Full wwPDB EM Validation Report ⓘ

Jul 30, 2022 – 02:04 pm BST

PDB ID	:	7QV7
EMDB ID	:	EMD-14169
Title	:	Cryo-EM structure of Hydrogen-dependent CO2 reductase.
Authors	:	Dietrich, H.M.; Righetto, R.D.; Kumar, A.; Wietrzynski, W.; Schuller, S.K.; Trischler, R.; Wagner, J.; Schwarz, F.M.; Engel, B.D.; Mueller, V.; Schuller, J.M.
Deposited on	:	2022-01-19
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

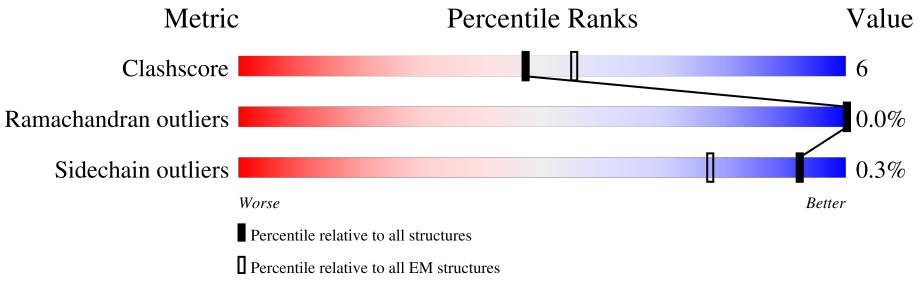
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	184	79% 15% 5%
1	G	184	77% 17% • 5%
2	B	210	78% 9% 13%
2	C	210	76% 11% 13%
2	J	210	79% 8% 13%
2	N	210	71% 16% 13%
2	P	210	72% 15% 13%
2	X	210	75% 12% 13%

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Mol	Chain	Length	Quality of chain
3	D	461	81% 16%
3	K	461	10% 83% 14%
3	Q	461	13% 81% 16%
3	R	461	82% 15%
3	V	461	81% 16%
3	Z	461	79% 18%
4	S	743	63% 14% 23%
4	Y	743	61% 16% 23%

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
5	SF4	C	304	-	-	X	-
5	SF4	S	801	-	-	X	-
5	SF4	V	504	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 41236 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Hydrogen dependent carbon dioxide reductase subunit HycB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	174	Total	C	N	O	S	0	0
			1338	844	225	250	19		
1	G	174	Total	C	N	O	S	0	0
			1338	844	225	250	19		

- Molecule 2 is a protein called Hydrogen dependent carbon dioxide reductase subunit HycB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	C	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	J	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	N	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	P	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	X	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		

- Molecule 3 is a protein called Hydrogen dependent carbon dioxide reductase subunit HydA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	K	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	Q	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	R	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	V	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		

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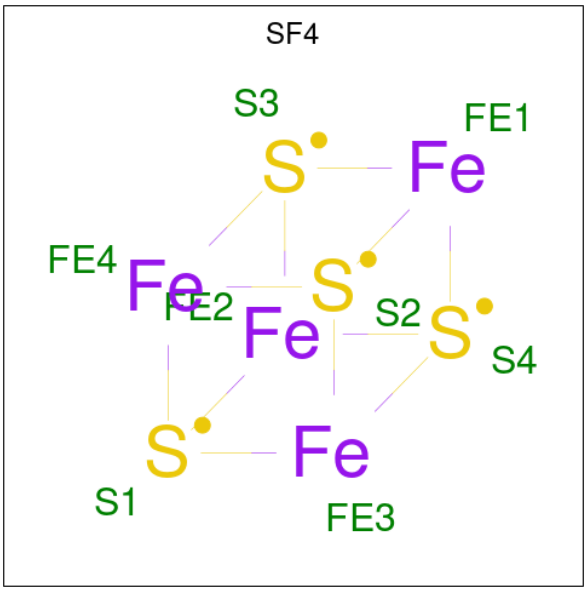
Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		

- Molecule 4 is a protein called Hydrogen dependent carbon dioxide reductase subunit FdhF.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	571	Total	C	N	O	S	0	0
			4429	2819	768	818	24		
4	Y	571	Total	C	N	O	S	0	0
			4429	2819	768	818	24		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	Fe	S		0
			32	16	16		
5	A	1	Total	Fe	S		0
			32	16	16		
5	A	1	Total	Fe	S		0
			32	16	16		
5	A	1	Total	Fe	S		0
			32	16	16		
5	B	1	Total	Fe	S		0
			32	16	16		
5	B	1	Total	Fe	S		0
			32	16	16		

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Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Fe S 32 16 16	0
5	B	1	Total Fe S 32 16 16	0
5	C	1	Total Fe S 32 16 16	0
5	C	1	Total Fe S 32 16 16	0
5	C	1	Total Fe S 32 16 16	0
5	C	1	Total Fe S 32 16 16	0
5	D	1	Total Fe S 24 12 12	0
5	D	1	Total Fe S 24 12 12	0
5	D	1	Total Fe S 24 12 12	0
5	G	1	Total Fe S 32 16 16	0
5	G	1	Total Fe S 32 16 16	0
5	G	1	Total Fe S 32 16 16	0
5	G	1	Total Fe S 32 16 16	0
5	J	1	Total Fe S 32 16 16	0
5	J	1	Total Fe S 32 16 16	0
5	J	1	Total Fe S 32 16 16	0
5	J	1	Total Fe S 32 16 16	0
5	K	1	Total Fe S 24 12 12	0
5	K	1	Total Fe S 24 12 12	0
5	K	1	Total Fe S 24 12 12	0
5	N	1	Total Fe S 32 16 16	0

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Mol	Chain	Residues	Atoms			AltConf
5	N	1	Total	Fe	S	0
			32	16	16	
5	N	1	Total	Fe	S	0
			32	16	16	
5	N	1	Total	Fe	S	0
			32	16	16	
5	P	1	Total	Fe	S	0
			32	16	16	
5	P	1	Total	Fe	S	0
			32	16	16	
5	P	1	Total	Fe	S	0
			32	16	16	
5	P	1	Total	Fe	S	0
			32	16	16	
5	Q	1	Total	Fe	S	0
			24	12	12	
5	Q	1	Total	Fe	S	0
			24	12	12	
5	Q	1	Total	Fe	S	0
			24	12	12	
5	R	1	Total	Fe	S	0
			24	12	12	
5	R	1	Total	Fe	S	0
			24	12	12	
5	R	1	Total	Fe	S	0
			24	12	12	
5	S	1	Total	Fe	S	0
			8	4	4	
5	V	1	Total	Fe	S	0
			24	12	12	
5	V	1	Total	Fe	S	0
			24	12	12	
5	V	1	Total	Fe	S	0
			24	12	12	
5	X	1	Total	Fe	S	0
			32	16	16	
5	X	1	Total	Fe	S	0
			32	16	16	
5	X	1	Total	Fe	S	0
			32	16	16	
5	X	1	Total	Fe	S	0
			32	16	16	

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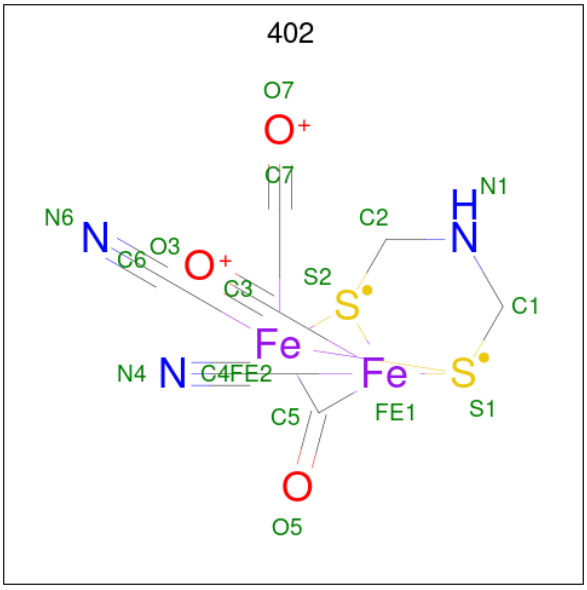
Mol	Chain	Residues	Atoms	AltConf
5	Y	1	Total Fe S 8 4 4	0
5	Z	1	Total Fe S 24 12 12	0
5	Z	1	Total Fe S 24 12 12	0
5	Z	1	Total Fe S 24 12 12	0

- Molecule 6 is dicarbonyl[bis(cyanide-kappaC)]-mu-(iminodimethanethiolatato-1kappaS:2kappaS)-mu-(oxomethylidene)diiron(2+) (three-letter code: 402) (formula: $C_7H_5Fe_2N_3O_3S_2$) (labeled as "Ligand of Interest" by depositor).



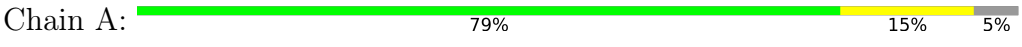
Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total C Fe N O S 17 7 2 3 3 2	0
6	K	1	Total C Fe N O S 17 7 2 3 3 2	0
6	Q	1	Total C Fe N O S 17 7 2 3 3 2	0
6	R	1	Total C Fe N O S 17 7 2 3 3 2	0
6	V	1	Total C Fe N O S 17 7 2 3 3 2	0
6	Z	1	Total C Fe N O S 17 7 2 3 3 2	0

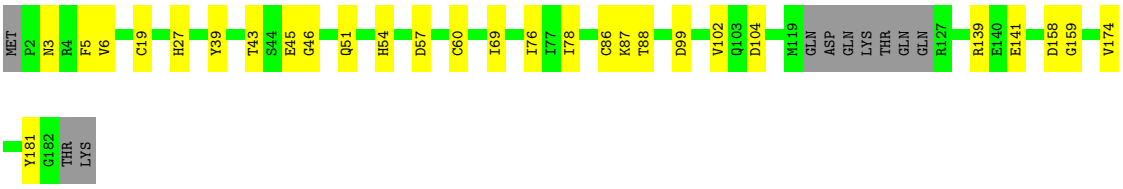
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Hydrogen dependent carbon dioxide reductase subunit HycB3

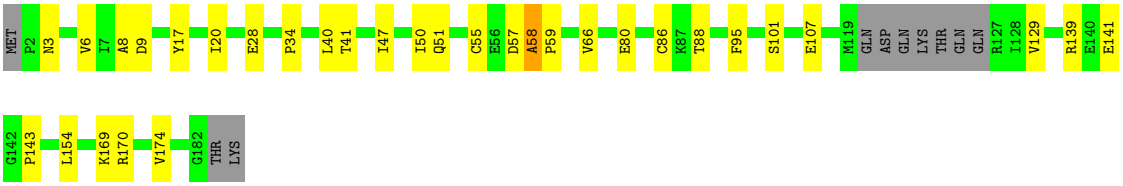
Chain A:





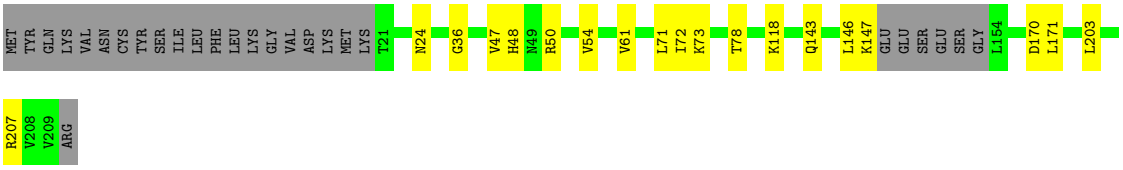
• Molecule 1: Hydrogen dependent carbon dioxide reductase subunit HycB3

Chain G:



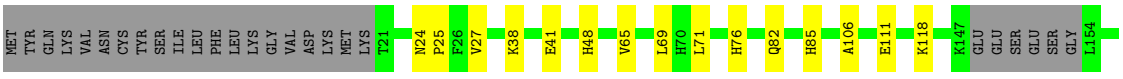
• Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

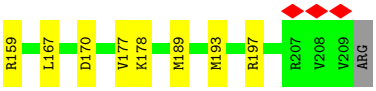
Chain B:



• Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

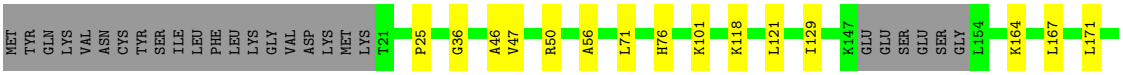
Chain C:

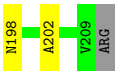




• Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

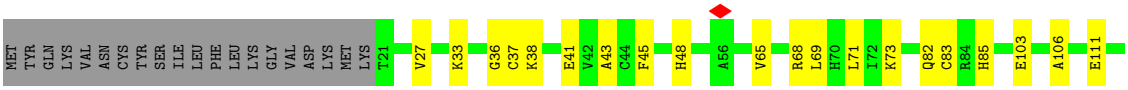
Chain J:

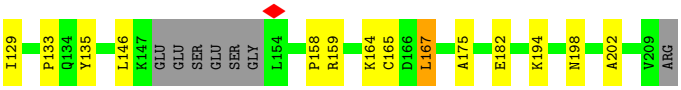




• Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

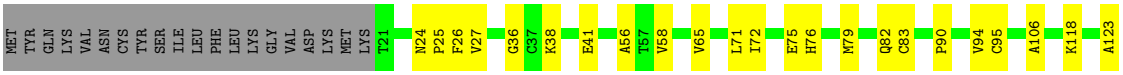
Chain N:

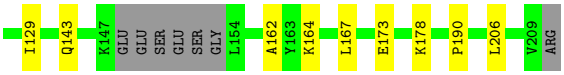




• Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

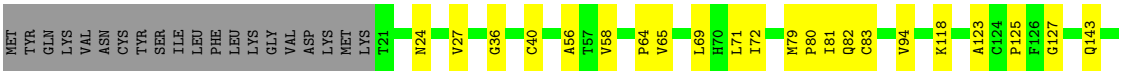
Chain P:

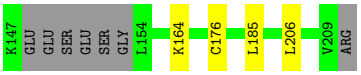




• Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

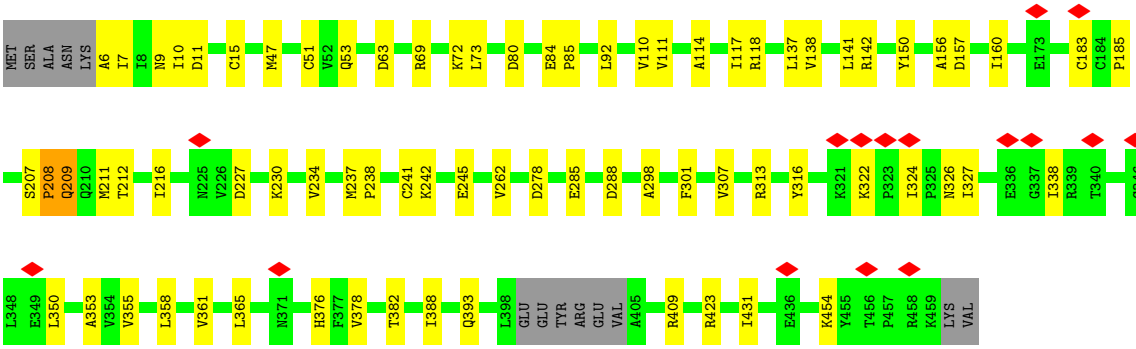
Chain X:





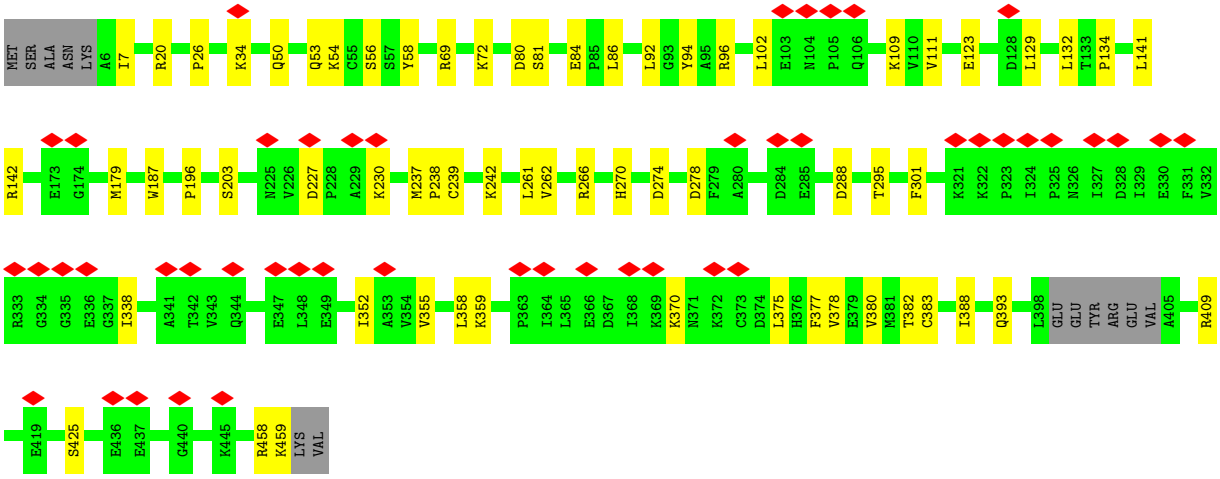
• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

Chain D:



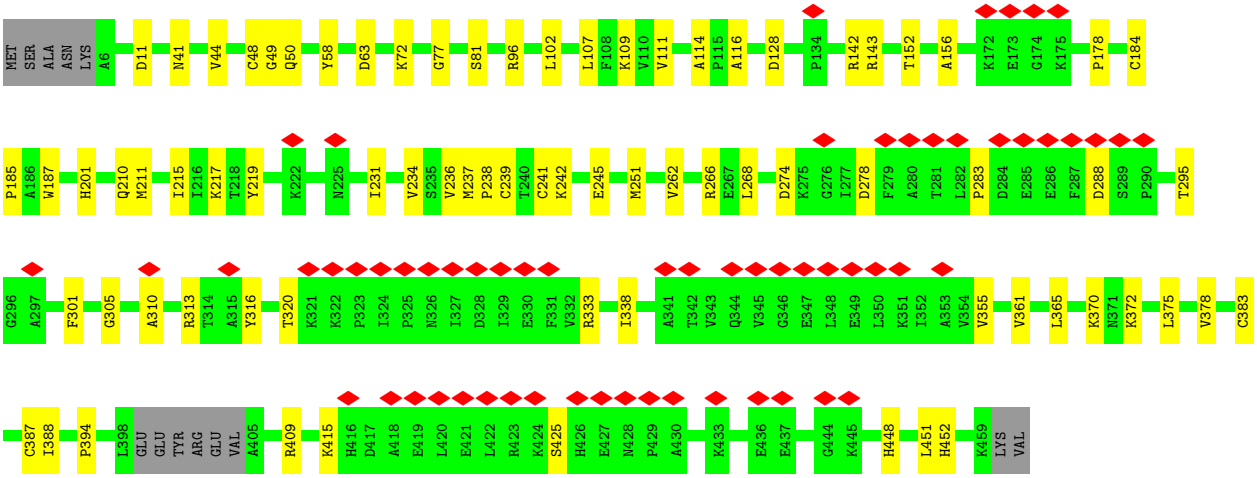
• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

Chain K:



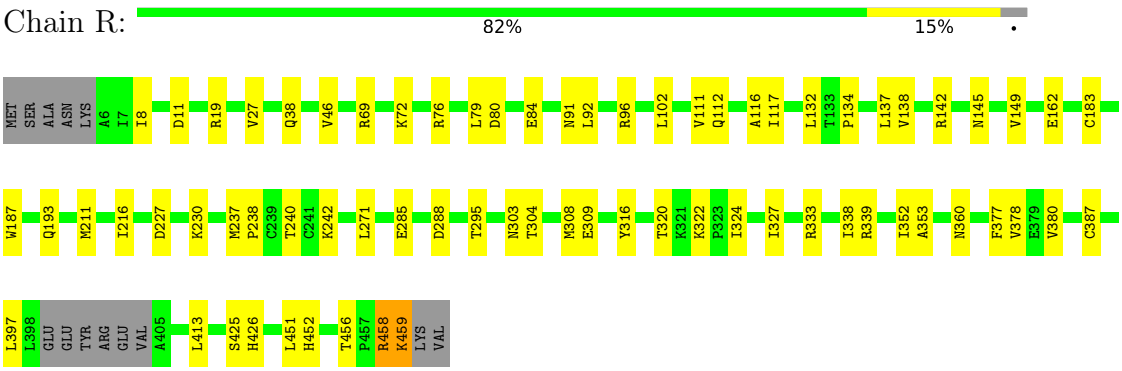
• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

Chain Q:



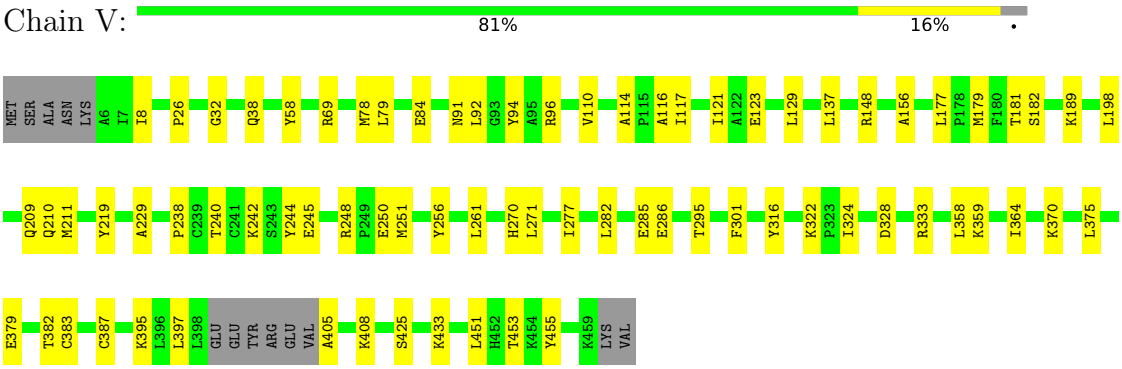
• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

Chain R:



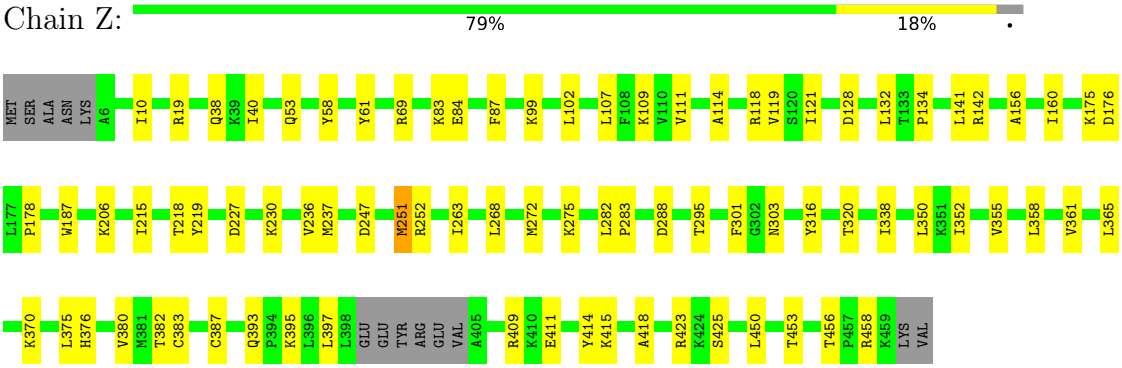
• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

Chain V:



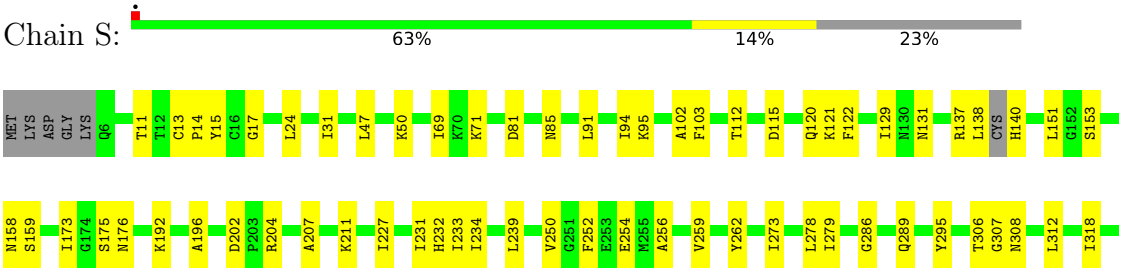
• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

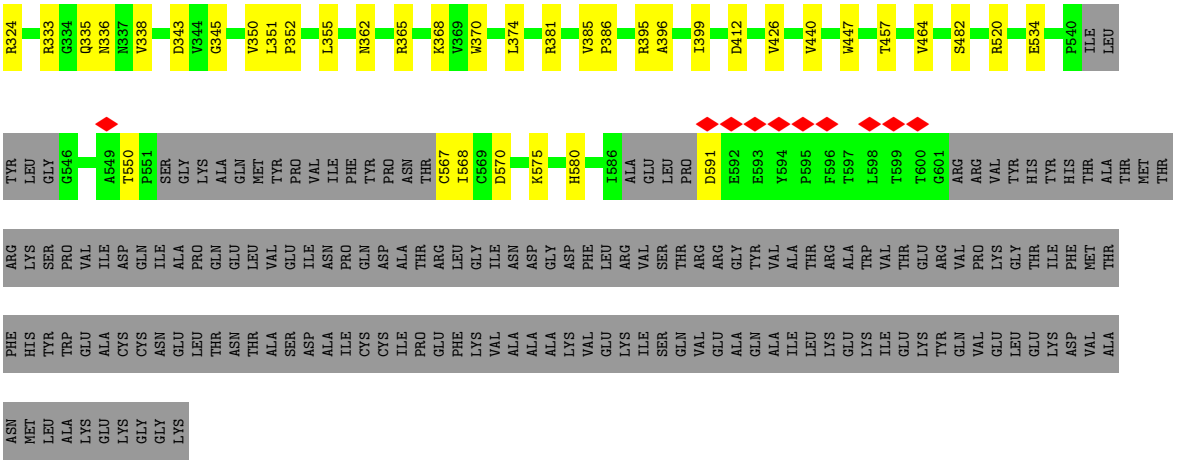
Chain Z:



• Molecule 4: Hydrogen dependent carbon dioxide reductase subunit FdhF

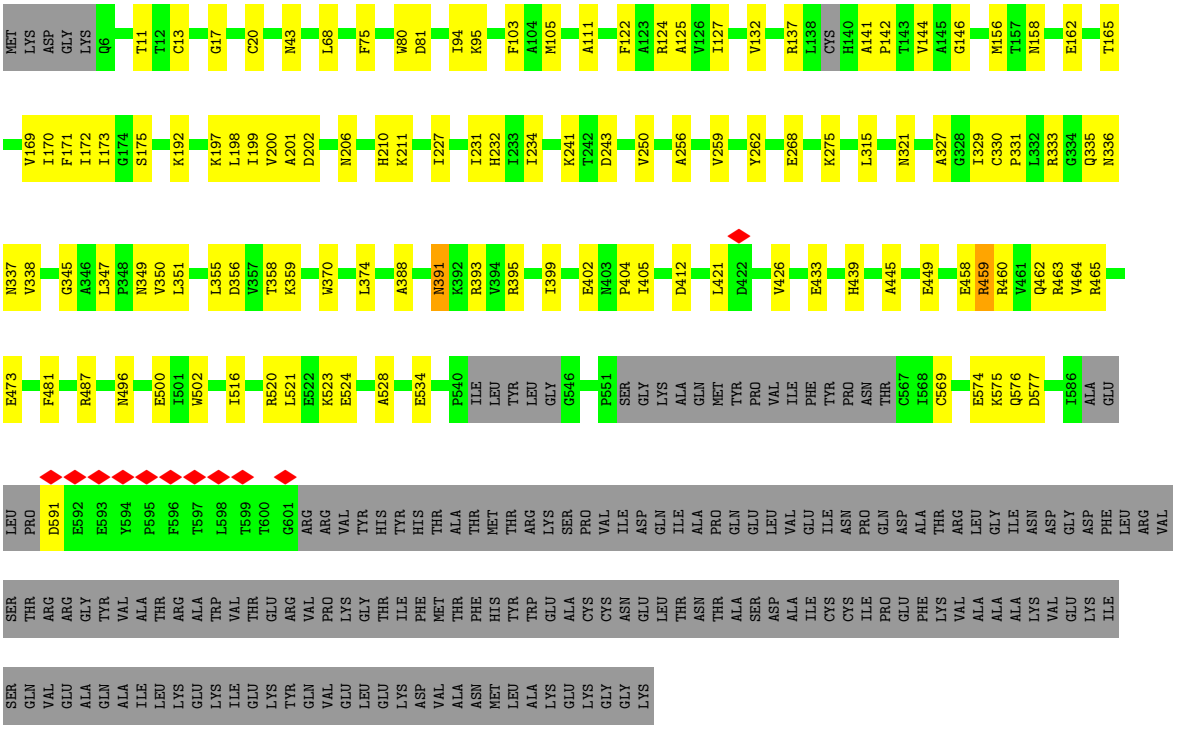
Chain S:





• Molecule 4: Hydrogen dependent carbon dioxide reductase subunit FdhF

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	719937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.398	Depositor
Minimum map value	-0.780	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	383.68002, 383.68002, 383.68002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 402, SF4

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	0.28	0/1359	0.50	0/1832
1	G	0.27	0/1359	0.51	0/1832
2	B	0.25	0/1400	0.50	0/1898
2	C	0.26	0/1400	0.52	0/1898
2	J	0.27	0/1400	0.51	0/1898
2	N	0.26	0/1400	0.51	1/1898 (0.1%)
2	P	0.28	0/1400	0.51	0/1898
2	X	0.26	0/1400	0.51	0/1898
3	D	0.25	0/3548	0.51	1/4788 (0.0%)
3	K	0.25	0/3548	0.47	0/4788
3	Q	0.25	0/3548	0.50	0/4788
3	R	0.26	0/3548	0.50	0/4788
3	V	0.27	0/3548	0.52	0/4788
3	Z	0.26	0/3548	0.52	1/4788 (0.0%)
4	S	0.26	0/4526	0.53	0/6136
4	Y	0.25	0/4526	0.51	0/6136
All	All	0.26	0/41458	0.51	3/56052 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	167	LEU	CA-CB-CG	5.46	127.86	115.30
3	Z	251	MET	CA-CB-CG	5.39	122.46	113.30
3	D	209	GLN	CB-CA-C	5.20	120.79	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	208	PRO	Peptide

