



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:24 PM UTC

PDB ID : 7RTH / pdb_00007rth
Title : Crystal structure of an anti-lysozyme nanobody in complex with an anti-nanobody Fab "NabFab"
Authors : Filippova, E.V.; Mukherjee, S.; Bloch, J.S.; Locher, K.P.; Kossiakoff, A.A.
Deposited on : 2021-08-13
Resolution : 3.19 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

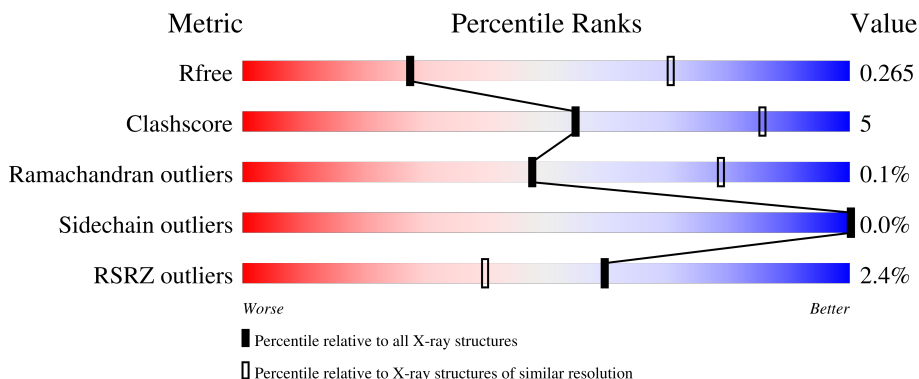
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	215	 7% 84% 10% 7%
1	C	215	 % 89% 6% 5%
1	E	215	 % 86% 12% .
1	G	215	 89% 8% .
1	I	215	 88% 6% 6%

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Mol	Chain	Length	Quality of chain
1	K	215	87% 10%
1	M	215	86% 10%
1	O	215	84% 10% 6%
1	Q	215	85% 10% 6%
2	B	239	78% 10% 11%
2	D	239	85% 10% 5%
2	F	239	82% 13% 6%
2	H	239	81% 13% 6%
2	J	239	82% 12% 5%
2	L	239	78% 15% 7%
2	N	239	82% 10% 8%
2	P	239	76% 15% 9%
2	R	239	82% 8% 9%
3	a	129	90% 7%
3	c	129	81% 16%
3	e	129	82% 13%
3	g	129	84% 11% 5%
3	i	129	87% 10%
3	k	129	83% 15%
3	m	129	77% 17% 6%
3	o	129	77% 19% 5%
3	q	129	86% 9% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	a	202	-	-	X	-
4	PO4	e	201	-	-	X	-
4	PO4	e	203	-	X	-	-
4	PO4	o	202	-	-	X	-
6	GOL	k	201	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 38455 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Fragment Antigen-Binding Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1533	959	258	312	4	0	0	0
1	C	204	1554	970	262	318	4	0	0	0
1	E	209	1587	989	268	326	4	0	0	0
1	G	209	1587	989	268	326	4	0	0	0
1	I	203	1548	967	261	316	4	0	0	0
1	K	210	1601	999	270	327	5	0	0	0
1	M	207	1574	982	266	322	4	0	0	0
1	O	202	1535	960	257	314	4	0	0	0
1	Q	203	1548	967	261	316	4	0	0	0

- Molecule 2 is a protein called Fragment Antigen-Binding Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1625	1039	268	313	5	0	0	0
2	D	228	1729	1100	286	338	5	0	0	0
2	F	225	1712	1091	283	332	6	0	0	0
2	H	225	1715	1093	283	334	5	0	0	0
2	J	226	1718	1094	284	335	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	223	Total	C	N	O	S	0	0	0
			1700	1085	281	329	5			
2	N	221	Total	C	N	O	S	0	0	0
			1682	1073	277	327	5			
2	P	218	Total	C	N	O	S	0	0	0
			1667	1067	275	320	5			
2	R	217	Total	C	N	O	S	0	0	0
			1663	1065	274	319	5			

- Molecule 3 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	125	Total	C	N	O	S	0	1	0
			967	608	164	190	5			
3	c	125	Total	C	N	O	S	0	1	0
			977	613	168	191	5			
3	e	124	Total	C	N	O	S	0	0	0
			959	604	163	187	5			
3	g	123	Total	C	N	O	S	0	0	0
			956	602	162	187	5			
3	i	125	Total	C	N	O	S	0	0	0
			966	607	164	190	5			
3	k	126	Total	C	N	O	S	0	1	0
			980	616	169	190	5			
3	m	121	Total	C	N	O	S	0	0	0
			943	595	160	183	5			
3	o	123	Total	C	N	O	S	0	1	0
			957	603	162	187	5			
3	q	123	Total	C	N	O	S	0	0	0
			953	601	162	185	5			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total 5	O 4	P 1	0	0
4	H	1	Total 5	O 4	P 1	0	0
4	I	1	Total 5	O 4	P 1	0	0
4	I	1	Total 5	O 4	P 1	0	0
4	I	1	Total 5	O 4	P 1	0	0
4	I	1	Total 5	O 4	P 1	0	0
4	J	1	Total 5	O 4	P 1	0	0
4	J	1	Total 5	O 4	P 1	0	0
4	K	1	Total 5	O 4	P 1	0	0
4	K	1	Total 5	O 4	P 1	0	0
4	L	1	Total 5	O 4	P 1	0	0
4	M	1	Total 5	O 4	P 1	0	0
4	M	1	Total 5	O 4	P 1	0	0
4	M	1	Total 5	O 4	P 1	0	0
4	O	1	Total 5	O 4	P 1	0	0
4	O	1	Total 5	O 4	P 1	0	0
4	Q	1	Total 5	O 4	P 1	0	0
4	R	1	Total 5	O 4	P 1	0	0
4	a	1	Total 5	O 4	P 1	0	0
4	a	1	Total 5	O 4	P 1	0	0
4	c	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	c	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	g	1	Total	O	P	0	0
			5	4	1		
4	g	1	Total	O	P	0	0
			5	4	1		
4	i	1	Total	O	P	0	0
			5	4	1		
4	i	1	Total	O	P	0	0
			5	4	1		
4	i	1	Total	O	P	0	0
			5	4	1		
4	m	1	Total	O	P	0	0
			5	4	1		
4	m	1	Total	O	P	0	0
			5	4	1		
4	o	1	Total	O	P	0	0
			5	4	1		
4	o	1	Total	O	P	0	0
			5	4	1		
4	o	1	Total	O	P	0	0
			5	4	1		
4	q	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

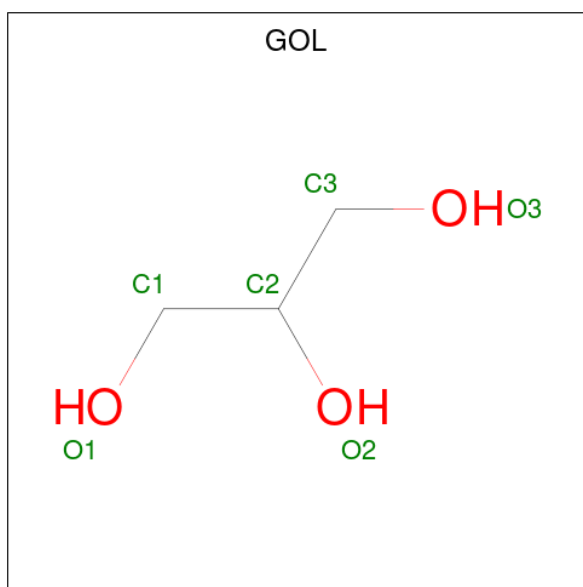
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	C	2	Total	Cl	0	0
			2	2		
5	D	2	Total	Cl	0	0
			2	2		
5	E	2	Total	Cl	0	0
			2	2		

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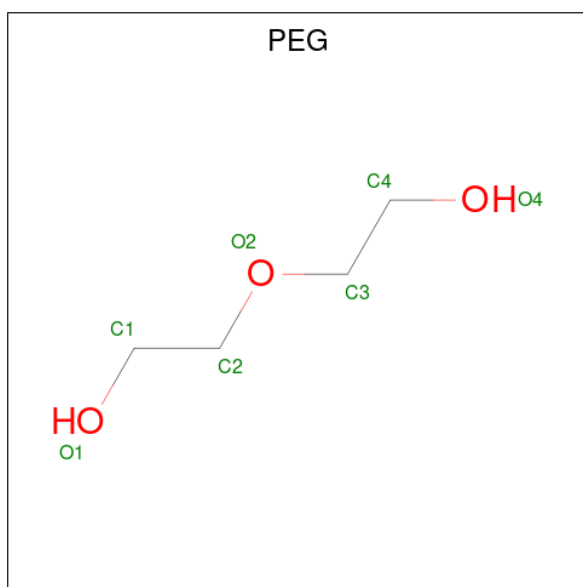
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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5	G	2	Total Cl 2 2	0	0
5	H	1	Total Cl 1 1	0	0
5	I	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0
5	K	2	Total Cl 2 2	0	0
5	L	1	Total Cl 1 1	0	0
5	M	1	Total Cl 1 1	0	0
5	N	2	Total Cl 2 2	0	0
5	P	1	Total Cl 1 1	0	0
5	R	3	Total Cl 3 3	0	0
5	e	1	Total Cl 1 1	0	0
5	g	2	Total Cl 2 2	0	0
5	q	2	Total Cl 2 2	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0
6	G	1	Total C O 6 3 3	0	0
6	G	1	Total C O 6 3 3	0	0
6	I	1	Total C O 6 3 3	0	0
6	L	1	Total C O 6 3 3	0	0
6	c	1	Total C O 6 3 3	0	0
6	k	1	Total C O 6 3 3	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 7 4 3	0	0
7	H	1	Total C O 7 4 3	0	0
7	N	1	Total C O 7 4 3	0	0

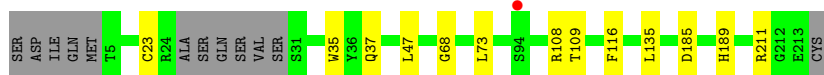
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0
8	B	3	Total O 3 3	0	0
8	C	8	Total O 8 8	0	0
8	D	6	Total O 6 6	0	0
8	E	9	Total O 9 9	0	0
8	F	5	Total O 5 5	0	0
8	G	16	Total O 16 16	0	0
8	H	10	Total O 10 10	0	0
8	I	13	Total O 13 13	0	0

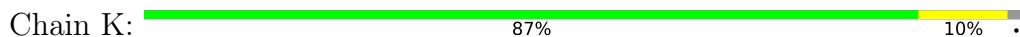
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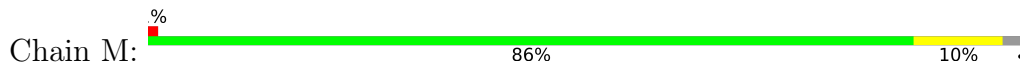
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8	K	12	Total O 12 12	0	0
8	L	8	Total O 8 8	0	0
8	M	5	Total O 5 5	0	0
8	N	4	Total O 4 4	0	0
8	O	3	Total O 3 3	0	0
8	P	8	Total O 8 8	0	0
8	Q	10	Total O 10 10	0	0
8	R	2	Total O 2 2	0	0
8	a	6	Total O 6 6	0	0
8	c	8	Total O 8 8	0	0
8	e	3	Total O 3 3	0	0
8	g	3	Total O 3 3	0	0
8	i	2	Total O 2 2	0	0
8	k	7	Total O 7 7	0	0
8	m	1	Total O 1 1	0	0
8	o	1	Total O 1 1	0	0
8	q	4	Total O 4 4	0	0



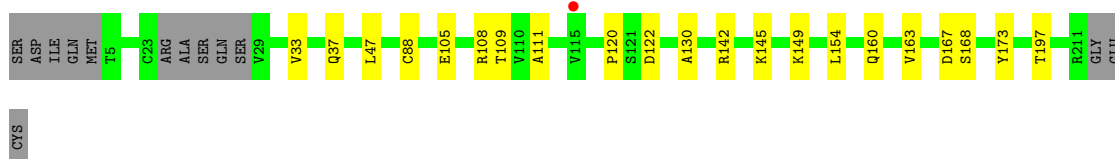
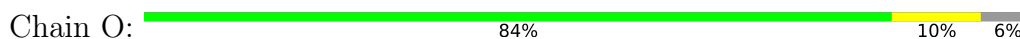
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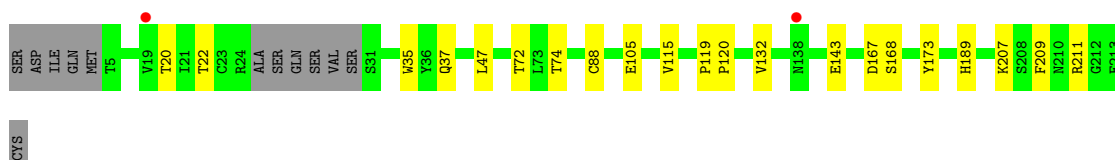
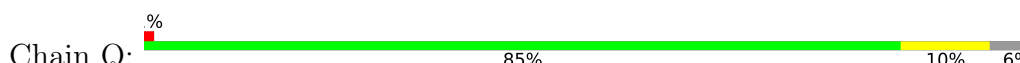
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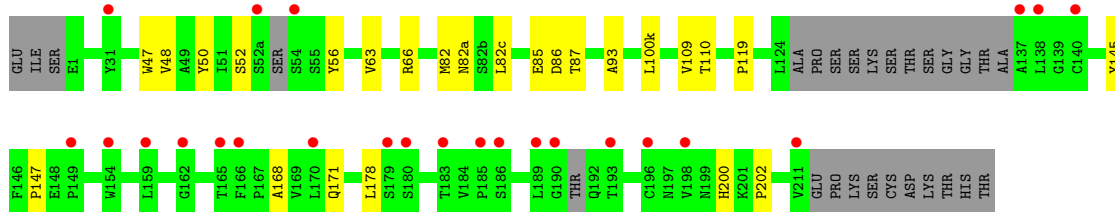
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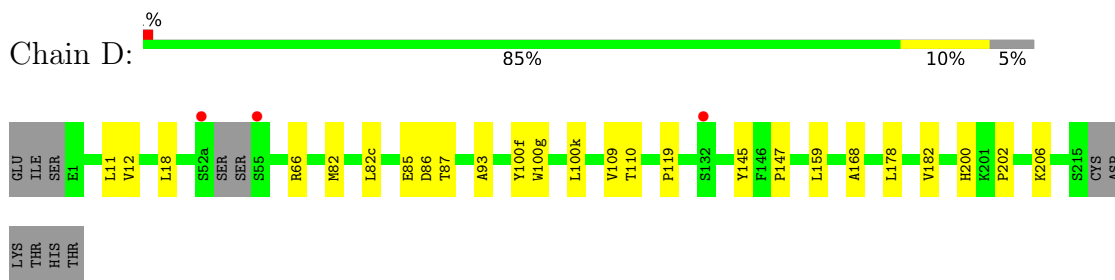
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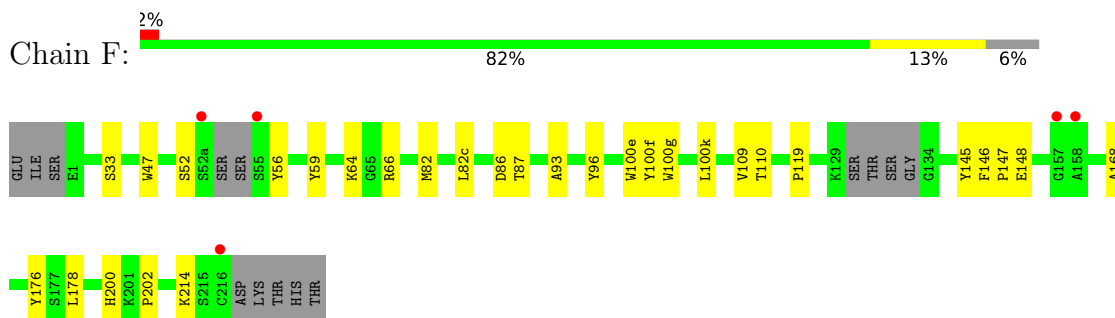
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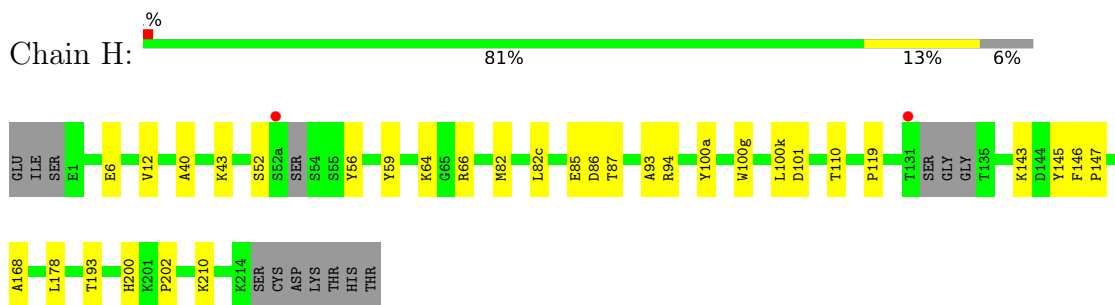
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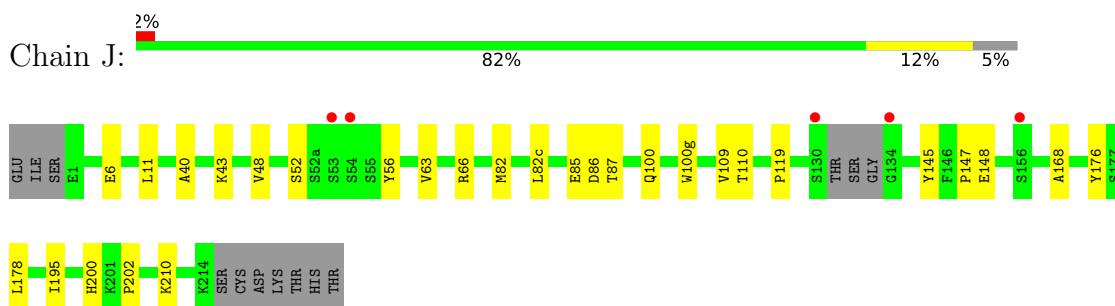
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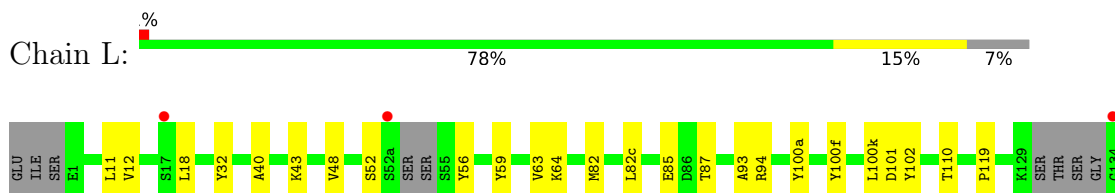
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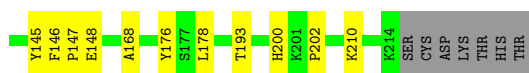


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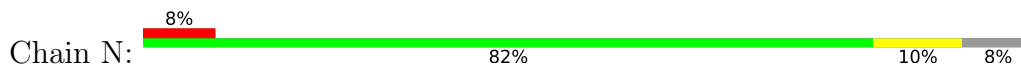


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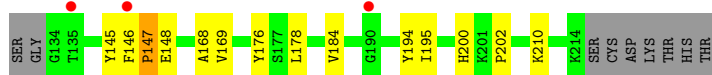
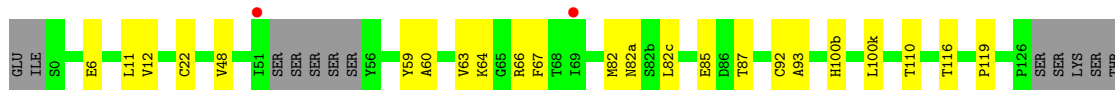
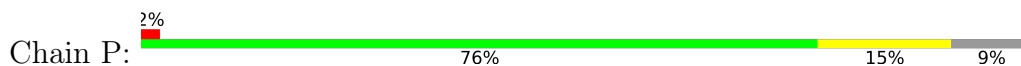




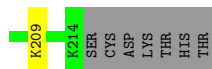
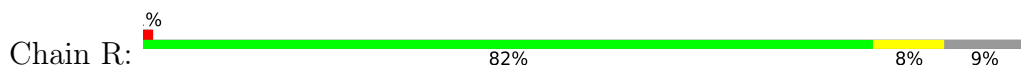
● Molecule 2: Fragment Antigen-Binding Heavy Chain



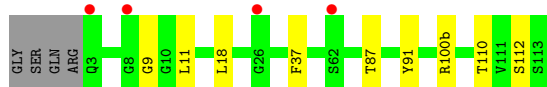
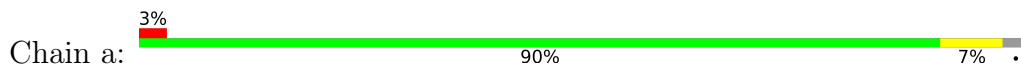
● Molecule 2: Fragment Antigen-Binding Heavy Chain



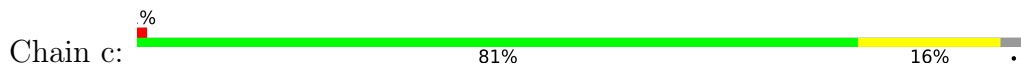
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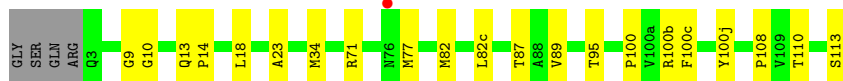


● Molecule 3: Nanobody

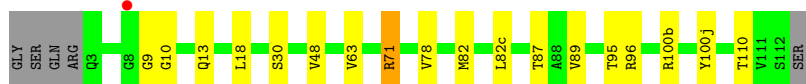
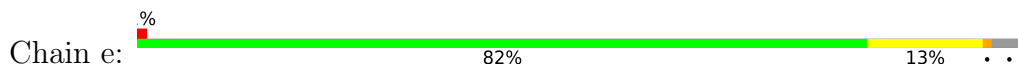


● Molecule 3: Nanobody

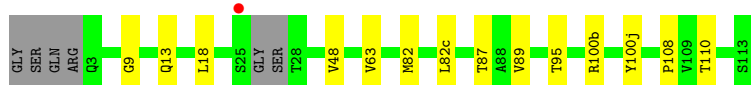
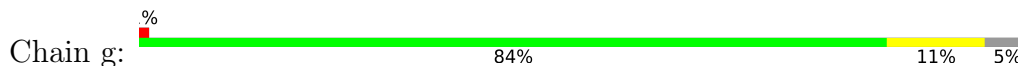




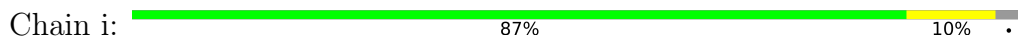
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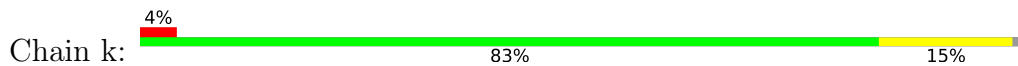
• Molecule 3: Nanobody



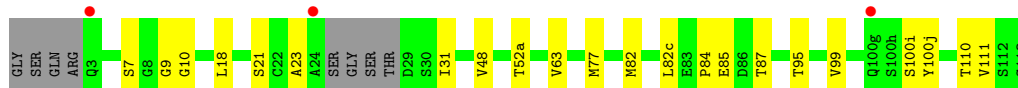
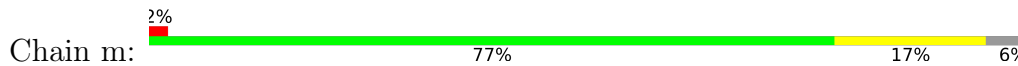
• Molecule 3: Nanobody



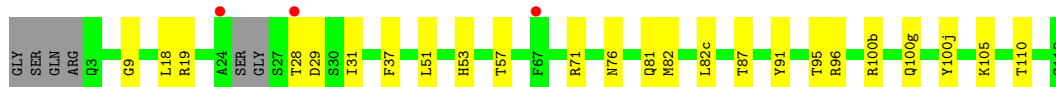
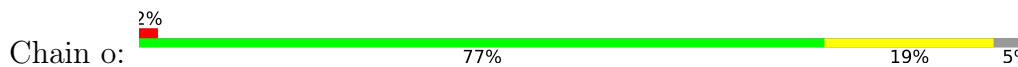
• Molecule 3: Nanobody




• Molecule 3: Nanobody

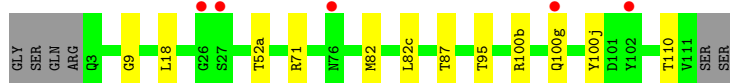


• Molecule 3: Nanobody



• Molecule 3: Nanobody

Chain q: 



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.53Å 130.28Å 223.98Å 90.00° 107.99° 90.00°	Depositor
Resolution (Å)	90.91 – 3.19 90.91 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.0 (90.91-3.19) 97.0 (90.91-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.216 , 0.267 0.216 , 0.265	Depositor DCC
R_{free} test set	5100 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.046 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.029 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	38455	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/1563	0.24	0/2118
1	C	0.08	0/1585	0.26	0/2149
1	E	0.07	0/1619	0.25	0/2197
1	G	0.09	0/1619	0.27	0/2197
1	I	0.08	0/1579	0.26	0/2141
1	K	0.08	0/1632	0.27	0/2212
1	M	0.08	0/1606	0.26	0/2180
1	O	0.08	0/1566	0.25	0/2125
1	Q	0.07	0/1579	0.25	0/2141
2	B	0.09	0/1670	0.26	0/2276
2	D	0.08	0/1778	0.26	0/2426
2	F	0.08	0/1760	0.25	0/2400
2	H	0.13	0/1763	0.28	0/2405
2	J	0.08	0/1767	0.24	0/2411
2	L	0.08	0/1748	0.25	0/2384
2	N	0.11	0/1731	0.25	0/2365
2	P	0.08	0/1715	0.24	0/2341
2	R	0.09	0/1711	0.26	0/2336
3	a	0.08	0/999	0.26	0/1351
3	c	0.08	0/999	0.27	0/1351
3	e	0.12	0/981	0.27	0/1329
3	g	0.14	0/977	0.29	0/1321
3	i	0.11	0/988	0.28	0/1337
3	k	0.08	0/1012	0.28	0/1369
3	m	0.12	0/964	0.30	0/1303
3	o	0.12	0/988	0.27	0/1335
3	q	0.08	0/975	0.26	0/1321
All	All	0.09	0/38874	0.26	0/52821

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1533	0	1502	12	0
1	C	1554	0	1518	7	0
1	E	1587	0	1551	15	0
1	G	1587	0	1551	12	0
1	I	1548	0	1513	9	0
1	K	1601	0	1568	13	0
1	M	1574	0	1542	13	0
1	O	1535	0	1498	12	0
1	Q	1548	0	1513	11	0
2	B	1625	0	1552	14	0
2	D	1729	0	1657	17	0
2	F	1712	0	1641	19	0
2	H	1715	0	1645	19	0
2	J	1718	0	1647	19	0
2	L	1700	0	1631	22	0
2	N	1682	0	1606	16	0
2	P	1667	0	1598	25	0
2	R	1663	0	1595	15	0
3	a	967	0	923	6	0
3	c	977	0	940	13	0
3	e	959	0	923	15	0
3	g	956	0	919	9	0
3	i	966	0	928	8	0
3	k	980	0	942	15	0
3	m	943	0	907	12	0
3	o	957	0	914	20	0
3	q	953	0	918	7	0
4	B	5	0	0	0	0
4	C	25	0	0	1	0
4	D	10	0	0	0	0
4	E	20	0	0	1	0
4	G	15	0	0	0	0
4	H	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	20	0	0	0	0
4	J	10	0	0	1	0
4	K	10	0	0	0	0
4	L	5	0	0	0	0
4	M	15	0	0	1	0
4	O	10	0	0	0	0
4	Q	5	0	0	0	0
4	R	5	0	0	1	0
4	a	10	0	0	2	0
4	c	10	0	0	1	0
4	e	15	0	0	5	0
4	g	10	0	0	1	0
4	i	15	0	0	1	0
4	m	10	0	0	0	0
4	o	15	0	0	3	0
4	q	5	0	0	1	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	2	0	0	0	0
5	P	1	0	0	0	0
5	R	3	0	0	0	0
5	e	1	0	0	0	0
5	g	2	0	0	0	0
5	q	2	0	0	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	E	6	0	8	0	0
6	G	12	0	16	3	0
6	I	6	0	8	0	0
6	L	6	0	8	1	0
6	c	6	0	8	0	0
6	k	6	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	7	0	10	0	0
7	H	7	0	10	1	0
7	N	7	0	10	2	0
8	A	1	0	0	0	0
8	B	3	0	0	0	0
8	C	8	0	0	0	0
8	D	6	0	0	0	0
8	E	9	0	0	0	0
8	F	5	0	0	0	0
8	G	16	0	0	0	0
8	H	10	0	0	1	0
8	I	13	0	0	0	0
8	J	7	0	0	0	0
8	K	12	0	0	0	0
8	L	8	0	0	0	0
8	M	5	0	0	0	0
8	N	4	0	0	0	0
8	O	3	0	0	0	0
8	P	8	0	0	0	0
8	Q	10	0	0	0	0
8	R	2	0	0	0	0
8	a	6	0	0	0	0
8	c	8	0	0	0	0
8	e	3	0	0	0	0
8	g	3	0	0	0	0
8	i	2	0	0	0	0
8	k	7	0	0	0	0
8	m	1	0	0	0	0
8	o	1	0	0	0	0
8	q	4	0	0	0	0
All	All	38455	0	36744	357	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 357 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:O:160:GLN:HG2	2:P:169:VAL:HG11	1.51	0.91
3:e:71:ARG:HD3	4:e:201:PO4:O3	1.80	0.81
3:o:19:ARG:HD2	3:o:81:GLN:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:71:ARG:CD	4:e:201:PO4:O3	2.34	0.74
3:q:9:GLY:HA2	3:q:18:LEU:HD21	1.69	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/215 (91%)	186 (95%)	9 (5%)	0	100	100
1	C	200/215 (93%)	193 (96%)	6 (3%)	1 (0%)	24	59
1	E	207/215 (96%)	199 (96%)	8 (4%)	0	100	100
1	G	207/215 (96%)	197 (95%)	10 (5%)	0	100	100
1	I	199/215 (93%)	188 (94%)	11 (6%)	0	100	100
1	K	206/215 (96%)	196 (95%)	9 (4%)	1 (0%)	24	59
1	M	205/215 (95%)	194 (95%)	11 (5%)	0	100	100
1	O	198/215 (92%)	187 (94%)	11 (6%)	0	100	100
1	Q	199/215 (93%)	187 (94%)	12 (6%)	0	100	100
2	B	204/239 (85%)	190 (93%)	13 (6%)	1 (0%)	24	59
2	D	224/239 (94%)	211 (94%)	13 (6%)	0	100	100
2	F	219/239 (92%)	207 (94%)	12 (6%)	0	100	100
2	H	219/239 (92%)	206 (94%)	13 (6%)	0	100	100
2	J	222/239 (93%)	208 (94%)	14 (6%)	0	100	100
2	L	217/239 (91%)	205 (94%)	12 (6%)	0	100	100
2	N	217/239 (91%)	203 (94%)	13 (6%)	1 (0%)	24	59
2	P	212/239 (89%)	200 (94%)	11 (5%)	1 (0%)	24	59
2	R	211/239 (88%)	200 (95%)	10 (5%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	124/129 (96%)	124 (100%)	0	0	100	100
3	c	124/129 (96%)	119 (96%)	5 (4%)	0	100	100
3	e	122/129 (95%)	120 (98%)	2 (2%)	0	100	100
3	g	119/129 (92%)	118 (99%)	1 (1%)	0	100	100
3	i	123/129 (95%)	122 (99%)	1 (1%)	0	100	100
3	k	125/129 (97%)	124 (99%)	1 (1%)	0	100	100
3	m	117/129 (91%)	114 (97%)	3 (3%)	0	100	100
3	o	120/129 (93%)	118 (98%)	2 (2%)	0	100	100
3	q	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
All	All	4856/5247 (92%)	4632 (95%)	218 (4%)	6 (0%)	48	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	92	SER
2	R	64	LYS
1	C	92	SER
2	B	147	PRO
2	N	147	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/190 (94%)	178 (100%)	0	100	100
1	C	180/190 (95%)	180 (100%)	0	100	100
1	E	184/190 (97%)	184 (100%)	0	100	100
1	G	184/190 (97%)	184 (100%)	0	100	100
1	I	179/190 (94%)	179 (100%)	0	100	100
1	K	186/190 (98%)	186 (100%)	0	100	100
1	M	183/190 (96%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	178/190 (94%)	178 (100%)	0	100	100
1	Q	179/190 (94%)	179 (100%)	0	100	100
2	B	177/200 (88%)	177 (100%)	0	100	100
2	D	189/200 (94%)	189 (100%)	0	100	100
2	F	187/200 (94%)	187 (100%)	0	100	100
2	H	188/200 (94%)	188 (100%)	0	100	100
2	J	188/200 (94%)	188 (100%)	0	100	100
2	L	185/200 (92%)	185 (100%)	0	100	100
2	N	183/200 (92%)	183 (100%)	0	100	100
2	P	180/200 (90%)	180 (100%)	0	100	100
2	R	180/200 (90%)	180 (100%)	0	100	100
3	a	103/105 (98%)	103 (100%)	0	100	100
3	c	103/105 (98%)	103 (100%)	0	100	100
3	e	101/105 (96%)	100 (99%)	1 (1%)	68	80
3	g	101/105 (96%)	101 (100%)	0	100	100
3	i	102/105 (97%)	102 (100%)	0	100	100
3	k	104/105 (99%)	104 (100%)	0	100	100
3	m	99/105 (94%)	99 (100%)	0	100	100
3	o	102/105 (97%)	102 (100%)	0	100	100
3	q	100/105 (95%)	100 (100%)	0	100	100
All	All	4203/4455 (94%)	4202 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	e	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
3	a	81	GLN
3	k	3	GLN
3	a	82(a)	ASN
3	e	81	GLN

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Mol	Chain	Res	Type
3	k	81	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 29 are monoatomic - leaving 62 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	a	201	-	4,4,4	0.98	0	6,6,6	0.45	0
4	PO4	g	201	-	4,4,4	0.97	0	6,6,6	0.44	0
4	PO4	o	201	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PO4	M	303	-	4,4,4	0.98	0	6,6,6	0.49	0
4	PO4	O	301	-	4,4,4	0.97	0	6,6,6	0.46	0
6	GOL	G	306	-	5,5,5	0.94	0	5,5,5	1.07	0
4	PO4	O	302	-	4,4,4	0.96	0	6,6,6	0.44	0
6	GOL	L	303	-	5,5,5	0.92	0	5,5,5	1.07	0
4	PO4	D	302	-	4,4,4	0.97	0	6,6,6	0.45	0
6	GOL	E	307	-	5,5,5	0.95	0	5,5,5	1.03	0
6	GOL	c	203	-	5,5,5	0.94	0	5,5,5	1.06	0
4	PO4	Q	301	-	4,4,4	0.96	0	6,6,6	0.47	0
4	PO4	i	201	-	4,4,4	0.98	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	k	201	-	5,5,5	0.93	0	5,5,5	1.09	0
4	PO4	H	301	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PO4	M	301	-	4,4,4	0.97	0	6,6,6	0.45	0
4	PO4	m	202	-	4,4,4	0.97	0	6,6,6	0.45	0
4	PO4	e	201	-	4,4,4	0.95	0	6,6,6	0.52	0
4	PO4	B	301	-	4,4,4	0.96	0	6,6,6	0.44	0
4	PO4	C	301	-	4,4,4	1.02	0	6,6,6	0.48	0
4	PO4	c	202	-	4,4,4	0.97	0	6,6,6	0.43	0
4	PO4	M	302	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	C	302	-	4,4,4	0.96	0	6,6,6	0.45	0
4	PO4	C	303	-	4,4,4	0.96	0	6,6,6	0.47	0
4	PO4	e	203	-	4,4,4	3.07	4 (100%)	6,6,6	0.47	0
7	PEG	F	302	-	6,6,6	0.50	0	5,5,5	0.29	0
4	PO4	E	302	-	4,4,4	0.96	0	6,6,6	0.47	0
4	PO4	q	201	-	4,4,4	0.99	0	6,6,6	0.41	0
4	PO4	a	202	-	4,4,4	0.98	0	6,6,6	0.53	0
4	PO4	D	301	-	4,4,4	0.99	0	6,6,6	0.42	0
4	PO4	C	304	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	K	302	-	4,4,4	0.96	0	6,6,6	0.45	0
4	PO4	J	301	-	4,4,4	0.96	0	6,6,6	0.45	0
4	PO4	R	301	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	g	202	-	4,4,4	0.96	0	6,6,6	0.54	0
4	PO4	G	303	-	4,4,4	0.96	0	6,6,6	0.47	0
6	GOL	G	307	-	5,5,5	0.79	0	5,5,5	1.18	1 (20%)
4	PO4	i	202	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PO4	I	302	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PO4	J	302	-	4,4,4	0.96	0	6,6,6	0.47	0
4	PO4	I	304	-	4,4,4	1.00	0	6,6,6	0.44	0
4	PO4	E	304	-	4,4,4	0.97	0	6,6,6	0.37	0
4	PO4	o	202	-	4,4,4	0.93	0	6,6,6	0.52	0
4	PO4	c	201	-	4,4,4	1.00	0	6,6,6	0.47	0
7	PEG	N	303	-	6,6,6	0.50	0	5,5,5	0.26	0
6	GOL	C	308	-	5,5,5	0.92	0	5,5,5	1.08	0
4	PO4	G	301	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	K	301	-	4,4,4	0.99	0	6,6,6	0.46	0
4	PO4	e	202	-	4,4,4	0.98	0	6,6,6	0.44	0
4	PO4	m	201	-	4,4,4	0.97	0	6,6,6	0.45	0
6	GOL	I	306	-	5,5,5	0.94	0	5,5,5	1.08	0
7	PEG	H	303	-	6,6,6	0.50	0	5,5,5	0.24	0
4	PO4	E	301	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PO4	G	302	-	4,4,4	0.97	0	6,6,6	0.45	0
4	PO4	I	301	-	4,4,4	0.97	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	i	203	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	L	301	-	4,4,4	0.96	0	6,6,6	0.47	0
4	PO4	o	203	-	4,4,4	0.97	0	6,6,6	0.49	0
6	GOL	B	304	-	5,5,5	0.09	0	5,5,5	0.37	0
4	PO4	I	303	-	4,4,4	0.98	0	6,6,6	0.45	0
4	PO4	C	305	-	4,4,4	0.96	0	6,6,6	0.46	0
4	PO4	E	303	-	4,4,4	0.97	0	6,6,6	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	G	307	-	-	2/4/4/4	-
6	GOL	G	306	-	-	0/4/4/4	-
6	GOL	I	306	-	-	0/4/4/4	-
7	PEG	H	303	-	-	2/4/4/4	-
6	GOL	L	303	-	-	0/4/4/4	-
6	GOL	B	304	-	-	0/4/4/4	-
6	GOL	E	307	-	-	1/4/4/4	-
6	GOL	c	203	-	-	2/4/4/4	-
6	GOL	k	201	-	-	2/4/4/4	-
7	PEG	F	302	-	-	2/4/4/4	-
7	PEG	N	303	-	-	1/4/4/4	-
6	GOL	C	308	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	203	PO4	P-O1	4.69	1.61	1.50
4	e	203	PO4	P-O2	2.35	1.61	1.54
4	e	203	PO4	P-O3	2.33	1.61	1.54
4	e	203	PO4	P-O4	-2.15	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	307	GOL	C3-C2-C1	-2.11	104.06	111.80

