wwPDB EM Validation Summary Report

Nov 20, 2022 – 03:39 pm GMT

PDB ID	:	5LER
EMDB ID	:	EMD-4044
Title	:	Structure of the bacterial sex F pilus (13.2 Angstrom rise)
Authors	:	Costa, T.R.D.; Ilangovan, I.; Ukleja, M.; Redzej, A.; Santini, J.M.; Smith, T.K.; Egelman, E.H.; Waksman, G.
Deposited on	:	2016-06-30
Resolution	:	5.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

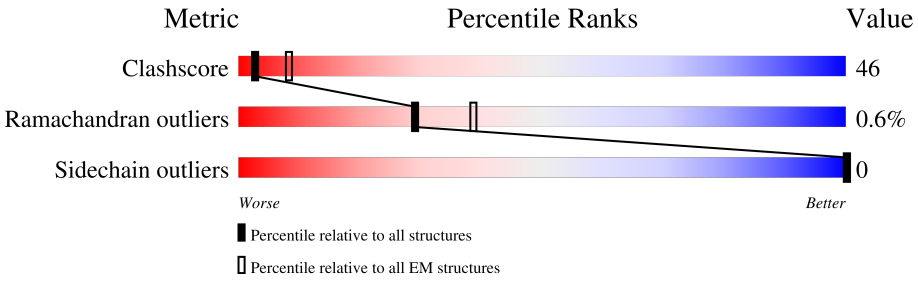
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.00 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	1A	65	15% 32% 66% ·
1	1B	65	9% 34% 65% ·
1	1C	65	12% 34% 65% ·
1	1D	65	11% 31% 66% ·
1	1E	65	11% 34% 65% ·
1	1F	65	12% 32% 65% ·
1	1G	65	8% 35% 62% ·
1	1H	65	12% 32% 66% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	1I	65	8% 34% 65%
1	1J	65	11% 32% 65%
1	1K	65	12% 34% 63%
1	1L	65	12% 35% 63%
1	1M	65	11% 32% 65%
1	1N	65	14% 37% 62%
1	1O	65	12% 40% 57%
1	2A	65	14% 32% 66%
1	2B	65	11% 34% 65%
1	2C	65	11% 32% 66%
1	2D	65	12% 31% 68%
1	2E	65	11% 34% 65%
1	2F	65	11% 32% 66%
1	2G	65	14% 35% 63%
1	2H	65	12% 32% 66%
1	2I	65	9% 34% 65%
1	2J	65	11% 34% 65%
1	2K	65	11% 35% 63%
1	2L	65	11% 35% 63%
1	2M	65	12% 32% 66%
1	2N	65	17% 37% 60%
1	2O	65	9% 40% 58%
1	3A	65	14% 32% 66%
1	3B	65	11% 34% 65%
1	3C	65	11% 32% 66%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	3D	65	15% 31% 68%
1	3E	65	12% 34% 65%
1	3F	65	9% 32% 66%
1	3G	65	8% 35% 63%
1	3H	65	15% 32% 66%
1	3I	65	15% 34% 65%
1	3J	65	9% 34% 63%
1	3K	65	11% 35% 62%
1	3L	65	11% 35% 63%
1	3M	65	11% 32% 65%
1	3N	65	15% 37% 60%
1	3O	65	9% 40% 57%
1	4A	65	12% 32% 65%
1	4B	65	9% 34% 65%
1	4C	65	14% 32% 66%
1	4D	65	8% 32% 66%
1	4E	65	11% 34% 65%
1	4F	65	11% 32% 66%
1	4G	65	12% 35% 63%
1	4H	65	12% 32% 66%
1	4I	65	14% 34% 65%
1	4J	65	11% 34% 63%
1	4K	65	11% 35% 62%
1	4L	65	14% 35% 63%
1	4M	65	11% 32% 66%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	4N	65	12% 37% 60%
1	4O	65	9% 40% 57%
1	5A	65	12% 32% 66%
1	5B	65	11% 35% 62%
1	5C	65	12% 32% 65%
1	5D	65	12% 31% 66%
1	5E	65	9% 34% 65%
1	5F	65	9% 32% 65%
1	5G	65	14% 35% 63%
1	5H	65	9% 32% 66%
1	5I	65	14% 34% 65%
1	5J	65	12% 34% 63%
1	5K	65	8% 35% 62%
1	5L	65	12% 34% 65%
1	5M	65	12% 31% 66%
1	5N	65	15% 37% 62%
1	5O	65	9% 40% 57%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 36539 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 Pilin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	65	Total	C	N	O	S	0	0
			475	314	73	83	5		
1	1B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	1O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2A	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	2O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3A	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		

Continued on next page...

Continued from previous page...

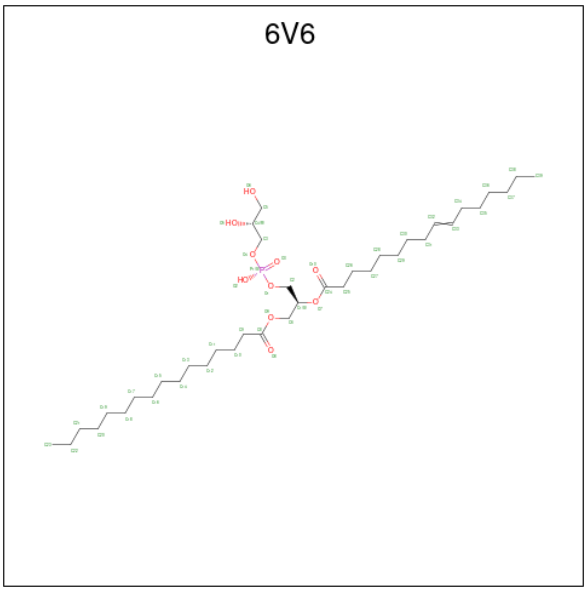
Mol	Chain	Residues	Atoms					AltConf	Trace
1	3I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	3O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4A	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	4N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5A	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5B	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5C	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5D	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5E	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5F	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5G	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5H	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5I	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5J	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5K	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5L	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5M	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5N	65	Total	C	N	O	S	0	0
			476	314	74	83	5		
1	5O	65	Total	C	N	O	S	0	0
			476	314	74	83	5		

- Molecule 2 is [(2 {S})-3-[[(2 {R})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-2-hexadec-9-enoyloxy-propyl] hexadecanoate (three-letter code: 6V6) (formula: $C_{38}H_{73}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
2	1A	1	Total	C	O	P	0
			12	5	6	1	
2	1B	1	Total	C	O	P	0
			12	5	6	1	
2	1C	1	Total	C	O	P	0
			12	5	6	1	
2	1D	1	Total	C	O	P	0
			12	5	6	1	
2	1E	1	Total	C	O	P	0
			12	5	6	1	
2	1F	1	Total	C	O	P	0
			12	5	6	1	
2	1G	1	Total	C	O	P	0
			12	5	6	1	
2	1H	1	Total	C	O	P	0
			12	5	6	1	
2	1I	1	Total	C	O	P	0
			12	5	6	1	
2	1J	1	Total	C	O	P	0
			12	5	6	1	
2	1K	1	Total	C	O	P	0
			12	5	6	1	
2	1L	1	Total	C	O	P	0
			12	5	6	1	
2	1M	1	Total	C	O	P	0
			12	5	6	1	
2	1N	1	Total	C	O	P	0
			12	5	6	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	2A	1	Total	C	O	P	0
			12	5	6	1	
2	2B	1	Total	C	O	P	0
			12	5	6	1	
2	2C	1	Total	C	O	P	0
			12	5	6	1	
2	2D	1	Total	C	O	P	0
			12	5	6	1	
2	2E	1	Total	C	O	P	0
			12	5	6	1	
2	2F	1	Total	C	O	P	0
			12	5	6	1	
2	2G	1	Total	C	O	P	0
			12	5	6	1	
2	2H	1	Total	C	O	P	0
			12	5	6	1	
2	2I	1	Total	C	O	P	0
			12	5	6	1	
2	2J	1	Total	C	O	P	0
			12	5	6	1	
2	2K	1	Total	C	O	P	0
			12	5	6	1	
2	2L	1	Total	C	O	P	0
			12	5	6	1	
2	2M	1	Total	C	O	P	0
			12	5	6	1	
2	2N	1	Total	C	O	P	0
			12	5	6	1	
2	3A	1	Total	C	O	P	0
			12	5	6	1	
2	3B	1	Total	C	O	P	0
			12	5	6	1	
2	3C	1	Total	C	O	P	0
			12	5	6	1	
2	3D	1	Total	C	O	P	0
			12	5	6	1	
2	3E	1	Total	C	O	P	0
			12	5	6	1	
2	3F	1	Total	C	O	P	0
			12	5	6	1	
2	3G	1	Total	C	O	P	0
			12	5	6	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	3H	1	Total	C	O	P	0
			12	5	6	1	
2	3I	1	Total	C	O	P	0
			12	5	6	1	
2	3J	1	Total	C	O	P	0
			12	5	6	1	
2	3K	1	Total	C	O	P	0
			12	5	6	1	
2	3L	1	Total	C	O	P	0
			12	5	6	1	
2	3M	1	Total	C	O	P	0
			12	5	6	1	
2	3N	1	Total	C	O	P	0
			12	5	6	1	
2	4A	1	Total	C	O	P	0
			12	5	6	1	
2	4B	1	Total	C	O	P	0
			12	5	6	1	
2	4C	1	Total	C	O	P	0
			12	5	6	1	
2	4D	1	Total	C	O	P	0
			12	5	6	1	
2	4E	1	Total	C	O	P	0
			12	5	6	1	
2	4F	1	Total	C	O	P	0
			12	5	6	1	
2	4G	1	Total	C	O	P	0
			12	5	6	1	
2	4H	1	Total	C	O	P	0
			12	5	6	1	
2	4I	1	Total	C	O	P	0
			12	5	6	1	
2	4J	1	Total	C	O	P	0
			12	5	6	1	
2	4K	1	Total	C	O	P	0
			12	5	6	1	
2	4L	1	Total	C	O	P	0
			12	5	6	1	
2	4M	1	Total	C	O	P	0
			12	5	6	1	
2	4N	1	Total	C	O	P	0
			12	5	6	1	

Continued on next page...

Continued from previous page...

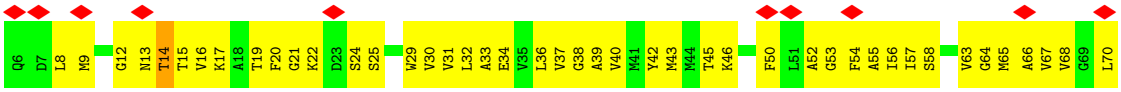
Mol	Chain	Residues	Atoms				AltConf
2	5A	1	Total	C	O	P	0
			12	5	6	1	
2	5B	1	Total	C	O	P	0
			12	5	6	1	
2	5C	1	Total	C	O	P	0
			12	5	6	1	
2	5D	1	Total	C	O	P	0
			12	5	6	1	
2	5E	1	Total	C	O	P	0
			12	5	6	1	
2	5F	1	Total	C	O	P	0
			12	5	6	1	
2	5G	1	Total	C	O	P	0
			12	5	6	1	
2	5H	1	Total	C	O	P	0
			12	5	6	1	
2	5I	1	Total	C	O	P	0
			12	5	6	1	
2	5J	1	Total	C	O	P	0
			12	5	6	1	
2	5K	1	Total	C	O	P	0
			12	5	6	1	
2	5L	1	Total	C	O	P	0
			12	5	6	1	
2	5M	1	Total	C	O	P	0
			12	5	6	1	
2	5N	1	Total	C	O	P	0
			12	5	6	1	

3 Residue-property plots

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.

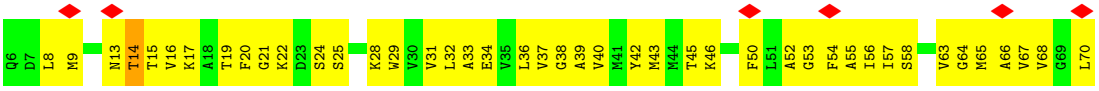
- Molecule 1: Pilin

Chain 1A:



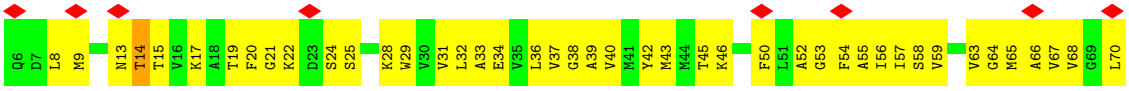
- Molecule 1: Pilin

Chain 1B:



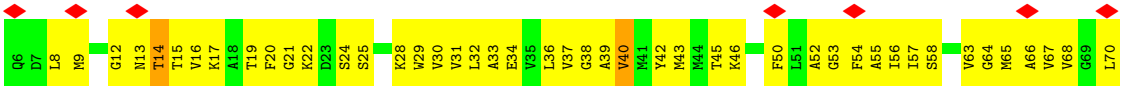
- Molecule 1: Pilin

Chain 1C:



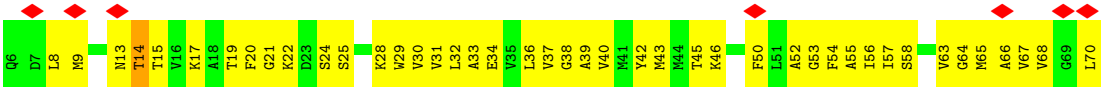
- Molecule 1: Pilin

Chain 1D:



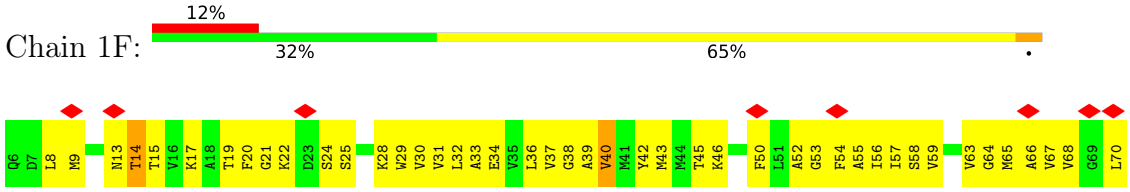
- Molecule 1: Pilin

Chain 1E:



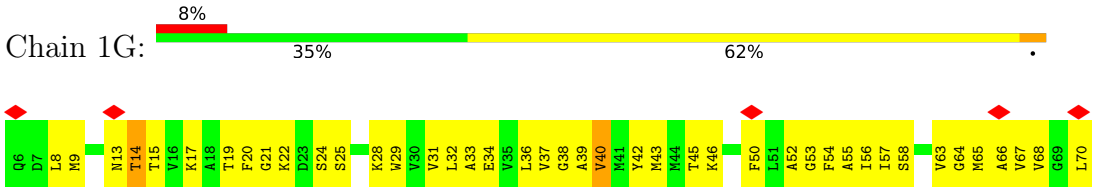
- Molecule 1: Pilin

Chain 1F:



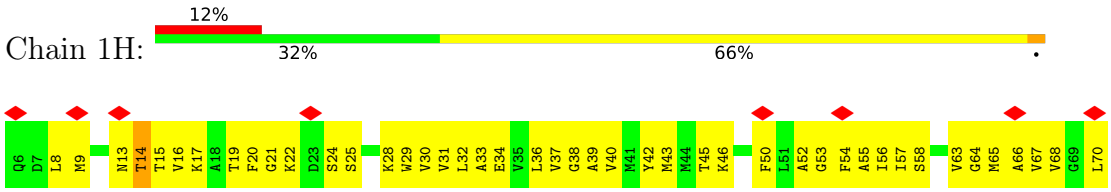
• Molecule 1: Pilin

Chain 1G:



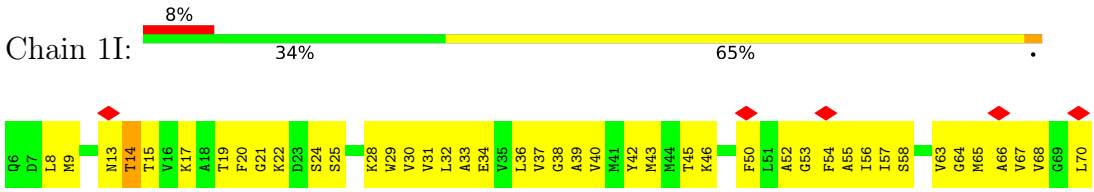
• Molecule 1: Pilin

Chain 1H:



• Molecule 1: Pilin

Chain 1I:

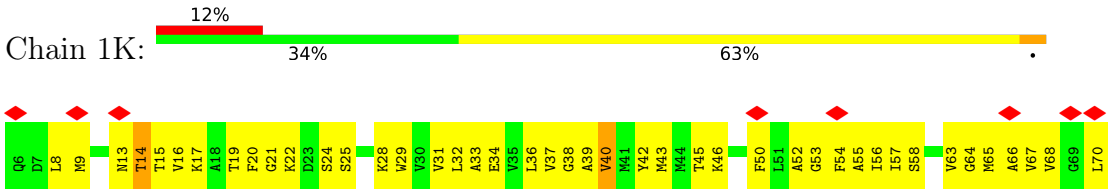


• Molecule 1: Pilin

Chain 1J:

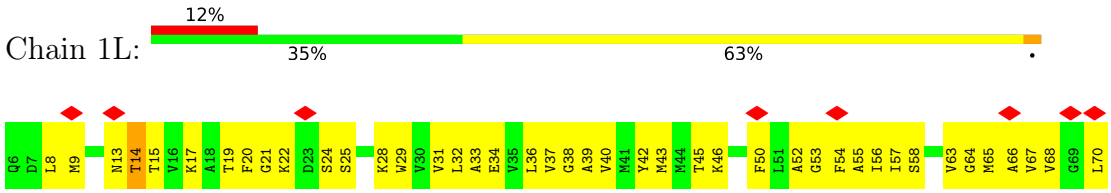
• Molecule 1: Pilin

Chain 1K:



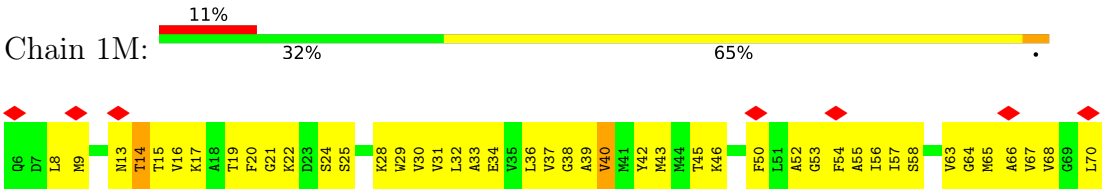
• Molecule 1: Pilin

Chain 1L:



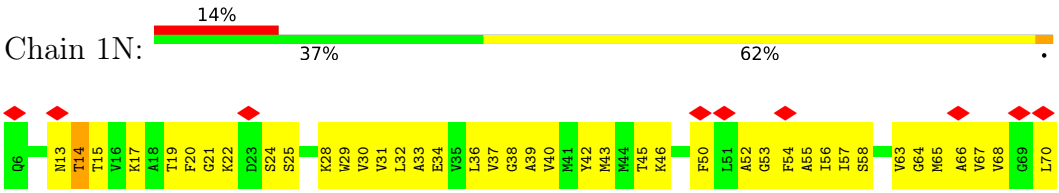
• Molecule 1: Pilin

Chain 1M:



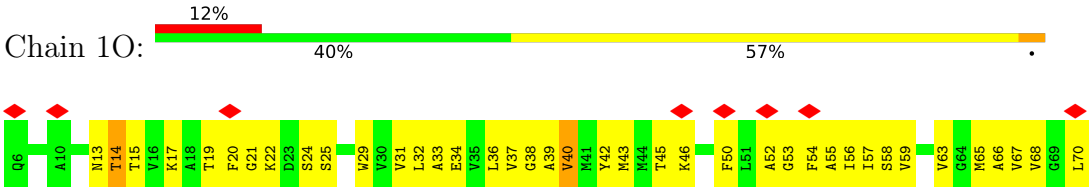
• Molecule 1: Pilin

Chain 1N:



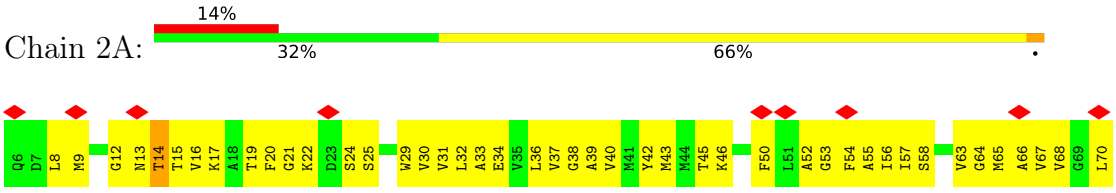
• Molecule 1: Pilin

Chain 1O:



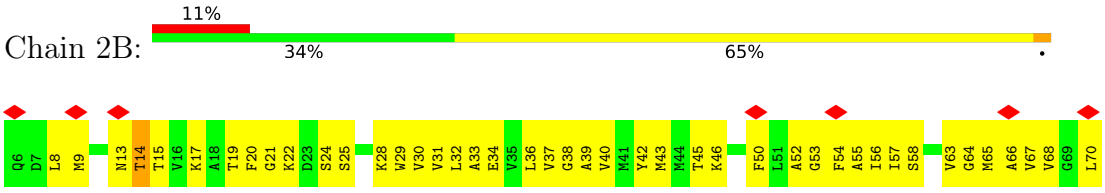
• Molecule 1: Pilin

Chain 2A:



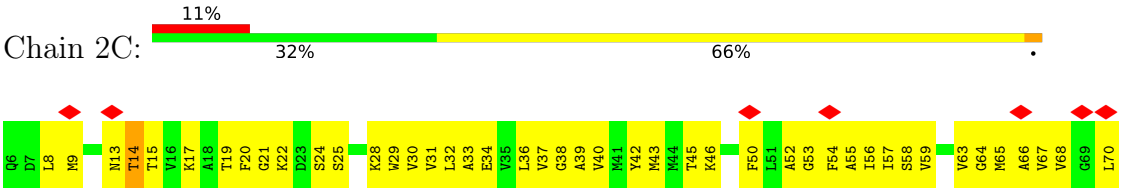
• Molecule 1: Pilin

Chain 2B:



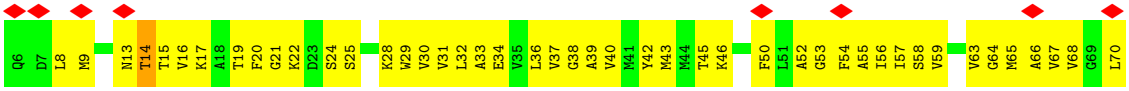
• Molecule 1: Pilin

Chain 2C:



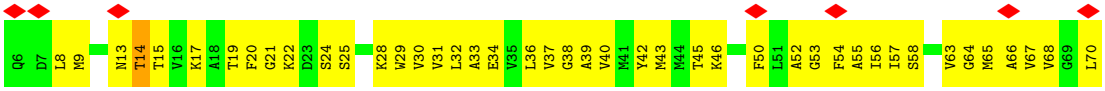
• Molecule 1: Pilin

Chain 2D:



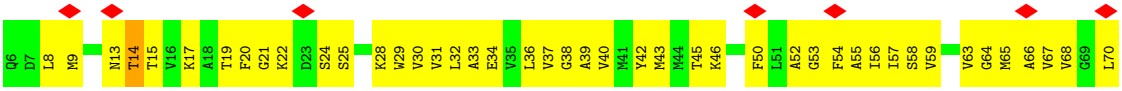
• Molecule 1: Pilin

Chain 2E:



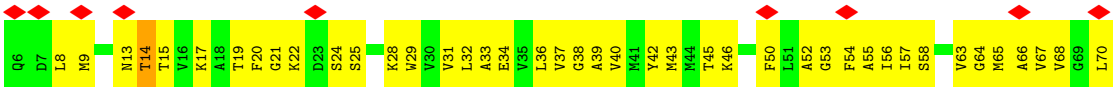
• Molecule 1: Pilin

Chain 2F:



• Molecule 1: Pilin

Chain 2G:

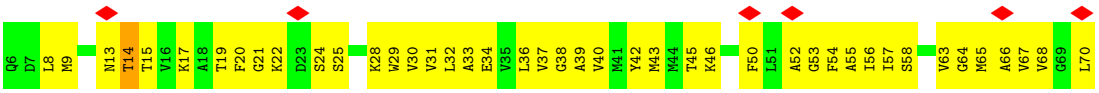


• Molecule 1: Pilin

Chain 2H:

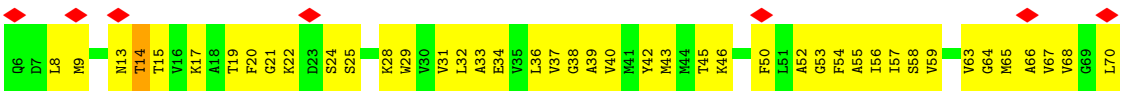
• Molecule 1: Pilin

Chain 2I:



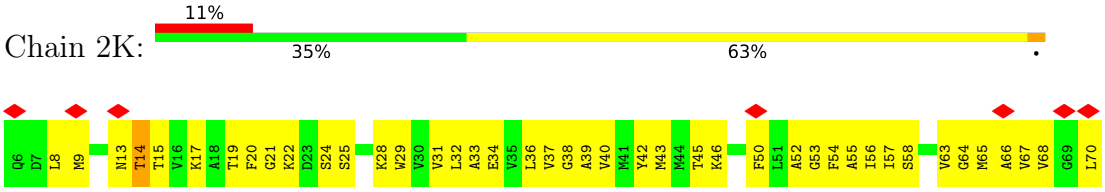
• Molecule 1: Pilin

Chain 2J:



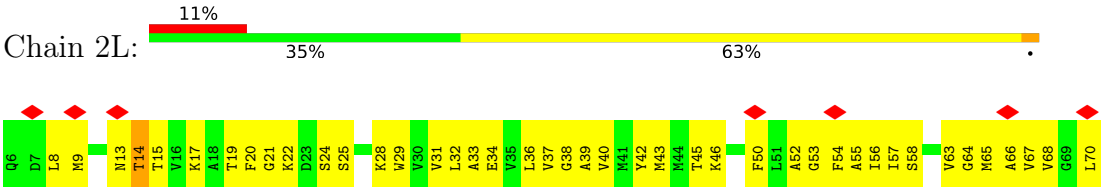
• Molecule 1: Pilin

Chain 2K:



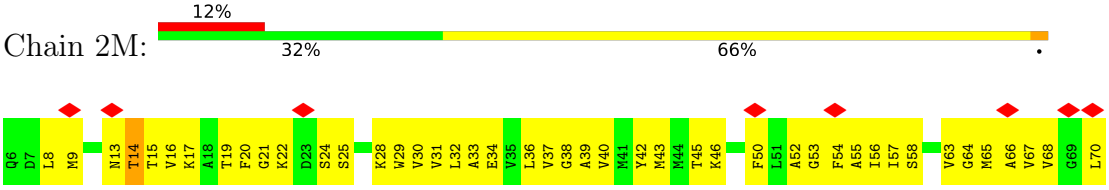
• Molecule 1: Pilin

Chain 2L:



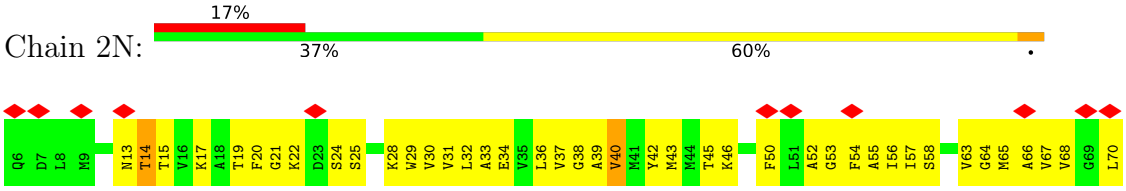
• Molecule 1: Pilin

Chain 2M:



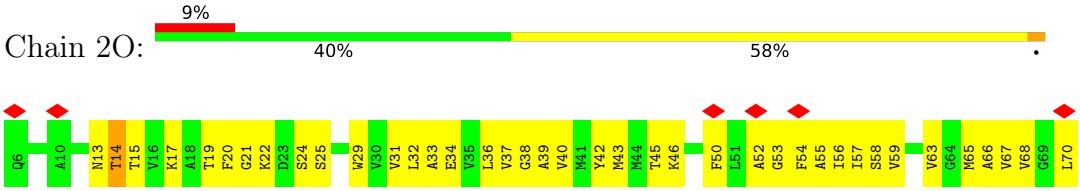
• Molecule 1: Pilin

Chain 2N:



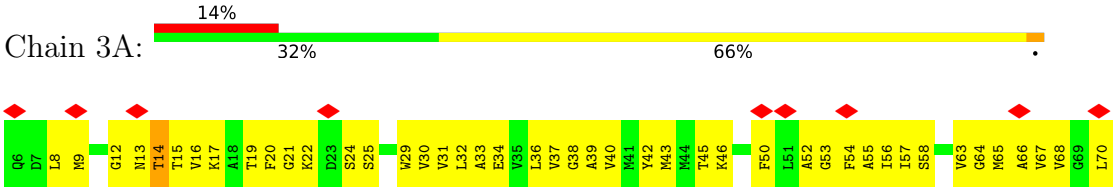
• Molecule 1: Pilin

Chain 2O:



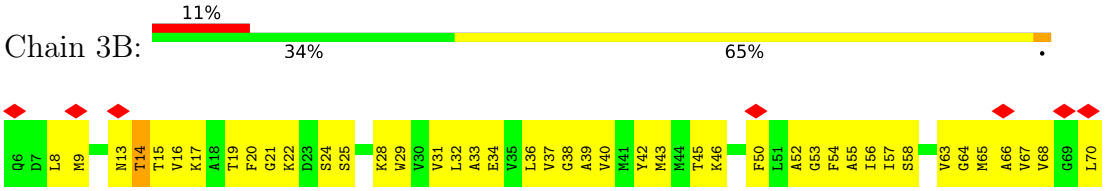
• Molecule 1: Pilin

Chain 3A:



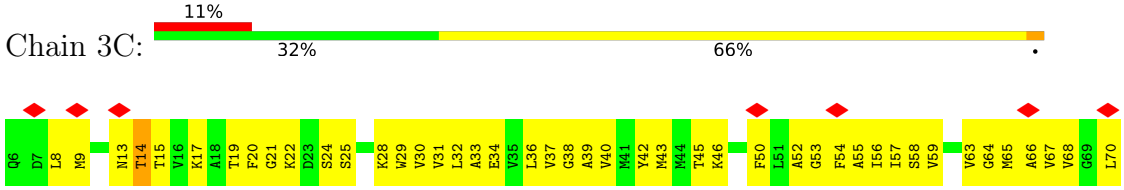
• Molecule 1: Pilin

Chain 3B:



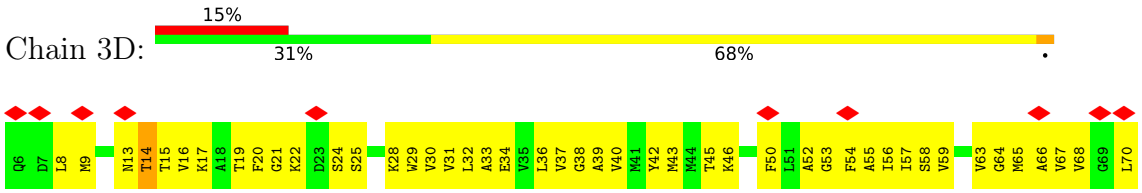
• Molecule 1: Pilin

Chain 3C:



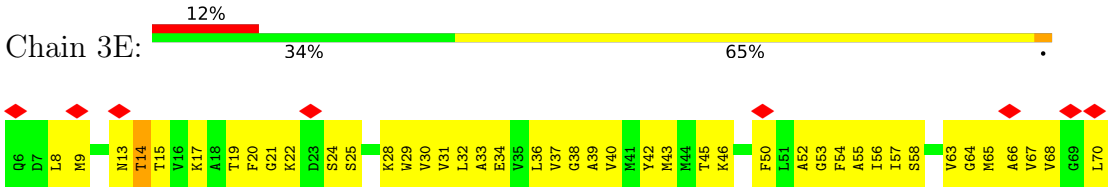
• Molecule 1: Pilin

Chain 3D:



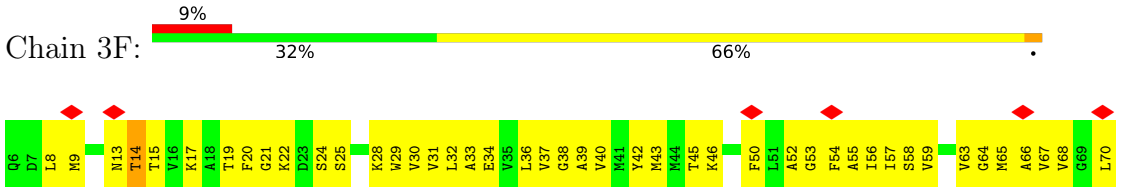
• Molecule 1: Pilin

Chain 3E:



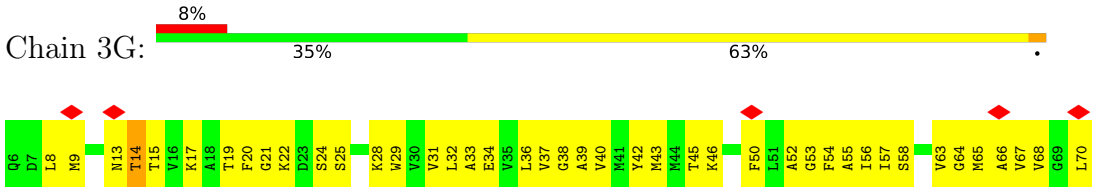
• Molecule 1: Pilin

Chain 3F:



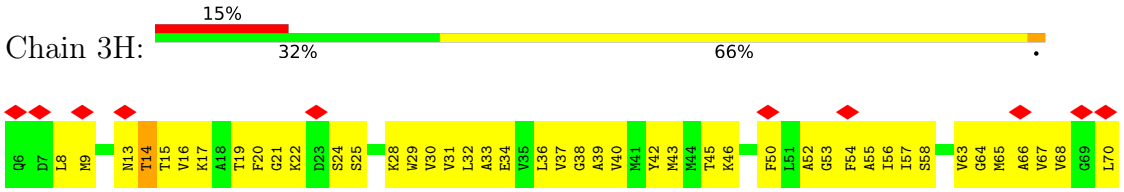
• Molecule 1: Pilin

Chain 3G:



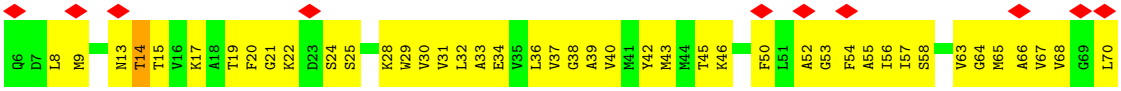
• Molecule 1: Pilin

Chain 3H:

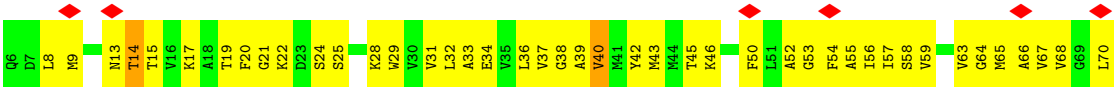


• Molecule 1: Pilin

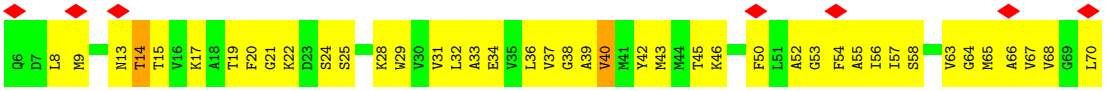
Chain 3I:



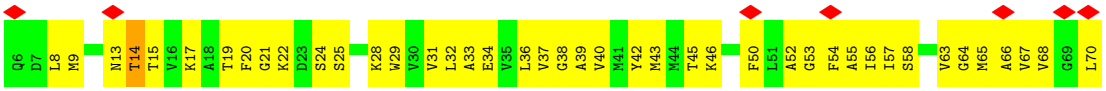
• Molecule 1: Pilin



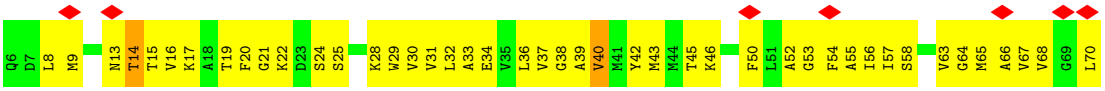
• Molecule 1: Pilin



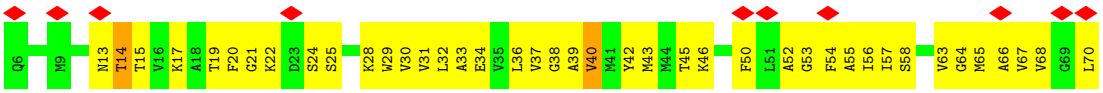
• Molecule 1: Pilin



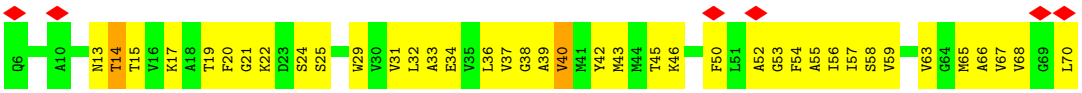
• Molecule 1: Pilin



• Molecule 1: Pilin

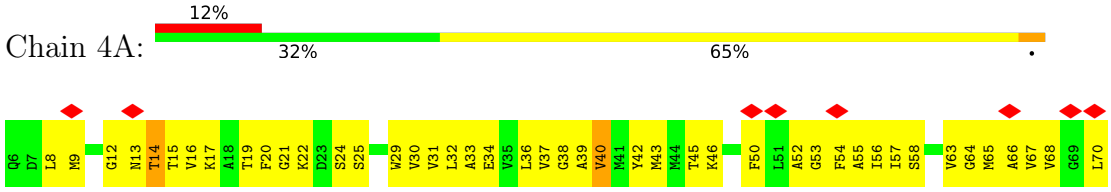


• Molecule 1: Pilin



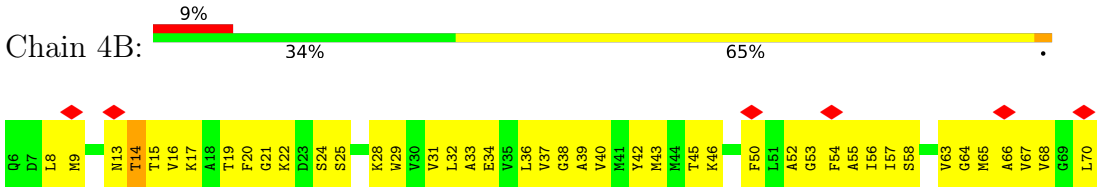
• Molecule 1: Pilin

Chain 4A:



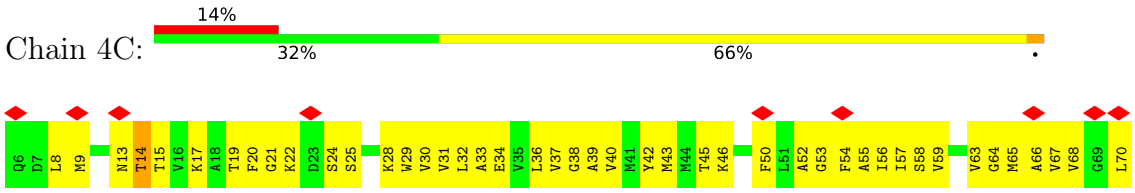
• Molecule 1: Pilin

Chain 4B:



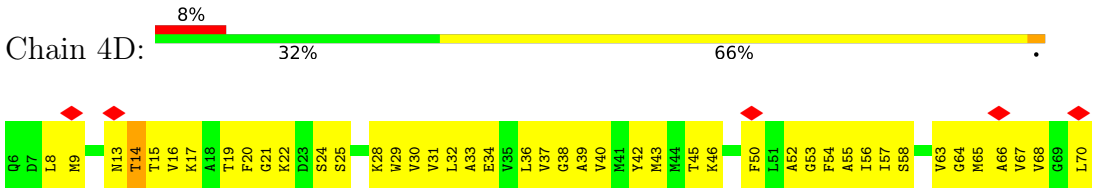
• Molecule 1: Pilin

Chain 4C:



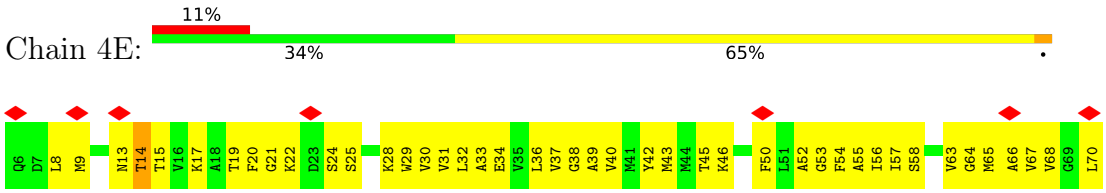
• Molecule 1: Pilin

Chain 4D:



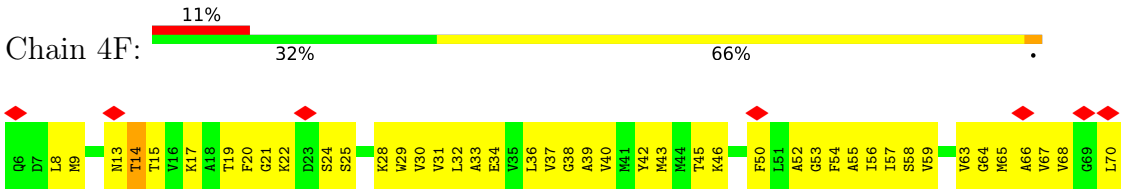
• Molecule 1: Pilin

Chain 4E:



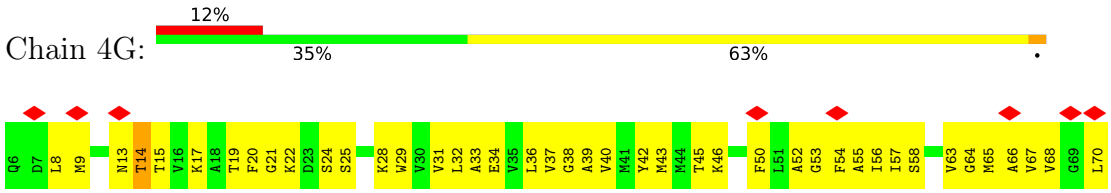
• Molecule 1: Pilin

Chain 4F:



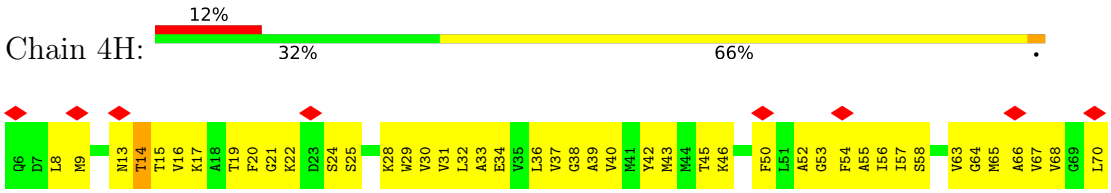
• Molecule 1: Pilin

Chain 4G:



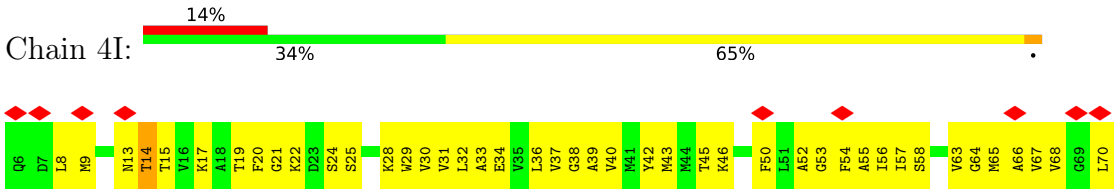
• Molecule 1: Pilin

Chain 4H:



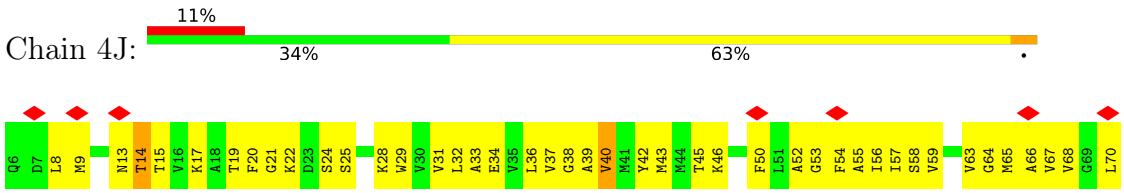
• Molecule 1: Pilin

Chain 4I:



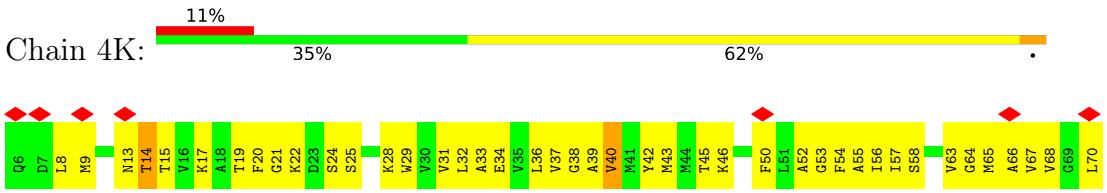
• Molecule 1: Pilin

Chain 4J:



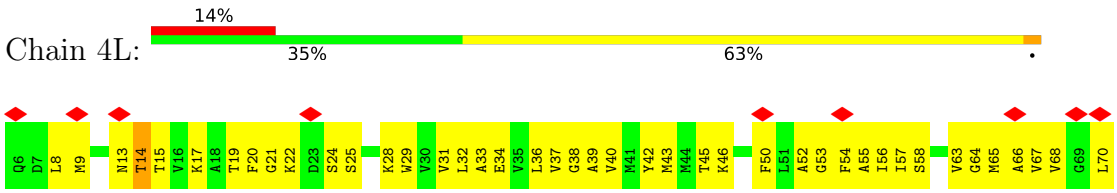
• Molecule 1: Pilin

Chain 4K:



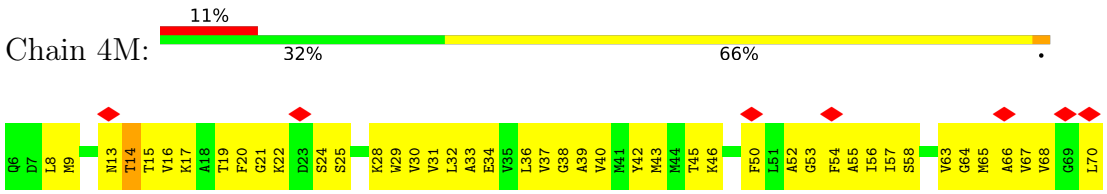
• Molecule 1: Pilin

Chain 4L:



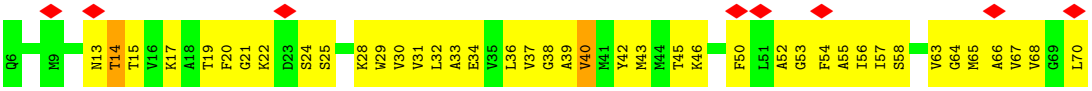
• Molecule 1: Pilin

Chain 4M:



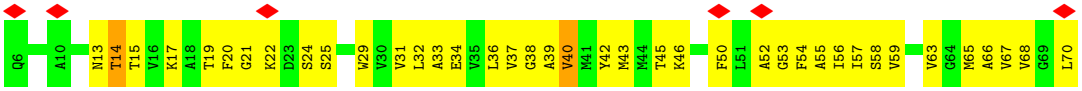
• Molecule 1: Pilin

Chain 4N:



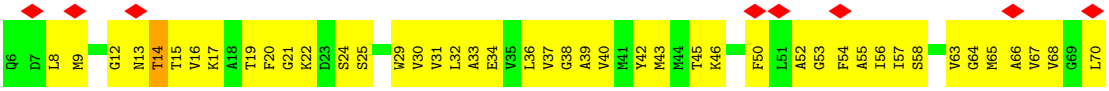
• Molecule 1: Pilin

Chain 4O:



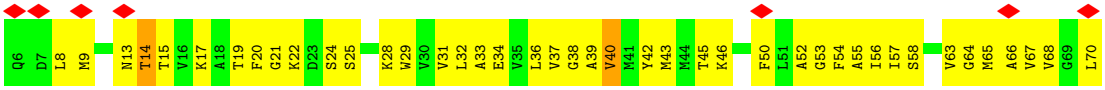
• Molecule 1: Pilin

Chain 5A:



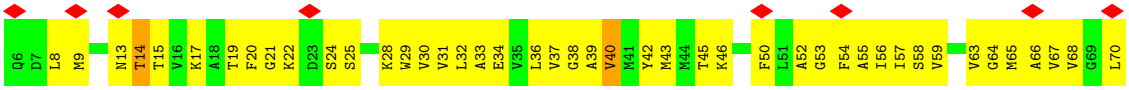
• Molecule 1: Pilin

Chain 5B:



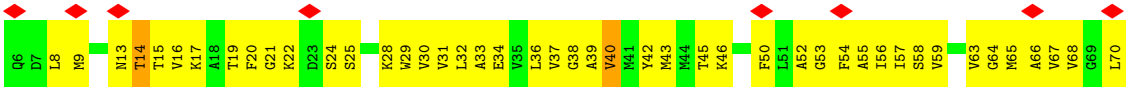
• Molecule 1: Pilin

Chain 5C:



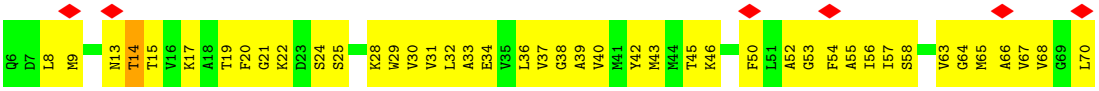
• Molecule 1: Pilin

Chain 5D:



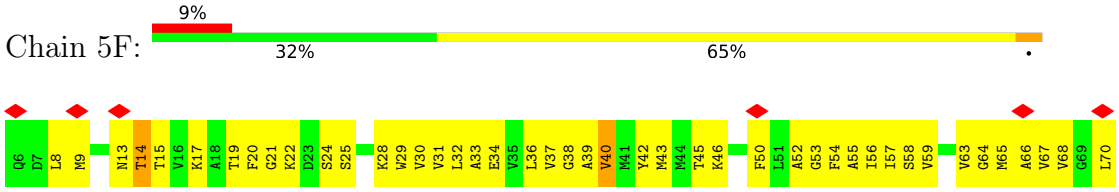
• Molecule 1: Pilin

Chain 5E:



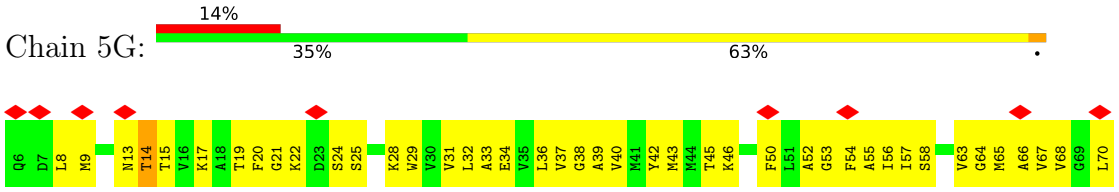
• Molecule 1: Pilin

Chain 5F:



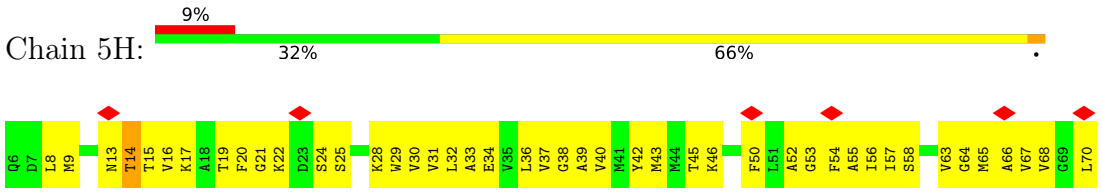
• Molecule 1: Pilin

Chain 5G:



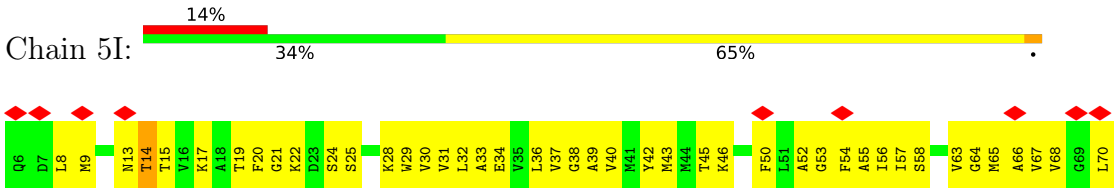
• Molecule 1: Pilin

Chain 5H:



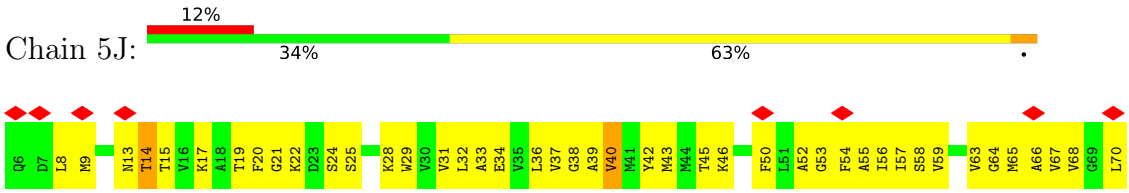
• Molecule 1: Pilin

Chain 5I:



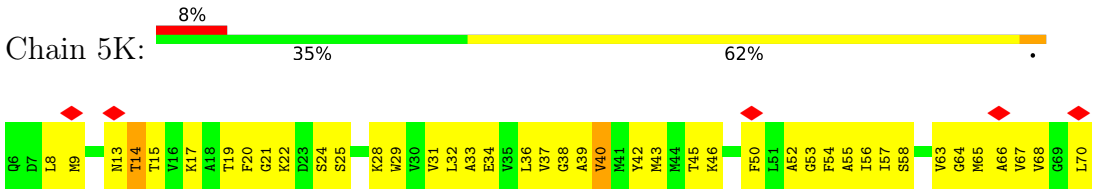
• Molecule 1: Pilin

Chain 5J:



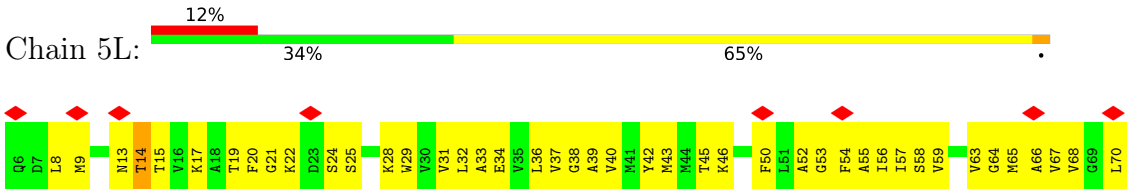
• Molecule 1: Pilin

Chain 5K:



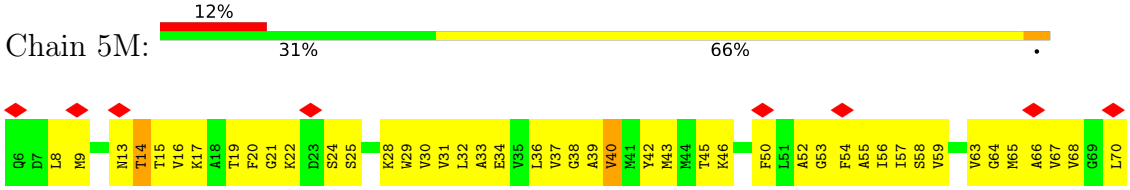
• Molecule 1: Pilin

Chain 5L:



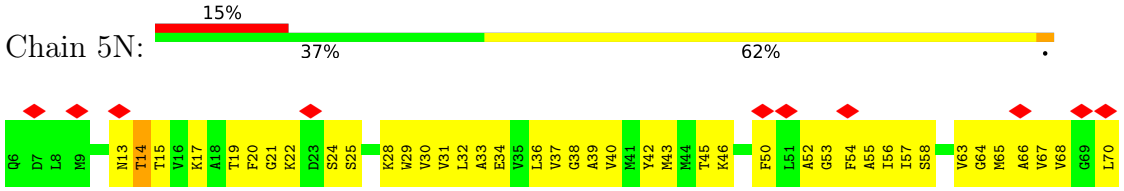
• Molecule 1: Pilin

Chain 5M:



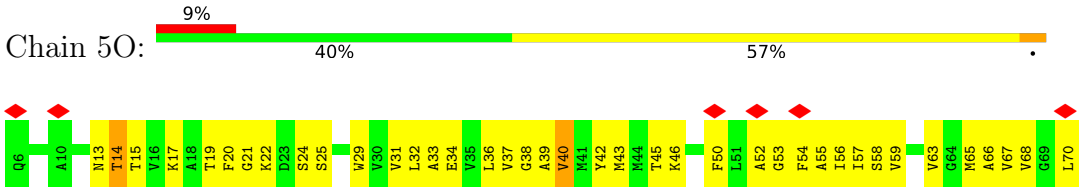
• Molecule 1: Pilin

Chain 5N:



• Molecule 1: Pilin

Chain 5O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=27.9°, rise=13.2 Å, axial sym=C5	Depositor
Number of segments used	11969	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	120.630	Depositor
Minimum map value	-46.547	Depositor
Average map value	4.592	Depositor
Map value standard deviation	16.741	Depositor
Recommended contour level	44.0	Depositor
Map size (Å)	140.8, 140.8, 281.6	wwPDB
Map dimensions	128, 128, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6V6

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	1A	0.52	0/481	0.61	0/649
1	1B	0.52	0/482	0.61	0/651
1	1C	0.52	0/482	0.61	0/651
1	1D	0.52	0/482	0.61	0/651
1	1E	0.52	0/482	0.61	0/651
1	1F	0.52	0/482	0.61	0/651
1	1G	0.52	0/482	0.61	0/651
1	1H	0.52	0/482	0.61	0/651
1	1I	0.52	0/482	0.61	0/651
1	1J	0.52	0/482	0.61	0/651
1	1K	0.52	0/482	0.61	0/651
1	1L	0.52	0/482	0.61	0/651
1	1M	0.52	0/482	0.61	0/651
1	1N	0.52	0/482	0.61	0/651
1	1O	0.52	0/482	0.61	0/651
1	2A	0.52	0/482	0.61	0/651
1	2B	0.52	0/482	0.61	0/651
1	2C	0.52	0/482	0.61	0/651
1	2D	0.52	0/482	0.61	0/651
1	2E	0.52	0/482	0.61	0/651
1	2F	0.52	0/482	0.61	0/651
1	2G	0.52	0/482	0.61	0/651
1	2H	0.52	0/482	0.61	0/651
1	2I	0.52	0/482	0.61	0/651
1	2J	0.52	0/482	0.61	0/651
1	2K	0.52	0/482	0.61	0/651
1	2L	0.52	0/482	0.61	0/651
1	2M	0.52	0/482	0.61	0/651
1	2N	0.52	0/482	0.61	0/651
1	2O	0.52	0/482	0.61	0/651
1	3A	0.52	0/482	0.61	0/651
1	3B	0.52	0/482	0.61	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	3C	0.52	0/482	0.61	0/651
1	3D	0.52	0/482	0.61	0/651
1	3E	0.52	0/482	0.61	0/651
1	3F	0.52	0/482	0.61	0/651
1	3G	0.52	0/482	0.61	0/651
1	3H	0.52	0/482	0.61	0/651
1	3I	0.52	0/482	0.61	0/651
1	3J	0.52	0/482	0.61	0/651
1	3K	0.52	0/482	0.61	0/651
1	3L	0.52	0/482	0.61	0/651
1	3M	0.52	0/482	0.61	0/651
1	3N	0.52	0/482	0.61	0/651
1	3O	0.52	0/482	0.61	0/651
1	4A	0.52	0/482	0.61	0/651
1	4B	0.52	0/482	0.61	0/651
1	4C	0.52	0/482	0.61	0/651
1	4D	0.52	0/482	0.61	0/651
1	4E	0.52	0/482	0.61	0/651
1	4F	0.52	0/482	0.61	0/651
1	4G	0.52	0/482	0.61	0/651
1	4H	0.52	0/482	0.61	0/651
1	4I	0.52	0/482	0.61	0/651
1	4J	0.52	0/482	0.61	0/651
1	4K	0.52	0/482	0.61	0/651
1	4L	0.52	0/482	0.61	0/651
1	4M	0.52	0/482	0.61	0/651
1	4N	0.52	0/482	0.61	0/651
1	4O	0.52	0/482	0.61	0/651
1	5A	0.52	0/482	0.61	0/651
1	5B	0.52	0/482	0.61	0/651
1	5C	0.52	0/482	0.61	0/651
1	5D	0.52	0/482	0.61	0/651
1	5E	0.52	0/482	0.61	0/651
1	5F	0.52	0/482	0.61	0/651
1	5G	0.52	0/482	0.61	0/651
1	5H	0.52	0/482	0.61	0/651
1	5I	0.52	0/482	0.61	0/651
1	5J	0.52	0/482	0.61	0/651
1	5K	0.52	0/482	0.61	0/651
1	5L	0.52	0/482	0.61	0/651
1	5M	0.52	0/482	0.61	0/651
1	5N	0.52	0/482	0.61	0/651
1	5O	0.52	0/482	0.61	0/651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.52	0/36149	0.61	0/48823

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
1	1A	0	1
1	1B	0	1
1	1C	0	1
1	1D	0	1
1	1E	0	1
1	1F	0	1
1	1G	0	1
1	1H	0	1
1	1I	0	1
1	1J	0	1
1	1K	0	1
1	1L	0	1
1	1M	0	1
1	1N	0	1
1	1O	0	1
1	2A	0	1
1	2B	0	1
1	2C	0	1
1	2D	0	1
1	2E	0	1
1	2F	0	1
1	2G	0	1
1	2H	0	1
1	2I	0	1
1	2J	0	1
1	2K	0	1
1	2L	0	1
1	2M	0	1
1	2N	0	1
1	2O	0	1
1	3A	0	1
1	3B	0	1
1	3C	0	1
1	3D	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3E	0	1
1	3F	0	1
1	3G	0	1
1	3H	0	1
1	3I	0	1
1	3J	0	1
1	3K	0	1
1	3L	0	1
1	3M	0	1
1	3N	0	1
1	3O	0	1
1	4A	0	1
1	4B	0	1
1	4C	0	1
1	4D	0	1
1	4E	0	1
1	4F	0	1
1	4G	0	1
1	4H	0	1
1	4I	0	1
1	4J	0	1
1	4K	0	1
1	4L	0	1
1	4M	0	1
1	4N	0	1
1	4O	0	1
1	5A	0	1
1	5B	0	1
1	5C	0	1
1	5D	0	1
1	5E	0	1
1	5F	0	1
1	5G	0	1
1	5H	0	1
1	5I	0	1
1	5J	0	1
1	5K	0	1
1	5L	0	1
1	5M	0	1
1	5N	0	1
1	5O	0	1
All	All	0	75

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	14	THR	Peptide
1	1B	14	THR	Peptide
1	1C	14	THR	Peptide
1	1D	14	THR	Peptide
1	1E	14	THR	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	1A	475	0	508	55	0
1	1B	476	0	509	56	0
1	1C	476	0	509	65	0
1	1D	476	0	509	64	0
1	1E	476	0	509	60	0
1	1F	476	0	509	61	0
1	1G	476	0	509	58	0
1	1H	476	0	509	59	0
1	1I	476	0	509	59	0
1	1J	476	0	509	62	0
1	1K	476	0	509	57	0
1	1L	476	0	509	56	0
1	1M	476	0	509	65	0
1	1N	476	0	509	51	0
1	1O	476	0	509	52	0
1	2A	476	0	509	52	0
1	2B	476	0	509	53	0
1	2C	476	0	509	65	0
1	2D	476	0	509	61	0
1	2E	476	0	509	58	0
1	2F	476	0	509	61	0
1	2G	476	0	509	56	0
1	2H	476	0	509	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2I	476	0	509	57	0
1	2J	476	0	509	61	0
1	2K	476	0	509	56	0
1	2L	476	0	509	56	0
1	2M	476	0	509	66	0
1	2N	476	0	509	52	0
1	2O	476	0	509	51	0
1	3A	476	0	509	52	0
1	3B	476	0	509	56	0
1	3C	476	0	509	65	0
1	3D	476	0	509	64	0
1	3E	476	0	509	58	0
1	3F	476	0	509	61	0
1	3G	476	0	509	57	0
1	3H	476	0	509	59	0
1	3I	476	0	509	57	0
1	3J	476	0	509	61	0
1	3K	476	0	509	58	0
1	3L	476	0	509	56	0
1	3M	476	0	509	63	0
1	3N	476	0	509	53	0
1	3O	476	0	509	50	0
1	4A	476	0	509	53	0
1	4B	476	0	509	55	0
1	4C	476	0	509	63	0
1	4D	476	0	509	65	0
1	4E	476	0	509	59	0
1	4F	476	0	509	62	0
1	4G	476	0	509	59	0
1	4H	476	0	509	62	0
1	4I	476	0	509	60	0
1	4J	476	0	509	58	0
1	4K	476	0	509	55	0
1	4L	476	0	509	55	0
1	4M	476	0	509	63	0
1	4N	476	0	509	48	0
1	4O	476	0	509	51	0
1	5A	476	0	509	50	0
1	5B	476	0	509	53	0
1	5C	476	0	509	67	0
1	5D	476	0	509	66	0
1	5E	476	0	509	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5F	476	0	509	65	0
1	5G	476	0	509	59	0
1	5H	476	0	509	61	0
1	5I	476	0	509	58	0
1	5J	476	0	509	59	0
1	5K	476	0	509	57	0
1	5L	476	0	509	60	0
1	5M	476	0	509	67	0
1	5N	476	0	509	53	0
1	5O	476	0	509	50	0
2	1A	12	0	0	0	0
2	1B	12	0	0	1	0
2	1C	12	0	0	1	0
2	1D	12	0	0	1	0
2	1E	12	0	0	1	0
2	1F	12	0	0	1	0
2	1G	12	0	0	2	0
2	1H	12	0	0	1	0
2	1I	12	0	0	2	0
2	1J	12	0	0	1	0
2	1K	12	0	0	1	0
2	1L	12	0	0	1	0
2	1M	12	0	0	1	0
2	1N	12	0	0	1	0
2	2A	12	0	0	0	0
2	2B	12	0	0	1	0
2	2C	12	0	0	1	0
2	2D	12	0	0	1	0
2	2E	12	0	0	1	0
2	2F	12	0	0	1	0
2	2G	12	0	0	1	0
2	2H	12	0	0	1	0
2	2I	12	0	0	2	0
2	2J	12	0	0	1	0
2	2K	12	0	0	1	0
2	2L	12	0	0	1	0
2	2M	12	0	0	1	0
2	2N	12	0	0	1	0
2	3A	12	0	0	0	0
2	3B	12	0	0	1	0
2	3C	12	0	0	1	0
2	3D	12	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3E	12	0	0	1	0
2	3F	12	0	0	1	0
2	3G	12	0	0	1	0
2	3H	12	0	0	1	0
2	3I	12	0	0	2	0
2	3J	12	0	0	1	0
2	3K	12	0	0	1	0
2	3L	12	0	0	1	0
2	3M	12	0	0	1	0
2	3N	12	0	0	1	0
2	4A	12	0	0	0	0
2	4B	12	0	0	1	0
2	4C	12	0	0	1	0
2	4D	12	0	0	1	0
2	4E	12	0	0	1	0
2	4F	12	0	0	1	0
2	4G	12	0	0	1	0
2	4H	12	0	0	1	0
2	4I	12	0	0	2	0
2	4J	12	0	0	1	0
2	4K	12	0	0	1	0
2	4L	12	0	0	1	0
2	4M	12	0	0	1	0
2	4N	12	0	0	1	0
2	5A	12	0	0	0	0
2	5B	12	0	0	1	0
2	5C	12	0	0	1	0
2	5D	12	0	0	1	0
2	5E	12	0	0	1	0
2	5F	12	0	0	1	0
2	5G	12	0	0	1	0
2	5H	12	0	0	1	0
2	5I	12	0	0	1	0
2	5J	12	0	0	1	0
2	5K	12	0	0	1	0
2	5L	12	0	0	1	0
2	5M	12	0	0	1	0
2	5N	12	0	0	1	0
All	All	36539	0	38174	3428	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 46.

The worst 5 of 3428 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3C:67:VAL:HG13	1:4A:9:MET:CE	1.15	1.63
1:2C:67:VAL:HG13	1:3A:9:MET:CE	1.15	1.61
1:4C:67:VAL:HG13	1:5A:9:MET:CE	1.17	1.60
1:1A:9:MET:CE	1:5C:67:VAL:HG13	1.15	1.60
1:3D:67:VAL:HG13	1:4B:9:MET:CE	1.39	1.53

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	1A	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1B	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1C	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1D	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9	44
1	1E	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1F	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9	44
1	1G	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9	44
1	1H	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1I	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9	44
1	1K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9	44
1	1L	63/65 (97%)	52 (82%)	11 (18%)	0	100	100
1	1M	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9	44
1	1N	63/65 (97%)	52 (82%)	11 (18%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	2A	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2B	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2C	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2D	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2E	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2F	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2G	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2H	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2I	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2J	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2K	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2L	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2M	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	2N	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	2O	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3A	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3B	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3C	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3D	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3E	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3F	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3G	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3H	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3I	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	3K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	3L	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	3M	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	3N	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	3O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	4A	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	4B	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4C	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4D	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4E	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4F	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4G	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4H	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4I	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	4K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	4L	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4M	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	4N	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	4O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5A	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	5B	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5C	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5D	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5E	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	5F	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5G	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	5H	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	5I	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	5J	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5K	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5L	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	5M	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
1	5N	63/65 (97%)	52 (82%)	11 (18%)	0	100 100
1	5O	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	9 44
All	All	4725/4875 (97%)	3900 (82%)	799 (17%)	26 (1%)	29 65

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1D	40	VAL
1	1F	40	VAL
1	1G	40	VAL
1	1J	40	VAL
1	1K	40	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1A	50/51 (98%)	50 (100%)	0	100	100
1	1B	51/51 (100%)	51 (100%)	0	100	100
1	1C	51/51 (100%)	51 (100%)	0	100	100
1	1D	51/51 (100%)	51 (100%)	0	100	100
1	1E	51/51 (100%)	51 (100%)	0	100	100
1	1F	51/51 (100%)	51 (100%)	0	100	100
1	1G	51/51 (100%)	51 (100%)	0	100	100
1	1H	51/51 (100%)	51 (100%)	0	100	100
1	1I	51/51 (100%)	51 (100%)	0	100	100
1	1J	51/51 (100%)	51 (100%)	0	100	100
1	1K	51/51 (100%)	51 (100%)	0	100	100
1	1L	51/51 (100%)	51 (100%)	0	100	100
1	1M	51/51 (100%)	51 (100%)	0	100	100
1	1N	51/51 (100%)	51 (100%)	0	100	100
1	1O	51/51 (100%)	51 (100%)	0	100	100
1	2A	51/51 (100%)	51 (100%)	0	100	100
1	2B	51/51 (100%)	51 (100%)	0	100	100
1	2C	51/51 (100%)	51 (100%)	0	100	100
1	2D	51/51 (100%)	51 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2E	51/51 (100%)	51 (100%)	0	100	100
1	2F	51/51 (100%)	51 (100%)	0	100	100
1	2G	51/51 (100%)	51 (100%)	0	100	100
1	2H	51/51 (100%)	51 (100%)	0	100	100
1	2I	51/51 (100%)	51 (100%)	0	100	100
1	2J	51/51 (100%)	51 (100%)	0	100	100
1	2K	51/51 (100%)	51 (100%)	0	100	100
1	2L	51/51 (100%)	51 (100%)	0	100	100
1	2M	51/51 (100%)	51 (100%)	0	100	100
1	2N	51/51 (100%)	51 (100%)	0	100	100
1	2O	51/51 (100%)	51 (100%)	0	100	100
1	3A	51/51 (100%)	51 (100%)	0	100	100
1	3B	51/51 (100%)	51 (100%)	0	100	100
1	3C	51/51 (100%)	51 (100%)	0	100	100
1	3D	51/51 (100%)	51 (100%)	0	100	100
1	3E	51/51 (100%)	51 (100%)	0	100	100
1	3F	51/51 (100%)	51 (100%)	0	100	100
1	3G	51/51 (100%)	51 (100%)	0	100	100
1	3H	51/51 (100%)	51 (100%)	0	100	100
1	3I	51/51 (100%)	51 (100%)	0	100	100
1	3J	51/51 (100%)	51 (100%)	0	100	100
1	3K	51/51 (100%)	51 (100%)	0	100	100
1	3L	51/51 (100%)	51 (100%)	0	100	100
1	3M	51/51 (100%)	51 (100%)	0	100	100
1	3N	51/51 (100%)	51 (100%)	0	100	100
1	3O	51/51 (100%)	51 (100%)	0	100	100
1	4A	51/51 (100%)	51 (100%)	0	100	100
1	4B	51/51 (100%)	51 (100%)	0	100	100
1	4C	51/51 (100%)	51 (100%)	0	100	100
1	4D	51/51 (100%)	51 (100%)	0	100	100
1	4E	51/51 (100%)	51 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4F	51/51 (100%)	51 (100%)	0	100	100
1	4G	51/51 (100%)	51 (100%)	0	100	100
1	4H	51/51 (100%)	51 (100%)	0	100	100
1	4I	51/51 (100%)	51 (100%)	0	100	100
1	4J	51/51 (100%)	51 (100%)	0	100	100
1	4K	51/51 (100%)	51 (100%)	0	100	100
1	4L	51/51 (100%)	51 (100%)	0	100	100
1	4M	51/51 (100%)	51 (100%)	0	100	100
1	4N	51/51 (100%)	51 (100%)	0	100	100
1	4O	51/51 (100%)	51 (100%)	0	100	100
1	5A	51/51 (100%)	51 (100%)	0	100	100
1	5B	51/51 (100%)	51 (100%)	0	100	100
1	5C	51/51 (100%)	51 (100%)	0	100	100
1	5D	51/51 (100%)	51 (100%)	0	100	100
1	5E	51/51 (100%)	51 (100%)	0	100	100
1	5F	51/51 (100%)	51 (100%)	0	100	100
1	5G	51/51 (100%)	51 (100%)	0	100	100
1	5H	51/51 (100%)	51 (100%)	0	100	100
1	5I	51/51 (100%)	51 (100%)	0	100	100
1	5J	51/51 (100%)	51 (100%)	0	100	100
1	5K	51/51 (100%)	51 (100%)	0	100	100
1	5L	51/51 (100%)	51 (100%)	0	100	100
1	5M	51/51 (100%)	51 (100%)	0	100	100
1	5N	51/51 (100%)	51 (100%)	0	100	100
1	5O	51/51 (100%)	51 (100%)	0	100	100
All	All	3824/3825 (100%)	3824 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

70 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	6V6	2C	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	5N	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	1G	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	4K	101	-	11,11,48	0.53	0	12,14,54	0.50	0
2	6V6	5A	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	1F	101	-	11,11,48	0.53	0	12,14,54	0.53	0
2	6V6	5L	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	4D	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	3H	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	4A	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	4N	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	5G	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	5D	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	3L	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	5B	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	4C	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	2G	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	5K	101	-	11,11,48	0.54	0	12,14,54	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	6V6	1I	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	2J	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	4G	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	1N	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	1K	101	-	11,11,48	0.53	0	12,14,54	0.50	0
2	6V6	4J	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	2D	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	1E	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	2K	101	-	11,11,48	0.53	0	12,14,54	0.50	0
2	6V6	4M	101	-	11,11,48	0.53	0	12,14,54	0.50	0
2	6V6	5E	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	2A	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	2F	101	-	11,11,48	0.53	0	12,14,54	0.53	0
2	6V6	5J	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	1A	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	5I	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	1D	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	3C	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	4E	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	2M	101	-	11,11,48	0.53	0	12,14,54	0.50	0
2	6V6	1H	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	1J	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	4H	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	5C	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	3M	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	5F	101	-	11,11,48	0.53	0	12,14,54	0.53	0
2	6V6	2I	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	1C	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	1L	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	3F	101	-	11,11,48	0.54	0	12,14,54	0.53	0
2	6V6	2B	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	3J	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	3B	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	3K	101	-	11,11,48	0.53	0	12,14,54	0.50	0
2	6V6	2H	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	4L	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	1M	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	1B	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	3D	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	3N	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	4B	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	4I	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	5M	101	-	11,11,48	0.54	0	12,14,54	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	6V6	2L	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	3A	101	-	11,11,48	0.54	0	12,14,54	0.52	0
2	6V6	2E	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	3E	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	3G	101	-	11,11,48	0.53	0	12,14,54	0.51	0
2	6V6	4F	101	-	11,11,48	0.54	0	12,14,54	0.53	0
2	6V6	5H	101	-	11,11,48	0.54	0	12,14,54	0.51	0
2	6V6	3I	101	-	11,11,48	0.53	0	12,14,54	0.52	0
2	6V6	2N	101	-	11,11,48	0.53	0	12,14,54	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	2C	101	-	-	2/12/12/53	-
2	6V6	5N	101	-	-	2/12/12/53	-
2	6V6	1G	101	-	-	2/12/12/53	-
2	6V6	4K	101	-	-	2/12/12/53	-
2	6V6	5A	101	-	-	2/12/12/53	-
2	6V6	1F	101	-	-	2/12/12/53	-
2	6V6	5L	101	-	-	2/12/12/53	-
2	6V6	4D	101	-	-	2/12/12/53	-
2	6V6	3H	101	-	-	2/12/12/53	-
2	6V6	4A	101	-	-	2/12/12/53	-
2	6V6	4N	101	-	-	2/12/12/53	-
2	6V6	5G	101	-	-	2/12/12/53	-
2	6V6	5D	101	-	-	2/12/12/53	-
2	6V6	3L	101	-	-	2/12/12/53	-
2	6V6	5B	101	-	-	2/12/12/53	-
2	6V6	4C	101	-	-	2/12/12/53	-
2	6V6	2G	101	-	-	2/12/12/53	-
2	6V6	5K	101	-	-	2/12/12/53	-
2	6V6	1I	101	-	-	2/12/12/53	-
2	6V6	2J	101	-	-	2/12/12/53	-
2	6V6	4G	101	-	-	2/12/12/53	-
2	6V6	1N	101	-	-	2/12/12/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	1K	101	-	-	2/12/12/53	-
2	6V6	4J	101	-	-	2/12/12/53	-
2	6V6	2D	101	-	-	2/12/12/53	-
2	6V6	1E	101	-	-	2/12/12/53	-
2	6V6	2K	101	-	-	2/12/12/53	-
2	6V6	4M	101	-	-	2/12/12/53	-
2	6V6	5E	101	-	-	2/12/12/53	-
2	6V6	2A	101	-	-	2/12/12/53	-
2	6V6	2F	101	-	-	2/12/12/53	-
2	6V6	5J	101	-	-	2/12/12/53	-
2	6V6	1A	101	-	-	2/12/12/53	-
2	6V6	5I	101	-	-	2/12/12/53	-
2	6V6	1D	101	-	-	2/12/12/53	-
2	6V6	3C	101	-	-	2/12/12/53	-
2	6V6	4E	101	-	-	2/12/12/53	-
2	6V6	2M	101	-	-	2/12/12/53	-
2	6V6	1H	101	-	-	2/12/12/53	-
2	6V6	1J	101	-	-	2/12/12/53	-
2	6V6	4H	101	-	-	2/12/12/53	-
2	6V6	5C	101	-	-	2/12/12/53	-
2	6V6	3M	101	-	-	2/12/12/53	-
2	6V6	5F	101	-	-	2/12/12/53	-
2	6V6	2I	101	-	-	2/12/12/53	-
2	6V6	1C	101	-	-	2/12/12/53	-
2	6V6	1L	101	-	-	2/12/12/53	-
2	6V6	3F	101	-	-	2/12/12/53	-
2	6V6	2B	101	-	-	2/12/12/53	-
2	6V6	3J	101	-	-	2/12/12/53	-
2	6V6	3B	101	-	-	2/12/12/53	-
2	6V6	3K	101	-	-	2/12/12/53	-
2	6V6	2H	101	-	-	2/12/12/53	-
2	6V6	4L	101	-	-	2/12/12/53	-
2	6V6	1M	101	-	-	2/12/12/53	-
2	6V6	1B	101	-	-	2/12/12/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6V6	3D	101	-	-	2/12/12/53	-
2	6V6	3N	101	-	-	2/12/12/53	-
2	6V6	4B	101	-	-	2/12/12/53	-
2	6V6	4I	101	-	-	2/12/12/53	-
2	6V6	5M	101	-	-	2/12/12/53	-
2	6V6	2L	101	-	-	2/12/12/53	-
2	6V6	3A	101	-	-	2/12/12/53	-
2	6V6	2E	101	-	-	2/12/12/53	-
2	6V6	3E	101	-	-	2/12/12/53	-
2	6V6	3G	101	-	-	2/12/12/53	-
2	6V6	4F	101	-	-	2/12/12/53	-
2	6V6	5H	101	-	-	2/12/12/53	-
2	6V6	3I	101	-	-	2/12/12/53	-
2	6V6	2N	101	-	-	2/12/12/53	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 140 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1A	101	6V6	O4-C3-C4-O5
2	1B	101	6V6	O4-C3-C4-O5
2	1D	101	6V6	O4-C3-C4-O5
2	1E	101	6V6	O4-C3-C4-O5
2	1G	101	6V6	O4-C3-C4-C5

There are no ring outliers.

65 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2C	101	6V6	1	0
2	5N	101	6V6	1	0
2	1G	101	6V6	2	0
2	4K	101	6V6	1	0
2	1F	101	6V6	1	0
2	5L	101	6V6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4D	101	6V6	1	0
2	3H	101	6V6	1	0
2	4N	101	6V6	1	0
2	5G	101	6V6	1	0
2	5D	101	6V6	1	0
2	3L	101	6V6	1	0
2	5B	101	6V6	1	0
2	4C	101	6V6	1	0
2	2G	101	6V6	1	0
2	5K	101	6V6	1	0
2	1I	101	6V6	2	0
2	2J	101	6V6	1	0
2	4G	101	6V6	1	0
2	1N	101	6V6	1	0
2	1K	101	6V6	1	0
2	4J	101	6V6	1	0
2	2D	101	6V6	1	0
2	1E	101	6V6	1	0
2	2K	101	6V6	1	0
2	4M	101	6V6	1	0
2	5E	101	6V6	1	0
2	2F	101	6V6	1	0
2	5J	101	6V6	1	0
2	5I	101	6V6	1	0
2	1D	101	6V6	1	0
2	3C	101	6V6	1	0
2	4E	101	6V6	1	0
2	2M	101	6V6	1	0
2	1H	101	6V6	1	0
2	1J	101	6V6	1	0
2	4H	101	6V6	1	0
2	5C	101	6V6	1	0
2	3M	101	6V6	1	0
2	5F	101	6V6	1	0
2	2I	101	6V6	2	0
2	1C	101	6V6	1	0
2	1L	101	6V6	1	0
2	3F	101	6V6	1	0
2	2B	101	6V6	1	0
2	3J	101	6V6	1	0
2	3B	101	6V6	1	0
2	3K	101	6V6	1	0

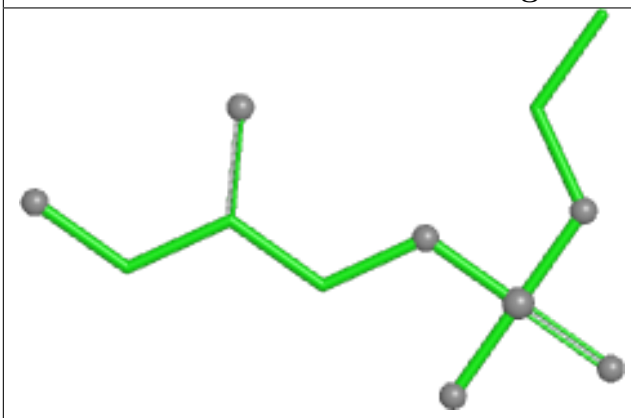
Continued on next page...

Continued from previous page...

