



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 8, 2023 – 10:34 PM EDT

PDB ID : 8FK4  
Title : Structure of the catalytic domain of Streptococcus mutans GtfB complexed to acarbose in orthorhombic space group P21212  
Authors : Schormann, N.; Deivanayagam, C.  
Deposited on : 2022-12-20  
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

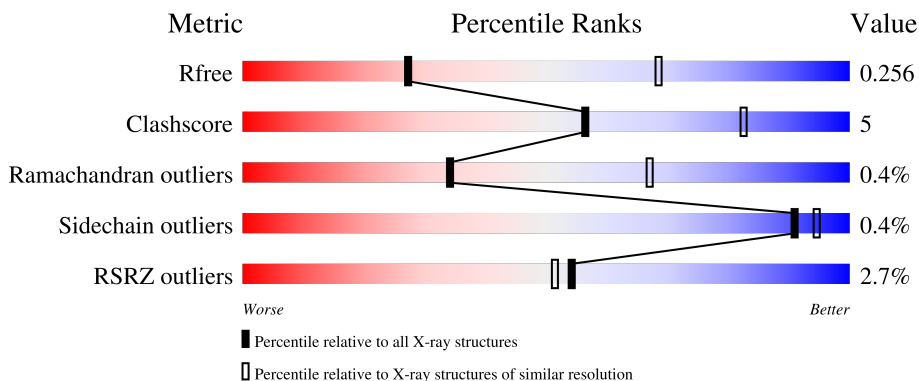
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

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



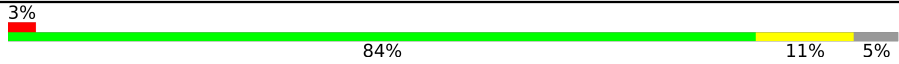
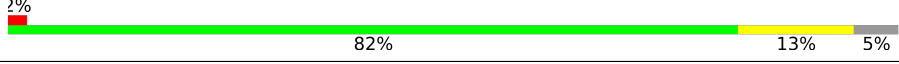


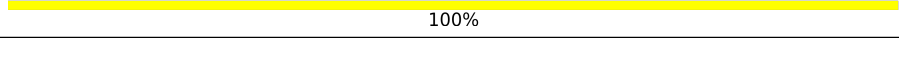
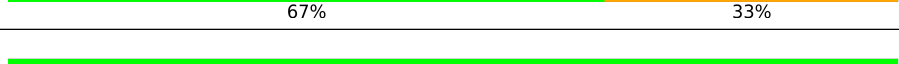
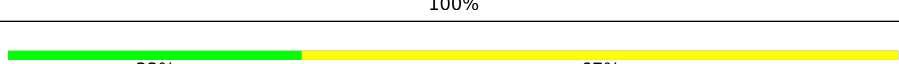
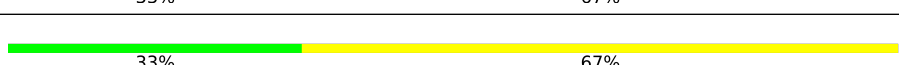
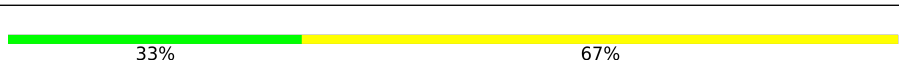
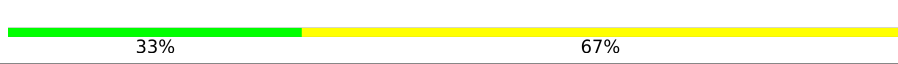

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	869	 83% 12% 5%
1	B	869	 82% 12% 6%
1	C	869	 81% 14% 5%
1	D	869	 81% 14% 5%
1	E	869	 84% 11% 5%

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Mol	Chain	Length	Quality of chain
1	F	869	 3% 84% 11% 5%
1	G	869	 2% 82% 13% 5%
1	H	869	 6% 80% 14% 6%
2	I	3	 67% 33%
2	J	3	 100%
2	K	3	 67% 33%
2	L	3	 100%
2	M	3	 33% 67%
2	N	3	 33% 67%
2	O	3	 33% 67%
2	P	3	 33% 67%

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
4	SO4	A	1207	-	-	X	-
4	SO4	G	1204	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52614 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 Glucosyltransferase-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	827	Total 6521	C 4107	N 1119	O 1279	S 16	0	0	0
1	B	821	Total 6440	C 4050	N 1106	O 1268	S 16	0	0	0
1	C	828	Total 6530	C 4113	N 1121	O 1280	S 16	0	0	0
1	D	828	Total 6529	C 4107	N 1123	O 1283	S 16	0	0	0
1	E	829	Total 6548	C 4127	N 1122	O 1283	S 16	0	0	0
1	F	826	Total 6513	C 4103	N 1117	O 1277	S 16	0	0	0
1	G	828	Total 6536	C 4118	N 1121	O 1281	S 16	0	0	0
1	H	817	Total 6427	C 4044	N 1105	O 1262	S 16	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1052	LEU	-	expression tag	UNP P08987
A	1053	GLU	-	expression tag	UNP P08987
A	1054	HIS	-	expression tag	UNP P08987
A	1055	HIS	-	expression tag	UNP P08987
A	1056	HIS	-	expression tag	UNP P08987
A	1057	HIS	-	expression tag	UNP P08987
A	1058	HIS	-	expression tag	UNP P08987
A	1059	HIS	-	expression tag	UNP P08987
B	1052	LEU	-	expression tag	UNP P08987
B	1053	GLU	-	expression tag	UNP P08987
B	1054	HIS	-	expression tag	UNP P08987
B	1055	HIS	-	expression tag	UNP P08987
B	1056	HIS	-	expression tag	UNP P08987

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1057	HIS	-	expression tag	UNP P08987
B	1058	HIS	-	expression tag	UNP P08987
B	1059	HIS	-	expression tag	UNP P08987
C	1052	LEU	-	expression tag	UNP P08987
C	1053	GLU	-	expression tag	UNP P08987
C	1054	HIS	-	expression tag	UNP P08987
C	1055	HIS	-	expression tag	UNP P08987
C	1056	HIS	-	expression tag	UNP P08987
C	1057	HIS	-	expression tag	UNP P08987
C	1058	HIS	-	expression tag	UNP P08987
C	1059	HIS	-	expression tag	UNP P08987
D	1052	LEU	-	expression tag	UNP P08987
D	1053	GLU	-	expression tag	UNP P08987
D	1054	HIS	-	expression tag	UNP P08987
D	1055	HIS	-	expression tag	UNP P08987
D	1056	HIS	-	expression tag	UNP P08987
D	1057	HIS	-	expression tag	UNP P08987
D	1058	HIS	-	expression tag	UNP P08987
D	1059	HIS	-	expression tag	UNP P08987
E	1052	LEU	-	expression tag	UNP P08987
E	1053	GLU	-	expression tag	UNP P08987
E	1054	HIS	-	expression tag	UNP P08987
E	1055	HIS	-	expression tag	UNP P08987
E	1056	HIS	-	expression tag	UNP P08987
E	1057	HIS	-	expression tag	UNP P08987
E	1058	HIS	-	expression tag	UNP P08987
E	1059	HIS	-	expression tag	UNP P08987
F	1052	LEU	-	expression tag	UNP P08987
F	1053	GLU	-	expression tag	UNP P08987
F	1054	HIS	-	expression tag	UNP P08987
F	1055	HIS	-	expression tag	UNP P08987
F	1056	HIS	-	expression tag	UNP P08987
F	1057	HIS	-	expression tag	UNP P08987
F	1058	HIS	-	expression tag	UNP P08987
F	1059	HIS	-	expression tag	UNP P08987
G	1052	LEU	-	expression tag	UNP P08987
G	1053	GLU	-	expression tag	UNP P08987
G	1054	HIS	-	expression tag	UNP P08987
G	1055	HIS	-	expression tag	UNP P08987
G	1056	HIS	-	expression tag	UNP P08987
G	1057	HIS	-	expression tag	UNP P08987
G	1058	HIS	-	expression tag	UNP P08987

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1059	HIS	-	expression tag	UNP P08987
H	1052	LEU	-	expression tag	UNP P08987
H	1053	GLU	-	expression tag	UNP P08987
H	1054	HIS	-	expression tag	UNP P08987
H	1055	HIS	-	expression tag	UNP P08987
H	1056	HIS	-	expression tag	UNP P08987
H	1057	HIS	-	expression tag	UNP P08987
H	1058	HIS	-	expression tag	UNP P08987
H	1059	HIS	-	expression tag	UNP P08987

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	3	44	25	1	18	0	0	0
2	J	3	44	25	1	18	0	0	0
2	K	3	44	25	1	18	0	0	0
2	L	3	44	25	1	18	0	0	0
2	M	3	44	25	1	18	0	0	0
2	N	3	44	25	1	18	0	0	0
2	O	3	44	25	1	18	0	0	0
2	P	3	44	25	1	18	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

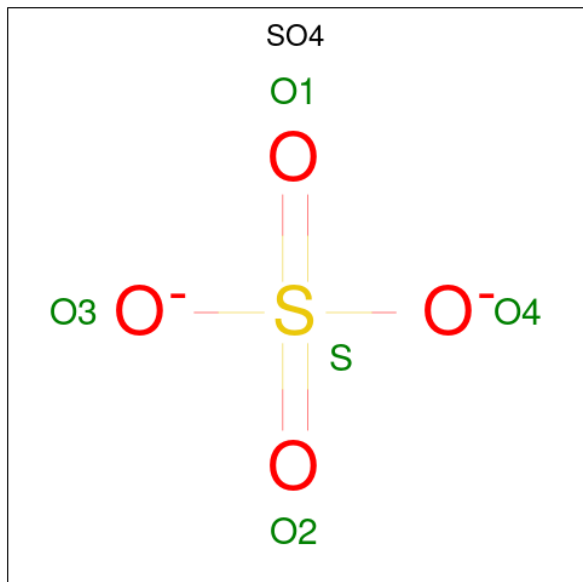
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

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



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

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

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

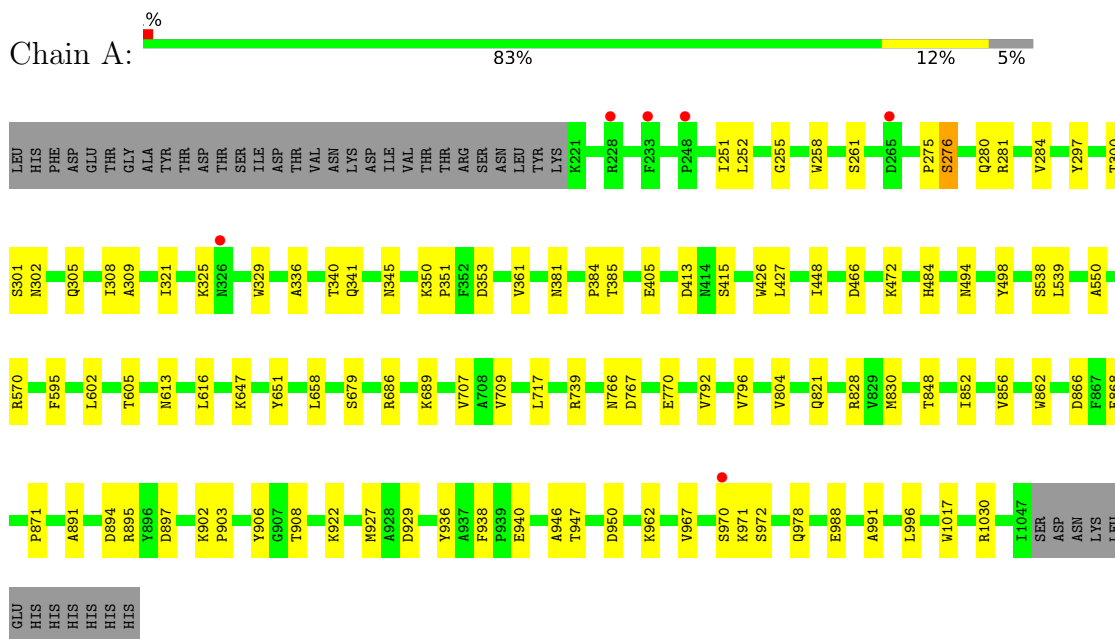
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	E	2	Total O 2 2	0	0

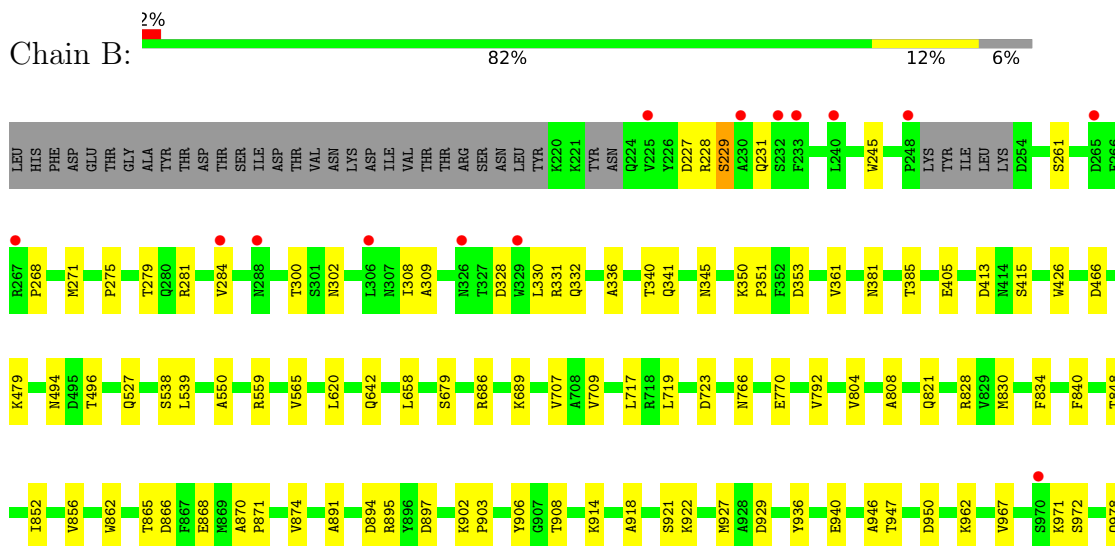
### 3 Residue-property plots [i](#)

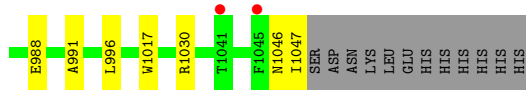
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

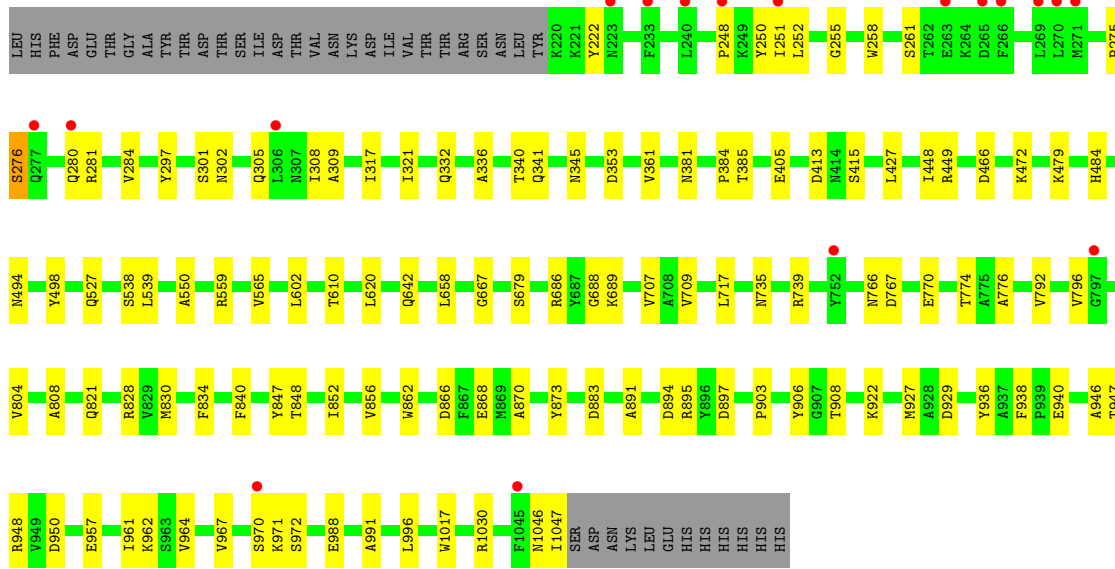
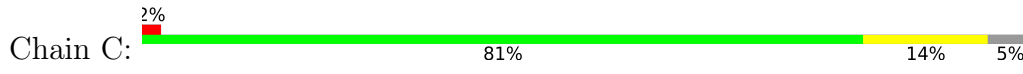


- Molecule 1: Glucosyltransferase-I

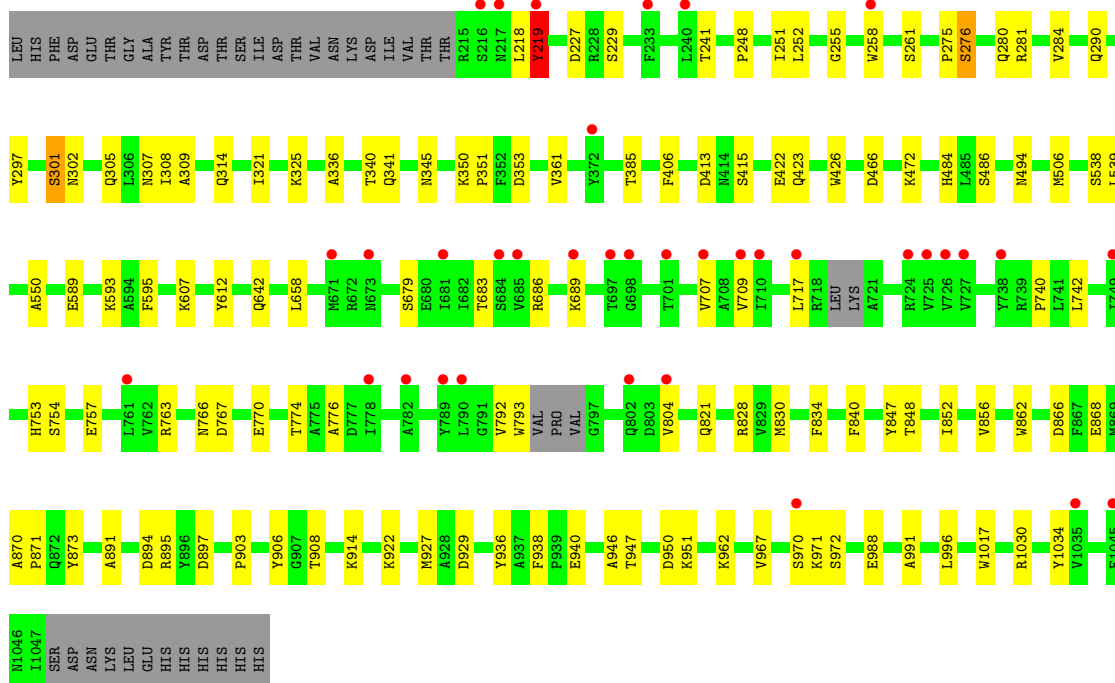
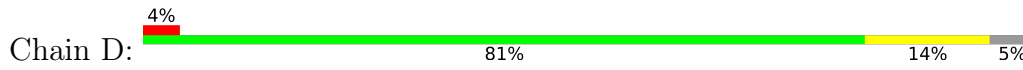




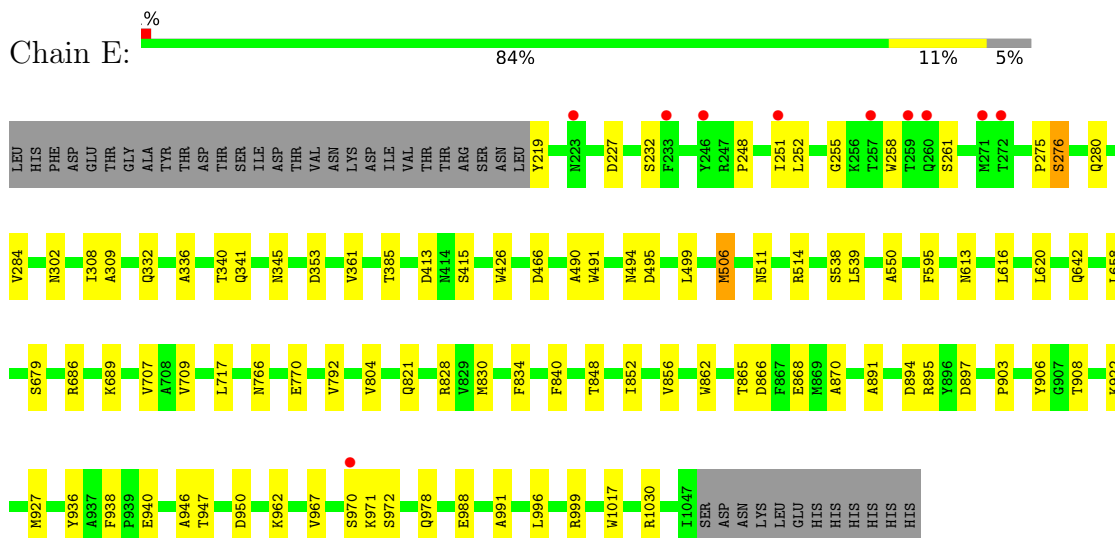
- Molecule 1: Glucosyltransferase-I



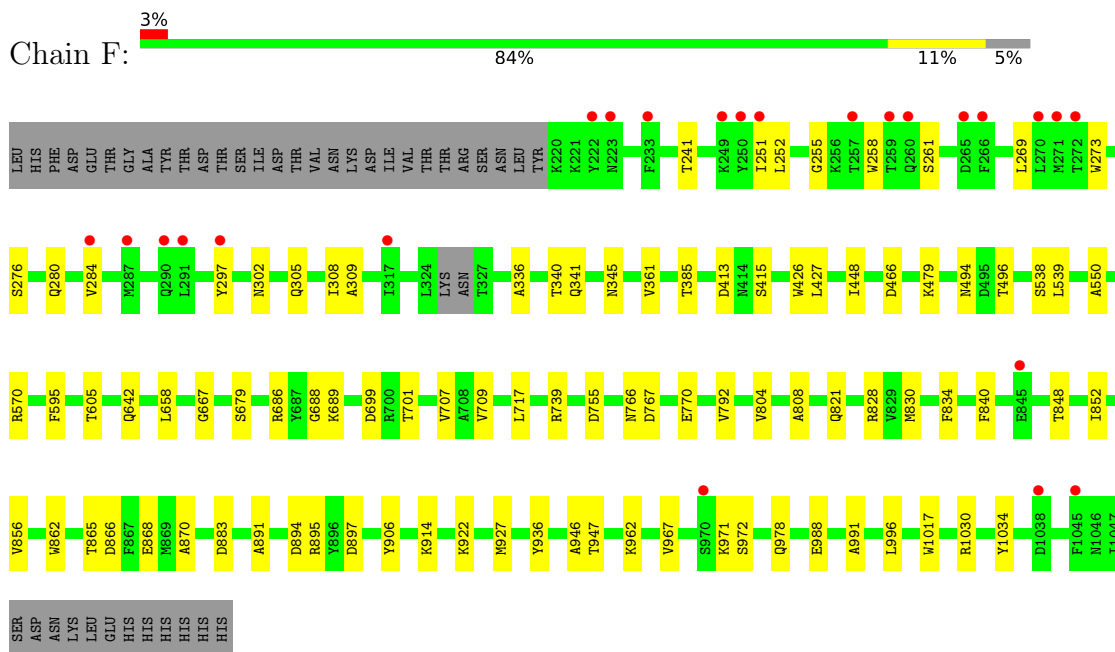
- Molecule 1: Glucosyltransferase-I



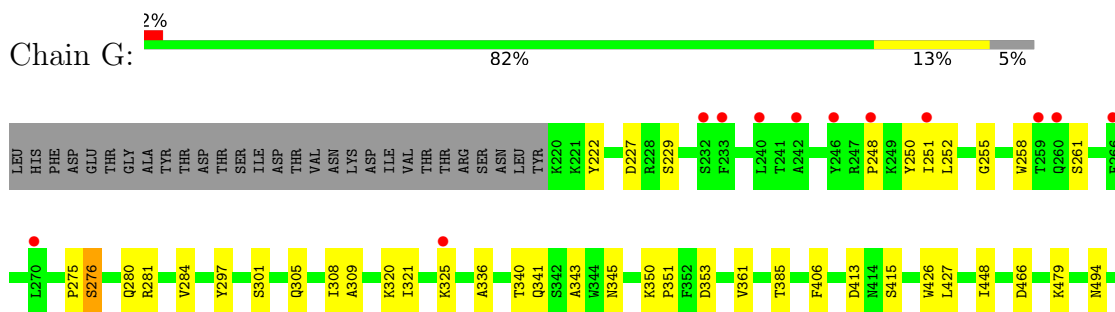
- Molecule 1: Glucosyltransferase-I

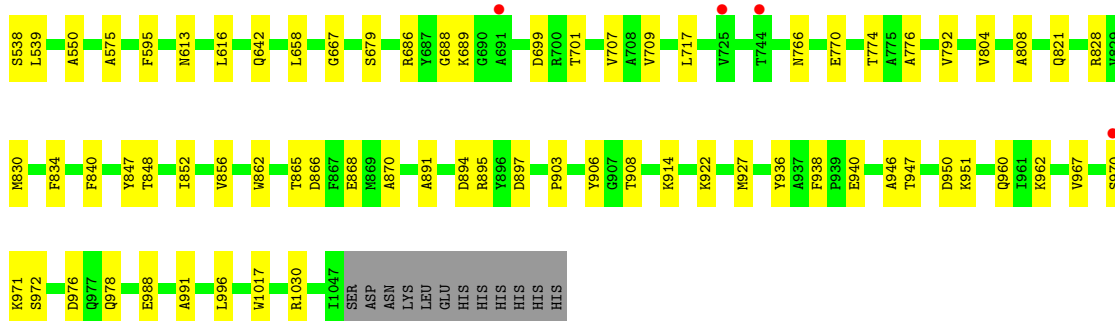


- Molecule 1: Glucosyltransferase-I

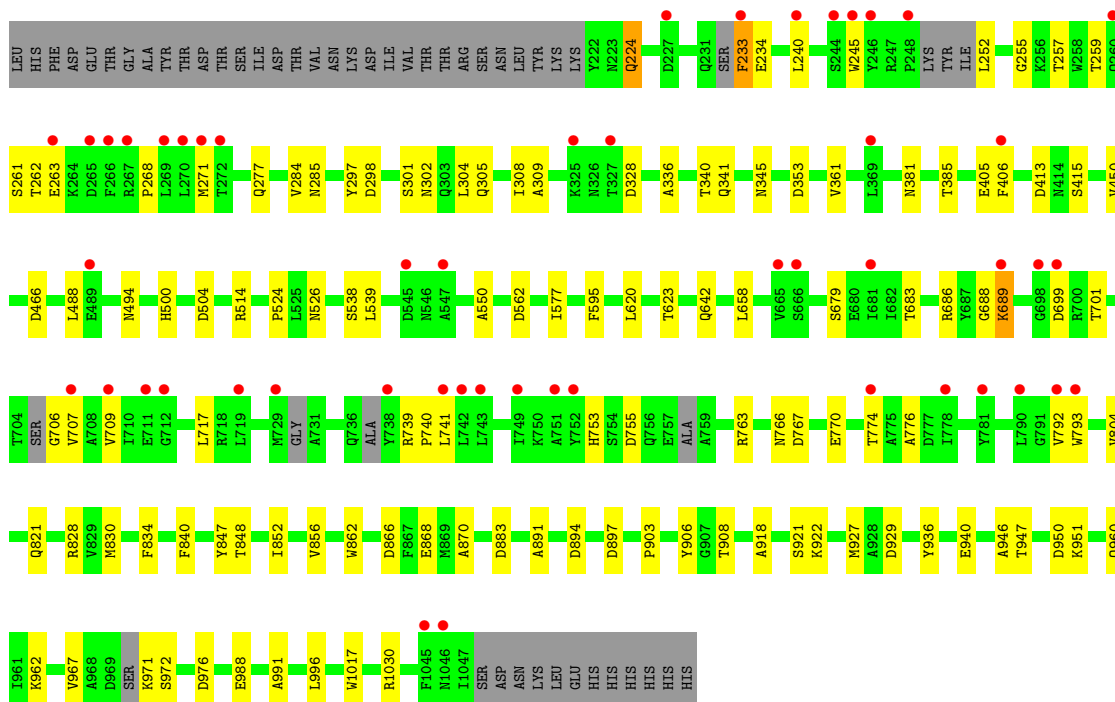
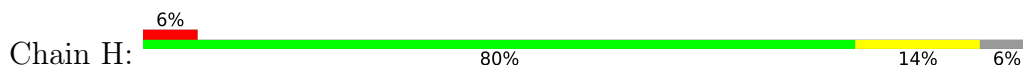


- Molecule 1: Glucosyltransferase-I





- Molecule 1: Glucosyltransferase-I



- Molecule 2: 4,6-dideoxy-4-{\{(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl\}amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: 4,6-dideoxy-4-{\{(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl\}amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain K:  67% 33%


GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain L:  100%

GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain M:  33% 67%

GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain N:  33% 67%

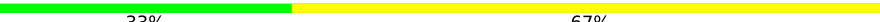
GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain O:  33% 67%

GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain P:  33% 67%

GLC1  
GLC2  
AC13

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	299.31Å 215.77Å 219.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 3.25 49.44 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.88-3.25) 99.9 (49.44-3.25)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.224 , 0.255 0.225 , 0.256	Depositor DCC
$R_{free}$ test set	11053 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.3	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.001 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	52614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.11 % 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 2.8710e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4, GLC, AC1

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	0.24	0/6658	0.43	0/9035
1	B	0.25	0/6573	0.44	1/8921 (0.0%)
1	C	0.25	0/6667	0.44	1/9046 (0.0%)
1	D	0.25	0/6664	0.43	0/9039
1	E	0.25	0/6687	0.44	0/9074
1	F	0.25	0/6649	0.44	0/9021
1	G	0.25	0/6674	0.44	0/9056
1	H	0.26	0/6554	0.46	0/8884
All	All	0.25	0/53126	0.44	2/72076 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	527	GLN	N-CA-CB	-5.79	100.17	110.60
1	B	527	GLN	N-CA-CB	-5.15	101.33	110.60

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	6521	0	6346	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6440	0	6230	59	1
1	C	6530	0	6359	66	0
1	D	6529	0	6330	83	0
1	E	6548	0	6373	62	0
1	F	6513	0	6339	52	0
1	G	6536	0	6364	74	0
1	H	6427	0	6221	76	1
2	I	44	0	30	0	0
2	J	44	0	30	0	0
2	K	44	0	30	1	0
2	L	44	0	30	0	0
2	M	44	0	30	1	0
2	N	44	0	30	1	0
2	O	44	0	30	0	0
2	P	44	0	30	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	30	0	0	4	0
4	B	35	0	0	0	0
4	C	25	0	0	0	0
4	D	25	0	0	1	0
4	E	35	0	0	1	0
4	F	30	0	0	2	0
4	G	20	0	0	2	0
4	H	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
All	All	52614	0	50802	520	1

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.

The worst 5 of 520 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:E:332:GLN:NE2	1:G:320:LYS:NZ	2.13	0.96
1:D:422:GLU:HG3	1:D:895:ARG:HH12	1.31	0.94
1:D:871:PRO:HD3	1:D:929:ASP:OD2	1.73	0.88
1:A:871:PRO:HD3	1:A:929:ASP:OD2	1.74	0.87
1:B:871:PRO:HD3	1:B:929:ASP:OD2	1.74	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:OG1	1:H:960:GLN:NE2[2_555]	2.16	0.04

### 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	825/869 (95%)	766 (93%)	57 (7%)	2 (0%)	47	77
1	B	815/869 (94%)	756 (93%)	55 (7%)	4 (0%)	29	62
1	C	826/869 (95%)	766 (93%)	57 (7%)	3 (0%)	34	67
1	D	822/869 (95%)	765 (93%)	53 (6%)	4 (0%)	29	62
1	E	827/869 (95%)	770 (93%)	55 (7%)	2 (0%)	47	77
1	F	822/869 (95%)	766 (93%)	54 (7%)	2 (0%)	47	77
1	G	826/869 (95%)	769 (93%)	56 (7%)	1 (0%)	51	82
1	H	801/869 (92%)	745 (93%)	50 (6%)	6 (1%)	22	56
All	All	6564/6952 (94%)	6103 (93%)	437 (7%)	24 (0%)	34	67

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	SER

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Mol	Chain	Res	Type
1	C	276	SER
1	D	276	SER
1	D	302	ASN
1	E	276	SER

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	697/738 (94%)	696 (100%)	1 (0%)	93	97
1	B	685/738 (93%)	685 (100%)	0	100	100
1	C	698/738 (95%)	695 (100%)	3 (0%)	91	94
1	D	696/738 (94%)	693 (100%)	3 (0%)	91	94
1	E	700/738 (95%)	697 (100%)	3 (0%)	91	94
1	F	696/738 (94%)	695 (100%)	1 (0%)	93	97
1	G	699/738 (95%)	697 (100%)	2 (0%)	92	96
1	H	683/738 (92%)	676 (99%)	7 (1%)	76	85
All	All	5554/5904 (94%)	5534 (100%)	20 (0%)	91	94

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	233	PHE
1	H	767	ASP
1	H	929	ASP
1	H	847	TYR
1	D	847	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	290	GLN

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Mol	Chain	Res	Type
1	H	302	ASN
1	H	305	GLN
1	E	332	GLN
1	E	290	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLC	I	1	2	12,12,12	0.17	0	17,17,17	0.54	0
2	GLC	I	2	2	11,11,12	0.34	0	15,15,17	0.93	2 (13%)
2	AC1	I	3	2	21,22,23	0.28	0	22,32,34	0.53	0
2	GLC	J	1	2	12,12,12	0.28	0	17,17,17	0.82	1 (5%)
2	GLC	J	2	2	11,11,12	0.36	0	15,15,17	0.80	1 (6%)
2	AC1	J	3	2	21,22,23	0.31	0	22,32,34	1.11	2 (9%)
2	GLC	K	1	2	12,12,12	0.21	0	17,17,17	0.58	0
2	GLC	K	2	2	11,11,12	0.36	0	15,15,17	0.58	0
2	AC1	K	3	2	21,22,23	0.33	0	22,32,34	0.80	2 (9%)
2	GLC	L	1	2	12,12,12	0.20	0	17,17,17	0.29	0
2	GLC	L	2	2	11,11,12	0.43	0	15,15,17	0.45	0
2	AC1	L	3	2	21,22,23	0.28	0	22,32,34	0.59	0
2	GLC	M	1	2	12,12,12	0.18	0	17,17,17	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	M	2	2	11,11,12	0.40	0	15,15,17	0.69	1 (6%)
2	AC1	M	3	2	21,22,23	0.33	0	22,32,34	0.65	0
2	GLC	N	1	2	12,12,12	0.26	0	17,17,17	0.63	1 (5%)
2	GLC	N	2	2	11,11,12	0.41	0	15,15,17	0.45	0
2	AC1	N	3	2	21,22,23	0.28	0	22,32,34	0.51	0
2	GLC	O	1	2	12,12,12	0.16	0	17,17,17	0.63	1 (5%)
2	GLC	O	2	2	11,11,12	0.32	0	15,15,17	1.16	2 (13%)
2	AC1	O	3	2	21,22,23	0.28	0	22,32,34	0.56	0
2	GLC	P	1	2	12,12,12	0.23	0	17,17,17	0.37	0
2	GLC	P	2	2	11,11,12	0.43	0	15,15,17	0.77	0
2	AC1	P	3	2	21,22,23	0.31	0	22,32,34	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	1	2	-	1/2/22/22	0/1/1/1
2	GLC	I	2	2	-	1/2/19/22	0/1/1/1
2	AC1	I	3	2	-	4/6/43/46	0/2/2/2
2	GLC	J	1	2	-	2/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	AC1	J	3	2	-	3/6/43/46	0/2/2/2
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	1/2/19/22	0/1/1/1
2	AC1	K	3	2	-	3/6/43/46	0/2/2/2
2	GLC	L	1	2	-	0/2/22/22	0/1/1/1
2	GLC	L	2	2	-	1/2/19/22	0/1/1/1
2	AC1	L	3	2	-	1/6/43/46	0/2/2/2
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	1/2/19/22	0/1/1/1
2	AC1	M	3	2	-	2/6/43/46	0/2/2/2
2	GLC	N	1	2	-	0/2/22/22	0/1/1/1
2	GLC	N	2	2	-	0/2/19/22	0/1/1/1
2	AC1	N	3	2	-	4/6/43/46	0/2/2/2
2	GLC	O	1	2	-	1/2/22/22	0/1/1/1
2	GLC	O	2	2	-	1/2/19/22	0/1/1/1
2	AC1	O	3	2	-	3/6/43/46	0/2/2/2
2	GLC	P	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	P	2	2	-	0/2/19/22	0/1/1/1
2	AC1	P	3	2	-	3/6/43/46	0/2/2/2

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	3	AC1	C7B-C1B-N4A	3.57	116.04	110.68
2	O	2	GLC	C1-O5-C5	3.06	116.34	112.19
2	O	2	GLC	O4-C4-C3	-2.76	103.97	110.35
2	J	1	GLC	O4-C4-C3	2.61	116.38	110.35
2	O	1	GLC	O4-C4-C3	-2.43	104.74	110.35

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

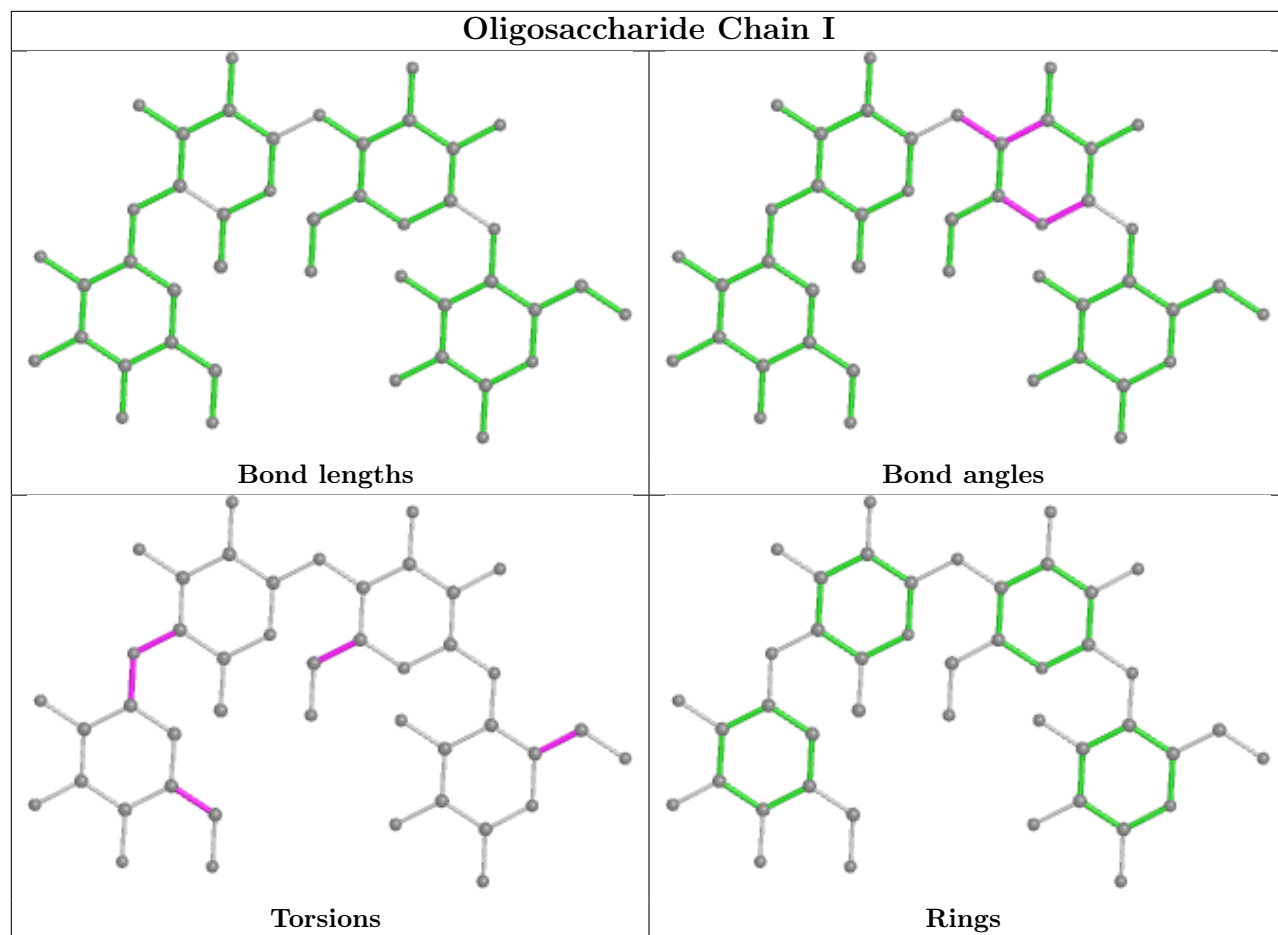
Mol	Chain	Res	Type	Atoms
2	I	3	AC1	C7B-C1B-N4A-C4
2	I	3	AC1	C7B-C5B-C6B-O6B
2	J	3	AC1	C7B-C1B-N4A-C4
2	J	3	AC1	C4A-C5B-C6B-O6B
2	J	3	AC1	C7B-C5B-C6B-O6B

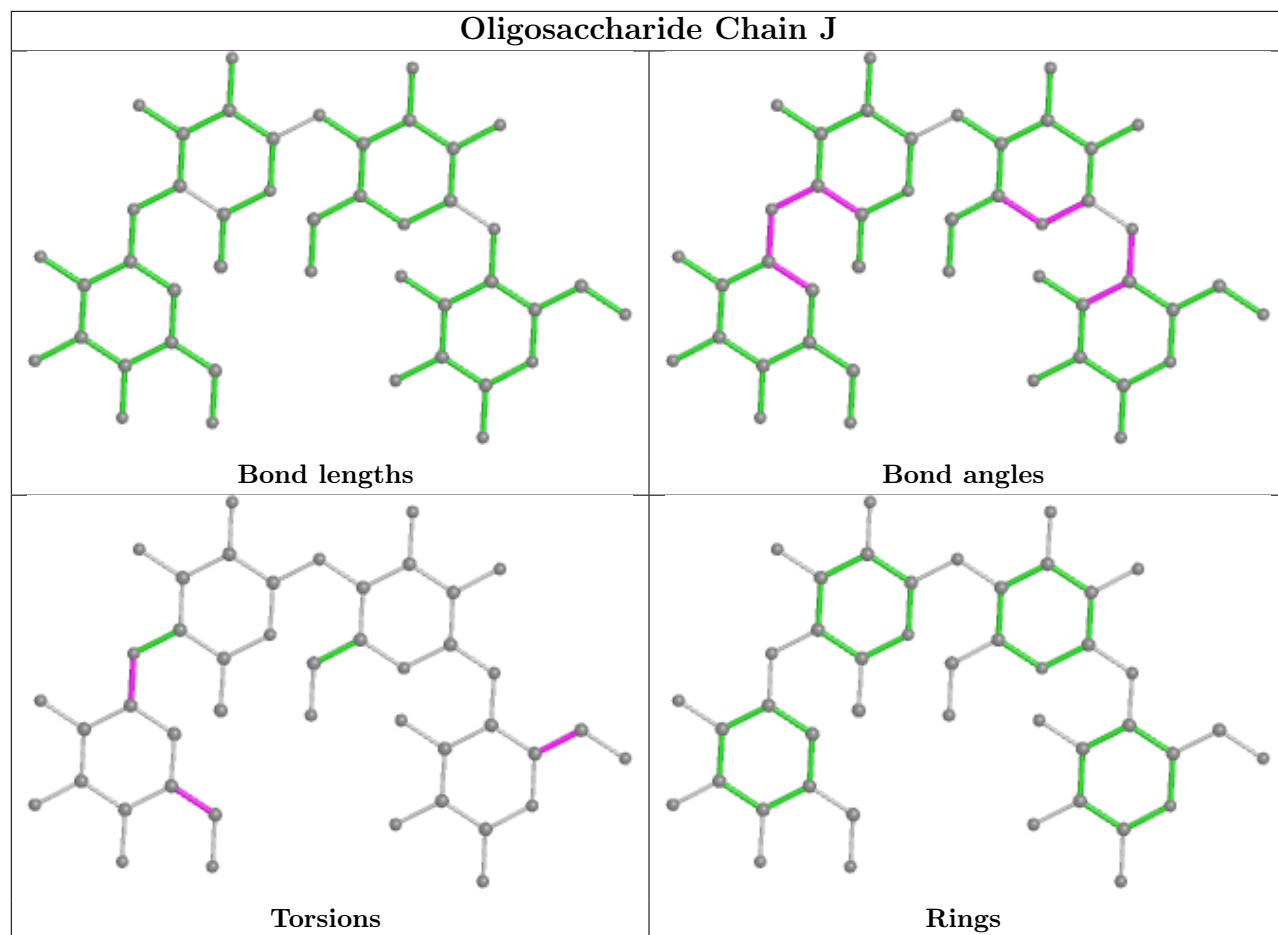
There are no ring outliers.