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	k	201	GOL	O1-C1-C2-C3
6	c	203	GOL	O1-C1-C2-C3
6	k	201	GOL	O1-C1-C2-O2
6	G	307	GOL	O1-C1-C2-O2
7	H	303	PEG	O1-C1-C2-O2

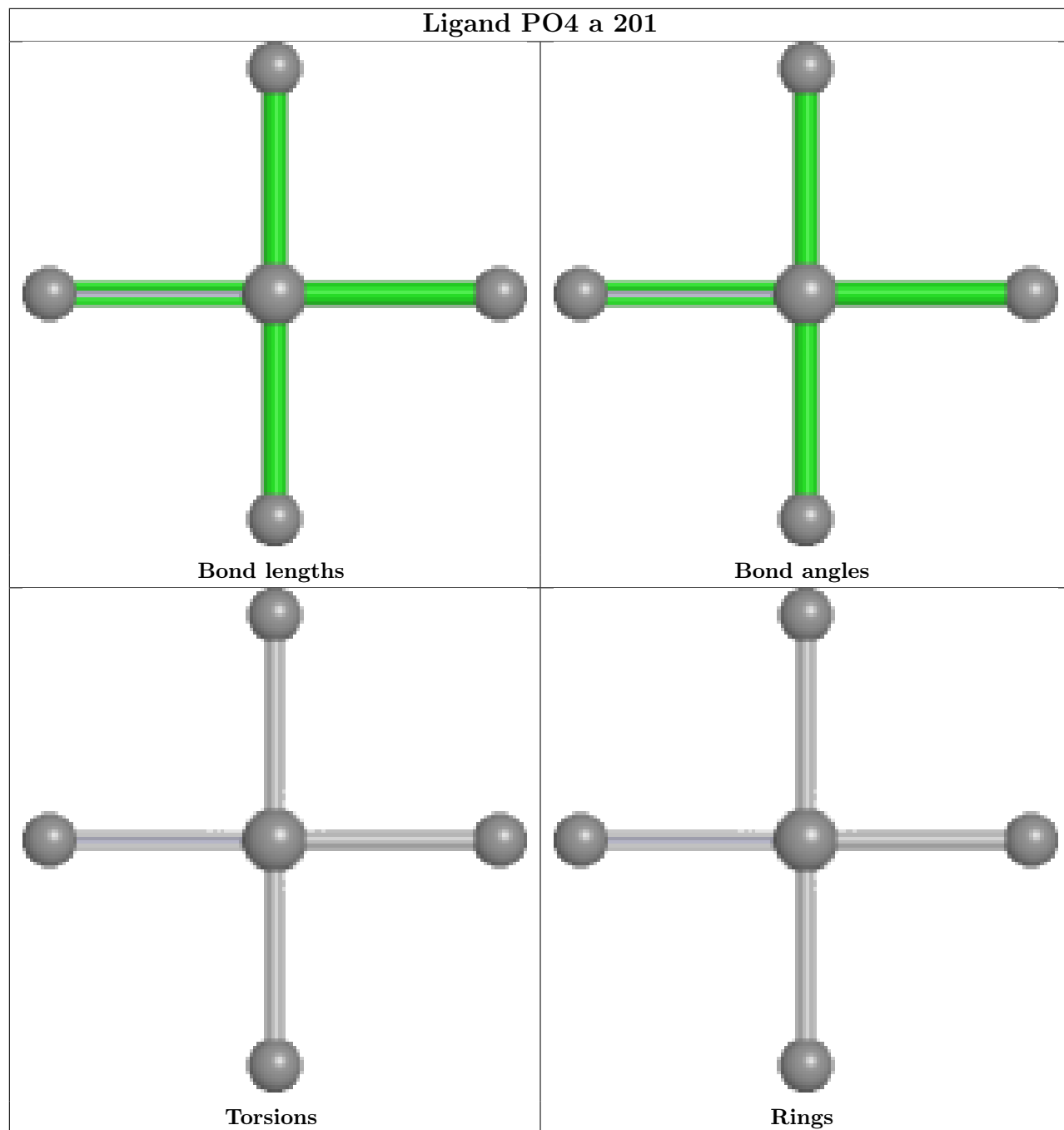
There are no ring outliers.

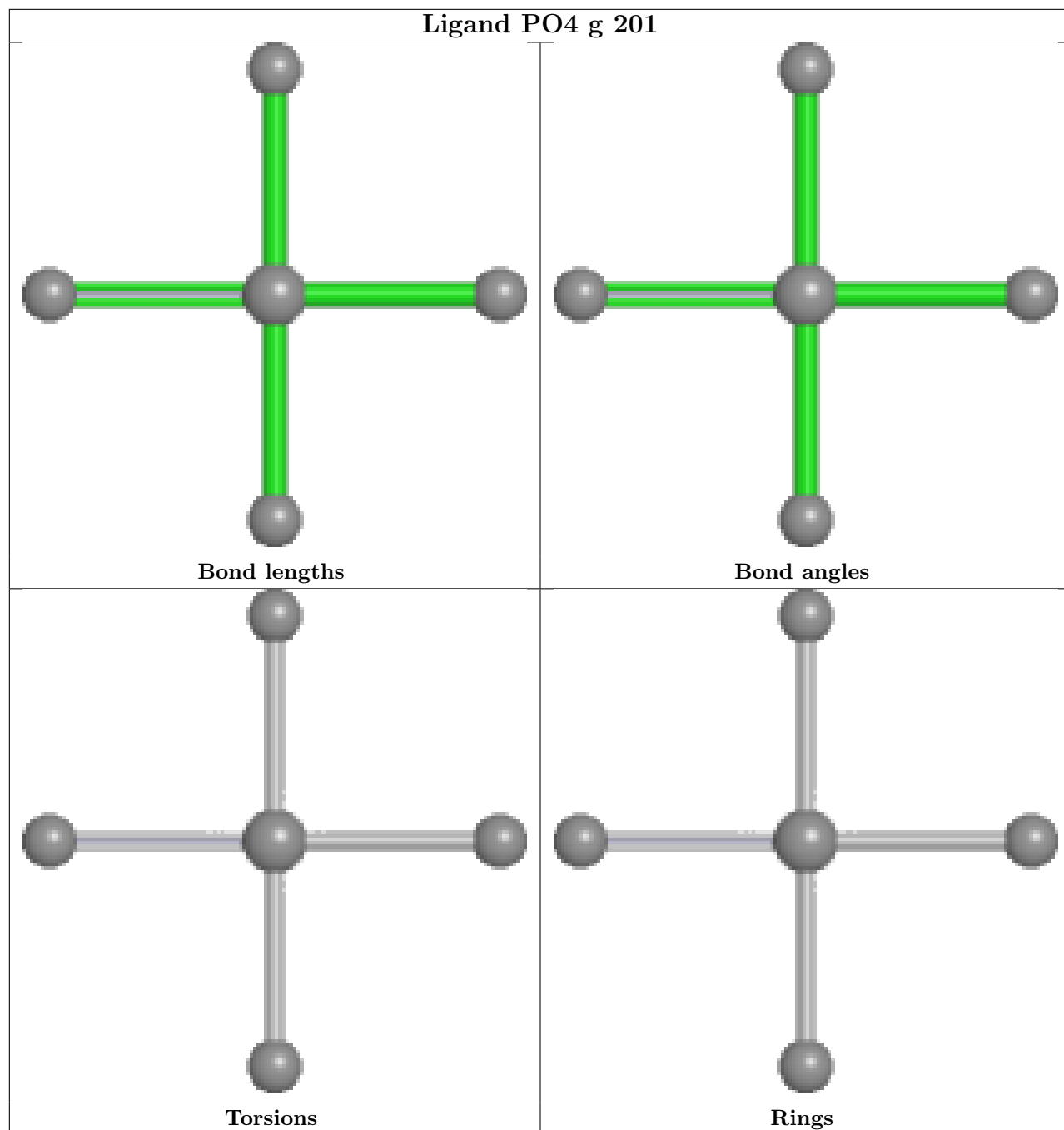
20 monomers are involved in 30 short contacts:

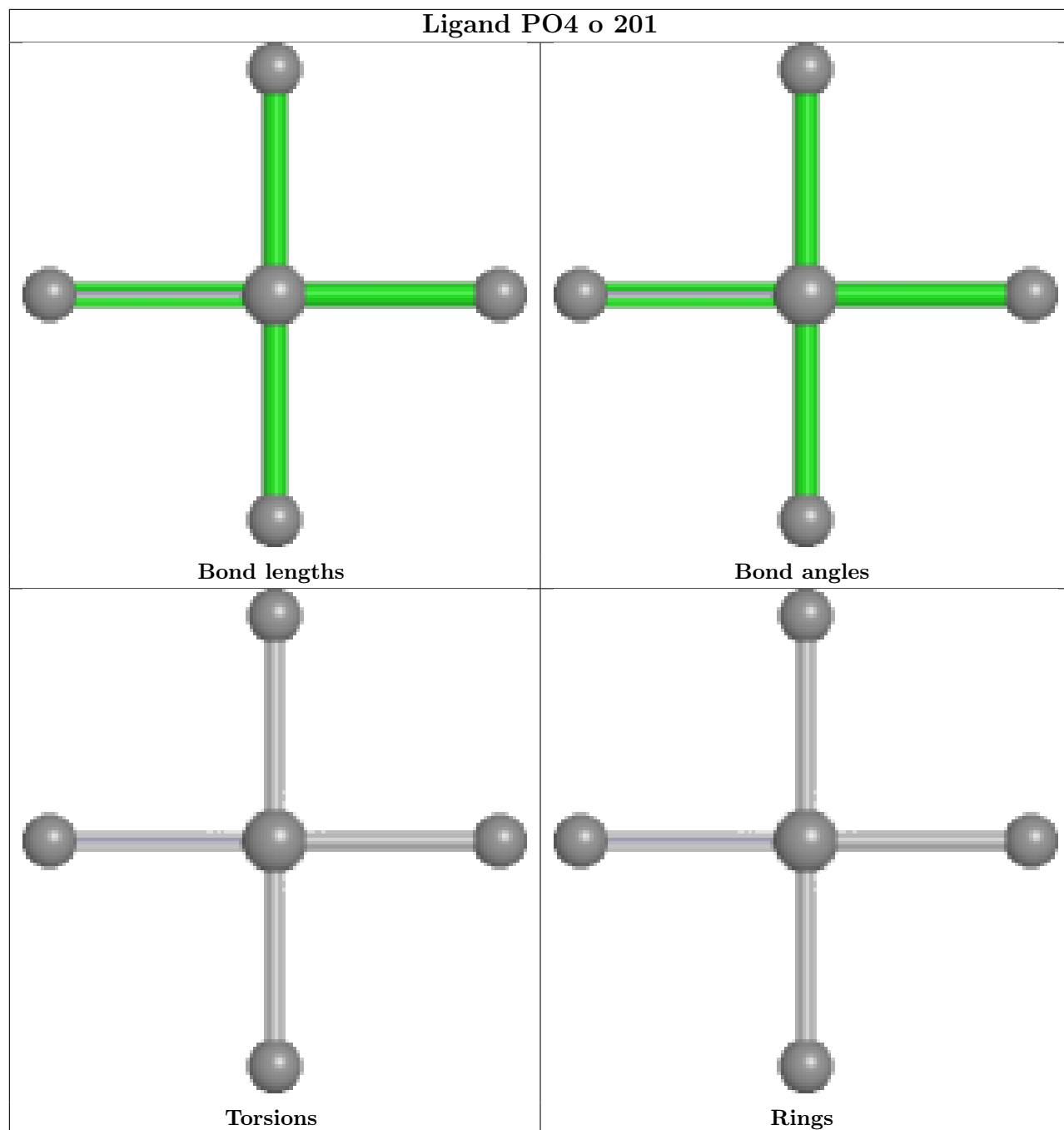
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	306	GOL	3	0
6	L	303	GOL	1	0
6	k	201	GOL	4	0
4	e	201	PO4	3	0
4	C	301	PO4	1	0
4	M	302	PO4	1	0
4	e	203	PO4	1	0
4	q	201	PO4	1	0
4	a	202	PO4	2	0
4	R	301	PO4	1	0
4	g	202	PO4	1	0
4	J	302	PO4	1	0
4	E	304	PO4	1	0
4	o	202	PO4	2	0
4	c	201	PO4	1	0
7	N	303	PEG	2	0
4	e	202	PO4	1	0
7	H	303	PEG	1	0
4	i	203	PO4	1	0
4	o	203	PO4	1	0

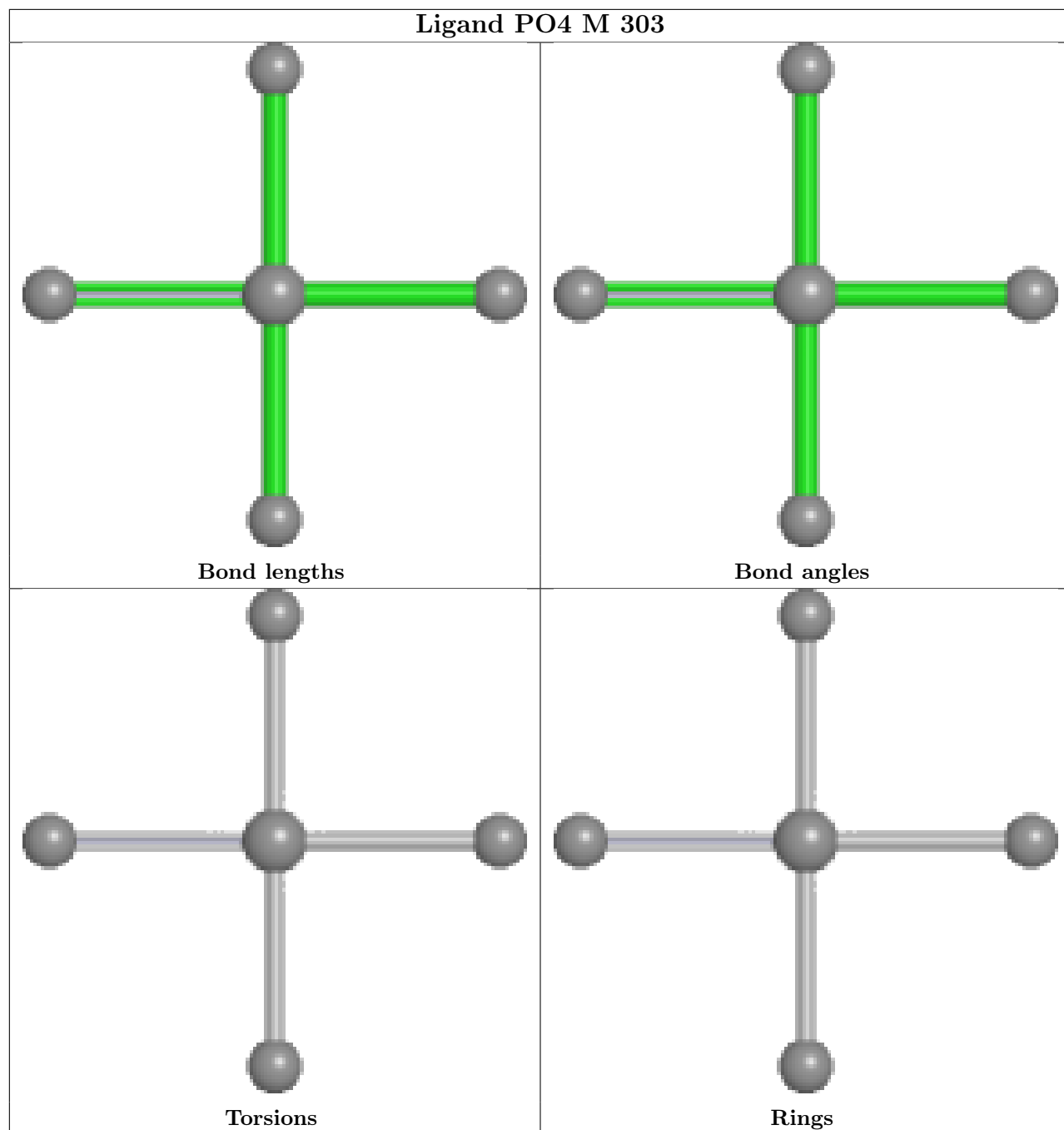
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

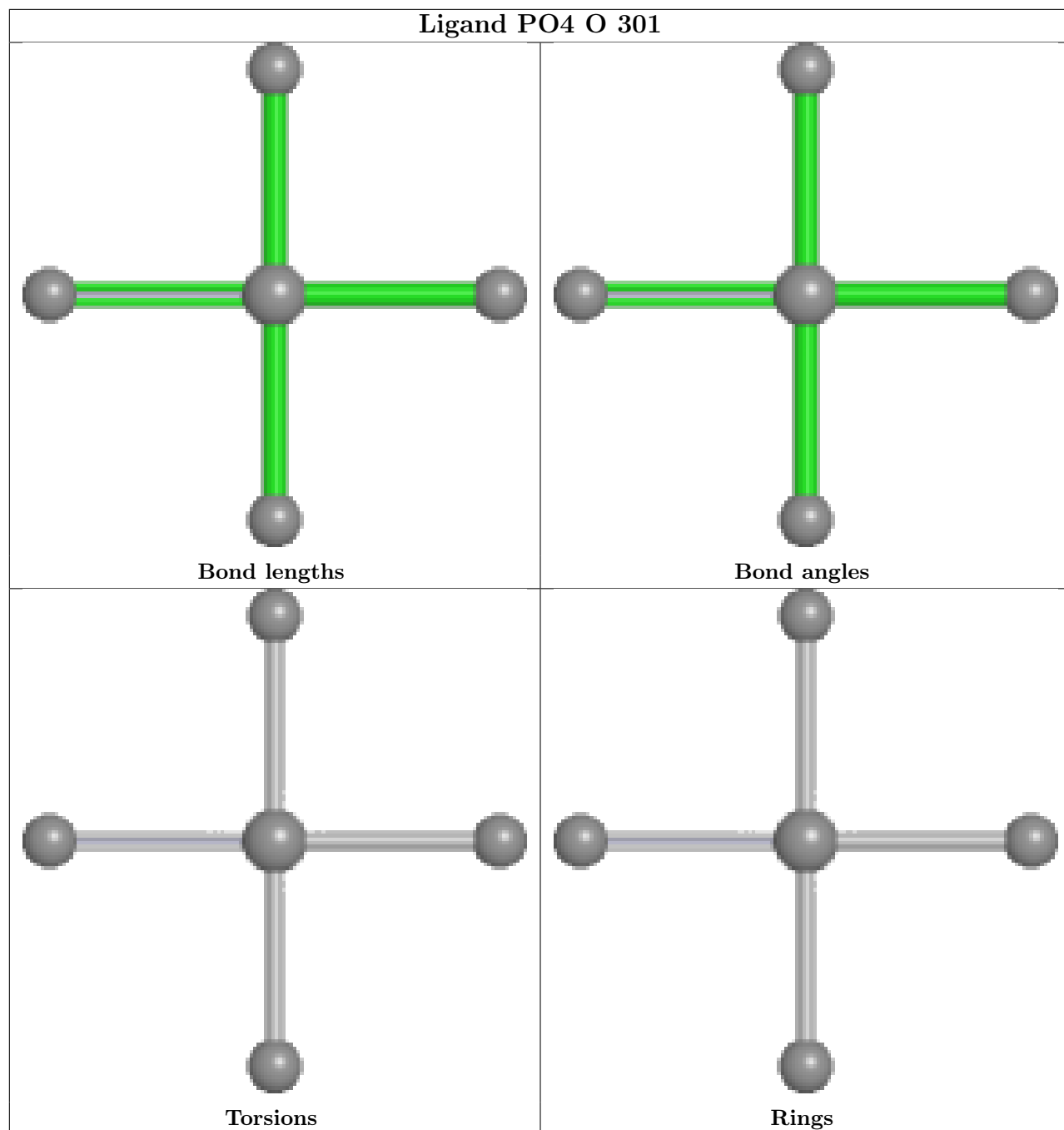
equivalents in the CSD to analyse the geometry.