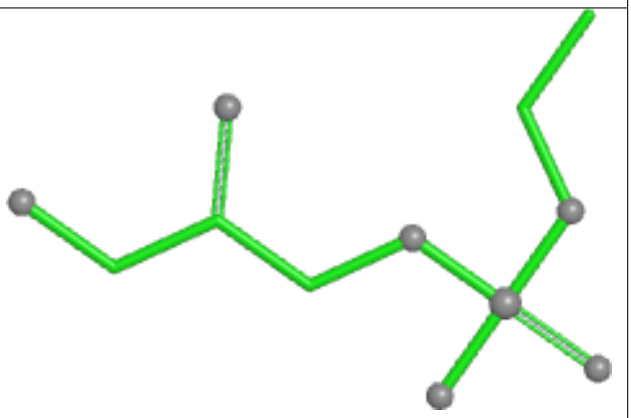
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2H	101	6V6	1	0
2	4L	101	6V6	1	0
2	1M	101	6V6	1	0
2	1B	101	6V6	1	0
2	3D	101	6V6	1	0
2	3N	101	6V6	1	0
2	4B	101	6V6	1	0
2	4I	101	6V6	2	0
2	5M	101	6V6	1	0
2	2L	101	6V6	1	0
2	2E	101	6V6	1	0
2	3E	101	6V6	1	0
2	3G	101	6V6	1	0
2	4F	101	6V6	1	0
2	5H	101	6V6	1	0
2	3I	101	6V6	2	0
2	2N	101	6V6	1	0

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

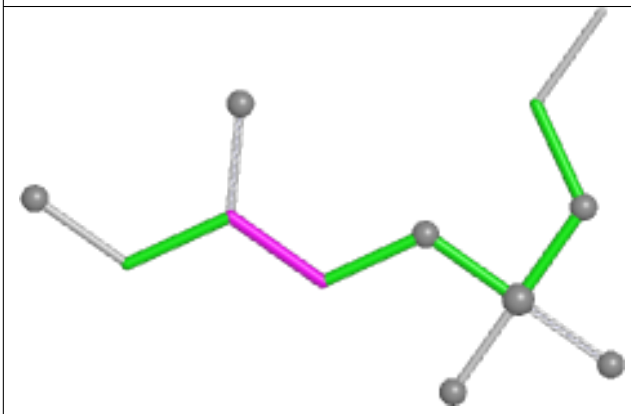
Ligand 6V6 2C 101



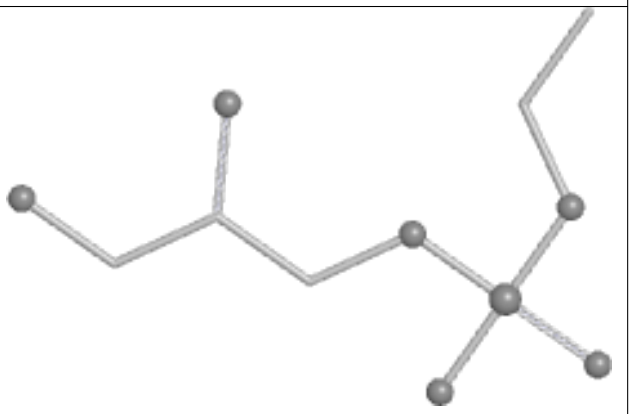
Bond lengths



Bond angles

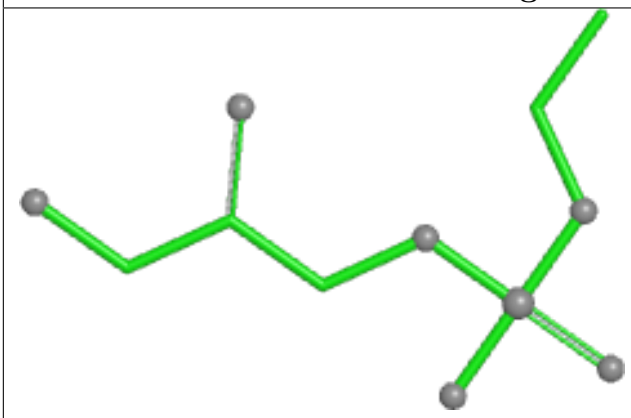


Torsions

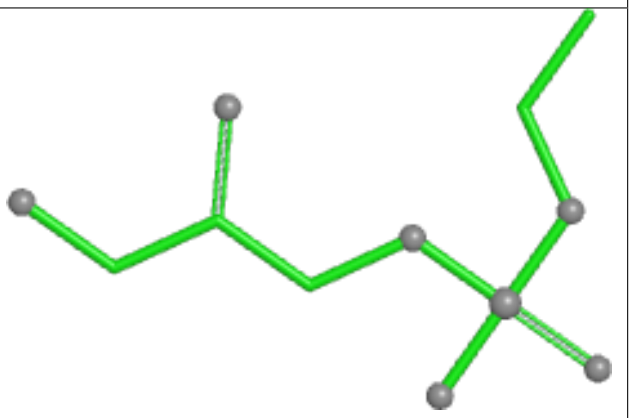


Rings

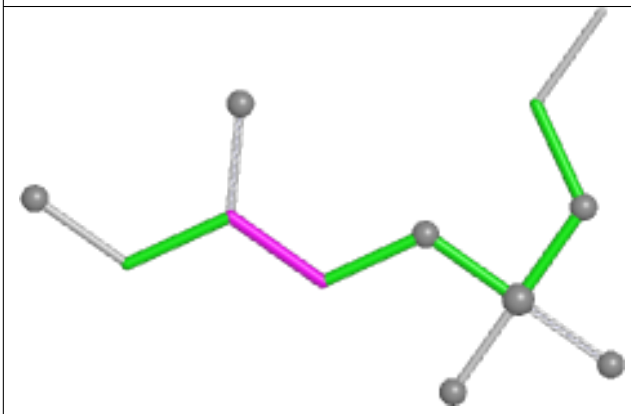
Ligand 6V6 5N 101



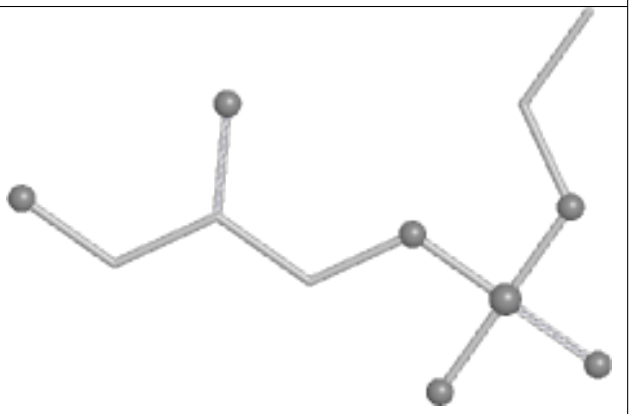
Bond lengths



Bond angles

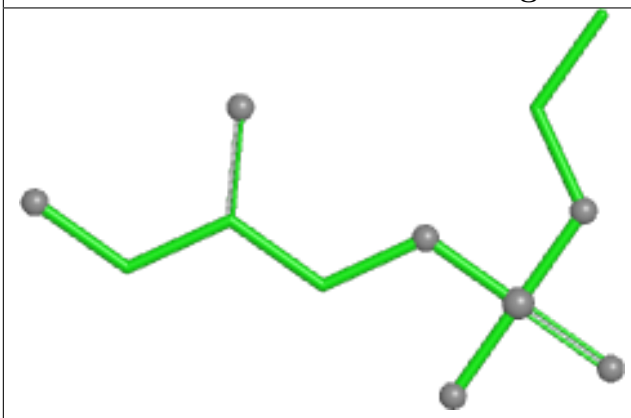


Torsions

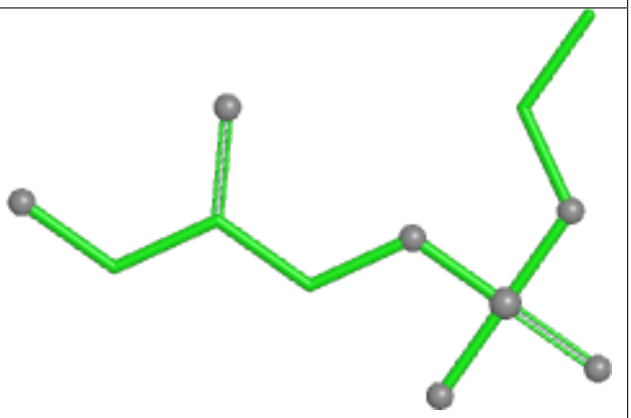


Rings

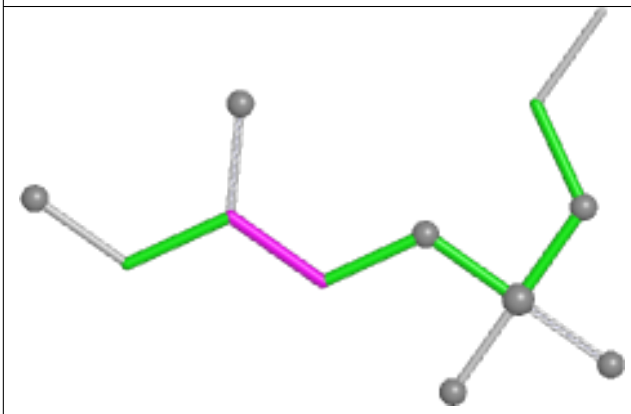
Ligand 6V6 1G 101



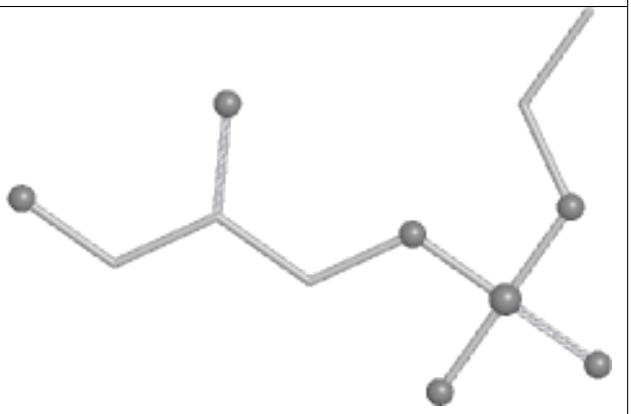
Bond lengths



Bond angles

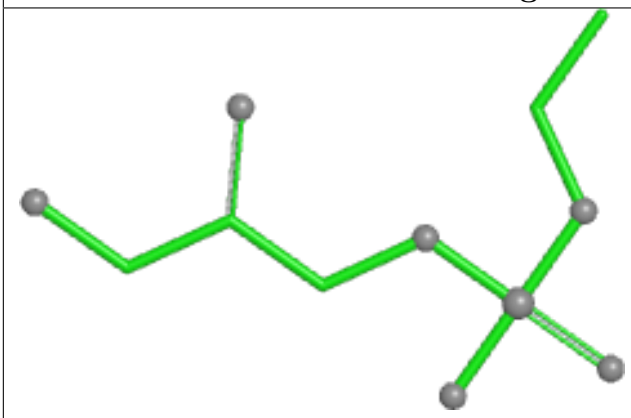


Torsions

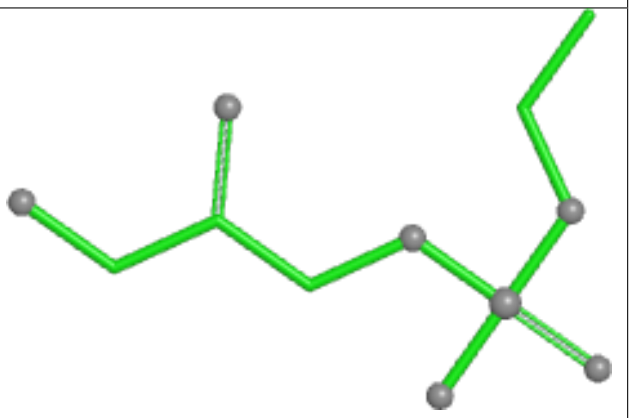


Rings

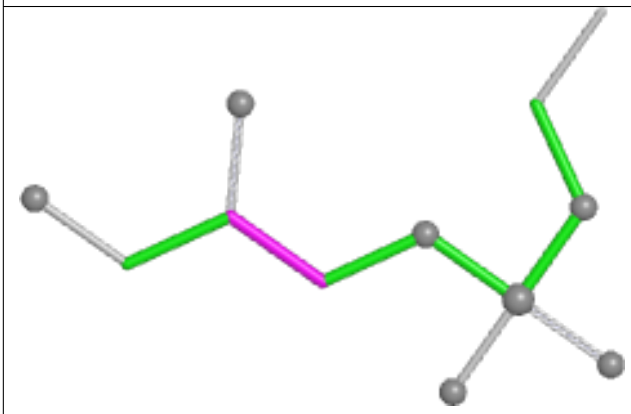
Ligand 6V6 4K 101



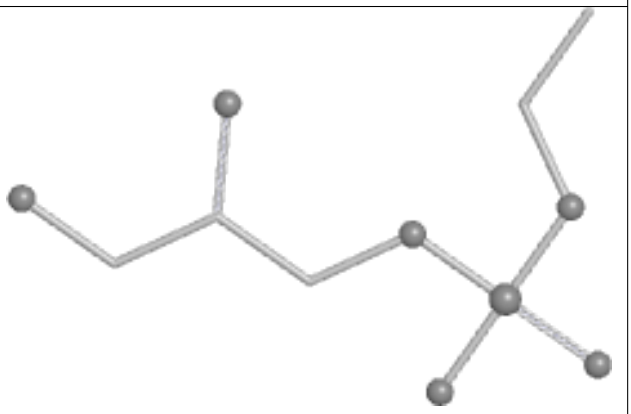
Bond lengths



Bond angles

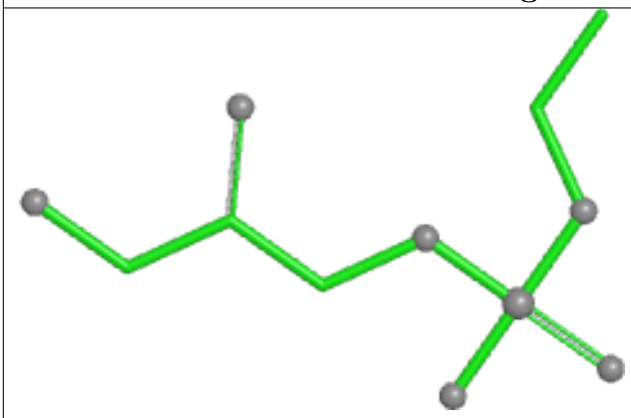


Torsions

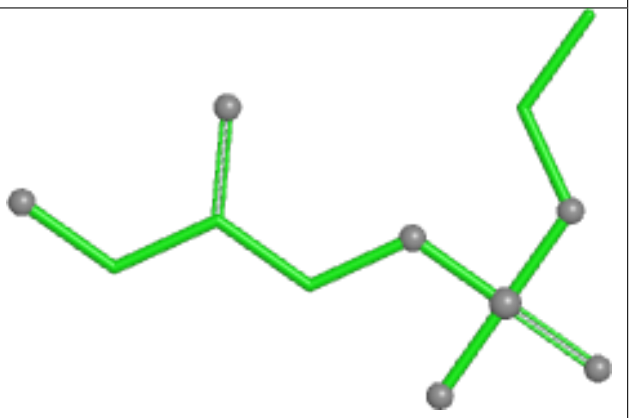


Rings

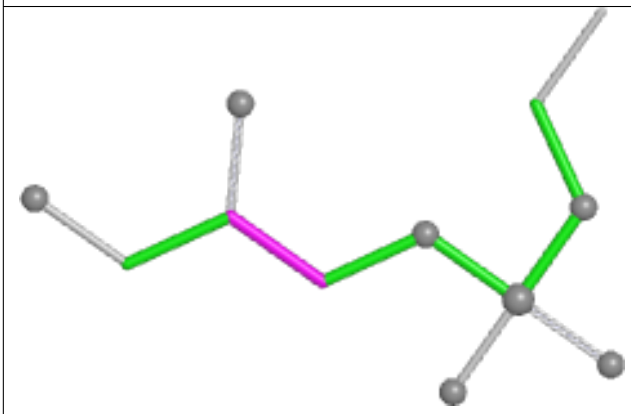
Ligand 6V6 5A 101



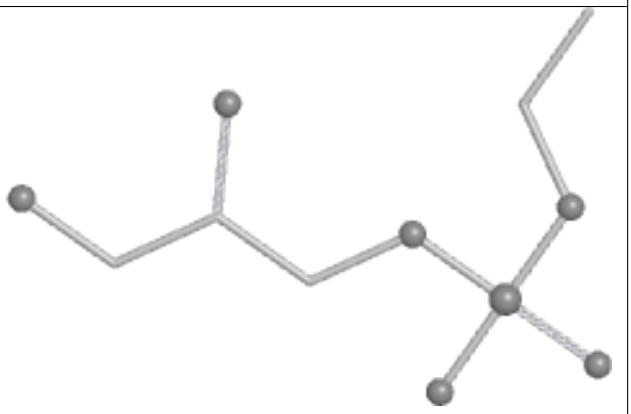
Bond lengths



Bond angles

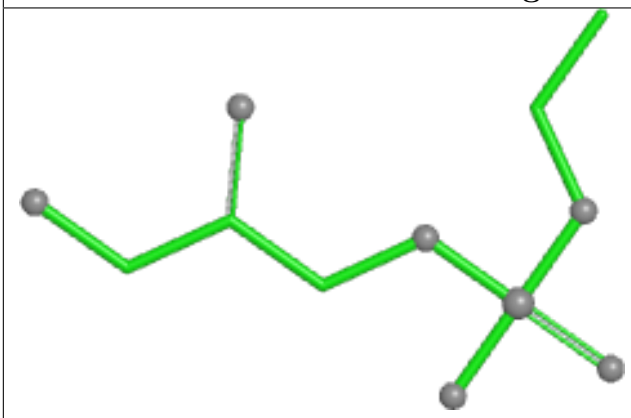


Torsions

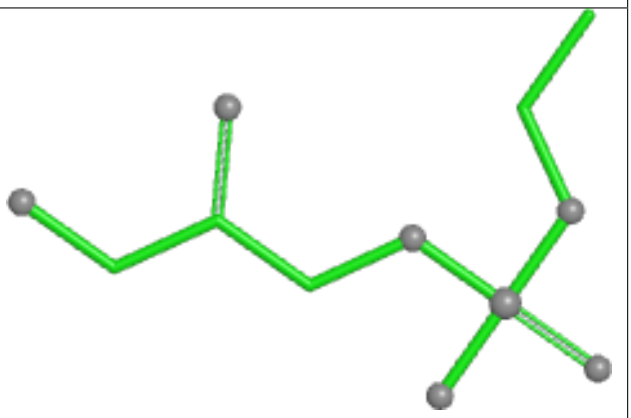


Rings

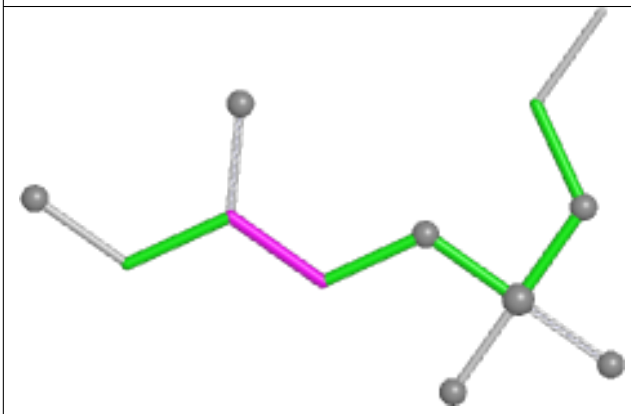
Ligand 6V6 1F 101



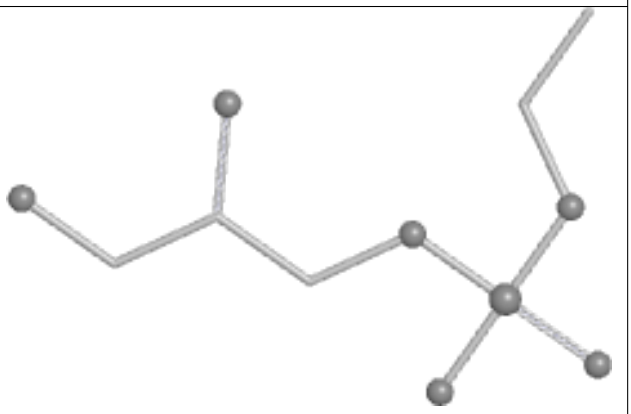
Bond lengths



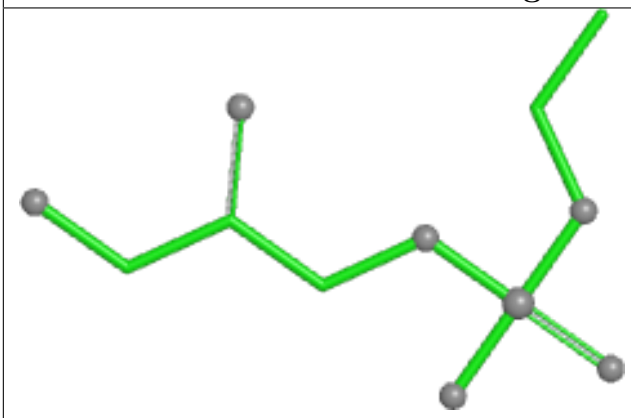
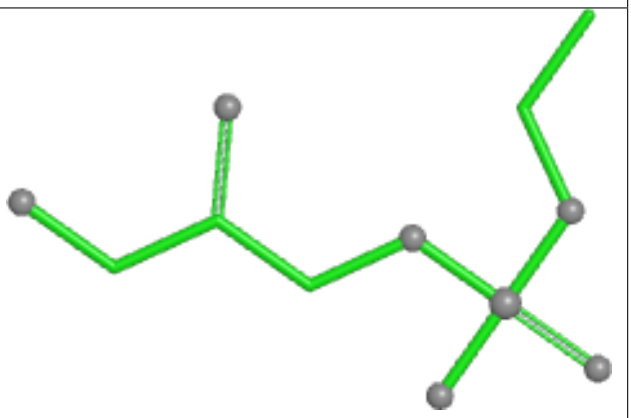
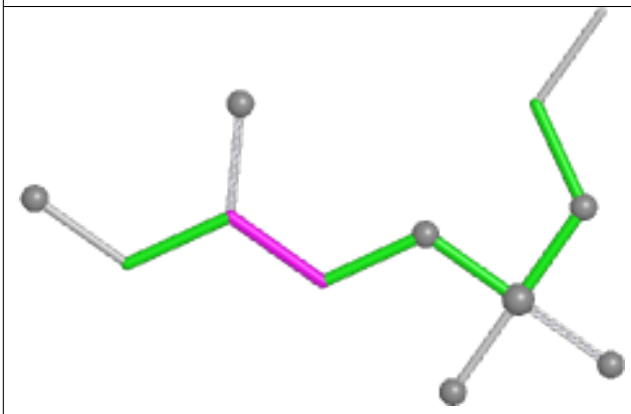
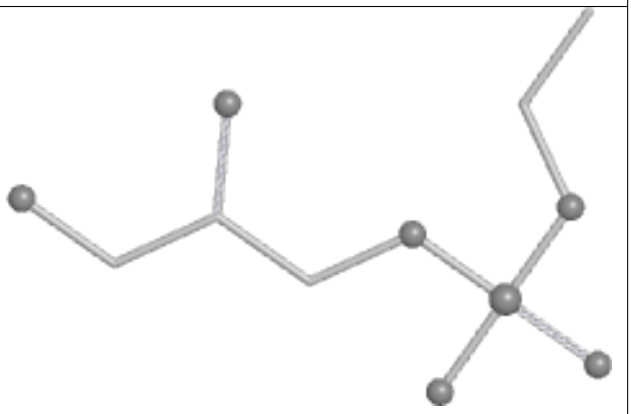
Bond angles