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	1338	0	1333	24	0
1	G	1338	0	1333	27	0
2	B	1378	0	1401	15	0
2	C	1378	0	1401	17	0
2	J	1378	0	1401	14	0
2	N	1378	0	1401	25	0
2	P	1378	0	1401	27	0
2	X	1378	0	1401	21	0
3	D	3486	0	3527	49	0
3	K	3486	0	3527	39	0
3	Q	3486	0	3527	46	0
3	R	3486	0	3527	40	0
3	V	3486	0	3527	46	0
3	Z	3486	0	3526	52	0
4	S	4429	0	4414	62	0
4	Y	4429	0	4414	71	0
5	A	32	0	0	2	0
5	B	32	0	0	1	0
5	C	32	0	0	2	0
5	D	24	0	0	1	0
5	G	32	0	0	1	0
5	J	32	0	0	0	0
5	K	24	0	0	1	0
5	N	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	32	0	0	2	0
5	Q	24	0	0	0	0
5	R	24	0	0	1	0
5	S	8	0	0	2	0
5	V	24	0	0	2	0
5	X	32	0	0	1	0
5	Y	8	0	0	1	0
5	Z	24	0	0	1	0
6	D	17	0	5	3	0
6	K	17	0	5	1	0
6	Q	17	0	5	2	0
6	R	17	0	5	2	0
6	V	17	0	5	3	0
6	Z	17	0	3	3	0
All	All	41236	0	41089	528	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (528) 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)
2:J:118:LYS:NZ	2:P:24:ASN:O	2.14	0.80
3:K:239:CYS:HB2	5:K:504:SF4:S3	2.26	0.74
4:Y:137:ARG:O	4:Y:141:ALA:HB2	1.89	0.71
2:N:27:VAL:HG23	2:N:82:GLN:HE21	1.60	0.67
2:P:83:CYS:SG	2:P:164:LYS:NZ	2.68	0.66
4:S:399:ILE:HB	4:S:426:VAL:HG12	1.76	0.65
3:V:110:VAL:HG12	3:V:148:ARG:HB2	1.76	0.65
4:Y:13:CYS:HB3	5:Y:801:SF4:S4	2.37	0.65
4:Y:122:PHE:HD2	4:Y:481:PHE:HB3	1.62	0.65
4:Y:202:ASP:OD2	4:Y:206:ASN:ND2	2.30	0.64
3:R:316:TYR:HE2	3:R:324:ILE:HD12	1.62	0.64
4:Y:175:SER:O	4:Y:206:ASN:ND2	2.31	0.64
3:K:50:GLN:NE2	3:K:383:CYS:SG	2.70	0.64
2:C:76:HIS:HB2	2:X:206:LEU:HD13	1.79	0.63
4:S:158:ASN:OD1	4:S:159:SER:N	2.32	0.63
3:V:358:LEU:HD13	3:V:382:THR:HG22	1.80	0.63
3:Z:338:ILE:HG22	3:Z:355:VAL:HG12	1.79	0.63
3:Z:114:ALA:O	3:Z:118:ARG:NH1	2.32	0.62
3:Q:50:GLN:NE2	3:Q:383:CYS:SG	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:335:GLN:HB2	4:Y:338:VAL:HG23	1.82	0.62
3:V:211:MET:HG2	3:V:451:LEU:HD22	1.81	0.62
4:S:129:ILE:HG23	4:S:131:ASN:H	1.63	0.62
2:C:27:VAL:HG23	2:C:82:GLN:HE21	1.64	0.62
3:R:295:THR:HG21	3:R:425:SER:HA	1.81	0.61
1:G:3:ASN:O	2:X:118:LYS:NZ	2.33	0.61
4:S:13:CYS:HB3	5:S:801:SF4:S4	2.39	0.61
3:V:387:CYS:CB	6:V:503:402:C4	2.78	0.61
1:A:19:CYS:HB3	5:A:201:SF4:S3	2.39	0.61
2:B:36:GLY:HA2	2:B:71:LEU:HD11	1.83	0.61
3:Q:338:ILE:HG22	3:Q:355:VAL:HG12	1.81	0.60
2:B:48:HIS:CD2	5:B:304:SF4:S1	2.84	0.60
4:Y:459:ARG:HG2	4:Y:528:ALA:HB1	1.84	0.60
3:Z:19:ARG:NH1	3:Z:38:GLN:OE1	2.34	0.60
2:N:33:LYS:NZ	2:N:182:GLU:O	2.35	0.60
4:S:91:LEU:HD13	4:S:94:ILE:HD11	1.84	0.60
4:S:232:HIS:ND1	4:S:262:TYR:O	2.34	0.60
4:S:239:LEU:HD13	4:S:286:GLY:HA3	1.84	0.59
3:Z:132:LEU:HG	3:Z:134:PRO:HD3	1.82	0.59
3:Q:116:ALA:HB3	3:Q:238:PRO:HG2	1.85	0.59
3:Z:301:PHE:HB3	6:Z:504:402:H11	1.84	0.59
4:S:103:PHE:HB3	4:S:396:ALA:HB3	1.84	0.59
4:Y:405:ILE:HG21	4:Y:433:GLU:HB3	1.84	0.59
4:S:14:PRO:O	4:S:336:ASN:ND2	2.36	0.58
3:Z:69:ARG:HH12	3:Z:83:LYS:HG2	1.68	0.58
3:V:277:ILE:HD11	3:V:282:LEU:HD21	1.86	0.58
4:Y:523:LYS:HG3	4:Y:524:GLU:HG2	1.86	0.58
4:Y:172:ILE:HD13	4:Y:200:VAL:HG22	1.86	0.58
3:Z:387:CYS:CB	6:Z:504:402:C4	2.82	0.58
3:V:248:ARG:HB2	3:V:251:MET:HB2	1.86	0.58
3:V:219:TYR:OH	3:V:433:LYS:NZ	2.37	0.57
2:P:38:LYS:HG3	2:P:71:LEU:HD13	1.86	0.57
2:C:106:ALA:HB2	2:C:167:LEU:HD13	1.86	0.57
3:D:338:ILE:HG22	3:D:355:VAL:HG12	1.86	0.57
3:Q:355:VAL:HG21	3:Q:361:VAL:HG22	1.86	0.57
2:C:24:ASN:ND2	2:C:85:HIS:O	2.38	0.57
2:X:58:VAL:HB	3:Z:395:LYS:HB2	1.86	0.57
4:Y:20:CYS:HB3	4:Y:43:ASN:HD22	1.69	0.57
3:Q:370:LYS:HG3	3:Q:375:LEU:HD12	1.85	0.57
3:Z:383:CYS:HB2	5:Z:503:SF4:S3	2.45	0.57
3:V:382:THR:OG1	5:V:504:SF4:S4	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:53:GLN:NE2	3:Z:393:GLN:O	2.37	0.57
3:D:11:ASP:OD2	3:D:72:LYS:NZ	2.37	0.57
2:P:173:GLU:OE2	2:P:178:LYS:NZ	2.35	0.57
3:K:266:ARG:O	3:K:270:HIS:ND1	2.30	0.56
3:K:20:ARG:HE	2:N:37:CYS:HB2	1.70	0.56
2:C:38:LYS:HG3	2:C:71:LEU:HD13	1.87	0.56
4:S:15:TYR:HB3	4:S:50:LYS:HD2	1.88	0.56
3:V:328:ASP:OD1	3:V:333:ARG:NH1	2.39	0.56
4:Y:156:MET:HG3	4:Y:330:CYS:HA	1.86	0.56
3:Z:175:LYS:NZ	3:Z:176:ASP:OD2	2.38	0.56
3:Q:11:ASP:OD2	3:Q:72:LYS:NZ	2.39	0.56
3:D:350:LEU:HB3	3:D:376:HIS:HD2	1.70	0.56
3:K:196:PRO:O	3:K:458:ARG:NH1	2.38	0.56
4:Y:520:ARG:NH1	4:Y:534:GLU:O	2.39	0.56
3:D:157:ASP:HB3	3:D:431:ILE:HD11	1.87	0.56
3:V:210:GLN:NE2	3:V:245:GLU:OE1	2.37	0.56
4:Y:232:HIS:ND1	4:Y:262:TYR:O	2.37	0.56
3:K:26:PRO:HA	3:K:359:LYS:HE3	1.88	0.56
3:Q:236:VAL:HG21	3:Q:268:LEU:HD22	1.87	0.56
2:B:50:ARG:HH21	2:B:54:VAL:HG23	1.71	0.56
3:D:110:VAL:HG11	3:D:216:ILE:HG21	1.88	0.56
3:R:69:ARG:NH2	3:R:84:GLU:O	2.39	0.56
4:Y:402:GLU:HG3	4:Y:404:PRO:HD3	1.88	0.56
3:R:142:ARG:NH2	3:R:288:ASP:OD1	2.39	0.55
4:S:520:ARG:NH1	4:S:534:GLU:O	2.39	0.55
2:C:25:PRO:HG2	2:C:167:LEU:HD11	1.88	0.55
3:R:187:TRP:CG	3:R:380:VAL:HG21	2.41	0.55
4:S:362:ASN:HA	4:S:365:ARG:HE	1.71	0.55
1:G:6:VAL:HG13	1:G:51:GLN:HE21	1.72	0.55
3:K:295:THR:HG21	3:K:425:SER:HA	1.88	0.55
2:X:83:CYS:SG	2:X:164:LYS:NZ	2.76	0.55
3:R:80:ASP:OD1	3:R:96:ARG:NH1	2.38	0.55
4:Y:569:CYS:HB2	4:Y:574:GLU:HB3	1.88	0.55
3:Q:210:GLN:NE2	3:Q:251:MET:O	2.40	0.55
3:Q:388:ILE:O	3:Q:409:ARG:NH1	2.40	0.55
3:R:183:CYS:HB3	6:R:503:402:H8	1.88	0.55
1:A:3:ASN:O	2:P:118:LYS:NZ	2.40	0.55
3:Q:361:VAL:HG12	3:Q:365:LEU:HB2	1.89	0.54
4:S:256:ALA:HA	4:S:259:VAL:HG12	1.90	0.54
4:Y:169:VAL:HG22	4:Y:197:LYS:HB2	1.89	0.54
3:Z:121:ILE:HD11	3:Z:272:MET:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:OD1	2:P:143:GLN:NE2	2.39	0.54
1:A:69:ILE:HG12	1:A:78:ILE:HD12	1.89	0.54
4:Y:463:ARG:HG2	4:Y:521:LEU:HG	1.88	0.54
3:Z:456:THR:OG1	3:Z:458:ARG:NH1	2.41	0.54
1:A:57:ASP:HA	2:P:143:GLN:HE22	1.72	0.54
2:C:25:PRO:HB3	2:C:189:MET:HB2	1.90	0.54
3:D:47:MET:HG3	3:D:241:CYS:HA	1.90	0.54
2:C:118:LYS:NZ	2:X:24:ASN:O	2.31	0.54
3:D:183:CYS:O	6:D:503:402:H8	2.08	0.54
2:J:56:ALA:HA	3:R:397:LEU:HD12	1.88	0.54
4:S:121:LYS:NZ	4:S:370:TRP:O	2.41	0.54
4:Y:144:VAL:HB	4:Y:333:ARG:HH22	1.71	0.54
4:Y:399:ILE:HB	4:Y:426:VAL:HG12	1.90	0.54
3:Z:393:GLN:OE1	3:Z:409:ARG:NH1	2.41	0.54
4:S:17:GLY:HA2	4:S:336:ASN:HA	1.89	0.53
3:Z:215:ILE:HG23	3:Z:219:TYR:HB3	1.90	0.53
3:Q:310:ALA:HA	3:Q:313:ARG:HD2	1.89	0.53
2:J:129:ILE:HG12	2:J:164:LYS:HB3	1.90	0.53
3:Z:227:ASP:OD1	3:Z:230:LYS:NZ	2.37	0.53
3:Q:185:PRO:HG3	3:Q:245:GLU:HB2	1.89	0.53
3:Q:387:CYS:HB2	6:Q:504:402:C4	2.38	0.53
4:Y:111:ALA:O	4:Y:337:ASN:ND2	2.28	0.53
3:D:7:ILE:HG13	3:D:92:LEU:HB3	1.90	0.53
1:A:5:PHE:HE1	2:P:118:LYS:HD2	1.74	0.53
2:B:72:ILE:HD13	2:N:198:ASN:HB3	1.90	0.53
3:Q:185:PRO:HG2	3:Q:241:CYS:HB2	1.90	0.53
3:K:7:ILE:HG12	3:K:92:LEU:HD22	1.91	0.53
2:P:41:GLU:OE1	3:V:58:TYR:OH	2.23	0.53
4:Y:17:GLY:HA2	4:Y:336:ASN:HA	1.91	0.53
4:Y:463:ARG:O	4:Y:465:ARG:NH1	2.42	0.53
2:N:106:ALA:HB2	2:N:167:LEU:HD23	1.90	0.53
4:S:102:ALA:HB1	4:S:395:ARG:HB2	1.91	0.53
3:Z:350:LEU:HB3	3:Z:352:ILE:HD11	1.91	0.53
2:B:47:VAL:HG22	2:B:171:LEU:HD13	1.91	0.53
3:R:387:CYS:CB	6:R:503:402:C4	2.88	0.52
3:Z:247:ASP:HA	3:Z:252:ARG:HH22	1.74	0.52
3:D:313:ARG:HH12	3:D:326:ASN:H	1.57	0.52
2:P:36:GLY:HA2	2:P:71:LEU:HD11	1.92	0.52
3:Z:370:LYS:HG3	3:Z:375:LEU:HD12	1.91	0.52
1:A:43:THR:OG1	1:A:46:GLY:O	2.26	0.52
2:C:27:VAL:O	2:C:82:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:237:MET:HG3	3:K:242:LYS:HG3	1.90	0.52
4:S:69:ILE:HG22	4:S:440:VAL:HG13	1.91	0.52
3:Q:48:CYS:SG	3:Q:49:GLY:N	2.83	0.52
3:V:94:TYR:HB3	3:V:261:LEU:HD13	1.91	0.52
3:Z:114:ALA:HB2	3:Z:237:MET:HB2	1.91	0.52
2:X:71:LEU:HA	2:X:80:PRO:HA	1.92	0.52
1:A:27:HIS:NE2	5:A:204:SF4:S4	2.70	0.52
3:K:132:LEU:HG	3:K:134:PRO:HD3	1.91	0.52
3:K:142:ARG:NH2	3:K:288:ASP:OD1	2.42	0.52
2:J:46:ALA:O	2:J:50:ARG:NH1	2.42	0.52
3:R:8:ILE:HD11	3:R:240:THR:HG21	1.91	0.52
3:K:370:LYS:HG3	3:K:375:LEU:HD12	1.92	0.51
3:Q:305:GLY:O	3:Q:333:ARG:NH1	2.43	0.51
3:R:338:ILE:HD11	3:R:360:ASN:HB3	1.92	0.51
3:V:78:MET:O	3:V:96:ARG:NH1	2.42	0.51
1:A:46:GLY:H	4:Y:210:HIS:CE1	2.28	0.51
3:Q:239:CYS:HB3	3:Q:242:LYS:HG2	1.92	0.51
3:R:11:ASP:OD2	3:R:72:LYS:NZ	2.43	0.51
3:Z:236:VAL:HG11	3:Z:268:LEU:HD22	1.92	0.51
3:D:63:ASP:OD1	3:D:63:ASP:N	2.44	0.51
3:K:72:LYS:HD3	3:K:86:LEU:HD12	1.92	0.51
4:Y:391:ASN:ND2	4:Y:391:ASN:O	2.44	0.51
1:G:50:ILE:HD11	2:J:202:ALA:HB2	1.92	0.51
2:P:56:ALA:HA	3:V:397:LEU:HD12	1.92	0.51
3:K:69:ARG:NH2	3:K:84:GLU:O	2.44	0.51
3:Q:387:CYS:CB	6:Q:504:402:C4	2.89	0.51
4:S:102:ALA:O	4:S:396:ALA:N	2.41	0.51
4:S:231:ILE:HA	4:S:234:ILE:HG12	1.91	0.51
4:S:333:ARG:HB2	4:S:457:THR:HG22	1.92	0.51
3:V:116:ALA:HB3	3:V:238:PRO:HG2	1.93	0.51
3:R:132:LEU:HG	3:R:134:PRO:HD3	1.93	0.51
4:S:175:SER:H	4:S:202:ASP:HB3	1.76	0.51
4:Y:158:ASN:O	4:Y:459:ARG:NH1	2.36	0.51
3:D:117:ILE:HG22	3:D:137:LEU:HD11	1.93	0.51
4:S:153:SER:OG	4:S:570:ASP:OD2	2.29	0.51
3:K:338:ILE:HG22	3:K:355:VAL:HG12	1.91	0.50
4:S:138:LEU:O	4:S:140:HIS:N	2.44	0.50
2:P:106:ALA:HB2	2:P:167:LEU:HD23	1.91	0.50
4:S:173:ILE:HB	4:S:295:TYR:HB3	1.92	0.50
2:X:40:CYS:HB3	5:X:301:SF4:S3	2.51	0.50
2:C:48:HIS:NE2	5:C:304:SF4:S1	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:242:LYS:NZ	6:D:503:402:S2	2.77	0.50
3:R:116:ALA:HB3	3:R:238:PRO:HG2	1.92	0.50
4:Y:11:THR:HG23	4:Y:464:VAL:HG13	1.92	0.50
1:G:9:ASP:N	1:G:9:ASP:OD1	2.42	0.50
3:D:183:CYS:C	6:D:503:402:H8	2.31	0.50
4:S:120:GLN:HE22	4:S:352:PRO:HD3	1.77	0.50
4:Y:241:LYS:HZ3	4:Y:243:ASP:HB2	1.77	0.50
1:G:95:PHE:O	2:J:198:ASN:ND2	2.44	0.50
3:D:111:VAL:HG11	3:D:141:LEU:HD22	1.94	0.50
3:D:207:SER:O	3:D:211:MET:HG2	2.12	0.50
1:A:5:PHE:CE1	2:P:118:LYS:HD2	2.47	0.50
3:Z:142:ARG:NH2	3:Z:288:ASP:OD1	2.45	0.50
2:X:176:CYS:HB2	2:X:185:LEU:HD13	1.92	0.49
3:Z:282:LEU:HD12	3:Z:283:PRO:HD2	1.92	0.49
3:K:20:ARG:NH1	3:K:54:LYS:O	2.45	0.49
3:Q:266:ARG:HD3	3:Q:394:PRO:HA	1.94	0.49
3:V:285:GLU:HG2	3:V:286:GLU:H	1.77	0.49
2:B:170:ASP:N	2:B:170:ASP:OD1	2.45	0.49
3:Q:81:SER:OG	3:Q:274:ASP:OD1	2.30	0.49
3:Q:242:LYS:HB2	3:Q:262:VAL:HG21	1.95	0.49
3:R:327:ILE:HD12	3:R:327:ILE:H	1.77	0.49
1:A:6:VAL:O	1:A:51:GLN:NE2	2.46	0.49
3:Q:375:LEU:HD22	3:Q:378:VAL:HG21	1.93	0.49
4:S:151:LEU:HB3	4:S:568:ILE:HD11	1.94	0.49
4:S:254:GLU:O	4:S:580:HIS:NE2	2.46	0.49
4:Y:370:TRP:HD1	4:Y:374:LEU:HD21	1.77	0.49
2:X:36:GLY:HA2	2:X:71:LEU:HD11	1.94	0.49
4:Y:94:ILE:HG23	4:Y:395:ARG:HE	1.77	0.49
3:Z:361:VAL:HG12	3:Z:365:LEU:HB2	1.95	0.49
3:R:227:ASP:OD1	3:R:230:LYS:NZ	2.42	0.49
4:S:412:ASP:OD1	4:S:412:ASP:N	2.46	0.49
1:A:174:VAL:HG22	2:P:79:MET:HE3	1.94	0.49
3:K:123:GLU:HG2	3:K:129:LEU:HA	1.95	0.49
3:R:304:THR:OG1	3:R:339:ARG:NH2	2.45	0.49
1:A:45:GLU:OE2	2:B:207:ARG:NH1	2.46	0.48
3:K:81:SER:OG	3:K:274:ASP:OD1	2.31	0.48
2:P:129:ILE:HD11	2:P:162:ALA:HB1	1.94	0.48
4:S:192:LYS:NZ	4:S:211:LYS:O	2.46	0.48
3:D:353:ALA:HB3	3:D:378:VAL:HG22	1.95	0.48
4:Y:496:ASN:ND2	4:Y:500:GLU:OE2	2.46	0.48
3:Q:107:LEU:O	3:Q:109:LYS:NZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:103:PHE:HZ	4:Y:127:ILE:HG21	1.78	0.48
4:Y:576:GLN:NE2	4:Y:577:ASP:O	2.46	0.48
2:B:73:LYS:HZ2	2:B:78:THR:HG1	1.55	0.48
4:S:176:ASN:HB2	4:S:204:ARG:HH21	1.79	0.48
4:S:207:ALA:O	4:S:211:LYS:NZ	2.41	0.48
3:D:227:ASP:OD1	3:D:230:LYS:NZ	2.47	0.48
3:Q:128:ASP:OD1	3:Q:128:ASP:N	2.47	0.48
3:R:309:GLU:OE1	3:R:333:ARG:NH2	2.46	0.48
3:V:8:ILE:HD11	3:V:240:THR:HG21	1.96	0.48
4:S:335:GLN:HB2	4:S:338:VAL:HG23	1.95	0.48
2:J:36:GLY:HA2	2:J:71:LEU:HD11	1.95	0.48
3:Z:303:ASN:ND2	3:Z:414:TYR:OH	2.47	0.48
3:R:456:THR:OG1	3:R:458:ARG:NE	2.47	0.48
3:K:278:ASP:OD1	3:K:278:ASP:N	2.47	0.48
3:K:352:ILE:HG22	3:K:377:PHE:HB3	1.96	0.48
4:S:370:TRP:HE1	4:S:374:LEU:HD21	1.78	0.48
3:V:189:LYS:HD3	3:V:244:TYR:HE2	1.79	0.48
3:V:295:THR:HG21	3:V:425:SER:HA	1.96	0.48
4:S:289:GLN:OE1	4:S:324:ARG:NH2	2.47	0.47
1:G:28:GLU:HG3	1:G:34:PRO:HB3	1.96	0.47
3:Z:206:LYS:HE2	3:Z:453:THR:HB	1.95	0.47
3:V:316:TYR:CE2	3:V:324:ILE:HB	2.49	0.47
4:Y:81:ASP:OD1	4:Y:487:ARG:NH2	2.47	0.47
4:Y:388:ALA:HB1	4:Y:393:ARG:HB2	1.96	0.47
1:A:54:HIS:CE1	1:A:76:ILE:H	2.32	0.47
1:G:80:GLU:HG3	1:G:129:VAL:HG21	1.97	0.47
2:N:194:LYS:NZ	2:N:198:ASN:OD1	2.48	0.47
3:R:19:ARG:NH1	3:R:38:GLN:OE1	2.46	0.47
4:Y:421:LEU:HD11	4:Y:439:HIS:HB2	1.95	0.47
3:Z:295:THR:HG21	3:Z:425:SER:HA	1.97	0.47
3:K:58:TYR:OH	2:N:41:GLU:OE1	2.22	0.47
3:Q:142:ARG:NH2	3:Q:288:ASP:OD1	2.47	0.47
4:S:343:ASP:OD1	4:S:343:ASP:N	2.48	0.47
3:V:383:CYS:HB2	5:V:504:SF4:S3	2.54	0.47
2:X:56:ALA:HA	3:Z:397:LEU:HD12	1.96	0.47
4:Y:68:LEU:HB3	4:Y:75:PHE:HB3	1.97	0.47
4:Y:227:ILE:HG13	4:Y:315:LEU:HD12	1.96	0.47
4:Y:329:ILE:HG22	4:Y:331:PRO:HD3	1.95	0.47
2:C:111:GLU:O	2:C:159:ARG:NH2	2.47	0.47
1:G:17:TYR:OH	1:G:107:GLU:OE2	2.32	0.47
1:G:57:ASP:O	2:X:143:GLN:NE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:58:VAL:HB	3:V:395:LYS:HB2	1.96	0.47
3:Q:295:THR:HG21	3:Q:425:SER:HA	1.96	0.47
3:R:303:ASN:OD1	3:R:304:THR:N	2.48	0.47
4:S:351:LEU:HB3	4:S:355:LEU:HB2	1.95	0.47
3:V:322:LYS:HE3	3:V:322:LYS:HA	1.95	0.47
3:V:364:ILE:HB	3:V:375:LEU:HD11	1.97	0.47
4:Y:162:GLU:O	4:Y:165:THR:OG1	2.31	0.47
4:Y:458:GLU:O	4:Y:459:ARG:HD3	2.14	0.47
3:Z:251:MET:O	3:Z:251:MET:HG3	2.15	0.47
3:Q:217:LYS:NZ	3:Q:231:ILE:O	2.47	0.47
3:D:185:PRO:HG3	3:D:245:GLU:HB2	1.96	0.47
3:D:207:SER:HB2	3:D:209:GLN:HG3	1.96	0.47
3:D:242:LYS:HB2	3:D:262:VAL:HG21	1.95	0.47
2:P:75:GLU:OE2	2:P:76:HIS:ND1	2.48	0.47
4:S:14:PRO:HG3	4:S:447:TRP:CG	2.50	0.47
3:V:209:GLN:HE22	3:V:242:LYS:HB3	1.79	0.47
1:A:181:TYR:HE1	1:G:66:VAL:HG23	1.80	0.46
3:D:208:PRO:O	3:D:212:THR:OG1	2.26	0.46
3:Q:77:GLY:HA2	3:Q:96:ARG:HH21	1.79	0.46
4:Y:137:ARG:O	4:Y:141:ALA:CB	2.62	0.46
3:Z:102:LEU:HD23	3:Z:109:LYS:HD2	1.96	0.46
1:A:174:VAL:HG21	2:P:72:ILE:HG21	1.98	0.46
3:Z:107:LEU:O	3:Z:109:LYS:NZ	2.36	0.46
1:A:39:TYR:OH	1:A:99:ASP:OD1	2.32	0.46
1:G:174:VAL:HG22	2:X:79:MET:HE2	1.97	0.46
3:K:375:LEU:HD22	3:K:378:VAL:HG21	1.98	0.46
4:Y:321:ASN:HB3	4:Y:327:ALA:HB1	1.96	0.46
3:V:182:SER:OG	3:V:455:TYR:OH	2.27	0.46
3:V:316:TYR:HE2	3:V:324:ILE:HB	1.80	0.46
4:Y:80:TRP:HE1	4:Y:473:GLU:HB3	1.79	0.46
3:D:150:TYR:HE1	3:D:288:ASP:HB2	1.81	0.46
3:K:80:ASP:OD1	3:K:96:ARG:NH1	2.42	0.46
3:V:250:GLU:OE1	3:V:453:THR:OG1	2.33	0.46
4:Y:94:ILE:HD12	4:Y:395:ARG:HE	1.80	0.46
3:R:79:LEU:HD11	3:R:271:LEU:HD23	1.98	0.46
2:X:94:VAL:HG21	2:X:123:ALA:HB2	1.97	0.46
1:G:139:ARG:HD3	1:G:141:GLU:HB3	1.98	0.46
2:J:25:PRO:HG2	2:J:167:LEU:HD21	1.98	0.46
2:J:121:LEU:HD12	2:P:190:PRO:HB2	1.97	0.46
3:K:301:PHE:HB3	6:K:503:402:H11	1.98	0.46
2:B:118:LYS:NZ	2:N:85:HIS:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:CYS:HB3	5:D:502:SF4:S3	2.56	0.45
3:D:237:MET:HG3	3:D:242:LYS:HG3	1.96	0.45
1:G:170:ARG:HG3	2:X:81:ILE:HD11	1.98	0.45
2:P:94:VAL:HG21	2:P:123:ALA:HB2	1.98	0.45
3:Q:102:LEU:HD23	3:Q:109:LYS:HD2	1.98	0.45
3:V:91:ASN:OD1	3:V:92:LEU:N	2.50	0.45
4:Y:351:LEU:N	4:Y:355:LEU:O	2.46	0.45
1:G:8:ALA:HB2	1:G:154:LEU:HG	1.99	0.45
3:V:84:GLU:OE1	3:V:270:HIS:NE2	2.37	0.45
3:K:358:LEU:HB2	3:K:382:THR:HG23	1.97	0.45
3:K:102:LEU:HD23	3:K:109:LYS:HD2	1.98	0.45
3:Z:236:VAL:HG22	3:Z:263:ILE:HD11	1.98	0.45
1:A:158:ASP:OD1	1:A:159:GLY:N	2.41	0.45
3:D:388:ILE:O	3:D:409:ARG:NH1	2.49	0.45
3:K:111:VAL:HG11	3:K:141:LEU:HD22	1.98	0.45
2:N:133:PRO:HB3	2:N:158:PRO:HB2	1.98	0.45
4:S:351:LEU:HD23	4:S:355:LEU:HD12	1.99	0.45
4:Y:250:VAL:HG12	4:Y:575:LYS:HD3	1.99	0.45
4:Y:445:ALA:HB1	4:Y:449:GLU:HG3	1.98	0.45
3:Z:156:ALA:HB1	3:Z:301:PHE:CE2	2.51	0.45
2:B:147:LYS:HE2	2:N:103:GLU:HA	1.99	0.45
2:N:83:CYS:HB3	2:N:165:CYS:HB3	1.98	0.45
3:D:316:TYR:HE2	3:D:324:ILE:HB	1.81	0.45
1:G:41:THR:HG21	2:J:198:ASN:HB3	1.98	0.45
3:V:121:ILE:HG21	3:V:137:LEU:HD12	1.99	0.45
1:A:86:CYS:O	1:A:88:THR:N	2.45	0.45
3:D:6:ALA:HA	3:D:9:ASN:HD21	1.82	0.45
3:D:454:LYS:HE3	3:D:454:LYS:HA	1.98	0.45
3:K:56:SER:OG	2:N:38:LYS:O	2.35	0.45
3:Q:278:ASP:OD1	3:Q:278:ASP:N	2.47	0.45
4:S:351:LEU:N	4:S:355:LEU:O	2.47	0.45
3:D:301:PHE:CD1	3:D:307:VAL:HG22	2.52	0.45
3:Q:63:ASP:OD1	3:Q:63:ASP:N	2.49	0.45
4:Y:268:GLU:HG3	4:Y:275:LYS:HB3	1.98	0.45
1:G:41:THR:HG21	1:G:50:ILE:HD12	1.99	0.44
3:Z:316:TYR:O	3:Z:320:THR:HG22	2.17	0.44
3:Z:387:CYS:HB2	6:Z:504:402:C4	2.46	0.44
2:C:69:LEU:HD23	5:C:304:SF4:S4	2.57	0.44
1:G:20:ILE:HD11	1:G:40:LEU:HB2	1.98	0.44
3:Q:111:VAL:HA	3:Q:234:VAL:O	2.17	0.44
4:S:227:ILE:HD12	4:S:312:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:64:PRO:HB3	3:Z:61:TYR:HE1	1.81	0.44
1:A:87:LYS:NZ	2:B:24:ASN:O	2.45	0.44
1:A:60:CYS:HB3	1:A:69:ILE:HD13	1.99	0.44
3:D:327:ILE:HD11	3:D:423:ARG:HG3	2.00	0.44
4:Y:171:PHE:HD1	4:Y:199:ILE:HB	1.82	0.44
2:B:54:VAL:HG12	2:B:61:VAL:HG22	1.99	0.44
3:K:34:LYS:HE3	3:K:34:LYS:HA	1.99	0.44
3:R:237:MET:HG3	3:R:242:LYS:HG3	1.98	0.44
4:Y:142:PRO:O	4:Y:146:GLY:N	2.51	0.44
3:Z:358:LEU:HB2	3:Z:382:THR:HG23	1.98	0.44
3:K:53:GLN:HE22	3:K:393:GLN:HB2	1.81	0.44
2:N:36:GLY:HA3	2:N:73:LYS:HZ3	1.82	0.44
3:Q:143:ARG:HH12	3:Q:283:PRO:HD2	1.83	0.44
1:G:86:CYS:O	1:G:88:THR:N	2.49	0.44
2:N:69:LEU:HD23	5:N:304:SF4:S4	2.58	0.44
3:R:352:ILE:HG22	3:R:377:PHE:HB3	2.00	0.44
3:V:123:GLU:HG2	3:V:129:LEU:HA	2.00	0.44
3:D:69:ARG:NH1	3:D:84:GLU:O	2.51	0.44
1:G:55:CYS:HB2	1:G:58:ALA:HA	2.00	0.44
3:Q:215:ILE:HG23	3:Q:219:TYR:HB3	2.00	0.44
3:R:353:ALA:HB3	3:R:378:VAL:HG22	2.00	0.44
4:S:81:ASP:O	4:S:85:ASN:ND2	2.40	0.44
1:A:139:ARG:HD3	1:A:141:GLU:HB3	1.98	0.44
2:C:170:ASP:OD1	2:C:170:ASP:N	2.51	0.44
4:S:370:TRP:NE1	4:S:374:LEU:HD21	2.33	0.44
4:S:385:VAL:HG23	4:S:386:PRO:HD3	2.00	0.44
3:Z:111:VAL:HG11	3:Z:141:LEU:HD22	1.99	0.44
3:D:157:ASP:HA	3:D:160:ILE:HD12	2.00	0.43
3:K:187:TRP:CD1	3:K:380:VAL:HG21	2.53	0.43
4:S:273:ILE:HD11	4:S:278:LEU:HD11	2.00	0.43
3:Z:118:ARG:HG3	3:Z:119:VAL:HG13	2.00	0.43
3:Z:128:ASP:OD1	3:Z:128:ASP:N	2.50	0.43
3:K:227:ASP:OD1	3:K:230:LYS:NZ	2.47	0.43
3:Z:418:ALA:HA	3:Z:423:ARG:HH21	1.83	0.43
3:D:10:ILE:HD11	3:D:15:CYS:HB2	2.01	0.43
2:N:129:ILE:HG22	2:N:164:LYS:HB3	2.00	0.43
3:Q:178:PRO:HG2	3:Q:201:HIS:CE1	2.52	0.43
3:Q:448:HIS:HA	3:Q:452:HIS:HB2	2.00	0.43
4:S:47:LEU:HB3	5:S:801:SF4:S2	2.58	0.43
4:S:137:ARG:HH12	4:S:381:ARG:HG2	1.84	0.43
4:Y:170:ILE:HB	4:Y:198:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:32:GLY:HA3	3:V:38:GLN:HG3	2.01	0.43
1:G:170:ARG:NH2	2:X:127:GLY:O	2.40	0.43
2:N:36:GLY:HA3	2:N:73:LYS:NZ	2.34	0.43
2:P:90:PRO:HD2	5:P:302:SF4:S1	2.59	0.43
3:Z:350:LEU:HA	3:Z:376:HIS:CD2	2.53	0.43
1:G:6:VAL:HG13	1:G:51:GLN:NE2	2.34	0.43
3:R:211:MET:SD	3:R:451:LEU:HG	2.59	0.43
4:S:24:LEU:HD22	4:S:31:ILE:HD13	2.00	0.43
3:Q:114:ALA:HA	3:Q:152:THR:HG22	2.00	0.43
4:S:192:LYS:HA	4:S:196:ALA:HB3	2.01	0.43
3:Z:156:ALA:O	3:Z:160:ILE:HG12	2.18	0.43
1:A:102:VAL:HG12	1:A:104:ASP:H	1.83	0.43
2:X:27:VAL:HG23	2:X:82:GLN:NE2	2.33	0.43
4:Y:105:MET:SD	4:Y:132:VAL:HG23	2.59	0.43
3:D:361:VAL:O	3:D:365:LEU:N	2.49	0.43
2:N:146:LEU:HD23	2:N:146:LEU:HA	1.92	0.43
2:P:25:PRO:HG2	2:P:167:LEU:HD21	2.01	0.43
3:R:193:GLN:HA	3:R:459:LYS:HE3	2.00	0.43
2:X:69:LEU:HB3	2:X:82:GLN:HB3	1.99	0.43
2:C:177:VAL:O	2:C:178:LYS:HG2	2.18	0.42
2:C:193:MET:SD	2:C:197:ARG:NH1	2.91	0.42
3:D:138:VAL:HG13	3:D:285:GLU:HB2	2.01	0.42
3:D:393:GLN:OE1	3:D:409:ARG:NH1	2.51	0.42
2:N:36:GLY:HA2	2:N:71:LEU:HD11	2.01	0.42
2:N:43:ALA:HB1	2:N:175:ALA:HB1	2.01	0.42
4:S:345:GLY:HA2	4:S:350:VAL:HG13	2.01	0.42
4:Y:349:ASN:OD1	4:Y:349:ASN:N	2.51	0.42
3:Z:10:ILE:HG13	3:Z:40:ILE:HD11	2.01	0.42
2:B:203:LEU:HD23	2:B:203:LEU:HA	1.87	0.42
4:S:591:ASP:OD1	4:S:591:ASP:N	2.53	0.42
3:V:301:PHE:HB3	6:V:503:402:H11	2.01	0.42
3:D:114:ALA:O	3:D:118:ARG:NH1	2.52	0.42
3:V:114:ALA:HB3	3:V:117:ILE:HG12	2.01	0.42
2:C:41:GLU:OE2	3:Q:58:TYR:OH	2.31	0.42
3:D:142:ARG:NH2	3:D:288:ASP:OD1	2.53	0.42
3:D:238:PRO:HB3	3:D:393:GLN:HE21	1.83	0.42
3:K:58:TYR:HD2	2:N:65:VAL:HG11	1.84	0.42
2:N:133:PRO:HB2	2:N:135:TYR:HE2	1.83	0.42
3:R:27:VAL:HG21	3:R:46:VAL:HB	2.01	0.42
3:R:308:MET:HE1	3:R:352:ILE:HD12	2.00	0.42
4:S:250:VAL:HG12	4:S:575:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:26:PRO:HA	3:V:359:LYS:HE3	2.00	0.42
4:Y:125:ALA:HB2	4:Y:370:TRP:CD1	2.54	0.42
3:Z:187:TRP:CD2	3:Z:380:VAL:HG21	2.55	0.42
2:B:143:GLN:HG2	2:B:146:LEU:HD12	2.02	0.42
1:G:170:ARG:HG2	2:X:72:ILE:HD13	2.02	0.42
4:S:112:THR:OG1	4:S:115:ASP:OD1	2.22	0.42
4:Y:192:LYS:NZ	4:Y:211:LYS:O	2.52	0.42
2:B:72:ILE:HD11	2:N:202:ALA:HB2	2.00	0.42
3:D:111:VAL:HA	3:D:234:VAL:O	2.20	0.42
1:G:169:LYS:HD2	2:X:125:PRO:HA	2.02	0.42
3:Q:316:TYR:O	3:Q:320:THR:HG22	2.20	0.42
3:V:181:THR:HG21	3:V:379:GLU:HG3	2.02	0.42
3:D:156:ALA:HB3	3:D:298:ALA:HB1	2.02	0.42
2:J:101:LYS:HE2	2:J:101:LYS:HB3	1.92	0.42
3:K:94:TYR:HB3	3:K:261:LEU:HD13	2.01	0.42
3:Q:41:ASN:HB3	3:Q:44:VAL:HG12	2.01	0.42
3:V:79:LEU:HD11	3:V:271:LEU:HD23	2.01	0.42
4:Y:95:LYS:HE2	4:Y:127:ILE:HG12	2.01	0.42
2:C:65:VAL:HG11	3:Q:58:TYR:HD2	1.84	0.42
3:D:358:LEU:HD12	3:D:382:THR:HG23	2.00	0.42
3:K:7:ILE:HG23	3:K:92:LEU:HB2	2.02	0.42
4:S:233:ILE:HD13	4:S:279:ILE:HD13	2.02	0.42
4:Y:370:TRP:CD1	4:Y:374:LEU:HD21	2.55	0.42
3:Z:87:PHE:CE2	3:Z:395:LYS:HE2	2.55	0.42
2:J:76:HIS:HB2	2:P:206:LEU:HD13	2.02	0.41
4:Y:345:GLY:HA2	4:Y:350:VAL:HG13	2.01	0.41
3:V:405:ALA:N	3:V:408:LYS:HZ2	2.18	0.41
2:X:65:VAL:HG11	3:Z:58:TYR:HD2	1.85	0.41
2:P:27:VAL:HG23	2:P:82:GLN:HE21	1.85	0.41
4:Y:460:ARG:HD2	4:Y:462:GLN:HE21	1.85	0.41
3:R:112:GLN:HE21	3:R:216:ILE:HD12	1.84	0.41
4:S:11:THR:HG23	4:S:464:VAL:HG13	2.01	0.41
4:Y:124:ARG:HB3	4:Y:374:LEU:HD22	2.02	0.41
3:K:242:LYS:HB3	3:K:262:VAL:HG11	2.02	0.41
2:N:48:HIS:CE1	2:N:68:ARG:HG3	2.56	0.41
2:P:65:VAL:HG11	3:V:58:TYR:HD2	1.85	0.41
3:D:69:ARG:HH12	3:D:85:PRO:HA	1.86	0.41
2:P:95:CYS:HB2	5:P:303:SF4:S2	2.59	0.41
3:Q:237:MET:HG3	3:Q:242:LYS:HG3	2.01	0.41
4:S:95:LYS:HE2	4:S:95:LYS:HB3	1.91	0.41
4:Y:137:ARG:HE	4:Y:347:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:SER:OG	1:G:129:VAL:N	2.48	0.41
1:G:139:ARG:NH1	1:G:141:GLU:OE1	2.54	0.41
3:Q:415:LYS:HD3	3:Q:415:LYS:HA	1.90	0.41
3:V:177:LEU:O	3:V:179:MET:N	2.53	0.41
3:D:73:LEU:HD13	3:D:80:ASP:HA	2.03	0.41
3:D:118:ARG:HG3	3:D:137:LEU:HD13	2.01	0.41
3:R:46:VAL:HG12	5:R:502:SF4:S4	2.61	0.41
3:V:198:LEU:HD13	3:V:370:LYS:HZ3	1.86	0.41
3:V:245:GLU:O	3:V:251:MET:HG2	2.20	0.41
4:Y:359:LYS:HE3	4:Y:359:LYS:HB2	1.86	0.41
3:Z:411:GLU:O	3:Z:415:LYS:HG2	2.21	0.41
3:D:278:ASP:OD1	3:D:278:ASP:N	2.45	0.41
1:G:143:PRO:HB3	5:G:204:SF4:S1	2.61	0.41
3:K:388:ILE:O	3:K:409:ARG:NH1	2.54	0.41
3:Q:184:CYS:HB3	3:Q:187:TRP:CE2	2.55	0.41
3:Q:211:MET:SD	3:Q:451:LEU:HG	2.61	0.41
3:R:316:TYR:O	3:R:320:THR:HG22	2.20	0.41
4:S:71:LYS:HA	4:S:71:LYS:HD2	1.83	0.41
4:S:252:PHE:HE1	4:S:318:ILE:HD11	1.85	0.41
4:S:550:THR:O	4:S:567:CYS:HB3	2.21	0.41
4:Y:122:PHE:CD2	4:Y:481:PHE:HB3	2.50	0.41
3:Z:69:ARG:NH2	3:Z:84:GLU:O	2.54	0.41
3:Z:99:LYS:HE3	3:Z:275:LYS:HE2	2.03	0.41
3:Z:178:PRO:HB3	3:Z:375:LEU:HB2	2.02	0.41
3:D:237:MET:HA	3:D:238:PRO:HD3	1.94	0.41
2:J:118:LYS:HE3	2:P:26:PHE:CE1	2.56	0.41
2:N:111:GLU:O	2:N:159:ARG:NH2	2.54	0.41
3:R:102:LEU:HD11	3:R:145:ASN:HB2	2.03	0.41
3:R:111:VAL:HG13	3:R:149:VAL:HG23	2.02	0.41
4:S:122:PHE:HE2	4:S:482:SER:HA	1.86	0.41
4:Y:256:ALA:HA	4:Y:259:VAL:HG22	2.03	0.41
4:Y:502:TRP:NE1	4:Y:516:ILE:O	2.48	0.41
1:G:47:ILE:HD13	4:S:207:ALA:HA	2.01	0.40
3:R:117:ILE:HG22	3:R:137:LEU:HD11	2.02	0.40
4:S:17:GLY:O	4:S:457:THR:HG23	2.21	0.40
4:S:306:THR:OG1	4:S:307:GLY:N	2.54	0.40
4:Y:173:ILE:HD13	4:Y:201:ALA:HB3	2.02	0.40
4:Y:356:ASP:HB3	4:Y:358:THR:HG22	2.02	0.40
3:Z:218:THR:HG21	3:Z:450:LEU:HD13	2.03	0.40
1:A:6:VAL:HG13	1:A:51:GLN:NE2	2.35	0.40
3:D:53:GLN:NE2	3:D:393:GLN:O	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:316:TYR:CE2	3:D:324:ILE:HB	2.56	0.40
2:J:47:VAL:HG22	2:J:171:LEU:HD22	2.02	0.40
3:R:91:ASN:OD1	3:R:92:LEU:N	2.55	0.40
3:V:156:ALA:HB1	3:V:301:PHE:CE2	2.56	0.40
3:V:229:ALA:HA	3:V:256:TYR:HE2	1.86	0.40
4:Y:591:ASP:N	4:Y:591:ASP:OD1	2.55	0.40
3:R:413:LEU:HD23	3:R:413:LEU:HA	1.93	0.40
3:R:138:VAL:HG13	3:R:285:GLU:HB2	2.03	0.40
3:R:426:HIS:O	3:R:426:HIS:ND1	2.54	0.40
4:Y:231:ILE:HA	4:Y:234:ILE:HG12	2.03	0.40
3:K:179:MET:SD	3:K:203:SER:HB2	2.62	0.40
3:K:237:MET:HA	3:K:238:PRO:HD3	1.97	0.40
2:N:45:PHE:CD2	2:N:65:VAL:HG23	2.57	0.40
3:Q:156:ALA:HB1	3:Q:301:PHE:CE2	2.56	0.40
3:R:162:GLU:OE1	3:R:452:HIS:NE2	2.55	0.40
3:V:387:CYS:HB2	6:V:503:402:C4	2.50	0.40
4:Y:412:ASP:N	4:Y:412:ASP:OD1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	170/184 (92%)	162 (95%)	8 (5%)	0	100	100
1	G	170/184 (92%)	159 (94%)	9 (5%)	2 (1%)	13	41
2	B	179/210 (85%)	169 (94%)	10 (6%)	0	100	100
2	C	179/210 (85%)	166 (93%)	13 (7%)	0	100	100
2	J	179/210 (85%)	171 (96%)	8 (4%)	0	100	100
2	N	179/210 (85%)	172 (96%)	7 (4%)	0	100	100
2	P	179/210 (85%)	173 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	179/210 (85%)	172 (96%)	7 (4%)	0	100	100
3	D	444/461 (96%)	419 (94%)	25 (6%)	0	100	100
3	K	444/461 (96%)	420 (95%)	24 (5%)	0	100	100
3	Q	444/461 (96%)	420 (95%)	24 (5%)	0	100	100
3	R	444/461 (96%)	419 (94%)	25 (6%)	0	100	100
3	V	444/461 (96%)	413 (93%)	31 (7%)	0	100	100
3	Z	444/461 (96%)	420 (95%)	24 (5%)	0	100	100
4	S	561/743 (76%)	527 (94%)	34 (6%)	0	100	100
4	Y	561/743 (76%)	534 (95%)	27 (5%)	0	100	100
All	All	5200/5880 (88%)	4916 (94%)	282 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	58	ALA
1	G	59	PRO

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 PDB entries followed by that with respect to all EM entries.

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	151/161 (94%)	151 (100%)	0	100	100
1	G	151/161 (94%)	151 (100%)	0	100	100
2	B	154/179 (86%)	154 (100%)	0	100	100
2	C	154/179 (86%)	154 (100%)	0	100	100
2	J	154/179 (86%)	154 (100%)	0	100	100
2	N	154/179 (86%)	154 (100%)	0	100	100
2	P	154/179 (86%)	154 (100%)	0	100	100
2	X	154/179 (86%)	154 (100%)	0	100	100
3	D	384/396 (97%)	383 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	384/396 (97%)	383 (100%)	1 (0%)	92	97
3	Q	384/396 (97%)	383 (100%)	1 (0%)	92	97
3	R	384/396 (97%)	380 (99%)	4 (1%)	76	88
3	V	384/396 (97%)	383 (100%)	1 (0%)	92	97
3	Z	384/396 (97%)	384 (100%)	0	100	100
4	S	470/616 (76%)	468 (100%)	2 (0%)	91	95
4	Y	470/616 (76%)	468 (100%)	2 (0%)	91	95
All	All	4470/5004 (89%)	4458 (100%)	12 (0%)	92	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	322	LYS
3	K	459	LYS
3	Q	372	LYS
3	R	76	ARG
3	R	322	LYS
3	R	458	ARG
3	R	459	LYS
4	S	308	ASN
4	S	368	LYS
3	V	69	ARG
4	Y	391	ASN
4	Y	459	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	209	GLN
3	D	376	HIS
3	K	53	GLN
2	P	143	GLN
3	Q	210	GLN
4	Y	206	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

58 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	$\#\|Z\| > 2$
5	SF4	X	304	2	0,12,12	-	-	-		
5	SF4	N	301	2	0,12,12	-	-	-		
5	SF4	C	303	2	0,12,12	-	-	-		
5	SF4	G	204	1	0,12,12	-	-	-		
5	SF4	N	303	2	0,12,12	-	-	-		
5	SF4	P	304	2	0,12,12	-	-	-		
5	SF4	Y	801	4	0,12,12	-	-	-		
5	SF4	V	502	3	0,12,12	-	-	-		
5	SF4	A	202	1	0,12,12	-	-	-		
5	SF4	G	201	1	0,12,12	-	-	-		
6	402	K	503	3	13,19,19	2.55	10 (76%)	2,36,36	0.79	0
5	SF4	B	301	2	0,12,12	-	-	-		
5	SF4	D	502	3	0,12,12	-	-	-		
5	SF4	B	303	2	0,12,12	-	-	-		
5	SF4	X	303	2	0,12,12	-	-	-		
5	SF4	G	202	1	0,12,12	-	-	-		
5	SF4	P	302	2	0,12,12	-	-	-		
5	SF4	Z	501	3	0,12,12	-	-	-		
5	SF4	B	302	2	0,12,12	-	-	-		
6	402	R	503	3	13,19,19	2.50	9 (69%)	2,36,36	0.88	0
5	SF4	A	204	1	0,12,12	-	-	-		
5	SF4	J	302	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SF4	R	501	3	0,12,12	-	-	-		
5	SF4	B	304	2	0,12,12	-	-	-		
5	SF4	Z	503	3	0,12,12	-	-	-		
6	402	V	503	5,3	13,19,19	2.51	9 (69%)	2,36,36	1.00	0
5	SF4	G	203	1	0,12,12	-	-	-		
5	SF4	D	504	3	0,12,12	-	-	-		
5	SF4	V	504	3,6	0,12,12	-	-	-		
5	SF4	Q	502	3	0,12,12	-	-	-		
5	SF4	X	302	2	0,12,12	-	-	-		
5	SF4	P	303	2	0,12,12	-	-	-		
5	SF4	X	301	2	0,12,12	-	-	-		
5	SF4	J	303	2	0,12,12	-	-	-		
5	SF4	N	302	2	0,12,12	-	-	-		
5	SF4	A	201	1	0,12,12	-	-	-		
5	SF4	K	501	3	0,12,12	-	-	-		
6	402	Z	504	3	13,19,19	2.52	9 (69%)	2,36,36	0.79	0
5	SF4	J	304	2	0,12,12	-	-	-		
5	SF4	C	304	2	0,12,12	-	-	-		
5	SF4	R	502	3	0,12,12	-	-	-		
5	SF4	N	304	2	0,12,12	-	-	-		
5	SF4	D	501	3	0,12,12	-	-	-		
6	402	D	503	3	13,19,19	2.38	8 (61%)	2,36,36	0.72	0
5	SF4	K	504	3	0,12,12	-	-	-		
5	SF4	C	302	2	0,12,12	-	-	-		
6	402	Q	504	3	13,19,19	2.53	9 (69%)	2,36,36	0.69	0
5	SF4	Z	502	3	0,12,12	-	-	-		
5	SF4	J	301	2	0,12,12	-	-	-		
5	SF4	K	502	3	0,12,12	-	-	-		
5	SF4	P	301	2	0,12,12	-	-	-		
5	SF4	Q	501	3	0,12,12	-	-	-		
5	SF4	R	504	3	0,12,12	-	-	-		
5	SF4	A	203	1	0,12,12	-	-	-		
5	SF4	V	501	3	0,12,12	-	-	-		
5	SF4	Q	503	3	0,12,12	-	-	-		
5	SF4	C	301	2	0,12,12	-	-	-		
5	SF4	S	801	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	X	304	2	-	-	0/6/5/5
5	SF4	N	301	2	-	-	0/6/5/5
5	SF4	C	303	2	-	-	0/6/5/5
5	SF4	G	204	1	-	-	0/6/5/5
5	SF4	N	303	2	-	-	0/6/5/5
5	SF4	P	304	2	-	-	0/6/5/5
5	SF4	Y	801	4	-	-	0/6/5/5
5	SF4	V	502	3	-	-	0/6/5/5
5	SF4	A	202	1	-	-	0/6/5/5
5	SF4	G	201	1	-	-	0/6/5/5
6	402	K	503	3	-	-	0/5/3/3
5	SF4	B	301	2	-	-	0/6/5/5
5	SF4	D	502	3	-	-	0/6/5/5
5	SF4	B	303	2	-	-	0/6/5/5
5	SF4	X	303	2	-	-	0/6/5/5
5	SF4	G	202	1	-	-	0/6/5/5
5	SF4	P	302	2	-	-	0/6/5/5
5	SF4	Z	501	3	-	-	0/6/5/5
5	SF4	B	302	2	-	-	0/6/5/5
6	402	R	503	3	-	-	0/5/3/3
5	SF4	A	204	1	-	-	0/6/5/5
5	SF4	J	302	2	-	-	0/6/5/5
5	SF4	R	501	3	-	-	0/6/5/5
5	SF4	B	304	2	-	-	0/6/5/5
5	SF4	Z	503	3	-	-	0/6/5/5
6	402	V	503	5,3	-	-	0/5/3/3
5	SF4	G	203	1	-	-	0/6/5/5
5	SF4	D	504	3	-	-	0/6/5/5
5	SF4	V	504	3,6	-	-	0/6/5/5
5	SF4	Q	502	3	-	-	0/6/5/5
5	SF4	X	302	2	-	-	0/6/5/5
5	SF4	P	303	2	-	-	0/6/5/5
5	SF4	X	301	2	-	-	0/6/5/5
5	SF4	J	303	2	-	-	0/6/5/5
5	SF4	N	302	2	-	-	0/6/5/5
5	SF4	A	201	1	-	-	0/6/5/5
5	SF4	K	501	3	-	-	0/6/5/5
6	402	Z	504	3	-	-	0/5/3/3
5	SF4	J	304	2	-	-	0/6/5/5
5	SF4	C	304	2	-	-	0/6/5/5
5	SF4	R	502	3	-	-	0/6/5/5
5	SF4	N	304	2	-	-	0/6/5/5
5	SF4	D	501	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	402	D	503	3	-	-	0/5/3/3
5	SF4	K	504	3	-	-	0/6/5/5
5	SF4	C	302	2	-	-	0/6/5/5
6	402	Q	504	3	-	-	0/5/3/3
5	SF4	Z	502	3	-	-	0/6/5/5
5	SF4	J	301	2	-	-	0/6/5/5
5	SF4	K	502	3	-	-	0/6/5/5
5	SF4	P	301	2	-	-	0/6/5/5
5	SF4	Q	501	3	-	-	0/6/5/5
5	SF4	R	504	3	-	-	0/6/5/5
5	SF4	A	203	1	-	-	0/6/5/5
5	SF4	V	501	3	-	-	0/6/5/5
5	SF4	Q	503	3	-	-	0/6/5/5
5	SF4	C	301	2	-	-	0/6/5/5
5	SF4	S	801	4	-	-	0/6/5/5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	503	402	S1-FE2	3.21	2.30	2.26
6	V	503	402	C4-N4	3.14	1.20	1.15
6	R	503	402	C4-N4	3.08	1.20	1.15
6	Q	504	402	C4-N4	3.06	1.20	1.15
6	Z	504	402	C4-N4	3.03	1.20	1.15
6	V	503	402	C3-FE1	-3.02	1.70	1.79
6	K	503	402	C4-N4	3.02	1.20	1.15
6	R	503	402	C3-FE1	-2.97	1.70	1.79
6	Z	504	402	C3-FE1	-2.96	1.70	1.79
6	Q	504	402	C2-S2	2.95	1.90	1.85
6	D	503	402	C4-N4	2.94	1.20	1.15
6	K	503	402	S1-FE2	2.94	2.30	2.26
6	D	503	402	C3-FE1	-2.94	1.70	1.79
6	K	503	402	S1-FE1	2.92	2.30	2.26
6	V	503	402	C6-N6	-2.92	1.10	1.15
6	Q	504	402	C3-FE1	-2.91	1.70	1.79
6	Q	504	402	S1-FE2	2.90	2.30	2.26
6	Z	504	402	S2-FE2	2.90	2.30	2.26
6	D	503	402	C2-S2	2.90	1.90	1.85
6	K	503	402	C3-FE1	-2.88	1.70	1.79
6	K	503	402	S2-FE1	2.88	2.30	2.26
6	R	503	402	S2-FE2	2.86	2.30	2.26
6	Z	504	402	S1-FE2	2.86	2.30	2.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	503	402	C2-S2	2.86	1.90	1.85
6	V	503	402	S2-FE2	2.85	2.30	2.26
6	Z	504	402	C2-S2	2.85	1.90	1.85
6	Q	504	402	S1-FE1	2.84	2.30	2.26
6	Z	504	402	S2-FE1	2.84	2.30	2.26
6	Q	504	402	S2-FE1	2.83	2.30	2.26
6	R	503	402	C6-N6	-2.82	1.10	1.15
6	V	503	402	C2-S2	2.81	1.90	1.85
6	K	503	402	S2-FE2	2.80	2.30	2.26
6	Z	504	402	C6-N6	-2.78	1.10	1.15
6	R	503	402	S1-FE2	2.78	2.30	2.26
6	R	503	402	C2-S2	2.78	1.90	1.85
6	Q	504	402	C6-N6	-2.76	1.10	1.15
6	Q	504	402	S2-FE2	2.76	2.30	2.26
6	V	503	402	S1-FE2	2.72	2.30	2.26
6	K	503	402	C6-N6	-2.72	1.10	1.15
6	R	503	402	S1-FE1	2.72	2.30	2.26
6	V	503	402	C1-S1	-2.71	1.80	1.85
6	D	503	402	C1-S1	-2.70	1.80	1.85
6	Z	504	402	C1-S1	-2.69	1.80	1.85
6	V	503	402	S2-FE1	2.67	2.30	2.26
6	V	503	402	S1-FE1	2.67	2.30	2.26
6	D	503	402	S1-FE1	2.66	2.30	2.26
6	R	503	402	S2-FE1	2.63	2.30	2.26
6	D	503	402	S2-FE1	2.63	2.30	2.26
6	R	503	402	C1-S1	-2.61	1.80	1.85
6	Q	504	402	C1-S1	-2.58	1.80	1.85
6	K	503	402	C1-S1	-2.57	1.80	1.85
6	D	503	402	S2-FE2	2.56	2.30	2.26
6	Z	504	402	S1-FE1	2.40	2.29	2.26
6	K	503	402	O5-C5	2.09	1.21	1.17

