



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 02:18 PM JST

PDB ID : 8YR5  
Title : Crystal structure of E. coli phosphatidylserine synthase in apo state  
Authors : Kim, J.; Lee, E.; Cho, G.  
Deposited on : 2024-03-20  
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

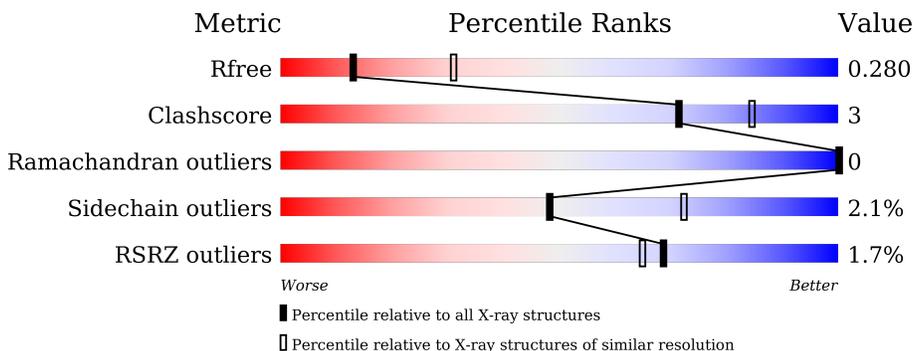
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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.



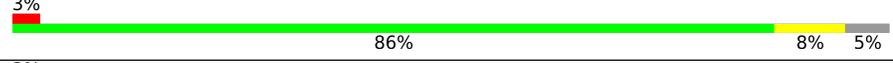
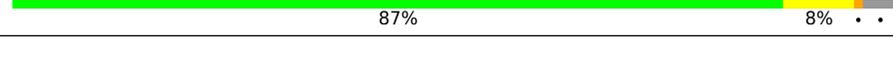
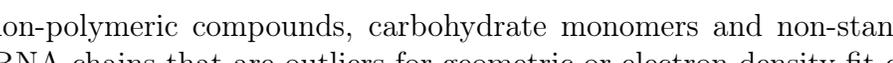
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1367 (2.86-2.82)
Clashscore	180529	1455 (2.86-2.82)
Ramachandran outliers	177936	1422 (2.86-2.82)
Sidechain outliers	177891	1423 (2.86-2.82)
RSRZ outliers	164620	1368 (2.86-2.82)

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	461	87% 7% • 5%
1	B	461	87% 8% • 5%
1	C	461	86% 8% • 5%
1	D	461	88% 8% •
1	E	461	88% 8% • •
1	F	461	86% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	G	461	 % 86% 8% 5%
1	H	461	 % 86% 8% 5%
1	I	461	 % 87% 8% . .
1	J	461	 3% 86% 9% . .
1	K	461	 3% 86% 8% 5%
1	L	461	 3% 87% 8% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	501	-	-	X	-
2	SO4	A	502	-	-	X	-
2	SO4	B	501	-	-	X	-
2	SO4	E	501	-	-	X	-
2	SO4	G	502	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 43895 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 CDP-diacylglycerol--serine O-phosphatidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3628	2309	658	650	11	0	0	0
1	B	439	3643	2319	662	651	11	0	0	0
1	C	440	3651	2323	664	653	11	0	0	0
1	D	446	3685	2343	671	660	11	0	0	0
1	E	445	3676	2337	669	659	11	0	0	0
1	F	437	3628	2309	658	650	11	0	0	0
1	G	437	3623	2306	655	651	11	0	0	0
1	H	436	3620	2305	656	648	11	0	0	0
1	I	444	3665	2331	665	658	11	0	0	0
1	J	443	3675	2340	668	656	11	0	0	0
1	K	437	3623	2306	655	651	11	0	0	0
1	L	441	3658	2329	663	655	11	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P23830
A	-8	GLY	-	expression tag	UNP P23830
A	-7	SER	-	expression tag	UNP P23830
A	-6	HIS	-	expression tag	UNP P23830
A	-5	HIS	-	expression tag	UNP P23830

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P23830
A	-3	HIS	-	expression tag	UNP P23830
A	-2	HIS	-	expression tag	UNP P23830
A	-1	HIS	-	expression tag	UNP P23830
A	0	GLY	-	expression tag	UNP P23830
A	1	SER	-	expression tag	UNP P23830
B	-9	MET	-	initiating methionine	UNP P23830
B	-8	GLY	-	expression tag	UNP P23830
B	-7	SER	-	expression tag	UNP P23830
B	-6	HIS	-	expression tag	UNP P23830
B	-5	HIS	-	expression tag	UNP P23830
B	-4	HIS	-	expression tag	UNP P23830
B	-3	HIS	-	expression tag	UNP P23830
B	-2	HIS	-	expression tag	UNP P23830
B	-1	HIS	-	expression tag	UNP P23830
B	0	GLY	-	expression tag	UNP P23830
B	1	SER	-	expression tag	UNP P23830
C	-9	MET	-	initiating methionine	UNP P23830
C	-8	GLY	-	expression tag	UNP P23830
C	-7	SER	-	expression tag	UNP P23830
C	-6	HIS	-	expression tag	UNP P23830
C	-5	HIS	-	expression tag	UNP P23830
C	-4	HIS	-	expression tag	UNP P23830
C	-3	HIS	-	expression tag	UNP P23830
C	-2	HIS	-	expression tag	UNP P23830
C	-1	HIS	-	expression tag	UNP P23830
C	0	GLY	-	expression tag	UNP P23830
C	1	SER	-	expression tag	UNP P23830
D	-9	MET	-	initiating methionine	UNP P23830
D	-8	GLY	-	expression tag	UNP P23830
D	-7	SER	-	expression tag	UNP P23830
D	-6	HIS	-	expression tag	UNP P23830
D	-5	HIS	-	expression tag	UNP P23830
D	-4	HIS	-	expression tag	UNP P23830
D	-3	HIS	-	expression tag	UNP P23830
D	-2	HIS	-	expression tag	UNP P23830
D	-1	HIS	-	expression tag	UNP P23830
D	0	GLY	-	expression tag	UNP P23830
D	1	SER	-	expression tag	UNP P23830
E	-9	MET	-	initiating methionine	UNP P23830
E	-8	GLY	-	expression tag	UNP P23830
E	-7	SER	-	expression tag	UNP P23830

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	HIS	-	expression tag	UNP P23830
E	-5	HIS	-	expression tag	UNP P23830
E	-4	HIS	-	expression tag	UNP P23830
E	-3	HIS	-	expression tag	UNP P23830
E	-2	HIS	-	expression tag	UNP P23830
E	-1	HIS	-	expression tag	UNP P23830
E	0	GLY	-	expression tag	UNP P23830
E	1	SER	-	expression tag	UNP P23830
F	-9	MET	-	initiating methionine	UNP P23830
F	-8	GLY	-	expression tag	UNP P23830
F	-7	SER	-	expression tag	UNP P23830
F	-6	HIS	-	expression tag	UNP P23830
F	-5	HIS	-	expression tag	UNP P23830
F	-4	HIS	-	expression tag	UNP P23830
F	-3	HIS	-	expression tag	UNP P23830
F	-2	HIS	-	expression tag	UNP P23830
F	-1	HIS	-	expression tag	UNP P23830
F	0	GLY	-	expression tag	UNP P23830
F	1	SER	-	expression tag	UNP P23830
G	-9	MET	-	initiating methionine	UNP P23830
G	-8	GLY	-	expression tag	UNP P23830
G	-7	SER	-	expression tag	UNP P23830
G	-6	HIS	-	expression tag	UNP P23830
G	-5	HIS	-	expression tag	UNP P23830
G	-4	HIS	-	expression tag	UNP P23830
G	-3	HIS	-	expression tag	UNP P23830
G	-2	HIS	-	expression tag	UNP P23830
G	-1	HIS	-	expression tag	UNP P23830
G	0	GLY	-	expression tag	UNP P23830
G	1	SER	-	expression tag	UNP P23830
H	-9	MET	-	initiating methionine	UNP P23830
H	-8	GLY	-	expression tag	UNP P23830
H	-7	SER	-	expression tag	UNP P23830
H	-6	HIS	-	expression tag	UNP P23830
H	-5	HIS	-	expression tag	UNP P23830
H	-4	HIS	-	expression tag	UNP P23830
H	-3	HIS	-	expression tag	UNP P23830
H	-2	HIS	-	expression tag	UNP P23830
H	-1	HIS	-	expression tag	UNP P23830
H	0	GLY	-	expression tag	UNP P23830
H	1	SER	-	expression tag	UNP P23830
I	-9	MET	-	initiating methionine	UNP P23830

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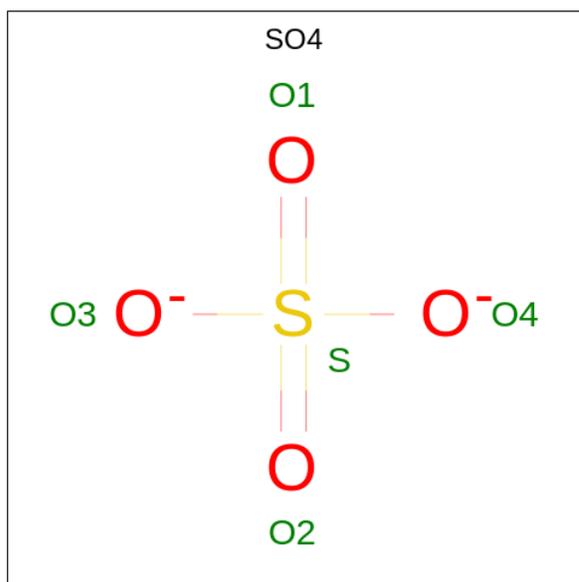
Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLY	-	expression tag	UNP P23830
I	-7	SER	-	expression tag	UNP P23830
I	-6	HIS	-	expression tag	UNP P23830
I	-5	HIS	-	expression tag	UNP P23830
I	-4	HIS	-	expression tag	UNP P23830
I	-3	HIS	-	expression tag	UNP P23830
I	-2	HIS	-	expression tag	UNP P23830
I	-1	HIS	-	expression tag	UNP P23830
I	0	GLY	-	expression tag	UNP P23830
I	1	SER	-	expression tag	UNP P23830
J	-9	MET	-	initiating methionine	UNP P23830
J	-8	GLY	-	expression tag	UNP P23830
J	-7	SER	-	expression tag	UNP P23830
J	-6	HIS	-	expression tag	UNP P23830
J	-5	HIS	-	expression tag	UNP P23830
J	-4	HIS	-	expression tag	UNP P23830
J	-3	HIS	-	expression tag	UNP P23830
J	-2	HIS	-	expression tag	UNP P23830
J	-1	HIS	-	expression tag	UNP P23830
J	0	GLY	-	expression tag	UNP P23830
J	1	SER	-	expression tag	UNP P23830
K	-9	MET	-	initiating methionine	UNP P23830
K	-8	GLY	-	expression tag	UNP P23830
K	-7	SER	-	expression tag	UNP P23830
K	-6	HIS	-	expression tag	UNP P23830
K	-5	HIS	-	expression tag	UNP P23830
K	-4	HIS	-	expression tag	UNP P23830
K	-3	HIS	-	expression tag	UNP P23830
K	-2	HIS	-	expression tag	UNP P23830
K	-1	HIS	-	expression tag	UNP P23830
K	0	GLY	-	expression tag	UNP P23830
K	1	SER	-	expression tag	UNP P23830
L	-9	MET	-	initiating methionine	UNP P23830
L	-8	GLY	-	expression tag	UNP P23830
L	-7	SER	-	expression tag	UNP P23830
L	-6	HIS	-	expression tag	UNP P23830
L	-5	HIS	-	expression tag	UNP P23830
L	-4	HIS	-	expression tag	UNP P23830
L	-3	HIS	-	expression tag	UNP P23830
L	-2	HIS	-	expression tag	UNP P23830
L	-1	HIS	-	expression tag	UNP P23830
L	0	GLY	-	expression tag	UNP P23830

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1	SER	-	expression tag	UNP P23830

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



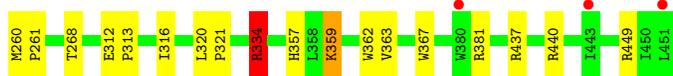
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

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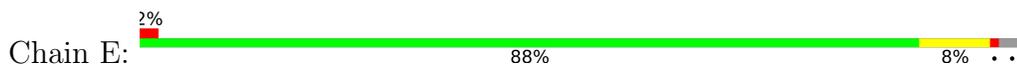
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0
2	I	1	Total 5	O 4	S 1	0	0
2	I	1	Total 5	O 4	S 1	0	0
2	J	1	Total 5	O 4	S 1	0	0
2	K	1	Total 5	O 4	S 1	0	0
2	K	1	Total 5	O 4	S 1	0	0
2	L	1	Total 5	O 4	S 1	0	0
2	L	1	Total 5	O 4	S 1	0	0

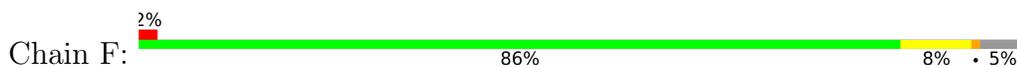




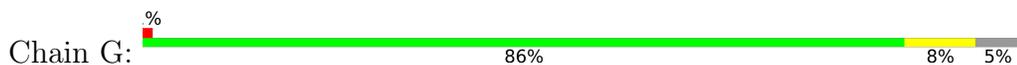
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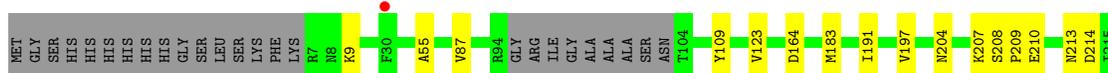
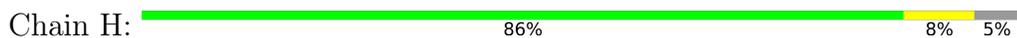
- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase



- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase

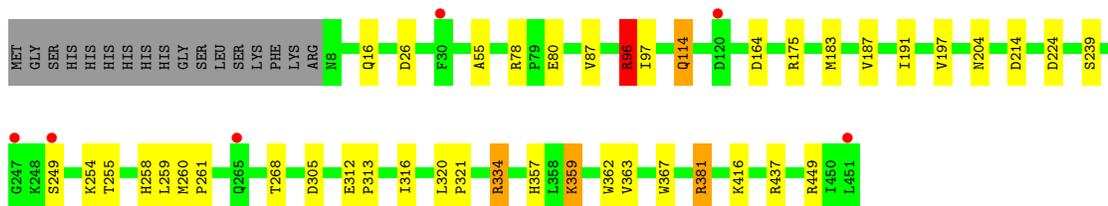


- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase



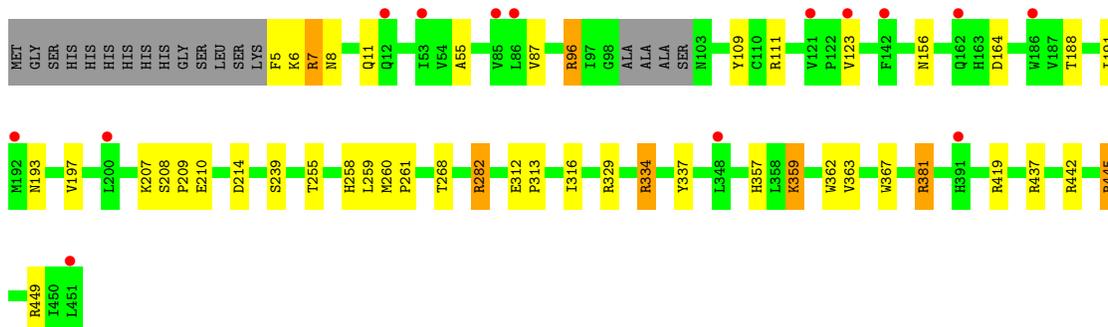
- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase

Chain I: 87% 8% . .



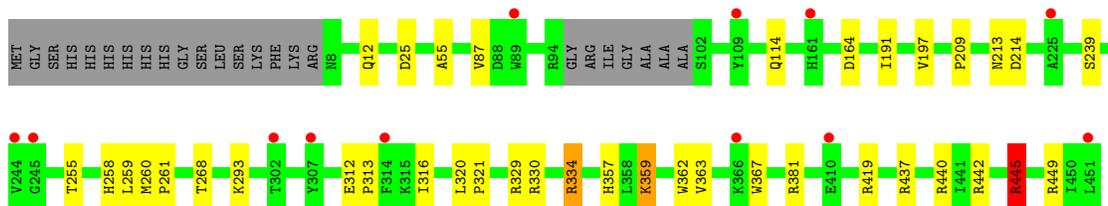
- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase

Chain J: 86% 9% . .



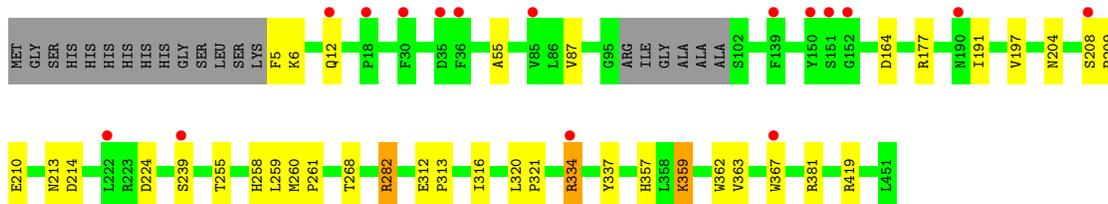
- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase

Chain K: 86% 8% 5%



- Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase

Chain L: 87% 8% . .



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.04Å 94.10Å 194.75Å 88.24° 87.70° 60.07°	Depositor
Resolution (Å)	48.64 – 2.83 48.64 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.64-2.83) 98.2 (48.64-2.83)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.242 , 0.285 0.242 , 0.280	Depositor DCC
$R_{free}$ test set	6358 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.7	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.014 for k,-h+k,l 0.014 for h-k,h,l 0.014 for -h+k,-h,l 0.014 for -k,h-k,l 0.023 for h,h-k,-l 0.083 for -h+k,k,-l 0.019 for -h,-k,l 0.016 for k,h,-l 0.019 for -k,-h,-l 0.023 for -h,-h+k,-l 0.024 for h-k,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	43895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/3705	0.76	7/5014 (0.1%)
1	B	0.36	0/3720	0.76	0/5033
1	C	0.37	0/3728	0.78	6/5044 (0.1%)
1	D	0.36	0/3763	0.76	4/5092 (0.1%)
1	E	0.36	0/3754	0.76	4/5081 (0.1%)
1	F	0.35	0/3705	0.74	6/5014 (0.1%)
1	G	0.35	0/3700	0.74	1/5008 (0.0%)
1	H	0.36	0/3697	0.76	5/5003 (0.1%)
1	I	0.36	0/3743	0.78	4/5067 (0.1%)
1	J	0.35	0/3753	0.77	3/5076 (0.1%)
1	K	0.35	0/3700	0.75	3/5008 (0.1%)
1	L	0.34	0/3736	0.72	1/5054 (0.0%)
All	All	0.35	0/44704	0.76	44/60494 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	1
1	E	0	4
1	H	0	1
1	I	0	1
1	J	0	2
1	K	0	1
1	L	0	2
All	All	0	14

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	419	ARG	CG-CD-NE	10.70	134.28	111.80
1	A	254	LYS	CA-CB-CG	7.79	130.53	113.40
1	D	437	ARG	CB-CG-CD	6.94	129.64	111.60
1	E	7	ARG	CG-CD-NE	6.64	125.75	111.80
1	A	329	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	D	96	ARG	CG-CD-NE	-6.35	98.46	111.80
1	F	449	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	F	177	ARG	CG-CD-NE	6.23	124.88	111.80
1	K	330	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	I	437	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	42	GLU	CG-CD-OE1	-5.93	106.44	118.30
1	K	293	LYS	CB-CG-CD	5.88	126.89	111.60
1	A	406	GLU	CG-CD-OE1	-5.84	106.62	118.30
1	A	42	GLU	CG-CD-OE2	5.81	129.91	118.30
1	I	114	GLN	CB-CA-C	5.80	122.00	110.40
1	C	442	ARG	CG-CD-NE	5.80	123.97	111.80
1	C	416	LYS	CD-CE-NZ	5.72	124.86	111.70
1	H	419	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	F	449	ARG	CG-CD-NE	5.59	123.55	111.80
1	A	406	GLU	CG-CD-OE2	5.59	129.49	118.30
1	E	78	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	334	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	D	96	ARG	CB-CG-CD	5.53	125.97	111.60
1	H	449	ARG	CG-CD-NE	5.52	123.39	111.80
1	H	449	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	J	334	ARG	CA-CB-CG	5.43	125.35	113.40
1	H	183	MET	CG-SD-CE	5.43	108.89	100.20
1	H	334	ARG	CA-CB-CG	5.40	125.28	113.40
1	L	334	ARG	CA-CB-CG	5.37	125.21	113.40
1	F	334	ARG	CA-CB-CG	5.36	125.18	113.40
1	D	334	ARG	CA-CB-CG	5.33	125.12	113.40
1	K	445	ARG	CG-CD-NE	5.31	122.95	111.80
1	C	334	ARG	CA-CB-CG	5.30	125.06	113.40
1	E	334	ARG	CA-CB-CG	5.29	125.05	113.40
1	J	207	LYS	CD-CE-NZ	5.29	123.86	111.70
1	I	334	ARG	CA-CB-CG	5.28	125.02	113.40
1	A	334	ARG	CA-CB-CG	5.27	125.00	113.40
1	G	334	ARG	CA-CB-CG	5.27	124.99	113.40
1	F	330	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	E	289	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	F	254	LYS	CA-CB-CG	5.06	124.54	113.40
1	C	406	GLU	CG-CD-OE1	-5.06	108.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	GLU	CG-CD-OE2	5.03	128.35	118.30
1	I	96	ARG	CG-CD-NE	5.01	122.33	111.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ARG	Sidechain
1	A	7	ARG	Sidechain
1	D	96	ARG	Sidechain
1	E	381	ARG	Sidechain
1	E	7	ARG	Sidechain
1	E	78	ARG	Sidechain
1	E	96	ARG	Sidechain
1	H	381	ARG	Sidechain
1	I	381	ARG	Sidechain
1	J	381	ARG	Sidechain
1	J	96	ARG	Sidechain
1	K	445	ARG	Sidechain
1	L	381	ARG	Sidechain
1	L	419	ARG	Sidechain

## 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	3628	0	3653	22	0
1	B	3643	0	3674	27	1
1	C	3651	0	3680	34	2
1	D	3685	0	3717	29	0
1	E	3676	0	3704	35	0
1	F	3628	0	3653	37	0
1	G	3623	0	3645	22	0
1	H	3620	0	3647	34	0
1	I	3665	0	3691	38	2
1	J	3675	0	3705	30	1
1	K	3623	0	3645	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3658	0	3683	24	0
2	A	10	0	0	5	0
2	B	10	0	0	3	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
2	E	10	0	0	3	0
2	F	10	0	0	2	0
2	G	15	0	0	2	0
2	H	10	0	0	2	0
2	I	10	0	0	0	0
2	J	5	0	0	0	0
2	K	10	0	0	1	0
2	L	10	0	0	1	0
All	All	43895	0	44097	282	3

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 3.

