



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:54 PM UTC

PDB ID : 8WT1 / pdb_00008wt1
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

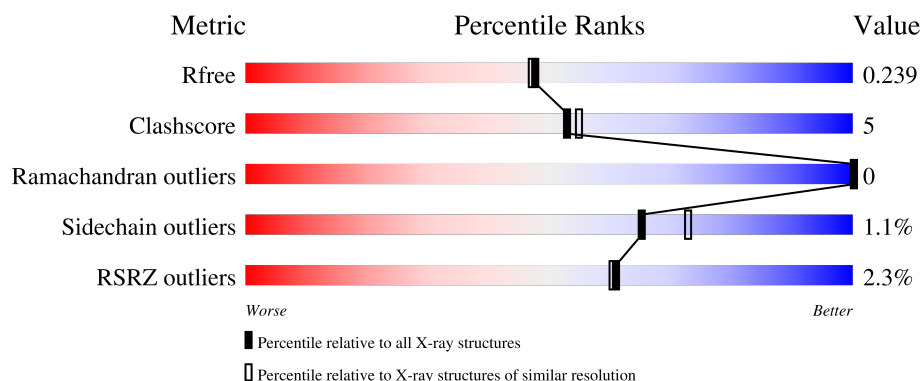
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 ≥ 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	0% 82% 12% 6%
1	B	691	0% 86% 9% 6%
1	C	691	0% 84% 10% 6%
1	D	691	2% 83% 11% 6%
1	E	691	0% 84% 10% 6%

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Mol	Chain	Length	Quality of chain
1	F	691	 2% 84% 10% 6%
1	G	691	 5% 82% 12% 6%
1	H	691	 4% 84% 10% 6%

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	-
4	GOL	A	715	-	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	-
5	ALA	G	709	-	X	-	-
6	FLC	A	717	-	X	-	-
6	FLC	H	713	-	X	-	-

2 Entry composition

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

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

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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

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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

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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

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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

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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

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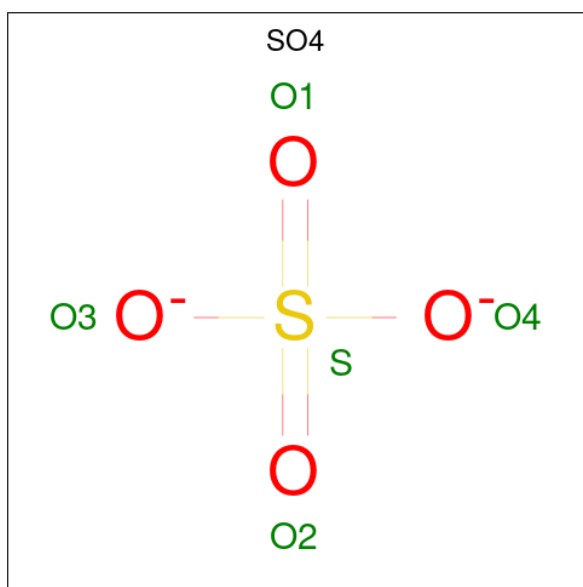
Chain	Residue	Modelled	Actual	Comment	Reference
F	13	PHE	-	expression tag	UNP A0A3L7D5Q2
F	14	GLN	-	expression tag	UNP A0A3L7D5Q2
F	15	GLY	-	expression tag	UNP A0A3L7D5Q2
F	16	THR	-	expression tag	UNP A0A3L7D5Q2
F	332	SER	LEU	conflict	UNP A0A3L7D5Q2
G	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
G	-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

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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 (CCD ID: SO4) (formula: O₄S) (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	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		

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

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

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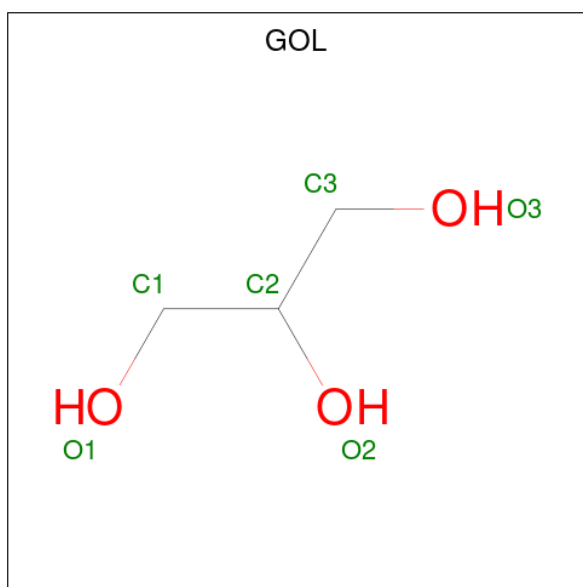
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0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

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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



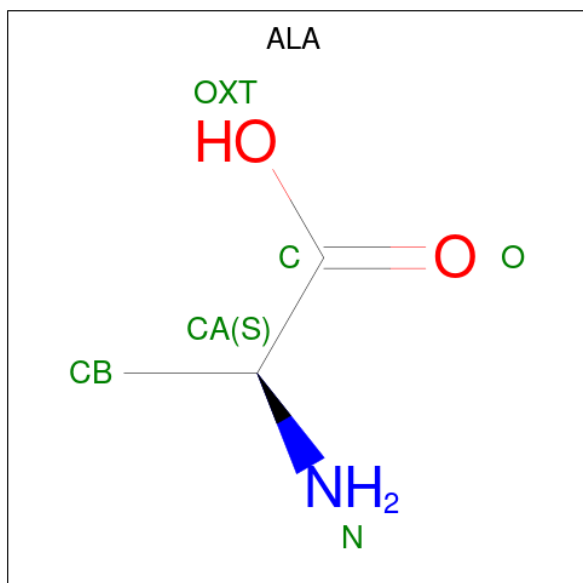
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total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

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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	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 (CCD ID: ALA) (formula: $C_3H_7NO_2$).



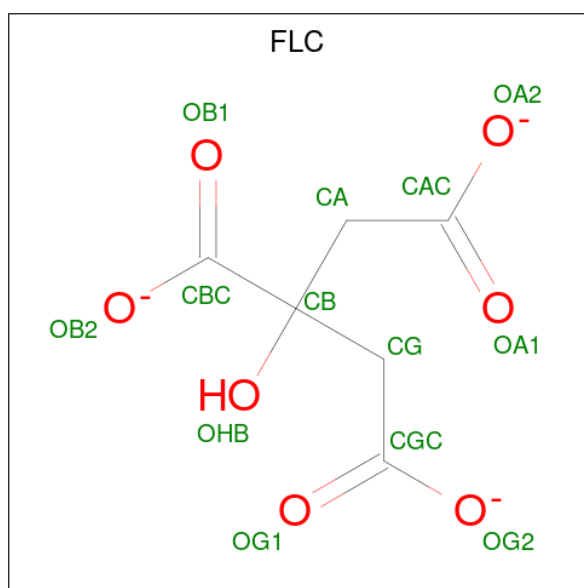
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			6	3	1	2		

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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 (CCD ID: 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		

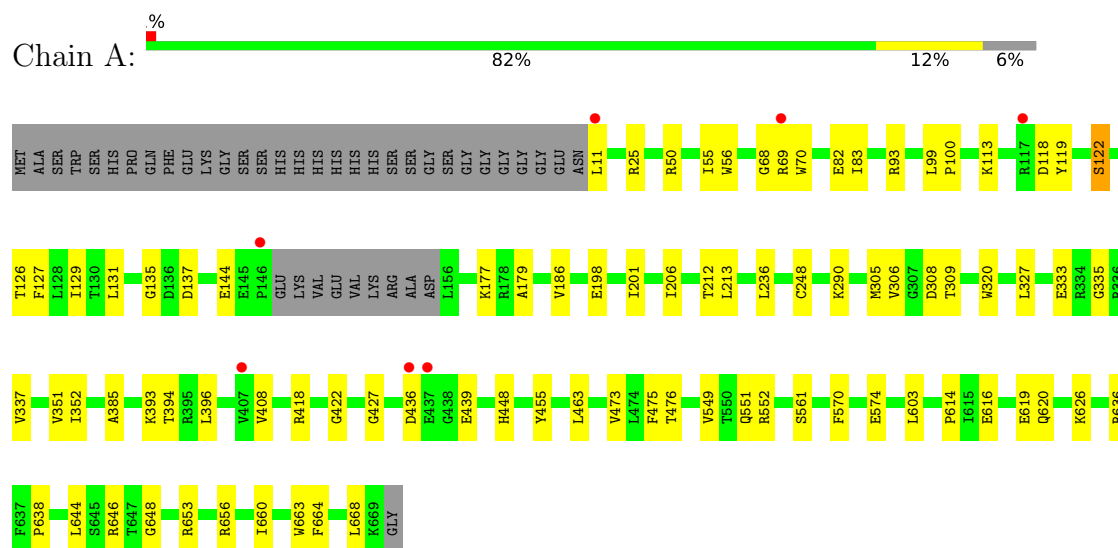
- Molecule 7 is water.

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

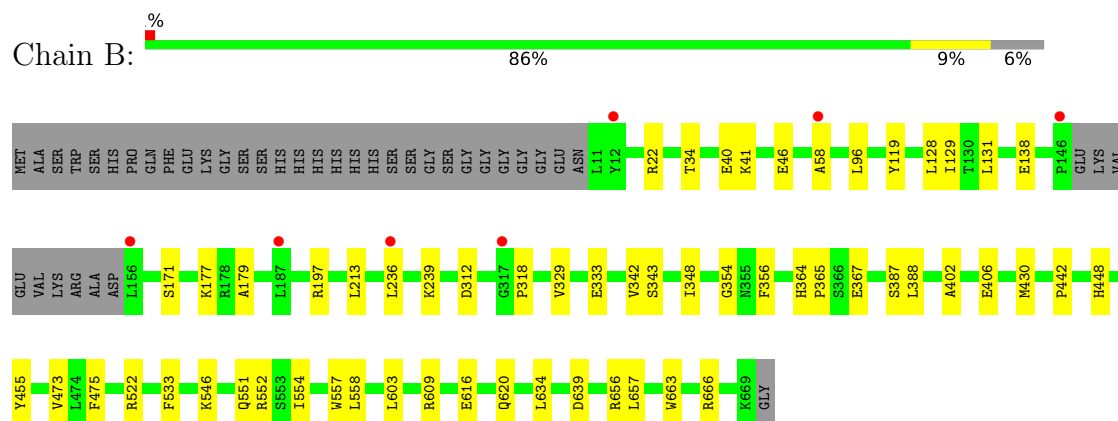
3 Residue-property plots [i](#)

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.

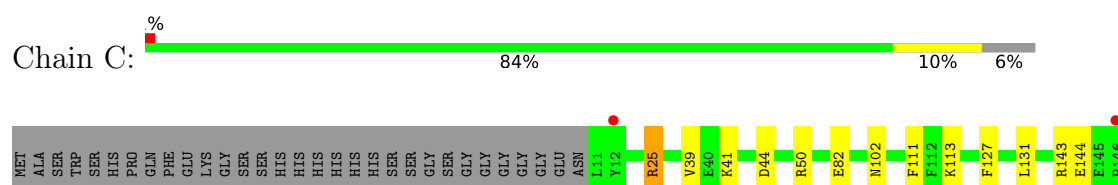
• Molecule 1: S9 family peptidase

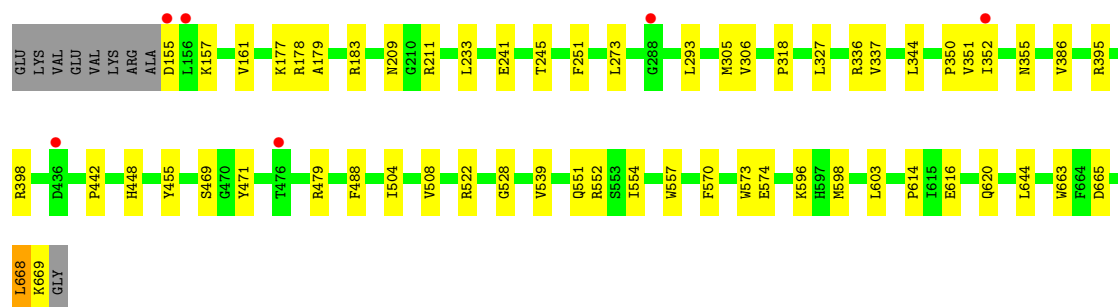


• Molecule 1: S9 family peptidase

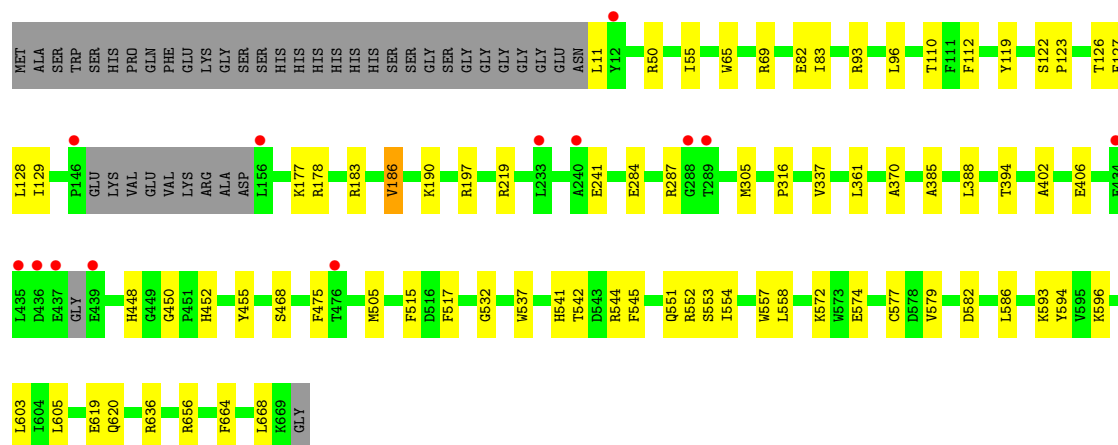
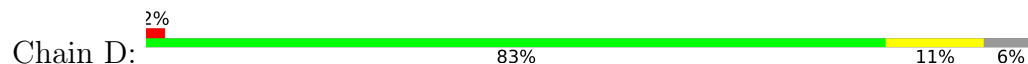


• Molecule 1: S9 family peptidase

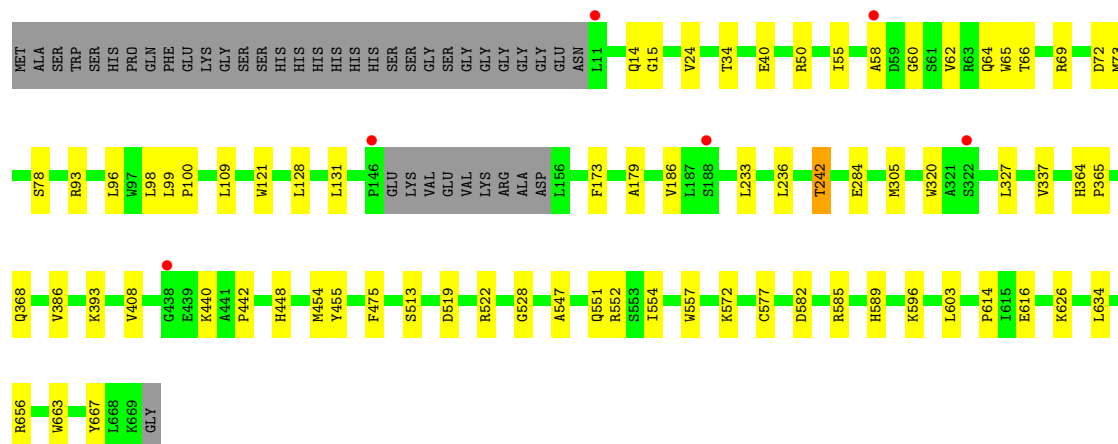
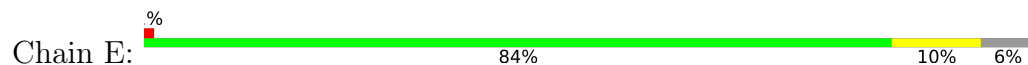




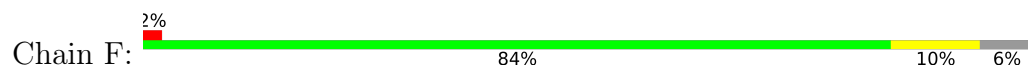
- Molecule 1: S9 family peptidase

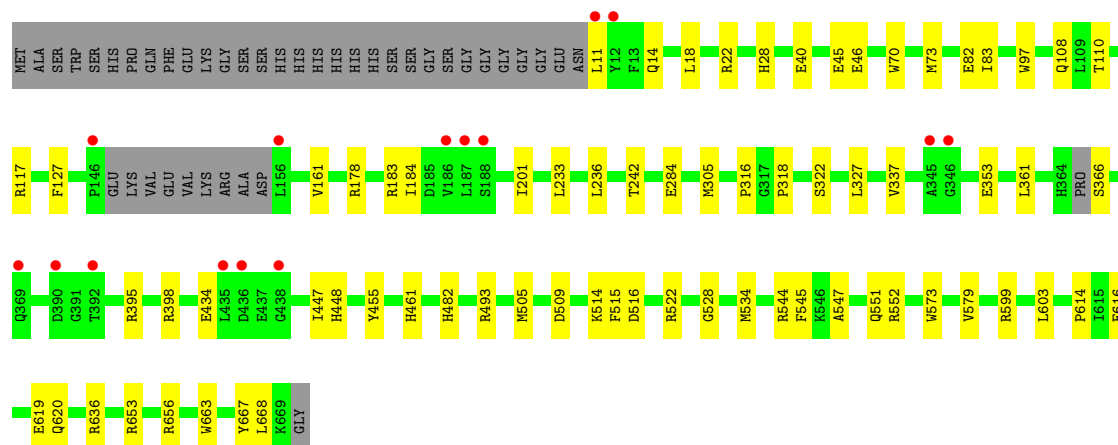


- Molecule 1: S9 family peptidase

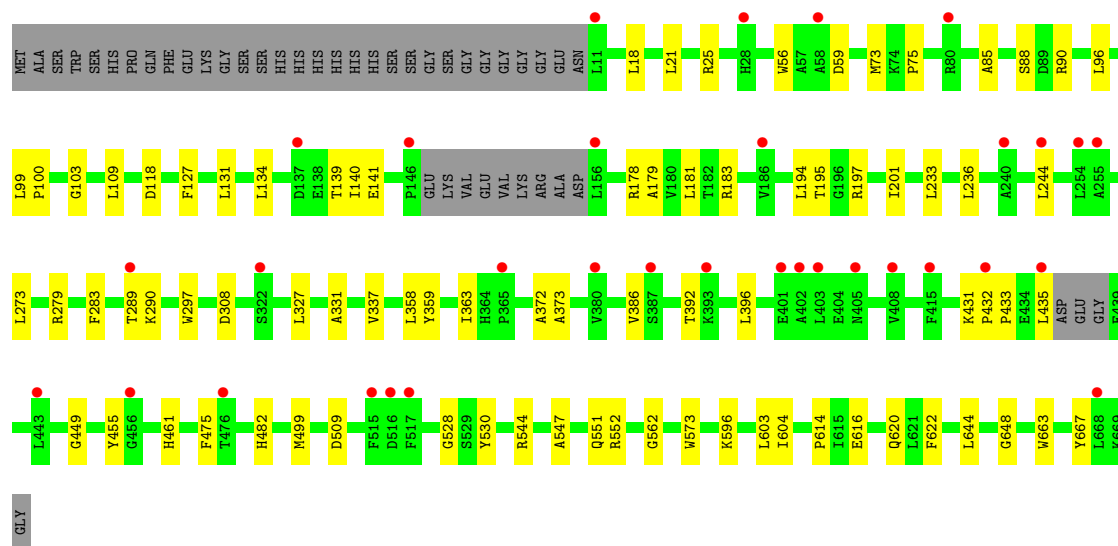
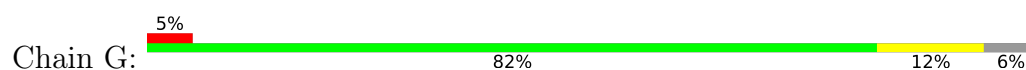


- Molecule 1: S9 family peptidase

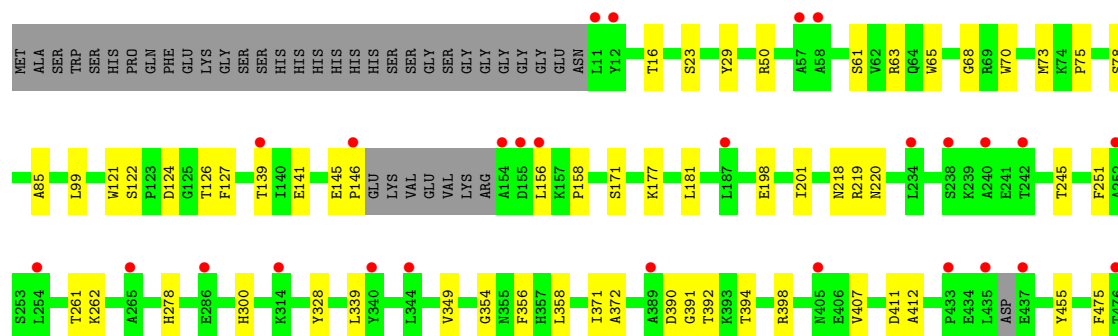
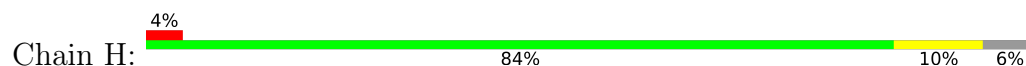




• Molecule 1: S9 family peptidase



• 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, α , β , γ	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) 90.5 (48.94-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.212 , 0.256 (Not available) , 0.239	Depositor DCC
R_{free} test set	19887 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42813	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, NA, GOL, 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	0.36	0/5201	0.54	0/7069
1	B	0.34	0/5197	0.54	0/7062
1	C	0.36	0/5187	0.53	1/7052 (0.0%)
1	D	0.34	0/5165	0.51	0/7022
1	E	0.34	0/5161	0.52	0/7020
1	F	0.35	0/5146	0.53	0/6990
1	G	0.30	0/5037	0.48	0/6862
1	H	0.30	0/5118	0.47	0/6963
All	All	0.34	0/41212	0.52	1/56040 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	ARG	CA-CB-CG	-6.29	101.51	114.10

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	57	0
1	B	5063	0	4830	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5053	0	4803	46	0
1	D	5032	0	4774	51	0
1	E	5027	0	4752	44	0
1	F	5014	0	4732	55	0
1	G	4904	0	4560	52	0
1	H	4985	0	4700	43	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	7	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	6	0
7	C	307	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	228	0	0	5	0
7	E	305	0	0	4	0
7	F	255	0	0	6	0
7	G	123	0	0	4	0
7	H	204	0	0	1	0
All	All	42813	0	38204	393	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 (393) 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
5:E:715:ALA:HB2	7:E:844:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:MET:HE2	1:C:337:VAL:HG23	1.77	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

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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:G:499:MET:HE2	1:G:499:MET:HA	1.87	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
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:F:505:MET:HA	1:F:505:MET:HE2	1.90	0.54
2:F:706:SO4:O4	4:F:708:GOL:O3	2.24	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:G:131:LEU:HD21	1:G:179:ALA:HB1	1.91	0.52
1:B:239:LYS:O	1:B:239:LYS:HG2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:305:MET:HE2	1:A:337:VAL:HG23	1.94	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:E:305:MET:HE2	1:E:337:VAL:HG23	1.94	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:D:305:MET:HE2	1:D:337:VAL:HG23	1.94	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:C:469:SER:O	1:C:669:LYS:NZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:505:MET:HE2	1:D:505:MET:HA	1.95	0.47
5:D:714:ALA:N	7:D:811:HOH:O	2.47	0.47
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
1:F:505:MET:HE1	1:F:545:PHE:CZ	2.50	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:390:ASP:CG	1:H:392:THR:HG23	2.39	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:B:551:GLN:O	1:B:552:ARG:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:58:ALA:C	1:E:60:GLY:H	2.22	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
1:C:131:LEU:HD11	1:C:179:ALA:HB1	1.97	0.45
1:F:305:MET:HE2	1:F:337:VAL:HG23	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:59:ASP:OD1	1:G:59:ASP:C	2.59	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:471:TYR:OH	1:C:665:ASP:OD1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:551:GLN:O	1:A:552:ARG:C	2.61	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
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:D:505:MET:HE1	1:D:545:PHE:CZ	2.52	0.43
1:F:318:PRO:HB2	1:F:327:LEU:HD22	1.99	0.43
1:H:551:GLN:O	1:H:552:ARG:C	2.61	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:A:305:MET:HE1	1:A:335:GLY:O	2.19	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:E:72:ASP:C	1:E:73:MET:HG3	2.42	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:H:124:ASP:CG	1:H:126:THR:HG22	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:58:ALA:C	1:E:60:GLY:N	2.77	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: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:305:MET:HE2	1:A:305:MET:HB2	1.99	0.42
1:A:549:VAL:HG11	1:A:660:ILE:HG12	2.02	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:MET:HE2	1:G:73:MET:HB3	1.79	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:A:137:ASP:OD2	1:A:137:ASP:C	2.63	0.41
1:B:333:GLU:HG2	7:B:1087:HOH:O	2.19	0.41
1:B:364:HIS:ND1	1:B:365:PRO:HD2	2.36	0.41
1:F:45:GLU:HG2	1:F:46:GLU:CD	2.45	0.41
1:H:358:LEU:CD1	1:H:372:ALA:HB1	2.49	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:F:73:MET:HE2	1:F:73:MET:HB2	1.92	0.41
1:B:46:GLU:N	1:B:46:GLU:CD	2.78	0.41
1:C:177:LYS:HB2	2:C:707:SO4:O1	2.20	0.41
1:C:551:GLN:O	1:C:552:ARG:C	2.62	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:G:551:GLN:O	1:G:552:ARG:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:70:TRP:CD1	1:F:70:TRP:C	2.99	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: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: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
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:73:MET:HE3	1:H:73:MET:HB2	1.87	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 ⓘ

5.3.1 Protein backbone ⓘ

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
All	All	5157/5528 (93%)	5007 (97%)	150 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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%)	503 (99%)	6 (1%)	63	70
1	B	509/568 (90%)	507 (100%)	2 (0%)	84	89
1	C	507/568 (89%)	504 (99%)	3 (1%)	78	85
1	D	504/568 (89%)	499 (99%)	5 (1%)	68	75
1	E	505/568 (89%)	496 (98%)	9 (2%)	51	58
1	F	496/568 (87%)	490 (99%)	6 (1%)	63	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	469/568 (83%)	464 (99%)	5 (1%)	65	73
1	H	486/568 (86%)	478 (98%)	8 (2%)	55	62
All	All	3985/4544 (88%)	3941 (99%)	44 (1%)	65	73

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	118	ASP
1	A	122	SER
1	A	333	GLU
1	A	394	THR
1	A	561	SER
1	B	171	SER
1	B	387	SER
1	C	178	ARG
1	C	351	VAL
1	C	668	LEU
1	D	11	LEU
1	D	93	ARG
1	D	122	SER
1	D	186	VAL
1	D	468	SER
1	E	62	VAL
1	E	93	ARG
1	E	186	VAL
1	E	236	LEU
1	E	242	THR
1	E	284	GLU
1	E	408	VAL
1	E	513	SER
1	E	626	LYS
1	F	11	LEU
1	F	236	LEU
1	F	284	GLU
1	F	322	SER
1	F	434	GLU
1	F	482	HIS
1	G	118	ASP
1	G	289	THR
1	G	327	LEU

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Mol	Chain	Res	Type
1	G	363	ILE
1	G	482	HIS
1	H	23	SER
1	H	50	ARG
1	H	122	SER
1	H	171	SER
1	H	349	VAL
1	H	394	THR
1	H	407	VAL
1	H	579	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	220	ASN
1	A	597	HIS
1	B	102	ASN
1	B	220	ASN
1	B	246	ASN
1	B	426	GLN
1	C	426	GLN
1	E	48	GLN
1	E	102	ASN
1	E	220	ASN
1	F	426	GLN
1	G	28	HIS
1	G	102	ASN
1	G	300	HIS
1	G	338	ASN
1	G	426	GLN
1	G	461	HIS
1	H	102	ASN
1	H	278	HIS
1	H	300	HIS
1	H	426	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	B	705	-	4,4,4	0.26	0	6,6,6	0.23	0
2	SO4	G	703	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	E	701	-	4,4,4	0.29	0	6,6,6	0.33	0
2	SO4	B	706	-	4,4,4	0.28	0	6,6,6	0.17	0
4	GOL	C	711	-	5,5,5	0.99	0	5,5,5	0.96	0
2	SO4	A	702	3	4,4,4	0.26	0	6,6,6	0.49	0
2	SO4	E	703	-	4,4,4	0.26	0	6,6,6	0.27	0
5	ALA	G	709	-	5,5,5	1.08	1 (20%)	6,6,6	1.69	2 (33%)
4	GOL	G	708	-	5,5,5	0.83	0	5,5,5	1.22	0
2	SO4	H	708	-	4,4,4	0.22	0	6,6,6	0.18	0
4	GOL	D	712	-	5,5,5	0.91	0	5,5,5	1.04	0
5	ALA	B	719	-	5,5,5	1.36	1 (20%)	6,6,6	1.68	2 (33%)
5	ALA	E	715	-	5,5,5	1.67	1 (20%)	6,6,6	1.09	1 (16%)
2	SO4	H	705	-	4,4,4	0.41	0	6,6,6	0.16	0
4	GOL	F	708	-	5,5,5	1.02	0	5,5,5	1.01	0
2	SO4	D	707	-	4,4,4	0.38	0	6,6,6	0.29	0
2	SO4	E	704	-	4,4,4	0.33	0	6,6,6	0.34	0
2	SO4	B	708	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	C	705	-	4,4,4	0.27	0	6,6,6	0.11	0
4	GOL	E	713	-	5,5,5	0.65	0	5,5,5	1.19	0
4	GOL	B	717	-	5,5,5	1.23	1 (20%)	5,5,5	1.22	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	702	-	4,4,4	0.15	0	6,6,6	0.32	0
4	GOL	F	710	-	5,5,5	1.02	0	5,5,5	1.07	0
2	SO4	G	702	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	E	702	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	G	705	-	4,4,4	0.27	0	6,6,6	0.25	0
4	GOL	C	709	-	5,5,5	0.96	0	5,5,5	0.87	0
2	SO4	C	704	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	E	709	-	4,4,4	0.39	0	6,6,6	0.35	0
2	SO4	B	710	-	4,4,4	0.29	0	6,6,6	0.16	0
4	GOL	F	711	-	5,5,5	0.83	0	5,5,5	1.16	0
5	ALA	H	712	-	5,5,5	1.31	1 (20%)	6,6,6	1.12	1 (16%)
4	GOL	F	709	-	5,5,5	0.99	0	5,5,5	1.05	0
2	SO4	A	703	-	4,4,4	0.20	0	6,6,6	0.26	0
6	FLC	A	717	-	12,12,12	2.10	6 (50%)	17,17,17	2.24	6 (35%)
2	SO4	H	704	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	B	711	-	4,4,4	0.29	0	6,6,6	0.16	0
2	SO4	H	703	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	D	704	-	4,4,4	0.30	0	6,6,6	0.12	0
2	SO4	A	705	-	4,4,4	0.30	0	6,6,6	0.35	0
2	SO4	C	702	-	4,4,4	0.26	0	6,6,6	0.35	0
5	ALA	D	714	-	5,5,5	2.03	2 (40%)	6,6,6	1.40	2 (33%)
2	SO4	F	701	-	4,4,4	0.31	0	6,6,6	0.31	0
5	ALA	F	713	-	5,5,5	1.55	1 (20%)	6,6,6	1.55	2 (33%)
5	ALA	A	716	3	5,5,5	1.90	2 (40%)	6,6,6	1.63	1 (16%)
4	GOL	G	707	-	5,5,5	0.62	0	5,5,5	1.52	1 (20%)
2	SO4	C	707	-	4,4,4	0.20	0	6,6,6	0.28	0
2	SO4	C	706	-	4,4,4	0.28	0	6,6,6	0.26	0
2	SO4	E	707	-	4,4,4	0.25	0	6,6,6	0.29	0
2	SO4	G	701	-	4,4,4	0.26	0	6,6,6	0.50	0
4	GOL	F	712	-	5,5,5	1.13	0	5,5,5	0.89	0
2	SO4	B	709	3	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	E	705	-	4,4,4	0.27	0	6,6,6	0.35	0
4	GOL	D	711	-	5,5,5	1.07	0	5,5,5	1.28	1 (20%)
2	SO4	H	702	-	4,4,4	0.30	0	6,6,6	0.26	0
2	SO4	A	701	-	4,4,4	0.43	0	6,6,6	0.24	0
2	SO4	D	703	-	4,4,4	0.34	0	6,6,6	0.30	0
2	SO4	F	704	-	4,4,4	0.27	0	6,6,6	0.28	0
4	GOL	A	713	-	5,5,5	1.43	1 (20%)	5,5,5	0.79	0
2	SO4	A	708	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	B	707	-	4,4,4	0.29	0	6,6,6	0.18	0
6	FLC	H	713	-	12,12,12	2.00	6 (50%)	17,17,17	2.07	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	F	702	-	4,4,4	0.20	0	6,6,6	0.50	0
2	SO4	H	709	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	C	701	-	4,4,4	0.23	0	6,6,6	0.21	0
2	SO4	B	704	-	4,4,4	0.34	0	6,6,6	0.17	0
2	SO4	E	706	-	4,4,4	0.27	0	6,6,6	0.12	0
4	GOL	E	714	-	5,5,5	0.78	0	5,5,5	1.06	0
2	SO4	C	703	-	4,4,4	0.34	0	6,6,6	0.20	0
2	SO4	E	708	-	4,4,4	0.24	0	6,6,6	0.56	0
2	SO4	B	702	-	4,4,4	0.26	0	6,6,6	0.30	0
2	SO4	A	707	-	4,4,4	0.24	0	6,6,6	0.30	0
4	GOL	A	715	-	5,5,5	1.23	1 (20%)	5,5,5	1.10	1 (20%)
2	SO4	A	704	-	4,4,4	0.32	0	6,6,6	0.21	0
2	SO4	G	704	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	H	707	-	4,4,4	0.30	0	6,6,6	0.11	0
4	GOL	D	713	-	5,5,5	1.00	0	5,5,5	1.00	0
2	SO4	D	705	-	4,4,4	0.38	0	6,6,6	0.28	0
2	SO4	B	703	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	D	708	-	4,4,4	0.24	0	6,6,6	0.21	0
4	GOL	A	714	-	5,5,5	0.90	0	5,5,5	1.24	1 (20%)
4	GOL	D	710	-	5,5,5	1.04	1 (20%)	5,5,5	1.24	1 (20%)
2	SO4	D	701	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	F	707	-	4,4,4	0.31	0	6,6,6	0.14	0
4	GOL	C	710	-	5,5,5	1.31	1 (20%)	5,5,5	1.19	1 (20%)
4	GOL	B	718	-	5,5,5	1.06	0	5,5,5	1.16	0
2	SO4	B	712	-	4,4,4	0.26	0	6,6,6	0.12	0
4	GOL	E	712	-	5,5,5	0.84	0	5,5,5	1.30	0
2	SO4	F	706	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	D	706	-	4,4,4	0.35	0	6,6,6	0.27	0
4	GOL	H	711	-	5,5,5	0.80	0	5,5,5	1.18	1 (20%)
2	SO4	H	701	-	4,4,4	0.25	0	6,6,6	0.31	0
5	ALA	C	713	-	5,5,5	1.29	1 (20%)	6,6,6	1.59	2 (33%)
2	SO4	B	701	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	F	705	-	4,4,4	0.30	0	6,6,6	0.23	0
2	SO4	H	706	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	A	706	-	4,4,4	0.27	0	6,6,6	0.33	0
4	GOL	C	712	-	5,5,5	0.87	0	5,5,5	1.11	0
2	SO4	F	703	3	4,4,4	0.29	0	6,6,6	0.16	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	F	710	-	-	4/4/4/4	-
5	ALA	A	716	3	-	0/4/4/4	-
4	GOL	G	707	-	-	4/4/4/4	-
4	GOL	A	715	-	-	4/4/4/4	-
4	GOL	D	713	-	-	1/4/4/4	-
4	GOL	C	709	-	-	3/4/4/4	-
4	GOL	F	712	-	-	0/4/4/4	-
4	GOL	D	711	-	-	2/4/4/4	-
4	GOL	D	710	-	-	1/4/4/4	-
4	GOL	A	714	-	-	4/4/4/4	-
4	GOL	C	711	-	-	3/4/4/4	-
4	GOL	C	710	-	-	2/4/4/4	-
4	GOL	F	711	-	-	2/4/4/4	-
4	GOL	B	718	-	-	0/4/4/4	-
5	ALA	G	709	-	-	4/4/4/4	-
4	GOL	G	708	-	-	4/4/4/4	-
4	GOL	A	713	-	-	0/4/4/4	-
5	ALA	H	712	-	-	1/4/4/4	-
4	GOL	D	712	-	-	2/4/4/4	-
4	GOL	F	709	-	-	3/4/4/4	-
6	FLC	A	717	-	-	7/16/16/16	-
5	ALA	B	719	-	-	0/4/4/4	-
5	ALA	E	715	-	-	4/4/4/4	-
4	GOL	E	712	-	-	3/4/4/4	-
6	FLC	H	713	-	-	9/16/16/16	-
4	GOL	H	711	-	-	4/4/4/4	-
4	GOL	F	708	-	-	4/4/4/4	-
4	GOL	E	714	-	-	4/4/4/4	-
5	ALA	C	713	-	-	4/4/4/4	-
4	GOL	E	713	-	-	2/4/4/4	-
5	ALA	D	714	-	-	3/4/4/4	-
4	GOL	B	717	-	-	2/4/4/4	-
4	GOL	C	712	-	-	2/4/4/4	-
5	ALA	F	713	-	-	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	3.36	1.33	1.22
5	D	714	ALA	CA-C	-3.28	1.50	1.54
6	H	713	FLC	OA1-CAC	3.12	1.32	1.22
6	A	717	FLC	OB1-CBC	3.09	1.31	1.22
6	A	717	FLC	CA-CB	3.04	1.57	1.54
6	H	713	FLC	OG1-CGC	3.01	1.31	1.22
6	H	713	FLC	OB1-CBC	3.00	1.31	1.22
5	A	716	ALA	OXT-C	-2.96	1.21	1.30
5	D	714	ALA	OXT-C	-2.86	1.21	1.30
6	H	713	FLC	OG2-CGC	-2.73	1.21	1.30
6	A	717	FLC	OG1-CGC	2.72	1.31	1.22
6	A	717	FLC	OG2-CGC	-2.60	1.22	1.30
5	A	716	ALA	CA-C	-2.52	1.51	1.54
4	C	710	GOL	O2-C2	-2.52	1.36	1.43
6	H	713	FLC	OA2-CAC	-2.50	1.22	1.30
5	E	715	ALA	OXT-C	-2.49	1.22	1.30
5	F	713	ALA	OXT-C	-2.43	1.22	1.30
5	C	713	ALA	OXT-C	-2.33	1.23	1.30
4	A	713	GOL	C1-C2	2.31	1.60	1.51
4	B	717	GOL	O2-C2	-2.30	1.36	1.43
4	A	715	GOL	O2-C2	-2.30	1.36	1.43
5	H	712	ALA	OXT-C	-2.24	1.23	1.30
5	B	719	ALA	OXT-C	-2.23	1.23	1.30
6	H	713	FLC	OB2-CBC	-2.20	1.22	1.30
4	D	710	GOL	C3-C2	2.13	1.59	1.51
5	G	709	ALA	OXT-C	-2.12	1.23	1.30
6	A	717	FLC	OB2-CBC	-2.05	1.23	1.30

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	713	FLC	OB2-CBC-CB	4.83	122.40	113.14
6	A	717	FLC	OB2-CBC-CB	4.49	121.76	113.14
6	A	717	FLC	OB1-CBC-CB	-4.35	113.67	122.09
6	H	713	FLC	OB1-CBC-CB	-4.30	113.76	122.09
6	A	717	FLC	OA1-CAC-CA	-3.40	113.31	122.95
5	G	709	ALA	OXT-C-O	-3.34	116.50	124.08
5	A	716	ALA	OXT-C-O	-3.30	116.58	124.08
6	A	717	FLC	OG1-CGC-CG	-3.18	113.96	122.95
5	C	713	ALA	OXT-C-O	-3.05	117.15	124.08
4	G	707	GOL	C3-C2-C1	-3.02	100.70	111.80
6	A	717	FLC	OA2-CAC-CA	2.91	123.56	114.35
6	A	717	FLC	OG2-CGC-CG	2.87	123.42	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	719	ALA	OXT-C-O	-2.86	117.59	124.08
6	H	713	FLC	OA1-CAC-CA	-2.83	114.93	122.95
5	F	713	ALA	OXT-C-CA	2.59	122.70	113.79
6	H	713	FLC	OG2-CGC-CG	2.54	122.41	114.35
6	H	713	FLC	OG1-CGC-CG	-2.43	116.06	122.95
5	G	709	ALA	OXT-C-CA	2.40	122.05	113.79
5	D	714	ALA	OXT-C-O	-2.40	118.64	124.08
5	H	712	ALA	OXT-C-O	-2.40	118.64	124.08
6	H	713	FLC	OA2-CAC-CA	2.39	121.92	114.35
5	C	713	ALA	OXT-C-CA	2.30	121.71	113.79
4	D	710	GOL	C3-C2-C1	-2.28	103.43	111.80
5	D	714	ALA	OXT-C-CA	2.27	121.62	113.79
5	F	713	ALA	OXT-C-O	-2.25	118.97	124.08
4	B	717	GOL	C3-C2-C1	-2.19	103.78	111.80
5	B	719	ALA	C-CA-N	2.15	115.54	107.93
4	A	714	GOL	C3-C2-C1	-2.15	103.91	111.80
5	E	715	ALA	OXT-C-O	-2.13	119.24	124.08
4	A	715	GOL	C3-C2-C1	-2.12	104.03	111.80
4	D	711	GOL	C3-C2-C1	-2.08	104.16	111.80
4	H	711	GOL	C3-C2-C1	-2.06	104.25	111.80
4	C	710	GOL	C3-C2-C1	-2.02	104.39	111.80

There are no chirality outliers.

All (94) 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	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

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Mol	Chain	Res	Type	Atoms
4	G	708	GOL	O2-C2-C3-O3
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	712	GOL	O1-C1-C2-C3
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	O-C-CA-CB
5	C	713	ALA	OXT-C-CA-CB
5	D	714	ALA	O-C-CA-CB
5	E	715	ALA	O-C-CA-CB

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

There are no ring outliers.

28 monomers are involved in 63 short contacts:

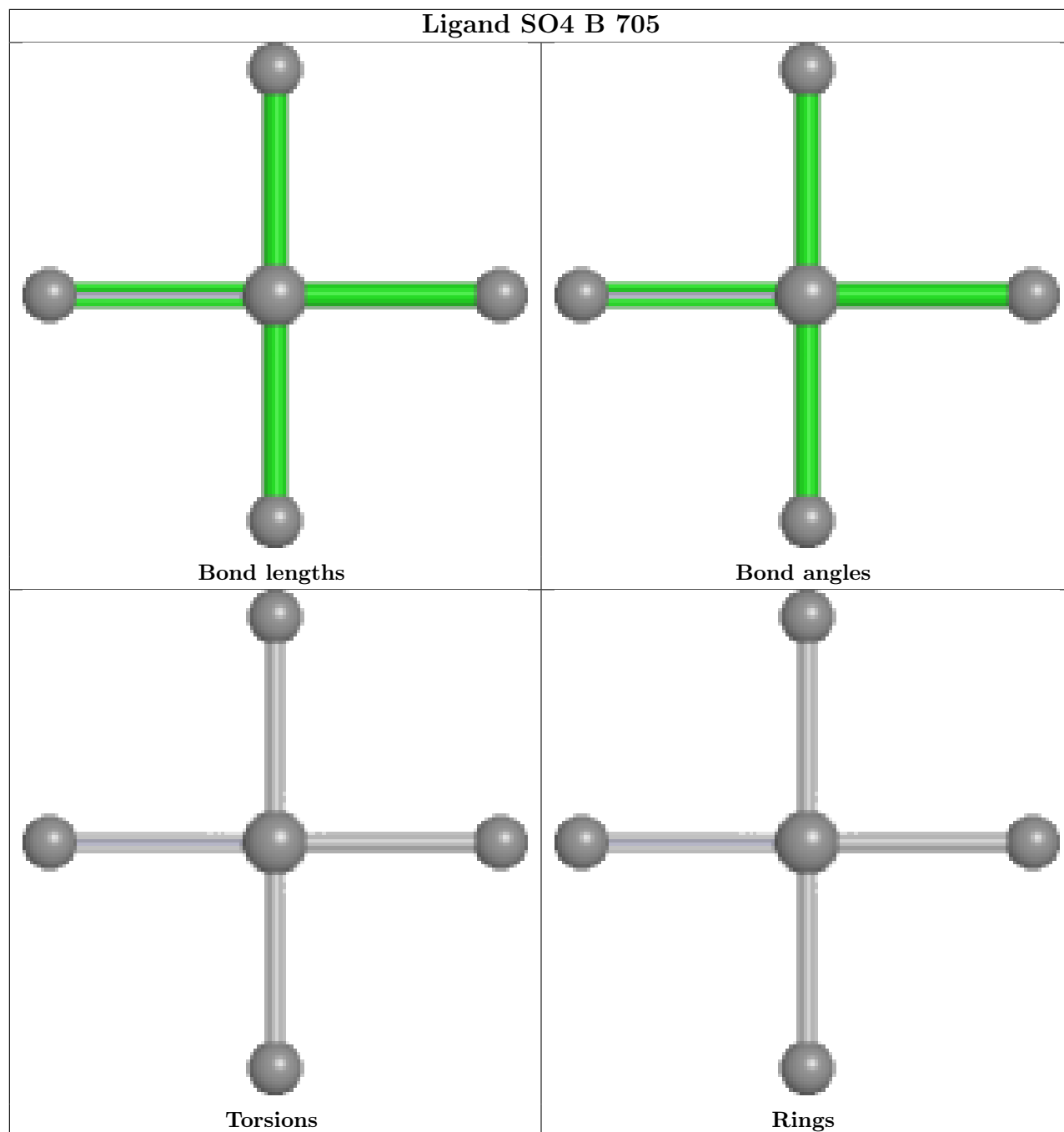
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	711	GOL	2	0

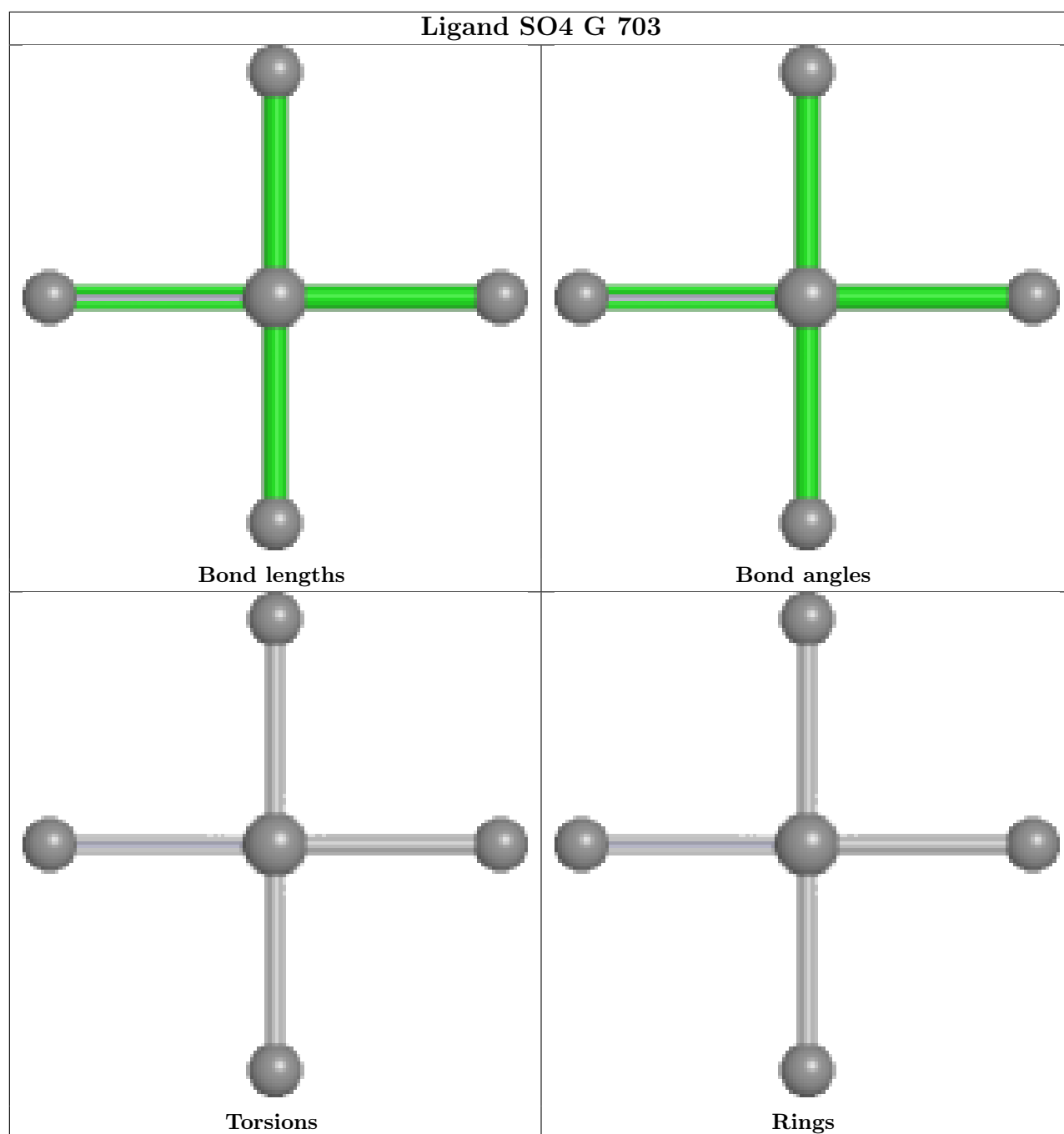
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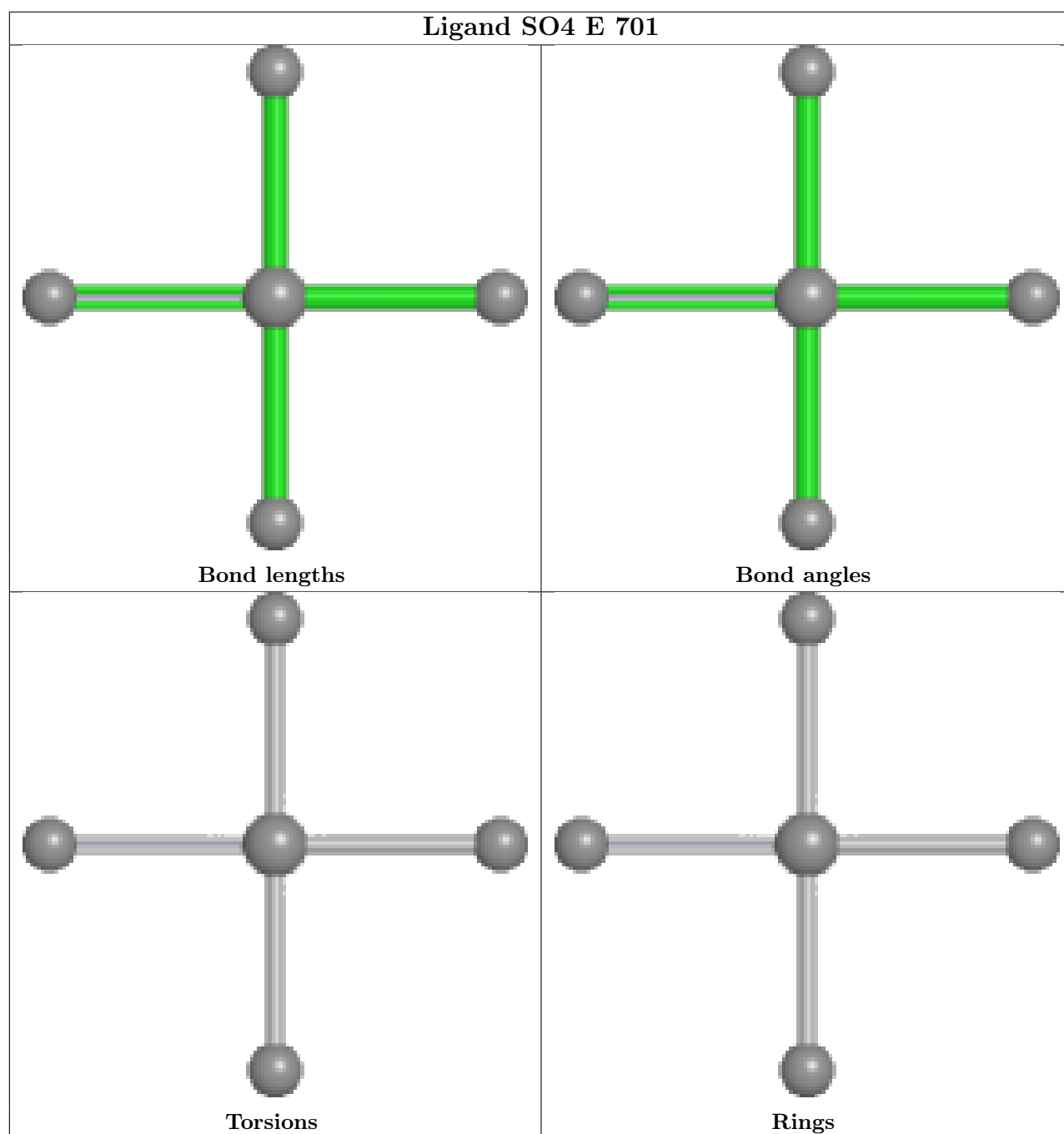
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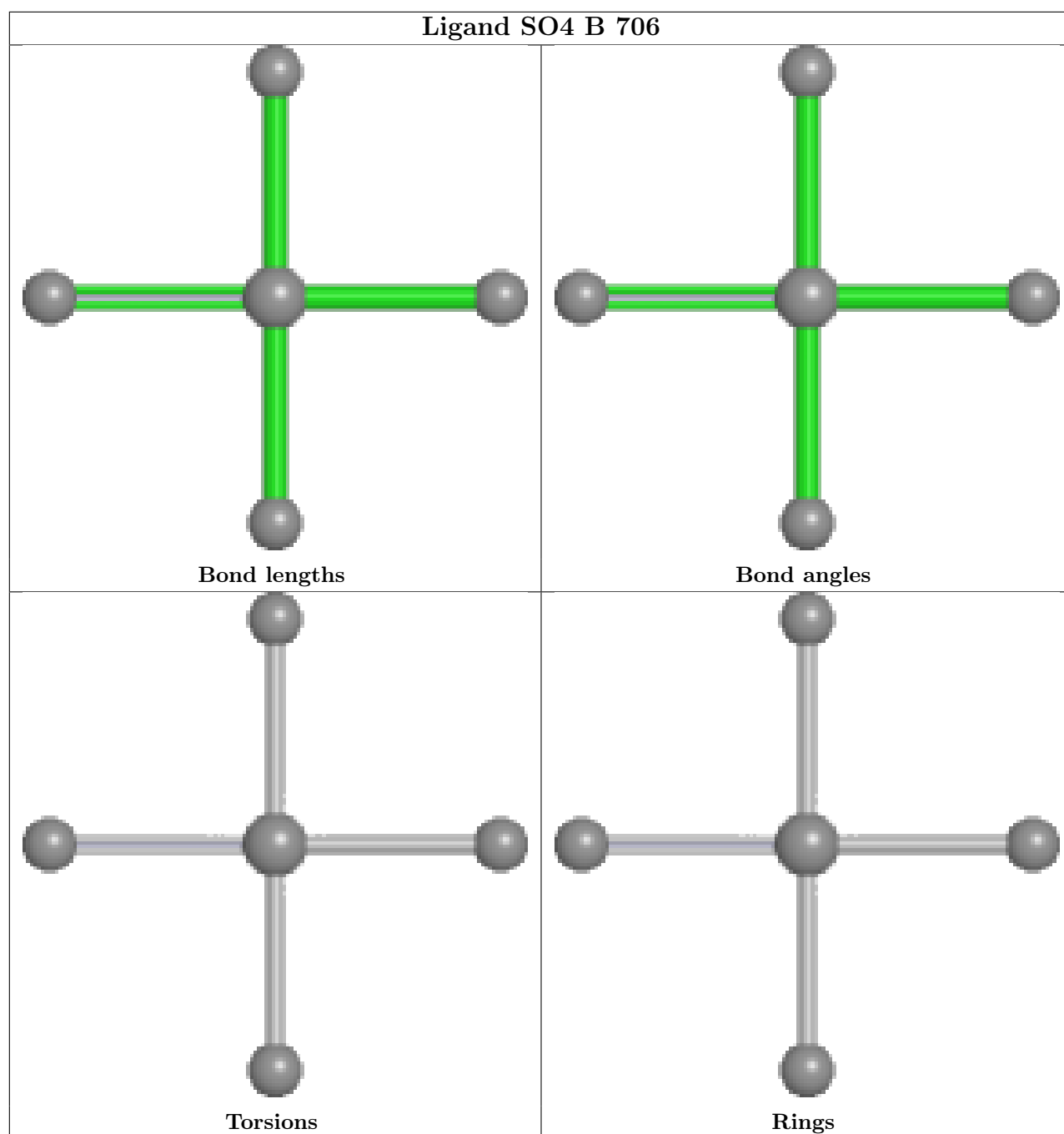
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	708	SO4	1	0
4	D	712	GOL	1	0
5	B	719	ALA	8	0
5	E	715	ALA	4	0
4	F	708	GOL	2	0
4	F	710	GOL	1	0
4	C	709	GOL	1	0
4	F	711	GOL	2	0
6	A	717	FLC	3	0
5	D	714	ALA	7	0
5	F	713	ALA	8	0
5	A	716	ALA	4	0
4	G	707	GOL	1	0
2	C	707	SO4	2	0
4	F	712	GOL	2	0
2	B	709	SO4	1	0
2	A	701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

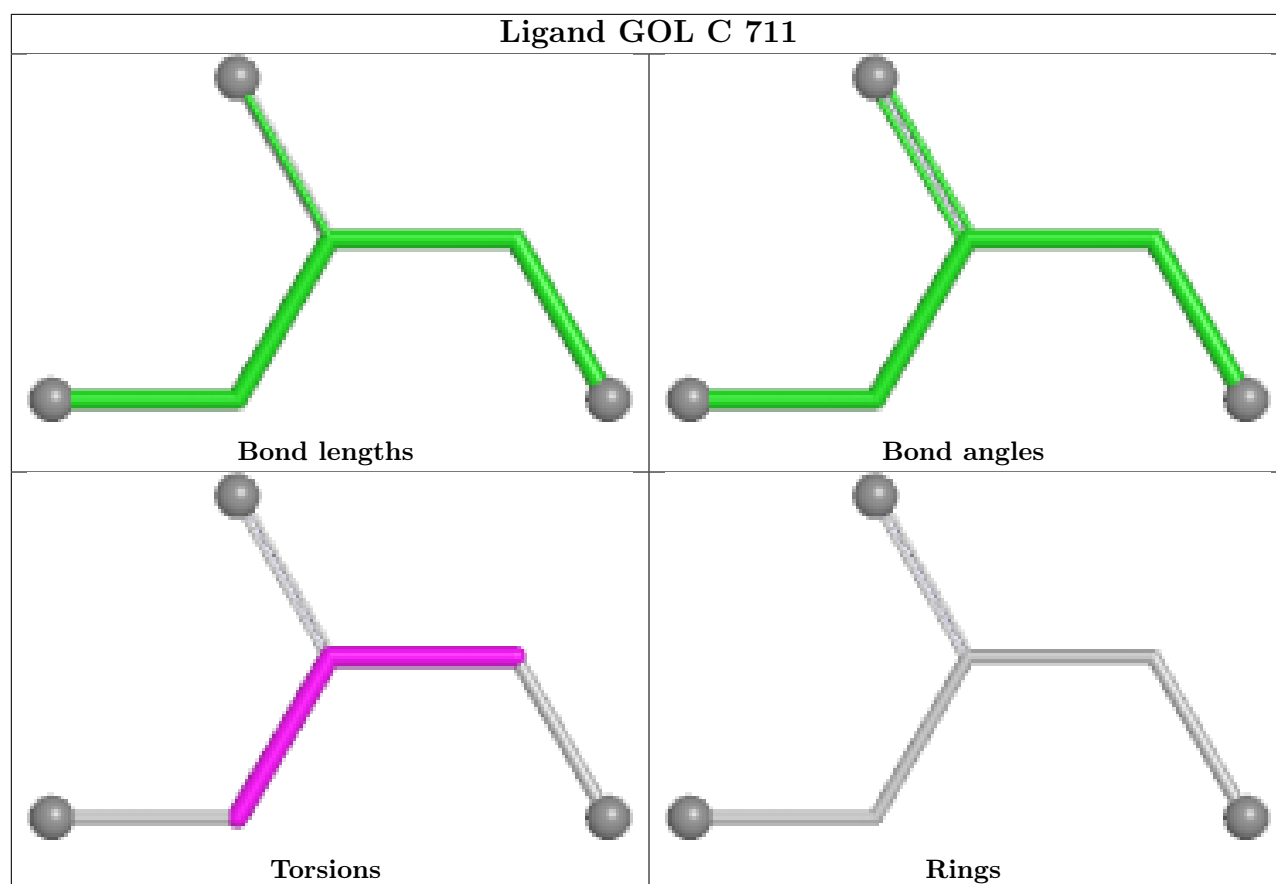
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