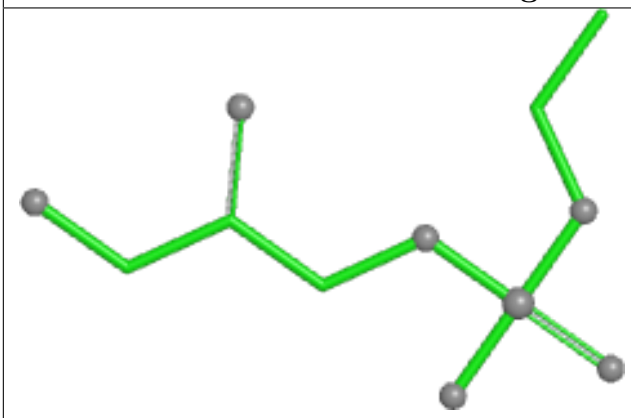
Torsions



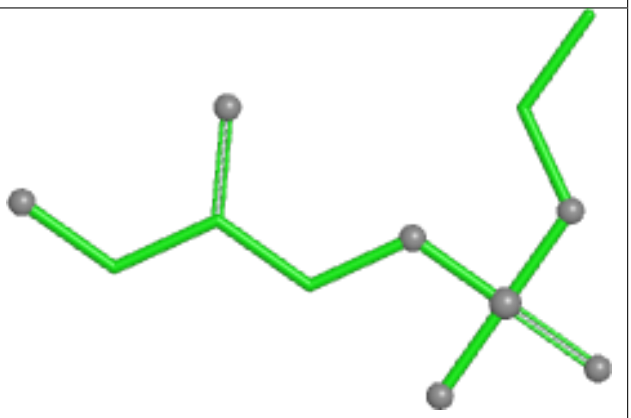
Rings

Ligand 6V6 5L 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

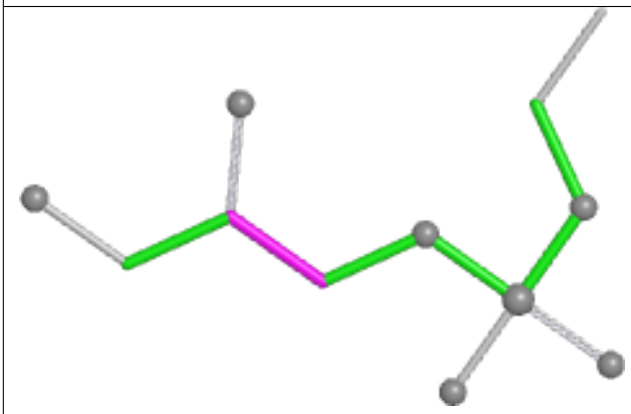
Ligand 6V6 4D 101



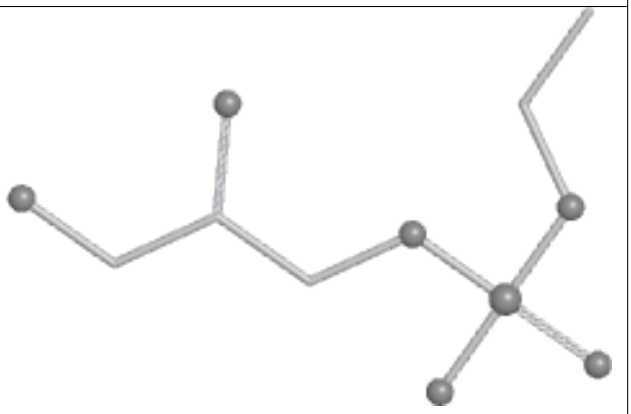
Bond lengths



Bond angles

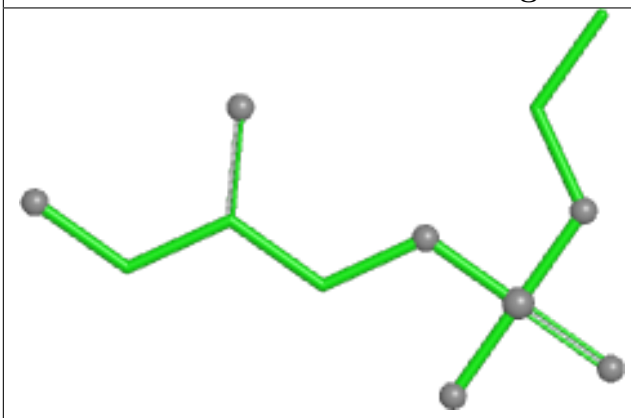


Torsions

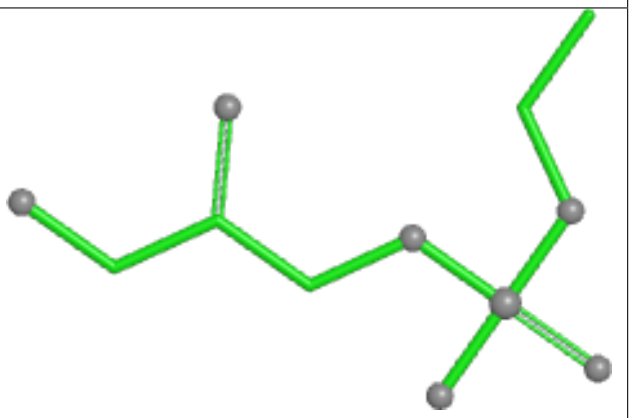


Rings

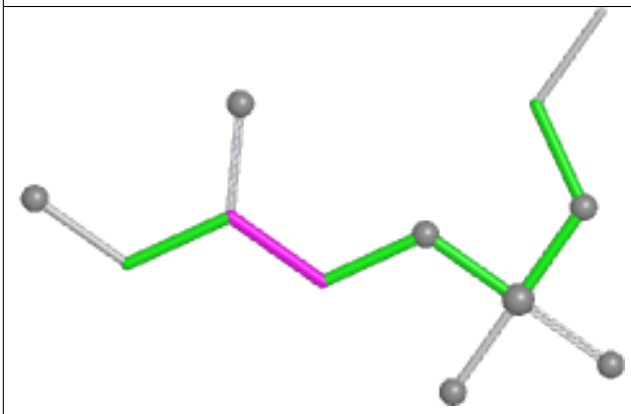
Ligand 6V6 3H 101



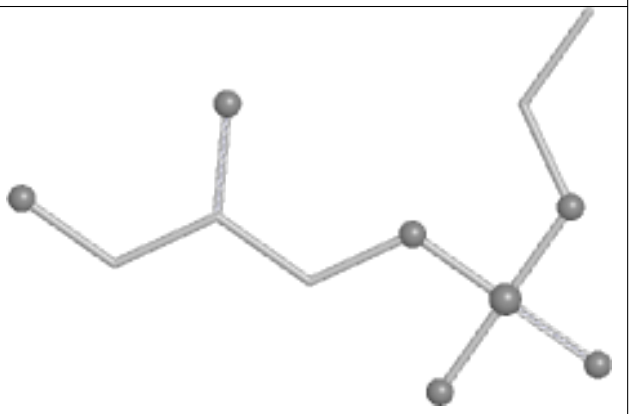
Bond lengths



Bond angles

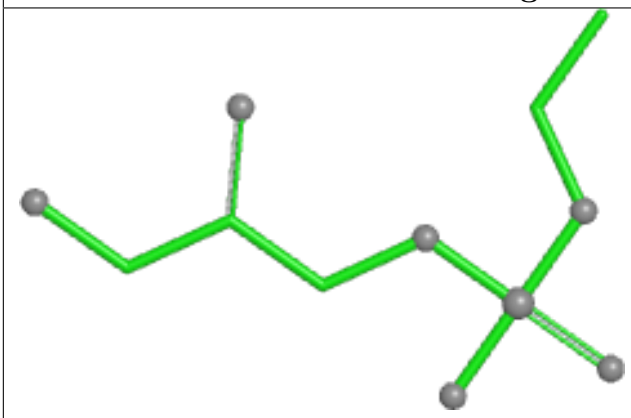


Torsions

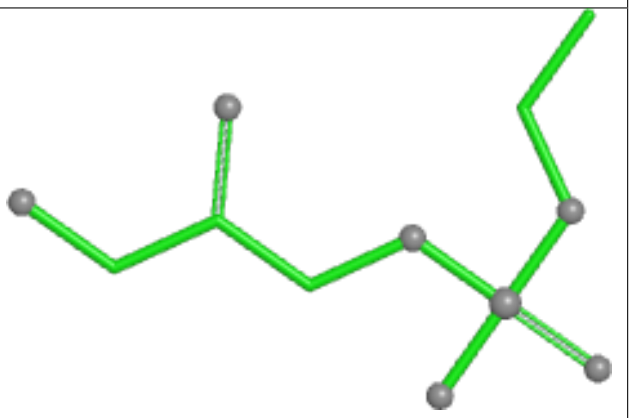


Rings

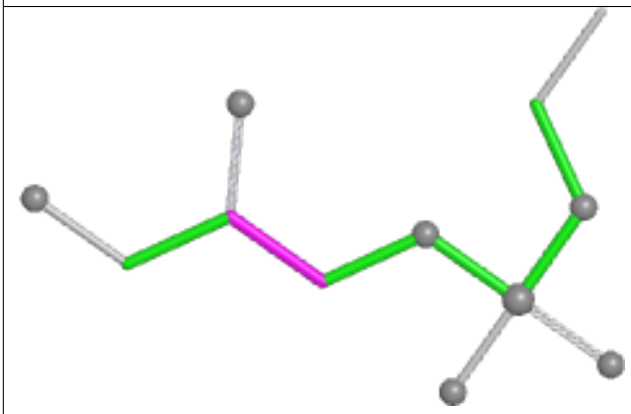
Ligand 6V6 4A 101



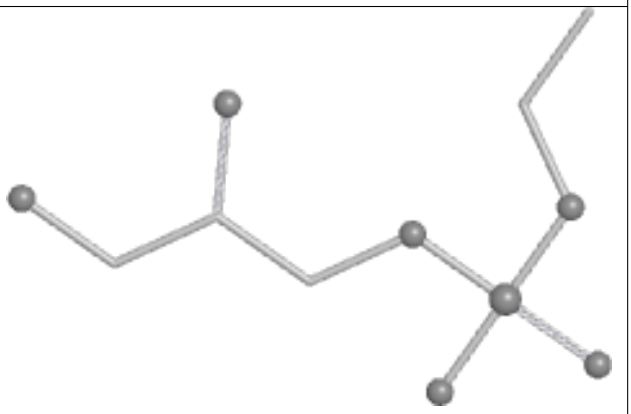
Bond lengths



Bond angles

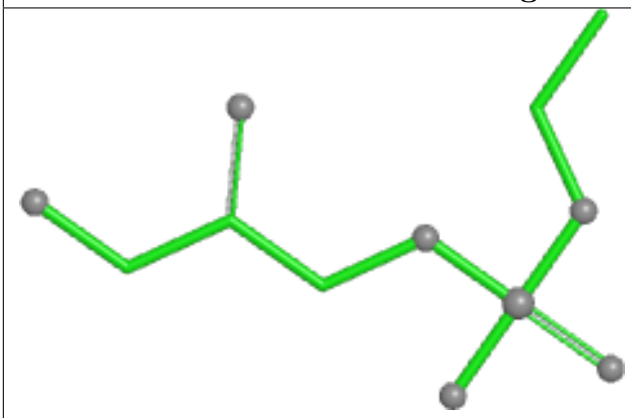


Torsions

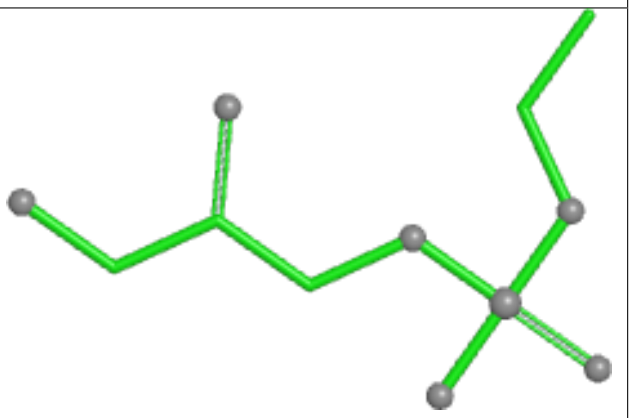


Rings

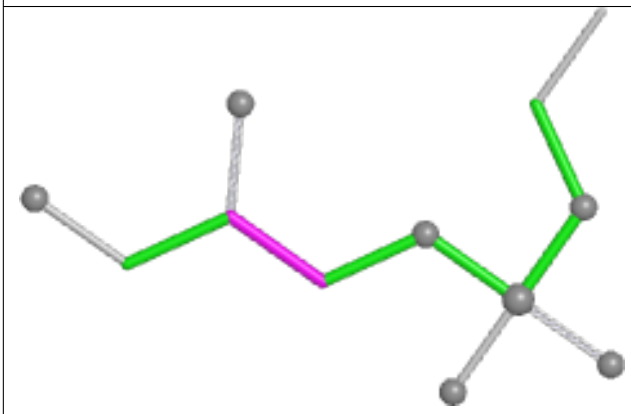
Ligand 6V6 4N 101



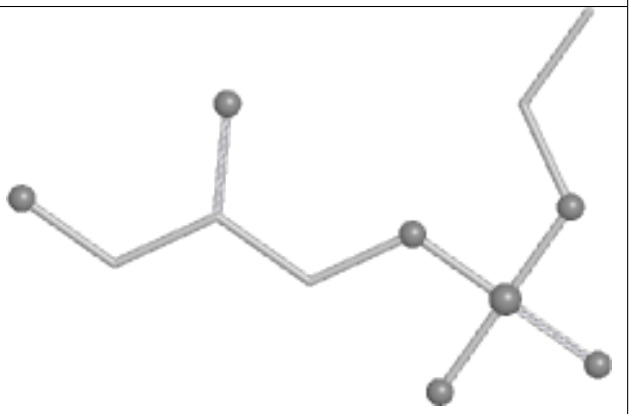
Bond lengths



Bond angles

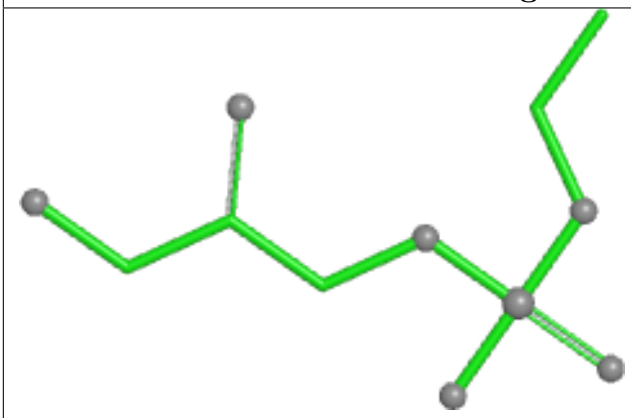


Torsions

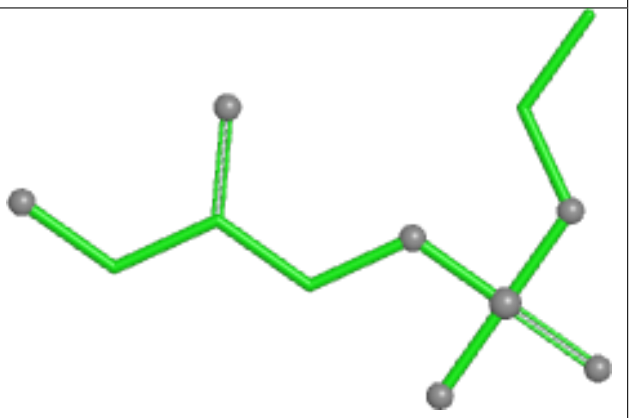


Rings

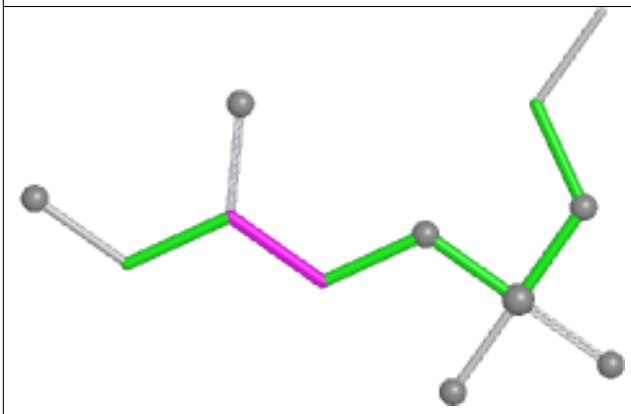
Ligand 6V6 5G 101



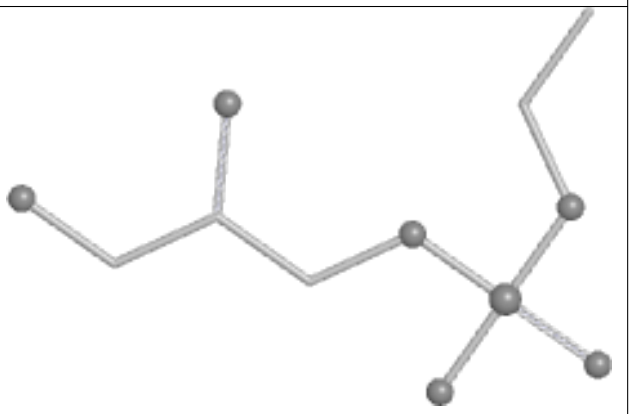
Bond lengths



Bond angles

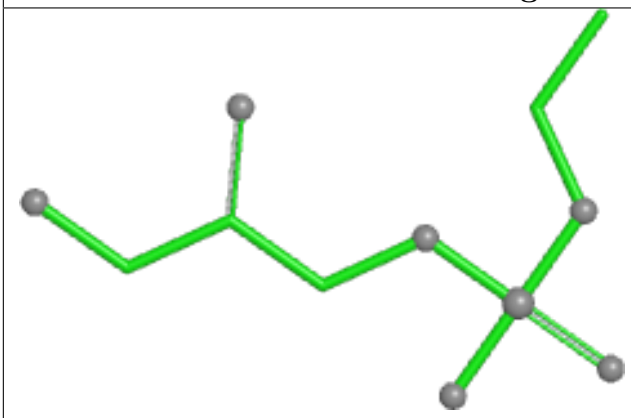


Torsions

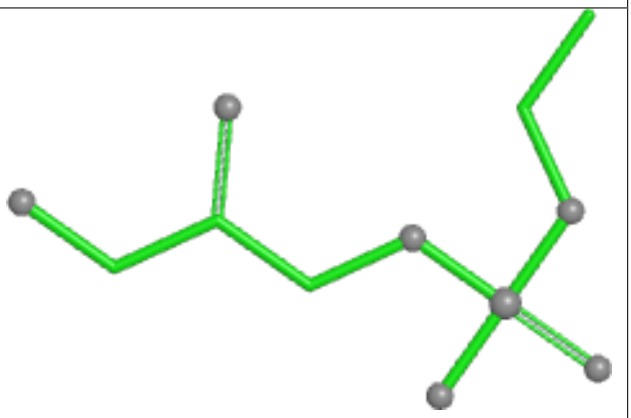


Rings

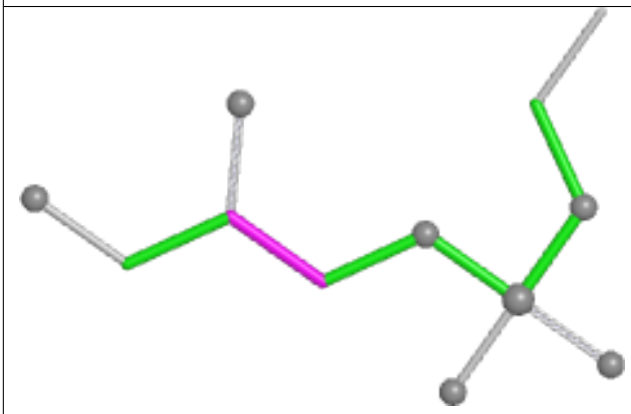
Ligand 6V6 5D 101



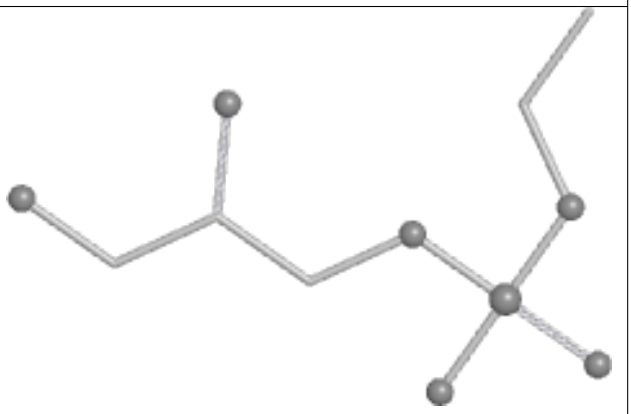
Bond lengths



Bond angles

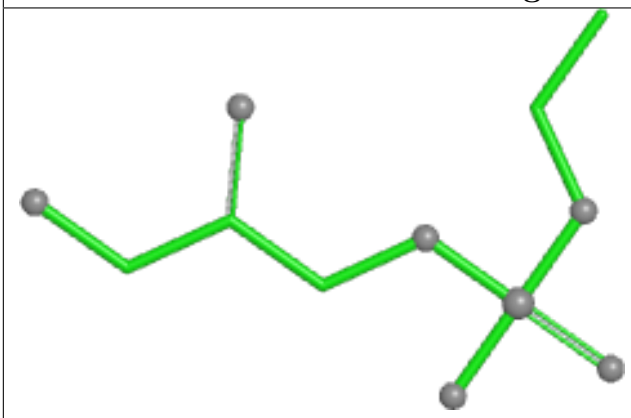


Torsions

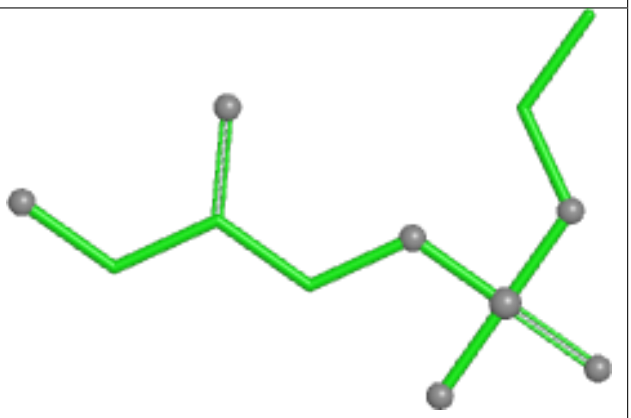


Rings

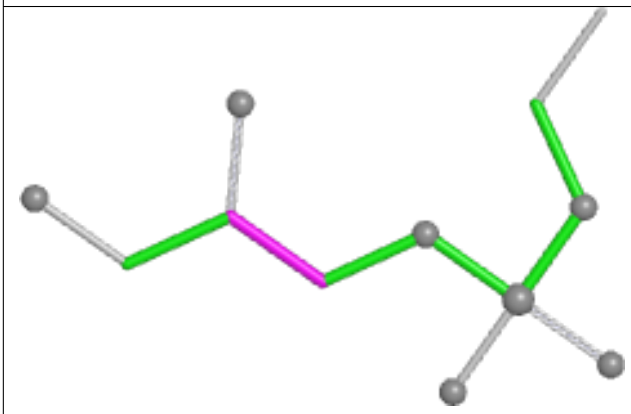
Ligand 6V6 3L 101



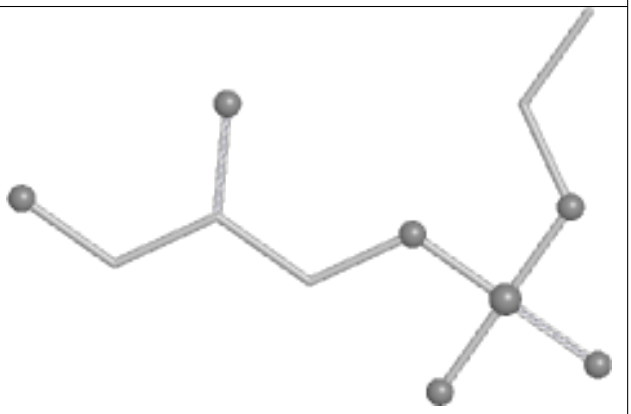
Bond lengths



Bond angles

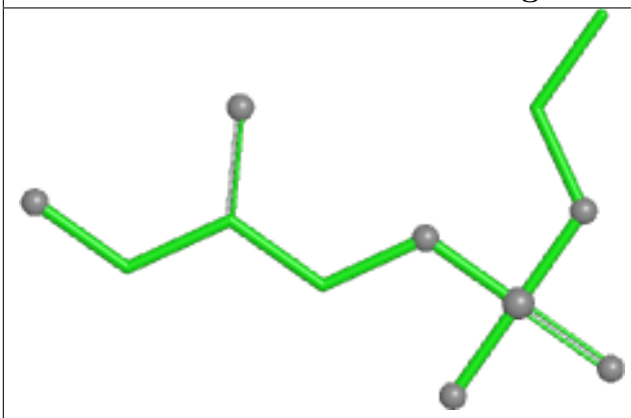


Torsions

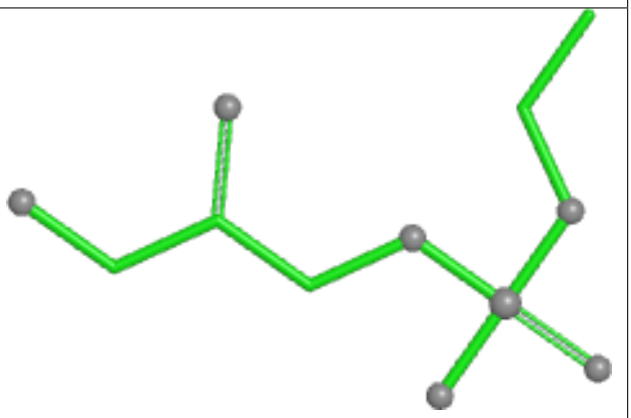


Rings

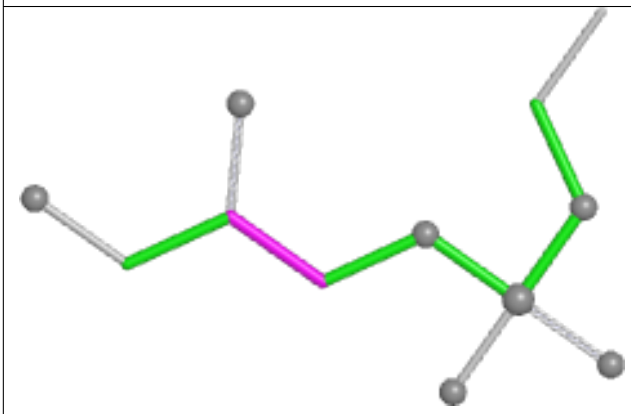
Ligand 6V6 5B 101



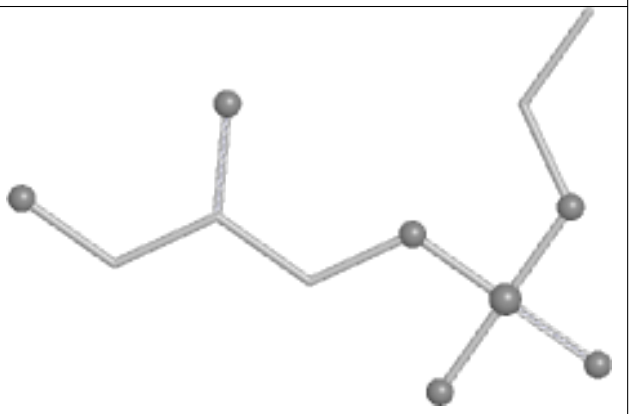
Bond lengths



Bond angles

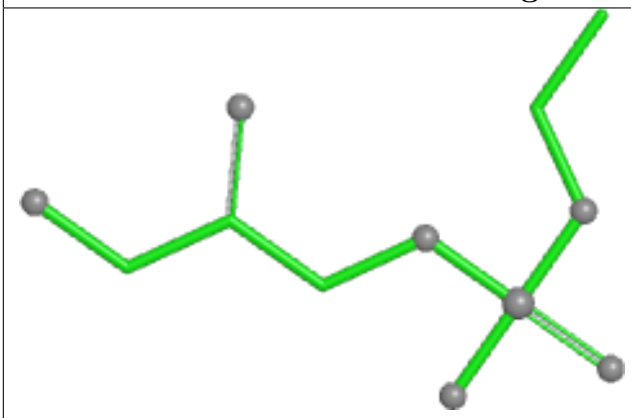


Torsions

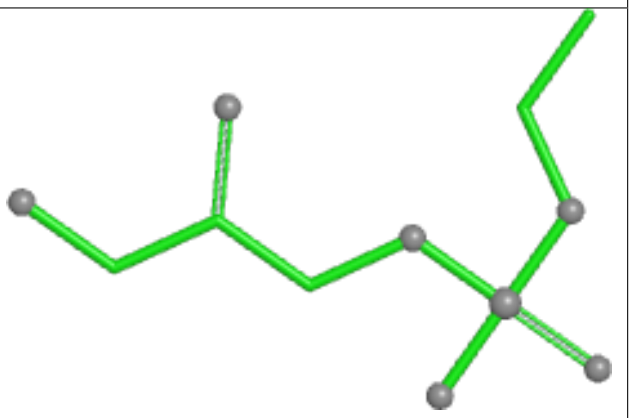


Rings

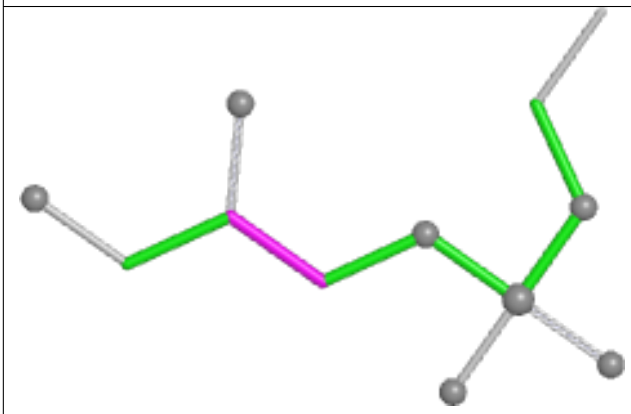
Ligand 6V6 4C 101



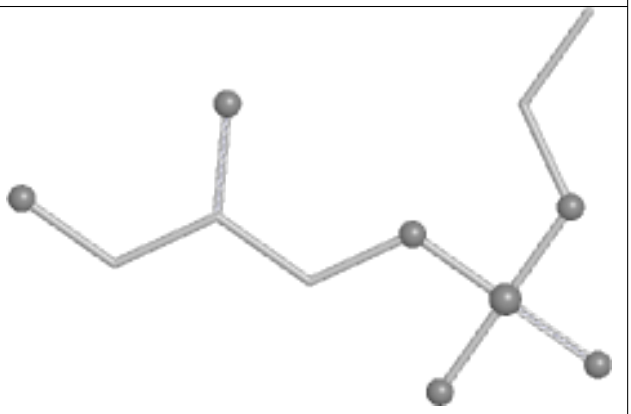
Bond lengths



Bond angles

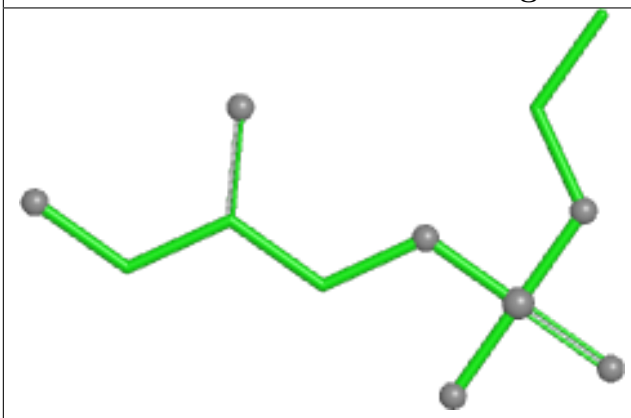


Torsions

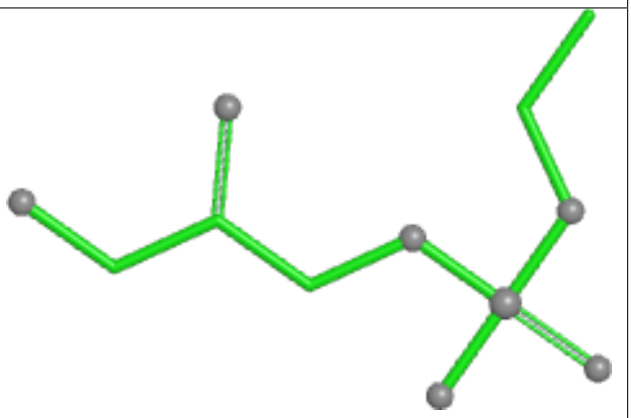


Rings

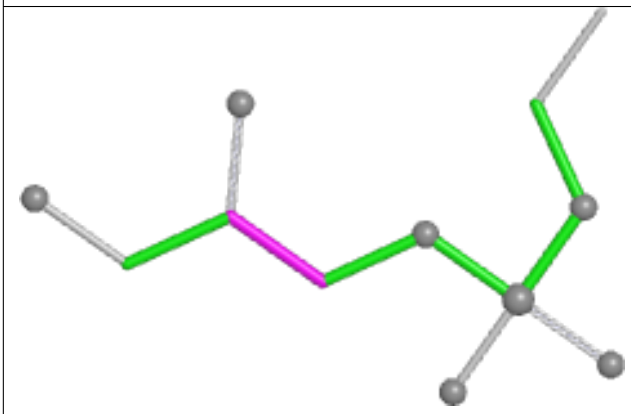
Ligand 6V6 2G 101



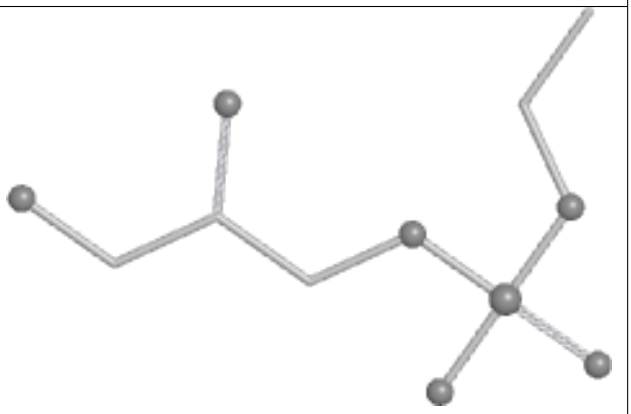
Bond lengths



Bond angles

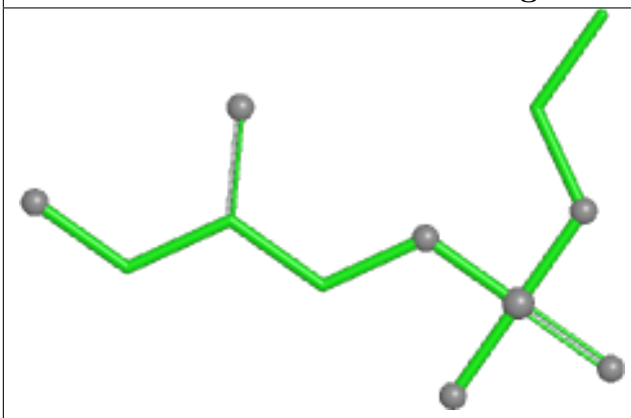


Torsions

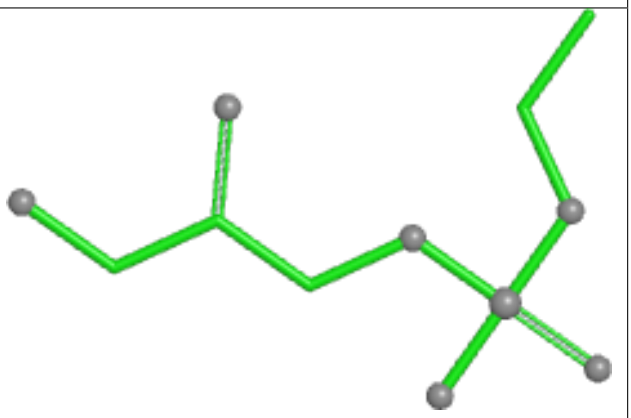


Rings

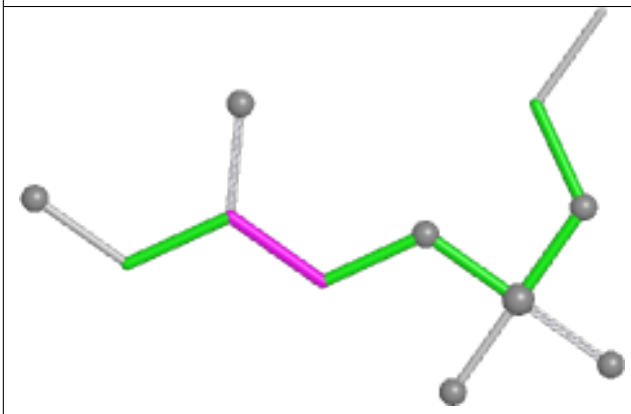
Ligand 6V6 5K 101



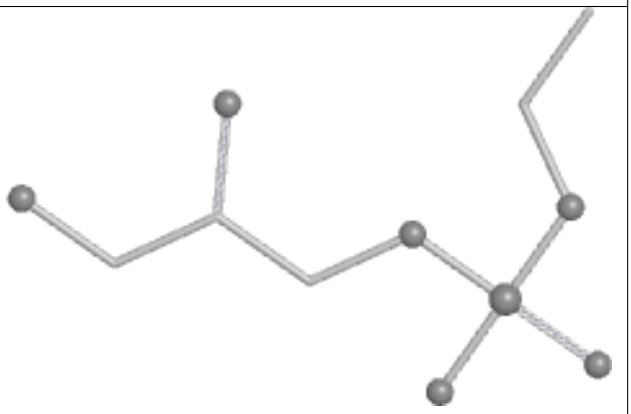
Bond lengths



Bond angles

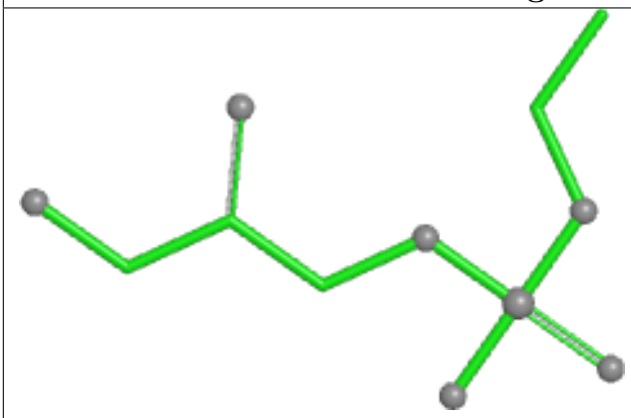


Torsions

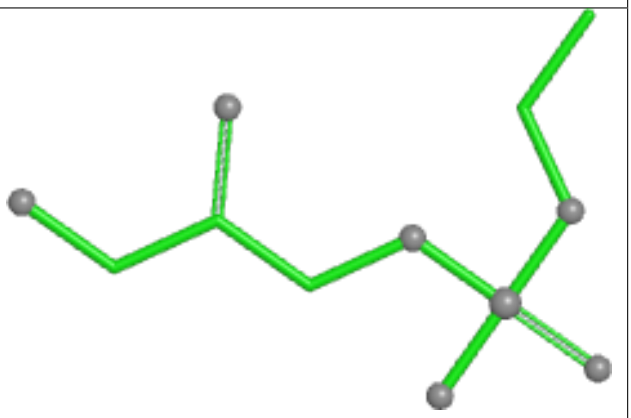


Rings

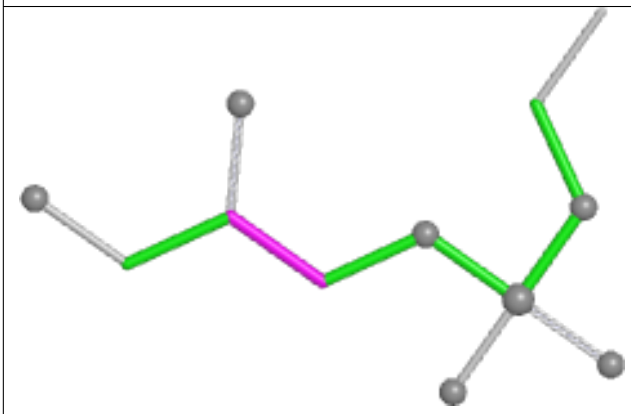
Ligand 6V6 1I 101



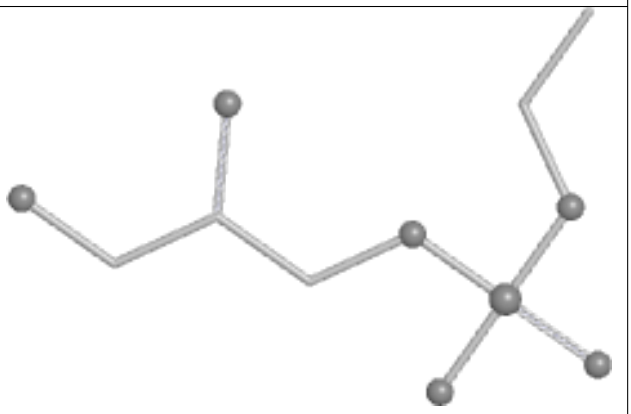
Bond lengths



Bond angles

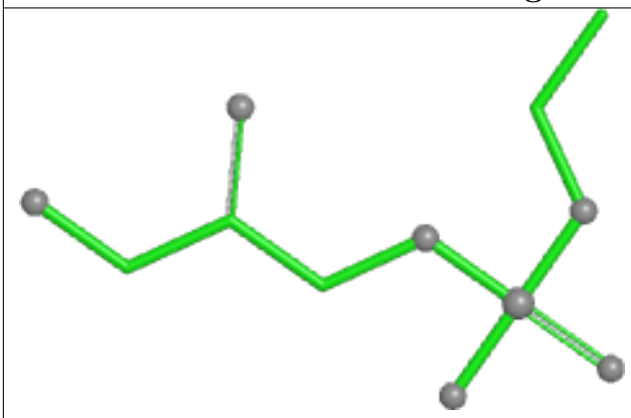


Torsions

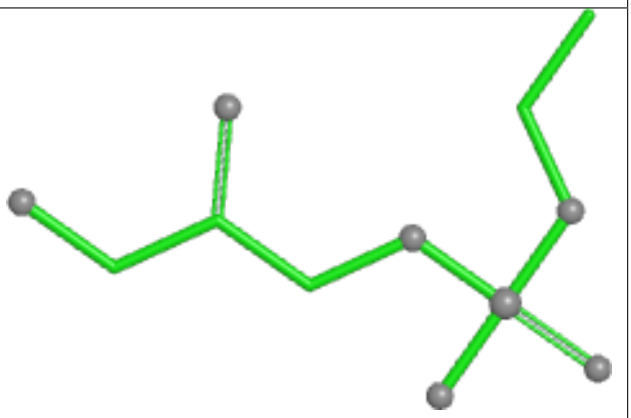


Rings

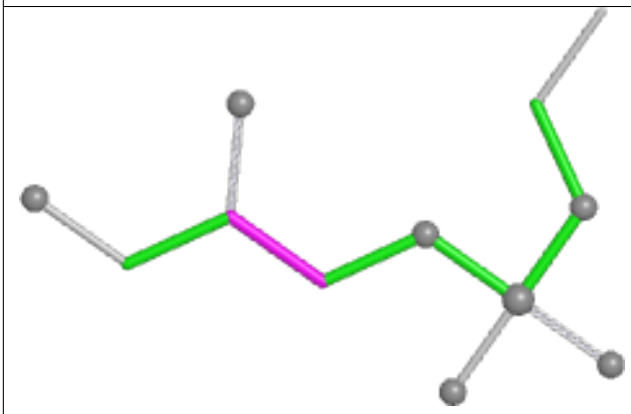
Ligand 6V6 2J 101



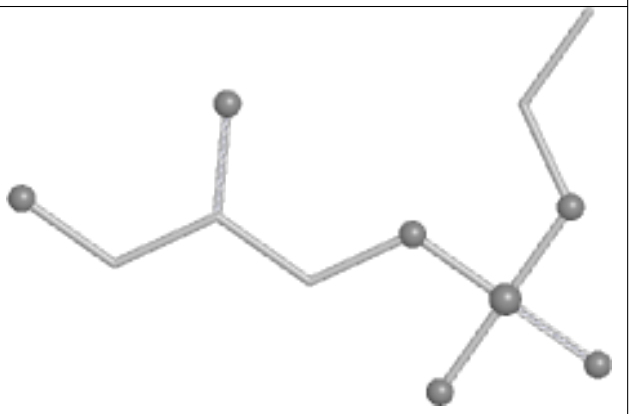
Bond lengths



Bond angles

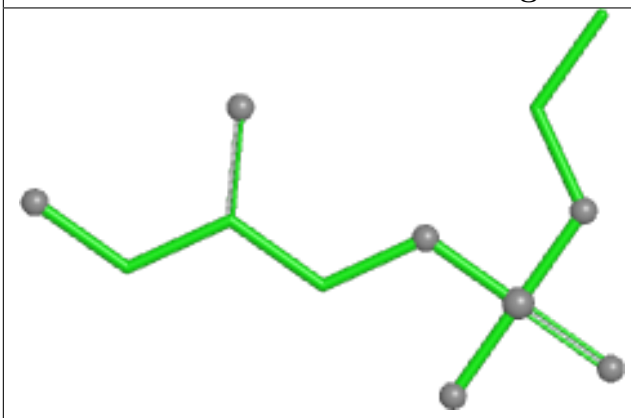


Torsions

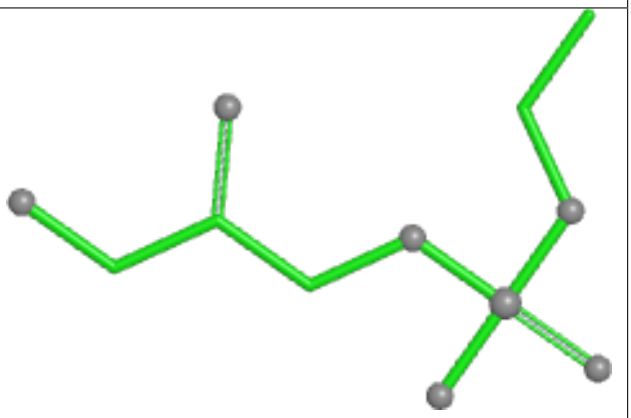


Rings

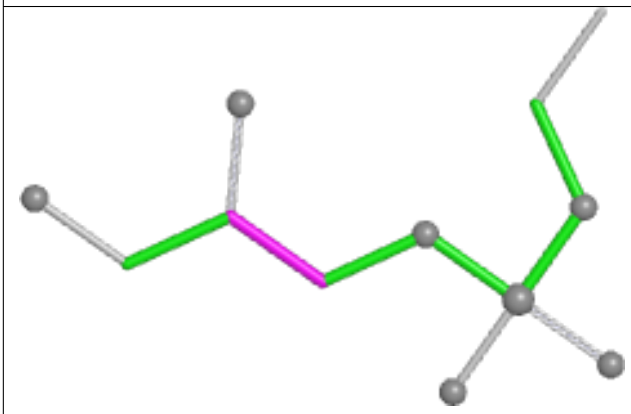
Ligand 6V6 4G 101



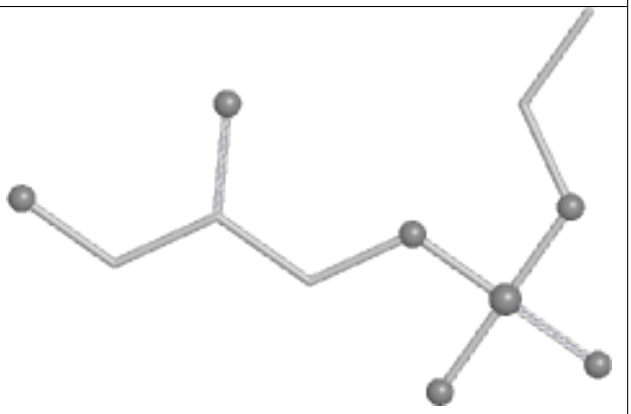
Bond lengths



Bond angles

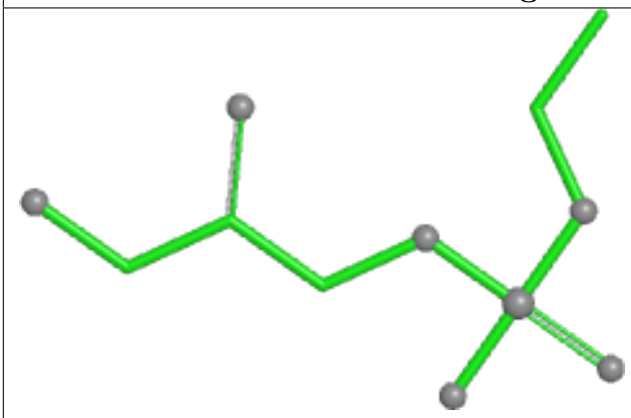


Torsions

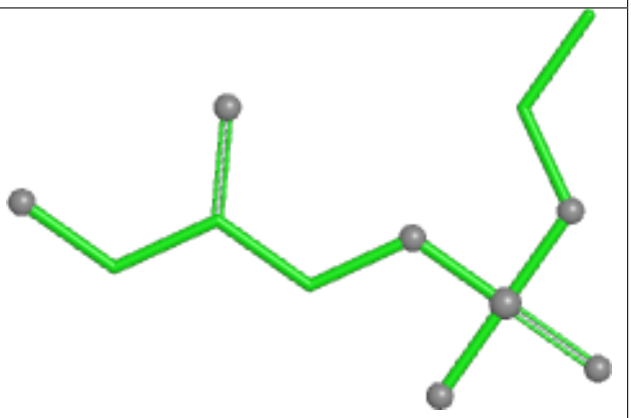


Rings

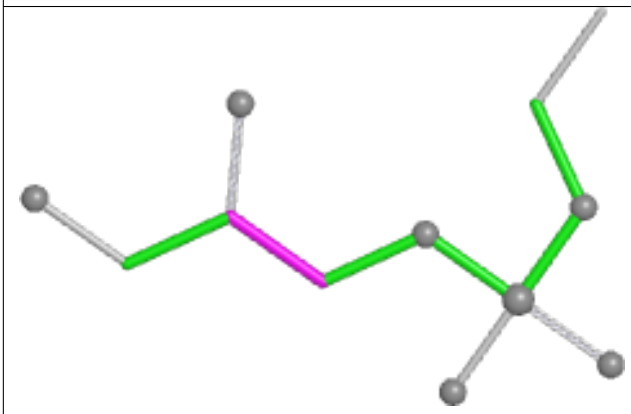
Ligand 6V6 1N 101



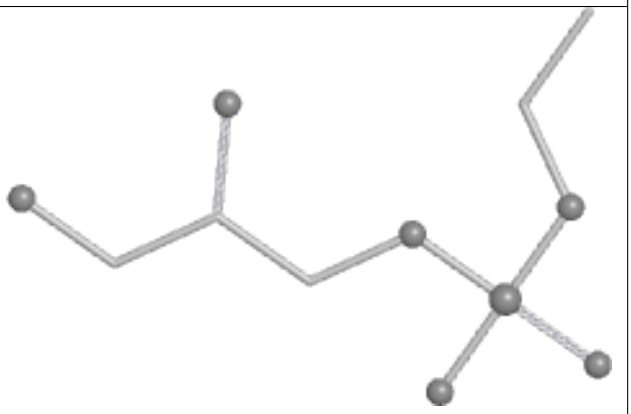
Bond lengths



Bond angles

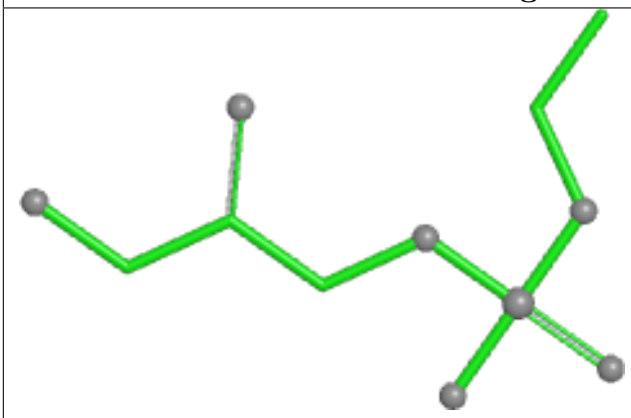


Torsions

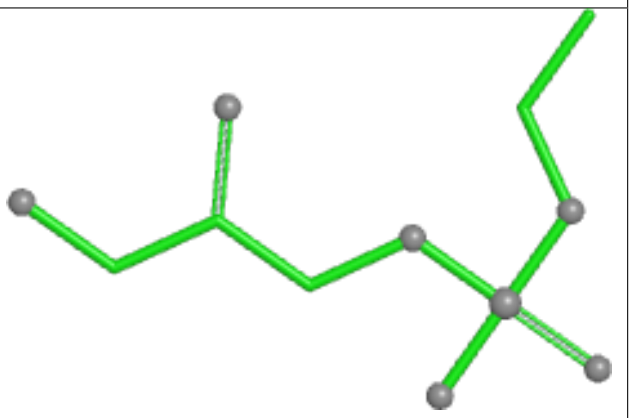


Rings

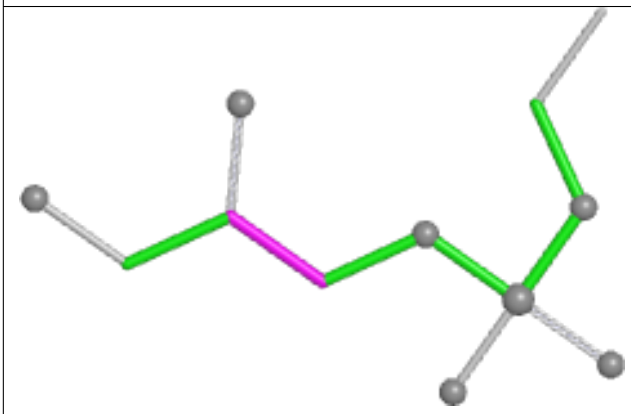
Ligand 6V6 1K 101



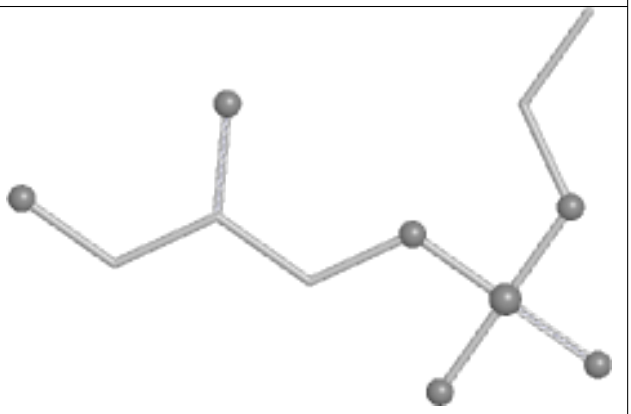
Bond lengths



Bond angles

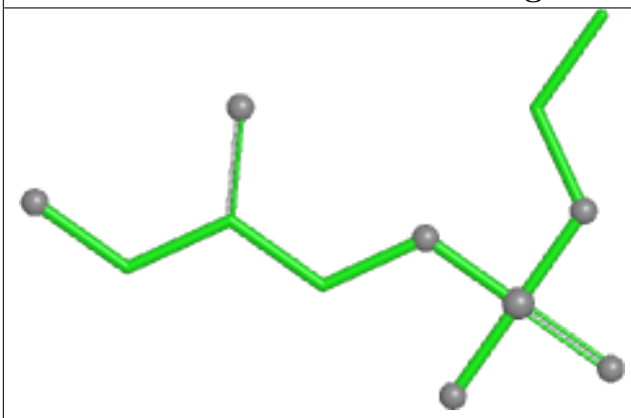


Torsions

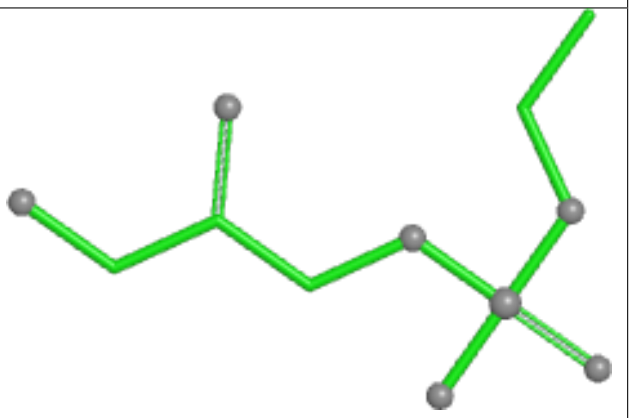


Rings

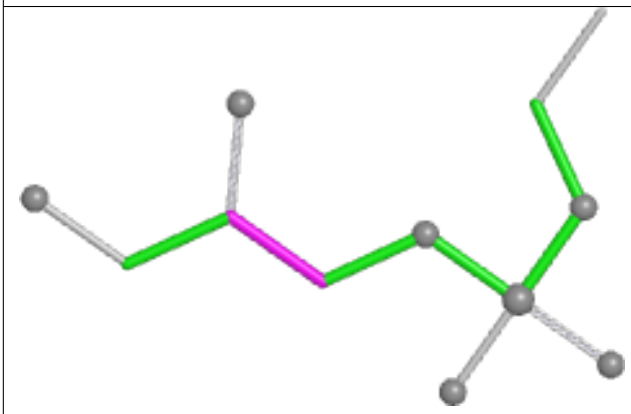
Ligand 6V6 4J 101