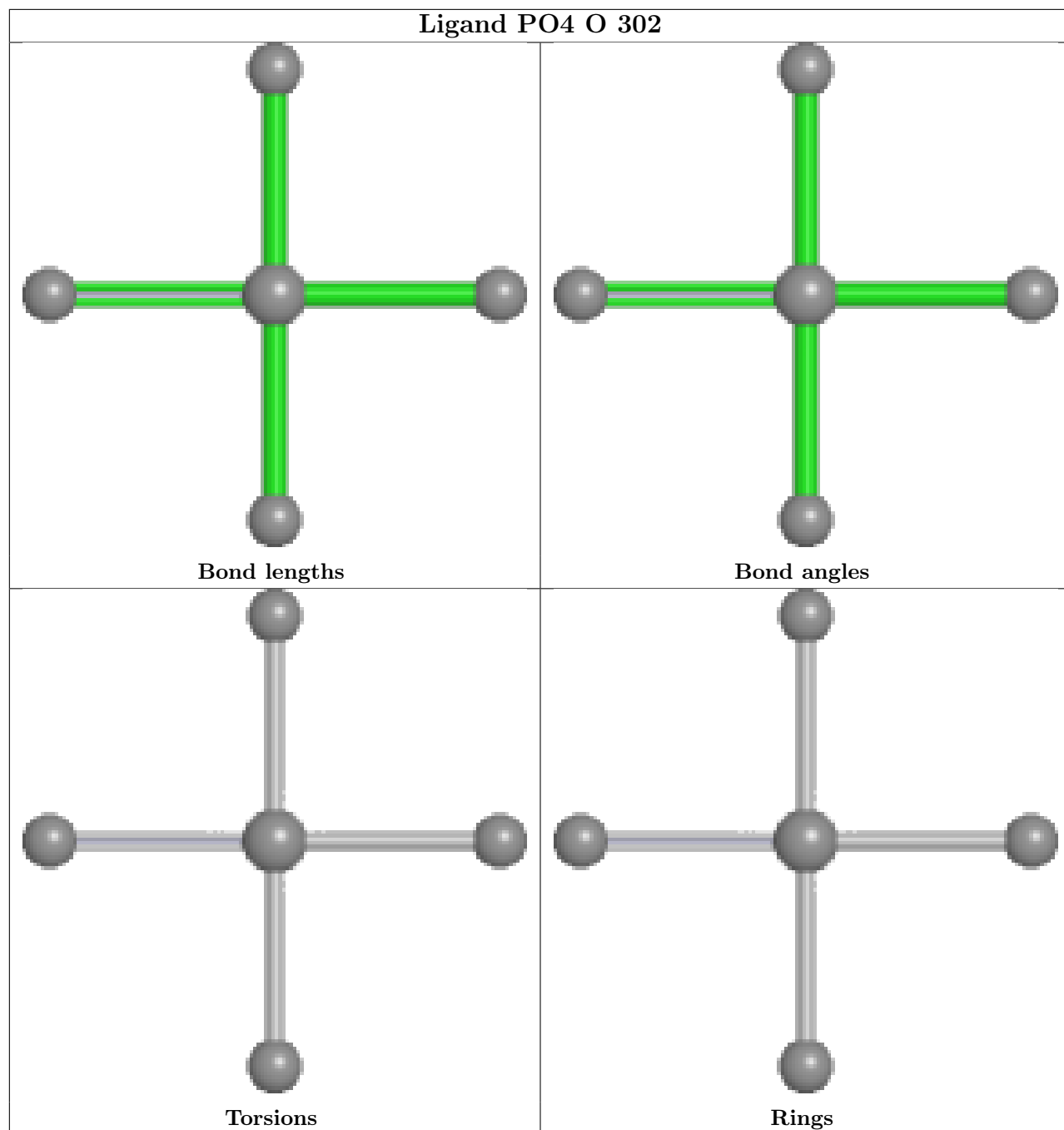


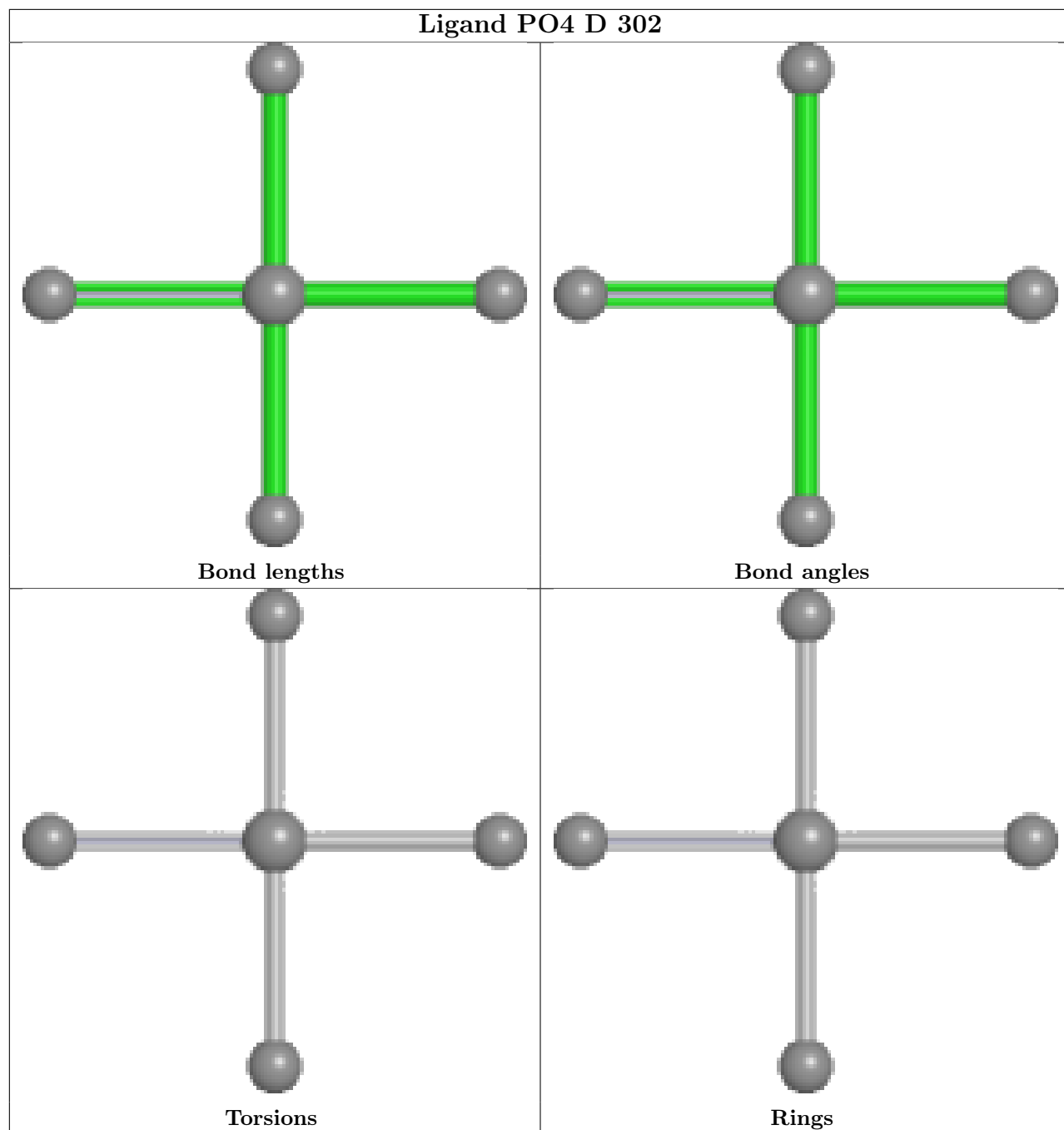


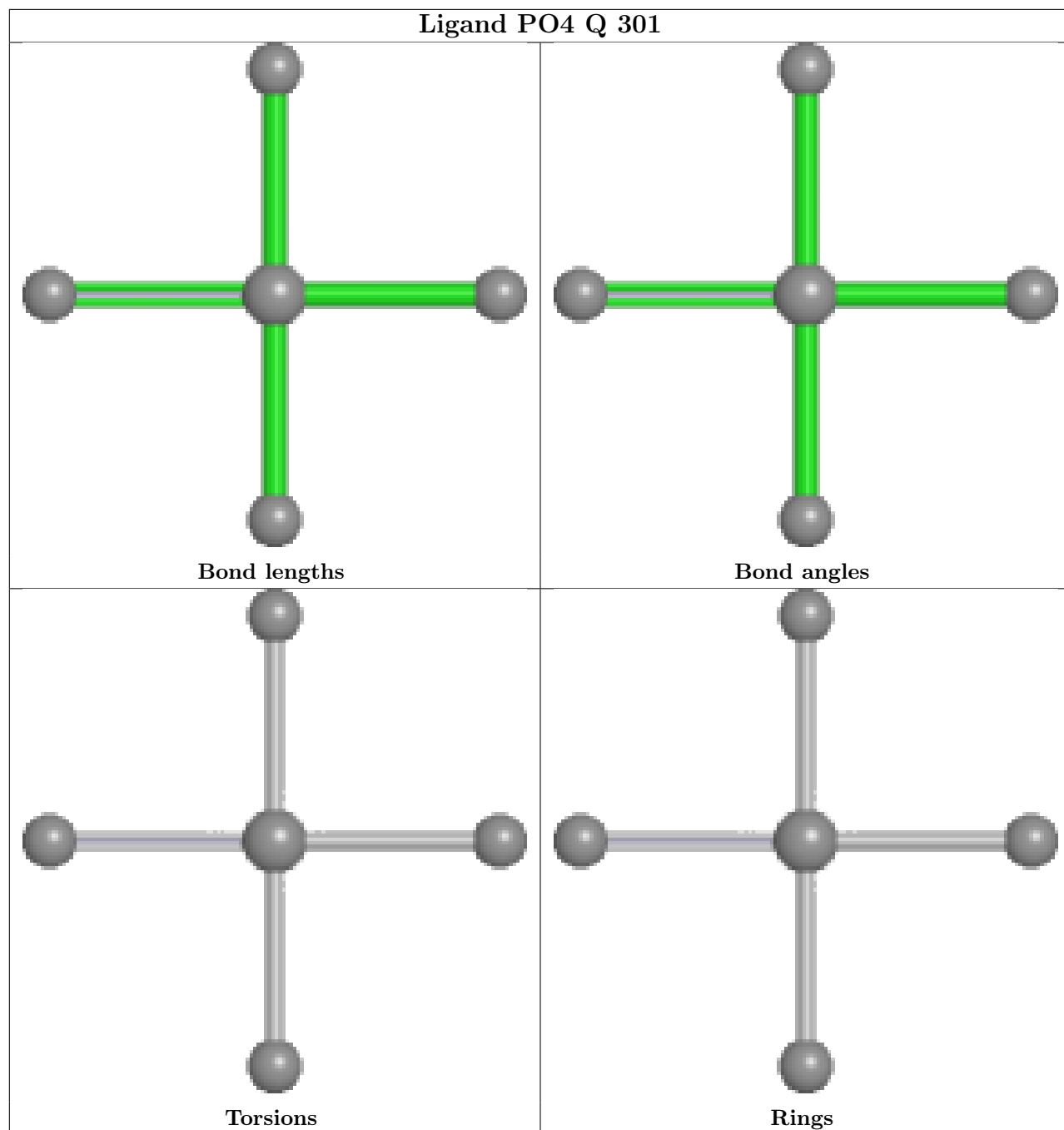


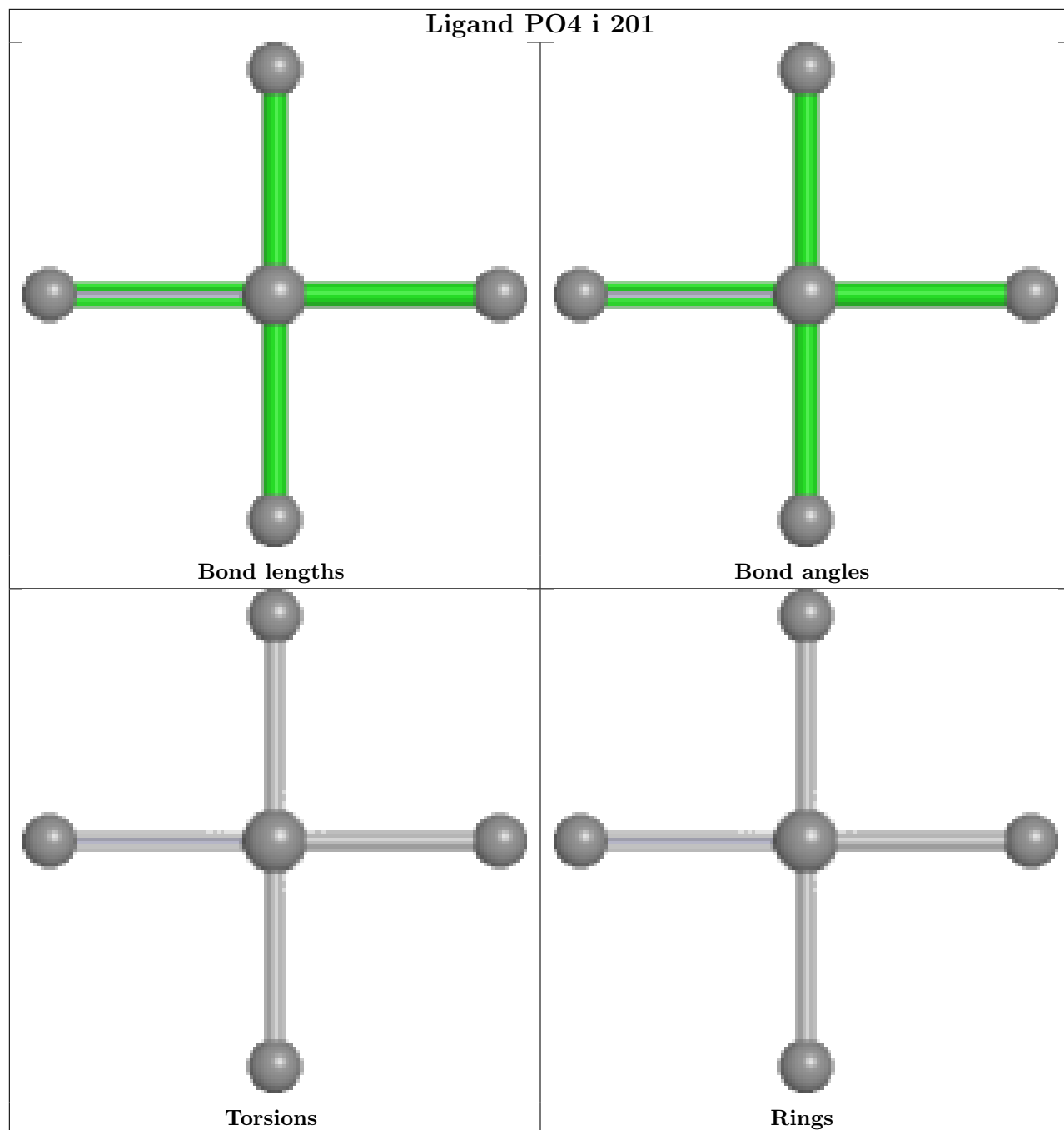


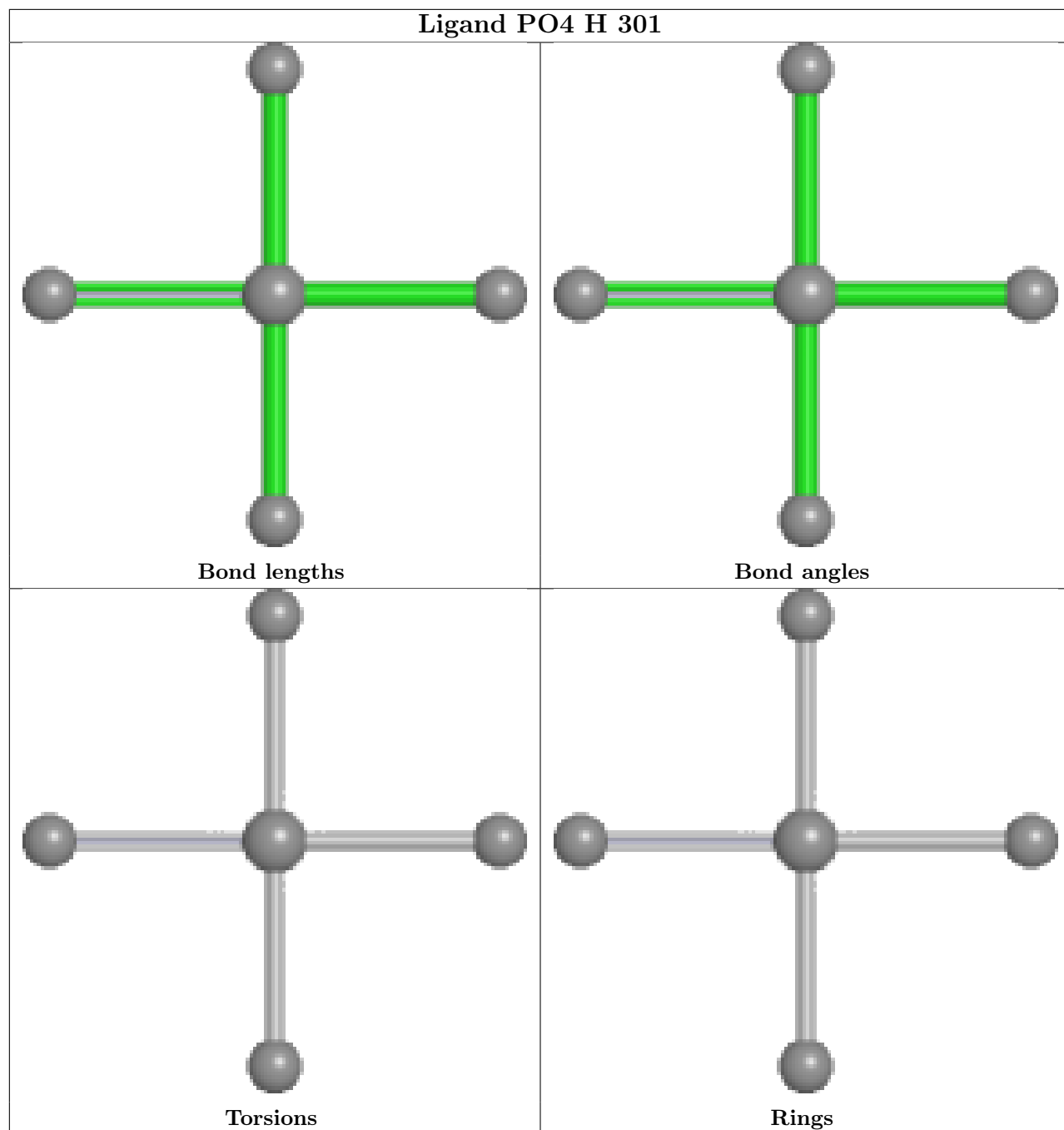


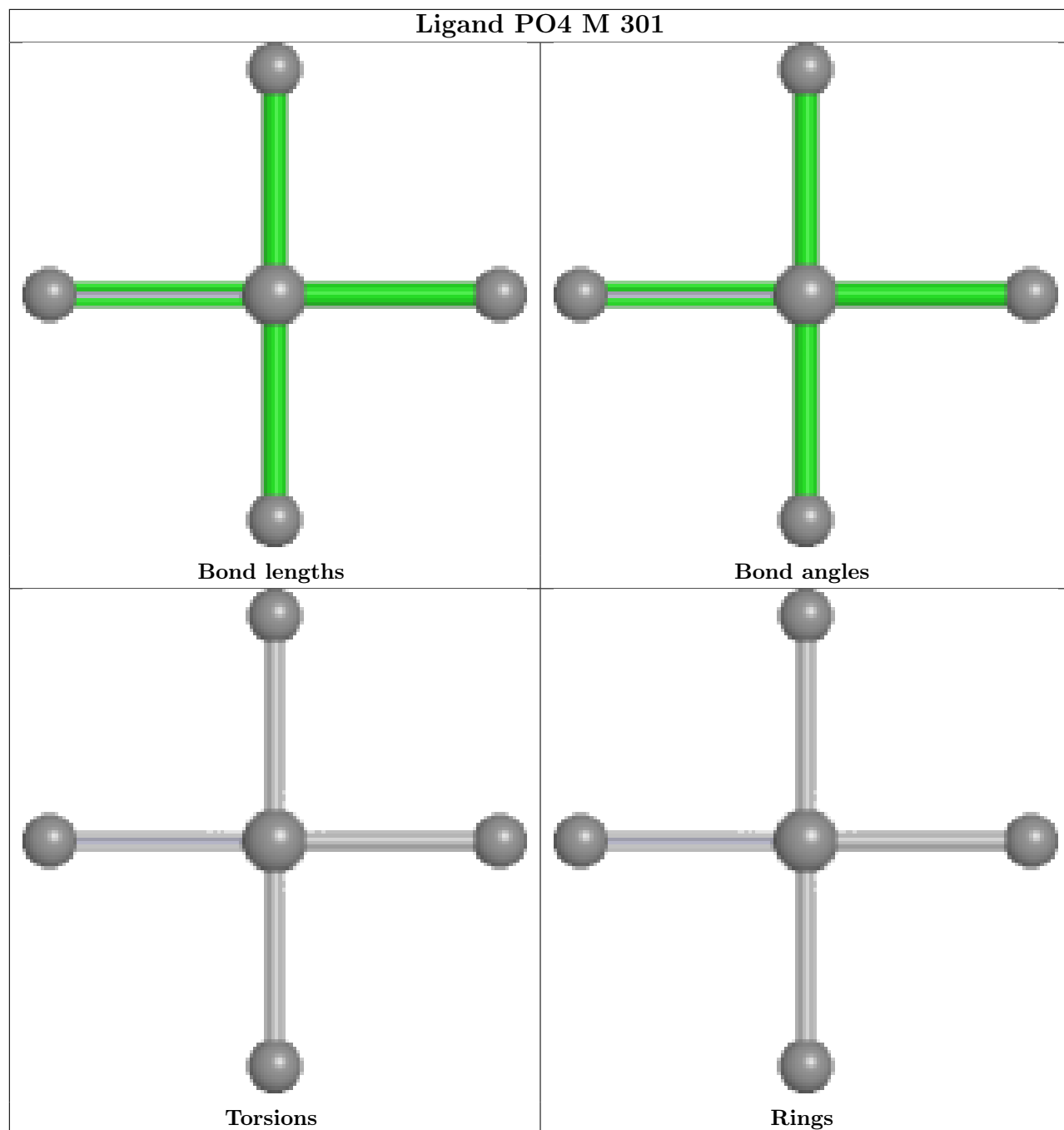


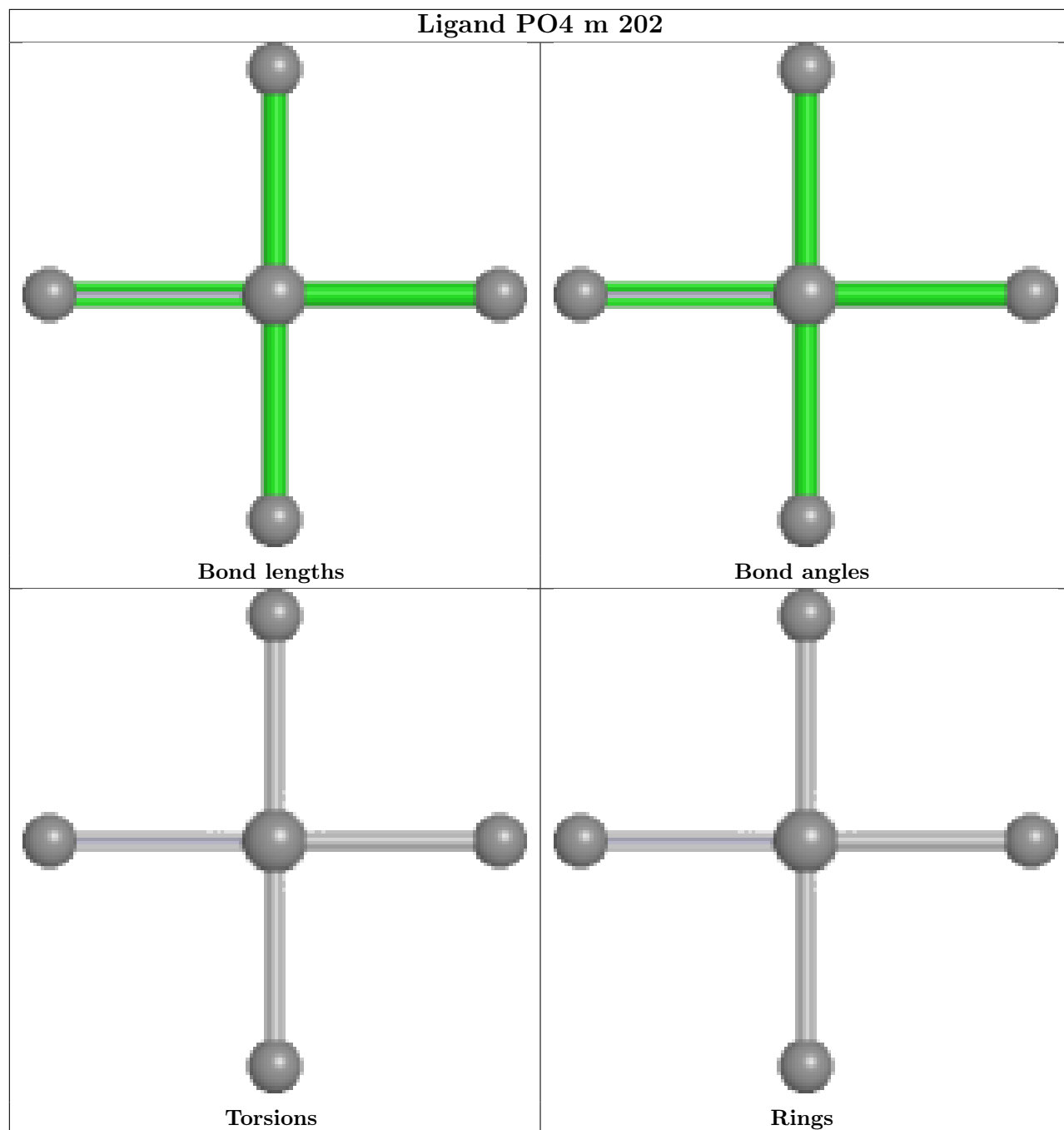


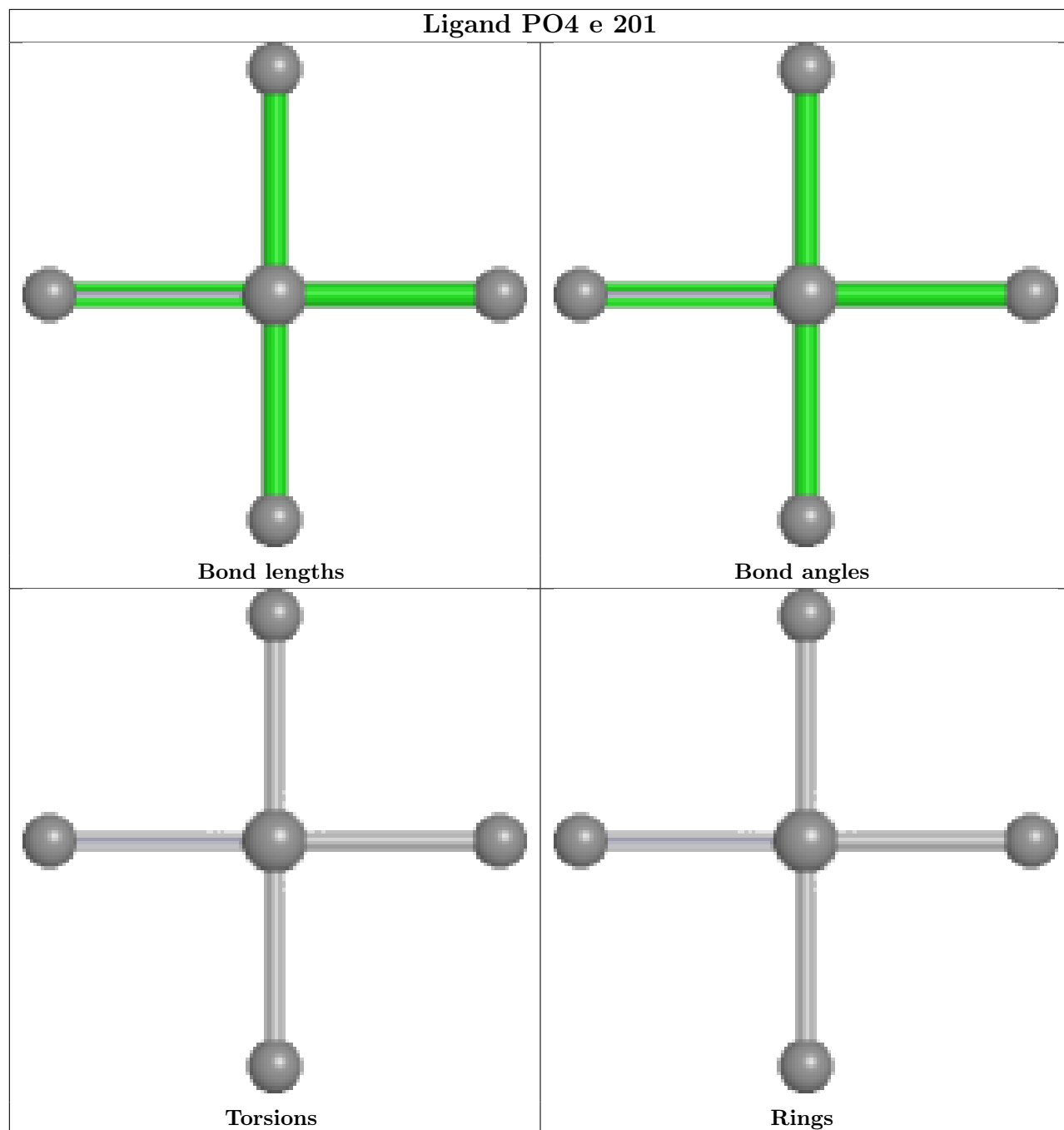


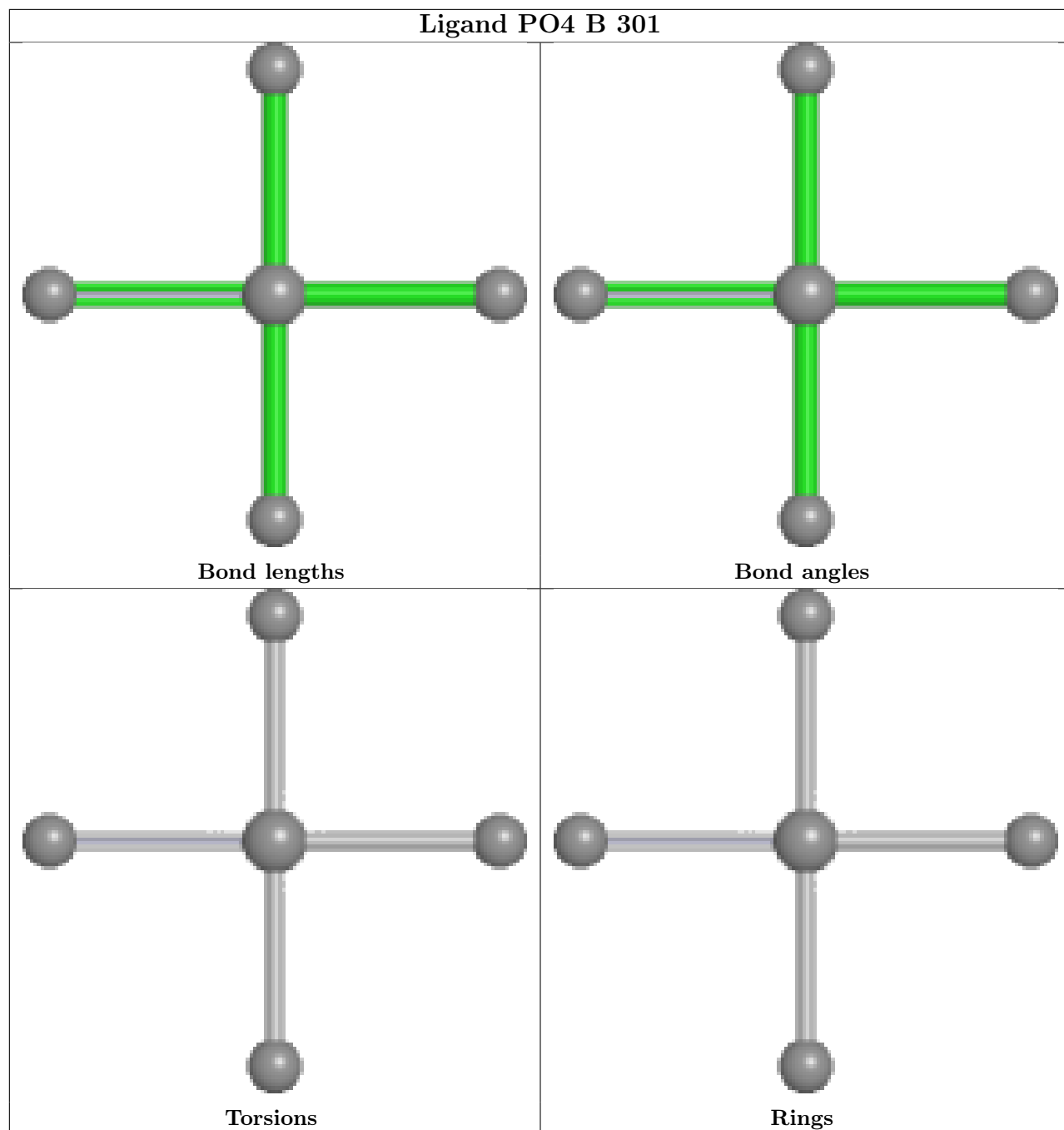


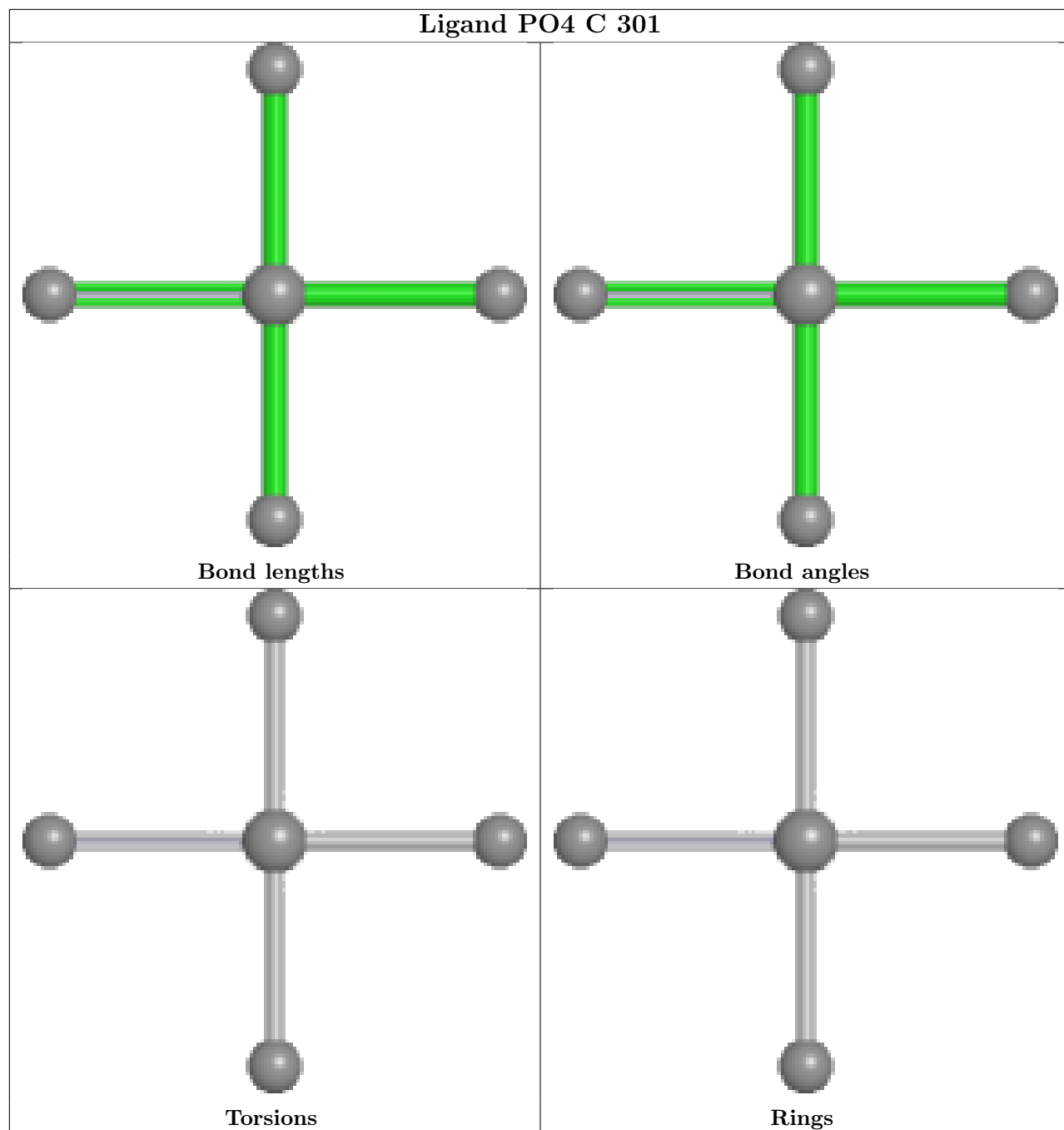


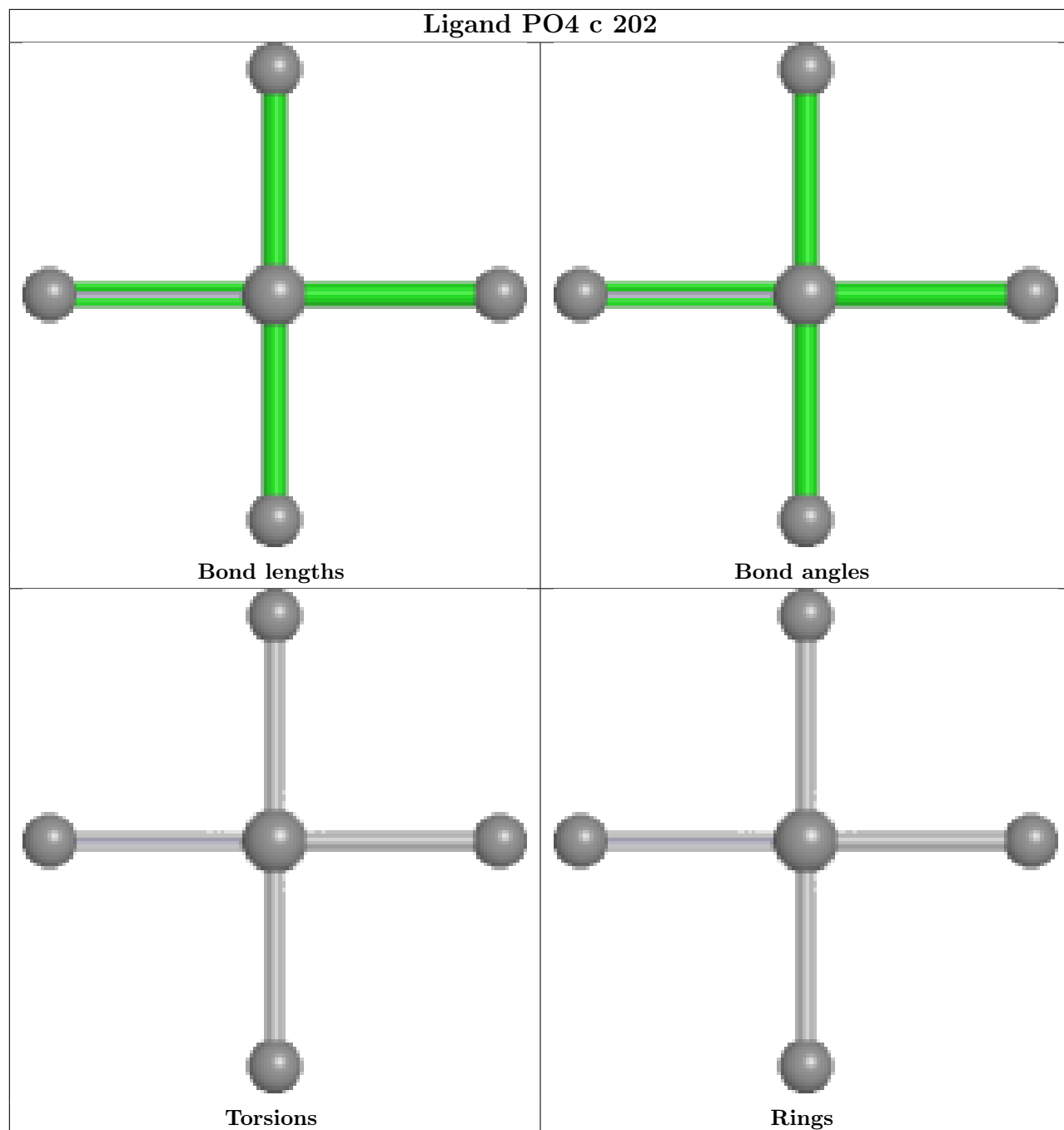


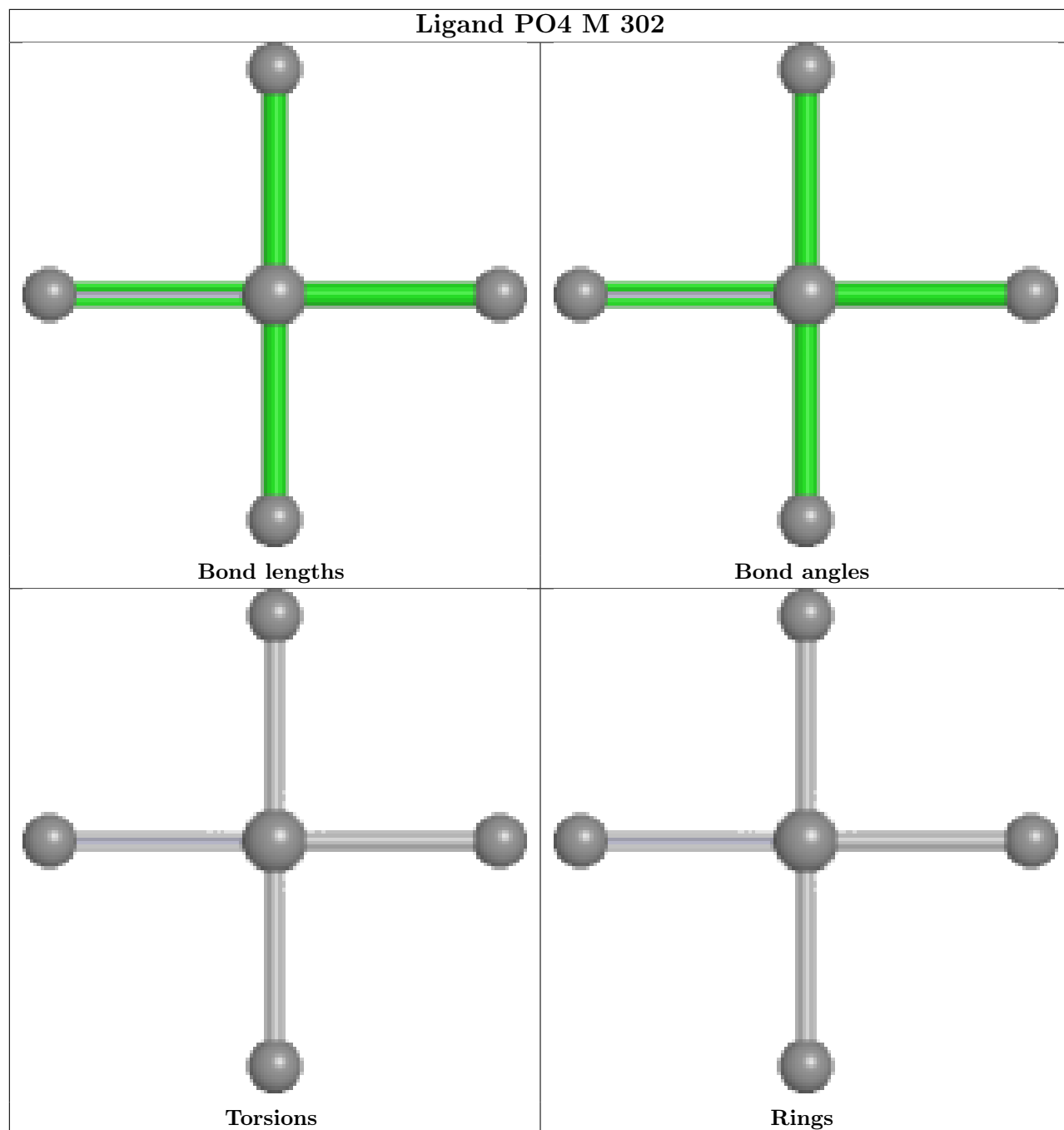


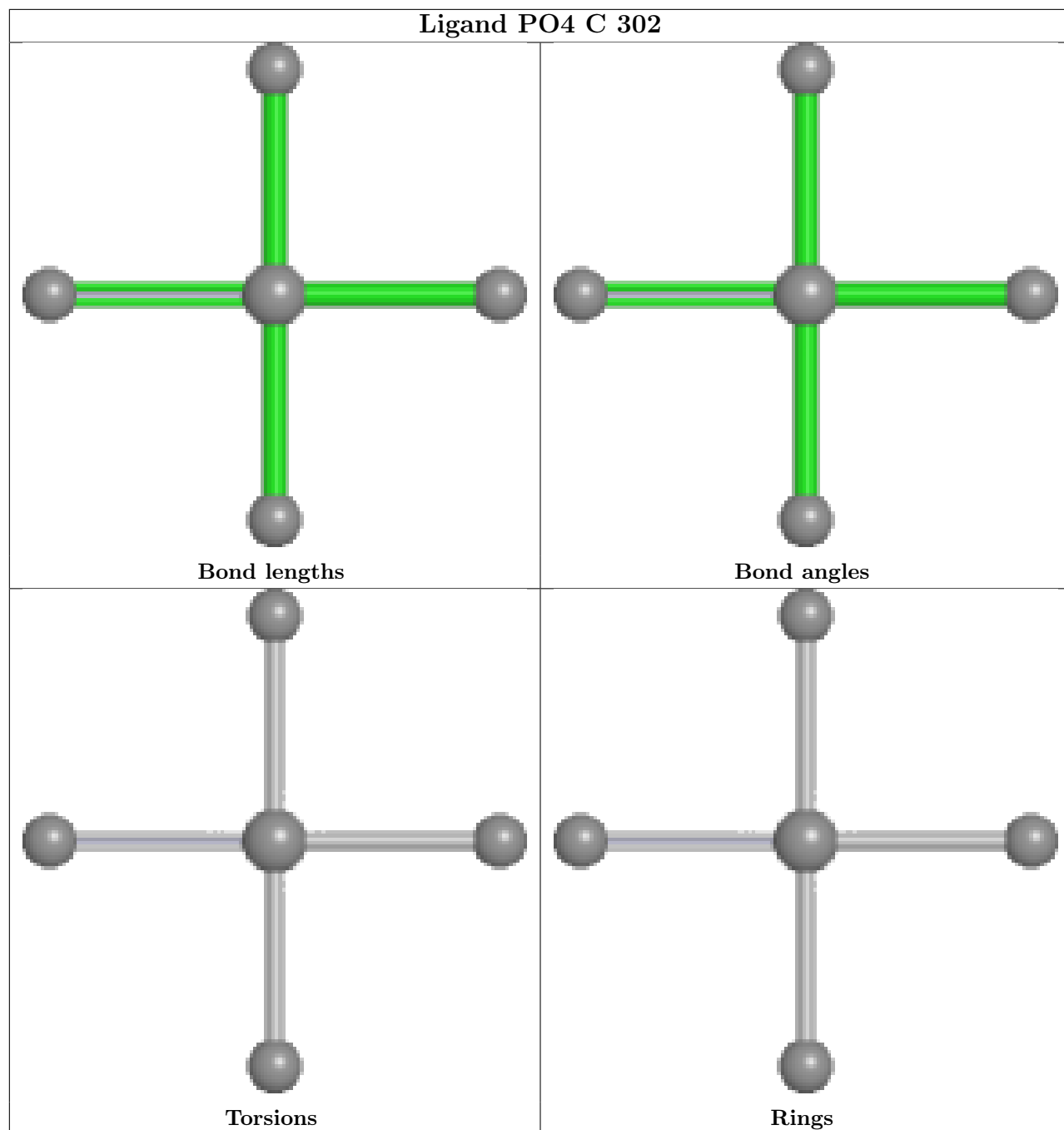


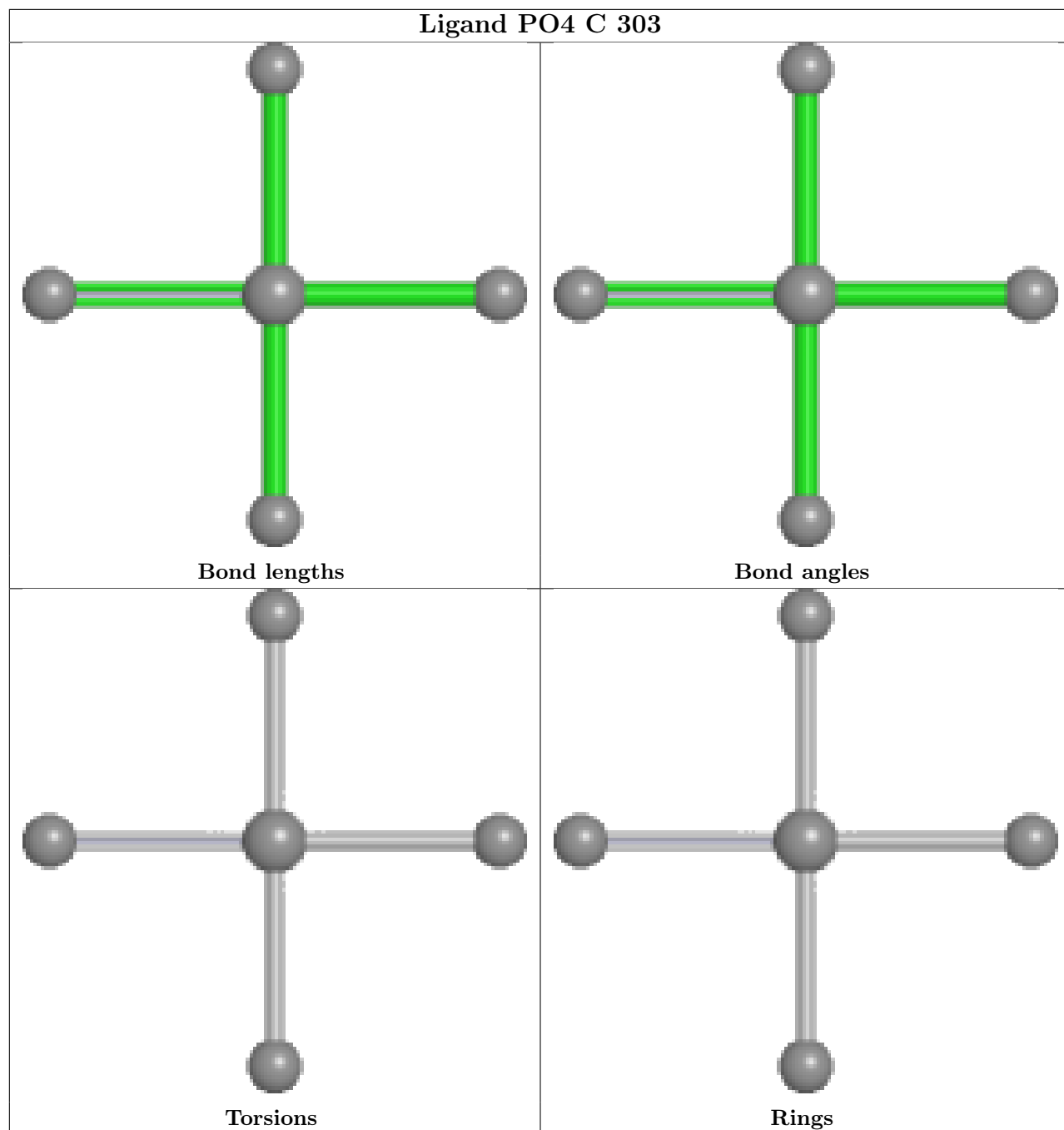


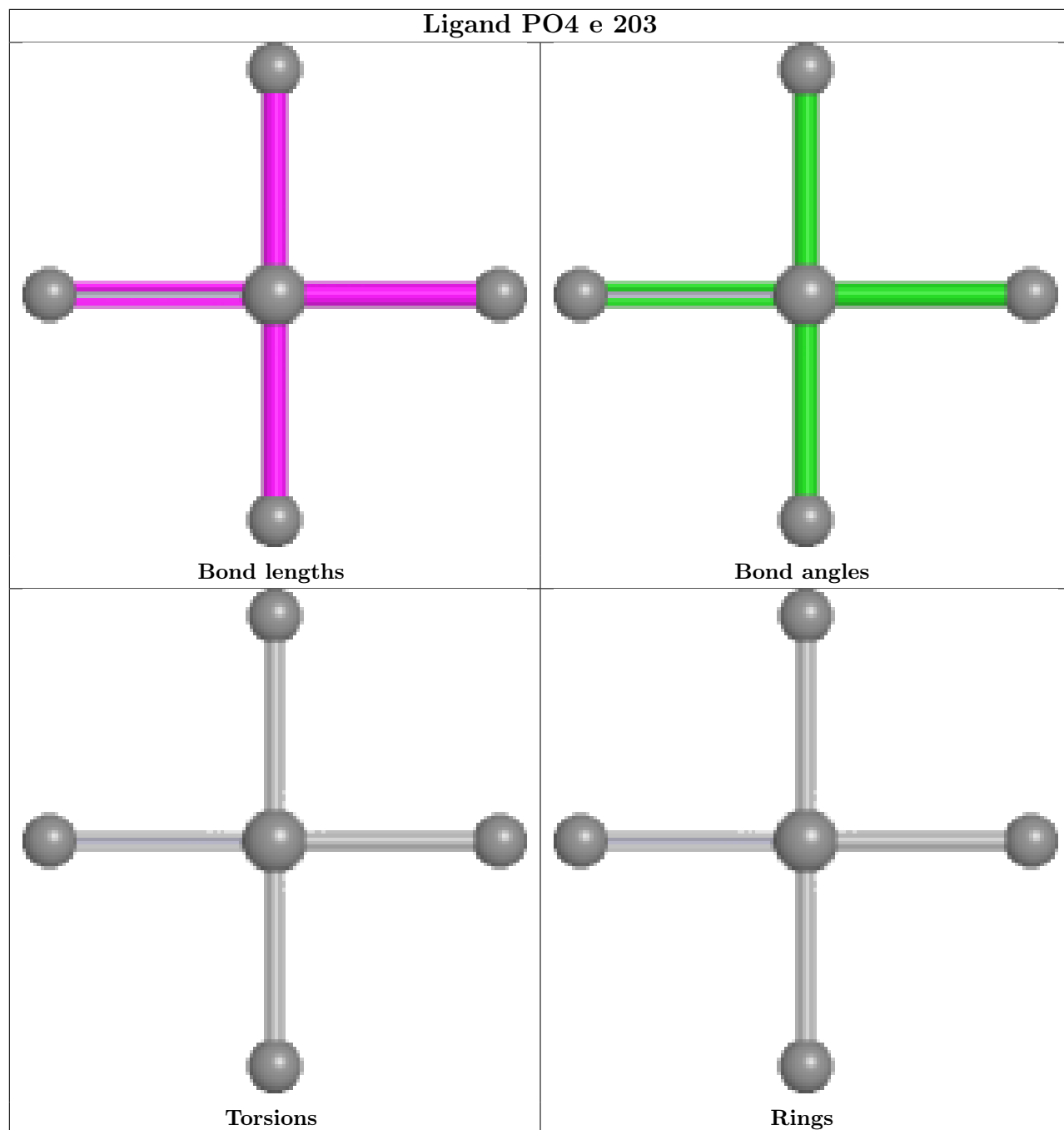


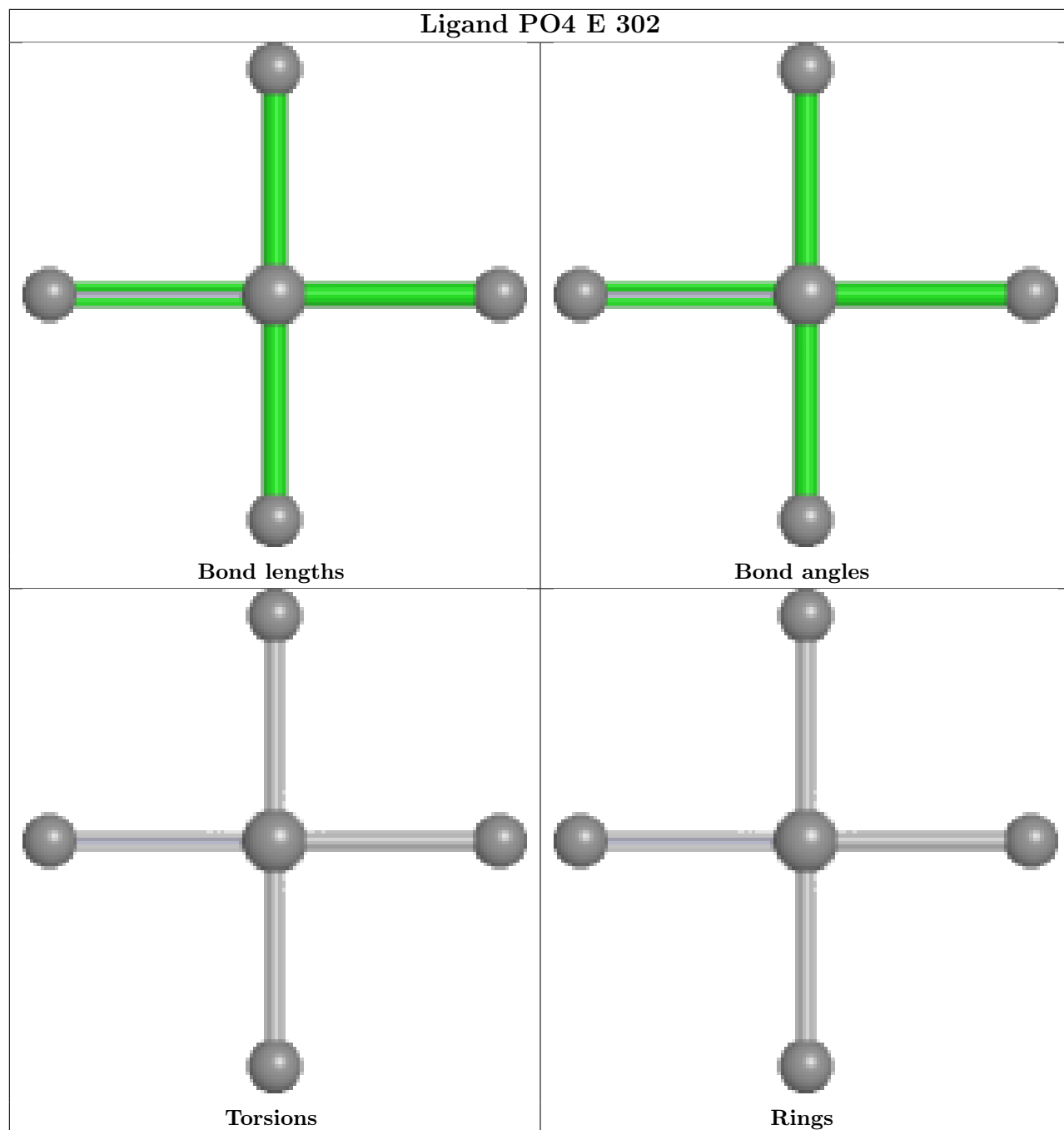


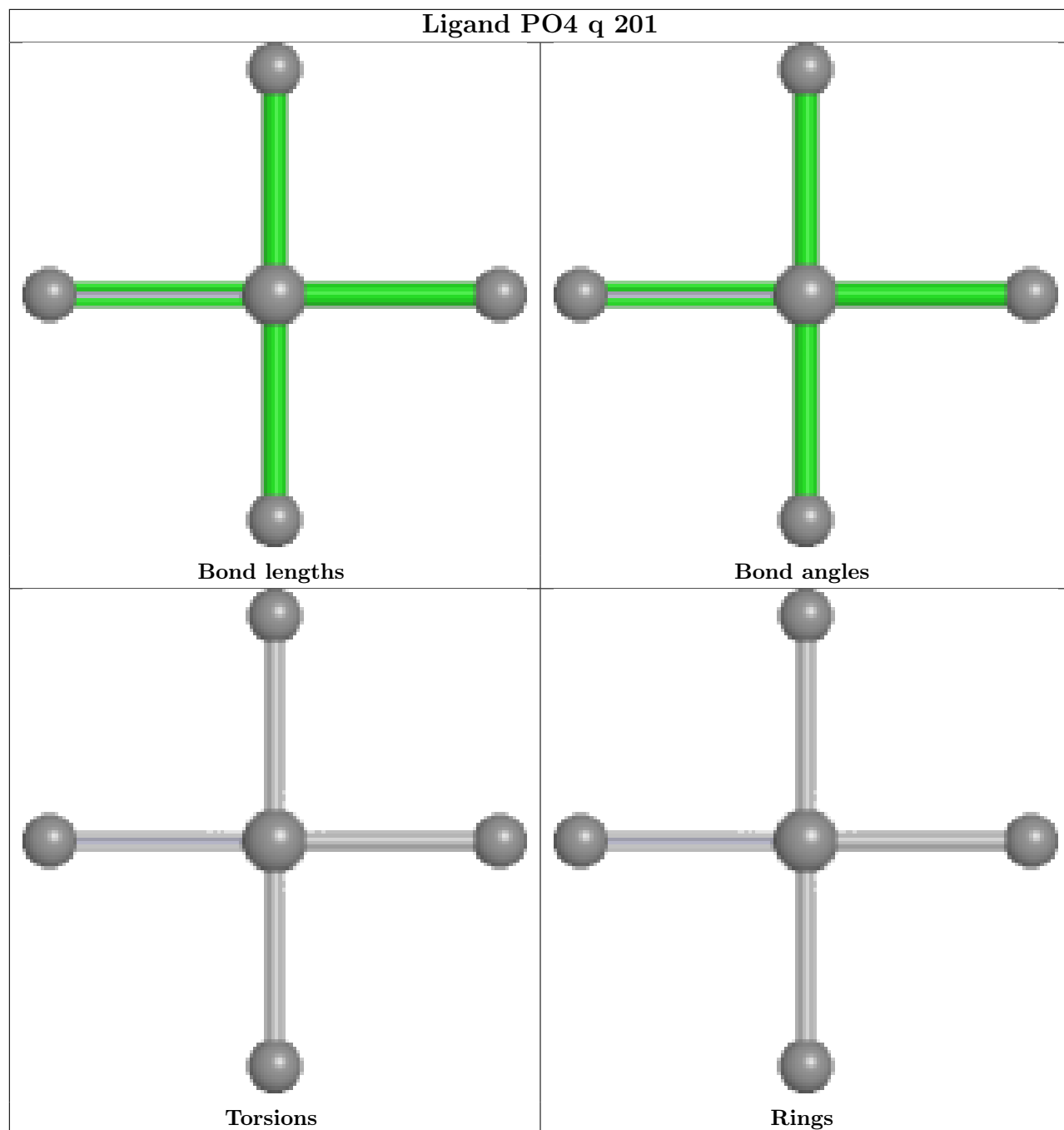


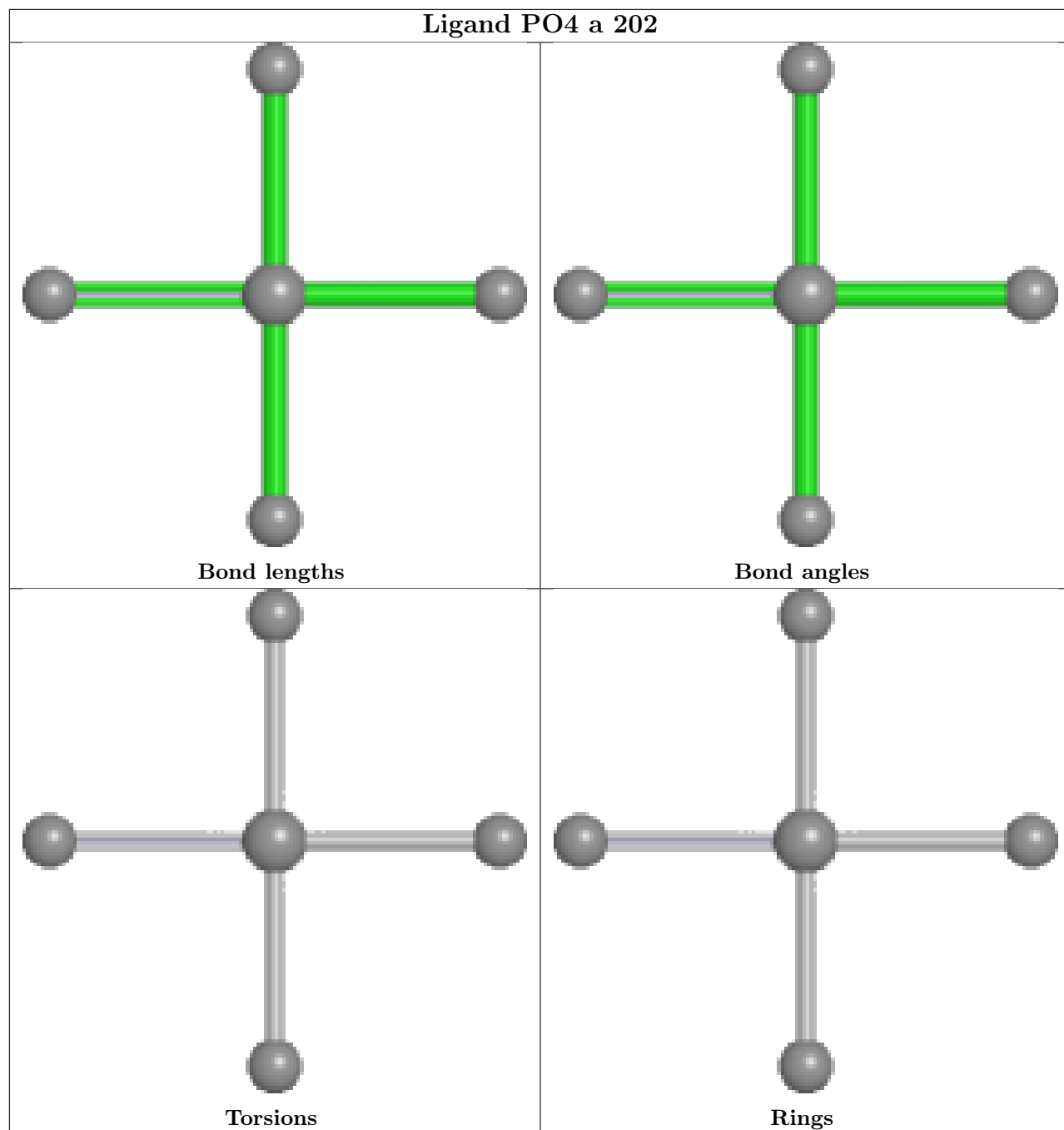


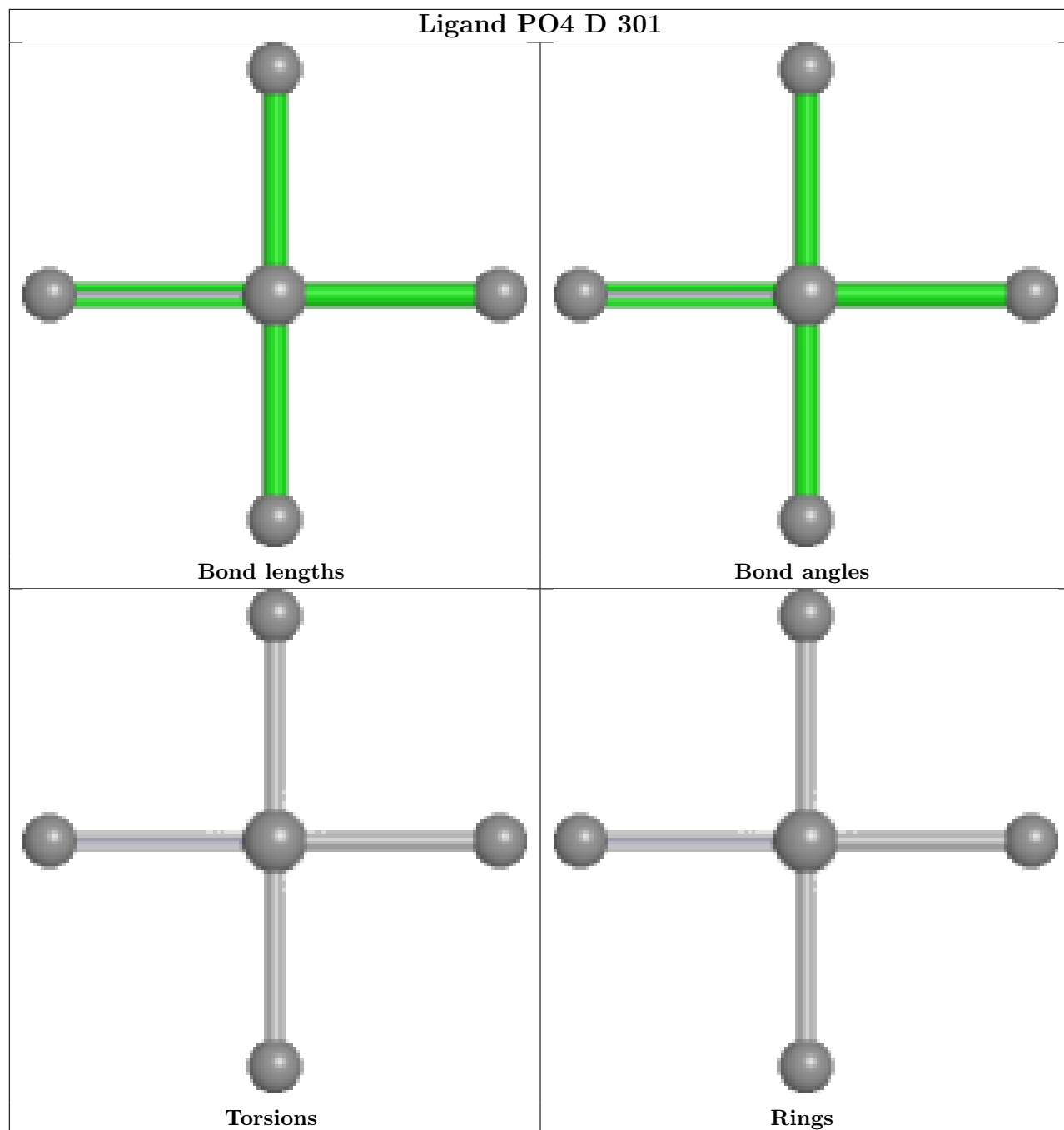


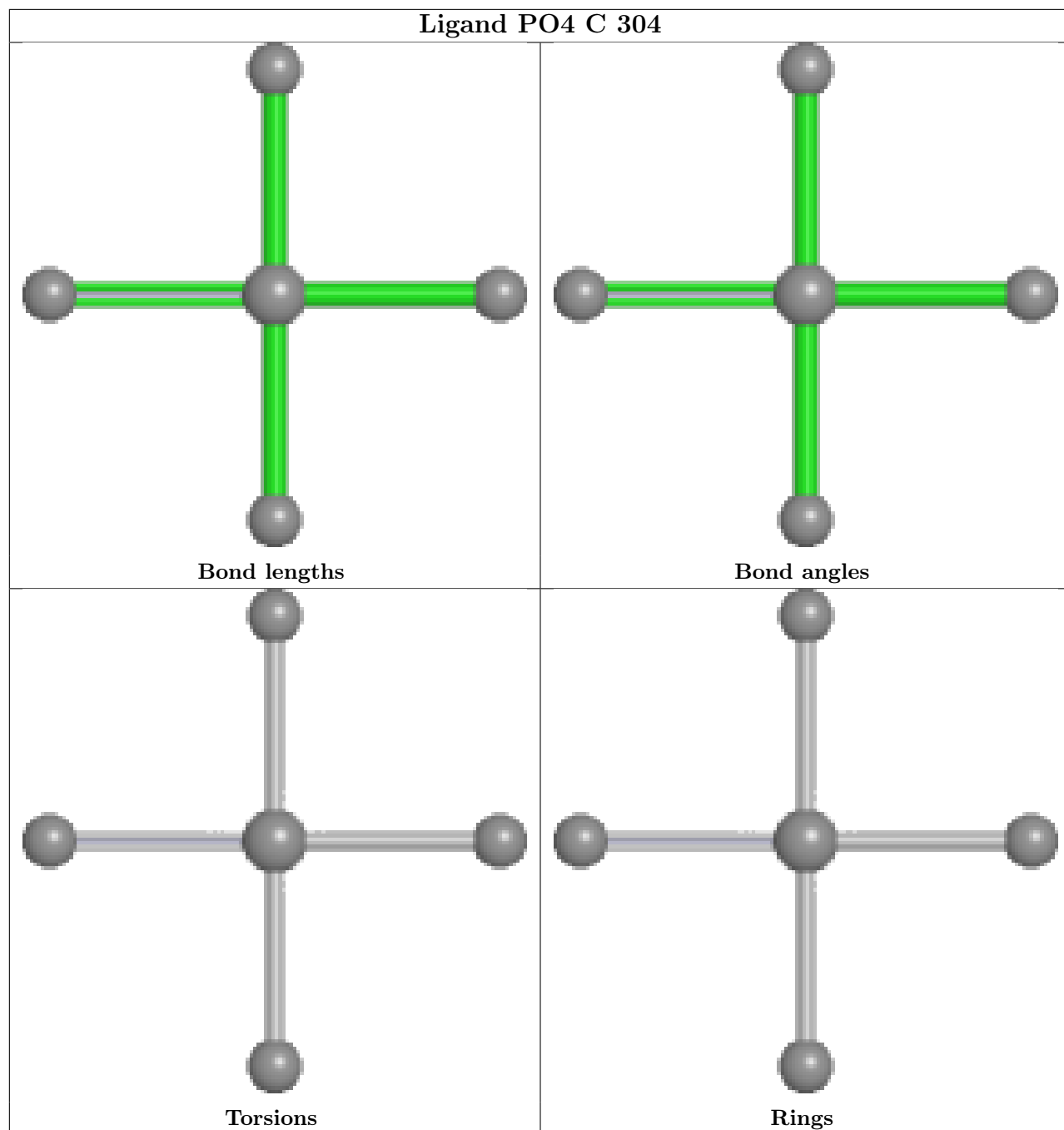


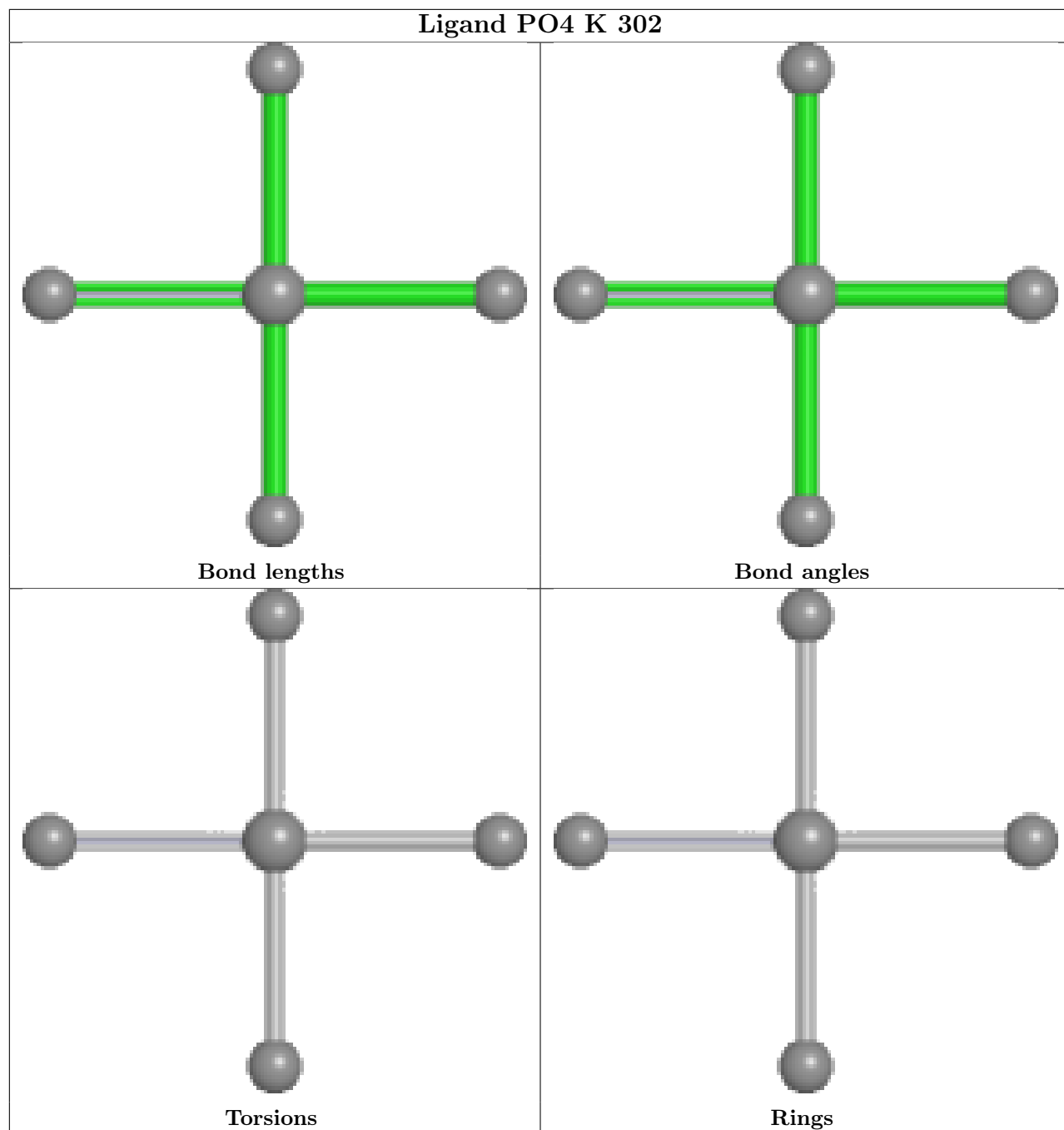