5 monomers are involved in 6 short contacts:

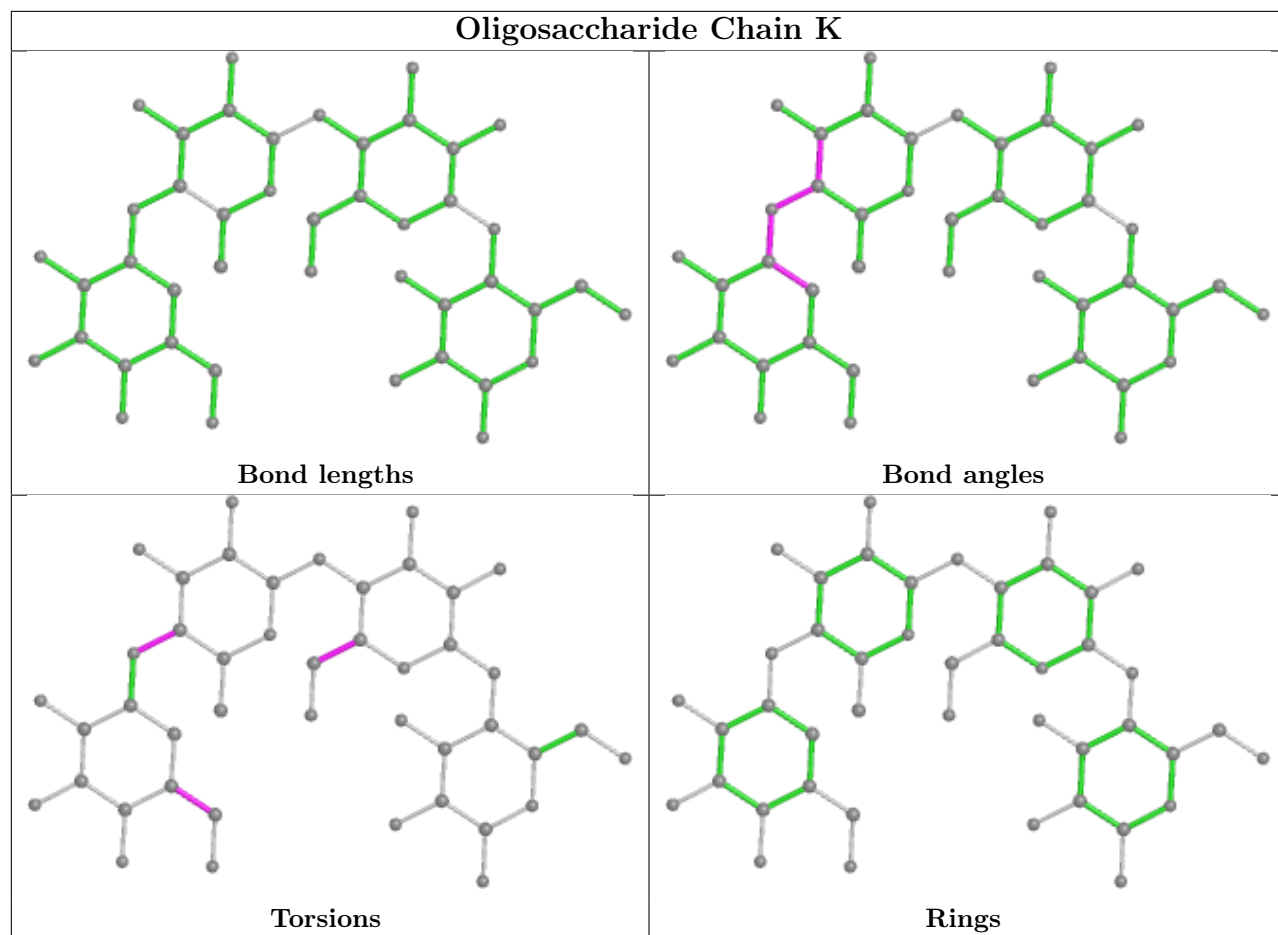
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	GLC	1	0
2	M	1	GLC	1	0
2	P	3	AC1	2	0
2	N	3	AC1	1	0
2	K	3	AC1	1	0

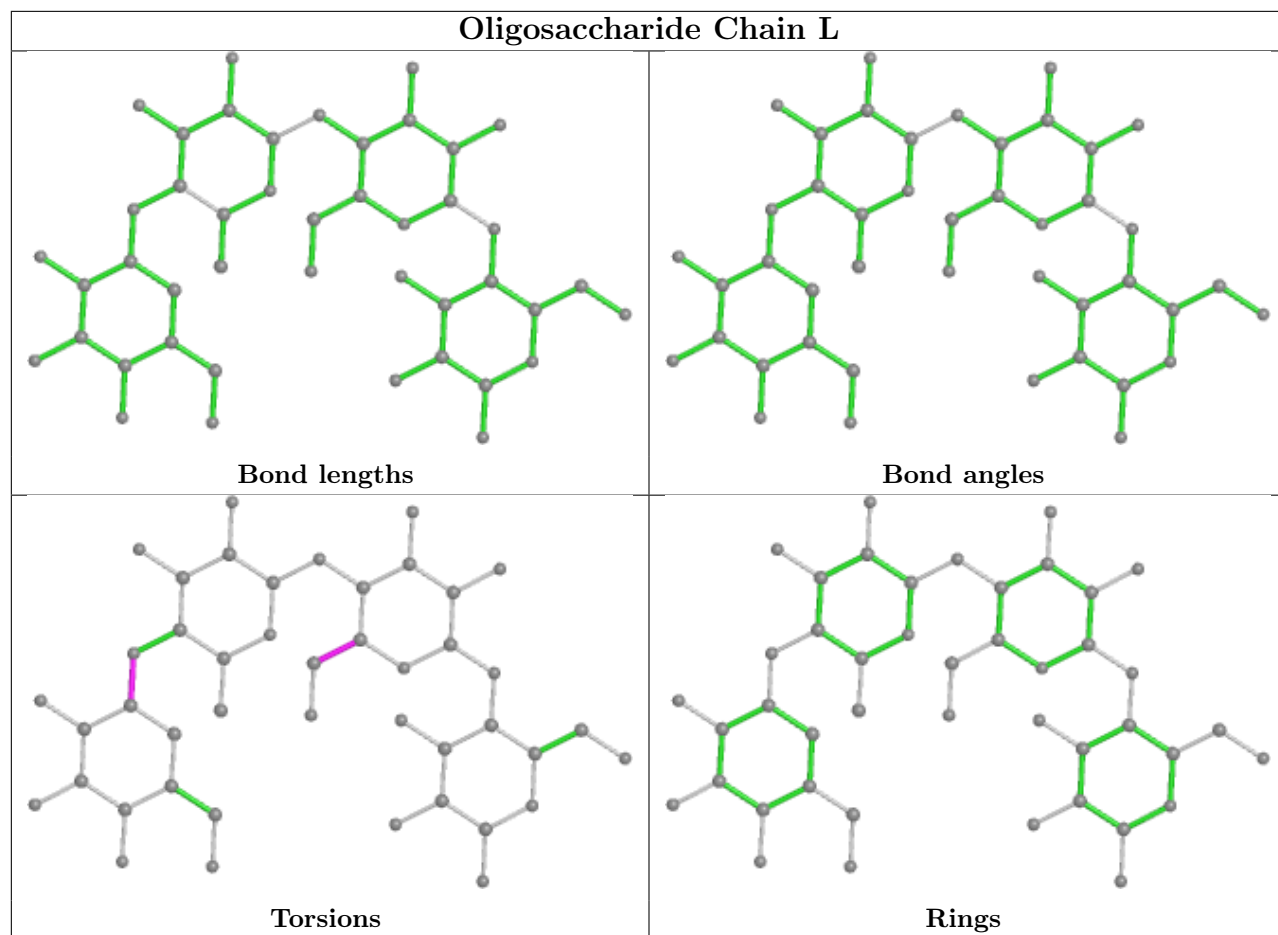
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

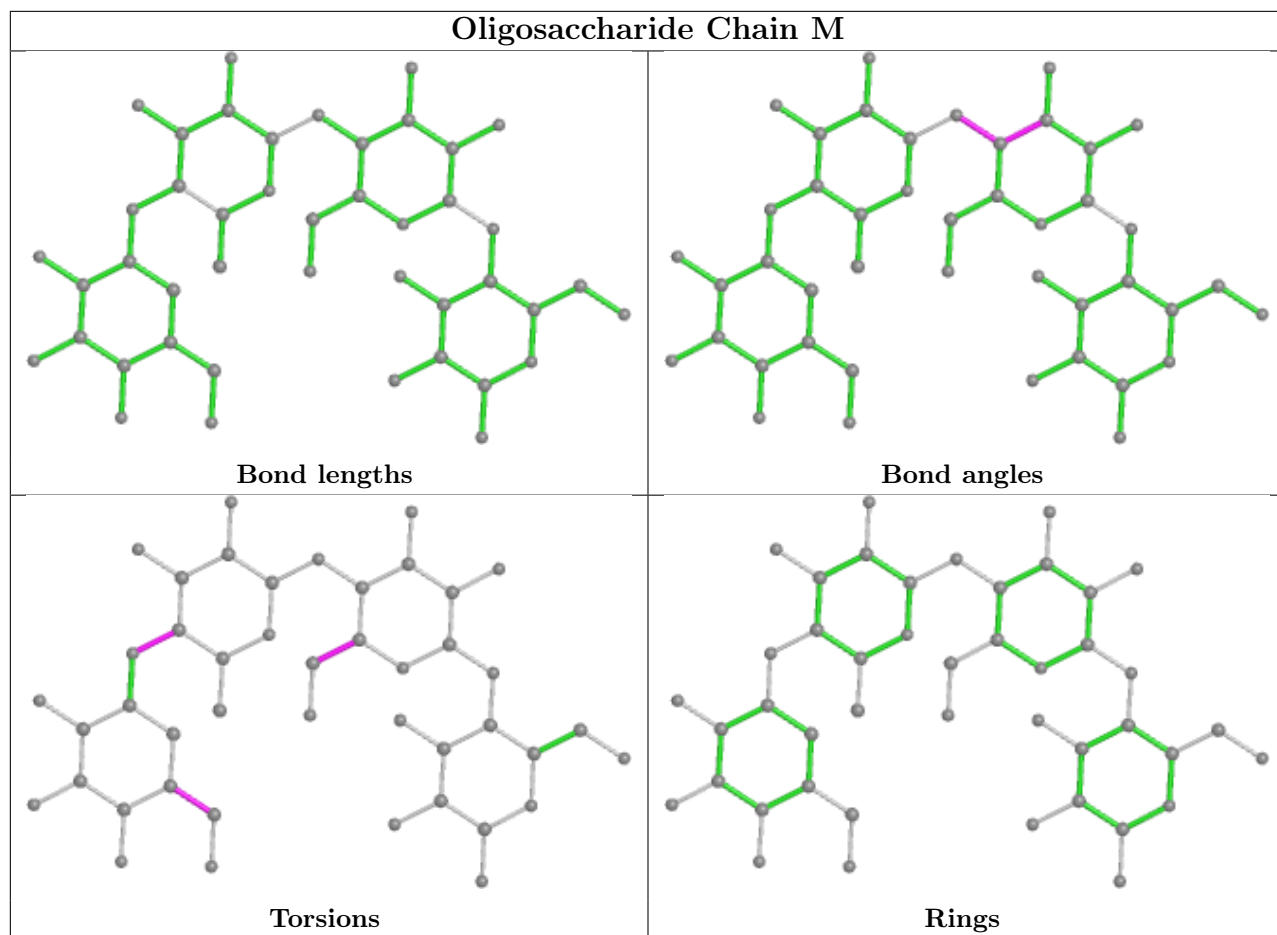


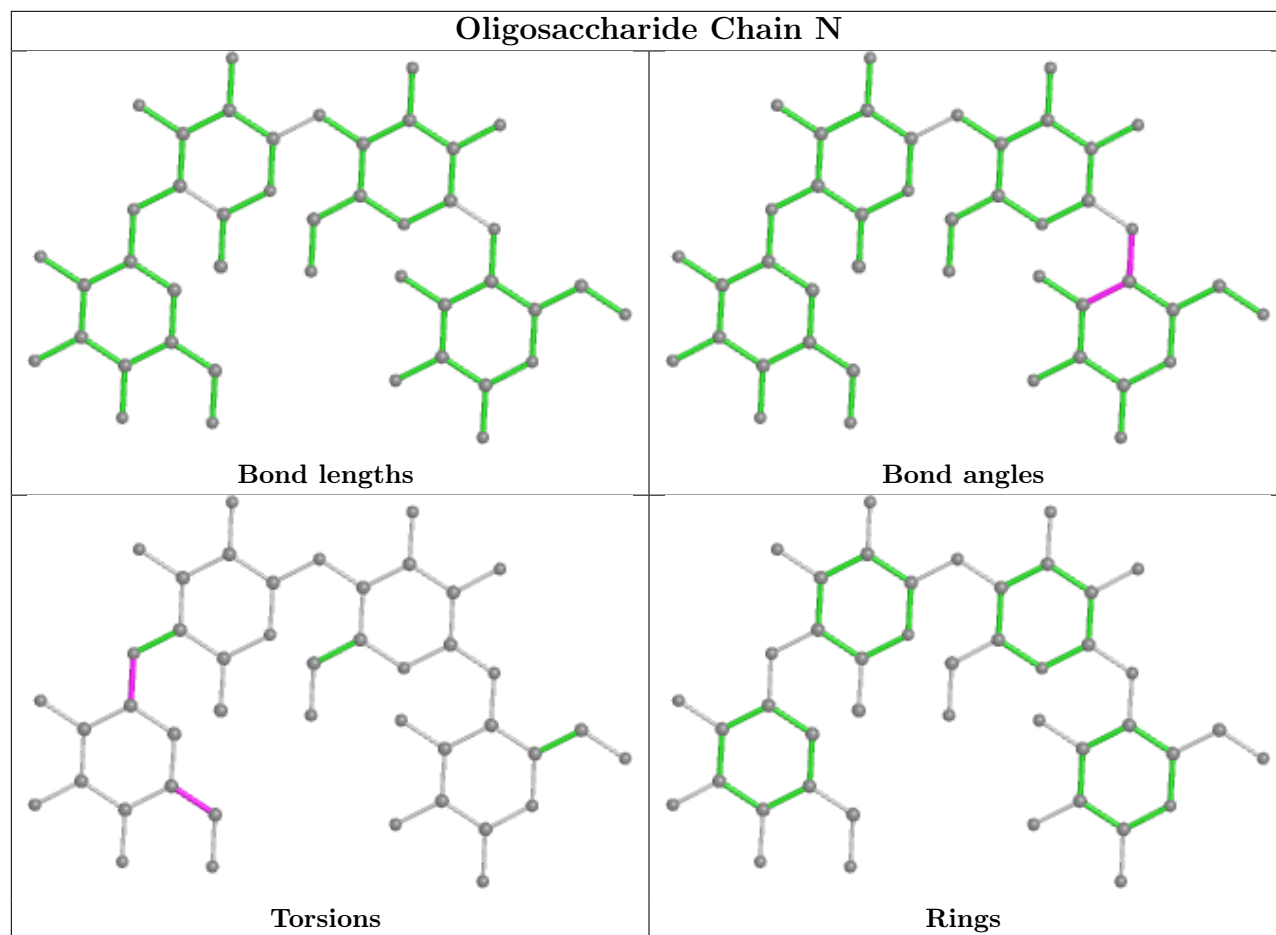


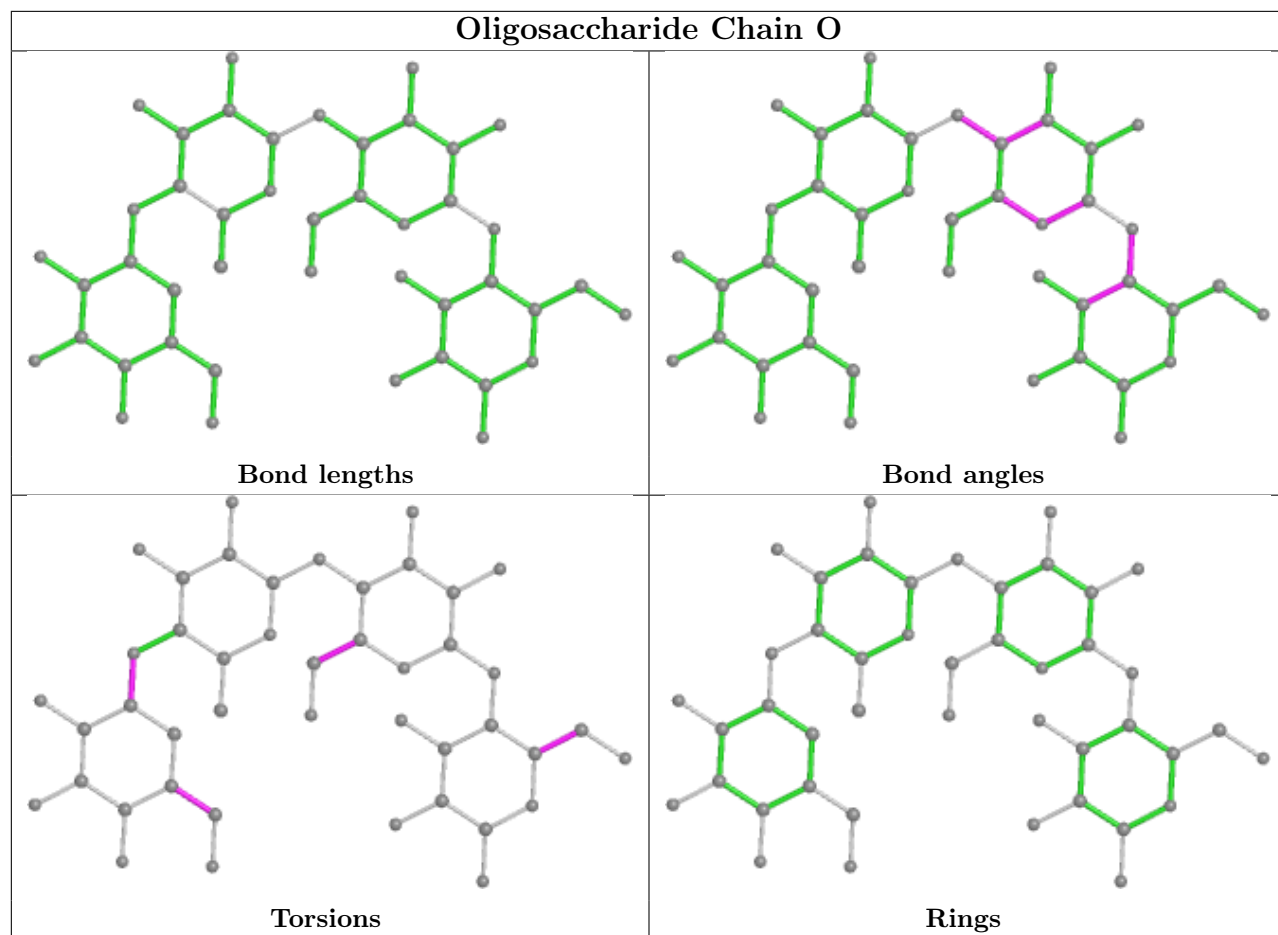


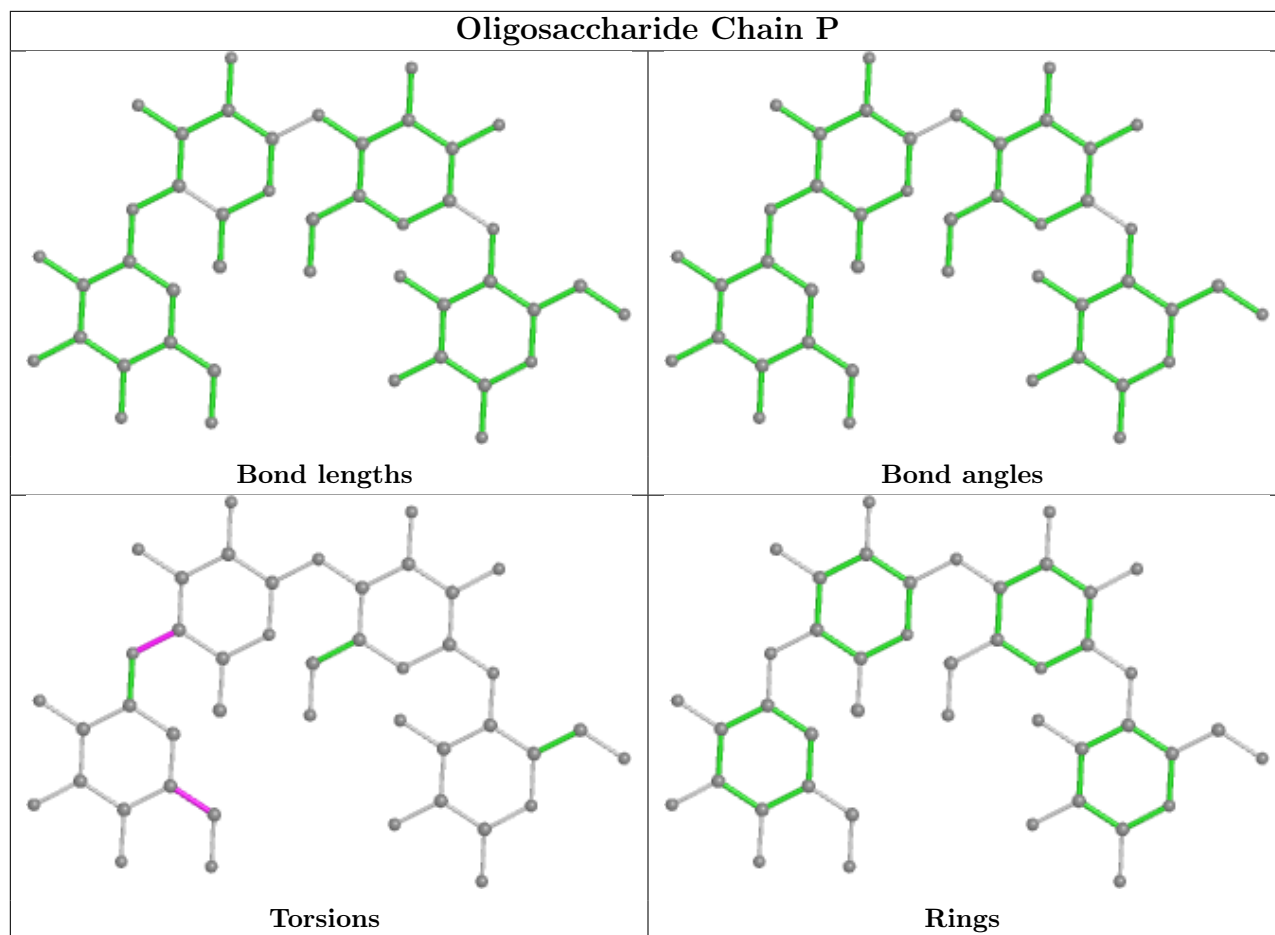












## 5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 8 are monoatomic - leaving 41 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	$\# Z  > 2$
4	SO4	G	1203	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	C	1206	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	E	1208	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	1206	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	F	1207	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	D	1202	-	4,4,4	0.15	0	6,6,6	0.04	0
4	SO4	F	1202	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	C	1202	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	A	1203	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	E	1203	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	1206	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	1204	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	F	1204	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	1203	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	B	1205	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	D	1206	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	F	1203	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	G	1205	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	1205	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	F	1206	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	E	1204	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	1204	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	E	1207	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	1203	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	E	1202	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	D	1205	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	H	1202	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	D	1203	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	G	1204	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	E	1206	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	F	1205	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	C	1205	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	1207	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	1202	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	1207	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	E	1205	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	1208	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	B	1204	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	G	1202	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	1202	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	1204	-	4,4,4	0.14	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

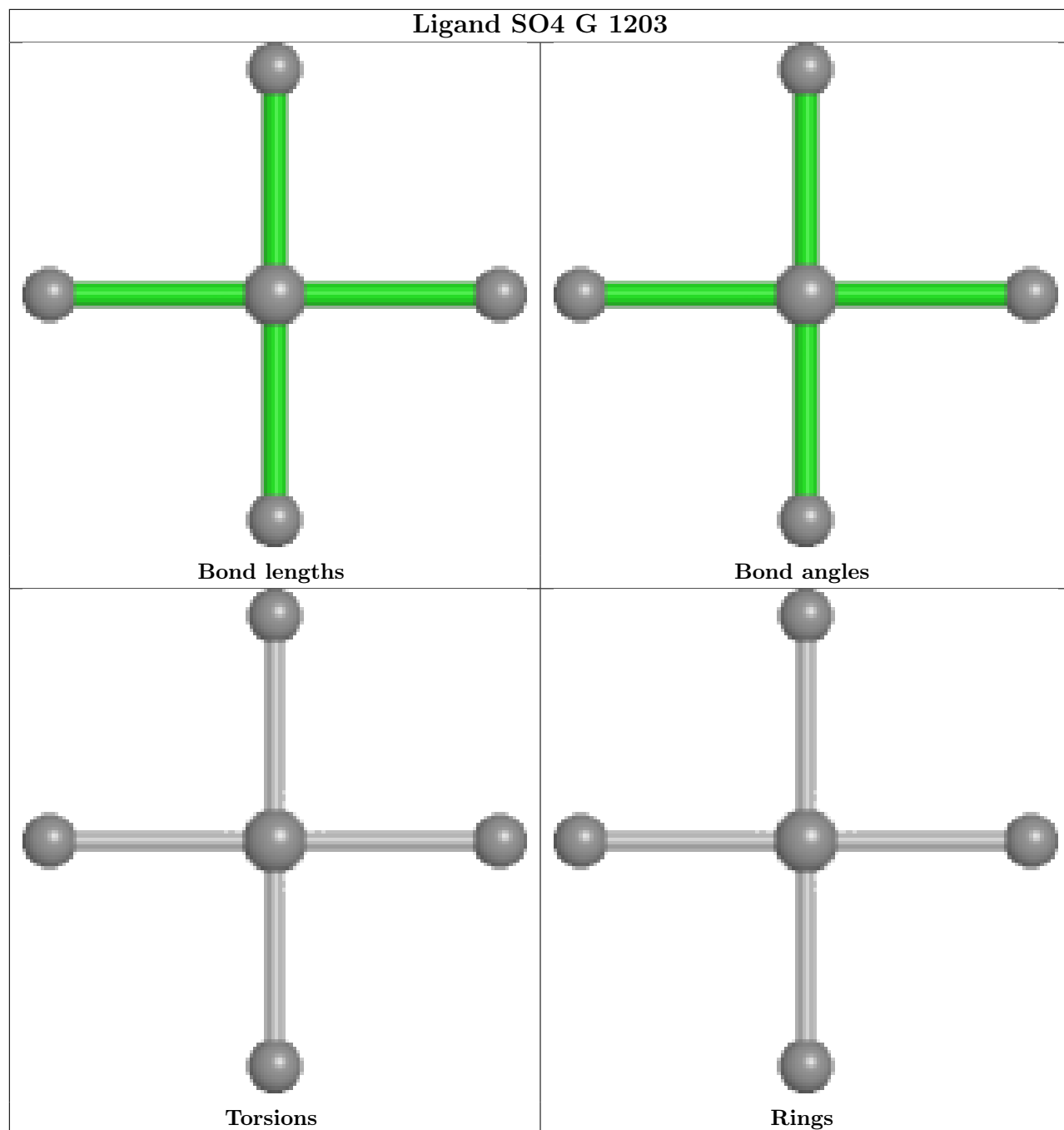
There are no ring outliers.

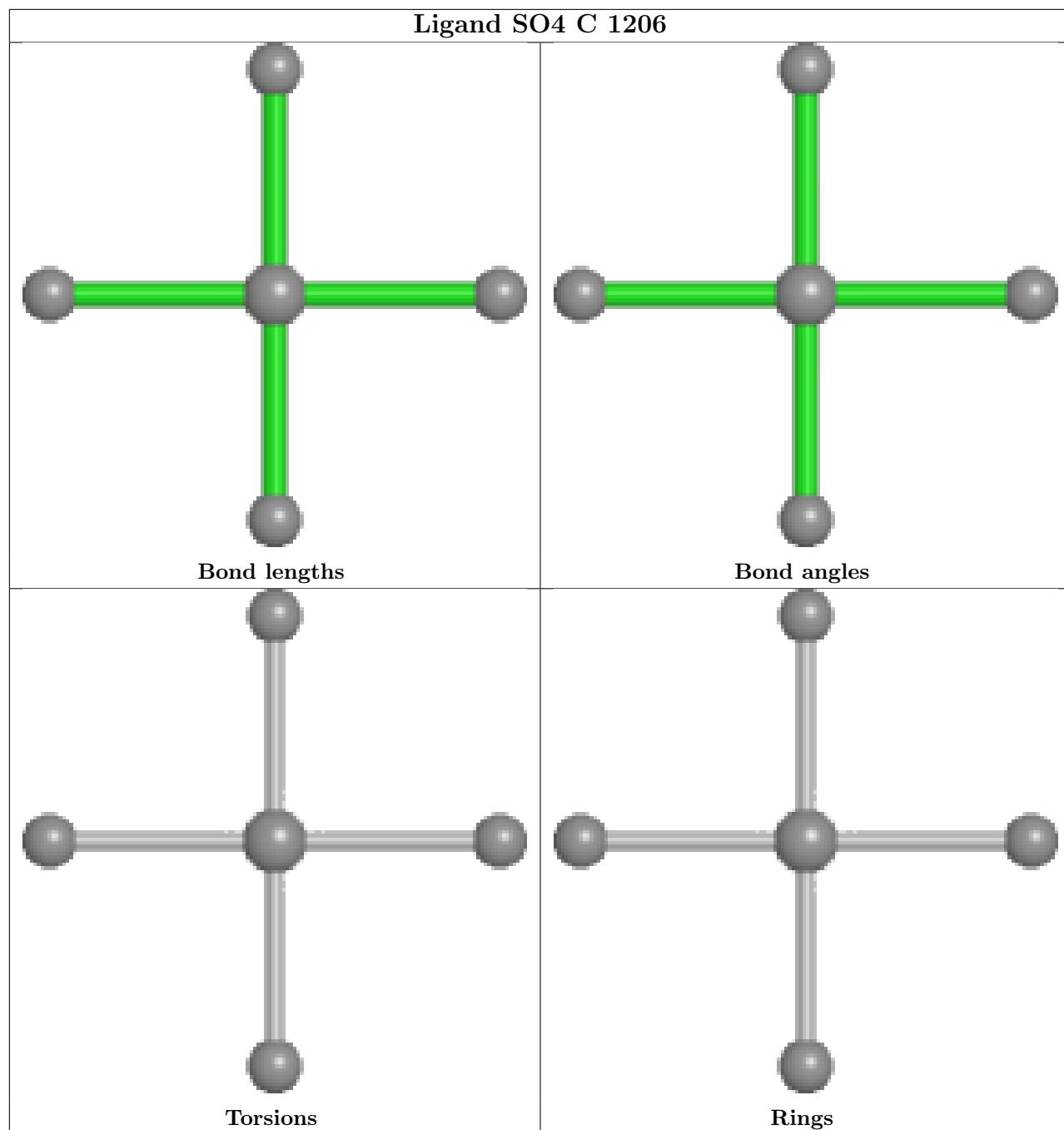
8 monomers are involved in 10 short contacts:

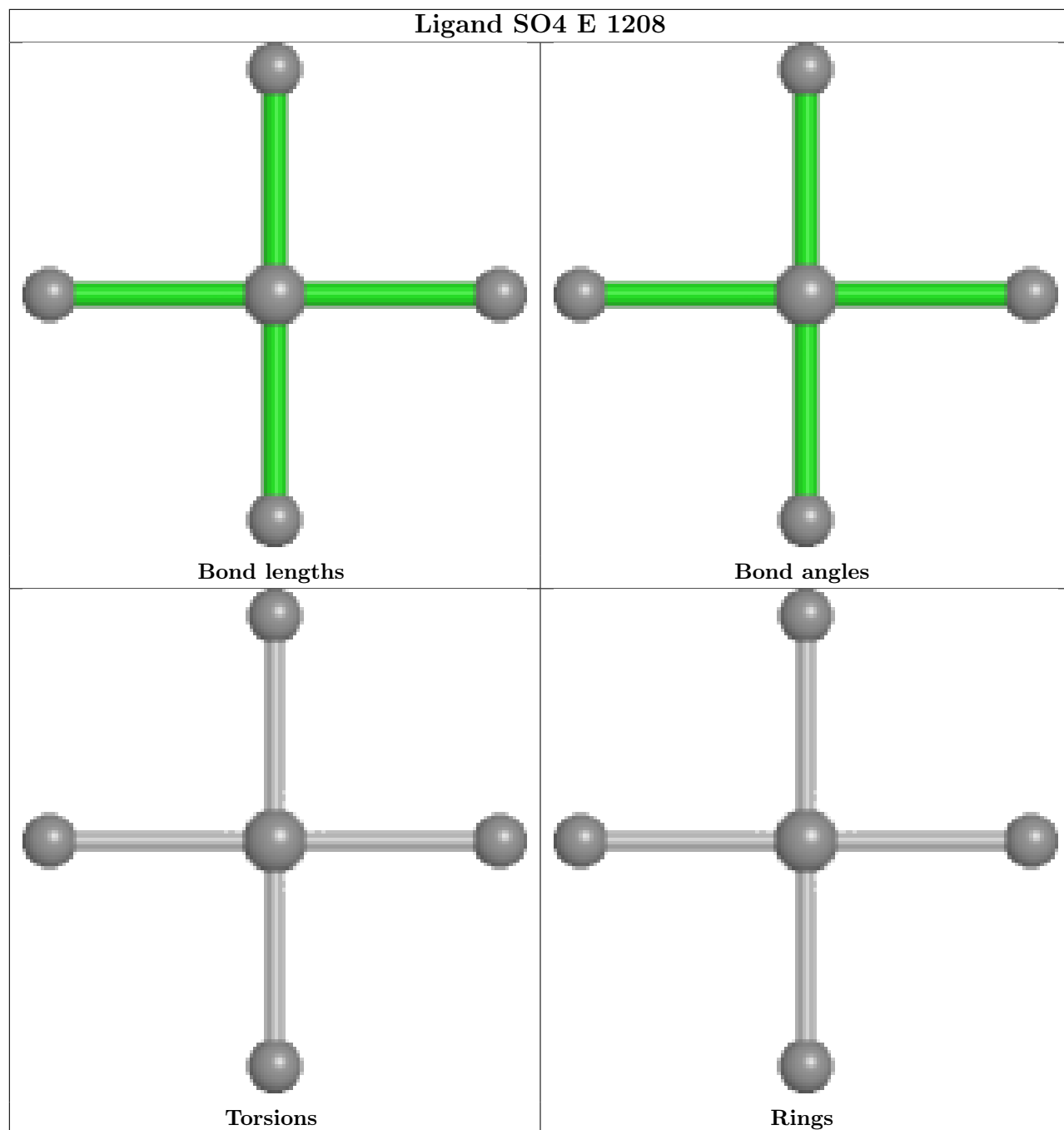
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1207	SO4	1	0
4	A	1203	SO4	1	0
4	D	1206	SO4	1	0
4	E	1207	SO4	1	0
4	G	1204	SO4	2	0
4	F	1205	SO4	1	0
4	A	1207	SO4	2	0
4	A	1204	SO4	1	0

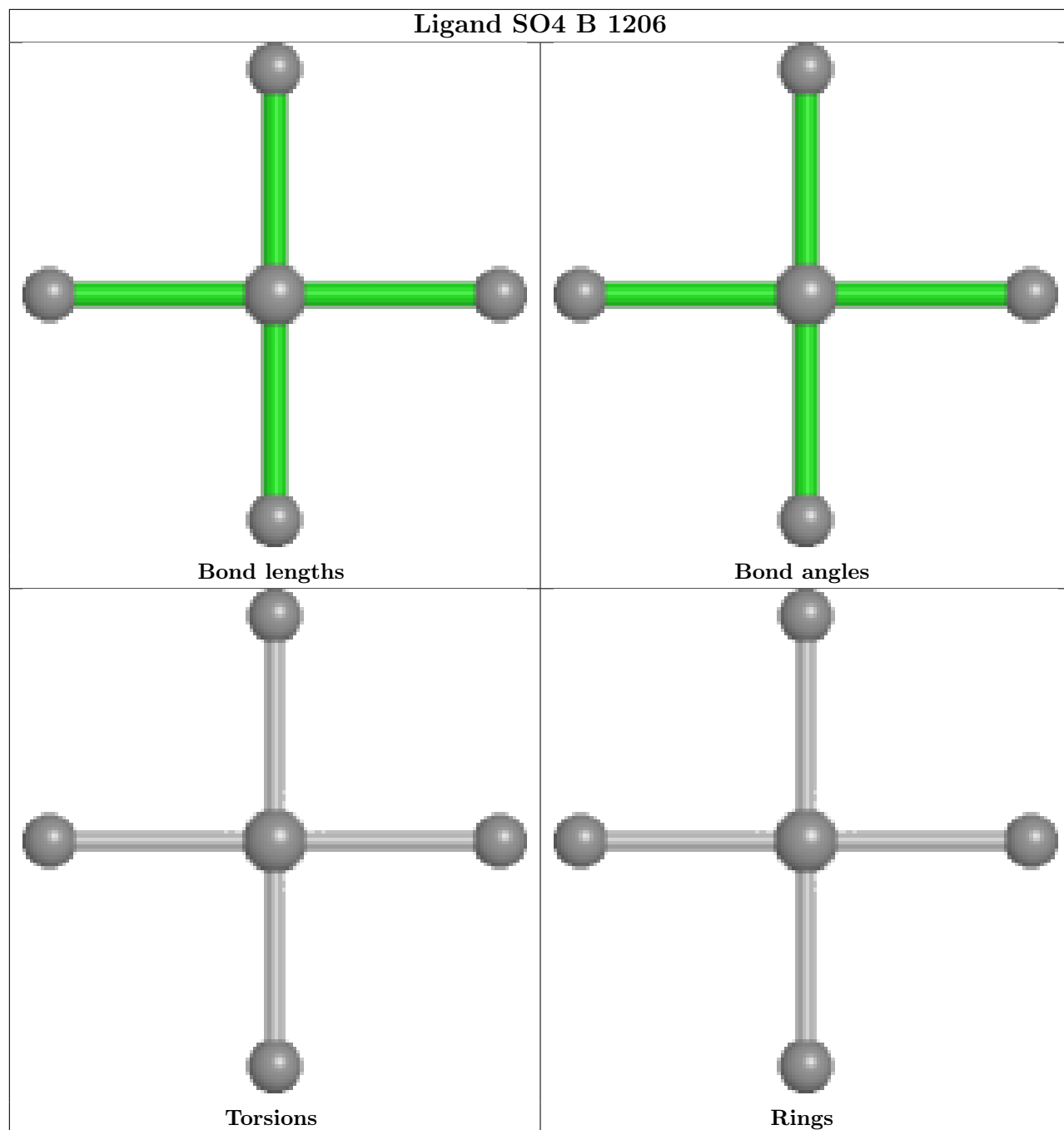
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