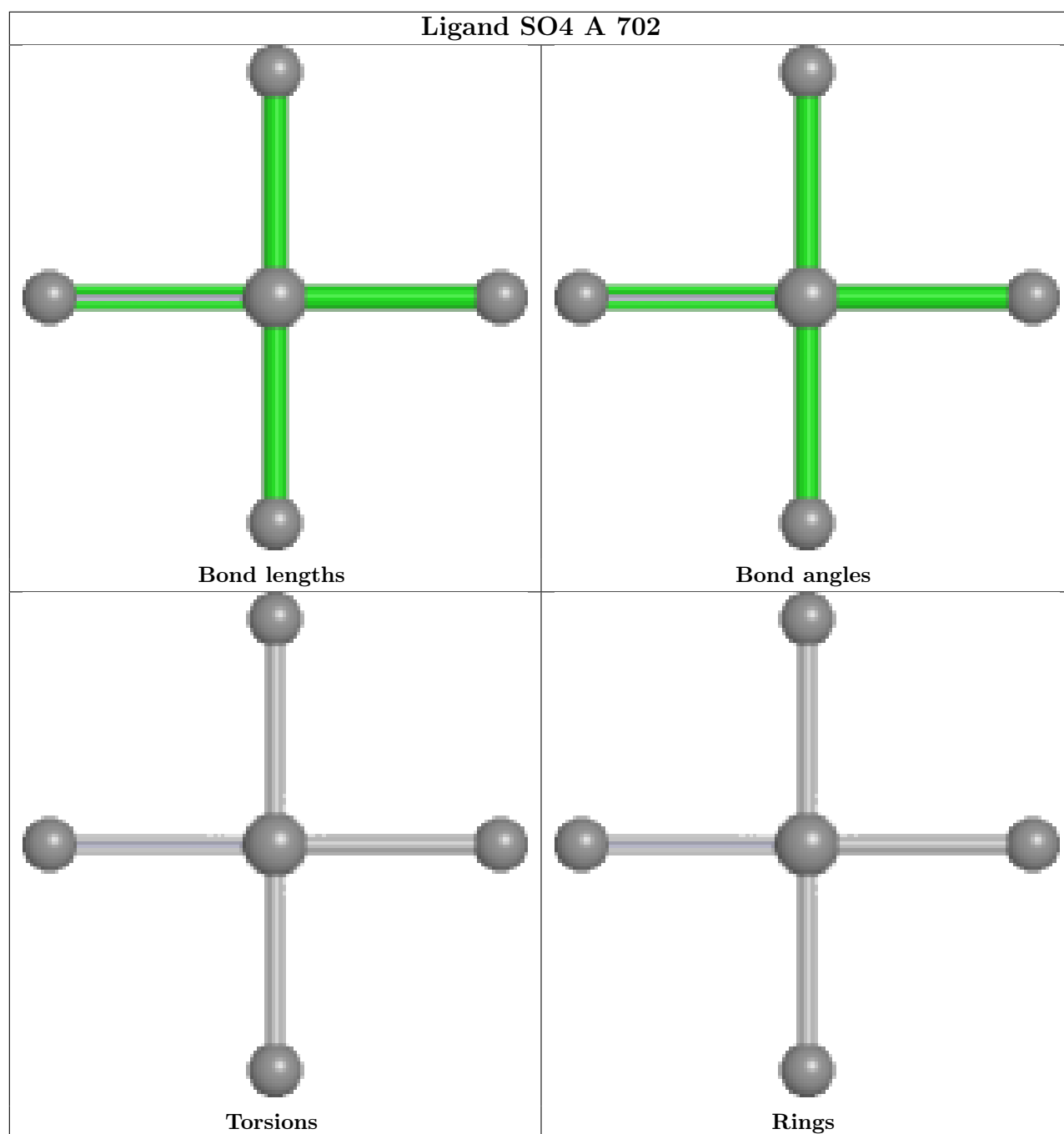


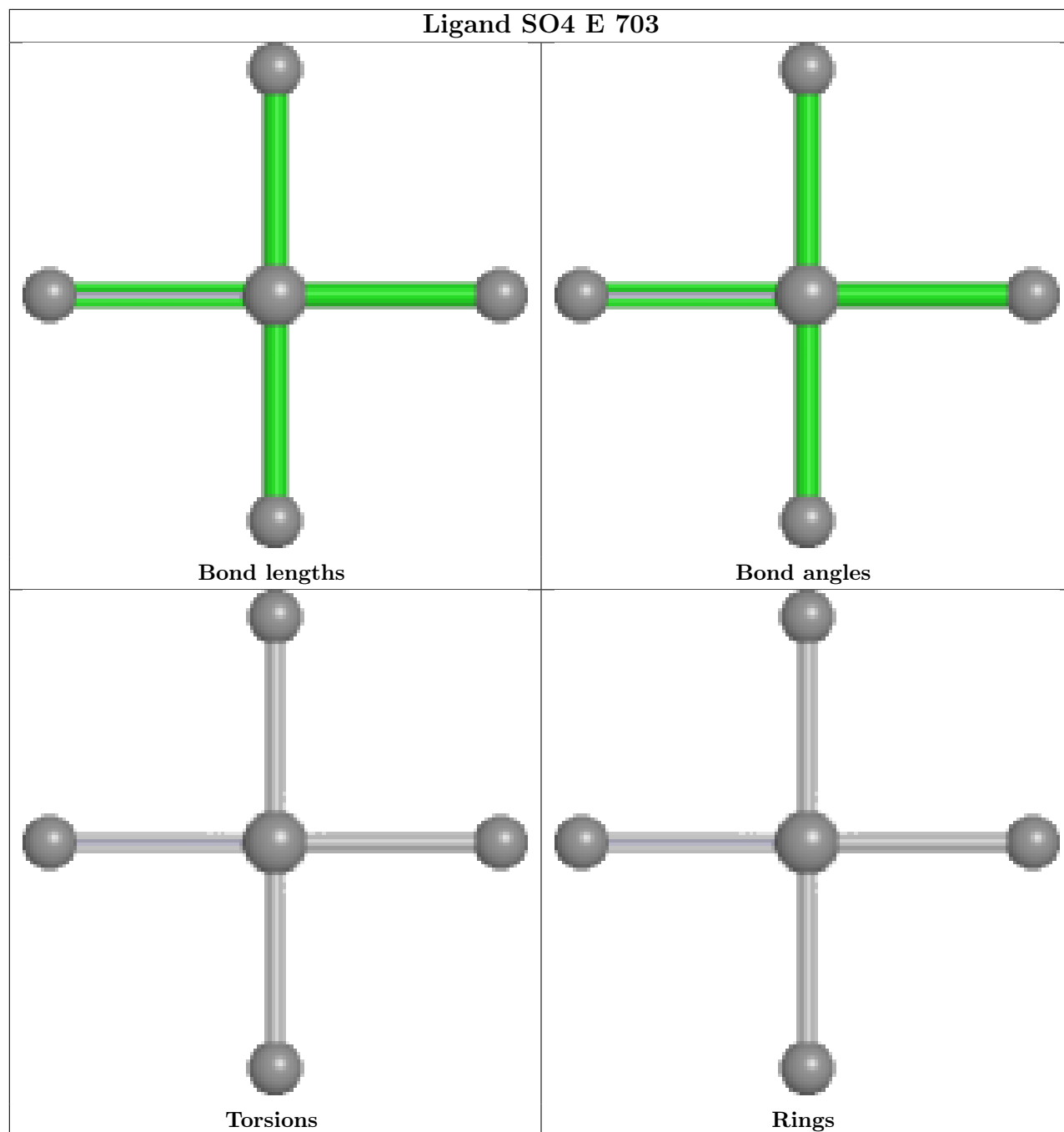


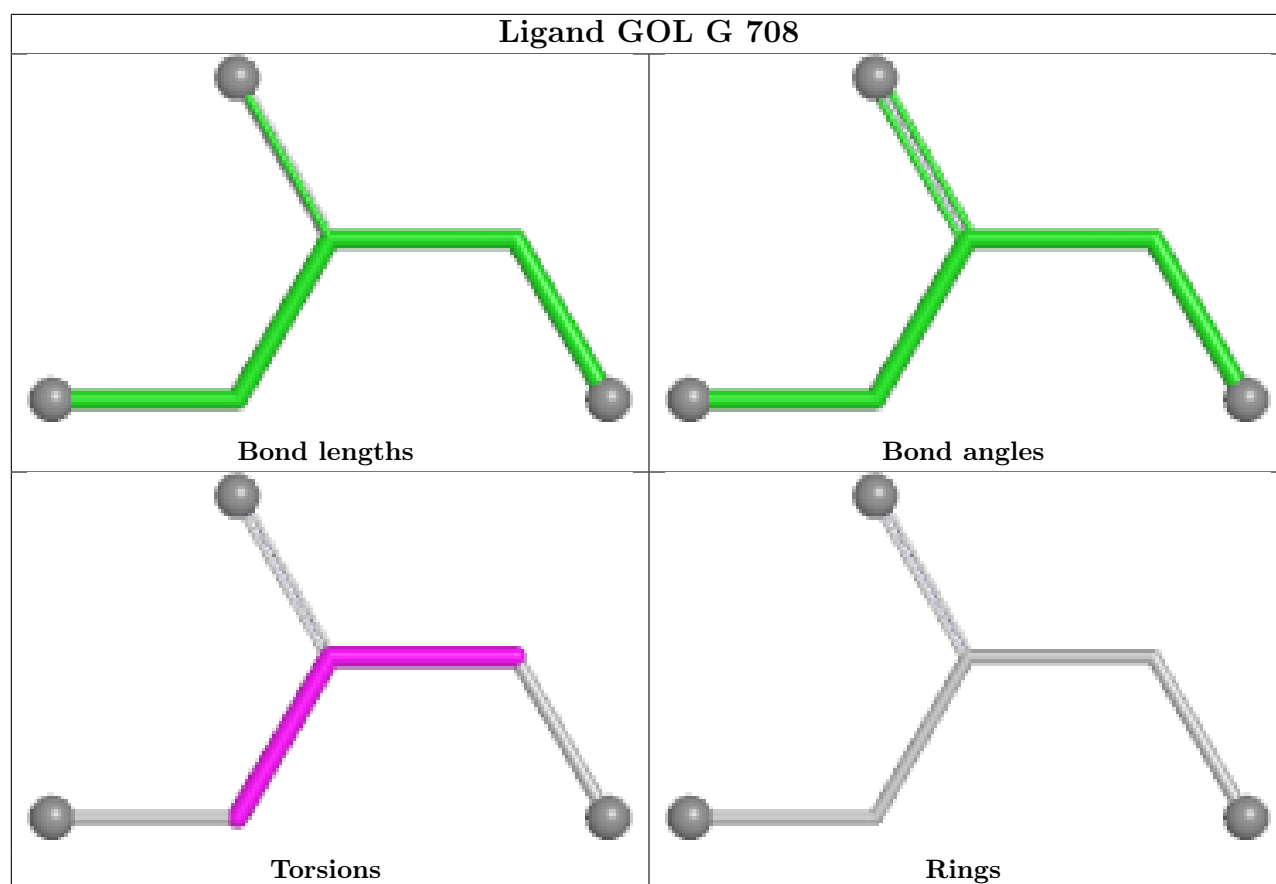


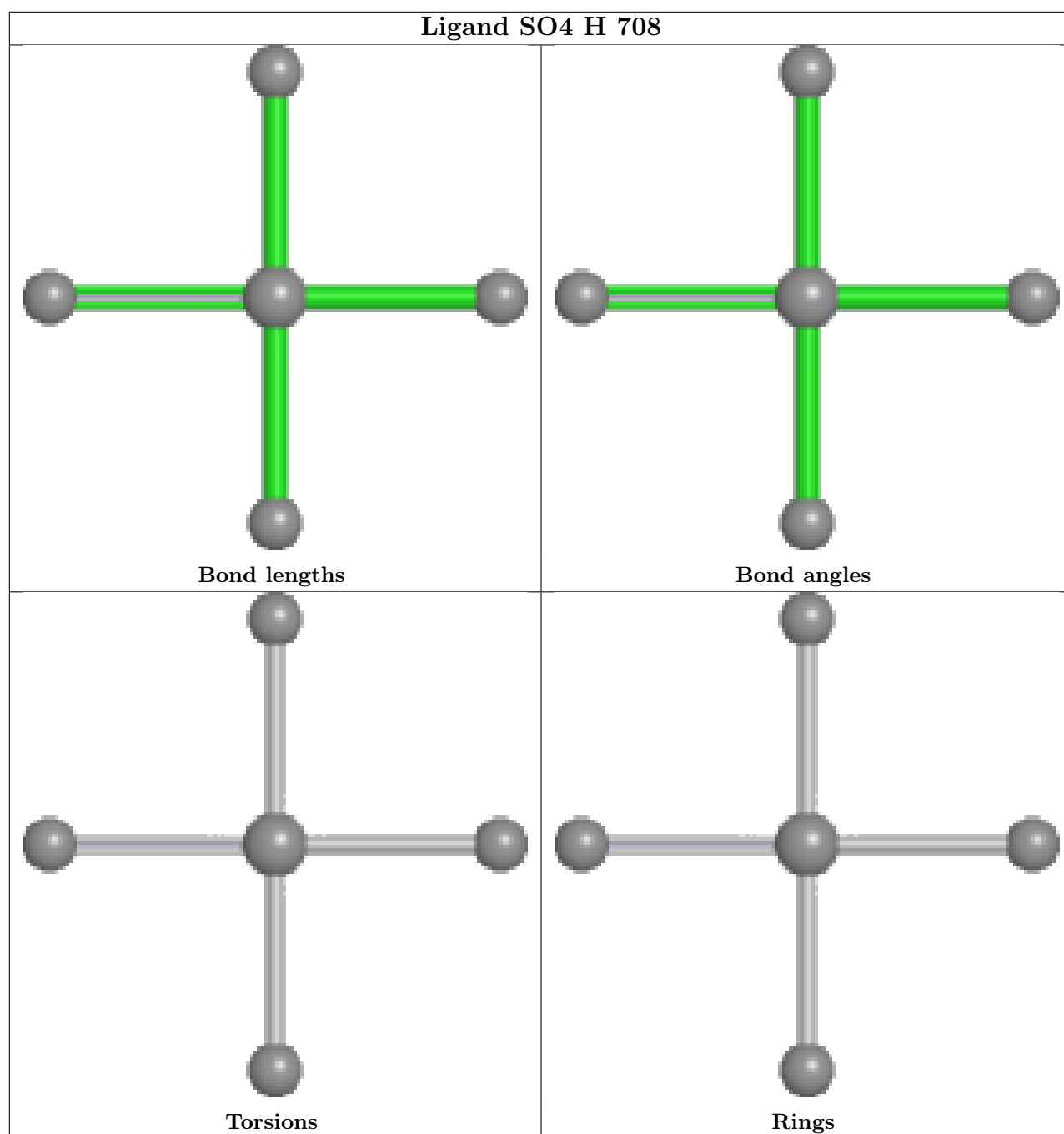


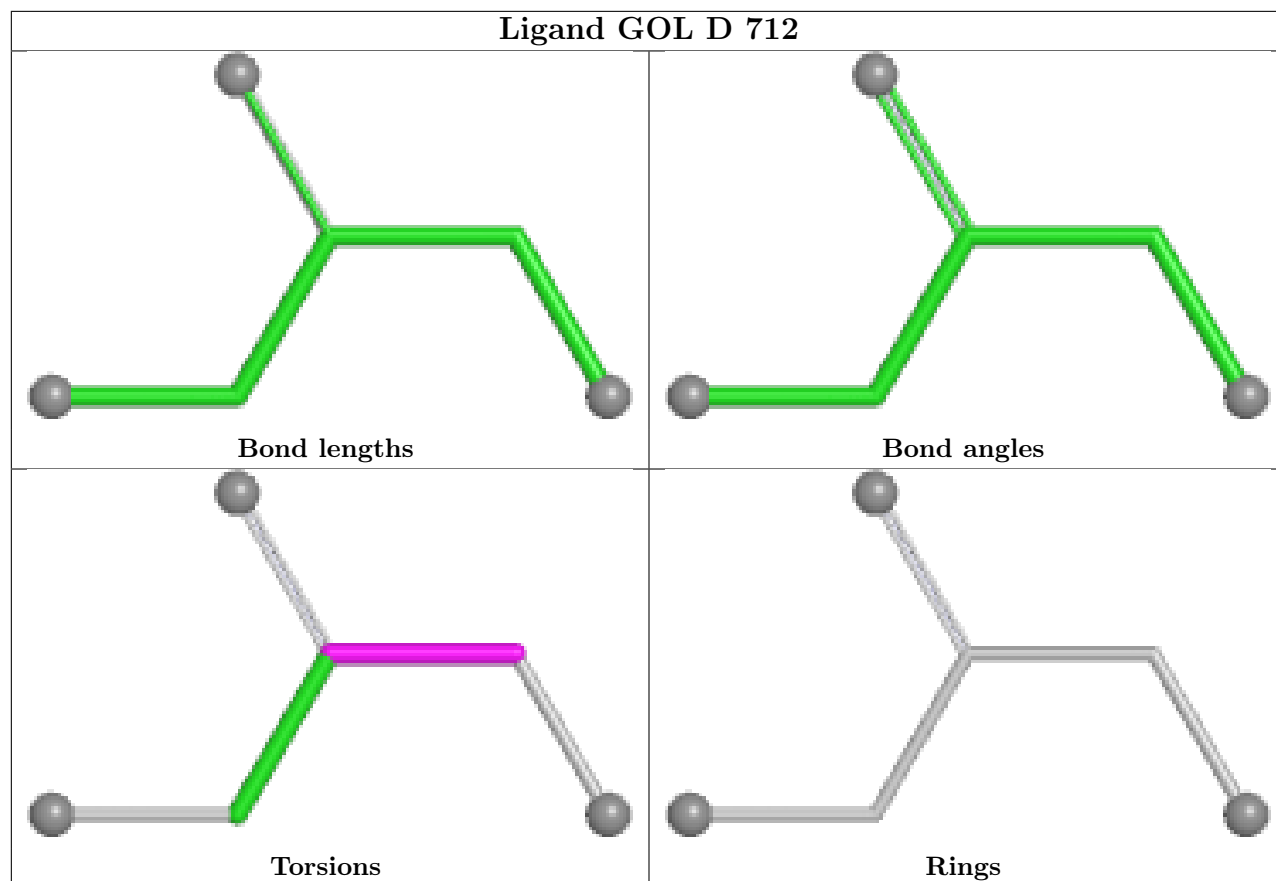


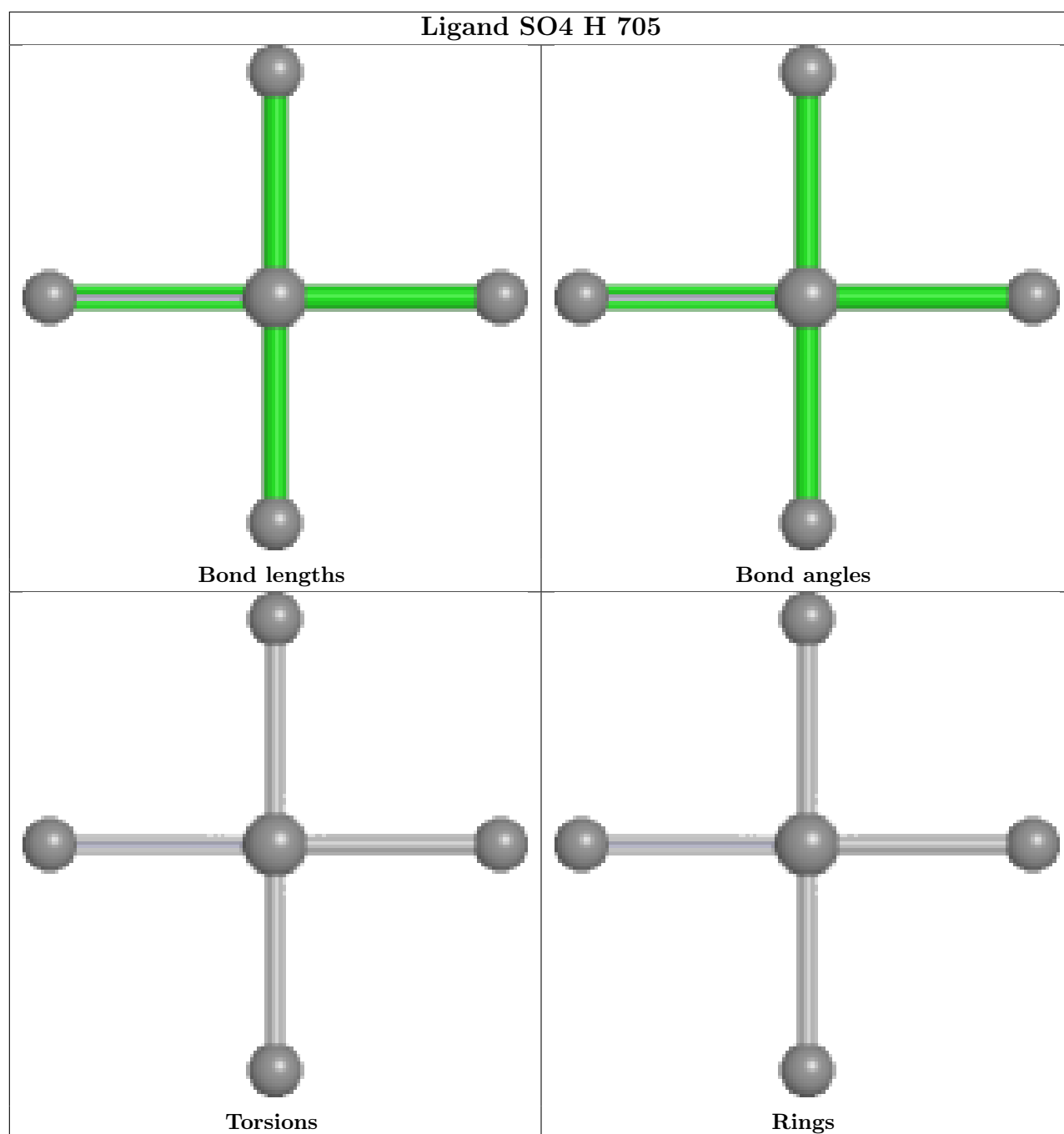


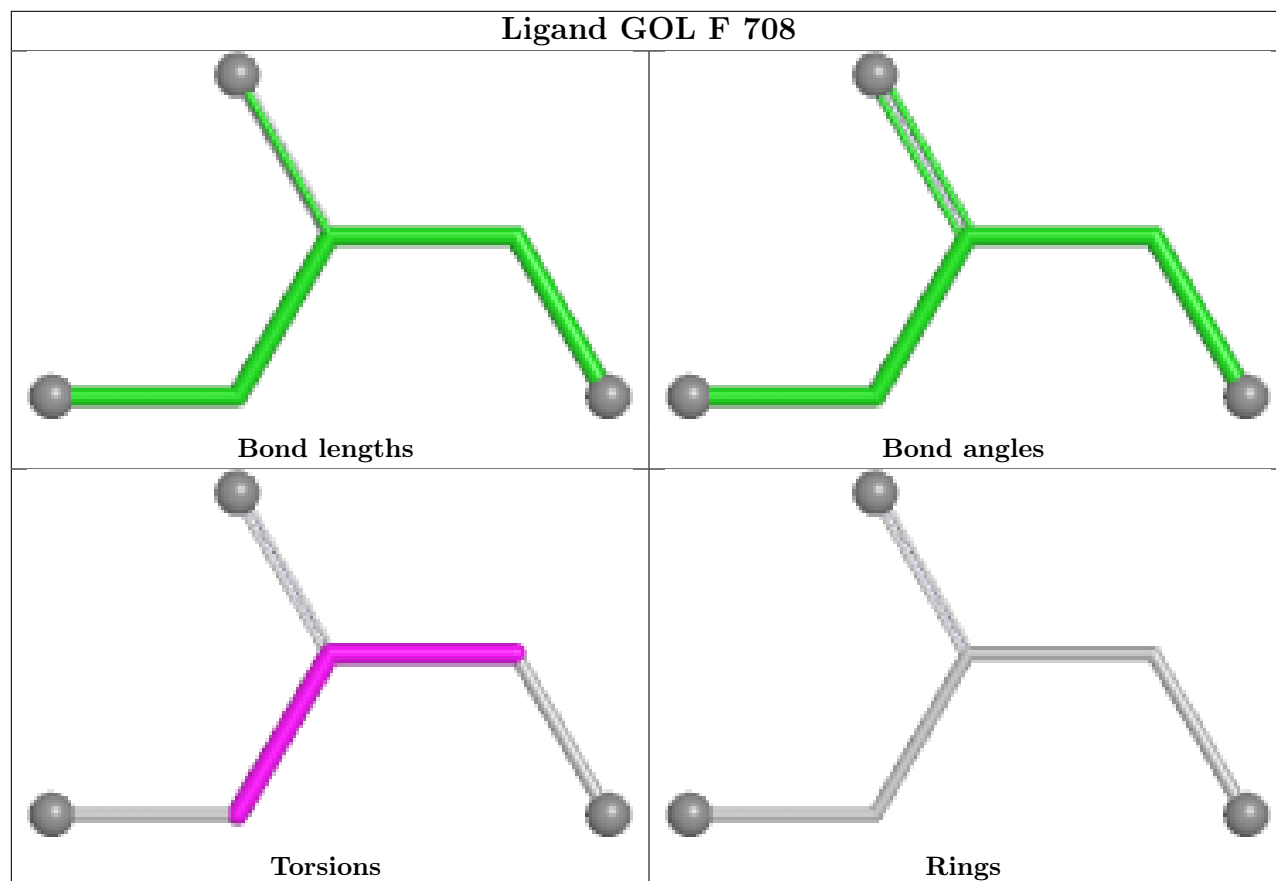


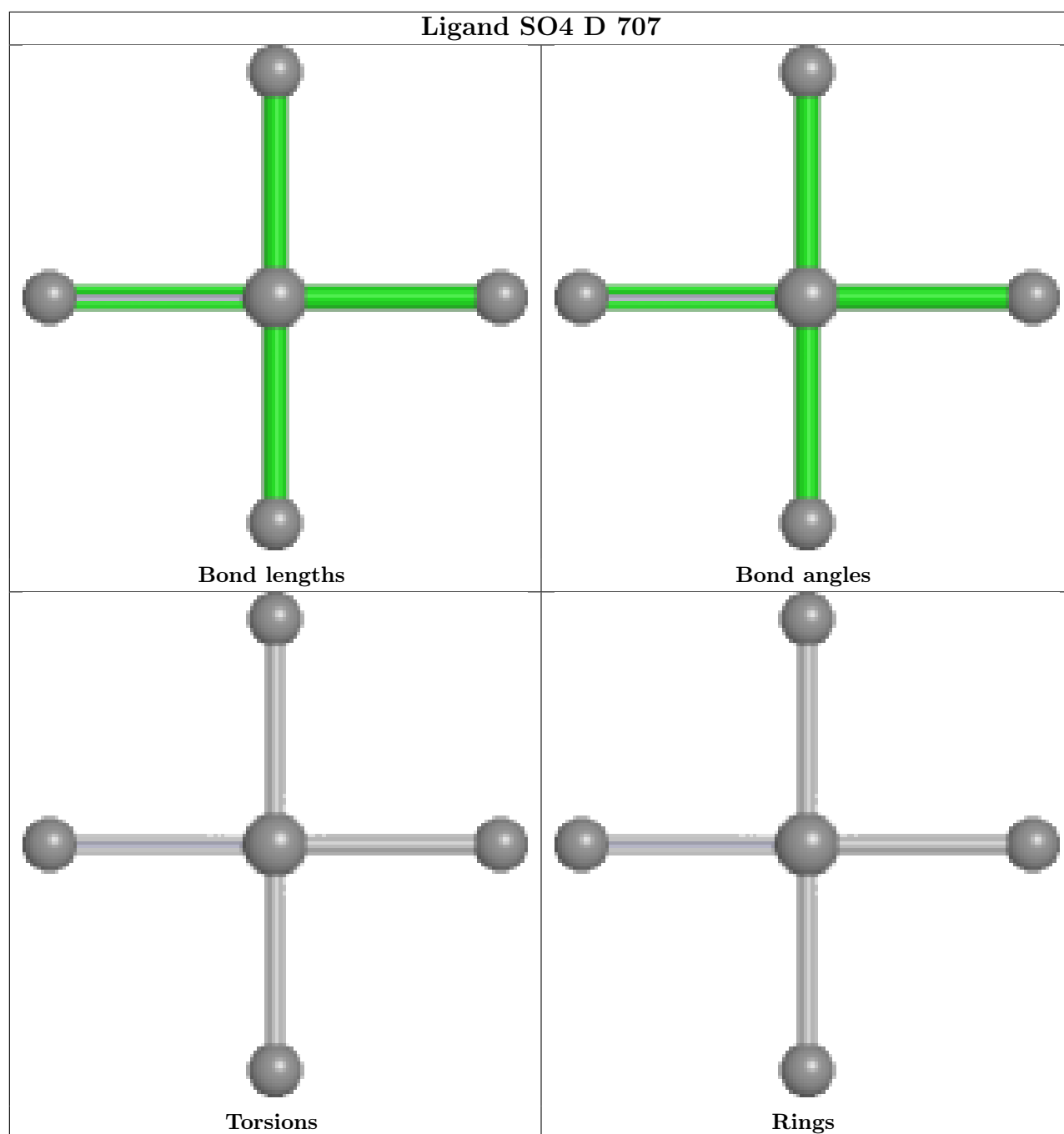


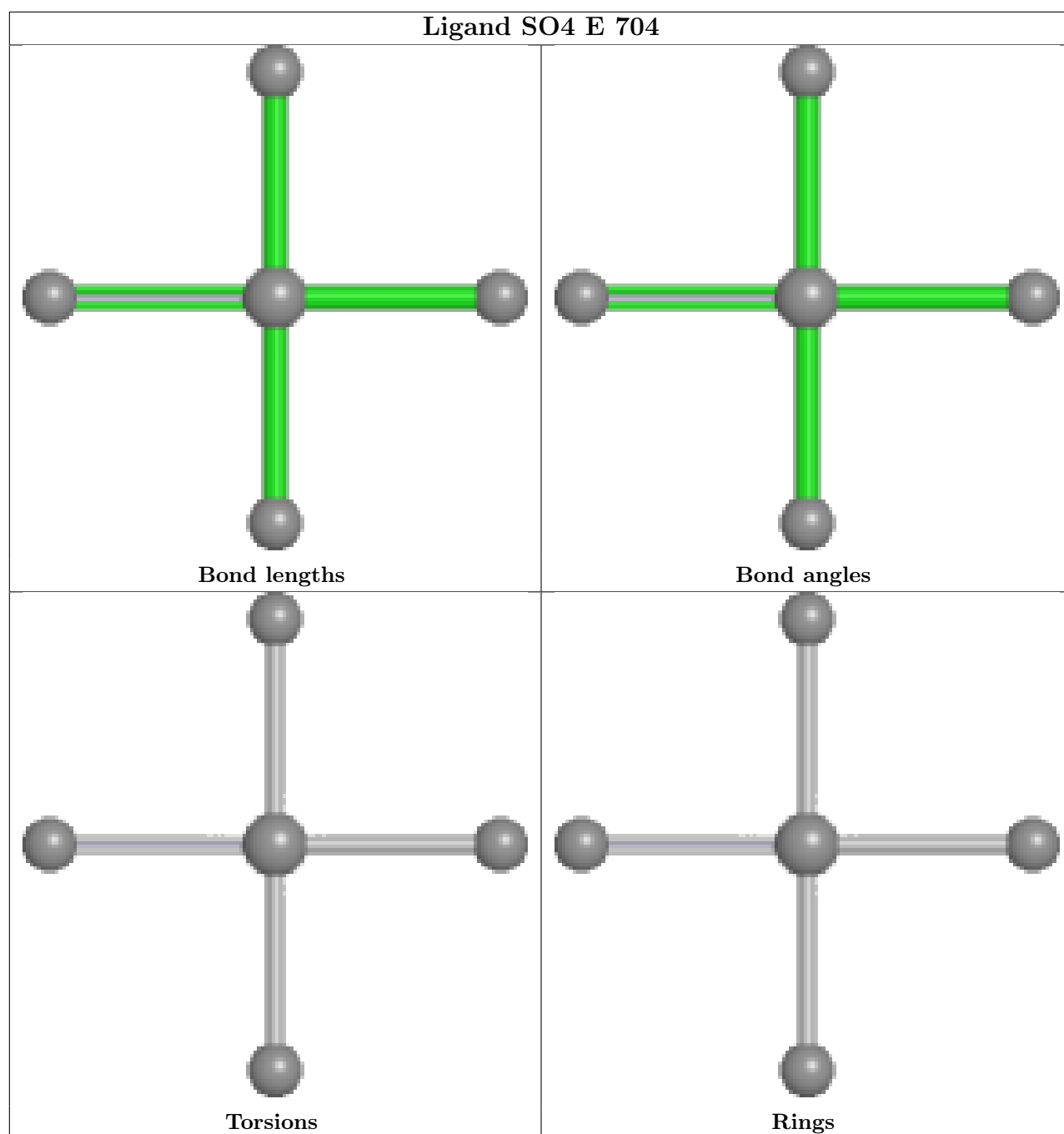


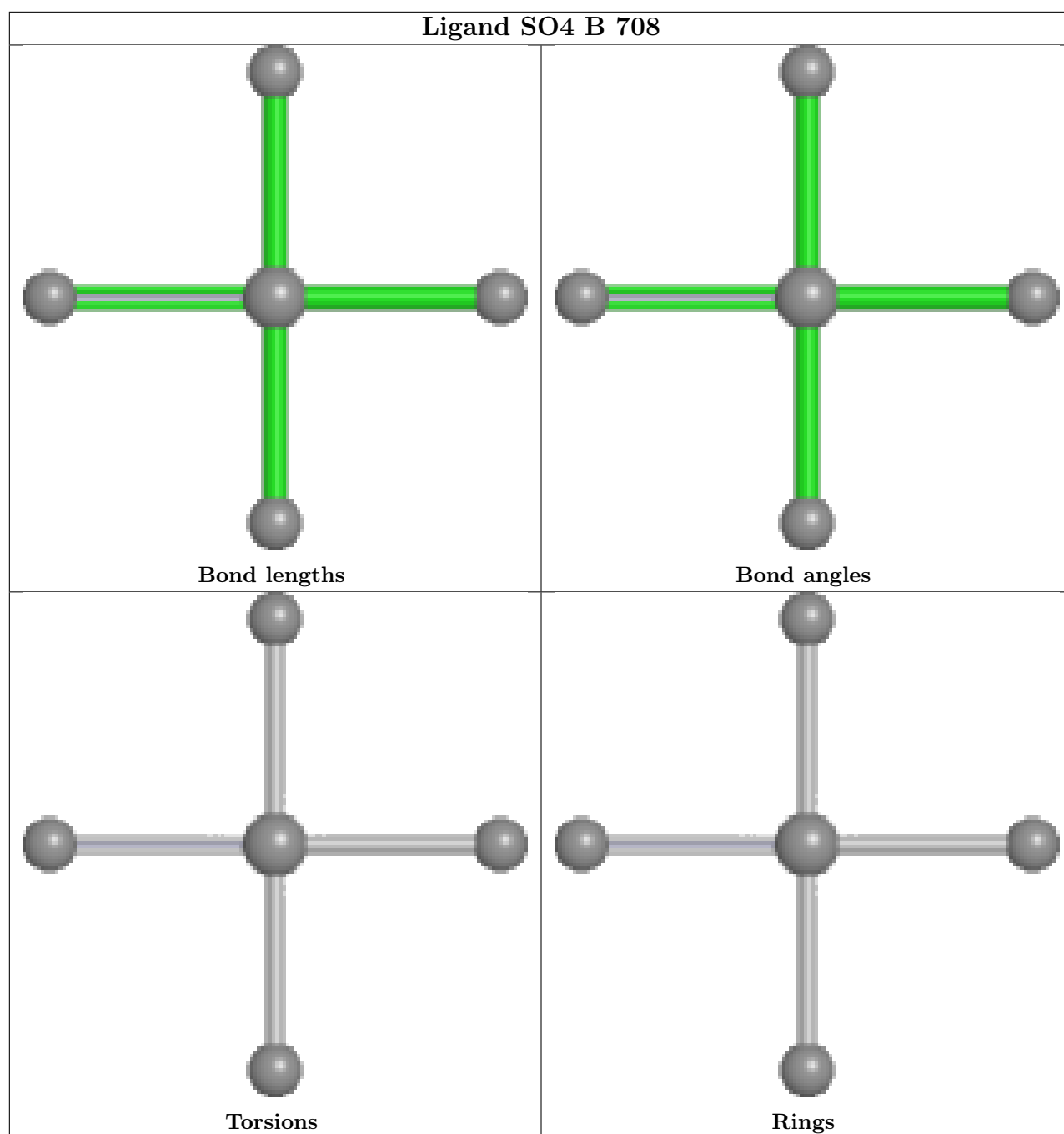


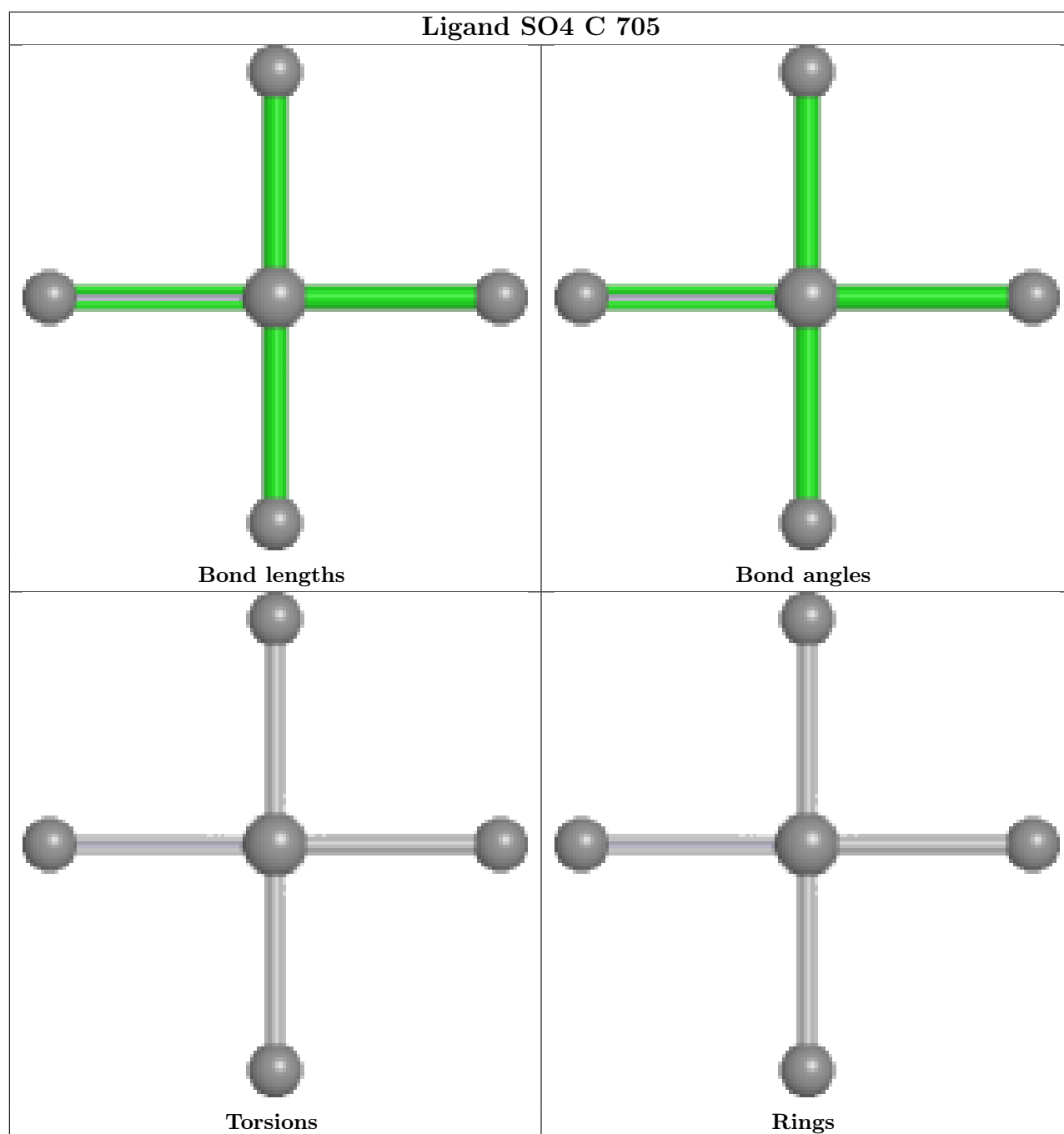


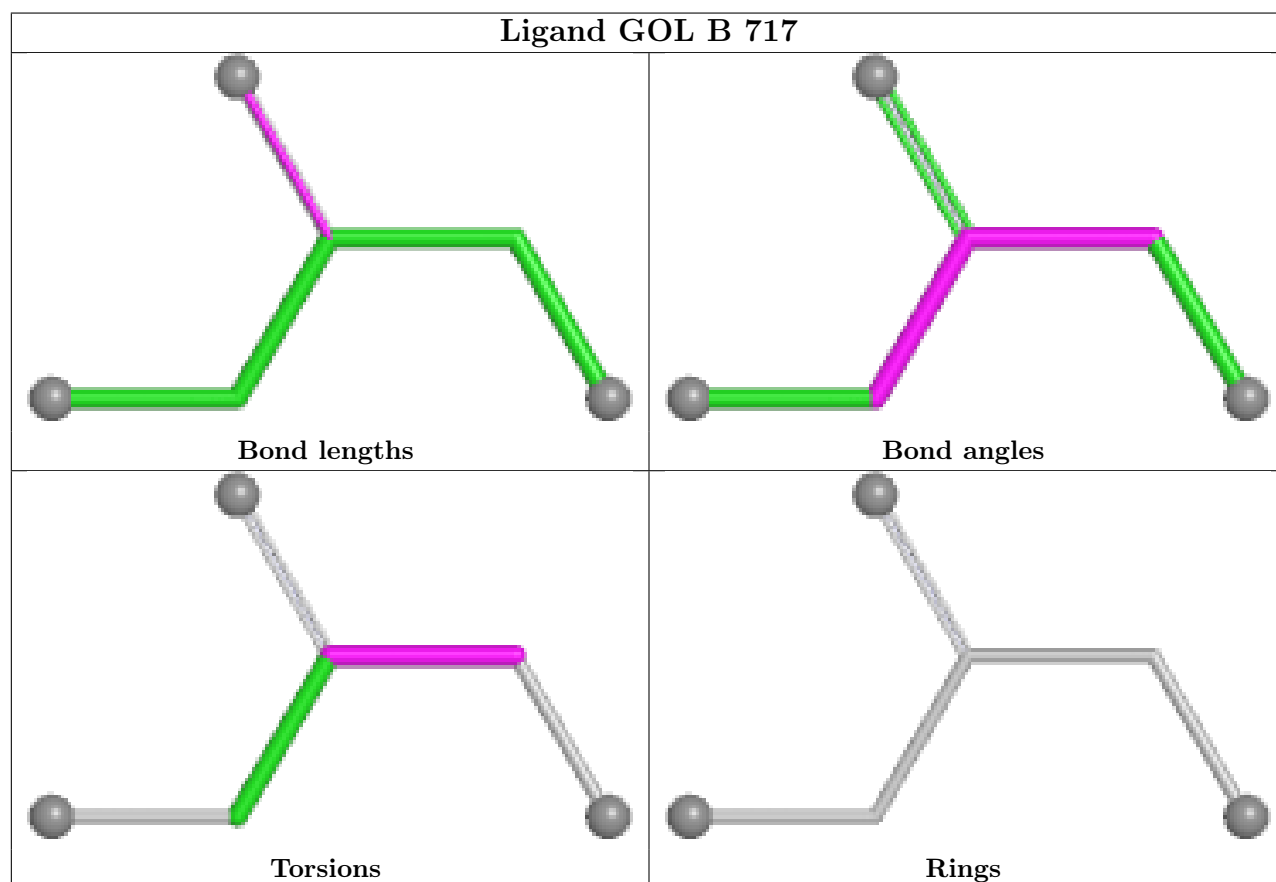
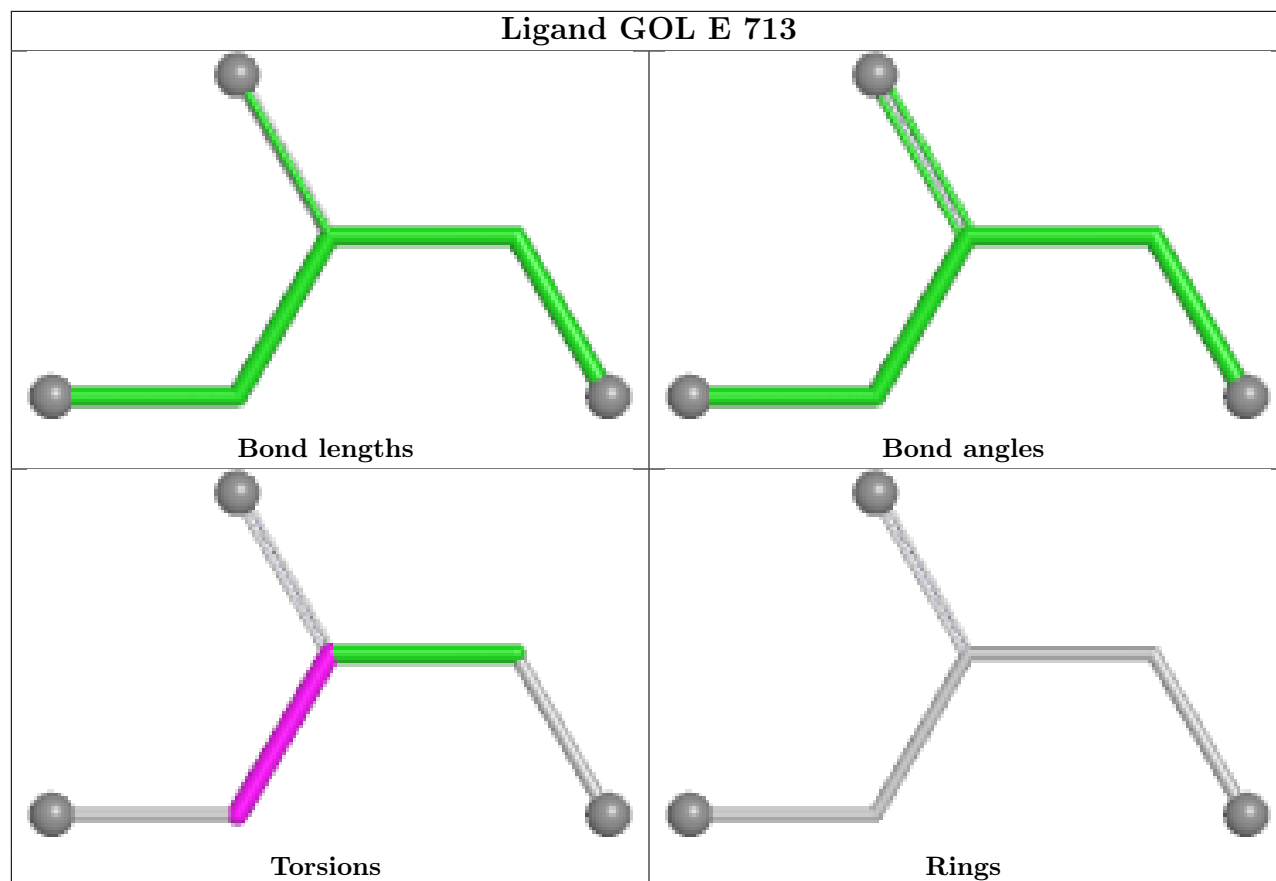


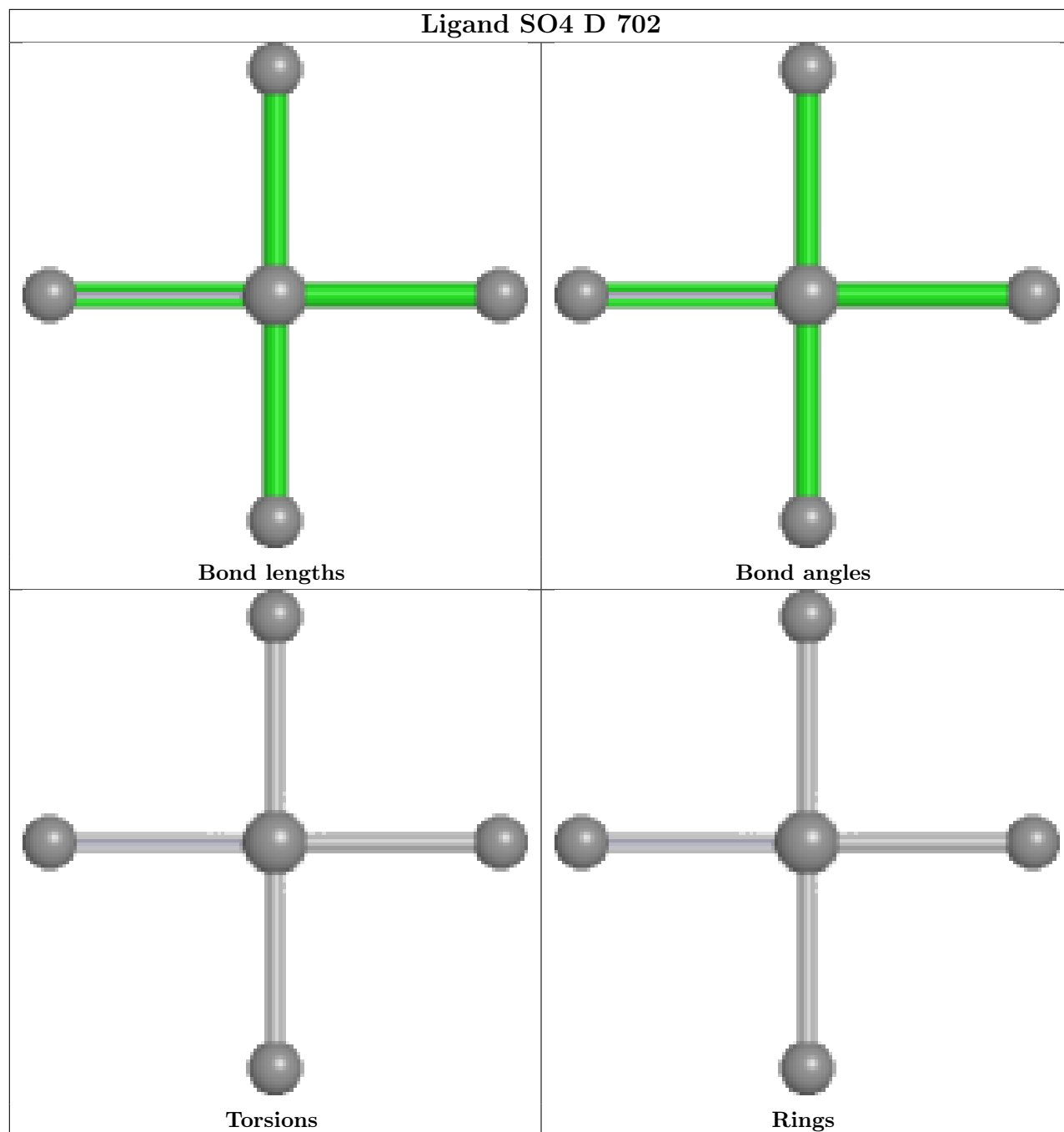


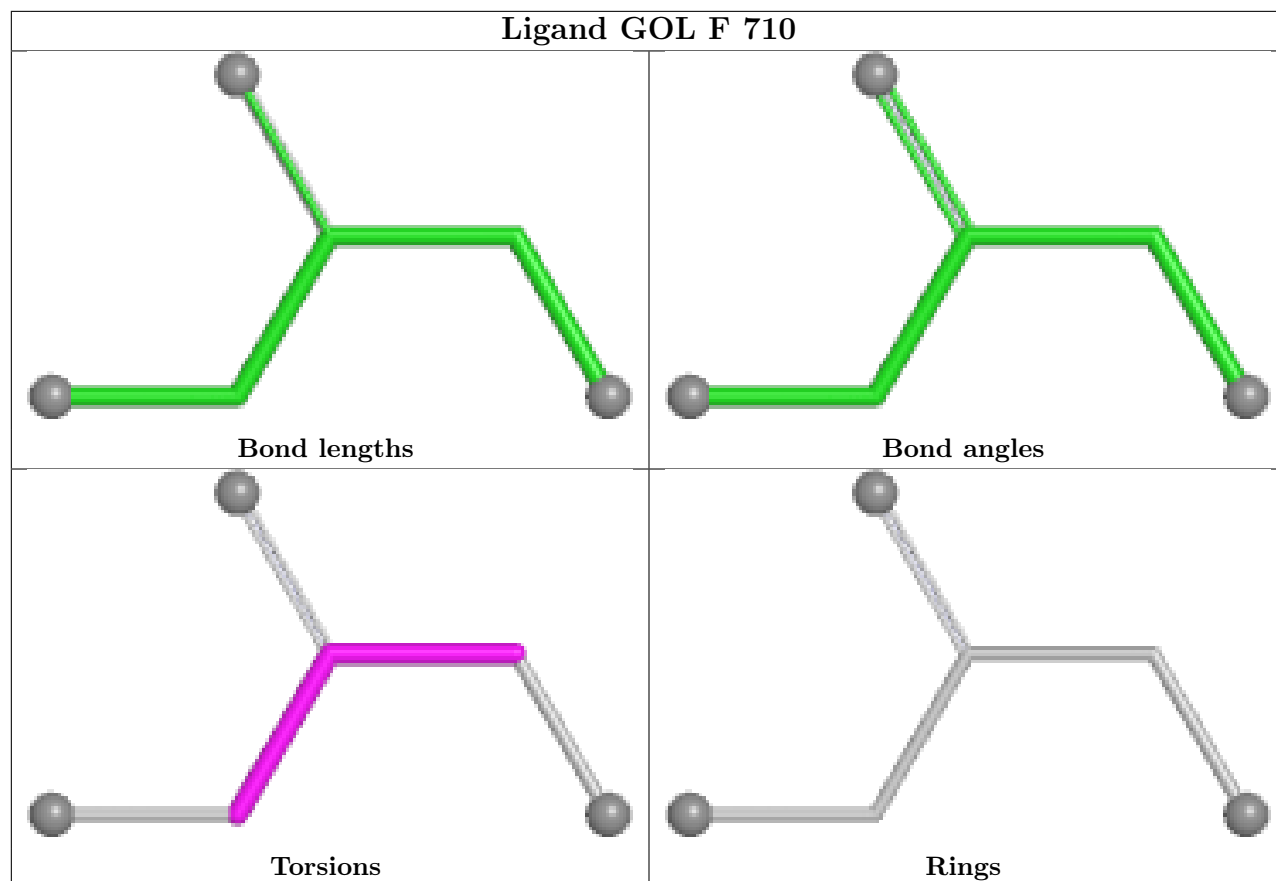


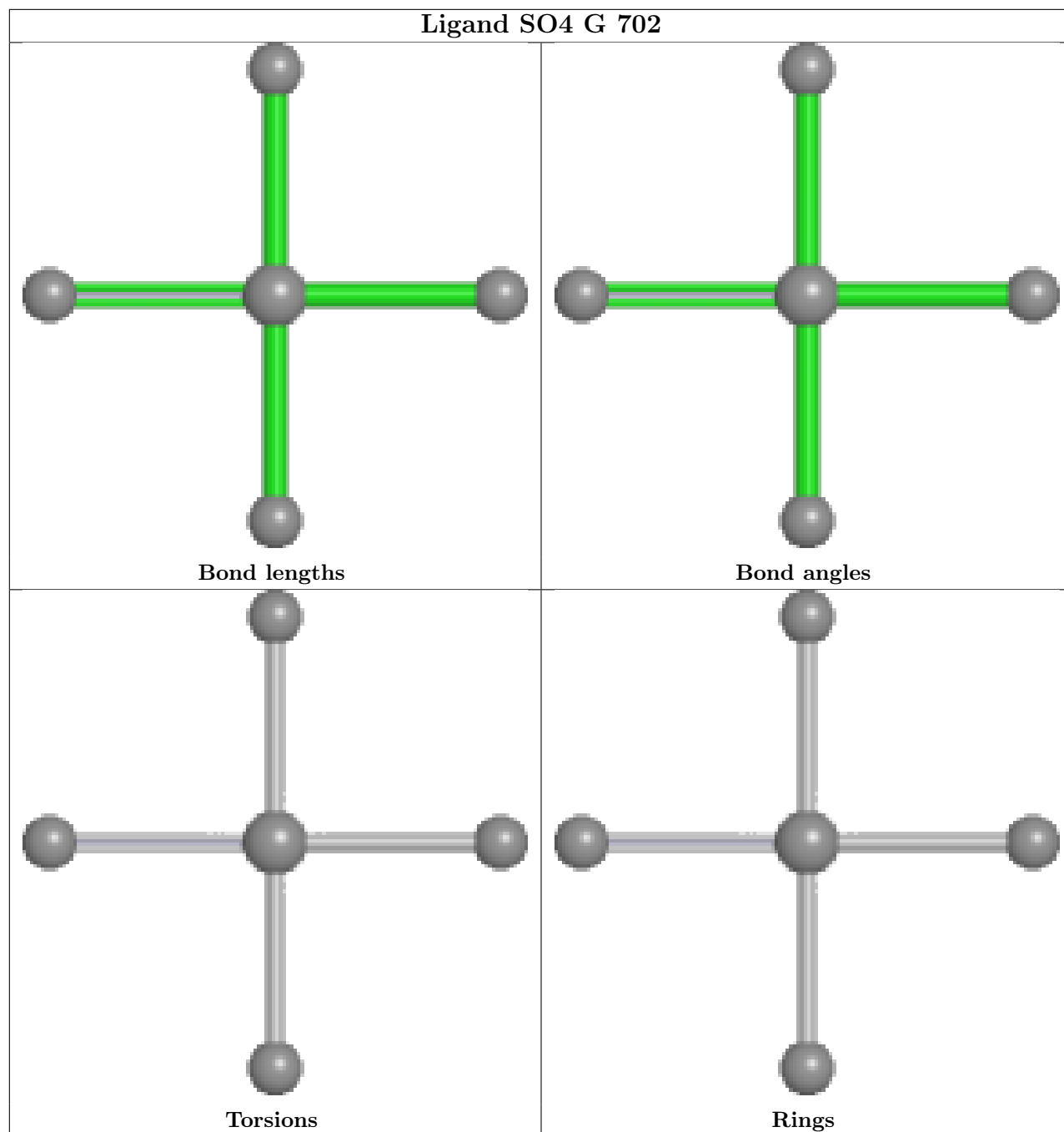


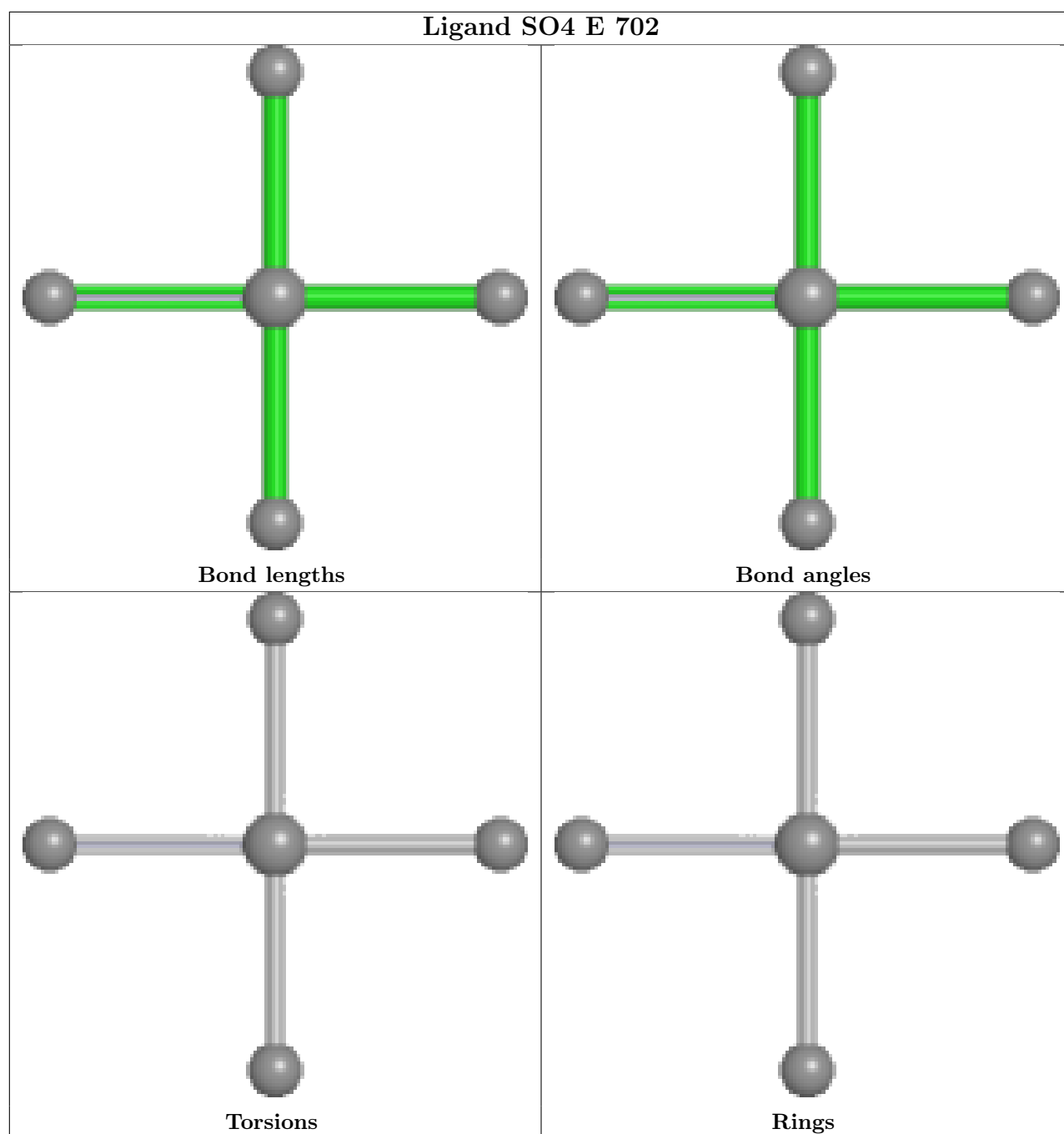


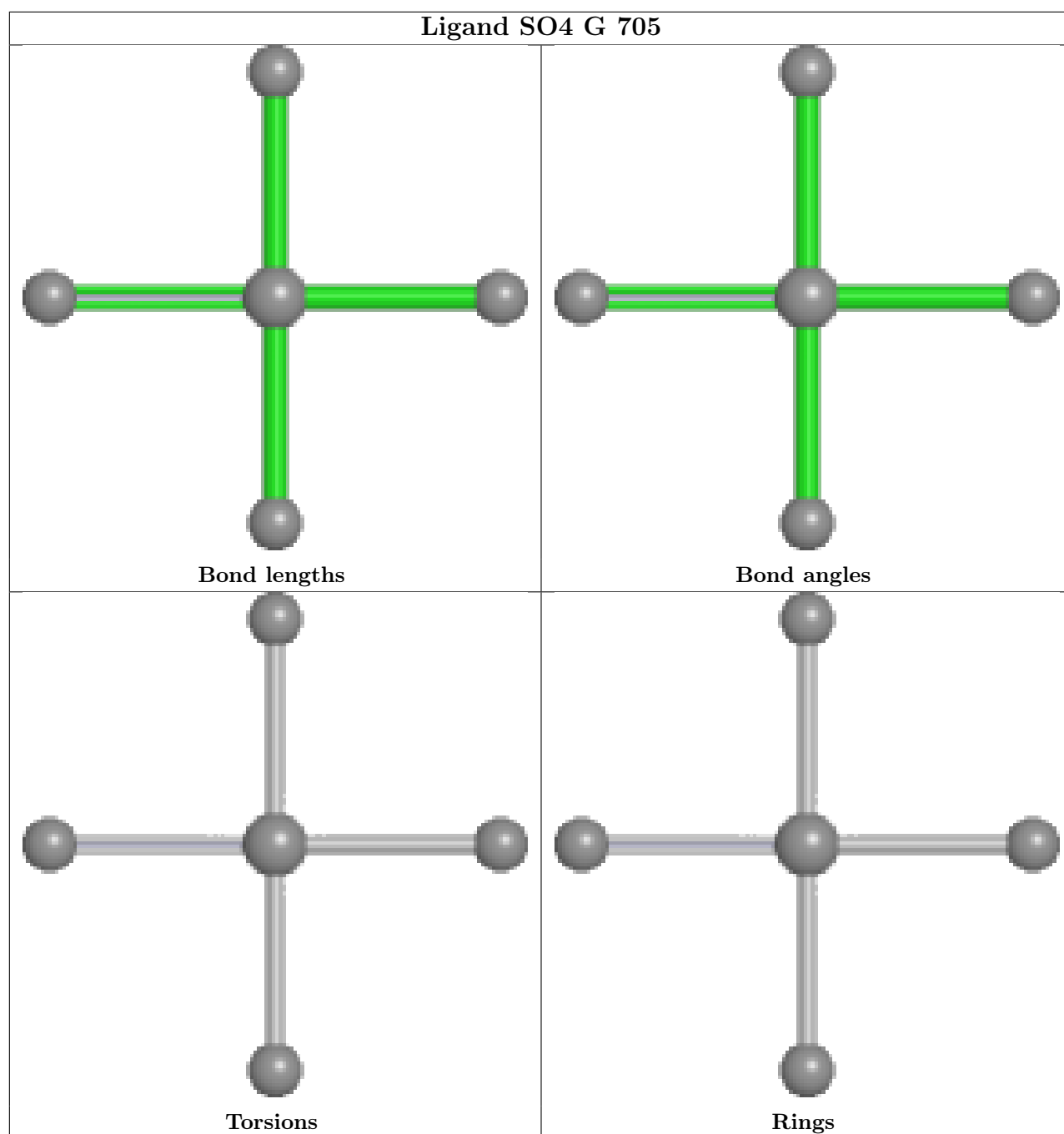


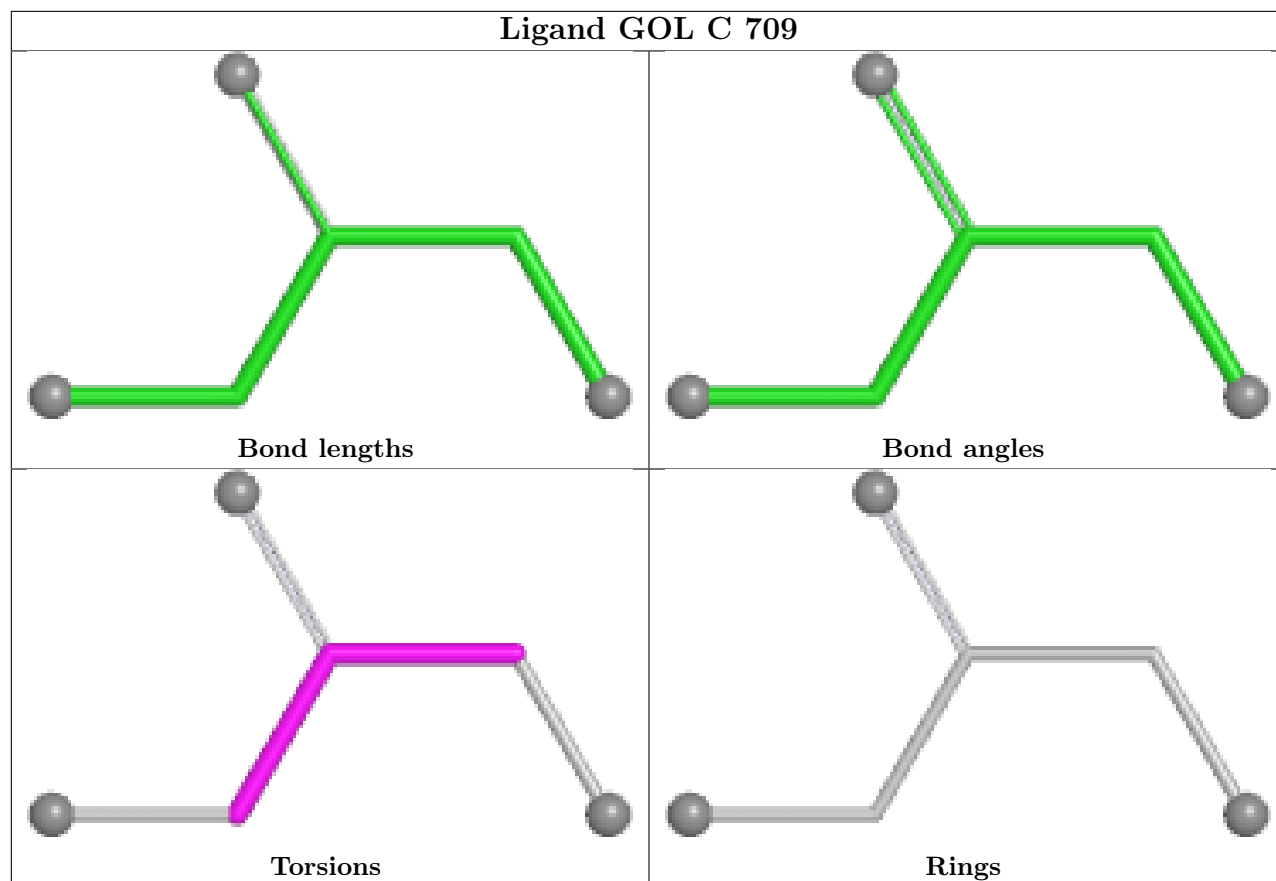


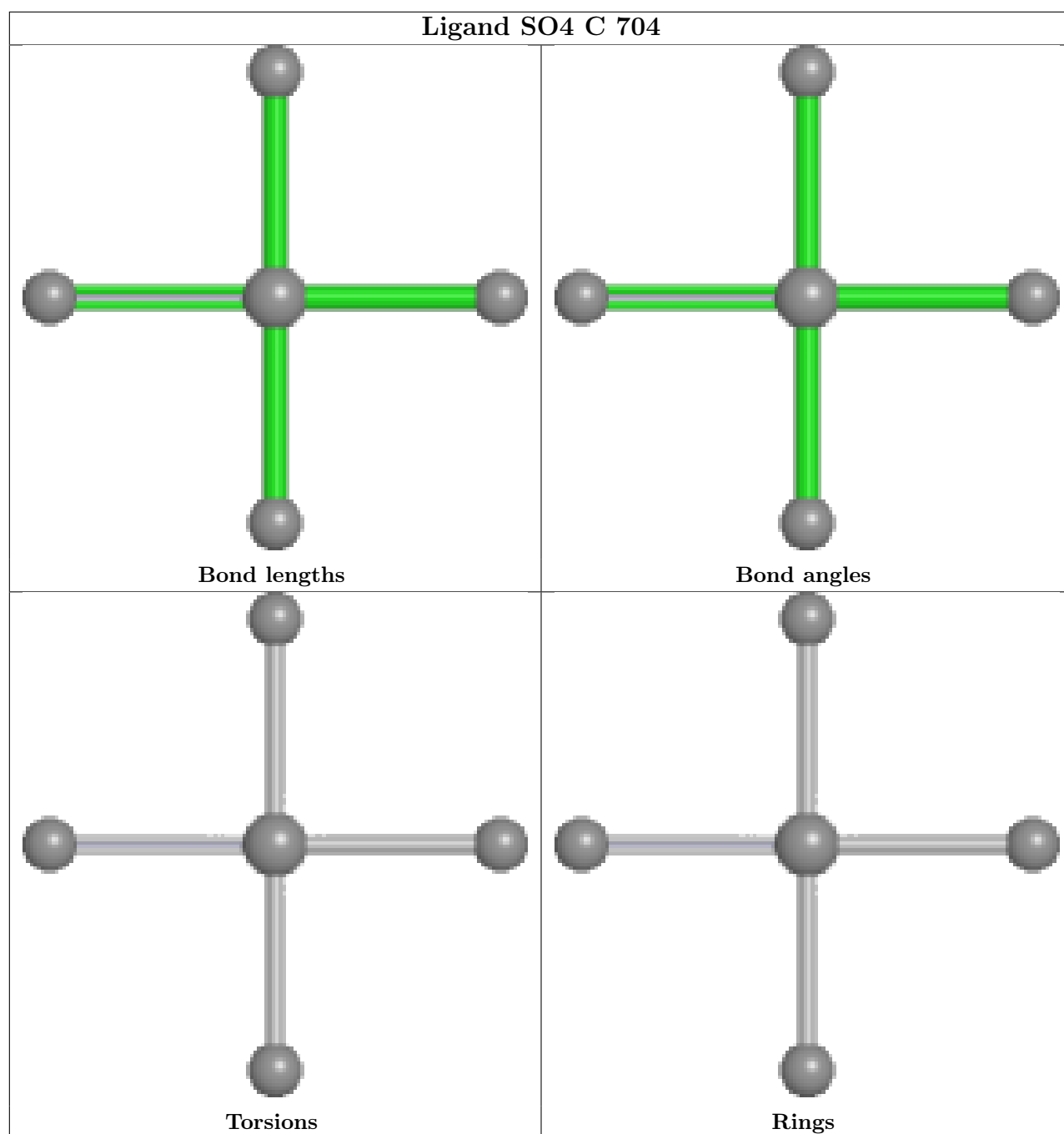


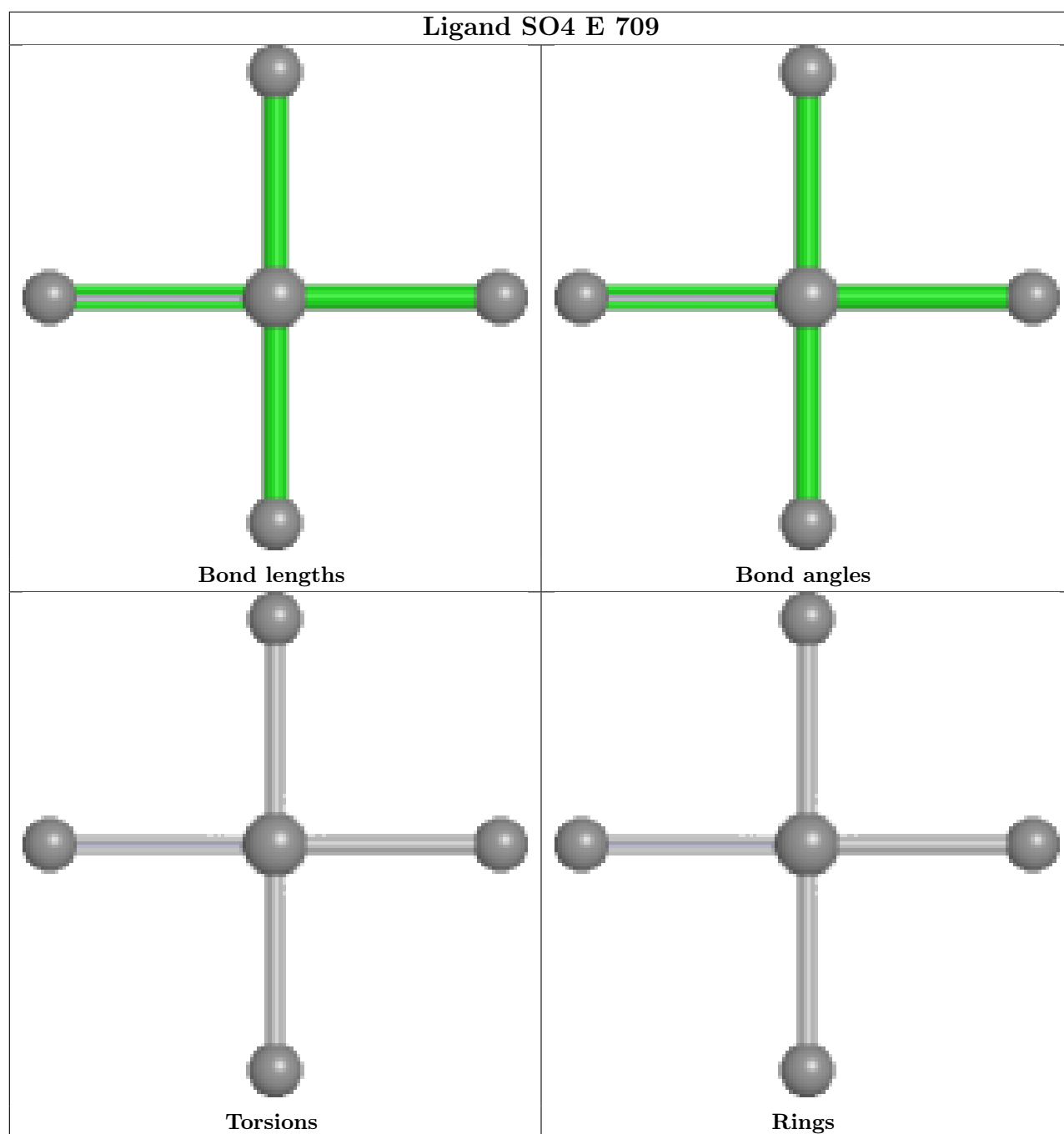


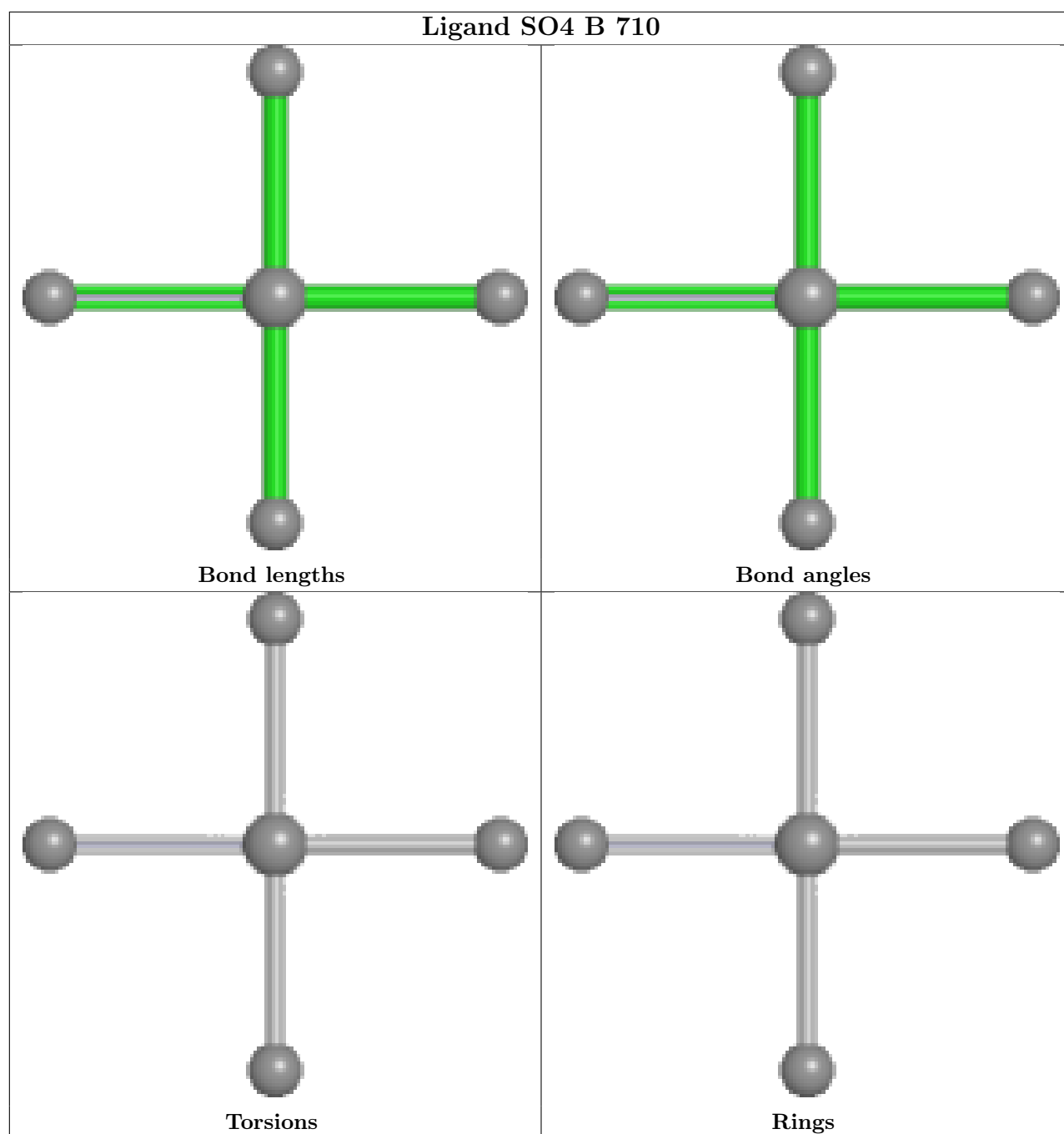


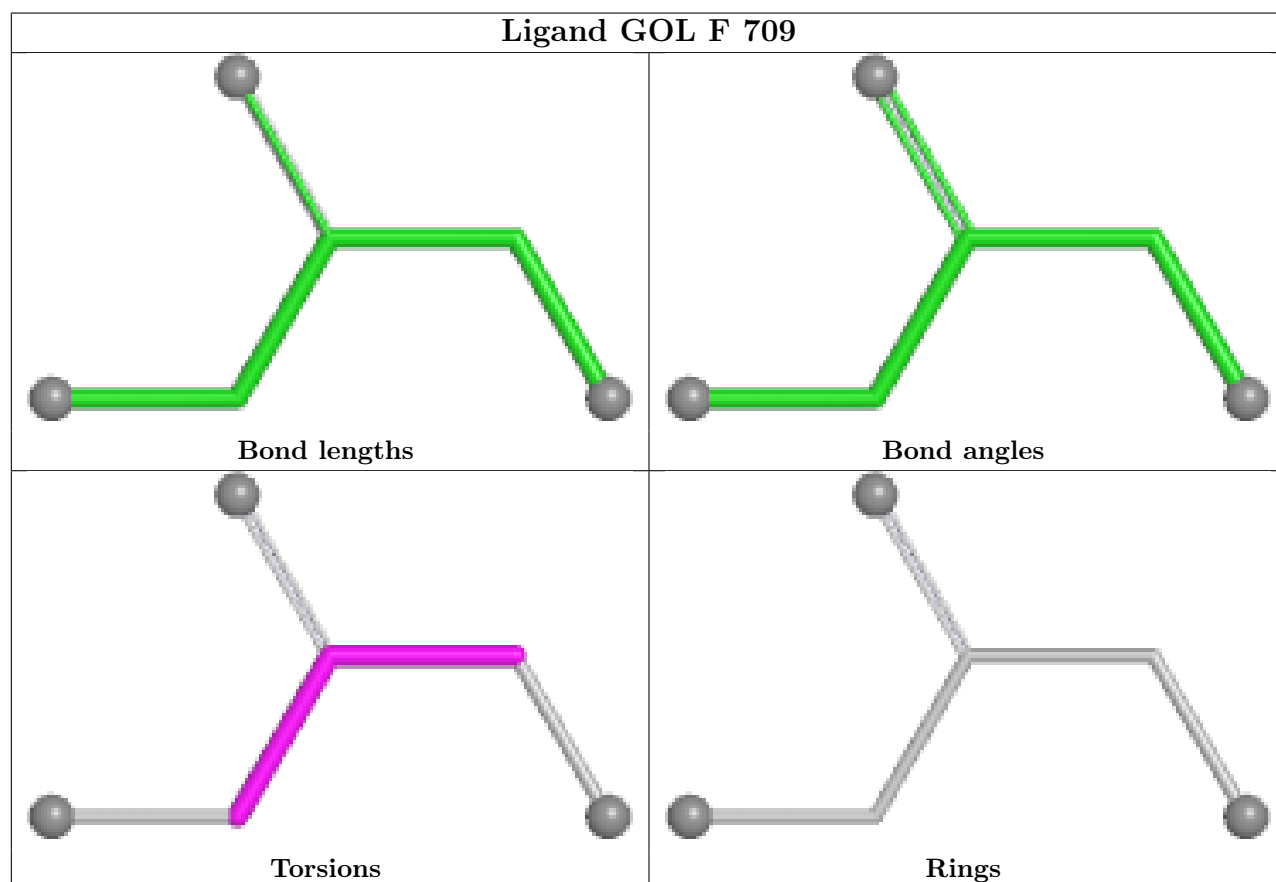
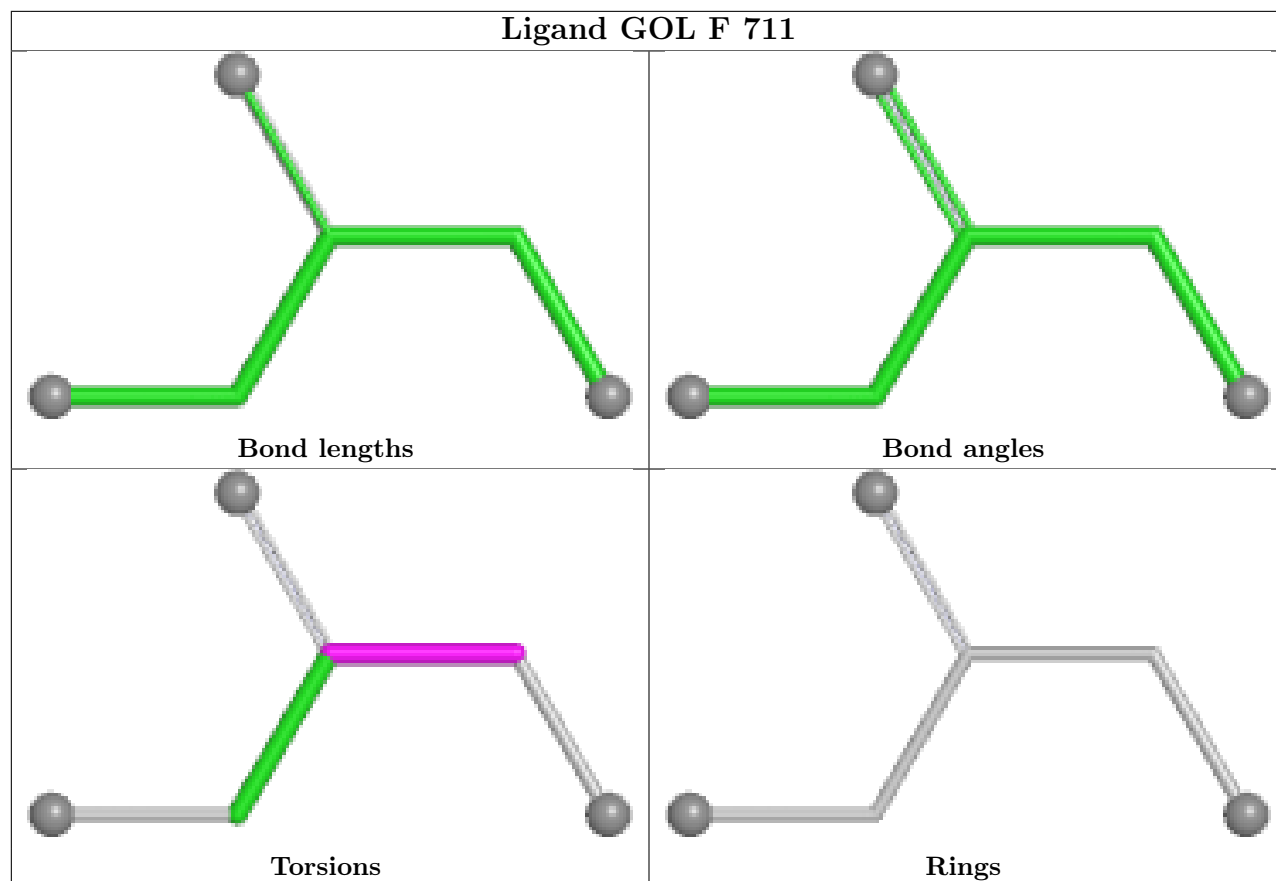


