



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 04:30 PM JST

PDB ID : 8WT1  
Title : Crystal structure of S9 carboxypeptidase from *Geobacillus sterothermophilus*  
Authors : Chandravanshi, K.; Kumar, A.; Sen, C.; Singh, R.; Bhange, G.B.; Makde, R.D.  
Deposited on : 2023-10-17  
Resolution : 2.00 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

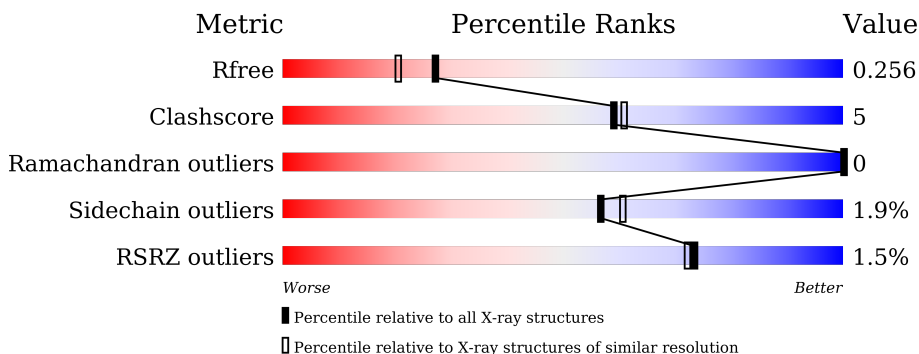
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.



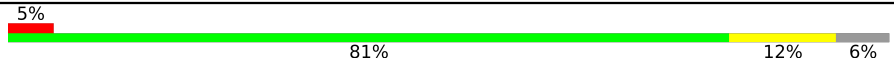

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	691	
1	B	691	
1	C	691	
1	D	691	
1	E	691	
1	F	691	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	691	
1	H	691	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	707	-	-	X	-
5	ALA	A	716	-	-	X	-
5	ALA	B	719	-	-	X	-
5	ALA	C	713	-	X	-	-
5	ALA	D	714	-	X	X	-
5	ALA	E	715	-	X	X	-
5	ALA	F	713	-	X	X	-
5	ALA	G	709	-	X	-	-
6	FLC	A	717	-	X	-	-
6	FLC	H	713	-	X	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 42813 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called S9 family peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	650	5067	3239	873	944	11	0	0	0
1	B	650	5063	3239	870	943	11	0	0	0
1	C	651	5053	3232	867	943	11	0	0	0
1	D	649	5032	3221	863	937	11	0	0	0
1	E	650	5027	3215	861	940	11	0	0	0
1	F	649	5014	3211	862	930	11	0	0	0
1	G	647	4904	3159	829	905	11	0	0	0
1	H	651	4985	3203	852	919	11	0	0	0

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
A	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
A	-18	SER	-	expression tag	UNP A0A3L7D5Q2
A	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
A	-16	SER	-	expression tag	UNP A0A3L7D5Q2
A	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
A	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
A	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
A	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
A	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
A	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
A	-8	SER	-	expression tag	UNP A0A3L7D5Q2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP A0A3L7D5Q2
A	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
A	0	SER	-	expression tag	UNP A0A3L7D5Q2
A	1	SER	-	expression tag	UNP A0A3L7D5Q2
A	2	GLY	-	expression tag	UNP A0A3L7D5Q2
A	3	SER	-	expression tag	UNP A0A3L7D5Q2
A	4	GLY	-	expression tag	UNP A0A3L7D5Q2
A	5	GLY	-	expression tag	UNP A0A3L7D5Q2
A	6	GLY	-	expression tag	UNP A0A3L7D5Q2
A	7	GLY	-	expression tag	UNP A0A3L7D5Q2
A	8	GLY	-	expression tag	UNP A0A3L7D5Q2
A	9	GLU	-	expression tag	UNP A0A3L7D5Q2
A	10	ASN	-	expression tag	UNP A0A3L7D5Q2
A	11	LEU	-	expression tag	UNP A0A3L7D5Q2
A	12	TYR	-	expression tag	UNP A0A3L7D5Q2
A	13	PHE	-	expression tag	UNP A0A3L7D5Q2
A	14	GLN	-	expression tag	UNP A0A3L7D5Q2
A	15	GLY	-	expression tag	UNP A0A3L7D5Q2
A	16	THR	-	expression tag	UNP A0A3L7D5Q2
A	332	SER	LEU	conflict	UNP A0A3L7D5Q2
B	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
B	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
B	-18	SER	-	expression tag	UNP A0A3L7D5Q2
B	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
B	-16	SER	-	expression tag	UNP A0A3L7D5Q2
B	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
B	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
B	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
B	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
B	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
B	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
B	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
B	-8	SER	-	expression tag	UNP A0A3L7D5Q2
B	-7	SER	-	expression tag	UNP A0A3L7D5Q2
B	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
B	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
B	-4	HIS	-	expression tag	UNP A0A3L7D5Q2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
B	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
B	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
B	0	SER	-	expression tag	UNP A0A3L7D5Q2
B	1	SER	-	expression tag	UNP A0A3L7D5Q2
B	2	GLY	-	expression tag	UNP A0A3L7D5Q2
B	3	SER	-	expression tag	UNP A0A3L7D5Q2
B	4	GLY	-	expression tag	UNP A0A3L7D5Q2
B	5	GLY	-	expression tag	UNP A0A3L7D5Q2
B	6	GLY	-	expression tag	UNP A0A3L7D5Q2
B	7	GLY	-	expression tag	UNP A0A3L7D5Q2
B	8	GLY	-	expression tag	UNP A0A3L7D5Q2
B	9	GLU	-	expression tag	UNP A0A3L7D5Q2
B	10	ASN	-	expression tag	UNP A0A3L7D5Q2
B	11	LEU	-	expression tag	UNP A0A3L7D5Q2
B	12	TYR	-	expression tag	UNP A0A3L7D5Q2
B	13	PHE	-	expression tag	UNP A0A3L7D5Q2
B	14	GLN	-	expression tag	UNP A0A3L7D5Q2
B	15	GLY	-	expression tag	UNP A0A3L7D5Q2
B	16	THR	-	expression tag	UNP A0A3L7D5Q2
B	332	SER	LEU	conflict	UNP A0A3L7D5Q2
C	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
C	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
C	-18	SER	-	expression tag	UNP A0A3L7D5Q2
C	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
C	-16	SER	-	expression tag	UNP A0A3L7D5Q2
C	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
C	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
C	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
C	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
C	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
C	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
C	-8	SER	-	expression tag	UNP A0A3L7D5Q2
C	-7	SER	-	expression tag	UNP A0A3L7D5Q2
C	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
C	0	SER	-	expression tag	UNP A0A3L7D5Q2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	-	expression tag	UNP A0A3L7D5Q2
C	2	GLY	-	expression tag	UNP A0A3L7D5Q2
C	3	SER	-	expression tag	UNP A0A3L7D5Q2
C	4	GLY	-	expression tag	UNP A0A3L7D5Q2
C	5	GLY	-	expression tag	UNP A0A3L7D5Q2
C	6	GLY	-	expression tag	UNP A0A3L7D5Q2
C	7	GLY	-	expression tag	UNP A0A3L7D5Q2
C	8	GLY	-	expression tag	UNP A0A3L7D5Q2
C	9	GLU	-	expression tag	UNP A0A3L7D5Q2
C	10	ASN	-	expression tag	UNP A0A3L7D5Q2
C	11	LEU	-	expression tag	UNP A0A3L7D5Q2
C	12	TYR	-	expression tag	UNP A0A3L7D5Q2
C	13	PHE	-	expression tag	UNP A0A3L7D5Q2
C	14	GLN	-	expression tag	UNP A0A3L7D5Q2
C	15	GLY	-	expression tag	UNP A0A3L7D5Q2
C	16	THR	-	expression tag	UNP A0A3L7D5Q2
C	332	SER	LEU	conflict	UNP A0A3L7D5Q2
D	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
D	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
D	-18	SER	-	expression tag	UNP A0A3L7D5Q2
D	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
D	-16	SER	-	expression tag	UNP A0A3L7D5Q2
D	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
D	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
D	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
D	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
D	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
D	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
D	-8	SER	-	expression tag	UNP A0A3L7D5Q2
D	-7	SER	-	expression tag	UNP A0A3L7D5Q2
D	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
D	0	SER	-	expression tag	UNP A0A3L7D5Q2
D	1	SER	-	expression tag	UNP A0A3L7D5Q2
D	2	GLY	-	expression tag	UNP A0A3L7D5Q2
D	3	SER	-	expression tag	UNP A0A3L7D5Q2
D	4	GLY	-	expression tag	UNP A0A3L7D5Q2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	GLY	-	expression tag	UNP A0A3L7D5Q2
D	6	GLY	-	expression tag	UNP A0A3L7D5Q2
D	7	GLY	-	expression tag	UNP A0A3L7D5Q2
D	8	GLY	-	expression tag	UNP A0A3L7D5Q2
D	9	GLU	-	expression tag	UNP A0A3L7D5Q2
D	10	ASN	-	expression tag	UNP A0A3L7D5Q2
D	11	LEU	-	expression tag	UNP A0A3L7D5Q2
D	12	TYR	-	expression tag	UNP A0A3L7D5Q2
D	13	PHE	-	expression tag	UNP A0A3L7D5Q2
D	14	GLN	-	expression tag	UNP A0A3L7D5Q2
D	15	GLY	-	expression tag	UNP A0A3L7D5Q2
D	16	THR	-	expression tag	UNP A0A3L7D5Q2
D	332	SER	LEU	conflict	UNP A0A3L7D5Q2
E	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
E	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
E	-18	SER	-	expression tag	UNP A0A3L7D5Q2
E	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
E	-16	SER	-	expression tag	UNP A0A3L7D5Q2
E	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
E	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
E	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
E	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
E	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
E	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
E	-8	SER	-	expression tag	UNP A0A3L7D5Q2
E	-7	SER	-	expression tag	UNP A0A3L7D5Q2
E	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
E	0	SER	-	expression tag	UNP A0A3L7D5Q2
E	1	SER	-	expression tag	UNP A0A3L7D5Q2
E	2	GLY	-	expression tag	UNP A0A3L7D5Q2
E	3	SER	-	expression tag	UNP A0A3L7D5Q2
E	4	GLY	-	expression tag	UNP A0A3L7D5Q2
E	5	GLY	-	expression tag	UNP A0A3L7D5Q2
E	6	GLY	-	expression tag	UNP A0A3L7D5Q2
E	7	GLY	-	expression tag	UNP A0A3L7D5Q2
E	8	GLY	-	expression tag	UNP A0A3L7D5Q2

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	GLU	-	expression tag	UNP A0A3L7D5Q2
E	10	ASN	-	expression tag	UNP A0A3L7D5Q2
E	11	LEU	-	expression tag	UNP A0A3L7D5Q2
E	12	TYR	-	expression tag	UNP A0A3L7D5Q2
E	13	PHE	-	expression tag	UNP A0A3L7D5Q2
E	14	GLN	-	expression tag	UNP A0A3L7D5Q2
E	15	GLY	-	expression tag	UNP A0A3L7D5Q2
E	16	THR	-	expression tag	UNP A0A3L7D5Q2
E	332	SER	LEU	conflict	UNP A0A3L7D5Q2
F	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
F	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
F	-18	SER	-	expression tag	UNP A0A3L7D5Q2
F	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
F	-16	SER	-	expression tag	UNP A0A3L7D5Q2
F	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
F	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
F	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
F	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
F	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
F	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
F	-8	SER	-	expression tag	UNP A0A3L7D5Q2
F	-7	SER	-	expression tag	UNP A0A3L7D5Q2
F	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
F	0	SER	-	expression tag	UNP A0A3L7D5Q2
F	1	SER	-	expression tag	UNP A0A3L7D5Q2
F	2	GLY	-	expression tag	UNP A0A3L7D5Q2
F	3	SER	-	expression tag	UNP A0A3L7D5Q2
F	4	GLY	-	expression tag	UNP A0A3L7D5Q2
F	5	GLY	-	expression tag	UNP A0A3L7D5Q2
F	6	GLY	-	expression tag	UNP A0A3L7D5Q2
F	7	GLY	-	expression tag	UNP A0A3L7D5Q2
F	8	GLY	-	expression tag	UNP A0A3L7D5Q2
F	9	GLU	-	expression tag	UNP A0A3L7D5Q2
F	10	ASN	-	expression tag	UNP A0A3L7D5Q2
F	11	LEU	-	expression tag	UNP A0A3L7D5Q2
F	12	TYR	-	expression tag	UNP A0A3L7D5Q2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	13	PHE	-	expression tag	UNP A0A3L7D5Q2
F	14	GLN	-	expression tag	UNP A0A3L7D5Q2
F	15	GLY	-	expression tag	UNP A0A3L7D5Q2
F	16	THR	-	expression tag	UNP A0A3L7D5Q2
F	332	SER	LEU	conflict	UNP A0A3L7D5Q2
G	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
G	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
G	-18	SER	-	expression tag	UNP A0A3L7D5Q2
G	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
G	-16	SER	-	expression tag	UNP A0A3L7D5Q2
G	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
G	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
G	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
G	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
G	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
G	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
G	-8	SER	-	expression tag	UNP A0A3L7D5Q2
G	-7	SER	-	expression tag	UNP A0A3L7D5Q2
G	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
G	0	SER	-	expression tag	UNP A0A3L7D5Q2
G	1	SER	-	expression tag	UNP A0A3L7D5Q2
G	2	GLY	-	expression tag	UNP A0A3L7D5Q2
G	3	SER	-	expression tag	UNP A0A3L7D5Q2
G	4	GLY	-	expression tag	UNP A0A3L7D5Q2
G	5	GLY	-	expression tag	UNP A0A3L7D5Q2
G	6	GLY	-	expression tag	UNP A0A3L7D5Q2
G	7	GLY	-	expression tag	UNP A0A3L7D5Q2
G	8	GLY	-	expression tag	UNP A0A3L7D5Q2
G	9	GLU	-	expression tag	UNP A0A3L7D5Q2
G	10	ASN	-	expression tag	UNP A0A3L7D5Q2
G	11	LEU	-	expression tag	UNP A0A3L7D5Q2
G	12	TYR	-	expression tag	UNP A0A3L7D5Q2
G	13	PHE	-	expression tag	UNP A0A3L7D5Q2
G	14	GLN	-	expression tag	UNP A0A3L7D5Q2
G	15	GLY	-	expression tag	UNP A0A3L7D5Q2
G	16	THR	-	expression tag	UNP A0A3L7D5Q2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	SER	LEU	conflict	UNP A0A3L7D5Q2
H	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
H	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
H	-18	SER	-	expression tag	UNP A0A3L7D5Q2
H	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
H	-16	SER	-	expression tag	UNP A0A3L7D5Q2
H	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
H	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
H	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
H	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
H	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
H	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
H	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
H	-8	SER	-	expression tag	UNP A0A3L7D5Q2
H	-7	SER	-	expression tag	UNP A0A3L7D5Q2
H	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
H	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
H	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
H	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
H	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
H	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
H	0	SER	-	expression tag	UNP A0A3L7D5Q2
H	1	SER	-	expression tag	UNP A0A3L7D5Q2
H	2	GLY	-	expression tag	UNP A0A3L7D5Q2
H	3	SER	-	expression tag	UNP A0A3L7D5Q2
H	4	GLY	-	expression tag	UNP A0A3L7D5Q2
H	5	GLY	-	expression tag	UNP A0A3L7D5Q2
H	6	GLY	-	expression tag	UNP A0A3L7D5Q2
H	7	GLY	-	expression tag	UNP A0A3L7D5Q2
H	8	GLY	-	expression tag	UNP A0A3L7D5Q2
H	9	GLU	-	expression tag	UNP A0A3L7D5Q2
H	10	ASN	-	expression tag	UNP A0A3L7D5Q2
H	11	LEU	-	expression tag	UNP A0A3L7D5Q2
H	12	TYR	-	expression tag	UNP A0A3L7D5Q2
H	13	PHE	-	expression tag	UNP A0A3L7D5Q2
H	14	GLN	-	expression tag	UNP A0A3L7D5Q2
H	15	GLY	-	expression tag	UNP A0A3L7D5Q2
H	16	THR	-	expression tag	UNP A0A3L7D5Q2
H	332	SER	LEU	conflict	UNP A0A3L7D5Q2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	G	1	5	4	1	0	0

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	2	Total Na 2 2	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

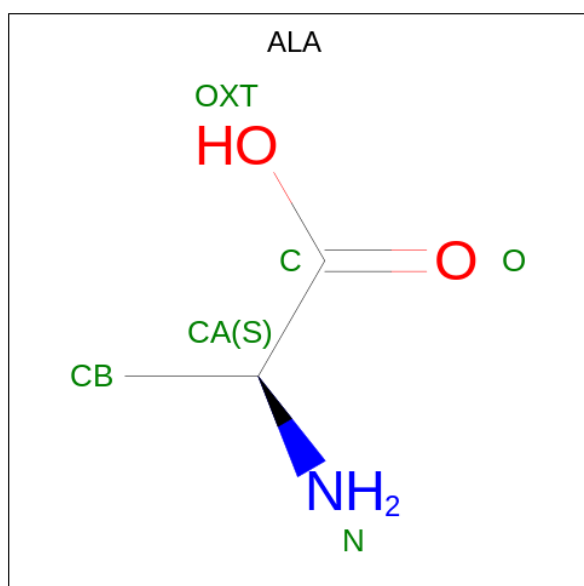
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



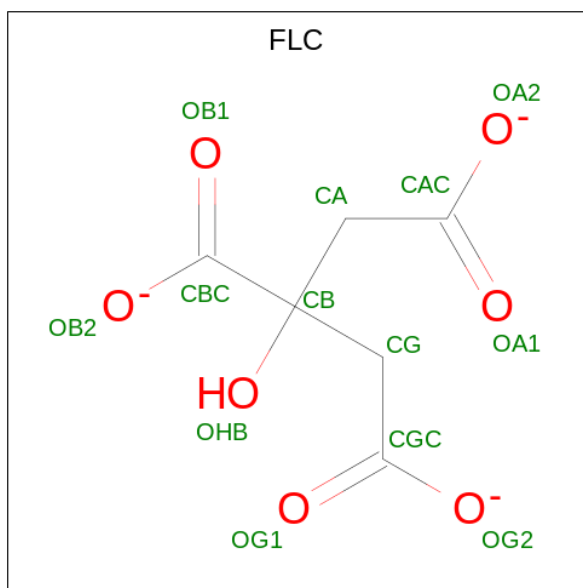
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			6	3	1	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			6	3	1	2		
5	C	1	Total	C	N	O	0	0
			6	3	1	2		
5	D	1	Total	C	N	O	0	0
			6	3	1	2		
5	E	1	Total	C	N	O	0	0
			6	3	1	2		
5	F	1	Total	C	N	O	0	0
			6	3	1	2		
5	G	1	Total	C	N	O	0	0
			6	3	1	2		
5	H	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	6	7		
6	H	1	Total	C	O	0	0
			13	6	7		

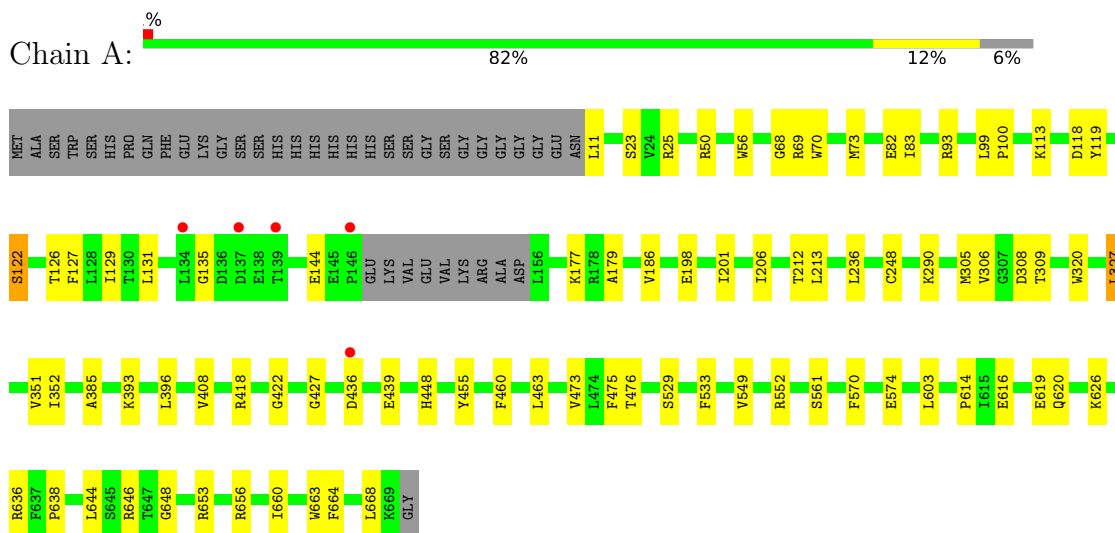
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	337	Total 342	O 342	0	5
7	B	342	Total 347	O 347	0	5
7	C	302	Total 307	O 307	0	5
7	D	225	Total 228	O 228	0	3
7	E	301	Total 305	O 305	0	4
7	F	250	Total 255	O 255	0	5
7	G	121	Total 123	O 123	0	2
7	H	203	Total 204	O 204	0	1

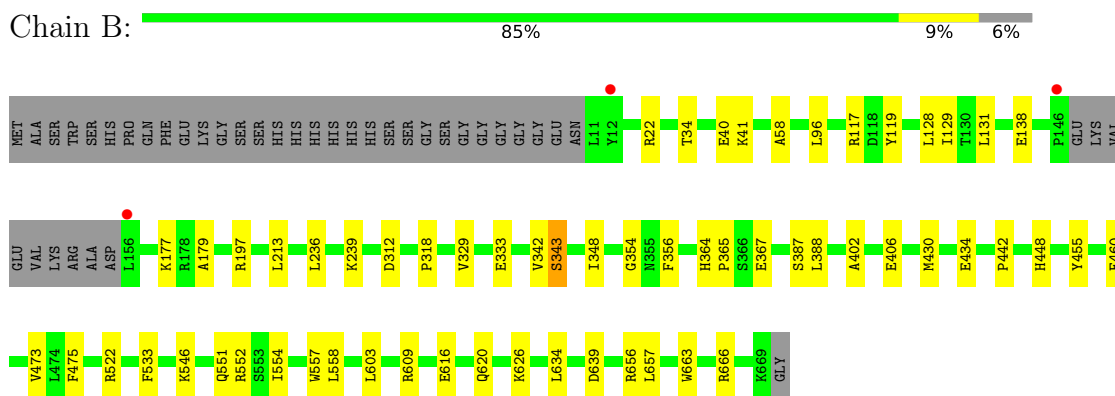
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

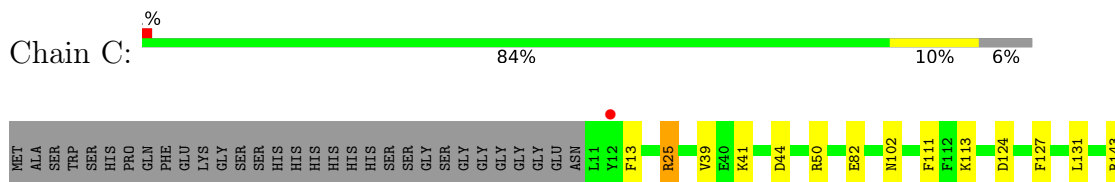
#### • Molecule 1: S9 family peptidase

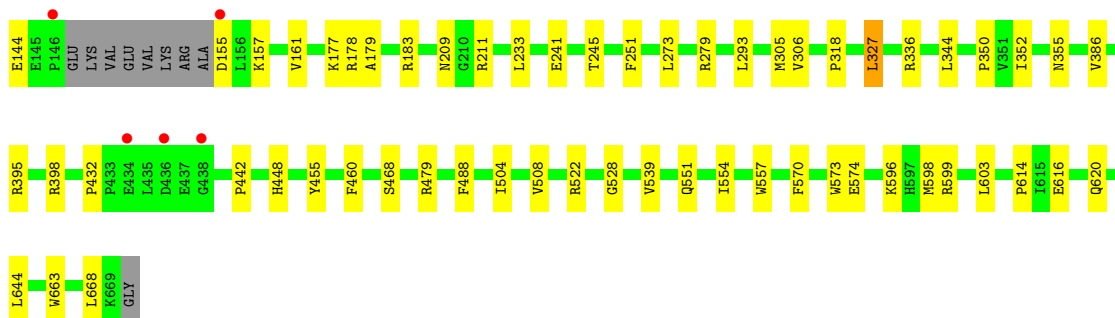


#### • Molecule 1: S9 family peptidase

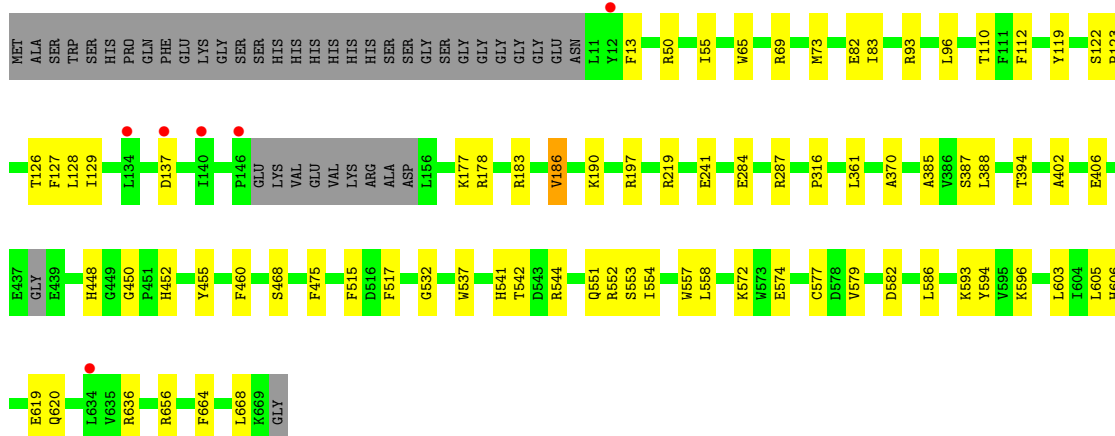
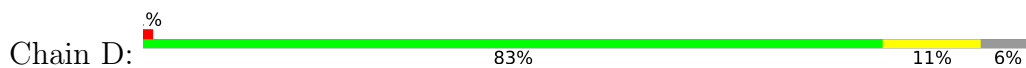


#### • Molecule 1: S9 family peptidase

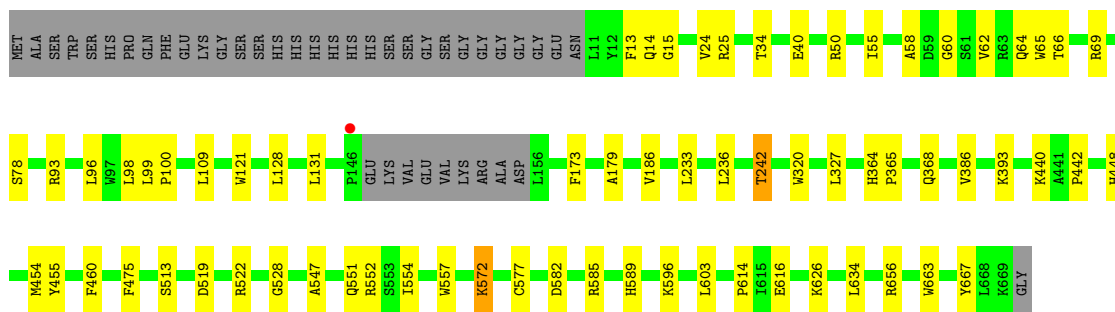
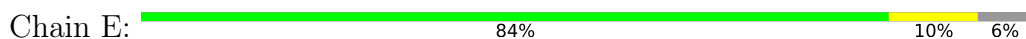




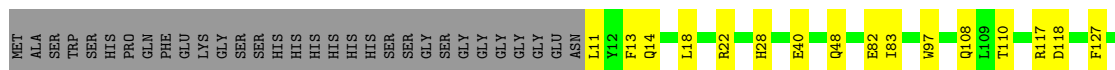
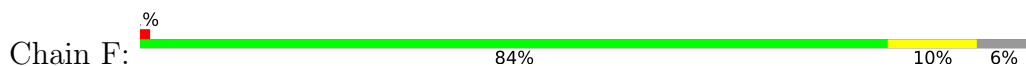
- Molecule 1: S9 family peptidase



- Molecule 1: S9 family peptidase

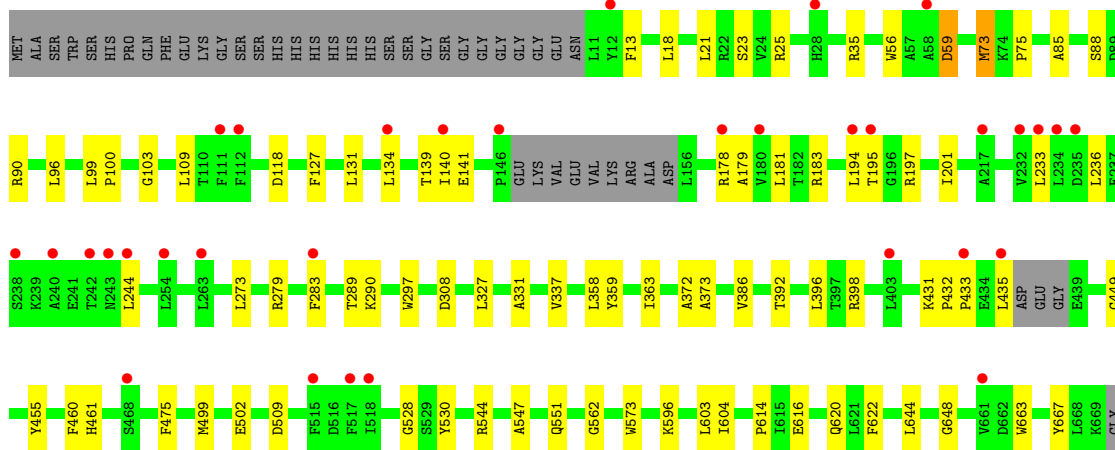
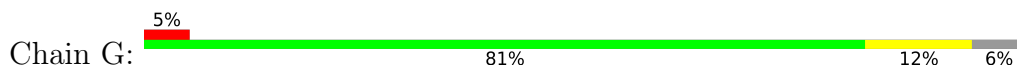


- Molecule 1: S9 family peptidase

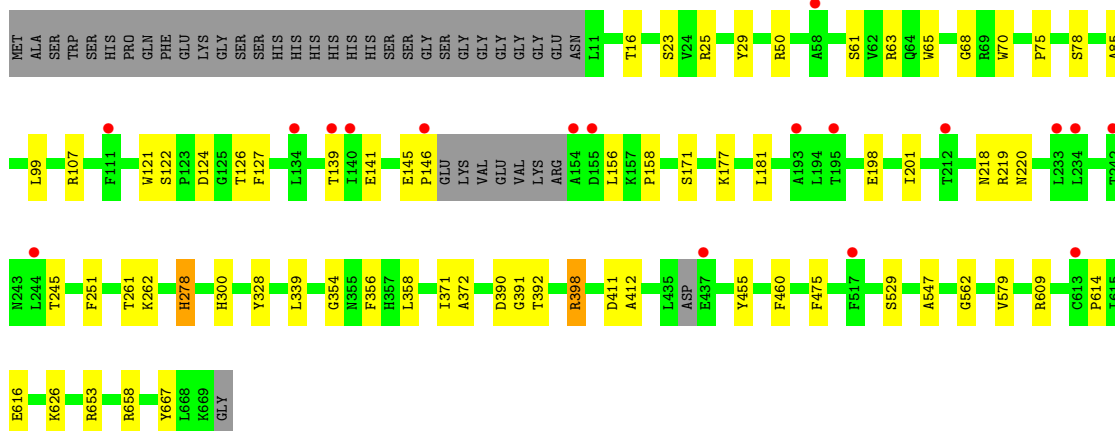
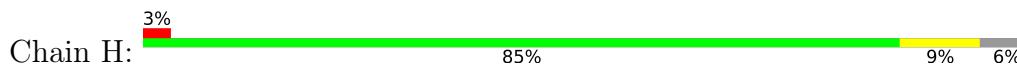




• Molecule 1: S9 family peptidase



• Molecule 1: S9 family peptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.12Å 75.44Å 219.74Å 90.00° 93.27° 90.00°	Depositor
Resolution (Å)	48.94 – 2.00 48.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (48.94-2.00) 91.9 (48.94-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.212 , 0.256 0.213 , 0.256	Depositor DCC
$R_{free}$ test set	19886 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	42813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5178e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL, SO4, FLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/5201	0.64	0/7069
1	B	0.42	0/5197	0.64	0/7062
1	C	0.43	0/5187	0.64	2/7052 (0.0%)
1	D	0.42	0/5165	0.62	0/7022
1	E	0.42	0/5161	0.63	0/7020
1	F	0.42	0/5146	0.64	0/6990
1	G	0.38	0/5037	0.59	0/6862
1	H	0.38	0/5118	0.60	0/6963
All	All	0.41	0/41212	0.62	2/56040 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	25	ARG	CA-CB-CG	-5.41	101.51	113.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5067	0	4822	52	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5063	0	4830	46	0
1	C	5053	0	4803	42	0
1	D	5032	0	4774	48	0
1	E	5027	0	4752	41	0
1	F	5014	0	4732	50	0
1	G	4904	0	4560	51	0
1	H	4985	0	4700	40	0
2	A	40	0	0	1	0
2	B	60	0	0	2	0
2	C	35	0	0	3	0
2	D	40	0	0	1	0
2	E	45	0	0	0	0
2	F	35	0	0	1	0
2	G	25	0	0	1	0
2	H	45	0	0	2	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	18	0	23	0	0
4	B	12	0	15	0	0
4	C	24	0	31	3	0
4	D	24	0	32	1	0
4	E	18	0	24	2	0
4	F	30	0	40	8	0
4	G	12	0	16	1	0
4	H	6	0	8	1	0
5	A	6	0	4	4	0
5	B	6	0	4	8	0
5	C	6	0	4	2	0
5	D	6	0	4	7	0
5	E	6	0	4	4	0
5	F	6	0	4	8	0
5	G	6	0	4	0	0
5	H	6	0	4	0	0
6	A	13	0	5	3	0
6	H	13	0	5	2	0
7	A	342	0	0	1	0
7	B	347	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	307	0	0	3	0
7	D	228	0	0	5	0
7	E	305	0	0	4	0
7	F	255	0	0	7	0
7	G	123	0	0	4	0
7	H	204	0	0	1	0
All	All	42813	0	38204	370	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 5.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:ARG:HH11	5:B:719:ALA:HB2	1.30	0.96
1:D:552:ARG:HH11	5:D:714:ALA:HB2	1.33	0.94
1:F:552:ARG:HH11	5:F:713:ALA:HB2	1.39	0.84
1:H:139:THR:HG23	1:H:141:GLU:H	1.45	0.82
1:C:82:GLU:OE1	1:C:102:ASN:ND2	2.12	0.82
1:G:139:THR:HG23	1:G:141:GLU:H	1.44	0.81
1:H:261:THR:HG23	1:H:262:LYS:HG3	1.63	0.80
1:F:551:GLN:HB3	5:F:713:ALA:HB1	1.65	0.78
1:B:552:ARG:NH1	5:B:719:ALA:HB2	2.00	0.77
1:D:50:ARG:HH11	1:D:69:ARG:HA	1.49	0.76
1:D:656:ARG:HE	5:D:714:ALA:HB3	1.51	0.76
1:F:233:LEU:HB2	1:F:242:THR:HG23	1.68	0.74
1:B:22:ARG:NH1	1:B:40:GLU:OE2	2.19	0.74
1:A:50:ARG:HG3	1:A:69:ARG:HH21	1.52	0.73
1:F:316:PRO:HG3	1:F:361:LEU:HB3	1.70	0.73
1:C:398:ARG:HH22	4:C:711:GOL:H31	1.54	0.73
1:D:551:GLN:HB3	5:D:714:ALA:HB1	1.71	0.72
1:B:402:ALA:O	1:B:406:GLU:HG3	1.90	0.71
1:F:656:ARG:HE	5:F:713:ALA:HB3	1.57	0.70
1:B:551:GLN:HB3	5:B:719:ALA:HB1	1.71	0.69
1:D:284:GLU:HG2	1:D:287:ARG:HB2	1.75	0.69
1:D:82:GLU:HG2	1:D:83:ILE:HG13	1.74	0.68
1:B:138:GLU:O	1:B:197:ARG:NH2	2.23	0.68
1:F:14:GLN:HB3	4:F:710:GOL:H32	1.74	0.68
1:D:316:PRO:HG3	1:D:361:LEU:HB3	1.74	0.68
1:F:599:ARG:HH12	4:F:712:GOL:H32	1.59	0.68
1:G:178:ARG:HD2	1:G:197:ARG:CB	2.24	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:715:ALA:HB2	7:E:844:HOH:O	1.93	0.67
1:F:552:ARG:NH1	5:F:713:ALA:HB2	2.09	0.67
1:H:124:ASP:OD1	1:H:126:THR:HG22	1.96	0.66
1:H:653:ARG:NH1	6:H:713:FLC:OG2	2.23	0.66
1:D:552:ARG:NH1	5:D:714:ALA:HB2	2.07	0.66
1:B:656:ARG:HE	5:B:719:ALA:HB3	1.62	0.65
1:E:656:ARG:HD2	5:E:715:ALA:HA	1.78	0.65
1:A:248:CYS:SG	1:A:290:LYS:NZ	2.69	0.64
1:H:614:PRO:HB2	1:H:616:GLU:HG3	1.80	0.64
1:A:656:ARG:HD2	5:A:716:ALA:HA	1.80	0.64
1:D:656:ARG:NE	5:D:714:ALA:HB3	2.12	0.64
1:D:177:LYS:HG3	2:D:706:SO4:O1	1.98	0.63
1:F:656:ARG:NE	5:F:713:ALA:HB3	2.12	0.63
1:C:448:HIS:HB3	1:C:455:TYR:CZ	2.32	0.63
1:A:99:LEU:HD12	1:A:100:PRO:HD2	1.81	0.63
1:A:131:LEU:HD11	1:A:179:ALA:HB1	1.80	0.63
1:A:82:GLU:HG2	1:A:83:ILE:HG13	1.80	0.63
2:B:709:SO4:O3	7:B:801:HOH:O	2.15	0.63
1:G:178:ARG:HD2	1:G:197:ARG:HB3	1.81	0.62
1:B:34:THR:O	1:B:58:ALA:HB2	2.00	0.62
1:F:366:SER:N	7:F:806:HOH:O	2.31	0.62
1:F:22:ARG:NE	1:F:40:GLU:OE2	2.33	0.62
1:G:308:ASP:OD2	7:G:801:HOH:O	2.16	0.62
1:F:448:HIS:HB3	1:F:455:TYR:CZ	2.33	0.62
1:B:22:ARG:HD3	1:B:40:GLU:OE2	1.99	0.62
1:F:398:ARG:HH22	4:F:711:GOL:H12	1.65	0.62
5:A:716:ALA:HB2	7:A:828:HOH:O	2.00	0.61
1:B:342:VAL:HG22	1:B:348:ILE:HG12	1.82	0.60
1:E:233:LEU:HB2	1:E:242:THR:HG23	1.84	0.60
1:A:206:ILE:HD12	1:A:212:THR:O	2.02	0.59
1:B:442:PRO:HB3	1:B:522:ARG:HB2	1.85	0.59
1:D:619:GLU:OE2	1:D:636:ARG:NH1	2.28	0.59
1:B:96:LEU:HD21	1:B:128:LEU:HD22	1.85	0.59
1:G:614:PRO:HB2	1:G:616:GLU:HG3	1.85	0.58
1:A:455:TYR:CE2	1:A:475:PHE:HB2	2.39	0.57
1:C:305:MET:HG3	1:C:306:VAL:N	2.19	0.57
1:H:16:THR:HG23	4:H:711:GOL:H32	1.86	0.57
1:B:609:ARG:HD3	1:B:639:ASP:HA	1.86	0.57
1:E:552:ARG:HH11	5:E:715:ALA:N	2.02	0.57
1:E:386:VAL:HG22	1:E:393:LYS:HG2	1.86	0.57
1:B:656:ARG:NE	5:B:719:ALA:HB3	2.20	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:PHE:HZ	1:F:636:ARG:CZ	2.18	0.57
1:B:343:SER:HB2	7:B:952:HOH:O	2.04	0.57
1:G:358:LEU:HD11	1:G:372:ALA:HB1	1.86	0.57
1:H:653:ARG:HH12	6:H:713:FLC:CGC	2.15	0.56
1:C:41:LYS:HD3	4:C:709:GOL:H32	1.86	0.56
1:A:436:ASP:N	1:A:439:GLU:OE2	2.35	0.56
1:A:653:ARG:HH12	6:A:717:FLC:CAC	2.18	0.56
1:H:126:THR:HG23	1:H:127:PHE:HD1	1.70	0.56
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.71	0.56
1:H:390:ASP:OD1	1:H:391:GLY:N	2.39	0.56
1:A:50:ARG:HG3	1:A:69:ARG:NH2	2.20	0.56
4:F:712:GOL:HO3	4:F:712:GOL:HO1	1.52	0.56
1:D:50:ARG:HH11	1:D:69:ARG:CA	2.17	0.55
1:F:110:THR:HG22	1:F:184:ILE:HD13	1.88	0.55
1:F:653:ARG:HH12	4:F:708:GOL:H11	1.72	0.55
1:A:448:HIS:HB3	1:A:455:TYR:CZ	2.42	0.54
1:A:305:MET:HG3	1:A:306:VAL:N	2.21	0.54
1:B:177:LYS:HE2	2:B:703:SO4:O4	2.08	0.54
1:E:14:GLN:HB3	4:E:712:GOL:H12	1.88	0.54
1:C:448:HIS:HB3	1:C:455:TYR:CE2	2.43	0.54
1:D:596:LYS:NZ	7:D:806:HOH:O	2.40	0.53
1:E:572:LYS:HD3	1:E:577:CYS:HA	1.90	0.53
1:G:181:LEU:HD12	1:G:195:THR:HG21	1.91	0.53
1:F:395:ARG:HE	4:F:711:GOL:H32	1.73	0.53
1:E:242:THR:HG22	7:E:1065:HOH:O	2.09	0.53
1:A:664:PHE:O	1:A:668:LEU:HB2	2.09	0.52
1:D:385:ALA:HB3	1:D:394:THR:HG23	1.91	0.52
1:E:24:VAL:HG12	1:E:40:GLU:HG3	1.90	0.52
1:A:436:ASP:O	1:A:439:GLU:HG3	2.09	0.52
1:H:547:ALA:HB2	1:H:667:TYR:HB2	1.91	0.52
1:B:239:LYS:O	1:B:239:LYS:HG2	2.10	0.52
1:G:131:LEU:HD21	1:G:179:ALA:HB1	1.91	0.52
1:E:50:ARG:HD2	1:E:69:ARG:HA	1.90	0.52
1:F:447:ILE:HD13	1:F:534:MET:HG3	1.92	0.52
1:G:56:TRP:NE1	1:G:396:LEU:HD22	2.25	0.52
1:D:452:HIS:NE2	1:D:574:GLU:OE2	2.32	0.51
1:C:25:ARG:HD3	2:C:701:SO4:O2	2.10	0.51
1:D:450:GLY:O	4:D:712:GOL:H31	2.09	0.51
1:E:547:ALA:HB2	1:E:667:TYR:HB2	1.91	0.51
1:A:122:SER:HB2	1:A:127:PHE:CZ	2.46	0.51
1:C:395:ARG:HE	4:C:711:GOL:H2	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TRP:NE1	1:A:396:LEU:HD22	2.26	0.51
1:D:127:PHE:CD2	1:D:183:ARG:HG3	2.46	0.51
1:F:233:LEU:HB2	1:F:242:THR:CG2	2.38	0.51
1:A:552:ARG:HH11	5:A:716:ALA:N	2.09	0.51
1:H:65:TRP:HE3	1:H:99:LEU:HD21	1.76	0.51
1:D:593:LYS:HD3	1:D:594:TYR:CZ	2.45	0.51
1:F:614:PRO:HB2	1:F:616:GLU:HG3	1.93	0.50
1:F:82:GLU:HG2	1:F:83:ILE:HG13	1.93	0.50
1:F:127:PHE:CD2	1:F:183:ARG:HG3	2.46	0.50
1:F:572:LYS:NZ	7:F:807:HOH:O	2.44	0.50
1:A:455:TYR:CD2	1:A:475:PHE:HB2	2.46	0.50
1:D:55:ILE:HG13	1:D:65:TRP:CE2	2.46	0.50
1:E:15:GLY:H	4:E:712:GOL:H2	1.76	0.50
1:G:75:PRO:HA	1:G:85:ALA:O	2.11	0.50
1:E:455:TYR:CE2	1:E:475:PHE:HB2	2.47	0.50
1:C:539:VAL:HG23	1:C:598:MET:HG2	1.93	0.49
1:F:579:VAL:HG23	7:F:948:HOH:O	2.12	0.49
1:F:656:ARG:HE	5:F:713:ALA:CB	2.23	0.49
1:F:117:ARG:NH1	1:F:201:ILE:O	2.44	0.49
1:G:604:ILE:HD12	1:G:622:PHE:HB2	1.95	0.49
1:A:463:LEU:HD22	1:A:473:VAL:HG11	1.94	0.49
1:A:113:LYS:HA	1:A:144:GLU:HA	1.94	0.49
1:B:634:LEU:HB3	1:C:161:VAL:HB	1.95	0.49
1:G:127:PHE:CD1	1:G:183:ARG:HG3	2.48	0.49
1:D:402:ALA:O	1:D:406:GLU:HG3	2.13	0.49
1:D:579:VAL:HG22	1:D:586:LEU:HD12	1.95	0.48
1:E:440:LYS:HB3	1:E:519:ASP:HB2	1.93	0.48
1:G:432:PRO:HG2	1:G:435:LEU:HD22	1.95	0.48
1:H:658:ARG:HG2	1:H:658:ARG:HH11	1.78	0.48
1:C:245:THR:HG21	1:C:251:PHE:CE2	2.47	0.48
1:D:455:TYR:CE2	1:D:475:PHE:HB2	2.49	0.48
1:B:41:LYS:NZ	1:B:312:ASP:OD2	2.47	0.48
1:C:209:ASN:ND2	1:C:211:ARG:HD3	2.27	0.48
1:E:131:LEU:HD11	1:E:179:ALA:HB1	1.94	0.48
1:G:99:LEU:HD12	1:G:100:PRO:HD2	1.94	0.48
1:F:599:ARG:NH1	4:F:712:GOL:H32	2.27	0.48
1:E:368:GLN:NE2	7:E:815:HOH:O	2.47	0.48
1:C:44:ASP:HB3	1:C:50:ARG:HD2	1.95	0.47
1:E:78:SER:HB3	1:E:121:TRP:CZ2	2.49	0.47
1:B:364:HIS:CE1	1:B:367:GLU:HG3	2.49	0.47
5:D:714:ALA:N	7:D:811:HOH:O	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:HIS:HB3	1:D:455:TYR:CZ	2.49	0.47
1:G:181:LEU:HB2	1:G:195:THR:HG23	1.96	0.47
1:H:177:LYS:HE2	2:H:707:SO4:O3	2.13	0.47
1:D:96:LEU:HD21	1:D:128:LEU:HD22	1.96	0.47
1:F:616:GLU:O	1:F:620:GLN:HG3	2.14	0.47
1:A:309:THR:HA	6:A:717:FLC:HA2	1.96	0.47
1:C:318:PRO:HB2	1:C:327:LEU:HD22	1.95	0.47
1:C:614:PRO:HB2	1:C:616:GLU:HG3	1.97	0.47
1:D:126:THR:O	1:D:186:VAL:HG22	2.14	0.47
1:E:603:LEU:HD22	1:E:663:TRP:HB2	1.97	0.47
1:G:455:TYR:CD2	1:G:475:PHE:HB2	2.50	0.47
1:B:552:ARG:HH11	5:B:719:ALA:CB	2.14	0.47
1:D:123:PRO:HD2	7:D:999:HOH:O	2.14	0.47
2:F:706:SO4:O4	4:F:708:GOL:O3	2.24	0.47
1:C:127:PHE:CD2	1:C:183:ARG:HG3	2.49	0.47
1:G:18:LEU:HA	1:G:21:LEU:HG	1.96	0.47
1:A:351:VAL:HG12	1:A:352:ILE:HG13	1.97	0.46
1:G:358:LEU:CD1	1:G:372:ALA:HB1	2.44	0.46
1:H:61:SER:HB2	1:H:63:ARG:HE	1.81	0.46
1:B:666:ARG:HD2	1:B:666:ARG:O	2.14	0.46
1:C:570:PHE:CZ	1:C:574:GLU:HG3	2.50	0.46
1:H:68:GLY:HA3	1:H:70:TRP:CH2	2.50	0.46
1:A:198:GLU:HG3	1:A:201:ILE:HD11	1.98	0.46
1:D:542:THR:OG1	1:D:544:ARG:HG3	2.15	0.46
1:F:18:LEU:HB3	1:F:461:HIS:CE1	2.51	0.46
1:G:88:SER:OG	1:G:90:ARG:HG2	2.15	0.46
1:D:119:TYR:HA	1:D:129:ILE:O	2.16	0.46
1:F:552:ARG:HD3	5:F:713:ALA:HA	1.97	0.46
1:A:135:GLY:N	1:A:177:LYS:HG2	2.30	0.46
1:B:430:MET:HB2	1:B:473:VAL:HB	1.97	0.46
1:C:336:ARG:HD3	1:C:355:ASN:OD1	2.15	0.46
1:D:385:ALA:HB3	1:D:394:THR:CG2	2.46	0.46
1:E:448:HIS:HB3	1:E:455:TYR:CZ	2.50	0.46
1:G:455:TYR:CE2	1:G:475:PHE:HB2	2.51	0.46
1:A:614:PRO:HB2	1:A:616:GLU:HG3	1.97	0.46
1:C:554:ILE:HD13	1:C:557:TRP:CH2	2.51	0.46
1:B:455:TYR:CE2	1:B:475:PHE:HB2	2.51	0.45
1:D:656:ARG:HE	5:D:714:ALA:CB	2.24	0.45
1:G:283:PHE:CD2	1:G:290:LYS:HB3	2.51	0.45
1:G:547:ALA:HB2	1:G:667:TYR:HB2	1.98	0.45
1:H:609:ARG:HD2	7:H:987:HOH:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LEU:HD11	1:C:179:ALA:HB1	1.97	0.45
1:E:96:LEU:HD21	1:E:128:LEU:HD22	1.96	0.45
1:F:619:GLU:OE2	1:F:636:ARG:NH1	2.39	0.45
1:H:75:PRO:HA	1:H:85:ALA:O	2.16	0.45
1:C:273:LEU:HD13	1:C:573:TRP:CD1	2.52	0.45
1:D:664:PHE:O	1:D:668:LEU:HB2	2.17	0.45
1:G:449:GLY:HA2	1:G:530:TYR:HB3	1.98	0.45
1:A:25:ARG:HD3	2:A:701:SO4:O2	2.17	0.45
1:A:213:LEU:HB2	1:A:236:LEU:HD11	1.98	0.45
1:F:547:ALA:HB2	1:F:667:TYR:HB2	1.97	0.45
1:G:179:ALA:HB3	1:G:201:ILE:HG13	1.99	0.45
1:A:126:THR:O	1:A:186:VAL:HG22	2.17	0.45
1:C:293:LEU:HD11	1:C:344:LEU:HD23	1.98	0.45
1:D:558:LEU:HD23	1:D:579:VAL:HG13	1.98	0.45
1:G:236:LEU:HD23	1:G:236:LEU:HA	1.80	0.45
1:H:358:LEU:HD11	1:H:372:ALA:HB1	1.99	0.45
1:A:418:ARG:HG2	1:A:422:GLY:O	2.16	0.45
1:B:603:LEU:HB2	1:B:663:TRP:CD2	2.51	0.45
1:D:178:ARG:HD2	1:D:197:ARG:HB3	1.98	0.45
1:G:178:ARG:HD2	1:G:197:ARG:HB2	1.98	0.45
1:B:552:ARG:HD3	5:B:719:ALA:HA	1.99	0.45
1:B:558:LEU:HD12	1:B:558:LEU:H	1.81	0.45
1:C:350:PRO:HG3	1:F:353:GLU:OE1	2.16	0.45
1:D:572:LYS:HD2	1:D:577:CYS:HA	1.99	0.45
1:H:455:TYR:CE2	1:H:475:PHE:HB2	2.51	0.45
1:B:354:GLY:HA3	1:B:356:PHE:CE2	2.52	0.45
1:C:479:ARG:HA	1:C:488:PHE:CE2	2.52	0.45
1:A:570:PHE:CE2	1:A:574:GLU:HG3	2.51	0.44
1:G:603:LEU:HB2	1:G:663:TRP:CD2	2.52	0.44
1:C:616:GLU:O	1:C:620:GLN:HG3	2.16	0.44
1:A:644:LEU:HD12	1:A:648:GLY:HA3	1.98	0.44
1:B:626:LYS:NZ	7:B:808:HOH:O	2.36	0.44
1:G:73:MET:HE2	1:G:73:MET:HB3	1.91	0.44
1:C:113:LYS:HA	1:C:144:GLU:HA	1.99	0.44
1:D:219:ARG:NH2	1:D:241:GLU:OE1	2.50	0.44
1:F:522:ARG:HD2	1:F:668:LEU:O	2.16	0.44
1:C:177:LYS:HE2	2:C:707:SO4:O1	2.18	0.44
1:F:97:TRP:CH2	1:F:108:GLN:HB2	2.52	0.44
1:H:626:LYS:HA	1:H:626:LYS:HD2	1.83	0.44
1:D:96:LEU:HB3	1:D:110:THR:HG23	1.98	0.44
1:A:619:GLU:OE2	1:A:636:ARG:NH1	2.40	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:HIS:ND1	1:E:365:PRO:HD2	2.33	0.44
1:G:431:LYS:O	1:G:433:PRO:HD3	2.18	0.44
1:D:537:TRP:CE2	1:D:541:HIS:CE1	3.06	0.44
1:E:34:THR:O	1:E:58:ALA:HB2	2.18	0.44
1:E:55:ILE:HG13	1:E:65:TRP:CE2	2.53	0.44
1:B:318:PRO:HB3	1:B:329:VAL:HG12	2.00	0.43
1:F:318:PRO:HB2	1:F:327:LEU:HD22	1.99	0.43
1:C:111:PHE:O	1:C:143:ARG:HA	2.18	0.43
1:F:22:ARG:HD3	7:F:1026:HOH:O	2.19	0.43
1:G:96:LEU:HD23	1:G:109:LEU:HD23	2.00	0.43
1:F:97:TRP:CZ2	1:F:108:GLN:HB2	2.53	0.43
1:G:461:HIS:HD2	7:G:801:HOH:O	2.01	0.43
1:H:78:SER:HB3	1:H:121:TRP:CZ2	2.54	0.43
1:E:78:SER:HB3	1:E:121:TRP:CH2	2.54	0.43
1:F:448:HIS:HB3	1:F:455:TYR:CE2	2.52	0.43
1:B:455:TYR:CD2	1:B:475:PHE:HB2	2.54	0.43
1:B:448:HIS:HB3	1:B:455:TYR:CZ	2.53	0.43
1:H:156:LEU:HA	1:H:156:LEU:HD23	1.73	0.43
1:B:213:LEU:HB2	1:B:236:LEU:HD11	2.00	0.43
1:B:616:GLU:O	1:B:620:GLN:HG3	2.17	0.43
1:C:442:PRO:HB2	1:C:668:LEU:HD13	2.00	0.43
1:A:620:GLN:HA	1:H:562:GLY:HA3	2.01	0.43
1:D:370:ALA:HB2	1:D:388:LEU:HD21	2.01	0.43
1:C:442:PRO:HB3	1:C:522:ARG:HB3	2.01	0.43
1:E:99:LEU:HD12	1:E:100:PRO:HD2	2.01	0.43
1:E:448:HIS:HB3	1:E:455:TYR:CE2	2.54	0.43
1:B:656:ARG:HE	5:B:719:ALA:CB	2.31	0.42
1:H:181:LEU:HG	1:H:201:ILE:HD13	2.00	0.42
1:H:398:ARG:NH2	2:H:708:SO4:O3	2.51	0.42
1:A:56:TRP:HE1	1:A:396:LEU:HD22	1.84	0.42
1:A:320:TRP:CE2	1:A:327:LEU:HD21	2.54	0.42
1:F:509:ASP:OD2	1:F:544:ARG:NH2	2.53	0.42
1:G:509:ASP:OD1	1:G:544:ARG:NH1	2.51	0.42
1:B:131:LEU:HD11	1:B:179:ALA:HB1	2.01	0.42
1:F:178:ARG:HD2	7:F:1022:HOH:O	2.18	0.42
1:F:603:LEU:HB2	1:F:663:TRP:CD2	2.54	0.42
1:H:390:ASP:OD1	1:H:392:THR:HG23	2.20	0.42
1:H:390:ASP:CG	1:H:392:THR:HG23	2.39	0.42
1:H:658:ARG:HG2	1:H:658:ARG:NH1	2.34	0.42
1:A:122:SER:HB3	1:A:127:PHE:O	2.19	0.42
1:A:549:VAL:HG11	1:A:660:ILE:HG12	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:LEU:O	7:B:802:HOH:O	2.22	0.42
1:C:603:LEU:HB2	1:C:663:TRP:CD2	2.55	0.42
1:H:218:ASN:OD1	1:H:220:ASN:ND2	2.52	0.42
1:A:552:ARG:HD3	5:A:716:ALA:HB3	2.01	0.42
1:C:157:LYS:N	7:C:803:HOH:O	2.35	0.42
1:C:273:LEU:HD13	1:C:573:TRP:CG	2.55	0.42
1:D:50:ARG:HD3	1:D:69:ARG:HA	2.02	0.42
1:D:515:PHE:HB3	1:D:517:PHE:CE2	2.54	0.42
1:E:596:LYS:HB2	7:E:905:HOH:O	2.19	0.42
1:F:528:GLY:HA2	1:F:551:GLN:O	2.19	0.42
1:G:233:LEU:HG	1:G:244:LEU:HD23	2.01	0.42
1:A:427:GLY:HA2	1:A:476:THR:HA	2.01	0.42
1:C:155:ASP:HB3	7:C:1044:HOH:O	2.19	0.42
1:A:68:GLY:HA3	1:A:70:TRP:CH2	2.55	0.42
1:D:656:ARG:HD3	7:D:891:HOH:O	2.18	0.42
1:E:552:ARG:HD3	5:E:715:ALA:CB	2.49	0.42
1:F:516:ASP:OD1	7:F:801:HOH:O	2.21	0.42
1:G:528:GLY:HA2	1:G:551:GLN:O	2.19	0.42
1:G:616:GLU:O	1:G:620:GLN:HG3	2.20	0.42
1:H:245:THR:HG21	1:H:251:PHE:CE2	2.54	0.42
1:A:626:LYS:HA	1:A:626:LYS:HD2	1.87	0.42
1:B:609:ARG:NE	7:B:823:HOH:O	2.51	0.42
1:D:603:LEU:HD21	1:D:605:LEU:HD21	2.02	0.42
1:H:29:TYR:CZ	1:H:371:ILE:HG13	2.55	0.42
1:A:638:PRO:HD3	1:H:158:PRO:HA	2.02	0.42
1:D:190:LYS:HB3	1:D:190:LYS:HE2	1.75	0.42
1:G:25:ARG:HD3	2:G:704:SO4:O2	2.19	0.42
1:B:546:LYS:NZ	7:B:818:HOH:O	2.47	0.41
1:C:25:ARG:HG3	1:C:39:VAL:HB	2.01	0.41
1:F:514:LYS:HG2	1:F:515:PHE:CZ	2.55	0.41
1:G:386:VAL:HA	1:G:392:THR:O	2.19	0.41
1:G:596:LYS:HB2	7:G:828:HOH:O	2.19	0.41
1:G:644:LEU:HD12	1:G:648:GLY:HA3	2.02	0.41
1:H:145:GLU:HA	1:H:146:PRO:HD3	1.91	0.41
1:A:570:PHE:CZ	1:A:574:GLU:HG3	2.55	0.41
1:C:644:LEU:HD23	5:C:713:ALA:HB3	2.02	0.41
1:D:554:ILE:HD13	1:D:557:TRP:CH2	2.55	0.41
1:G:331:ALA:O	1:G:337:VAL:HA	2.21	0.41
1:E:577:CYS:SG	1:E:582:ASP:HB3	2.61	0.41
1:G:183:ARG:HB2	1:G:194:LEU:HD21	2.02	0.41
1:B:333:GLU:HG2	7:B:1087:HOH:O	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:HIS:ND1	1:B:365:PRO:HD2	2.36	0.41
1:H:358:LEU:CD1	1:H:372:ALA:HB1	2.49	0.41
1:B:551:GLN:O	1:B:552:ARG:C	2.58	0.41
5:C:713:ALA:HB1	7:C:930:HOH:O	2.21	0.41
1:E:98:LEU:HD11	1:E:109:LEU:HD22	2.03	0.41
1:E:554:ILE:HD13	1:E:557:TRP:CH2	2.56	0.41
1:C:177:LYS:HB2	2:C:707:SO4:O1	2.20	0.41
1:E:58:ALA:C	1:E:60:GLY:H	2.22	0.41
1:E:454:MET:HG2	1:E:455:TYR:O	2.21	0.41
1:F:28:HIS:HB3	7:F:923:HOH:O	2.20	0.41
1:H:198:GLU:OE2	1:H:219:ARG:NH2	2.53	0.41
1:A:646:ARG:O	6:A:717:FLC:HA1	2.21	0.41
1:D:620:GLN:HA	1:G:562:GLY:HA3	2.01	0.41
1:E:455:TYR:CD2	1:E:475:PHE:HB2	2.55	0.41
1:E:585:ARG:O	1:E:589:HIS:HD2	2.03	0.41
1:G:279:ARG:NH1	1:G:297:TRP:O	2.53	0.41
1:A:603:LEU:HB2	1:A:663:TRP:CD2	2.56	0.41
1:D:577:CYS:SG	1:D:582:ASP:HB3	2.61	0.41
1:F:656:ARG:CD	5:F:713:ALA:HB3	2.50	0.41
1:H:354:GLY:HA3	1:H:356:PHE:CE2	2.56	0.41
1:C:528:GLY:HA2	1:C:551:GLN:O	2.20	0.41
1:D:532:GLY:HA3	1:D:553:SER:HB3	2.03	0.41
1:E:320:TRP:CE2	1:E:327:LEU:HD21	2.56	0.41
1:H:328:TYR:HB3	1:H:339:LEU:HD11	2.03	0.41
1:H:411:ASP:OD1	1:H:412:ALA:N	2.50	0.41
1:B:533:PHE:HB2	1:B:554:ILE:HB	2.01	0.41
1:C:352:ILE:CG1	1:C:386:VAL:HG11	2.51	0.41
1:G:59:ASP:OD1	1:G:59:ASP:C	2.59	0.41
1:A:119:TYR:HA	1:A:129:ILE:O	2.22	0.40
1:B:657:LEU:HD23	1:B:657:LEU:HA	1.91	0.40
1:E:64:GLN:NE2	1:E:66:THR:O	2.48	0.40
1:G:103:GLY:HA2	7:G:820:HOH:O	2.21	0.40
1:G:359:TYR:CZ	1:G:373:ALA:HB1	2.56	0.40
1:G:499:MET:HE1	1:G:502:GLU:HB2	2.03	0.40
1:A:308:ASP:HA	1:A:646:ARG:HG2	2.04	0.40
1:C:596:LYS:HB2	1:C:596:LYS:HE2	1.88	0.40
1:G:273:LEU:HD13	1:G:573:TRP:CD1	2.56	0.40
1:H:139:THR:HG23	1:H:141:GLU:N	2.25	0.40
1:A:11:LEU:O	1:A:408:VAL:HG23	2.21	0.40
1:A:93:ARG:HH11	1:A:93:ARG:CG	2.35	0.40
1:C:233:LEU:O	1:C:241:GLU:HA	2.20	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:493:ARG:HD2	1:F:573:TRP:O	2.21	0.40
1:G:25:ARG:NH2	4:G:707:GOL:H32	2.35	0.40
1:G:134:LEU:HD11	1:G:140:ILE:HG22	2.02	0.40
1:A:385:ALA:O	1:A:393:LYS:HA	2.21	0.40
1:B:119:TYR:HA	1:B:129:ILE:O	2.21	0.40
1:B:554:ILE:HD13	1:B:557:TRP:CH2	2.56	0.40
1:C:504:ILE:O	1:C:508:VAL:HG23	2.21	0.40
1:E:528:GLY:HA2	1:E:551:GLN:O	2.21	0.40
1:H:278:HIS:CG	1:H:300:HIS:HE1	2.39	0.40
1:D:112:PHE:HB3	7:D:867:HOH:O	2.22	0.40
1:E:442:PRO:HB3	1:E:522:ARG:HB3	2.03	0.40
1:E:614:PRO:HB2	1:E:616:GLU:HG3	2.02	0.40
1:E:634:LEU:HB3	1:F:161:VAL:HB	2.03	0.40
1:F:514:LYS:HG2	1:F:515:PHE:CE1	2.57	0.40
1:G:283:PHE:CE2	1:G:290:LYS:HD3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	646/691 (94%)	623 (96%)	23 (4%)	0	100	100
1	B	646/691 (94%)	631 (98%)	15 (2%)	0	100	100
1	C	647/691 (94%)	631 (98%)	16 (2%)	0	100	100
1	D	643/691 (93%)	623 (97%)	20 (3%)	0	100	100
1	E	646/691 (94%)	631 (98%)	15 (2%)	0	100	100
1	F	643/691 (93%)	627 (98%)	16 (2%)	0	100	100
1	G	641/691 (93%)	621 (97%)	20 (3%)	0	100	100
1	H	645/691 (93%)	620 (96%)	25 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5157/5528 (93%)	5007 (97%)	150 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/568 (90%)	500 (98%)	9 (2%)	59	63
1	B	509/568 (90%)	504 (99%)	5 (1%)	76	81
1	C	507/568 (89%)	499 (98%)	8 (2%)	62	67
1	D	504/568 (89%)	494 (98%)	10 (2%)	55	58
1	E	505/568 (89%)	494 (98%)	11 (2%)	52	55
1	F	496/568 (87%)	487 (98%)	9 (2%)	59	63
1	G	469/568 (83%)	458 (98%)	11 (2%)	50	53
1	H	486/568 (86%)	475 (98%)	11 (2%)	50	53
All	All	3985/4544 (88%)	3911 (98%)	74 (2%)	57	61

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	73	MET
1	A	118	ASP
1	A	122	SER
1	A	327	LEU
1	A	460	PHE
1	A	529	SER
1	A	533	PHE
1	A	561	SER
1	B	117	ARG
1	B	343	SER
1	B	387	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	434	GLU
1	B	460	PHE
1	C	13	PHE
1	C	178	ARG
1	C	279	ARG
1	C	327	LEU
1	C	432	PRO
1	C	460	PHE
1	C	468	SER
1	C	599	ARG
1	D	13	PHE
1	D	73	MET
1	D	93	ARG
1	D	122	SER
1	D	137	ASP
1	D	186	VAL
1	D	387	SER
1	D	460	PHE
1	D	468	SER
1	D	606	HIS
1	E	13	PHE
1	E	25	ARG
1	E	62	VAL
1	E	93	ARG
1	E	186	VAL
1	E	236	LEU
1	E	242	THR
1	E	460	PHE
1	E	513	SER
1	E	572	LYS
1	E	626	LYS
1	F	11	LEU
1	F	13	PHE
1	F	48	GLN
1	F	118	ASP
1	F	322	SER
1	F	343	SER
1	F	434	GLU
1	F	460	PHE
1	F	468	SER
1	G	13	PHE
1	G	23	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	35	ARG
1	G	59	ASP
1	G	73	MET
1	G	118	ASP
1	G	289	THR
1	G	327	LEU
1	G	363	ILE
1	G	398	ARG
1	G	460	PHE
1	H	23	SER
1	H	25	ARG
1	H	50	ARG
1	H	107	ARG
1	H	122	SER
1	H	171	SER
1	H	278	HIS
1	H	398	ARG
1	H	460	PHE
1	H	529	SER
1	H	579	VAL

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

Mol	Chain	Res	Type
1	A	368	GLN
1	B	28	HIS
1	E	14	GLN
1	E	48	GLN
1	G	28	HIS
1	H	278	HIS
1	H	300	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 14 are monoatomic - leaving 99 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	G	703	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	B	706	-	4,4,4	0.16	0	6,6,6	0.21	0
4	GOL	C	709	-	5,5,5	0.91	0	5,5,5	0.81	0
4	GOL	F	712	-	5,5,5	1.09	0	5,5,5	0.83	0
4	GOL	B	718	-	5,5,5	1.02	0	5,5,5	1.08	0
2	SO4	H	709	-	4,4,4	0.22	0	6,6,6	0.14	0
5	ALA	G	709	-	5,5,5	1.10	1 (20%)	6,6,6	1.65	2 (33%)
2	SO4	G	704	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	A	702	3	4,4,4	0.14	0	6,6,6	0.49	0
4	GOL	G	707	-	5,5,5	0.59	0	5,5,5	1.42	1 (20%)
5	ALA	E	715	-	5,5,5	1.73	1 (20%)	6,6,6	1.07	1 (16%)
2	SO4	C	707	-	4,4,4	0.14	0	6,6,6	0.28	0
6	FLC	A	717	-	12,12,12	2.06	5 (41%)	17,17,17	2.52	7 (41%)
2	SO4	H	707	-	4,4,4	0.19	0	6,6,6	0.14	0
4	GOL	D	710	-	5,5,5	0.97	0	5,5,5	1.15	1 (20%)
2	SO4	G	701	-	4,4,4	0.15	0	6,6,6	0.50	0
2	SO4	A	708	-	4,4,4	0.11	0	6,6,6	0.27	0
2	SO4	C	701	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	G	702	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	A	706	-	4,4,4	0.15	0	6,6,6	0.36	0
4	GOL	E	713	-	5,5,5	0.63	0	5,5,5	1.10	0
2	SO4	C	706	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	B	710	-	4,4,4	0.18	0	6,6,6	0.21	0
2	SO4	C	705	-	4,4,4	0.15	0	6,6,6	0.09	0
4	GOL	C	710	-	5,5,5	1.28	1 (20%)	5,5,5	1.10	0
2	SO4	D	707	-	4,4,4	0.28	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	H	708	-	4,4,4	0.11	0	6,6,6	0.18	0
2	SO4	D	701	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	B	711	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	H	704	-	4,4,4	0.14	0	6,6,6	0.15	0
4	GOL	E	712	-	5,5,5	0.82	0	5,5,5	1.21	0
2	SO4	E	709	-	4,4,4	0.28	0	6,6,6	0.30	0
5	ALA	A	716	3	5,5,5	1.94	2 (40%)	6,6,6	1.60	1 (16%)
2	SO4	E	707	-	4,4,4	0.13	0	6,6,6	0.28	0
2	SO4	E	702	-	4,4,4	0.15	0	6,6,6	0.32	0
2	SO4	A	704	-	4,4,4	0.20	0	6,6,6	0.27	0
2	SO4	F	704	-	4,4,4	0.16	0	6,6,6	0.27	0
5	ALA	B	719	-	5,5,5	1.53	2 (40%)	6,6,6	1.64	2 (33%)
2	SO4	H	703	-	4,4,4	0.15	0	6,6,6	0.21	0
2	SO4	D	705	-	4,4,4	0.27	0	6,6,6	0.24	0
2	SO4	E	703	-	4,4,4	0.17	0	6,6,6	0.27	0
2	SO4	H	702	-	4,4,4	0.18	0	6,6,6	0.31	0
2	SO4	B	704	-	4,4,4	0.23	0	6,6,6	0.14	0
2	SO4	B	702	-	4,4,4	0.14	0	6,6,6	0.28	0
2	SO4	F	702	-	4,4,4	0.11	0	6,6,6	0.46	0
2	SO4	E	708	-	4,4,4	0.13	0	6,6,6	0.57	0
4	GOL	F	711	-	5,5,5	0.81	0	5,5,5	1.08	0
2	SO4	B	712	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	B	709	3	4,4,4	0.13	0	6,6,6	0.29	0
2	SO4	B	708	-	4,4,4	0.16	0	6,6,6	0.07	0
4	GOL	G	708	-	5,5,5	0.82	0	5,5,5	1.13	0
5	ALA	C	713	-	5,5,5	1.39	1 (20%)	6,6,6	1.55	2 (33%)
2	SO4	B	703	-	4,4,4	0.18	0	6,6,6	0.31	0
2	SO4	D	702	-	4,4,4	0.13	0	6,6,6	0.30	0
4	GOL	E	714	-	5,5,5	0.75	0	5,5,5	0.98	0
4	GOL	F	709	-	5,5,5	0.96	0	5,5,5	0.97	0
2	SO4	E	704	-	4,4,4	0.23	0	6,6,6	0.35	0
2	SO4	G	705	-	4,4,4	0.17	0	6,6,6	0.21	0
5	ALA	F	713	-	5,5,5	1.68	2 (40%)	6,6,6	1.48	2 (33%)
2	SO4	D	708	-	4,4,4	0.13	0	6,6,6	0.20	0
6	FLC	H	713	-	12,12,12	1.95	6 (50%)	17,17,17	2.36	6 (35%)
4	GOL	D	713	-	5,5,5	0.96	0	5,5,5	0.93	0
2	SO4	F	705	-	4,4,4	0.19	0	6,6,6	0.22	0
4	GOL	B	717	-	5,5,5	1.21	1 (20%)	5,5,5	1.13	1 (20%)
2	SO4	H	701	-	4,4,4	0.14	0	6,6,6	0.31	0
2	SO4	C	704	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	F	707	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	D	704	-	4,4,4	0.19	0	6,6,6	0.19	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	E	706	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	H	705	-	4,4,4	0.31	0	6,6,6	0.17	0
2	SO4	E	701	-	4,4,4	0.18	0	6,6,6	0.35	0
2	SO4	C	703	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	B	701	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	F	701	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	D	703	-	4,4,4	0.24	0	6,6,6	0.27	0
4	GOL	D	712	-	5,5,5	0.87	0	5,5,5	0.97	0
2	SO4	F	706	-	4,4,4	0.29	0	6,6,6	0.13	0
4	GOL	A	714	-	5,5,5	0.88	0	5,5,5	1.15	1 (20%)
2	SO4	A	703	-	4,4,4	0.11	0	6,6,6	0.27	0
4	GOL	C	712	-	5,5,5	0.85	0	5,5,5	1.03	0
2	SO4	A	707	-	4,4,4	0.13	0	6,6,6	0.31	0
2	SO4	H	706	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	C	702	-	4,4,4	0.15	0	6,6,6	0.34	0
4	GOL	F	708	-	5,5,5	0.98	0	5,5,5	0.94	0
4	GOL	H	711	-	5,5,5	0.77	0	5,5,5	1.10	0
2	SO4	A	701	-	4,4,4	0.34	0	6,6,6	0.27	0
4	GOL	A	713	-	5,5,5	1.36	1 (20%)	5,5,5	0.73	0
5	ALA	D	714	-	5,5,5	2.05	2 (40%)	6,6,6	1.34	2 (33%)
2	SO4	F	703	3	4,4,4	0.17	0	6,6,6	0.16	0
5	ALA	H	712	-	5,5,5	1.32	1 (20%)	6,6,6	1.10	1 (16%)
2	SO4	E	705	-	4,4,4	0.15	0	6,6,6	0.42	0
2	SO4	A	705	-	4,4,4	0.18	0	6,6,6	0.31	0
2	SO4	D	706	-	4,4,4	0.24	0	6,6,6	0.32	0
4	GOL	D	711	-	5,5,5	1.05	0	5,5,5	1.19	0
2	SO4	B	707	-	4,4,4	0.18	0	6,6,6	0.23	0
4	GOL	F	710	-	5,5,5	1.00	0	5,5,5	0.99	0
4	GOL	A	715	-	5,5,5	1.20	1 (20%)	5,5,5	1.02	0
4	GOL	C	711	-	5,5,5	0.96	0	5,5,5	0.89	0
2	SO4	B	705	-	4,4,4	0.15	0	6,6,6	0.25	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
4	GOL	C	710	-	-	2/4/4/4	-
4	GOL	D	712	-	-	2/4/4/4	-
4	GOL	A	714	-	-	4/4/4/4	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	709	-	-	3/4/4/4	-
4	GOL	G	708	-	-	4/4/4/4	-
4	GOL	F	712	-	-	0/4/4/4	-
4	GOL	B	718	-	-	0/4/4/4	-
4	GOL	C	712	-	-	2/4/4/4	-
5	ALA	C	713	-	-	4/4/4/4	-
5	ALA	G	709	-	-	4/4/4/4	-
4	GOL	F	708	-	-	4/4/4/4	-
4	GOL	H	711	-	-	4/4/4/4	-
4	GOL	E	712	-	-	3/4/4/4	-
4	GOL	G	707	-	-	4/4/4/4	-
4	GOL	E	714	-	-	4/4/4/4	-
5	ALA	A	716	3	-	0/4/4/4	-
5	ALA	E	715	-	-	4/4/4/4	-
4	GOL	A	713	-	-	0/4/4/4	-
4	GOL	F	709	-	-	4/4/4/4	-
5	ALA	D	714	-	-	3/4/4/4	-
5	ALA	B	719	-	-	0/4/4/4	-
5	ALA	F	713	-	-	3/4/4/4	-
6	FLC	A	717	-	-	8/16/16/16	-
6	FLC	H	713	-	-	9/16/16/16	-
4	GOL	D	713	-	-	2/4/4/4	-
5	ALA	H	712	-	-	2/4/4/4	-
4	GOL	B	717	-	-	2/4/4/4	-
4	GOL	D	710	-	-	2/4/4/4	-
4	GOL	D	711	-	-	2/4/4/4	-
4	GOL	F	710	-	-	4/4/4/4	-
4	GOL	A	715	-	-	4/4/4/4	-
4	GOL	C	711	-	-	3/4/4/4	-
4	GOL	E	713	-	-	2/4/4/4	-
4	GOL	F	711	-	-	2/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	717	FLC	OA1-CAC	3.30	1.33	1.22

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	714	ALA	CA-C	-3.29	1.50	1.54
6	A	717	FLC	CA-CB	3.13	1.57	1.53
6	H	713	FLC	OA1-CAC	3.06	1.32	1.22
6	A	717	FLC	OB1-CBC	2.98	1.31	1.22
6	H	713	FLC	OG1-CGC	2.95	1.31	1.22
6	H	713	FLC	OB1-CBC	2.89	1.31	1.22
5	A	716	ALA	OXT-C	-2.85	1.21	1.30
5	D	714	ALA	OXT-C	-2.75	1.21	1.30
6	H	713	FLC	OG2-CGC	-2.66	1.21	1.30
6	A	717	FLC	OG1-CGC	2.66	1.31	1.22
5	A	716	ALA	CA-C	-2.53	1.51	1.54
6	A	717	FLC	OG2-CGC	-2.53	1.22	1.30
4	C	710	GOL	O2-C2	-2.46	1.36	1.43
6	H	713	FLC	OA2-CAC	-2.43	1.22	1.30
5	B	719	ALA	CB-CA	-2.39	1.43	1.52
5	E	715	ALA	OXT-C	-2.39	1.22	1.30
5	F	713	ALA	OXT-C	-2.33	1.22	1.30
5	F	713	ALA	CB-CA	-2.29	1.43	1.52
4	B	717	GOL	O2-C2	-2.25	1.36	1.43
4	A	715	GOL	O2-C2	-2.24	1.36	1.43
5	C	713	ALA	OXT-C	-2.23	1.23	1.30
4	A	713	GOL	C1-C2	2.16	1.60	1.51
5	H	712	ALA	OXT-C	-2.15	1.23	1.30
5	B	719	ALA	OXT-C	-2.14	1.23	1.30
6	H	713	FLC	OB2-CBC	-2.08	1.22	1.30
5	G	709	ALA	OXT-C	-2.03	1.23	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	717	FLC	OB1-CBC-CB	-6.06	113.67	122.25
6	H	713	FLC	OB1-CBC-CB	-6.00	113.76	122.25
6	H	713	FLC	OB2-CBC-CB	5.39	122.41	113.05
6	A	717	FLC	OB2-CBC-CB	5.01	121.75	113.05
5	G	709	ALA	OXT-C-O	-3.34	116.50	124.09
5	A	716	ALA	OXT-C-O	-3.31	116.58	124.09
6	A	717	FLC	OA1-CAC-CA	-3.30	113.31	122.94
6	A	717	FLC	OG1-CGC-CG	-3.07	113.96	122.94
5	C	713	ALA	OXT-C-O	-3.05	117.15	124.09
6	A	717	FLC	OA2-CAC-CA	2.87	123.56	114.35
5	B	719	ALA	OXT-C-O	-2.86	117.59	124.09
4	G	707	GOL	C3-C2-C1	-2.83	100.70	111.70

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	717	FLC	OG2-CGC-CG	2.82	123.42	114.35
6	H	713	FLC	OA1-CAC-CA	-2.74	114.93	122.94
6	H	713	FLC	OG2-CGC-CG	2.51	122.41	114.35
5	D	714	ALA	OXT-C-O	-2.40	118.64	124.09
5	H	712	ALA	OXT-C-O	-2.40	118.64	124.09
5	F	713	ALA	OXT-C-CA	2.39	122.70	114.06
6	H	713	FLC	OA2-CAC-CA	2.36	121.92	114.35
6	H	713	FLC	OG1-CGC-CG	-2.35	116.06	122.94
5	F	713	ALA	OXT-C-O	-2.26	118.97	124.09
5	G	709	ALA	OXT-C-CA	2.21	122.05	114.06
5	E	715	ALA	OXT-C-O	-2.14	119.24	124.09
4	D	710	GOL	C3-C2-C1	-2.13	103.43	111.70
5	B	719	ALA	C-CA-N	2.12	115.54	107.60
5	C	713	ALA	OXT-C-CA	2.12	121.71	114.06
5	D	714	ALA	OXT-C-CA	2.09	121.62	114.06
6	A	717	FLC	CB-CA-CAC	2.08	118.85	113.81
4	B	717	GOL	C3-C2-C1	-2.04	103.78	111.70
4	A	714	GOL	C3-C2-C1	-2.00	103.91	111.70

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	715	GOL	O1-C1-C2-C3
4	A	715	GOL	C1-C2-C3-O3
4	B	717	GOL	O1-C1-C2-C3
4	C	710	GOL	O1-C1-C2-C3
4	C	712	GOL	O1-C1-C2-C3
4	D	711	GOL	C1-C2-C3-O3
4	D	712	GOL	O1-C1-C2-O2
4	D	712	GOL	O1-C1-C2-C3
4	E	713	GOL	C1-C2-C3-O3
4	E	714	GOL	C1-C2-C3-O3
4	F	708	GOL	O1-C1-C2-C3
4	F	708	GOL	C1-C2-C3-O3
4	F	708	GOL	O2-C2-C3-O3
4	F	711	GOL	O1-C1-C2-C3
4	G	707	GOL	O1-C1-C2-C3
4	G	708	GOL	O1-C1-C2-C3
4	G	708	GOL	C1-C2-C3-O3
4	G	708	GOL	O2-C2-C3-O3
5	C	713	ALA	O-C-CA-N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	714	ALA	OXT-C-CA-N
5	D	714	ALA	OXT-C-CA-CB
5	E	715	ALA	O-C-CA-N
5	E	715	ALA	OXT-C-CA-N
5	G	709	ALA	OXT-C-CA-N
6	A	717	FLC	CA-CB-CBC-OB1
6	A	717	FLC	CA-CB-CBC-OB2
6	A	717	FLC	OHB-CB-CBC-OB1
6	A	717	FLC	OHB-CB-CBC-OB2
6	H	713	FLC	CAC-CA-CB-CBC
6	H	713	FLC	CAC-CA-CB-CG
6	H	713	FLC	CA-CB-CBC-OB1
6	H	713	FLC	CA-CB-CBC-OB2
6	H	713	FLC	OHB-CB-CBC-OB1
6	H	713	FLC	OHB-CB-CBC-OB2
4	A	714	GOL	O2-C2-C3-O3
6	H	713	FLC	CAC-CA-CB-OHB
4	A	714	GOL	O1-C1-C2-C3
4	A	714	GOL	C1-C2-C3-O3
4	C	709	GOL	C1-C2-C3-O3
4	C	711	GOL	C1-C2-C3-O3
4	E	712	GOL	C1-C2-C3-O3
4	E	714	GOL	O1-C1-C2-C3
4	F	709	GOL	O1-C1-C2-C3
4	F	710	GOL	O1-C1-C2-C3
4	F	710	GOL	C1-C2-C3-O3
4	G	707	GOL	C1-C2-C3-O3
4	H	711	GOL	O1-C1-C2-C3
4	H	711	GOL	C1-C2-C3-O3
4	A	715	GOL	O1-C1-C2-O2
4	A	715	GOL	O2-C2-C3-O3
4	B	717	GOL	O1-C1-C2-O2
4	C	710	GOL	O1-C1-C2-O2
4	F	709	GOL	O1-C1-C2-O2
4	G	707	GOL	O1-C1-C2-O2
4	H	711	GOL	O1-C1-C2-O2
4	H	711	GOL	O2-C2-C3-O3
5	C	713	ALA	OXT-C-CA-N
6	A	717	FLC	CAC-CA-CB-CG
5	C	713	ALA	O-C-CA-CB
5	C	713	ALA	OXT-C-CA-CB
5	D	714	ALA	O-C-CA-CB

*Continued on next page...*

*Continued from previous page...*

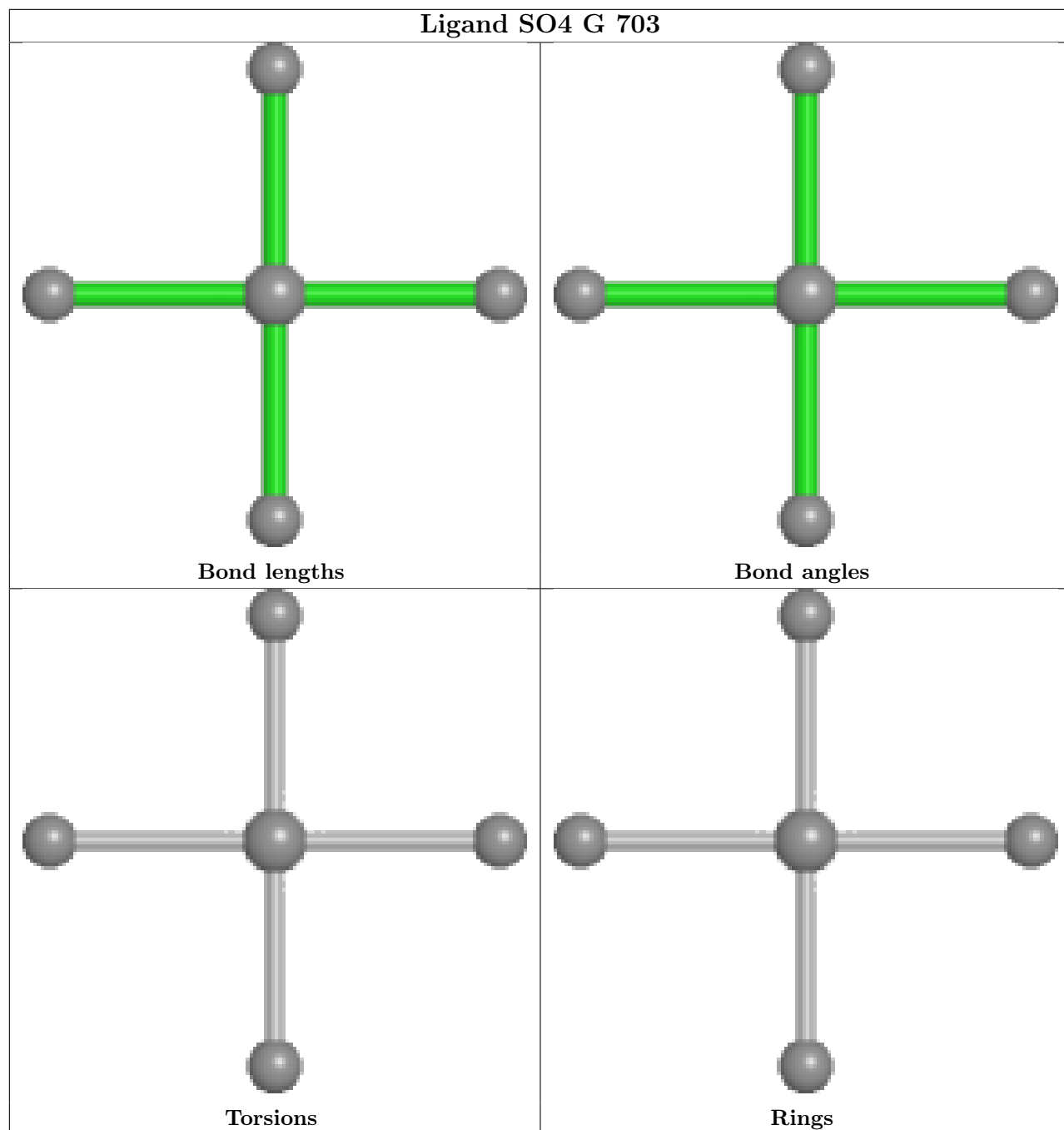
Mol	Chain	Res	Type	Atoms
5	E	715	ALA	O-C-CA-CB
5	E	715	ALA	OXT-C-CA-CB
4	D	711	GOL	O2-C2-C3-O3
4	F	708	GOL	O1-C1-C2-O2
4	F	710	GOL	O1-C1-C2-O2
4	F	710	GOL	O2-C2-C3-O3
4	F	711	GOL	O1-C1-C2-O2
6	H	713	FLC	CG-CB-CBC-OB1
6	H	713	FLC	CG-CB-CBC-OB2
4	A	714	GOL	O1-C1-C2-O2
4	C	709	GOL	O1-C1-C2-O2
4	C	711	GOL	O2-C2-C3-O3
4	D	713	GOL	O2-C2-C3-O3
4	E	714	GOL	O2-C2-C3-O3
4	F	709	GOL	O2-C2-C3-O3
5	H	712	ALA	OXT-C-CA-N
6	A	717	FLC	CAC-CA-CB-CBC
5	H	712	ALA	O-C-CA-N
5	F	713	ALA	OXT-C-CA-CB
5	G	709	ALA	O-C-CA-CB
5	G	709	ALA	OXT-C-CA-CB
4	C	712	GOL	O1-C1-C2-O2
4	E	713	GOL	O2-C2-C3-O3
4	G	707	GOL	O2-C2-C3-O3
4	G	708	GOL	O1-C1-C2-O2
6	A	717	FLC	CAC-CA-CB-OHB
4	E	712	GOL	O1-C1-C2-C3
4	E	712	GOL	O2-C2-C3-O3
4	D	710	GOL	C1-C2-C3-O3
4	D	713	GOL	C1-C2-C3-O3
5	F	713	ALA	O-C-CA-CB
4	C	709	GOL	O2-C2-C3-O3
4	D	710	GOL	O2-C2-C3-O3
4	E	714	GOL	O1-C1-C2-O2
6	A	717	FLC	CA-CB-CG-CGC
4	F	709	GOL	C1-C2-C3-O3
5	G	709	ALA	O-C-CA-N
5	F	713	ALA	OXT-C-CA-N
4	C	711	GOL	O1-C1-C2-O2

There are no ring outliers.