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 33 short contacts:

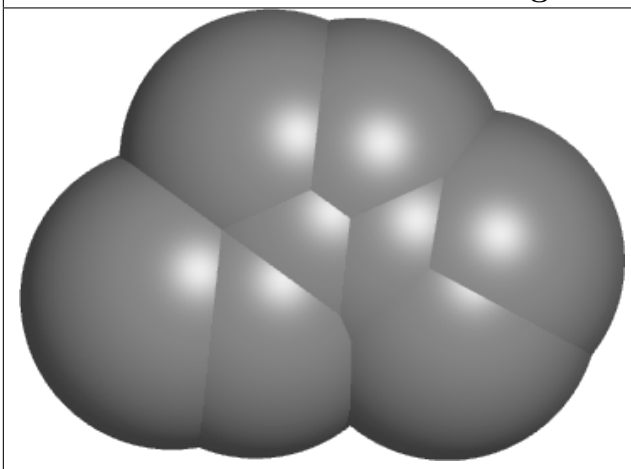
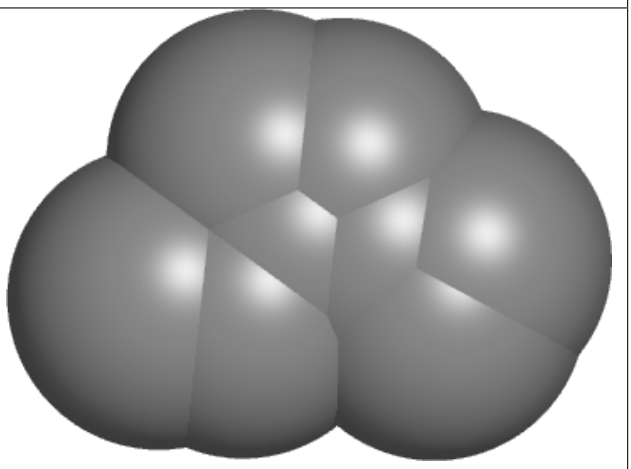
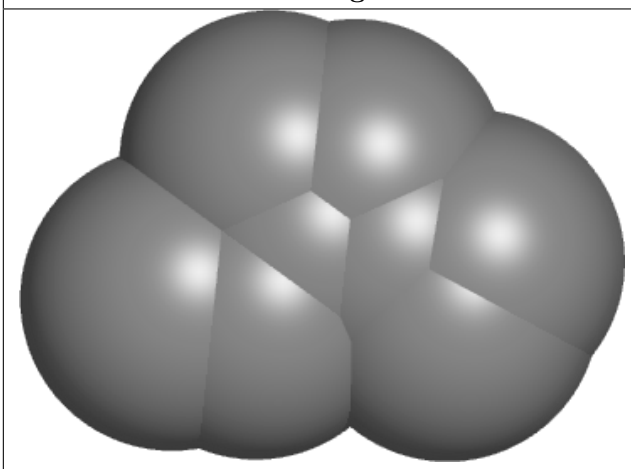
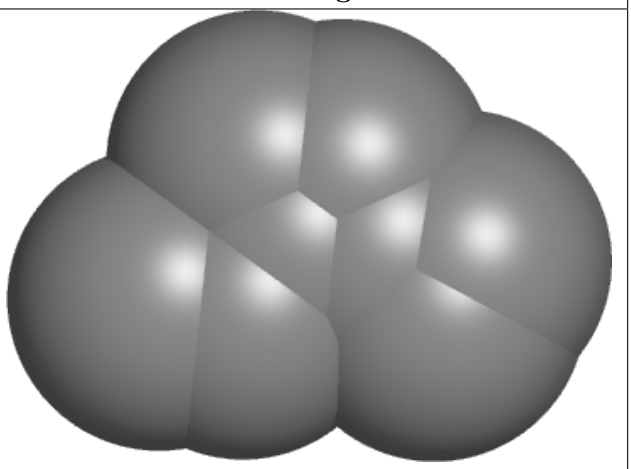
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	204	SF4	1	0
5	Y	801	SF4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	503	402	1	0
5	D	502	SF4	1	0
5	P	302	SF4	1	0
6	R	503	402	2	0
5	A	204	SF4	1	0
5	B	304	SF4	1	0
5	Z	503	SF4	1	0
6	V	503	402	3	0
5	V	504	SF4	2	0
5	P	303	SF4	1	0
5	X	301	SF4	1	0
5	A	201	SF4	1	0
6	Z	504	402	3	0
5	C	304	SF4	2	0
5	R	502	SF4	1	0
5	N	304	SF4	1	0
6	D	503	402	3	0
5	K	504	SF4	1	0
6	Q	504	402	2	0
5	S	801	SF4	2	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 SF4 X 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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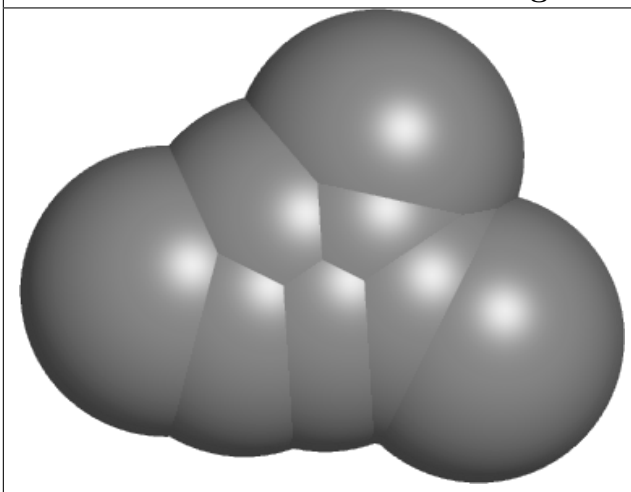
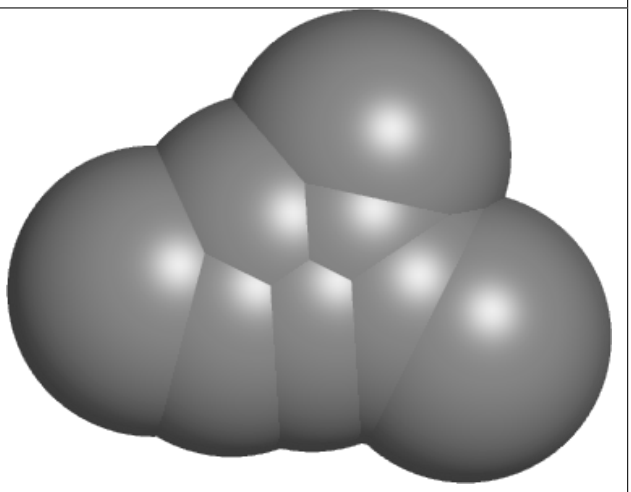
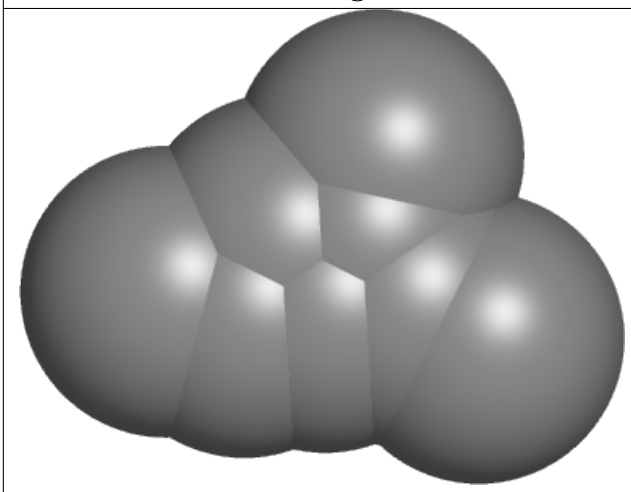
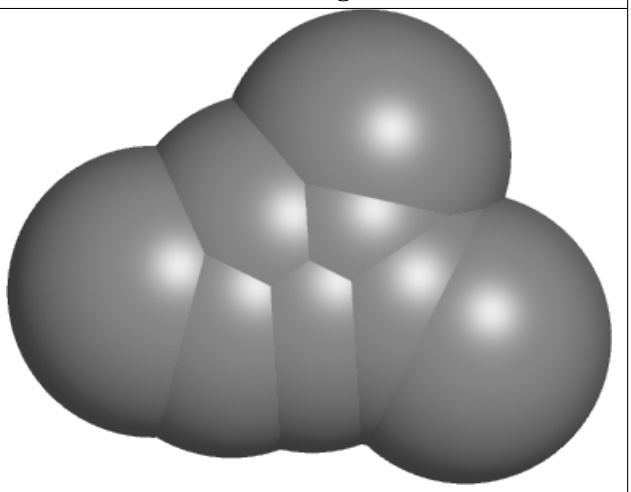
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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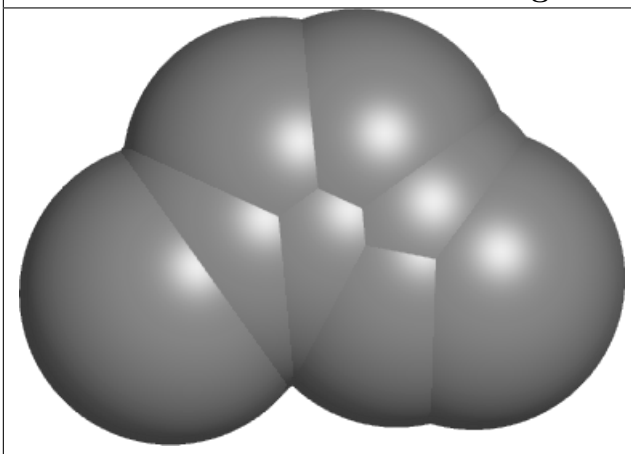
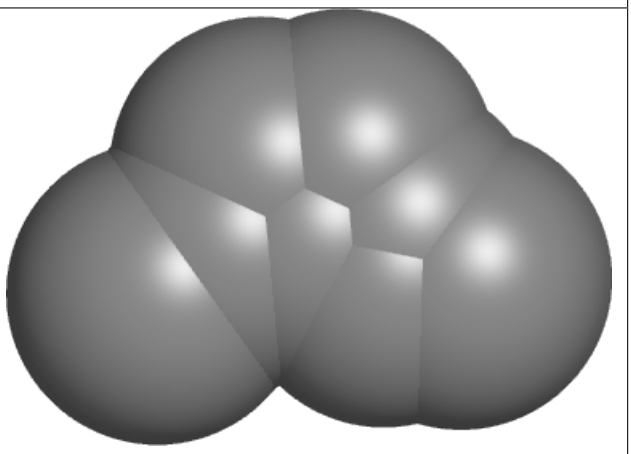
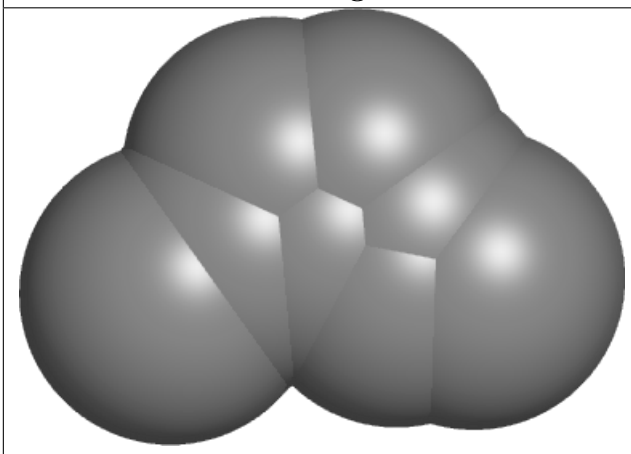
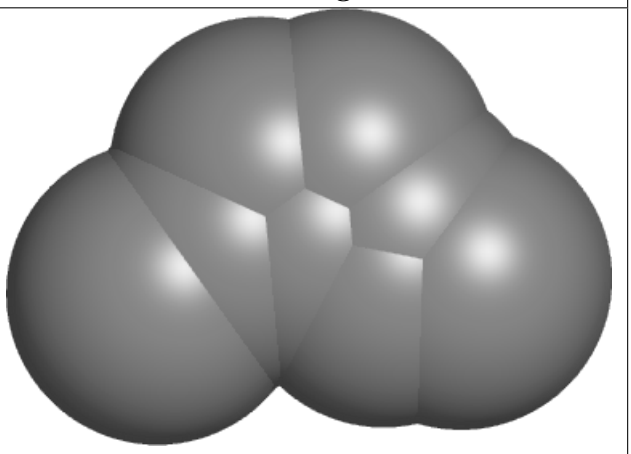
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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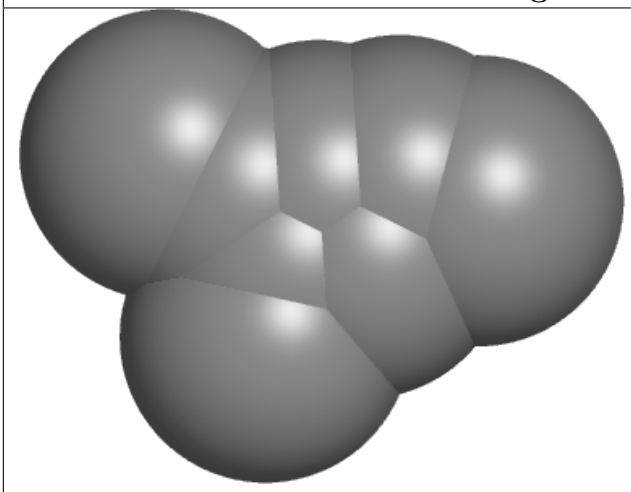
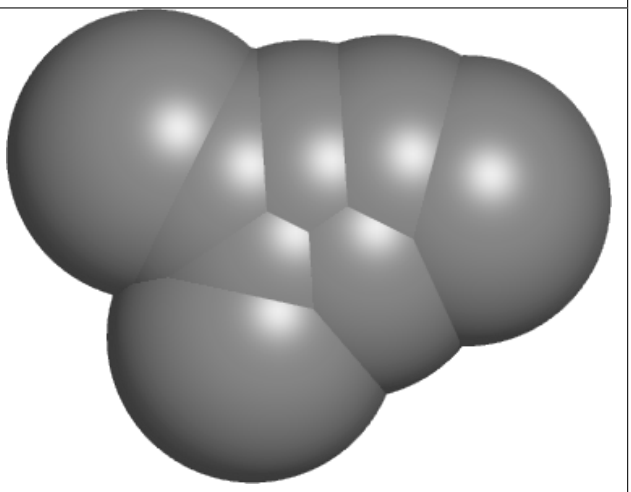
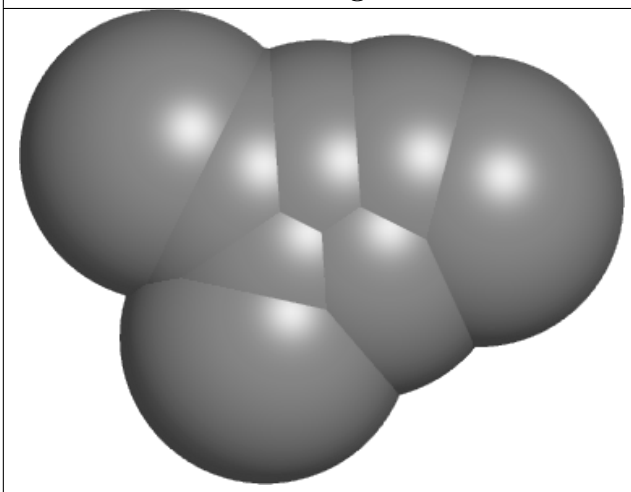
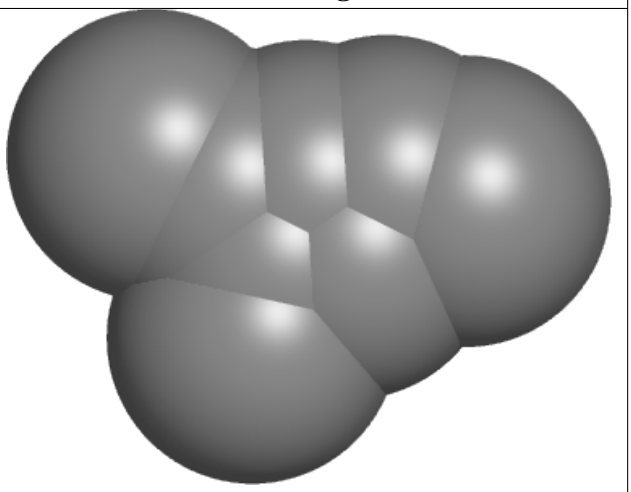
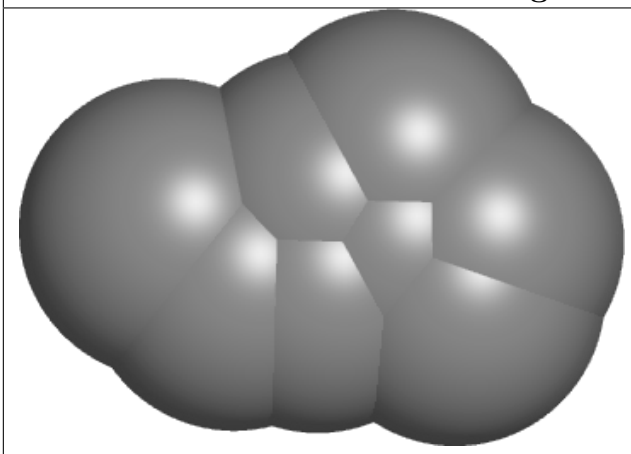
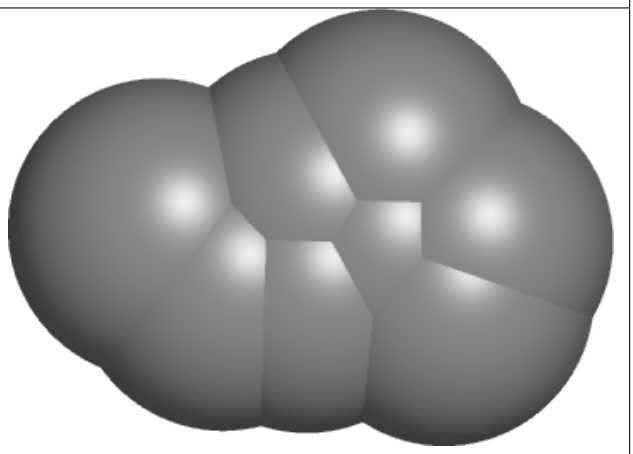
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

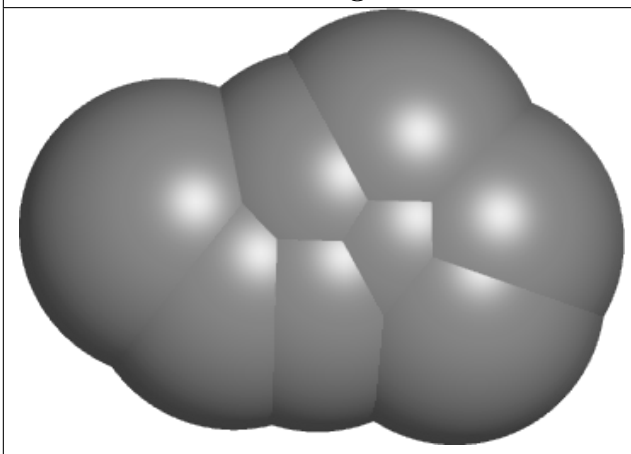
Ligand SF4 N 303



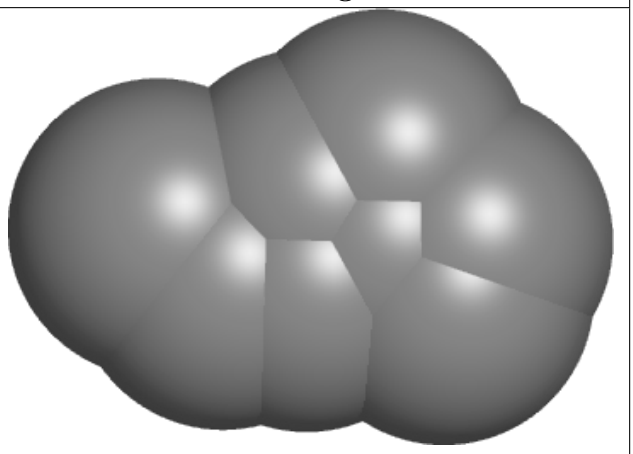
Bond lengths



Bond angles



Torsions



Rings

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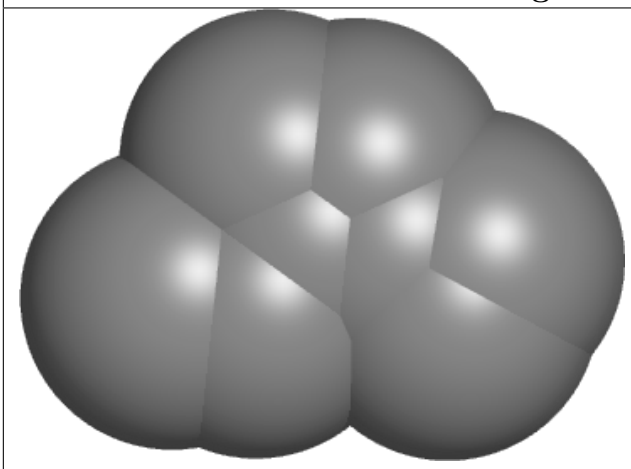
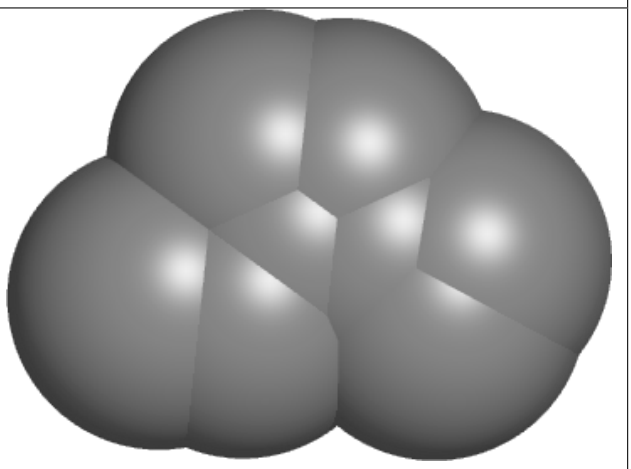
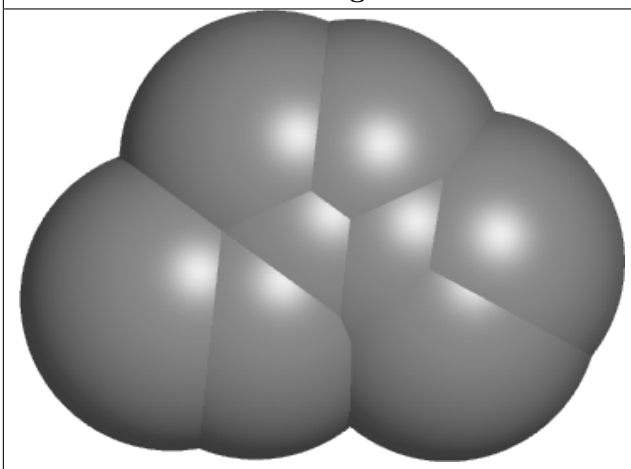
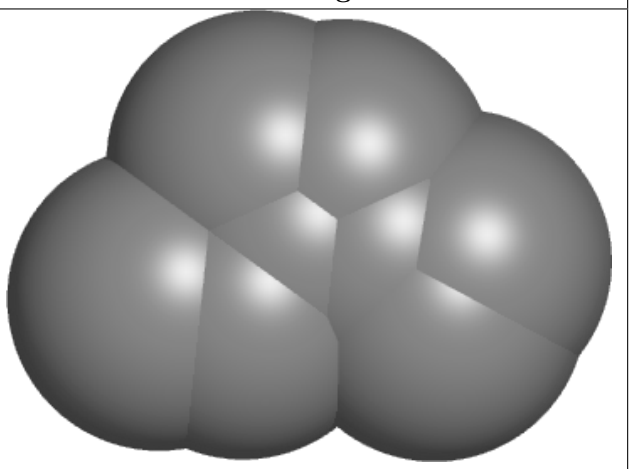
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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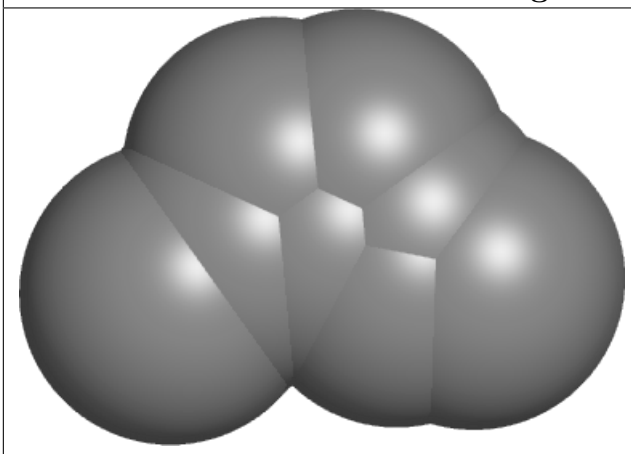
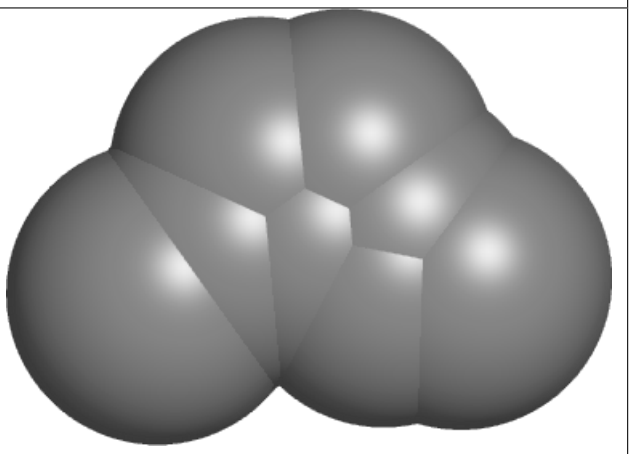
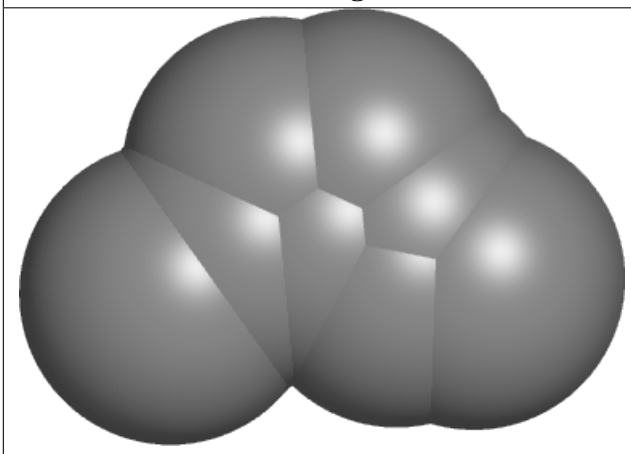
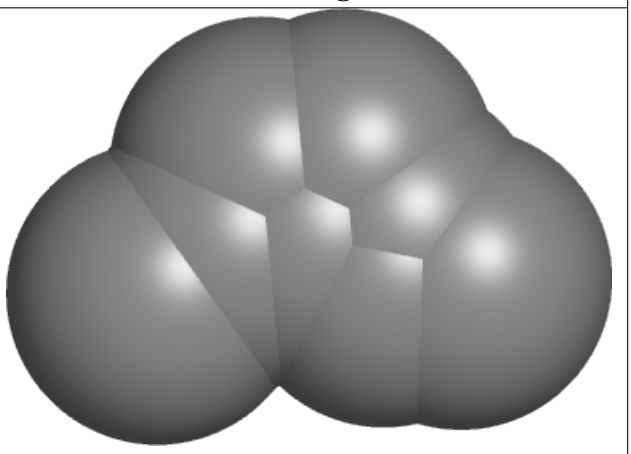
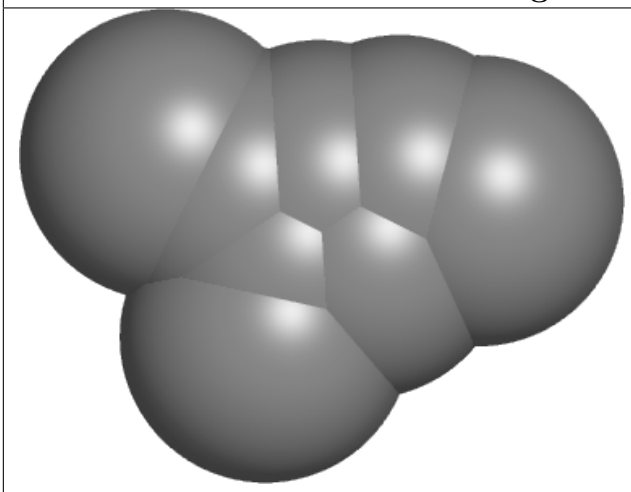
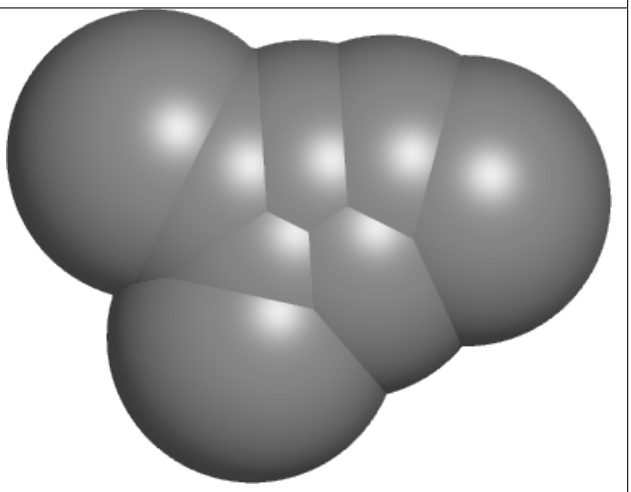
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

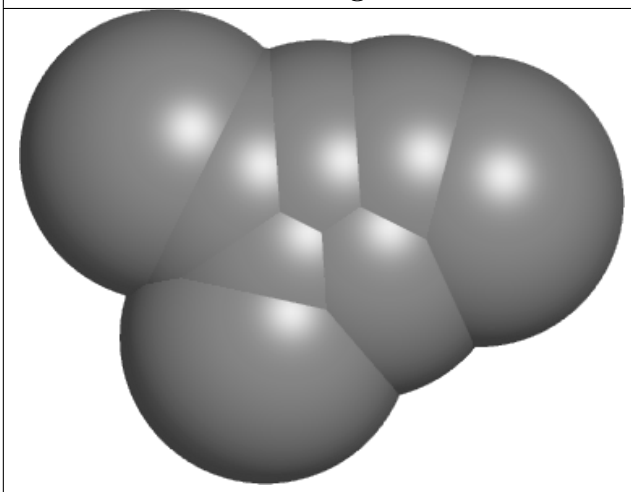
Ligand SF4 V 502



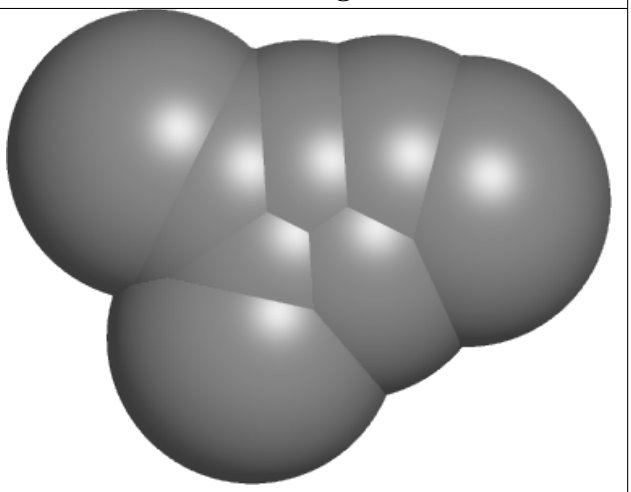
Bond lengths



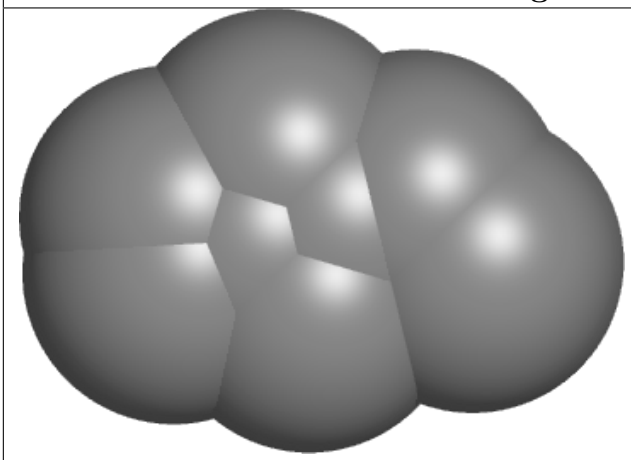
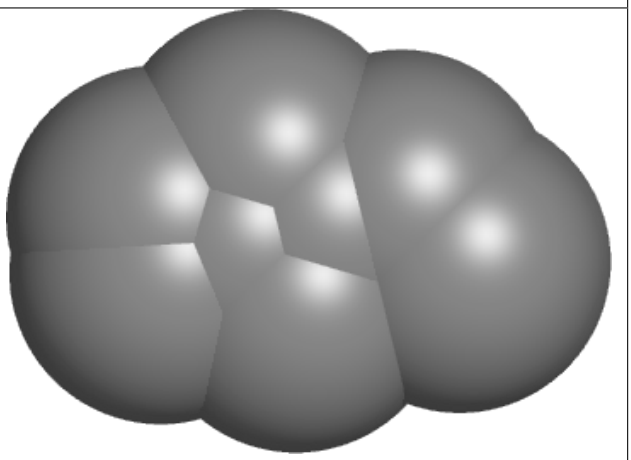
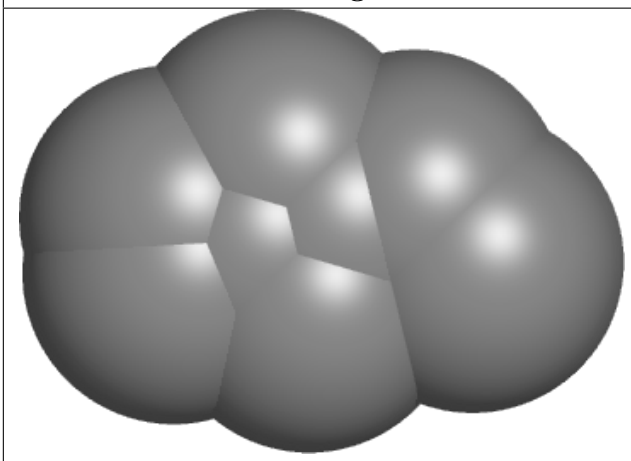
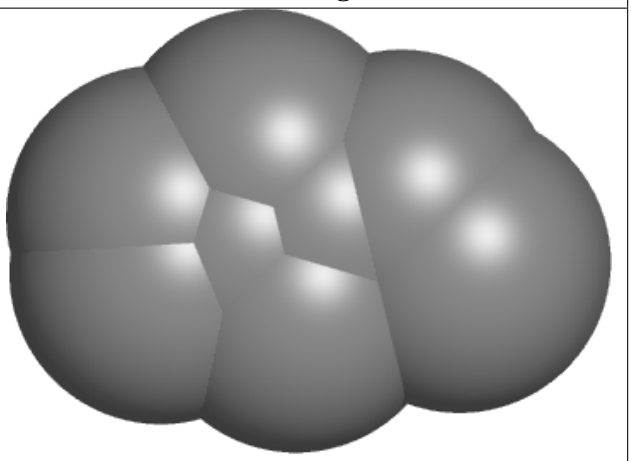
Bond angles



Torsions



Rings

Ligand SF4 A 202	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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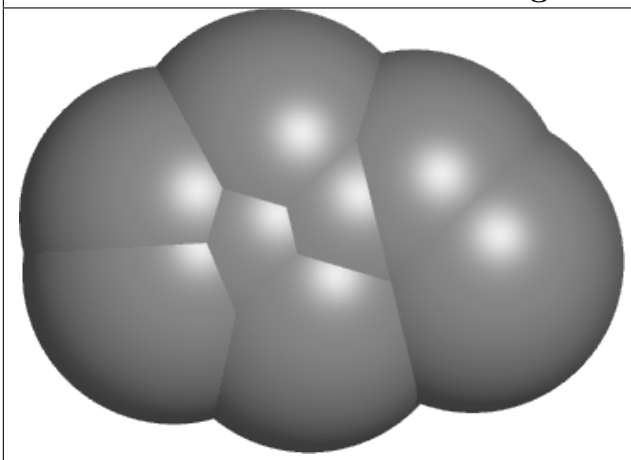
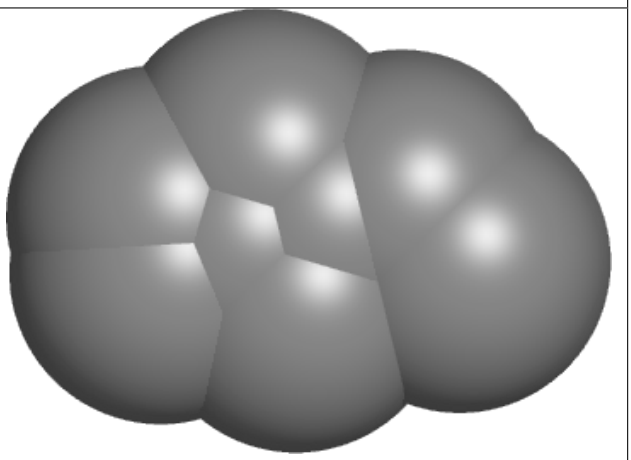
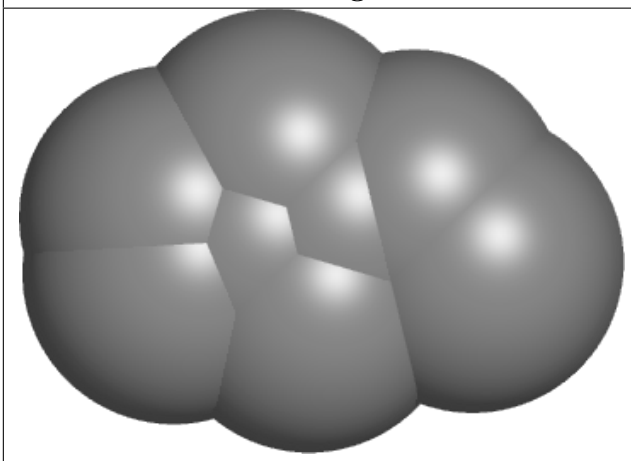
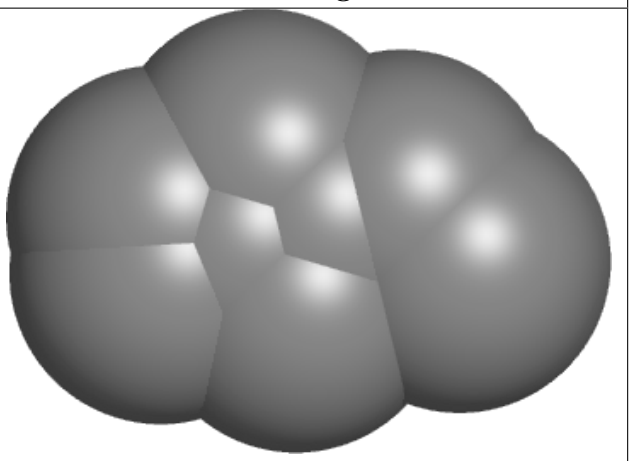
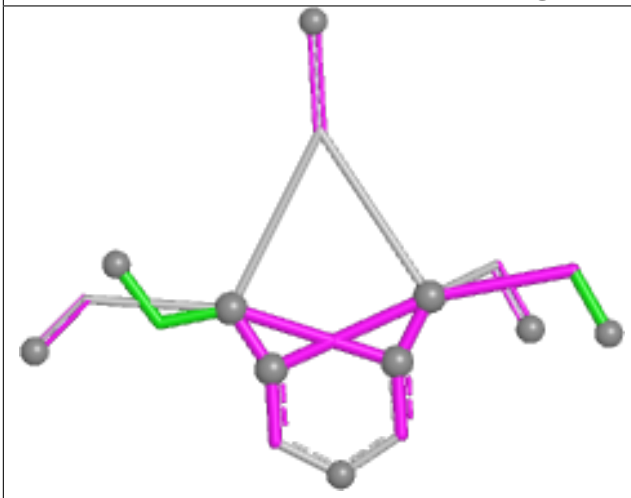
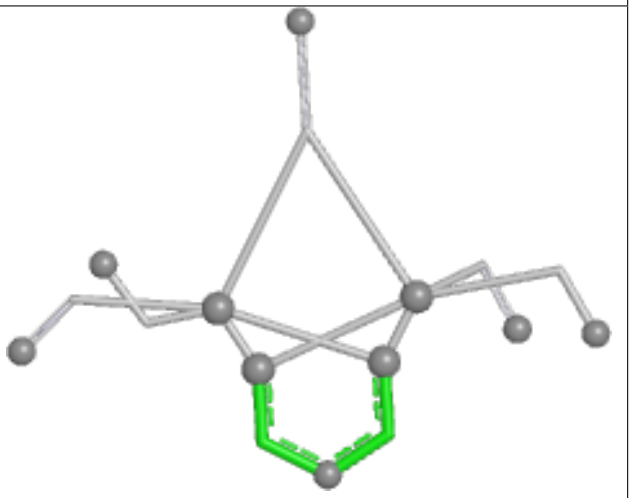
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