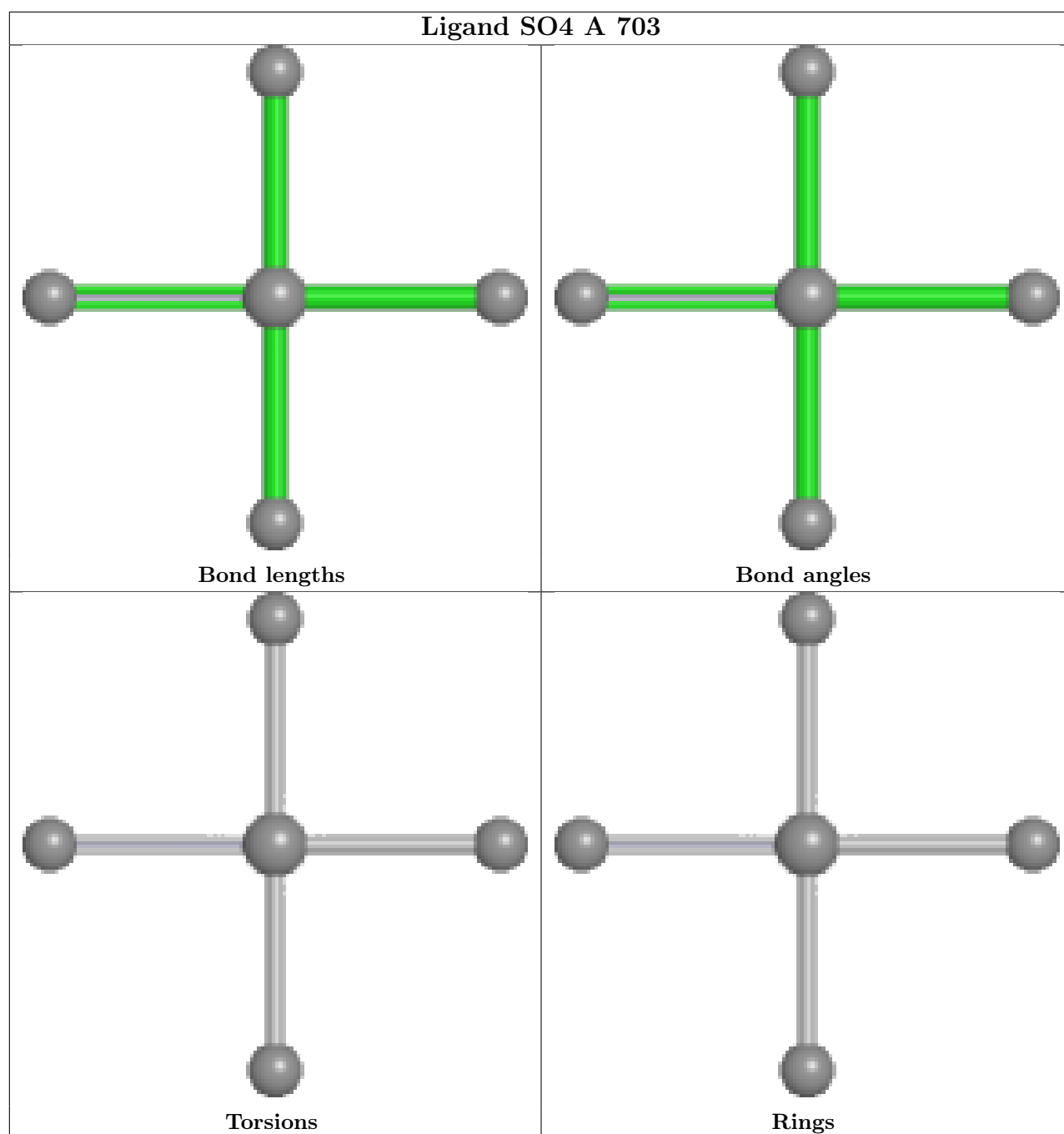


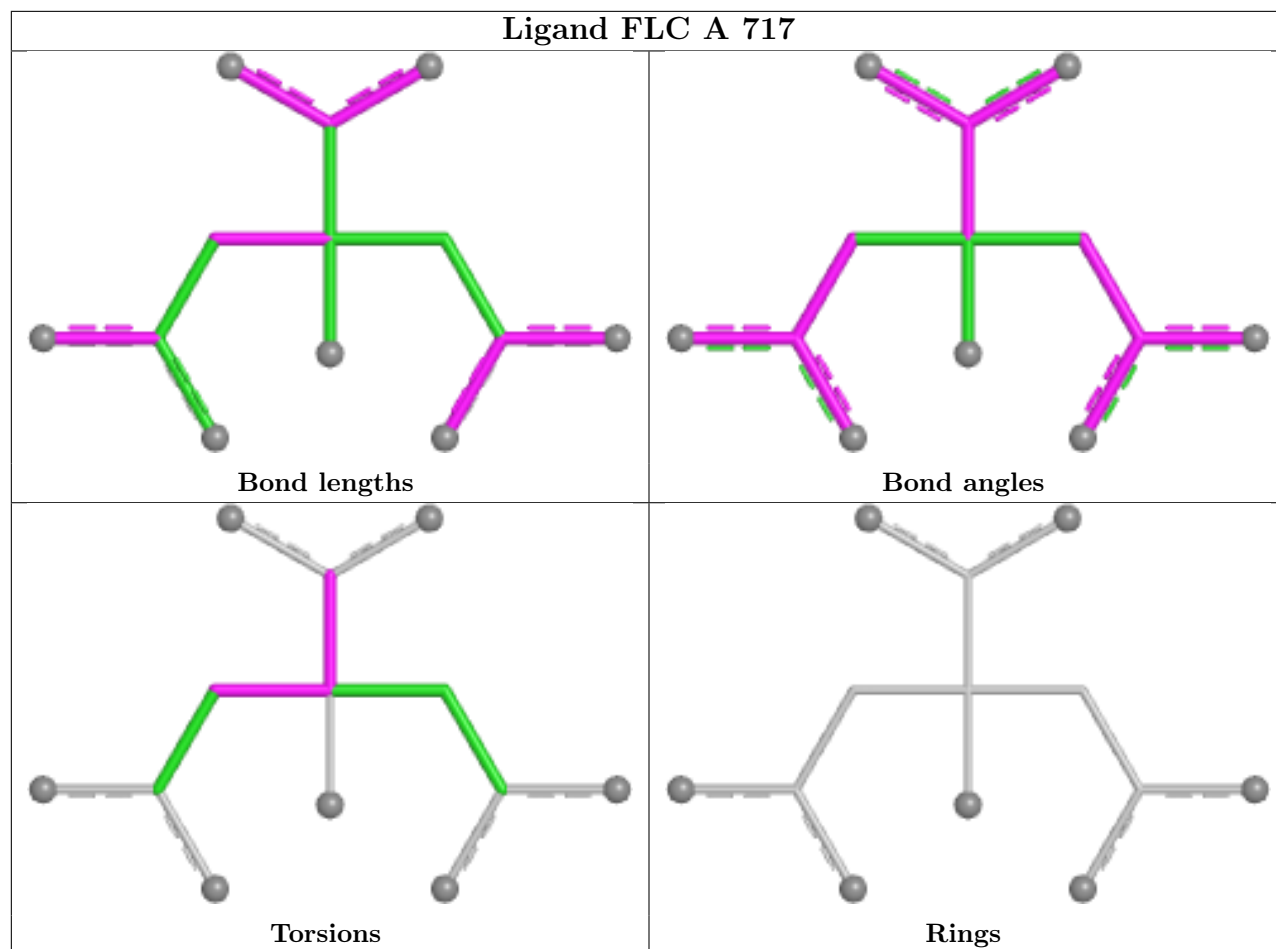


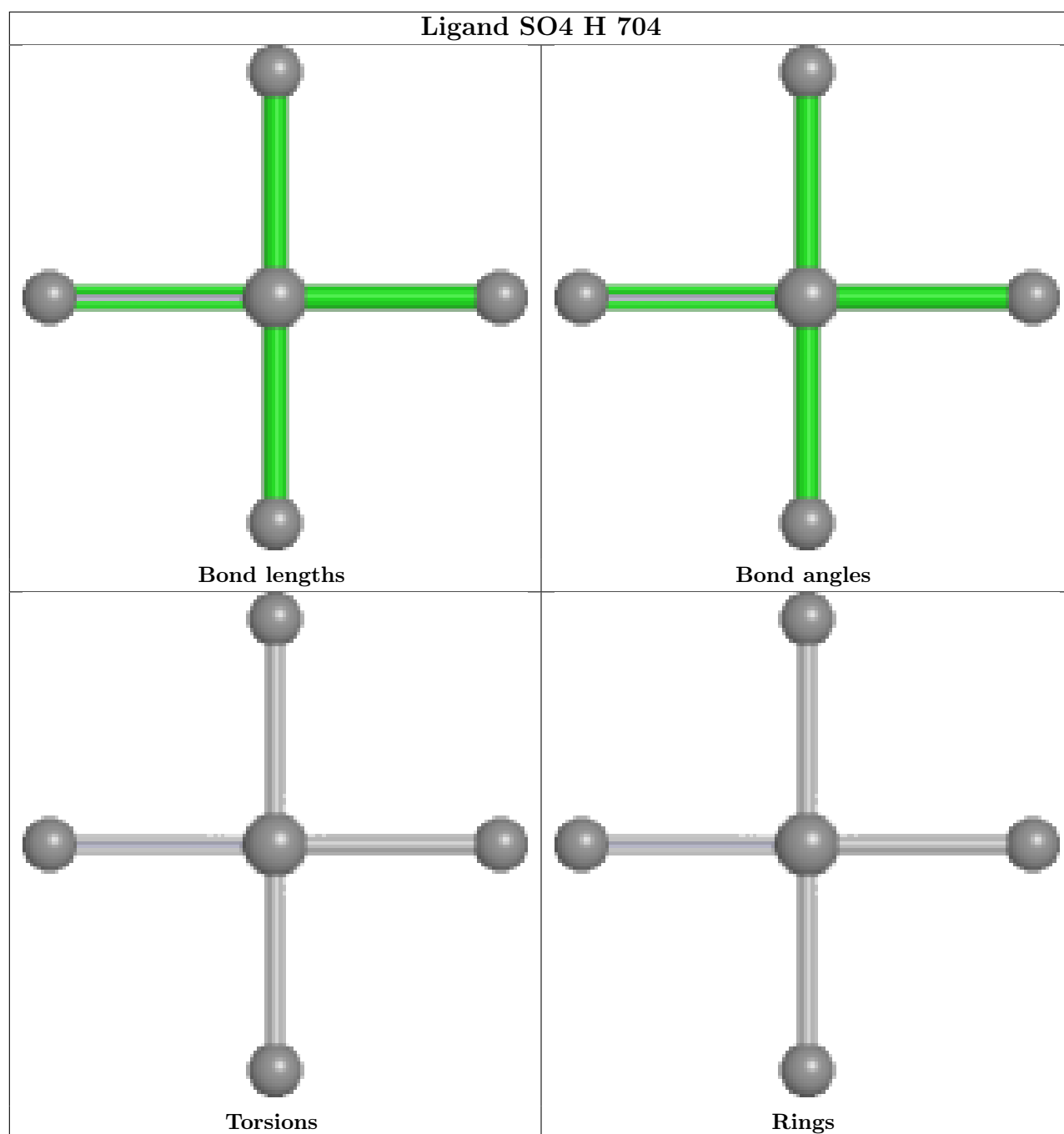


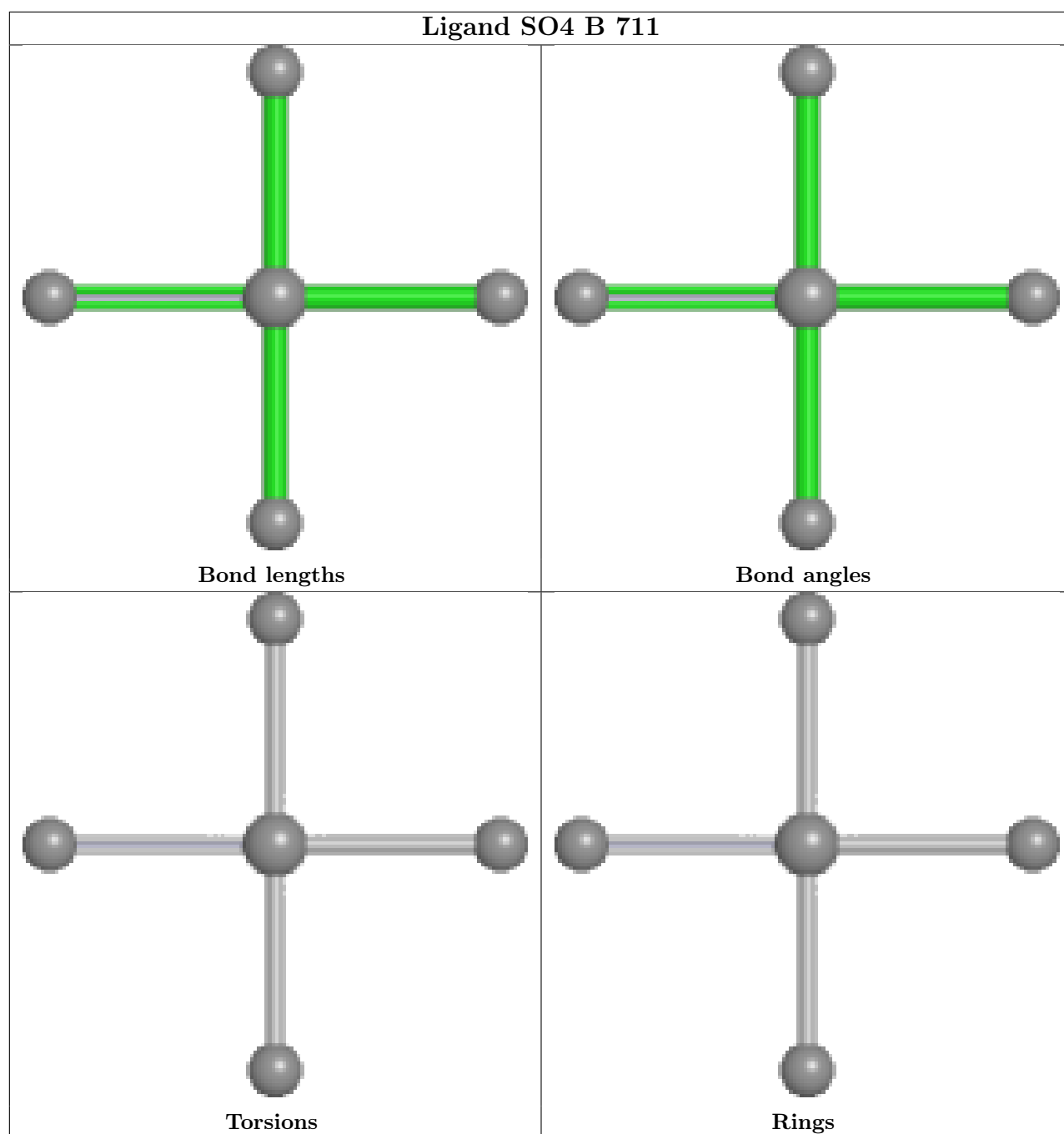


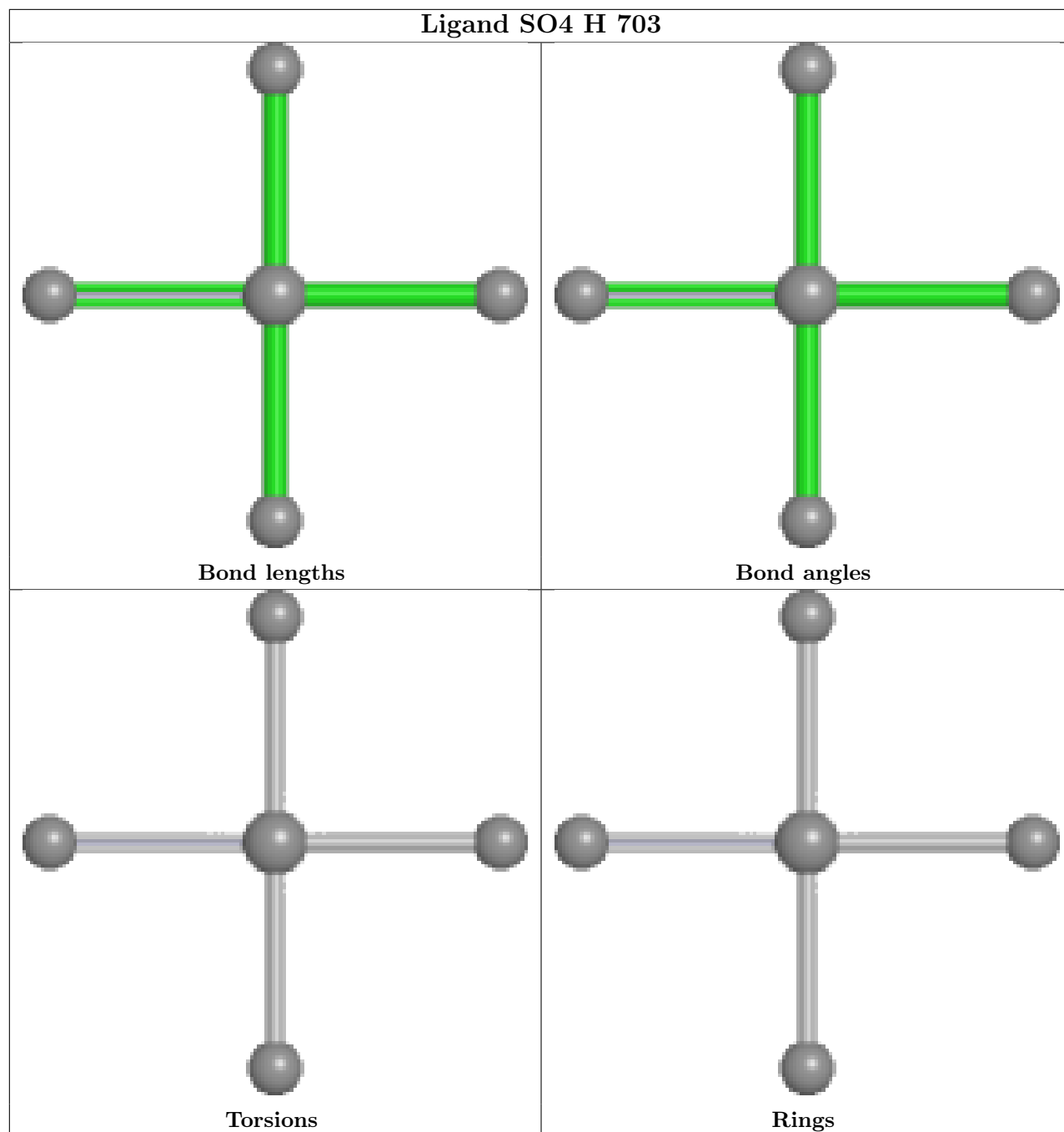


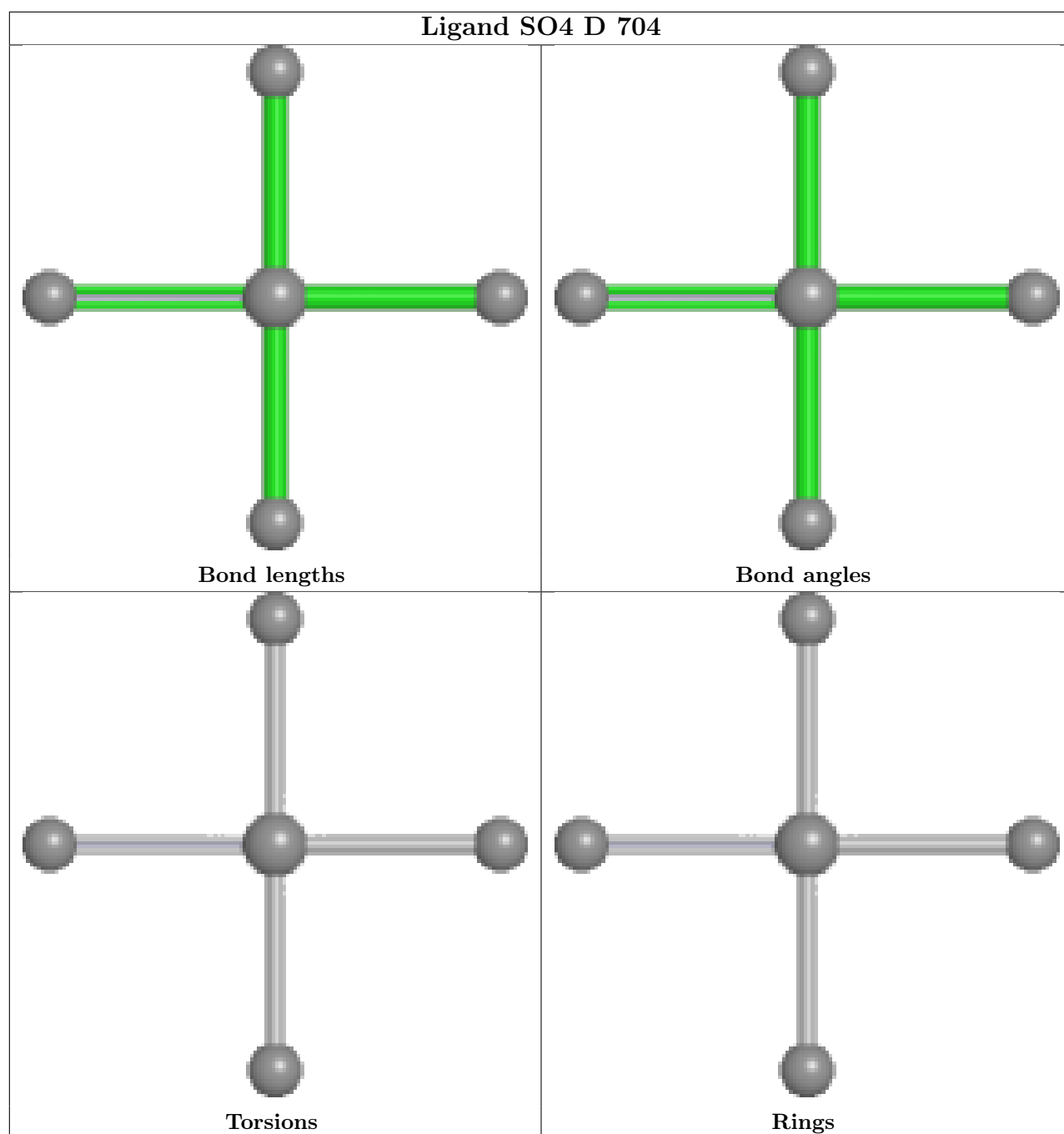


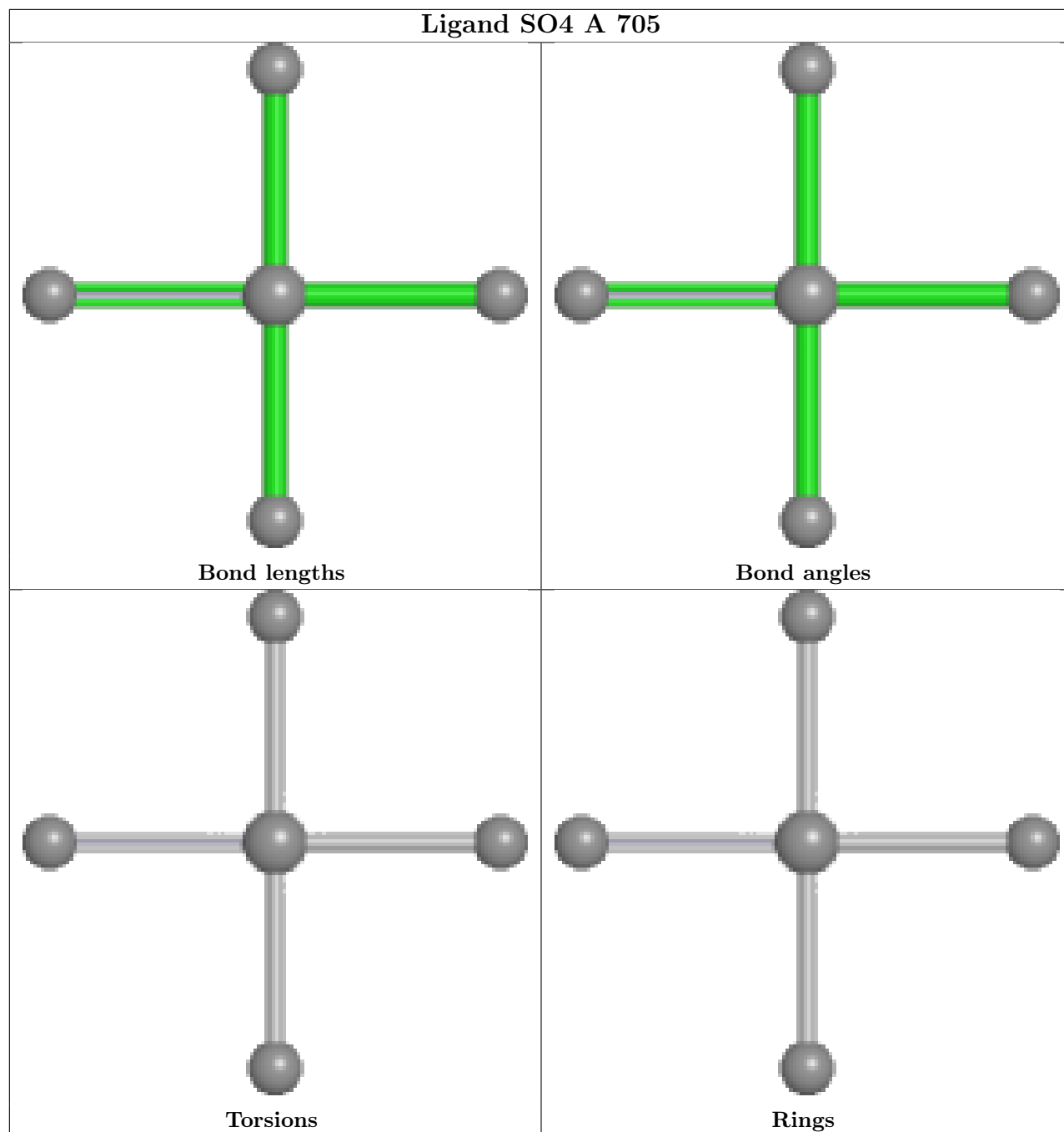


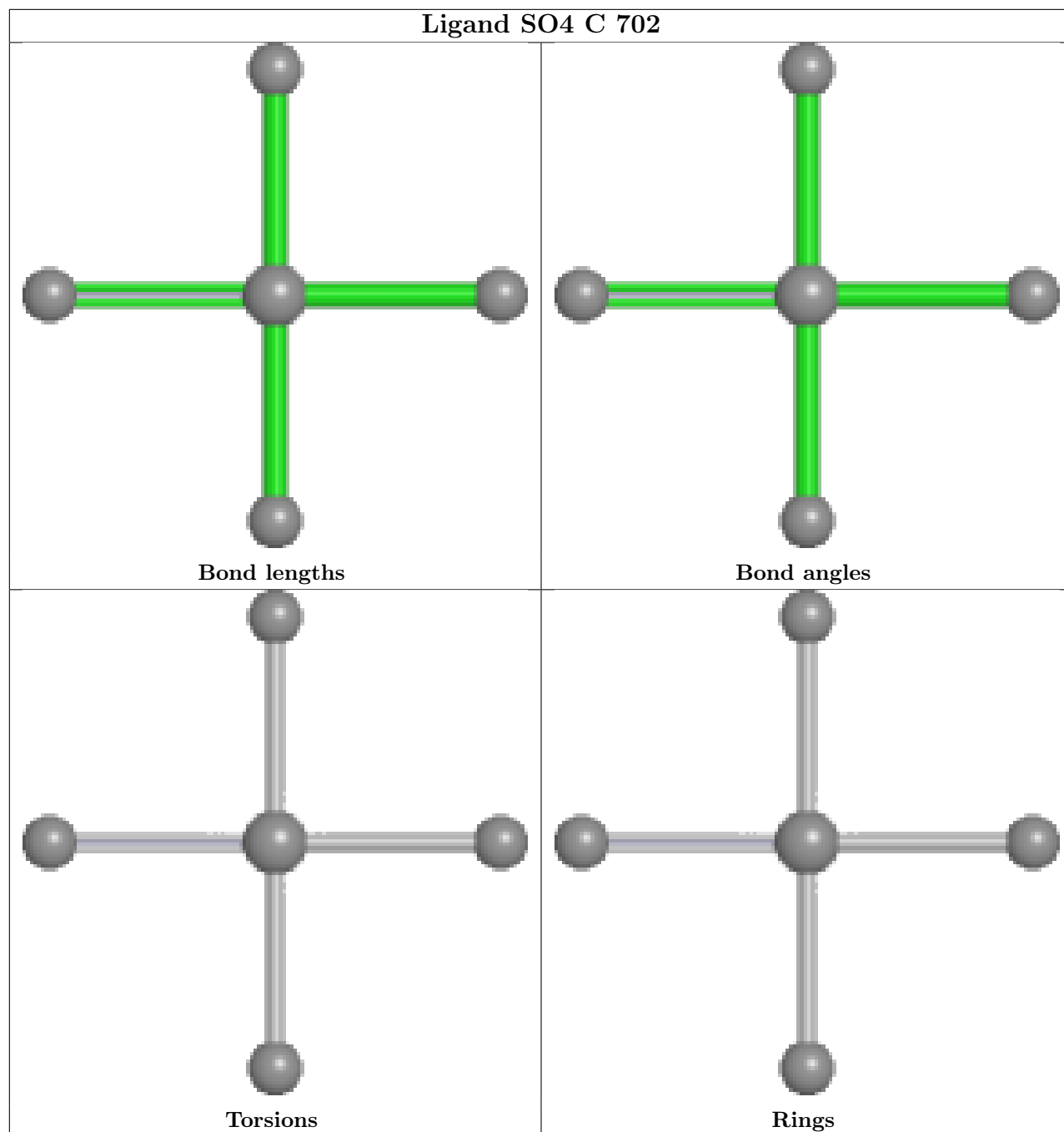


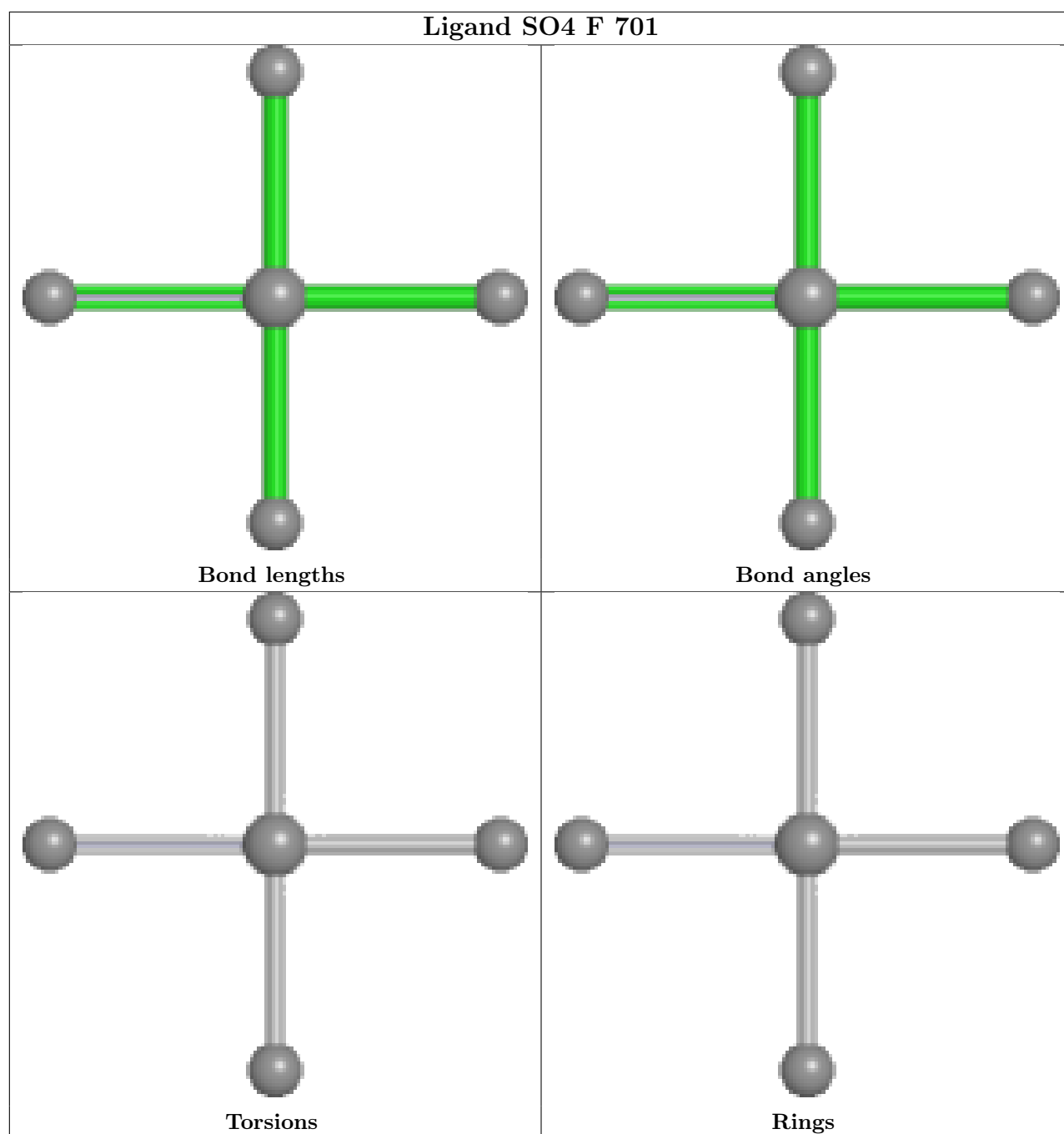


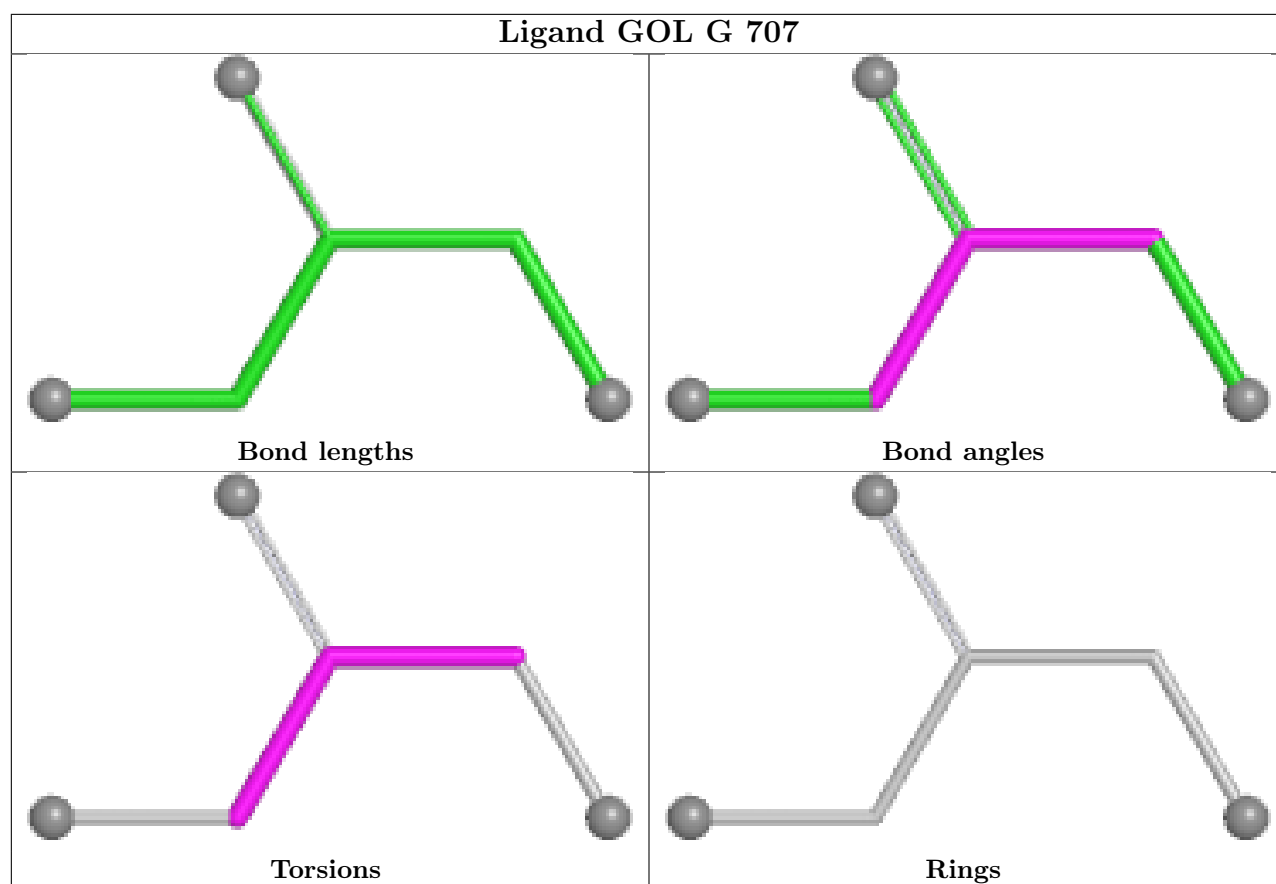


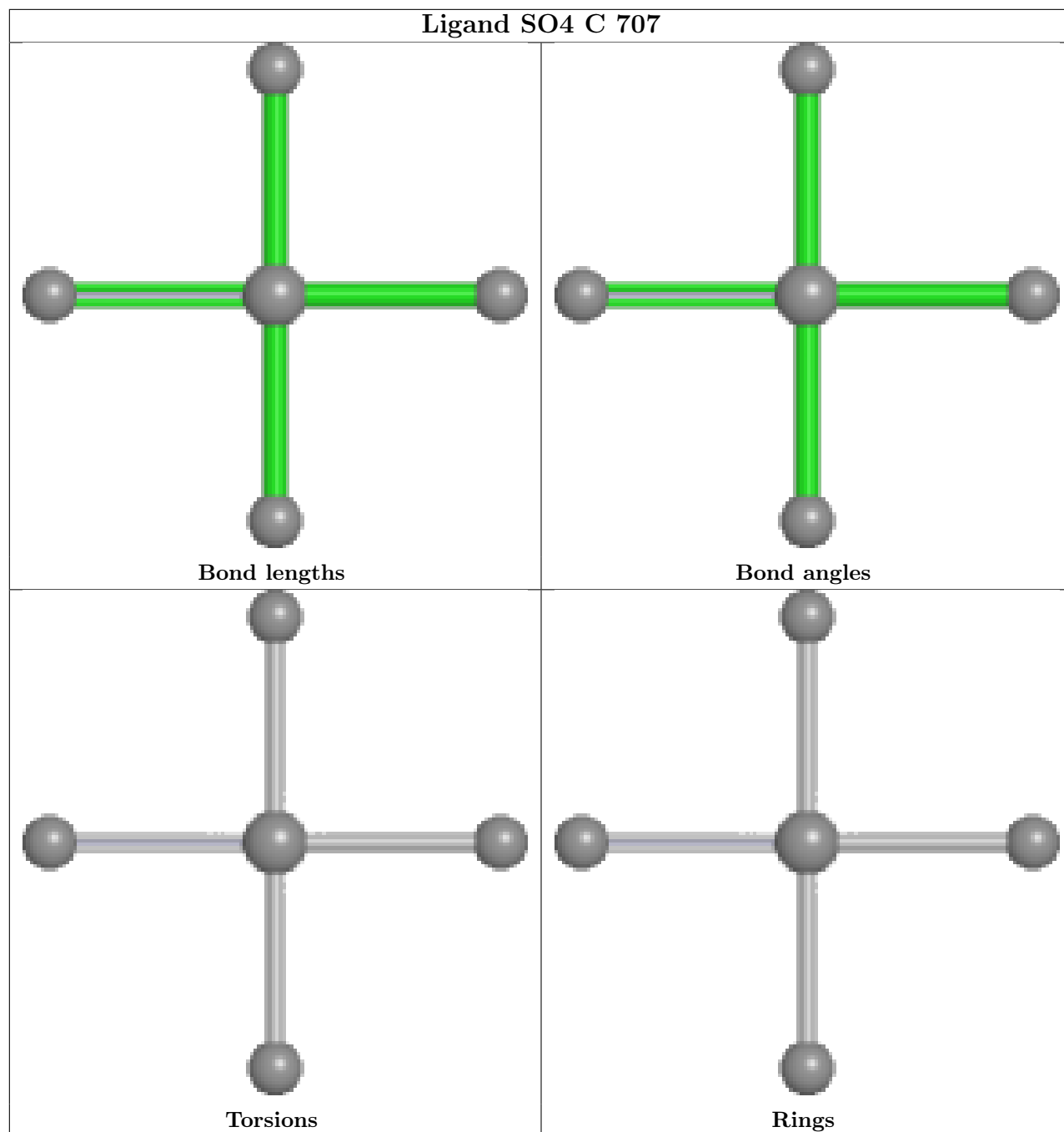


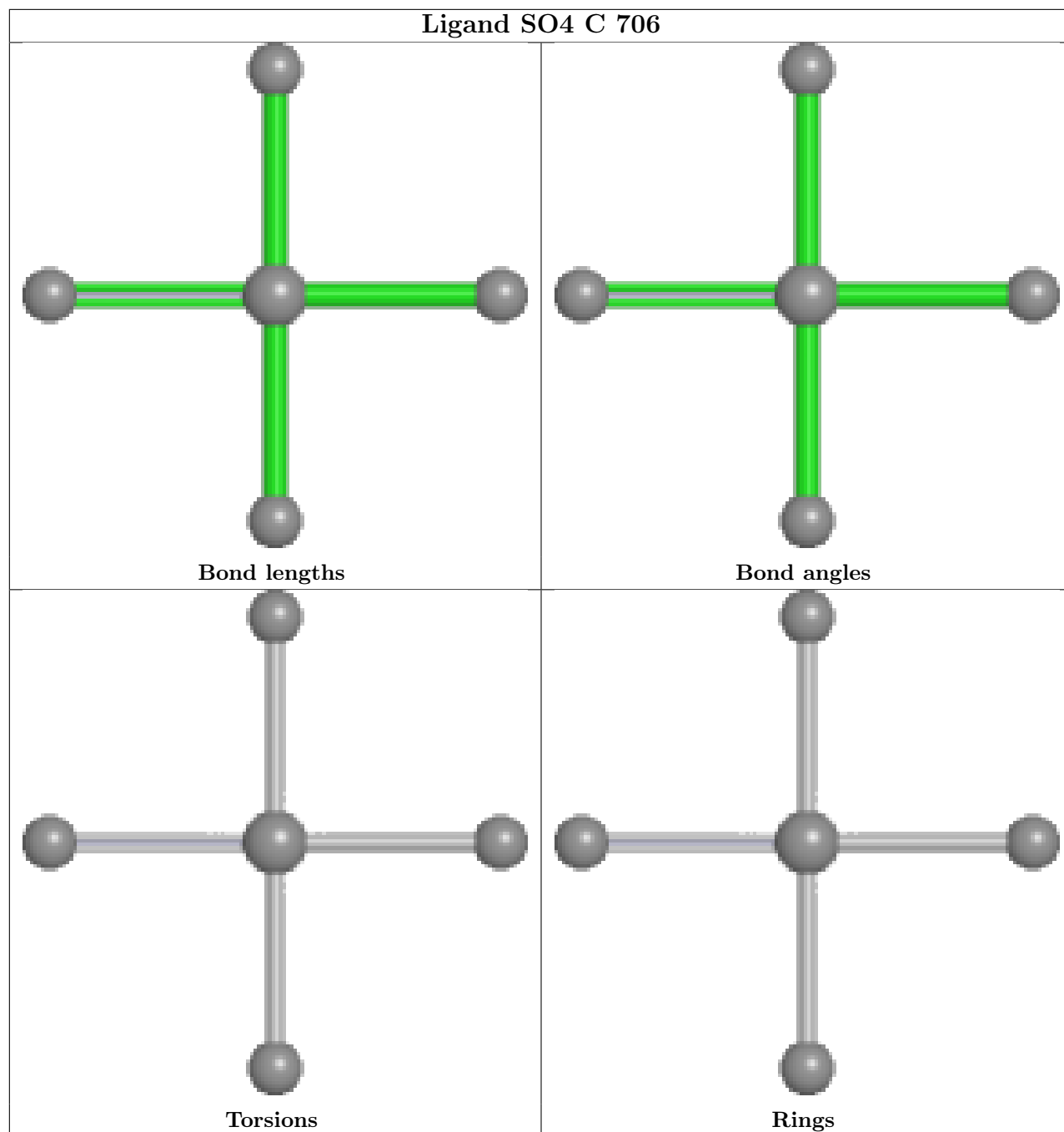


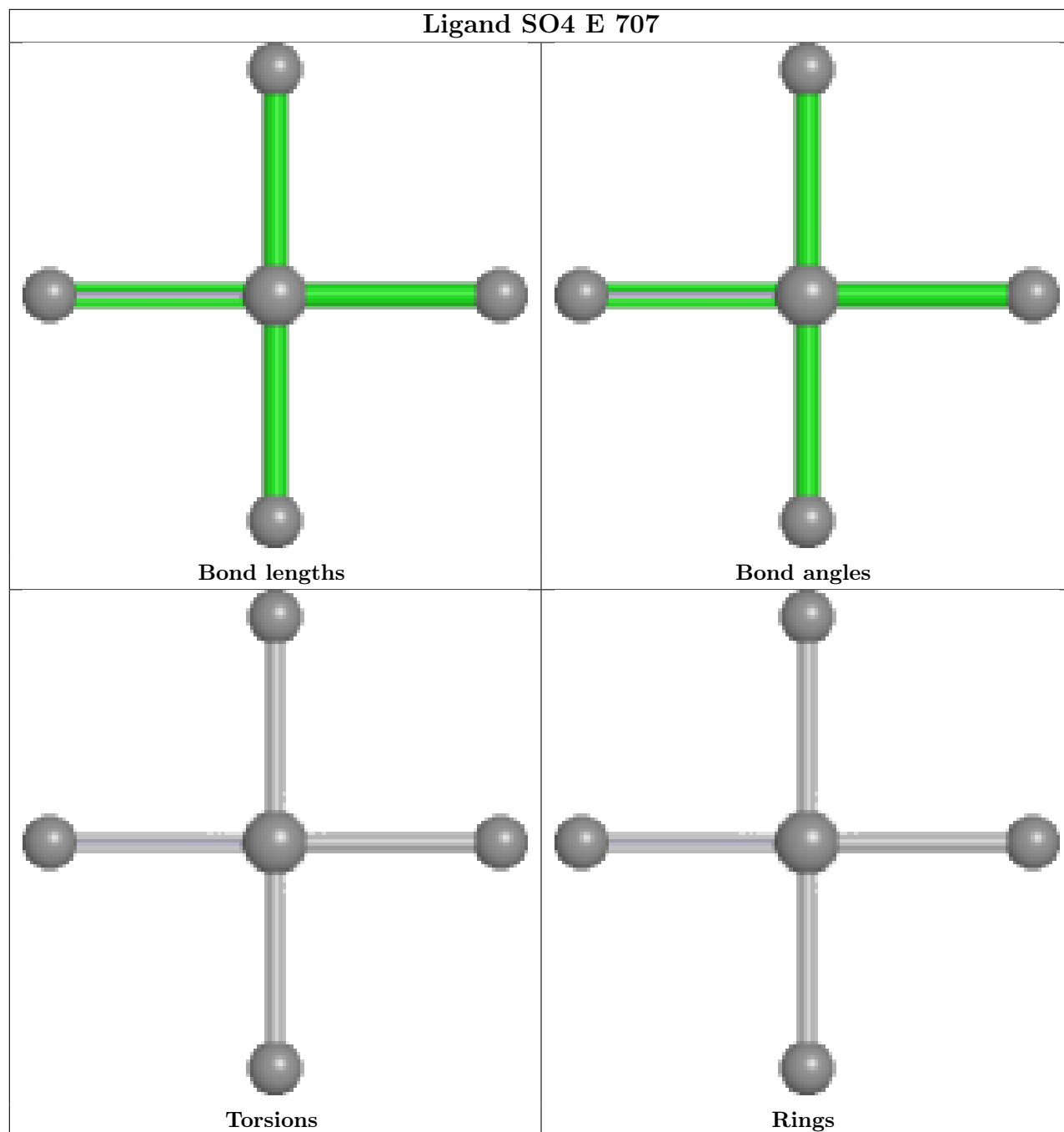


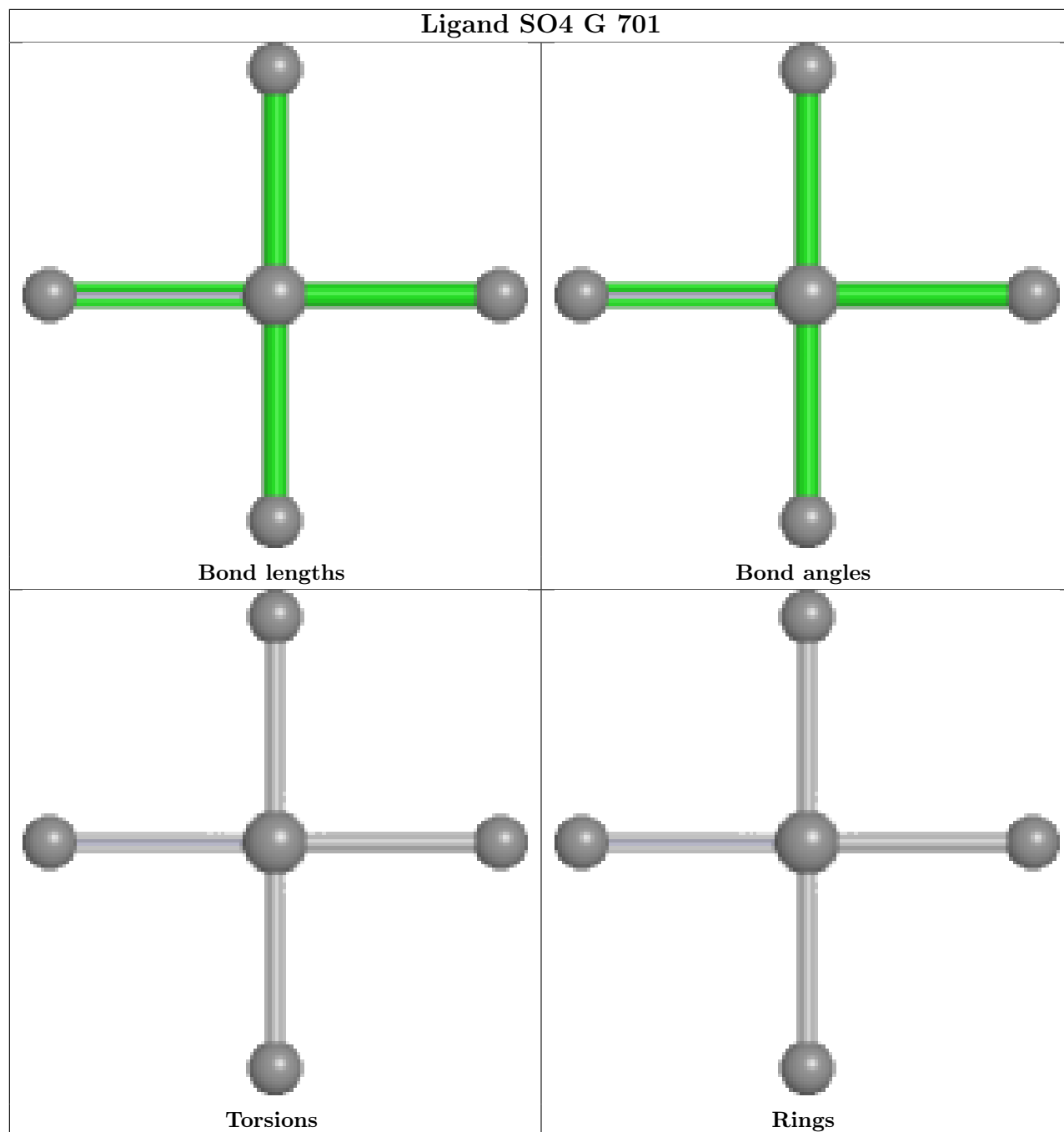


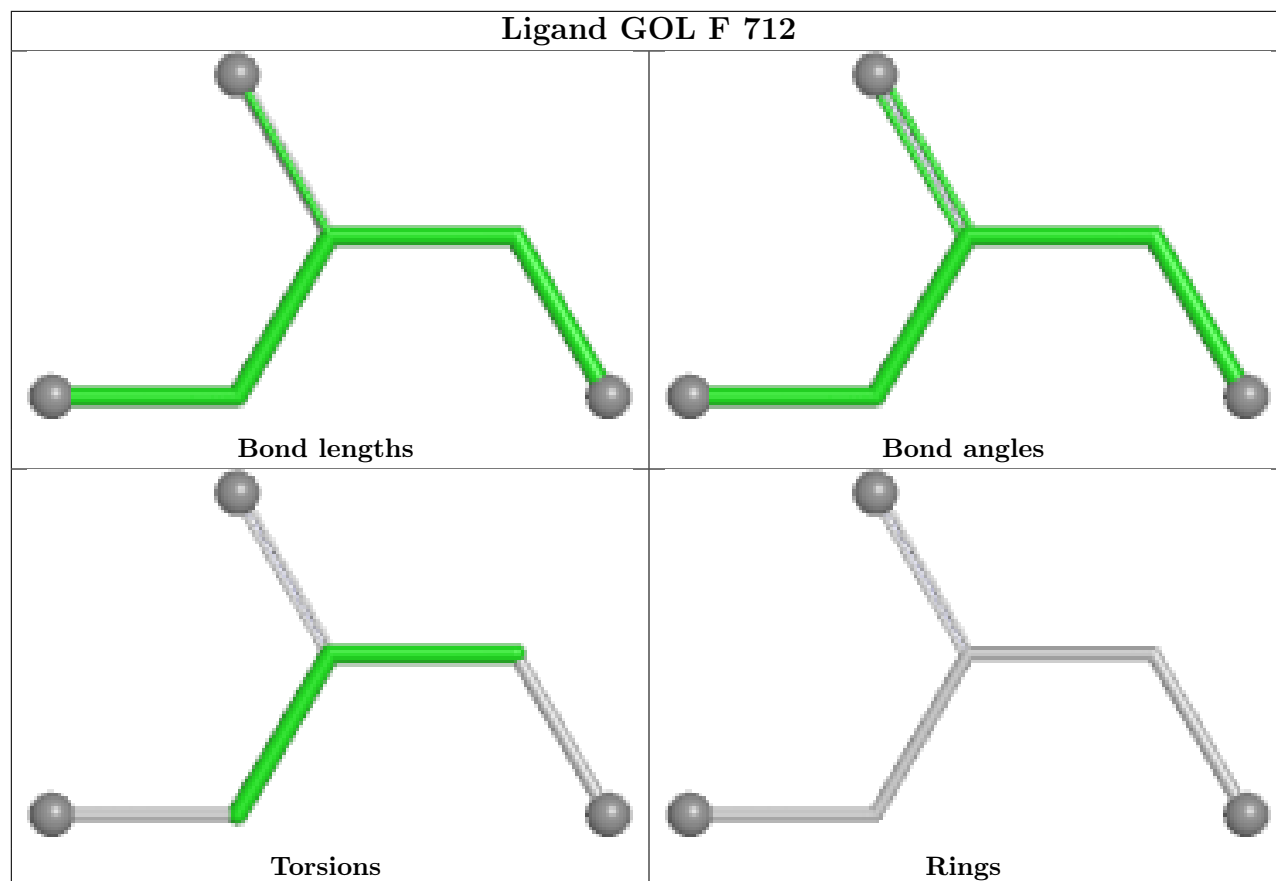


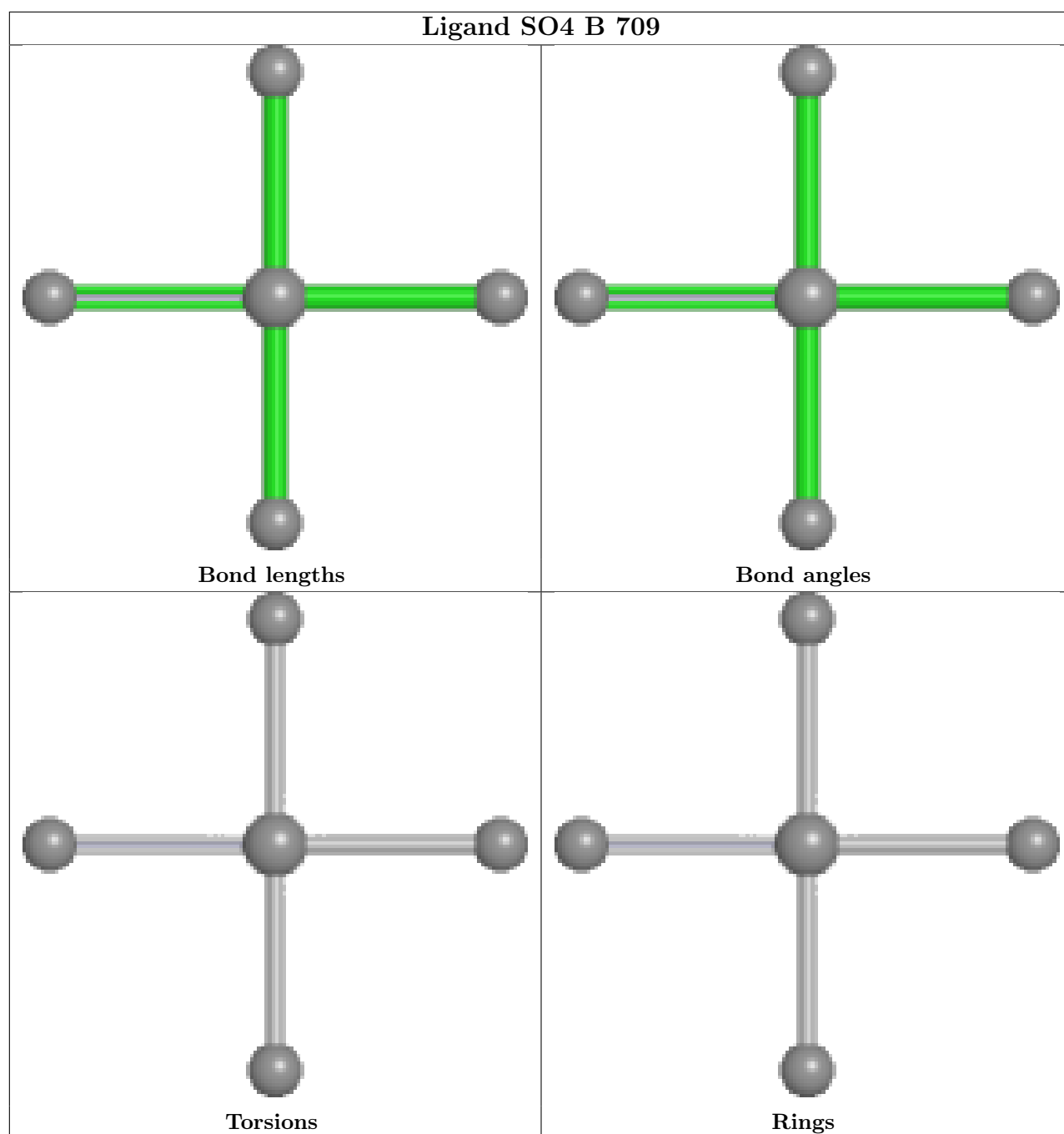


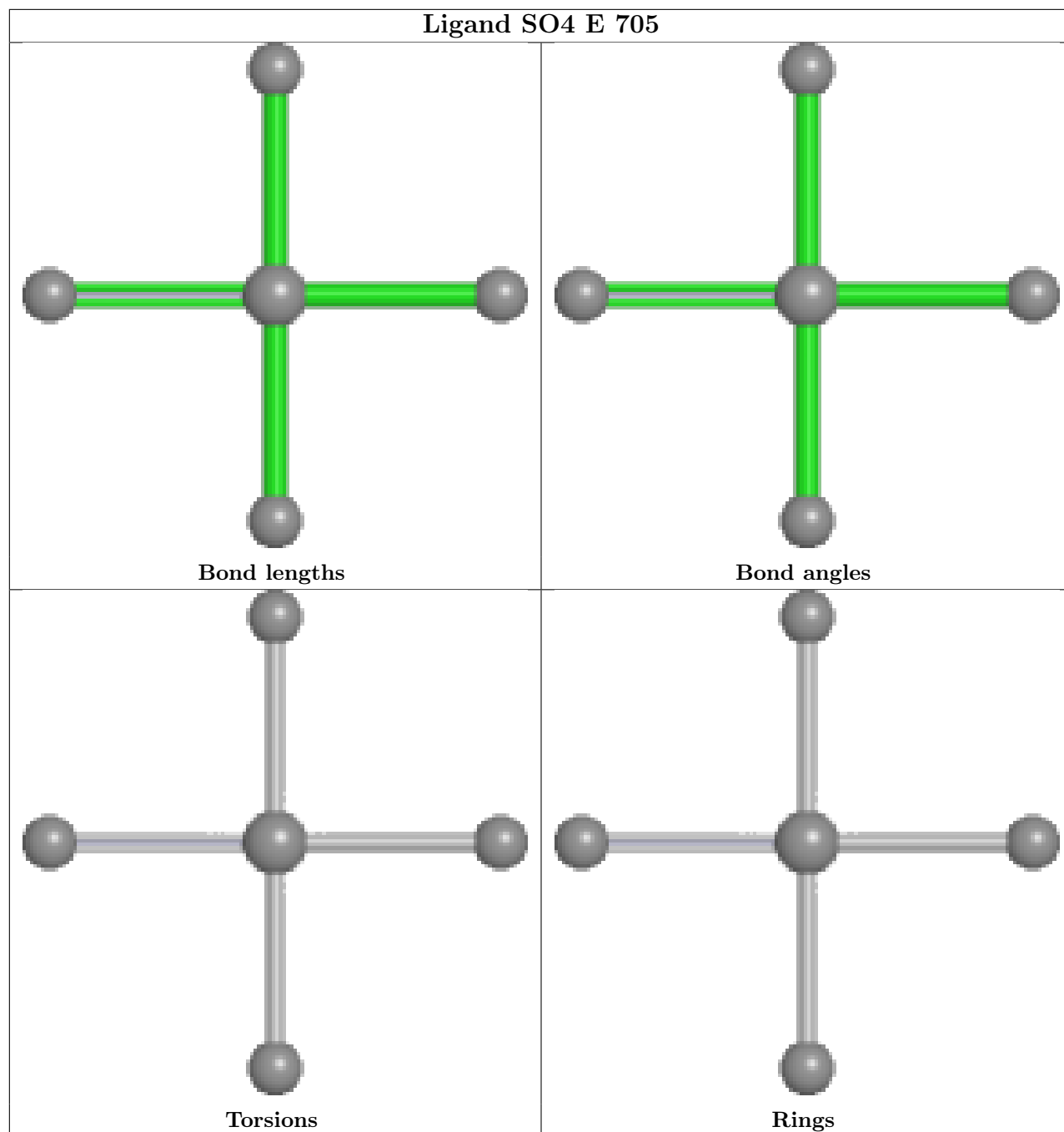


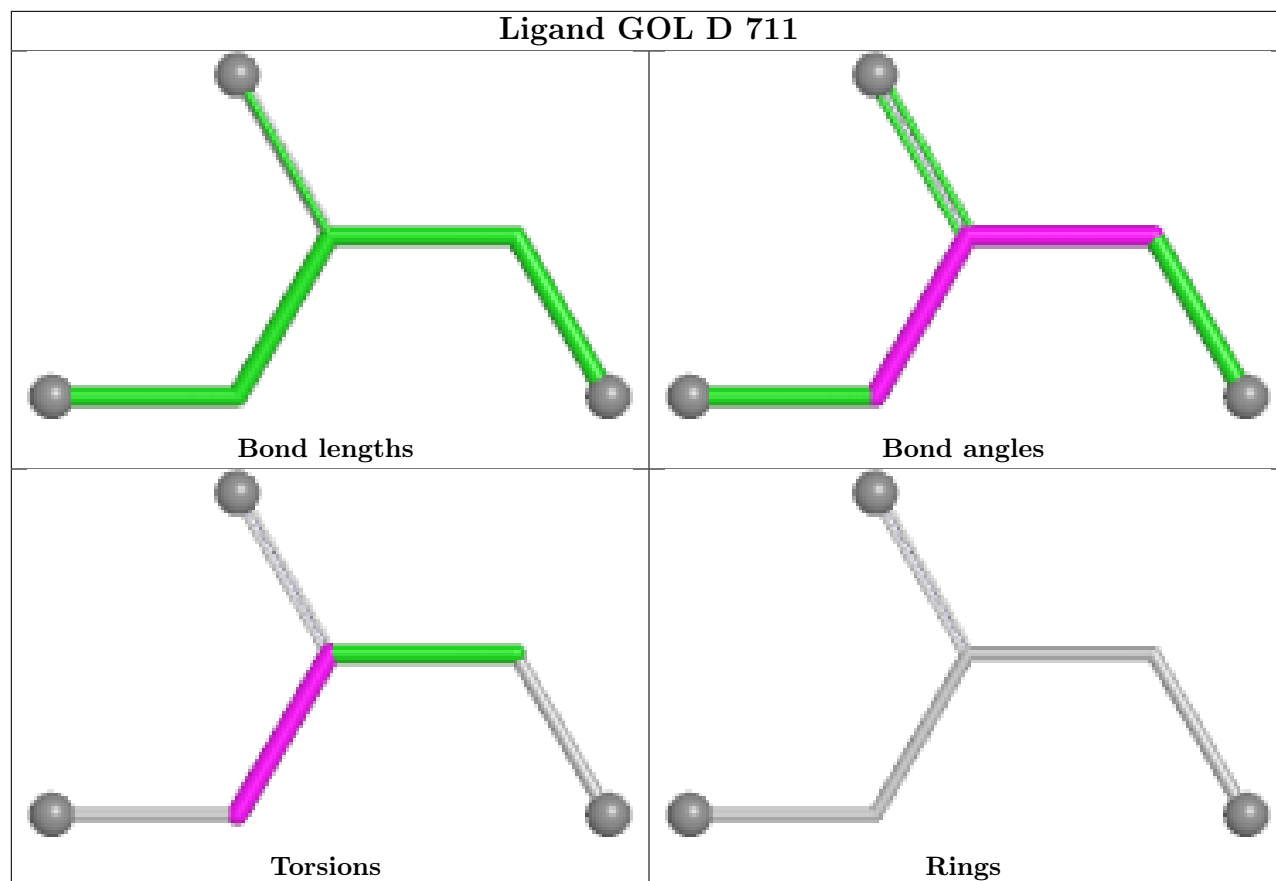


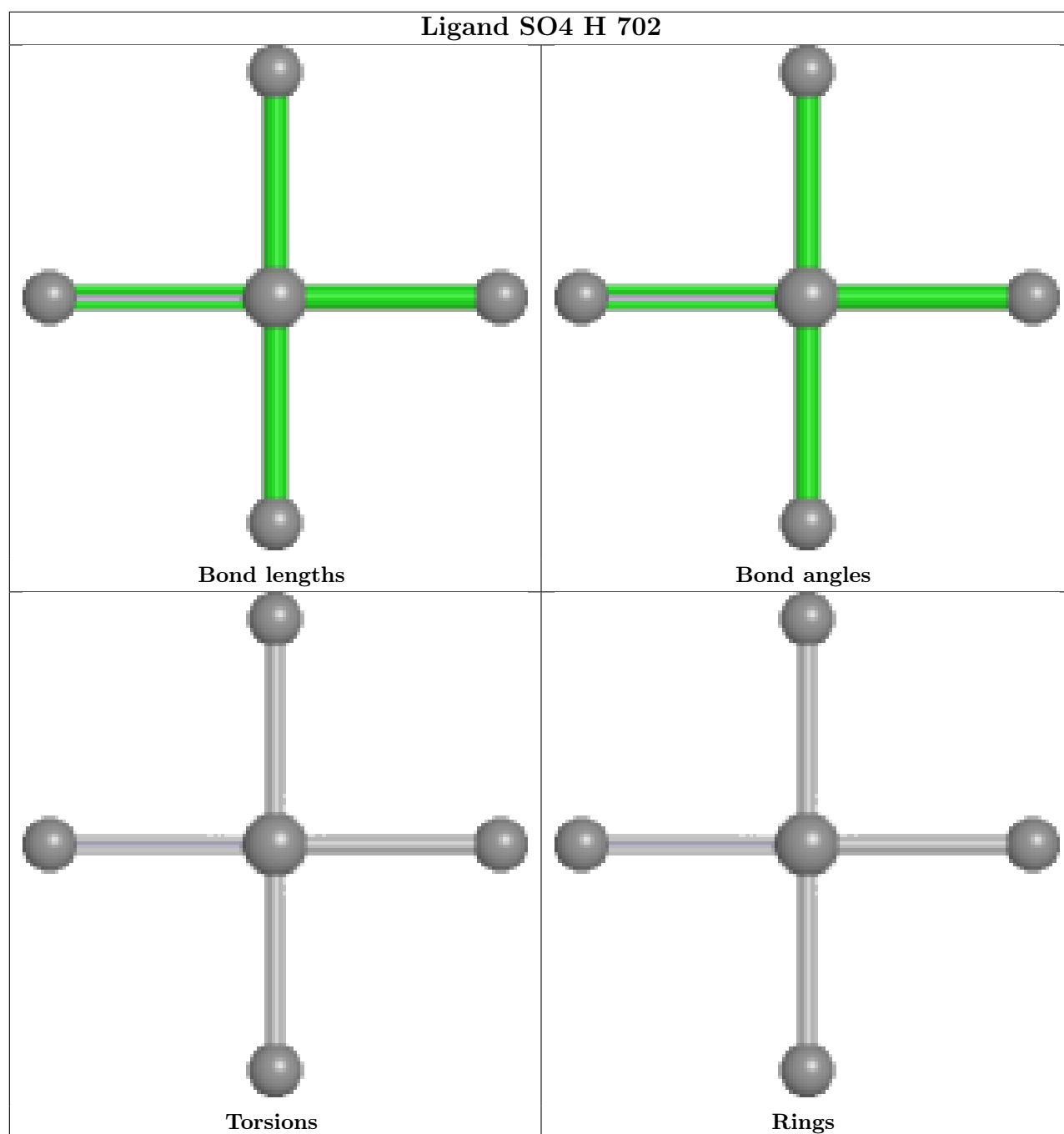


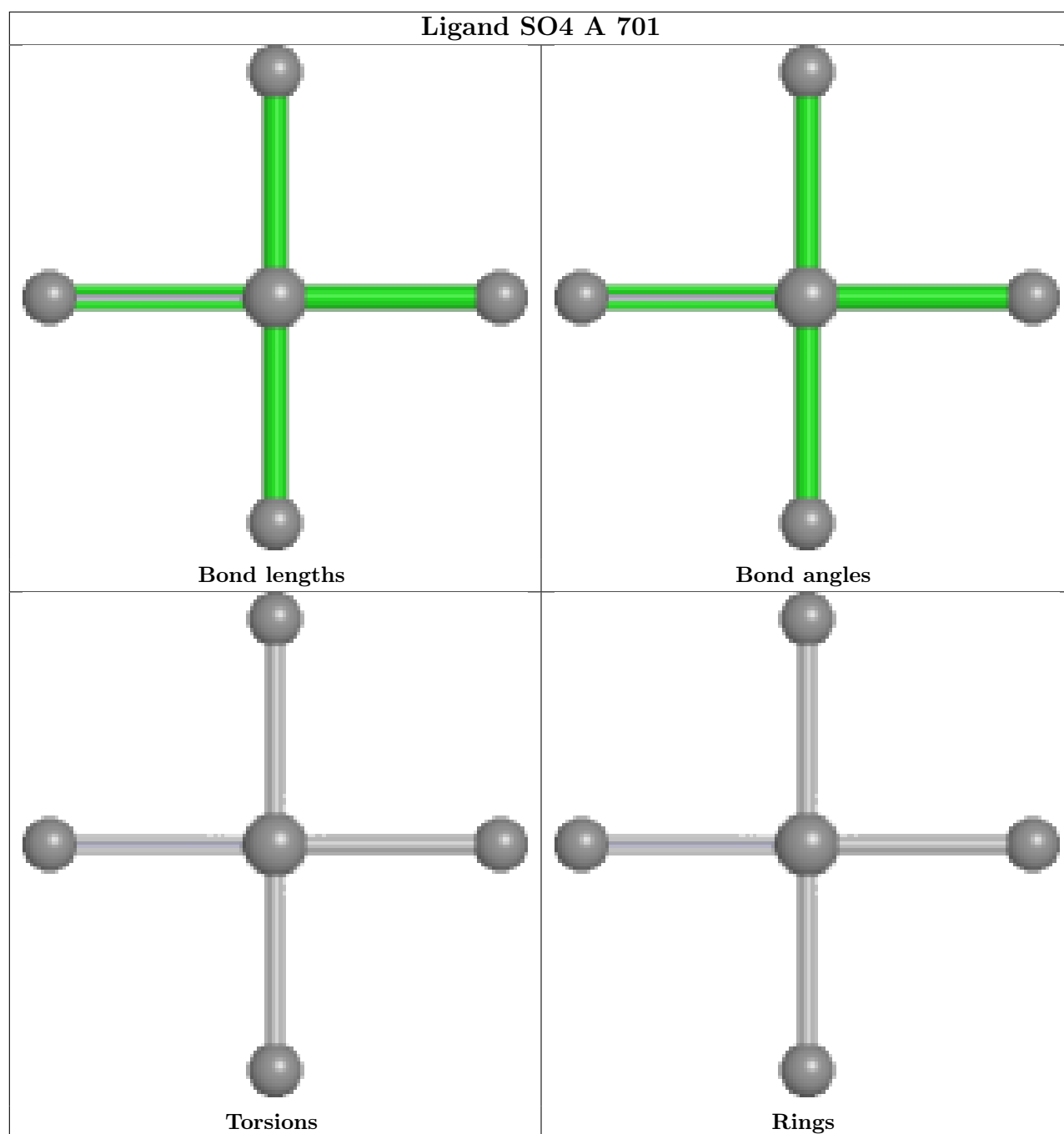


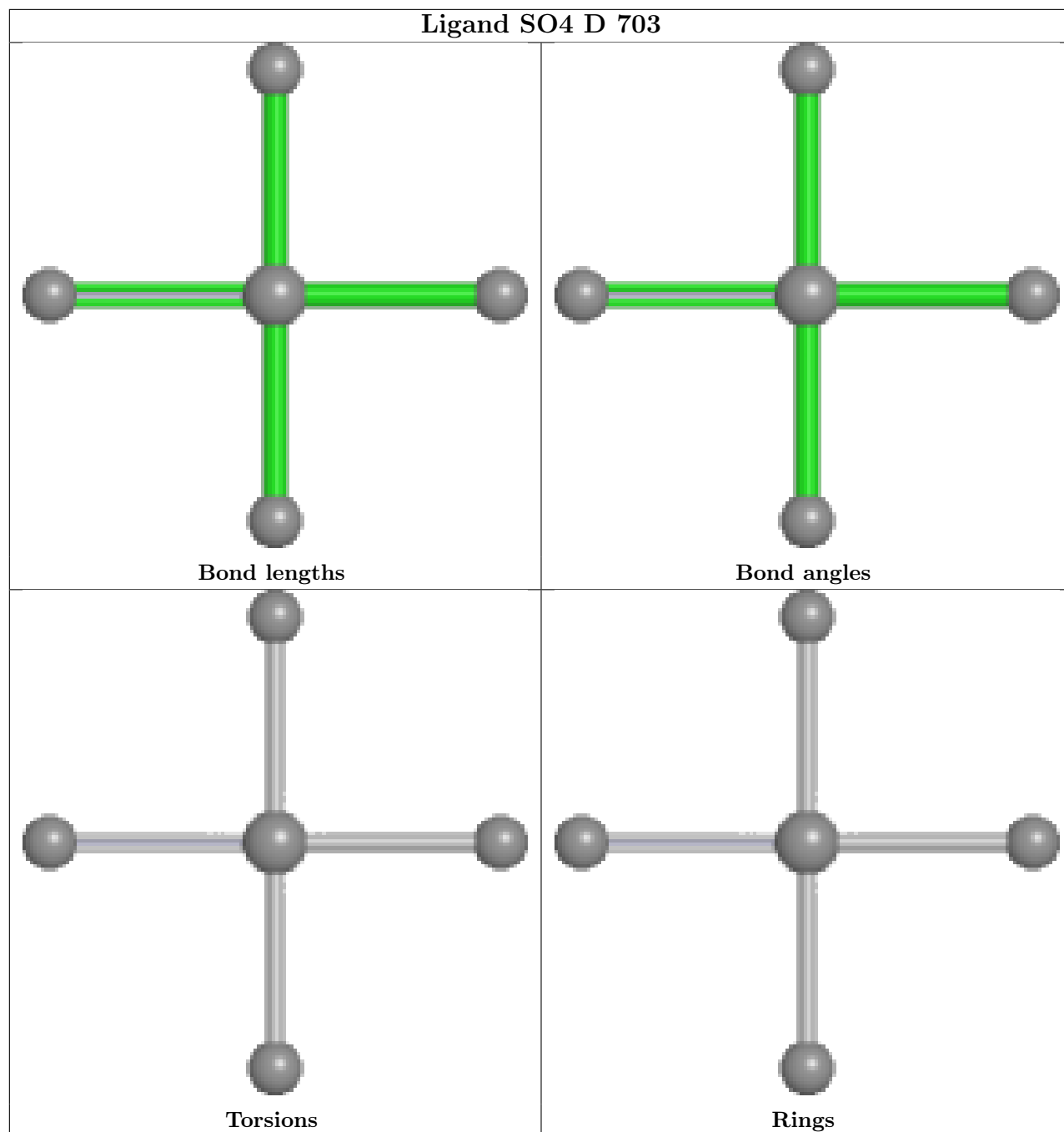


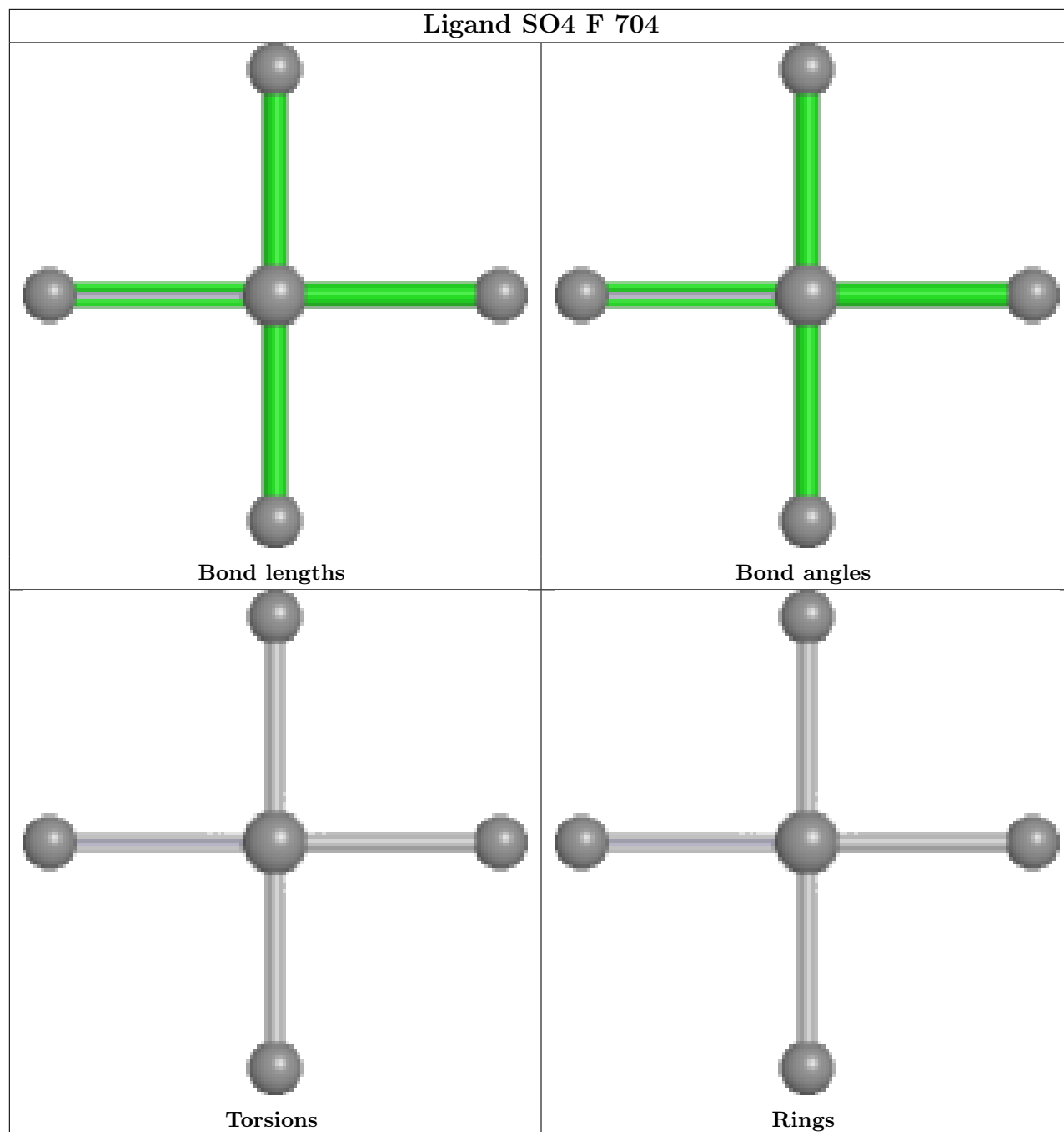


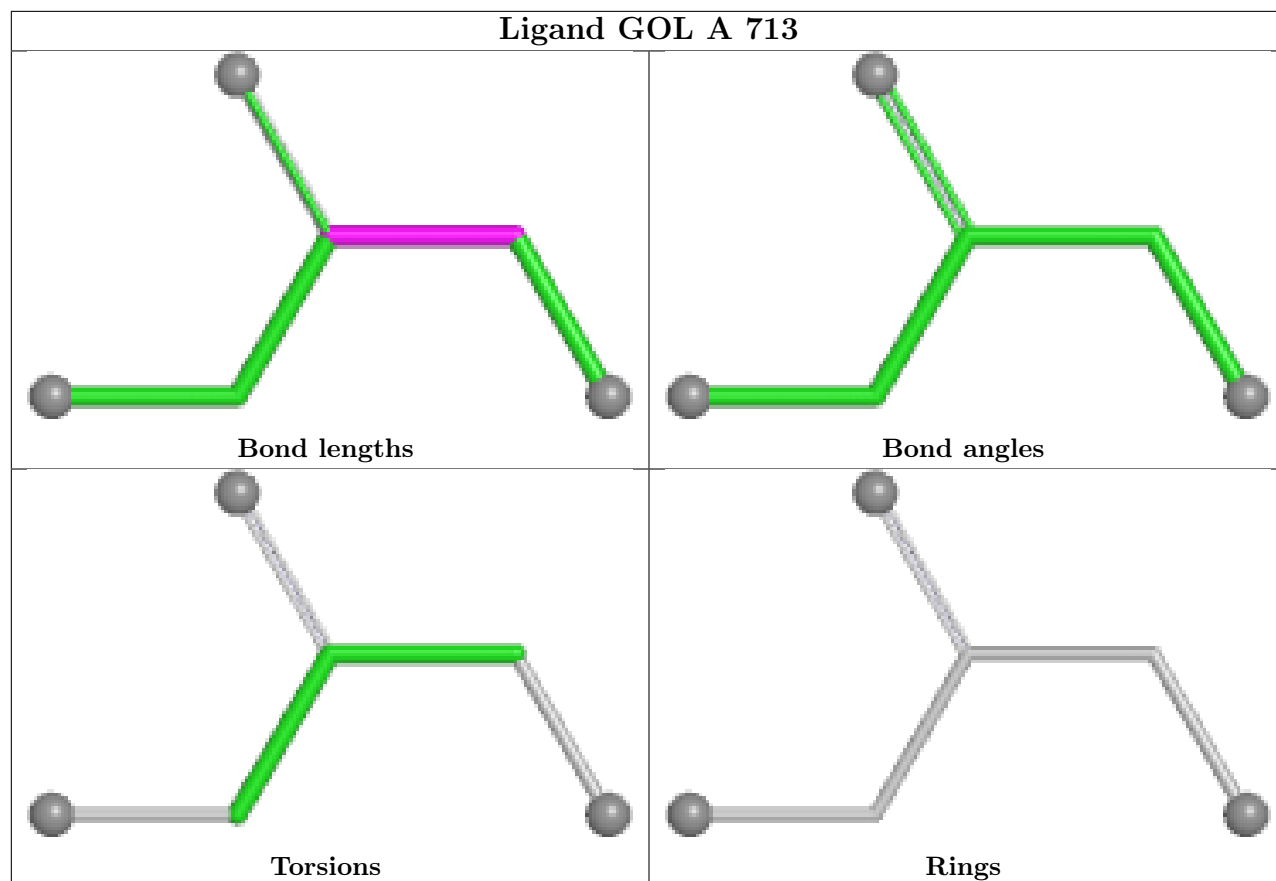


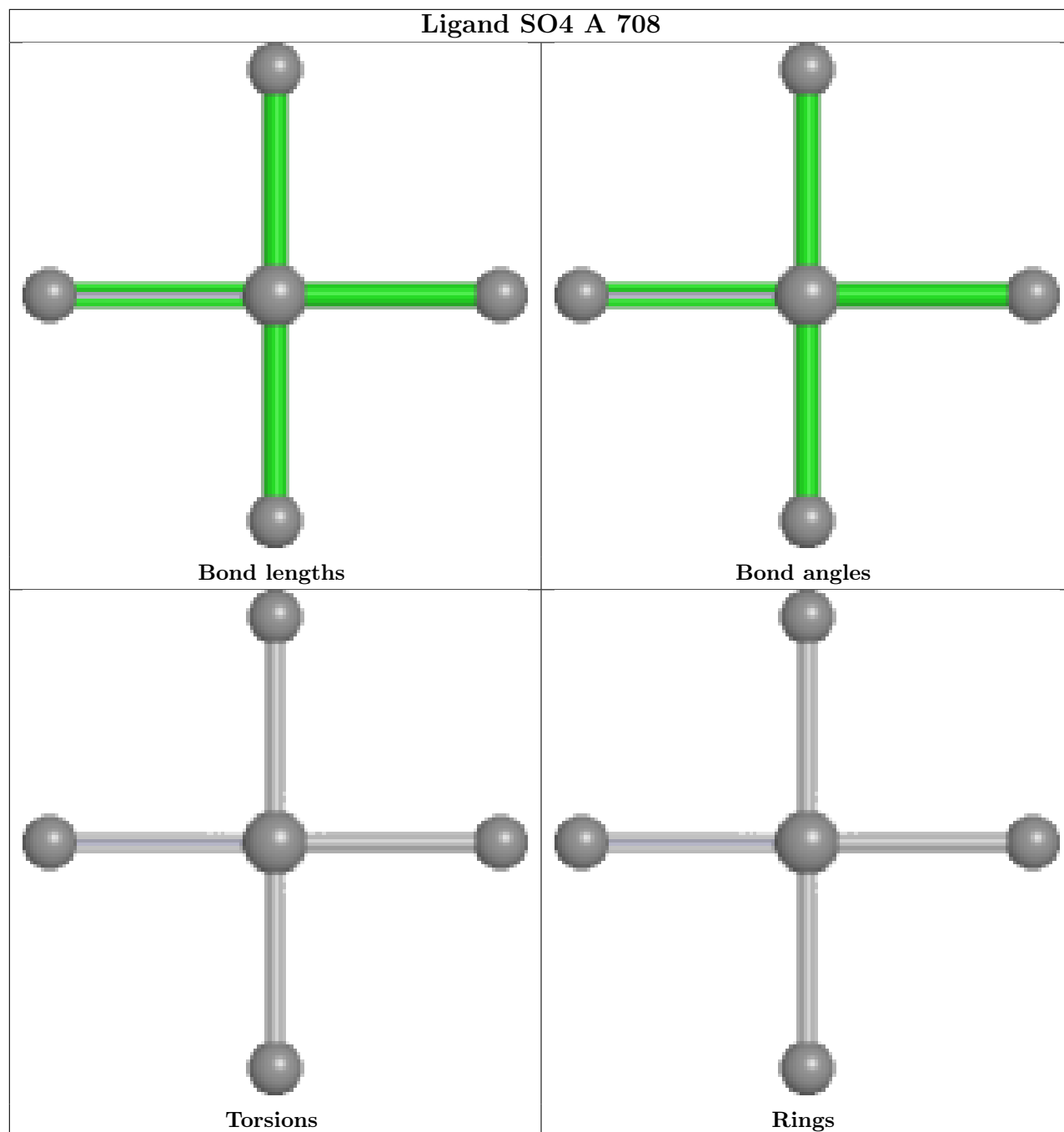


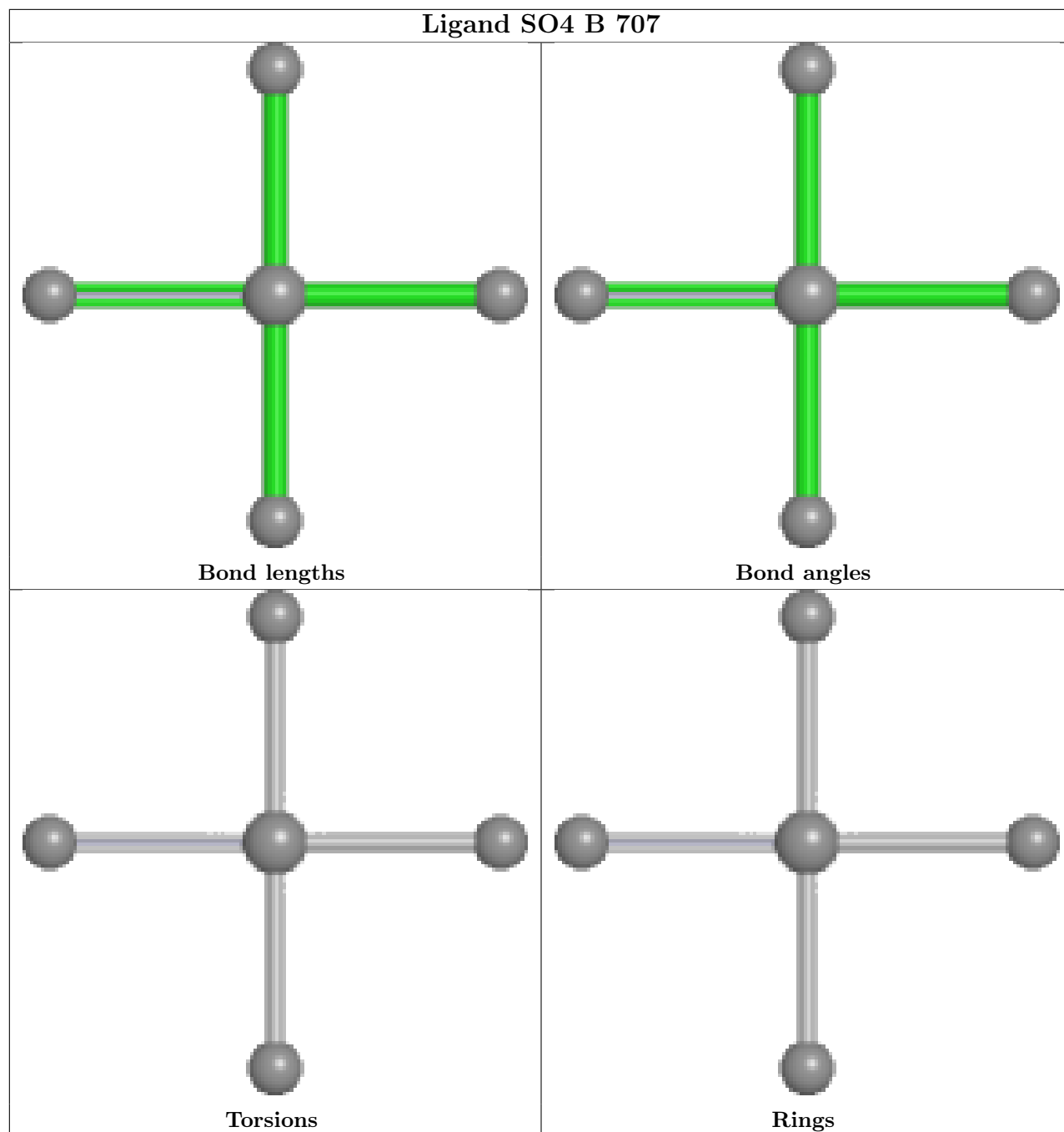