All (282) 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:D:12:GLN:NE2	1:F:204:ASN:O	1.72	1.22
1:C:224:ASP:OD2	1:E:213:ASN:CB	1.94	1.15
1:C:224:ASP:OD2	1:E:213:ASN:HB3	1.48	1.11
1:F:16:GLN:CD	1:L:204:ASN:HD21	1.54	1.09
1:H:213:ASN:CB	1:I:224:ASP:OD2	2.03	1.07
1:F:249:SER:HB2	1:L:210:GLU:HA	1.42	1.01
1:A:204:ASN:O	1:B:12:GLN:NE2	1.95	0.98
1:F:16:GLN:CD	1:L:204:ASN:ND2	2.17	0.98
1:F:16:GLN:NE2	1:L:204:ASN:HD21	1.60	0.97
1:H:213:ASN:HB3	1:I:224:ASP:OD2	1.65	0.96
1:H:334:ARG:NH2	2:H:501:SO4:O3	2.00	0.93
1:I:78:ARG:HG3	1:I:80:GLU:OE1	1.67	0.93
1:F:78:ARG:HG2	1:J:193:ASN:ND2	1.84	0.92
1:E:224:ASP:HB3	1:G:195:ARG:HH21	1.42	0.84
1:H:213:ASN:N	1:I:224:ASP:OD2	2.11	0.84
1:C:16:GLN:HB3	1:E:204:ASN:OD1	1.80	0.81
1:C:224:ASP:OD2	1:E:213:ASN:N	2.13	0.81
1:H:210:GLU:O	1:I:224:ASP:HB2	1.81	0.80
1:I:78:ARG:NH1	1:I:80:GLU:OE1	2.14	0.79
1:E:224:ASP:HB3	1:G:195:ARG:NH2	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:381:ARG:HH22	1:K:449:ARG:HH11	1.28	0.77
1:F:78:ARG:CG	1:J:193:ASN:ND2	2.47	0.77
1:C:224:ASP:OD2	1:E:213:ASN:CA	2.32	0.76
1:D:96:ARG:HH22	1:D:156:ASN:HD22	1.33	0.75
1:F:357:HIS:NE2	2:F:502:SO4:O3	2.17	0.74
1:C:224:ASP:CG	1:E:213:ASN:HB3	2.08	0.73
1:F:16:GLN:NE2	1:L:204:ASN:ND2	2.36	0.73
1:D:381:ARG:HH21	1:D:449:ARG:HH11	1.38	0.71
1:E:7:ARG:HH11	1:E:7:ARG:HB2	1.57	0.69
1:H:213:ASN:CA	1:I:224:ASP:OD2	2.41	0.68
2:G:502:SO4:O2	1:J:329:ARG:NH2	2.29	0.66
1:A:138:HIS:HE1	2:A:502:SO4:O1	1.79	0.66
1:I:78:ARG:CG	1:I:80:GLU:OE1	2.43	0.65
1:C:249:SER:HB2	1:E:209:PRO:HB2	1.79	0.65
1:K:329:ARG:NH2	2:L:501:SO4:O1	2.29	0.65
1:F:77:GLN:O	1:J:193:ASN:ND2	2.29	0.65
1:H:207:LYS:HB2	1:I:254:LYS:NZ	2.11	0.65
1:H:213:ASN:HB3	1:I:224:ASP:CG	2.18	0.64
1:C:224:ASP:HB2	1:E:210:GLU:O	1.96	0.64
1:H:209:PRO:HB3	1:I:249:SER:OG	1.96	0.64
1:H:204:ASN:OD1	1:I:16:GLN:HB3	1.97	0.64
1:E:334:ARG:NH2	2:E:501:SO4:O2	2.28	0.63
1:F:16:GLN:OE1	1:L:204:ASN:ND2	2.32	0.62
1:A:7:ARG:NH2	1:A:15:ALA:HB2	2.16	0.61
1:B:23:SER:HB2	1:D:24:VAL:CG1	2.30	0.61
1:D:96:ARG:HH22	1:D:156:ASN:ND2	1.97	0.61
1:C:249:SER:OG	1:E:209:PRO:HB3	1.98	0.61
1:D:381:ARG:NH2	1:D:449:ARG:HH11	1.99	0.60
1:A:204:ASN:O	1:B:12:GLN:CD	2.40	0.59
1:D:96:ARG:NH2	1:D:156:ASN:HD22	2.00	0.59
1:C:260:MET:HB2	1:C:261:PRO:HD3	1.85	0.59
1:I:260:MET:HB2	1:I:261:PRO:HD3	1.85	0.59
1:K:442:ARG:HH11	1:K:445:ARG:HH21	1.49	0.59
1:A:316:ILE:HD12	1:A:316:ILE:H	1.68	0.58
1:G:338:TYR:OH	2:G:502:SO4:O3	2.19	0.58
1:K:260:MET:HB2	1:K:261:PRO:HD3	1.84	0.58
1:H:260:MET:HB2	1:H:261:PRO:HD3	1.85	0.58
1:B:329:ARG:NH2	2:E:501:SO4:O4	2.37	0.58
1:G:260:MET:HB2	1:G:261:PRO:HD3	1.85	0.58
1:H:213:ASN:HB2	1:I:224:ASP:OD2	1.97	0.58
1:F:377:PRO:HB3	1:F:381:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:316:ILE:H	1:L:316:ILE:HD12	1.70	0.57
1:A:231:GLY:O	1:F:177:ARG:HG2	2.04	0.57
1:L:260:MET:HB2	1:L:261:PRO:HD3	1.87	0.57
1:B:440:ARG:HD3	1:G:209:PRO:HG3	1.86	0.57
1:F:260:MET:HB2	1:F:261:PRO:HD3	1.85	0.57
1:A:329:ARG:NH2	2:C:501:SO4:O1	2.37	0.57
1:C:224:ASP:OD2	1:E:213:ASN:HB2	1.99	0.56
1:H:209:PRO:CB	1:I:249:SER:OG	2.53	0.56
1:B:260:MET:HB2	1:B:261:PRO:HD3	1.86	0.56
1:E:260:MET:HB2	1:E:261:PRO:HD3	1.86	0.56
1:J:260:MET:HB2	1:J:261:PRO:HD3	1.88	0.56
1:B:237:GLN:HB3	1:D:175:ARG:HH21	1.71	0.56
1:A:260:MET:HB2	1:A:261:PRO:HD3	1.88	0.56
1:I:316:ILE:HD12	1:I:316:ILE:H	1.70	0.55
1:F:377:PRO:HB3	1:F:381:ARG:NH1	2.21	0.55
1:E:316:ILE:HD12	1:E:316:ILE:H	1.72	0.55
1:D:260:MET:HB2	1:D:261:PRO:HD3	1.88	0.55
1:D:316:ILE:HD12	1:D:316:ILE:H	1.71	0.55
1:E:12:GLN:OE1	1:G:204:ASN:ND2	2.39	0.55
1:L:282:ARG:NH1	1:L:282:ARG:HB2	2.22	0.54
1:C:249:SER:CB	1:E:209:PRO:HB2	2.38	0.54
1:I:78:ARG:HG3	1:I:80:GLU:CD	2.27	0.54
1:C:191:ILE:O	1:C:197:VAL:HG21	2.08	0.54
1:F:250:SER:O	1:F:254:LYS:HG3	2.08	0.54
1:F:191:ILE:O	1:F:197:VAL:HG21	2.08	0.54
1:B:316:ILE:HD12	1:B:316:ILE:H	1.72	0.54
1:D:191:ILE:O	1:D:197:VAL:HG21	2.08	0.53
1:C:249:SER:OG	1:E:209:PRO:CB	2.56	0.53
1:K:191:ILE:O	1:K:197:VAL:HG21	2.08	0.53
1:B:191:ILE:O	1:B:197:VAL:HG21	2.08	0.53
1:H:191:ILE:O	1:H:197:VAL:HG21	2.09	0.53
1:H:316:ILE:HD12	1:H:316:ILE:H	1.74	0.53
1:F:316:ILE:HD12	1:F:316:ILE:H	1.73	0.53
1:G:191:ILE:O	1:G:197:VAL:HG21	2.08	0.53
1:L:191:ILE:O	1:L:197:VAL:HG21	2.08	0.53
1:I:191:ILE:O	1:I:197:VAL:HG21	2.08	0.53
1:I:204:ASN:ND2	1:K:12:GLN:OE1	2.41	0.53
1:J:191:ILE:O	1:J:197:VAL:HG21	2.09	0.53
1:D:334:ARG:NH2	2:D:501:SO4:O4	2.43	0.52
1:A:191:ILE:O	1:A:197:VAL:HG21	2.08	0.52
1:A:249:SER:HB2	1:J:210:GLU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:316:ILE:HD12	1:K:316:ILE:H	1.74	0.52
1:J:282:ARG:NH1	1:J:282:ARG:HB2	2.24	0.52
1:B:237:GLN:HB3	1:D:175:ARG:NH2	2.25	0.52
1:I:96:ARG:NH1	1:I:305:ASP:OD2	2.43	0.51
1:E:191:ILE:O	1:E:197:VAL:HG21	2.09	0.51
1:J:255:THR:O	1:J:259:LEU:HB2	2.10	0.51
1:C:204:ASN:HD22	1:G:12:GLN:HE21	1.58	0.51
1:B:96:ARG:NH2	1:B:156:ASN:HD22	2.08	0.51
1:J:316:ILE:HD12	1:J:316:ILE:H	1.74	0.51
1:B:255:THR:O	1:B:259:LEU:HB2	2.11	0.51
1:E:255:THR:O	1:E:259:LEU:HB2	2.11	0.51
1:A:255:THR:O	1:A:259:LEU:HB2	2.11	0.51
1:J:96:ARG:NH2	1:J:156:ASN:HD22	2.08	0.51
1:F:77:GLN:OE1	1:J:188:THR:HB	2.11	0.51
1:H:209:PRO:HB2	1:I:249:SER:HB2	1.92	0.50
1:D:255:THR:O	1:D:259:LEU:HB2	2.11	0.50
1:G:255:THR:O	1:G:259:LEU:HB2	2.11	0.50
1:L:255:THR:O	1:L:259:LEU:HB2	2.11	0.50
1:K:255:THR:O	1:K:259:LEU:HB2	2.11	0.50
1:H:213:ASN:HD22	1:H:216:ARG:HH11	1.57	0.50
1:B:357:HIS:CE1	1:B:359:LYS:HE3	2.47	0.50
1:H:210:GLU:O	1:I:224:ASP:CB	2.56	0.50
1:I:312:GLU:HB3	1:I:313:PRO:HD2	1.94	0.50
1:B:97:ILE:HD12	1:B:97:ILE:H	1.77	0.50
1:C:255:THR:O	1:C:259:LEU:HB2	2.11	0.50
1:I:255:THR:O	1:I:259:LEU:HB2	2.12	0.50
1:K:381:ARG:HH22	1:K:449:ARG:NH1	2.05	0.50
1:A:7:ARG:NH2	1:A:15:ALA:CB	2.74	0.49
1:H:255:THR:O	1:H:259:LEU:HB2	2.11	0.49
1:K:381:ARG:NH2	1:K:449:ARG:HH11	2.05	0.49
2:B:501:SO4:O3	1:E:329:ARG:NH2	2.44	0.49
1:F:255:THR:O	1:F:259:LEU:HB2	2.12	0.49
1:F:312:GLU:HB3	1:F:313:PRO:HD2	1.94	0.49
1:C:312:GLU:HB3	1:C:313:PRO:HD2	1.94	0.49
1:G:357:HIS:CE1	1:G:359:LYS:HE3	2.48	0.49
1:J:312:GLU:HB3	1:J:313:PRO:HD2	1.95	0.49
1:K:419:ARG:HD2	1:L:337:TYR:CE1	2.48	0.49
1:I:268:THR:HB	1:I:362:TRP:HB2	1.95	0.49
1:D:312:GLU:HB3	1:D:313:PRO:HD2	1.95	0.48
1:E:357:HIS:NE2	2:E:502:SO4:O4	2.46	0.48
1:H:207:LYS:HB2	1:I:254:LYS:HZ3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:HB3	1:A:313:PRO:HD2	1.94	0.48
1:C:268:THR:HB	1:C:362:TRP:HB2	1.96	0.48
1:F:268:THR:HB	1:F:362:TRP:HB2	1.96	0.48
1:H:381:ARG:HH22	1:H:449:ARG:HG2	1.79	0.48
1:C:316:ILE:HD12	1:C:316:ILE:H	1.78	0.48
1:G:316:ILE:H	1:G:316:ILE:HD12	1.79	0.48
1:H:312:GLU:HB3	1:H:313:PRO:HD2	1.95	0.48
1:A:357:HIS:NE2	2:A:502:SO4:O3	2.25	0.48
2:A:501:SO4:O4	1:C:329:ARG:NH2	2.46	0.48
1:C:249:SER:CB	1:E:209:PRO:CB	2.92	0.48
1:E:312:GLU:HB3	1:E:313:PRO:HD2	1.95	0.48
1:F:78:ARG:HG3	1:J:193:ASN:ND2	2.28	0.48
1:L:268:THR:HB	1:L:362:TRP:HB2	1.96	0.48
1:C:204:ASN:HD22	1:G:12:GLN:NE2	2.11	0.48
1:G:312:GLU:HB3	1:G:313:PRO:HD2	1.96	0.48
1:K:312:GLU:HB3	1:K:313:PRO:HD2	1.95	0.48
1:B:312:GLU:HB3	1:B:313:PRO:HD2	1.95	0.48
1:F:78:ARG:HG3	1:J:193:ASN:HD21	1.78	0.48
1:D:268:THR:HB	1:D:362:TRP:HB2	1.95	0.47
1:E:7:ARG:HH12	1:E:12:GLN:HG3	1.78	0.47
1:D:363:VAL:HB	1:D:367:TRP:HB2	1.96	0.47
1:H:268:THR:HB	1:H:362:TRP:HB2	1.96	0.47
1:E:268:THR:HB	1:E:362:TRP:HB2	1.96	0.47
1:J:268:THR:HB	1:J:362:TRP:HB2	1.95	0.47
1:B:131:ARG:NH2	1:G:441:ILE:HG22	2.30	0.47
1:G:268:THR:HB	1:G:362:TRP:HB2	1.96	0.47
1:K:357:HIS:CE1	1:K:359:LYS:HE3	2.49	0.47
1:L:312:GLU:HB3	1:L:313:PRO:HD2	1.96	0.47
1:K:268:THR:HB	1:K:362:TRP:HB2	1.97	0.47
1:A:268:THR:HB	1:A:362:TRP:HB2	1.97	0.47
1:B:268:THR:HB	1:B:362:TRP:HB2	1.96	0.47
1:B:363:VAL:HB	1:B:367:TRP:HB2	1.97	0.47
1:H:204:ASN:OD1	1:I:16:GLN:O	2.34	0.46
1:E:363:VAL:HB	1:E:367:TRP:HB2	1.97	0.46
1:H:363:VAL:HB	1:H:367:TRP:HB2	1.97	0.46
1:I:363:VAL:HB	1:I:367:TRP:HB2	1.97	0.46
1:J:7:ARG:NH1	1:J:11:GLN:OE1	2.49	0.46
1:D:357:HIS:CE1	1:D:359:LYS:HE3	2.50	0.46
1:F:77:GLN:OE1	1:J:188:THR:CG2	2.64	0.46
1:H:248:LYS:HB2	1:K:213:ASN:CG	2.35	0.46
1:H:357:HIS:NE2	2:H:502:SO4:O1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:357:HIS:CE1	1:J:359:LYS:HE3	2.51	0.46
1:C:363:VAL:HB	1:C:367:TRP:HB2	1.98	0.46
1:J:381:ARG:HH22	1:J:449:ARG:CZ	2.29	0.46
1:F:363:VAL:HB	1:F:367:TRP:HB2	1.98	0.46
1:L:357:HIS:CE1	1:L:359:LYS:HE3	2.51	0.46
1:B:334:ARG:NH2	2:B:501:SO4:O3	2.45	0.45
1:H:357:HIS:CE1	1:H:359:LYS:HE3	2.51	0.45
1:B:289:ARG:NE	2:B:501:SO4:O2	2.42	0.45
1:E:357:HIS:CE1	1:E:359:LYS:HE3	2.51	0.45
1:J:363:VAL:HB	1:J:367:TRP:HB2	1.99	0.45
1:K:363:VAL:HB	1:K:367:TRP:HB2	1.98	0.45
1:L:363:VAL:HB	1:L:367:TRP:HB2	1.99	0.45
1:C:357:HIS:CE1	1:C:359:LYS:HE3	2.52	0.45
1:I:357:HIS:CE1	1:I:359:LYS:HE3	2.52	0.45
1:F:357:HIS:CE1	1:F:359:LYS:HE3	2.52	0.44
1:I:96:ARG:HH21	1:I:96:ARG:HG3	1.82	0.44
1:G:363:VAL:HB	1:G:367:TRP:HB2	1.98	0.44
1:F:338:TYR:OH	2:F:501:SO4:O4	2.29	0.44
2:A:501:SO4:O3	1:C:418:TYR:CE2	2.70	0.44
1:A:357:HIS:CE1	1:A:359:LYS:HE3	2.53	0.44
1:F:55:ALA:O	1:F:87:VAL:HA	2.18	0.44
1:D:12:GLN:CD	1:F:204:ASN:O	2.47	0.44
1:H:209:PRO:HB2	1:I:249:SER:CB	2.47	0.44
1:K:419:ARG:HD2	1:L:337:TYR:CD1	2.53	0.44
1:I:55:ALA:O	1:I:87:VAL:HA	2.18	0.43
1:A:55:ALA:O	1:A:87:VAL:HA	2.18	0.43
1:D:195:ARG:NH2	1:L:224:ASP:HB3	2.33	0.43
1:J:55:ALA:O	1:J:87:VAL:HA	2.19	0.43
1:B:258:HIS:O	1:B:261:PRO:HD2	2.18	0.43
1:E:208:SER:HB2	1:E:209:PRO:HD3	2.01	0.43
1:C:55:ALA:O	1:C:87:VAL:HA	2.18	0.43
1:G:55:ALA:O	1:G:87:VAL:HA	2.18	0.43
1:L:258:HIS:O	1:L:261:PRO:HD2	2.18	0.43
1:F:258:HIS:O	1:F:261:PRO:HD2	2.18	0.43
1:B:55:ALA:O	1:B:87:VAL:HA	2.18	0.43
1:H:55:ALA:O	1:H:87:VAL:HA	2.18	0.43
1:E:55:ALA:O	1:E:87:VAL:HA	2.18	0.43
1:H:208:SER:HB2	1:H:209:PRO:HD3	2.01	0.43
1:J:442:ARG:NH1	1:J:445:ARG:HH21	2.17	0.43
2:A:501:SO4:O3	1:C:418:TYR:HE2	2.01	0.42
1:G:213:ASN:HD22	1:G:216:ARG:HH11	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:HIS:O	1:E:261:PRO:HD2	2.19	0.42
1:J:258:HIS:O	1:J:261:PRO:HD2	2.19	0.42
1:L:55:ALA:O	1:L:87:VAL:HA	2.18	0.42
1:C:16:GLN:CB	1:E:204:ASN:OD1	2.60	0.42
1:D:55:ALA:O	1:D:87:VAL:HA	2.18	0.42
1:D:320:LEU:N	1:D:321:PRO:CD	2.82	0.42
1:C:258:HIS:O	1:C:261:PRO:HD2	2.19	0.42
1:I:258:HIS:O	1:I:261:PRO:HD2	2.19	0.42
1:B:97:ILE:HD12	1:B:97:ILE:N	2.34	0.42
1:A:363:VAL:HB	1:A:367:TRP:HB2	1.99	0.42
1:B:320:LEU:N	1:B:321:PRO:CD	2.83	0.42
1:D:258:HIS:O	1:D:261:PRO:HD2	2.19	0.42
1:I:97:ILE:H	1:I:97:ILE:HD12	1.85	0.42
1:F:77:GLN:OE1	1:J:188:THR:HG21	2.19	0.42
1:A:208:SER:HB2	1:A:209:PRO:HD3	2.02	0.42
1:E:109:TYR:CD2	1:E:123:VAL:HG11	2.55	0.42
1:F:320:LEU:N	1:F:321:PRO:CD	2.83	0.42
1:H:258:HIS:O	1:H:261:PRO:HD2	2.19	0.42
1:A:258:HIS:O	1:A:261:PRO:HD2	2.19	0.41
1:C:208:SER:HB2	1:C:209:PRO:HD3	2.02	0.41
1:H:320:LEU:N	1:H:321:PRO:CD	2.83	0.41
1:I:183:MET:O	1:I:187:VAL:HG23	2.20	0.41
1:I:320:LEU:N	1:I:321:PRO:CD	2.83	0.41
1:K:55:ALA:O	1:K:87:VAL:HA	2.19	0.41
1:J:109:TYR:CD2	1:J:123:VAL:HG11	2.55	0.41
1:G:258:HIS:O	1:G:261:PRO:HD2	2.19	0.41
1:D:440:ARG:HD3	1:K:209:PRO:HG3	2.02	0.41
1:G:320:LEU:N	1:G:321:PRO:CD	2.84	0.41
1:F:224:ASP:OD2	1:L:213:ASN:OD1	2.37	0.41
1:G:419:ARG:HD2	1:J:337:TYR:CD1	2.56	0.41
1:I:97:ILE:HD12	1:I:97:ILE:N	2.35	0.41
1:K:320:LEU:N	1:K:321:PRO:CD	2.84	0.41
1:G:409:ARG:O	1:G:412:THR:OG1	2.34	0.41
1:A:230:GLN:HB3	1:F:177:ARG:NE	2.35	0.41
1:A:320:LEU:N	1:A:321:PRO:CD	2.83	0.41
1:C:97:ILE:HD12	1:C:97:ILE:H	1.85	0.41
1:C:97:ILE:HD12	1:C:97:ILE:N	2.36	0.41
1:C:320:LEU:N	1:C:321:PRO:CD	2.83	0.41
1:D:97:ILE:HD12	1:D:97:ILE:N	2.36	0.41
1:D:204:ASN:ND2	1:L:12:GLN:OE1	2.54	0.41
1:D:208:SER:HB2	1:D:209:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:TYR:CD2	1:H:123:VAL:HG11	2.56	0.41
1:J:208:SER:HB2	1:J:209:PRO:HD3	2.02	0.41
1:K:258:HIS:O	1:K:261:PRO:HD2	2.20	0.41
1:K:334:ARG:NH2	2:K:501:SO4:O2	2.54	0.41
1:L:320:LEU:N	1:L:321:PRO:CD	2.84	0.41
1:B:23:SER:HB2	1:D:24:VAL:HG11	2.01	0.41
1:J:96:ARG:HH22	1:J:156:ASN:HD22	1.69	0.41
1:C:183:MET:O	1:C:187:VAL:HG23	2.21	0.40
1:D:109:TYR:CD2	1:D:123:VAL:HG11	2.56	0.40
1:B:96:ARG:HH21	1:B:156:ASN:HD22	1.68	0.40
1:F:78:ARG:NH1	1:J:193:ASN:OD1	2.52	0.40
1:L:208:SER:HB2	1:L:209:PRO:HD3	2.04	0.40
1:B:424:ILE:HA	1:B:427:TYR:CD2	2.56	0.40
1:E:183:MET:O	1:E:187:VAL:HG23	2.22	0.40
1:F:208:SER:HB2	1:F:209:PRO:HD3	2.03	0.40
1:I:381:ARG:NH2	1:I:449:ARG:NH2	2.69	0.40

All (3) 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:C:175:ARG:NH2	1:I:26:ASP:OD2[1_556]	1.86	0.34
1:C:26:ASP:OD2	1:I:175:ARG:NH2[1_556]	1.92	0.28
1:B:164:ASP:OD2	1:J:111:ARG:CD[1_565]	2.07	0.13

## 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	433/461 (94%)	413 (95%)	20 (5%)	0	100 100
1	B	435/461 (94%)	415 (95%)	20 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	436/461 (95%)	414 (95%)	22 (5%)	0	100	100
1	D	444/461 (96%)	424 (96%)	20 (4%)	0	100	100
1	E	443/461 (96%)	420 (95%)	23 (5%)	0	100	100
1	F	433/461 (94%)	413 (95%)	20 (5%)	0	100	100
1	G	433/461 (94%)	413 (95%)	20 (5%)	0	100	100
1	H	432/461 (94%)	412 (95%)	20 (5%)	0	100	100
1	I	442/461 (96%)	420 (95%)	22 (5%)	0	100	100
1	J	439/461 (95%)	417 (95%)	22 (5%)	0	100	100
1	K	433/461 (94%)	413 (95%)	20 (5%)	0	100	100
1	L	437/461 (95%)	417 (95%)	20 (5%)	0	100	100
All	All	5240/5532 (95%)	4991 (95%)	249 (5%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/412 (96%)	390 (99%)	5 (1%)	65	83
1	B	396/412 (96%)	388 (98%)	8 (2%)	50	74
1	C	397/412 (96%)	390 (98%)	7 (2%)	54	76
1	D	399/412 (97%)	392 (98%)	7 (2%)	54	76
1	E	398/412 (97%)	390 (98%)	8 (2%)	50	74
1	F	395/412 (96%)	387 (98%)	8 (2%)	50	74
1	G	395/412 (96%)	386 (98%)	9 (2%)	45	70
1	H	394/412 (96%)	386 (98%)	8 (2%)	50	74
1	I	397/412 (96%)	389 (98%)	8 (2%)	50	74
1	J	399/412 (97%)	387 (97%)	12 (3%)	36	61
1	K	395/412 (96%)	386 (98%)	9 (2%)	45	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	398/412 (97%)	389 (98%)	9 (2%)	45 70
All	All	4758/4944 (96%)	4660 (98%)	98 (2%)	48 72

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ASP
1	A	214	ASP
1	A	239	SER
1	A	334	ARG
1	A	359	LYS
1	B	38	GLU
1	B	164	ASP
1	B	177	ARG
1	B	214	ASP
1	B	239	SER
1	B	334	ARG
1	B	359	LYS
1	B	437	ARG
1	C	9	LYS
1	C	38	GLU
1	C	164	ASP
1	C	214	ASP
1	C	239	SER
1	C	334	ARG
1	C	359	LYS
1	D	6	LYS
1	D	38	GLU
1	D	164	ASP
1	D	214	ASP
1	D	239	SER
1	D	334	ARG
1	D	359	LYS
1	E	78	ARG
1	E	164	ASP
1	E	214	ASP
1	E	230	GLN
1	E	239	SER
1	E	334	ARG
1	E	359	LYS
1	E	416	LYS
1	F	164	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	177	ARG
1	F	214	ASP
1	F	239	SER
1	F	334	ARG
1	F	359	LYS
1	F	437	ARG
1	F	449	ARG
1	G	25	ASP
1	G	164	ASP
1	G	177	ARG
1	G	214	ASP
1	G	239	SER
1	G	334	ARG
1	G	342	ASP
1	G	359	LYS
1	G	437	ARG
1	H	9	LYS
1	H	164	ASP
1	H	214	ASP
1	H	239	SER
1	H	334	ARG
1	H	359	LYS
1	H	440	ARG
1	H	449	ARG
1	I	96	ARG
1	I	114	GLN
1	I	164	ASP
1	I	214	ASP
1	I	239	SER
1	I	334	ARG
1	I	359	LYS
1	I	416	LYS
1	J	5	PHE
1	J	6	LYS
1	J	7	ARG
1	J	8	ASN
1	J	164	ASP
1	J	214	ASP
1	J	239	SER
1	J	282	ARG
1	J	334	ARG
1	J	359	LYS

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Mol	Chain	Res	Type
1	J	437	ARG
1	J	445	ARG
1	K	25	ASP
1	K	114	GLN
1	K	164	ASP
1	K	214	ASP
1	K	239	SER
1	K	334	ARG
1	K	359	LYS
1	K	437	ARG
1	K	440	ARG
1	L	5	PHE
1	L	6	LYS
1	L	164	ASP
1	L	177	ARG
1	L	214	ASP
1	L	239	SER
1	L	282	ARG
1	L	334	ARG
1	L	359	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	213	ASN
1	A	343	GLN
1	B	12	GLN
1	B	138	HIS
1	B	343	GLN
1	C	138	HIS
1	C	204	ASN
1	C	343	GLN
1	D	138	HIS
1	D	343	GLN
1	E	138	HIS
1	E	343	GLN
1	F	138	HIS
1	F	343	GLN
1	G	138	HIS
1	G	213	ASN
1	G	343	GLN

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Mol	Chain	Res	Type
1	H	138	HIS
1	H	213	ASN
1	H	343	GLN
1	I	138	HIS
1	I	204	ASN
1	I	343	GLN
1	J	138	HIS
1	J	343	GLN
1	K	12	GLN
1	K	138	HIS
1	K	343	GLN
1	L	138	HIS
1	L	204	ASN
1	L	213	ASN
1	L	343	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](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	L	502	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	D	502	-	4,4,4	0.35	0	6,6,6	0.19	0
2	SO4	E	501	-	4,4,4	0.48	0	6,6,6	0.43	0
2	SO4	A	501	-	4,4,4	0.44	0	6,6,6	0.34	0
2	SO4	G	503	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	B	501	-	4,4,4	0.37	0	6,6,6	0.30	0
2	SO4	L	501	-	4,4,4	0.40	0	6,6,6	0.15	0
2	SO4	I	501	-	4,4,4	0.44	0	6,6,6	0.16	0
2	SO4	C	502	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	D	501	-	4,4,4	0.37	0	6,6,6	0.29	0
2	SO4	C	501	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	F	502	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	K	501	-	4,4,4	0.38	0	6,6,6	0.18	0
2	SO4	I	502	-	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	B	502	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	G	502	-	4,4,4	0.41	0	6,6,6	0.24	0
2	SO4	K	502	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	A	502	-	4,4,4	0.34	0	6,6,6	0.16	0
2	SO4	F	501	-	4,4,4	0.28	0	6,6,6	0.47	0
2	SO4	H	501	-	4,4,4	0.50	0	6,6,6	0.21	0
2	SO4	E	502	-	4,4,4	0.35	0	6,6,6	0.10	0
2	SO4	G	501	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	J	501	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	H	502	-	4,4,4	0.35	0	6,6,6	0.15	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.