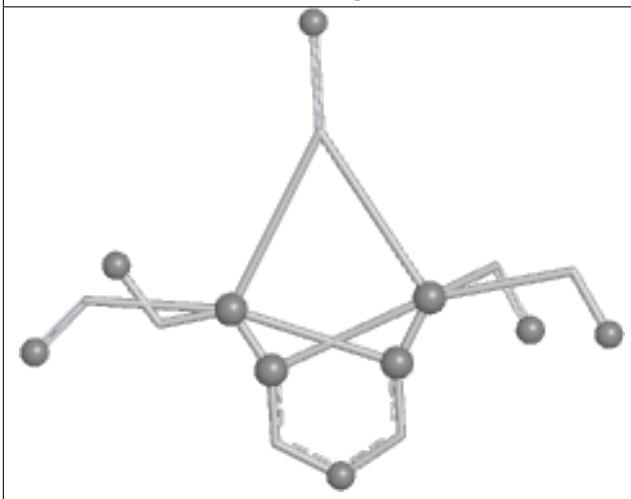
Ligand 402 K 503



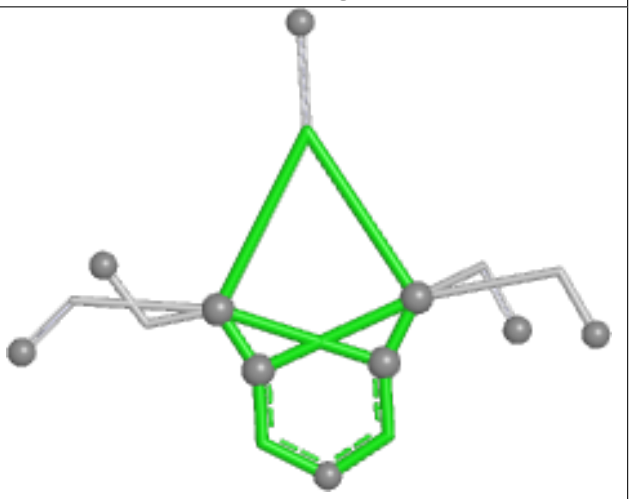
Bond lengths



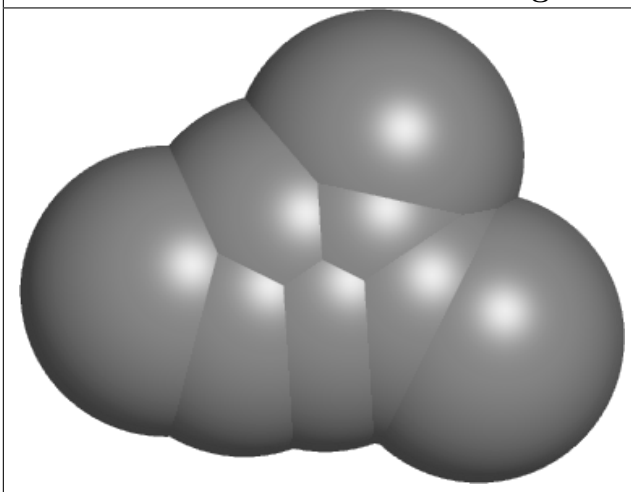
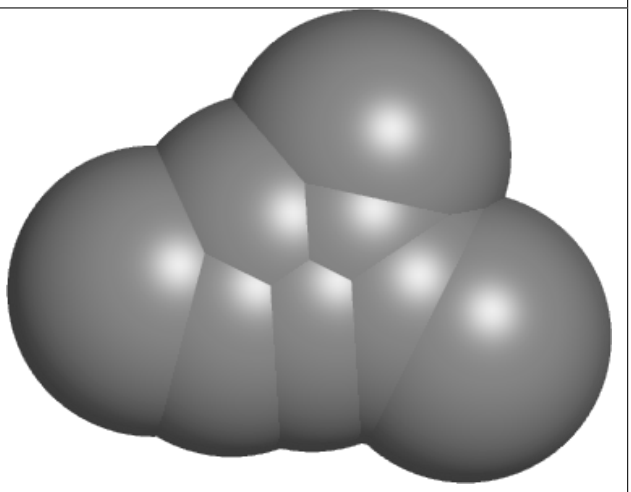
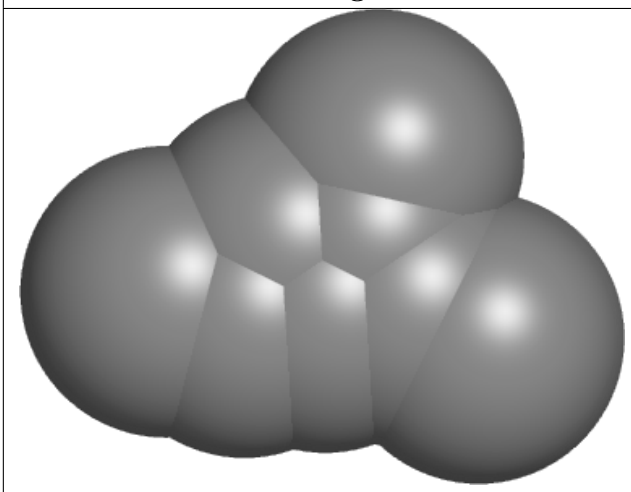
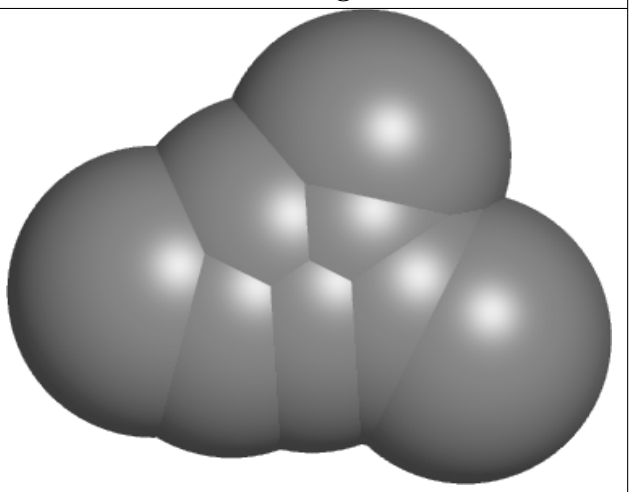
Bond angles

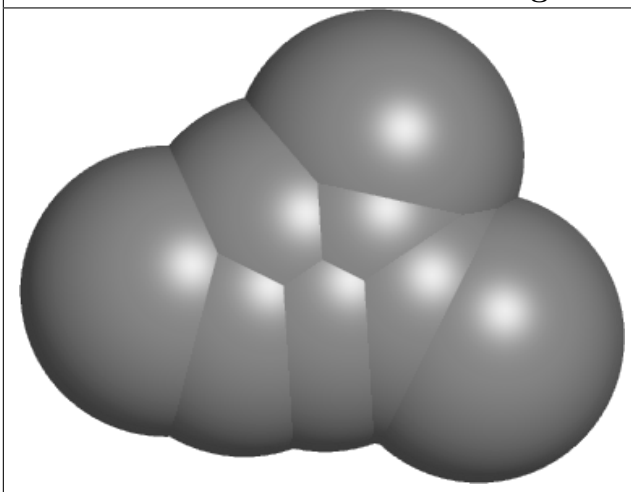
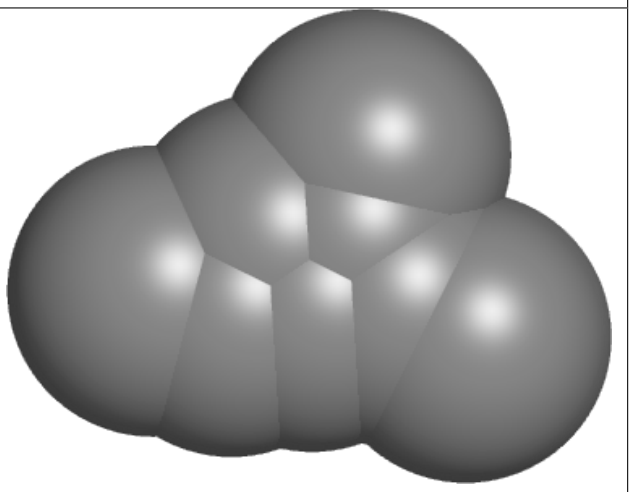
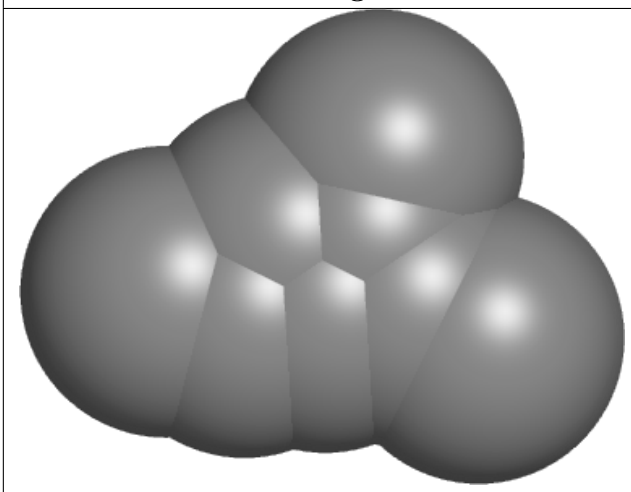
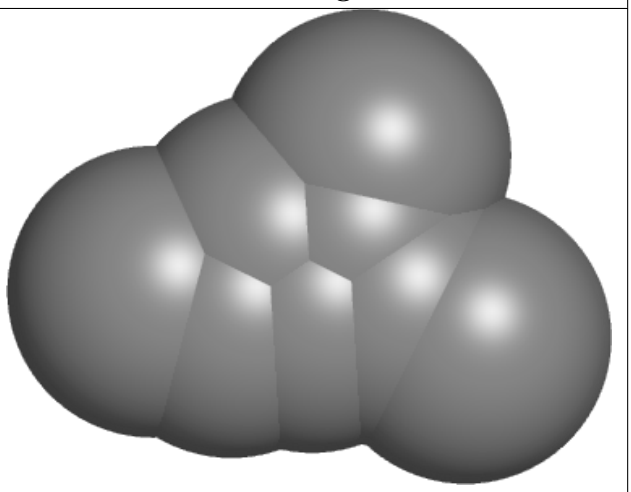


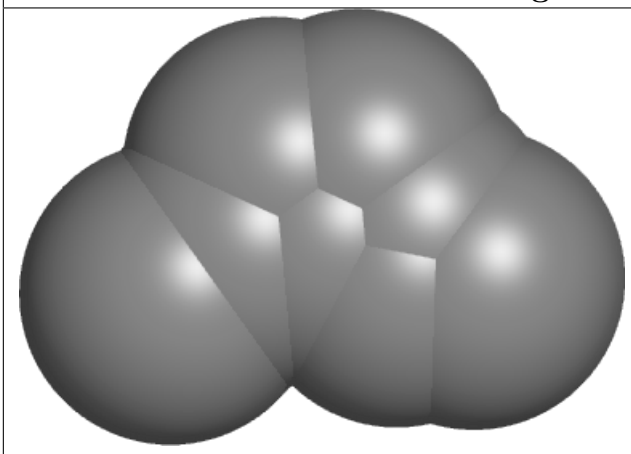
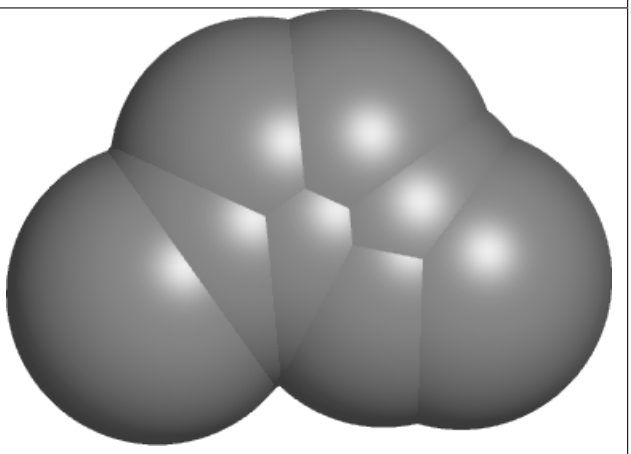
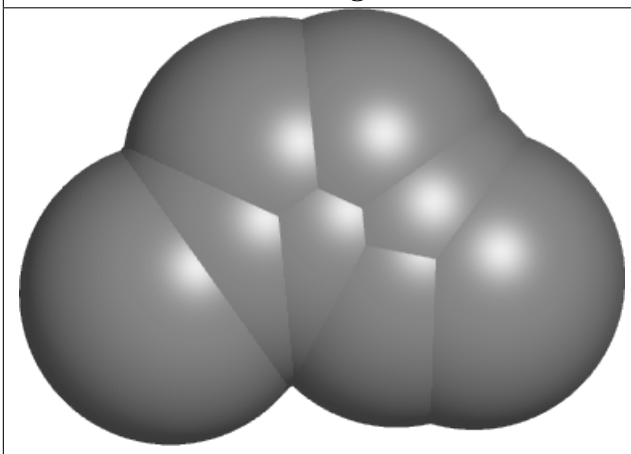
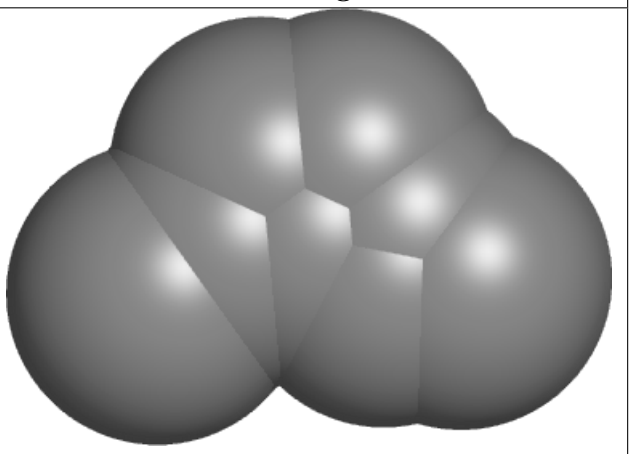
Torsions

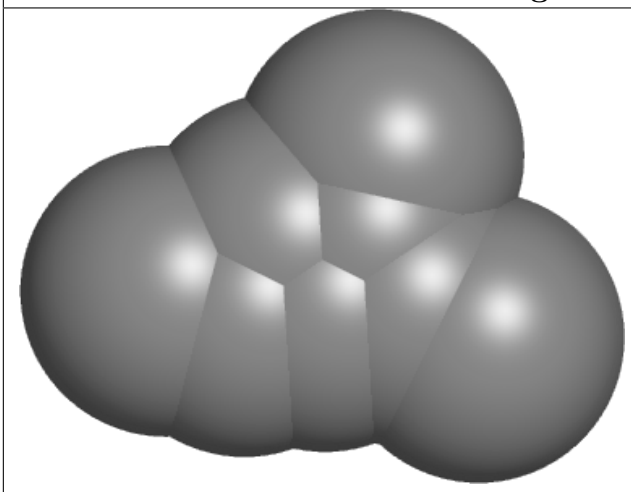
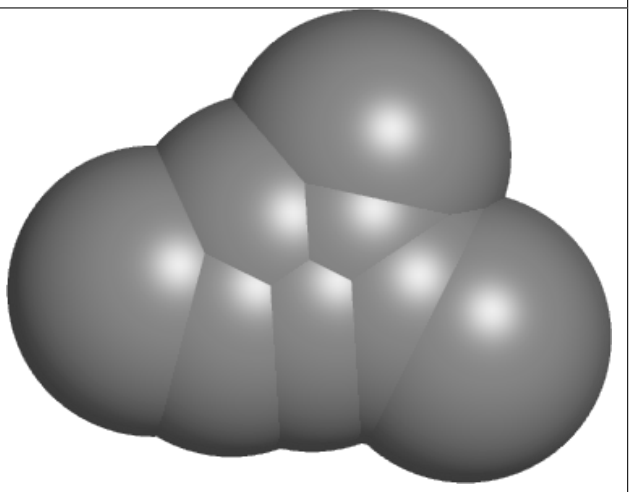
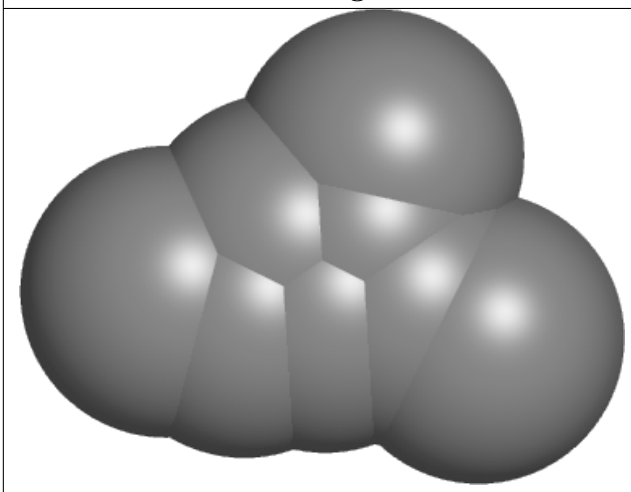
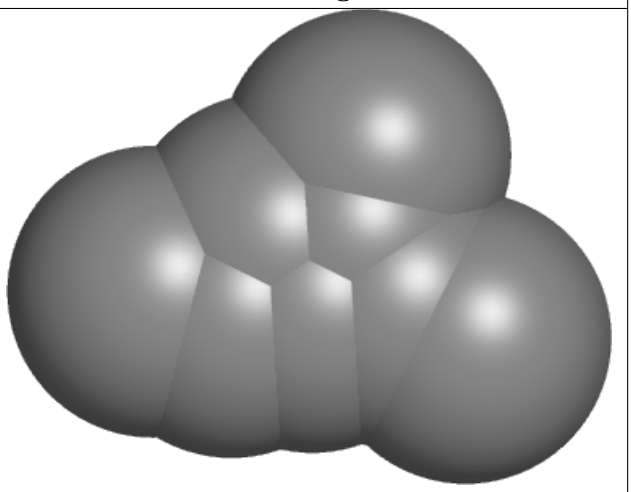


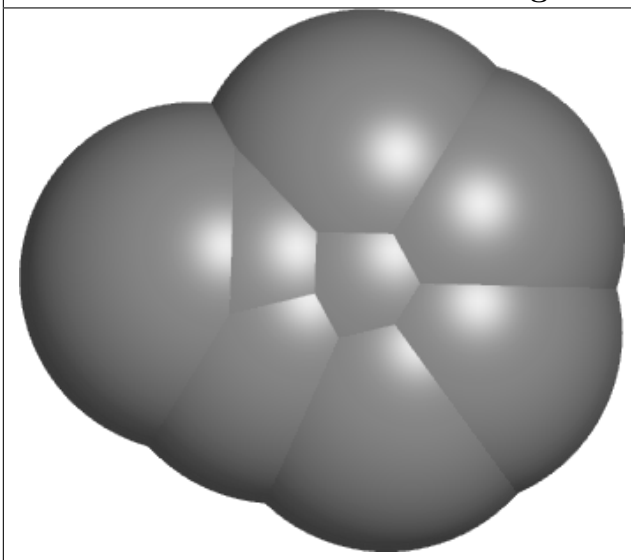
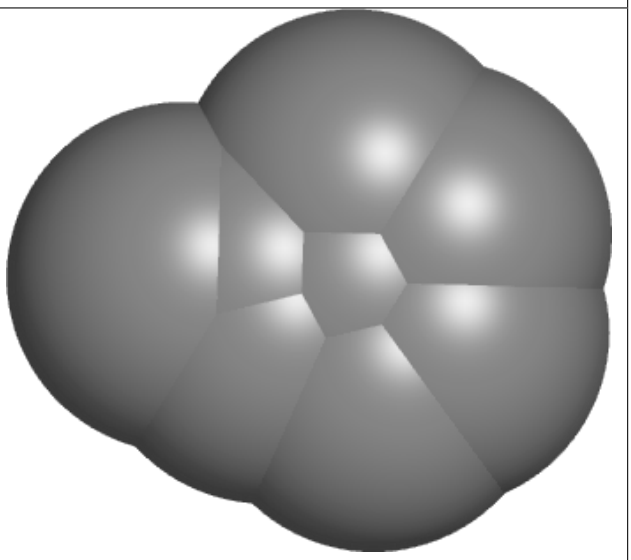
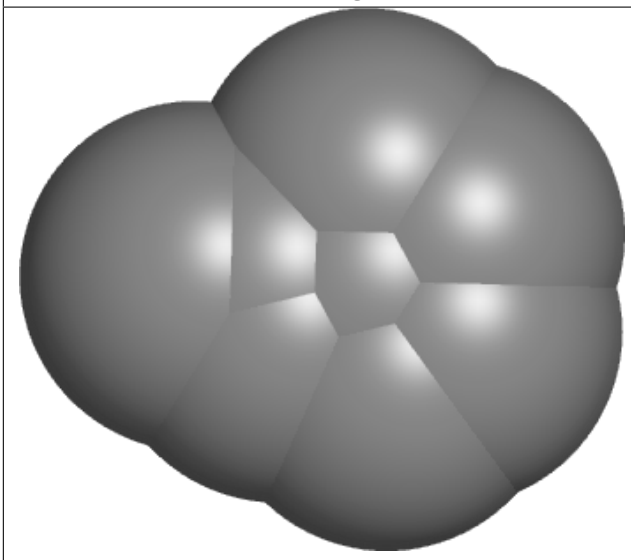
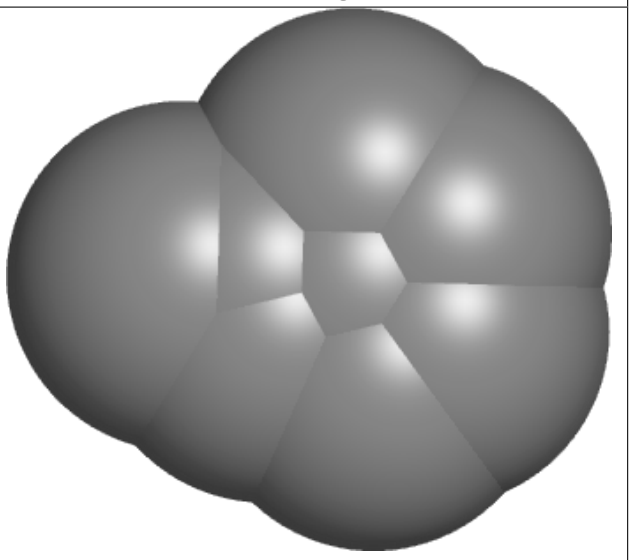
Rings

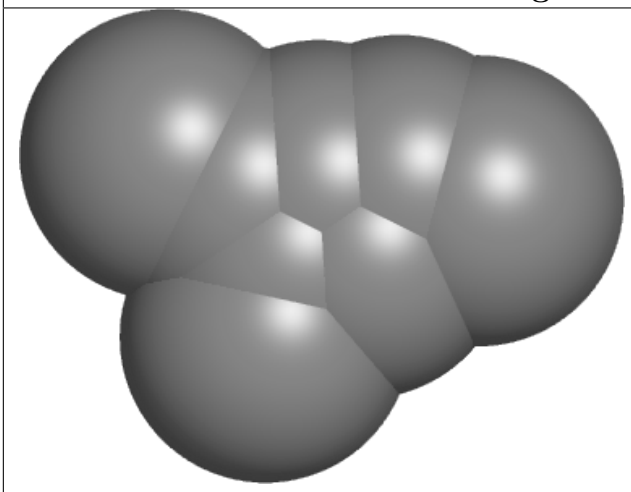
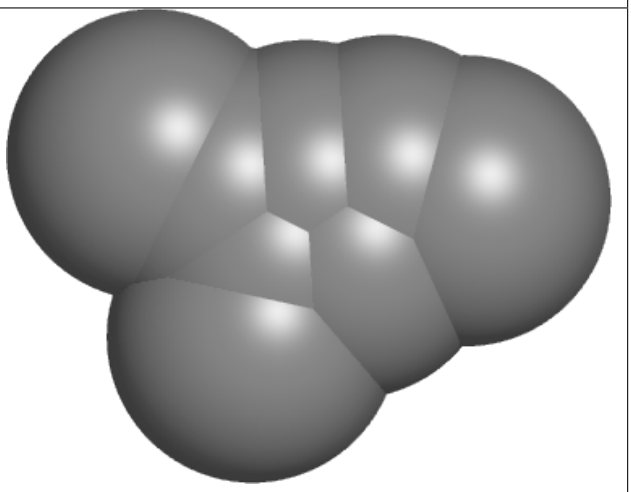
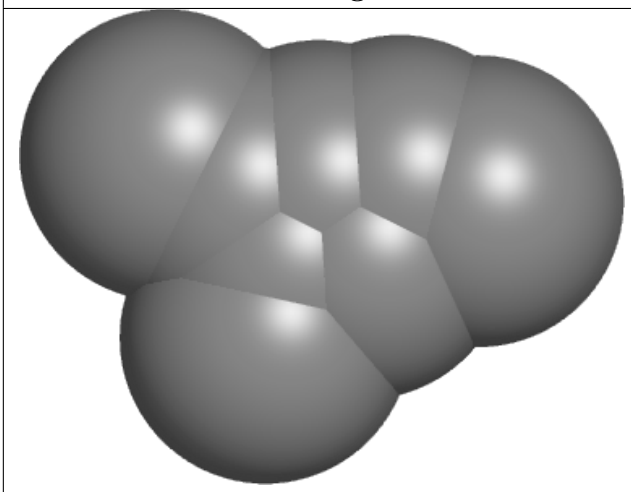
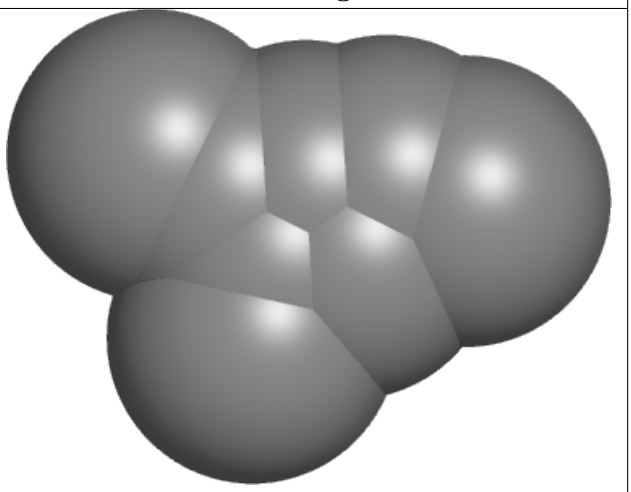
Ligand SF4 B 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

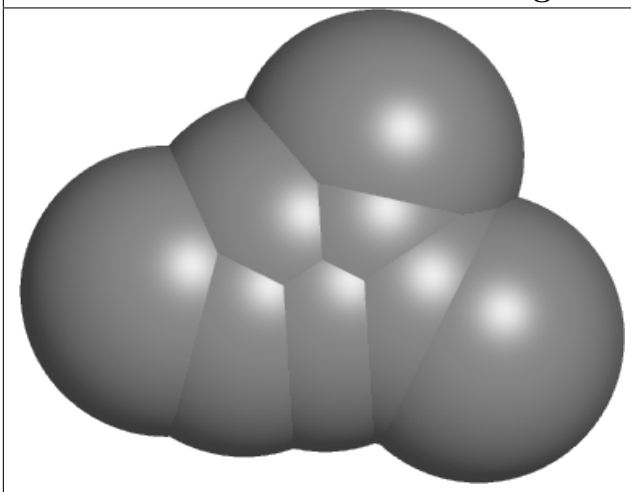
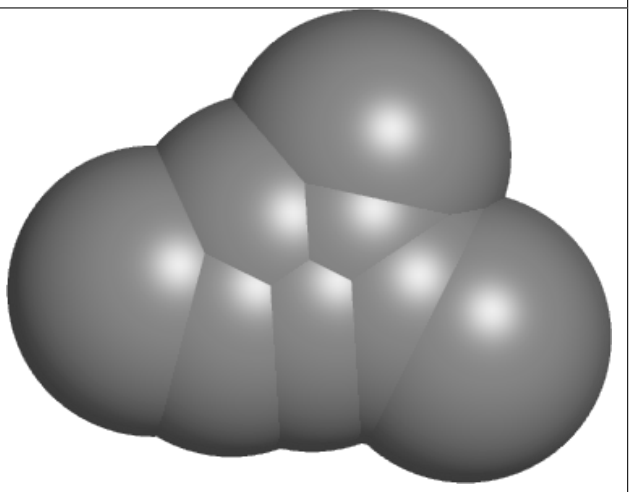
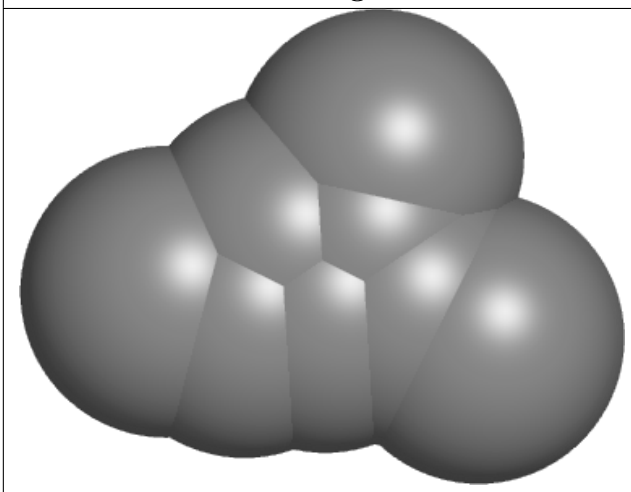
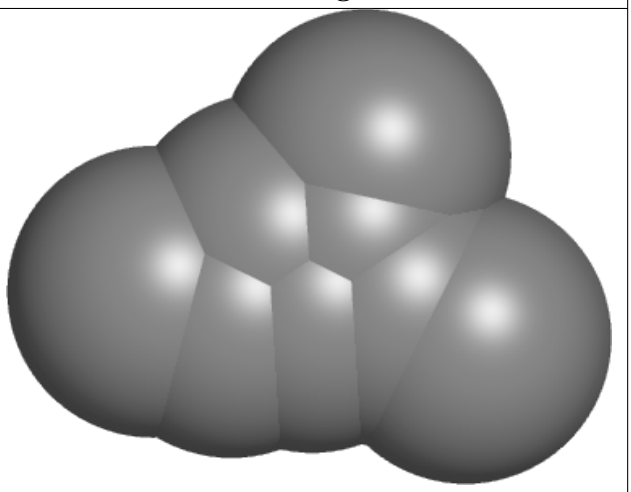
Ligand SF4 D 502	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

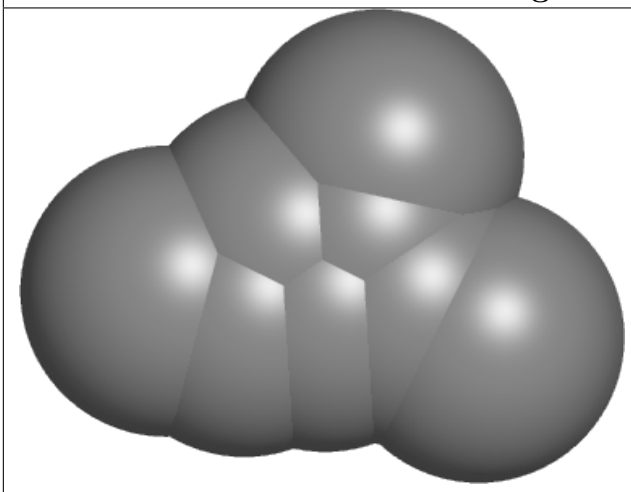
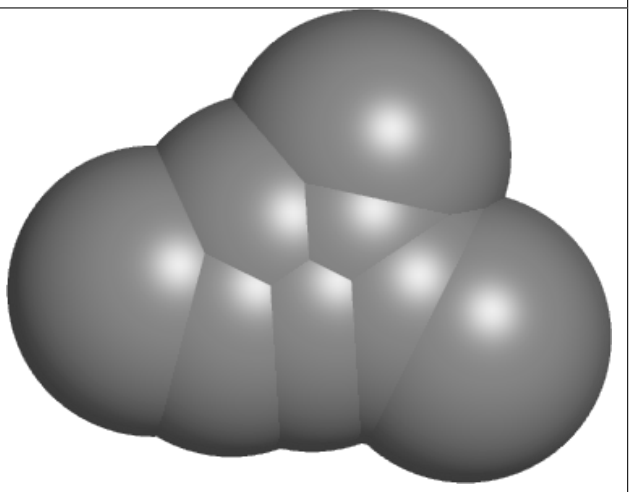
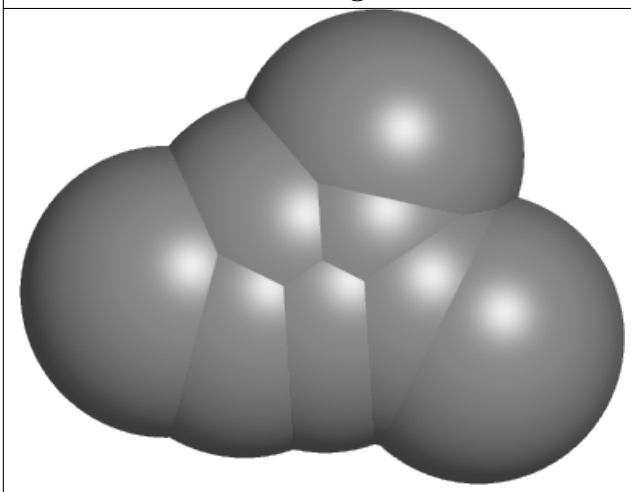
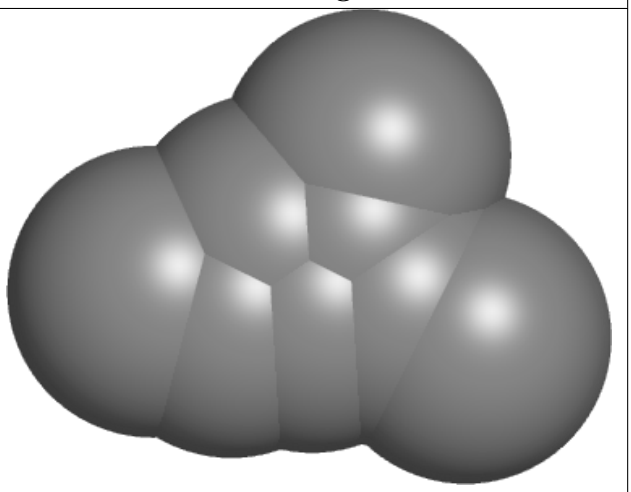
Ligand SF4 B 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 X 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

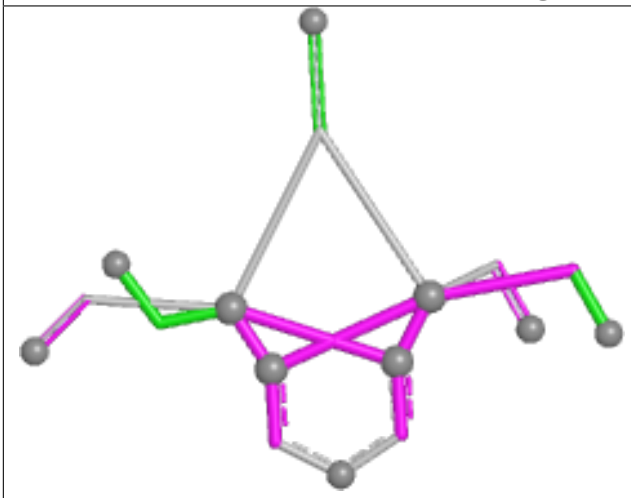
Ligand SF4 G 202	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 P 302	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

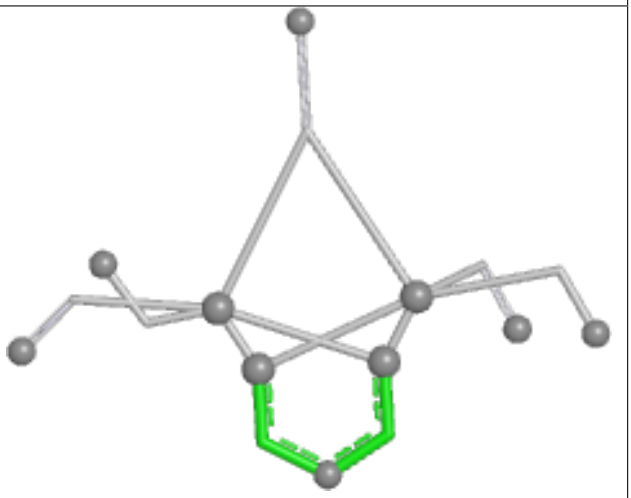
Ligand SF4 Z 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 B 302	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

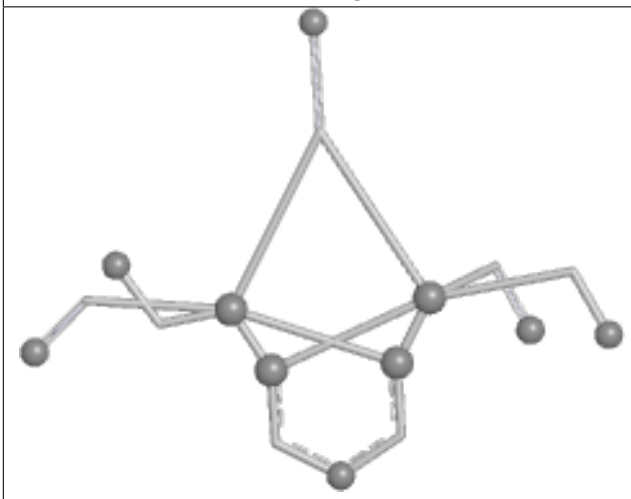
Ligand 402 R 503



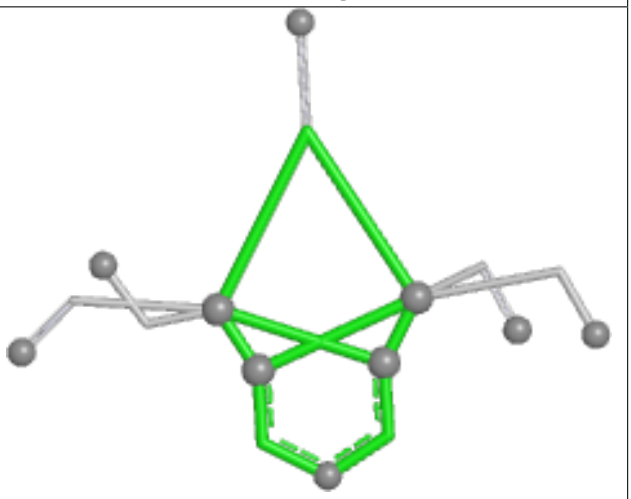
Bond lengths



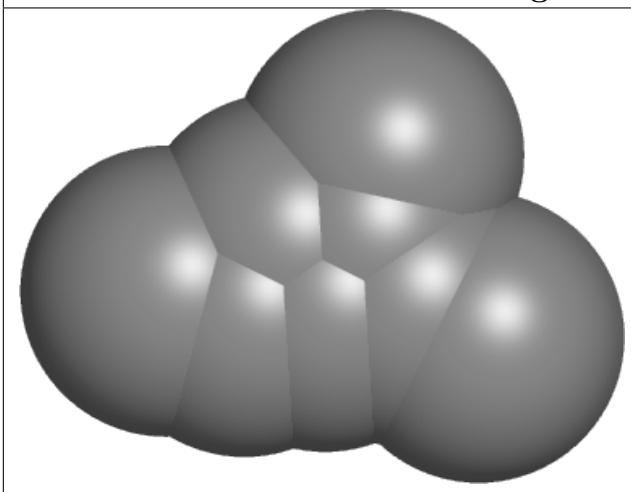
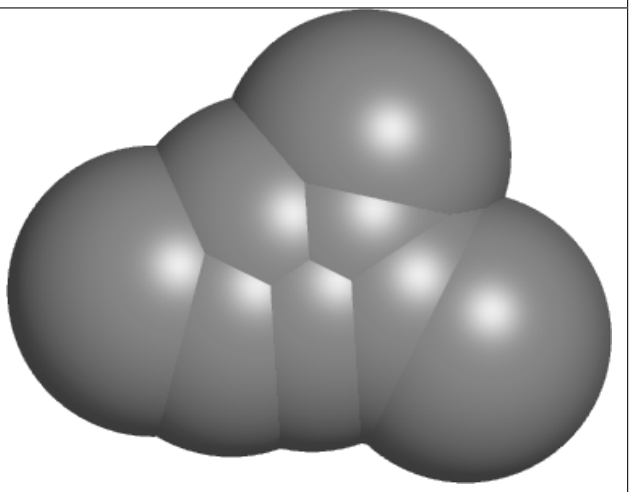
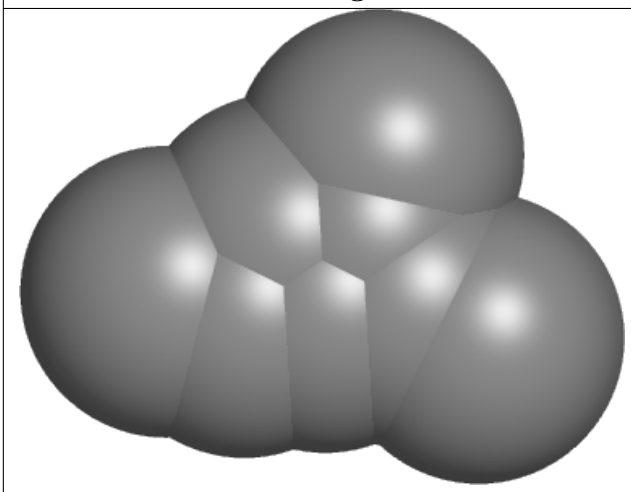
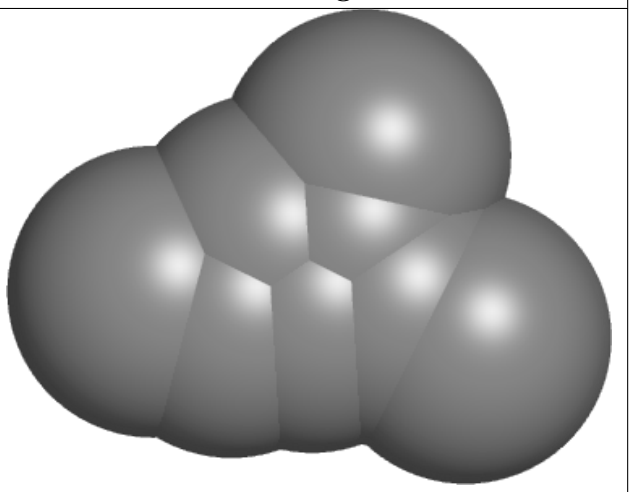
Bond angles