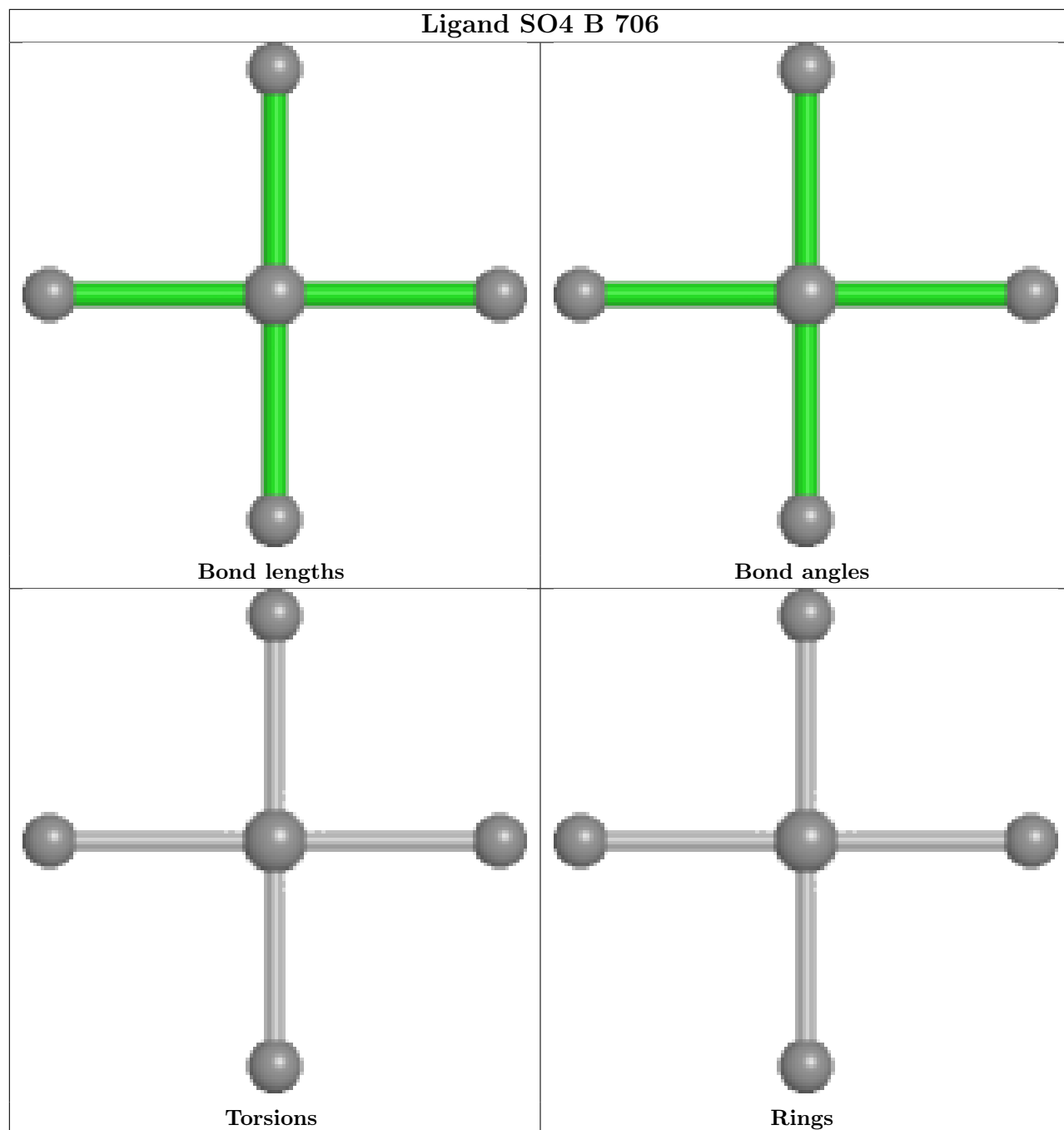
28 monomers are involved in 64 short contacts:

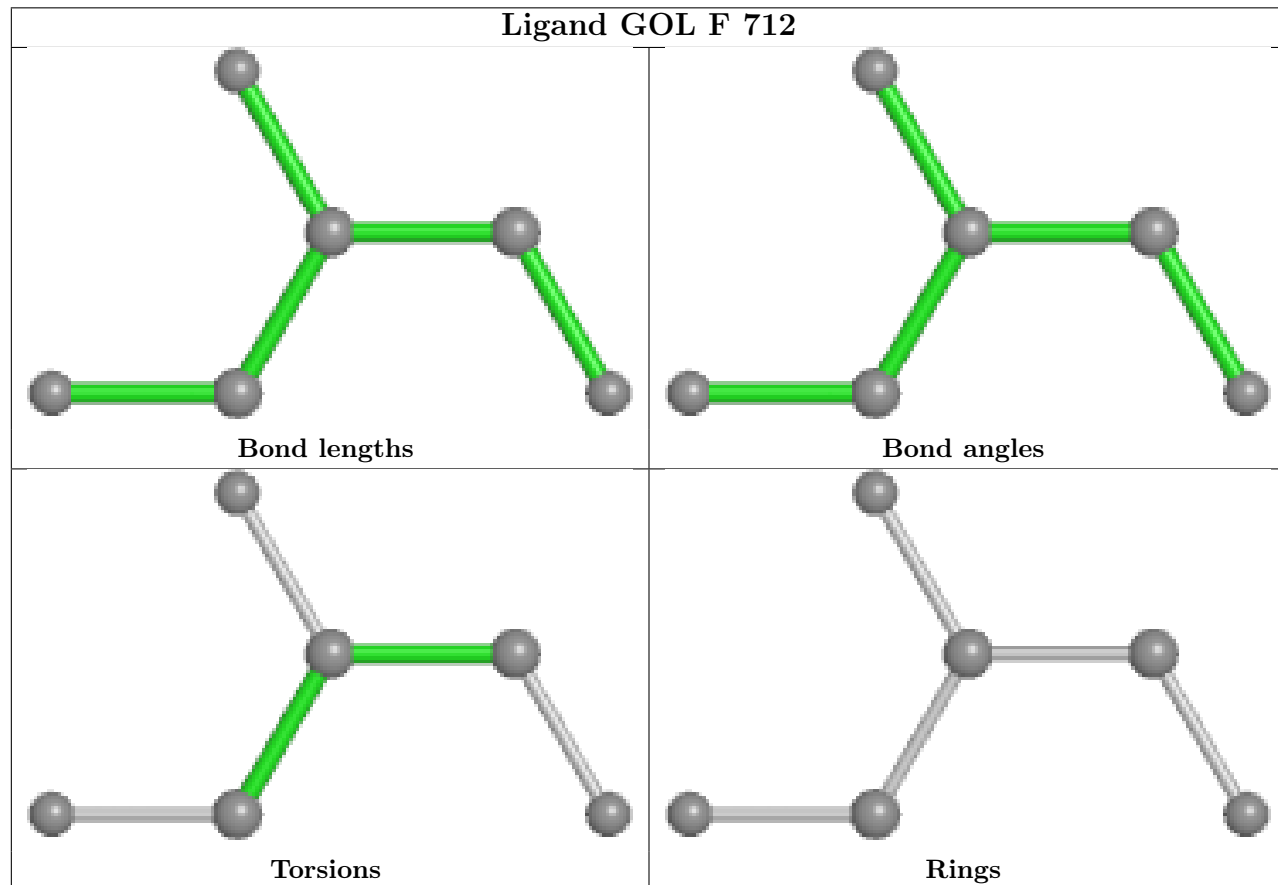
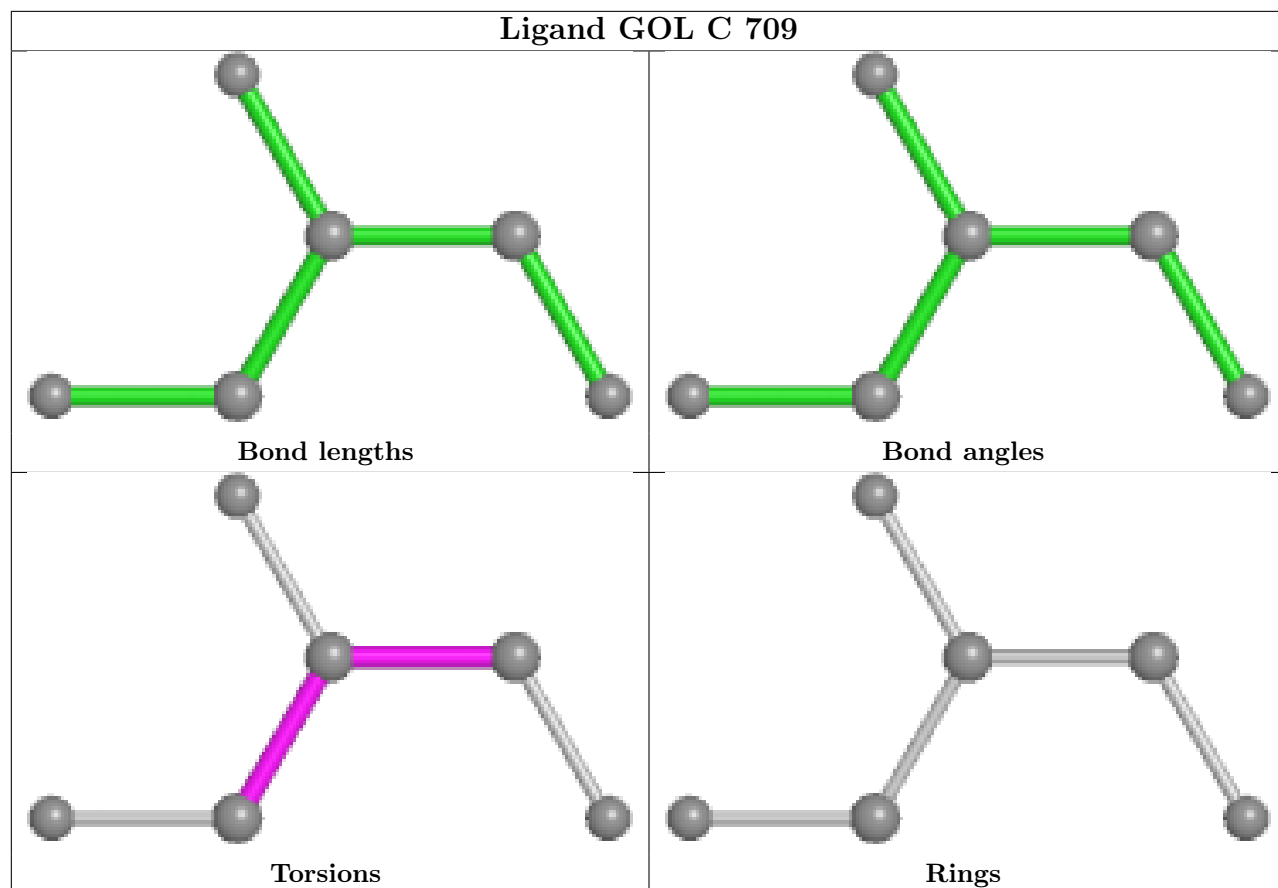
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	709	GOL	1	0
4	F	712	GOL	3	0
2	G	704	SO4	1	0
4	G	707	GOL	1	0
5	E	715	ALA	4	0
2	C	707	SO4	2	0
6	A	717	FLC	3	0
2	H	707	SO4	1	0
2	C	701	SO4	1	0
2	H	708	SO4	1	0
4	E	712	GOL	2	0
5	A	716	ALA	4	0
5	B	719	ALA	8	0
4	F	711	GOL	2	0
2	B	709	SO4	1	0
5	C	713	ALA	2	0
2	B	703	SO4	1	0
5	F	713	ALA	8	0
6	H	713	FLC	2	0
4	D	712	GOL	1	0
2	F	706	SO4	1	0
4	F	708	GOL	2	0
4	H	711	GOL	1	0
2	A	701	SO4	1	0
5	D	714	ALA	7	0
2	D	706	SO4	1	0
4	F	710	GOL	1	0
4	C	711	GOL	2	0

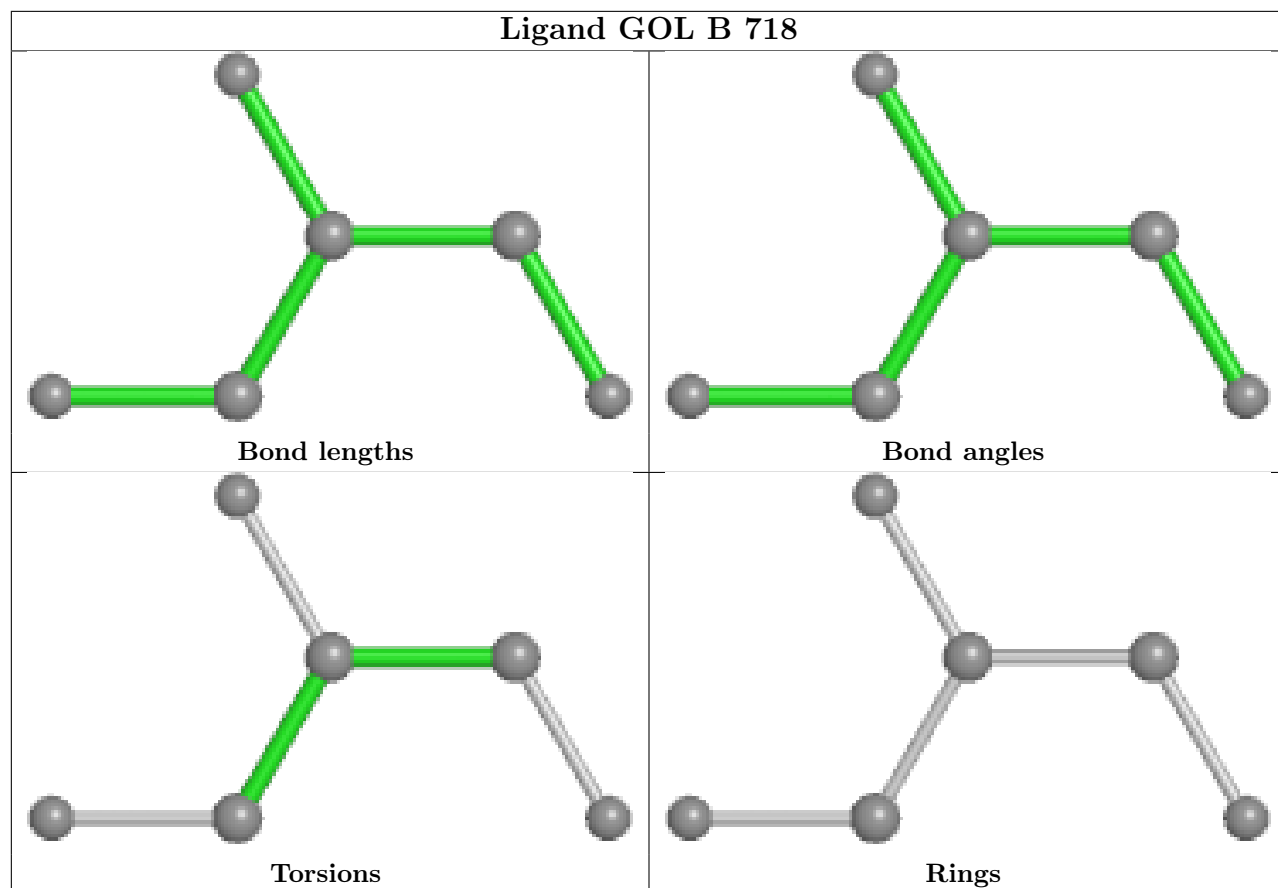
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