14 monomers are involved in 21 short contacts:

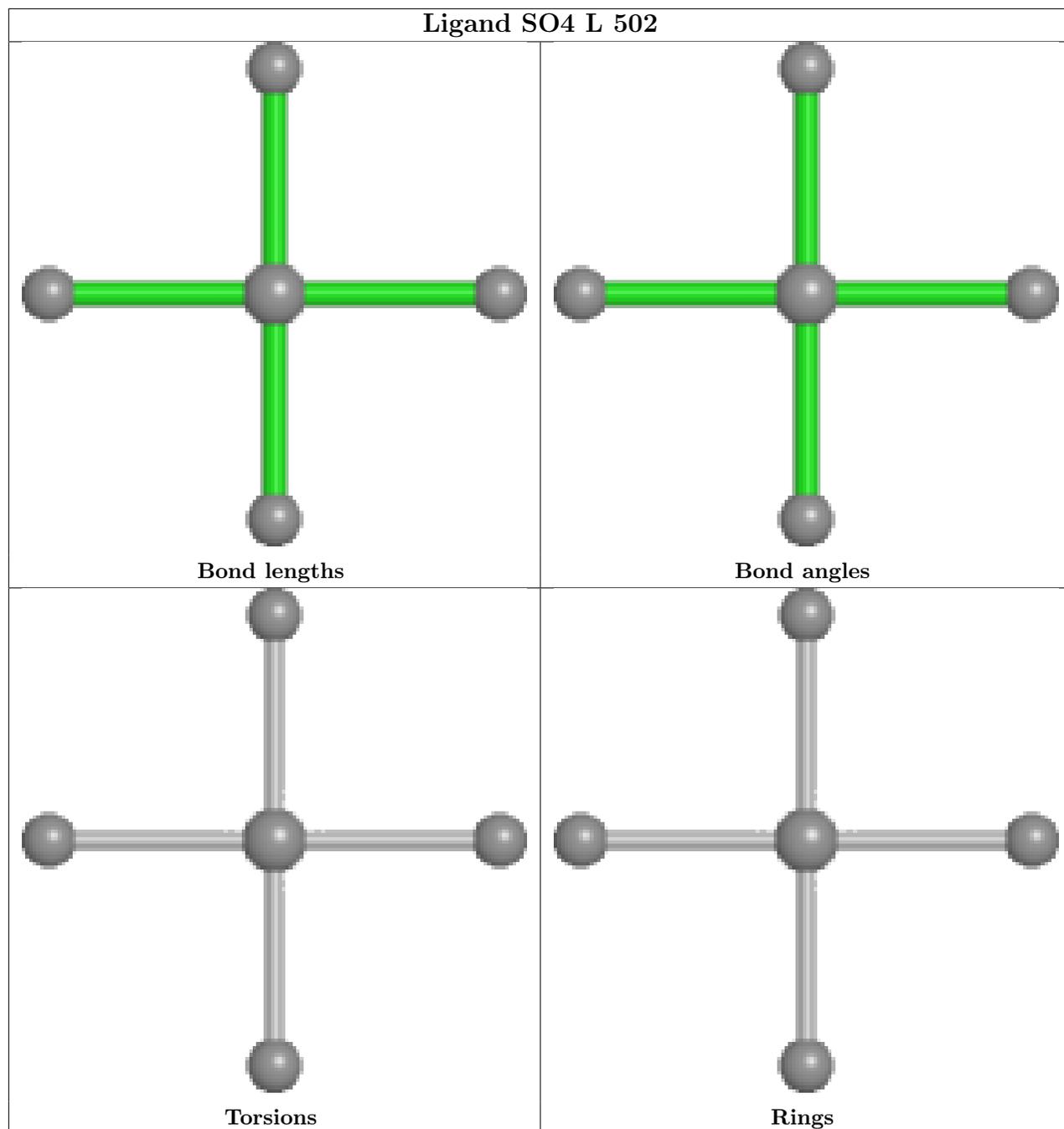
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	SO4	2	0
2	A	501	SO4	3	0
2	B	501	SO4	3	0
2	L	501	SO4	1	0
2	D	501	SO4	1	0
2	C	501	SO4	1	0
2	F	502	SO4	1	0

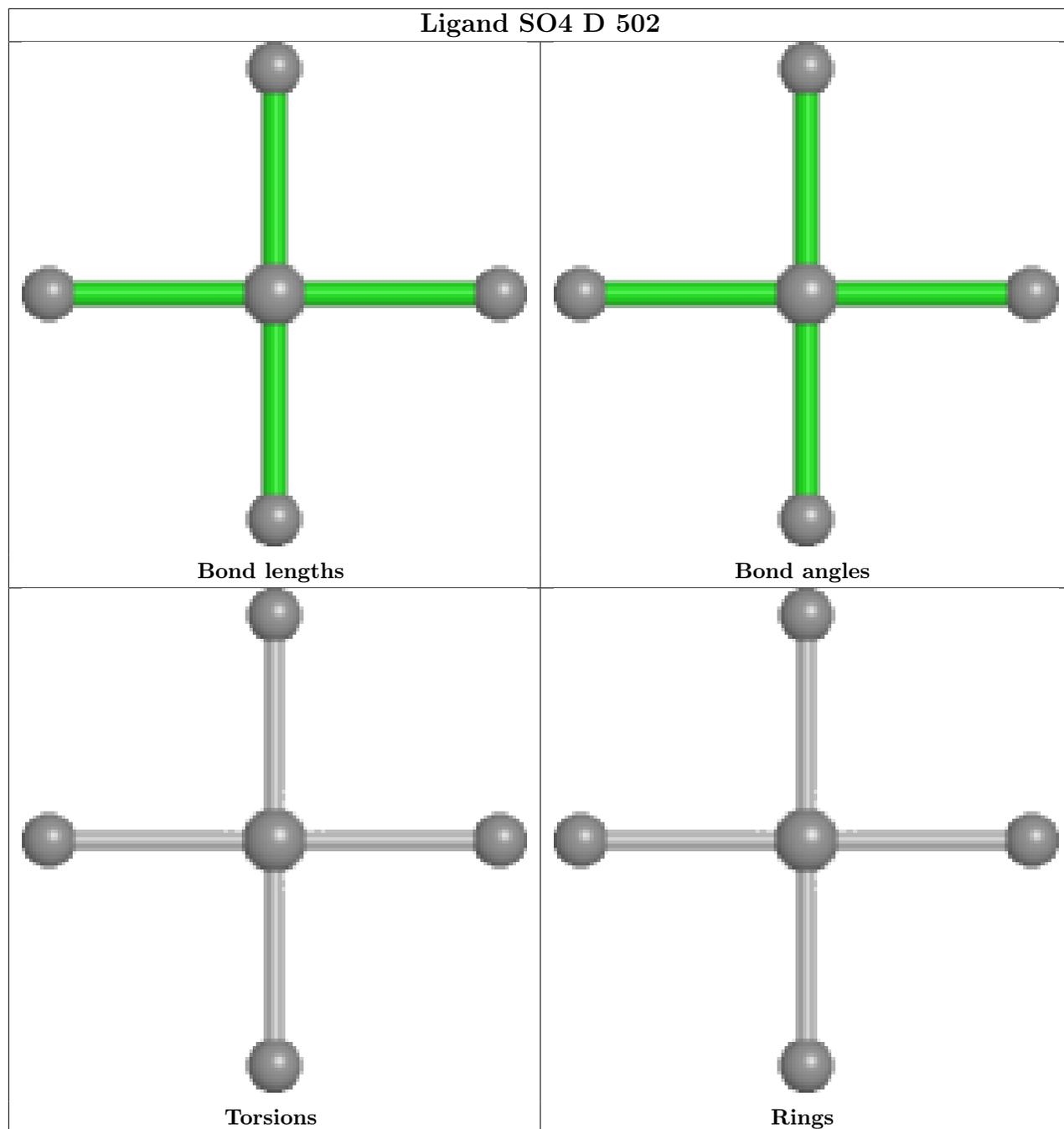
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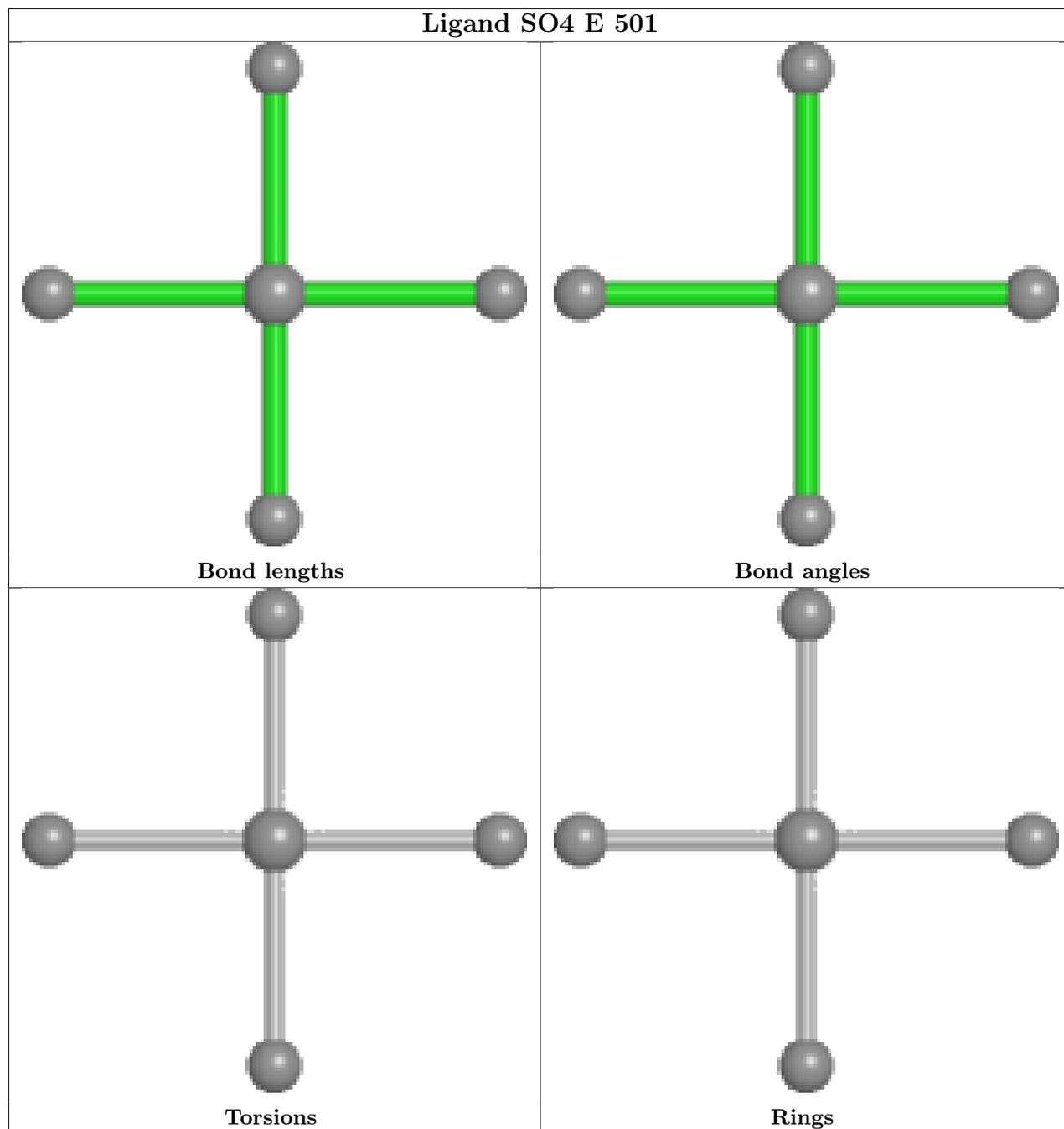
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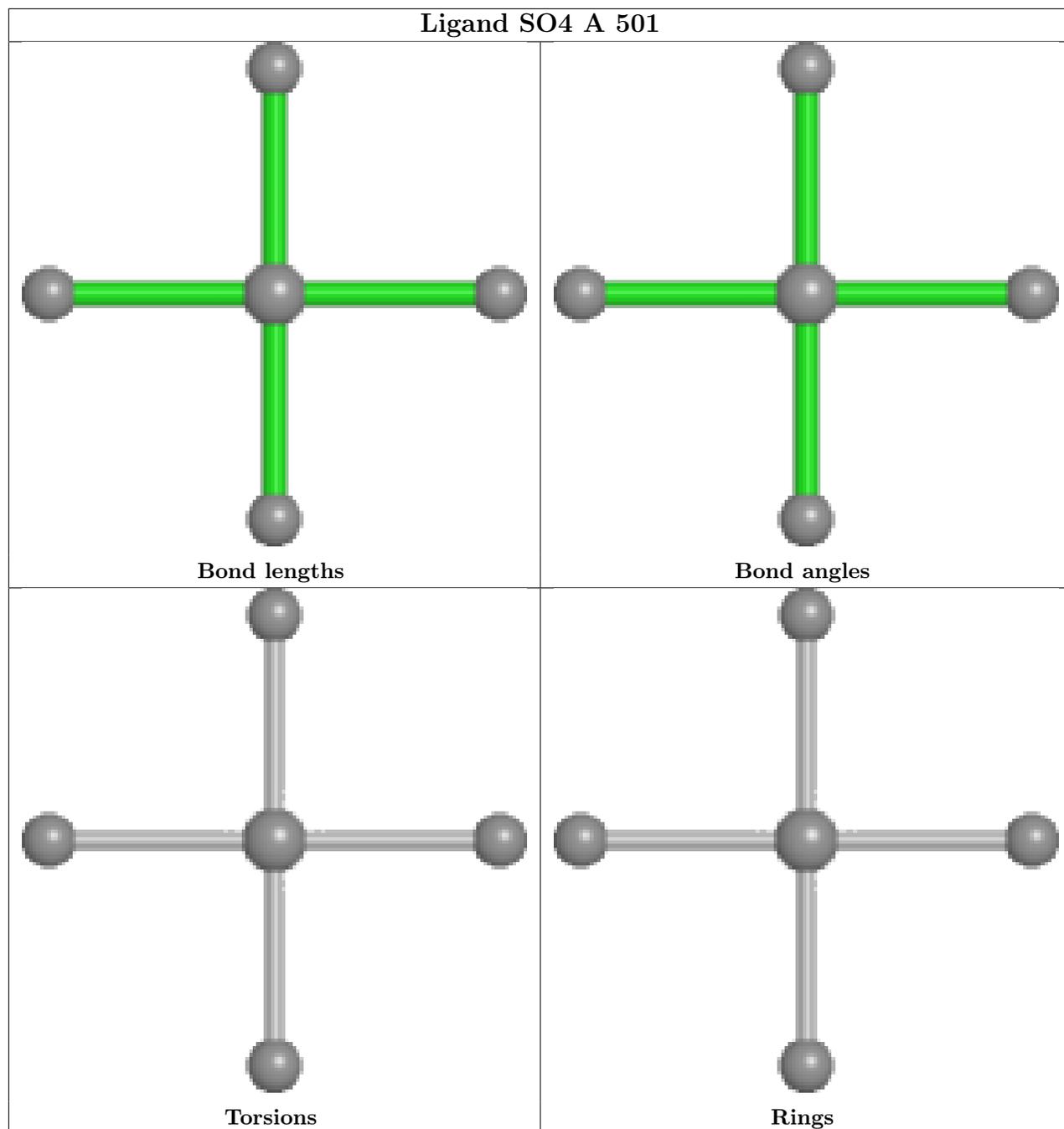
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	501	SO4	1	0
2	G	502	SO4	2	0
2	A	502	SO4	2	0
2	F	501	SO4	1	0
2	H	501	SO4	1	0
2	E	502	SO4	1	0
2	H	502	SO4	1	0

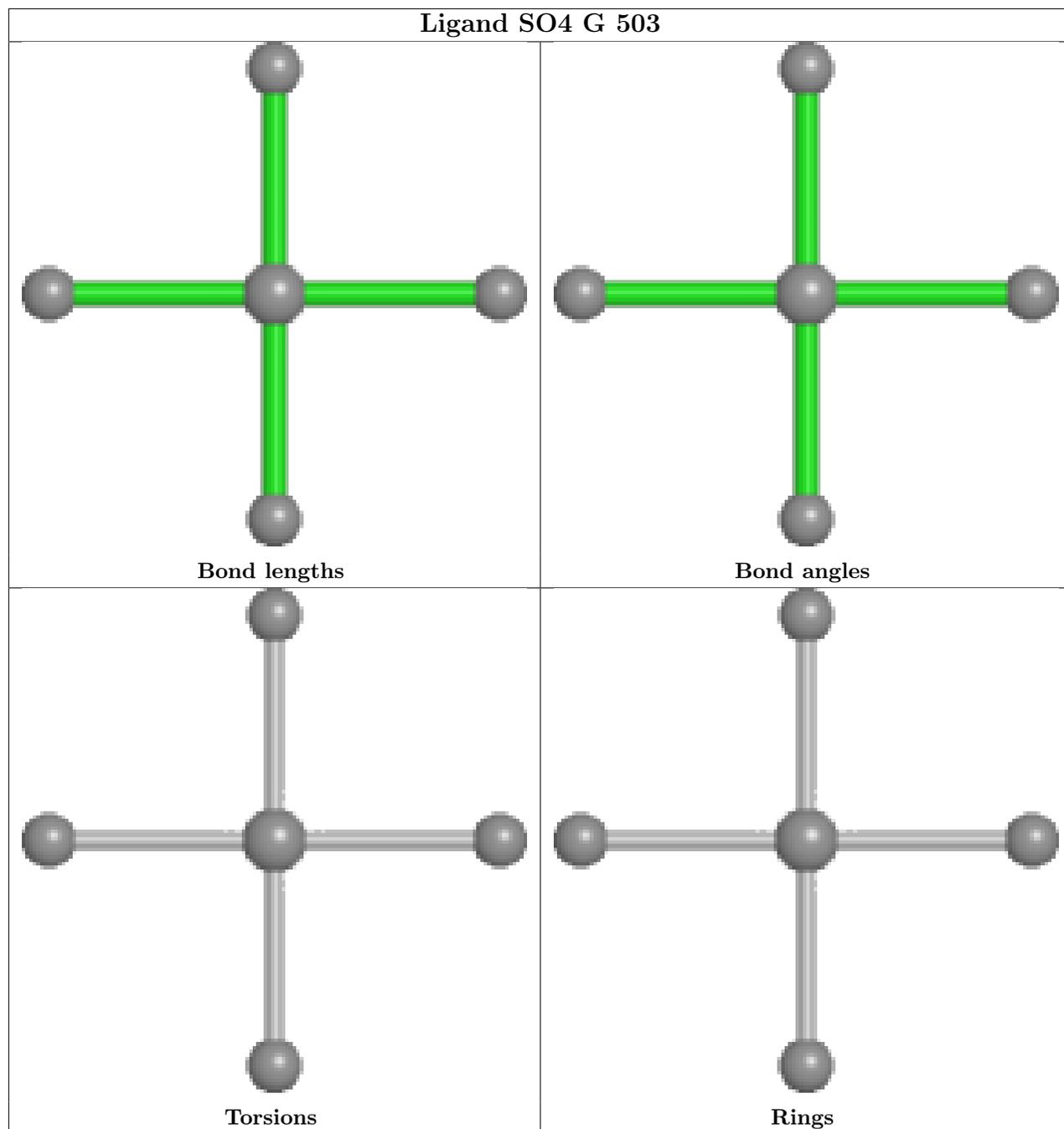
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