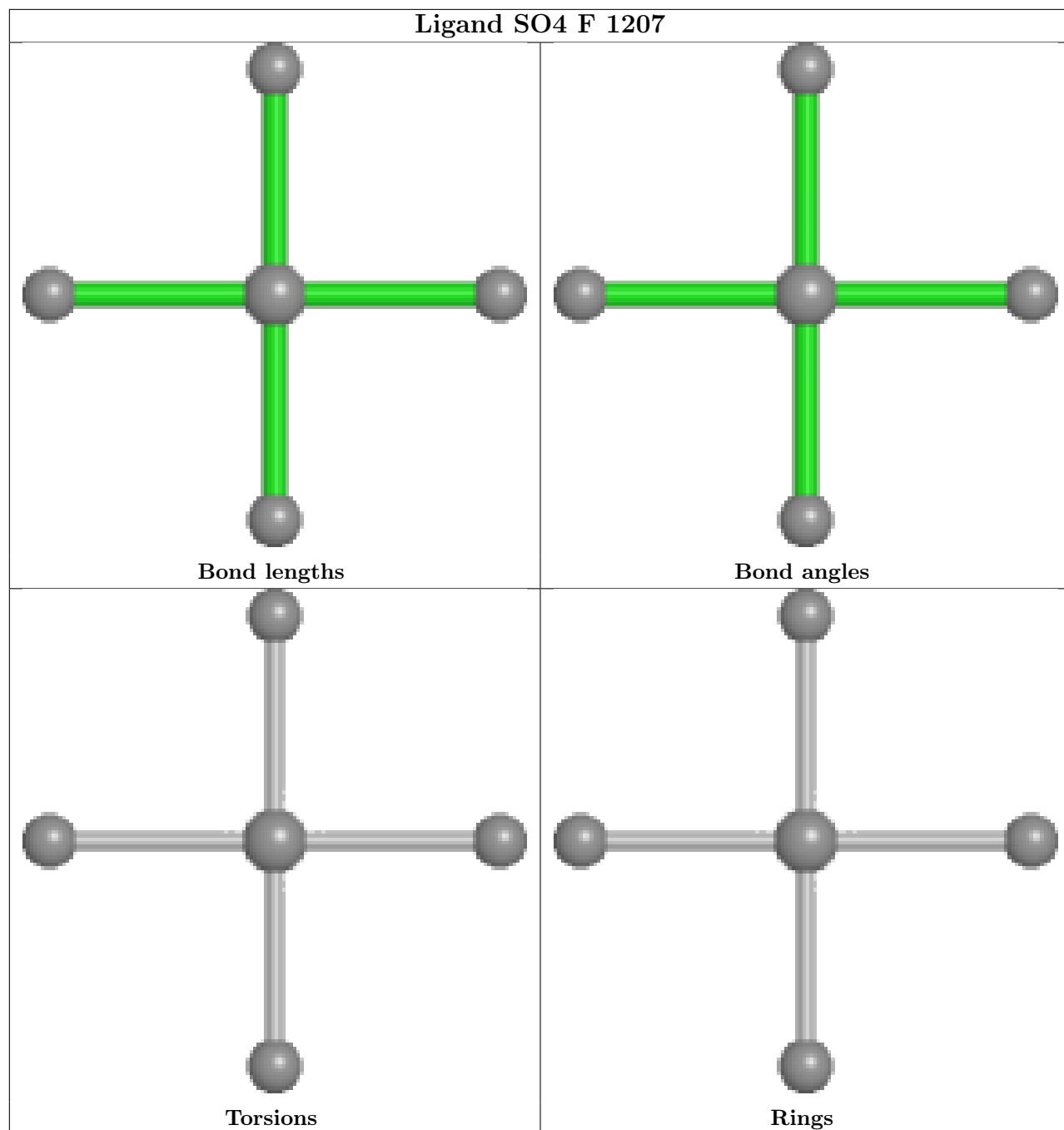


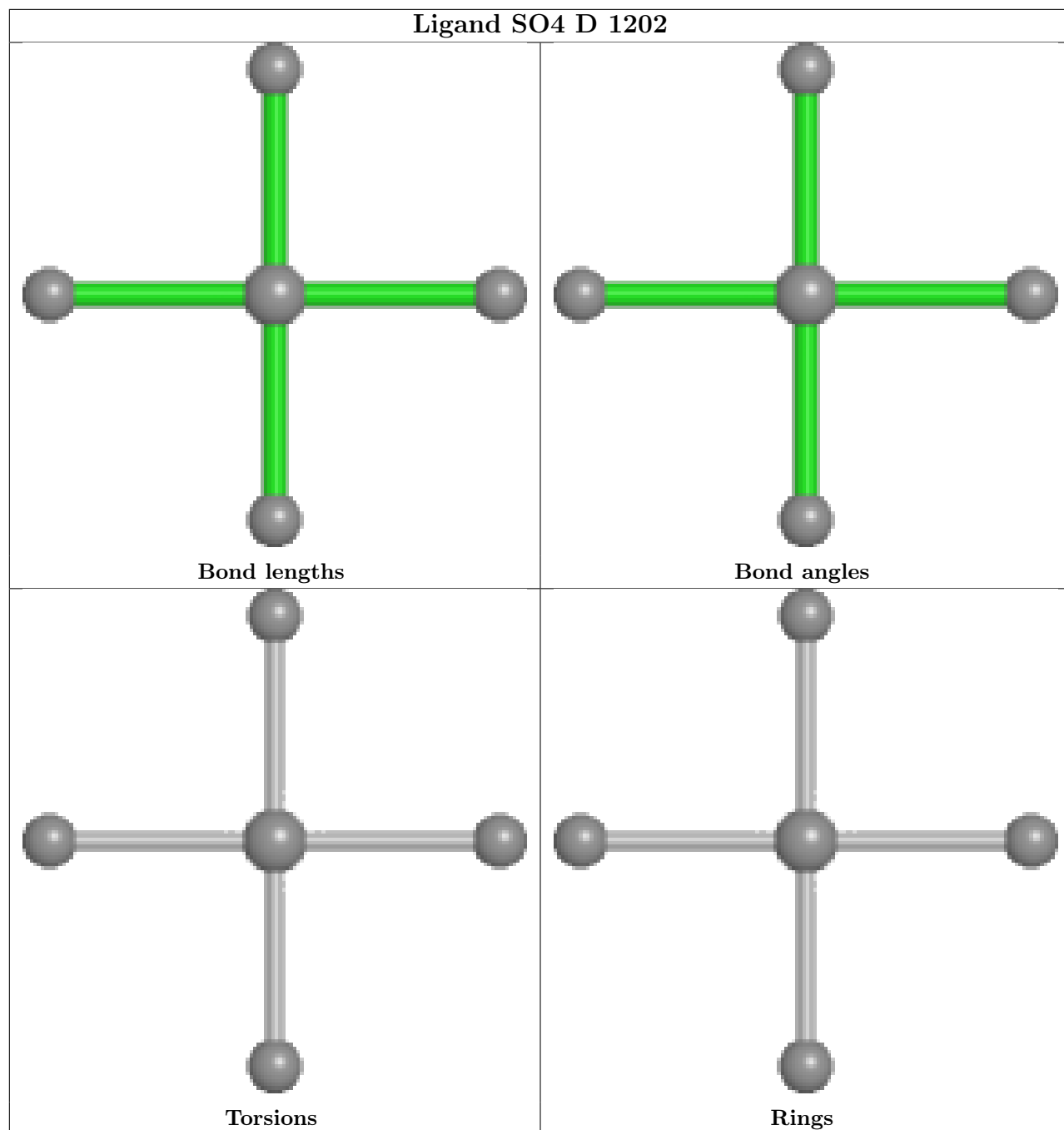


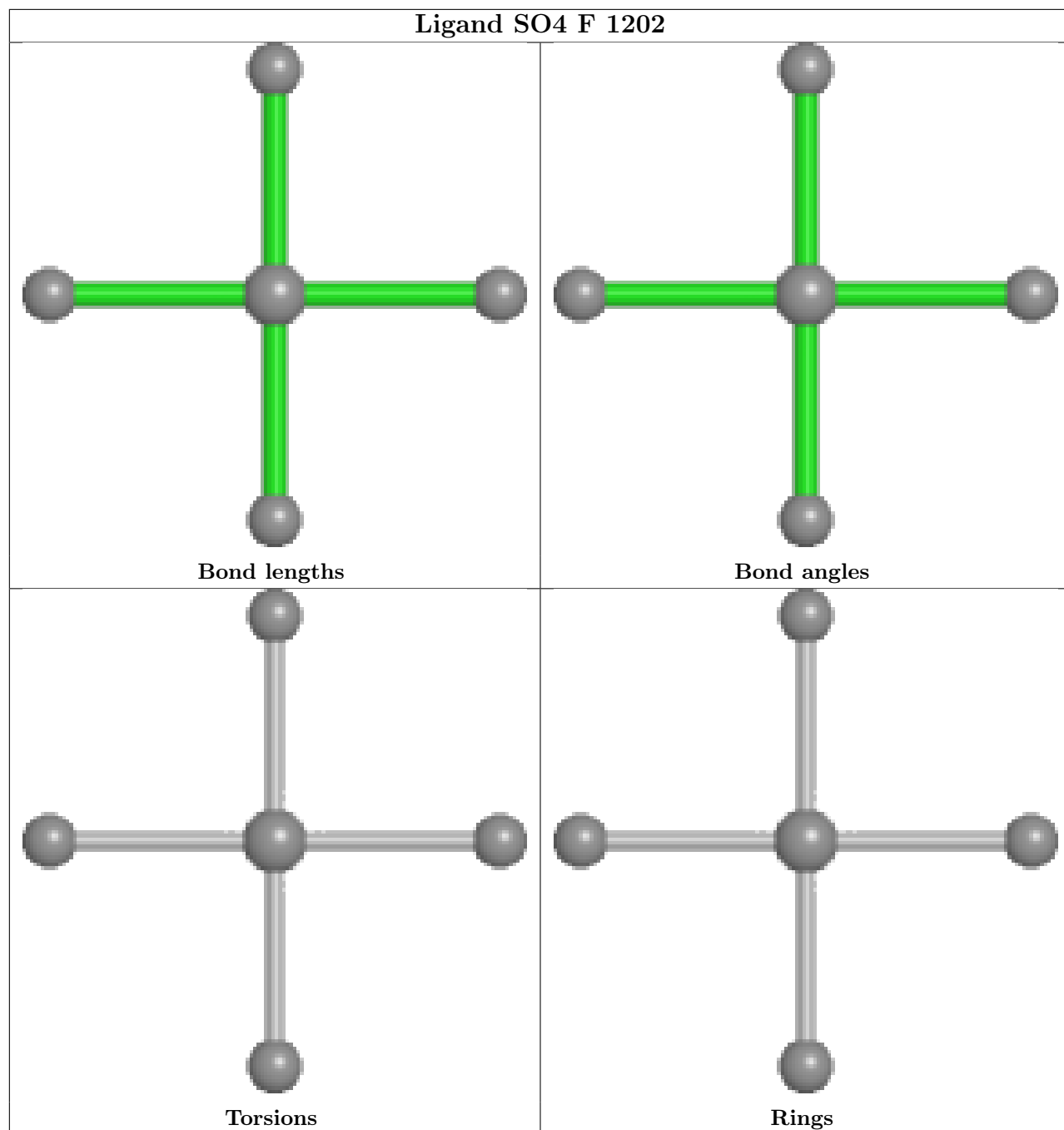


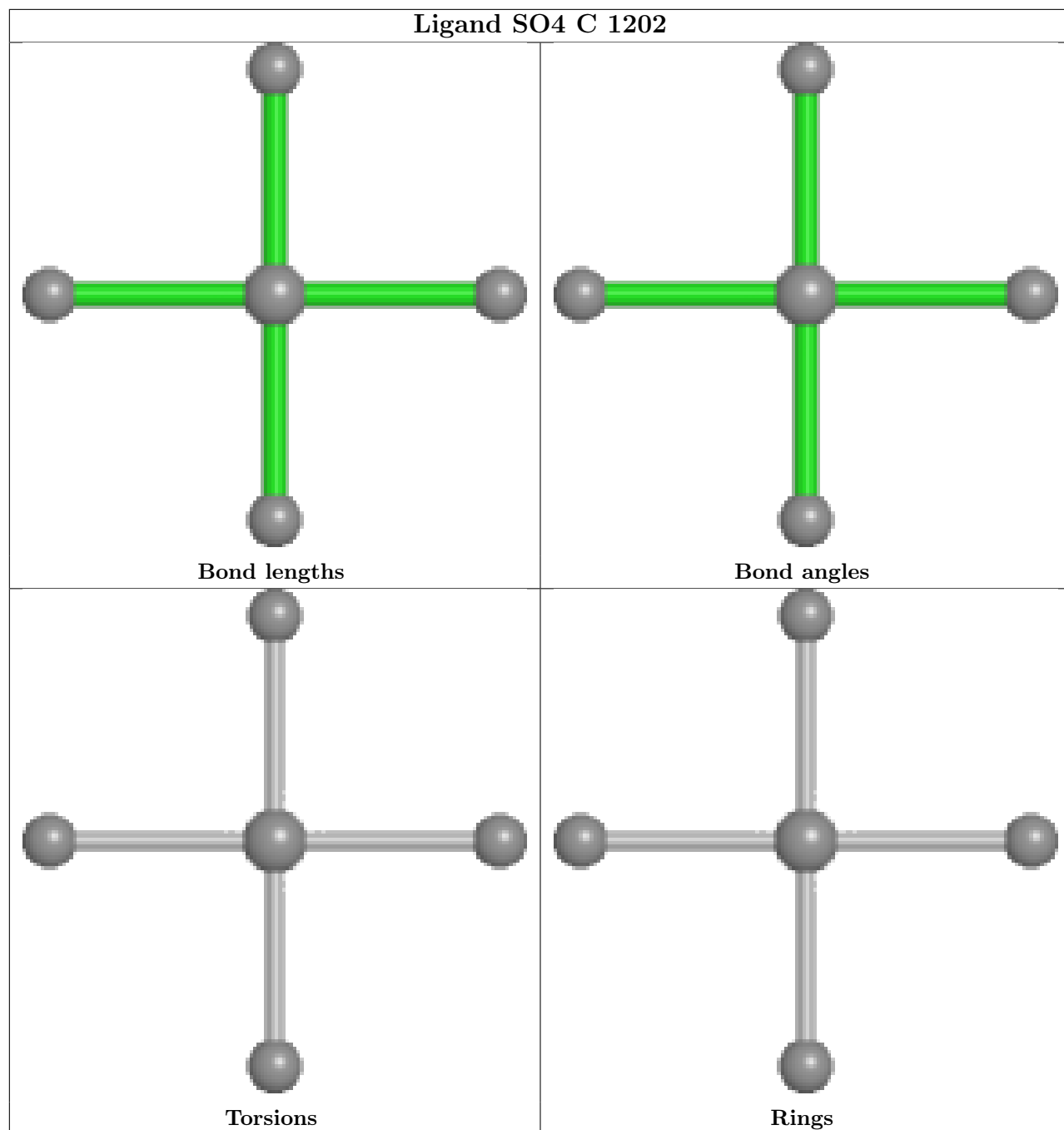




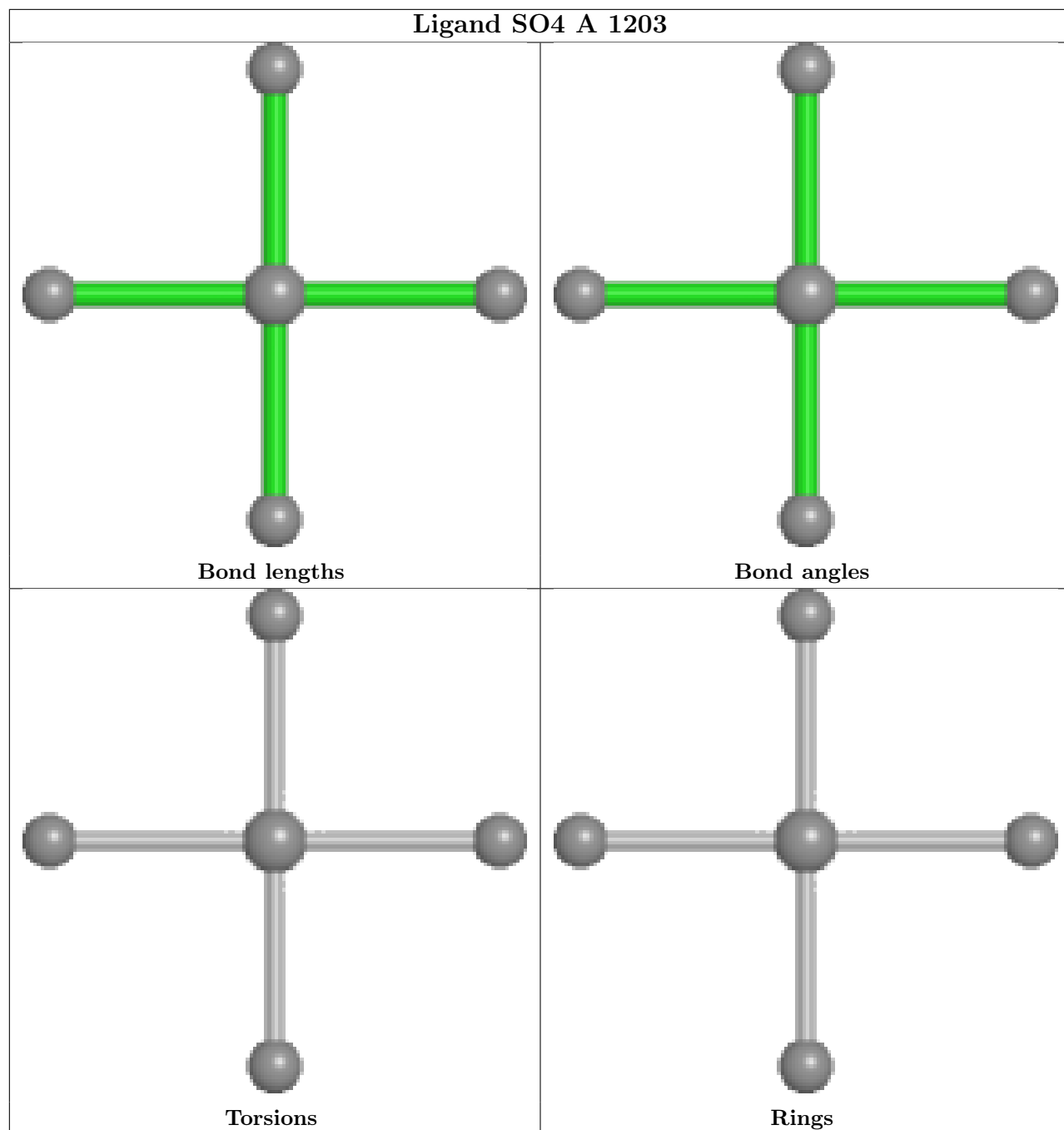


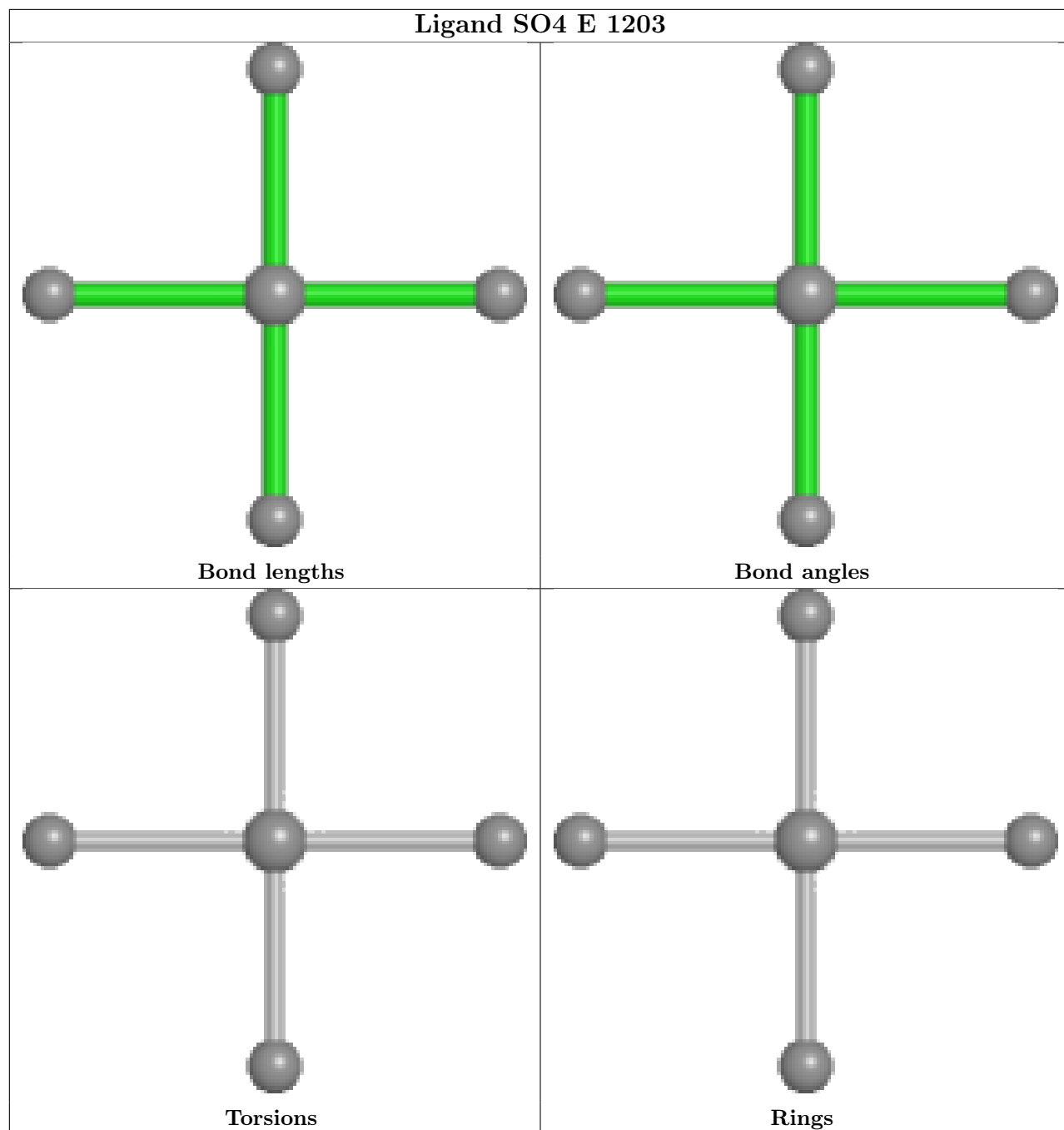


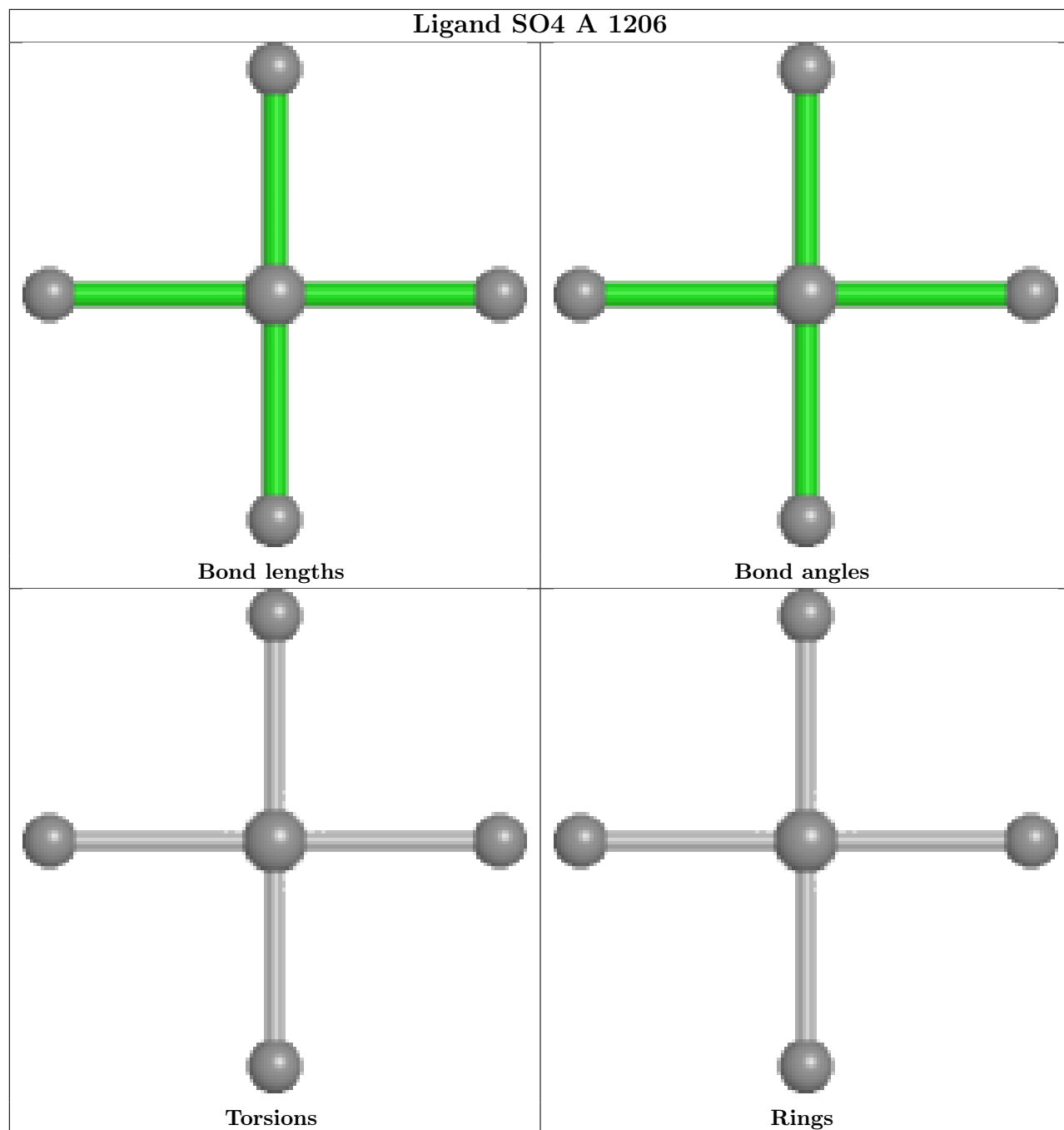


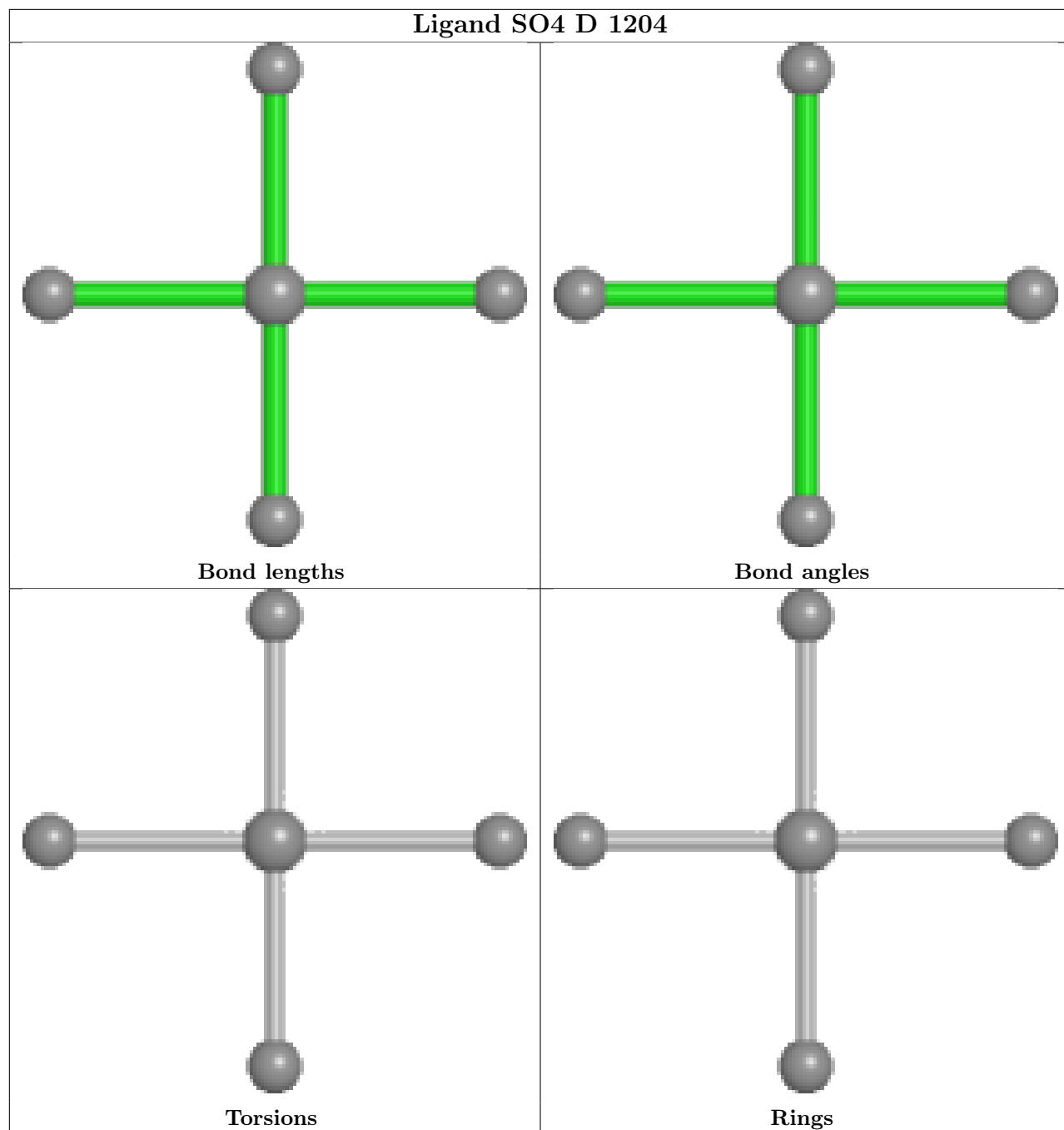


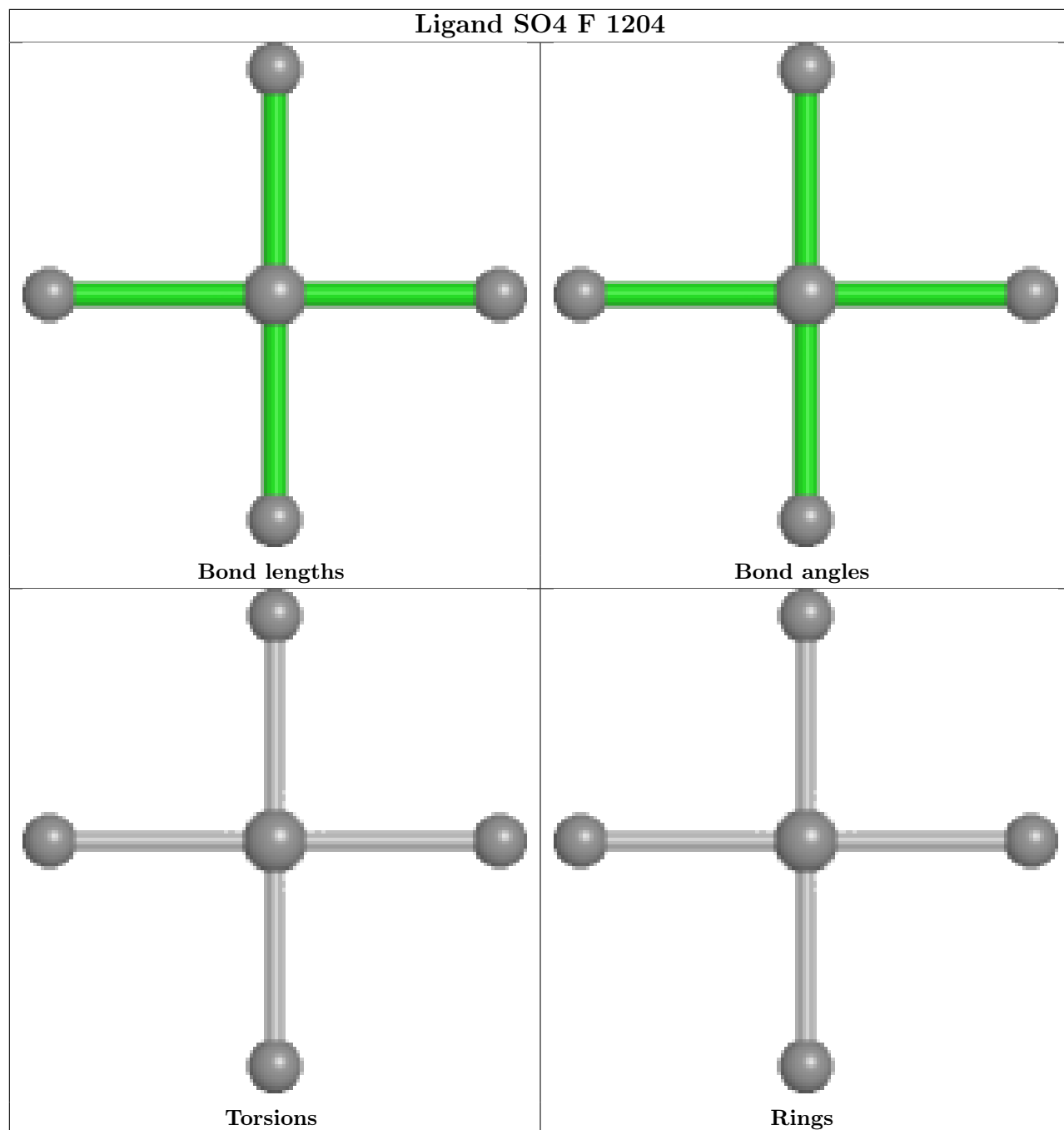


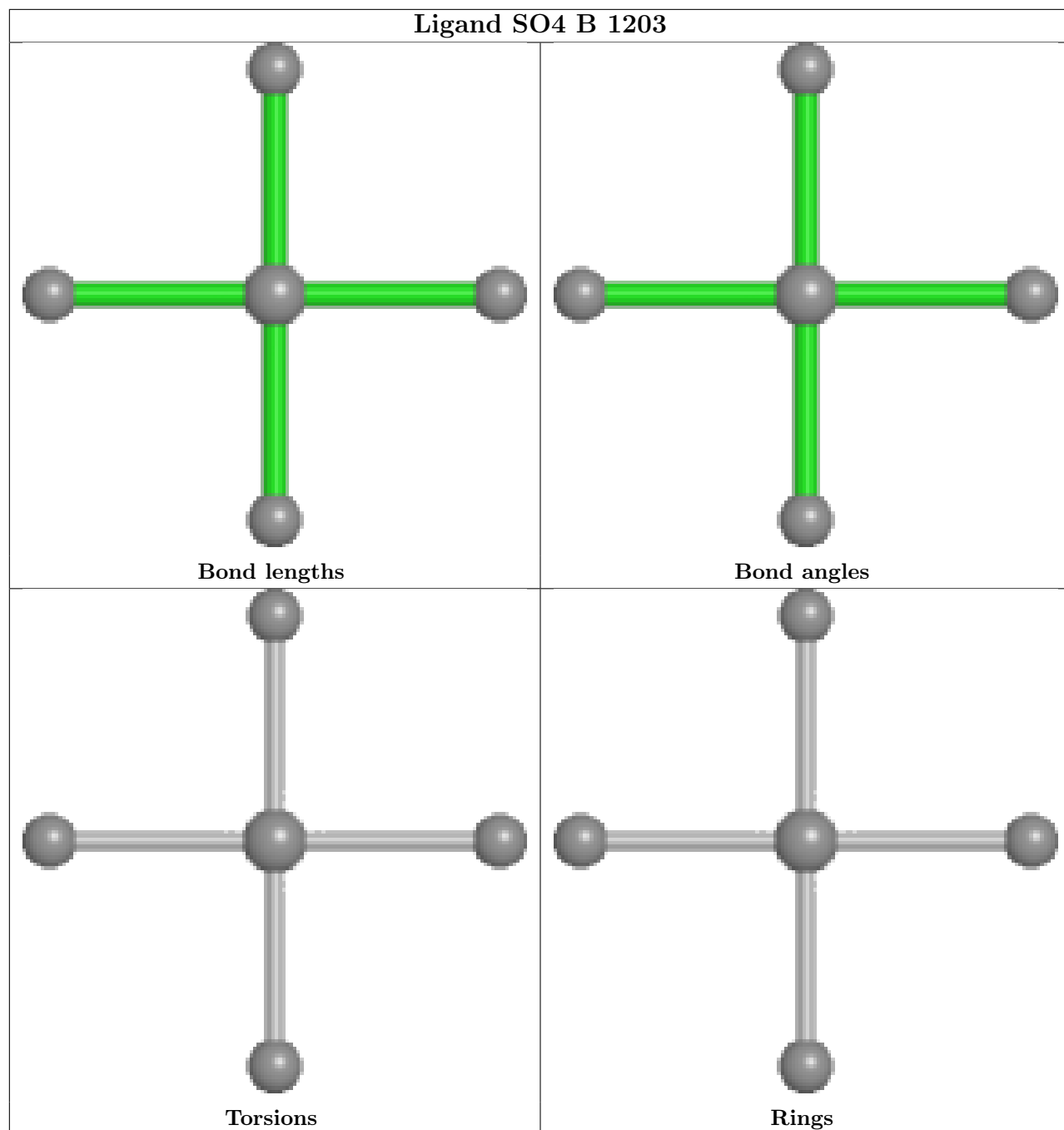


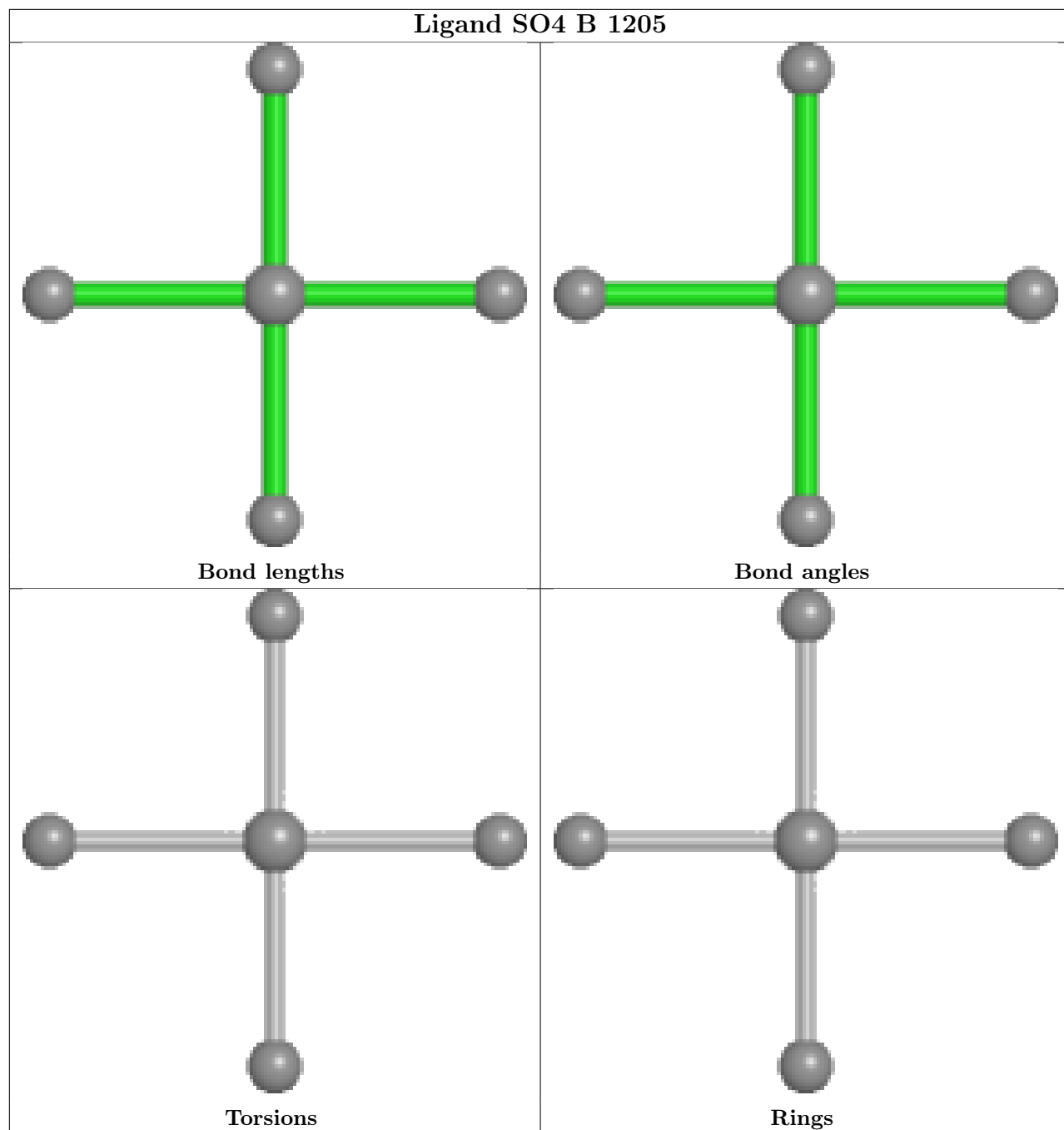


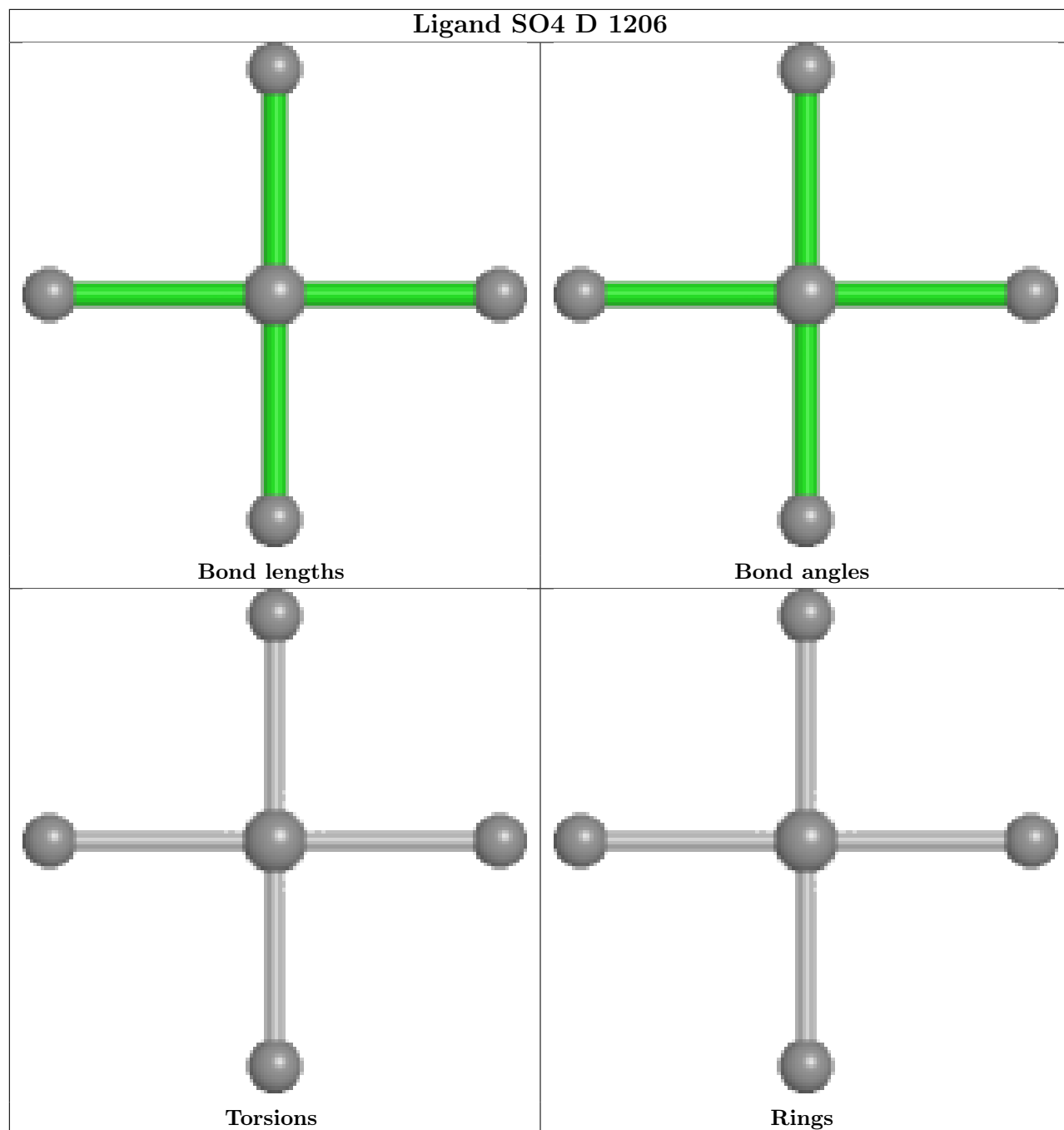




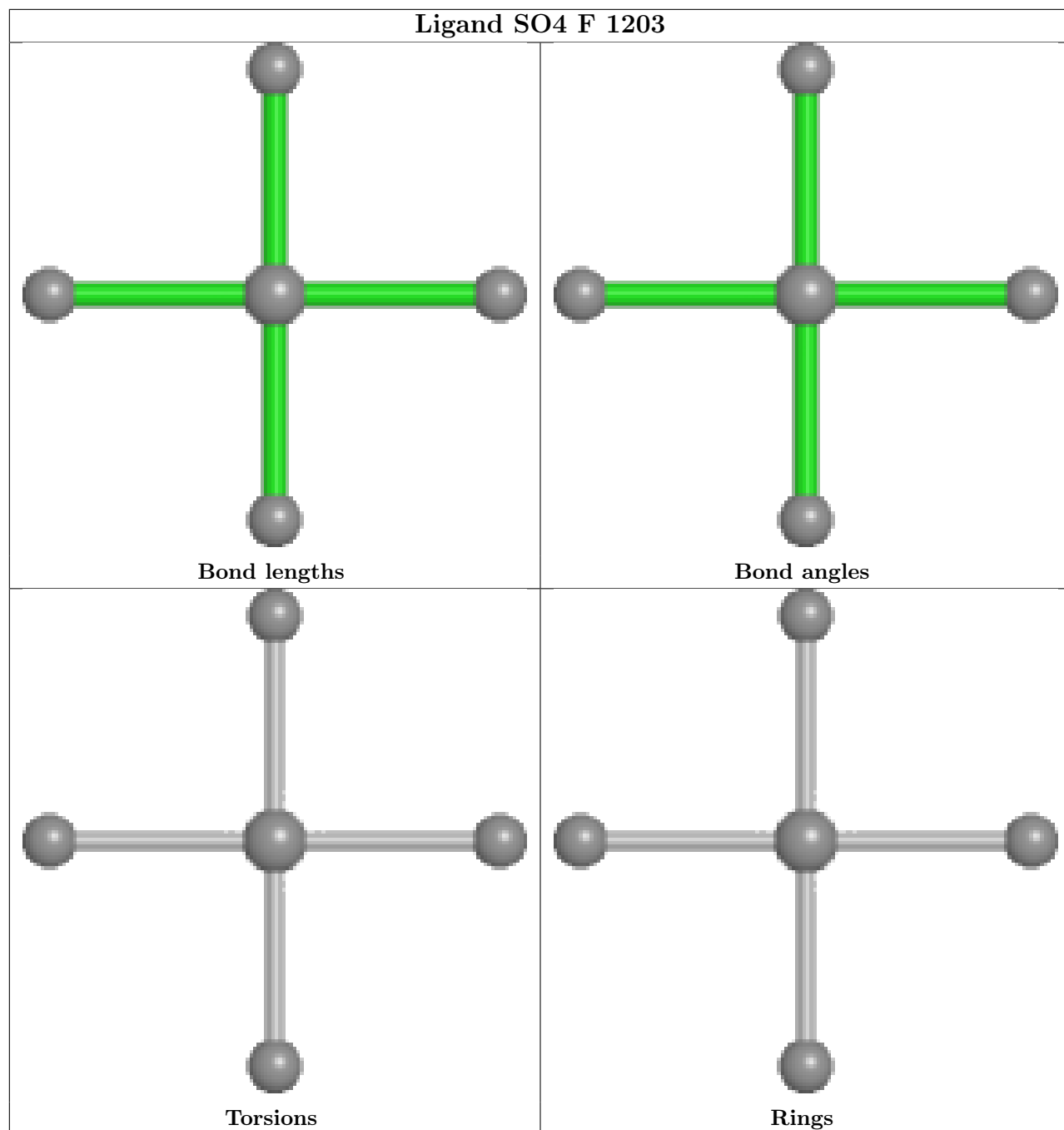


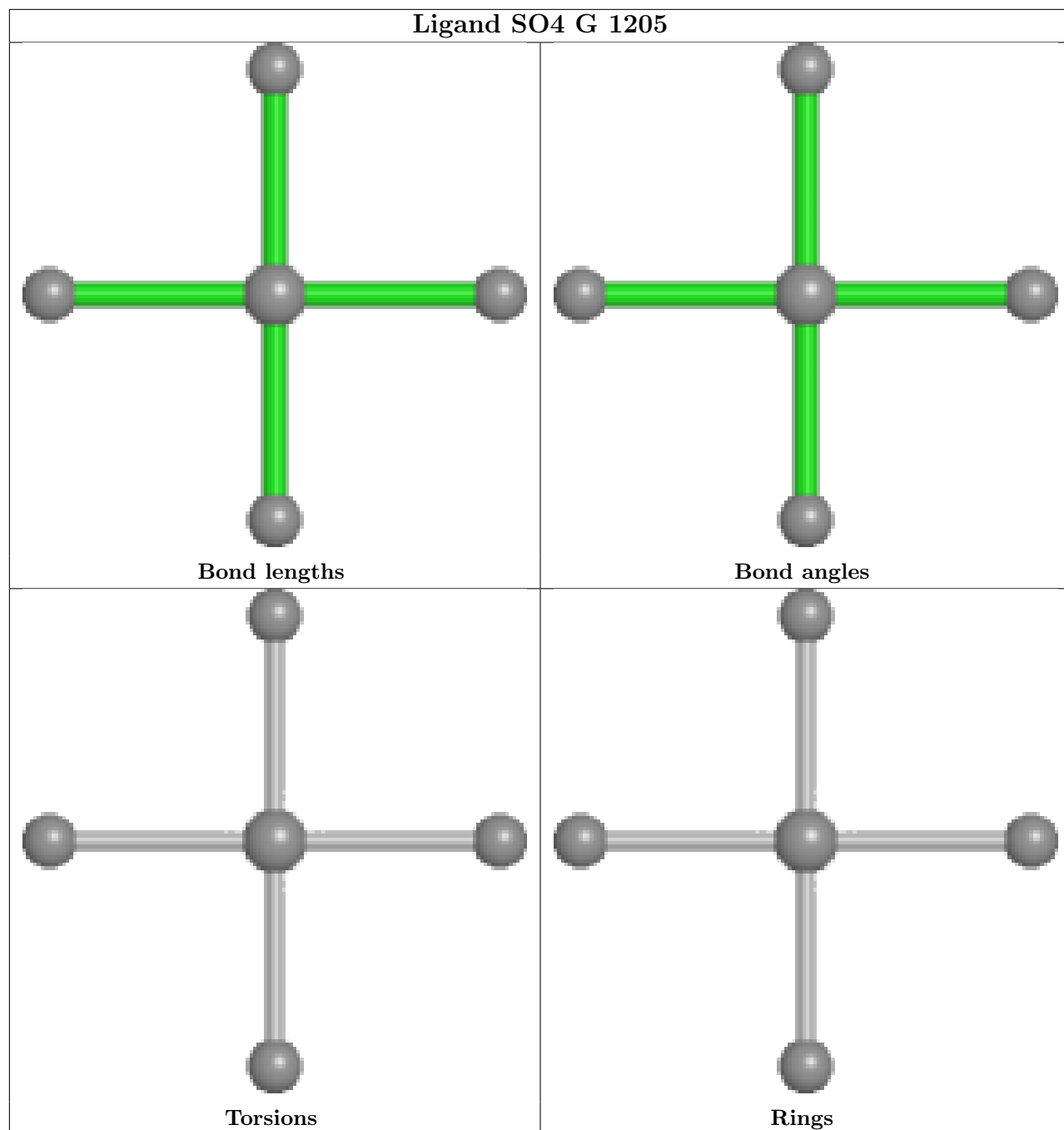


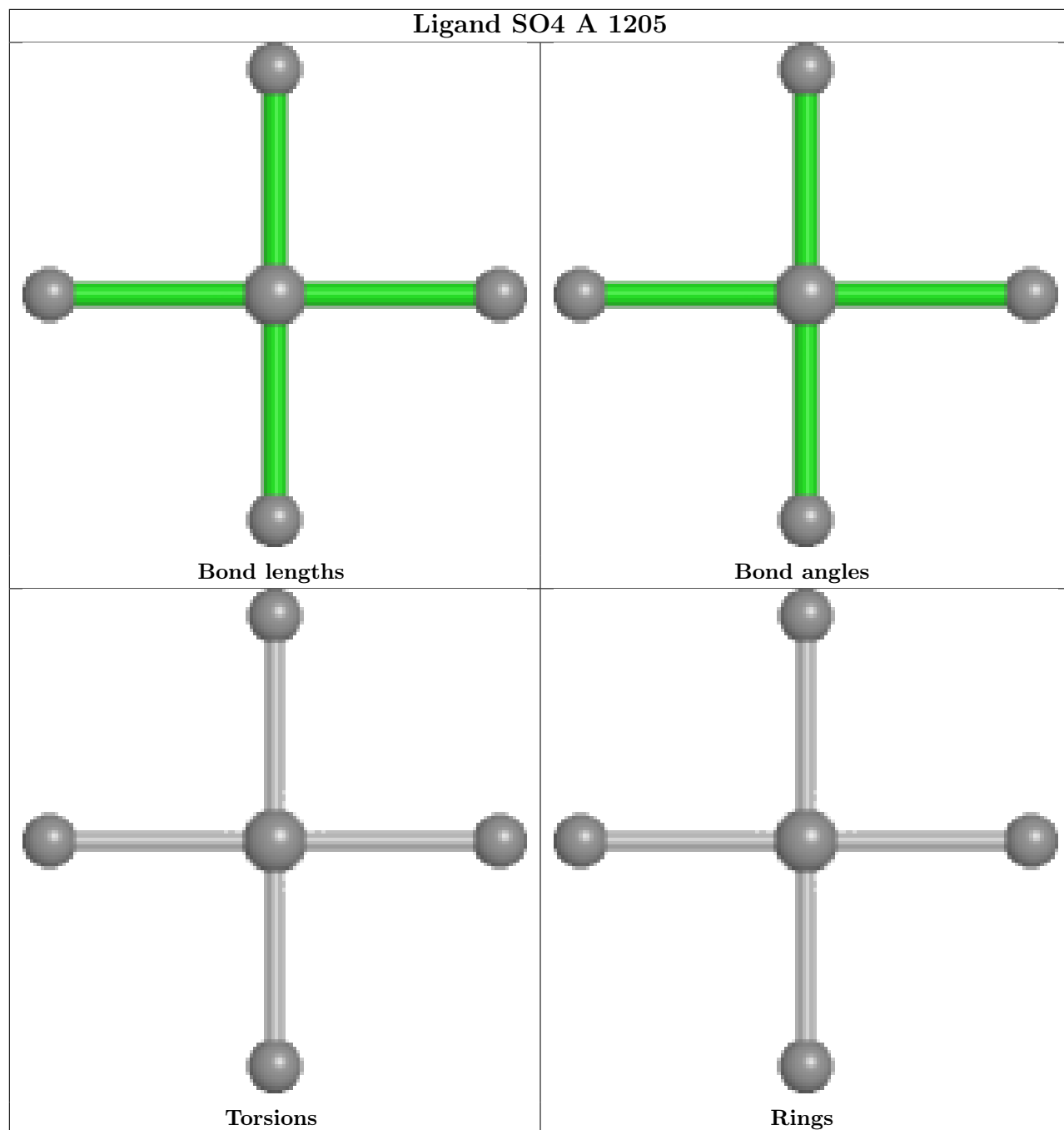


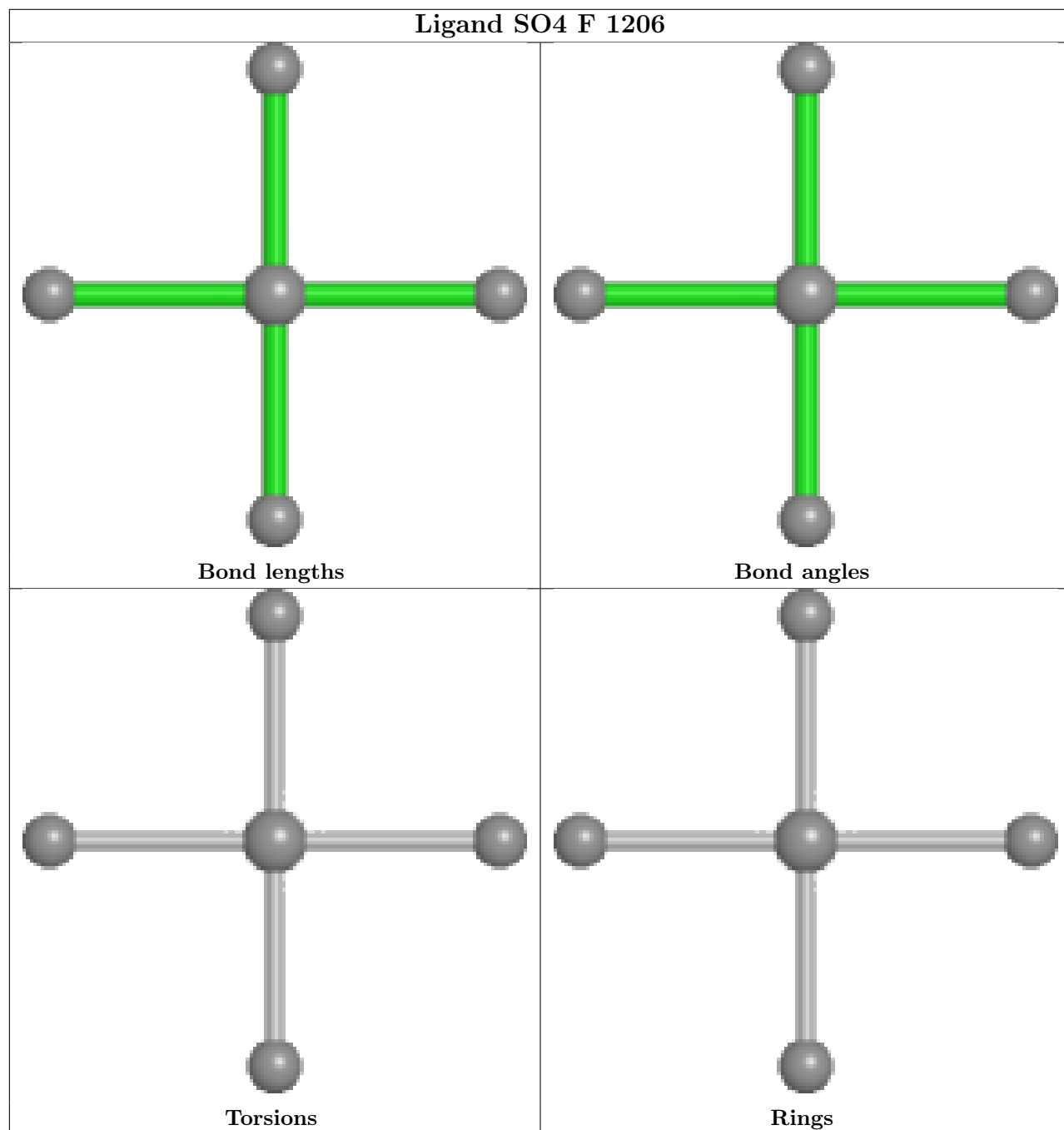


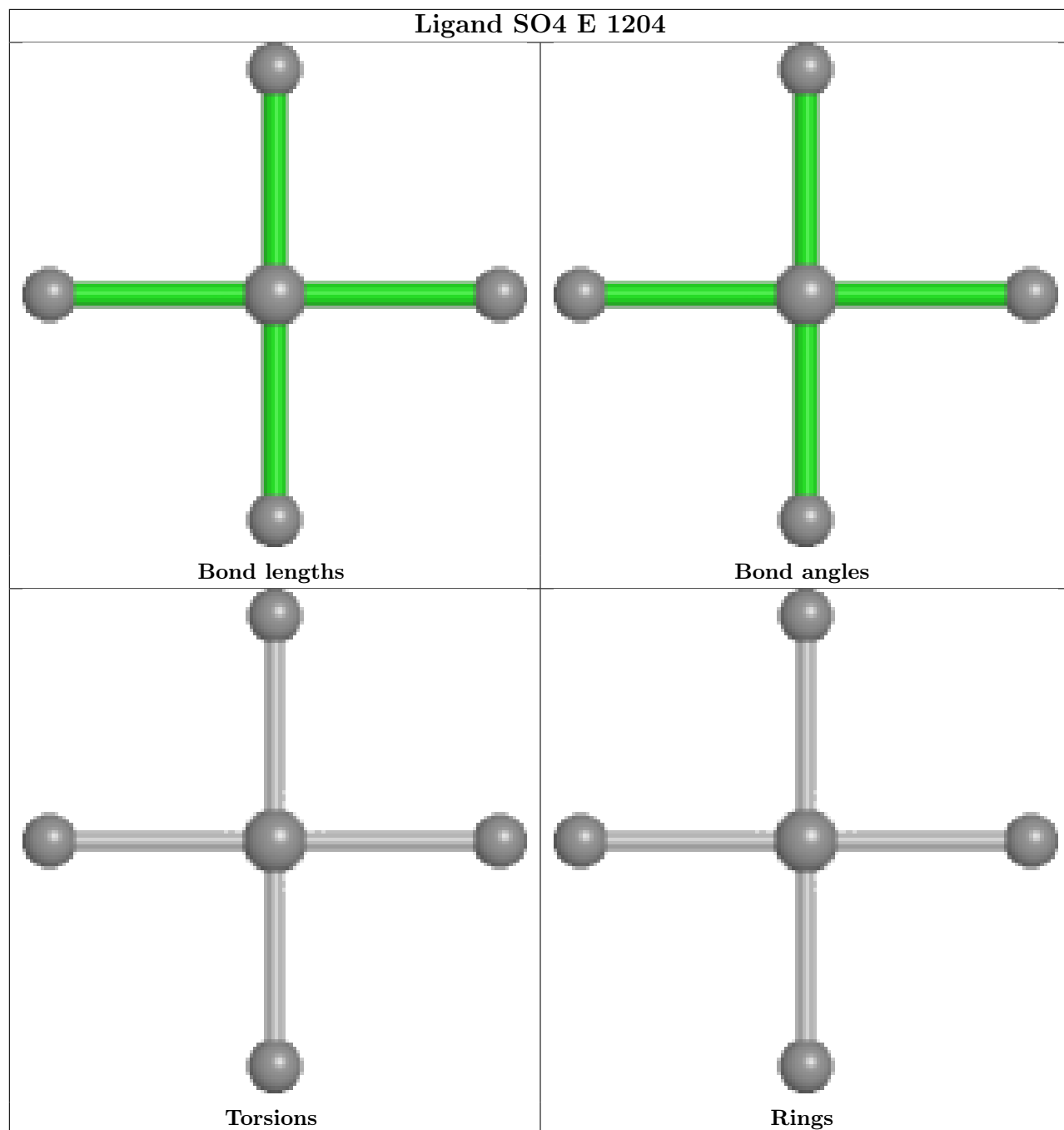


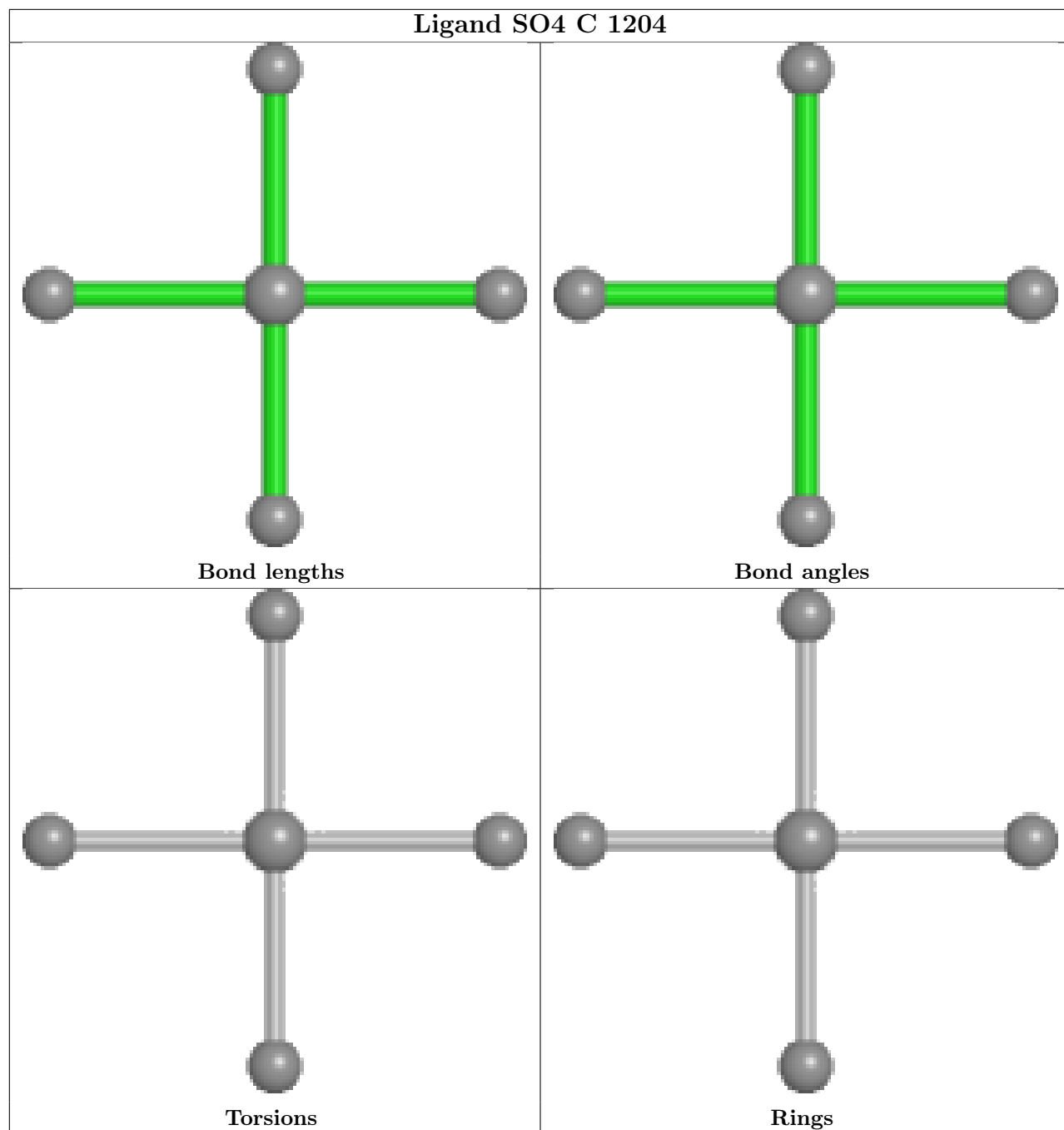


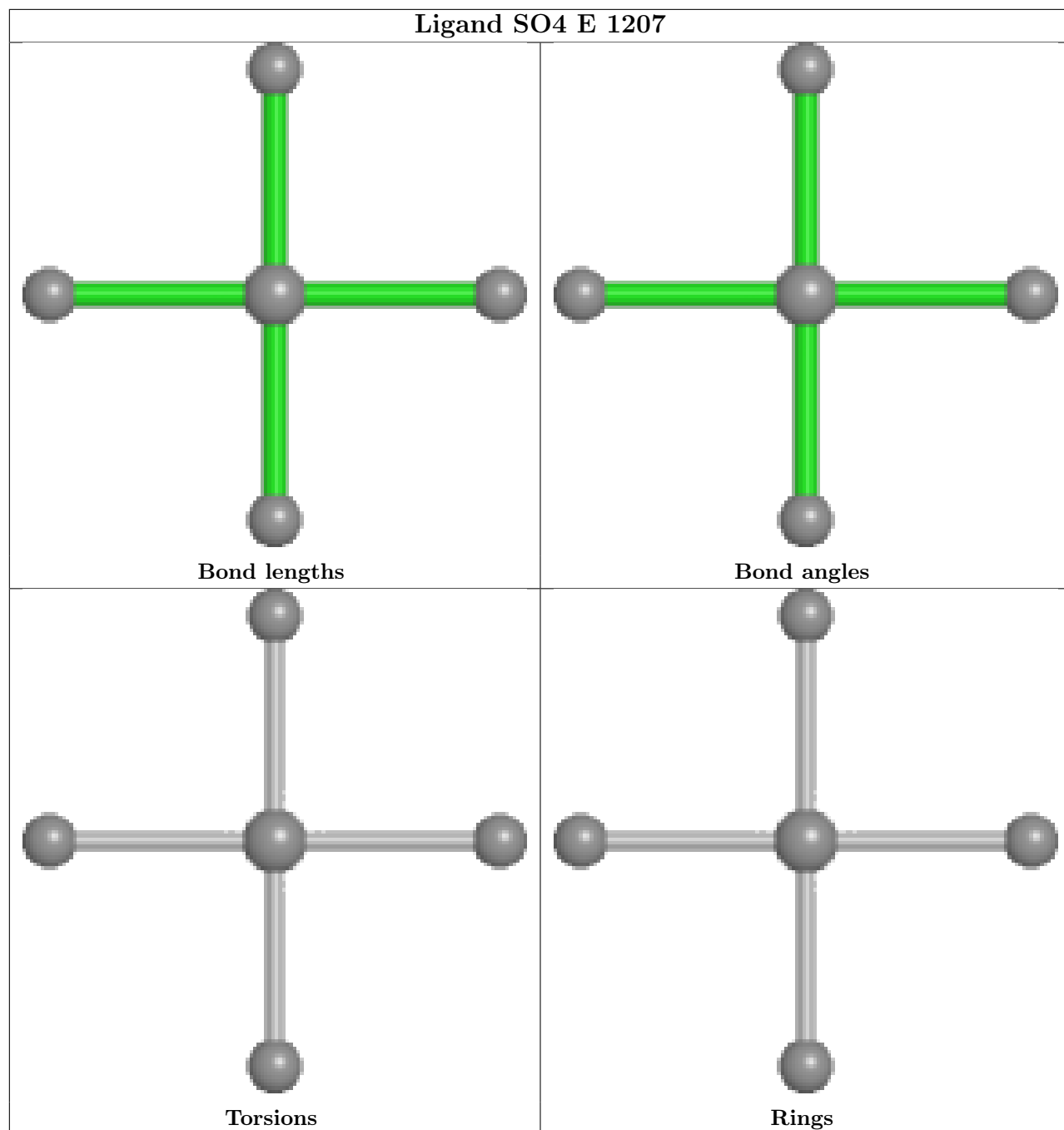


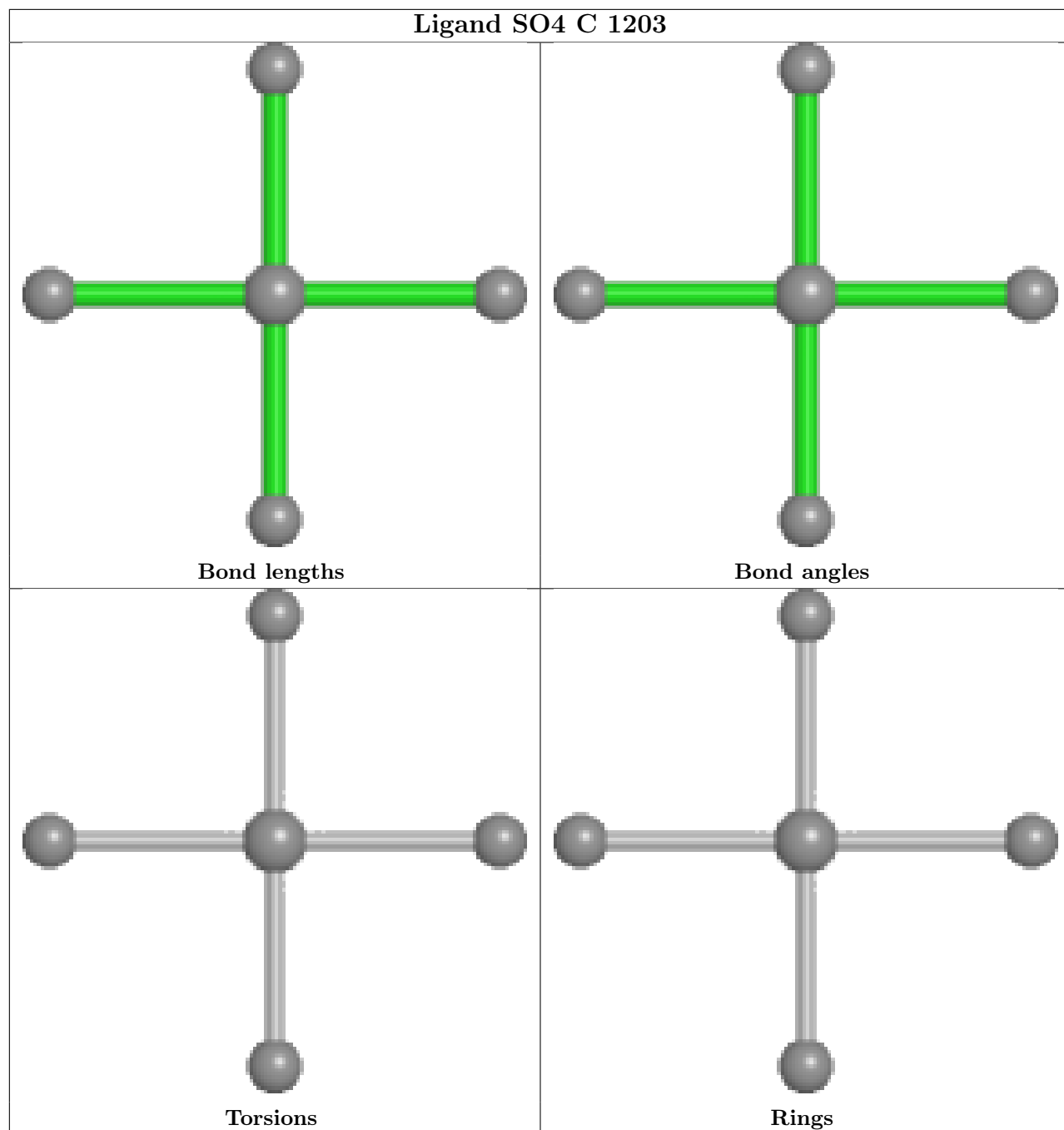




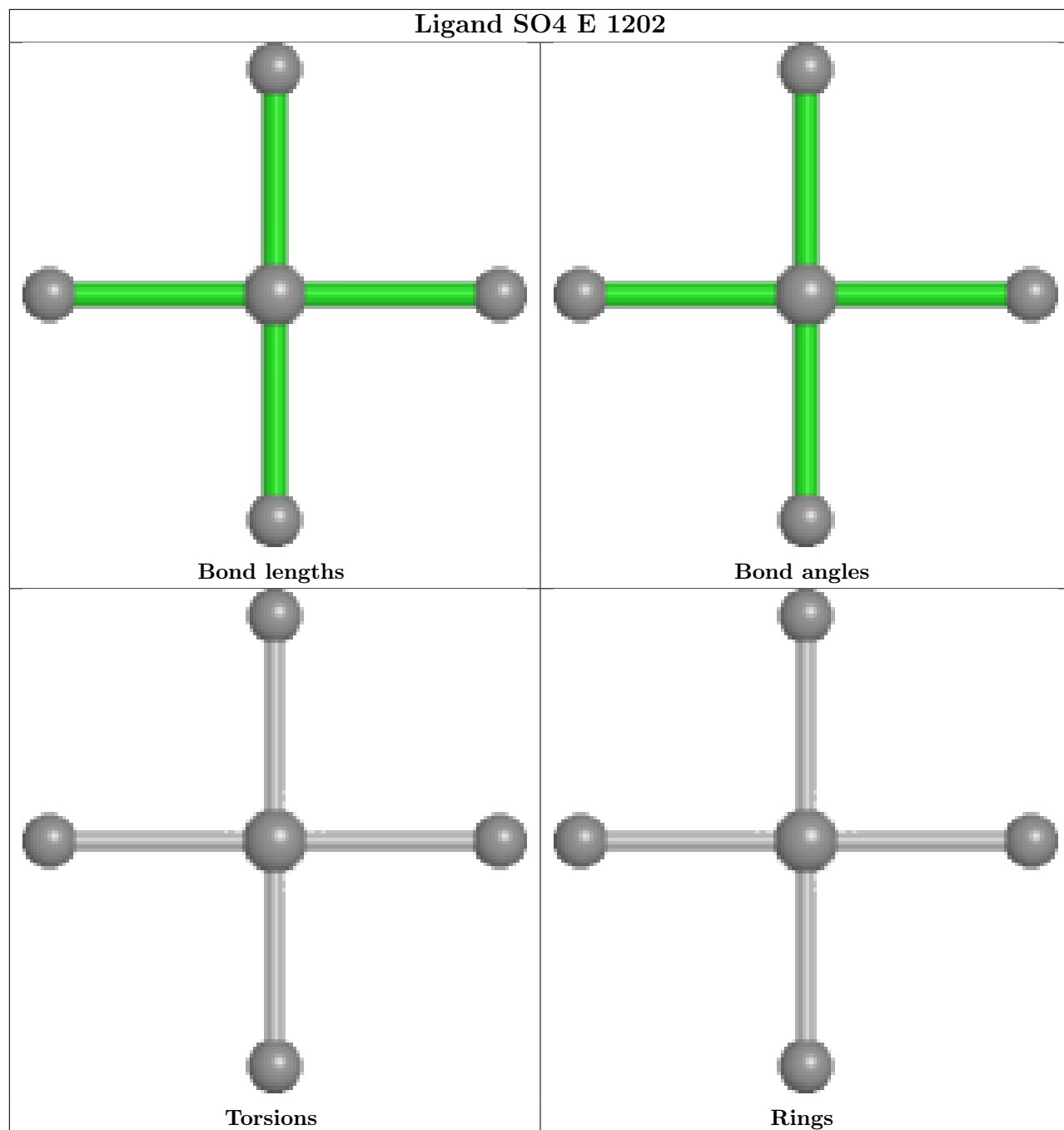


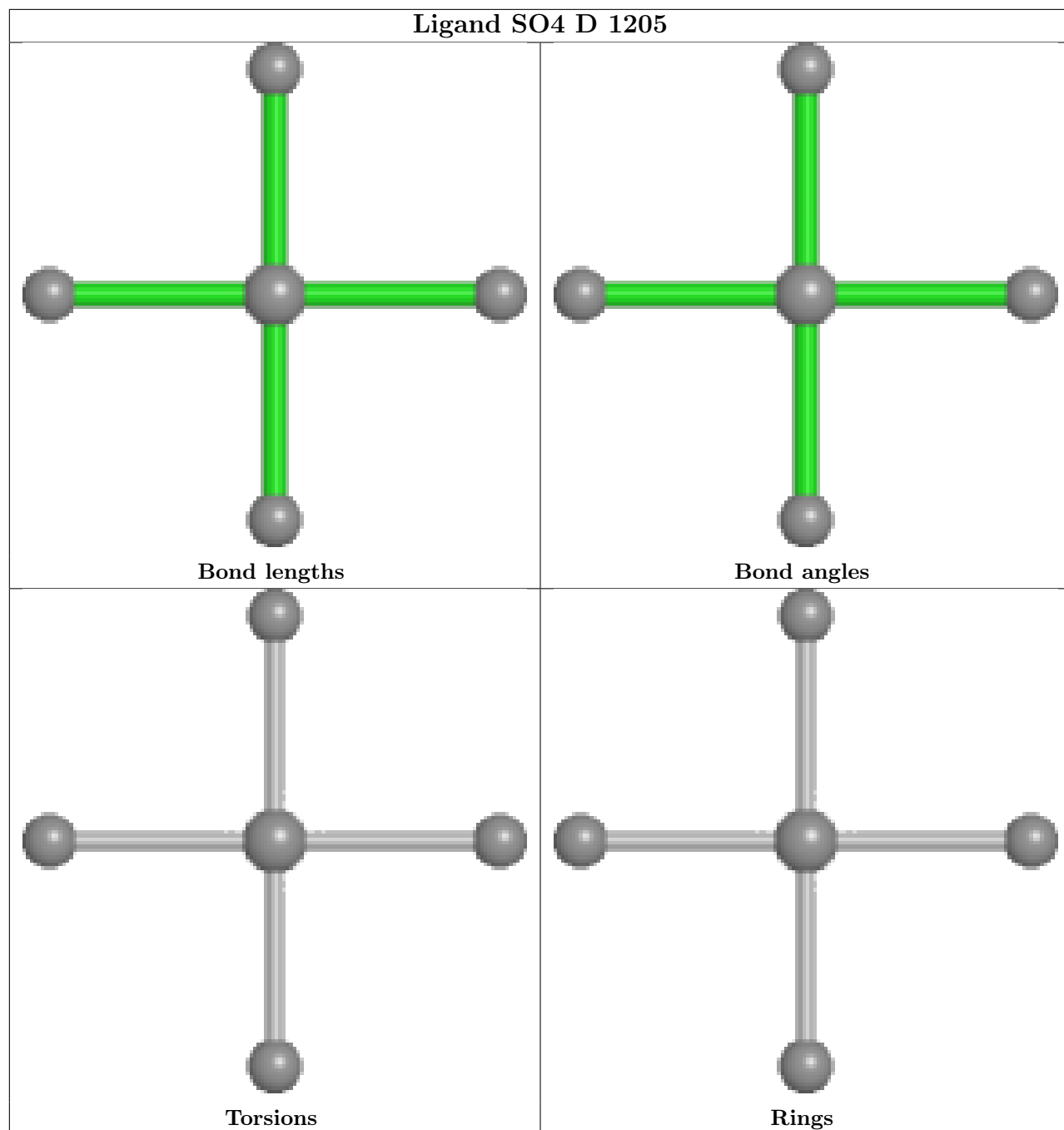


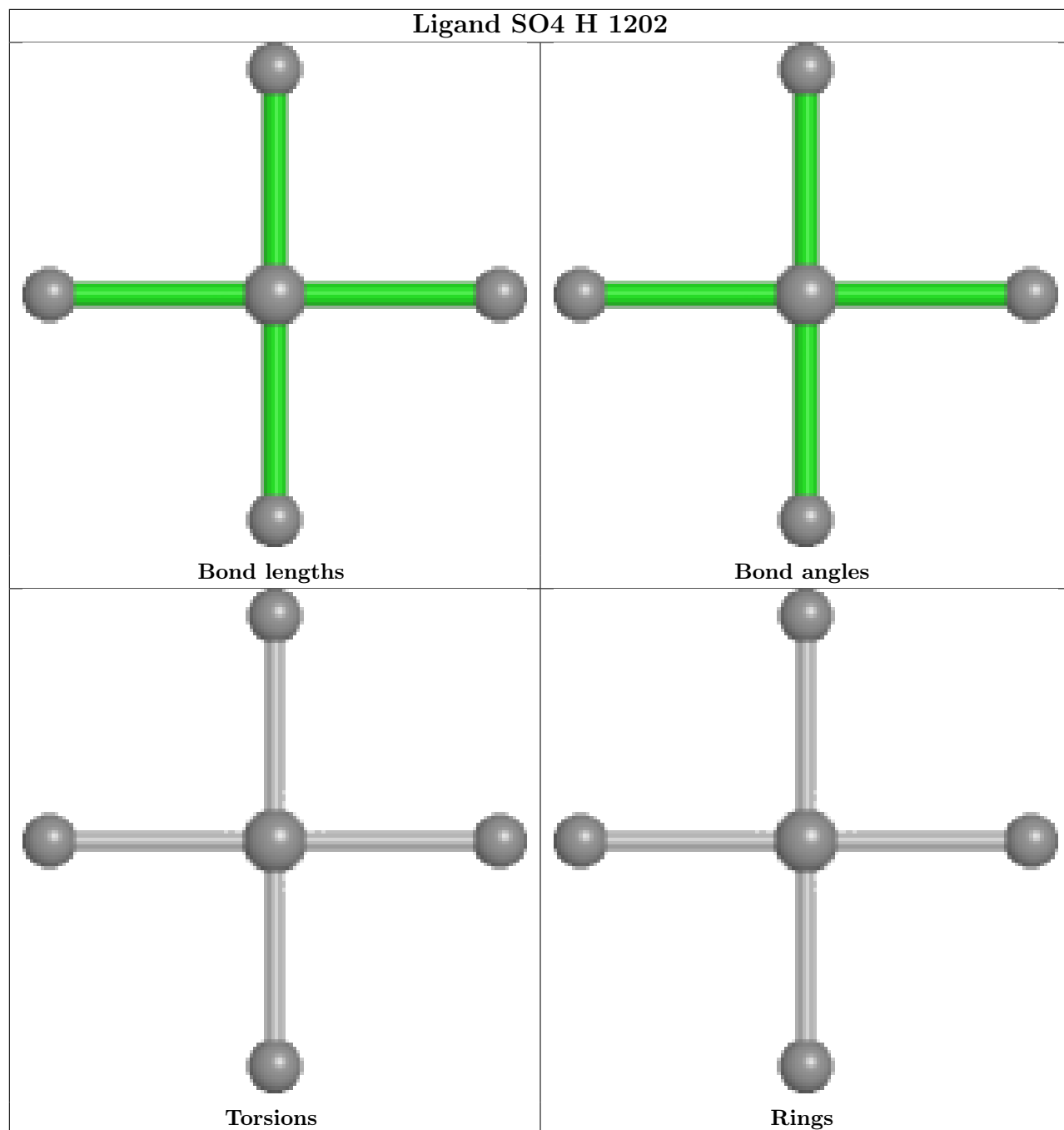


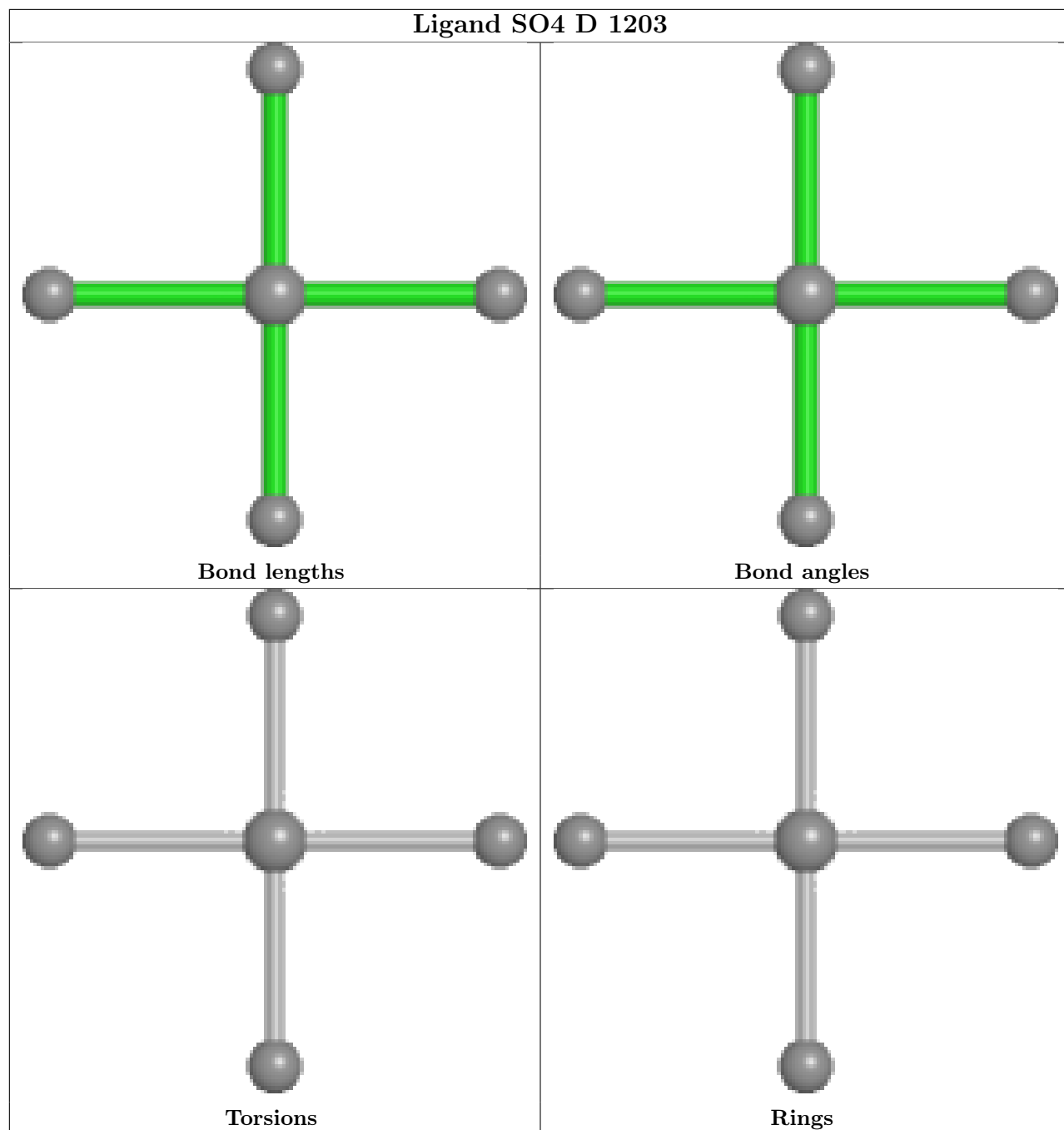


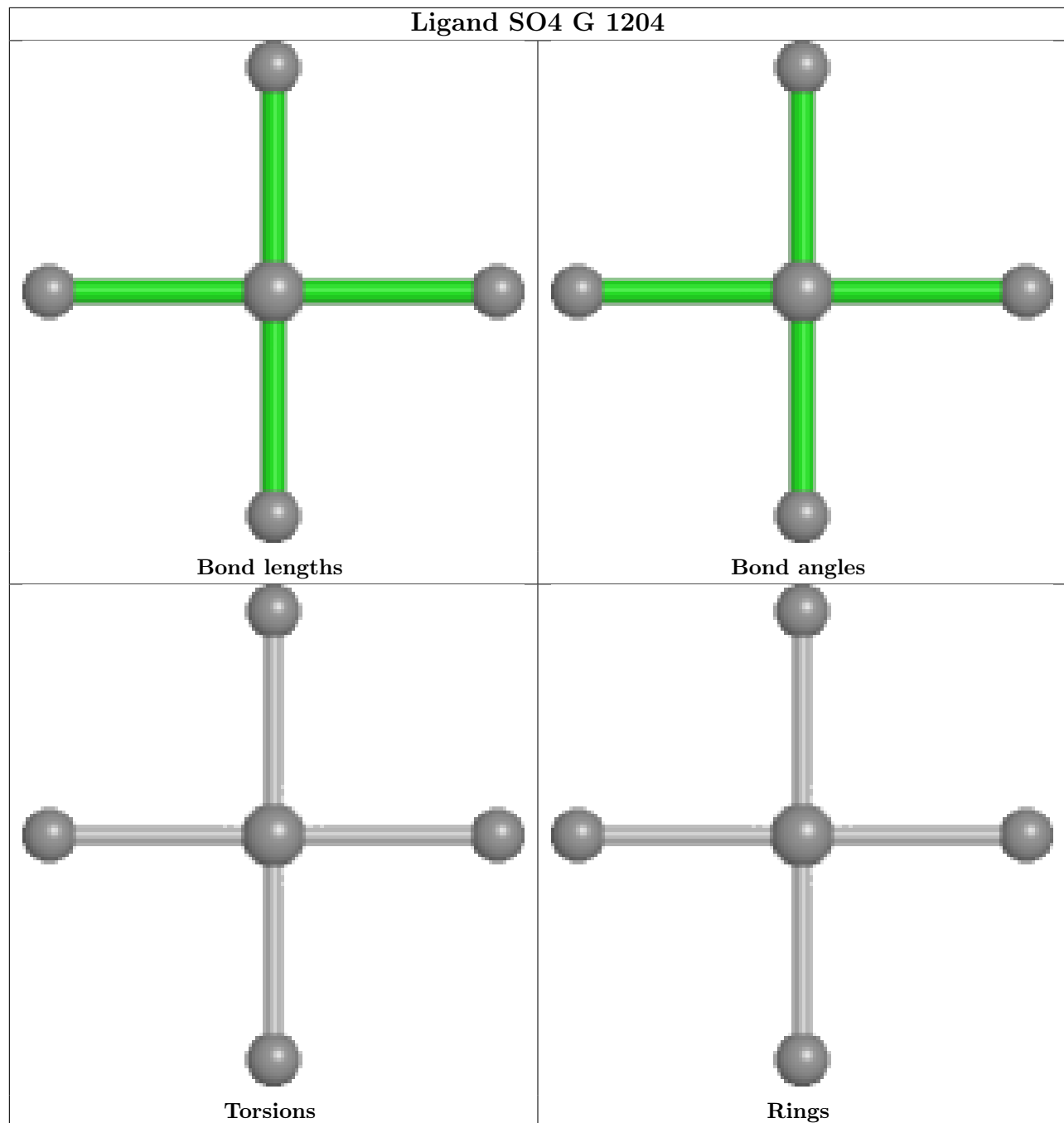


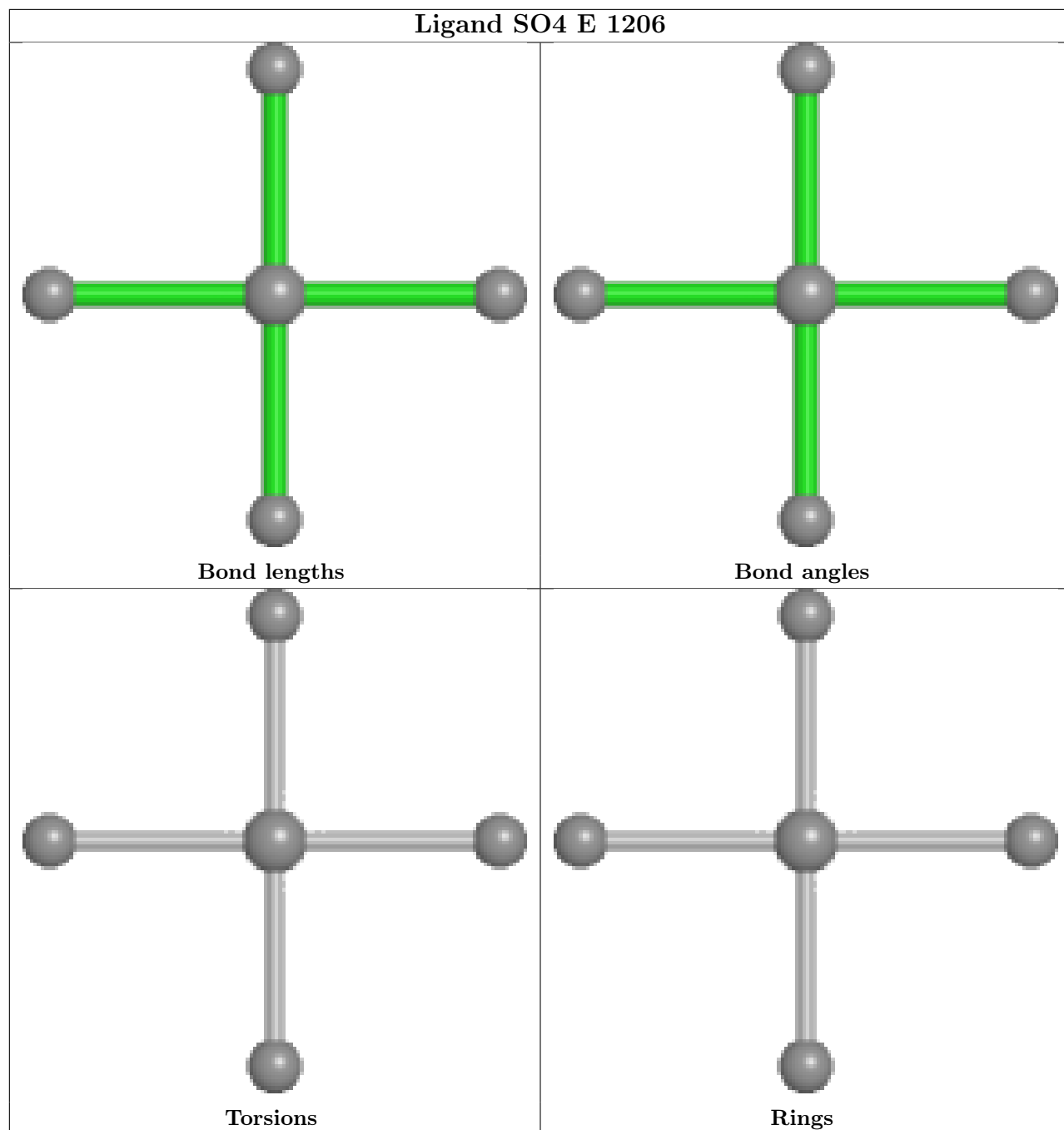


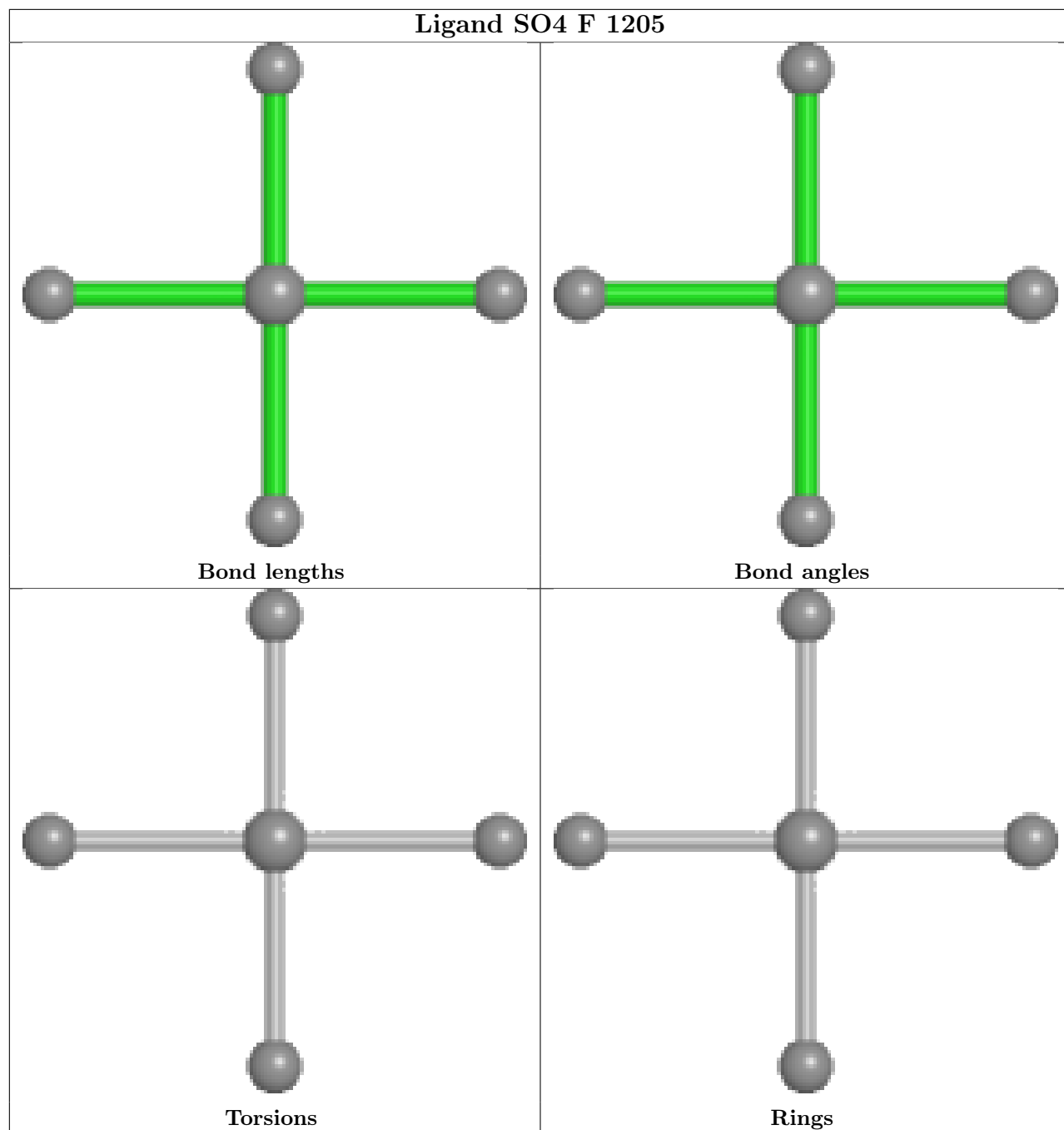


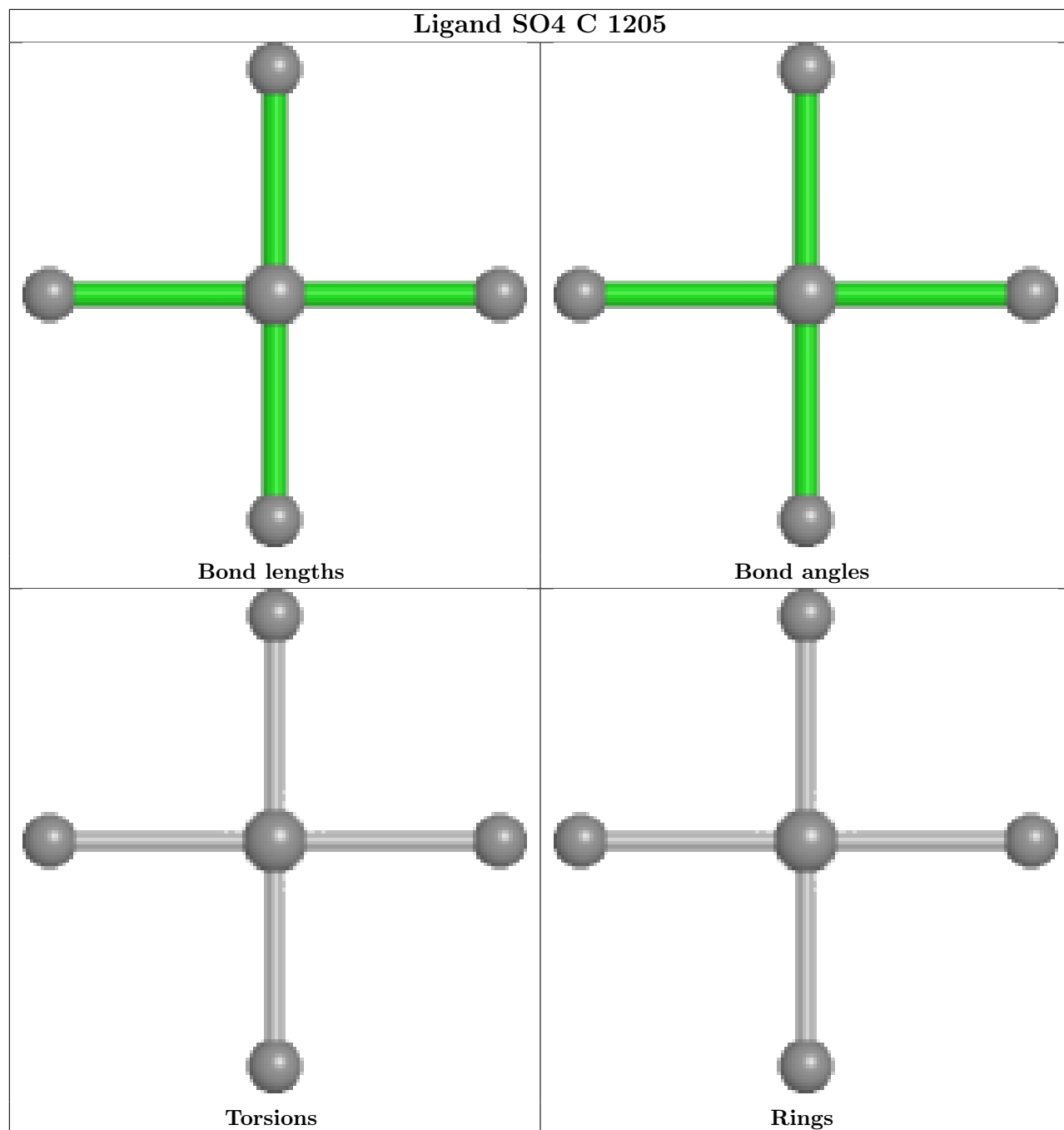




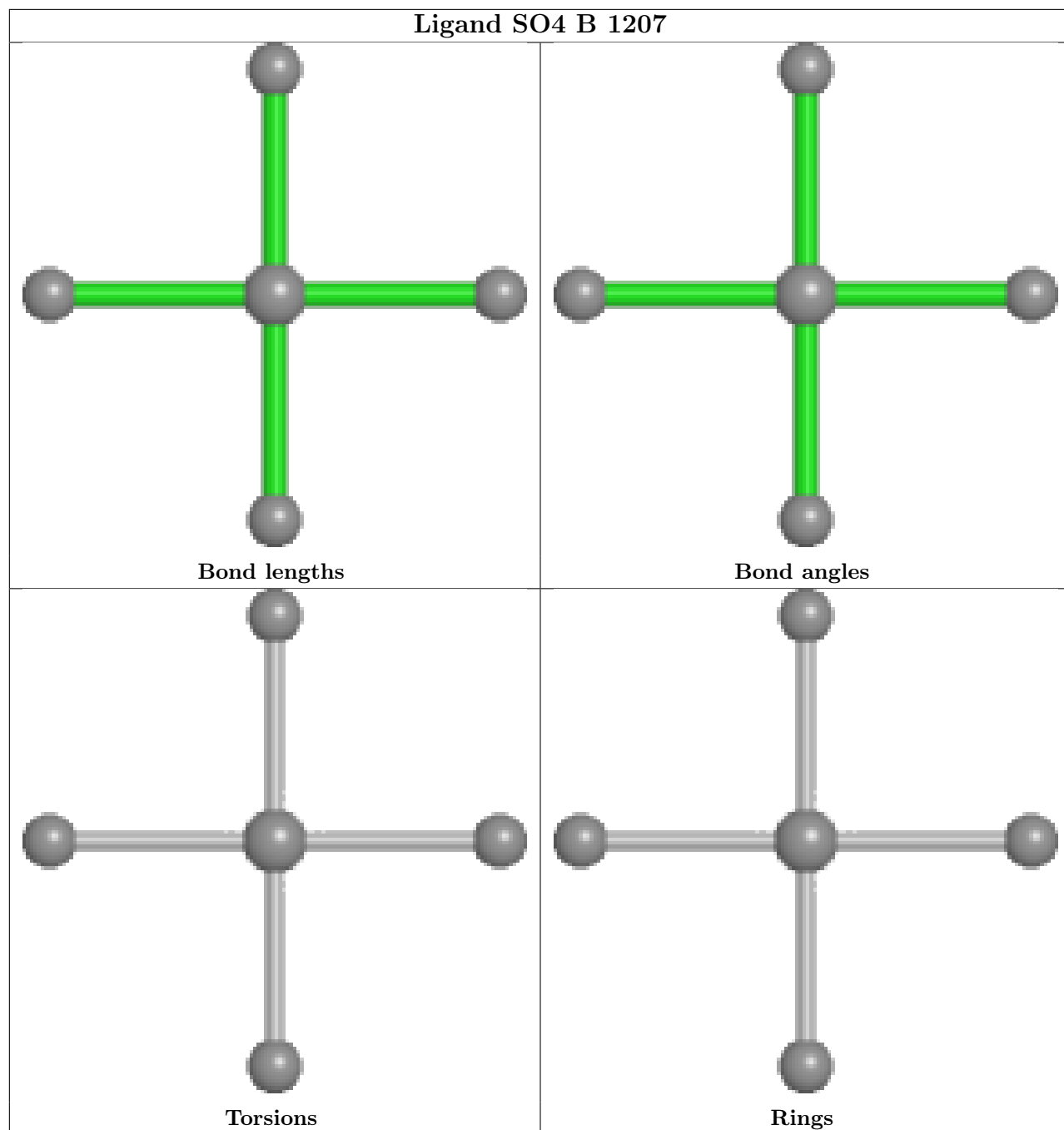


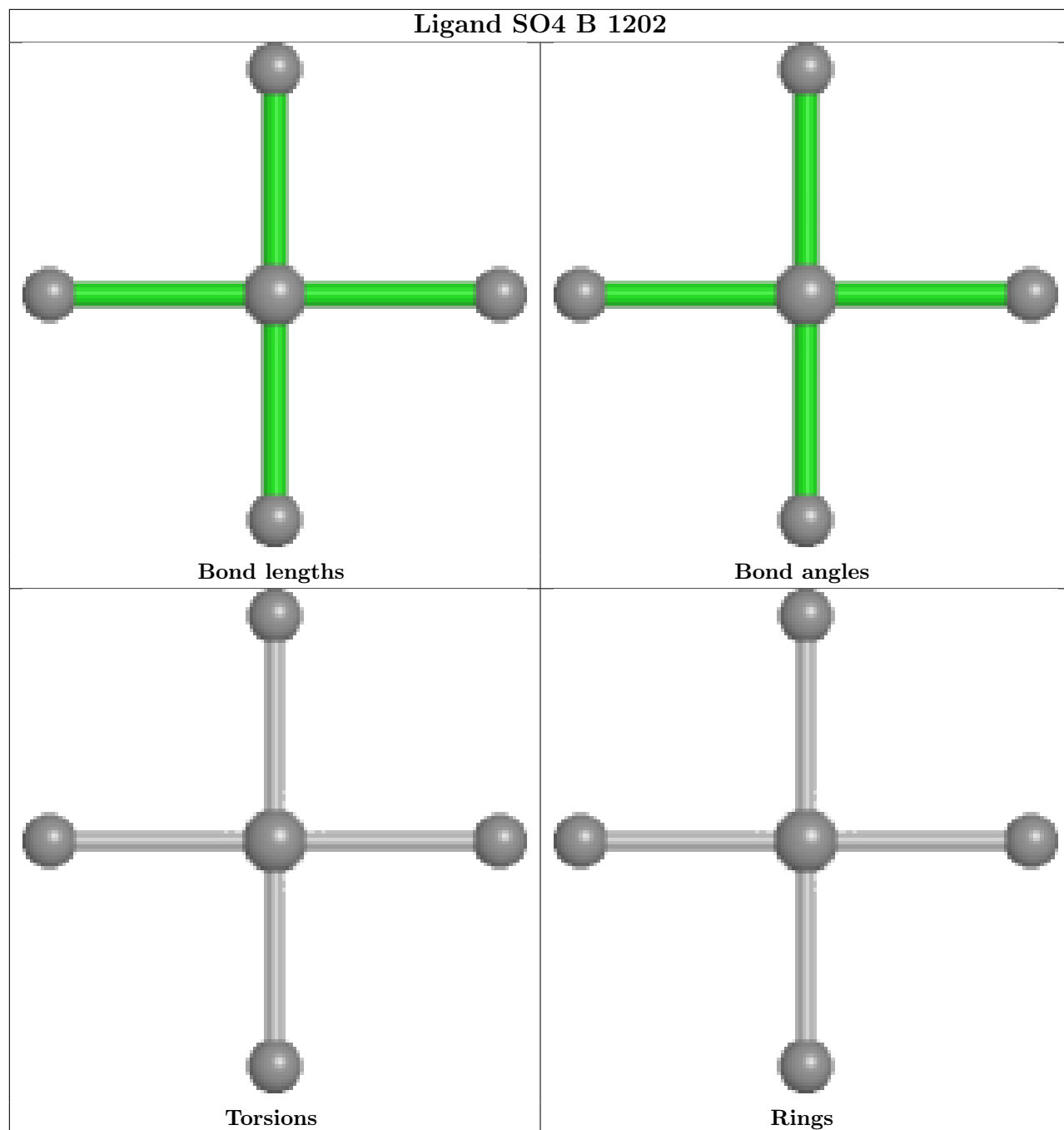


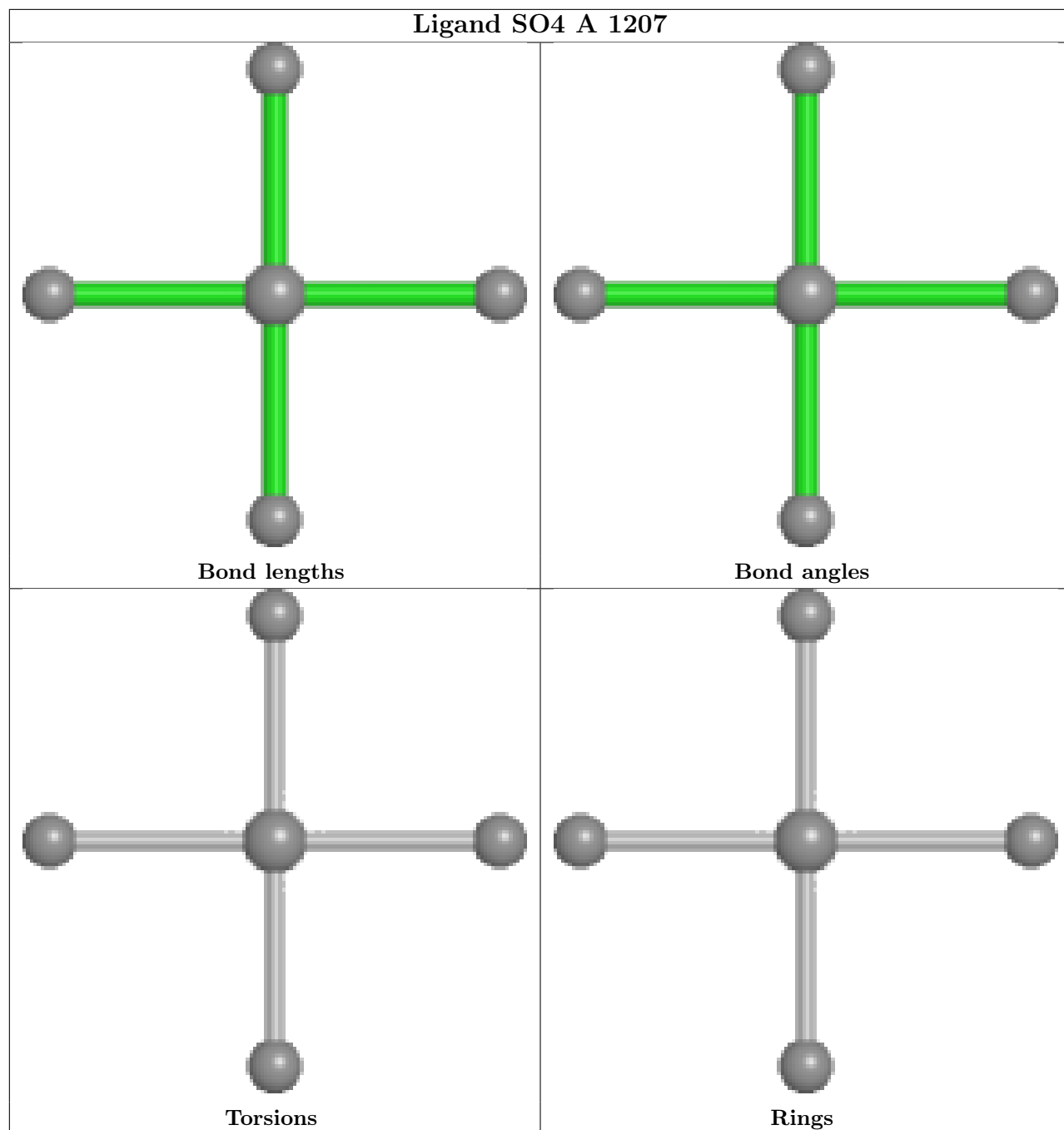


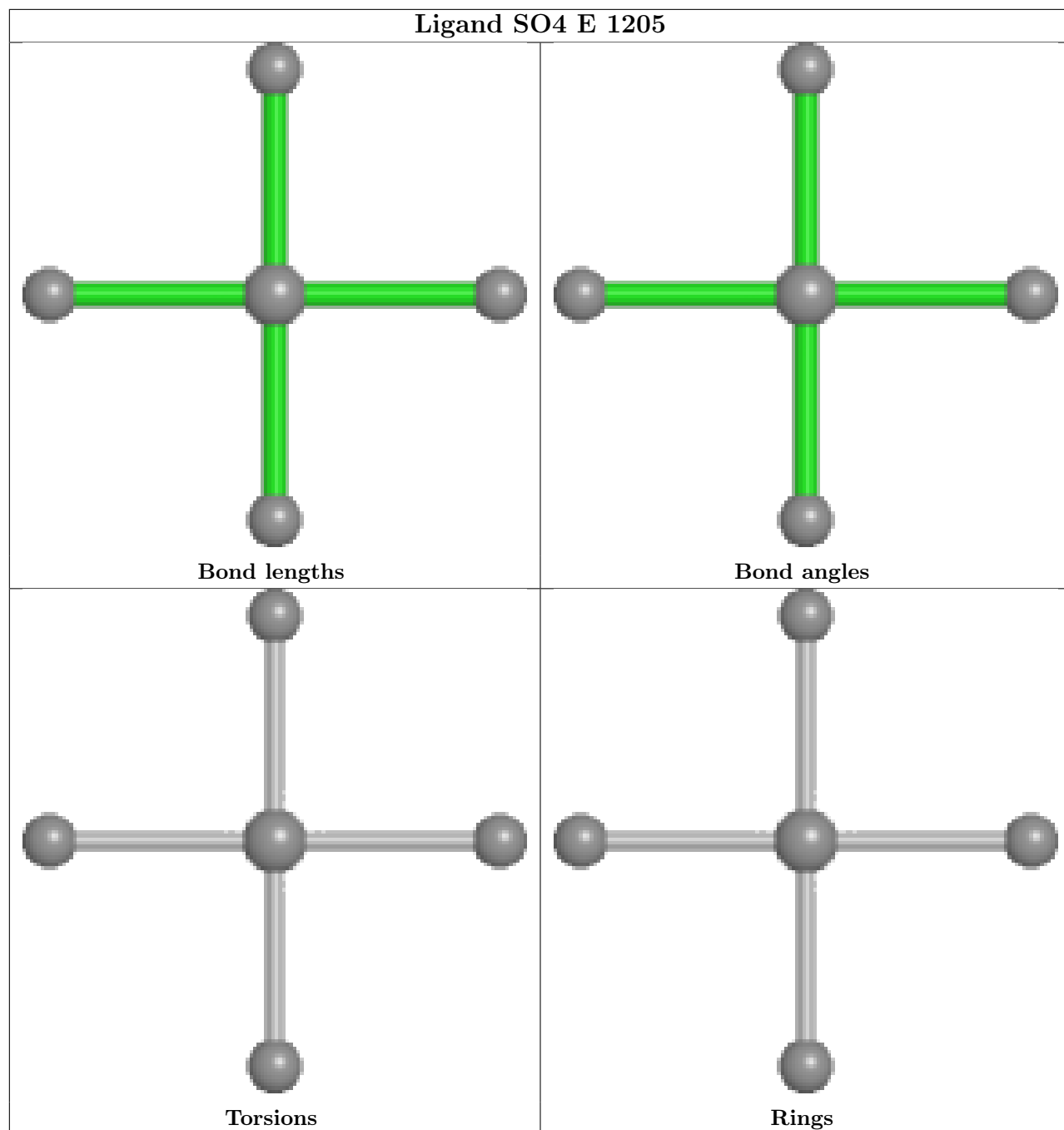


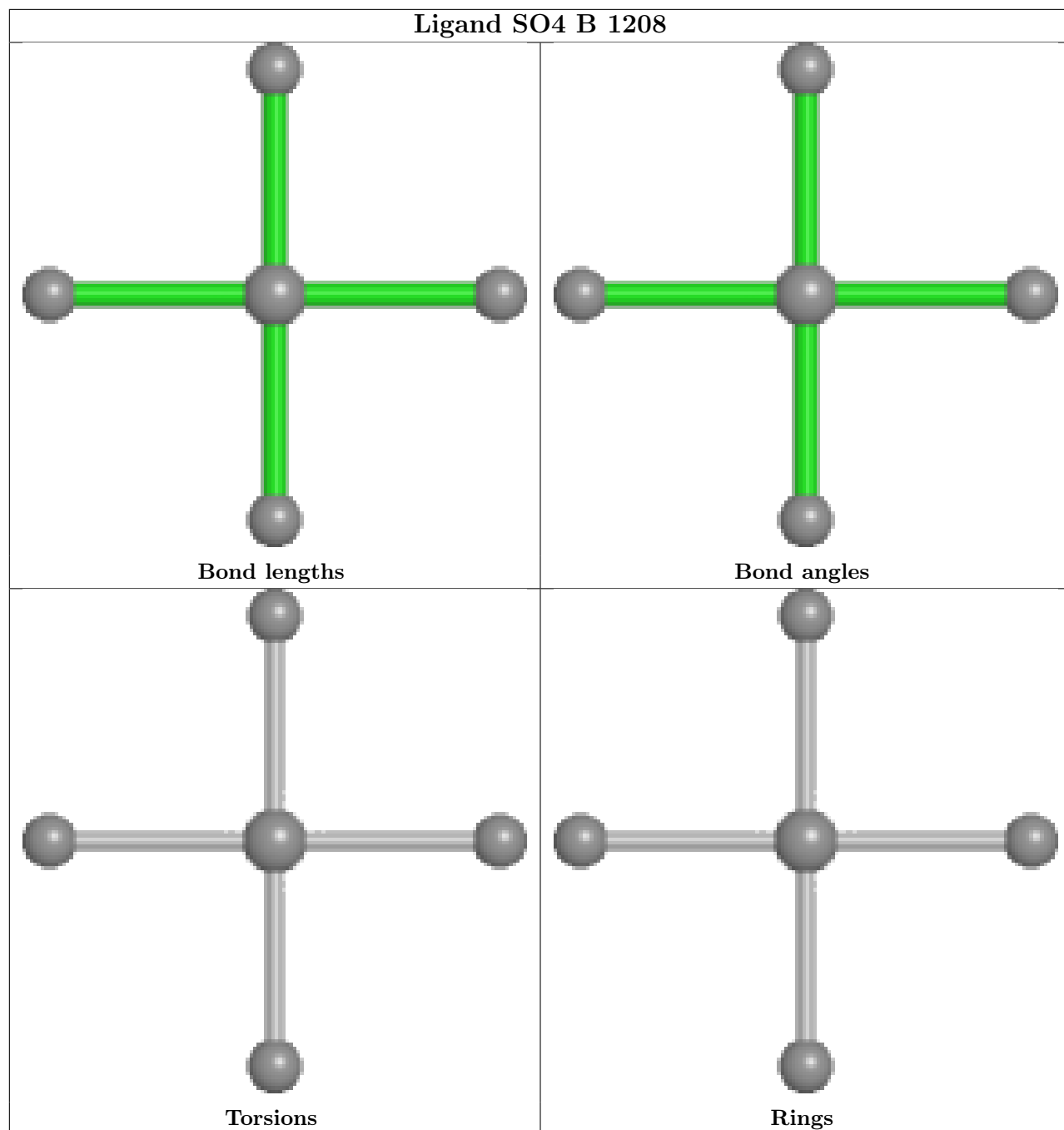


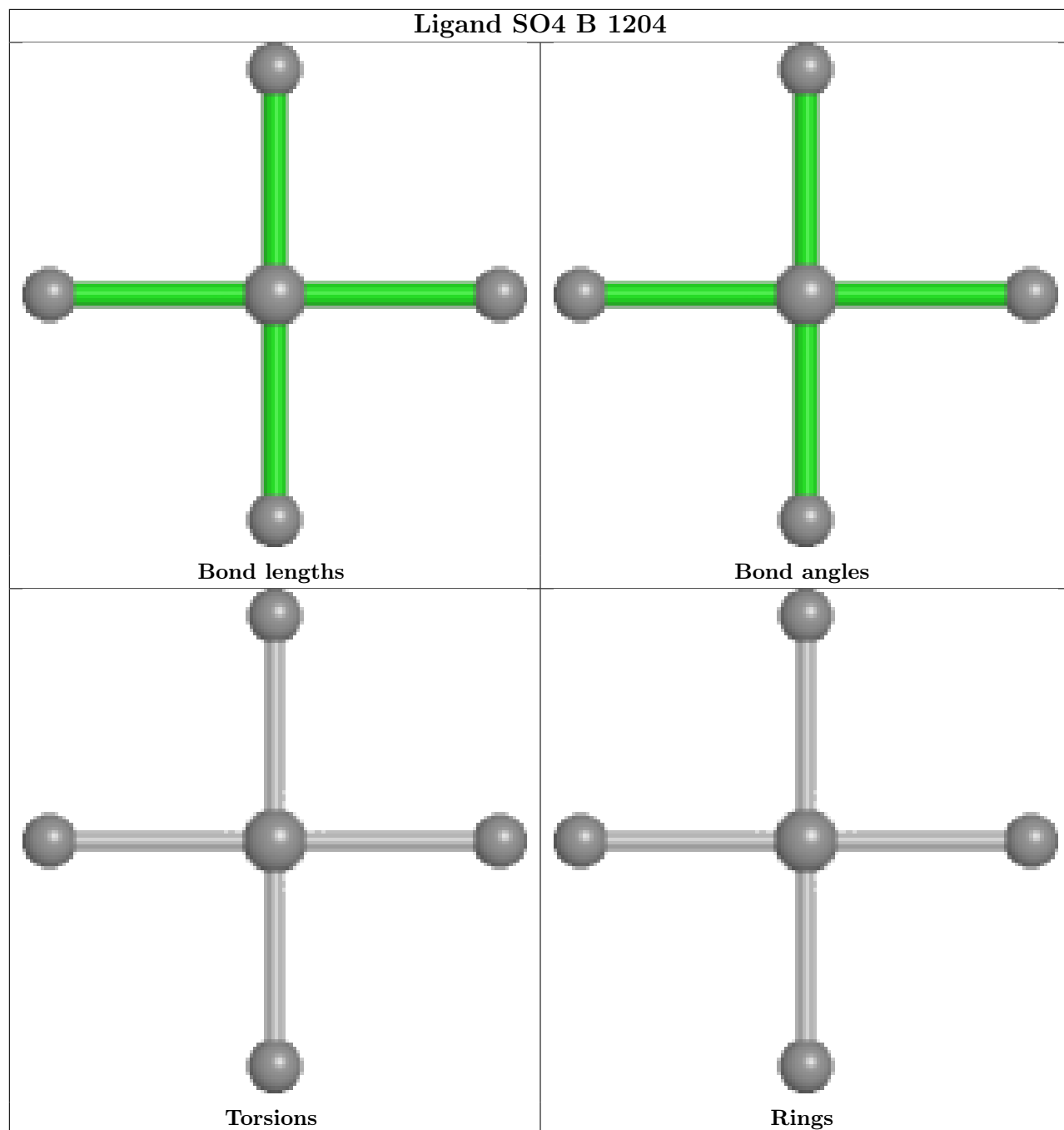


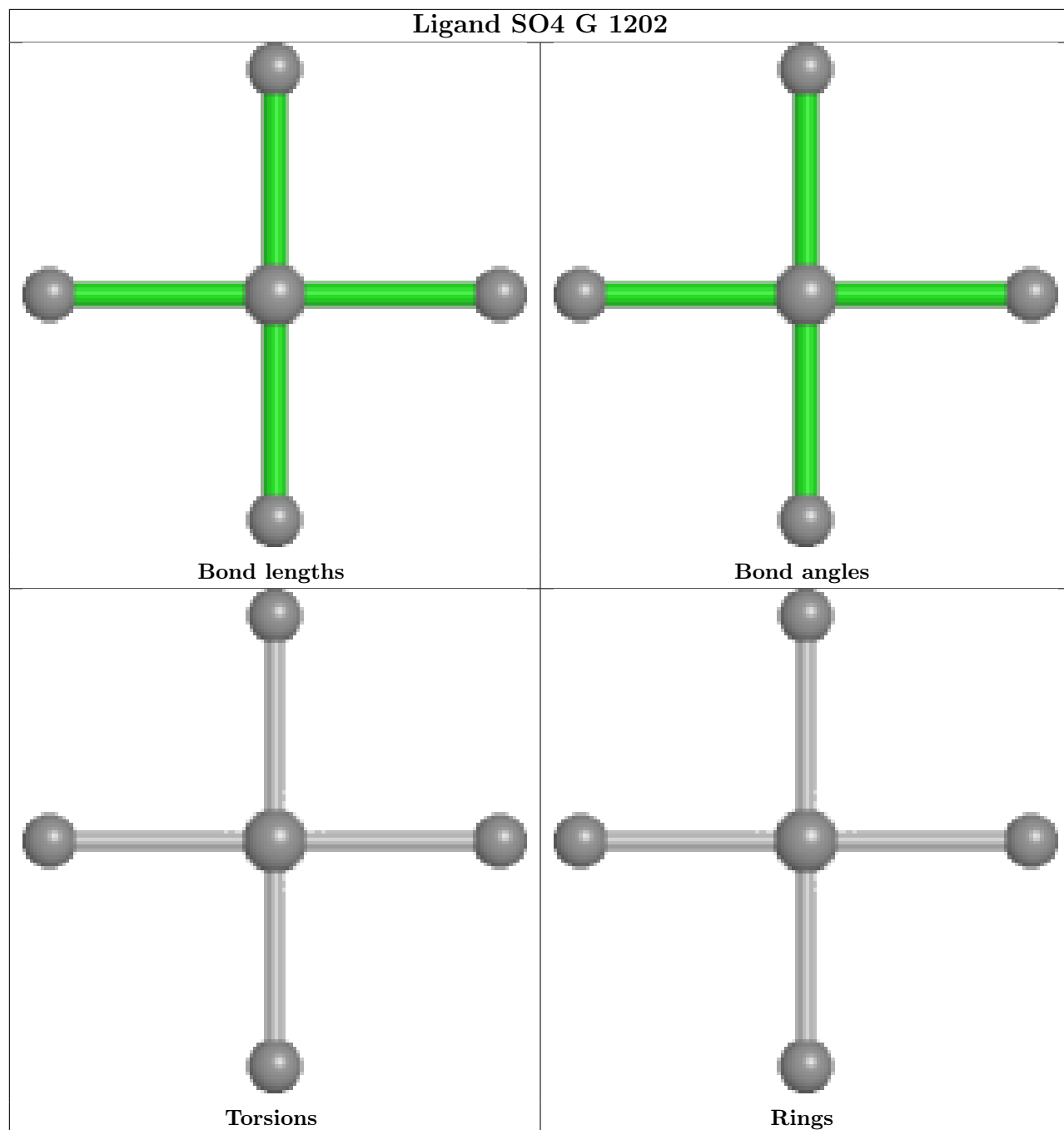


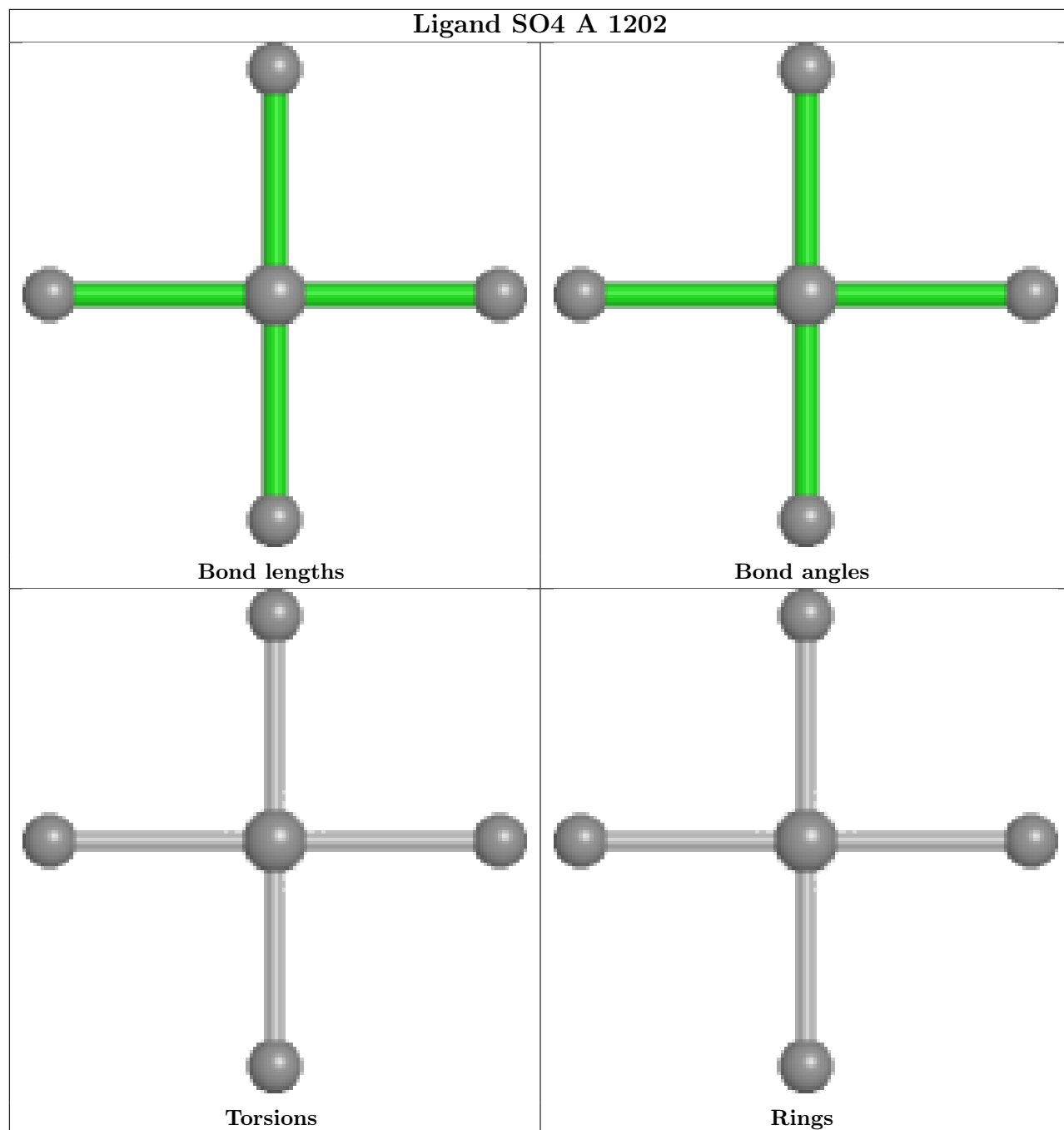




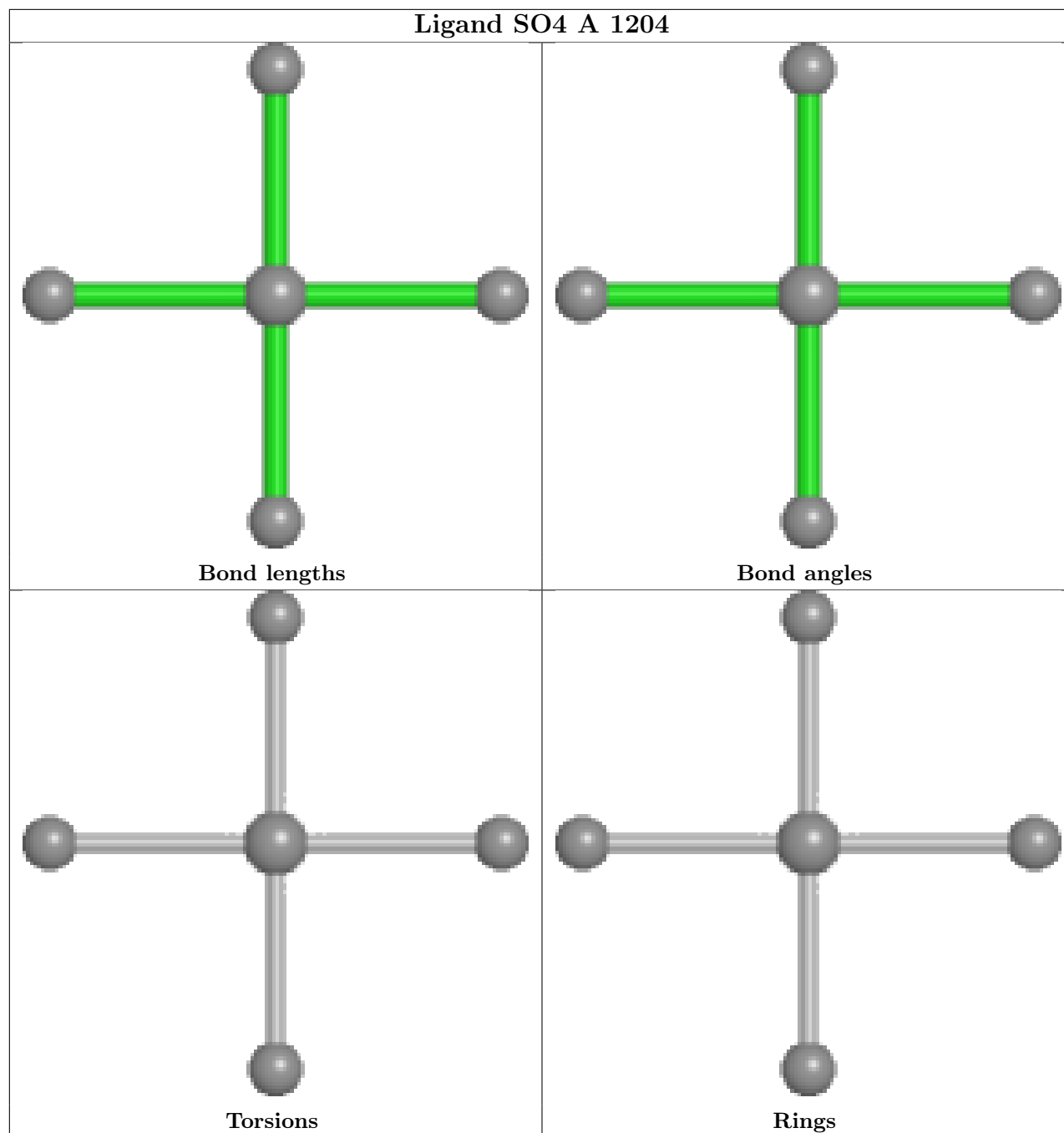












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	827/869 (95%)	-0.08	6 (0%) 87 88	52, 86, 130, 176	0
1	B	821/869 (94%)	-0.07	16 (1%) 66 64	49, 84, 175, 204	0
1	C	828/869 (95%)	-0.00	18 (2%) 62 59	60, 95, 149, 176	0
1	D	828/869 (95%)	0.22	36 (4%) 35 33	72, 119, 167, 196	0
1	E	829/869 (95%)	-0.08	10 (1%) 79 77	52, 84, 134, 170	0
1	F	826/869 (95%)	0.04	24 (2%) 51 50	49, 95, 166, 190	0
1	G	828/869 (95%)	-0.01	16 (1%) 66 64	61, 94, 135, 165	0
1	H	817/869 (94%)	0.42	50 (6%) 21 20	85, 134, 185, 214	0
All	All	6604/6952 (94%)	0.05	176 (2%) 54 51	49, 98, 164, 214	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	271	MET	6.1
1	B	233	PHE	5.2
1	H	742	LEU	4.9
1	H	271	MET	4.9
1	D	778	ILE	4.8

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

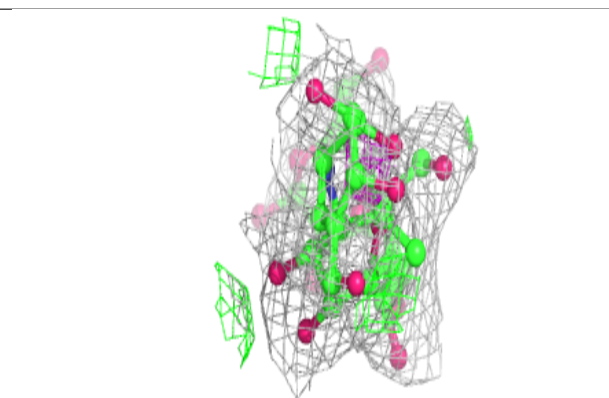
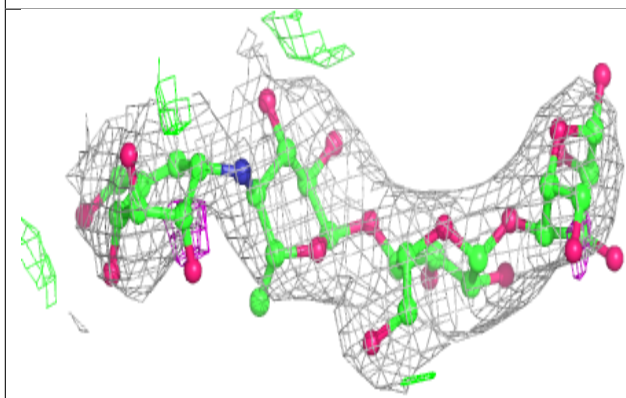
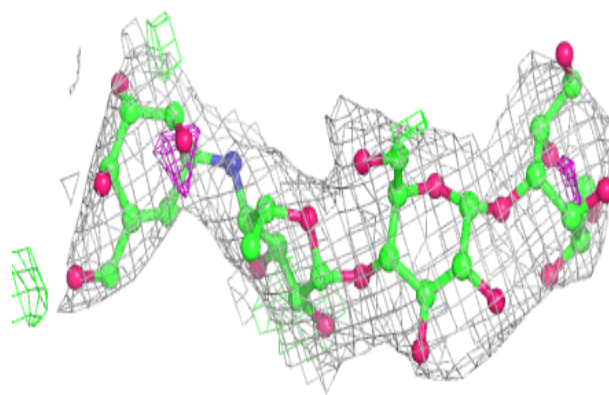
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AC1	P	3	21/22	0.75	0.38	120,152,170,185	0
