



wwPDB EM Validation Summary Report ⓘ

Jul 18, 2026 – 08:06 am BST

PDB ID : 9RYW / pdb_00009ryw
EMDB ID : EMD-54394
Title : Aquifex aeolicus lumazine synthase I125A mutant 12-pentamer cage
Authors : Koziej, L.; Azuma, Y.
Deposited on : 2025-07-15
Resolution : 1.71 Å(reported)
Based on initial model : 1HQK

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

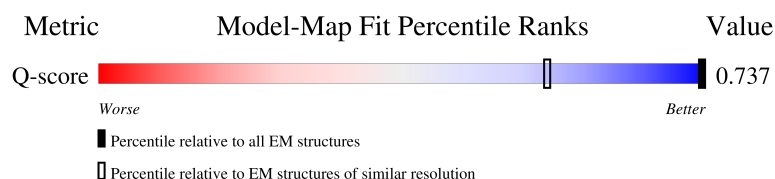
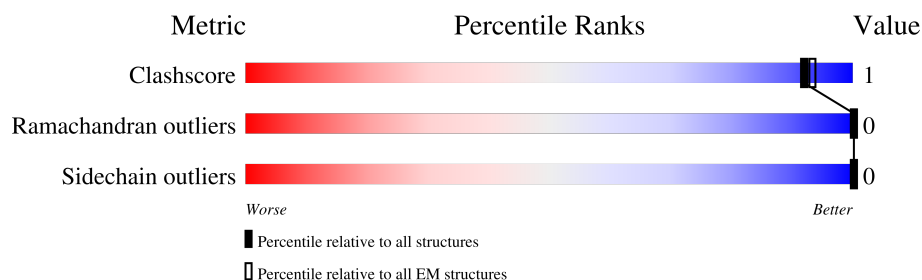
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

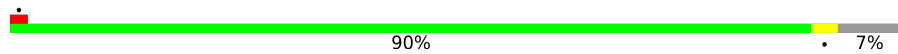
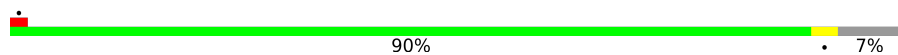
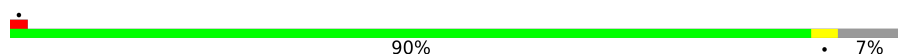
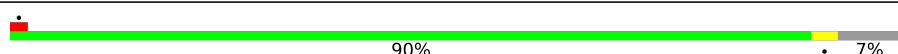
The reported resolution of this entry is 1.71 Å.

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



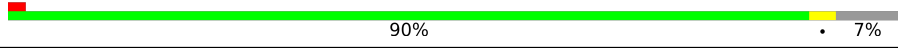
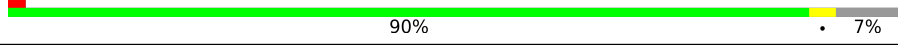
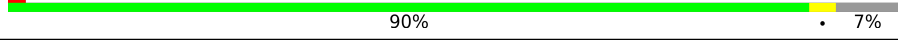
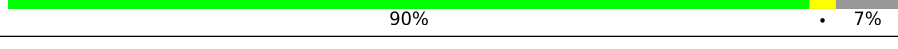
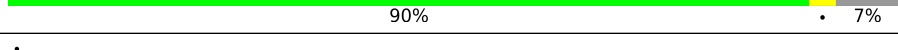
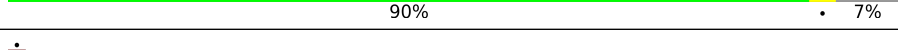
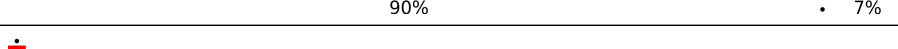
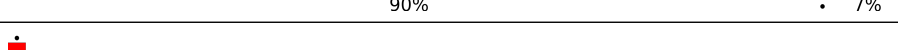
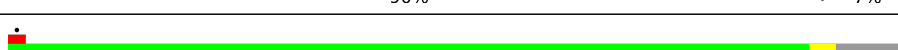
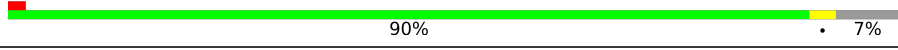
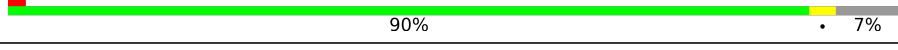
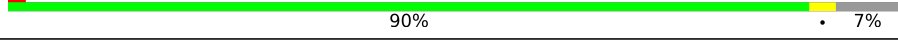
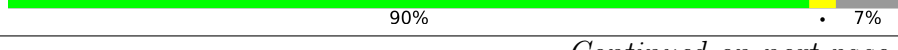
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	612 (1.21 - 2.21)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	166	
1	A2	166	
1	A3	166	
1	A4	166	

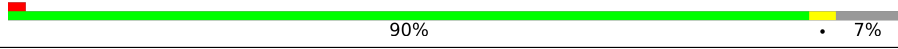
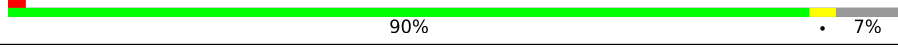
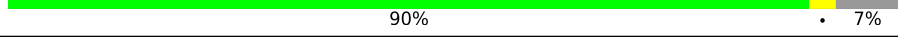
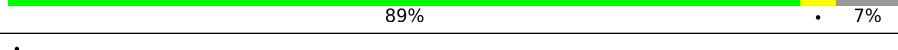
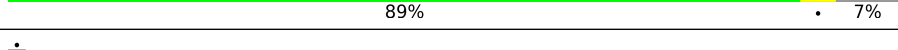
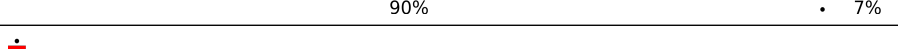
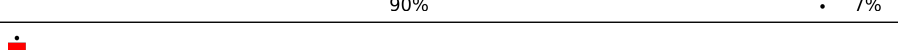
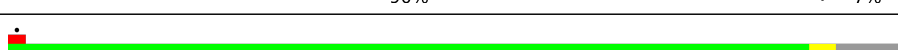
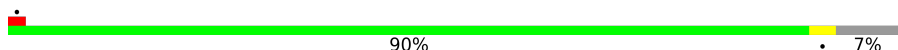
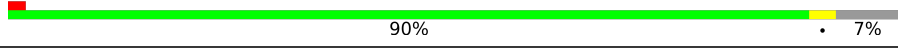
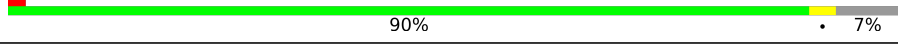
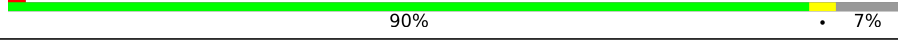
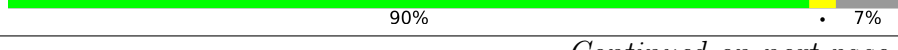
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Mol	Chain	Length	Quality of chain
1	A5	166	
1	B1	166	
1	B2	166	
1	B3	166	
1	B4	166	
1	B5	166	
1	C1	166	
1	C2	166	
1	C3	166	
1	C4	166	
1	C5	166	
1	D1	166	
1	D2	166	
1	D3	166	
1	D4	166	
1	D5	166	
1	E1	166	
1	E2	166	
1	E3	166	
1	E4	166	
1	E5	166	
1	F1	166	
1	F2	166	
1	F3	166	
1	F4	166	

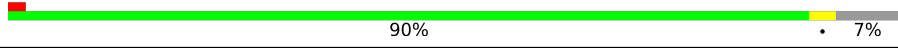
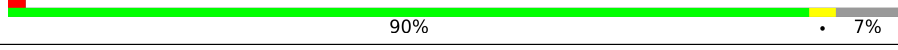
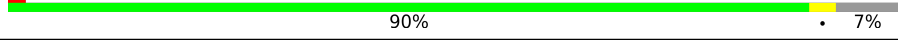
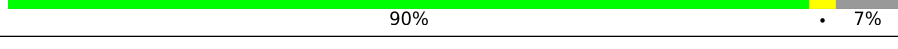
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Mol	Chain	Length	Quality of chain
1	F5	166	
1	G1	166	
1	G2	166	
1	G3	166	
1	G4	166	
1	G5	166	
1	H1	166	
1	H2	166	
1	H3	166	
1	H4	166	
1	H5	166	
1	I1	166	
1	I2	166	
1	I3	166	
1	I4	166	
1	I5	166	
1	J1	166	
1	J2	166	
1	J3	166	
1	J4	166	
1	J5	166	
1	K1	166	
1	K2	166	
1	K3	166	
1	K4	166	

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Mol	Chain	Length	Quality of chain
1	K5	166	 90%7%
1	L1	166	 90%7%
1	L2	166	 90%7%
1	L3	166	 90%7%
1	L4	166	 90%7%
1	L5	166	 90%7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 72750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 6,7-dimethyl-8-ribityllumazine synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	A2	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	A3	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	A4	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	A5	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	B1	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	B2	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	B3	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	B4	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	B5	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	C1	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	C2	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	C3	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	C4	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	C5	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	D1	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		
1	D2	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	D3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	D4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	D5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	E1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	E2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	E3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	E4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	E5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	F1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	F2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	F3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	F4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	F5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	G1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	G2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	G3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	G4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	G5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	H1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	H2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	H3	154	Total 1173	C 742	N 209	O 219	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	H4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	H5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	I1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	I2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	I3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	I4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	I5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	J1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	J2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	J3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	J4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	J5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	K1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	K2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	K3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	K4	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	K5	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	L1	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	L2	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	L3	154	Total 1173	C 742	N 209	O 219	S 3	0	0
1	L4	154	Total 1173	C 742	N 209	O 219	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	154	Total	C	N	O	S	0	0
			1173	742	209	219	3		

There are 840 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	2	GLU	GLN	conflict	UNP O66529
A1	125	ALA	ILE	engineered mutation	UNP O66529
A1	155	LEU	-	expression tag	UNP O66529
A1	156	GLU	-	expression tag	UNP O66529
A1	157	GLY	-	expression tag	UNP O66529
A1	158	GLY	-	expression tag	UNP O66529
A1	159	TRP	-	expression tag	UNP O66529
A1	160	SER	-	expression tag	UNP O66529
A1	161	HIS	-	expression tag	UNP O66529
A1	162	PRO	-	expression tag	UNP O66529
A1	163	GLN	-	expression tag	UNP O66529
A1	164	PHE	-	expression tag	UNP O66529
A1	165	GLU	-	expression tag	UNP O66529
A1	166	LYS	-	expression tag	UNP O66529
A2	2	GLU	GLN	conflict	UNP O66529
A2	125	ALA	ILE	engineered mutation	UNP O66529
A2	155	LEU	-	expression tag	UNP O66529
A2	156	GLU	-	expression tag	UNP O66529
A2	157	GLY	-	expression tag	UNP O66529
A2	158	GLY	-	expression tag	UNP O66529
A2	159	TRP	-	expression tag	UNP O66529
A2	160	SER	-	expression tag	UNP O66529
A2	161	HIS	-	expression tag	UNP O66529
A2	162	PRO	-	expression tag	UNP O66529
A2	163	GLN	-	expression tag	UNP O66529
A2	164	PHE	-	expression tag	UNP O66529
A2	165	GLU	-	expression tag	UNP O66529
A2	166	LYS	-	expression tag	UNP O66529
A3	2	GLU	GLN	conflict	UNP O66529
A3	125	ALA	ILE	engineered mutation	UNP O66529
A3	155	LEU	-	expression tag	UNP O66529
A3	156	GLU	-	expression tag	UNP O66529
A3	157	GLY	-	expression tag	UNP O66529
A3	158	GLY	-	expression tag	UNP O66529
A3	159	TRP	-	expression tag	UNP O66529
A3	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
A3	161	HIS	-	expression tag	UNP O66529
A3	162	PRO	-	expression tag	UNP O66529
A3	163	GLN	-	expression tag	UNP O66529
A3	164	PHE	-	expression tag	UNP O66529
A3	165	GLU	-	expression tag	UNP O66529
A3	166	LYS	-	expression tag	UNP O66529
A4	2	GLU	GLN	conflict	UNP O66529
A4	125	ALA	ILE	engineered mutation	UNP O66529
A4	155	LEU	-	expression tag	UNP O66529
A4	156	GLU	-	expression tag	UNP O66529
A4	157	GLY	-	expression tag	UNP O66529
A4	158	GLY	-	expression tag	UNP O66529
A4	159	TRP	-	expression tag	UNP O66529
A4	160	SER	-	expression tag	UNP O66529
A4	161	HIS	-	expression tag	UNP O66529
A4	162	PRO	-	expression tag	UNP O66529
A4	163	GLN	-	expression tag	UNP O66529
A4	164	PHE	-	expression tag	UNP O66529
A4	165	GLU	-	expression tag	UNP O66529
A4	166	LYS	-	expression tag	UNP O66529
A5	2	GLU	GLN	conflict	UNP O66529
A5	125	ALA	ILE	engineered mutation	UNP O66529
A5	155	LEU	-	expression tag	UNP O66529
A5	156	GLU	-	expression tag	UNP O66529
A5	157	GLY	-	expression tag	UNP O66529
A5	158	GLY	-	expression tag	UNP O66529
A5	159	TRP	-	expression tag	UNP O66529
A5	160	SER	-	expression tag	UNP O66529
A5	161	HIS	-	expression tag	UNP O66529
A5	162	PRO	-	expression tag	UNP O66529
A5	163	GLN	-	expression tag	UNP O66529
A5	164	PHE	-	expression tag	UNP O66529
A5	165	GLU	-	expression tag	UNP O66529
A5	166	LYS	-	expression tag	UNP O66529
B1	2	GLU	GLN	conflict	UNP O66529
B1	125	ALA	ILE	engineered mutation	UNP O66529
B1	155	LEU	-	expression tag	UNP O66529
B1	156	GLU	-	expression tag	UNP O66529
B1	157	GLY	-	expression tag	UNP O66529
B1	158	GLY	-	expression tag	UNP O66529
B1	159	TRP	-	expression tag	UNP O66529
B1	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
B1	161	HIS	-	expression tag	UNP O66529
B1	162	PRO	-	expression tag	UNP O66529
B1	163	GLN	-	expression tag	UNP O66529
B1	164	PHE	-	expression tag	UNP O66529
B1	165	GLU	-	expression tag	UNP O66529
B1	166	LYS	-	expression tag	UNP O66529
B2	2	GLU	GLN	conflict	UNP O66529
B2	125	ALA	ILE	engineered mutation	UNP O66529
B2	155	LEU	-	expression tag	UNP O66529
B2	156	GLU	-	expression tag	UNP O66529
B2	157	GLY	-	expression tag	UNP O66529
B2	158	GLY	-	expression tag	UNP O66529
B2	159	TRP	-	expression tag	UNP O66529
B2	160	SER	-	expression tag	UNP O66529
B2	161	HIS	-	expression tag	UNP O66529
B2	162	PRO	-	expression tag	UNP O66529
B2	163	GLN	-	expression tag	UNP O66529
B2	164	PHE	-	expression tag	UNP O66529
B2	165	GLU	-	expression tag	UNP O66529
B2	166	LYS	-	expression tag	UNP O66529
B3	2	GLU	GLN	conflict	UNP O66529
B3	125	ALA	ILE	engineered mutation	UNP O66529
B3	155	LEU	-	expression tag	UNP O66529
B3	156	GLU	-	expression tag	UNP O66529
B3	157	GLY	-	expression tag	UNP O66529
B3	158	GLY	-	expression tag	UNP O66529
B3	159	TRP	-	expression tag	UNP O66529
B3	160	SER	-	expression tag	UNP O66529
B3	161	HIS	-	expression tag	UNP O66529
B3	162	PRO	-	expression tag	UNP O66529
B3	163	GLN	-	expression tag	UNP O66529
B3	164	PHE	-	expression tag	UNP O66529
B3	165	GLU	-	expression tag	UNP O66529
B3	166	LYS	-	expression tag	UNP O66529
B4	2	GLU	GLN	conflict	UNP O66529
B4	125	ALA	ILE	engineered mutation	UNP O66529
B4	155	LEU	-	expression tag	UNP O66529
B4	156	GLU	-	expression tag	UNP O66529
B4	157	GLY	-	expression tag	UNP O66529
B4	158	GLY	-	expression tag	UNP O66529
B4	159	TRP	-	expression tag	UNP O66529
B4	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
B4	161	HIS	-	expression tag	UNP O66529
B4	162	PRO	-	expression tag	UNP O66529
B4	163	GLN	-	expression tag	UNP O66529
B4	164	PHE	-	expression tag	UNP O66529
B4	165	GLU	-	expression tag	UNP O66529
B4	166	LYS	-	expression tag	UNP O66529
B5	2	GLU	GLN	conflict	UNP O66529
B5	125	ALA	ILE	engineered mutation	UNP O66529
B5	155	LEU	-	expression tag	UNP O66529
B5	156	GLU	-	expression tag	UNP O66529
B5	157	GLY	-	expression tag	UNP O66529
B5	158	GLY	-	expression tag	UNP O66529
B5	159	TRP	-	expression tag	UNP O66529
B5	160	SER	-	expression tag	UNP O66529
B5	161	HIS	-	expression tag	UNP O66529
B5	162	PRO	-	expression tag	UNP O66529
B5	163	GLN	-	expression tag	UNP O66529
B5	164	PHE	-	expression tag	UNP O66529
B5	165	GLU	-	expression tag	UNP O66529
B5	166	LYS	-	expression tag	UNP O66529
C1	2	GLU	GLN	conflict	UNP O66529
C1	125	ALA	ILE	engineered mutation	UNP O66529
C1	155	LEU	-	expression tag	UNP O66529
C1	156	GLU	-	expression tag	UNP O66529
C1	157	GLY	-	expression tag	UNP O66529
C1	158	GLY	-	expression tag	UNP O66529
C1	159	TRP	-	expression tag	UNP O66529
C1	160	SER	-	expression tag	UNP O66529
C1	161	HIS	-	expression tag	UNP O66529
C1	162	PRO	-	expression tag	UNP O66529
C1	163	GLN	-	expression tag	UNP O66529
C1	164	PHE	-	expression tag	UNP O66529
C1	165	GLU	-	expression tag	UNP O66529
C1	166	LYS	-	expression tag	UNP O66529
C2	2	GLU	GLN	conflict	UNP O66529
C2	125	ALA	ILE	engineered mutation	UNP O66529
C2	155	LEU	-	expression tag	UNP O66529
C2	156	GLU	-	expression tag	UNP O66529
C2	157	GLY	-	expression tag	UNP O66529
C2	158	GLY	-	expression tag	UNP O66529
C2	159	TRP	-	expression tag	UNP O66529
C2	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
C2	161	HIS	-	expression tag	UNP O66529
C2	162	PRO	-	expression tag	UNP O66529
C2	163	GLN	-	expression tag	UNP O66529
C2	164	PHE	-	expression tag	UNP O66529
C2	165	GLU	-	expression tag	UNP O66529
C2	166	LYS	-	expression tag	UNP O66529
C3	2	GLU	GLN	conflict	UNP O66529
C3	125	ALA	ILE	engineered mutation	UNP O66529
C3	155	LEU	-	expression tag	UNP O66529
C3	156	GLU	-	expression tag	UNP O66529
C3	157	GLY	-	expression tag	UNP O66529
C3	158	GLY	-	expression tag	UNP O66529
C3	159	TRP	-	expression tag	UNP O66529
C3	160	SER	-	expression tag	UNP O66529
C3	161	HIS	-	expression tag	UNP O66529
C3	162	PRO	-	expression tag	UNP O66529
C3	163	GLN	-	expression tag	UNP O66529
C3	164	PHE	-	expression tag	UNP O66529
C3	165	GLU	-	expression tag	UNP O66529
C3	166	LYS	-	expression tag	UNP O66529
C4	2	GLU	GLN	conflict	UNP O66529
C4	125	ALA	ILE	engineered mutation	UNP O66529
C4	155	LEU	-	expression tag	UNP O66529
C4	156	GLU	-	expression tag	UNP O66529
C4	157	GLY	-	expression tag	UNP O66529
C4	158	GLY	-	expression tag	UNP O66529
C4	159	TRP	-	expression tag	UNP O66529
C4	160	SER	-	expression tag	UNP O66529
C4	161	HIS	-	expression tag	UNP O66529
C4	162	PRO	-	expression tag	UNP O66529
C4	163	GLN	-	expression tag	UNP O66529
C4	164	PHE	-	expression tag	UNP O66529
C4	165	GLU	-	expression tag	UNP O66529
C4	166	LYS	-	expression tag	UNP O66529
C5	2	GLU	GLN	conflict	UNP O66529
C5	125	ALA	ILE	engineered mutation	UNP O66529
C5	155	LEU	-	expression tag	UNP O66529
C5	156	GLU	-	expression tag	UNP O66529
C5	157	GLY	-	expression tag	UNP O66529
C5	158	GLY	-	expression tag	UNP O66529
C5	159	TRP	-	expression tag	UNP O66529
C5	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
C5	161	HIS	-	expression tag	UNP O66529
C5	162	PRO	-	expression tag	UNP O66529
C5	163	GLN	-	expression tag	UNP O66529
C5	164	PHE	-	expression tag	UNP O66529
C5	165	GLU	-	expression tag	UNP O66529
C5	166	LYS	-	expression tag	UNP O66529
D1	2	GLU	GLN	conflict	UNP O66529
D1	125	ALA	ILE	engineered mutation	UNP O66529
D1	155	LEU	-	expression tag	UNP O66529
D1	156	GLU	-	expression tag	UNP O66529
D1	157	GLY	-	expression tag	UNP O66529
D1	158	GLY	-	expression tag	UNP O66529
D1	159	TRP	-	expression tag	UNP O66529
D1	160	SER	-	expression tag	UNP O66529
D1	161	HIS	-	expression tag	UNP O66529
D1	162	PRO	-	expression tag	UNP O66529
D1	163	GLN	-	expression tag	UNP O66529
D1	164	PHE	-	expression tag	UNP O66529
D1	165	GLU	-	expression tag	UNP O66529
D1	166	LYS	-	expression tag	UNP O66529
D2	2	GLU	GLN	conflict	UNP O66529
D2	125	ALA	ILE	engineered mutation	UNP O66529
D2	155	LEU	-	expression tag	UNP O66529
D2	156	GLU	-	expression tag	UNP O66529
D2	157	GLY	-	expression tag	UNP O66529
D2	158	GLY	-	expression tag	UNP O66529
D2	159	TRP	-	expression tag	UNP O66529
D2	160	SER	-	expression tag	UNP O66529
D2	161	HIS	-	expression tag	UNP O66529
D2	162	PRO	-	expression tag	UNP O66529
D2	163	GLN	-	expression tag	UNP O66529
D2	164	PHE	-	expression tag	UNP O66529
D2	165	GLU	-	expression tag	UNP O66529
D2	166	LYS	-	expression tag	UNP O66529
D3	2	GLU	GLN	conflict	UNP O66529
D3	125	ALA	ILE	engineered mutation	UNP O66529
D3	155	LEU	-	expression tag	UNP O66529
D3	156	GLU	-	expression tag	UNP O66529
D3	157	GLY	-	expression tag	UNP O66529
D3	158	GLY	-	expression tag	UNP O66529
D3	159	TRP	-	expression tag	UNP O66529
D3	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
D3	161	HIS	-	expression tag	UNP O66529
D3	162	PRO	-	expression tag	UNP O66529
D3	163	GLN	-	expression tag	UNP O66529
D3	164	PHE	-	expression tag	UNP O66529
D3	165	GLU	-	expression tag	UNP O66529
D3	166	LYS	-	expression tag	UNP O66529
D4	2	GLU	GLN	conflict	UNP O66529
D4	125	ALA	ILE	engineered mutation	UNP O66529
D4	155	LEU	-	expression tag	UNP O66529
D4	156	GLU	-	expression tag	UNP O66529
D4	157	GLY	-	expression tag	UNP O66529
D4	158	GLY	-	expression tag	UNP O66529
D4	159	TRP	-	expression tag	UNP O66529
D4	160	SER	-	expression tag	UNP O66529
D4	161	HIS	-	expression tag	UNP O66529
D4	162	PRO	-	expression tag	UNP O66529
D4	163	GLN	-	expression tag	UNP O66529
D4	164	PHE	-	expression tag	UNP O66529
D4	165	GLU	-	expression tag	UNP O66529
D4	166	LYS	-	expression tag	UNP O66529
D5	2	GLU	GLN	conflict	UNP O66529
D5	125	ALA	ILE	engineered mutation	UNP O66529
D5	155	LEU	-	expression tag	UNP O66529
D5	156	GLU	-	expression tag	UNP O66529
D5	157	GLY	-	expression tag	UNP O66529
D5	158	GLY	-	expression tag	UNP O66529
D5	159	TRP	-	expression tag	UNP O66529
D5	160	SER	-	expression tag	UNP O66529
D5	161	HIS	-	expression tag	UNP O66529
D5	162	PRO	-	expression tag	UNP O66529
D5	163	GLN	-	expression tag	UNP O66529
D5	164	PHE	-	expression tag	UNP O66529
D5	165	GLU	-	expression tag	UNP O66529
D5	166	LYS	-	expression tag	UNP O66529
E1	2	GLU	GLN	conflict	UNP O66529
E1	125	ALA	ILE	engineered mutation	UNP O66529
E1	155	LEU	-	expression tag	UNP O66529
E1	156	GLU	-	expression tag	UNP O66529
E1	157	GLY	-	expression tag	UNP O66529
E1	158	GLY	-	expression tag	UNP O66529
E1	159	TRP	-	expression tag	UNP O66529
E1	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
E1	161	HIS	-	expression tag	UNP O66529
E1	162	PRO	-	expression tag	UNP O66529
E1	163	GLN	-	expression tag	UNP O66529
E1	164	PHE	-	expression tag	UNP O66529
E1	165	GLU	-	expression tag	UNP O66529
E1	166	LYS	-	expression tag	UNP O66529
E2	2	GLU	GLN	conflict	UNP O66529
E2	125	ALA	ILE	engineered mutation	UNP O66529
E2	155	LEU	-	expression tag	UNP O66529
E2	156	GLU	-	expression tag	UNP O66529
E2	157	GLY	-	expression tag	UNP O66529
E2	158	GLY	-	expression tag	UNP O66529
E2	159	TRP	-	expression tag	UNP O66529
E2	160	SER	-	expression tag	UNP O66529
E2	161	HIS	-	expression tag	UNP O66529
E2	162	PRO	-	expression tag	UNP O66529
E2	163	GLN	-	expression tag	UNP O66529
E2	164	PHE	-	expression tag	UNP O66529
E2	165	GLU	-	expression tag	UNP O66529
E2	166	LYS	-	expression tag	UNP O66529
E3	2	GLU	GLN	conflict	UNP O66529
E3	125	ALA	ILE	engineered mutation	UNP O66529
E3	155	LEU	-	expression tag	UNP O66529
E3	156	GLU	-	expression tag	UNP O66529
E3	157	GLY	-	expression tag	UNP O66529
E3	158	GLY	-	expression tag	UNP O66529
E3	159	TRP	-	expression tag	UNP O66529
E3	160	SER	-	expression tag	UNP O66529
E3	161	HIS	-	expression tag	UNP O66529
E3	162	PRO	-	expression tag	UNP O66529
E3	163	GLN	-	expression tag	UNP O66529
E3	164	PHE	-	expression tag	UNP O66529
E3	165	GLU	-	expression tag	UNP O66529
E3	166	LYS	-	expression tag	UNP O66529
E4	2	GLU	GLN	conflict	UNP O66529
E4	125	ALA	ILE	engineered mutation	UNP O66529
E4	155	LEU	-	expression tag	UNP O66529
E4	156	GLU	-	expression tag	UNP O66529
E4	157	GLY	-	expression tag	UNP O66529
E4	158	GLY	-	expression tag	UNP O66529
E4	159	TRP	-	expression tag	UNP O66529
E4	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
E4	161	HIS	-	expression tag	UNP O66529
E4	162	PRO	-	expression tag	UNP O66529
E4	163	GLN	-	expression tag	UNP O66529
E4	164	PHE	-	expression tag	UNP O66529
E4	165	GLU	-	expression tag	UNP O66529
E4	166	LYS	-	expression tag	UNP O66529
E5	2	GLU	GLN	conflict	UNP O66529
E5	125	ALA	ILE	engineered mutation	UNP O66529
E5	155	LEU	-	expression tag	UNP O66529
E5	156	GLU	-	expression tag	UNP O66529
E5	157	GLY	-	expression tag	UNP O66529
E5	158	GLY	-	expression tag	UNP O66529
E5	159	TRP	-	expression tag	UNP O66529
E5	160	SER	-	expression tag	UNP O66529
E5	161	HIS	-	expression tag	UNP O66529
E5	162	PRO	-	expression tag	UNP O66529
E5	163	GLN	-	expression tag	UNP O66529
E5	164	PHE	-	expression tag	UNP O66529
E5	165	GLU	-	expression tag	UNP O66529
E5	166	LYS	-	expression tag	UNP O66529
F1	2	GLU	GLN	conflict	UNP O66529
F1	125	ALA	ILE	engineered mutation	UNP O66529
F1	155	LEU	-	expression tag	UNP O66529
F1	156	GLU	-	expression tag	UNP O66529
F1	157	GLY	-	expression tag	UNP O66529
F1	158	GLY	-	expression tag	UNP O66529
F1	159	TRP	-	expression tag	UNP O66529
F1	160	SER	-	expression tag	UNP O66529
F1	161	HIS	-	expression tag	UNP O66529
F1	162	PRO	-	expression tag	UNP O66529
F1	163	GLN	-	expression tag	UNP O66529
F1	164	PHE	-	expression tag	UNP O66529
F1	165	GLU	-	expression tag	UNP O66529
F1	166	LYS	-	expression tag	UNP O66529
F2	2	GLU	GLN	conflict	UNP O66529
F2	125	ALA	ILE	engineered mutation	UNP O66529
F2	155	LEU	-	expression tag	UNP O66529
F2	156	GLU	-	expression tag	UNP O66529
F2	157	GLY	-	expression tag	UNP O66529
F2	158	GLY	-	expression tag	UNP O66529
F2	159	TRP	-	expression tag	UNP O66529
F2	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
F2	161	HIS	-	expression tag	UNP O66529
F2	162	PRO	-	expression tag	UNP O66529
F2	163	GLN	-	expression tag	UNP O66529
F2	164	PHE	-	expression tag	UNP O66529
F2	165	GLU	-	expression tag	UNP O66529
F2	166	LYS	-	expression tag	UNP O66529
F3	2	GLU	GLN	conflict	UNP O66529
F3	125	ALA	ILE	engineered mutation	UNP O66529
F3	155	LEU	-	expression tag	UNP O66529
F3	156	GLU	-	expression tag	UNP O66529
F3	157	GLY	-	expression tag	UNP O66529
F3	158	GLY	-	expression tag	UNP O66529
F3	159	TRP	-	expression tag	UNP O66529
F3	160	SER	-	expression tag	UNP O66529
F3	161	HIS	-	expression tag	UNP O66529
F3	162	PRO	-	expression tag	UNP O66529
F3	163	GLN	-	expression tag	UNP O66529
F3	164	PHE	-	expression tag	UNP O66529
F3	165	GLU	-	expression tag	UNP O66529
F3	166	LYS	-	expression tag	UNP O66529
F4	2	GLU	GLN	conflict	UNP O66529
F4	125	ALA	ILE	engineered mutation	UNP O66529
F4	155	LEU	-	expression tag	UNP O66529
F4	156	GLU	-	expression tag	UNP O66529
F4	157	GLY	-	expression tag	UNP O66529
F4	158	GLY	-	expression tag	UNP O66529
F4	159	TRP	-	expression tag	UNP O66529
F4	160	SER	-	expression tag	UNP O66529
F4	161	HIS	-	expression tag	UNP O66529
F4	162	PRO	-	expression tag	UNP O66529
F4	163	GLN	-	expression tag	UNP O66529
F4	164	PHE	-	expression tag	UNP O66529
F4	165	GLU	-	expression tag	UNP O66529
F4	166	LYS	-	expression tag	UNP O66529
F5	2	GLU	GLN	conflict	UNP O66529
F5	125	ALA	ILE	engineered mutation	UNP O66529
F5	155	LEU	-	expression tag	UNP O66529
F5	156	GLU	-	expression tag	UNP O66529
F5	157	GLY	-	expression tag	UNP O66529
F5	158	GLY	-	expression tag	UNP O66529
F5	159	TRP	-	expression tag	UNP O66529
F5	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
F5	161	HIS	-	expression tag	UNP O66529
F5	162	PRO	-	expression tag	UNP O66529
F5	163	GLN	-	expression tag	UNP O66529
F5	164	PHE	-	expression tag	UNP O66529
F5	165	GLU	-	expression tag	UNP O66529
F5	166	LYS	-	expression tag	UNP O66529
G1	2	GLU	GLN	conflict	UNP O66529
G1	125	ALA	ILE	engineered mutation	UNP O66529
G1	155	LEU	-	expression tag	UNP O66529
G1	156	GLU	-	expression tag	UNP O66529
G1	157	GLY	-	expression tag	UNP O66529
G1	158	GLY	-	expression tag	UNP O66529
G1	159	TRP	-	expression tag	UNP O66529
G1	160	SER	-	expression tag	UNP O66529
G1	161	HIS	-	expression tag	UNP O66529
G1	162	PRO	-	expression tag	UNP O66529
G1	163	GLN	-	expression tag	UNP O66529
G1	164	PHE	-	expression tag	UNP O66529
G1	165	GLU	-	expression tag	UNP O66529
G1	166	LYS	-	expression tag	UNP O66529
G2	2	GLU	GLN	conflict	UNP O66529
G2	125	ALA	ILE	engineered mutation	UNP O66529
G2	155	LEU	-	expression tag	UNP O66529
G2	156	GLU	-	expression tag	UNP O66529
G2	157	GLY	-	expression tag	UNP O66529
G2	158	GLY	-	expression tag	UNP O66529
G2	159	TRP	-	expression tag	UNP O66529
G2	160	SER	-	expression tag	UNP O66529
G2	161	HIS	-	expression tag	UNP O66529
G2	162	PRO	-	expression tag	UNP O66529
G2	163	GLN	-	expression tag	UNP O66529
G2	164	PHE	-	expression tag	UNP O66529
G2	165	GLU	-	expression tag	UNP O66529
G2	166	LYS	-	expression tag	UNP O66529
G3	2	GLU	GLN	conflict	UNP O66529
G3	125	ALA	ILE	engineered mutation	UNP O66529
G3	155	LEU	-	expression tag	UNP O66529
G3	156	GLU	-	expression tag	UNP O66529
G3	157	GLY	-	expression tag	UNP O66529
G3	158	GLY	-	expression tag	UNP O66529
G3	159	TRP	-	expression tag	UNP O66529
G3	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
G3	161	HIS	-	expression tag	UNP O66529
G3	162	PRO	-	expression tag	UNP O66529
G3	163	GLN	-	expression tag	UNP O66529
G3	164	PHE	-	expression tag	UNP O66529
G3	165	GLU	-	expression tag	UNP O66529
G3	166	LYS	-	expression tag	UNP O66529
G4	2	GLU	GLN	conflict	UNP O66529
G4	125	ALA	ILE	engineered mutation	UNP O66529
G4	155	LEU	-	expression tag	UNP O66529
G4	156	GLU	-	expression tag	UNP O66529
G4	157	GLY	-	expression tag	UNP O66529
G4	158	GLY	-	expression tag	UNP O66529
G4	159	TRP	-	expression tag	UNP O66529
G4	160	SER	-	expression tag	UNP O66529
G4	161	HIS	-	expression tag	UNP O66529
G4	162	PRO	-	expression tag	UNP O66529
G4	163	GLN	-	expression tag	UNP O66529
G4	164	PHE	-	expression tag	UNP O66529
G4	165	GLU	-	expression tag	UNP O66529
G4	166	LYS	-	expression tag	UNP O66529
G5	2	GLU	GLN	conflict	UNP O66529
G5	125	ALA	ILE	engineered mutation	UNP O66529
G5	155	LEU	-	expression tag	UNP O66529
G5	156	GLU	-	expression tag	UNP O66529
G5	157	GLY	-	expression tag	UNP O66529
G5	158	GLY	-	expression tag	UNP O66529
G5	159	TRP	-	expression tag	UNP O66529
G5	160	SER	-	expression tag	UNP O66529
G5	161	HIS	-	expression tag	UNP O66529
G5	162	PRO	-	expression tag	UNP O66529
G5	163	GLN	-	expression tag	UNP O66529
G5	164	PHE	-	expression tag	UNP O66529
G5	165	GLU	-	expression tag	UNP O66529
G5	166	LYS	-	expression tag	UNP O66529
H1	2	GLU	GLN	conflict	UNP O66529
H1	125	ALA	ILE	engineered mutation	UNP O66529
H1	155	LEU	-	expression tag	UNP O66529
H1	156	GLU	-	expression tag	UNP O66529
H1	157	GLY	-	expression tag	UNP O66529
H1	158	GLY	-	expression tag	UNP O66529
H1	159	TRP	-	expression tag	UNP O66529
H1	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
H1	161	HIS	-	expression tag	UNP O66529
H1	162	PRO	-	expression tag	UNP O66529
H1	163	GLN	-	expression tag	UNP O66529
H1	164	PHE	-	expression tag	UNP O66529
H1	165	GLU	-	expression tag	UNP O66529
H1	166	LYS	-	expression tag	UNP O66529
H2	2	GLU	GLN	conflict	UNP O66529
H2	125	ALA	ILE	engineered mutation	UNP O66529
H2	155	LEU	-	expression tag	UNP O66529
H2	156	GLU	-	expression tag	UNP O66529
H2	157	GLY	-	expression tag	UNP O66529
H2	158	GLY	-	expression tag	UNP O66529
H2	159	TRP	-	expression tag	UNP O66529
H2	160	SER	-	expression tag	UNP O66529
H2	161	HIS	-	expression tag	UNP O66529
H2	162	PRO	-	expression tag	UNP O66529
H2	163	GLN	-	expression tag	UNP O66529
H2	164	PHE	-	expression tag	UNP O66529
H2	165	GLU	-	expression tag	UNP O66529
H2	166	LYS	-	expression tag	UNP O66529
H3	2	GLU	GLN	conflict	UNP O66529
H3	125	ALA	ILE	engineered mutation	UNP O66529
H3	155	LEU	-	expression tag	UNP O66529
H3	156	GLU	-	expression tag	UNP O66529
H3	157	GLY	-	expression tag	UNP O66529
H3	158	GLY	-	expression tag	UNP O66529
H3	159	TRP	-	expression tag	UNP O66529
H3	160	SER	-	expression tag	UNP O66529
H3	161	HIS	-	expression tag	UNP O66529
H3	162	PRO	-	expression tag	UNP O66529
H3	163	GLN	-	expression tag	UNP O66529
H3	164	PHE	-	expression tag	UNP O66529
H3	165	GLU	-	expression tag	UNP O66529
H3	166	LYS	-	expression tag	UNP O66529
H4	2	GLU	GLN	conflict	UNP O66529
H4	125	ALA	ILE	engineered mutation	UNP O66529
H4	155	LEU	-	expression tag	UNP O66529
H4	156	GLU	-	expression tag	UNP O66529
H4	157	GLY	-	expression tag	UNP O66529
H4	158	GLY	-	expression tag	UNP O66529
H4	159	TRP	-	expression tag	UNP O66529
H4	160	SER	-	expression tag	UNP O66529

