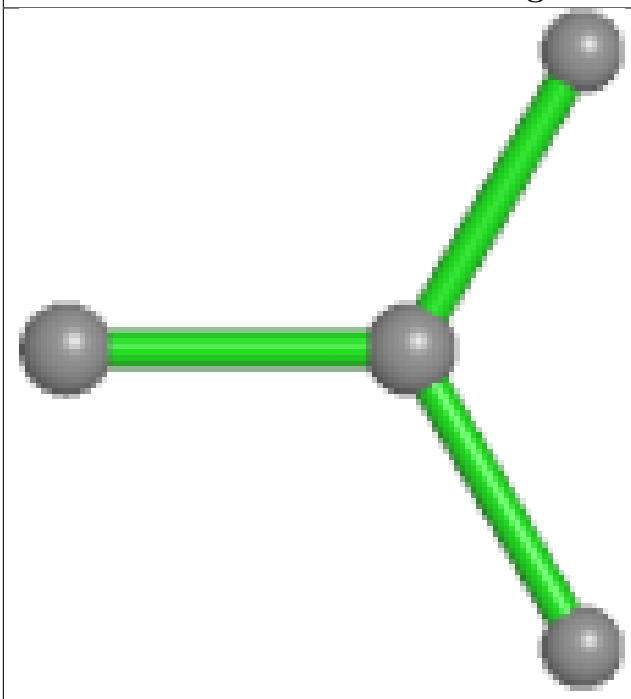


Torsions

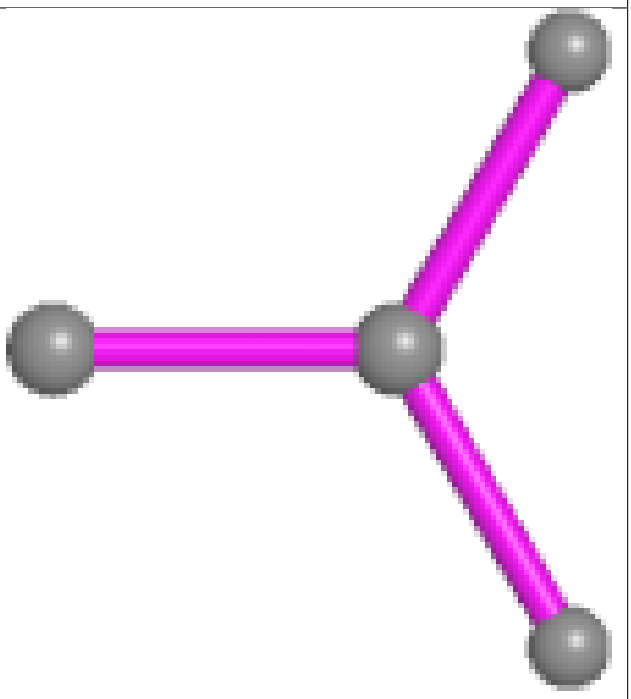


Rings

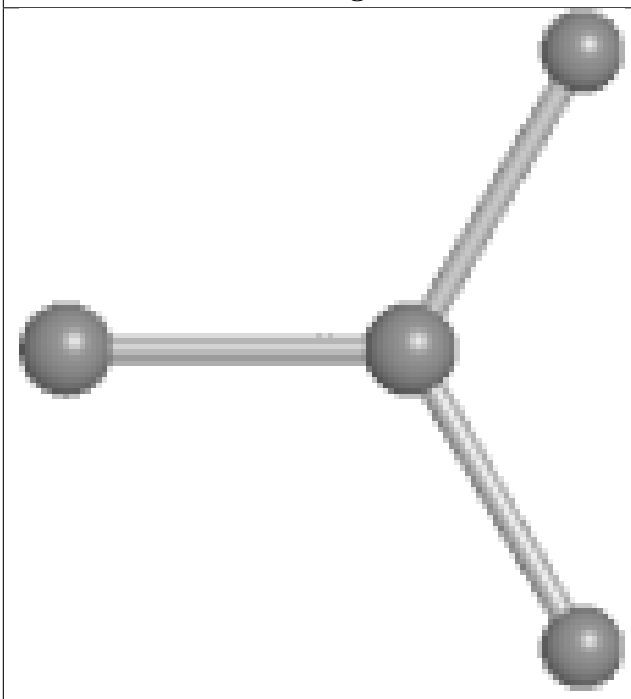
Ligand ACT J 301



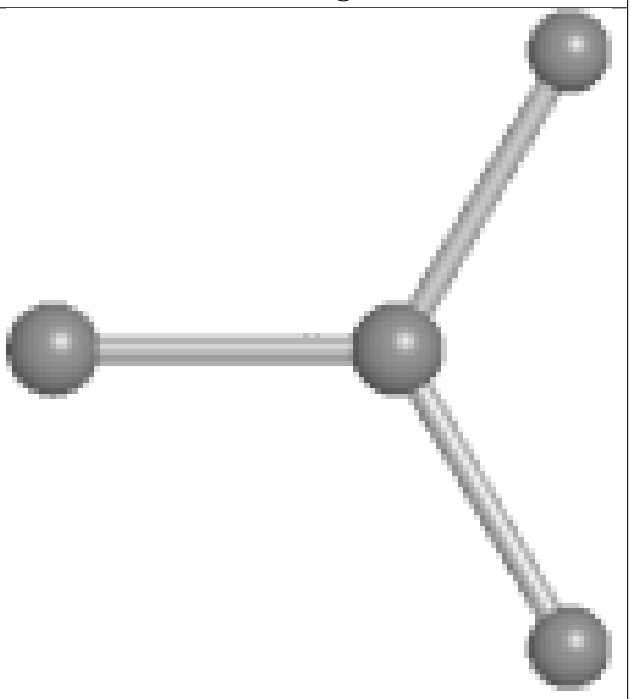
Bond lengths



Bond angles

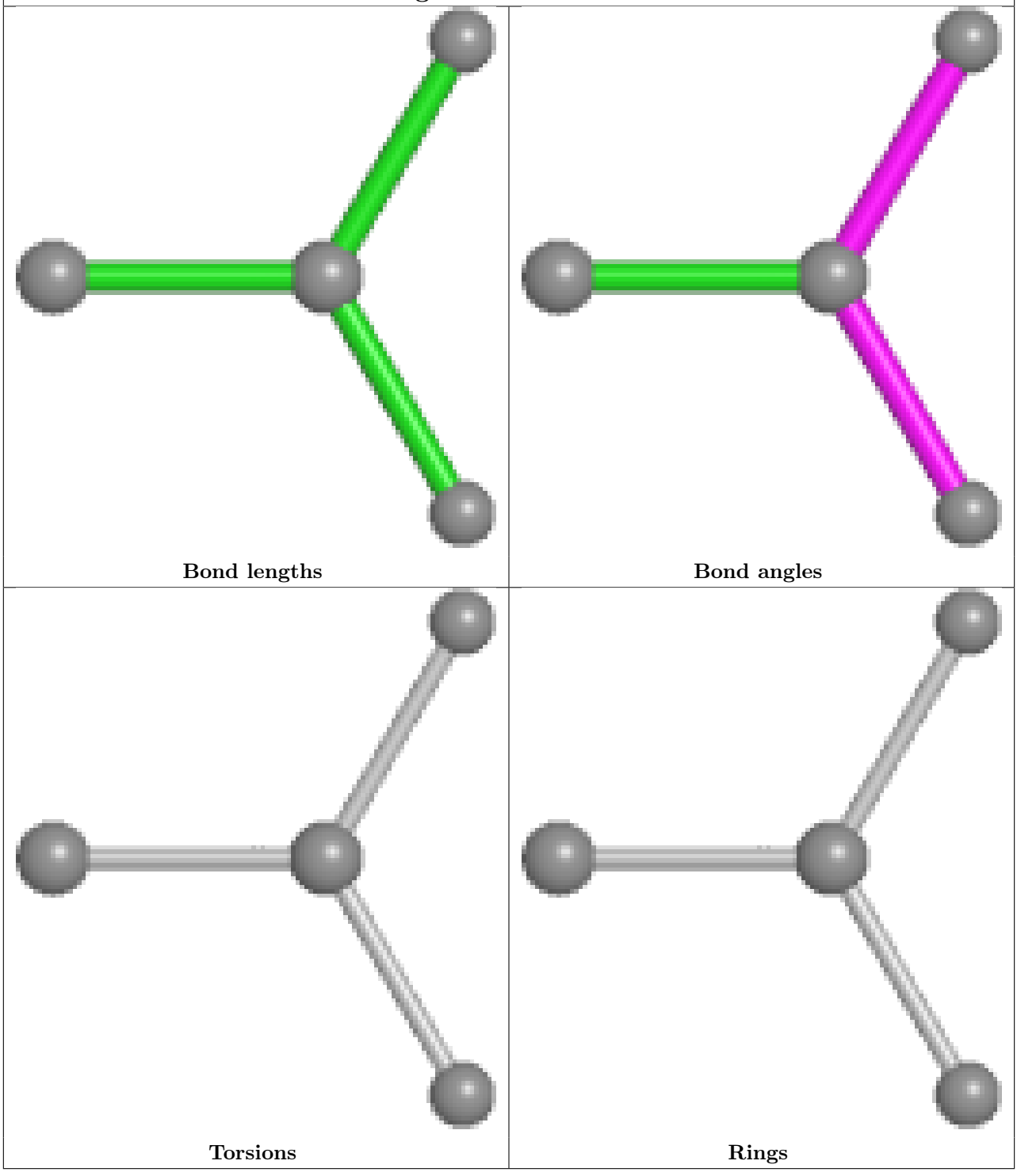


Torsions



Rings

Ligand ACT C 302



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

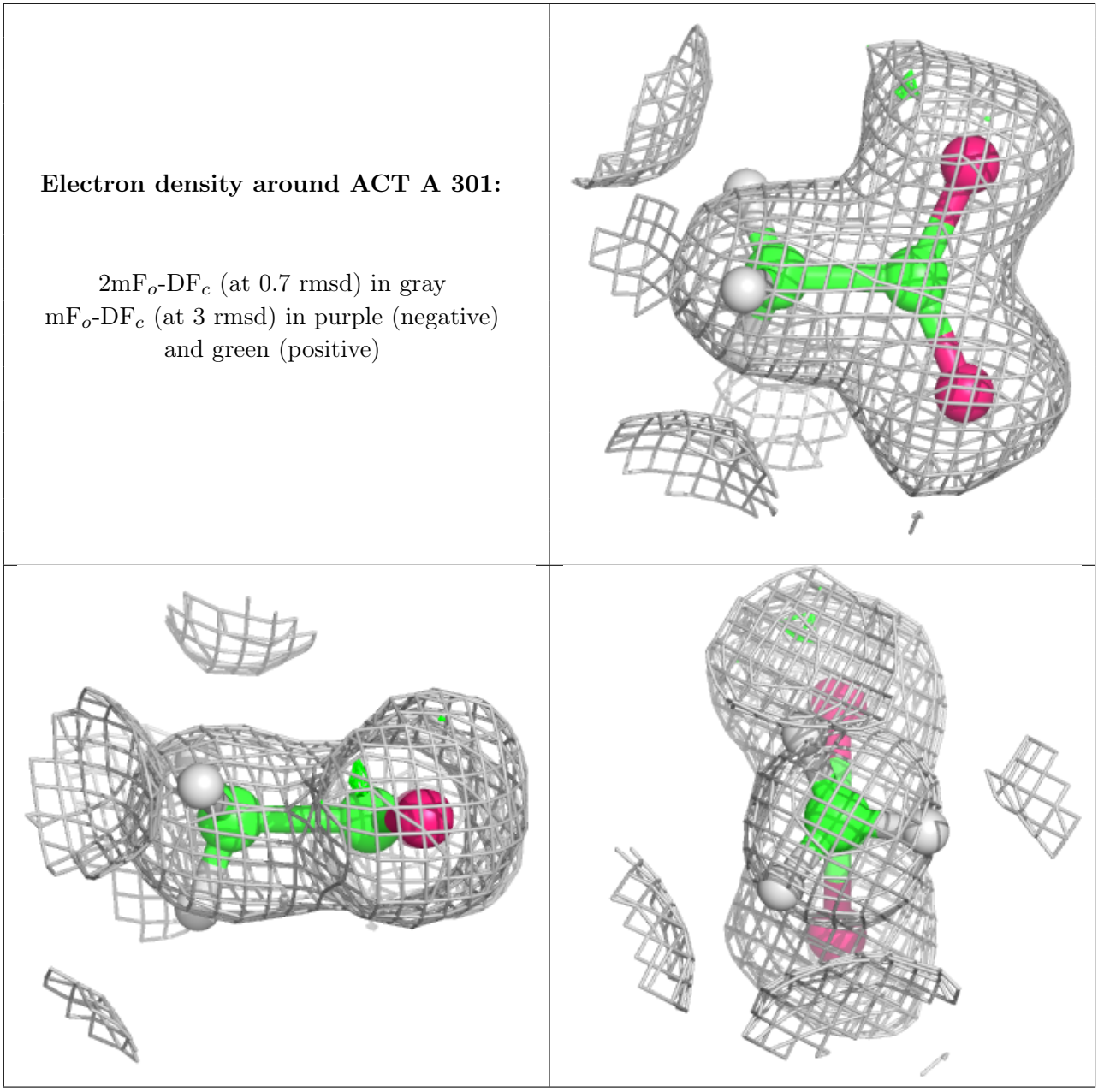
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