2	GLC	K	2	11/12	0.79	0.33	100,125,140,141	0
2	GLC	L	1	12/12	0.80	0.37	121,140,149,156	0
2	GLC	P	2	11/12	0.81	0.46	121,139,152,163	0
2	GLC	O	1	12/12	0.82	0.28	120,138,149,151	0
2	GLC	L	2	11/12	0.85	0.36	116,128,141,143	0
2	GLC	P	1	12/12	0.85	0.28	142,159,173,183	0
2	GLC	O	2	11/12	0.86	0.31	104,125,135,136	0
2	GLC	N	1	12/12	0.87	0.26	103,131,137,154	0
2	GLC	K	1	12/12	0.87	0.23	116,131,135,139	0
2	AC1	K	3	21/22	0.88	0.26	97,119,143,152	0
2	GLC	M	1	12/12	0.89	0.25	99,124,133,138	0
2	GLC	M	2	11/12	0.89	0.35	81,111,131,131	0
2	GLC	J	2	11/12	0.89	0.28	100,117,123,134	0
2	AC1	L	3	21/22	0.89	0.26	102,133,147,154	0
2	GLC	I	1	12/12	0.90	0.24	109,127,151,153	0
2	AC1	J	3	21/22	0.90	0.27	89,106,128,131	0
2	GLC	I	2	11/12	0.91	0.37	102,108,118,120	0
2	GLC	N	2	11/12	0.91	0.22	86,105,135,139	0
2	AC1	N	3	21/22	0.91	0.24	75,105,121,131	0
2	AC1	I	3	21/22	0.91	0.28	76,103,124,135	0
2	AC1	O	3	21/22	0.92	0.22	77,110,125,147	0
2	AC1	M	3	21/22	0.92	0.26	77,100,115,124	0
2	GLC	J	1	12/12	0.93	0.25	112,126,139,143	0

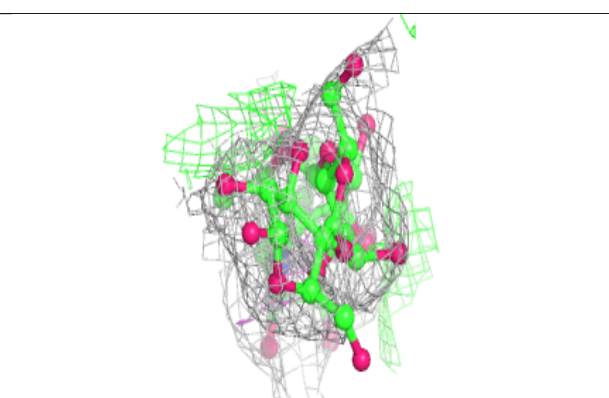
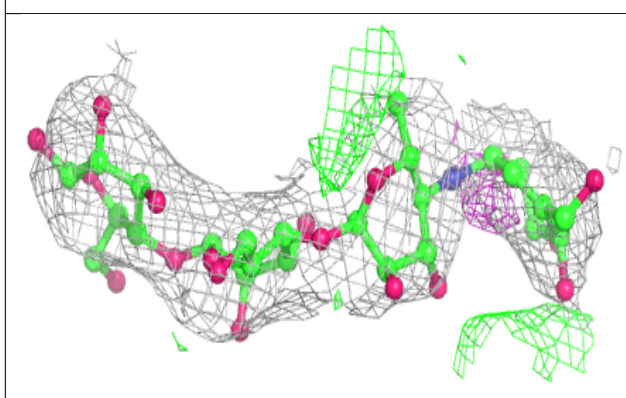
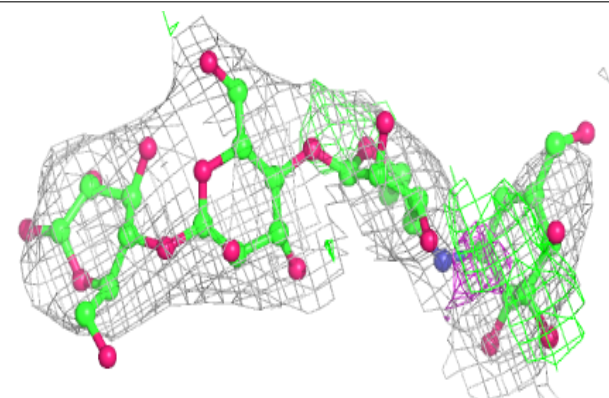
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain I:**

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

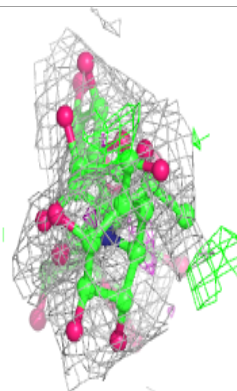
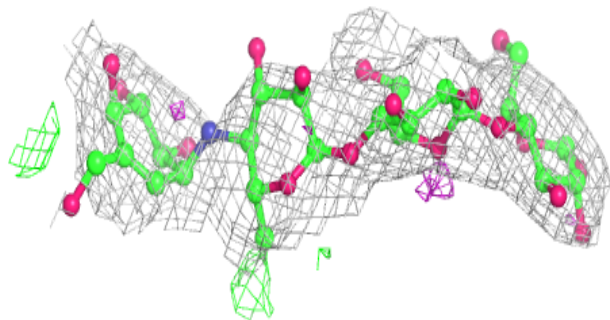
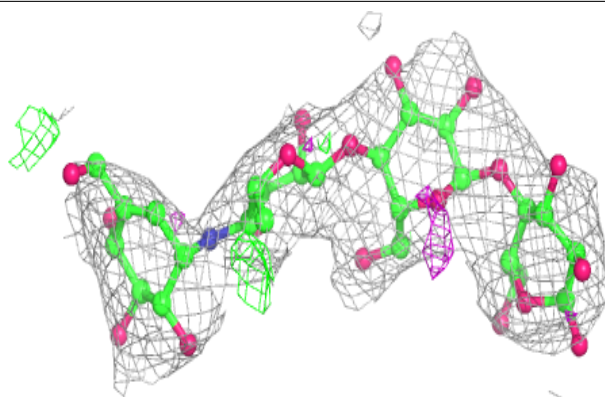
**Electron density around Chain J:**

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

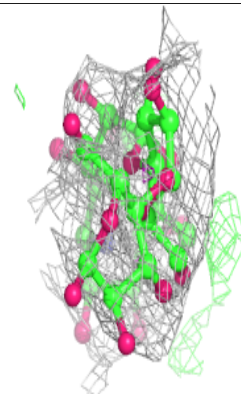
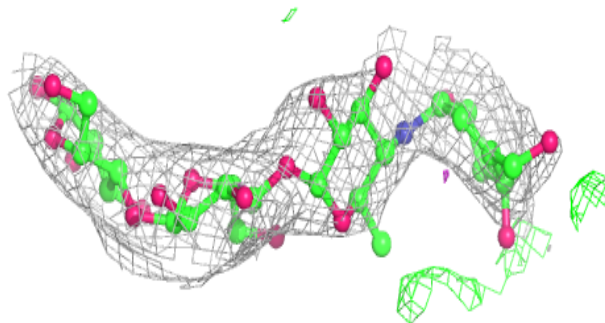
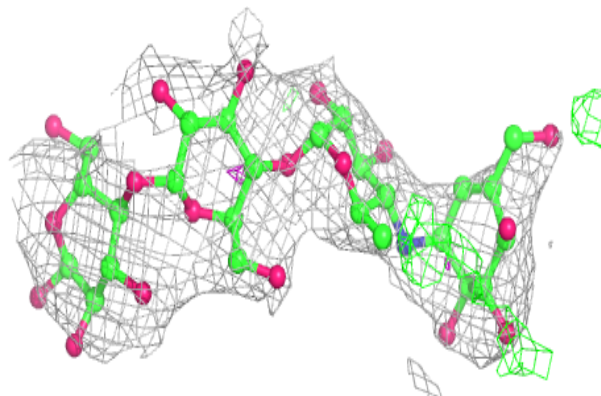


**Electron density around Chain K:**

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

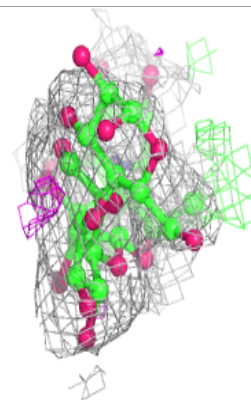
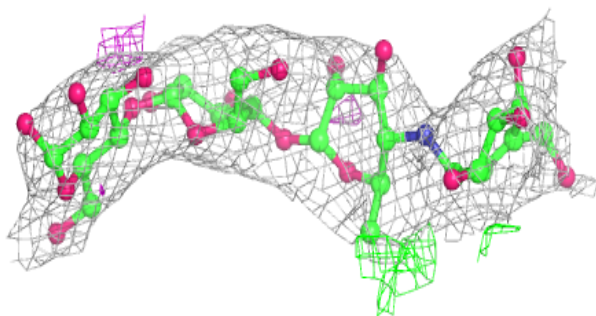
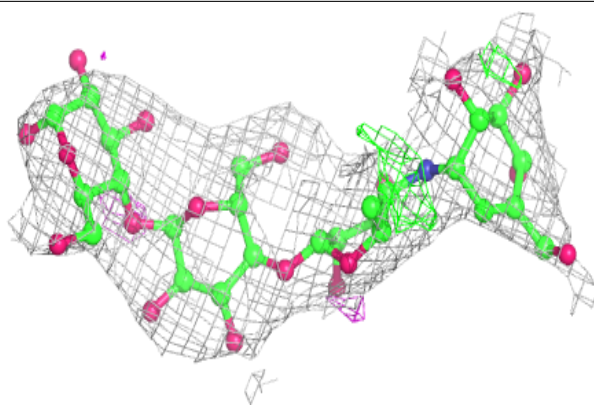
**Electron density around Chain L:**

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

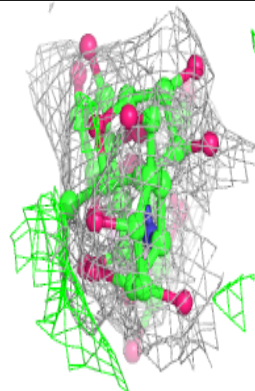
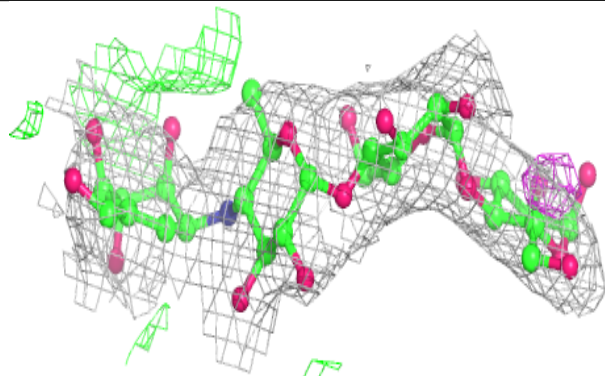
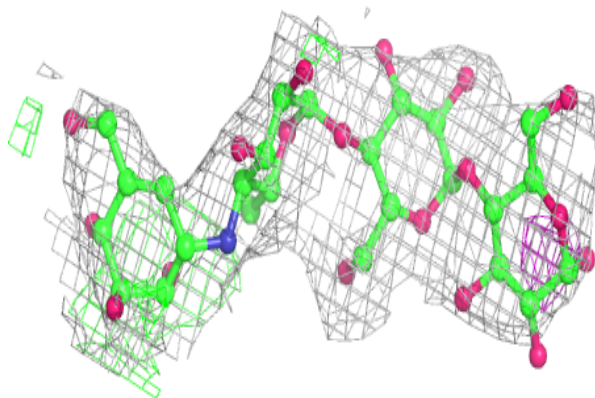


**Electron density around Chain M:**

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

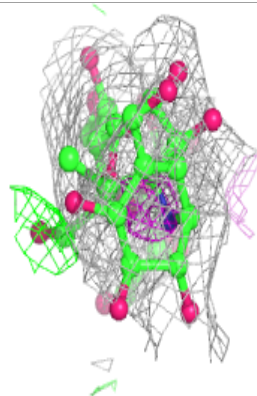
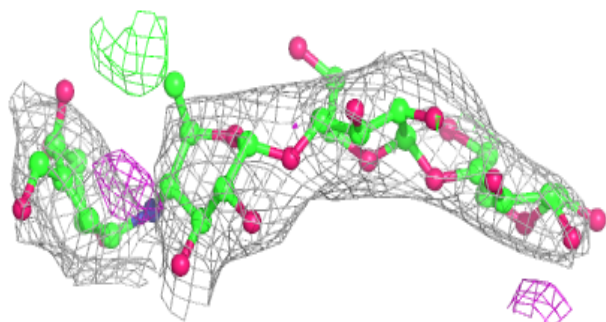
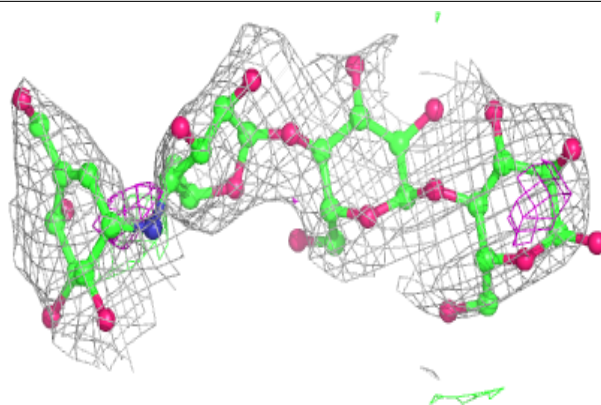
**Electron density around Chain N:**

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

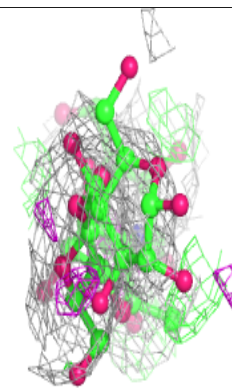
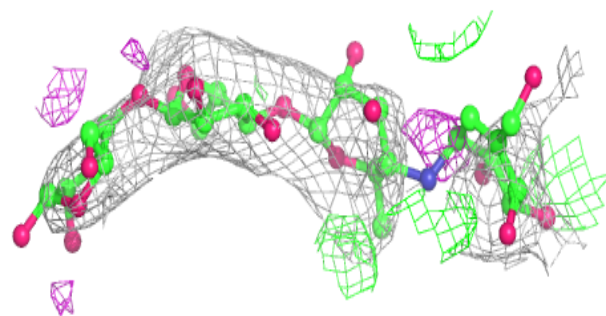
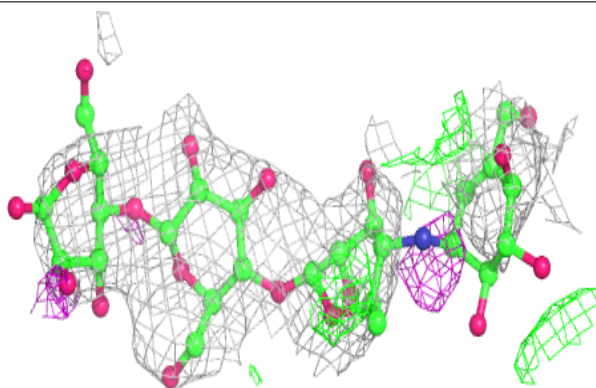


**Electron density around Chain O:**

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