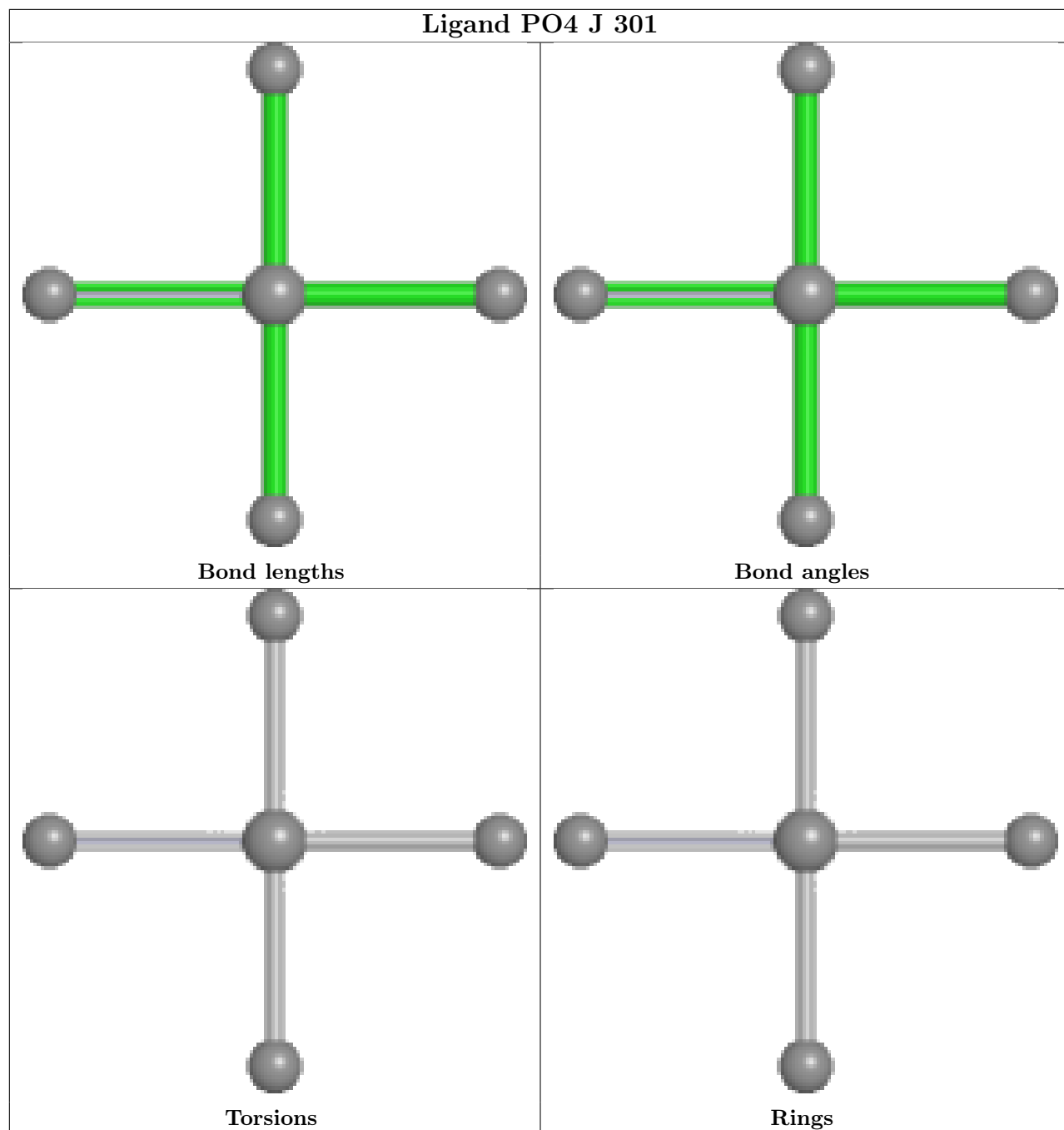


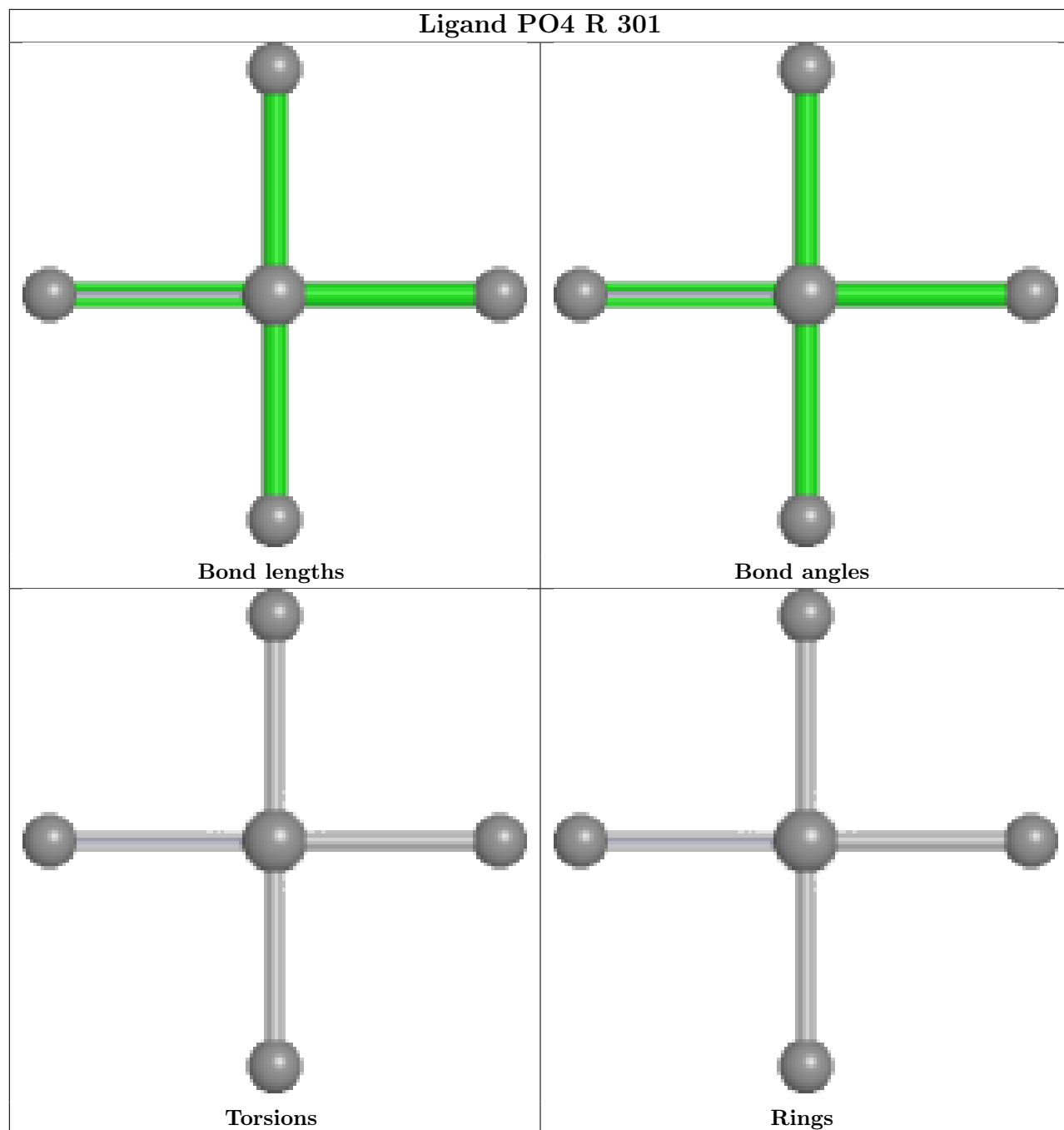


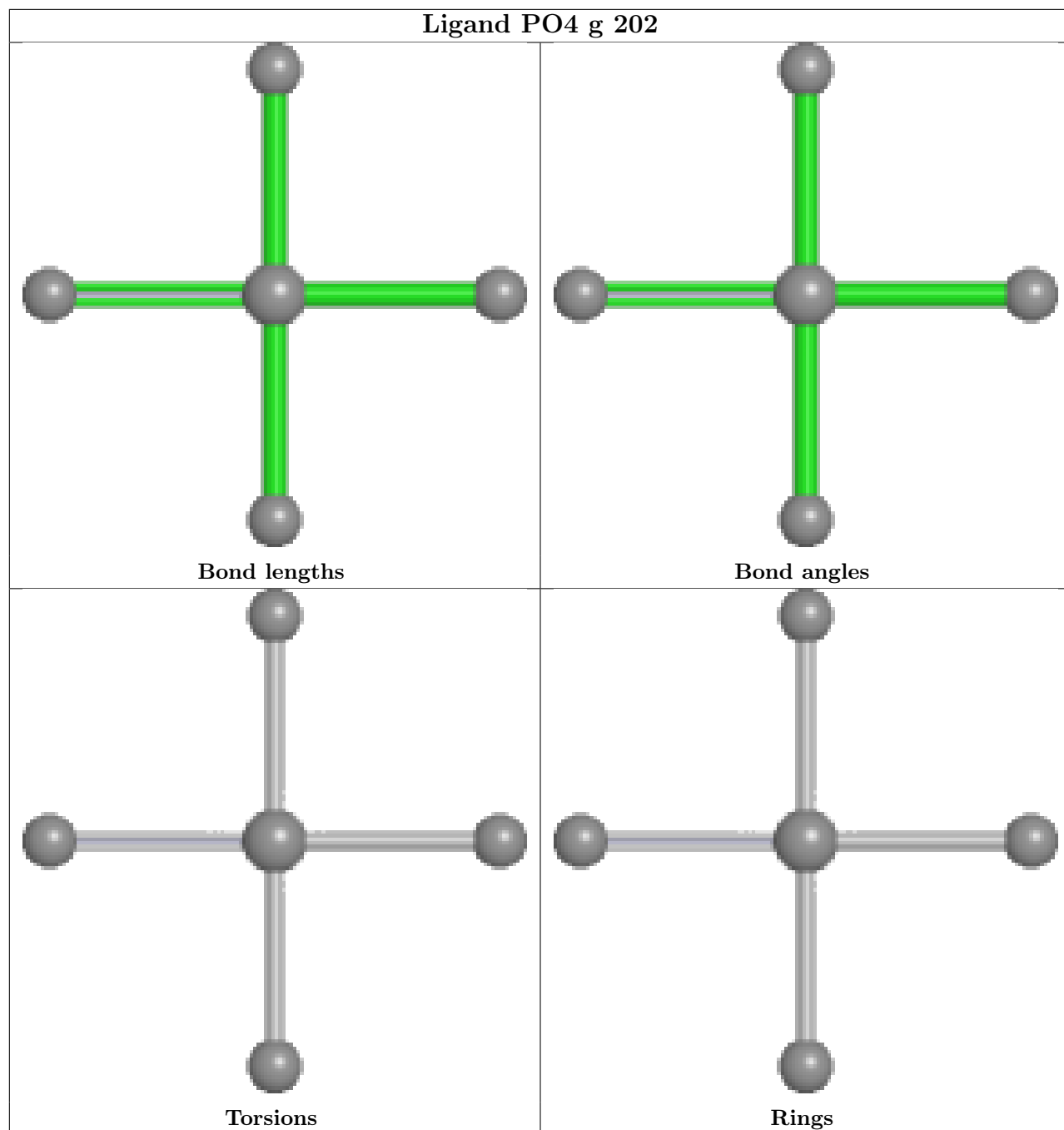


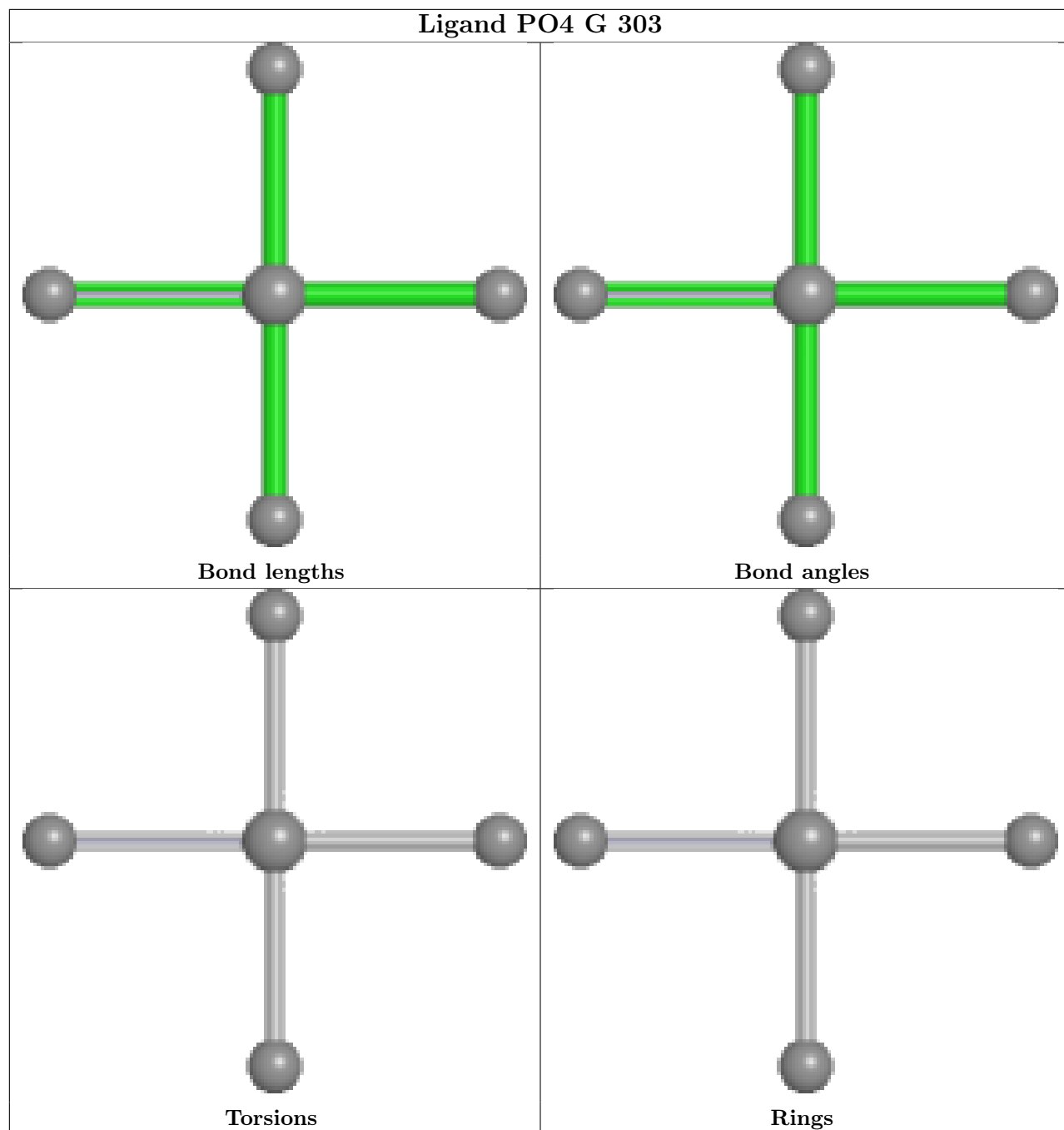


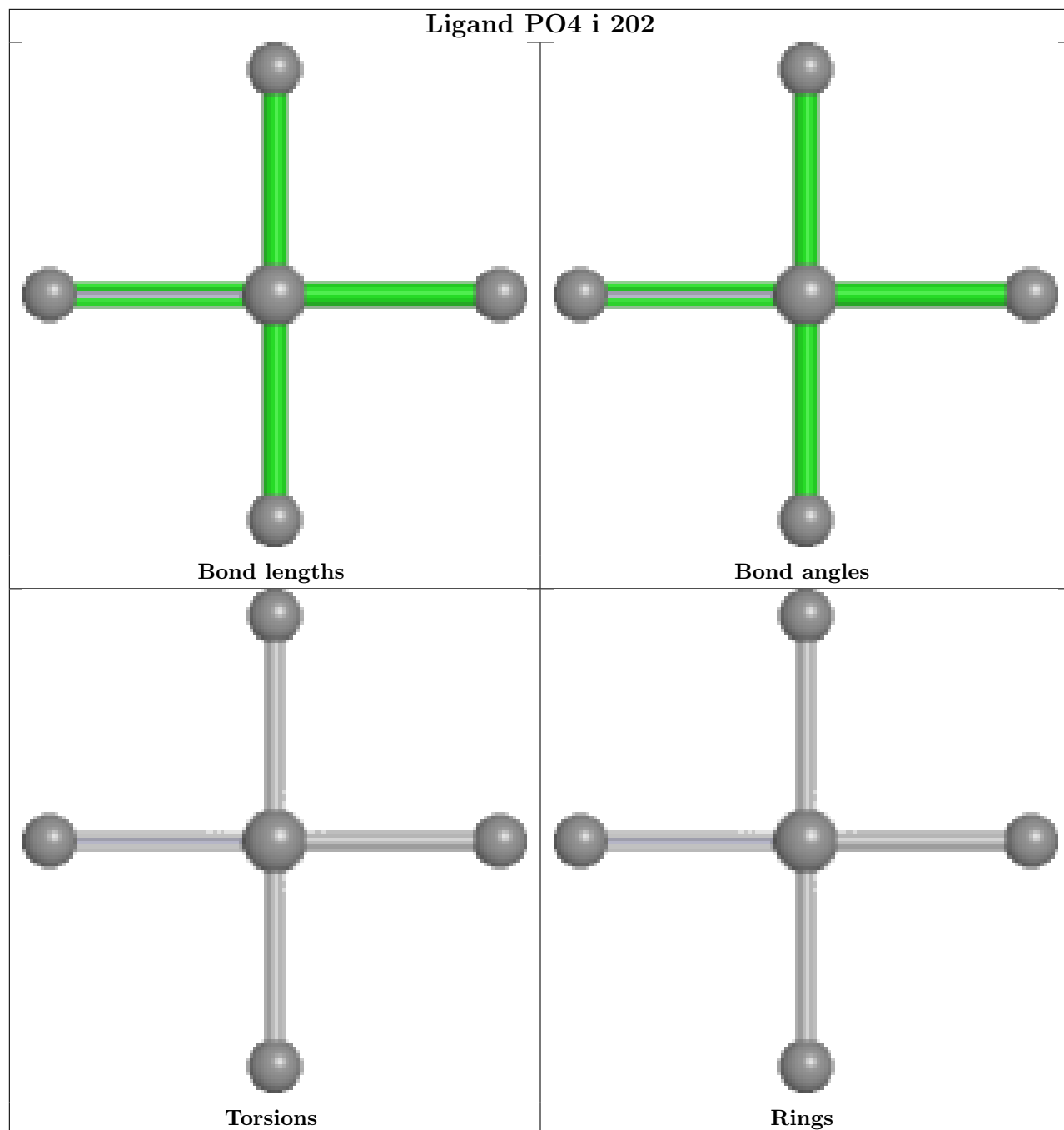


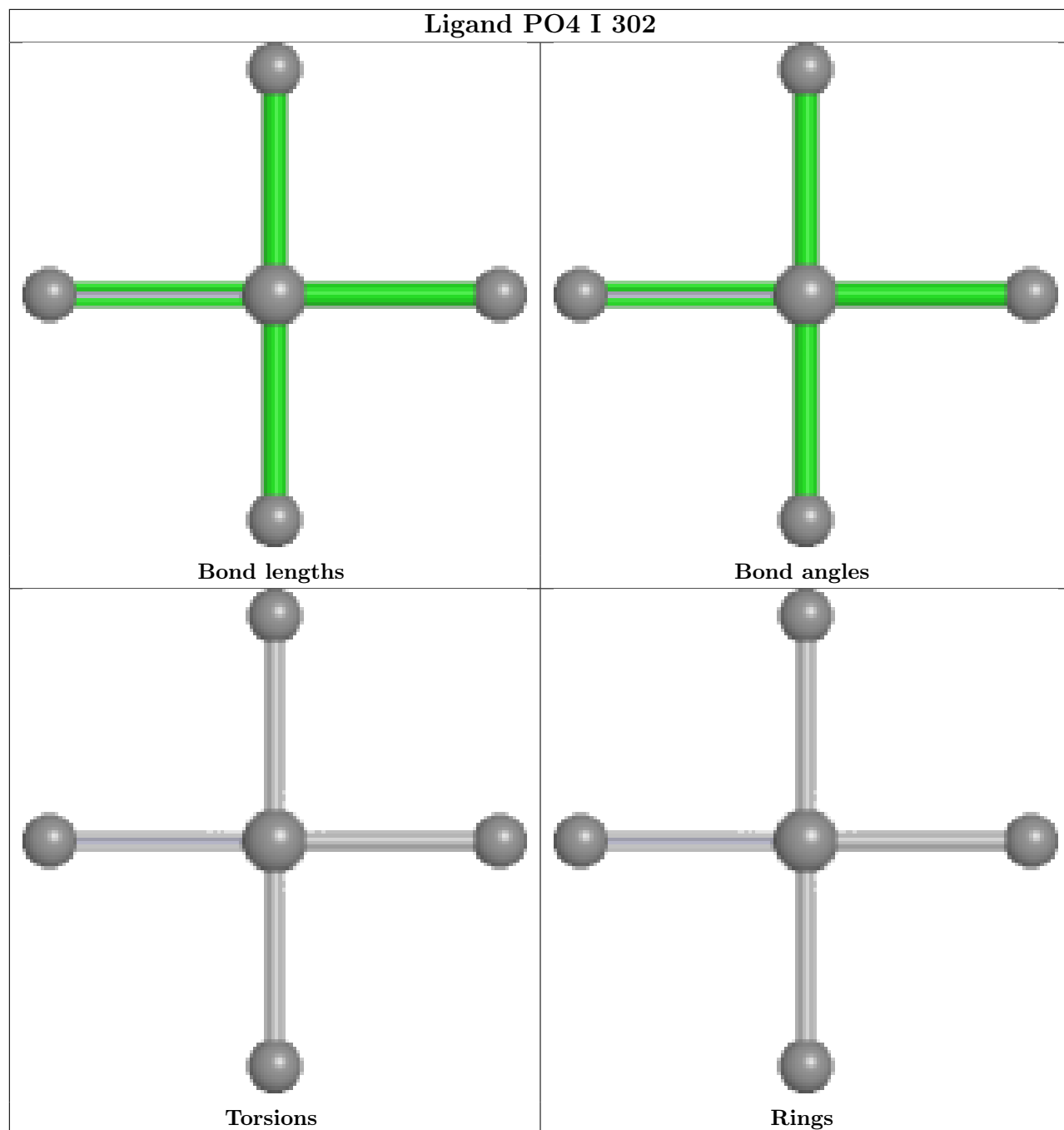


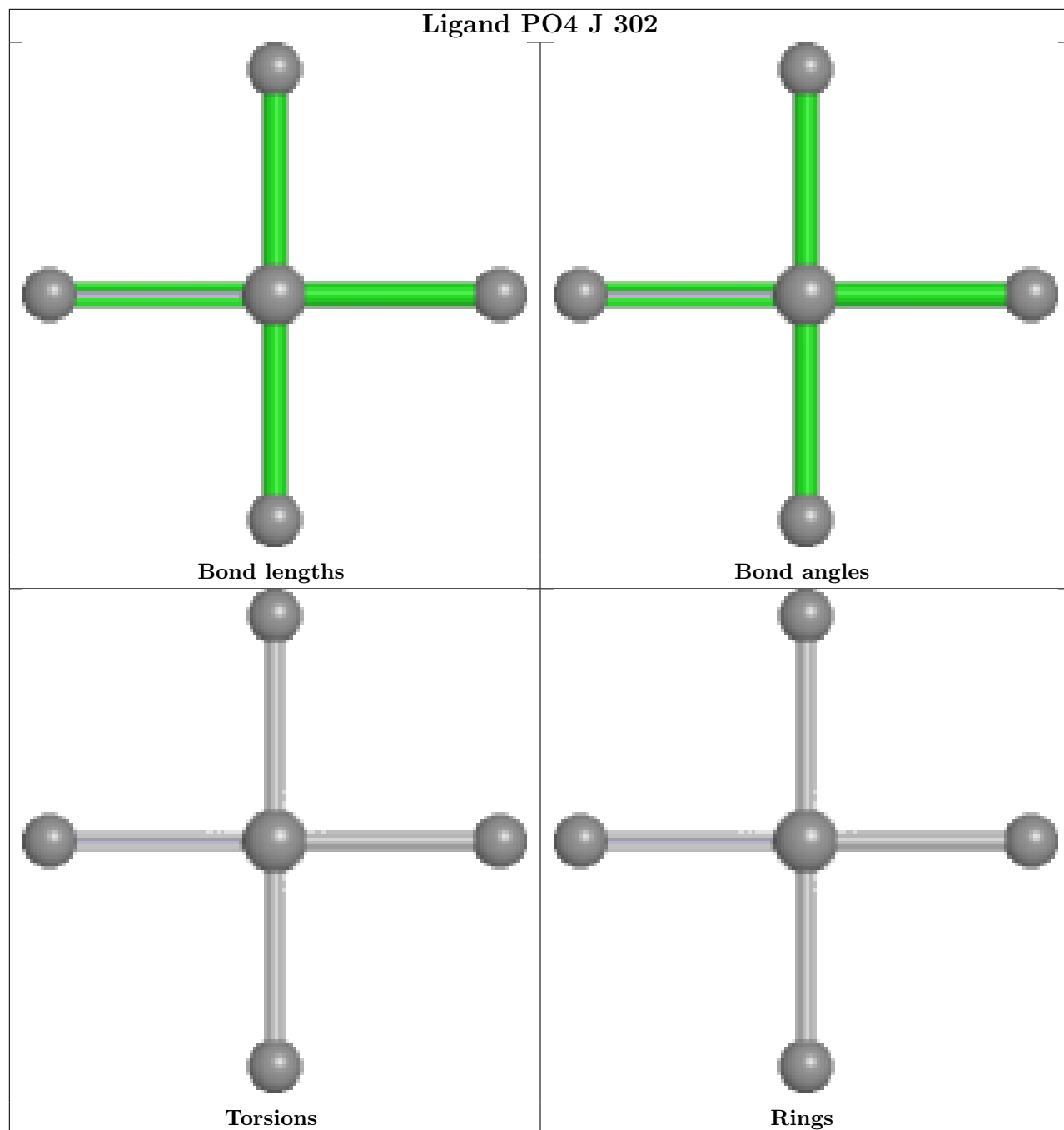


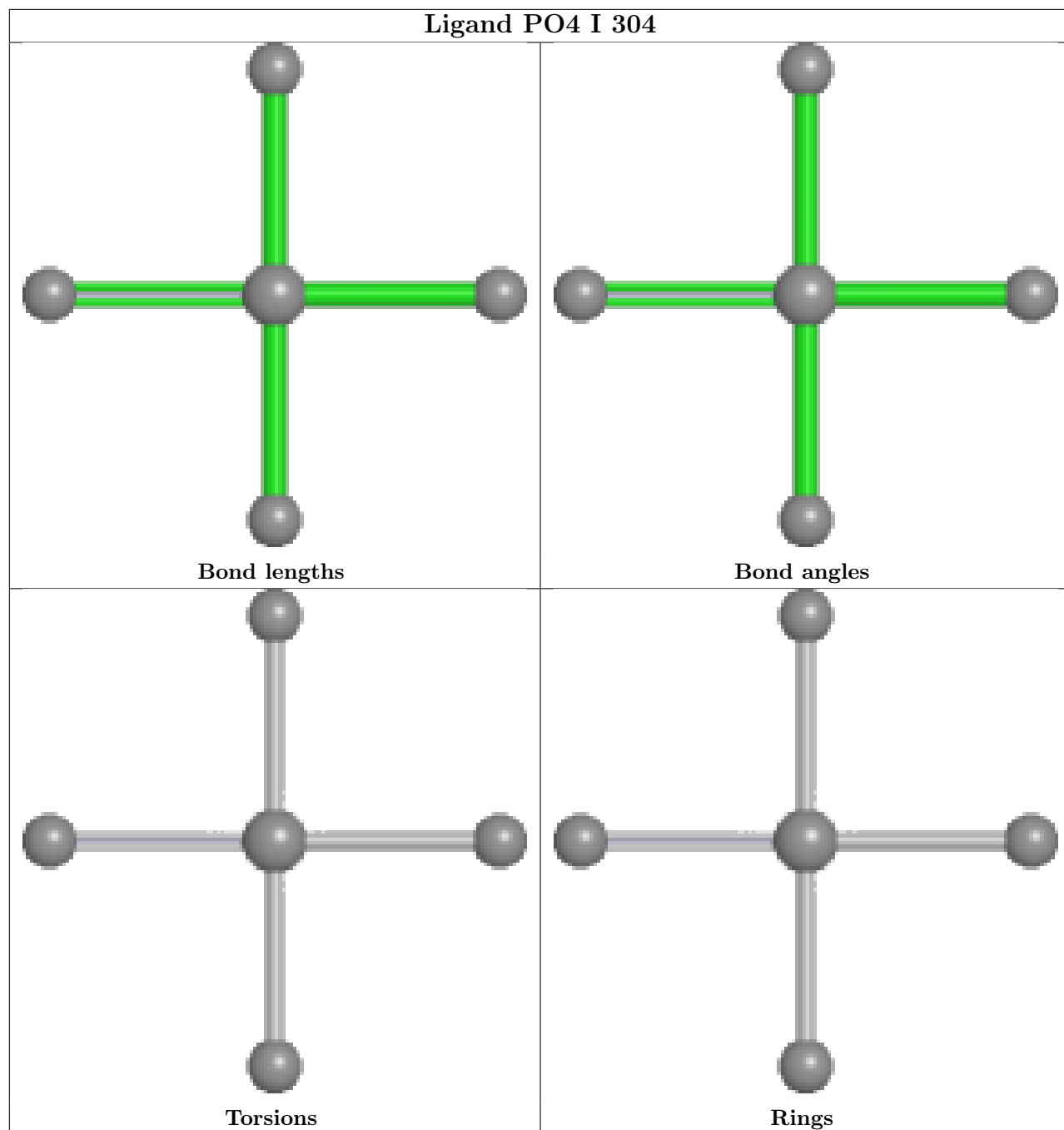


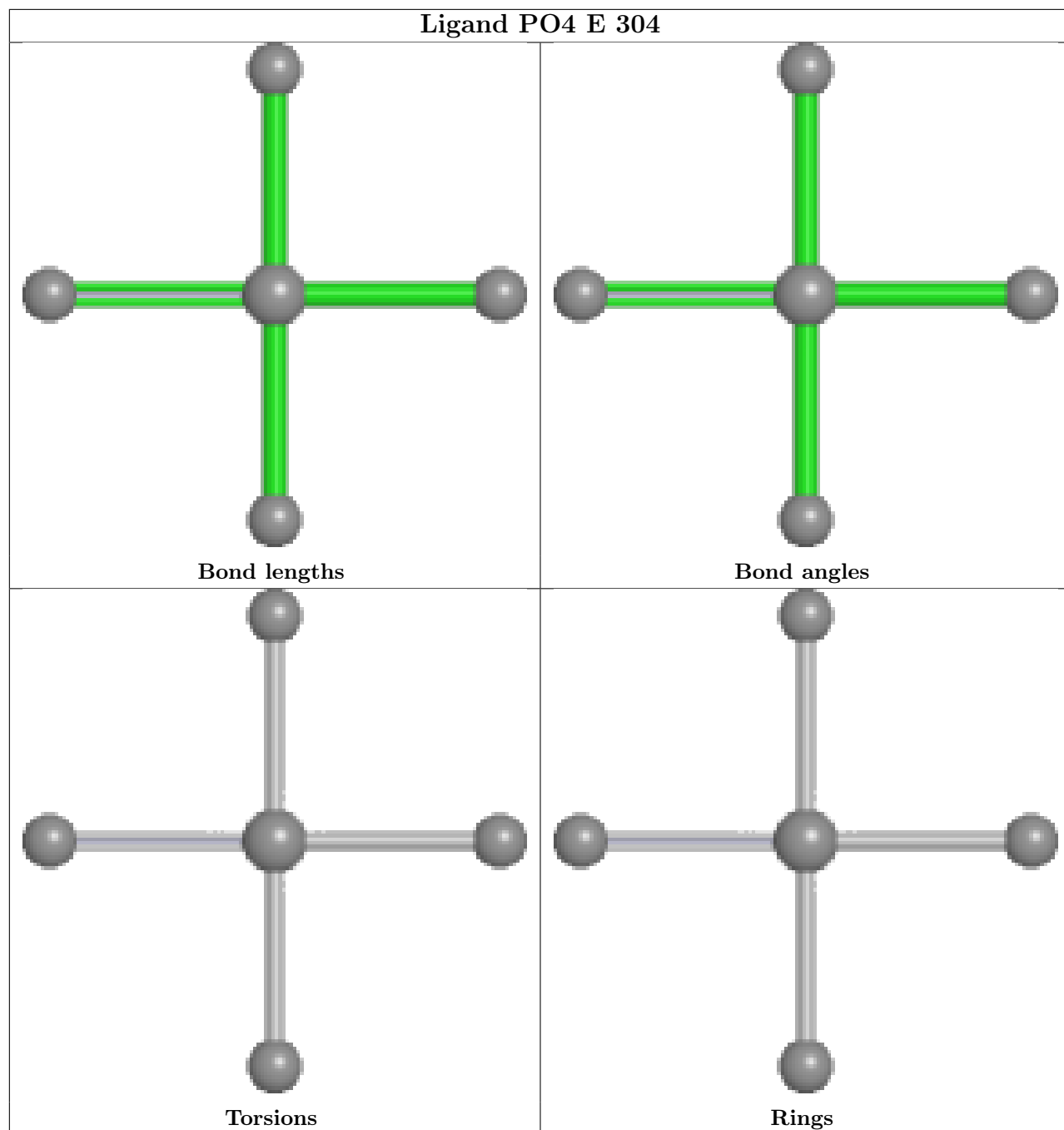


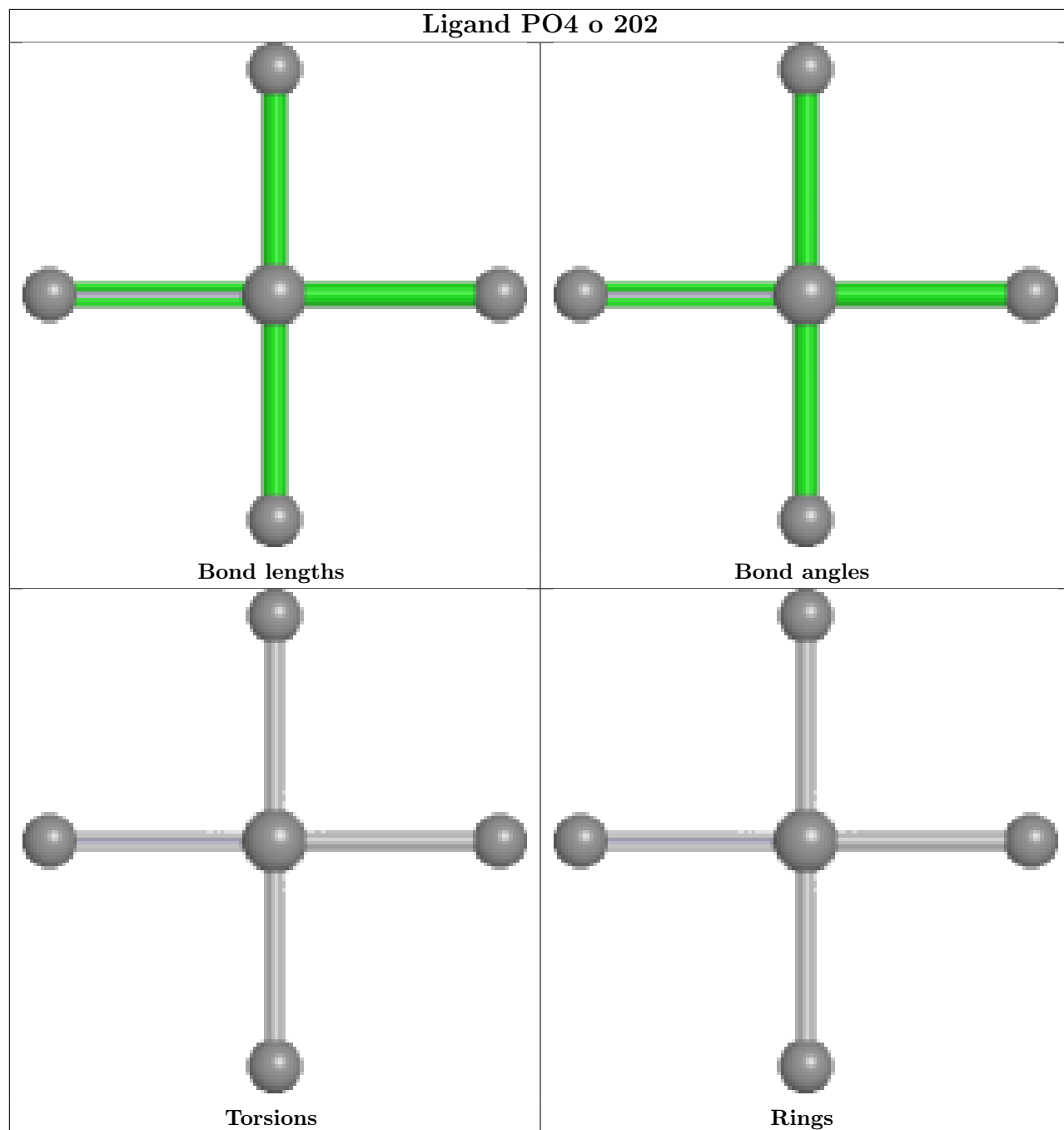


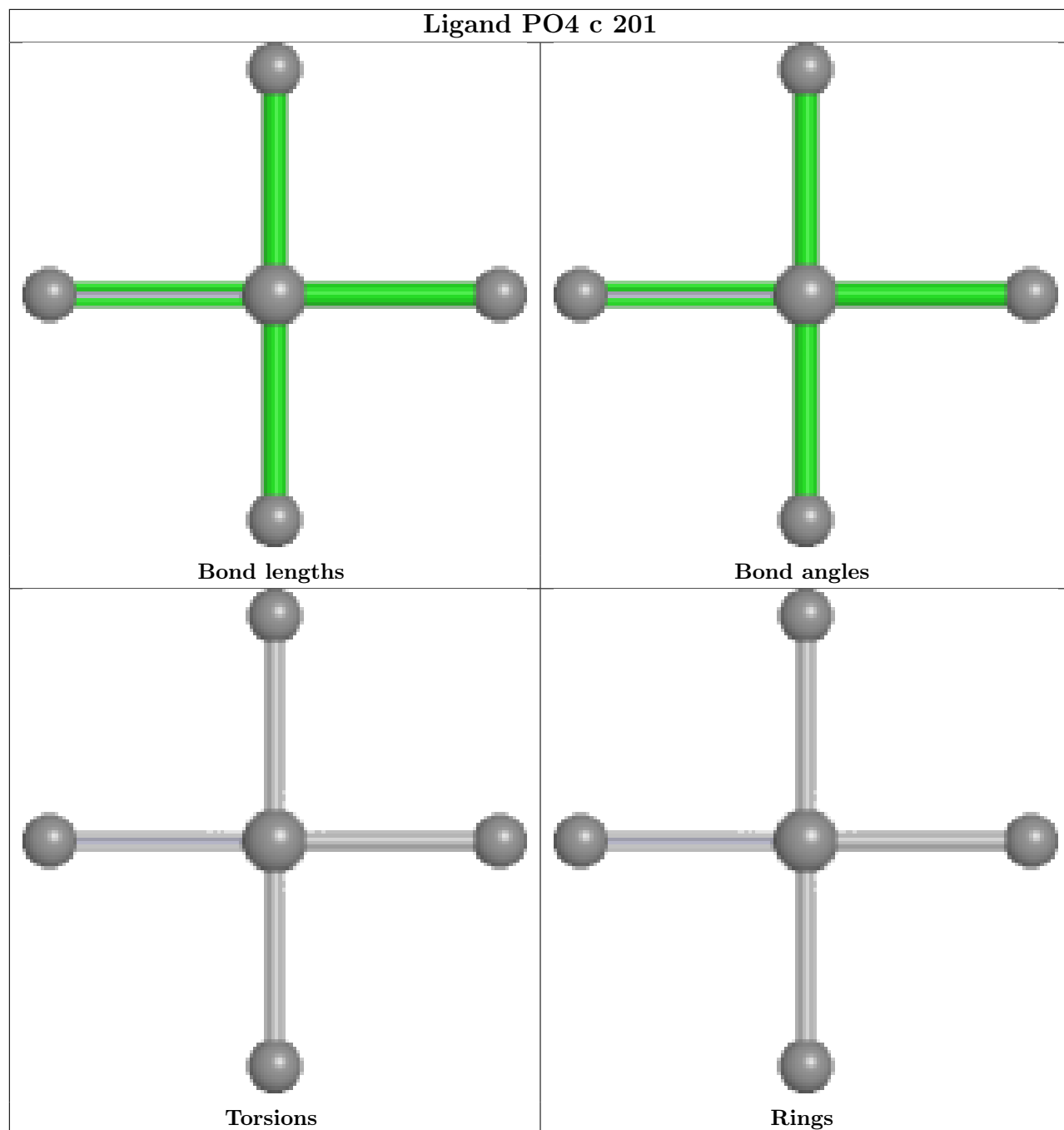


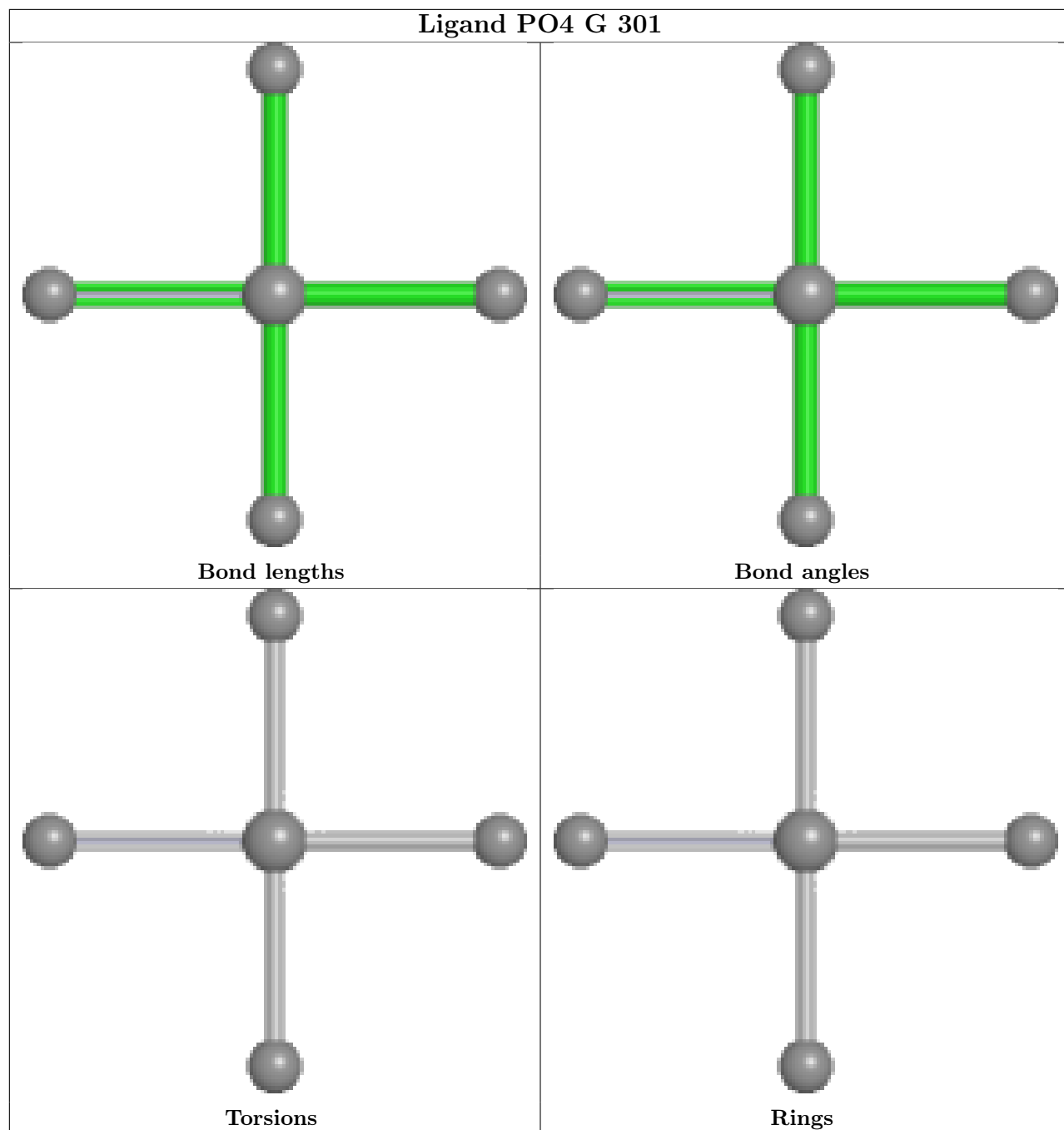


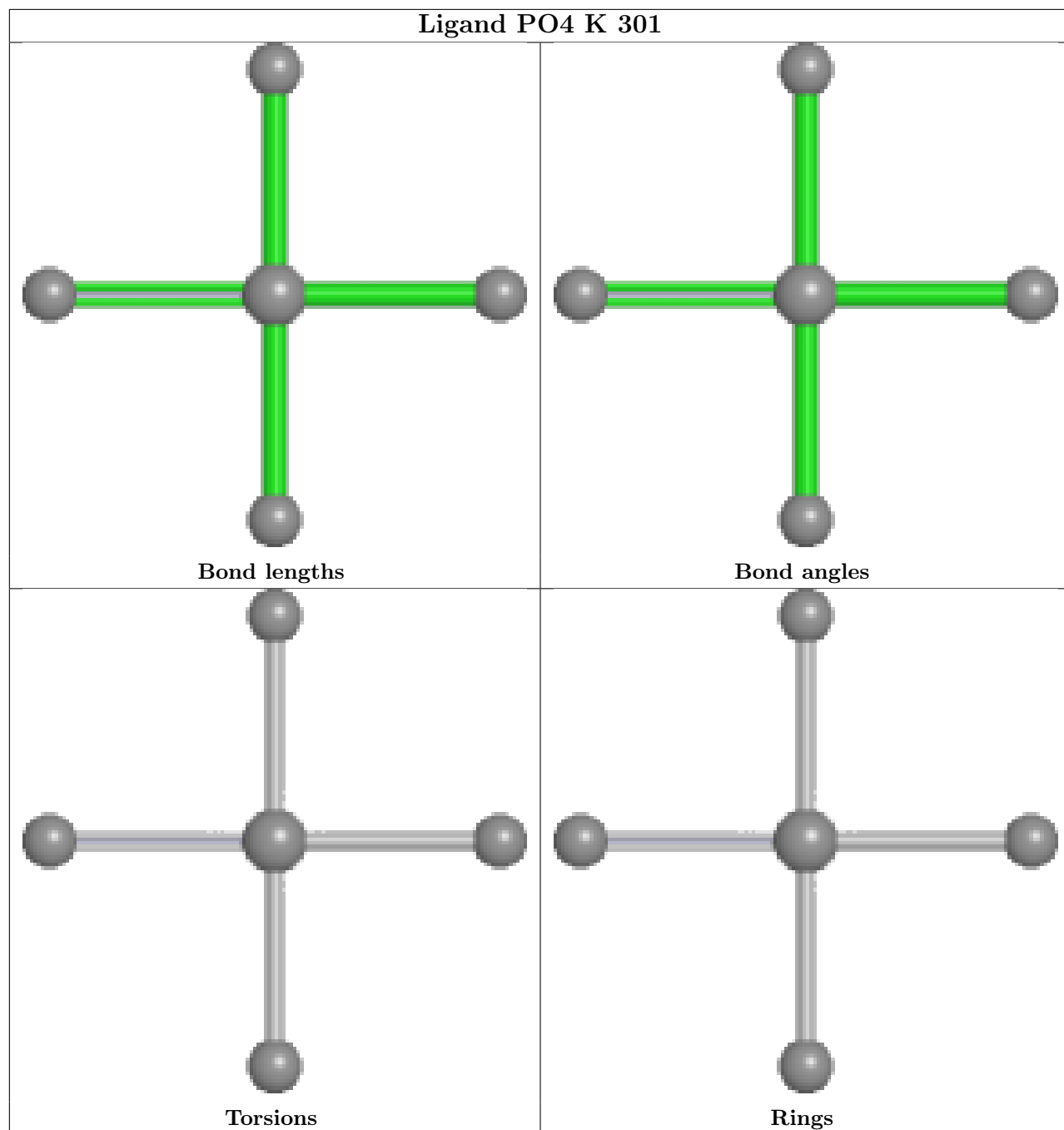


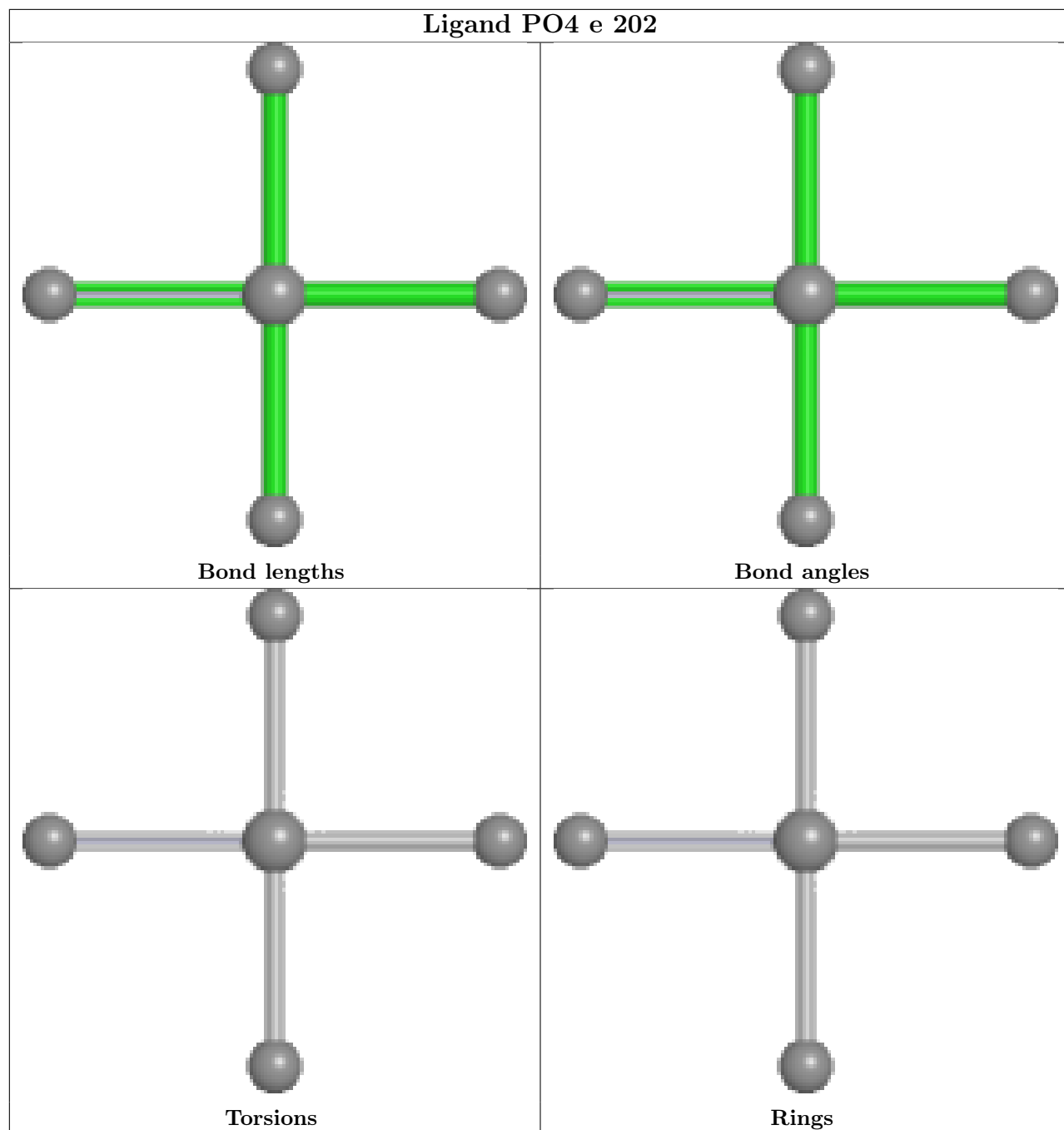


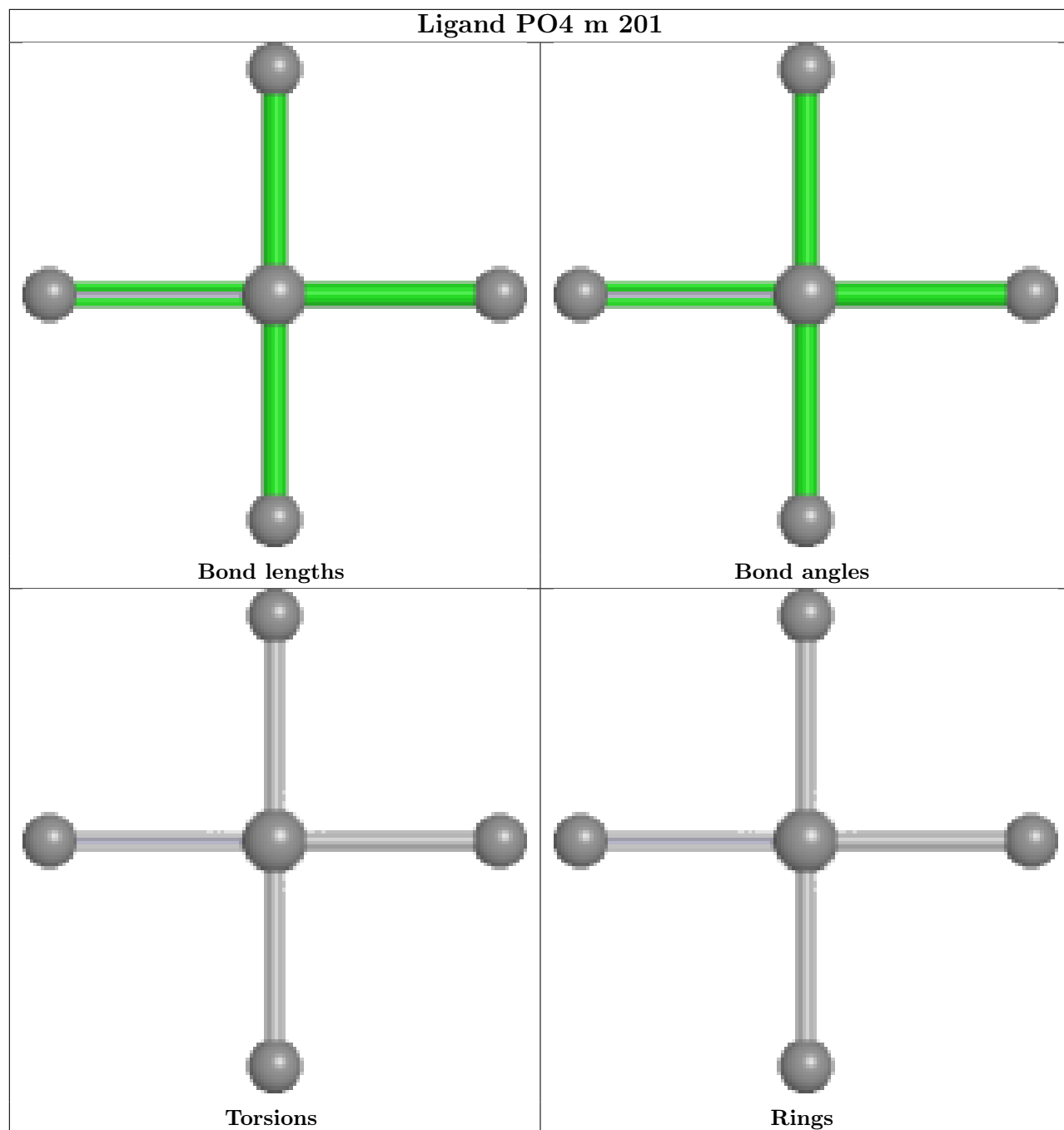


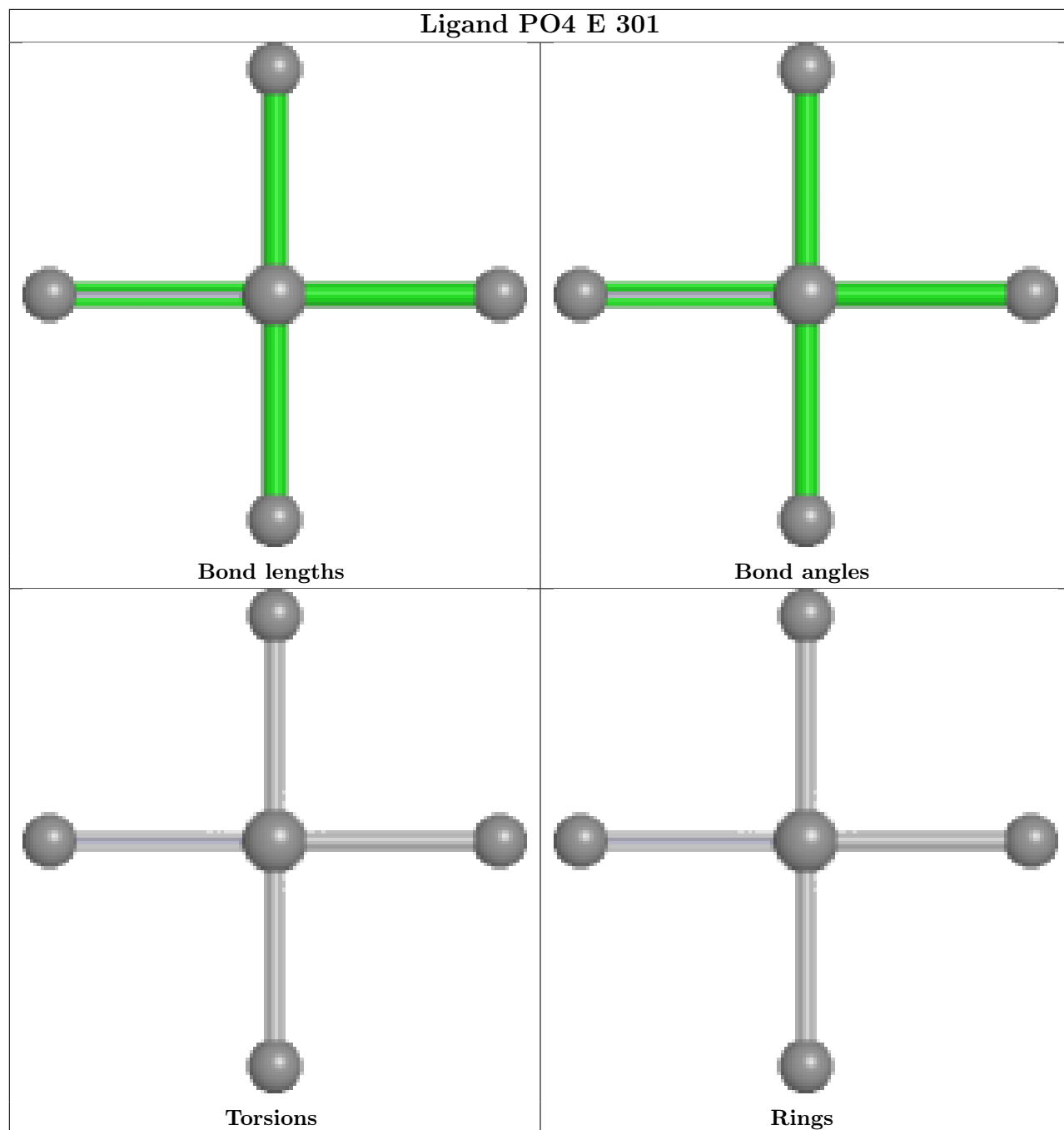


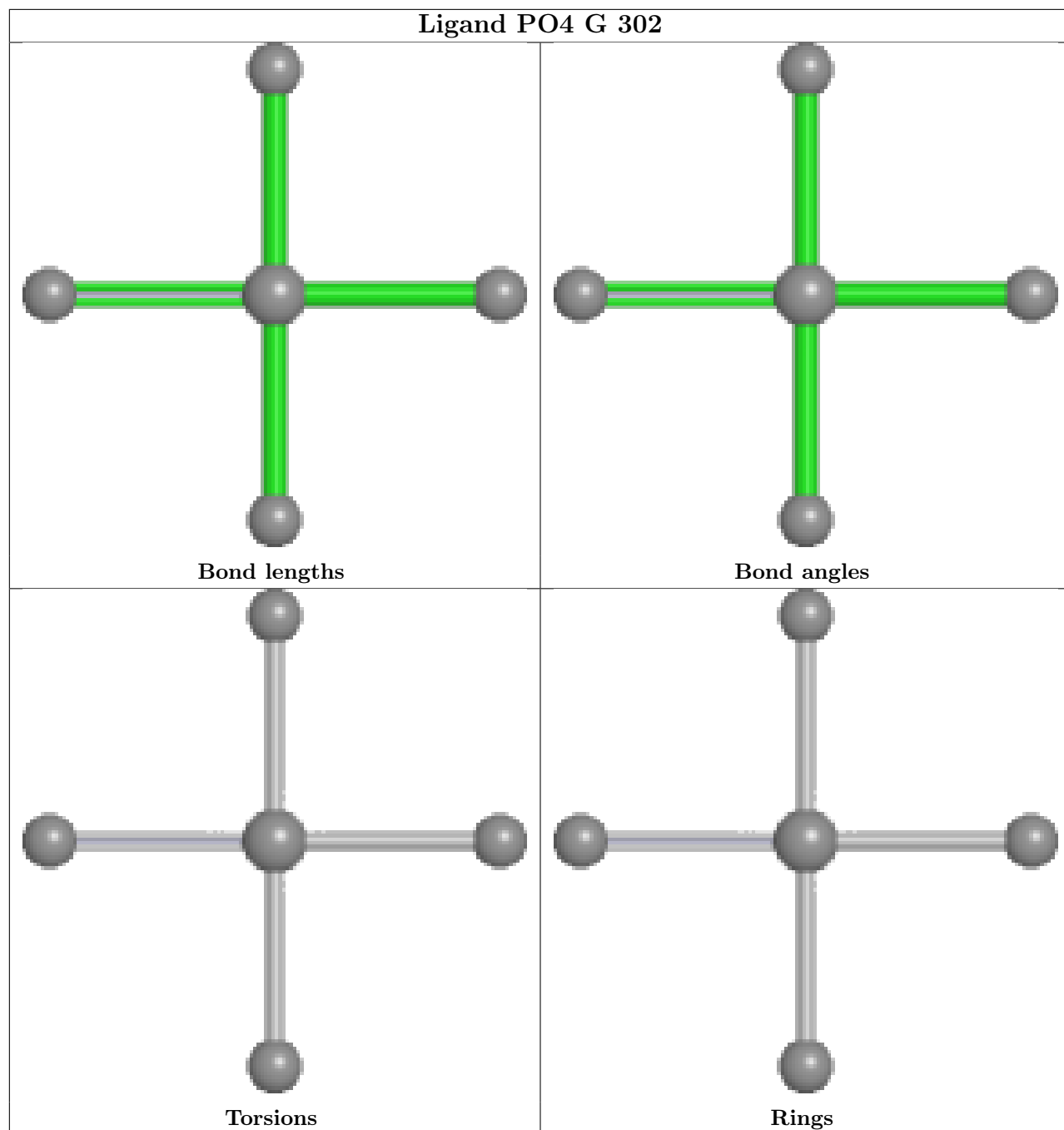


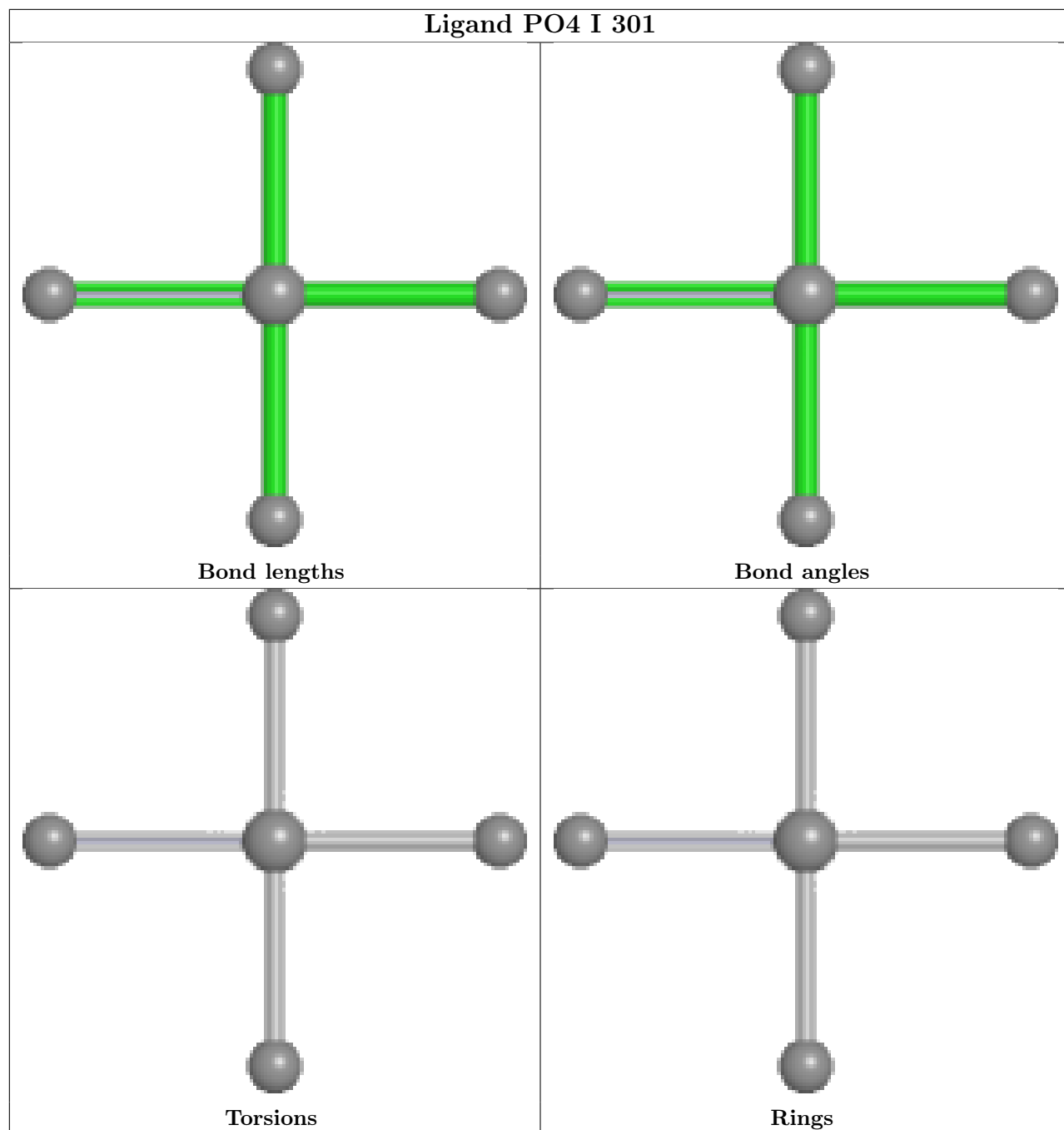


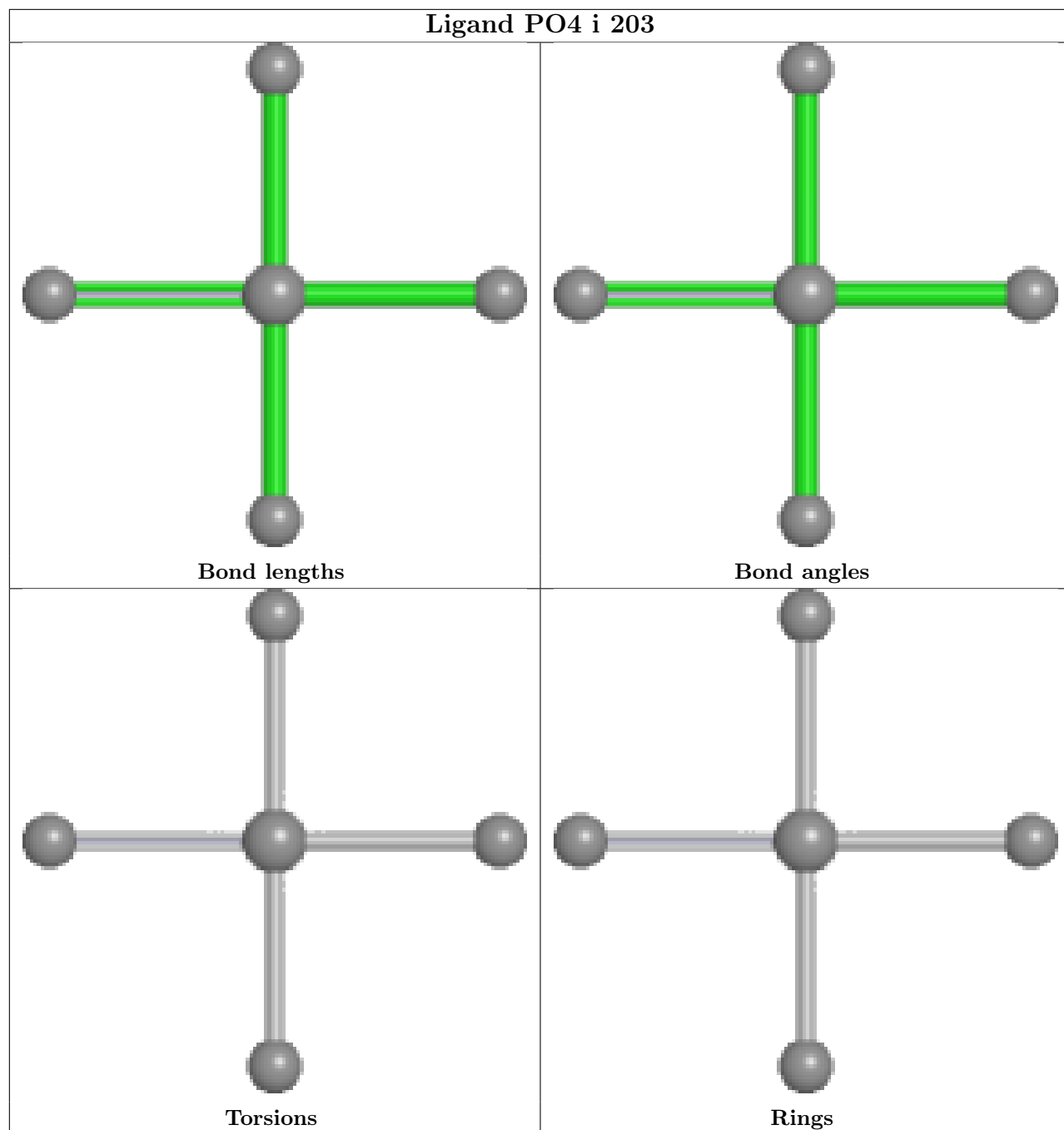


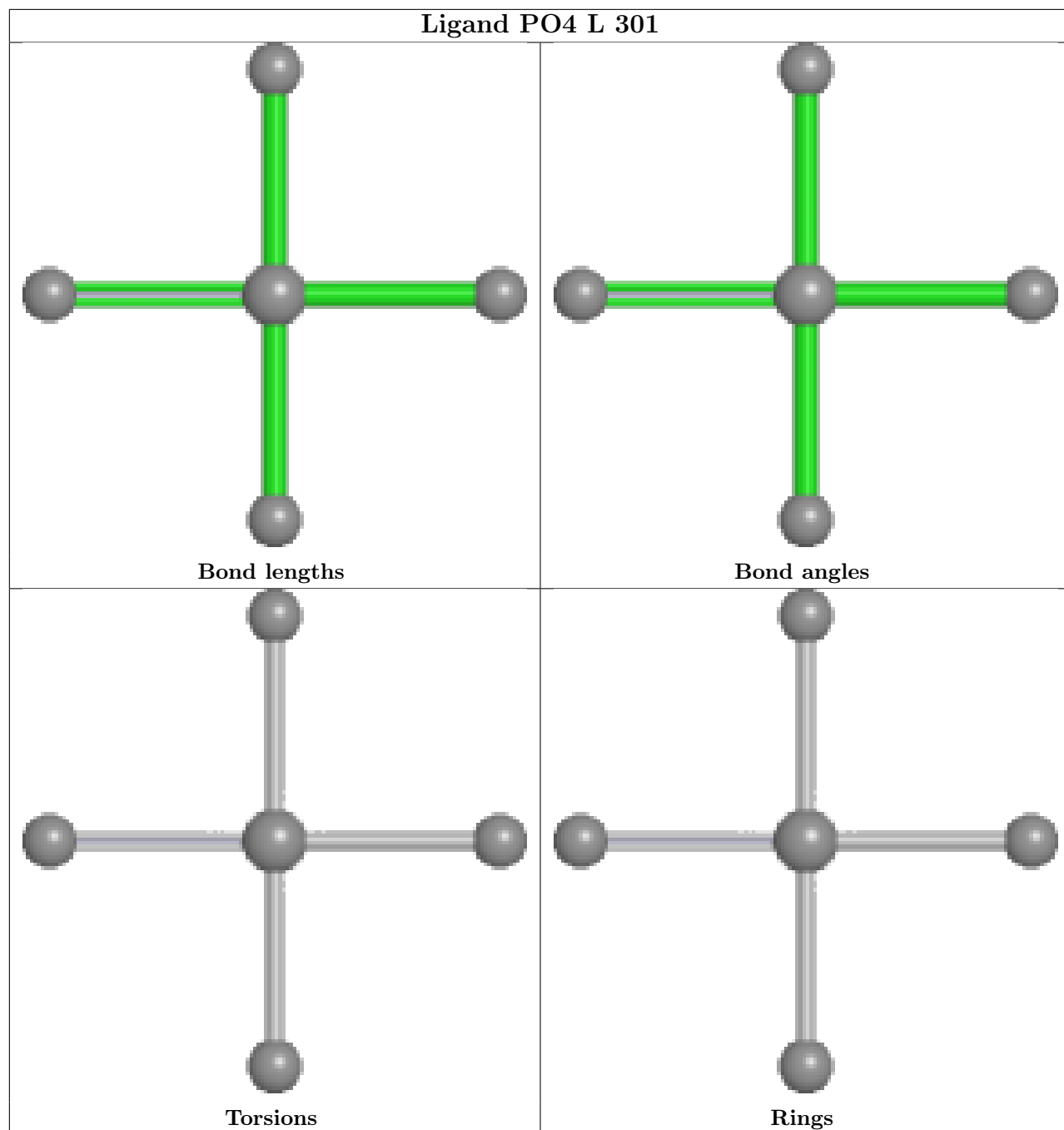


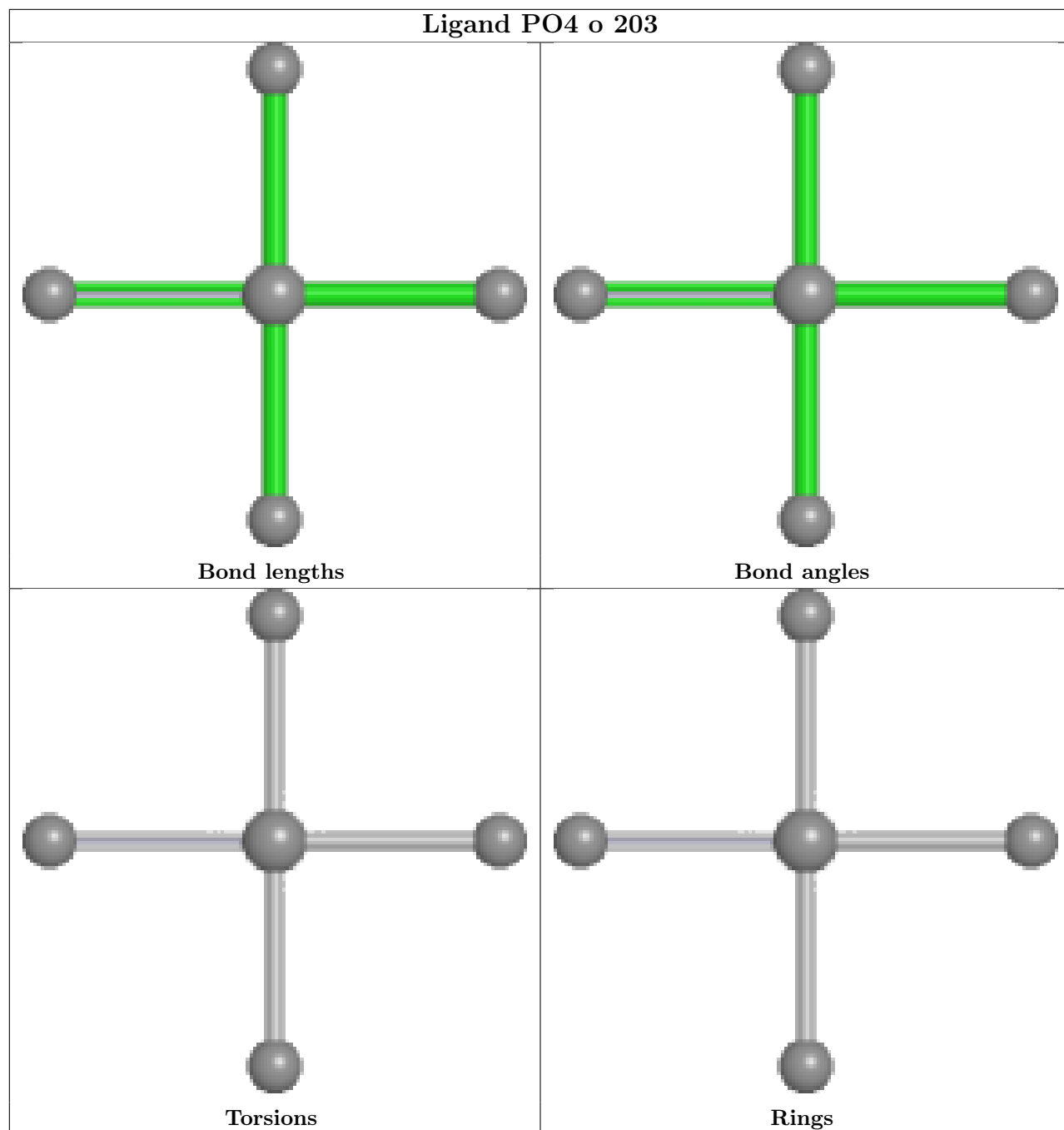