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Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H4	161	HIS	-	expression tag	UNP O66529
H4	162	PRO	-	expression tag	UNP O66529
H4	163	GLN	-	expression tag	UNP O66529
H4	164	PHE	-	expression tag	UNP O66529
H4	165	GLU	-	expression tag	UNP O66529
H4	166	LYS	-	expression tag	UNP O66529
H5	2	GLU	GLN	conflict	UNP O66529
H5	125	ALA	ILE	engineered mutation	UNP O66529
H5	155	LEU	-	expression tag	UNP O66529
H5	156	GLU	-	expression tag	UNP O66529
H5	157	GLY	-	expression tag	UNP O66529
H5	158	GLY	-	expression tag	UNP O66529
H5	159	TRP	-	expression tag	UNP O66529
H5	160	SER	-	expression tag	UNP O66529
H5	161	HIS	-	expression tag	UNP O66529
H5	162	PRO	-	expression tag	UNP O66529
H5	163	GLN	-	expression tag	UNP O66529
H5	164	PHE	-	expression tag	UNP O66529
H5	165	GLU	-	expression tag	UNP O66529
H5	166	LYS	-	expression tag	UNP O66529
I1	2	GLU	GLN	conflict	UNP O66529
I1	125	ALA	ILE	engineered mutation	UNP O66529
I1	155	LEU	-	expression tag	UNP O66529
I1	156	GLU	-	expression tag	UNP O66529
I1	157	GLY	-	expression tag	UNP O66529
I1	158	GLY	-	expression tag	UNP O66529
I1	159	TRP	-	expression tag	UNP O66529
I1	160	SER	-	expression tag	UNP O66529
I1	161	HIS	-	expression tag	UNP O66529
I1	162	PRO	-	expression tag	UNP O66529
I1	163	GLN	-	expression tag	UNP O66529
I1	164	PHE	-	expression tag	UNP O66529
I1	165	GLU	-	expression tag	UNP O66529
I1	166	LYS	-	expression tag	UNP O66529
I2	2	GLU	GLN	conflict	UNP O66529
I2	125	ALA	ILE	engineered mutation	UNP O66529
I2	155	LEU	-	expression tag	UNP O66529
I2	156	GLU	-	expression tag	UNP O66529
I2	157	GLY	-	expression tag	UNP O66529
I2	158	GLY	-	expression tag	UNP O66529
I2	159	TRP	-	expression tag	UNP O66529
I2	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
I2	161	HIS	-	expression tag	UNP O66529
I2	162	PRO	-	expression tag	UNP O66529
I2	163	GLN	-	expression tag	UNP O66529
I2	164	PHE	-	expression tag	UNP O66529
I2	165	GLU	-	expression tag	UNP O66529
I2	166	LYS	-	expression tag	UNP O66529
I3	2	GLU	GLN	conflict	UNP O66529
I3	125	ALA	ILE	engineered mutation	UNP O66529
I3	155	LEU	-	expression tag	UNP O66529
I3	156	GLU	-	expression tag	UNP O66529
I3	157	GLY	-	expression tag	UNP O66529
I3	158	GLY	-	expression tag	UNP O66529
I3	159	TRP	-	expression tag	UNP O66529
I3	160	SER	-	expression tag	UNP O66529
I3	161	HIS	-	expression tag	UNP O66529
I3	162	PRO	-	expression tag	UNP O66529
I3	163	GLN	-	expression tag	UNP O66529
I3	164	PHE	-	expression tag	UNP O66529
I3	165	GLU	-	expression tag	UNP O66529
I3	166	LYS	-	expression tag	UNP O66529
I4	2	GLU	GLN	conflict	UNP O66529
I4	125	ALA	ILE	engineered mutation	UNP O66529
I4	155	LEU	-	expression tag	UNP O66529
I4	156	GLU	-	expression tag	UNP O66529
I4	157	GLY	-	expression tag	UNP O66529
I4	158	GLY	-	expression tag	UNP O66529
I4	159	TRP	-	expression tag	UNP O66529
I4	160	SER	-	expression tag	UNP O66529
I4	161	HIS	-	expression tag	UNP O66529
I4	162	PRO	-	expression tag	UNP O66529
I4	163	GLN	-	expression tag	UNP O66529
I4	164	PHE	-	expression tag	UNP O66529
I4	165	GLU	-	expression tag	UNP O66529
I4	166	LYS	-	expression tag	UNP O66529
I5	2	GLU	GLN	conflict	UNP O66529
I5	125	ALA	ILE	engineered mutation	UNP O66529
I5	155	LEU	-	expression tag	UNP O66529
I5	156	GLU	-	expression tag	UNP O66529
I5	157	GLY	-	expression tag	UNP O66529
I5	158	GLY	-	expression tag	UNP O66529
I5	159	TRP	-	expression tag	UNP O66529
I5	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
I5	161	HIS	-	expression tag	UNP O66529
I5	162	PRO	-	expression tag	UNP O66529
I5	163	GLN	-	expression tag	UNP O66529
I5	164	PHE	-	expression tag	UNP O66529
I5	165	GLU	-	expression tag	UNP O66529
I5	166	LYS	-	expression tag	UNP O66529
J1	2	GLU	GLN	conflict	UNP O66529
J1	125	ALA	ILE	engineered mutation	UNP O66529
J1	155	LEU	-	expression tag	UNP O66529
J1	156	GLU	-	expression tag	UNP O66529
J1	157	GLY	-	expression tag	UNP O66529
J1	158	GLY	-	expression tag	UNP O66529
J1	159	TRP	-	expression tag	UNP O66529
J1	160	SER	-	expression tag	UNP O66529
J1	161	HIS	-	expression tag	UNP O66529
J1	162	PRO	-	expression tag	UNP O66529
J1	163	GLN	-	expression tag	UNP O66529
J1	164	PHE	-	expression tag	UNP O66529
J1	165	GLU	-	expression tag	UNP O66529
J1	166	LYS	-	expression tag	UNP O66529
J2	2	GLU	GLN	conflict	UNP O66529
J2	125	ALA	ILE	engineered mutation	UNP O66529
J2	155	LEU	-	expression tag	UNP O66529
J2	156	GLU	-	expression tag	UNP O66529
J2	157	GLY	-	expression tag	UNP O66529
J2	158	GLY	-	expression tag	UNP O66529
J2	159	TRP	-	expression tag	UNP O66529
J2	160	SER	-	expression tag	UNP O66529
J2	161	HIS	-	expression tag	UNP O66529
J2	162	PRO	-	expression tag	UNP O66529
J2	163	GLN	-	expression tag	UNP O66529
J2	164	PHE	-	expression tag	UNP O66529
J2	165	GLU	-	expression tag	UNP O66529
J2	166	LYS	-	expression tag	UNP O66529
J3	2	GLU	GLN	conflict	UNP O66529
J3	125	ALA	ILE	engineered mutation	UNP O66529
J3	155	LEU	-	expression tag	UNP O66529
J3	156	GLU	-	expression tag	UNP O66529
J3	157	GLY	-	expression tag	UNP O66529
J3	158	GLY	-	expression tag	UNP O66529
J3	159	TRP	-	expression tag	UNP O66529
J3	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
J3	161	HIS	-	expression tag	UNP O66529
J3	162	PRO	-	expression tag	UNP O66529
J3	163	GLN	-	expression tag	UNP O66529
J3	164	PHE	-	expression tag	UNP O66529
J3	165	GLU	-	expression tag	UNP O66529
J3	166	LYS	-	expression tag	UNP O66529
J4	2	GLU	GLN	conflict	UNP O66529
J4	125	ALA	ILE	engineered mutation	UNP O66529
J4	155	LEU	-	expression tag	UNP O66529
J4	156	GLU	-	expression tag	UNP O66529
J4	157	GLY	-	expression tag	UNP O66529
J4	158	GLY	-	expression tag	UNP O66529
J4	159	TRP	-	expression tag	UNP O66529
J4	160	SER	-	expression tag	UNP O66529
J4	161	HIS	-	expression tag	UNP O66529
J4	162	PRO	-	expression tag	UNP O66529
J4	163	GLN	-	expression tag	UNP O66529
J4	164	PHE	-	expression tag	UNP O66529
J4	165	GLU	-	expression tag	UNP O66529
J4	166	LYS	-	expression tag	UNP O66529
J5	2	GLU	GLN	conflict	UNP O66529
J5	125	ALA	ILE	engineered mutation	UNP O66529
J5	155	LEU	-	expression tag	UNP O66529
J5	156	GLU	-	expression tag	UNP O66529
J5	157	GLY	-	expression tag	UNP O66529
J5	158	GLY	-	expression tag	UNP O66529
J5	159	TRP	-	expression tag	UNP O66529
J5	160	SER	-	expression tag	UNP O66529
J5	161	HIS	-	expression tag	UNP O66529
J5	162	PRO	-	expression tag	UNP O66529
J5	163	GLN	-	expression tag	UNP O66529
J5	164	PHE	-	expression tag	UNP O66529
J5	165	GLU	-	expression tag	UNP O66529
J5	166	LYS	-	expression tag	UNP O66529
K1	2	GLU	GLN	conflict	UNP O66529
K1	125	ALA	ILE	engineered mutation	UNP O66529
K1	155	LEU	-	expression tag	UNP O66529
K1	156	GLU	-	expression tag	UNP O66529
K1	157	GLY	-	expression tag	UNP O66529
K1	158	GLY	-	expression tag	UNP O66529
K1	159	TRP	-	expression tag	UNP O66529
K1	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
K1	161	HIS	-	expression tag	UNP O66529
K1	162	PRO	-	expression tag	UNP O66529
K1	163	GLN	-	expression tag	UNP O66529
K1	164	PHE	-	expression tag	UNP O66529
K1	165	GLU	-	expression tag	UNP O66529
K1	166	LYS	-	expression tag	UNP O66529
K2	2	GLU	GLN	conflict	UNP O66529
K2	125	ALA	ILE	engineered mutation	UNP O66529
K2	155	LEU	-	expression tag	UNP O66529
K2	156	GLU	-	expression tag	UNP O66529
K2	157	GLY	-	expression tag	UNP O66529
K2	158	GLY	-	expression tag	UNP O66529
K2	159	TRP	-	expression tag	UNP O66529
K2	160	SER	-	expression tag	UNP O66529
K2	161	HIS	-	expression tag	UNP O66529
K2	162	PRO	-	expression tag	UNP O66529
K2	163	GLN	-	expression tag	UNP O66529
K2	164	PHE	-	expression tag	UNP O66529
K2	165	GLU	-	expression tag	UNP O66529
K2	166	LYS	-	expression tag	UNP O66529
K3	2	GLU	GLN	conflict	UNP O66529
K3	125	ALA	ILE	engineered mutation	UNP O66529
K3	155	LEU	-	expression tag	UNP O66529
K3	156	GLU	-	expression tag	UNP O66529
K3	157	GLY	-	expression tag	UNP O66529
K3	158	GLY	-	expression tag	UNP O66529
K3	159	TRP	-	expression tag	UNP O66529
K3	160	SER	-	expression tag	UNP O66529
K3	161	HIS	-	expression tag	UNP O66529
K3	162	PRO	-	expression tag	UNP O66529
K3	163	GLN	-	expression tag	UNP O66529
K3	164	PHE	-	expression tag	UNP O66529
K3	165	GLU	-	expression tag	UNP O66529
K3	166	LYS	-	expression tag	UNP O66529
K4	2	GLU	GLN	conflict	UNP O66529
K4	125	ALA	ILE	engineered mutation	UNP O66529
K4	155	LEU	-	expression tag	UNP O66529
K4	156	GLU	-	expression tag	UNP O66529
K4	157	GLY	-	expression tag	UNP O66529
K4	158	GLY	-	expression tag	UNP O66529
K4	159	TRP	-	expression tag	UNP O66529
K4	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
K4	161	HIS	-	expression tag	UNP O66529
K4	162	PRO	-	expression tag	UNP O66529
K4	163	GLN	-	expression tag	UNP O66529
K4	164	PHE	-	expression tag	UNP O66529
K4	165	GLU	-	expression tag	UNP O66529
K4	166	LYS	-	expression tag	UNP O66529
K5	2	GLU	GLN	conflict	UNP O66529
K5	125	ALA	ILE	engineered mutation	UNP O66529
K5	155	LEU	-	expression tag	UNP O66529
K5	156	GLU	-	expression tag	UNP O66529
K5	157	GLY	-	expression tag	UNP O66529
K5	158	GLY	-	expression tag	UNP O66529
K5	159	TRP	-	expression tag	UNP O66529
K5	160	SER	-	expression tag	UNP O66529
K5	161	HIS	-	expression tag	UNP O66529
K5	162	PRO	-	expression tag	UNP O66529
K5	163	GLN	-	expression tag	UNP O66529
K5	164	PHE	-	expression tag	UNP O66529
K5	165	GLU	-	expression tag	UNP O66529
K5	166	LYS	-	expression tag	UNP O66529
L1	2	GLU	GLN	conflict	UNP O66529
L1	125	ALA	ILE	engineered mutation	UNP O66529
L1	155	LEU	-	expression tag	UNP O66529
L1	156	GLU	-	expression tag	UNP O66529
L1	157	GLY	-	expression tag	UNP O66529
L1	158	GLY	-	expression tag	UNP O66529
L1	159	TRP	-	expression tag	UNP O66529
L1	160	SER	-	expression tag	UNP O66529
L1	161	HIS	-	expression tag	UNP O66529
L1	162	PRO	-	expression tag	UNP O66529
L1	163	GLN	-	expression tag	UNP O66529
L1	164	PHE	-	expression tag	UNP O66529
L1	165	GLU	-	expression tag	UNP O66529
L1	166	LYS	-	expression tag	UNP O66529
L2	2	GLU	GLN	conflict	UNP O66529
L2	125	ALA	ILE	engineered mutation	UNP O66529
L2	155	LEU	-	expression tag	UNP O66529
L2	156	GLU	-	expression tag	UNP O66529
L2	157	GLY	-	expression tag	UNP O66529
L2	158	GLY	-	expression tag	UNP O66529
L2	159	TRP	-	expression tag	UNP O66529
L2	160	SER	-	expression tag	UNP O66529

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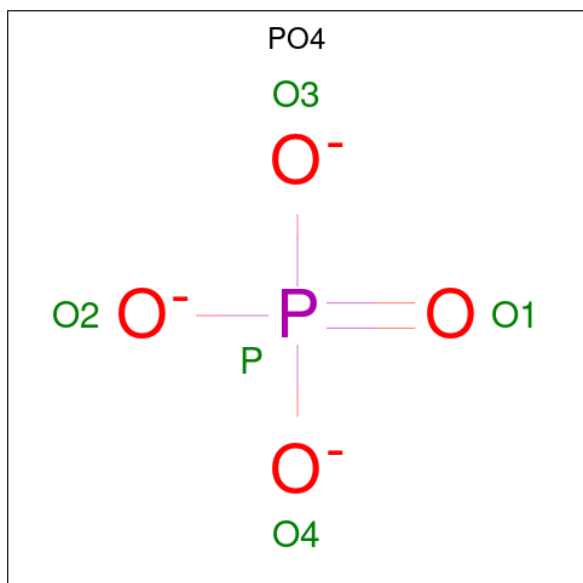
Chain	Residue	Modelled	Actual	Comment	Reference
L2	161	HIS	-	expression tag	UNP O66529
L2	162	PRO	-	expression tag	UNP O66529
L2	163	GLN	-	expression tag	UNP O66529
L2	164	PHE	-	expression tag	UNP O66529
L2	165	GLU	-	expression tag	UNP O66529
L2	166	LYS	-	expression tag	UNP O66529
L3	2	GLU	GLN	conflict	UNP O66529
L3	125	ALA	ILE	engineered mutation	UNP O66529
L3	155	LEU	-	expression tag	UNP O66529
L3	156	GLU	-	expression tag	UNP O66529
L3	157	GLY	-	expression tag	UNP O66529
L3	158	GLY	-	expression tag	UNP O66529
L3	159	TRP	-	expression tag	UNP O66529
L3	160	SER	-	expression tag	UNP O66529
L3	161	HIS	-	expression tag	UNP O66529
L3	162	PRO	-	expression tag	UNP O66529
L3	163	GLN	-	expression tag	UNP O66529
L3	164	PHE	-	expression tag	UNP O66529
L3	165	GLU	-	expression tag	UNP O66529
L3	166	LYS	-	expression tag	UNP O66529
L4	2	GLU	GLN	conflict	UNP O66529
L4	125	ALA	ILE	engineered mutation	UNP O66529
L4	155	LEU	-	expression tag	UNP O66529
L4	156	GLU	-	expression tag	UNP O66529
L4	157	GLY	-	expression tag	UNP O66529
L4	158	GLY	-	expression tag	UNP O66529
L4	159	TRP	-	expression tag	UNP O66529
L4	160	SER	-	expression tag	UNP O66529
L4	161	HIS	-	expression tag	UNP O66529
L4	162	PRO	-	expression tag	UNP O66529
L4	163	GLN	-	expression tag	UNP O66529
L4	164	PHE	-	expression tag	UNP O66529
L4	165	GLU	-	expression tag	UNP O66529
L4	166	LYS	-	expression tag	UNP O66529
L5	2	GLU	GLN	conflict	UNP O66529
L5	125	ALA	ILE	engineered mutation	UNP O66529
L5	155	LEU	-	expression tag	UNP O66529
L5	156	GLU	-	expression tag	UNP O66529
L5	157	GLY	-	expression tag	UNP O66529
L5	158	GLY	-	expression tag	UNP O66529
L5	159	TRP	-	expression tag	UNP O66529
L5	160	SER	-	expression tag	UNP O66529

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Chain	Residue	Modelled	Actual	Comment	Reference
L5	161	HIS	-	expression tag	UNP O66529
L5	162	PRO	-	expression tag	UNP O66529
L5	163	GLN	-	expression tag	UNP O66529
L5	164	PHE	-	expression tag	UNP O66529
L5	165	GLU	-	expression tag	UNP O66529
L5	166	LYS	-	expression tag	UNP O66529

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A1	1	Total	O	P	0
			5	4	1	
2	A2	1	Total	O	P	0
			5	4	1	
2	A3	1	Total	O	P	0
			5	4	1	
2	A4	1	Total	O	P	0
			5	4	1	
2	A5	1	Total	O	P	0
			5	4	1	
2	B1	1	Total	O	P	0
			5	4	1	
2	B2	1	Total	O	P	0
			5	4	1	
2	B3	1	Total	O	P	0
			5	4	1	

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Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
2	B4	1	5	4	1	0
2	B5	1	5	4	1	0
2	C1	1	5	4	1	0
2	C2	1	5	4	1	0
2	C3	1	5	4	1	0
2	C4	1	5	4	1	0
2	C5	1	5	4	1	0
2	D1	1	5	4	1	0
2	D2	1	5	4	1	0
2	D3	1	5	4	1	0
2	D4	1	5	4	1	0
2	D5	1	5	4	1	0
2	E1	1	5	4	1	0
2	E2	1	5	4	1	0
2	E3	1	5	4	1	0
2	E4	1	5	4	1	0
2	E5	1	5	4	1	0
2	F1	1	5	4	1	0
2	F2	1	5	4	1	0
2	F3	1	5	4	1	0
2	F4	1	5	4	1	0

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Mol	Chain	Residues	Atoms			AltConf
2	F5	1	Total	O	P	0
			5	4	1	
2	G1	1	Total	O	P	0
			5	4	1	
2	G2	1	Total	O	P	0
			5	4	1	
2	G3	1	Total	O	P	0
			5	4	1	
2	G4	1	Total	O	P	0
			5	4	1	
2	G5	1	Total	O	P	0
			5	4	1	
2	H1	1	Total	O	P	0
			5	4	1	
2	H2	1	Total	O	P	0
			5	4	1	
2	H3	1	Total	O	P	0
			5	4	1	
2	H4	1	Total	O	P	0
			5	4	1	
2	H5	1	Total	O	P	0
			5	4	1	
2	I1	1	Total	O	P	0
			5	4	1	
2	I2	1	Total	O	P	0
			5	4	1	
2	I3	1	Total	O	P	0
			5	4	1	
2	I4	1	Total	O	P	0
			5	4	1	
2	I5	1	Total	O	P	0
			5	4	1	
2	J1	1	Total	O	P	0
			5	4	1	
2	J2	1	Total	O	P	0
			5	4	1	
2	J3	1	Total	O	P	0
			5	4	1	
2	J4	1	Total	O	P	0
			5	4	1	
2	J5	1	Total	O	P	0
			5	4	1	

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Mol	Chain	Residues	Atoms			AltConf
2	K1	1	Total	O	P	0
			5	4	1	
2	K2	1	Total	O	P	0
			5	4	1	
2	K3	1	Total	O	P	0
			5	4	1	
2	K4	1	Total	O	P	0
			5	4	1	
2	K5	1	Total	O	P	0
			5	4	1	
2	L1	1	Total	O	P	0
			5	4	1	
2	L2	1	Total	O	P	0
			5	4	1	
2	L3	1	Total	O	P	0
			5	4	1	
2	L4	1	Total	O	P	0
			5	4	1	
2	L5	1	Total	O	P	0
			5	4	1	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A1	36	Total	O	0
			36	36	
3	A2	35	Total	O	0
			35	35	
3	A3	36	Total	O	0
			36	36	
3	A4	32	Total	O	0
			32	32	
3	A5	35	Total	O	0
			35	35	
3	B1	34	Total	O	0
			34	34	
3	B2	36	Total	O	0
			36	36	
3	B3	34	Total	O	0
			34	34	
3	B4	36	Total	O	0
			36	36	

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Mol	Chain	Residues	Atoms		AltConf
3	B5	32	Total 32	O 32	0
3	C1	34	Total 34	O 34	0
3	C2	36	Total 36	O 36	0
3	C3	32	Total 32	O 32	0
3	C4	34	Total 34	O 34	0
3	C5	36	Total 36	O 36	0
3	D1	32	Total 32	O 32	0
3	D2	34	Total 34	O 34	0
3	D3	36	Total 36	O 36	0
3	D4	35	Total 35	O 35	0
3	D5	36	Total 36	O 36	0
3	E1	36	Total 36	O 36	0
3	E2	32	Total 32	O 32	0
3	E3	35	Total 35	O 35	0
3	E4	36	Total 36	O 36	0
3	E5	35	Total 35	O 35	0
3	F1	36	Total 36	O 36	0
3	F2	34	Total 34	O 34	0
3	F3	36	Total 36	O 36	0
3	F4	32	Total 32	O 32	0
3	F5	33	Total 33	O 33	0

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Mol	Chain	Residues	Atoms		AltConf
3	G1	35	Total 35	O 35	0
3	G2	33	Total 33	O 33	0
3	G3	34	Total 34	O 34	0
3	G4	36	Total 36	O 36	0
3	G5	35	Total 35	O 35	0
3	H1	33	Total 33	O 33	0
3	H2	34	Total 34	O 34	0
3	H3	36	Total 36	O 36	0
3	H4	34	Total 34	O 34	0
3	H5	35	Total 35	O 35	0
3	I1	36	Total 36	O 36	0
3	I2	35	Total 35	O 35	0
3	I3	36	Total 36	O 36	0
3	I4	32	Total 32	O 32	0
3	I5	34	Total 34	O 34	0
3	J1	34	Total 34	O 34	0
3	J2	36	Total 36	O 36	0
3	J3	32	Total 32	O 32	0
3	J4	33	Total 33	O 33	0
3	J5	36	Total 36	O 36	0
3	K1	34	Total 34	O 34	0

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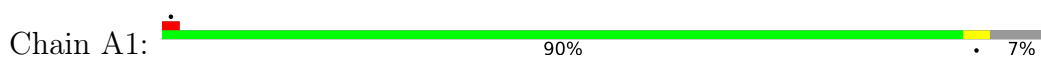
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Mol	Chain	Residues	Atoms		AltConf
3	K2	36	Total 36	O 36	0
3	K3	35	Total 35	O 35	0
3	K4	36	Total 36	O 36	0
3	K5	32	Total 32	O 32	0
3	L1	34	Total 34	O 34	0
3	L2	35	Total 35	O 35	0
3	L3	33	Total 33	O 33	0
3	L4	34	Total 34	O 34	0
3	L5	36	Total 36	O 36	0

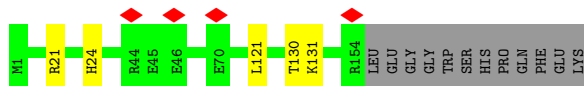
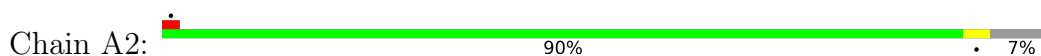
3 Residue-property plots [i](#)

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 atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

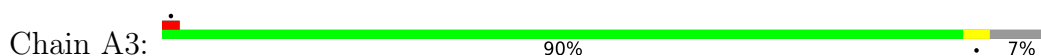
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



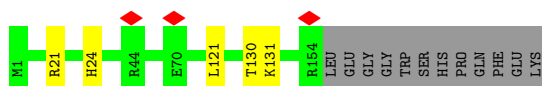
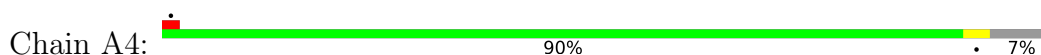
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



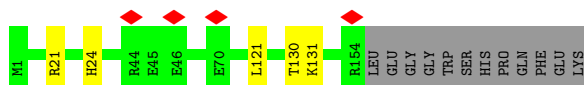
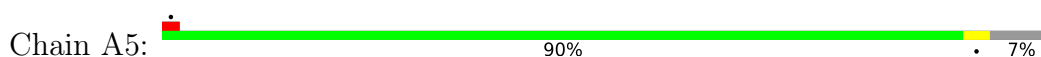
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B1:  89% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B2:  90% 7%



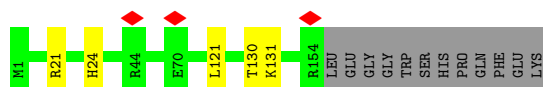
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B3:  90% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B4:  90% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B5:  90% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain C1:  90% 7%

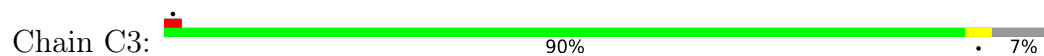


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

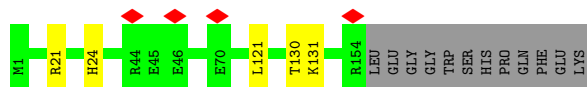
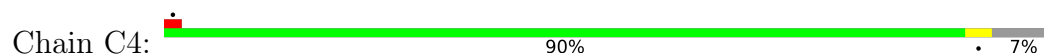
Chain C2:  90% 7%



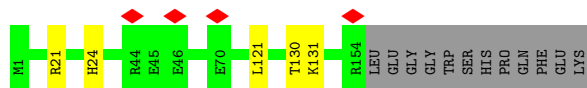
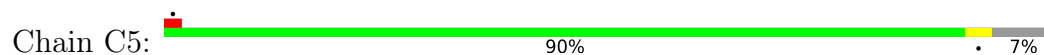
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



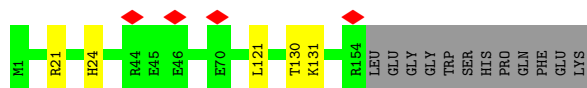
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



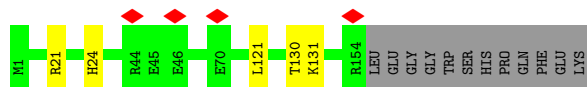
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



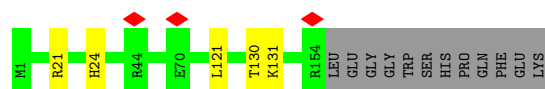
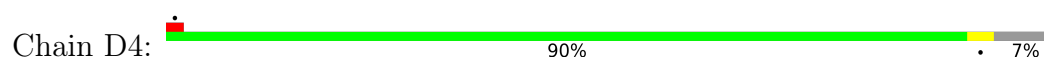
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



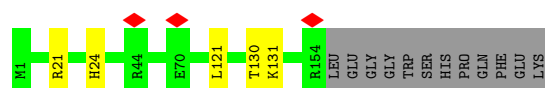
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



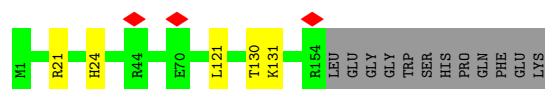
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



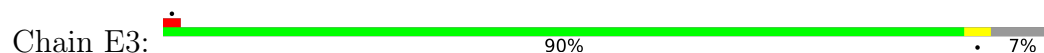
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



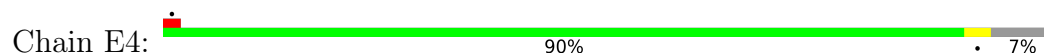
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



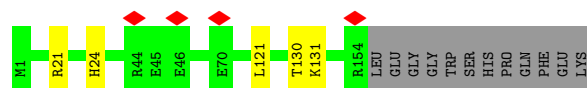
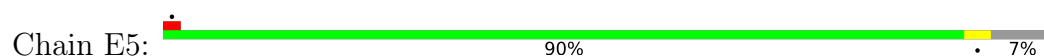
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



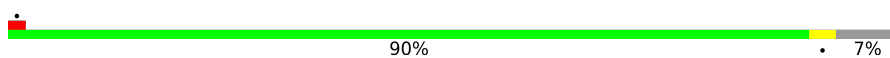
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

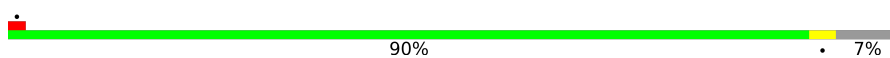


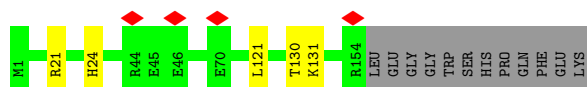
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F1:  90% 7%

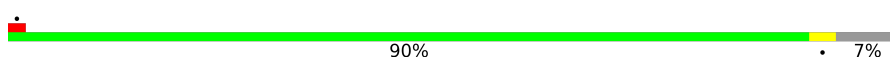


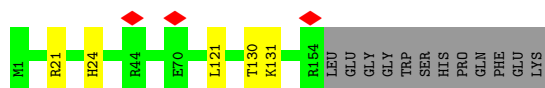
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F2:  90% 7%

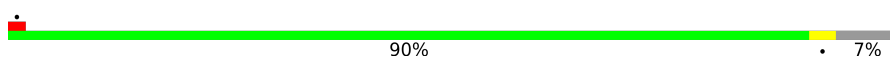


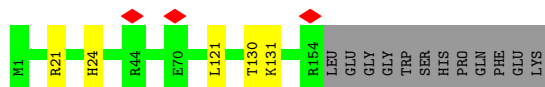
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F3:  90% 7%

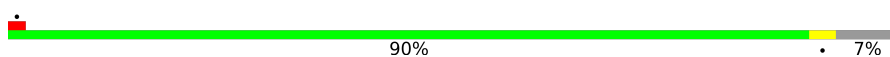


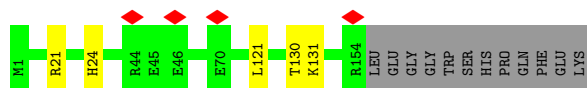
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F4:  90% 7%

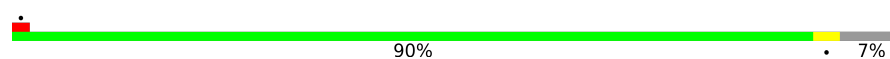


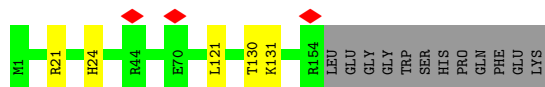
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain F5:  90% 7%

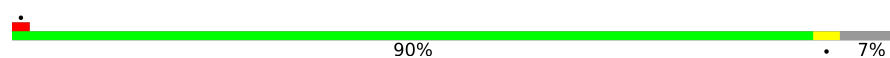


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain G1:  90% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain G2:  90% 7%



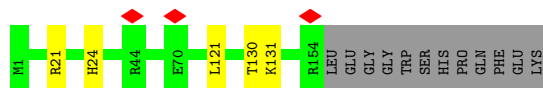
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



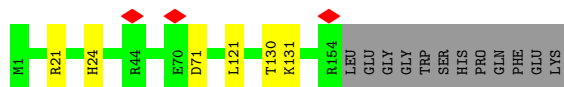
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



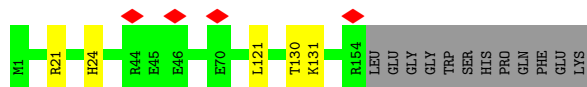
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



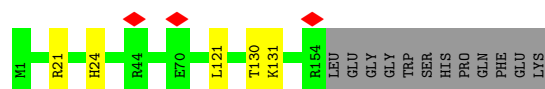
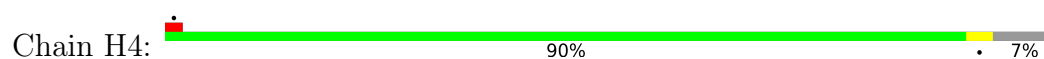
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



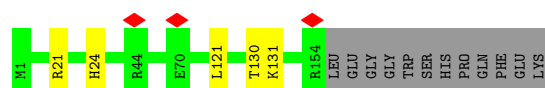
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



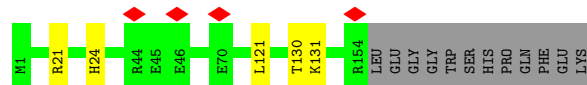
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



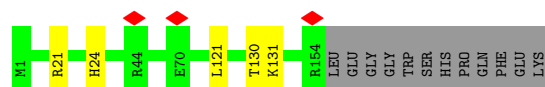
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



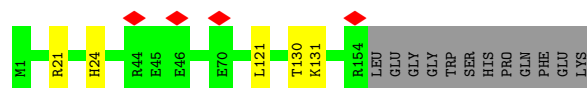
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J1:  89% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J2:  90% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J3:  90% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J4:  90% 7%

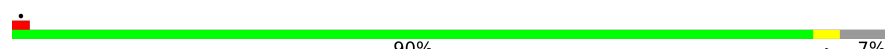


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain J5:  89% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain K1:  90% 7%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

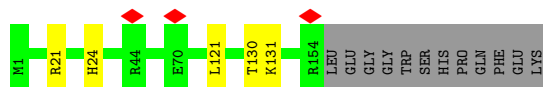
Chain K2:  90% 7%



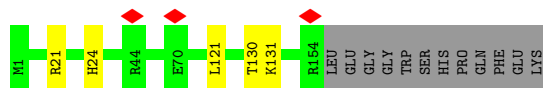
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



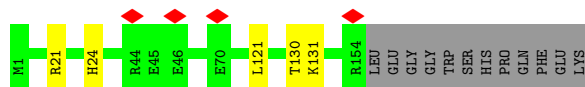
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



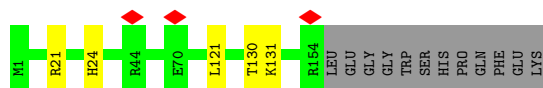
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



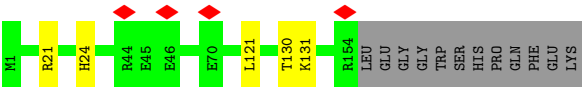
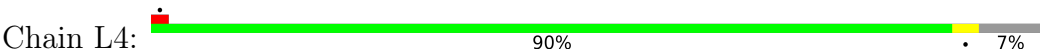
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



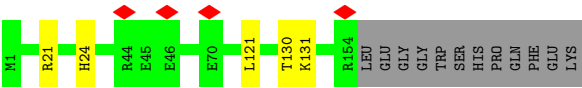
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



• Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1457813	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.061	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	314.5632, 314.5632, 314.5632	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8456, 0.8456, 0.8456	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	A1	0.18	0/1191	0.30	0/1609
1	A2	0.18	0/1191	0.30	0/1609
1	A3	0.18	0/1191	0.30	0/1609
1	A4	0.19	0/1191	0.30	0/1609
1	A5	0.18	0/1191	0.30	0/1609
1	B1	0.18	0/1191	0.30	0/1609
1	B2	0.18	0/1191	0.30	0/1609
1	B3	0.18	0/1191	0.30	0/1609
1	B4	0.19	0/1191	0.30	0/1609
1	B5	0.18	0/1191	0.30	0/1609
1	C1	0.18	0/1191	0.30	0/1609
1	C2	0.19	0/1191	0.30	0/1609
1	C3	0.19	0/1191	0.30	0/1609
1	C4	0.18	0/1191	0.30	0/1609
1	C5	0.19	0/1191	0.30	0/1609
1	D1	0.18	0/1191	0.30	0/1609
1	D2	0.18	0/1191	0.30	0/1609
1	D3	0.19	0/1191	0.30	0/1609
1	D4	0.18	0/1191	0.30	0/1609
1	D5	0.18	0/1191	0.30	0/1609
1	E1	0.18	0/1191	0.30	0/1609
1	E2	0.18	0/1191	0.30	0/1609
1	E3	0.18	0/1191	0.30	0/1609
1	E4	0.18	0/1191	0.30	0/1609
1	E5	0.18	0/1191	0.30	0/1609
1	F1	0.19	0/1191	0.30	0/1609
1	F2	0.18	0/1191	0.30	0/1609
1	F3	0.18	0/1191	0.30	0/1609
1	F4	0.18	0/1191	0.30	0/1609
1	F5	0.18	0/1191	0.30	0/1609
1	G1	0.19	0/1191	0.30	0/1609
1	G2	0.18	0/1191	0.30	0/1609

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G3	0.18	0/1191	0.30	0/1609
1	G4	0.18	0/1191	0.30	0/1609
1	G5	0.18	0/1191	0.30	0/1609
1	H1	0.18	0/1191	0.30	0/1609
1	H2	0.18	0/1191	0.30	0/1609
1	H3	0.18	0/1191	0.30	0/1609
1	H4	0.18	0/1191	0.30	0/1609
1	H5	0.18	0/1191	0.30	0/1609
1	I1	0.19	0/1191	0.30	0/1609
1	I2	0.18	0/1191	0.30	0/1609
1	I3	0.19	0/1191	0.30	0/1609
1	I4	0.18	0/1191	0.30	0/1609
1	I5	0.18	0/1191	0.30	0/1609
1	J1	0.18	0/1191	0.30	0/1609
1	J2	0.19	0/1191	0.30	0/1609
1	J3	0.18	0/1191	0.30	0/1609
1	J4	0.18	0/1191	0.30	0/1609
1	J5	0.18	0/1191	0.30	0/1609
1	K1	0.18	0/1191	0.30	0/1609
1	K2	0.19	0/1191	0.30	0/1609
1	K3	0.18	0/1191	0.30	0/1609
1	K4	0.18	0/1191	0.30	0/1609
1	K5	0.19	0/1191	0.30	0/1609
1	L1	0.18	0/1191	0.30	0/1609
1	L2	0.18	0/1191	0.30	0/1609
1	L3	0.18	0/1191	0.30	0/1609
1	L4	0.18	0/1191	0.30	0/1609
1	L5	0.18	0/1191	0.30	0/1609
All	All	0.18	0/71460	0.30	0/96540

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A1	1173	0	1195	4	0
1	A2	1173	0	1195	5	0
1	A3	1173	0	1195	4	0
1	A4	1173	0	1195	4	0
1	A5	1173	0	1195	5	0
1	B1	1173	0	1195	6	0
1	B2	1173	0	1195	4	0
1	B3	1173	0	1195	5	0
1	B4	1173	0	1195	5	0
1	B5	1173	0	1195	4	0
1	C1	1173	0	1195	5	0
1	C2	1173	0	1195	4	0
1	C3	1173	0	1195	4	0
1	C4	1173	0	1195	5	0
1	C5	1173	0	1195	4	0
1	D1	1173	0	1195	4	0
1	D2	1173	0	1195	5	0
1	D3	1173	0	1195	4	0
1	D4	1173	0	1195	5	0
1	D5	1173	0	1195	5	0
1	E1	1173	0	1195	4	0
1	E2	1173	0	1195	5	0
1	E3	1173	0	1195	5	0
1	E4	1173	0	1195	4	0
1	E5	1173	0	1195	4	0
1	F1	1173	0	1195	5	0
1	F2	1173	0	1195	4	0
1	F3	1173	0	1195	4	0
1	F4	1173	0	1195	5	0
1	F5	1173	0	1195	4	0
1	G1	1173	0	1195	4	0
1	G2	1173	0	1195	4	0
1	G3	1173	0	1195	4	0
1	G4	1173	0	1195	6	0
1	G5	1173	0	1195	4	0
1	H1	1173	0	1195	5	0
1	H2	1173	0	1195	5	0
1	H3	1173	0	1195	4	0
1	H4	1173	0	1195	4	0
1	H5	1173	0	1195	4	0
1	I1	1173	0	1195	5	0
1	I2	1173	0	1195	4	0
1	I3	1173	0	1195	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I4	1173	0	1195	5	0
1	I5	1173	0	1195	4	0
1	J1	1173	0	1195	5	0
1	J2	1173	0	1195	4	0
1	J3	1173	0	1195	4	0
1	J4	1173	0	1195	4	0
1	J5	1173	0	1195	6	0
1	K1	1173	0	1195	4	0
1	K2	1173	0	1195	4	0
1	K3	1173	0	1195	4	0
1	K4	1173	0	1195	5	0
1	K5	1173	0	1195	4	0
1	L1	1173	0	1195	4	0
1	L2	1173	0	1195	5	0
1	L3	1173	0	1195	4	0
1	L4	1173	0	1195	4	0
1	L5	1173	0	1195	4	0
2	A1	5	0	0	0	0
2	A2	5	0	0	0	0
2	A3	5	0	0	0	0
2	A4	5	0	0	0	0
2	A5	5	0	0	0	0
2	B1	5	0	0	0	0
2	B2	5	0	0	0	0
2	B3	5	0	0	0	0
2	B4	5	0	0	0	0
2	B5	5	0	0	0	0
2	C1	5	0	0	0	0
2	C2	5	0	0	0	0
2	C3	5	0	0	0	0
2	C4	5	0	0	0	0
2	C5	5	0	0	0	0
2	D1	5	0	0	0	0
2	D2	5	0	0	0	0
2	D3	5	0	0	0	0
2	D4	5	0	0	0	0
2	D5	5	0	0	0	0
2	E1	5	0	0	0	0
2	E2	5	0	0	0	0
2	E3	5	0	0	0	0
2	E4	5	0	0	0	0
2	E5	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F1	5	0	0	0	0
2	F2	5	0	0	0	0
2	F3	5	0	0	0	0
2	F4	5	0	0	0	0
2	F5	5	0	0	0	0
2	G1	5	0	0	0	0
2	G2	5	0	0	0	0
2	G3	5	0	0	0	0
2	G4	5	0	0	0	0
2	G5	5	0	0	0	0
2	H1	5	0	0	0	0
2	H2	5	0	0	0	0
2	H3	5	0	0	0	0
2	H4	5	0	0	0	0
2	H5	5	0	0	0	0
2	I1	5	0	0	0	0
2	I2	5	0	0	0	0
2	I3	5	0	0	0	0
2	I4	5	0	0	0	0
2	I5	5	0	0	0	0
2	J1	5	0	0	0	0
2	J2	5	0	0	0	0
2	J3	5	0	0	0	0
2	J4	5	0	0	0	0
2	J5	5	0	0	0	0
2	K1	5	0	0	0	0
2	K2	5	0	0	0	0
2	K3	5	0	0	0	0
2	K4	5	0	0	0	0
2	K5	5	0	0	0	0
2	L1	5	0	0	0	0
2	L2	5	0	0	0	0
2	L3	5	0	0	0	0
2	L4	5	0	0	0	0
2	L5	5	0	0	0	0
3	A1	36	0	0	0	0
3	A2	35	0	0	0	0
3	A3	36	0	0	0	0
3	A4	32	0	0	0	0
3	A5	35	0	0	0	0
3	B1	34	0	0	0	0
3	B2	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B3	34	0	0	0	0
3	B4	36	0	0	0	0
3	B5	32	0	0	0	0
3	C1	34	0	0	0	0
3	C2	36	0	0	0	0
3	C3	32	0	0	0	0
3	C4	34	0	0	0	0
3	C5	36	0	0	0	0
3	D1	32	0	0	0	0
3	D2	34	0	0	0	0
3	D3	36	0	0	0	0
3	D4	35	0	0	0	0
3	D5	36	0	0	0	0
3	E1	36	0	0	0	0
3	E2	32	0	0	0	0
3	E3	35	0	0	0	0
3	E4	36	0	0	0	0
3	E5	35	0	0	0	0
3	F1	36	0	0	0	0
3	F2	34	0	0	0	0
3	F3	36	0	0	0	0
3	F4	32	0	0	0	0
3	F5	33	0	0	0	0
3	G1	35	0	0	0	0
3	G2	33	0	0	0	0
3	G3	34	0	0	0	0
3	G4	36	0	0	0	0
3	G5	35	0	0	0	0
3	H1	33	0	0	0	0
3	H2	34	0	0	0	0
3	H3	36	0	0	0	0
3	H4	34	0	0	0	0
3	H5	35	0	0	0	0
3	I1	36	0	0	0	0
3	I2	35	0	0	0	0
3	I3	36	0	0	0	0
3	I4	32	0	0	0	0
3	I5	34	0	0	0	0
3	J1	34	0	0	0	0
3	J2	36	0	0	0	0
3	J3	32	0	0	0	0
3	J4	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J5	36	0	0	0	0
3	K1	34	0	0	0	0
3	K2	36	0	0	0	0
3	K3	35	0	0	0	0
3	K4	36	0	0	0	0
3	K5	32	0	0	0	0
3	L1	34	0	0	0	0
3	L2	35	0	0	0	0
3	L3	33	0	0	0	0
3	L4	34	0	0	0	0
3	L5	36	0	0	0	0
All	All	72750	0	71700	206	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 206 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:H3:130:THR:HG22	1:H3:131:LYS:H	1.63	0.64
1:I5:130:THR:HG22	1:I5:131:LYS:H	1.63	0.64
1:K5:130:THR:HG22	1:K5:131:LYS:H	1.63	0.64
1:E4:130:THR:HG22	1:E4:131:LYS:H	1.64	0.63
1:F5:130:THR:HG22	1:F5:131:LYS:H	1.63	0.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A1	152/166 (92%)	149 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	A3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	A4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	A5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	B1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	B2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	B3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	B4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	B5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	C1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	C2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	C3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	C4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	C5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	D1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	D2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	D3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	D4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	D5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	E1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	E2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	E3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	E4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	E5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	F1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	F2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	F3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	F4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	F5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	G1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	G2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	G4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	G5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	H1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	H2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	H3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	H4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	H5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	I1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	I2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	I3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	I4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	I5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	J1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	J2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	J3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	J4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	J5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	K1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	K2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	K3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	K4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	K5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	L1	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	L2	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	L3	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	L4	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
1	L5	152/166 (92%)	149 (98%)	3 (2%)	0	100	100
All	All	9120/9960 (92%)	8940 (98%)	180 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	119/129 (92%)	119 (100%)	0	100	100
1	A2	119/129 (92%)	119 (100%)	0	100	100
1	A3	119/129 (92%)	119 (100%)	0	100	100
1	A4	119/129 (92%)	119 (100%)	0	100	100
1	A5	119/129 (92%)	119 (100%)	0	100	100
1	B1	119/129 (92%)	119 (100%)	0	100	100
1	B2	119/129 (92%)	119 (100%)	0	100	100
1	B3	119/129 (92%)	119 (100%)	0	100	100
1	B4	119/129 (92%)	119 (100%)	0	100	100
1	B5	119/129 (92%)	119 (100%)	0	100	100
1	C1	119/129 (92%)	119 (100%)	0	100	100
1	C2	119/129 (92%)	119 (100%)	0	100	100
1	C3	119/129 (92%)	119 (100%)	0	100	100
1	C4	119/129 (92%)	119 (100%)	0	100	100
1	C5	119/129 (92%)	119 (100%)	0	100	100
1	D1	119/129 (92%)	119 (100%)	0	100	100
1	D2	119/129 (92%)	119 (100%)	0	100	100
1	D3	119/129 (92%)	119 (100%)	0	100	100
1	D4	119/129 (92%)	119 (100%)	0	100	100
1	D5	119/129 (92%)	119 (100%)	0	100	100
1	E1	119/129 (92%)	119 (100%)	0	100	100
1	E2	119/129 (92%)	119 (100%)	0	100	100
1	E3	119/129 (92%)	119 (100%)	0	100	100
1	E4	119/129 (92%)	119 (100%)	0	100	100
1	E5	119/129 (92%)	119 (100%)	0	100	100
1	F1	119/129 (92%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F2	119/129 (92%)	119 (100%)	0	100	100
1	F3	119/129 (92%)	119 (100%)	0	100	100
1	F4	119/129 (92%)	119 (100%)	0	100	100
1	F5	119/129 (92%)	119 (100%)	0	100	100
1	G1	119/129 (92%)	119 (100%)	0	100	100
1	G2	119/129 (92%)	119 (100%)	0	100	100
1	G3	119/129 (92%)	119 (100%)	0	100	100
1	G4	119/129 (92%)	119 (100%)	0	100	100
1	G5	119/129 (92%)	119 (100%)	0	100	100
1	H1	119/129 (92%)	119 (100%)	0	100	100
1	H2	119/129 (92%)	119 (100%)	0	100	100
1	H3	119/129 (92%)	119 (100%)	0	100	100
1	H4	119/129 (92%)	119 (100%)	0	100	100
1	H5	119/129 (92%)	119 (100%)	0	100	100
1	I1	119/129 (92%)	119 (100%)	0	100	100
1	I2	119/129 (92%)	119 (100%)	0	100	100
1	I3	119/129 (92%)	119 (100%)	0	100	100
1	I4	119/129 (92%)	119 (100%)	0	100	100
1	I5	119/129 (92%)	119 (100%)	0	100	100
1	J1	119/129 (92%)	119 (100%)	0	100	100
1	J2	119/129 (92%)	119 (100%)	0	100	100
1	J3	119/129 (92%)	119 (100%)	0	100	100
1	J4	119/129 (92%)	119 (100%)	0	100	100
1	J5	119/129 (92%)	119 (100%)	0	100	100
1	K1	119/129 (92%)	119 (100%)	0	100	100
1	K2	119/129 (92%)	119 (100%)	0	100	100
1	K3	119/129 (92%)	119 (100%)	0	100	100
1	K4	119/129 (92%)	119 (100%)	0	100	100
1	K5	119/129 (92%)	119 (100%)	0	100	100
1	L1	119/129 (92%)	119 (100%)	0	100	100
1	L2	119/129 (92%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L3	119/129 (92%)	119 (100%)	0	100	100
1	L4	119/129 (92%)	119 (100%)	0	100	100
1	L5	119/129 (92%)	119 (100%)	0	100	100
All	All	7140/7740 (92%)	7140 (100%)	0	100	100

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

60 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	PO4	B5	201	-	4,4,4	1.06	0	6,6,6	0.46	0
2	PO4	F3	201	-	4,4,4	1.09	0	6,6,6	0.40	0
2	PO4	D3	201	-	4,4,4	1.07	0	6,6,6	0.42	0
2	PO4	H2	201	-	4,4,4	1.07	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	L3	201	-	4,4,4	1.06	0	6,6,6	0.45	0
2	PO4	A3	201	-	4,4,4	1.08	0	6,6,6	0.40	0
2	PO4	A4	201	-	4,4,4	1.06	0	6,6,6	0.46	0
2	PO4	L1	201	-	4,4,4	1.08	0	6,6,6	0.41	0
2	PO4	G1	201	-	4,4,4	1.07	0	6,6,6	0.39	0
2	PO4	D4	201	-	4,4,4	1.07	0	6,6,6	0.40	0
2	PO4	E3	201	-	4,4,4	1.07	0	6,6,6	0.44	0
2	PO4	A2	201	-	4,4,4	1.07	0	6,6,6	0.41	0
2	PO4	E4	201	-	4,4,4	1.06	0	6,6,6	0.41	0
2	PO4	H4	201	-	4,4,4	1.08	0	6,6,6	0.41	0
2	PO4	C4	201	-	4,4,4	1.08	0	6,6,6	0.45	0
2	PO4	G2	201	-	4,4,4	1.06	0	6,6,6	0.45	0
2	PO4	C2	201	-	4,4,4	1.08	0	6,6,6	0.39	0
2	PO4	H3	201	-	4,4,4	1.06	0	6,6,6	0.42	0
2	PO4	E5	201	-	4,4,4	1.07	0	6,6,6	0.41	0
2	PO4	I3	201	-	4,4,4	1.08	0	6,6,6	0.40	0
2	PO4	B2	201	-	4,4,4	1.05	0	6,6,6	0.42	0
2	PO4	E2	201	-	4,4,4	1.07	0	6,6,6	0.46	0
2	PO4	J4	201	-	4,4,4	1.08	0	6,6,6	0.44	0
2	PO4	K1	201	-	4,4,4	1.07	0	6,6,6	0.44	0
2	PO4	K5	201	-	4,4,4	1.06	0	6,6,6	0.45	0
2	PO4	L4	201	-	4,4,4	1.07	0	6,6,6	0.44	0
2	PO4	I1	201	-	4,4,4	1.07	0	6,6,6	0.42	0
2	PO4	C3	201	-	4,4,4	1.06	0	6,6,6	0.45	0
2	PO4	J1	201	-	4,4,4	1.08	0	6,6,6	0.41	0
2	PO4	F2	201	-	4,4,4	1.08	0	6,6,6	0.41	0
2	PO4	L2	201	-	4,4,4	1.09	0	6,6,6	0.40	0
2	PO4	I5	201	-	4,4,4	1.07	0	6,6,6	0.45	0
2	PO4	G3	201	-	4,4,4	1.07	0	6,6,6	0.45	0
2	PO4	C1	201	-	4,4,4	1.08	0	6,6,6	0.41	0
2	PO4	B1	201	-	4,4,4	1.07	0	6,6,6	0.45	0
2	PO4	A5	201	-	4,4,4	1.07	0	6,6,6	0.45	0
2	PO4	K2	201	-	4,4,4	1.06	0	6,6,6	0.41	0
2	PO4	K3	201	-	4,4,4	1.08	0	6,6,6	0.41	0
2	PO4	L5	201	-	4,4,4	1.05	0	6,6,6	0.41	0
2	PO4	I2	201	-	4,4,4	1.08	0	6,6,6	0.41	0
2	PO4	F4	201	-	4,4,4	1.06	0	6,6,6	0.45	0
2	PO4	H5	201	-	4,4,4	1.08	0	6,6,6	0.40	0
2	PO4	D2	201	-	4,4,4	1.06	0	6,6,6	0.44	0
2	PO4	I4	201	-	4,4,4	1.07	0	6,6,6	0.45	0
2	PO4	A1	201	-	4,4,4	1.05	0	6,6,6	0.41	0
2	PO4	C5	201	-	4,4,4	1.06	0	6,6,6	0.42	0
2	PO4	G4	201	-	4,4,4	1.08	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	E1	201	-	4,4,4	1.08	0	6,6,6	0.40	0
2	PO4	J5	201	-	4,4,4	1.07	0	6,6,6	0.42	0
2	PO4	D1	201	-	4,4,4	1.07	0	6,6,6	0.46	0
2	PO4	D5	201	-	4,4,4	1.08	0	6,6,6	0.39	0
2	PO4	G5	201	-	4,4,4	1.07	0	6,6,6	0.41	0
2	PO4	B3	201	-	4,4,4	1.06	0	6,6,6	0.41	0
2	PO4	F1	201	-	4,4,4	1.07	0	6,6,6	0.41	0
2	PO4	F5	201	-	4,4,4	1.08	0	6,6,6	0.44	0
2	PO4	H1	201	-	4,4,4	1.06	0	6,6,6	0.45	0
2	PO4	K4	201	-	4,4,4	1.08	0	6,6,6	0.40	0
2	PO4	J2	201	-	4,4,4	1.08	0	6,6,6	0.40	0
2	PO4	B4	201	-	4,4,4	1.08	0	6,6,6	0.39	0
2	PO4	J3	201	-	4,4,4	1.06	0	6,6,6	0.45	0

There are no bond length outliers.