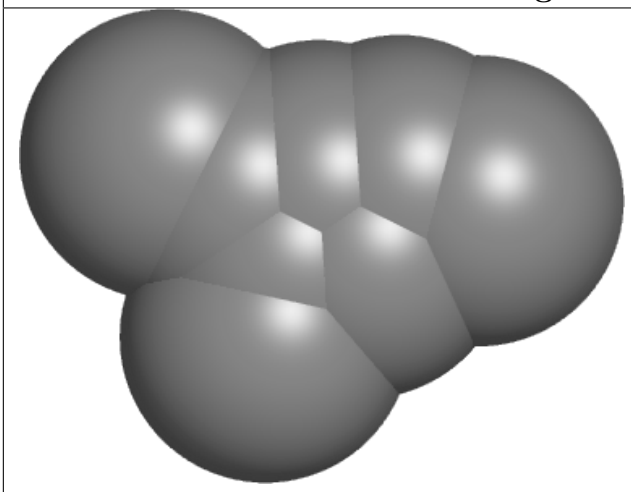
Torsions



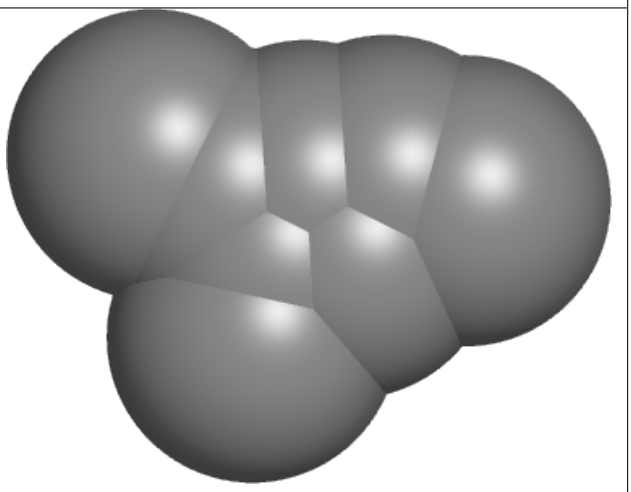
Rings

Ligand SF4 A 204	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

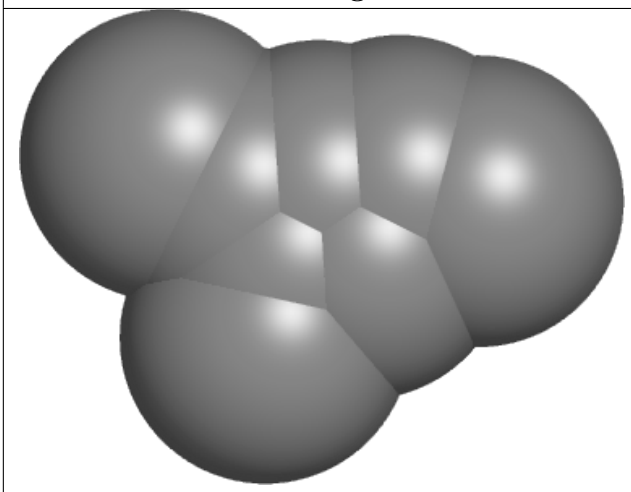
Ligand SF4 J 302



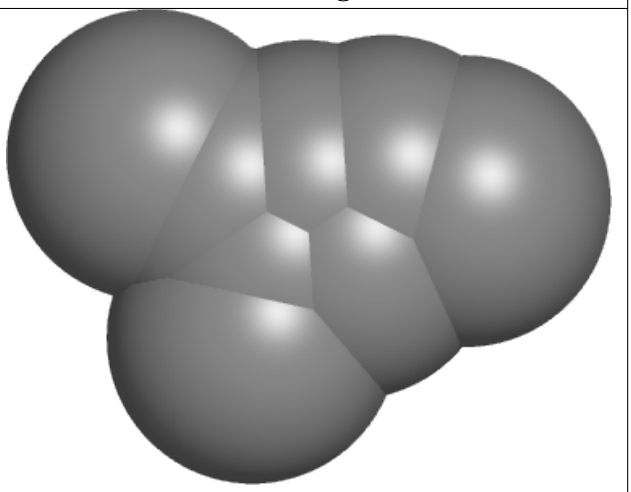
Bond lengths



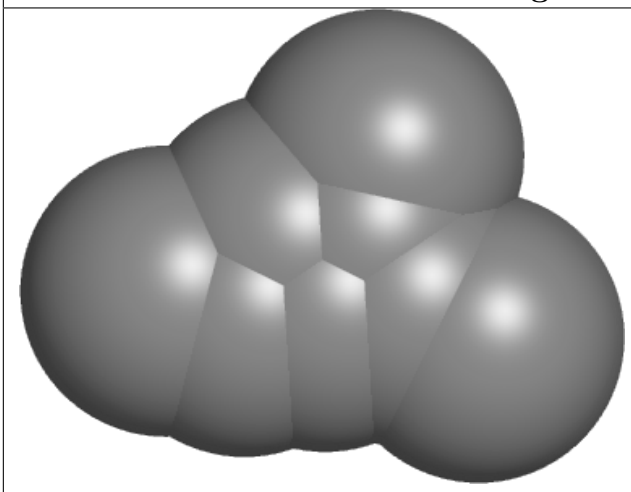
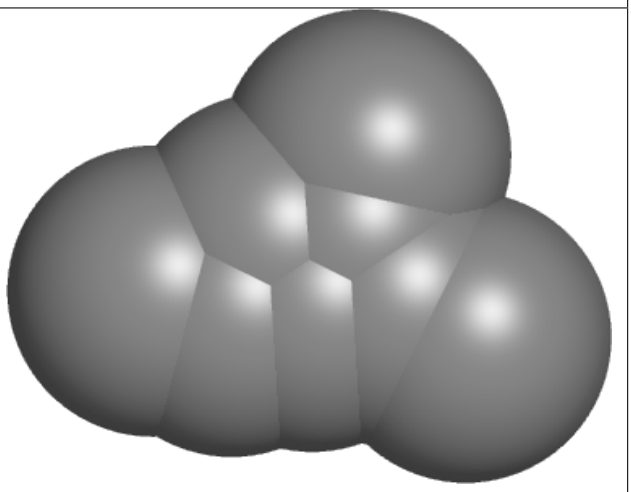
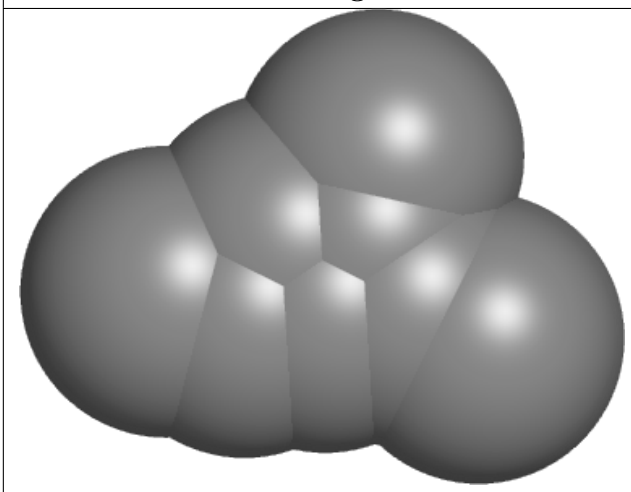
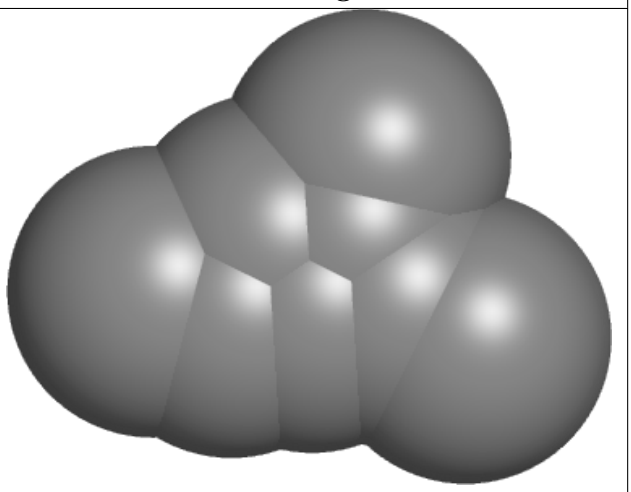
Bond angles

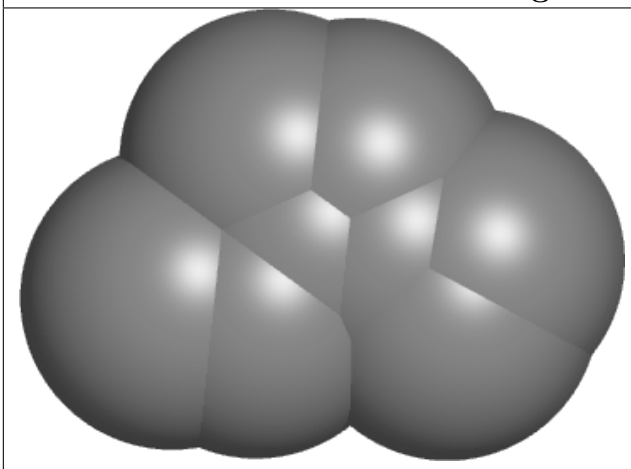
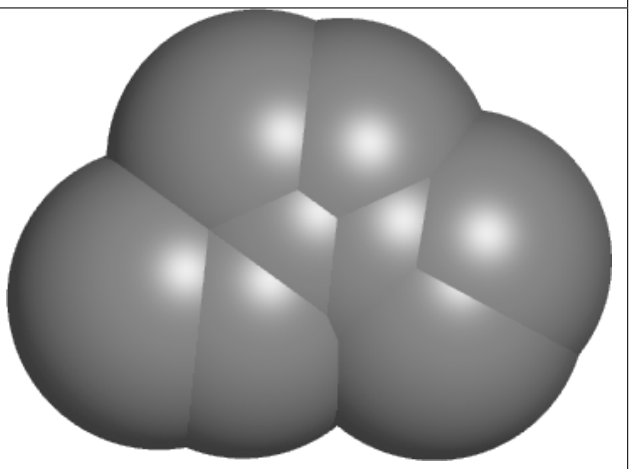
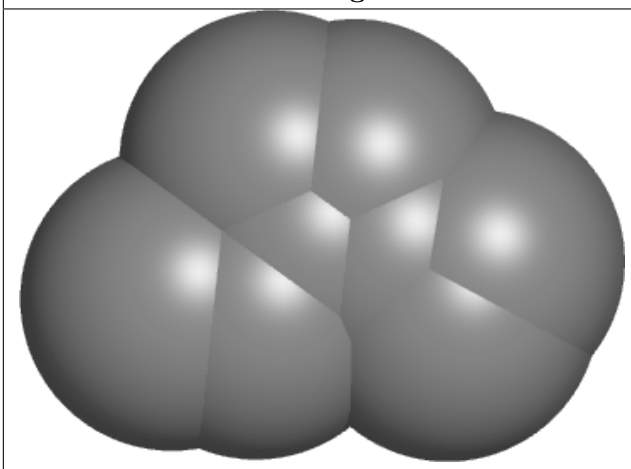
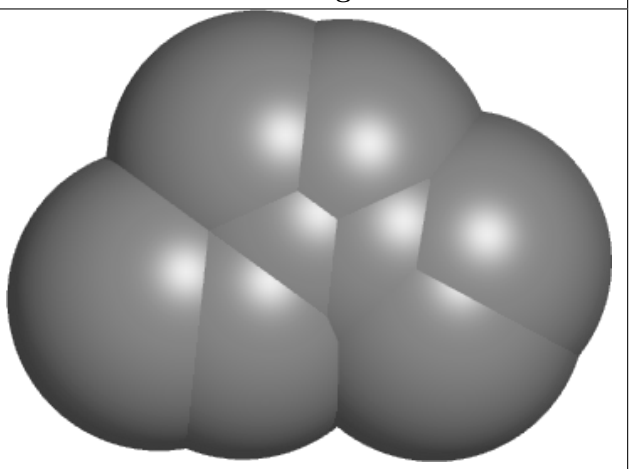


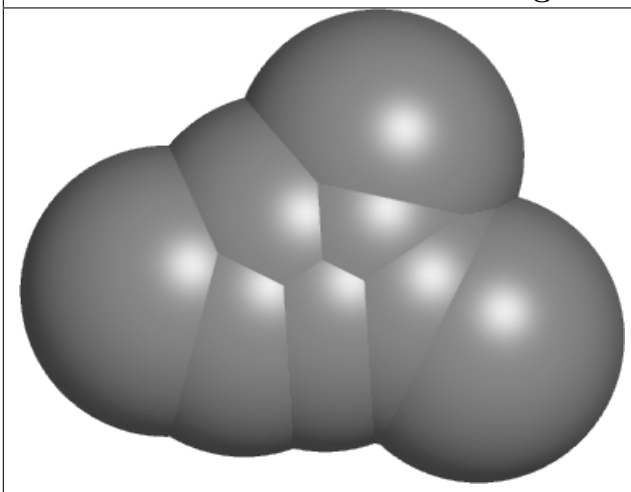
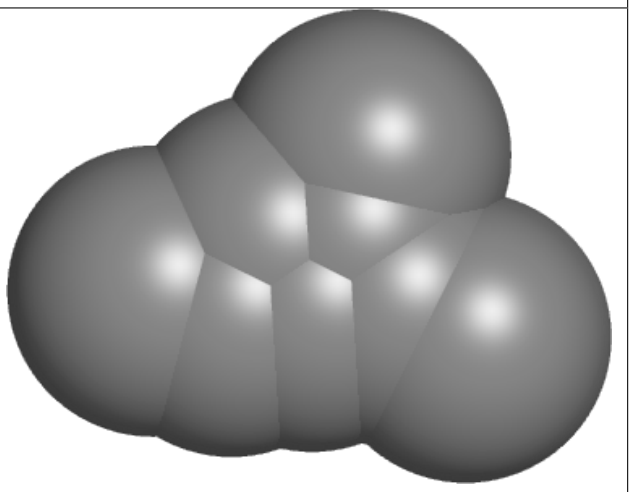
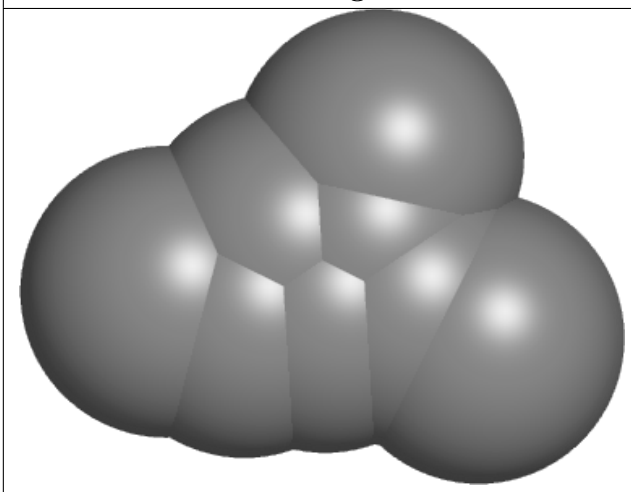
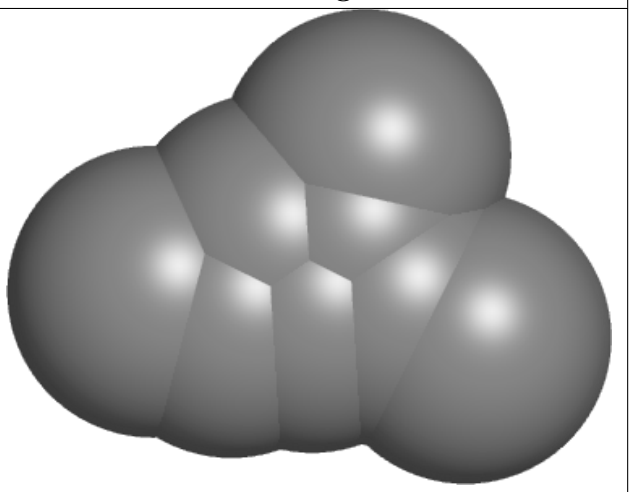
Torsions



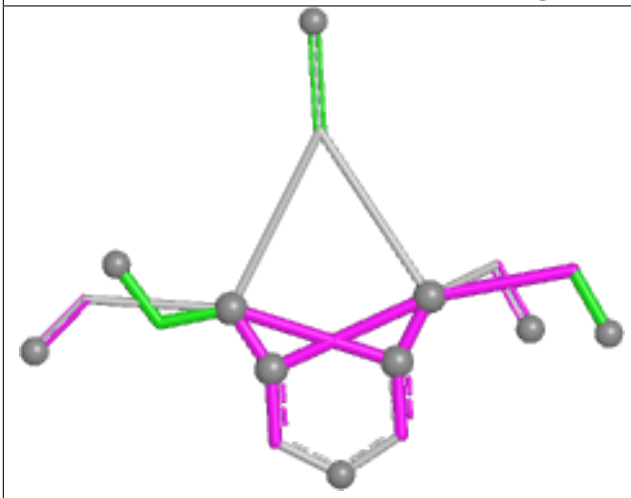
Rings

Ligand SF4 R 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

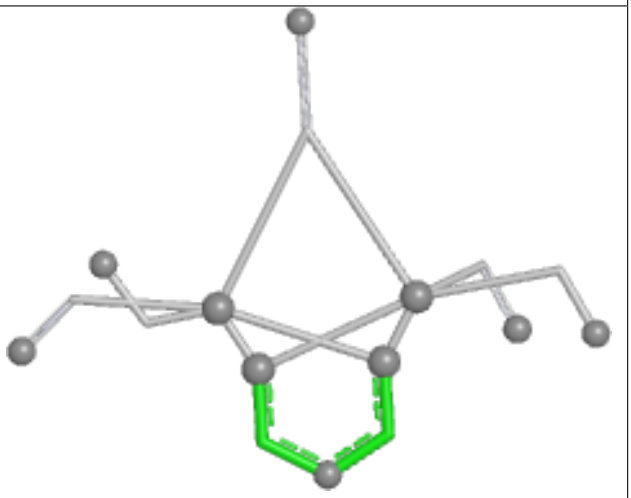
Ligand SF4 B 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 Z 503	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

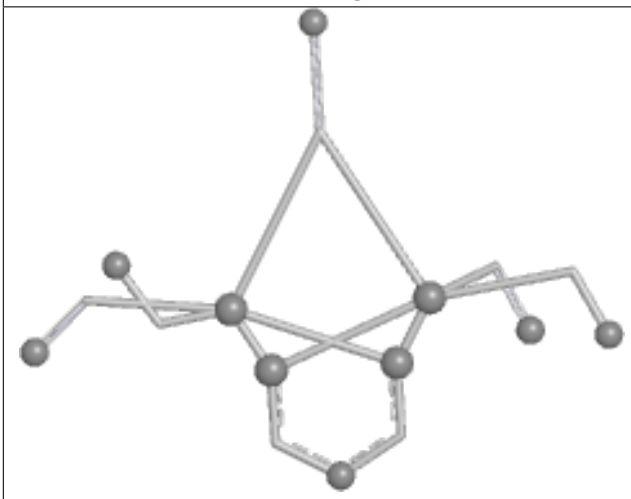
Ligand 402 V 503



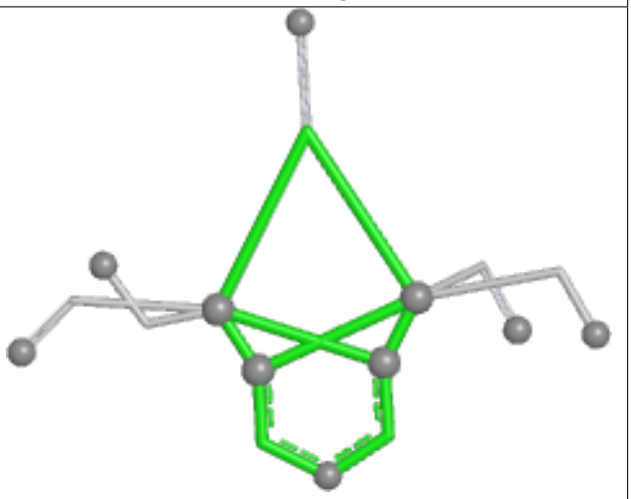
Bond lengths



Bond angles

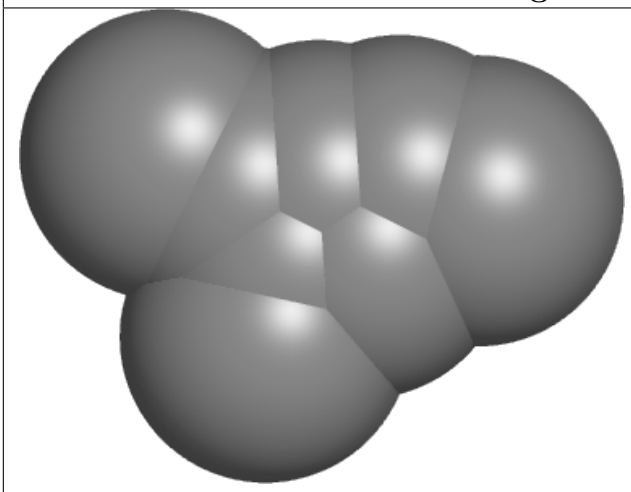


Torsions

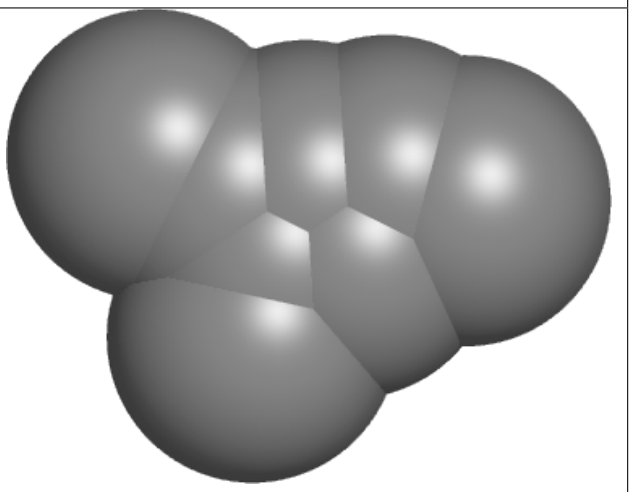


Rings

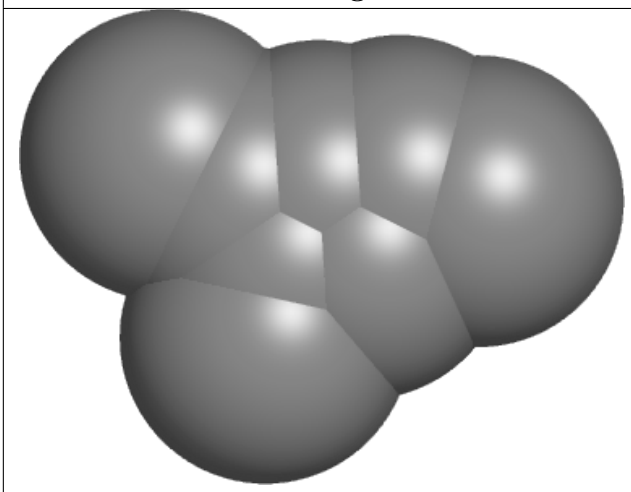
Ligand SF4 G 203



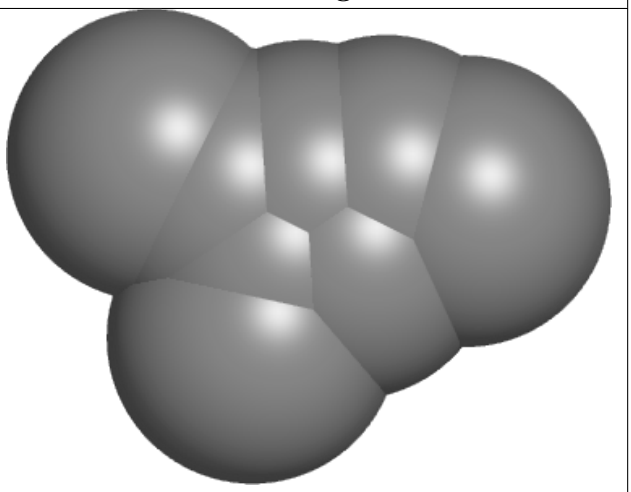
Bond lengths



Bond angles

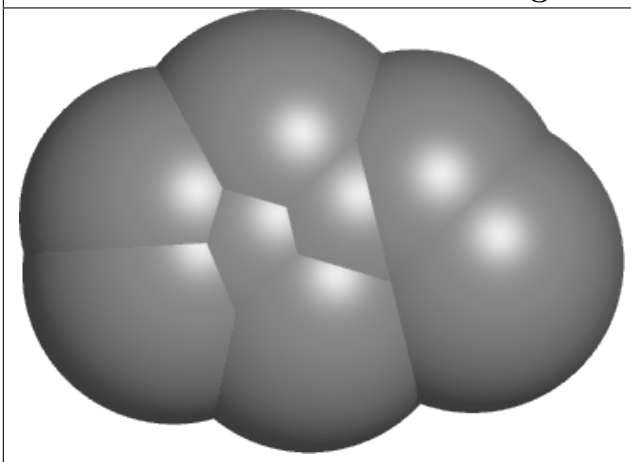


Torsions

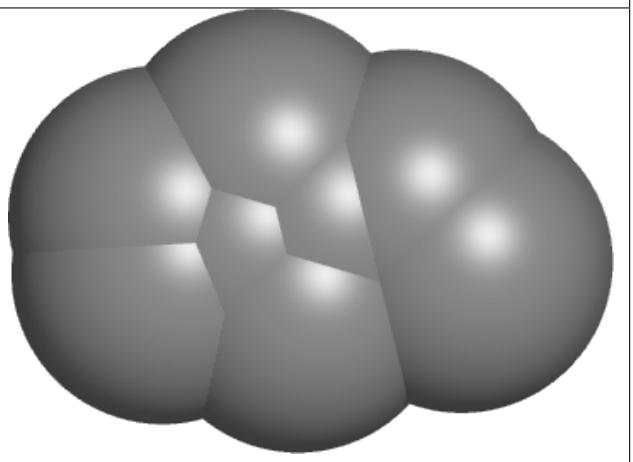


Rings

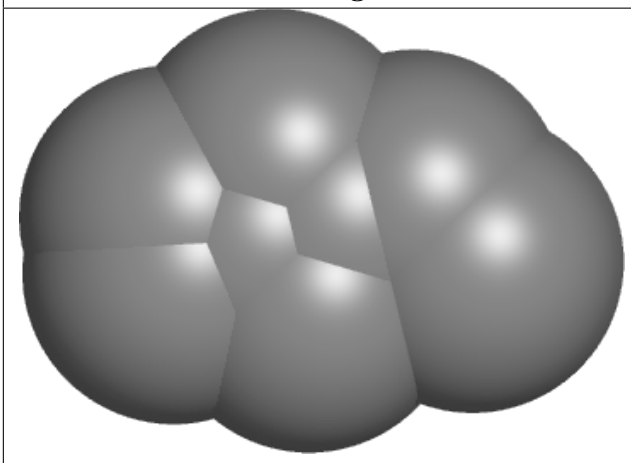
Ligand SF4 D 504



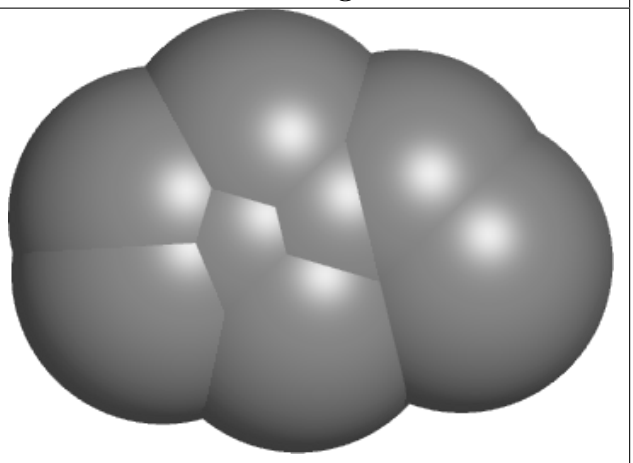
Bond lengths



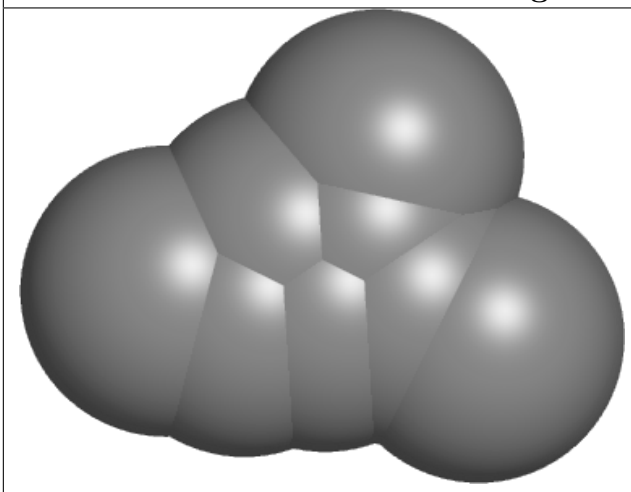
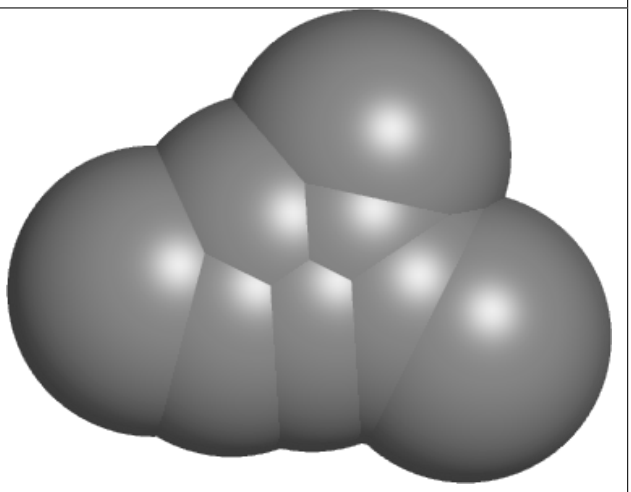
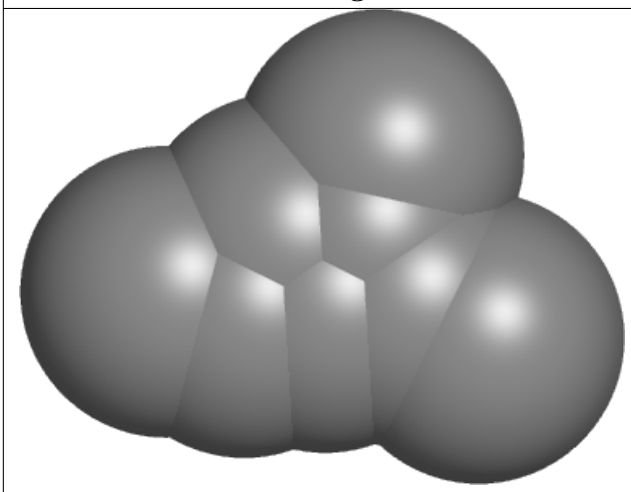
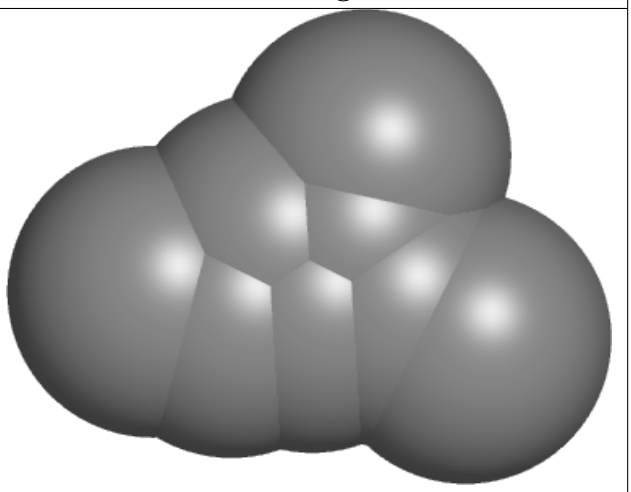
Bond angles

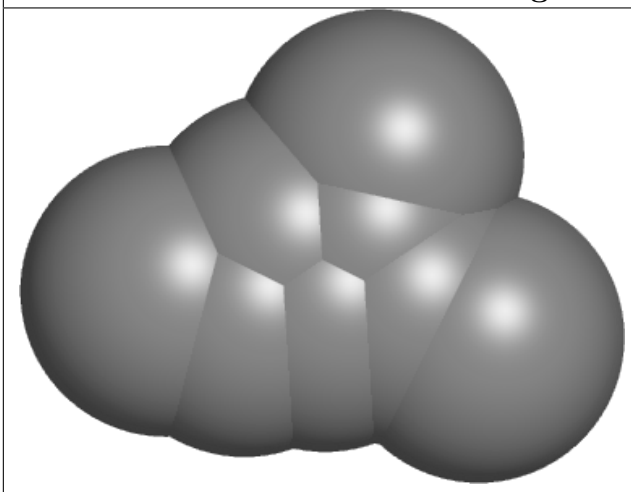
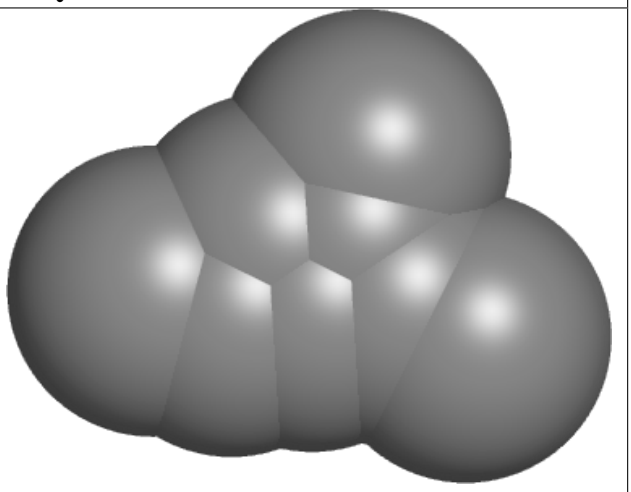
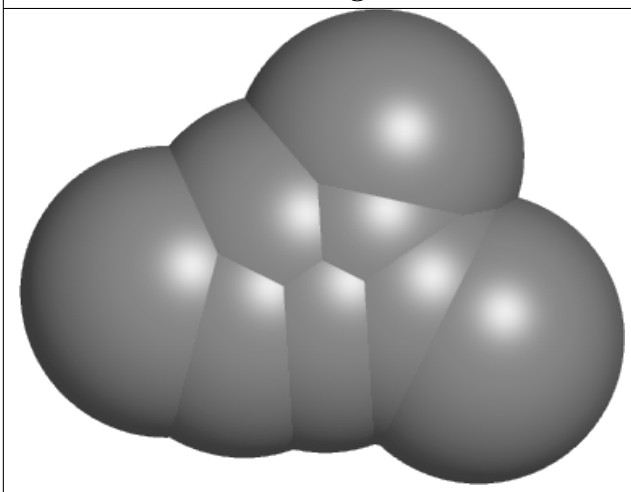
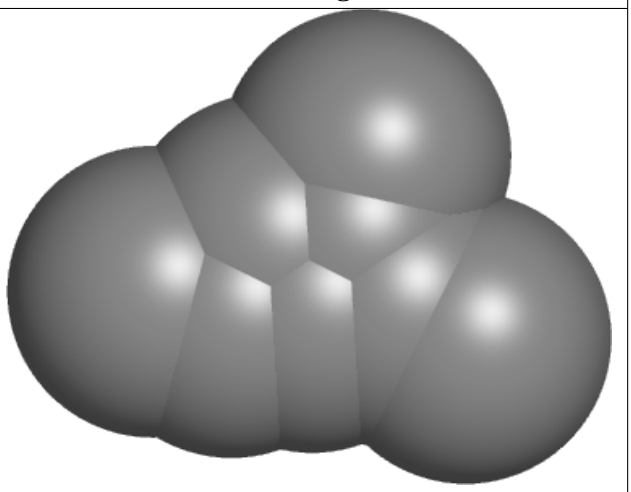


Torsions

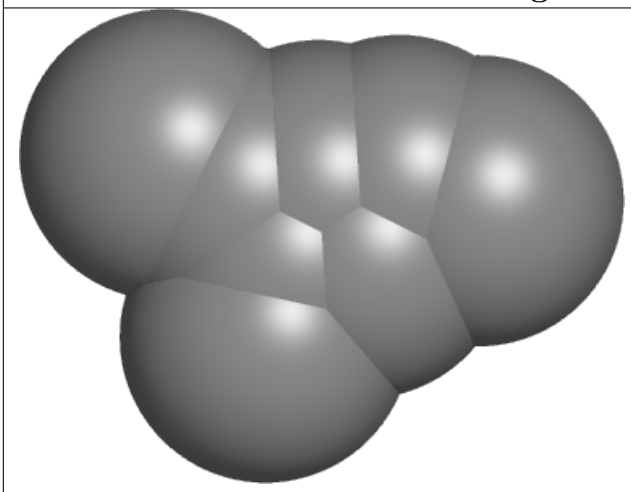


Rings

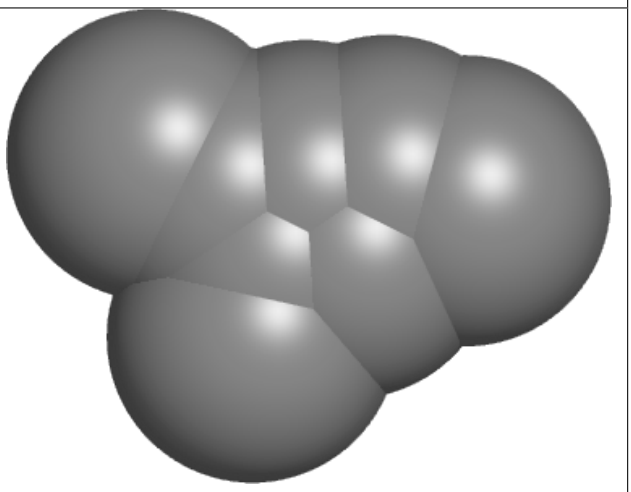
Ligand SF4 V 504	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 Q 502	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