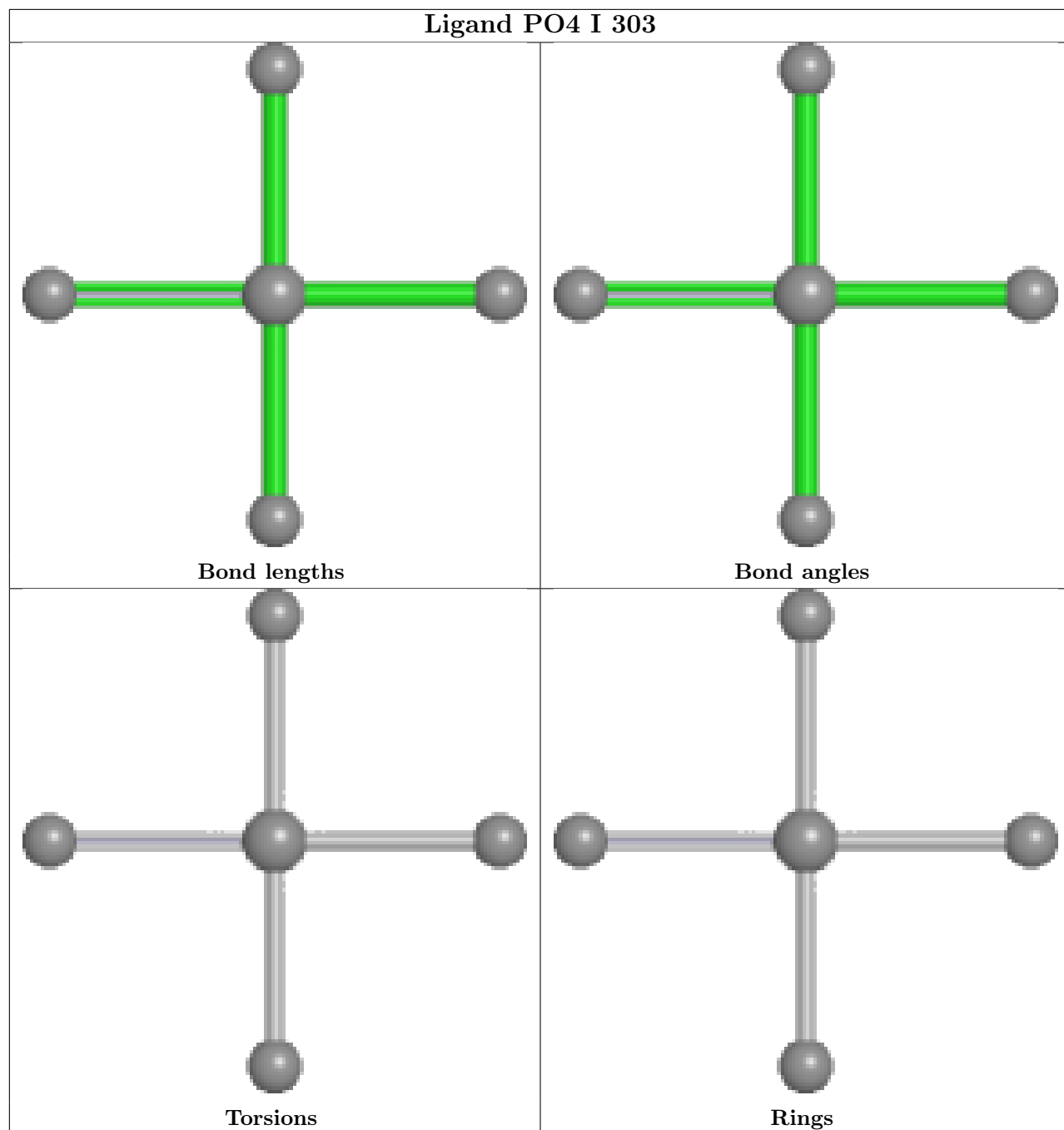


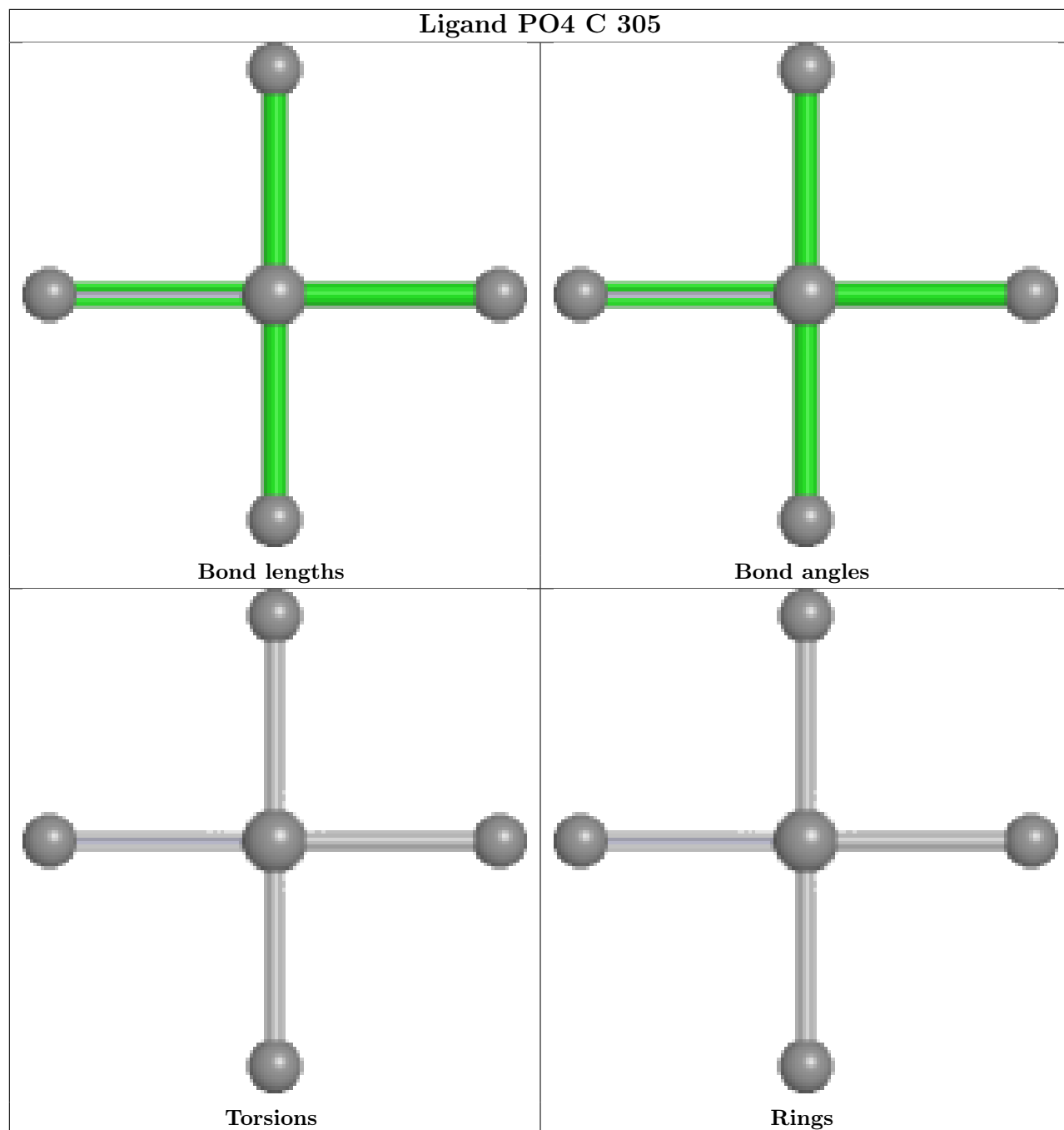


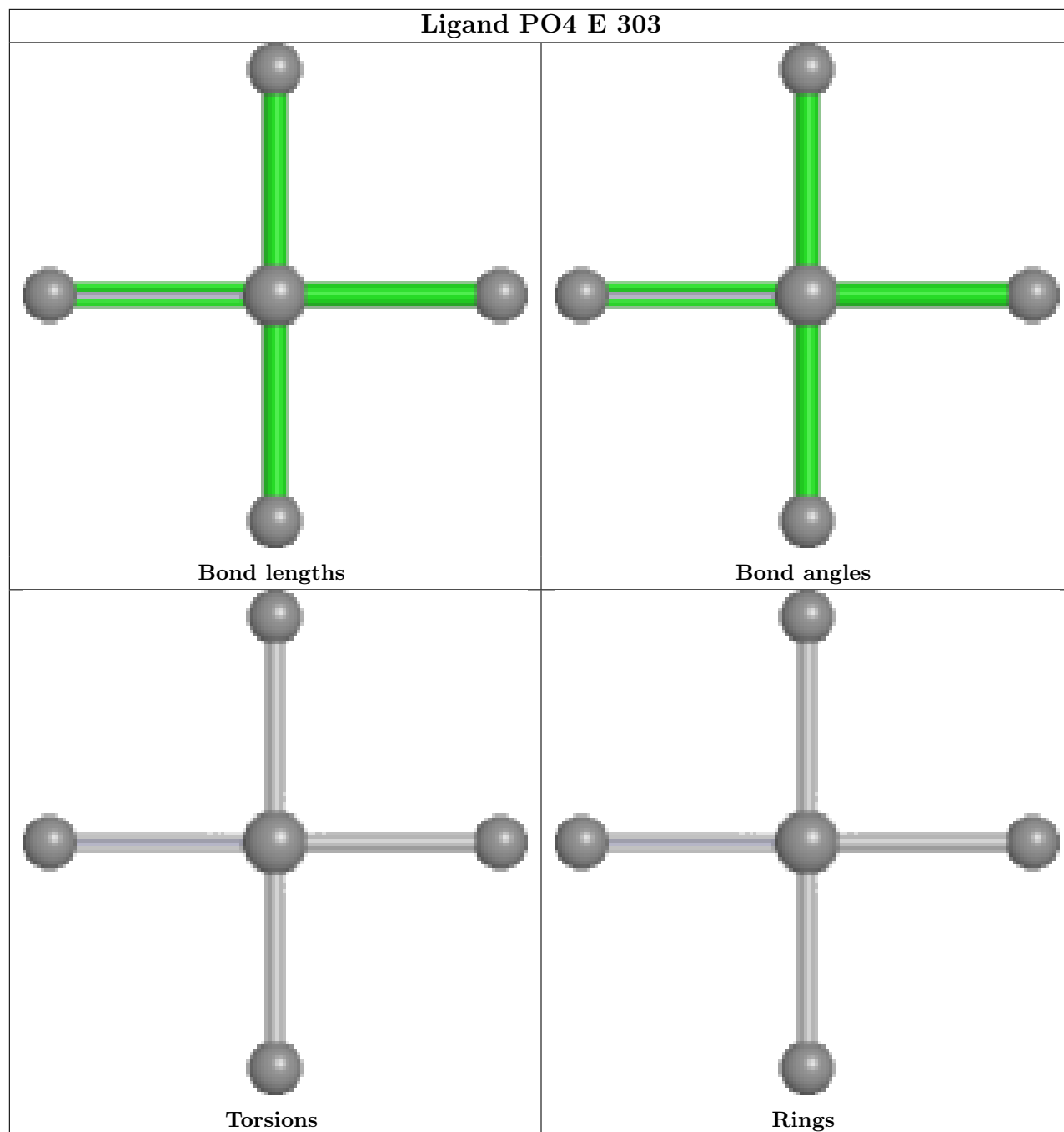












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	201/215 (93%)	0.62	15 (7%) 20 13	58, 105, 150, 198	0
1	C	204/215 (94%)	-0.21	3 (1%) 72 52	30, 49, 87, 138	0
1	E	209/215 (97%)	-0.19	2 (0%) 79 63	34, 55, 91, 143	0
1	G	209/215 (97%)	-0.29	1 (0%) 87 76	25, 49, 81, 151	0
1	I	203/215 (94%)	-0.19	1 (0%) 87 76	29, 50, 95, 122	0
1	K	210/215 (97%)	-0.11	1 (0%) 87 76	37, 58, 111, 139	0
1	M	207/215 (96%)	-0.02	3 (1%) 73 54	39, 71, 112, 161	0
1	O	202/215 (93%)	0.15	1 (0%) 87 76	61, 80, 123, 152	0
1	Q	203/215 (94%)	0.03	2 (0%) 79 63	46, 78, 108, 144	0
2	B	212/239 (88%)	0.59	24 (11%) 10 7	47, 92, 161, 195	0
2	D	228/239 (95%)	-0.10	3 (1%) 75 55	30, 59, 99, 133	0
2	F	225/239 (94%)	0.01	5 (2%) 62 42	36, 72, 106, 142	0
2	H	225/239 (94%)	-0.07	2 (0%) 81 64	32, 57, 99, 142	0