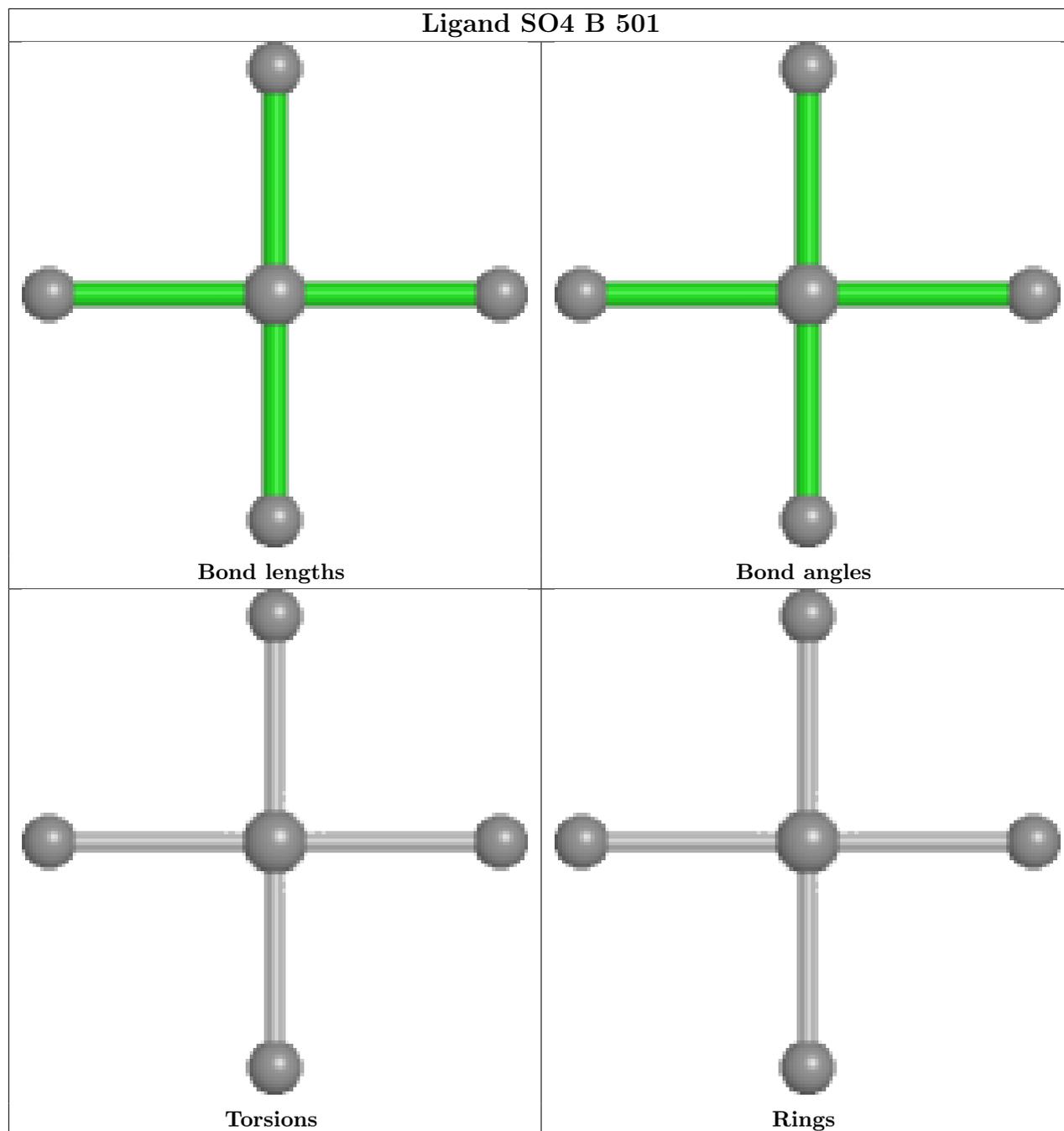


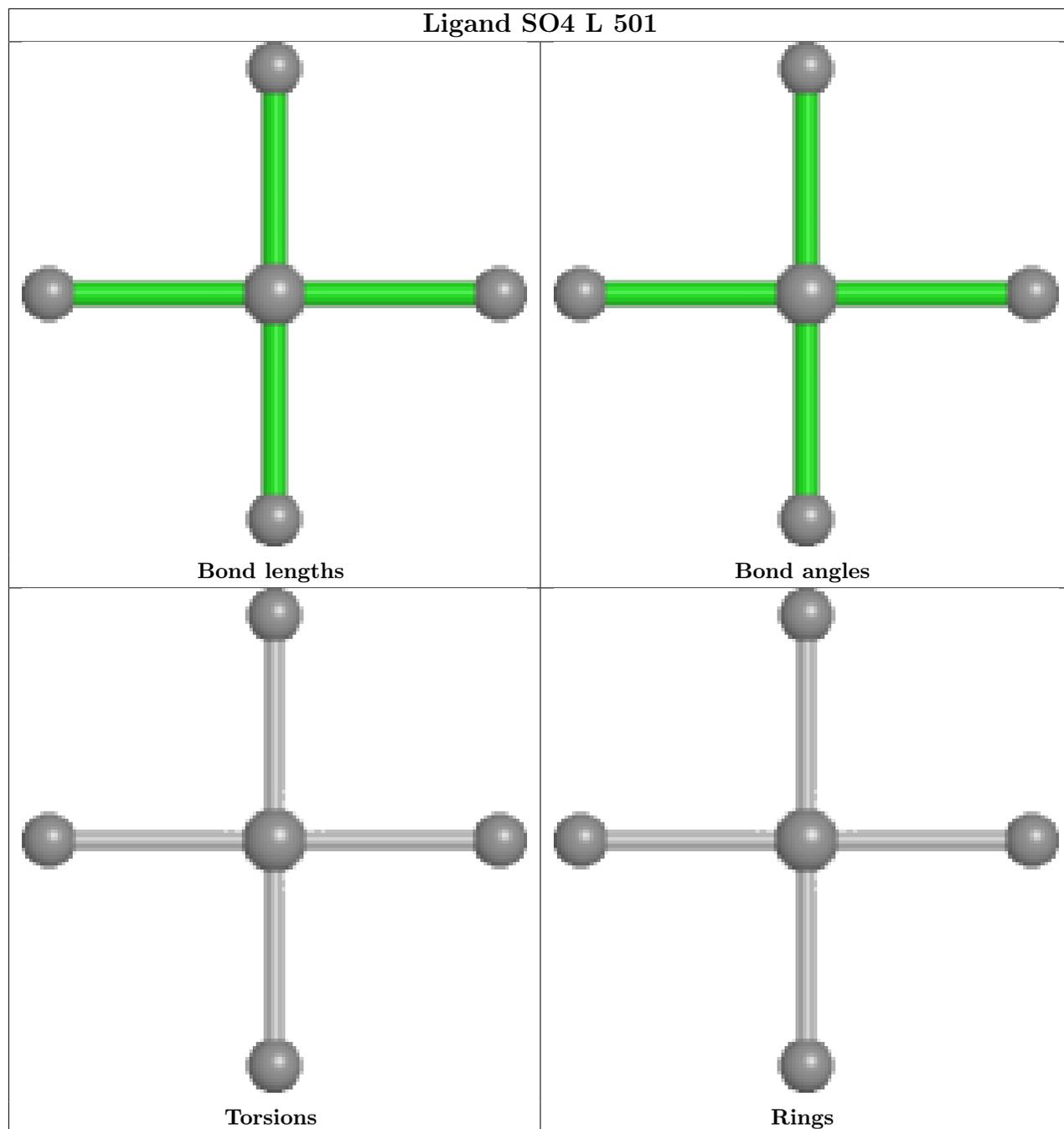


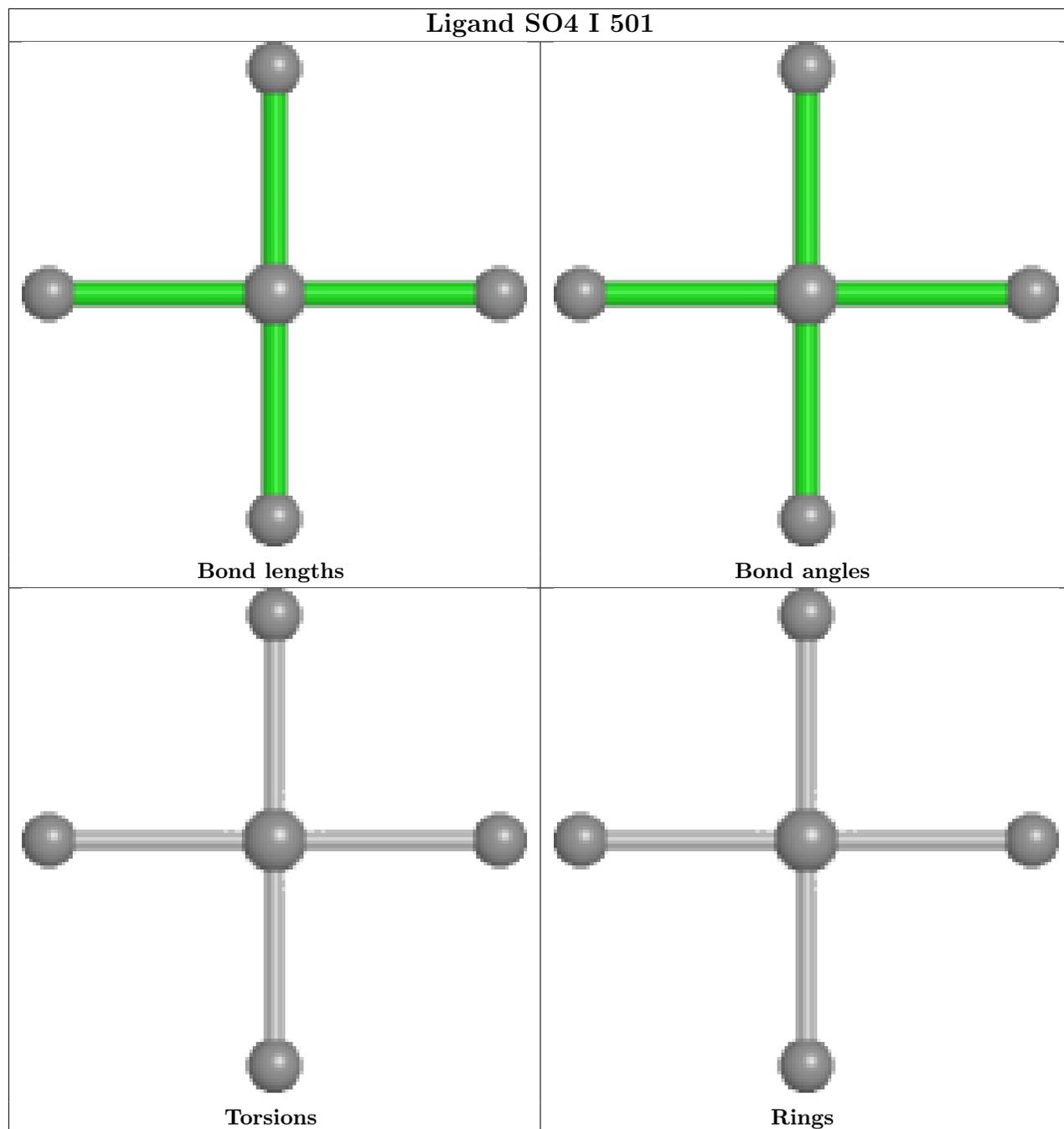


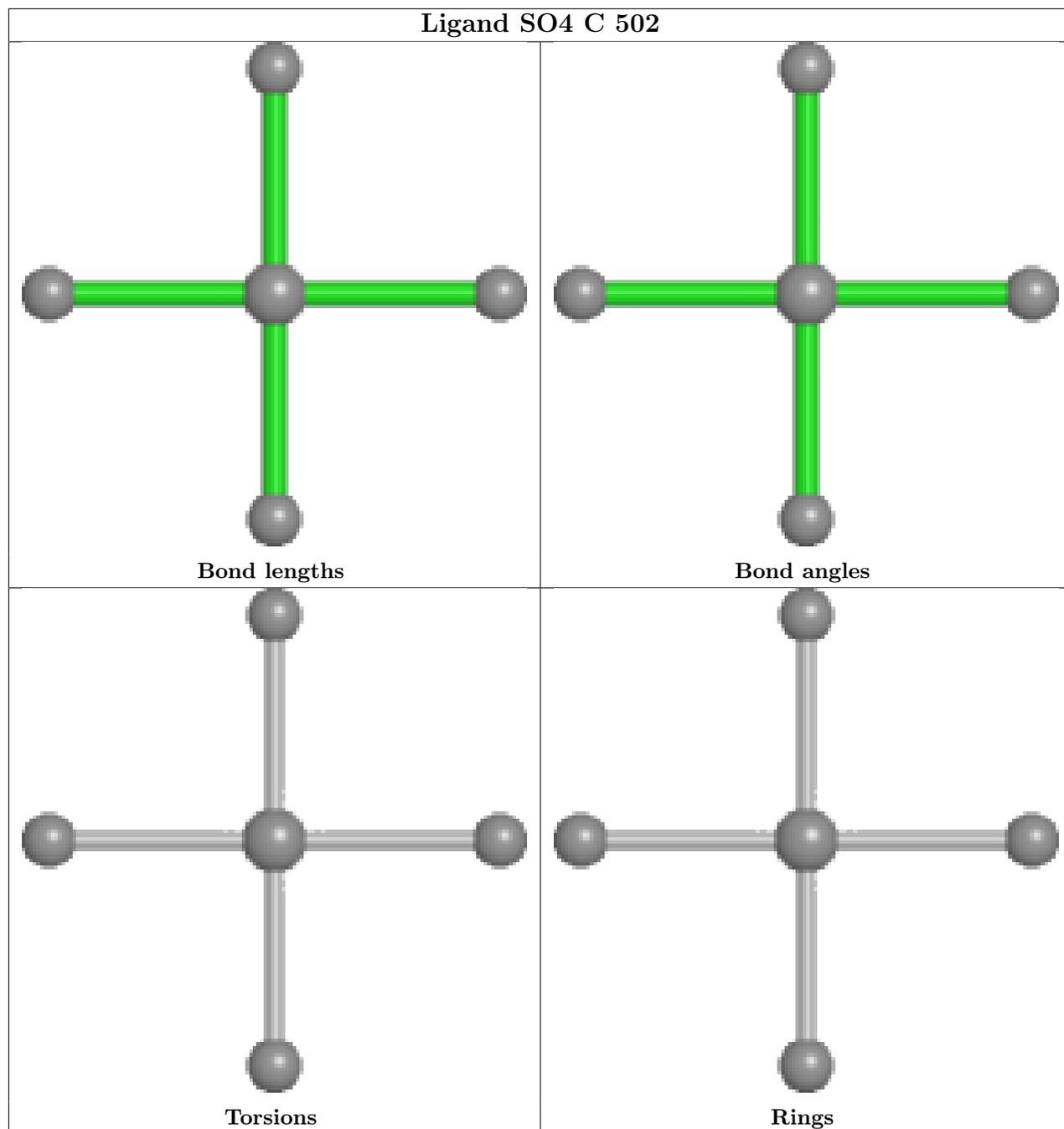


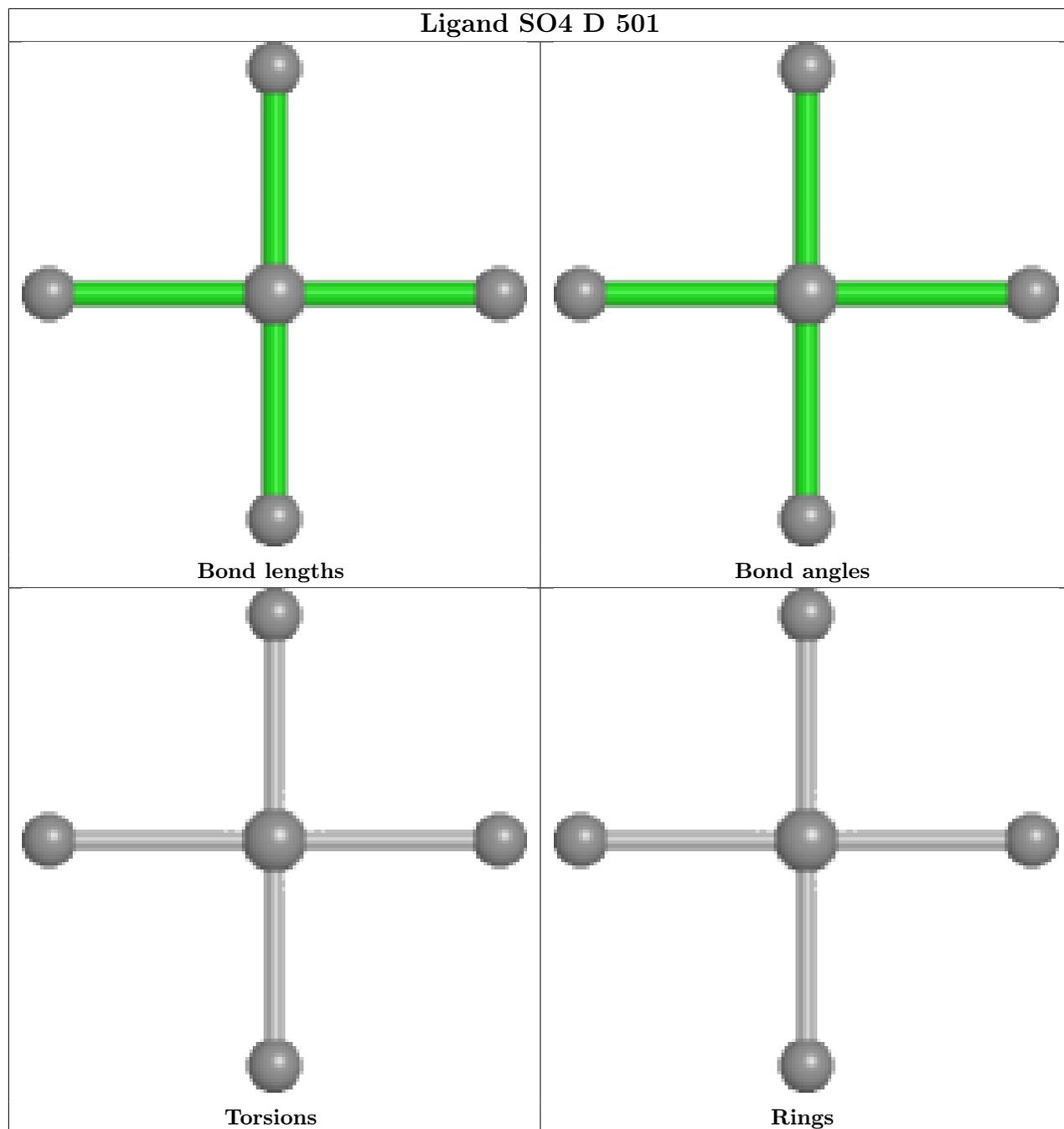


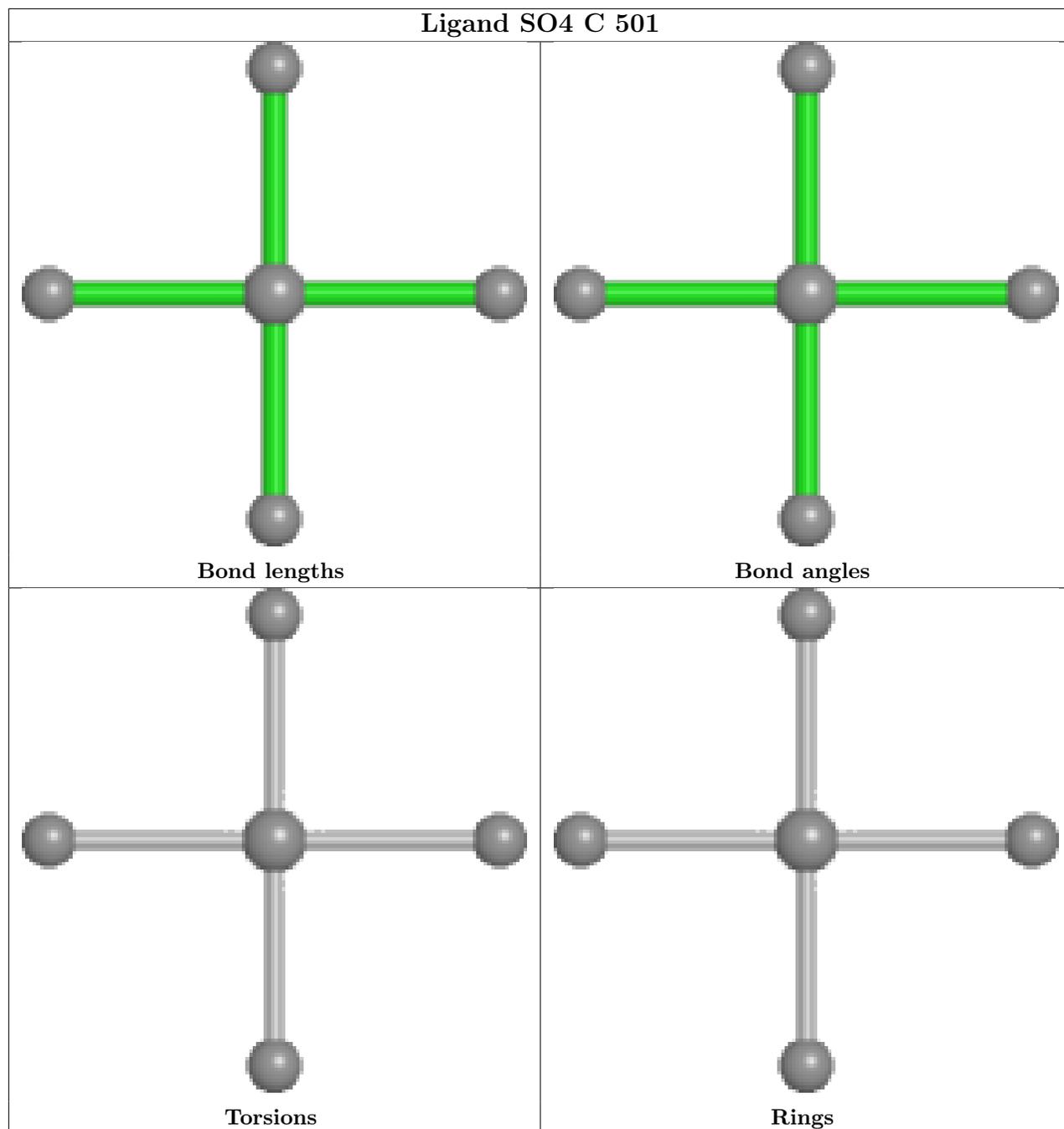


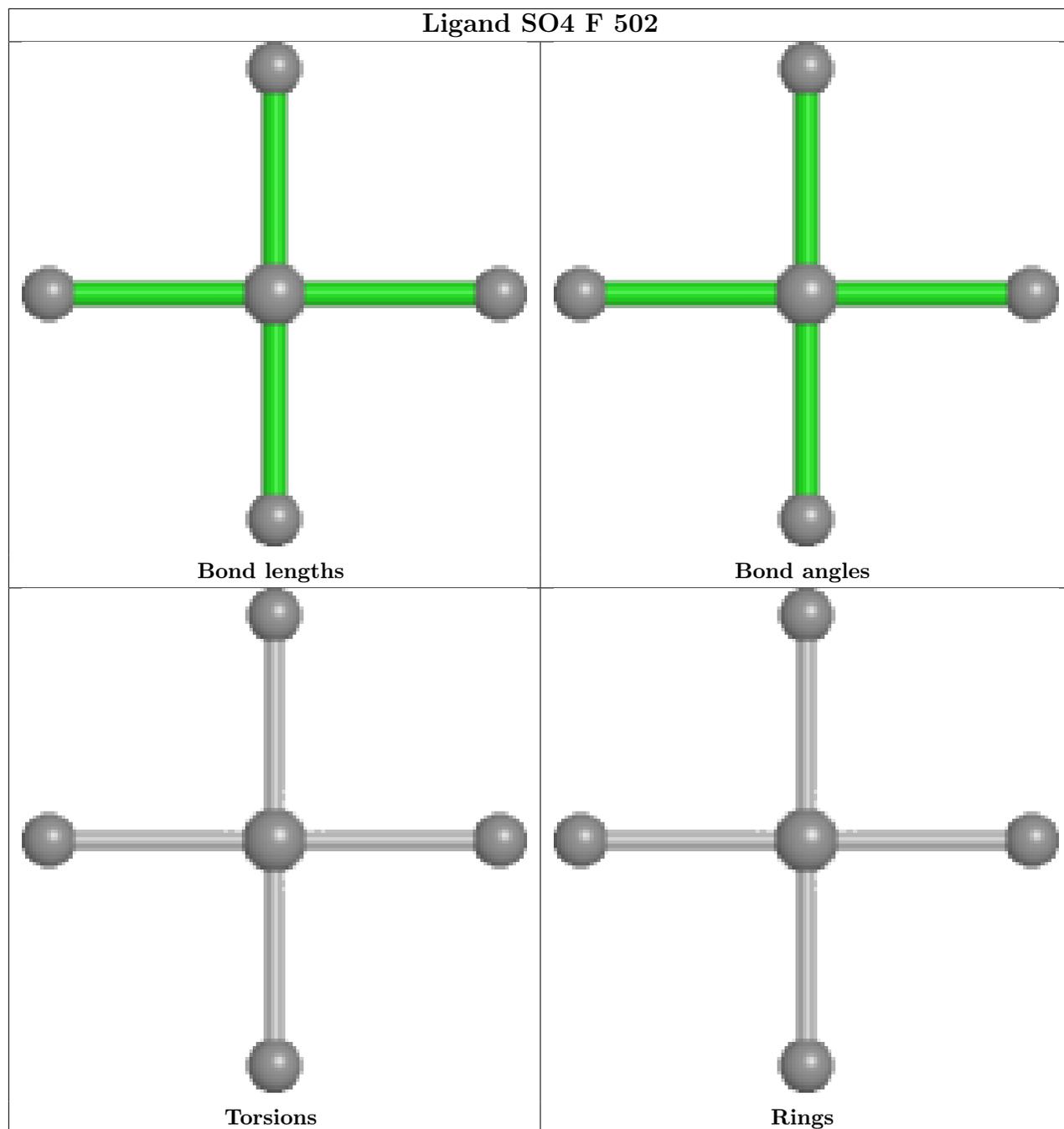


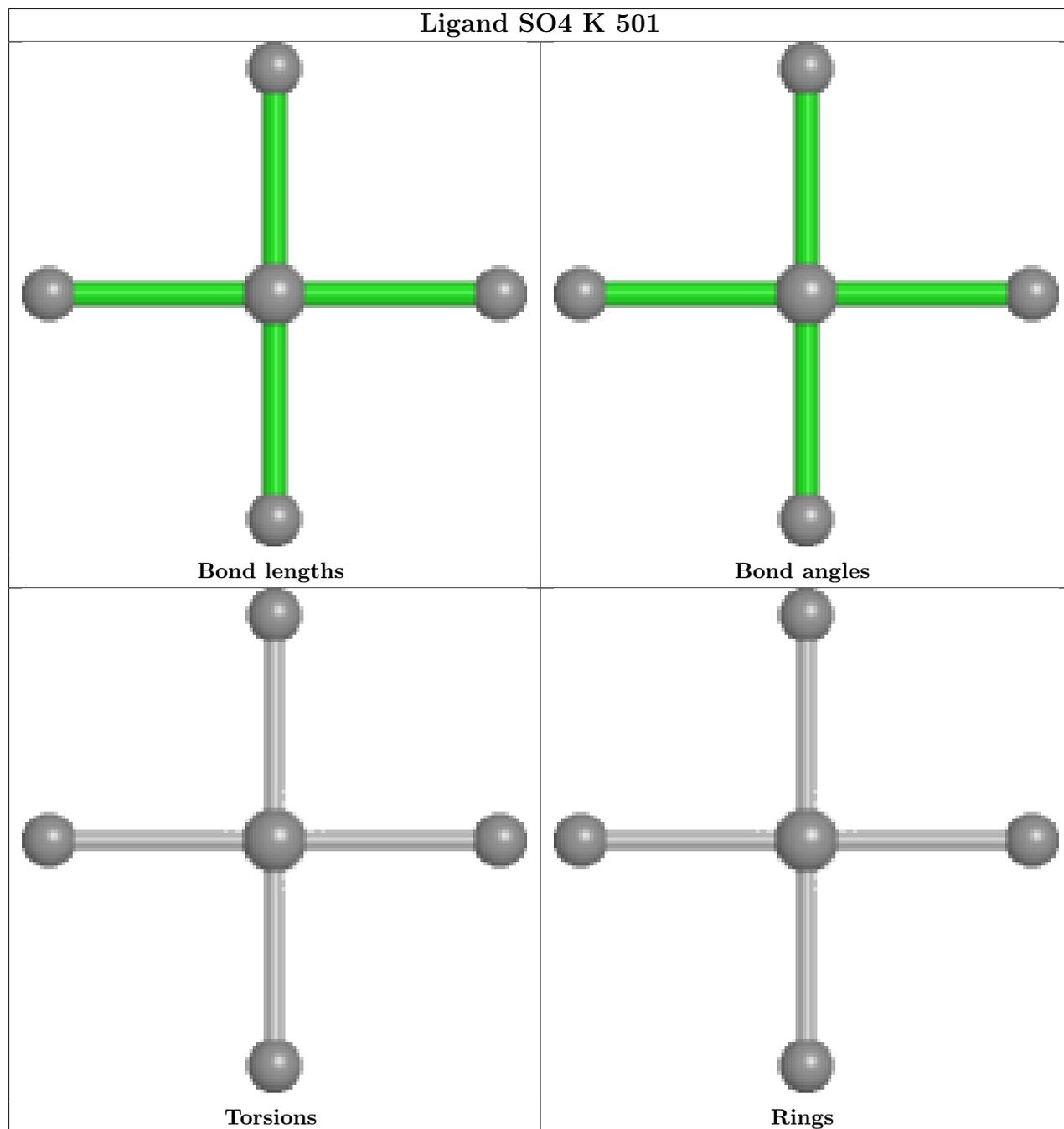


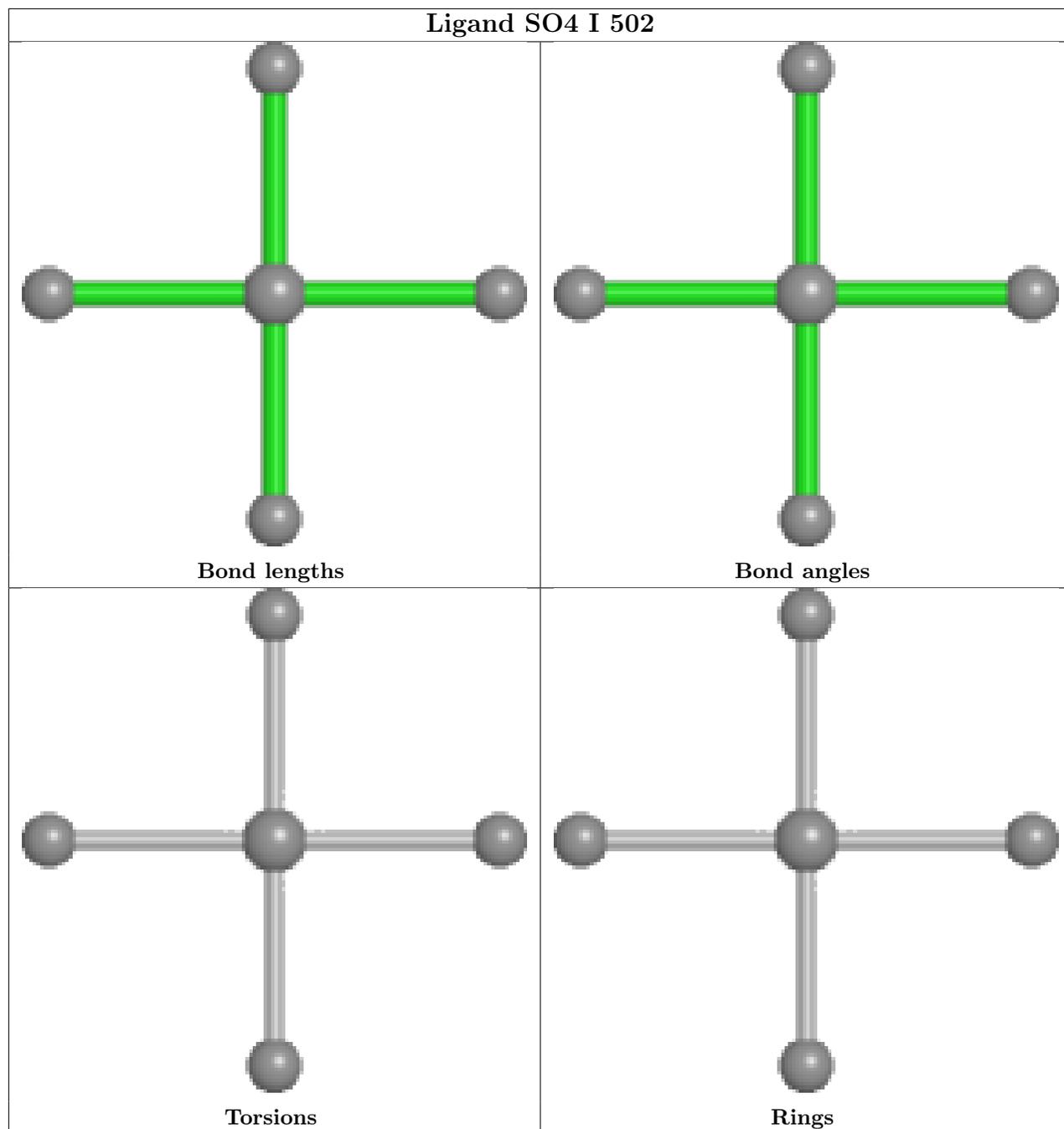


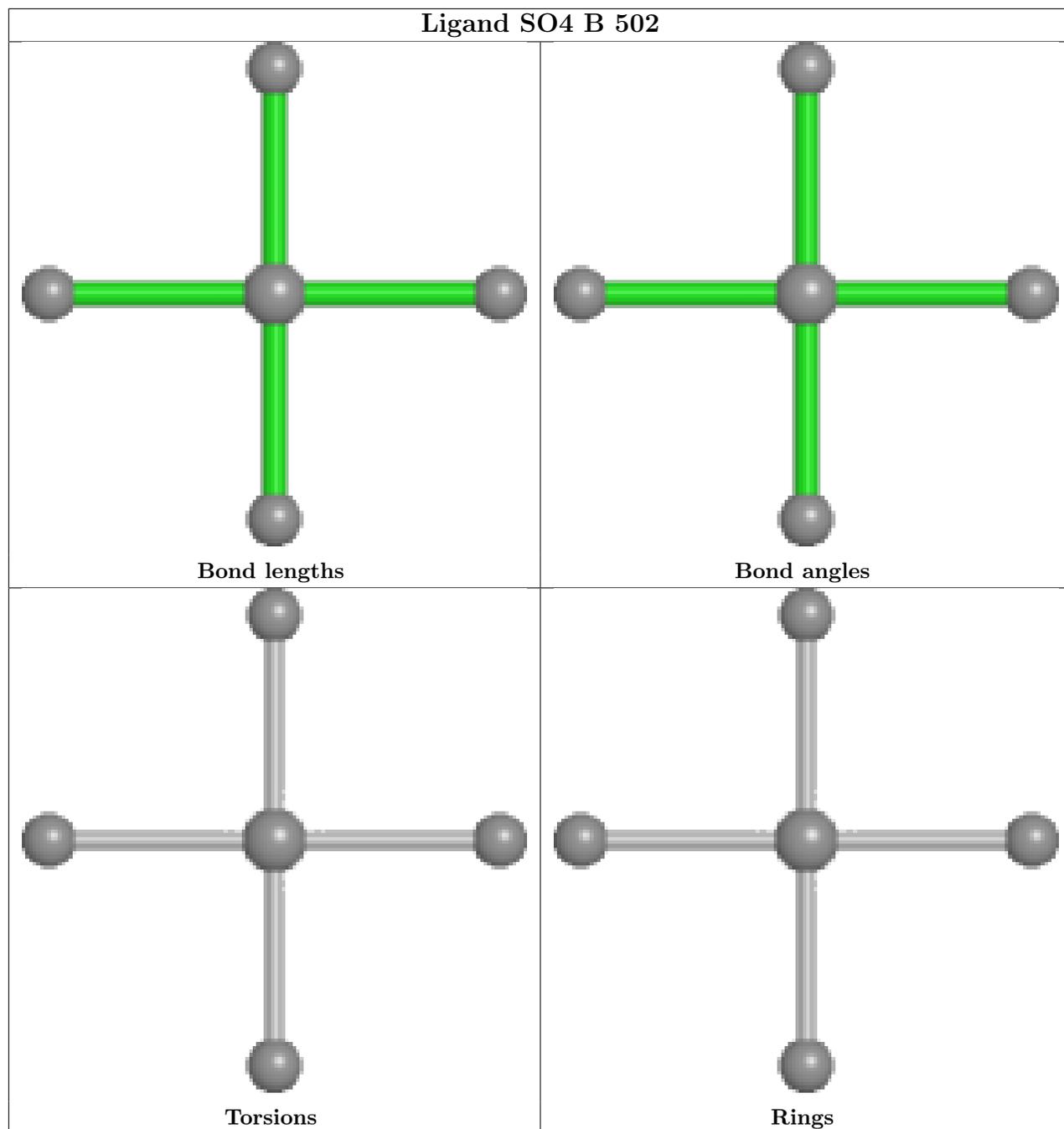


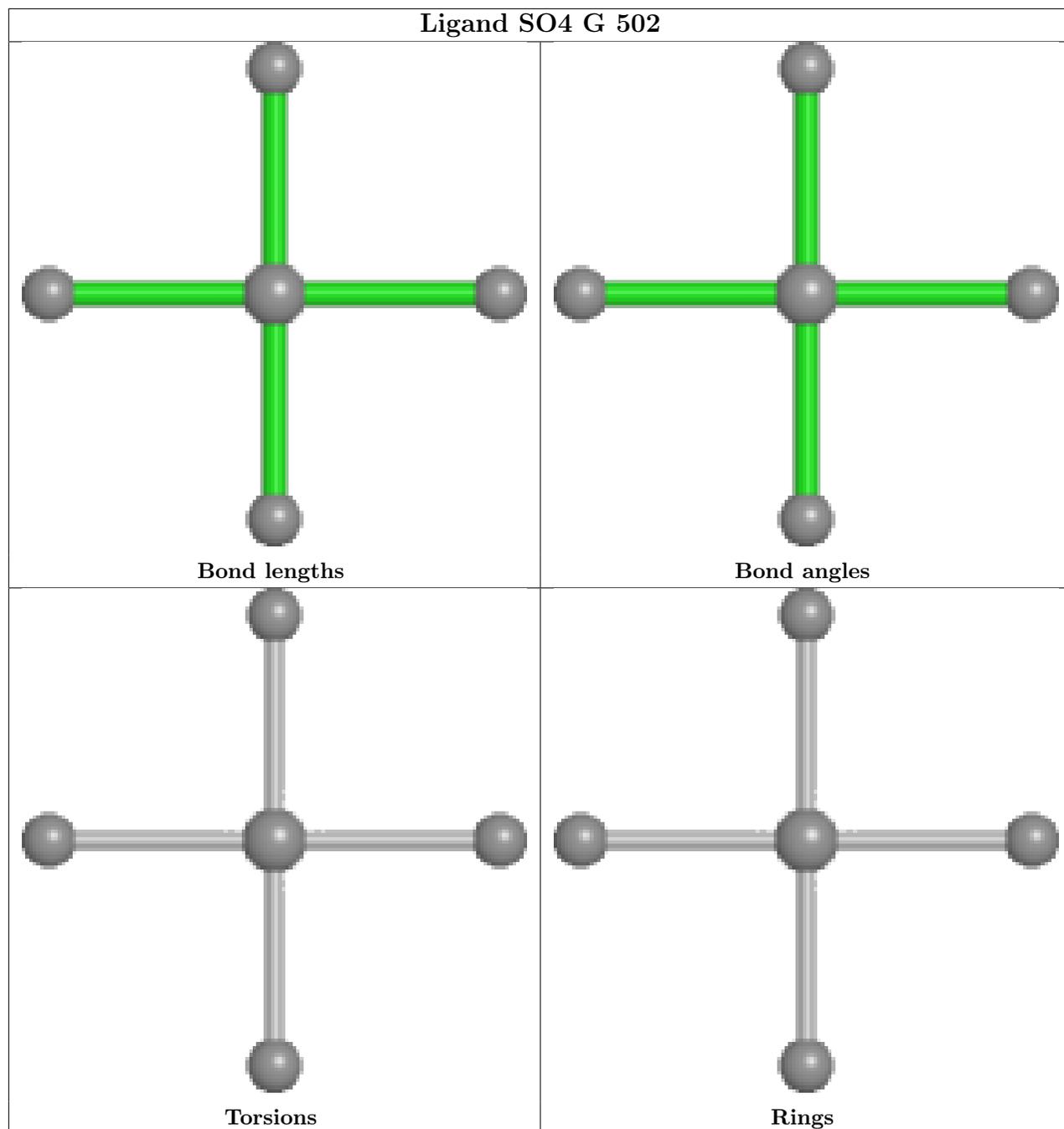


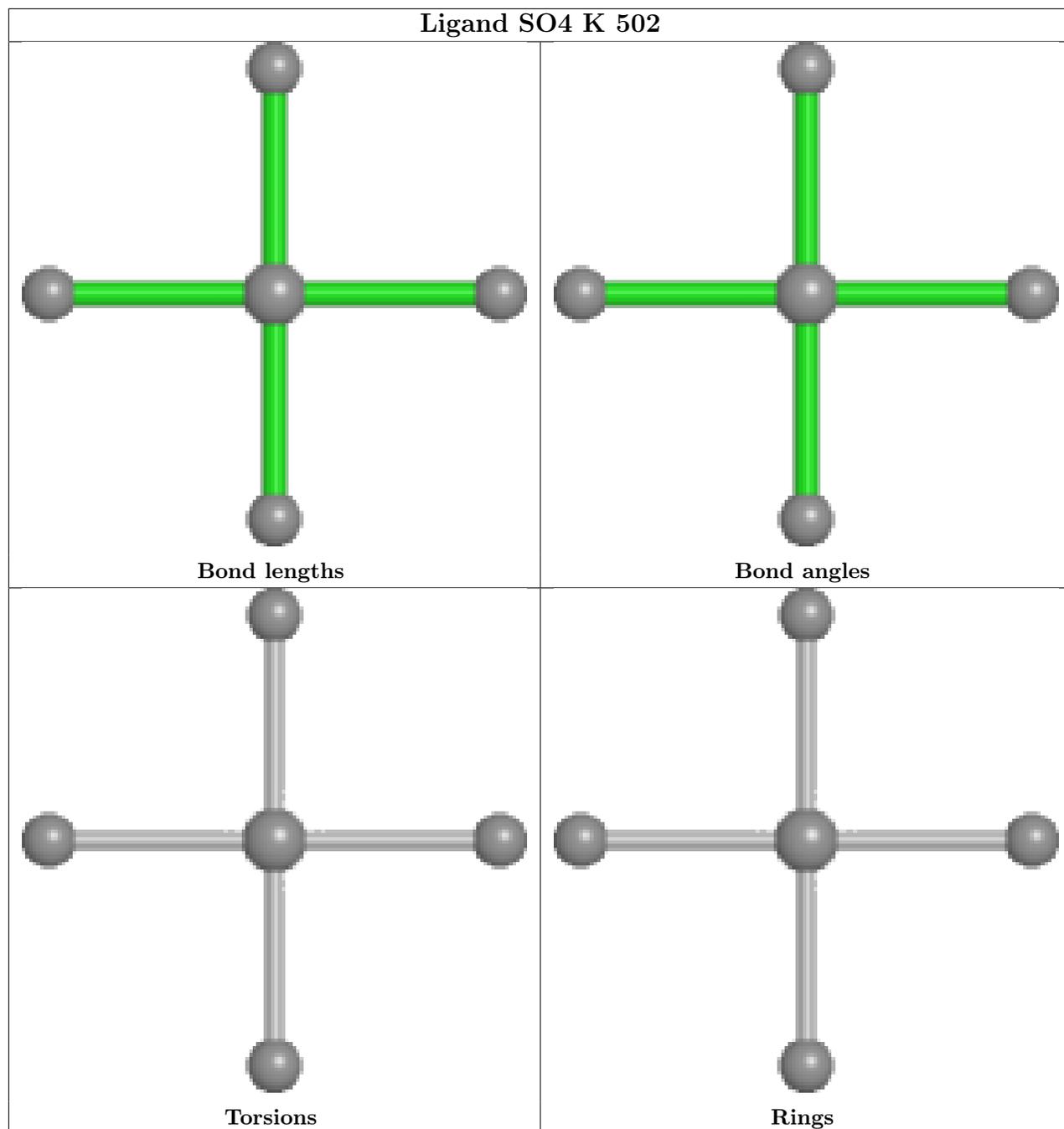


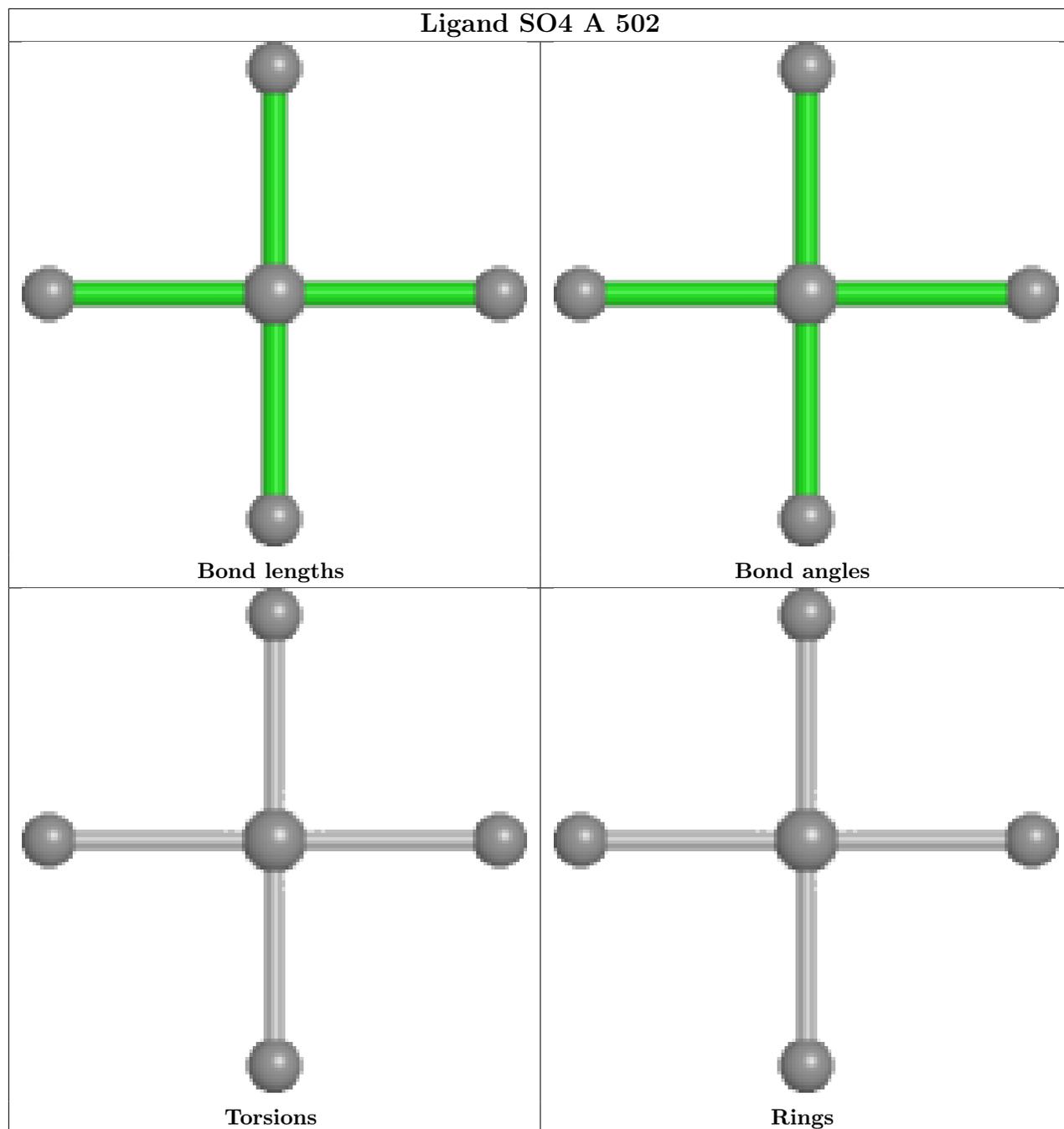


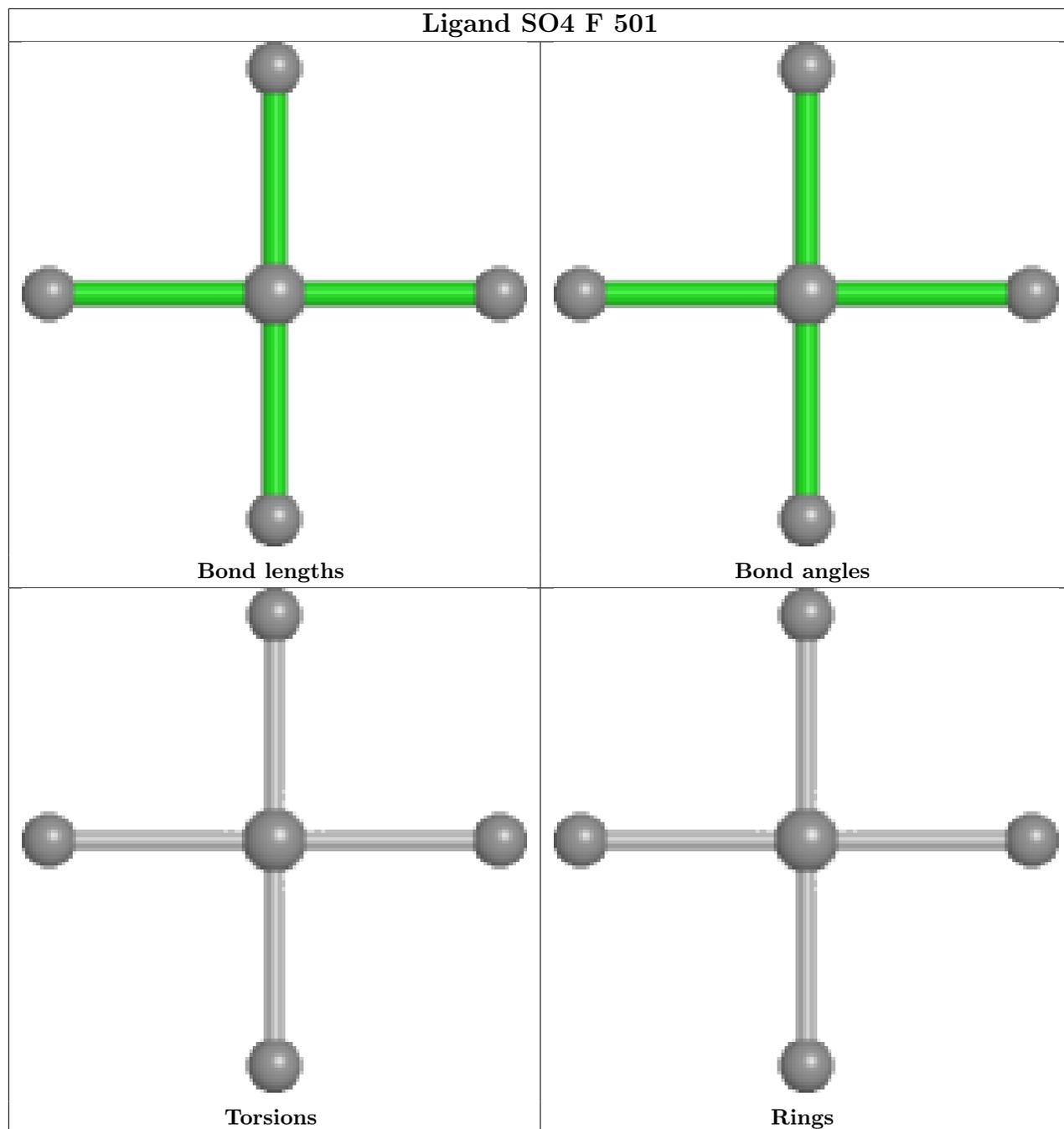


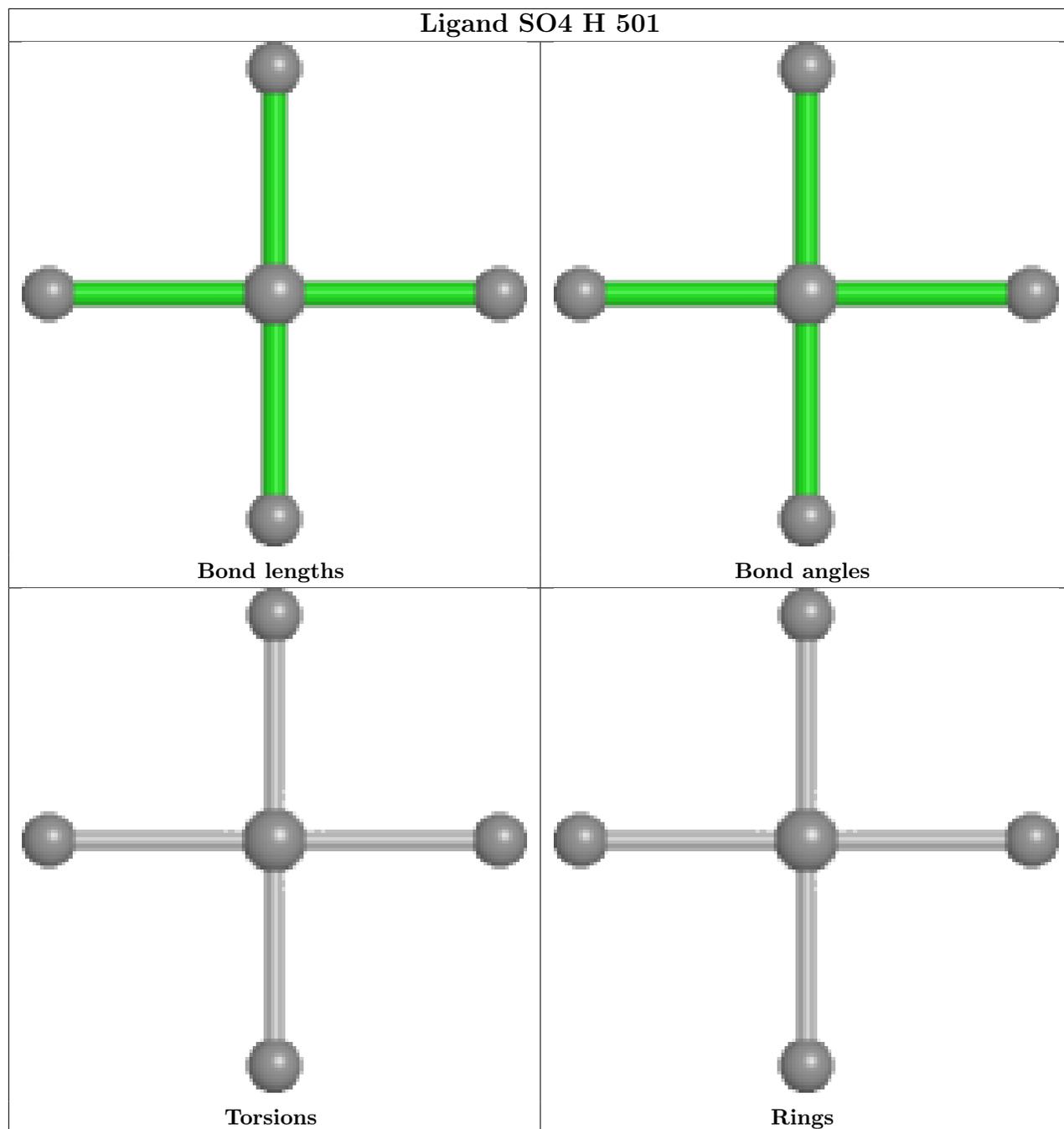


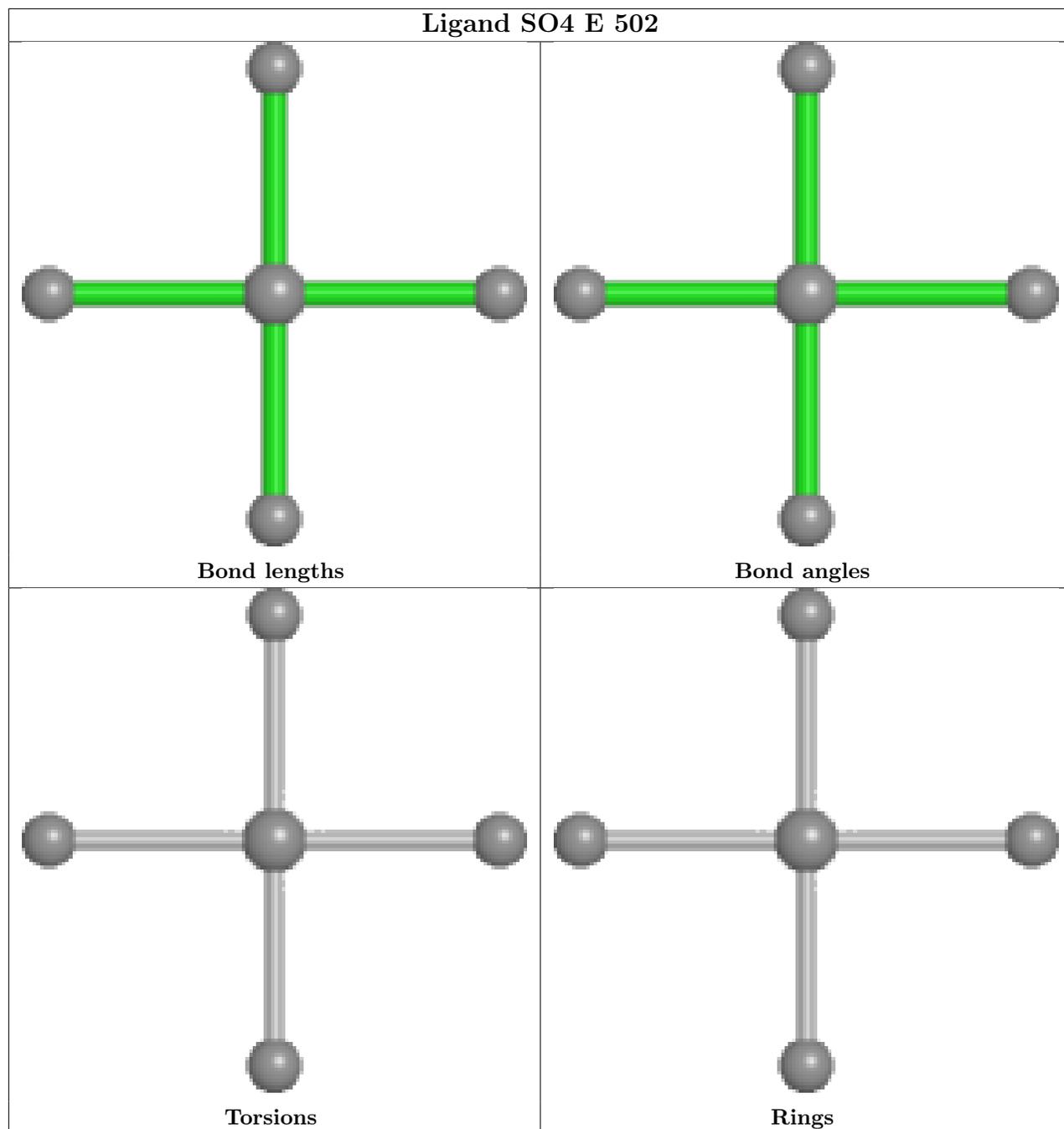


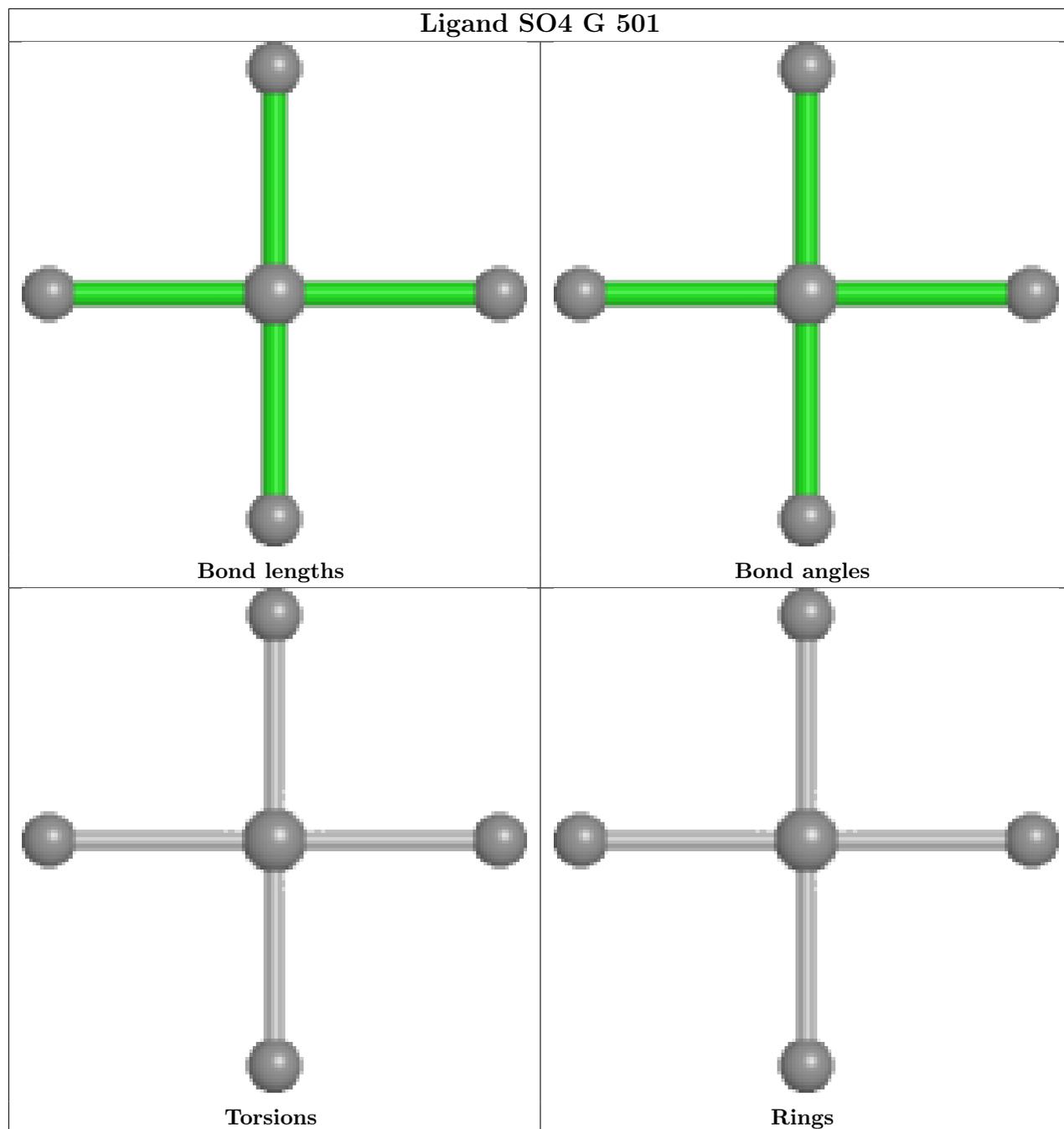


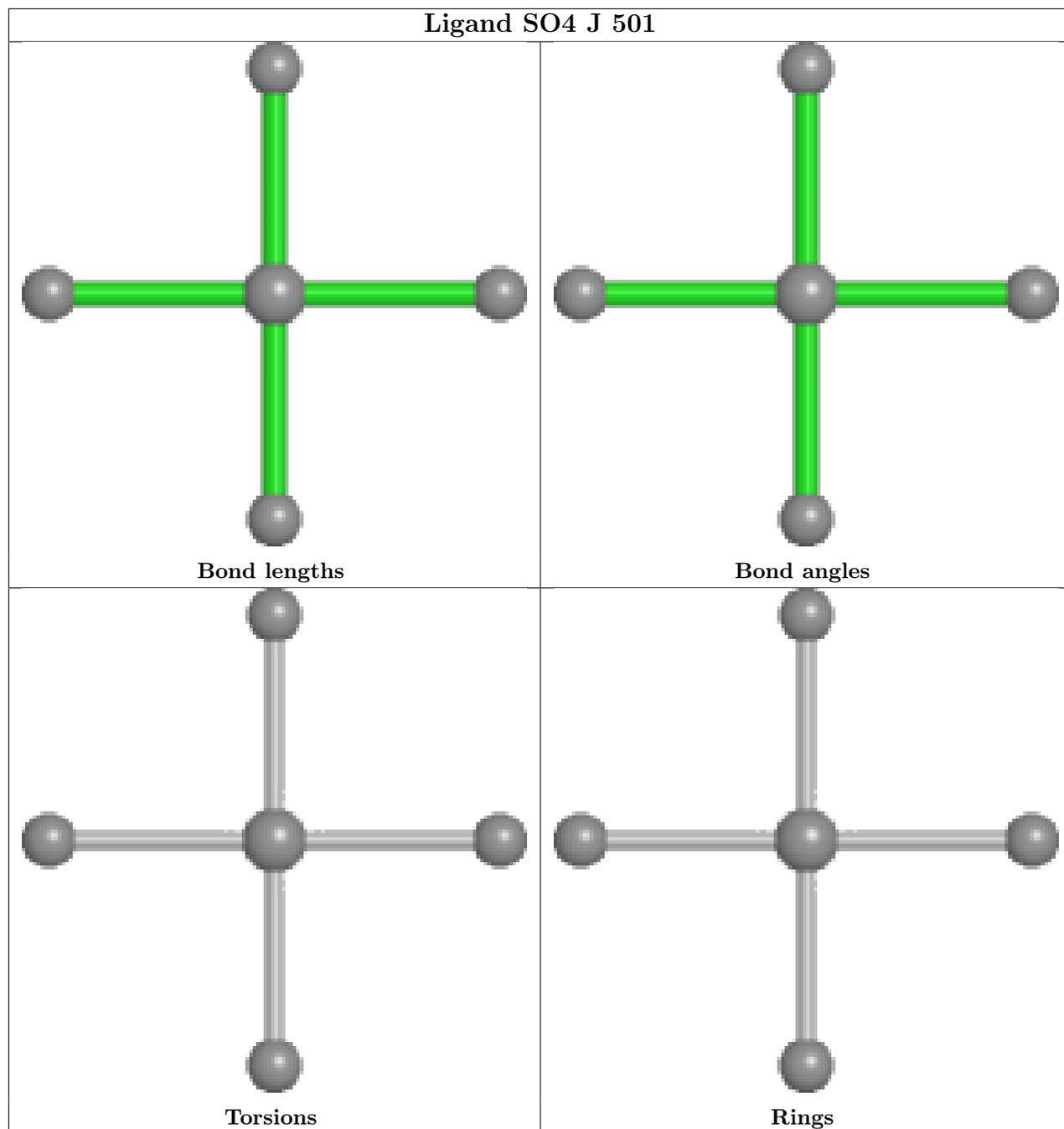


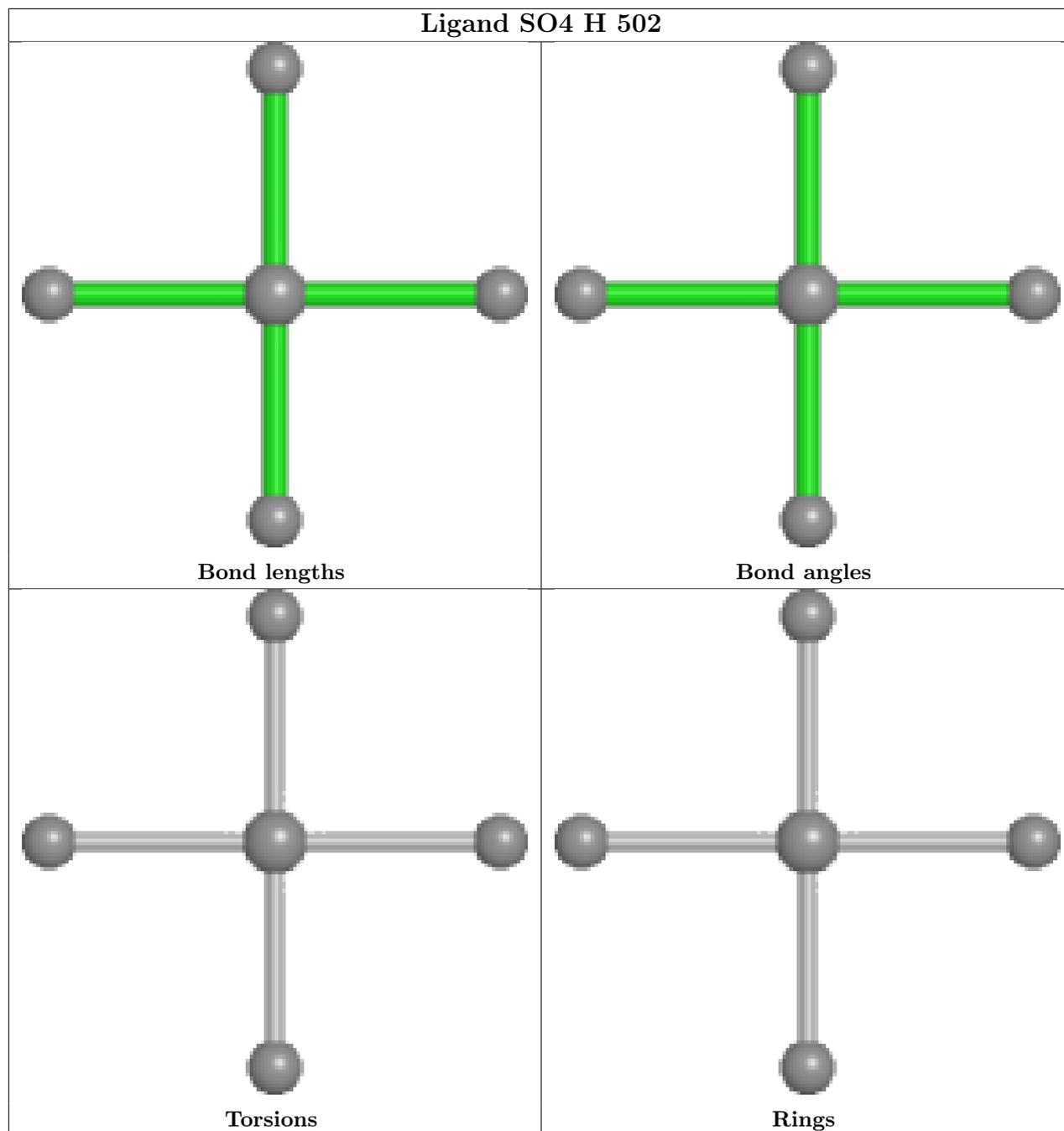












### 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/461 (94%)	-0.05	2 (0%) 87 86	29, 63, 103, 136	0
1	B	439/461 (95%)	0.02	7 (1%) 70 67	33, 59, 100, 122	0
1	C	440/461 (95%)	0.06	6 (1%) 73 69	32, 63, 106, 133	0
1	D	446/461 (96%)	0.10	4 (0%) 81 79	36, 66, 107, 158	0
1	E	445/461 (96%)	0.12	10 (2%) 62 59	34, 65, 108, 147	0
1	F	437/461 (94%)	0.16	8 (1%) 67 64	30, 71, 117, 155	0
1	G	437/461 (94%)	0.12	4 (0%) 81 79	36, 67, 111, 147	0
1	H	436/461 (94%)	0.07	2 (0%) 87 86	36, 65, 107, 135	0
1	I	444/461 (96%)	0.15	6 (1%) 73 69	34, 64, 104, 134	0
1	J	443/461 (96%)	0.36	14 (3%) 50 45	38, 74, 119, 158	0
1	K	437/461 (94%)	0.32	12 (2%) 56 52	41, 73, 120, 188	0
1	L	441/461 (95%)	0.44	16 (3%) 46 40	45, 85, 126, 160	0
All	All	5282/5532 (95%)	0.15	91 (1%) 69 65	29, 68, 114, 188	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	85	VAL	4.6
1	D	451	LEU	4.4
1	L	208	SER	4.2
1	I	451	LEU	4.1
1	J	53	ILE	4.1
1	L	150	TYR	3.9
1	E	196	GLY	3.8
1	K	245	GLY	3.5
1	I	120	ASP	3.5
1	B	12	GLN	3.5
1	L	151	SER	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	222	LEU	3.5
1	K	225	ALA	3.2