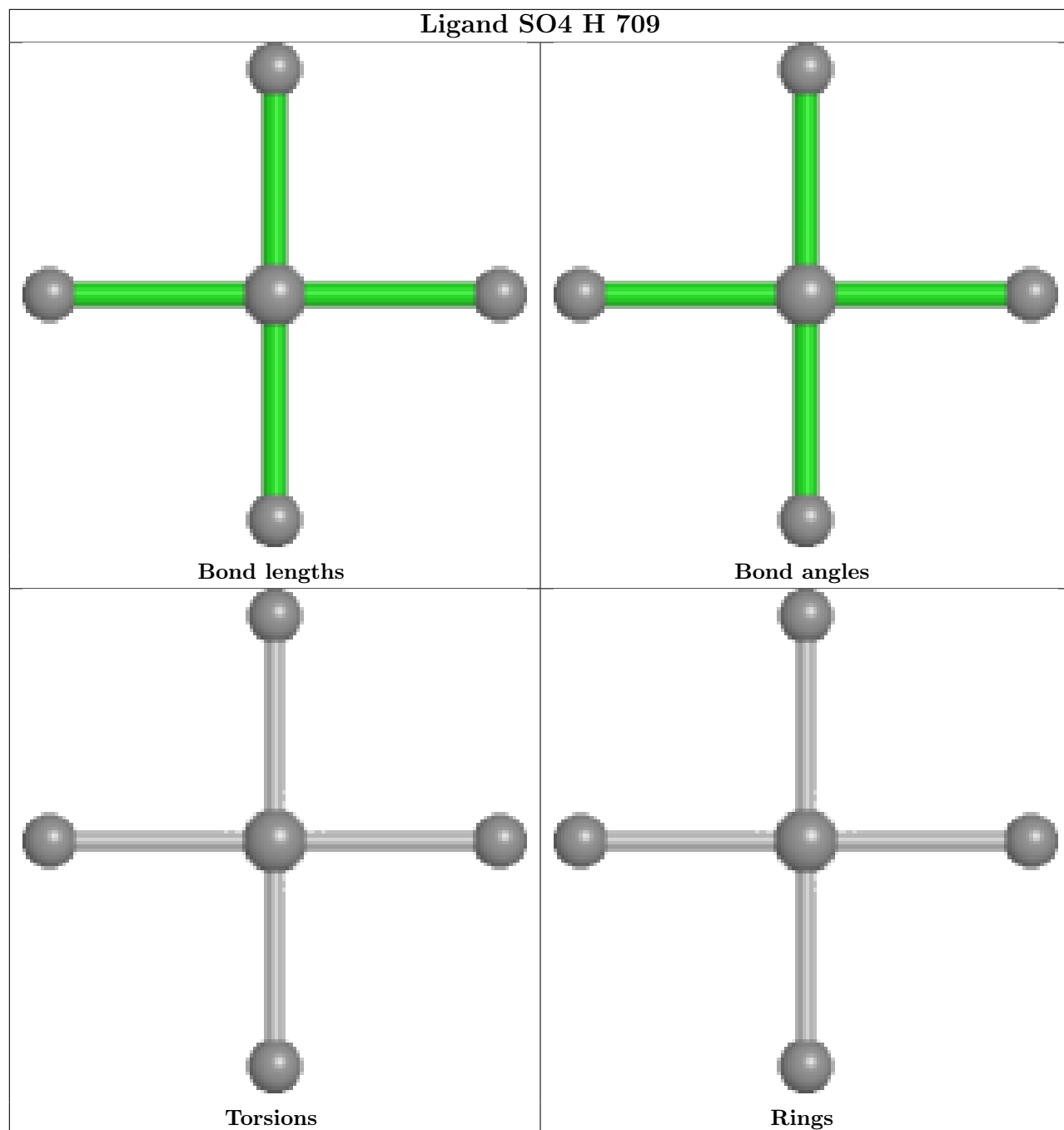


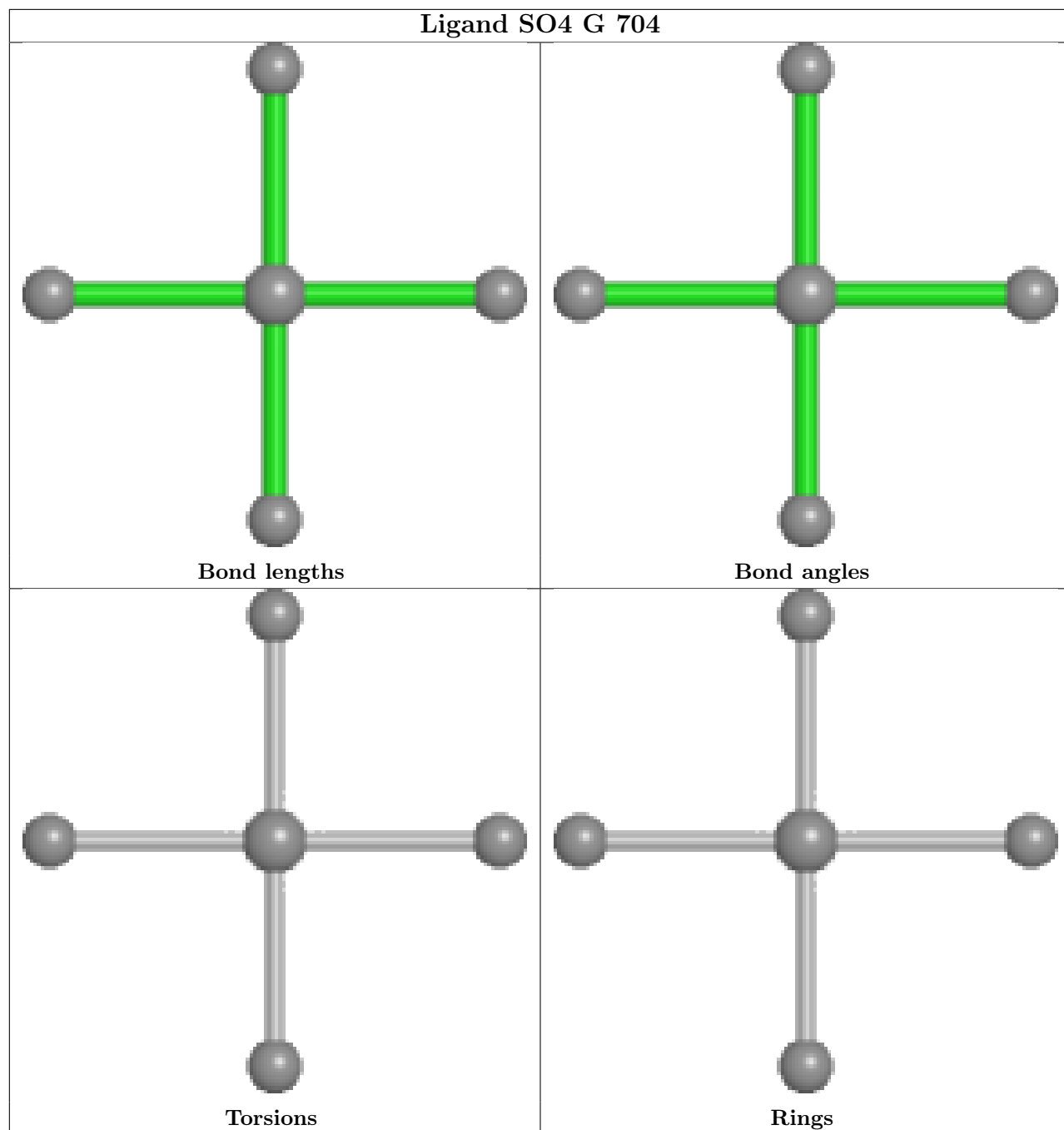


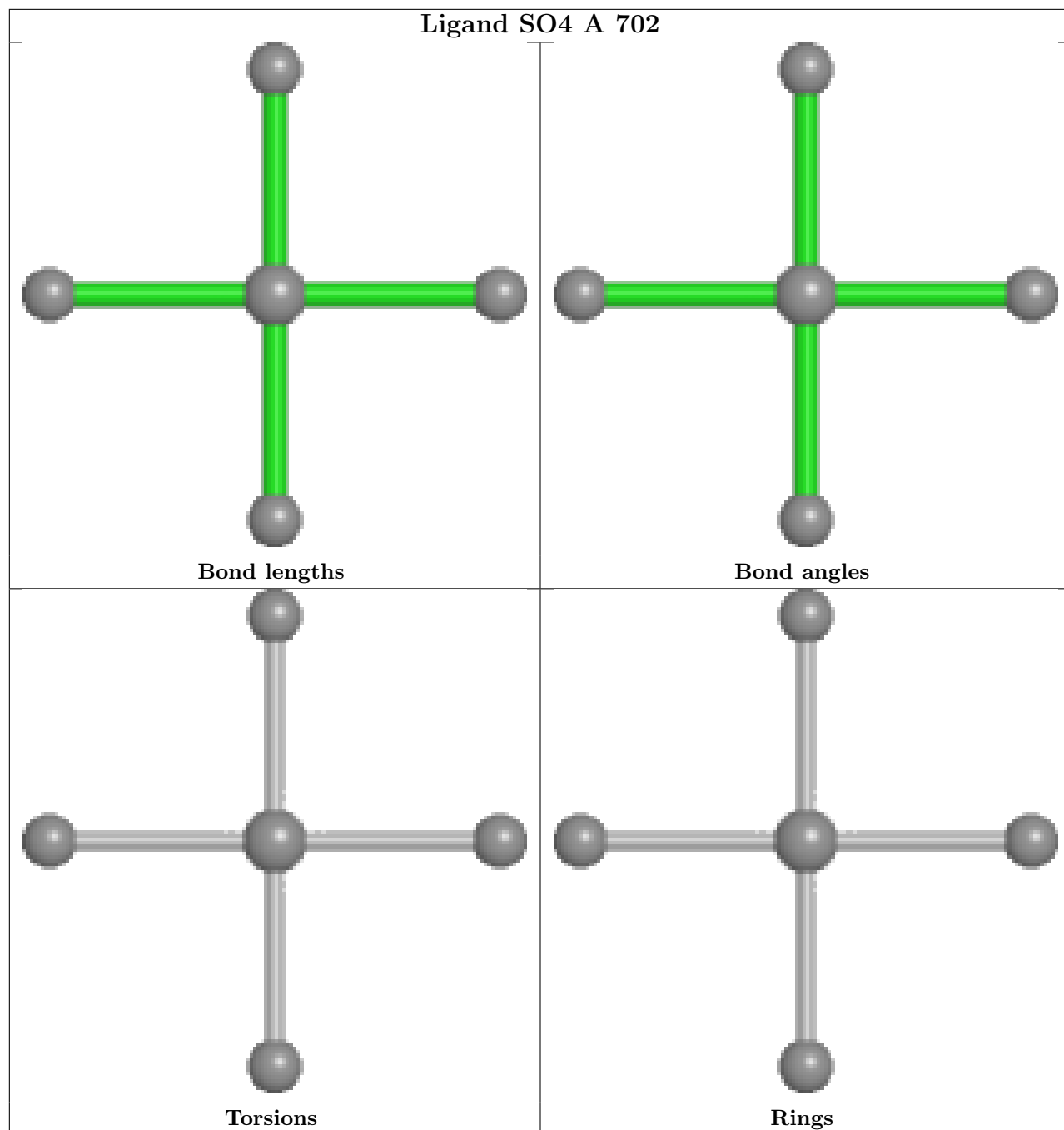


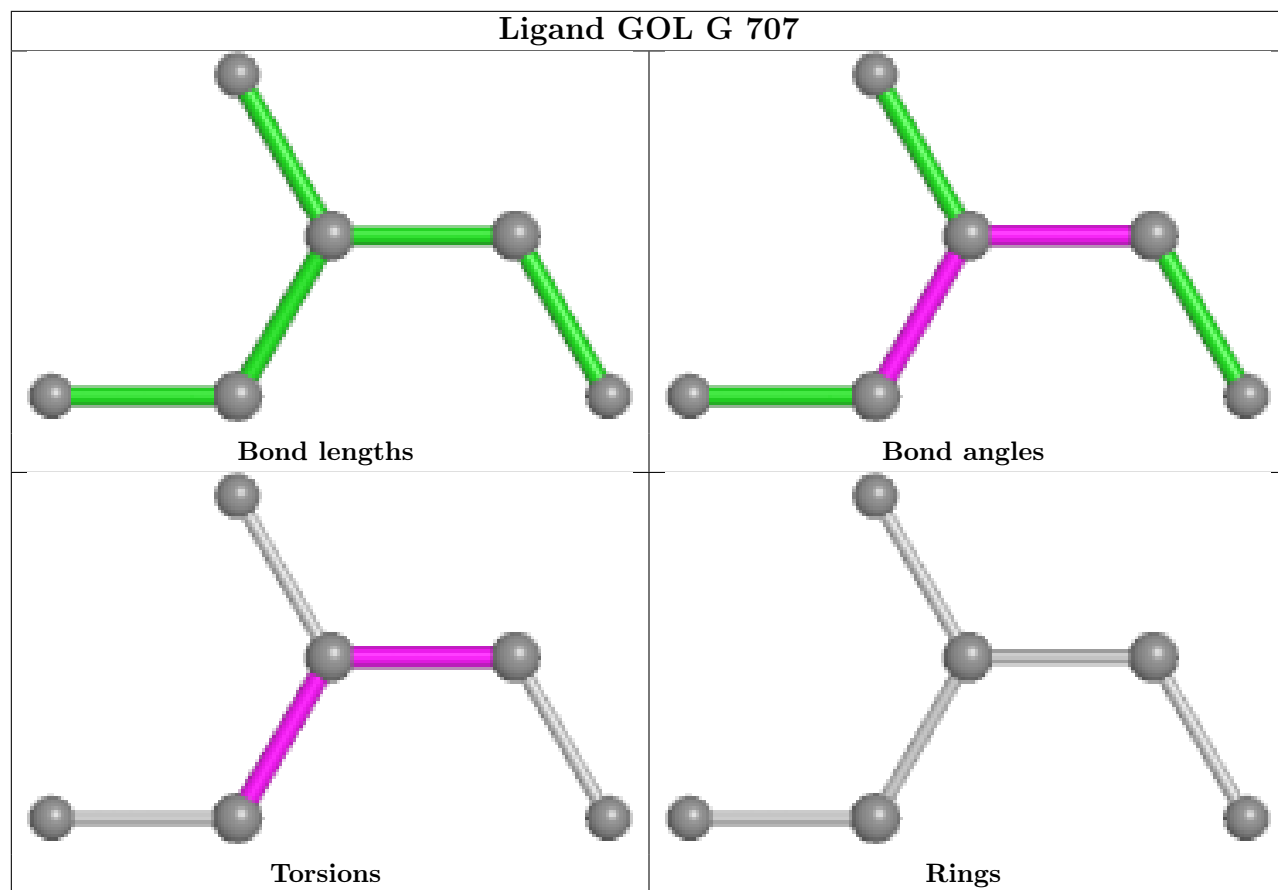


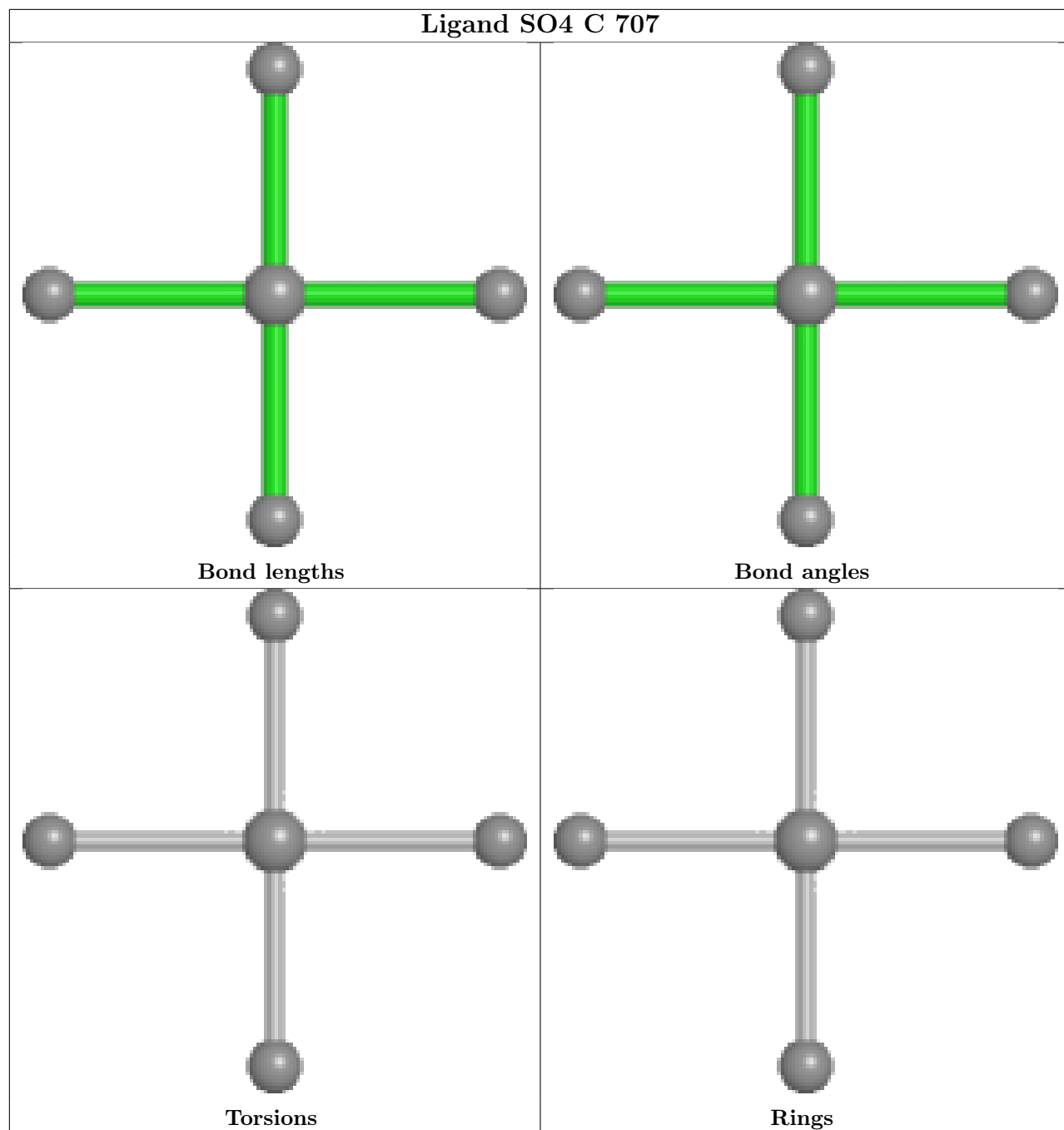




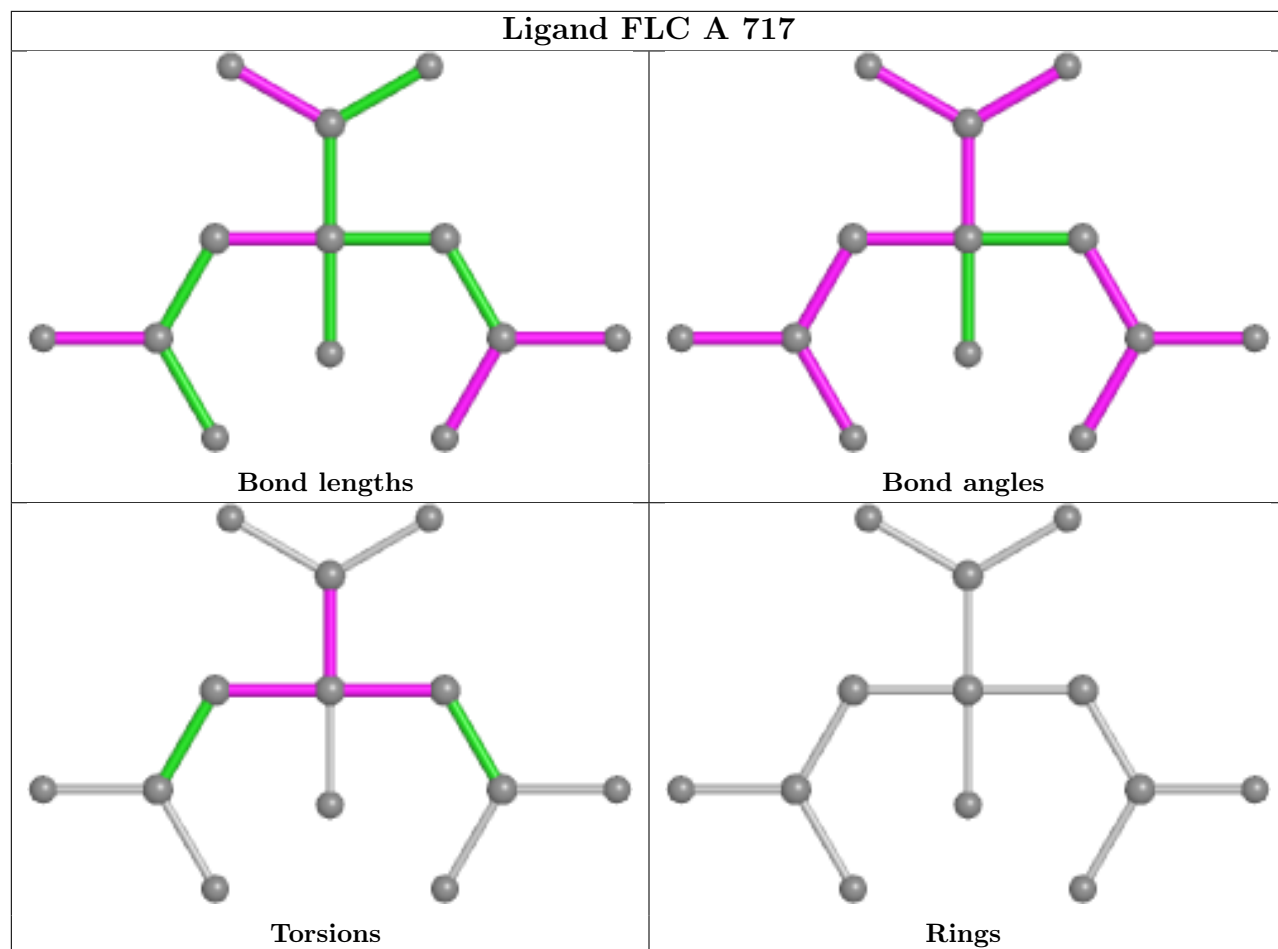


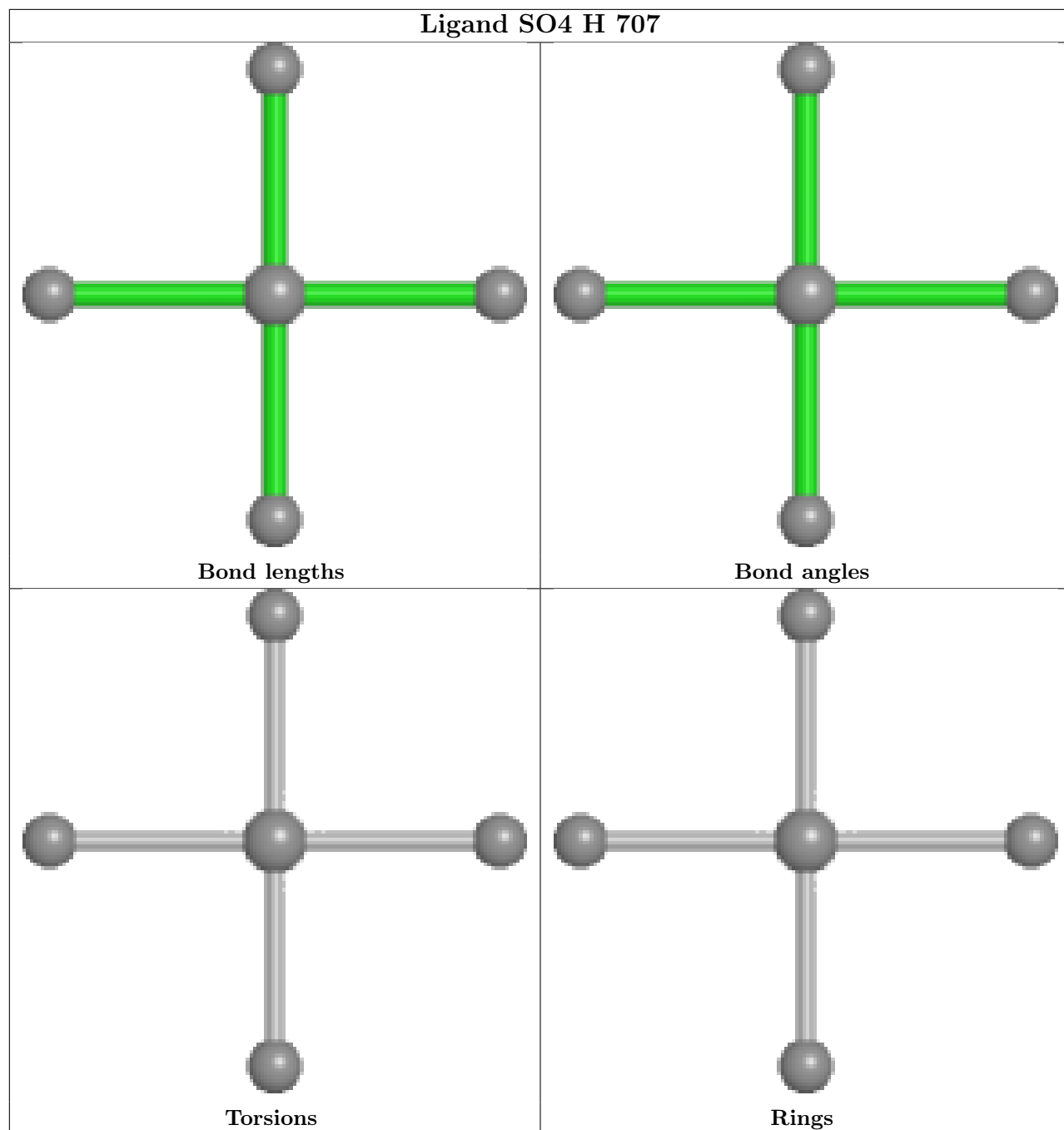


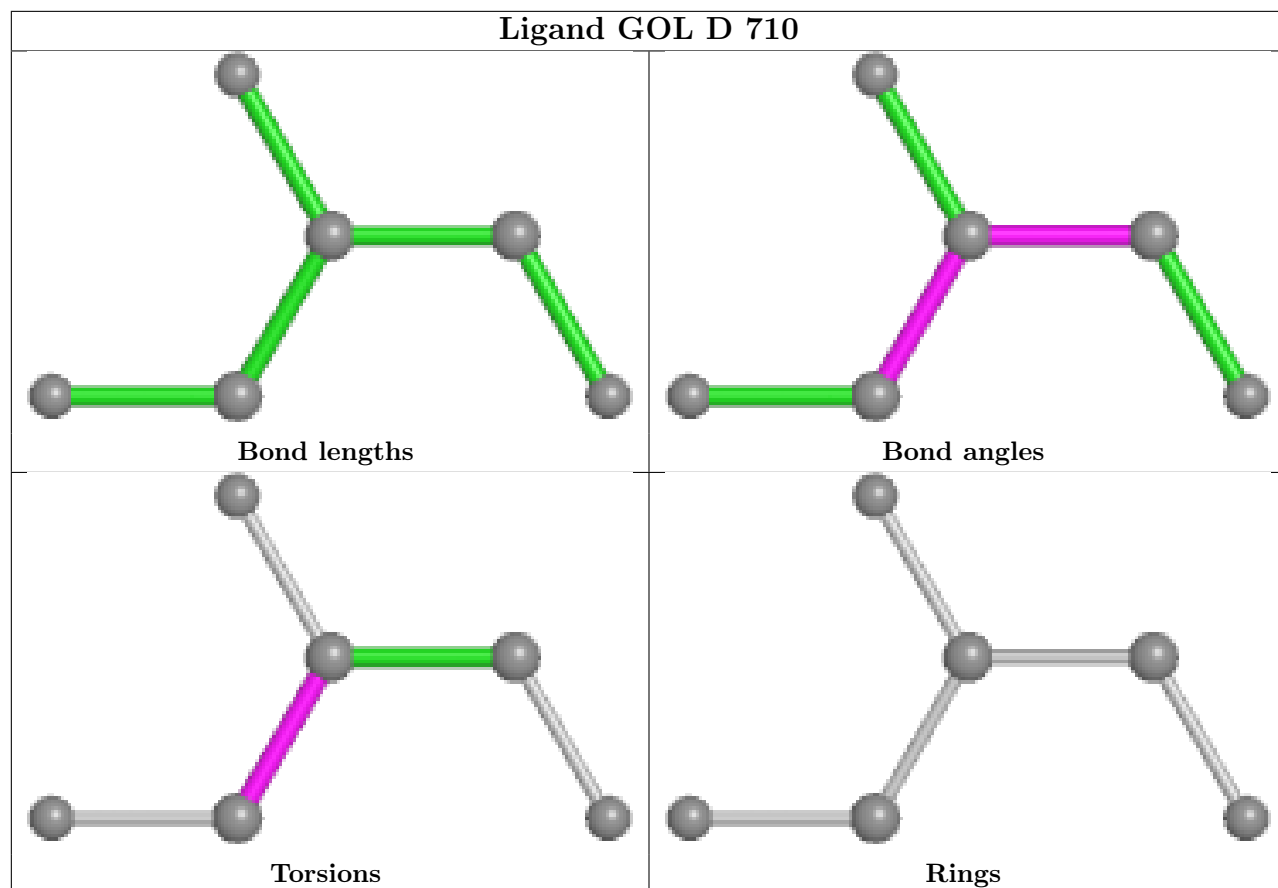


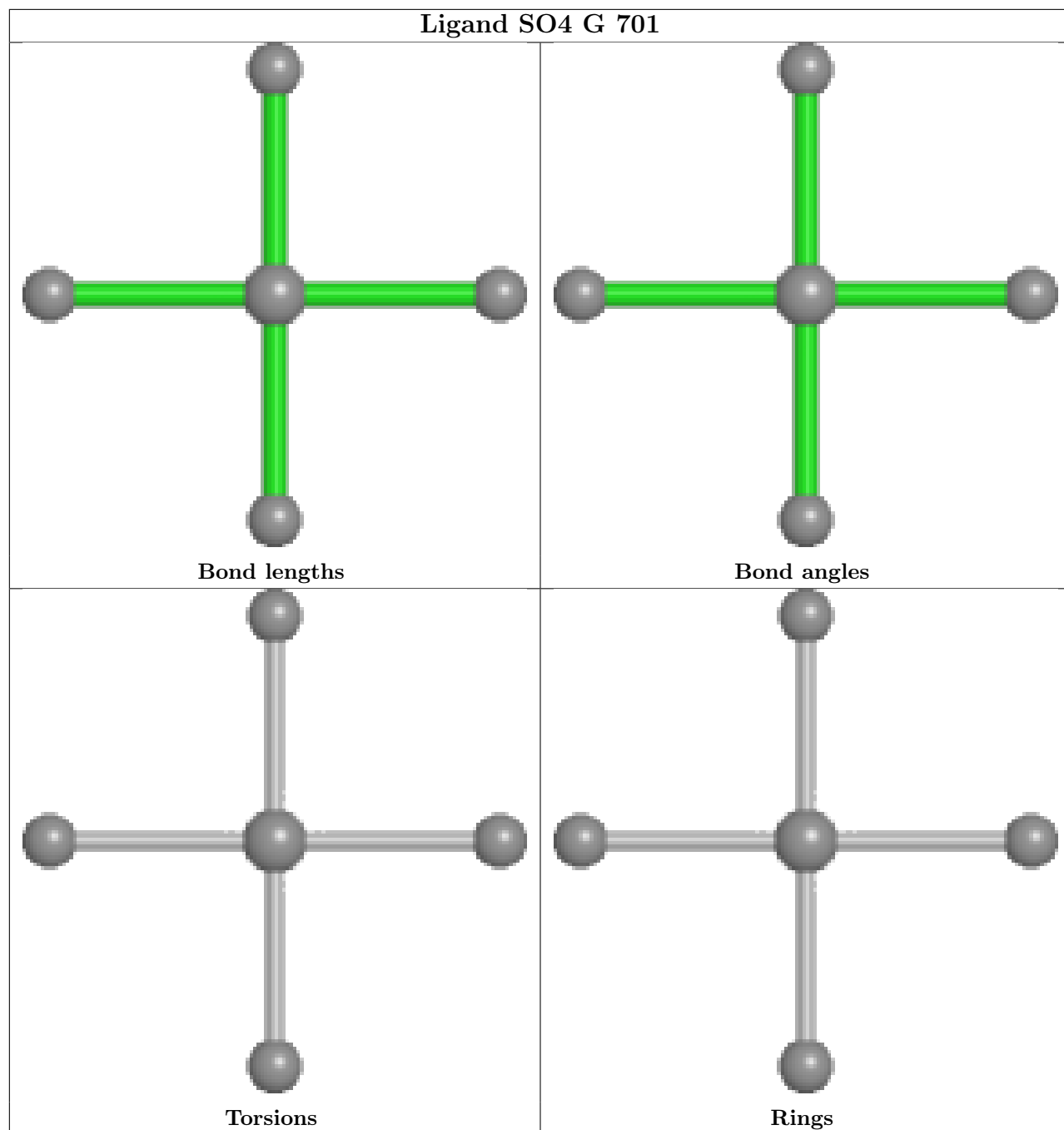


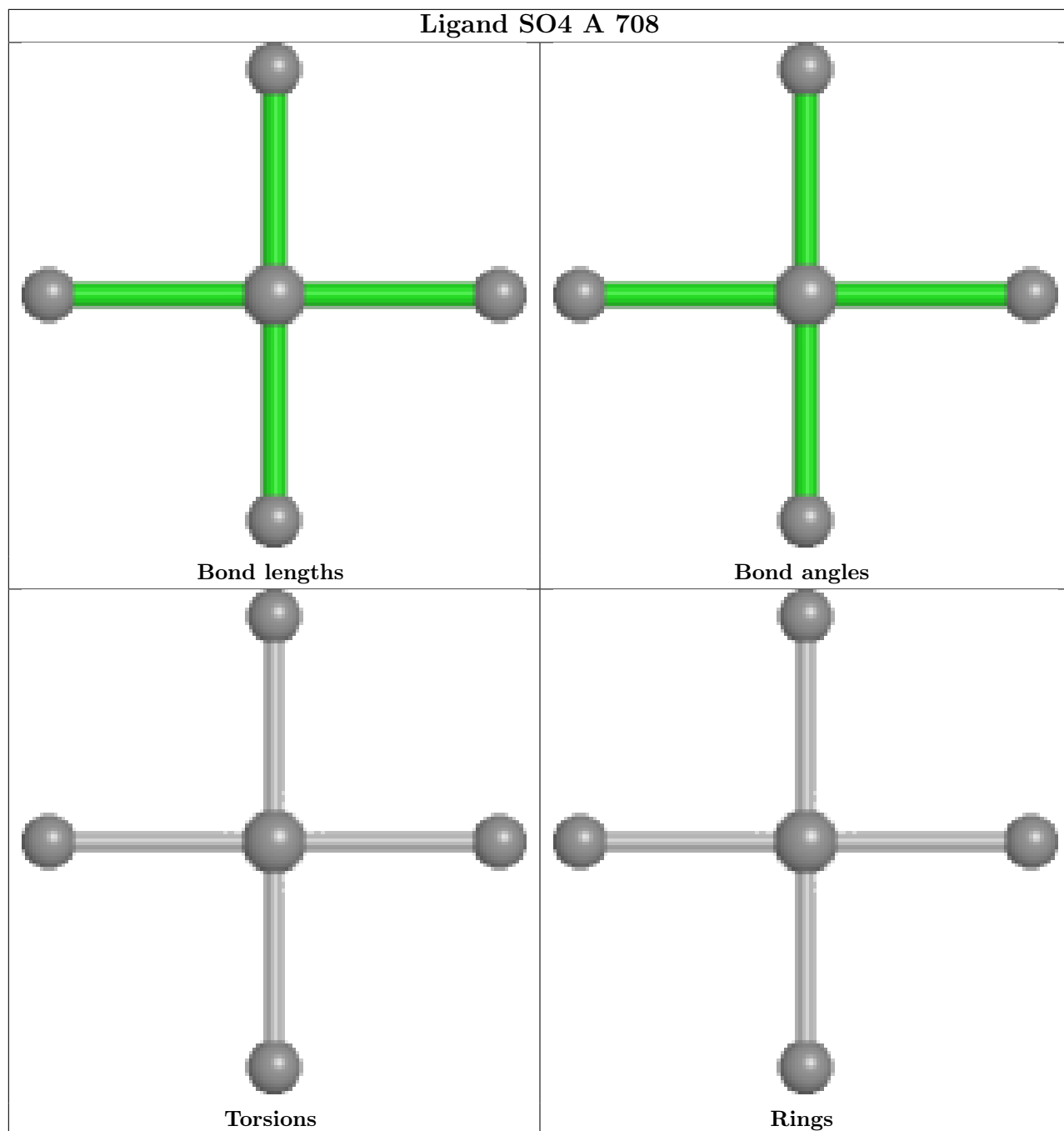


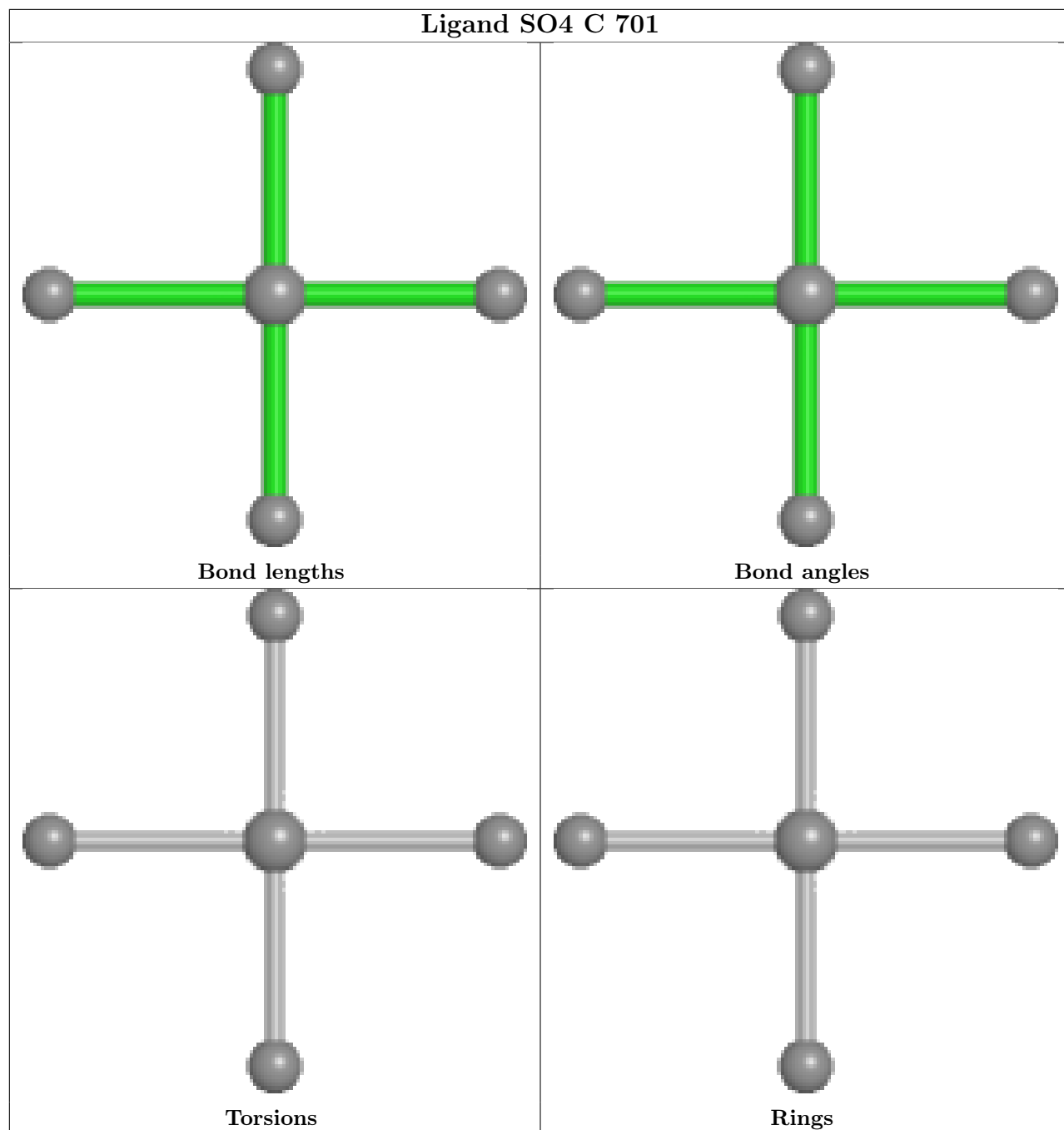


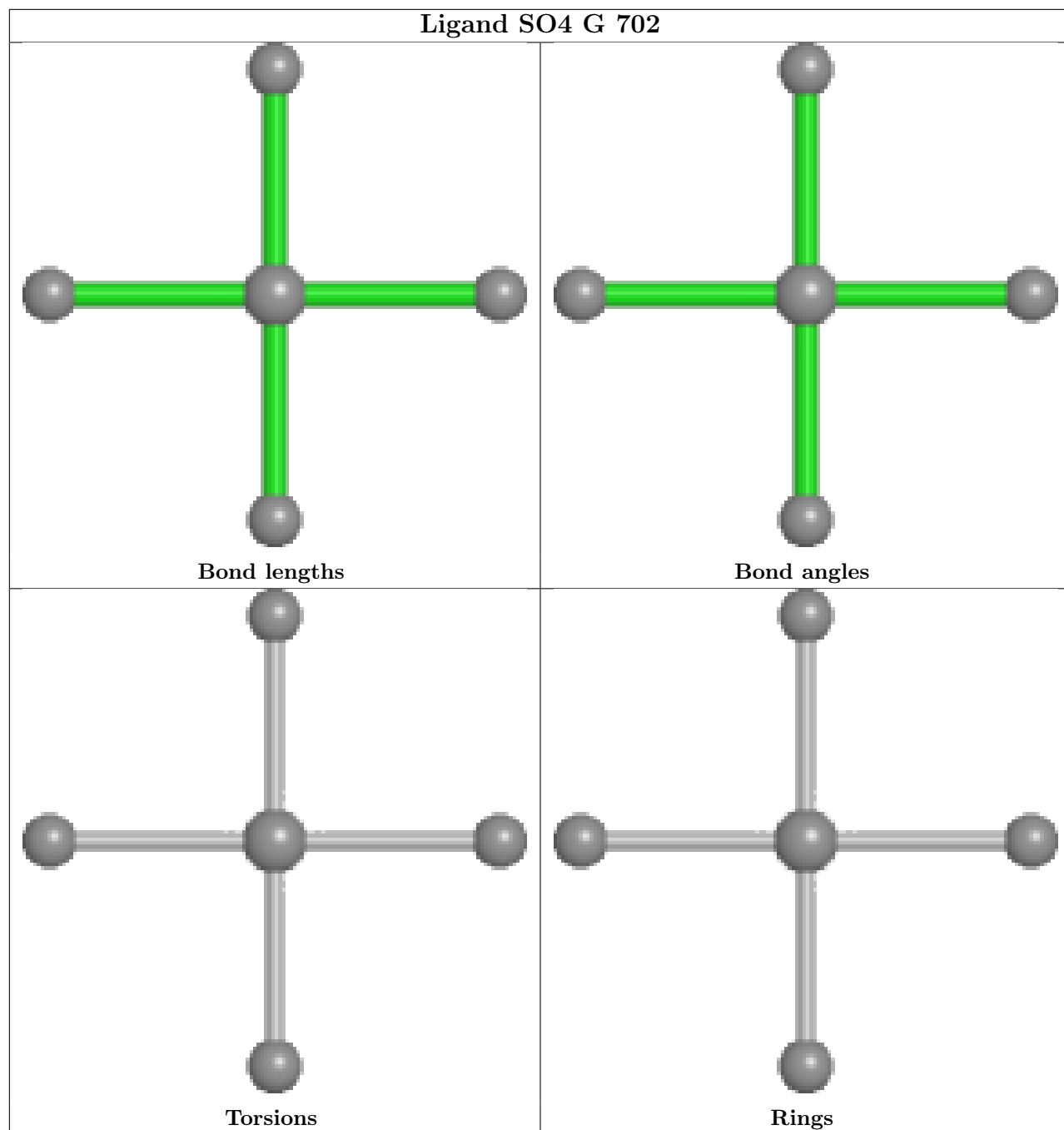


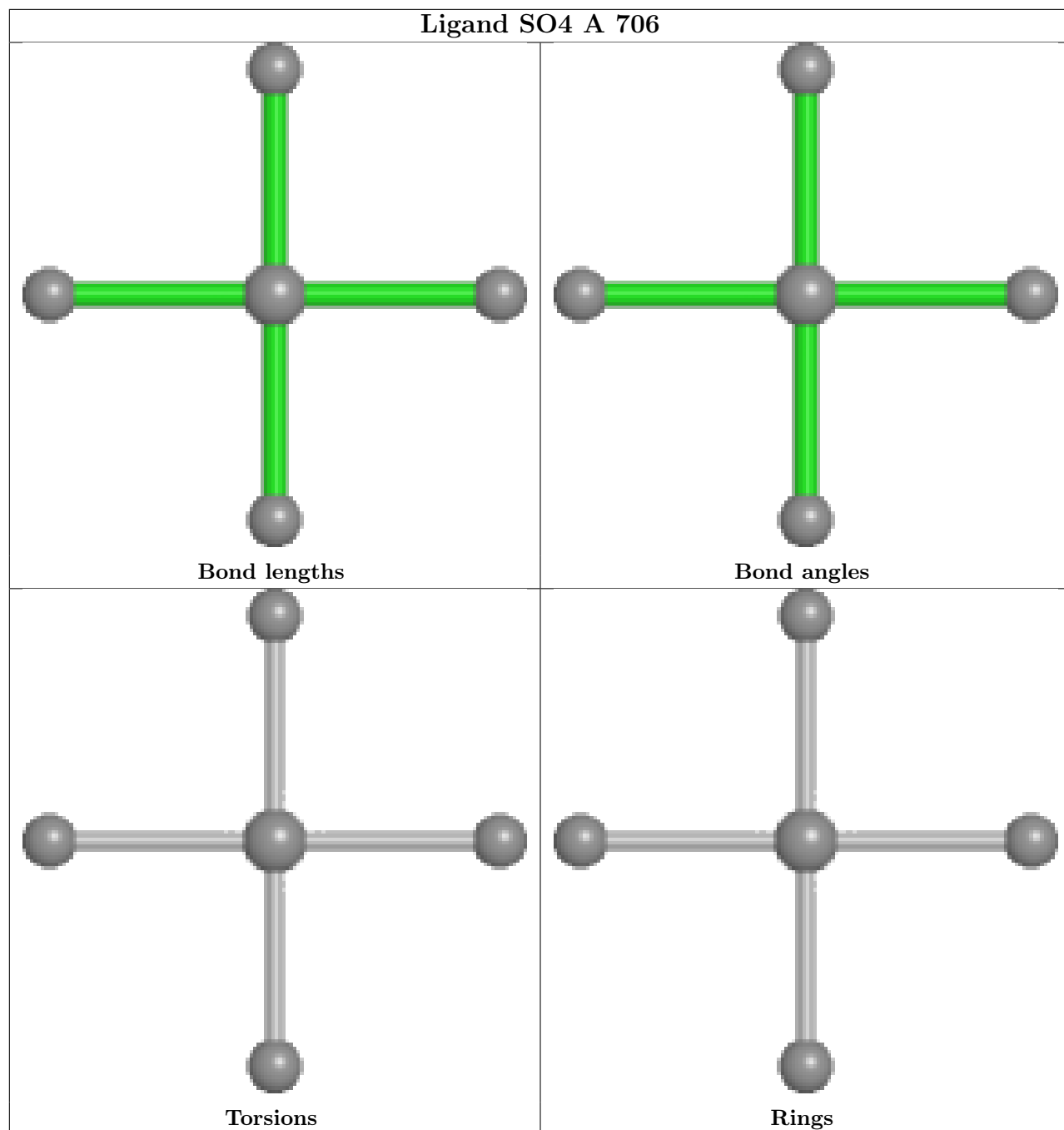




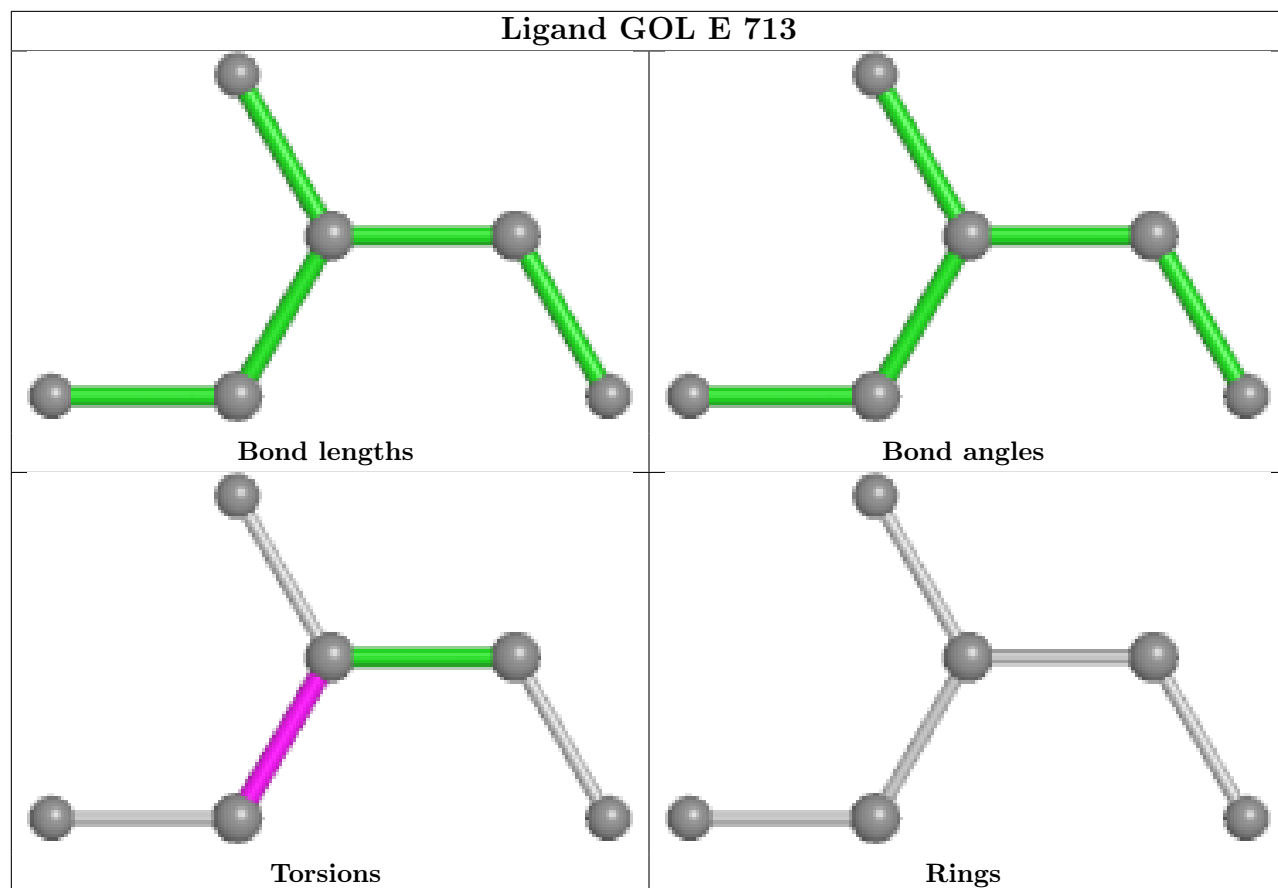


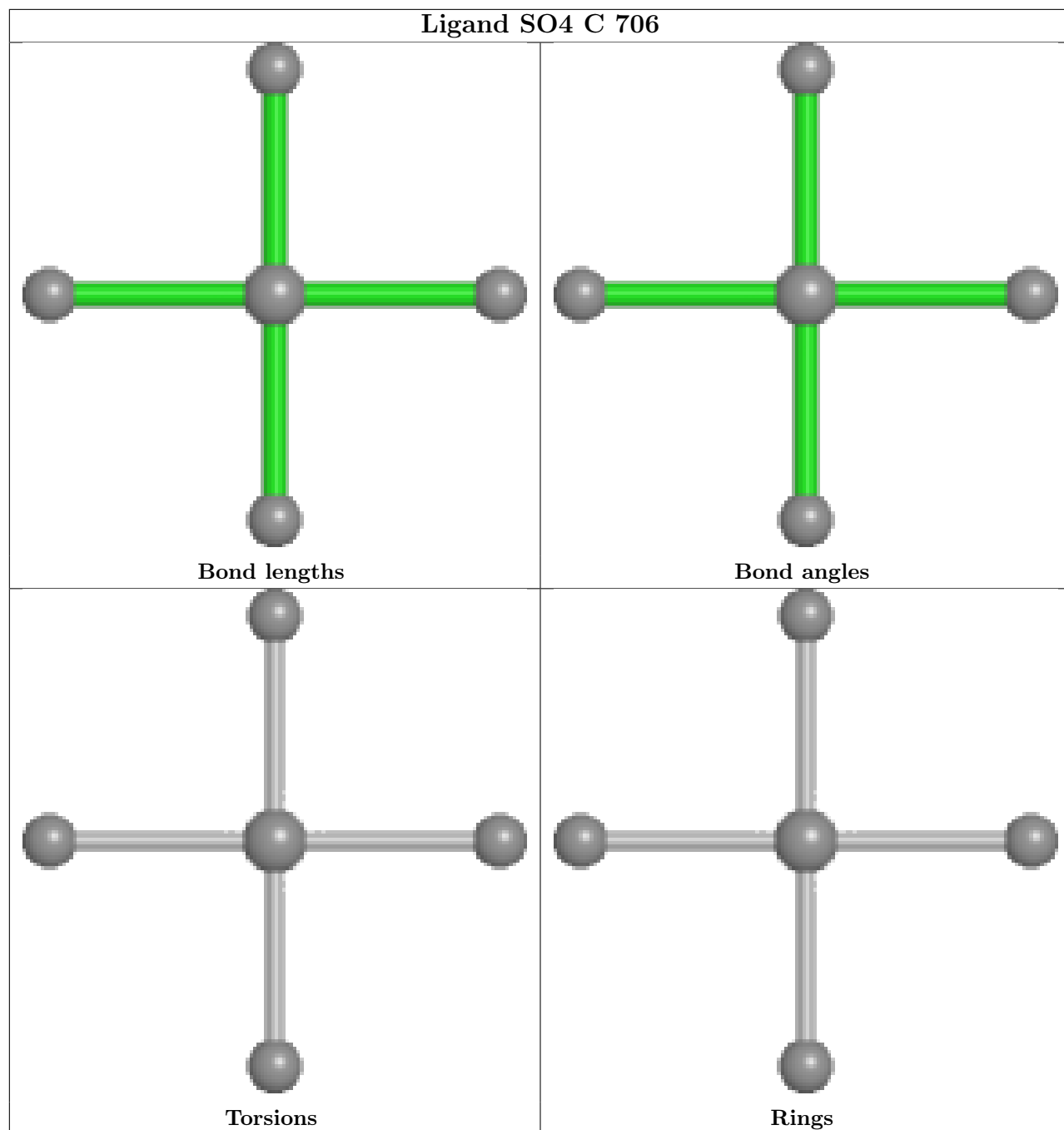


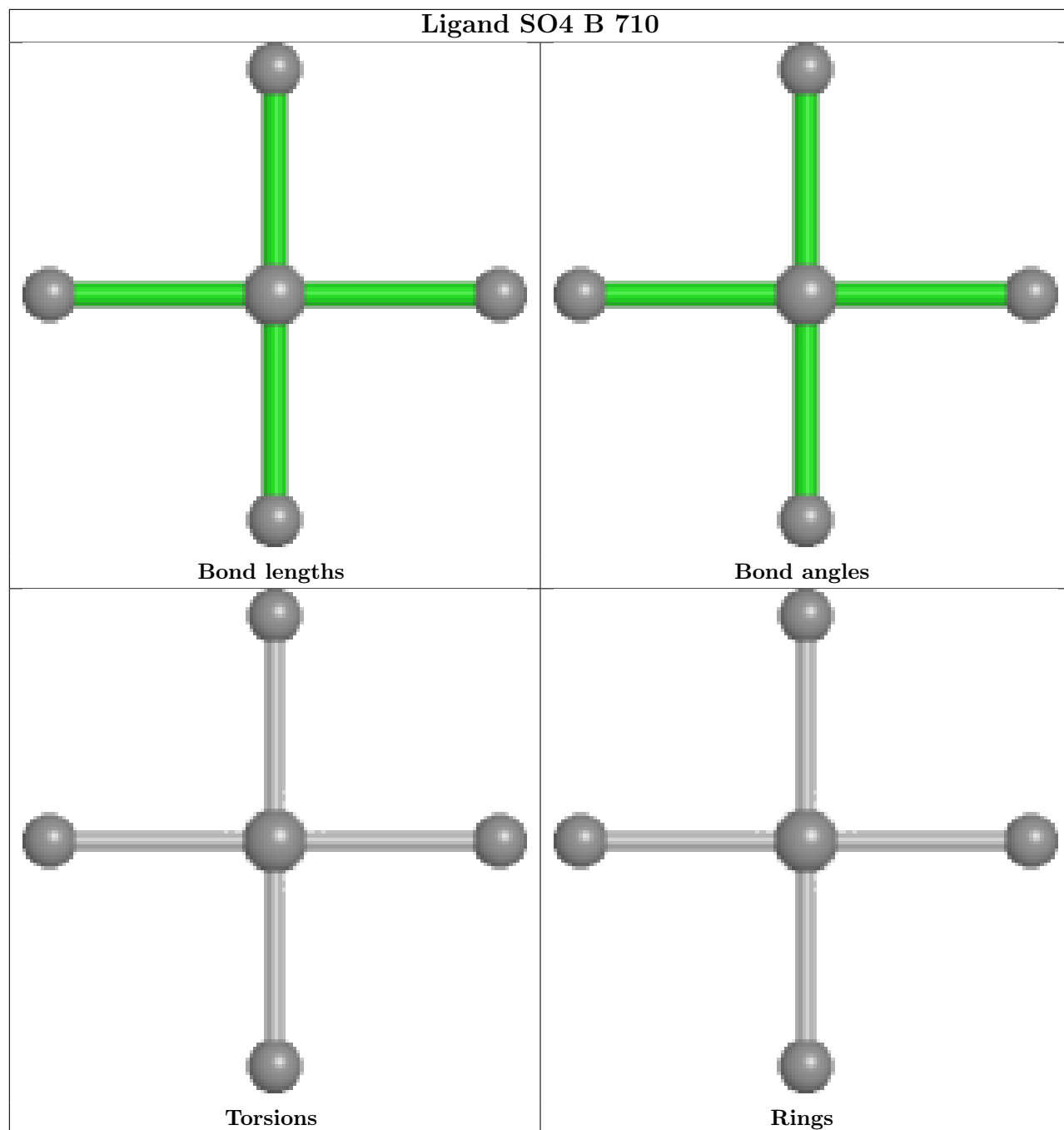


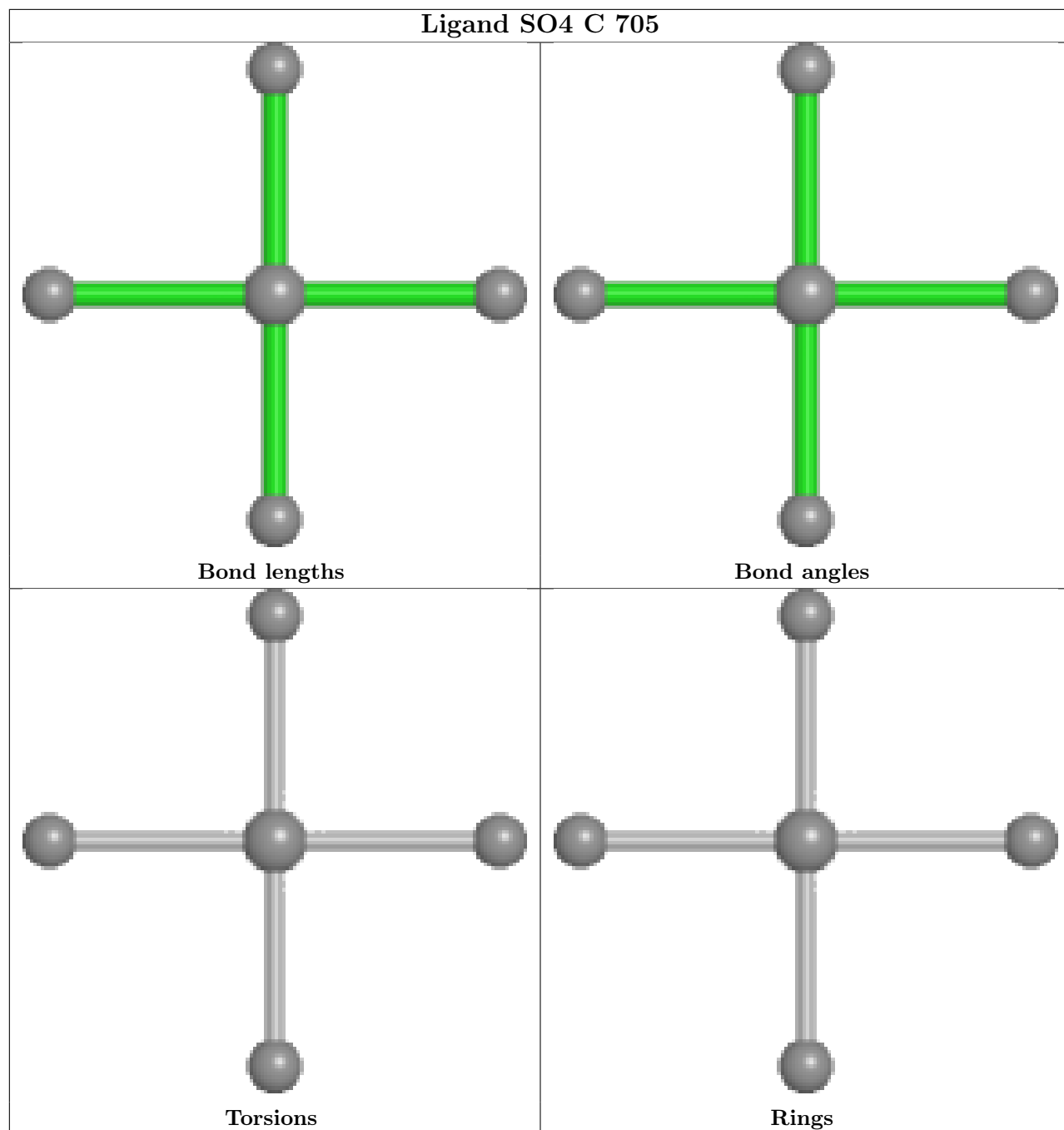


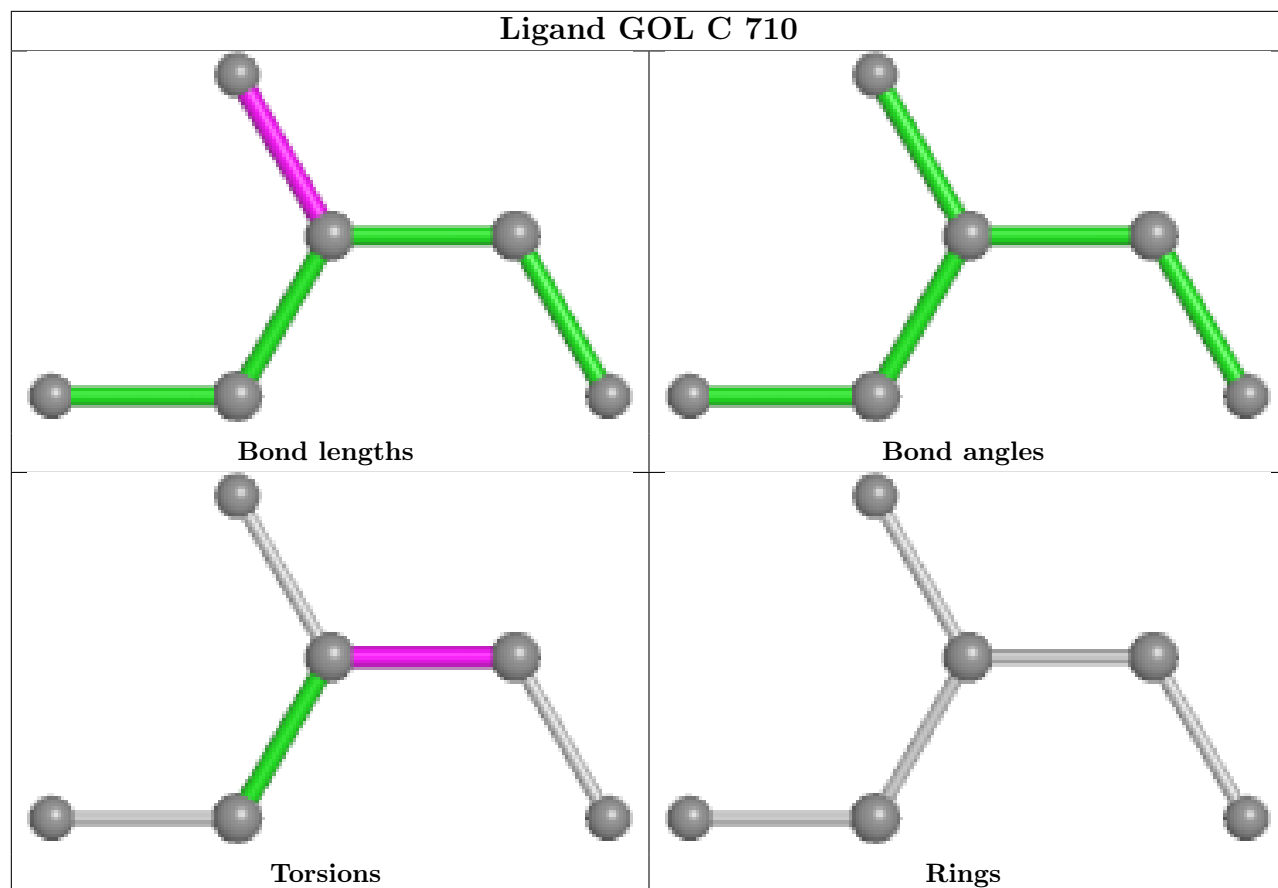


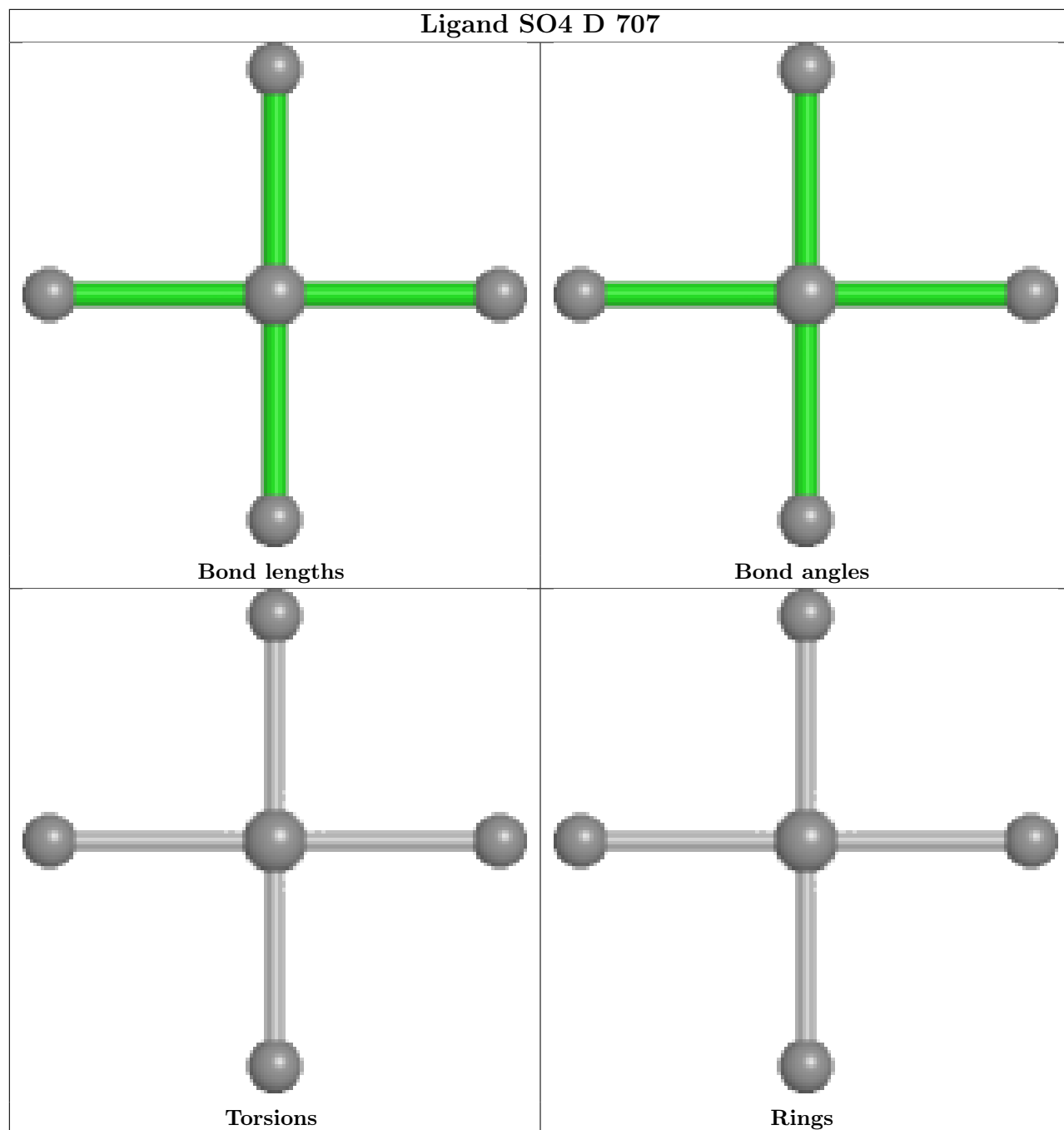


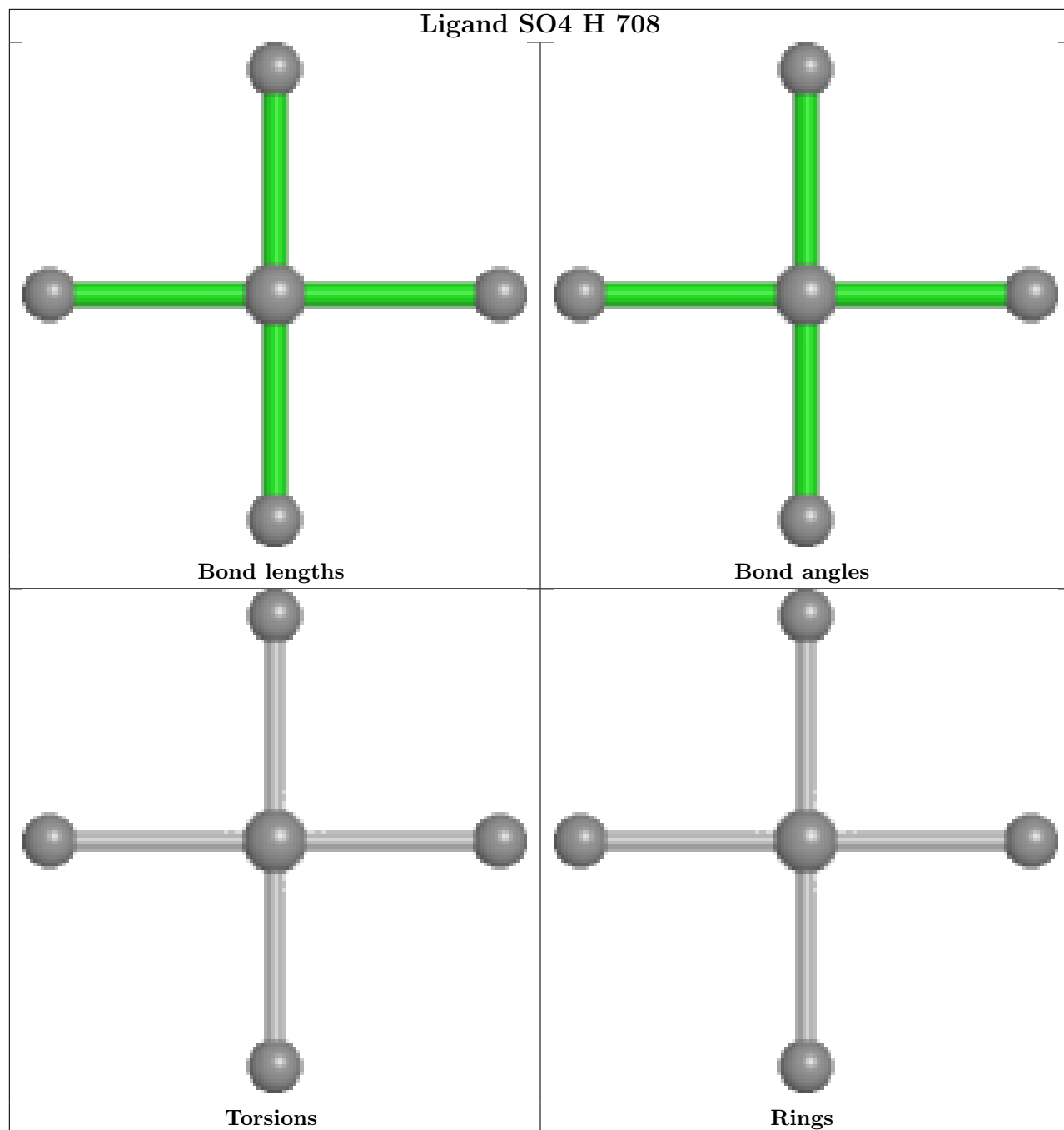


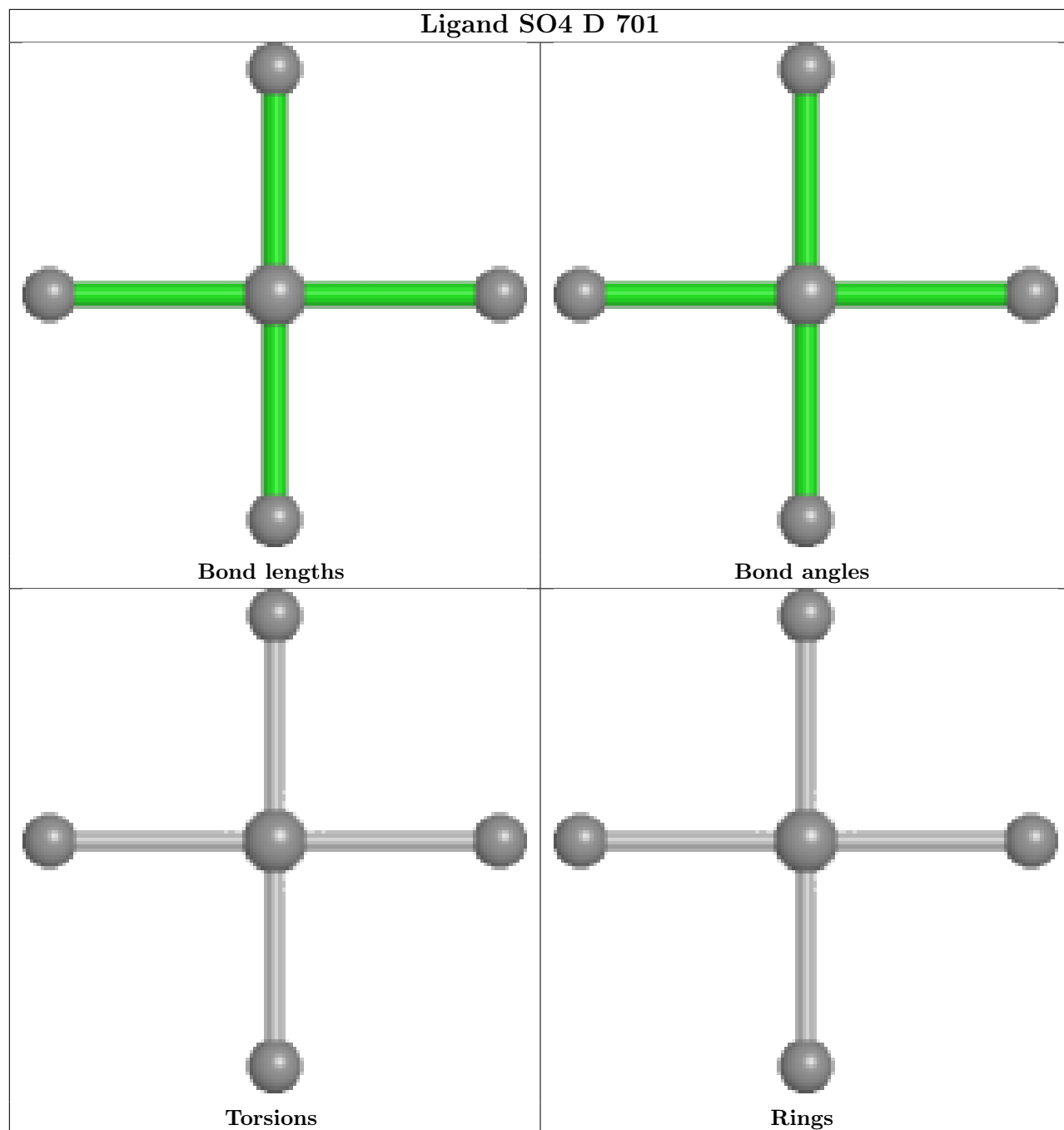




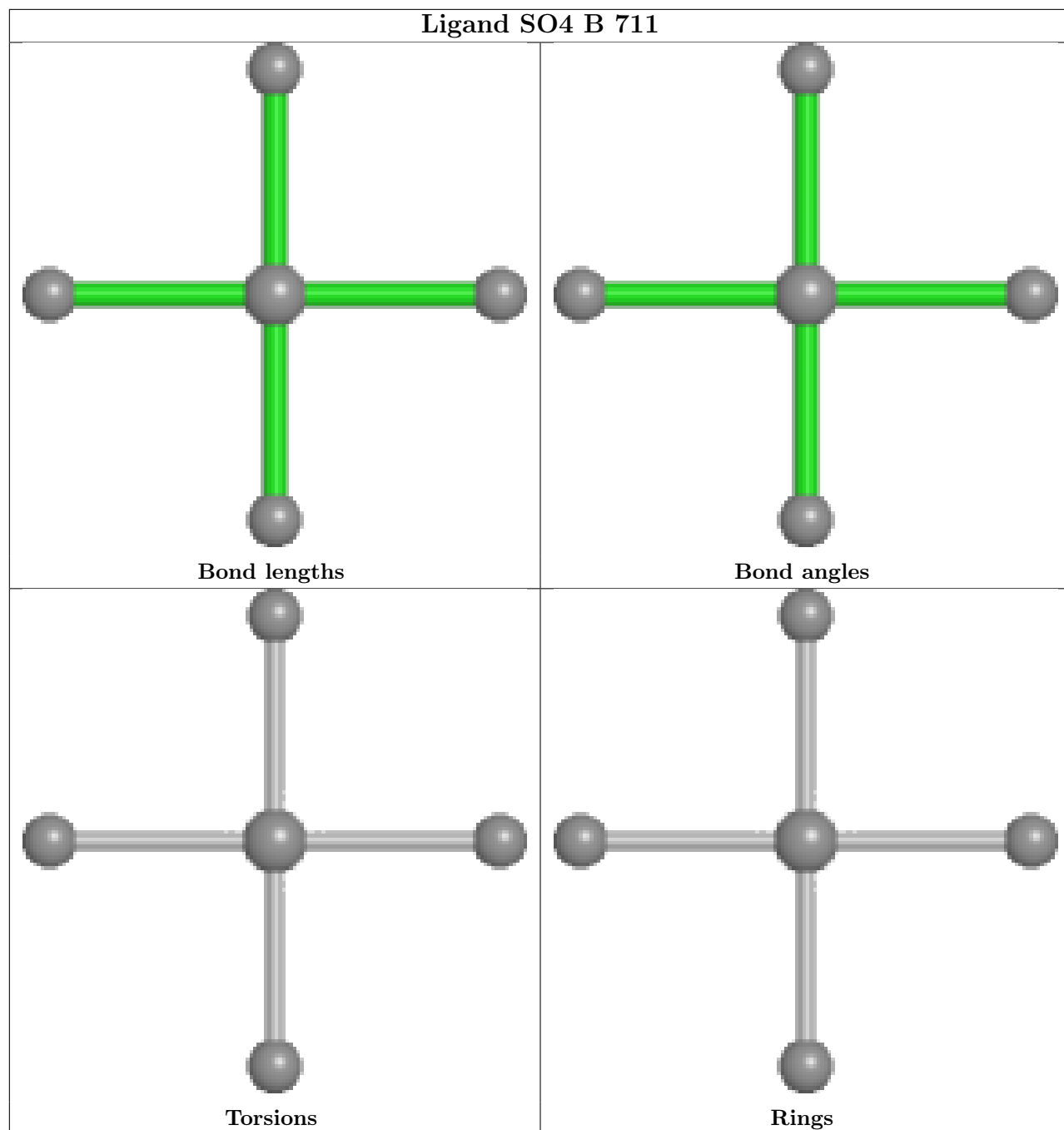


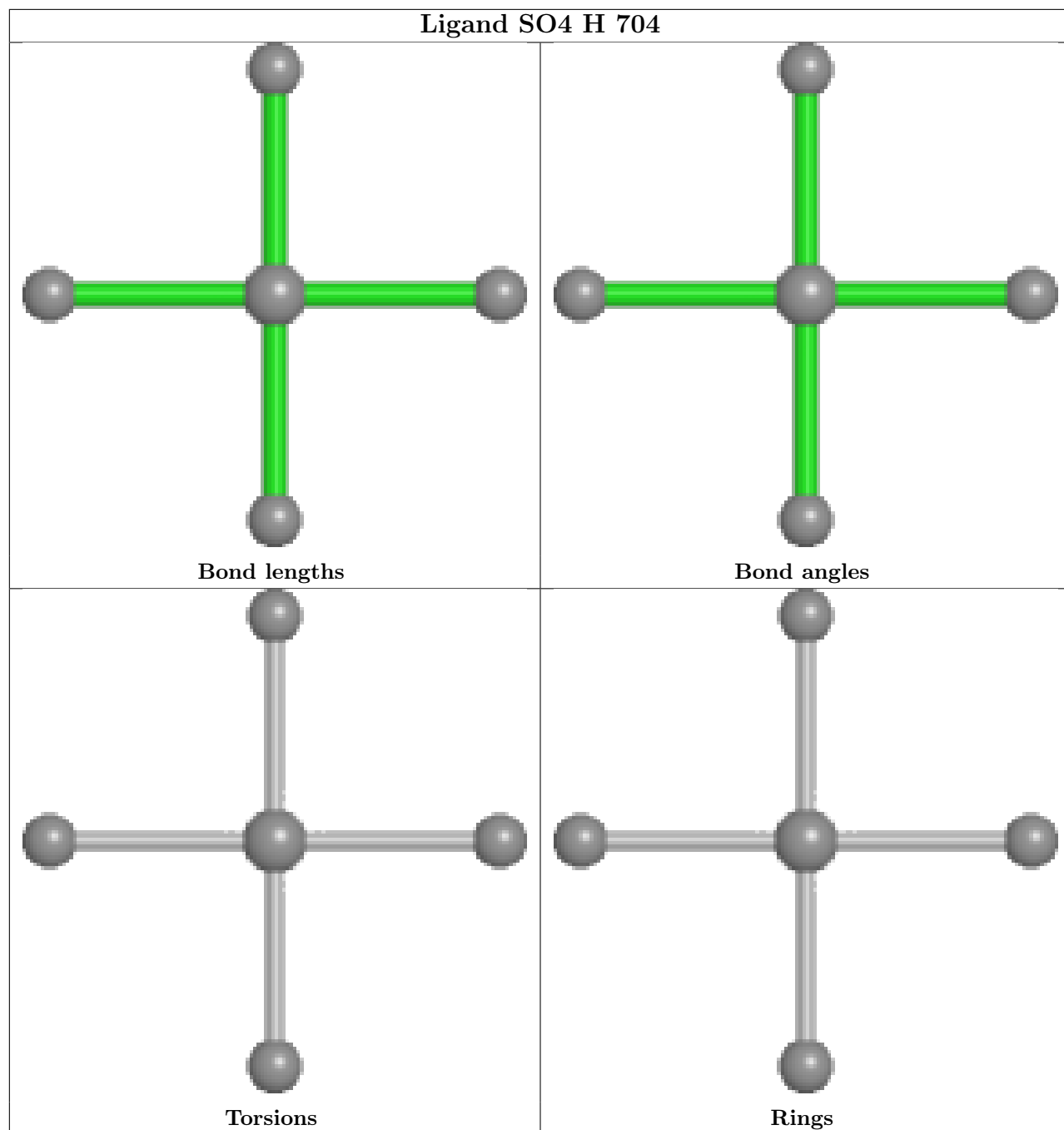


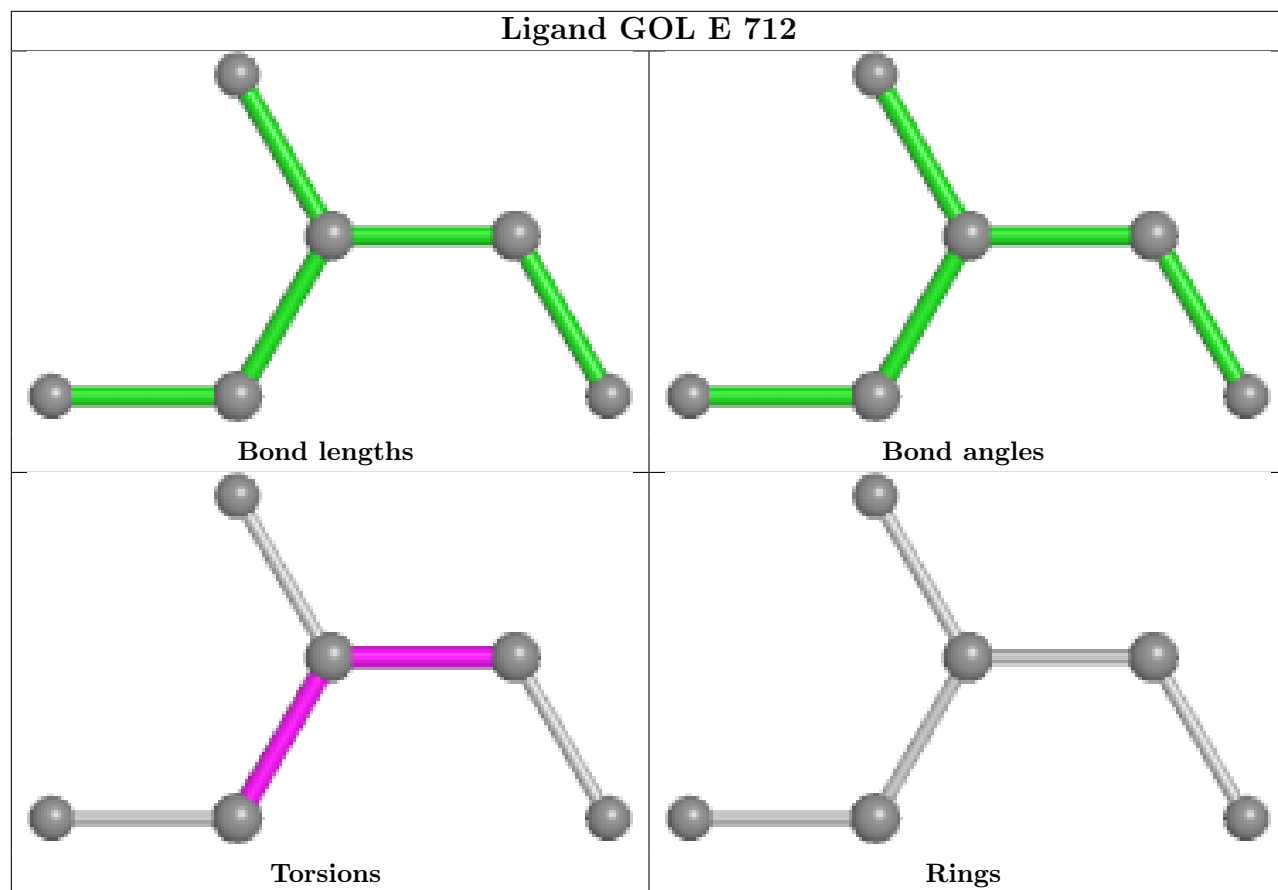


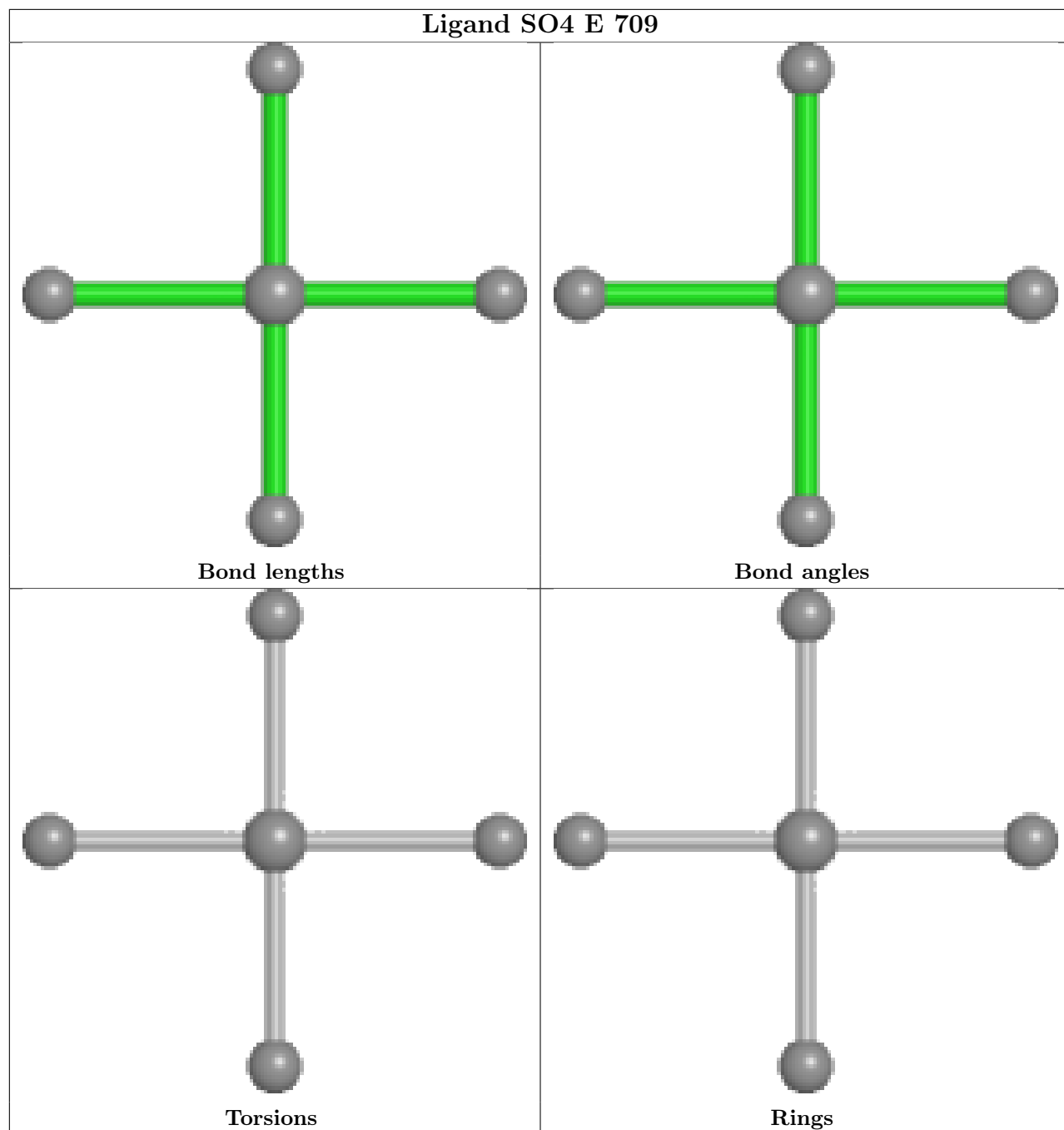


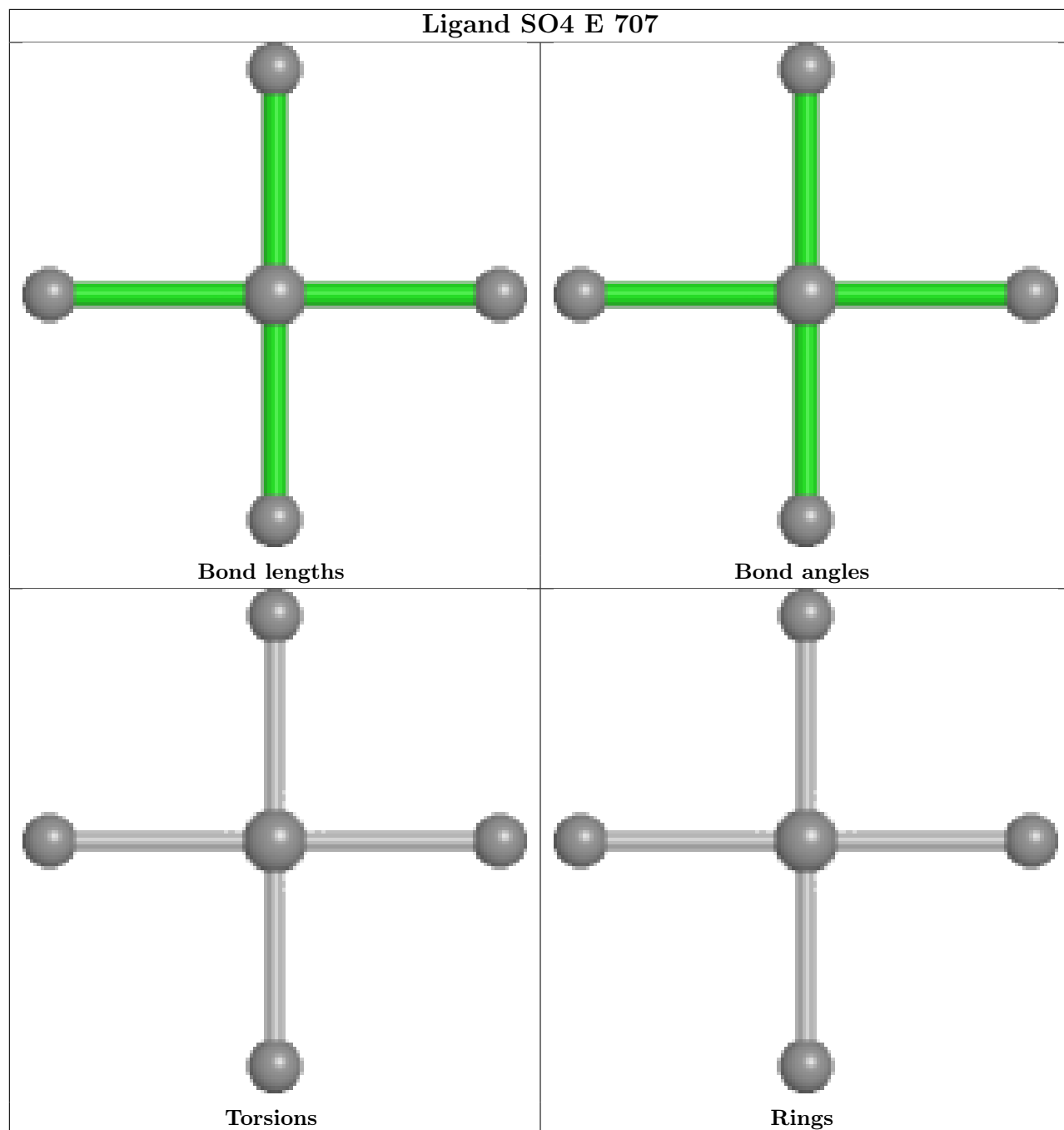


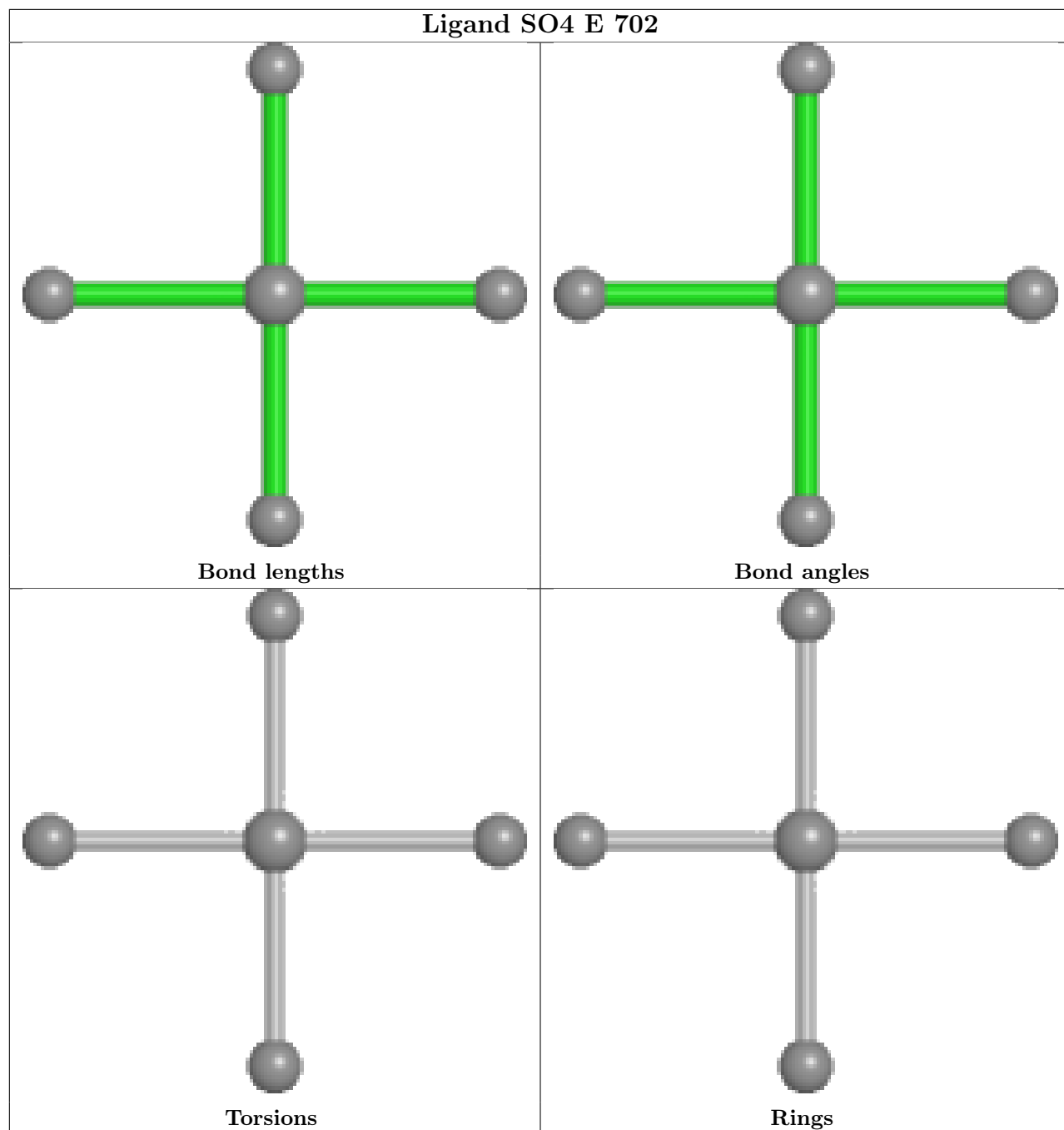


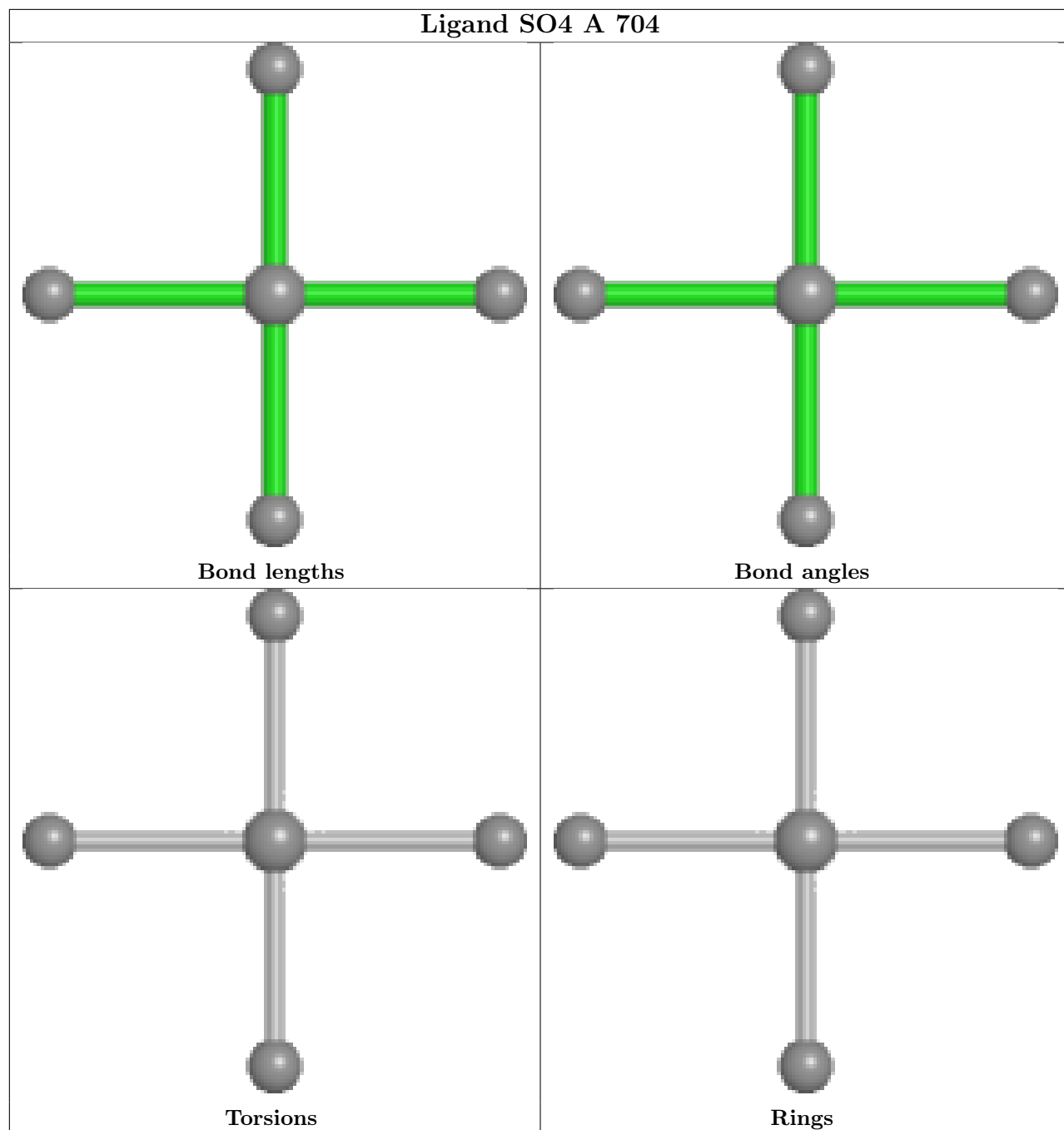


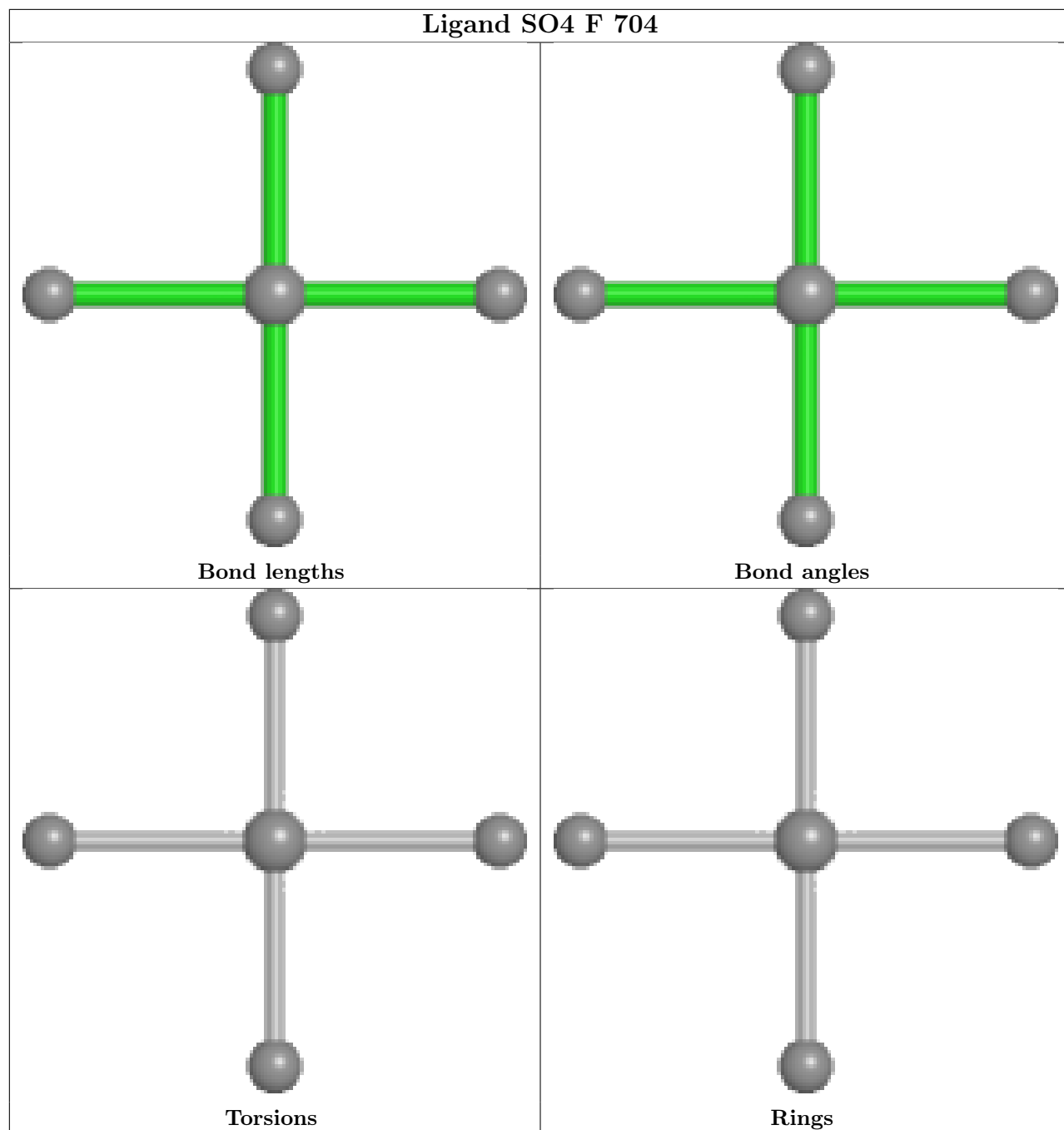




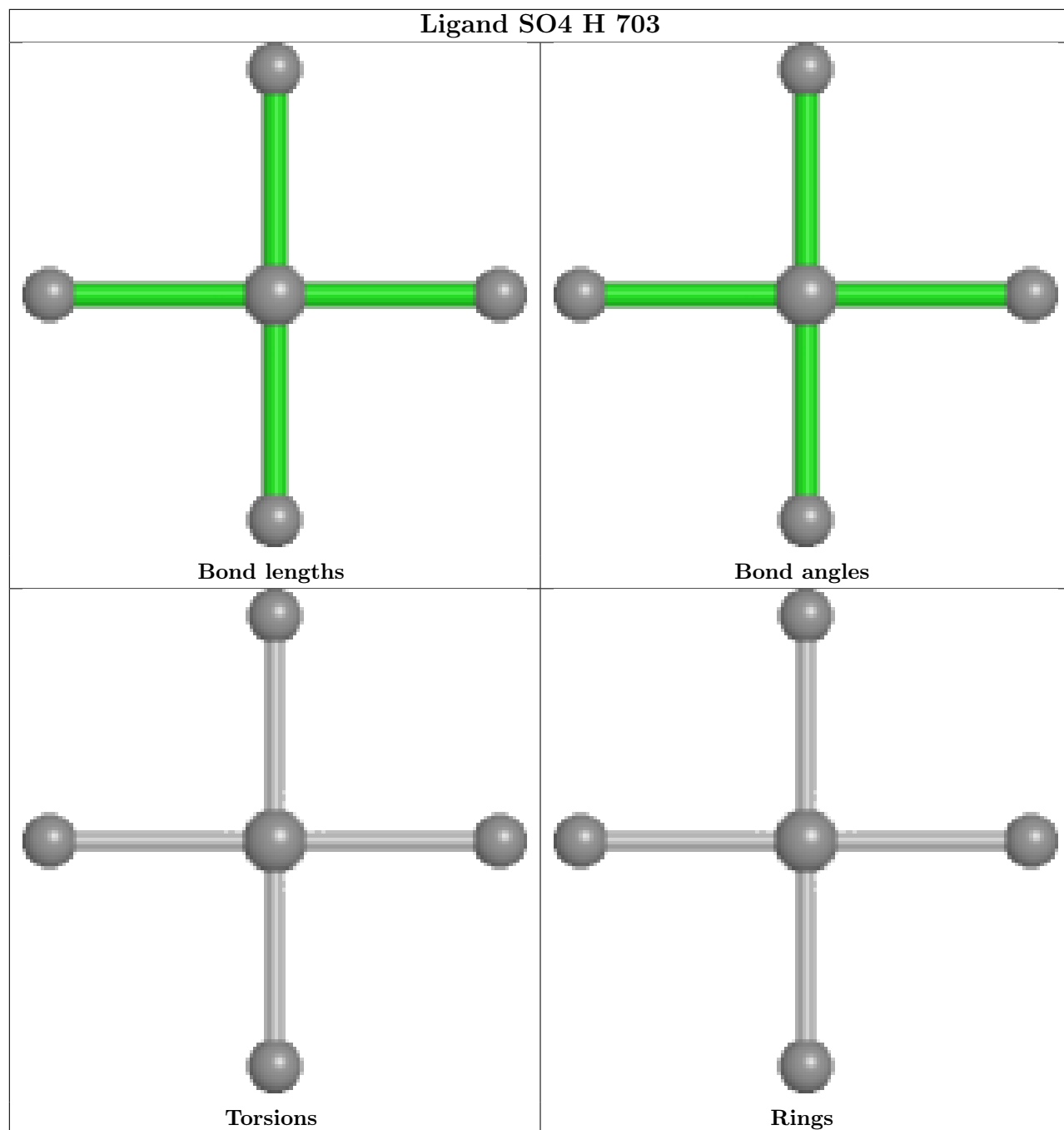


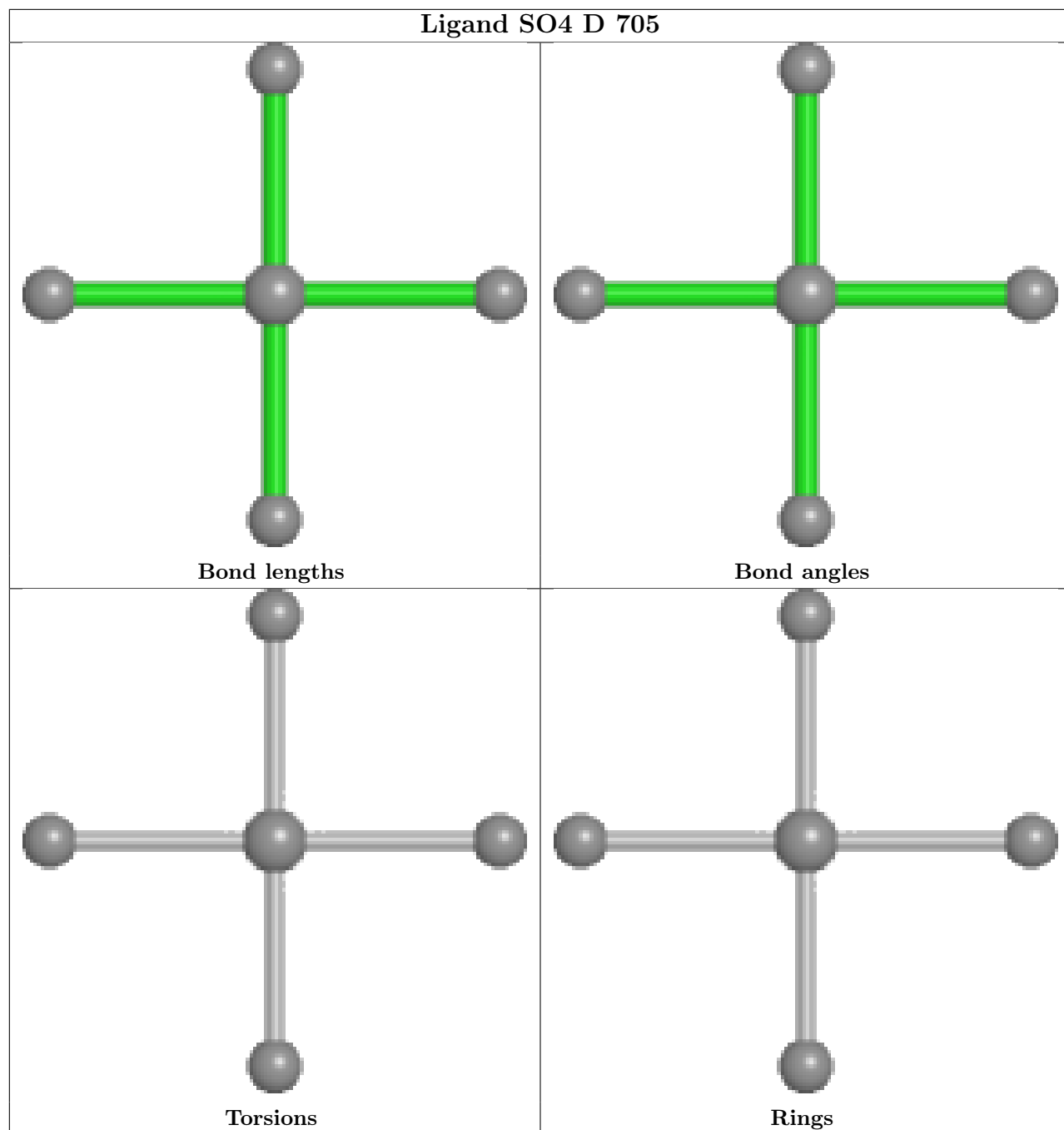


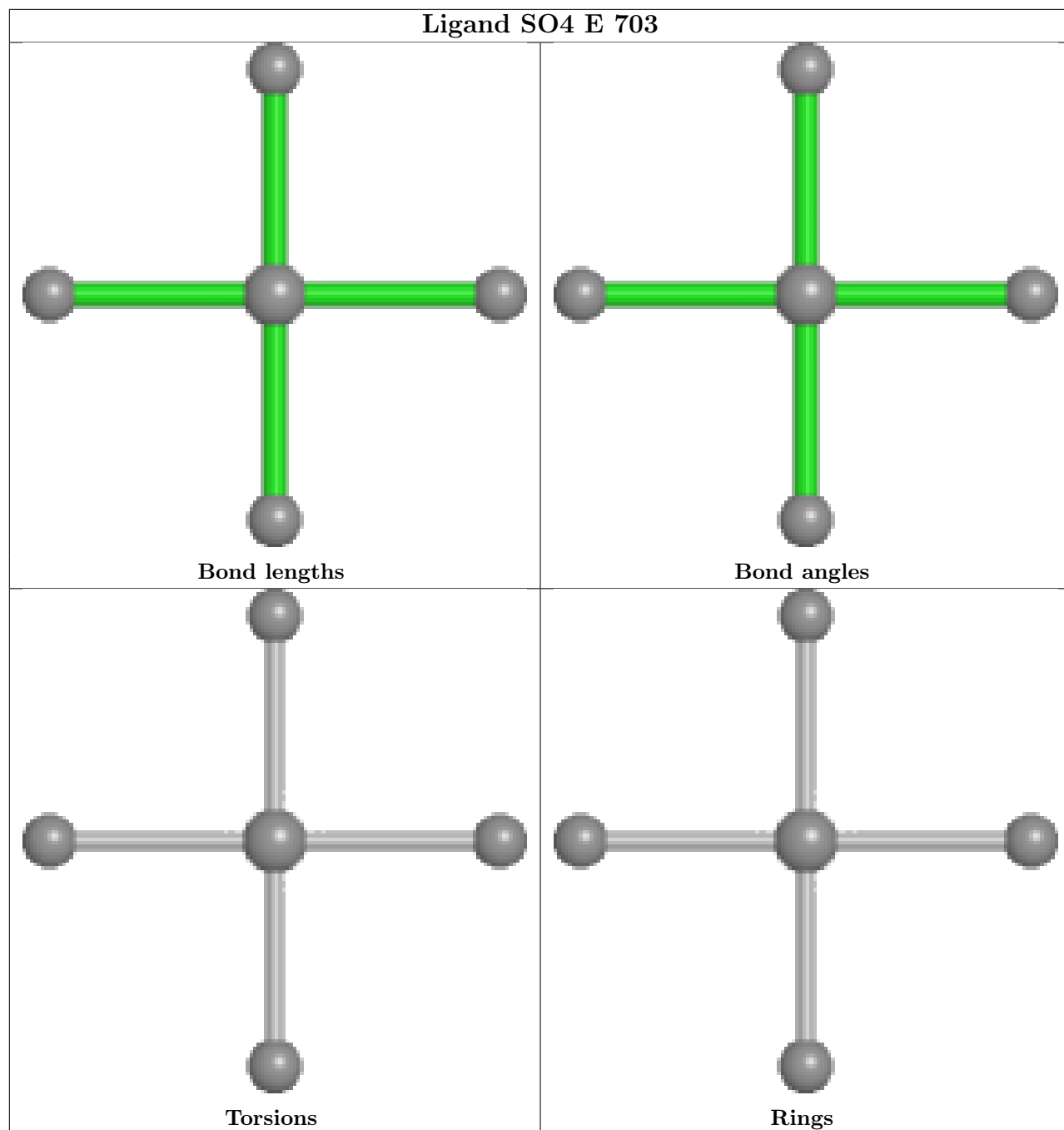


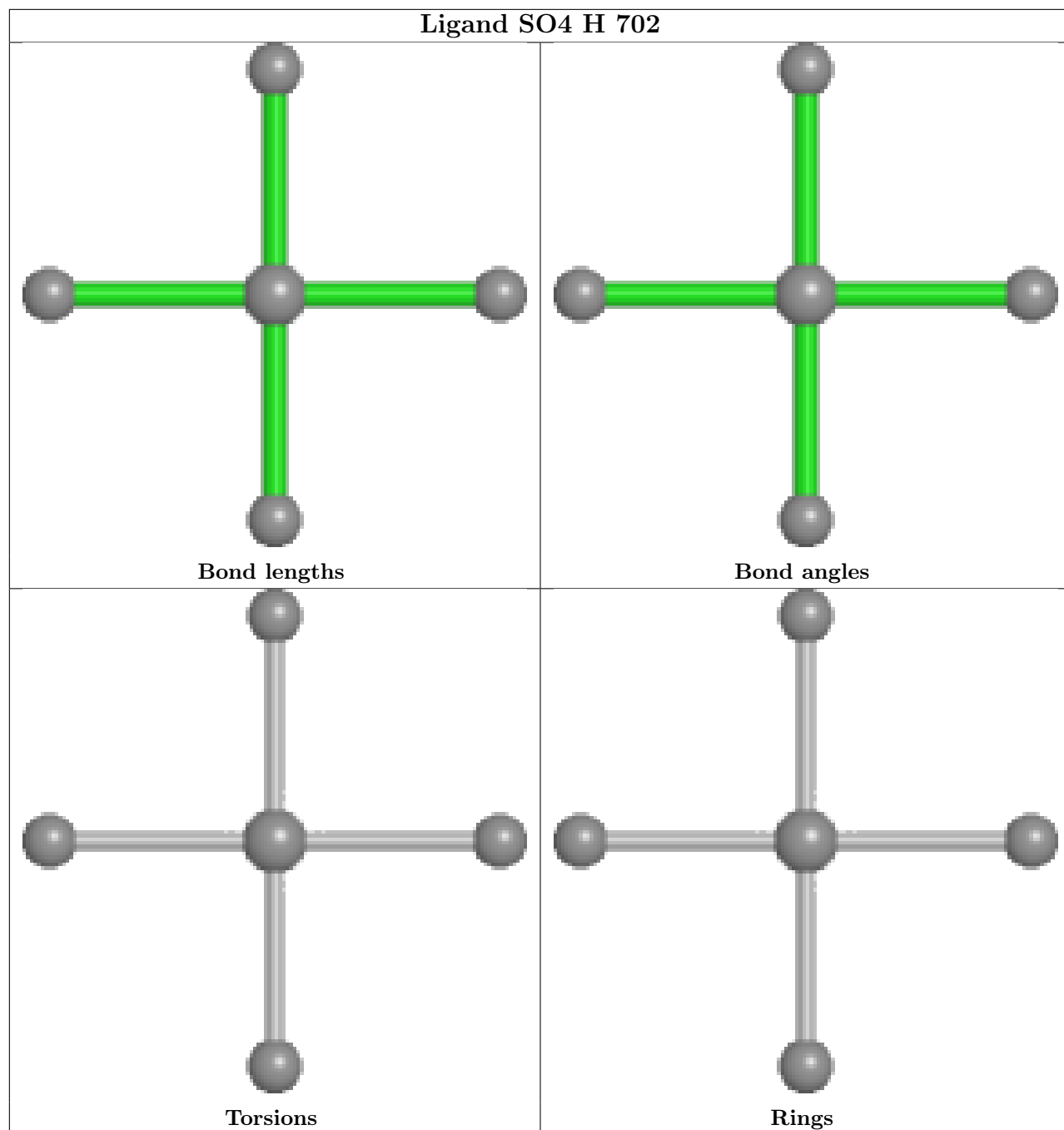


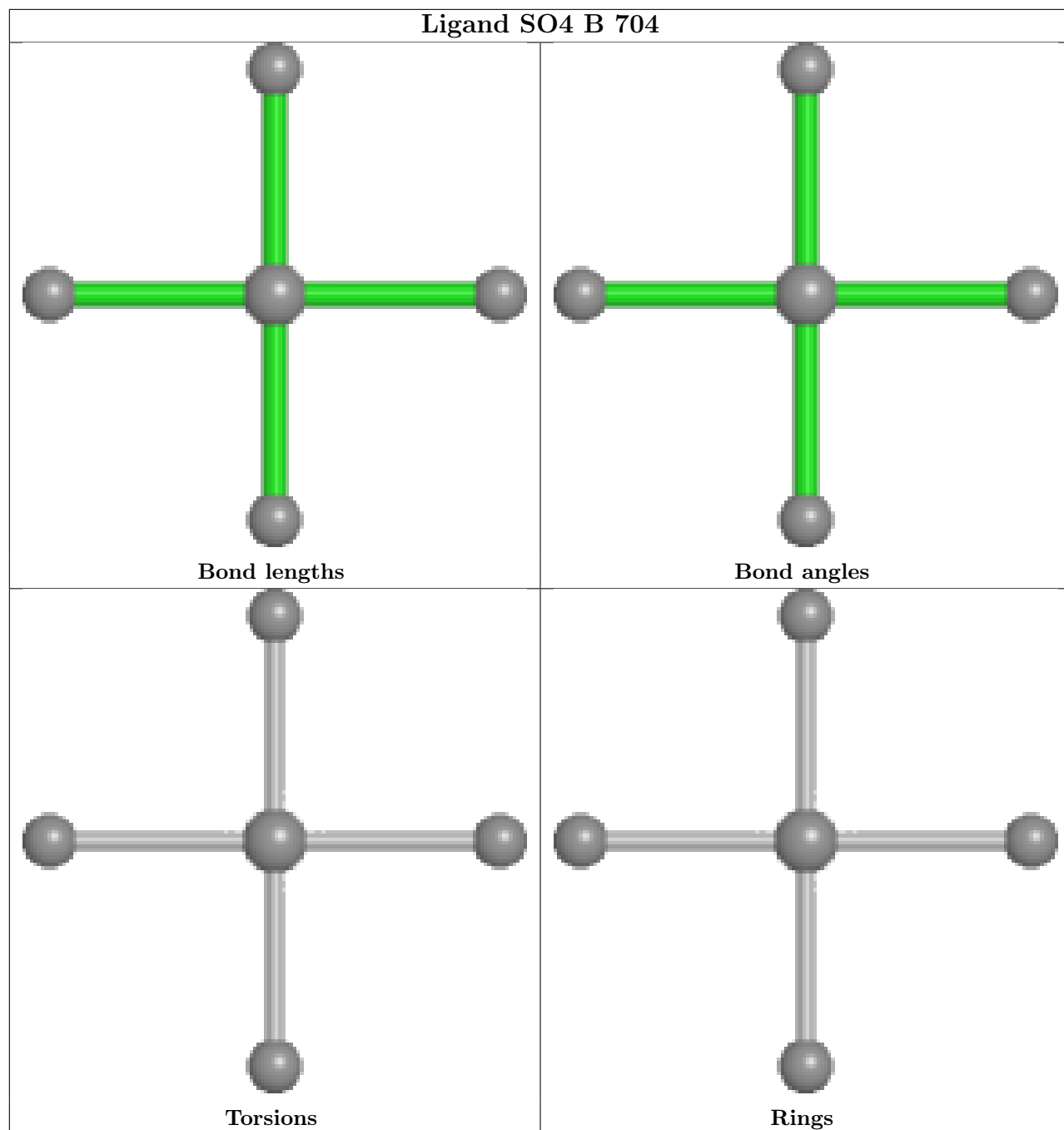


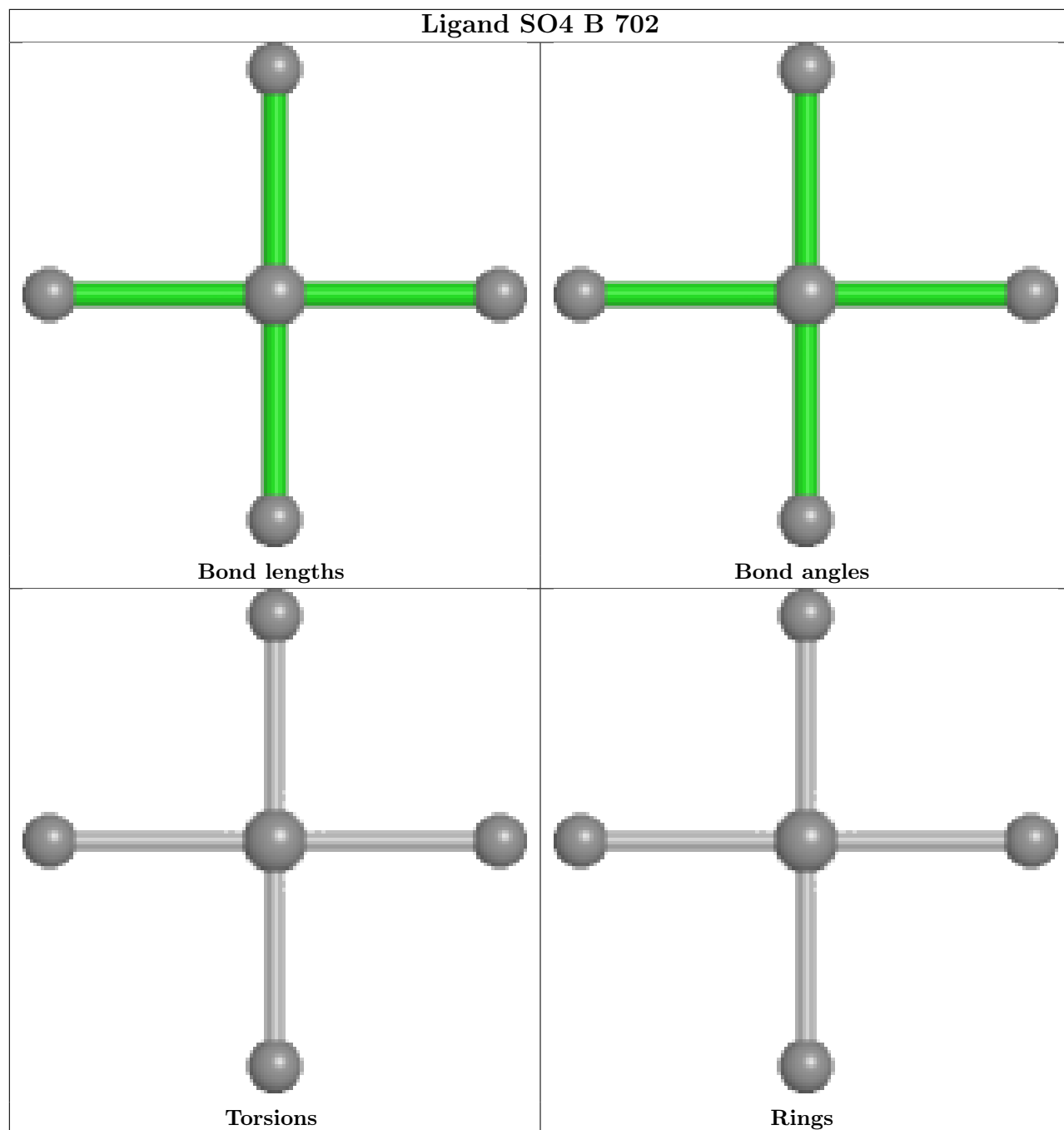


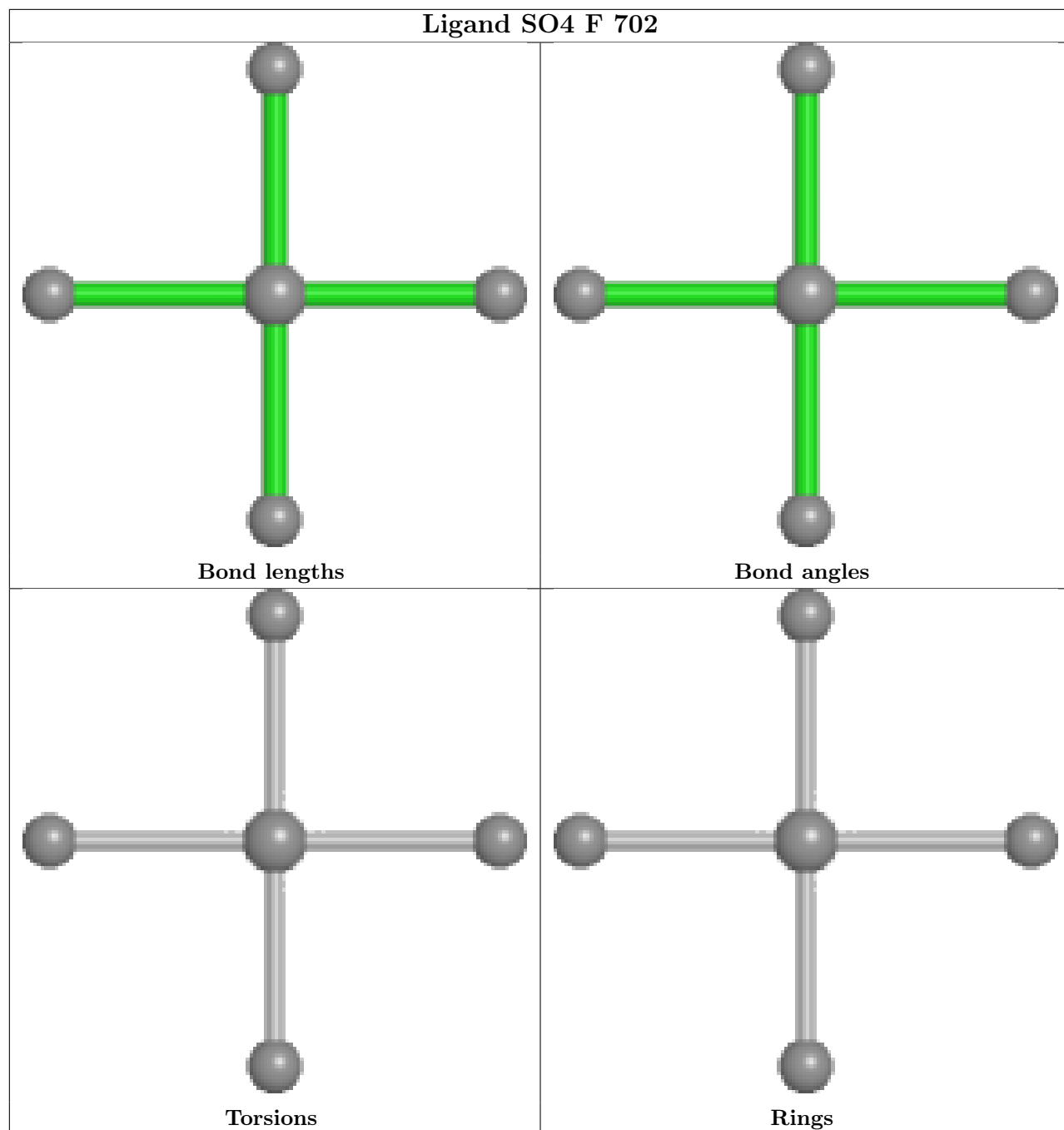


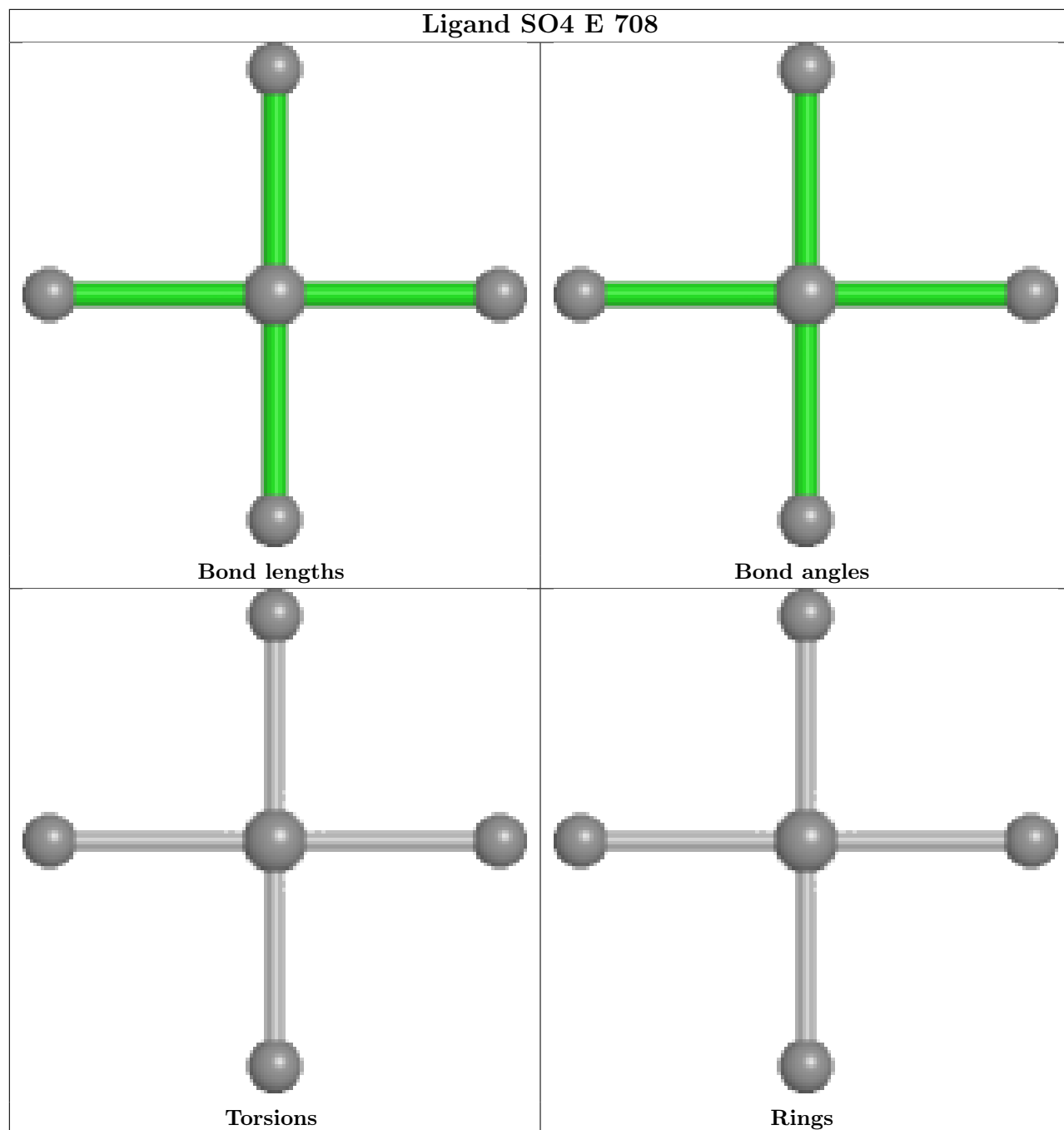




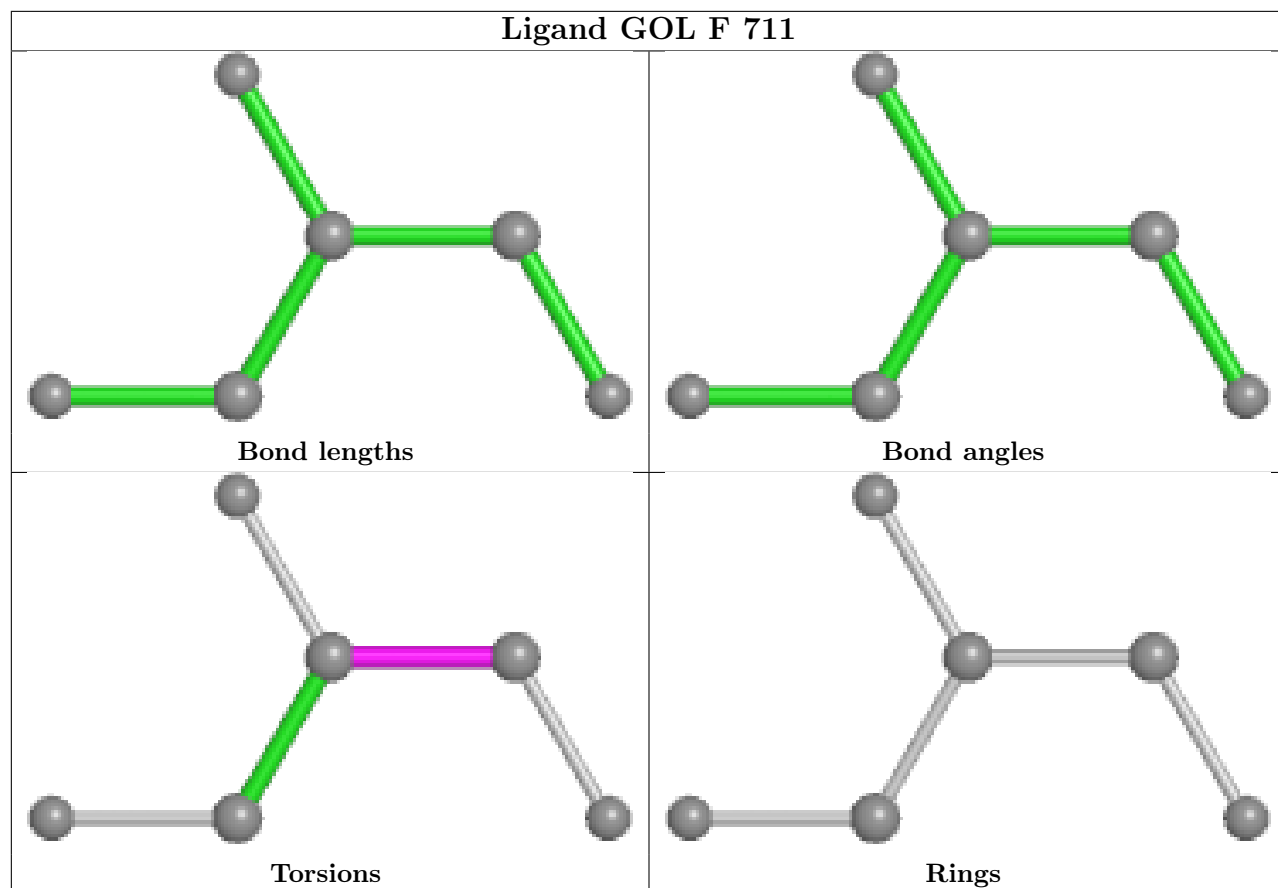


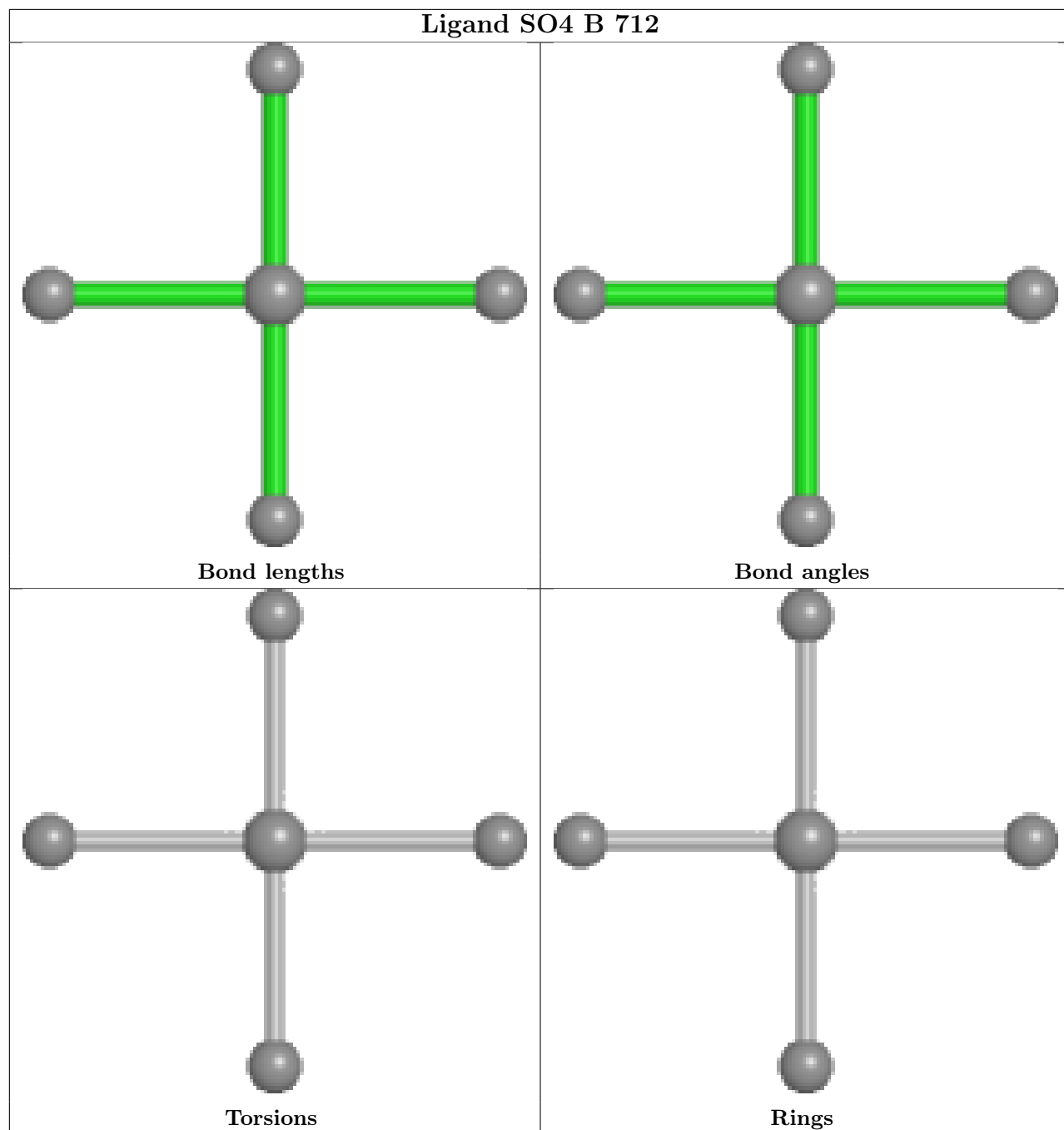


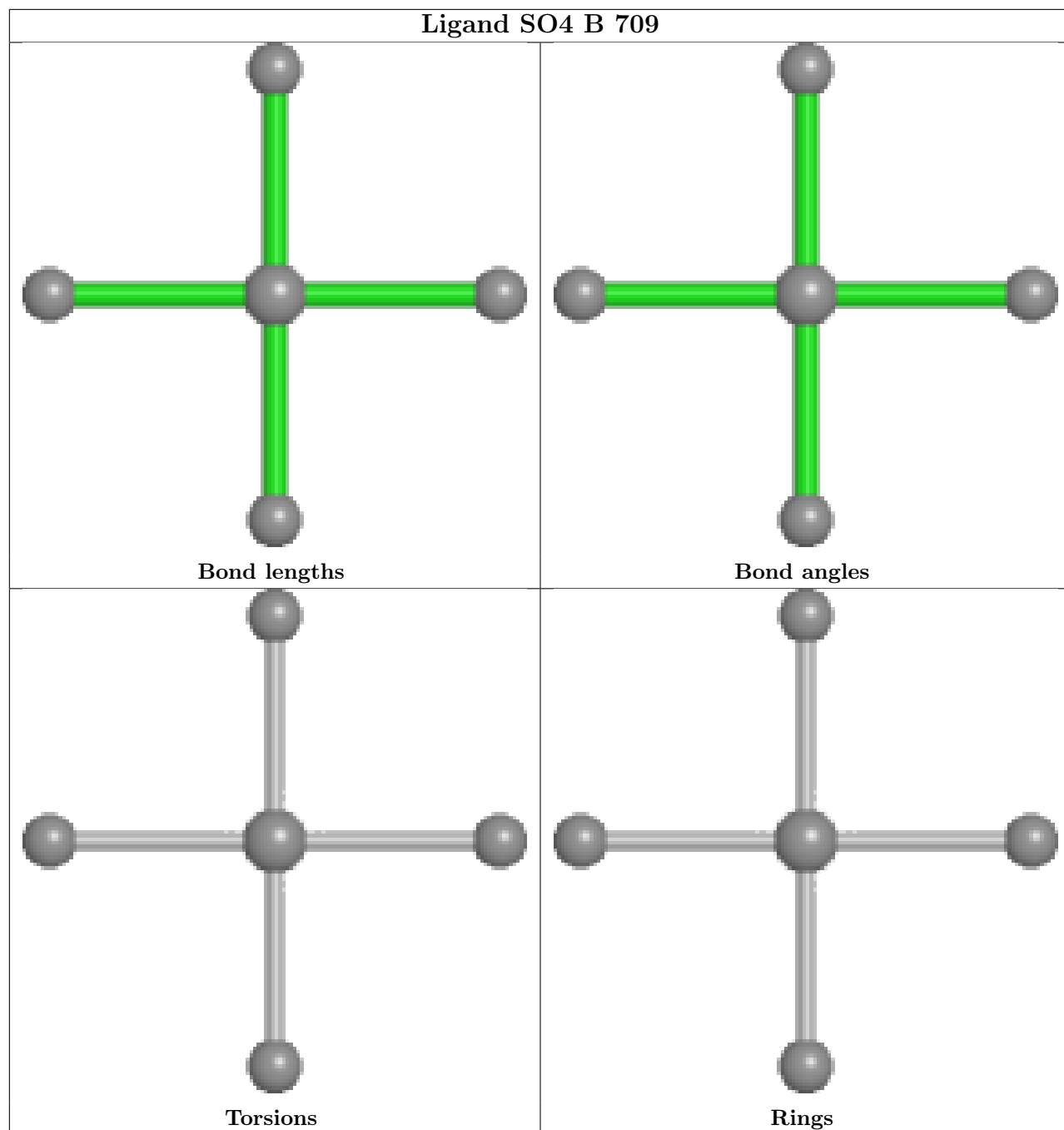


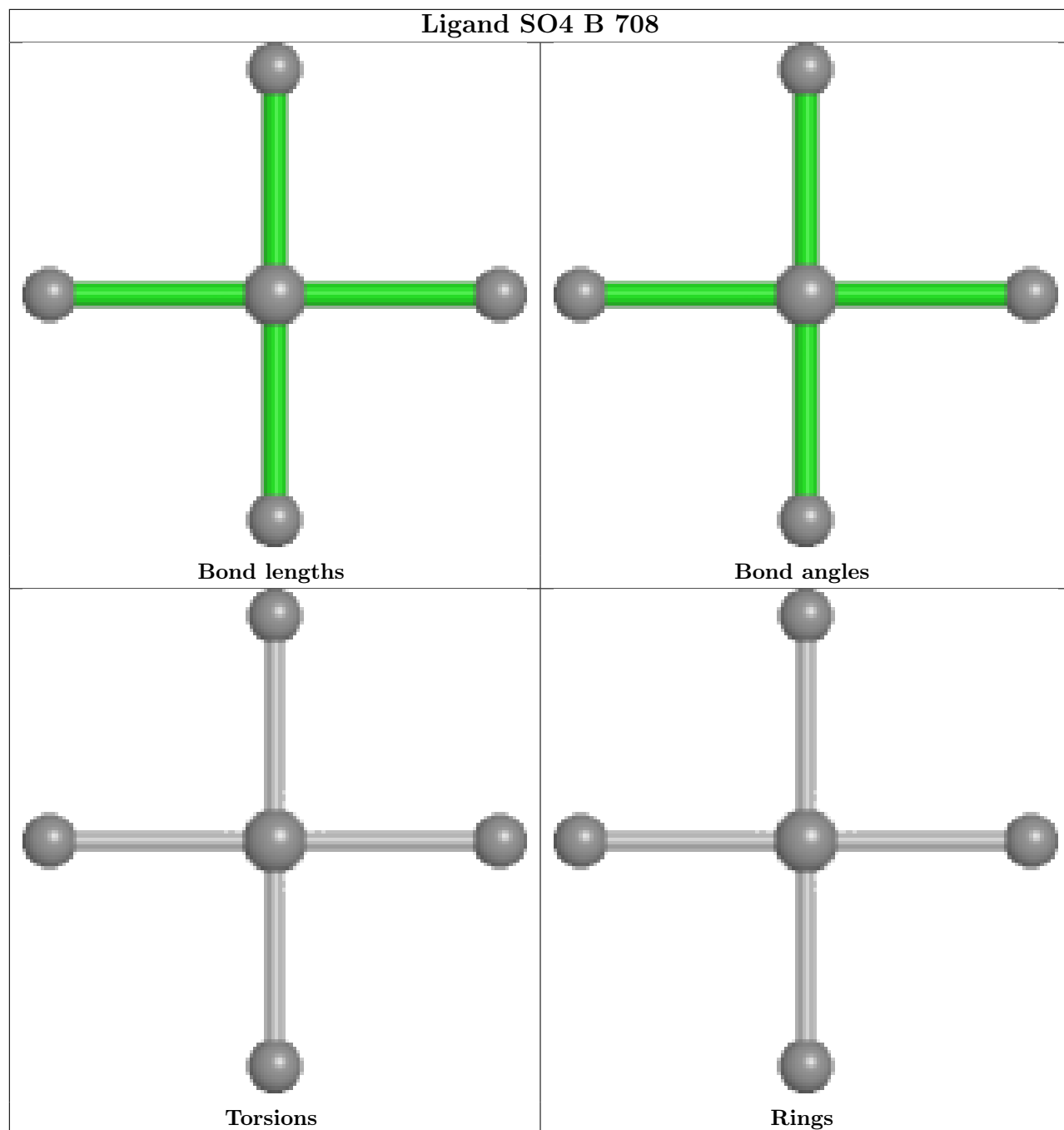


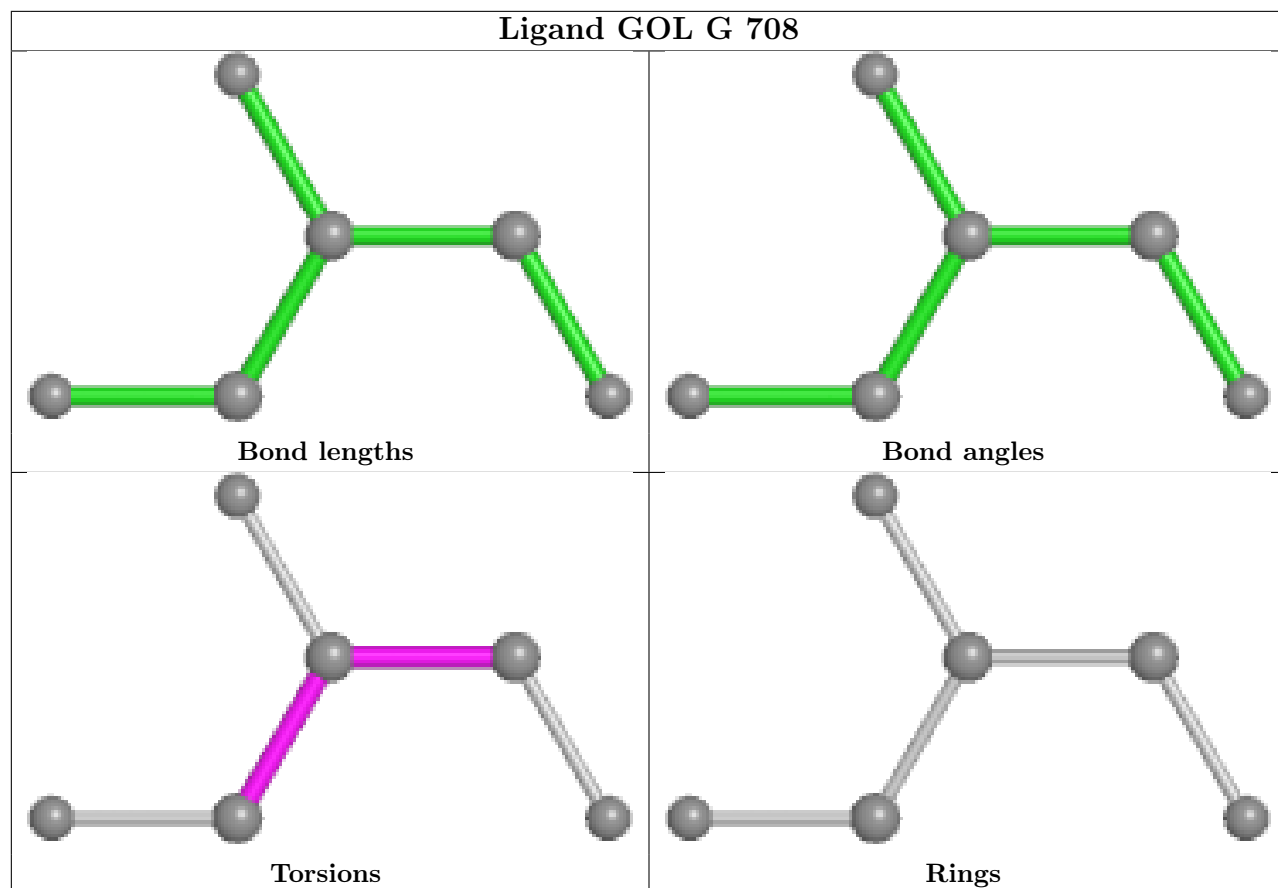


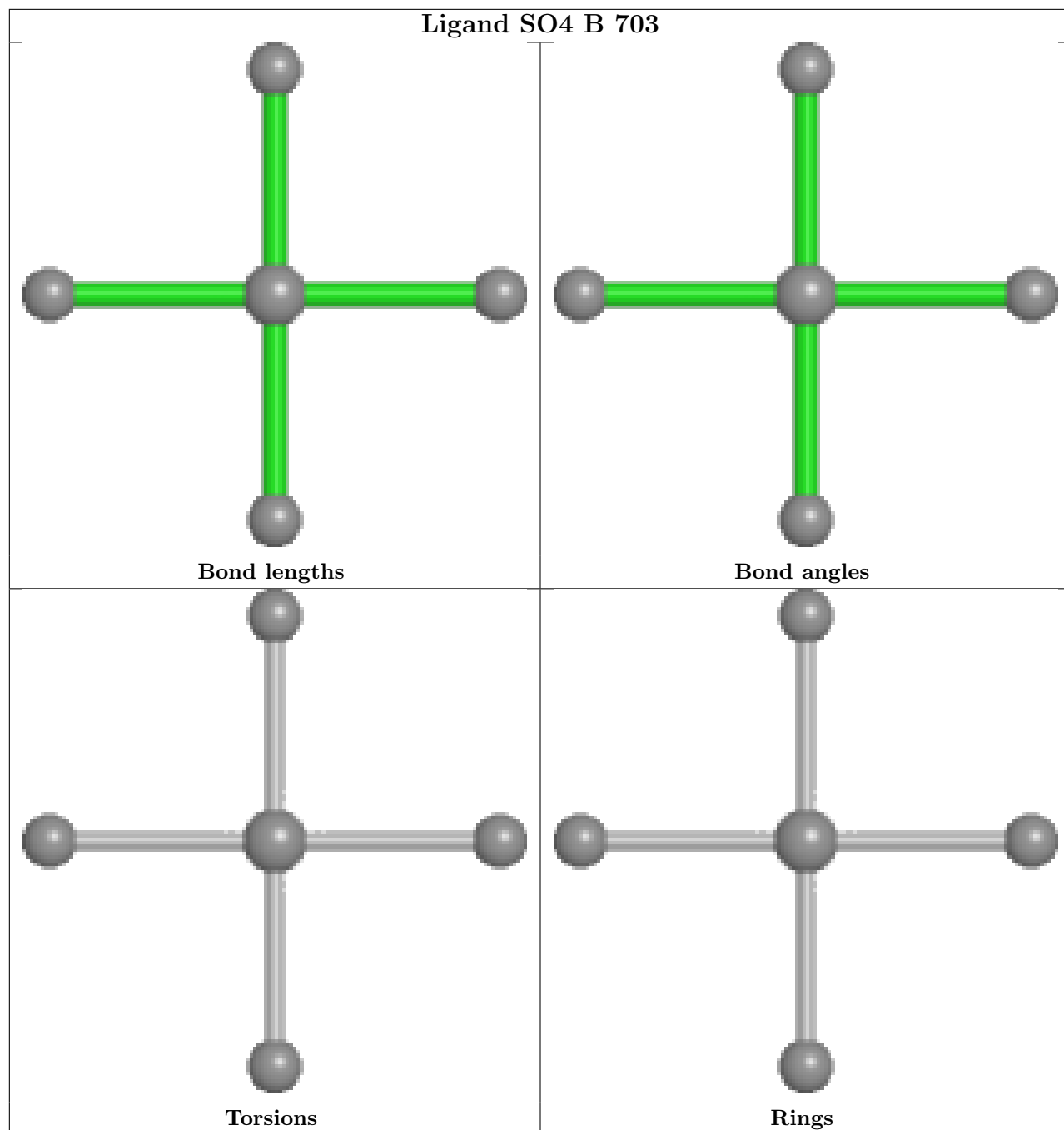


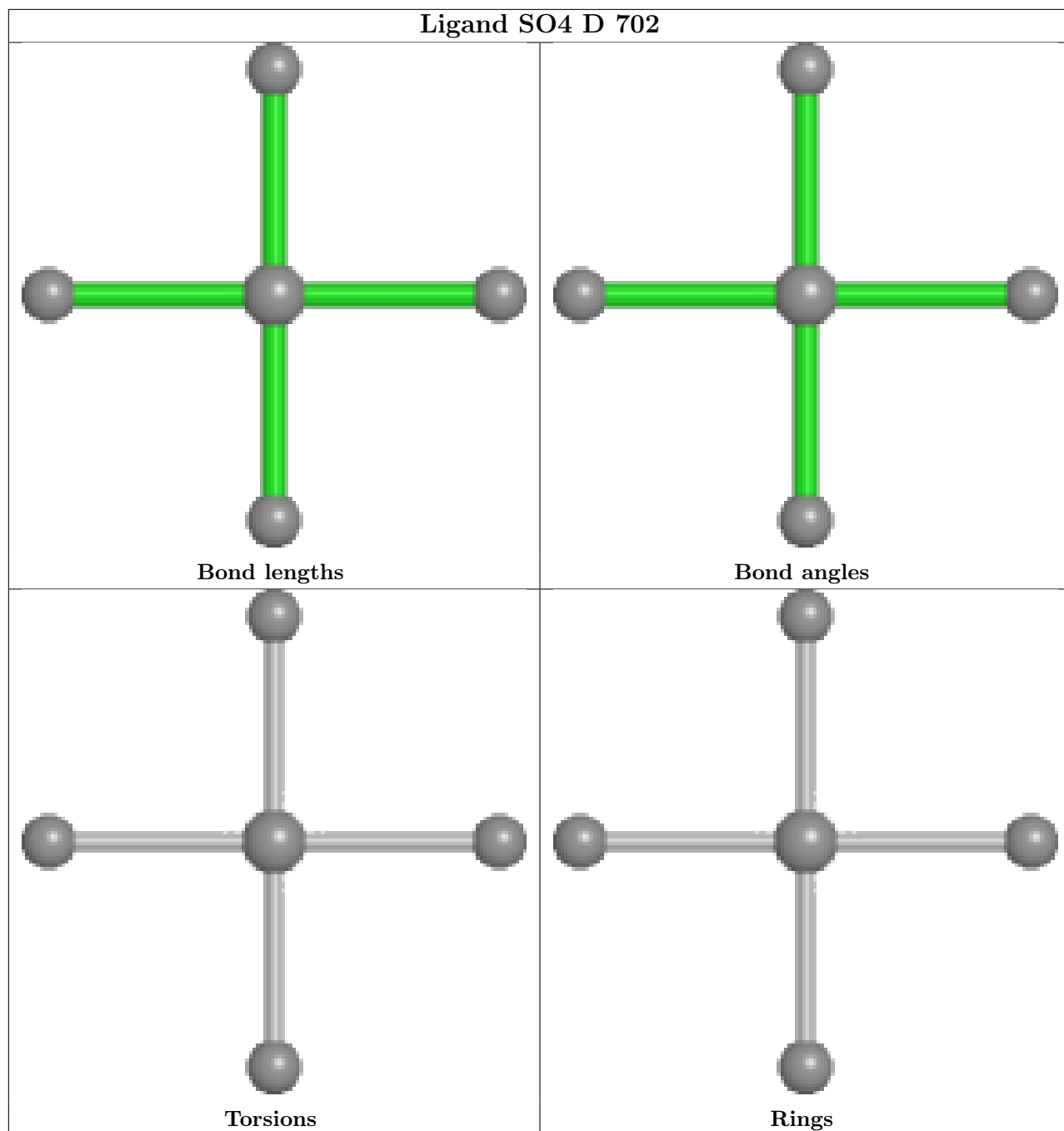


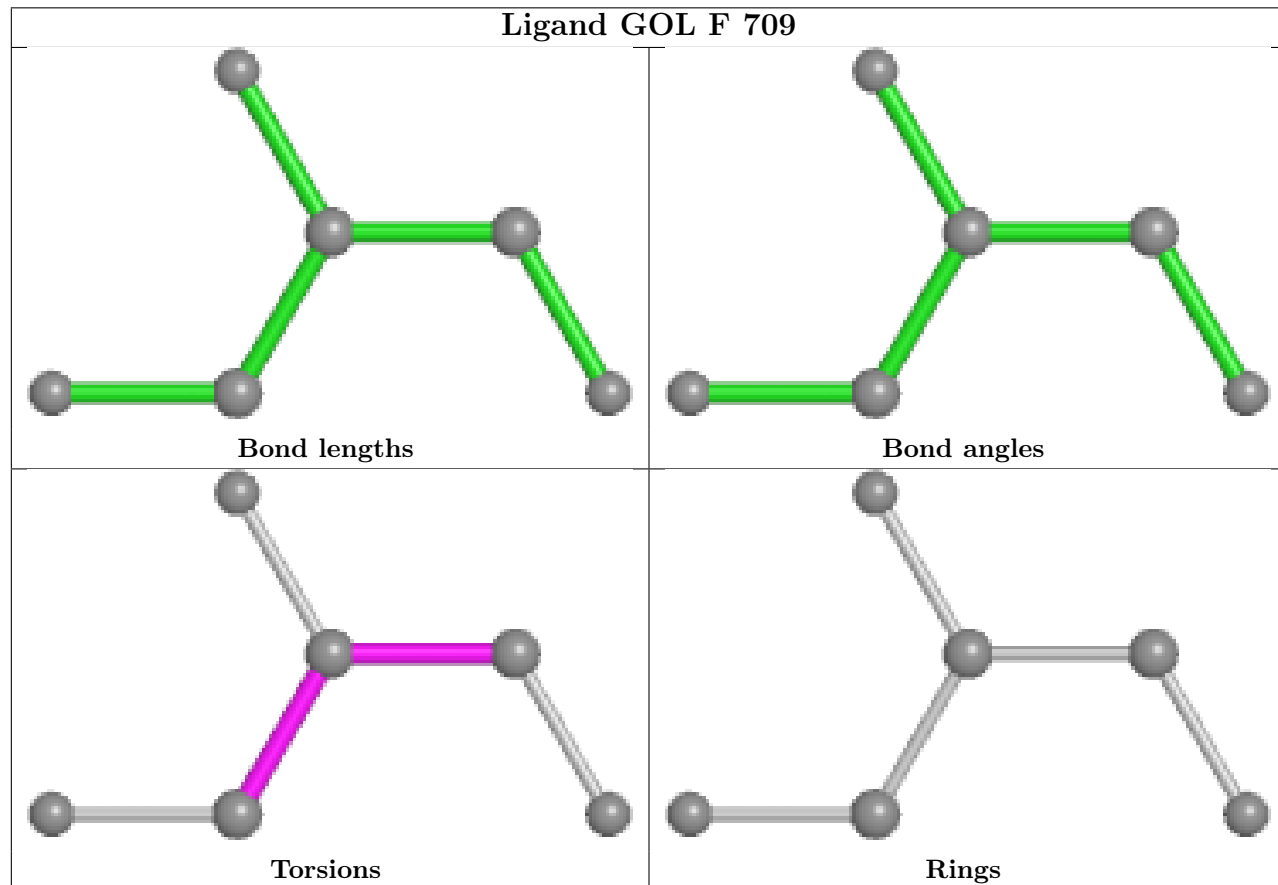
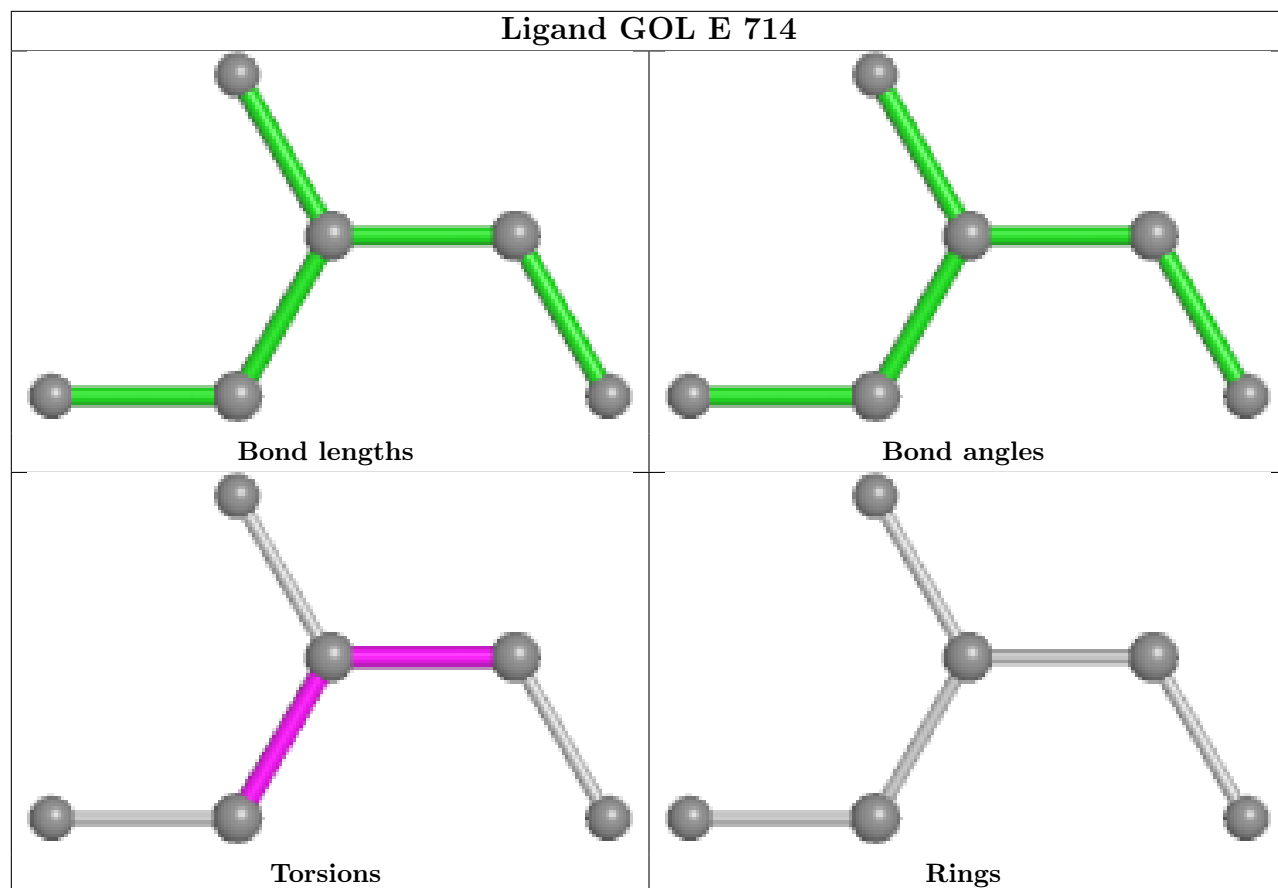