There are no bond angle outliers.

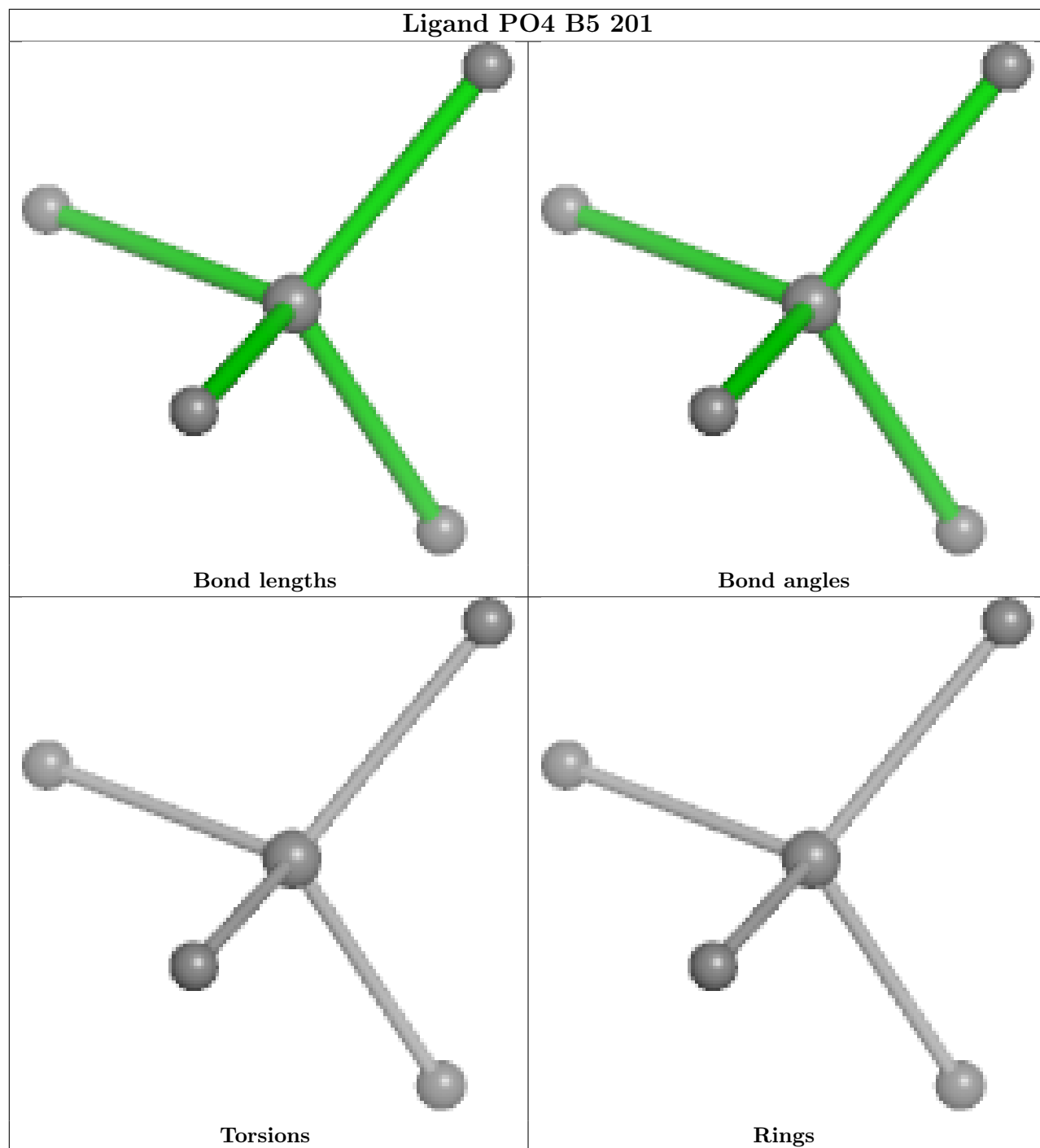
There are no chirality outliers.

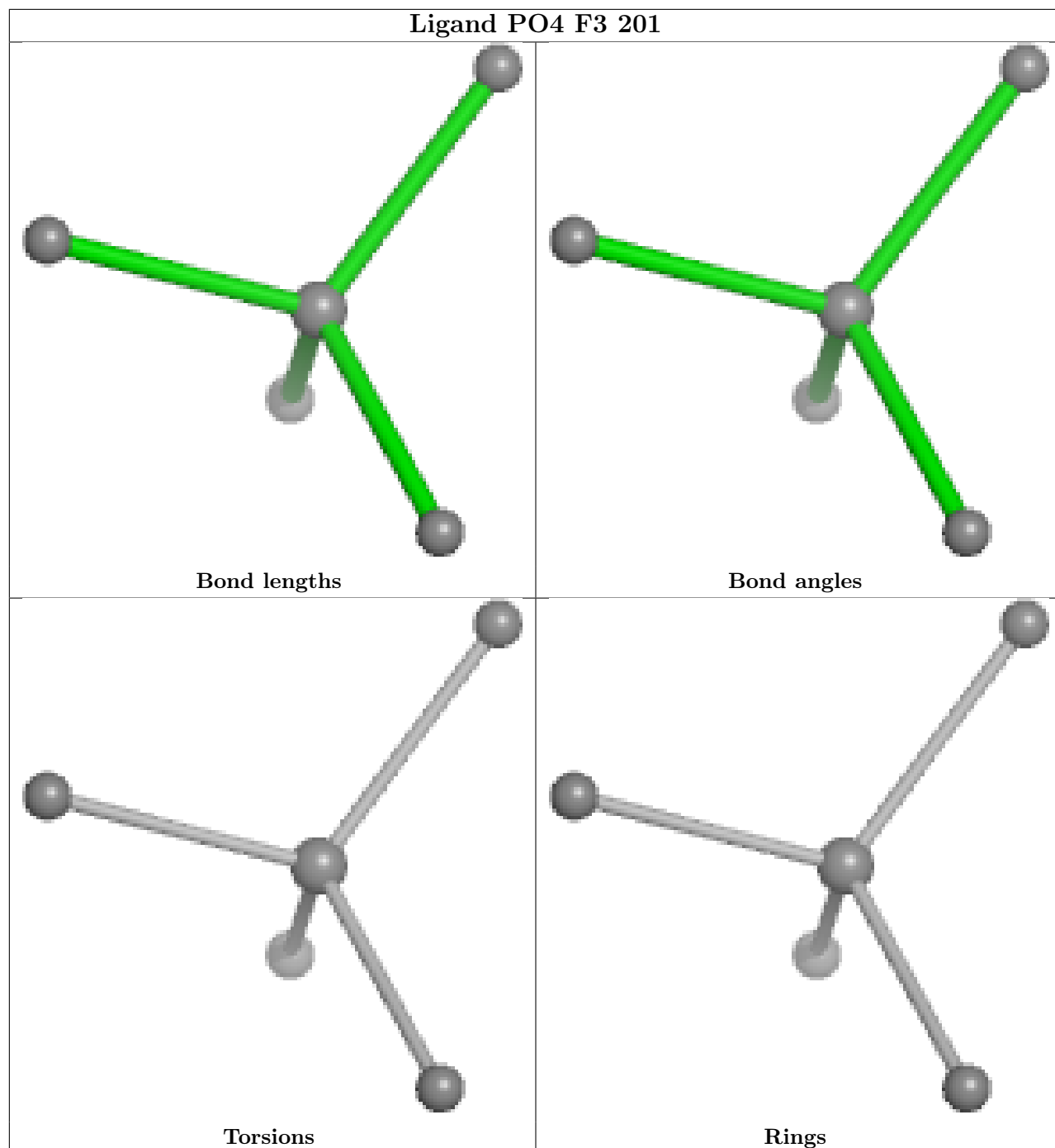
There are no torsion outliers.

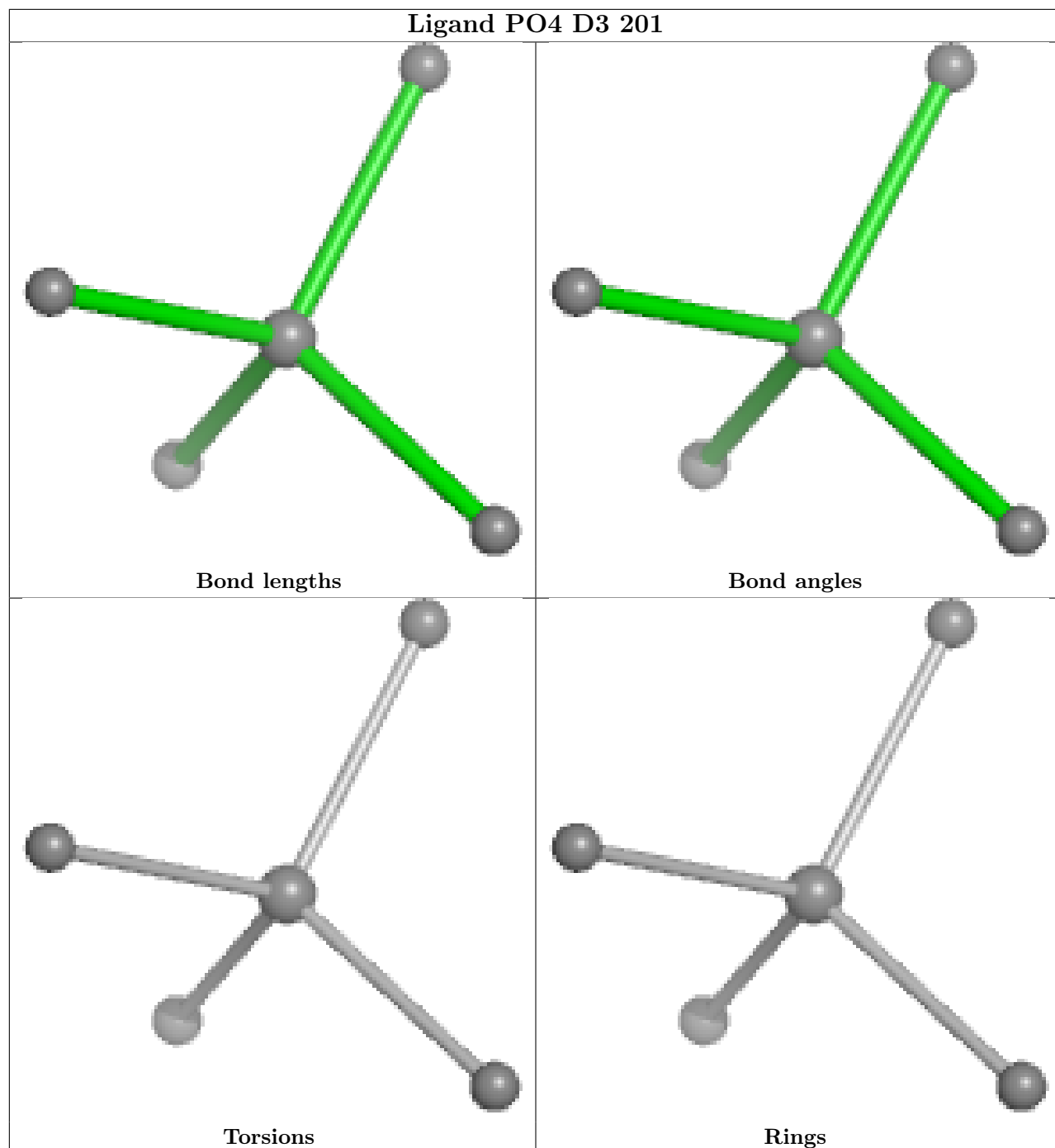
There are no ring outliers.

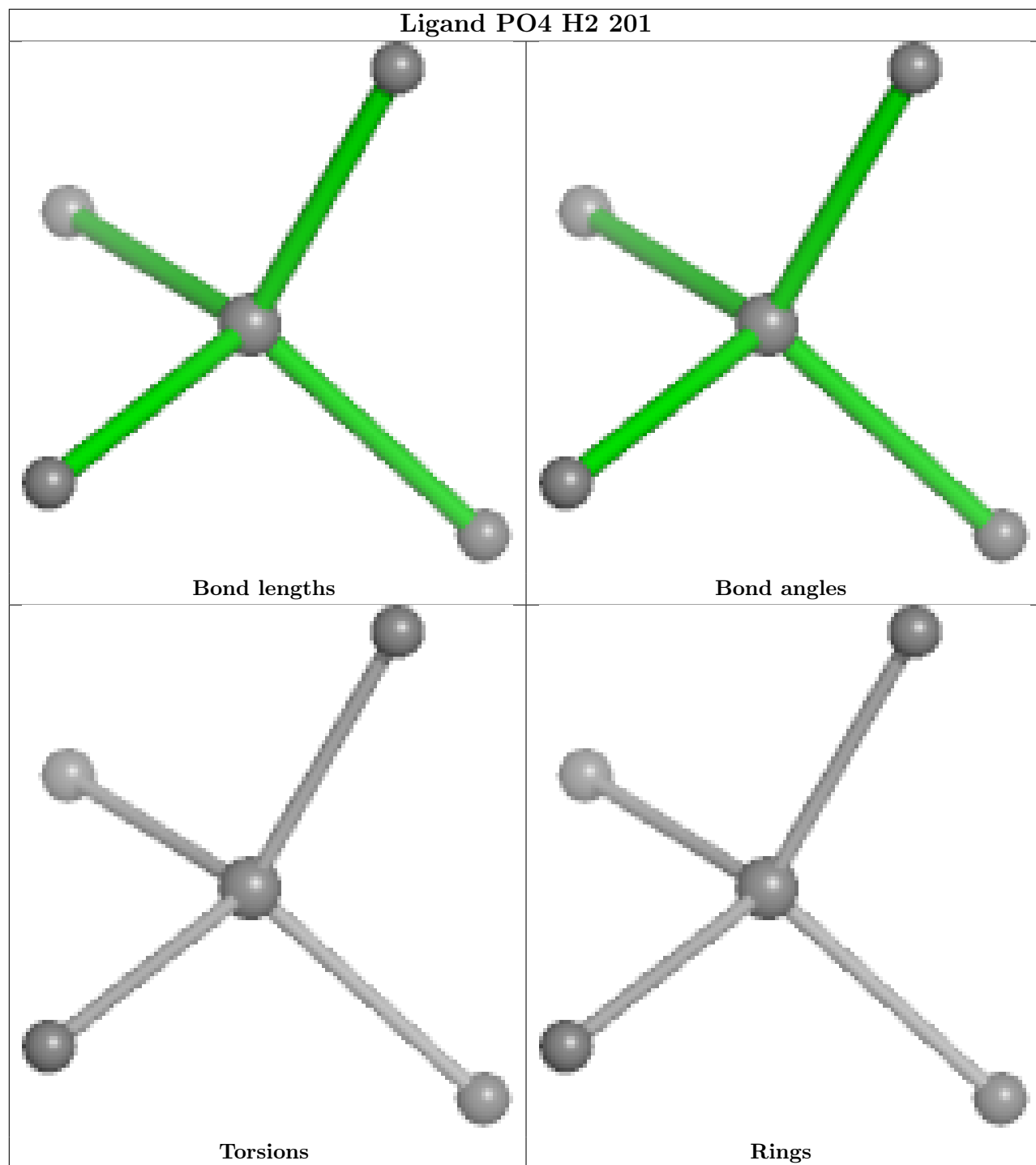
No monomer is involved in short contacts.

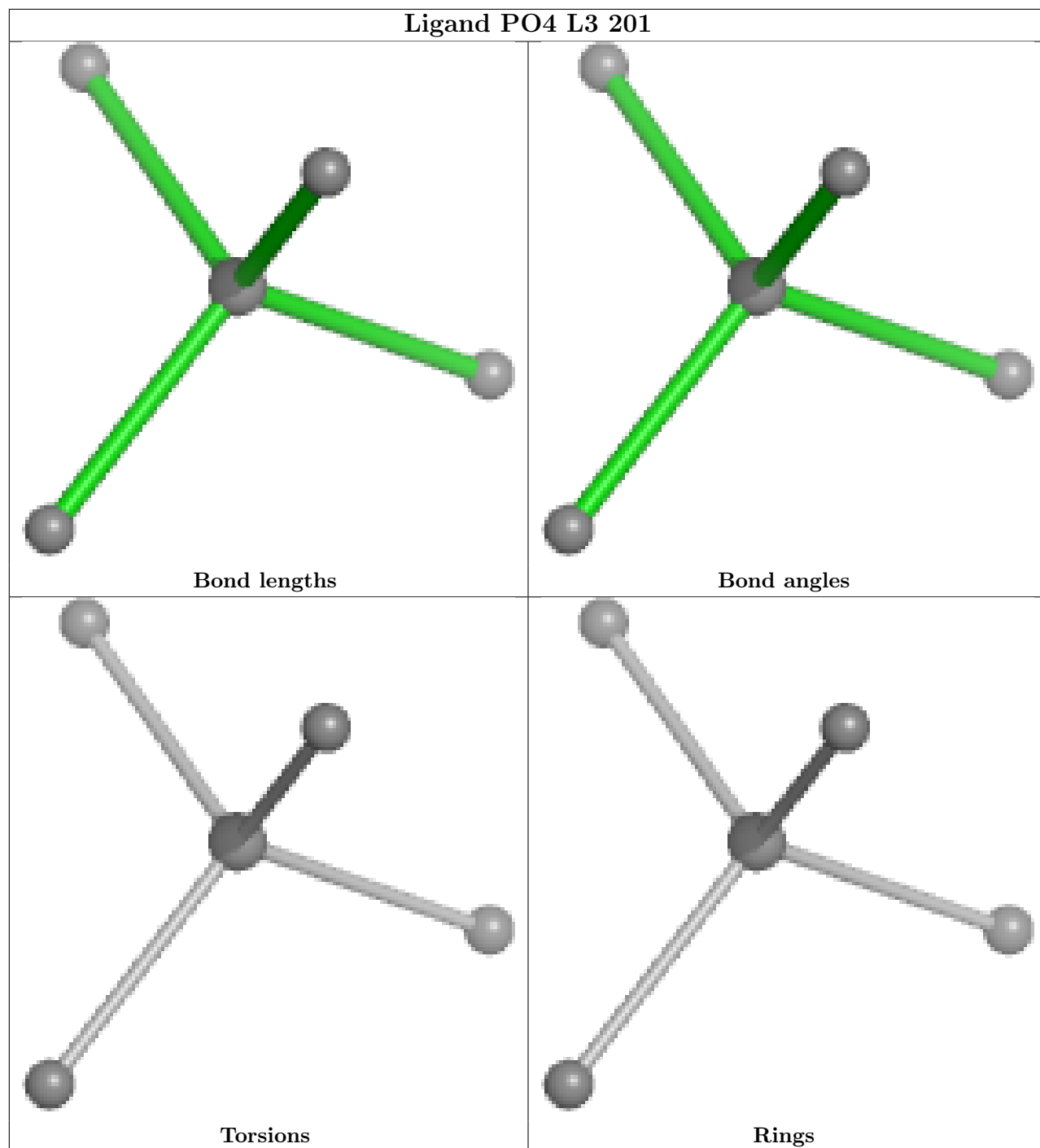
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