1	E	451	LEU	3.2
1	C	213	ASN	3.1
1	L	12	GLN	3.1
1	F	208	SER	3.0
1	J	200	LEU	3.0
1	F	211	ILE	3.0
1	K	302	THR	3.0
1	J	86	LEU	3.0
1	K	314	PHE	2.9
1	F	109	TYR	2.9
1	B	84	ARG	2.9
1	J	391	HIS	2.9
1	K	451	LEU	2.8
1	I	249	SER	2.8
1	B	249	SER	2.8
1	I	30	PHE	2.8
1	J	142	PHE	2.8
1	H	451	LEU	2.7
1	J	451	LEU	2.7
1	L	190	ASN	2.7
1	C	225	ALA	2.7
1	I	265	GLN	2.7
1	G	451	LEU	2.7
1	L	85	VAL	2.6
1	L	30	PHE	2.6
1	F	124	TYR	2.6
1	D	380	TRP	2.5
1	A	447	ILE	2.5
1	L	334	ARG	2.5
1	B	451	LEU	2.5
1	G	225	ALA	2.5
1	J	12	GLN	2.5
1	A	451	LEU	2.5
1	K	410	GLU	2.4
1	E	203	VAL	2.4
1	E	29	PHE	2.4
1	C	447	ILE	2.4
1	E	450	ILE	2.4
1	G	251	LEU	2.4
1	L	36	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	313	PRO	2.4
1	F	451	LEU	2.4
1	J	192	MET	2.4
1	F	196	GLY	2.4
1	I	247	GLY	2.3
1	E	446	LEU	2.3
1	C	119	VAL	2.3
1	K	244	VAL	2.3
1	L	239	SER	2.3
1	C	10	HIS	2.3
1	B	200	LEU	2.3
1	E	141	GLY	2.2
1	J	162	GLN	2.2
1	H	30	PHE	2.2
1	K	366	LYS	2.2
1	L	35	ASP	2.2
1	J	123	VAL	2.2
1	L	139	PHE	2.2
1	L	367	TRP	2.2
1	J	121	VAL	2.2
1	J	186	TRP	2.1
1	E	447	ILE	2.1
1	F	245	GLY	2.1
1	K	307	TYR	2.1
1	L	152	GLY	2.1
1	B	31	TYR	2.1
1	L	18	PRO	2.1
1	F	119	VAL	2.1
1	G	224	ASP	2.1
1	K	109	TYR	2.1
1	D	443	ILE	2.0
1	E	316	ILE	2.0
1	D	192	MET	2.0
1	K	89	TRP	2.0
1	J	348	LEU	2.0
1	K	161	HIS	2.0
1	B	333	SER	2.0
1	C	443	ILE	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

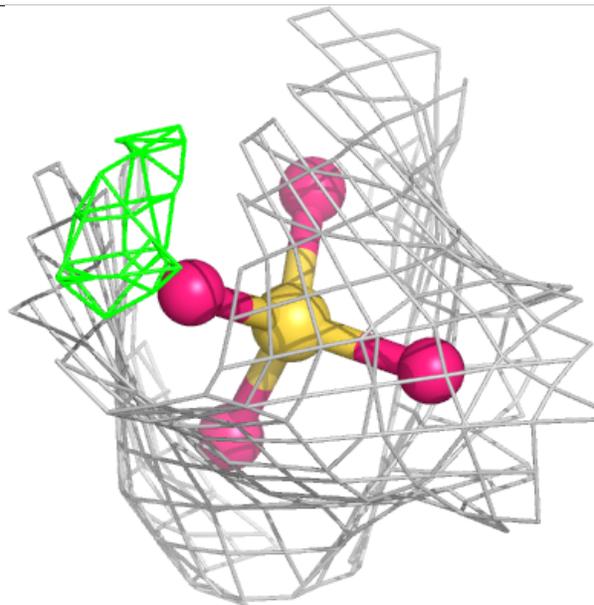
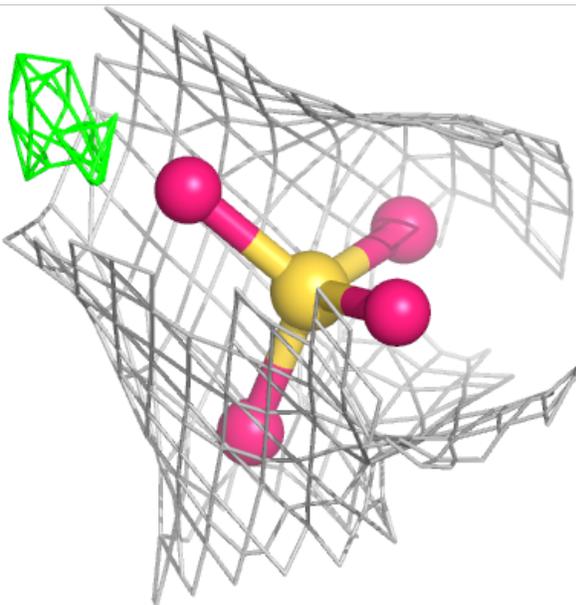
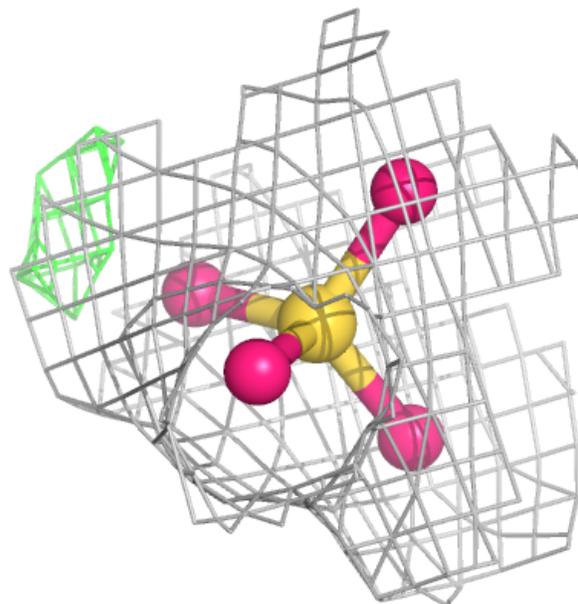
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	F	502	5/5	0.67	0.13	101,102,110,117	0
2	SO4	E	502	5/5	0.69	0.13	106,114,122,128	0
2	SO4	J	501	5/5	0.71	0.12	119,128,130,131	0
2	SO4	L	502	5/5	0.71	0.10	106,127,133,140	0
2	SO4	I	502	5/5	0.72	0.12	91,93,105,106	0
2	SO4	D	502	5/5	0.77	0.11	72,98,106,116	0
2	SO4	K	502	5/5	0.77	0.11	109,114,119,135	0
2	SO4	A	502	5/5	0.77	0.13	90,102,112,115	0
2	SO4	C	502	5/5	0.78	0.10	85,89,105,112	0