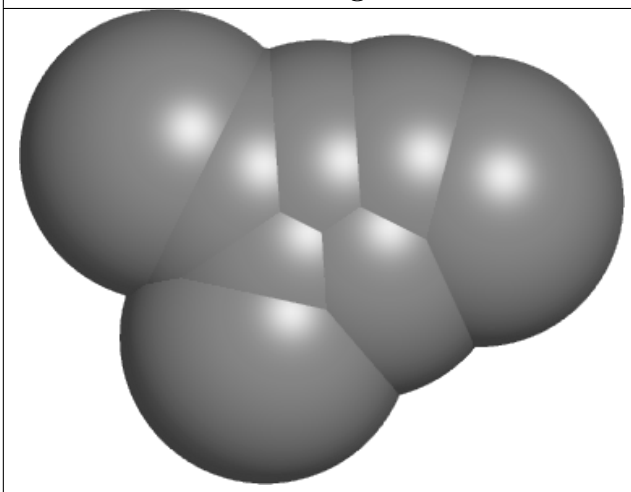
Ligand SF4 X 302



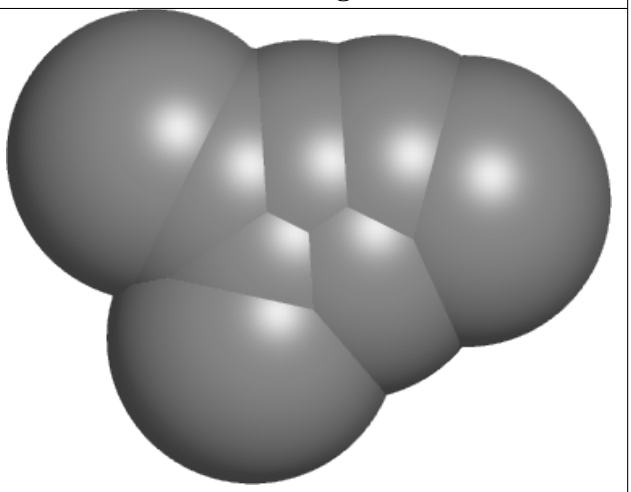
Bond lengths



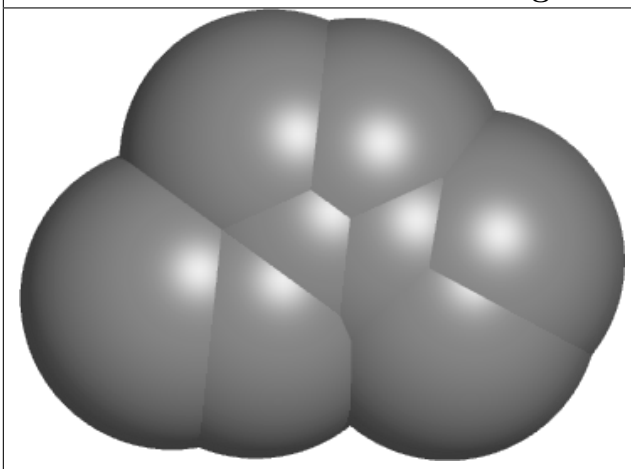
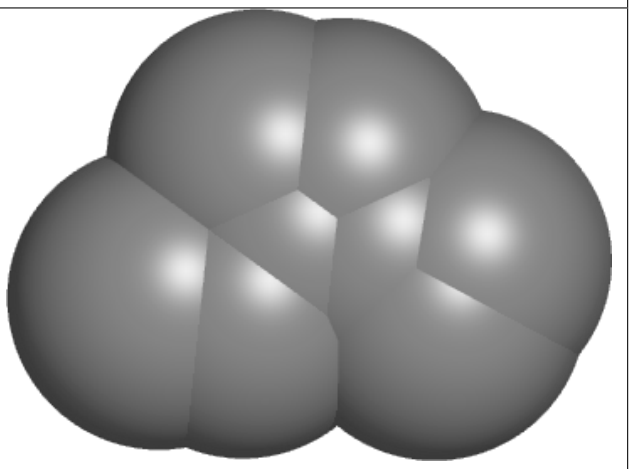
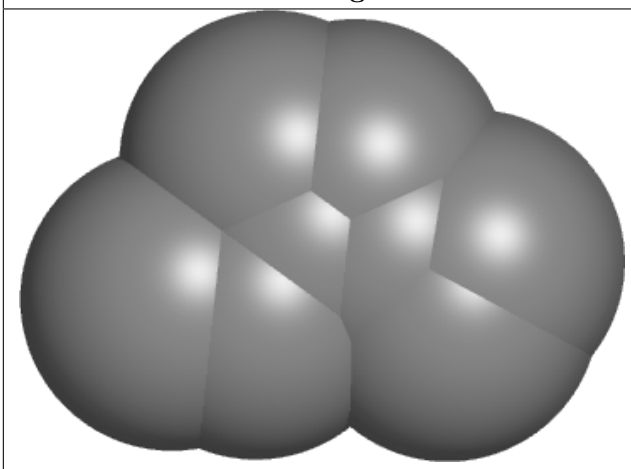
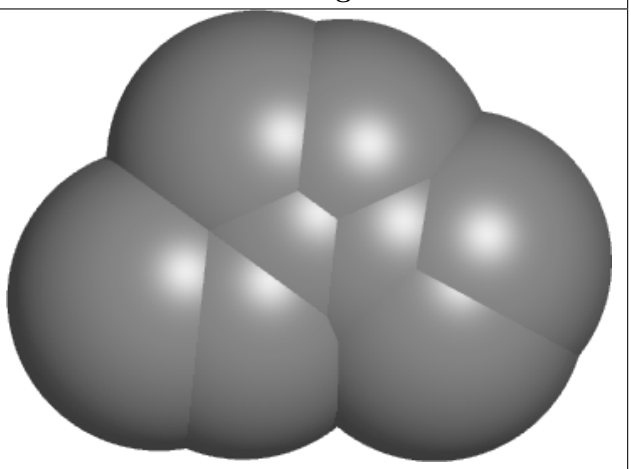
Bond angles

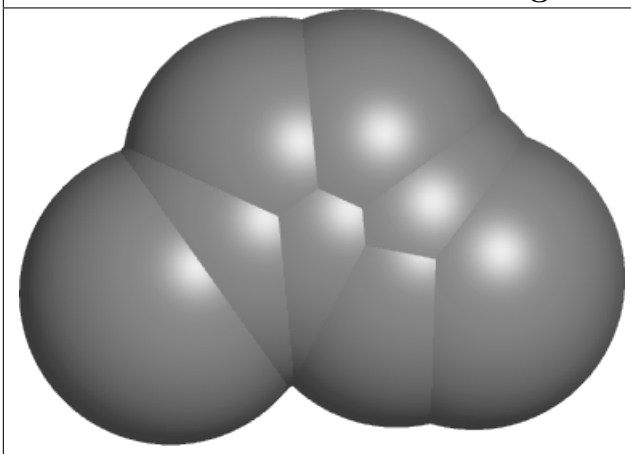
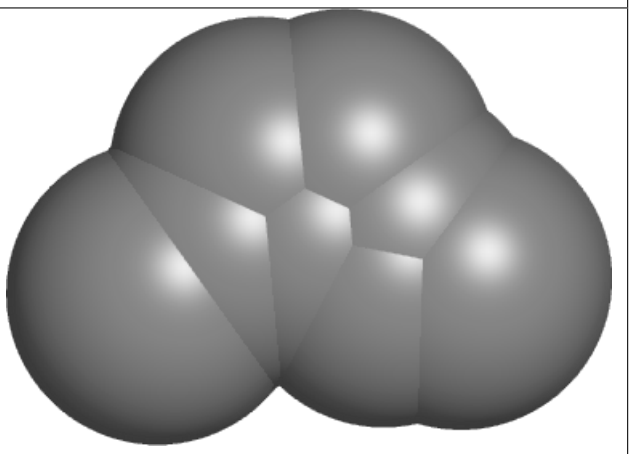
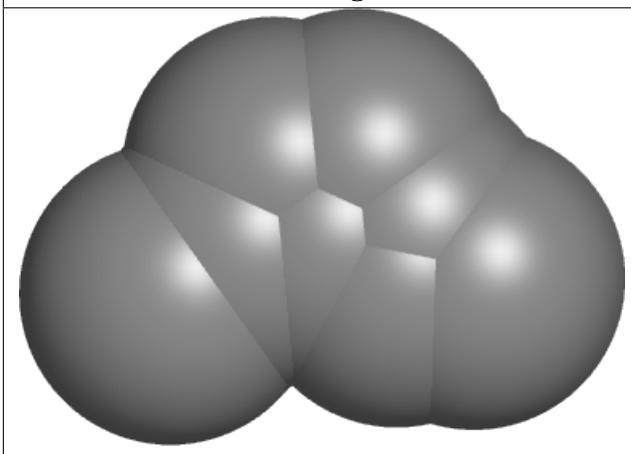
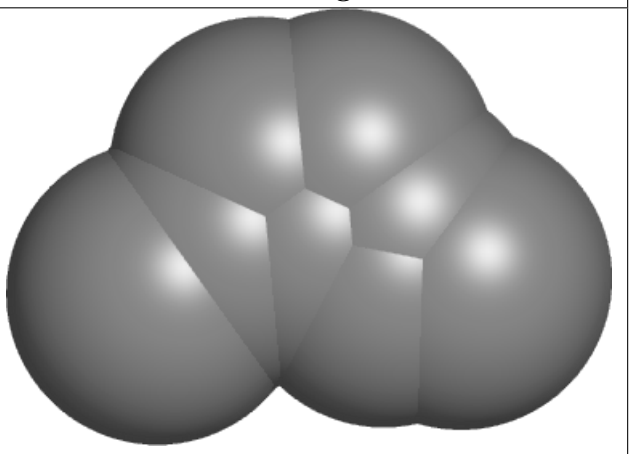


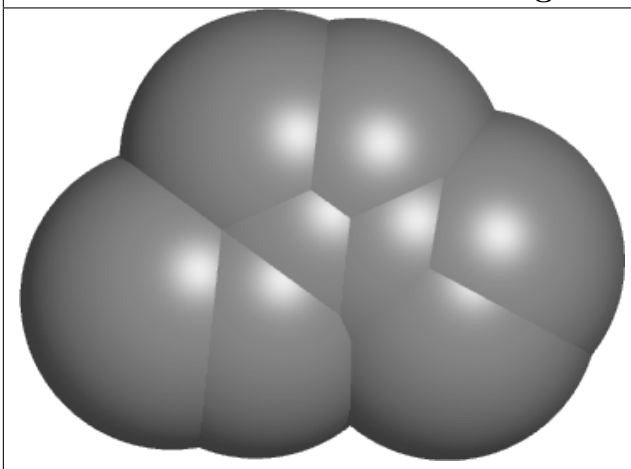
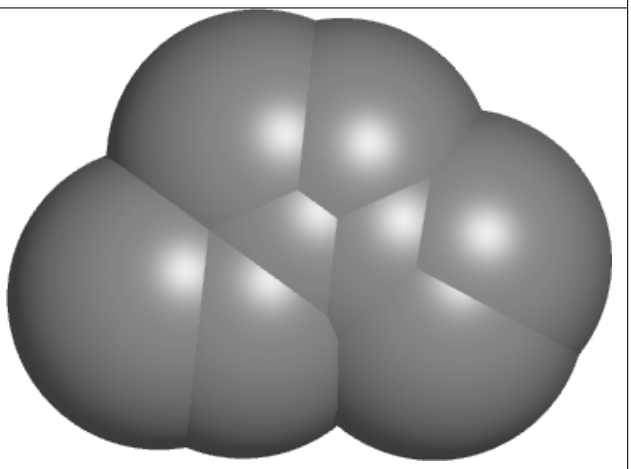
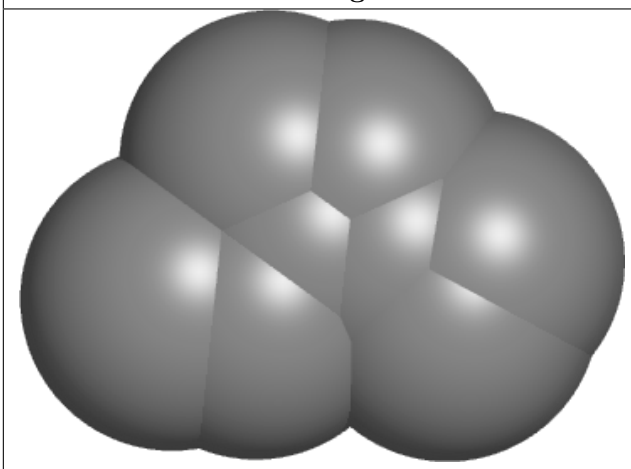
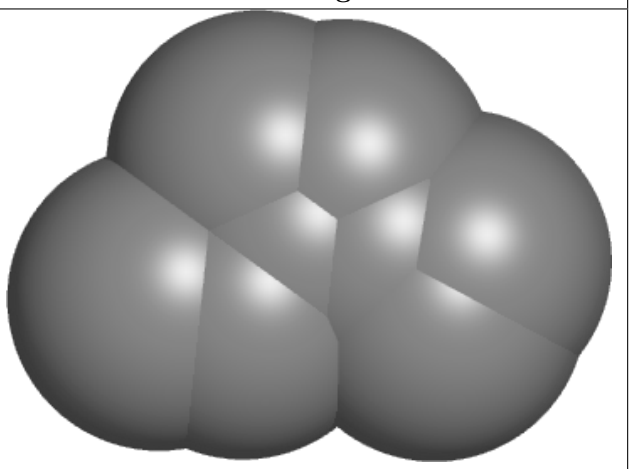
Torsions

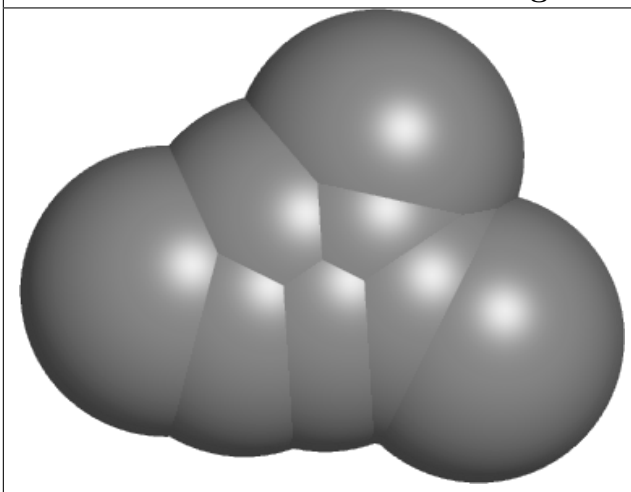
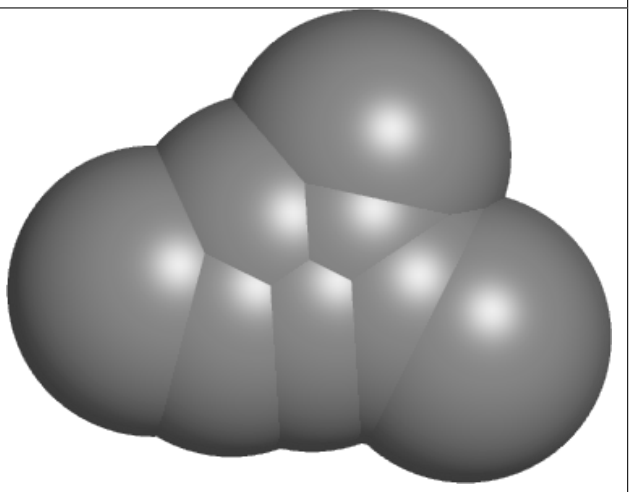
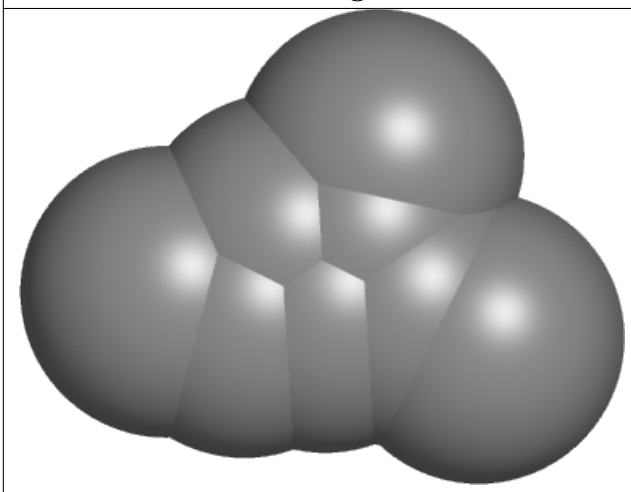
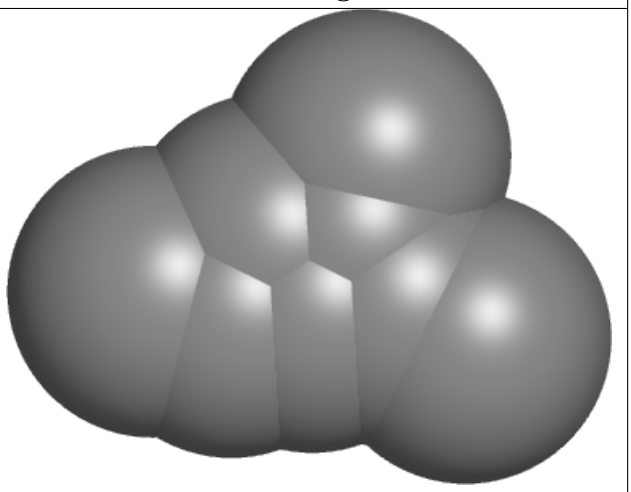


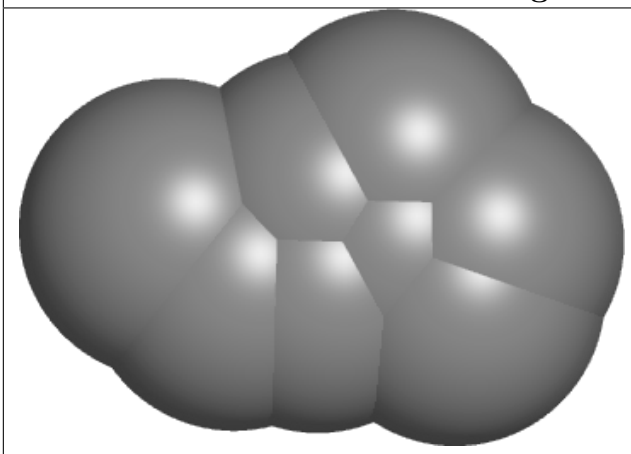
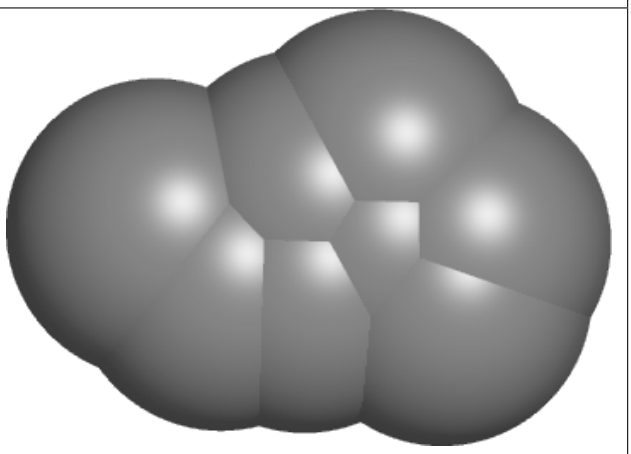
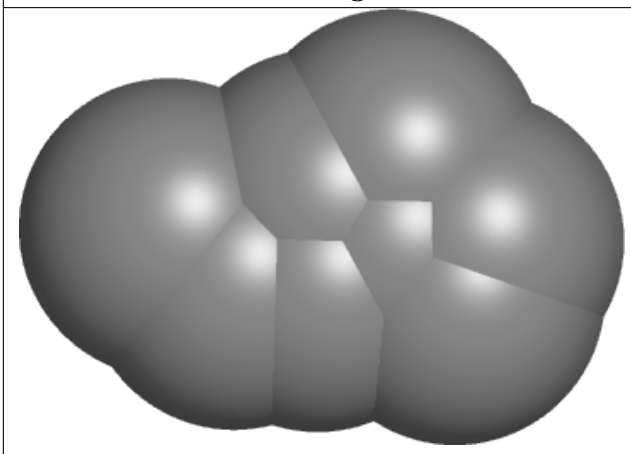
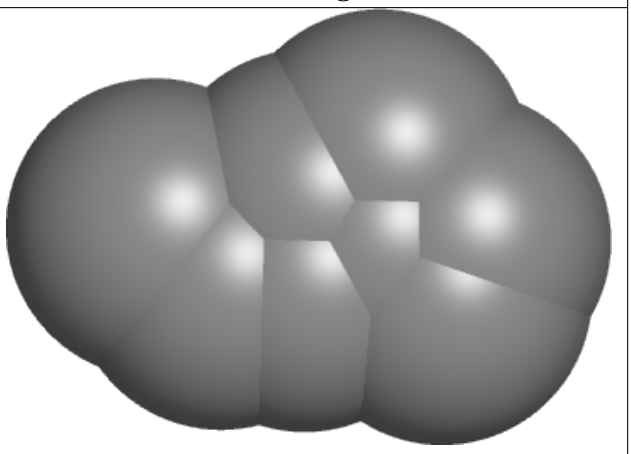
Rings

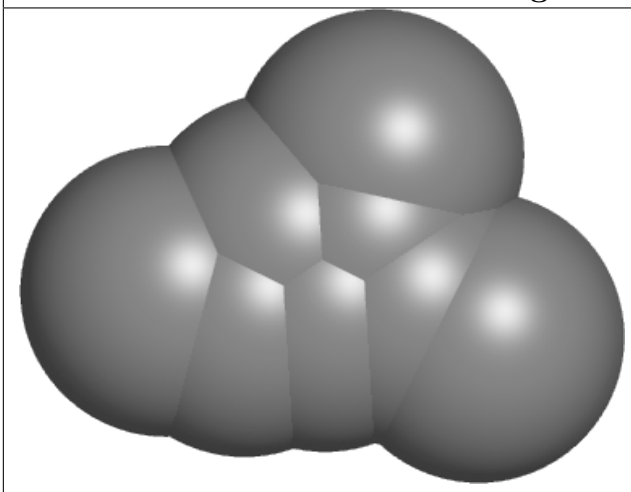
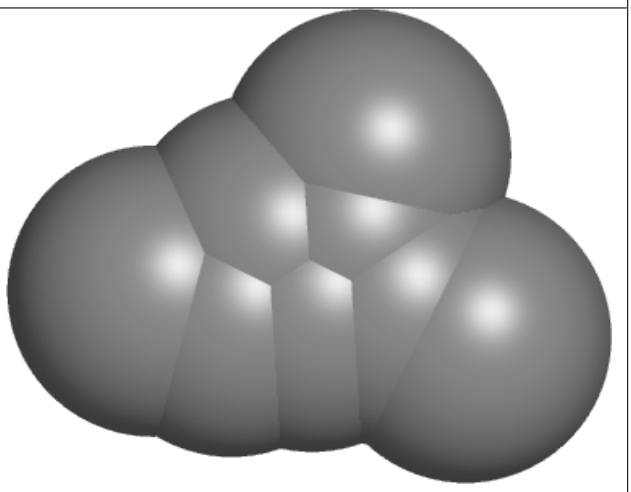
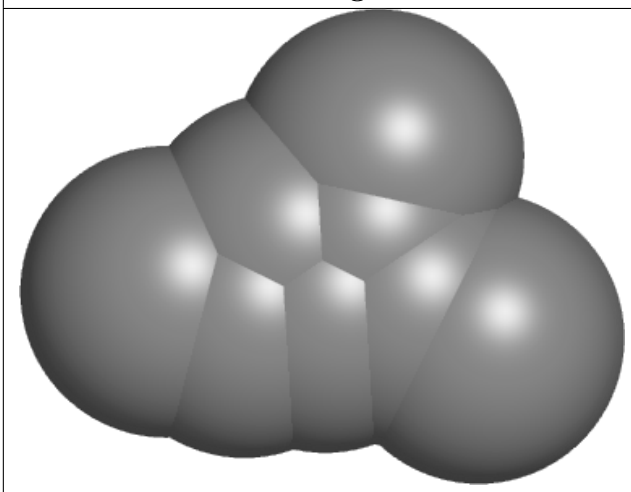
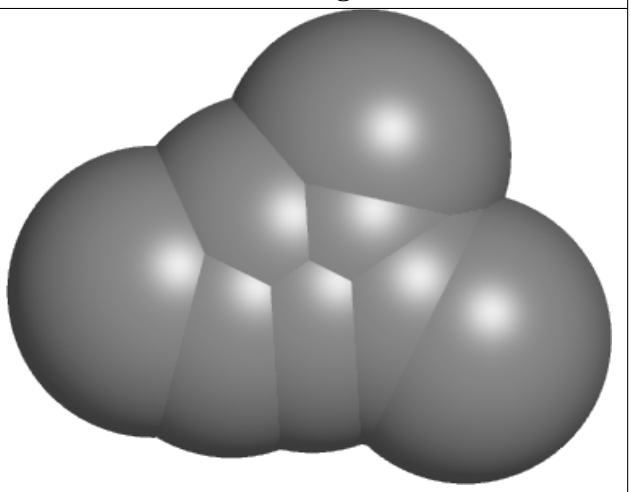
Ligand SF4 P 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 X 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

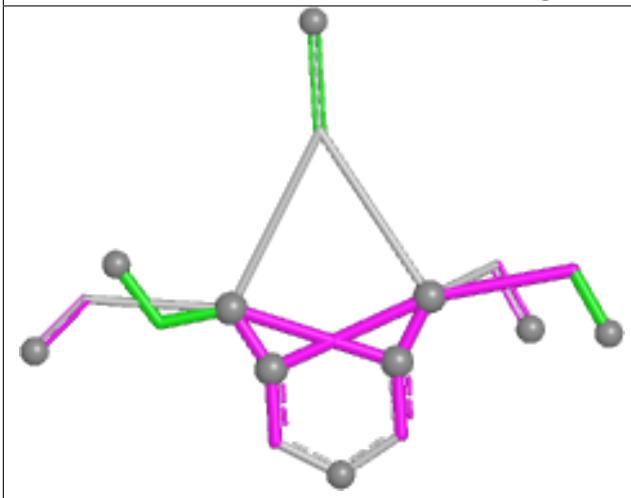
Ligand SF4 J 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 N 302	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

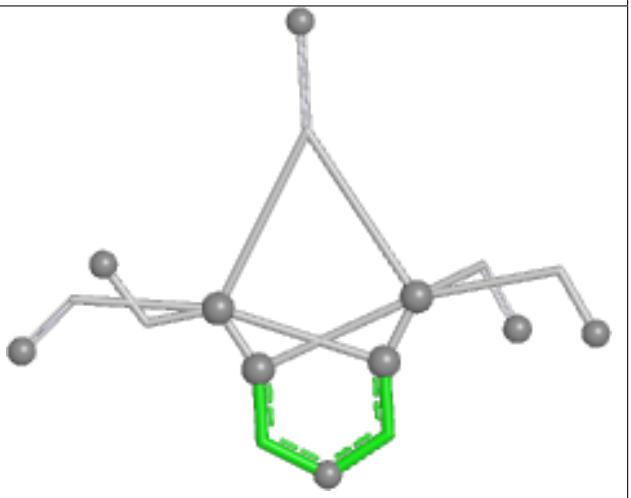
Ligand SF4 A 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 K 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

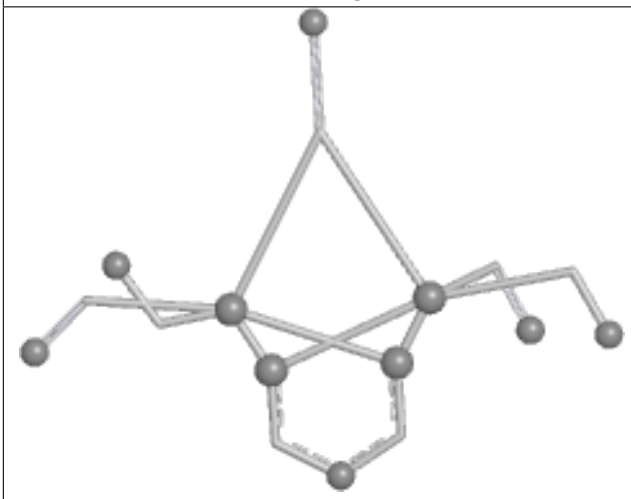
Ligand 402 Z 504



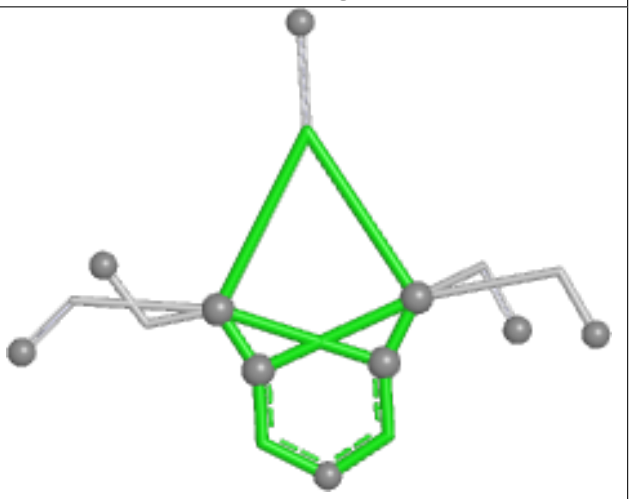
Bond lengths



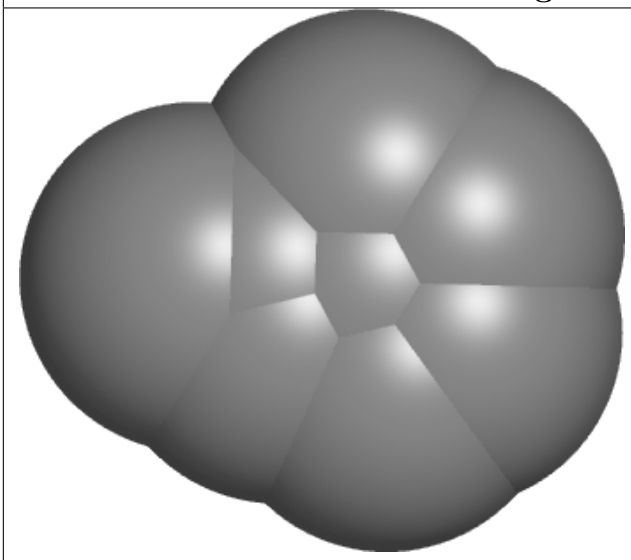
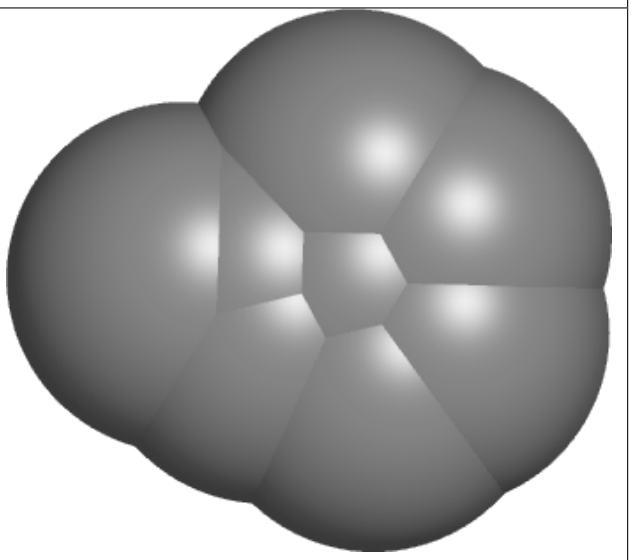
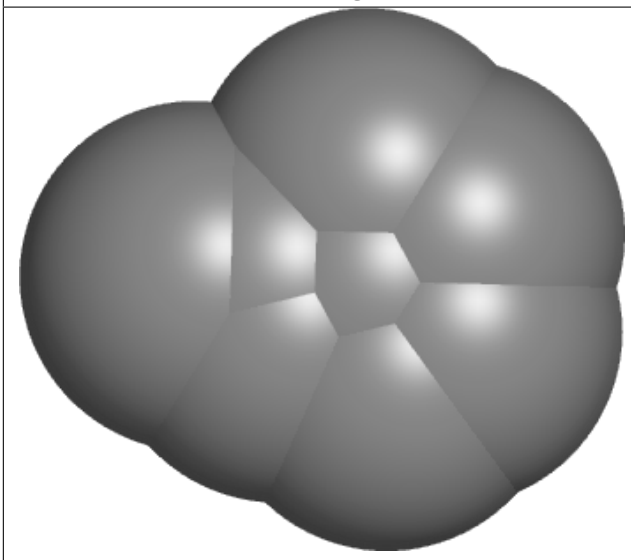
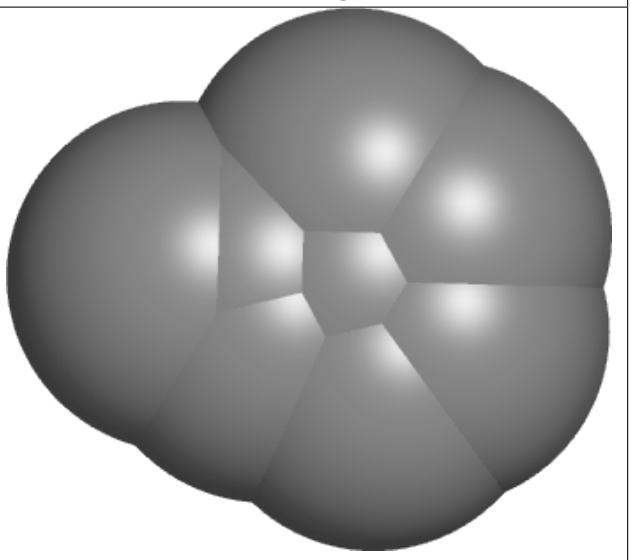
Bond angles

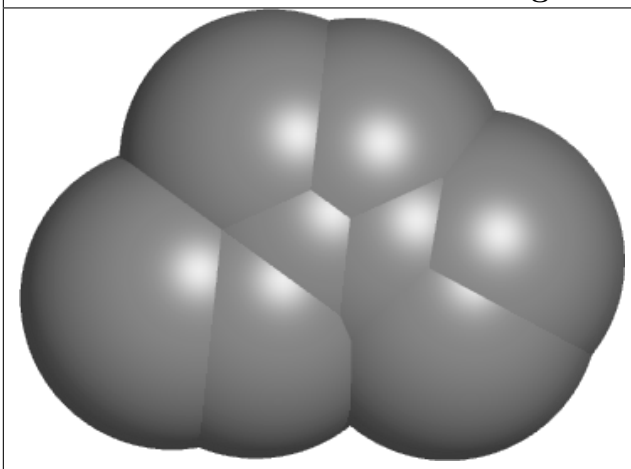
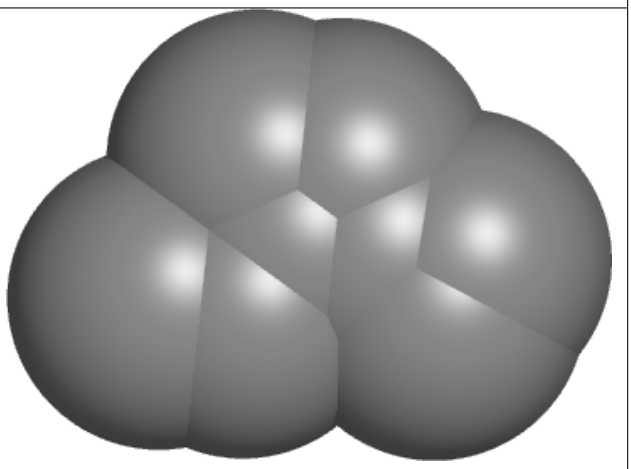
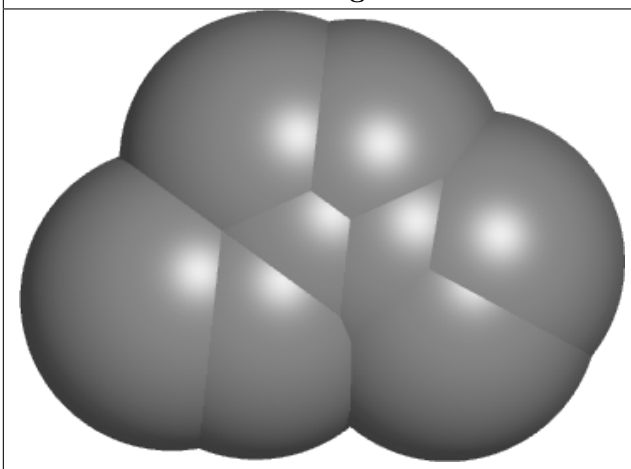
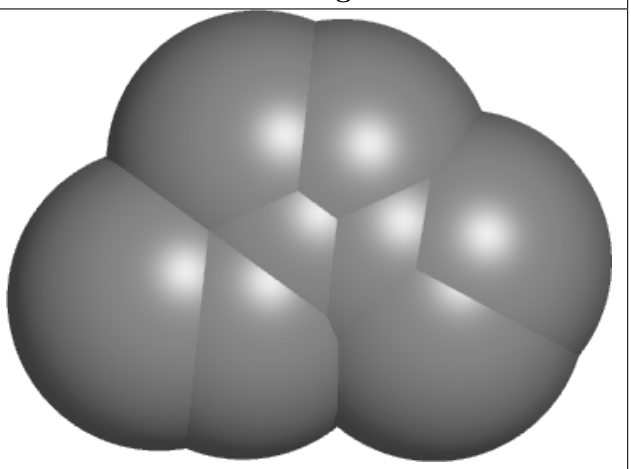


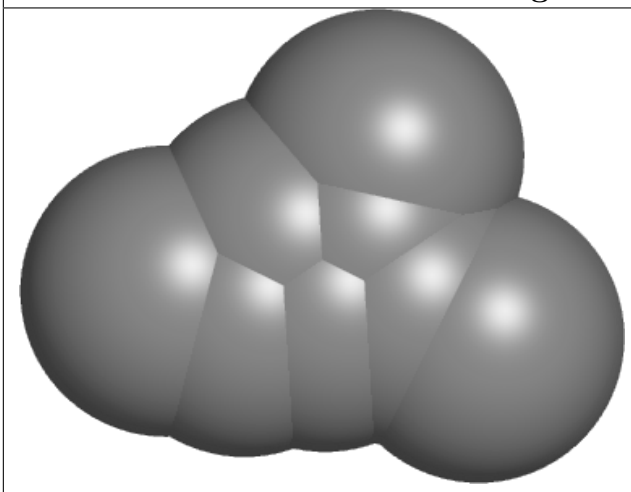
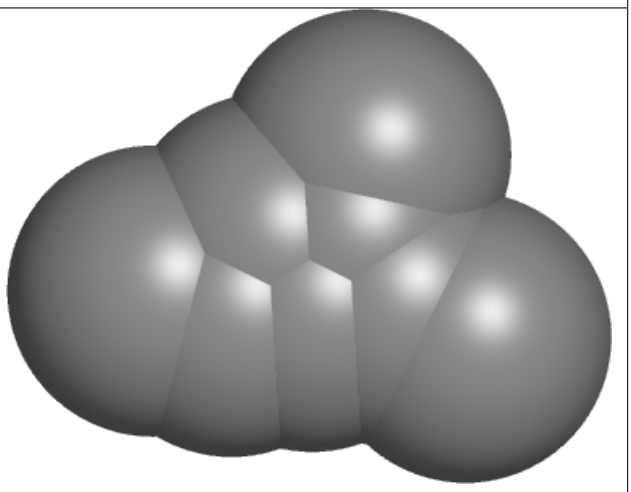
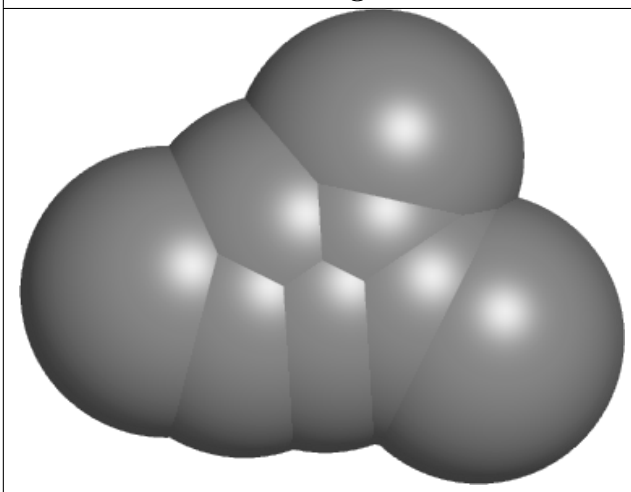
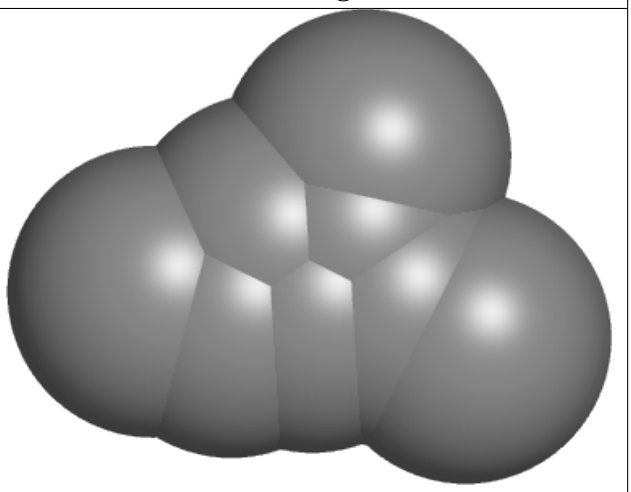
Torsions

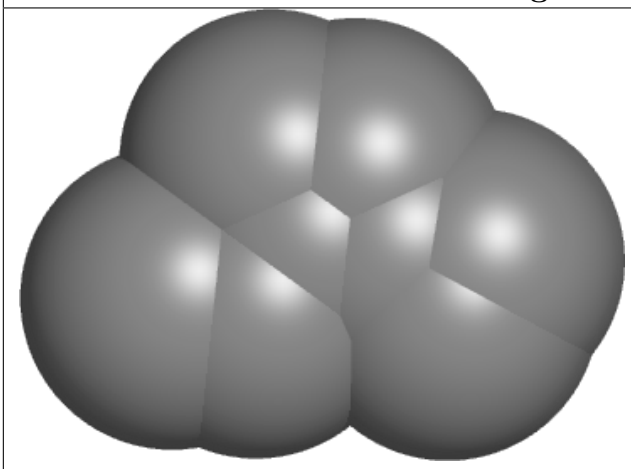
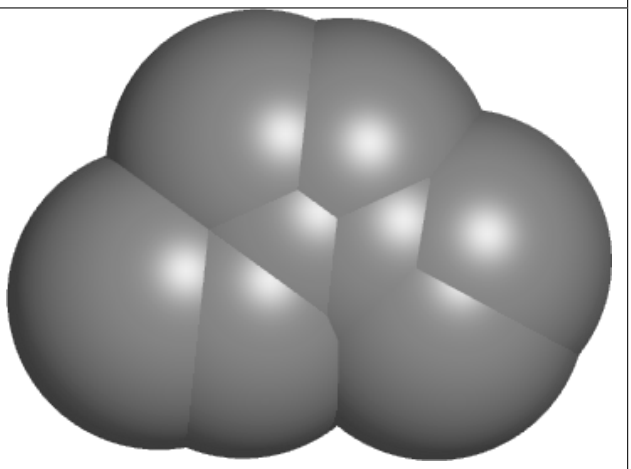
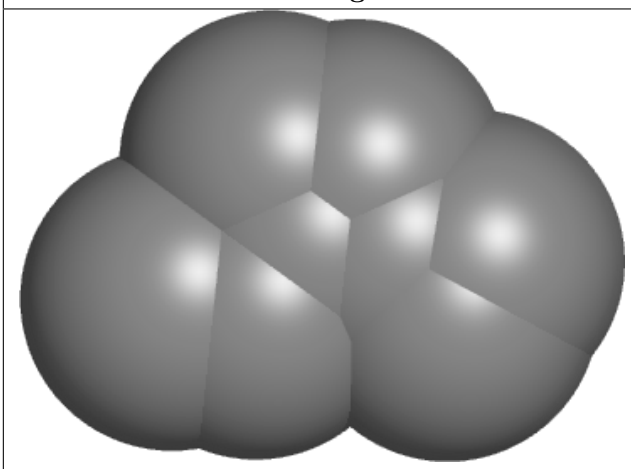
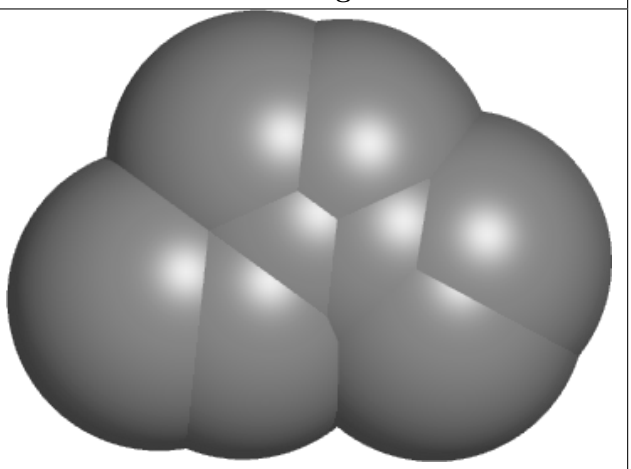