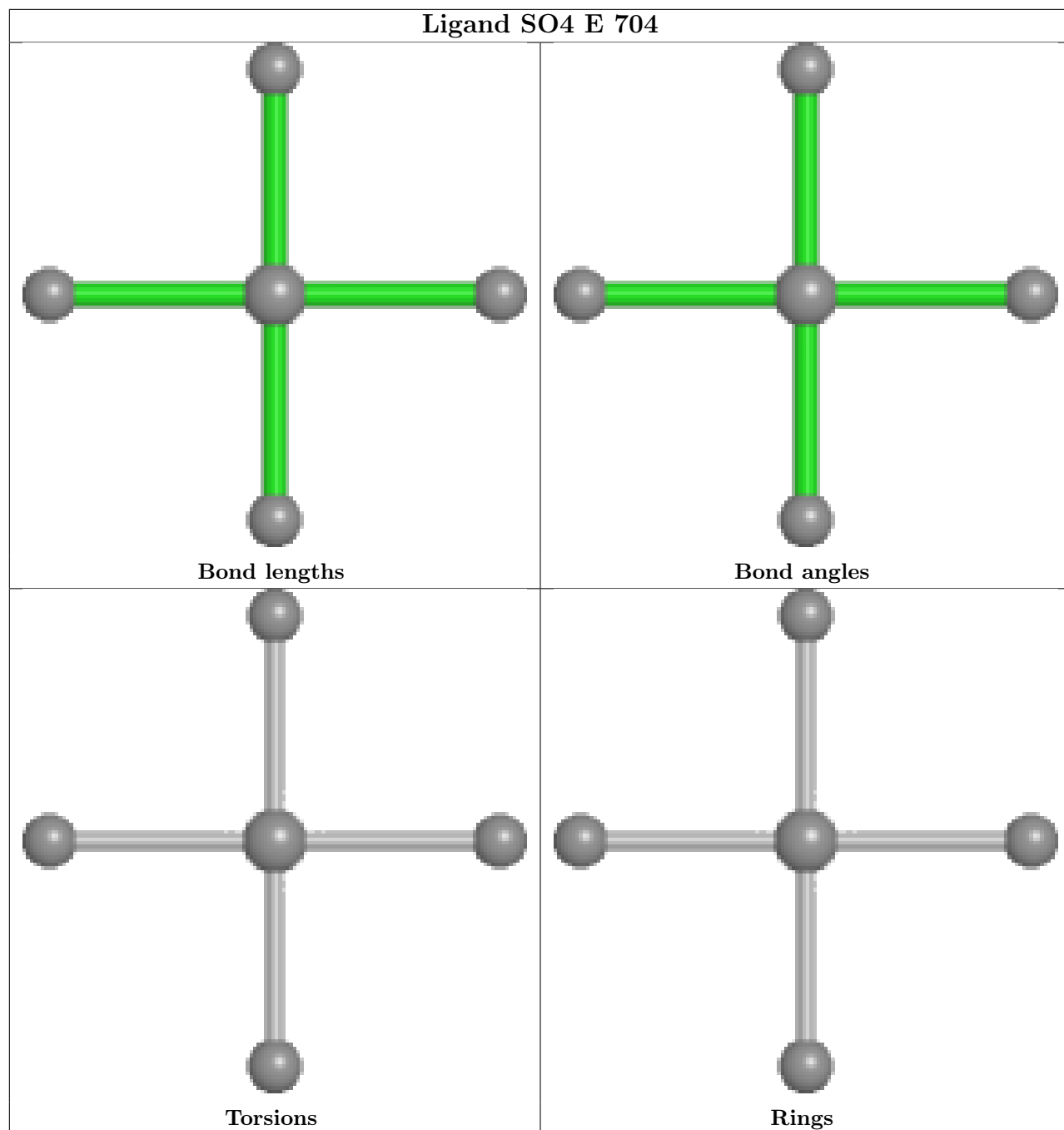


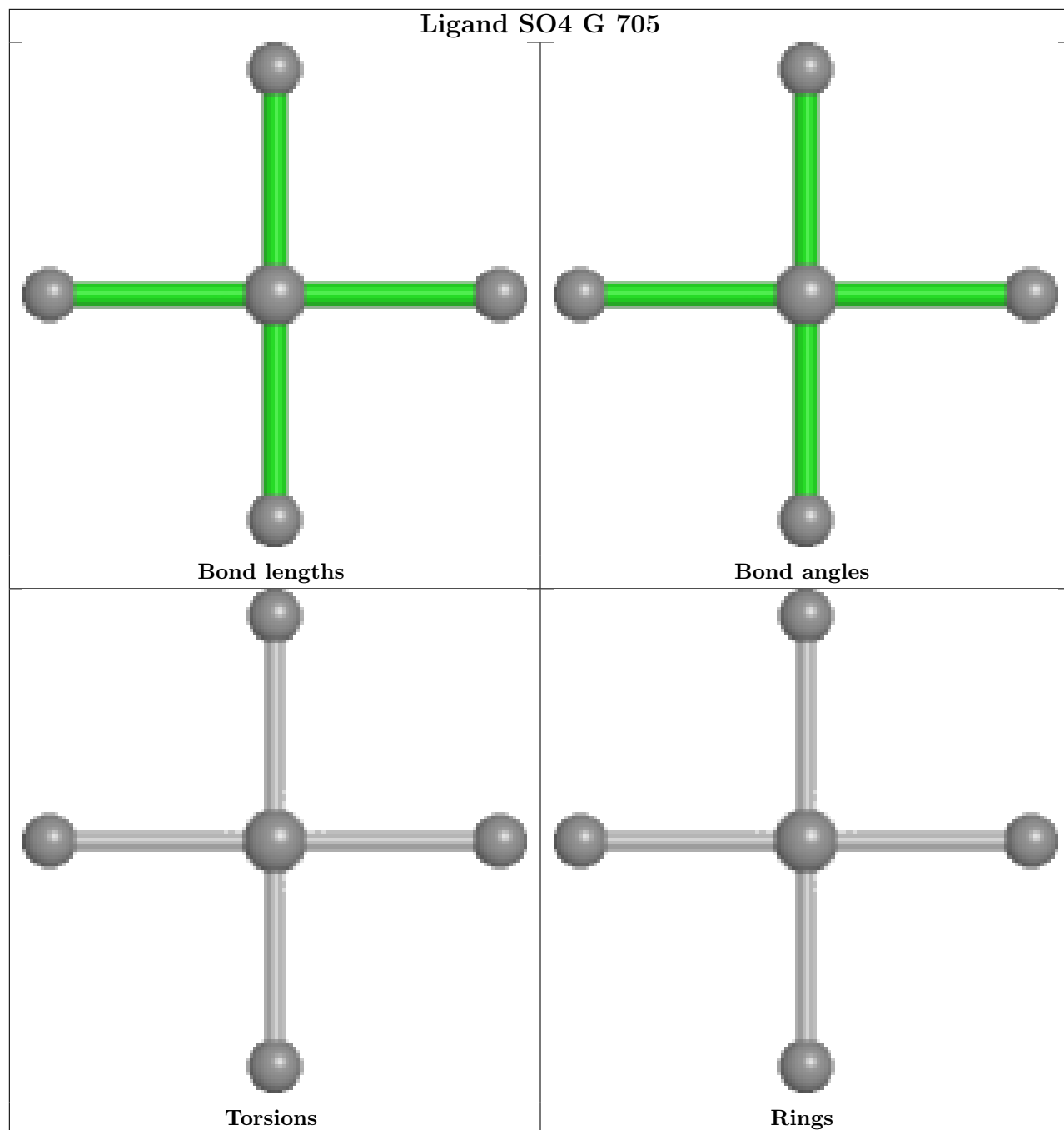


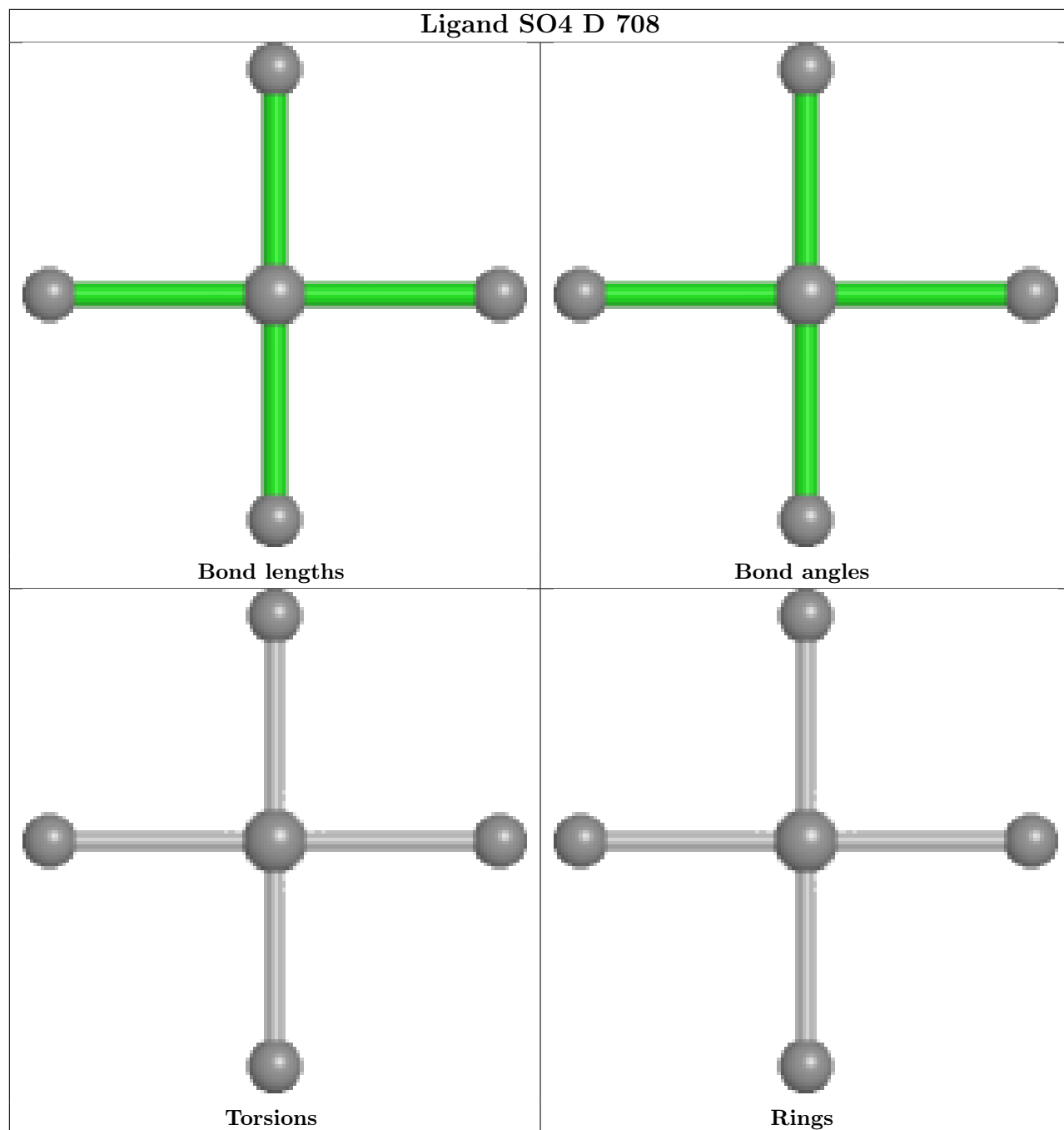


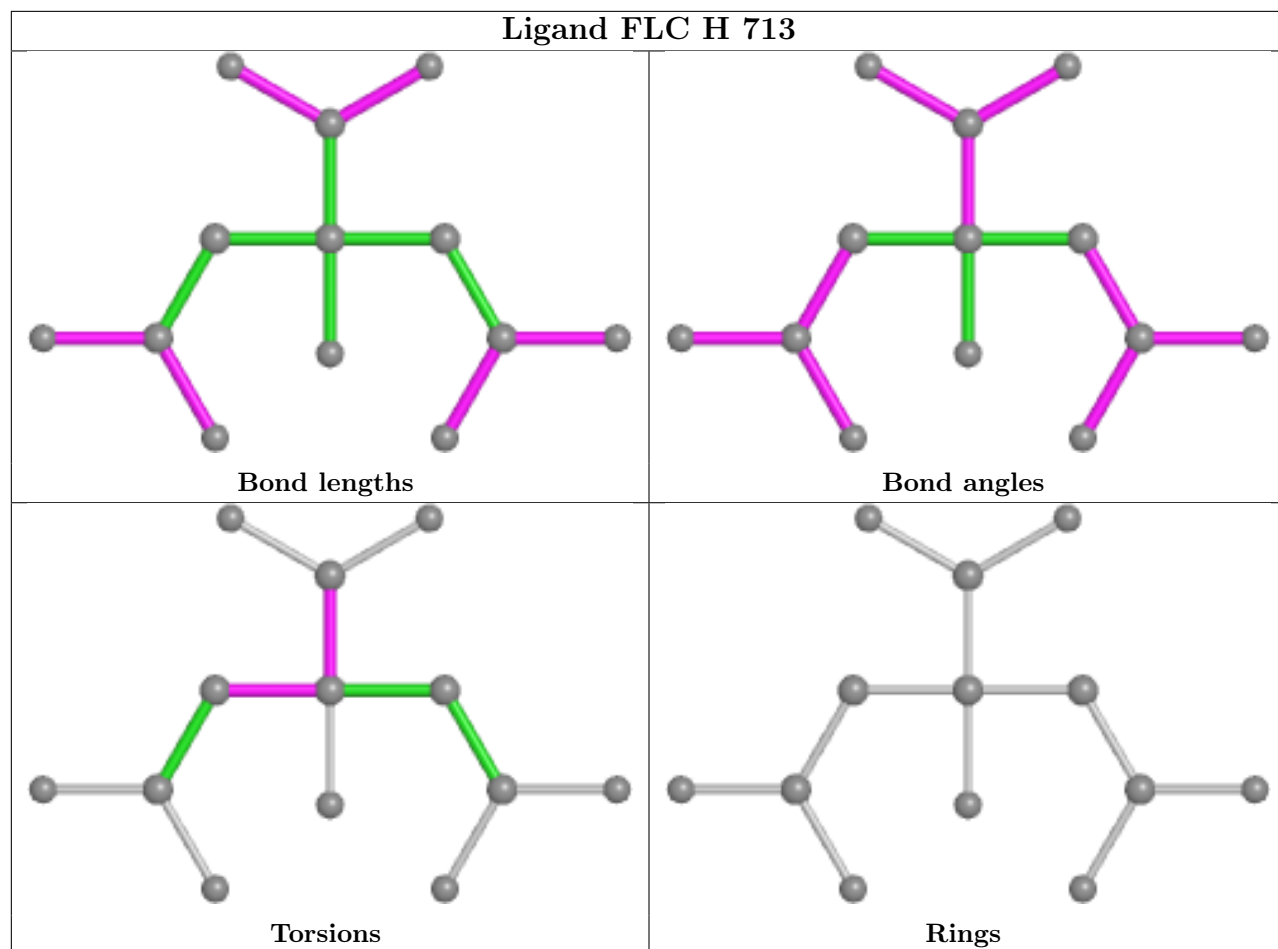


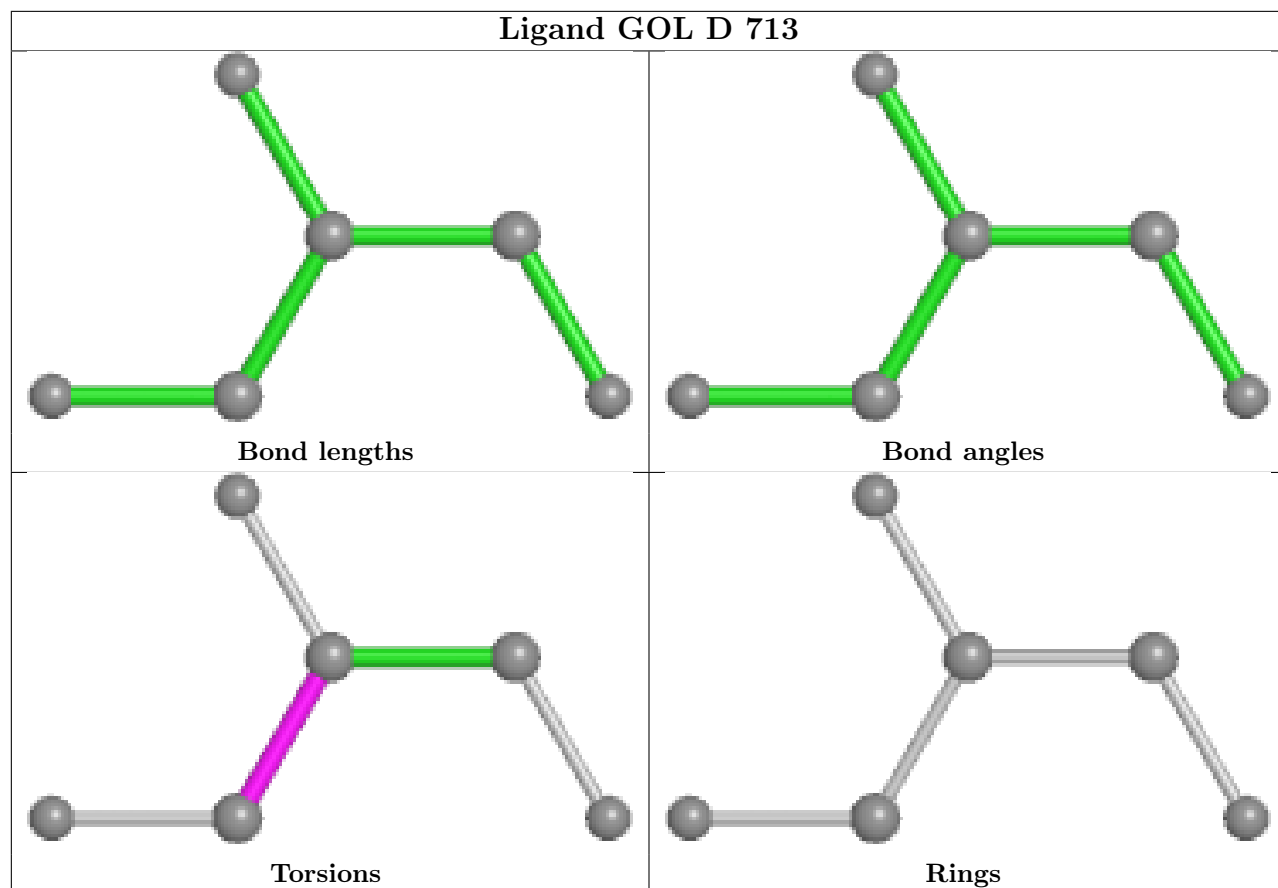


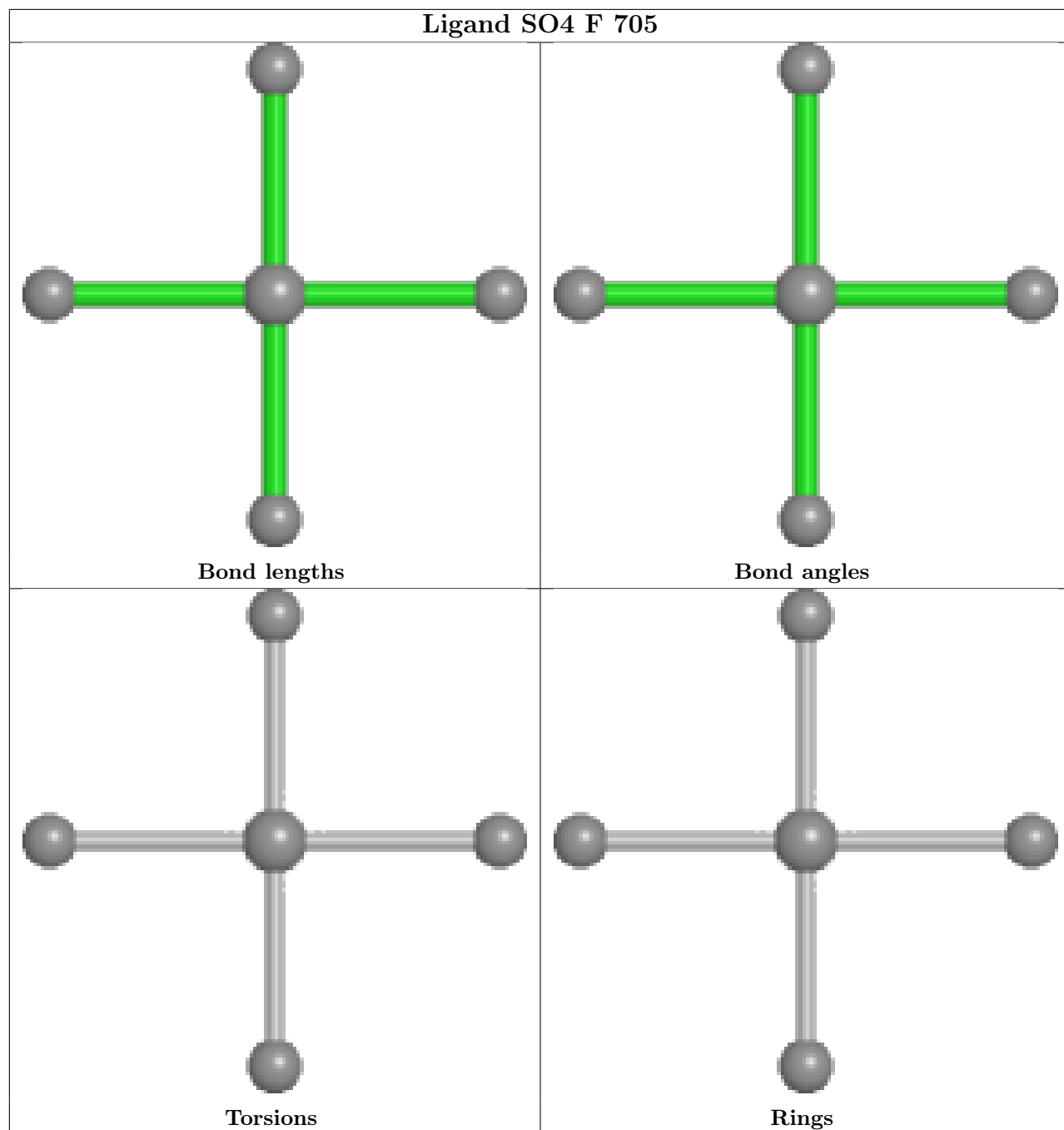


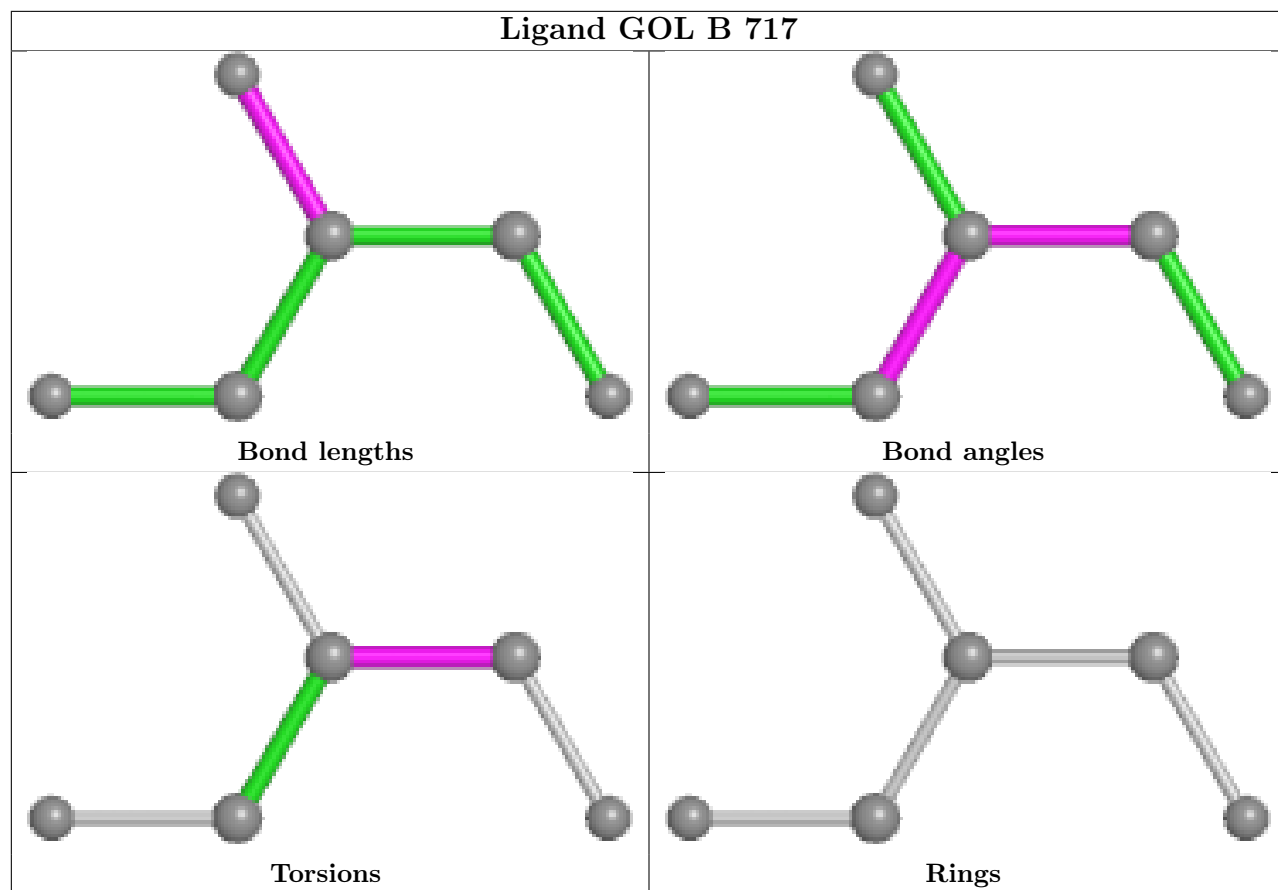


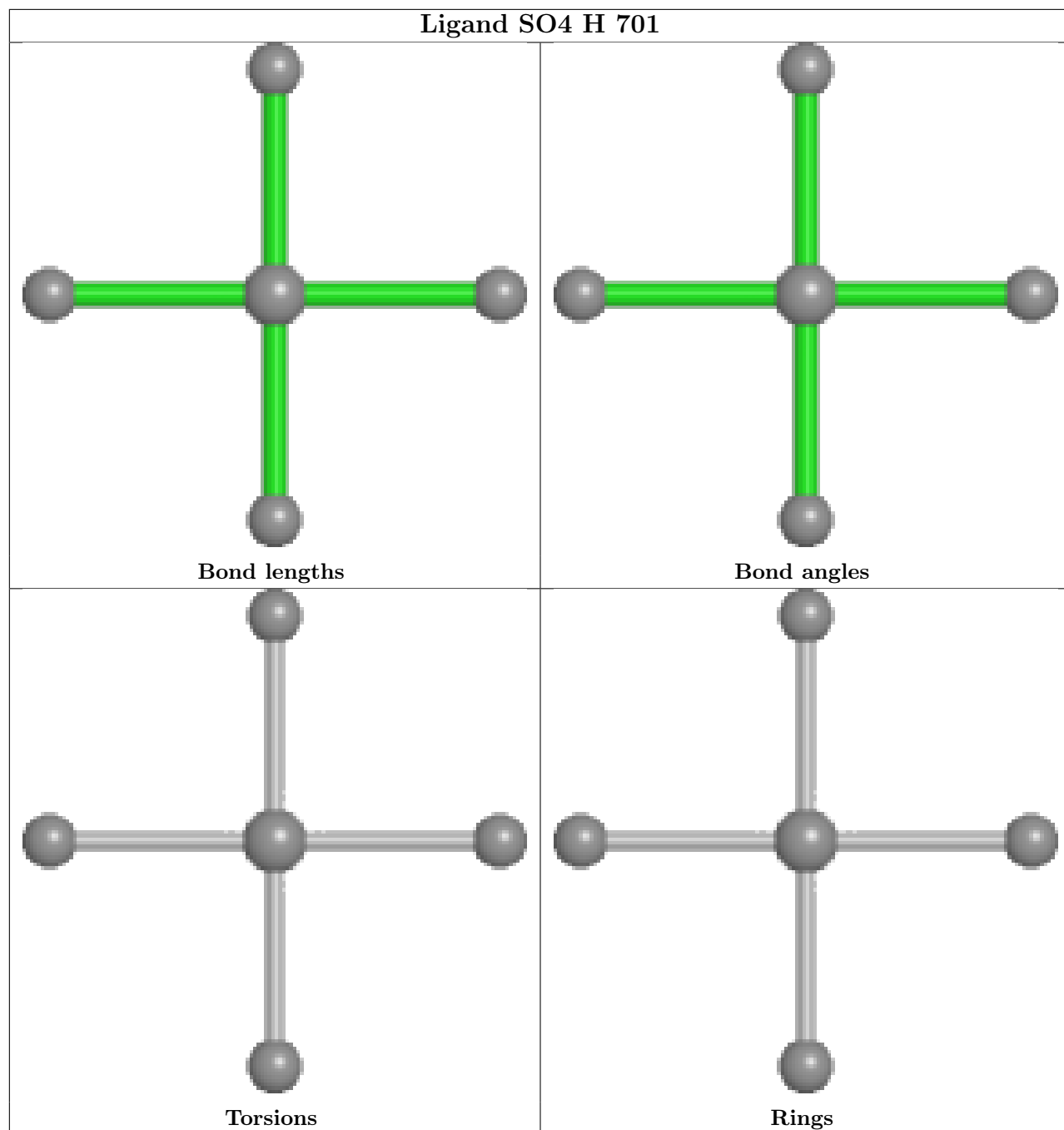




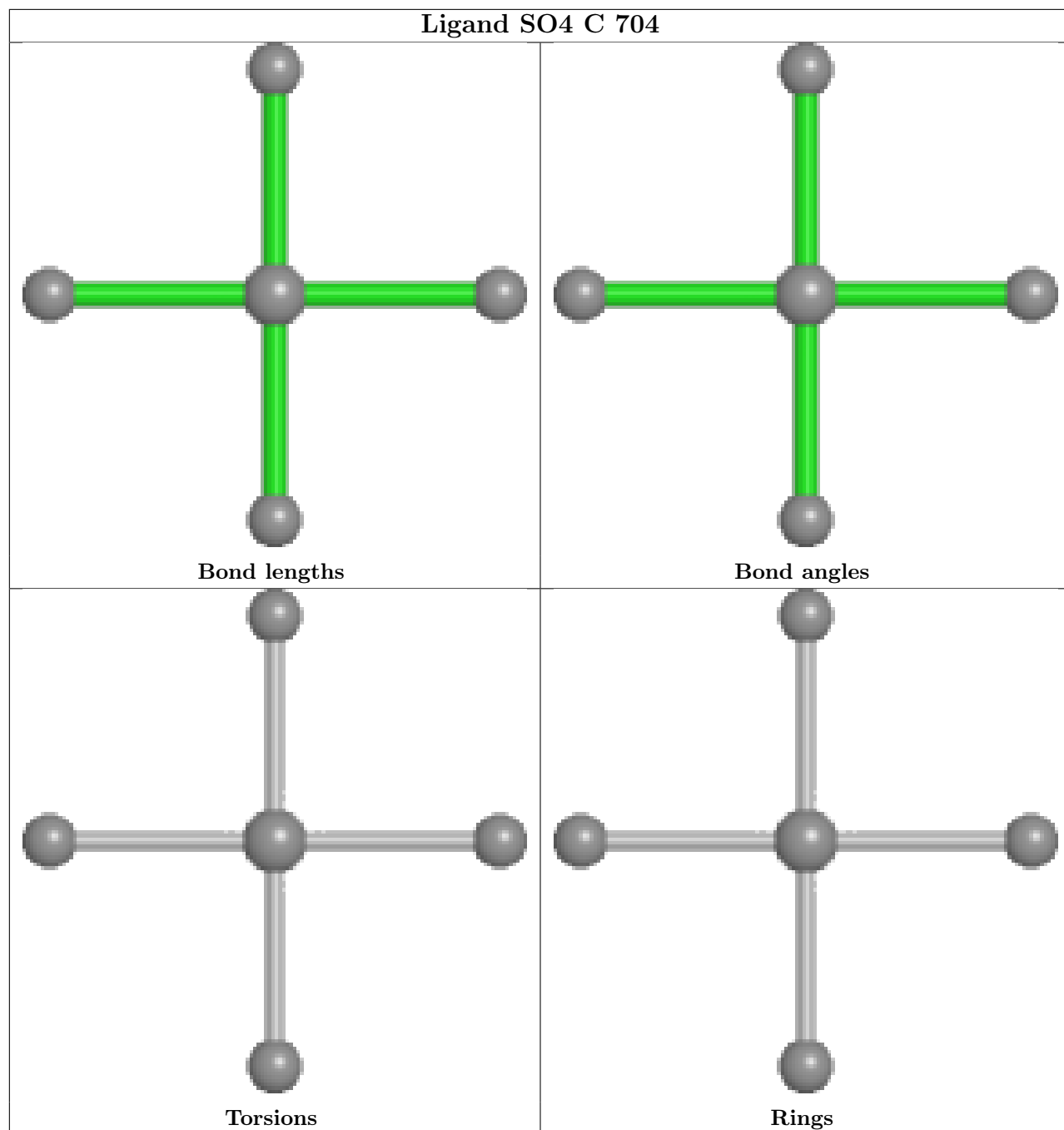


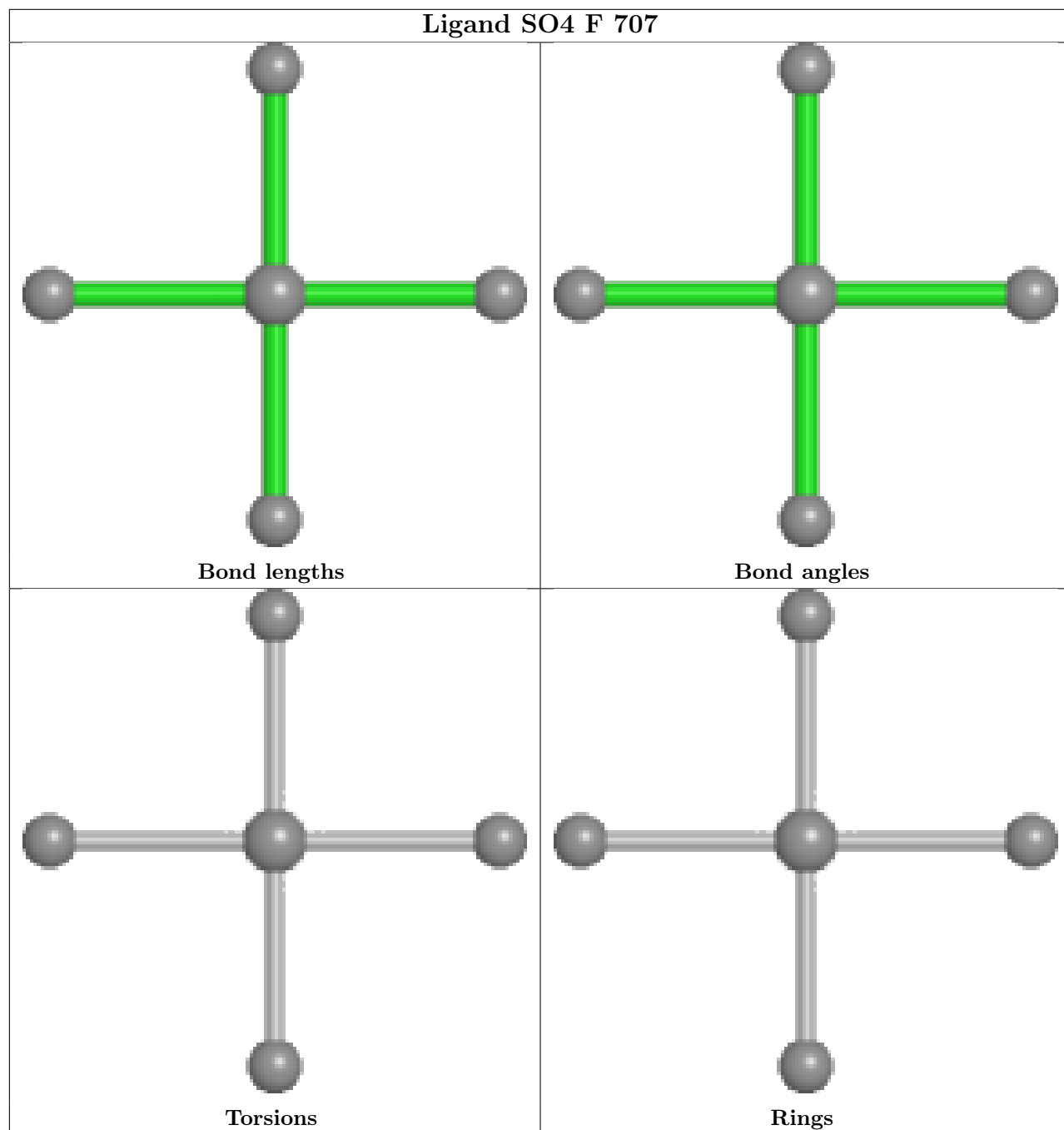


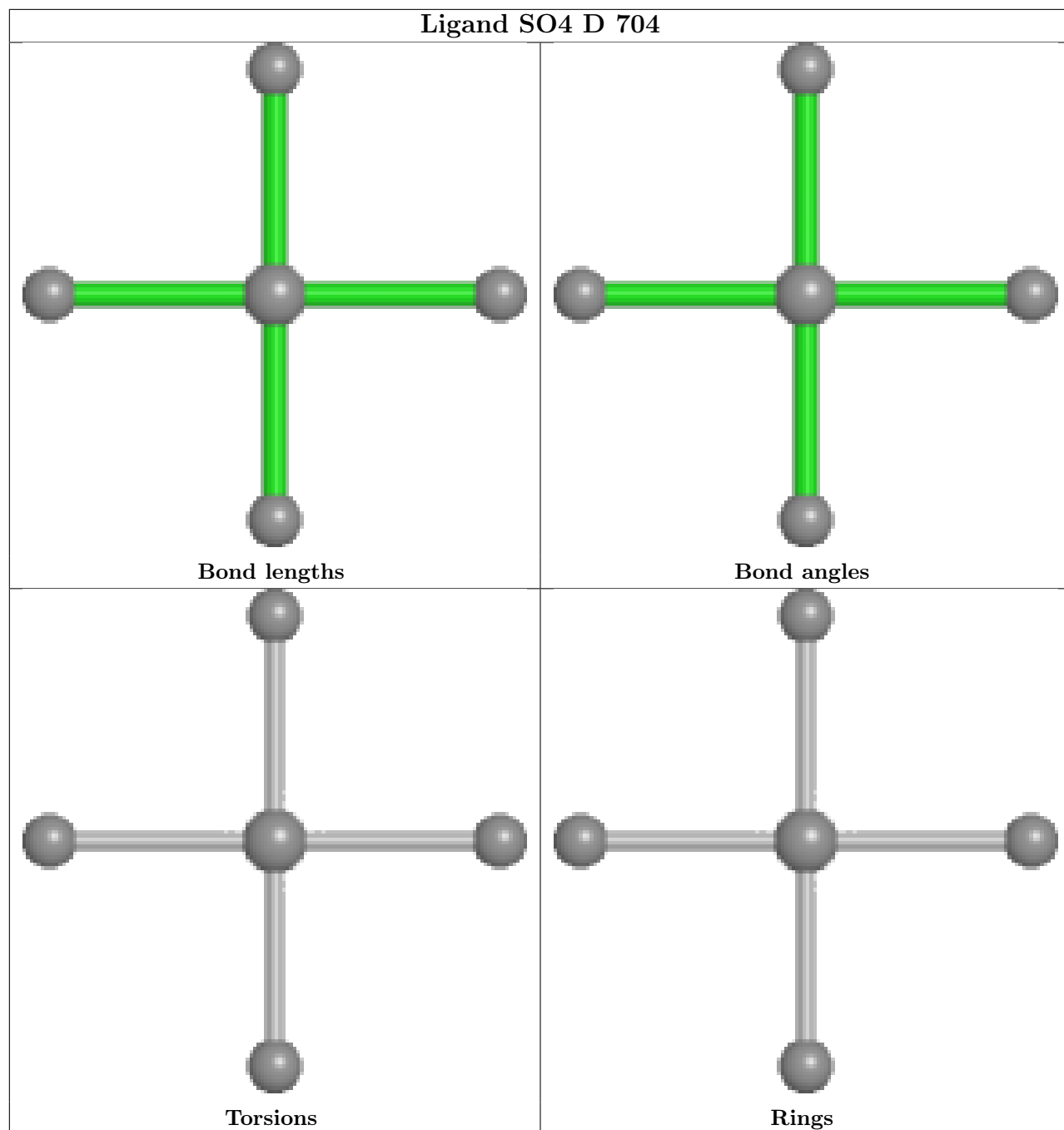


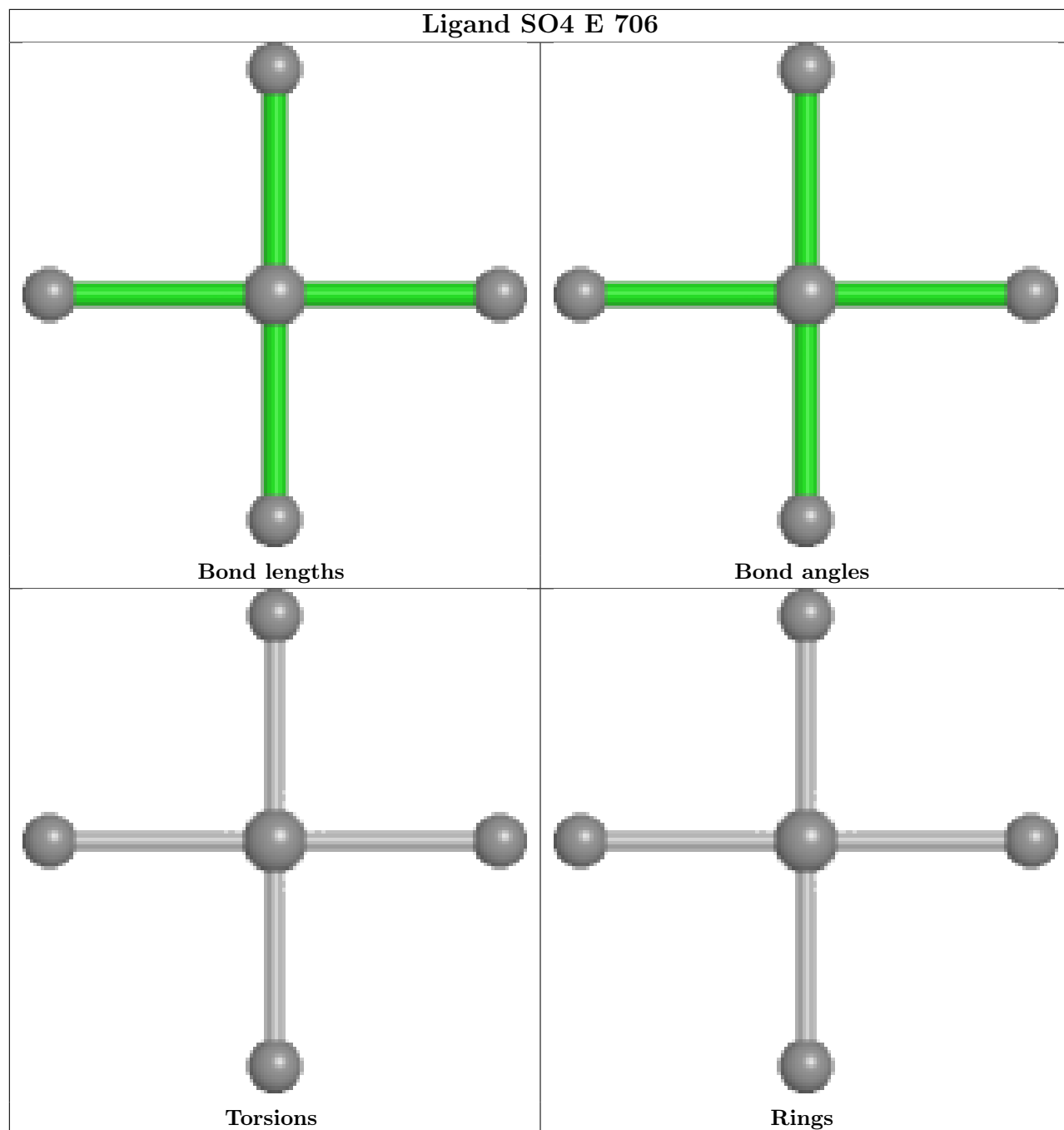


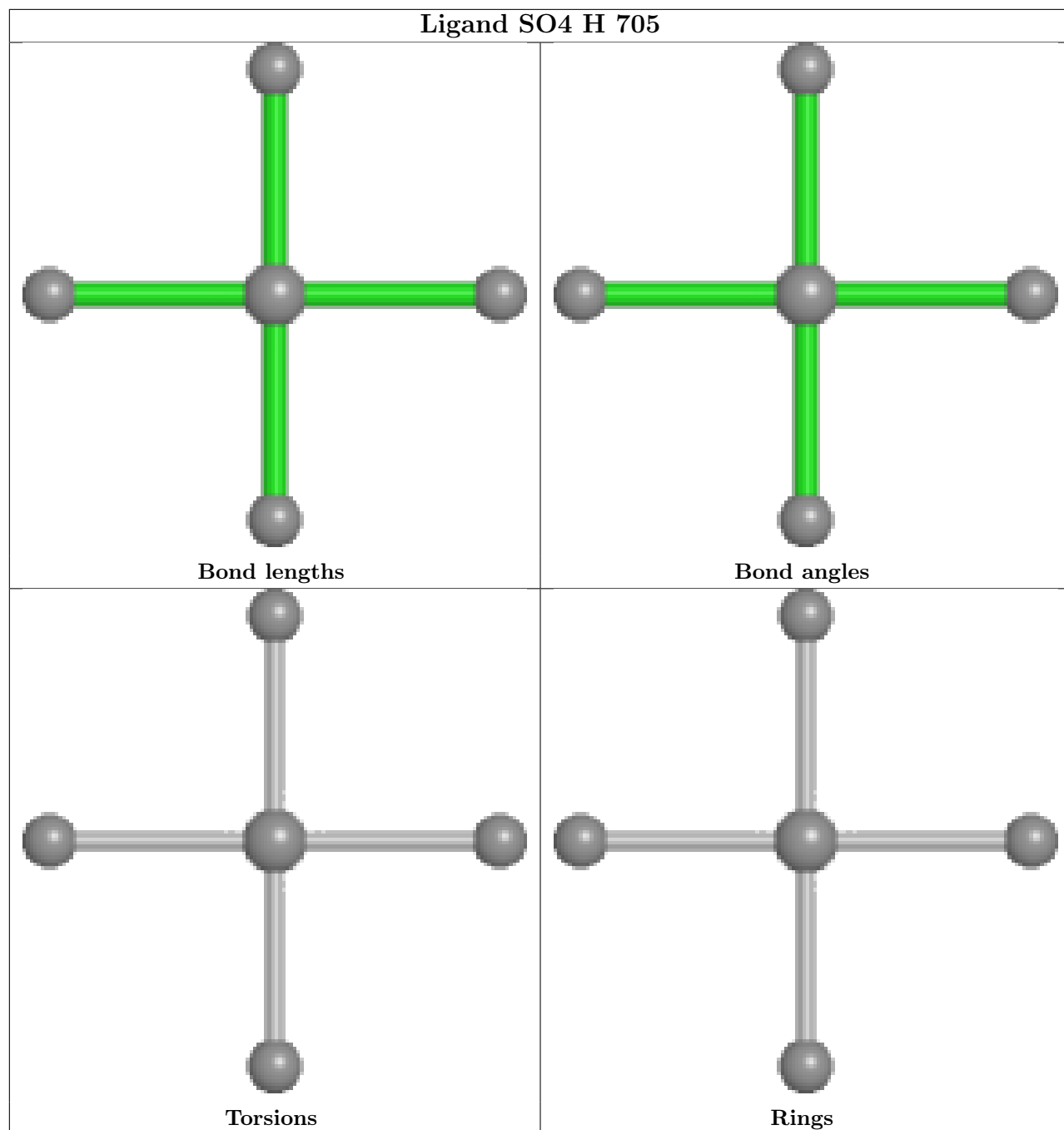


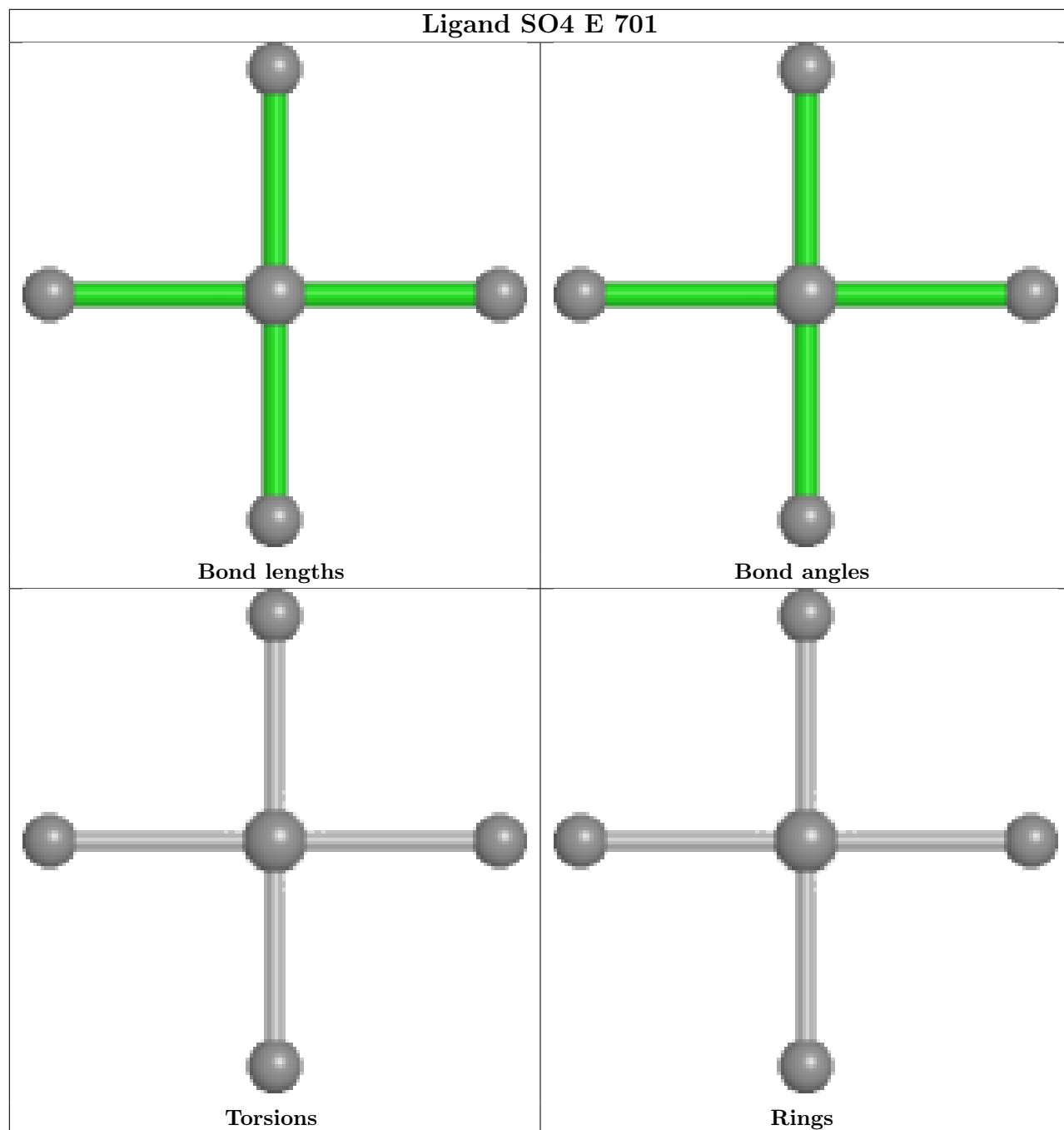


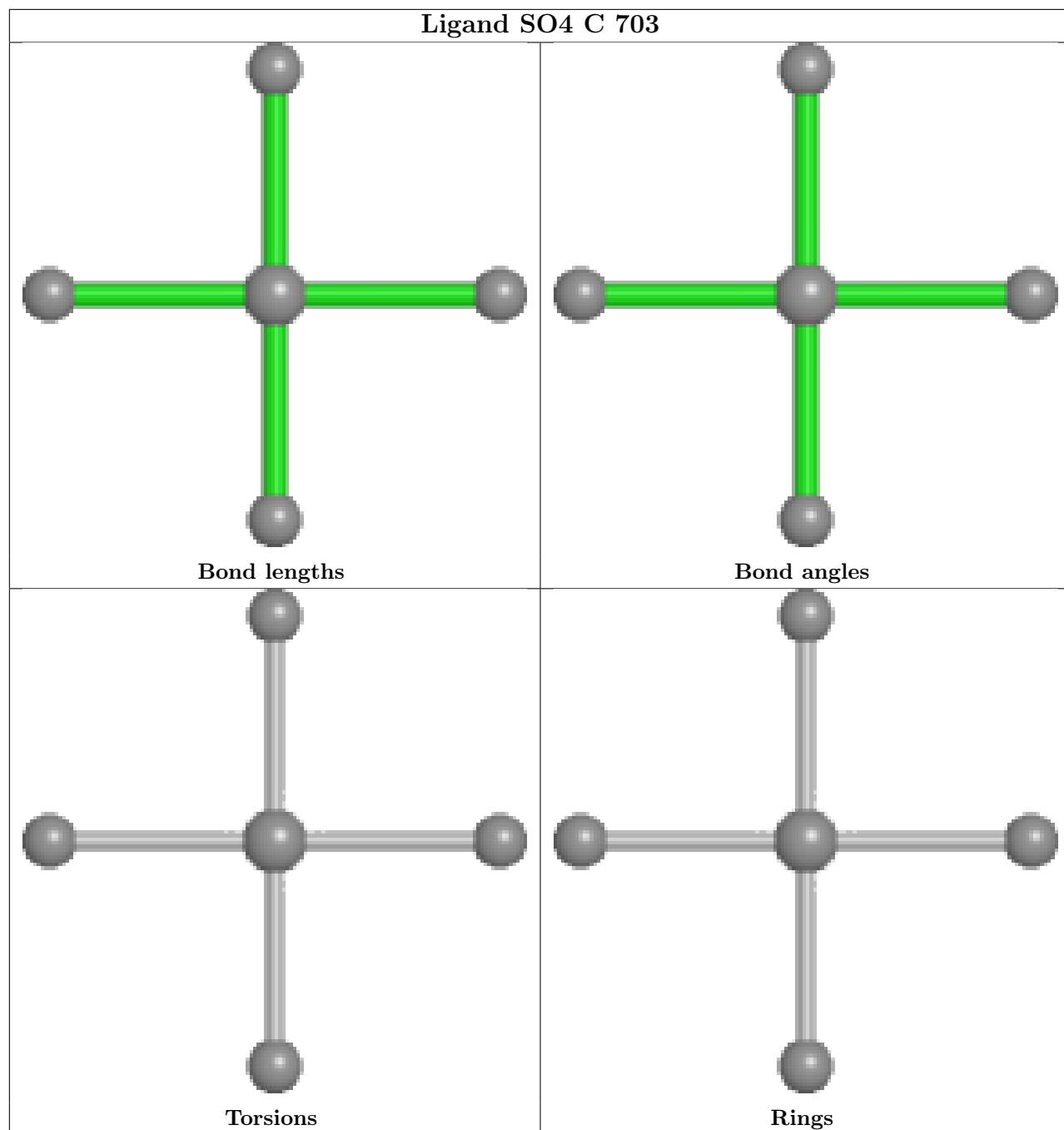


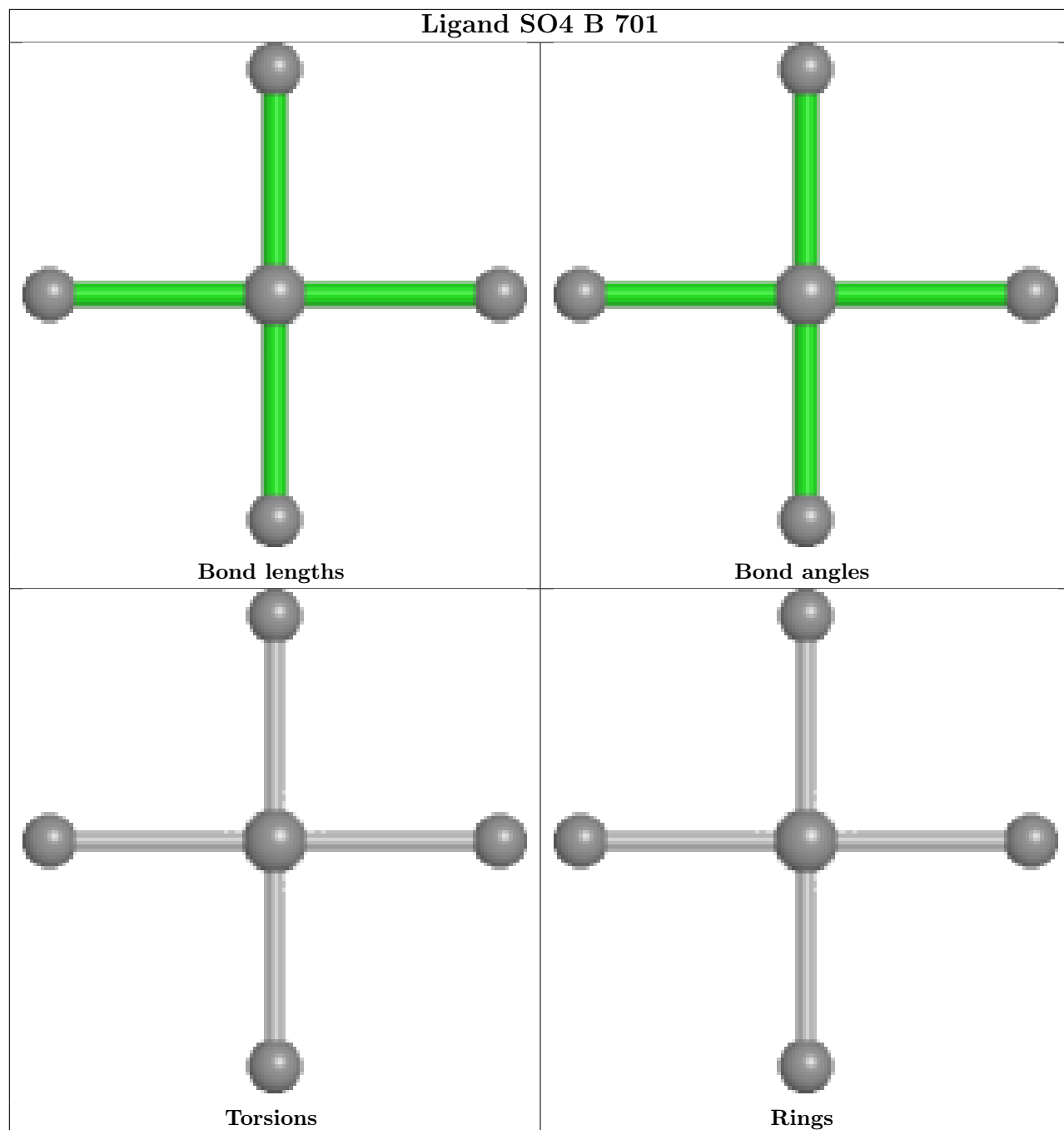




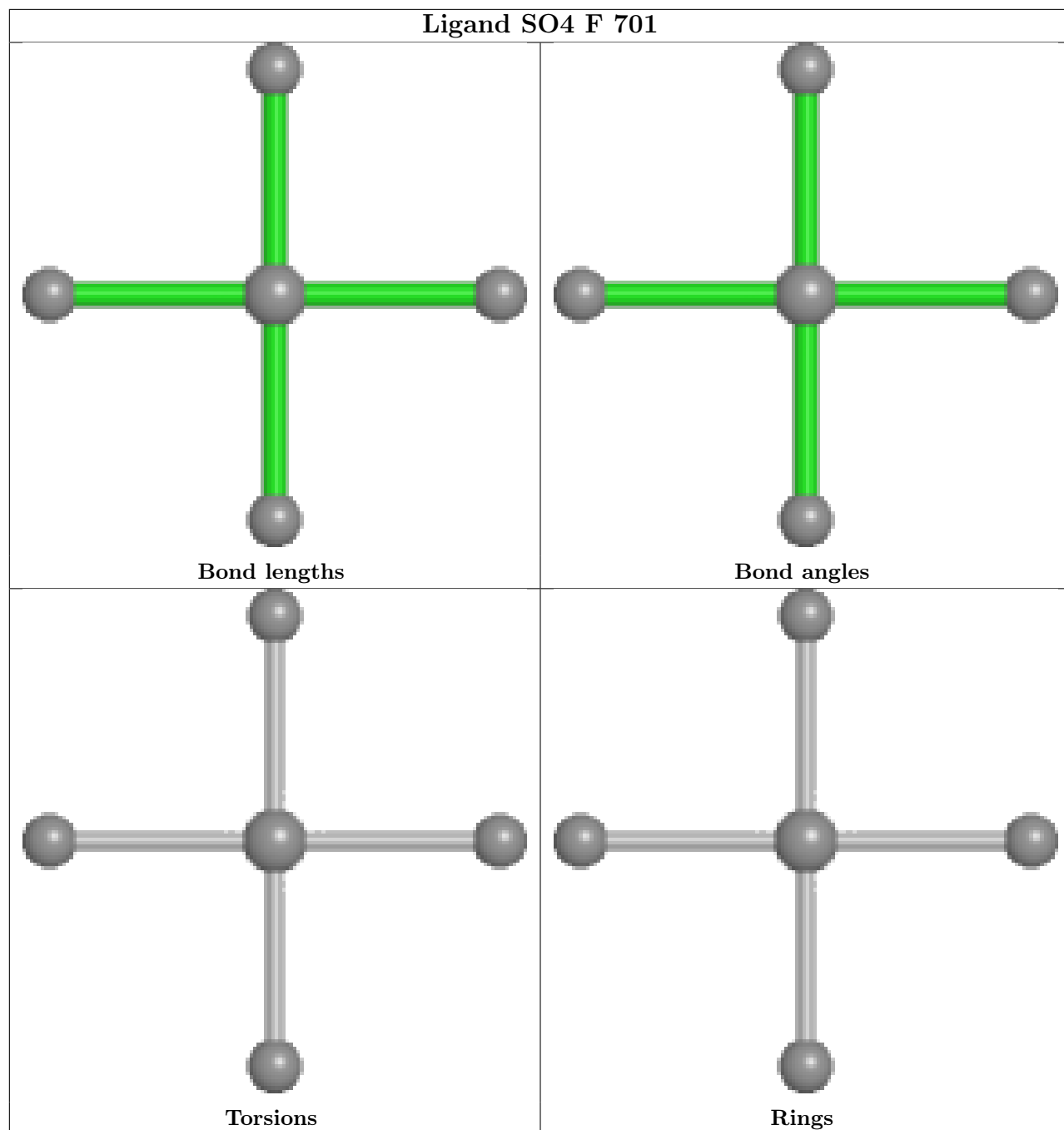


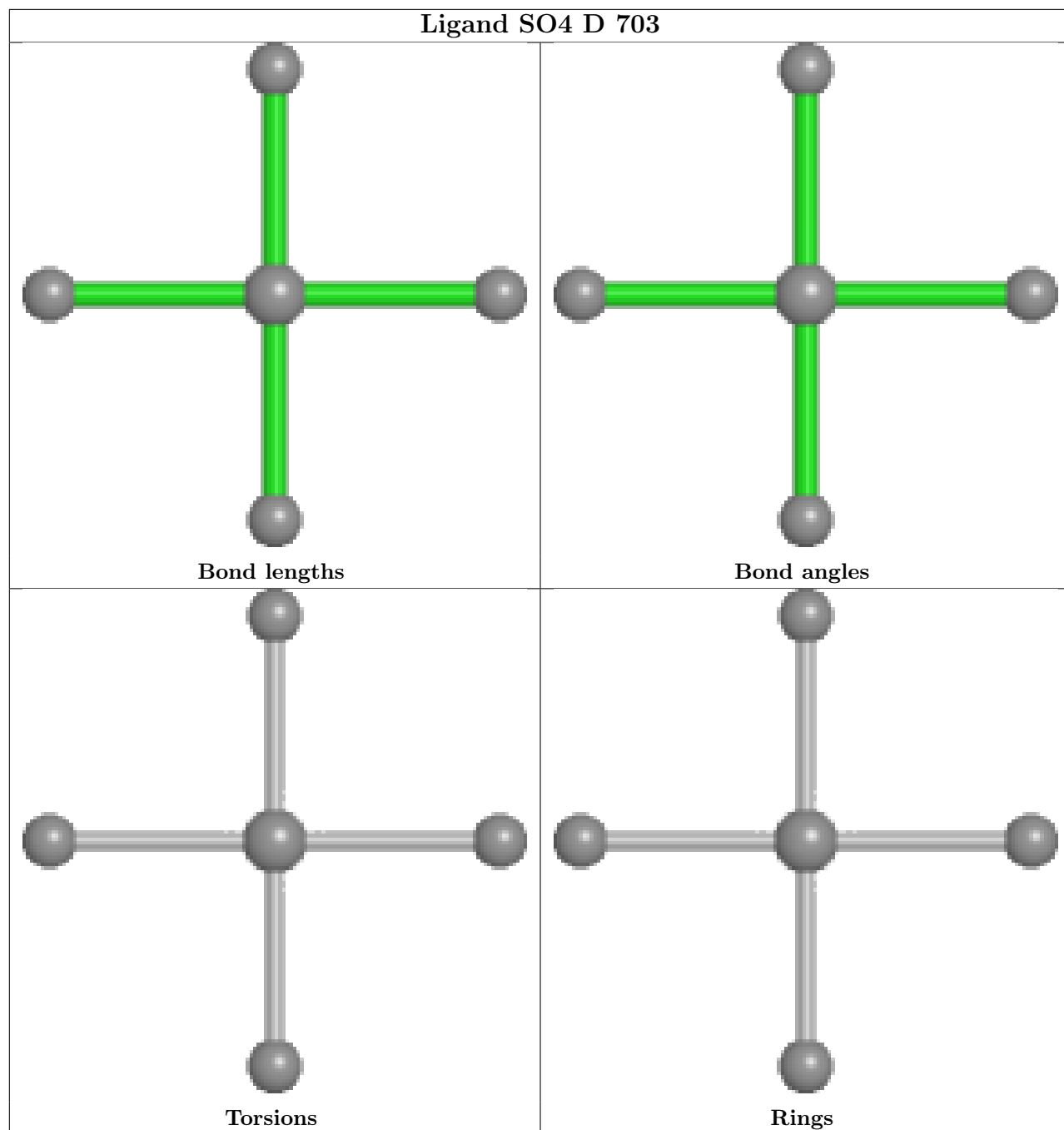


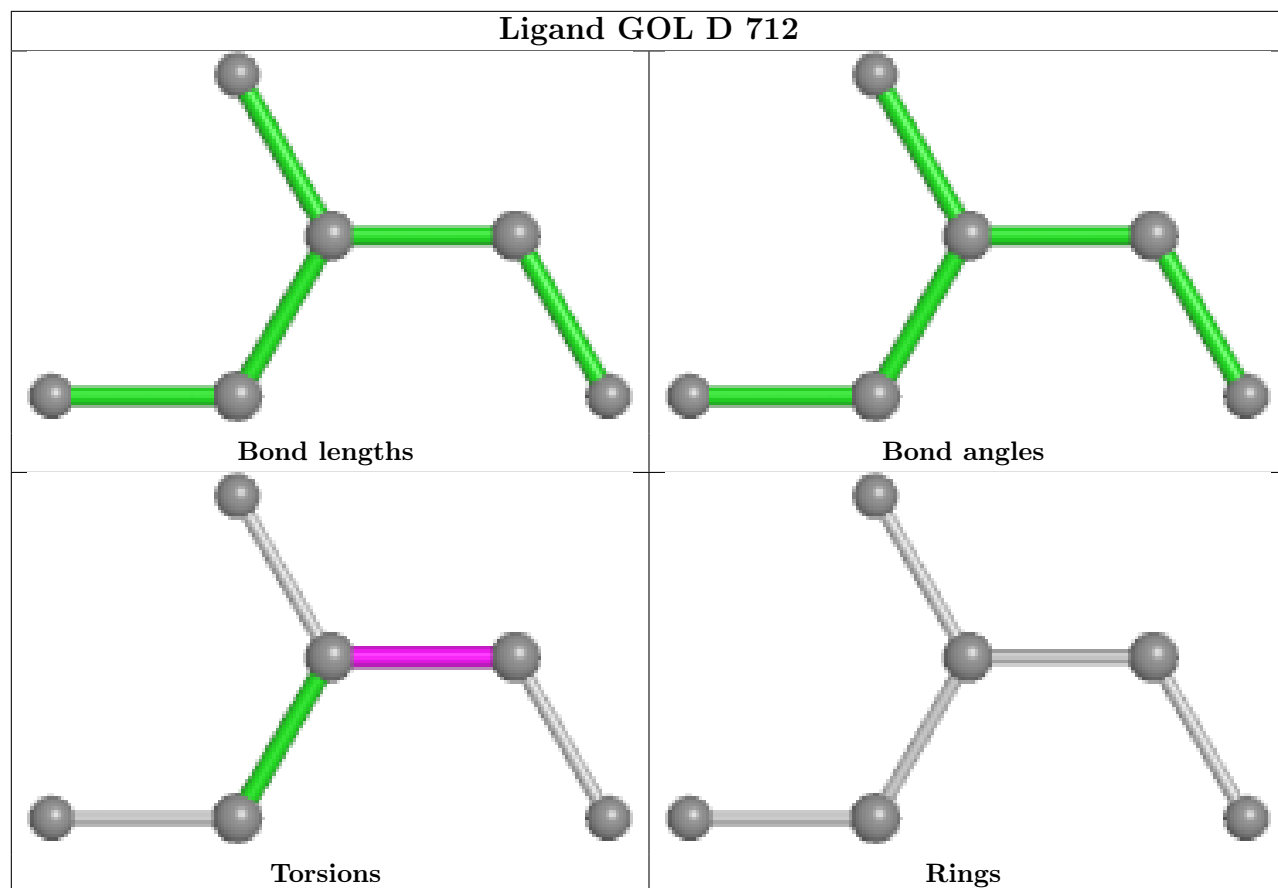


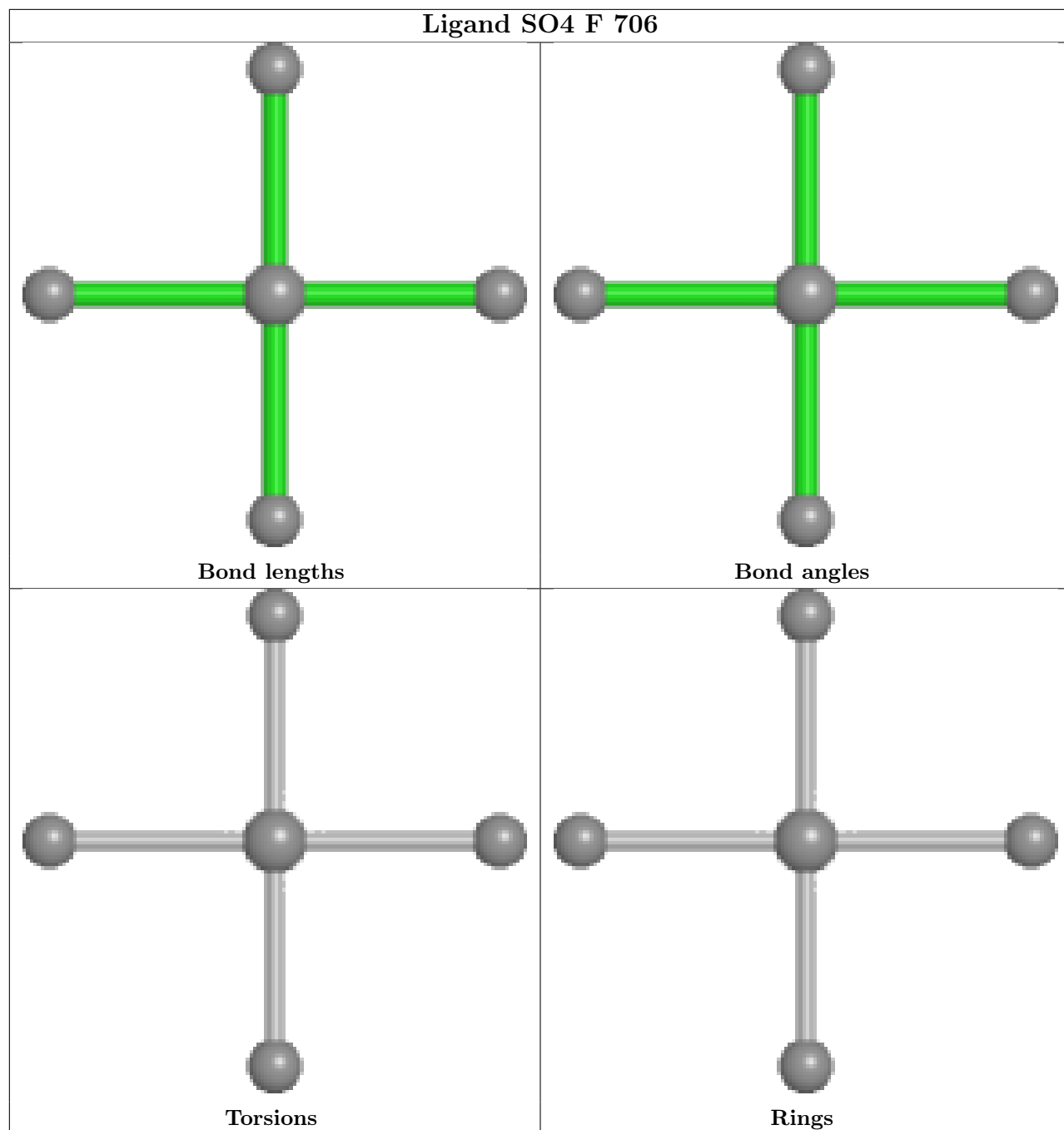


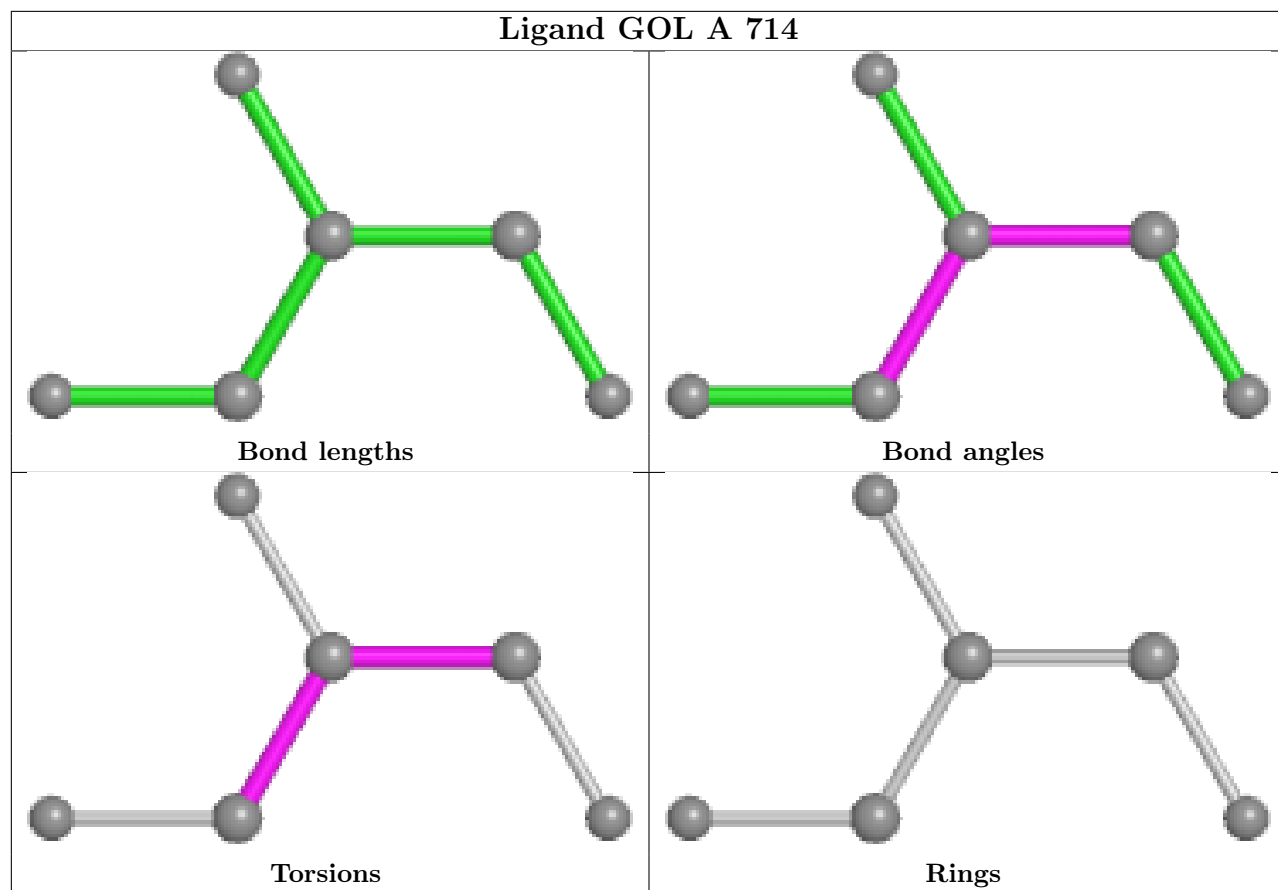


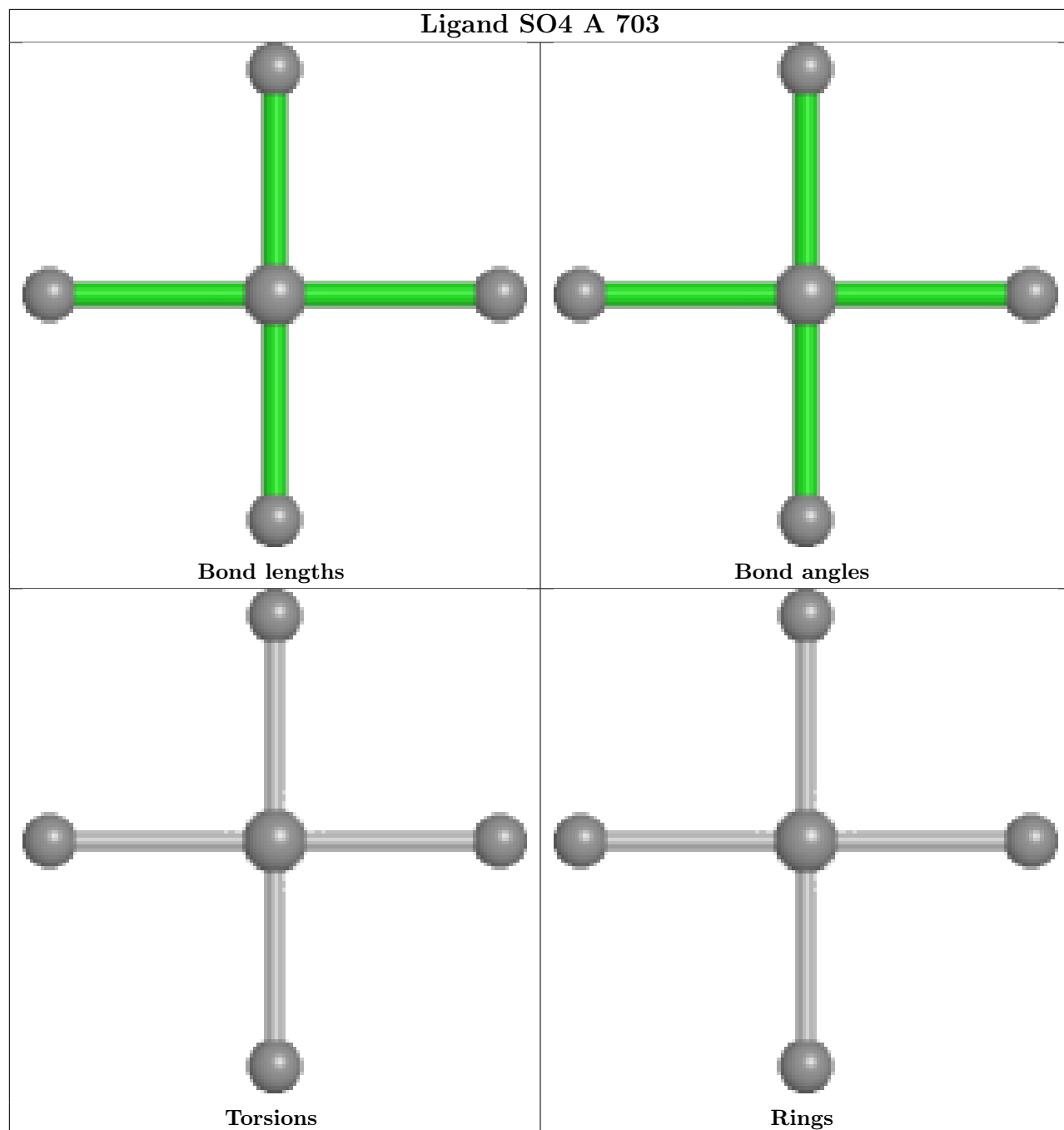


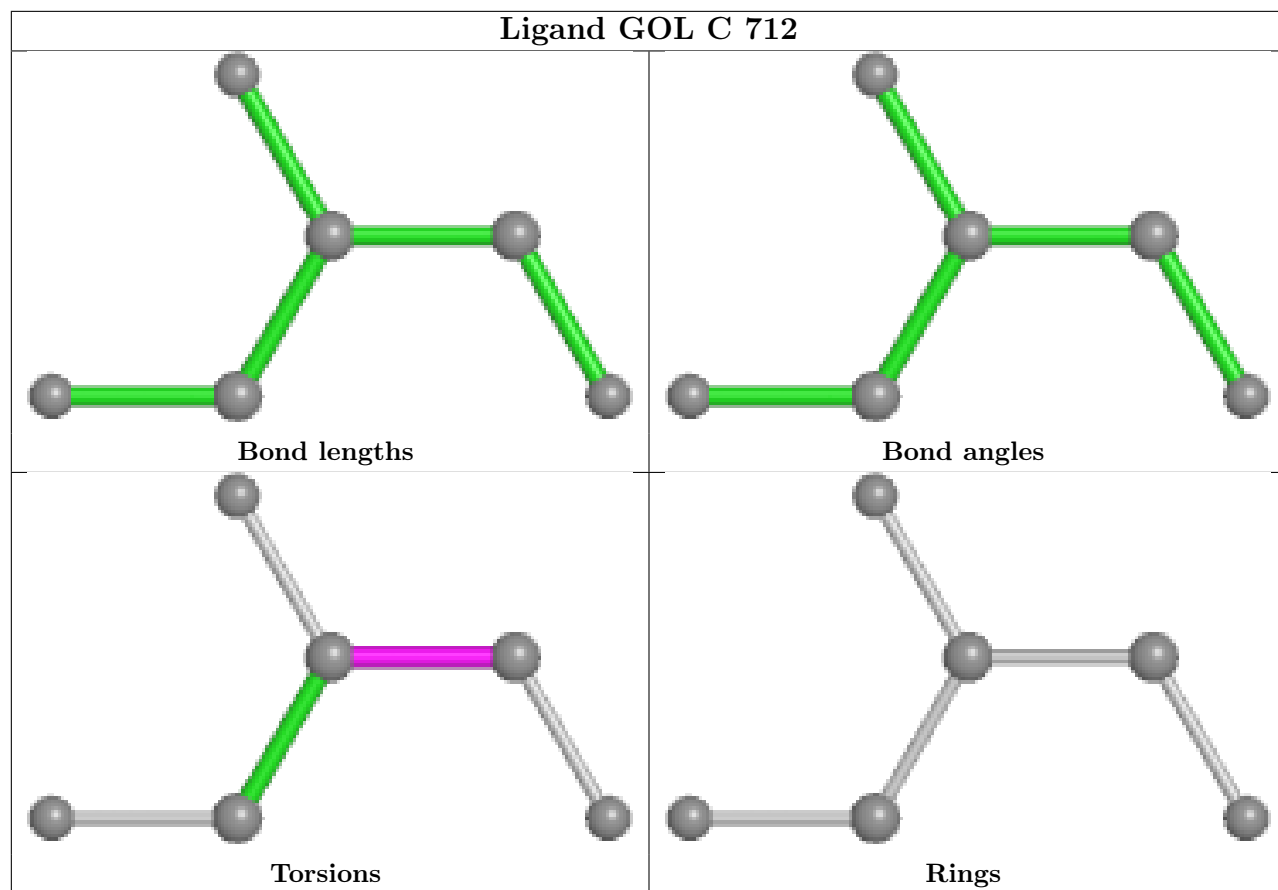


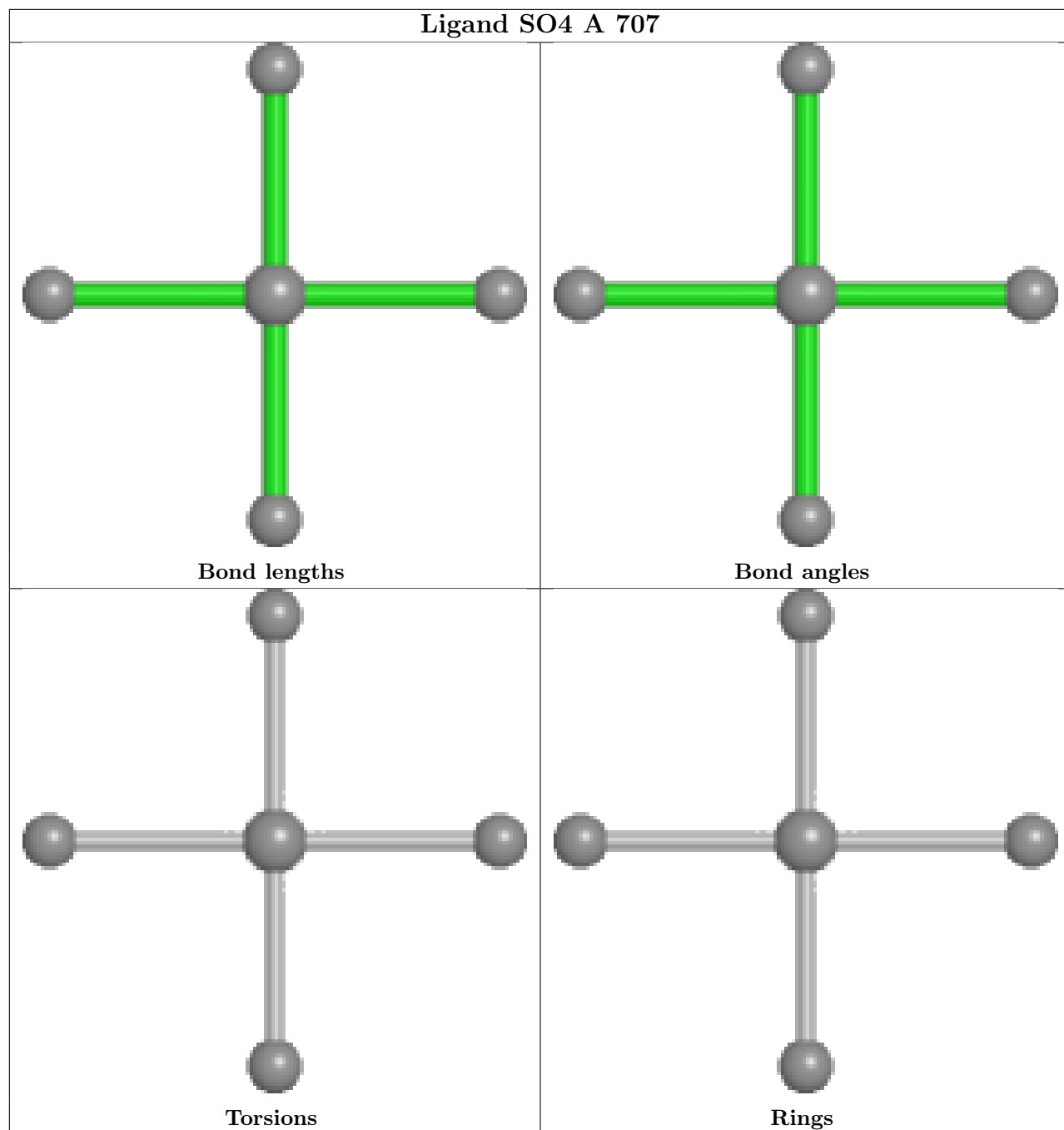




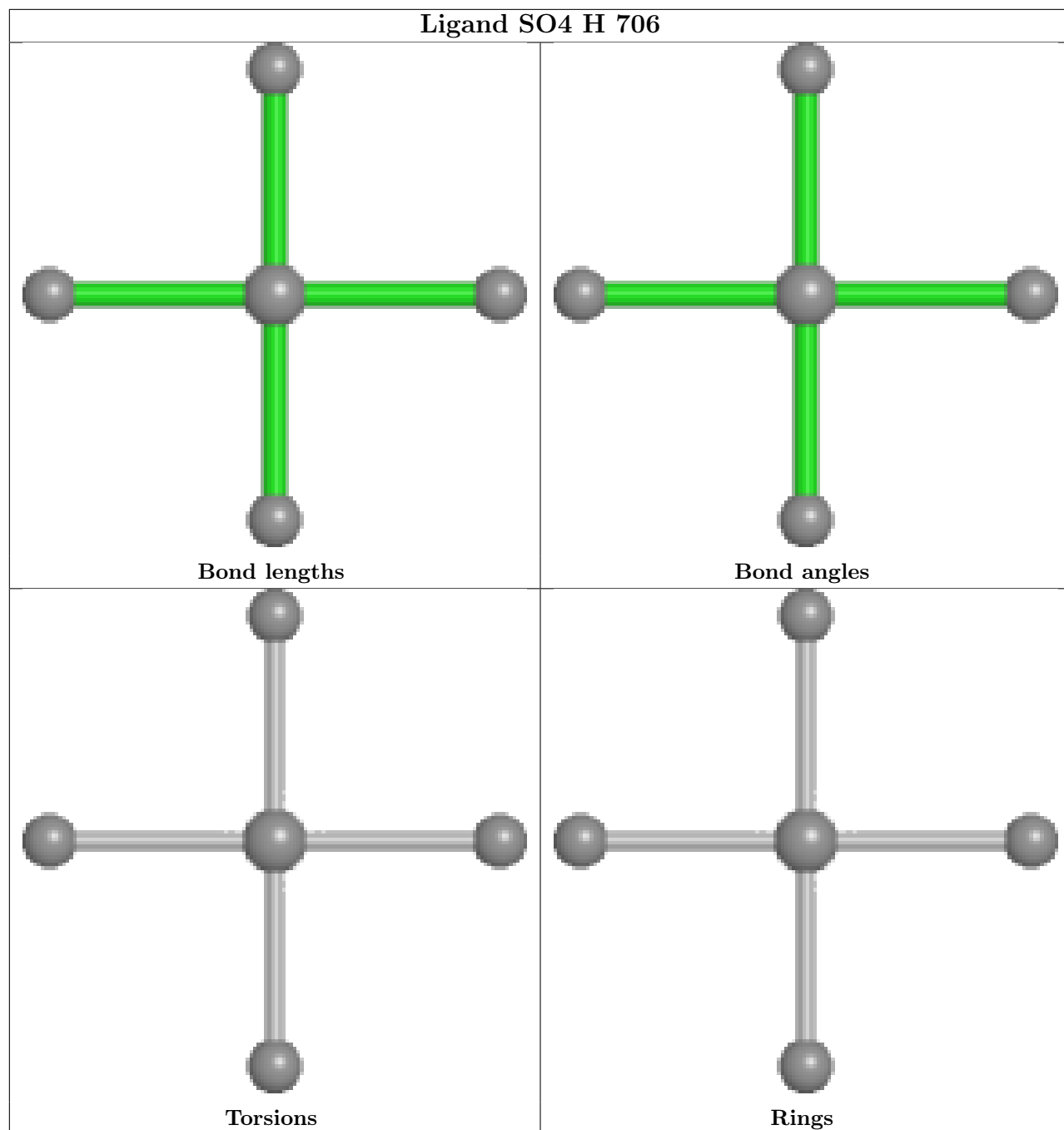


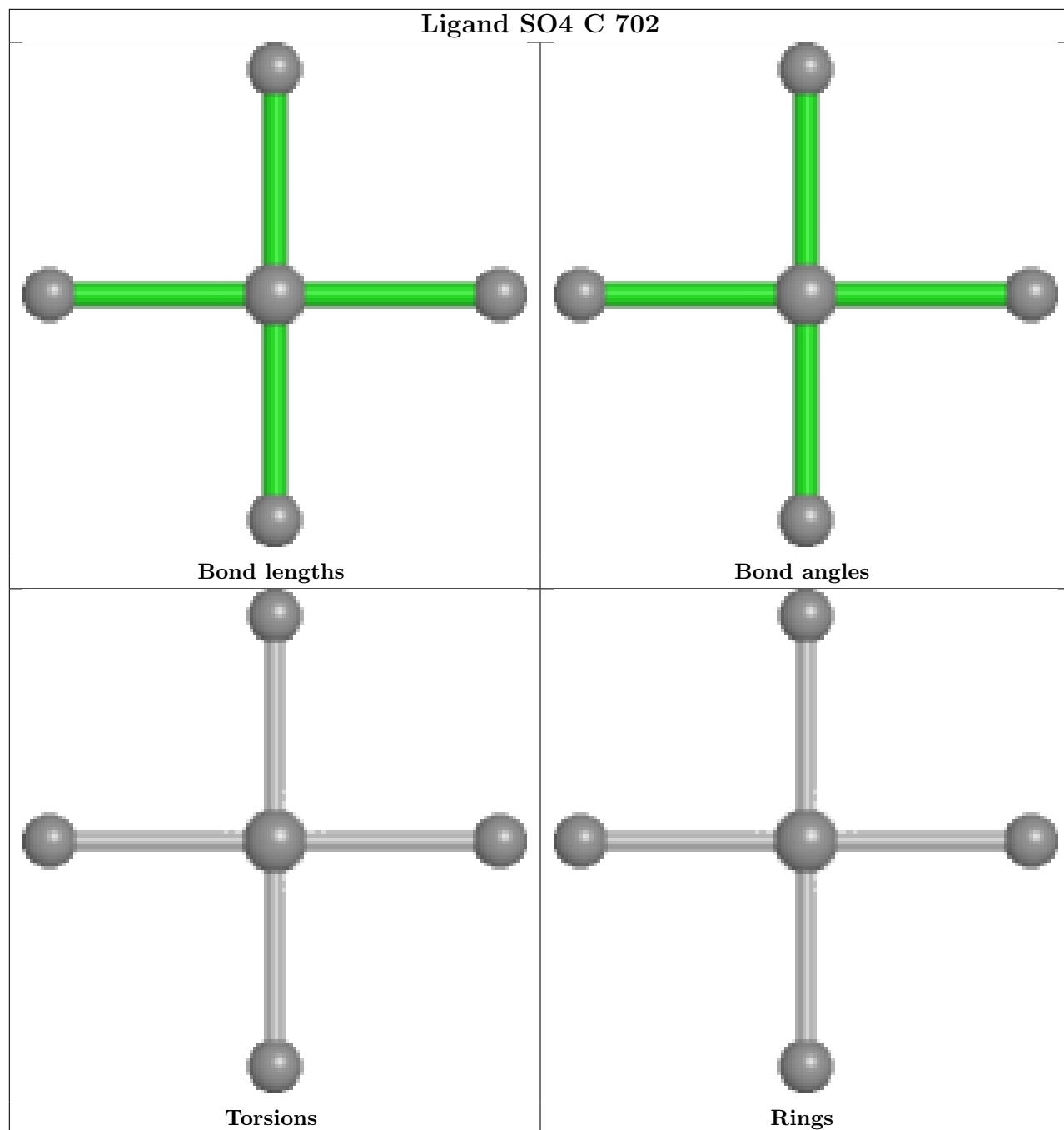


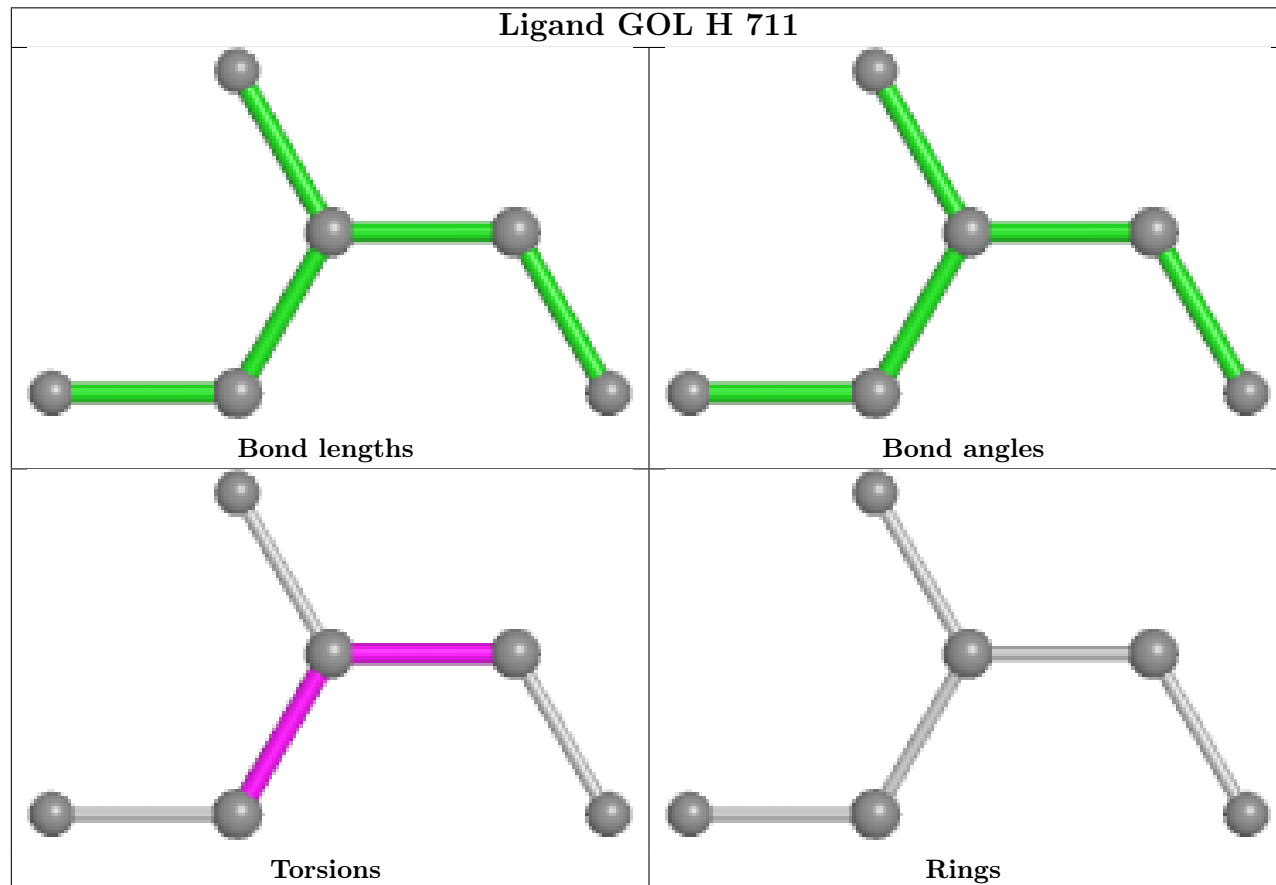
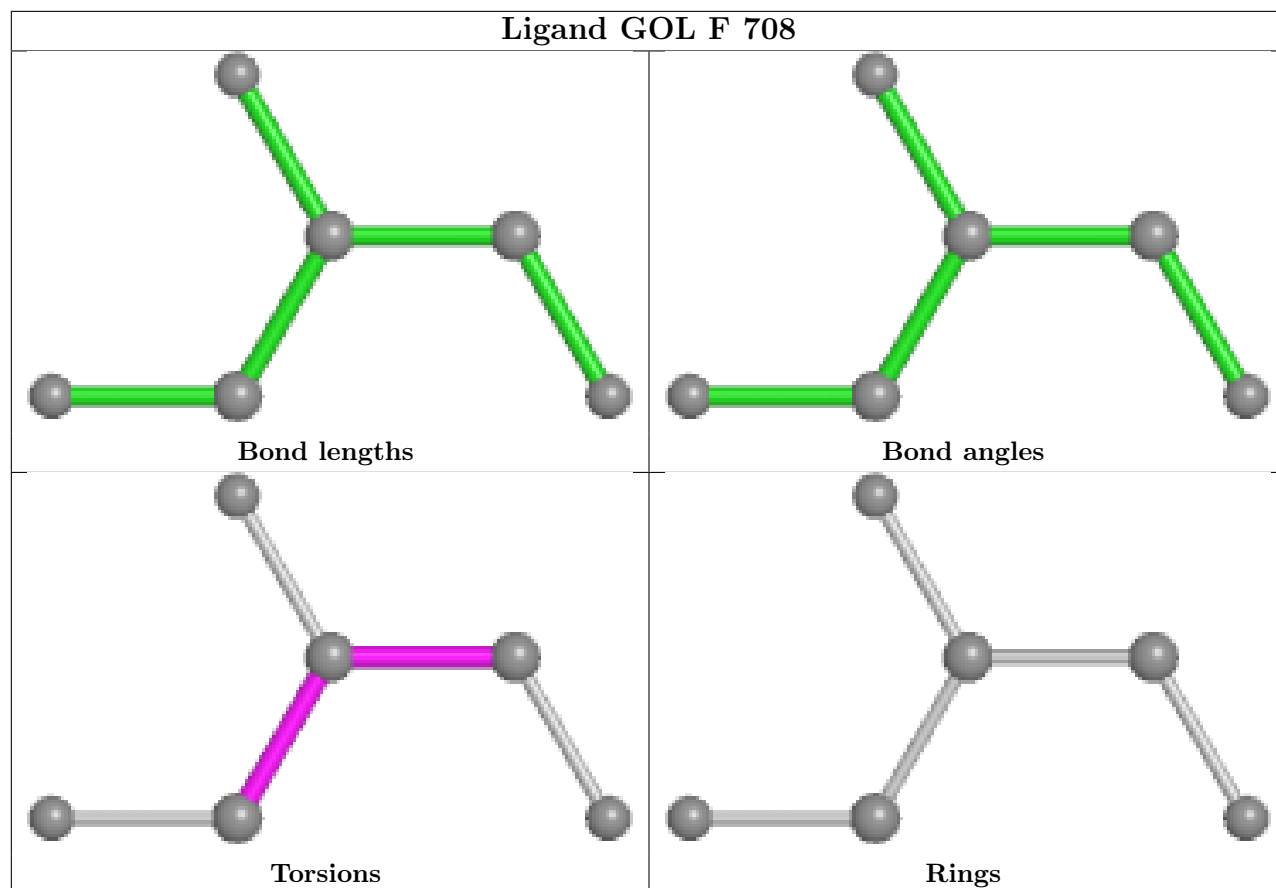