2	SO4	B	502	5/5	0.78	0.10	89,93,96,105	0
2	SO4	H	502	5/5	0.79	0.11	77,98,108,110	0
2	SO4	G	503	5/5	0.84	0.10	79,91,98,108	0
2	SO4	E	501	5/5	0.94	0.08	32,44,49,51	0
2	SO4	K	501	5/5	0.94	0.06	49,62,64,71	0
2	SO4	L	501	5/5	0.95	0.08	50,55,58,61	0
2	SO4	D	501	5/5	0.95	0.11	49,50,53,55	0
2	SO4	G	502	5/5	0.96	0.06	41,53,56,58	0
2	SO4	F	501	5/5	0.97	0.07	33,33,39,39	0
2	SO4	B	501	5/5	0.97	0.06	37,42,50,56	0
2	SO4	G	501	5/5	0.97	0.07	42,47,51,56	0
2	SO4	A	501	5/5	0.98	0.06	34,36,41,48	0
2	SO4	I	501	5/5	0.98	0.05	33,41,43,52	0
2	SO4	C	501	5/5	0.98	0.05	33,35,40,49	0
2	SO4	H	501	5/5	0.98	0.05	38,42,45,49	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.

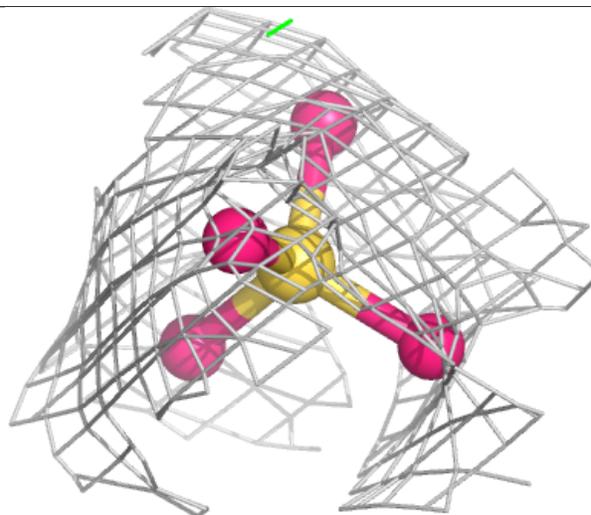
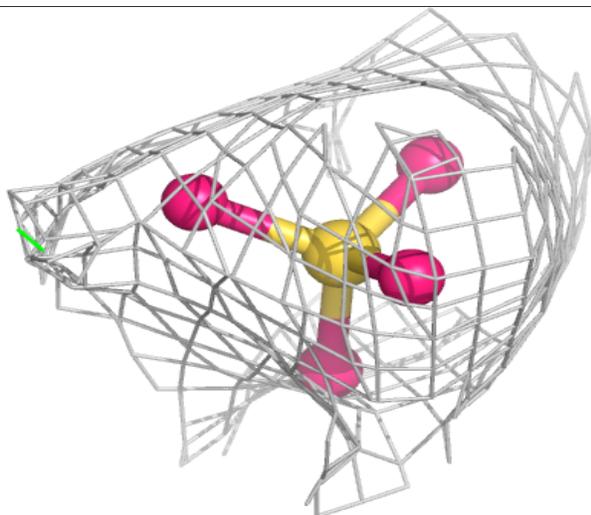
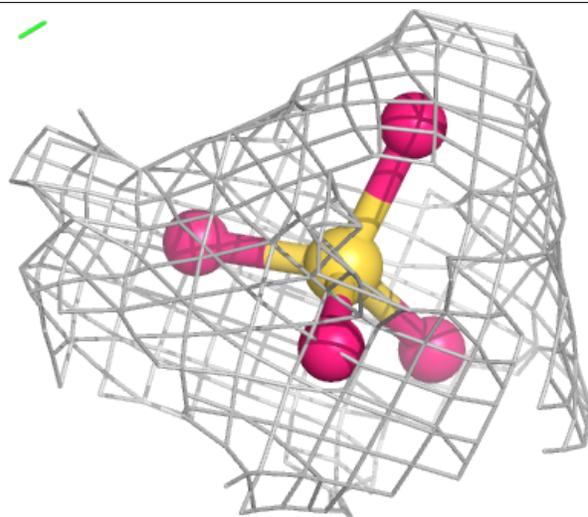
**Electron density around SO4 F 502:**

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



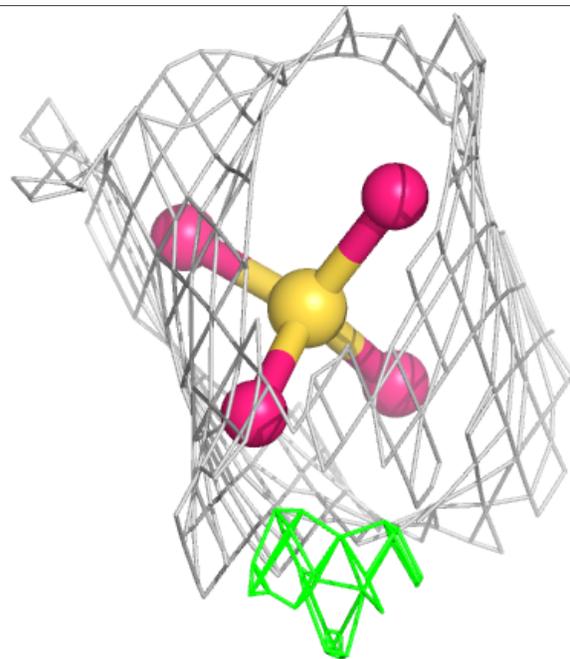
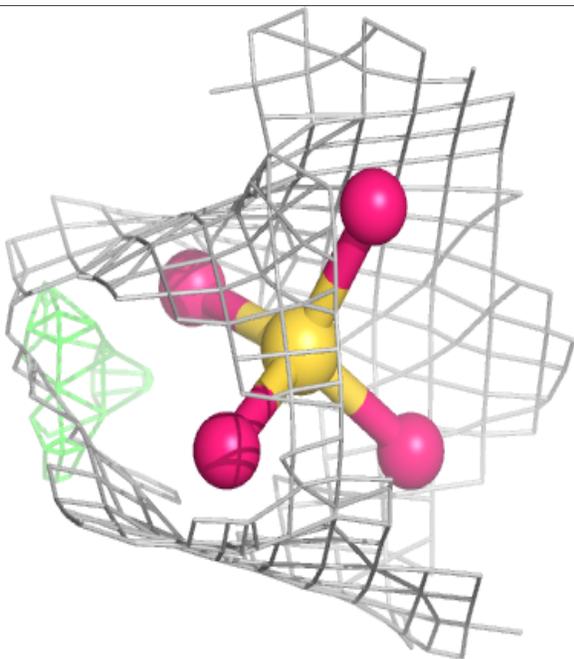
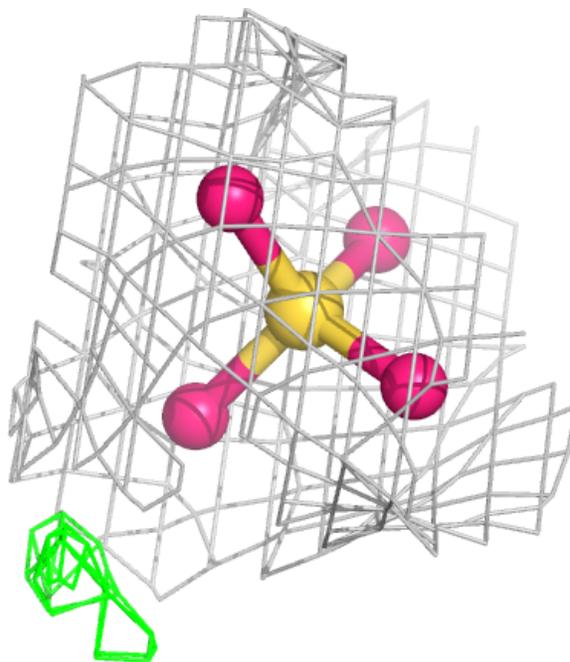
**Electron density around SO4 E 502:**

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



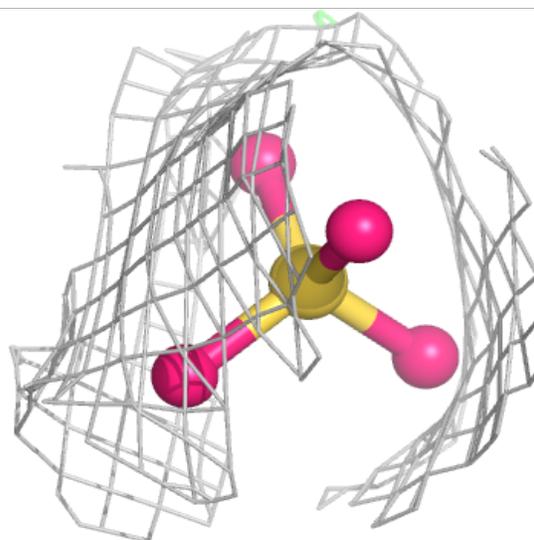
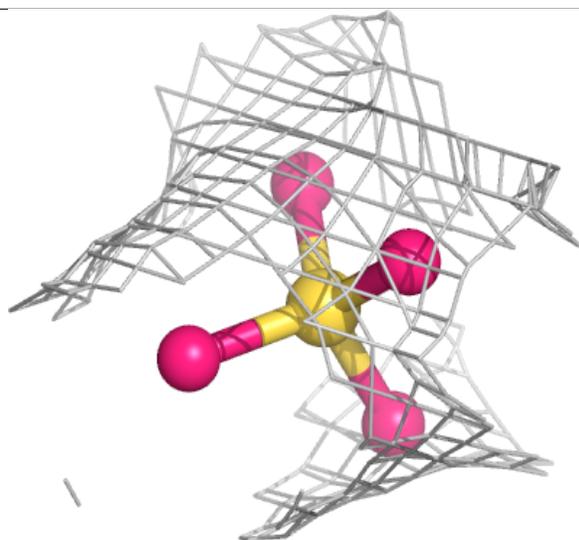
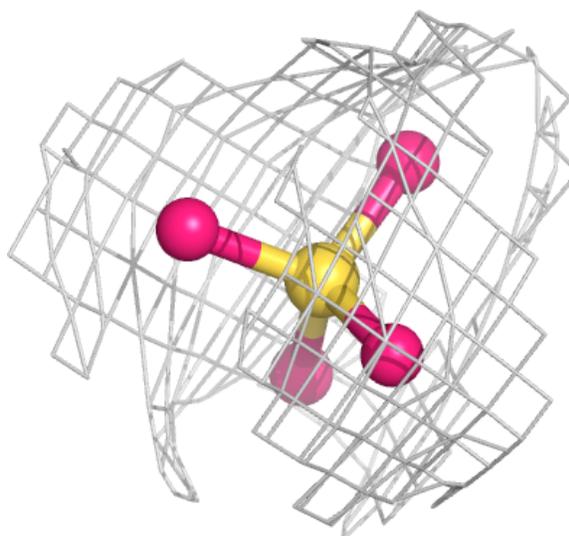
**Electron density around SO4 J 501:**

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



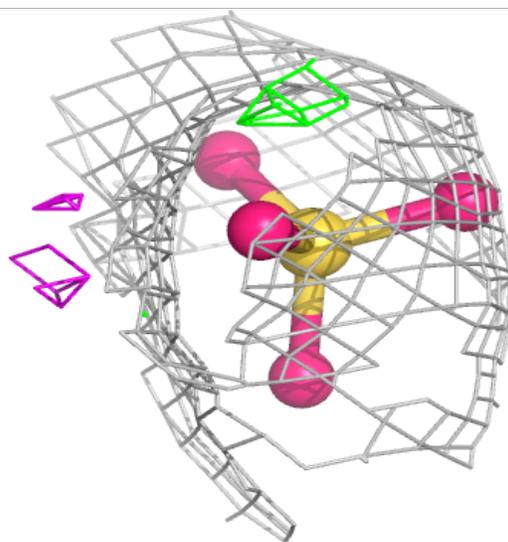
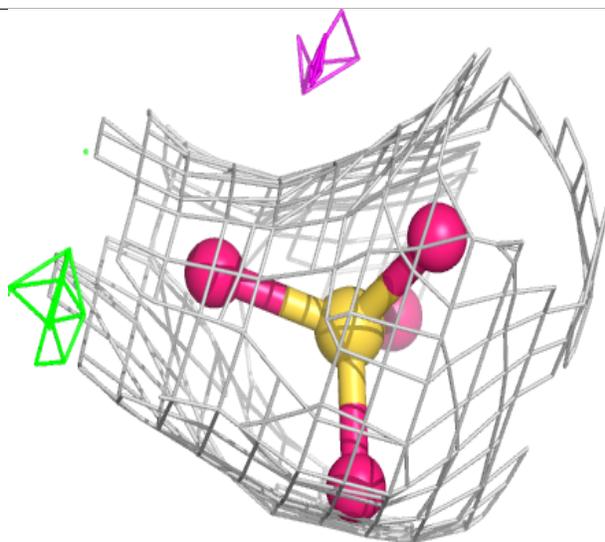
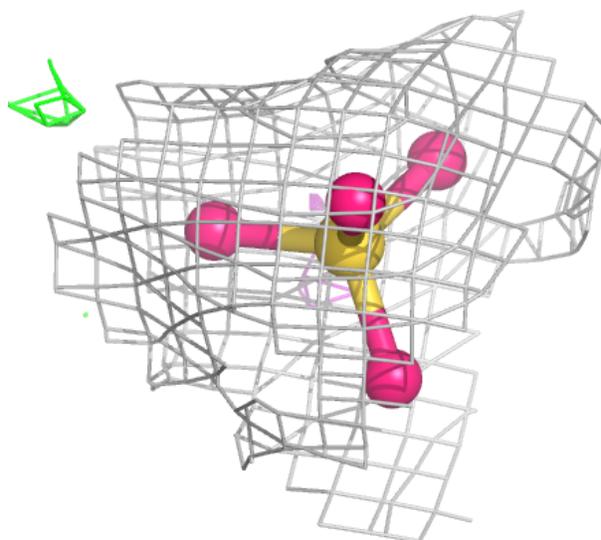
**Electron density around SO4 L 502:**

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and green (positive)



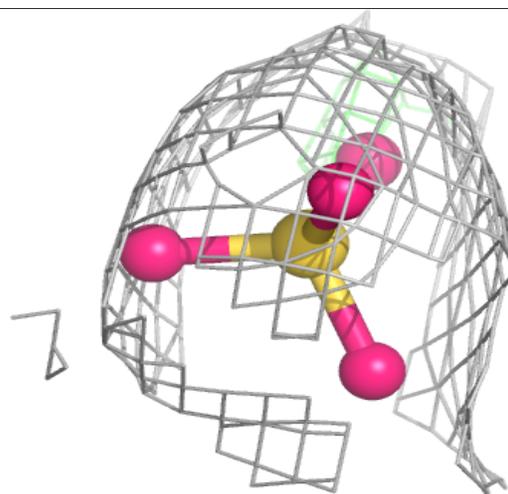
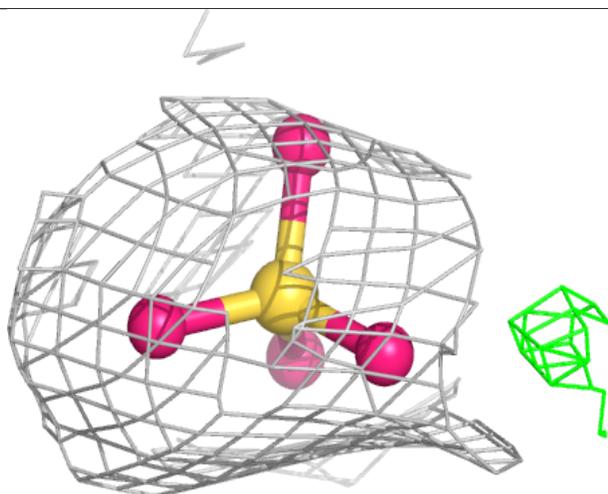
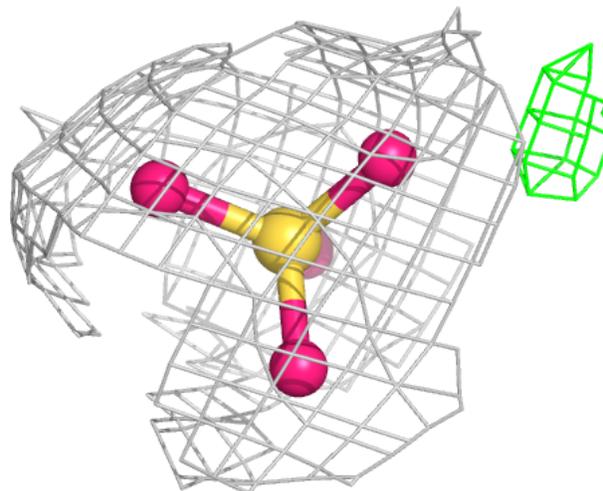
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and green (positive)



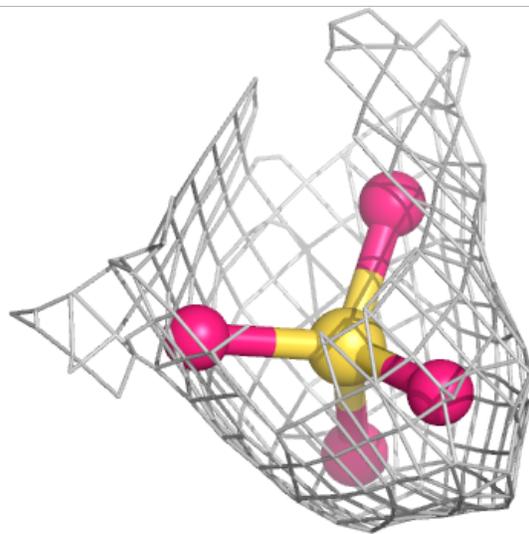
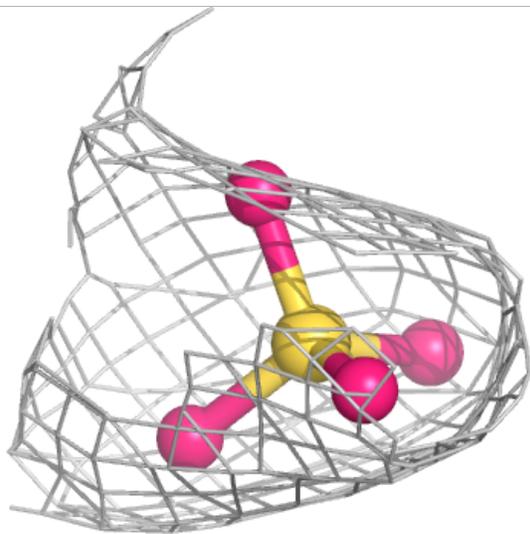
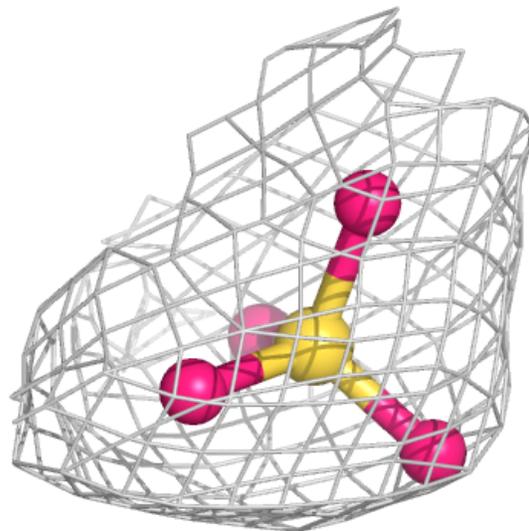
**Electron density around SO4 D 502:**