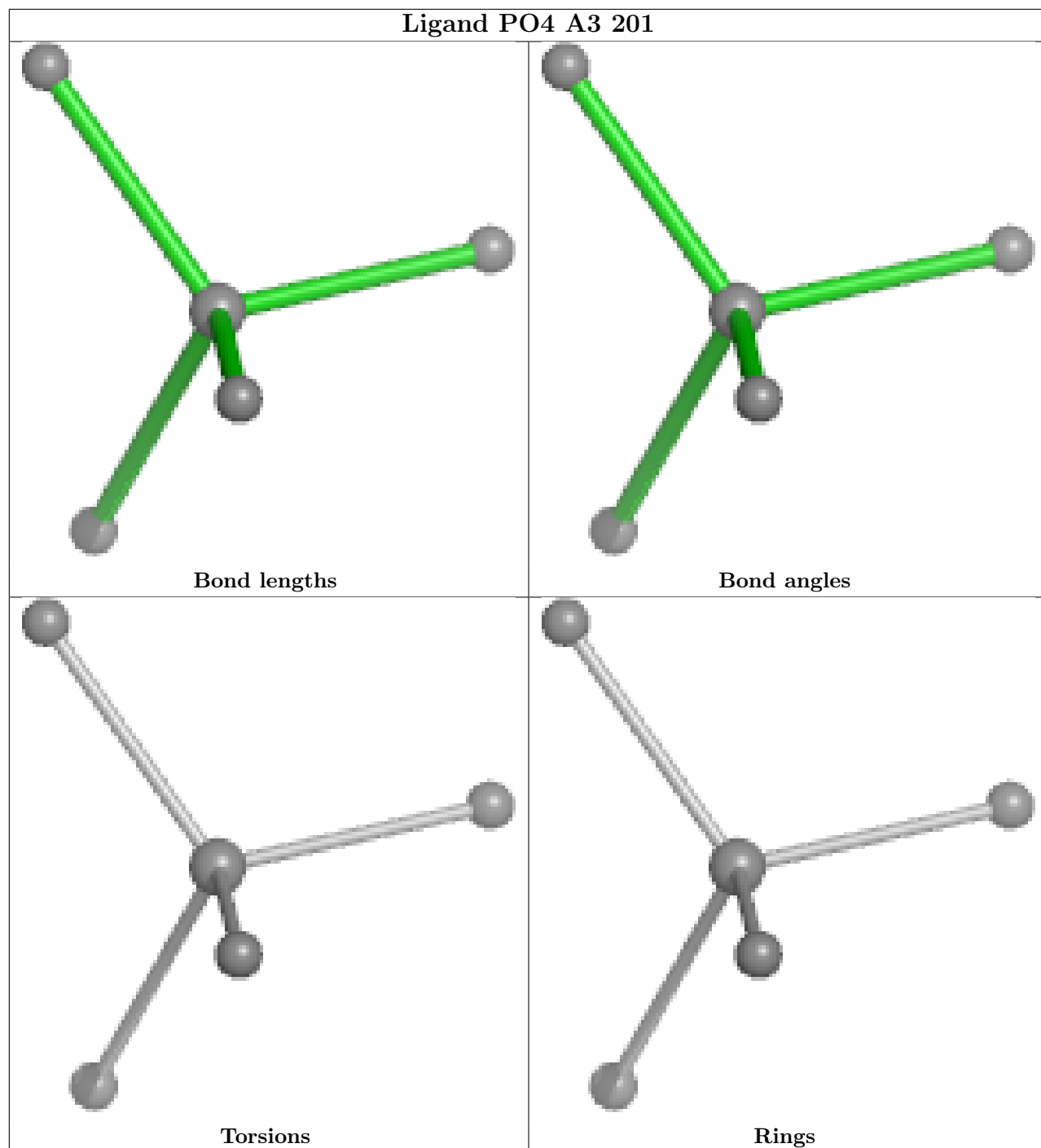


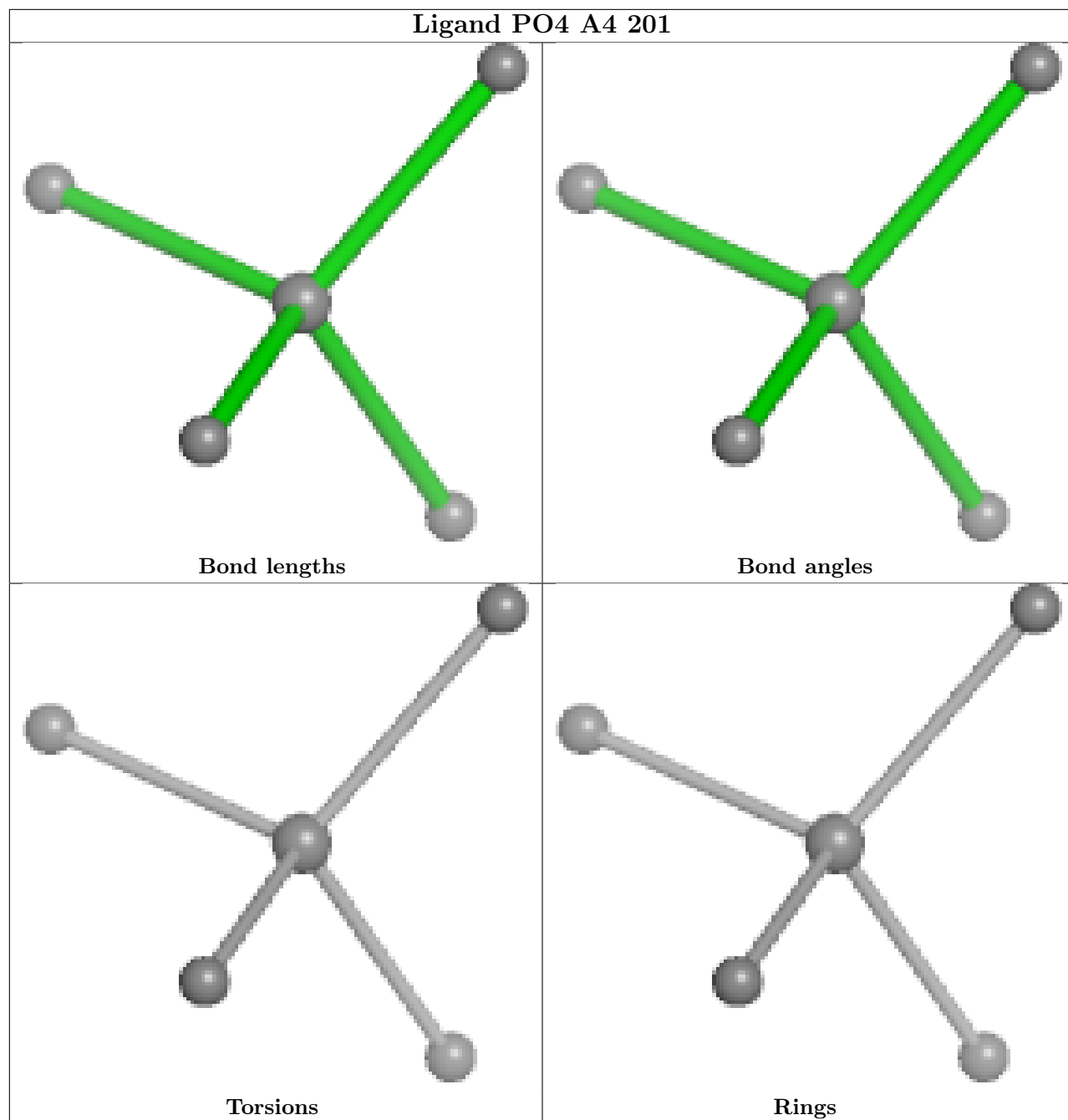


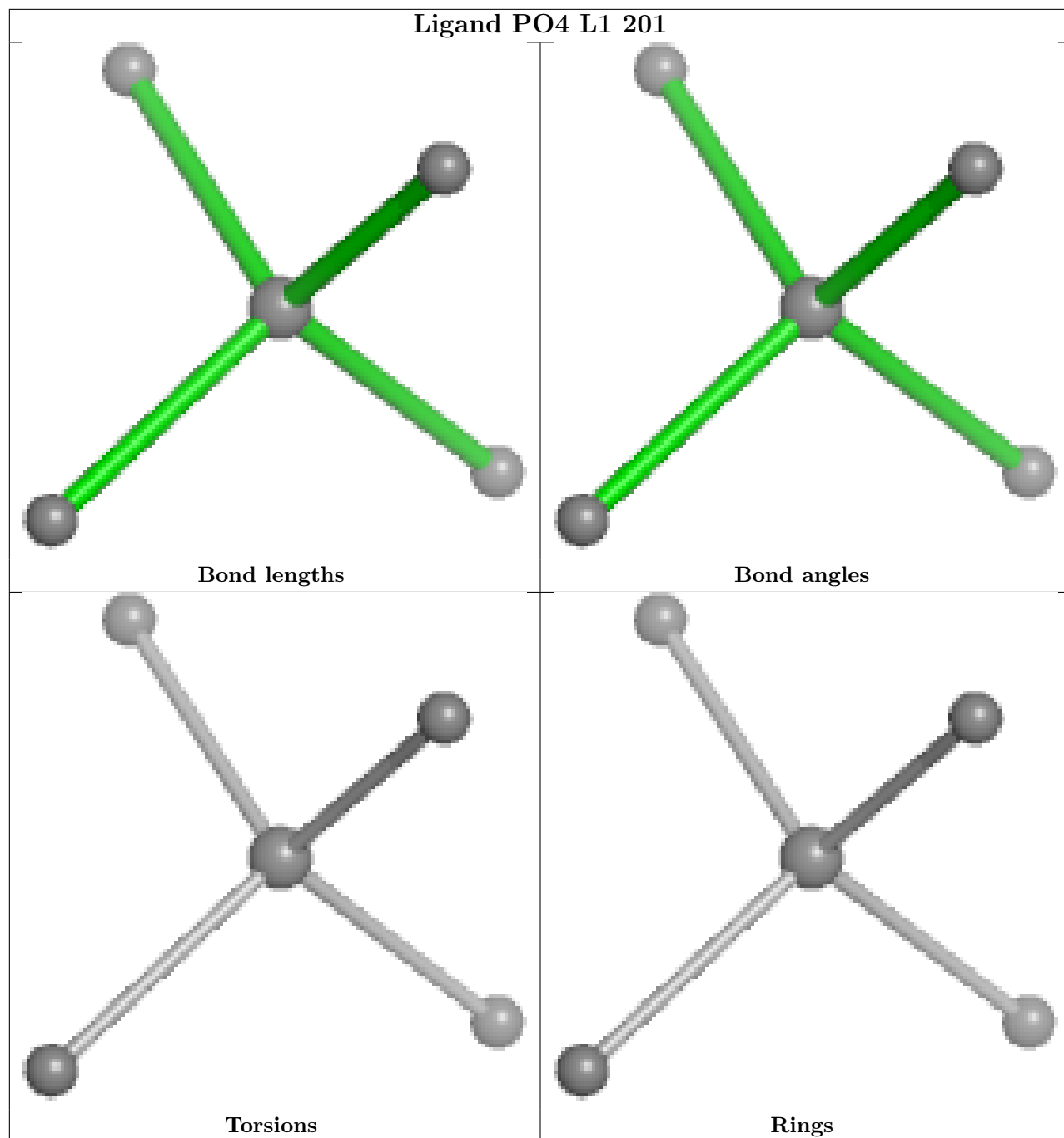


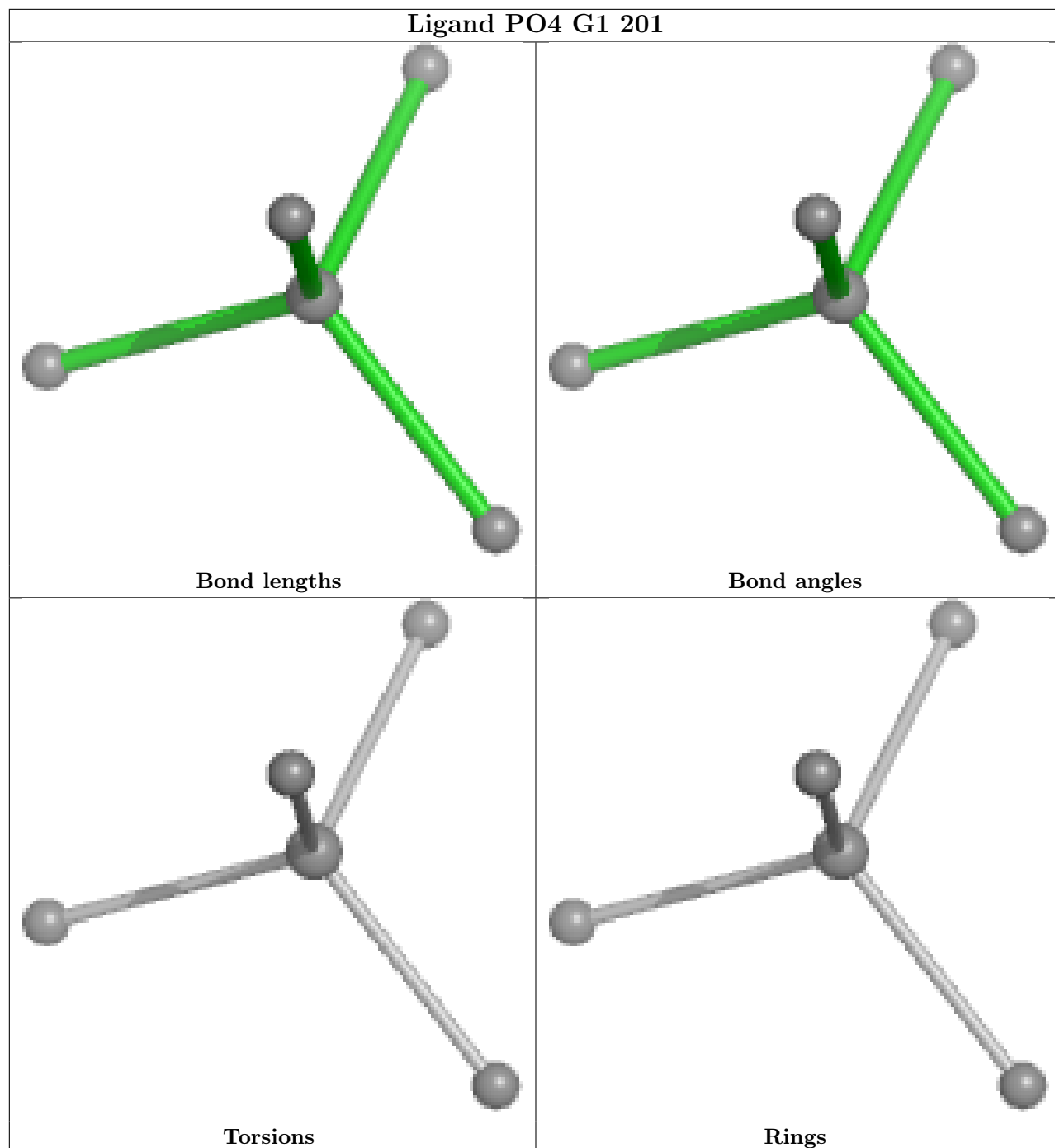


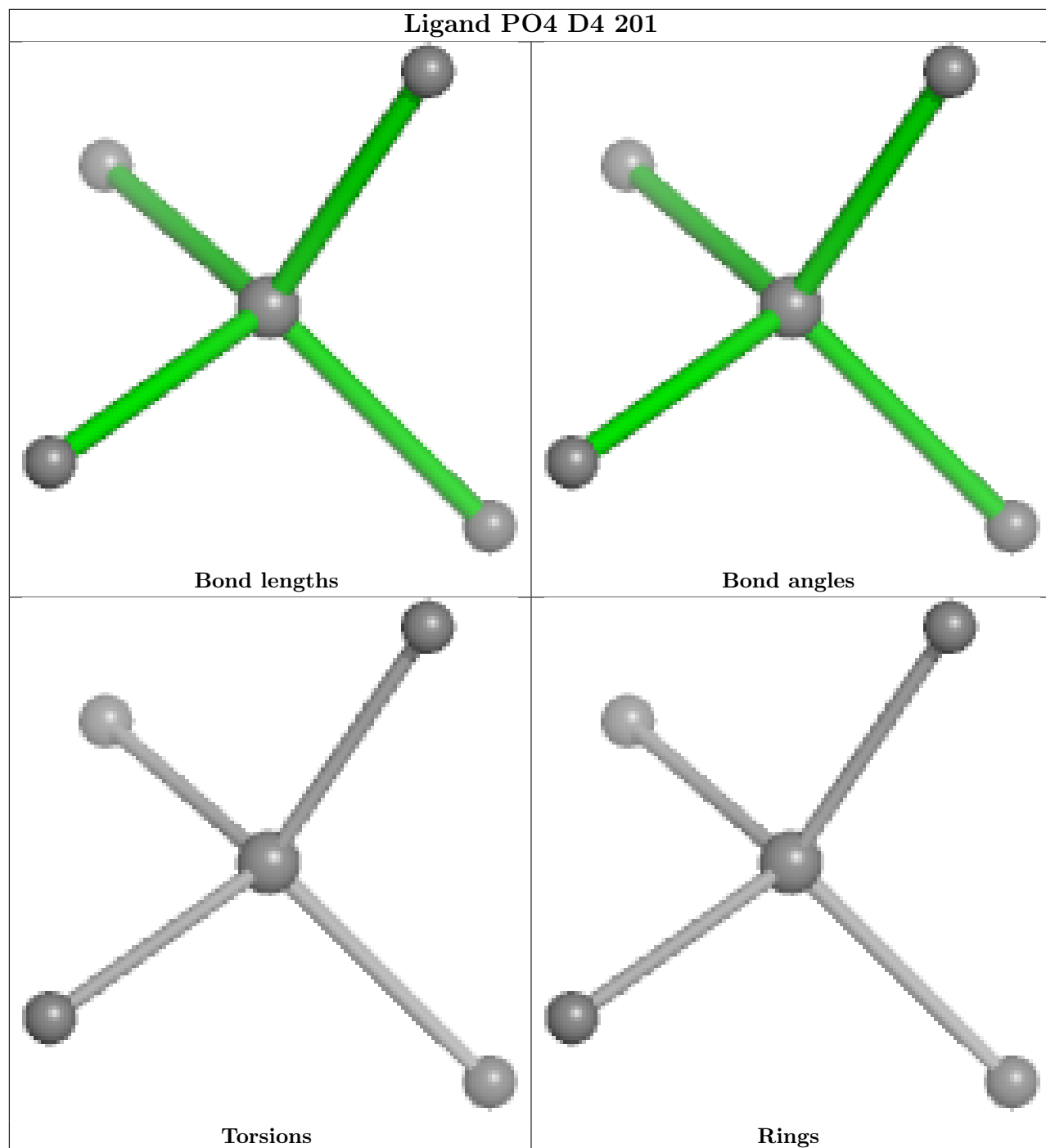


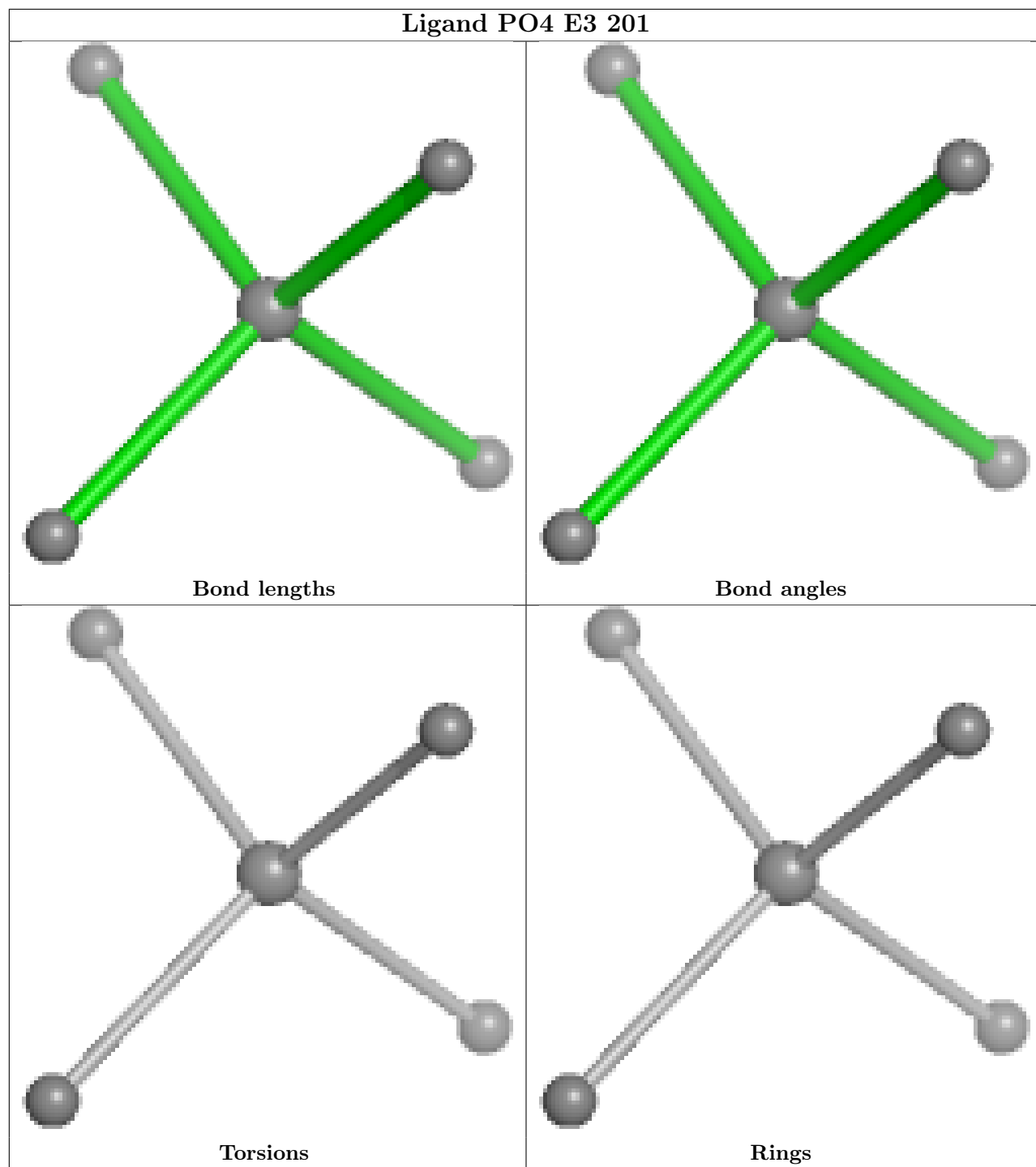


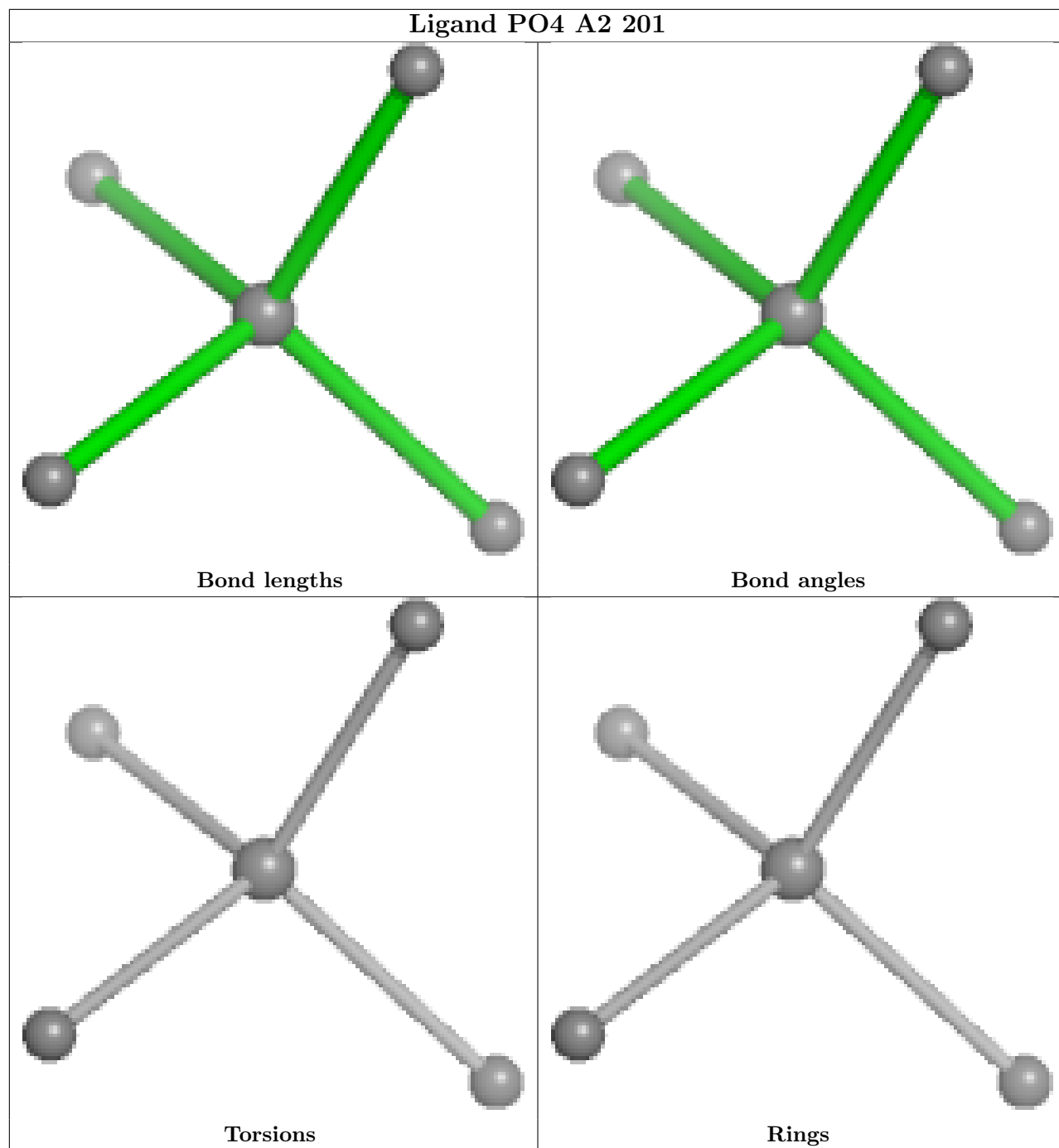


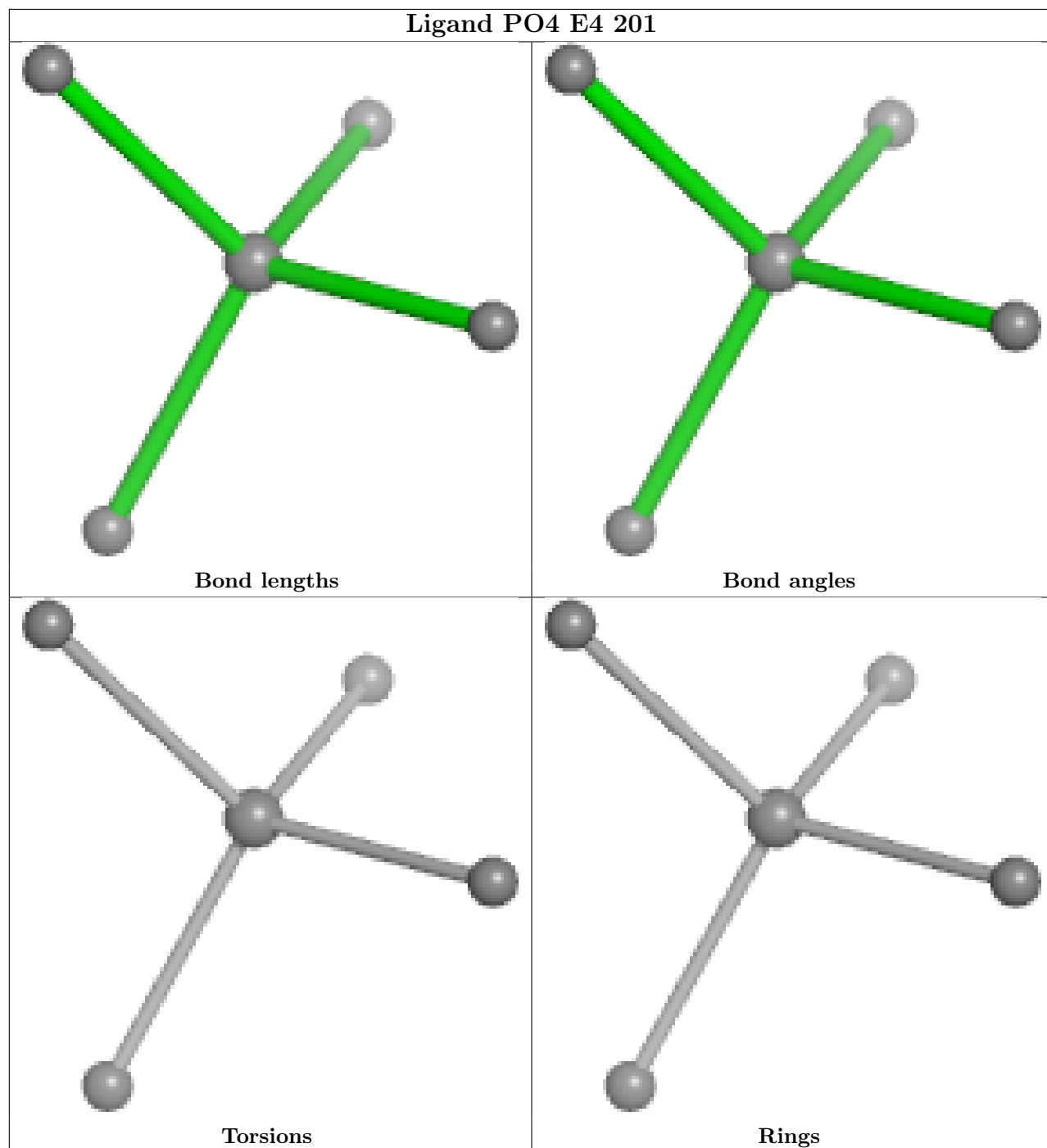


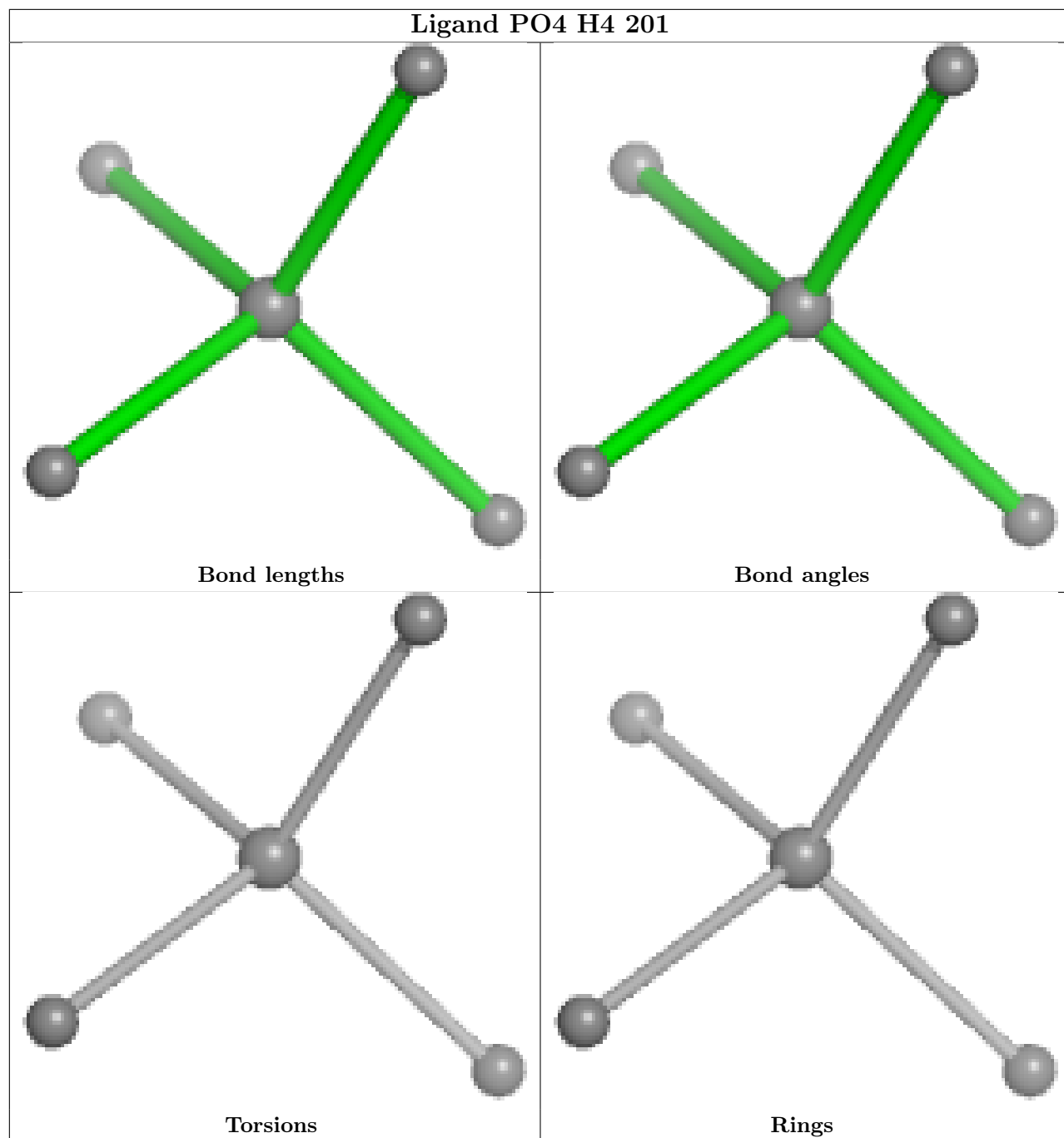


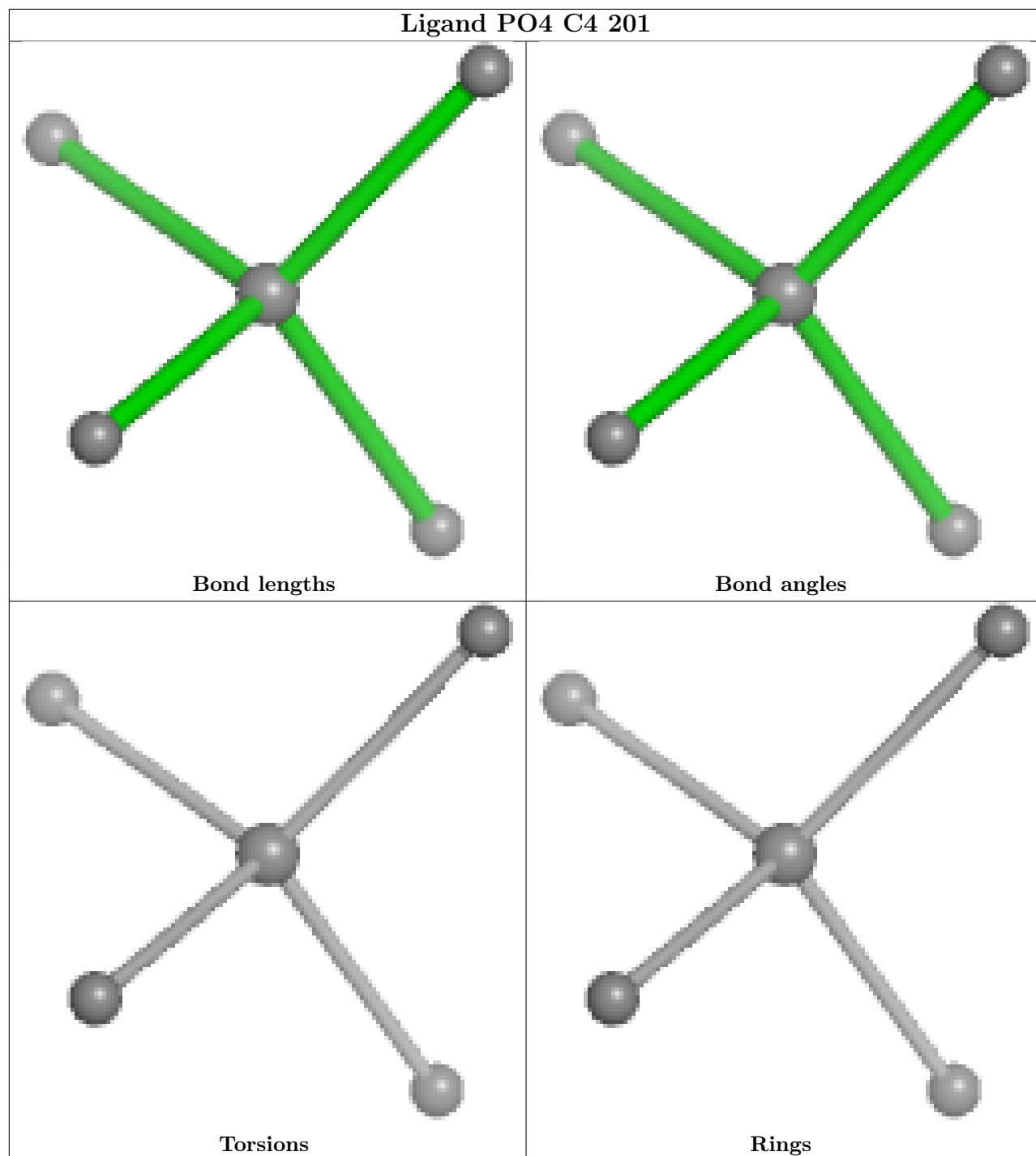


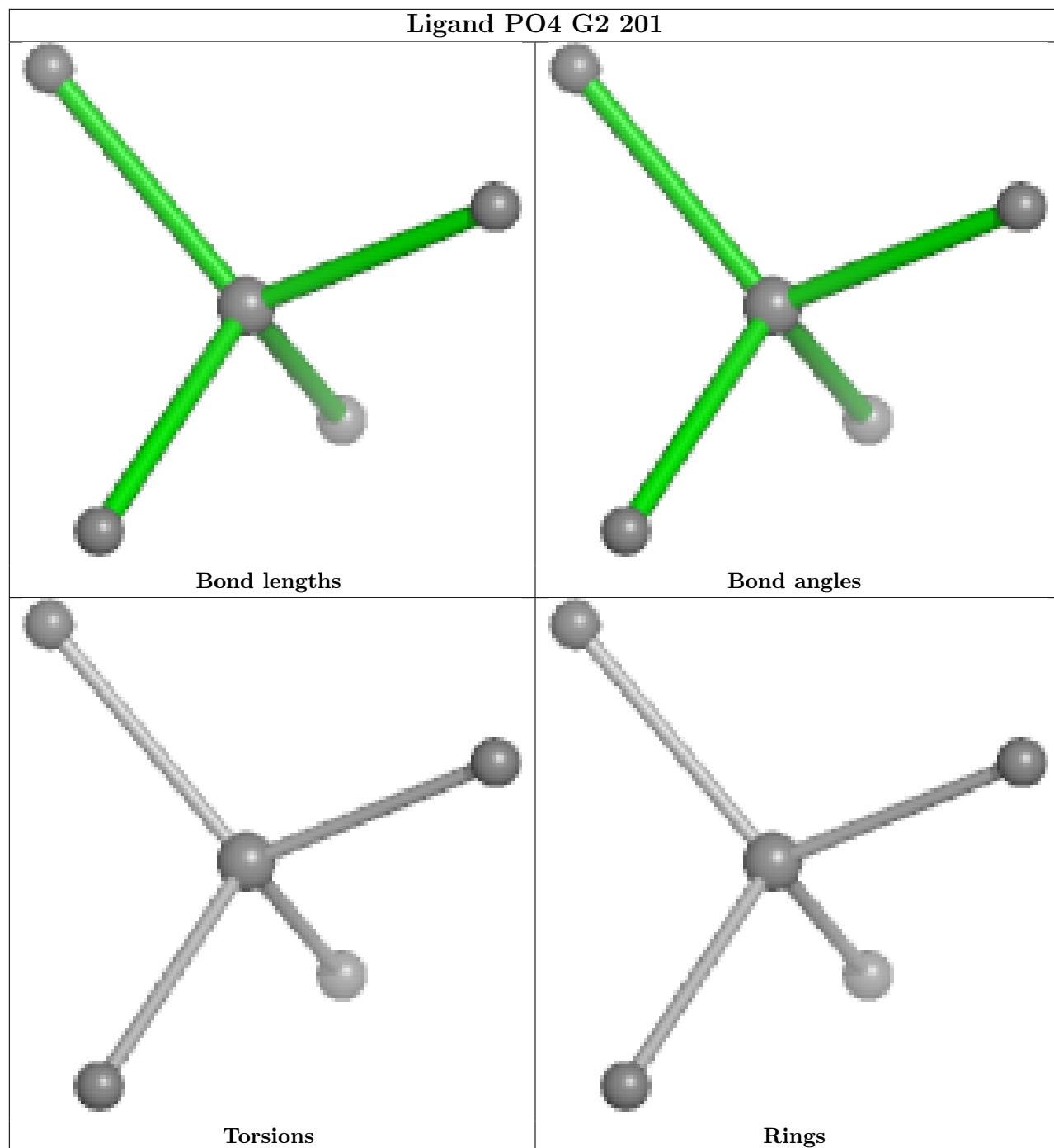


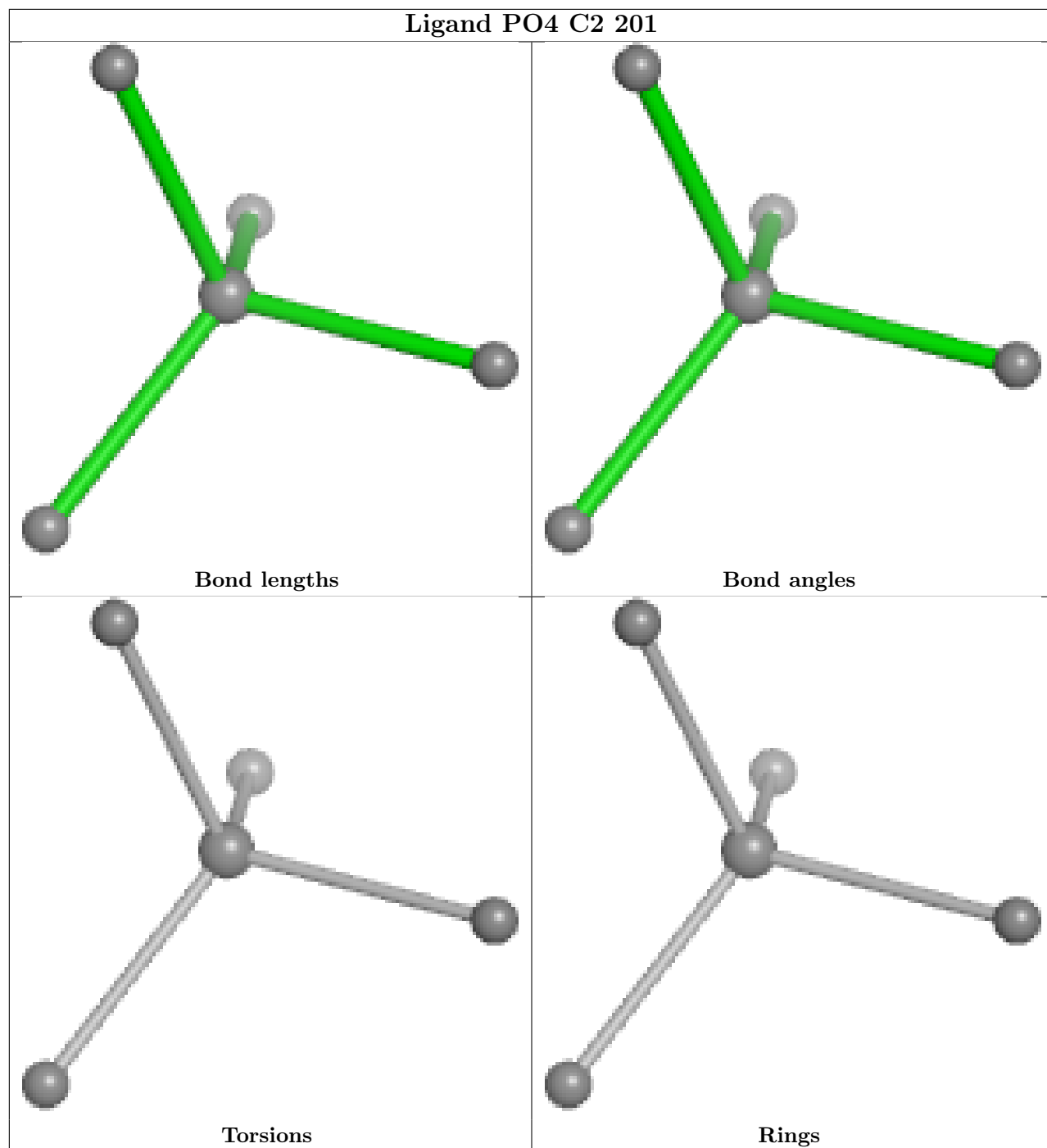


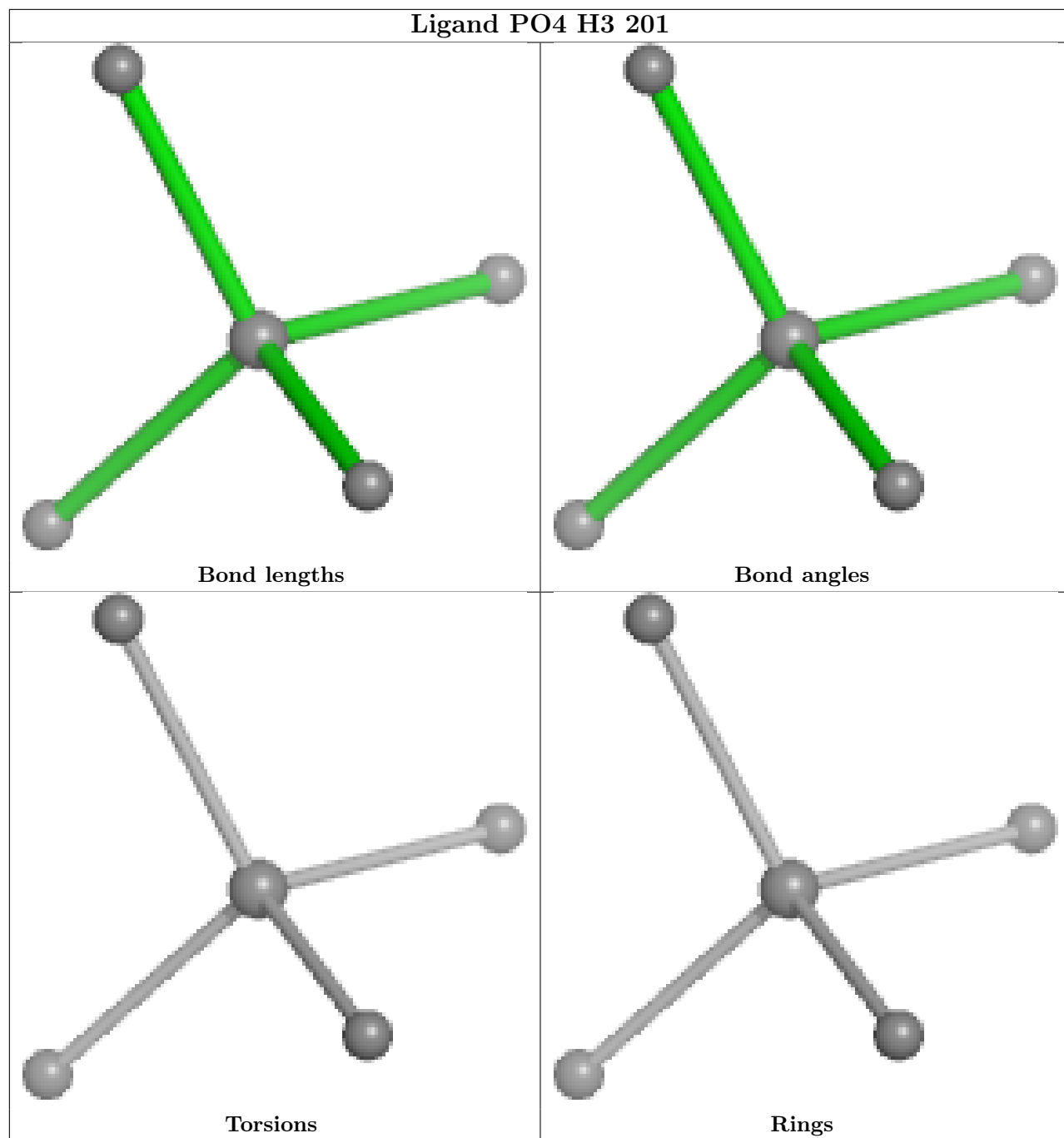


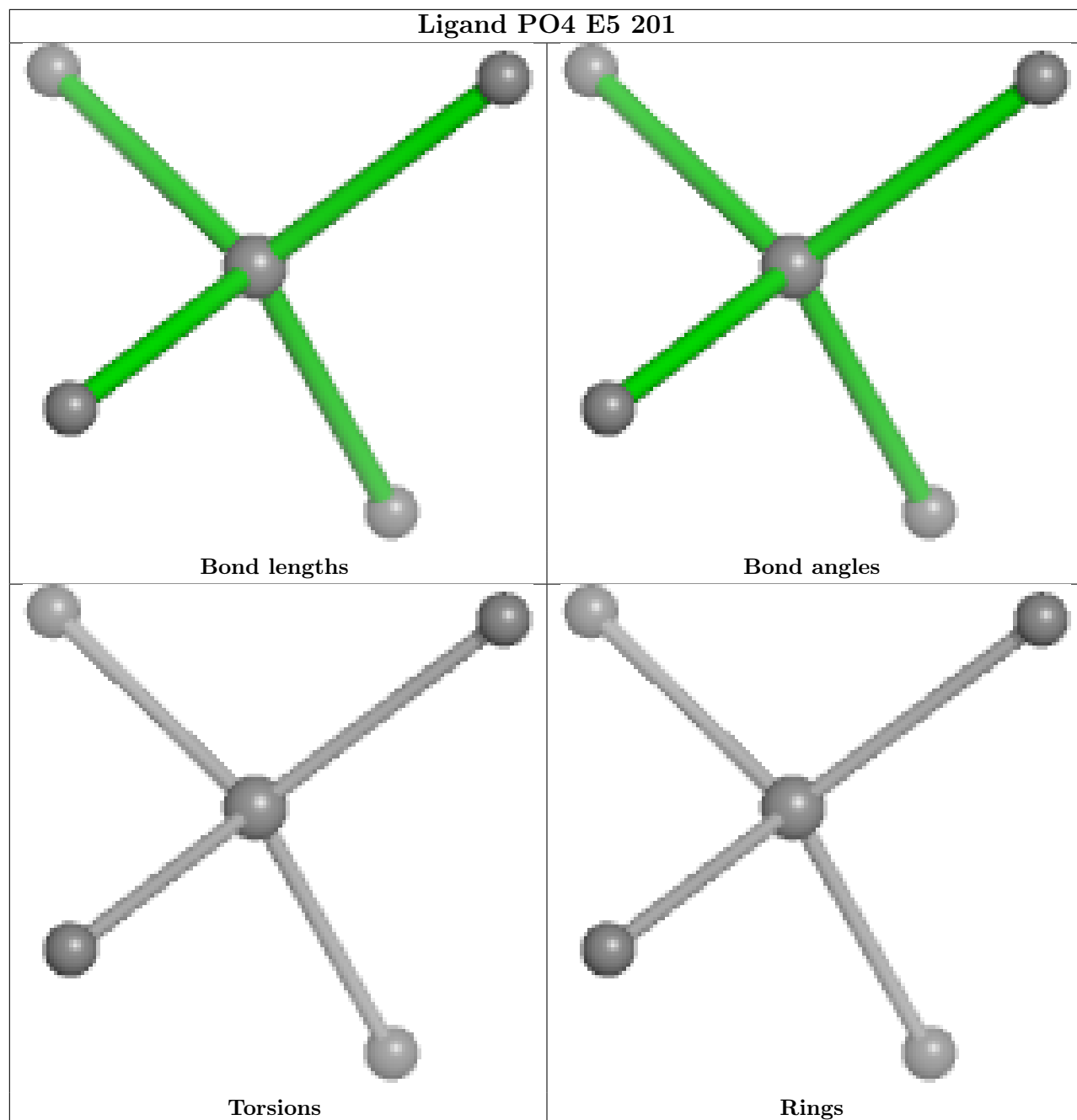


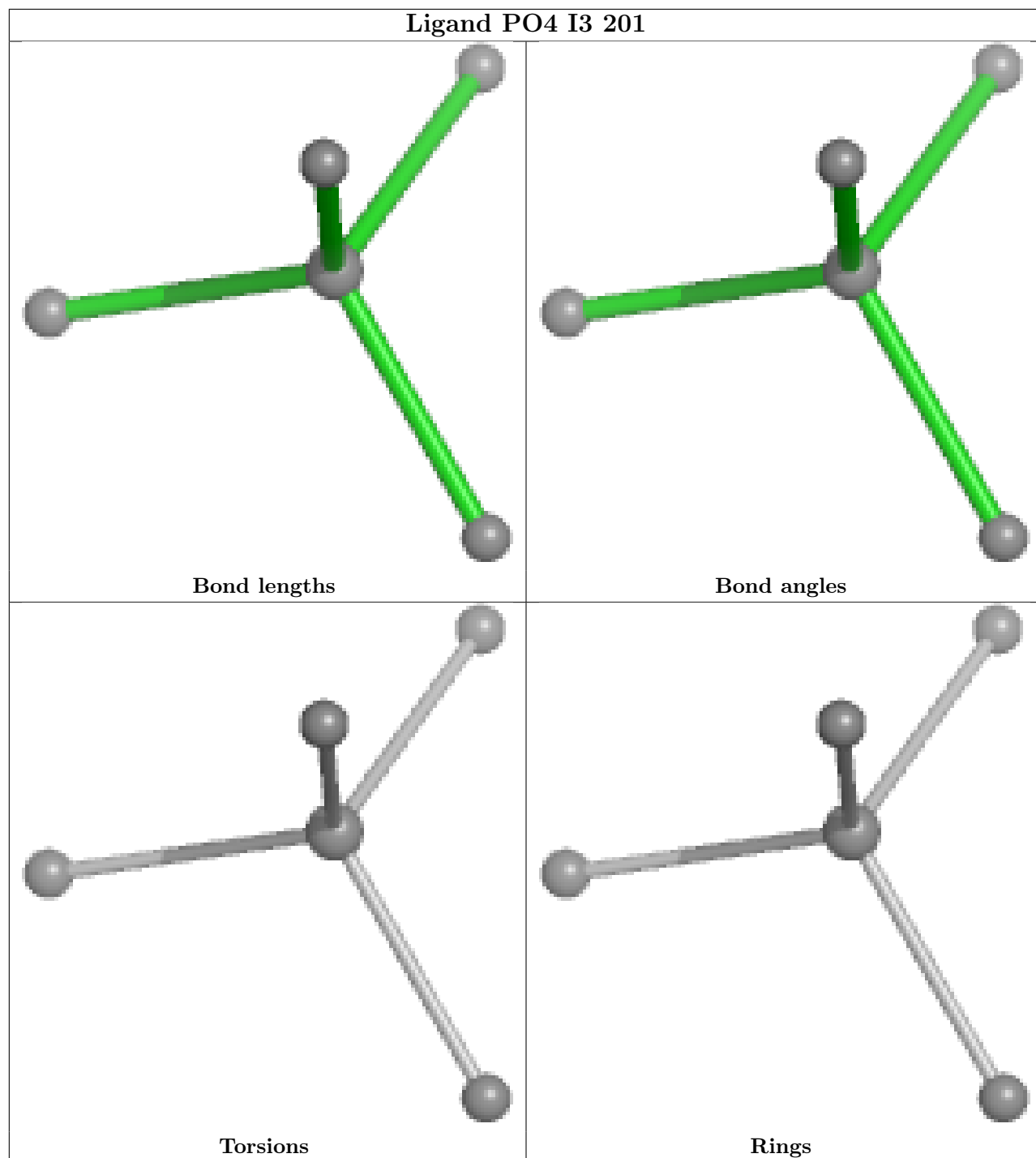