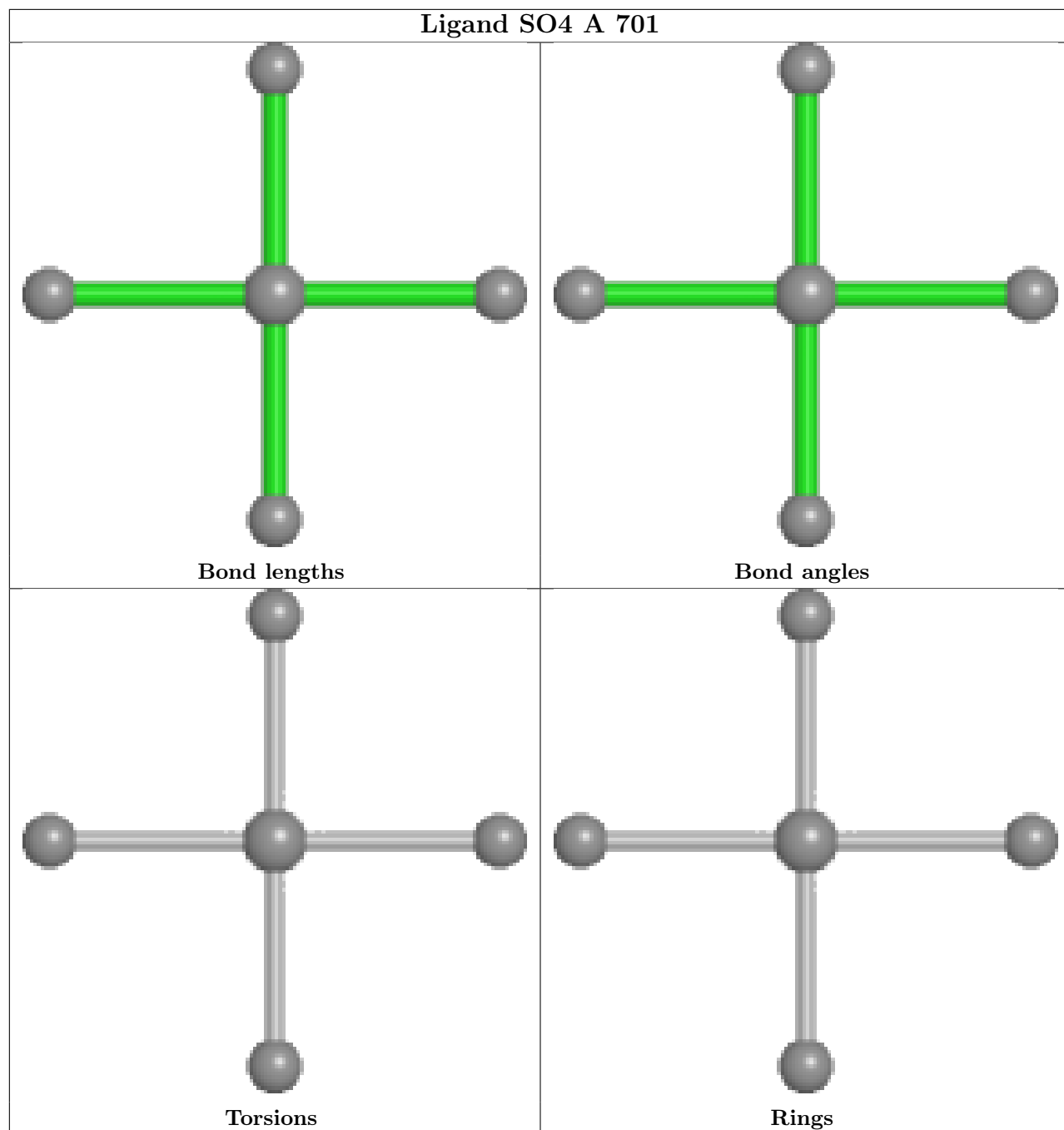


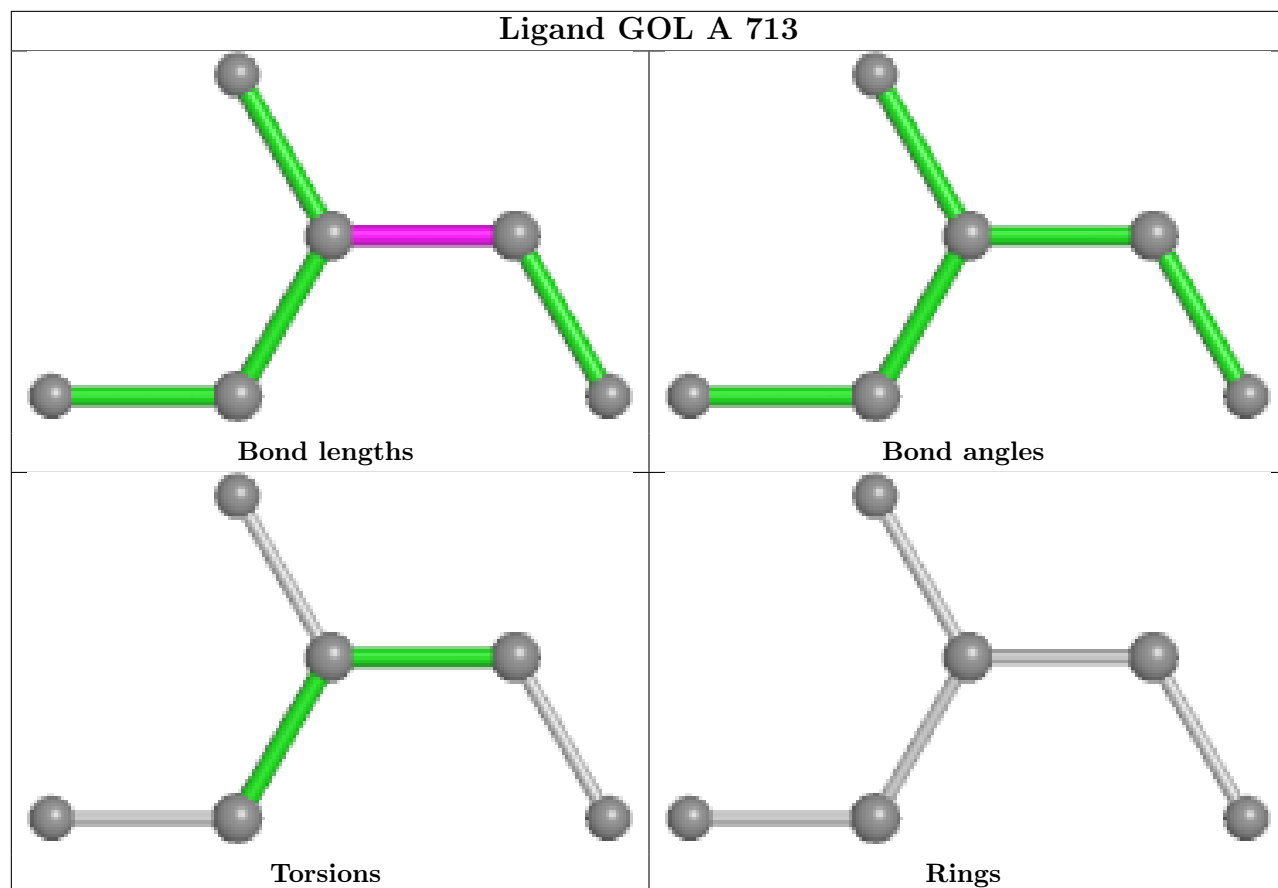


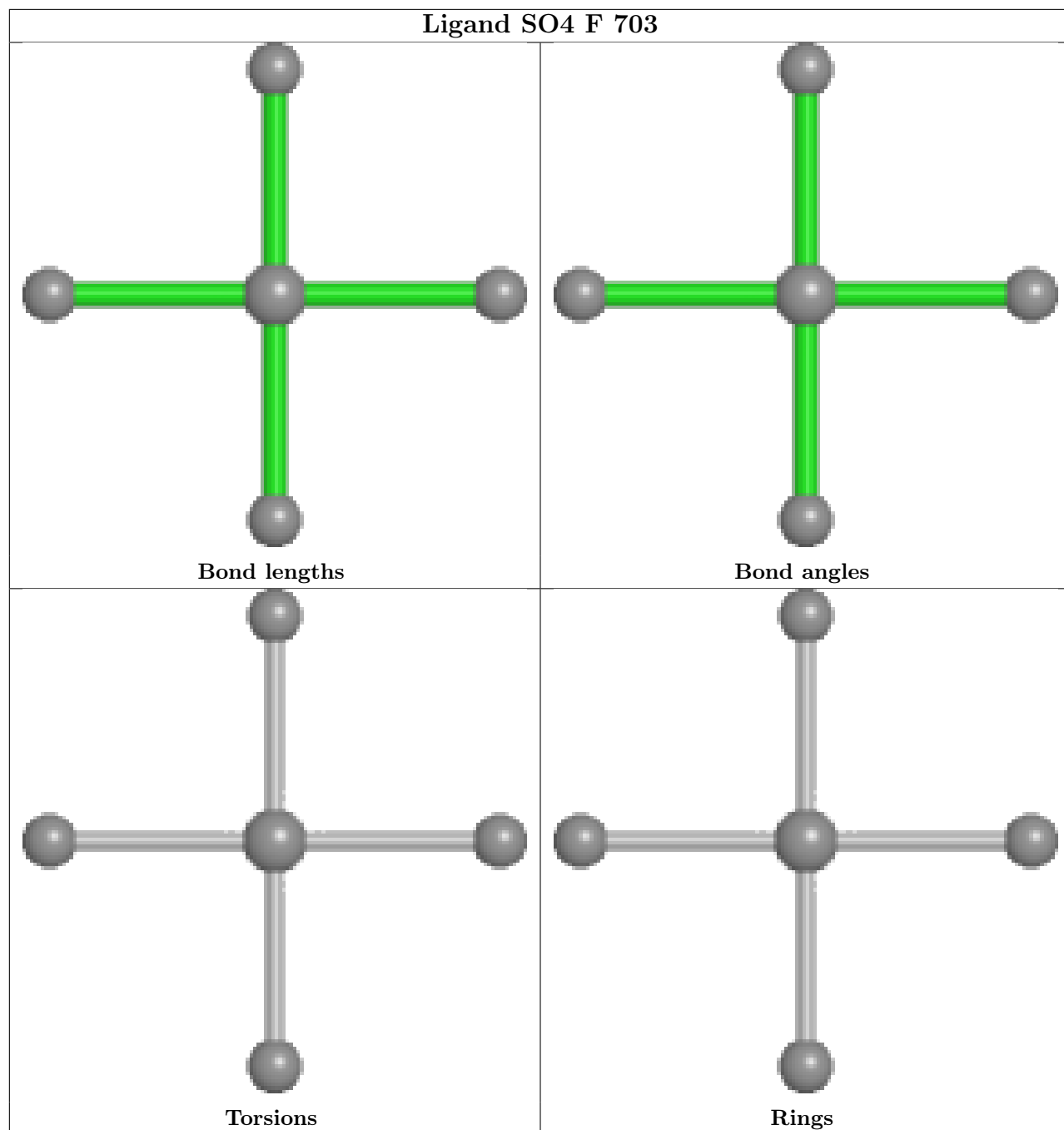


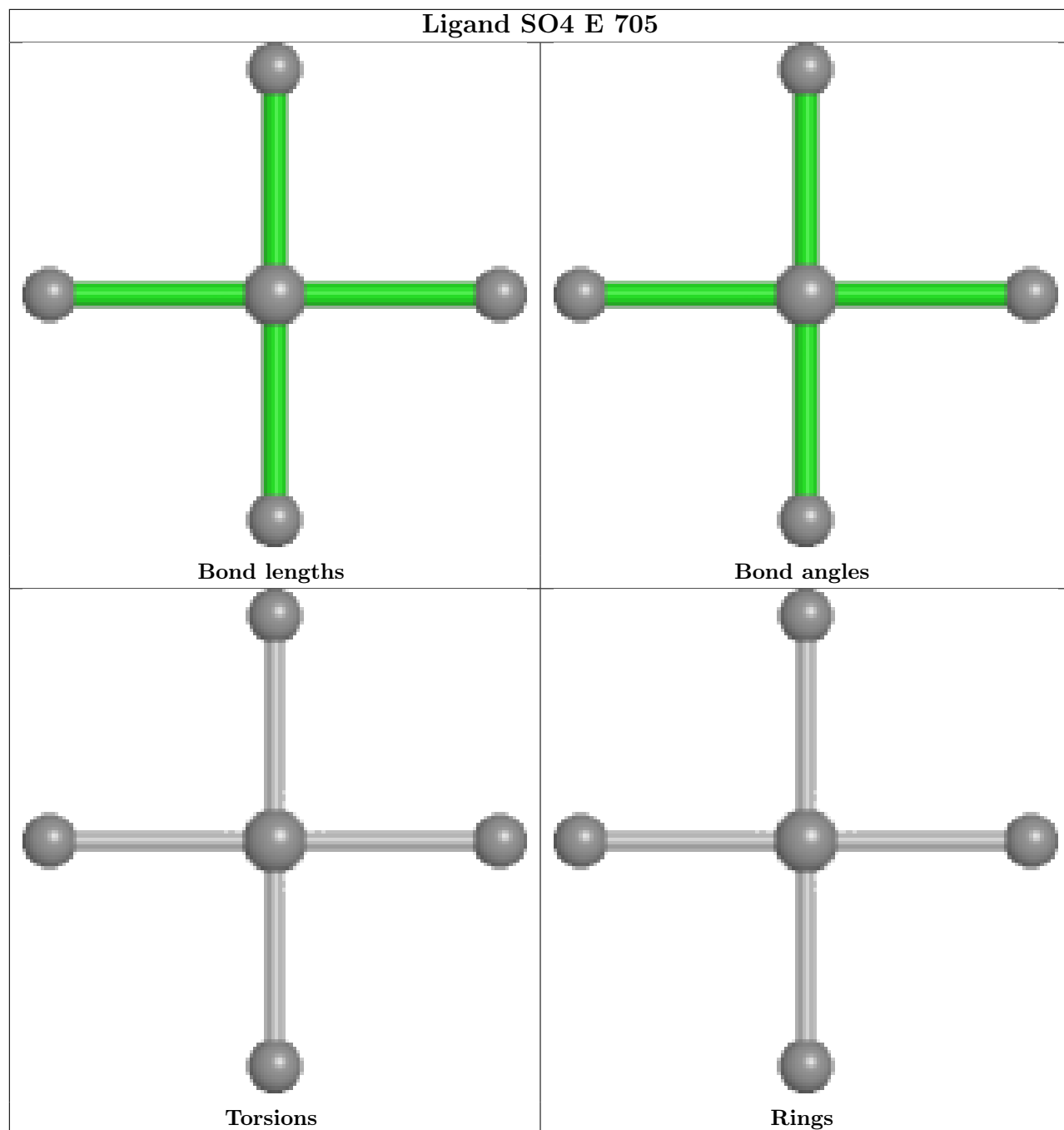


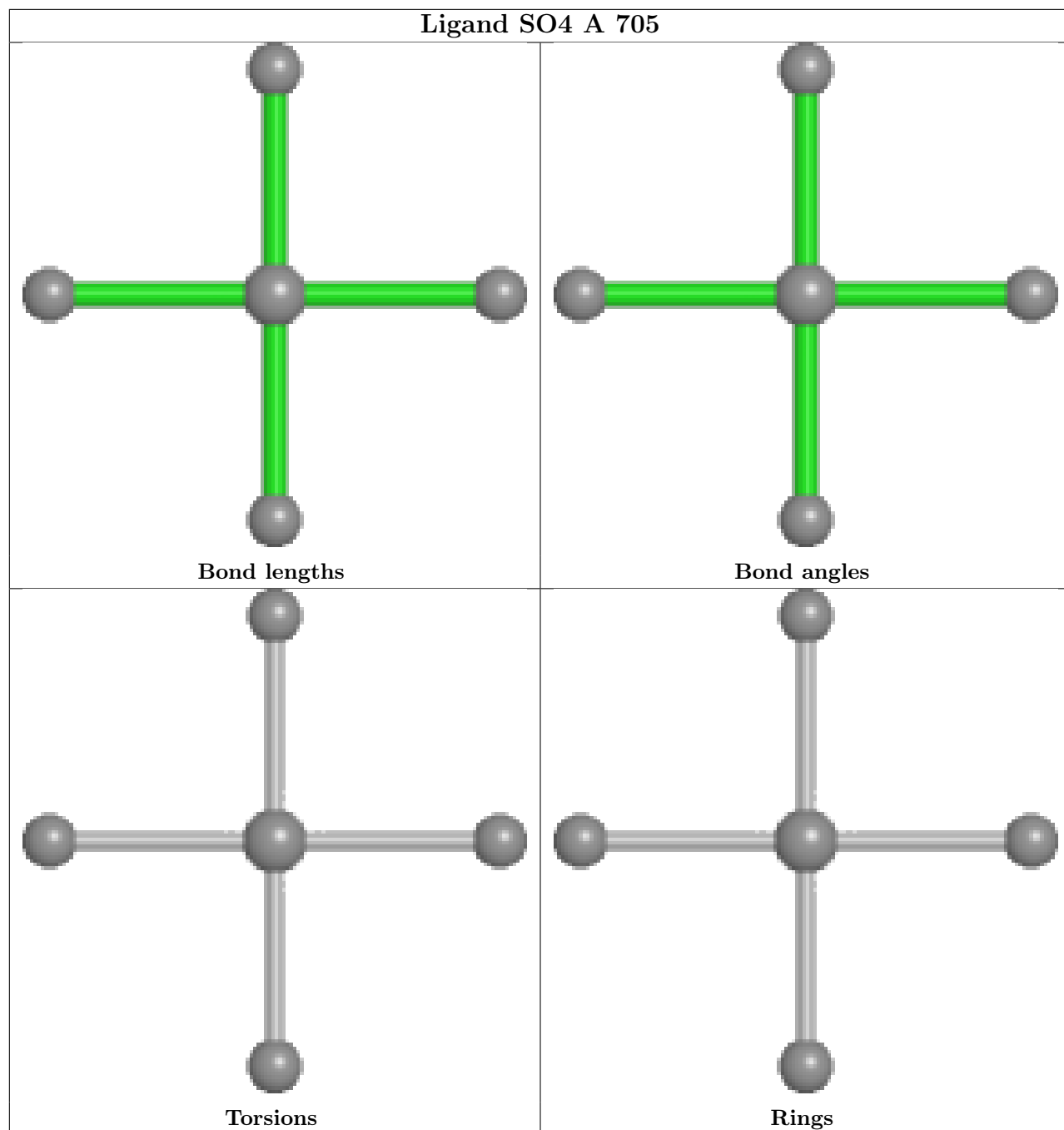




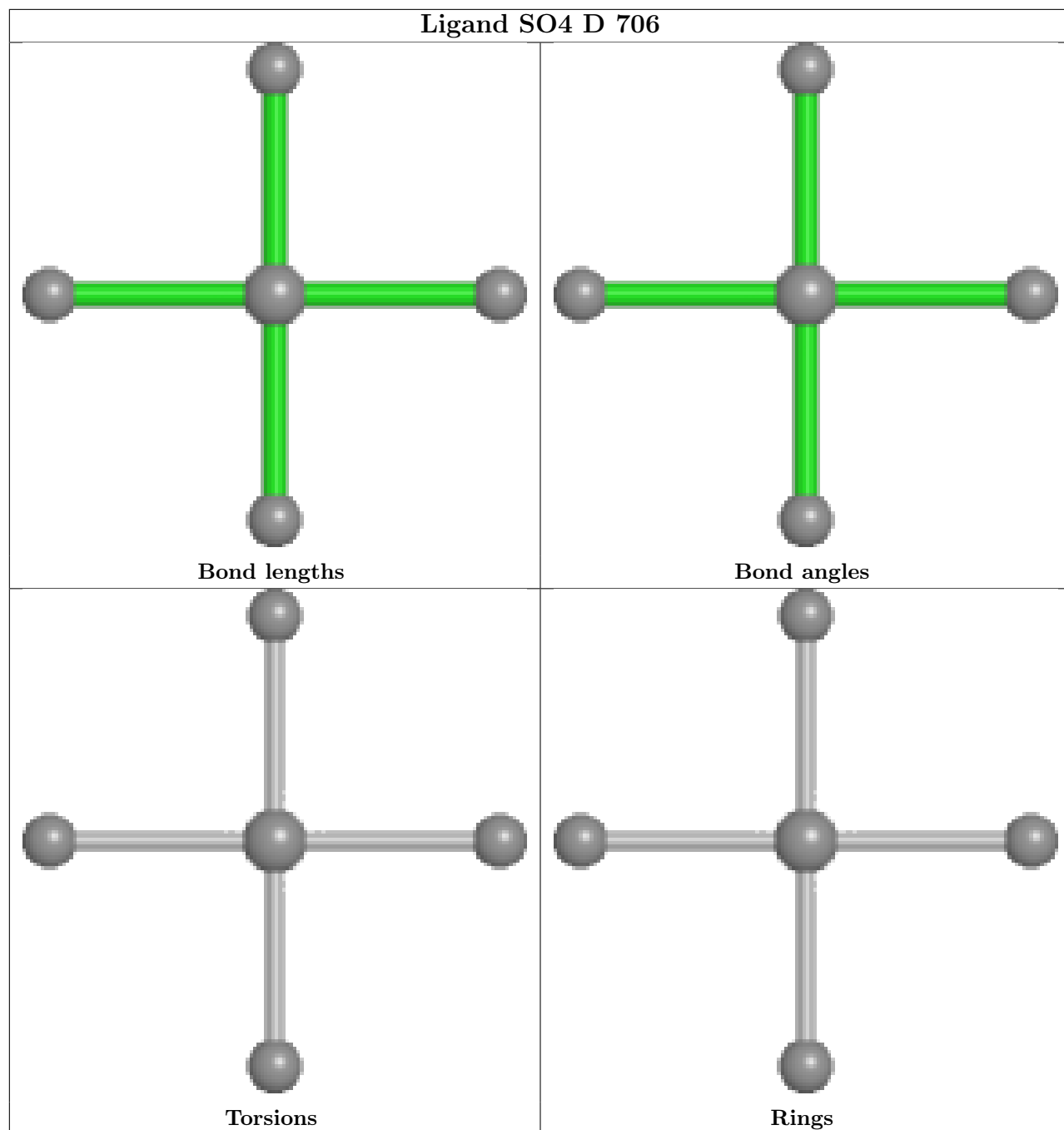


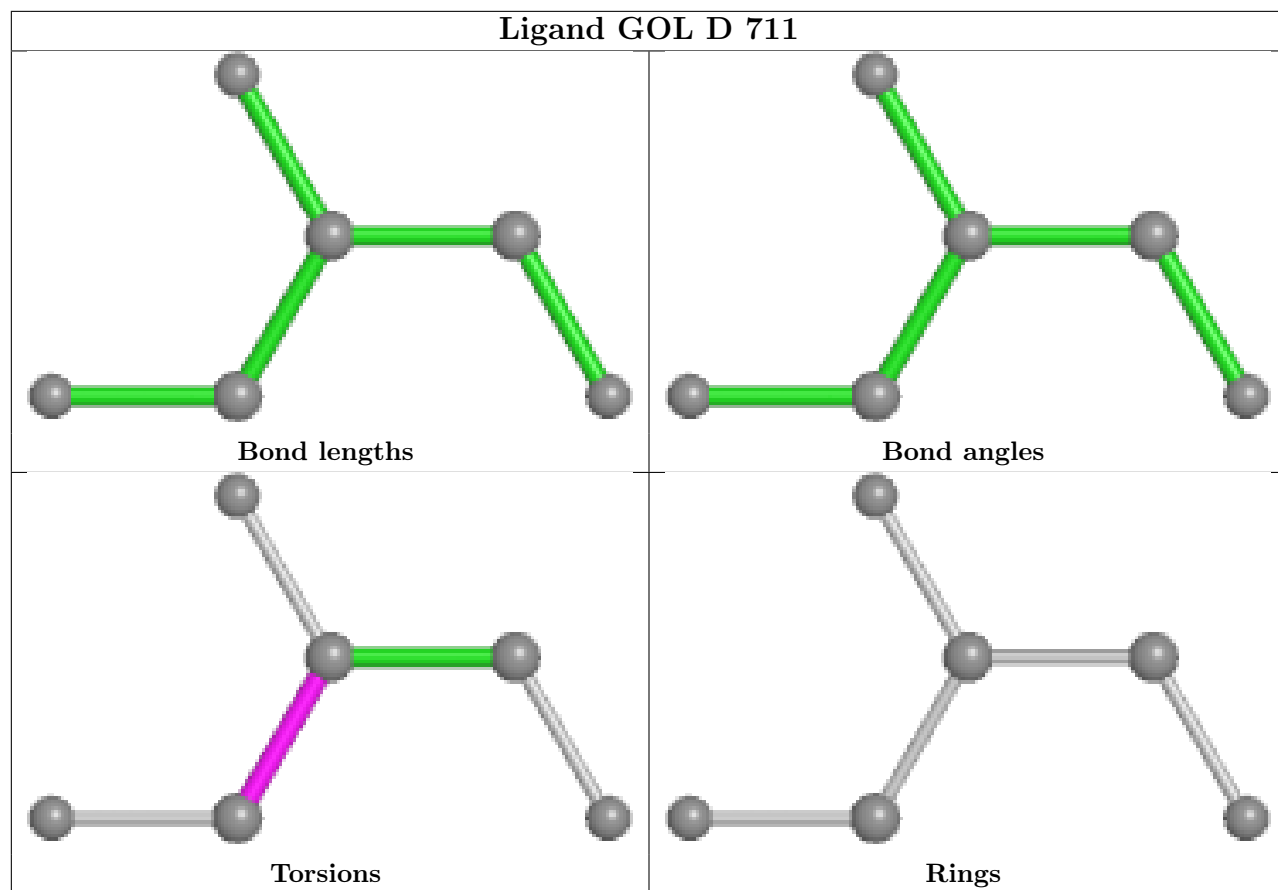


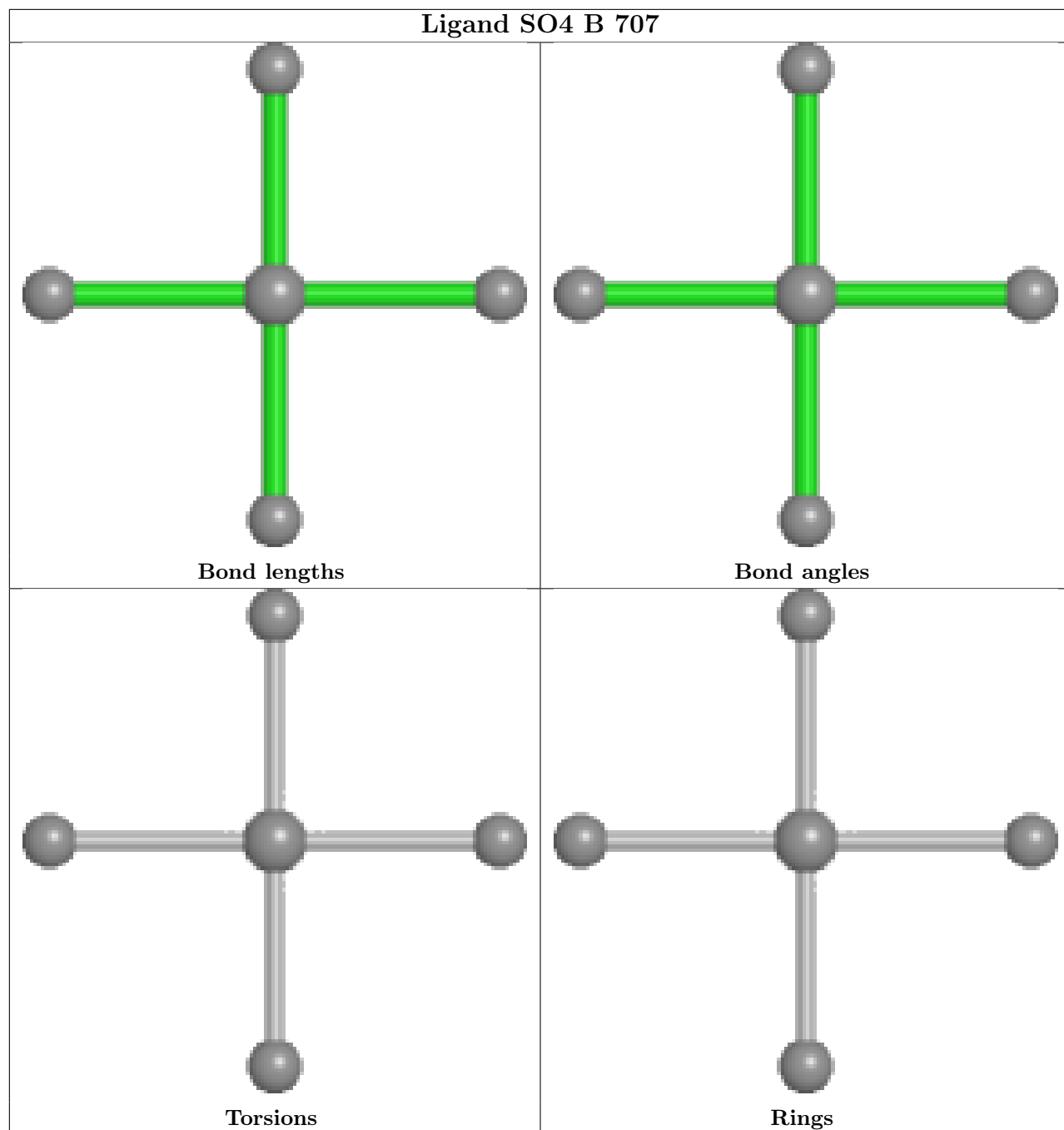


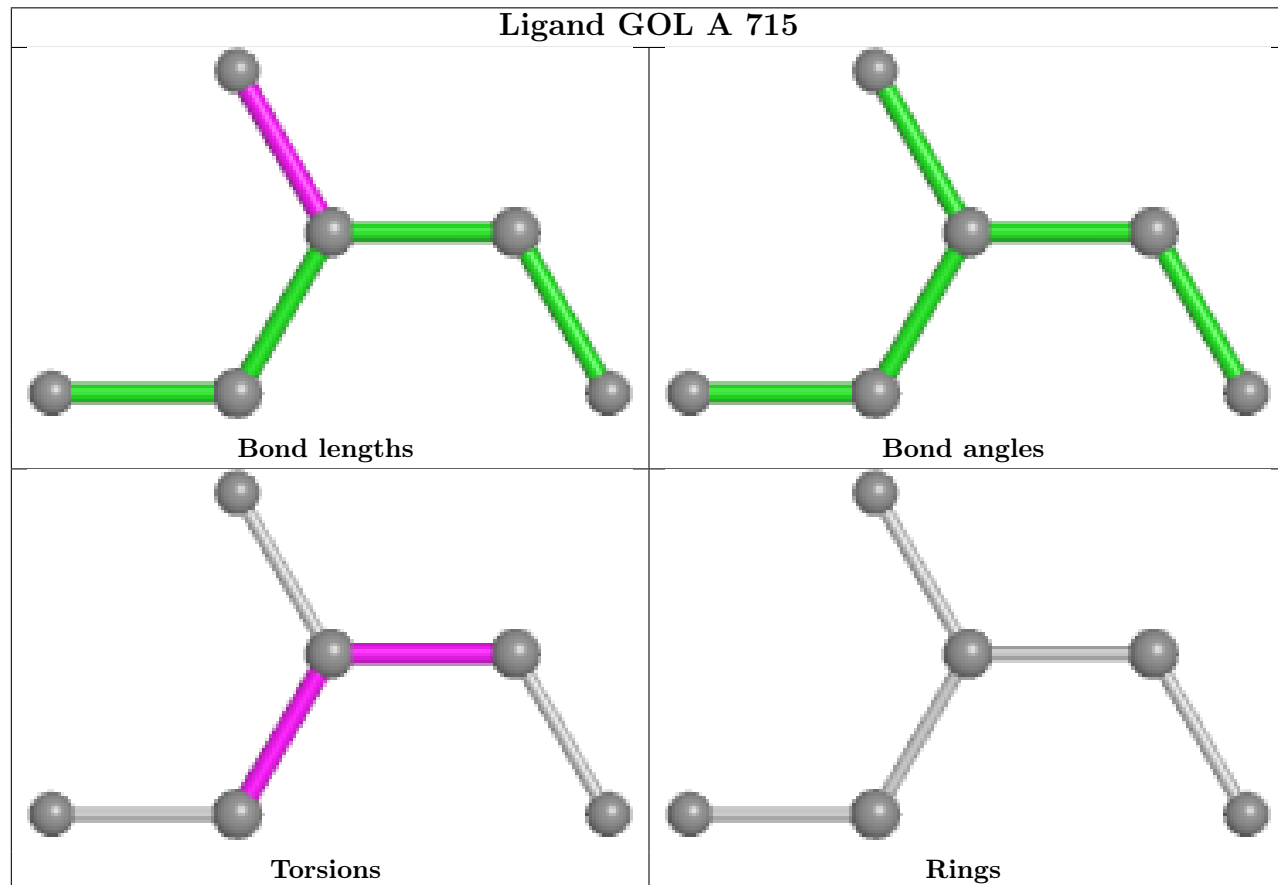
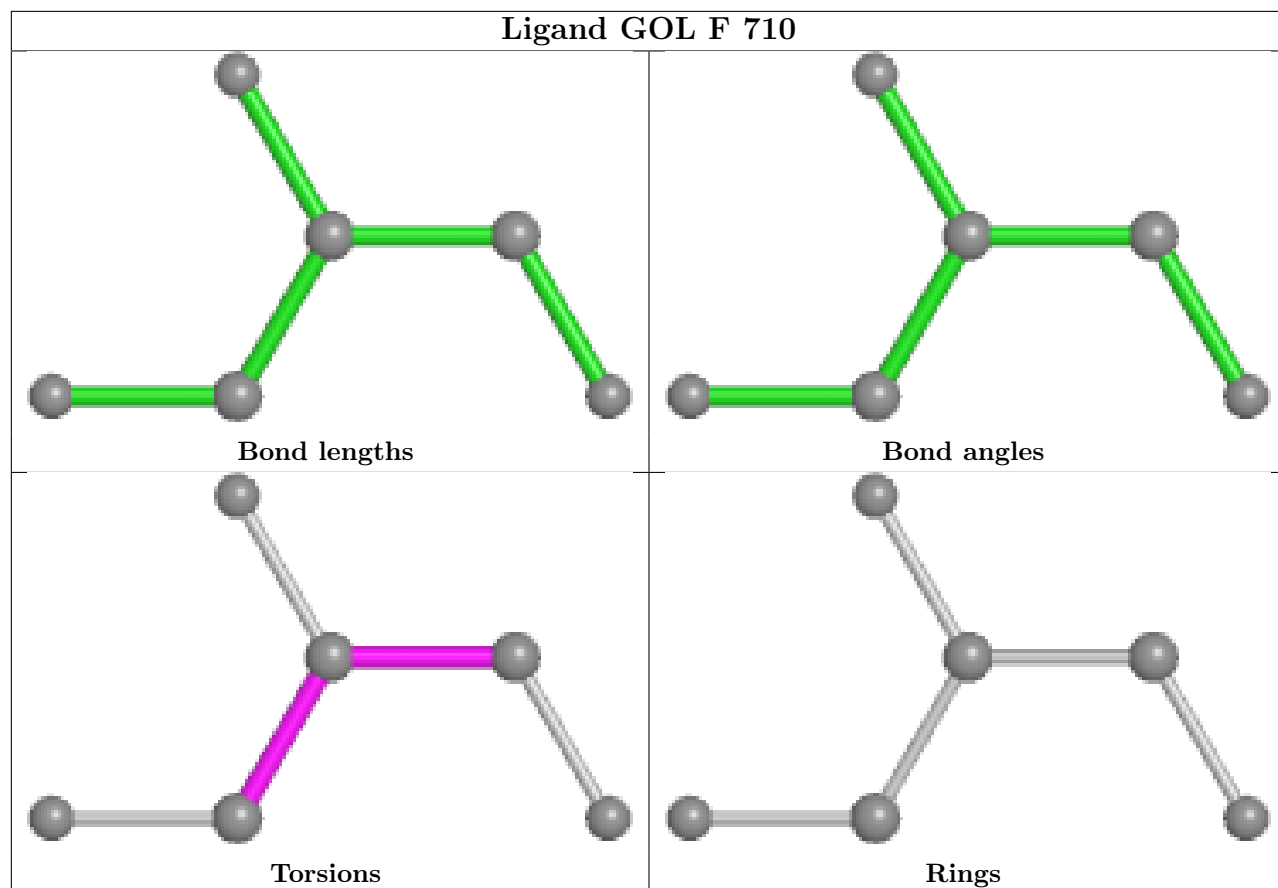


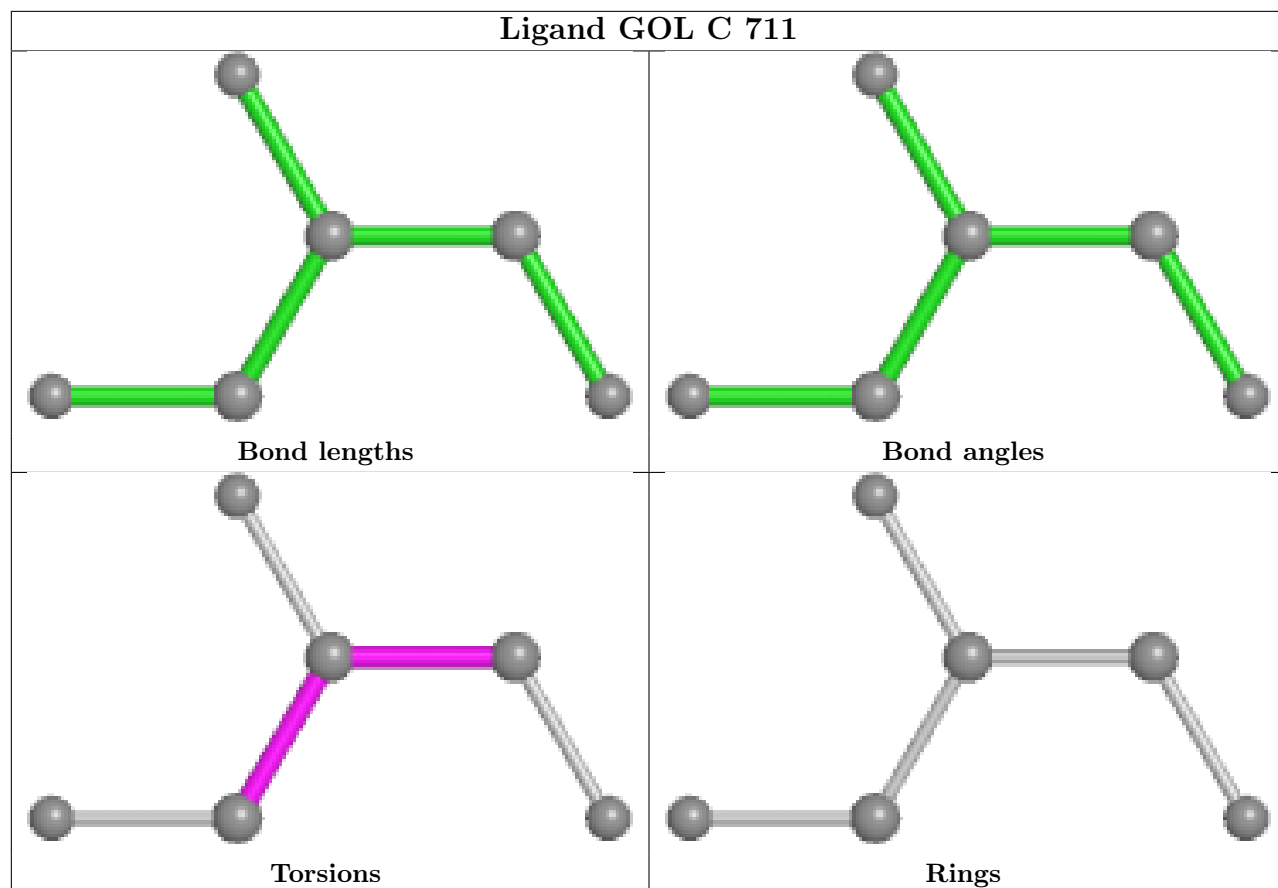


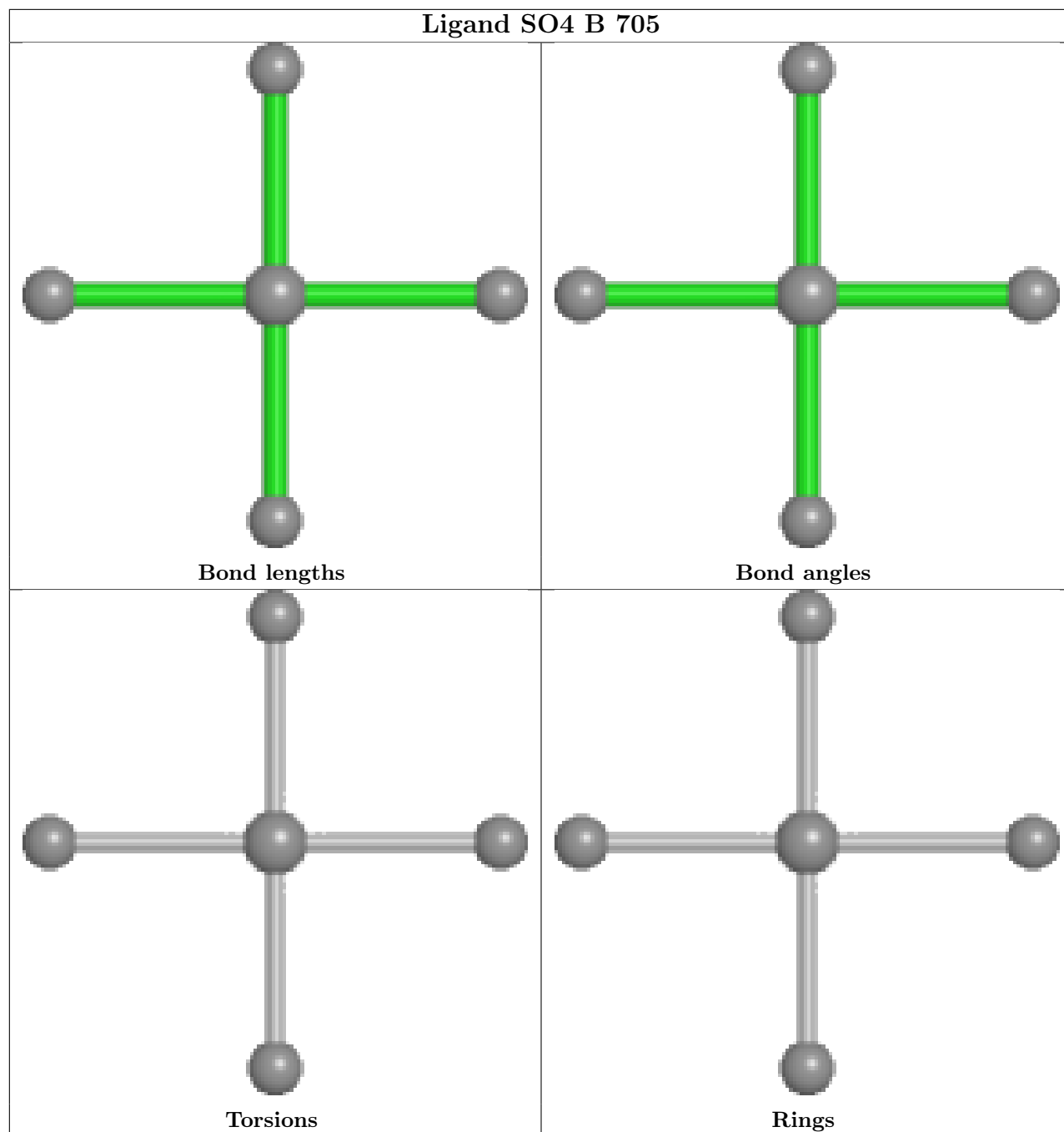












### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	650/691 (94%)	-0.13	5 (0%) 86 85	23, 32, 45, 62	0
1	B	650/691 (94%)	-0.25	3 (0%) 91 90	23, 33, 46, 69	0
1	C	651/691 (94%)	-0.13	6 (0%) 84 83	24, 32, 45, 68	0
1	D	649/691 (93%)	-0.07	6 (0%) 84 83	24, 35, 49, 75	0
1	E	650/691 (94%)	-0.23	1 (0%) 95 94	22, 33, 48, 74	0
1	F	649/691 (93%)	-0.05	5 (0%) 86 85	22, 34, 49, 67	0
1	G	647/691 (93%)	0.22	33 (5%) 28 27	31, 42, 58, 80	0
1	H	651/691 (94%)	0.10	18 (2%) 53 51	26, 39, 56, 71	0
All	All	5197/5528 (94%)	-0.07	77 (1%) 73 72	22, 35, 52, 80	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	ALA	6.2
1	E	146	PRO	4.7
1	D	146	PRO	4.5
1	A	146	PRO	3.9
1	F	146	PRO	3.5
1	G	146	PRO	3.5
1	G	140	ILE	3.5
1	H	437	GLU	3.5
1	G	433	PRO	3.4
1	G	518	ILE	3.3
1	C	155	ASP	3.3
1	G	283	PHE	3.3
1	G	517	PHE	3.3
1	D	12	TYR	3.3
1	G	232	VAL	3.3
1	G	240	ALA	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	242	THR	3.2
1	H	140	ILE	3.2
1	A	436	ASP	3.1
1	G	515	PHE	3.1
1	B	146	PRO	3.0
1	G	58	ALA	3.0
1	G	12	TYR	3.0
1	H	154	ALA	3.0
1	F	438	GLY	2.9
1	G	242	THR	2.9
1	C	434	GLU	2.9
1	H	155	ASP	2.9
1	A	137	ASP	2.9
1	H	234	LEU	2.8
1	G	238	SER	2.8
1	H	146	PRO	2.7
1	G	194	LEU	2.7
1	G	111	PHE	2.7
1	H	193	ALA	2.6
1	G	244	LEU	2.6
1	G	134	LEU	2.5
1	G	234	LEU	2.5
1	C	12	TYR	2.5
1	C	146	PRO	2.5
1	F	346	GLY	2.5
1	A	134	LEU	2.4
1	G	233	LEU	2.4
1	G	178	ARG	2.4
1	H	139	THR	2.4
1	G	254	LEU	2.4
1	G	195	THR	2.4
1	H	613	CYS	2.3
1	G	112	PHE	2.3
1	G	235	ASP	2.3
1	H	244	LEU	2.3
1	C	438	GLY	2.3
1	H	233	LEU	2.2
1	G	661	VAL	2.2
1	A	139	THR	2.2
1	G	243	ASN	2.2
1	D	134	LEU	2.2
1	C	436	ASP	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	263	LEU	2.2
1	G	403	LEU	2.2
1	H	517	PHE	2.2
1	B	12	TYR	2.1
1	G	217	ALA	2.1
1	G	435	LEU	2.1
1	G	180	VAL	2.1
1	H	111	PHE	2.1
1	D	137	ASP	2.1
1	H	212	THR	2.1
1	B	156	LEU	2.1
1	H	134	LEU	2.1
1	G	28	HIS	2.0
1	H	195	THR	2.0
1	F	436	ASP	2.0
1	G	468	SER	2.0
1	D	140	ILE	2.0
1	D	634	LEU	2.0
1	F	137	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	FLC	A	717	13/13	0.54	0.34	38,47,54,56	0
6	FLC	H	713	13/13	0.60	0.34	47,53,59,60	0
4	GOL	G	707	6/6	0.68	0.21	42,46,48,57	0
4	GOL	D	710	6/6	0.74	0.17	40,42,48,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	707	5/5	0.74	0.23	61,66,70,84	0
4	GOL	D	712	6/6	0.78	0.20	36,39,48,48	0
4	GOL	H	711	6/6	0.78	0.24	46,49,55,59	0
5	ALA	G	709	6/6	0.80	0.22	32,35,37,38	0
4	GOL	C	709	6/6	0.81	0.15	36,40,42,42	0
4	GOL	D	711	6/6	0.82	0.24	41,47,49,50	0
4	GOL	G	708	6/6	0.82	0.12	50,54,56,58	0
4	GOL	C	712	6/6	0.82	0.20	42,45,51,53	0
4	GOL	A	713	6/6	0.84	0.19	35,38,40,44	0
2	SO4	D	706	5/5	0.84	0.17	50,56,64,69	0
2	SO4	F	705	5/5	0.84	0.26	53,60,72,77	0
4	GOL	E	712	6/6	0.84	0.29	42,46,47,57	0
4	GOL	E	714	6/6	0.84	0.26	45,51,51,55	0
4	GOL	F	709	6/6	0.84	0.21	46,51,55,55	0
3	NA	A	712	1/1	0.85	0.13	41,41,41,41	0
4	GOL	D	713	6/6	0.86	0.17	44,45,48,61	0
4	GOL	C	710	6/6	0.86	0.16	38,42,45,46	0
4	GOL	F	712	6/6	0.86	0.27	47,52,54,63	0
4	GOL	F	711	6/6	0.87	0.12	50,52,57,58	0
2	SO4	H	708	5/5	0.87	0.20	72,74,82,86	0
5	ALA	C	713	6/6	0.88	0.19	22,28,30,30	0
2	SO4	G	702	5/5	0.88	0.21	58,63,71,74	0
2	SO4	E	709	5/5	0.88	0.20	41,51,55,67	0
4	GOL	B	718	6/6	0.88	0.12	39,42,46,46	0
3	NA	G	706	1/1	0.89	0.16	48,48,48,48	0
4	GOL	C	711	6/6	0.89	0.13	46,48,53,58	0
4	GOL	E	713	6/6	0.89	0.18	40,48,56,60	0
2	SO4	F	706	5/5	0.89	0.21	34,37,42,45	5
4	GOL	F	708	6/6	0.89	0.17	40,43,46,48	0
5	ALA	H	712	6/6	0.90	0.20	27,28,33,34	0
5	ALA	F	713	6/6	0.90	0.22	25,28,32,33	0
3	NA	H	710	1/1	0.90	0.29	49,49,49,49	0
4	GOL	F	710	6/6	0.91	0.28	40,51,57,64	0
4	GOL	A	715	6/6	0.91	0.15	38,41,42,50	0
2	SO4	B	712	5/5	0.91	0.20	60,61,73,80	0
4	GOL	A	714	6/6	0.91	0.21	36,41,46,48	0
2	SO4	H	709	5/5	0.92	0.17	58,64,78,82	0
2	SO4	F	707	5/5	0.92	0.34	59,60,76,86	0
2	SO4	A	705	5/5	0.92	0.18	53,54,60,63	0
4	GOL	B	717	6/6	0.92	0.20	39,48,50,52	0
2	SO4	A	707	5/5	0.92	0.21	62,70,74,86	0
5	ALA	E	715	6/6	0.93	0.22	21,29,36,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	706	5/5	0.93	0.17	50,57,66,70	0
3	NA	A	710	1/1	0.93	0.13	42,42,42,42	0
2	SO4	A	708	5/5	0.94	0.24	59,60,74,79	0
2	SO4	E	708	5/5	0.94	0.16	54,57,60,62	0
3	NA	A	711	1/1	0.94	0.10	43,43,43,43	0
5	ALA	B	719	6/6	0.94	0.20	26,27,30,32	0
2	SO4	B	707	5/5	0.94	0.10	46,48,65,65	0
3	NA	B	716	1/1	0.94	0.32	40,40,40,40	0
3	NA	D	709	1/1	0.94	0.31	47,47,47,47	0
3	NA	E	711	1/1	0.94	0.22	42,42,42,42	0
2	SO4	H	704	5/5	0.94	0.11	56,57,58,60	0
2	SO4	H	706	5/5	0.94	0.16	51,58,68,72	0
2	SO4	B	711	5/5	0.94	0.18	65,70,78,78	0
2	SO4	G	705	5/5	0.95	0.09	59,61,65,65	0
2	SO4	B	708	5/5	0.95	0.11	61,64,75,81	0
2	SO4	H	705	5/5	0.95	0.12	40,41,47,48	0
2	SO4	C	707	5/5	0.95	0.14	52,53,55,58	0
2	SO4	E	707	5/5	0.95	0.17	62,63,68,68	0
5	ALA	D	714	6/6	0.95	0.25	25,30,33,34	0
2	SO4	D	708	5/5	0.96	0.15	62,65,69,69	0
2	SO4	E	705	5/5	0.96	0.10	45,51,60,61	0
2	SO4	F	702	5/5	0.96	0.14	33,34,38,40	0
3	NA	B	713	1/1	0.96	0.12	40,40,40,40	0
3	NA	B	715	1/1	0.96	0.17	34,34,34,34	0
2	SO4	G	703	5/5	0.96	0.17	58,59,63,64	0
5	ALA	A	716	6/6	0.96	0.28	24,29,34,36	0
2	SO4	D	705	5/5	0.96	0.08	42,44,50,56	0
2	SO4	C	705	5/5	0.97	0.17	50,55,68,71	0
2	SO4	H	707	5/5	0.97	0.19	53,54,56,60	0
2	SO4	B	704	5/5	0.97	0.09	44,45,46,49	0
2	SO4	B	706	5/5	0.97	0.12	29,32,35,36	5
3	NA	A	709	1/1	0.97	0.09	35,35,35,35	0
2	SO4	F	703	5/5	0.97	0.08	41,42,48,51	0
2	SO4	D	702	5/5	0.97	0.10	44,49,53,53	0
2	SO4	A	702	5/5	0.97	0.14	36,37,41,43	0
2	SO4	A	706	5/5	0.97	0.11	23,35,40,43	5
3	NA	B	714	1/1	0.97	0.10	35,35,35,35	0
2	SO4	G	701	5/5	0.97	0.14	40,45,49,49	0
2	SO4	A	703	5/5	0.97	0.10	46,47,50,55	0
2	SO4	A	704	5/5	0.97	0.19	45,46,56,58	0
3	NA	E	710	1/1	0.97	0.11	40,40,40,40	0
2	SO4	E	701	5/5	0.97	0.12	26,30,33,36	5

*Continued on next page...*

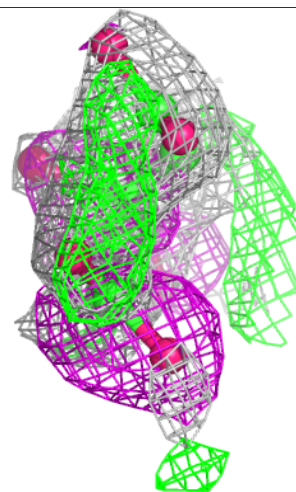
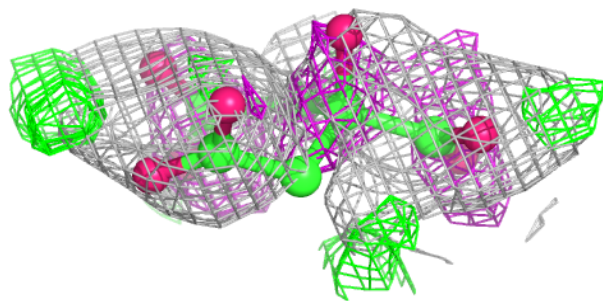
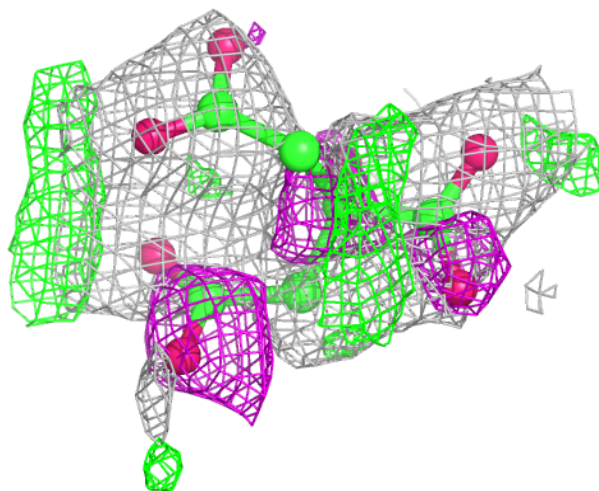
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	702	5/5	0.97	0.10	33,36,39,40	0
2	SO4	C	704	5/5	0.97	0.17	48,52,55,58	0
2	SO4	H	701	5/5	0.98	0.08	36,37,42,44	0
2	SO4	H	702	5/5	0.98	0.07	42,42,47,47	0
2	SO4	H	703	5/5	0.98	0.13	36,39,41,45	0
2	SO4	D	703	5/5	0.98	0.12	36,41,41,42	0
2	SO4	D	704	5/5	0.98	0.23	49,50,56,56	0
2	SO4	C	703	5/5	0.98	0.15	31,33,39,45	0
2	SO4	F	701	5/5	0.98	0.08	33,36,44,48	0
2	SO4	B	709	5/5	0.98	0.06	40,46,48,49	0
2	SO4	B	710	5/5	0.98	0.11	49,54,57,60	0
2	SO4	F	704	5/5	0.98	0.09	52,52,52,58	0
2	SO4	B	701	5/5	0.98	0.09	32,34,36,38	0
2	SO4	B	703	5/5	0.98	0.10	49,51,52,53	0
2	SO4	E	702	5/5	0.98	0.14	34,37,39,42	0
2	SO4	E	703	5/5	0.98	0.08	40,42,45,47	0
2	SO4	E	704	5/5	0.98	0.11	42,45,49,53	0
2	SO4	A	701	5/5	0.98	0.09	25,27,37,38	5
2	SO4	G	704	5/5	0.98	0.07	36,38,42,43	0
3	NA	C	708	1/1	0.98	0.06	39,39,39,39	0
2	SO4	E	706	5/5	0.98	0.10	31,32,36,36	5
2	SO4	B	702	5/5	0.99	0.09	35,37,39,42	0
2	SO4	C	701	5/5	0.99	0.08	29,32,37,38	0
2	SO4	D	701	5/5	0.99	0.07	24,31,40,41	0
2	SO4	B	705	5/5	0.99	0.11	36,36,41,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

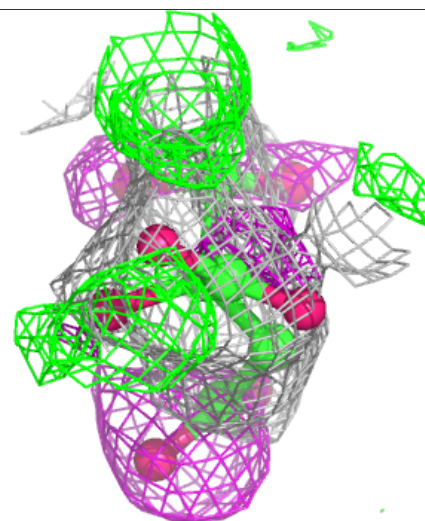
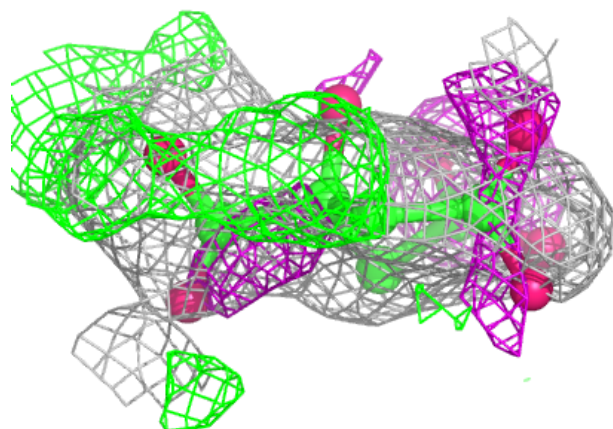
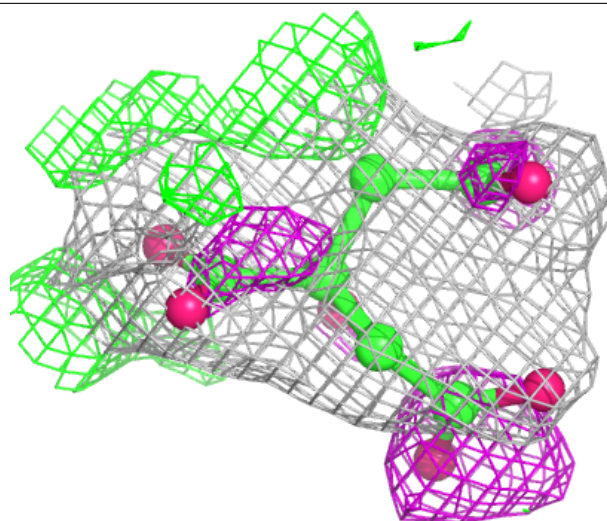
**Electron density around FLC A 717:**

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



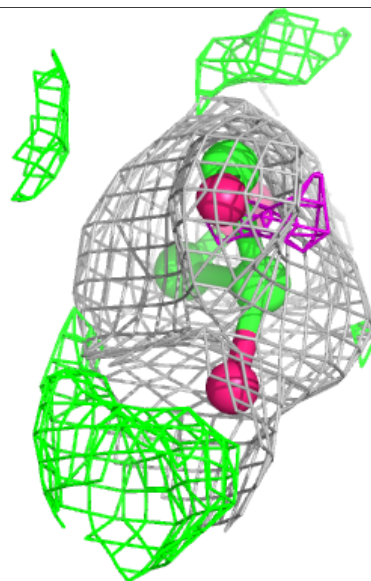
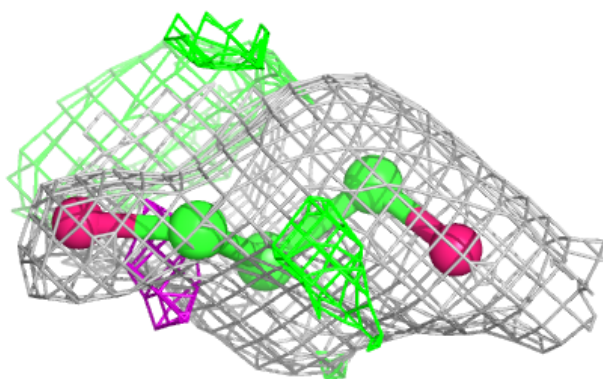
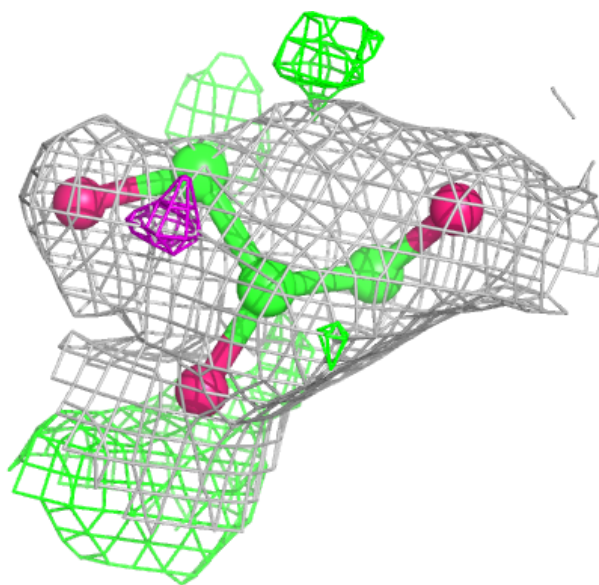
**Electron density around FLC H 713:**

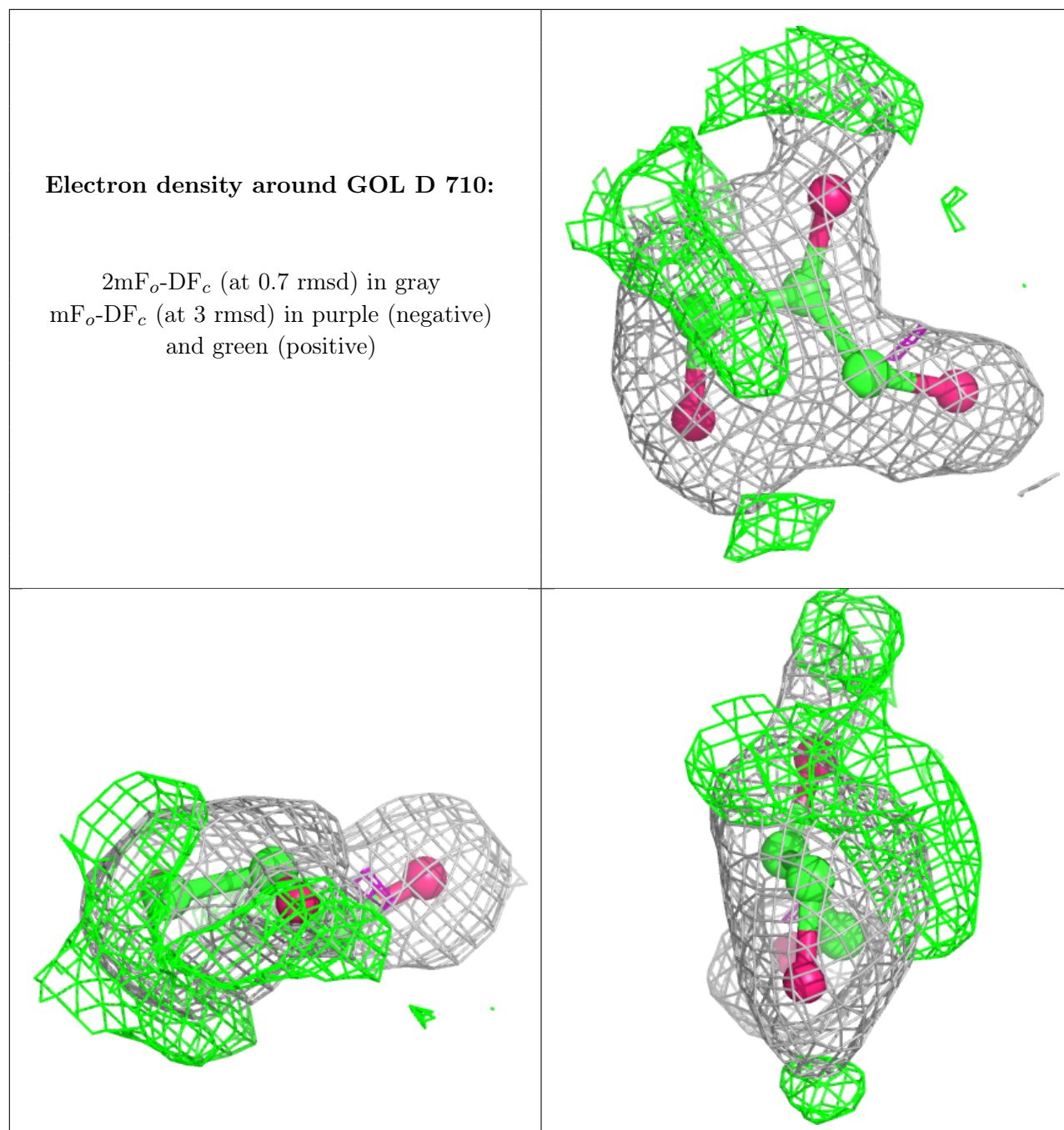
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GOL G 707:**

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

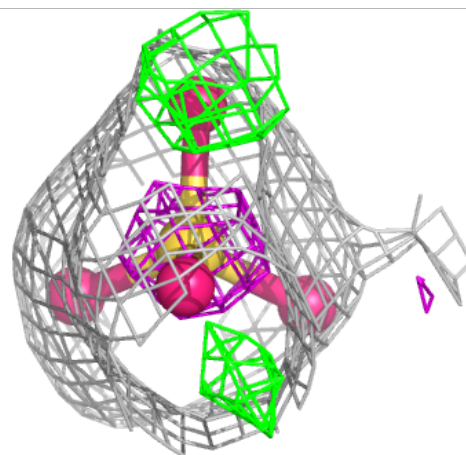
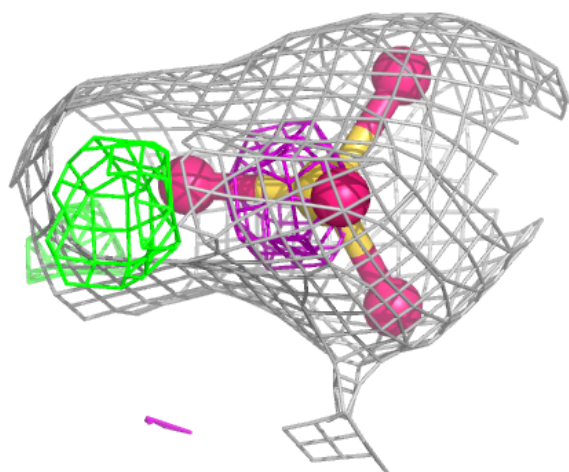
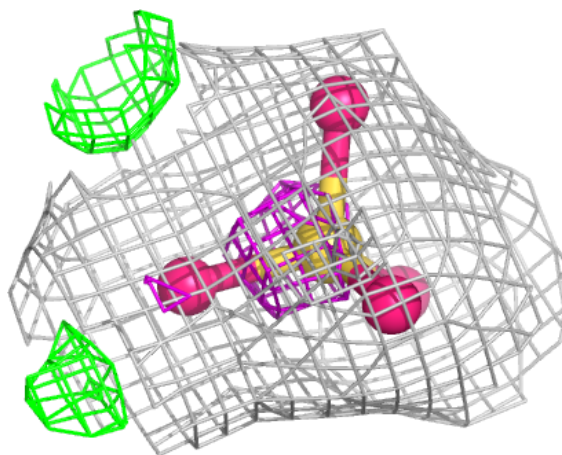


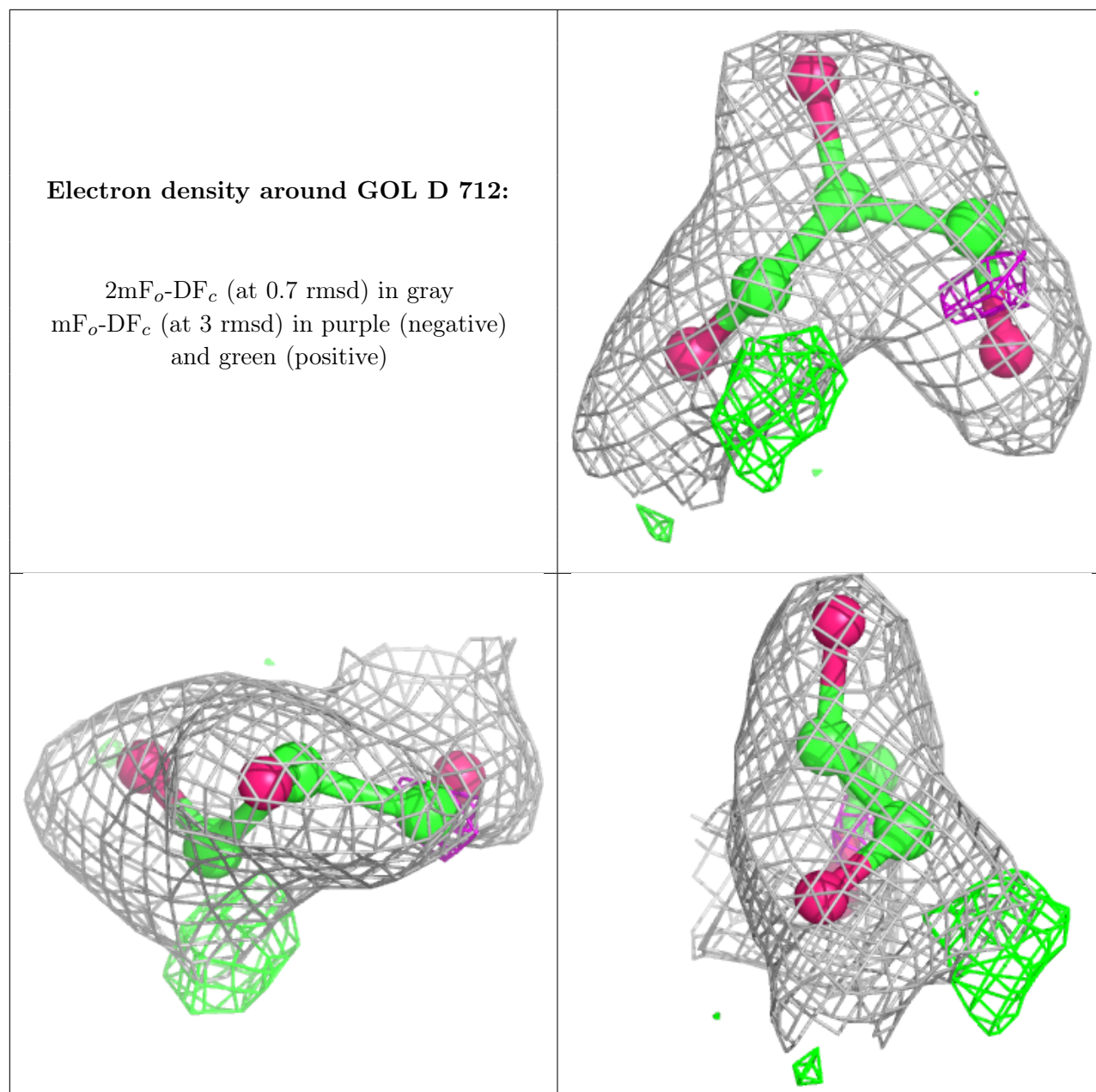




**Electron density around SO4 D 707:**

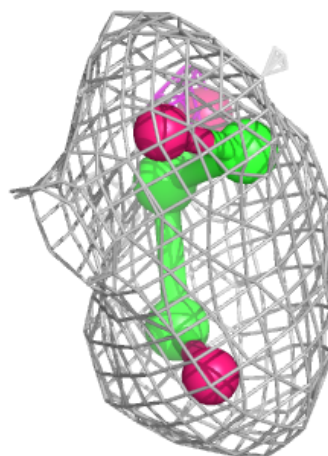
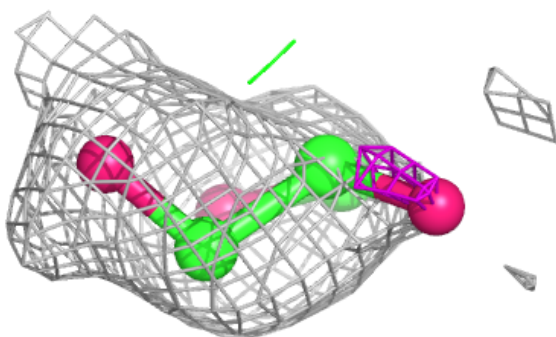
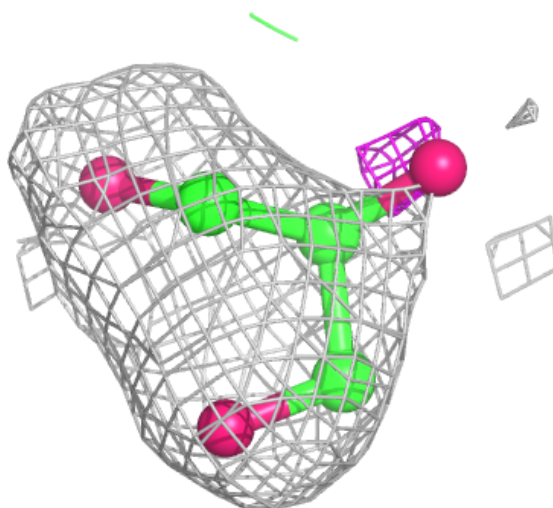
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





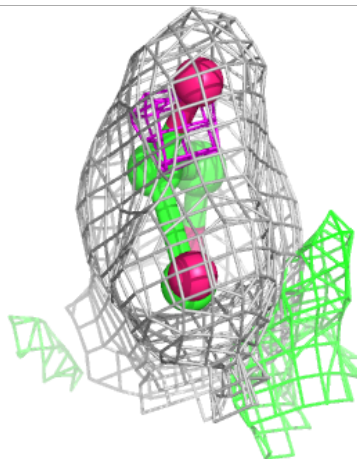
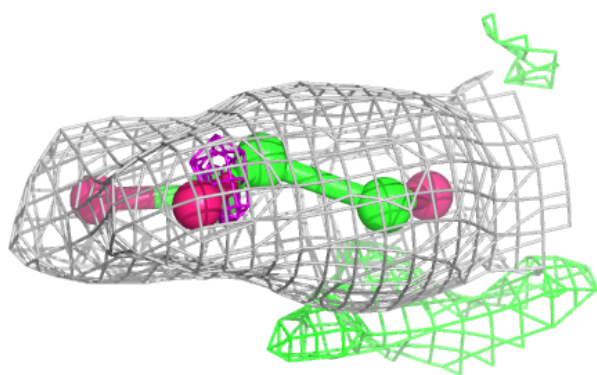
**Electron density around GOL H 711:**

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



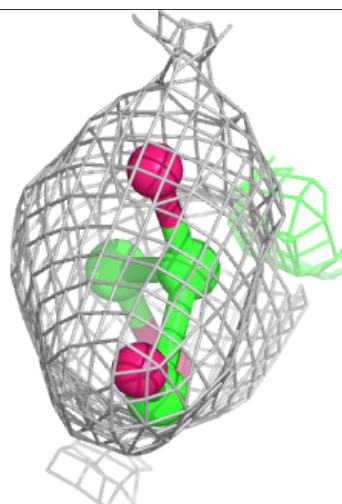
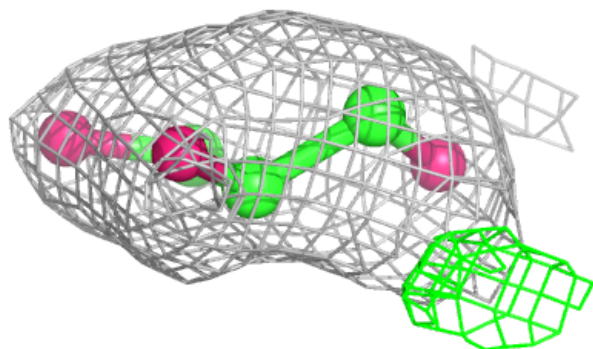
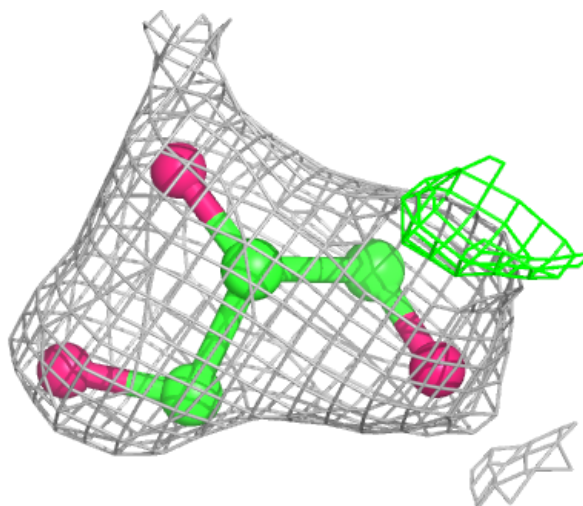
**Electron density around GOL C 709:**