Rings

Ligand SF4 J 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 C 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 R 502	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 N 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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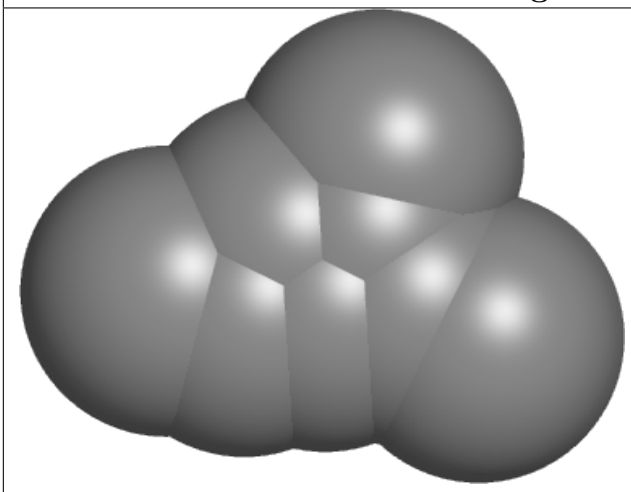
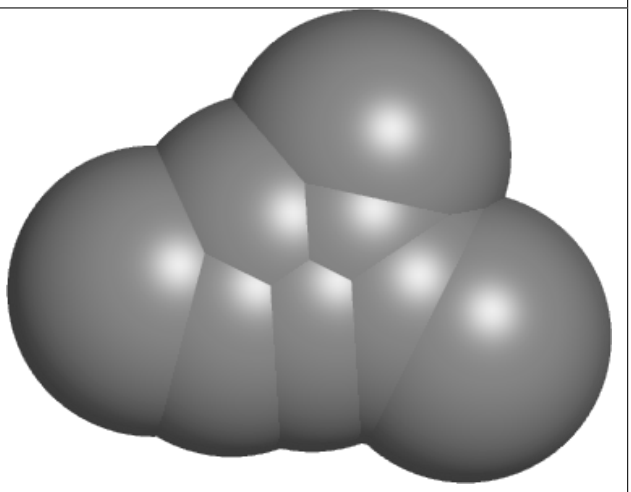
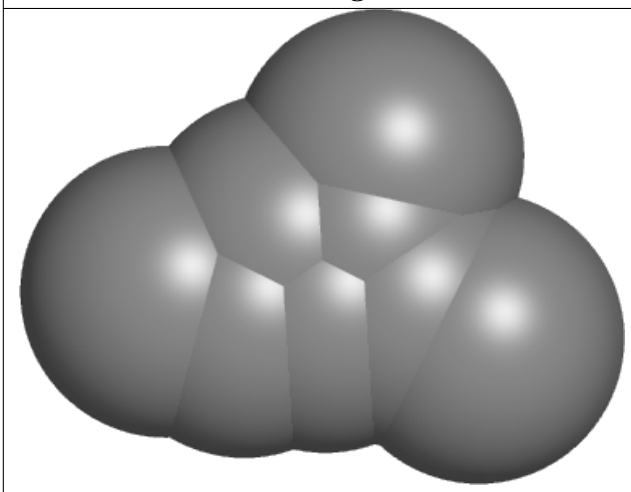
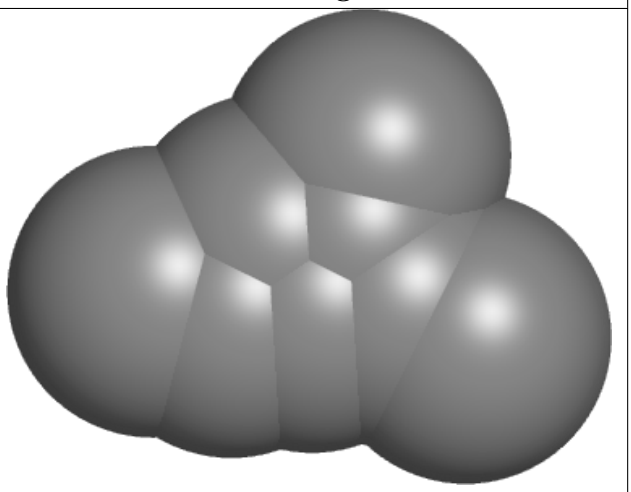
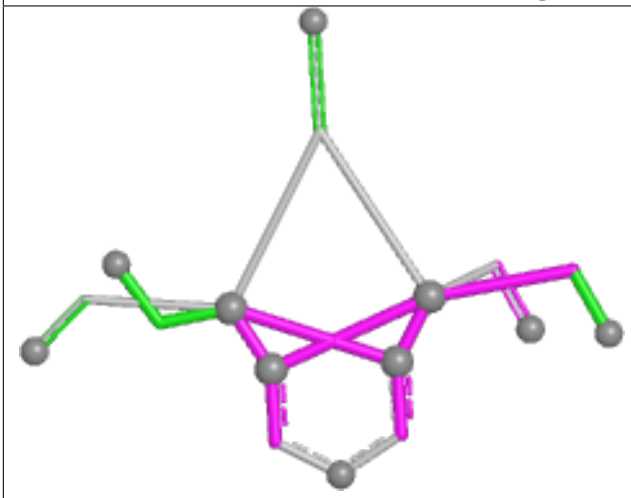
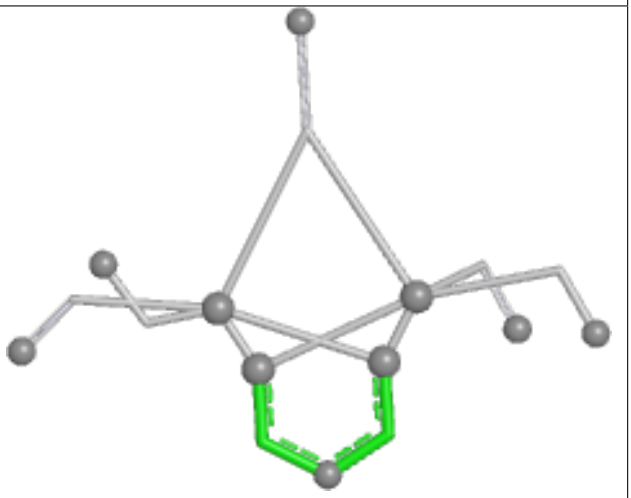
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

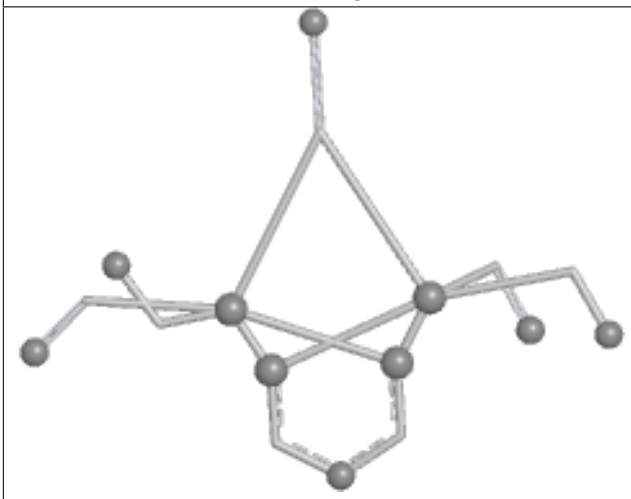
Ligand 402 D 503



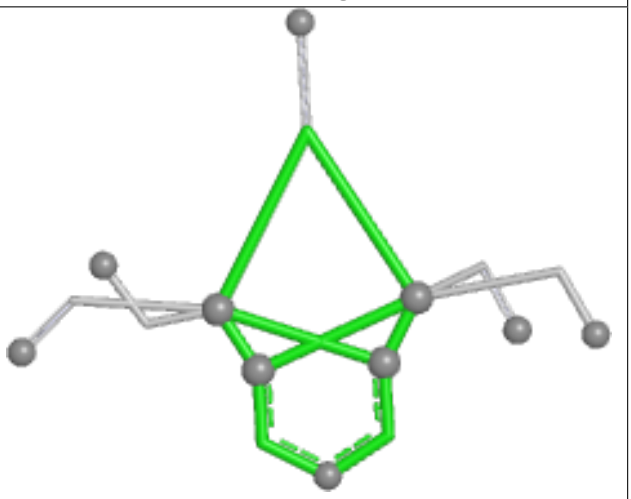
Bond lengths



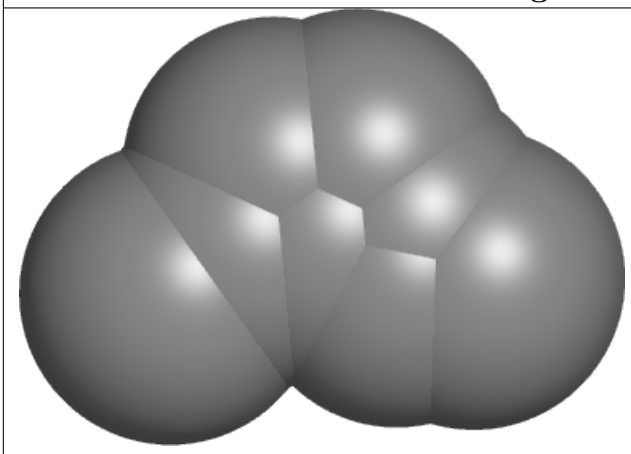
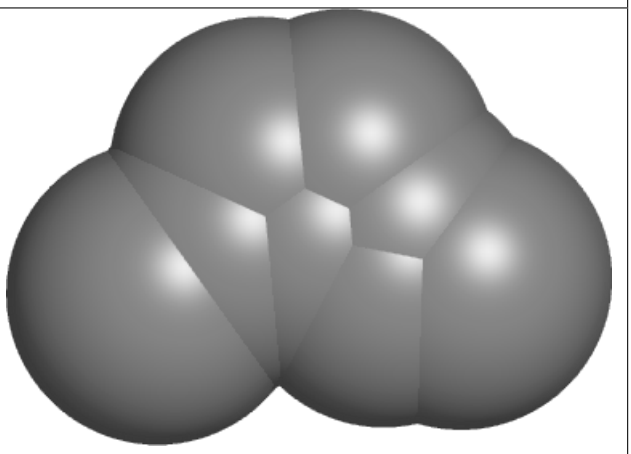
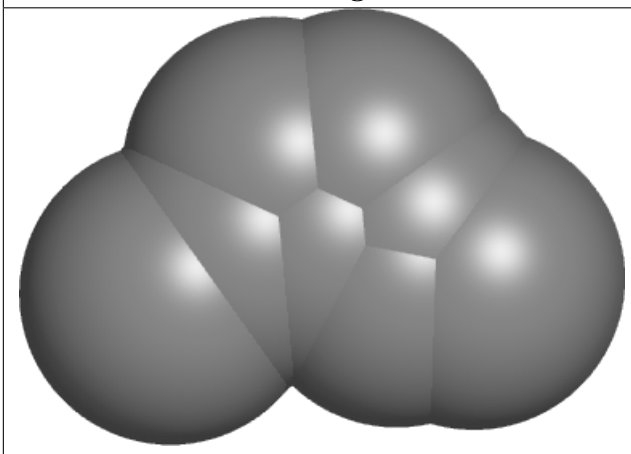
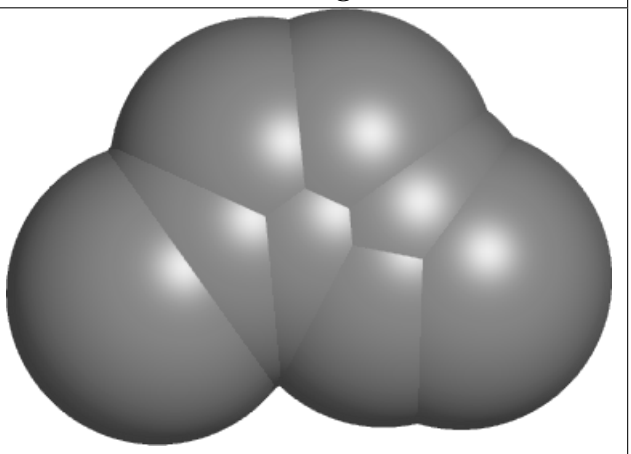
Bond angles



Torsions



Rings

Ligand SF4 K 504	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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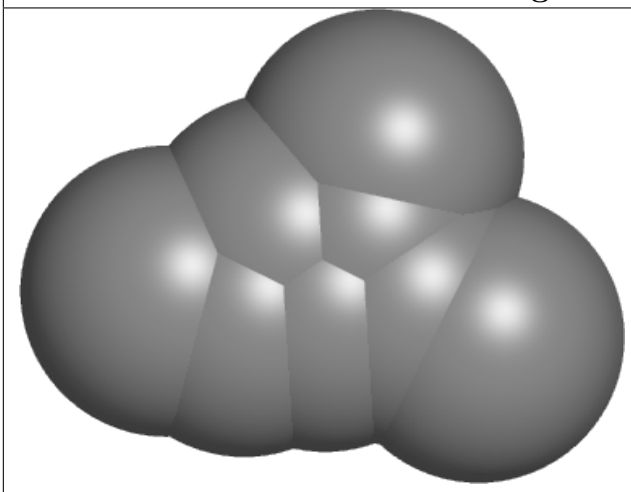
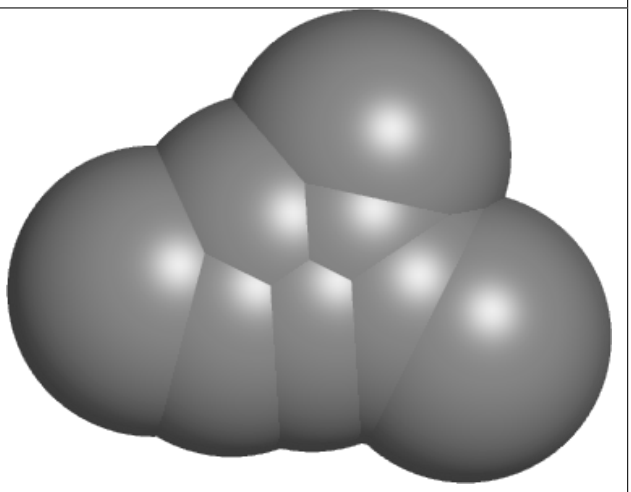
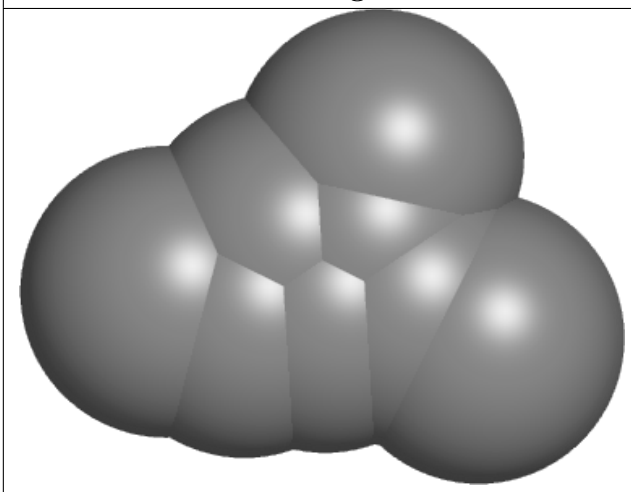
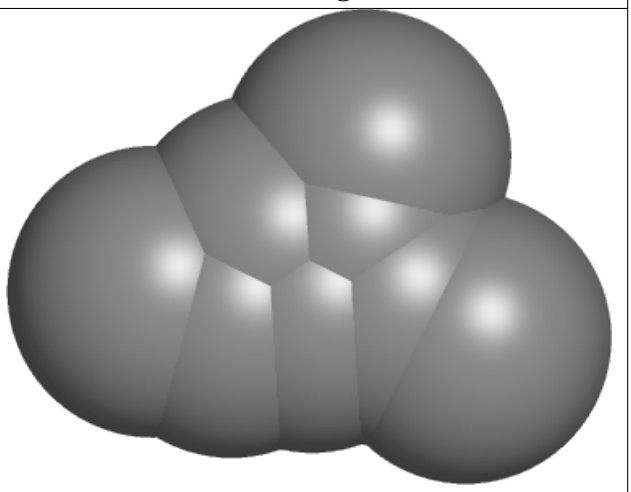
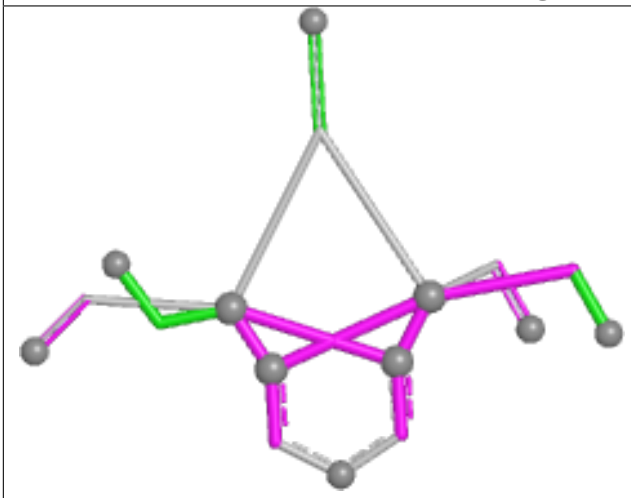
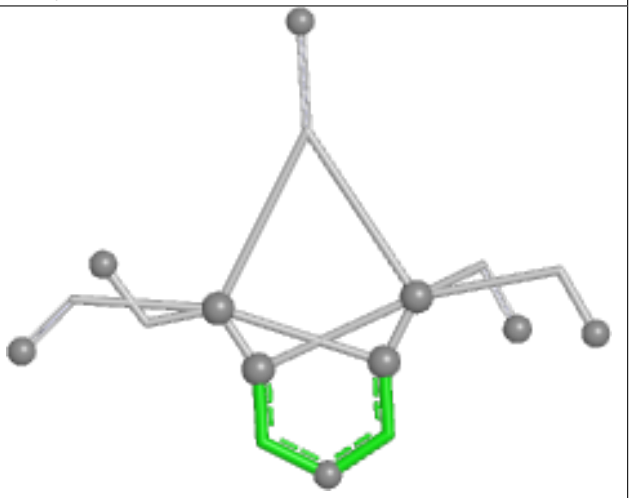
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

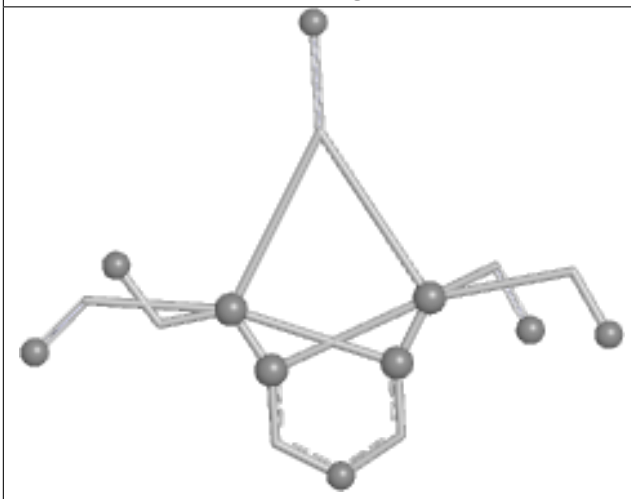
Ligand 402 Q 504



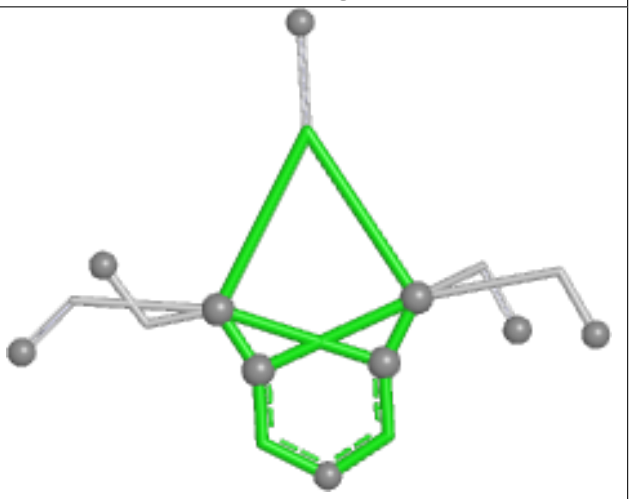
Bond lengths



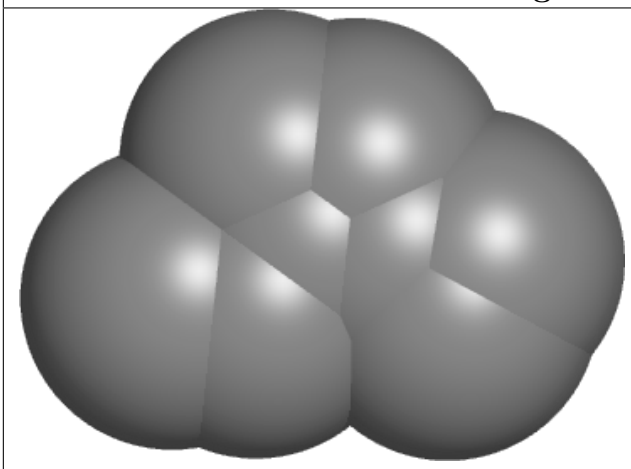
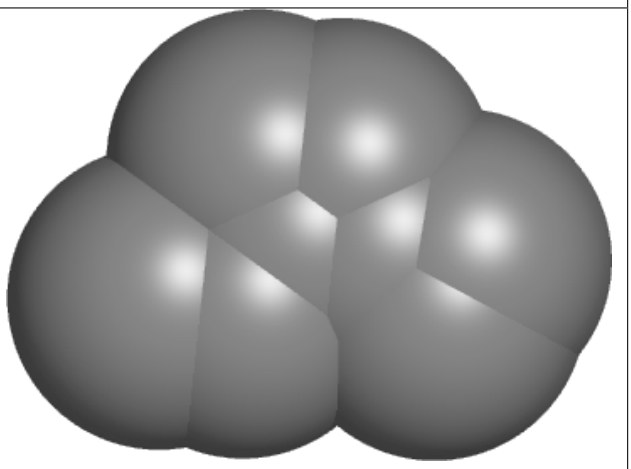
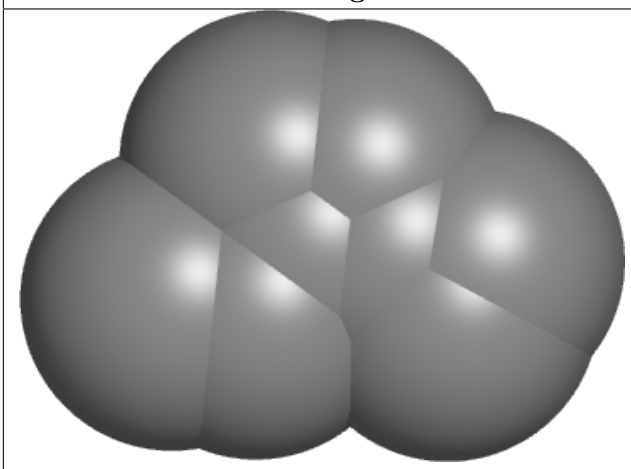
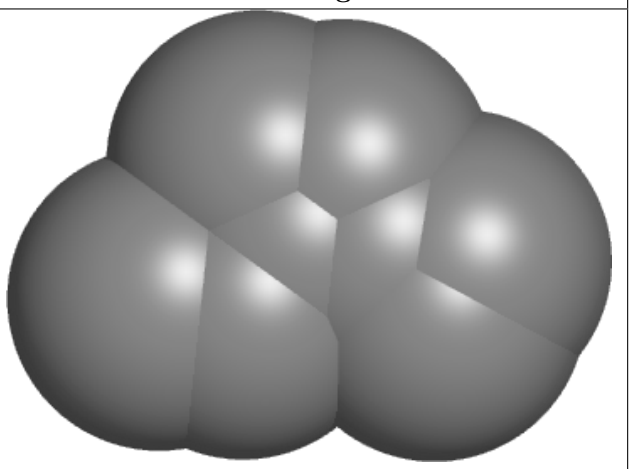
Bond angles

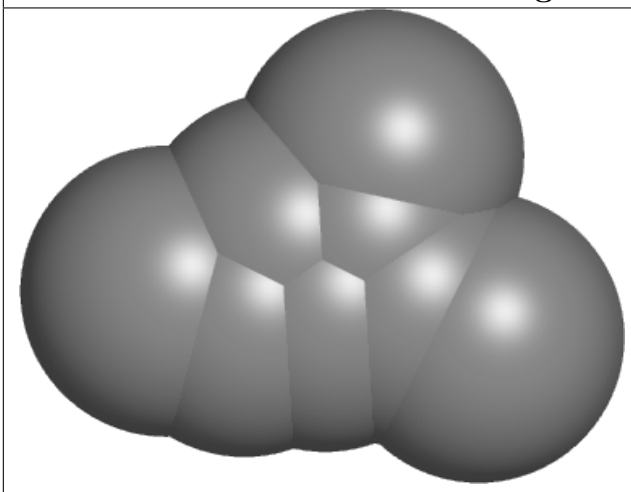
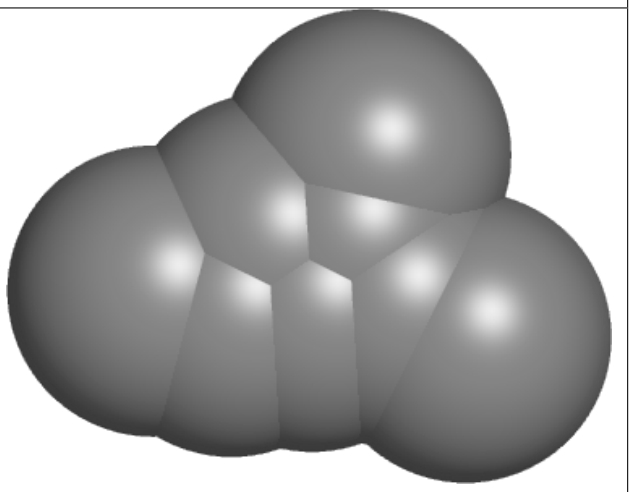
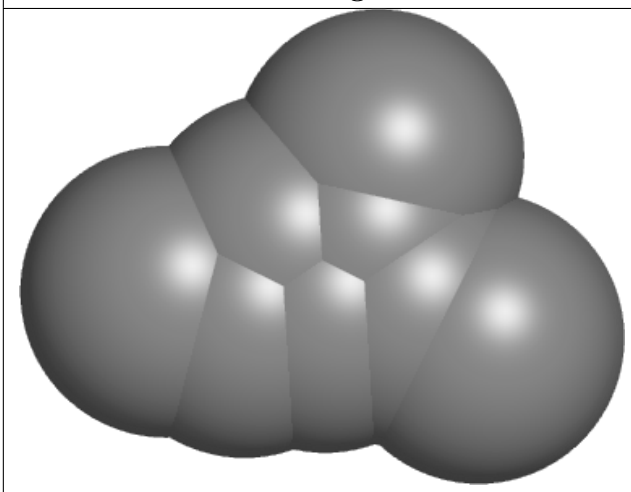
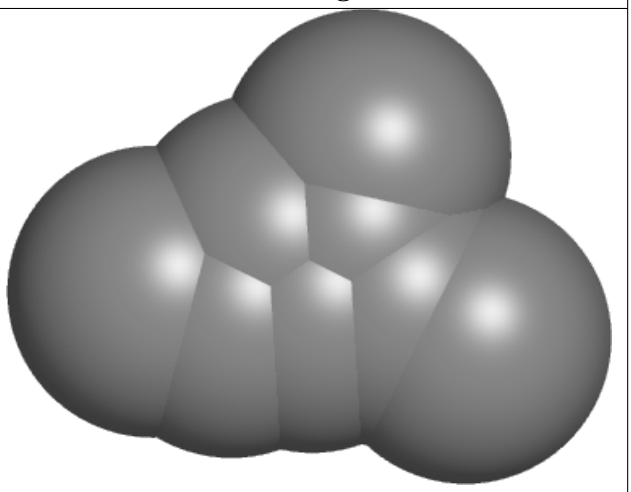


Torsions



Rings

Ligand SF4 Z 502	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 J 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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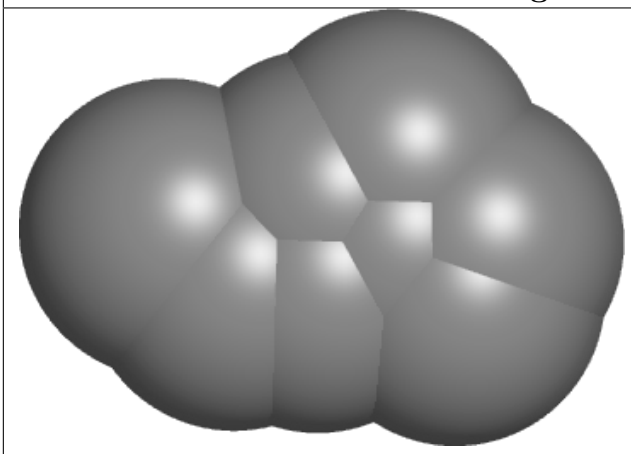
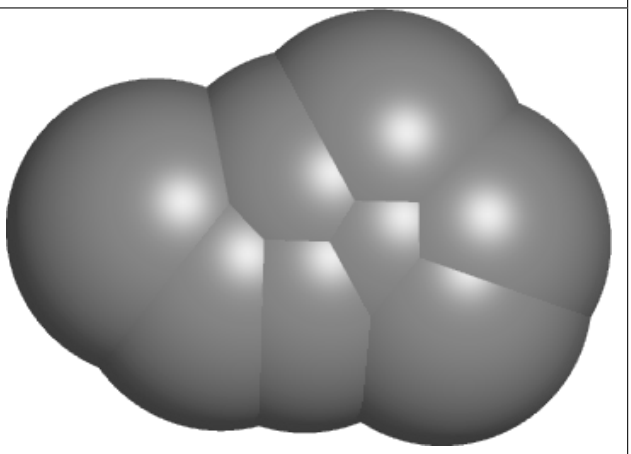
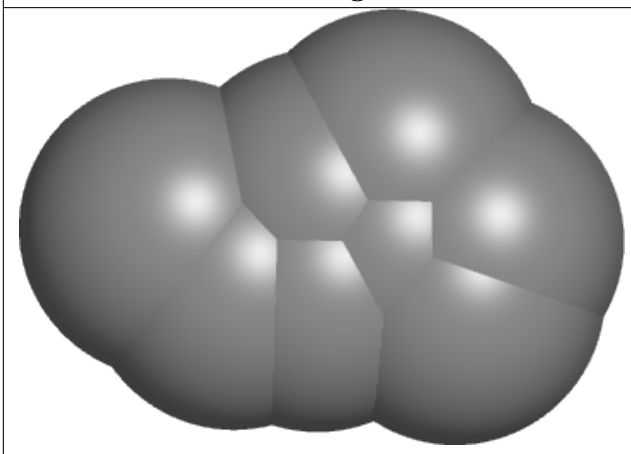
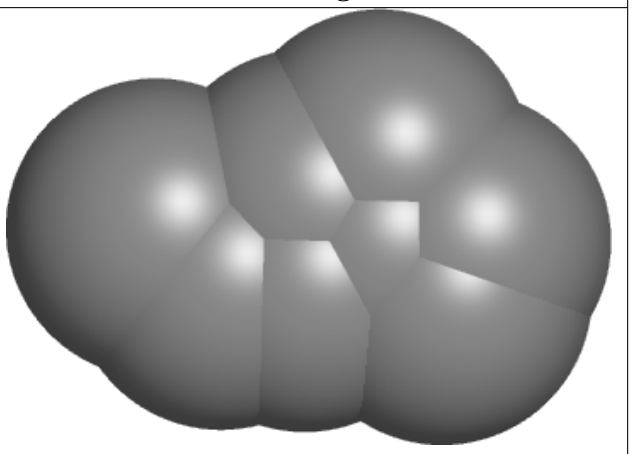
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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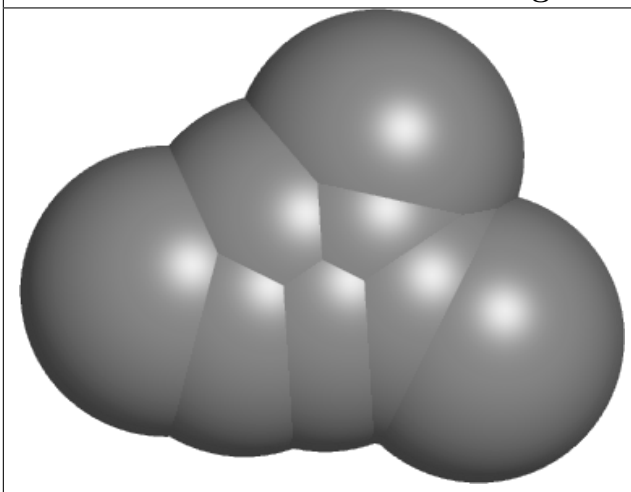
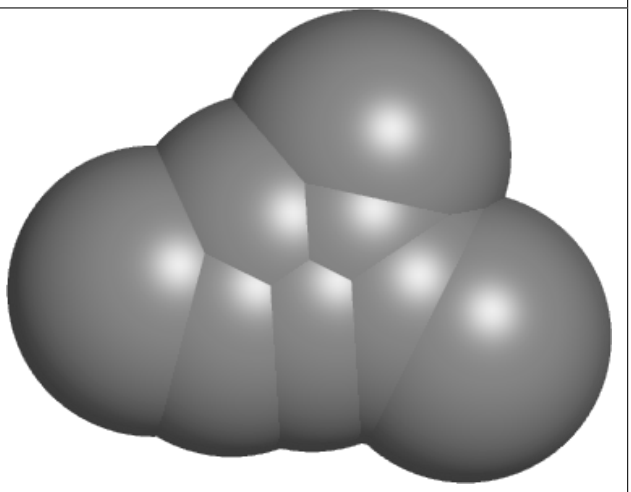
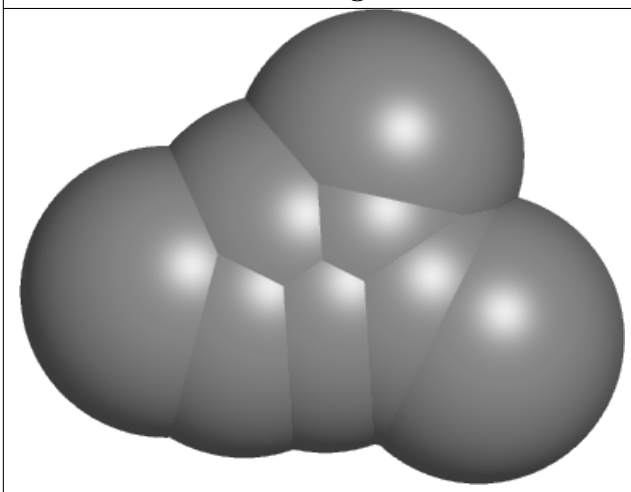
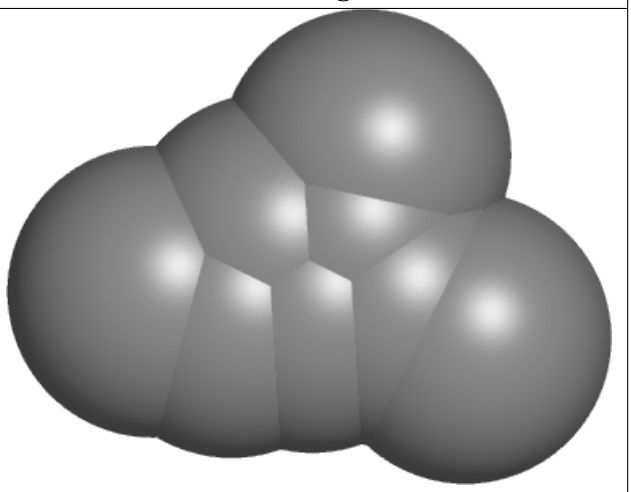
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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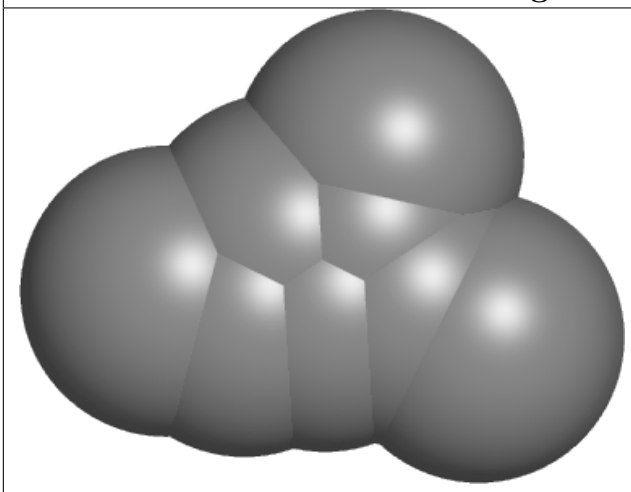
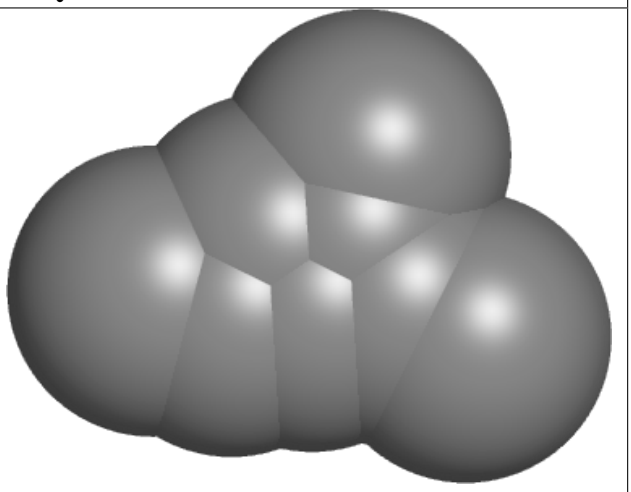
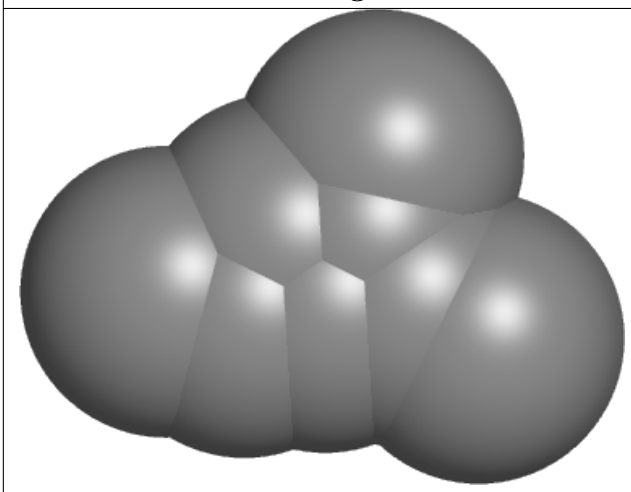
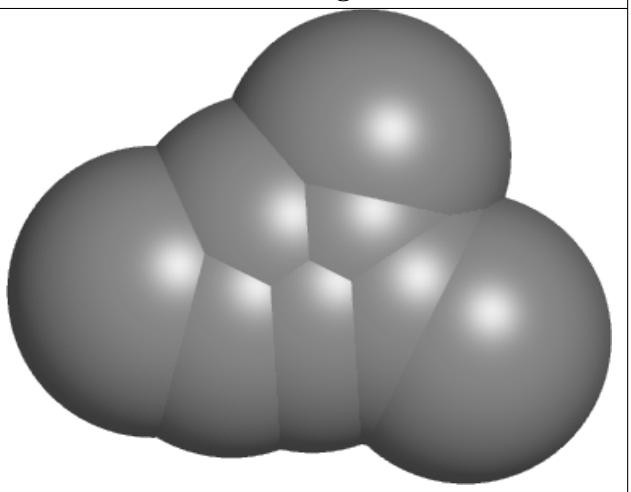
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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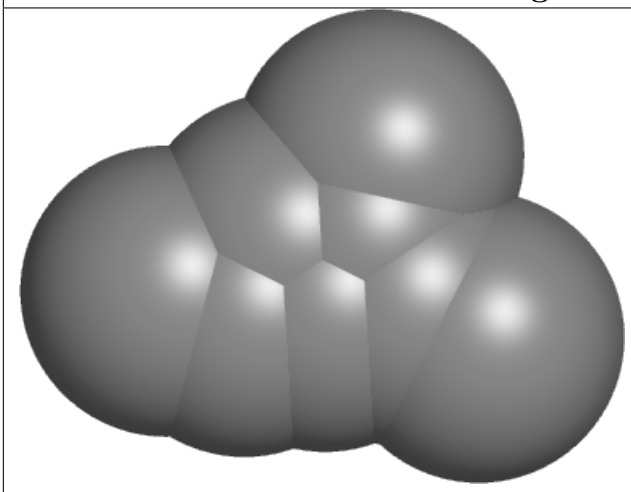
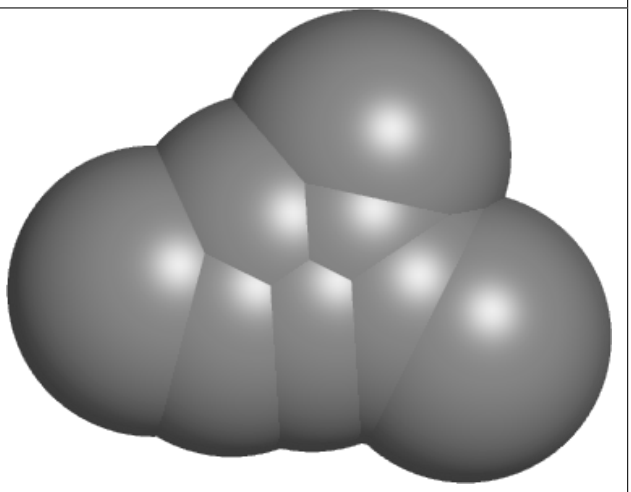
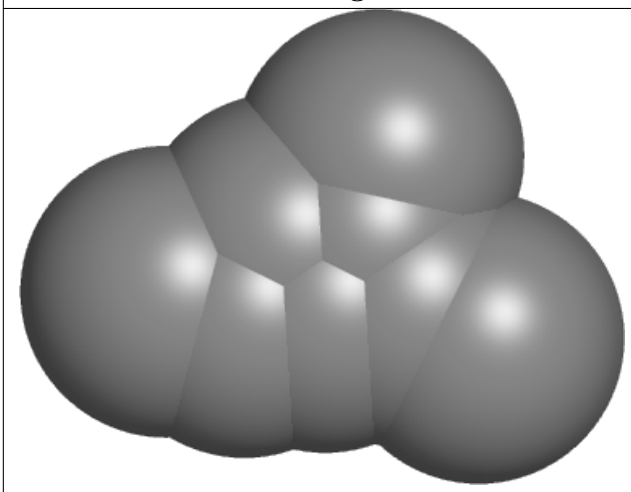
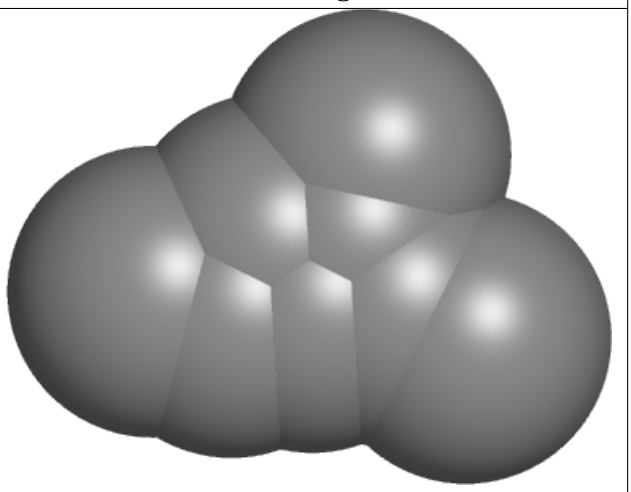
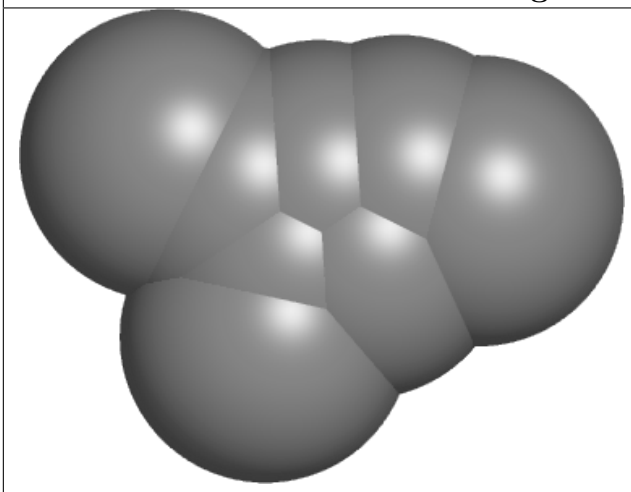
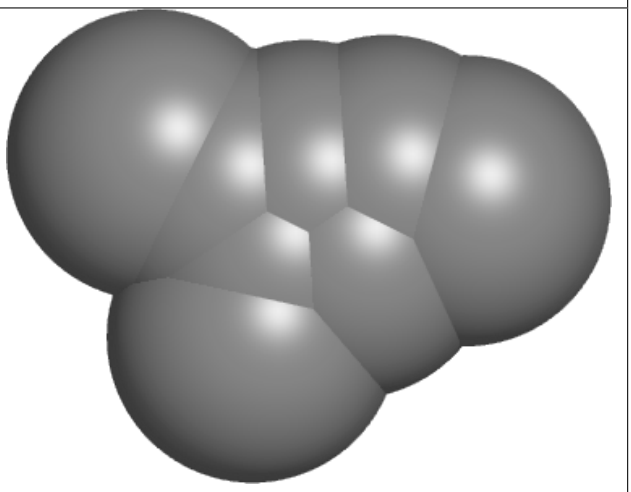
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