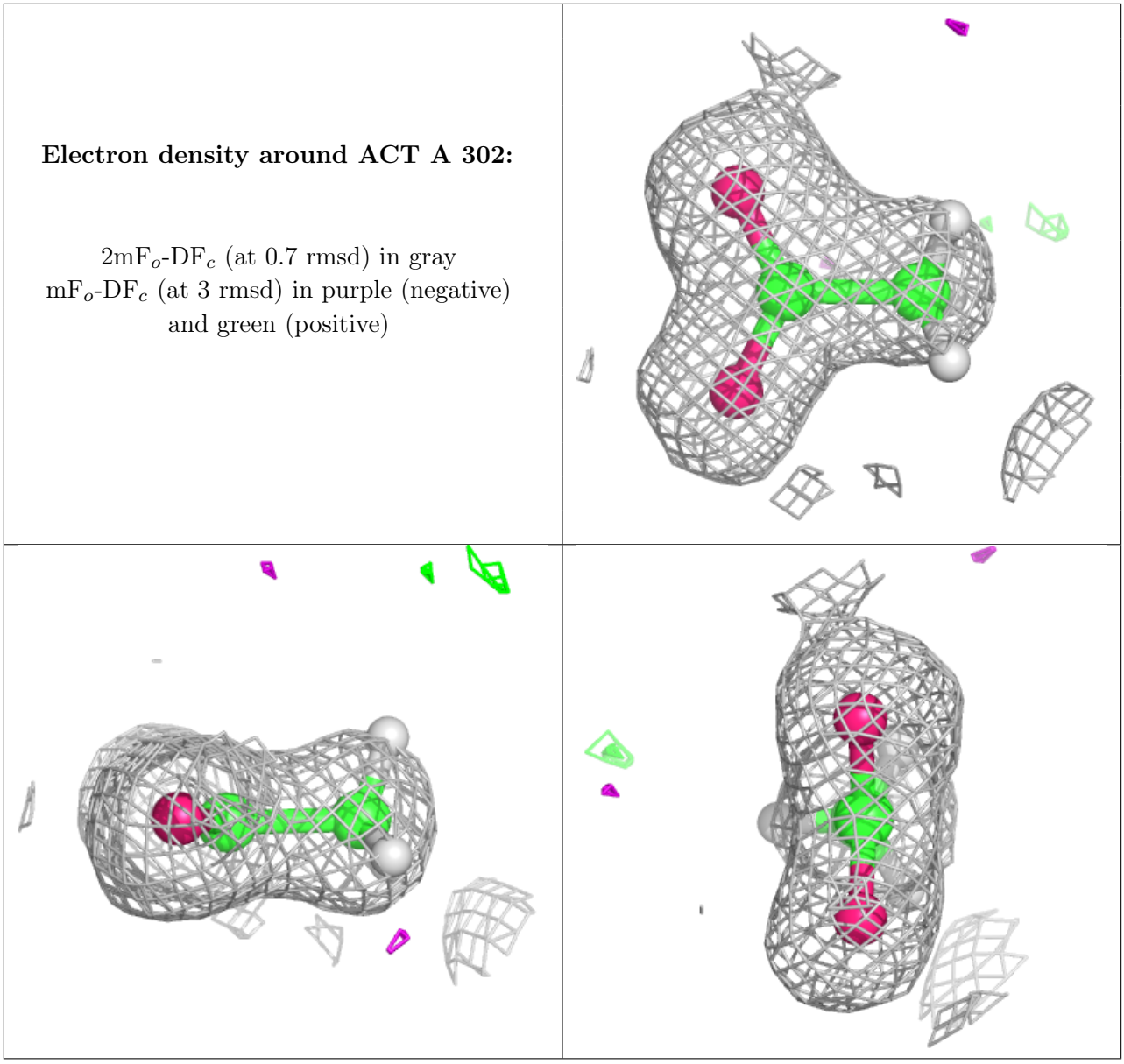
Electron density around ACT A 301:

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



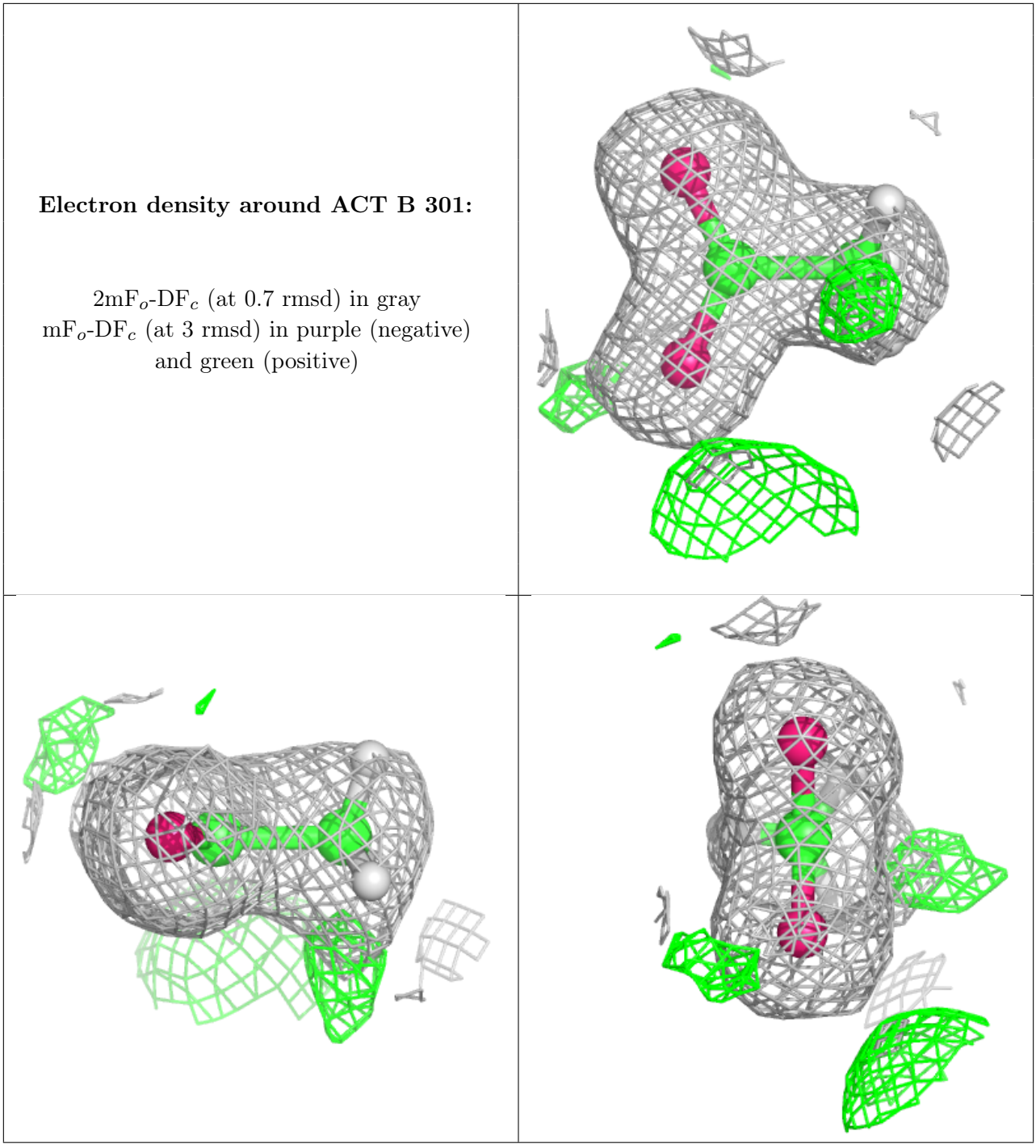
Electron density around ACT A 302:

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



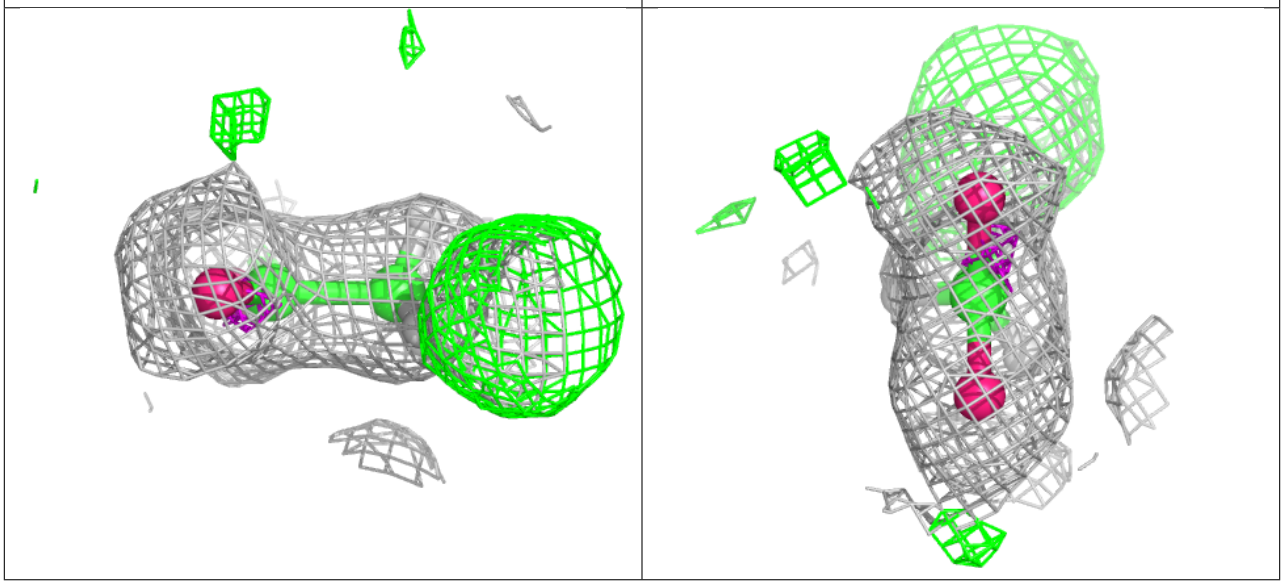
Electron density around ACT B 301:

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



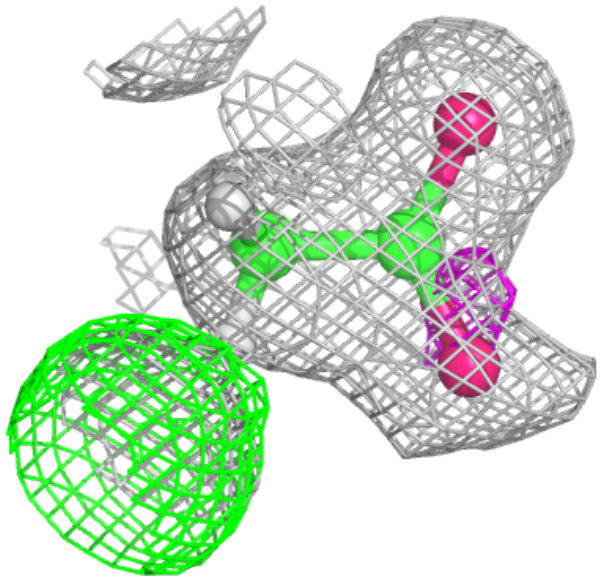
Electron density around ACT B 302:

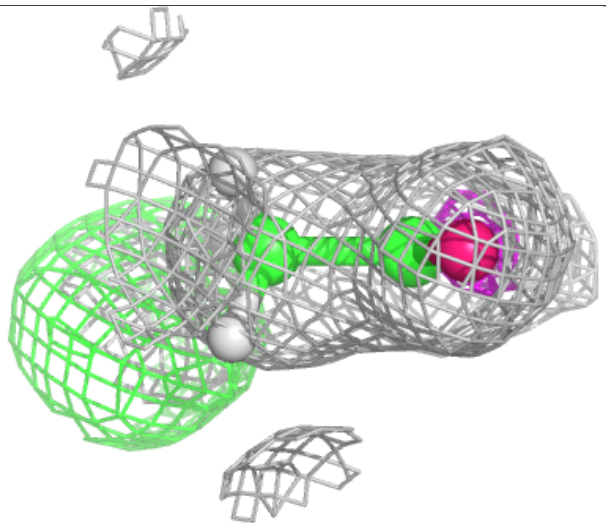
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

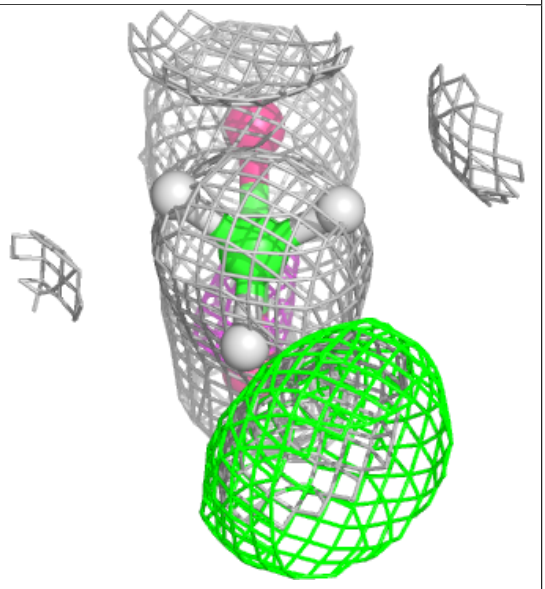


Electron density around ACT C 301:

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

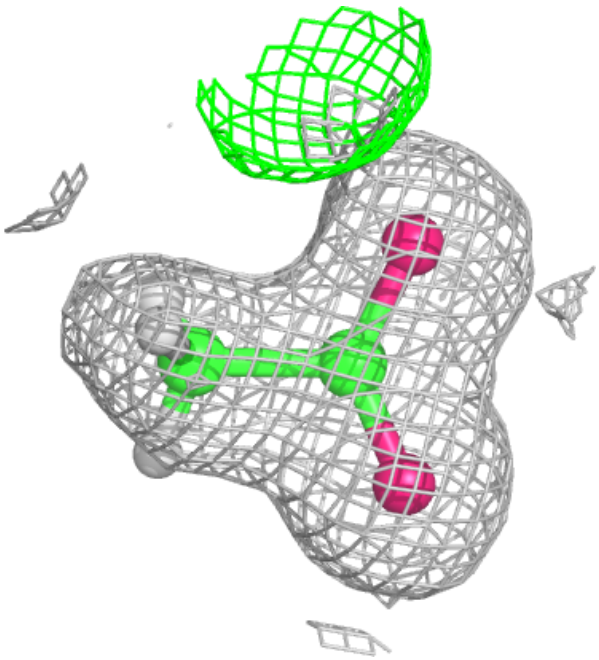


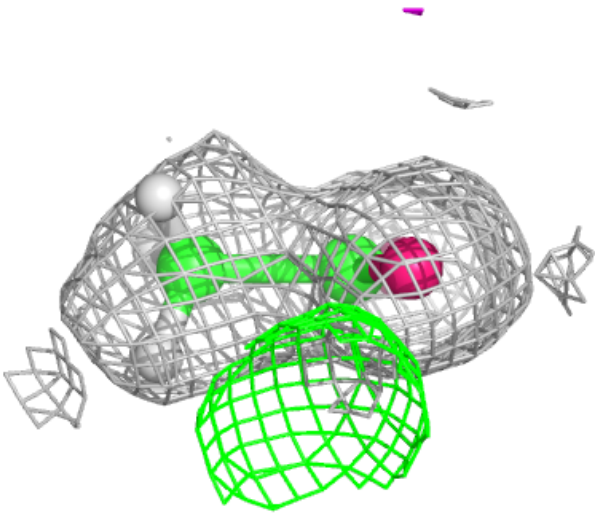


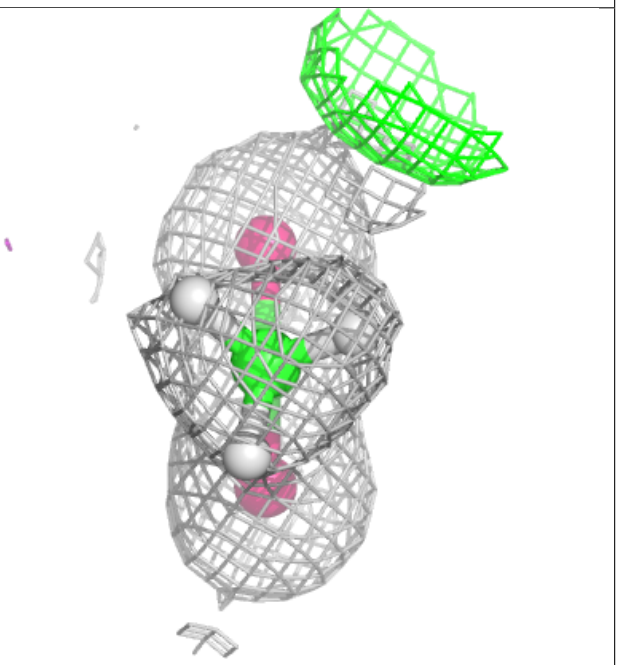


Electron density around ACT C 302:

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

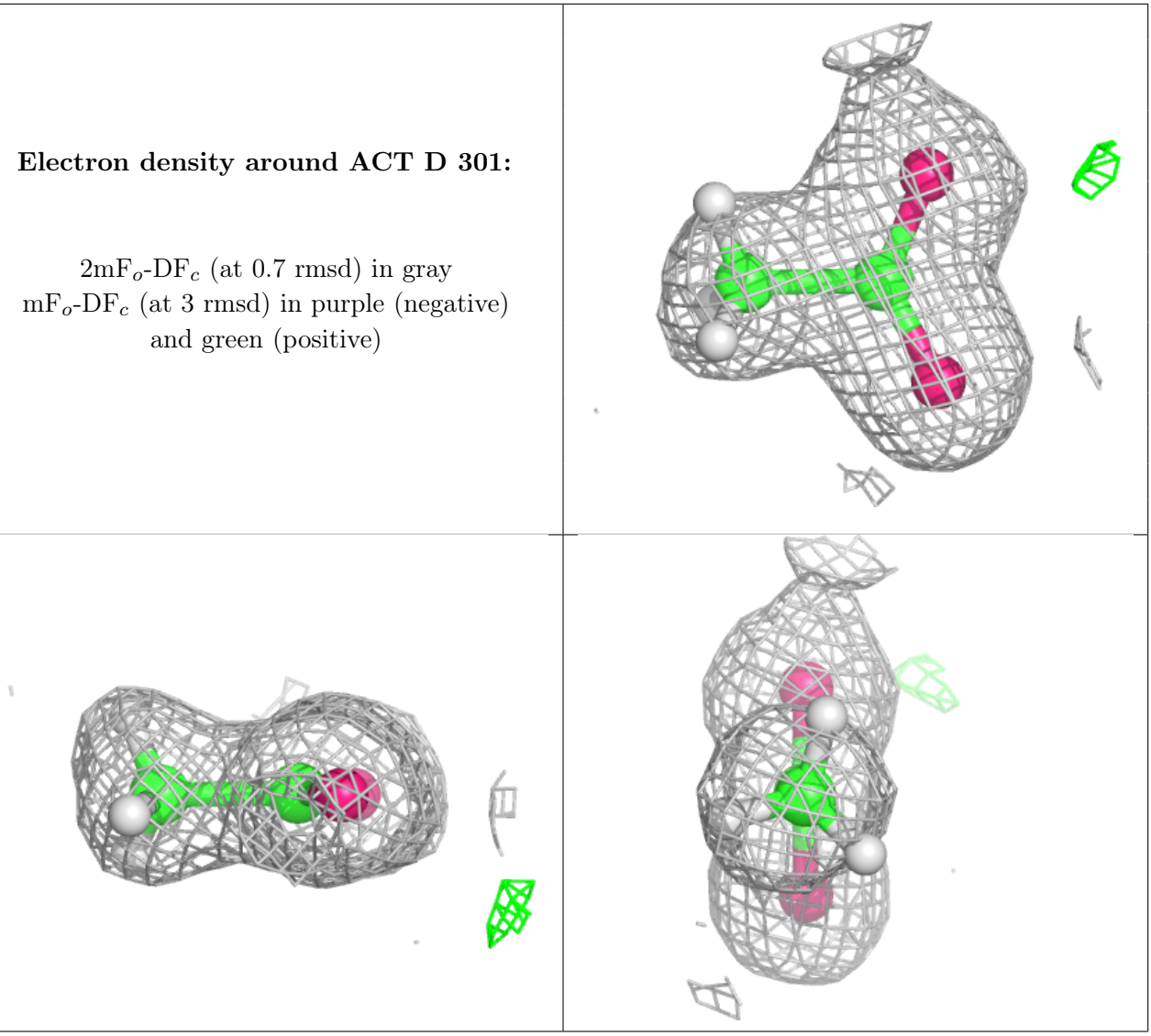






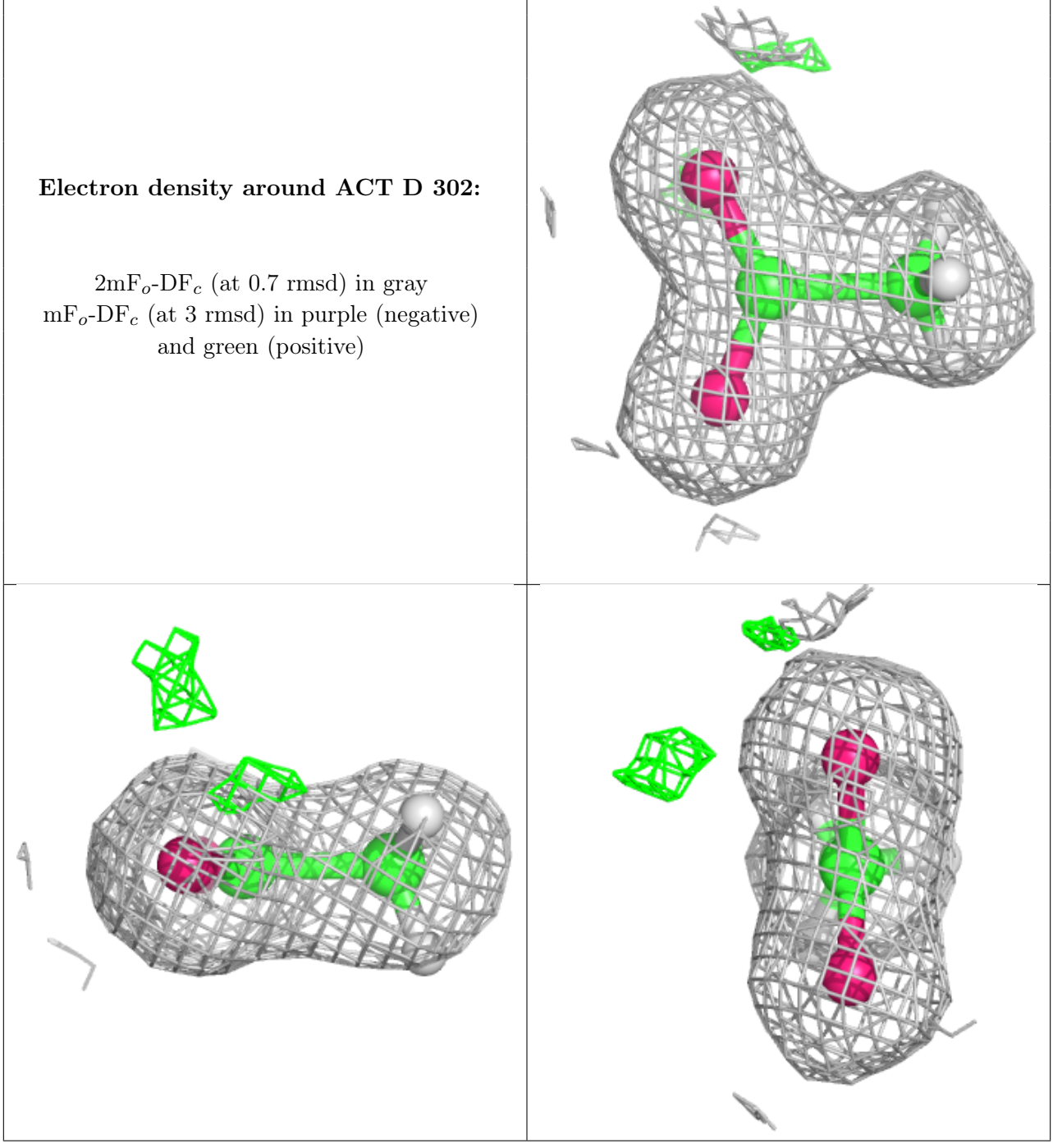
Electron density around ACT D 301:

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



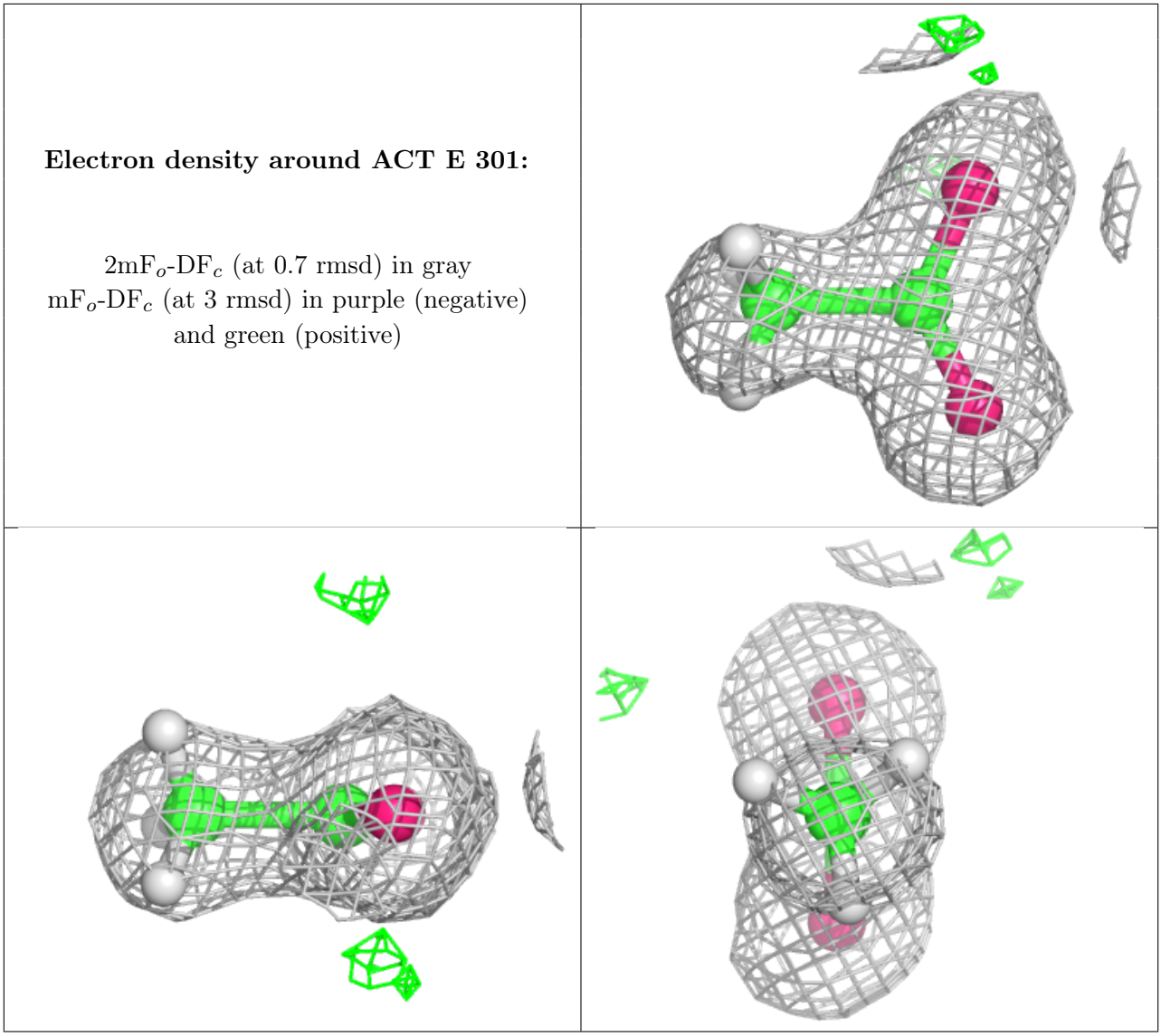
Electron density around ACT D 302:

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



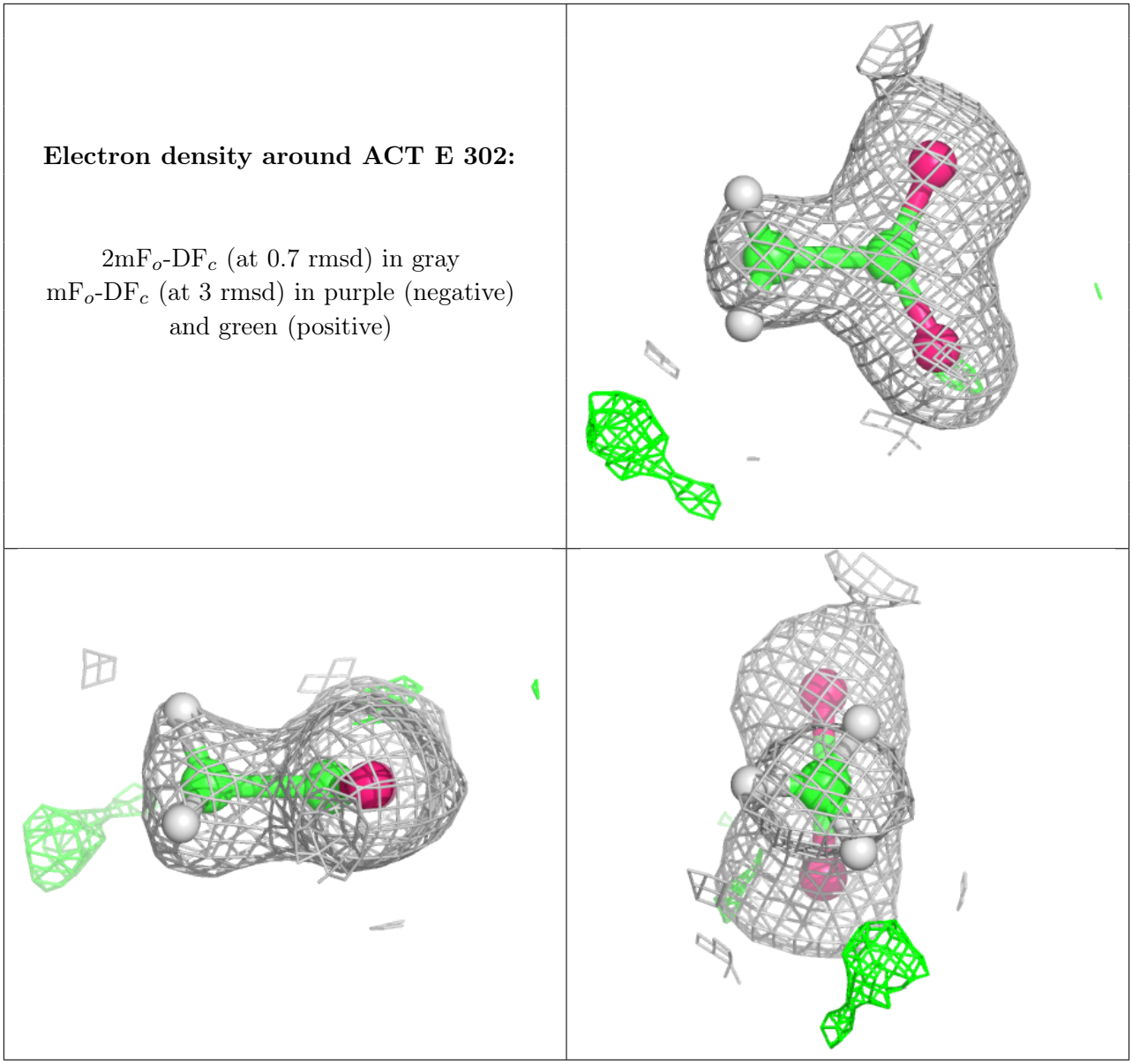
Electron density around ACT E 301:

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



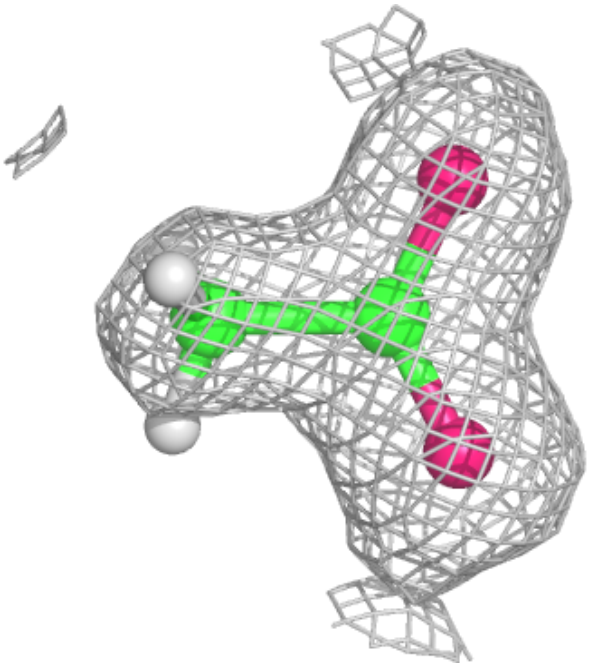
Electron density around ACT E 302:

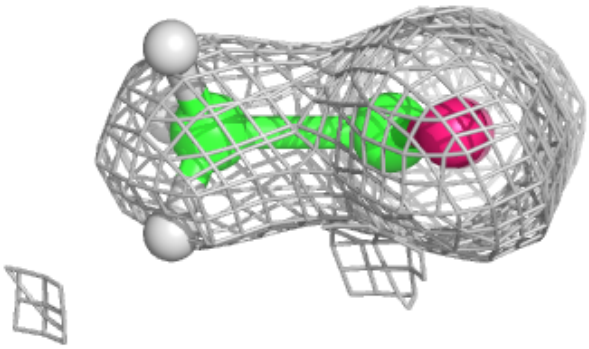
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

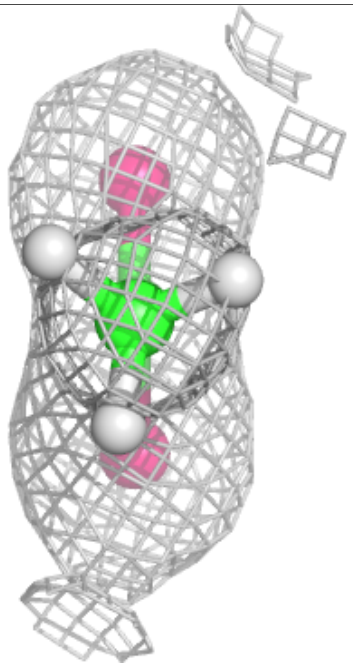


Electron density around ACT F 301:

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

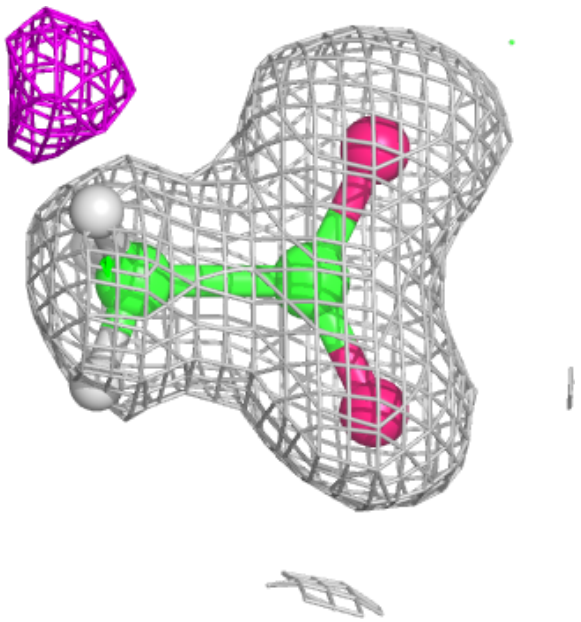


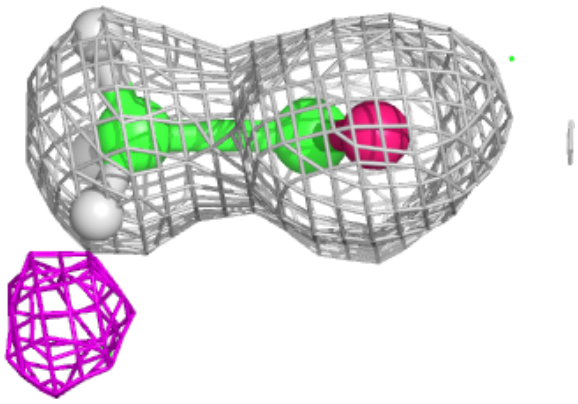


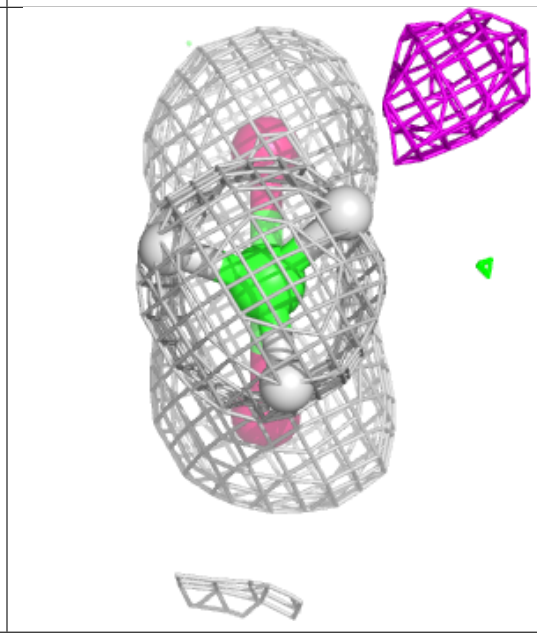


Electron density around ACT F 302:

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

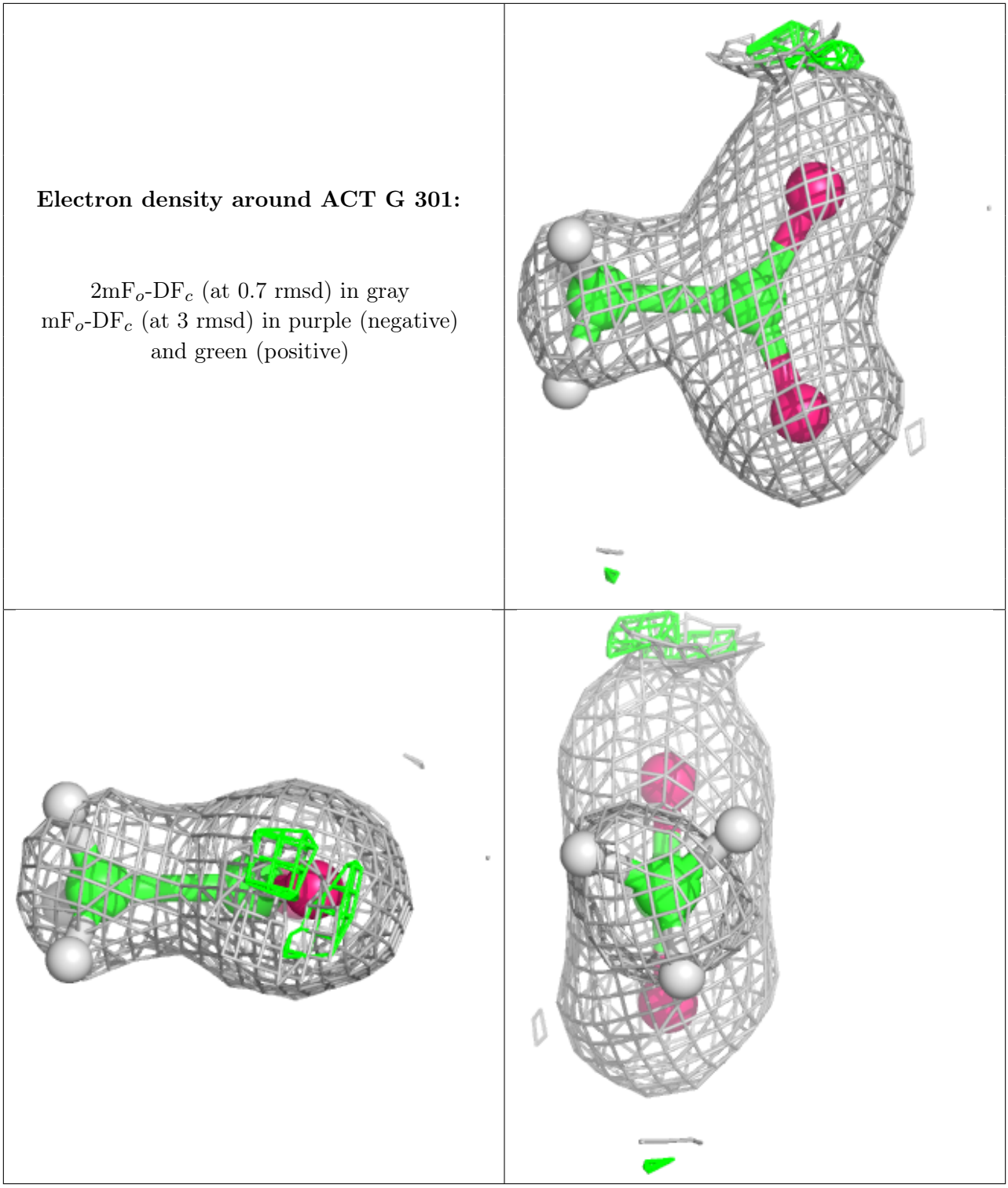






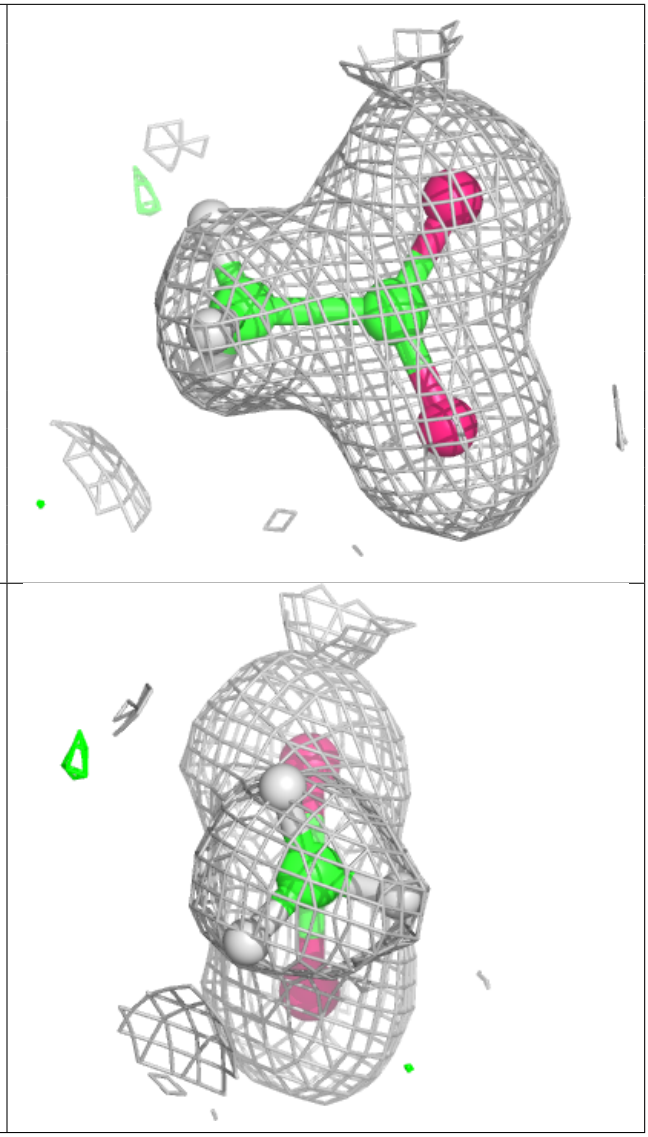
Electron density around ACT G 301:

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



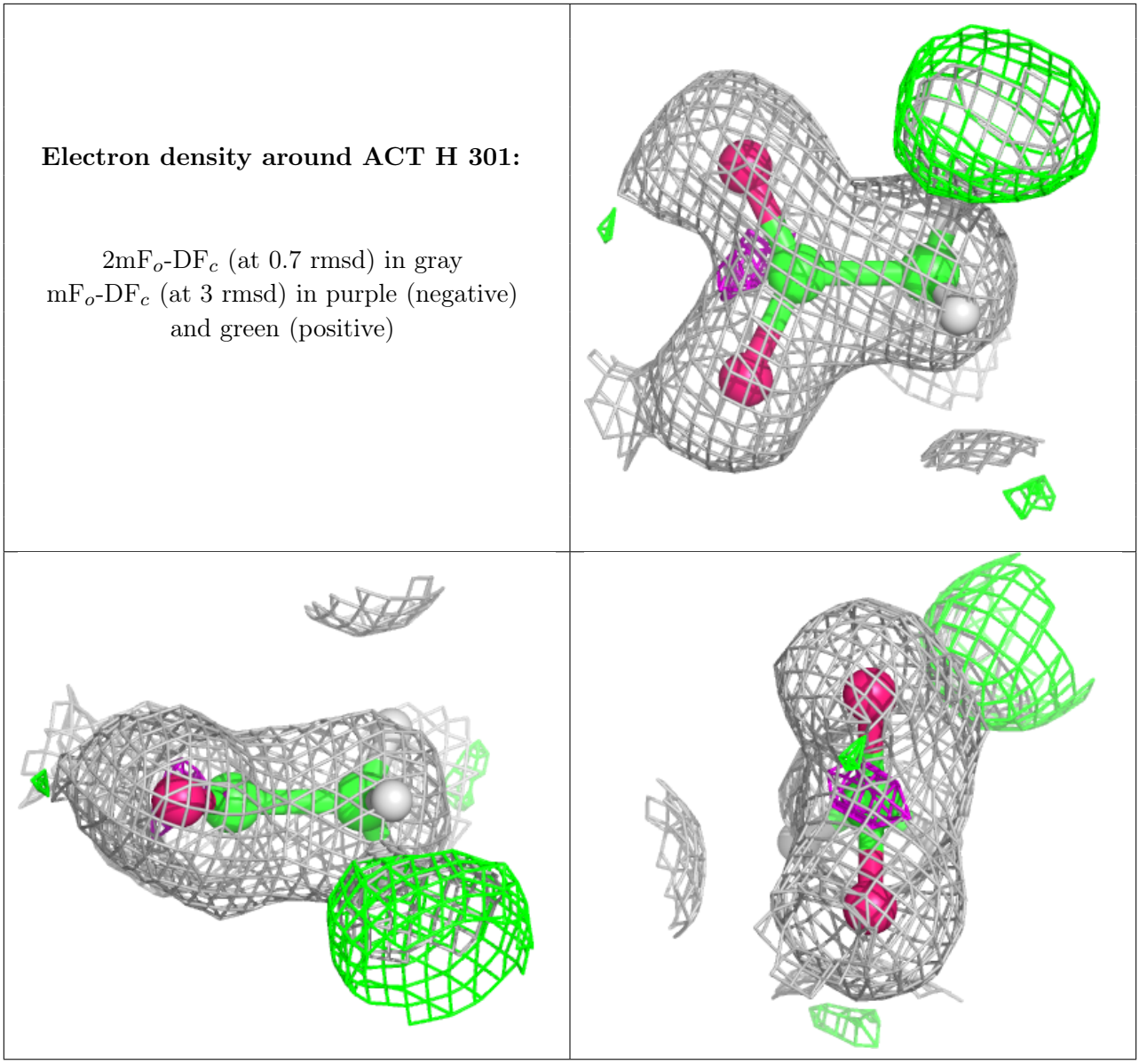
Electron density around ACT G 302:

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



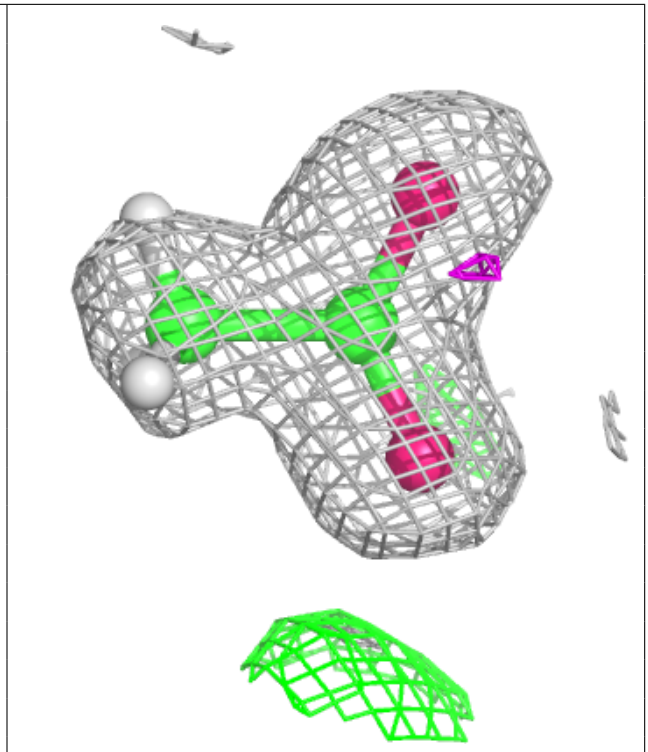
Electron density around ACT H 301:

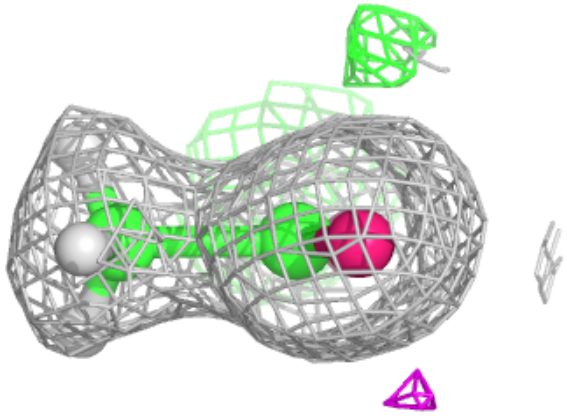
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

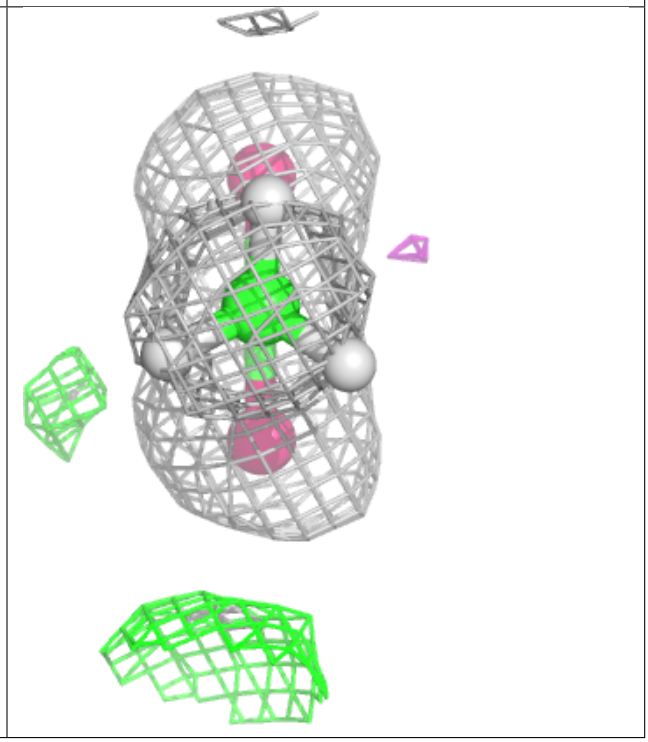


Electron density around ACT H 302:

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

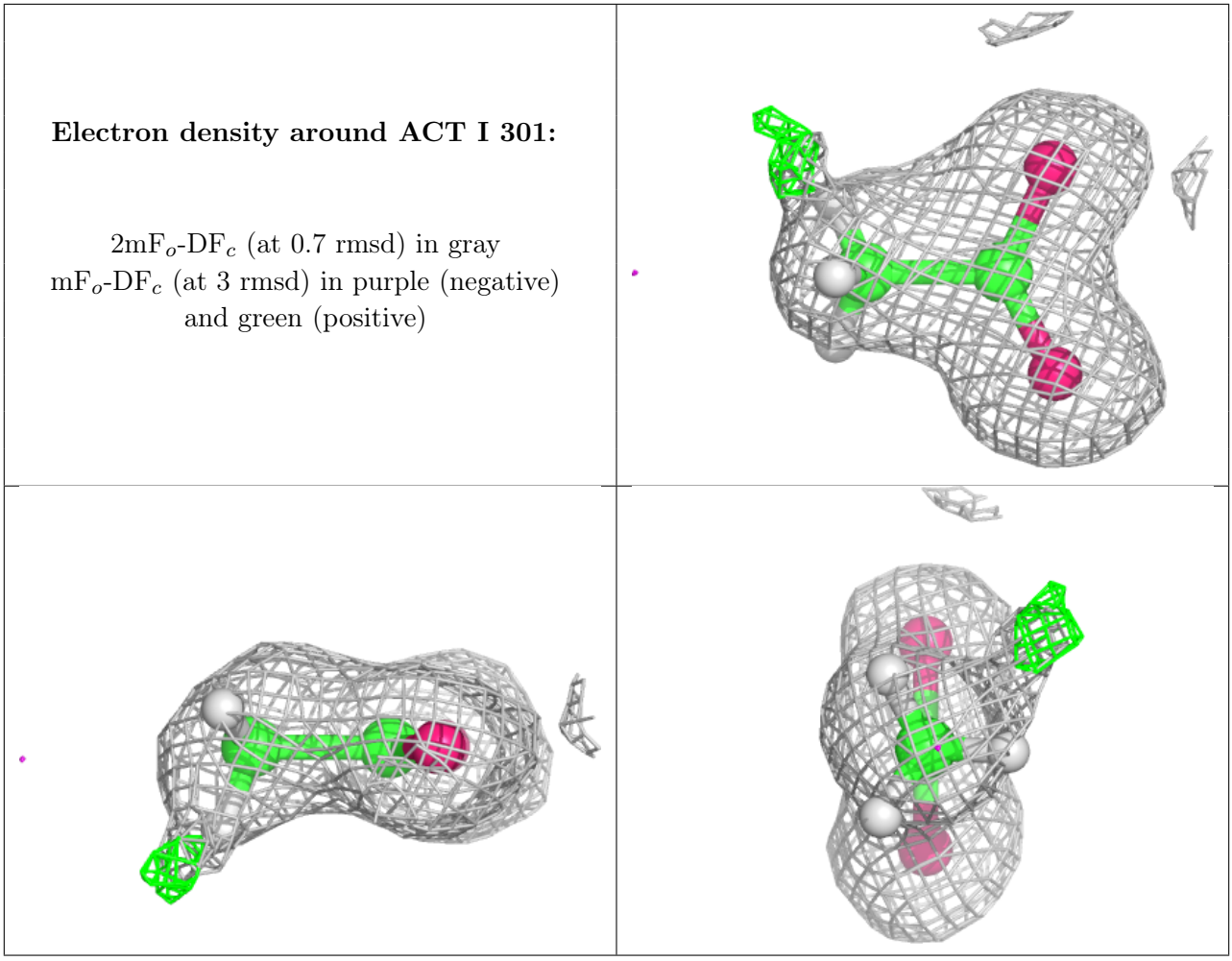






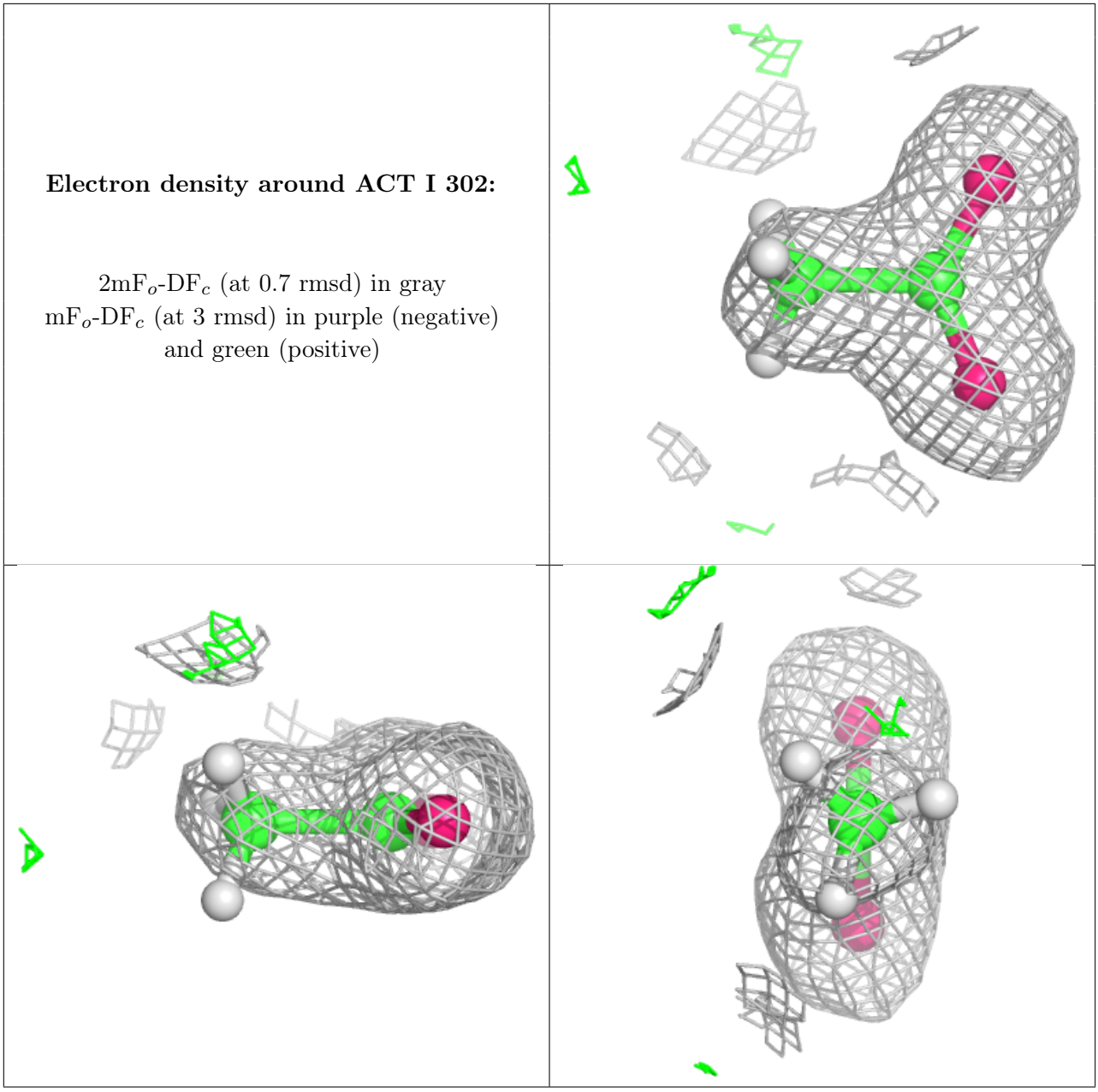
Electron density around ACT I 301:

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



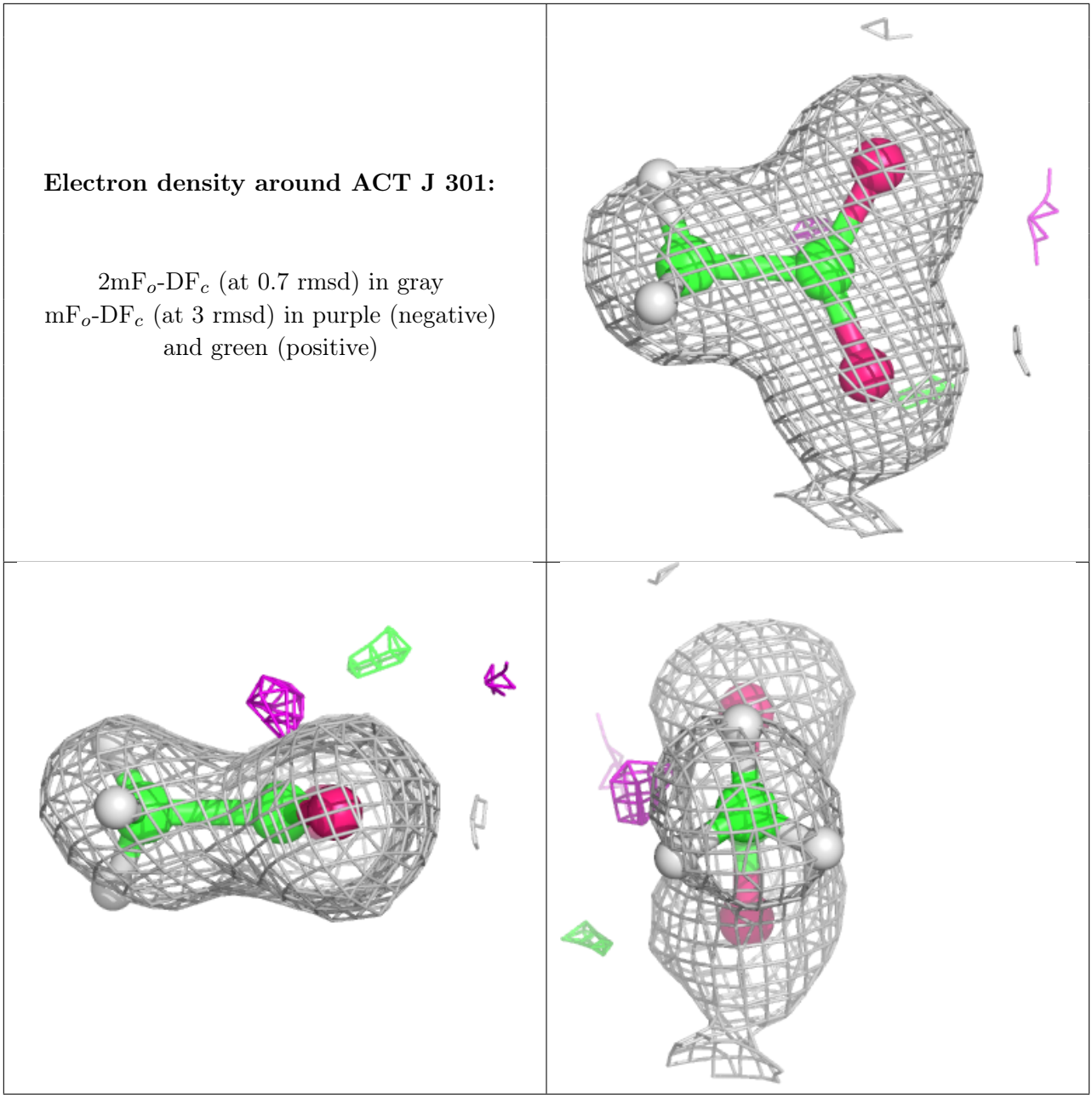
Electron density around ACT I 302:

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



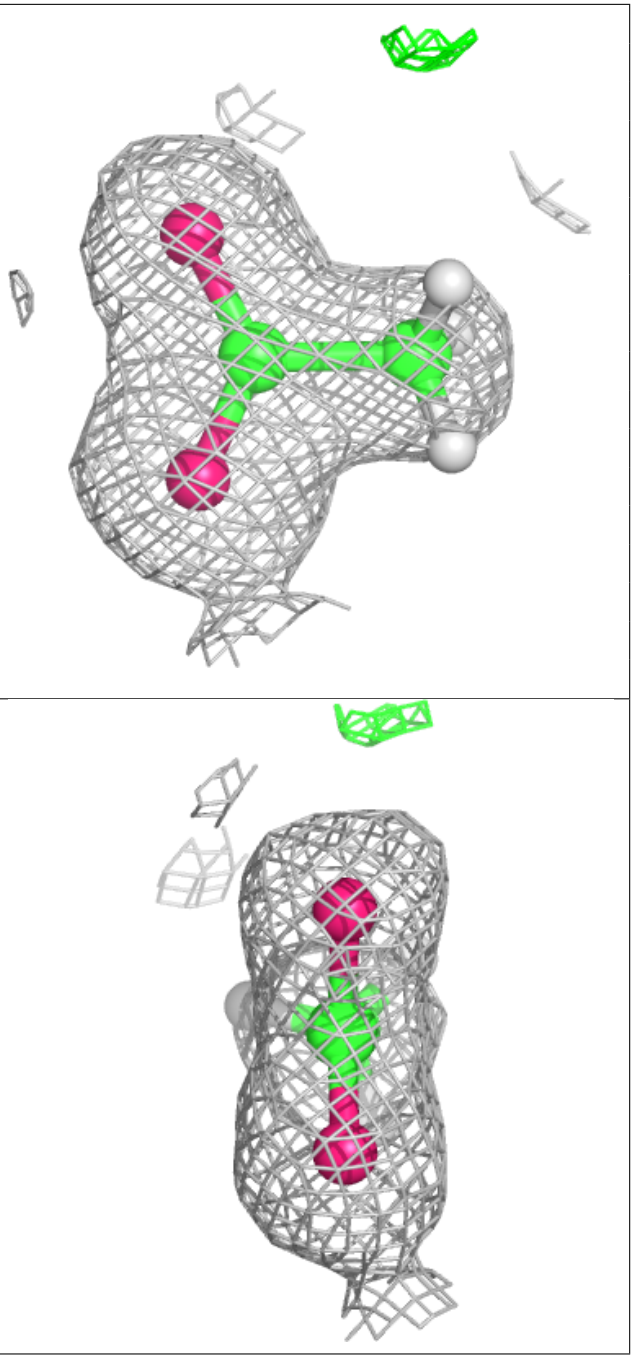
Electron density around ACT J 301:

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



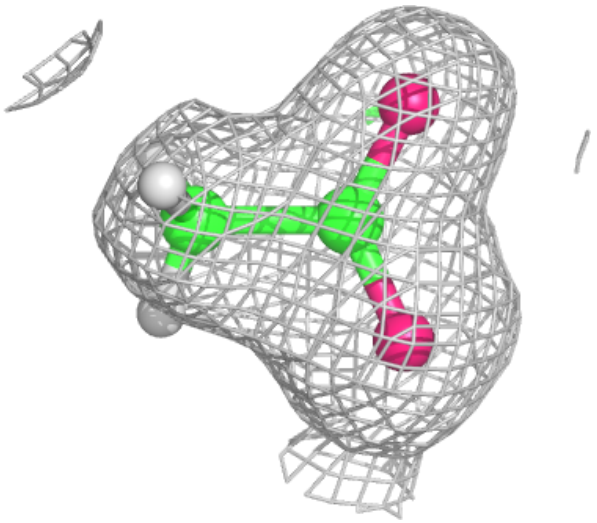
Electron density around ACT J 302:

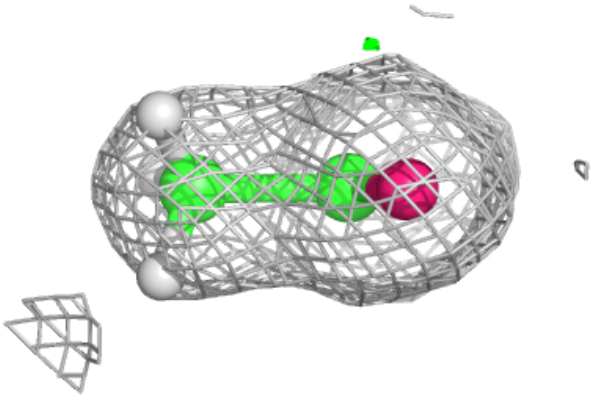
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

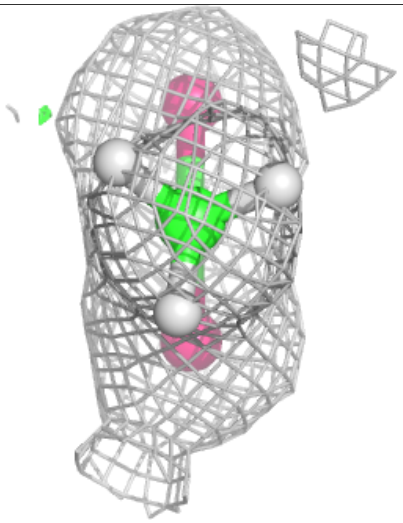


Electron density around ACT K 301:

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

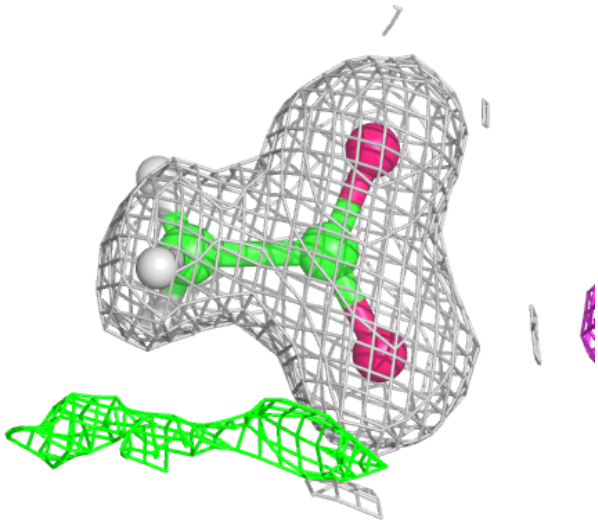


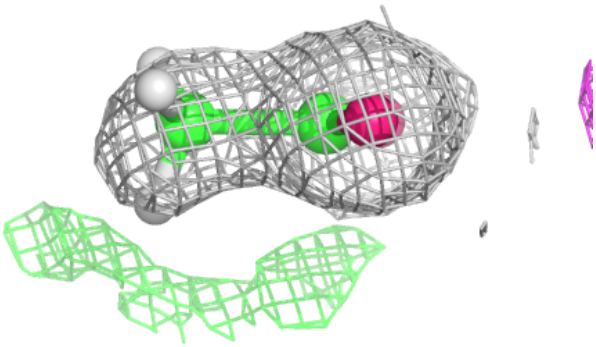


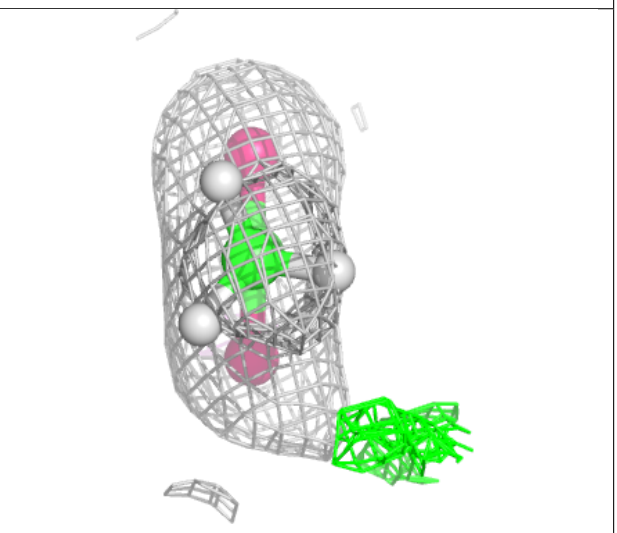


Electron density around ACT K 302:

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

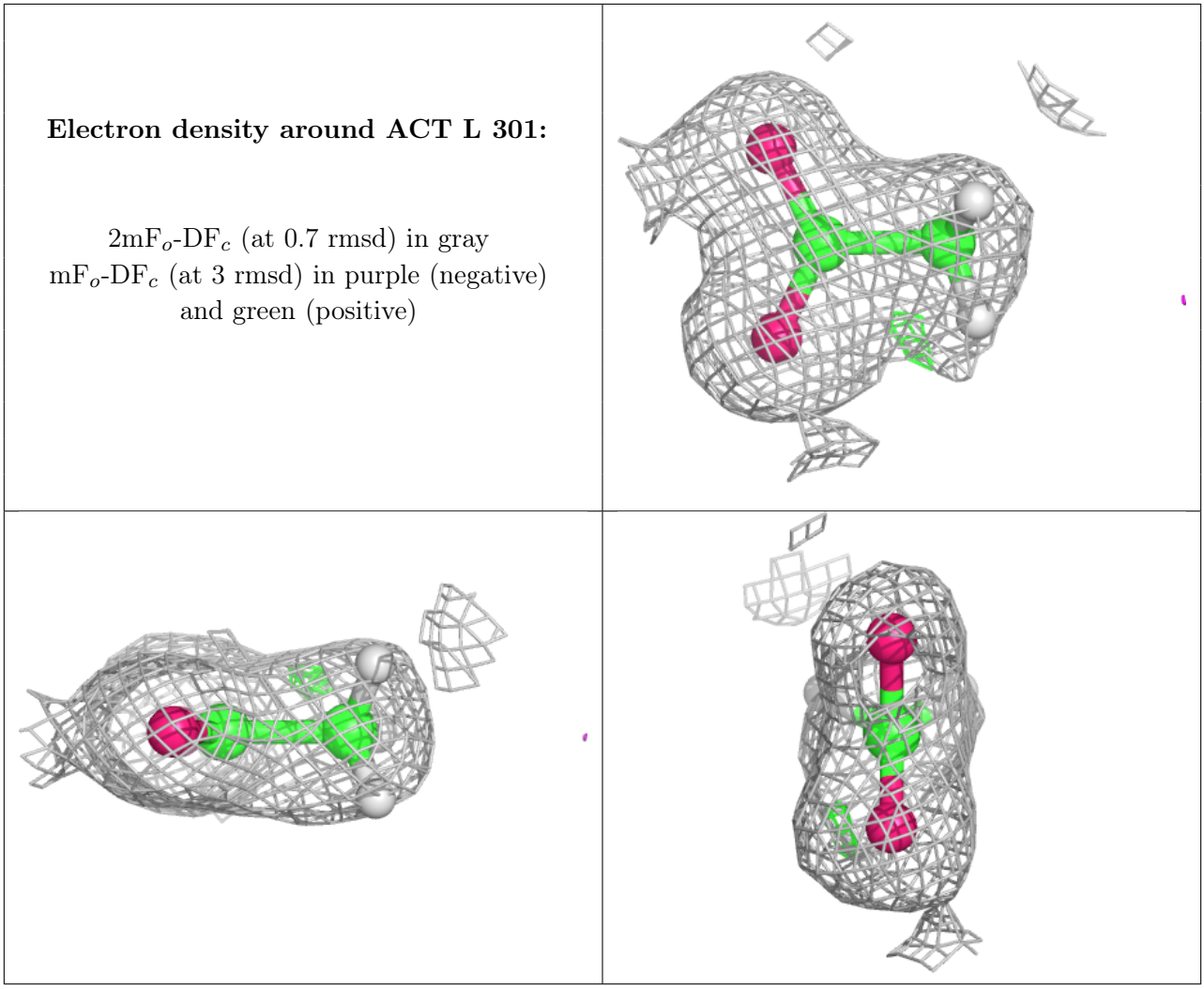






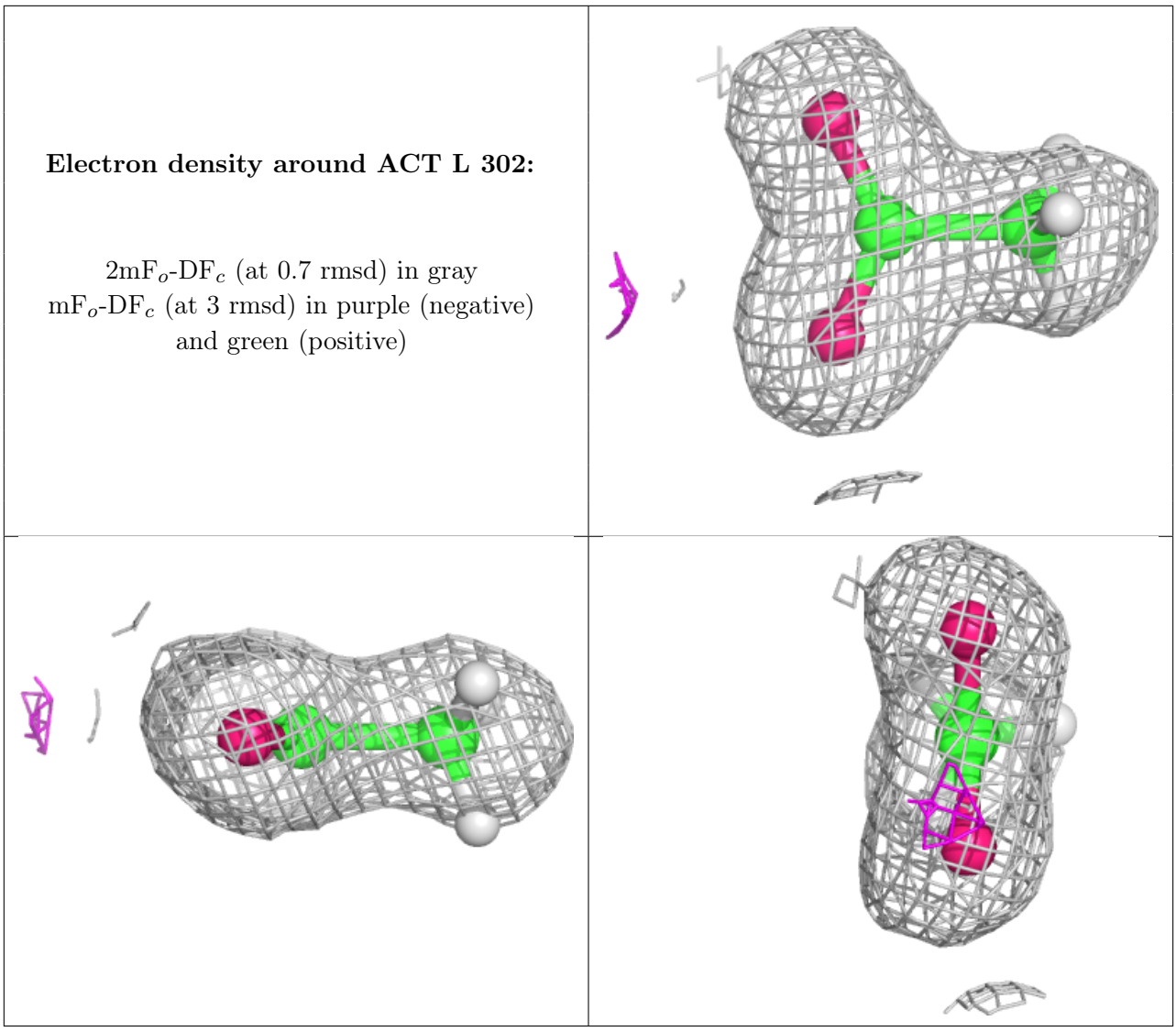
Electron density around ACT L 301:

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



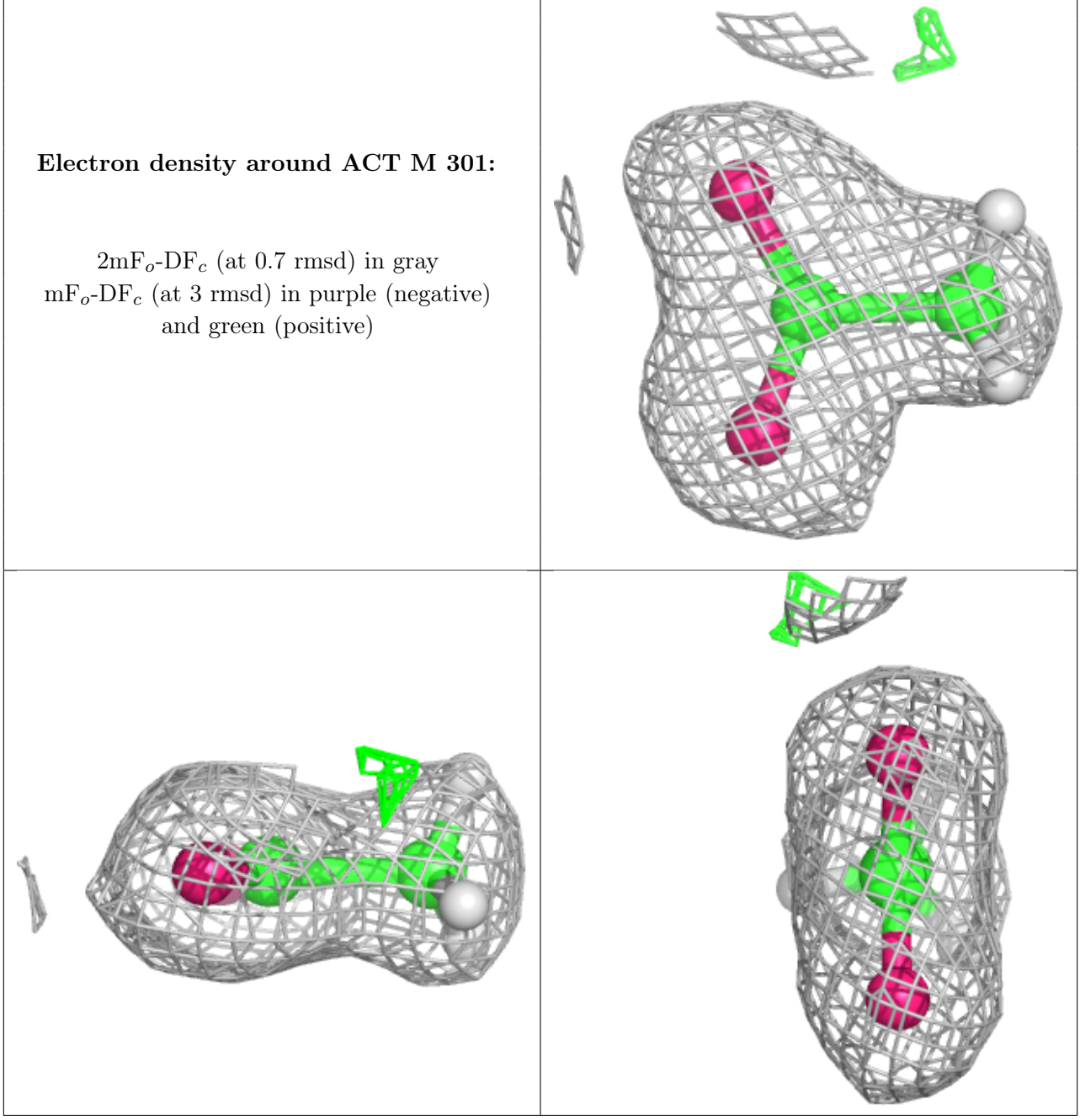
Electron density around ACT L 302:

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



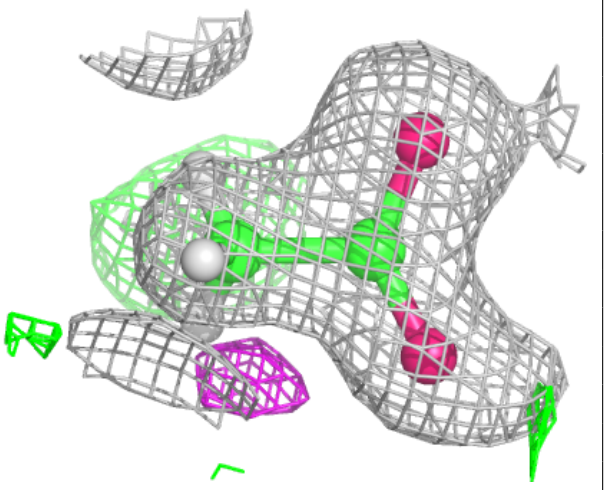
Electron density around ACT M 301:

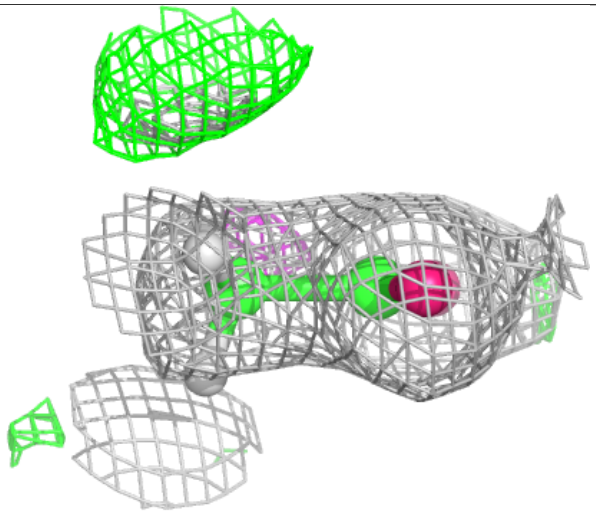
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

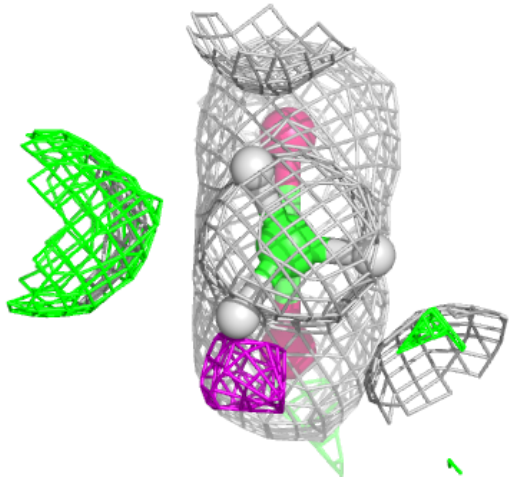


Electron density around ACT M 302:

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

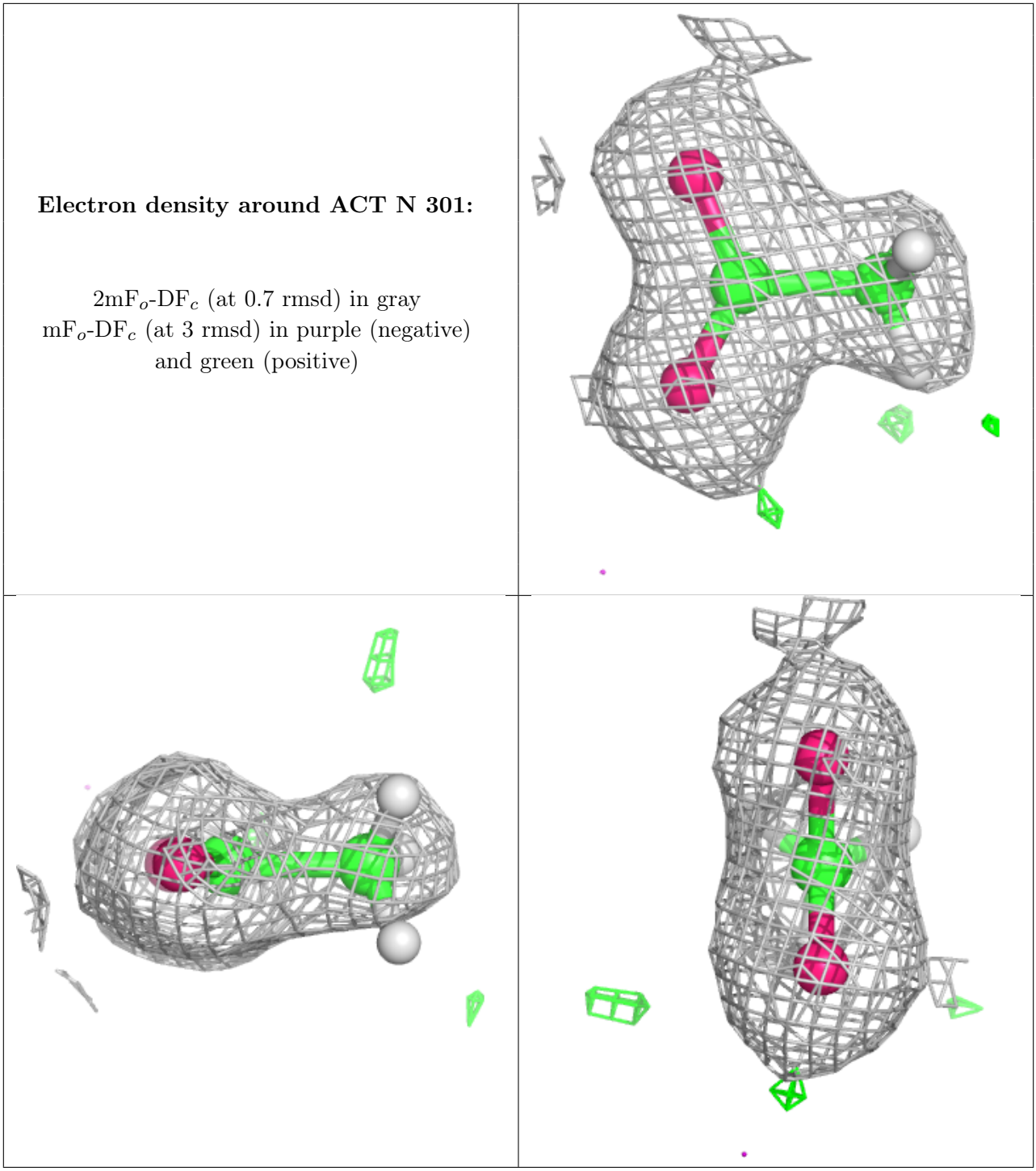






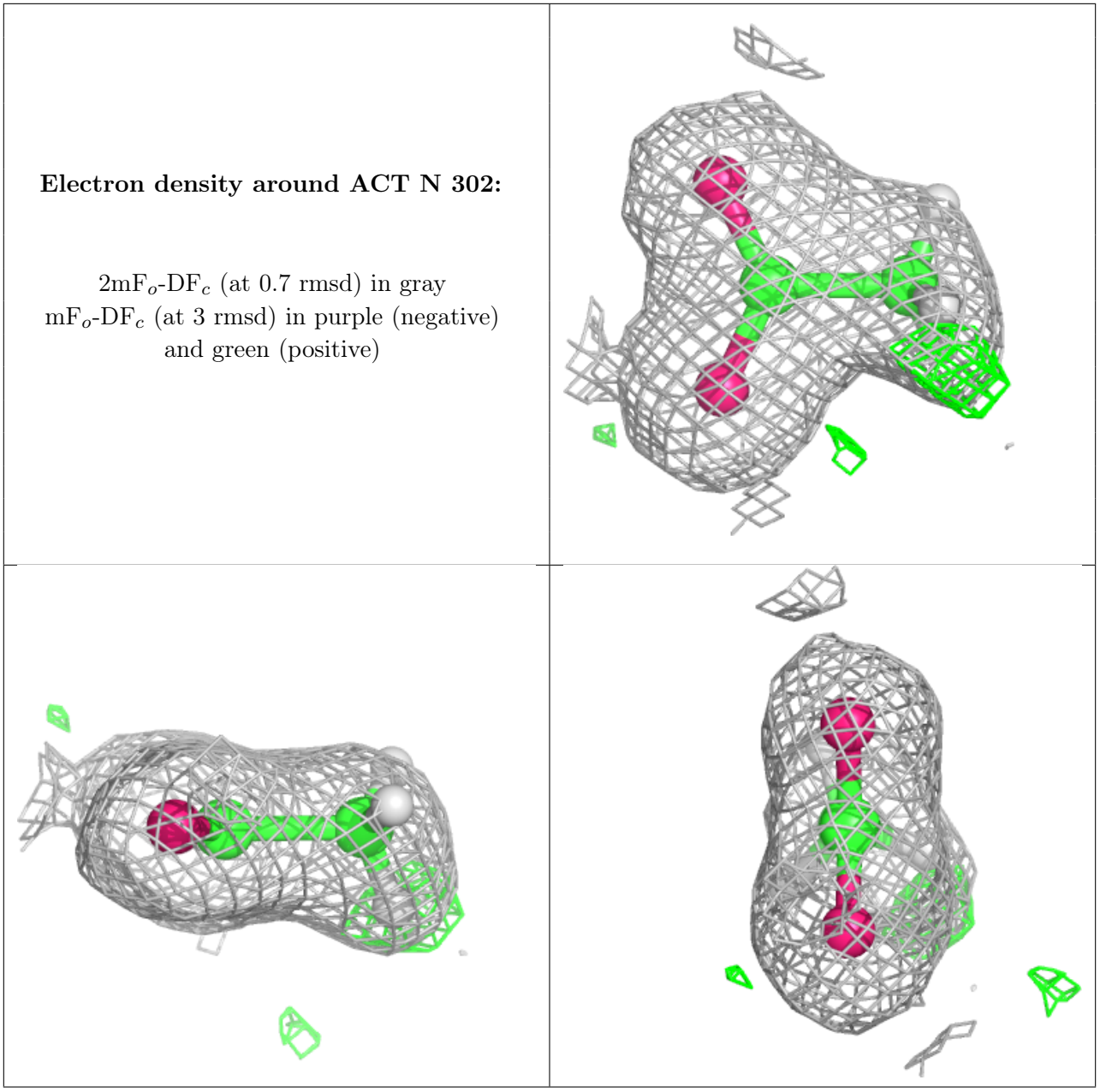
Electron density around ACT N 301:

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



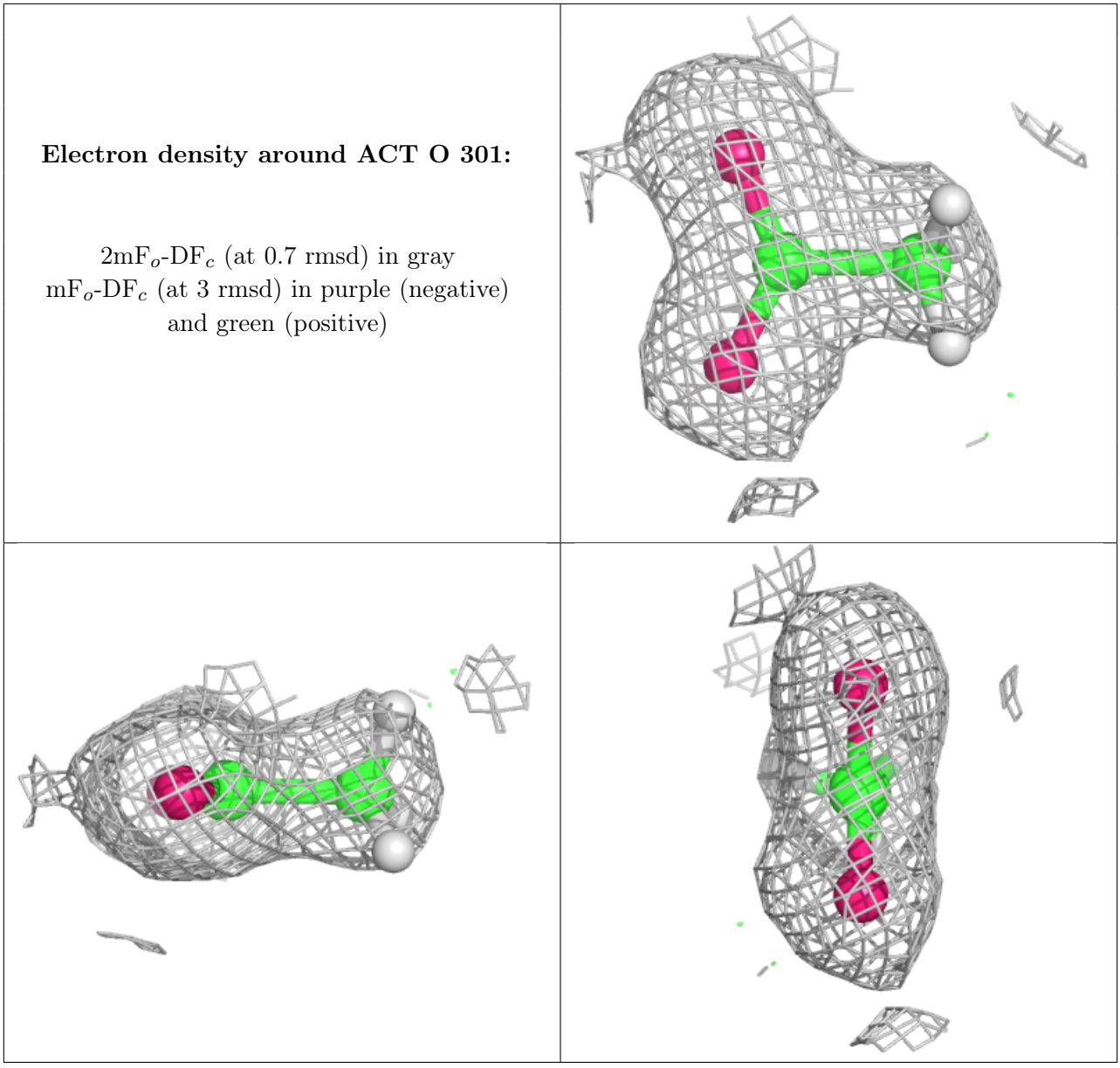
Electron density around ACT N 302:

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



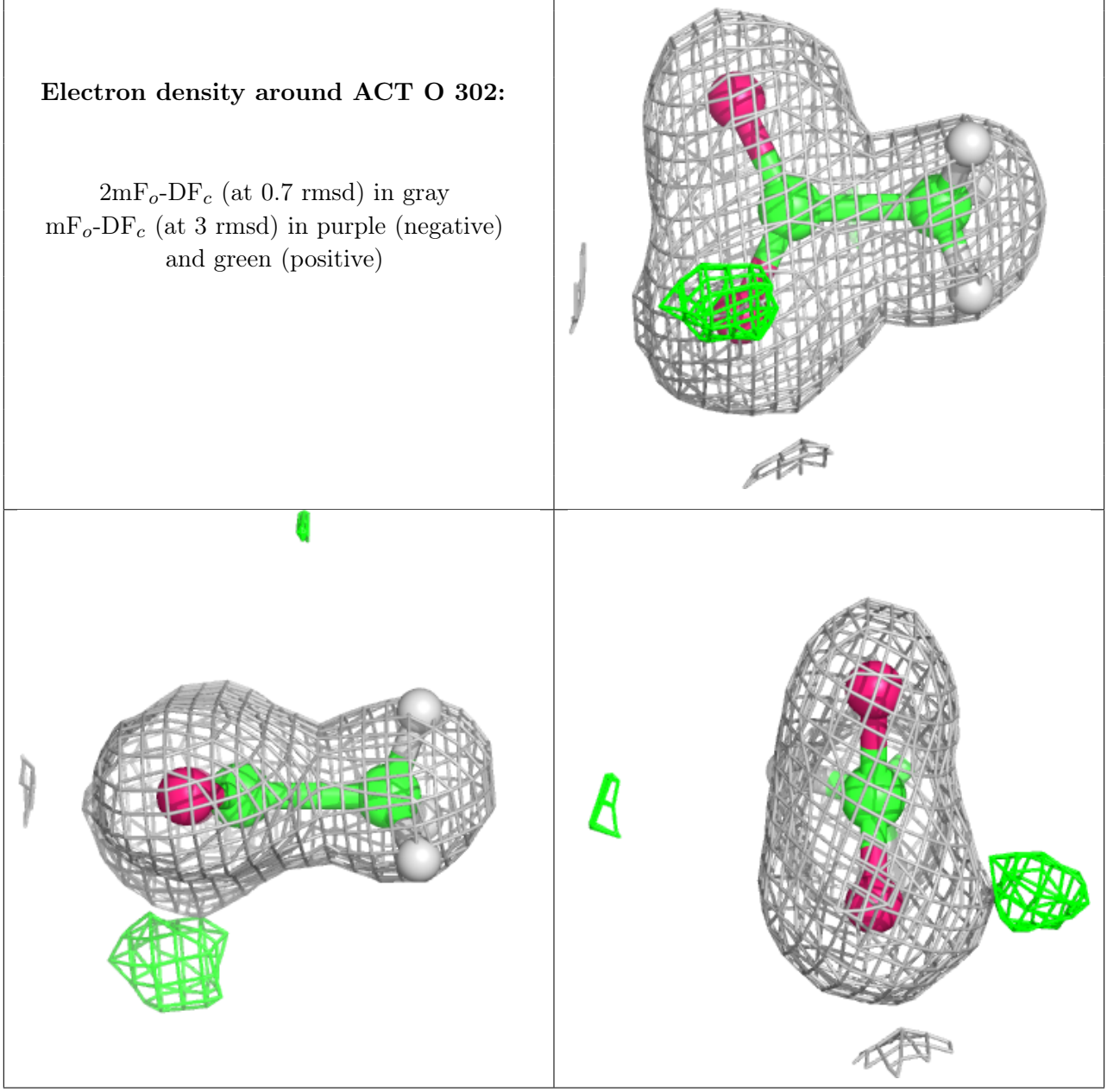
Electron density around ACT O 301:

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



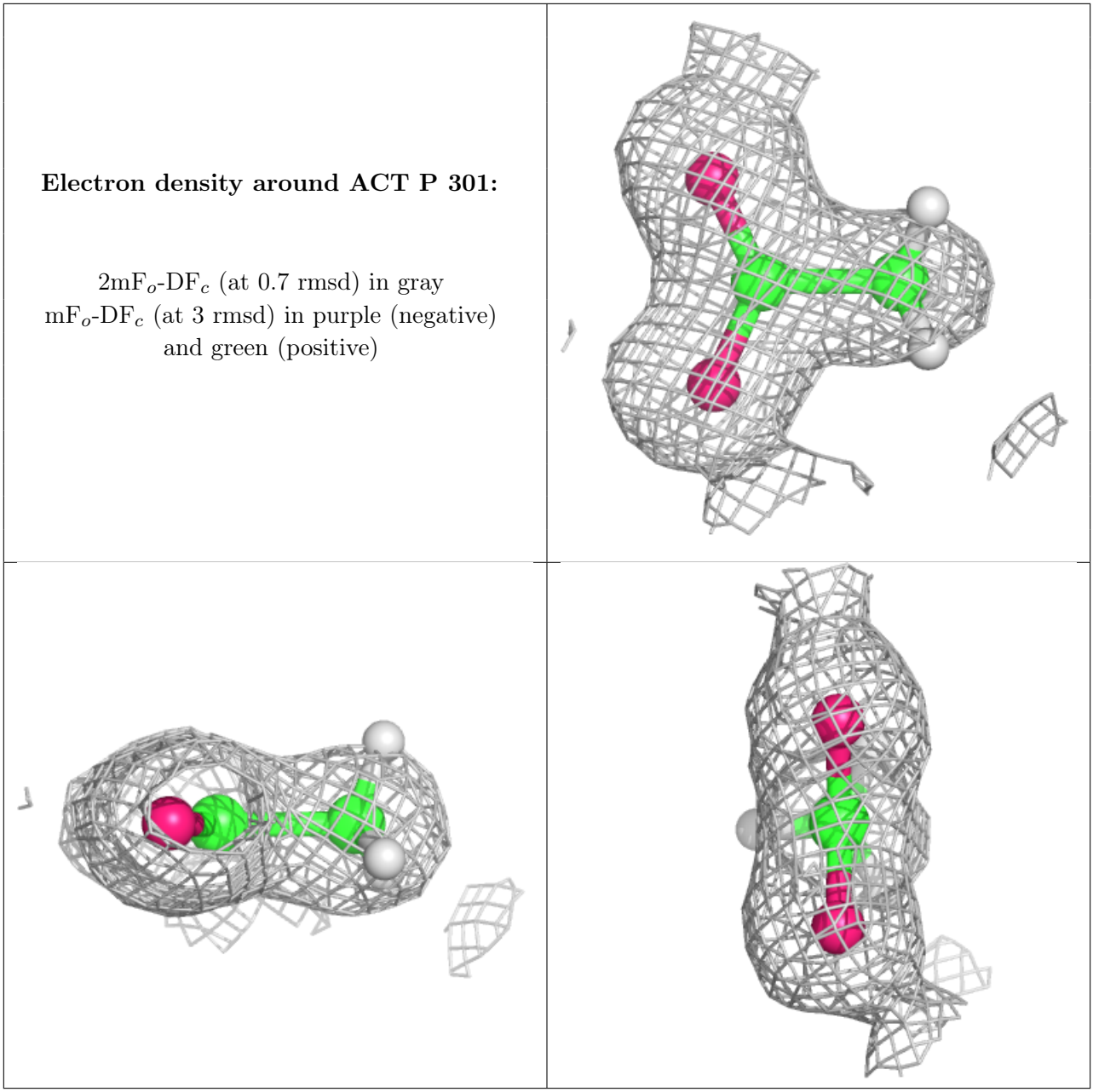
Electron density around ACT O 302:

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



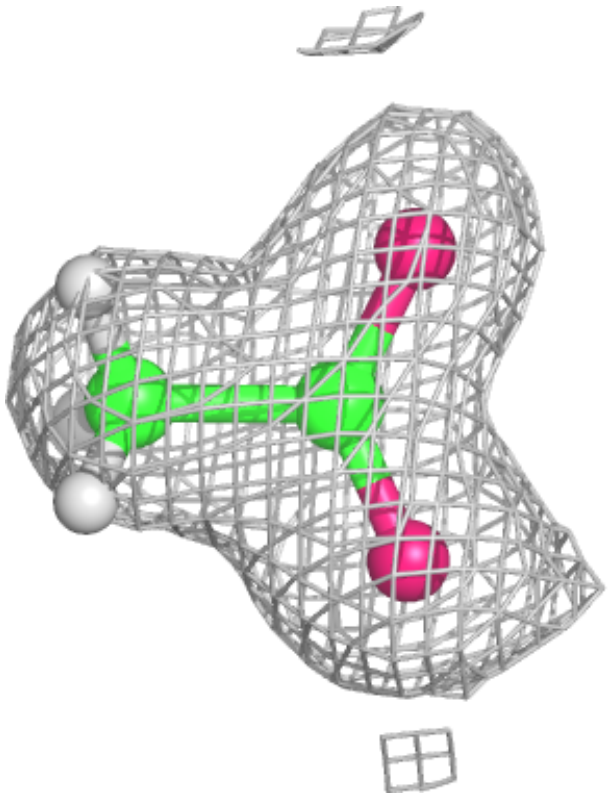
Electron density around ACT P 301:

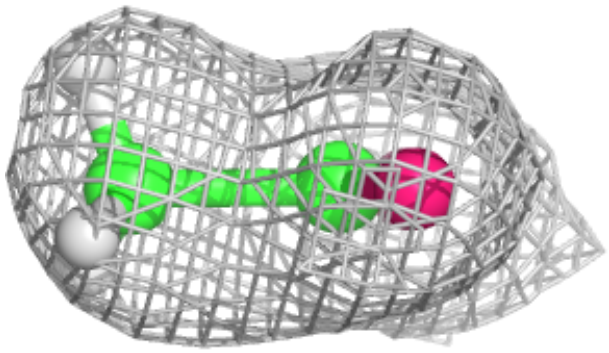
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

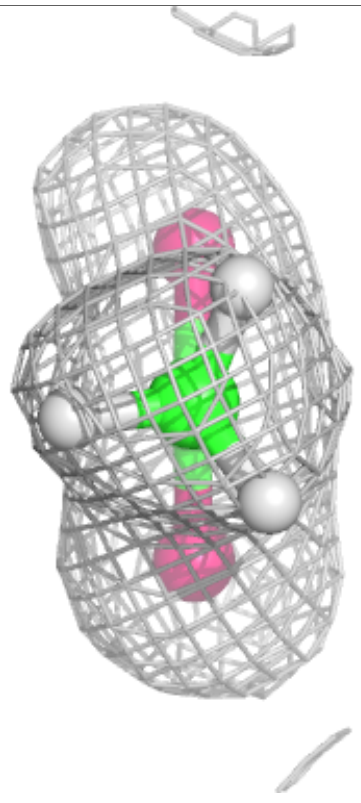


Electron density around ACT P 302:

$2mF_o$-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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.