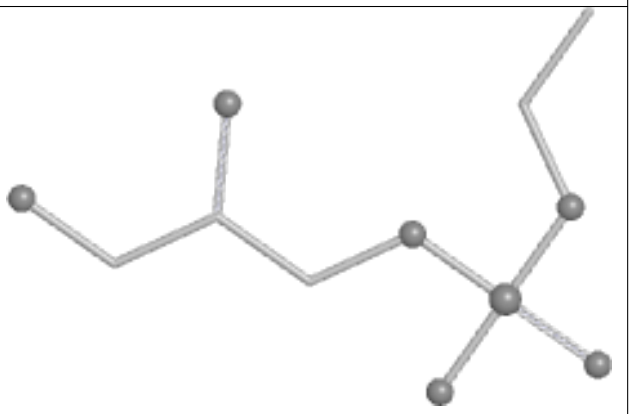
Bond lengths



Bond angles

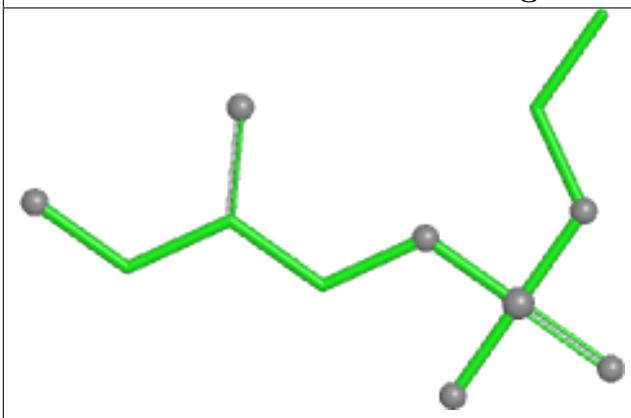


Torsions

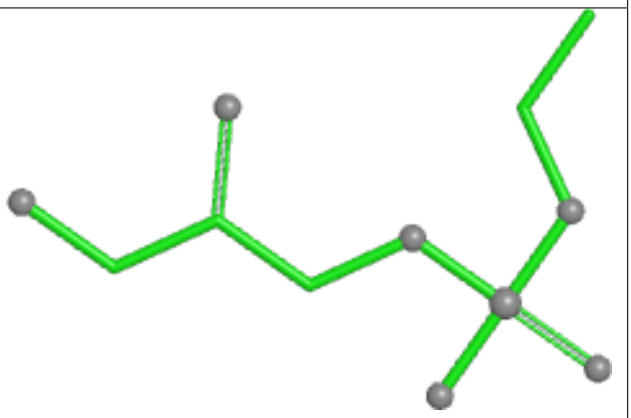


Rings

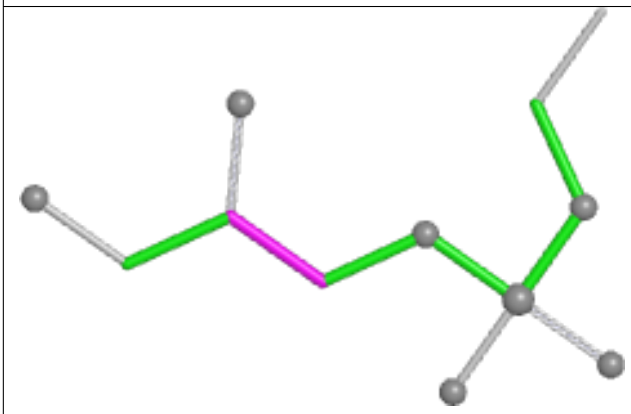
Ligand 6V6 2D 101



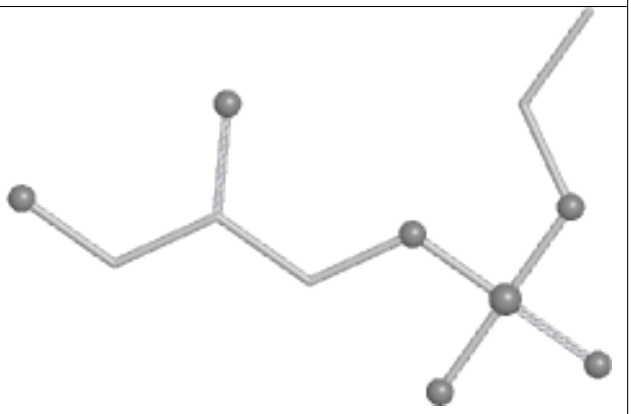
Bond lengths



Bond angles

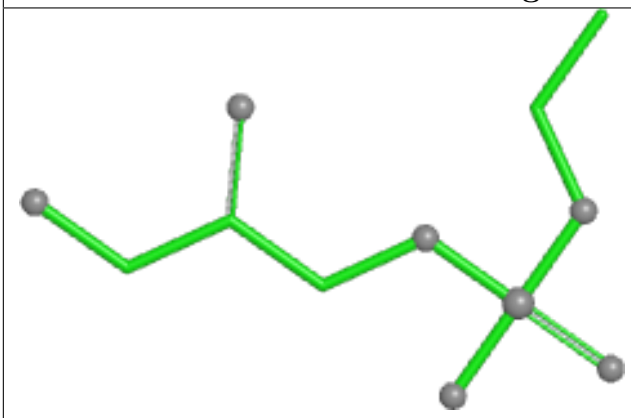


Torsions

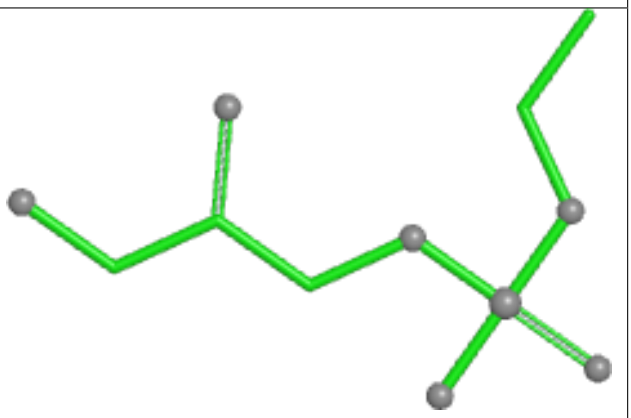


Rings

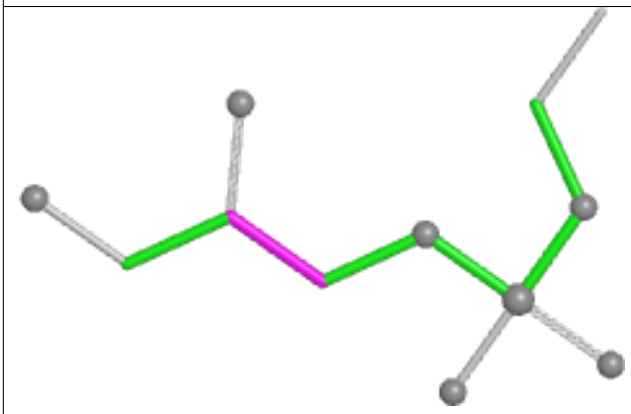
Ligand 6V6 1E 101



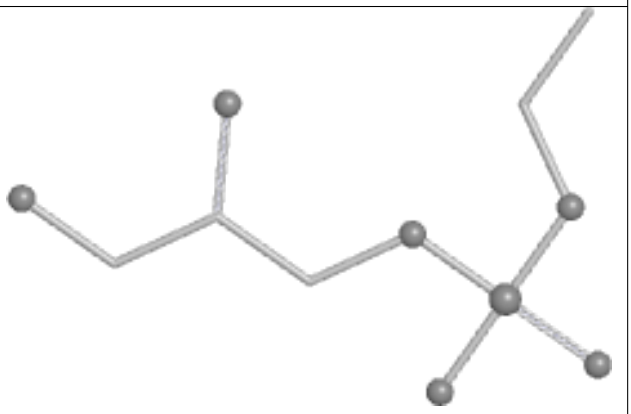
Bond lengths



Bond angles

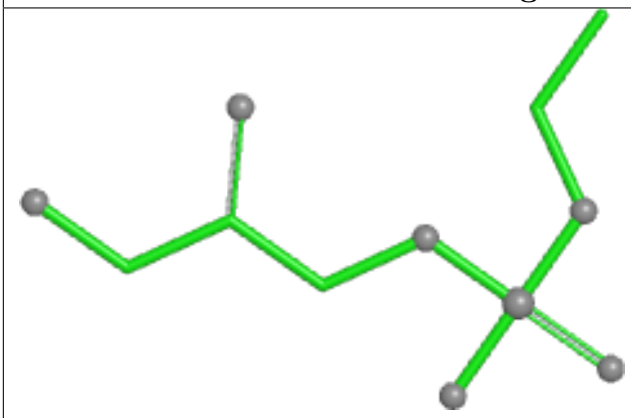


Torsions

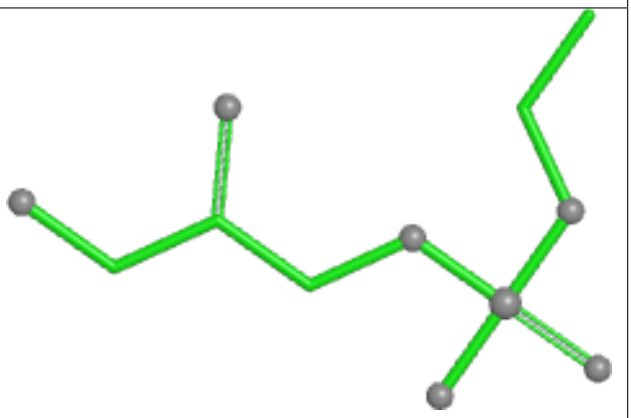


Rings

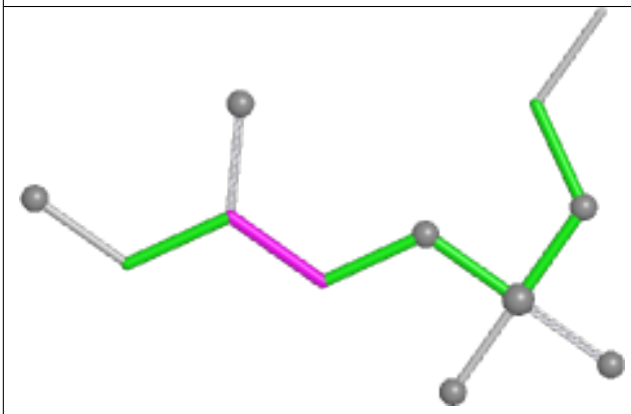
Ligand 6V6 2K 101



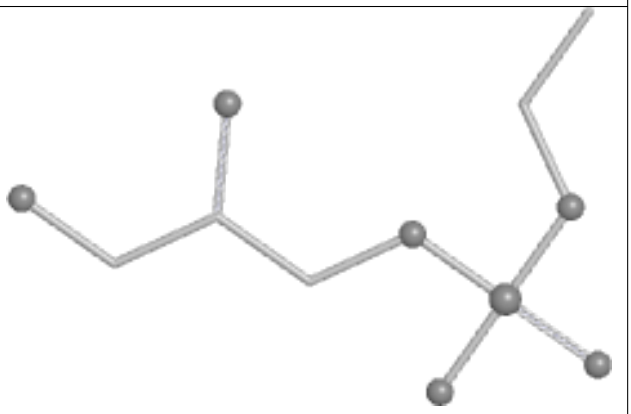
Bond lengths



Bond angles

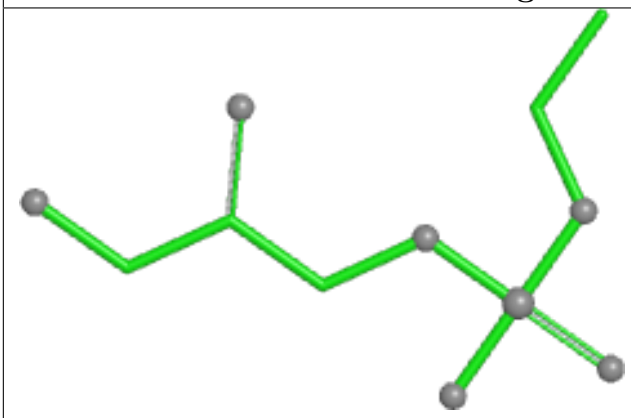


Torsions

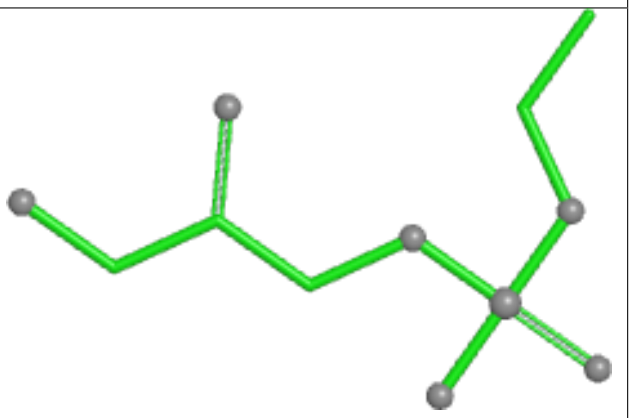


Rings

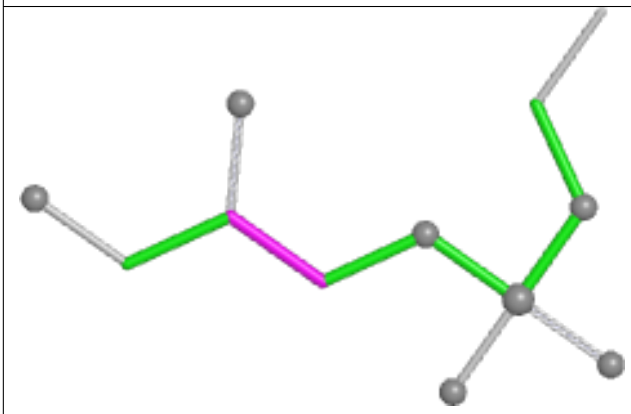
Ligand 6V6 4M 101



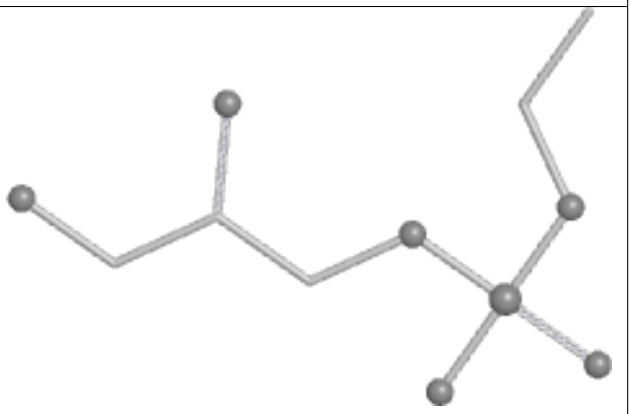
Bond lengths



Bond angles

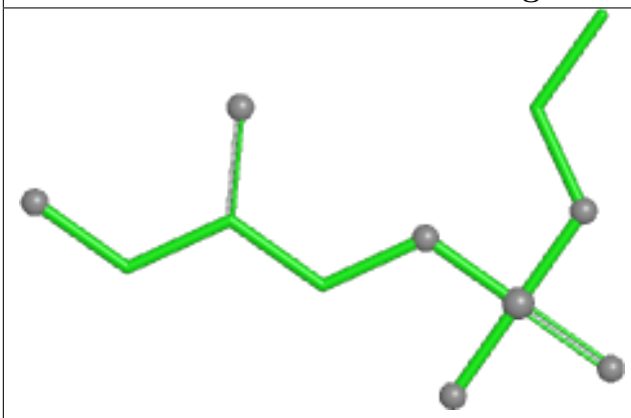


Torsions

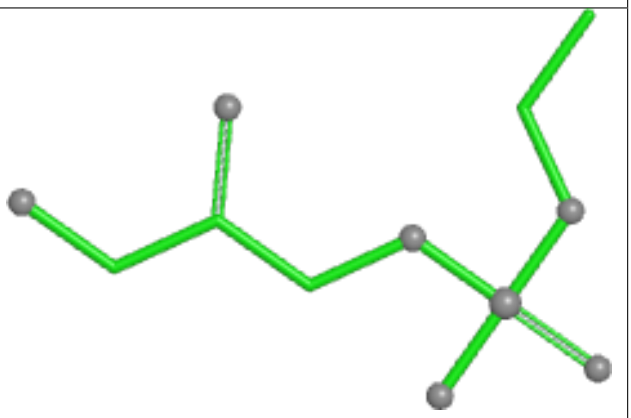


Rings

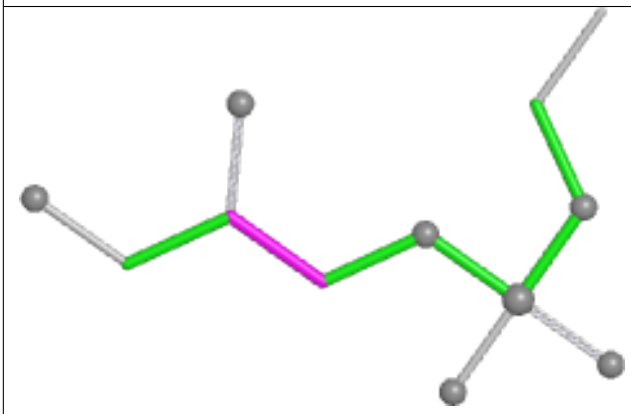
Ligand 6V6 5E 101



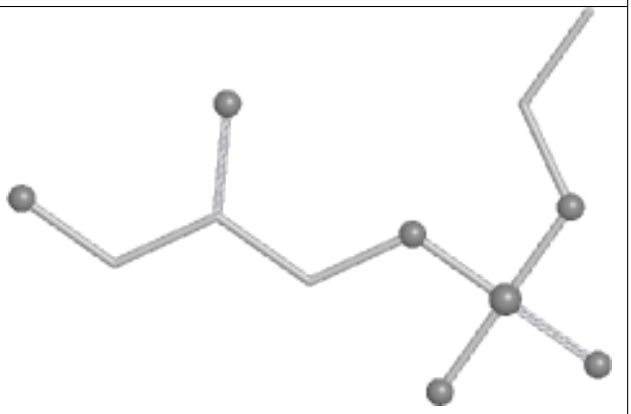
Bond lengths



Bond angles

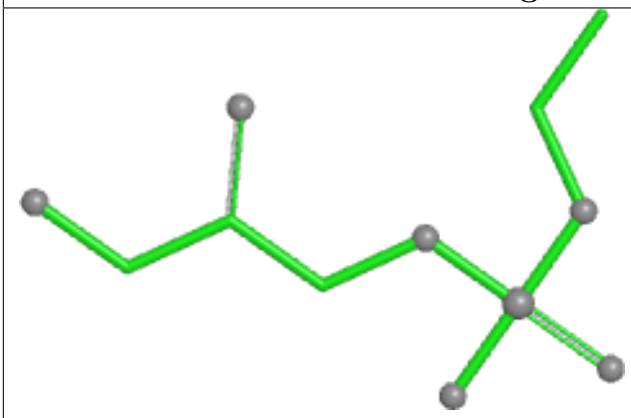


Torsions

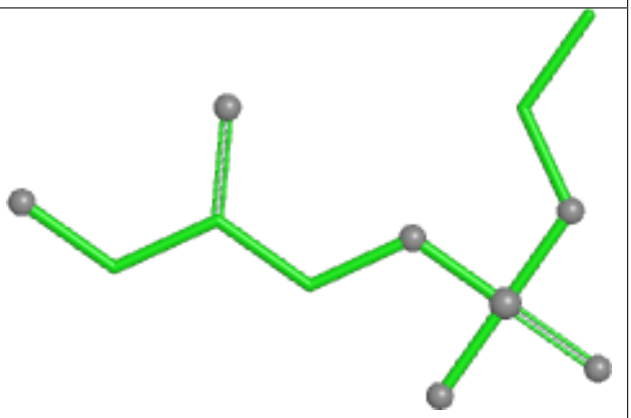


Rings

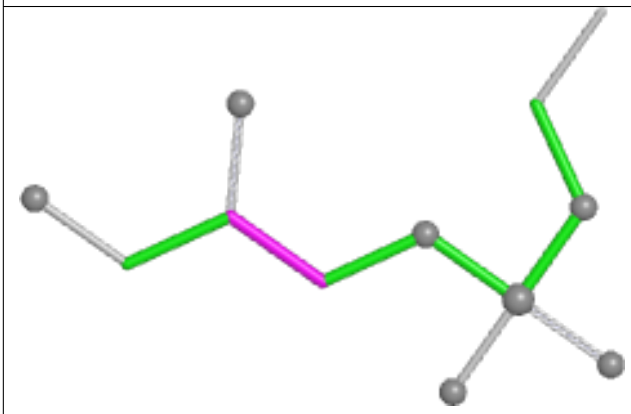
Ligand 6V6 2A 101



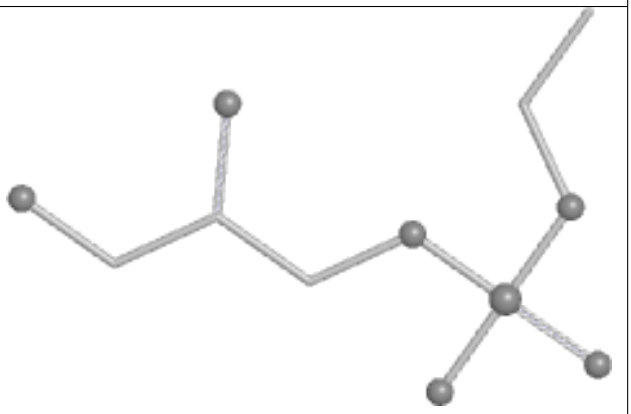
Bond lengths



Bond angles

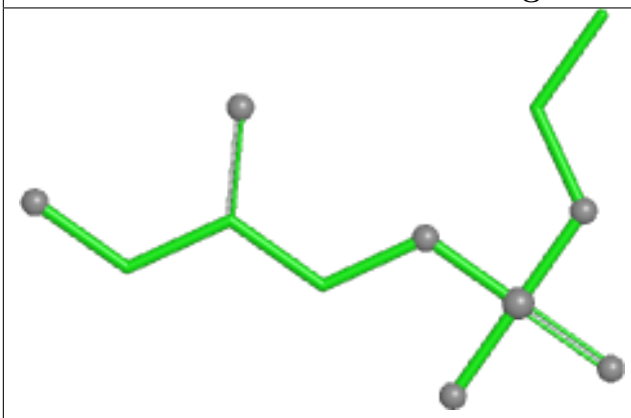


Torsions

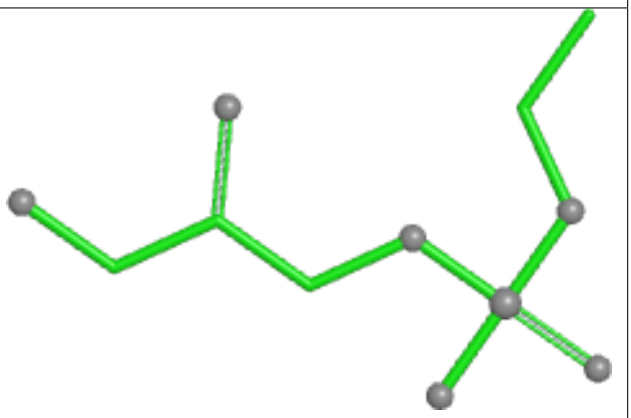


Rings

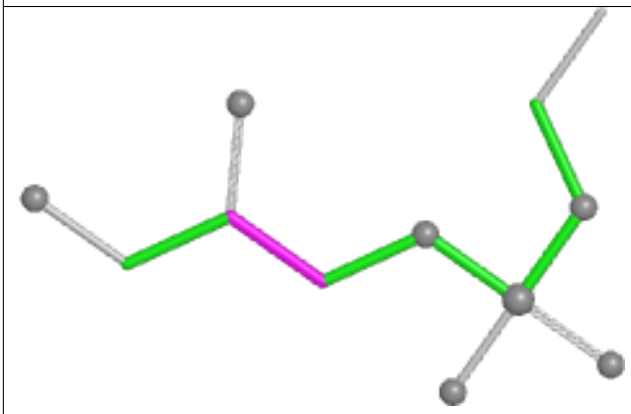
Ligand 6V6 2F 101



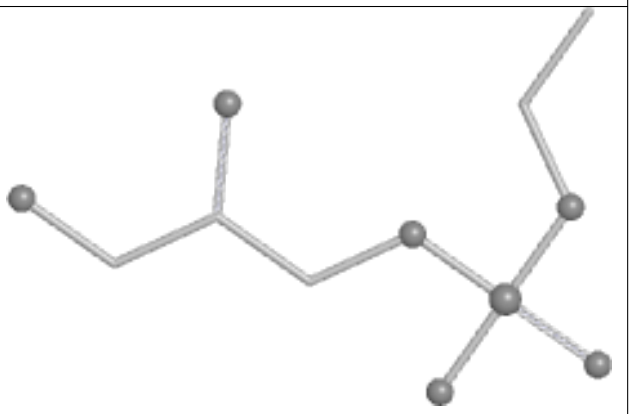
Bond lengths



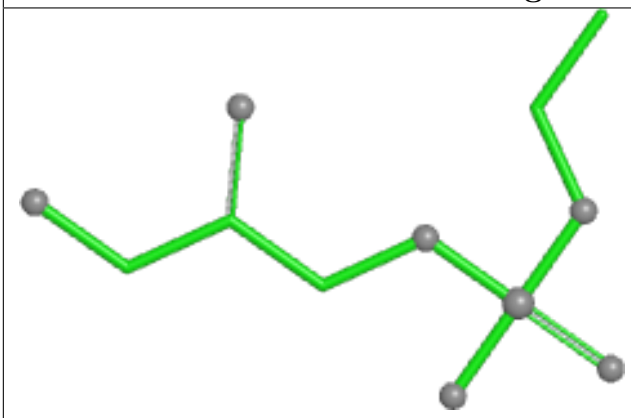
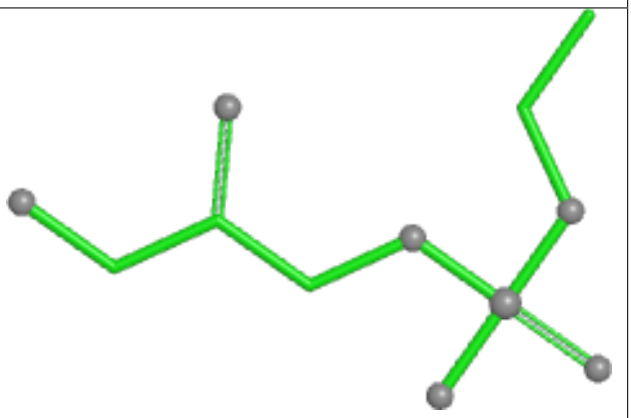
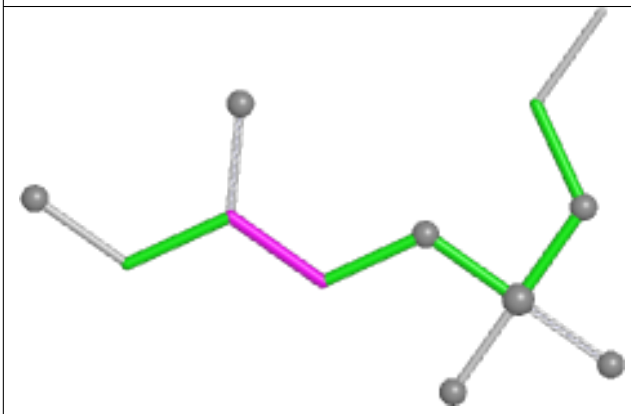
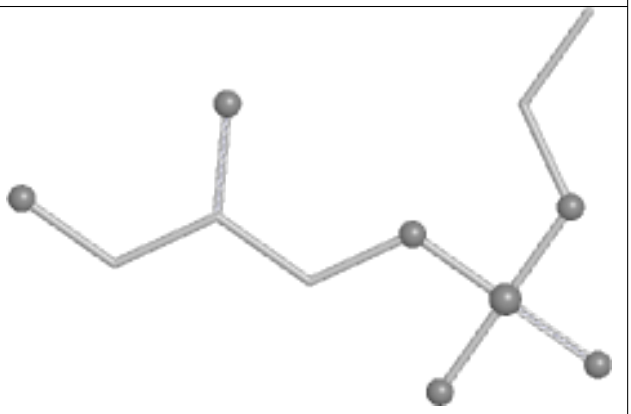
Bond angles

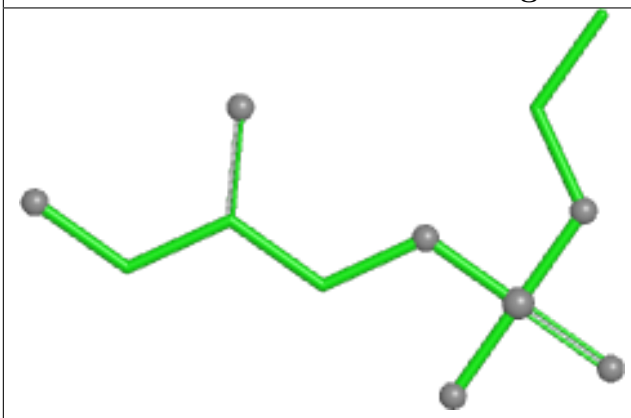
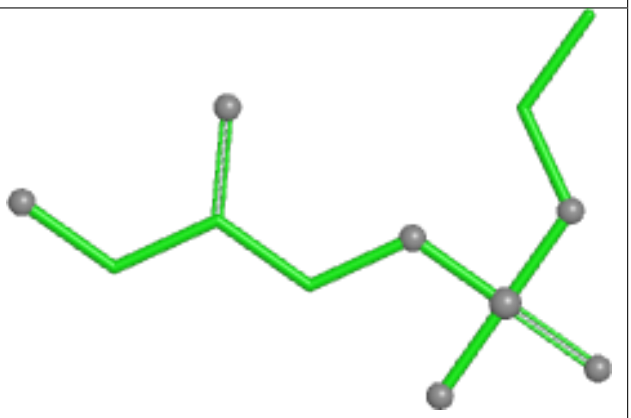
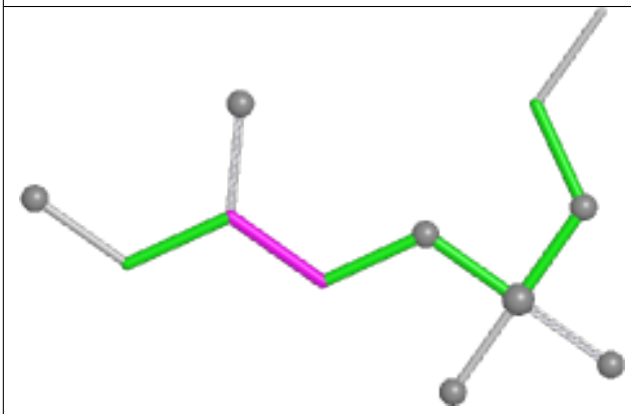
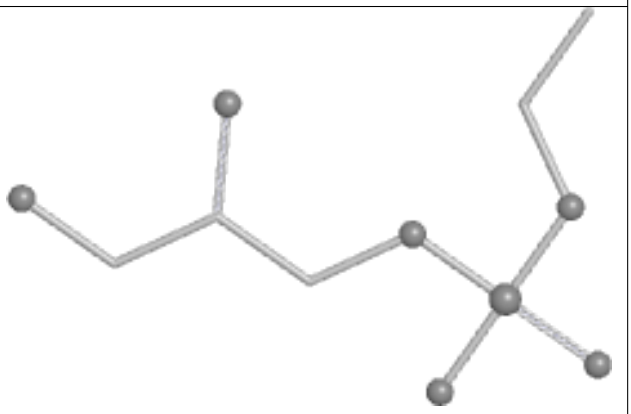


Torsions

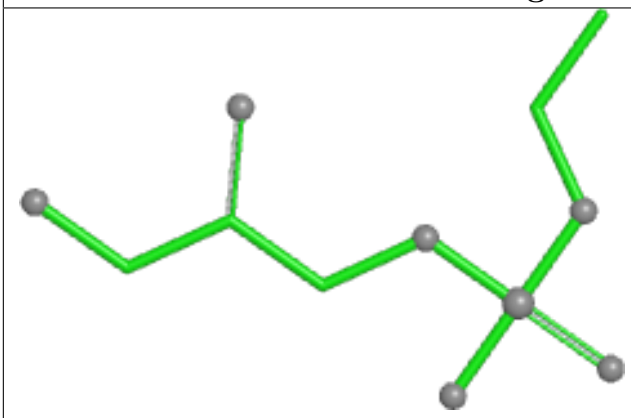


Rings

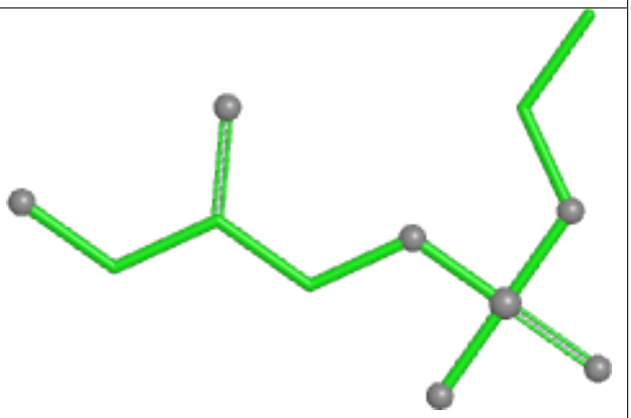
Ligand 6V6 5J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 6V6 1A 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

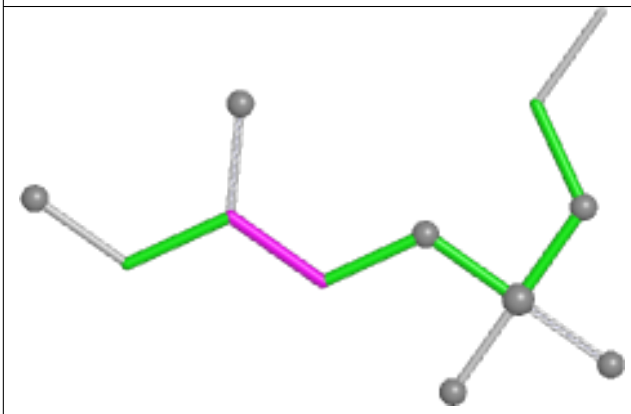
Ligand 6V6 5I 101



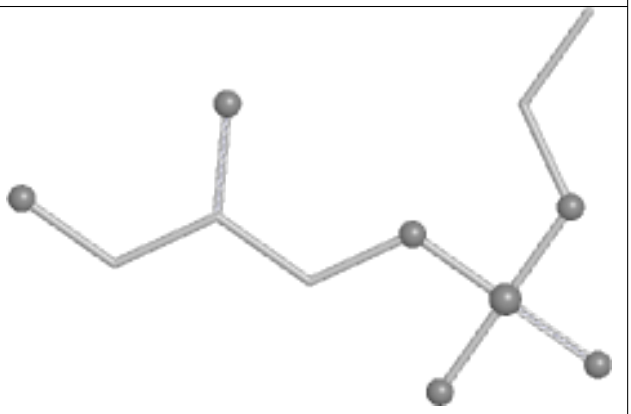
Bond lengths



Bond angles

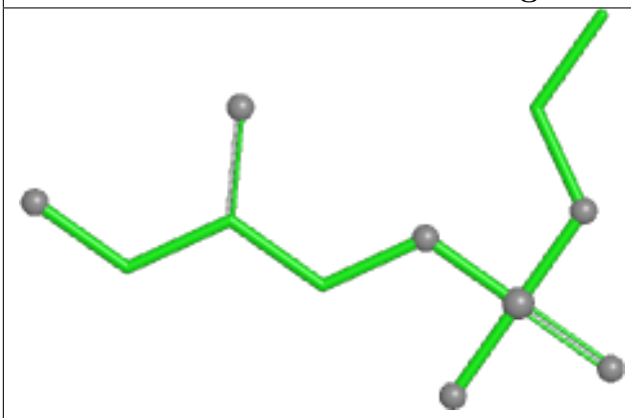


Torsions

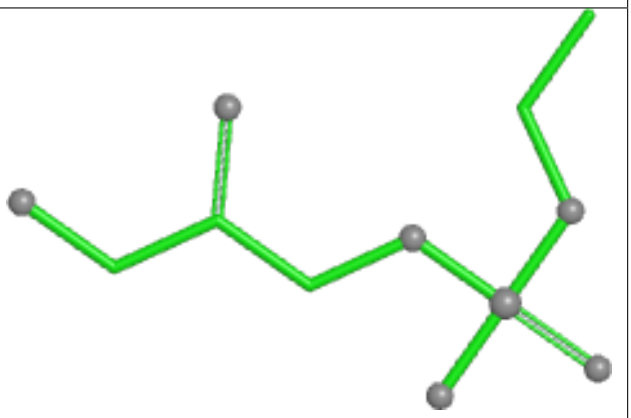


Rings

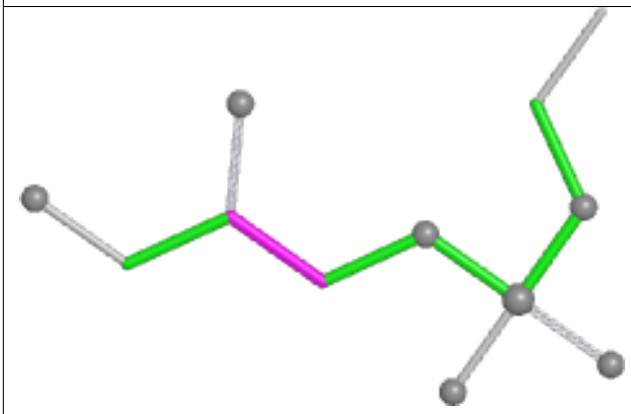
Ligand 6V6 1D 101



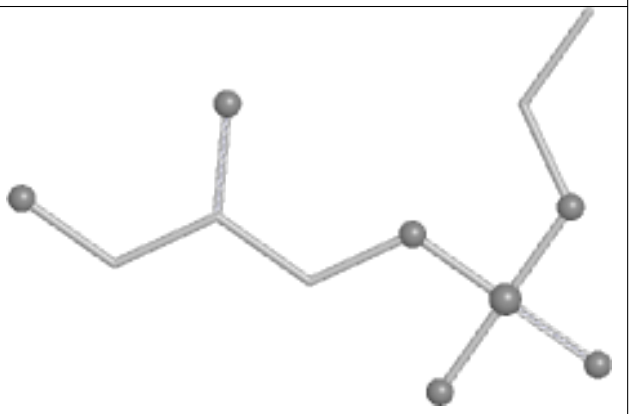
Bond lengths



Bond angles

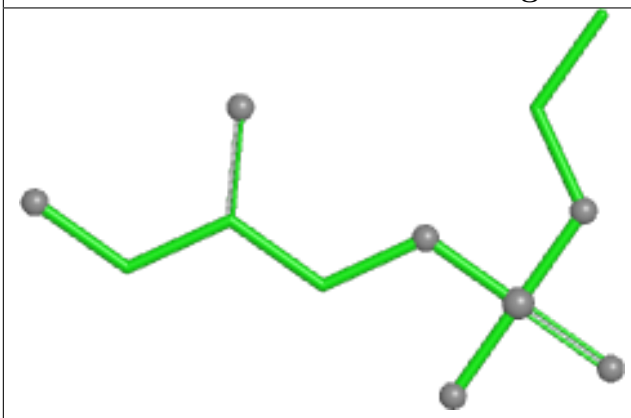


Torsions

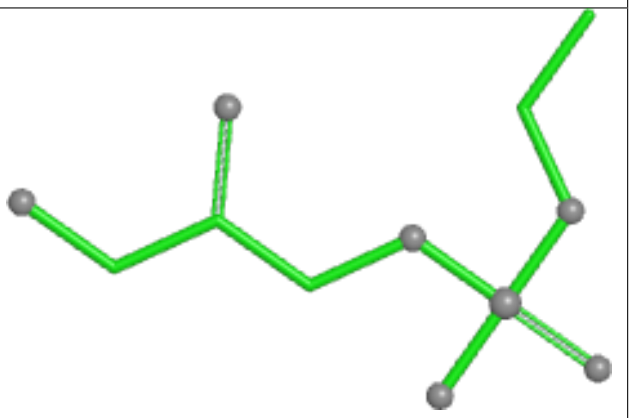


Rings

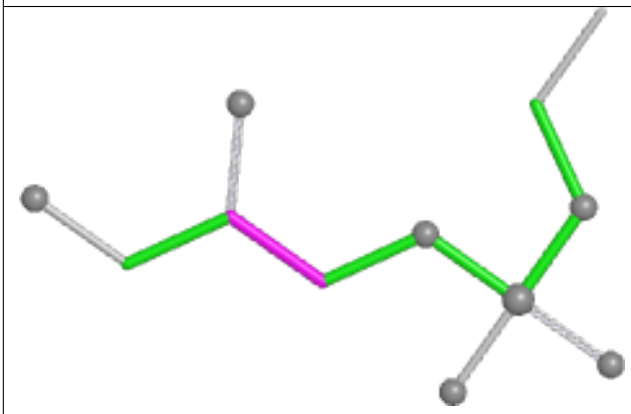
Ligand 6V6 3C 101



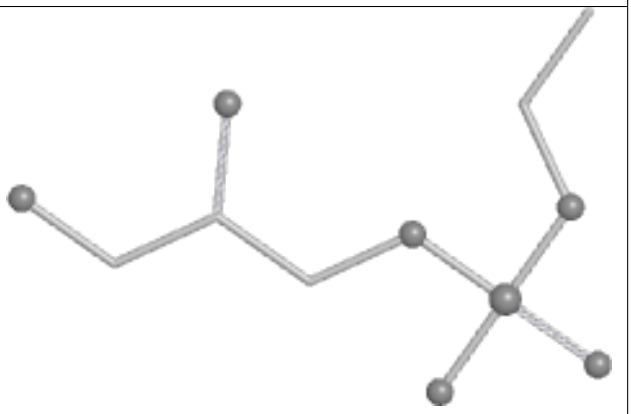
Bond lengths



Bond angles

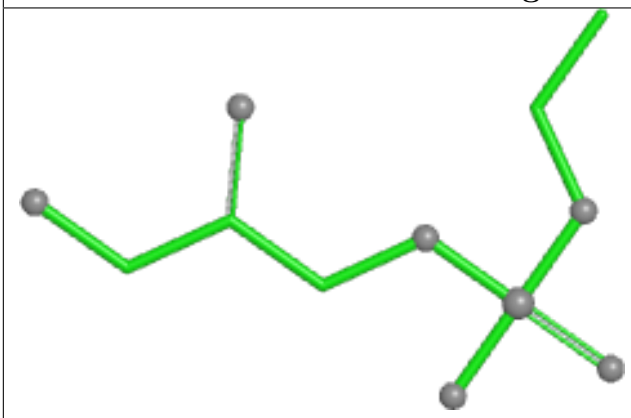


Torsions

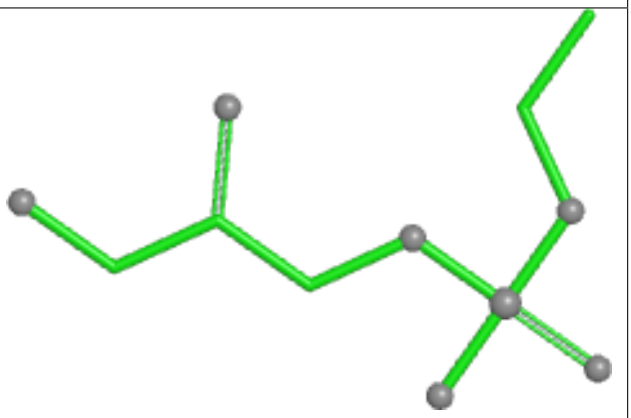


Rings

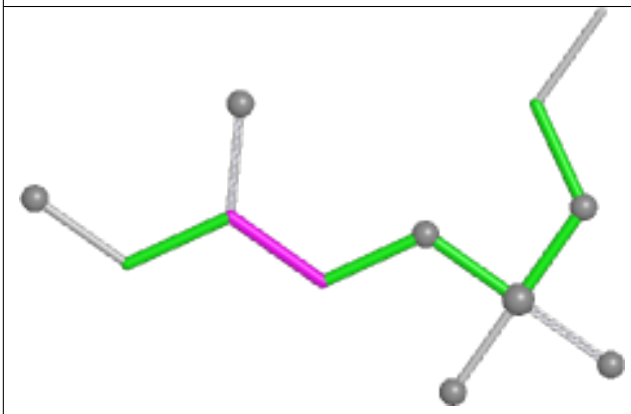
Ligand 6V6 4E 101



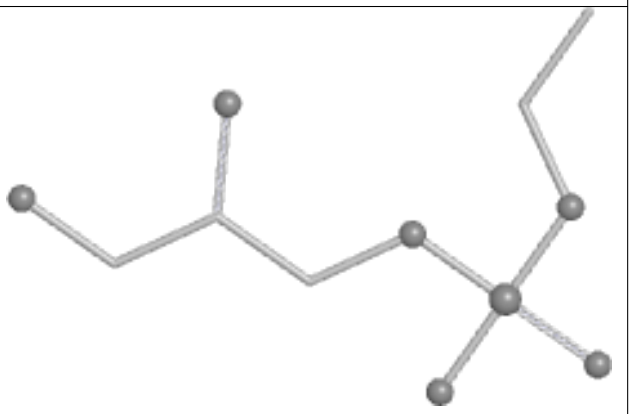
Bond lengths



Bond angles

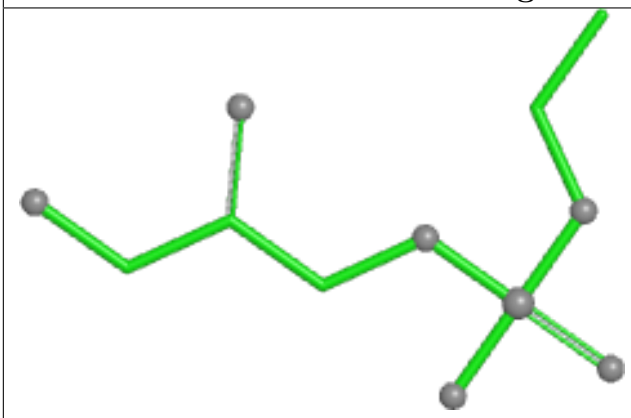


Torsions

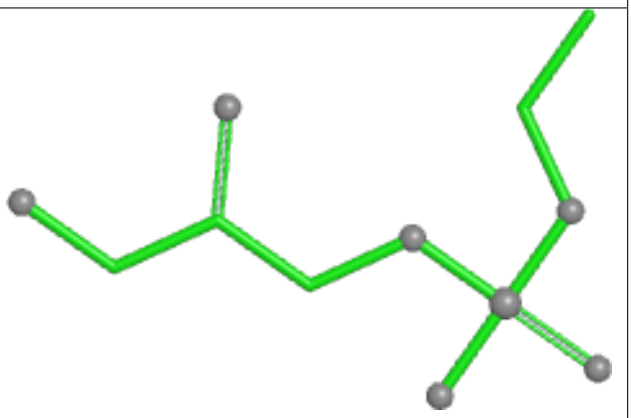


Rings

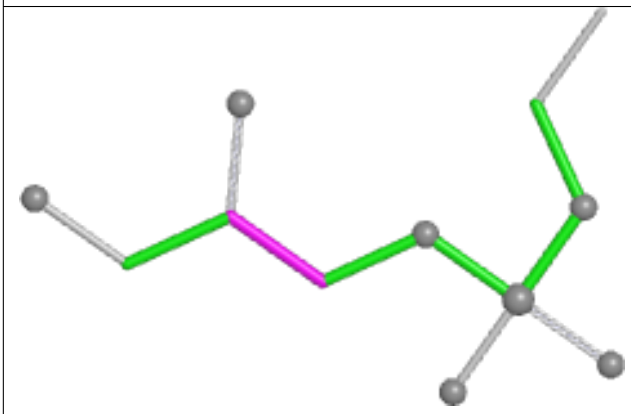
Ligand 6V6 2M 101



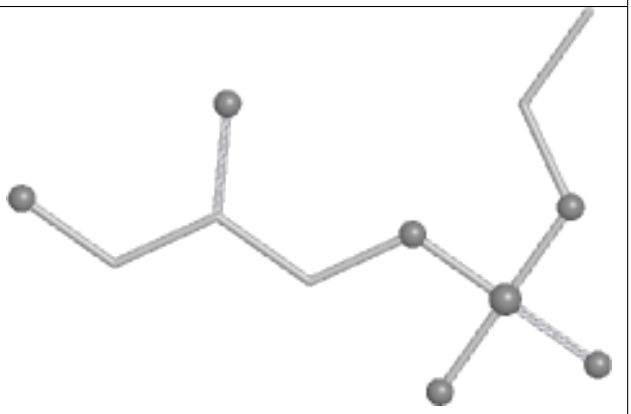
Bond lengths



Bond angles

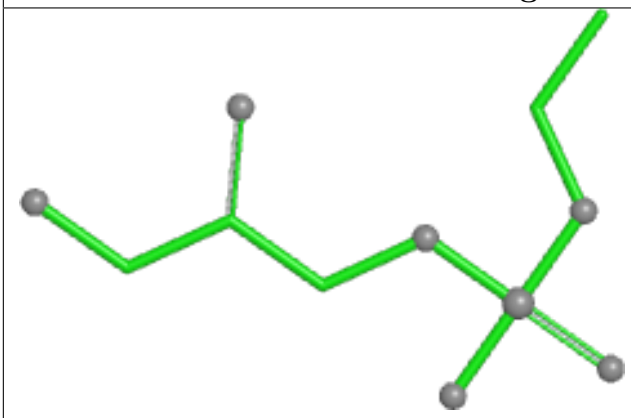


Torsions

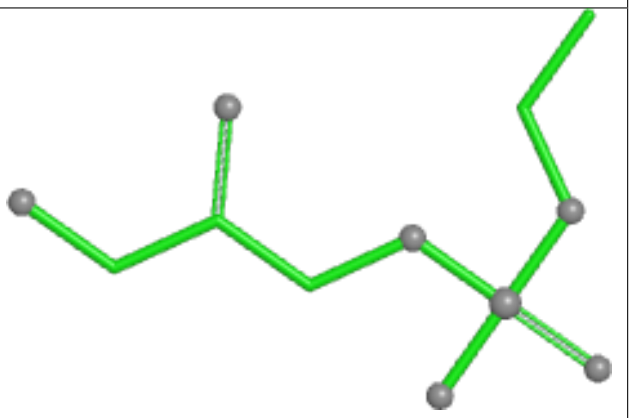


Rings

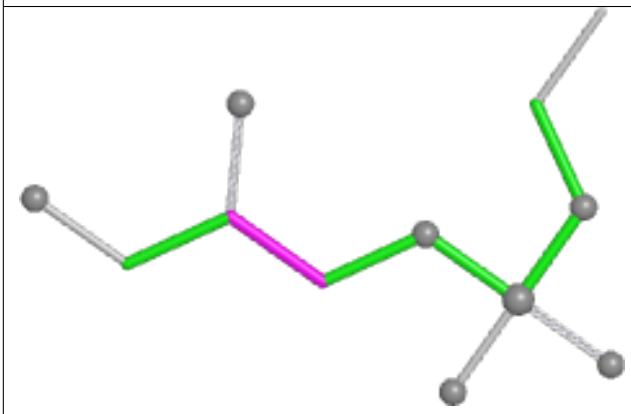
Ligand 6V6 1H 101



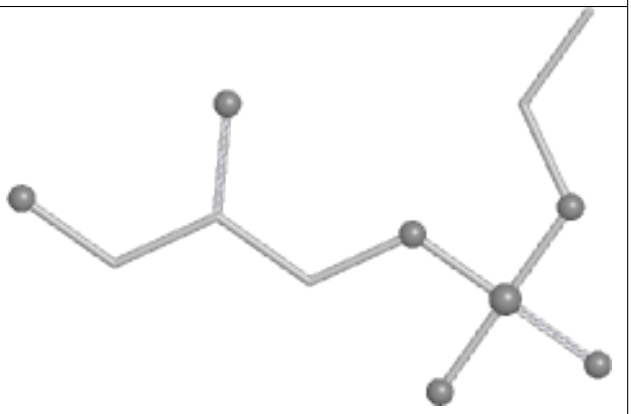
Bond lengths



Bond angles

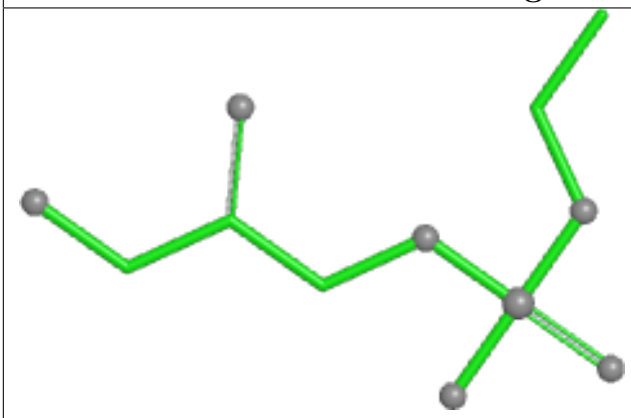


Torsions

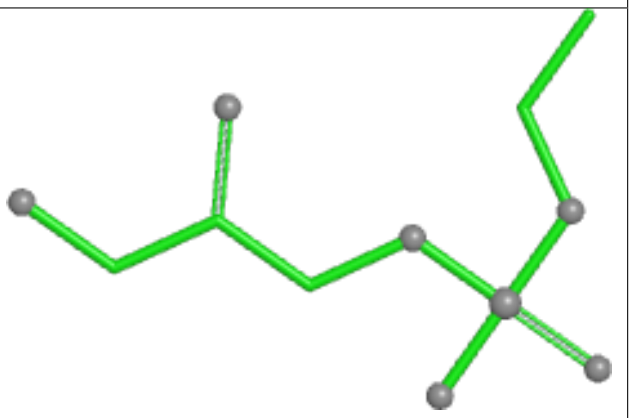


Rings

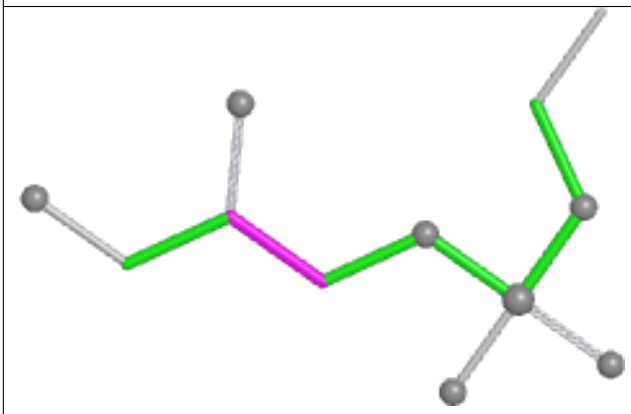
Ligand 6V6 1J 101



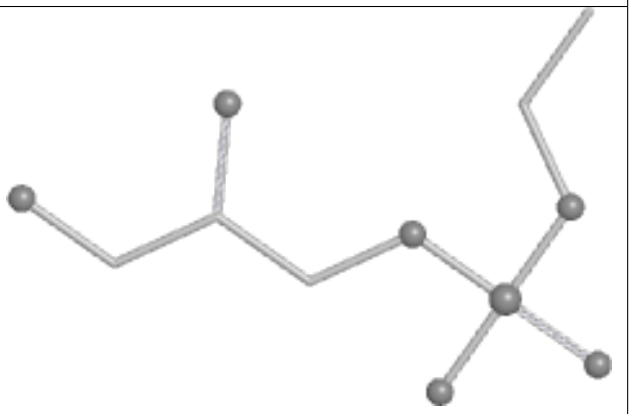
Bond lengths



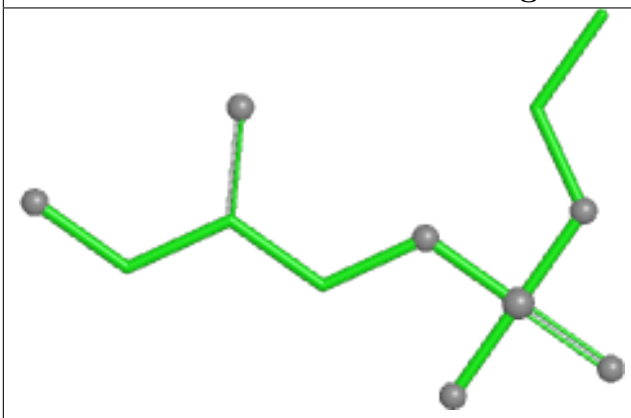
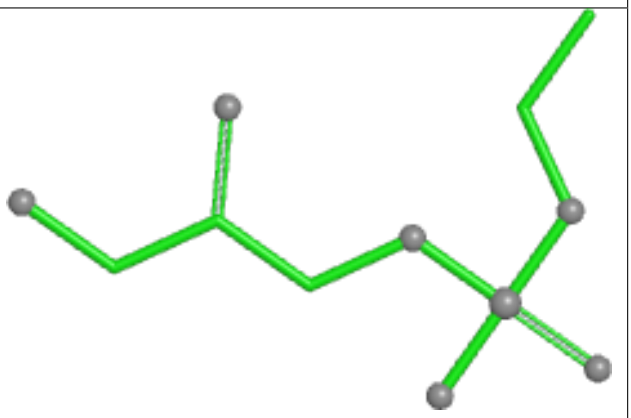
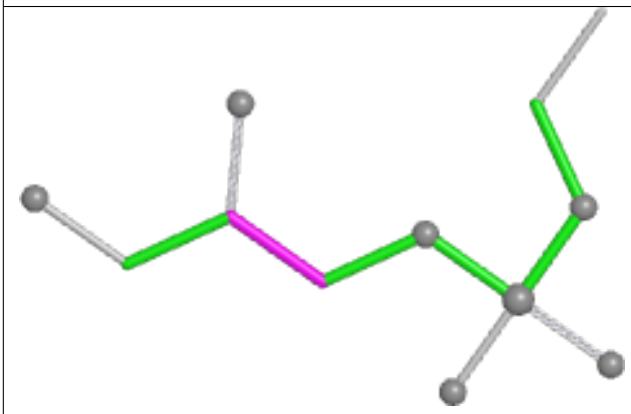
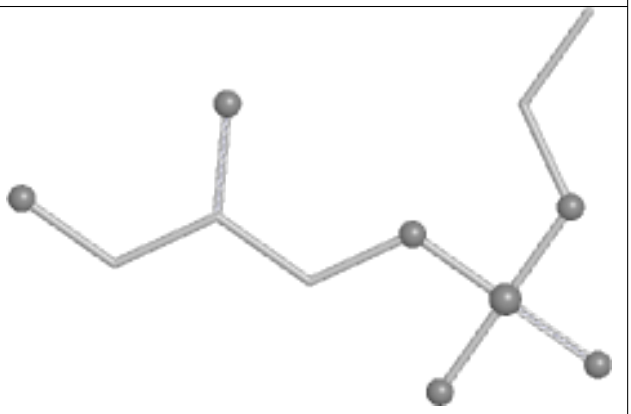
Bond angles