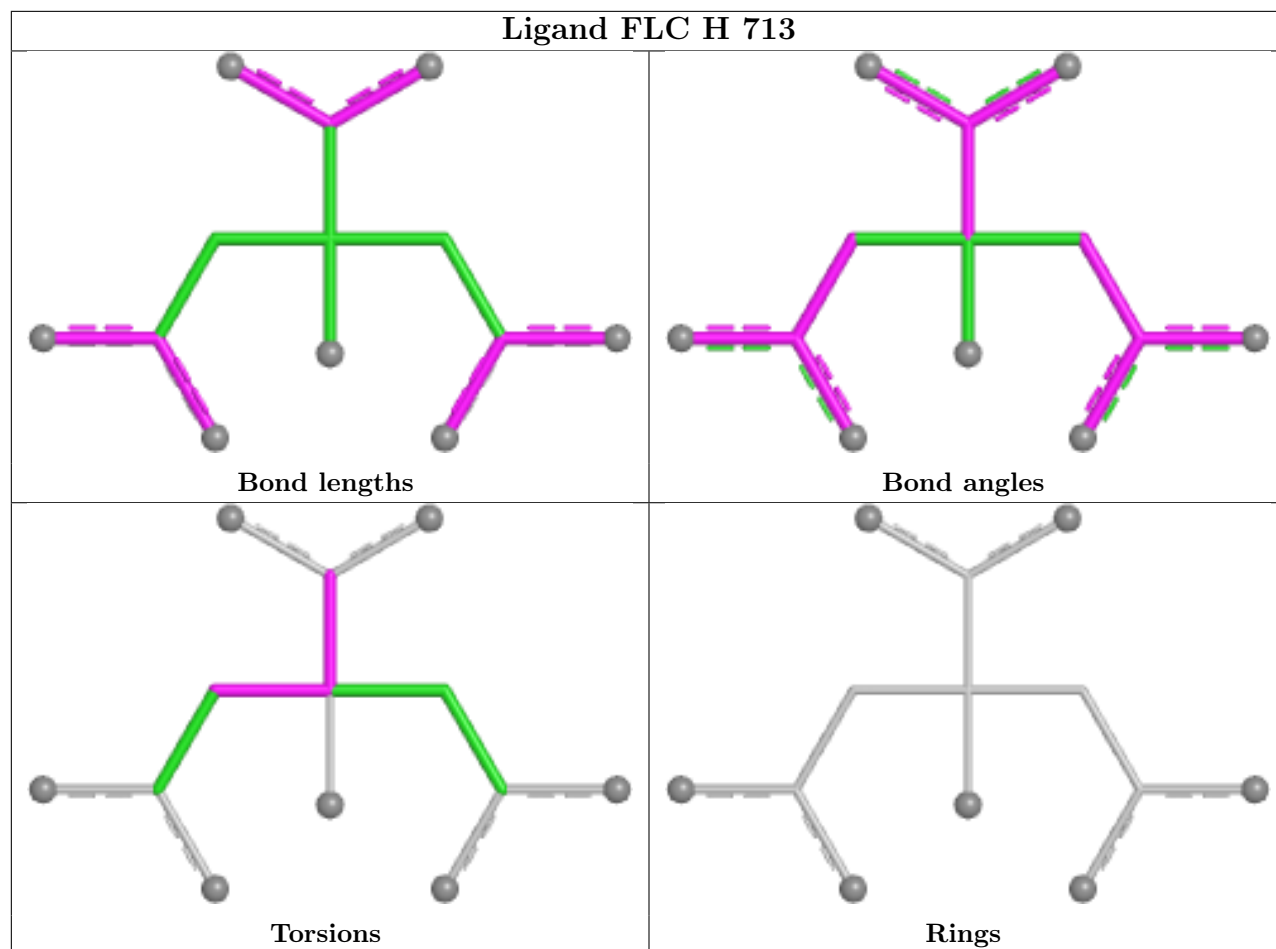


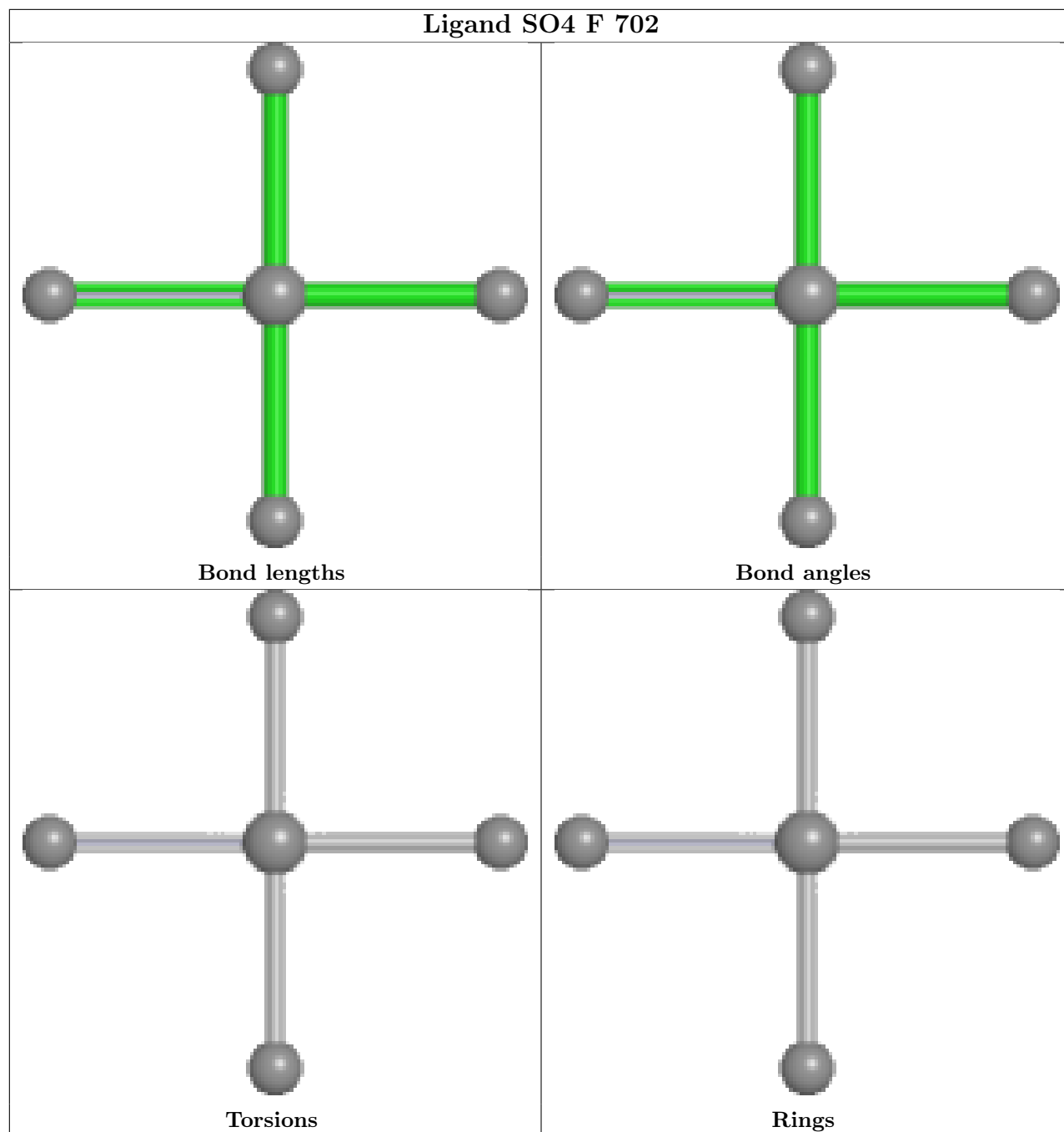


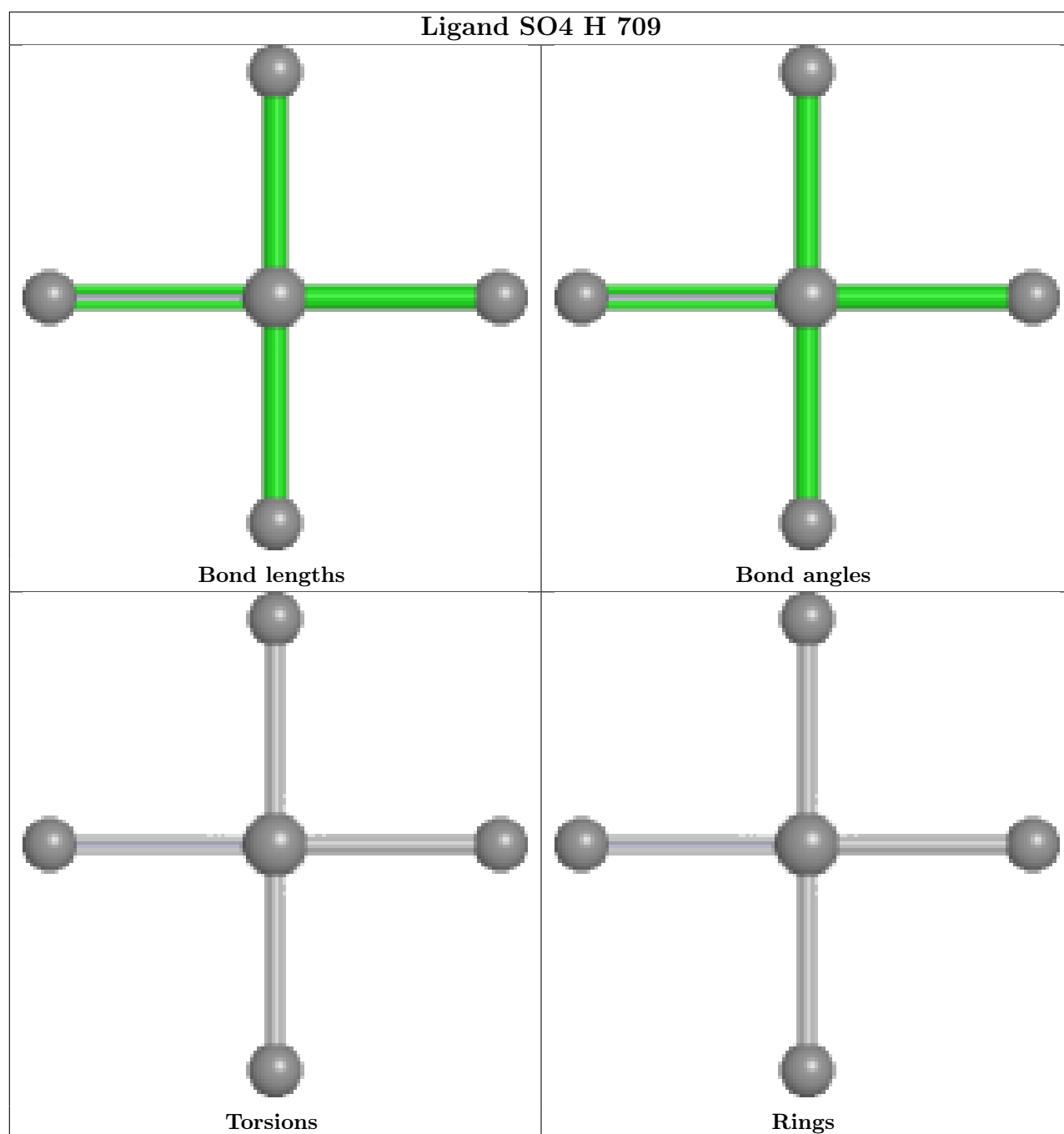


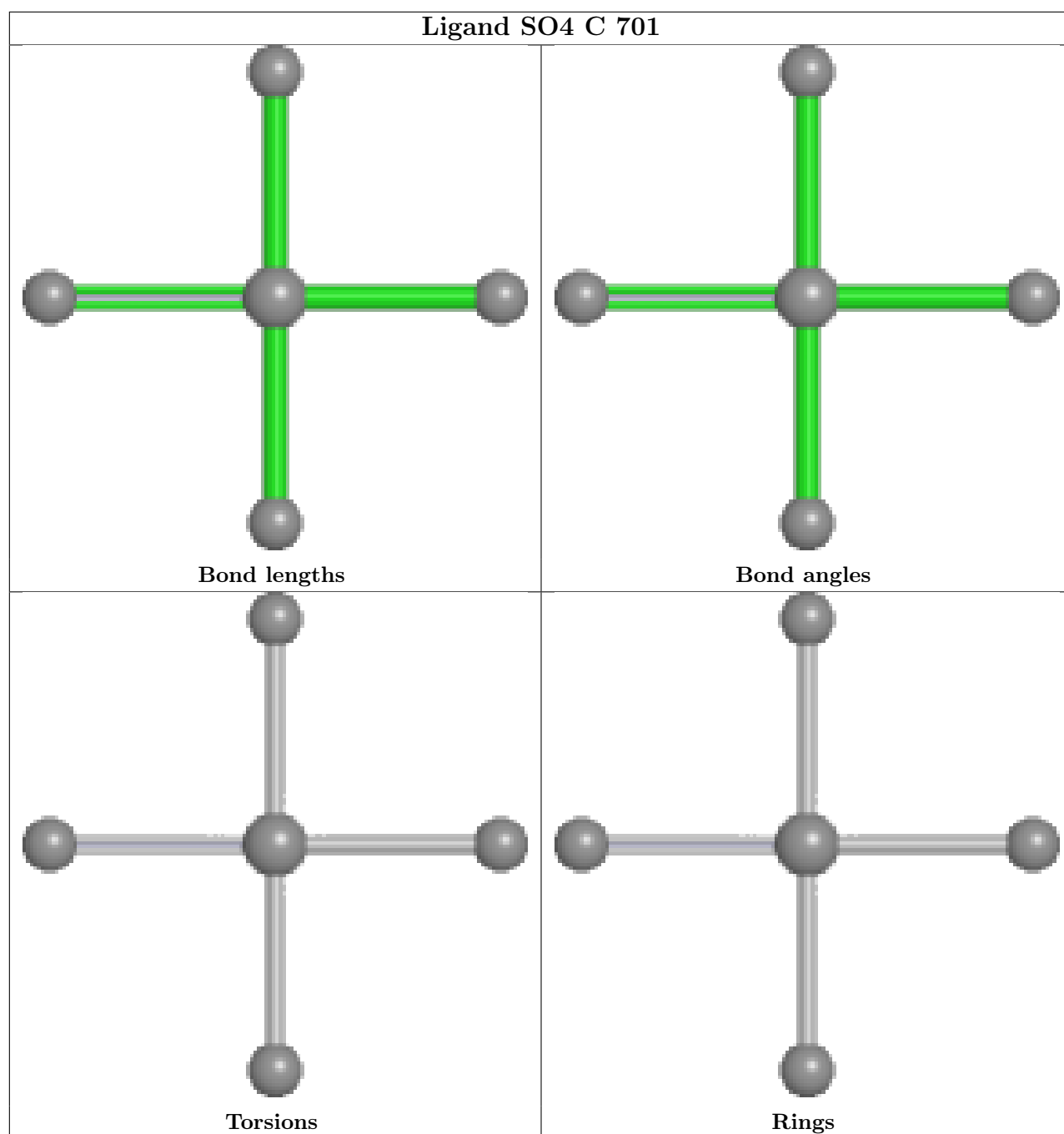


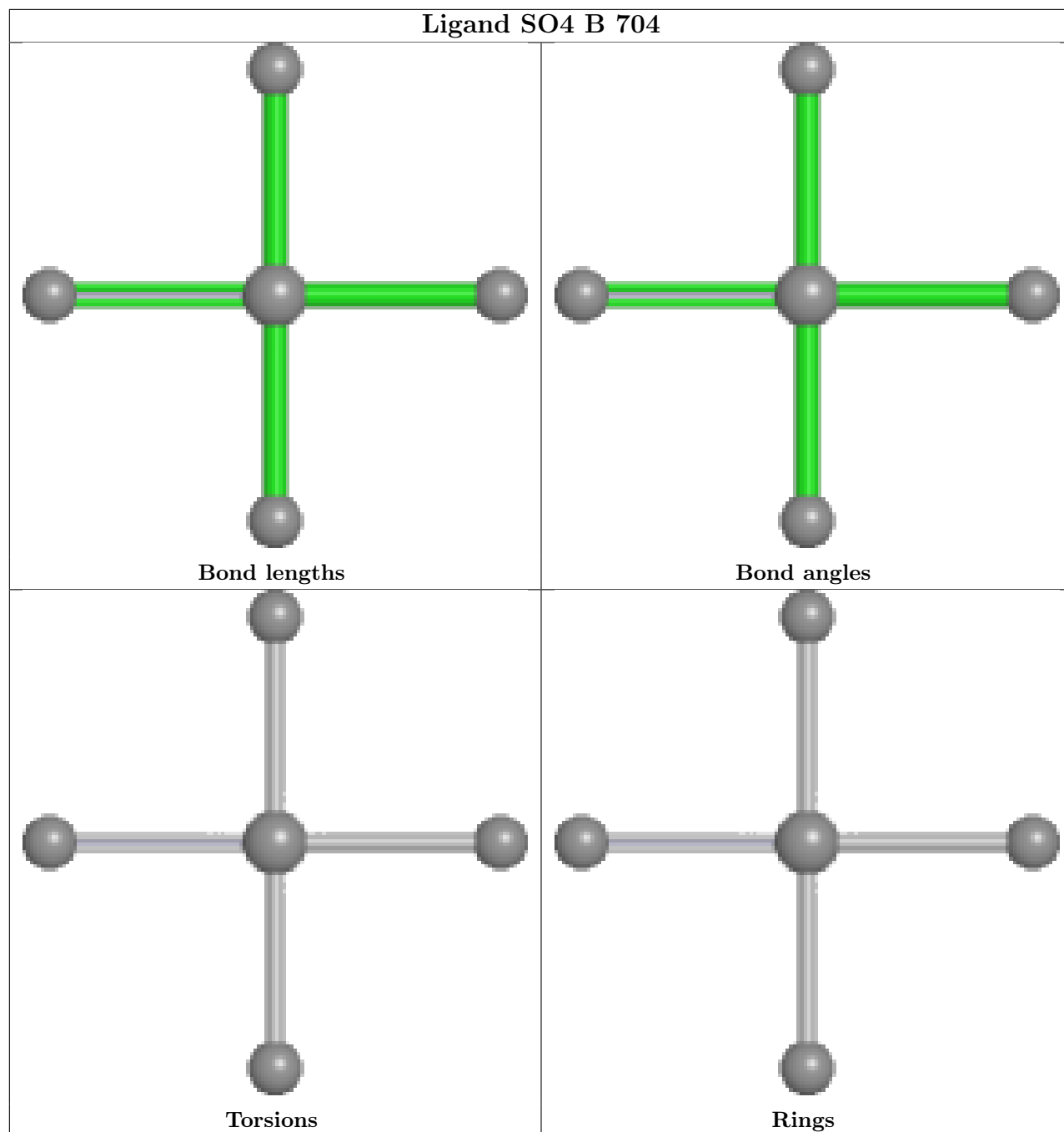


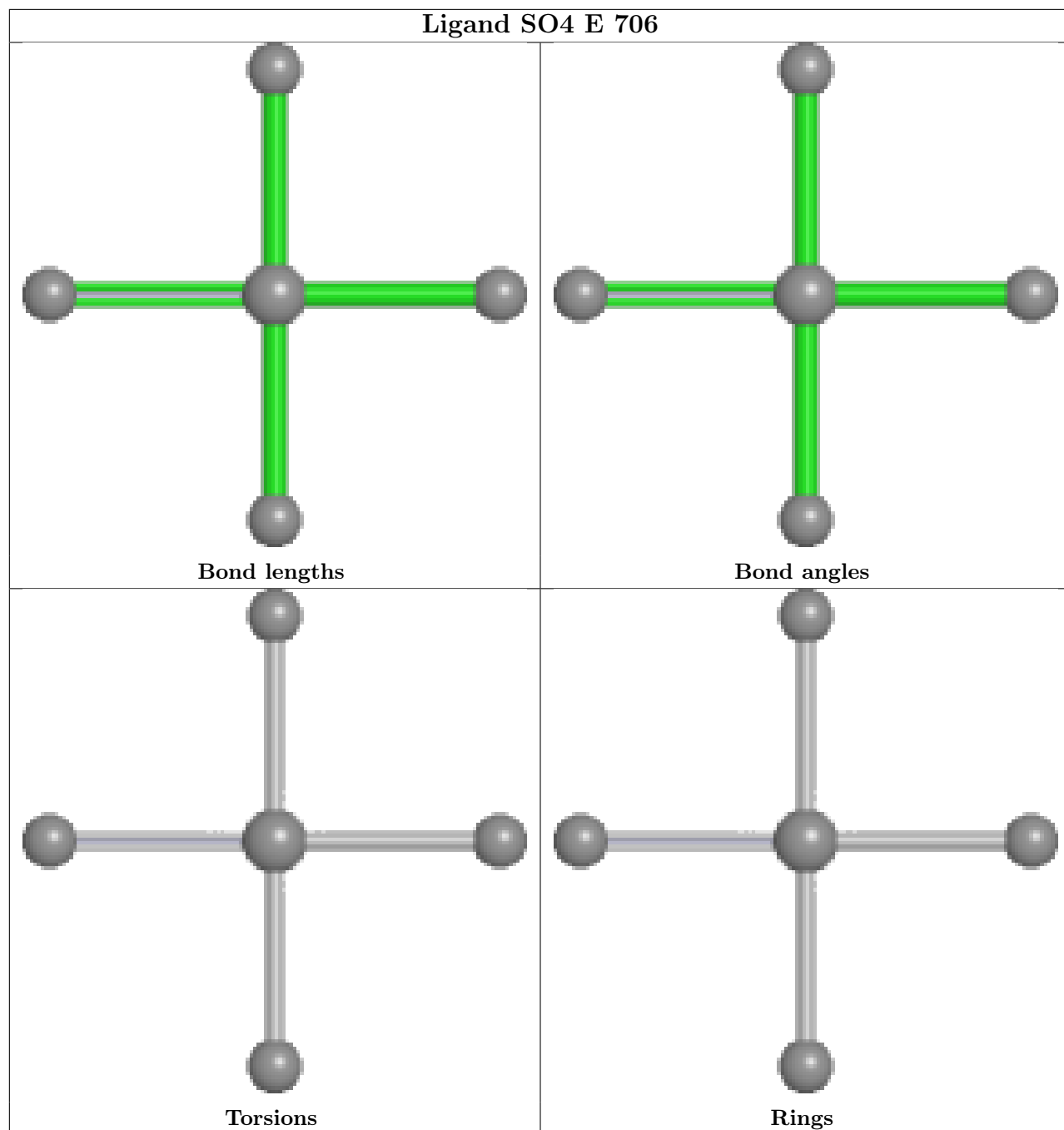


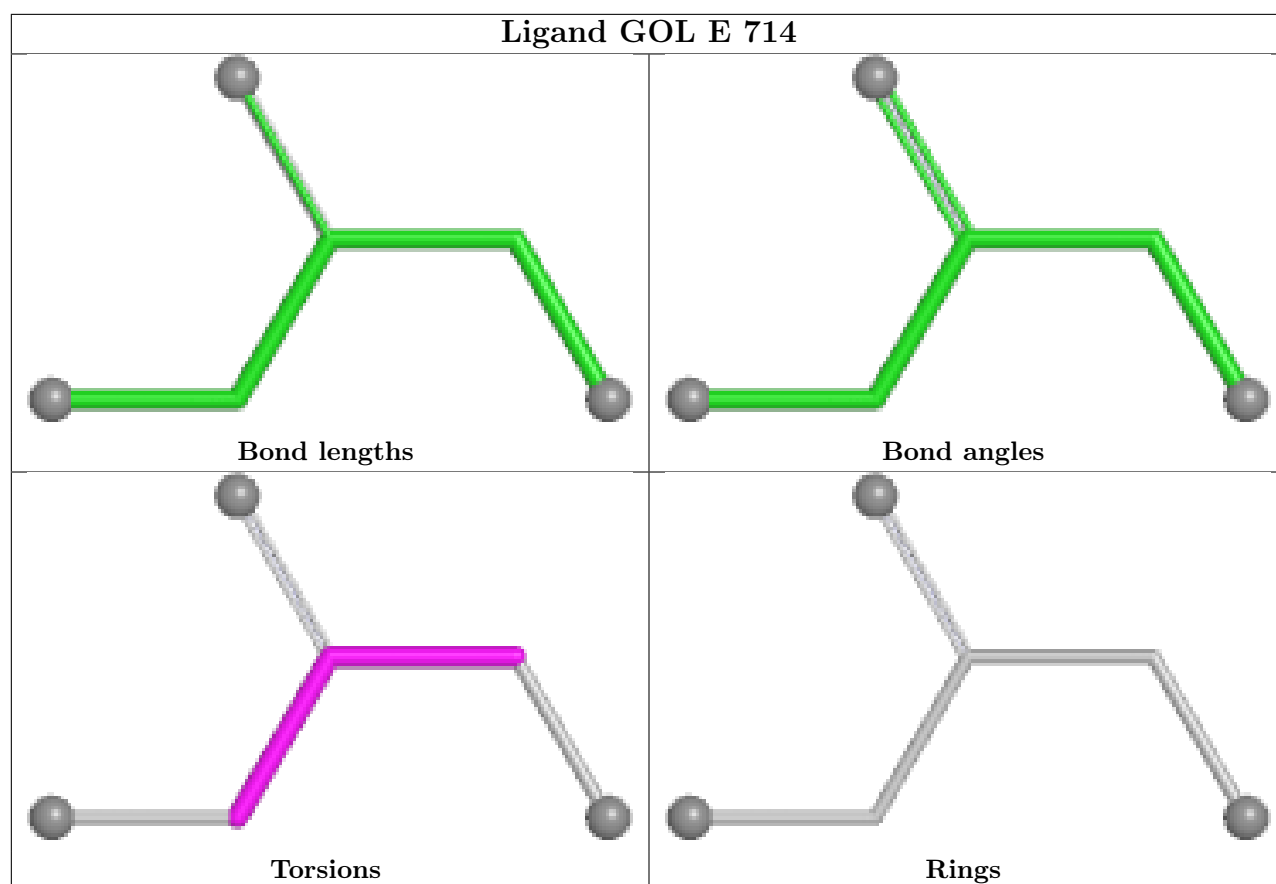


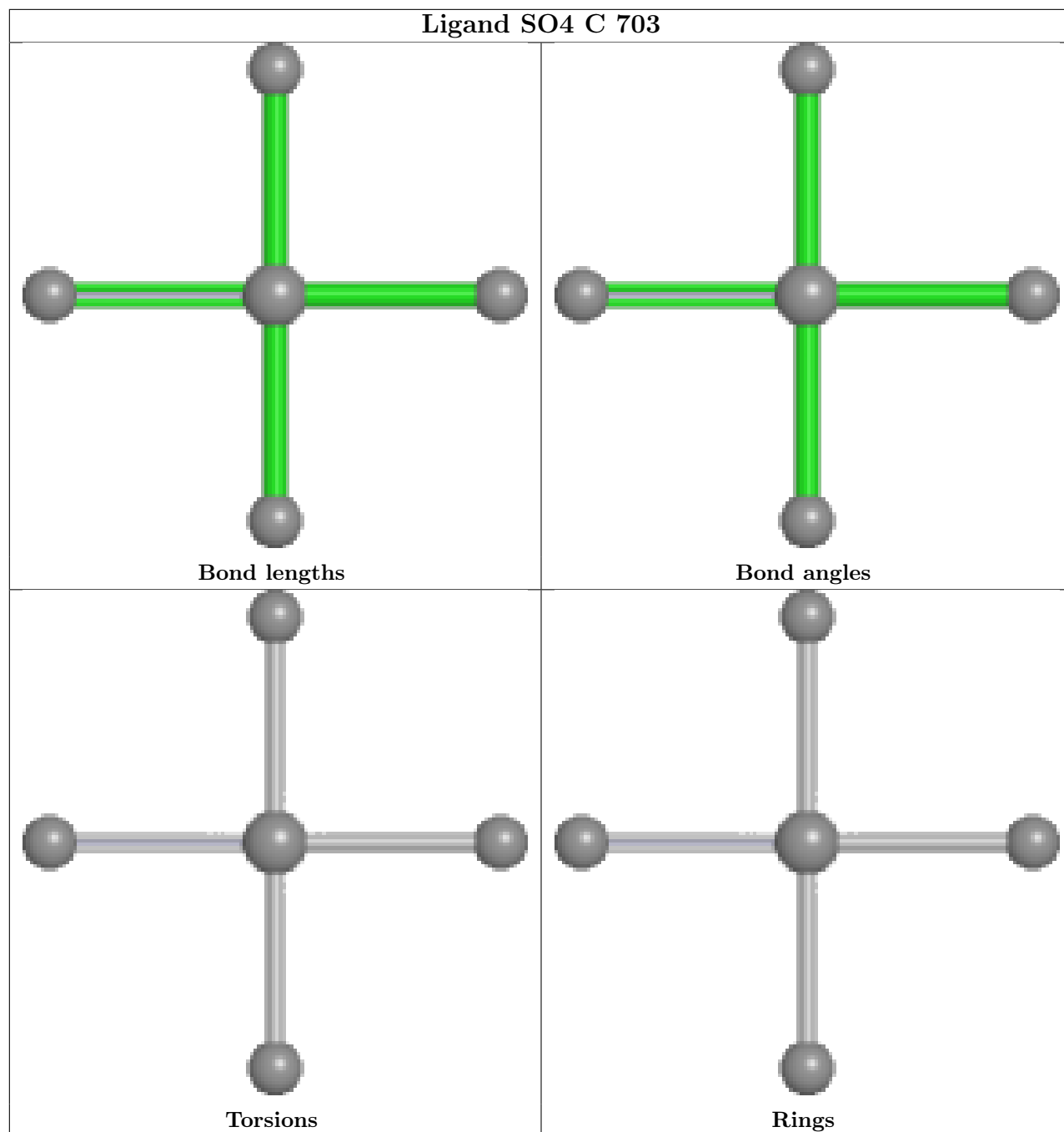


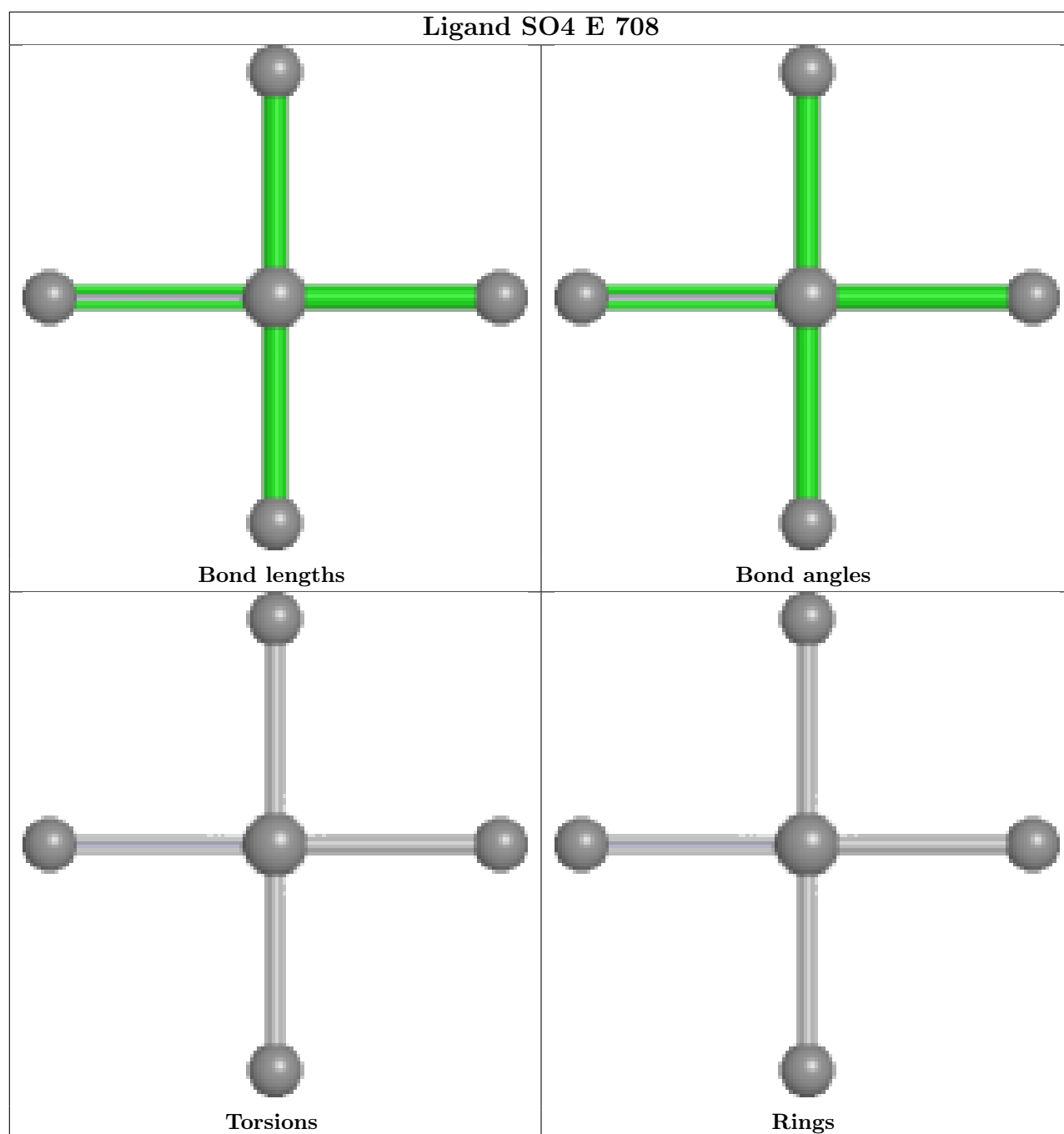


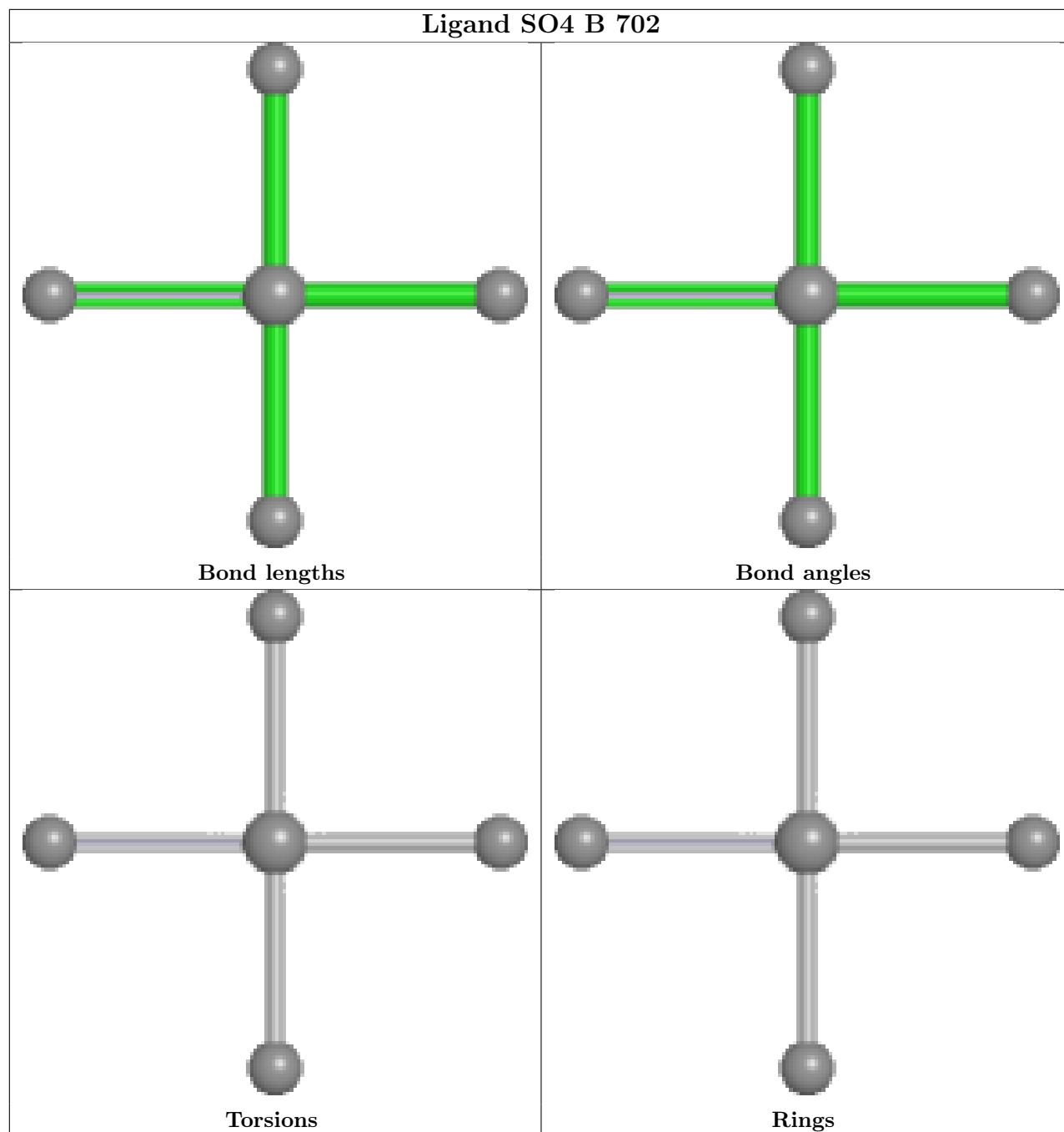


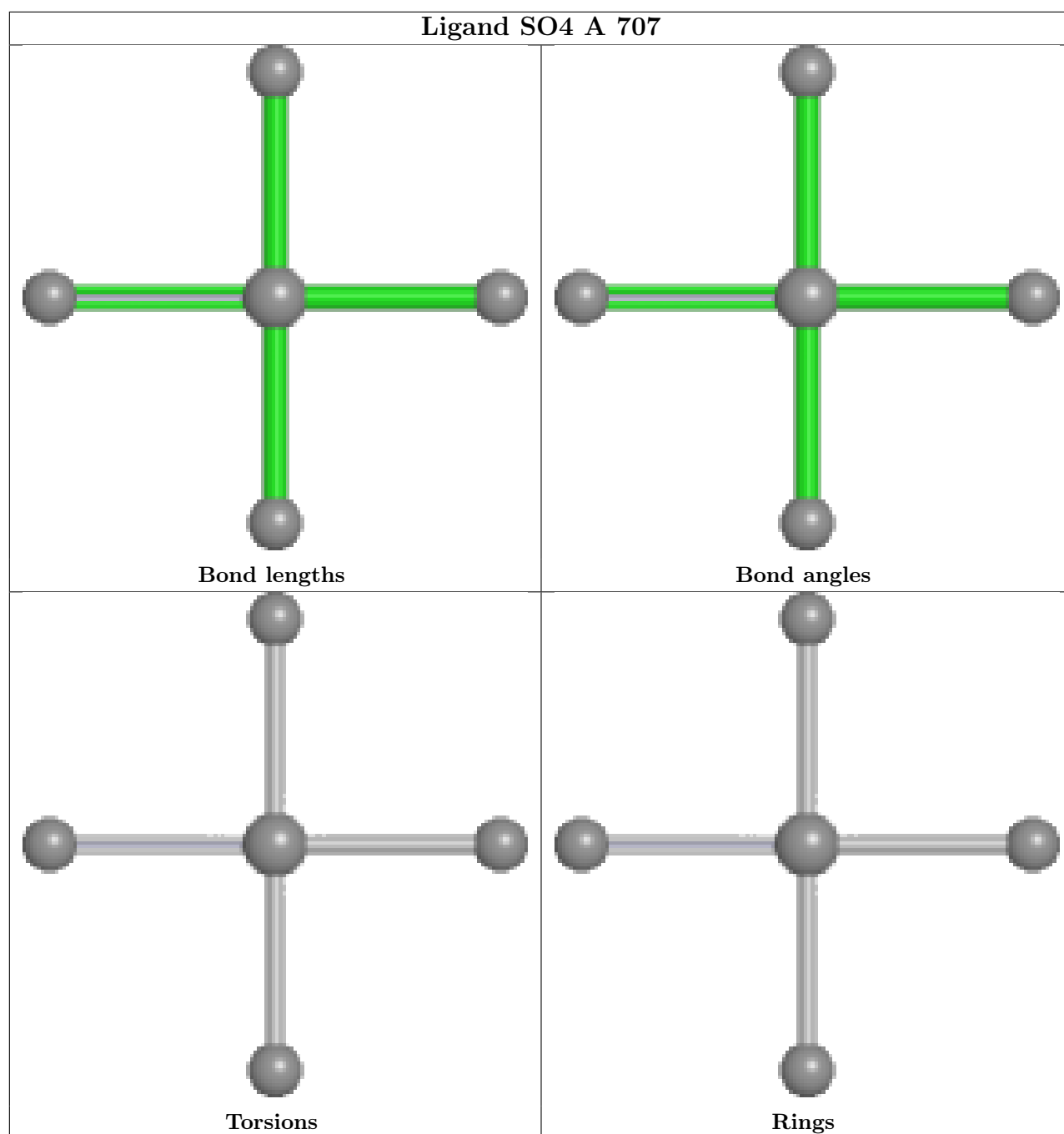


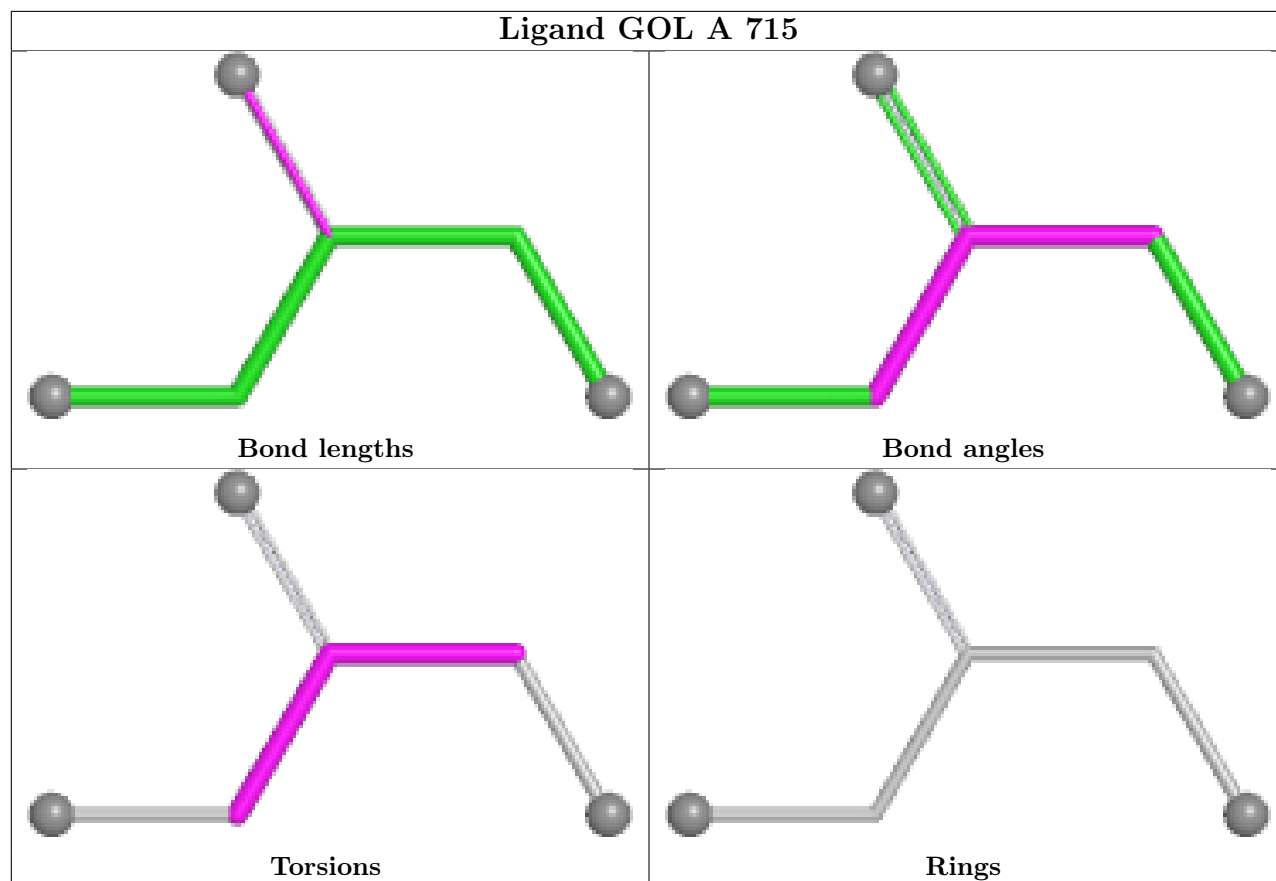


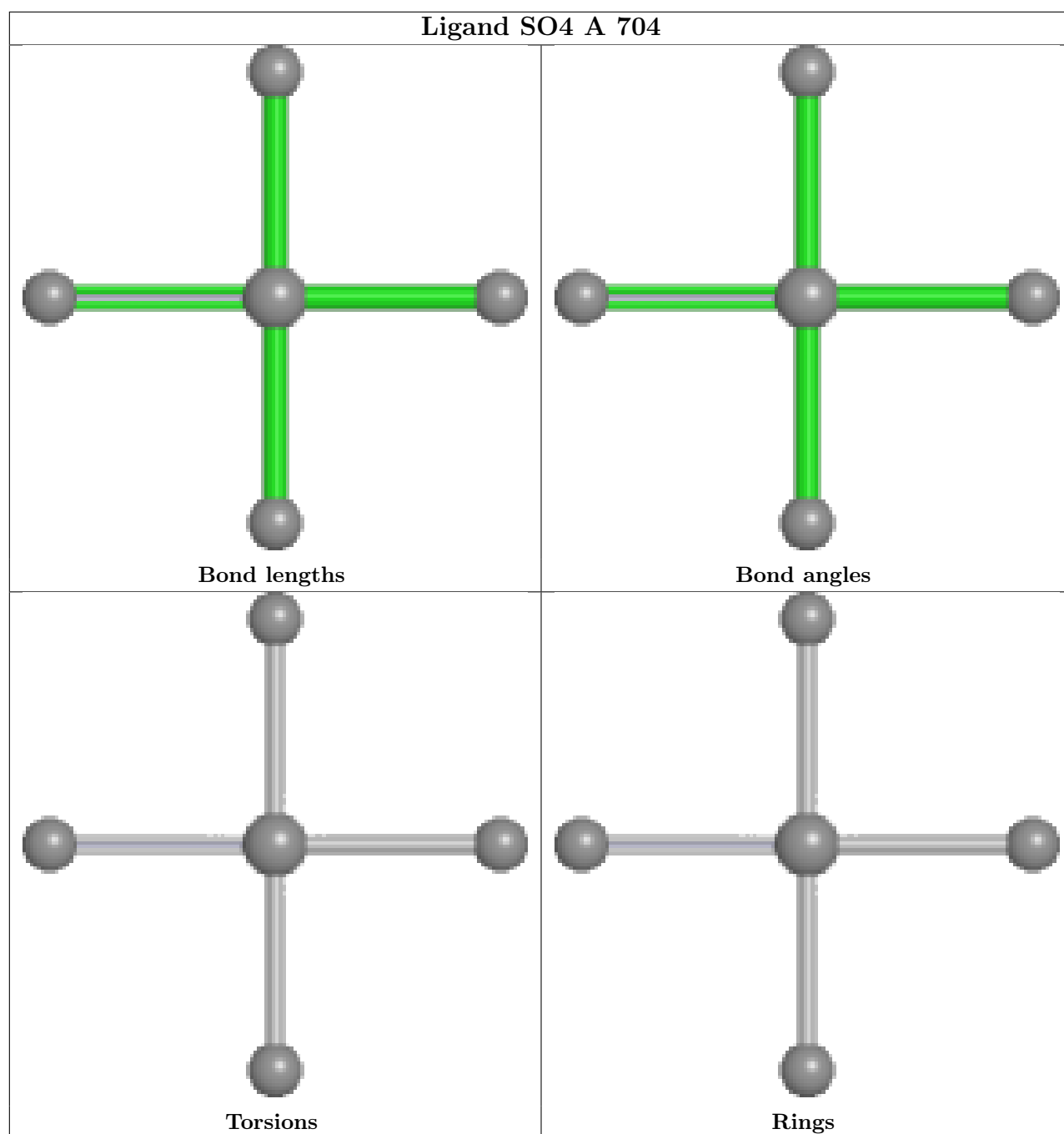


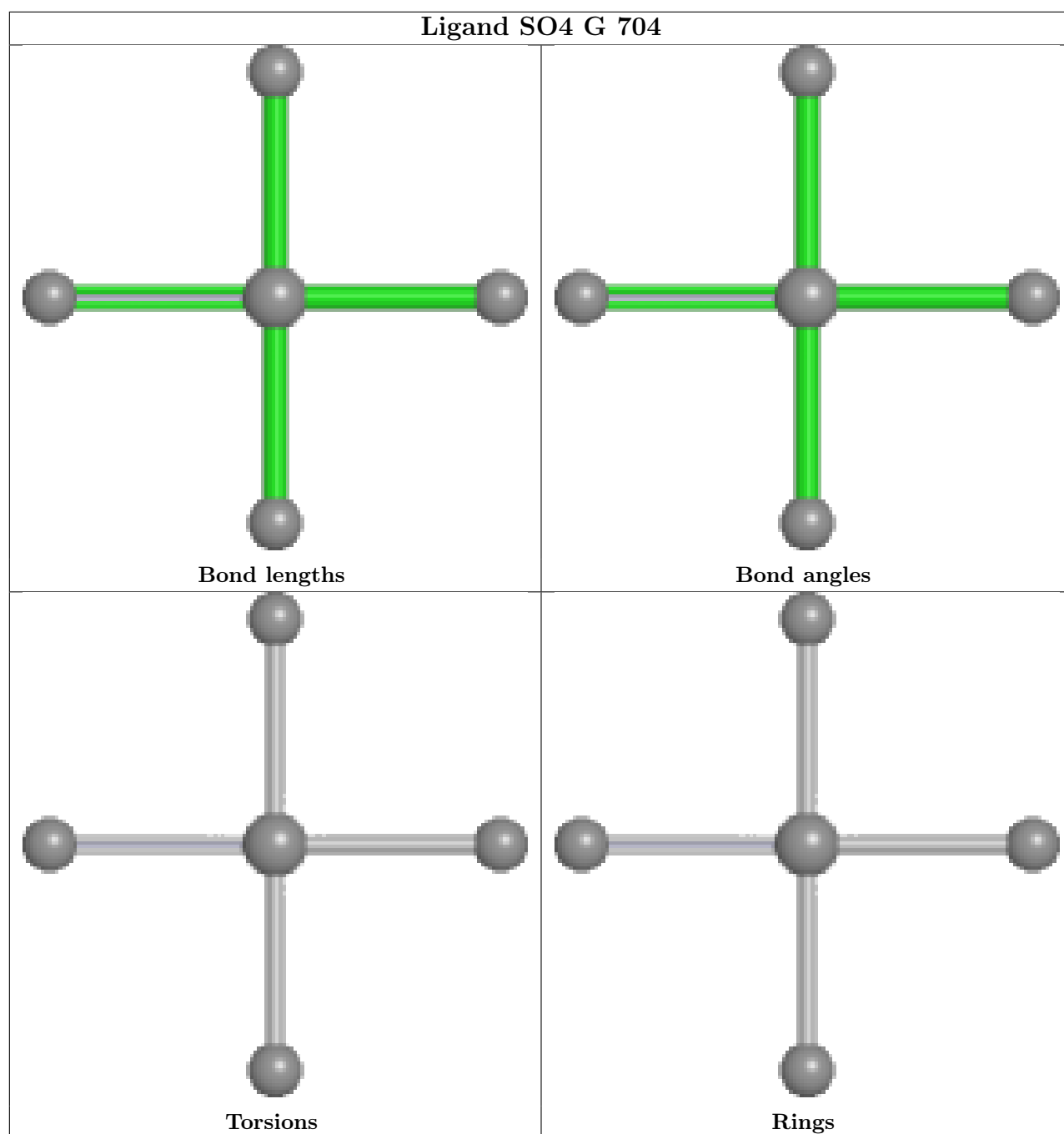


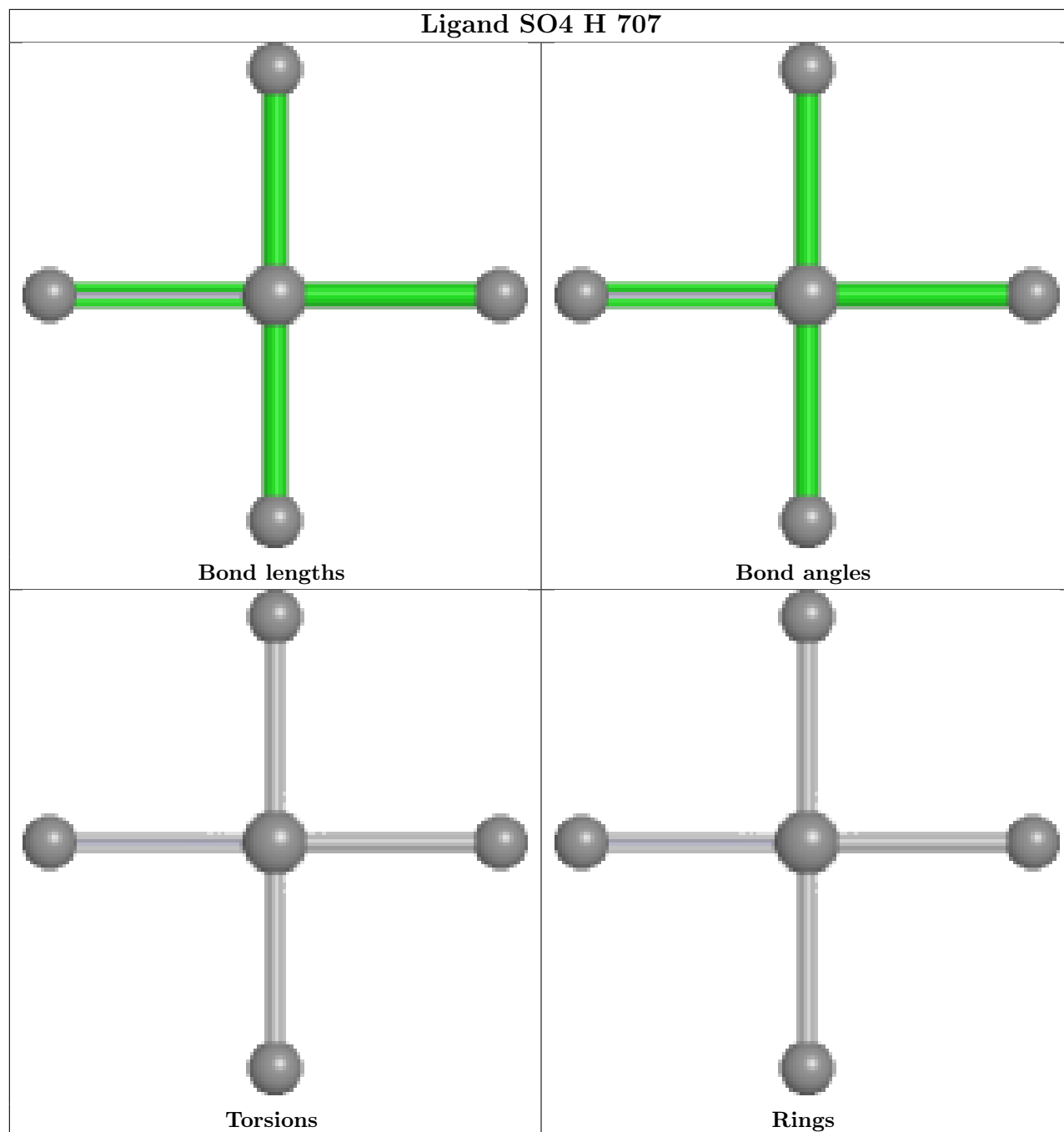


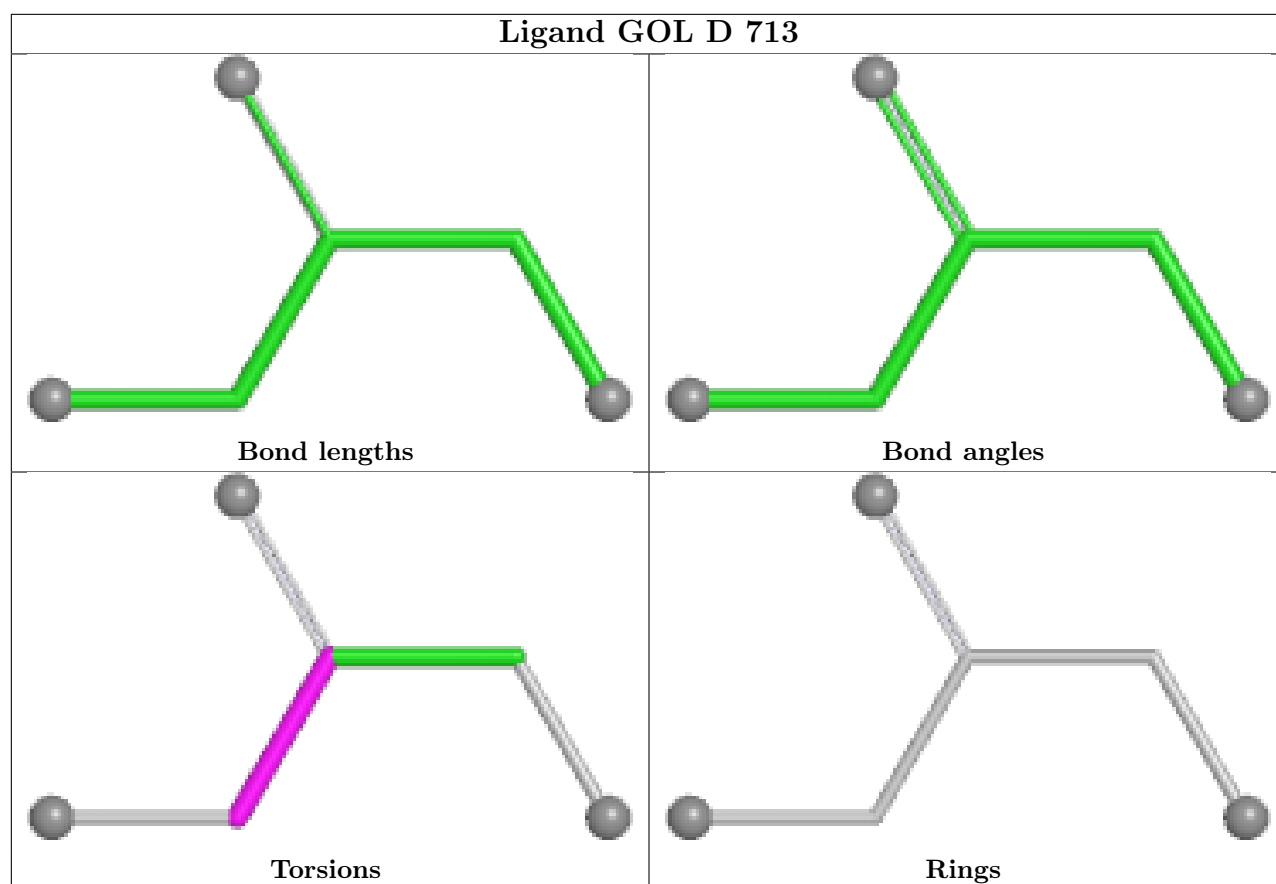


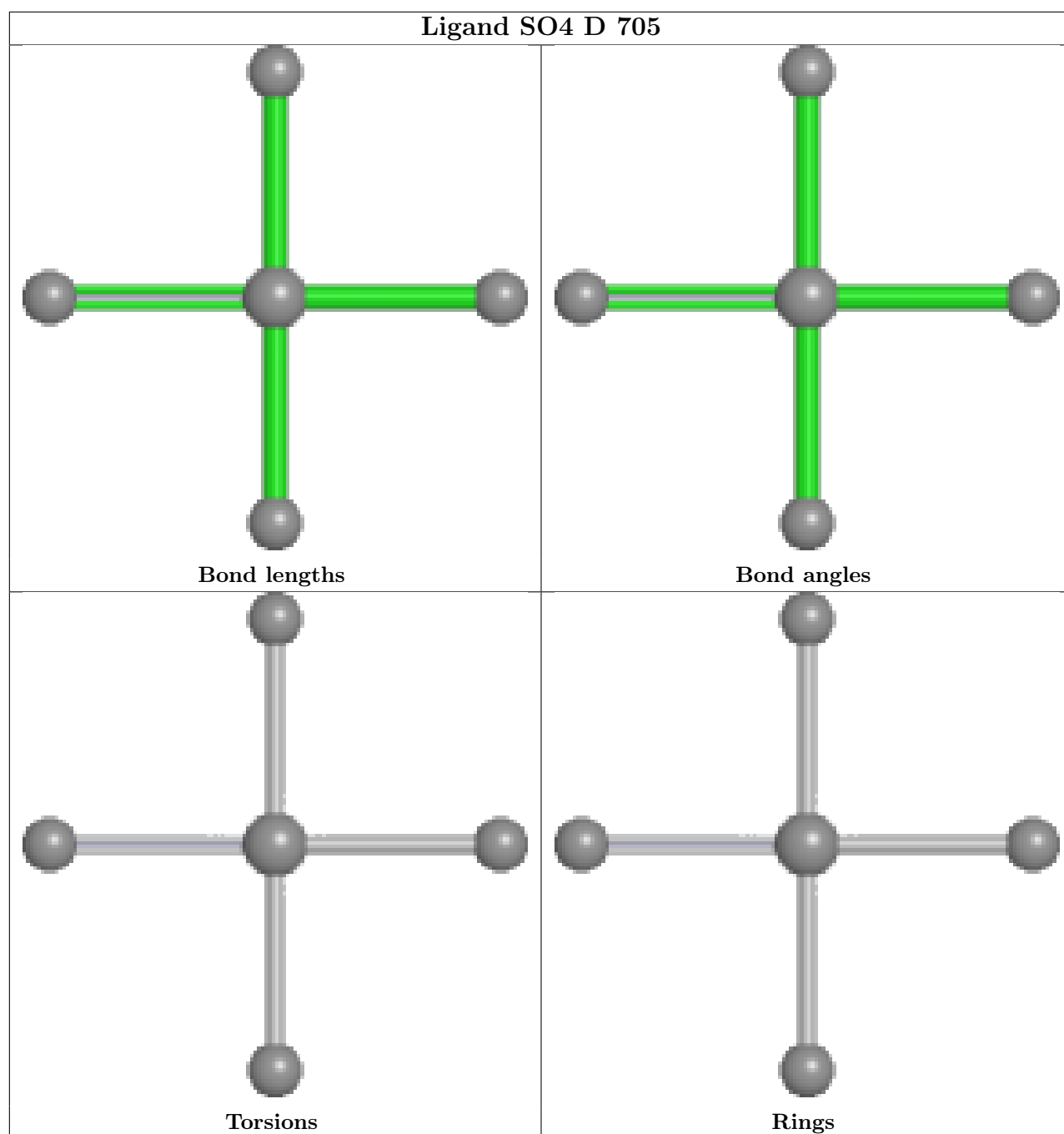


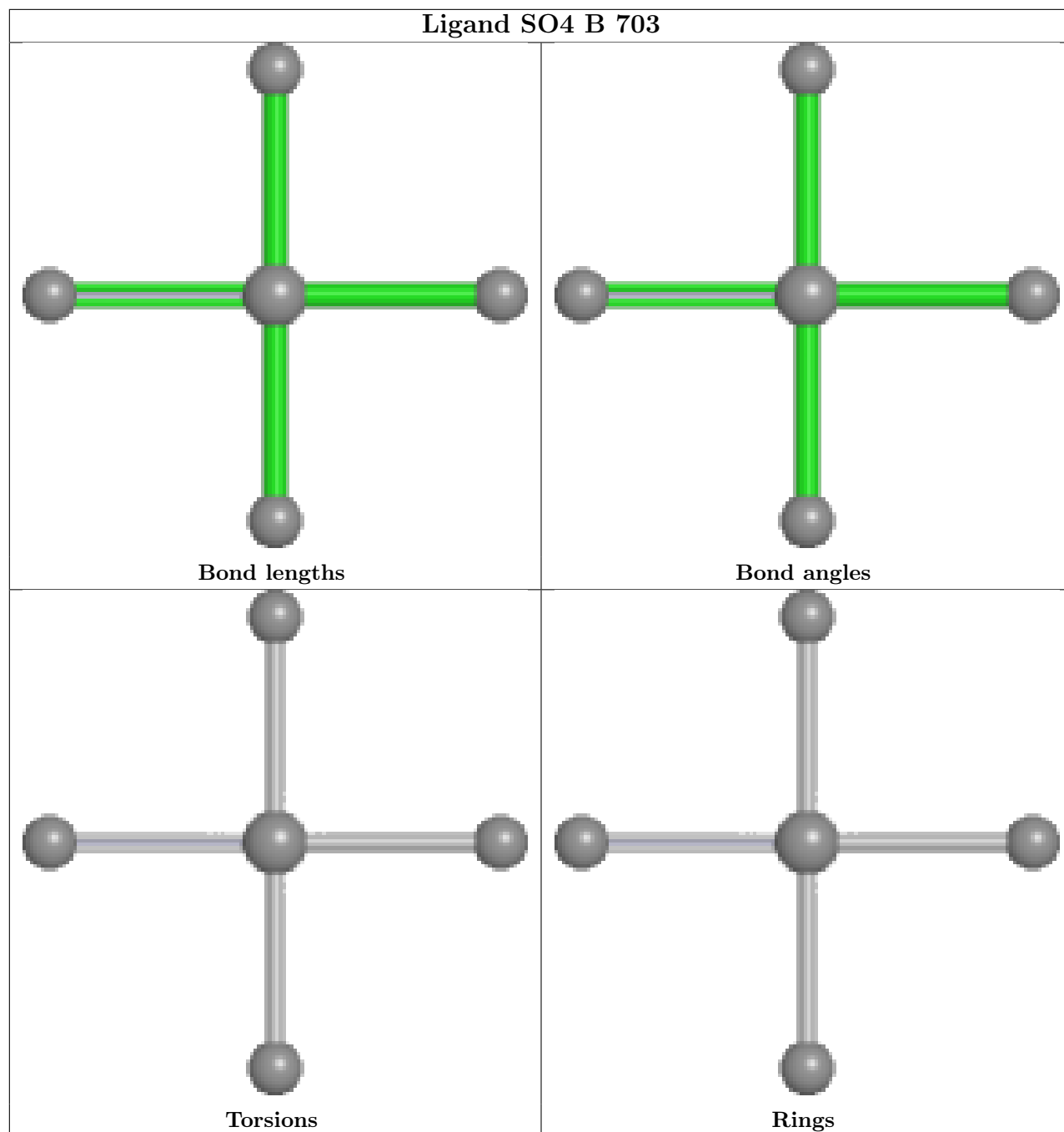


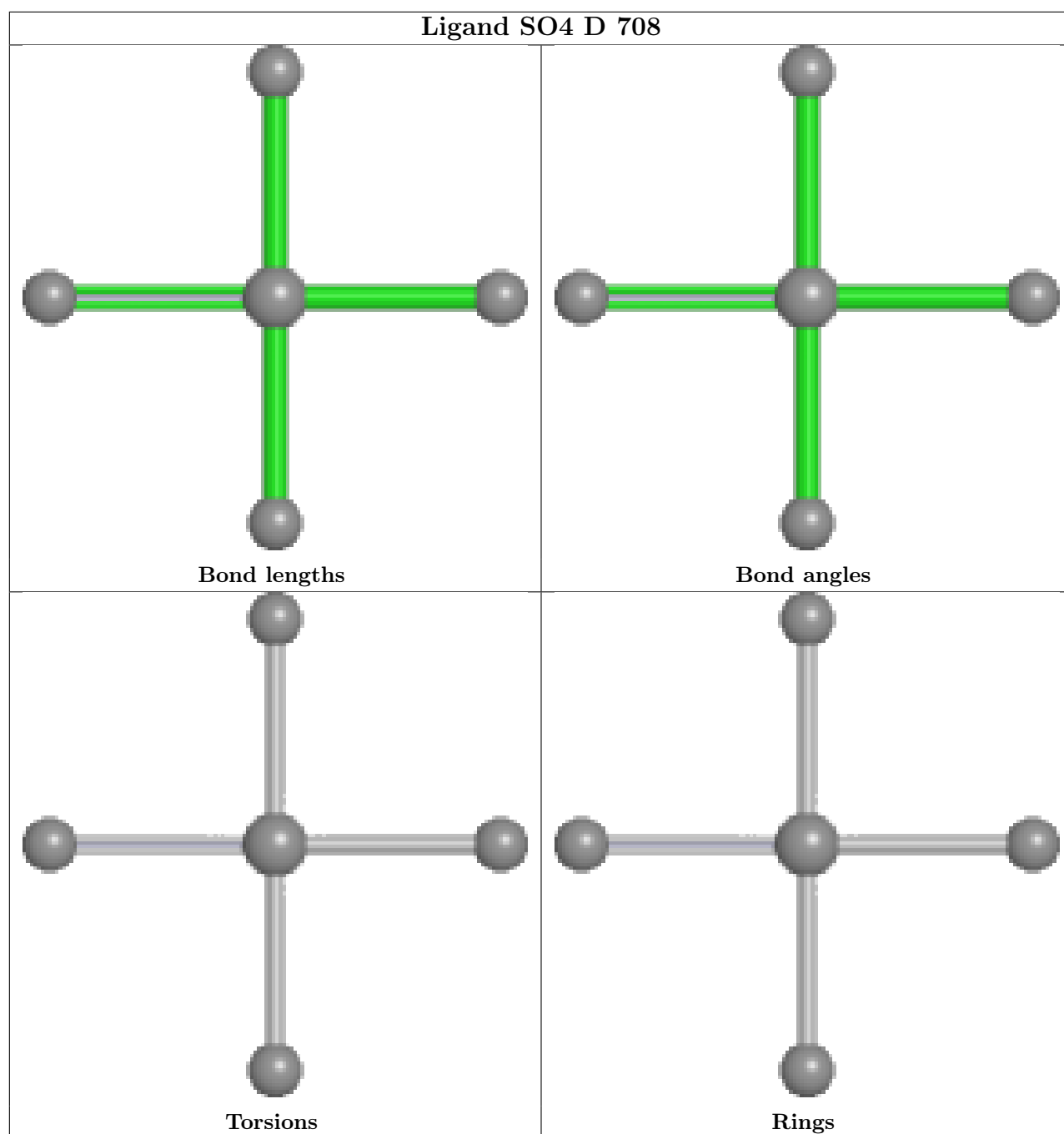


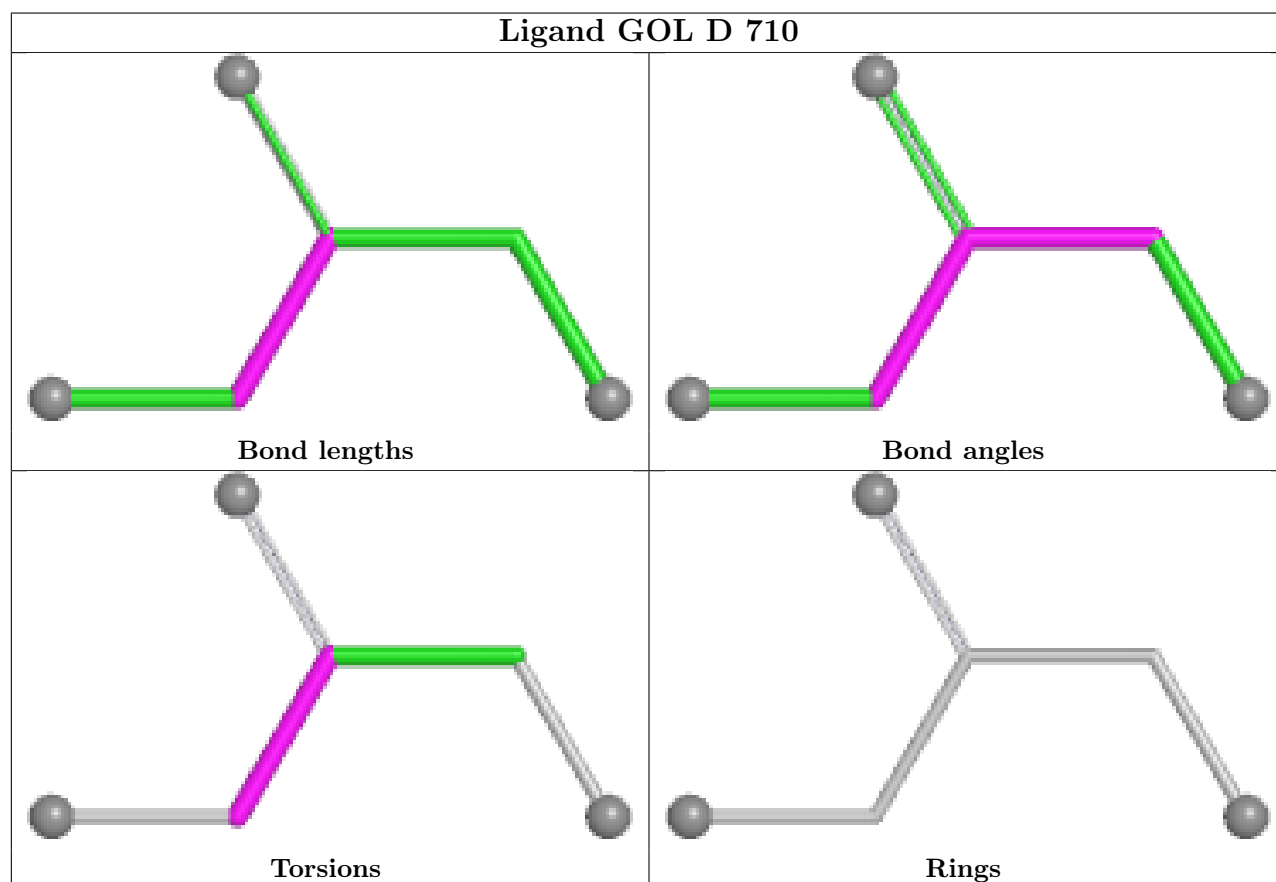
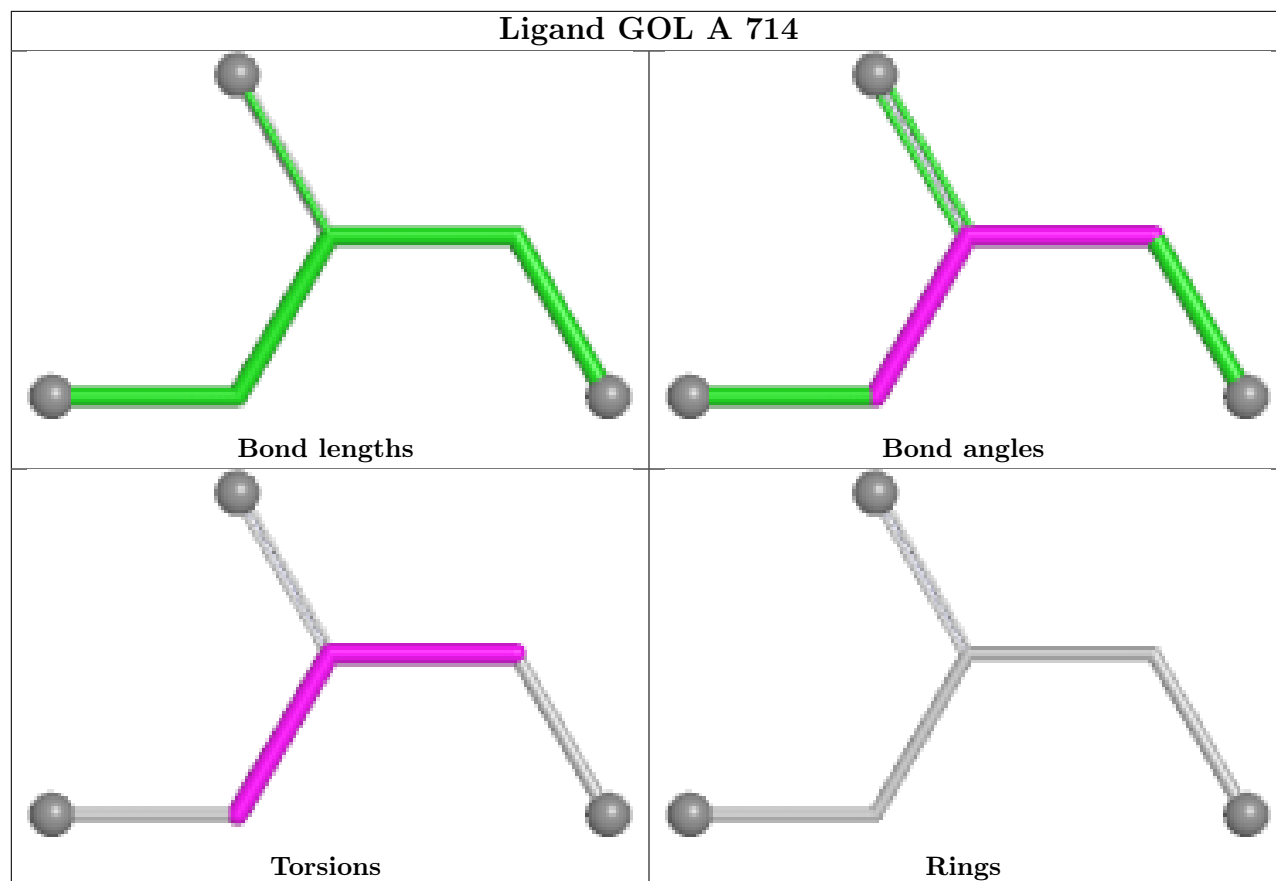


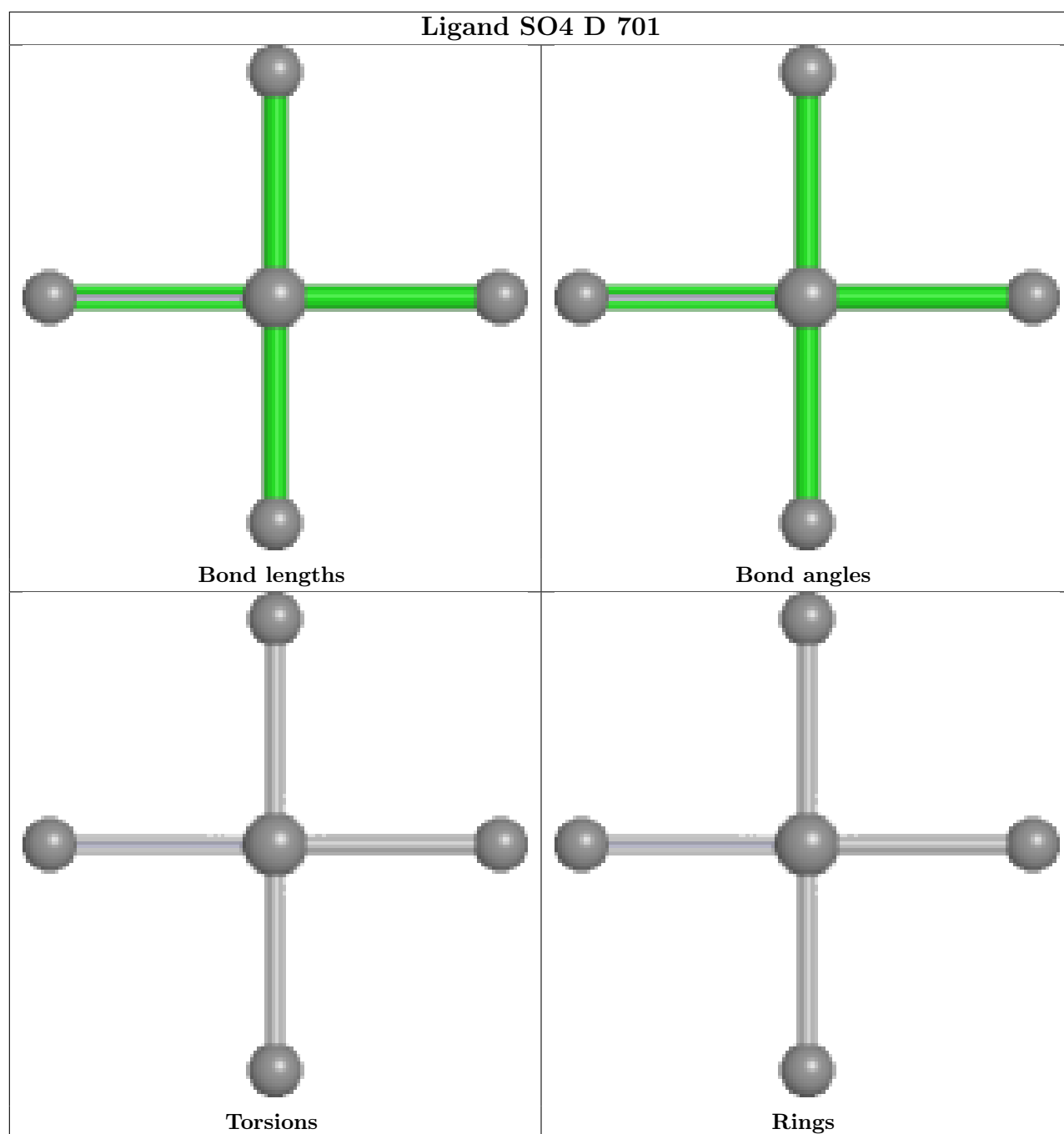


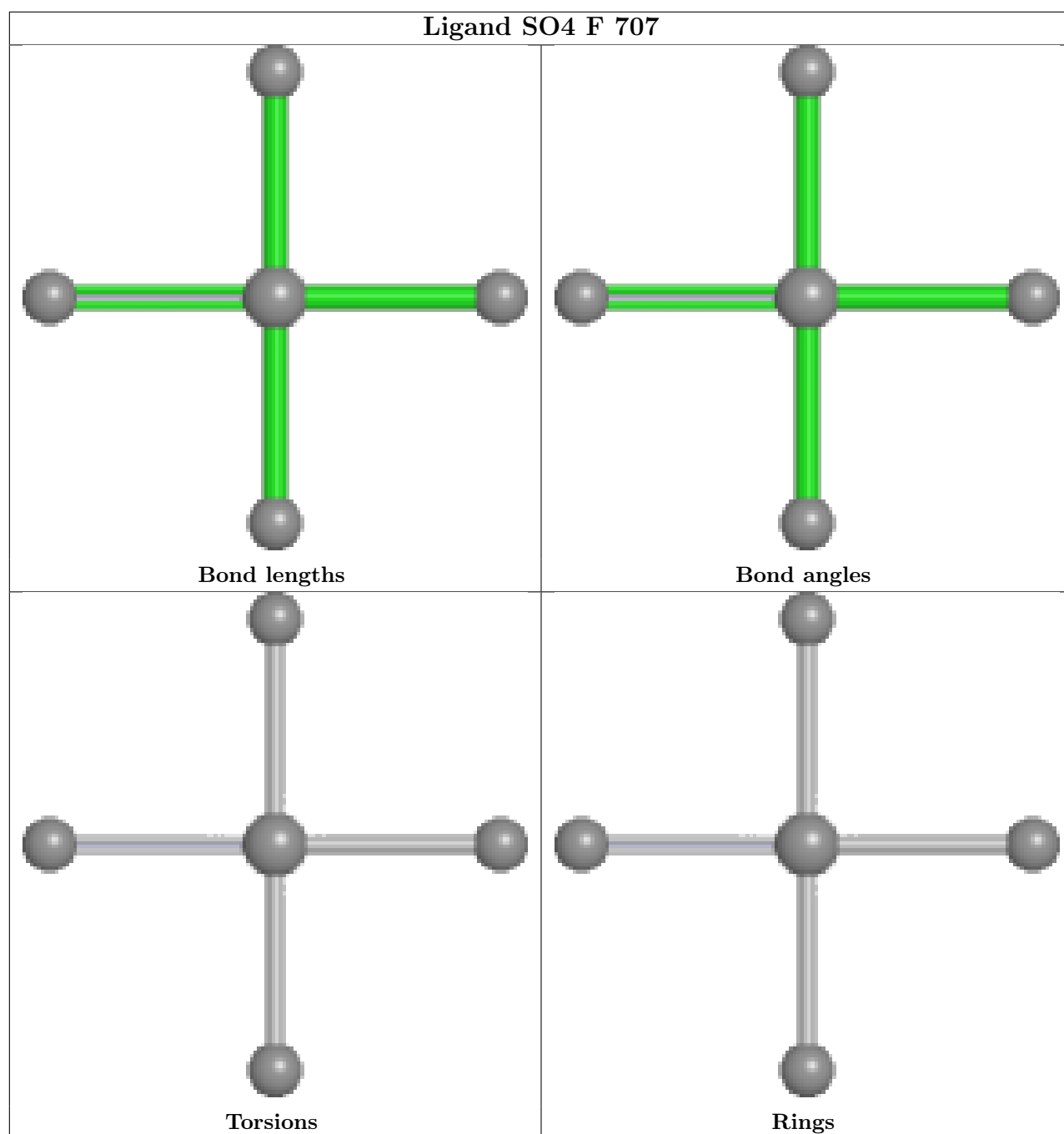


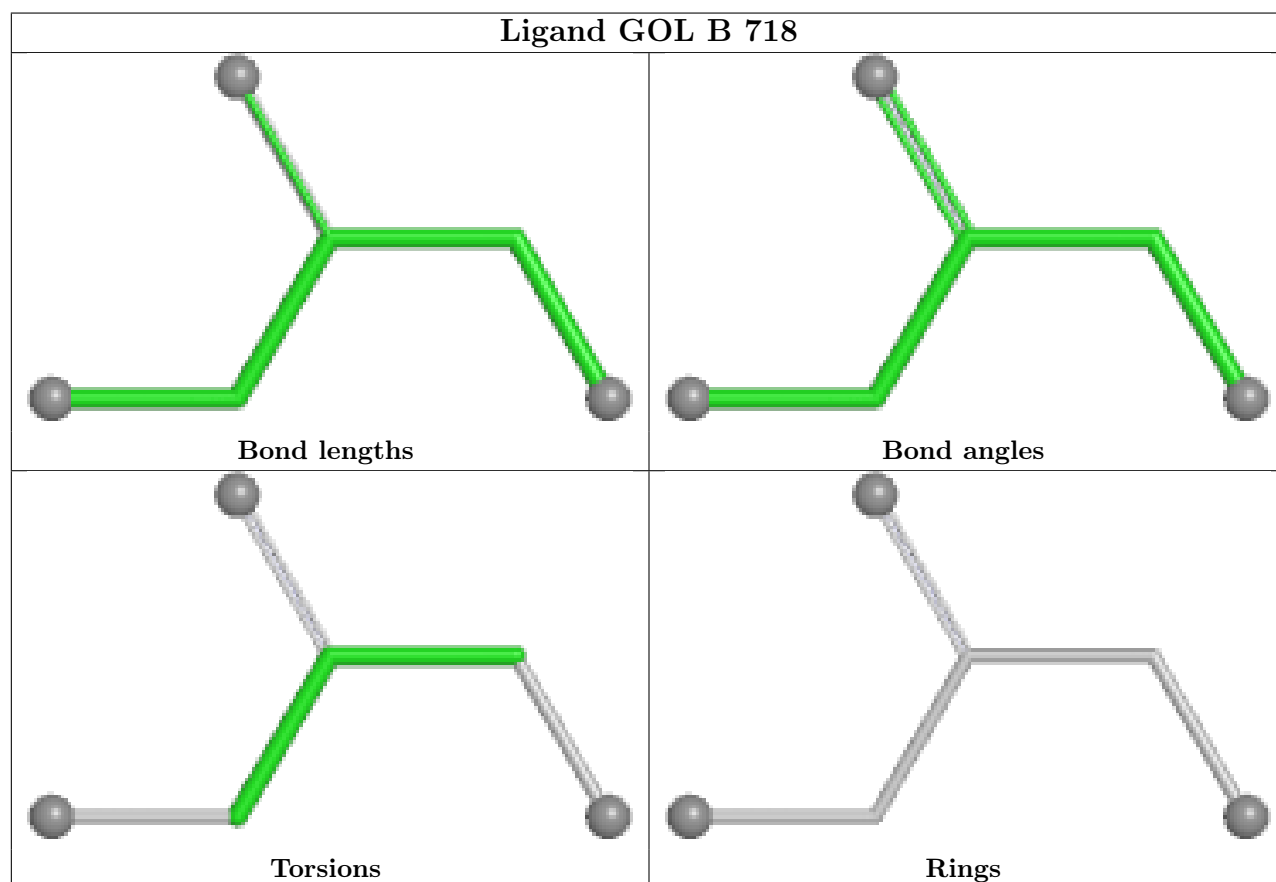
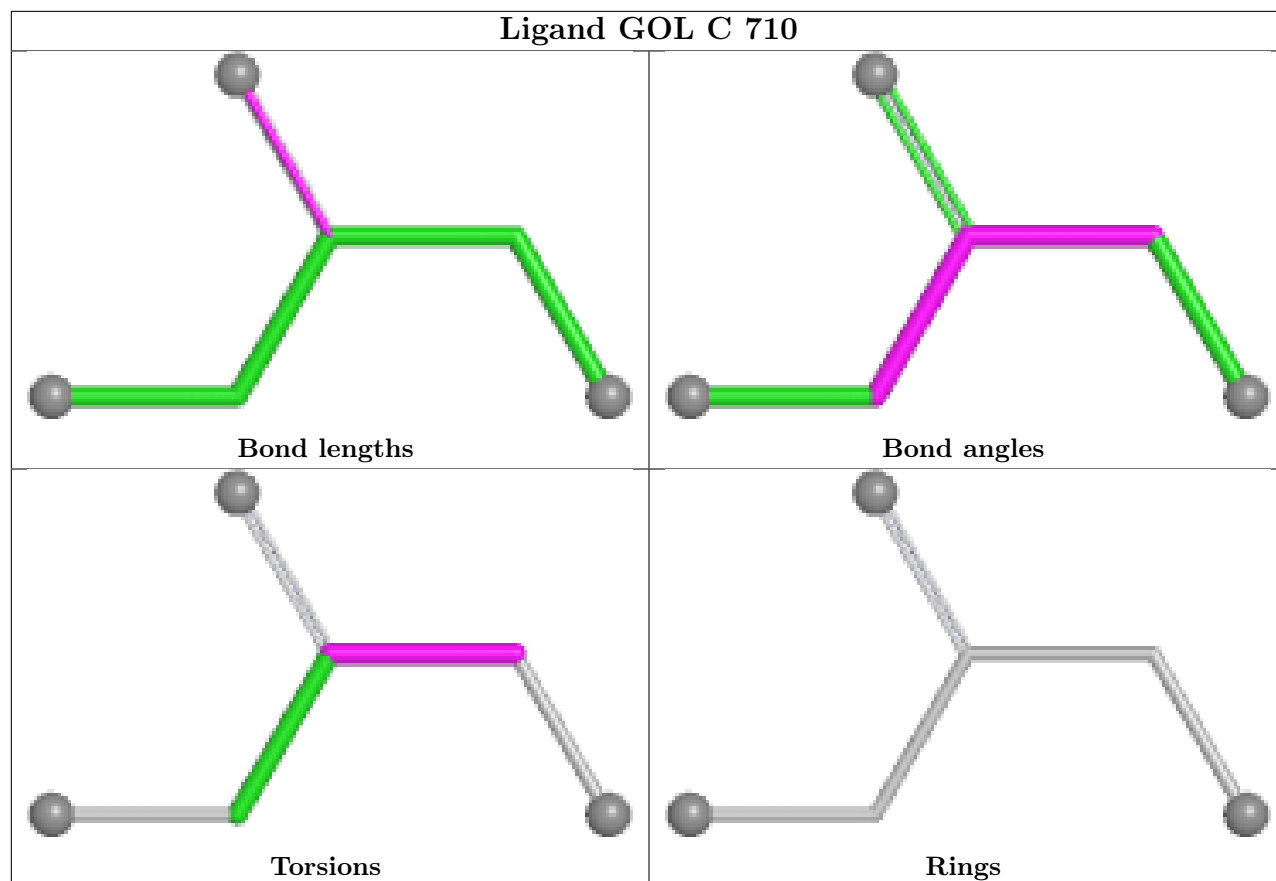