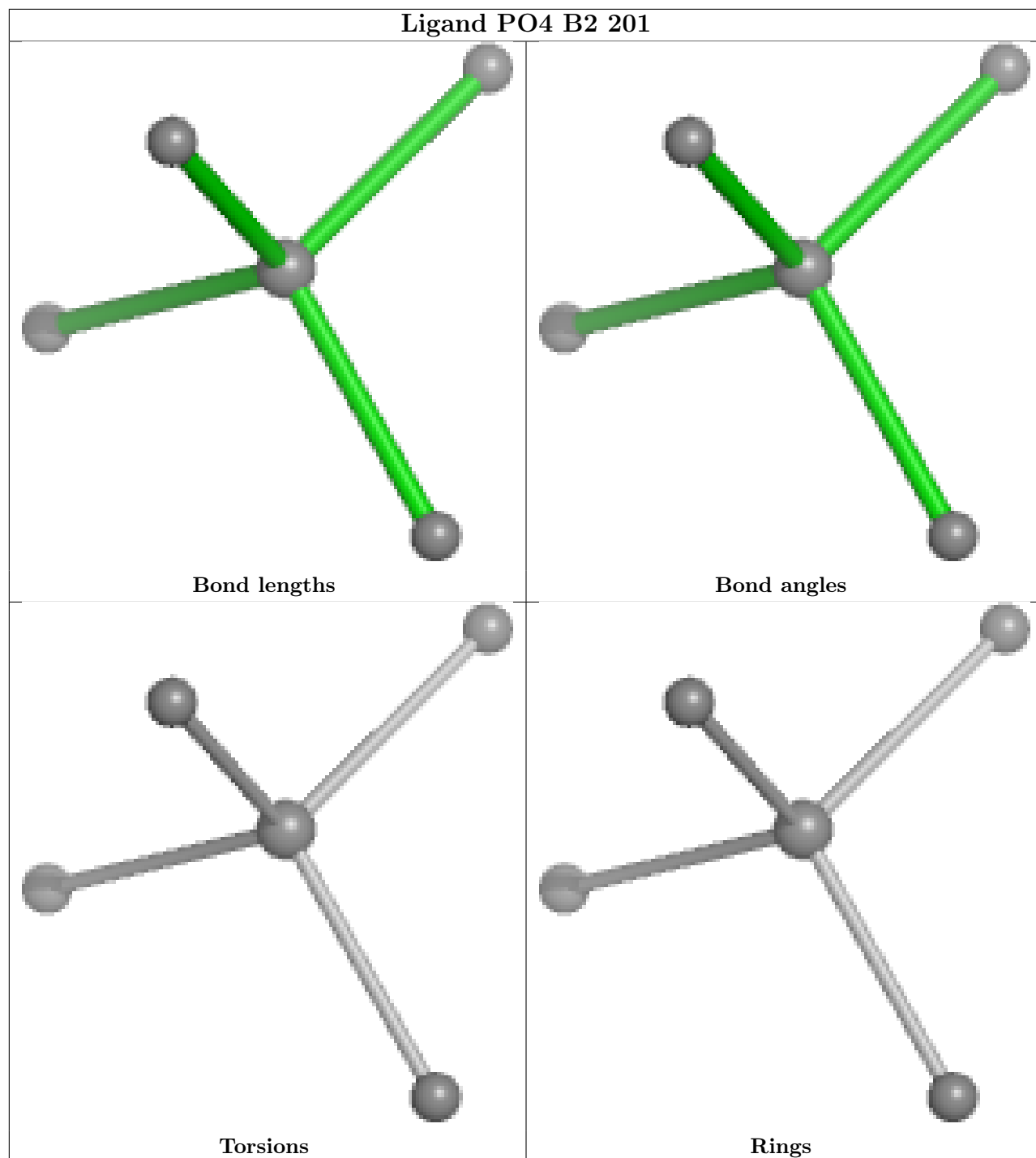


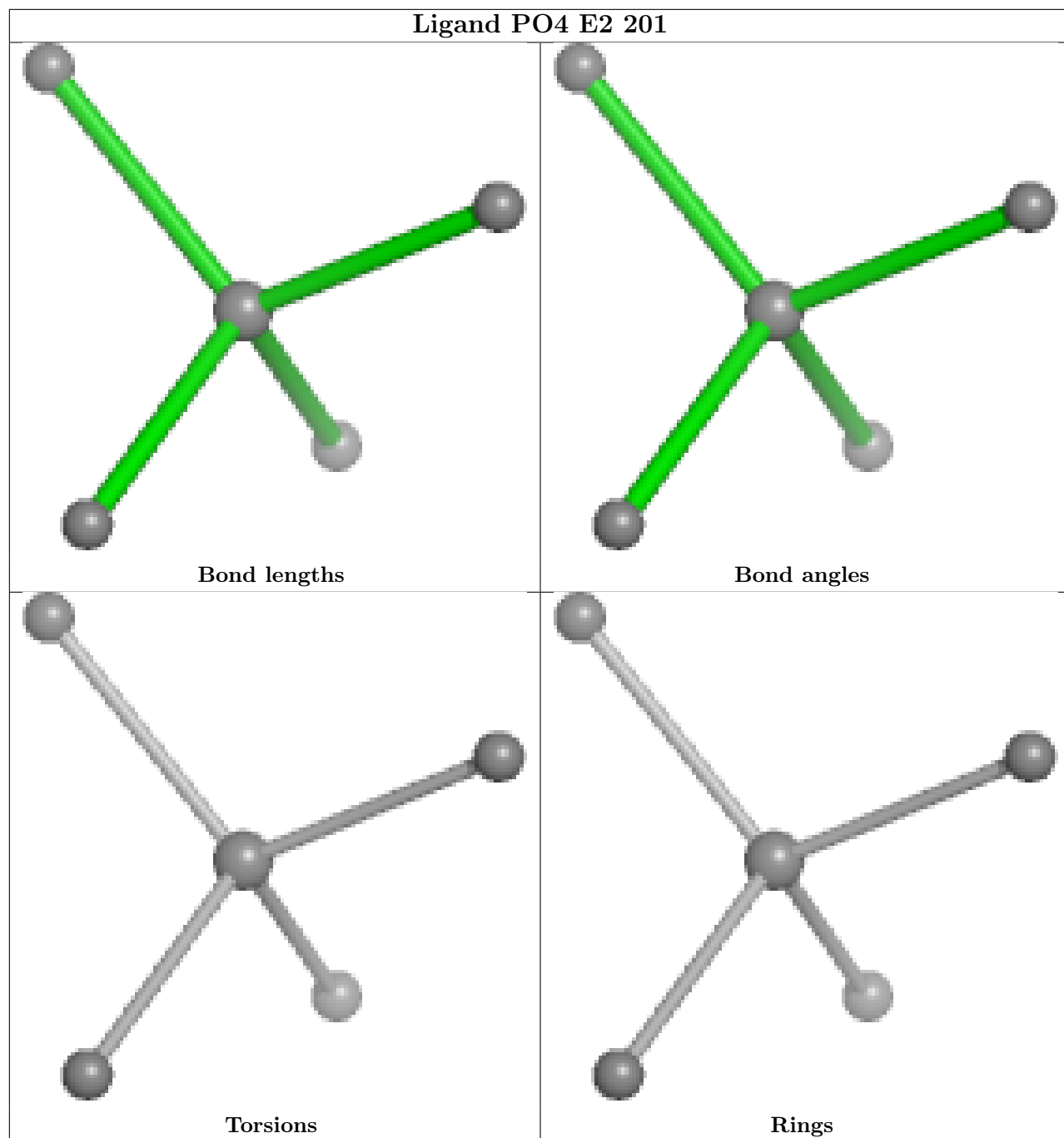


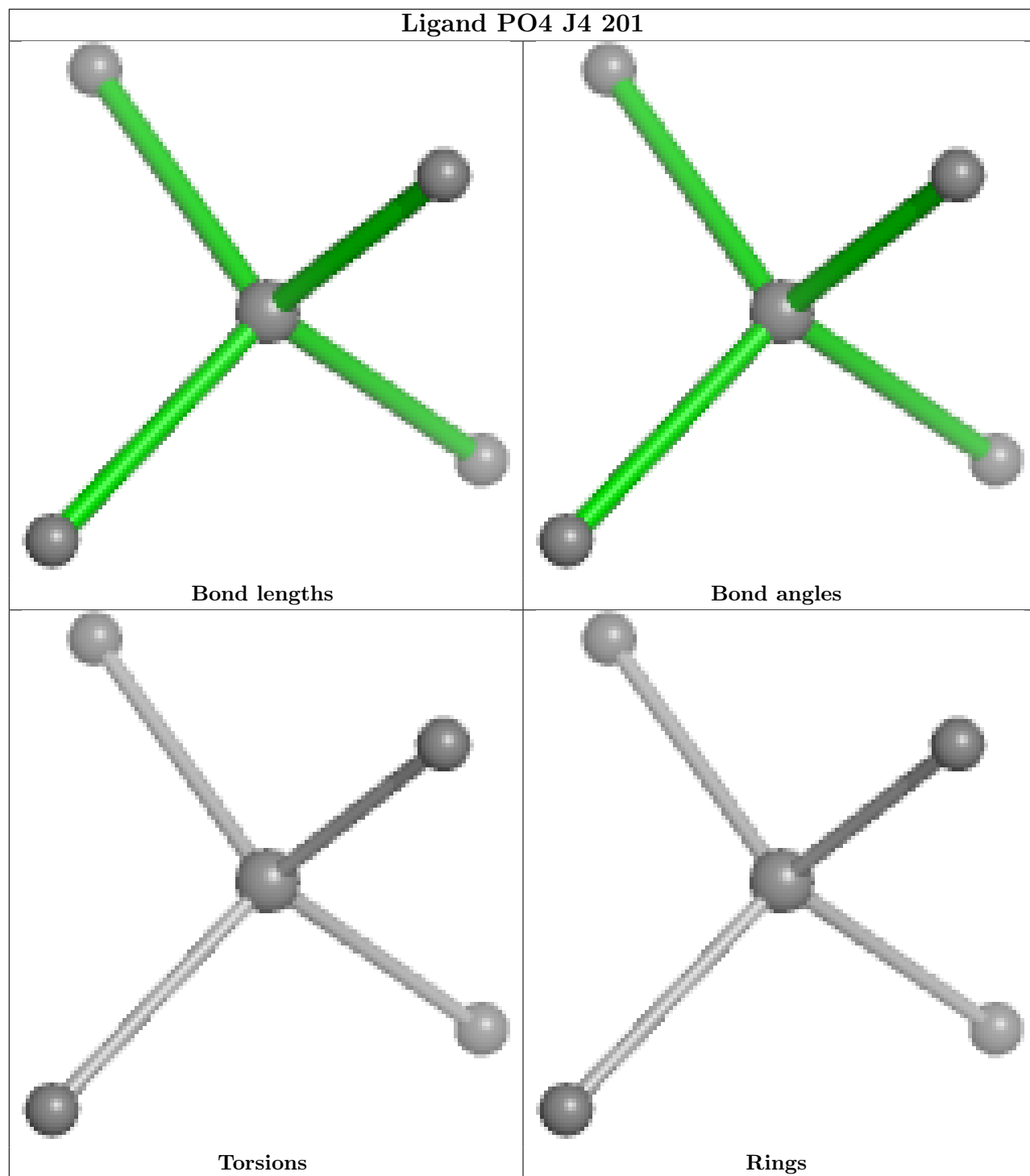


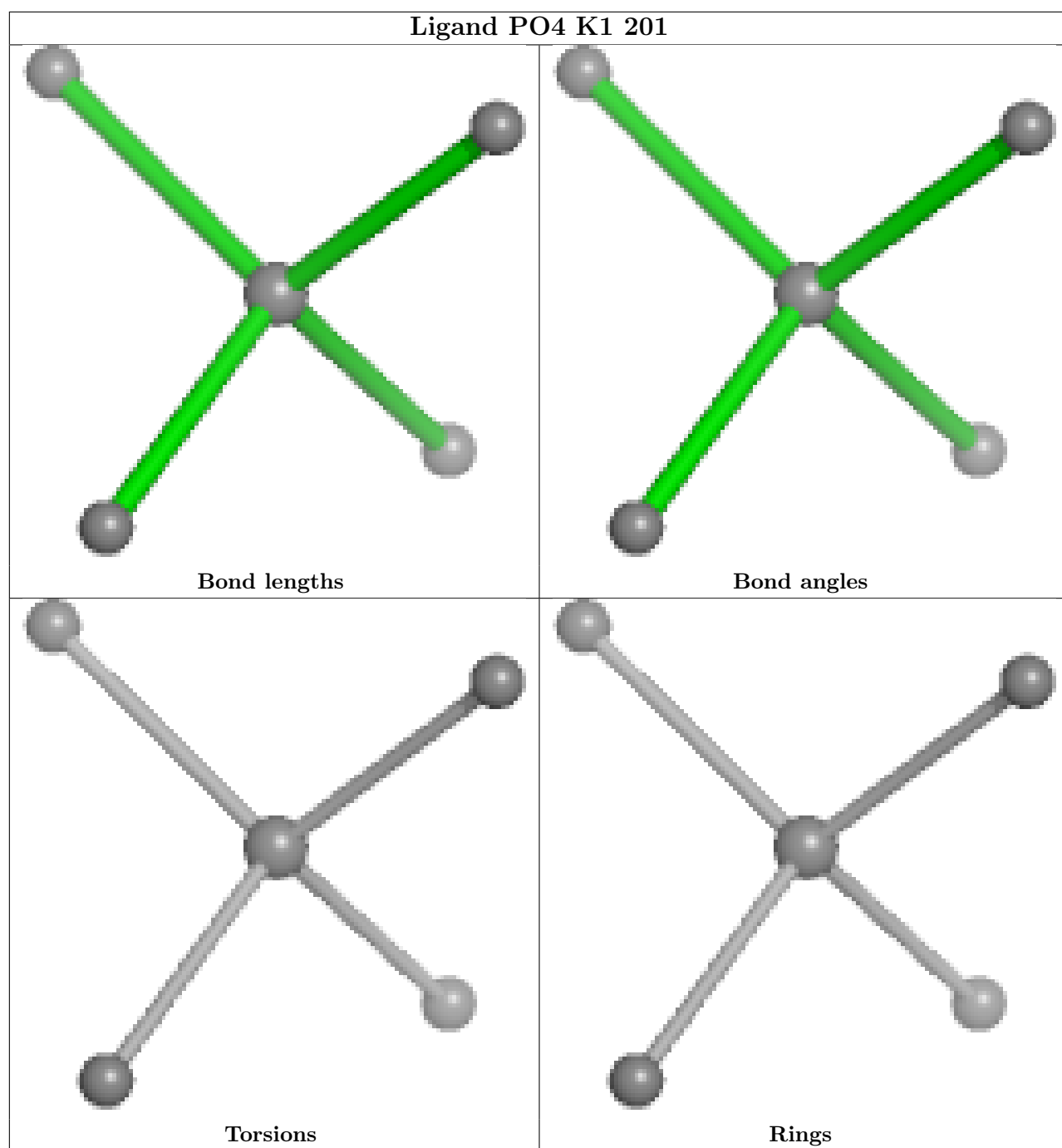


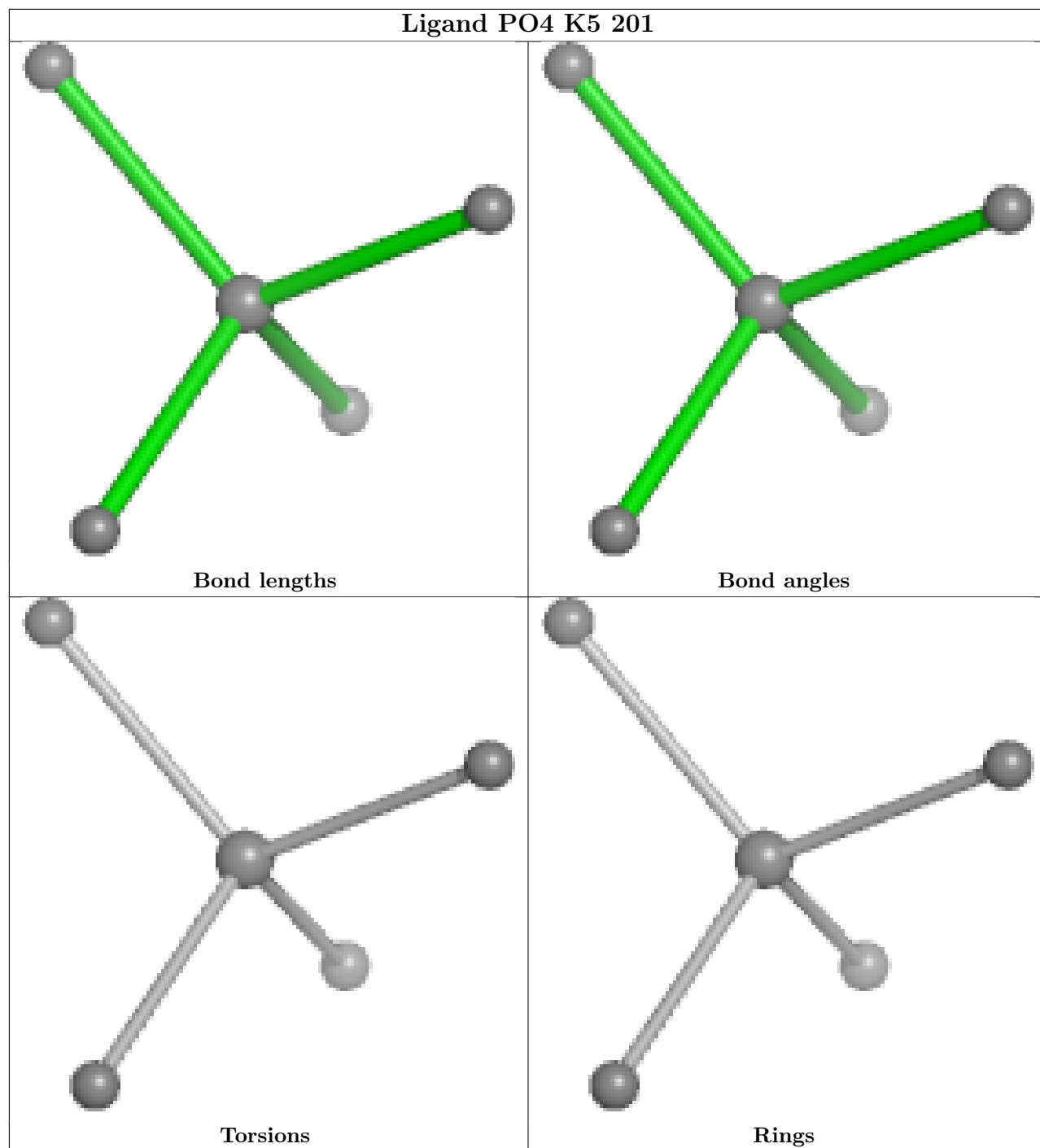


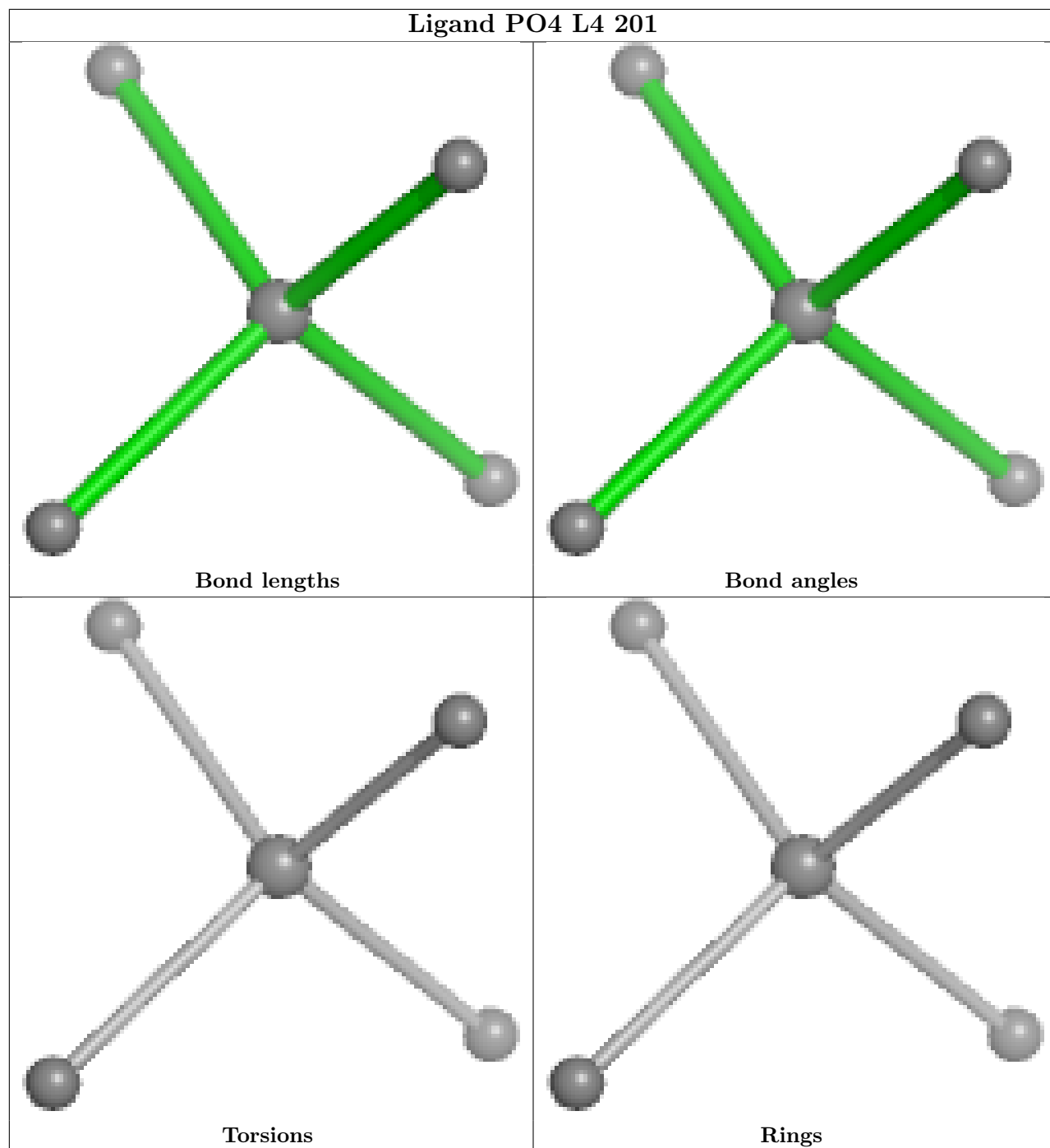


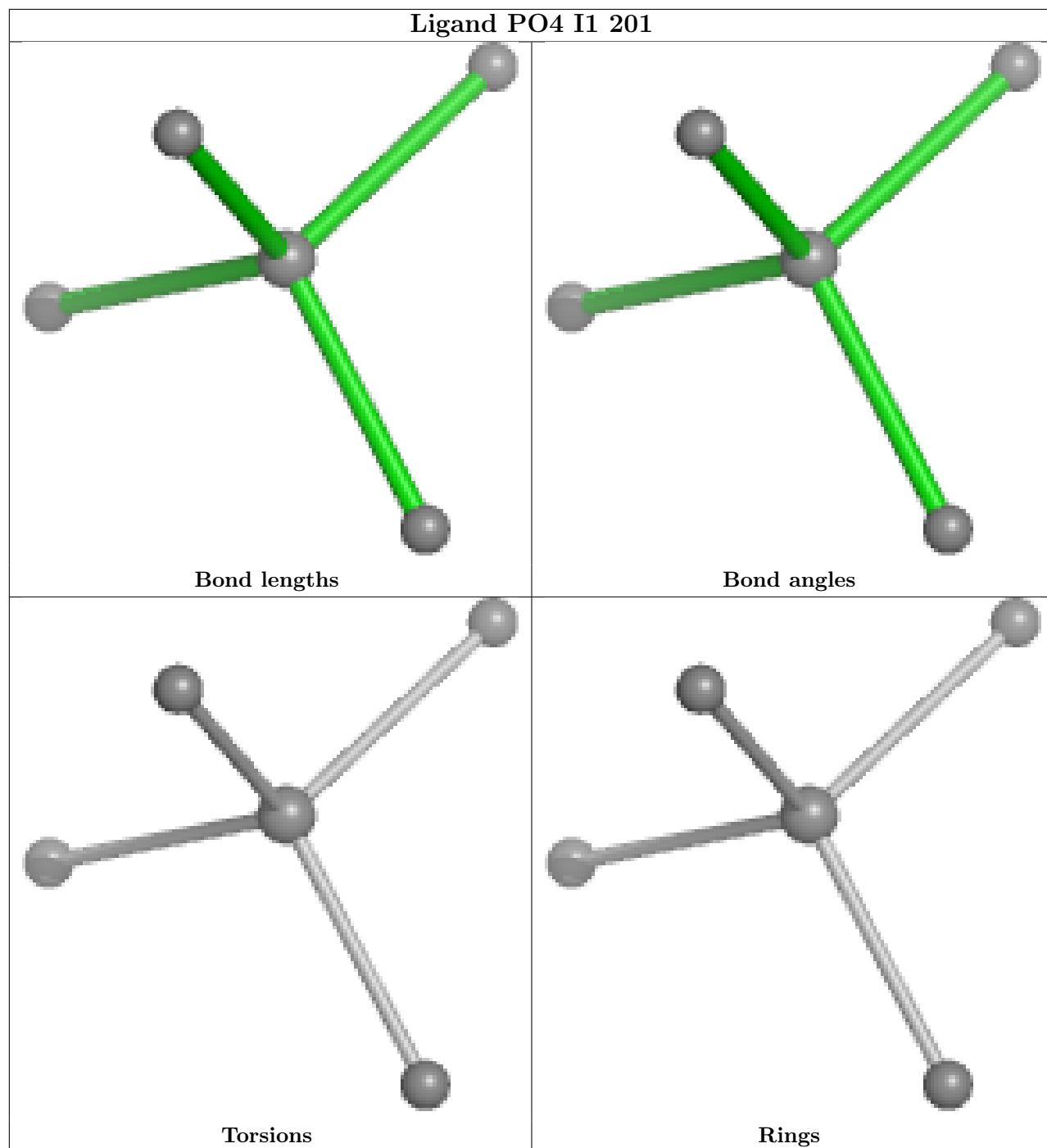


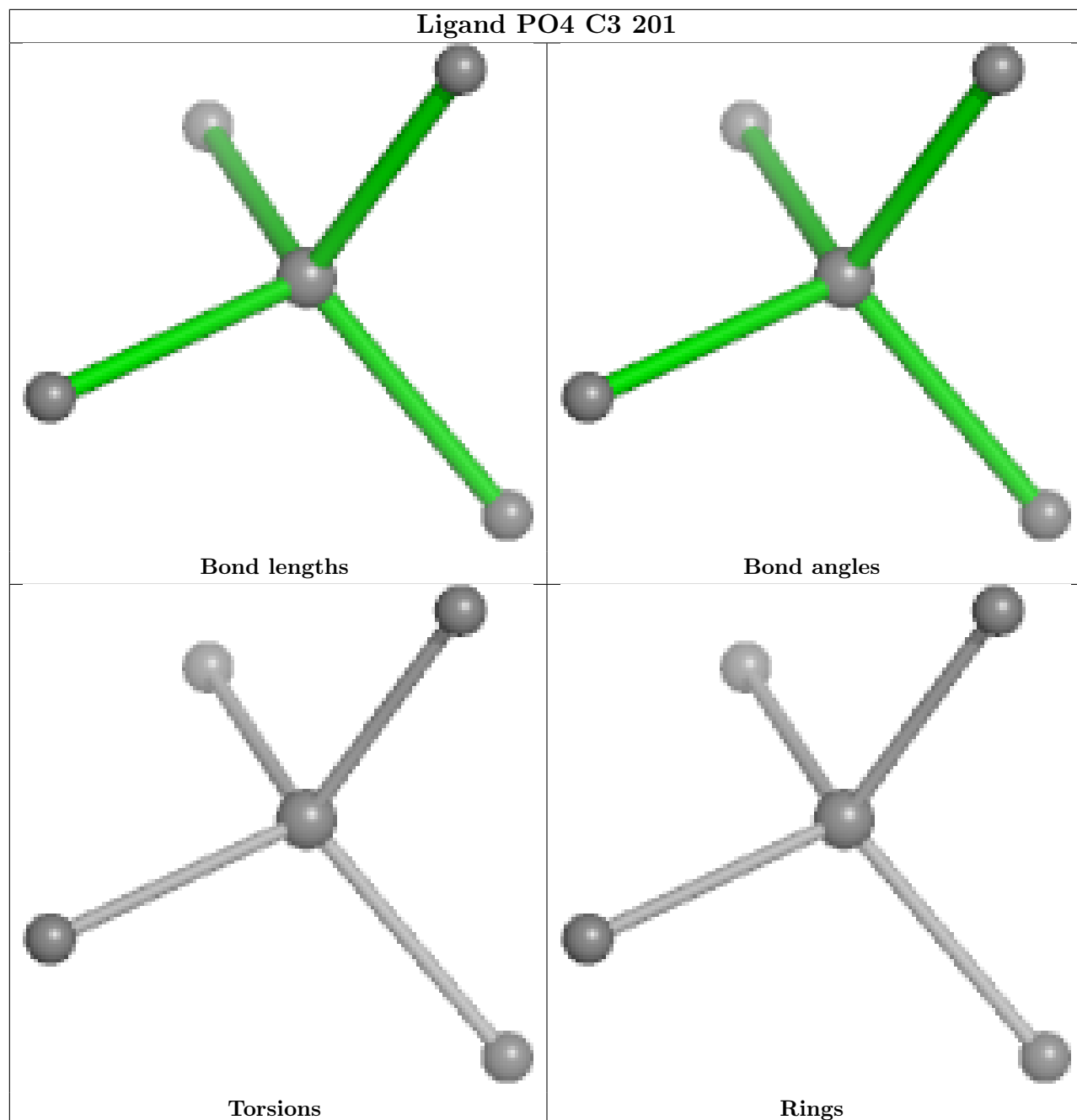


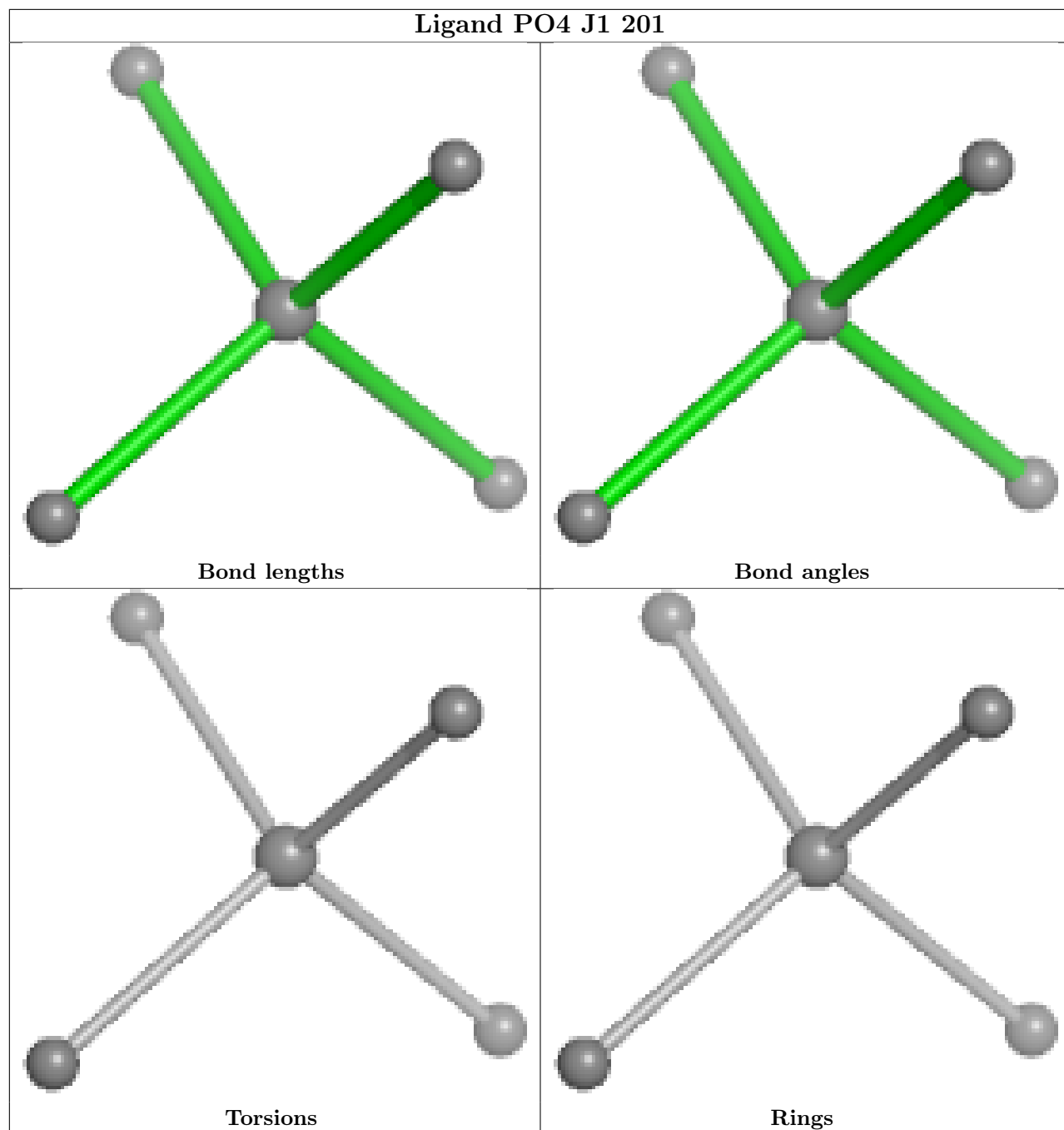


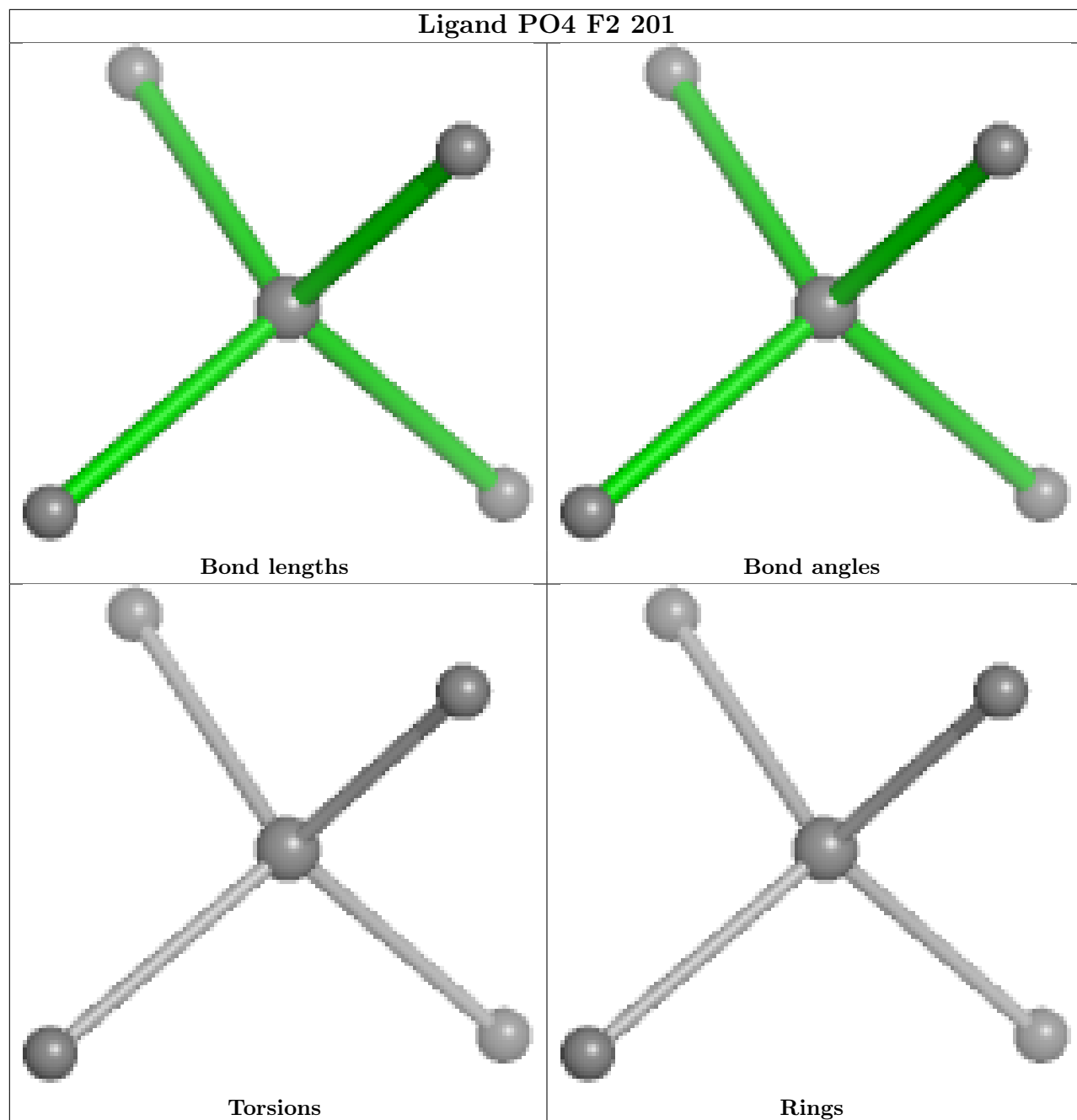


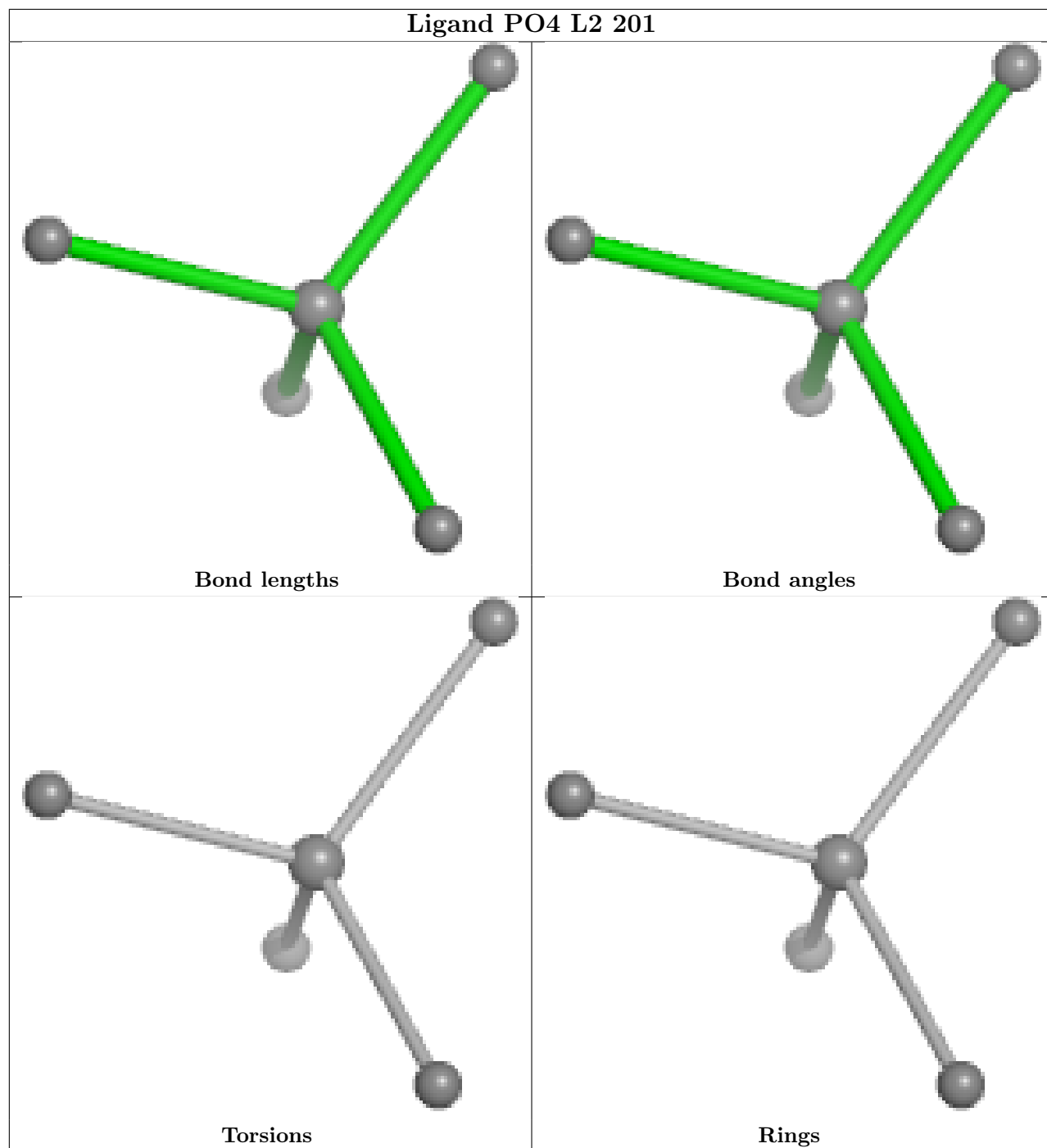


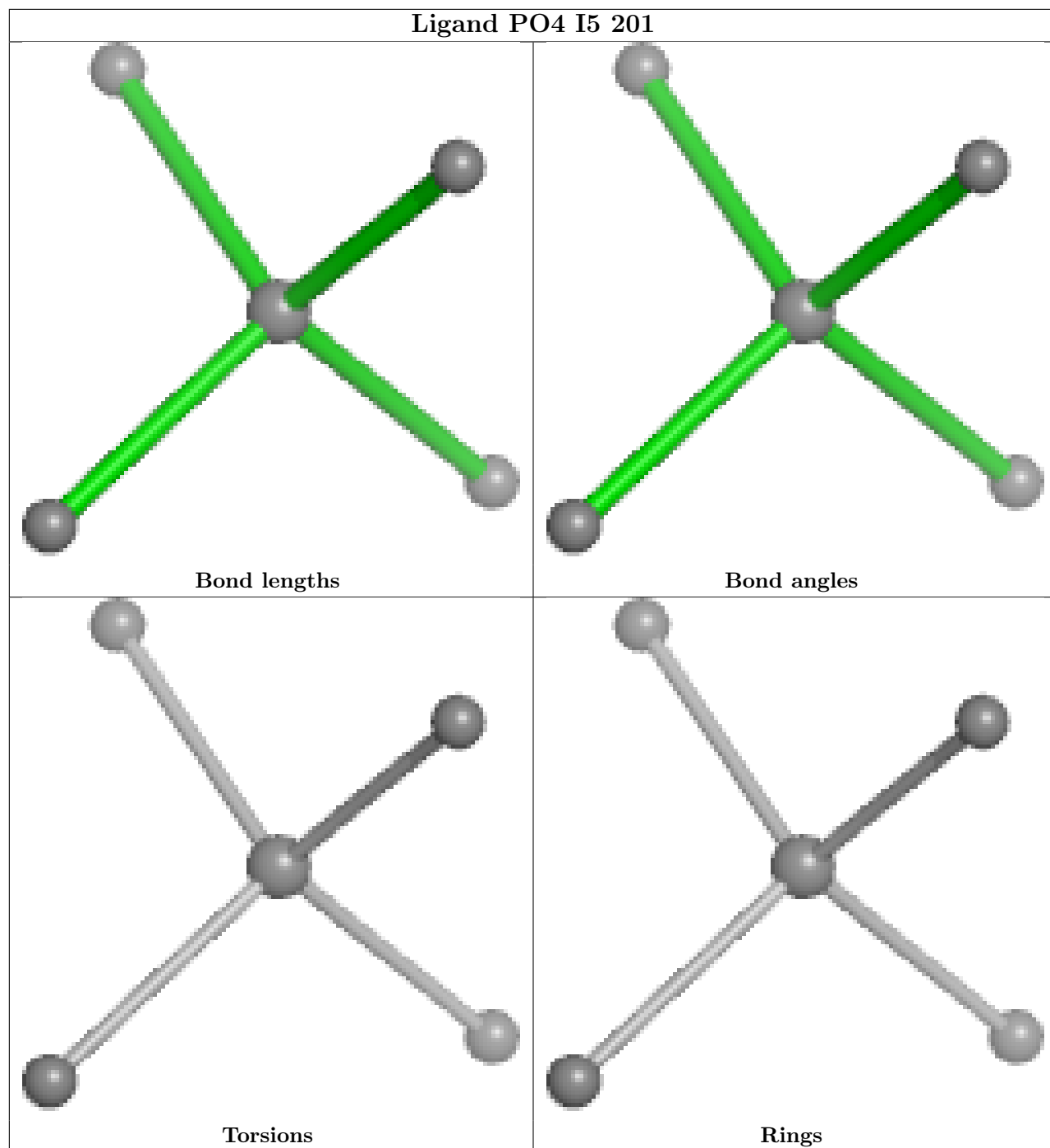


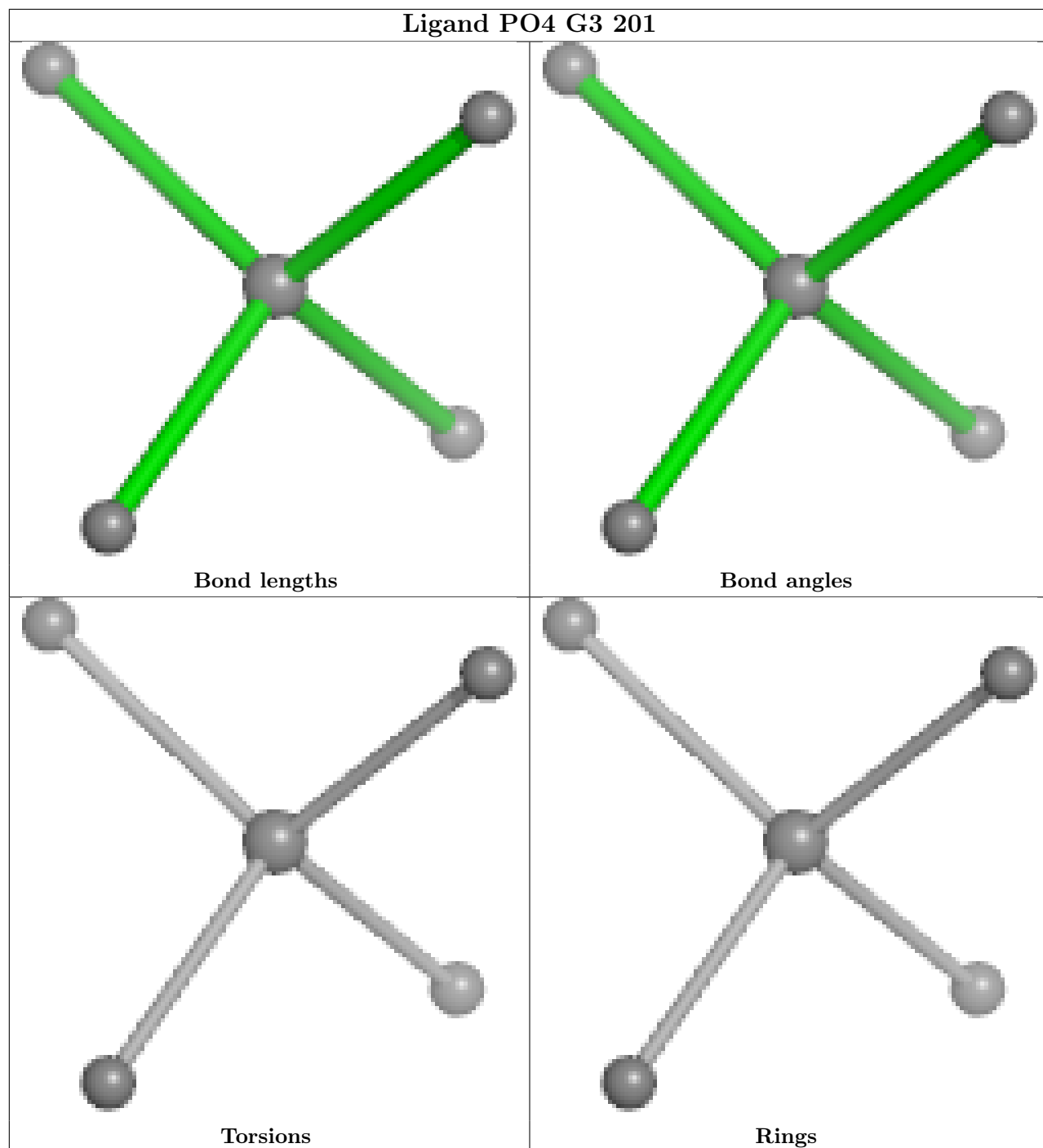


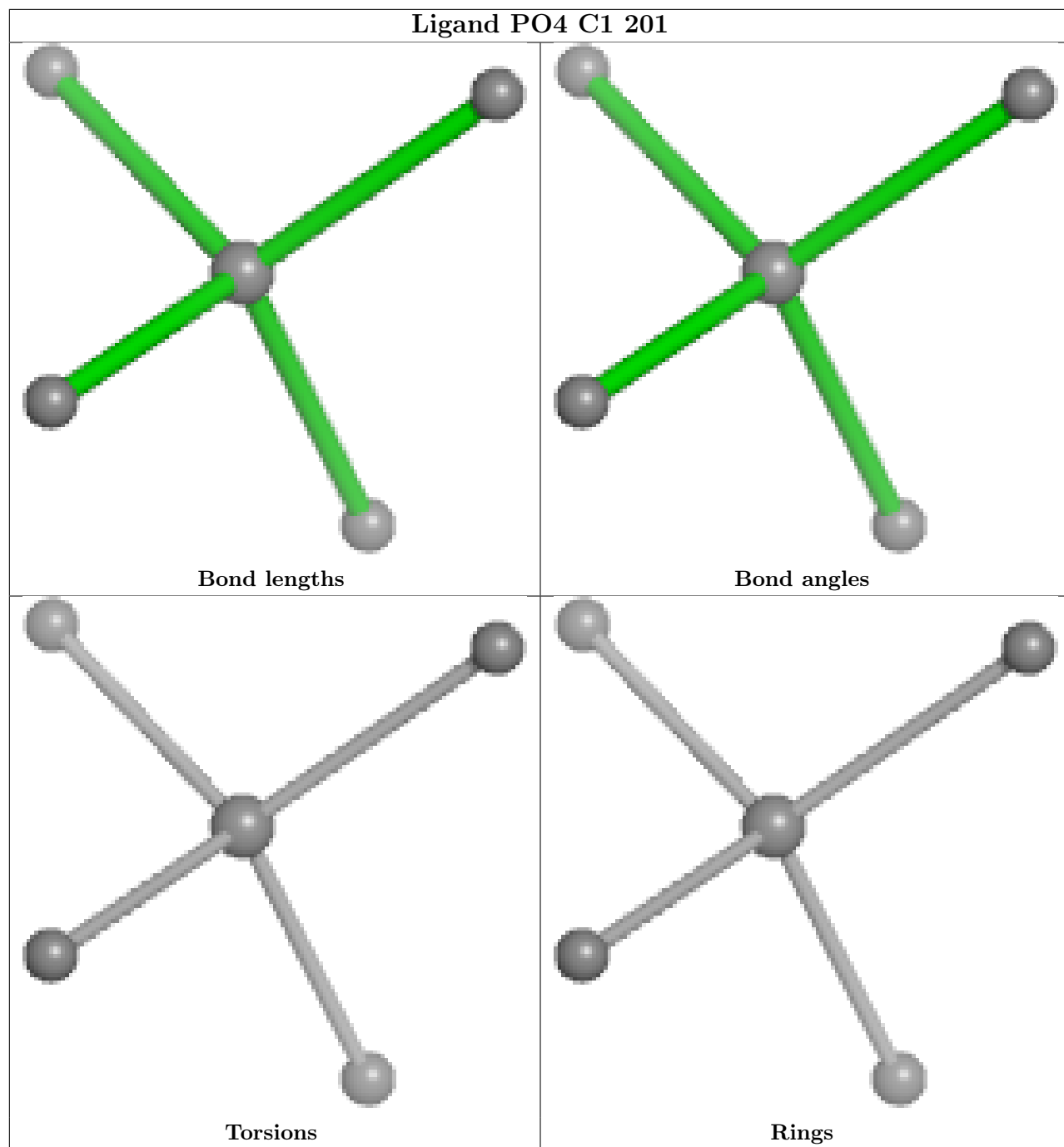


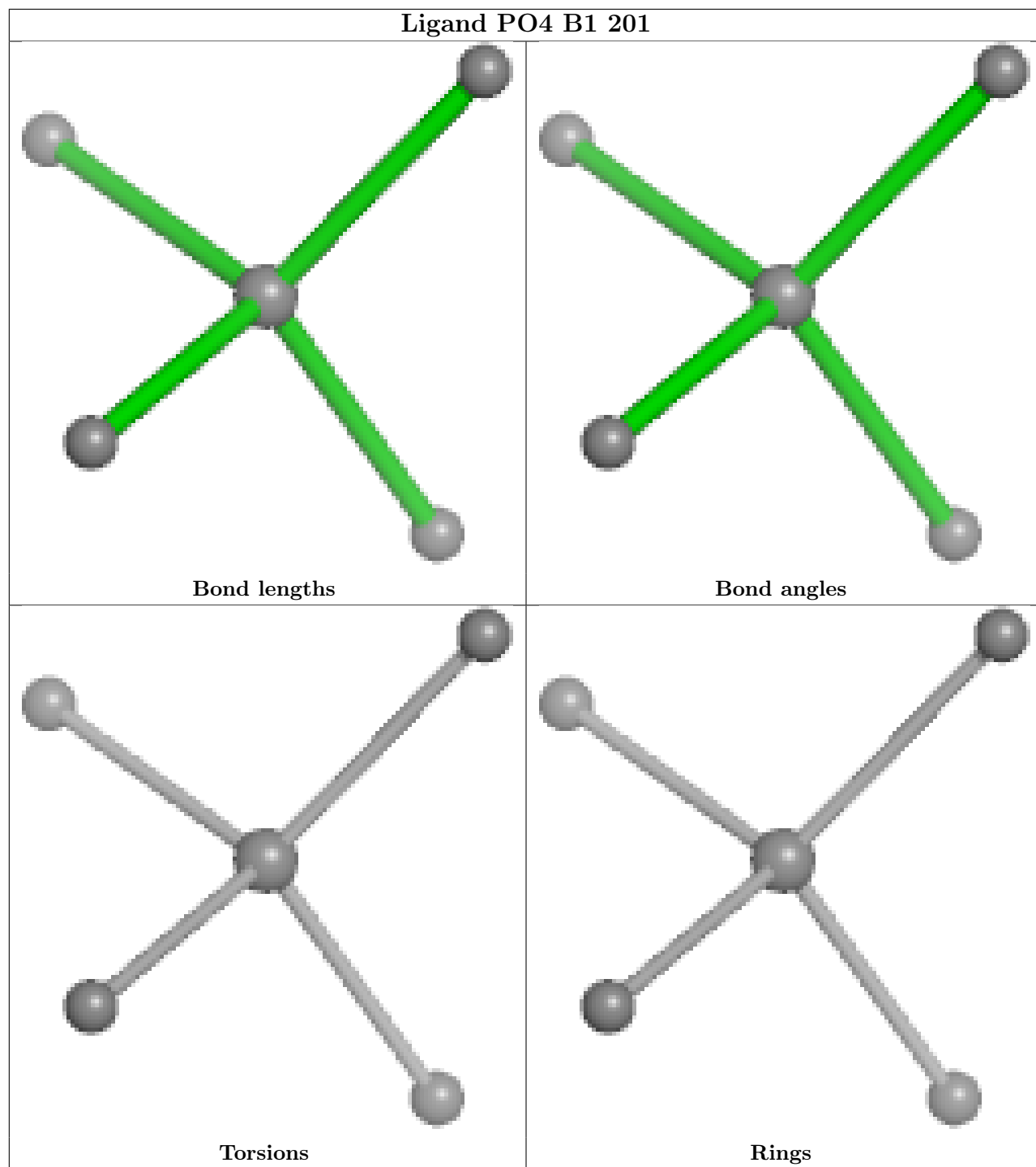


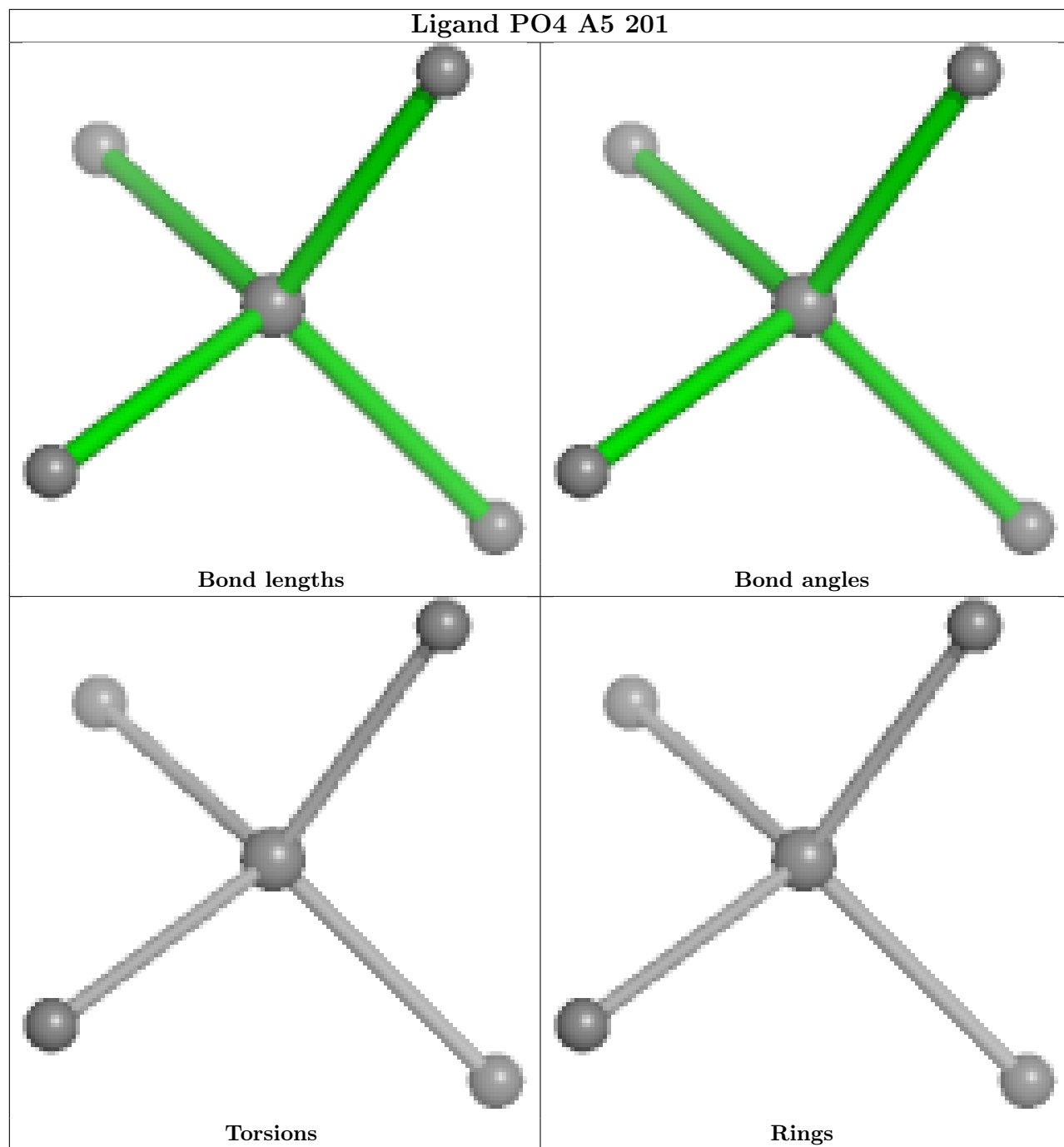