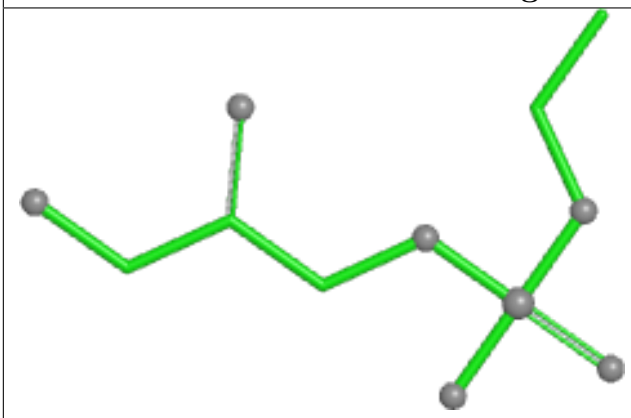
Torsions



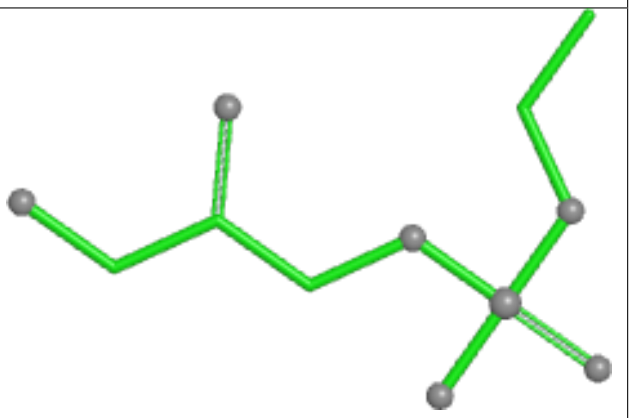
Rings

Ligand 6V6 4H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

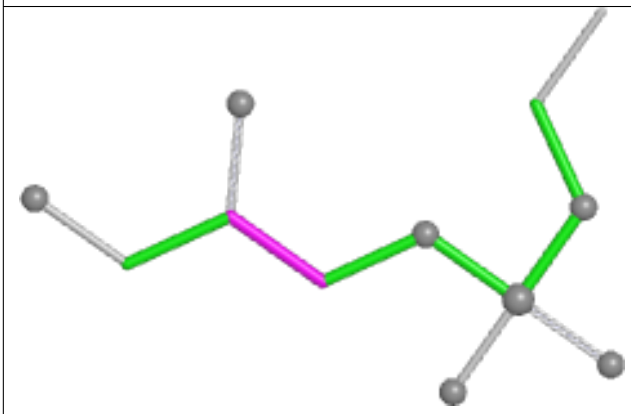
Ligand 6V6 5C 101



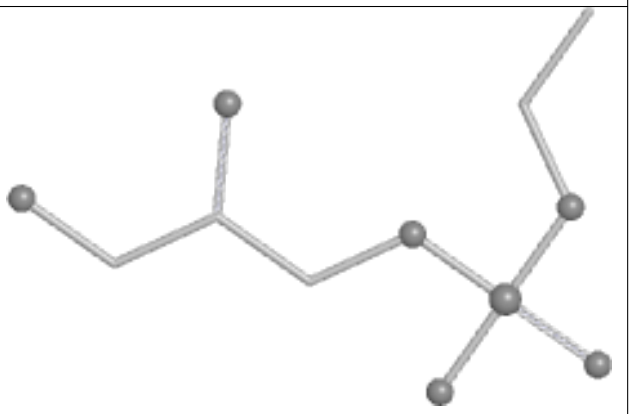
Bond lengths



Bond angles

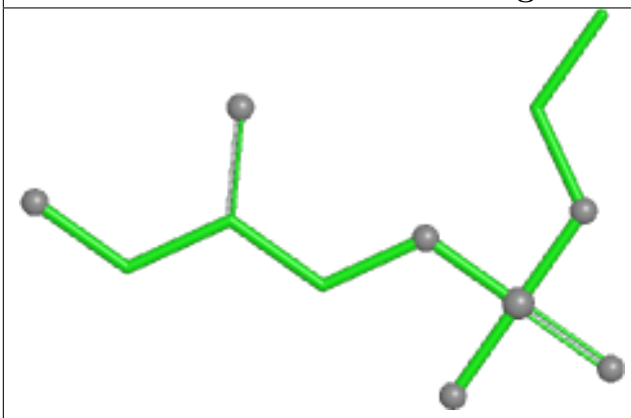


Torsions

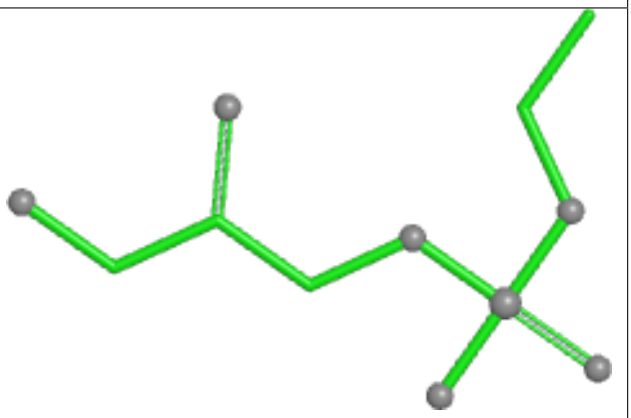


Rings

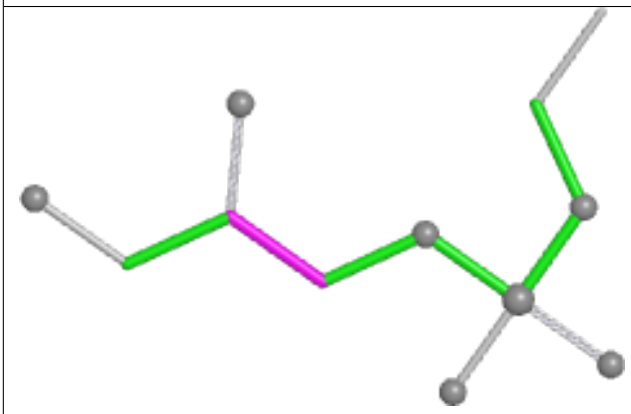
Ligand 6V6 3M 101



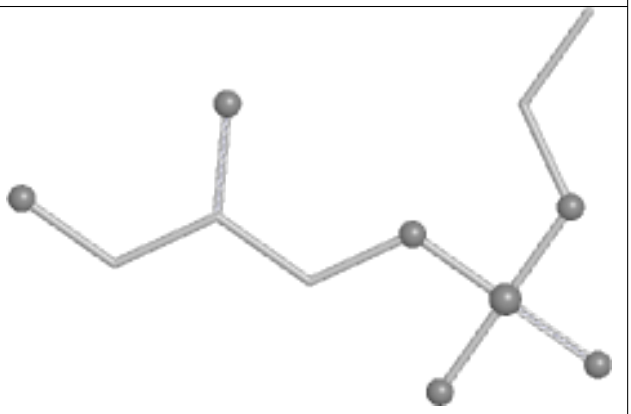
Bond lengths



Bond angles

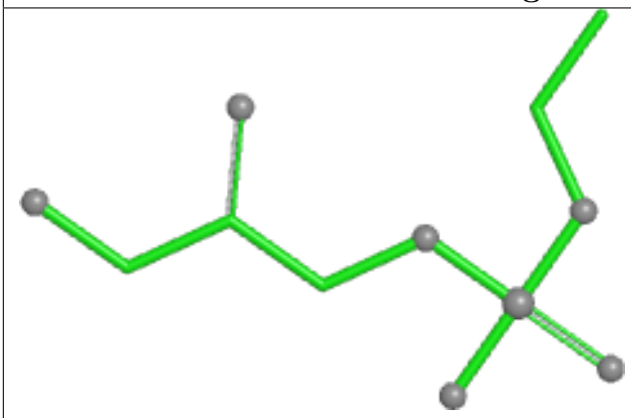


Torsions

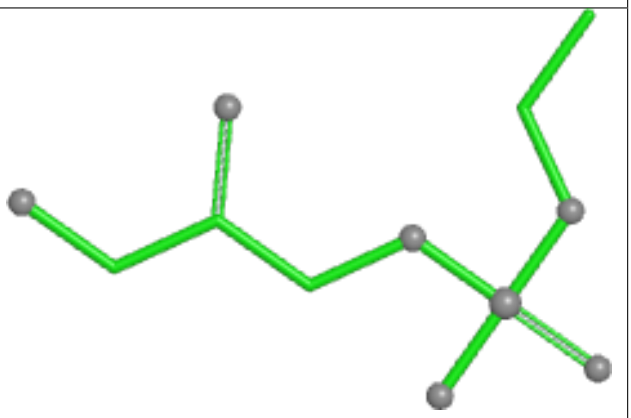


Rings

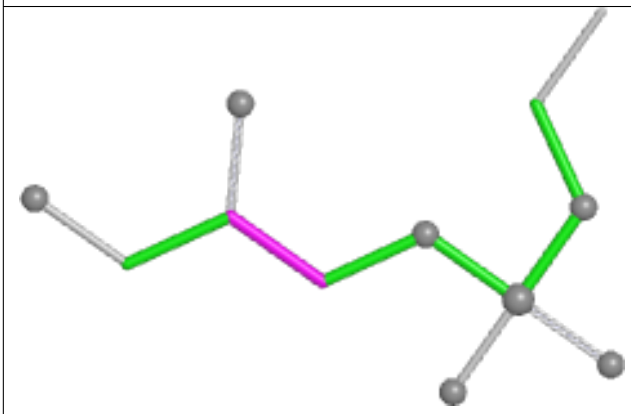
Ligand 6V6 5F 101



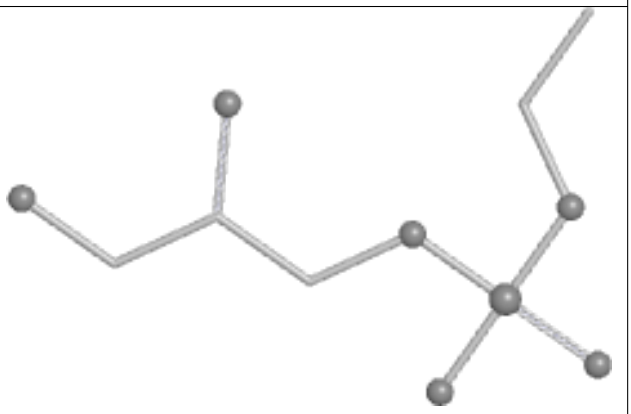
Bond lengths



Bond angles

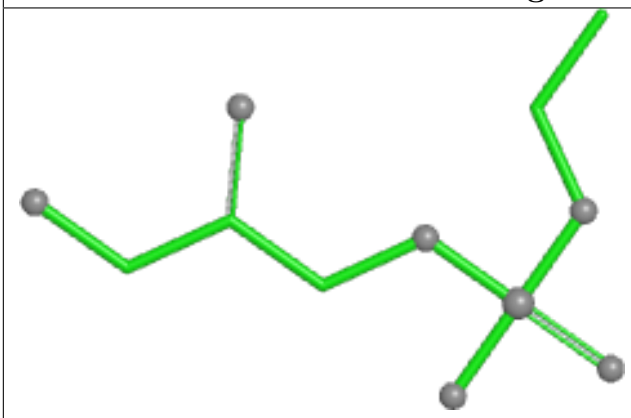


Torsions

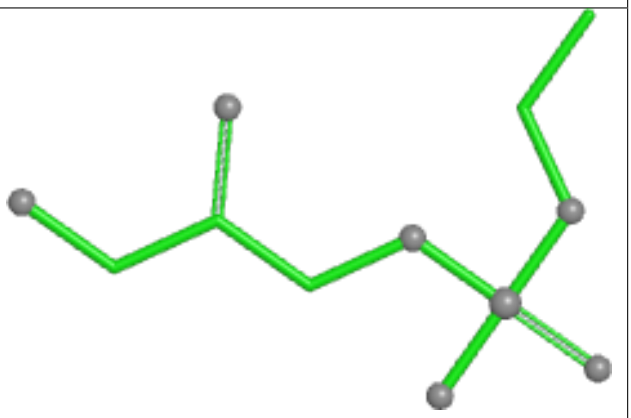


Rings

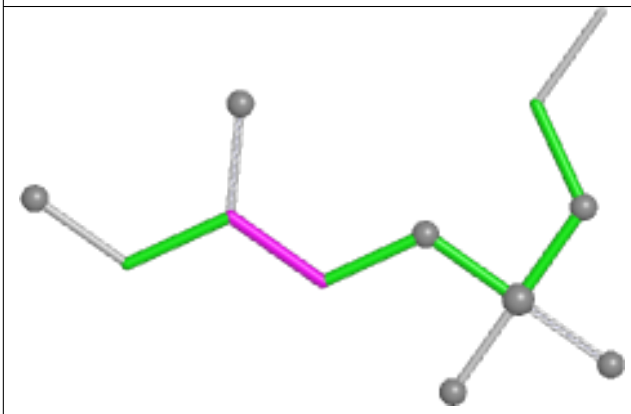
Ligand 6V6 2I 101



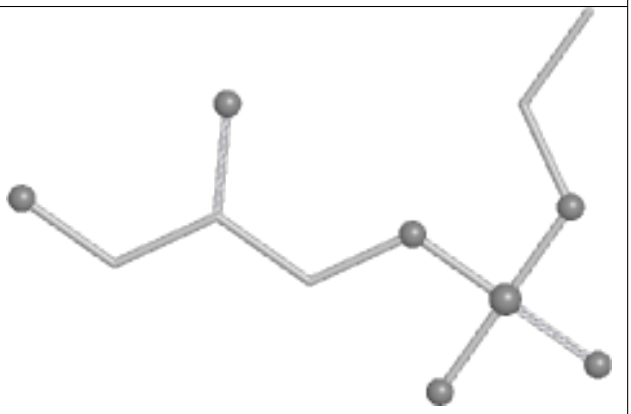
Bond lengths



Bond angles

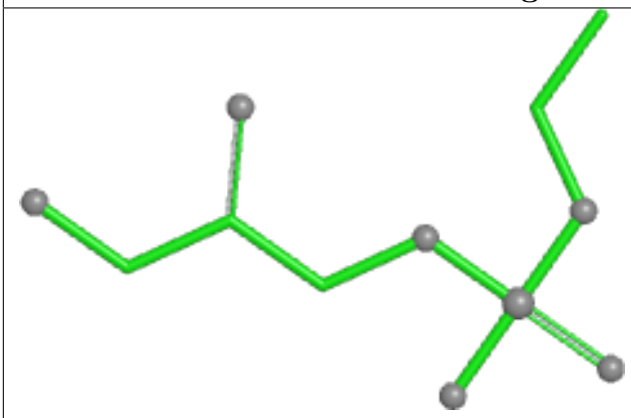


Torsions

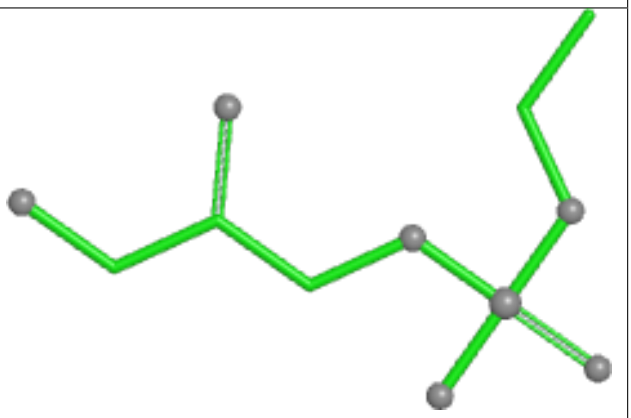


Rings

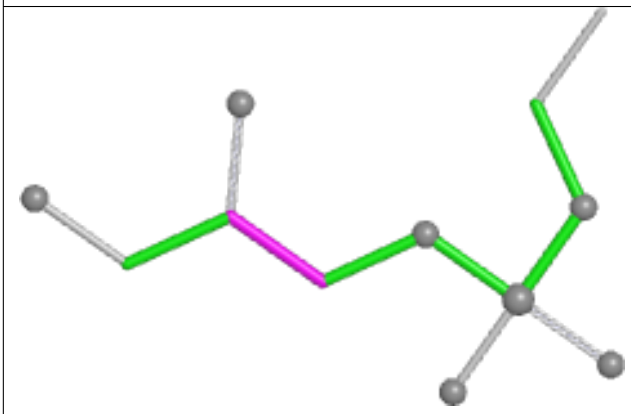
Ligand 6V6 1C 101



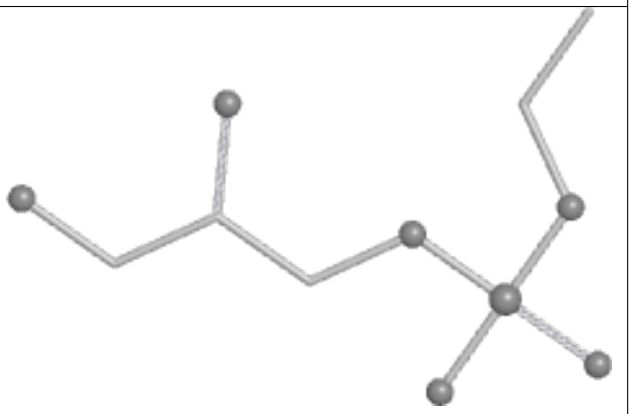
Bond lengths



Bond angles

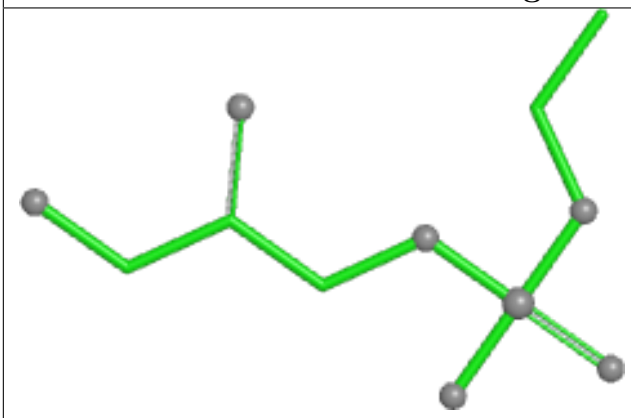


Torsions

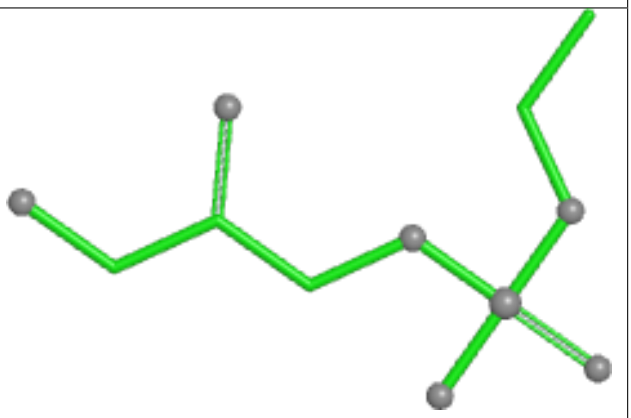


Rings

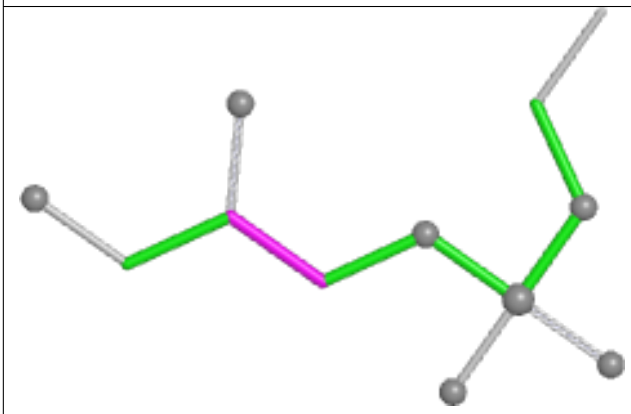
Ligand 6V6 1L 101



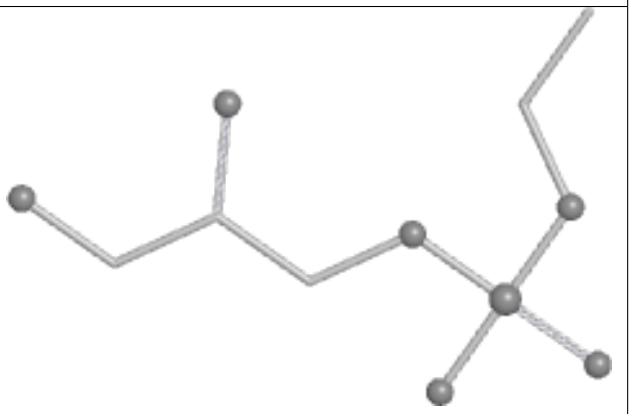
Bond lengths



Bond angles

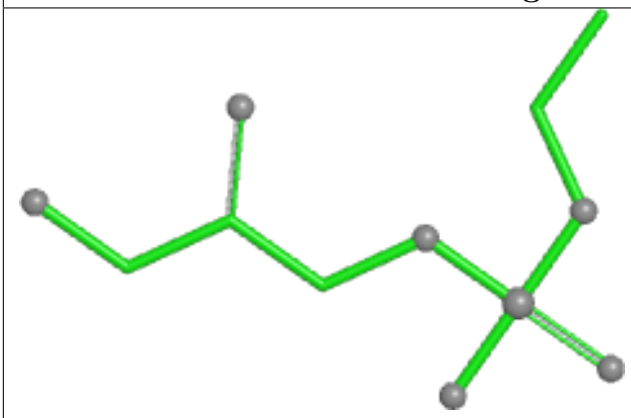


Torsions

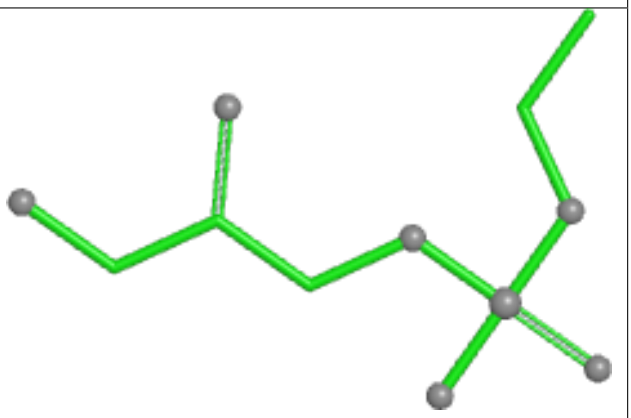


Rings

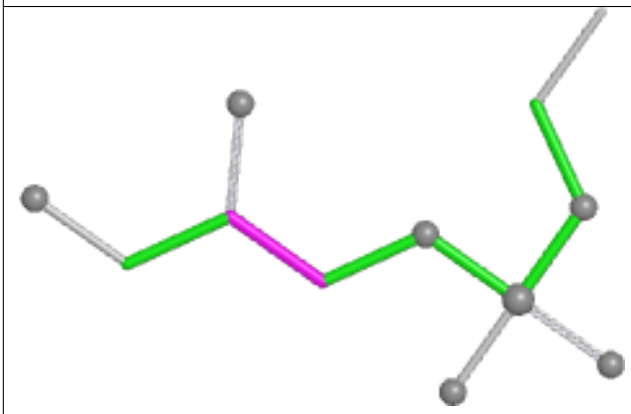
Ligand 6V6 3F 101



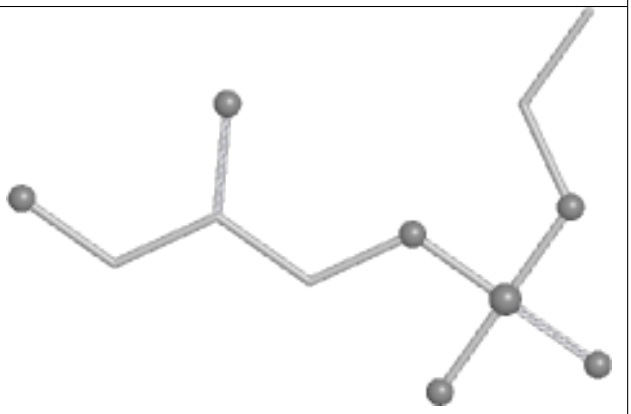
Bond lengths



Bond angles

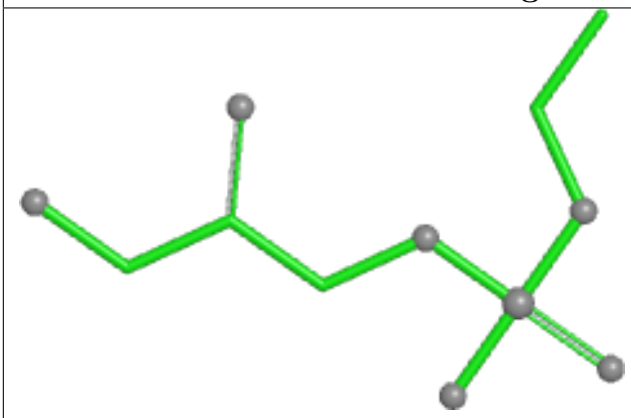


Torsions

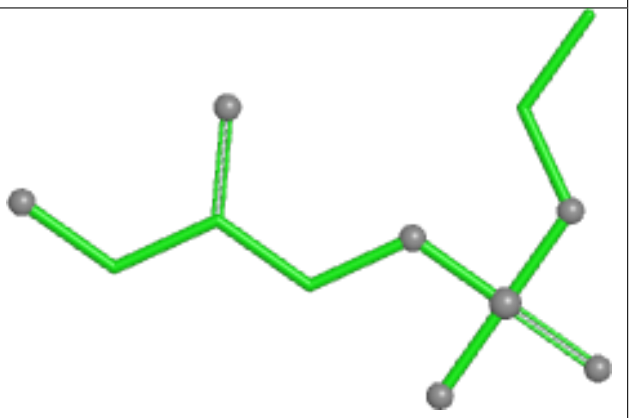


Rings

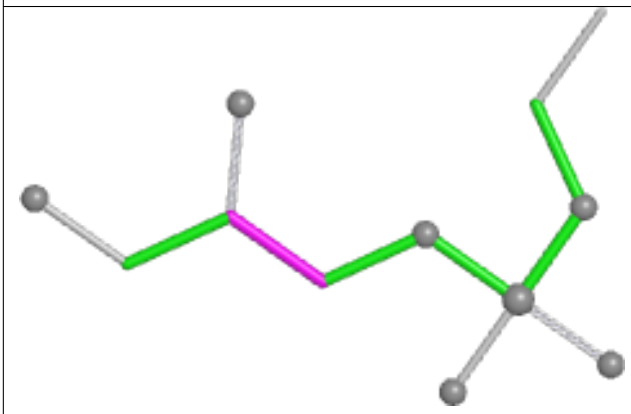
Ligand 6V6 2B 101



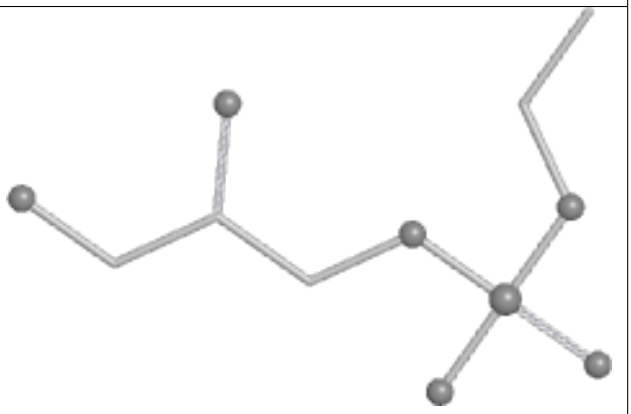
Bond lengths



Bond angles

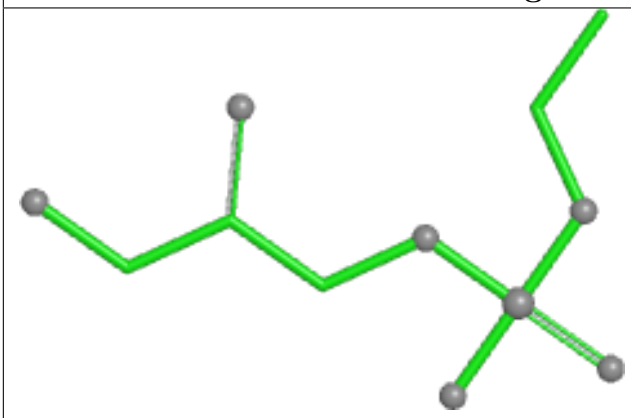


Torsions

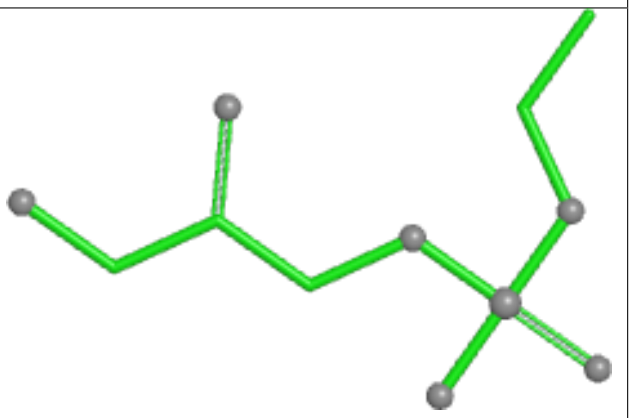


Rings

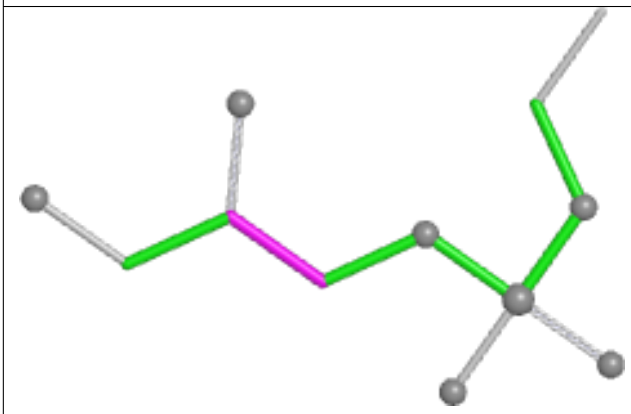
Ligand 6V6 3J 101



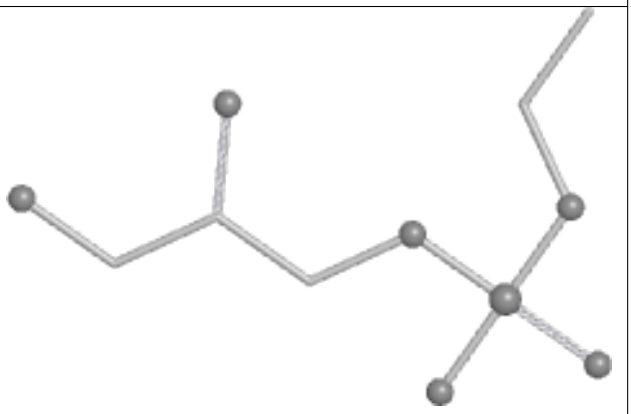
Bond lengths



Bond angles

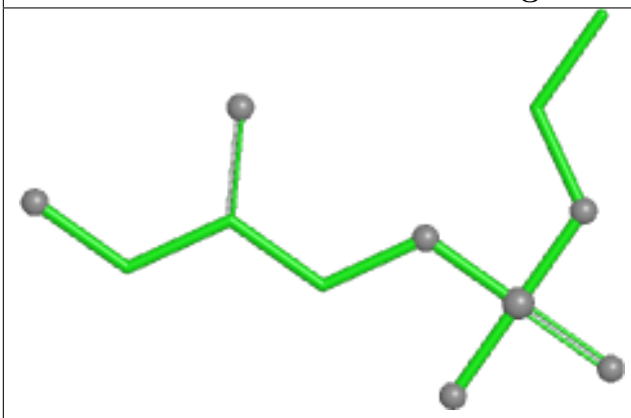


Torsions

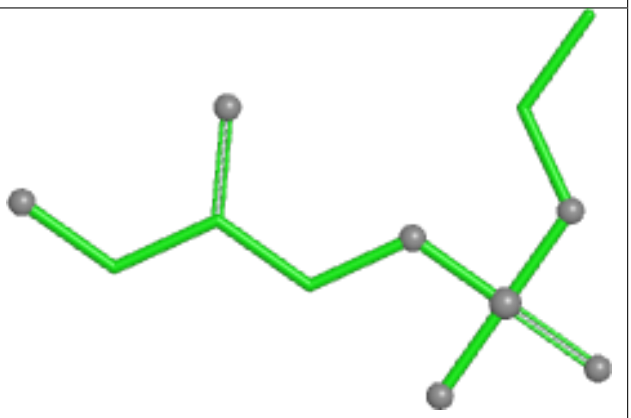


Rings

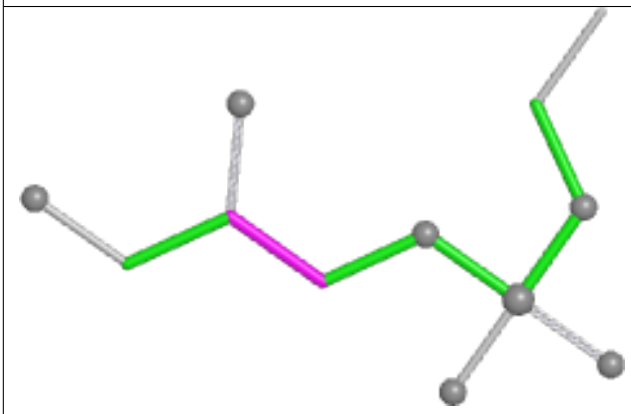
Ligand 6V6 3B 101



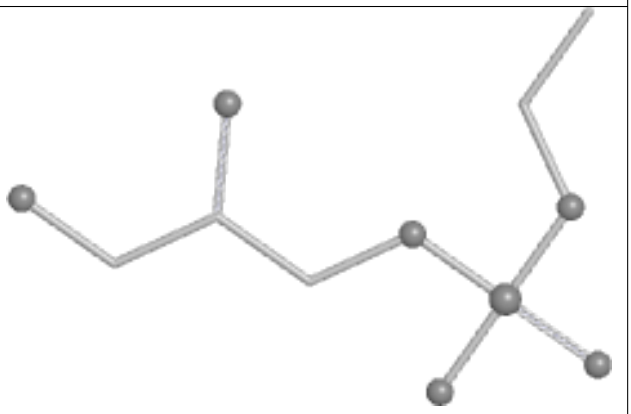
Bond lengths



Bond angles

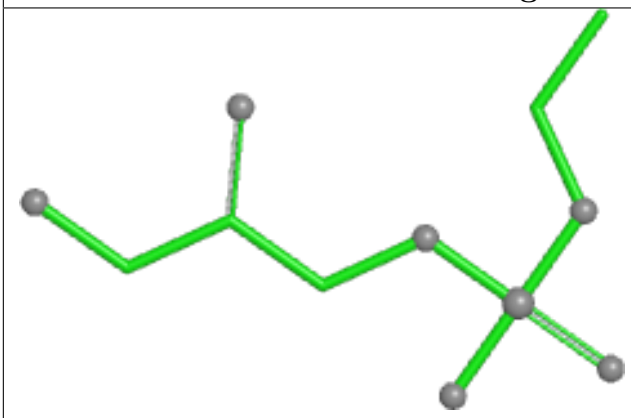


Torsions

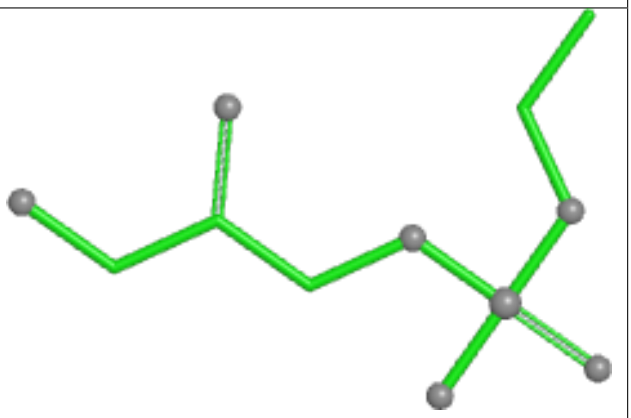


Rings

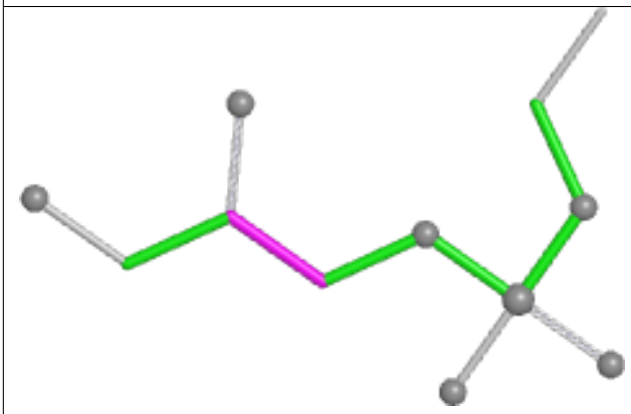
Ligand 6V6 3K 101



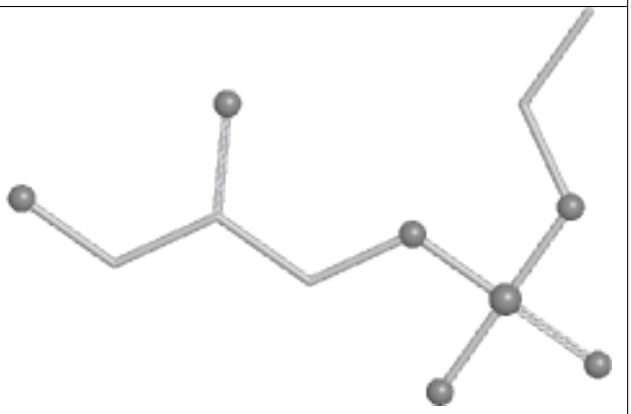
Bond lengths



Bond angles

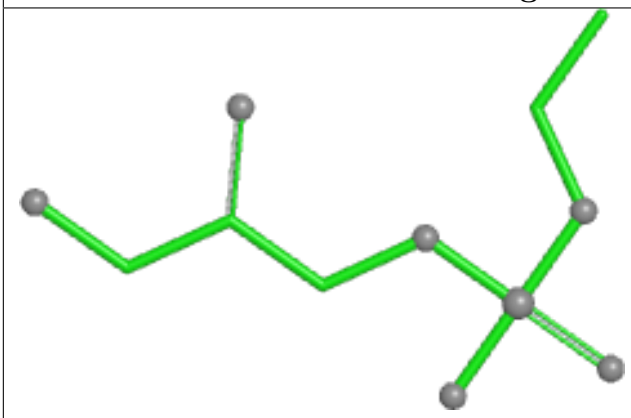


Torsions

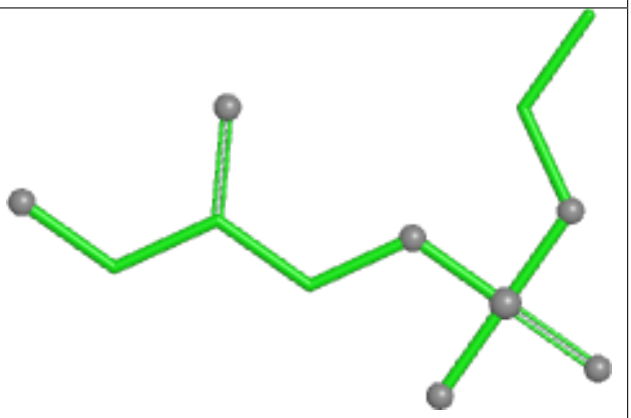


Rings

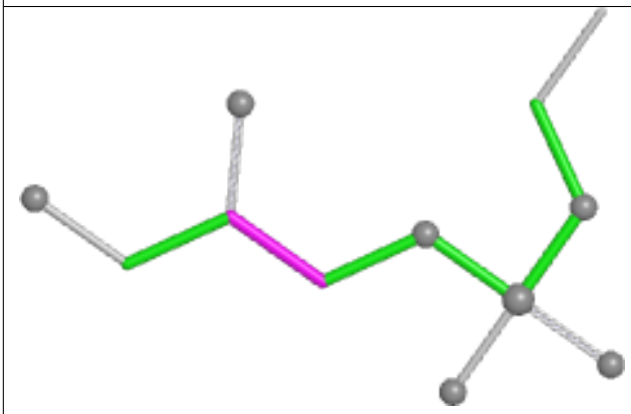
Ligand 6V6 2H 101



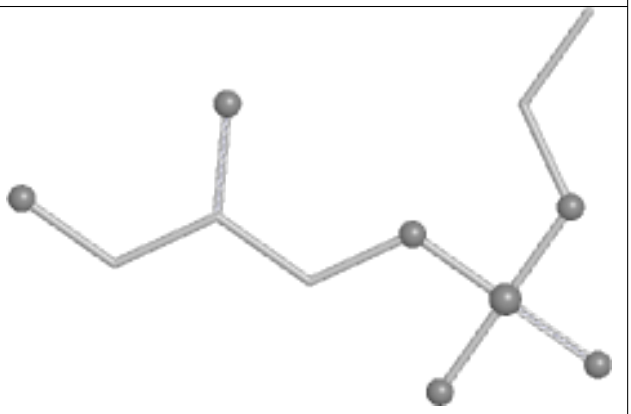
Bond lengths



Bond angles

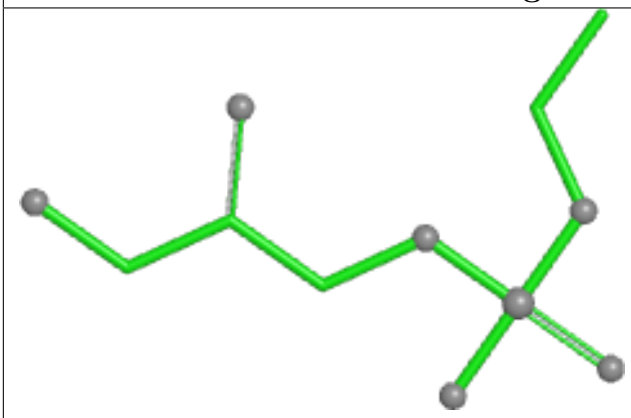


Torsions

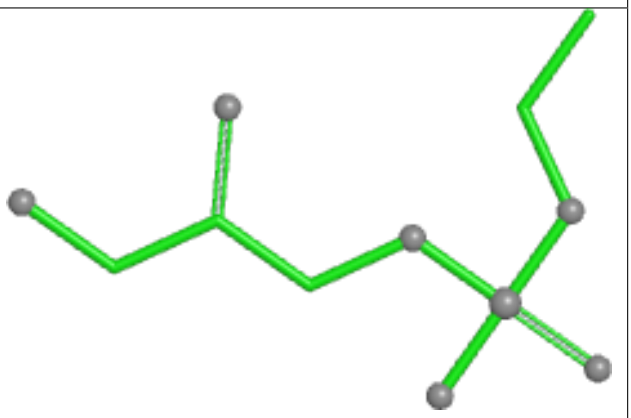


Rings

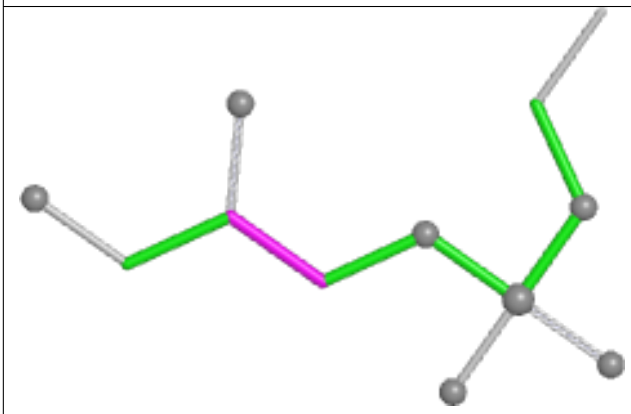
Ligand 6V6 4L 101



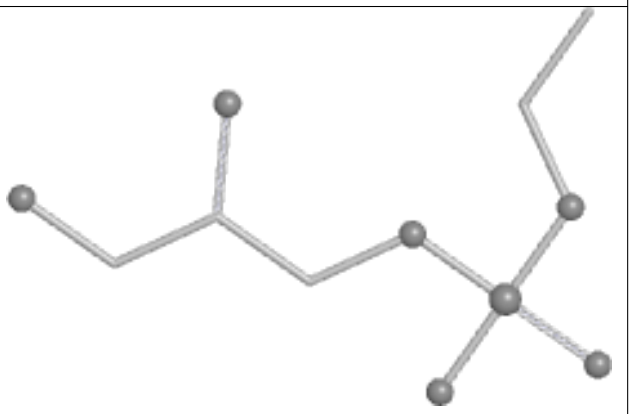
Bond lengths



Bond angles

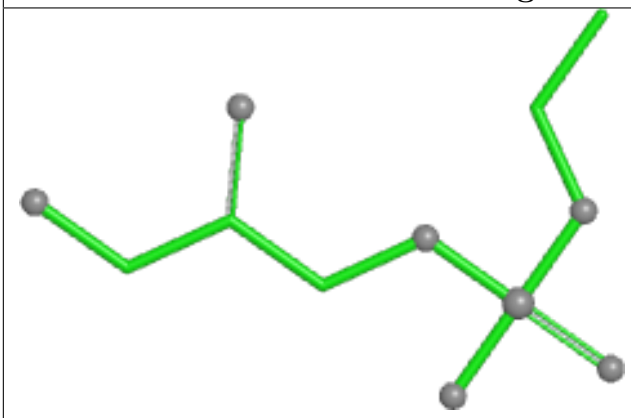


Torsions

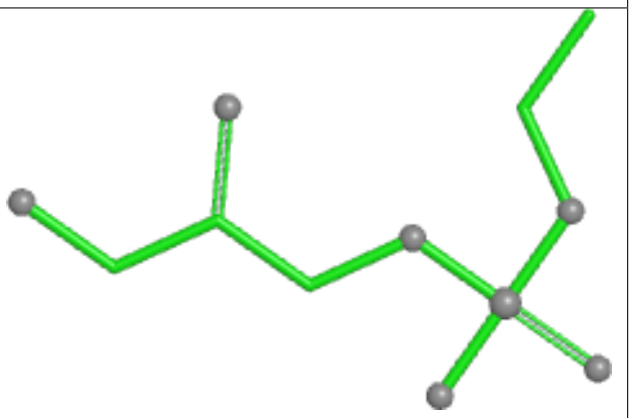


Rings

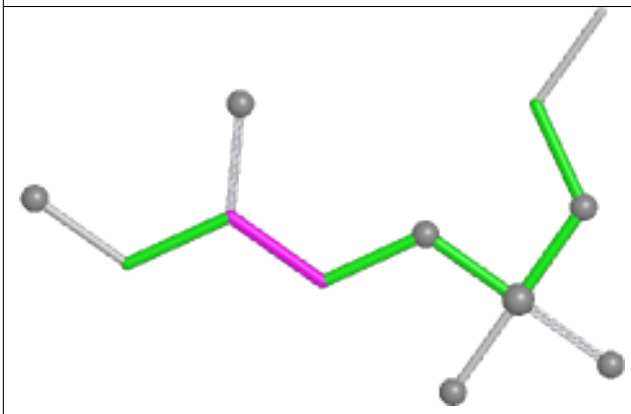
Ligand 6V6 1M 101



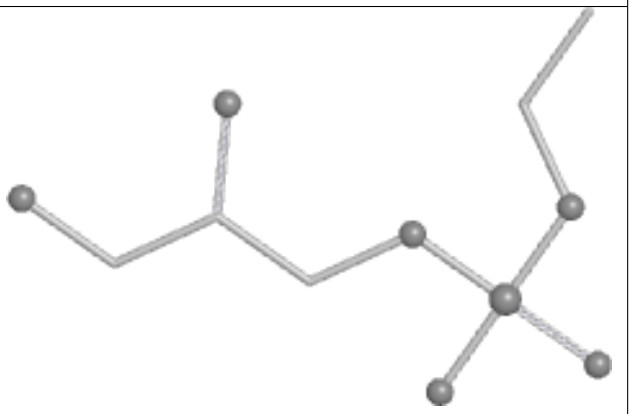
Bond lengths



Bond angles

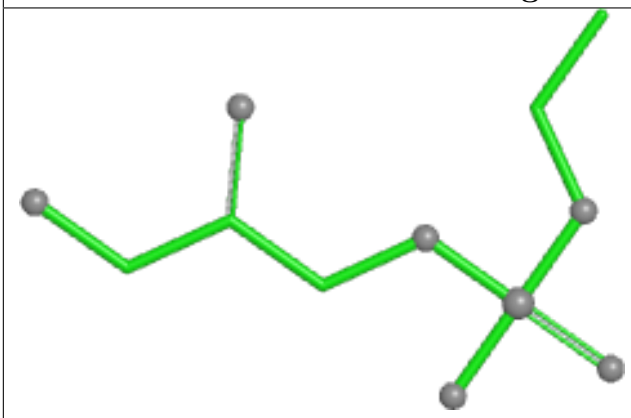


Torsions

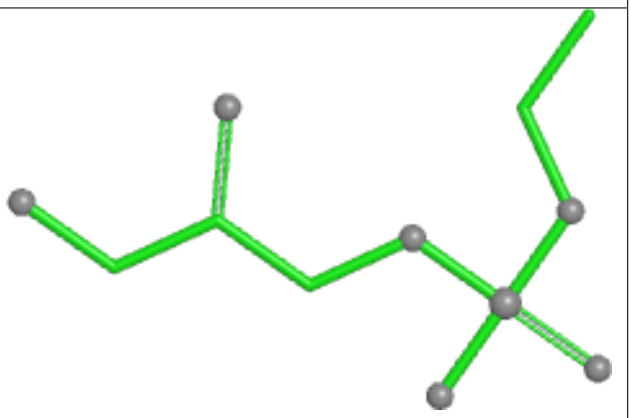


Rings

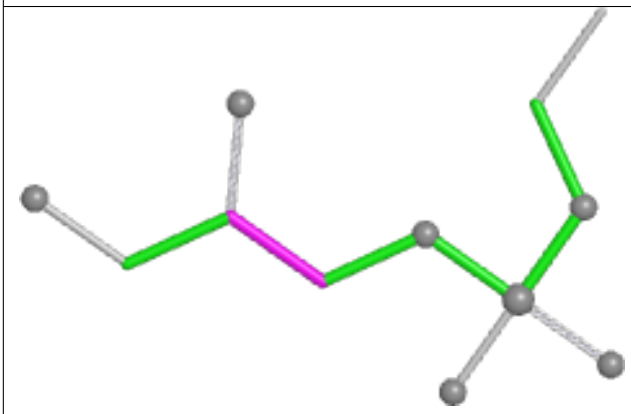
Ligand 6V6 1B 101



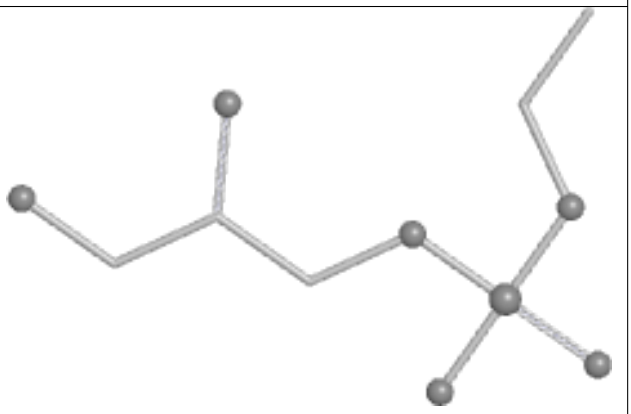
Bond lengths



Bond angles