**Electron density around Chain P:**

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



## 6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	C	1203	5/5	0.62	0.30	130,155,163,182	0
4	SO4	F	1203	5/5	0.62	0.29	118,139,178,179	0
4	SO4	F	1204	5/5	0.62	0.31	121,146,175,181	0
4	SO4	B	1207	5/5	0.65	0.37	137,158,168,187	0
4	SO4	D	1204	5/5	0.71	0.40	132,138,149,175	0
4	SO4	F	1205	5/5	0.72	0.29	129,147,157,171	0
4	SO4	E	1208	5/5	0.74	0.17	139,144,148,178	0
4	SO4	C	1204	5/5	0.78	0.32	140,141,164,181	0
4	SO4	C	1202	5/5	0.78	0.23	128,154,185,187	0
4	SO4	C	1206	5/5	0.79	0.32	114,122,164,168	0
4	SO4	C	1205	5/5	0.79	0.28	123,156,184,189	0
4	SO4	G	1204	5/5	0.79	0.32	144,152,175,178	0
4	SO4	G	1202	5/5	0.80	0.26	143,145,163,178	0
4	SO4	B	1205	5/5	0.80	0.23	156,166,173,186	0
4	SO4	G	1205	5/5	0.80	0.26	131,138,158,168	0
4	SO4	G	1203	5/5	0.81	0.17	108,116,154,157	0
4	SO4	B	1208	5/5	0.82	0.20	114,130,161,163	0
4	SO4	B	1203	5/5	0.83	0.17	101,110,138,164	0
4	SO4	D	1205	5/5	0.84	0.27	131,135,151,158	0
4	SO4	A	1202	5/5	0.85	0.22	79,114,144,148	0
4	SO4	D	1203	5/5	0.86	0.21	156,165,185,200	0
4	SO4	D	1206	5/5	0.86	0.20	144,149,172,180	0
4	SO4	A	1203	5/5	0.86	0.18	98,129,138,154	0
4	SO4	F	1206	5/5	0.86	0.21	125,136,153,164	0
4	SO4	H	1202	5/5	0.86	0.17	158,163,186,189	0
4	SO4	D	1202	5/5	0.87	0.23	124,143,148,156	0
4	SO4	B	1204	5/5	0.88	0.16	135,137,152,153	0
4	SO4	B	1202	5/5	0.88	0.18	57,108,129,142	0
4	SO4	A	1205	5/5	0.88	0.19	129,130,157,169	0
4	SO4	E	1203	5/5	0.89	0.15	88,111,118,135	0
4	SO4	A	1204	5/5	0.90	0.46	101,138,162,173	0
4	SO4	E	1204	5/5	0.90	0.32	119,137,159,161	0
4	SO4	E	1207	5/5	0.91	0.13	124,144,165,168	0
4	SO4	F	1202	5/5	0.92	0.17	140,147,166,169	0
3	CA	A	1201	1/1	0.92	0.36	116,116,116,116	0
4	SO4	E	1205	5/5	0.93	0.12	100,102,134,145	0
3	CA	H	1201	1/1	0.93	0.23	98,98,98,98	0

*Continued on next page...*



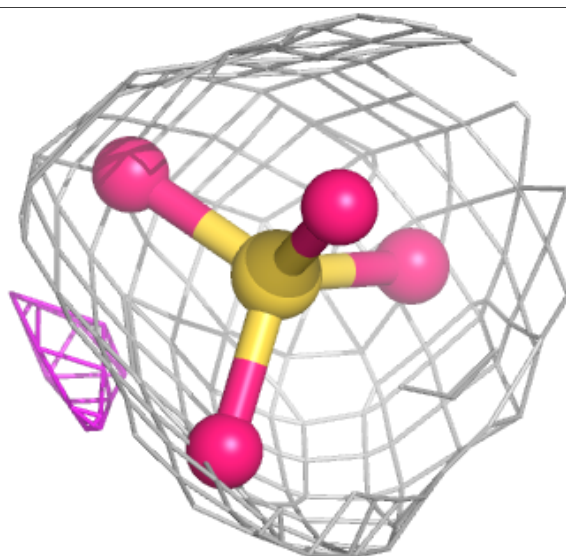
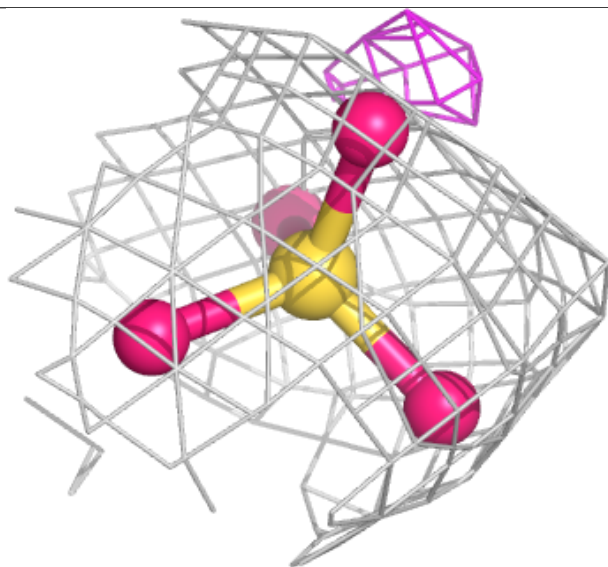
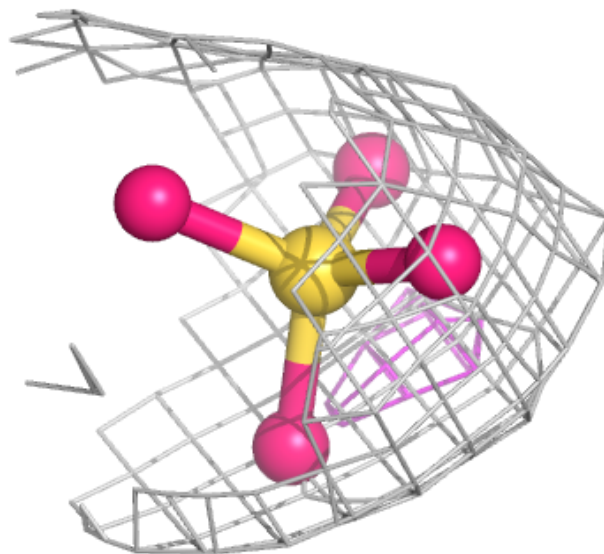
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	F	1207	5/5	0.93	0.36	105,123,131,142	0
4	SO4	E	1202	5/5	0.93	0.16	98,102,129,130	0
4	SO4	B	1206	5/5	0.94	0.24	123,124,137,140	0
4	SO4	A	1206	5/5	0.94	0.13	91,134,142,152	0
4	SO4	A	1207	5/5	0.94	0.21	144,150,168,169	0
3	CA	C	1201	1/1	0.97	0.22	80,80,80,80	0
4	SO4	E	1206	5/5	0.97	0.31	91,120,129,143	0
3	CA	B	1201	1/1	0.97	0.24	94,94,94,94	0
3	CA	D	1201	1/1	0.98	0.20	71,71,71,71	0
3	CA	E	1201	1/1	0.98	0.25	74,74,74,74	0
3	CA	F	1201	1/1	0.99	0.24	68,68,68,68	0
3	CA	G	1201	1/1	0.99	0.23	75,75,75,75	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.