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



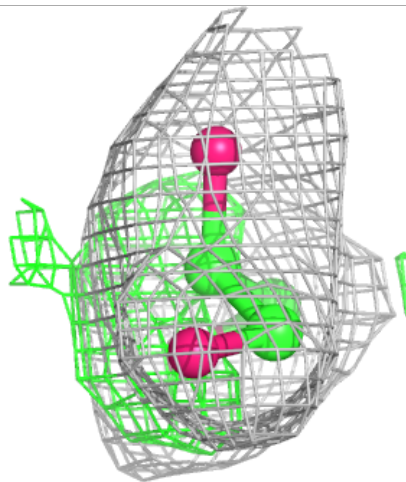
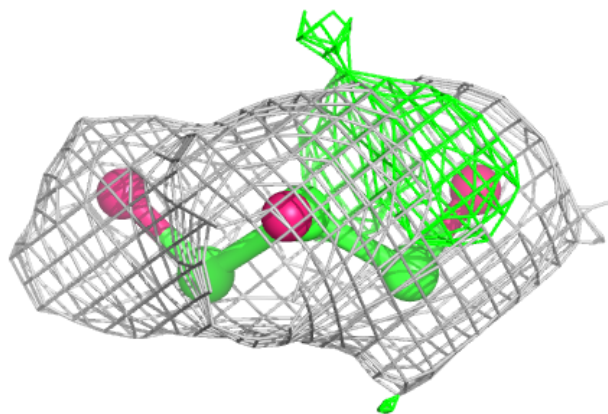
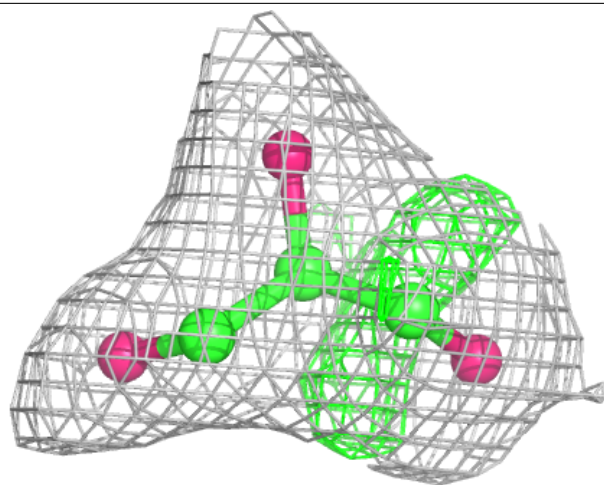
**Electron density around GOL D 711:**

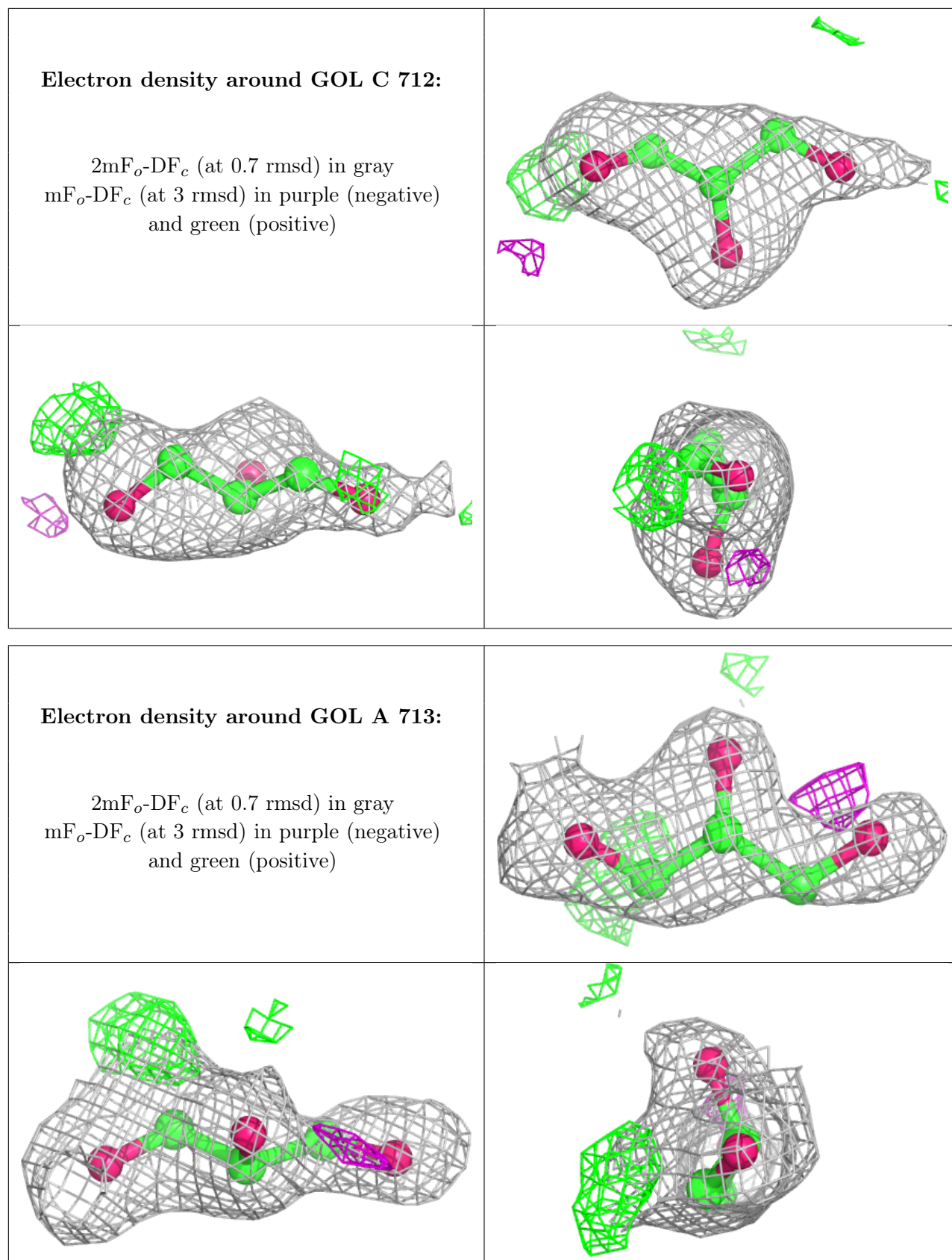
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GOL G 708:**

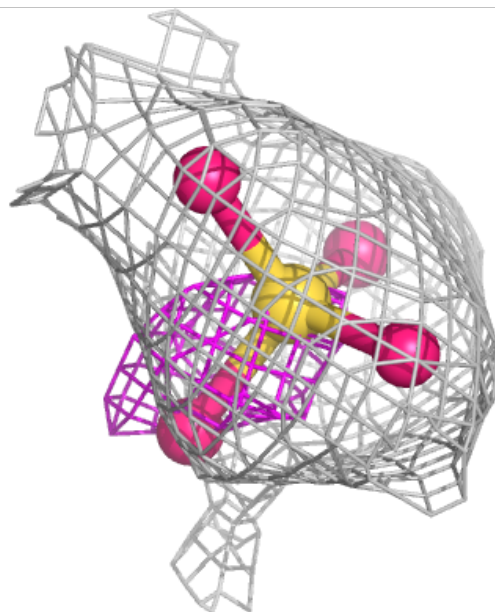
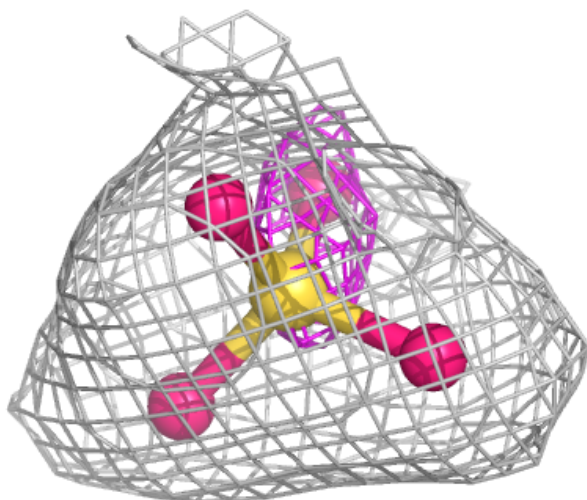
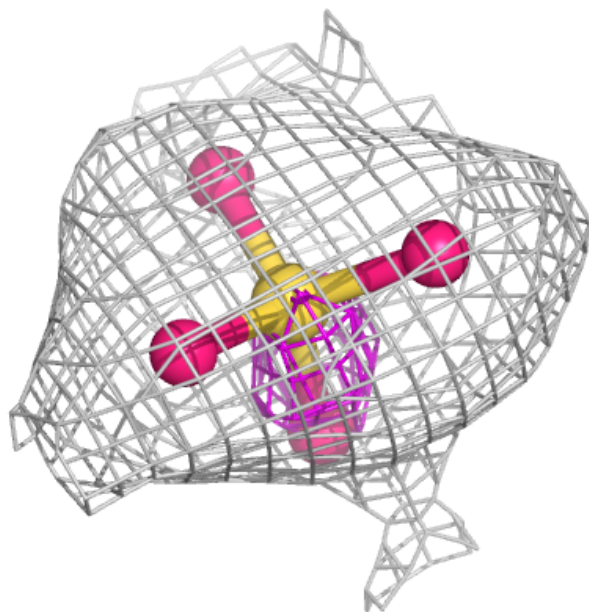
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SO4 D 706:**

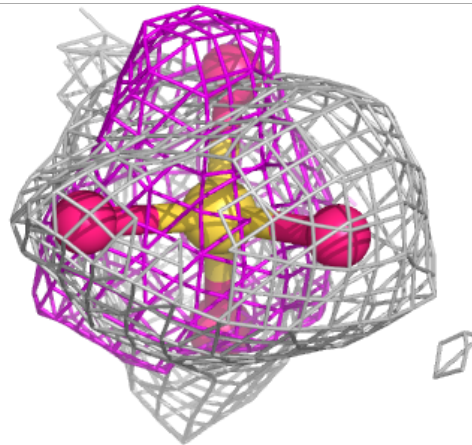
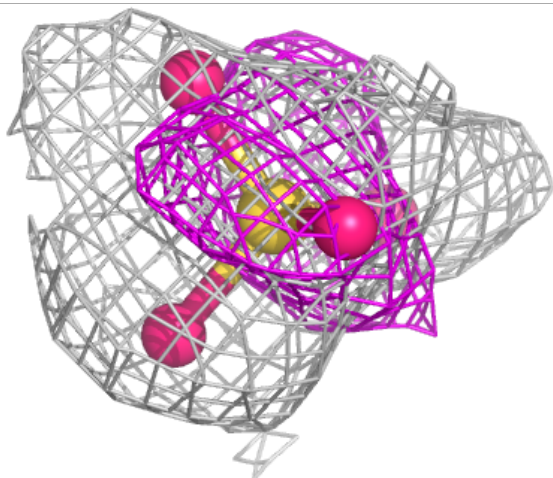
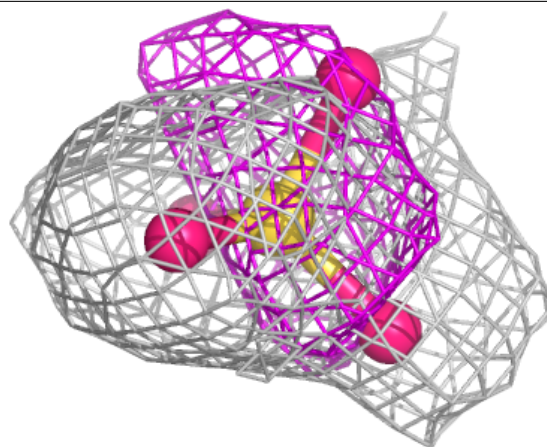
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





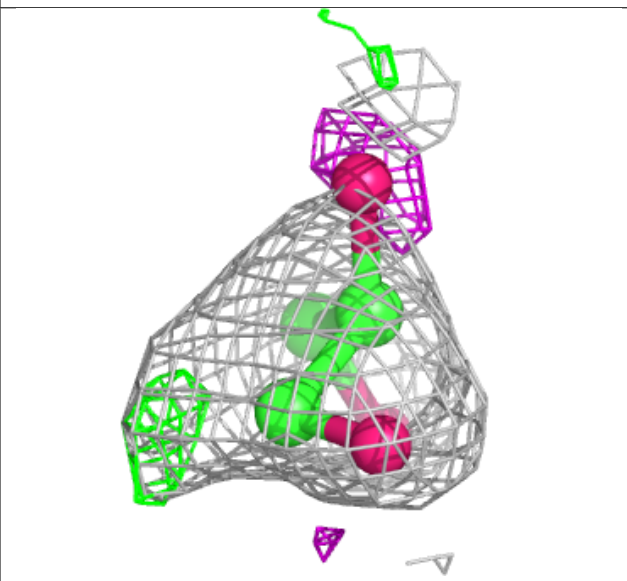
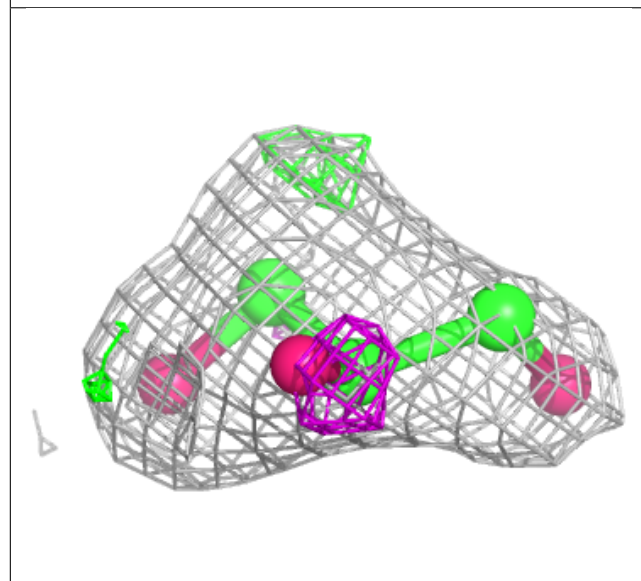
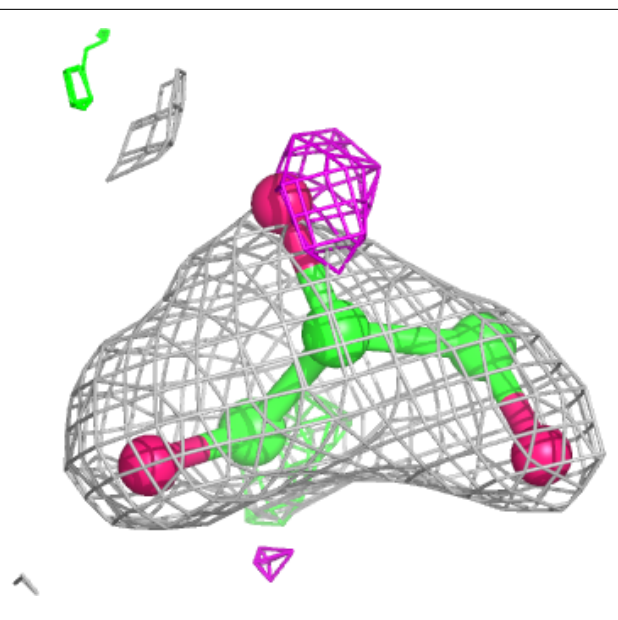
**Electron density around SO4 F 705:**

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



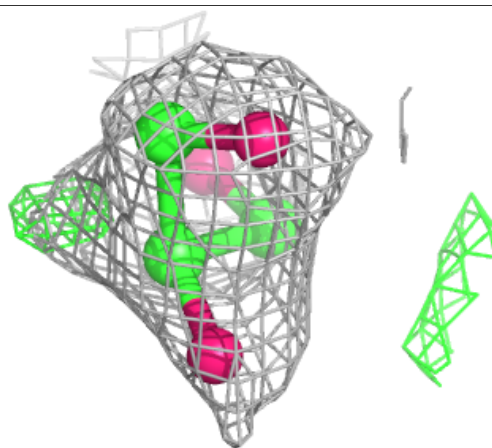
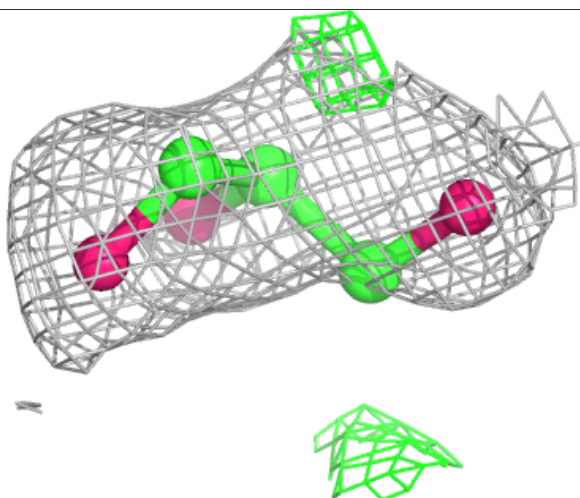
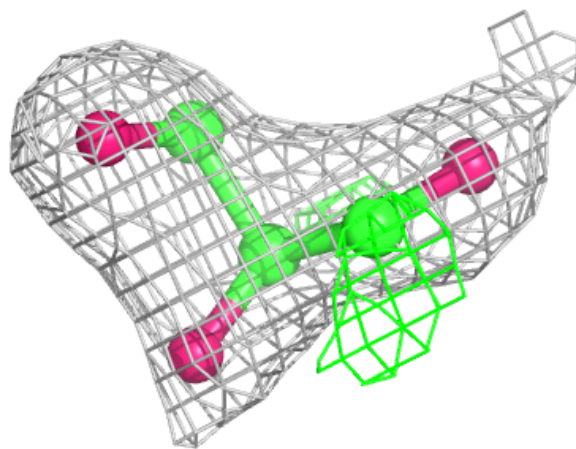
**Electron density around GOL E 712:**

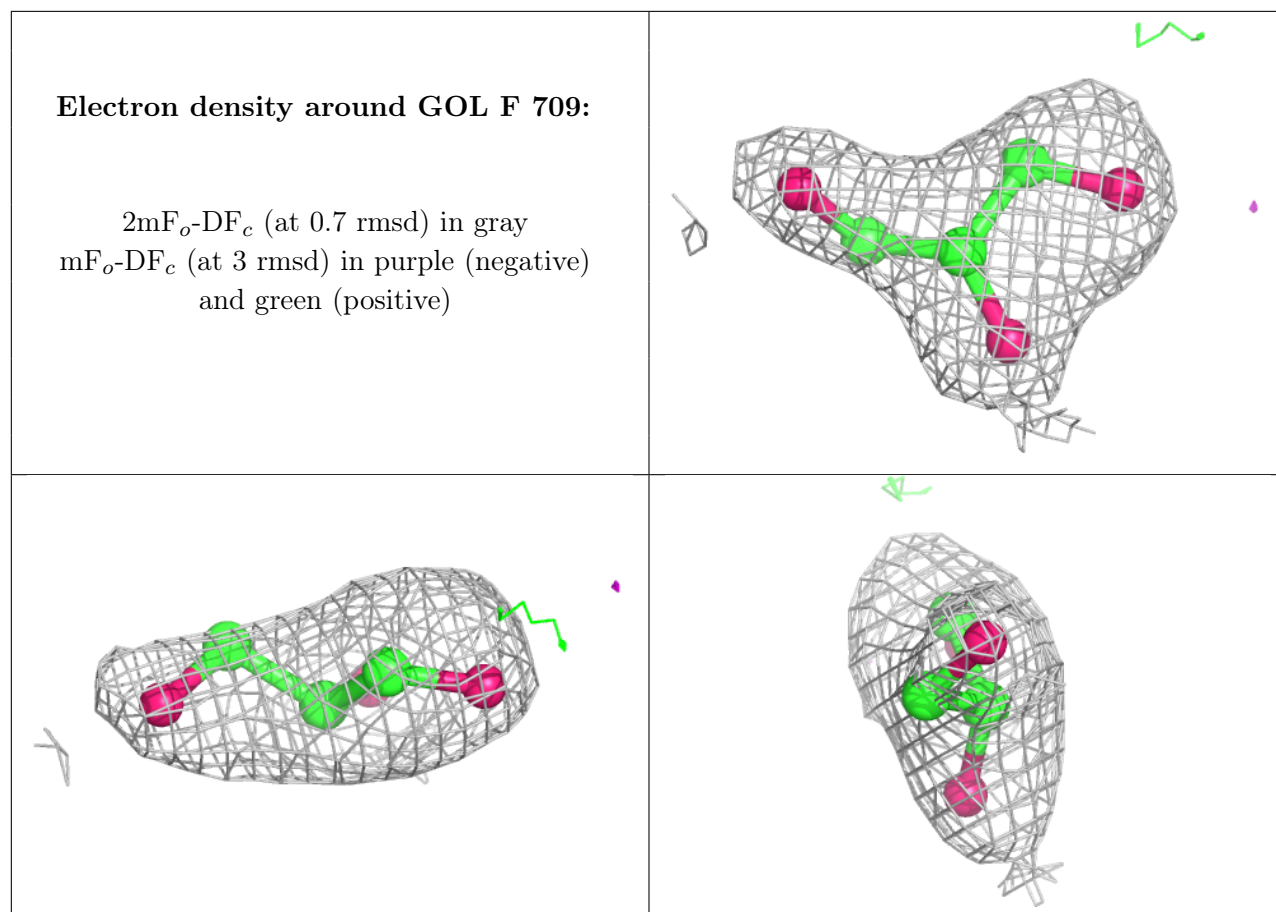
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GOL E 714:**

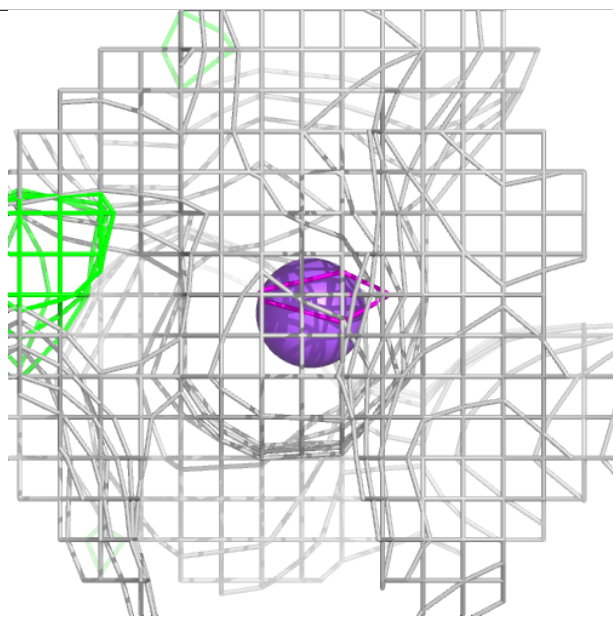
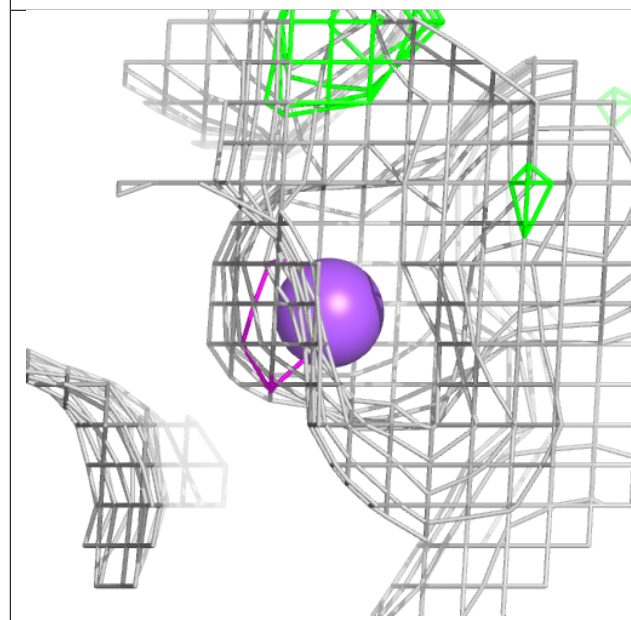
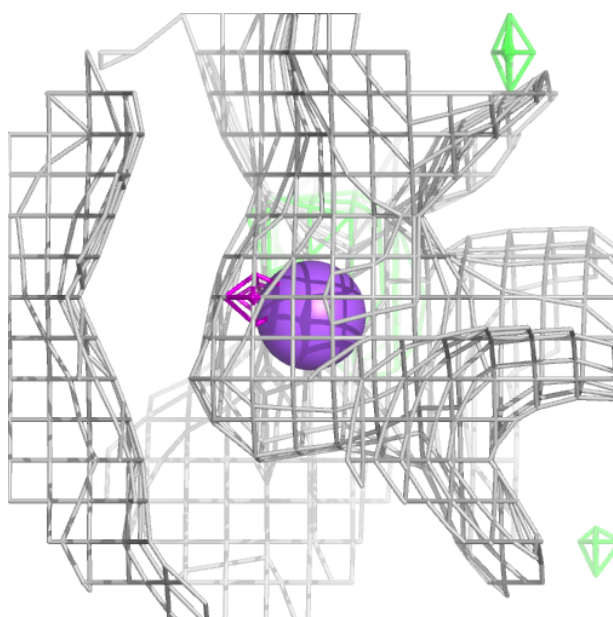
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

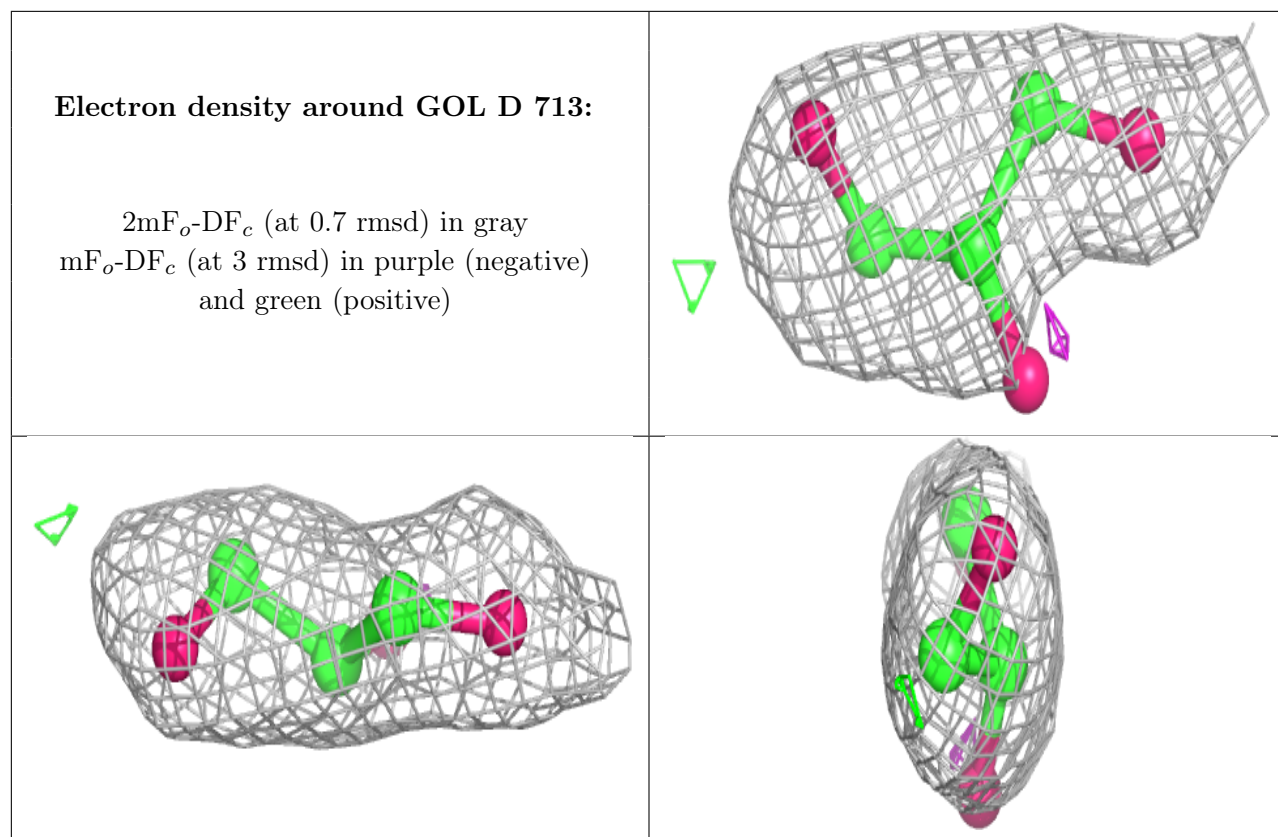




**Electron density around NA A 712:**

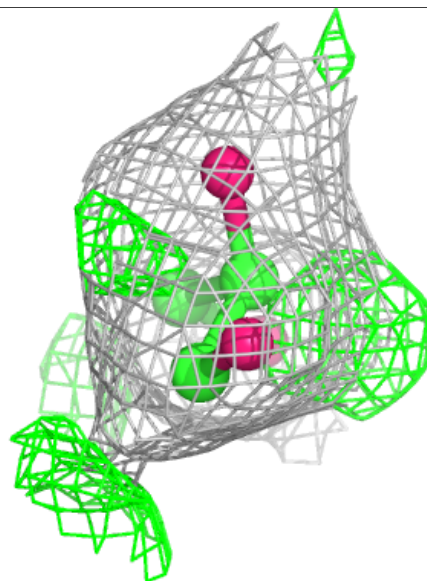
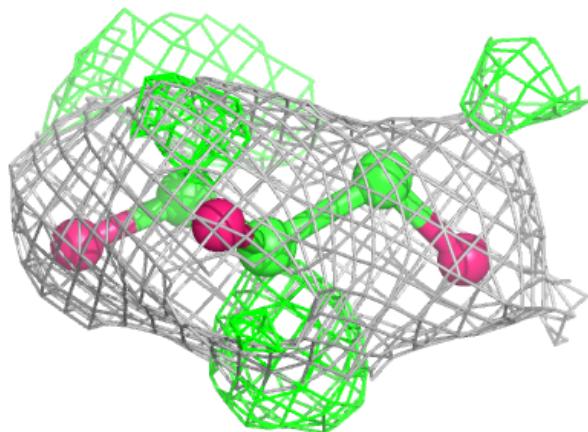
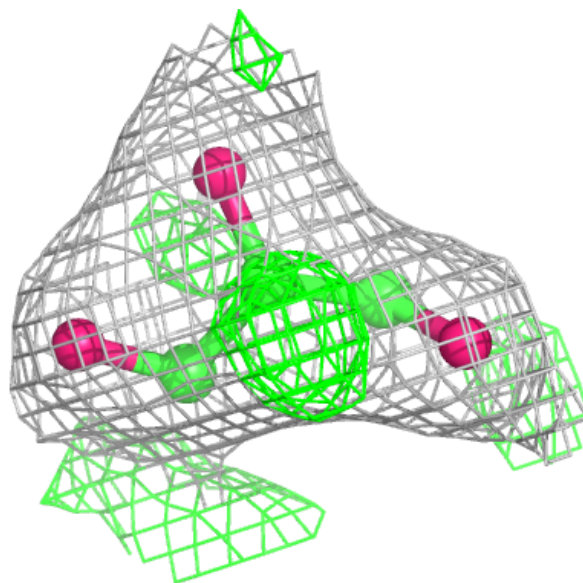
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





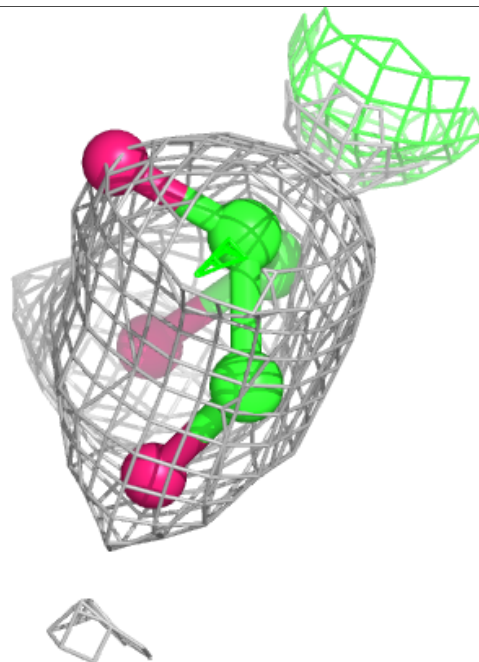
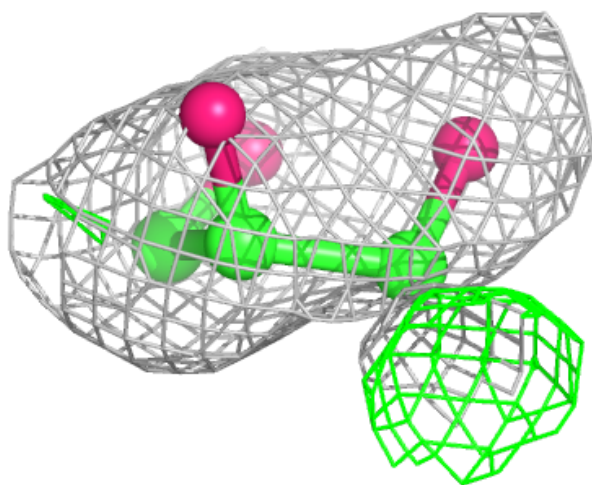
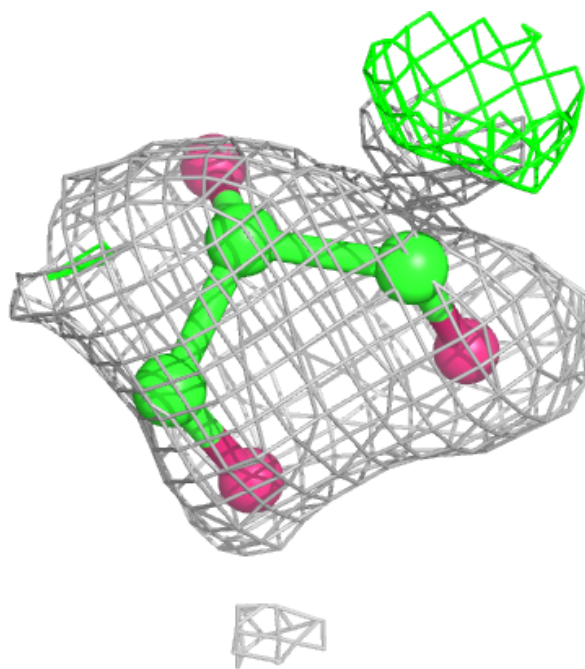
**Electron density around GOL C 710:**

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



**Electron density around GOL F 712:**

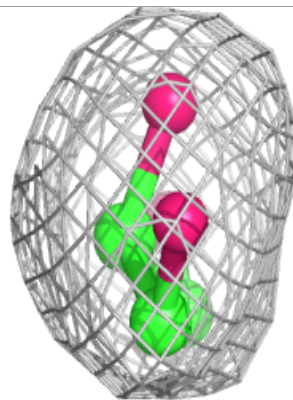
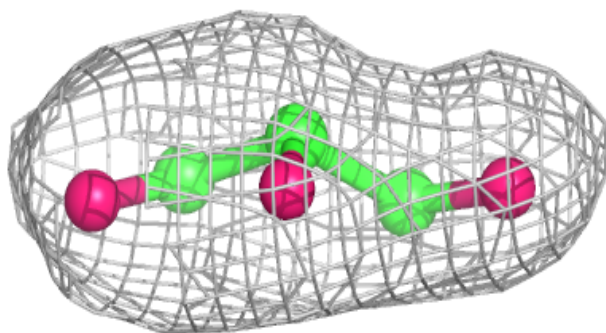
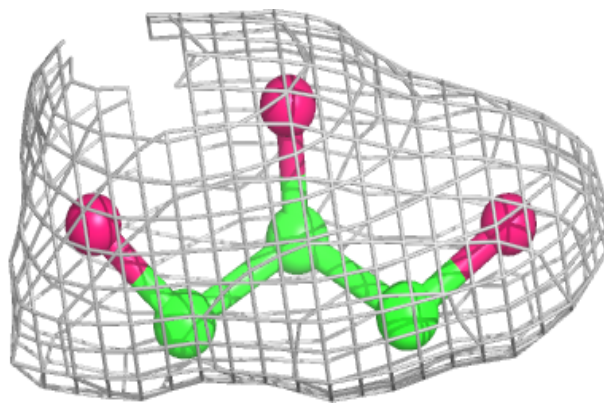
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





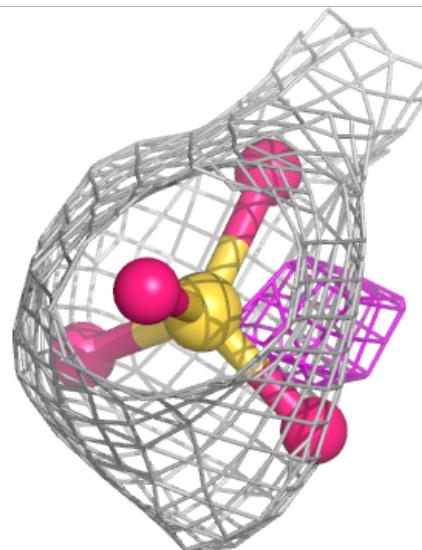
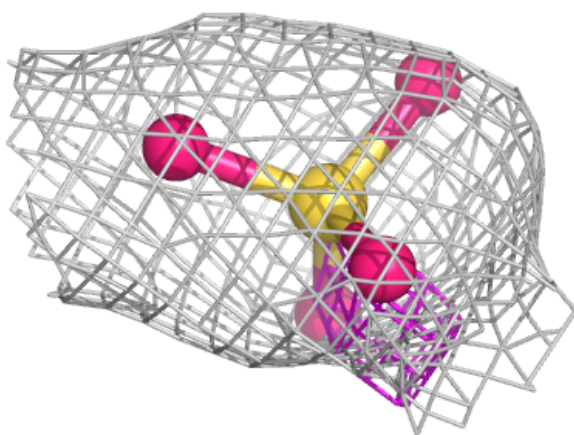
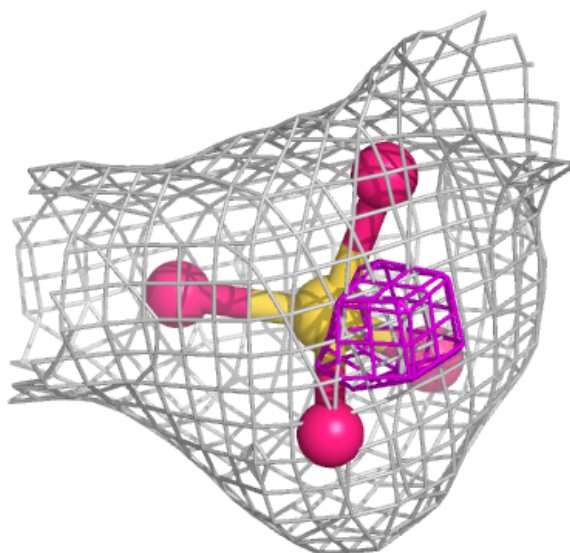
**Electron density around GOL F 711:**

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



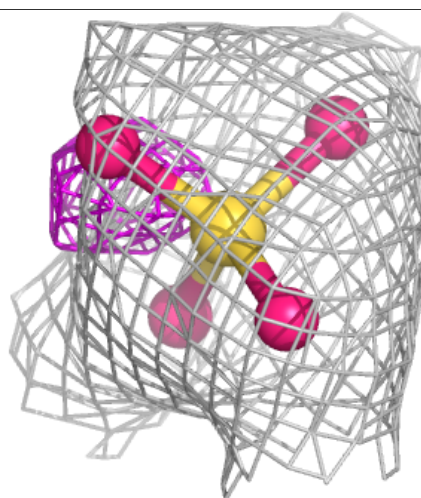
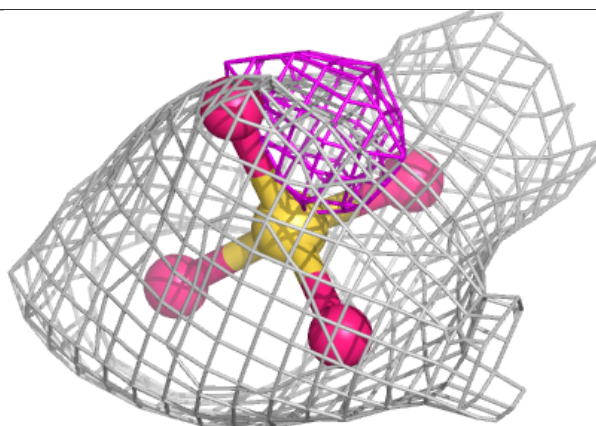
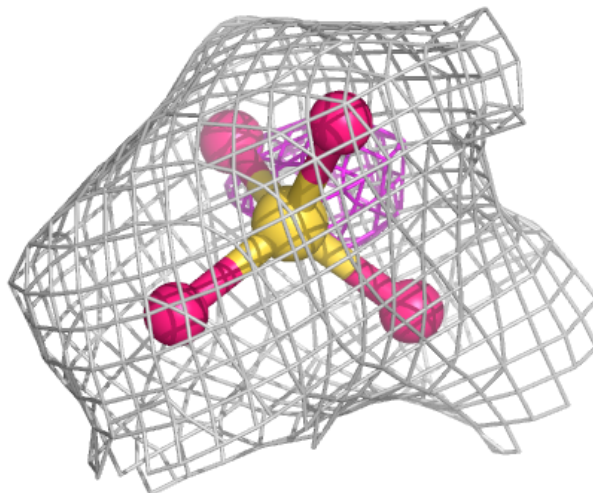
**Electron density around SO4 H 708:**

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



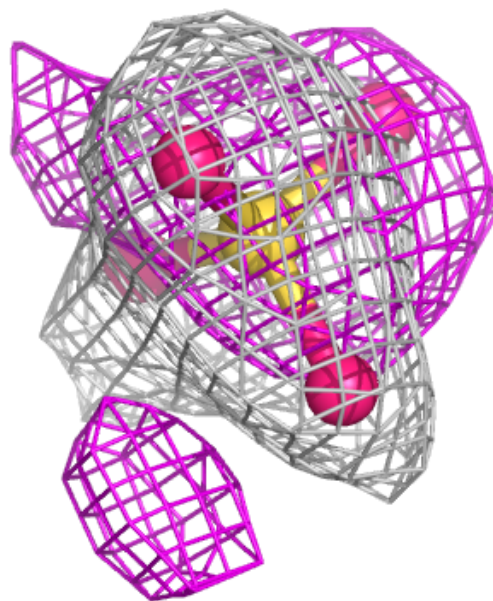
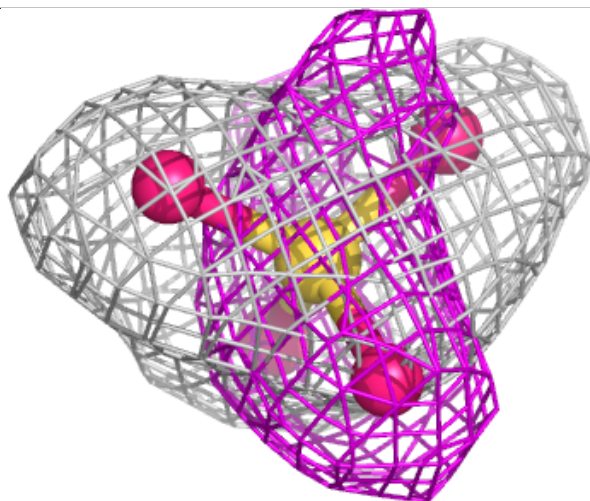
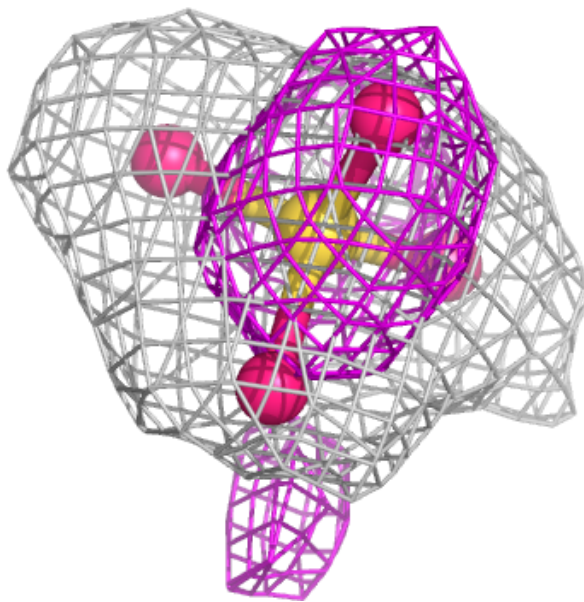
**Electron density around SO4 G 702:**

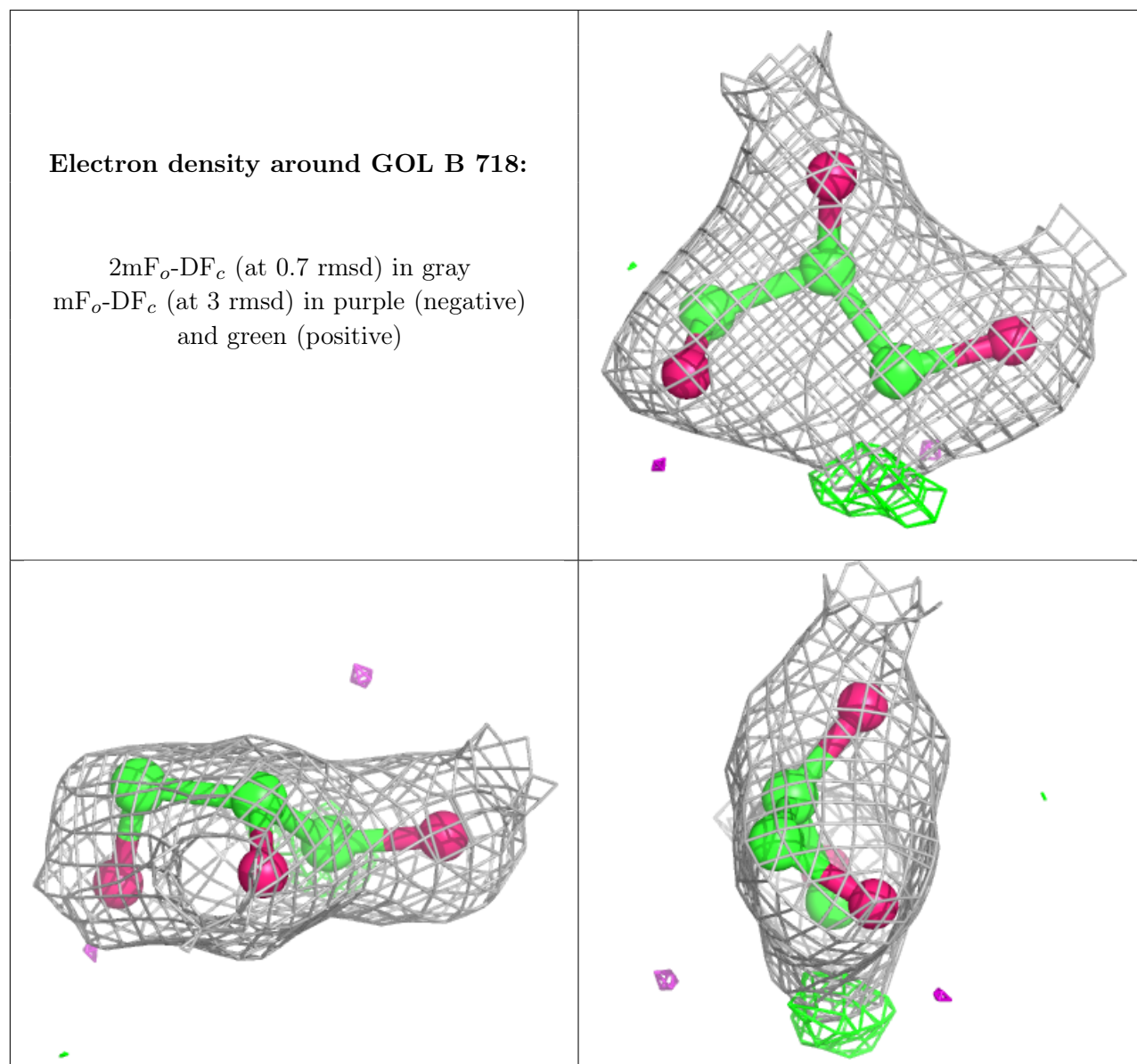
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 E 709:**

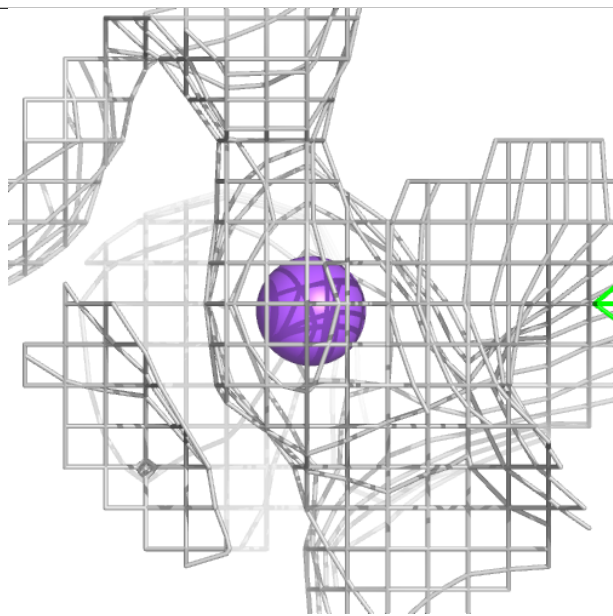
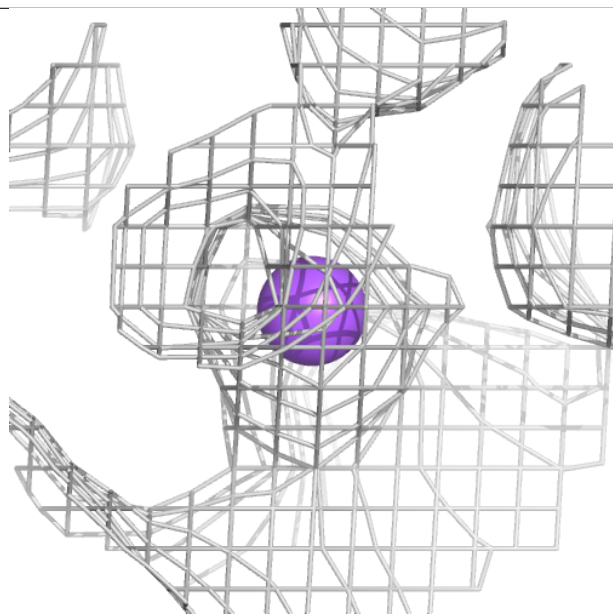
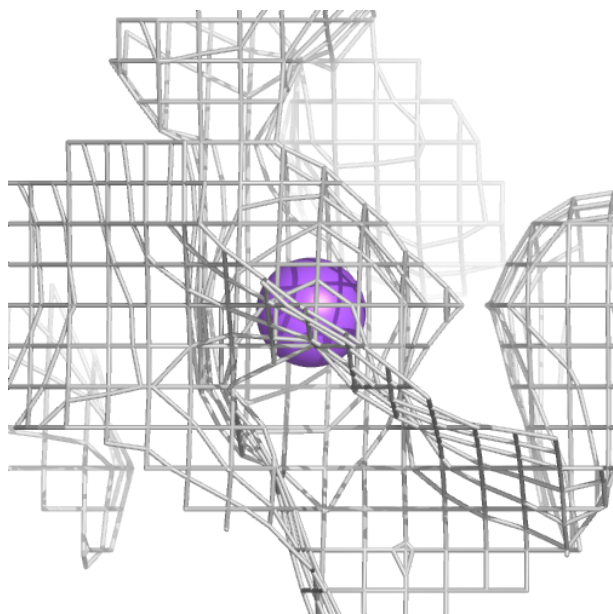
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





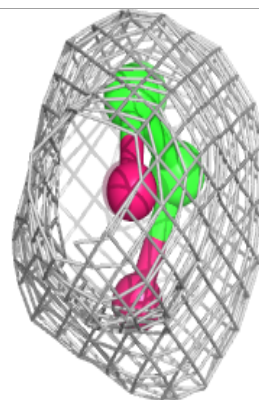
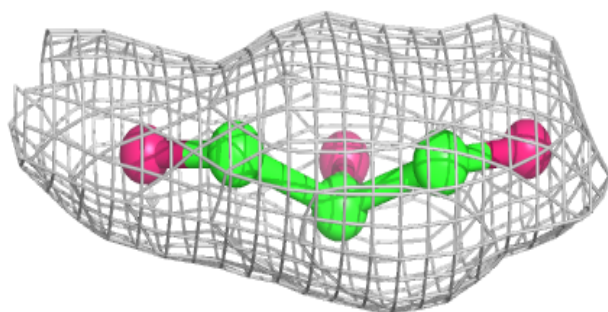
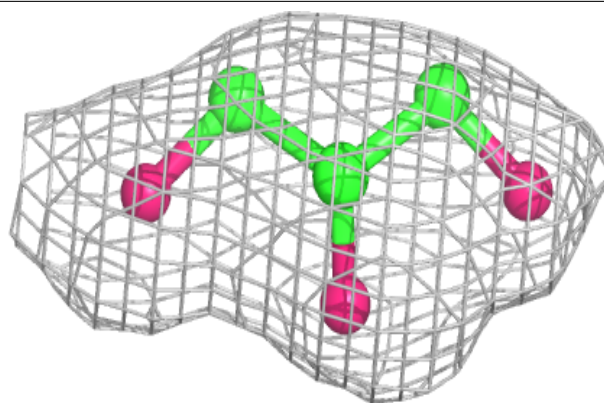
**Electron density around NA G 706:**

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

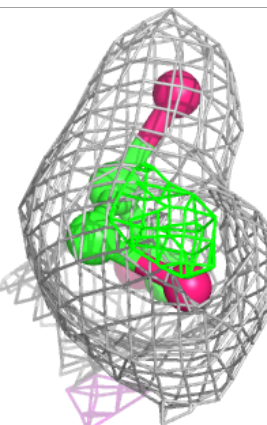
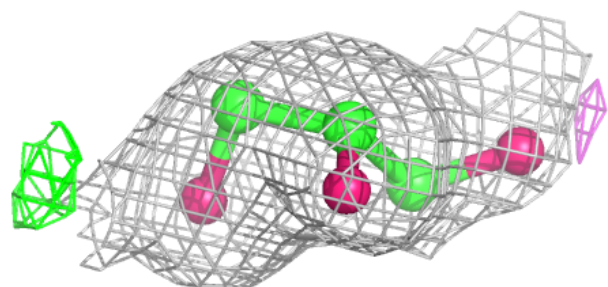
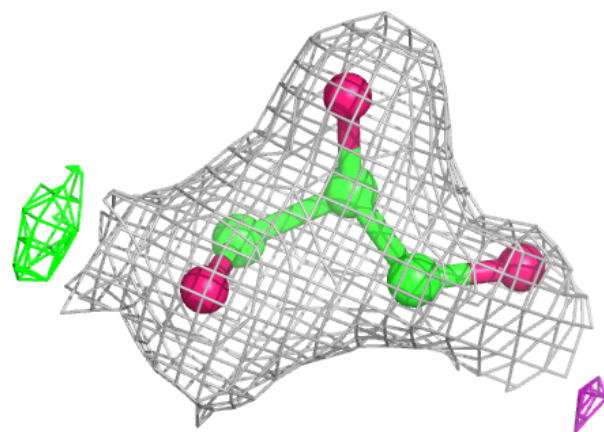


**Electron density around GOL C 711:**

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

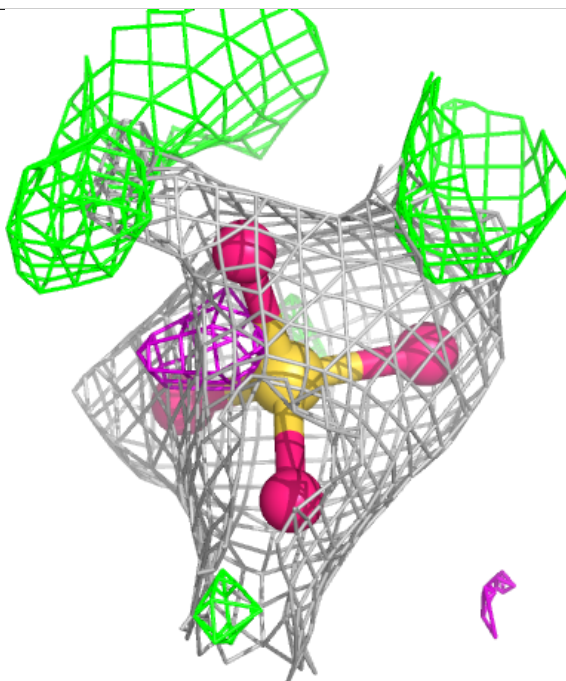
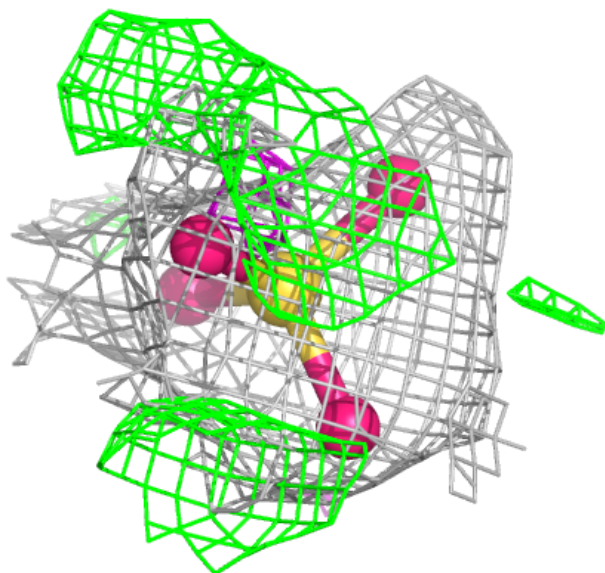
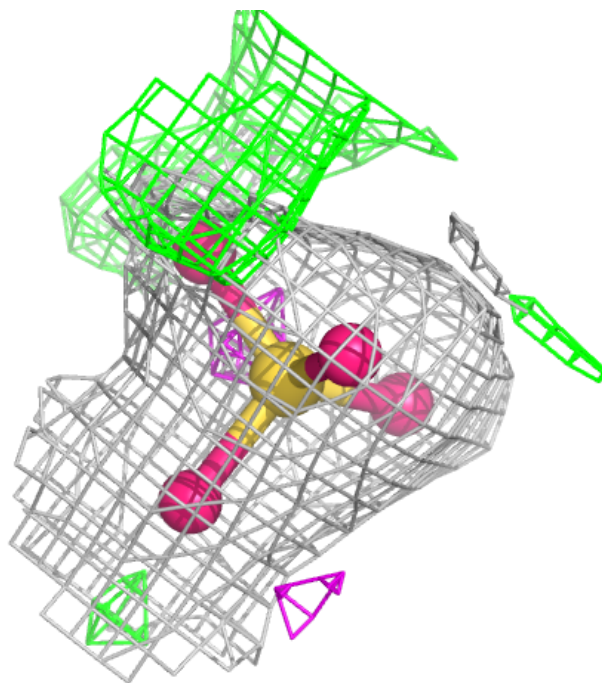
**Electron density around GOL E 713:**

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



**Electron density around SO4 F 706:**

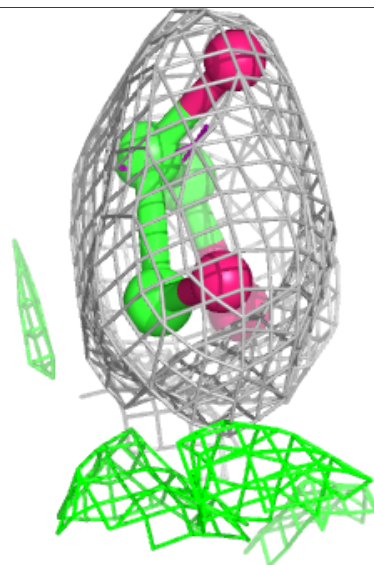
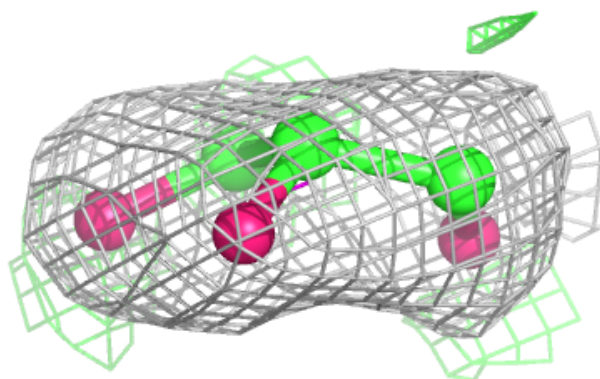
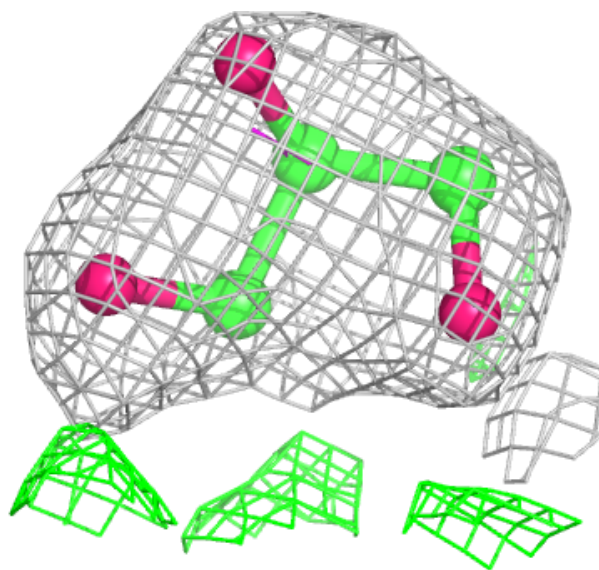
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





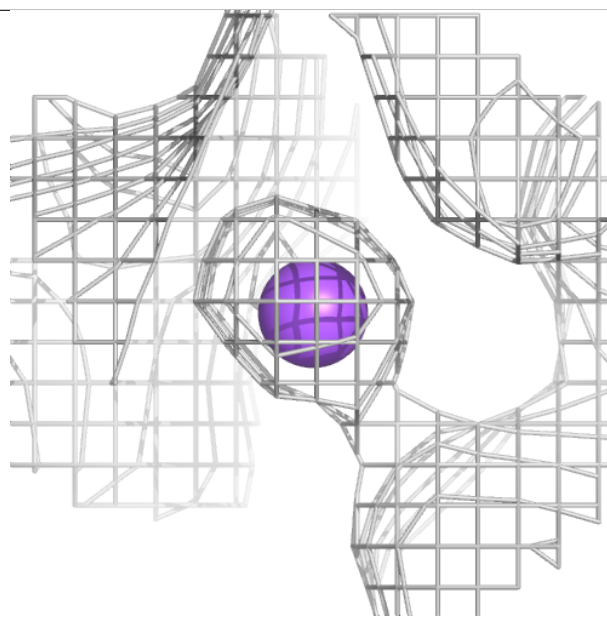
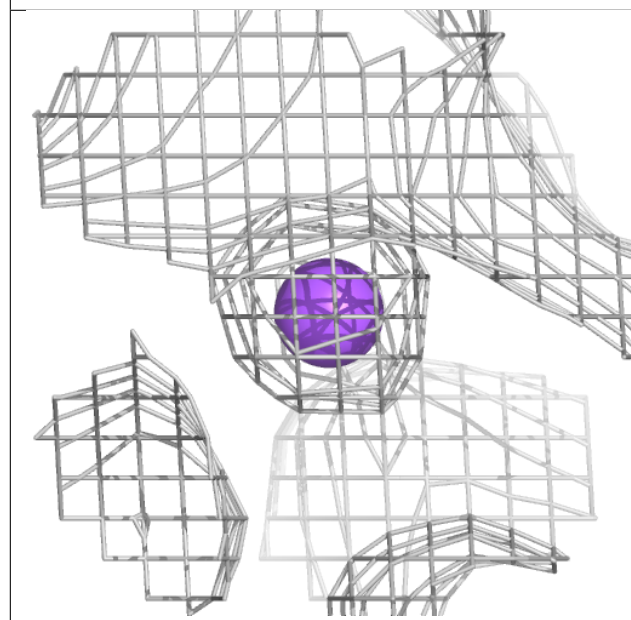
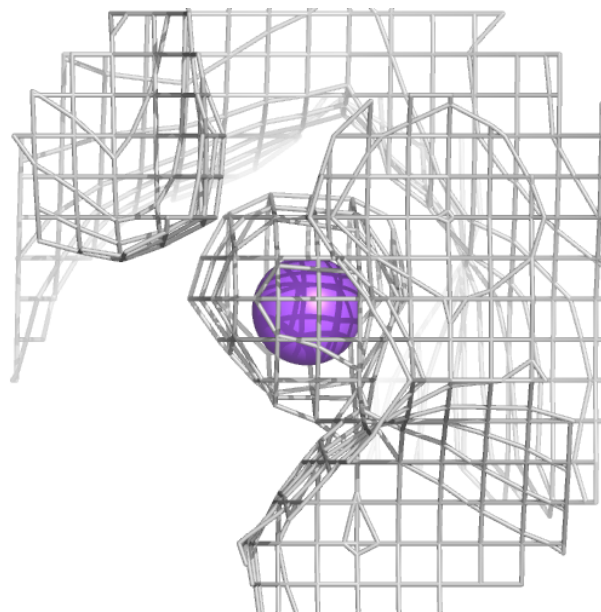
**Electron density around GOL F 708:**

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



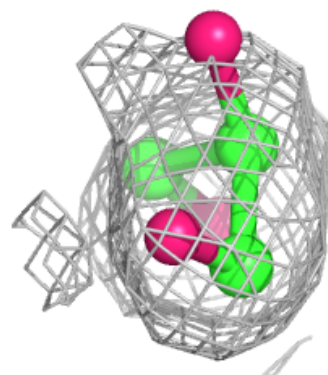
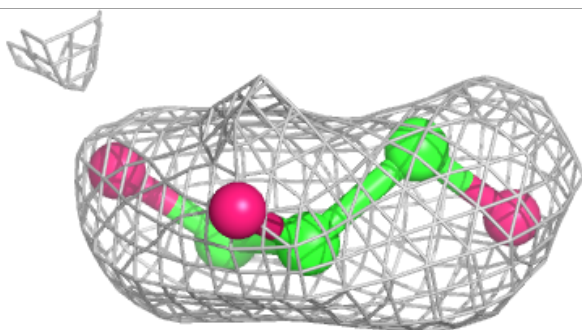
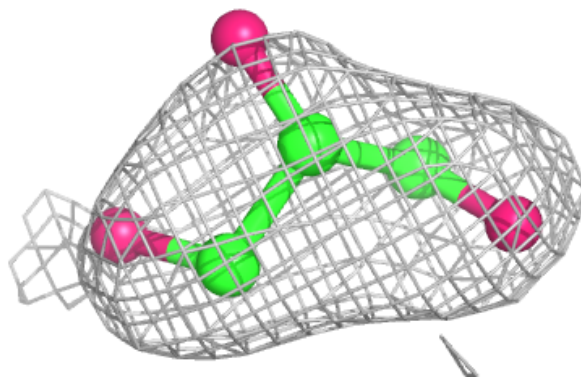
**Electron density around NA H 710:**

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

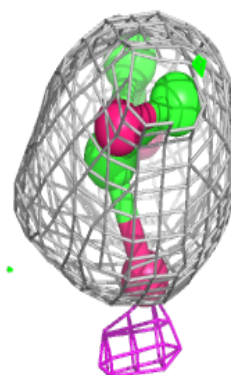
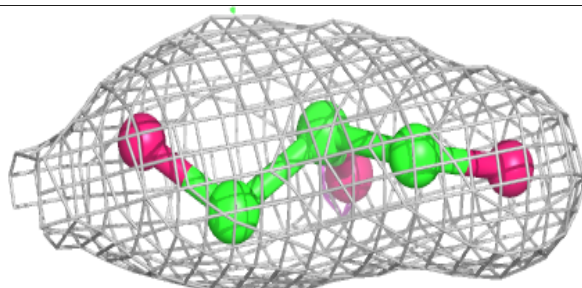
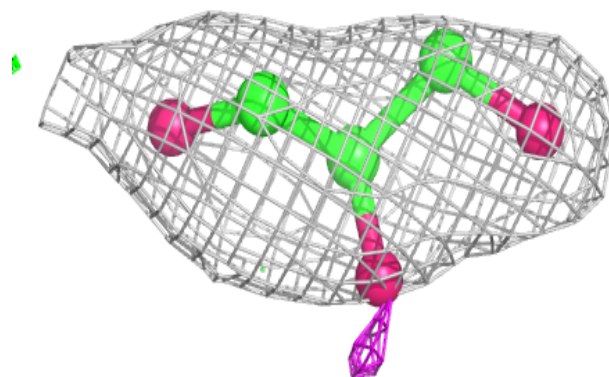


**Electron density around GOL F 710:**

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

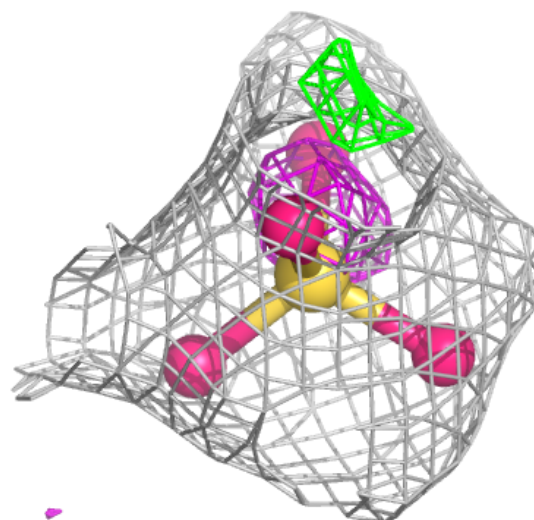
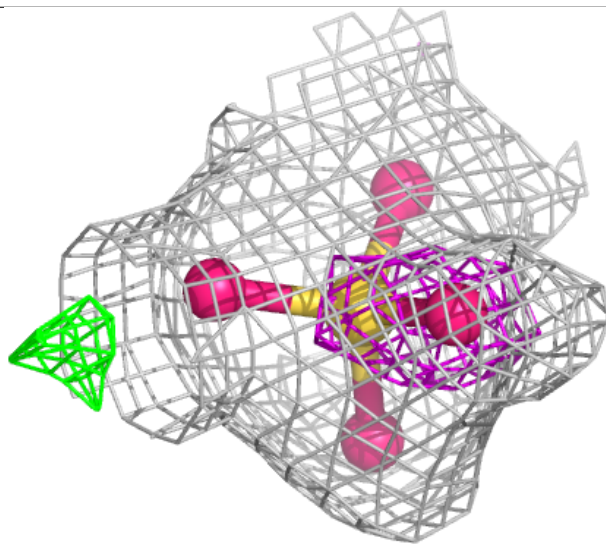
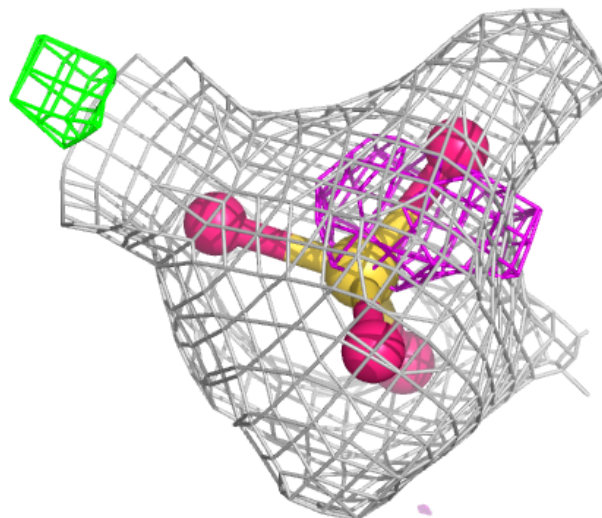
**Electron density around GOL A 715:**

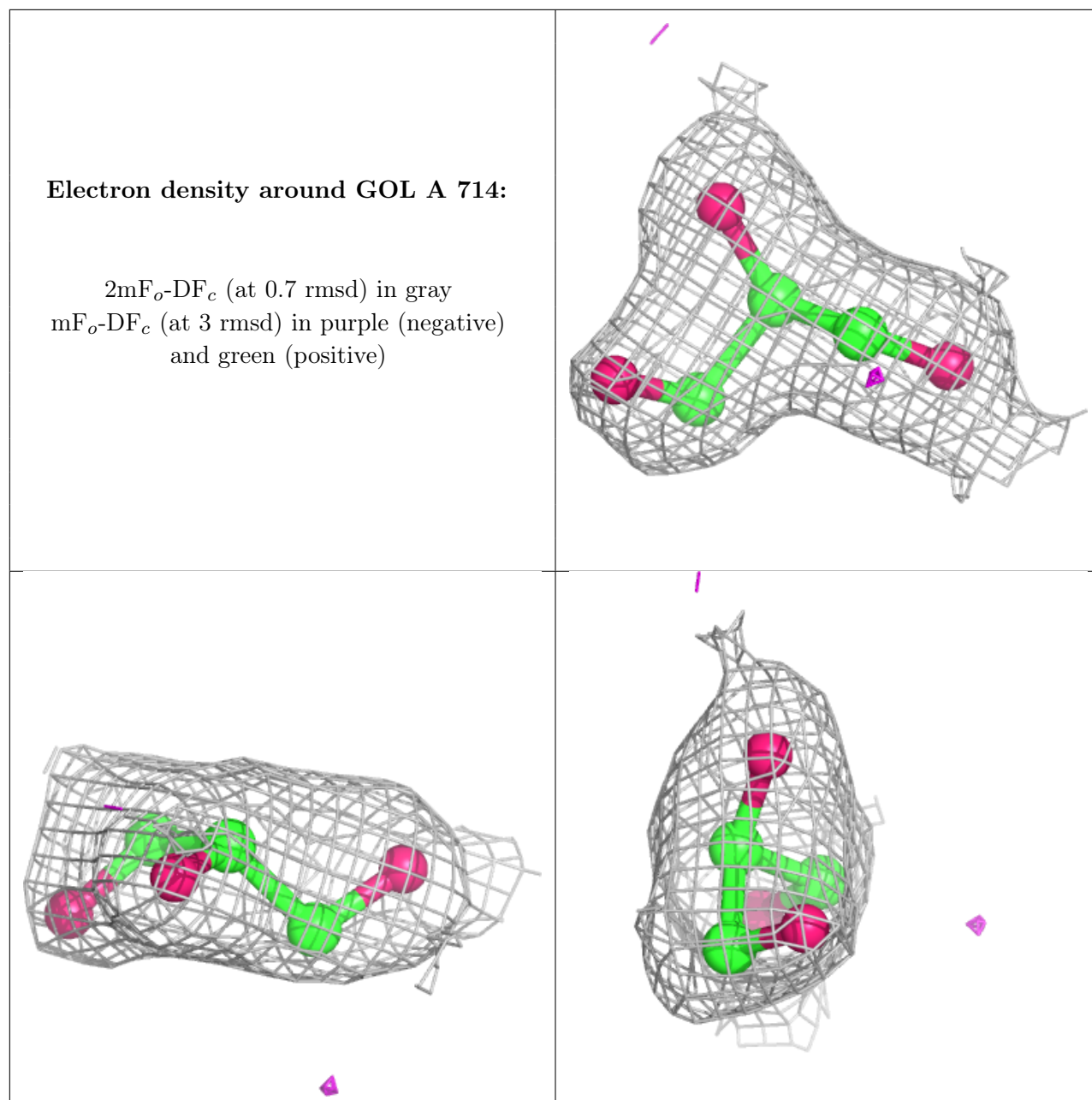
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 B 712:**

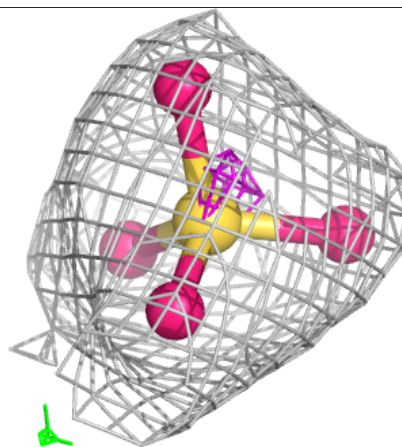
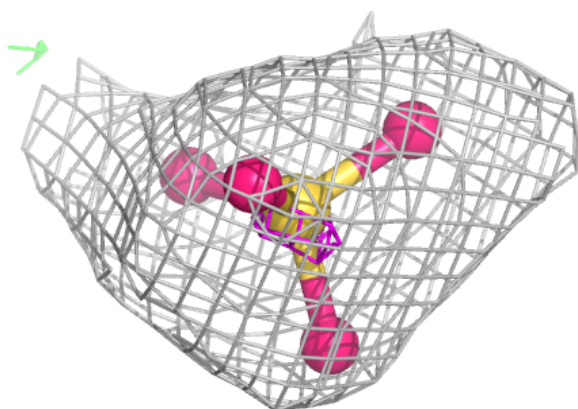
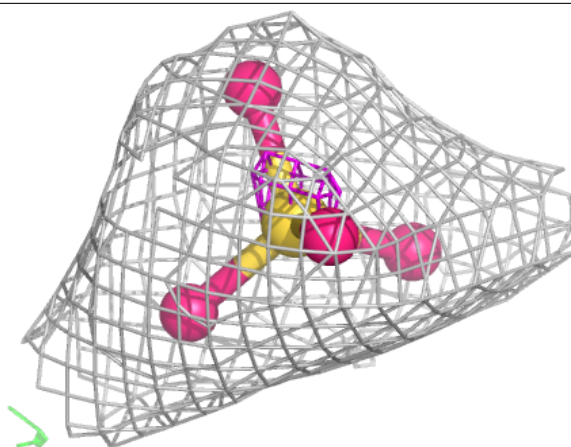
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





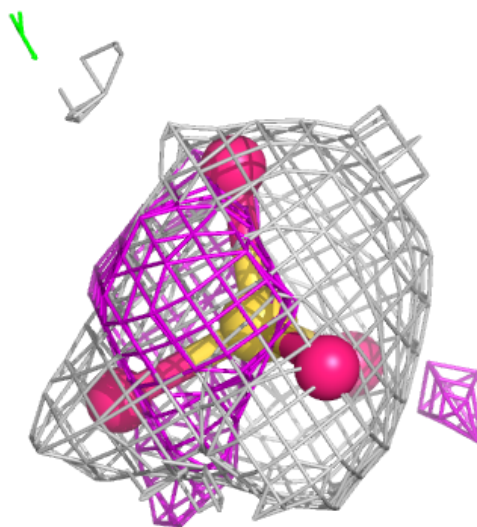
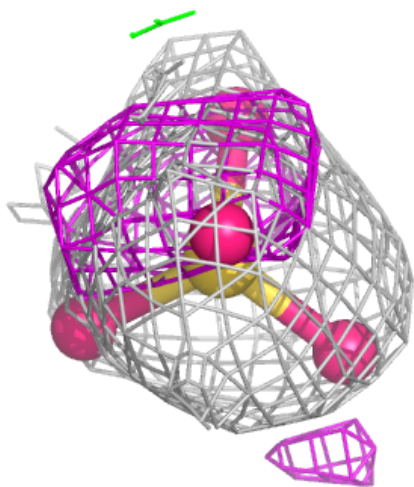
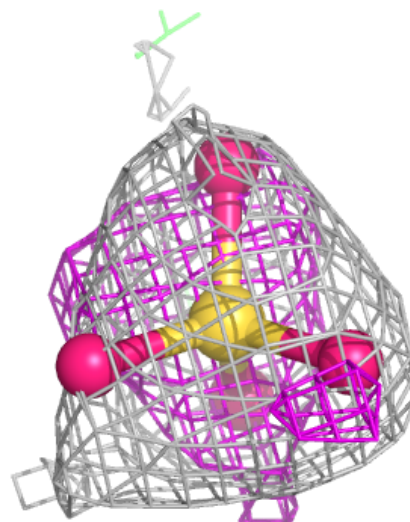
**Electron density around SO4 H 709:**

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



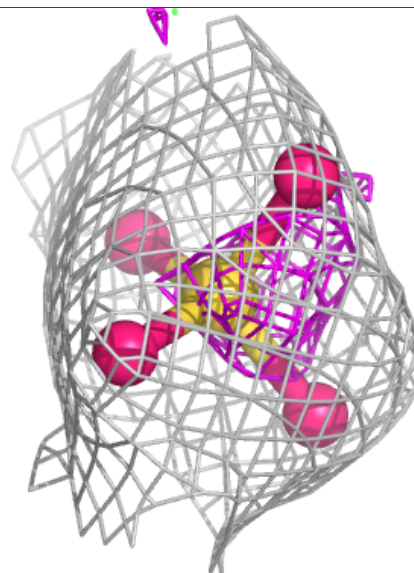
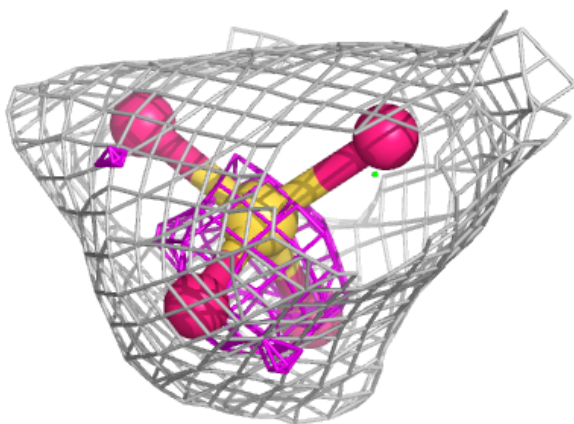
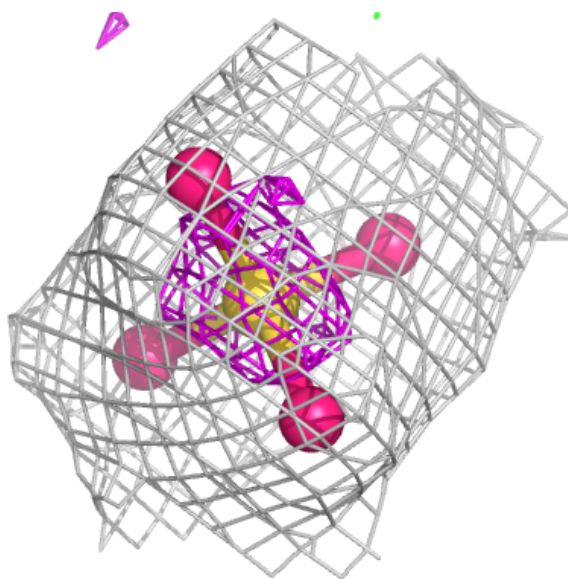
**Electron density around SO4 F 707:**

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

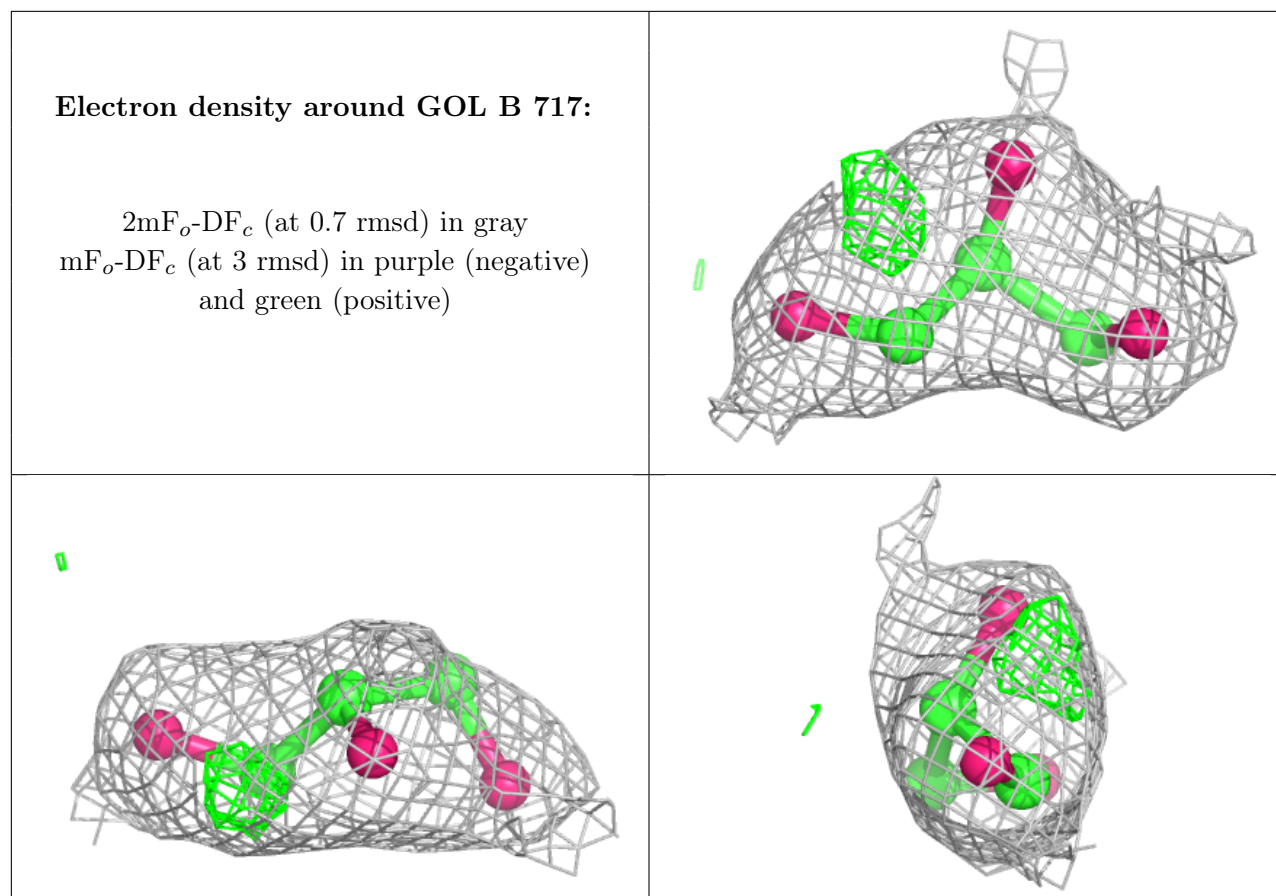


**Electron density around SO4 A 705:**

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

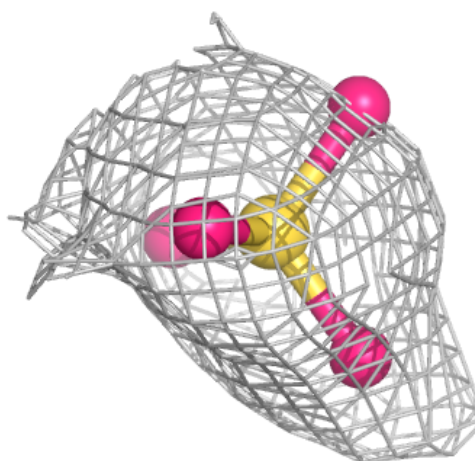
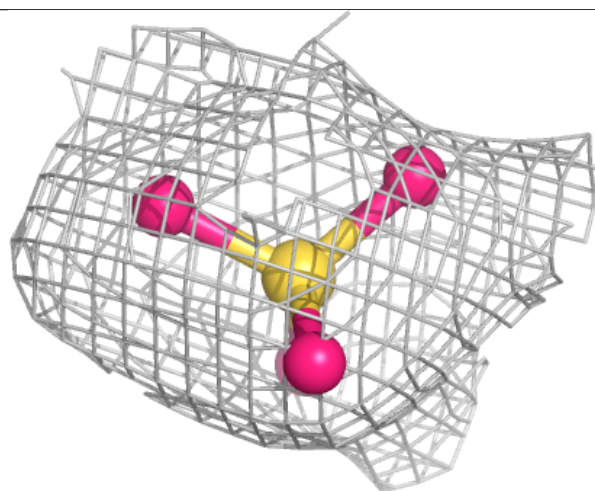
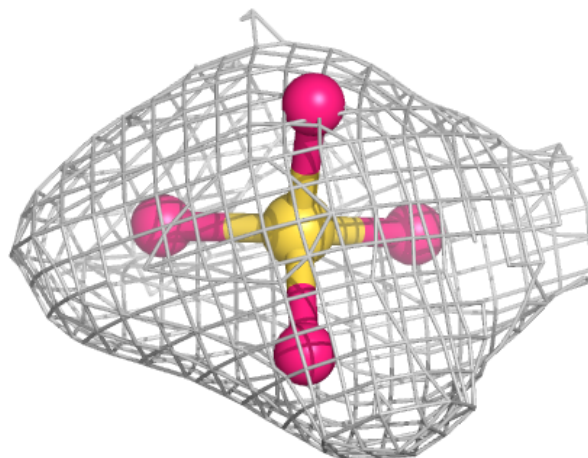






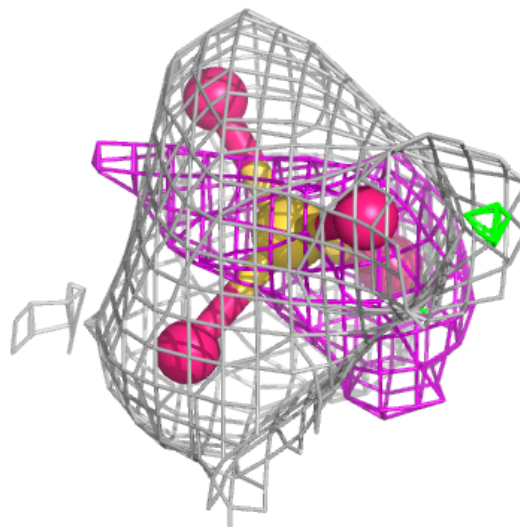
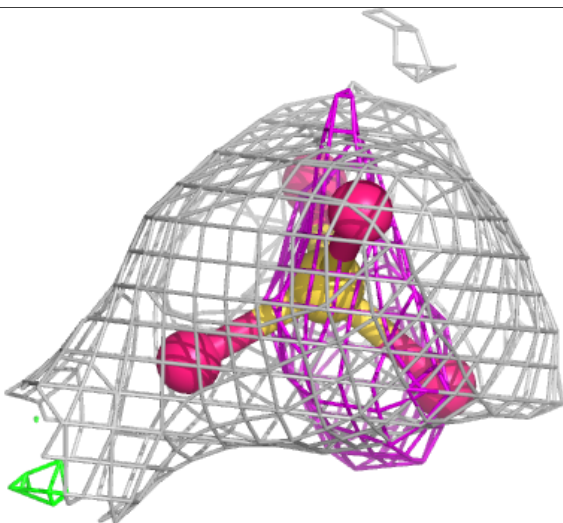
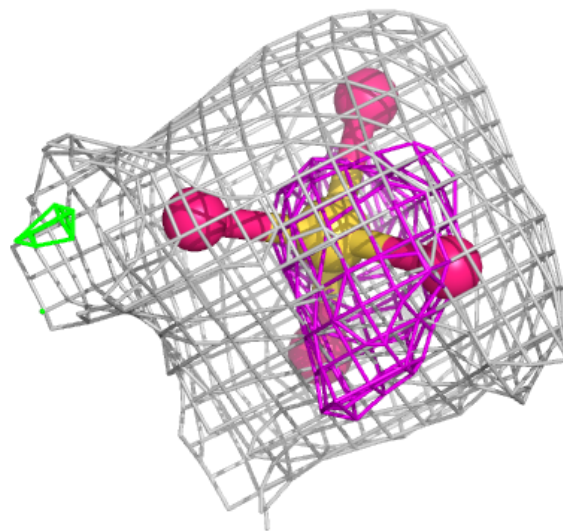
**Electron density around SO4 A 707:**