2	J	226/239 (94%)	0.10	5 (2%) 62 42	39, 77, 112, 197	0
2	L	223/239 (93%)	0.04	3 (1%) 75 55	44, 77, 111, 152	0
2	N	221/239 (92%)	0.56	19 (8%) 16 11	42, 97, 160, 216	0
2	P	218/239 (91%)	0.39	5 (2%) 61 41	68, 110, 140, 153	0
2	R	217/239 (90%)	0.18	2 (0%) 81 64	54, 92, 121, 150	0
3	a	125/129 (96%)	0.28	4 (3%) 50 31	48, 81, 125, 193	0
3	c	125/129 (96%)	-0.00	1 (0%) 82 67	33, 55, 90, 169	1 (0%)
3	e	124/129 (96%)	-0.12	1 (0%) 82 67	33, 54, 85, 112	0
3	g	123/129 (95%)	-0.16	1 (0%) 82 67	25, 54, 86, 108	0
3	i	125/129 (96%)	0.13	0 100 100	45, 77, 124, 149	0
3	k	126/129 (97%)	0.30	5 (3%) 42 26	37, 71, 115, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	m	121/129 (93%)	0.04	3 (2%) 58 39	34, 64, 112, 146	0
3	o	123/129 (95%)	0.52	3 (2%) 59 40	86, 115, 150, 217	0
3	q	123/129 (95%)	0.54	5 (4%) 41 25	67, 103, 140, 177	0
All	All	4958/5247 (94%)	0.10	120 (2%) 59 40	25, 73, 131, 217	1 (0%)