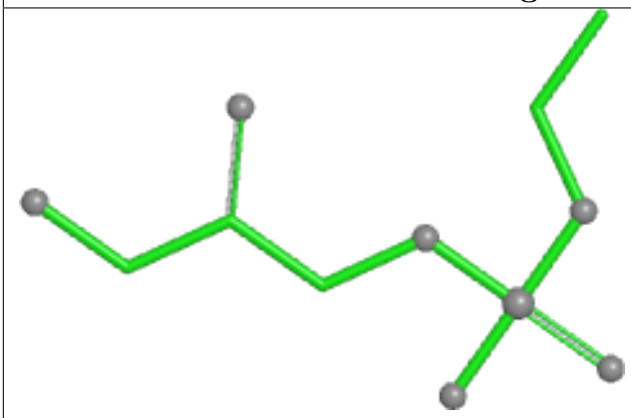


Torsions

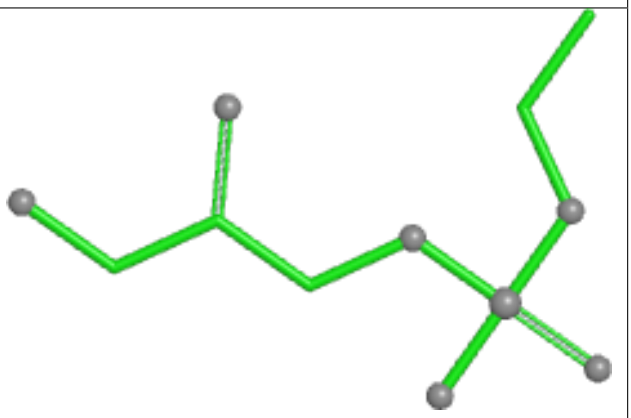


Rings

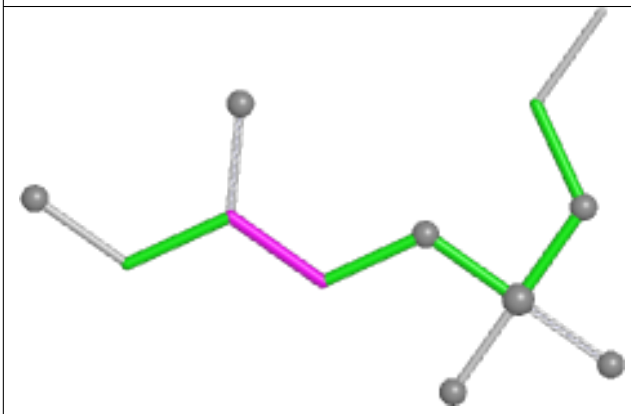
Ligand 6V6 3D 101



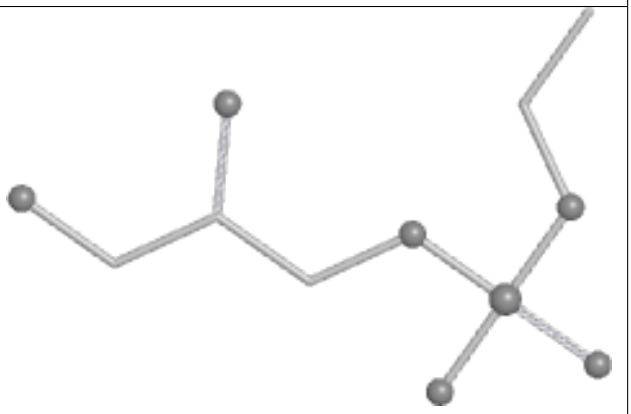
Bond lengths



Bond angles

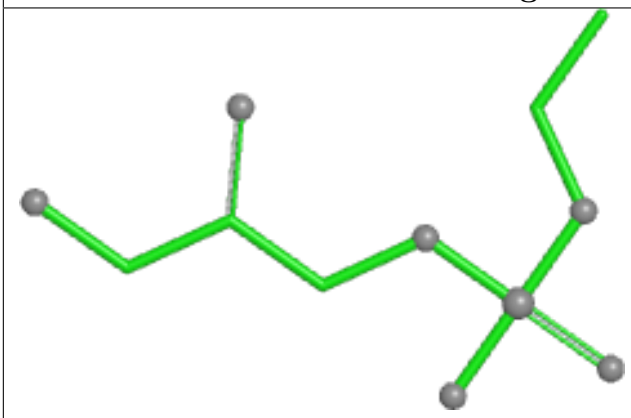


Torsions

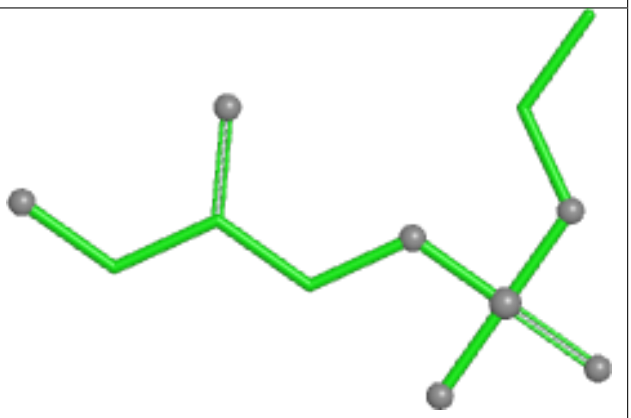


Rings

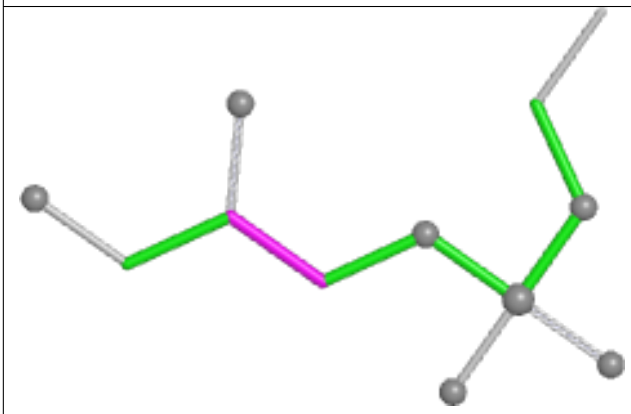
Ligand 6V6 3N 101



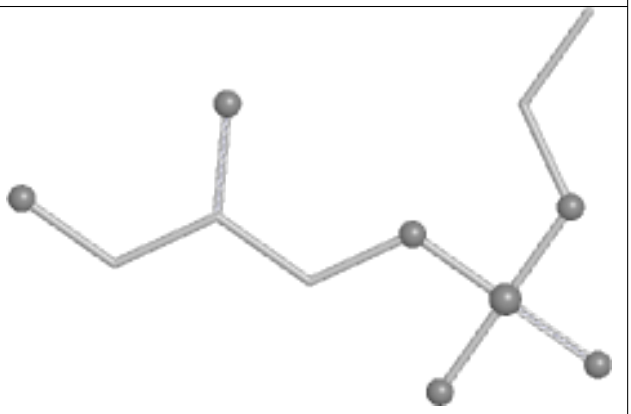
Bond lengths



Bond angles

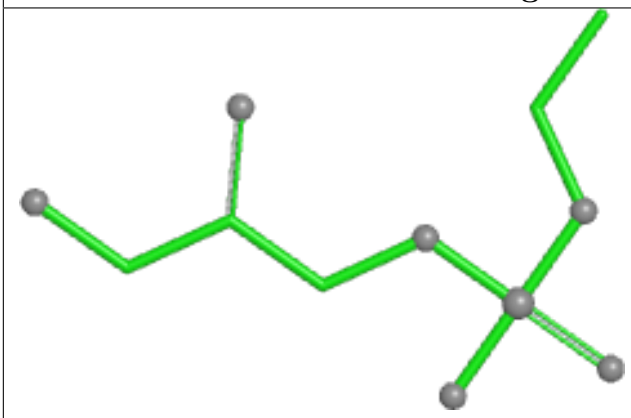


Torsions

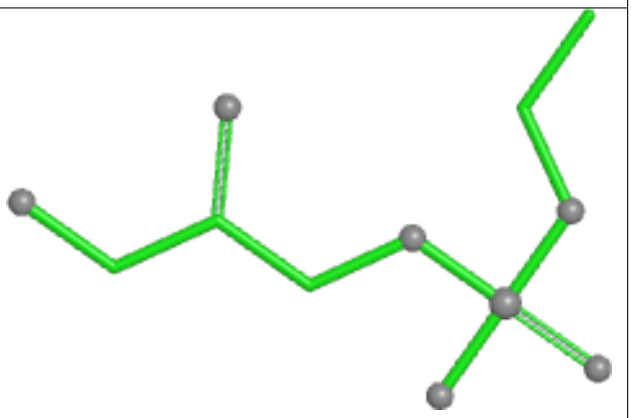


Rings

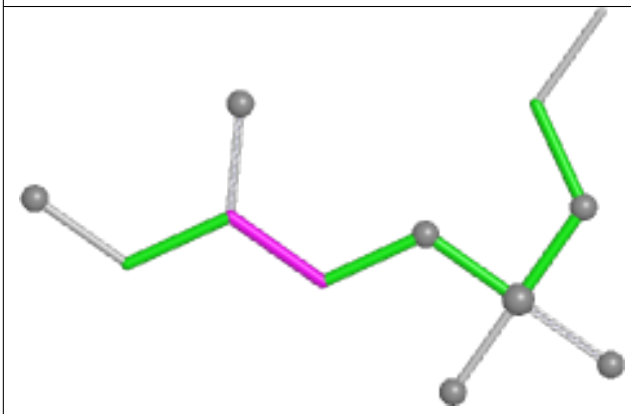
Ligand 6V6 4B 101



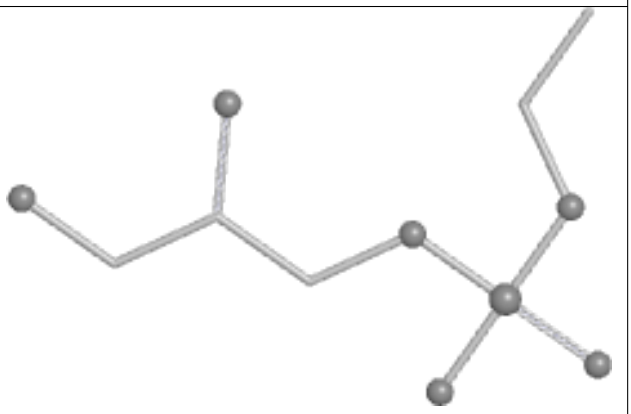
Bond lengths



Bond angles

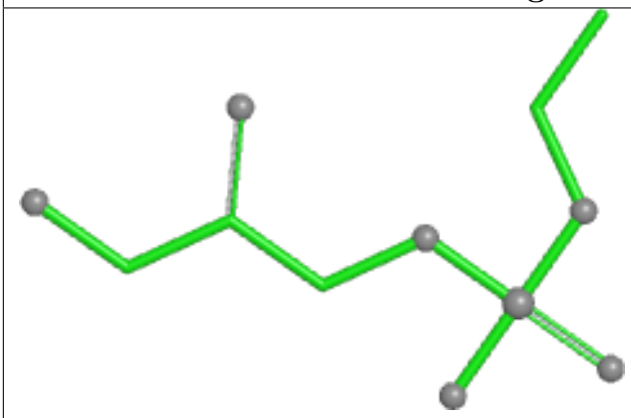


Torsions

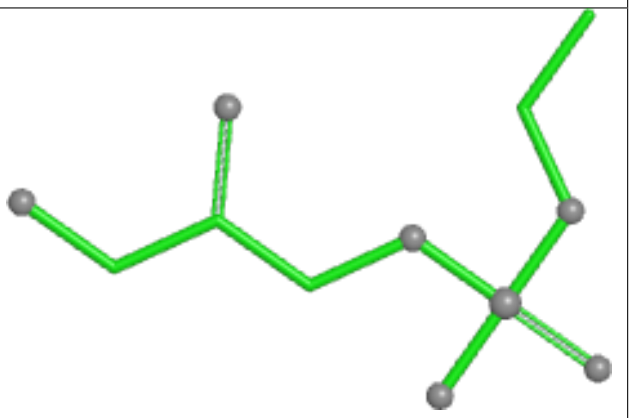


Rings

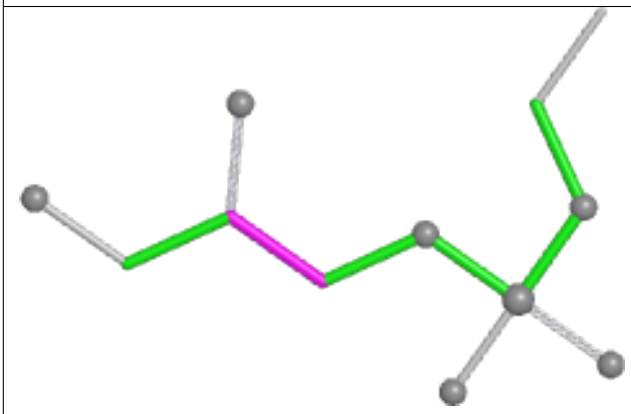
Ligand 6V6 4I 101



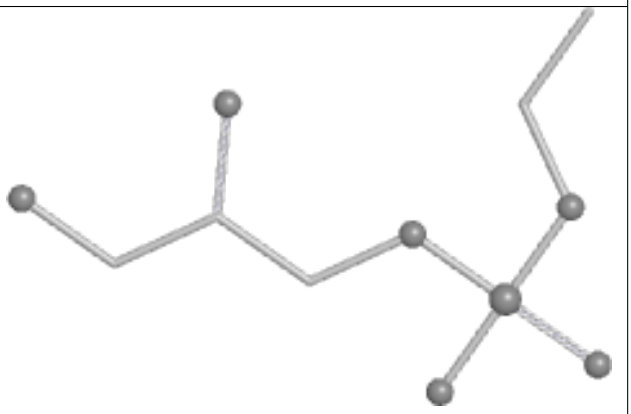
Bond lengths



Bond angles

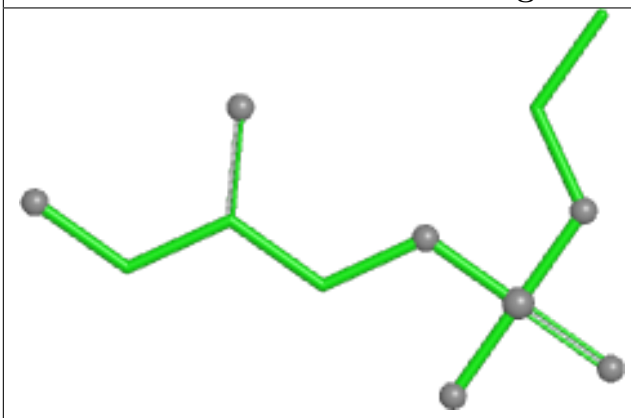


Torsions

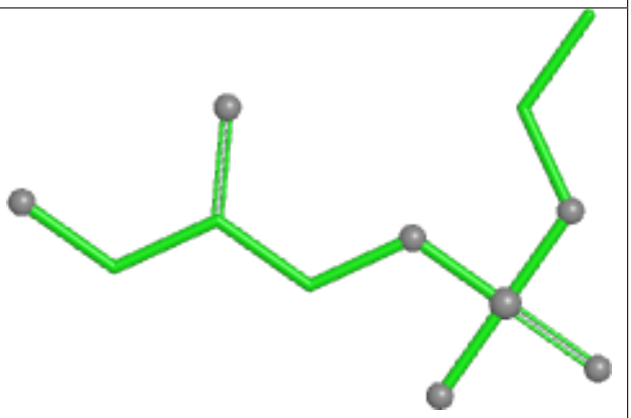


Rings

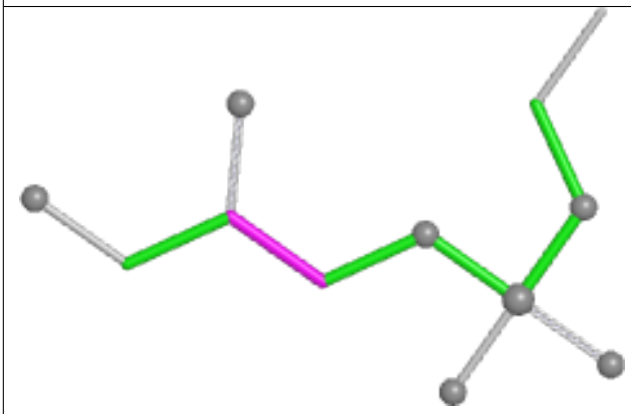
Ligand 6V6 5M 101



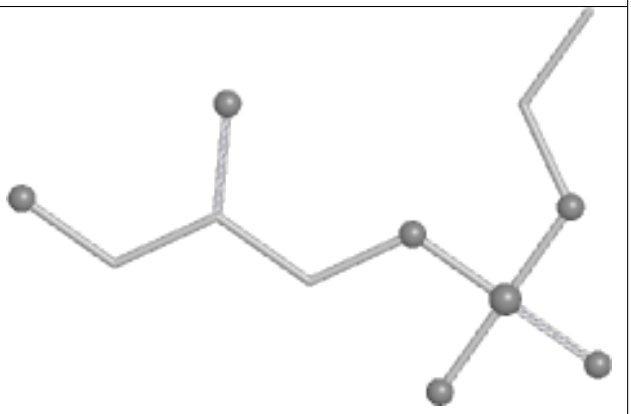
Bond lengths



Bond angles

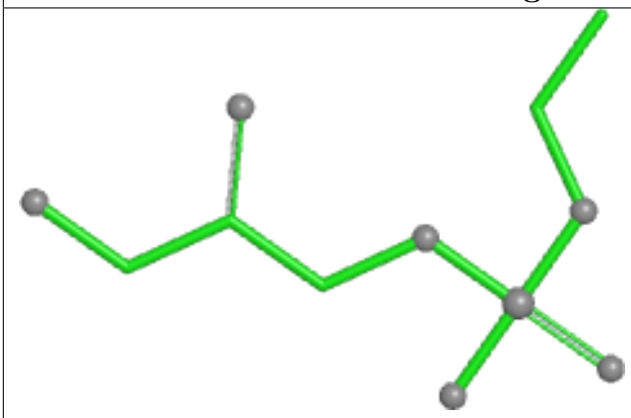


Torsions

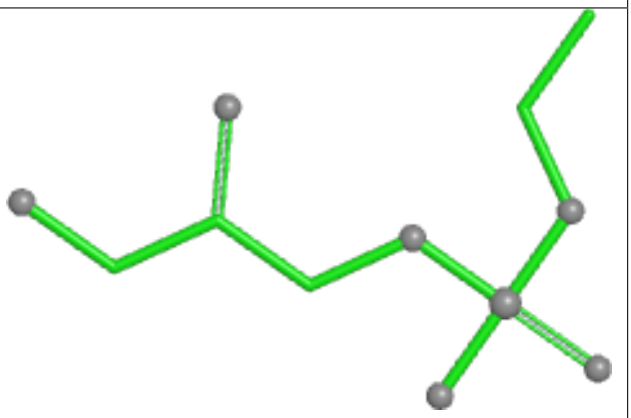


Rings

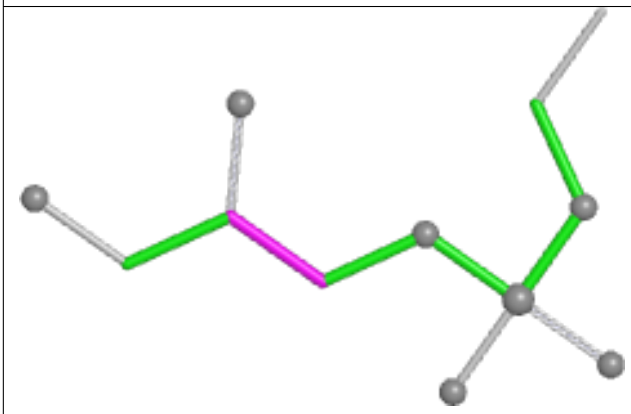
Ligand 6V6 2L 101



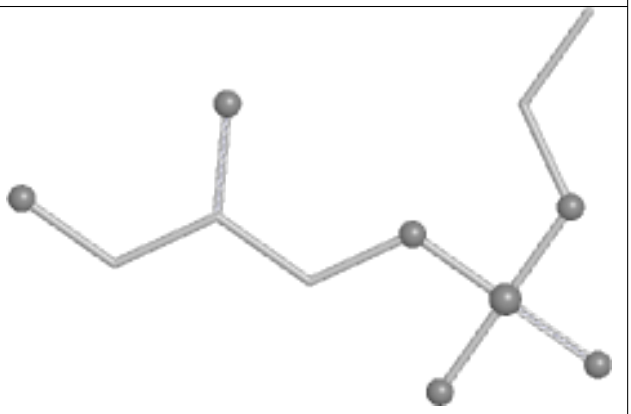
Bond lengths



Bond angles

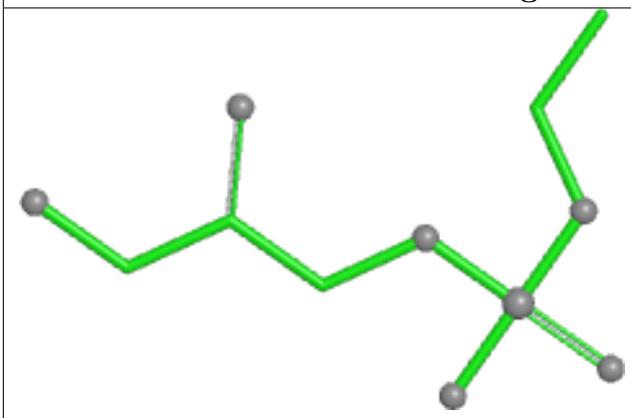


Torsions

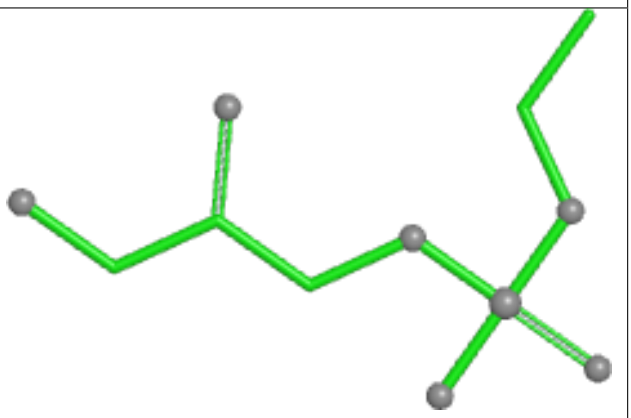


Rings

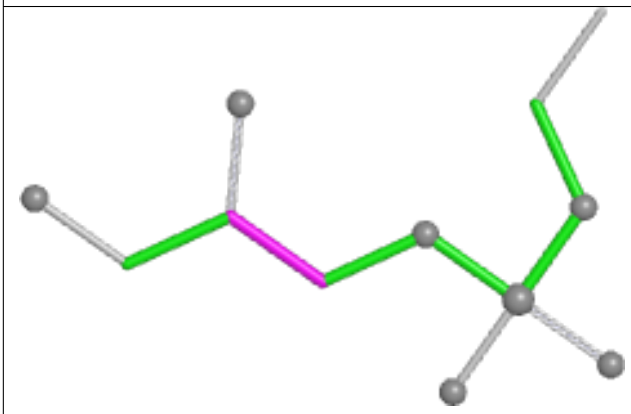
Ligand 6V6 3A 101



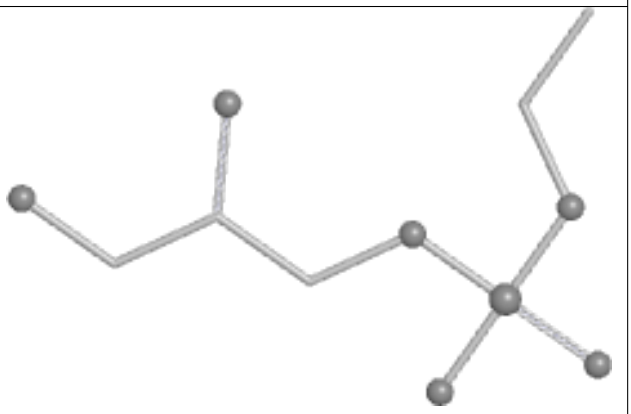
Bond lengths



Bond angles

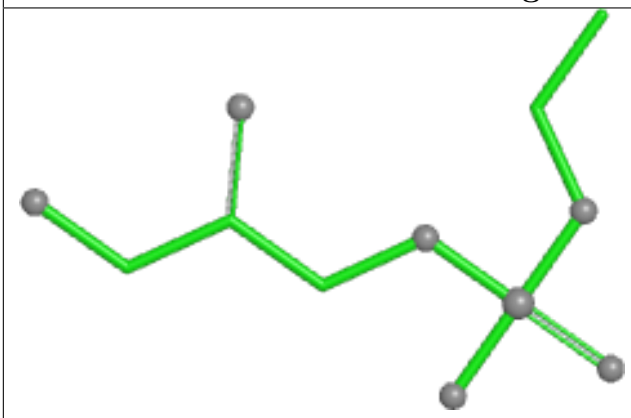


Torsions

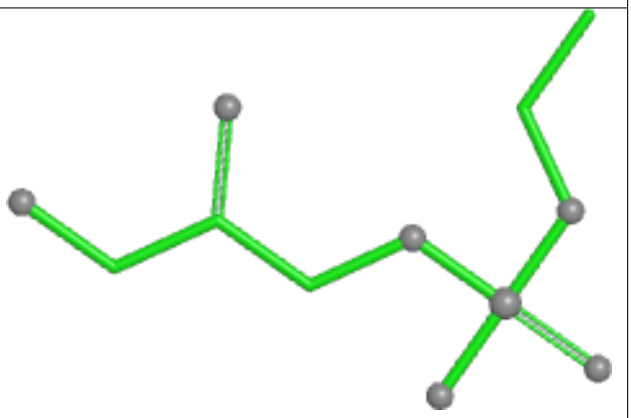


Rings

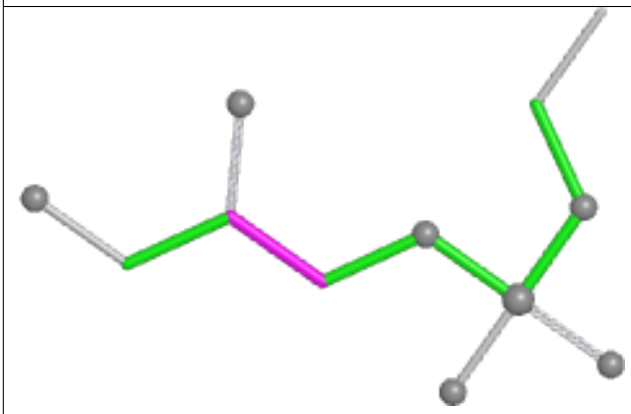
Ligand 6V6 2E 101



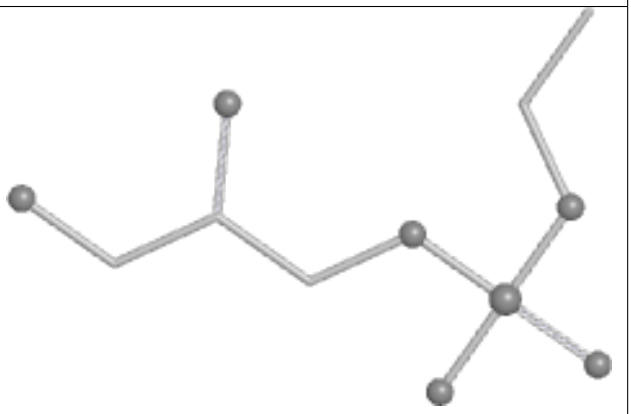
Bond lengths



Bond angles

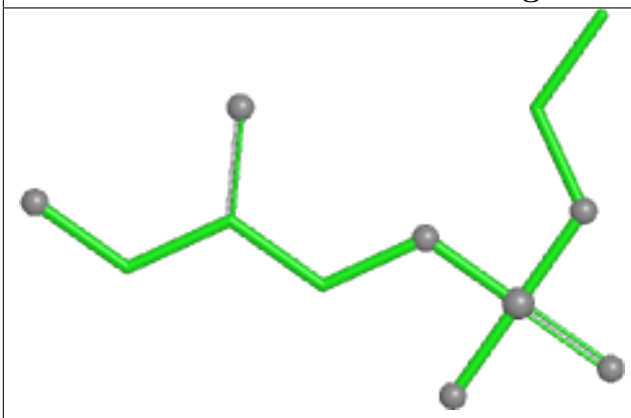


Torsions

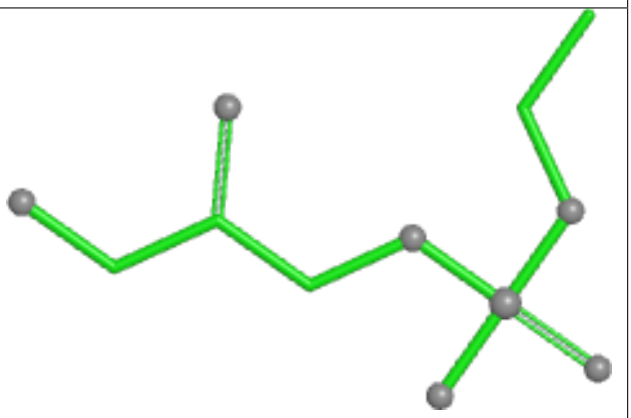


Rings

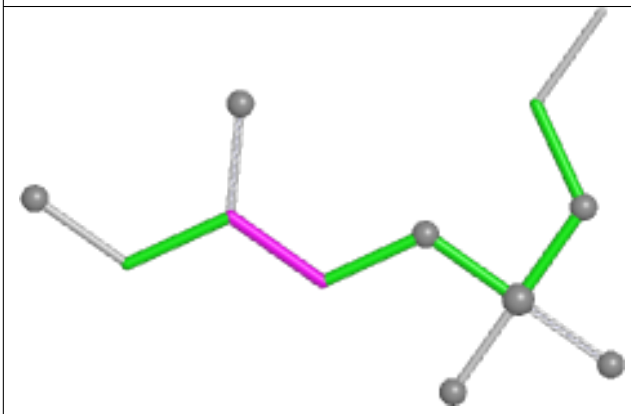
Ligand 6V6 3E 101



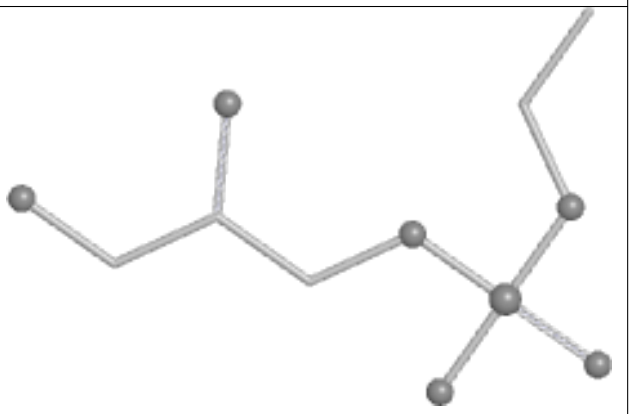
Bond lengths



Bond angles

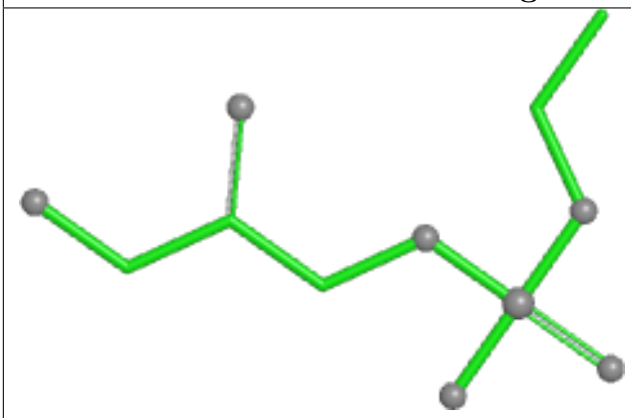


Torsions

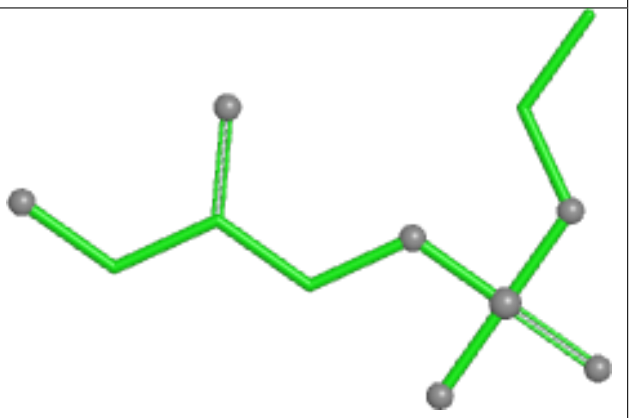


Rings

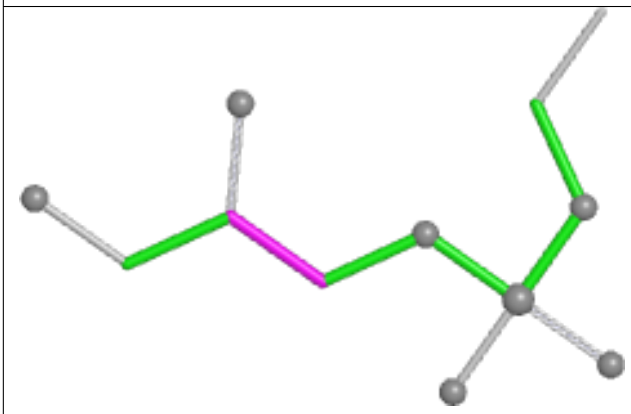
Ligand 6V6 3G 101



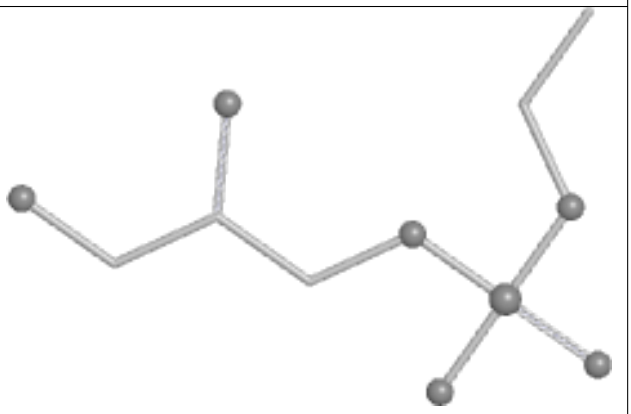
Bond lengths



Bond angles

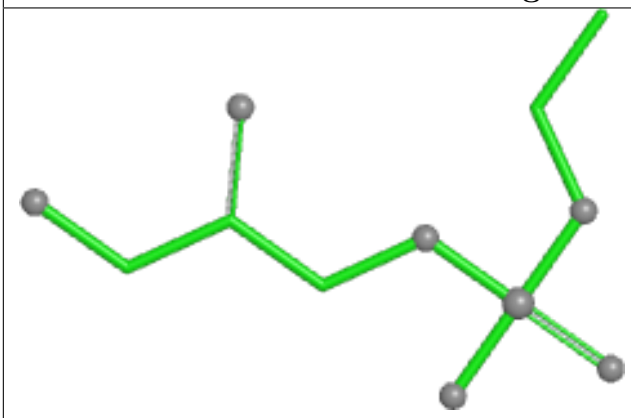


Torsions

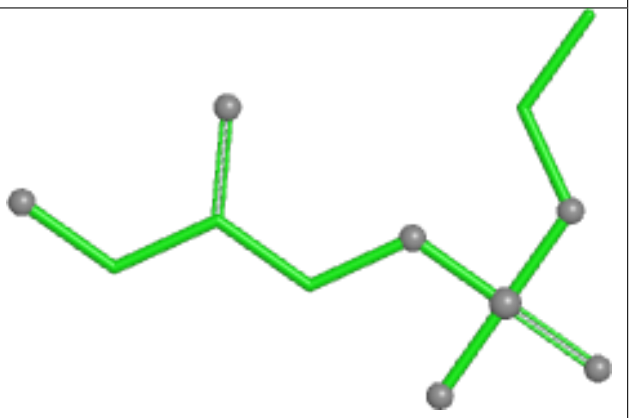


Rings

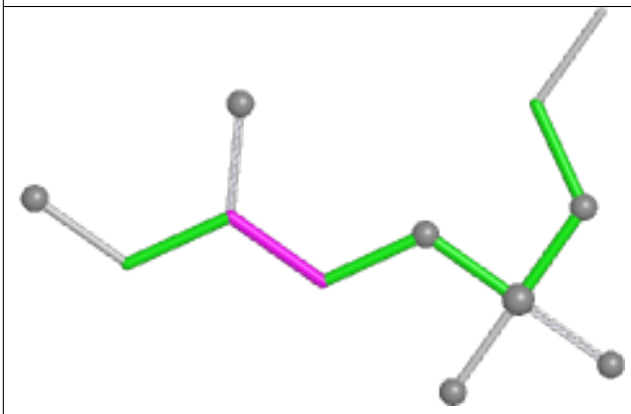
Ligand 6V6 4F 101



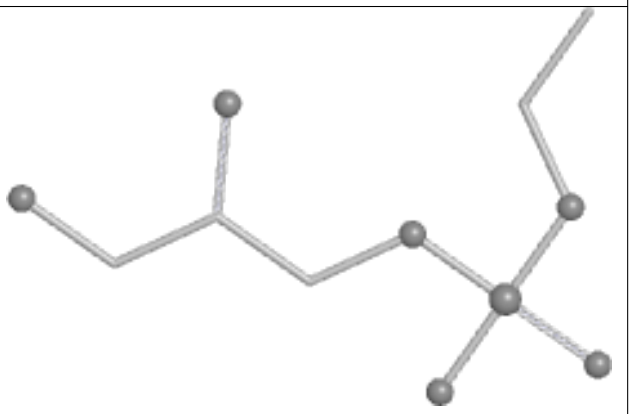
Bond lengths



Bond angles

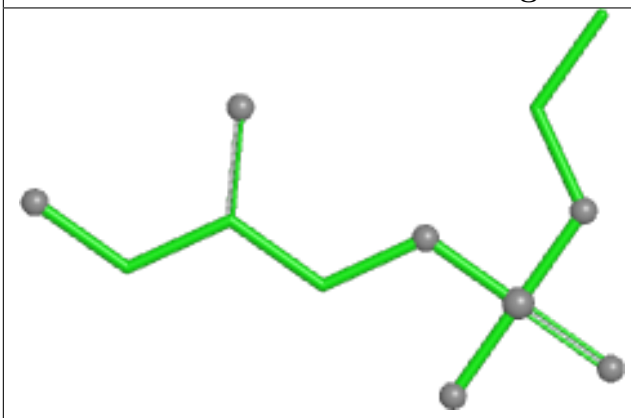


Torsions

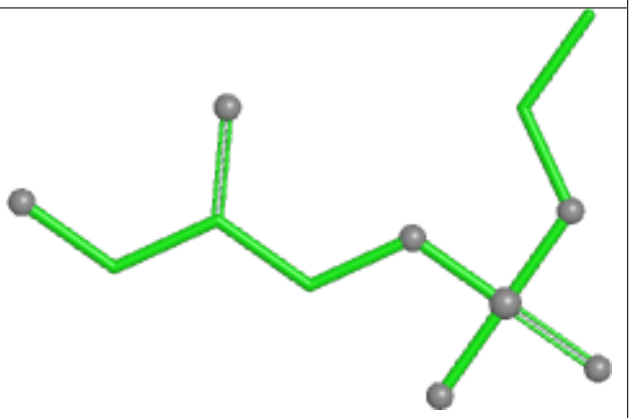


Rings

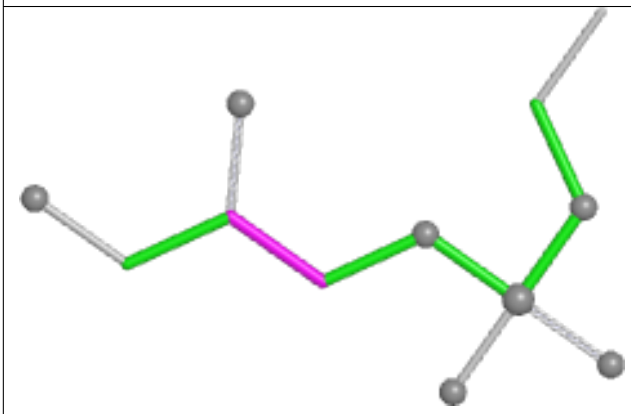
Ligand 6V6 5H 101



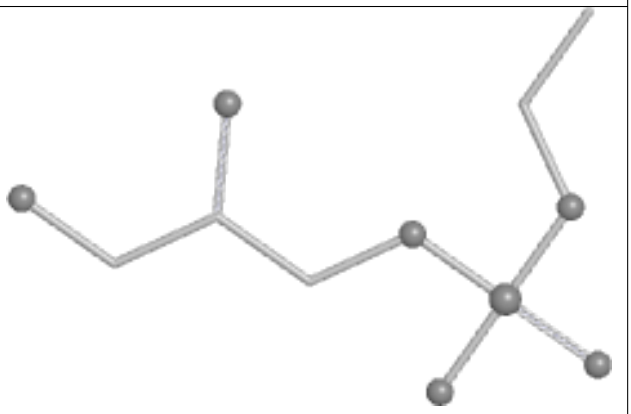
Bond lengths



Bond angles

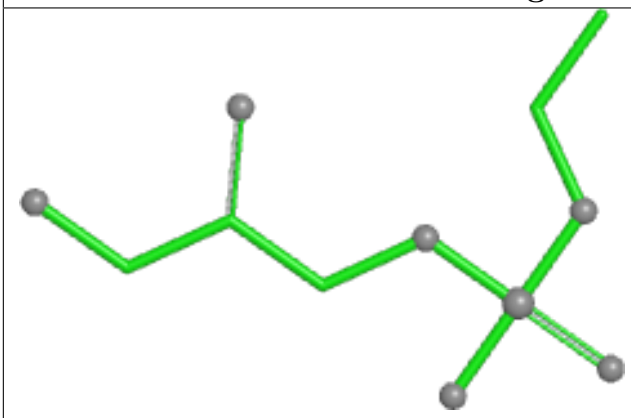


Torsions

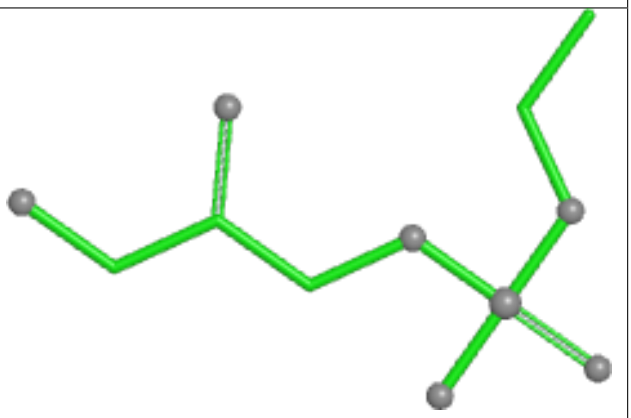


Rings

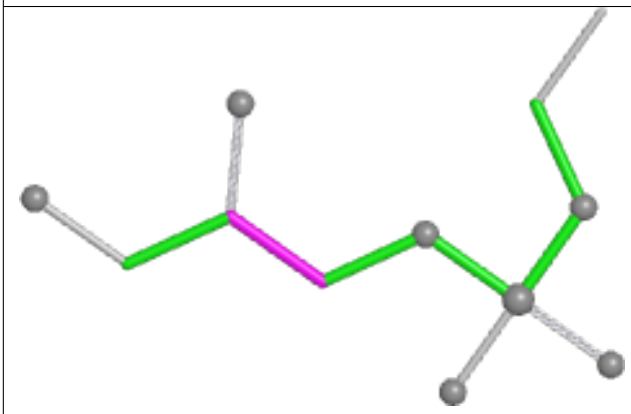
Ligand 6V6 3I 101



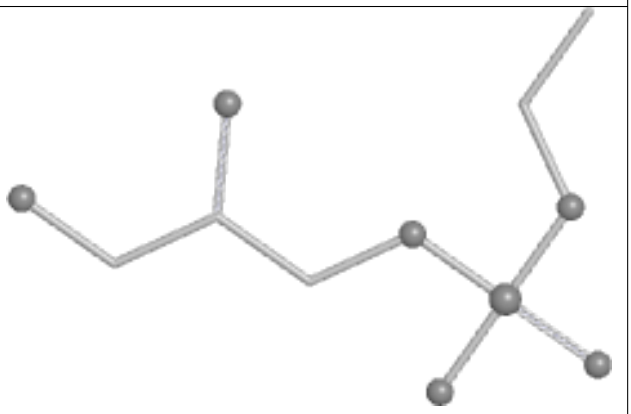
Bond lengths



Bond angles

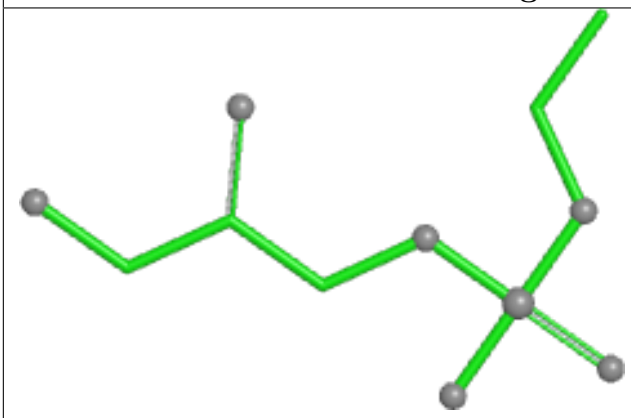


Torsions

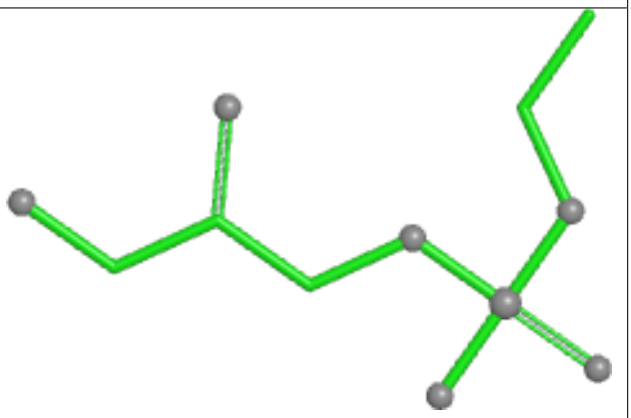


Rings

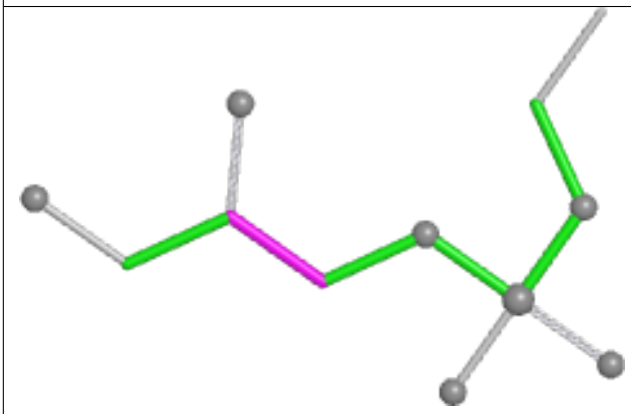
Ligand 6V6 2N 101



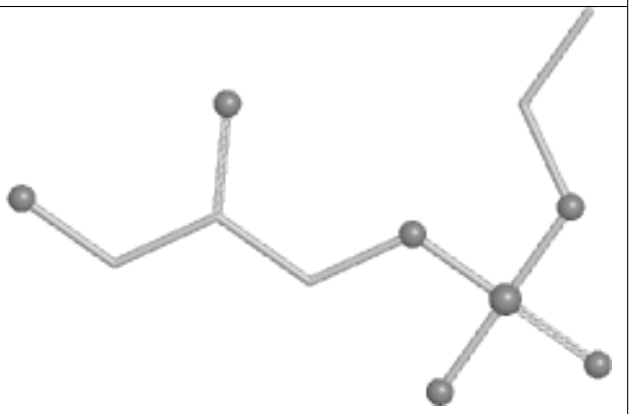
Bond lengths



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.

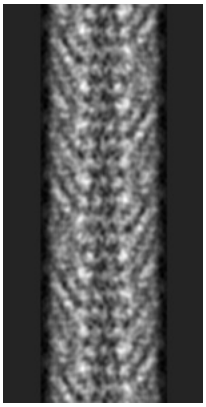
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4044. These allow visual inspection of the internal detail of the map and identification of artifacts.

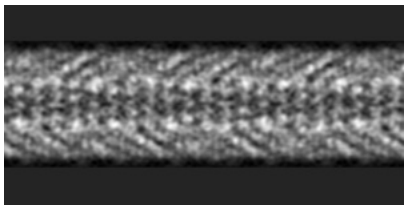
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



Y