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



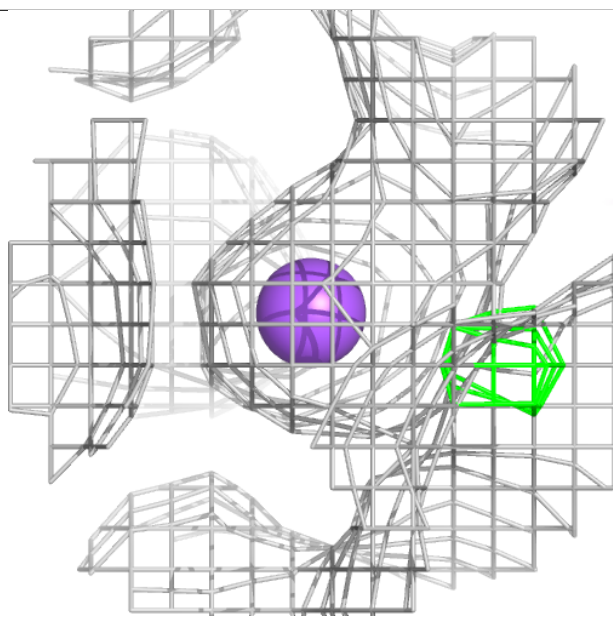
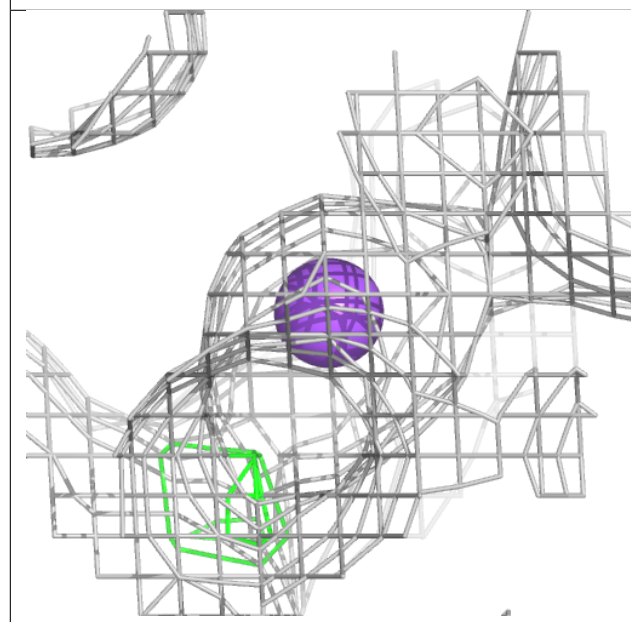
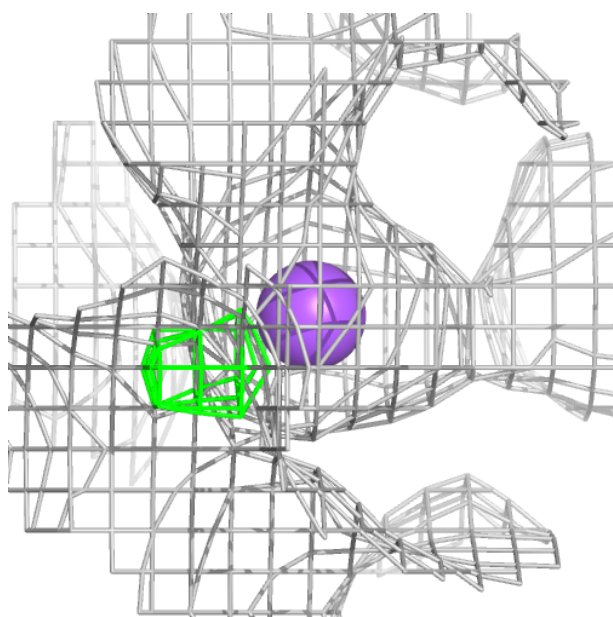
**Electron density around SO4 C 706:**

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



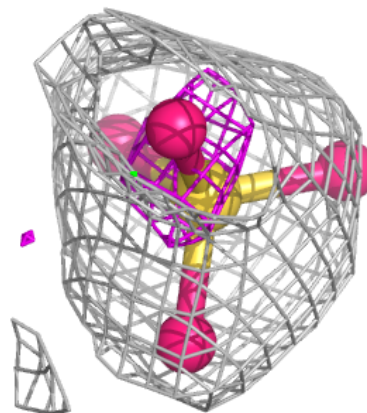
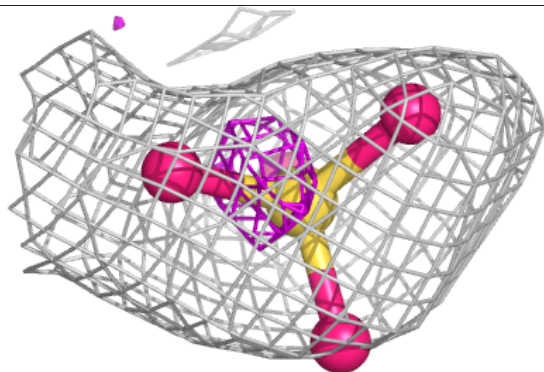
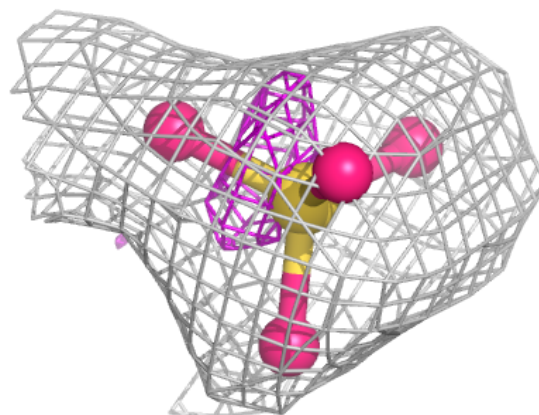
**Electron density around NA A 710:**

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



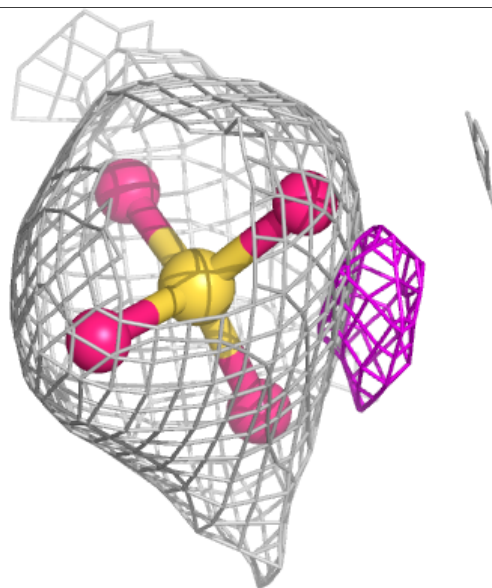
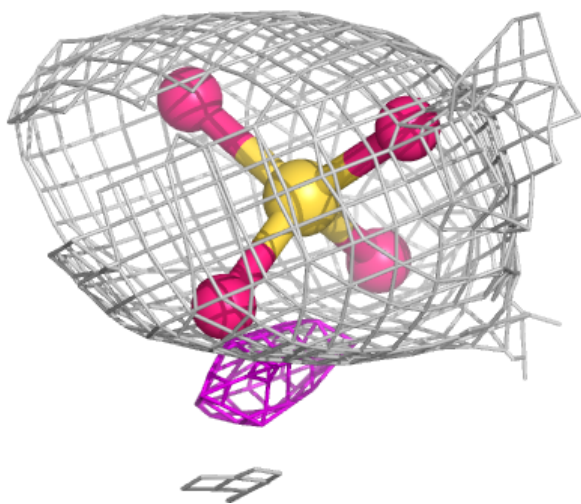
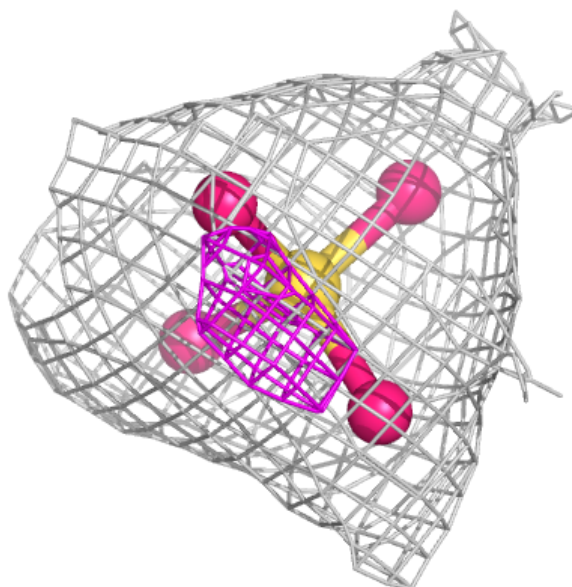
**Electron density around SO4 A 708:**

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



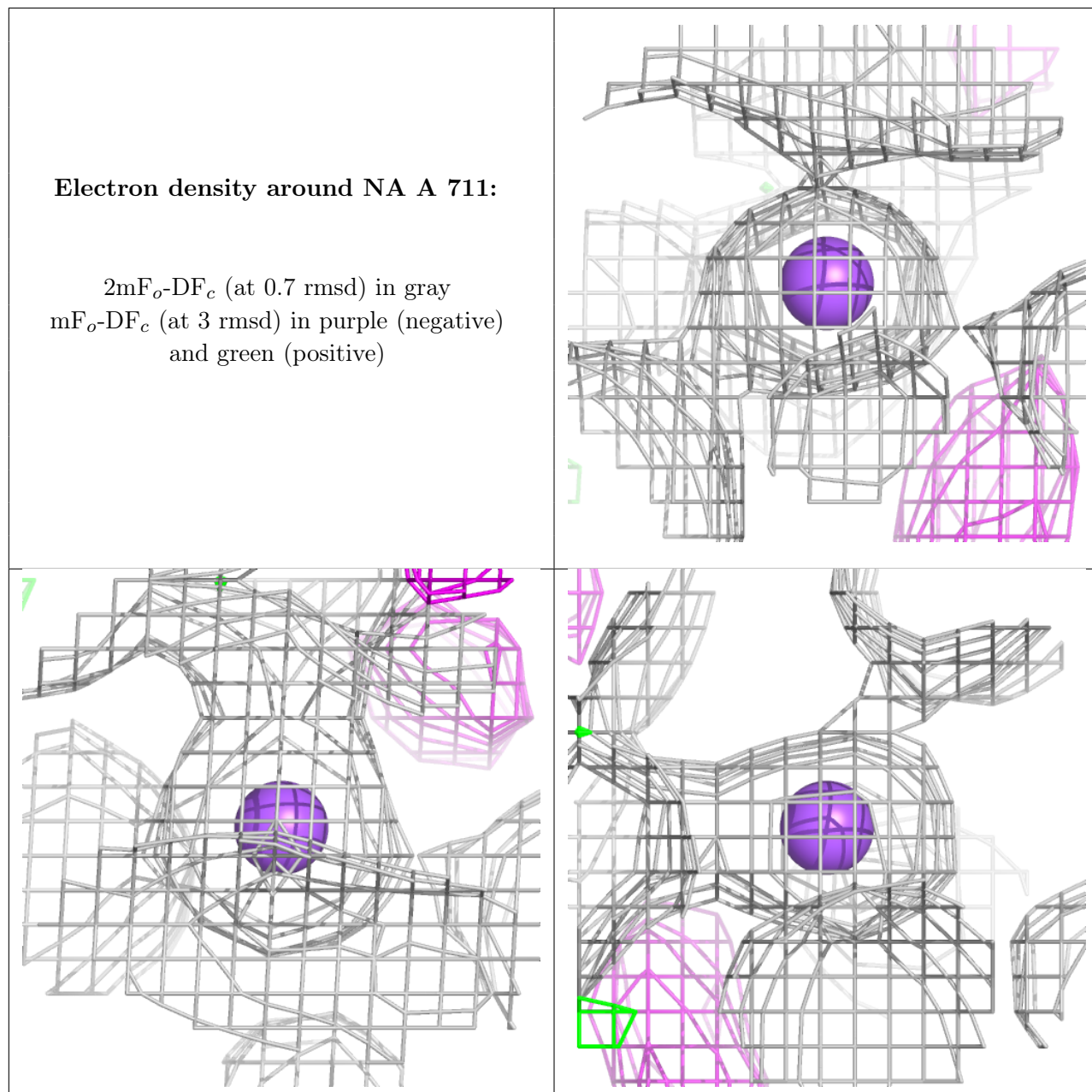
**Electron density around SO4 E 708:**

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



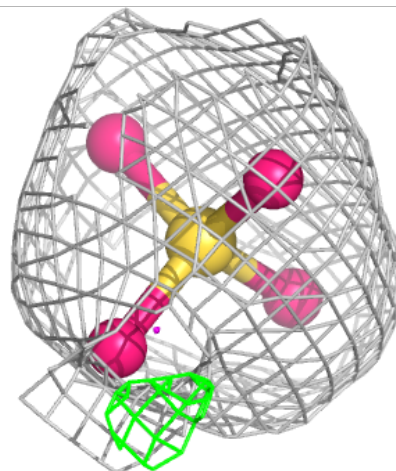
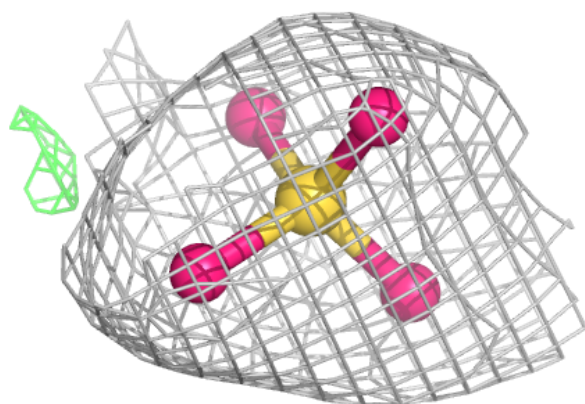
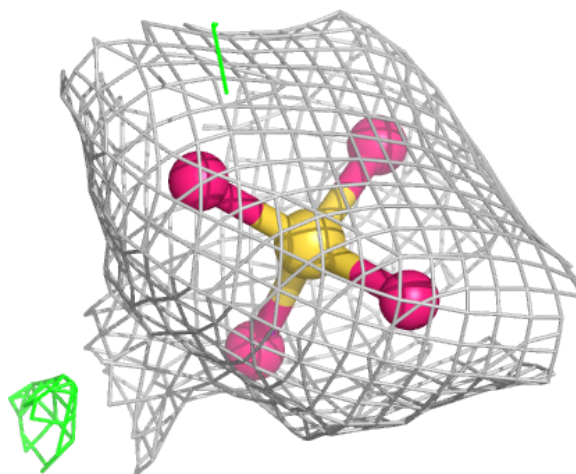
**Electron density around NA A 711:**

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



**Electron density around SO4 B 707:**

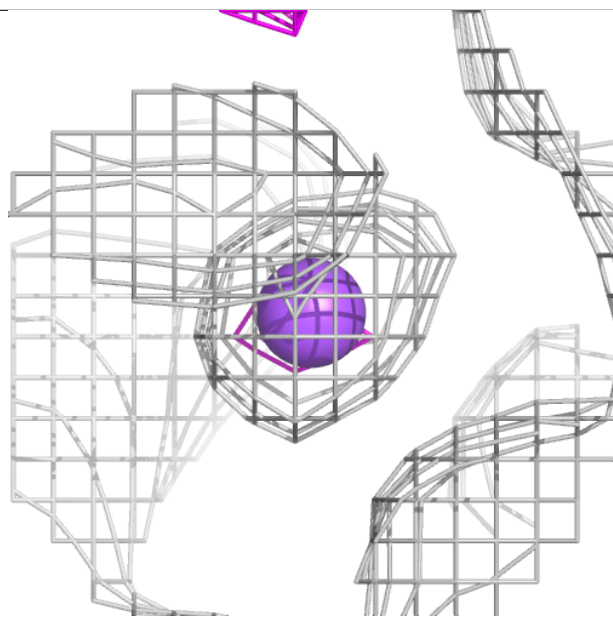
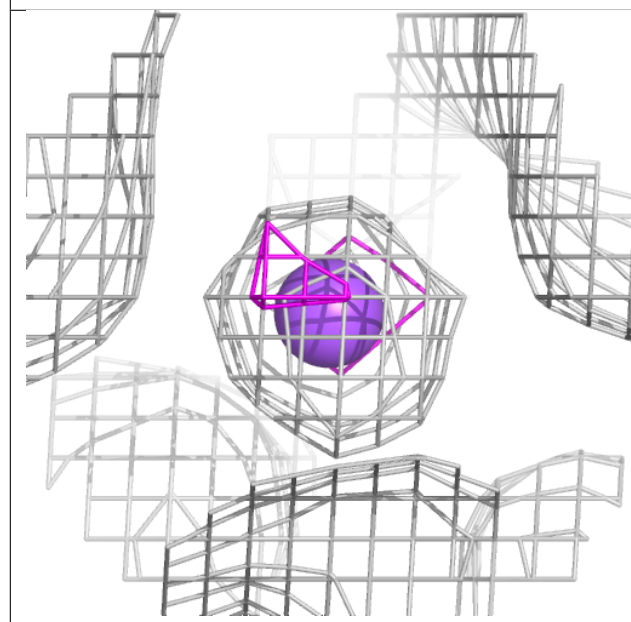
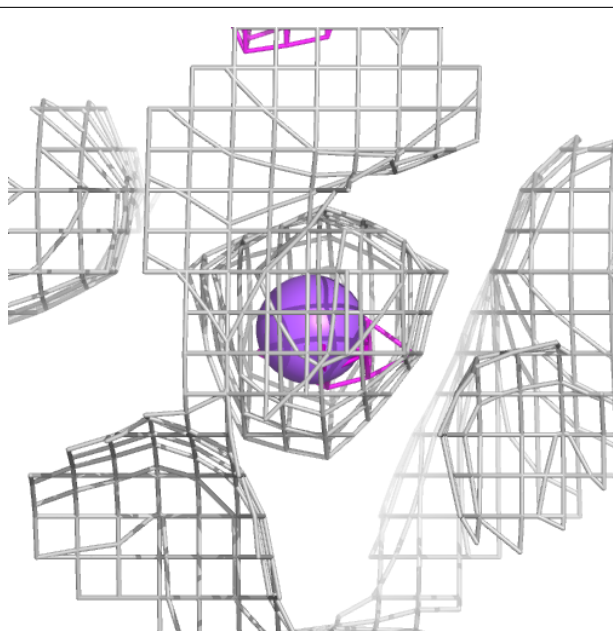
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





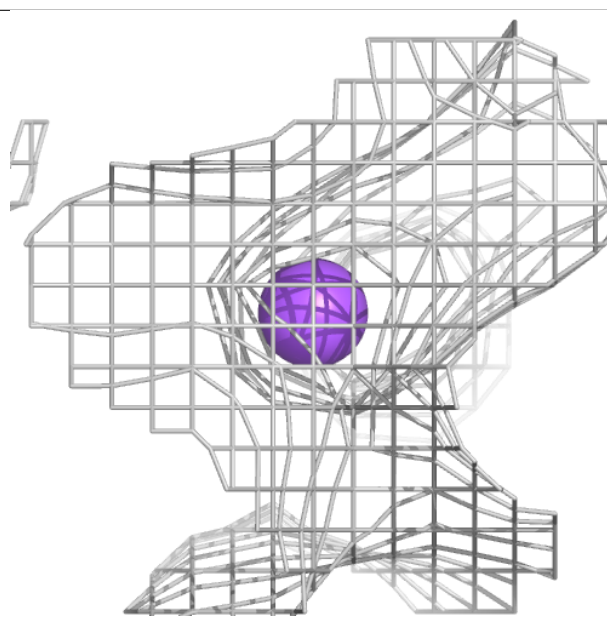
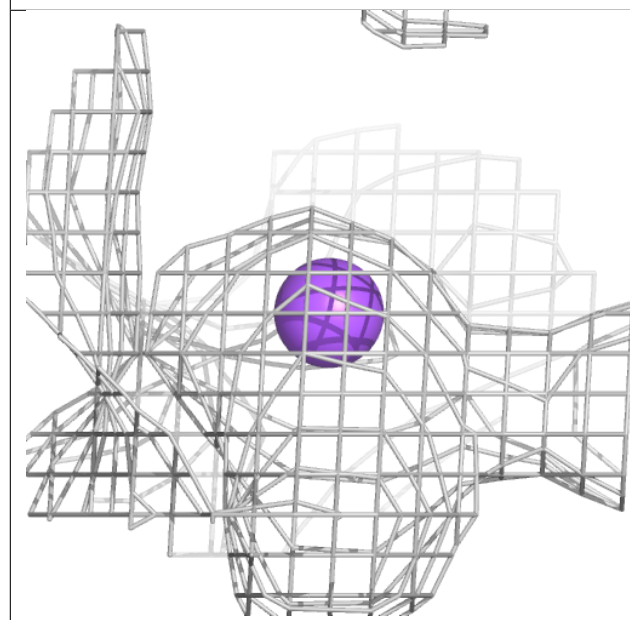
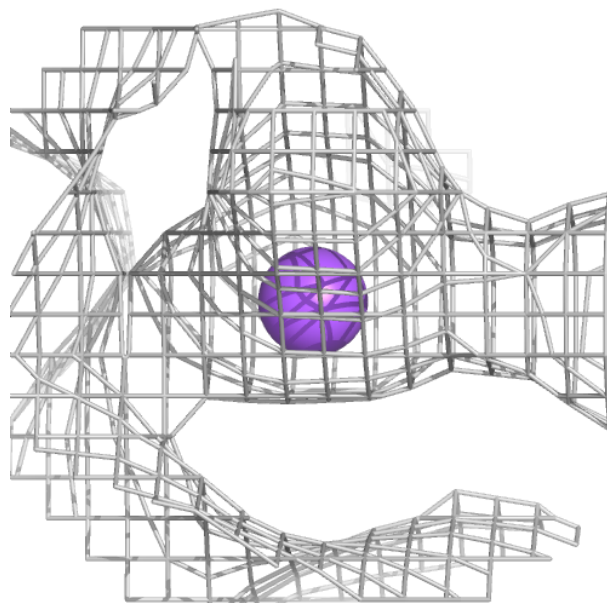
**Electron density around NA B 716:**

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



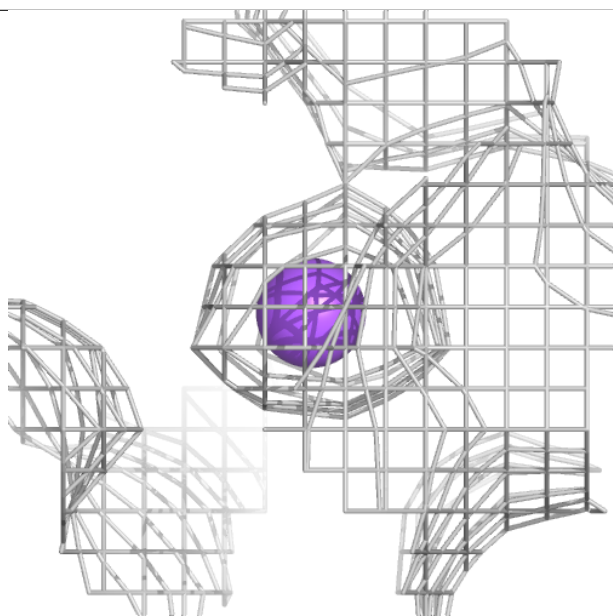
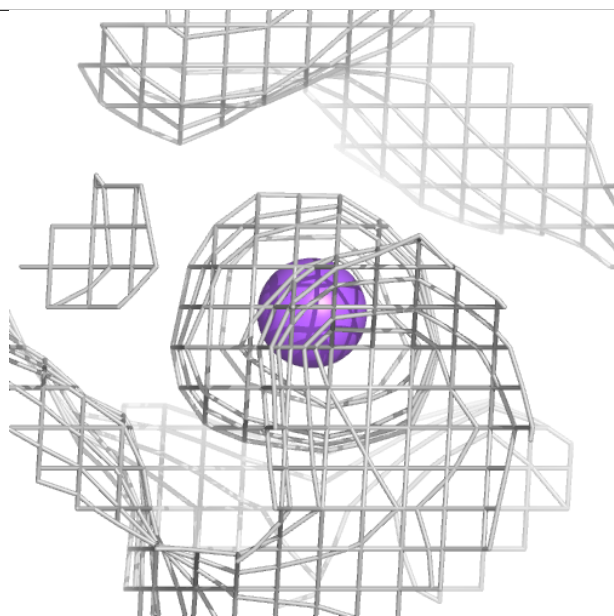
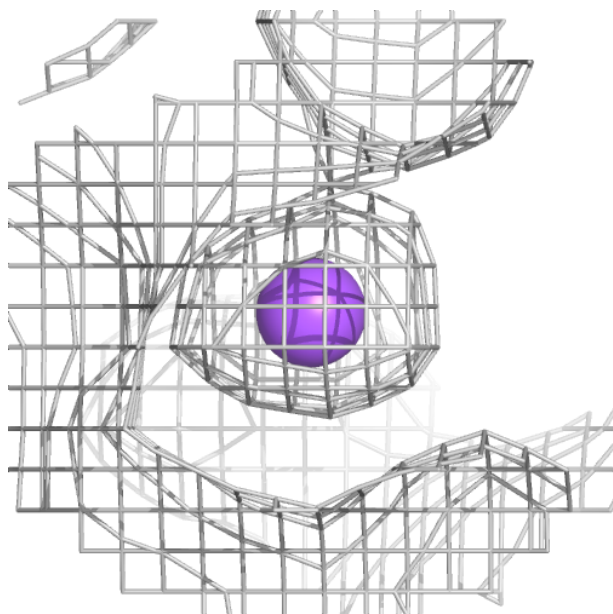
**Electron density around NA D 709:**

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



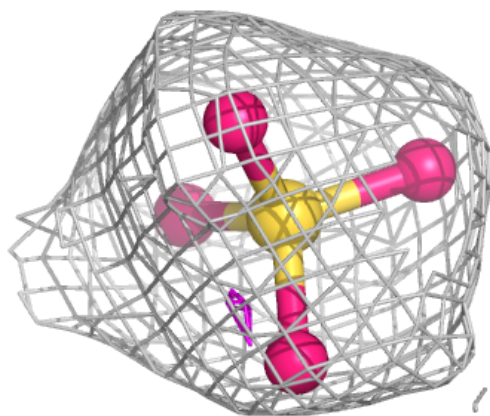
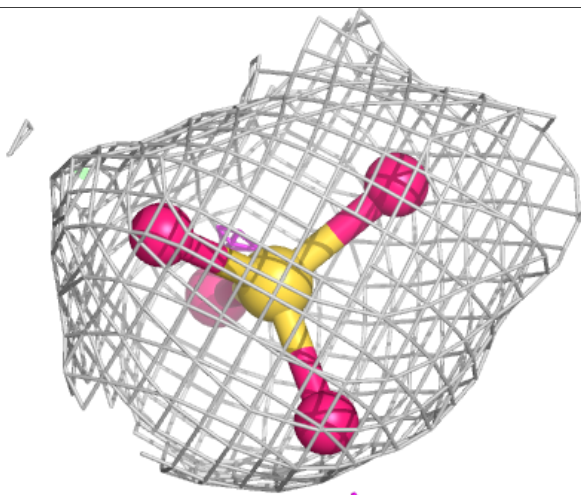
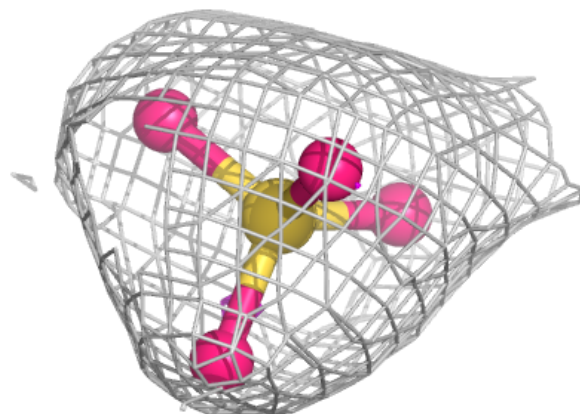
**Electron density around NA E 711:**

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



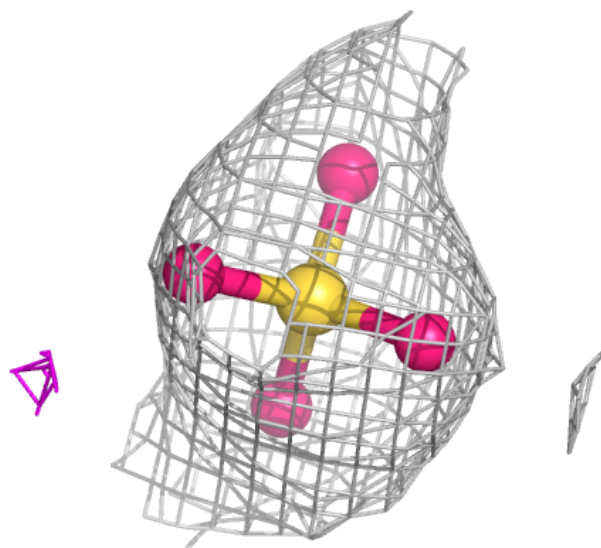
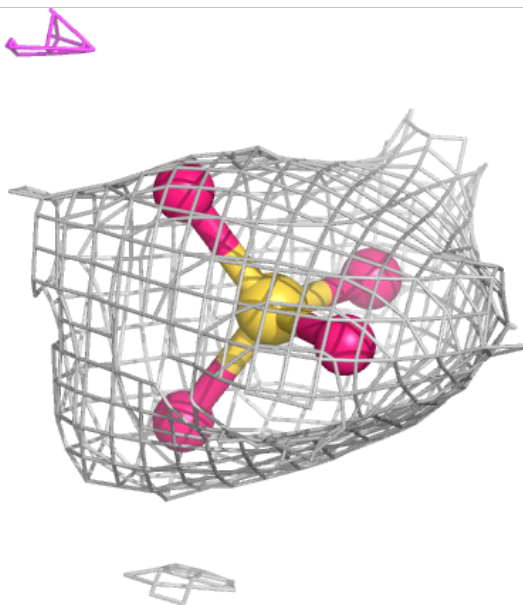
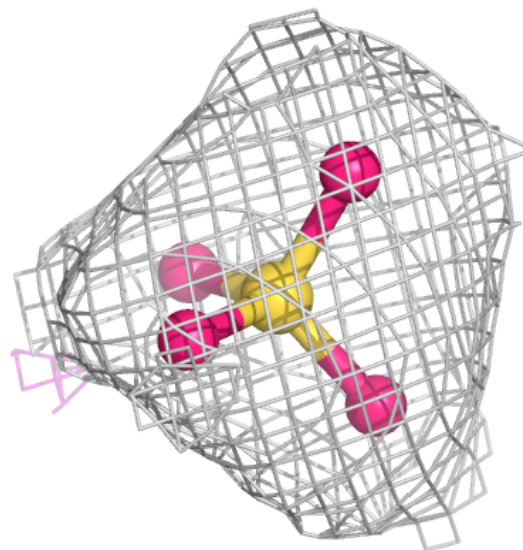
**Electron density around SO4 H 704:**

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



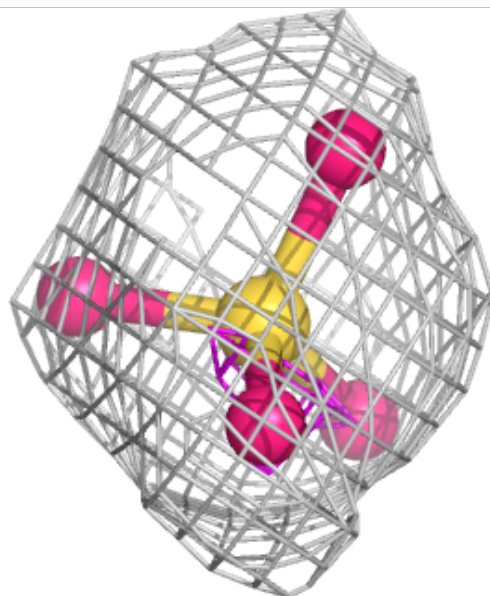
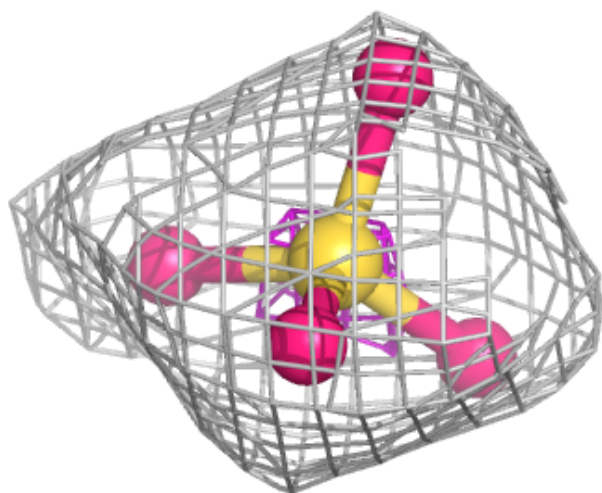
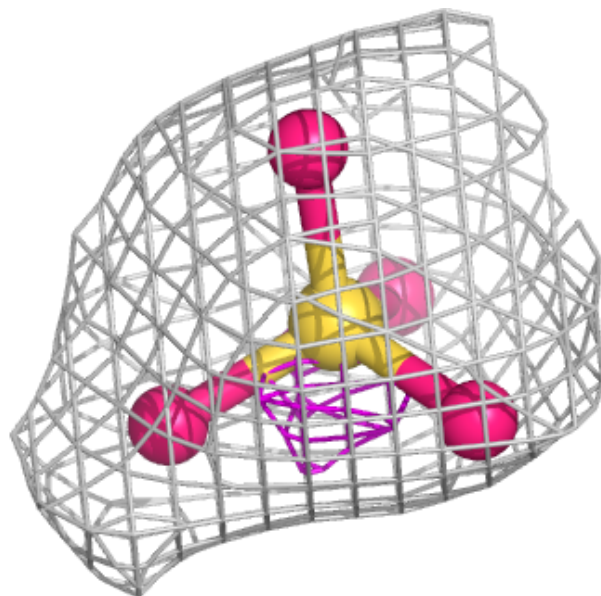
**Electron density around SO4 H 706:**

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



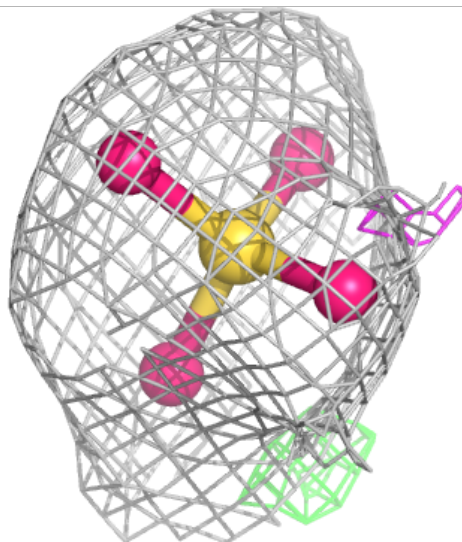
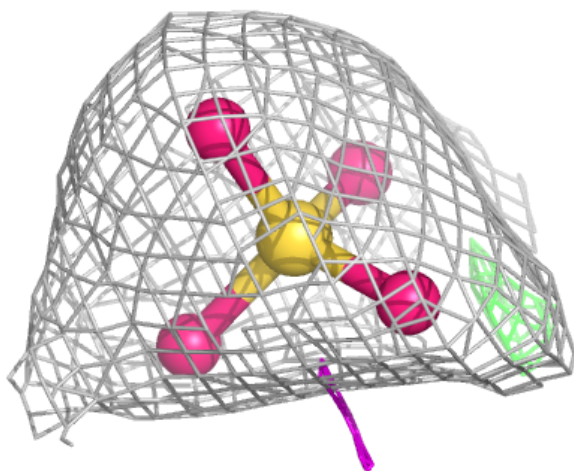
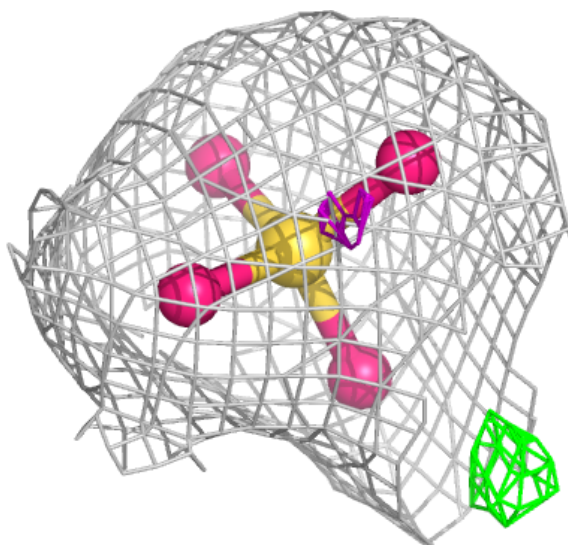
**Electron density around SO4 B 711:**

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



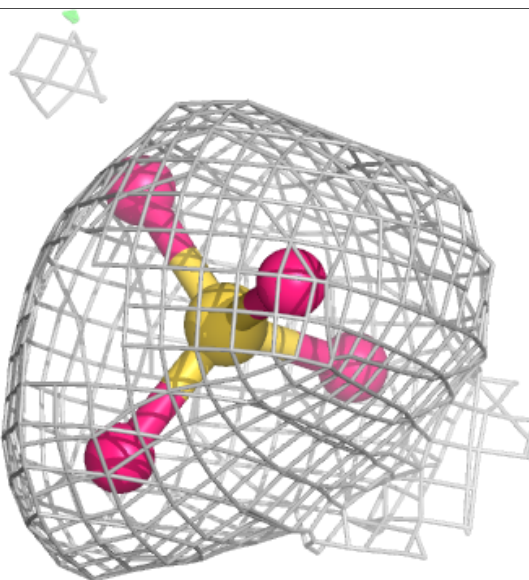
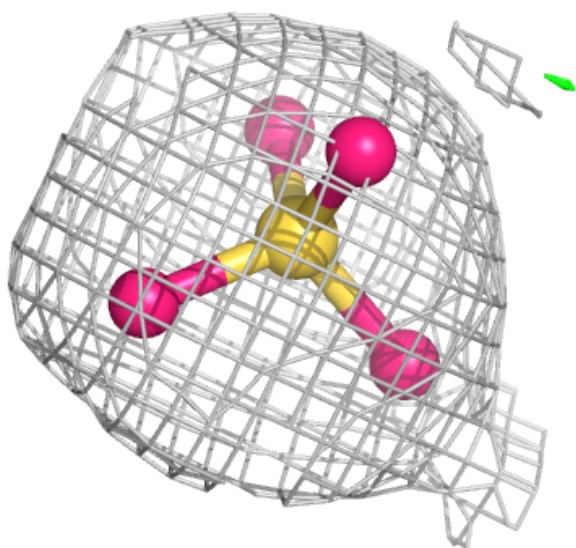
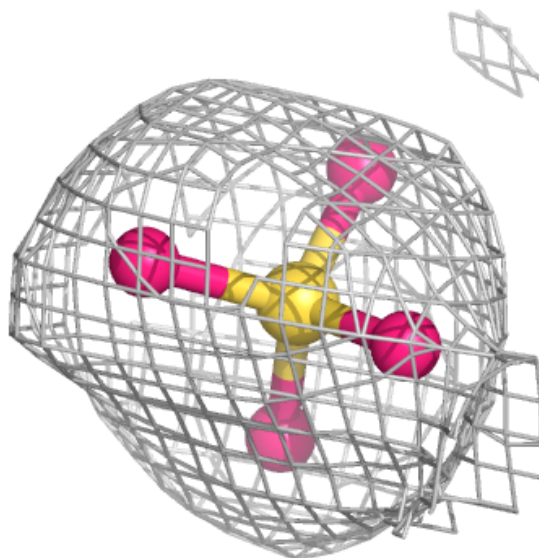
**Electron density around SO4 G 705:**

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



**Electron density around SO4 B 708:**

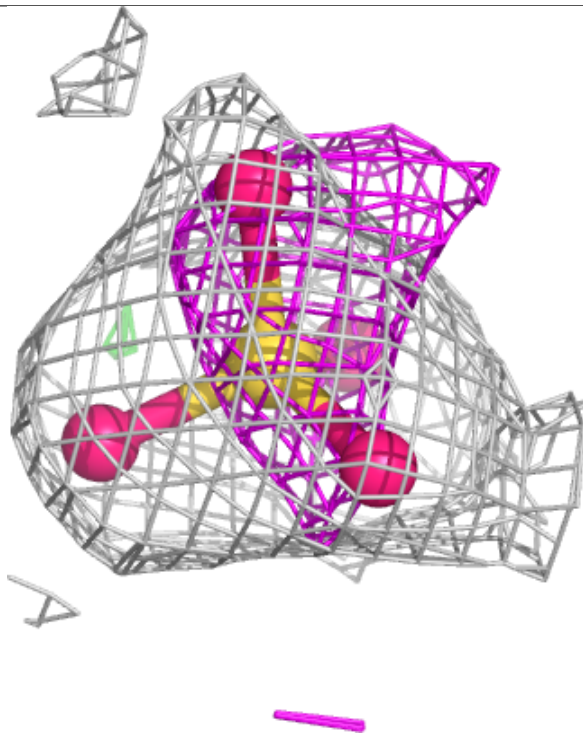
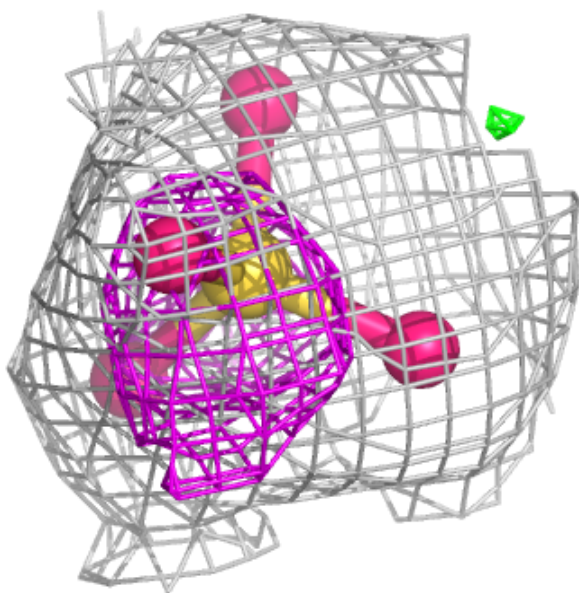
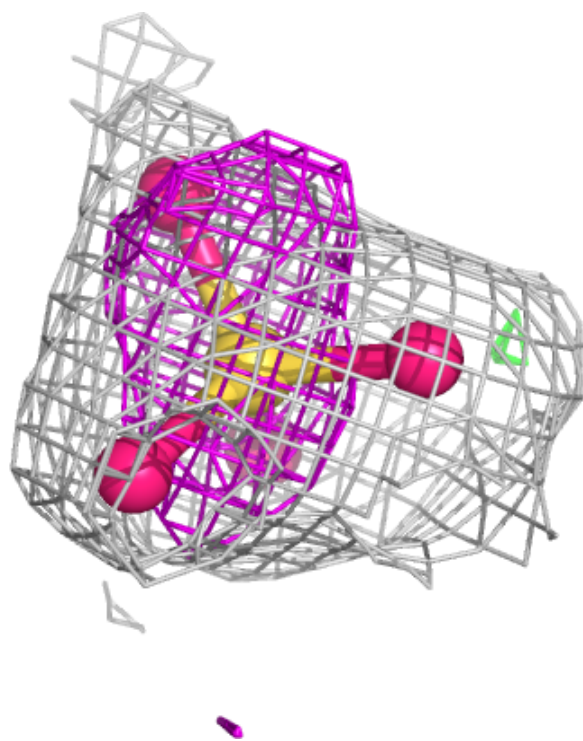
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





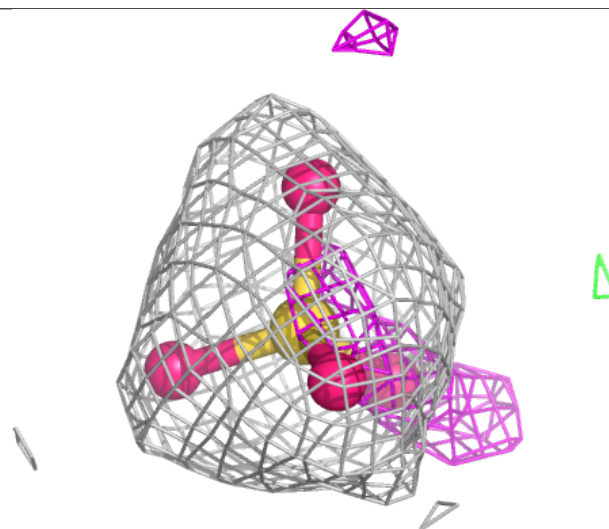
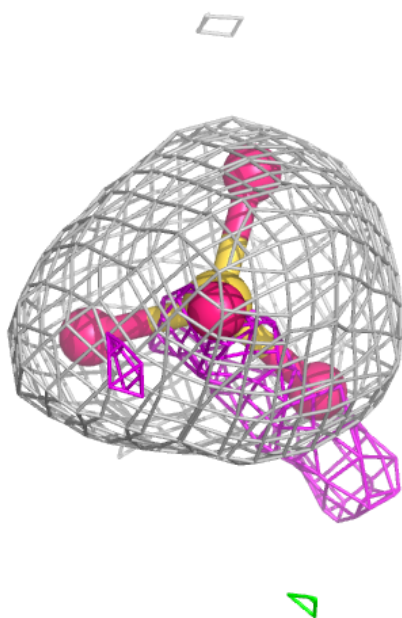
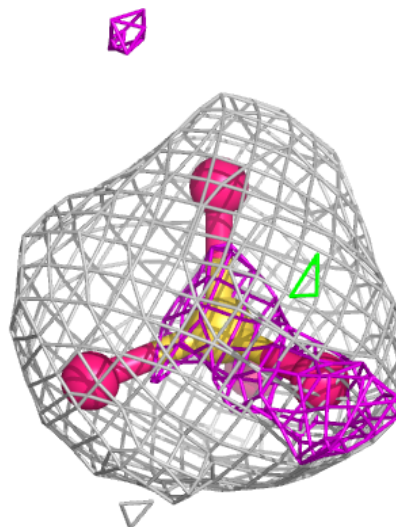
**Electron density around SO4 H 705:**

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



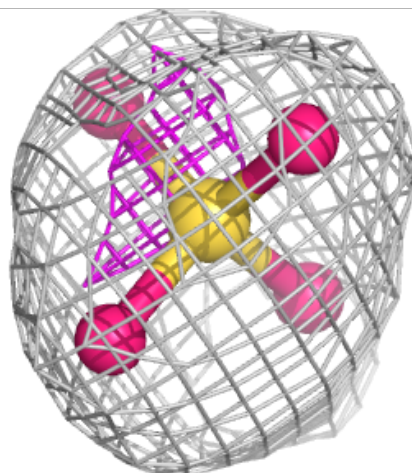
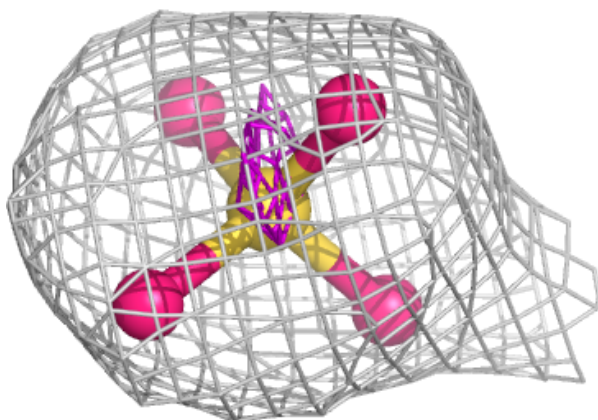
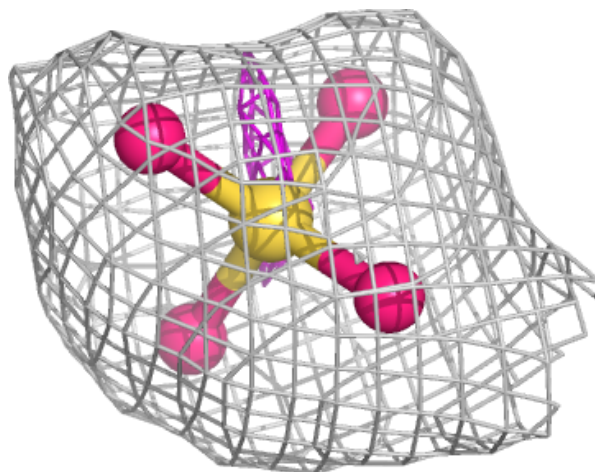
**Electron density around SO4 C 707:**

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



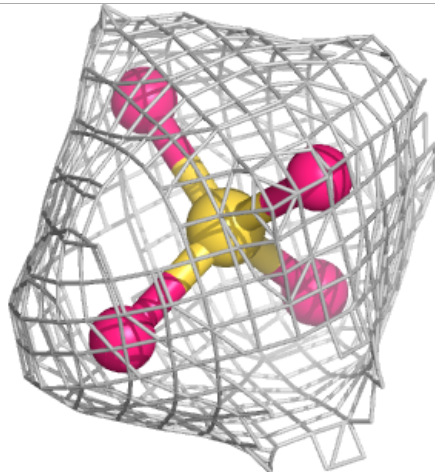
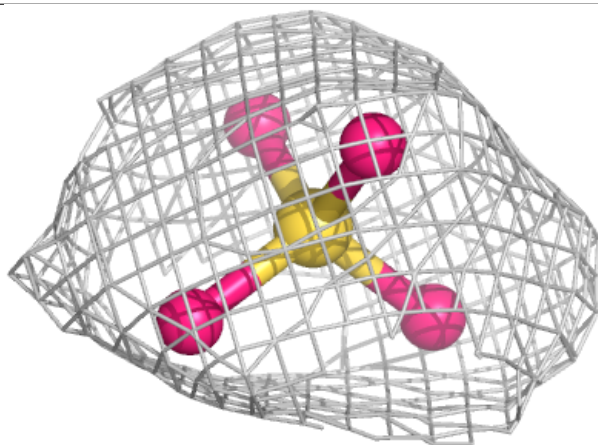
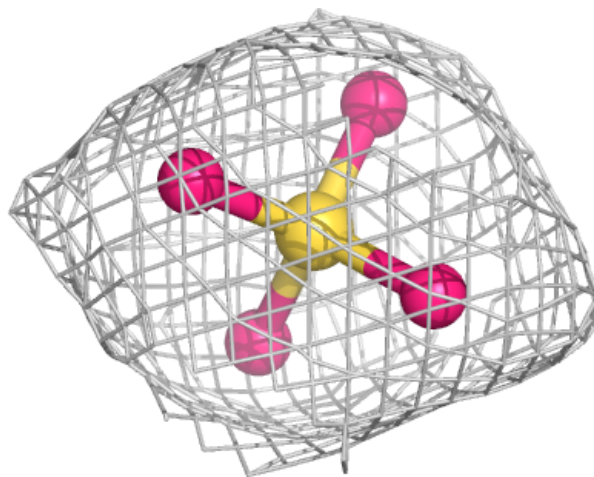
**Electron density around SO4 E 707:**

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



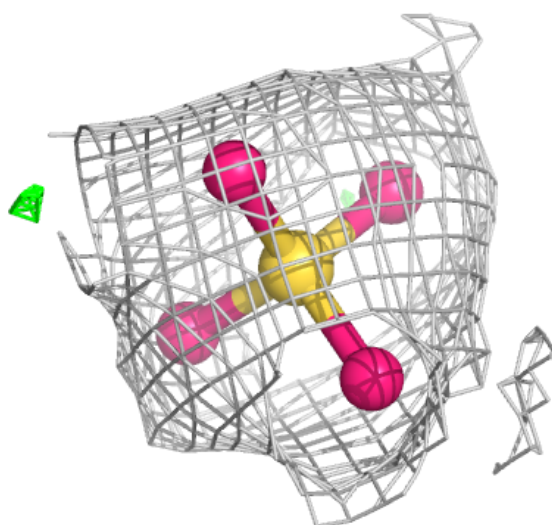
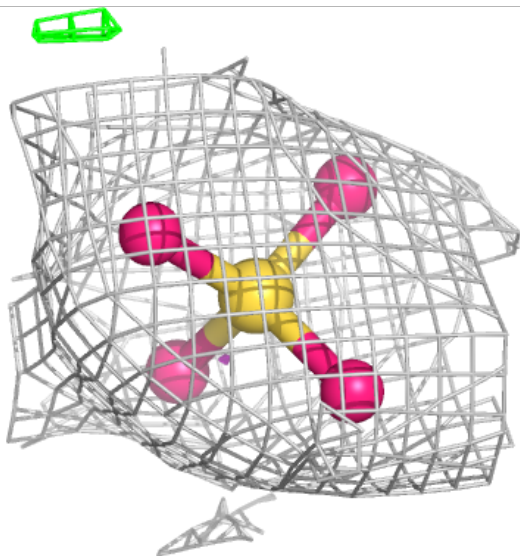
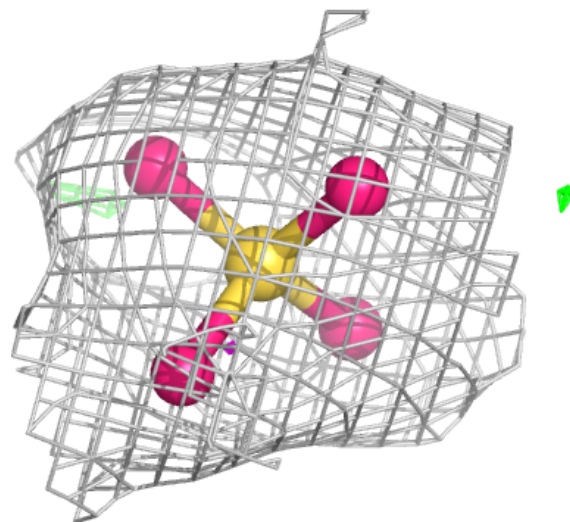
**Electron density around SO4 D 708:**

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



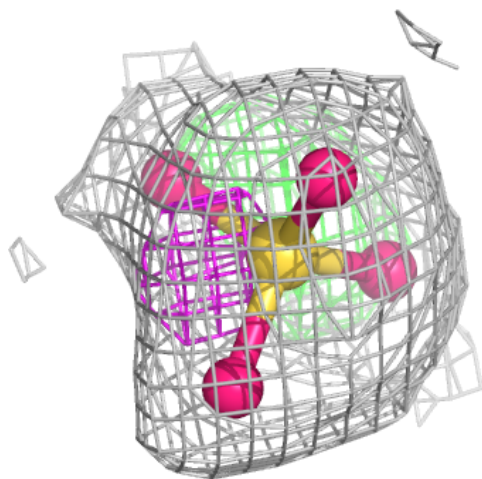
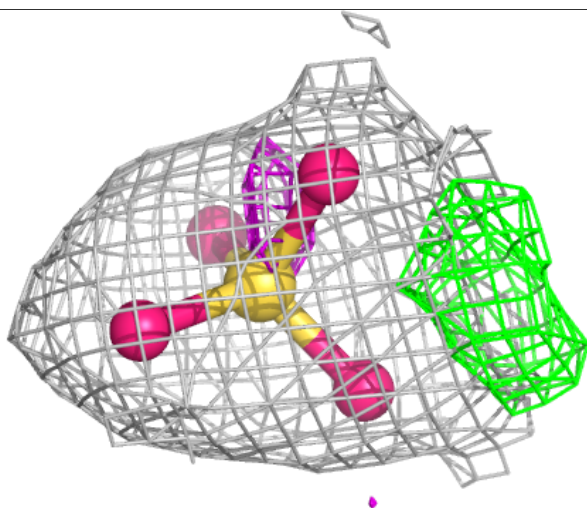
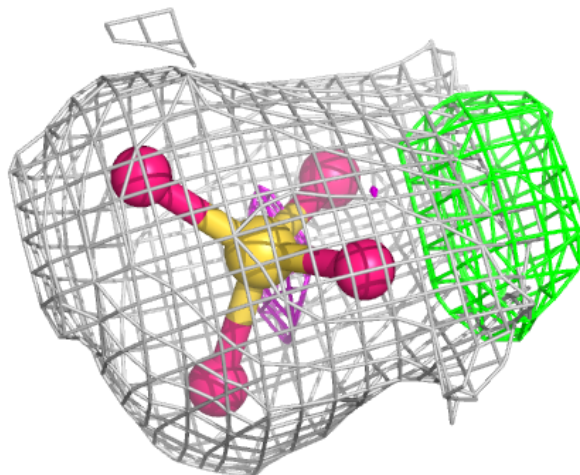
**Electron density around SO4 E 705:**

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



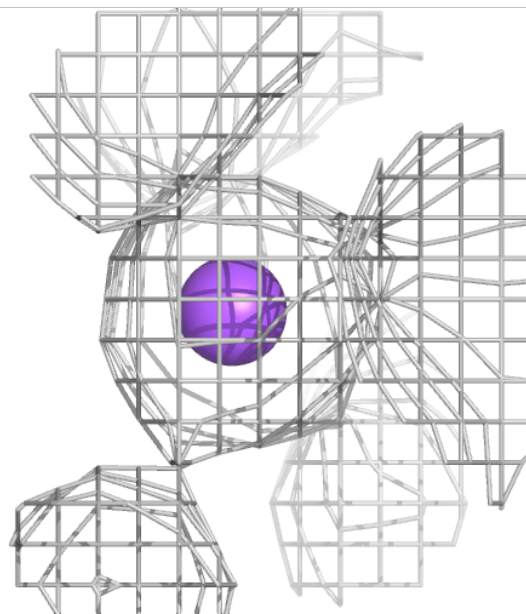
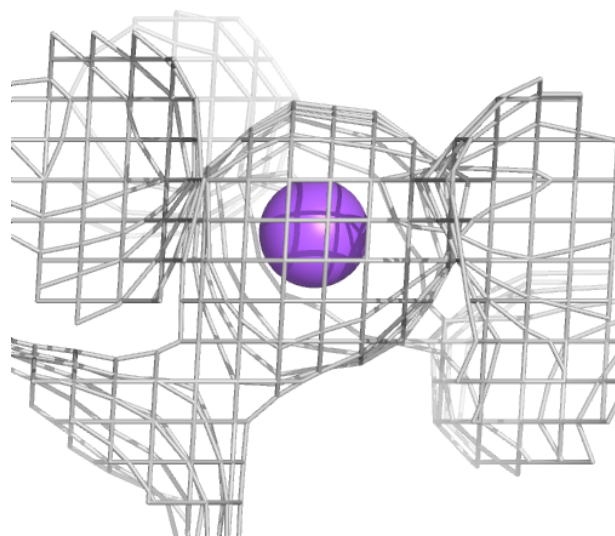
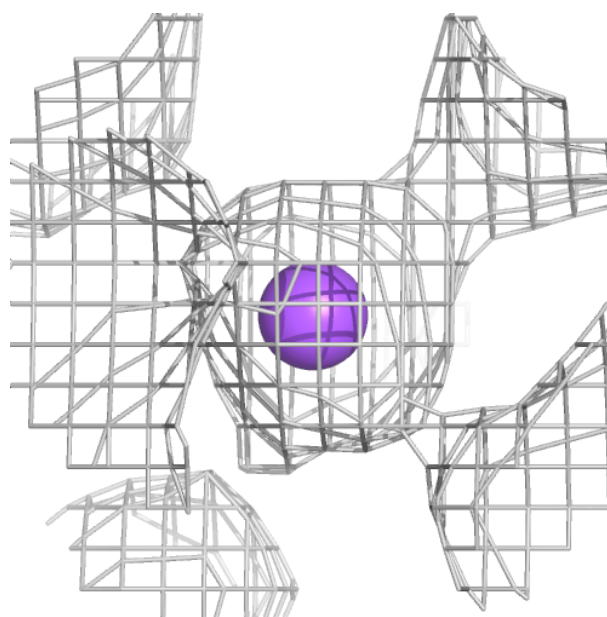
**Electron density around SO4 F 702:**

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



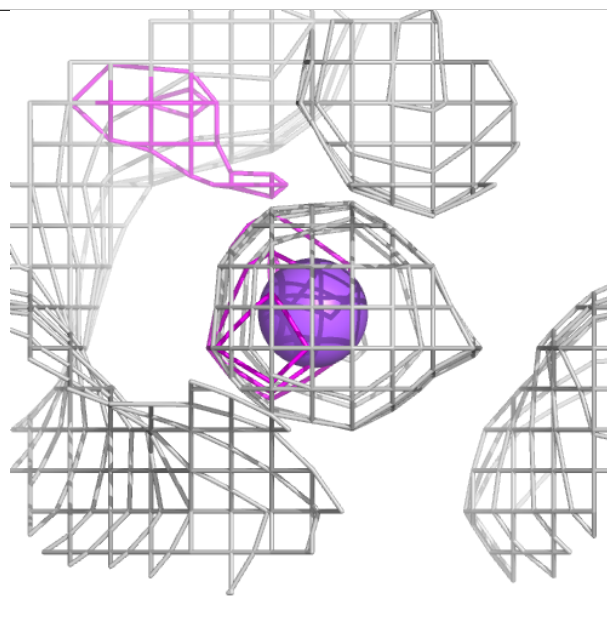
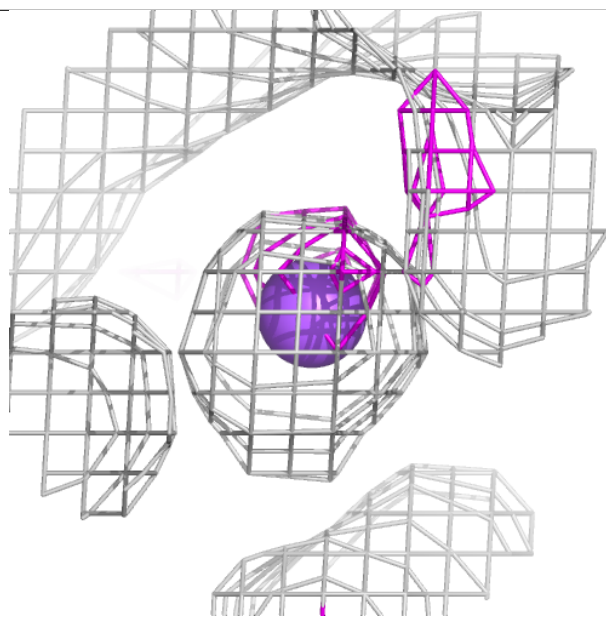
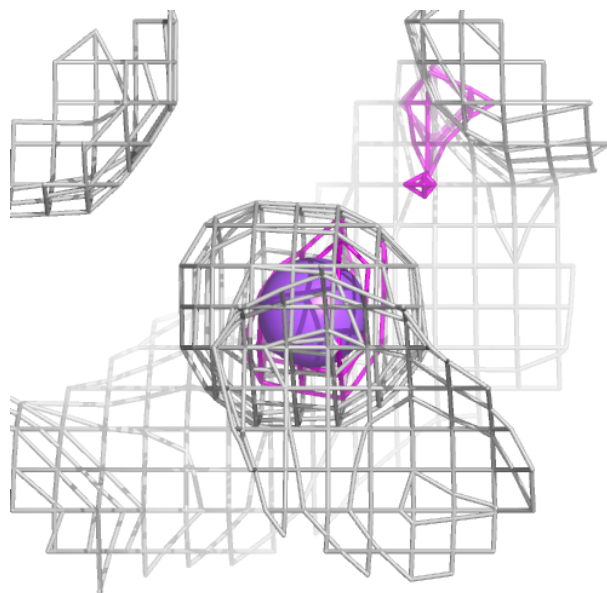
**Electron density around NA B 713:**

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



**Electron density around NA B 715:**

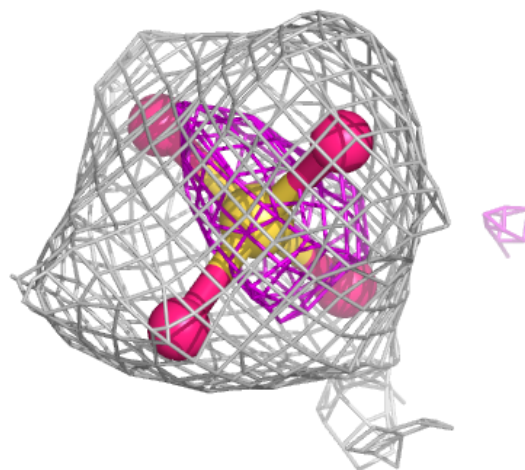
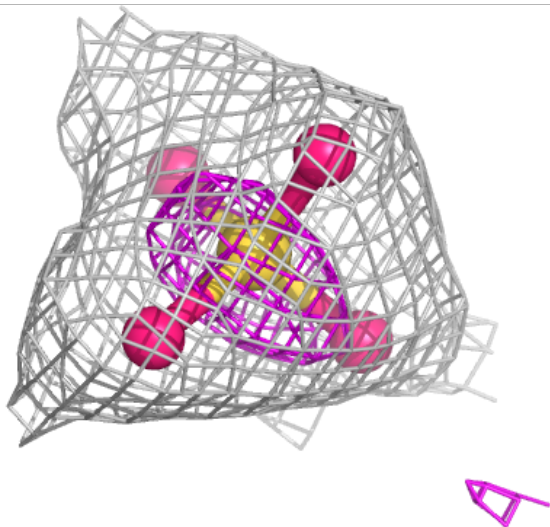
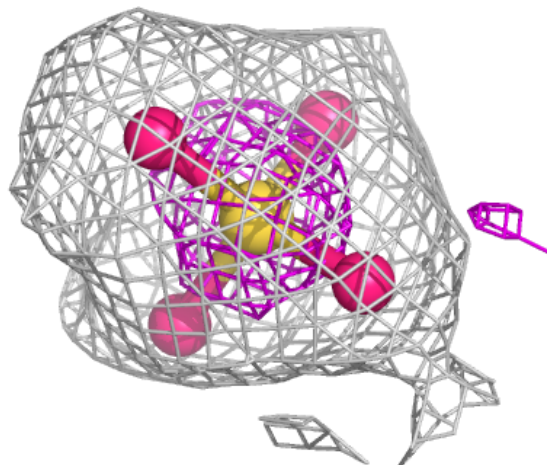
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





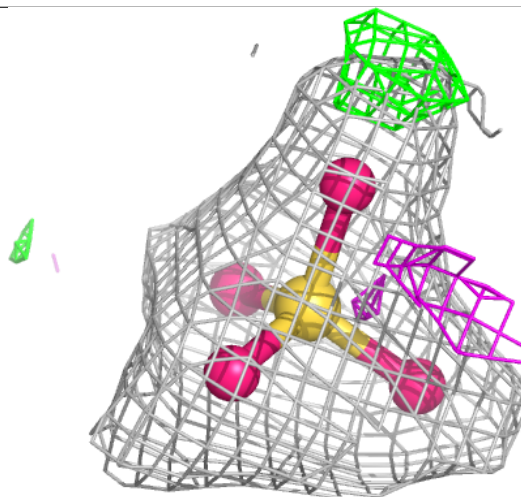
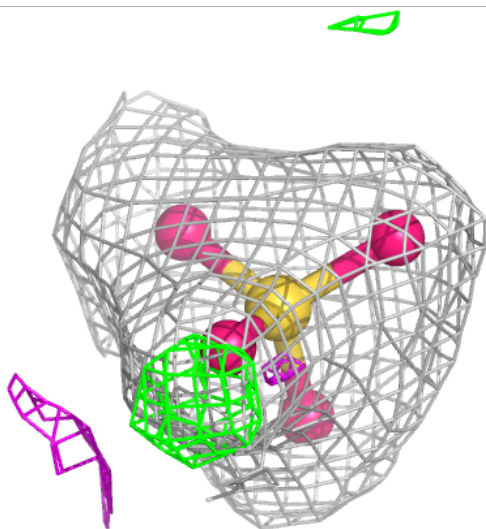
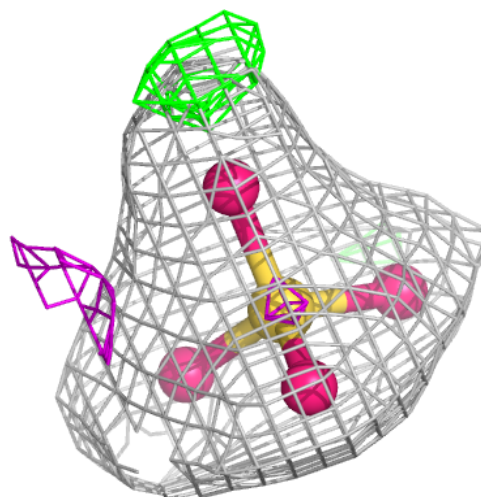
**Electron density around SO4 G 703:**

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



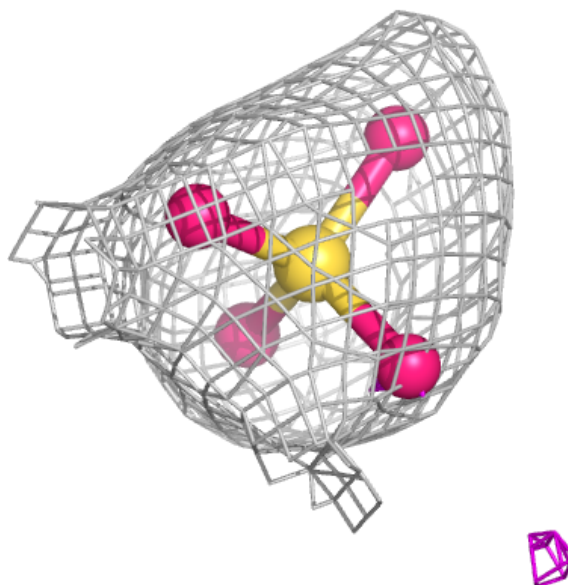
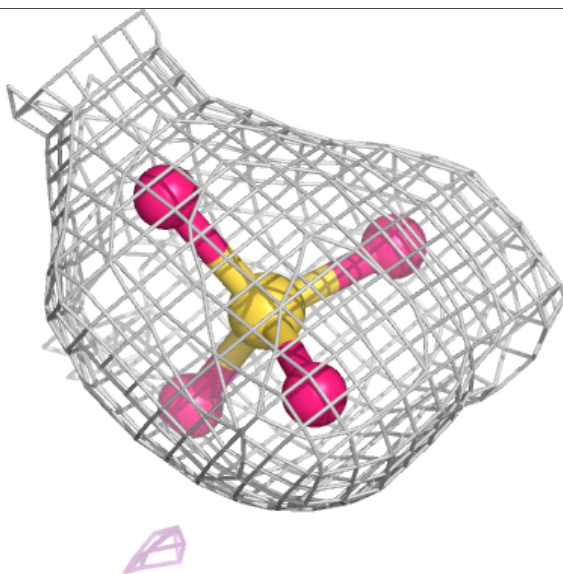
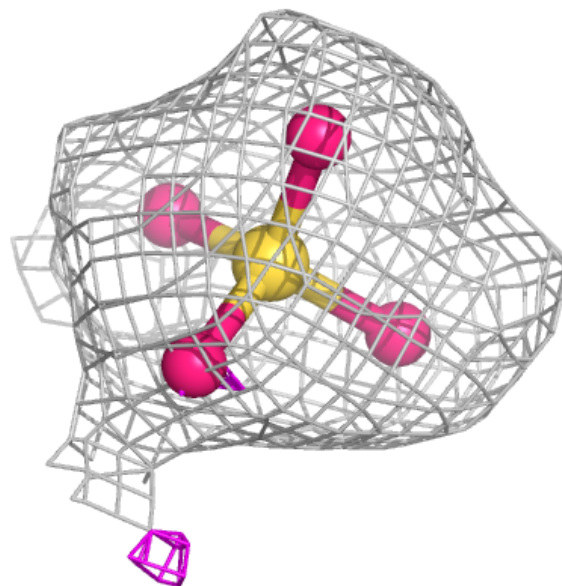
**Electron density around SO4 D 705:**

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



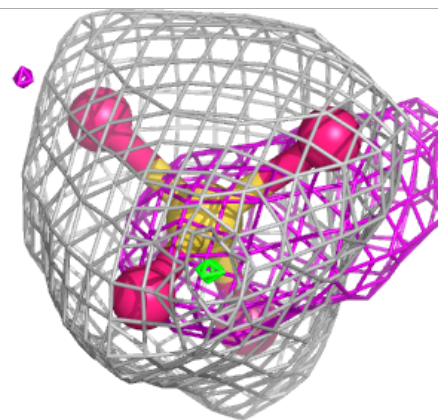
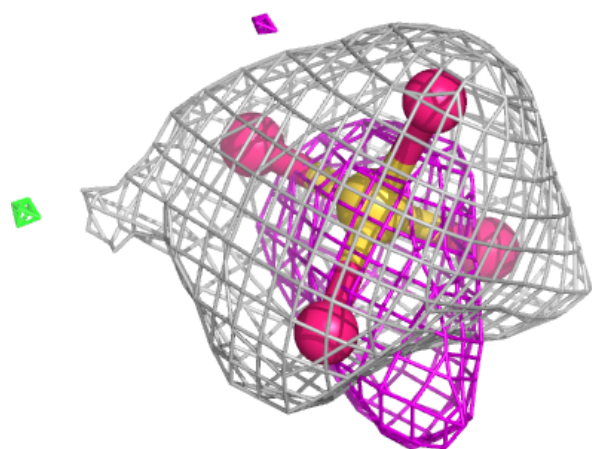
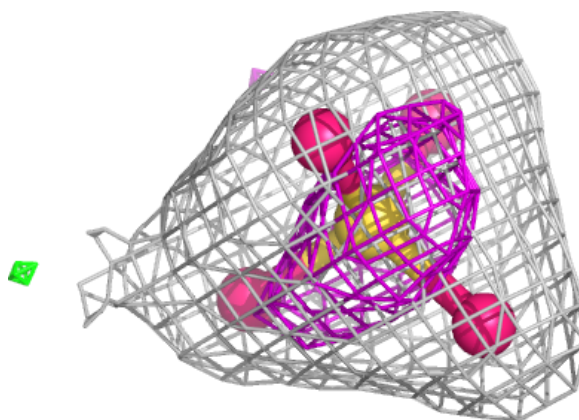
**Electron density around SO4 C 705:**

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



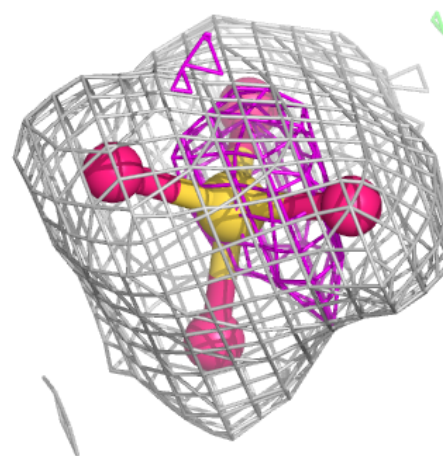
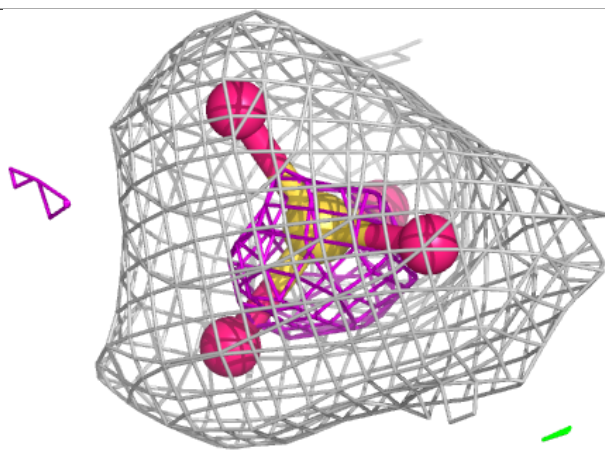
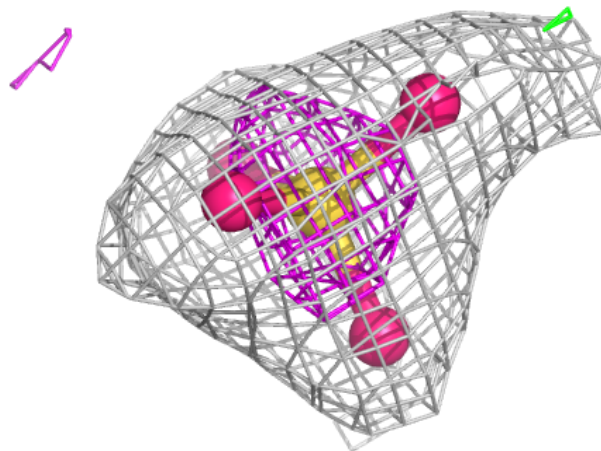
**Electron density around SO4 H 707:**

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



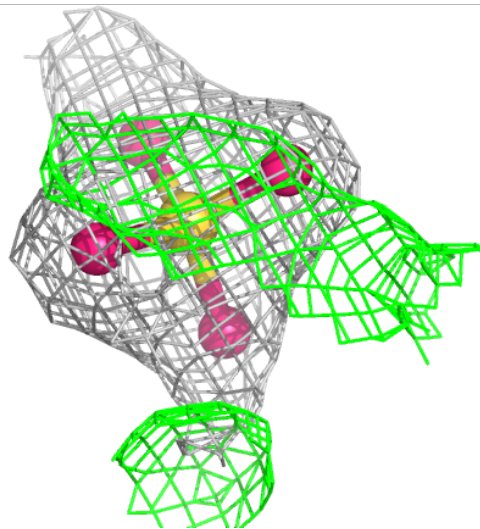
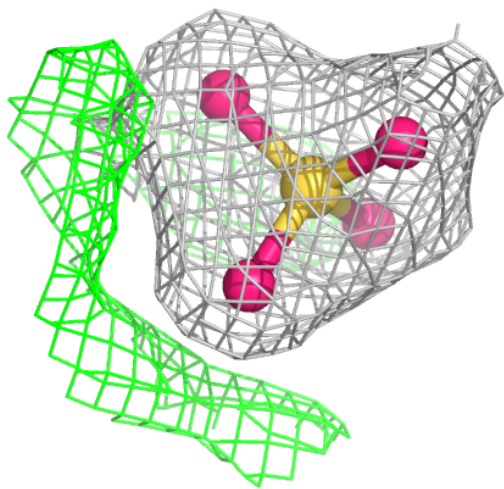
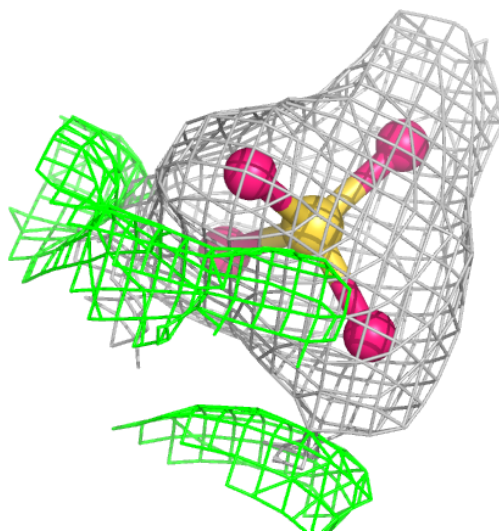
**Electron density around SO4 B 704:**

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



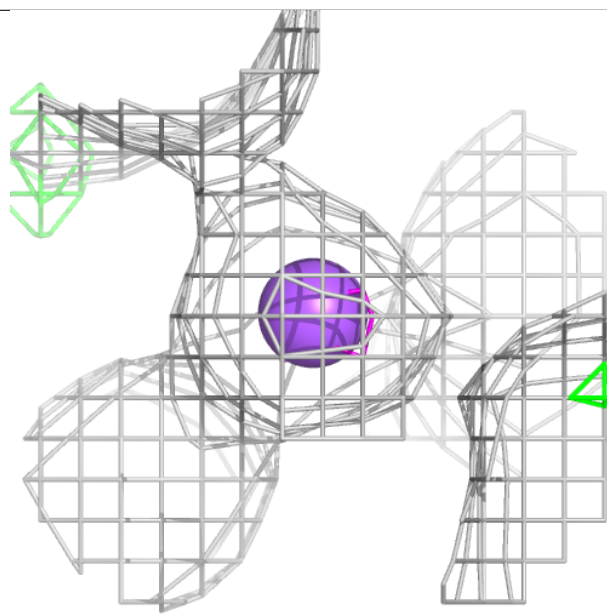
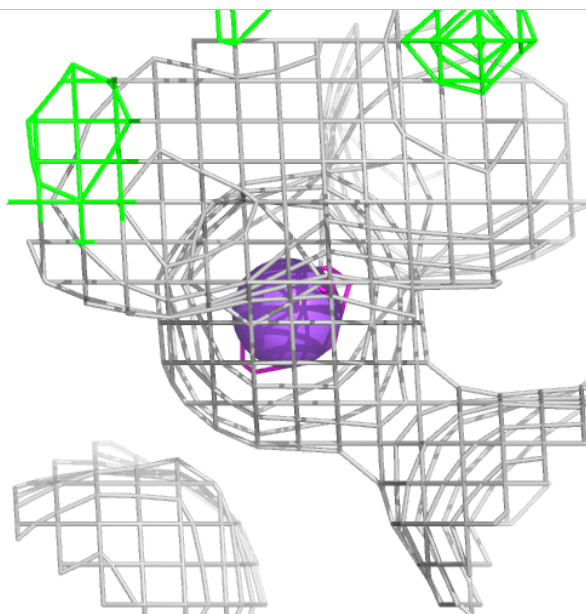
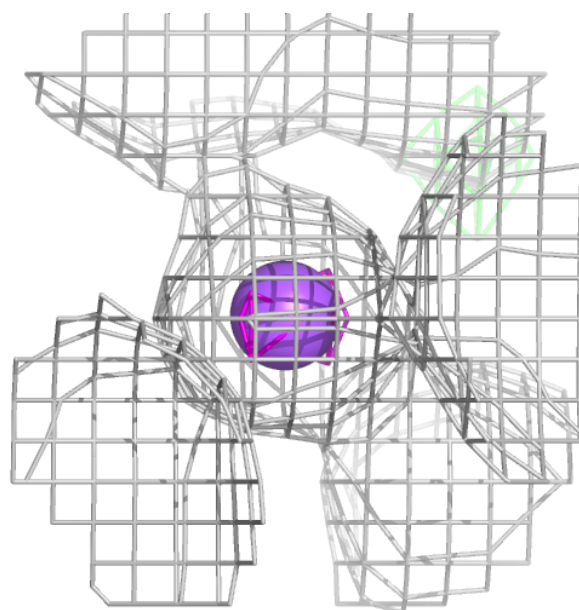
**Electron density around SO4 B 706:**

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



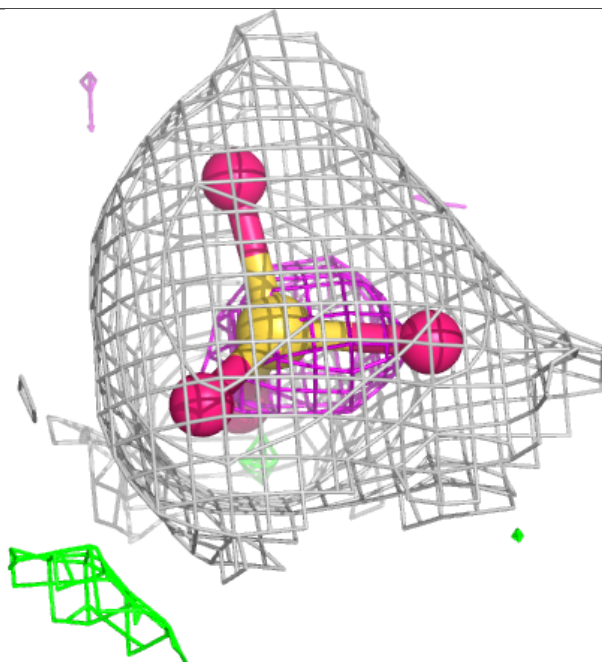
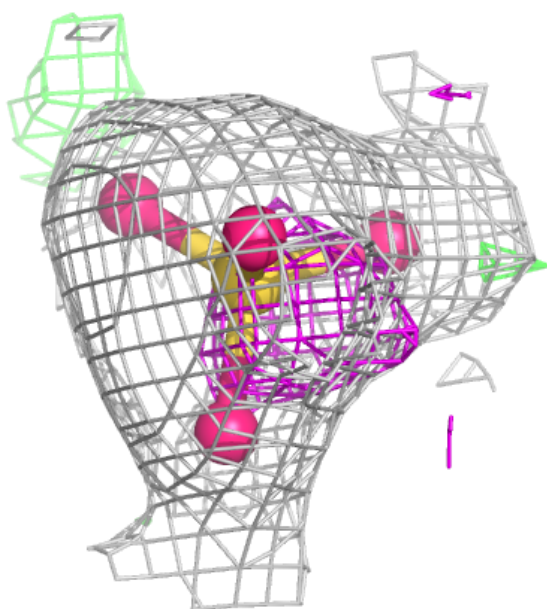
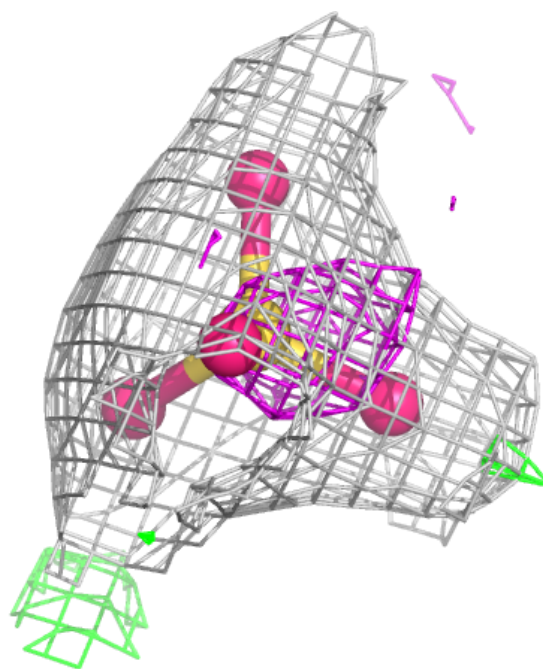
**Electron density around NA A 709:**

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



**Electron density around SO4 F 703:**

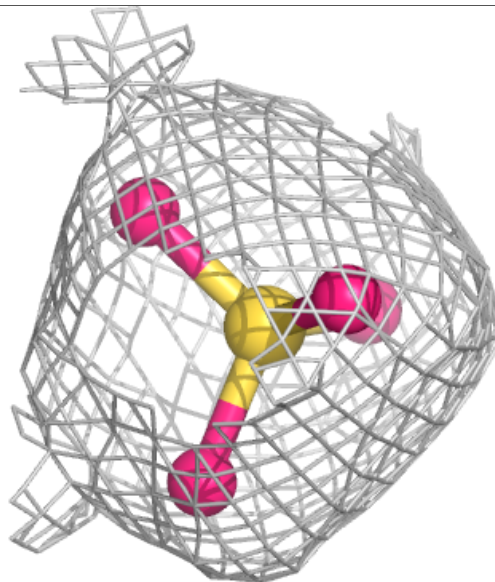
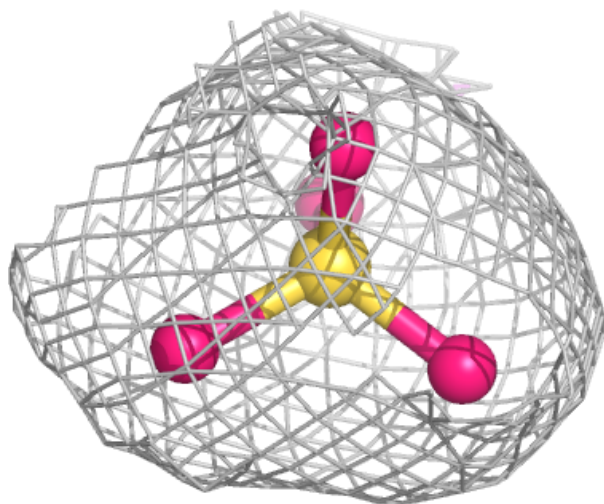
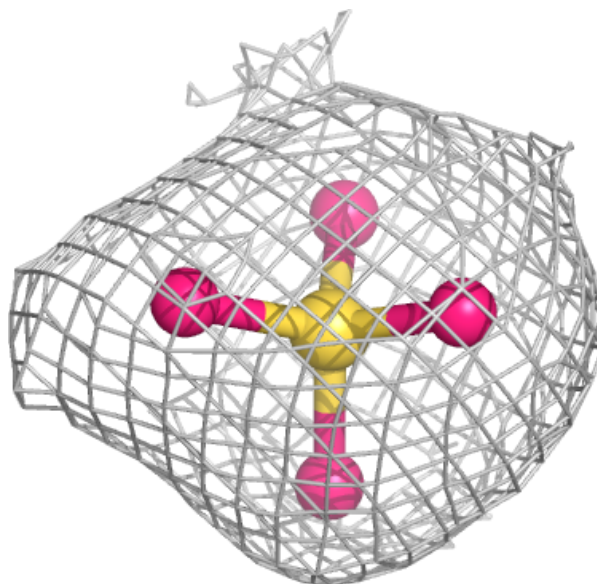
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





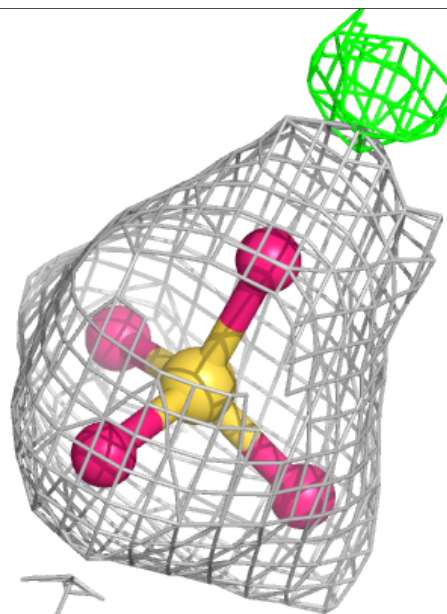
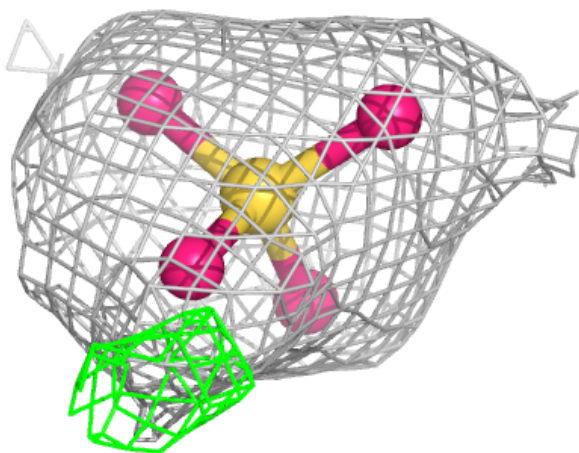
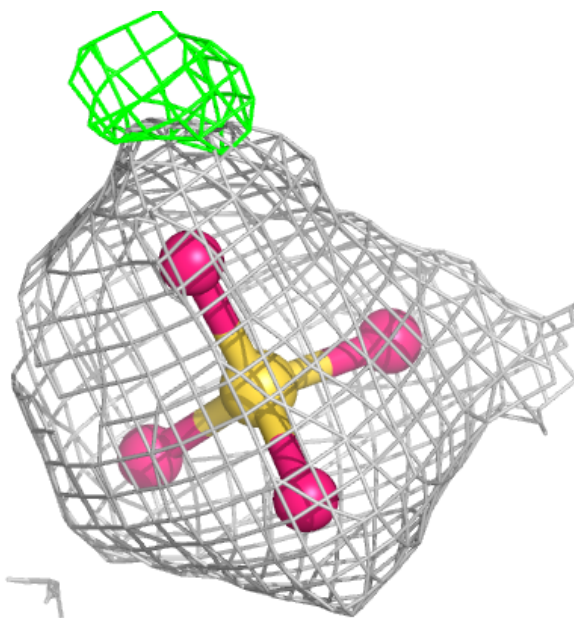
**Electron density around SO4 D 702:**