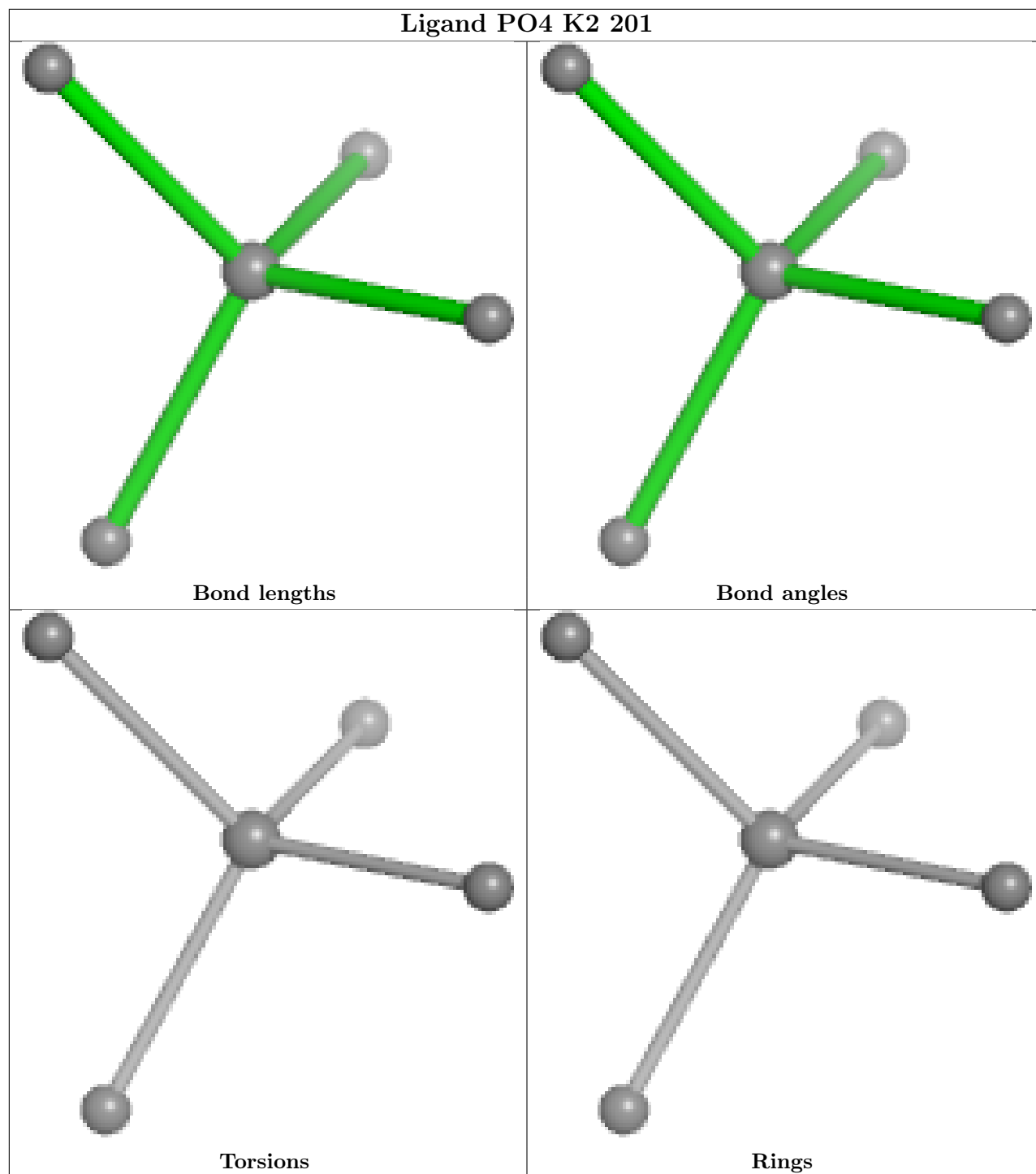


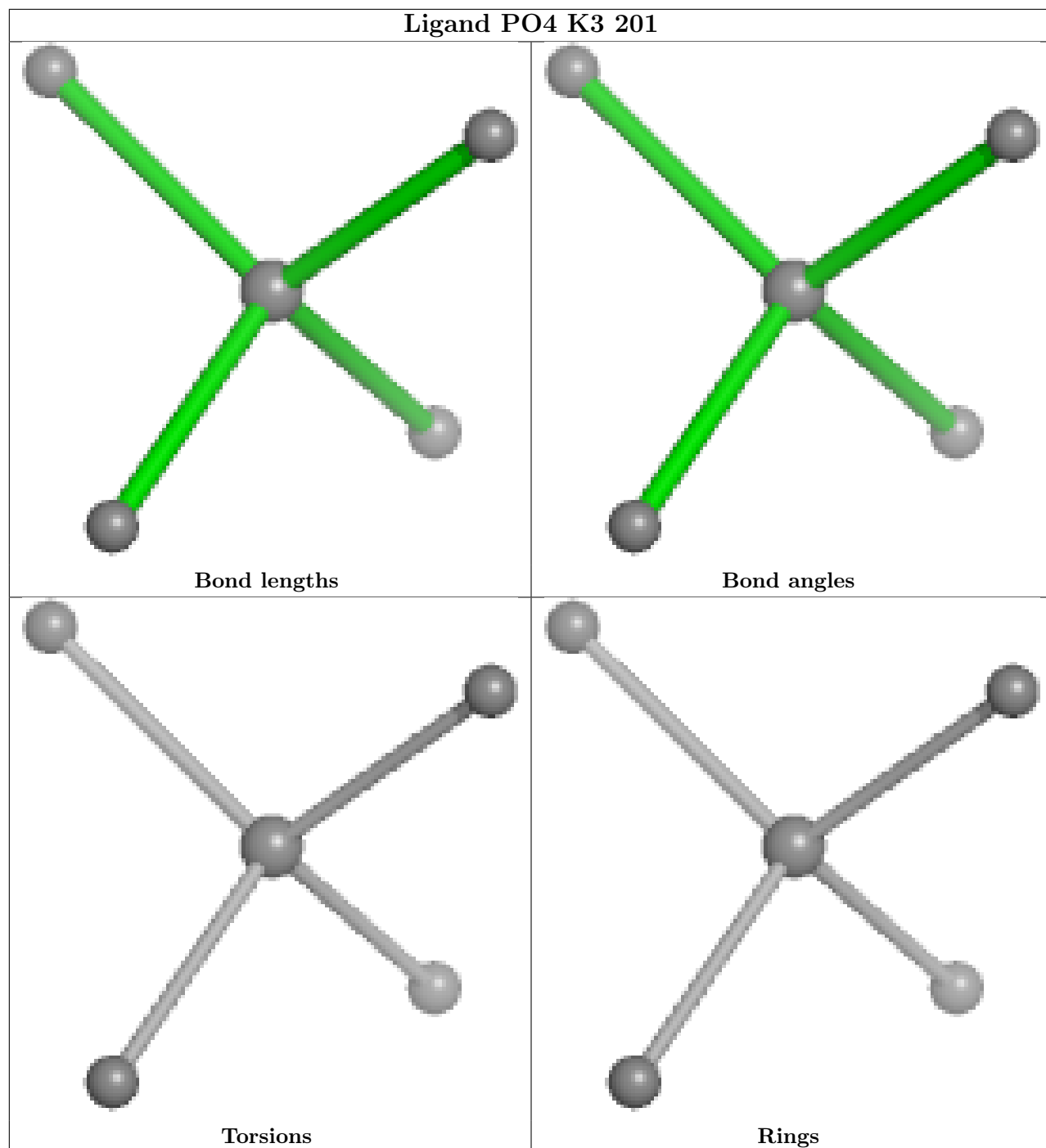


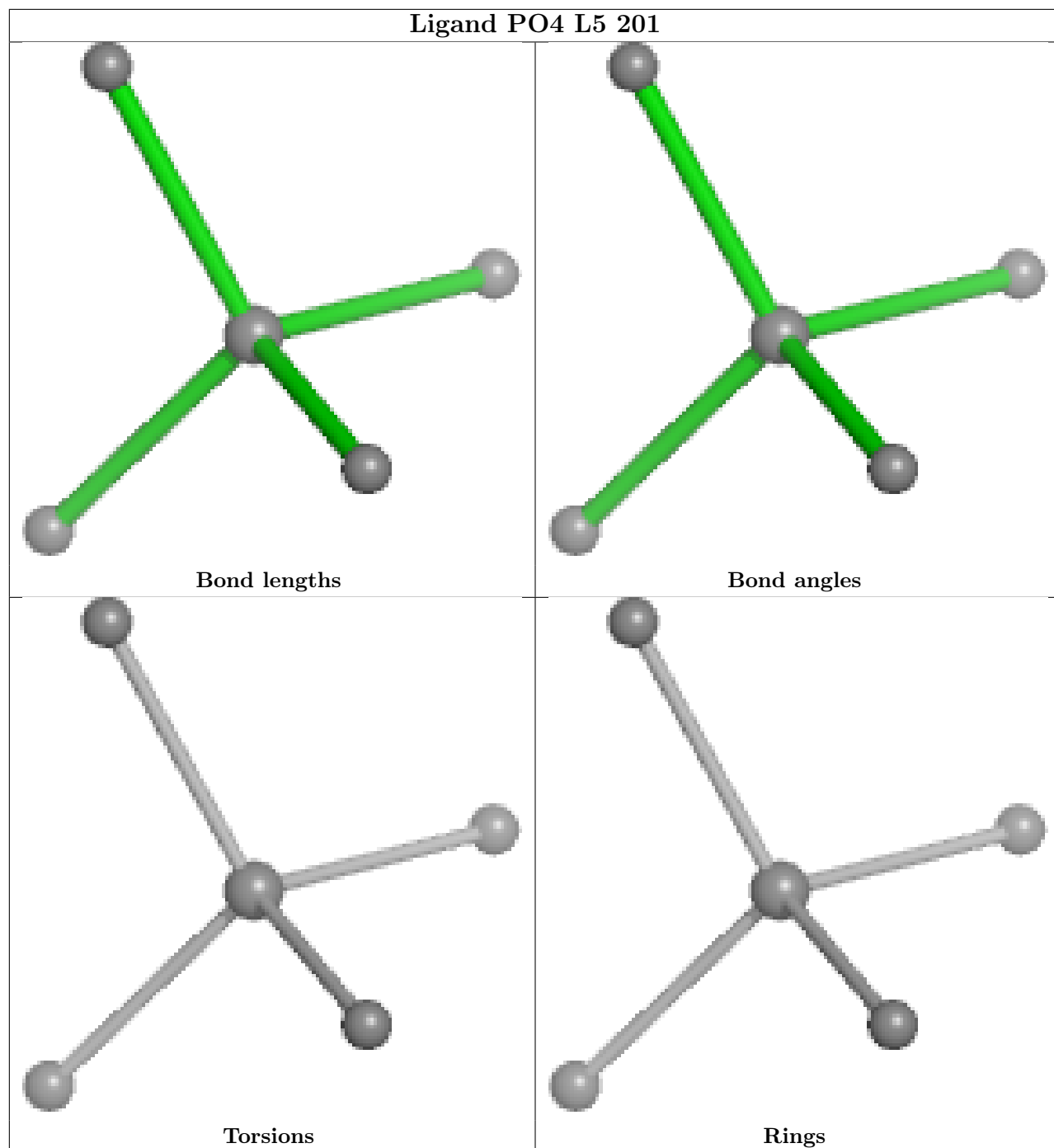


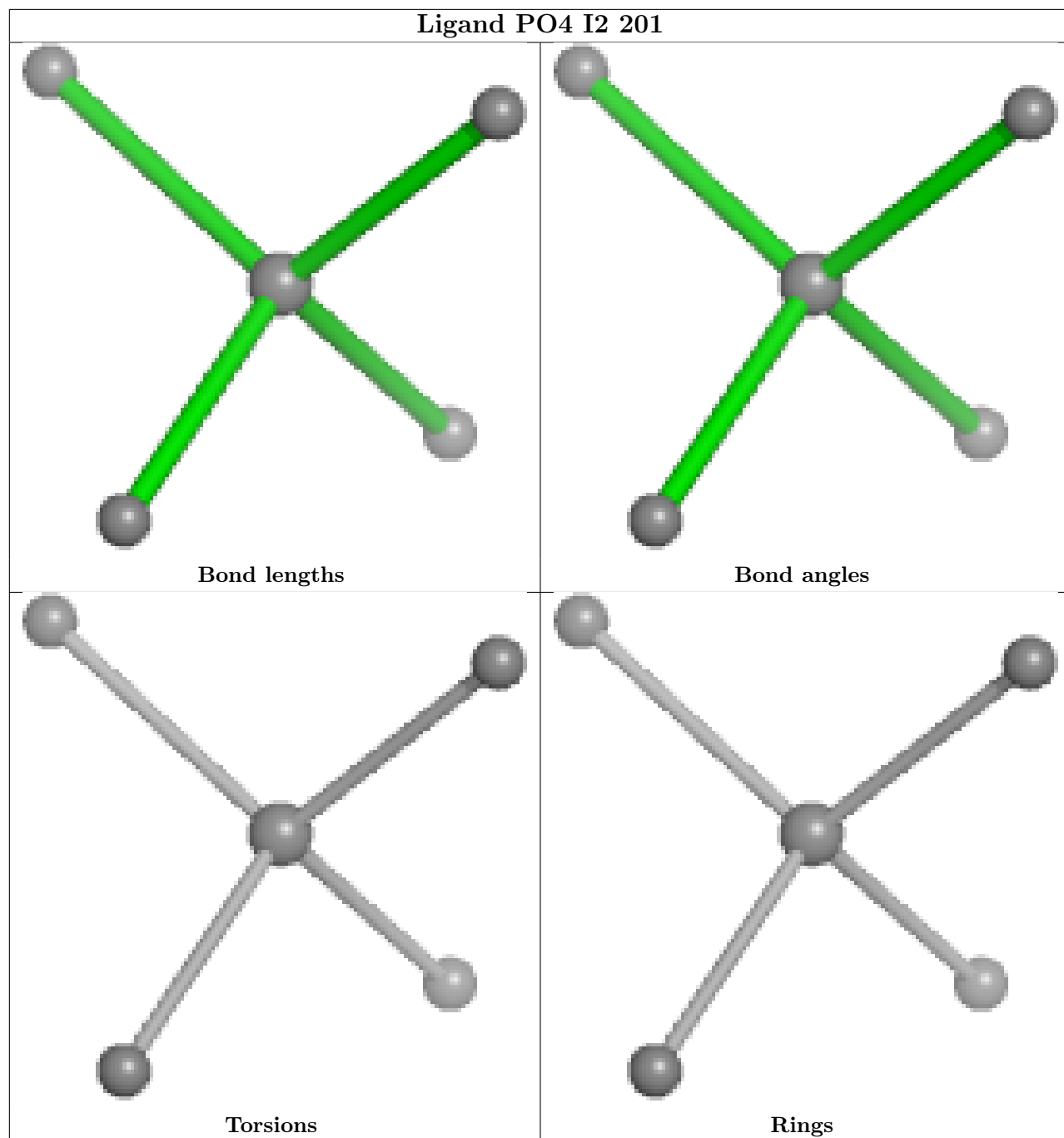


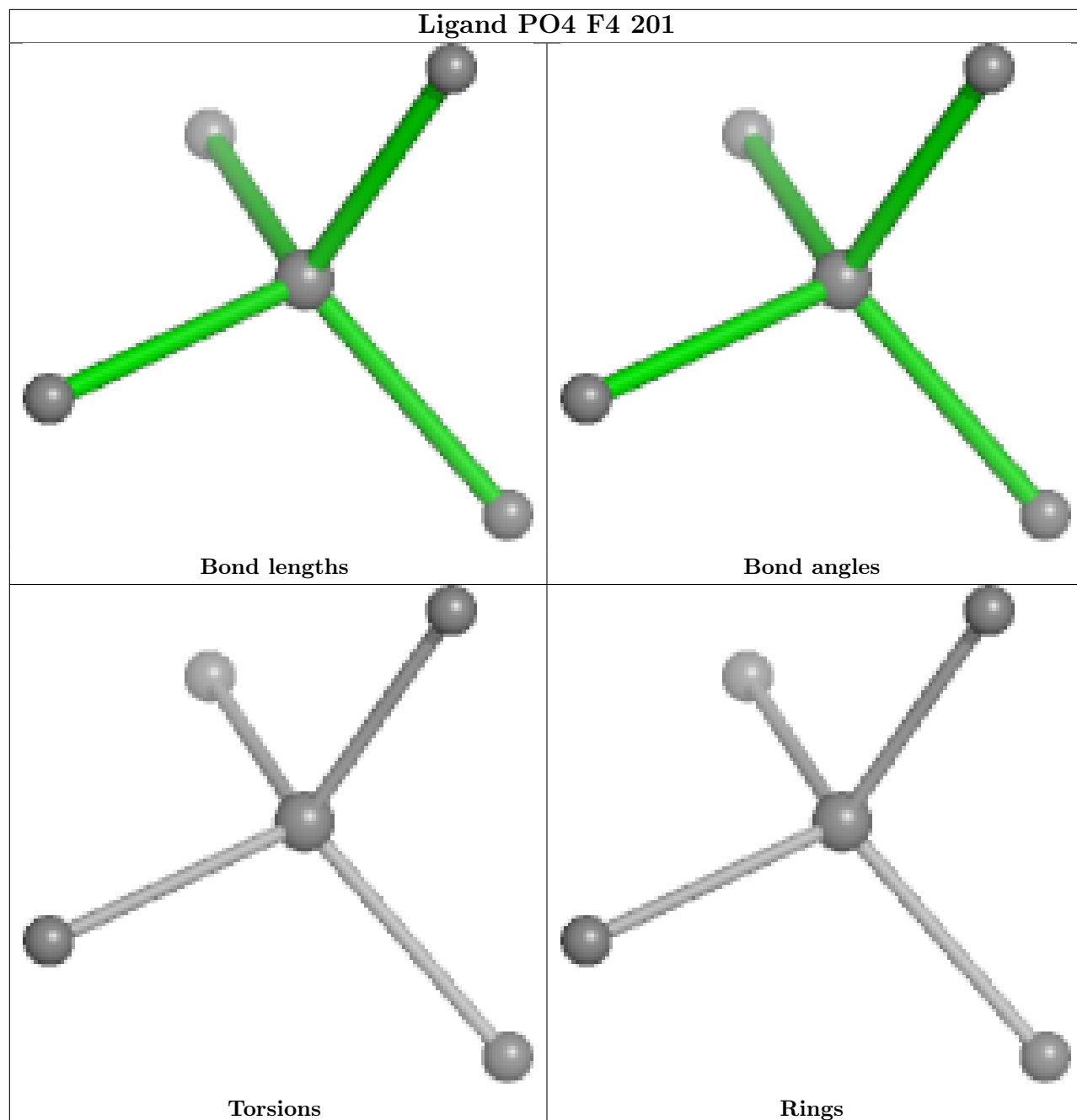


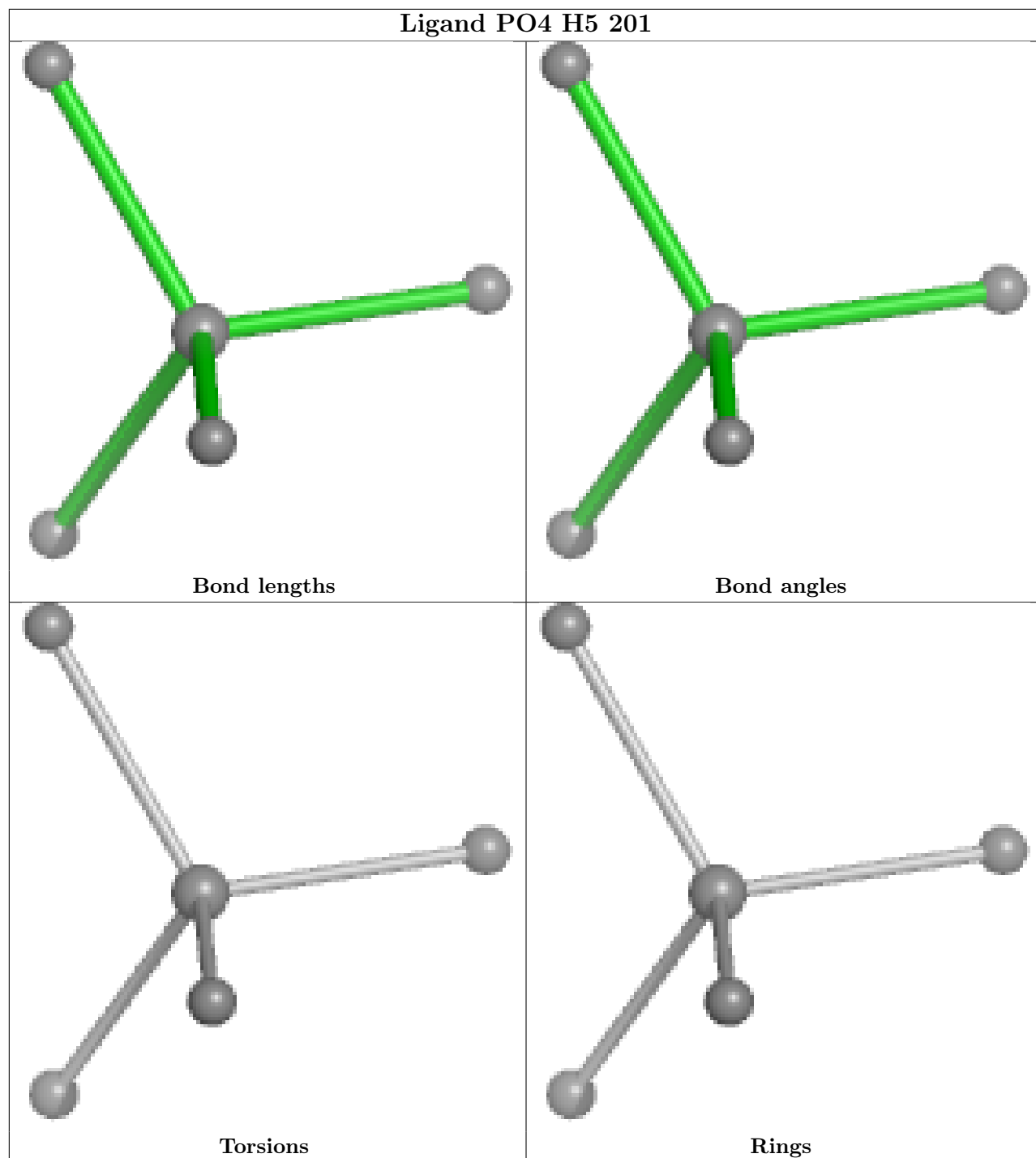


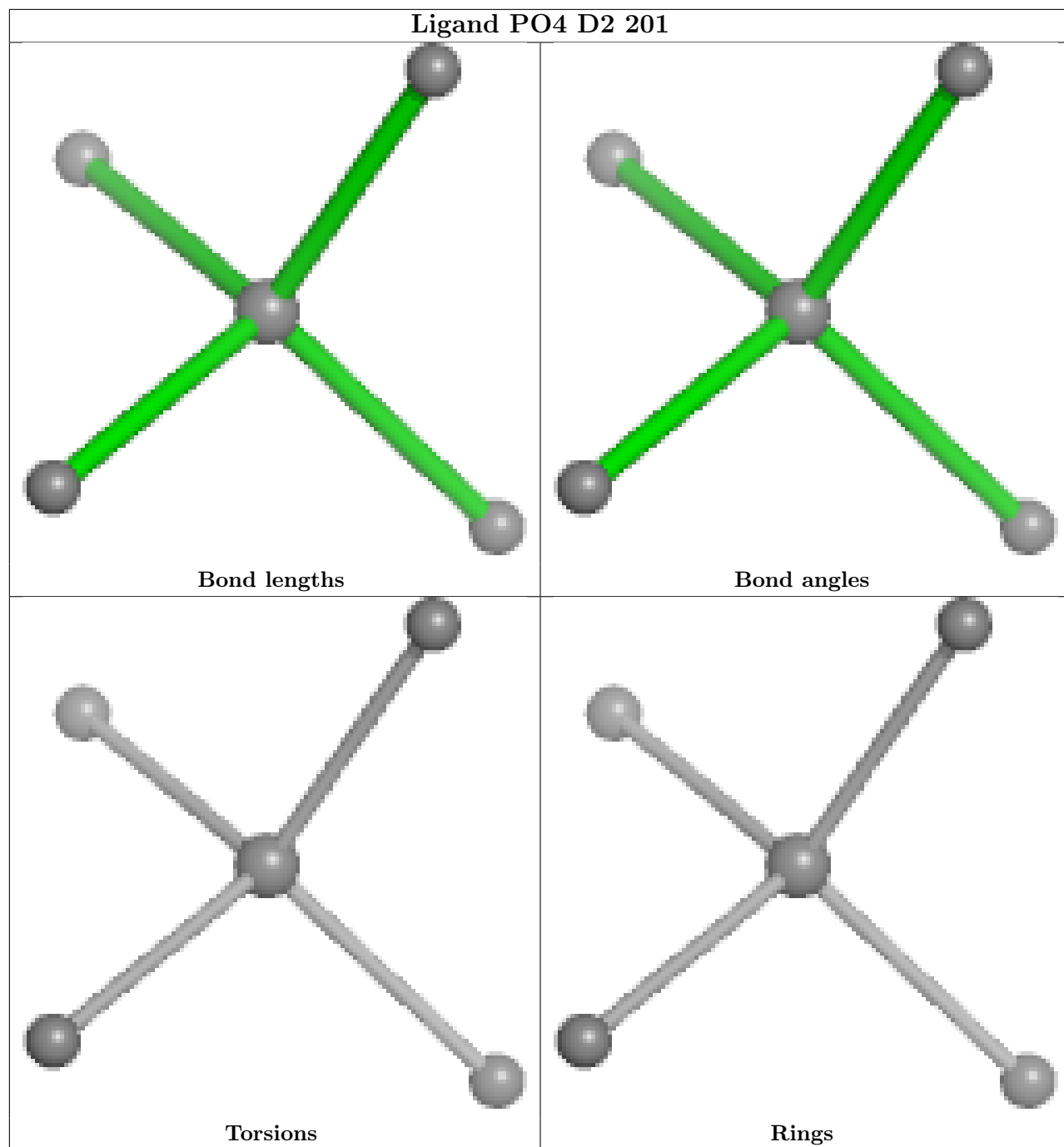


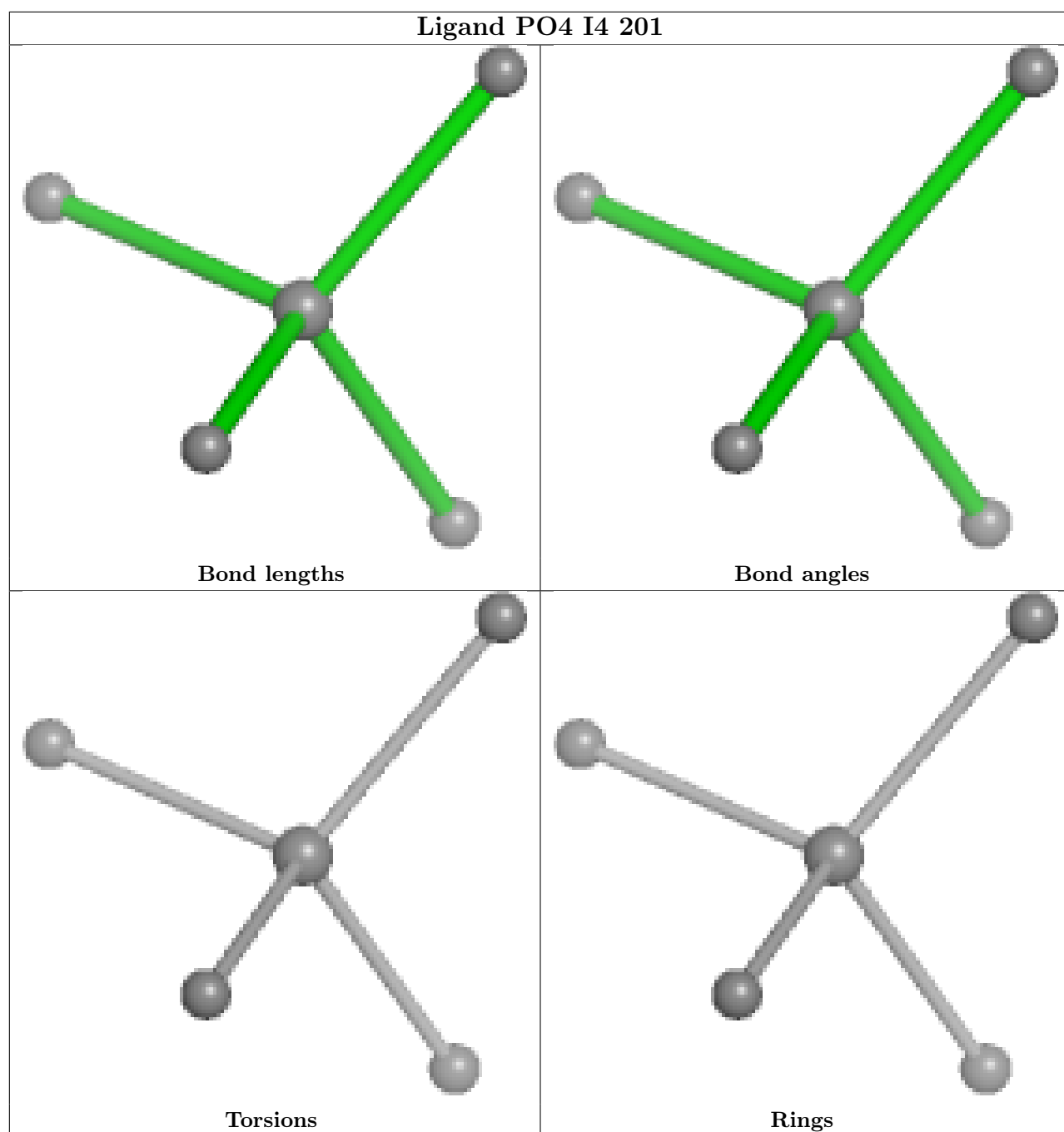


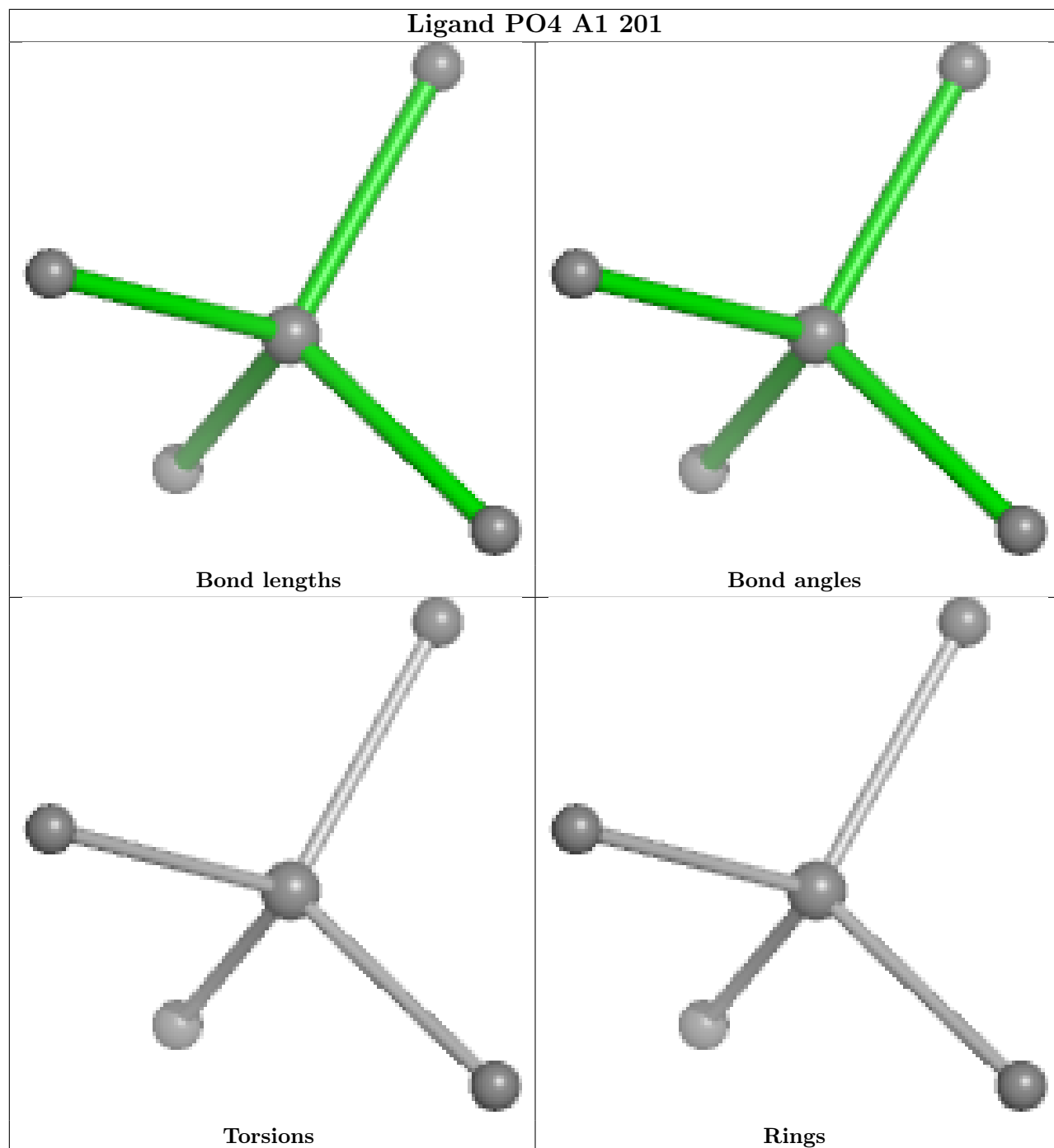


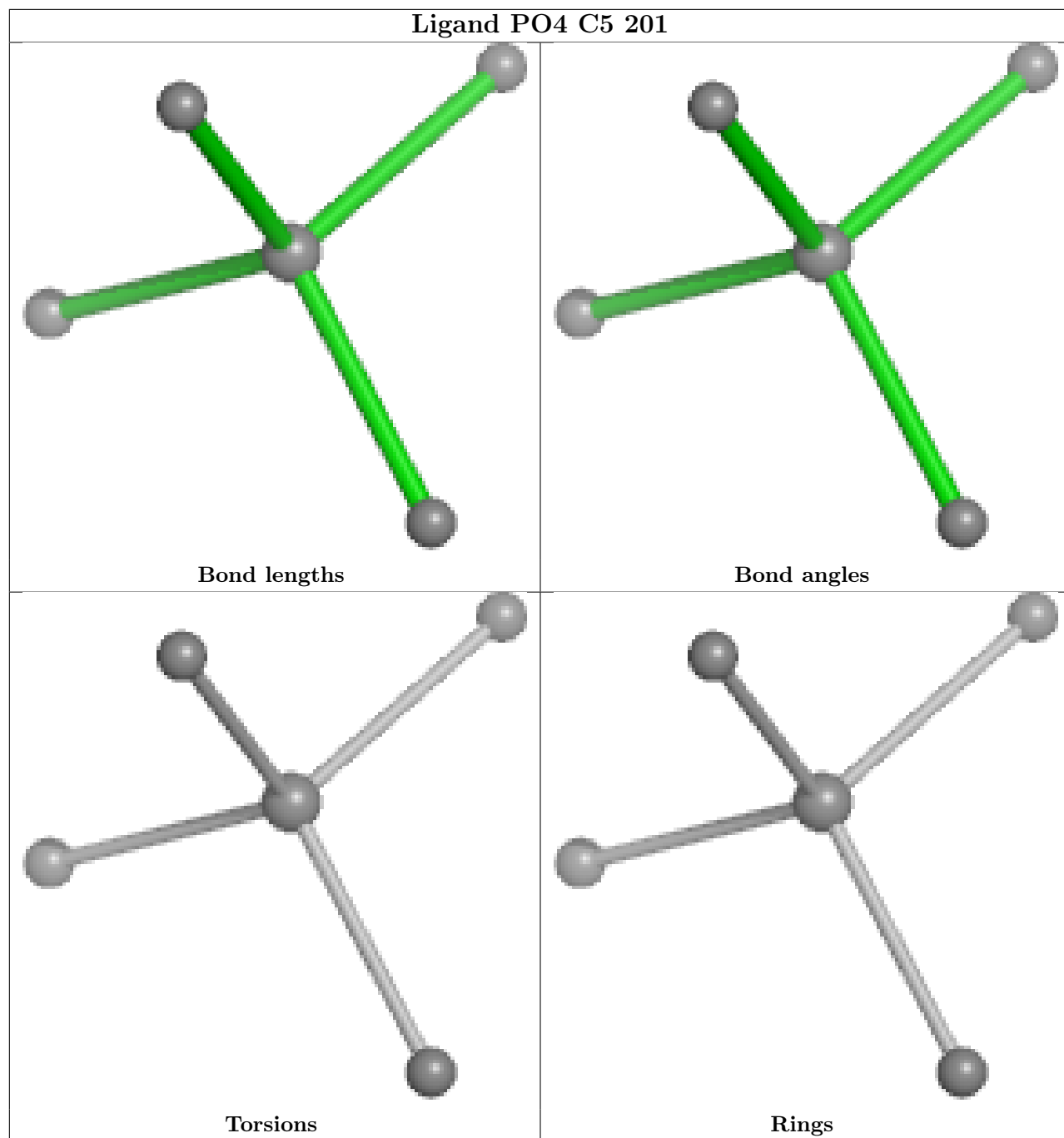


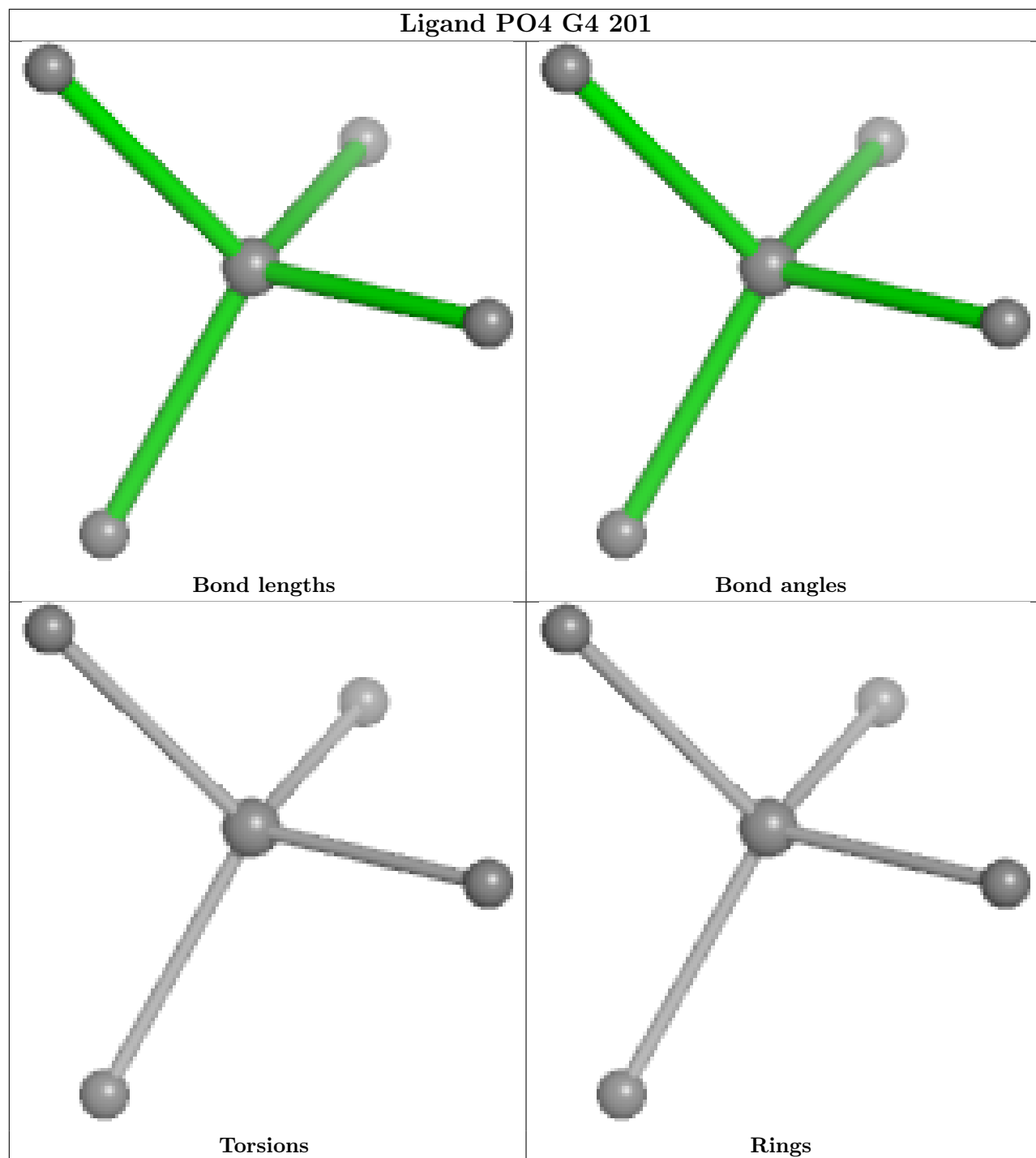


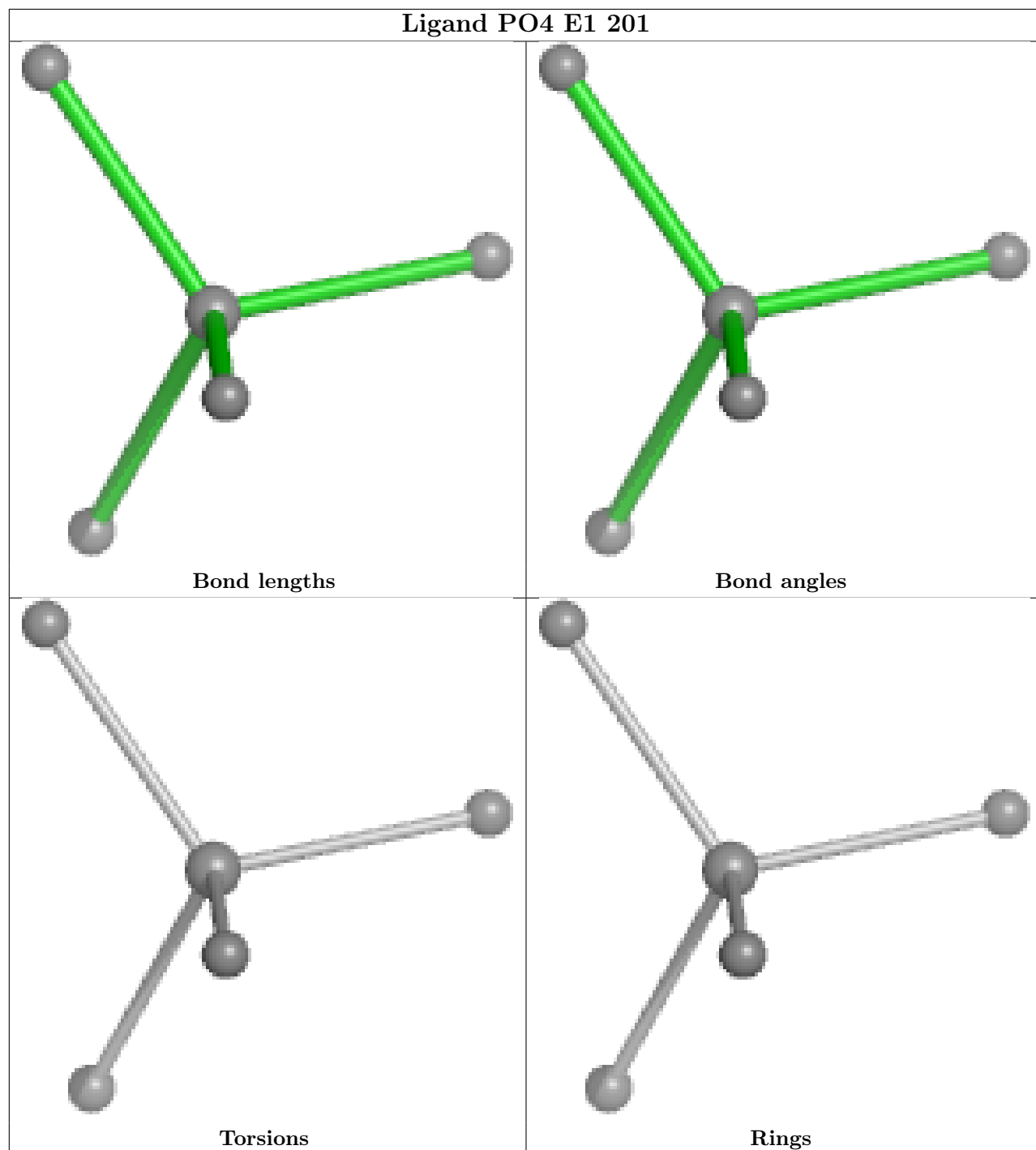


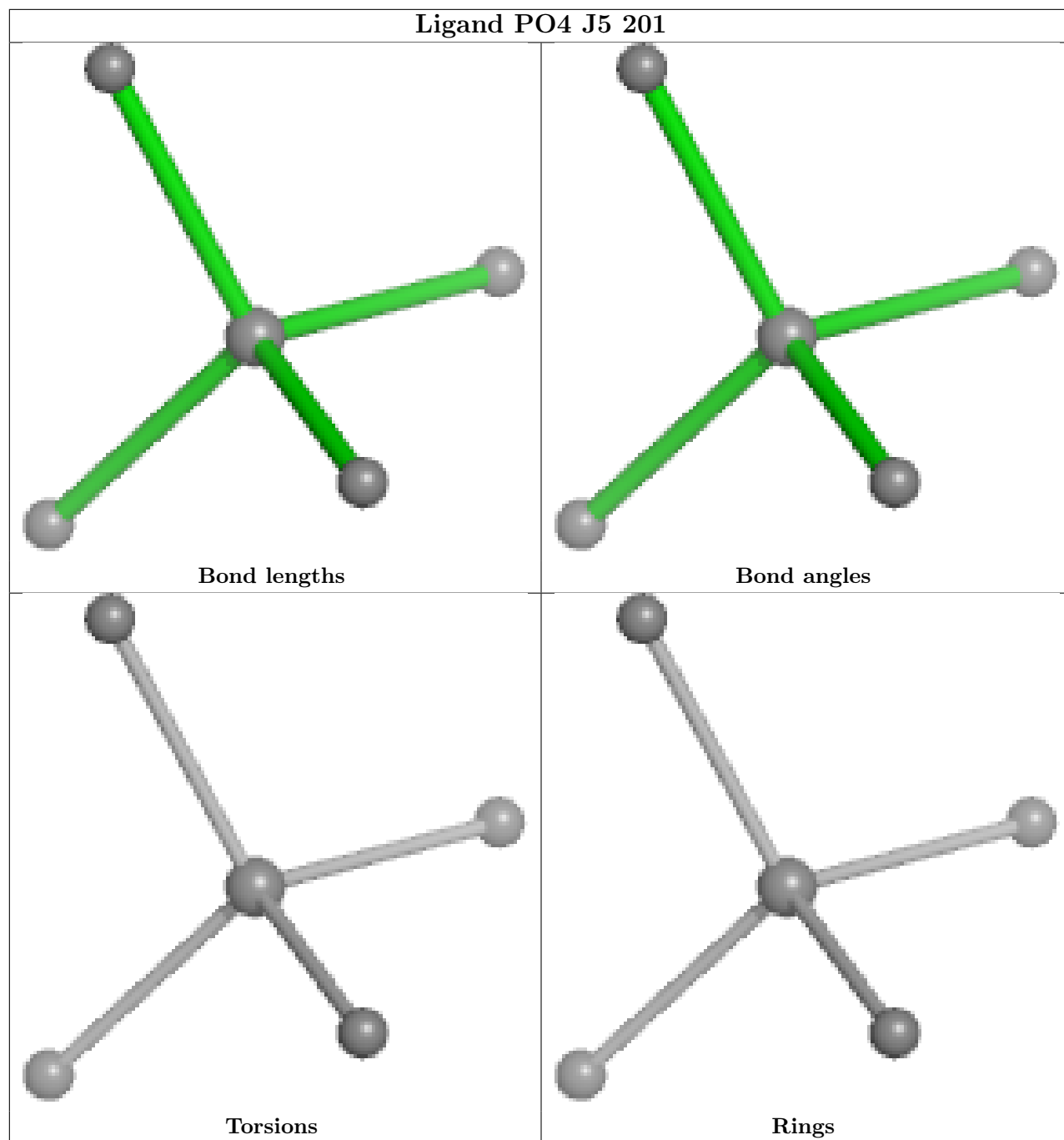


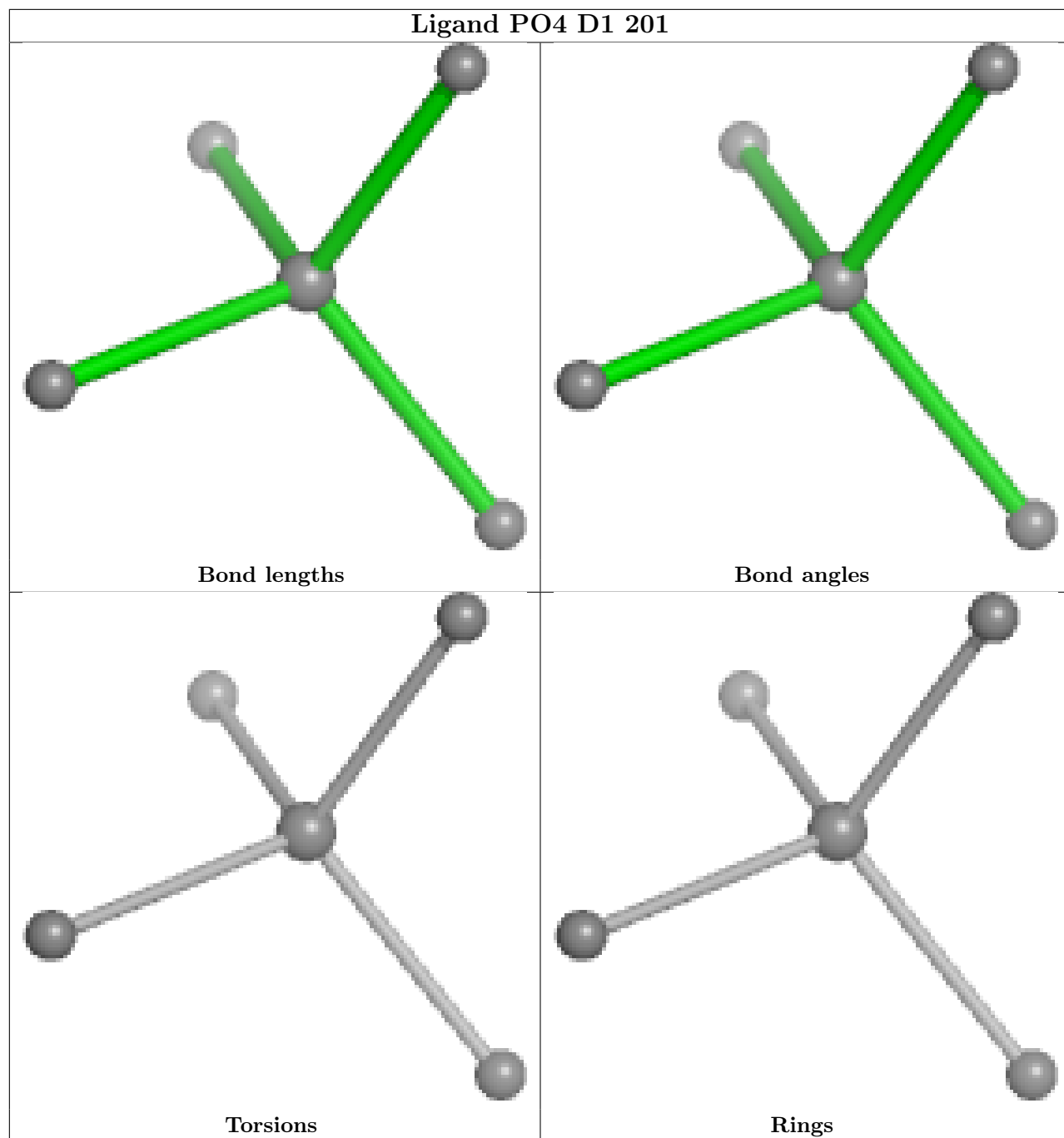


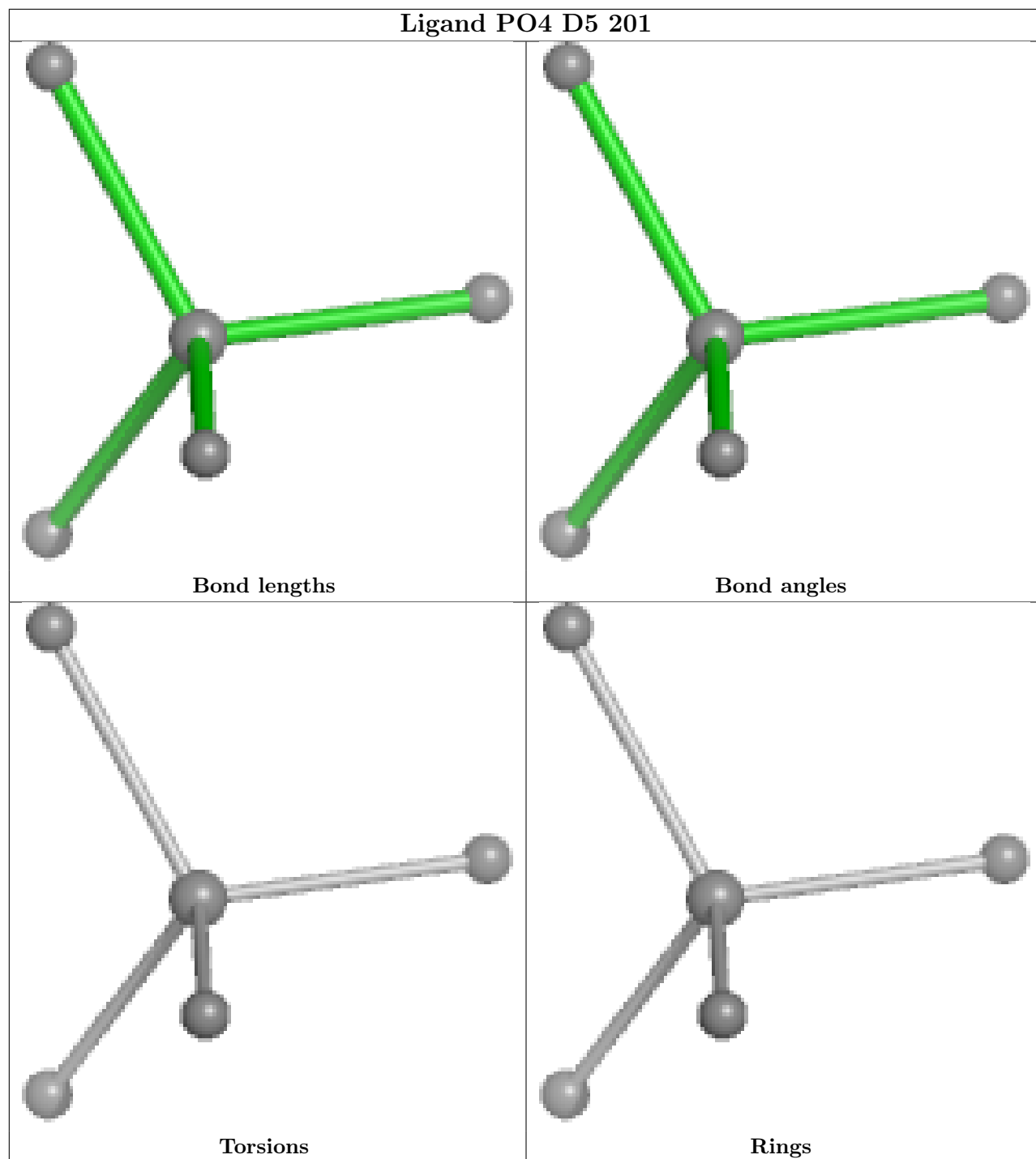