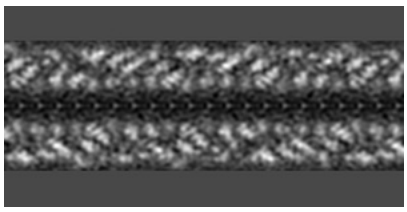
Z

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

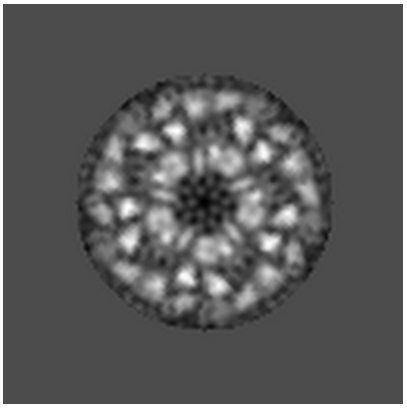
6.2 Central slices

6.2.1 Primary map

X Index: 64



Y Index: 64

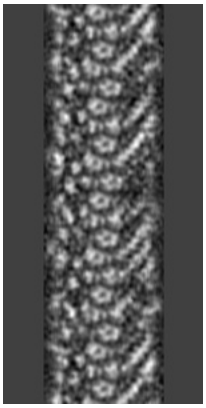


Z Index: 128

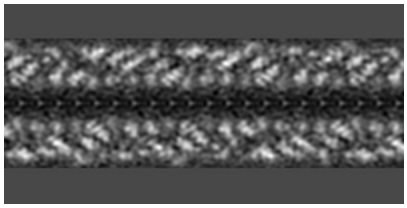
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

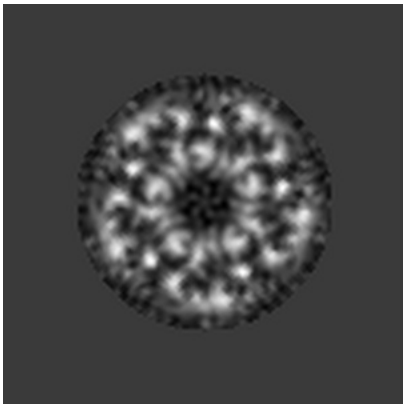
6.3.1 Primary map



X Index: 79



Y Index: 64



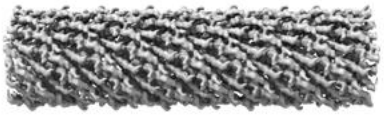
Z Index: 178

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

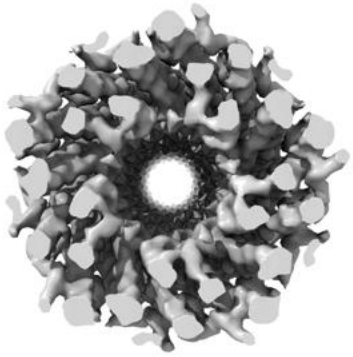
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 44.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

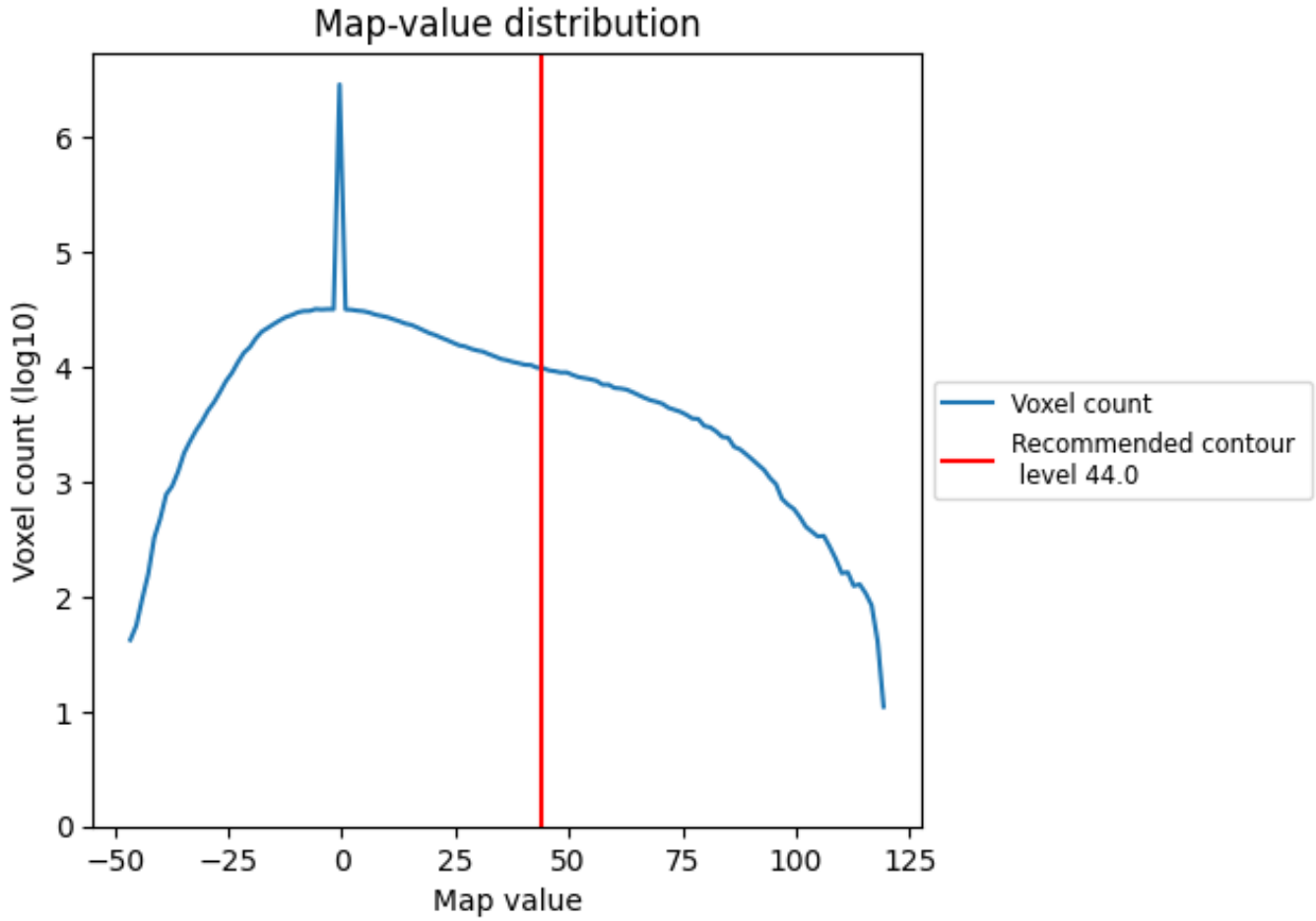
6.5 Mask visualisation (i)

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

7 Map analysis

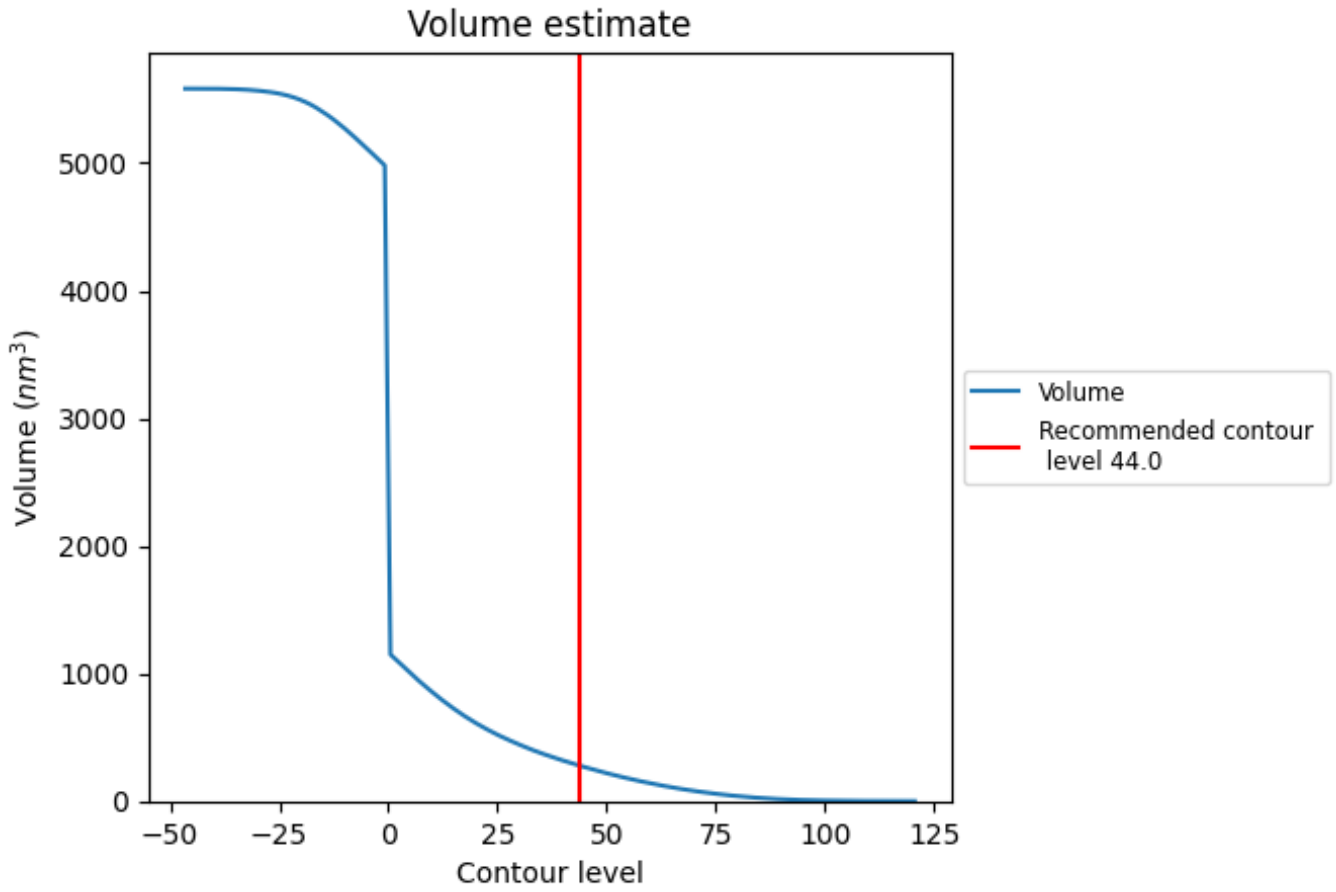
This section contains the results of statistical analysis of the map.

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 (i)



The volume at the recommended contour level is 276 nm^3; this corresponds to an approximate mass of 250 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.

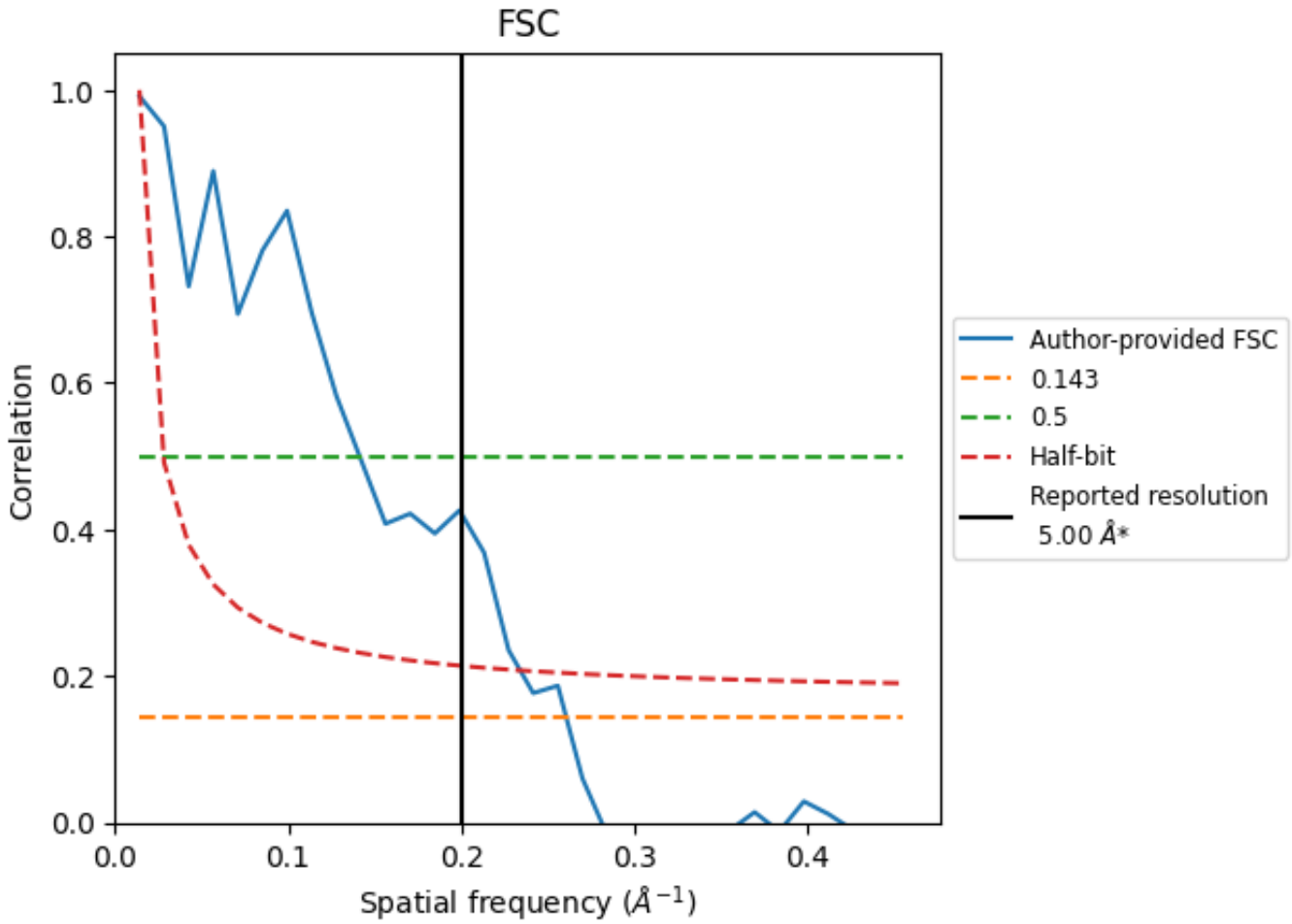
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.200 Å^{-1}

8.2 Resolution estimates (i)

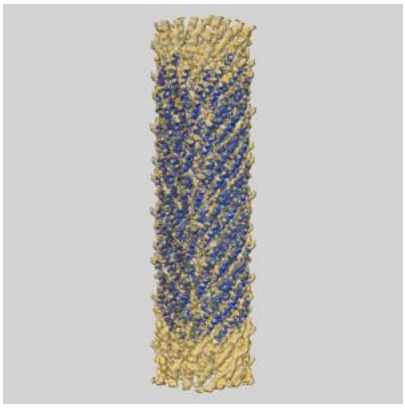
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	5.00
Author-provided FSC curve	3.84	7.08	4.28	-
Unmasked-calculated*	-	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

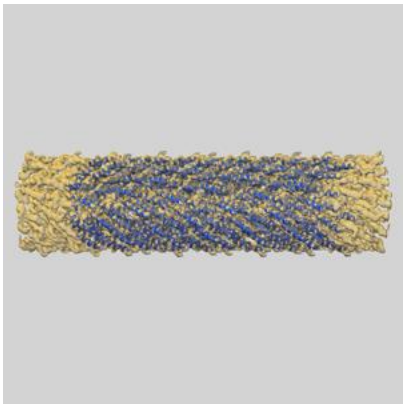
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4044 and PDB model 5LER. Per-residue inclusion information can be found in section 3 on page 14.

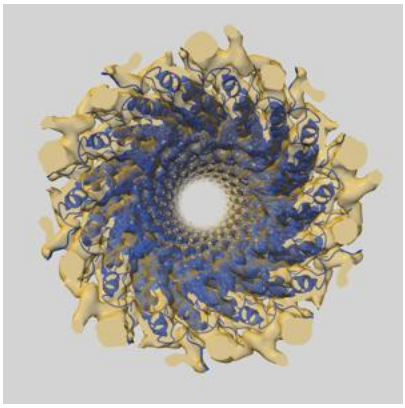
9.1 Map-model overlay



X



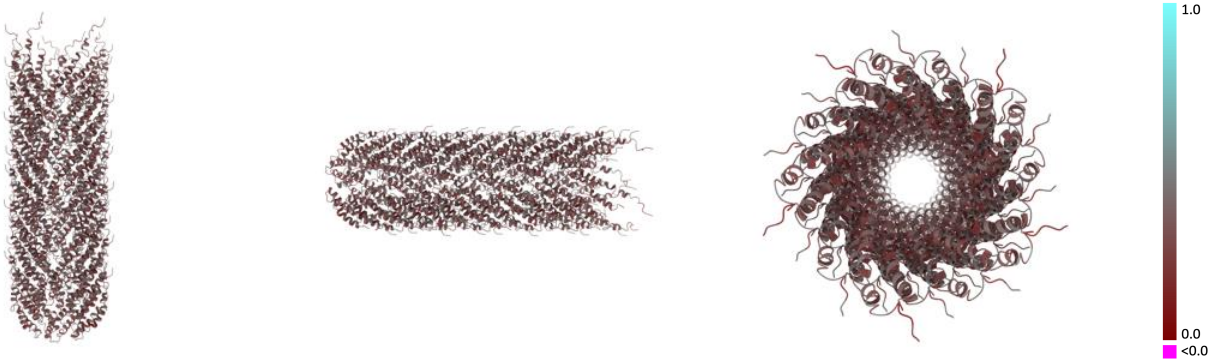
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 44.0 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.

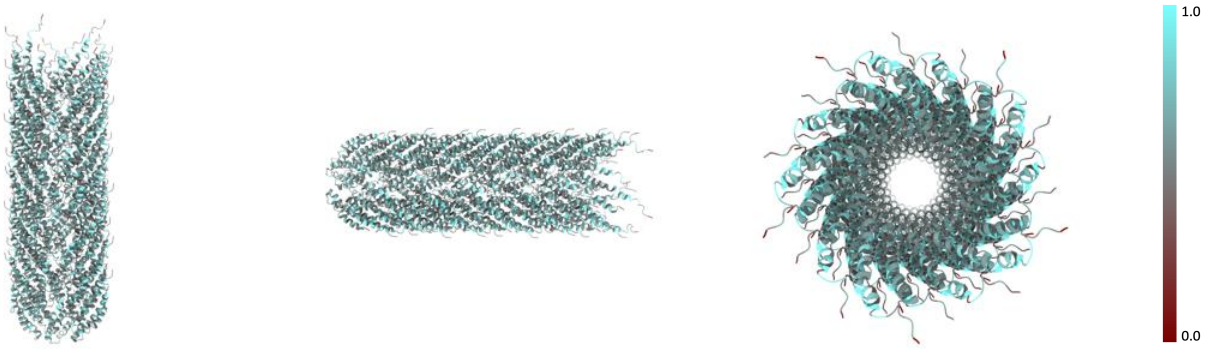
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

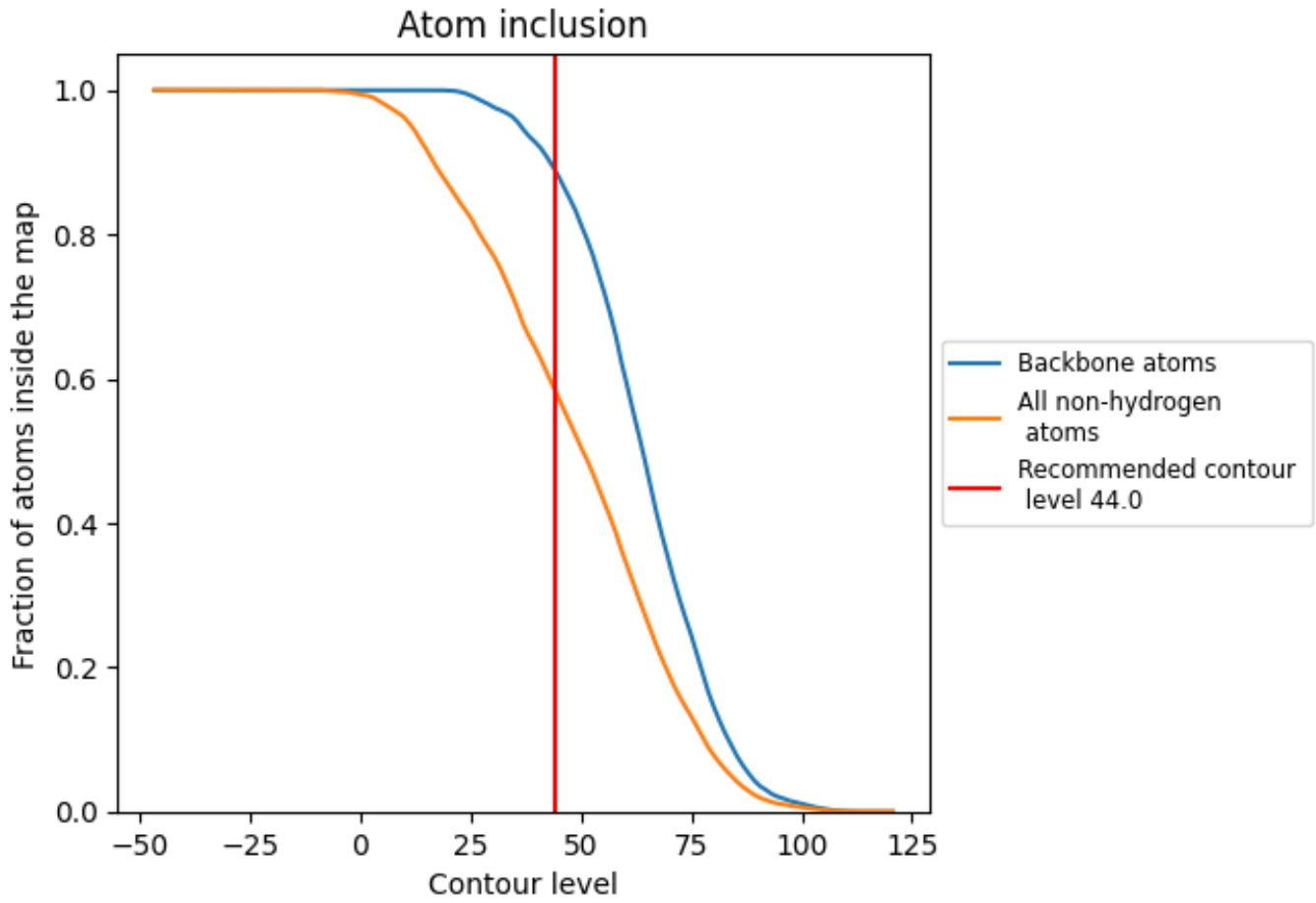
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (44.0).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (44.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5857	0.3440
1A	0.5794	0.3420
1B	0.5885	0.3500
1C	0.5782	0.3460
1D	0.5782	0.3480
1E	0.5823	0.3470
1F	0.5823	0.3450
1G	0.5947	0.3510
1H	0.5885	0.3510
1I	0.5885	0.3500
1J	0.5885	0.3480
1K	0.5885	0.3440
1L	0.5844	0.3410
1M	0.5823	0.3470
1N	0.5782	0.3450
1O	0.5802	0.3180
2A	0.5864	0.3440
2B	0.5864	0.3490
2C	0.5844	0.3440
2D	0.5823	0.3500
2E	0.5905	0.3450
2F	0.5864	0.3480
2G	0.5802	0.3440
2H	0.5885	0.3480
2I	0.5967	0.3460
2J	0.5988	0.3470
2K	0.5885	0.3440
2L	0.5802	0.3460
2M	0.5802	0.3440
2N	0.5761	0.3430
2O	0.5928	0.3220
3A	0.5823	0.3440
3B	0.5823	0.3450
3C	0.5761	0.3480
3D	0.5782	0.3450

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
3E	0.5885	0.3470
3F	0.5885	0.3440
3G	0.5988	0.3440
3H	0.5782	0.3450
3I	0.5864	0.3440
3J	0.5885	0.3420
3K	0.5905	0.3490
3L	0.5926	0.3430
3M	0.5905	0.3470
3N	0.5741	0.3440
3O	0.5865	0.3220
4A	0.5823	0.3440
4B	0.5844	0.3490
4C	0.5802	0.3450
4D	0.5967	0.3470
4E	0.5864	0.3460
4F	0.5844	0.3430
4G	0.5844	0.3390
4H	0.5926	0.3510
4I	0.5823	0.3430
4J	0.5844	0.3470
4K	0.5967	0.3460
4L	0.5782	0.3450
4M	0.5802	0.3450
4N	0.5844	0.3460
4O	0.5907	0.3210
5A	0.5926	0.3450
5B	0.5926	0.3450
5C	0.5782	0.3450
5D	0.5823	0.3420
5E	0.5885	0.3440
5F	0.5926	0.3480
5G	0.5823	0.3480
5H	0.5864	0.3450
5I	0.5926	0.3460
5J	0.5802	0.3460
5K	0.5947	0.3510
5L	0.5905	0.3450
5M	0.5782	0.3460
5N	0.5741	0.3410
5O	0.5886	0.3180