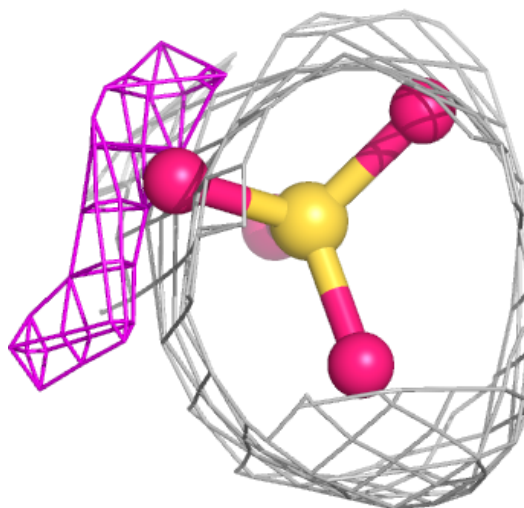
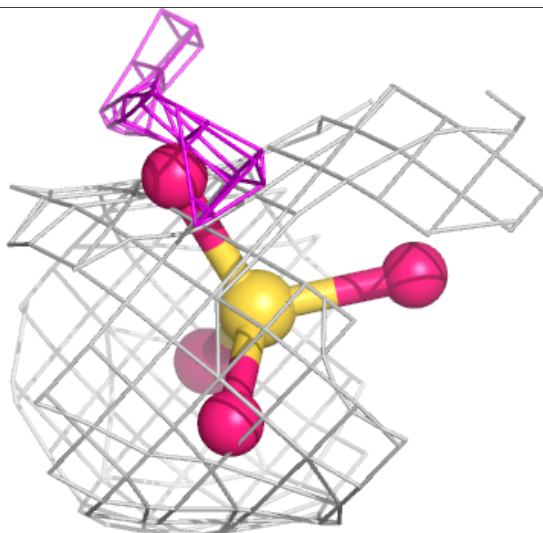
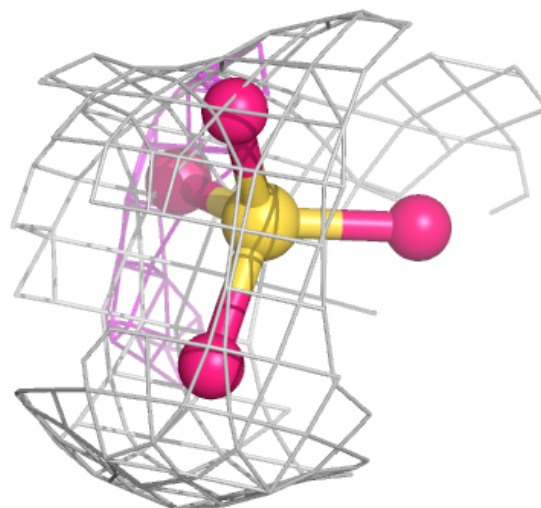
**Electron density around SO4 C 1203:**

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



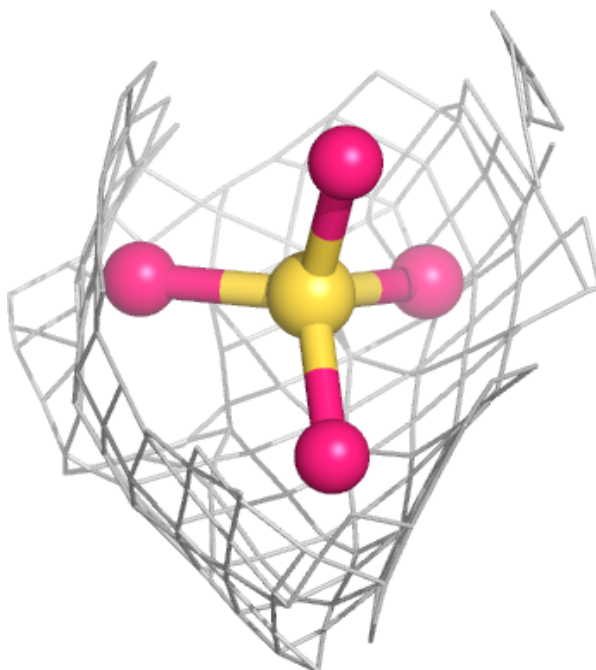
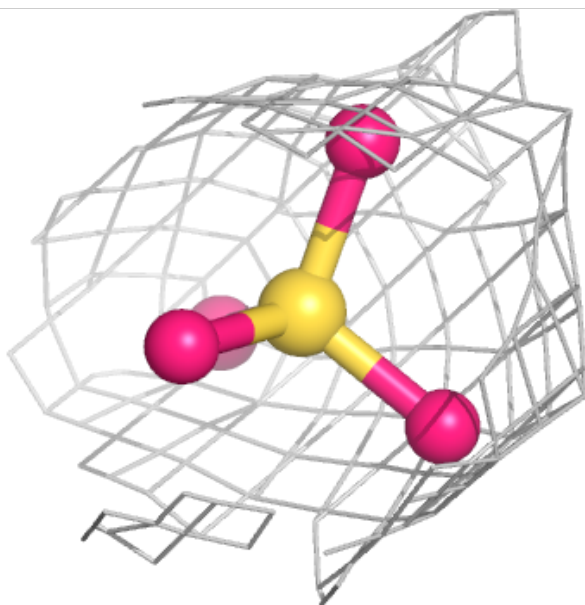
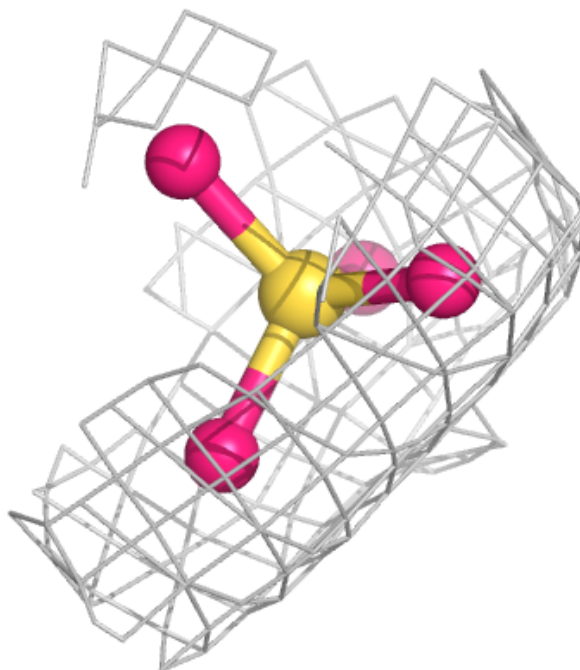
**Electron density around SO4 F 1203:**

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



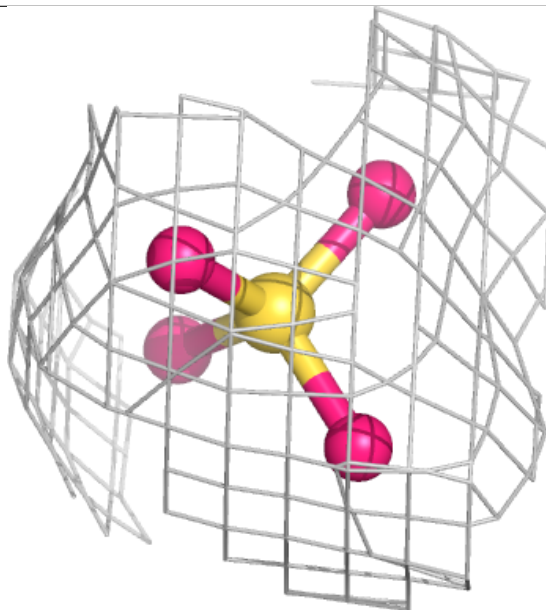
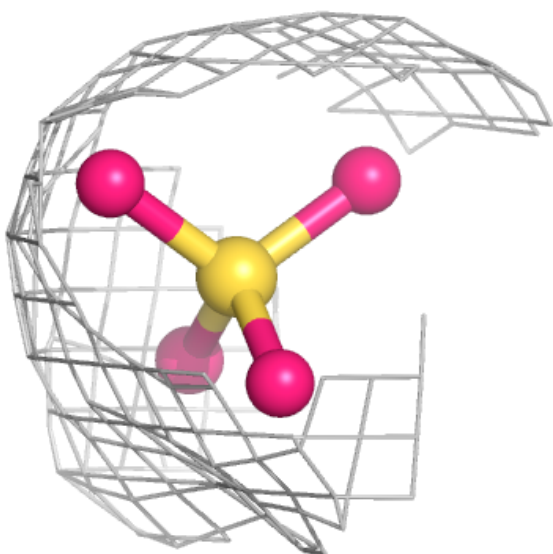
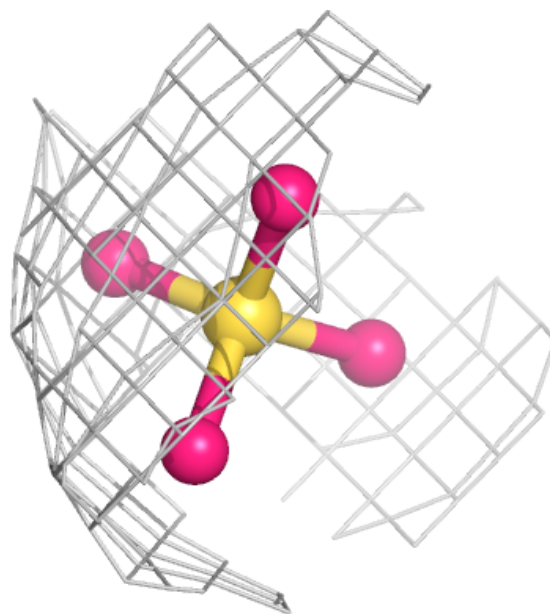
**Electron density around SO4 F 1204:**

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



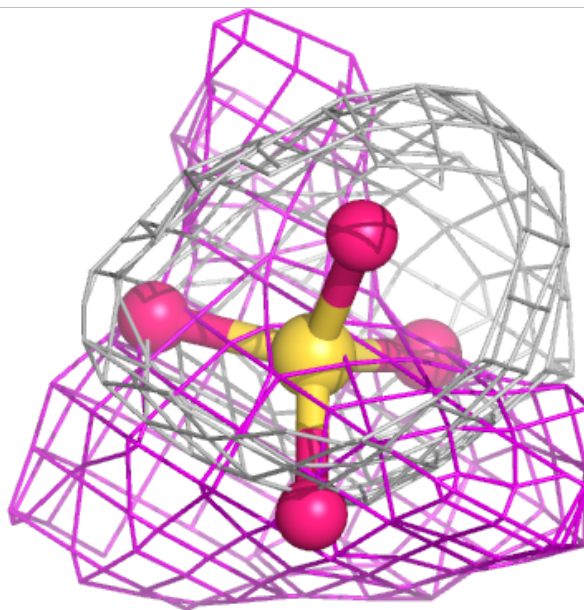
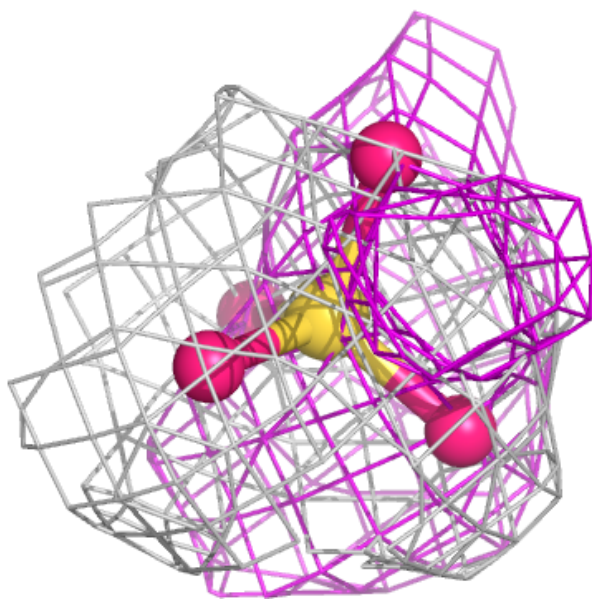
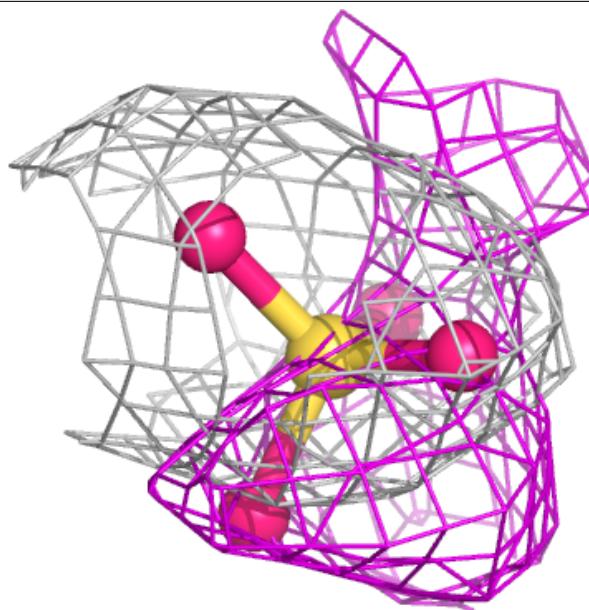
**Electron density around SO4 B 1207:**

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



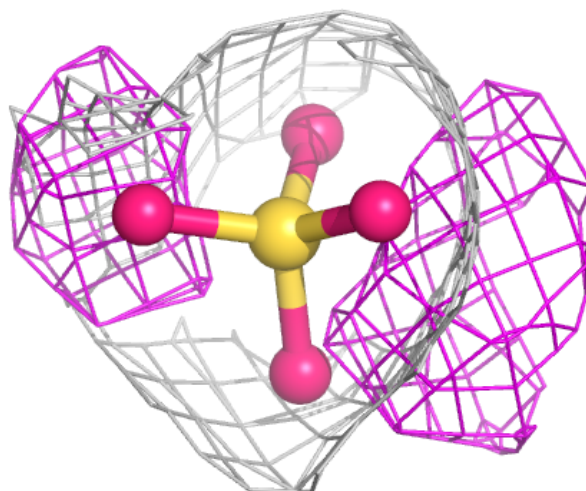
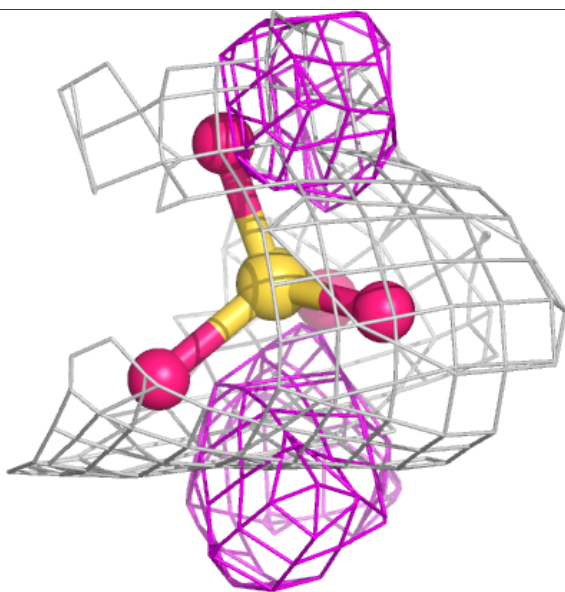
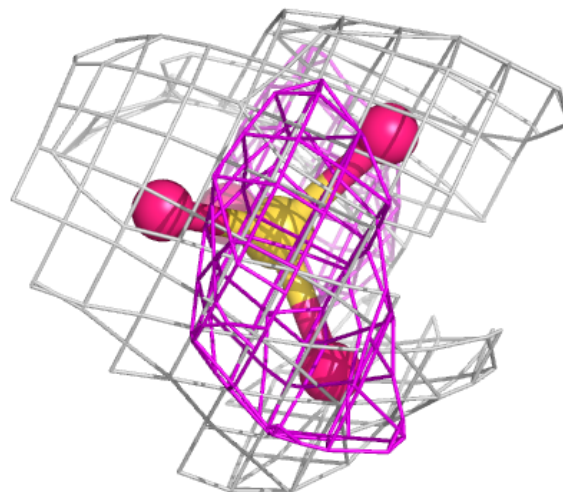
**Electron density around SO4 D 1204:**

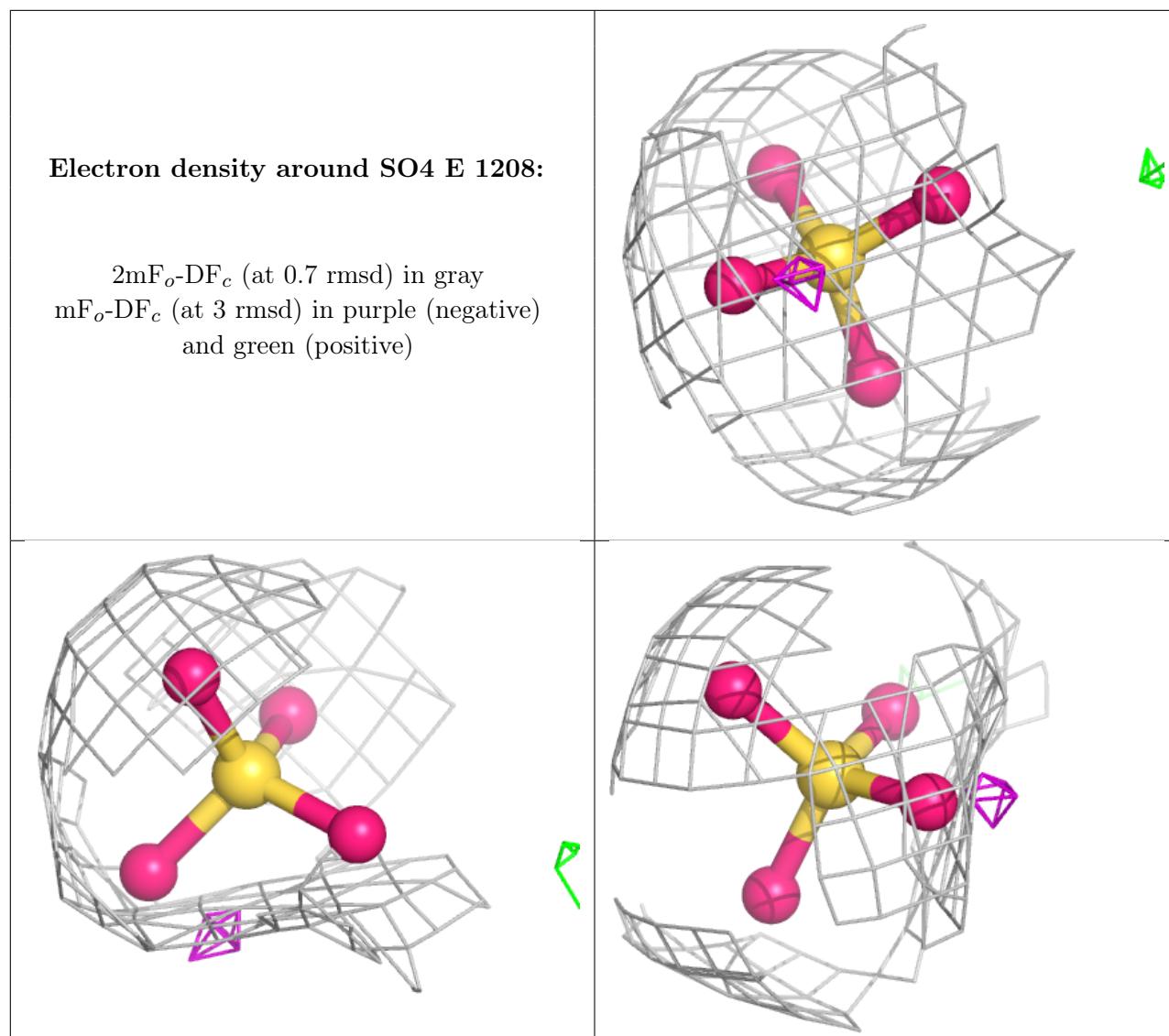
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 F 1205:**

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

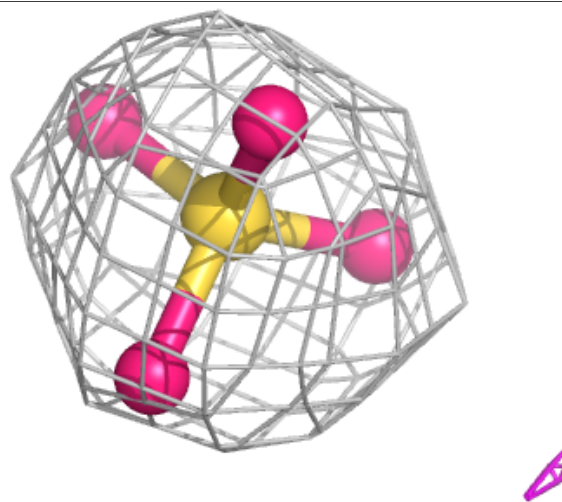
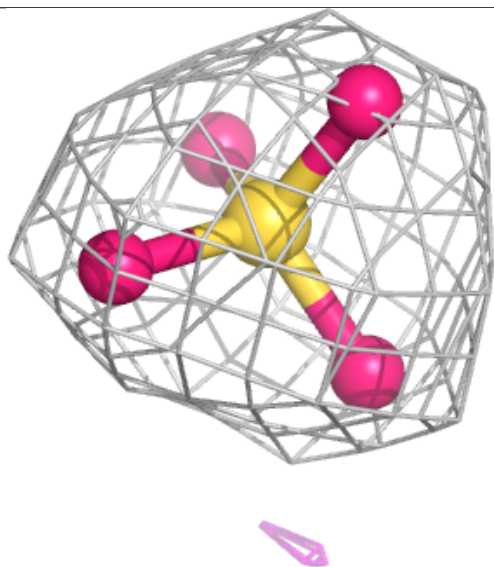
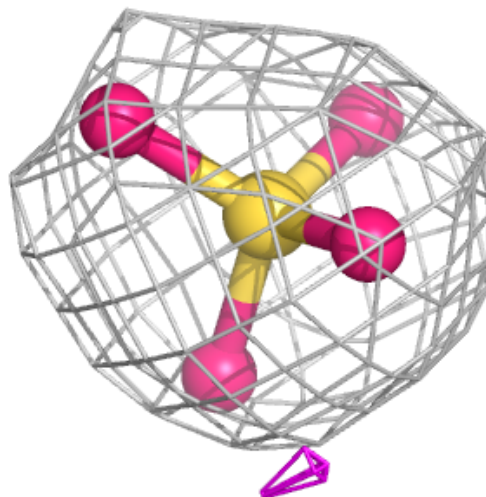


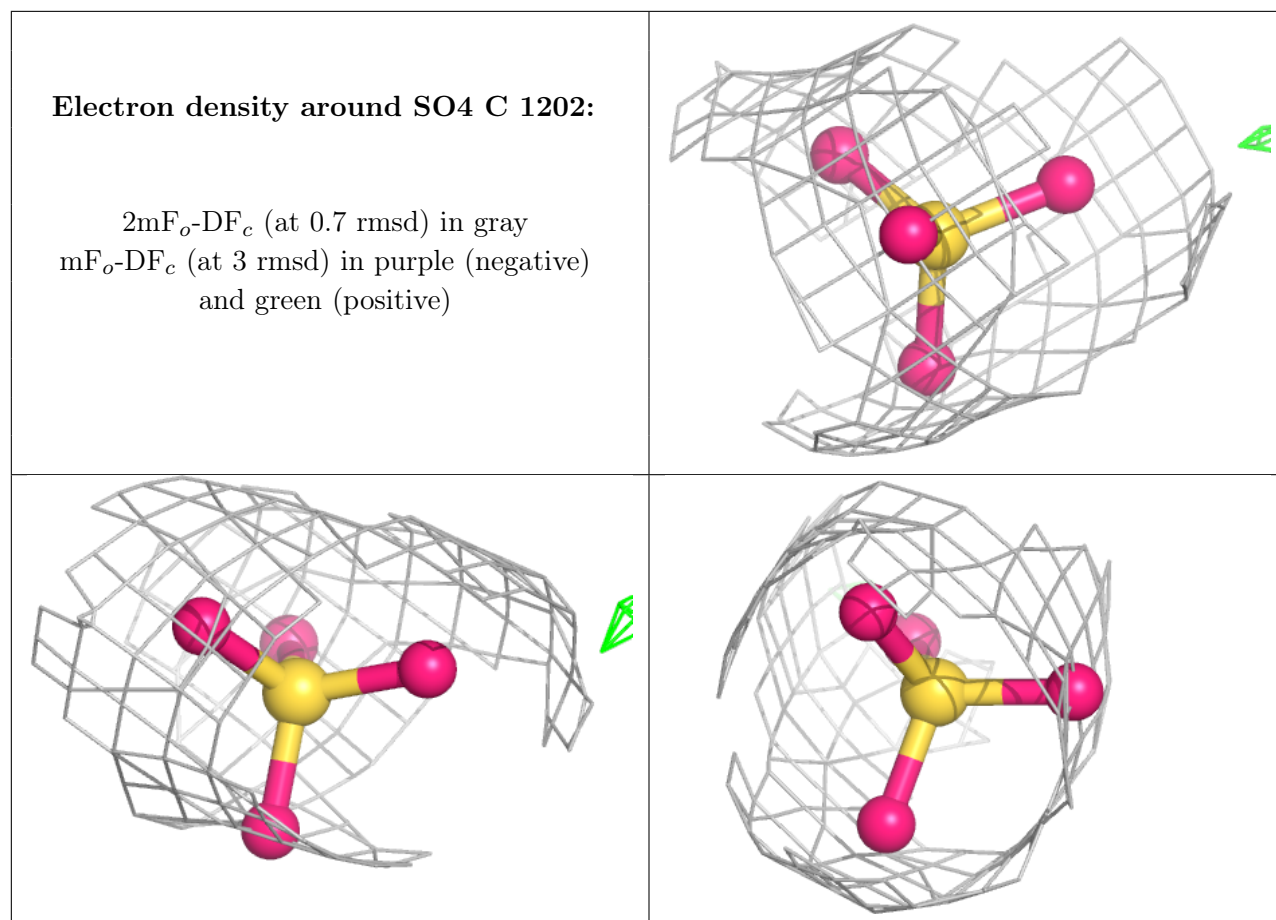




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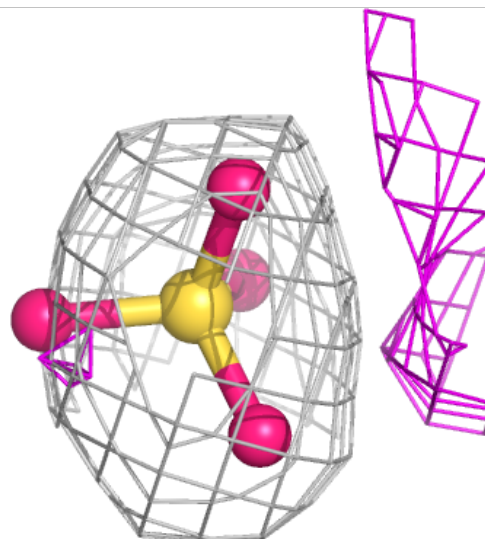
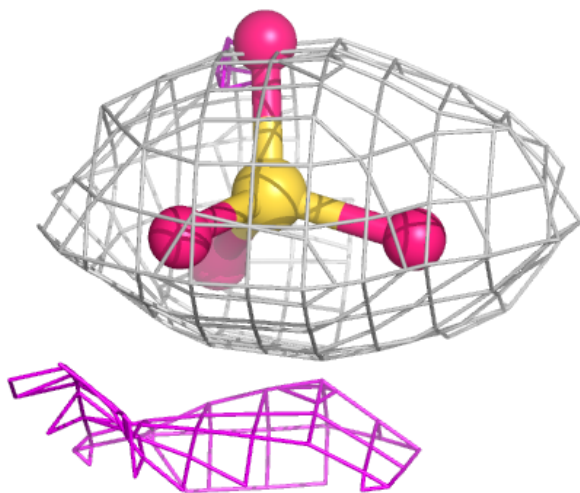
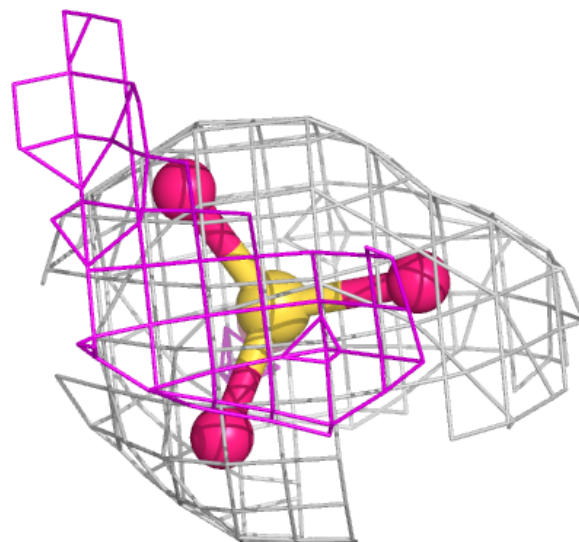
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





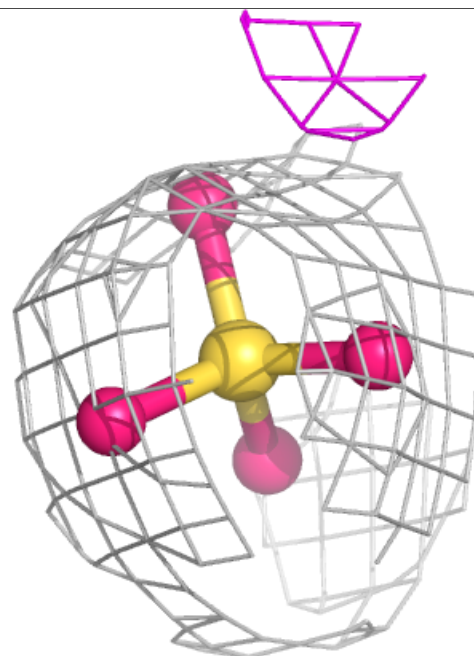
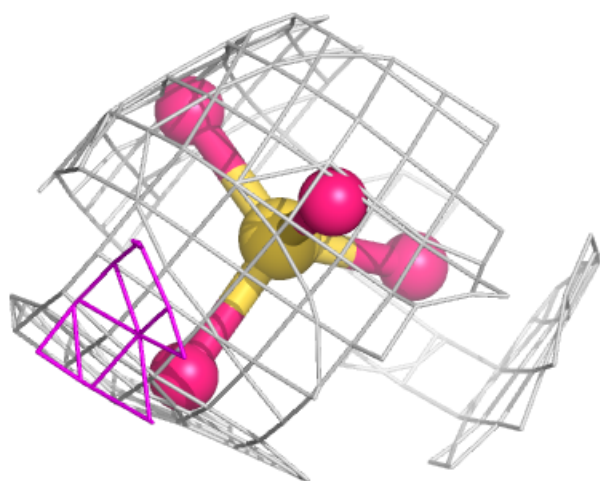
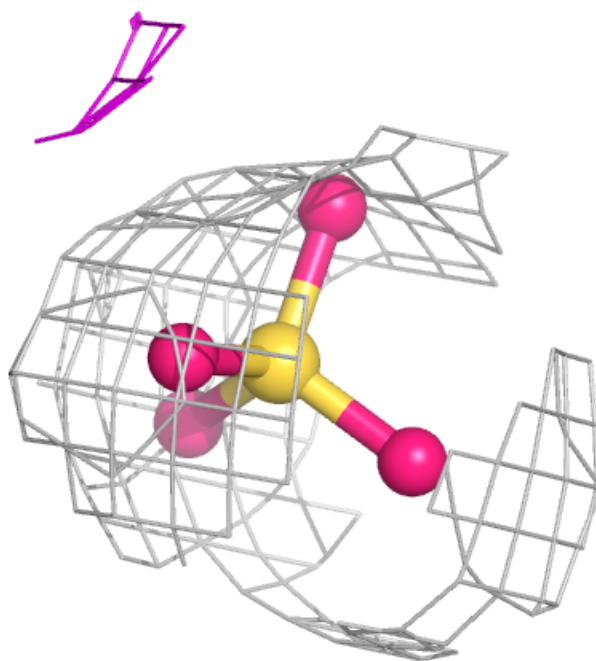
**Electron density around SO4 C 1206:**

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



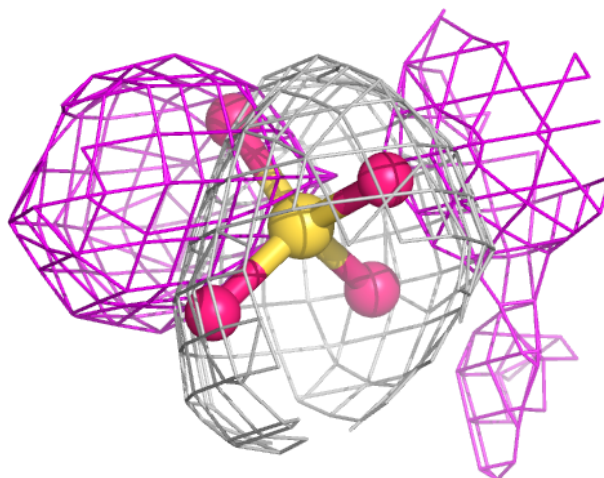
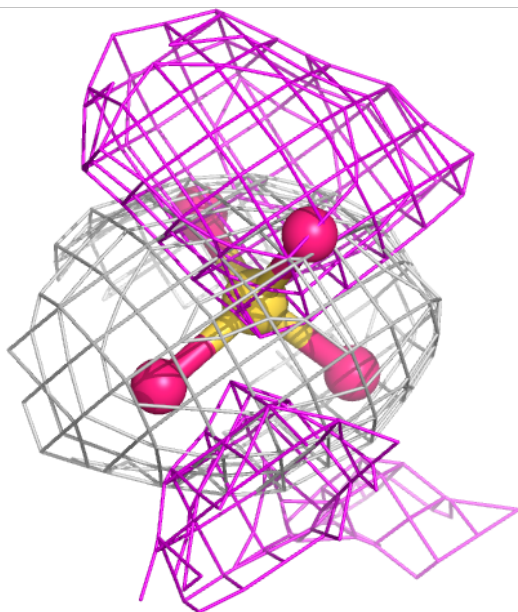
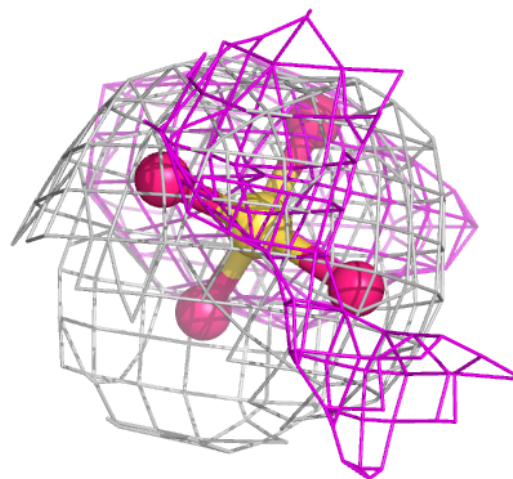
**Electron density around SO4 C 1205:**

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



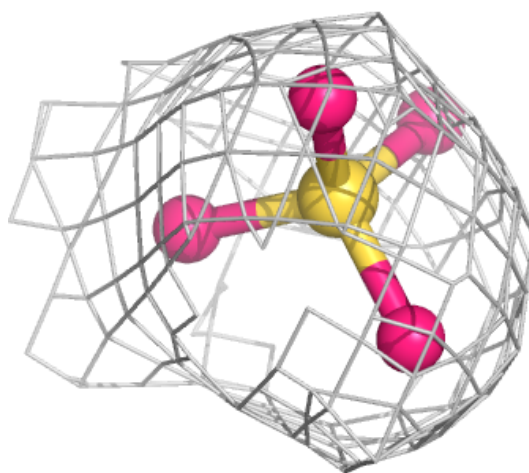
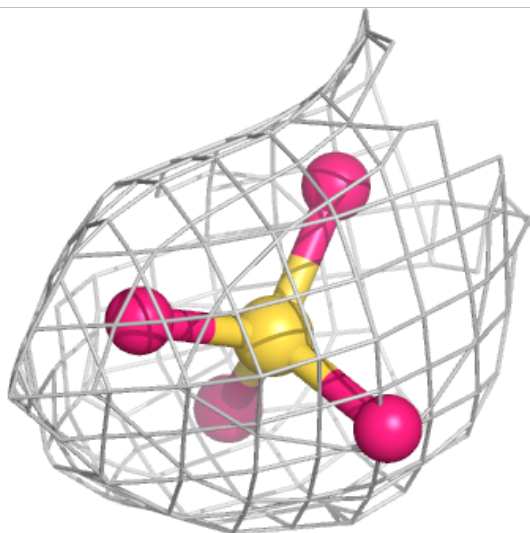
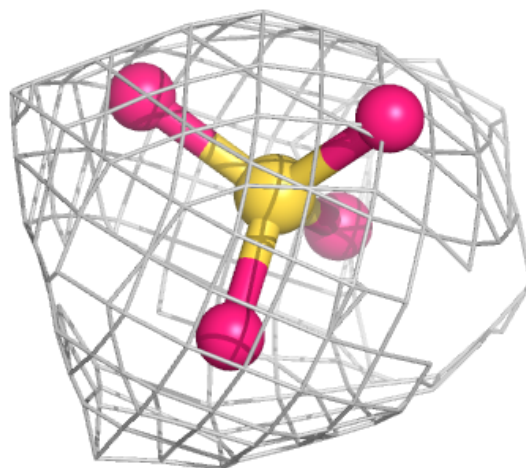
**Electron density around SO4 G 1204:**

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



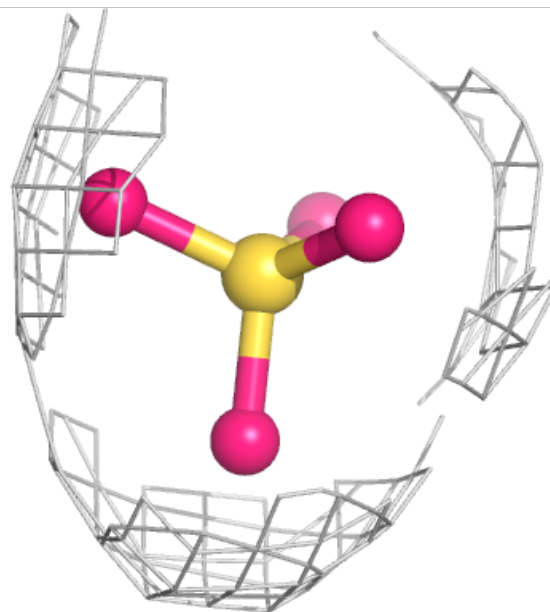
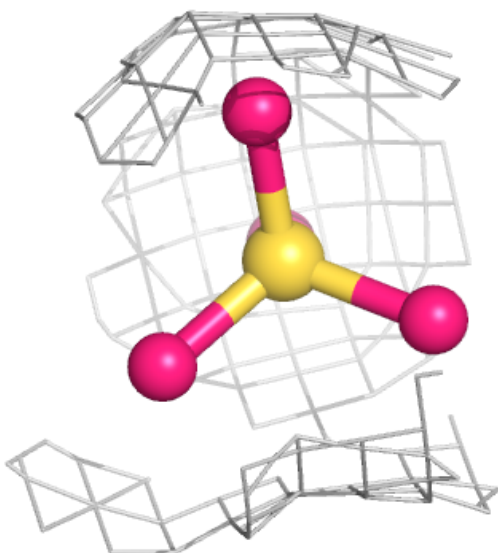
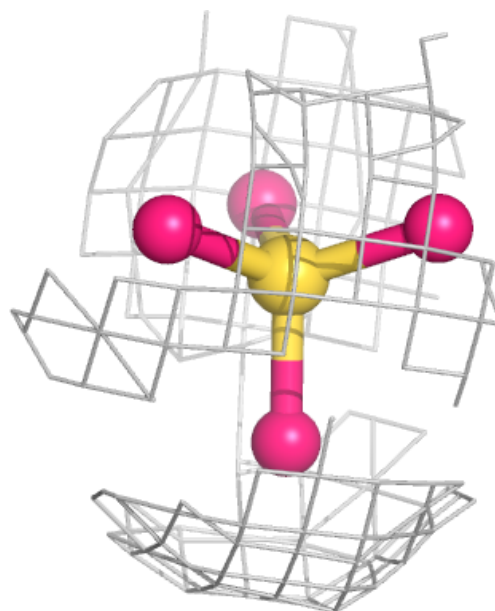
**Electron density around SO4 G 1202:**

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



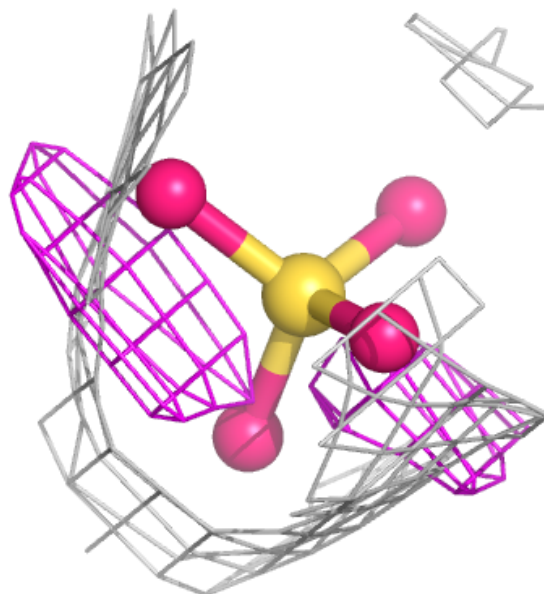
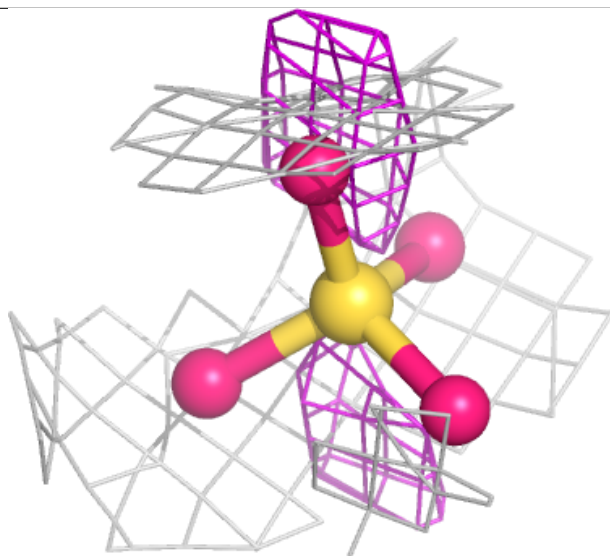
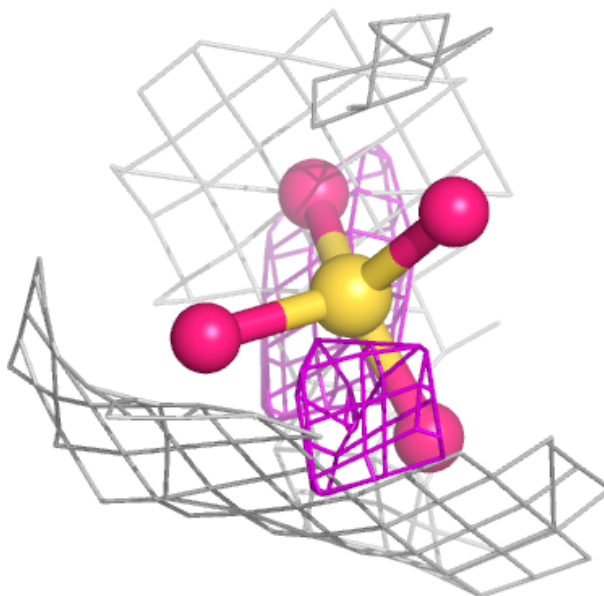
**Electron density around SO4 B 1205:**

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



**Electron density around SO4 G 1205:**

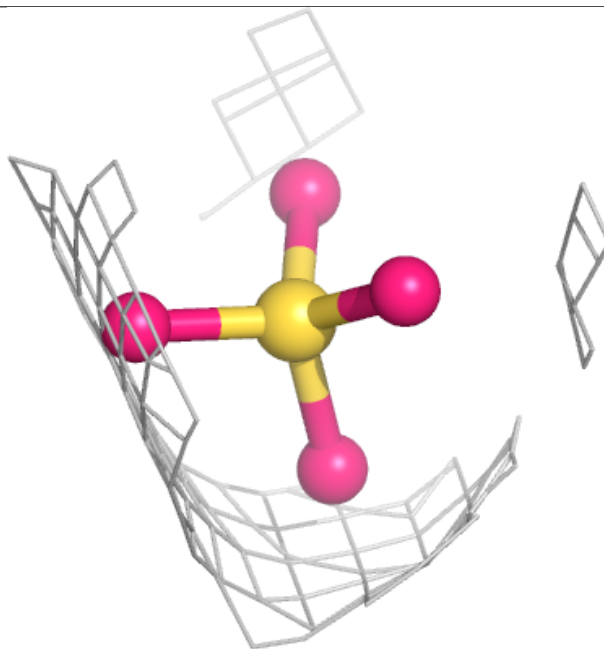
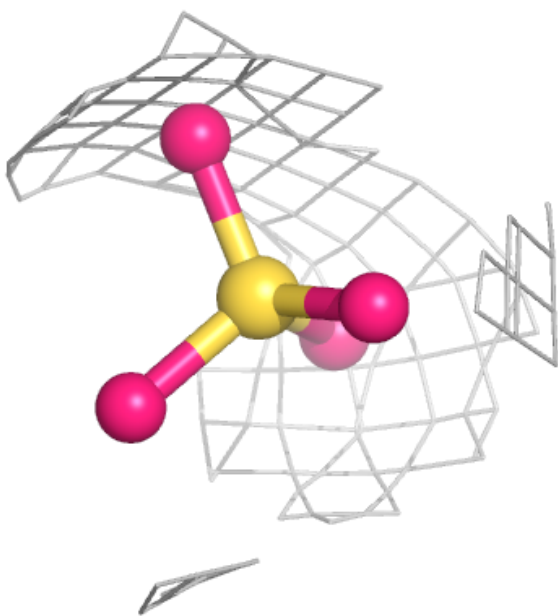
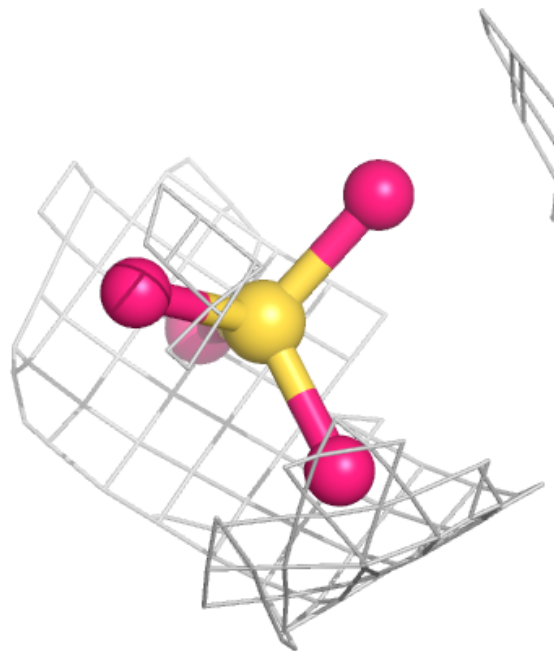
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





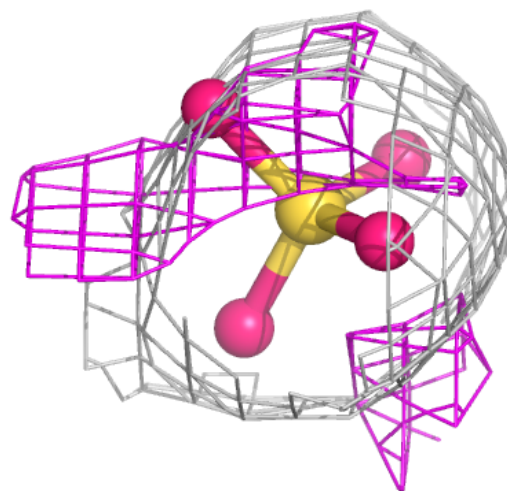
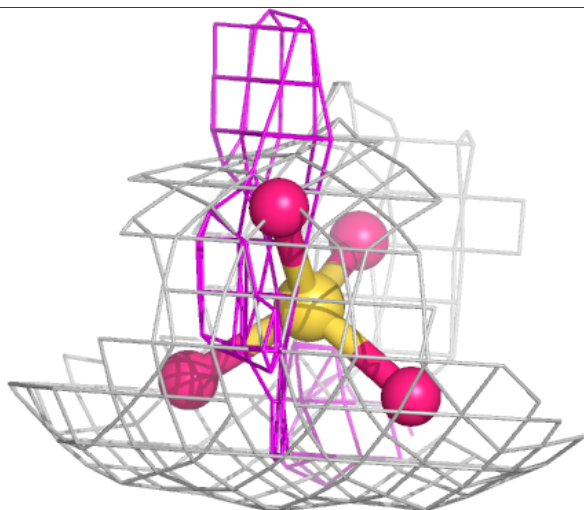
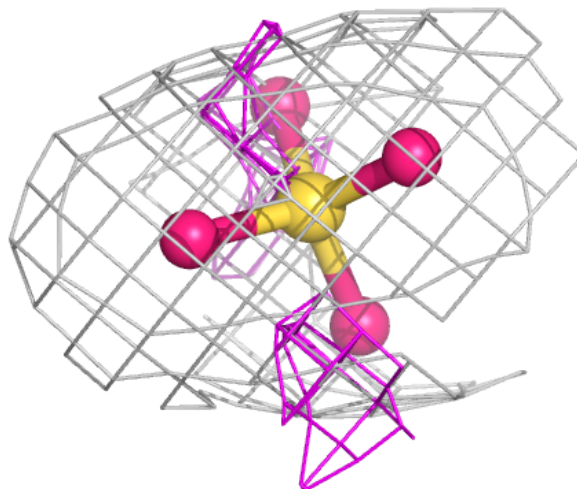
**Electron density around SO4 G 1203:**