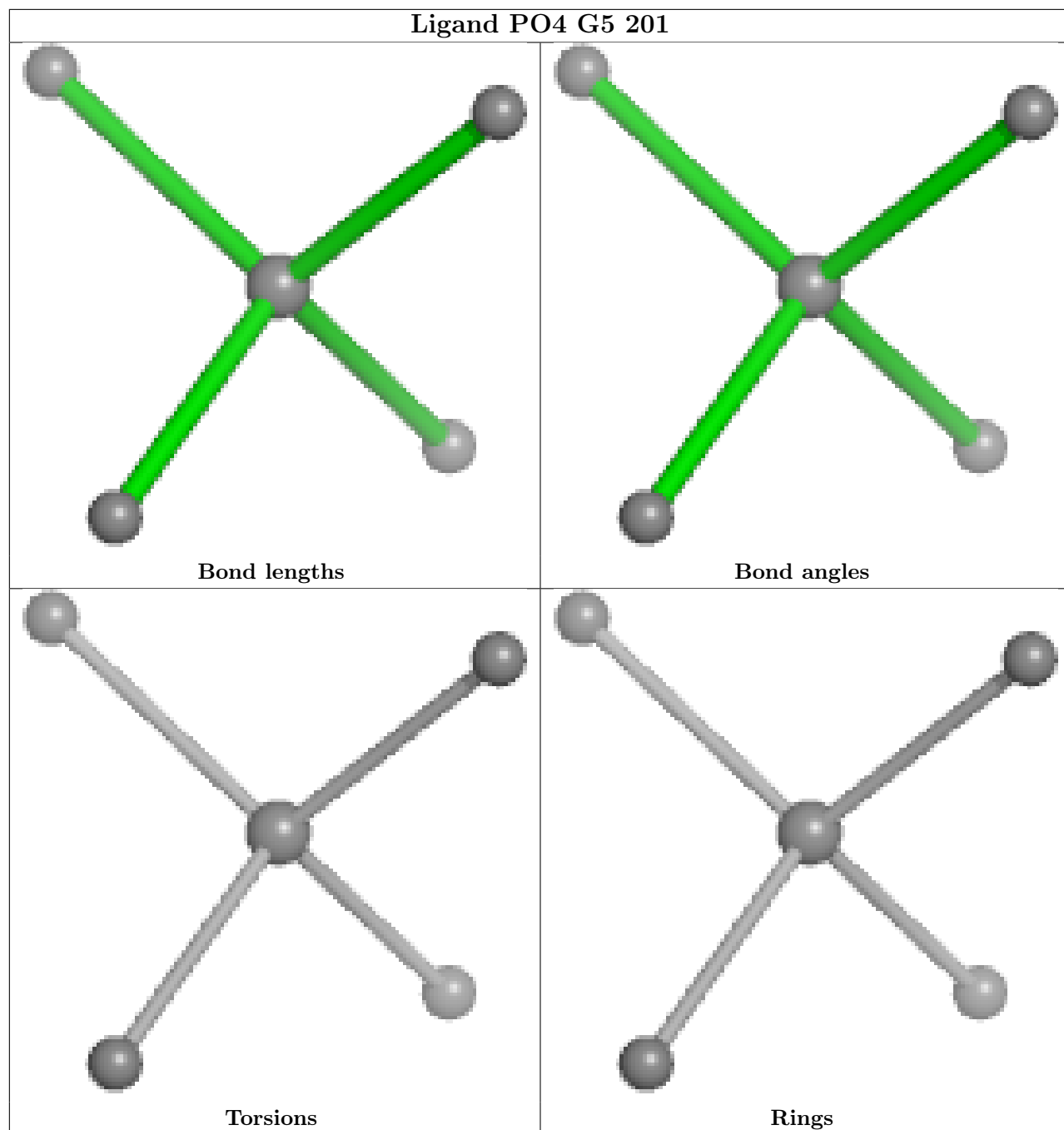


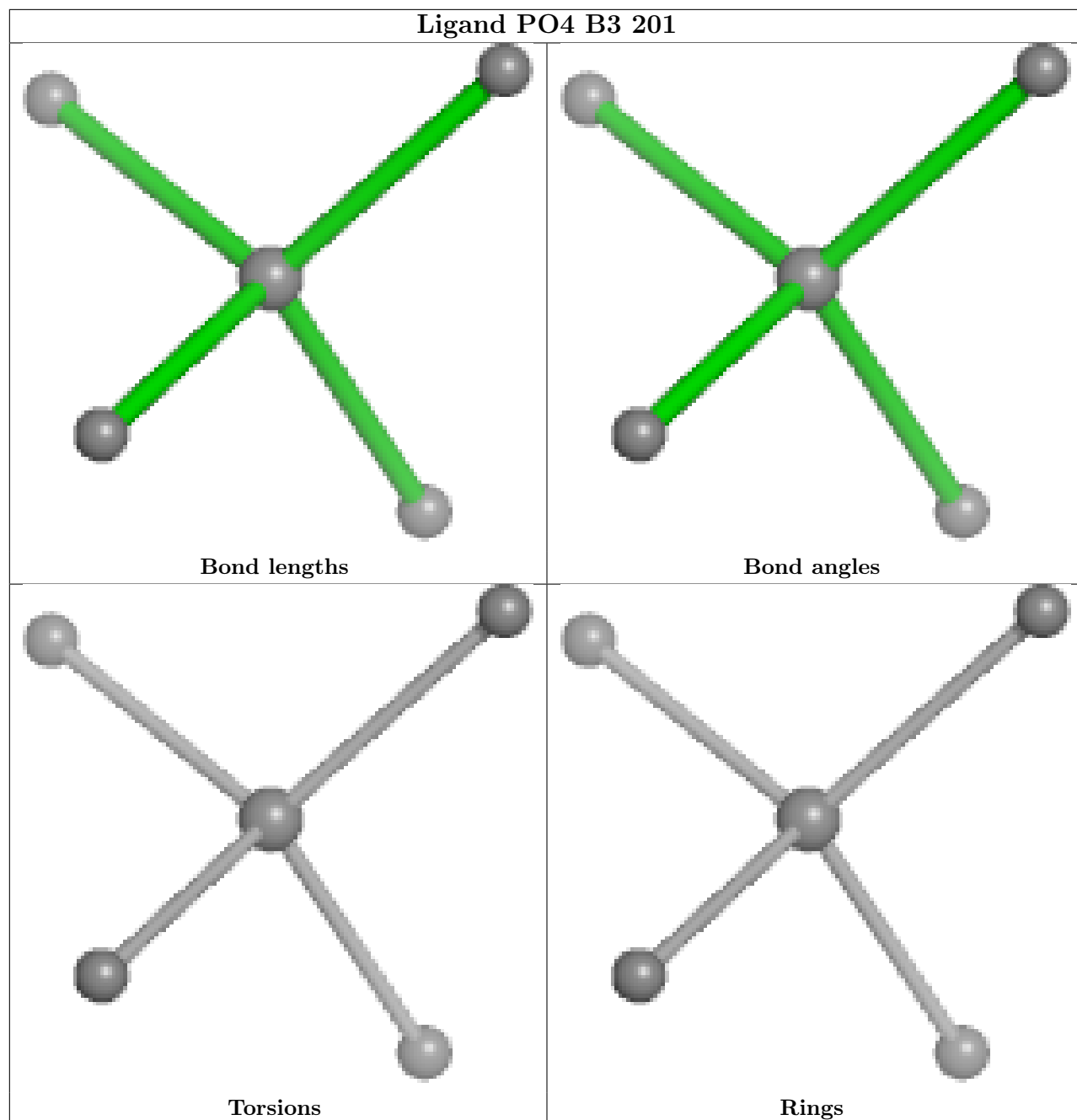


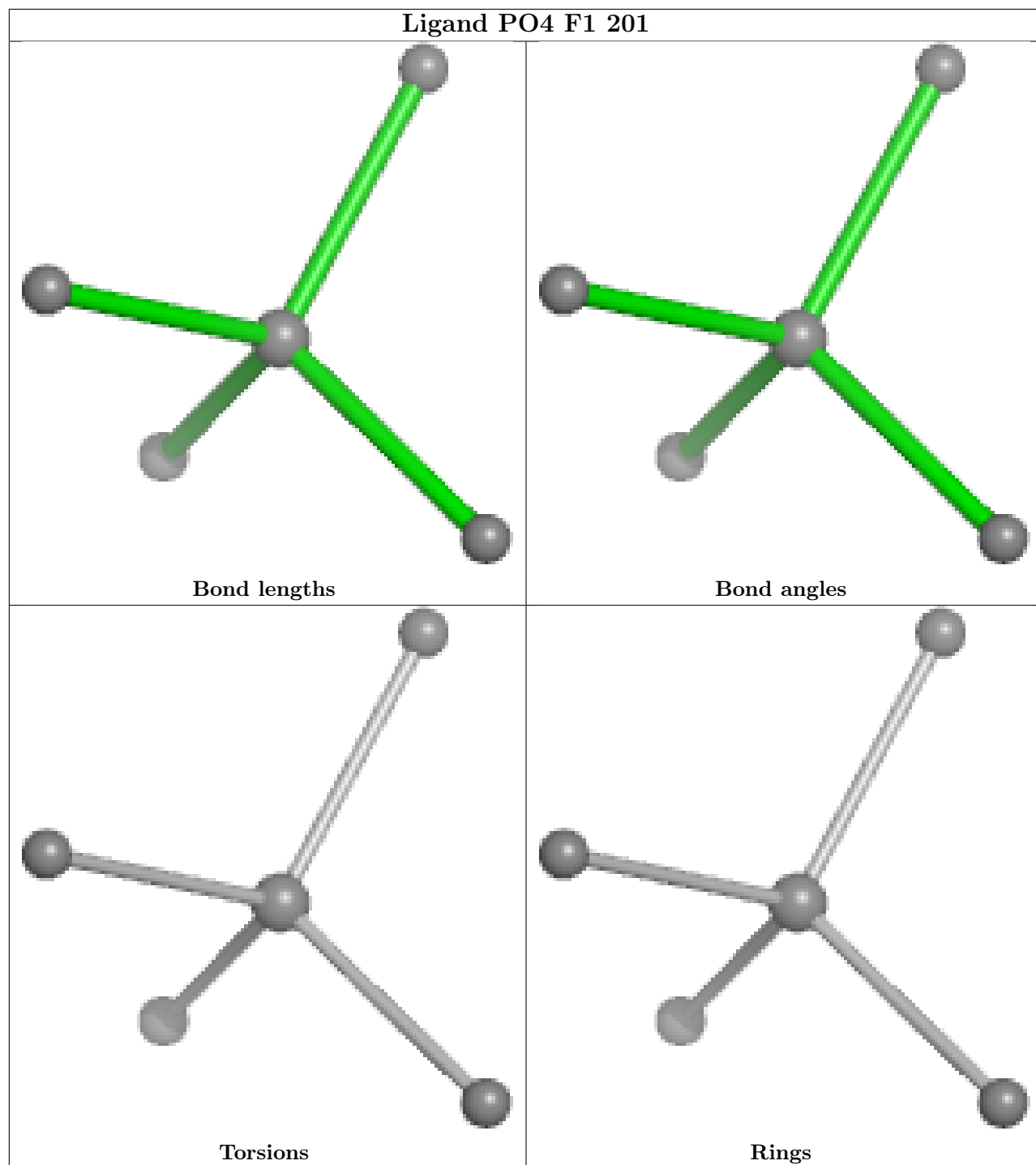


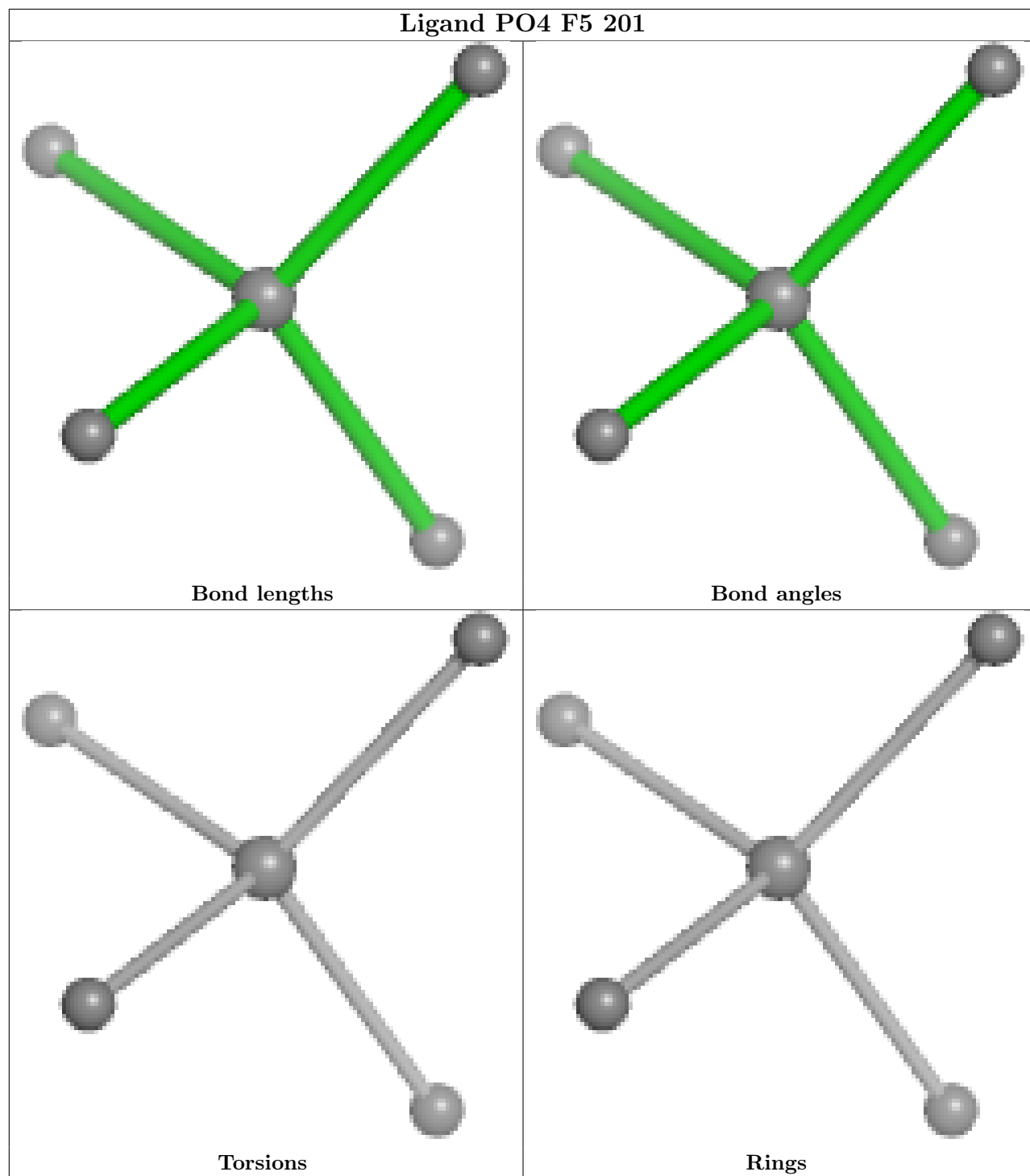


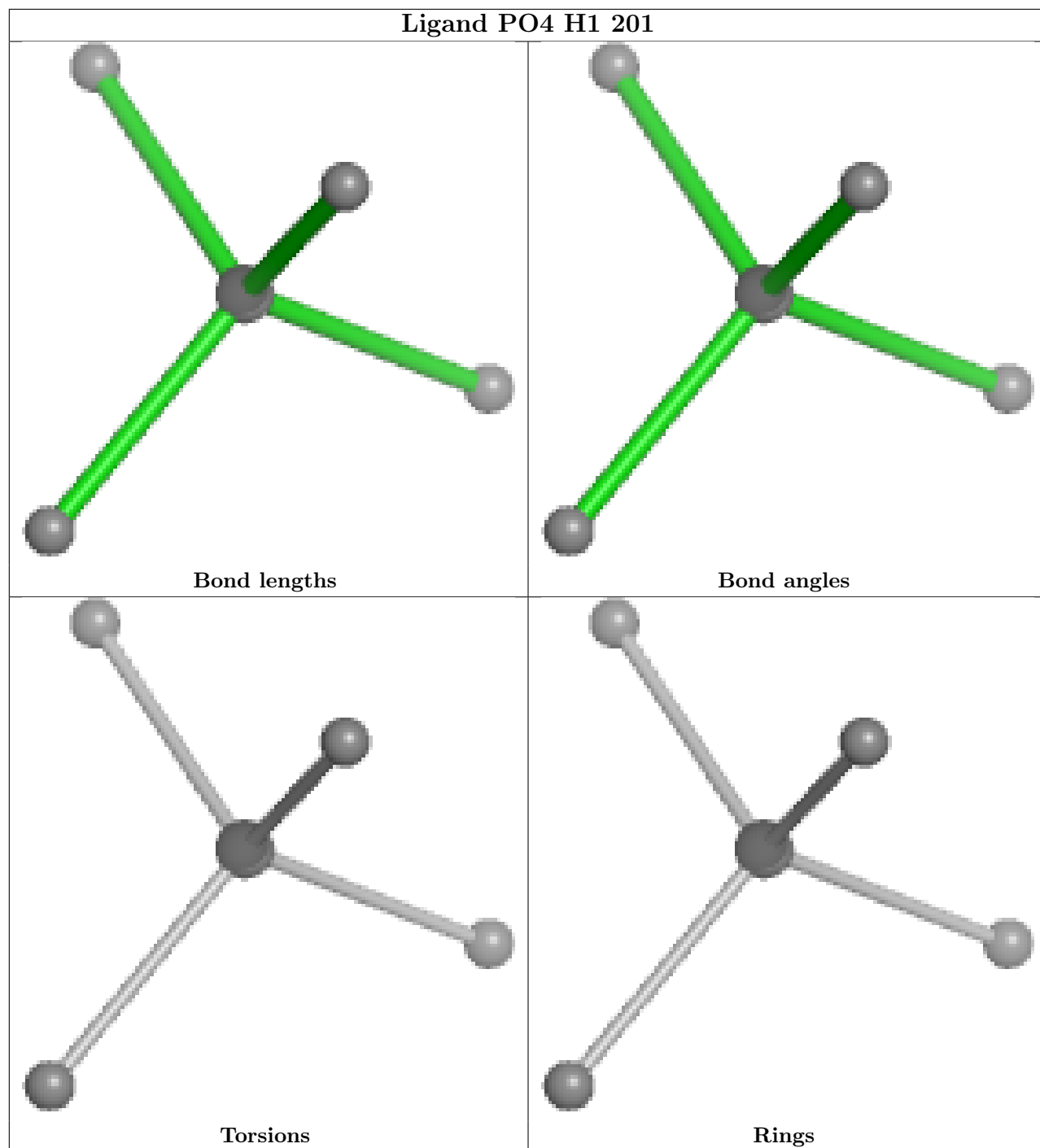


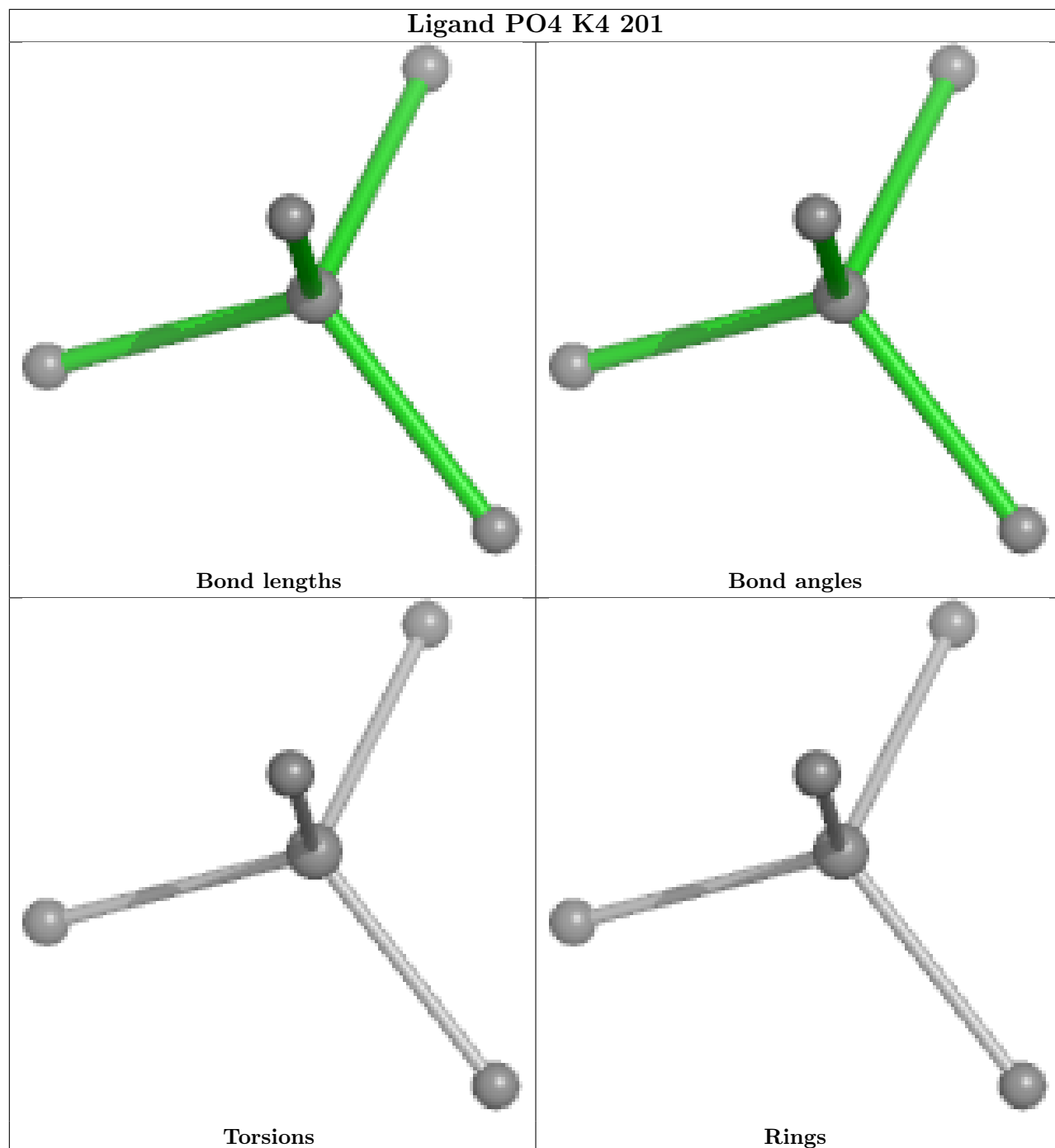


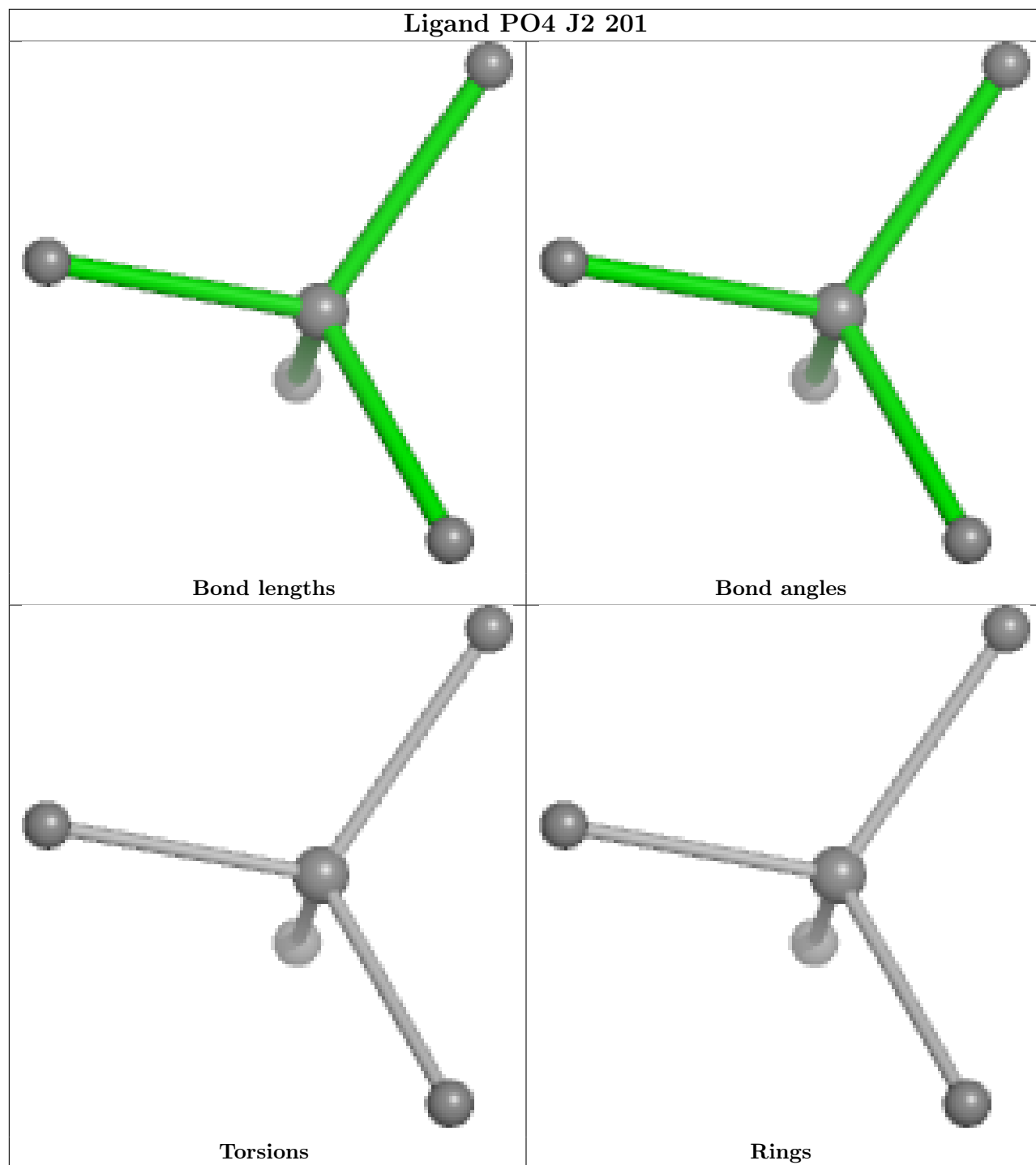


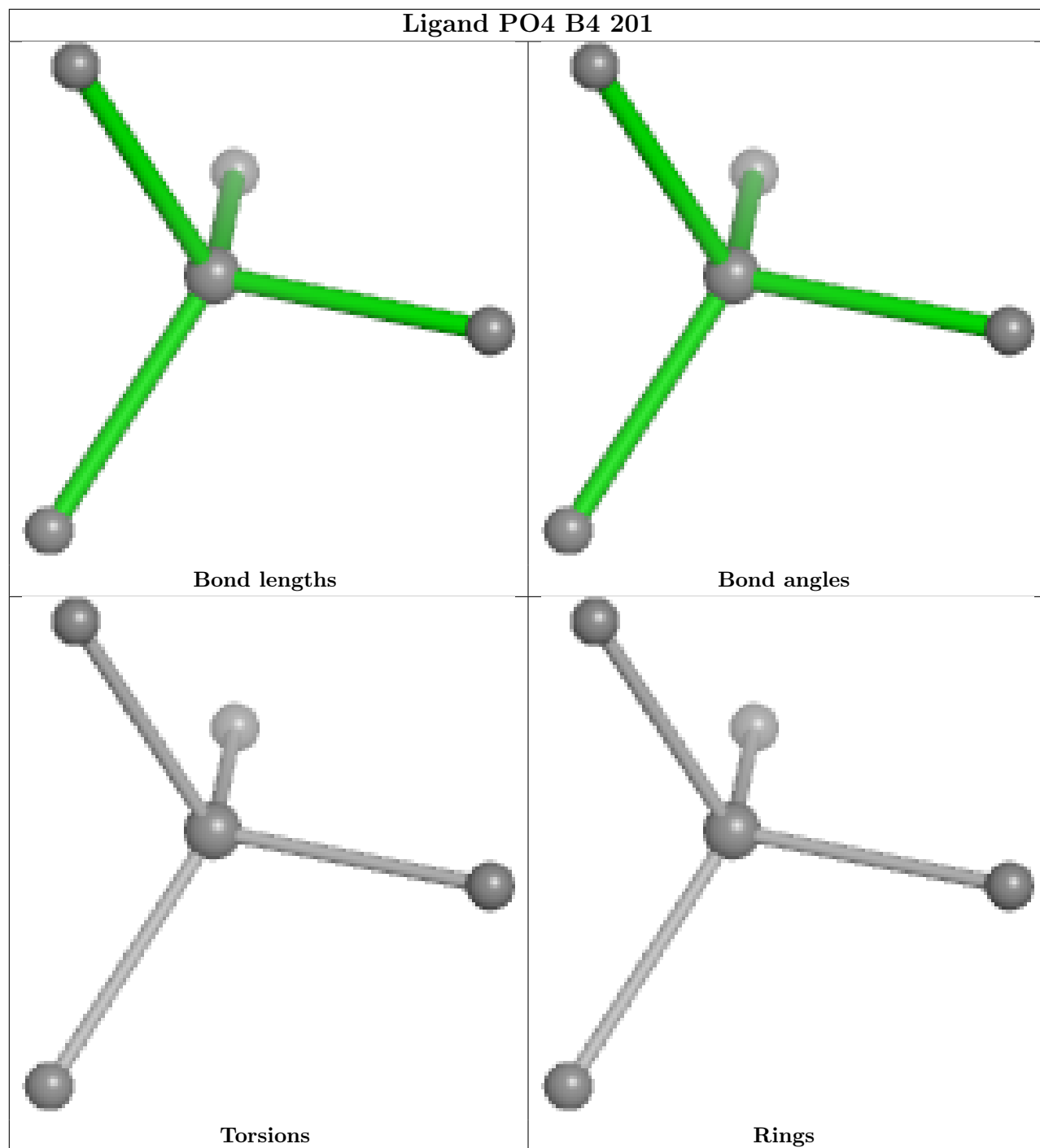


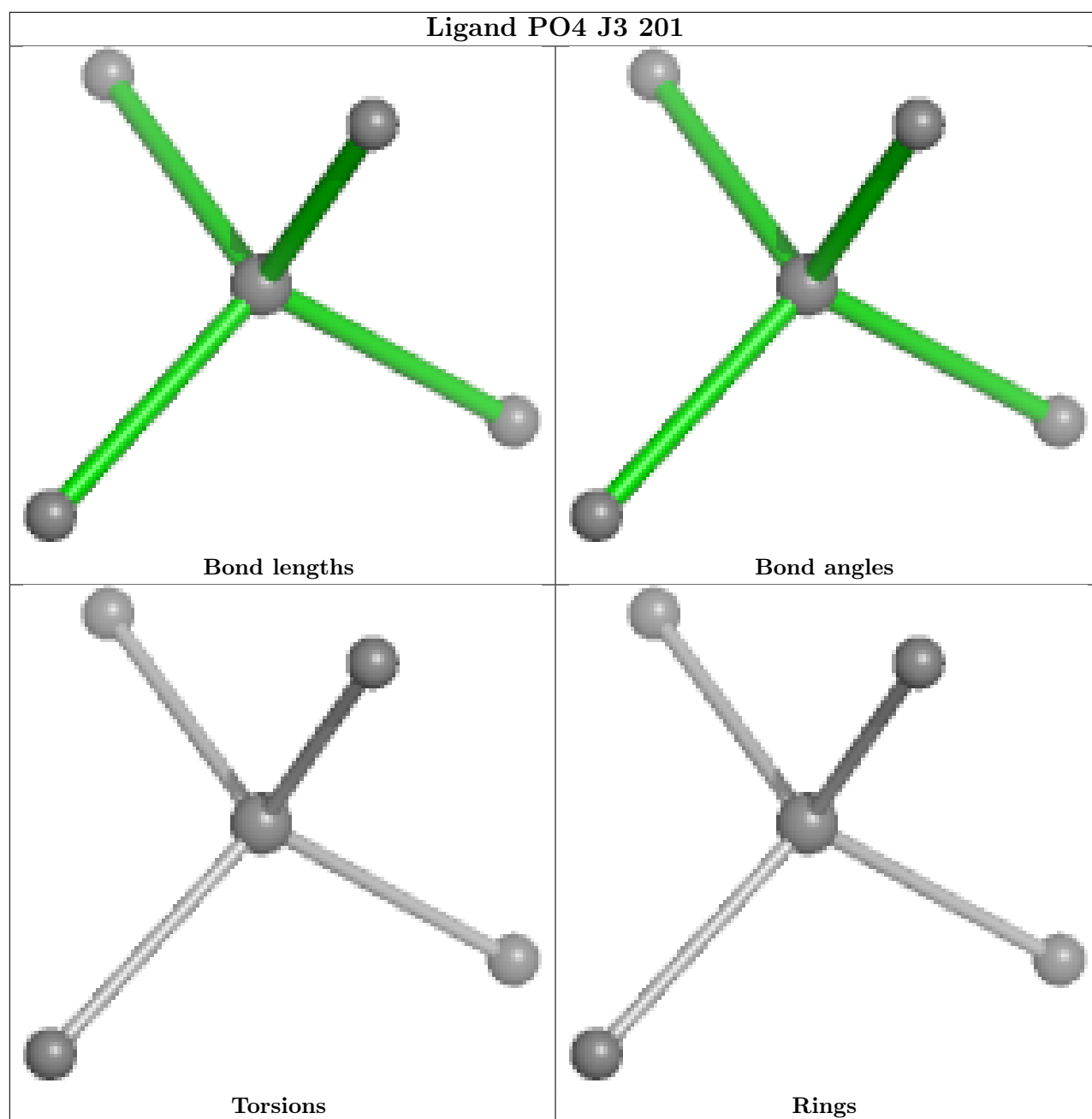












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

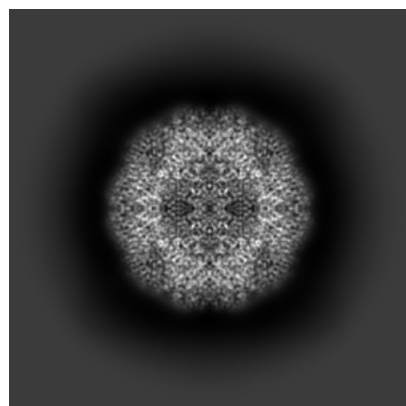
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54394. These allow visual inspection of the internal detail of the map and identification of artifacts.