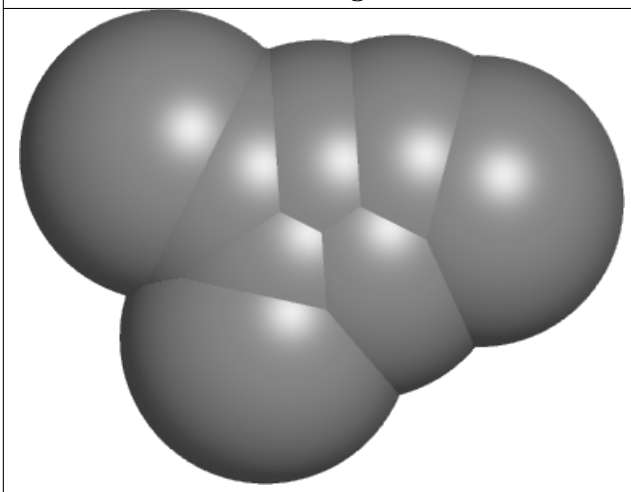
Ligand SF4 A 203



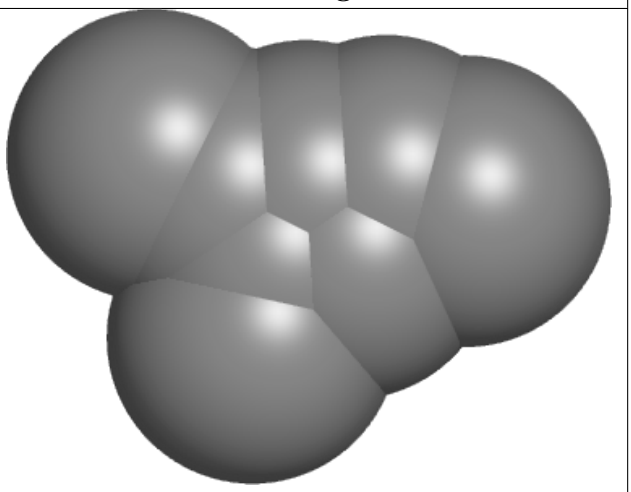
Bond lengths



Bond angles

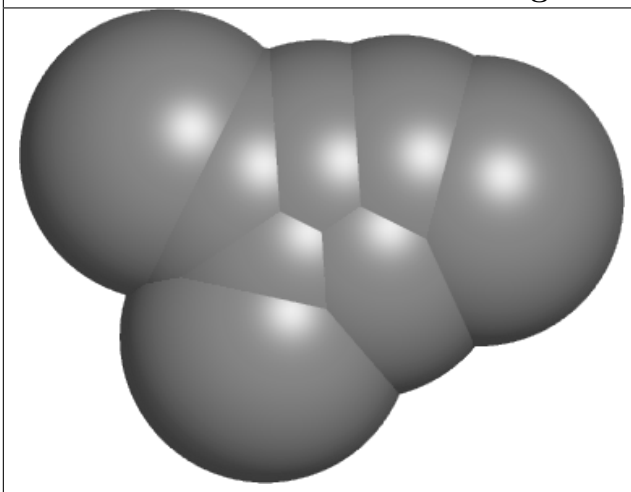


Torsions

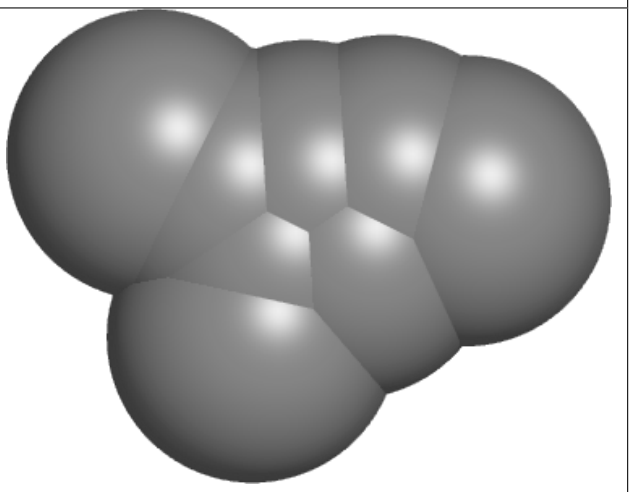


Rings

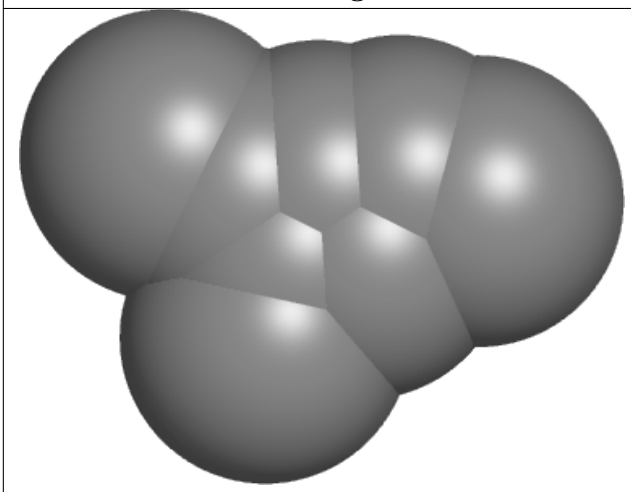
Ligand SF4 V 501



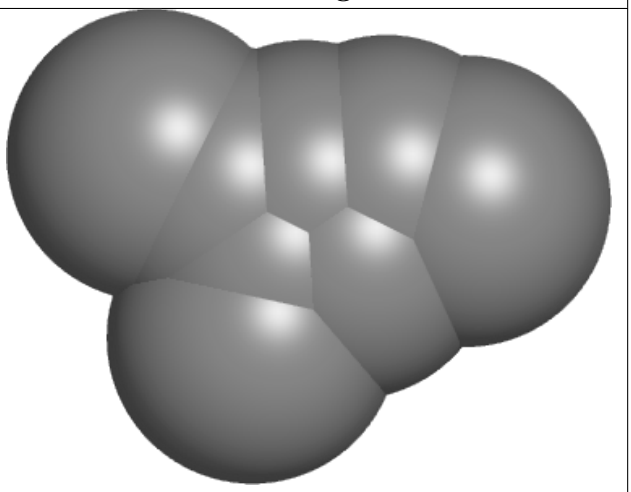
Bond lengths



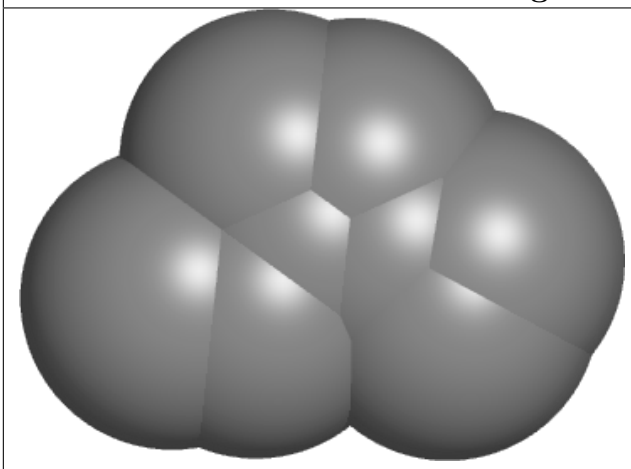
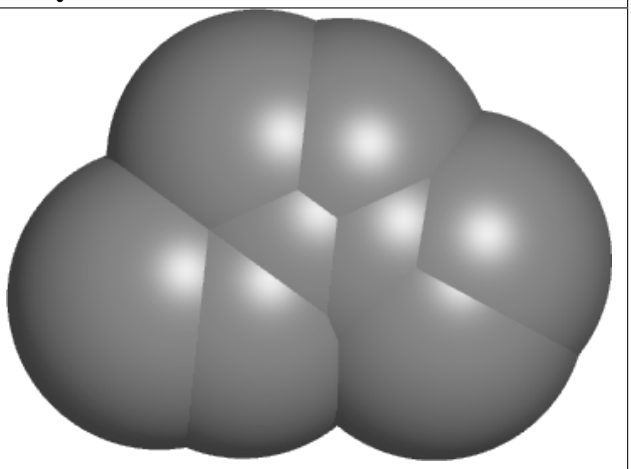
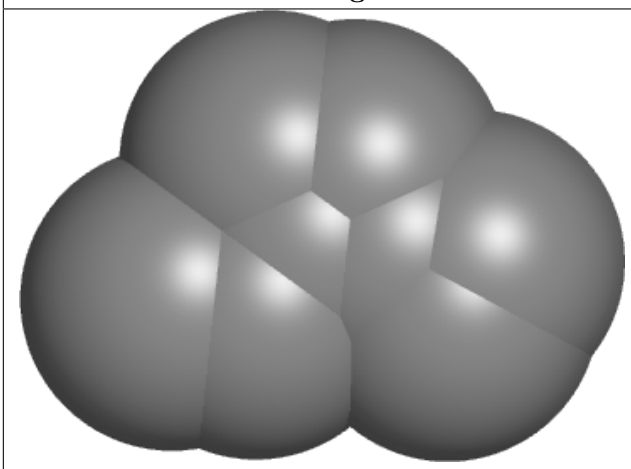
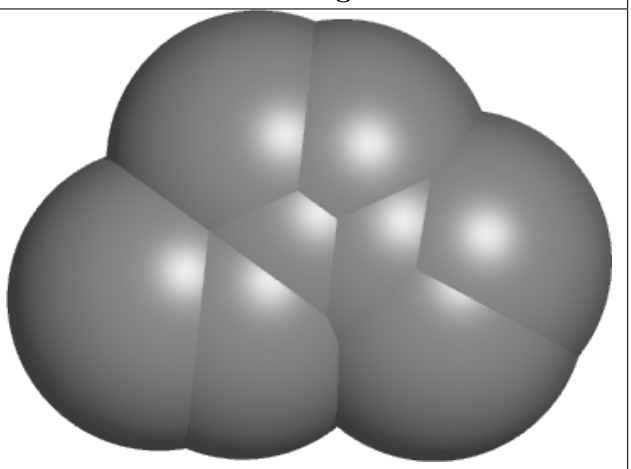
Bond angles

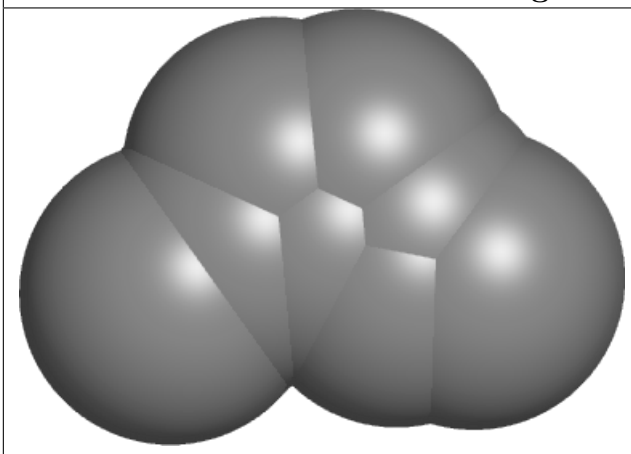
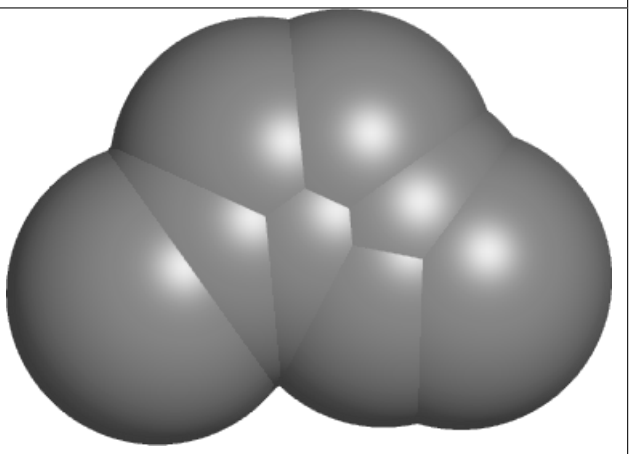
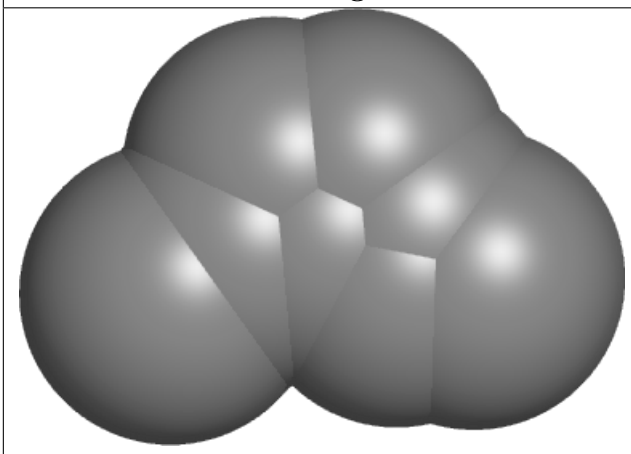
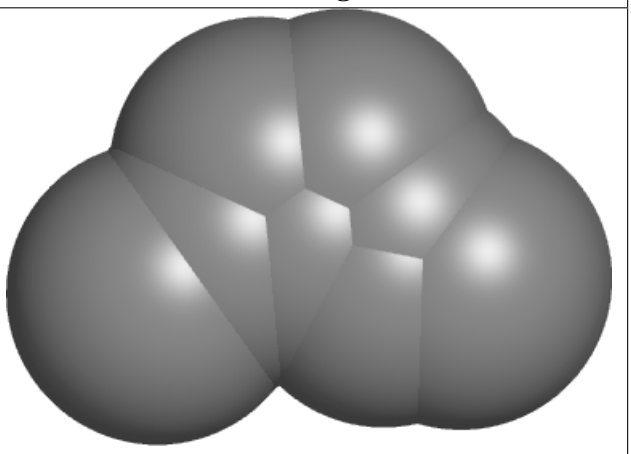


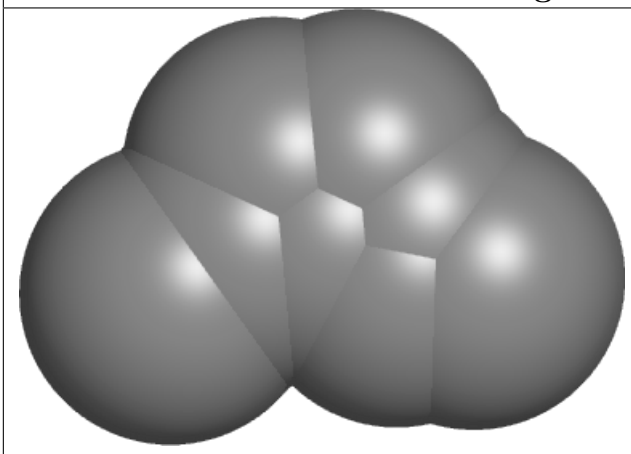
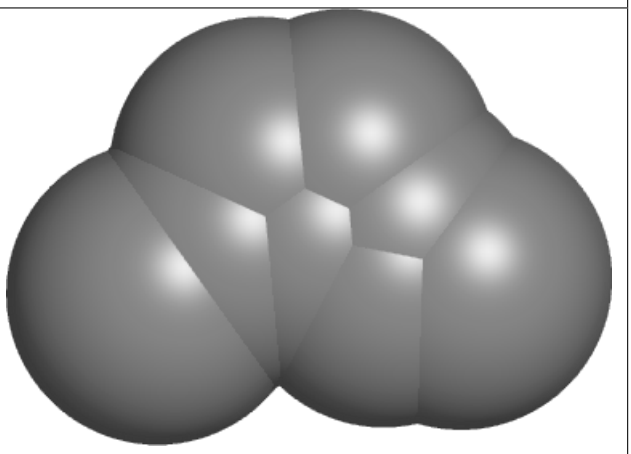
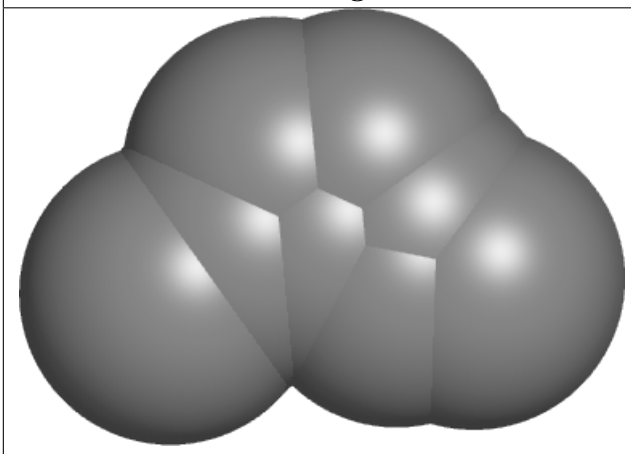
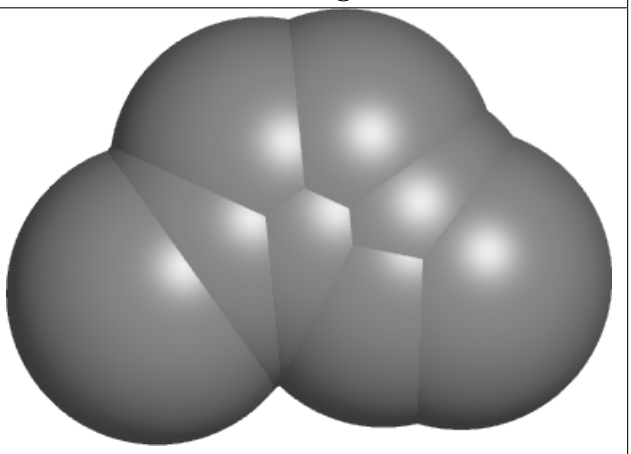
Torsions



Rings

Ligand SF4 Q 503	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 C 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 S 801	
	
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.

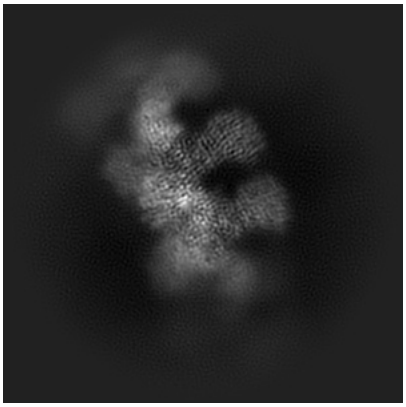
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14169. These allow visual inspection of the internal detail of the map and identification of artifacts.

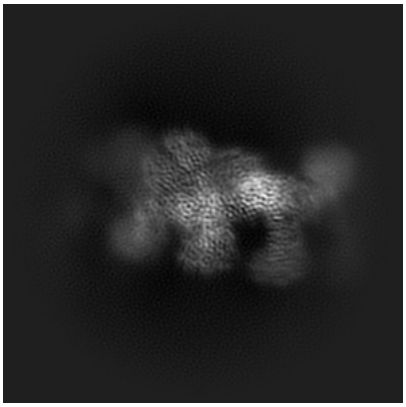
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

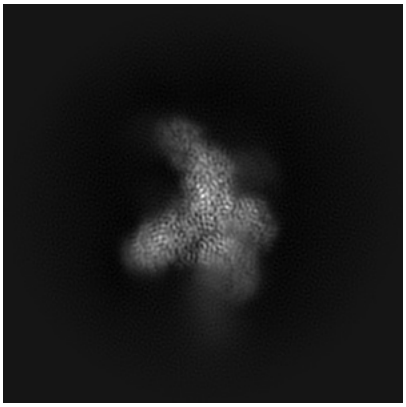
6.1.1 Primary map



X



Y

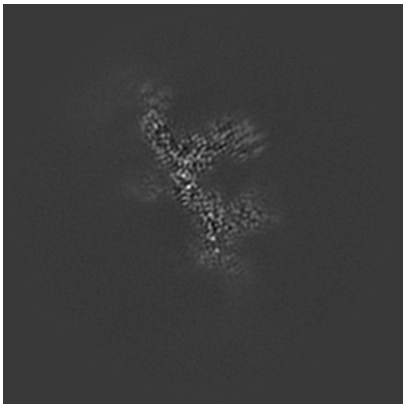


Z

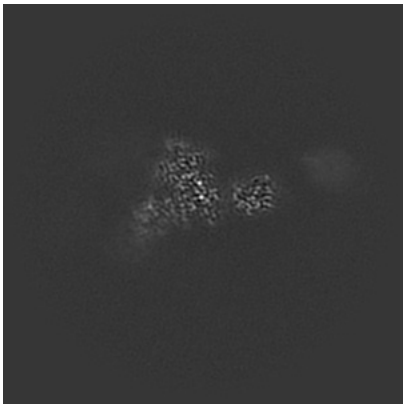
The images above show the map projected in three orthogonal directions.

6.2 Central slices

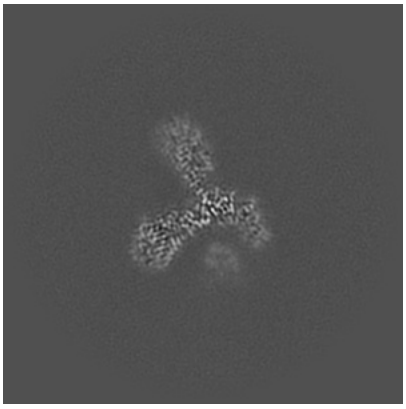
6.2.1 Primary map



X Index: 176



Y Index: 176

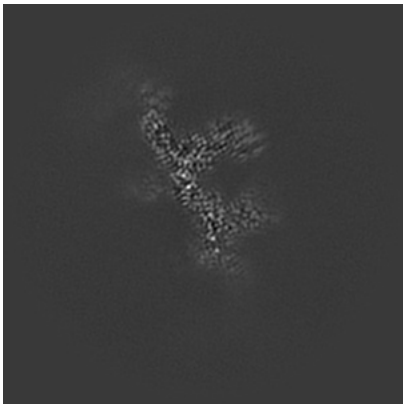


Z Index: 176

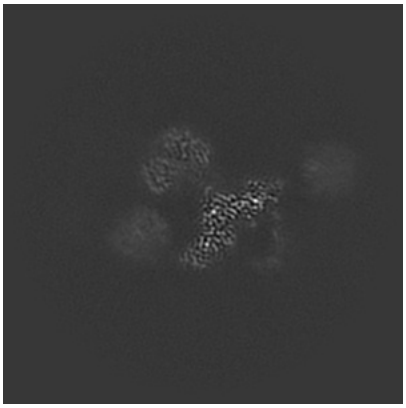
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

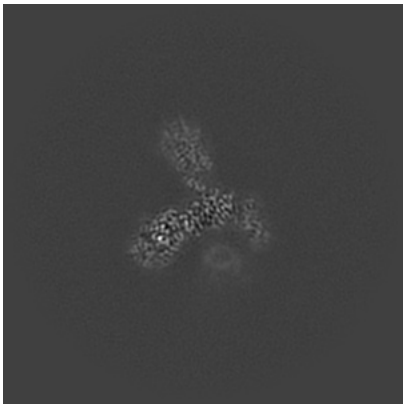
6.3.1 Primary map



X Index: 176



Y Index: 155



Z Index: 178

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

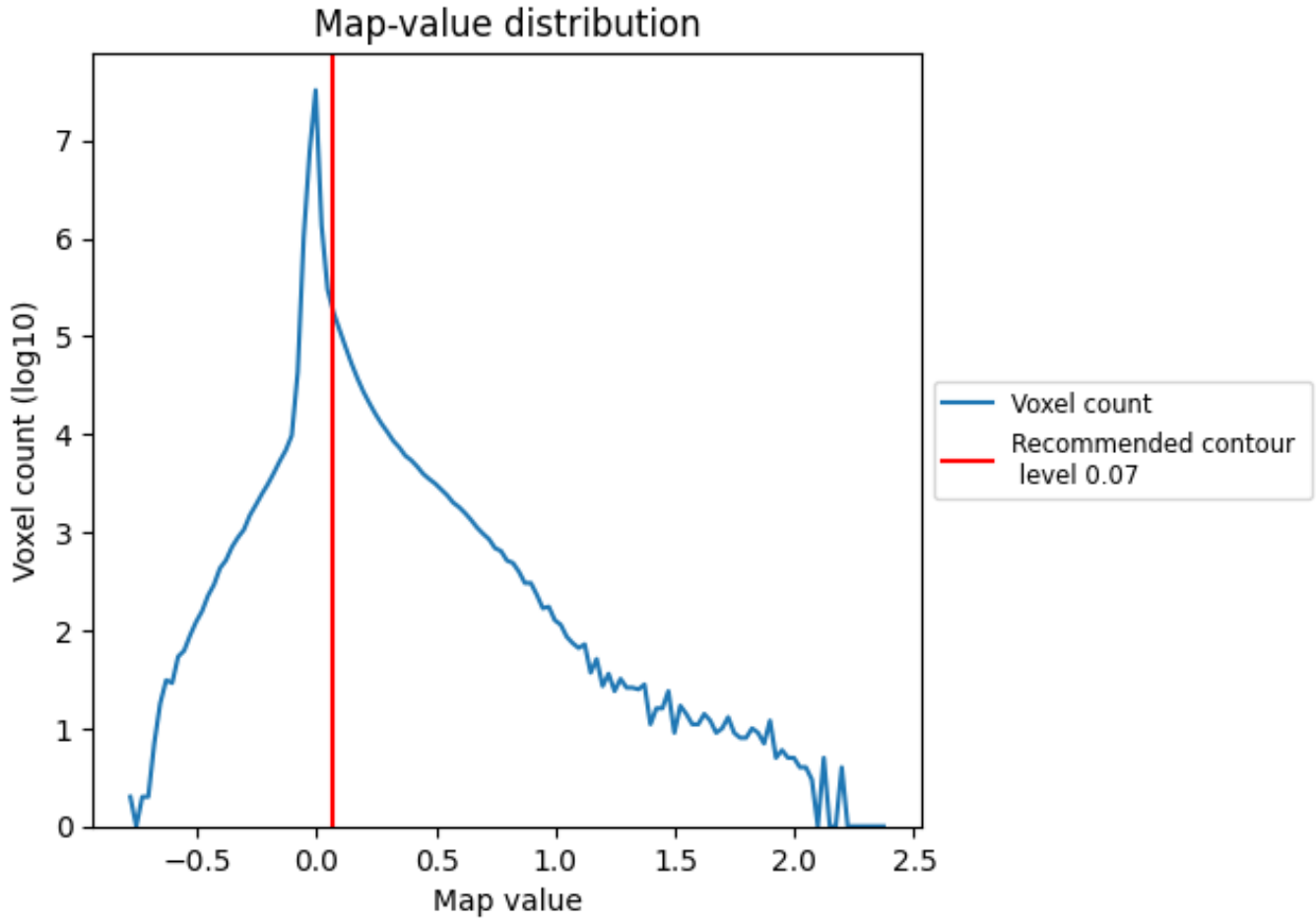
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

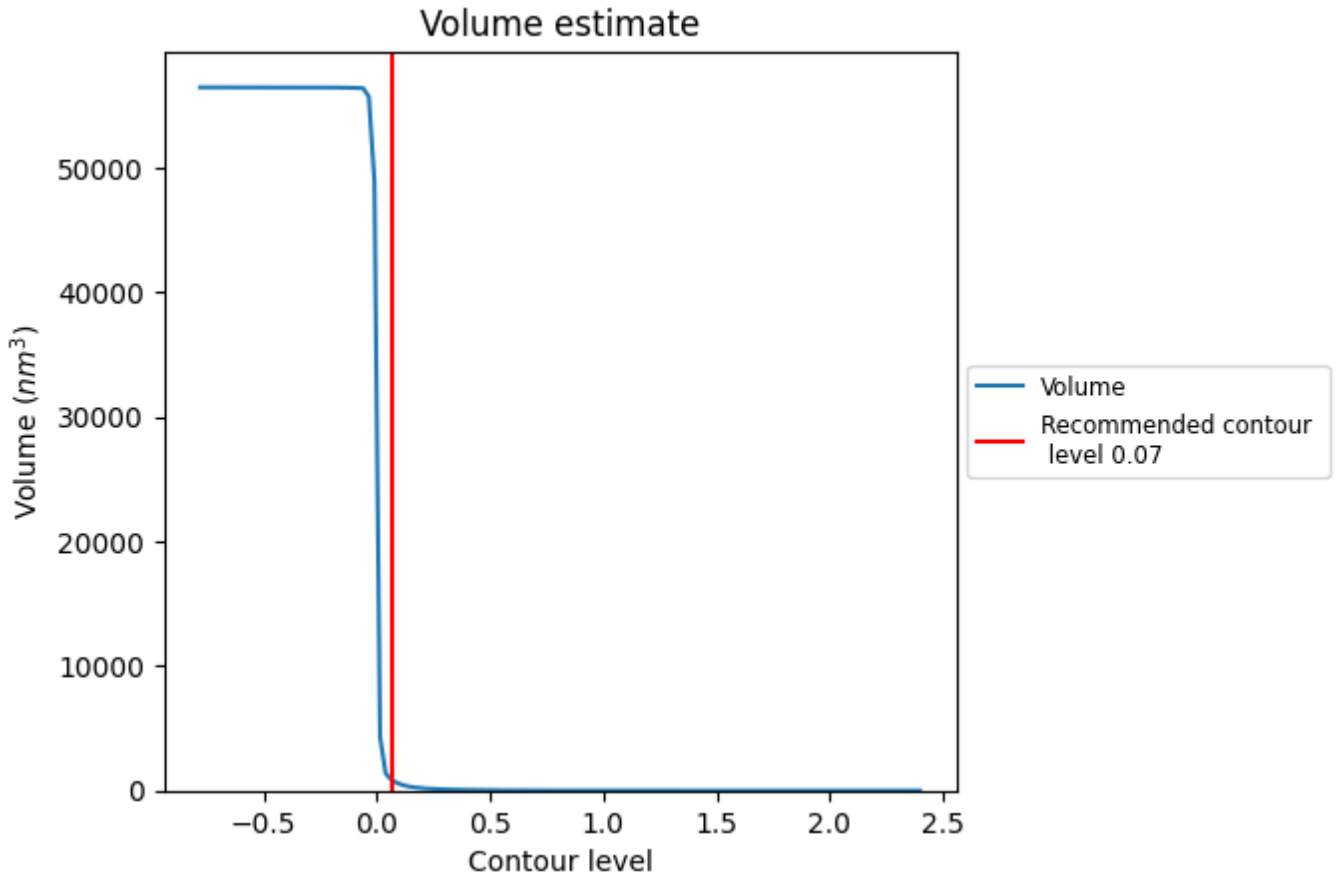
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

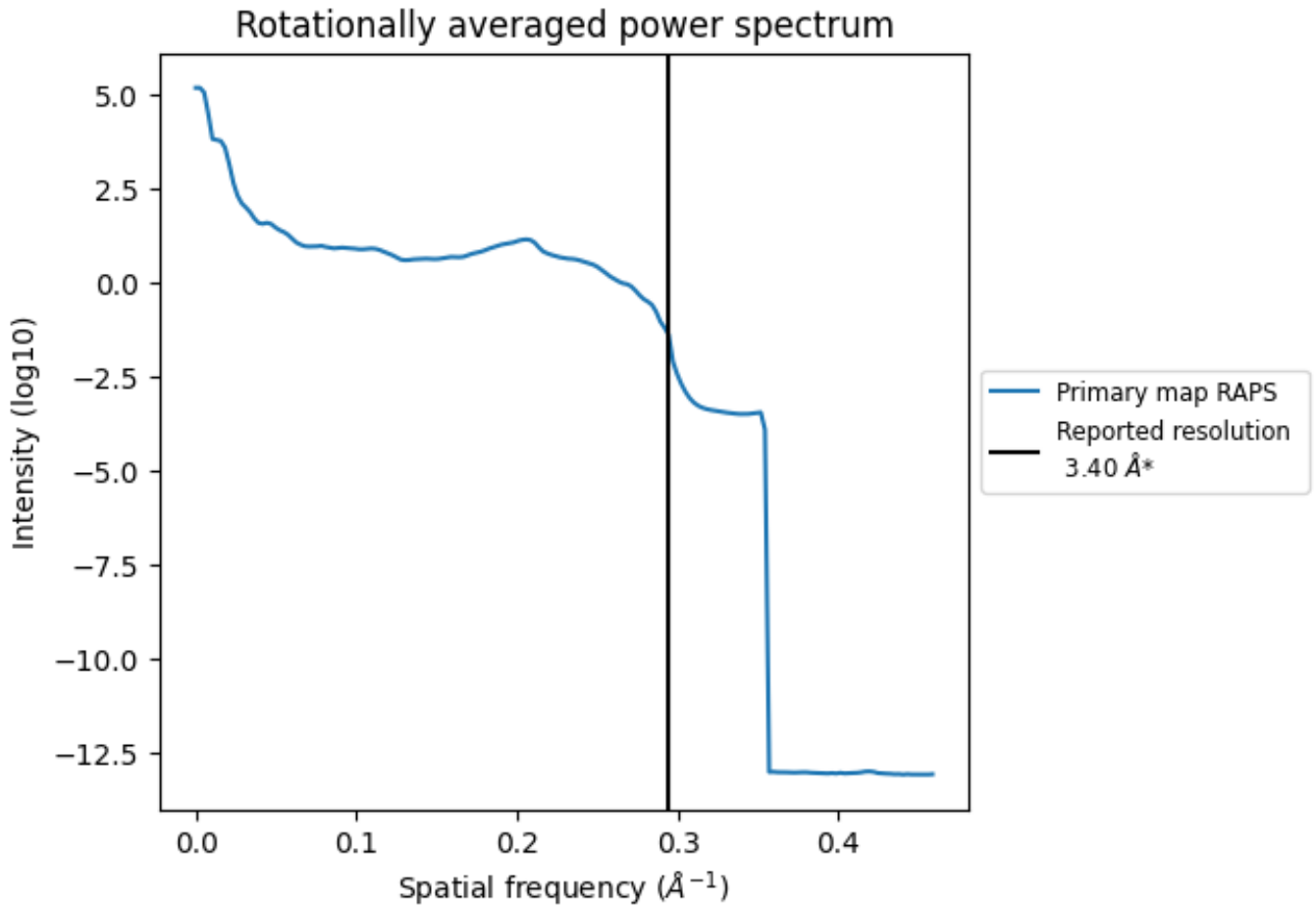
7.2 Volume estimate



The volume at the recommended contour level is 811 nm^3; this corresponds to an approximate mass of 733 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

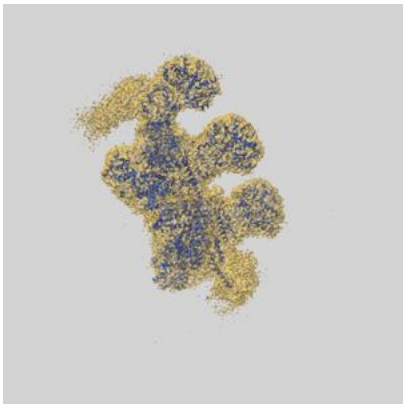
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

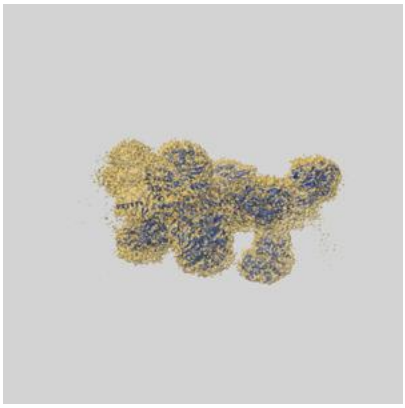
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14169 and PDB model 7QV7. Per-residue inclusion information can be found in section 3 on page 9.

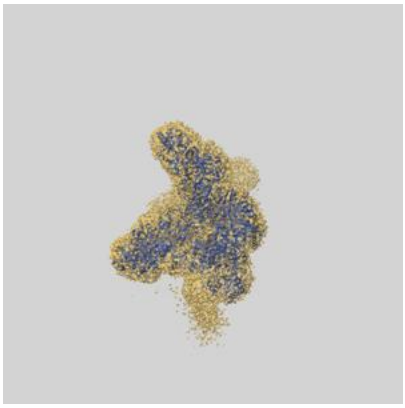
9.1 Map-model overlay



X



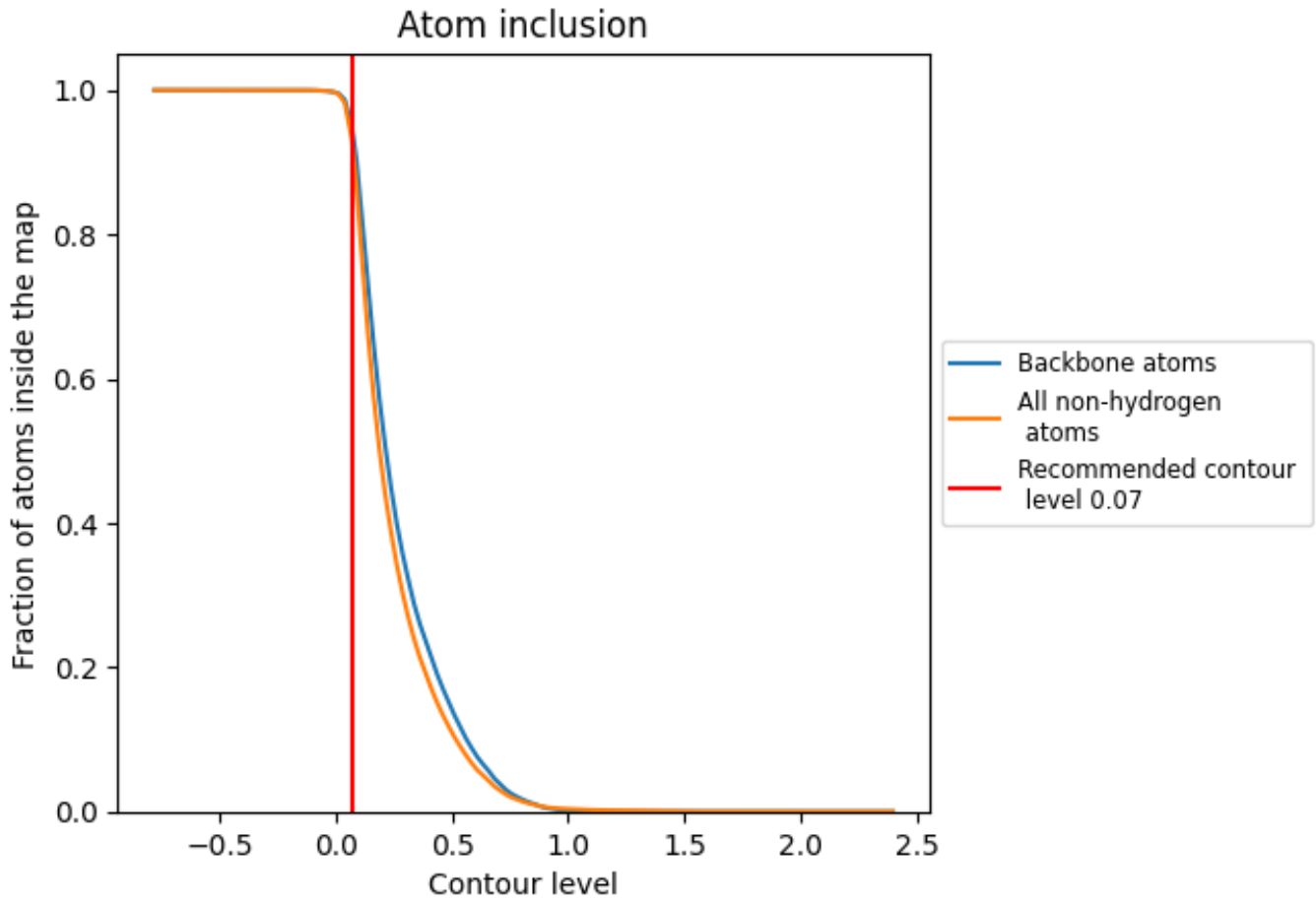
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.