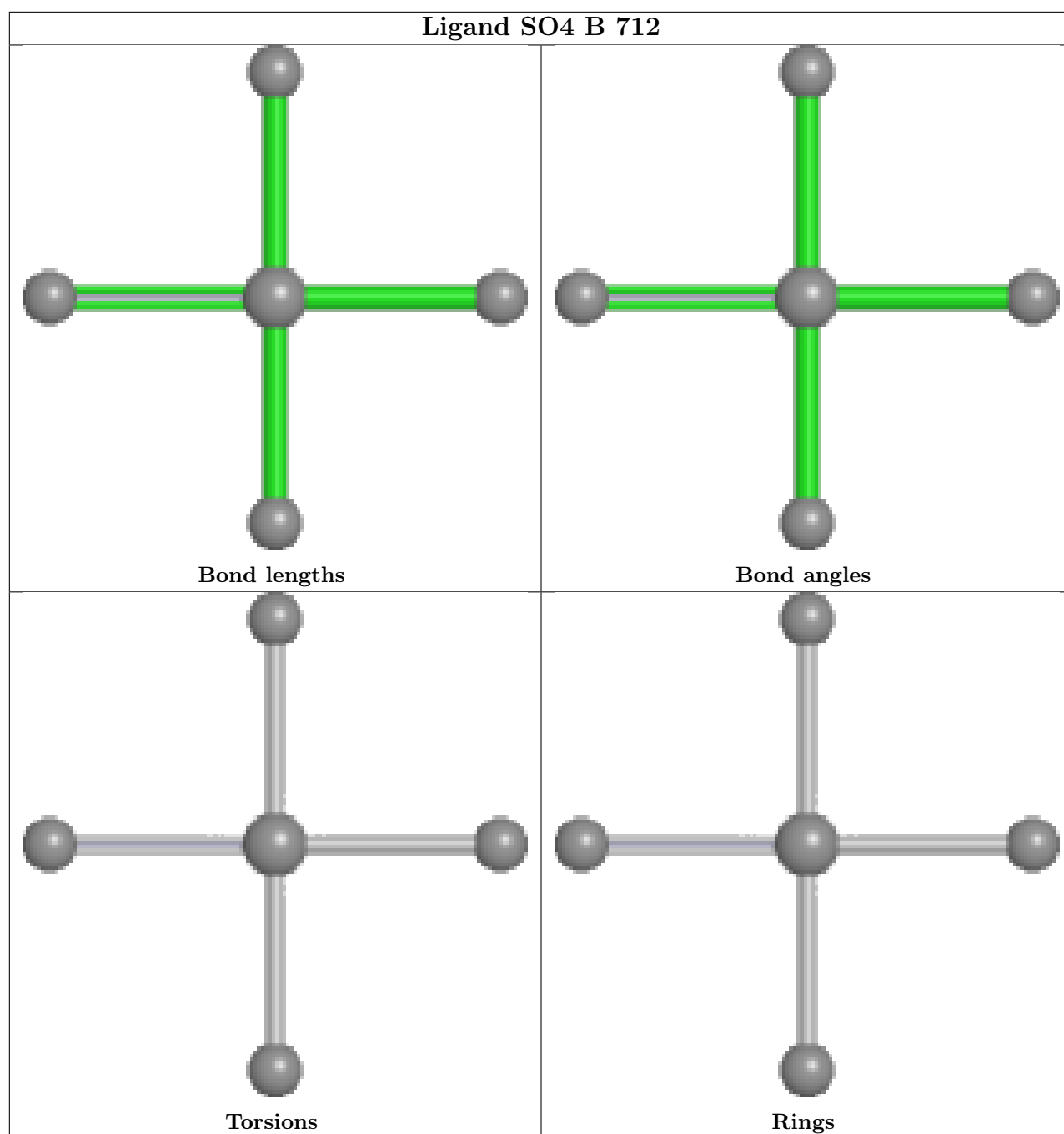


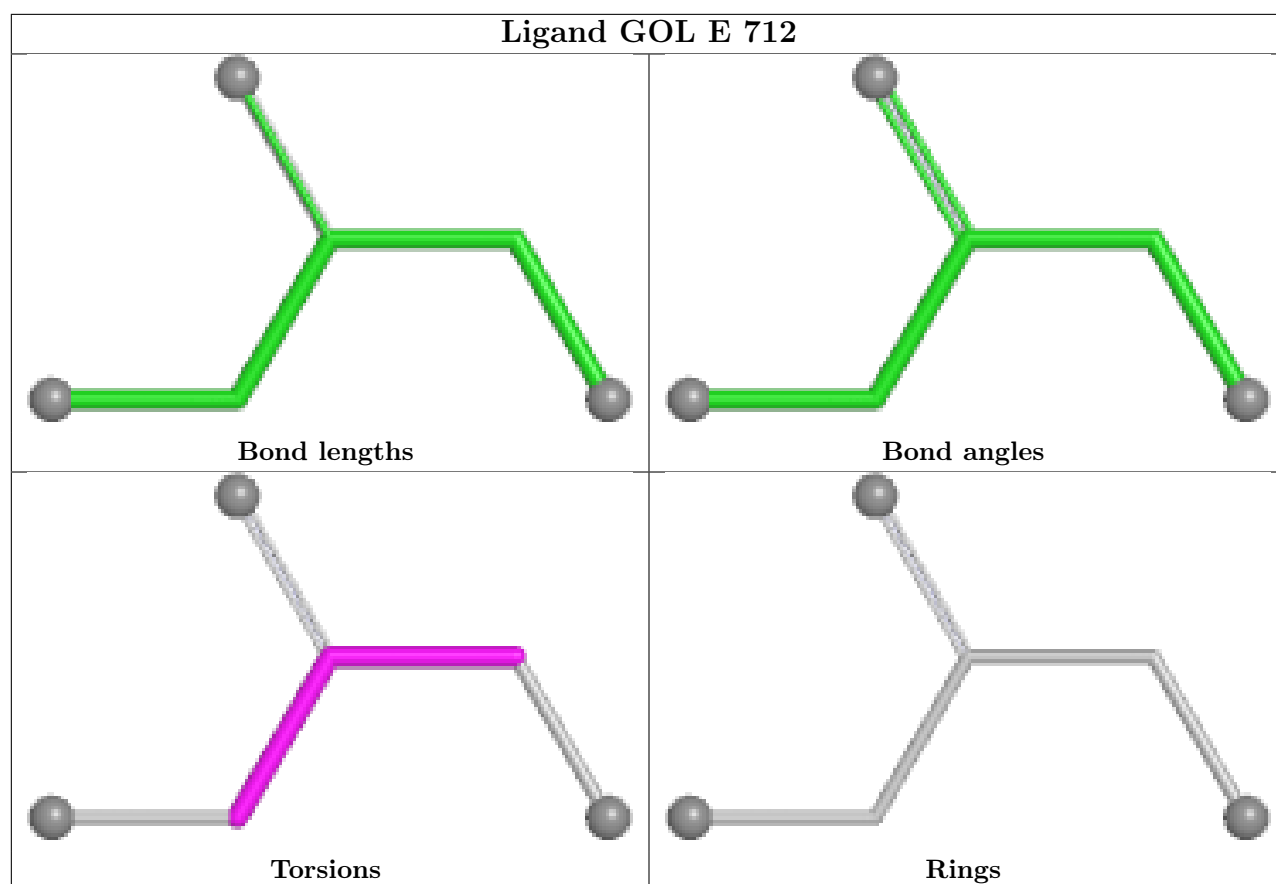


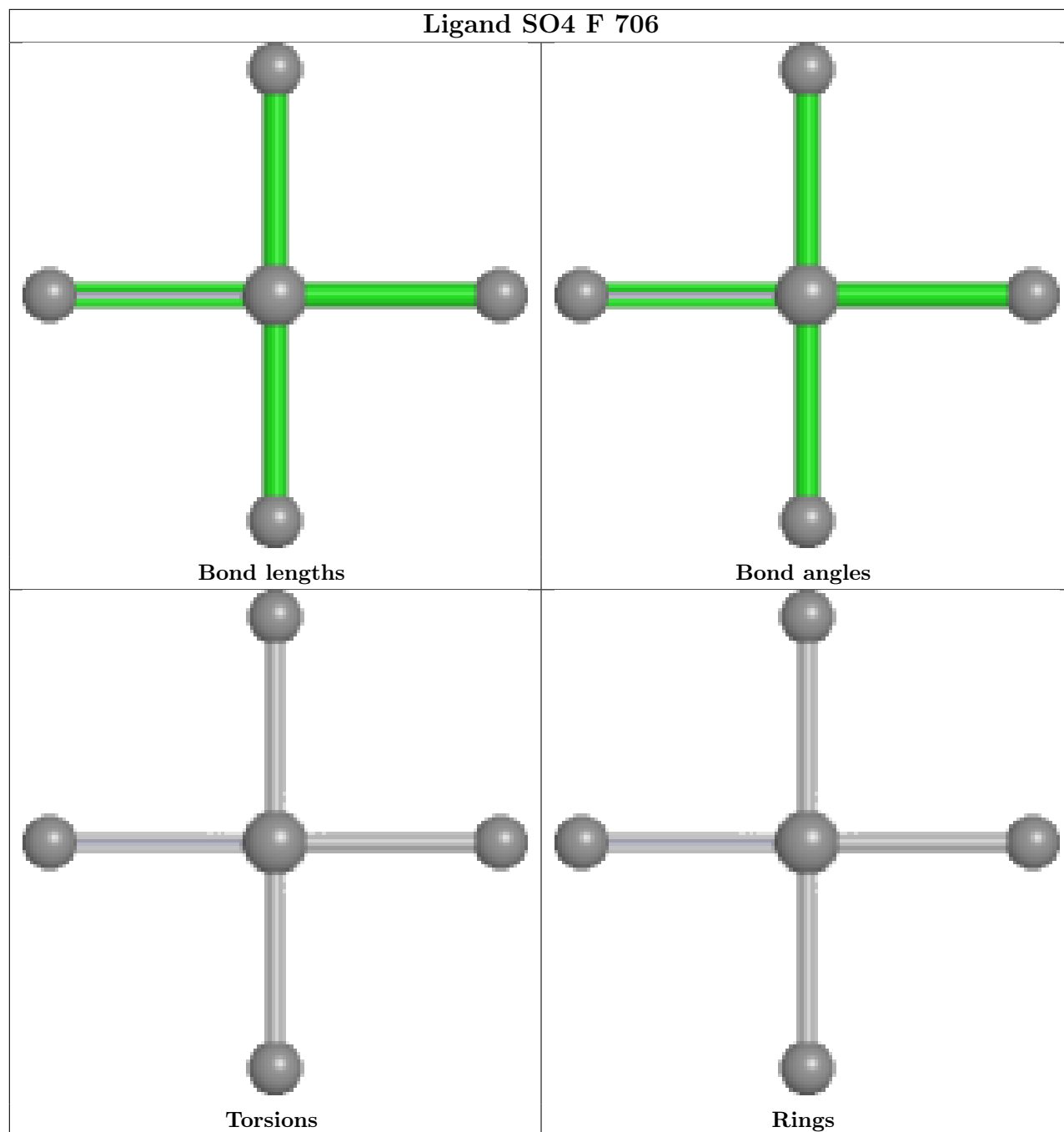


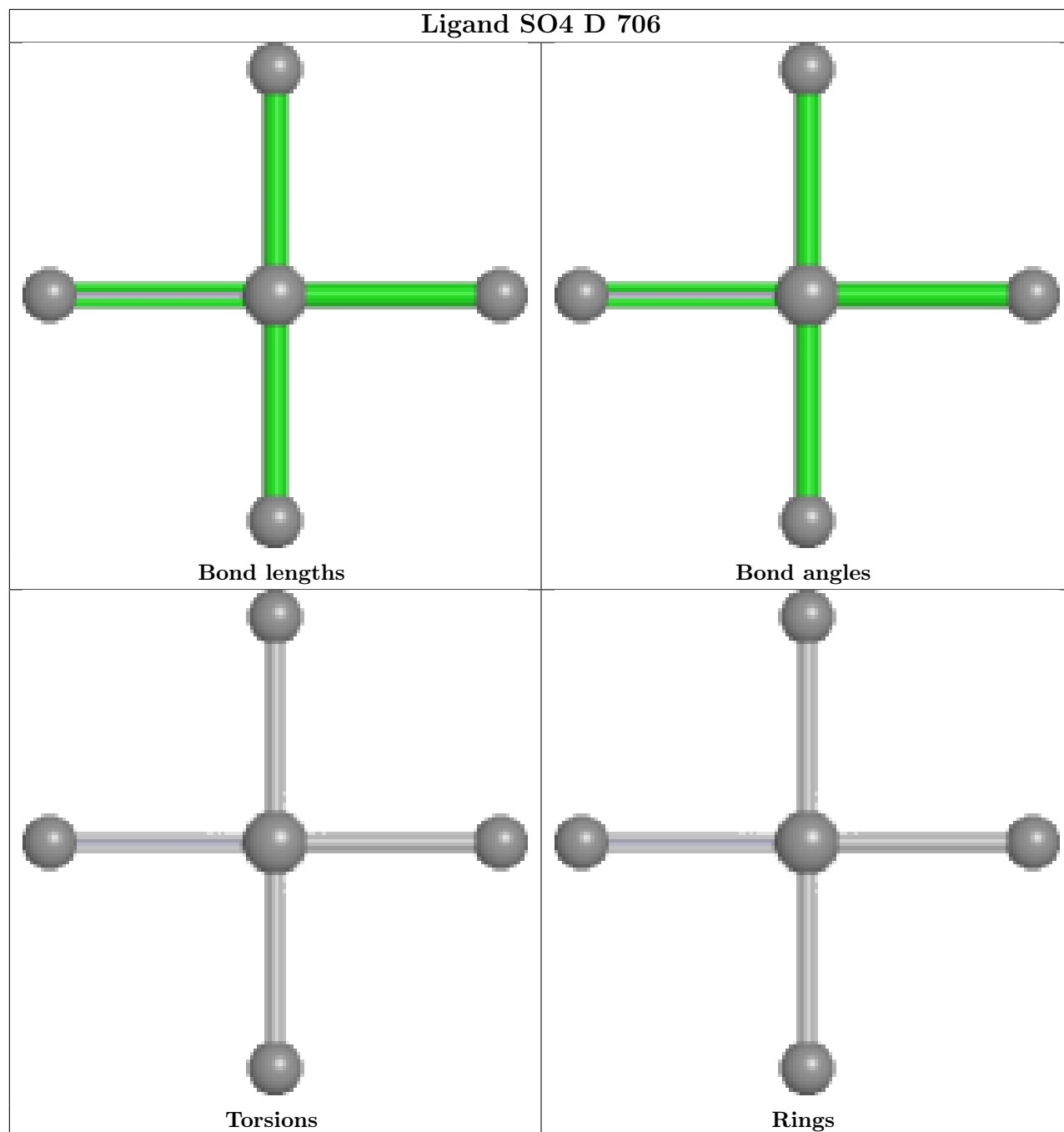


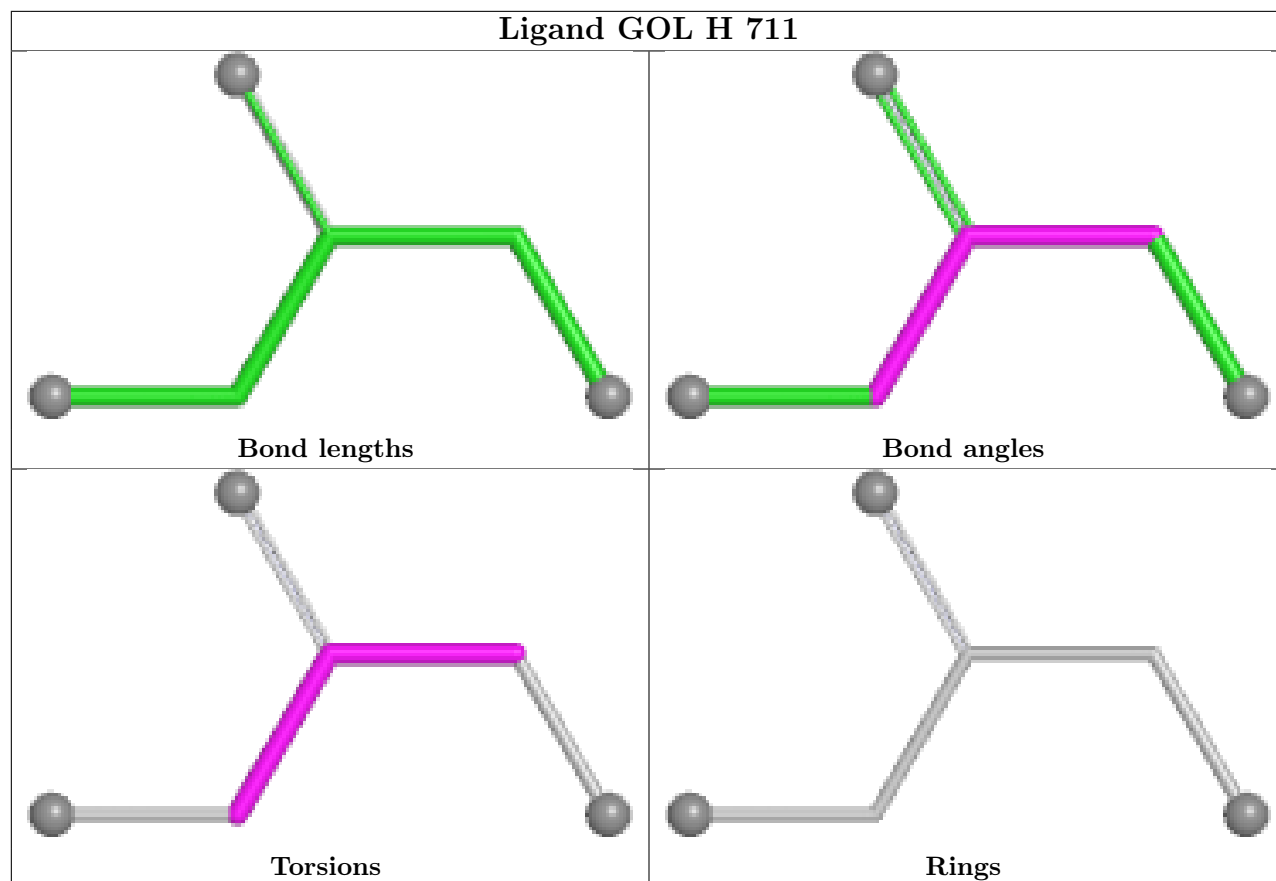


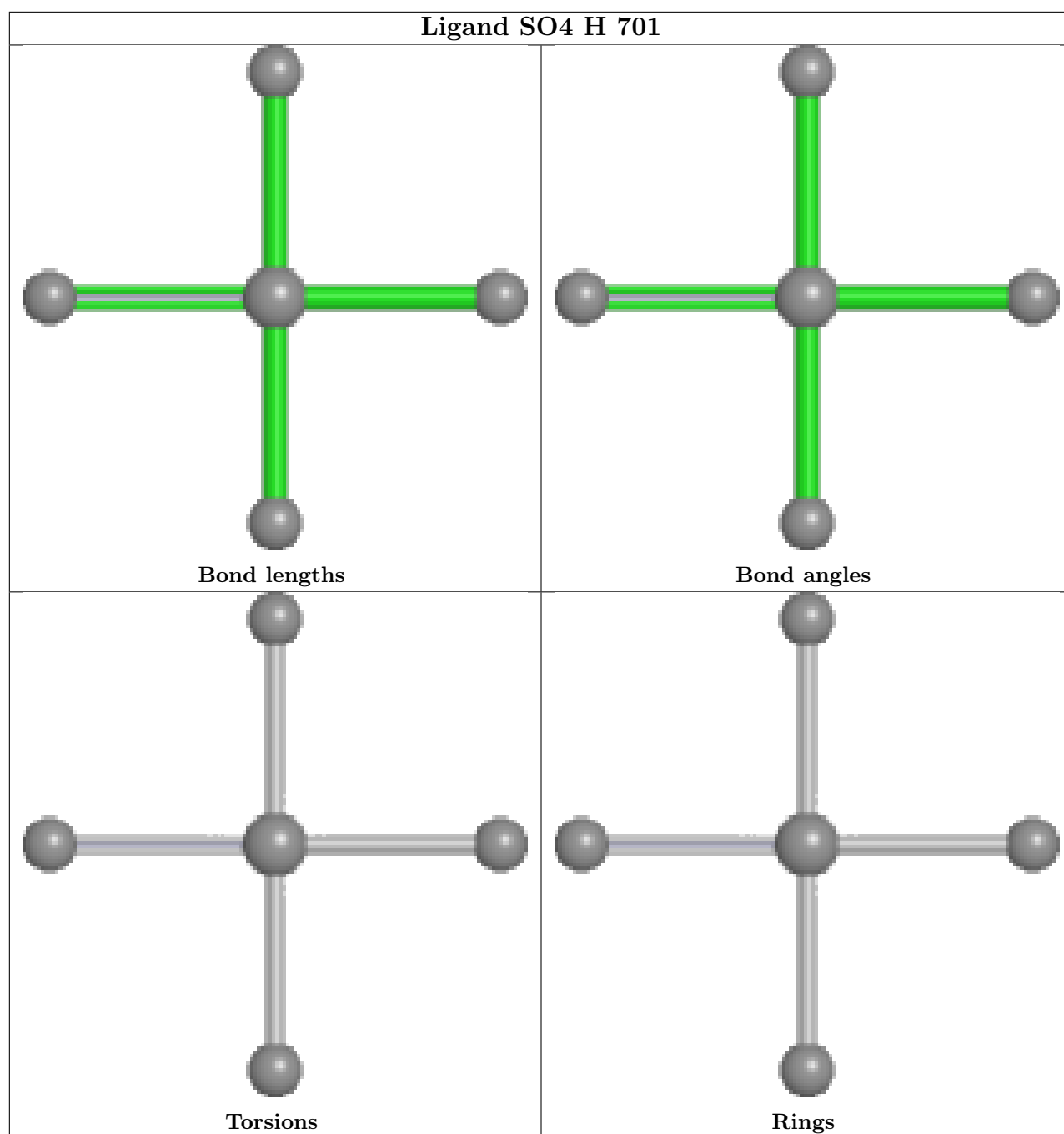


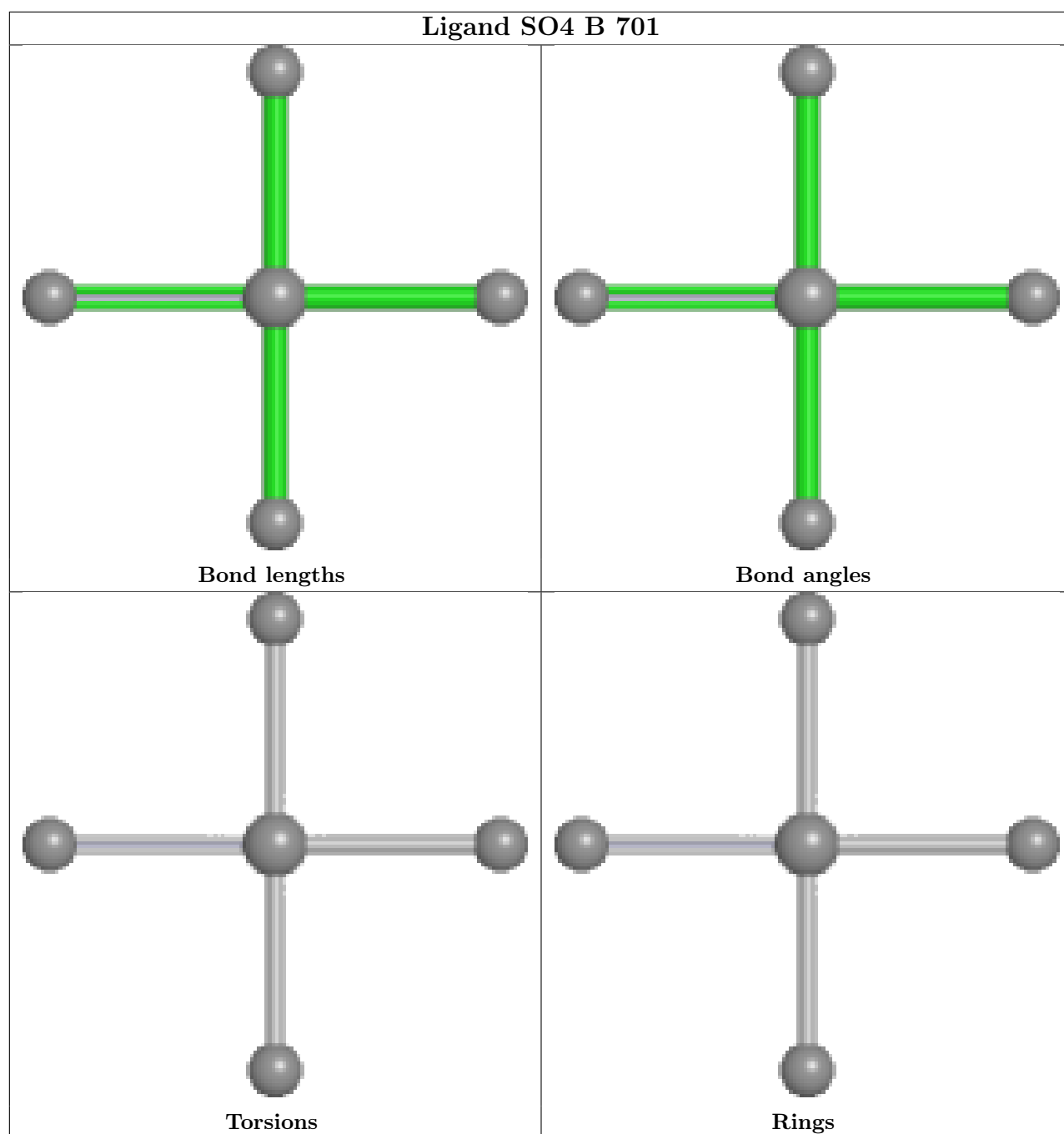


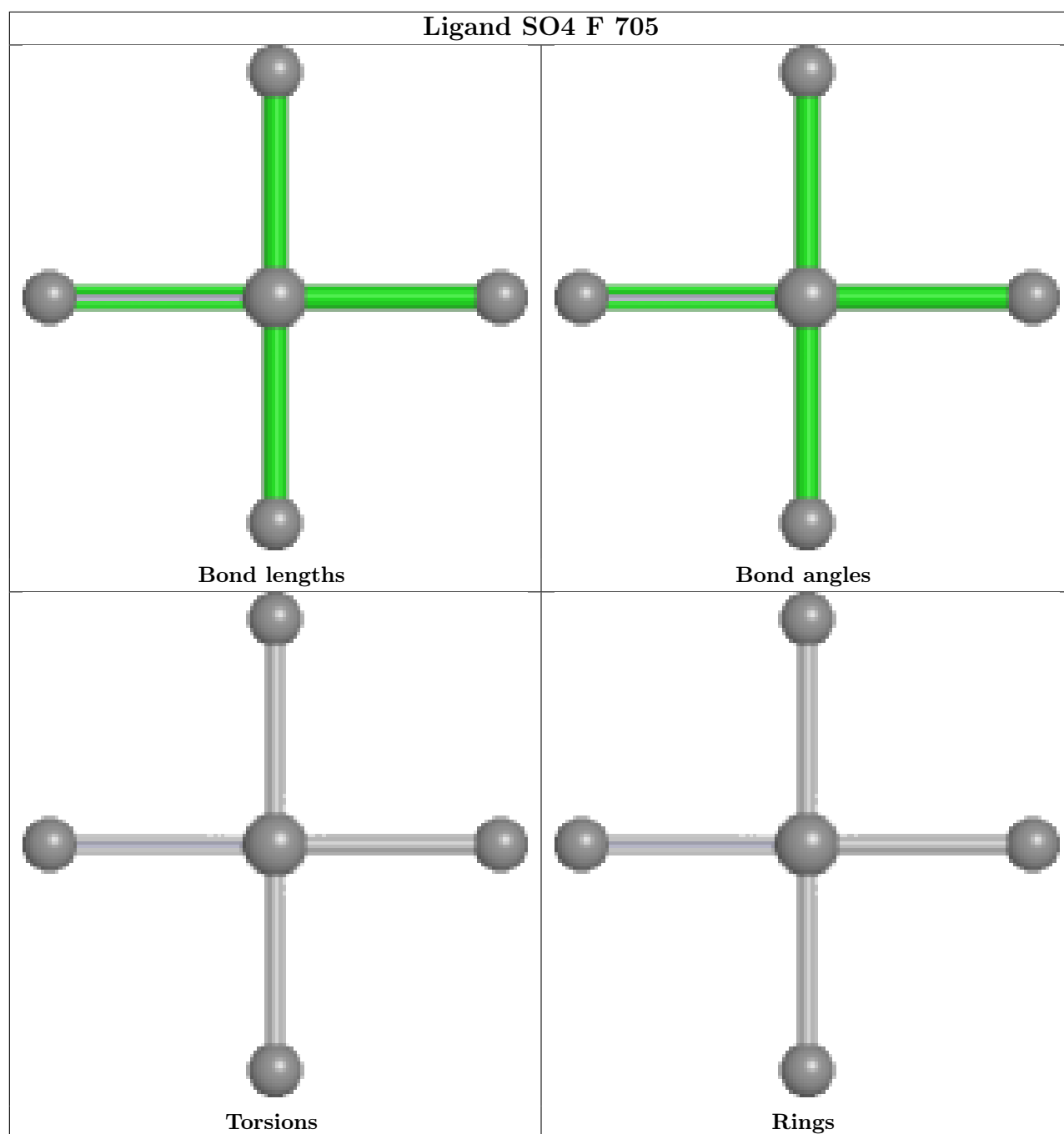


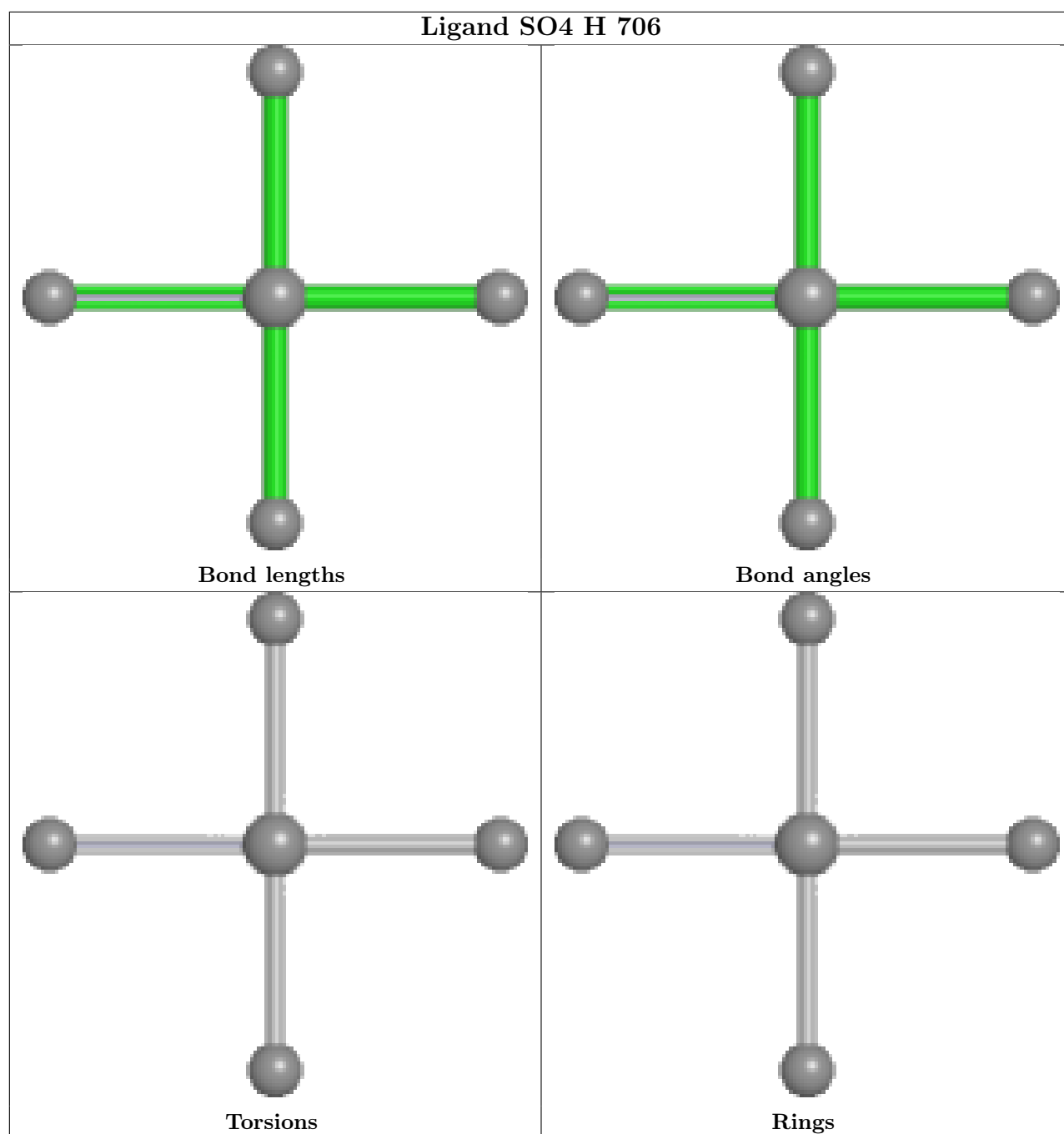


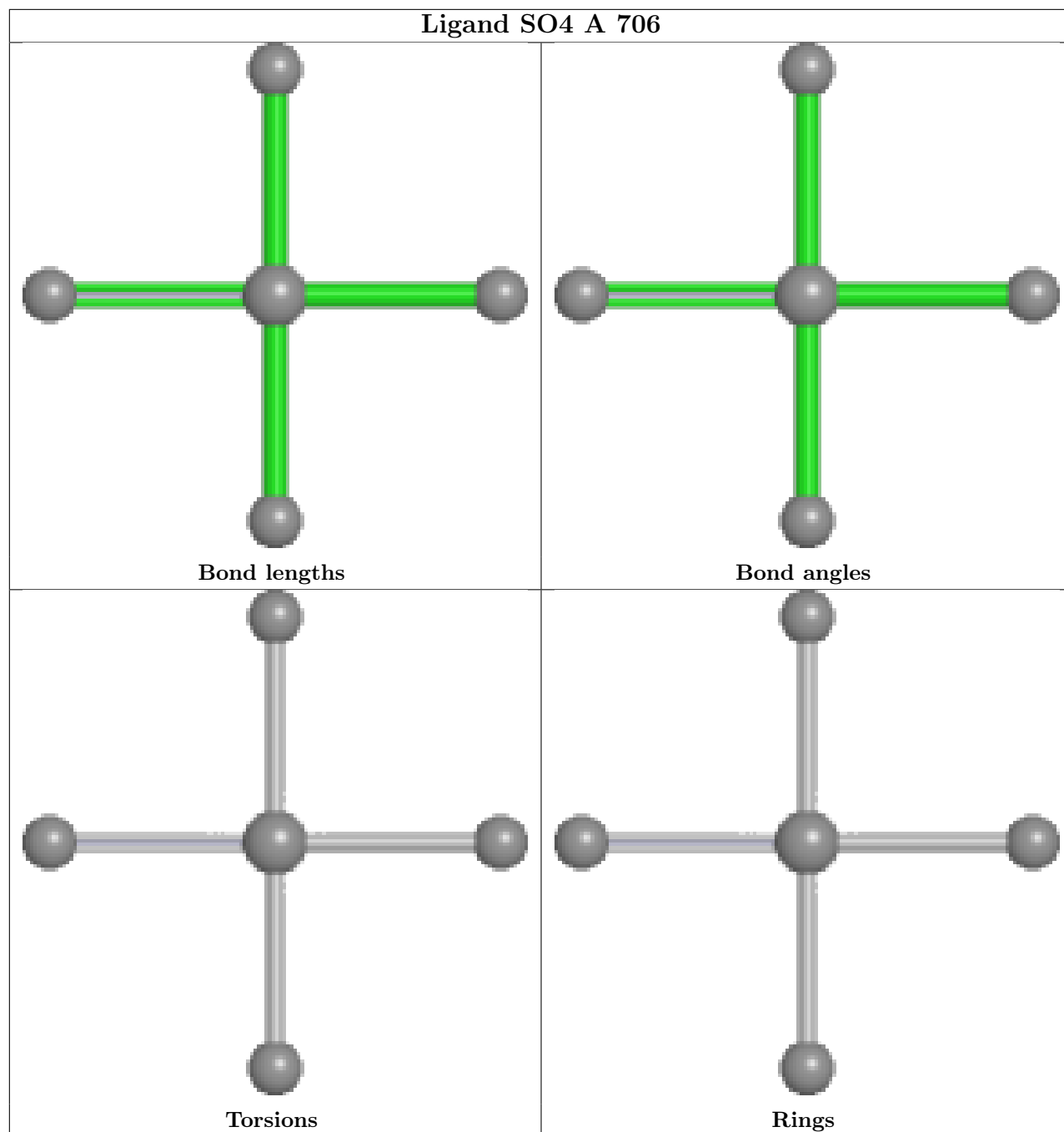


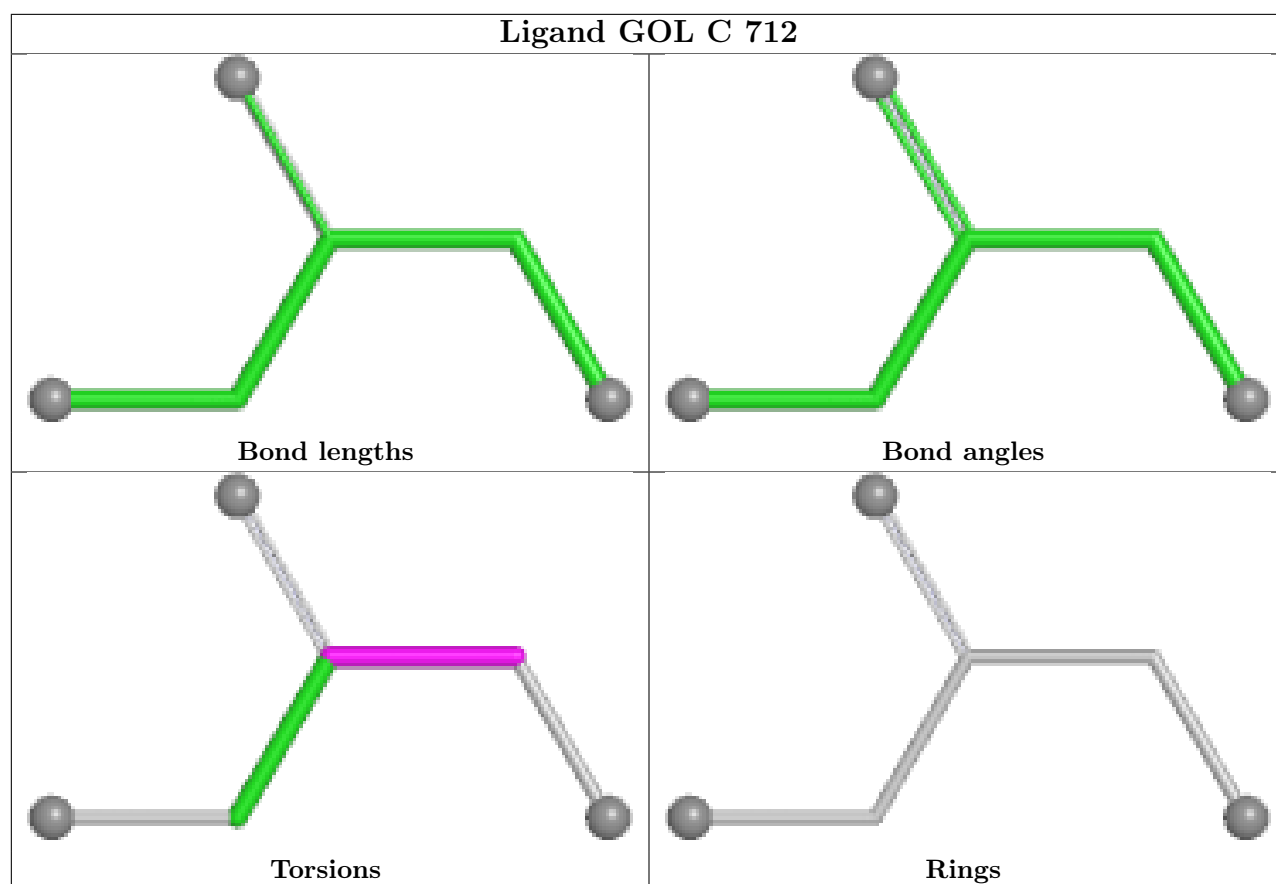


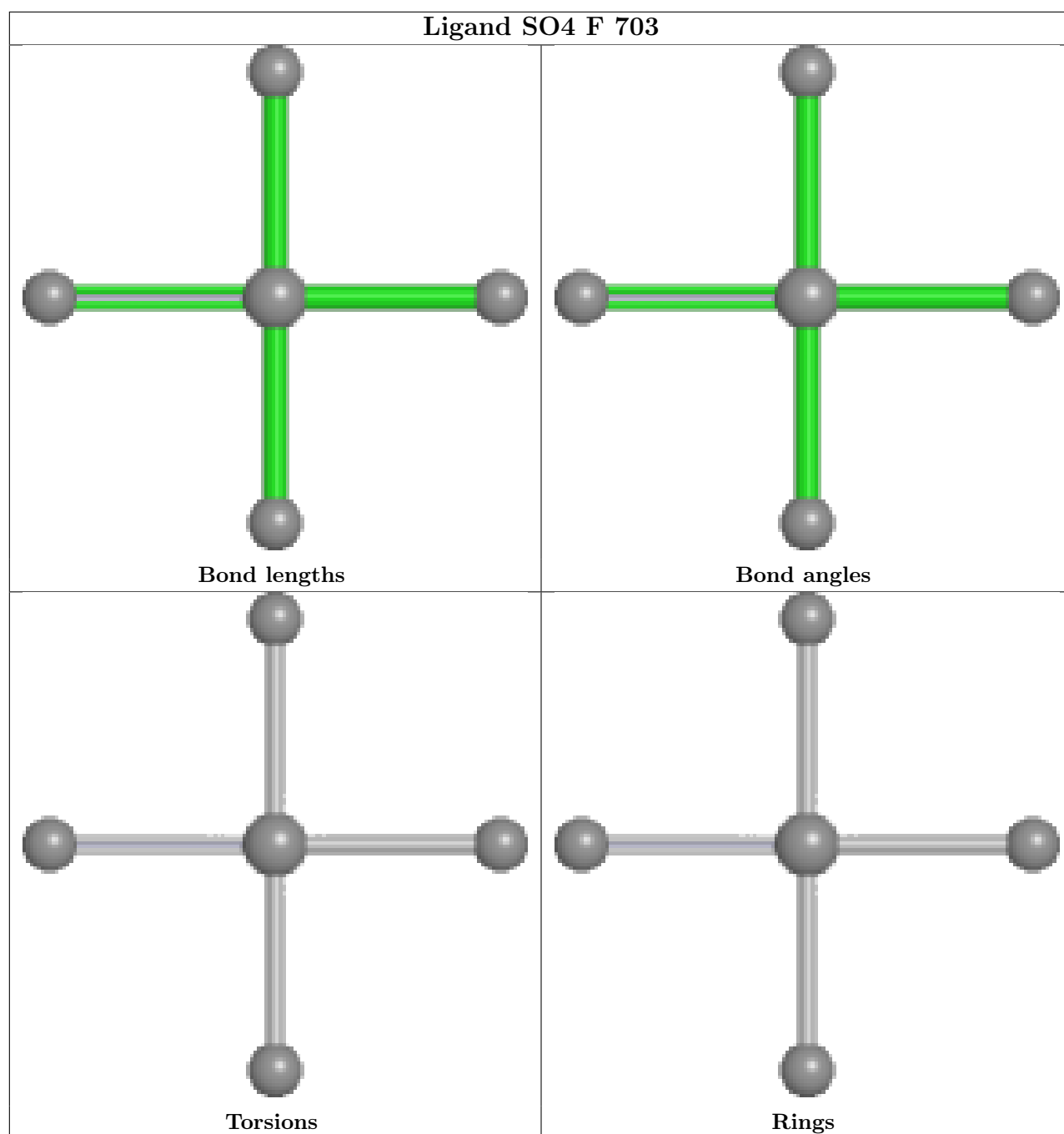












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	650/691 (94%)	0.23	7 (1%) 78 77	23, 32, 45, 62	0
1	B	650/691 (94%)	0.24	7 (1%) 78 77	23, 33, 46, 69	0
1	C	651/691 (94%)	0.34	8 (1%) 76 76	24, 32, 45, 68	0
1	D	649/691 (93%)	0.43	13 (2%) 65 64	24, 35, 49, 75	0
1	E	650/691 (94%)	0.28	6 (0%) 81 80	22, 33, 48, 74	0
1	F	649/691 (93%)	0.47	15 (2%) 61 60	22, 34, 49, 67	0
1	G	647/691 (93%)	0.76	33 (5%) 33 32	31, 42, 58, 80	0
1	H	651/691 (94%)	0.54	28 (4%) 40 39	26, 39, 56, 71	0
All	All	5197/5528 (94%)	0.41	117 (2%) 61 60	22, 35, 52, 80	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	ALA	5.0
1	H	240	ALA	4.4
1	G	146	PRO	3.9
1	C	146	PRO	3.8
1	F	390	ASP	3.5
1	C	12	TYR	3.4
1	F	346	GLY	3.4
1	H	154	ALA	3.4
1	B	156	LEU	3.3
1	H	156	LEU	3.3
1	D	437	GLU	3.3
1	D	436	ASP	3.3
1	G	28	HIS	3.2
1	F	156	LEU	3.2
1	D	439	GLU	3.2
1	H	433	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	3.2
1	G	435	LEU	3.2
1	D	146	PRO	3.2
1	E	58	ALA	3.1
1	E	146	PRO	3.1
1	F	146	PRO	3.1
1	E	438	GLY	3.0
1	H	155	ASP	3.0
1	D	476	THR	3.0
1	H	146	PRO	3.0
1	H	435	LEU	3.0
1	G	380	VAL	3.0
1	A	146	PRO	3.0
1	B	317	GLY	2.9
1	D	288	GLY	2.9
1	A	437	GLU	2.9
1	G	58	ALA	2.9
1	G	668	LEU	2.9
1	F	436	ASP	2.8
1	B	146	PRO	2.8
1	G	11	LEU	2.8
1	B	58	ALA	2.7
1	F	187	LEU	2.7
1	G	289	THR	2.7
1	H	139	THR	2.7
1	F	438	GLY	2.7
1	G	515	PHE	2.7
1	G	517	PHE	2.7
1	D	289	THR	2.7
1	G	408	VAL	2.7
1	C	155	ASP	2.7
1	G	403	LEU	2.6
1	A	436	ASP	2.6
1	A	117	ARG	2.6
1	H	476	THR	2.6
1	A	11	LEU	2.6
1	C	352	ILE	2.5
1	D	12	TYR	2.5
1	G	405	ASN	2.5
1	H	238	SER	2.5
1	B	12	TYR	2.5
1	G	516	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	255	ALA	2.5
1	H	437	GLU	2.4
1	B	187	LEU	2.4
1	H	314	LYS	2.4
1	H	340	TYR	2.4
1	E	11	LEU	2.4
1	G	322	SER	2.4
1	F	12	TYR	2.3
1	G	156	LEU	2.3
1	C	436	ASP	2.3
1	H	516	ASP	2.3
1	G	415	PHE	2.3
1	F	345	ALA	2.3
1	F	435	LEU	2.3
1	H	11	LEU	2.3
1	G	432	PRO	2.3
1	H	242	THR	2.3
1	H	252	ALA	2.3
1	G	80	ARG	2.3
1	G	186	VAL	2.3
1	G	244	LEU	2.3
1	H	234	LEU	2.3
1	G	387	SER	2.2
1	G	476	THR	2.2
1	G	137	ASP	2.2
1	G	456	GLY	2.2
1	H	57	ALA	2.2
1	F	188	SER	2.2
1	C	288	GLY	2.2
1	D	434	GLU	2.2
1	H	187	LEU	2.2
1	G	365	PRO	2.2
1	H	389	ALA	2.2
1	H	254	LEU	2.2
1	H	12	TYR	2.2
1	G	401	GLU	2.1
1	G	402	ALA	2.1
1	D	233	LEU	2.1
1	H	344	LEU	2.1
1	E	188	SER	2.1
1	C	476	THR	2.1
1	A	407	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	186	VAL	2.1
1	A	69	ARG	2.1
1	B	236	LEU	2.1
1	F	11	LEU	2.1
1	G	254	LEU	2.1
1	H	405	ASN	2.1
1	D	240	ALA	2.1
1	H	265	ALA	2.1
1	D	435	LEU	2.1
1	E	322	SER	2.1
1	F	369	GLN	2.1
1	H	286	GLU	2.0
1	D	156	LEU	2.0
1	F	392	THR	2.0
1	G	393	LYS	2.0
1	G	240	ALA	2.0
1	G	443	LEU	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	SO4	H	708	5/5	0.57	0.13	72,74,82,86	0
6	FLC	A	717	13/13	0.59	0.22	38,47,54,56	0
6	FLC	H	713	13/13	0.60	0.24	47,53,59,60	0
2	SO4	F	705	5/5	0.61	0.15	53,60,72,77	0
2	SO4	F	707	5/5	0.62	0.14	59,60,76,86	0
2	SO4	B	712	5/5	0.62	0.12	60,61,73,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	707	5/5	0.64	0.15	61,66,70,84	0
4	GOL	F	712	6/6	0.67	0.14	47,52,54,63	0
4	GOL	D	710	6/6	0.68	0.20	40,42,48,57	0
2	SO4	A	708	5/5	0.70	0.13	59,60,74,79	0
2	SO4	C	706	5/5	0.72	0.13	50,57,66,70	0
4	GOL	G	707	6/6	0.72	0.20	42,46,48,57	0
4	GOL	E	712	6/6	0.73	0.15	42,46,47,57	0
2	SO4	B	711	5/5	0.74	0.12	65,70,78,78	0
2	SO4	H	709	5/5	0.74	0.12	58,64,78,82	0
2	SO4	H	706	5/5	0.75	0.12	51,58,68,72	0
2	SO4	H	707	5/5	0.75	0.12	53,54,56,60	0
2	SO4	G	702	5/5	0.76	0.11	58,63,71,74	0
2	SO4	E	709	5/5	0.77	0.14	41,51,55,67	0
2	SO4	A	707	5/5	0.77	0.11	62,70,74,86	0
4	GOL	D	712	6/6	0.78	0.17	36,39,48,48	0
4	GOL	E	714	6/6	0.78	0.15	45,51,51,55	0
4	GOL	D	713	6/6	0.79	0.13	44,45,48,61	0
2	SO4	E	707	5/5	0.79	0.10	62,63,68,68	0
5	ALA	G	709	6/6	0.79	0.15	32,35,37,38	0
2	SO4	G	703	5/5	0.79	0.12	58,59,63,64	0
4	GOL	F	710	6/6	0.79	0.15	40,51,57,64	0
4	GOL	G	708	6/6	0.80	0.15	50,54,56,58	0
4	GOL	F	709	6/6	0.80	0.15	46,51,55,55	0
4	GOL	A	713	6/6	0.81	0.16	35,38,40,44	0
4	GOL	A	715	6/6	0.81	0.12	38,41,42,50	0
4	GOL	C	709	6/6	0.81	0.16	36,40,42,42	0
2	SO4	F	706	5/5	0.81	0.18	34,37,42,45	5
4	GOL	C	712	6/6	0.82	0.16	42,45,51,53	0
2	SO4	B	708	5/5	0.82	0.09	61,64,75,81	0
4	GOL	C	710	6/6	0.82	0.16	38,42,45,46	0
4	GOL	F	708	6/6	0.82	0.15	40,43,46,48	0
2	SO4	A	705	5/5	0.83	0.12	53,54,60,63	0
5	ALA	C	713	6/6	0.83	0.13	22,28,30,30	0
2	SO4	E	708	5/5	0.83	0.11	54,57,60,62	0
5	ALA	H	712	6/6	0.83	0.13	27,28,33,34	0
4	GOL	B	718	6/6	0.83	0.13	39,42,46,46	0
3	NA	A	712	1/1	0.83	0.14	41,41,41,41	0
5	ALA	F	713	6/6	0.84	0.13	25,28,32,33	0
2	SO4	G	705	5/5	0.84	0.09	59,61,65,65	0
4	GOL	D	711	6/6	0.84	0.13	41,47,49,50	0
2	SO4	D	705	5/5	0.84	0.14	42,44,50,56	0
4	GOL	F	711	6/6	0.84	0.12	50,52,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	E	705	5/5	0.86	0.09	45,51,60,61	0
4	GOL	H	711	6/6	0.86	0.13	46,49,55,59	0
2	SO4	D	706	5/5	0.86	0.09	50,56,64,69	0
2	SO4	C	705	5/5	0.86	0.08	50,55,68,71	0
2	SO4	C	704	5/5	0.87	0.10	48,52,55,58	0
2	SO4	D	708	5/5	0.87	0.08	62,65,69,69	0
3	NA	D	709	1/1	0.87	0.14	47,47,47,47	0
2	SO4	H	704	5/5	0.87	0.09	56,57,58,60	0
4	GOL	A	714	6/6	0.87	0.12	36,41,46,48	0
4	GOL	C	711	6/6	0.88	0.10	46,48,53,58	0
4	GOL	E	713	6/6	0.88	0.13	40,48,56,60	0
2	SO4	A	704	5/5	0.88	0.09	45,46,56,58	0
3	NA	A	710	1/1	0.88	0.14	42,42,42,42	0
5	ALA	E	715	6/6	0.88	0.13	21,29,36,37	0
2	SO4	B	707	5/5	0.89	0.09	46,48,65,65	0
2	SO4	F	704	5/5	0.89	0.10	52,52,52,58	0
2	SO4	C	707	5/5	0.89	0.09	52,53,55,58	0
4	GOL	B	717	6/6	0.89	0.12	39,48,50,52	0
5	ALA	B	719	6/6	0.89	0.11	26,27,30,32	0
2	SO4	B	710	5/5	0.89	0.10	49,54,57,60	0
3	NA	H	710	1/1	0.90	0.22	49,49,49,49	0
5	ALA	D	714	6/6	0.91	0.12	25,30,33,34	0
2	SO4	D	704	5/5	0.91	0.09	49,50,56,56	0
2	SO4	E	704	5/5	0.91	0.15	42,45,49,53	0
3	NA	G	706	1/1	0.91	0.11	48,48,48,48	0
2	SO4	B	703	5/5	0.91	0.09	49,51,52,53	0
2	SO4	F	703	5/5	0.91	0.14	41,42,48,51	0
2	SO4	H	705	5/5	0.91	0.19	40,41,47,48	0
3	NA	B	716	1/1	0.92	0.21	40,40,40,40	0
2	SO4	H	702	5/5	0.92	0.14	42,42,47,47	0
5	ALA	A	716	6/6	0.92	0.14	24,29,34,36	0
2	SO4	A	703	5/5	0.93	0.12	46,47,50,55	0
2	SO4	B	706	5/5	0.93	0.11	29,32,35,36	5
2	SO4	E	706	5/5	0.93	0.10	31,32,36,36	5
2	SO4	D	702	5/5	0.93	0.08	44,49,53,53	0
2	SO4	A	706	5/5	0.93	0.09	23,35,40,43	5
3	NA	E	711	1/1	0.93	0.13	42,42,42,42	0
3	NA	B	714	1/1	0.94	0.10	35,35,35,35	0
3	NA	B	715	1/1	0.94	0.19	34,34,34,34	0
2	SO4	F	701	5/5	0.94	0.12	33,36,44,48	0
3	NA	C	708	1/1	0.94	0.09	39,39,39,39	0
2	SO4	B	704	5/5	0.94	0.15	44,45,46,49	0

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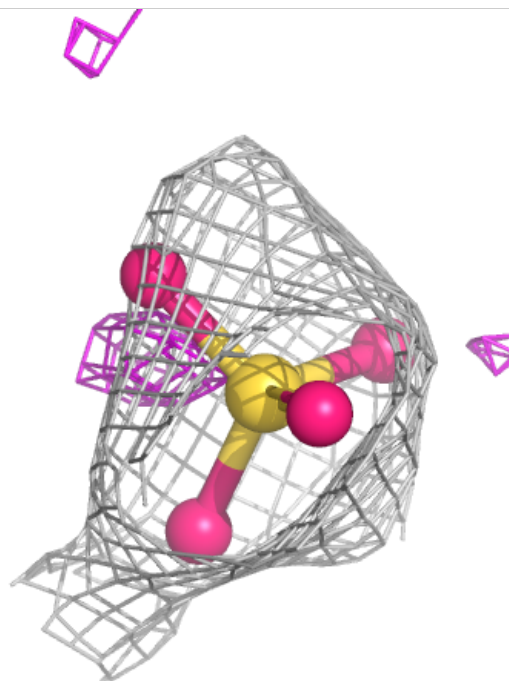
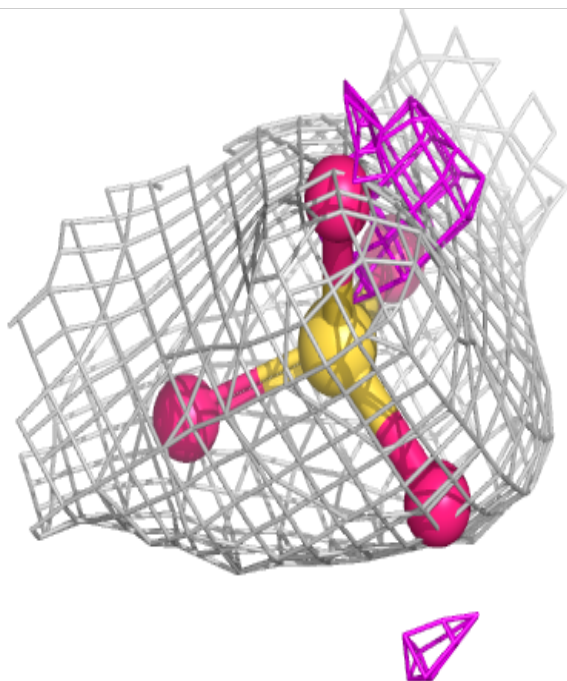
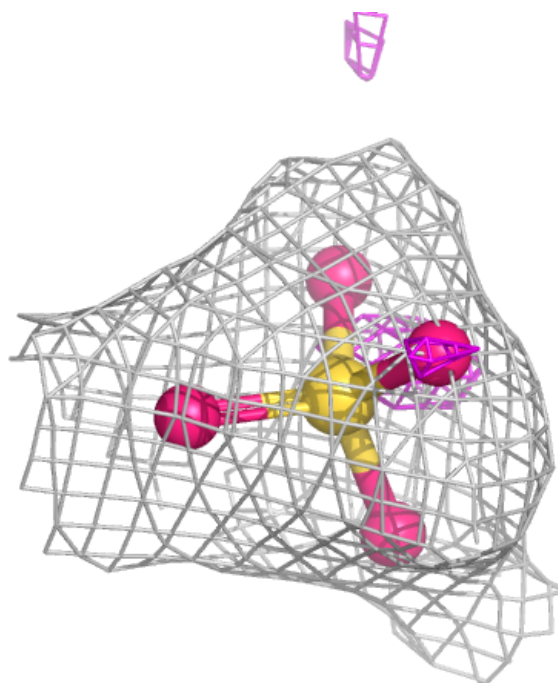
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	702	5/5	0.94	0.11	33,36,39,40	0
2	SO4	G	701	5/5	0.95	0.08	40,45,49,49	0
2	SO4	E	703	5/5	0.95	0.09	40,42,45,47	0
2	SO4	B	709	5/5	0.95	0.09	40,46,48,49	0
2	SO4	G	704	5/5	0.95	0.09	36,38,42,43	0
2	SO4	A	702	5/5	0.95	0.08	36,37,41,43	0
2	SO4	A	701	5/5	0.95	0.09	25,27,37,38	5
2	SO4	F	702	5/5	0.95	0.09	33,34,38,40	0
2	SO4	E	702	5/5	0.96	0.06	34,37,39,42	0
2	SO4	D	703	5/5	0.96	0.07	36,41,41,42	0
2	SO4	D	701	5/5	0.96	0.11	24,31,40,41	0
3	NA	A	711	1/1	0.96	0.07	43,43,43,43	0
3	NA	E	710	1/1	0.96	0.07	40,40,40,40	0
2	SO4	B	705	5/5	0.96	0.06	36,36,41,43	0
2	SO4	H	701	5/5	0.96	0.08	36,37,42,44	0
2	SO4	C	703	5/5	0.97	0.07	31,33,39,45	0
3	NA	A	709	1/1	0.97	0.12	35,35,35,35	0
2	SO4	E	701	5/5	0.97	0.08	26,30,33,36	5
2	SO4	B	702	5/5	0.97	0.06	35,37,39,42	0
2	SO4	B	701	5/5	0.97	0.08	32,34,36,38	0
3	NA	B	713	1/1	0.97	0.05	40,40,40,40	0
2	SO4	H	703	5/5	0.97	0.06	36,39,41,45	0
2	SO4	C	701	5/5	0.98	0.07	29,32,37,38	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.

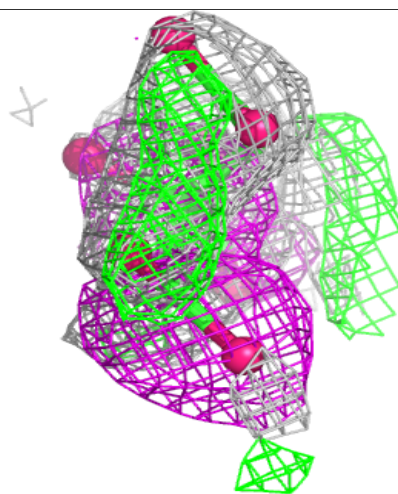
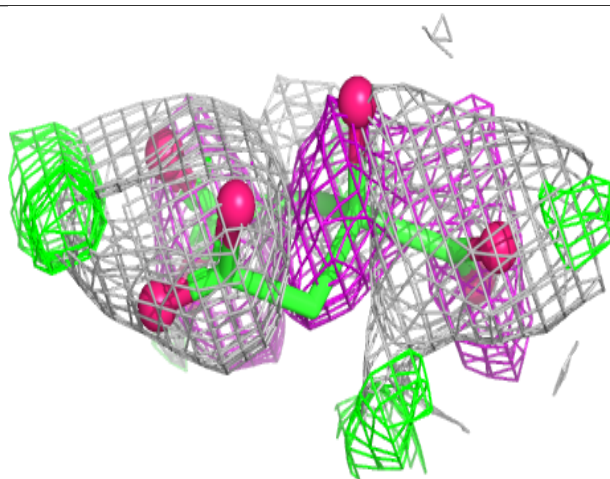
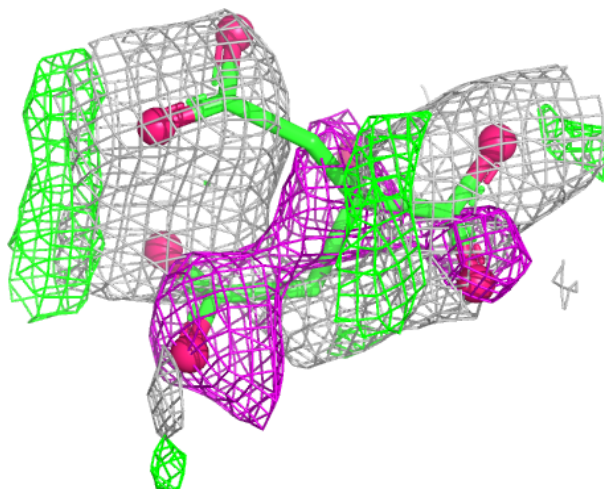
Electron density around SO4 H 708:

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



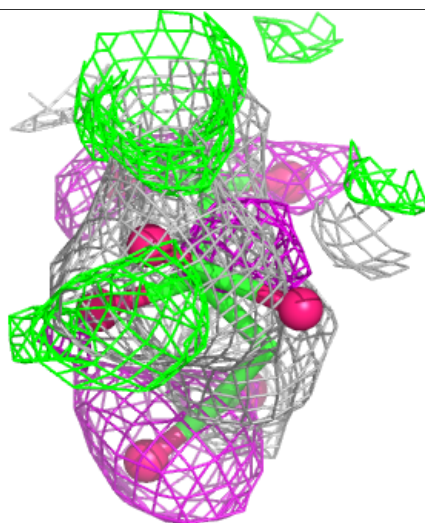
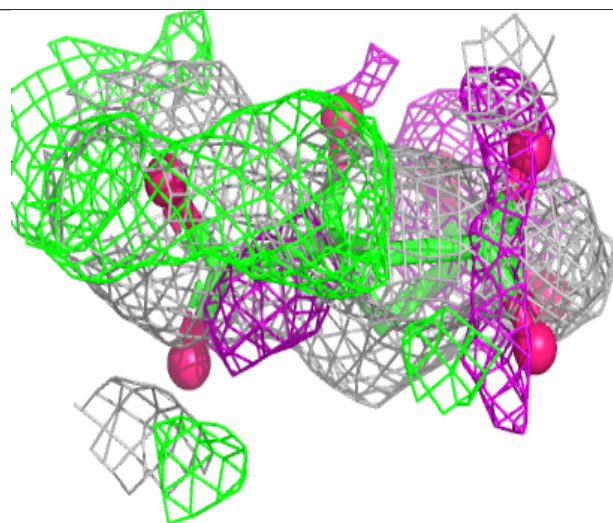
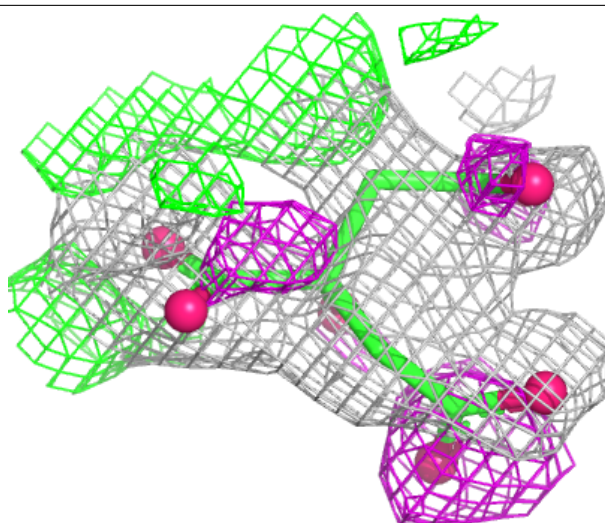
Electron density around FLC A 717:

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



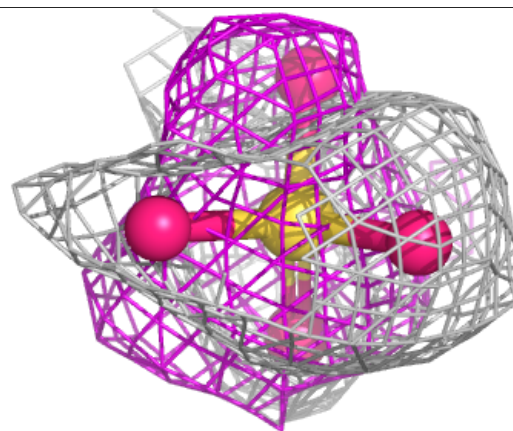
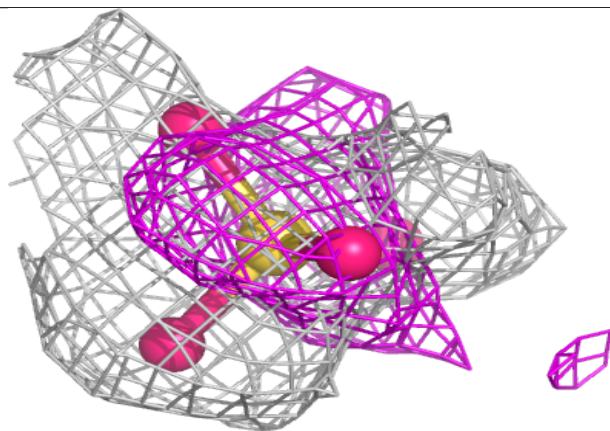
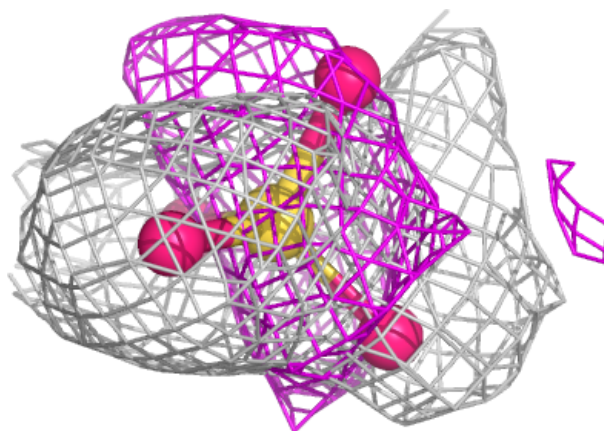
Electron density around FLC H 713:

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



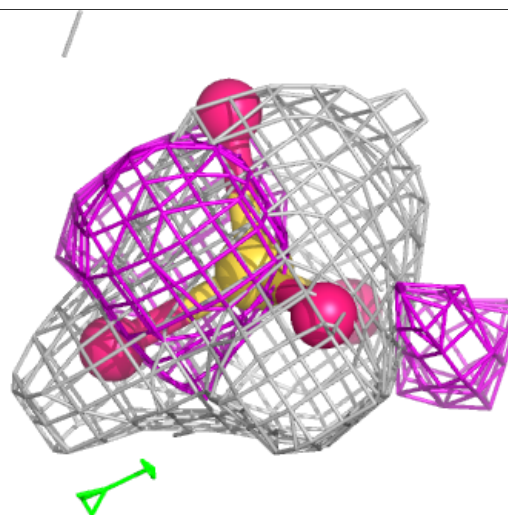
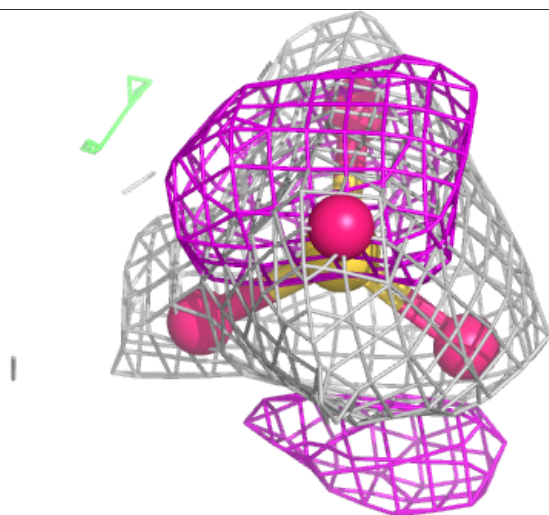
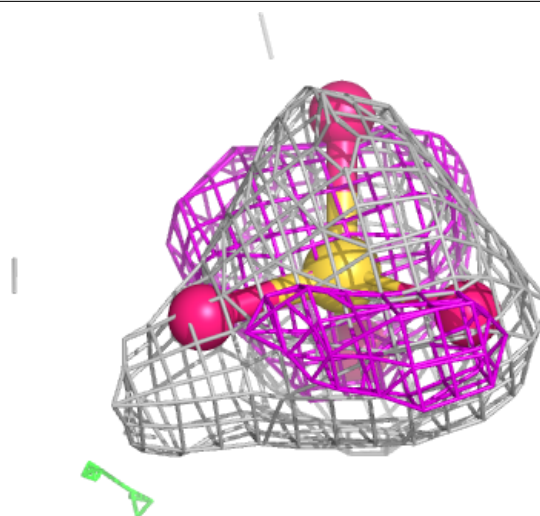
Electron density around SO4 F 705:

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



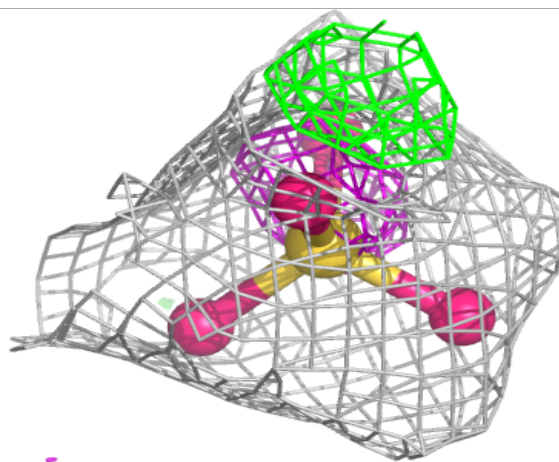
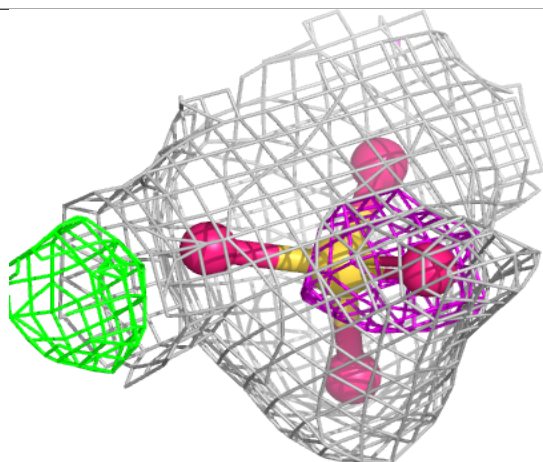
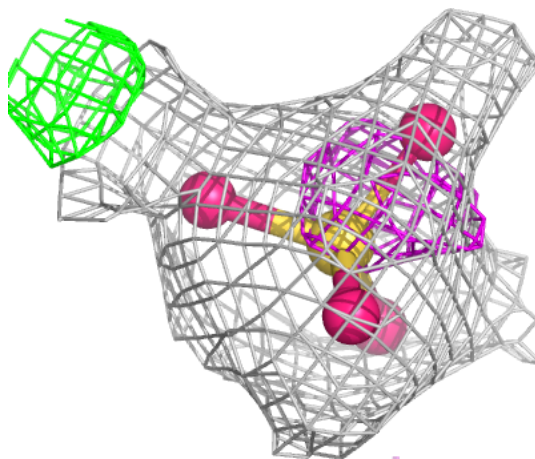
Electron density around SO4 F 707:

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



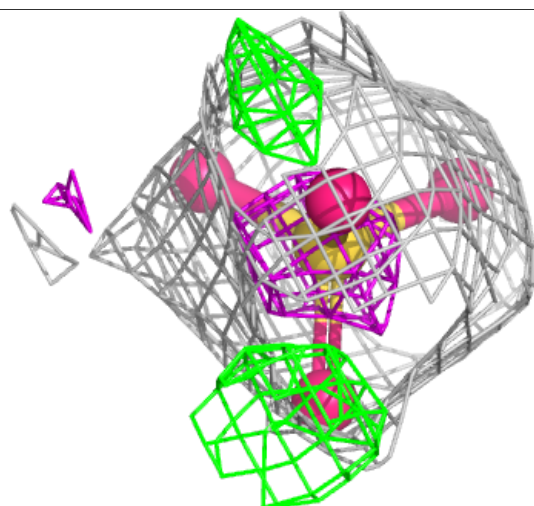
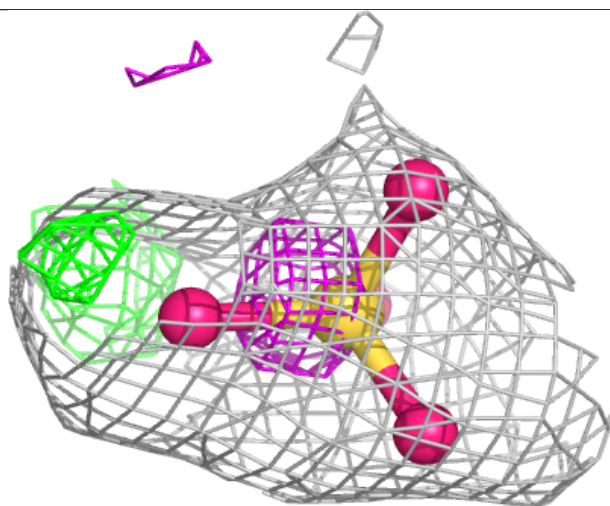
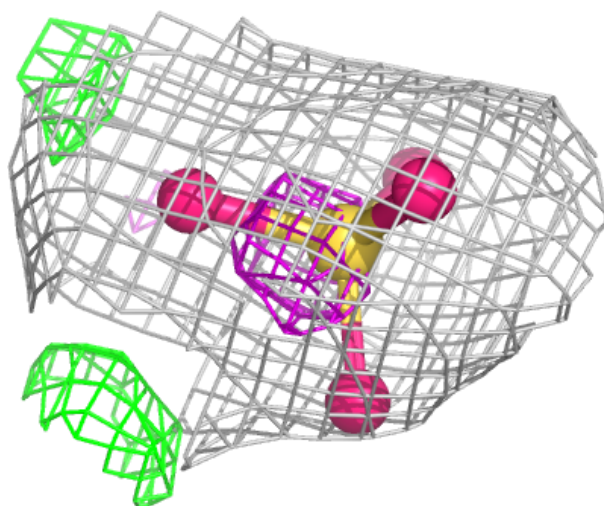
Electron density around SO4 B 712:

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



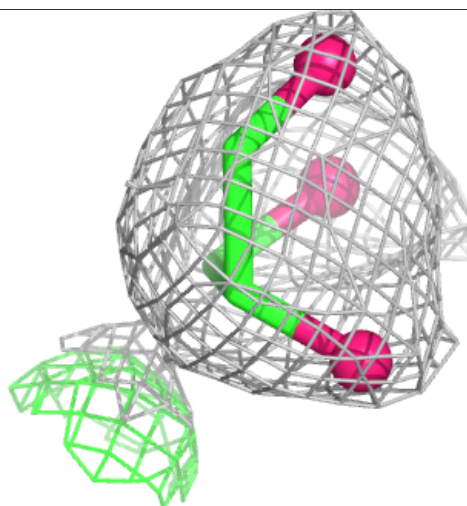
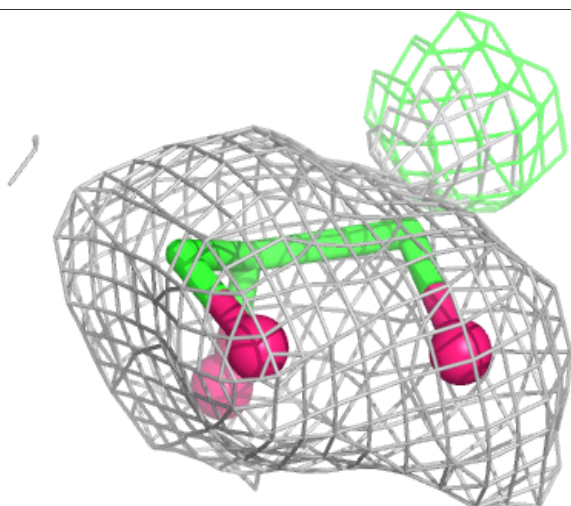
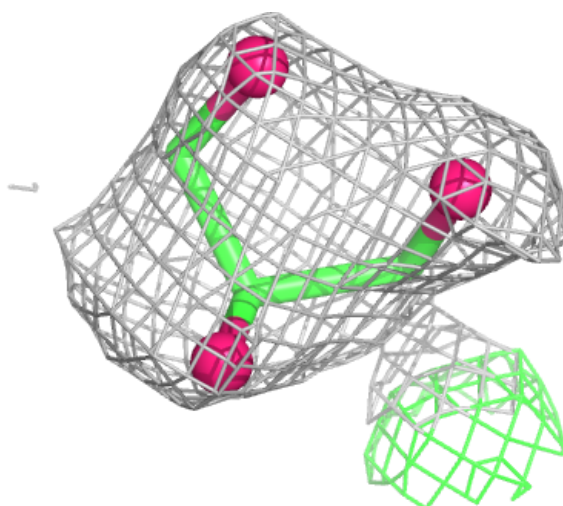
Electron density around SO4 D 707:

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



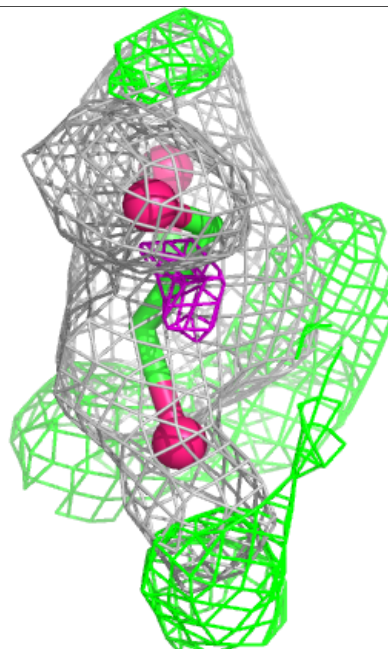
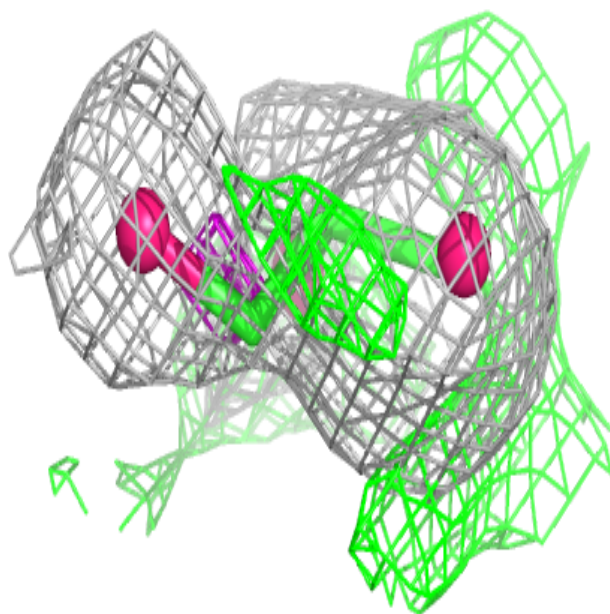
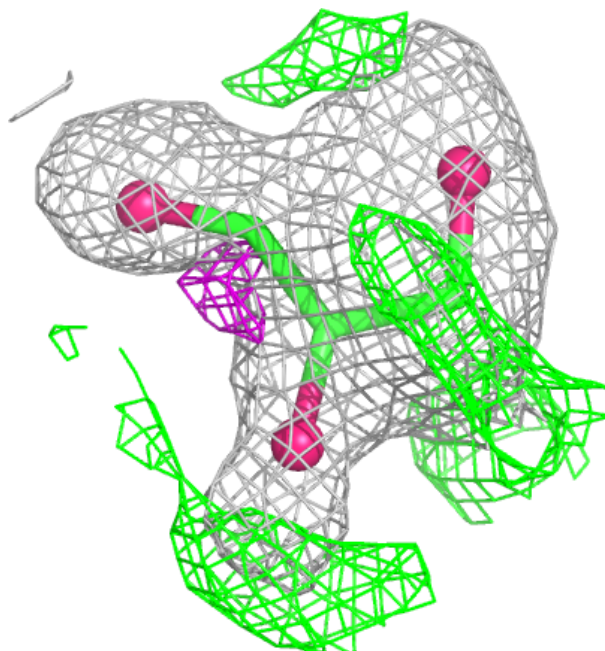
Electron density around GOL F 712:

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



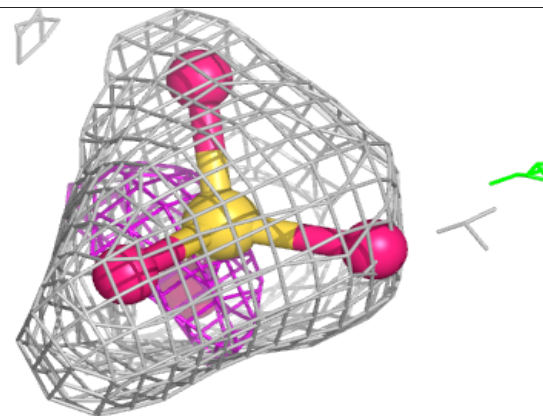
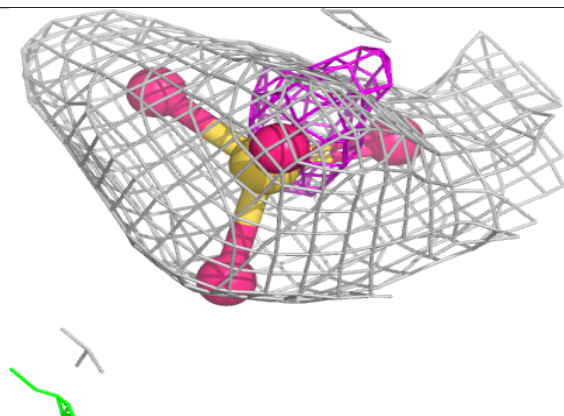
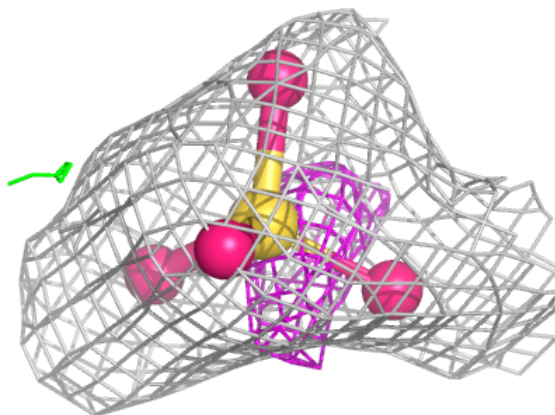
Electron density around GOL D 710:

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



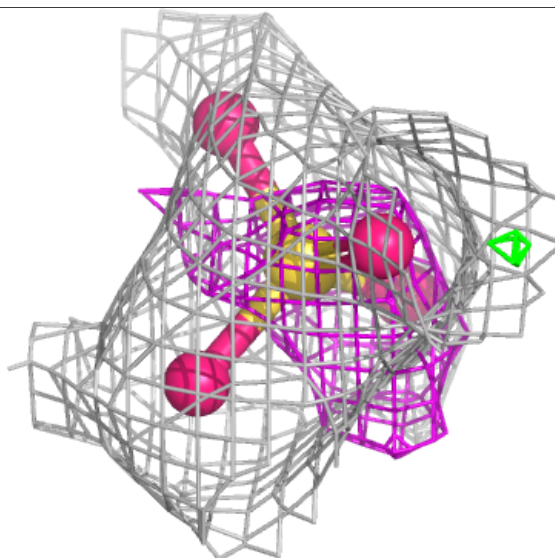
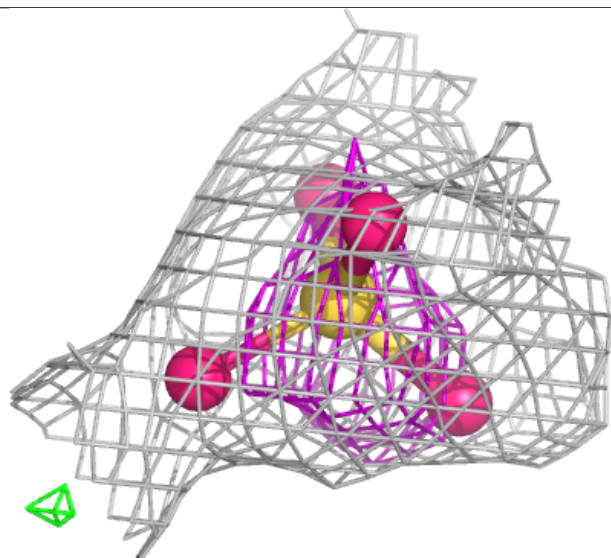
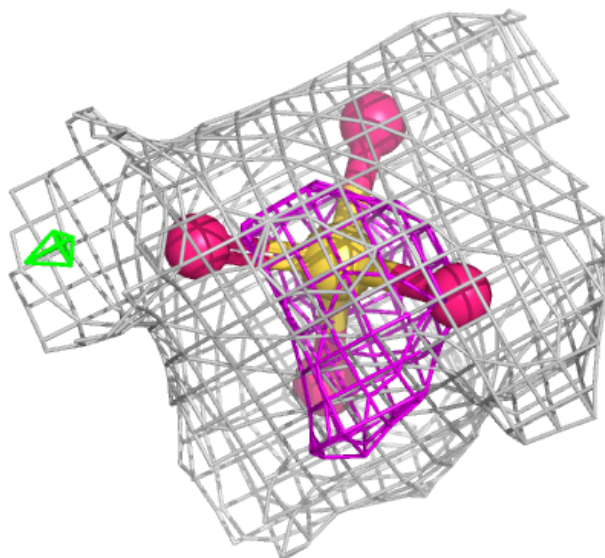
Electron density around SO4 A 708:

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



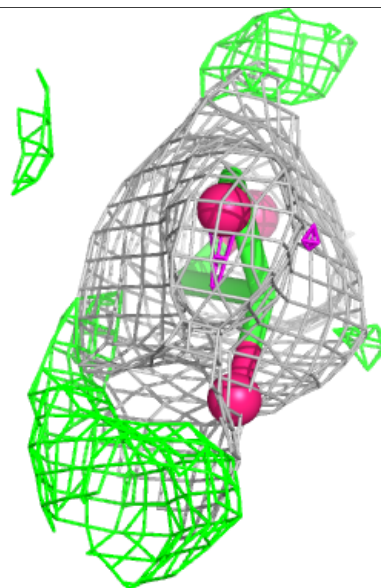
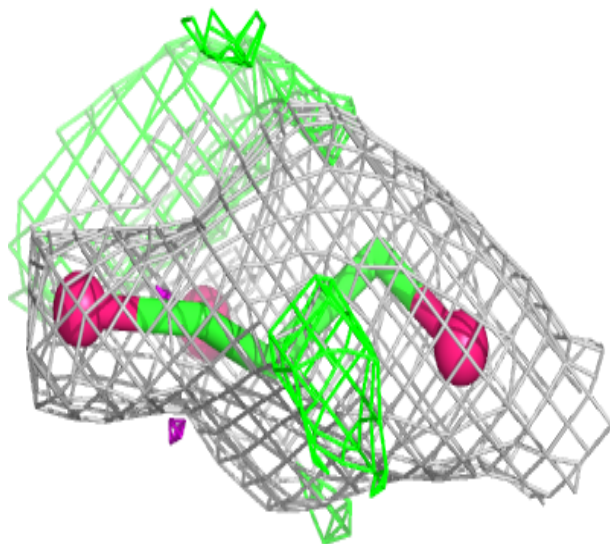
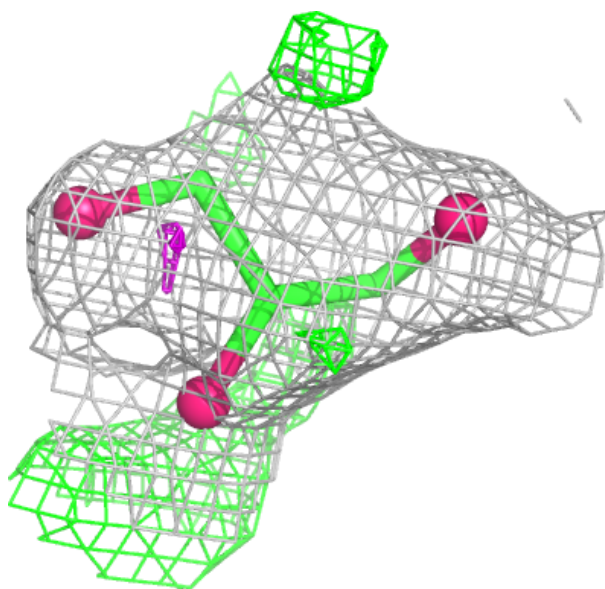
Electron density around SO4 C 706:

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



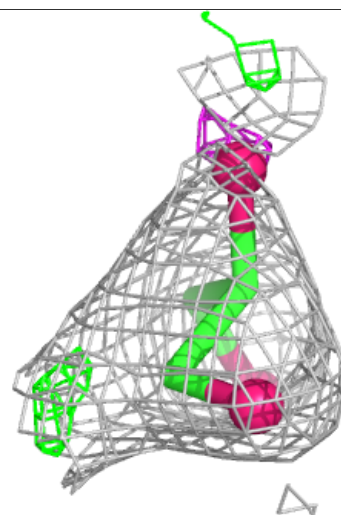
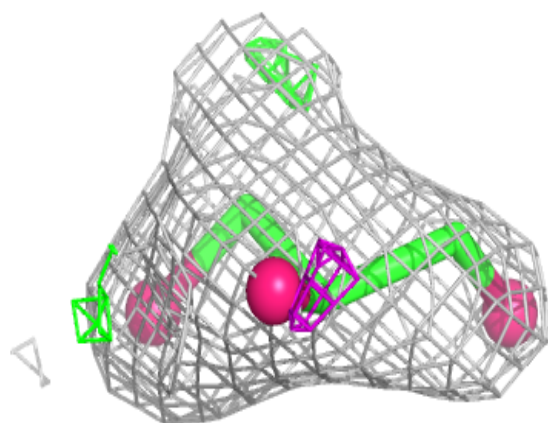
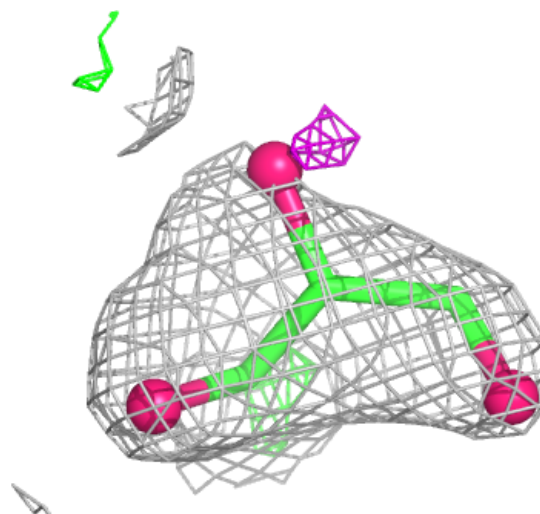
Electron density around GOL G 707:

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



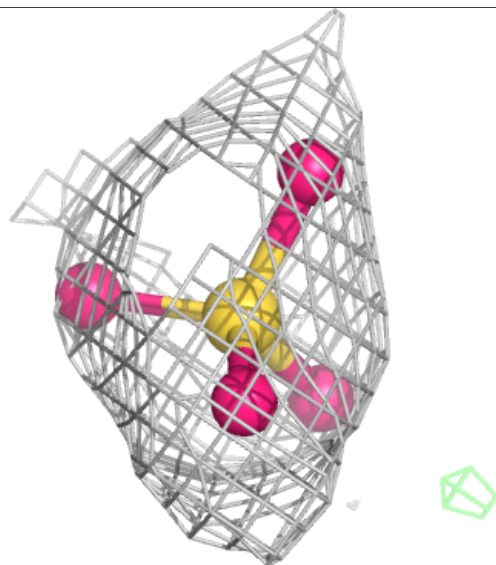
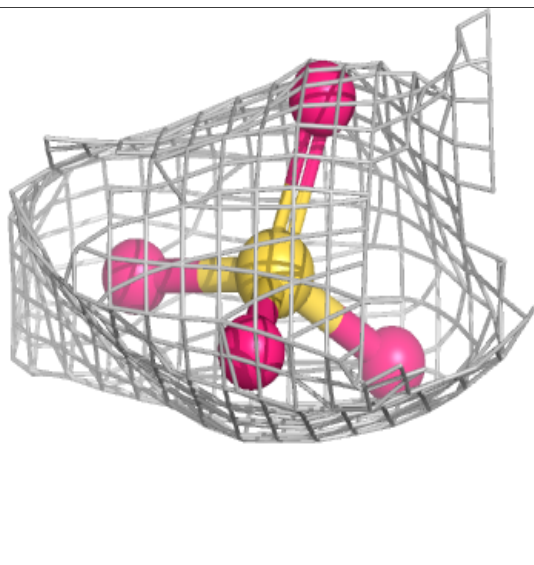
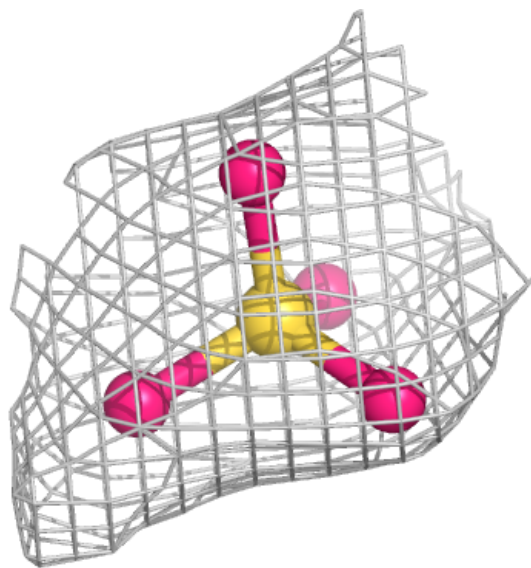
Electron density around GOL E 712:

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



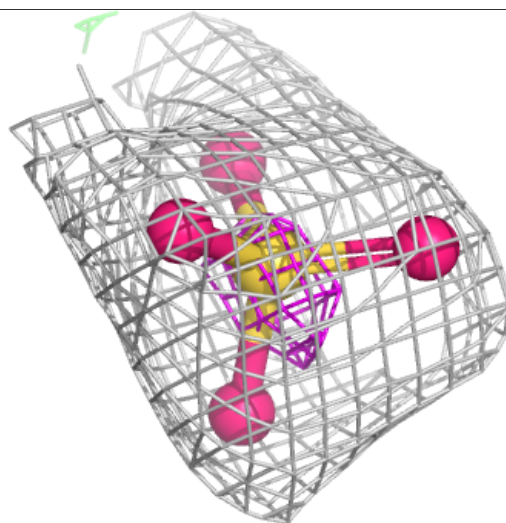
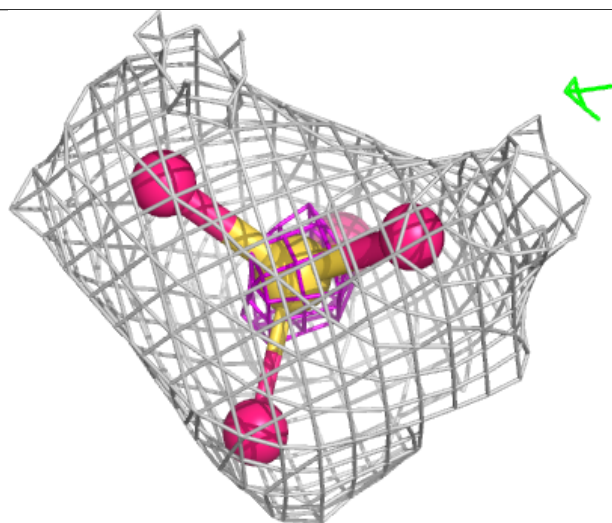
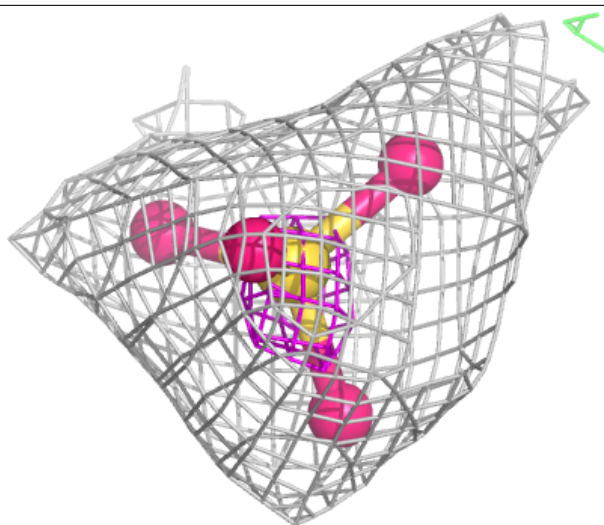
Electron density around SO4 B 711:

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



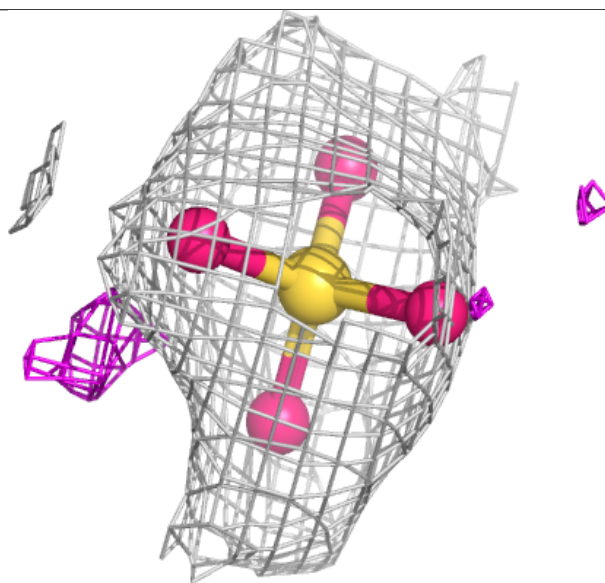
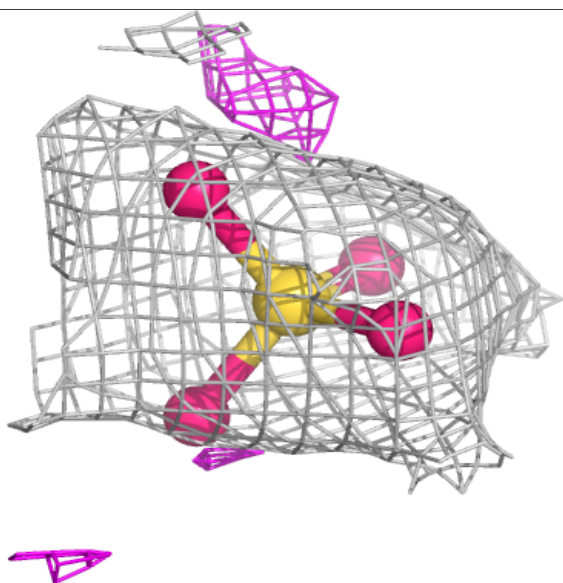
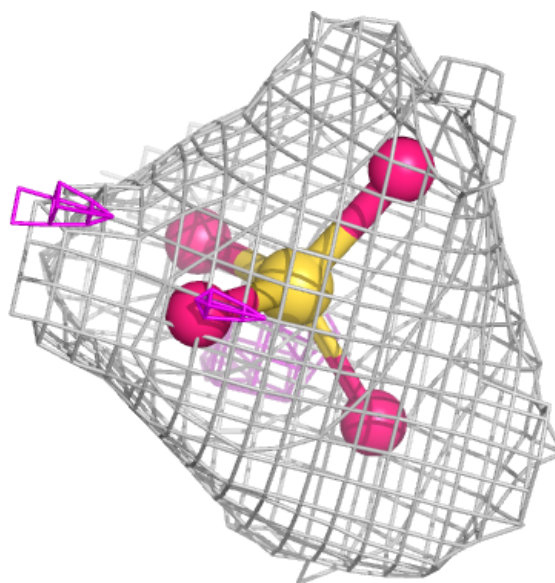
Electron density around SO4 H 709:

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



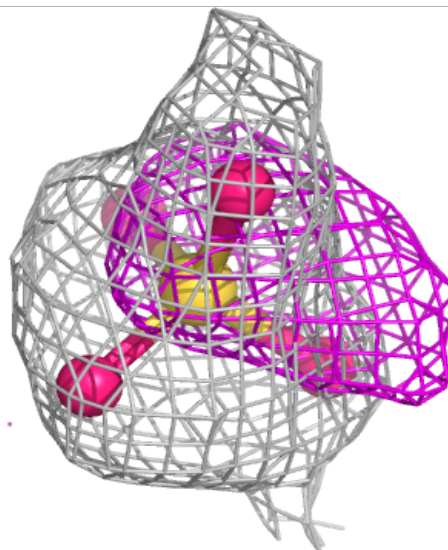
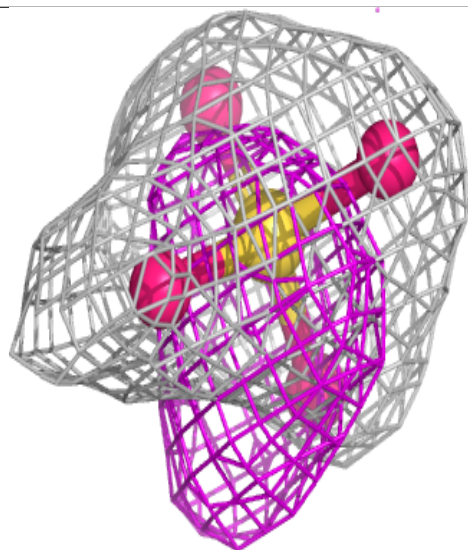
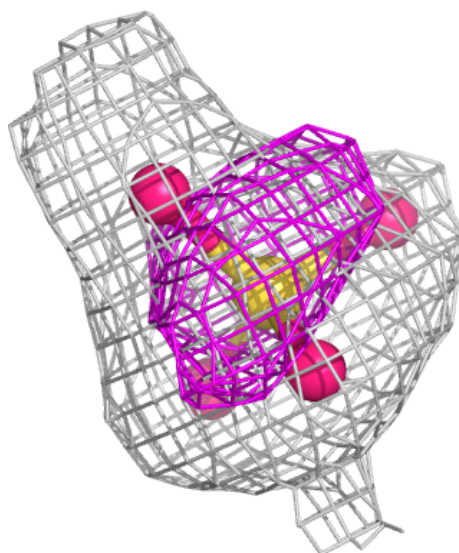
Electron density around SO4 H 706:

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



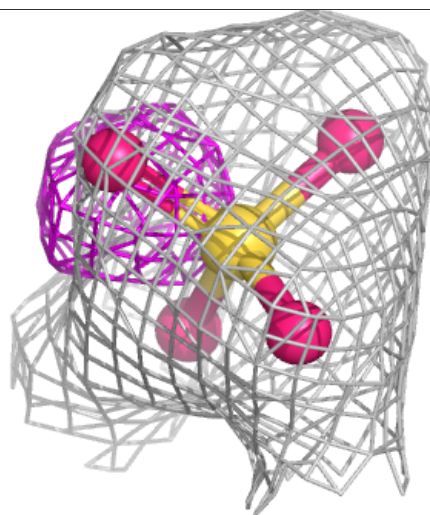
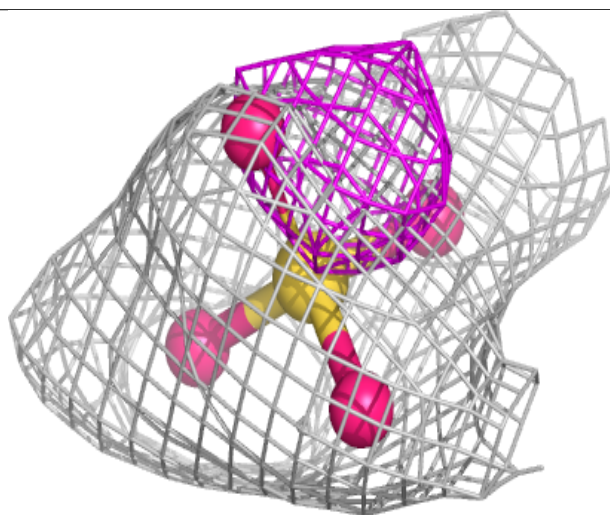
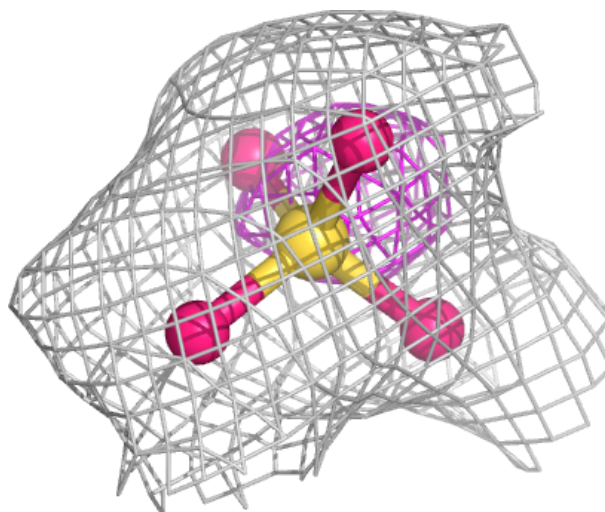
Electron density around SO4 H 707:

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



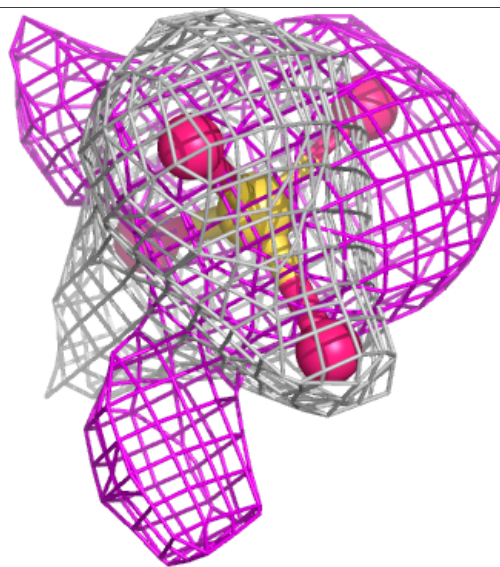
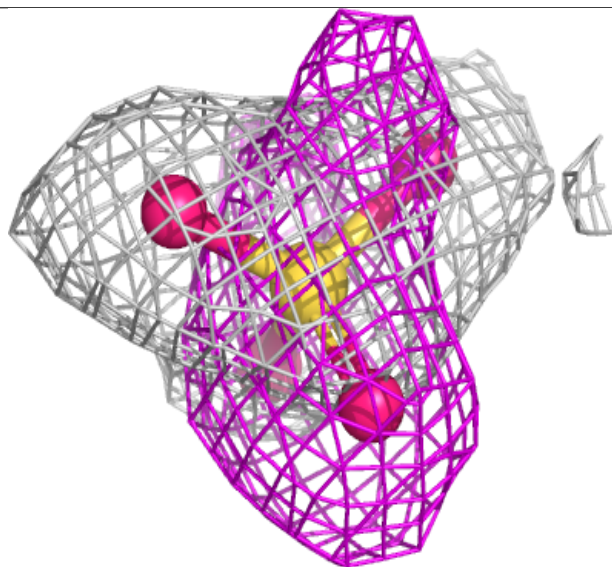
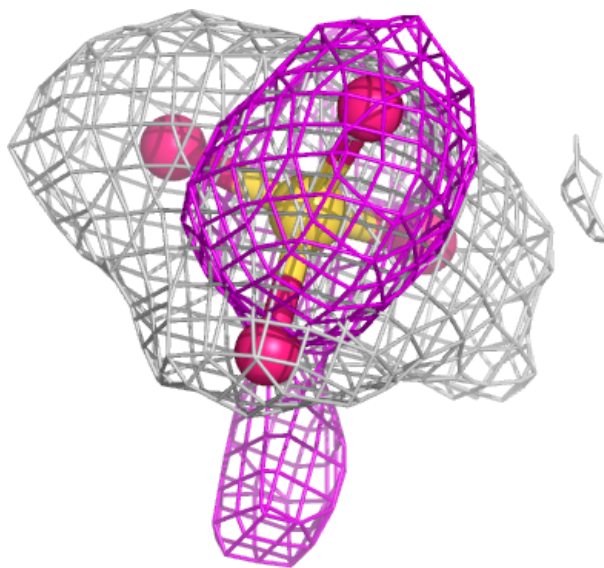
Electron density around SO4 G 702:

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



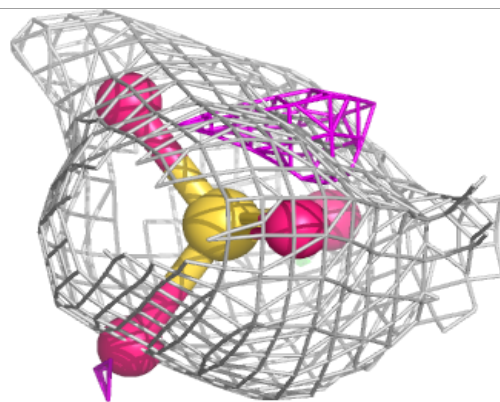
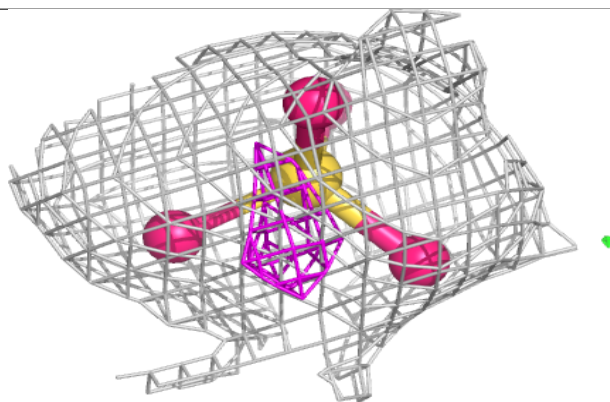
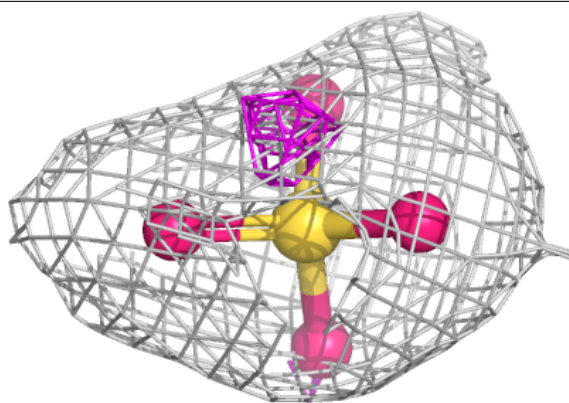
Electron density around SO4 E 709:

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



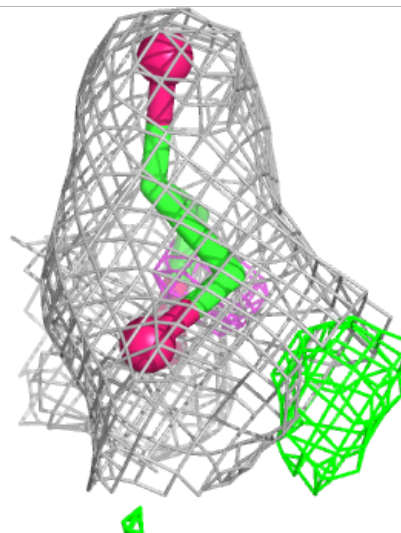
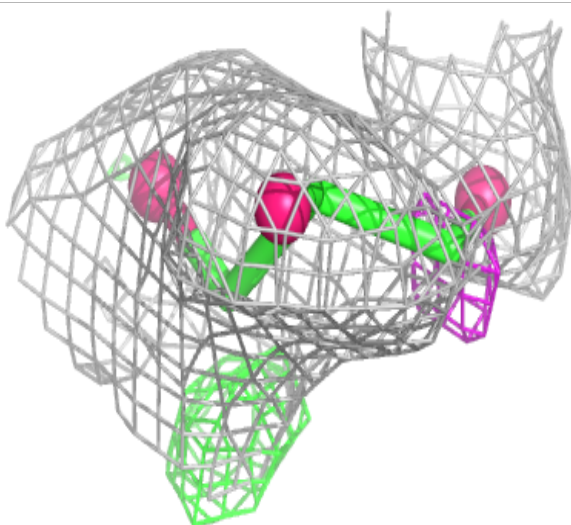
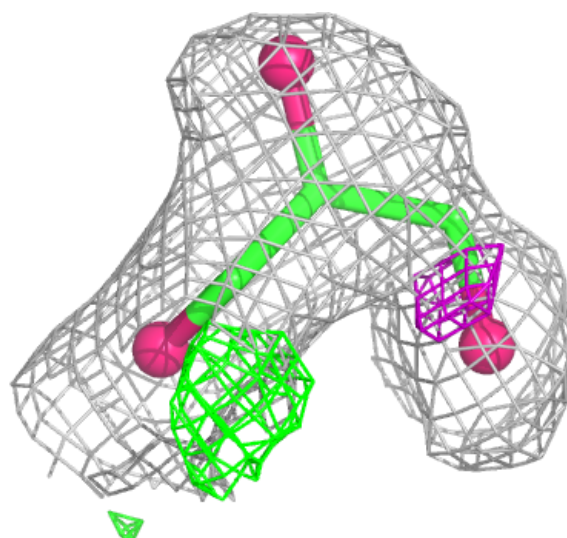
Electron density around SO4 A 707:

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



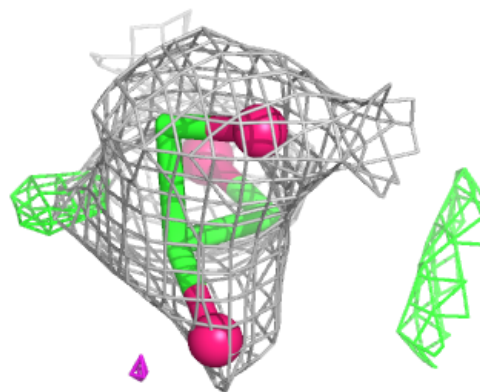
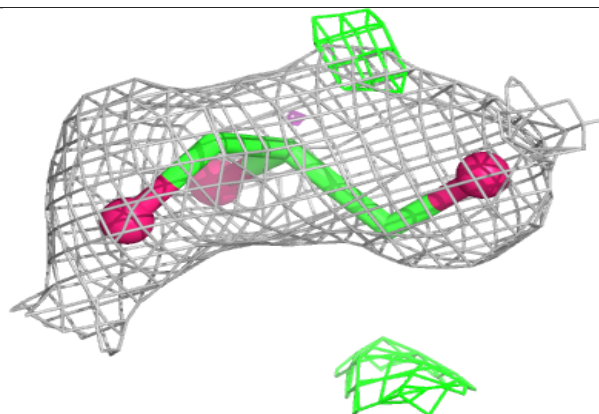
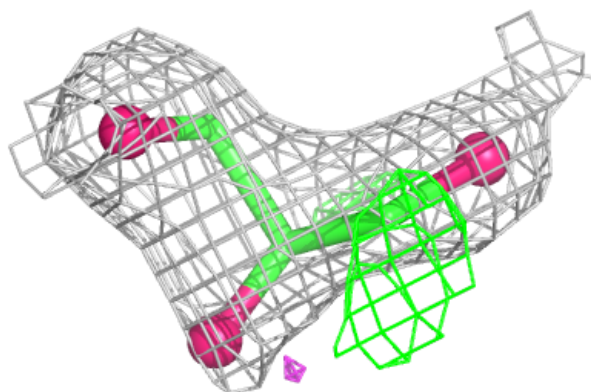
Electron density around GOL D 712:

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

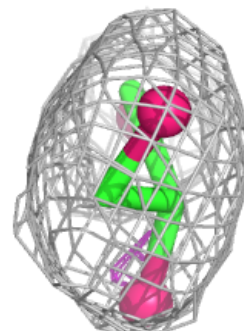
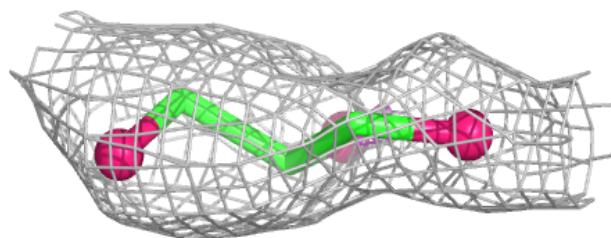
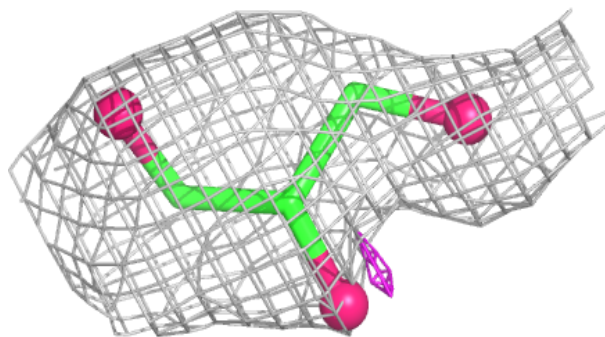


Electron density around GOL E 714:

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

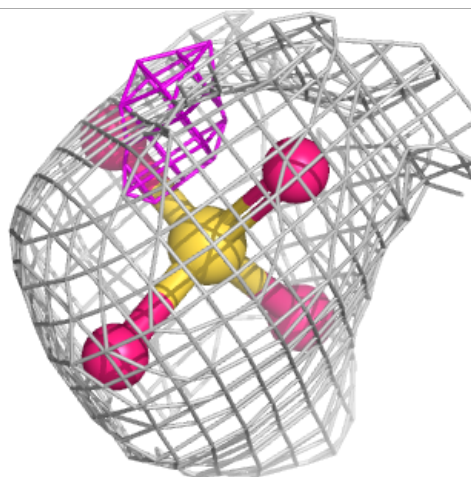
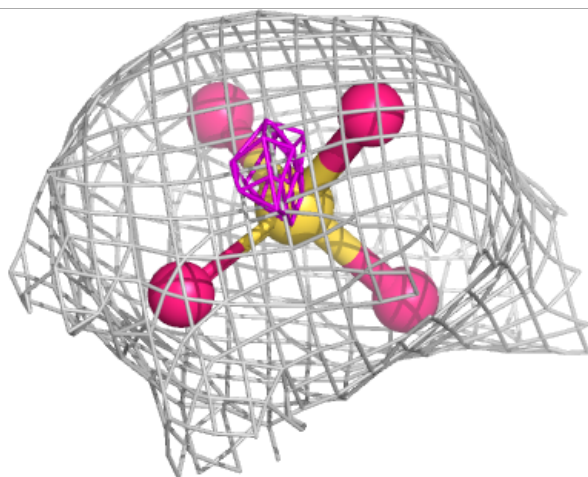
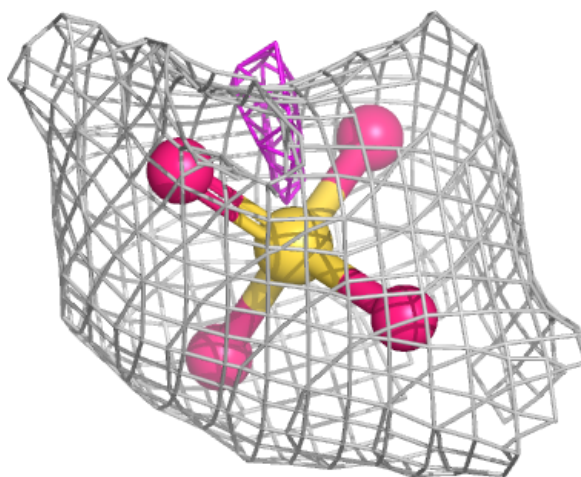
**Electron density around GOL D 713:**

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



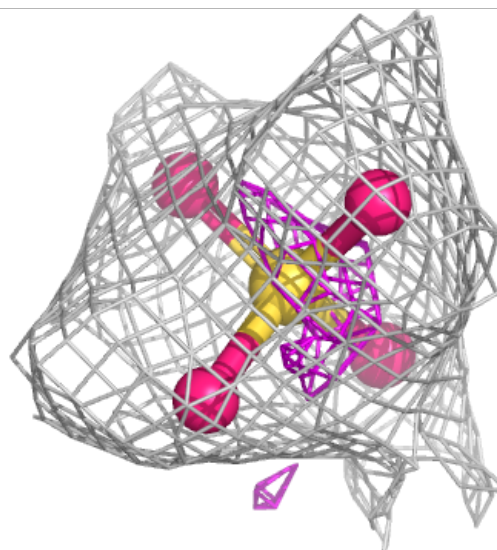
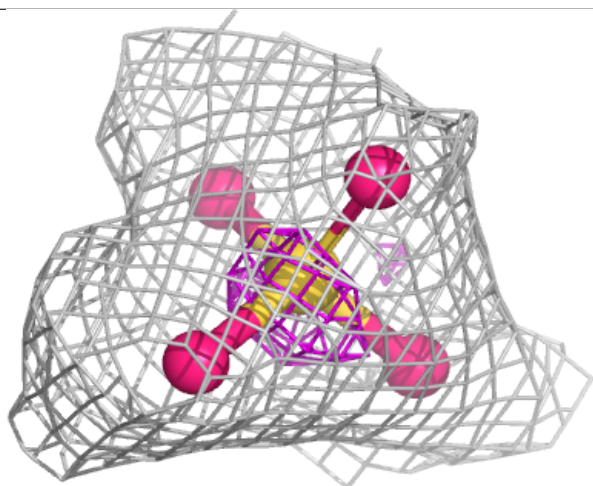
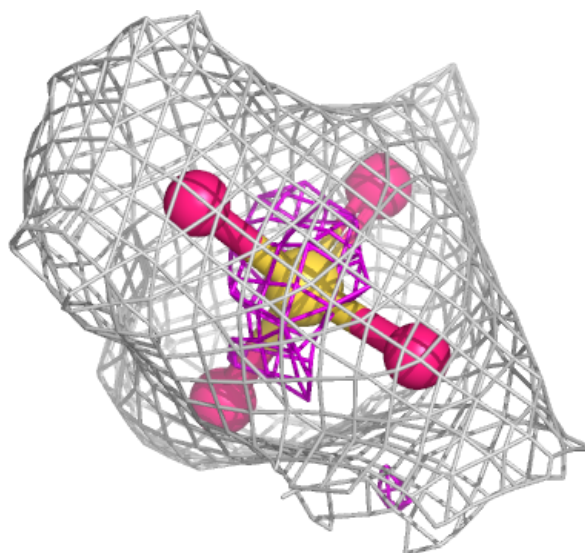
Electron density around SO4 E 707:

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



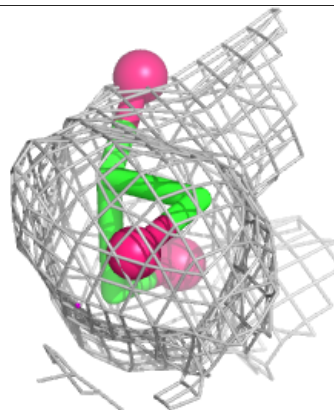
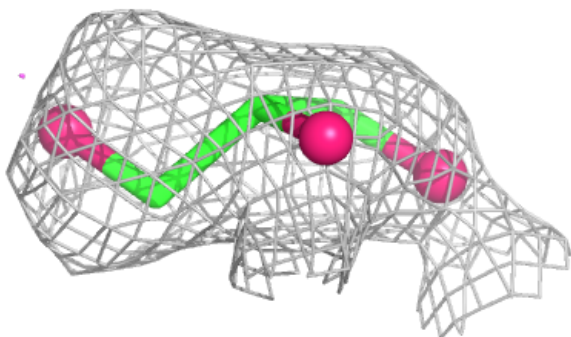
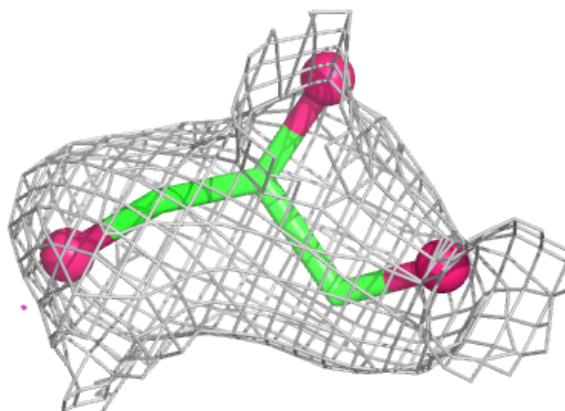
Electron density around SO4 G 703:

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



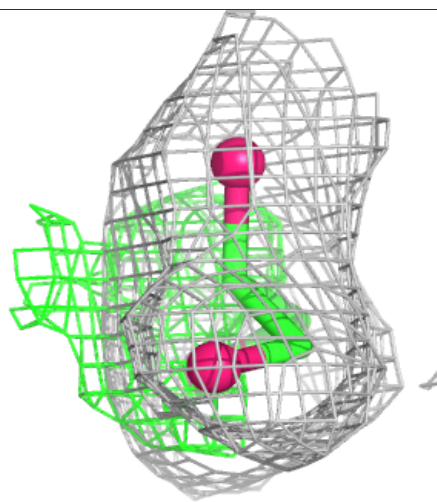
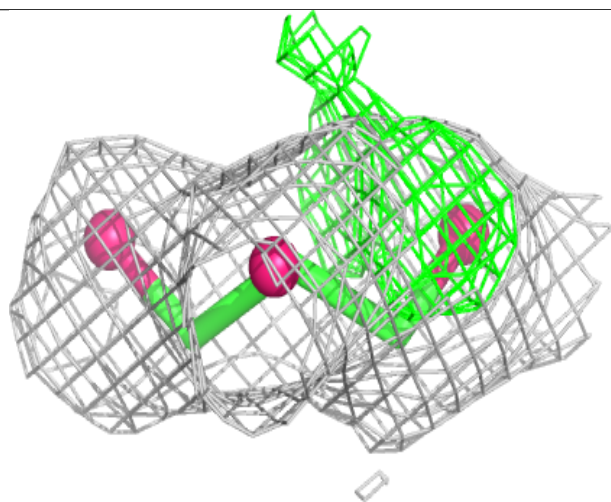
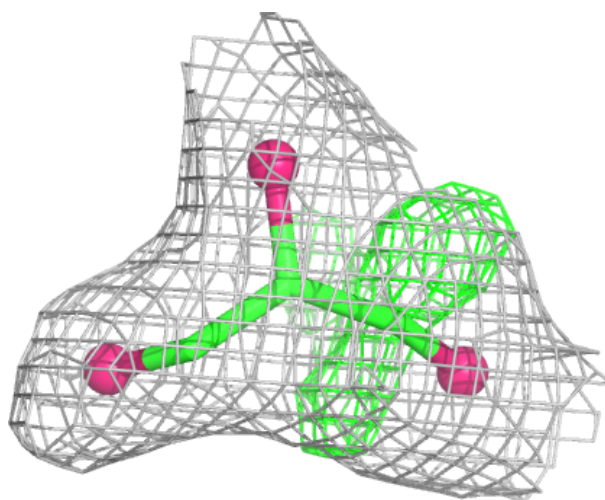
Electron density around GOL F 710:

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



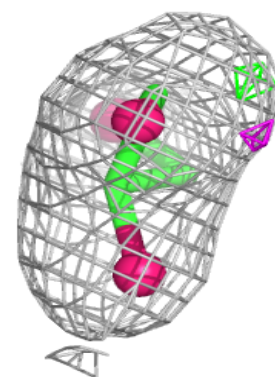
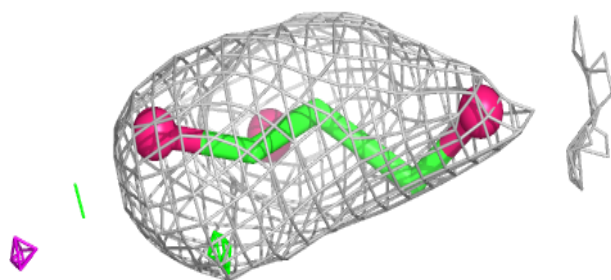
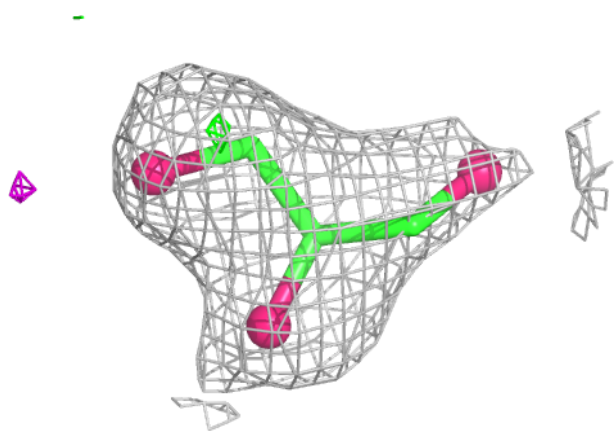
Electron density around GOL G 708:

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

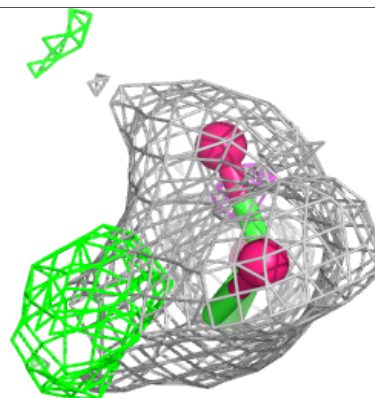
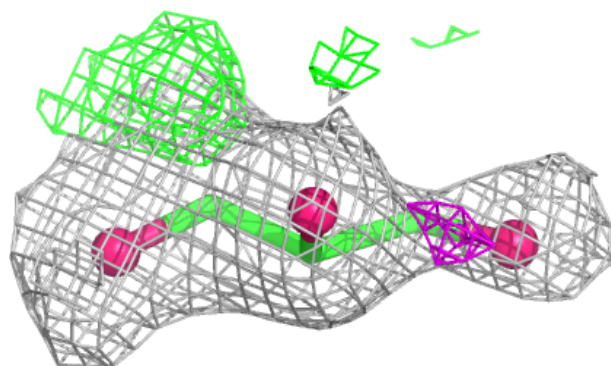
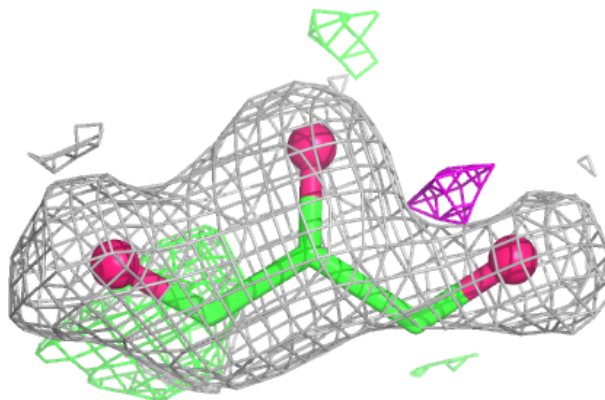


Electron density around GOL F 709:

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

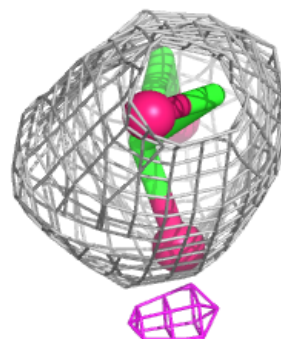
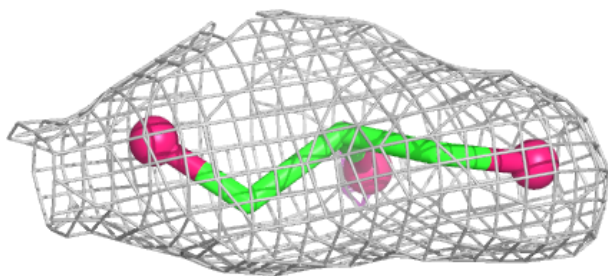
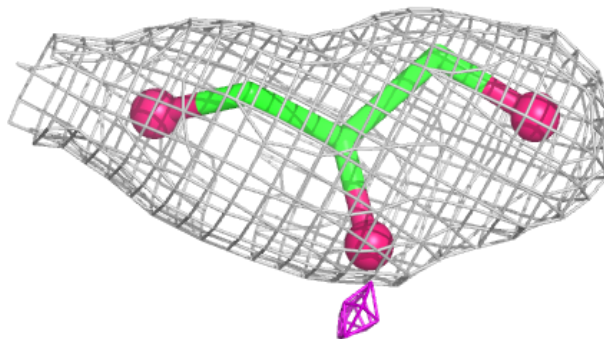
**Electron density around GOL A 713:**

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



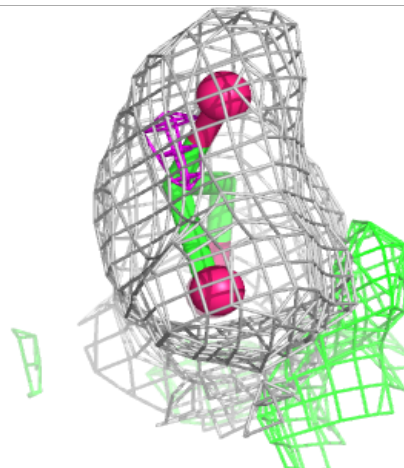
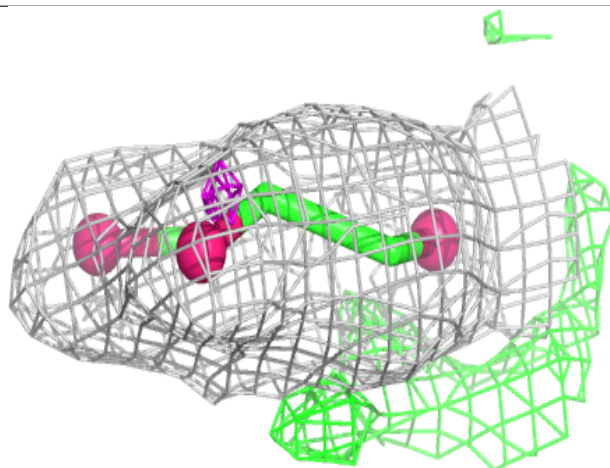
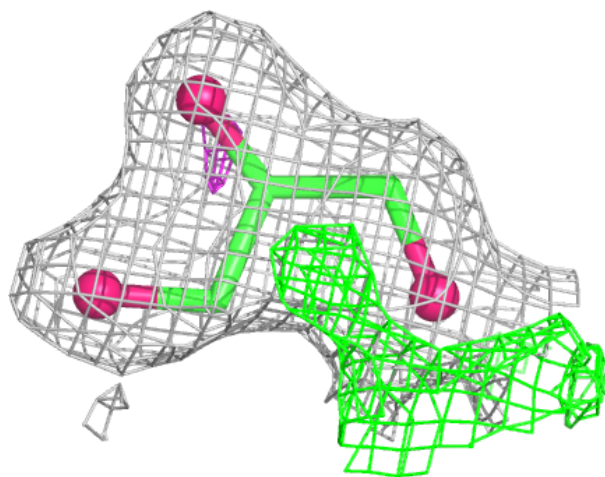
Electron density around GOL A 715:

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



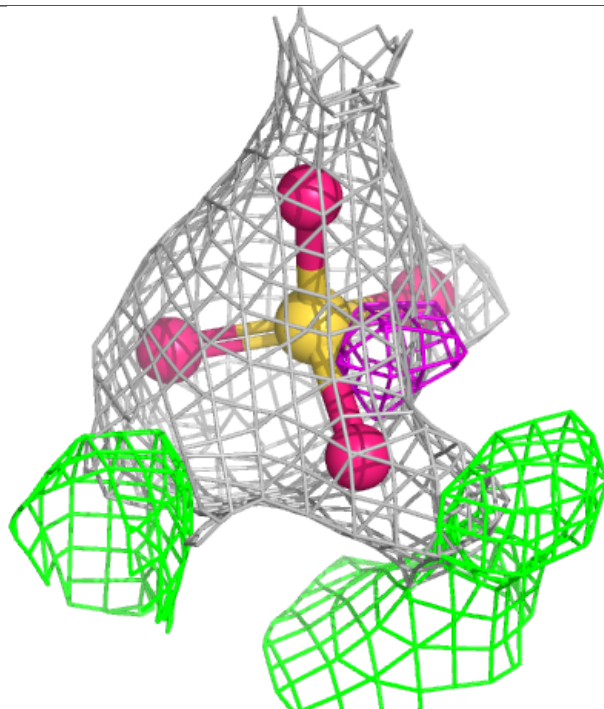
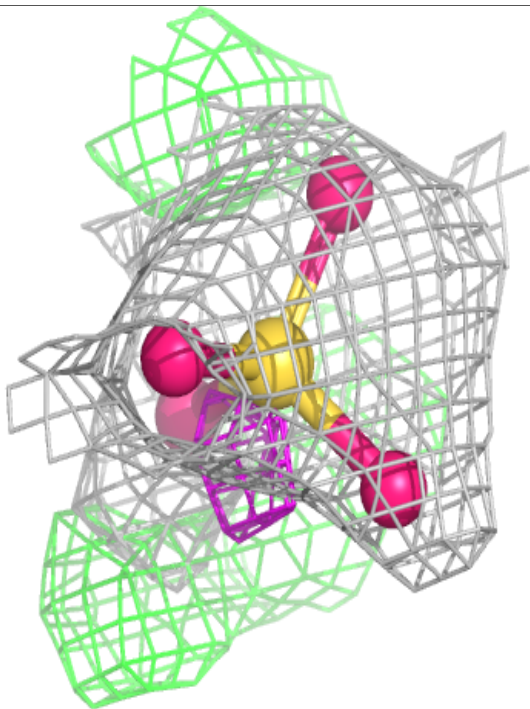
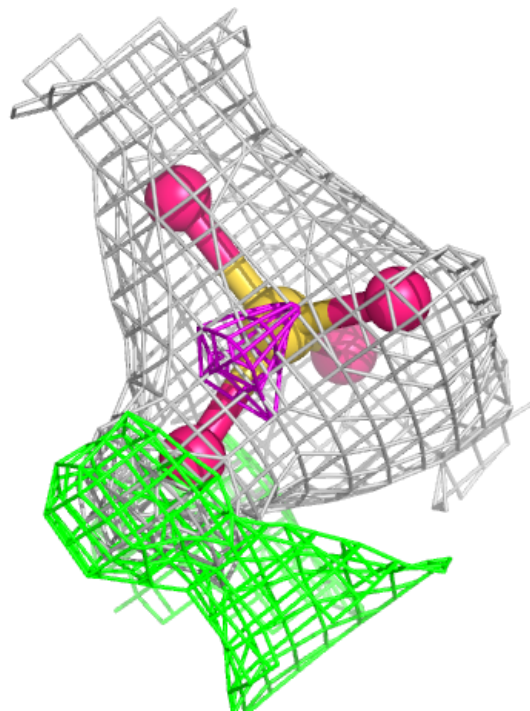
Electron density around GOL C 709:

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



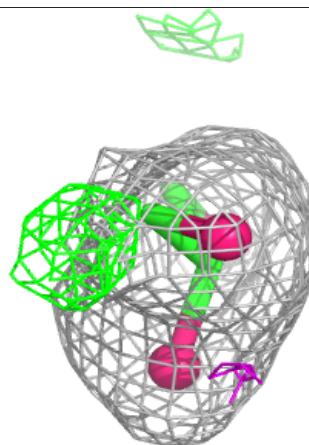
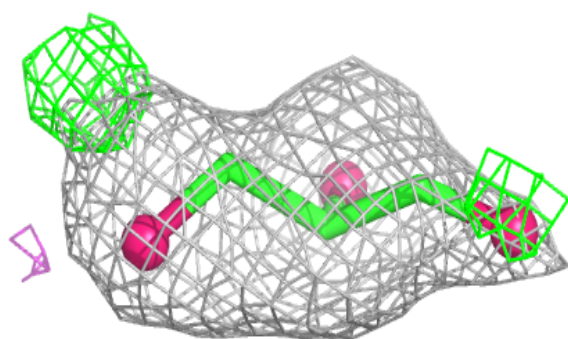
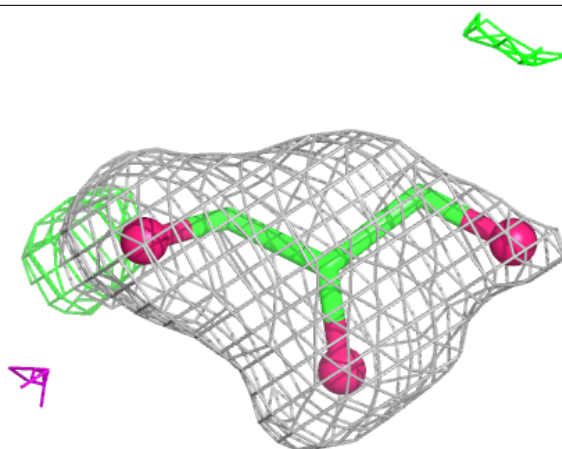
Electron density around SO4 F 706:

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



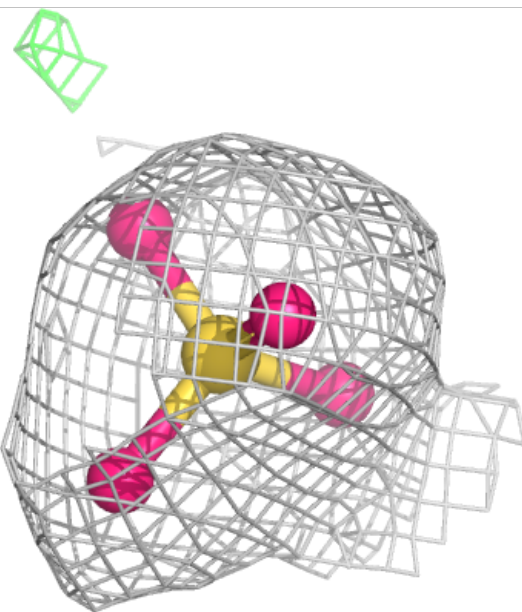
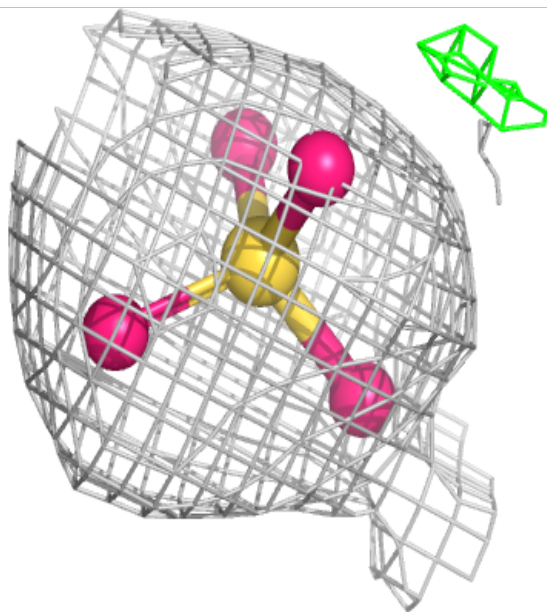
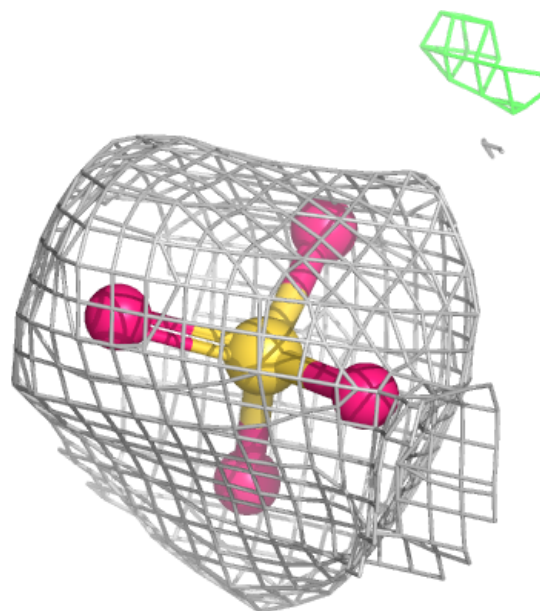
Electron density around GOL C 712:

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



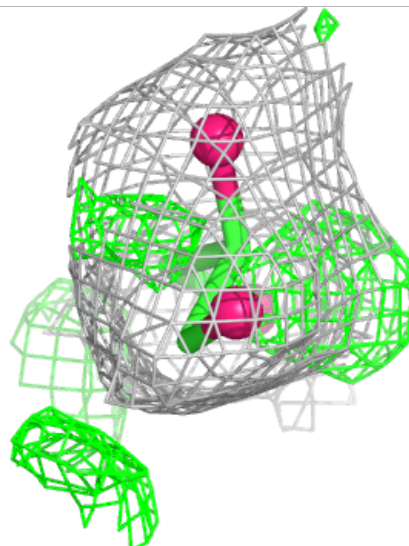
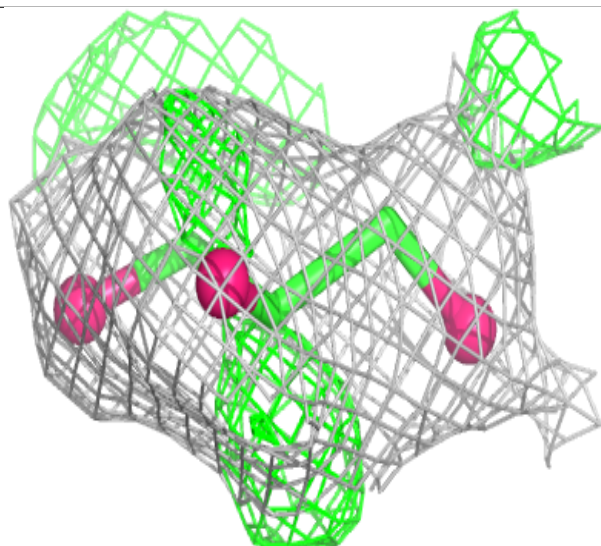
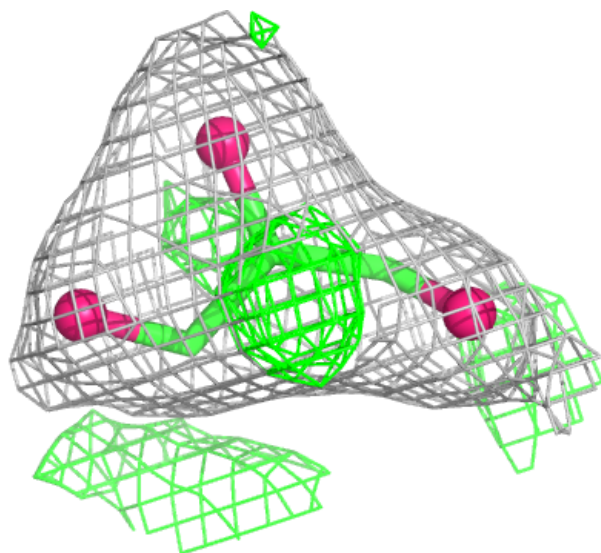
Electron density around SO4 B 708:

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



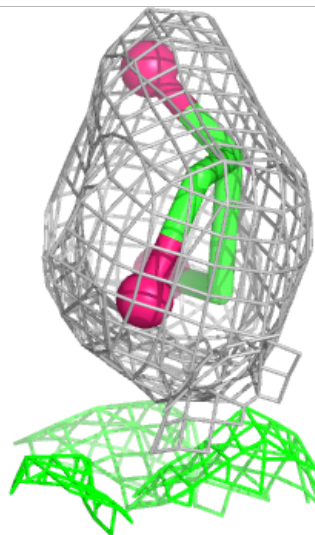
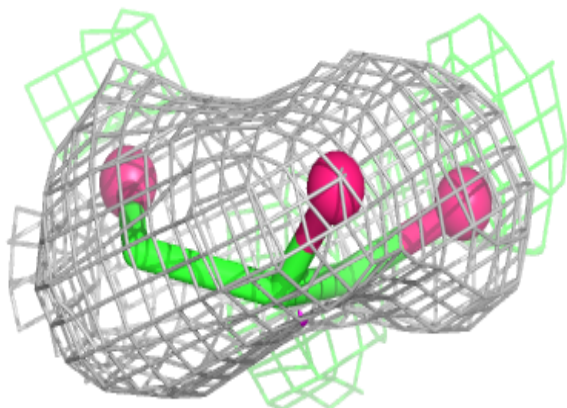
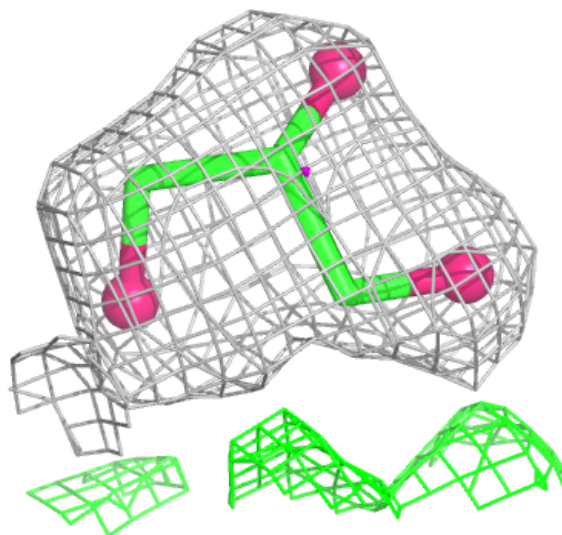
Electron density around GOL C 710:

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



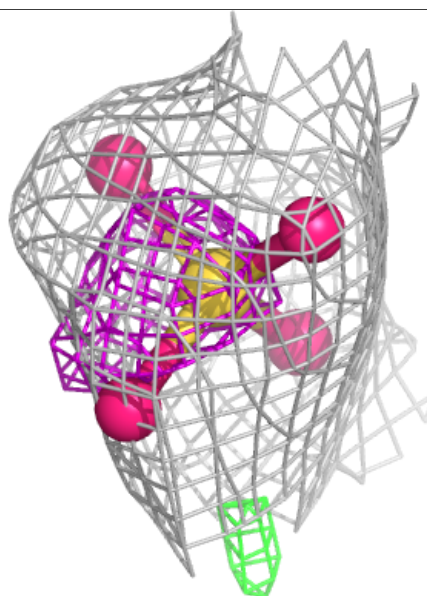
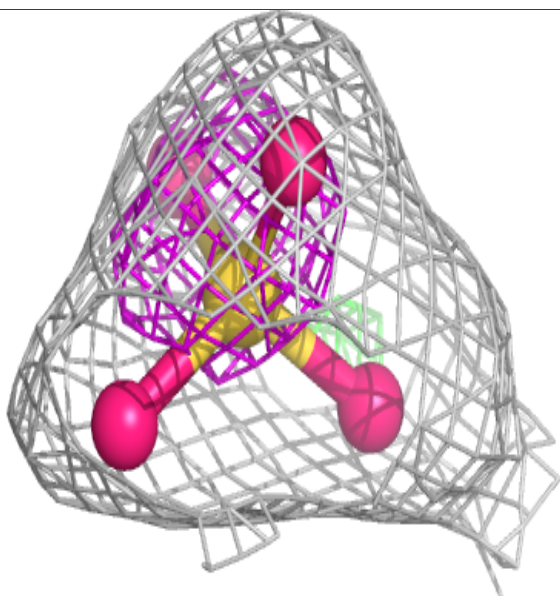
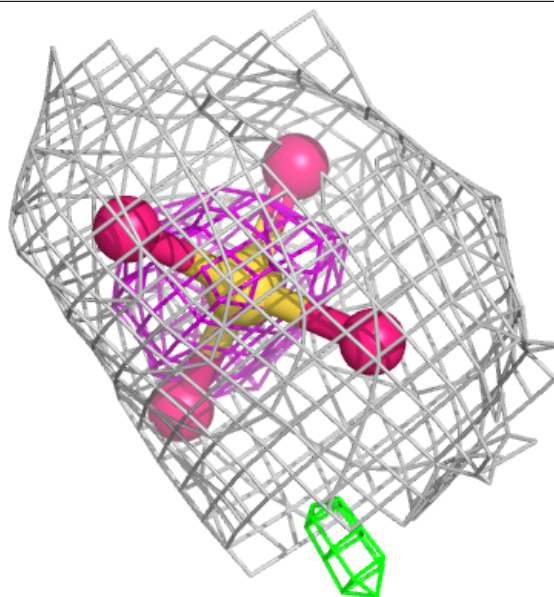
Electron density around GOL F 708:

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



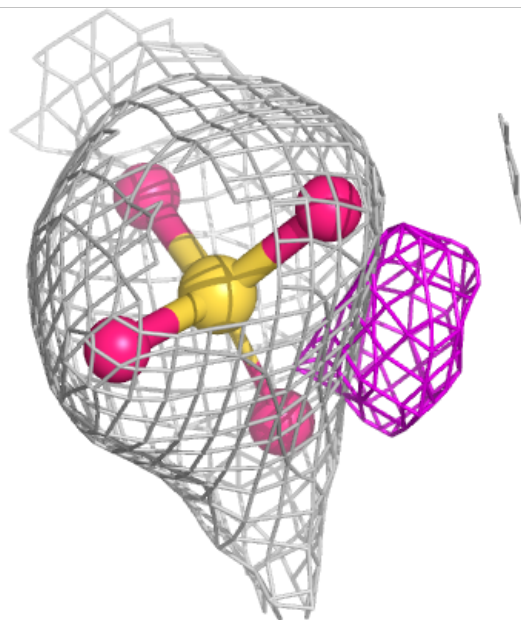
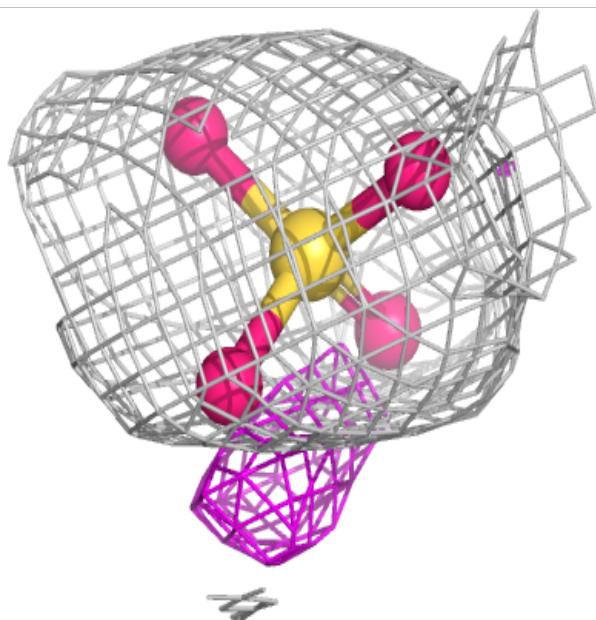
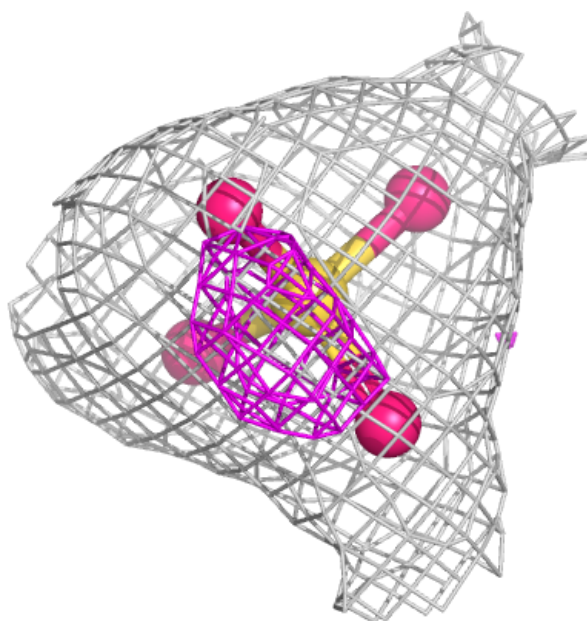
Electron density around SO4 A 705:

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



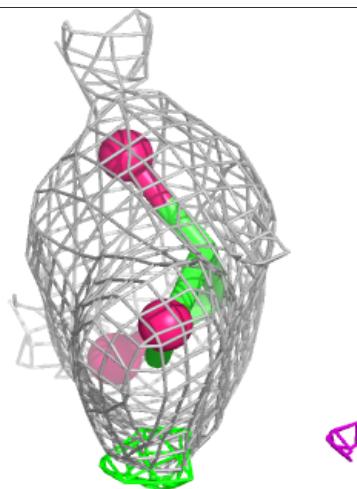
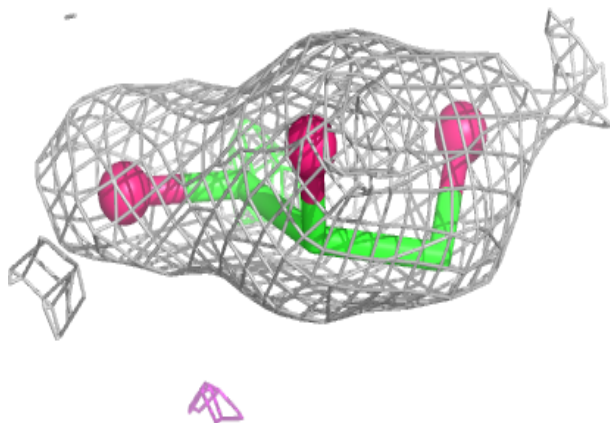
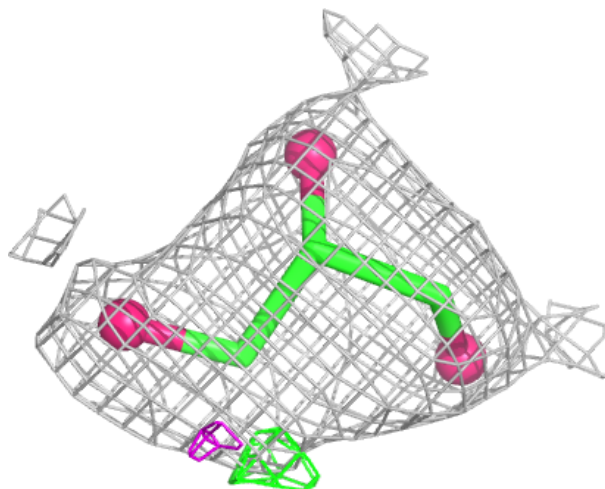
Electron density around SO4 E 708:

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



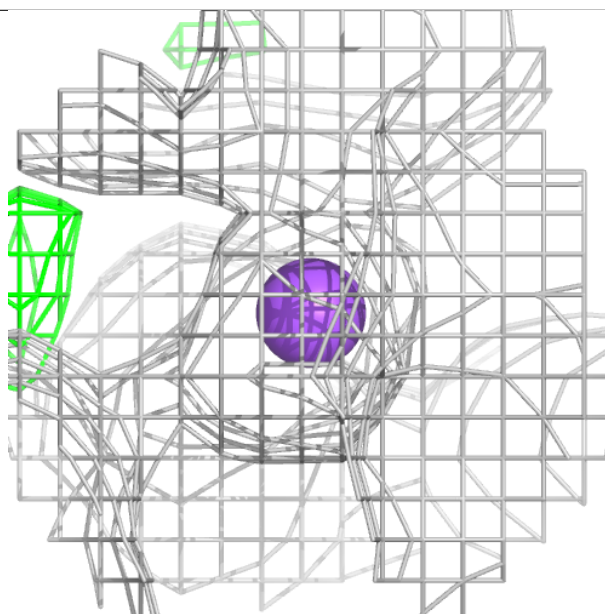
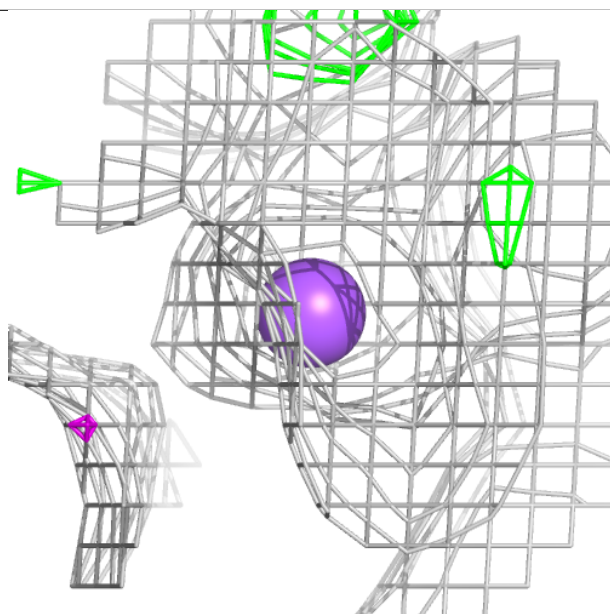
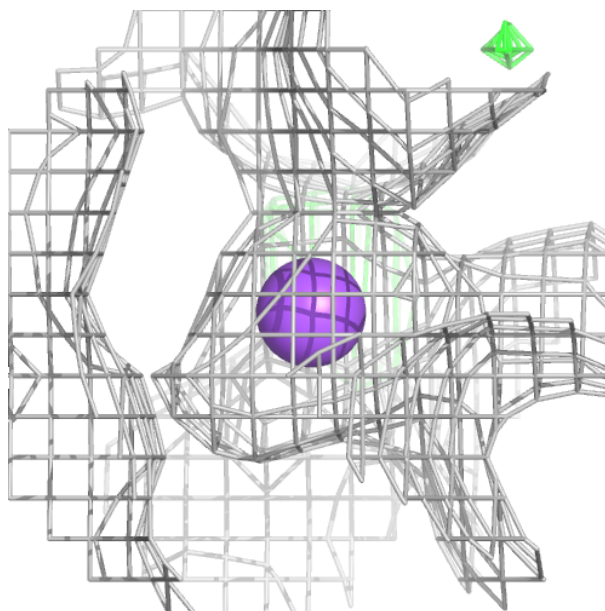
Electron density around GOL B 718:

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



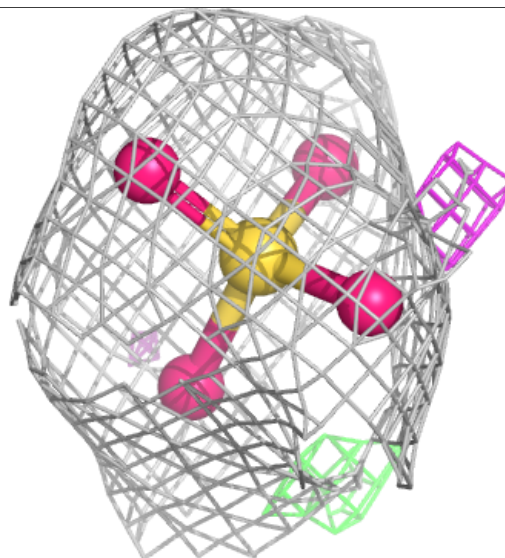
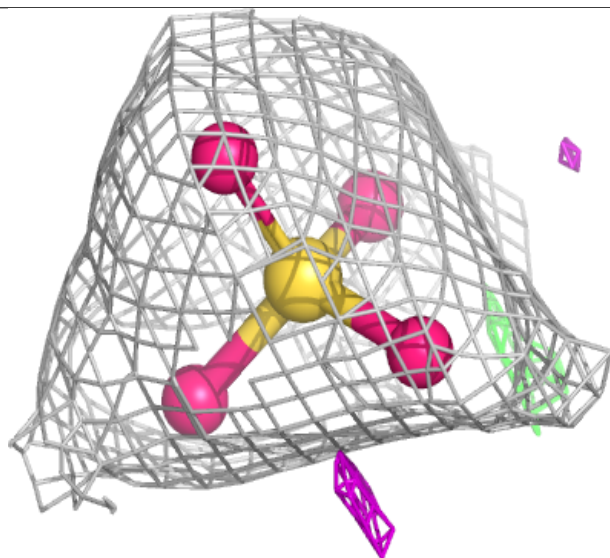
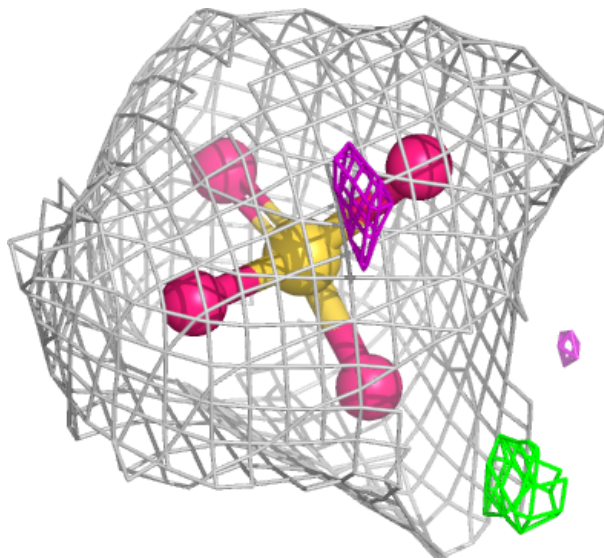
Electron density around NA A 712:

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



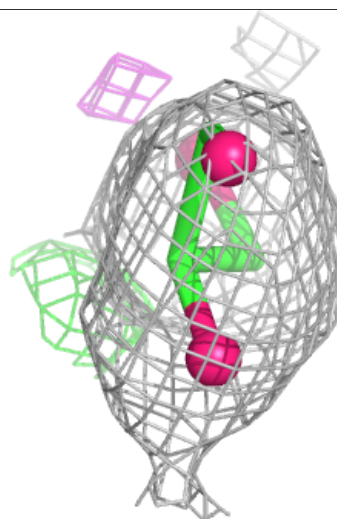
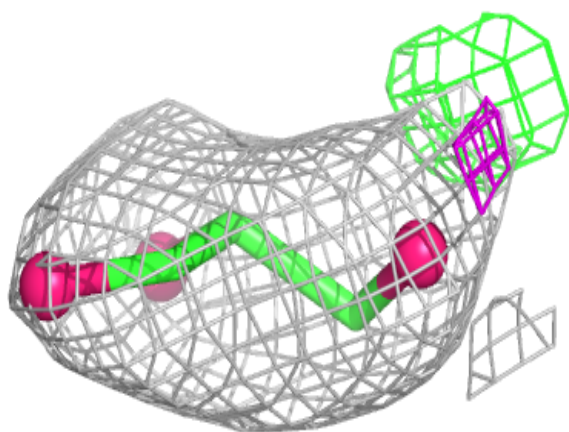
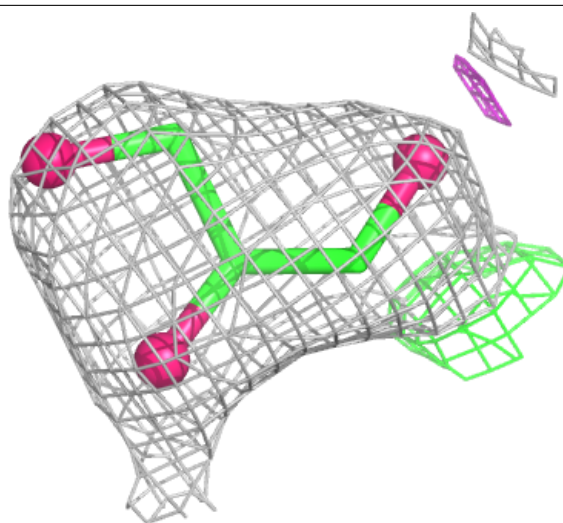
Electron density around SO4 G 705:

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



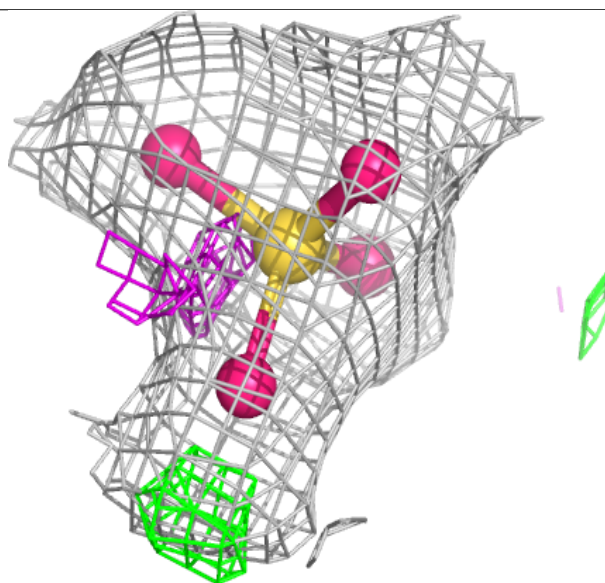
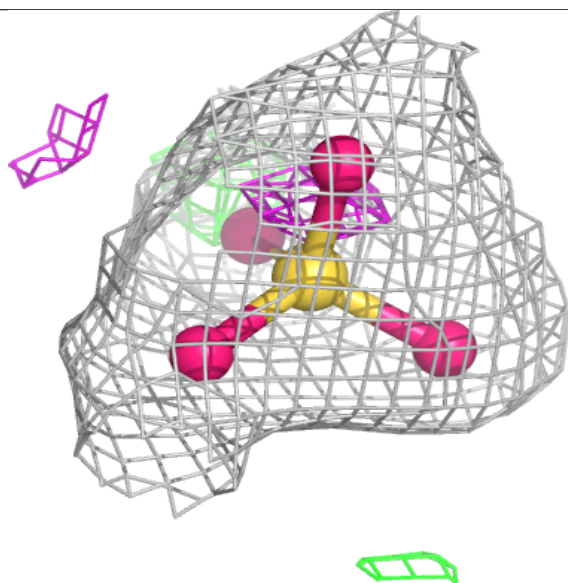
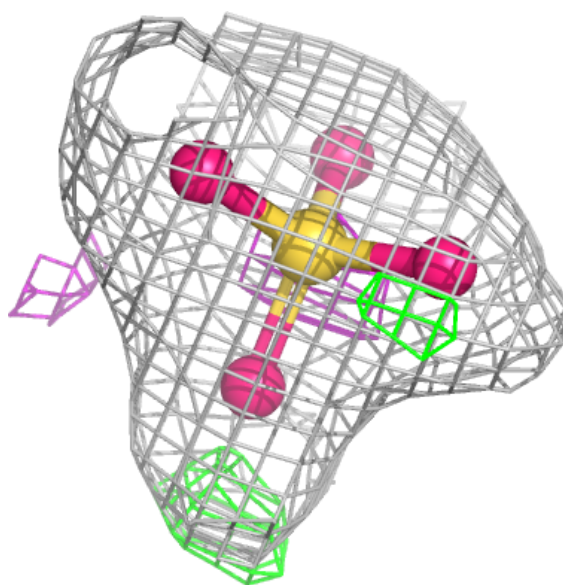
Electron density around GOL D 711:

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



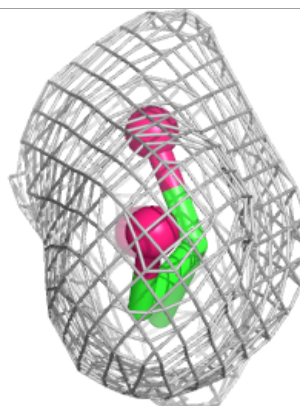
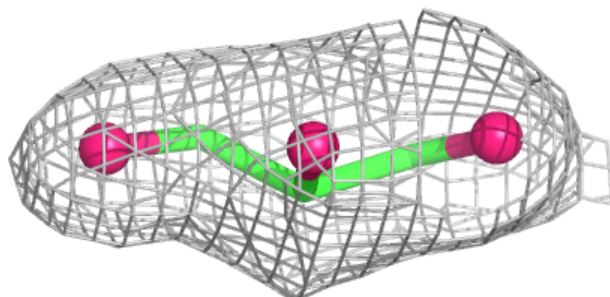
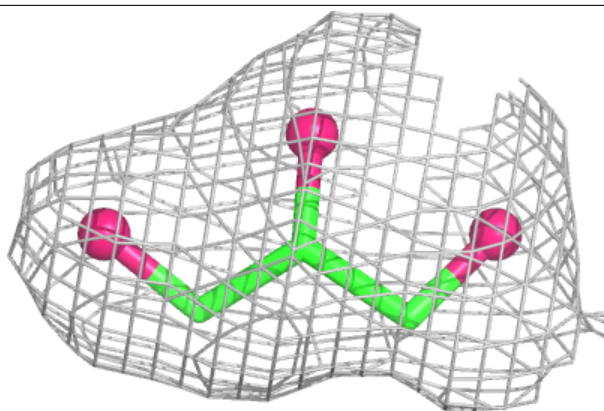
Electron density around SO4 D 705:

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



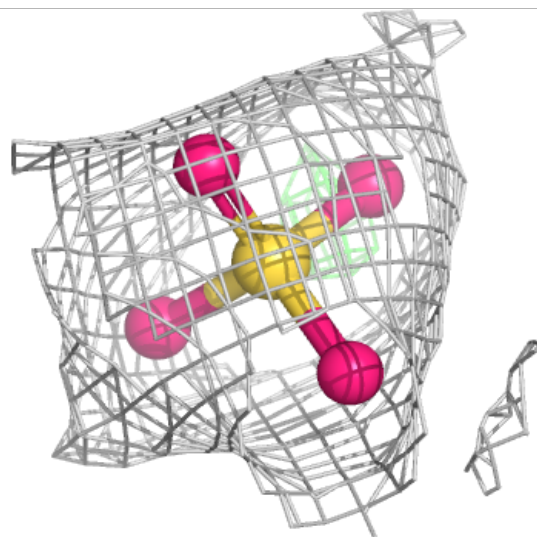
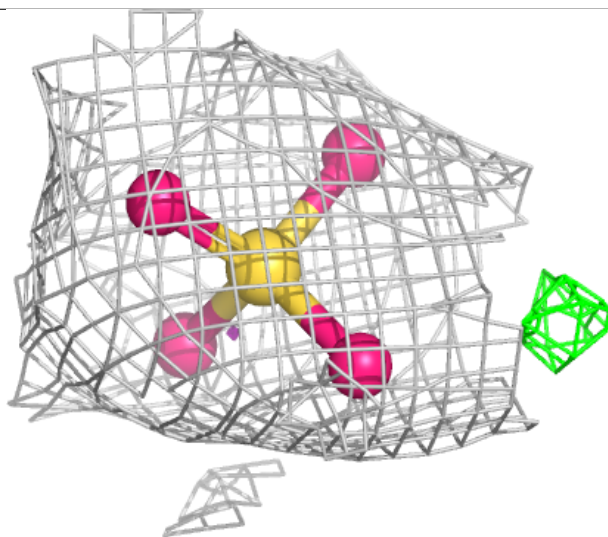
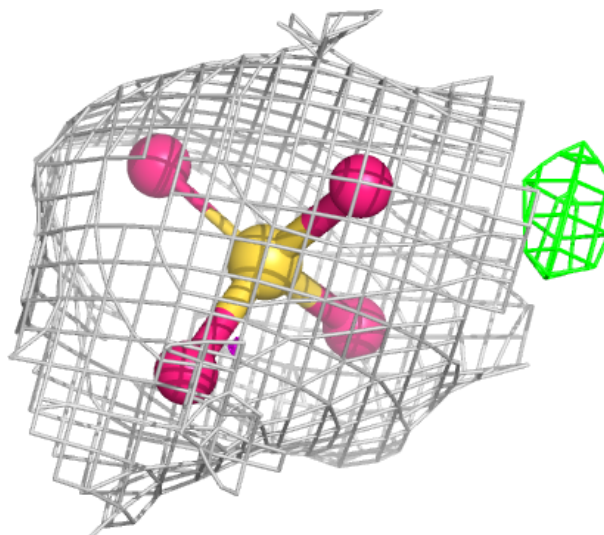
Electron density around GOL F 711:

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



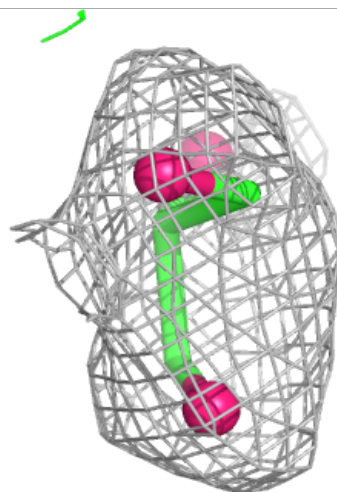
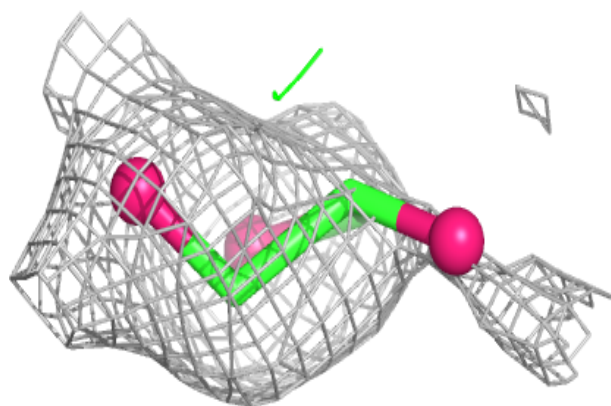
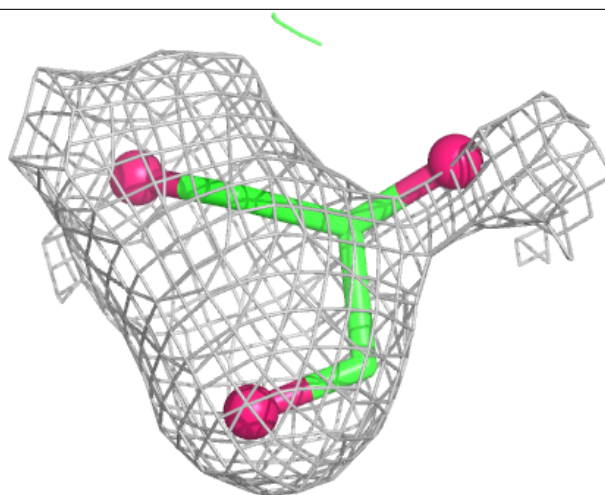
Electron density around SO4 E 705:

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



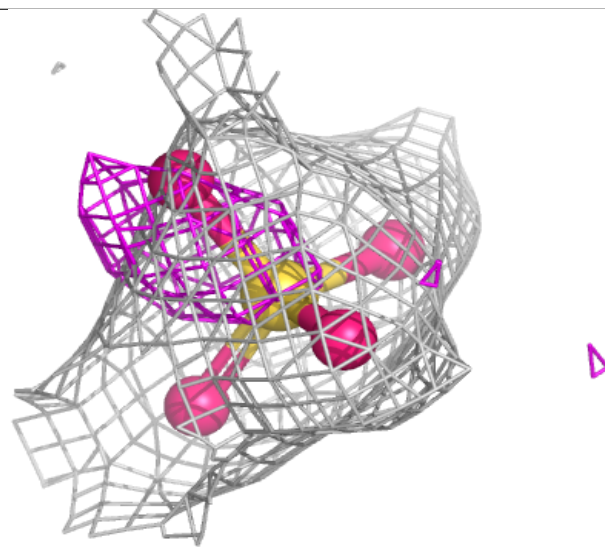
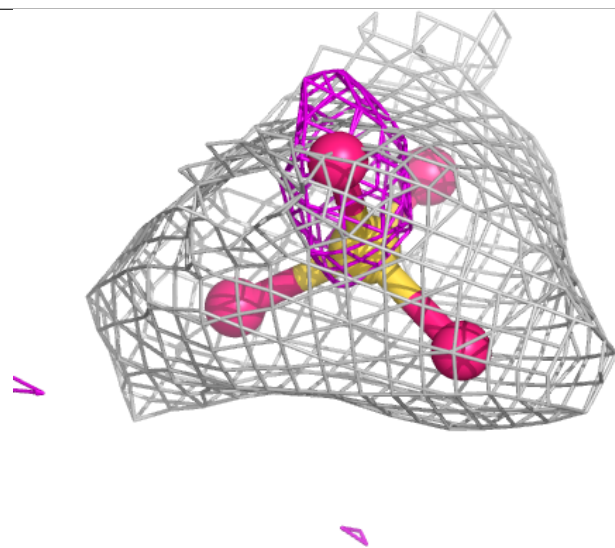
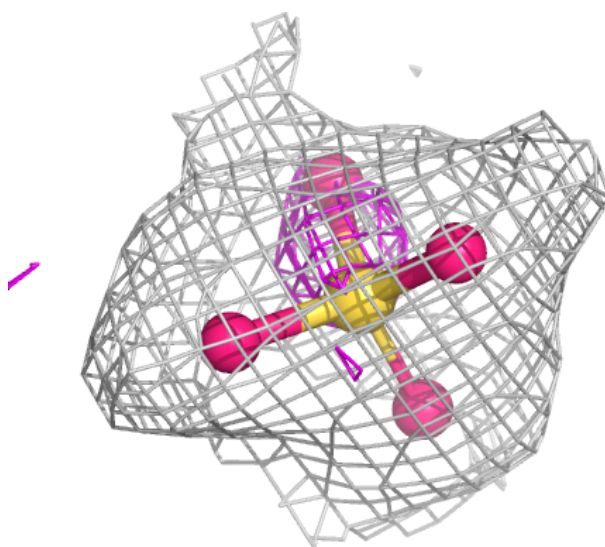
Electron density around GOL H 711:

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



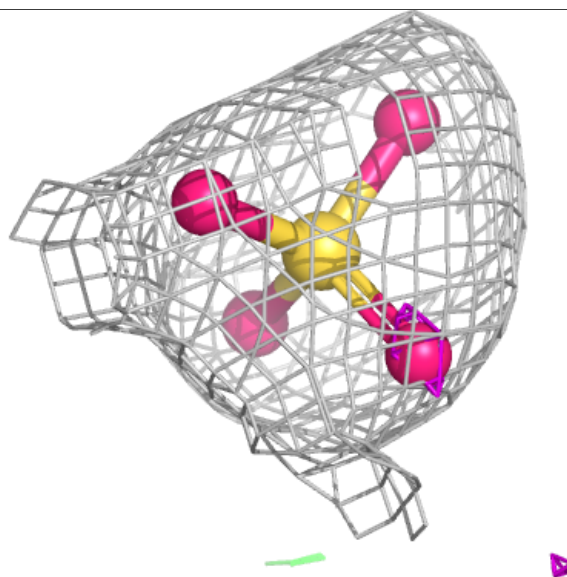
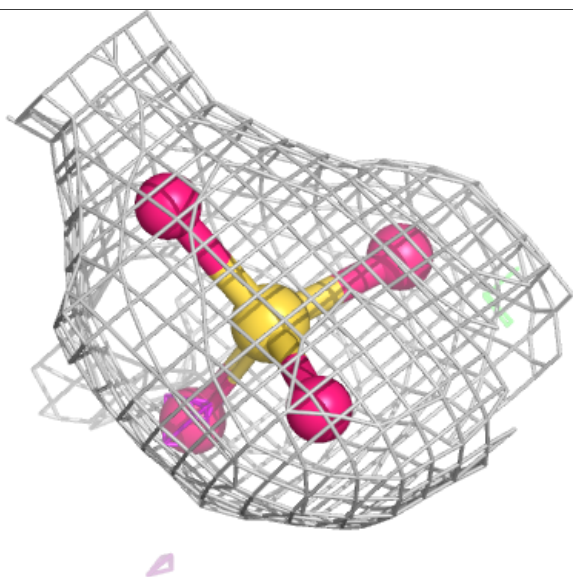
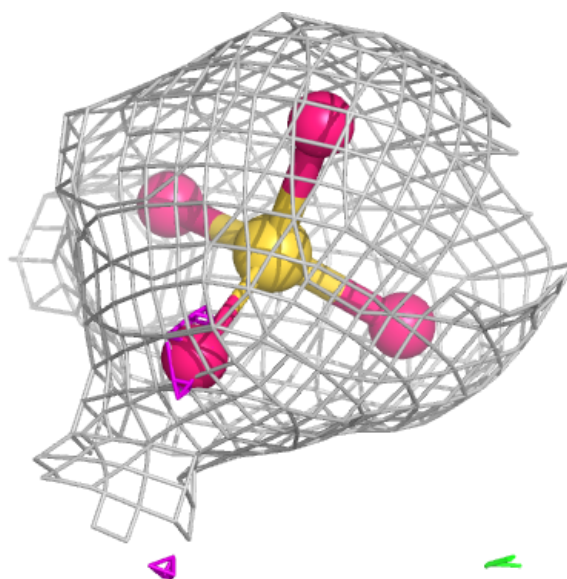
Electron density around SO4 D 706:

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



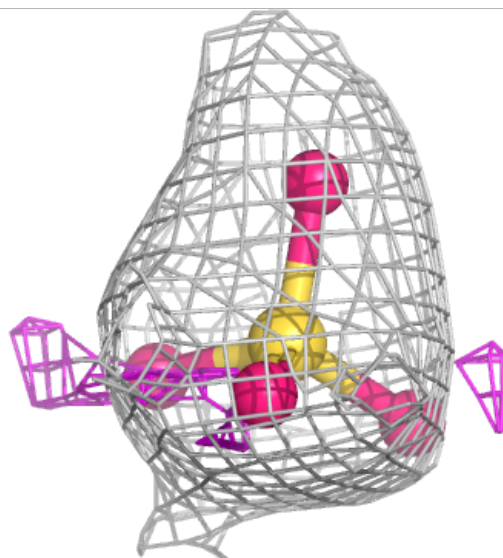
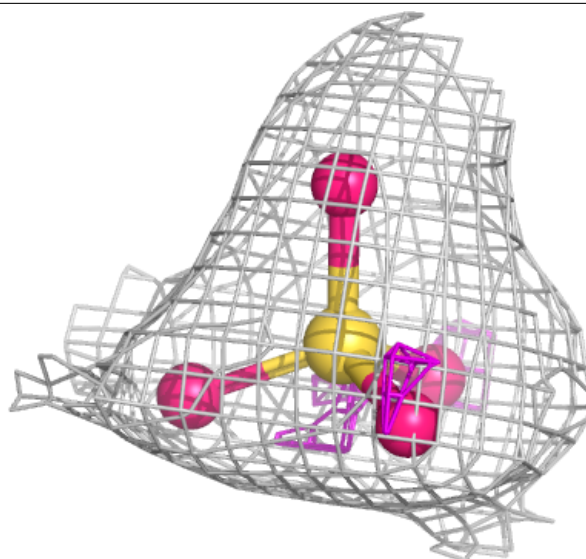
Electron density around SO4 C 705:

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



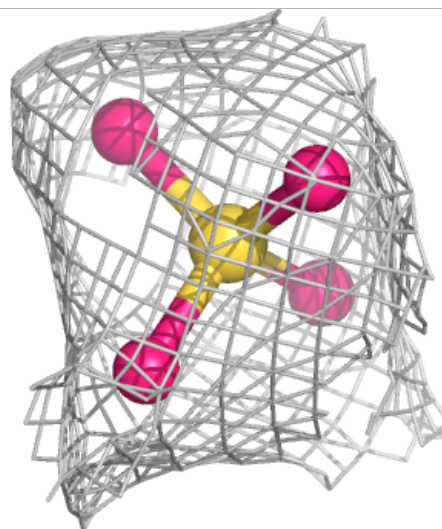
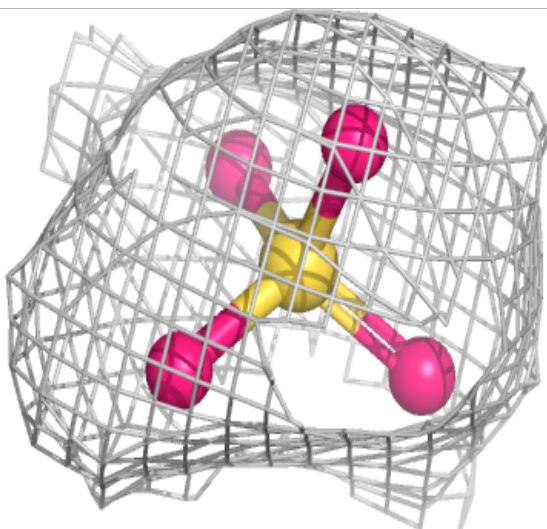
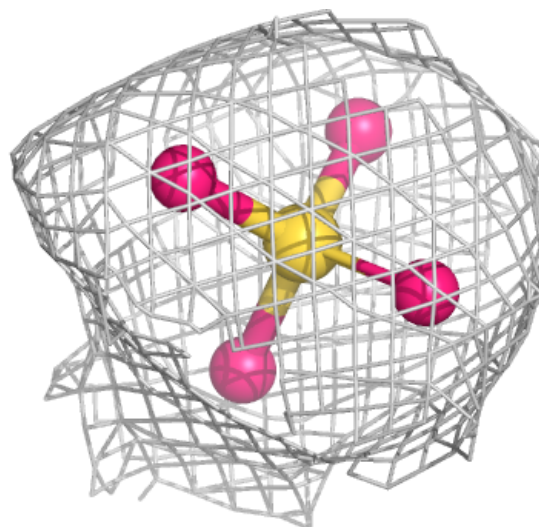
Electron density around SO4 C 704:

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



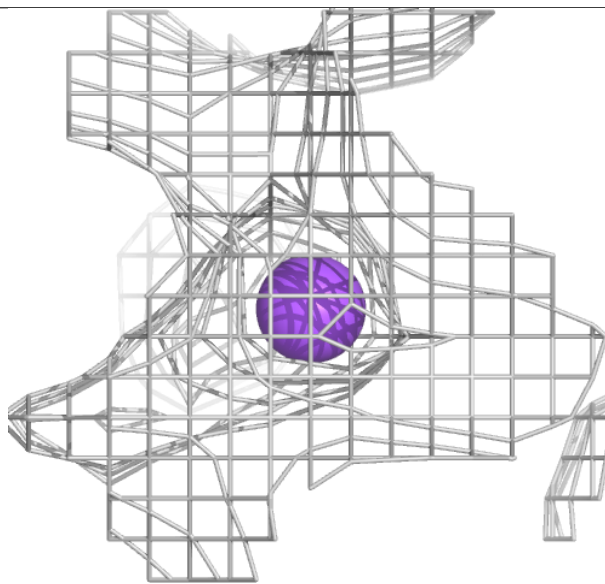
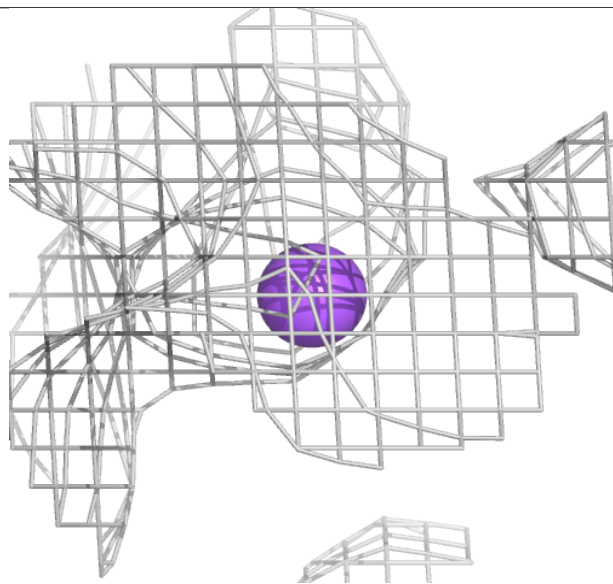
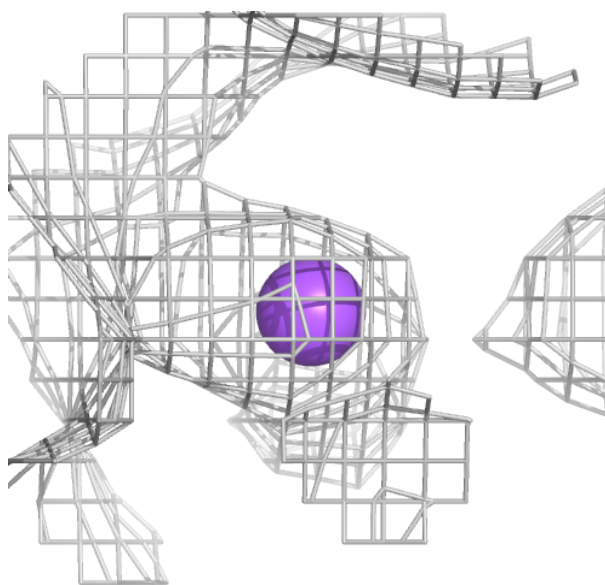
Electron density around SO4 D 708:

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



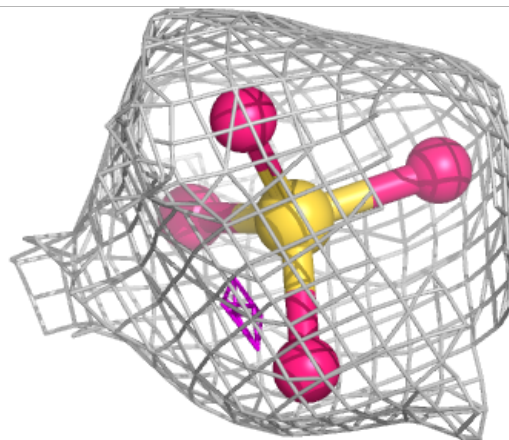
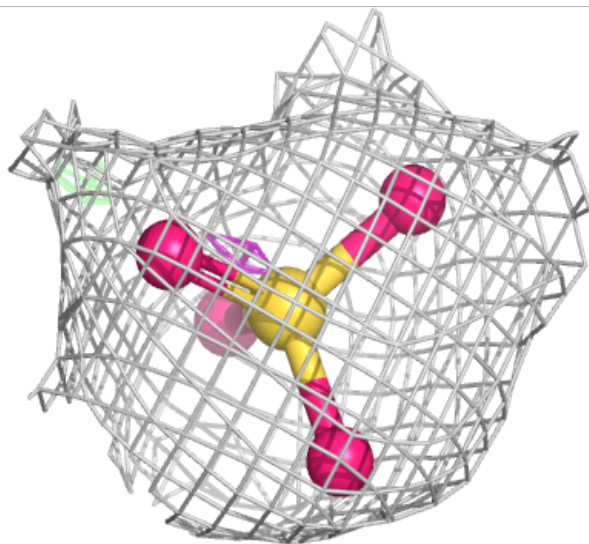
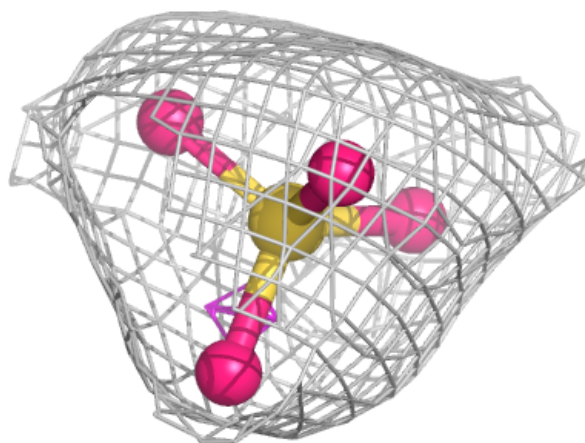
Electron density around NA D 709:

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



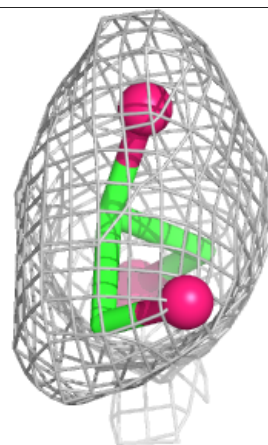
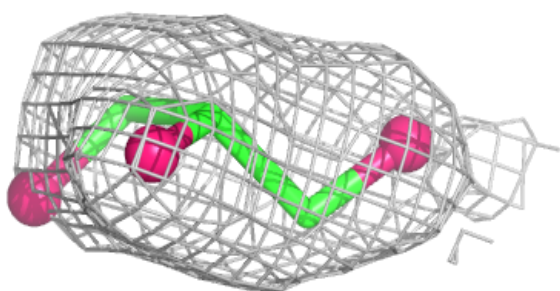
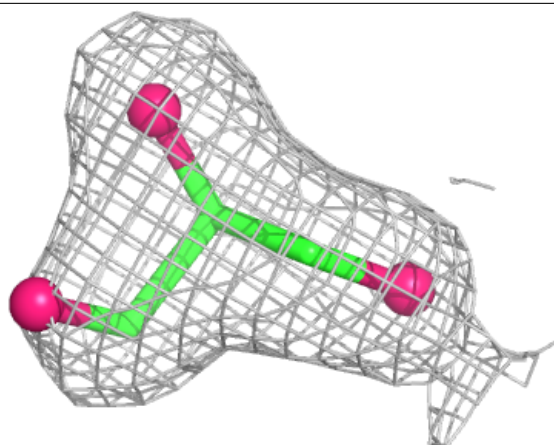
Electron density around SO4 H 704:

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

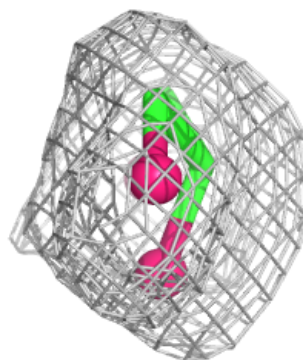
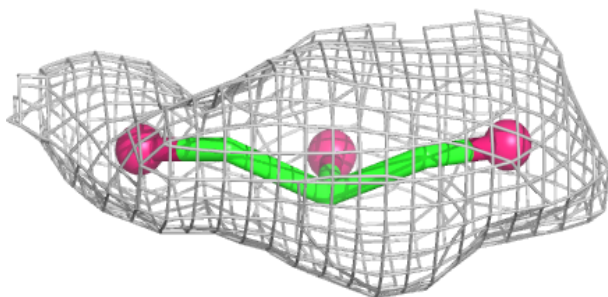
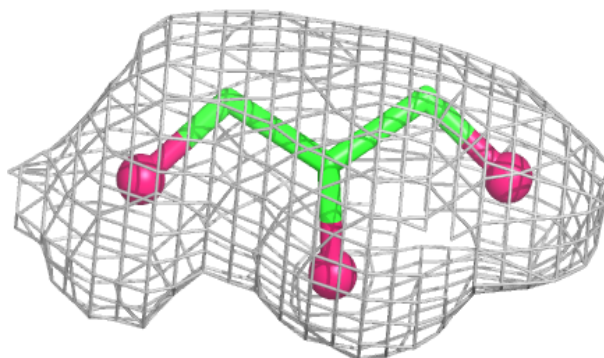


Electron density around GOL A 714:

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

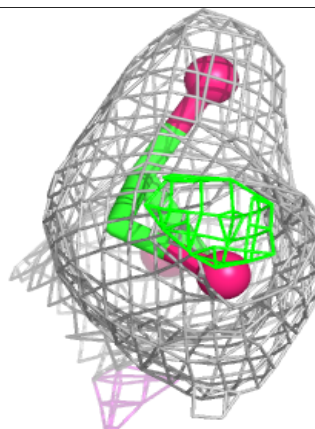
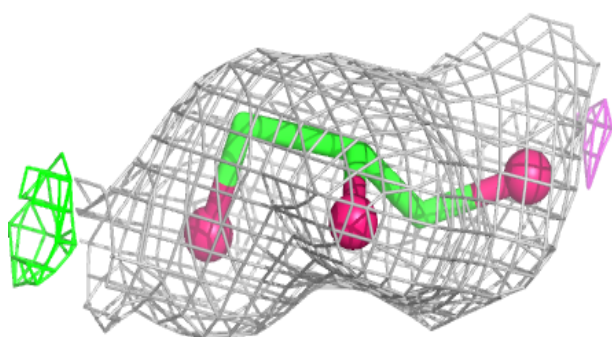
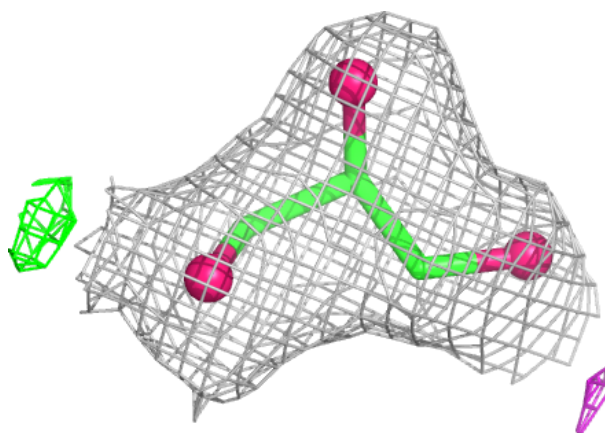
**Electron density around GOL C 711:**

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



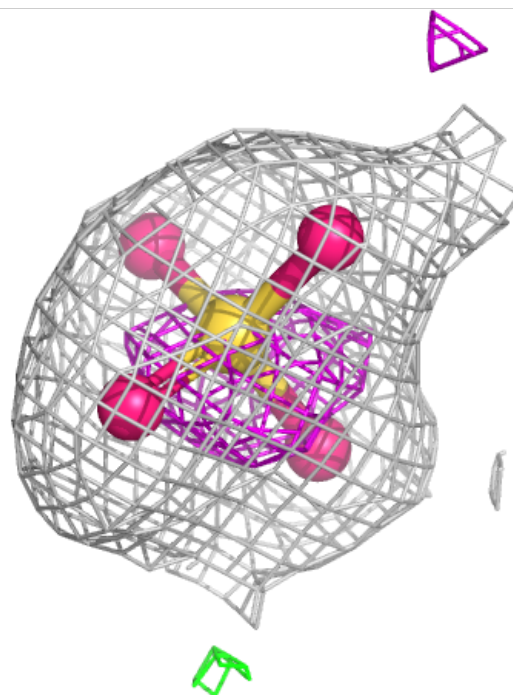
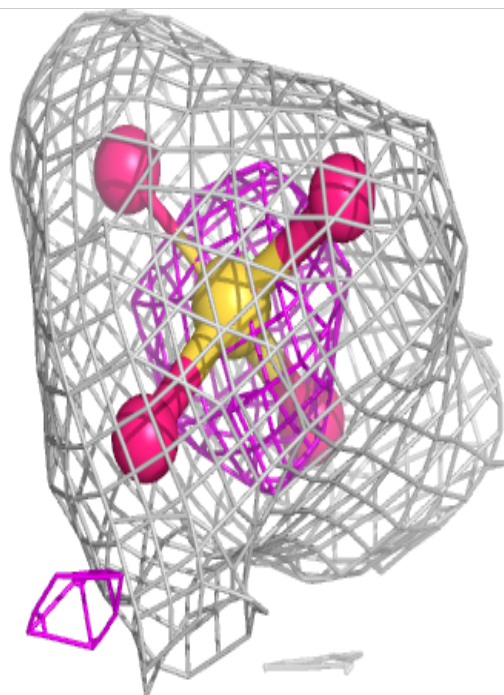
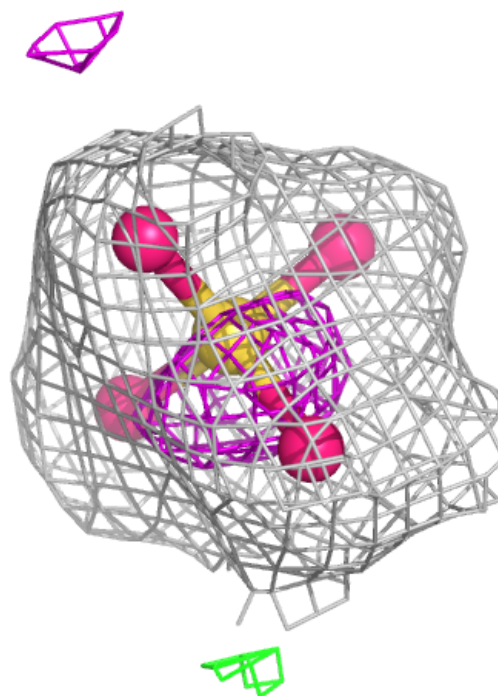
Electron density around GOL E 713:

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



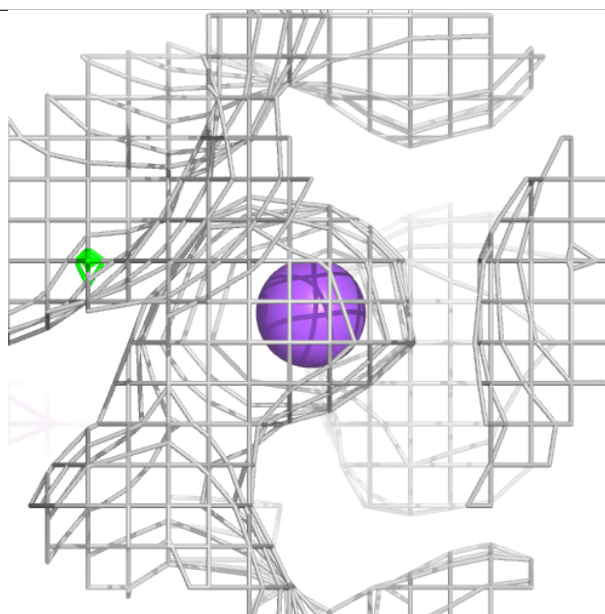
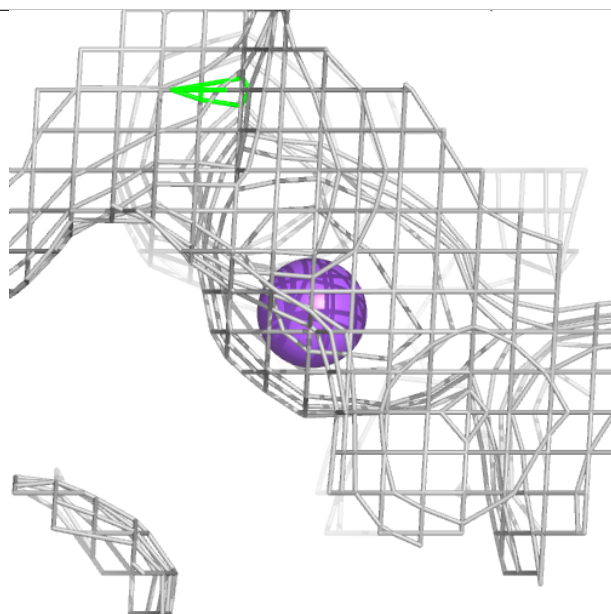
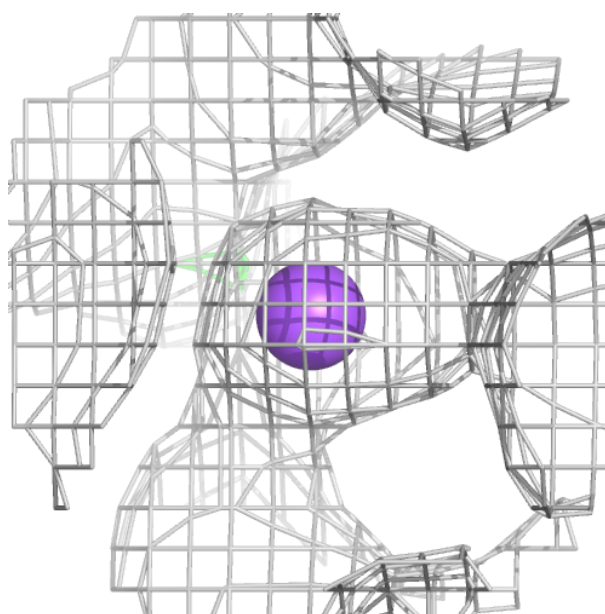
Electron density around SO4 A 704:

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



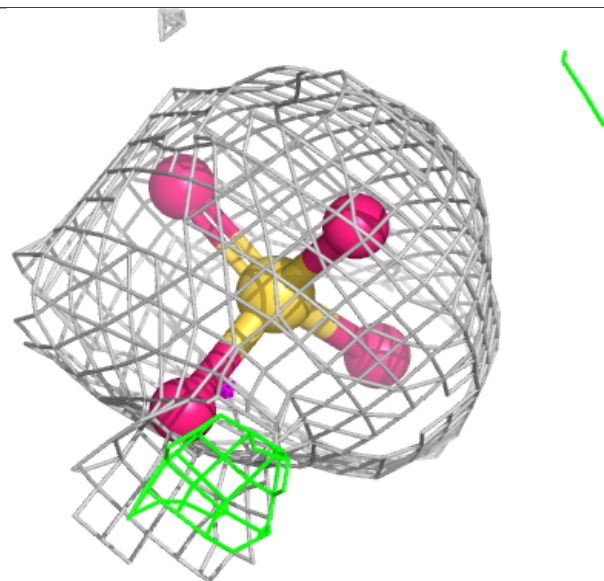
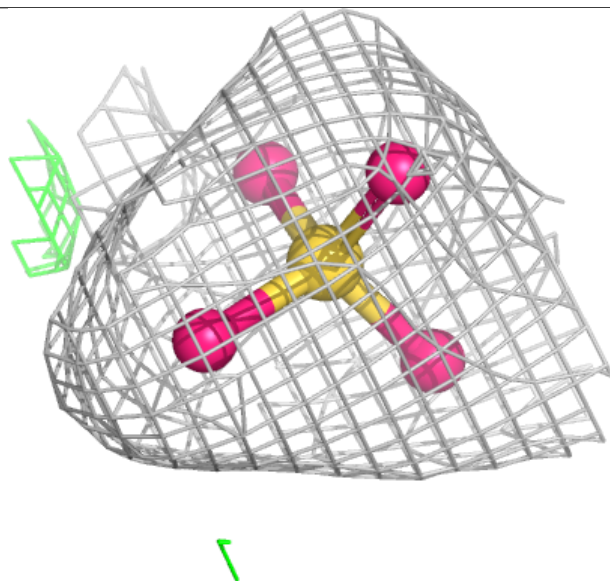
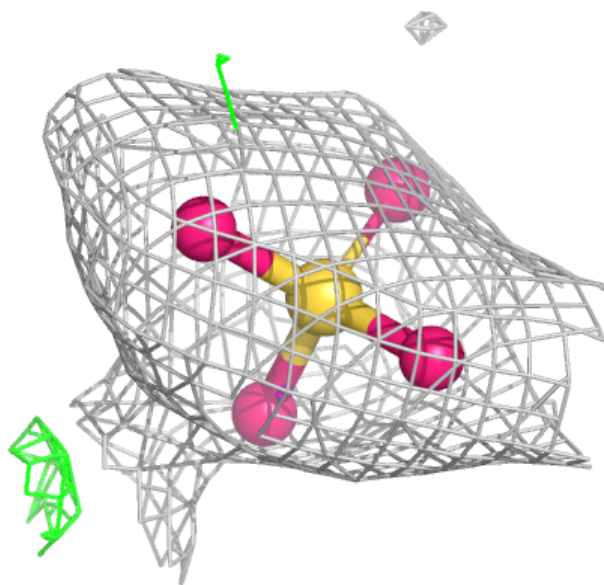
Electron density around NA A 710:

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



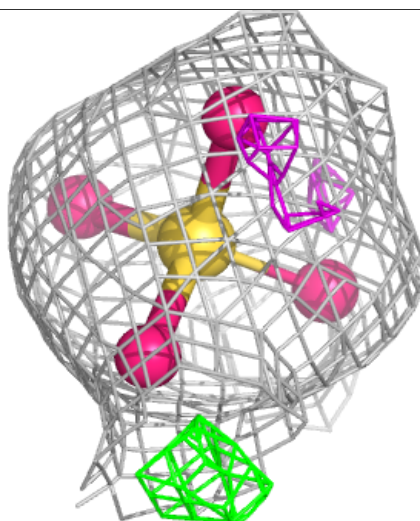
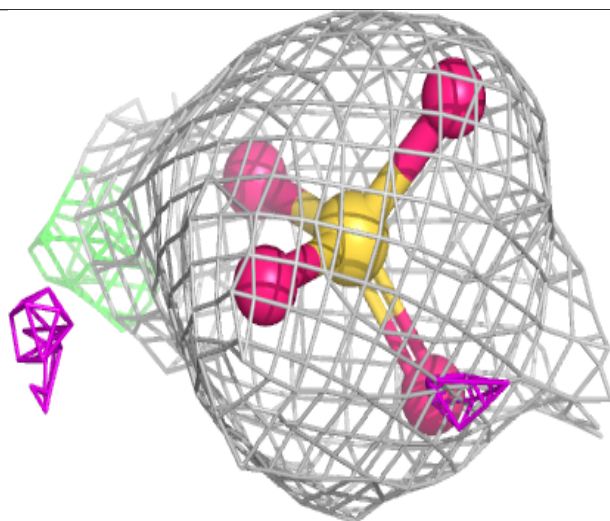
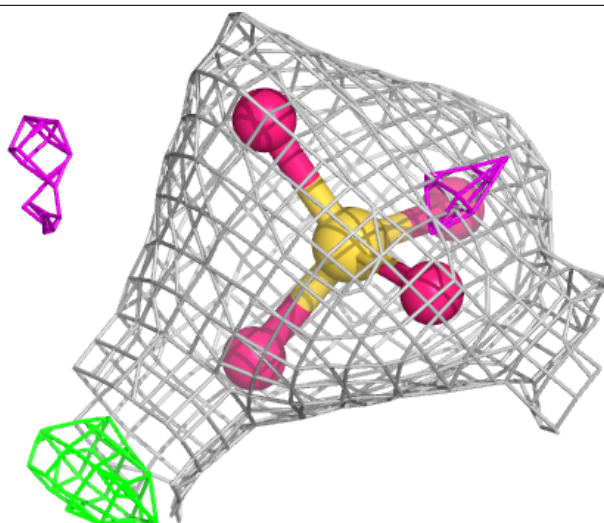
Electron density around SO4 B 707:

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



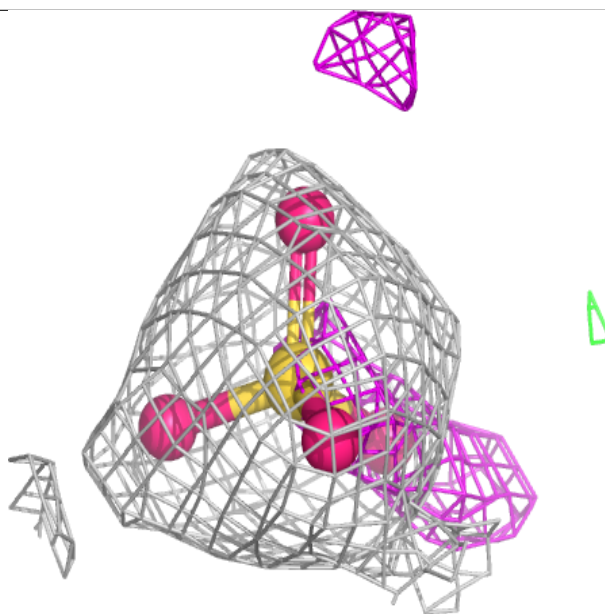
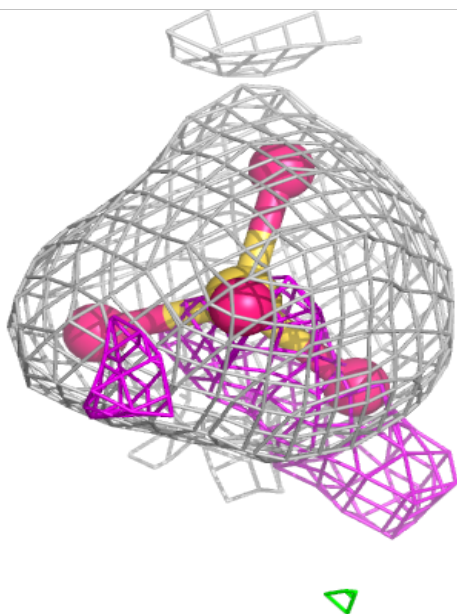
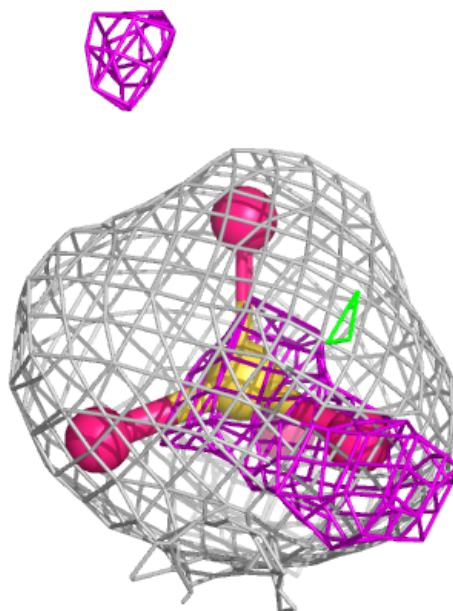
Electron density around SO4 F 704:

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



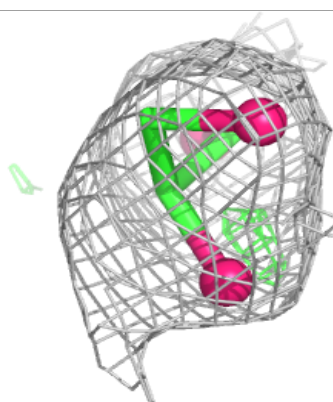
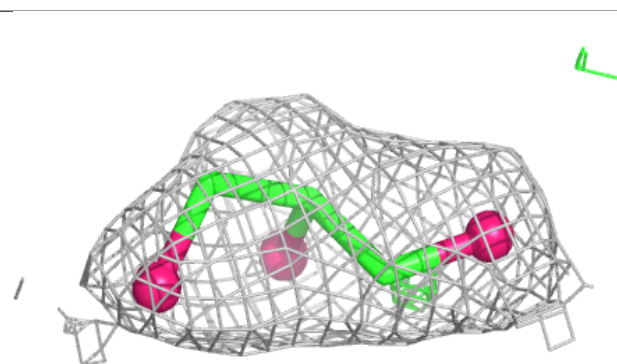
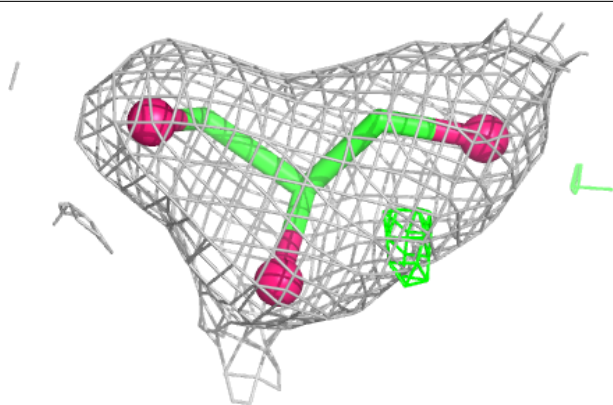
Electron density around SO4 C 707:

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



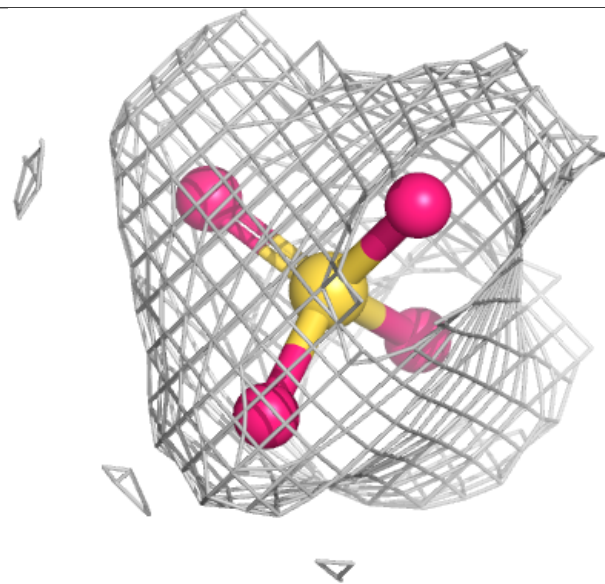
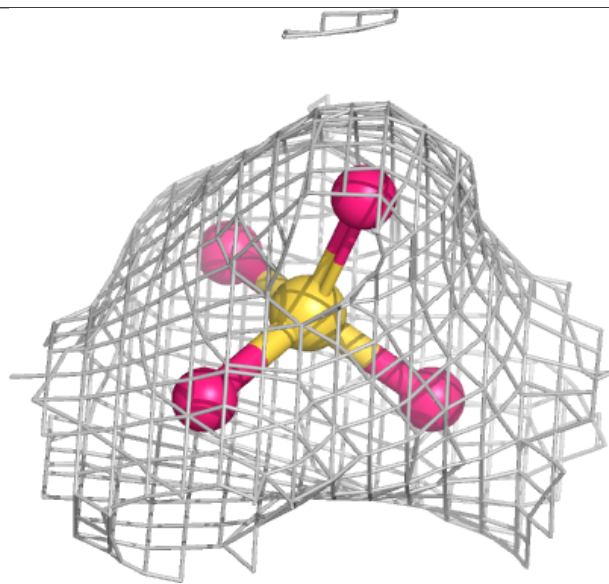
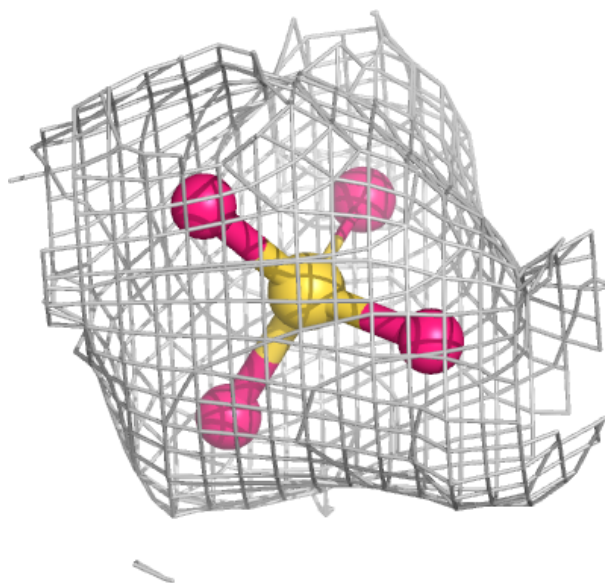
Electron density around GOL B 717:

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



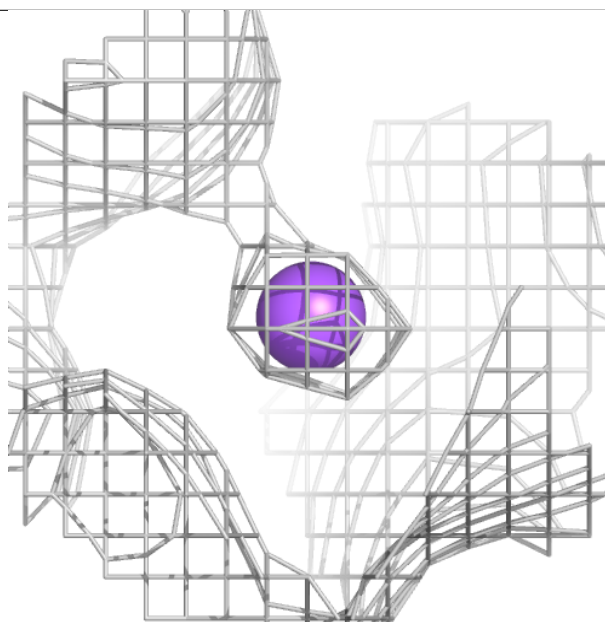
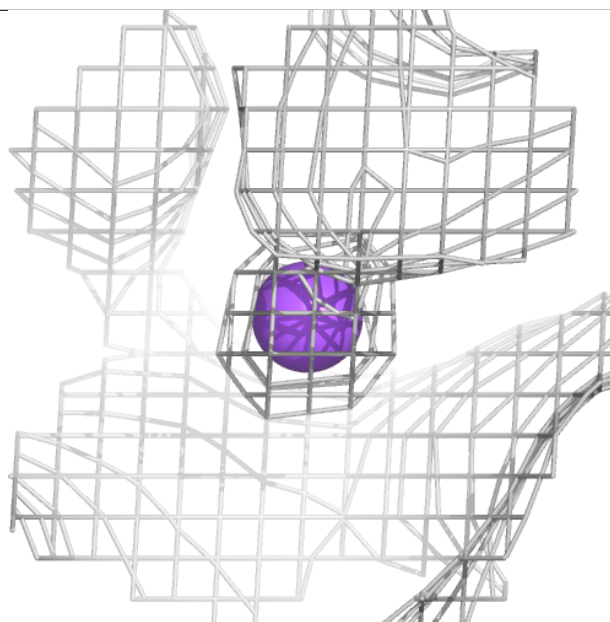
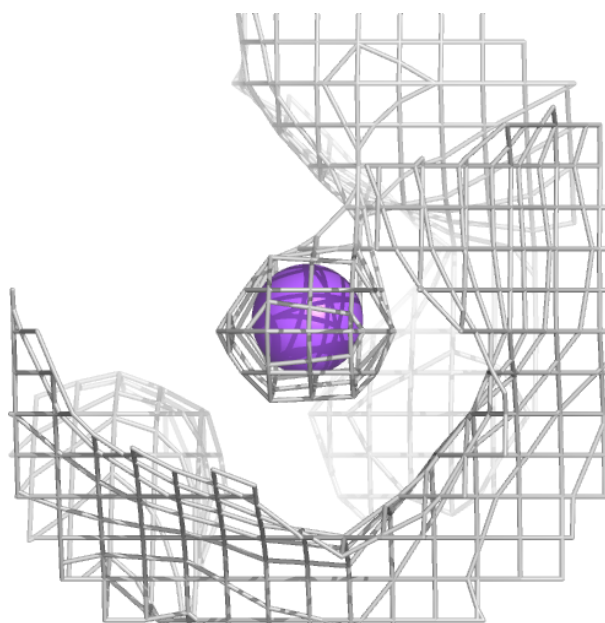
Electron density around SO4 B 710:

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



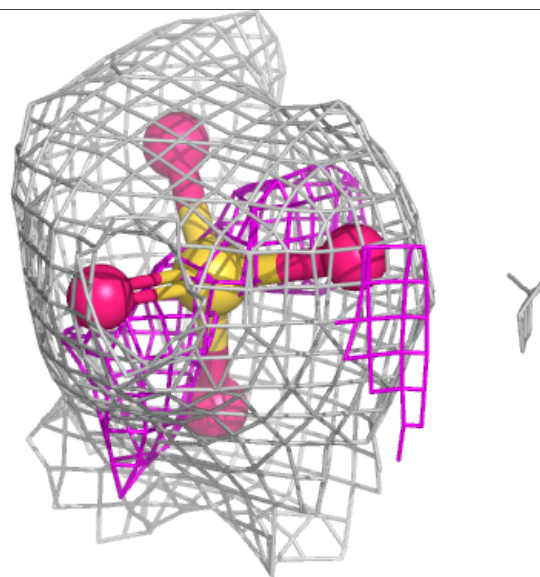
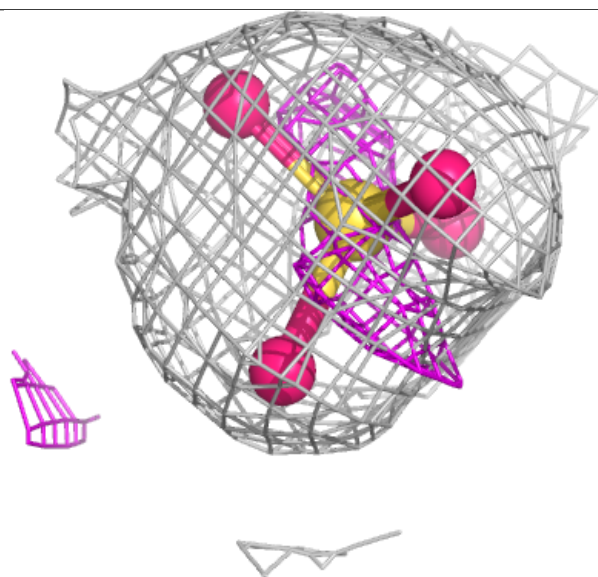
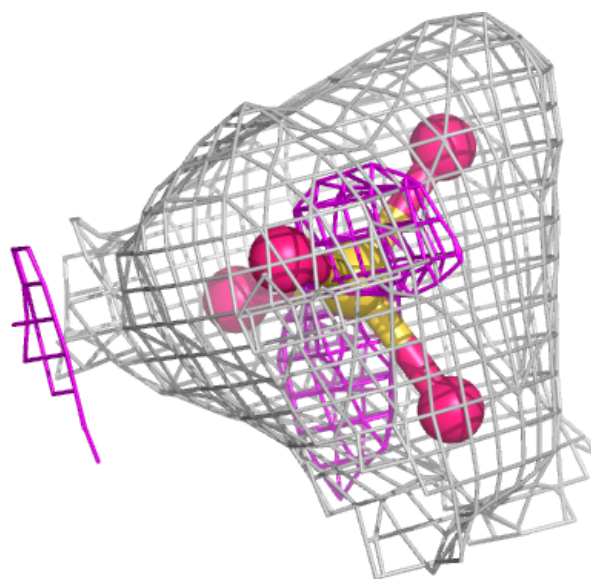
Electron density around NA H 710:

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



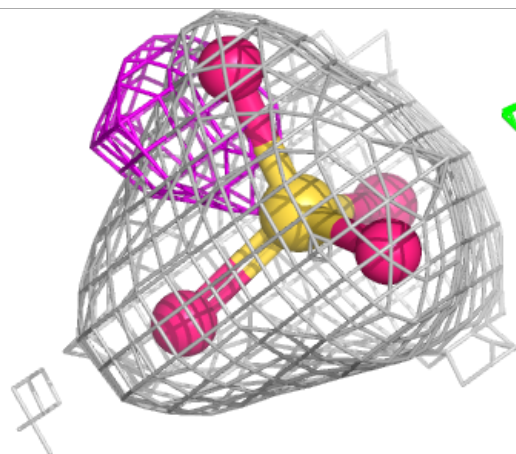
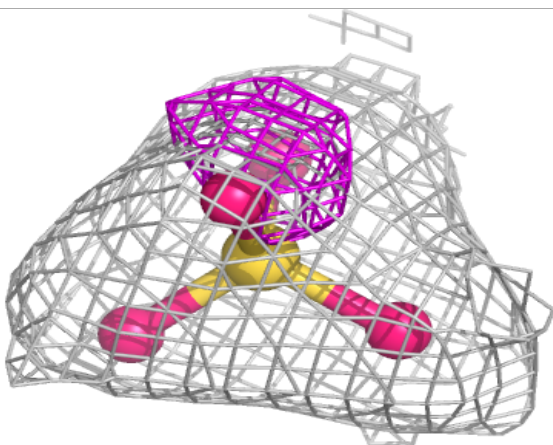
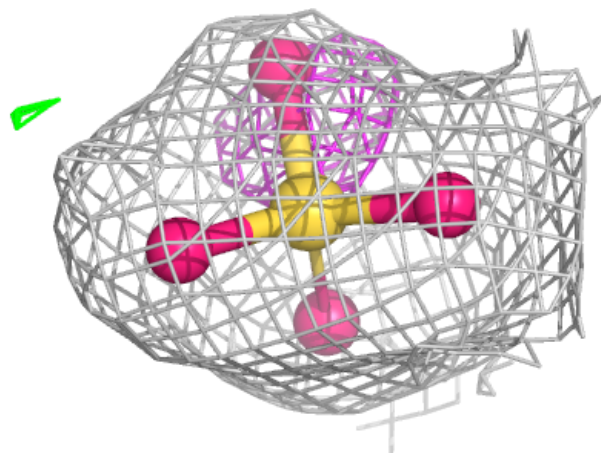
Electron density around SO4 D 704:

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



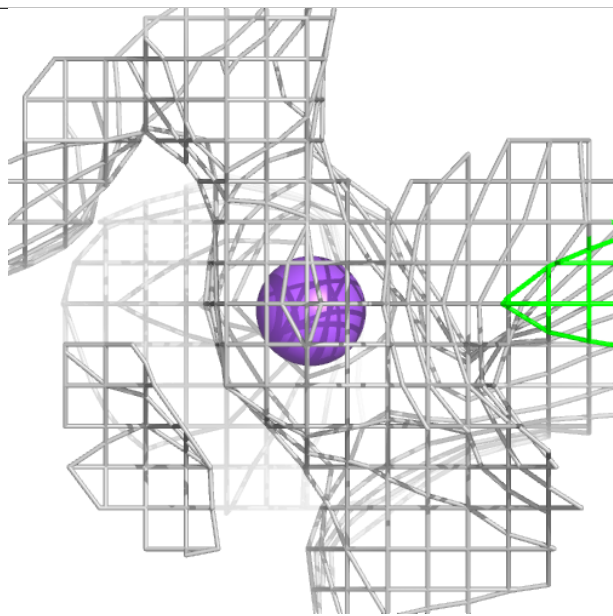
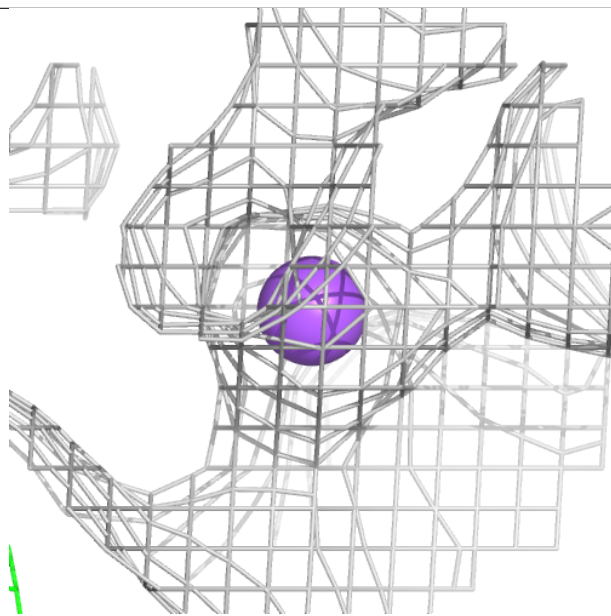
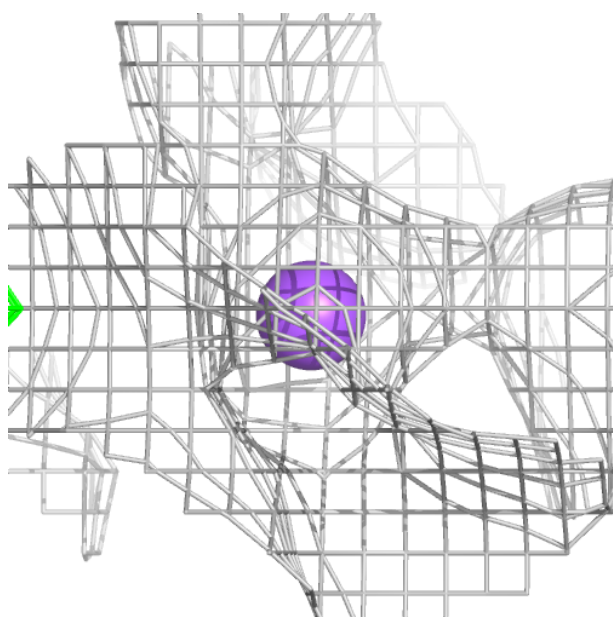
Electron density around SO4 E 704:

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



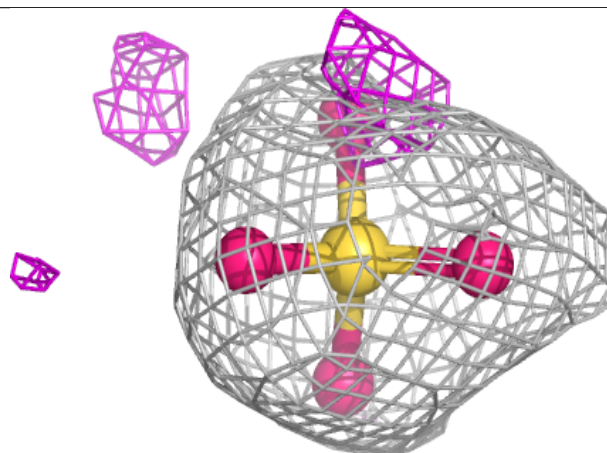
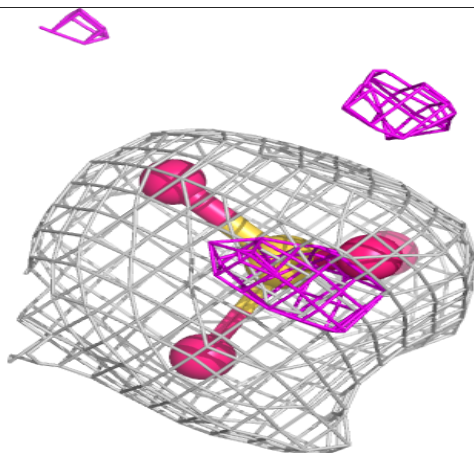
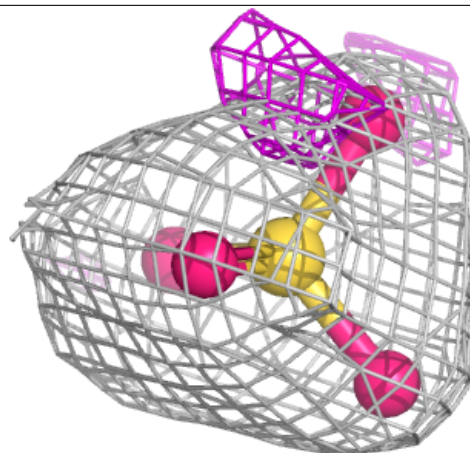
Electron density around NA G 706:

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



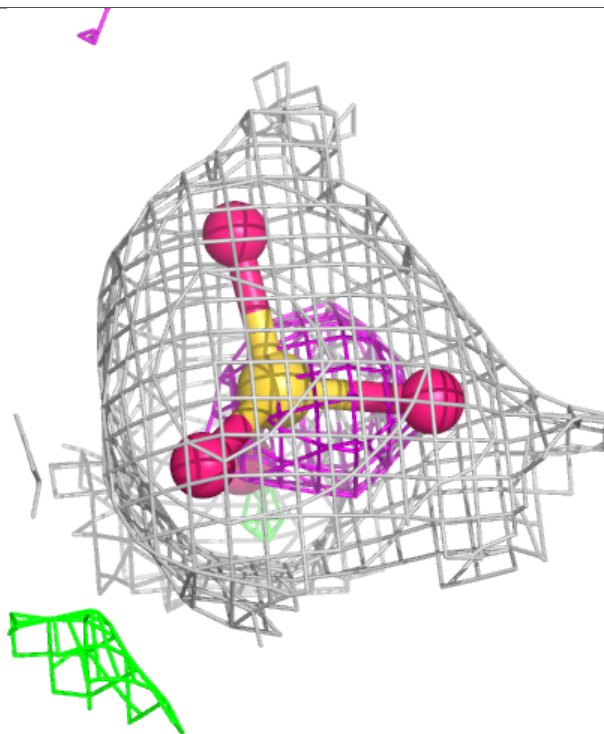
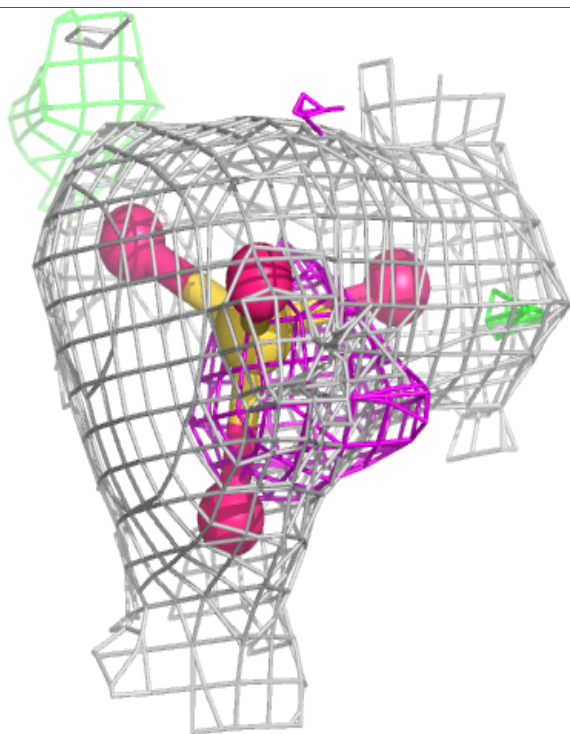
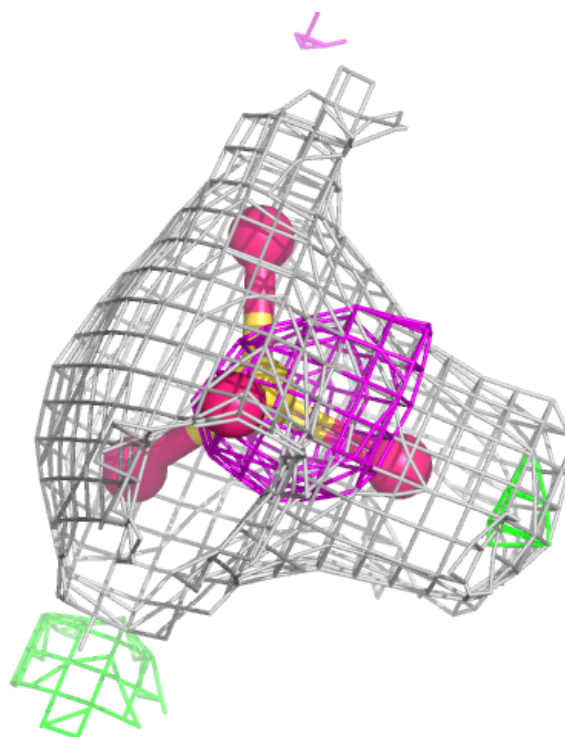
Electron density around SO4 B 703:

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



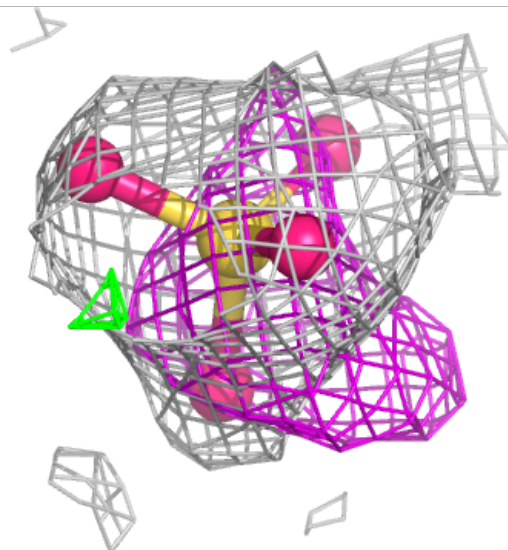
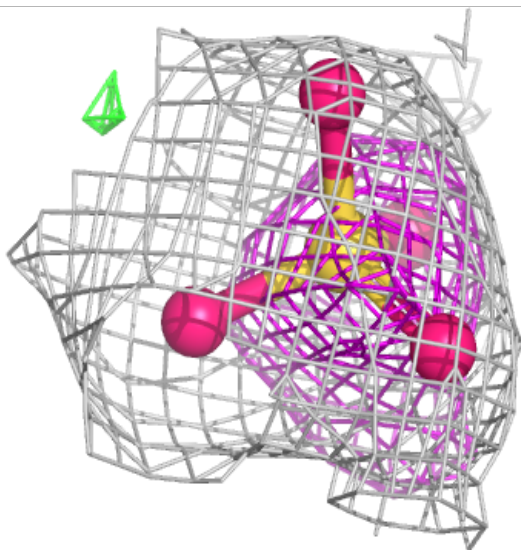
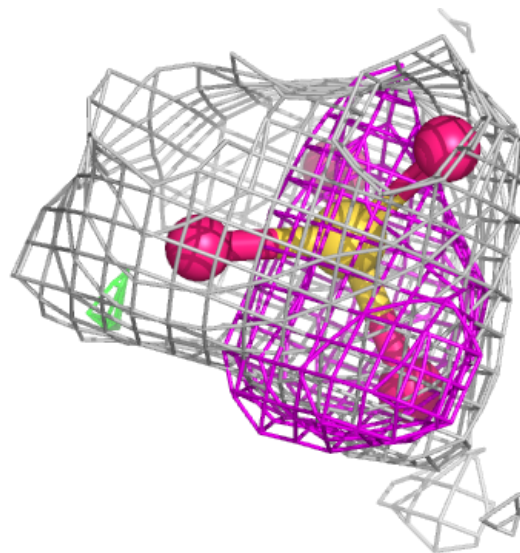
Electron density around SO4 F 703:

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



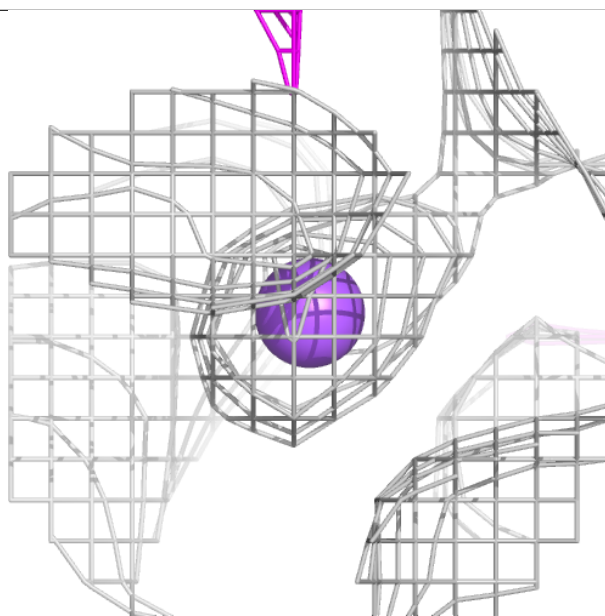
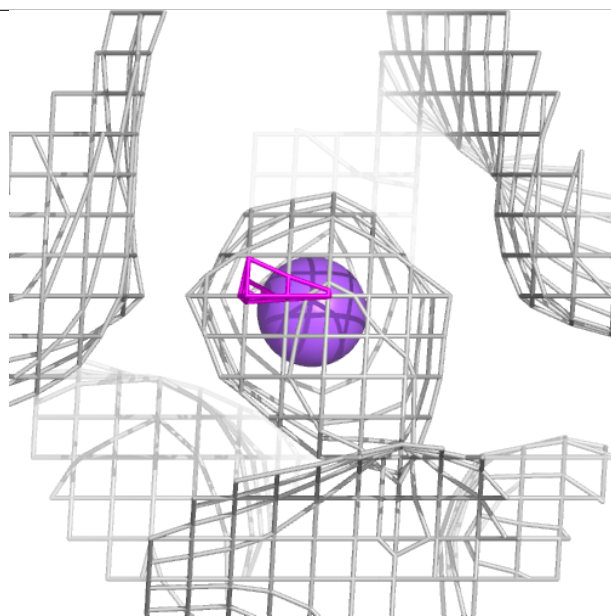
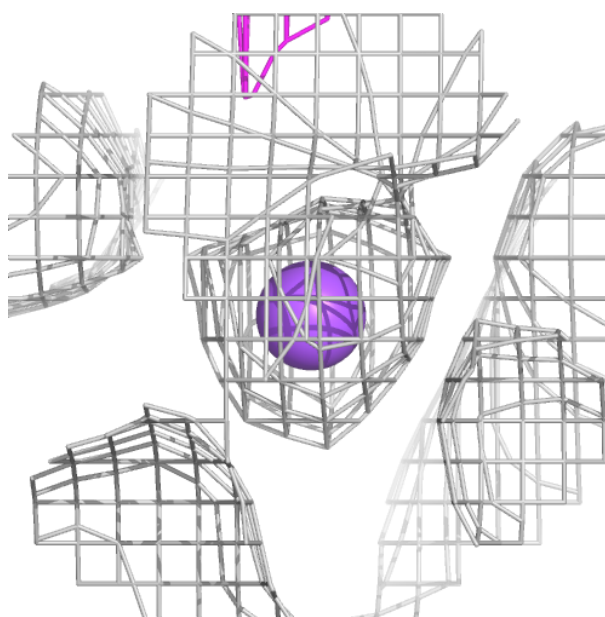
Electron density around SO4 H 705:

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



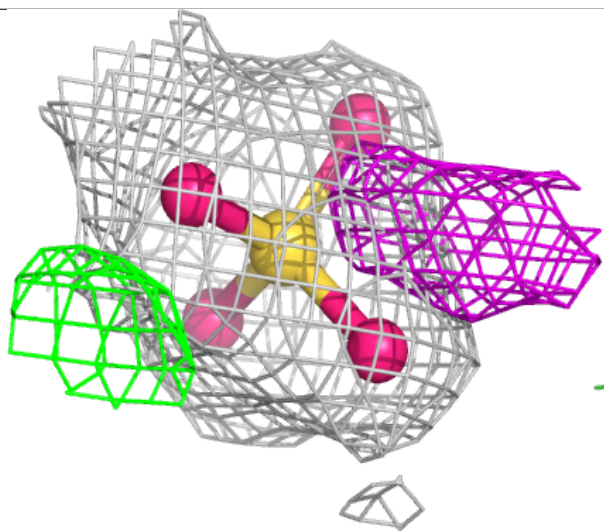
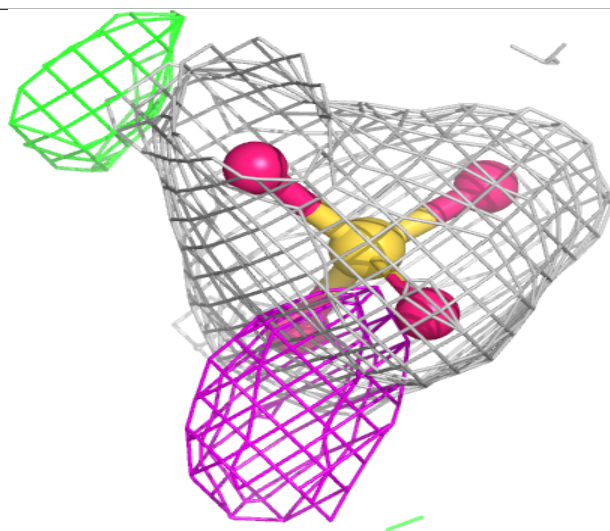
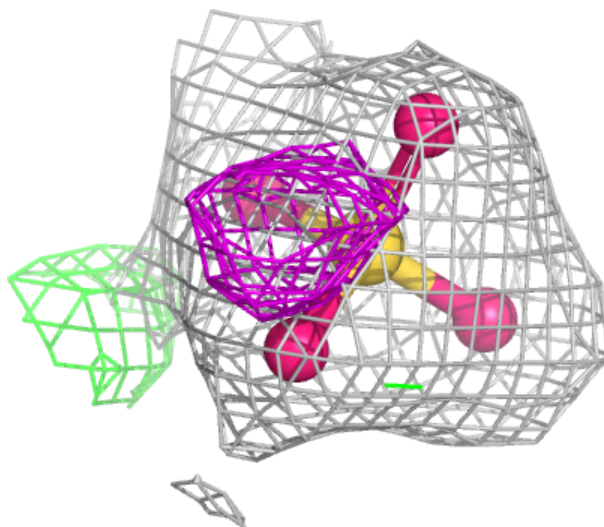
Electron density around NA B 716:

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



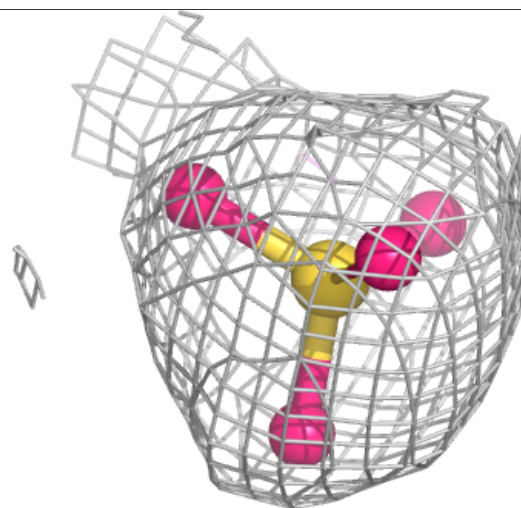
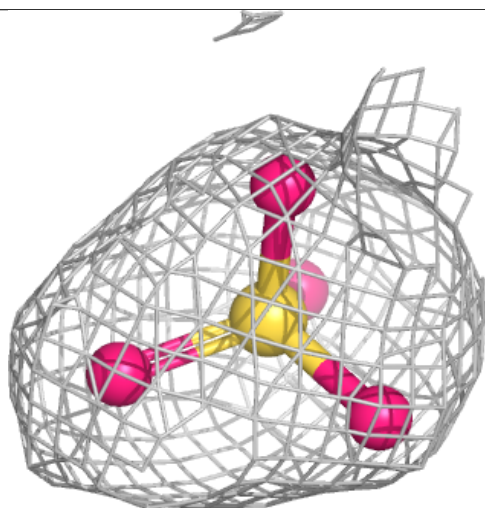
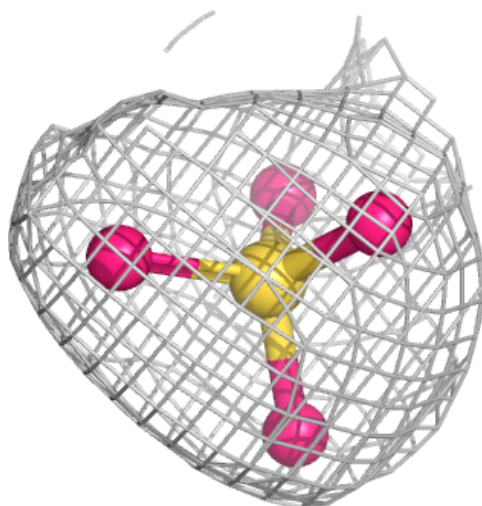
Electron density around SO4 H 702:

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



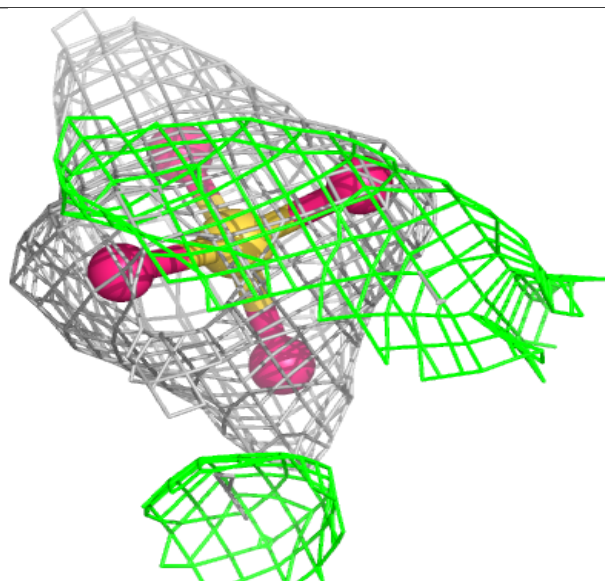
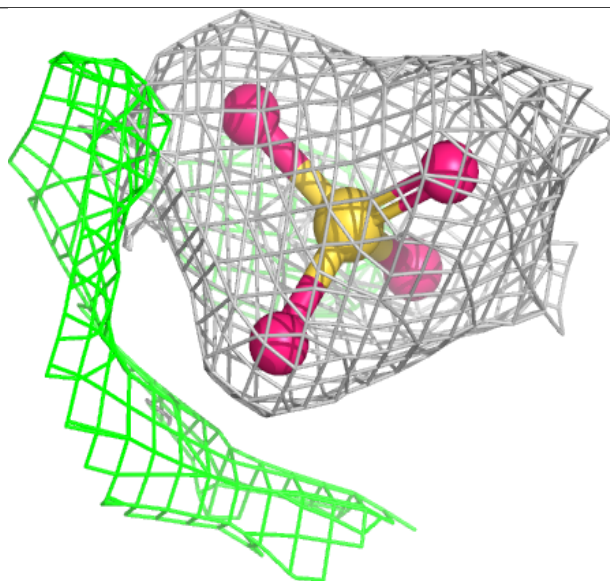
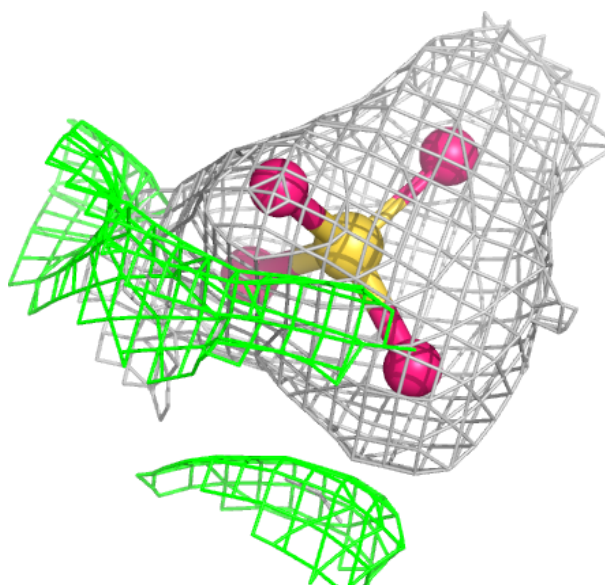
Electron density around SO4 A 703:

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



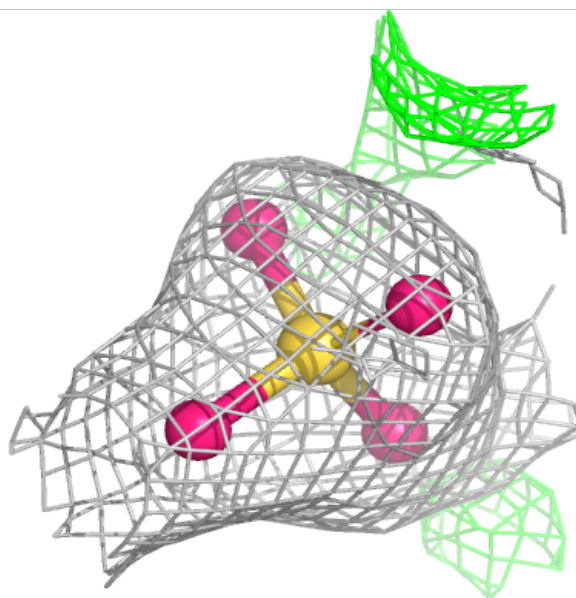
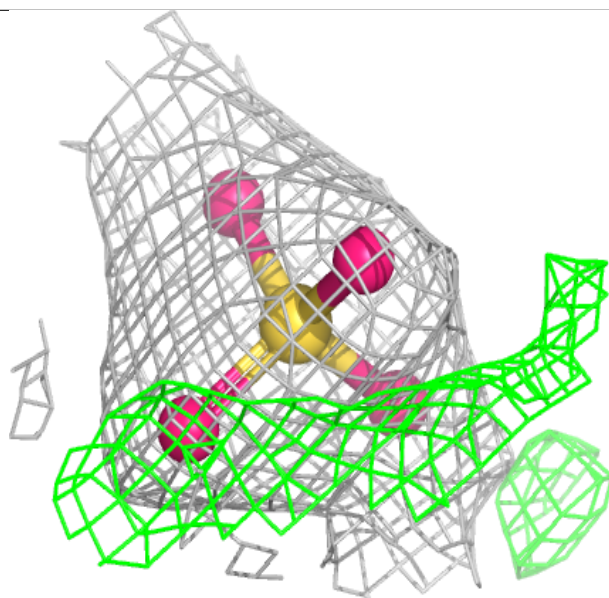
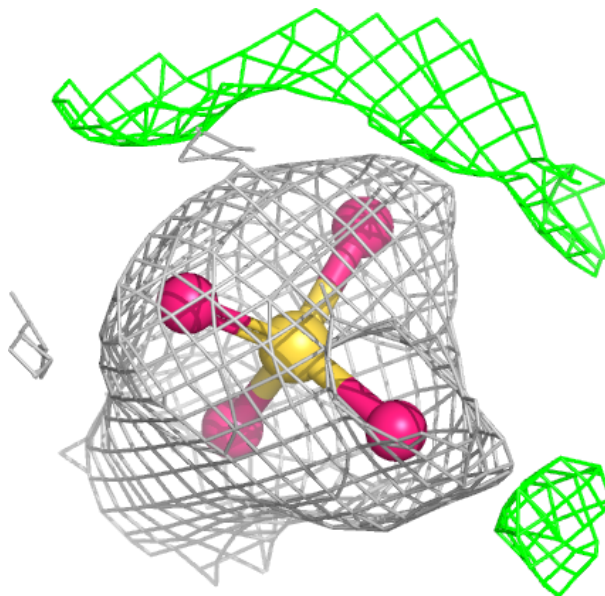
Electron density around SO4 B 706:

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



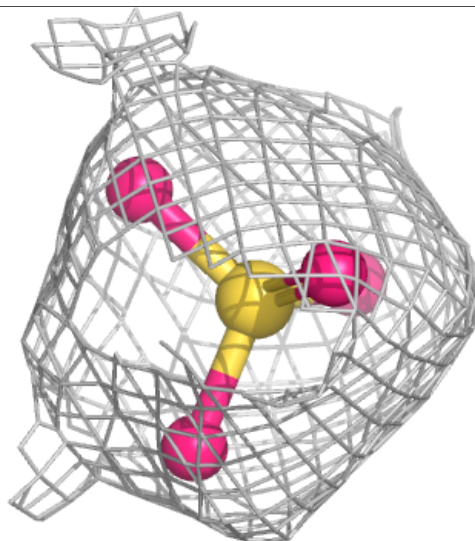
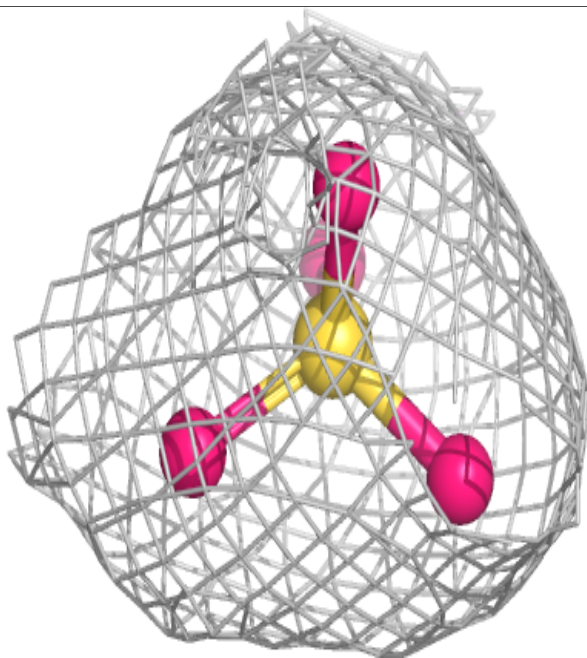
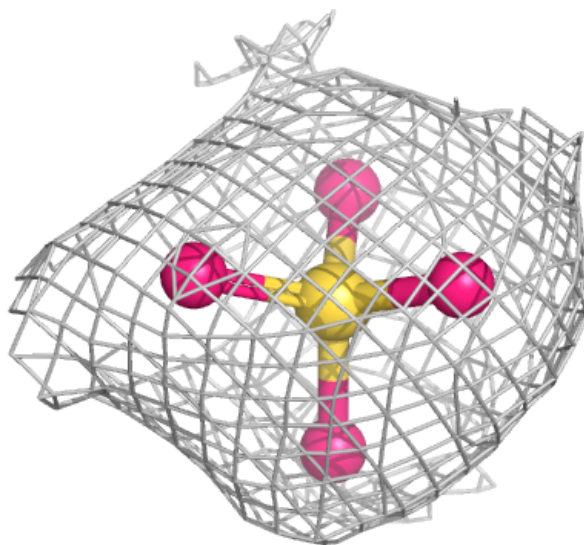
Electron density around SO4 E 706:

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



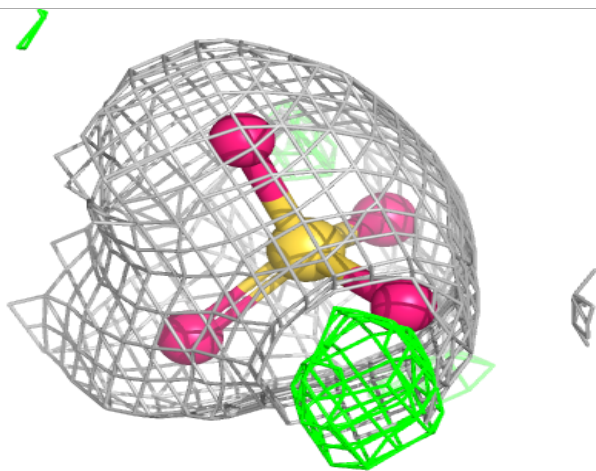
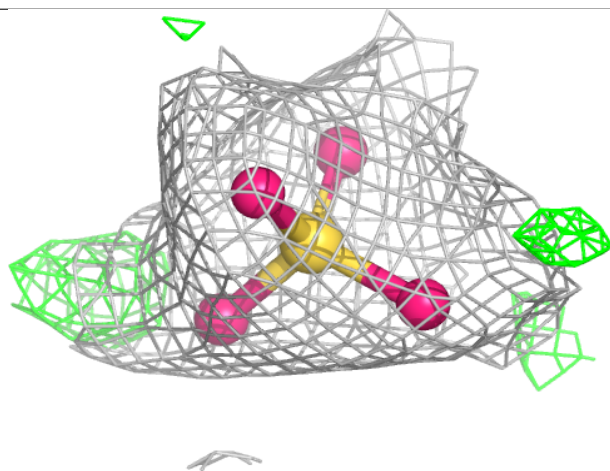
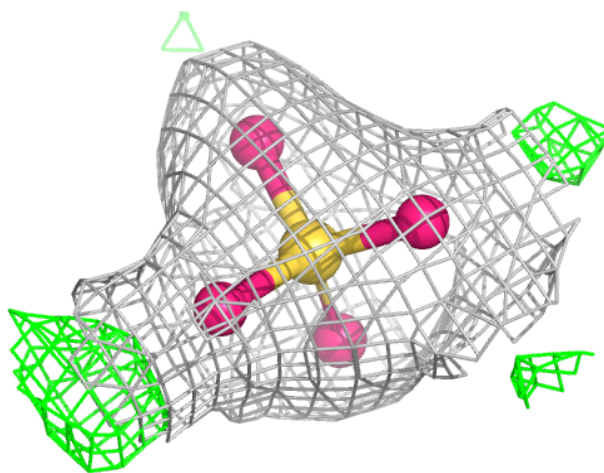
Electron density around SO4 D 702:

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



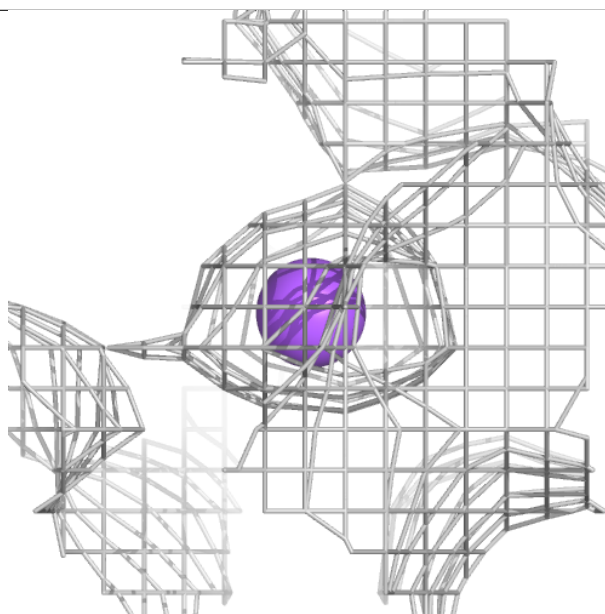
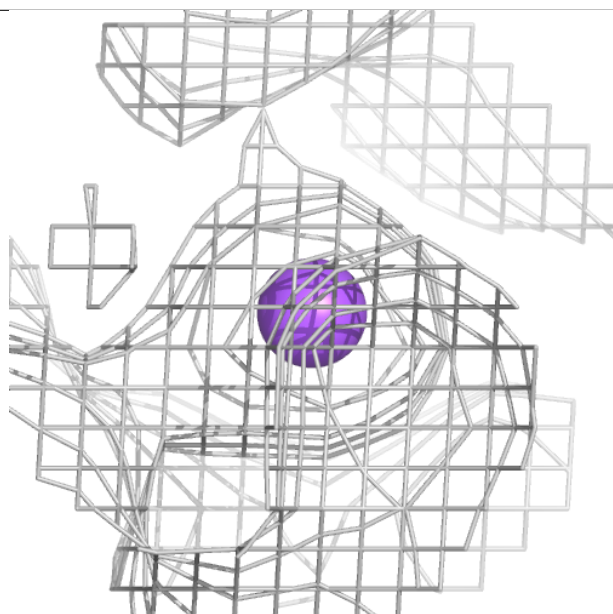
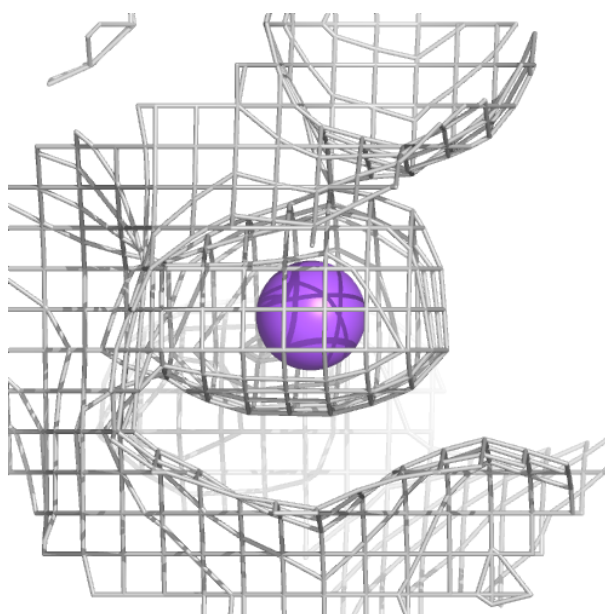
Electron density around SO4 A 706:

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



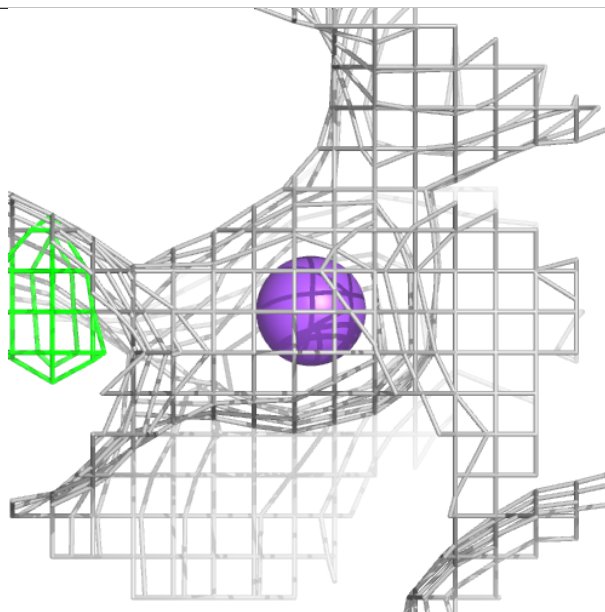
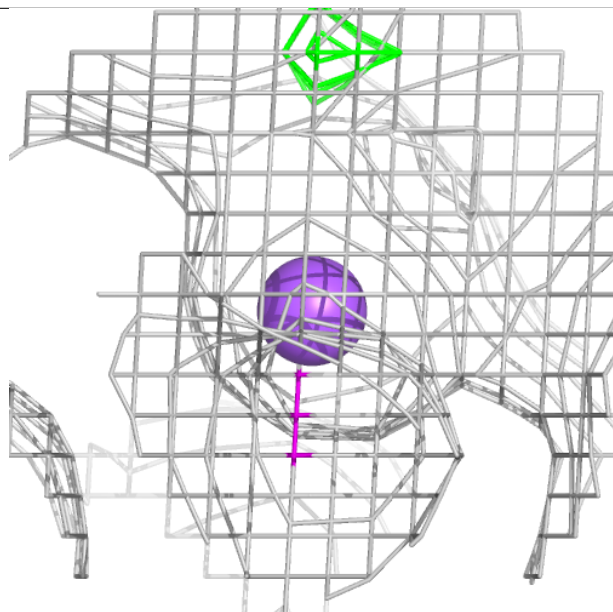
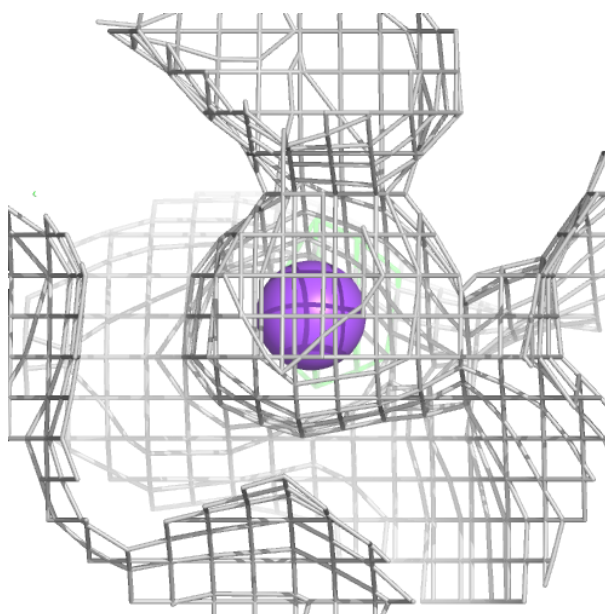
Electron density around NA E 711:

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



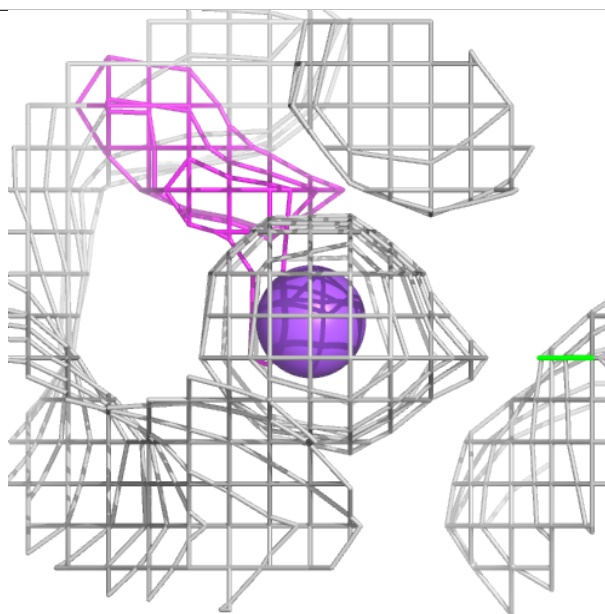
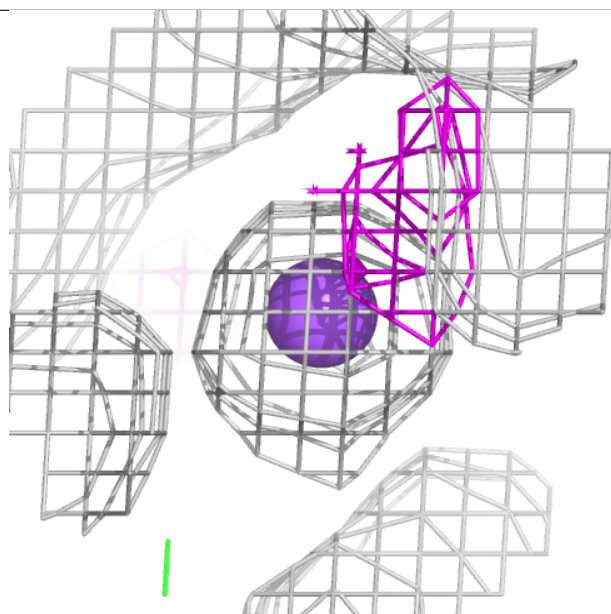
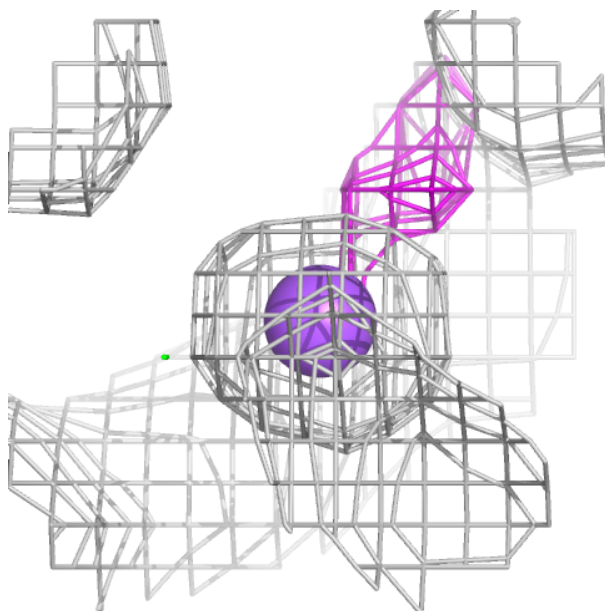
Electron density around NA B 714:

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



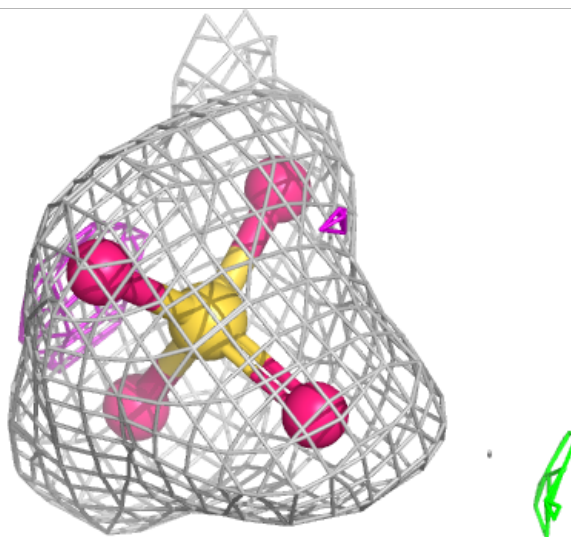
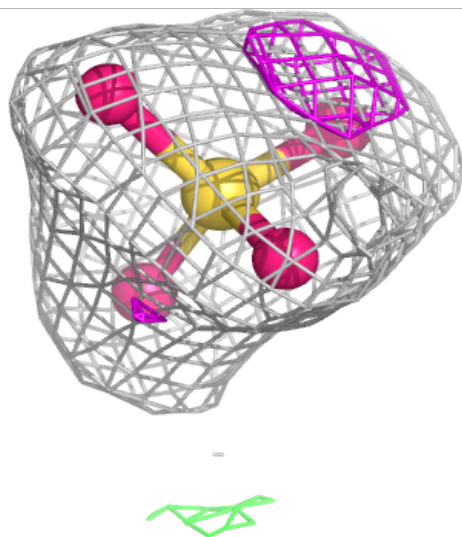
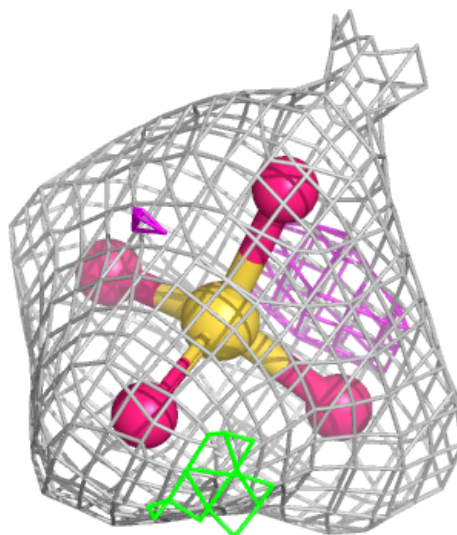
Electron density around NA B 715:

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



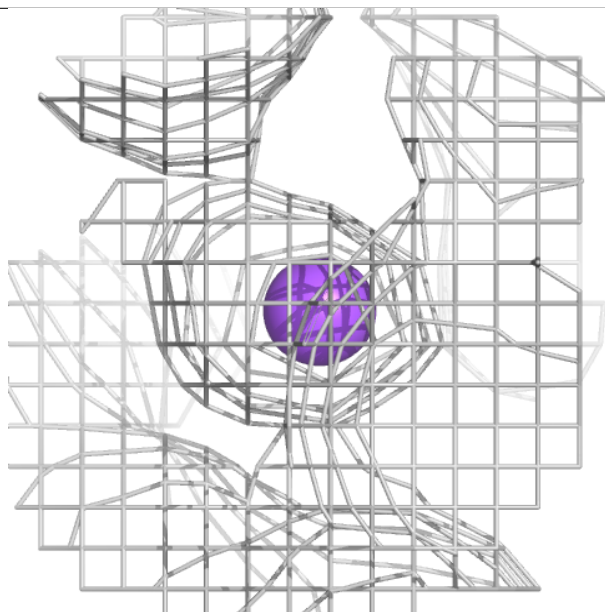
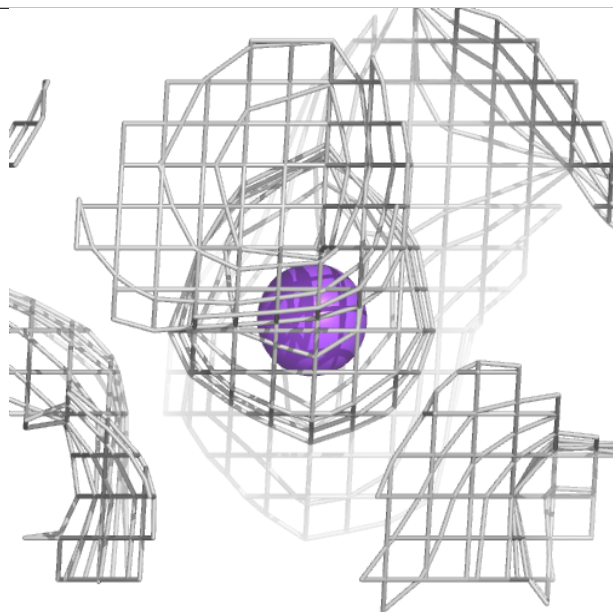
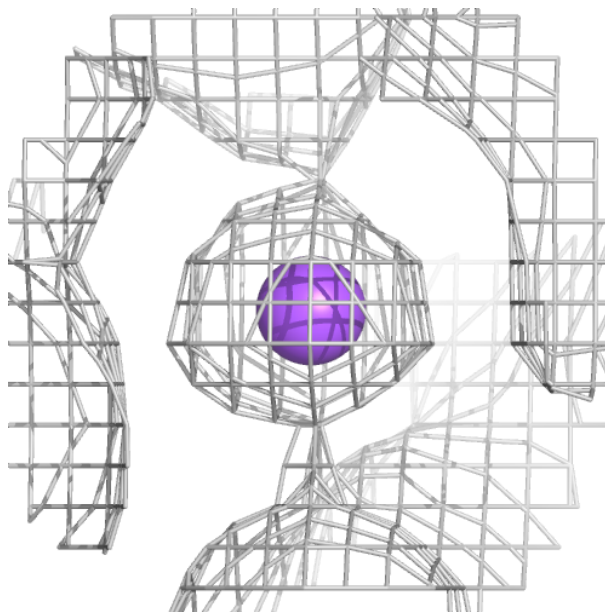
Electron density around SO4 F 701:

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



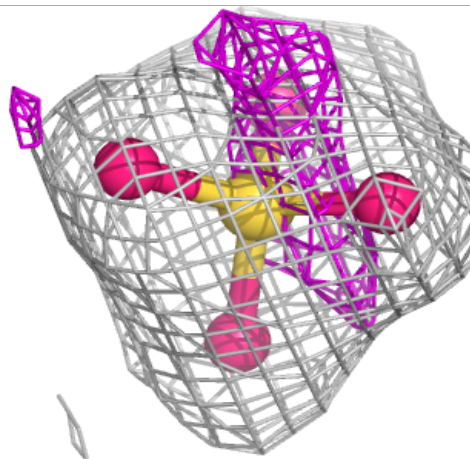
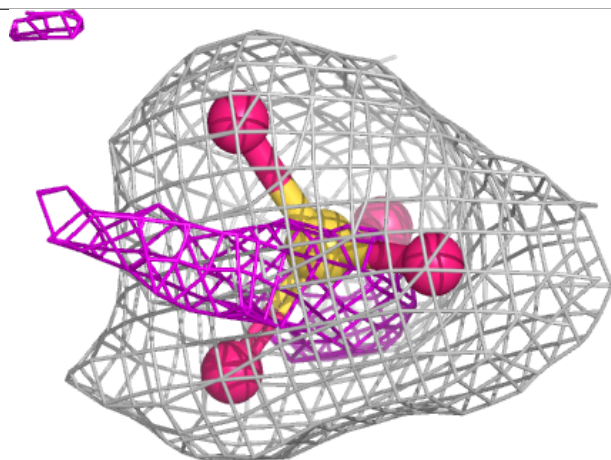
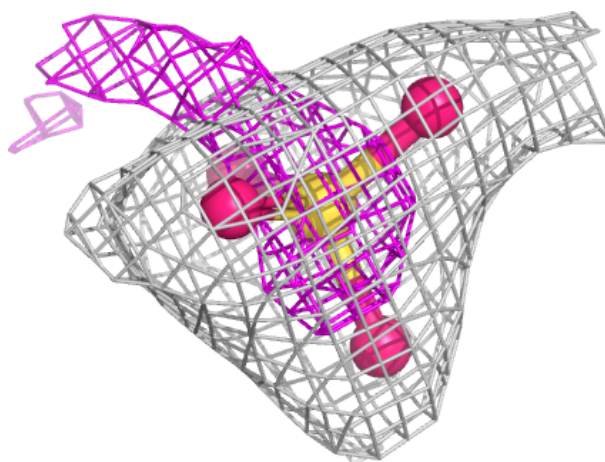
Electron density around NA C 708:

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



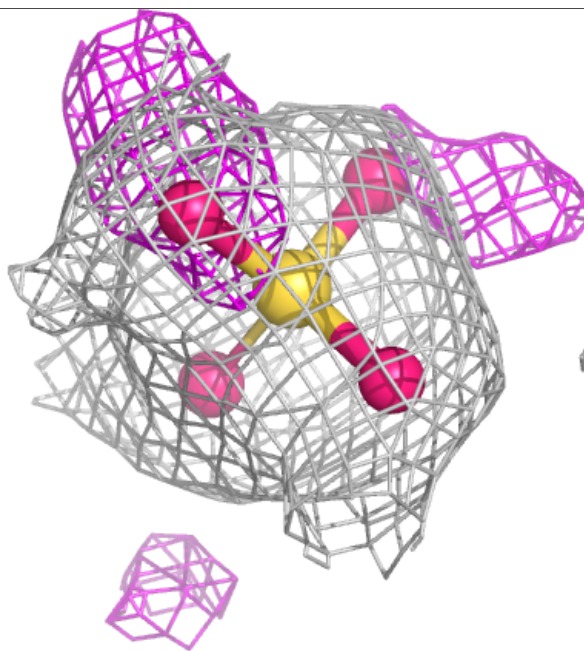
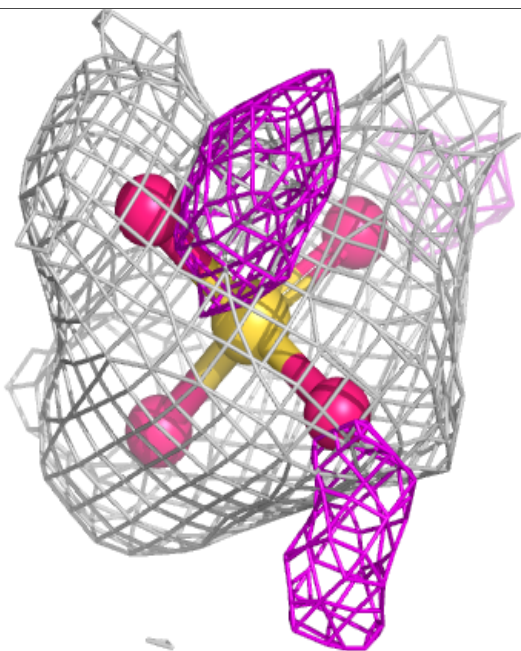
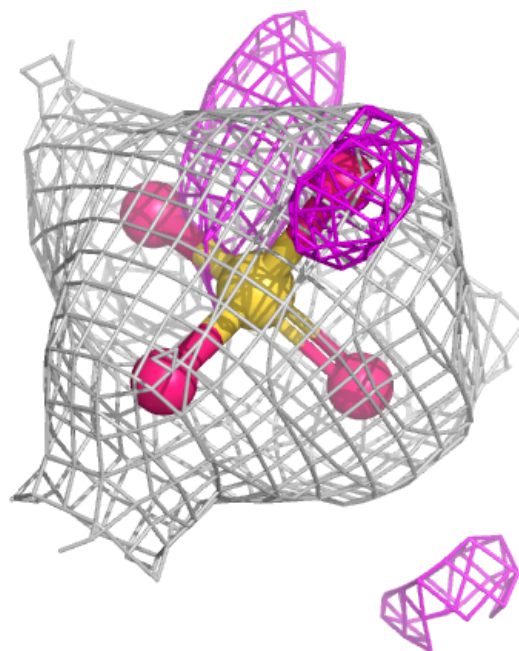
Electron density around SO4 B 704:

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



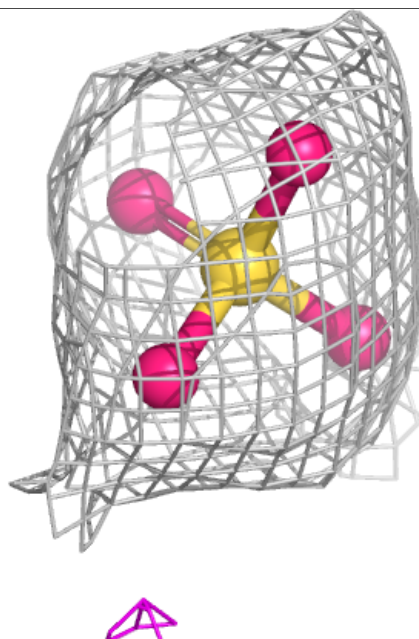
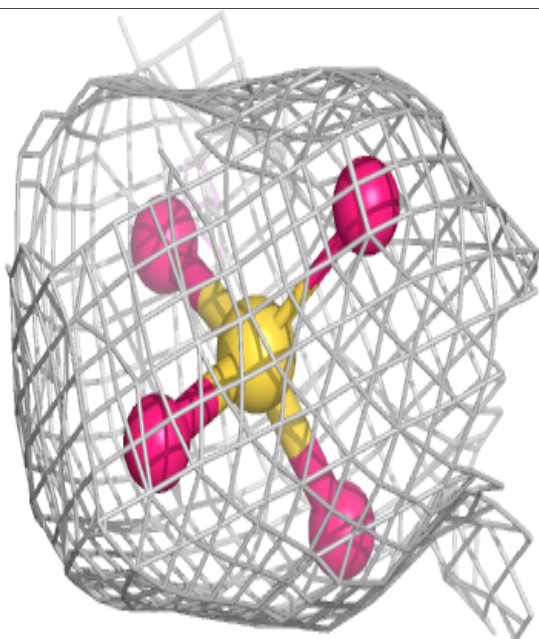
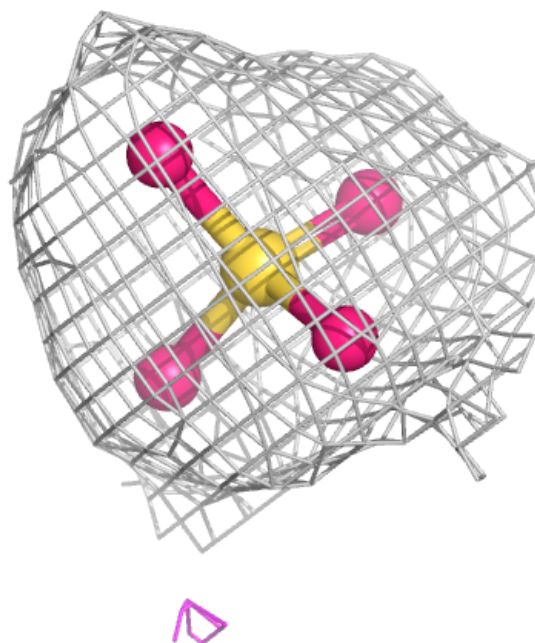
Electron density around SO4 C 702:

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



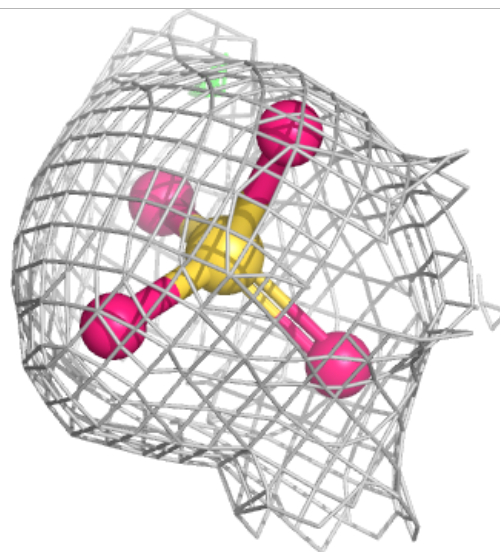
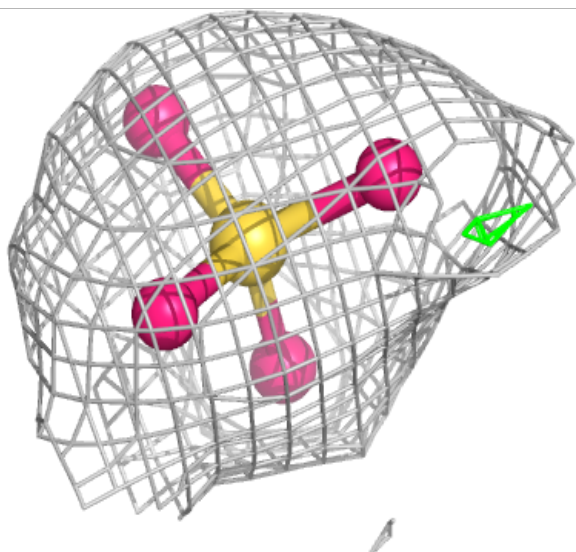
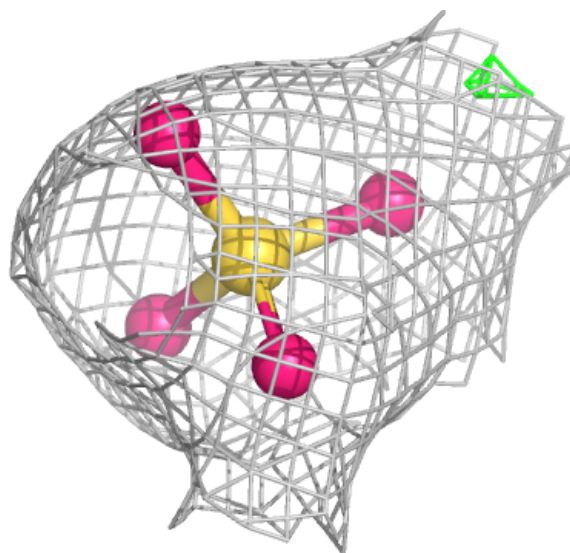
Electron density around SO4 G 701:

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



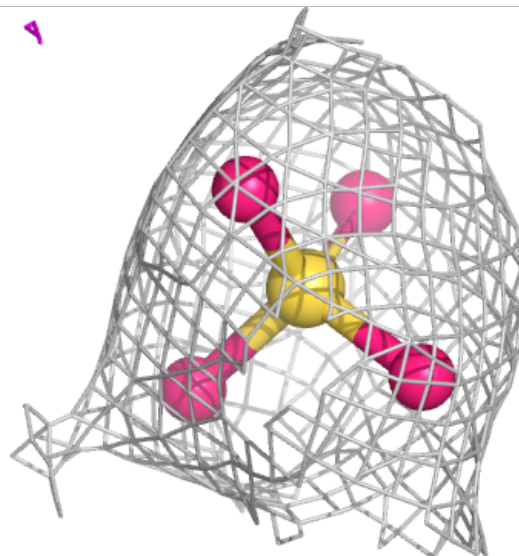
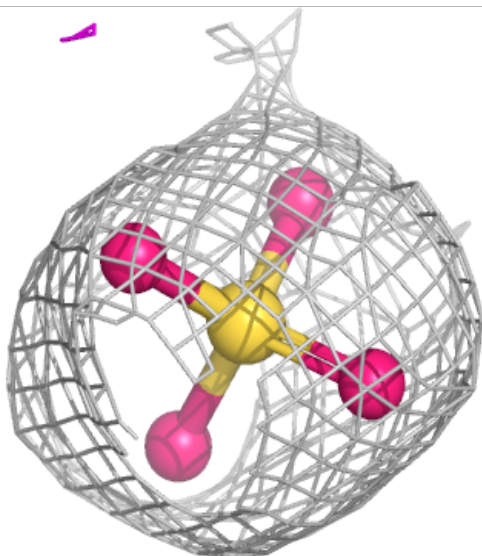
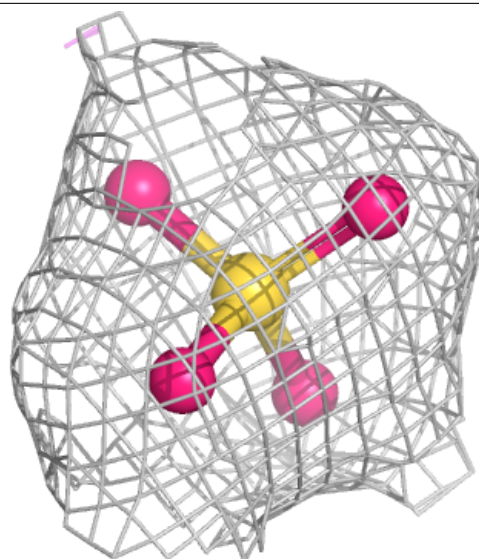
Electron density around SO4 E 703:

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



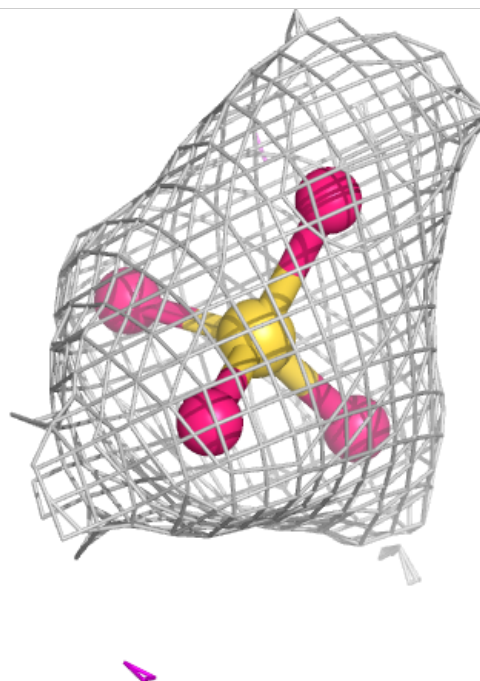
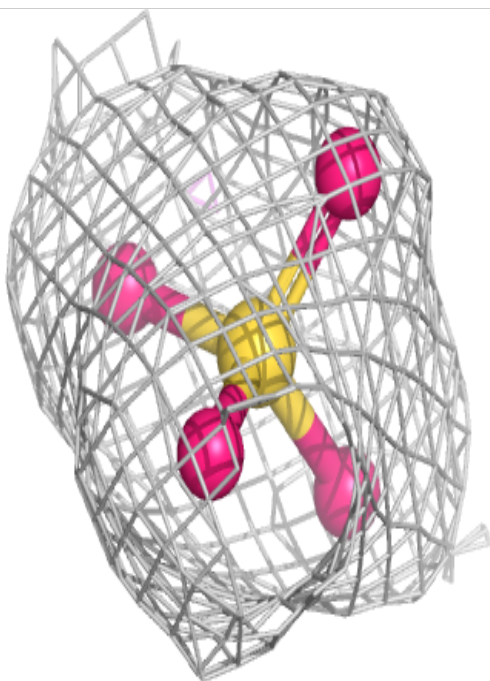
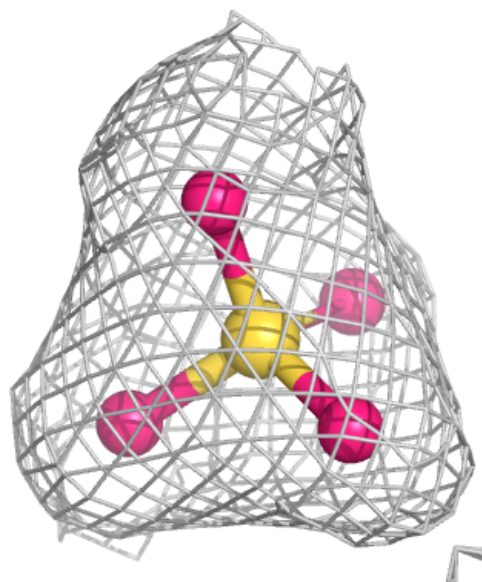
Electron density around SO4 B 709:

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



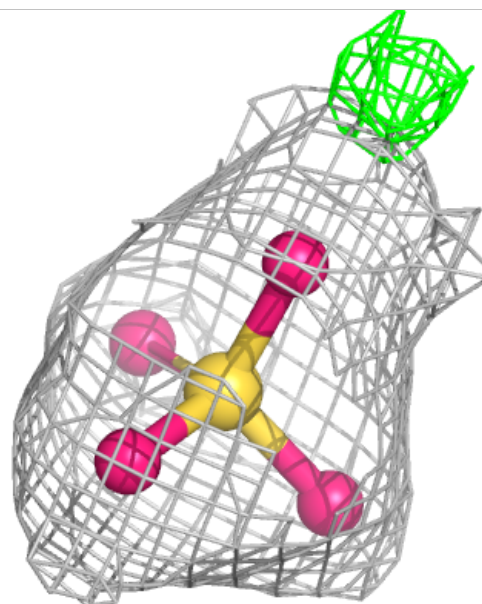
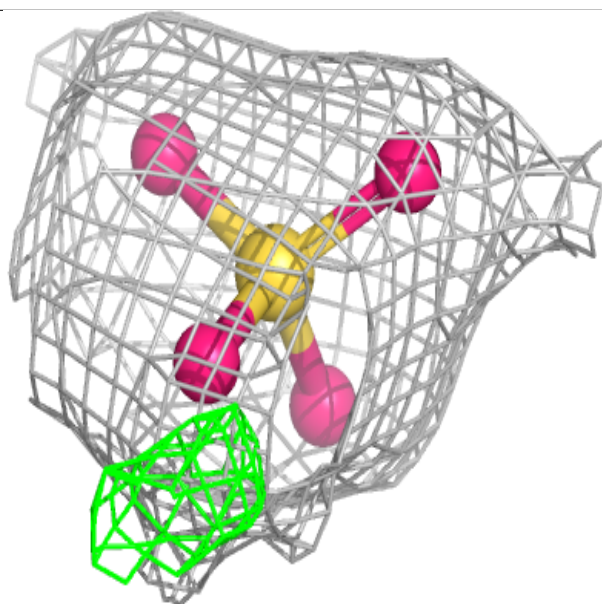
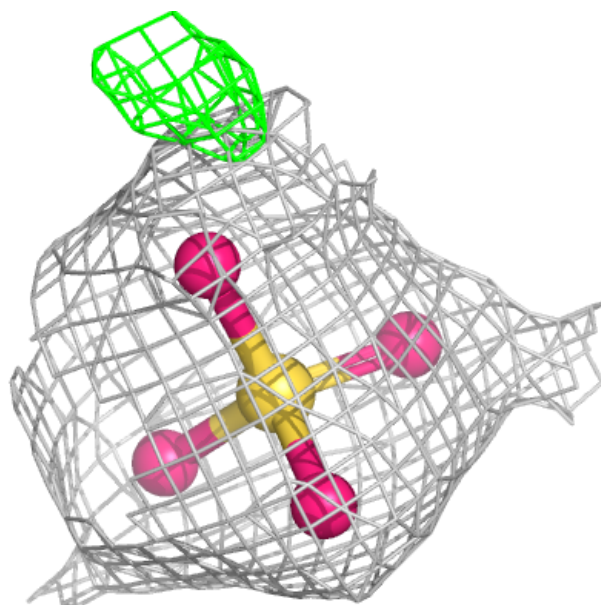
Electron density around SO4 G 704:

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



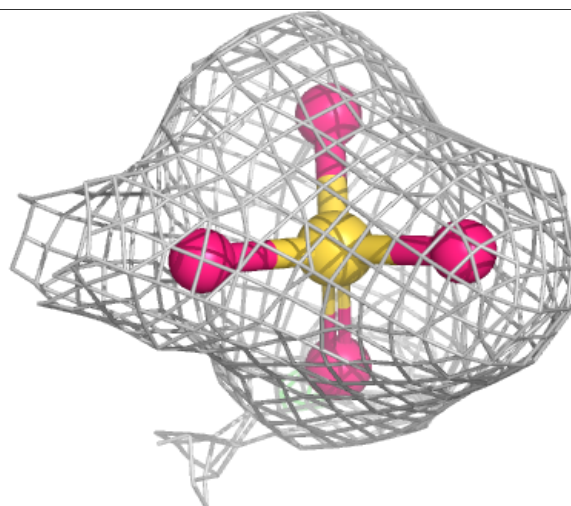
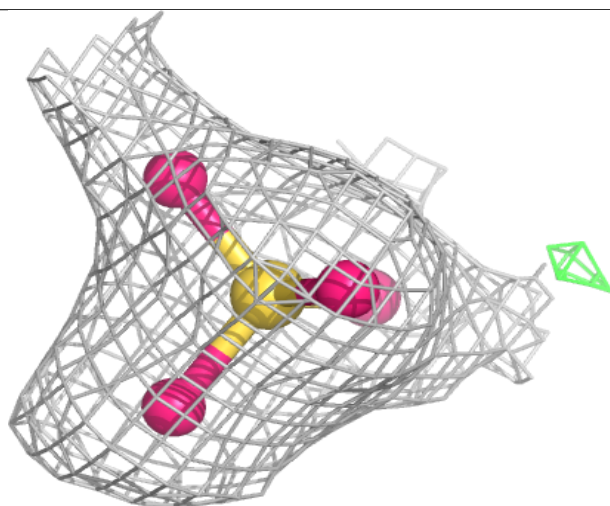
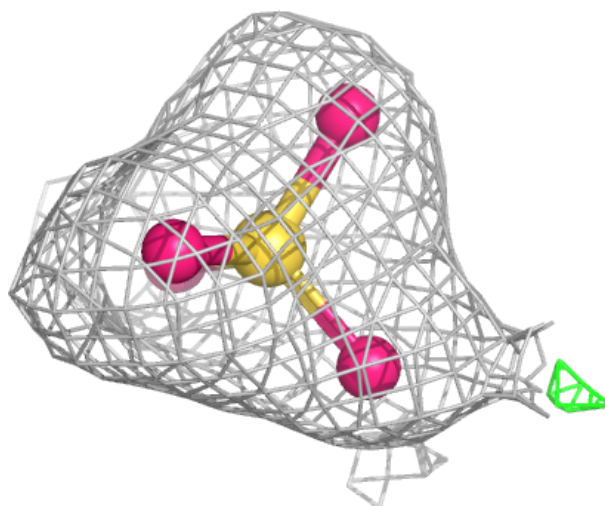
Electron density around SO4 A 702:

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



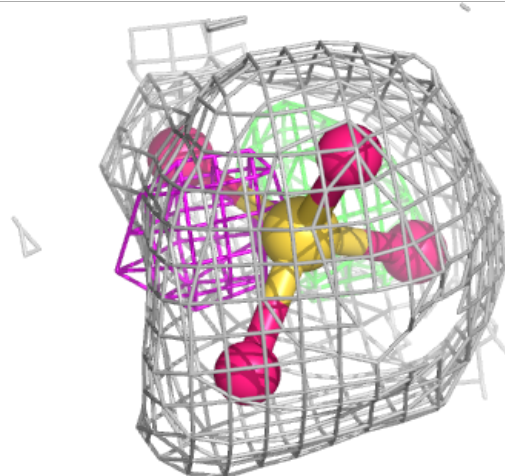
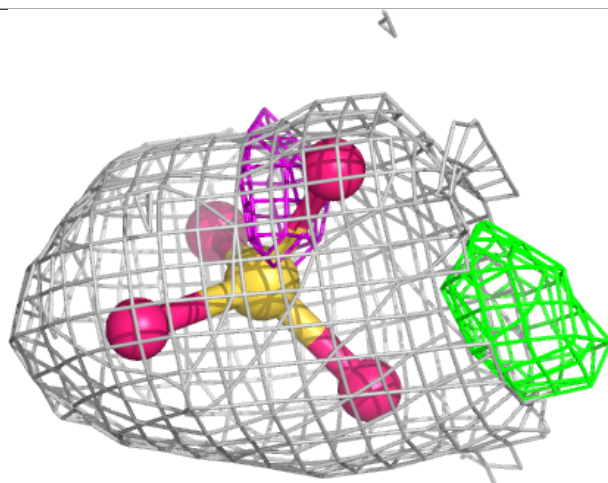
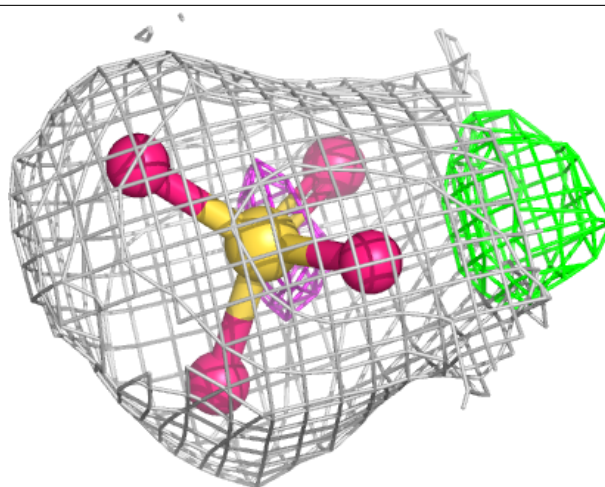
Electron density around SO4 A 701:

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



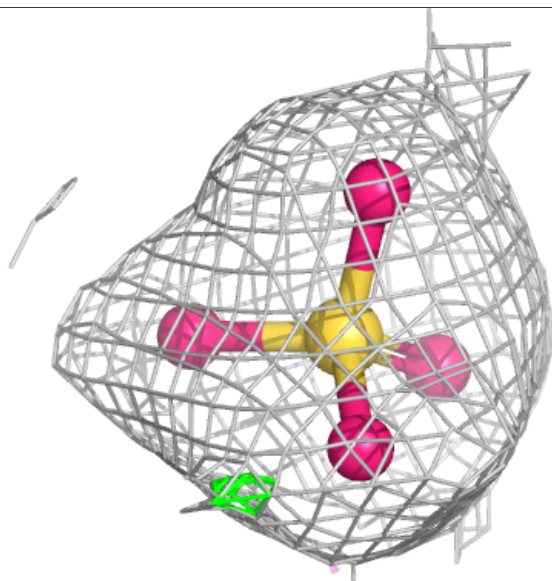
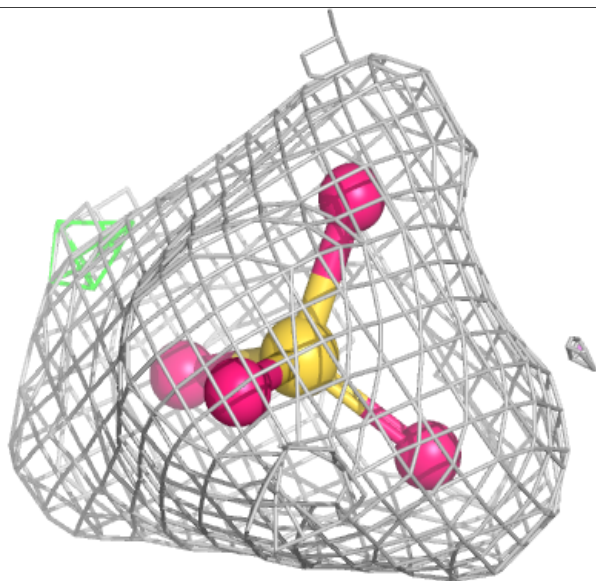
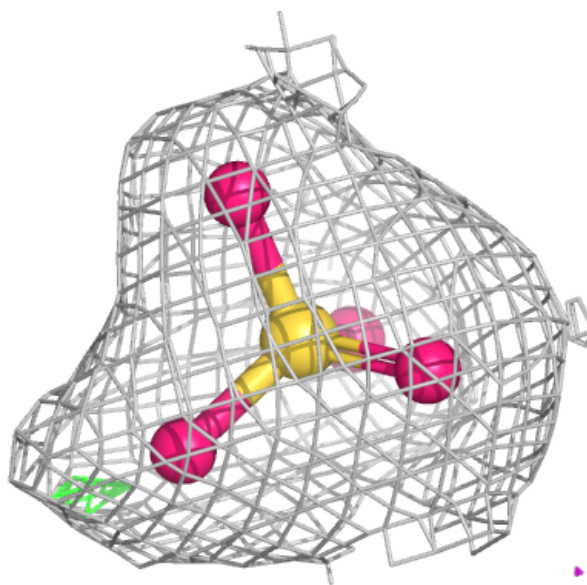
Electron density around SO4 F 702:

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



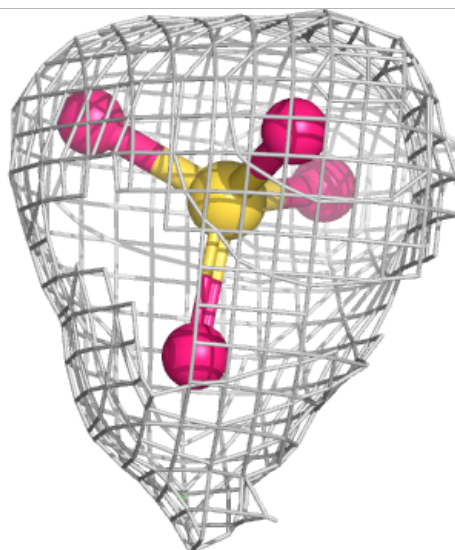
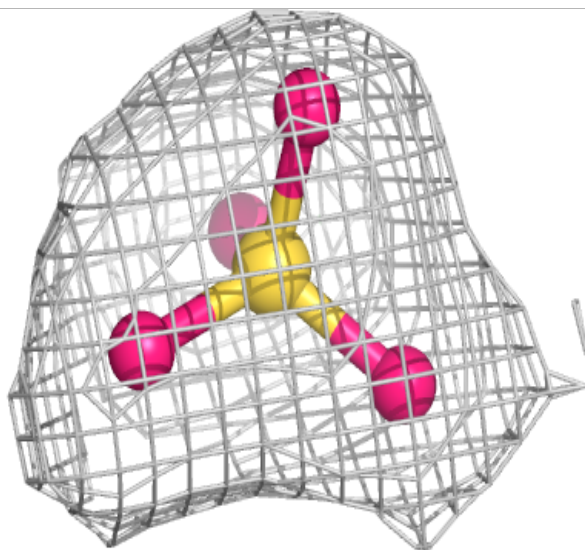
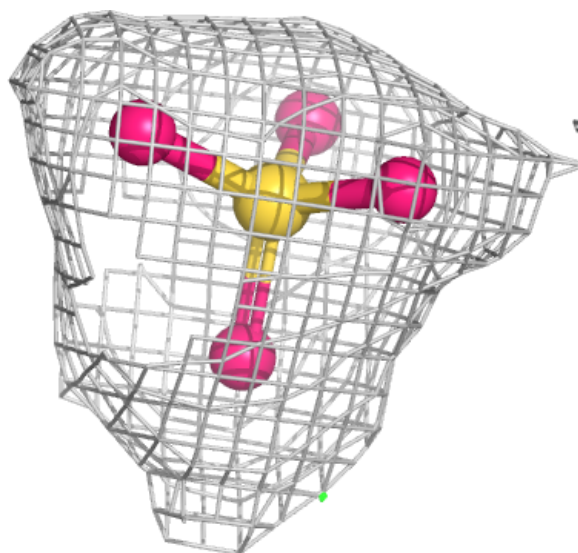
Electron density around SO4 E 702:

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



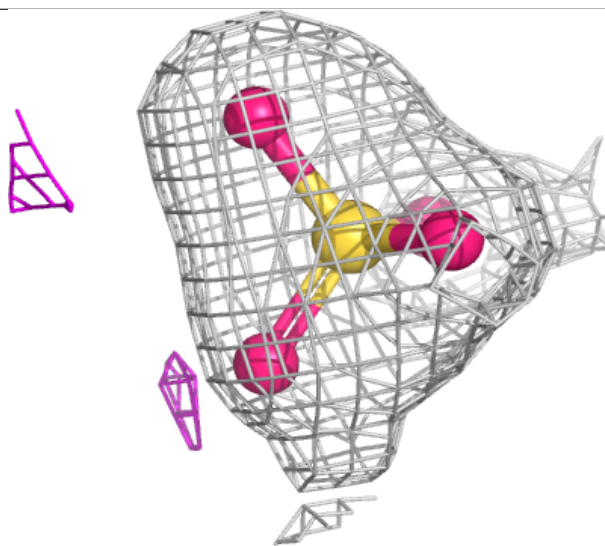
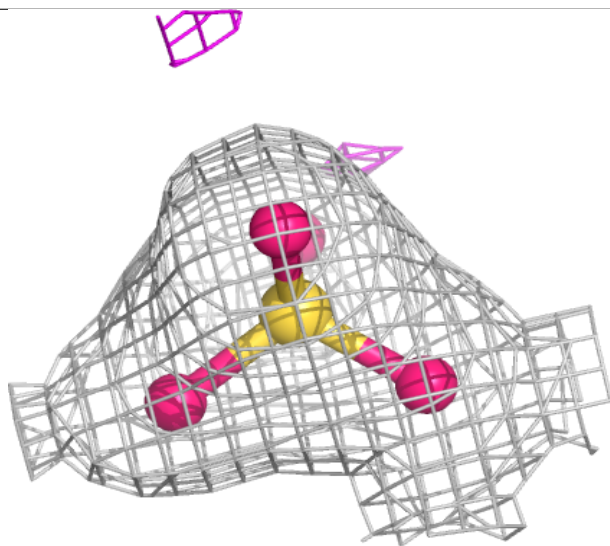
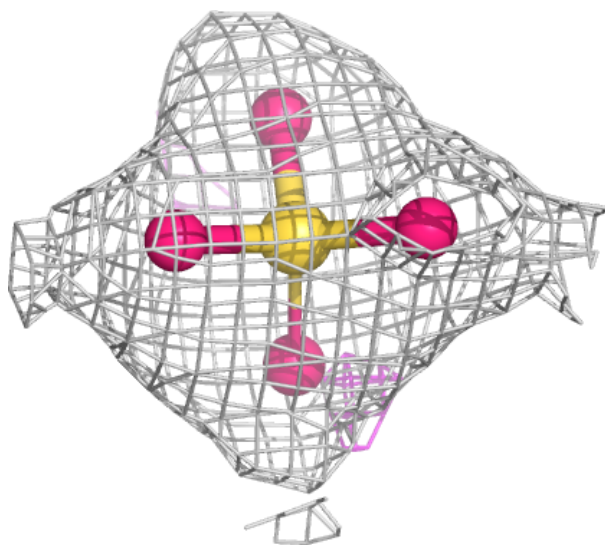
Electron density around SO4 D 703:

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



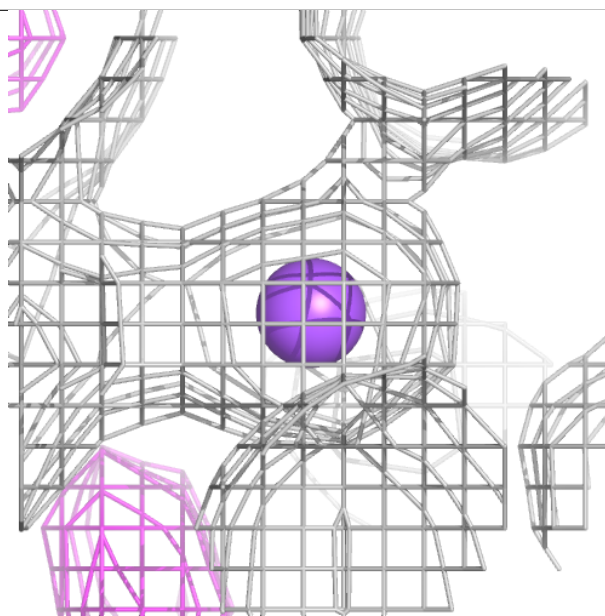
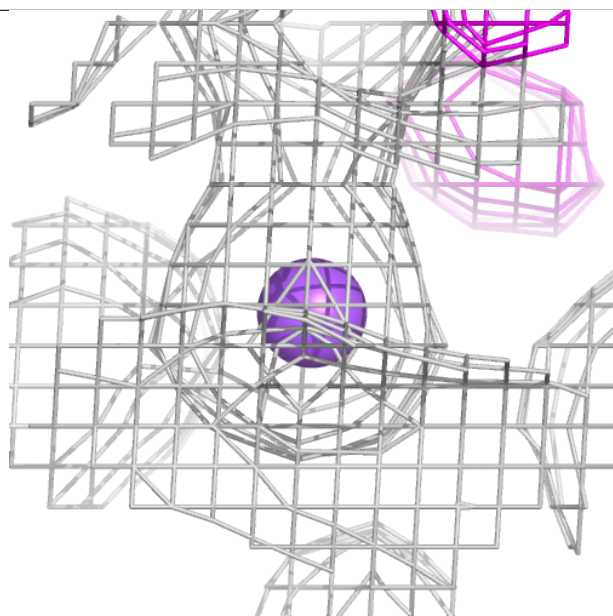
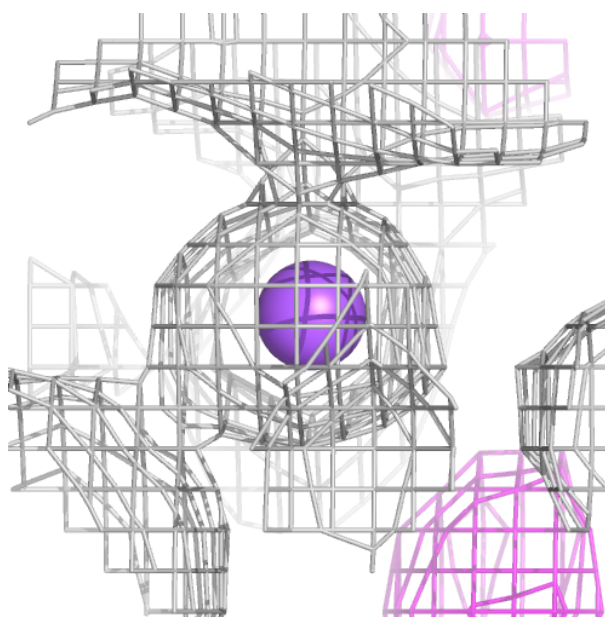
Electron density around SO4 D 701:

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



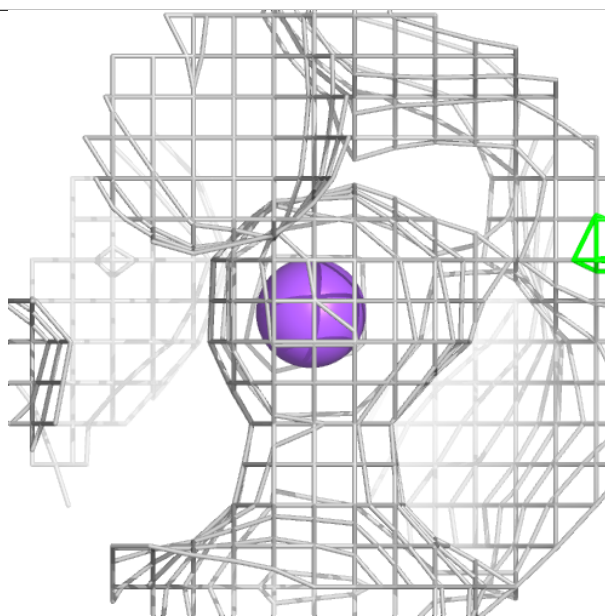
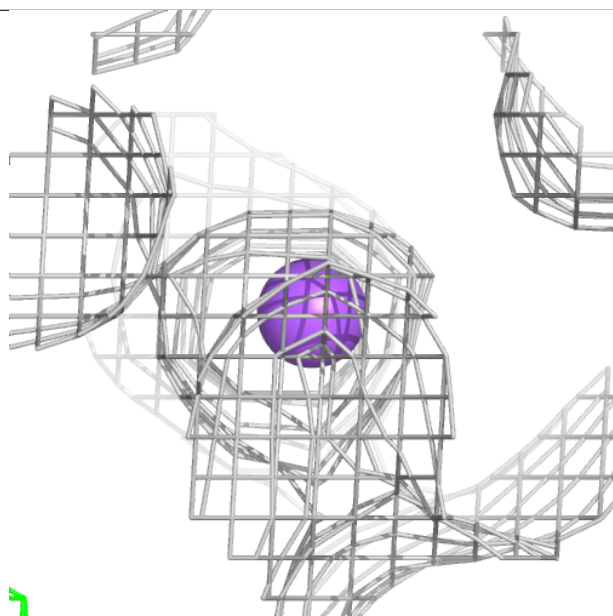
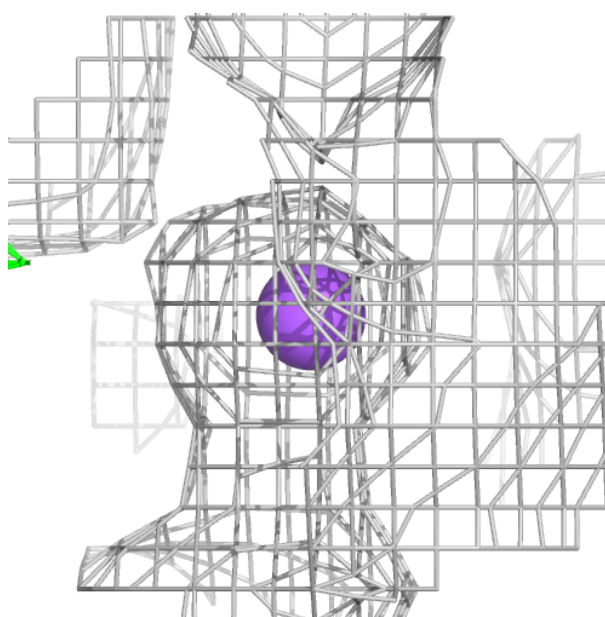
Electron density around NA A 711:

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



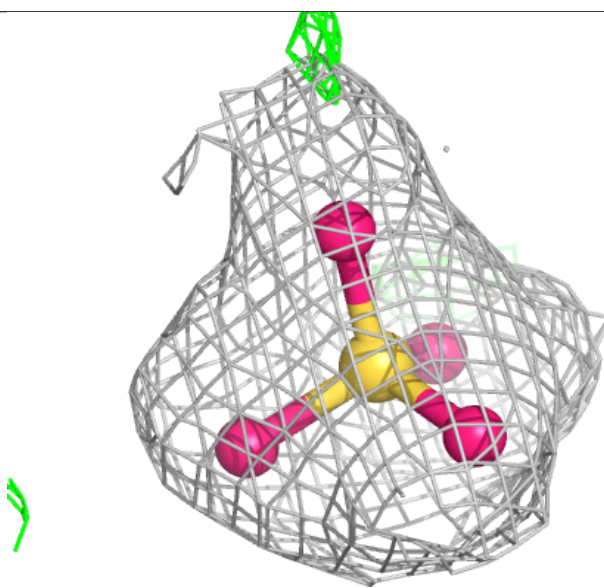
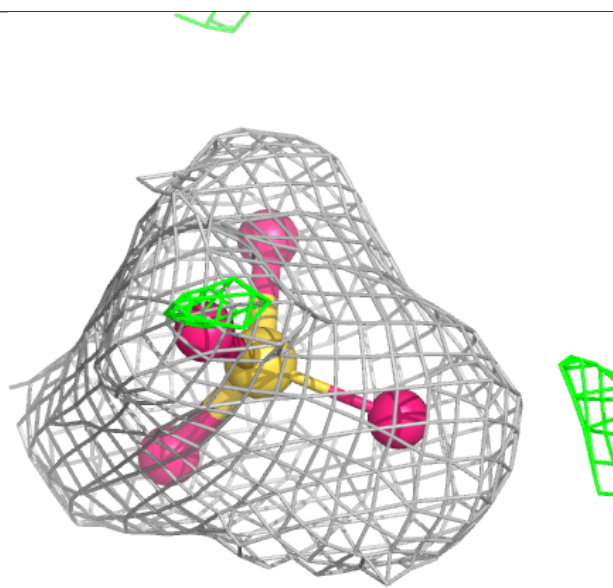
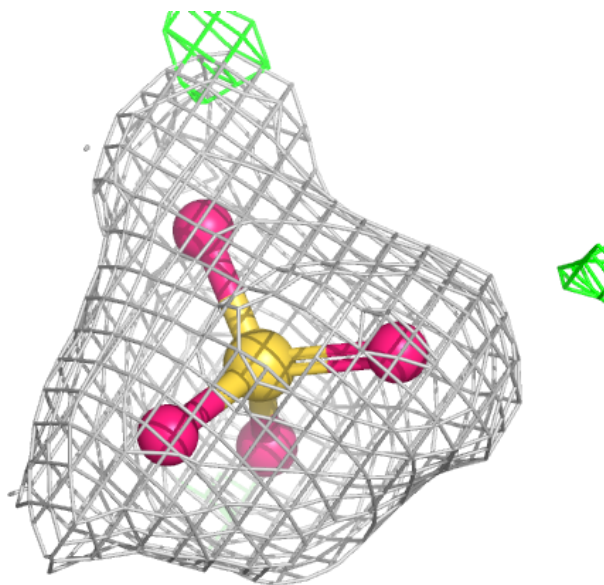
Electron density around NA E 710:

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



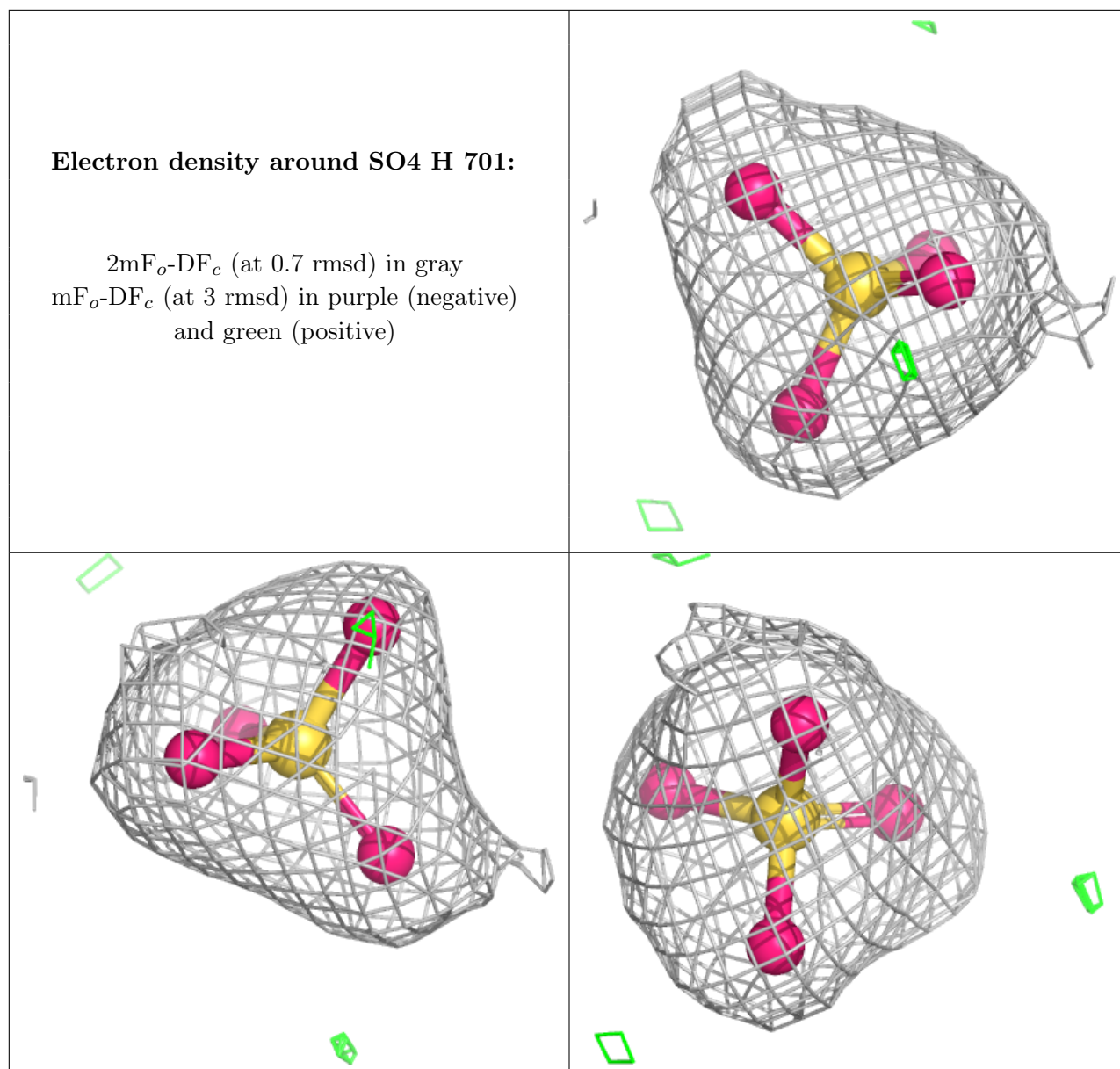
Electron density around SO4 B 705:

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



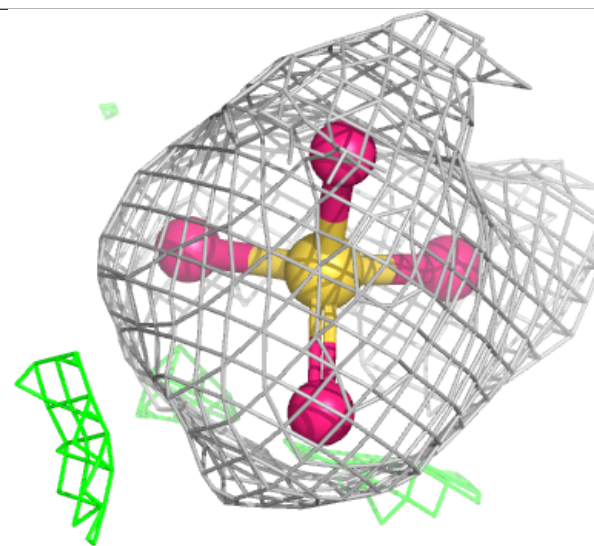
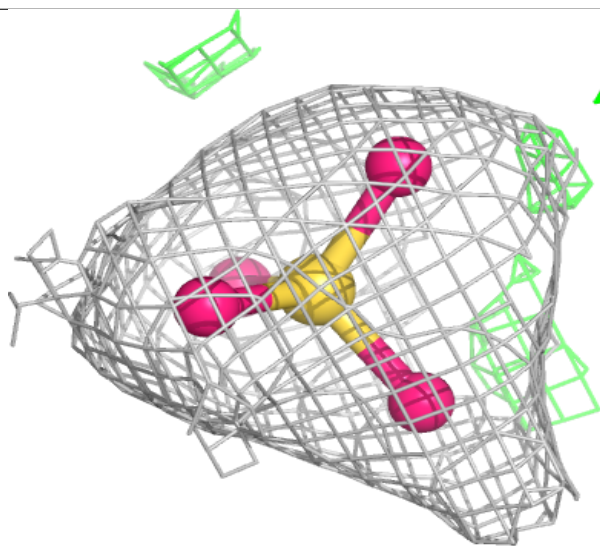
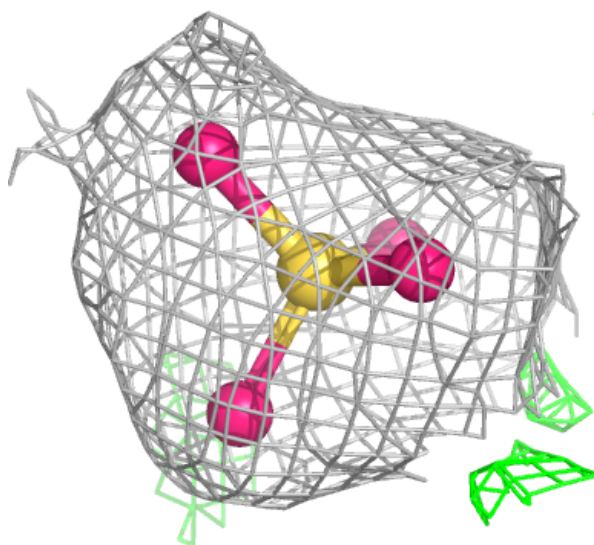
Electron density around SO4 H 701:

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



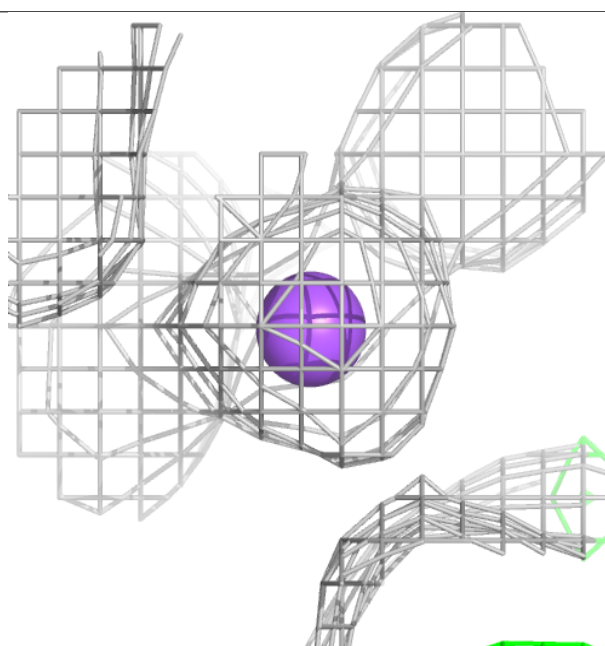
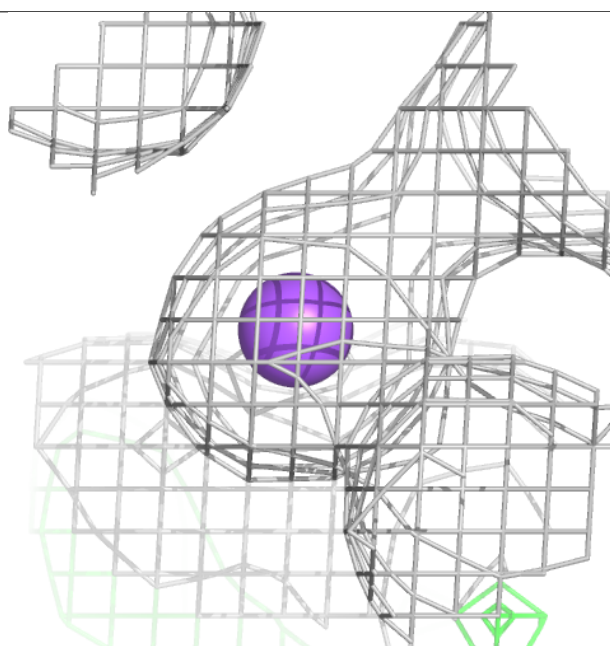
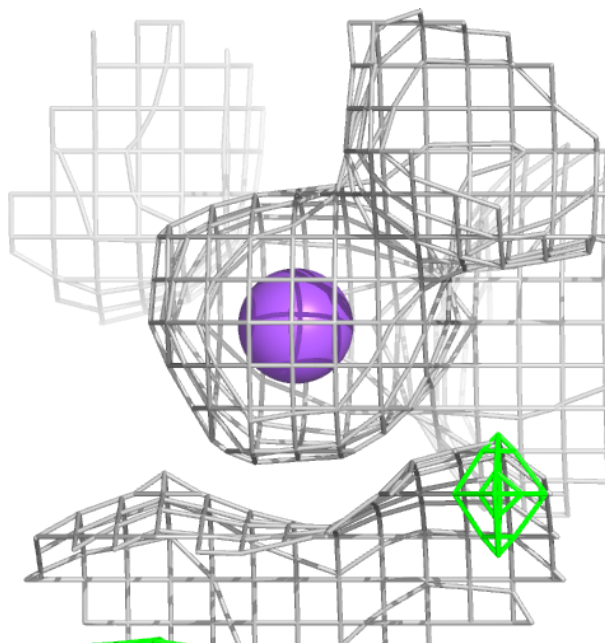
Electron density around SO4 C 703:

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



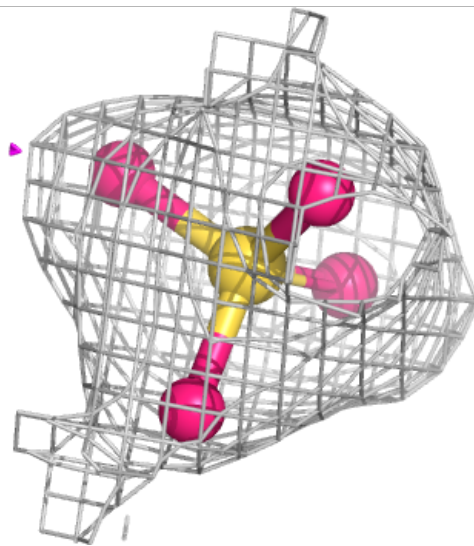
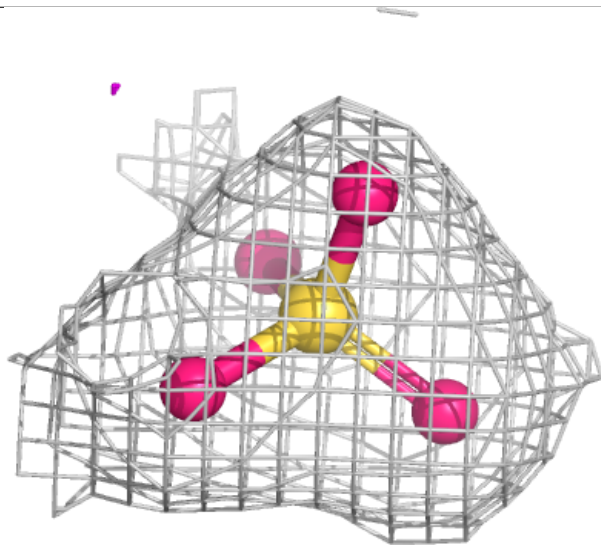
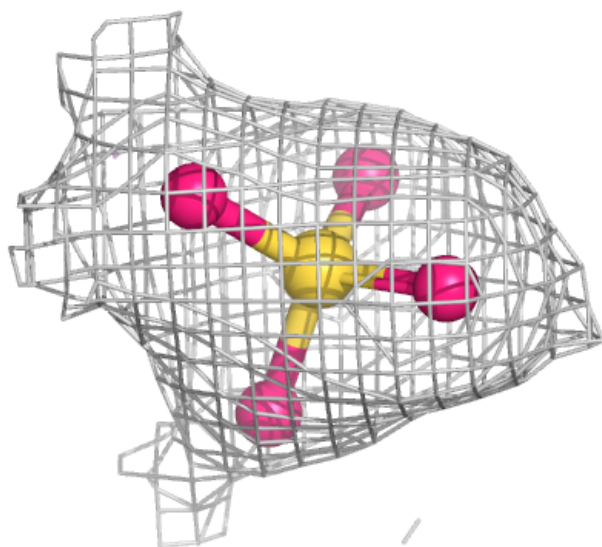
Electron density around NA A 709:

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



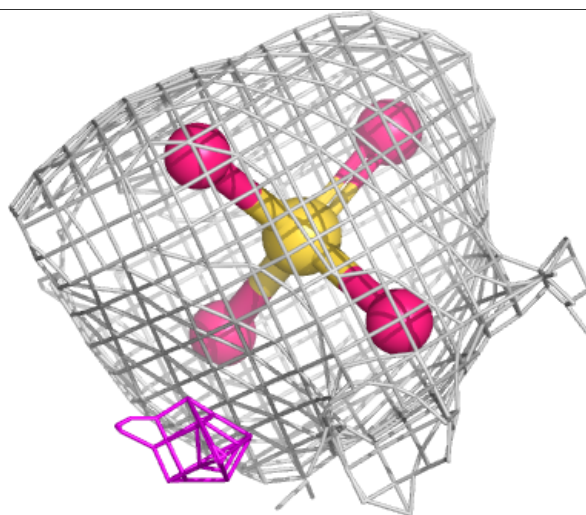
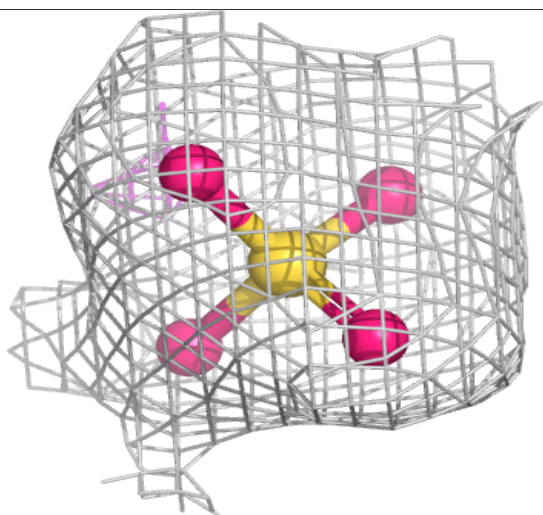
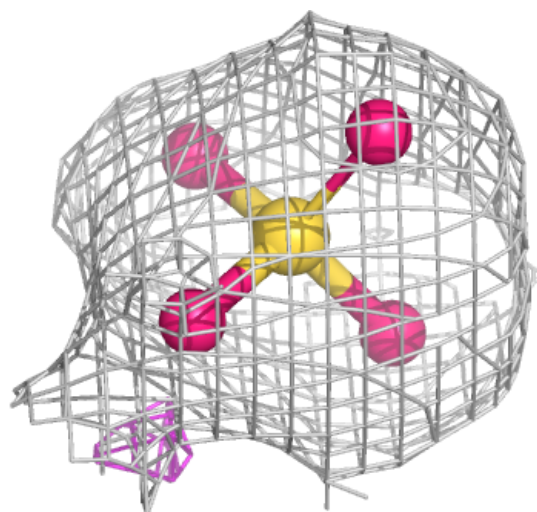
Electron density around SO4 E 701:

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



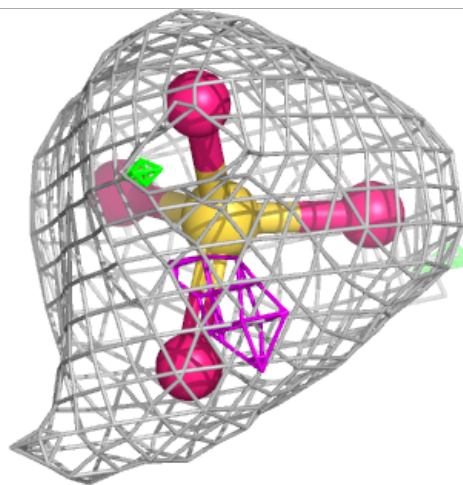
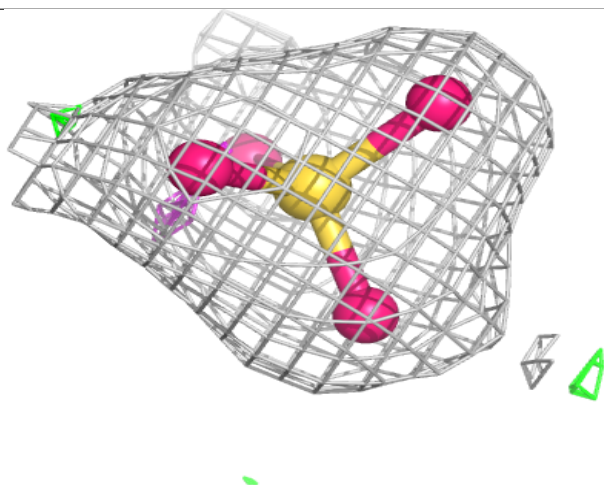
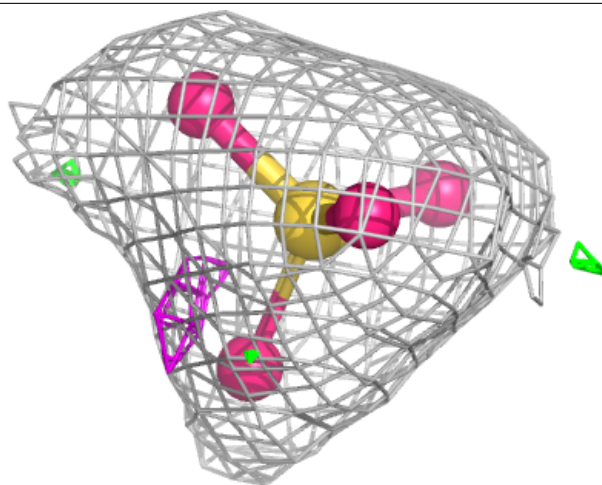
Electron density around SO4 B 702:

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



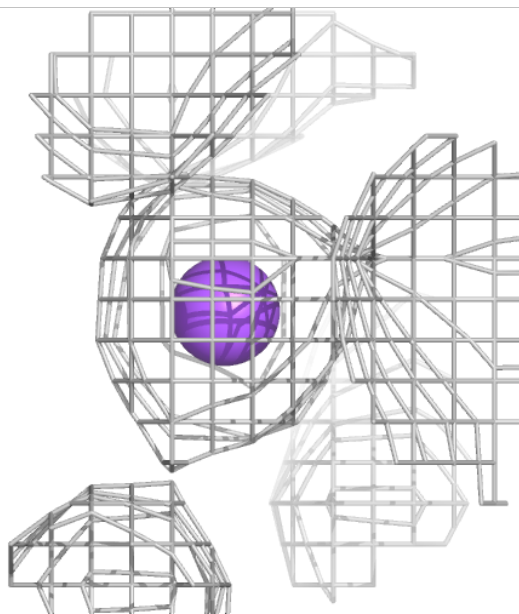
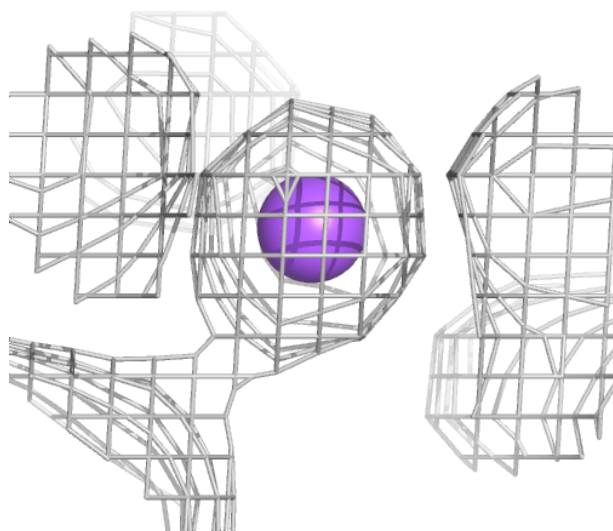
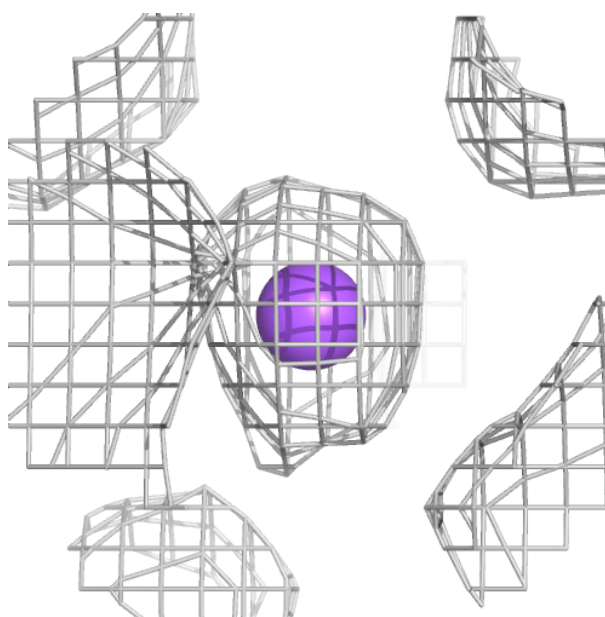
Electron density around SO4 B 701:

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



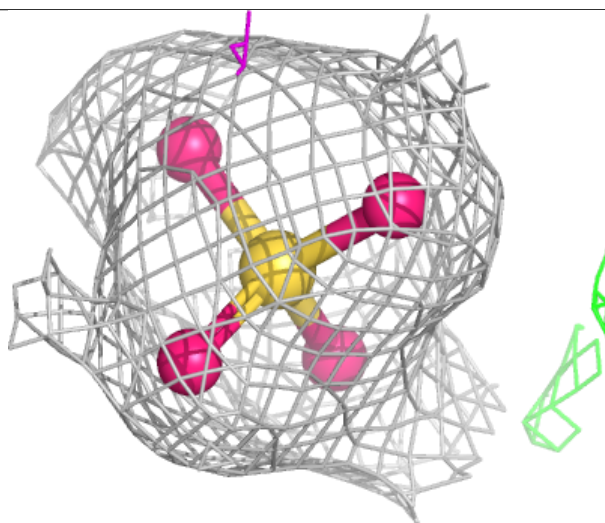
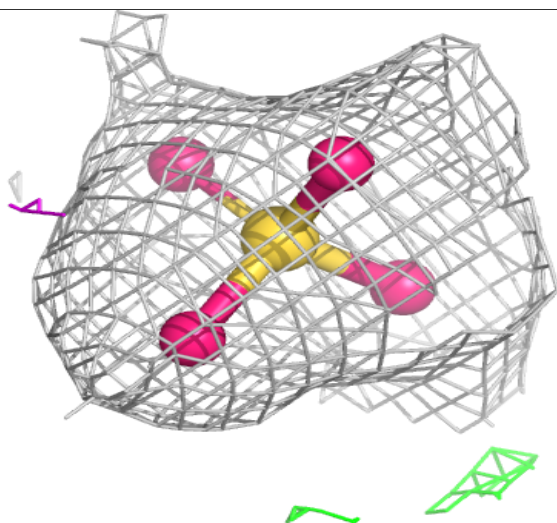
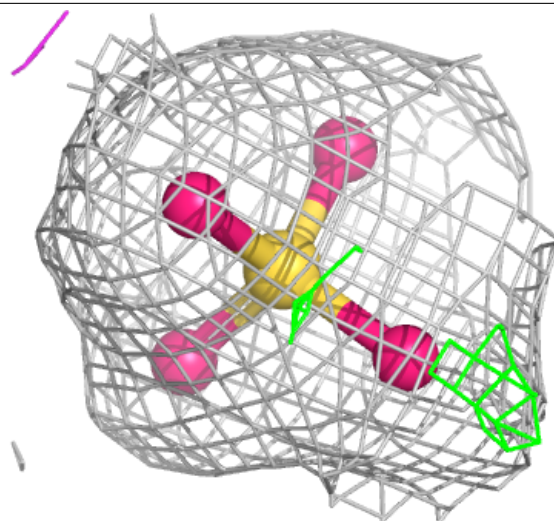
Electron density around NA B 713:

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



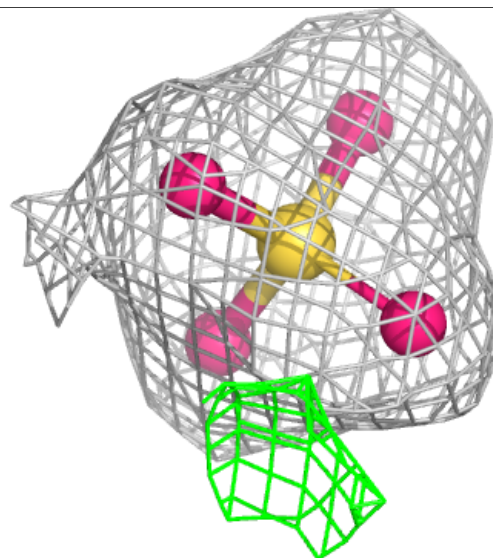
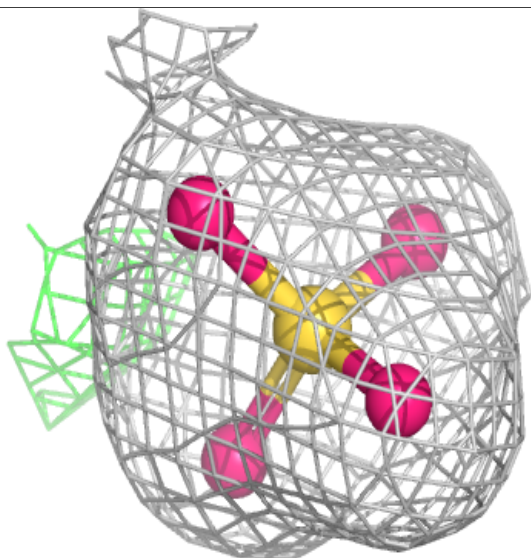
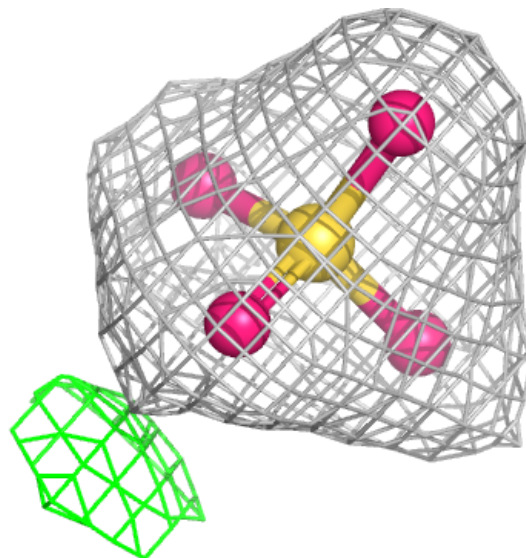
Electron density around SO4 H 703:

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



Electron density around SO4 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.