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



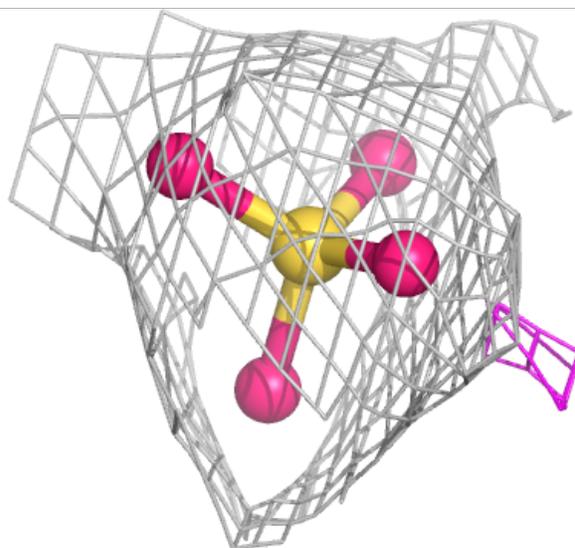
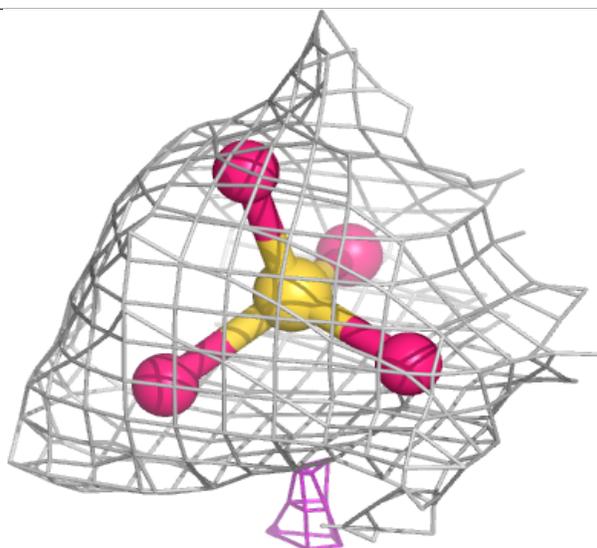
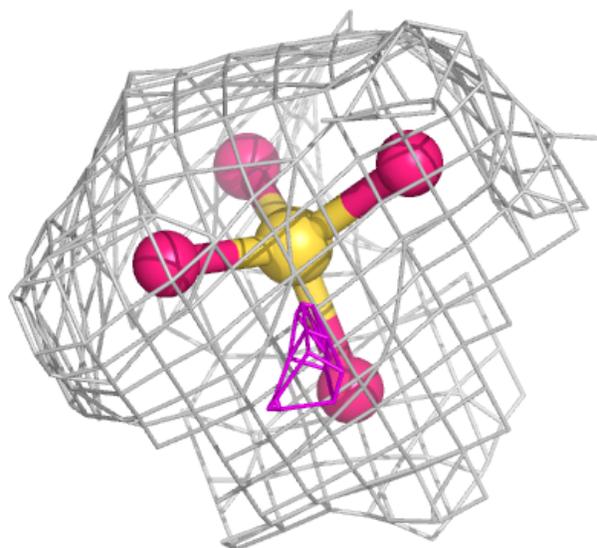
**Electron density around SO4 K 502:**

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and green (positive)



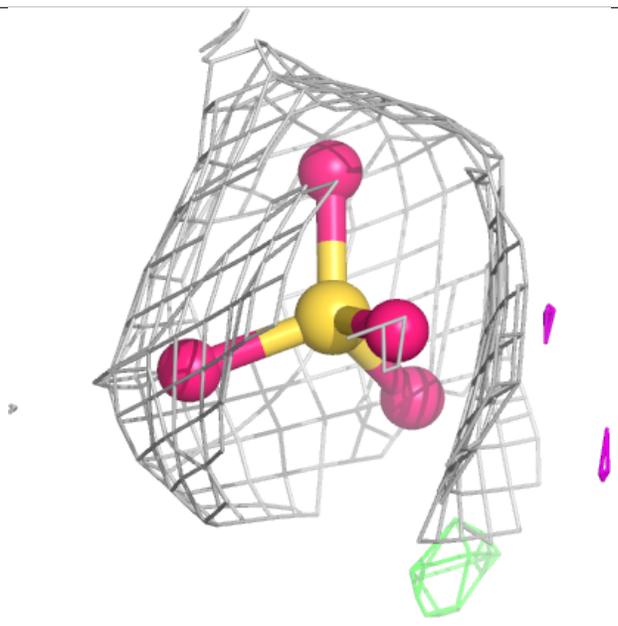
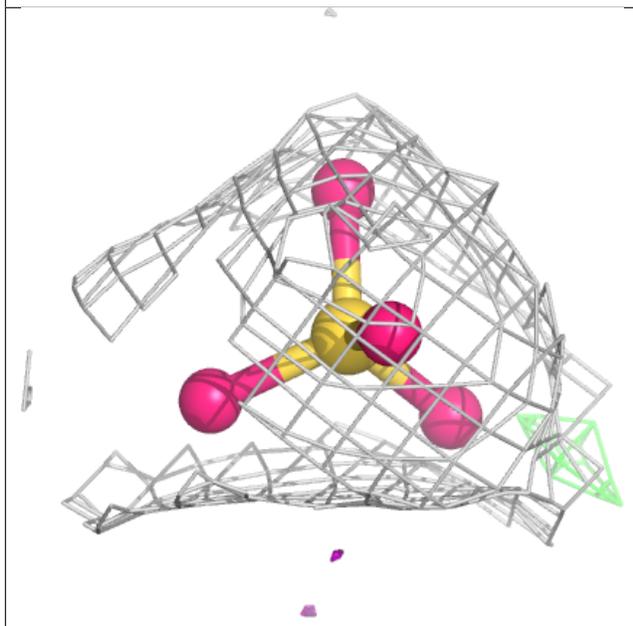
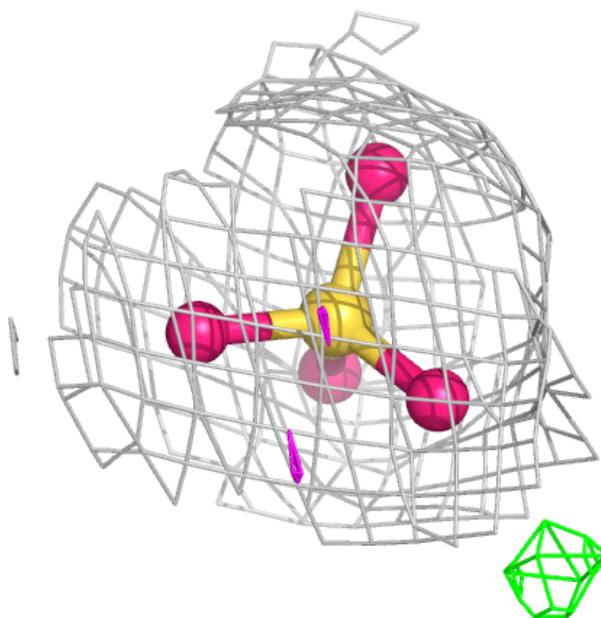
**Electron density around SO4 A 502:**

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and green (positive)



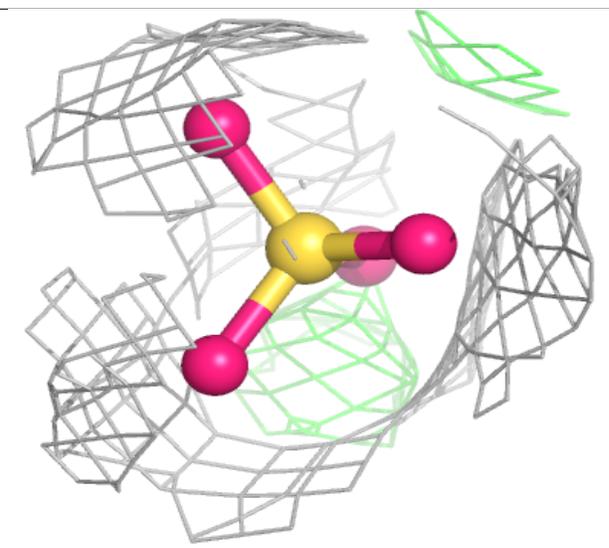
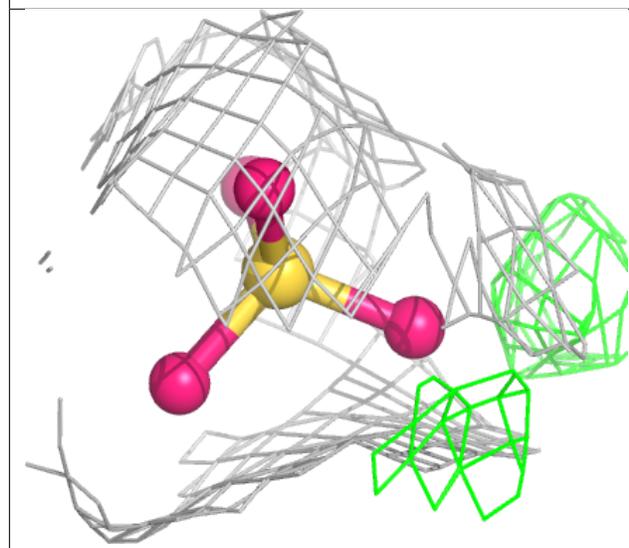
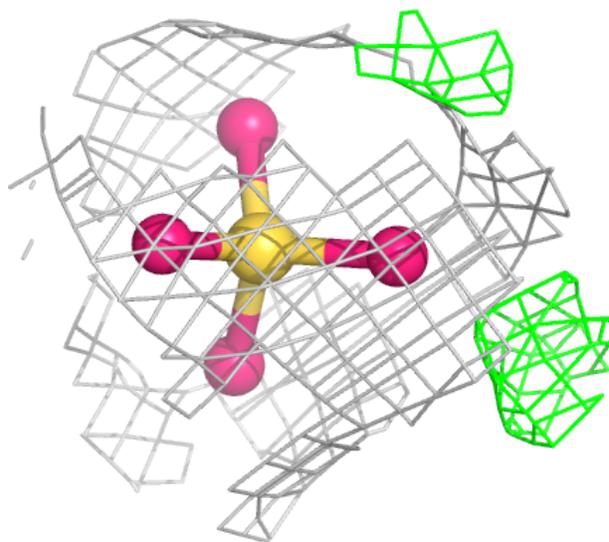
**Electron density around SO4 C 502:**

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



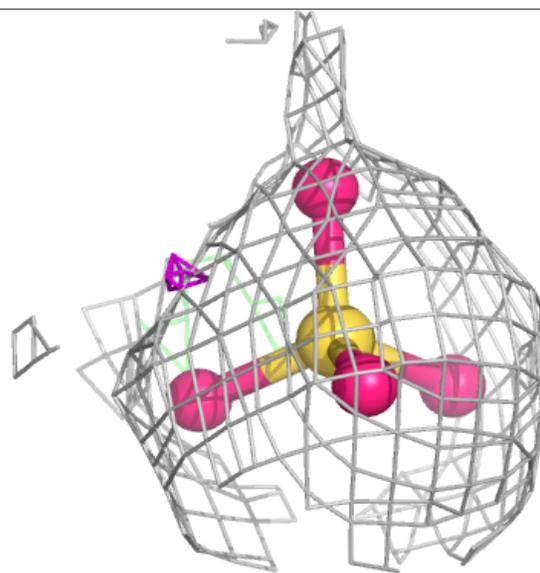
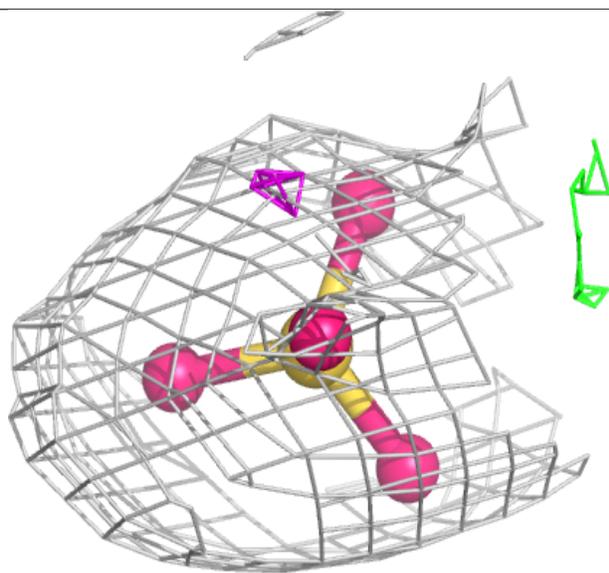
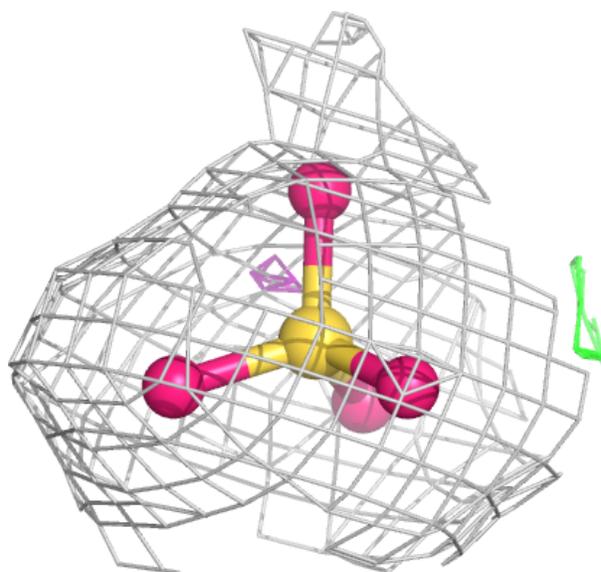
**Electron density around SO4 B 502:**

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



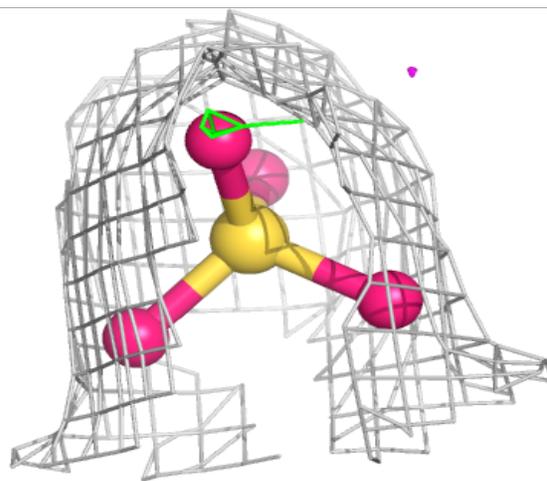
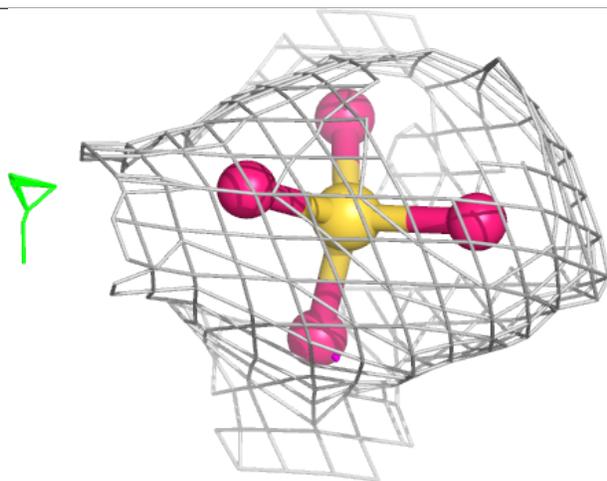
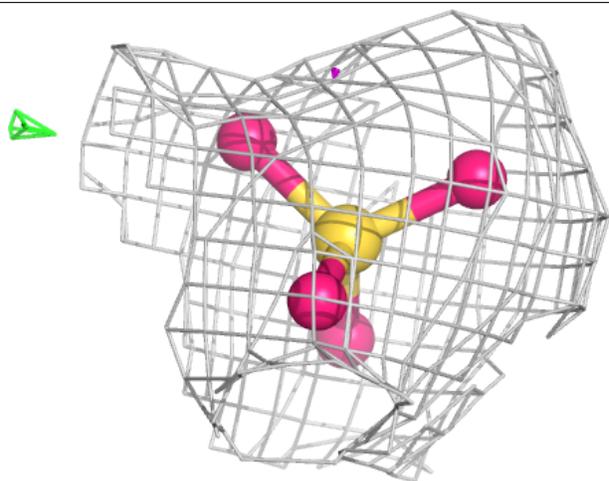
**Electron density around SO4 H 502:**

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



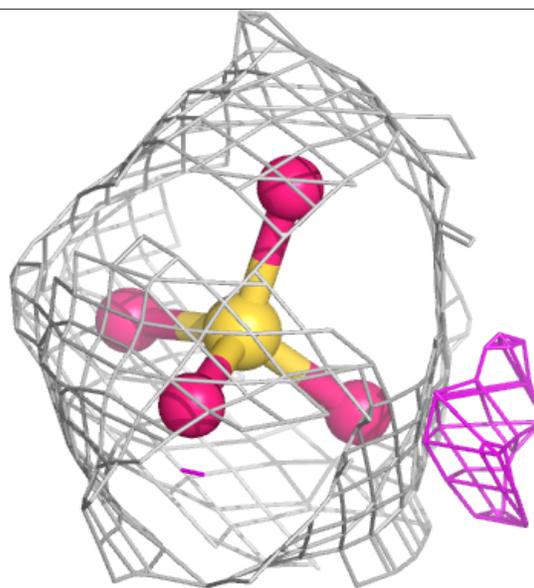
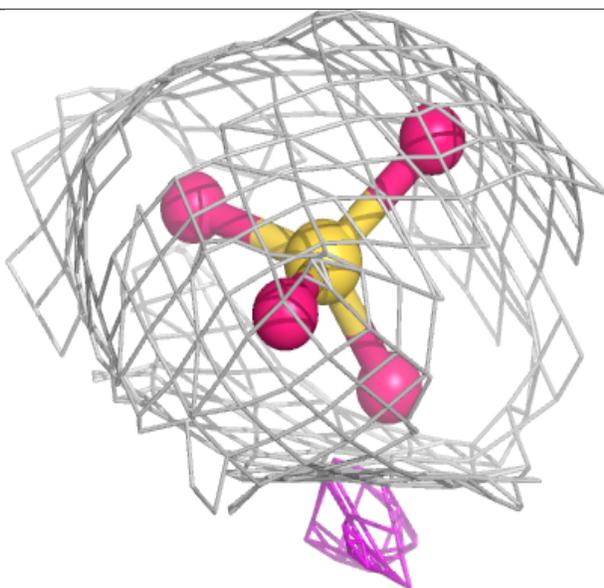
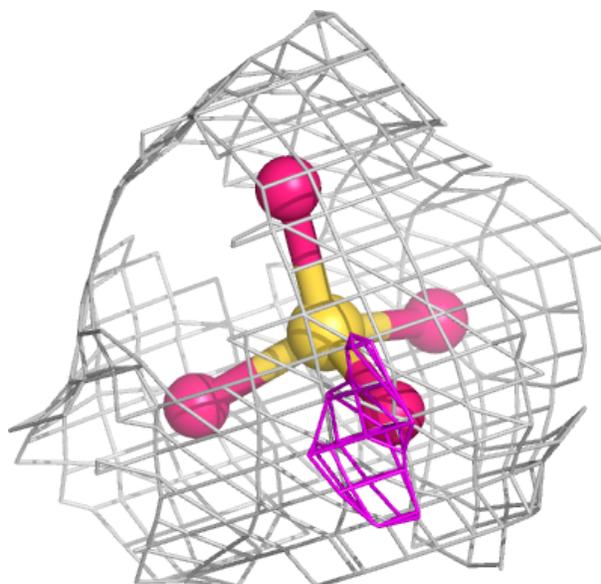
**Electron density around SO4 G 503:**

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



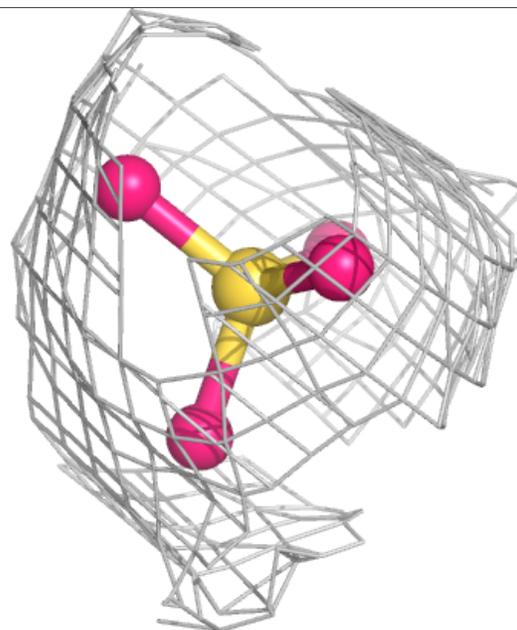
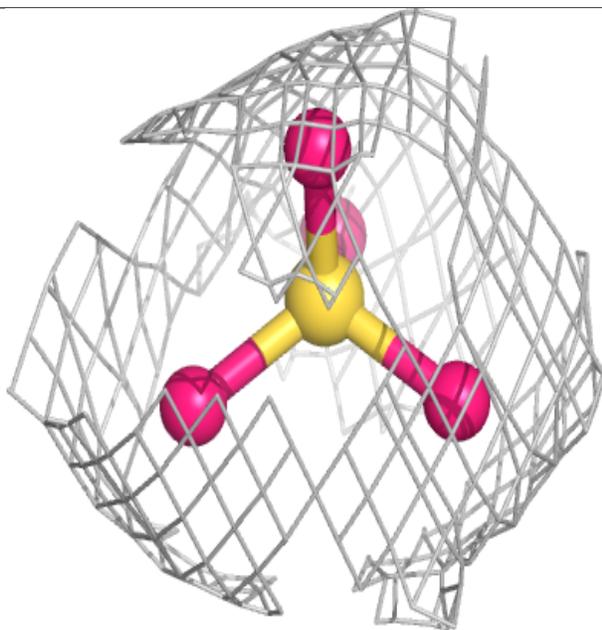
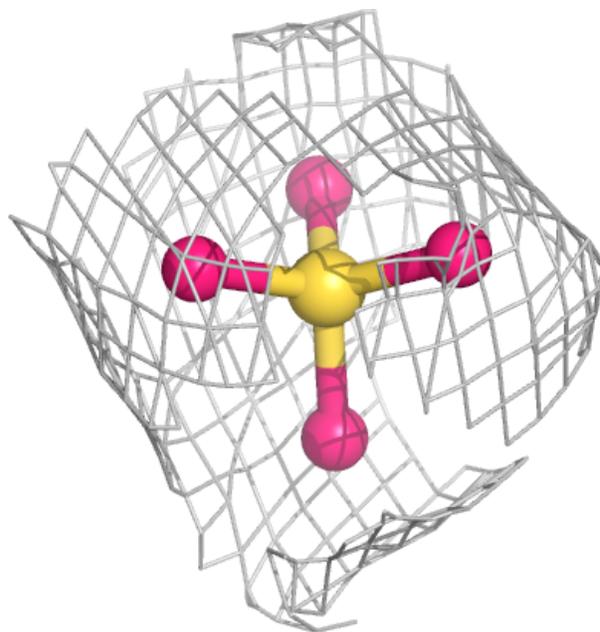
**Electron density around SO4 E 501:**

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



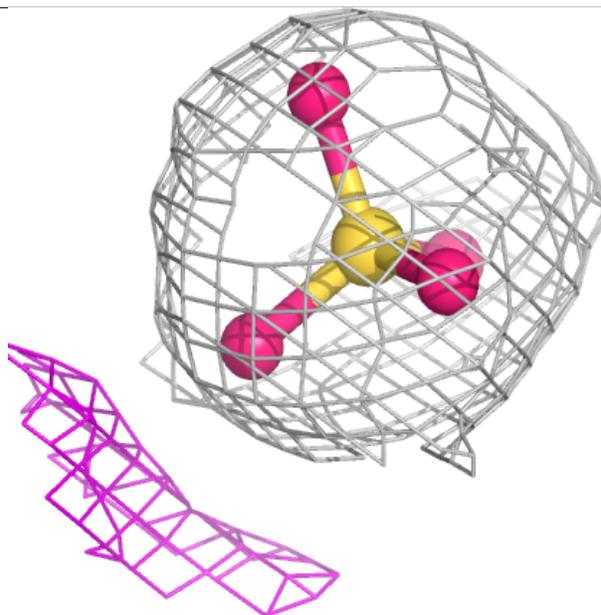
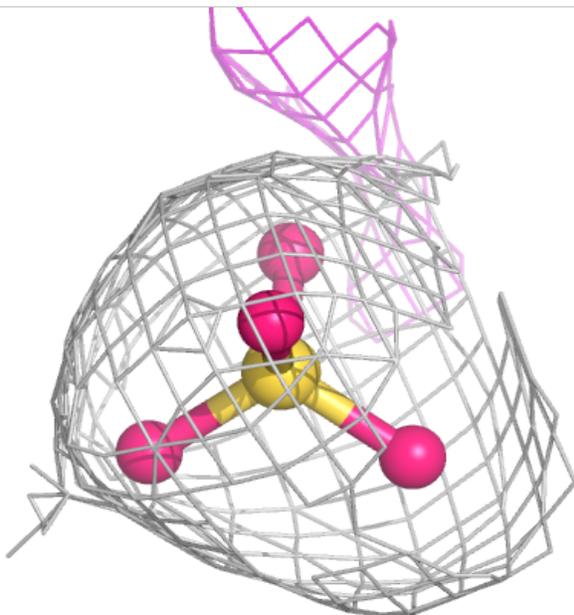
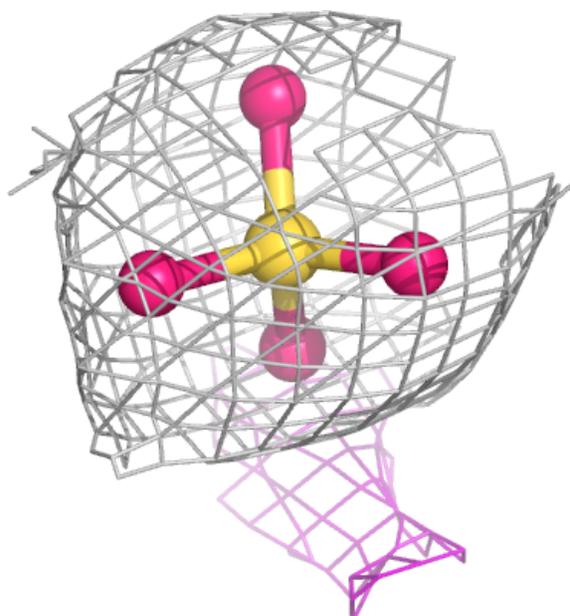
**Electron density around SO4 K 501:**