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



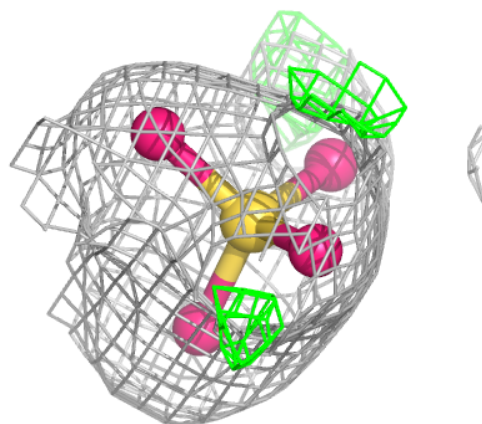
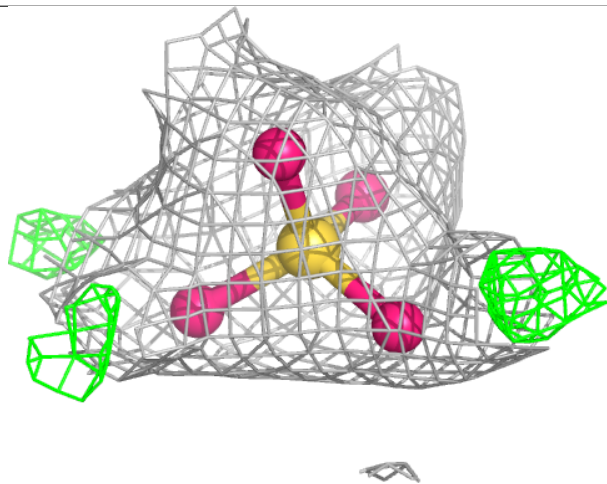
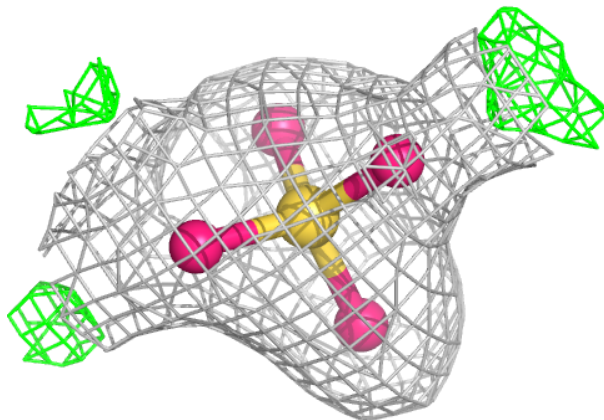
**Electron density around SO4 A 702:**

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



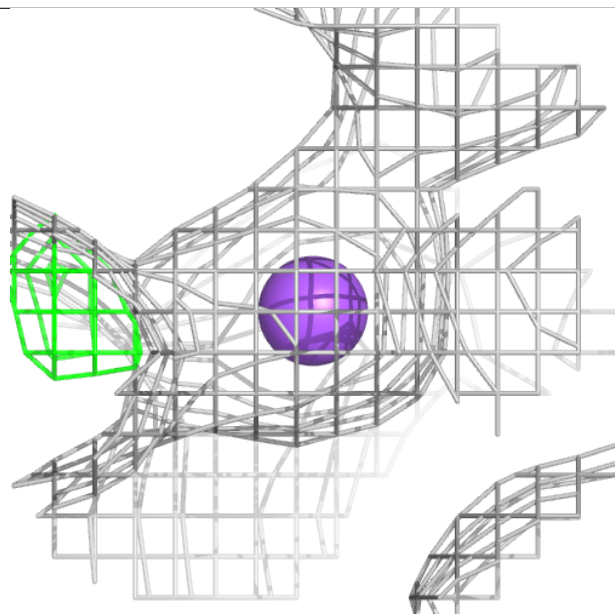
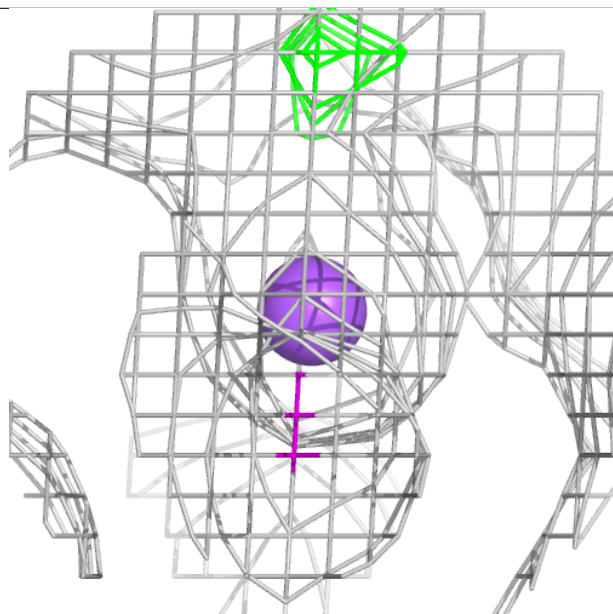
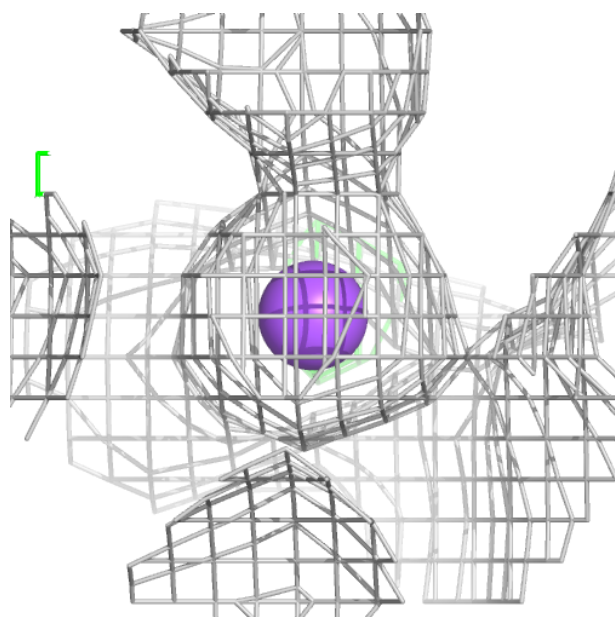
**Electron density around SO4 A 706:**

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



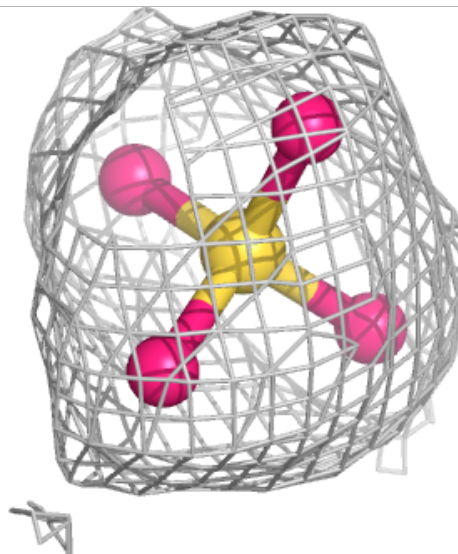
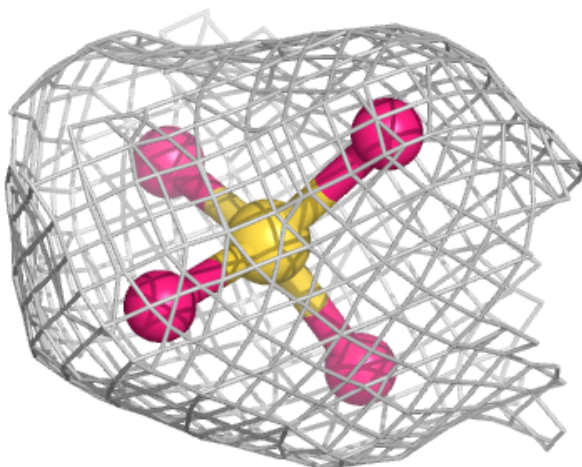
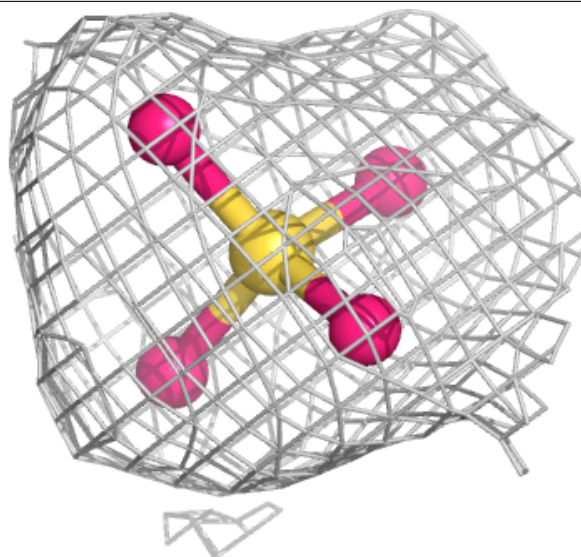
**Electron density around NA B 714:**

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



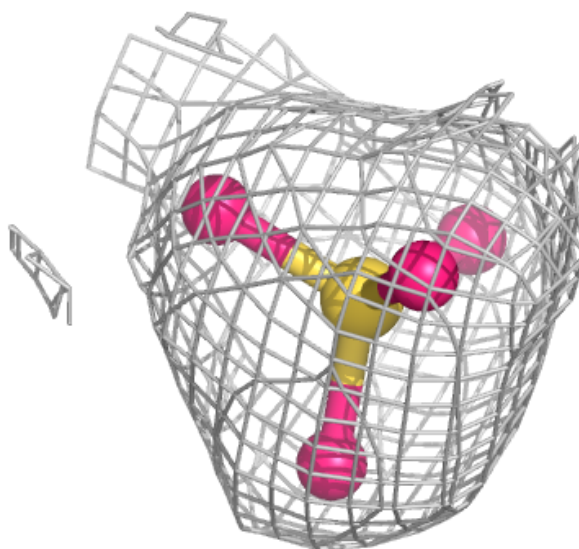
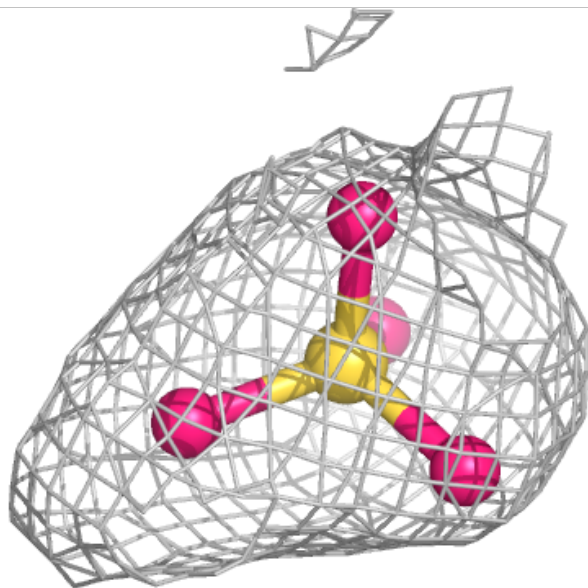
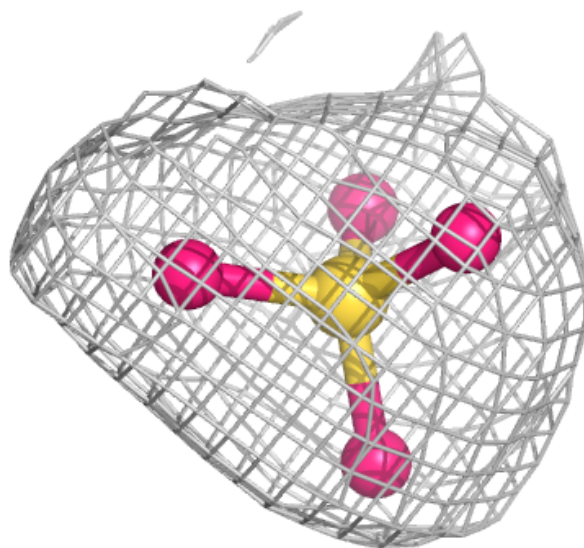
**Electron density around SO4 G 701:**

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



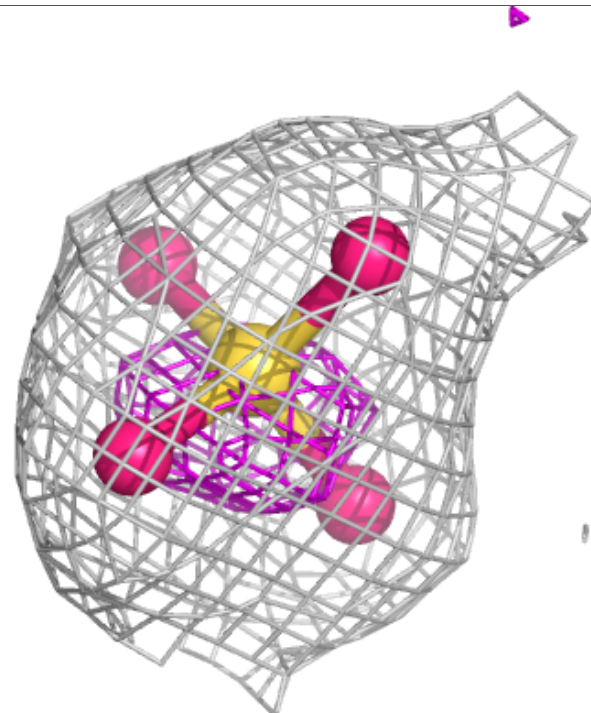
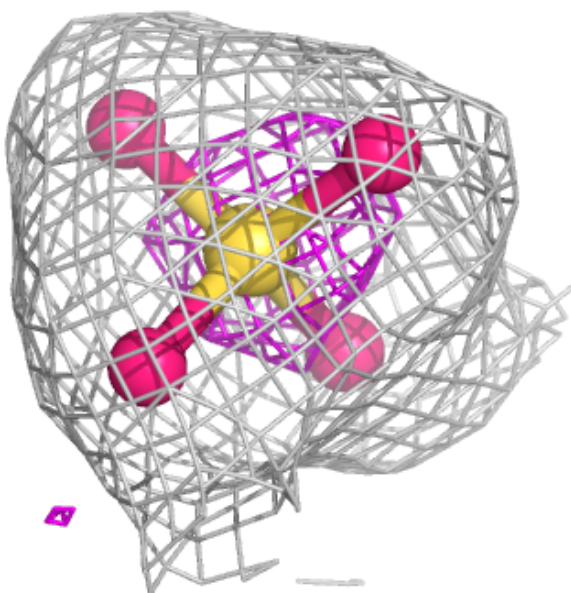
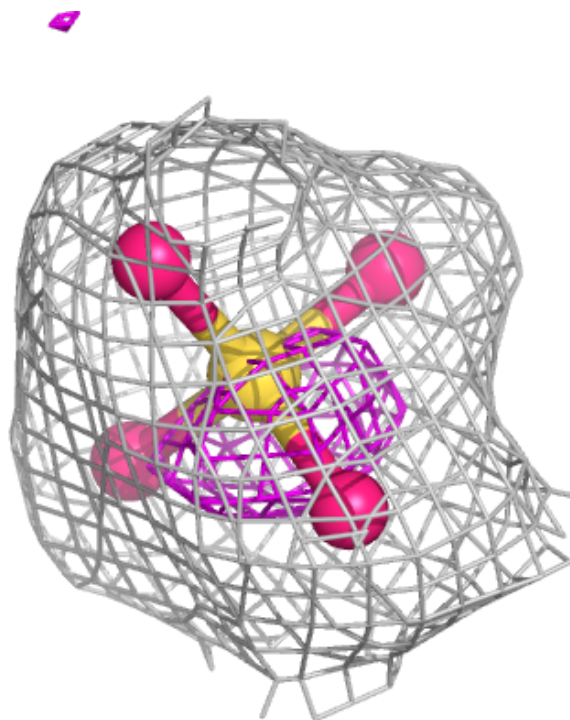
**Electron density around SO4 A 703:**

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



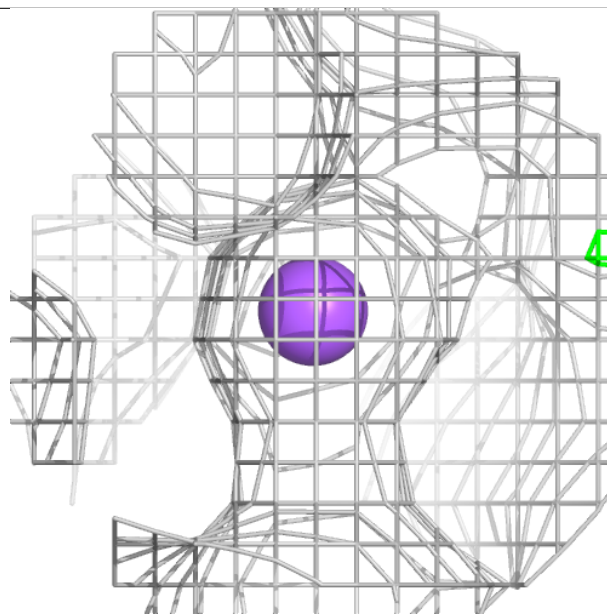
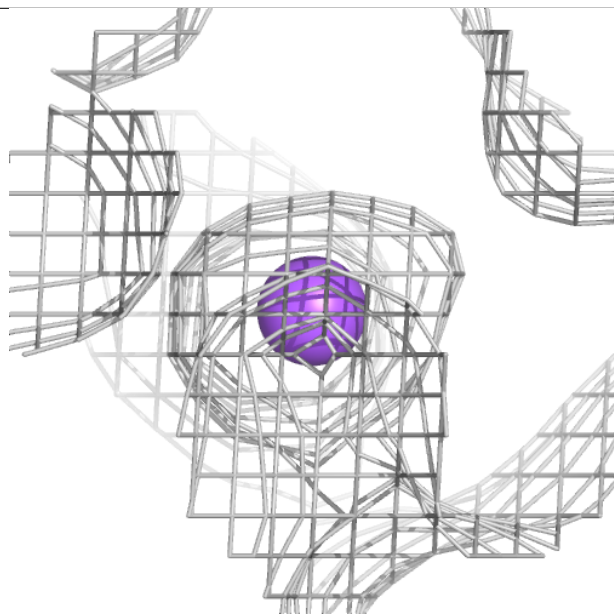
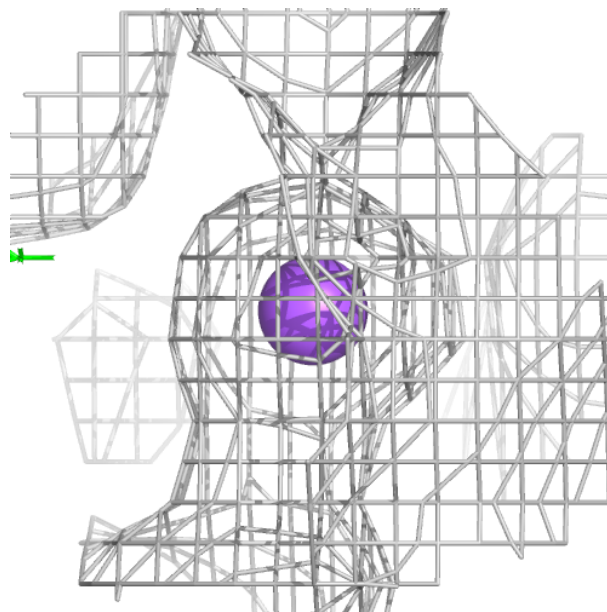
**Electron density around SO4 A 704:**

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



**Electron density around NA E 710:**

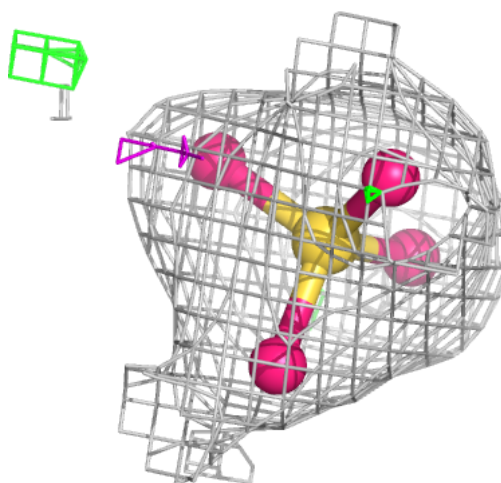
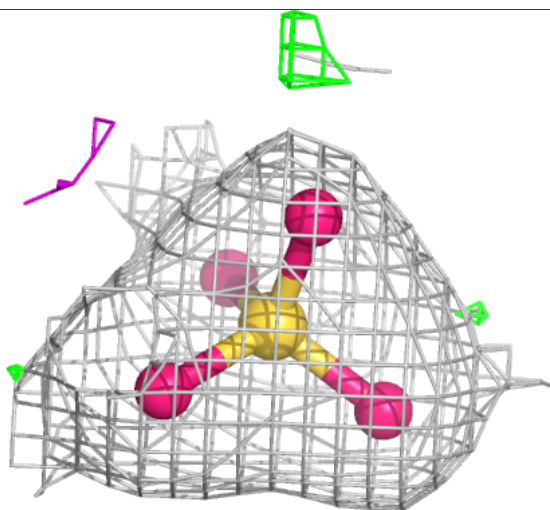
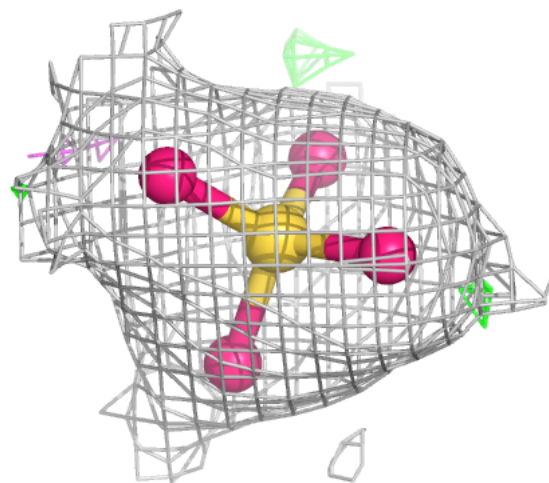
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





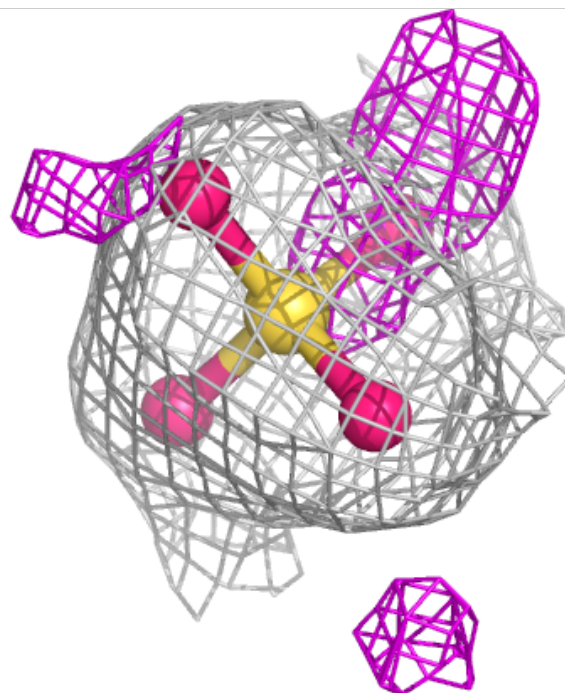
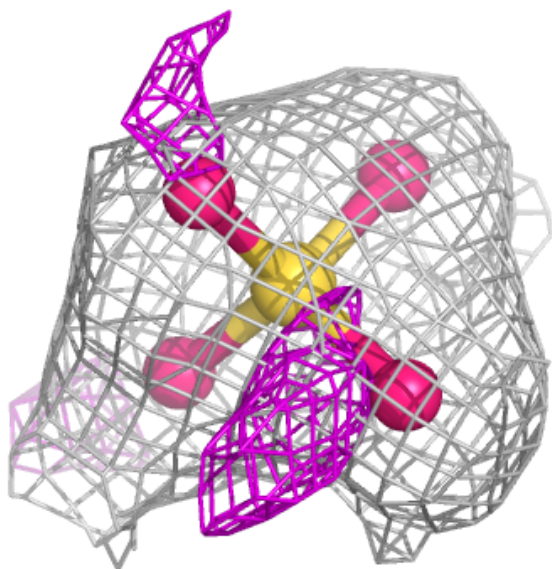
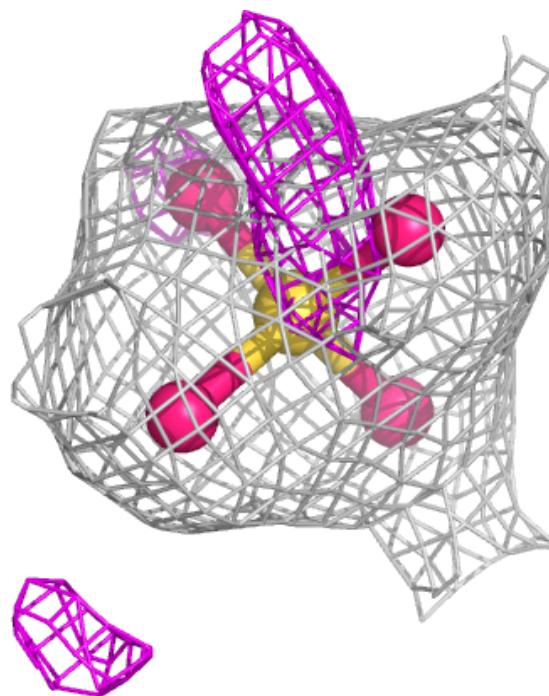
**Electron density around SO4 E 701:**

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



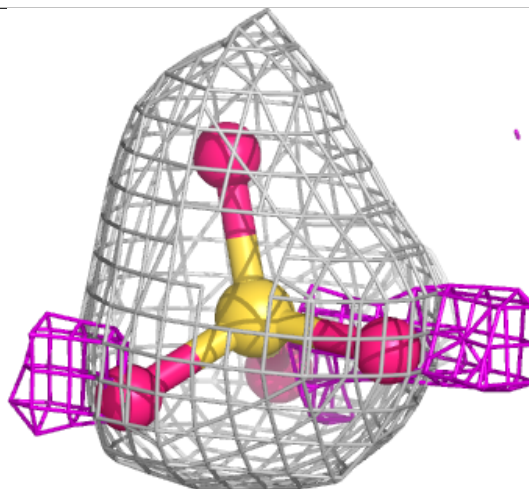
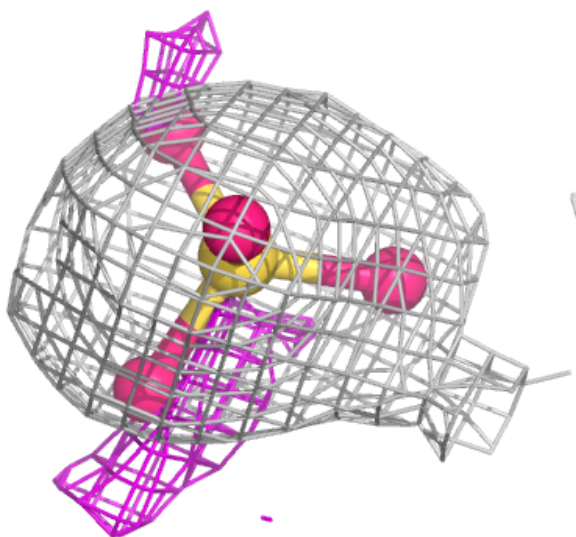
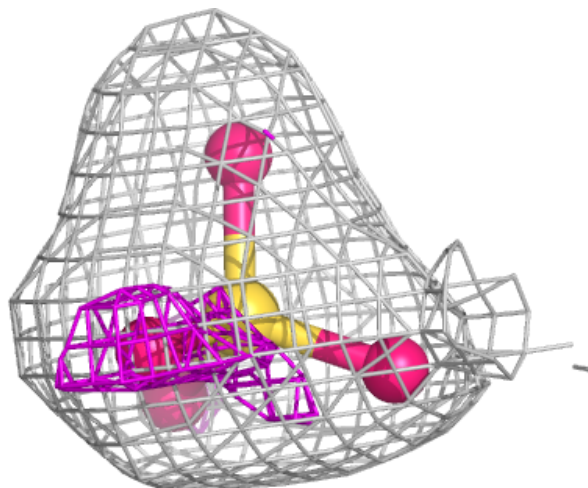
**Electron density around SO4 C 702:**

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



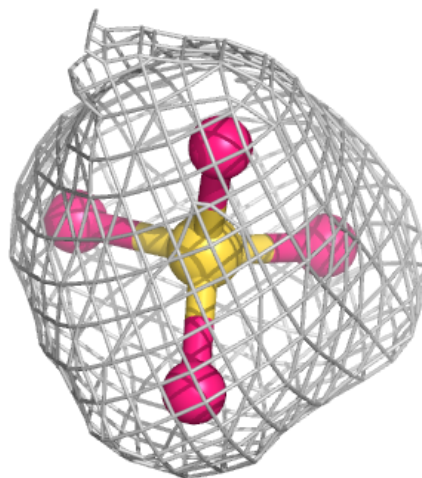
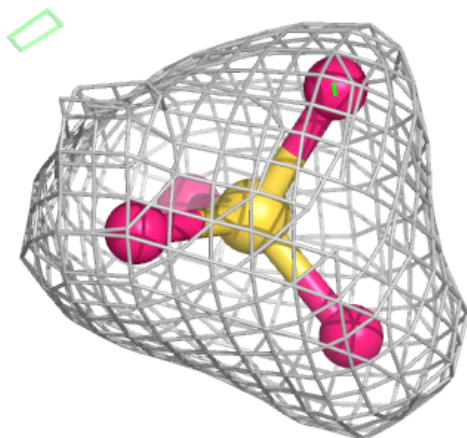
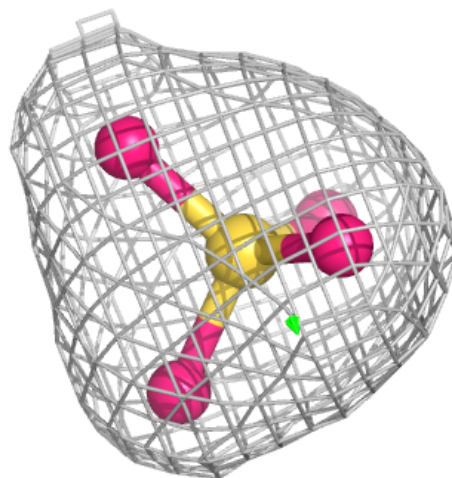
**Electron density around SO4 C 704:**

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



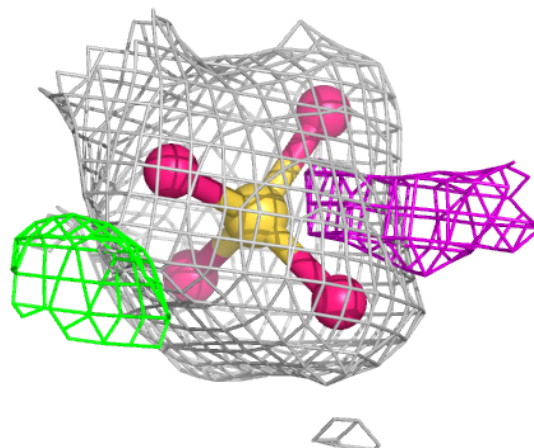
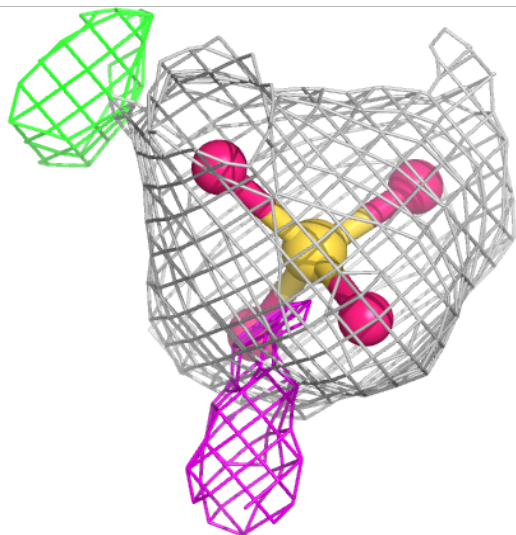
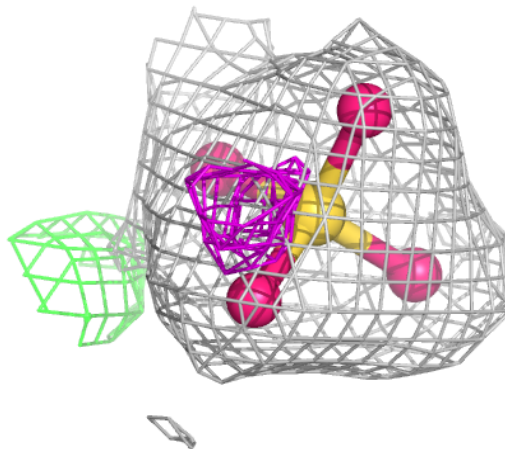
**Electron density around SO4 H 701:**

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



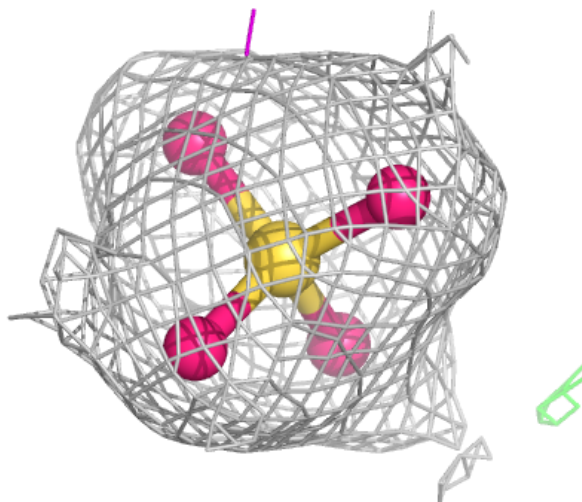
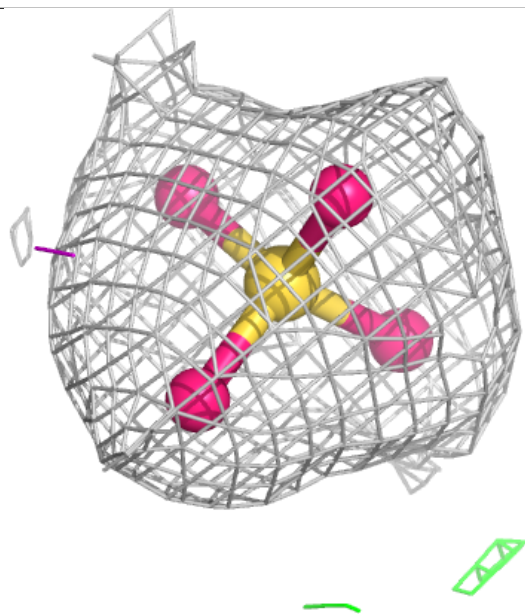
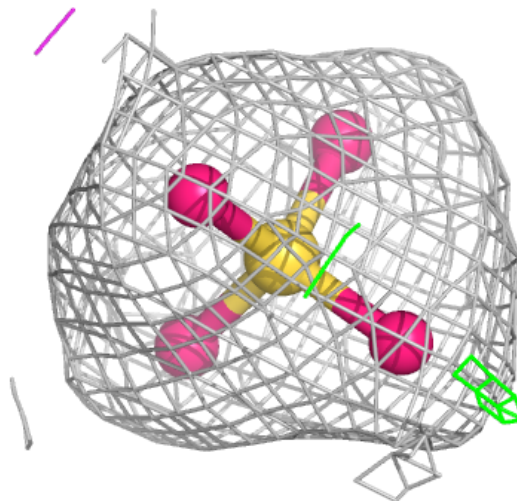
**Electron density around SO4 H 702:**

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



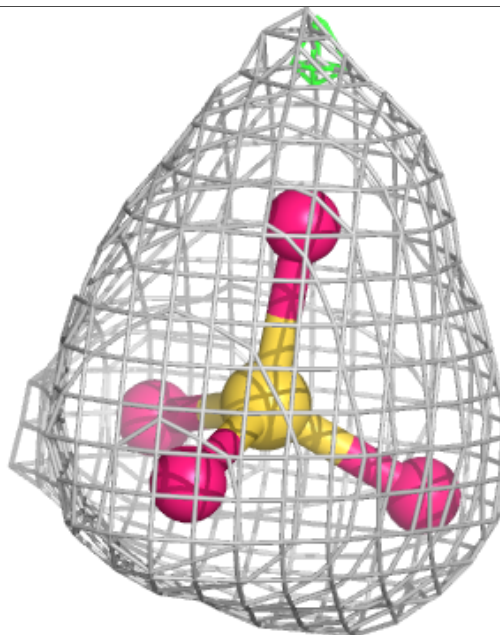
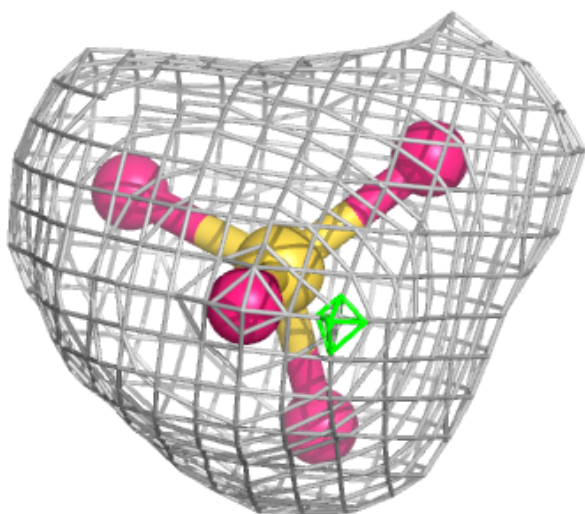
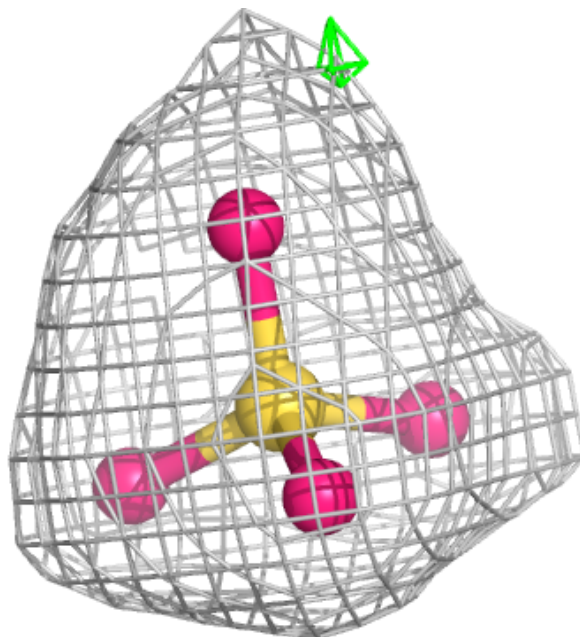
**Electron density around SO4 H 703:**

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



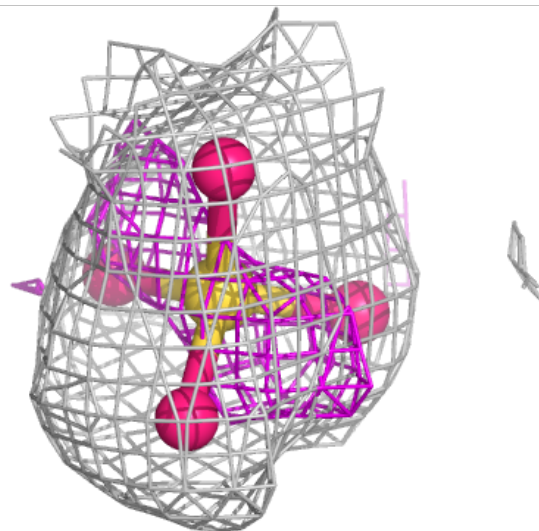
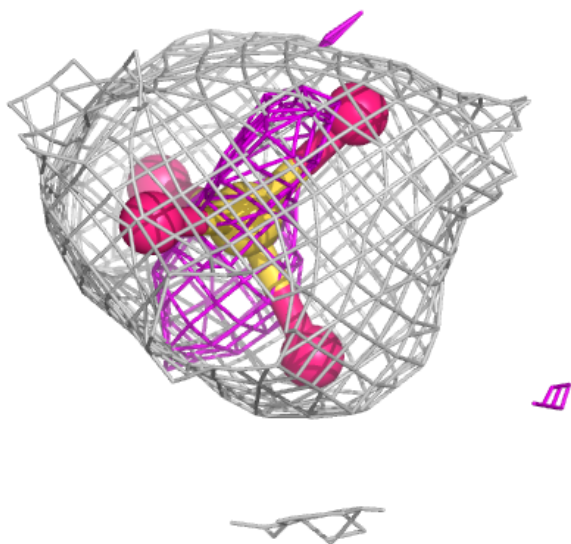
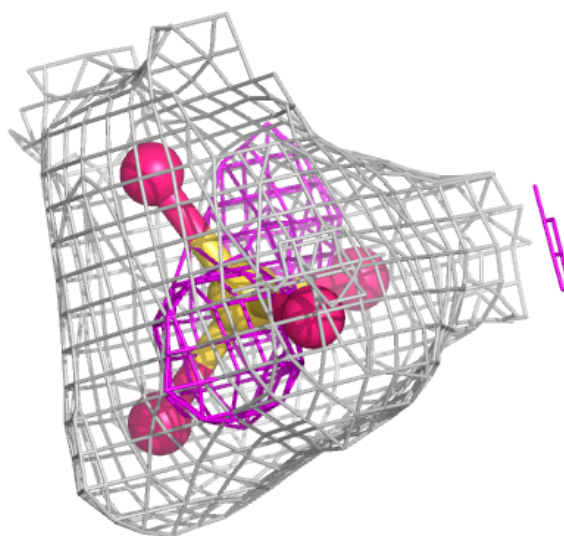
**Electron density around SO4 D 703:**

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



**Electron density around SO4 D 704:**

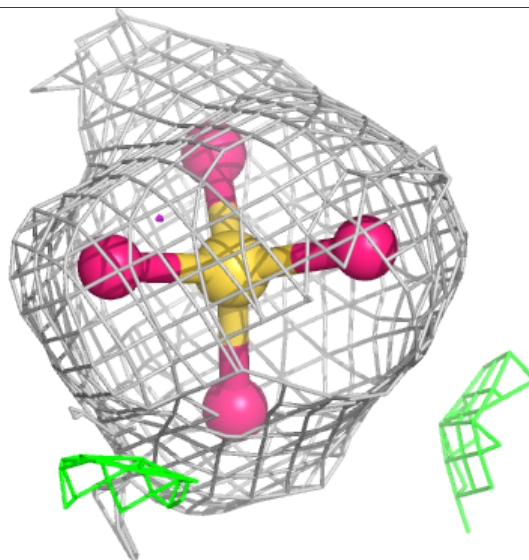
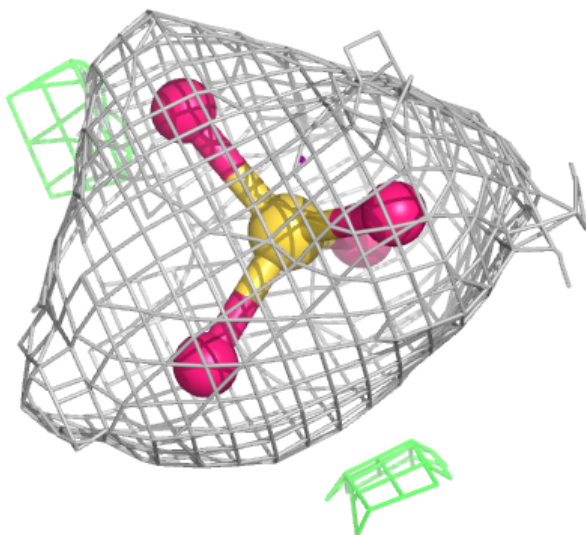
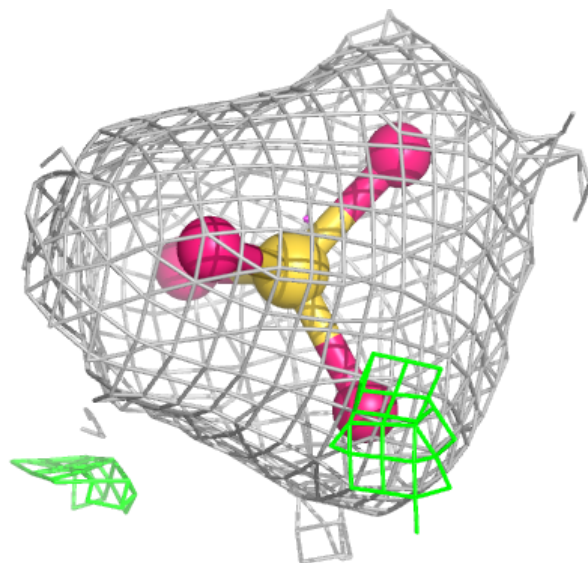
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





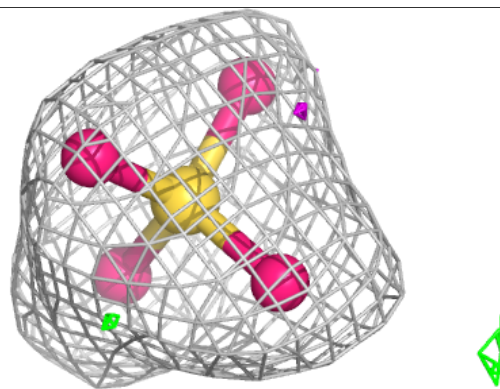
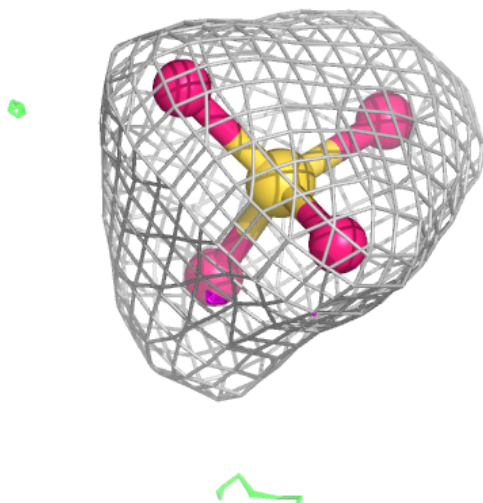
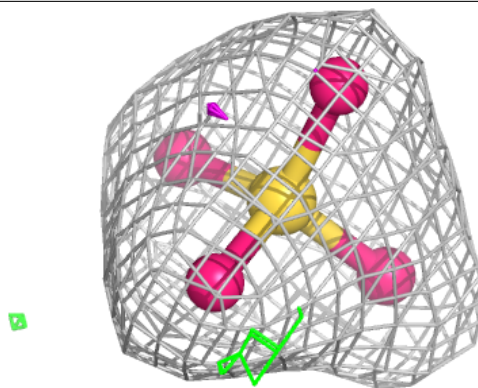
**Electron density around SO4 C 703:**

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



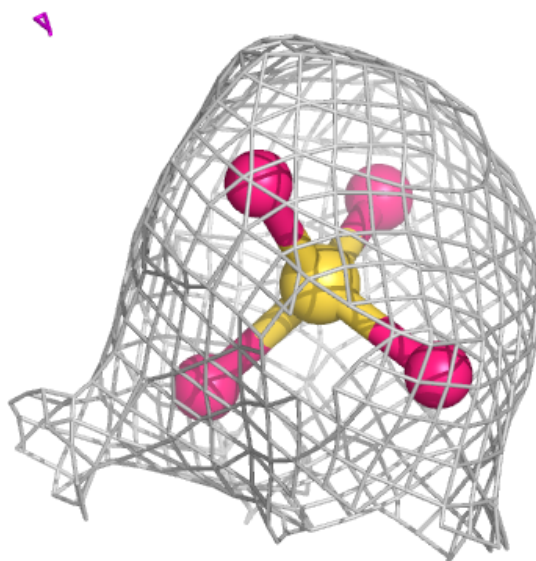
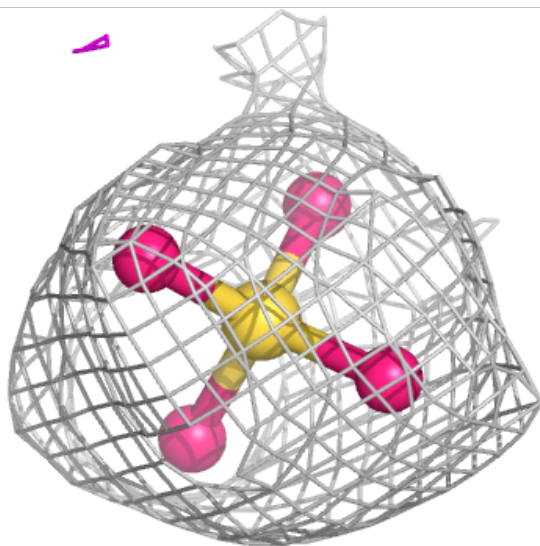
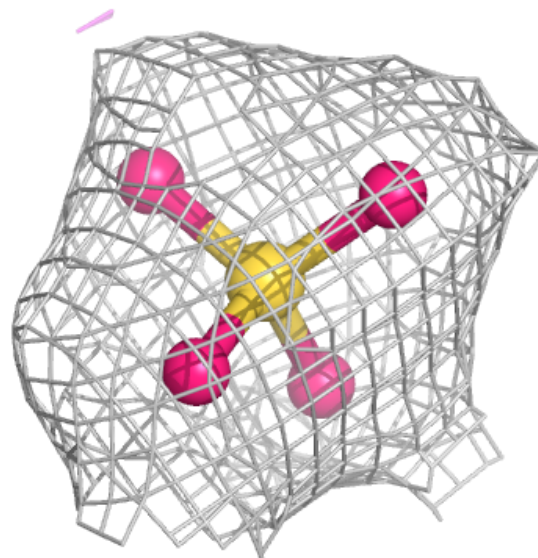
**Electron density around SO4 F 701:**

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



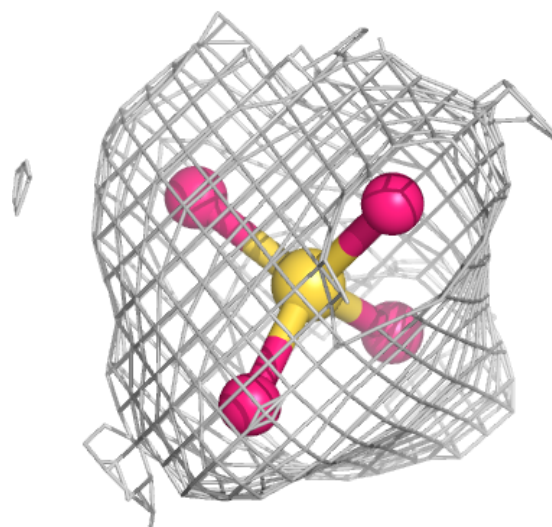
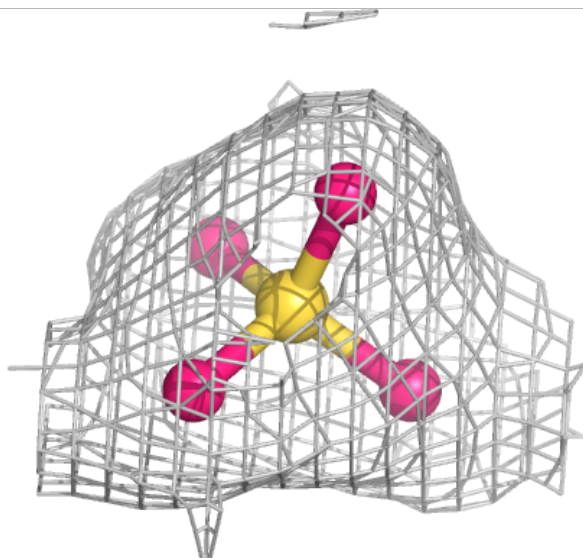
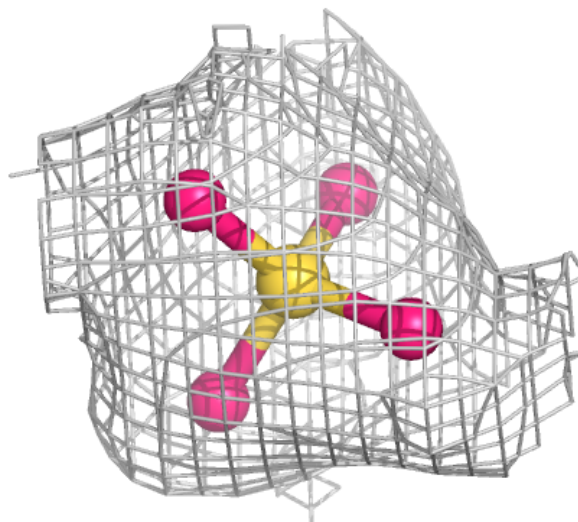
**Electron density around SO4 B 709:**

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



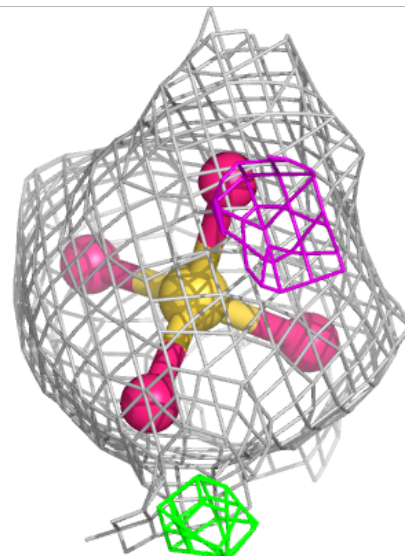
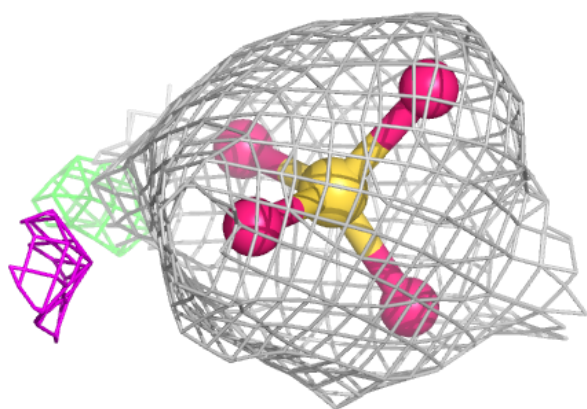
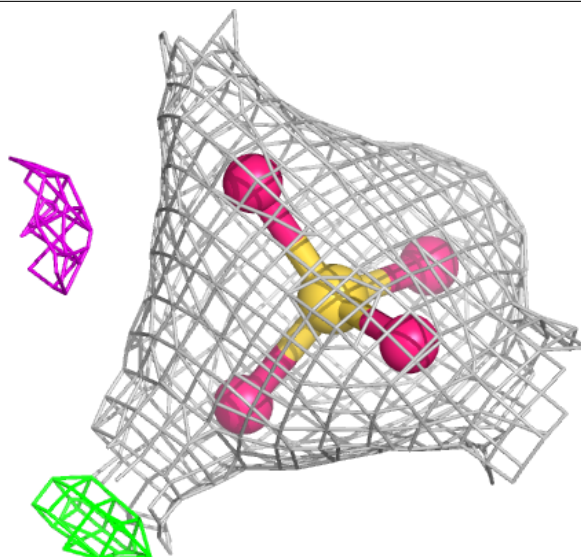
**Electron density around SO4 B 710:**

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



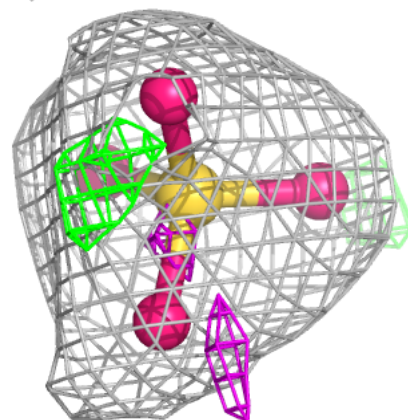
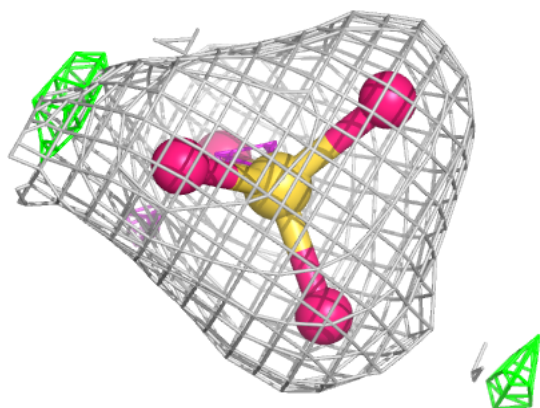
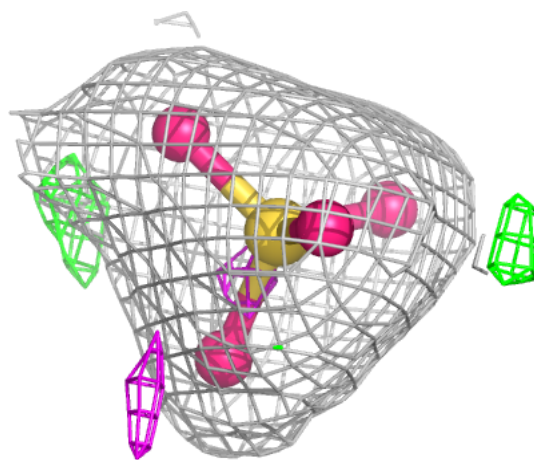
**Electron density around SO4 F 704:**

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



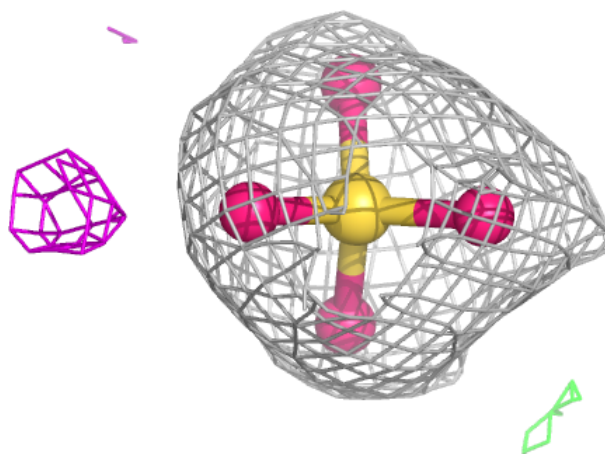
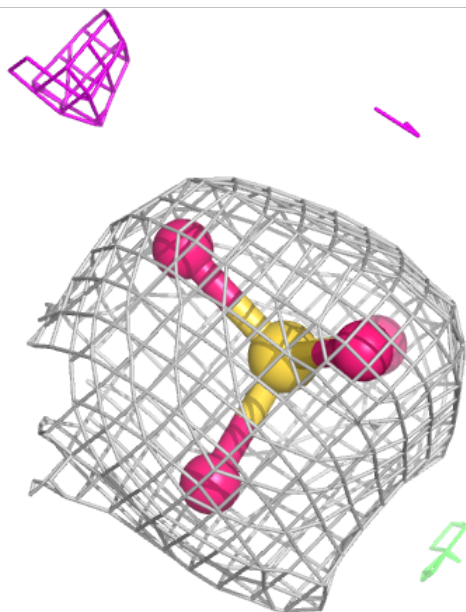
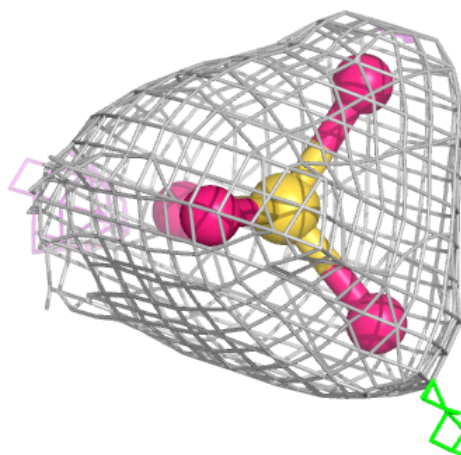
**Electron density around SO4 B 701:**

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



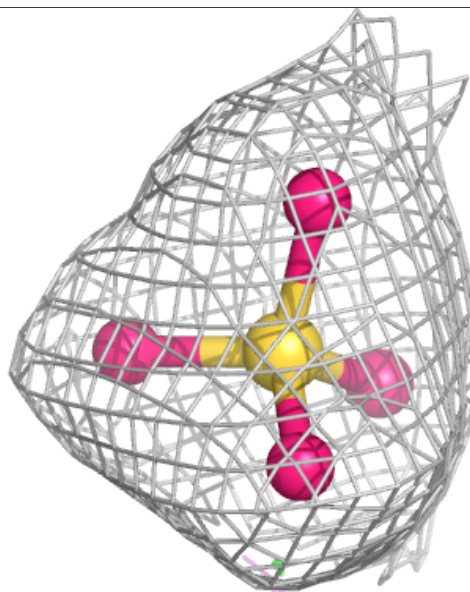
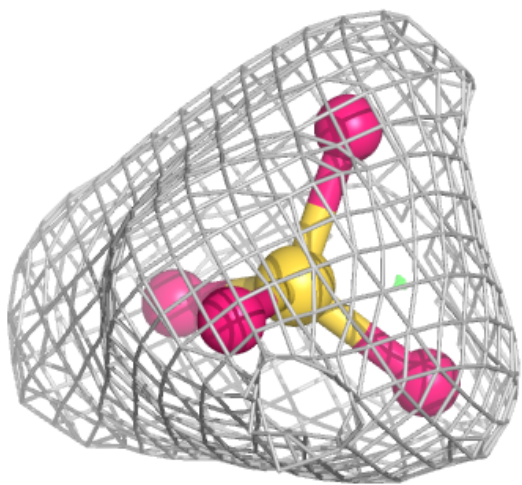
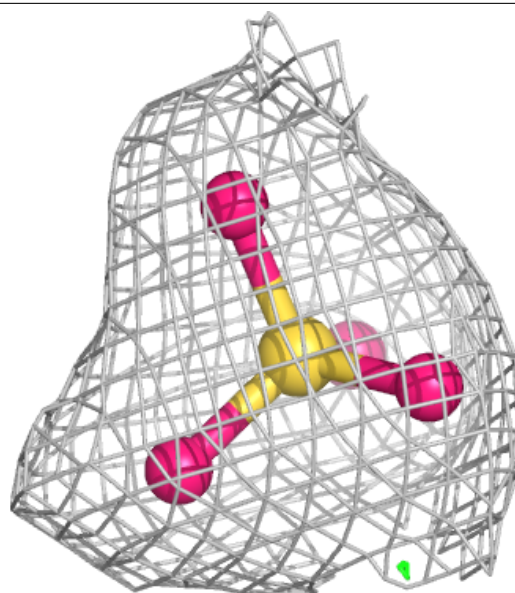
**Electron density around SO4 B 703:**

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



**Electron density around SO4 E 702:**

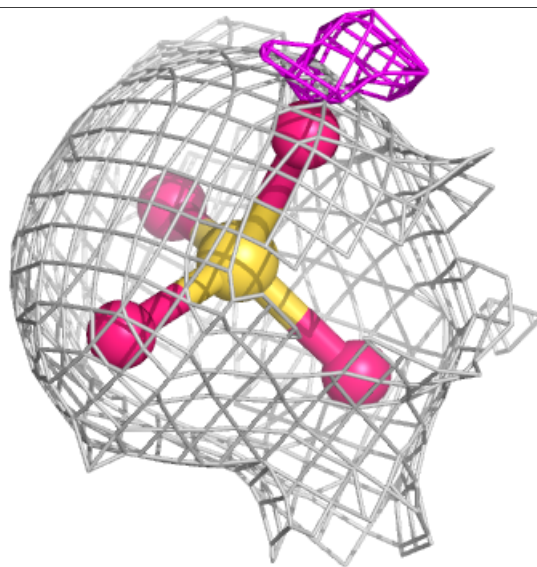
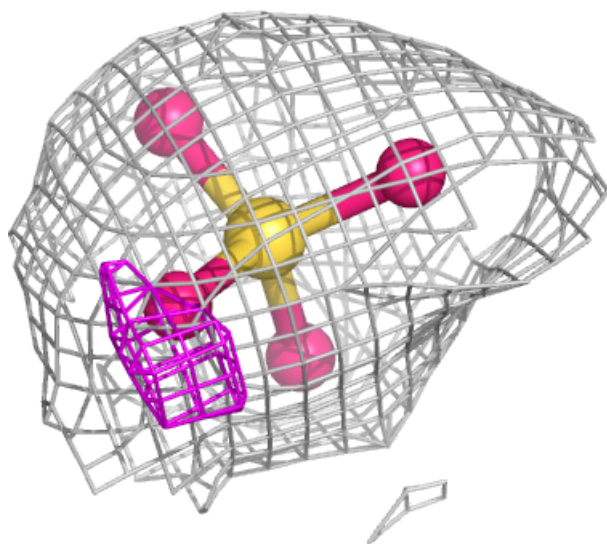
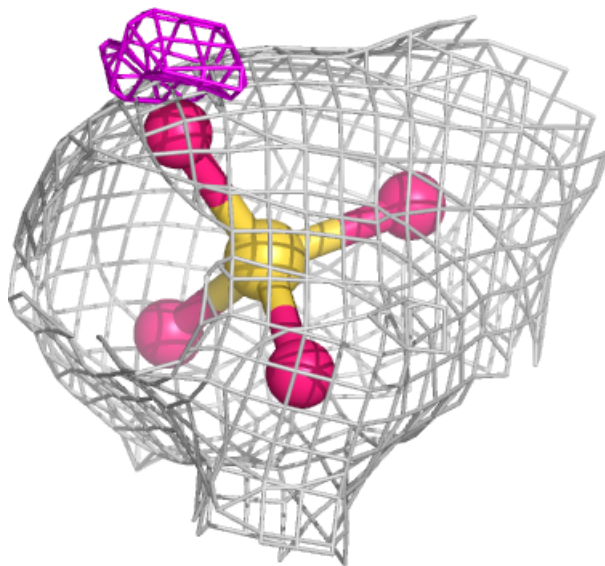
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





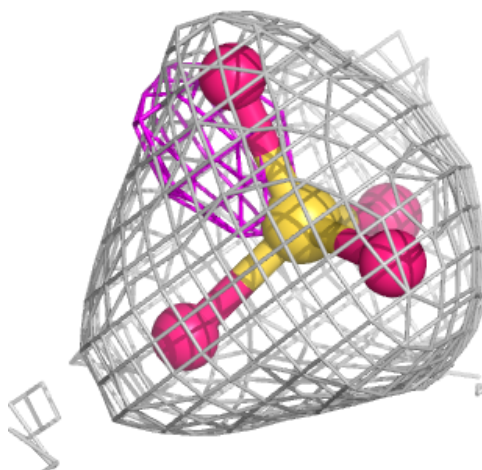
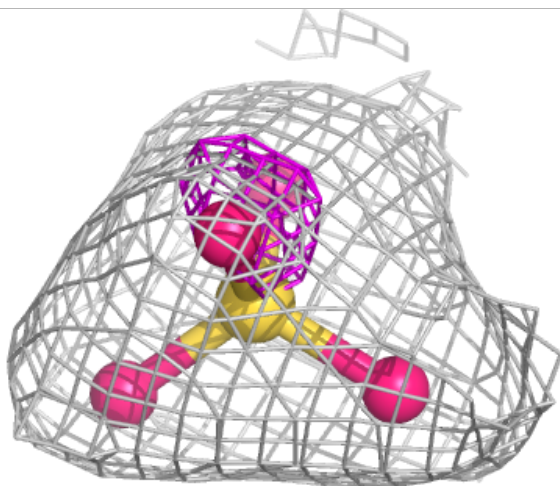
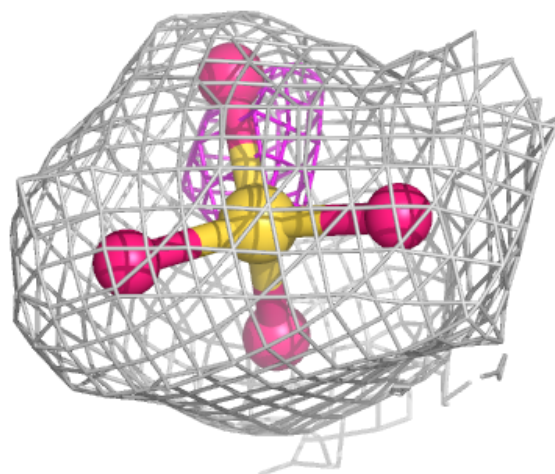
**Electron density around SO4 E 703:**

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



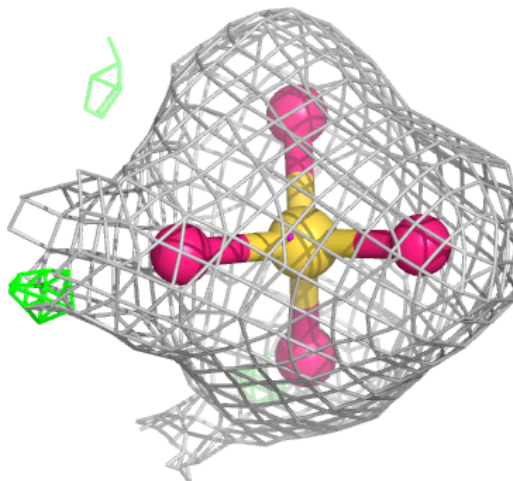
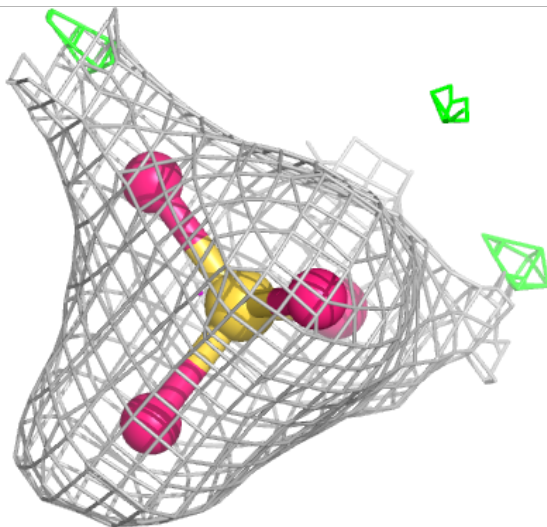
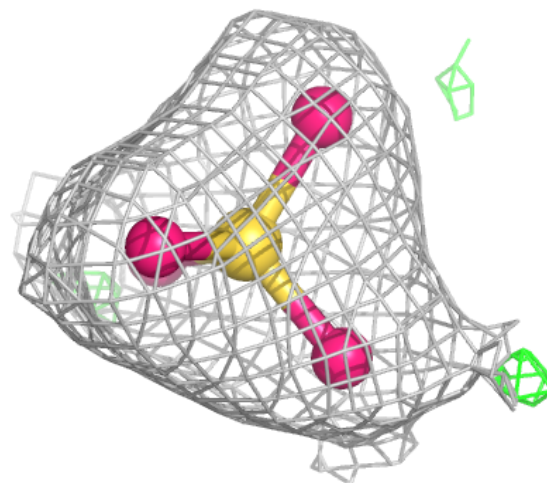
**Electron density around SO4 E 704:**

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



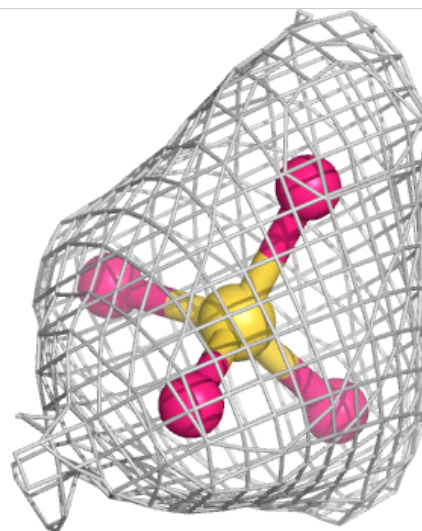
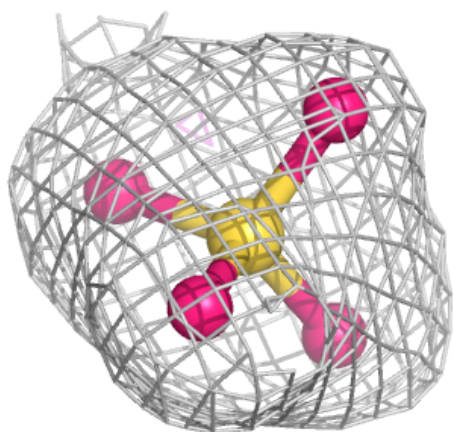
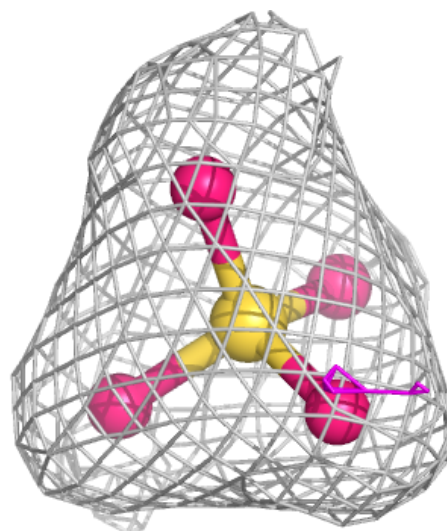
**Electron density around SO4 A 701:**

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



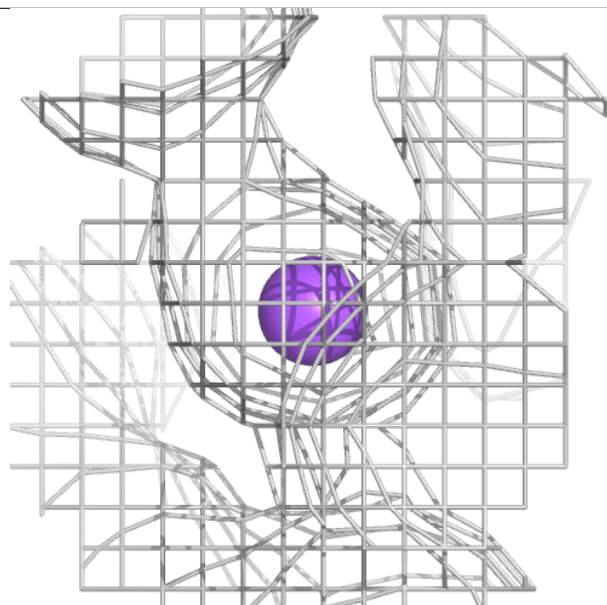
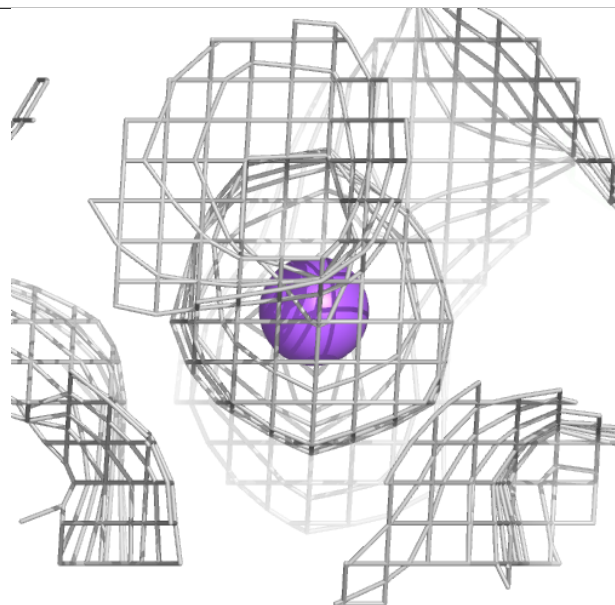
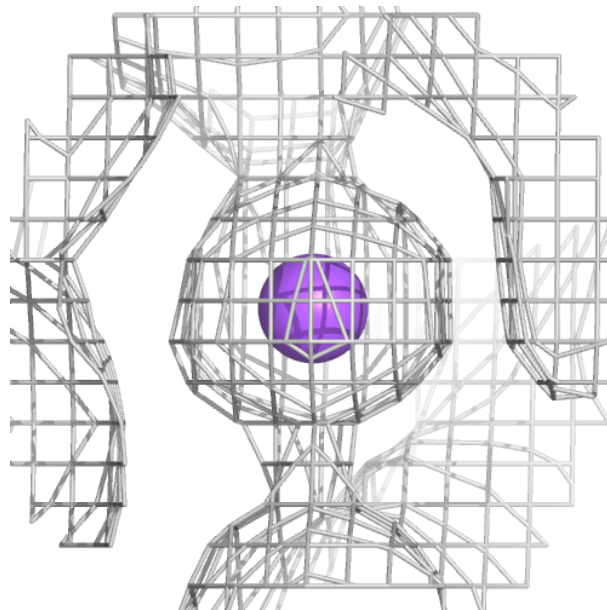
**Electron density around SO4 G 704:**

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



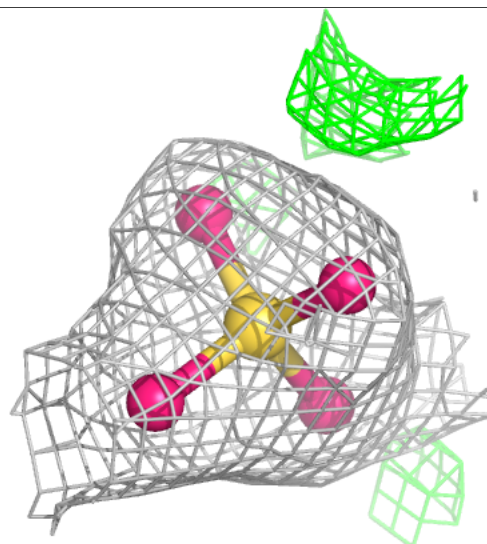
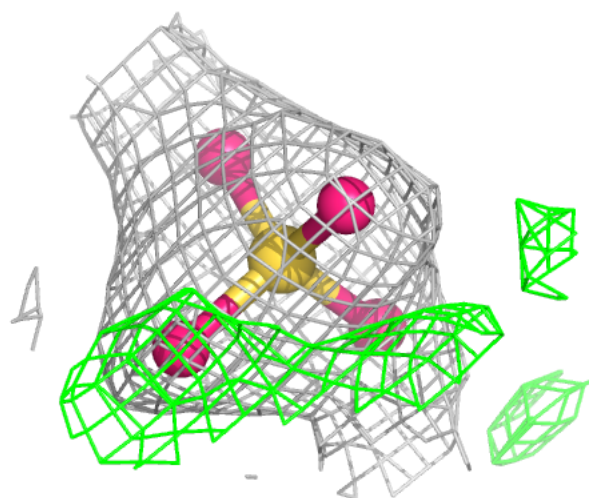
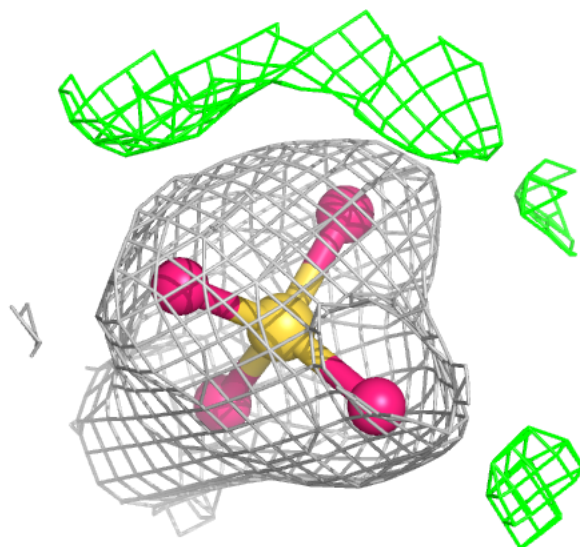
**Electron density around NA C 708:**

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



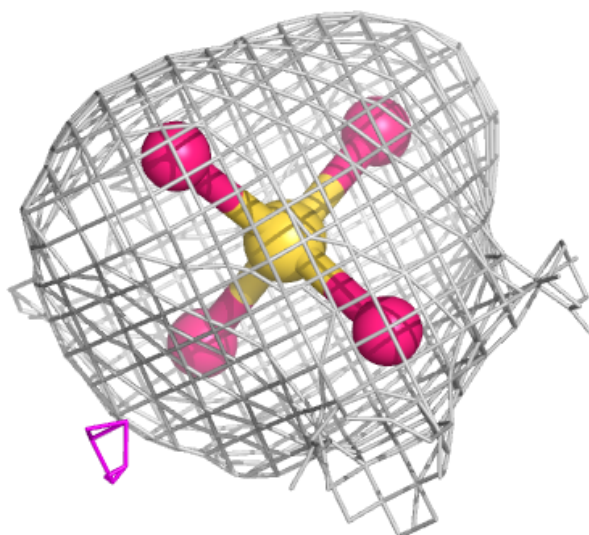
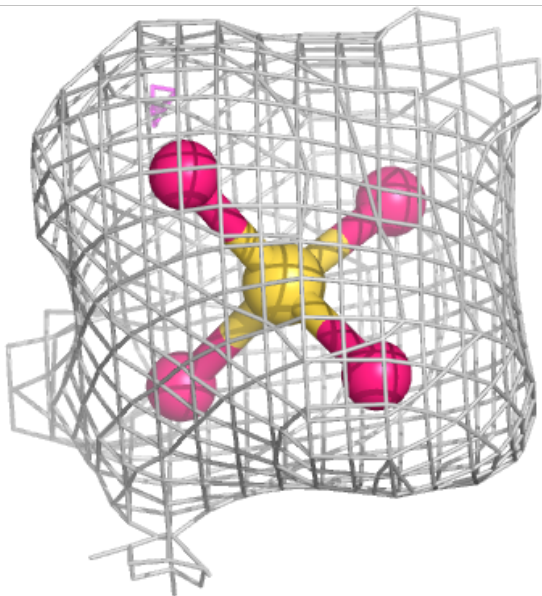
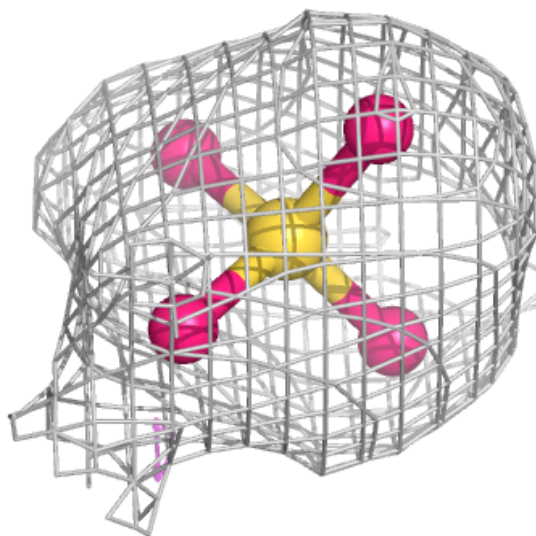
**Electron density around SO4 E 706:**

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



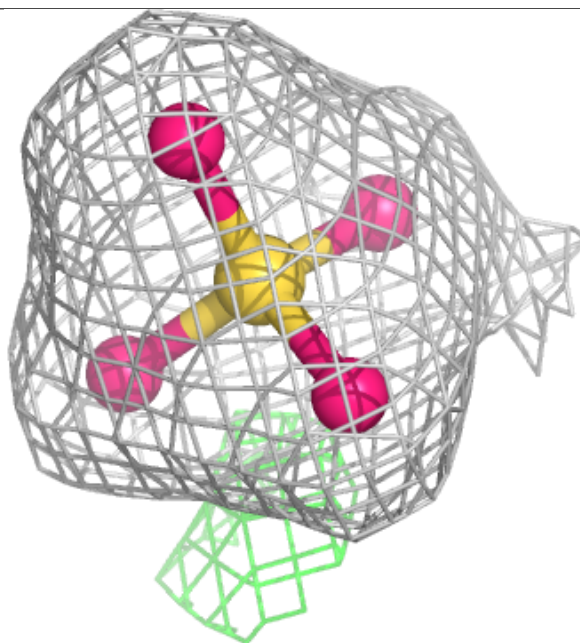
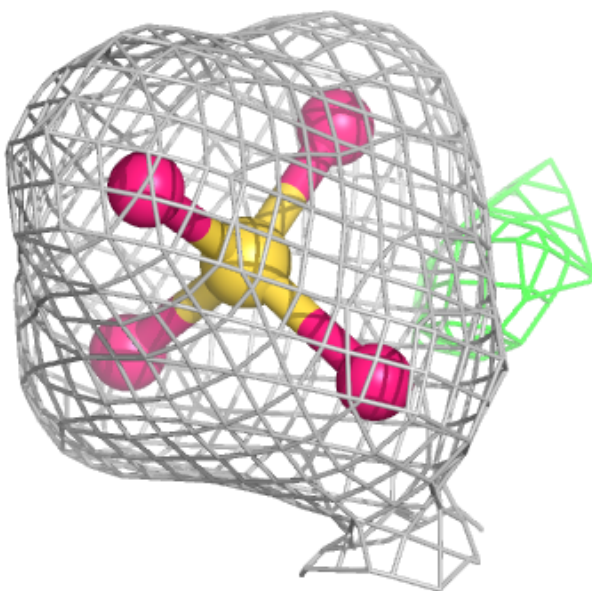
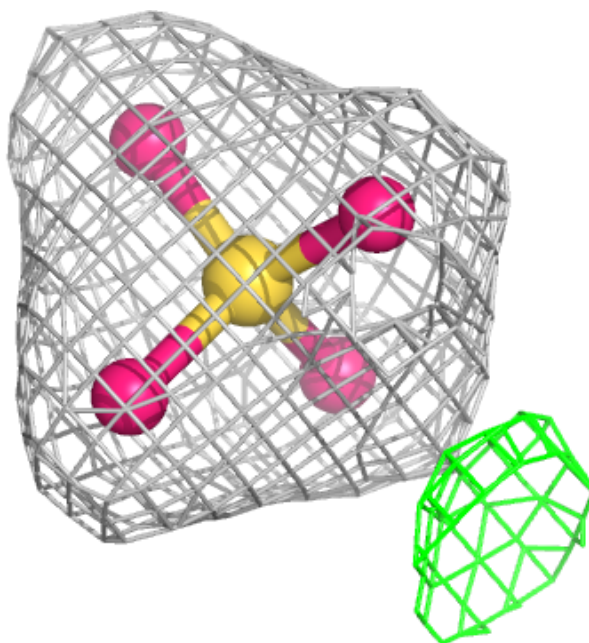
**Electron density around SO4 B 702:**

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



**Electron density around SO4 C 701:**

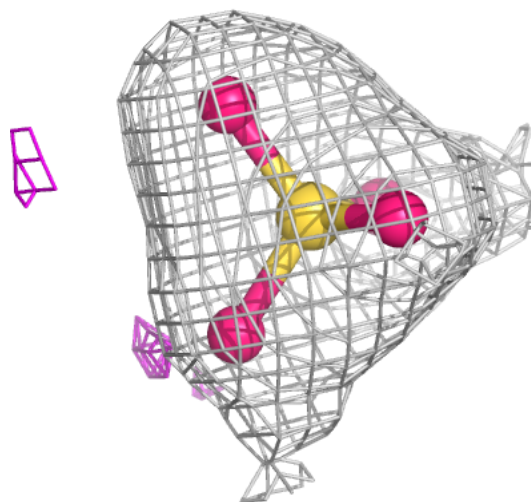
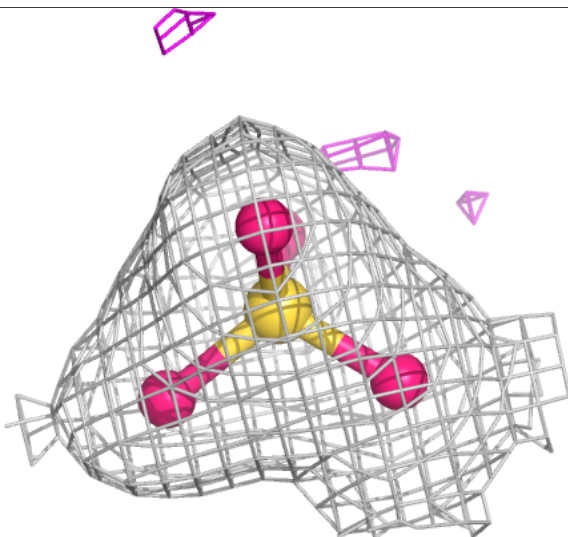
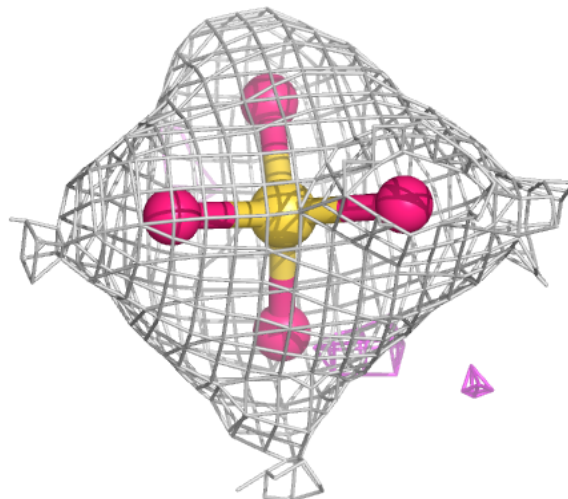
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





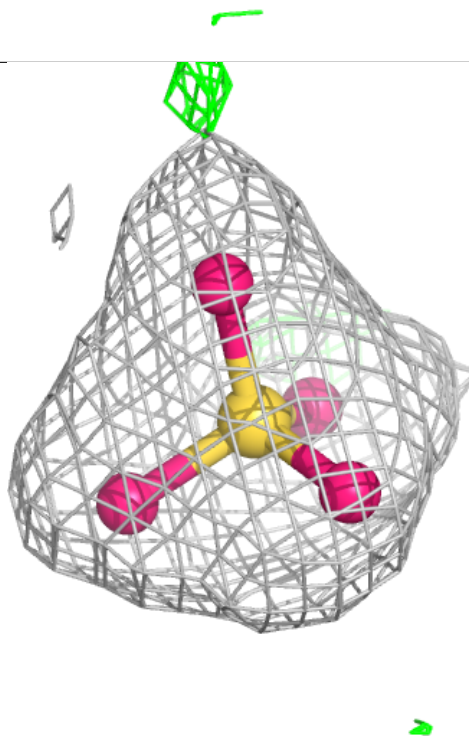
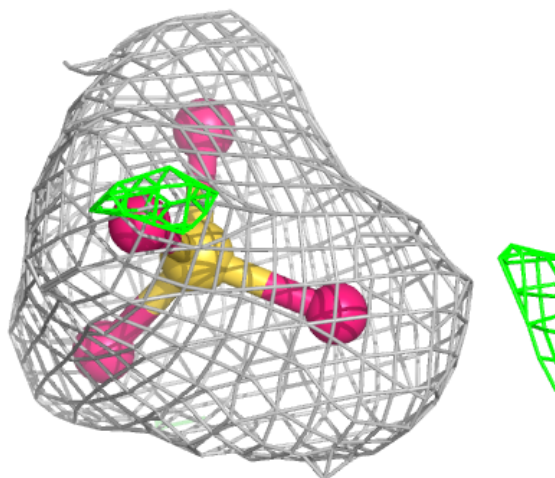
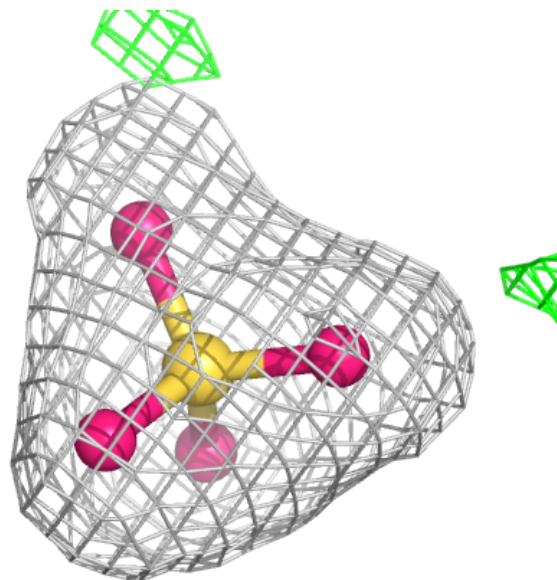
**Electron density around SO4 D 701:**

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



**Electron density around SO4 B 705:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.