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



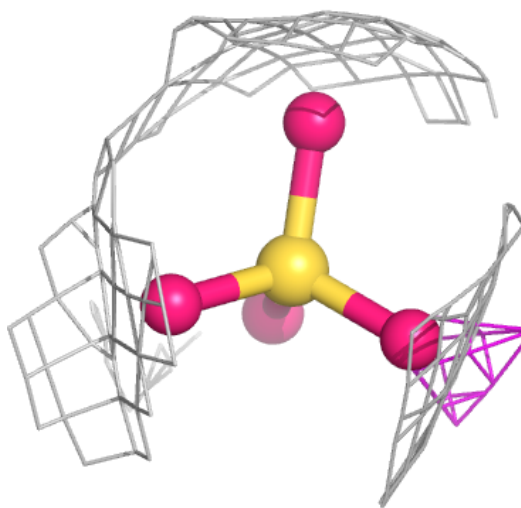
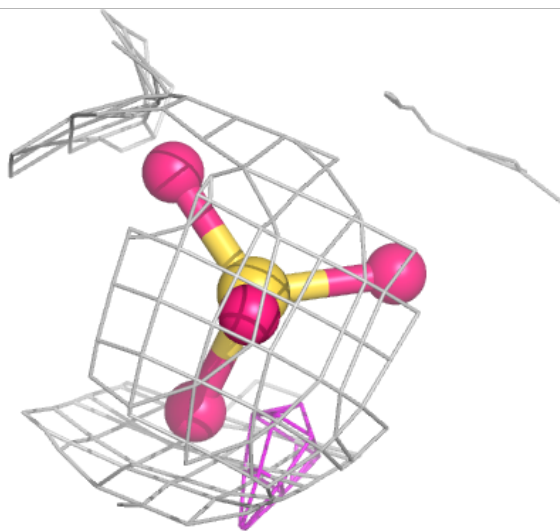
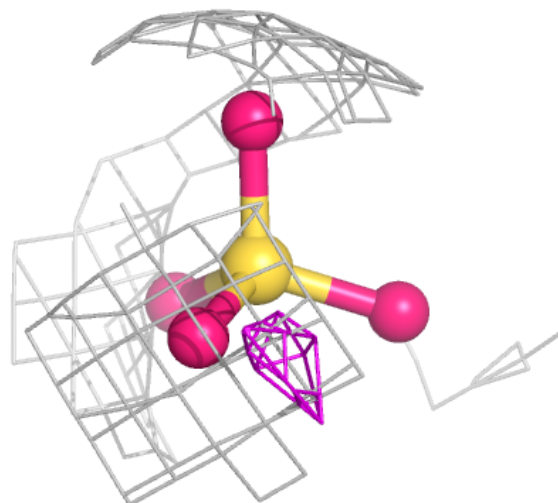
**Electron density around SO4 B 1208:**

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



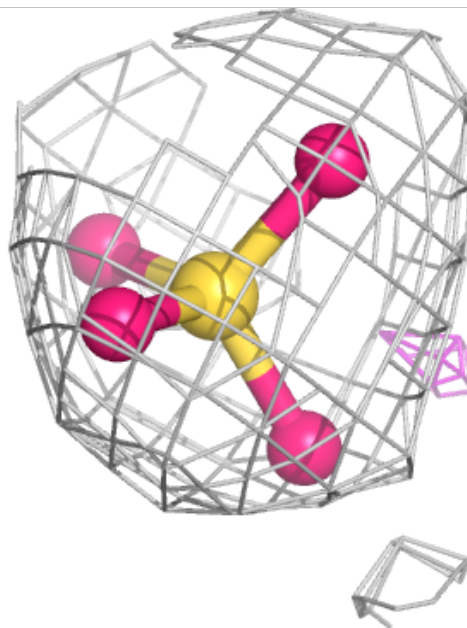
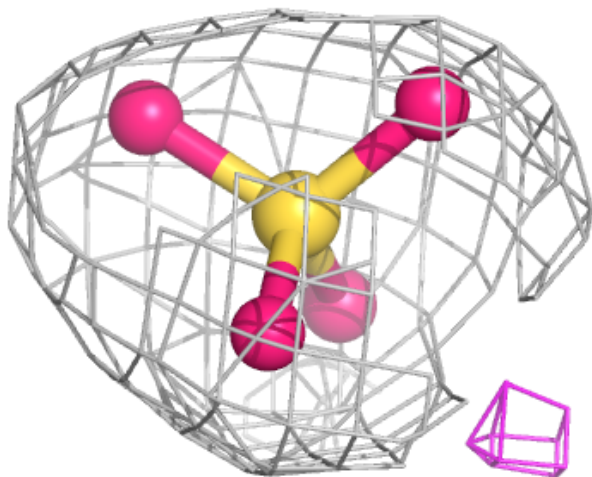
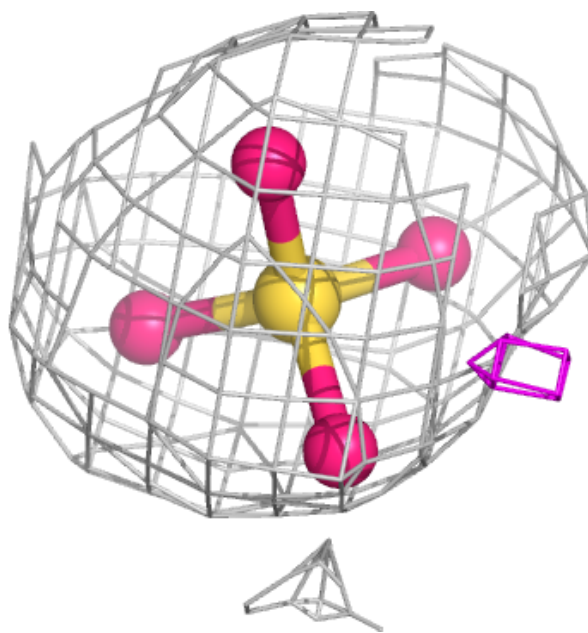
**Electron density around SO4 B 1203:**

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



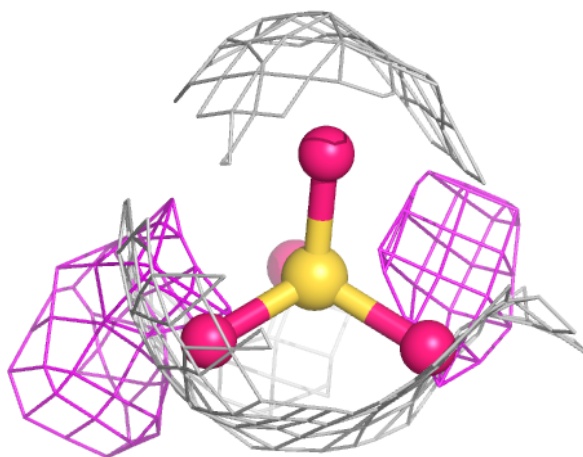
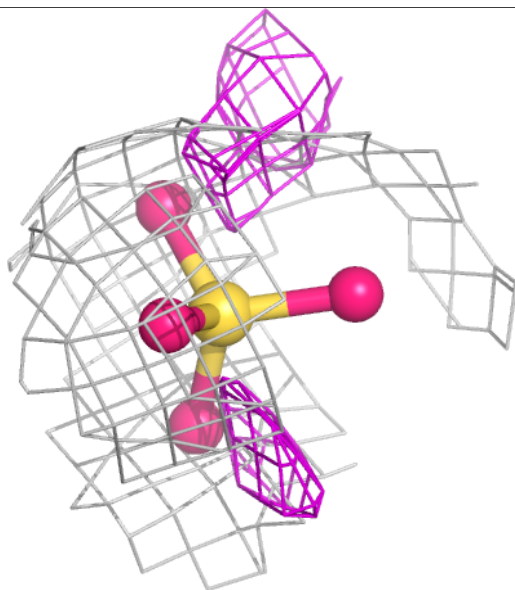
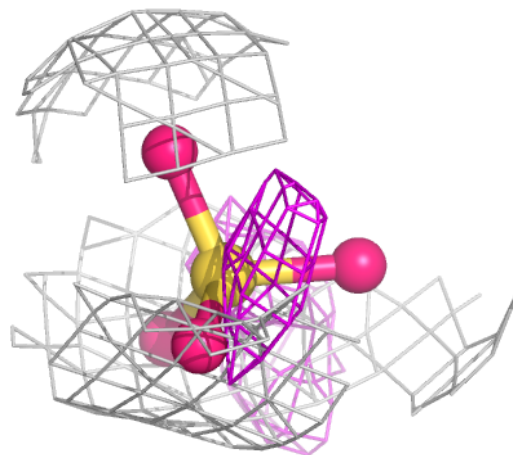
**Electron density around SO4 D 1205:**

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



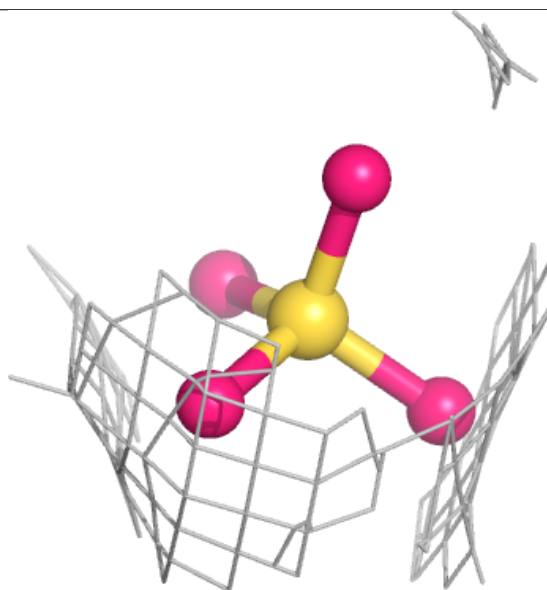
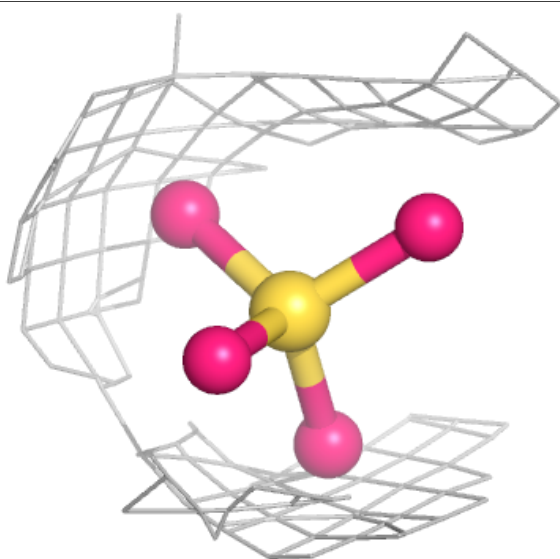
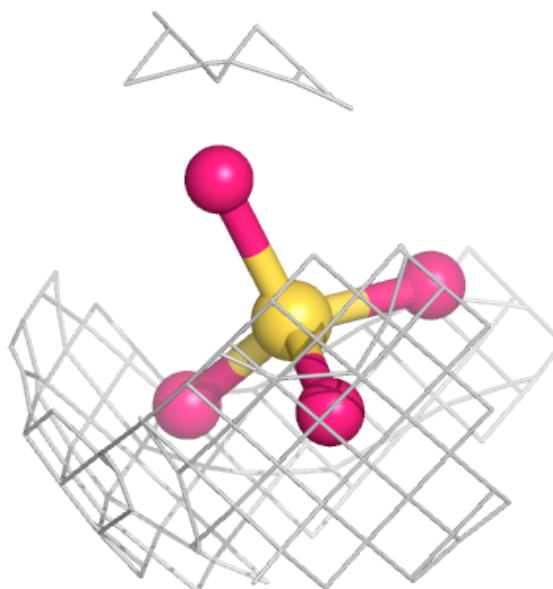
**Electron density around SO4 A 1202:**

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



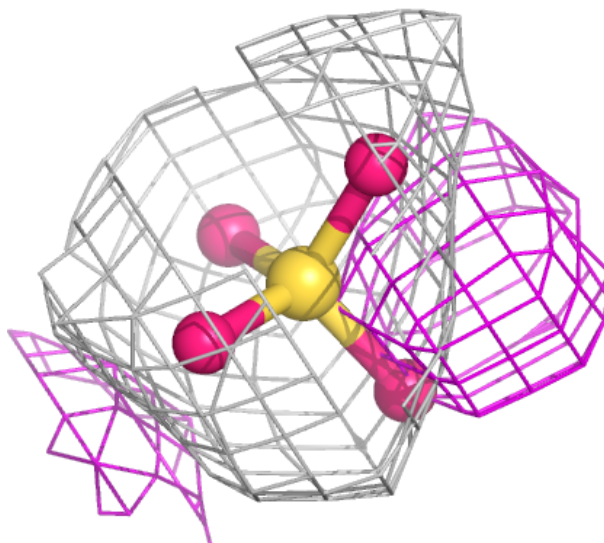
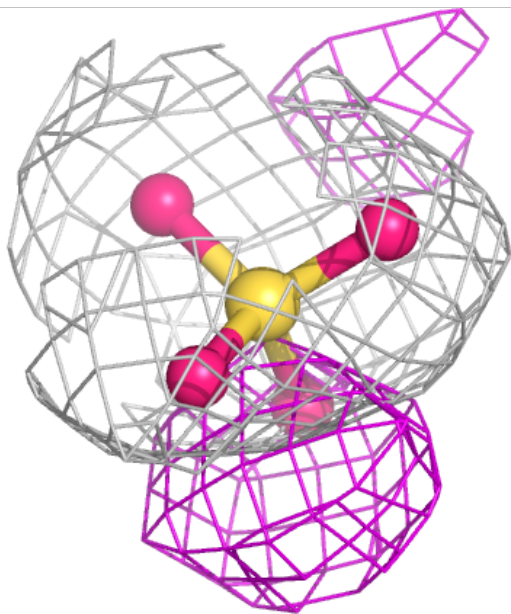
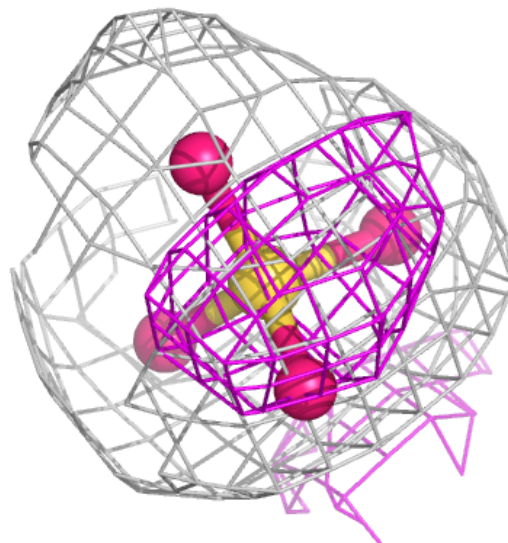
**Electron density around SO4 D 1203:**

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



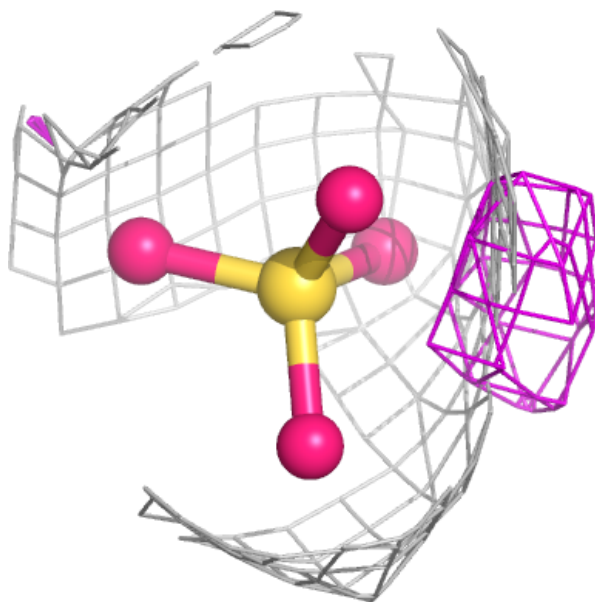
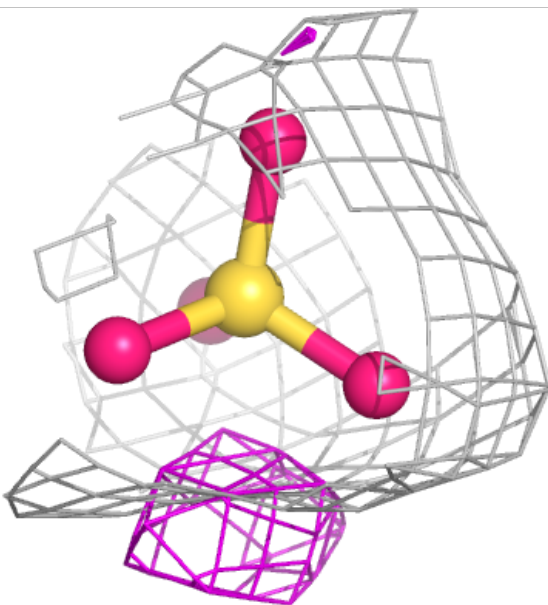
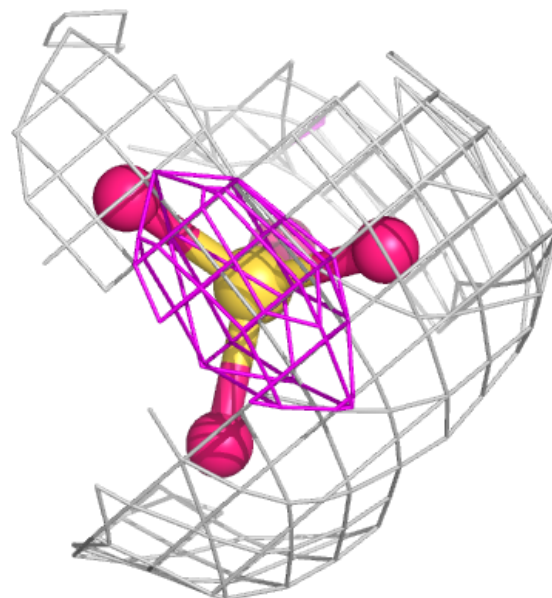
**Electron density around SO4 D 1206:**

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



**Electron density around SO4 A 1203:**

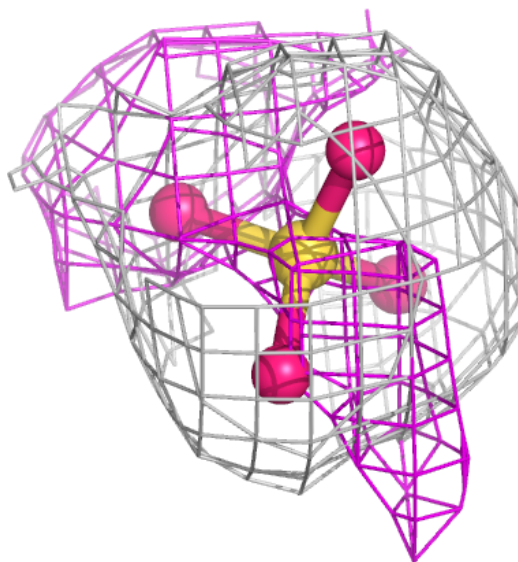
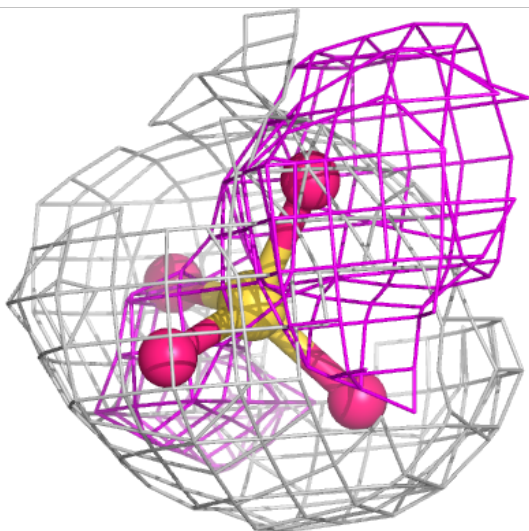
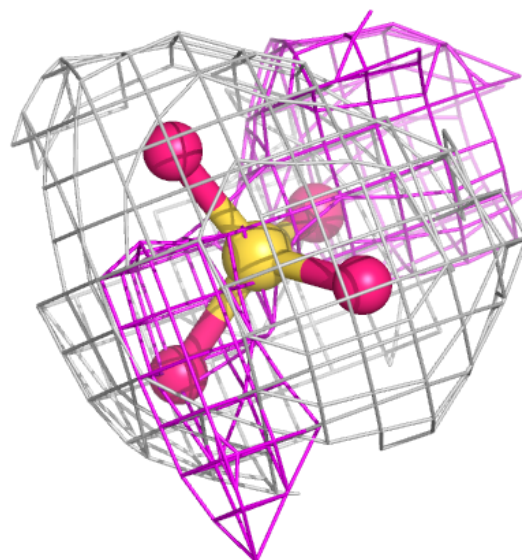
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





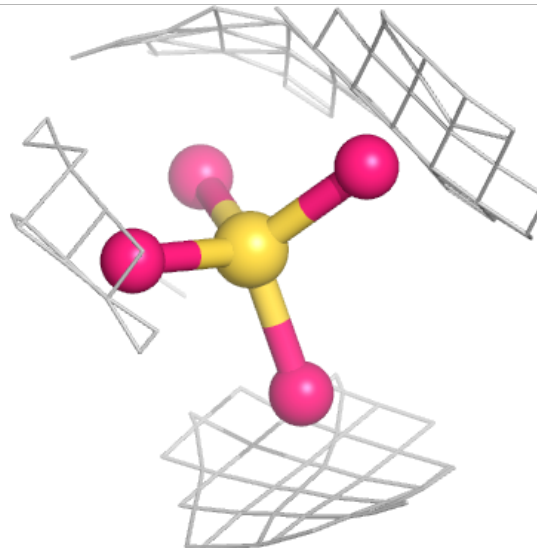
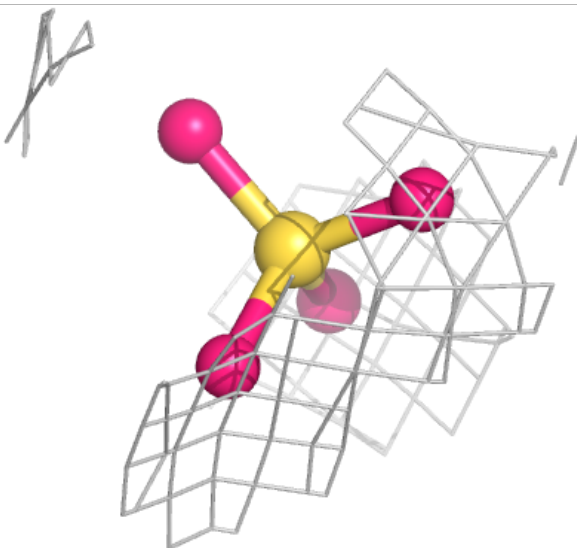
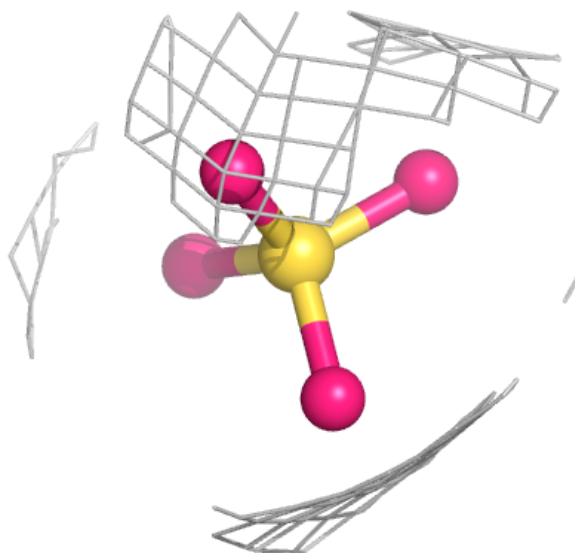
**Electron density around SO4 F 1206:**

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



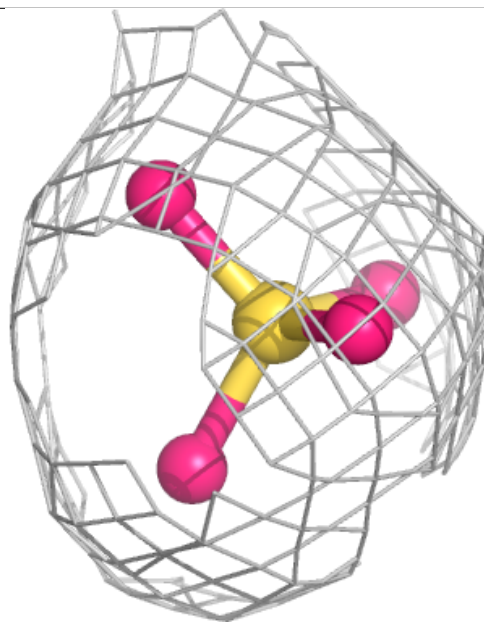
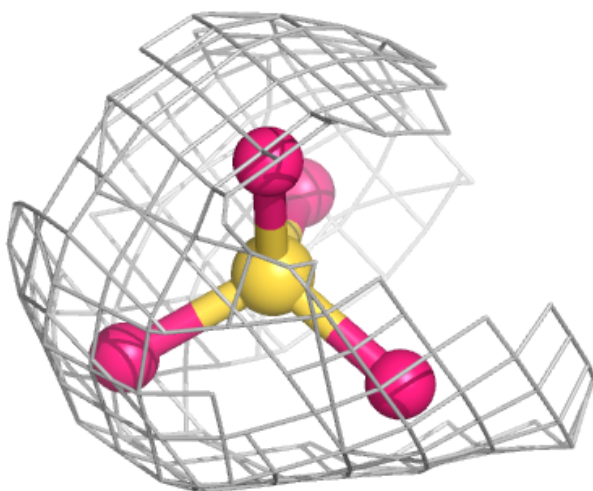
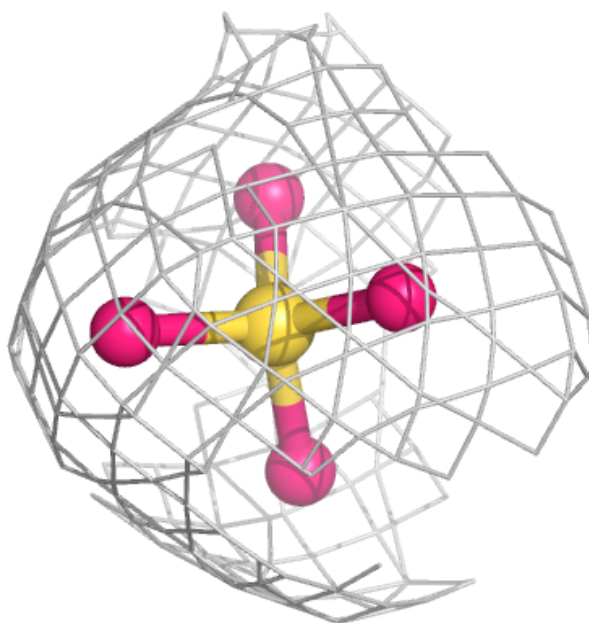
**Electron density around SO4 H 1202:**

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



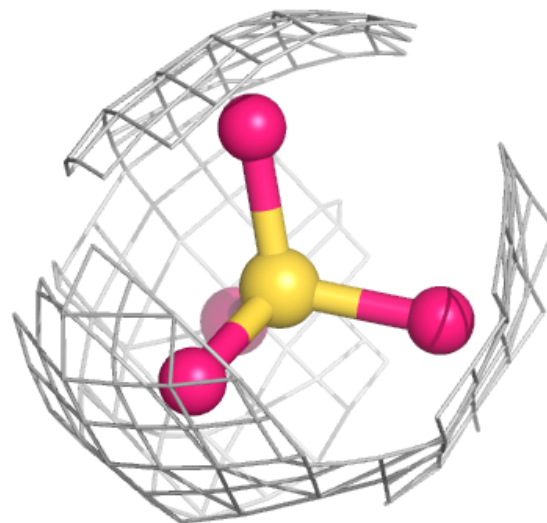
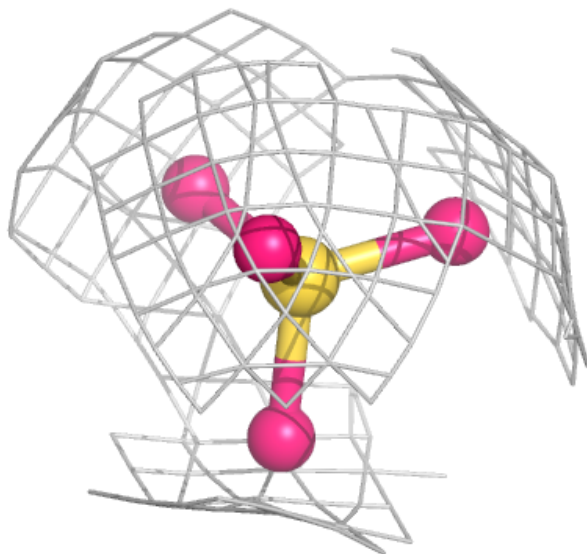
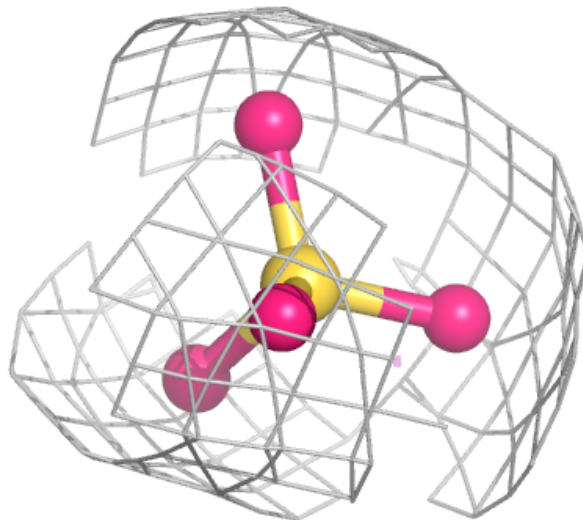
**Electron density around SO4 D 1202:**

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



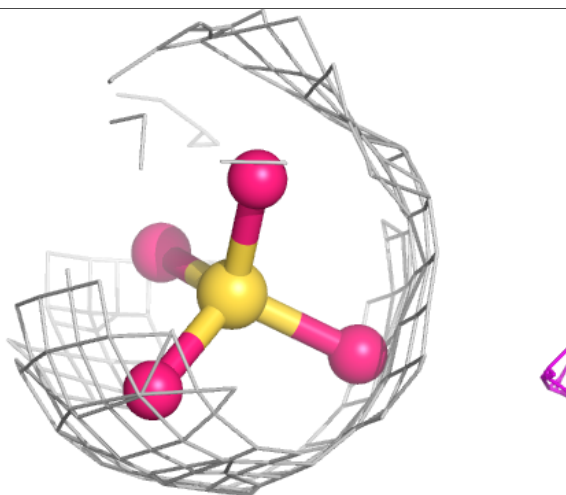
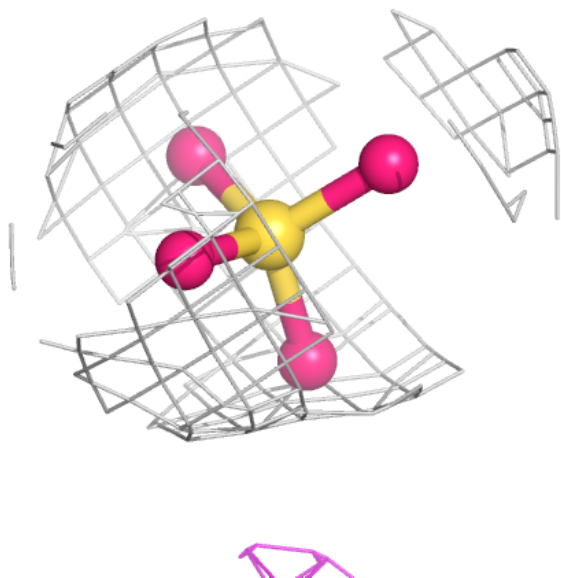
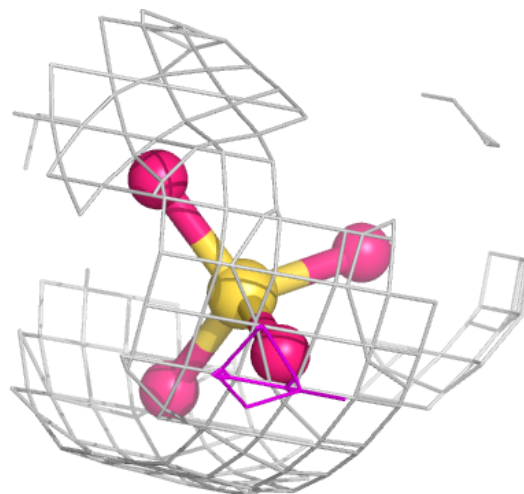
**Electron density around SO4 B 1204:**

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



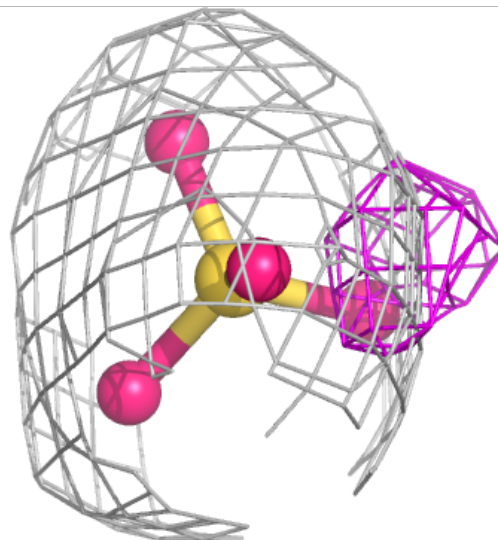
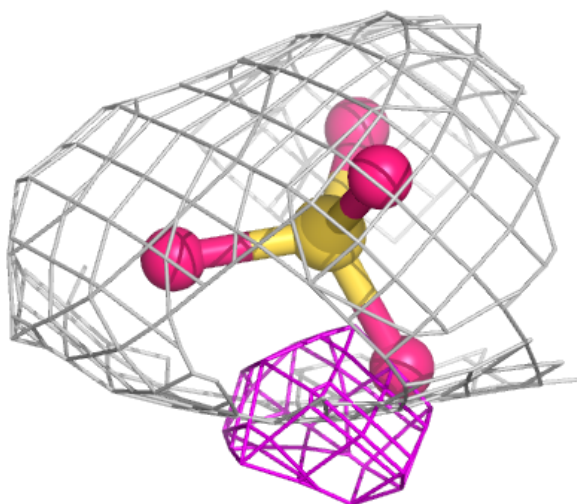
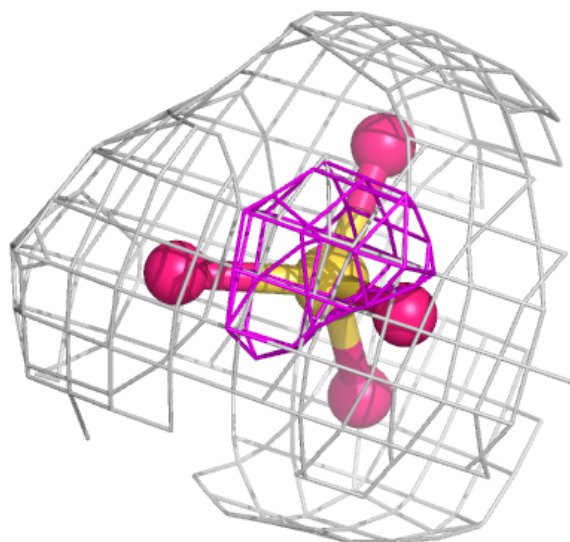
**Electron density around SO4 B 1202:**

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



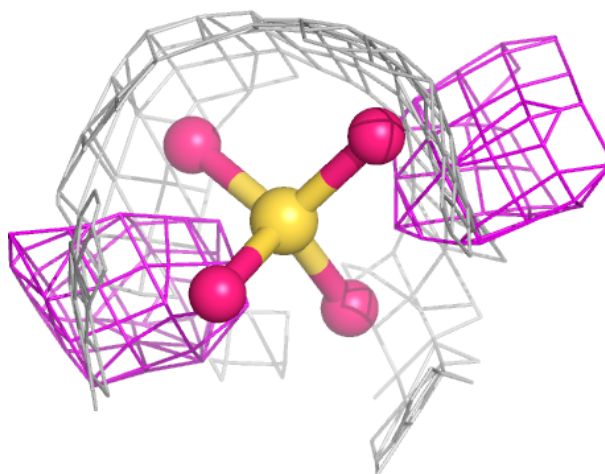
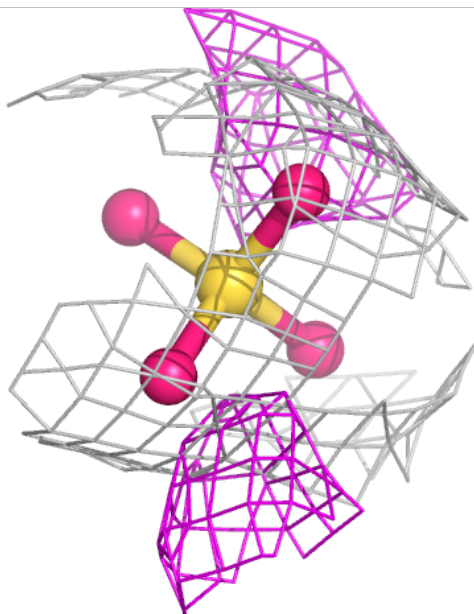
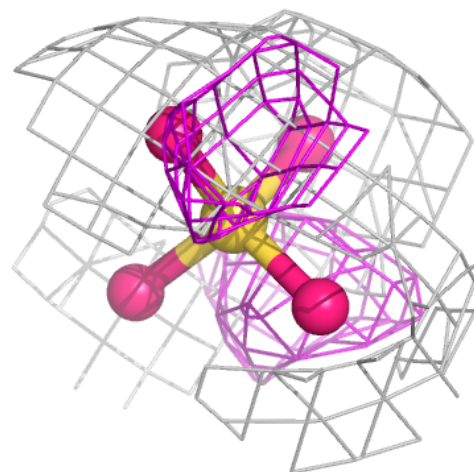
**Electron density around SO4 A 1205:**

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



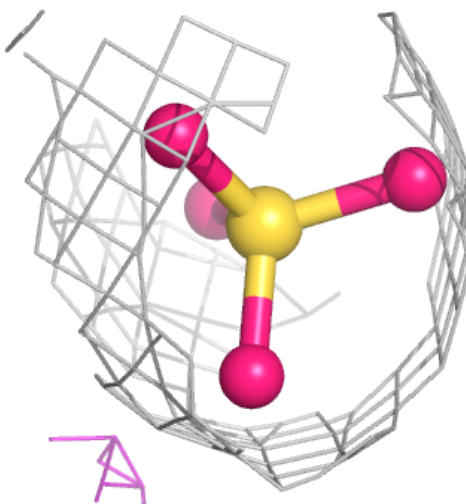
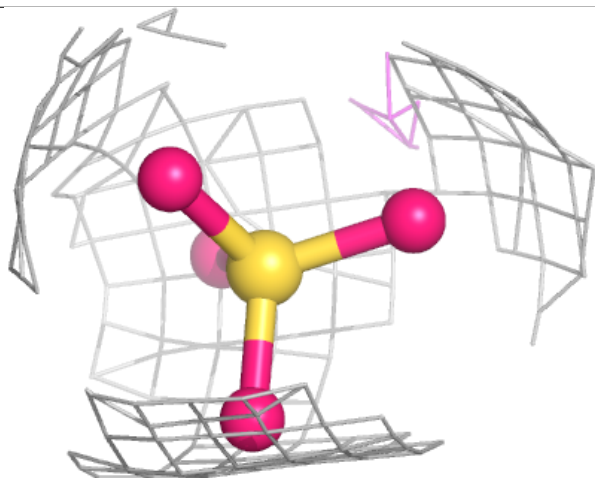
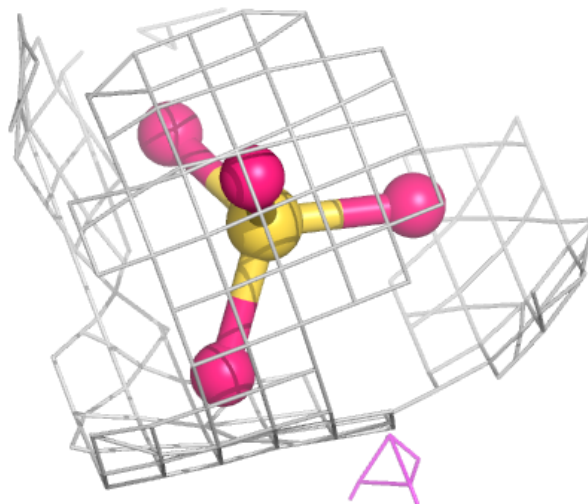
**Electron density around SO4 E 1203:**

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



**Electron density around SO4 A 1204:**

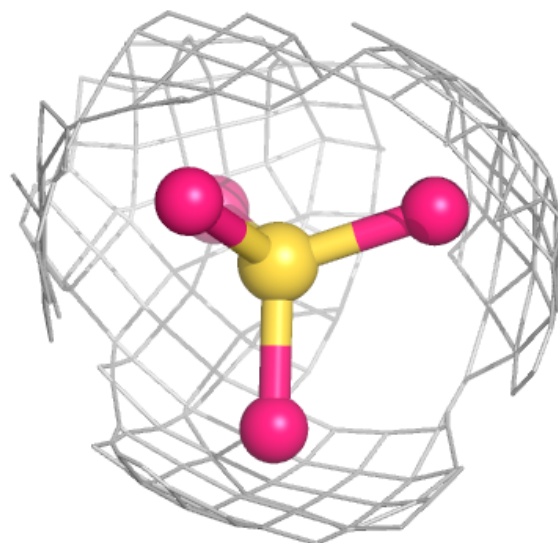
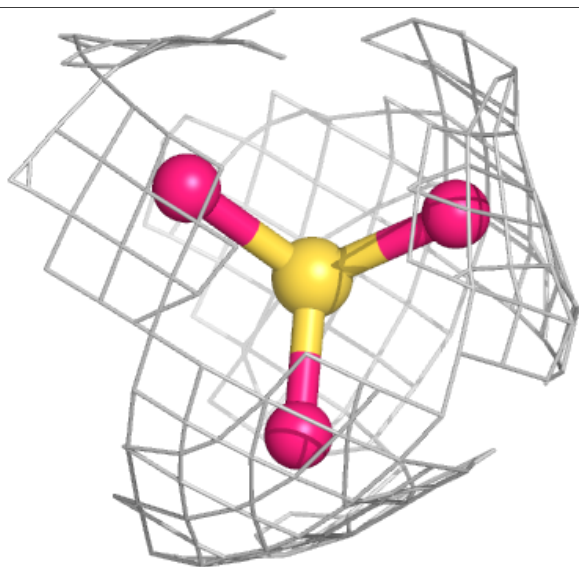
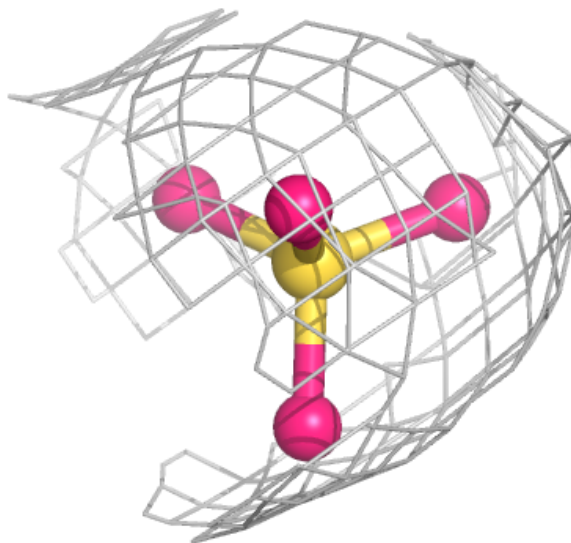
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





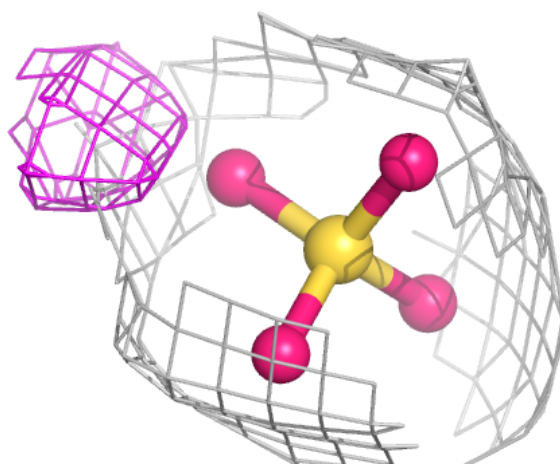
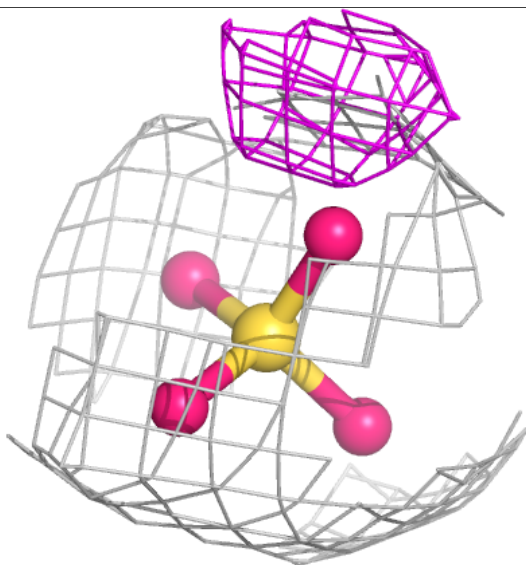
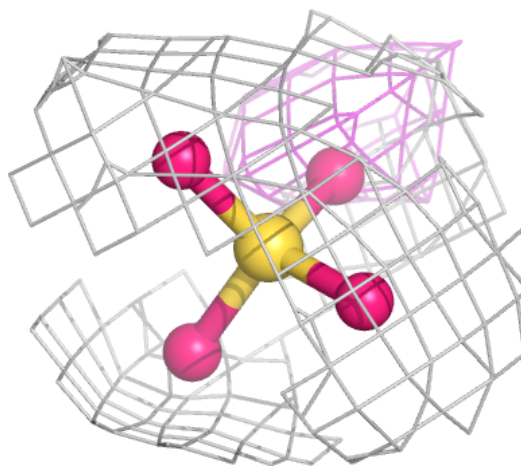
**Electron density around SO4 E 1204:**

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



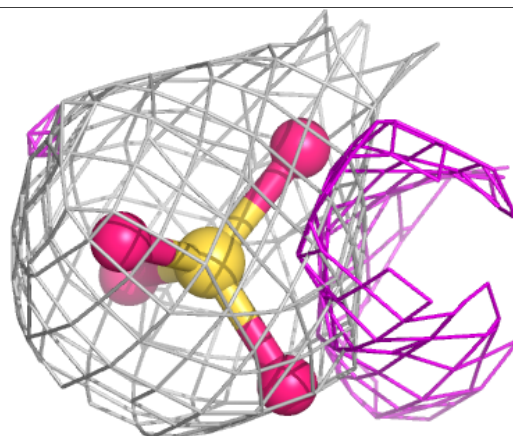
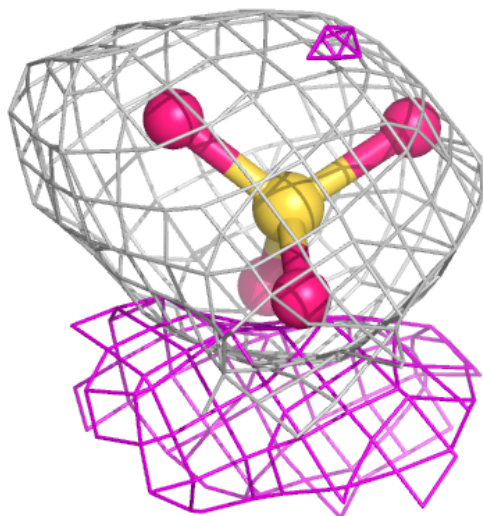
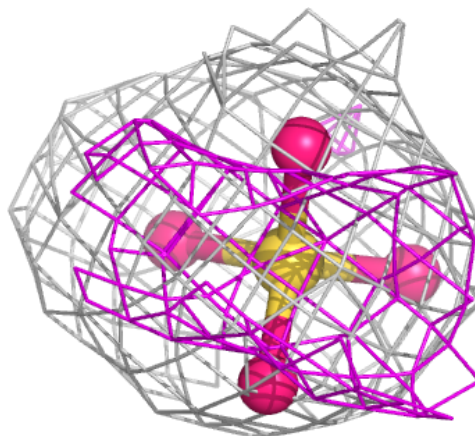
**Electron density around SO4 E 1207:**