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



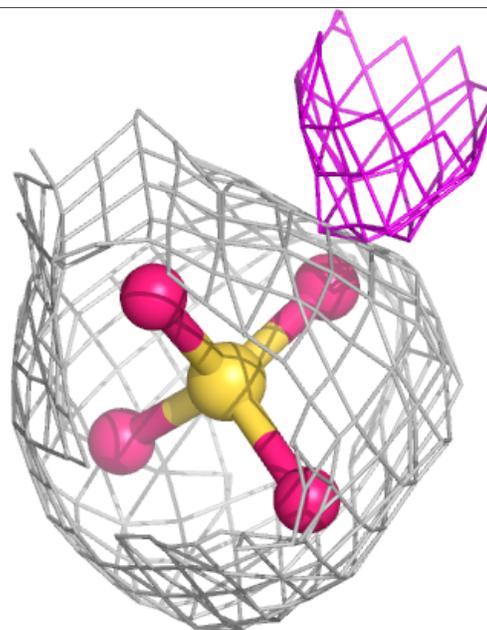
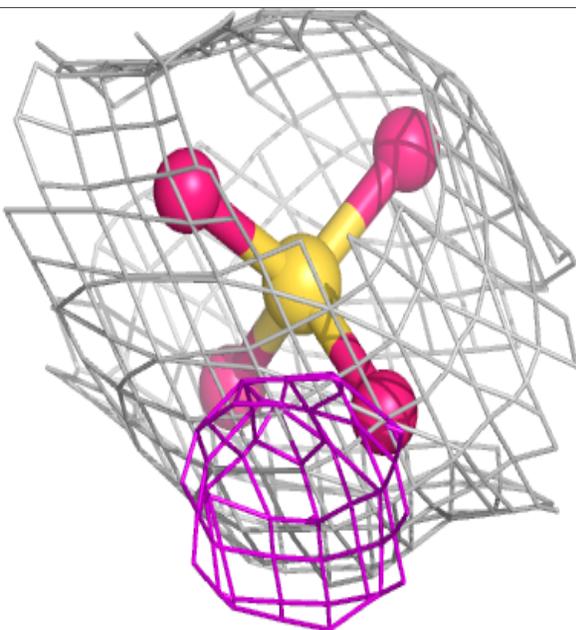
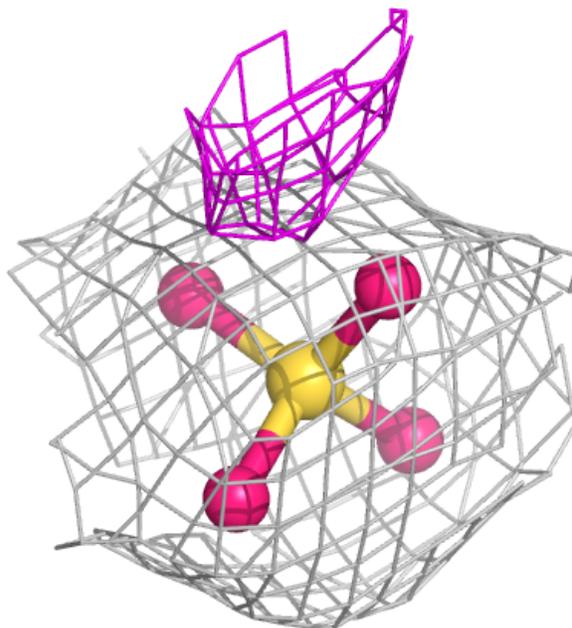
**Electron density around SO4 L 501:**

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



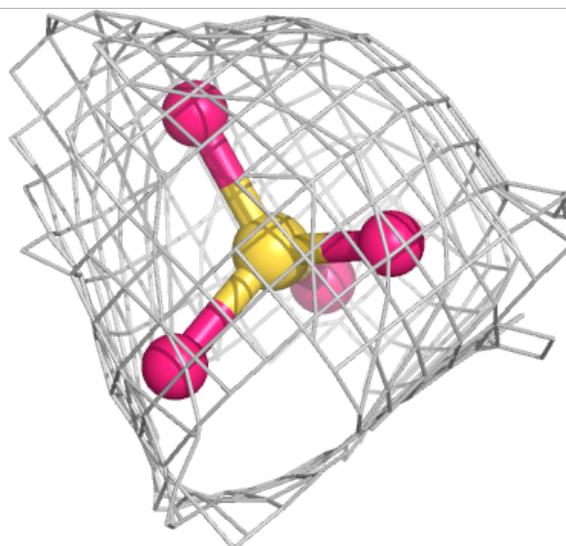
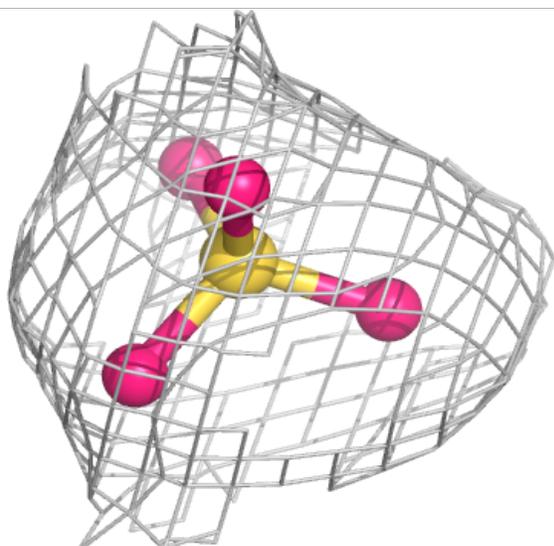
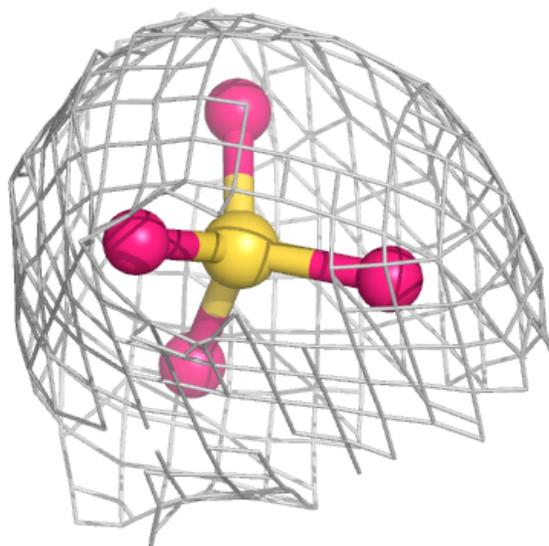
**Electron density around SO4 D 501:**

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



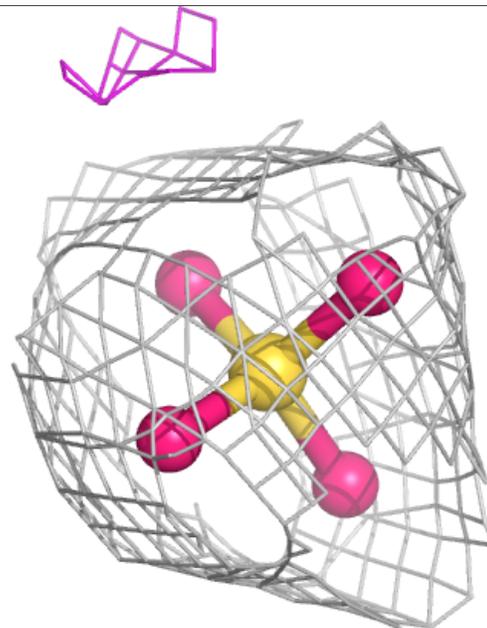
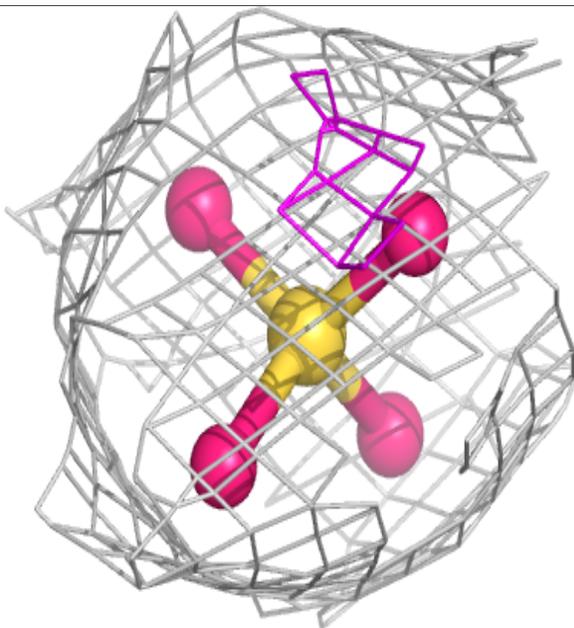
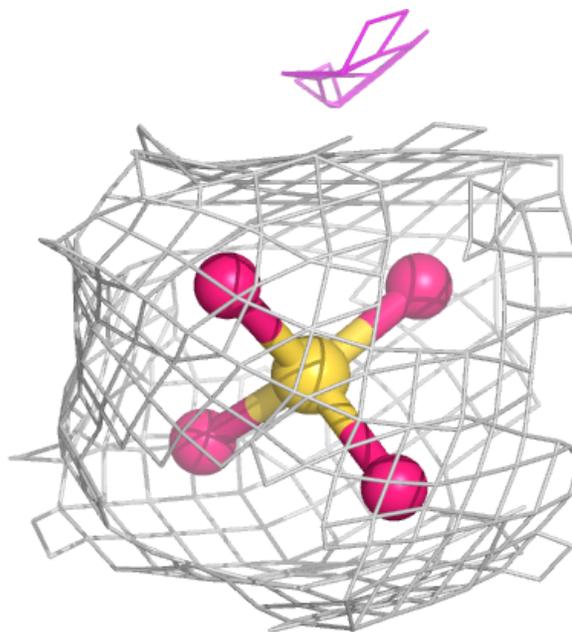
**Electron density around SO4 G 502:**

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



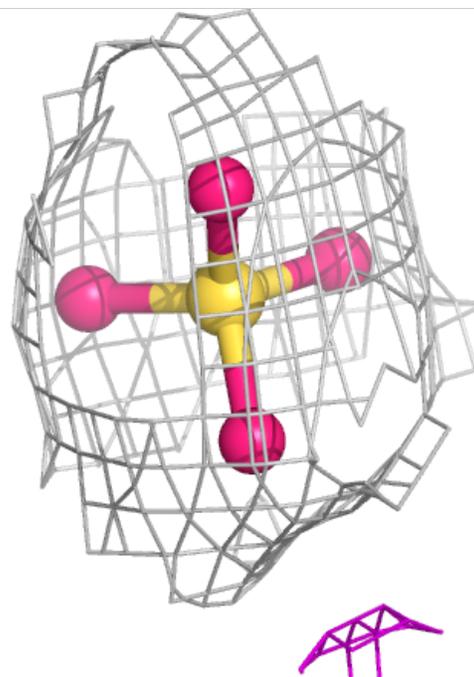
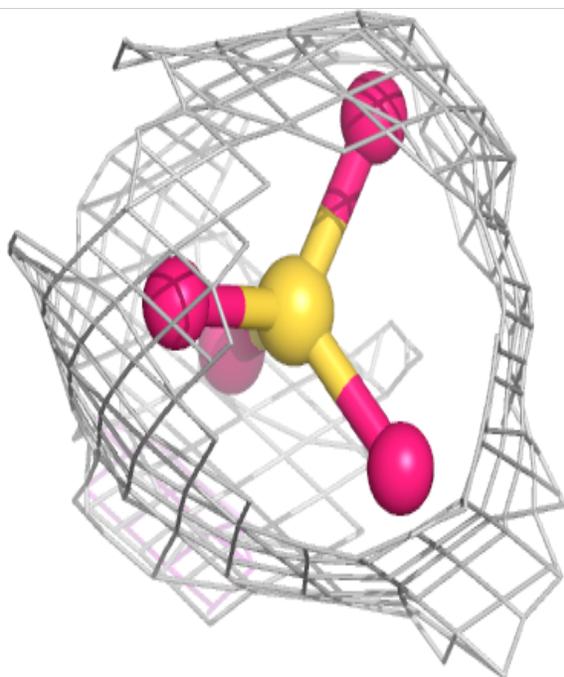
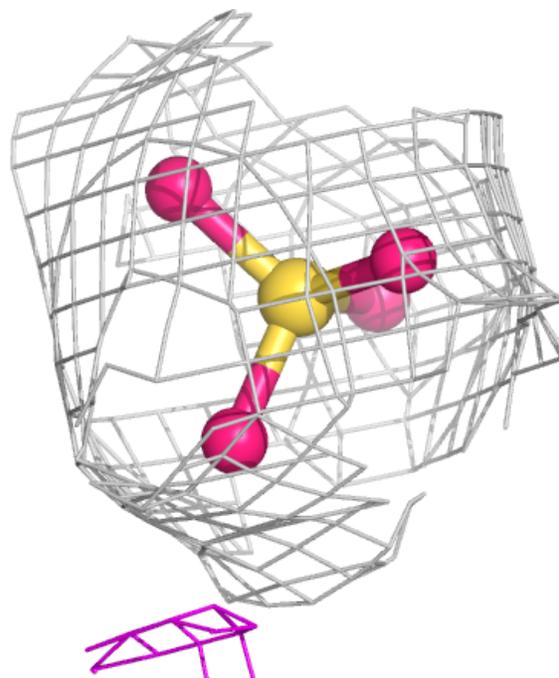
**Electron density around SO4 F 501:**

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



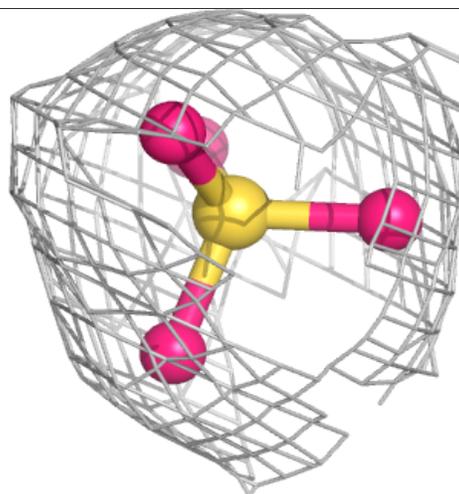
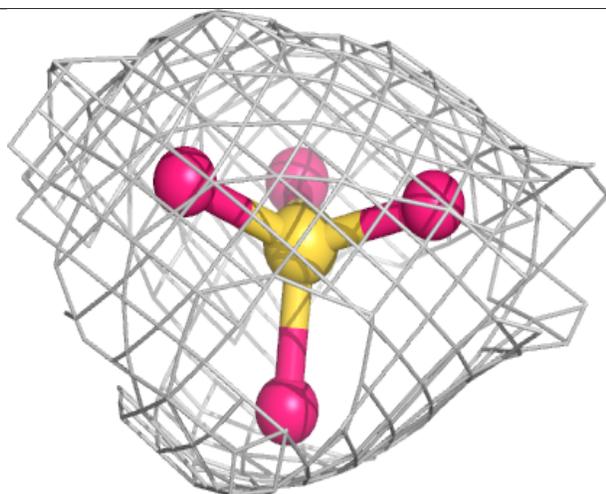
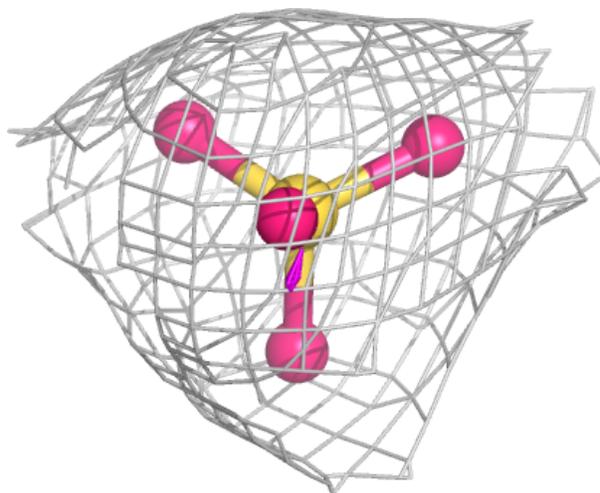
**Electron density around SO4 B 501:**

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



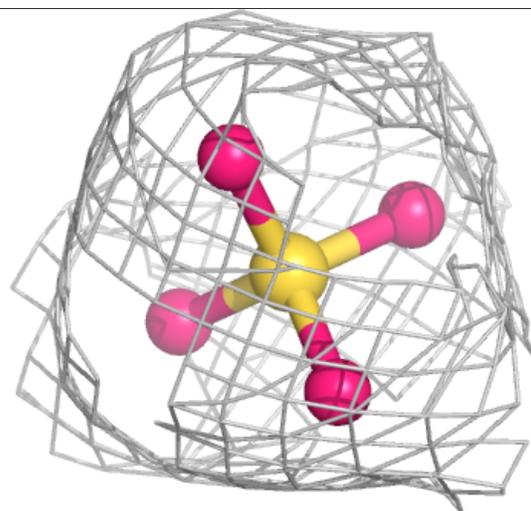
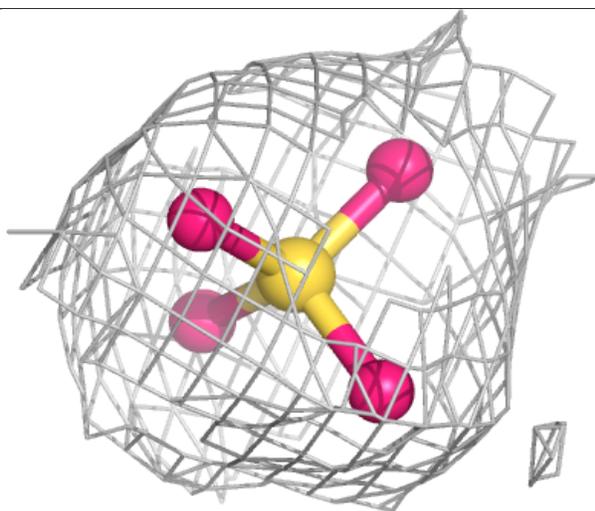
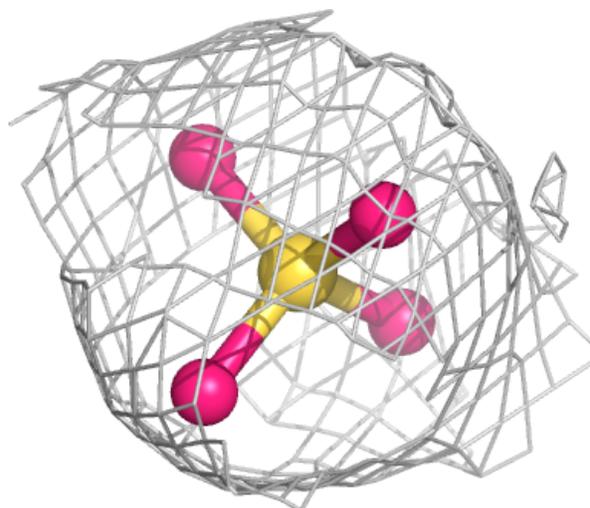
**Electron density around SO4 G 501:**

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



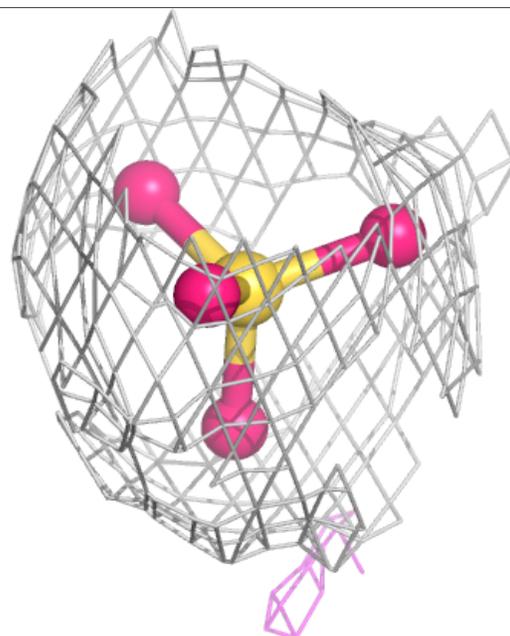
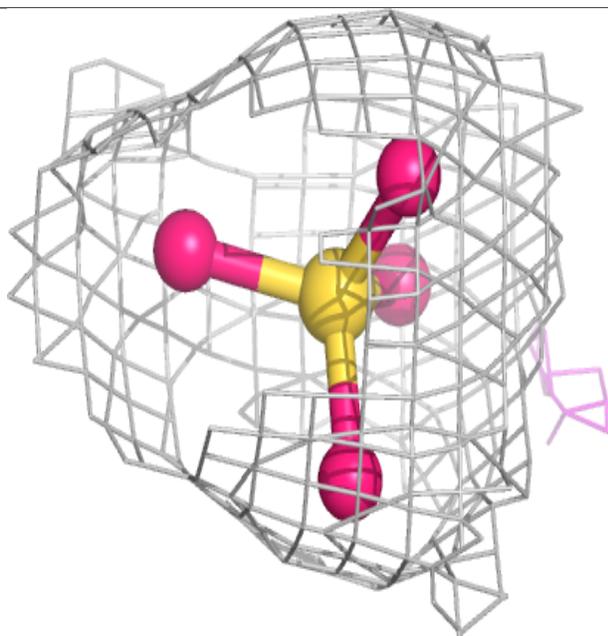
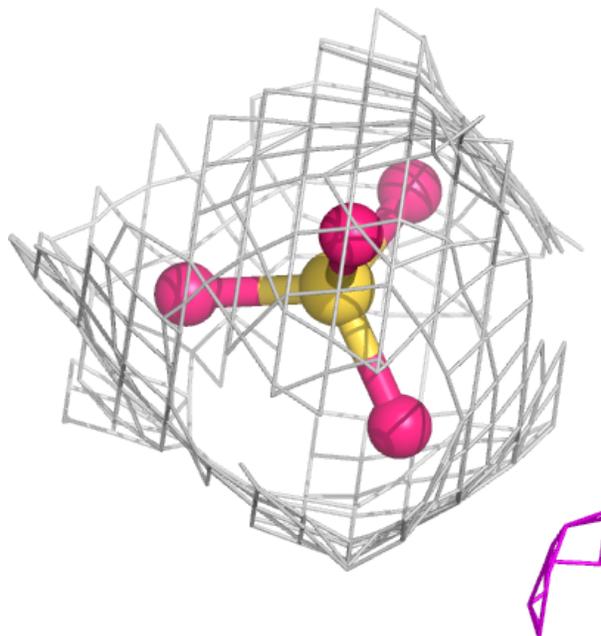
**Electron density around SO4 A 501:**

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



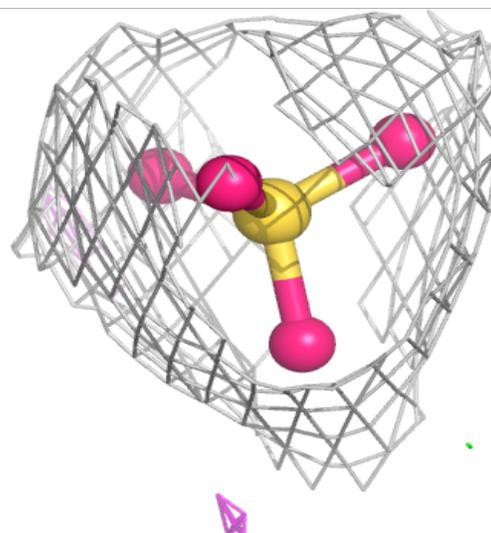
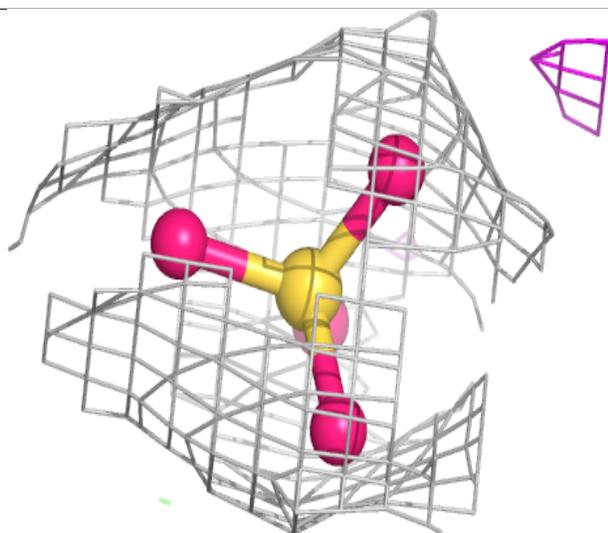
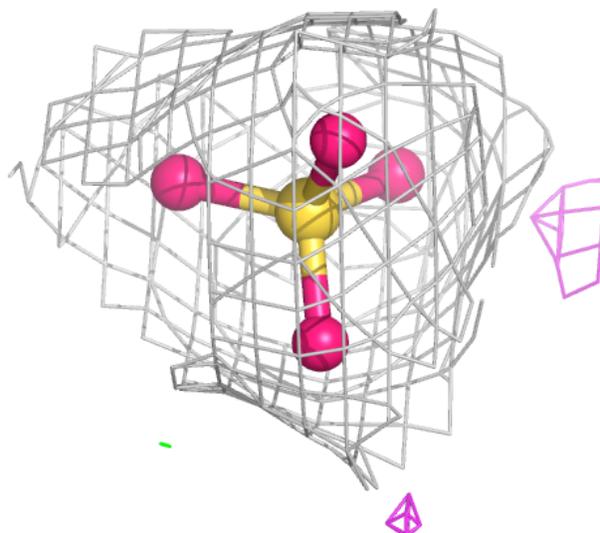
**Electron density around SO4 I 501:**

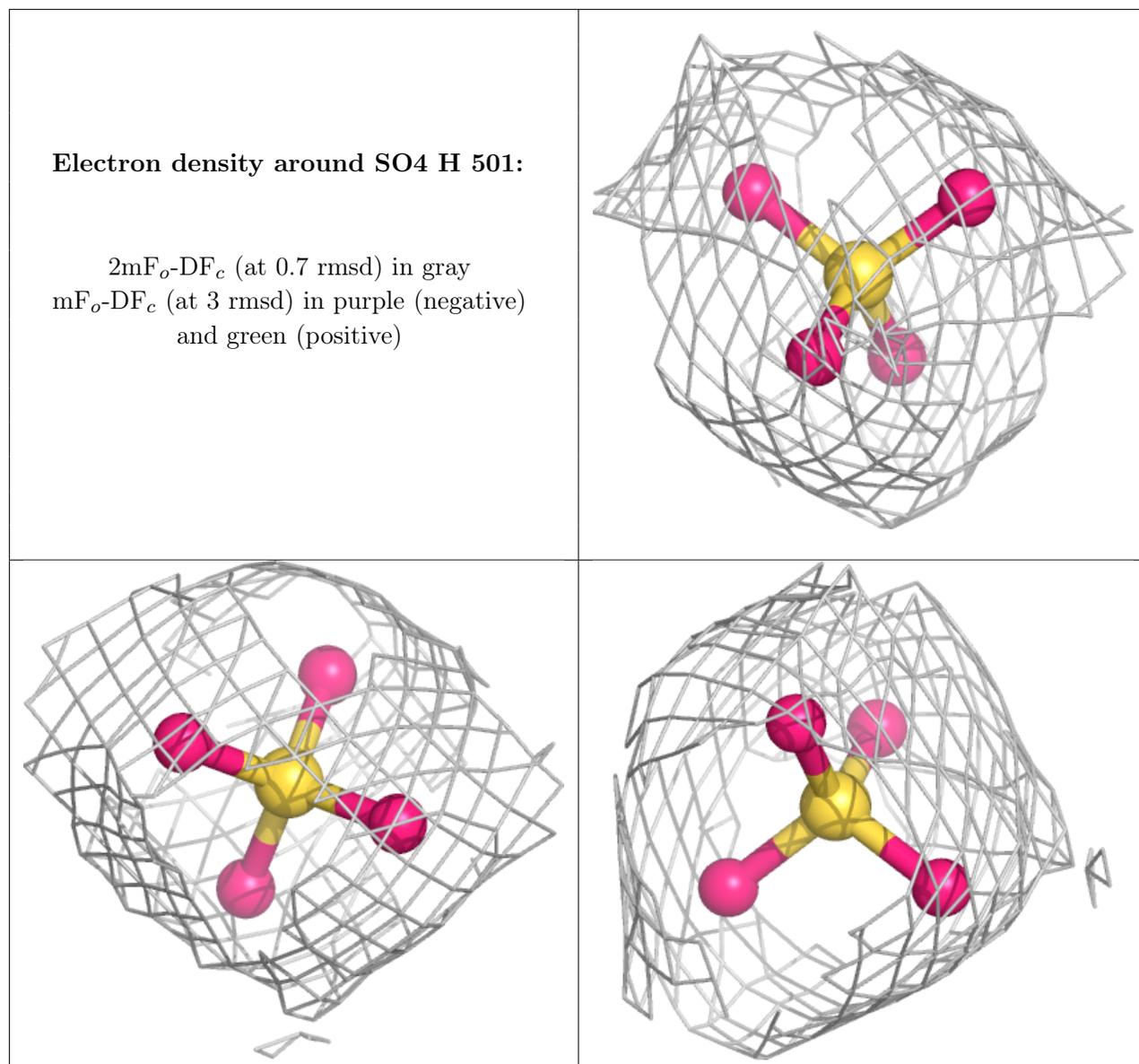
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 C 501:**

$2mF_o-DF_c$  (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.