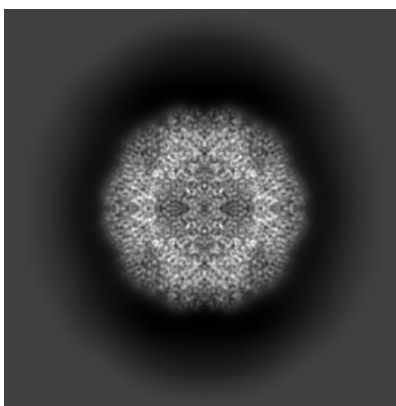
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

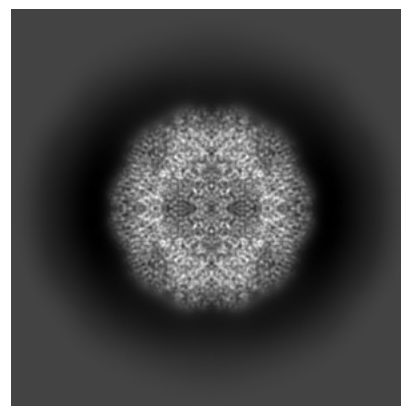
6.1.1 Primary map



X

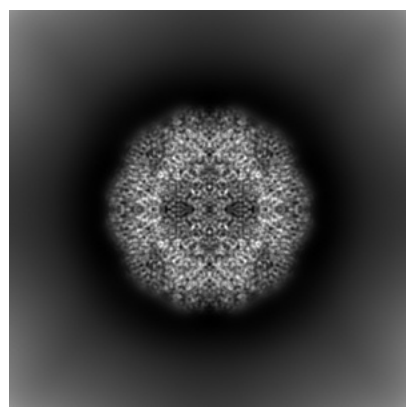


Y

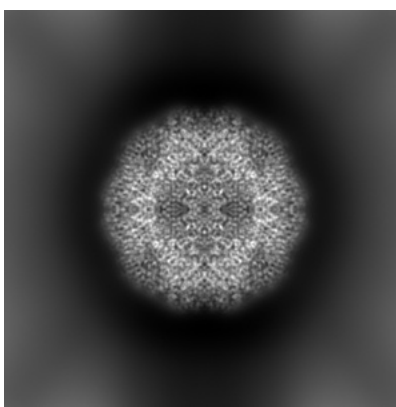


Z

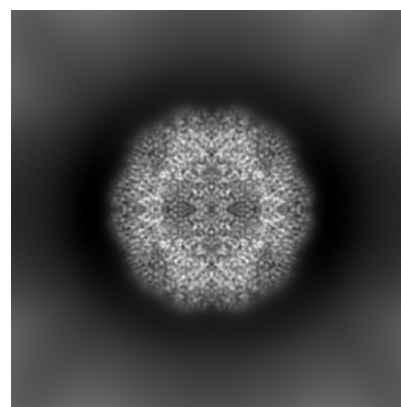
6.1.2 Raw map



X



Y

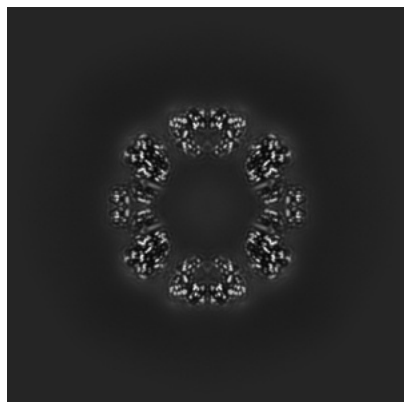


Z

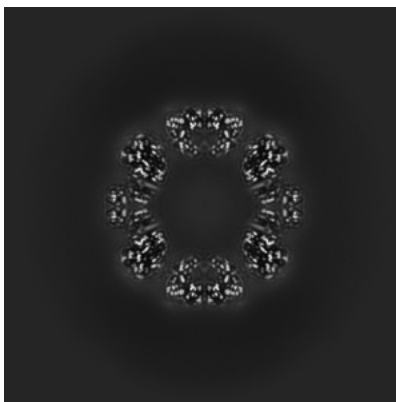
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

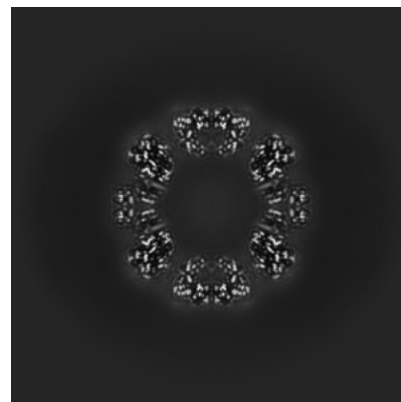
6.2.1 Primary map



X Index: 186

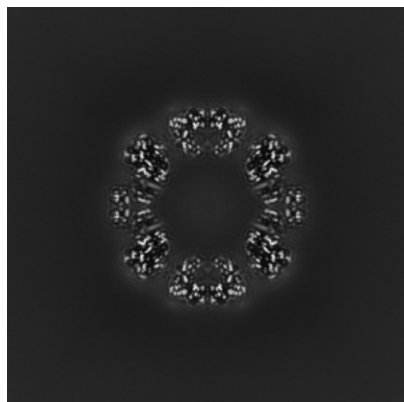


Y Index: 186

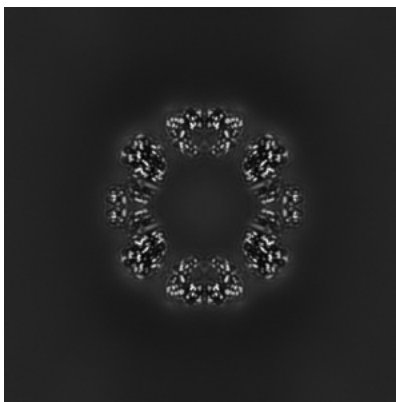


Z Index: 186

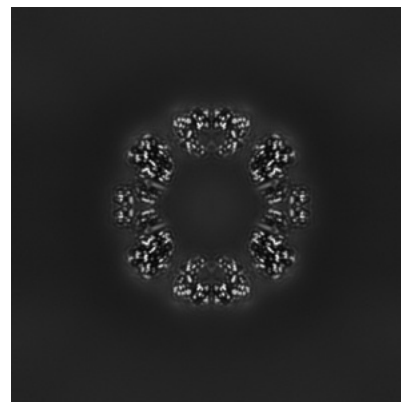
6.2.2 Raw map



X Index: 186



Y Index: 186

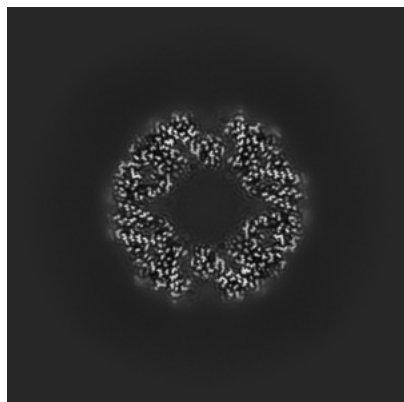


Z Index: 186

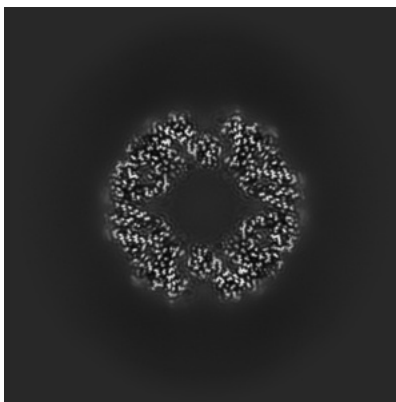
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

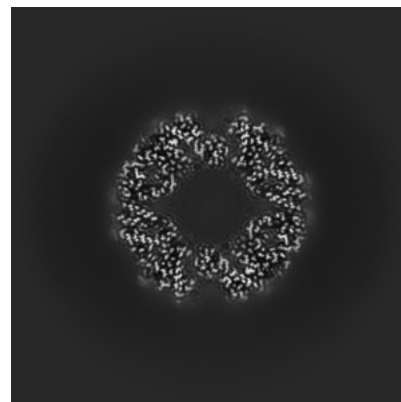
6.3.1 Primary map



X Index: 157

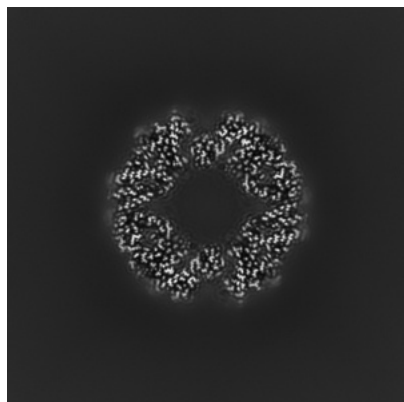


Y Index: 157

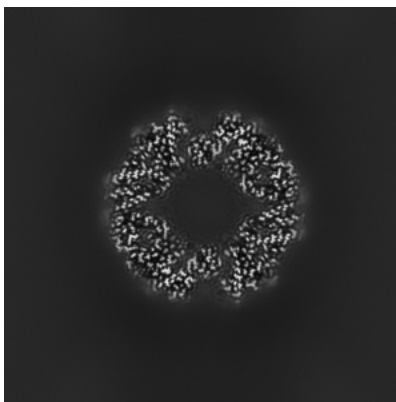


Z Index: 157

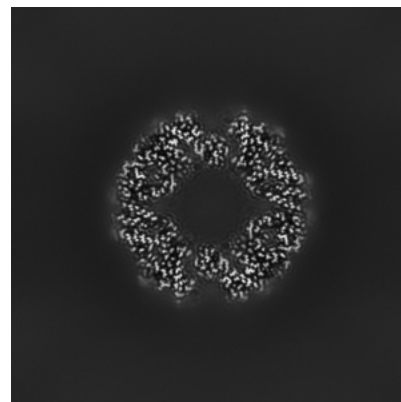
6.3.2 Raw map



X Index: 215



Y Index: 215

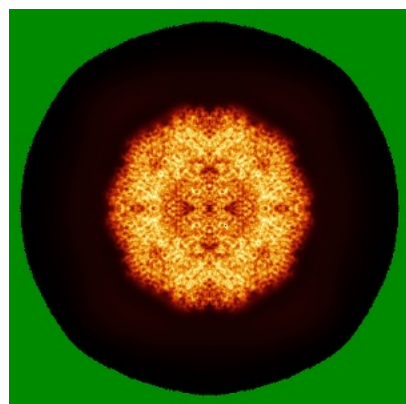


Z Index: 157

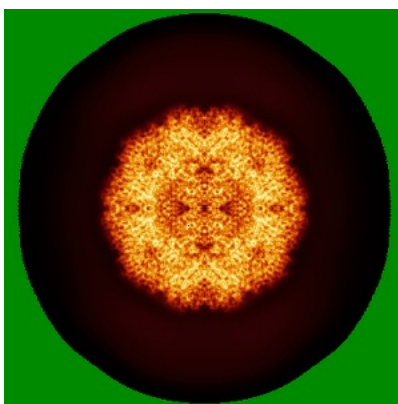
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

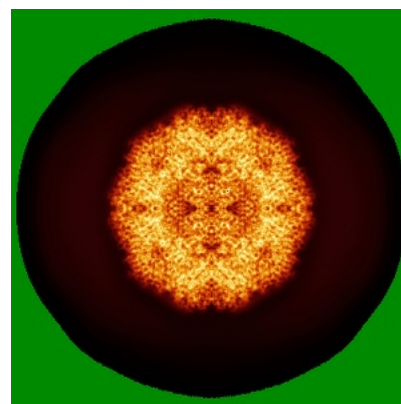
6.4.1 Primary map



X

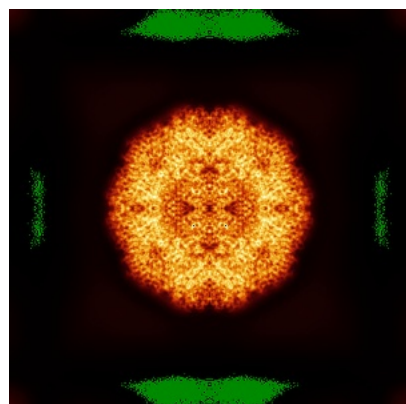


Y

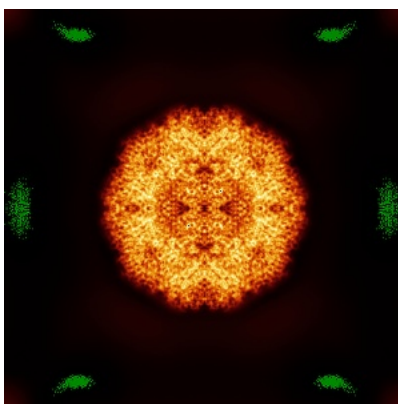


Z

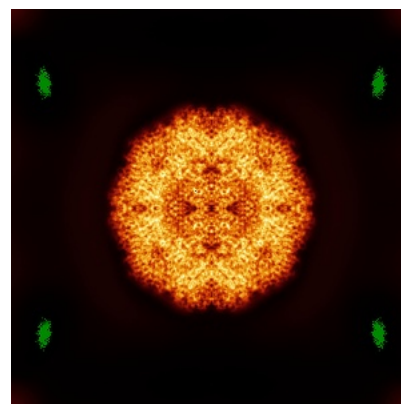
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

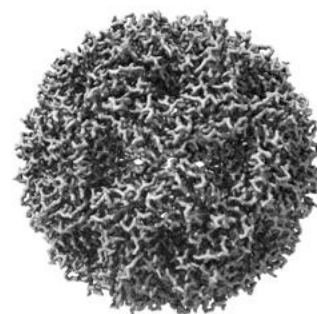
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

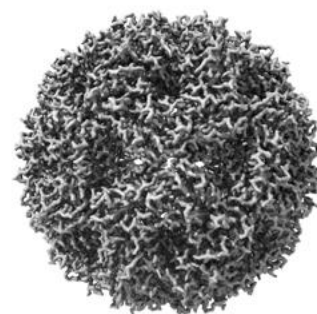
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

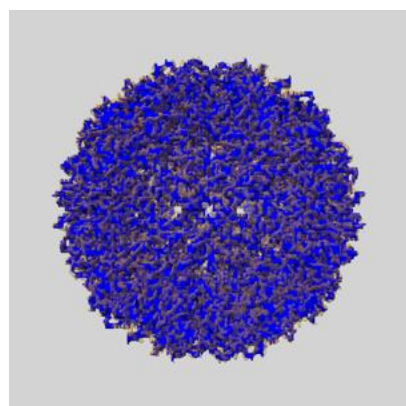
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

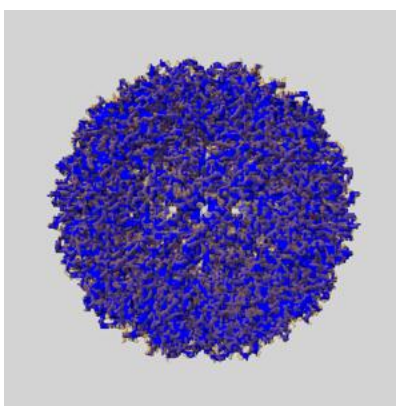
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

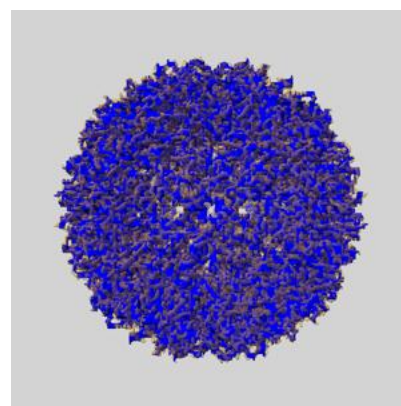
6.6.1 emd_54394_msk_1.map [i](#)



X



Y

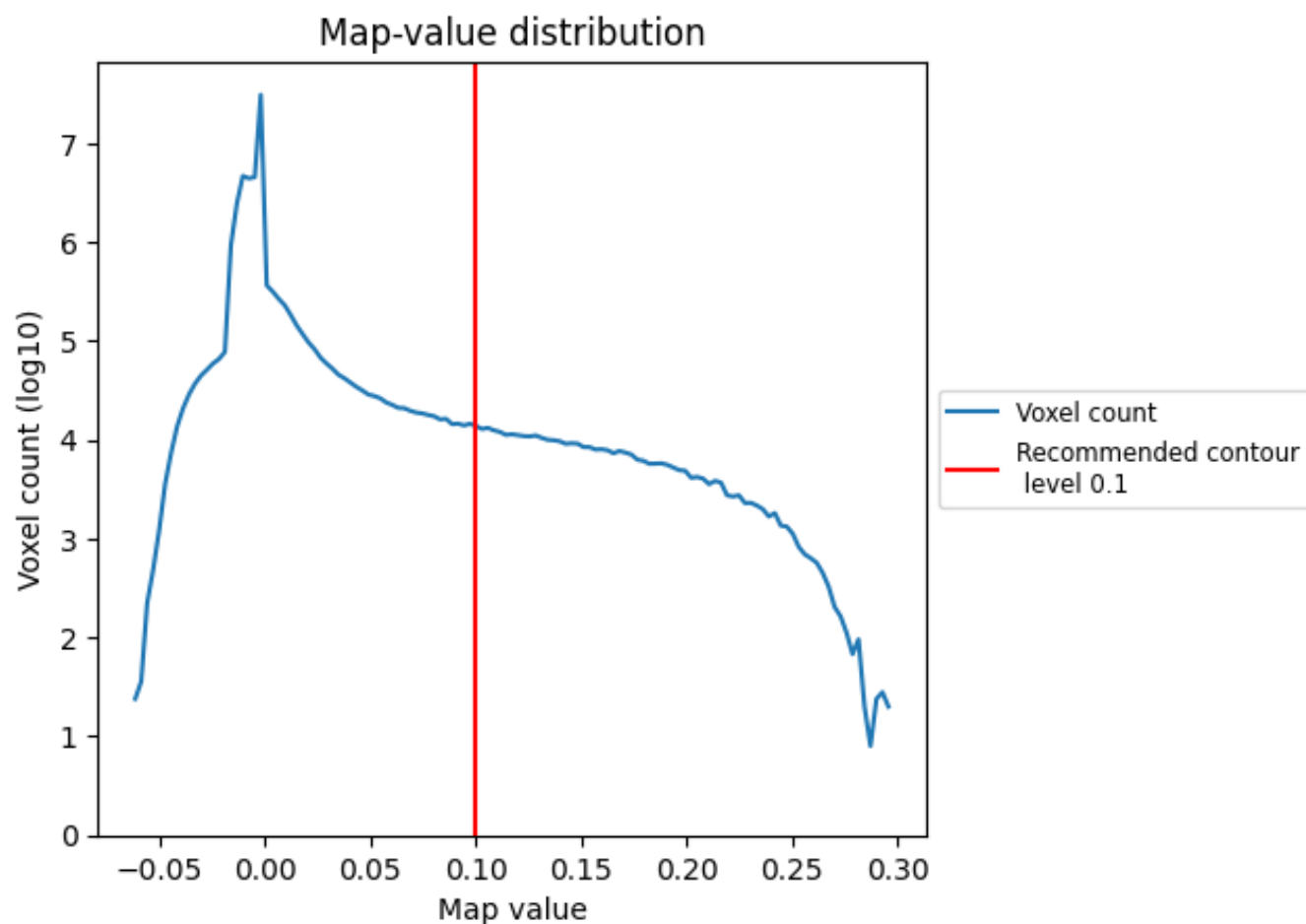


Z

7 Map analysis [i](#)

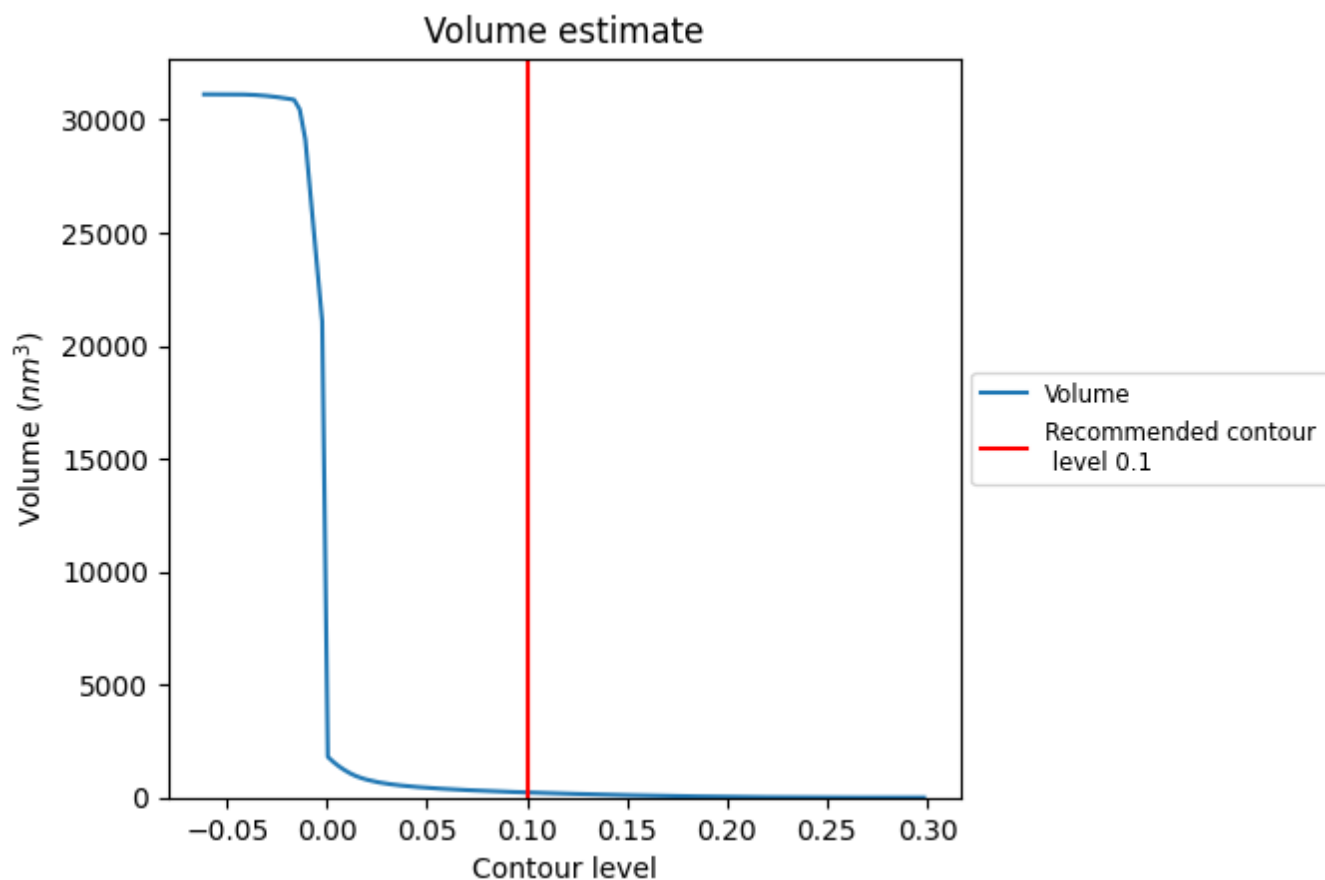
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

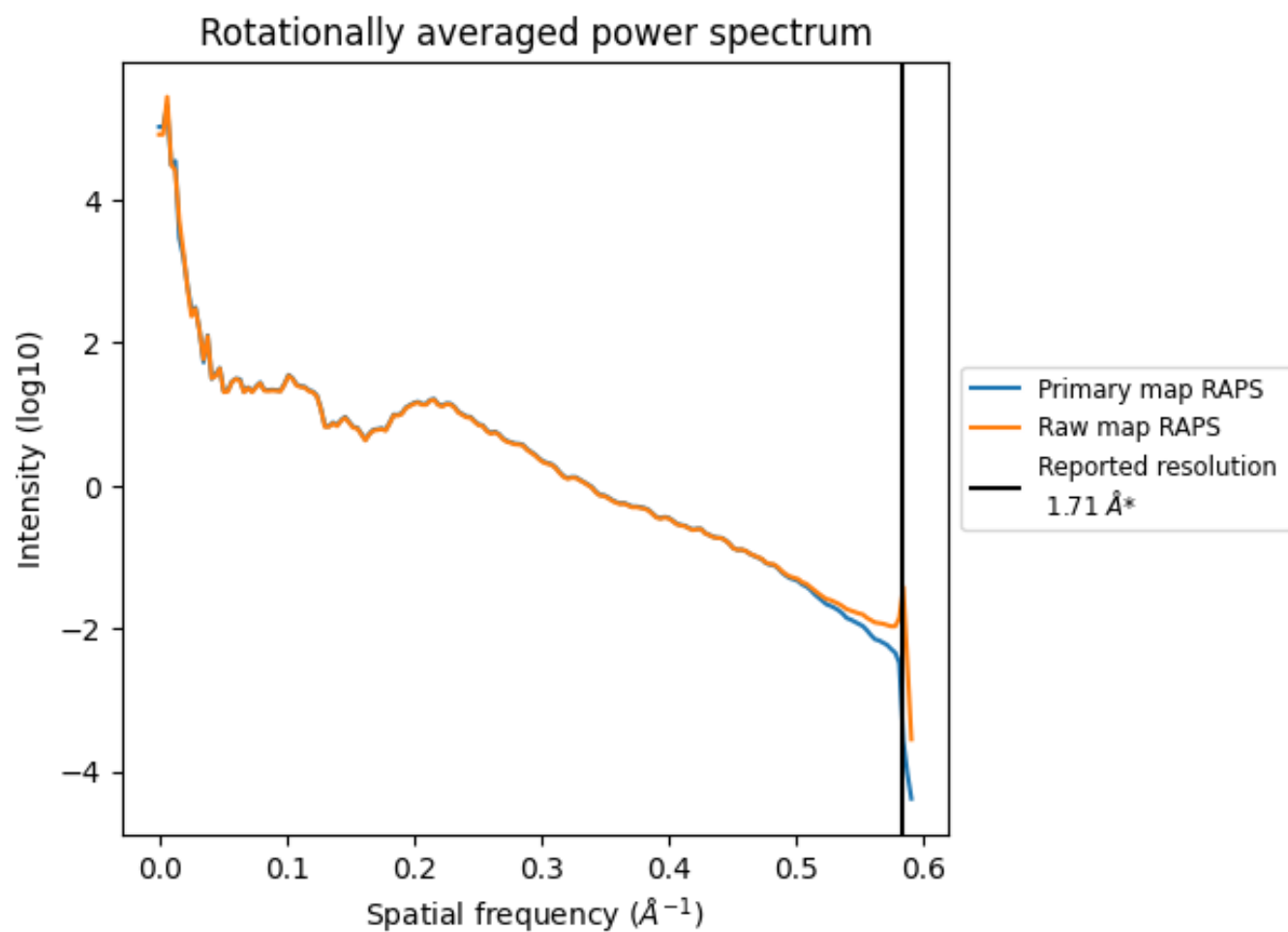
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm³; this corresponds to an approximate mass of 204 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

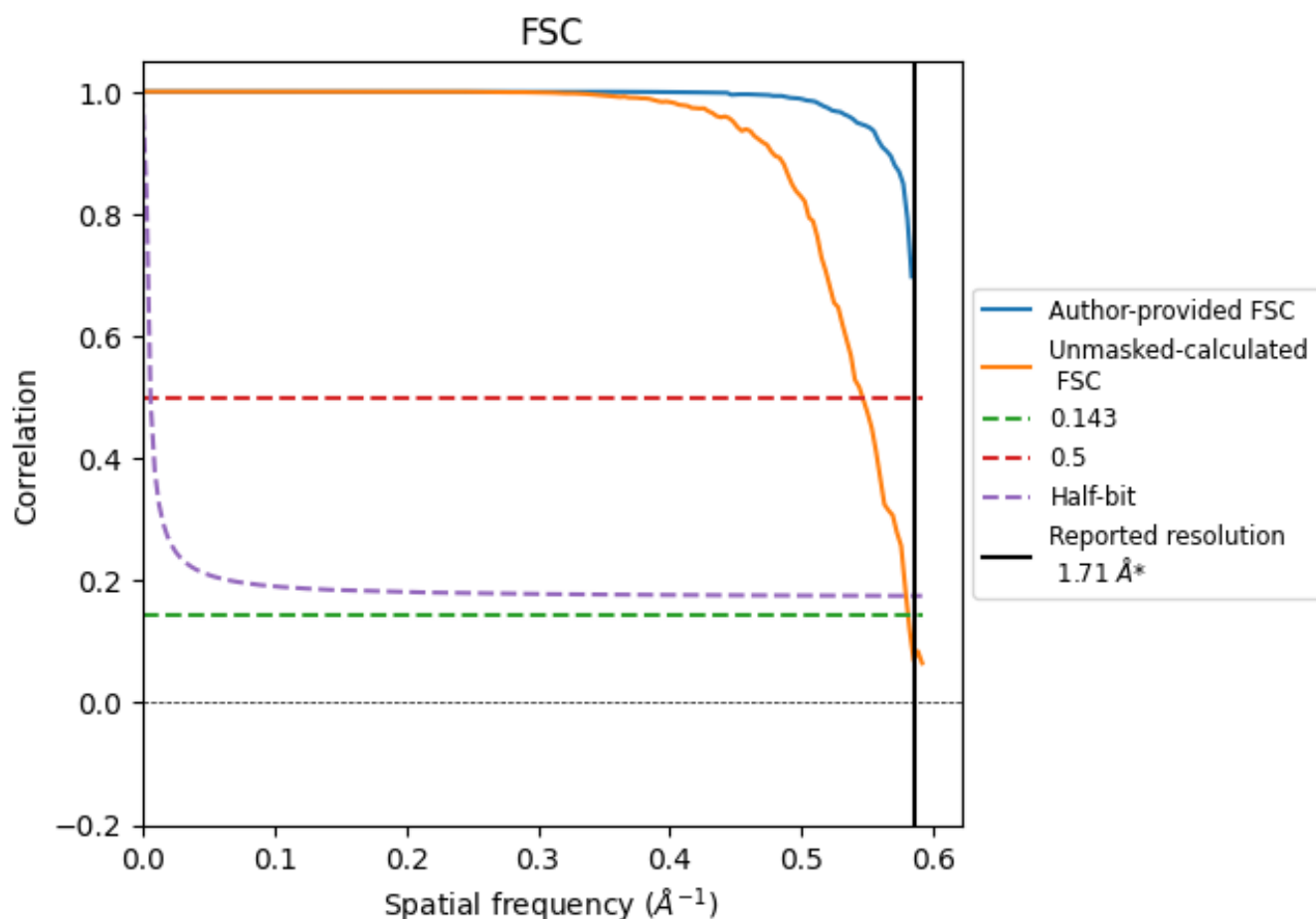


*Reported resolution corresponds to spatial frequency of 0.585 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.585 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

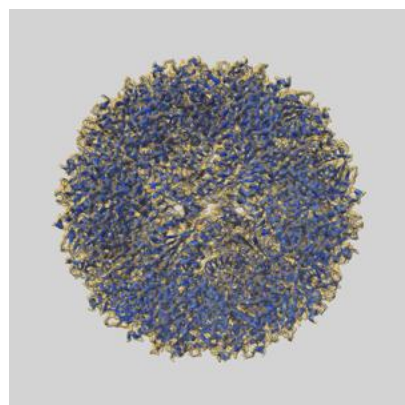
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	1.72	1.83	1.73

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

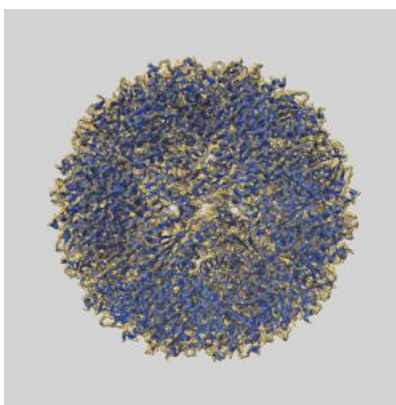
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54394 and PDB model 9RYW. Per-residue inclusion information can be found in section [3](#) on page [36](#).

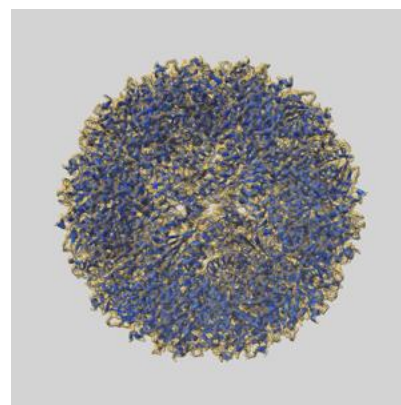
9.1 Map-model overlay [i](#)



X



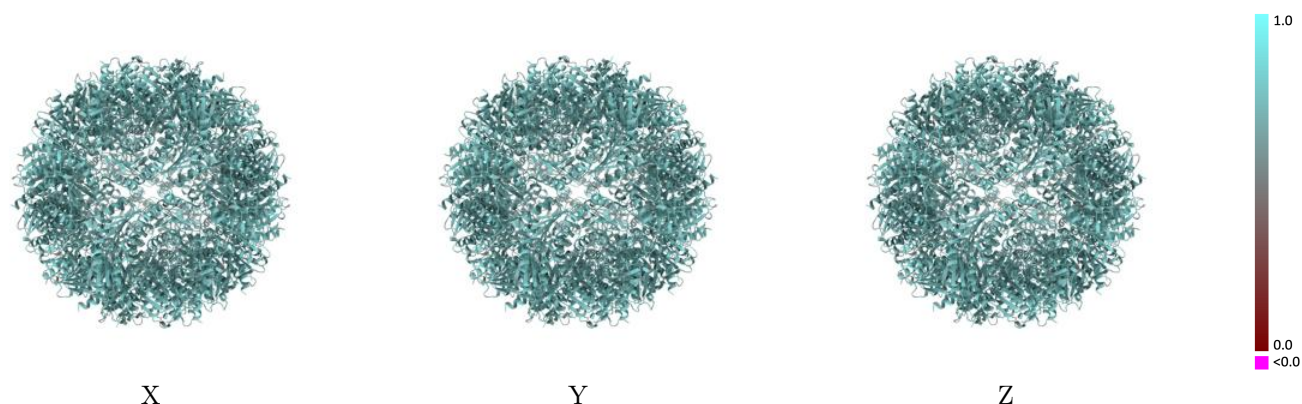
Y



Z

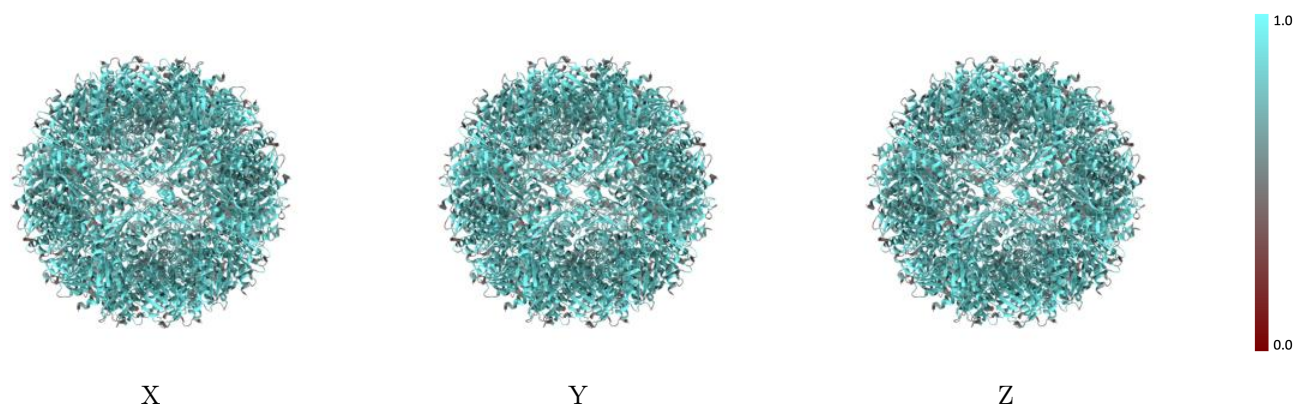
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



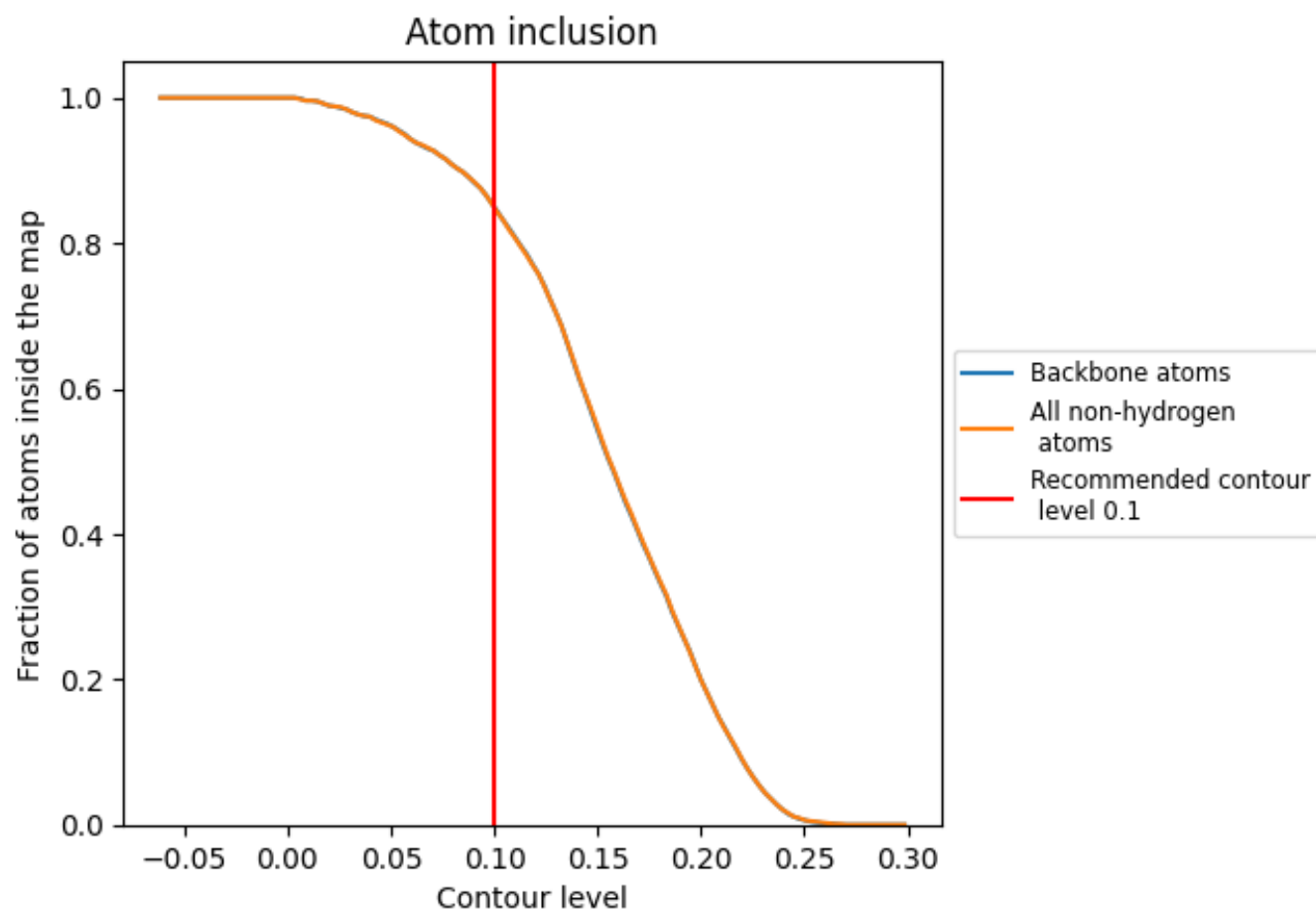
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.7370
A1	 0.8510	 0.7350
A2	 0.8590	 0.7380
A3	 0.8530	 0.7360
A4	 0.8590	 0.7370
A5	 0.8590	 0.7370
B1	 0.8600	 0.7380
B2	 0.8550	 0.7360
B3	 0.8650	 0.7380
B4	 0.8560	 0.7380
B5	 0.8540	 0.7360
C1	 0.8590	 0.7370
C2	 0.8540	 0.7370
C3	 0.8590	 0.7370
C4	 0.8580	 0.7380
C5	 0.8510	 0.7360
D1	 0.8570	 0.7360
D2	 0.8590	 0.7390
D3	 0.8550	 0.7360
D4	 0.8660	 0.7370
D5	 0.8570	 0.7370
E1	 0.8580	 0.7350
E2	 0.8610	 0.7360
E3	 0.8610	 0.7390
E4	 0.8540	 0.7350
E5	 0.8640	 0.7360
F1	 0.8540	 0.7360
F2	 0.8630	 0.7350
F3	 0.8570	 0.7370
F4	 0.8610	 0.7370
F5	 0.8600	 0.7390
G1	 0.8560	 0.7380
G2	 0.8580	 0.7370
G3	 0.8570	 0.7380
G4	 0.8540	 0.7360



Continued on next page...

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Chain	Atom inclusion	Q-score
G5	 0.8630	 0.7370
H1	 0.8600	 0.7370
H2	 0.8630	 0.7370
H3	 0.8540	 0.7360
H4	 0.8660	 0.7360
H5	 0.8570	 0.7350
I1	 0.8540	 0.7360
I2	 0.8630	 0.7360
I3	 0.8590	 0.7350
I4	 0.8610	 0.7360
I5	 0.8600	 0.7390
J1	 0.8660	 0.7370
J2	 0.8570	 0.7380
J3	 0.8550	 0.7360
J4	 0.8580	 0.7390
J5	 0.8550	 0.7360
K1	 0.8570	 0.7400
K2	 0.8510	 0.7380
K3	 0.8590	 0.7370
K4	 0.8520	 0.7360
K5	 0.8580	 0.7370
L1	 0.8580	 0.7370
L2	 0.8550	 0.7370
L3	 0.8550	 0.7360
L4	 0.8570	 0.7380
L5	 0.8510	 0.7370