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



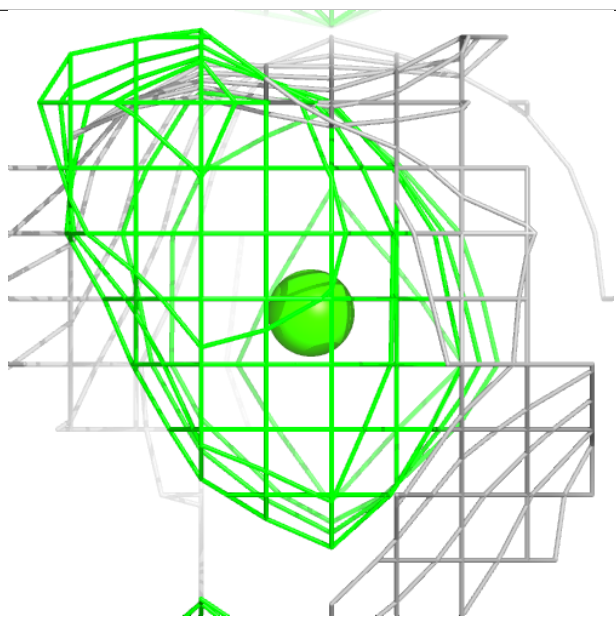
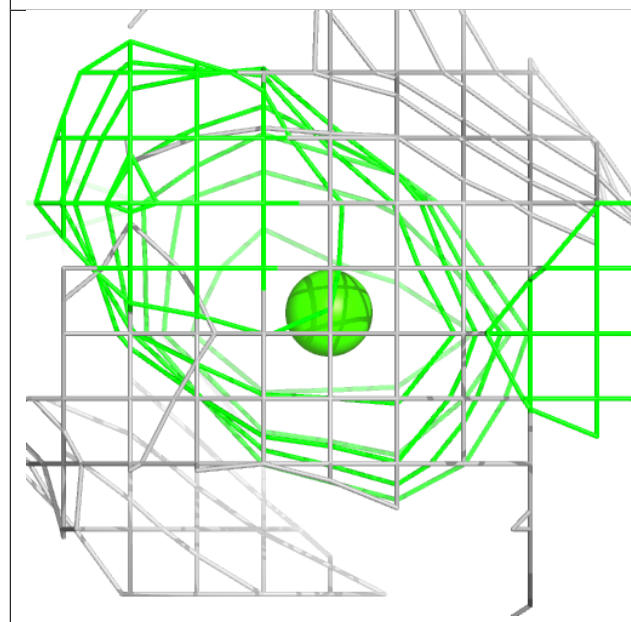
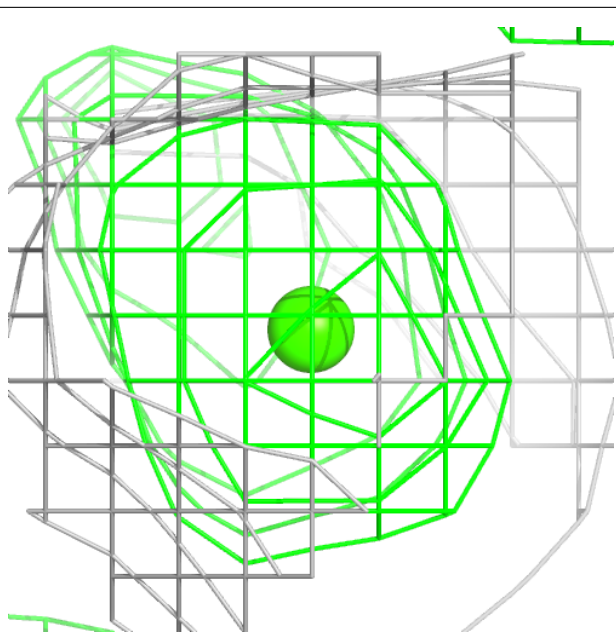
**Electron density around SO4 F 1202:**

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



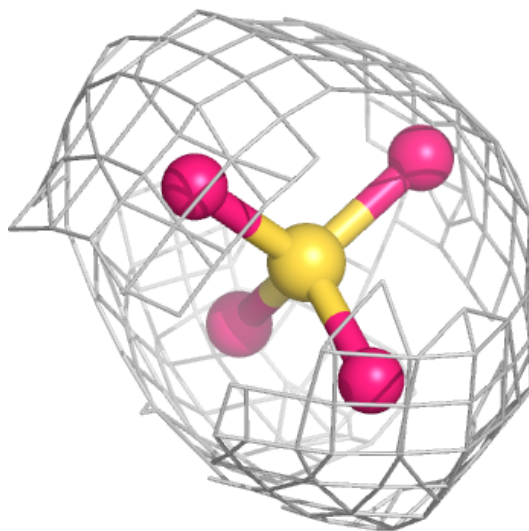
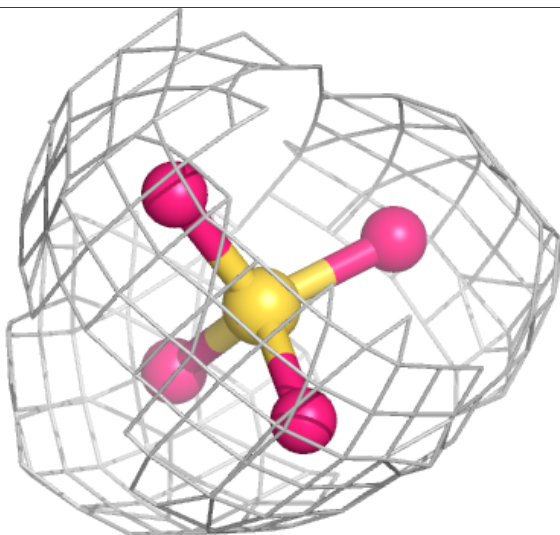
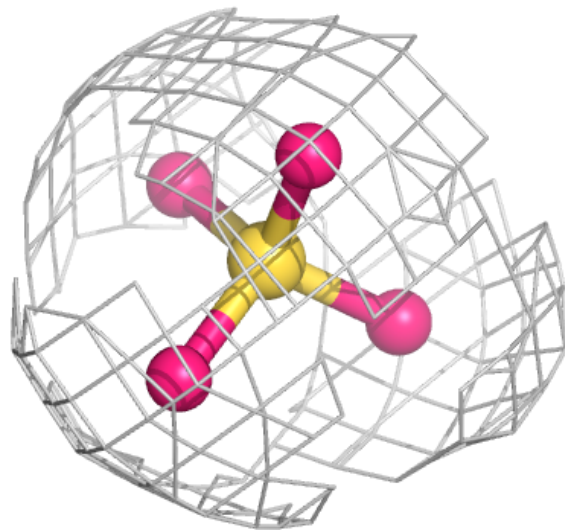
**Electron density around CA A 1201:**

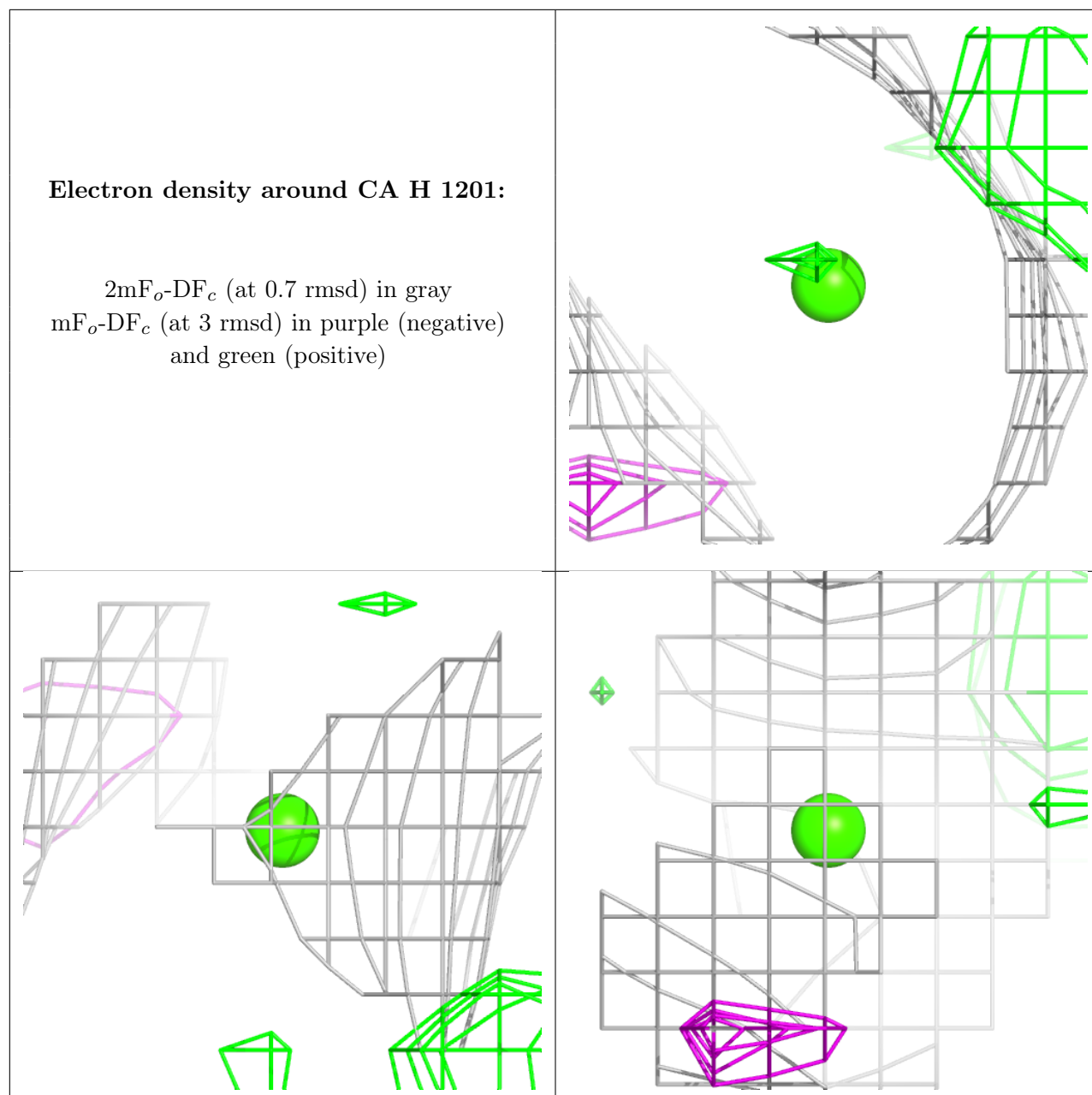
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 E 1205:**

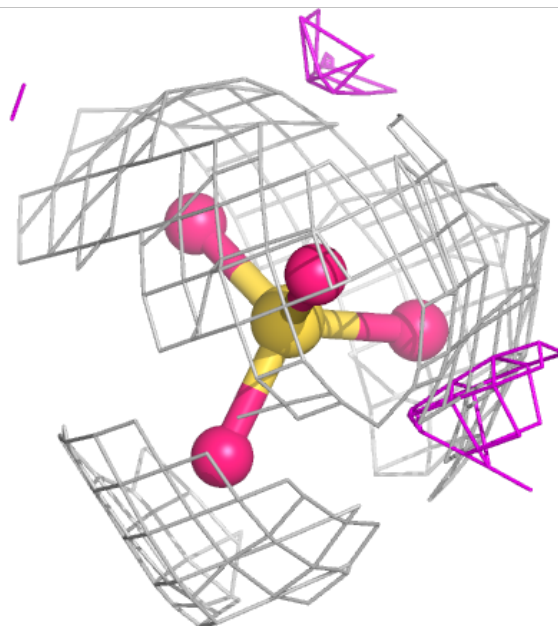
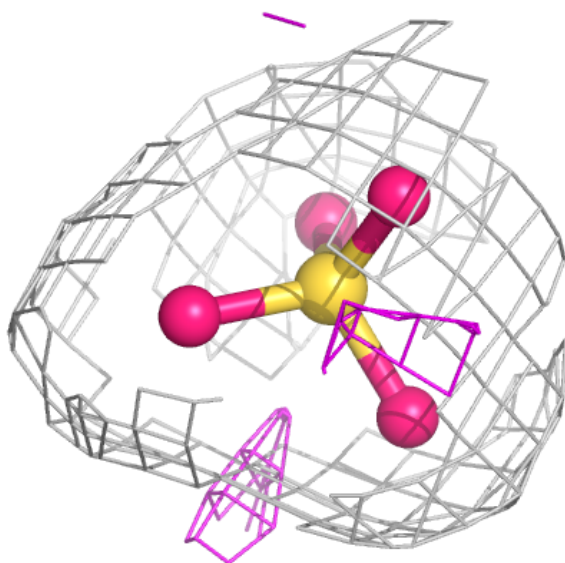
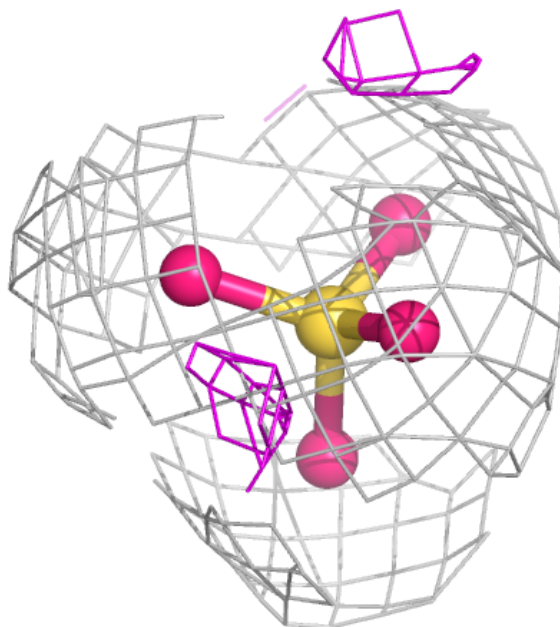
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





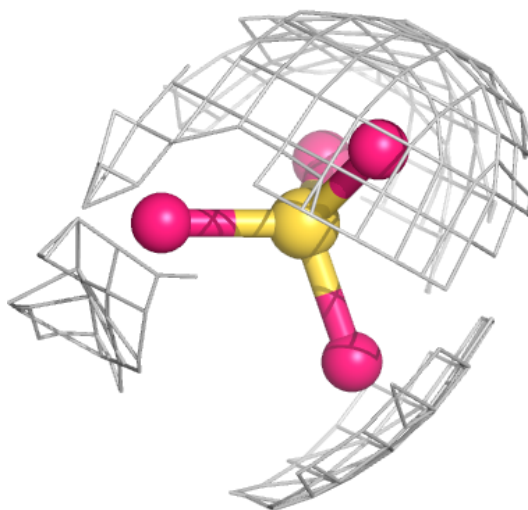
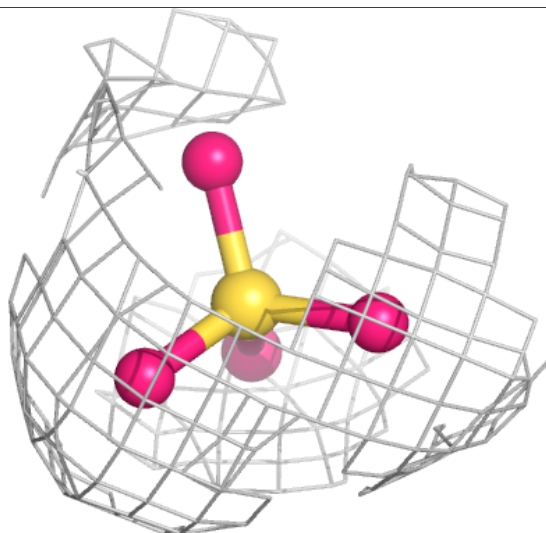
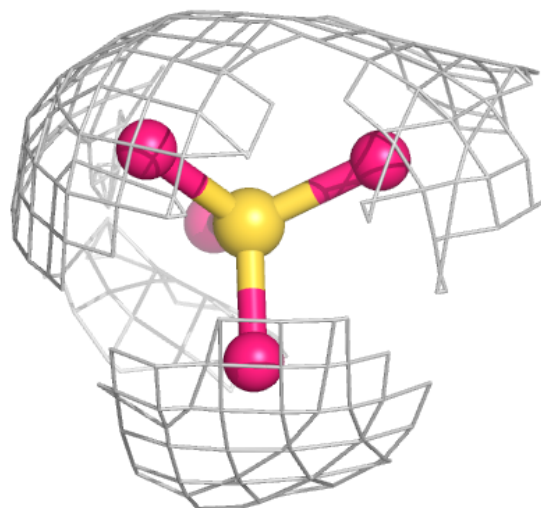
**Electron density around SO4 F 1207:**

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



**Electron density around SO4 E 1202:**

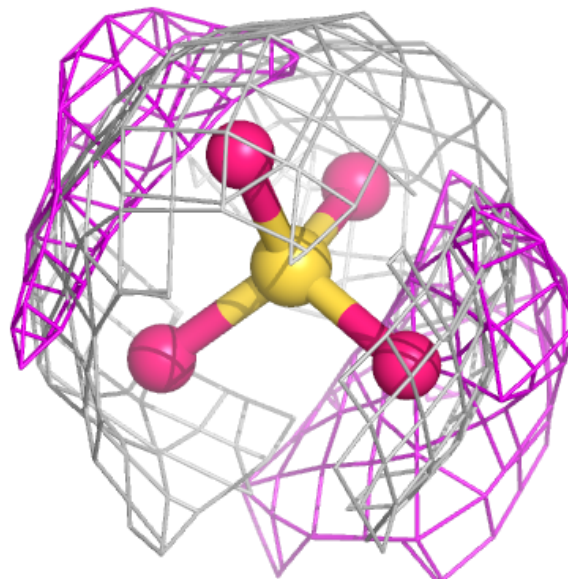
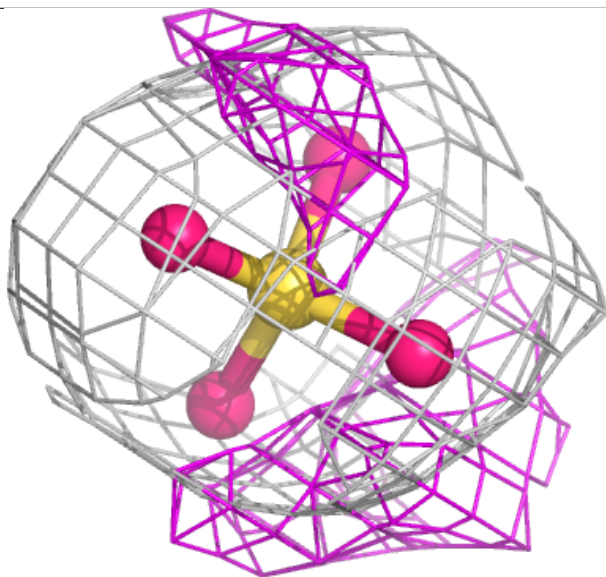
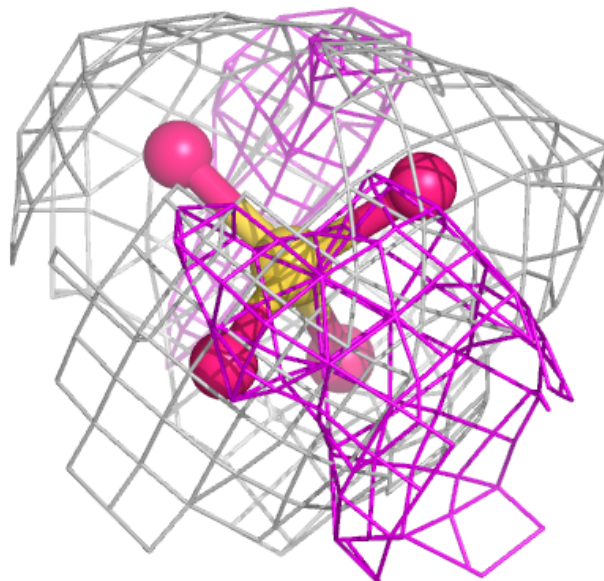
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





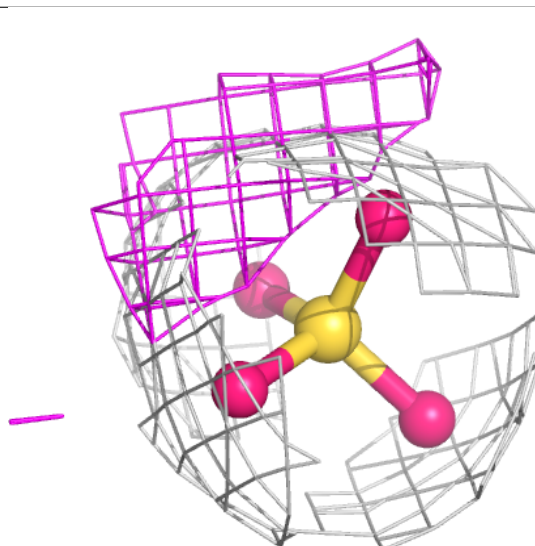
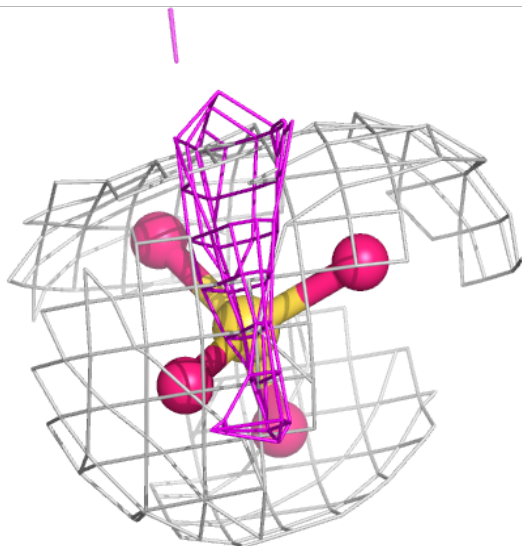
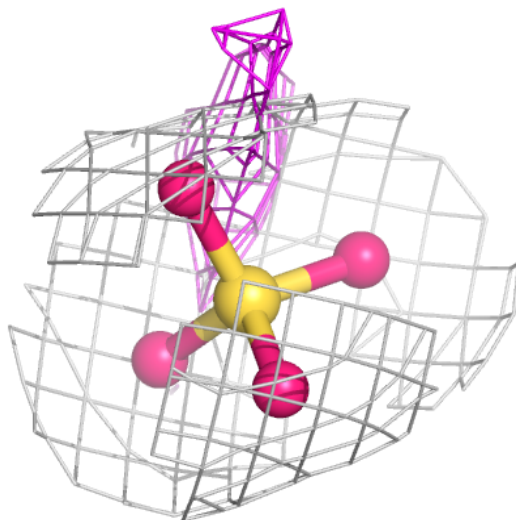
**Electron density around SO4 B 1206:**

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



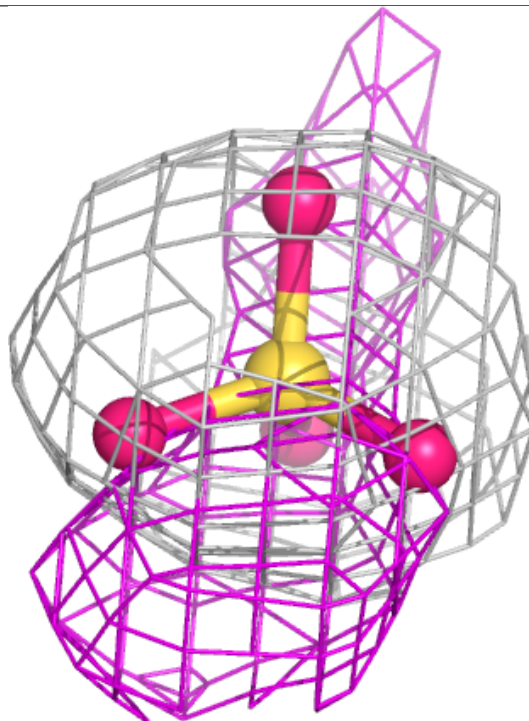
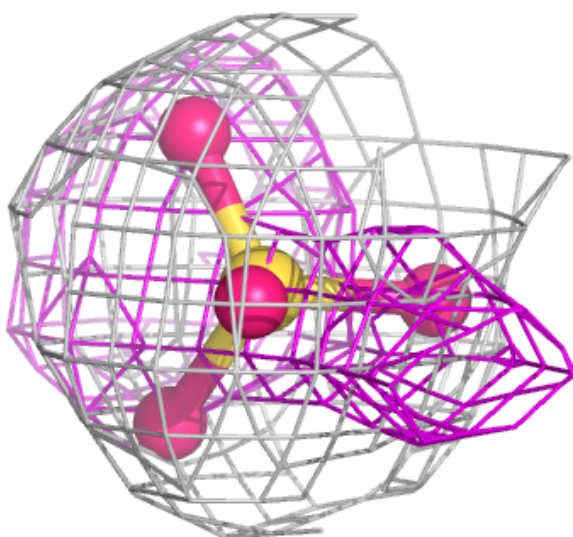
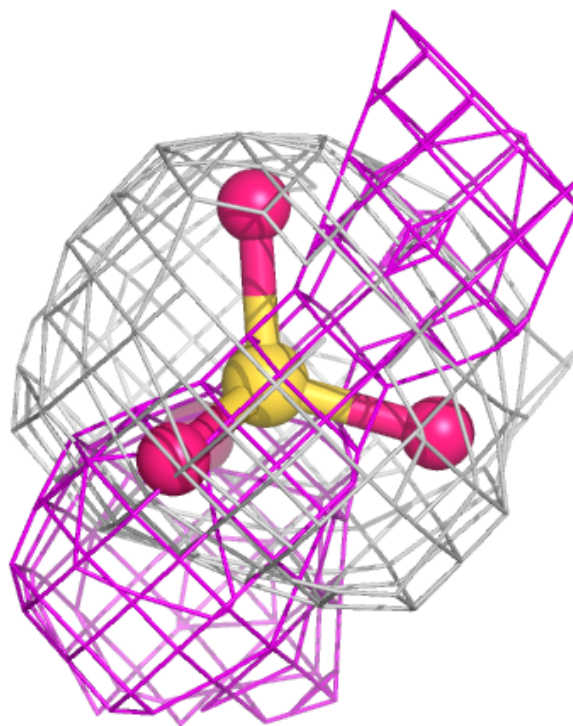
**Electron density around SO4 A 1206:**

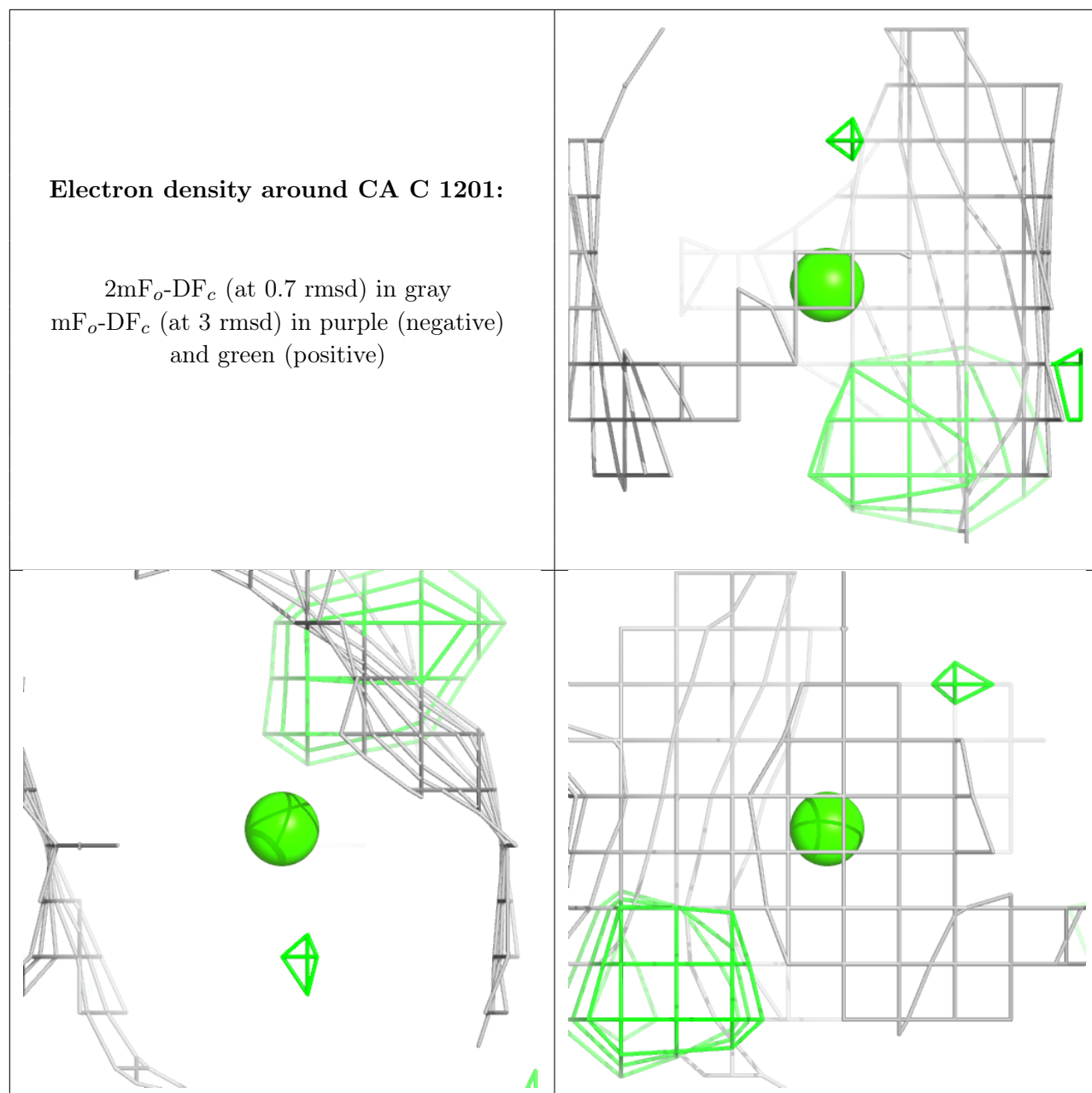
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 A 1207:**

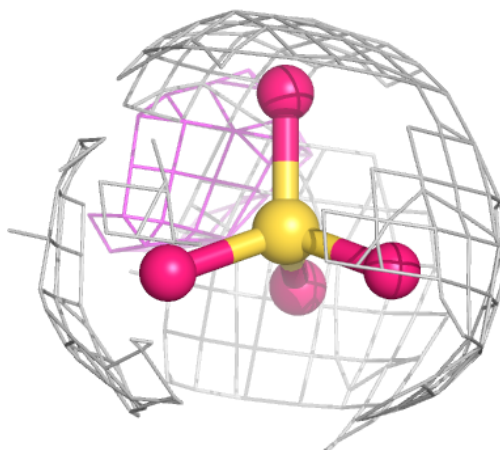
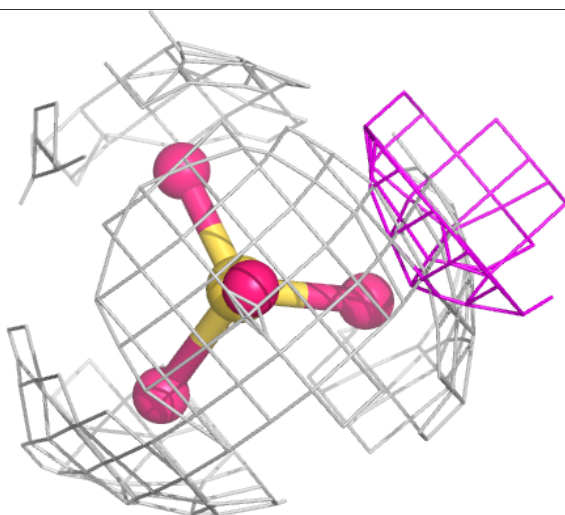
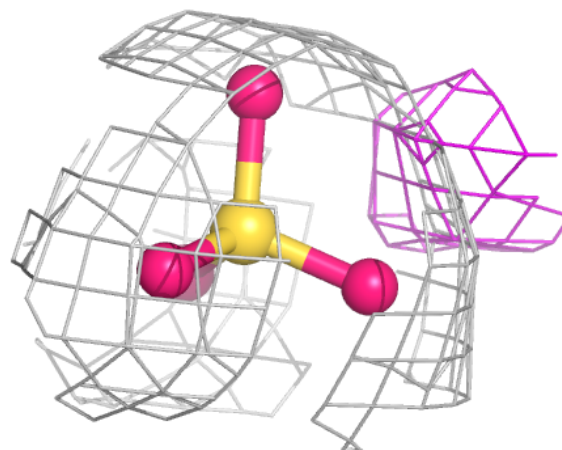
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





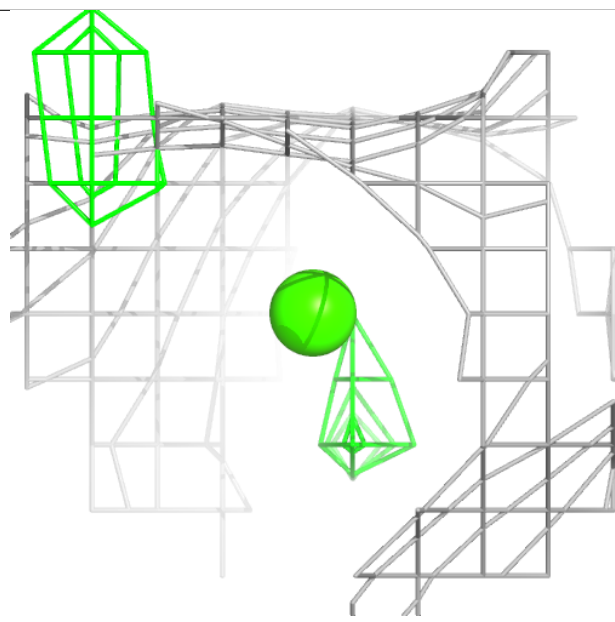
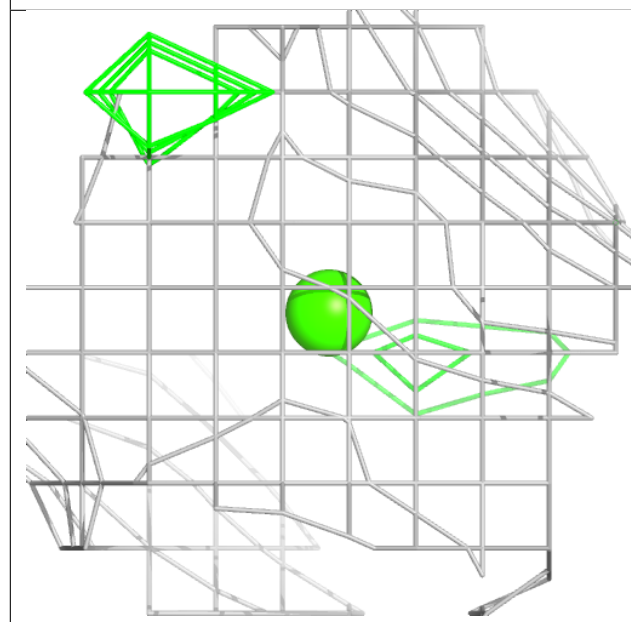
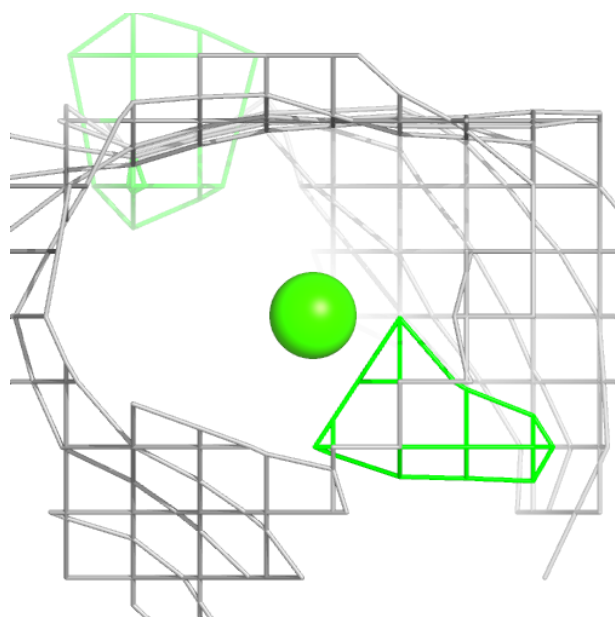
**Electron density around SO4 E 1206:**

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



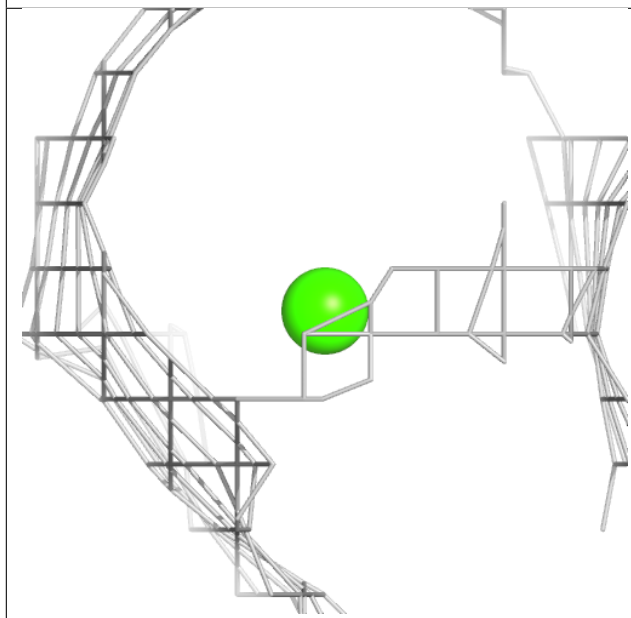
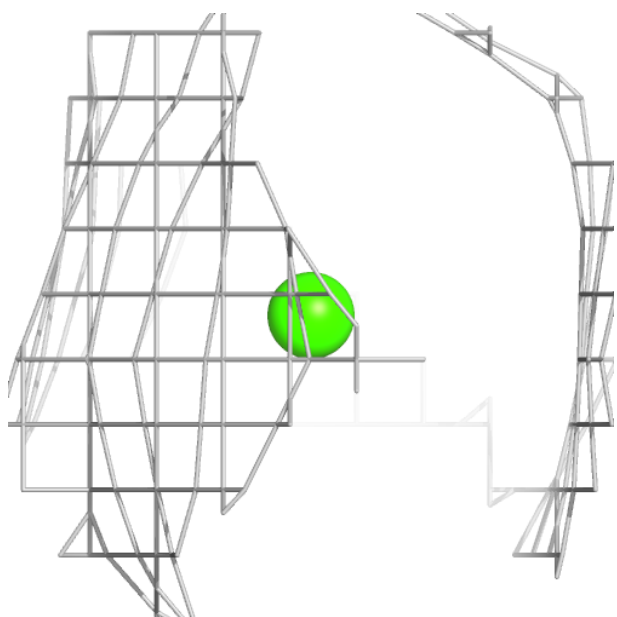
**Electron density around CA B 1201:**

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



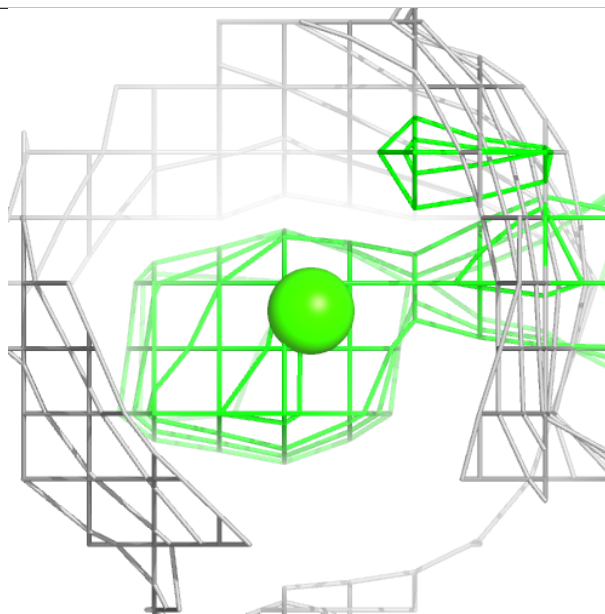
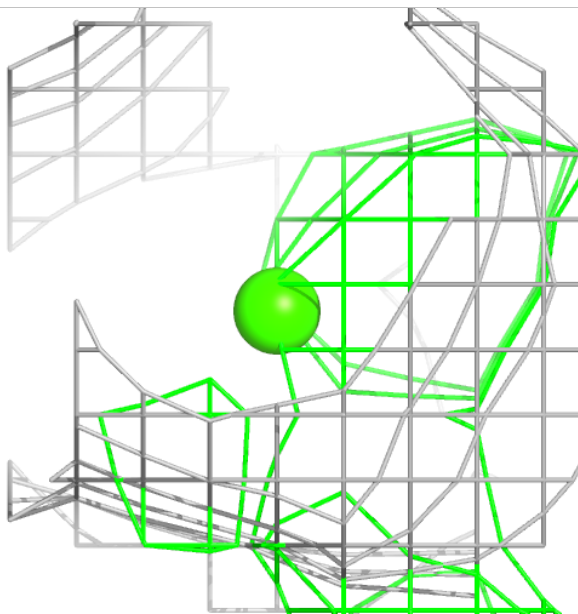
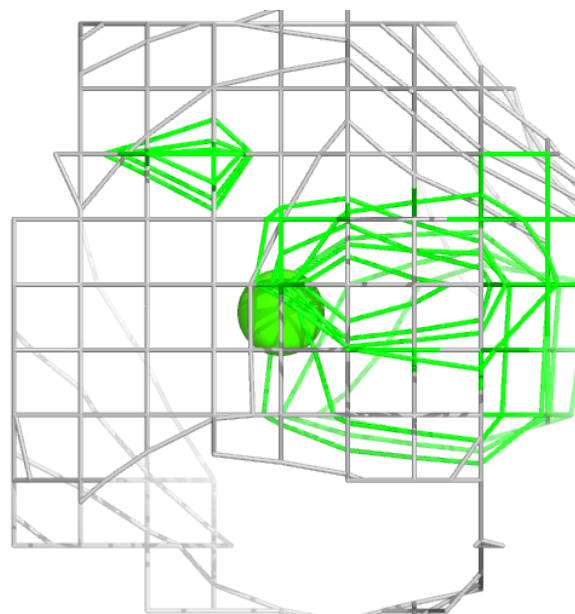
**Electron density around CA D 1201:**

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



**Electron density around CA E 1201:**

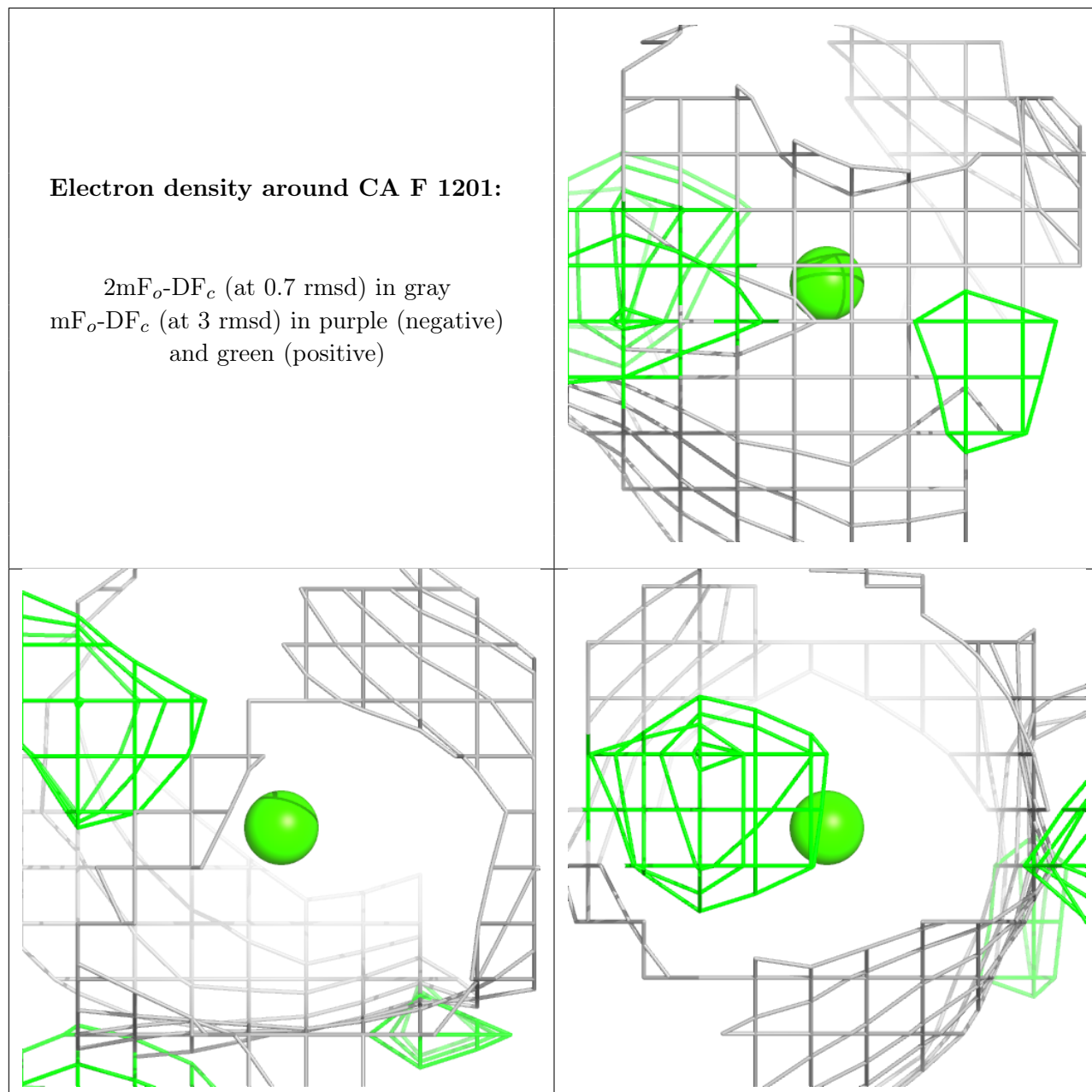
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

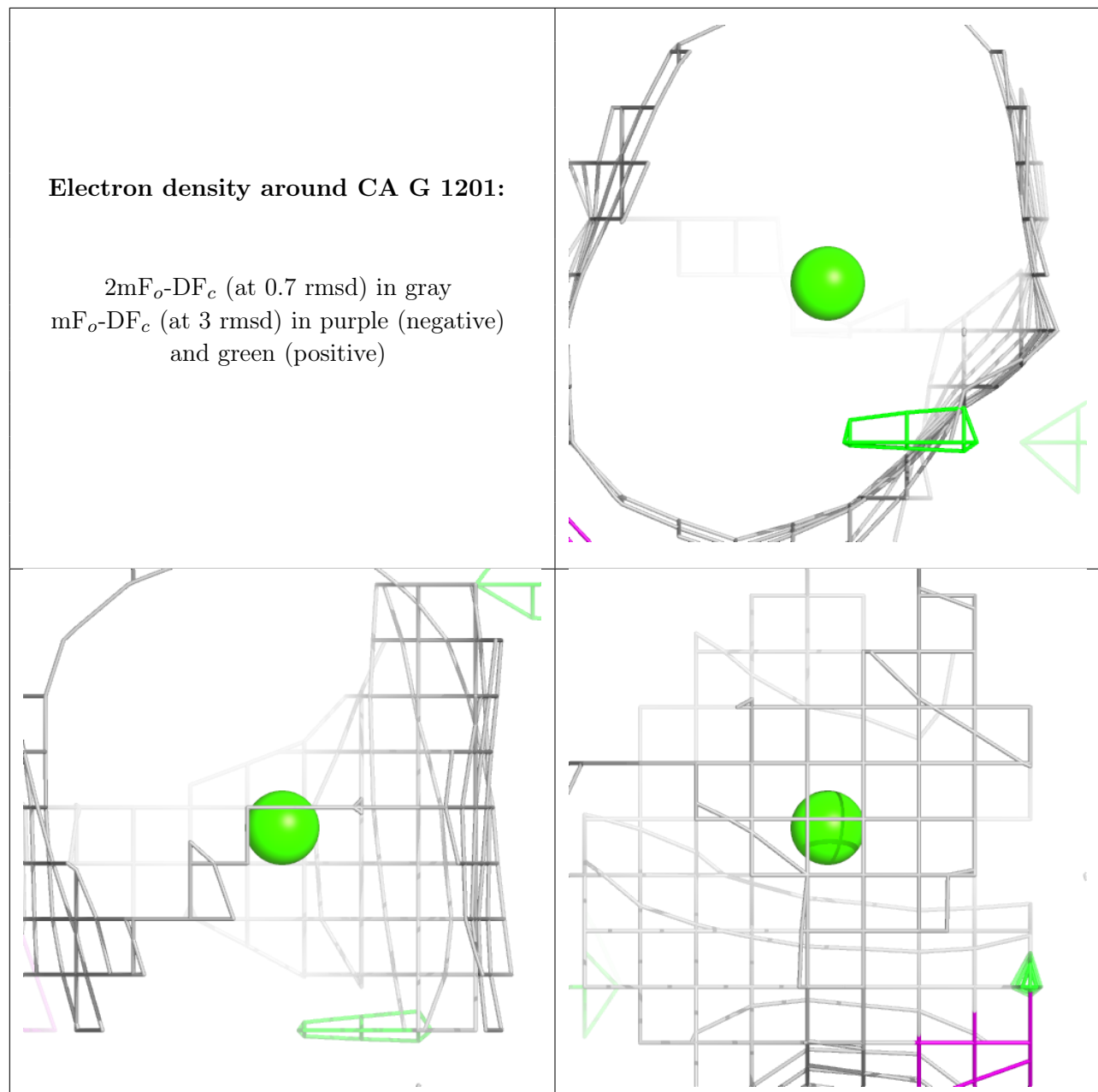




**Electron density around CA F 1201:**

$2mF_o-DF_c$  (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.