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	q	27	SER	4.9
3	c	76	ASN	4.4
2	N	126	PRO	4.3
1	E	112	ALA	4.2
3	q	26	GLY	4.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	E	304	5/5	0.65	0.13	147,149,151,152	0
4	PO4	E	302	5/5	0.70	0.18	118,118,121,123	0
4	PO4	H	301	5/5	0.73	0.15	115,119,121,121	0
4	PO4	Q	301	5/5	0.74	0.16	122,125,125,129	0
4	PO4	o	202	5/5	0.74	0.11	125,126,127,129	0
4	PO4	K	302	5/5	0.75	0.19	116,116,117,120	0
4	PO4	g	201	5/5	0.76	0.24	92,96,102,106	0
6	GOL	G	307	6/6	0.76	0.17	93,96,97,100	0
4	PO4	M	302	5/5	0.78	0.11	107,107,109,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	G	303	5/5	0.78	0.12	132,134,135,136	0
4	PO4	a	201	5/5	0.78	0.12	138,138,139,140	0
4	PO4	O	301	5/5	0.79	0.20	102,103,104,108	0
4	PO4	J	301	5/5	0.79	0.19	112,114,116,118	0
6	GOL	c	203	6/6	0.79	0.13	71,75,81,87	0
4	PO4	I	301	5/5	0.81	0.09	118,120,121,122	0
4	PO4	C	302	5/5	0.81	0.12	101,102,103,107	0
4	PO4	i	202	5/5	0.81	0.11	119,120,121,121	0
4	PO4	e	201	5/5	0.82	0.20	106,109,110,113	0
4	PO4	M	301	5/5	0.82	0.12	88,88,94,96	0
6	GOL	k	201	6/6	0.82	0.13	59,67,70,70	0
4	PO4	E	301	5/5	0.83	0.20	102,105,106,108	0
4	PO4	c	202	5/5	0.84	0.17	73,74,76,85	0
4	PO4	D	302	5/5	0.84	0.20	128,131,132,134	0
4	PO4	G	302	5/5	0.84	0.15	103,104,105,110	0
4	PO4	K	301	5/5	0.84	0.20	140,140,142,143	0
4	PO4	R	301	5/5	0.85	0.10	102,106,107,109	0
7	PEG	F	302	7/7	0.85	0.19	34,42,61,61	0
4	PO4	E	303	5/5	0.86	0.15	123,125,126,127	0
5	CL	K	304	1/1	0.86	0.21	76,76,76,76	0
4	PO4	J	302	5/5	0.86	0.18	95,99,103,106	0
7	PEG	H	303	7/7	0.86	0.16	28,41,50,51	0
4	PO4	o	201	5/5	0.87	0.13	156,157,158,160	0
4	PO4	O	302	5/5	0.87	0.14	94,95,99,101	0
4	PO4	m	201	5/5	0.88	0.12	97,97,98,100	0
4	PO4	C	304	5/5	0.88	0.19	98,105,109,110	0
4	PO4	C	303	5/5	0.88	0.14	109,112,115,116	0
4	PO4	o	203	5/5	0.88	0.10	69,70,75,80	0
4	PO4	I	302	5/5	0.88	0.34	103,103,105,108	0
7	PEG	N	303	7/7	0.88	0.12	61,65,67,68	0
4	PO4	i	201	5/5	0.89	0.13	82,84,90,91	0
4	PO4	e	203	5/5	0.89	0.16	67,76,78,79	0
6	GOL	I	306	6/6	0.89	0.09	51,53,55,55	0
4	PO4	B	301	5/5	0.89	0.11	66,71,79,81	0
4	PO4	m	202	5/5	0.90	0.10	59,69,72,81	0
6	GOL	B	304	6/6	0.90	0.09	63,66,68,68	0
6	GOL	L	303	6/6	0.90	0.12	38,55,59,66	0
6	GOL	G	306	6/6	0.90	0.10	45,54,56,58	0
4	PO4	C	305	5/5	0.91	0.18	77,80,80,84	0
5	CL	R	302	1/1	0.91	0.10	54,54,54,54	0
4	PO4	M	303	5/5	0.91	0.12	88,88,93,94	0
5	CL	G	304	1/1	0.91	0.07	61,61,61,61	0

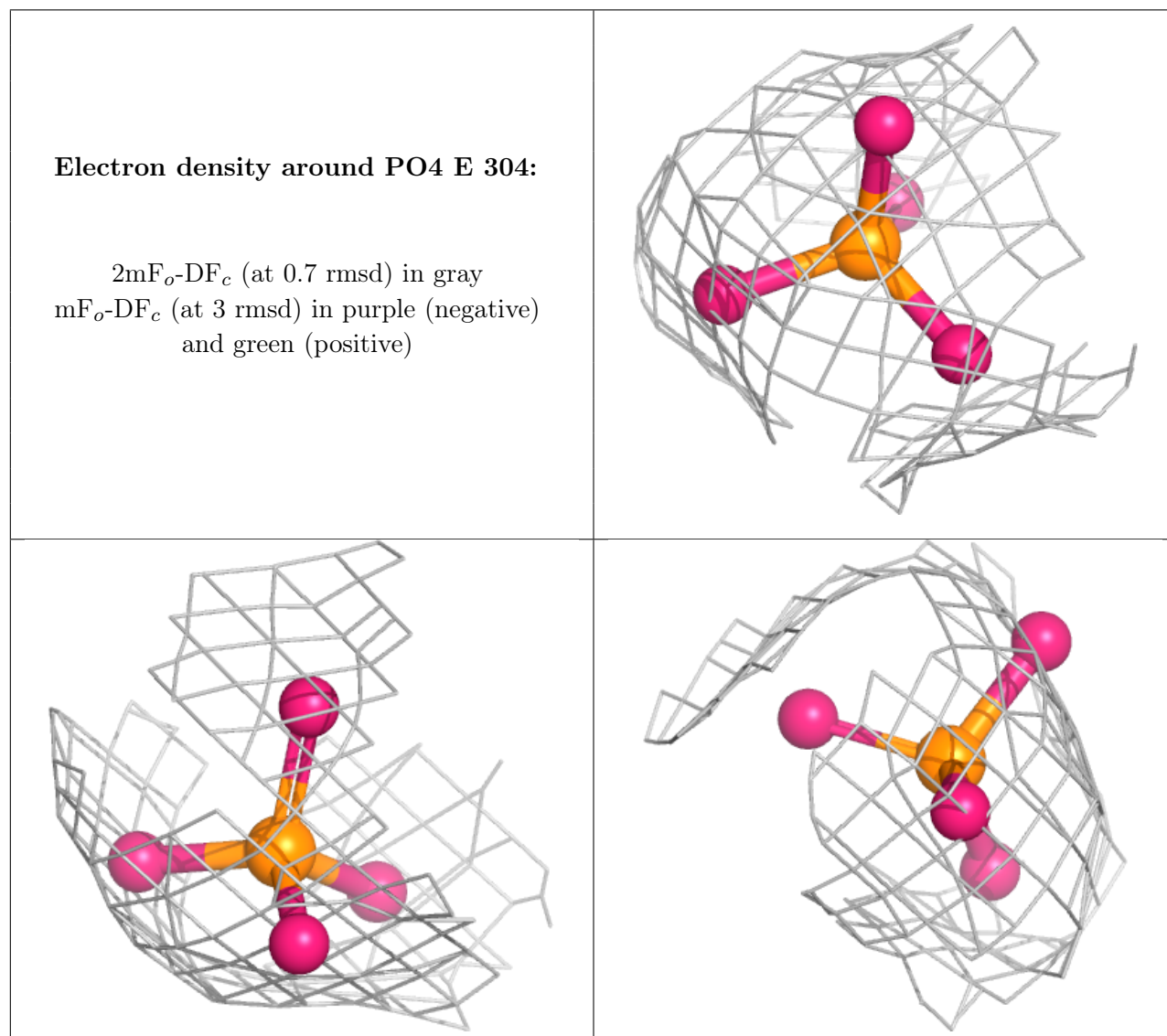
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	I	304	5/5	0.92	0.16	48,53,66,68	0
4	PO4	i	203	5/5	0.92	0.09	40,45,51,57	0
4	PO4	G	301	5/5	0.92	0.15	60,60,63,65	0
4	PO4	D	301	5/5	0.92	0.14	62,64,71,81	0
5	CL	M	304	1/1	0.93	0.07	53,53,53,53	0
4	PO4	e	202	5/5	0.93	0.10	17,34,44,50	0
6	GOL	E	307	6/6	0.94	0.11	47,59,64,65	0
5	CL	C	307	1/1	0.94	0.10	47,47,47,47	0
5	CL	q	202	1/1	0.94	0.09	58,58,58,58	0
5	CL	q	203	1/1	0.94	0.10	66,66,66,66	0
4	PO4	a	202	5/5	0.94	0.12	33,39,47,48	0
5	CL	C	306	1/1	0.95	0.07	42,42,42,42	0
5	CL	P	301	1/1	0.95	0.23	66,66,66,66	0
5	CL	H	302	1/1	0.95	0.07	37,37,37,37	0
5	CL	E	306	1/1	0.95	0.05	41,41,41,41	0
4	PO4	C	301	5/5	0.96	0.18	35,37,43,48	0
5	CL	R	303	1/1	0.96	0.04	55,55,55,55	0
5	CL	g	203	1/1	0.96	0.10	33,33,33,33	0
5	CL	J	303	1/1	0.96	0.06	45,45,45,45	0
4	PO4	L	301	5/5	0.96	0.13	48,50,53,60	0
4	PO4	I	303	5/5	0.96	0.07	41,44,48,51	0
5	CL	N	302	1/1	0.96	0.05	38,38,38,38	0
4	PO4	q	201	5/5	0.96	0.07	26,37,49,50	0
5	CL	e	204	1/1	0.97	0.04	42,42,42,42	0
5	CL	L	302	1/1	0.97	0.04	45,45,45,45	0
4	PO4	g	202	5/5	0.97	0.08	16,16,19,31	0
5	CL	B	302	1/1	0.97	0.13	53,53,53,53	0
5	CL	D	303	1/1	0.97	0.07	27,27,27,27	0
6	GOL	C	308	6/6	0.97	0.09	12,31,40,42	0
5	CL	D	304	1/1	0.97	0.05	42,42,42,42	0
5	CL	E	305	1/1	0.97	0.10	31,31,31,31	0
4	PO4	c	201	5/5	0.98	0.06	9,18,26,33	0
5	CL	B	303	1/1	0.98	0.10	55,55,55,55	0
5	CL	F	301	1/1	0.98	0.04	20,20,20,20	0
5	CL	R	304	1/1	0.98	0.03	33,33,33,33	0
5	CL	N	301	1/1	0.98	0.13	40,40,40,40	0
5	CL	K	303	1/1	0.98	0.04	41,41,41,41	0
5	CL	g	204	1/1	0.98	0.09	29,29,29,29	0
5	CL	G	305	1/1	0.99	0.08	29,29,29,29	0
5	CL	I	305	1/1	0.99	0.06	42,42,42,42	0

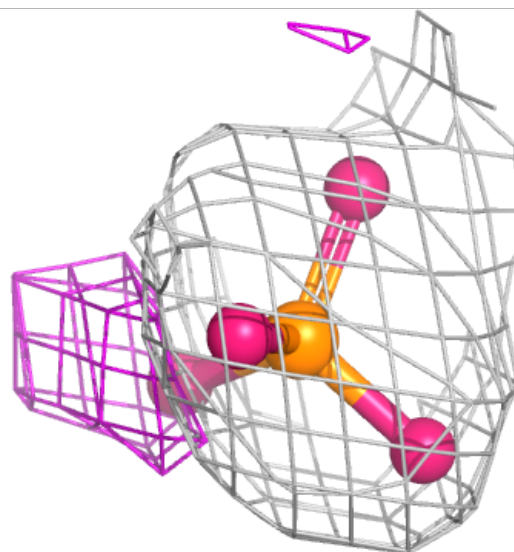
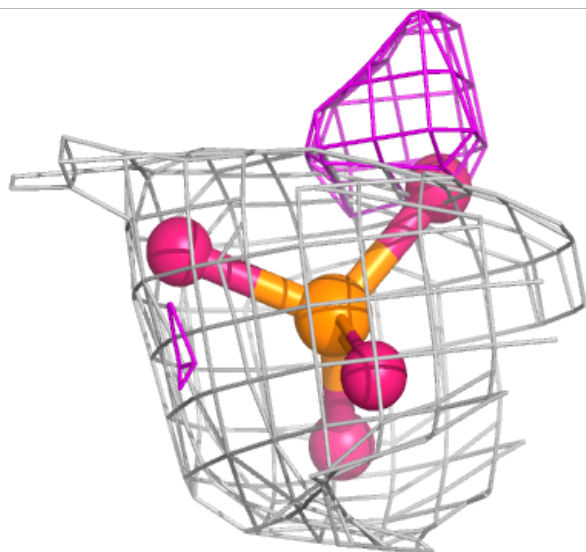
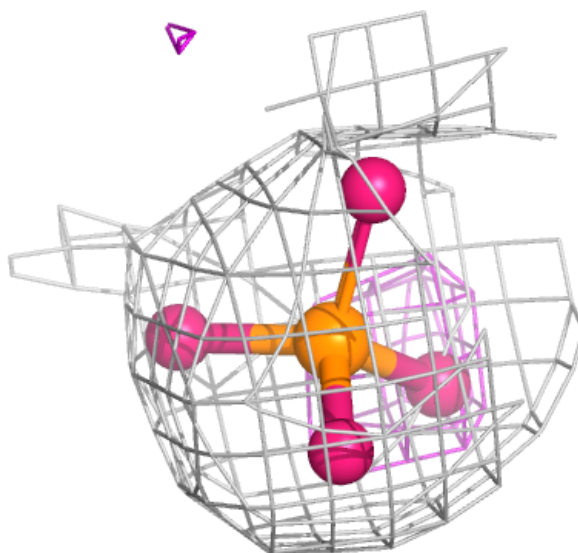
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



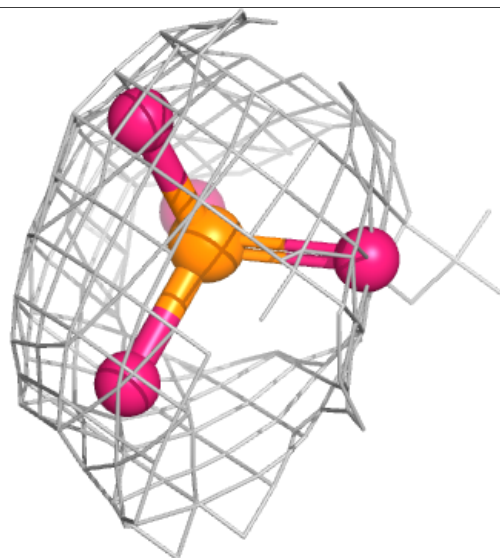
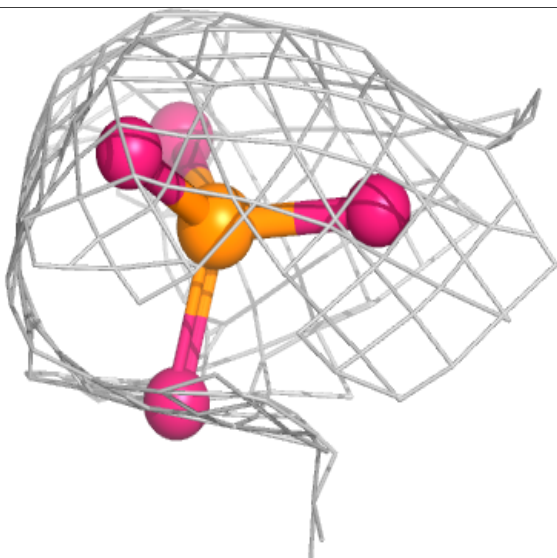
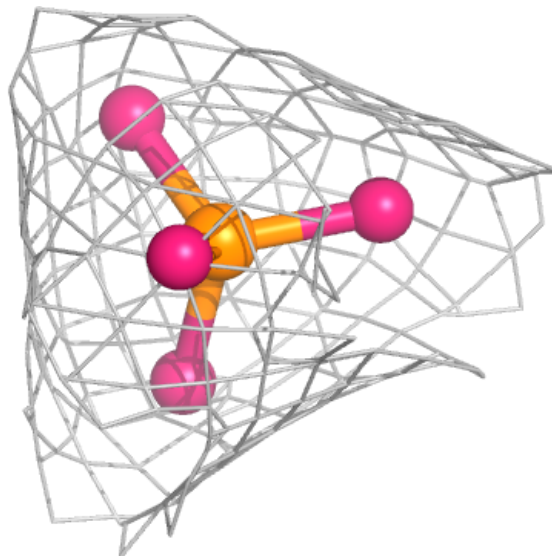
Electron density around PO4 E 302:

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



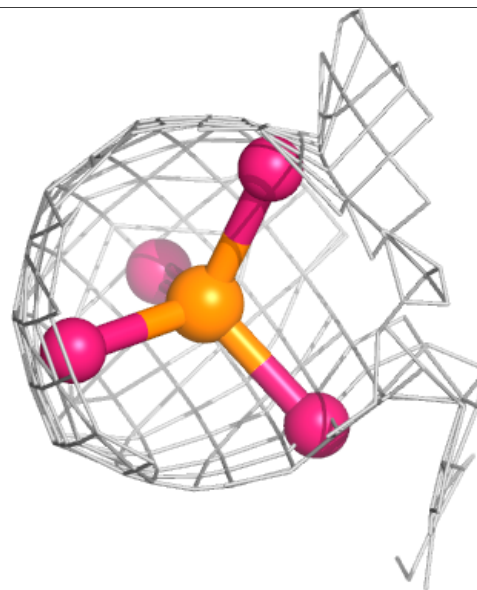
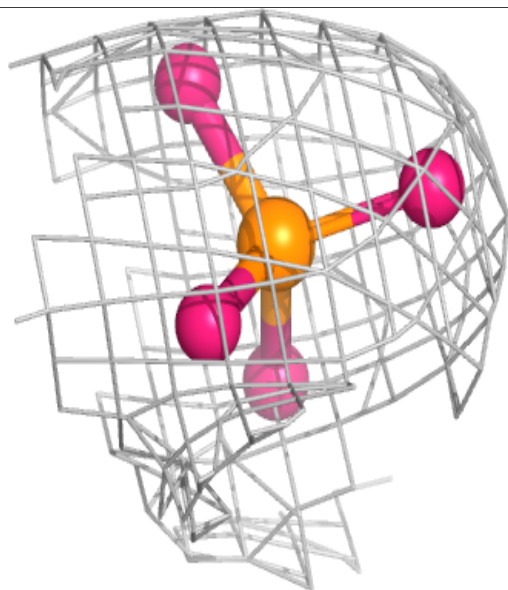
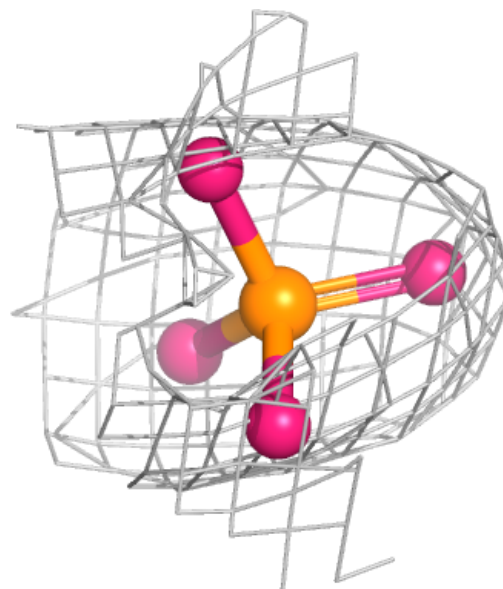
Electron density around PO4 H 301:

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



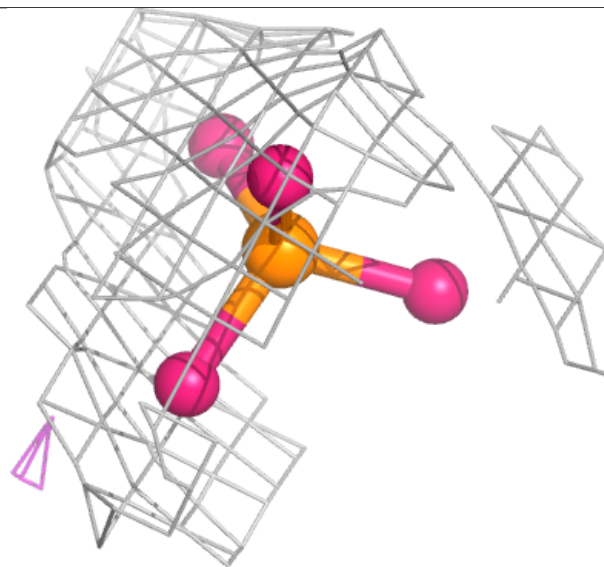
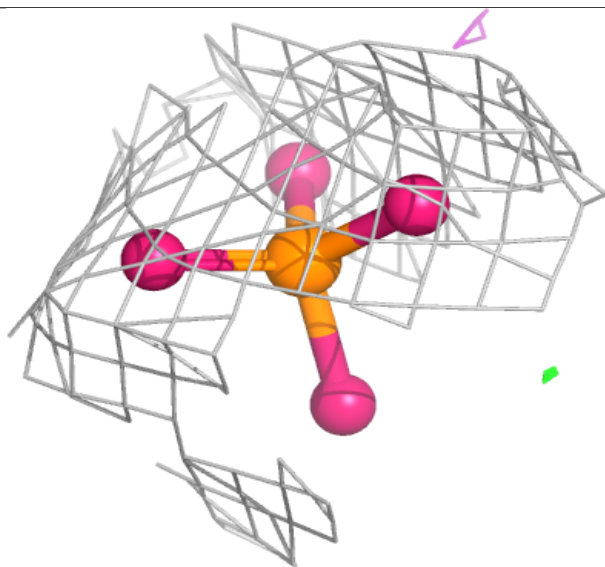
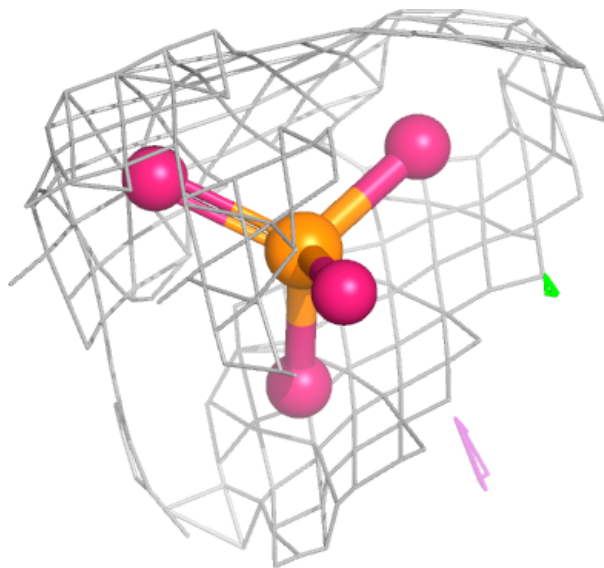
Electron density around PO4 Q 301:

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and green (positive)



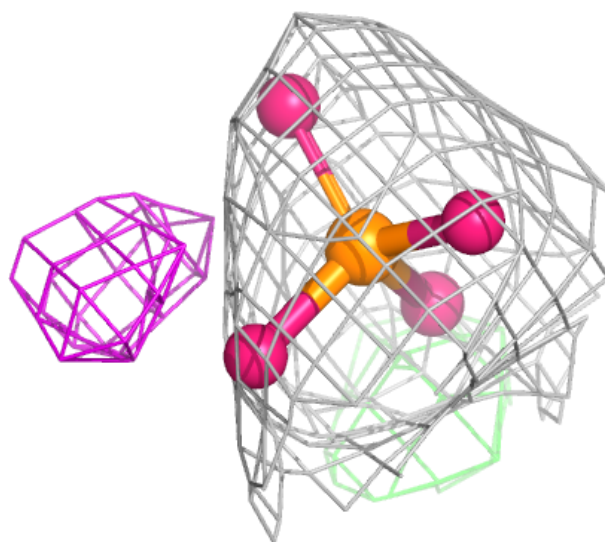
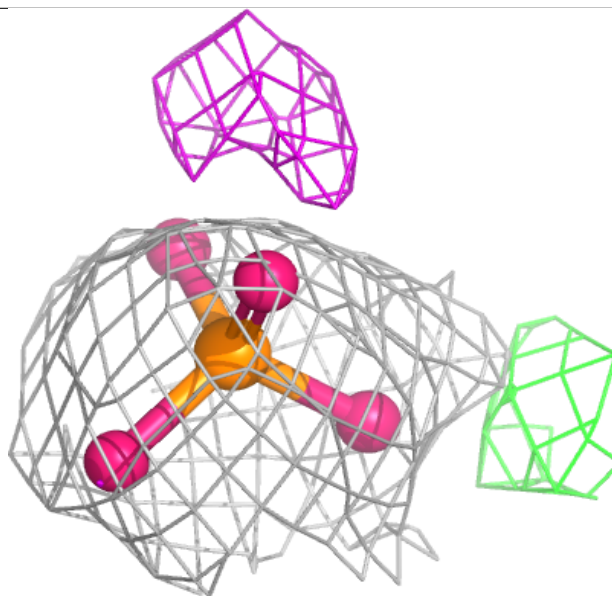
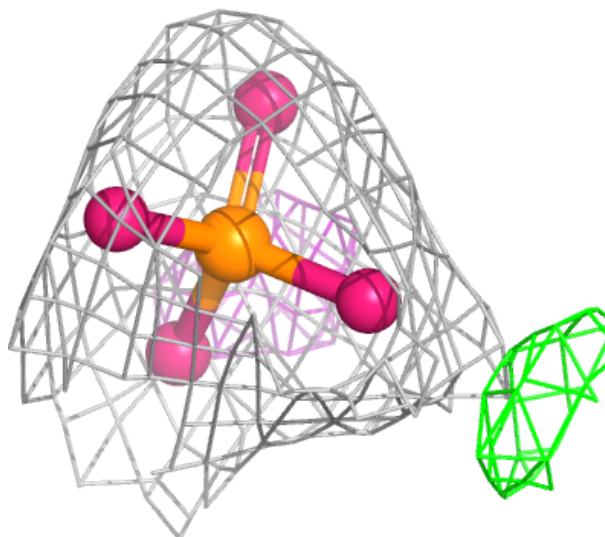
Electron density around PO4 o 202:

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



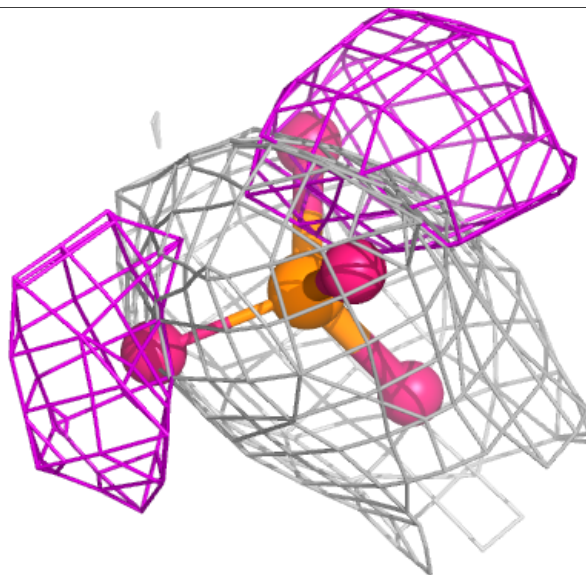
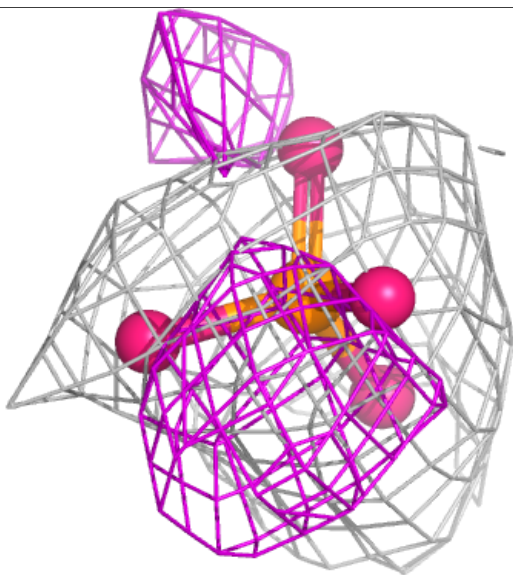
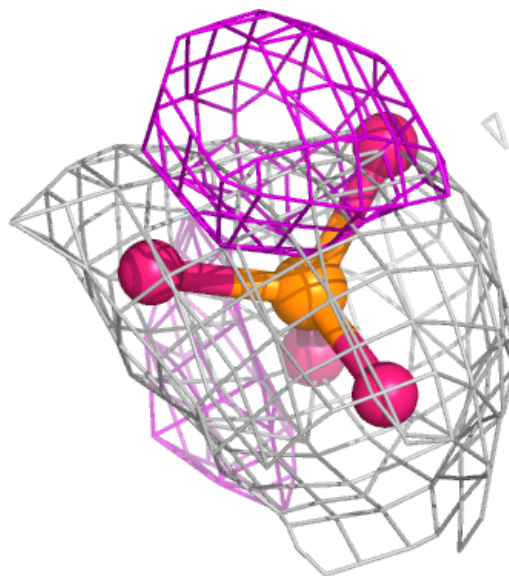
Electron density around PO4 K 302:

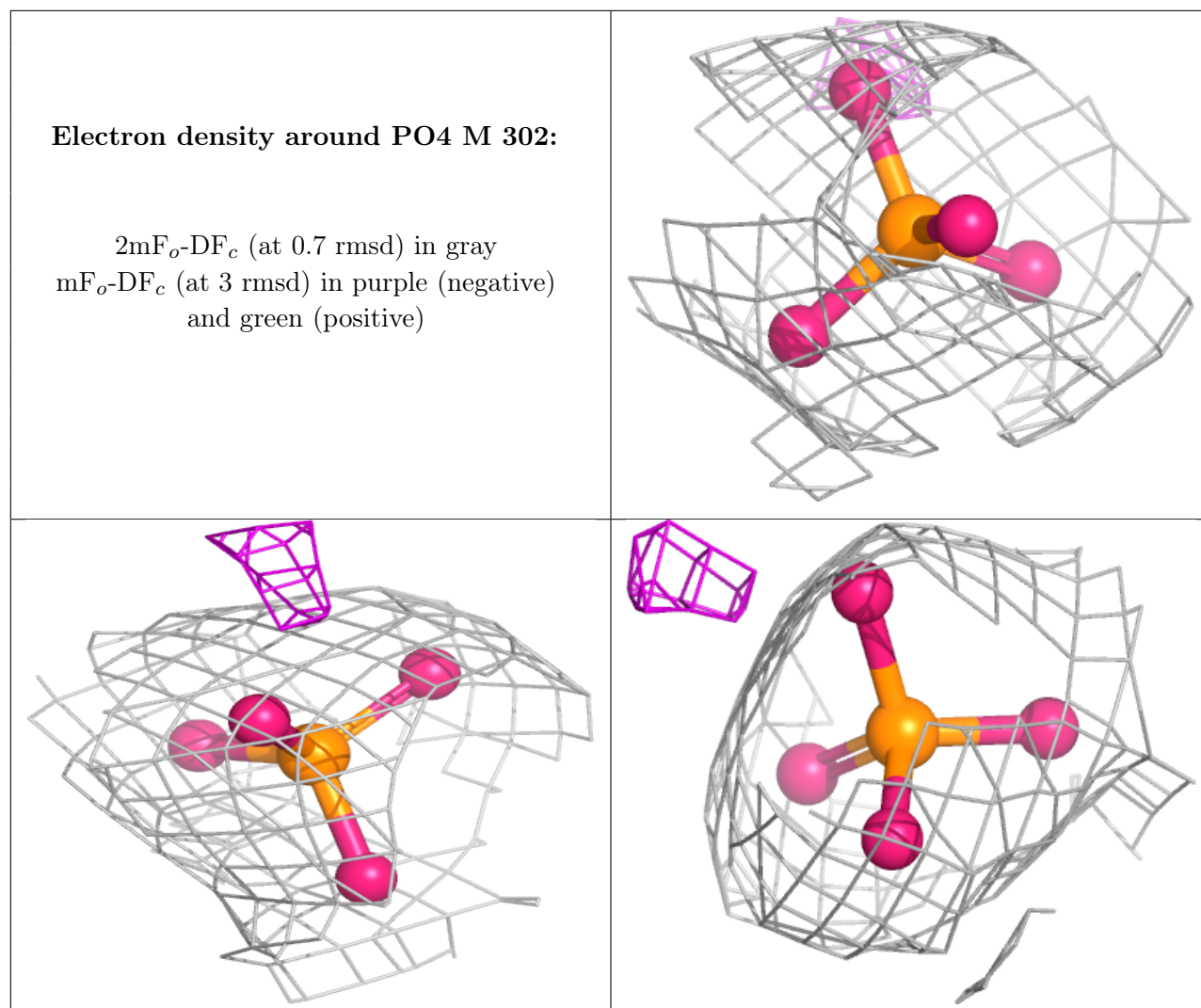
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and green (positive)



Electron density around PO4 g 201:

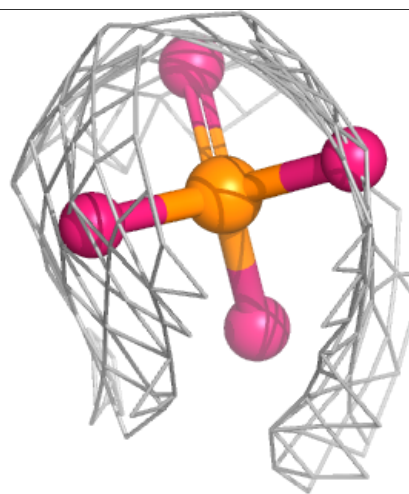
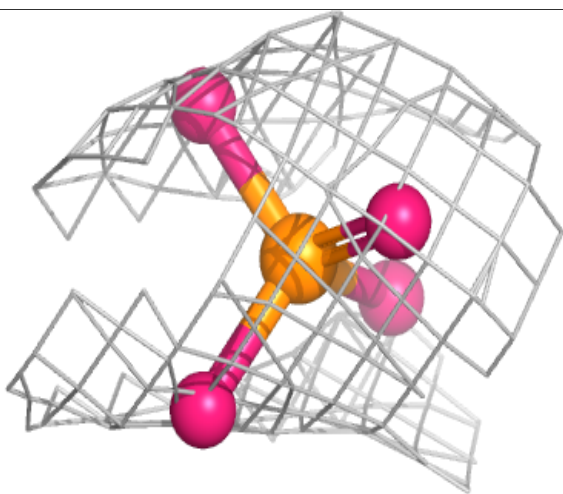
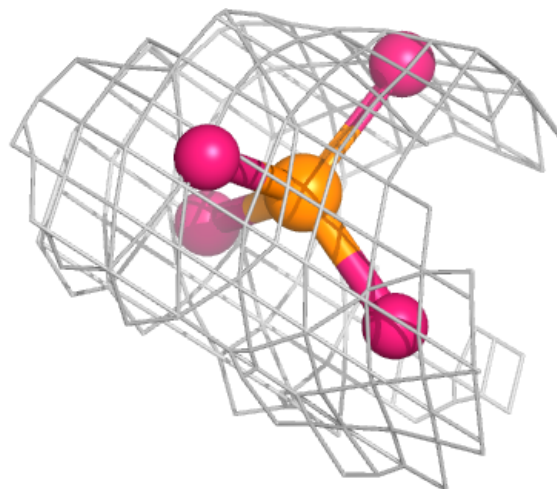
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





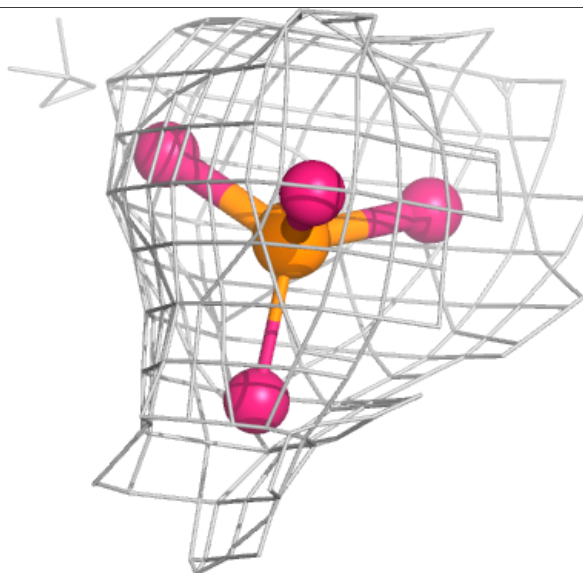
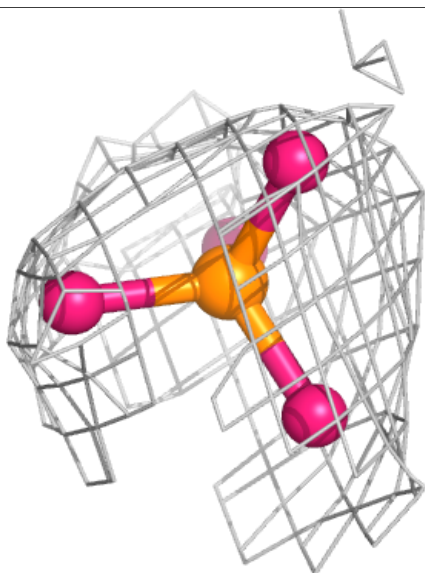
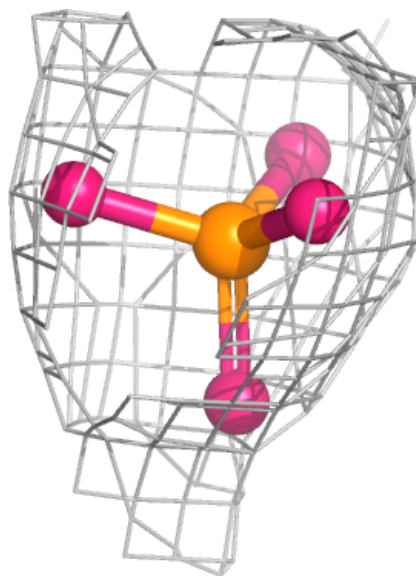
Electron density around PO4 G 303:

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



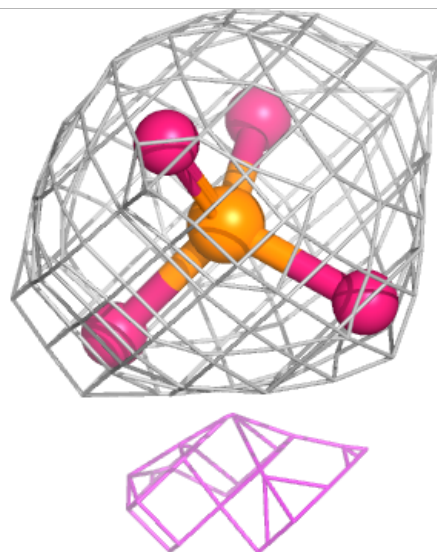
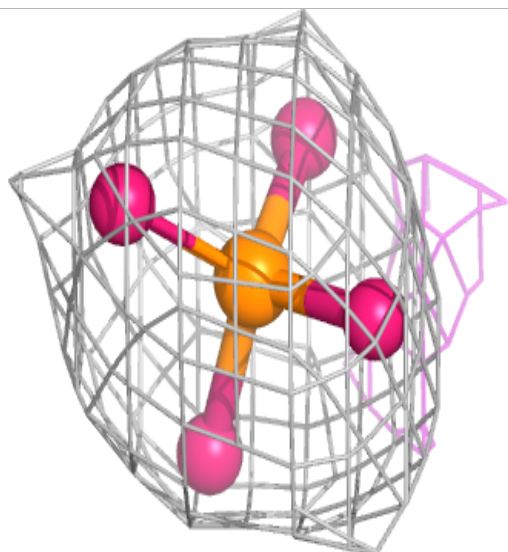
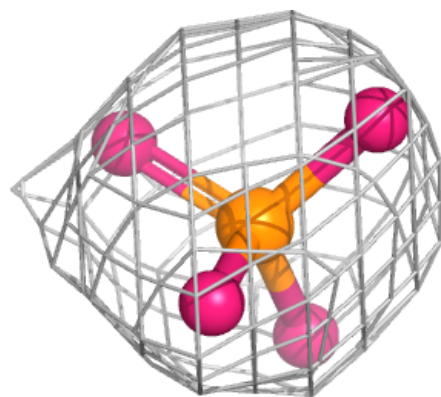
Electron density around PO4 a 201:

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



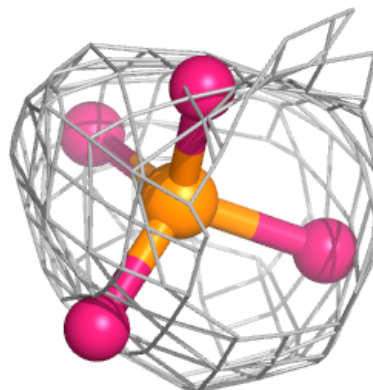
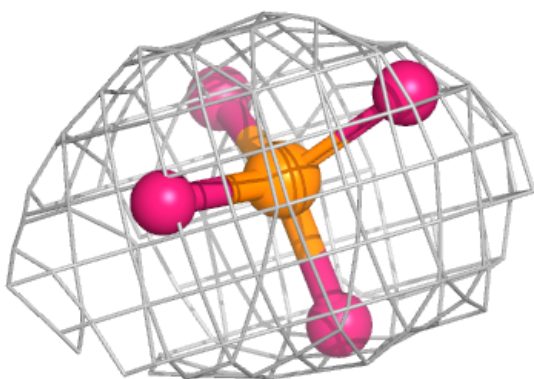
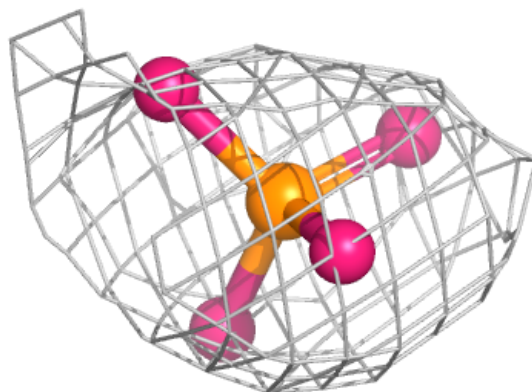
Electron density around PO4 O 301:

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and green (positive)



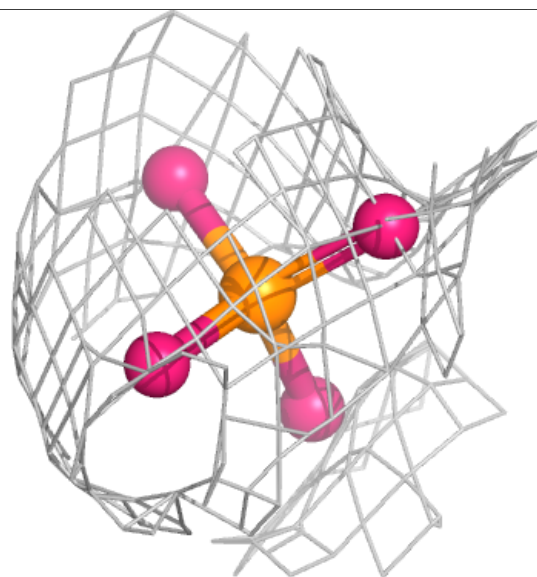
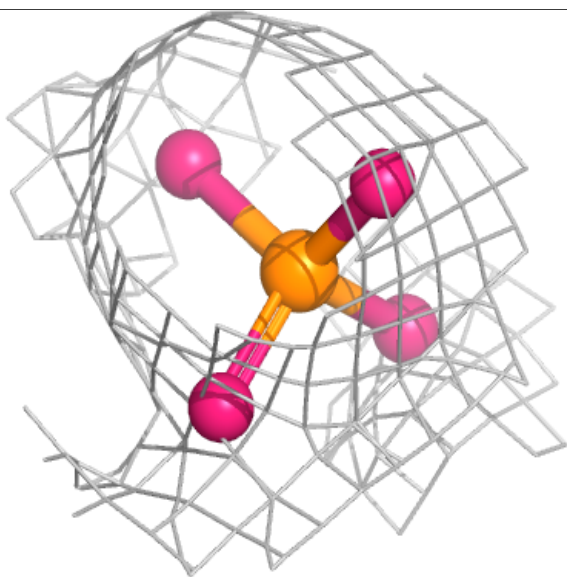
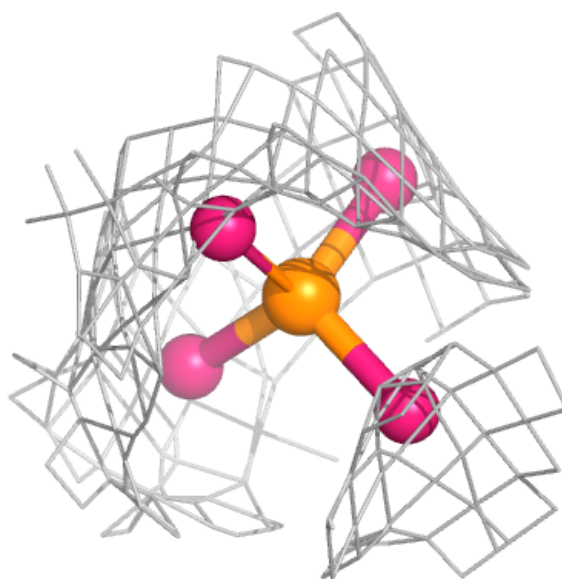
Electron density around PO4 J 301:

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



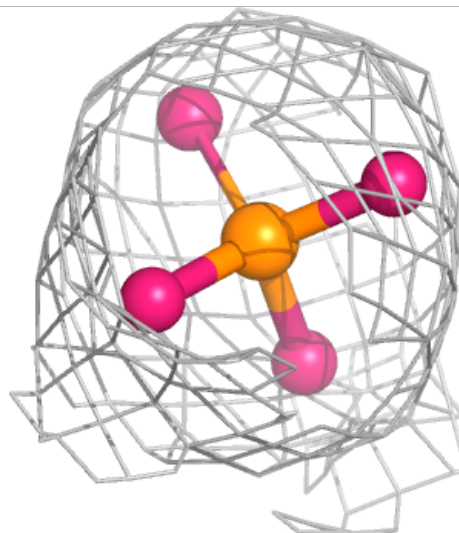
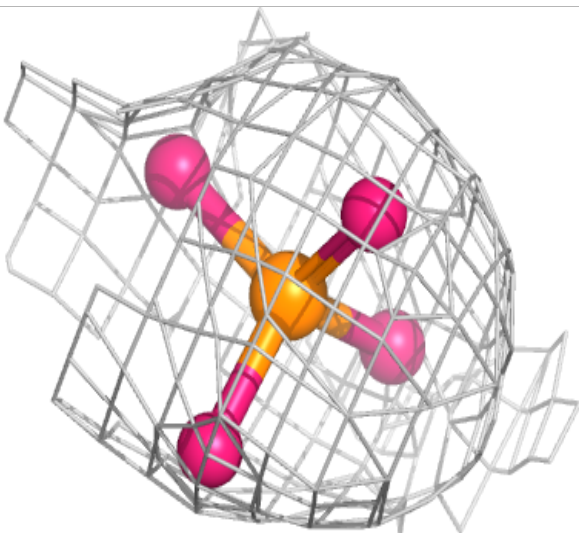
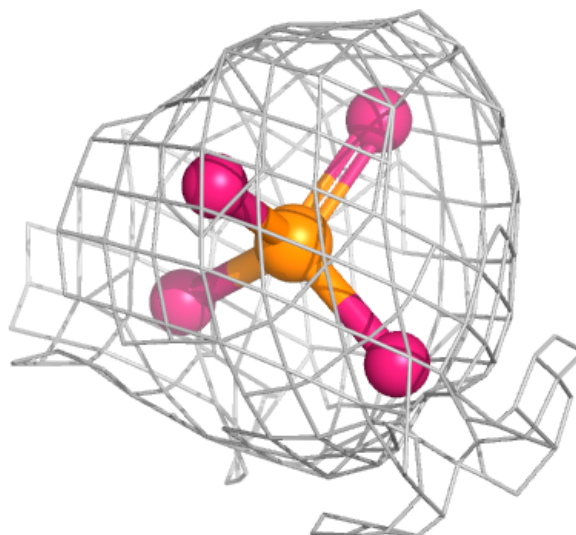
Electron density around PO4 I 301:

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and green (positive)



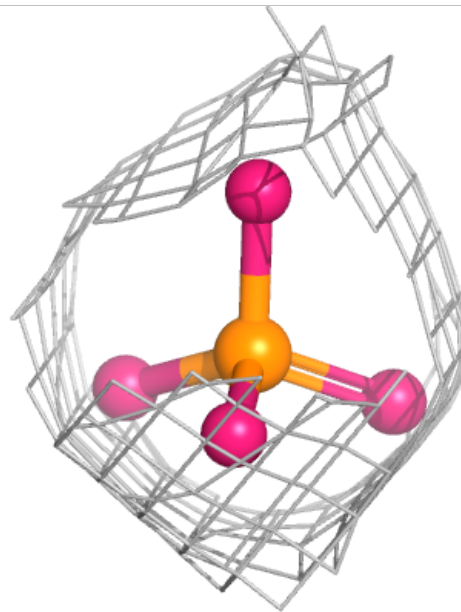
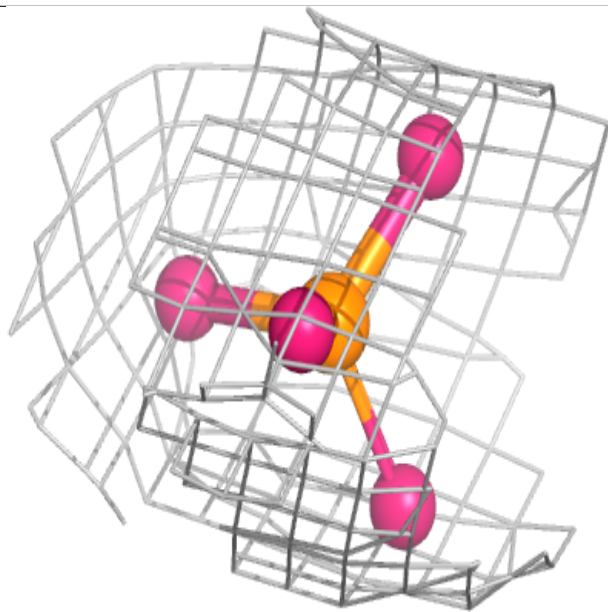
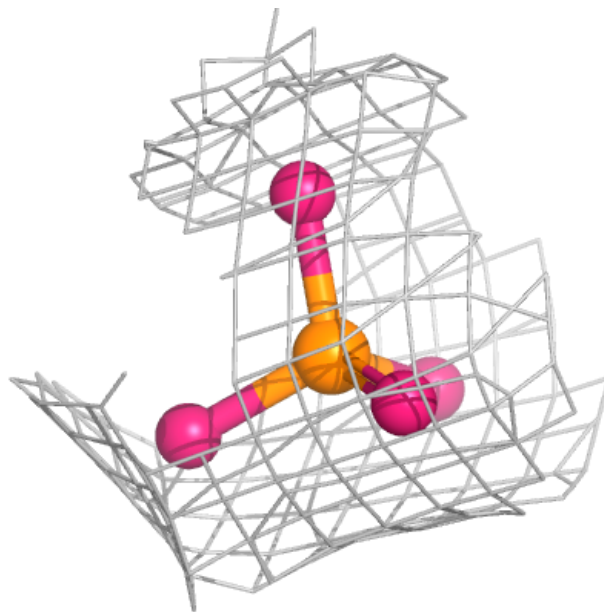
Electron density around PO4 C 302:

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and green (positive)



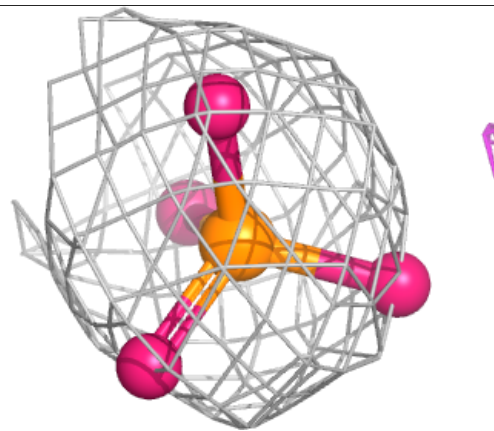
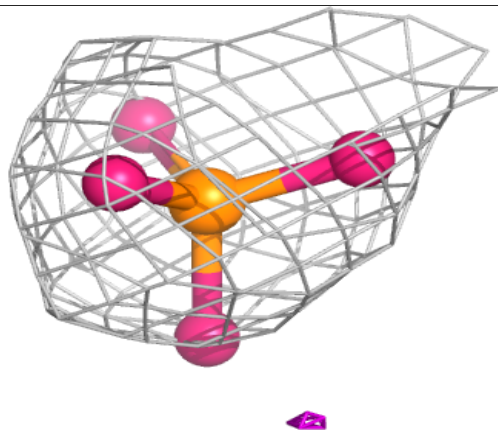
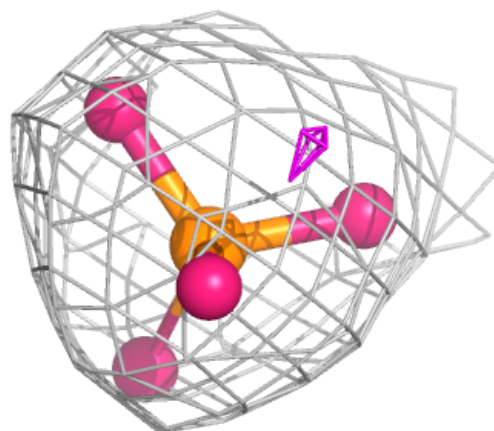
Electron density around PO4 i 202:

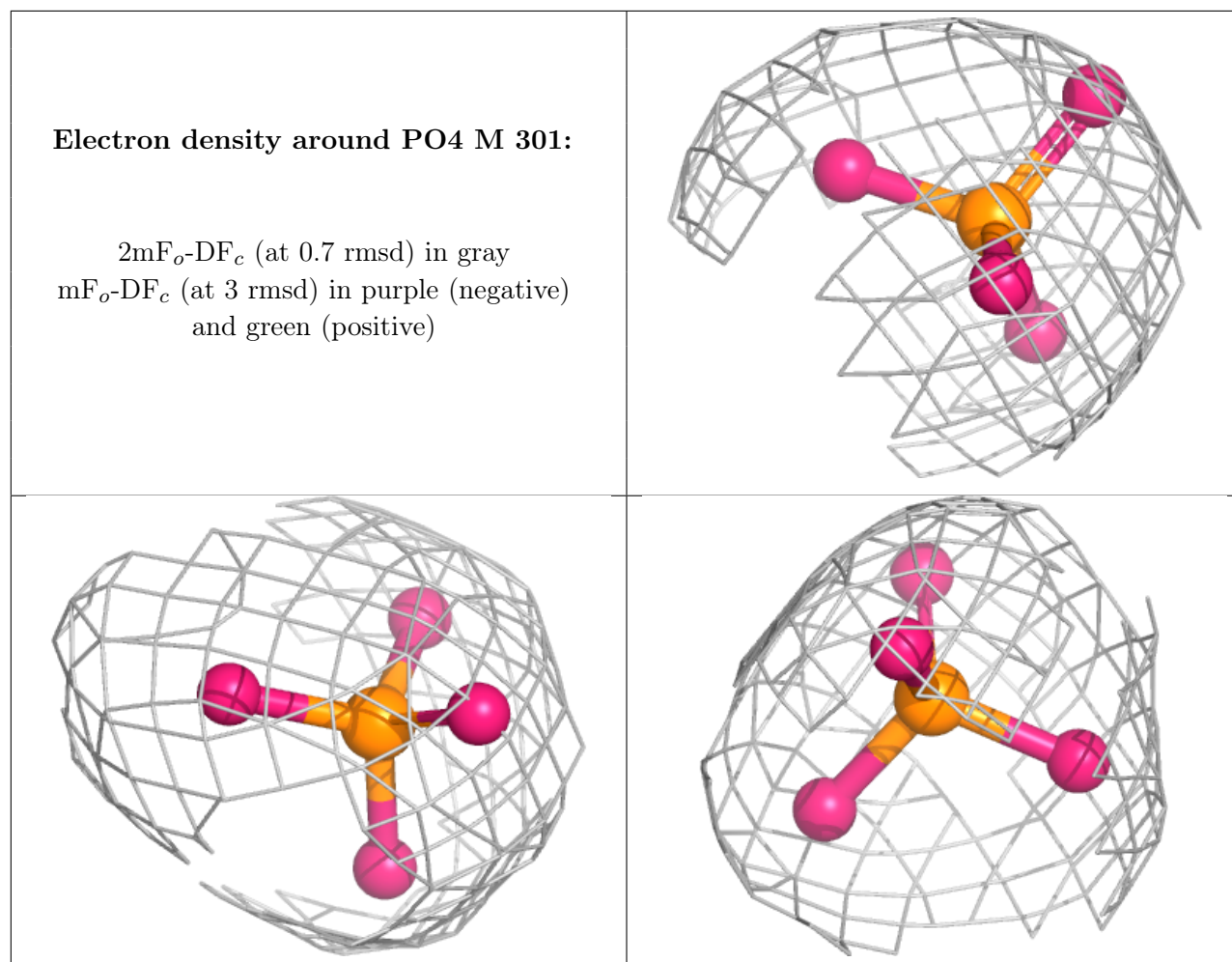
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



Electron density around PO4 e 201:

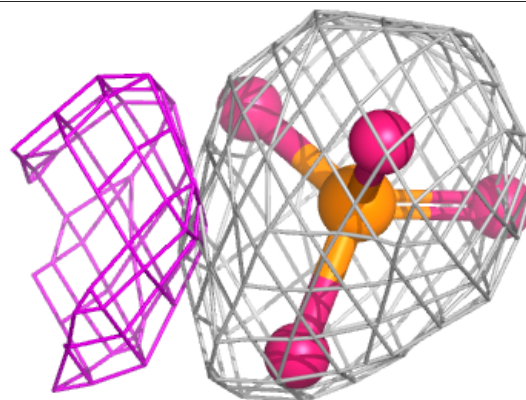
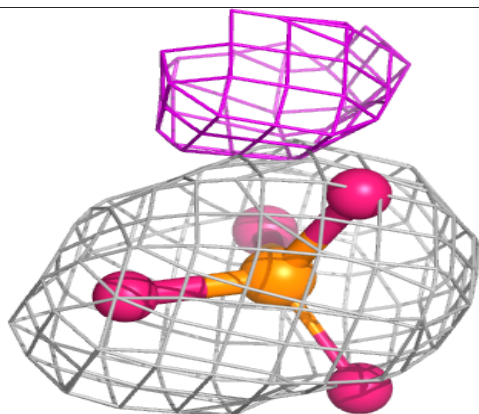
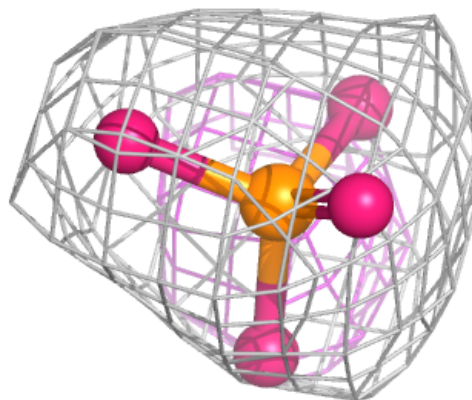
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and green (positive)





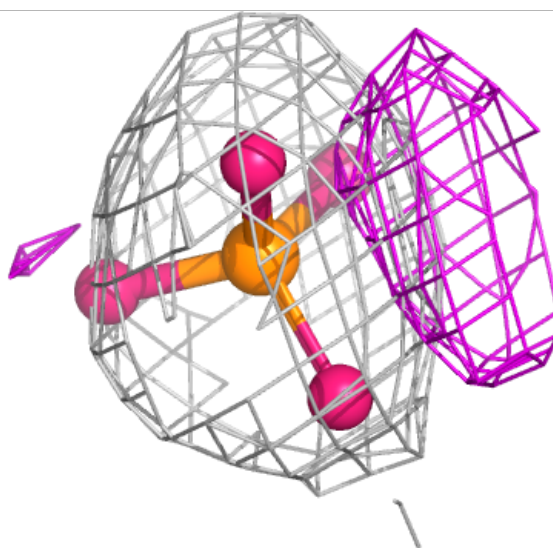
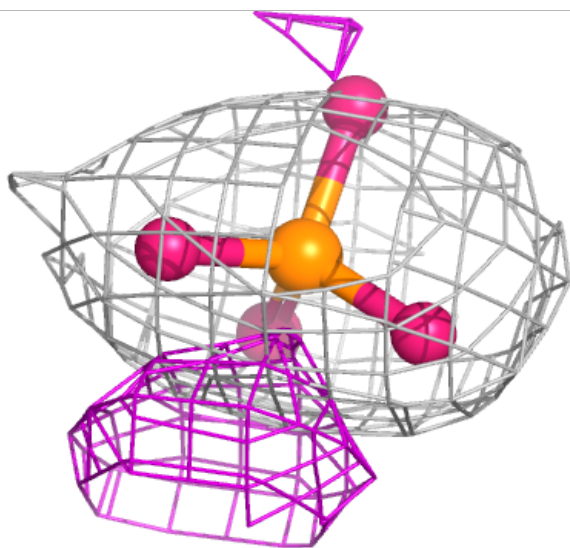
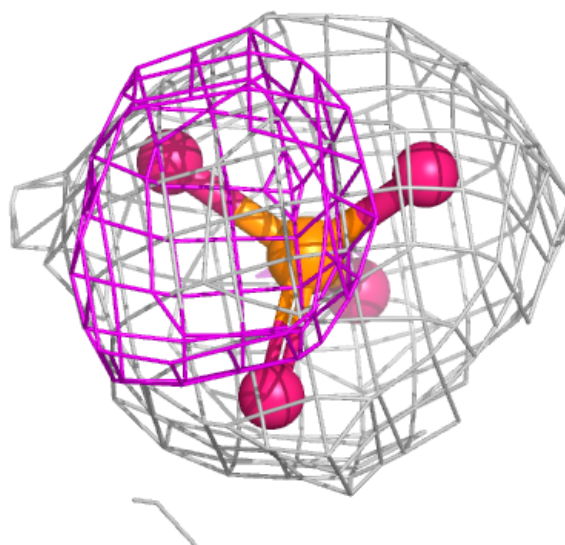
Electron density around PO4 E 301:

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and green (positive)



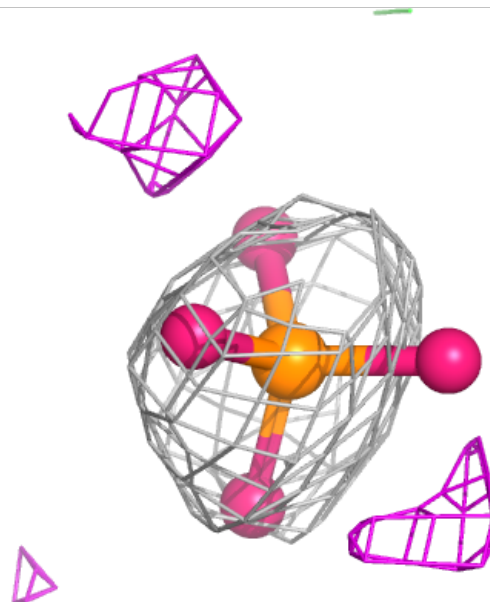
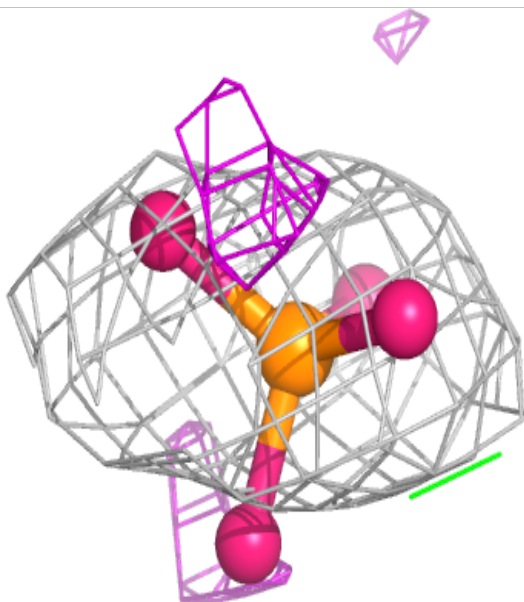
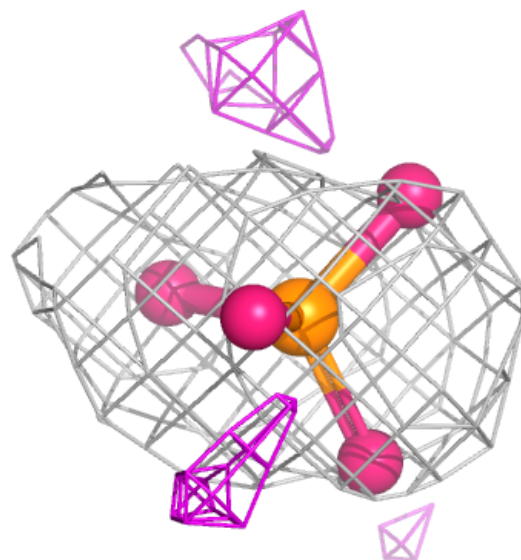
Electron density around PO4 c 202:

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



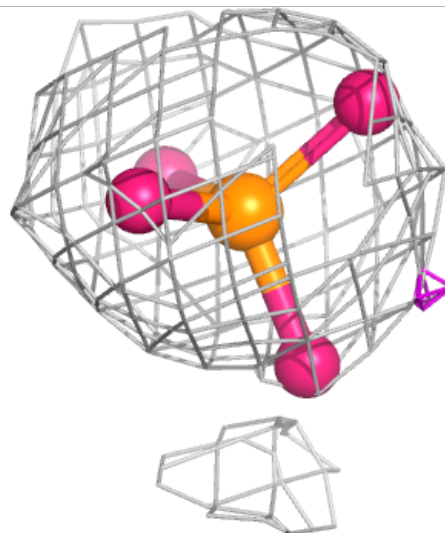
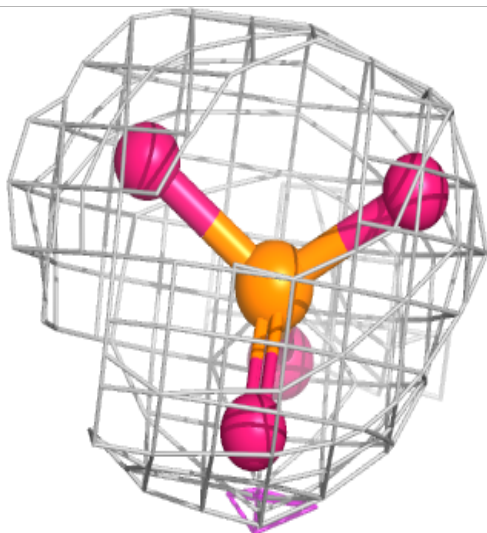
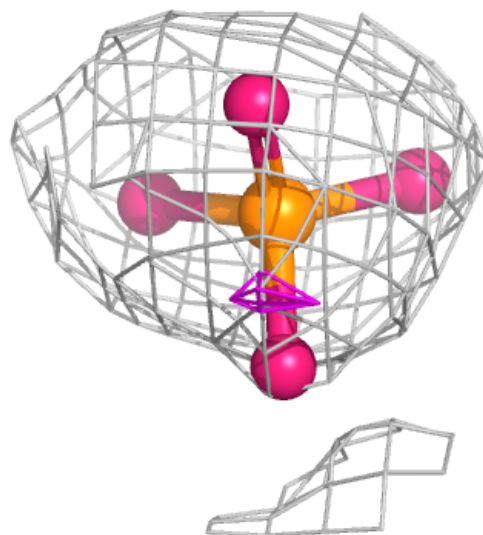
Electron density around PO4 D 302:

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



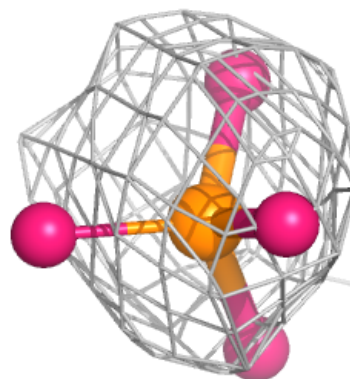
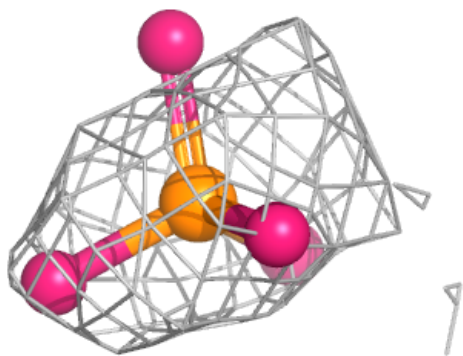
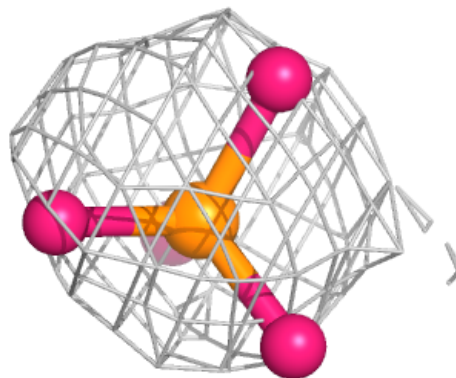
Electron density around PO4 G 302:

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



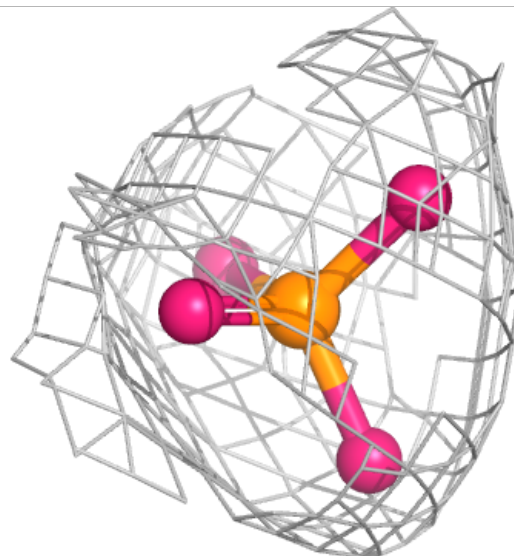
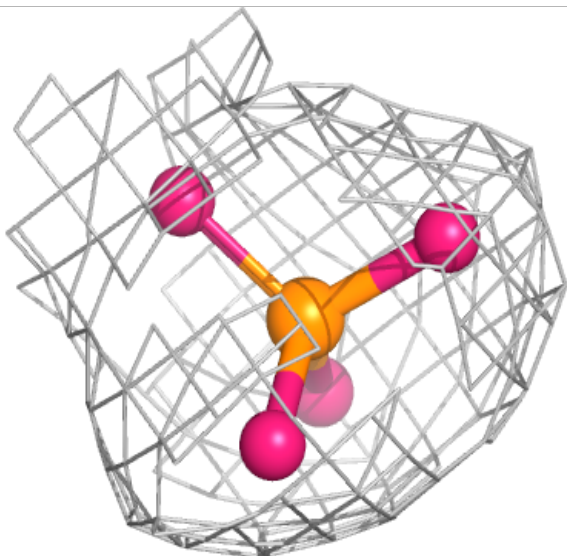
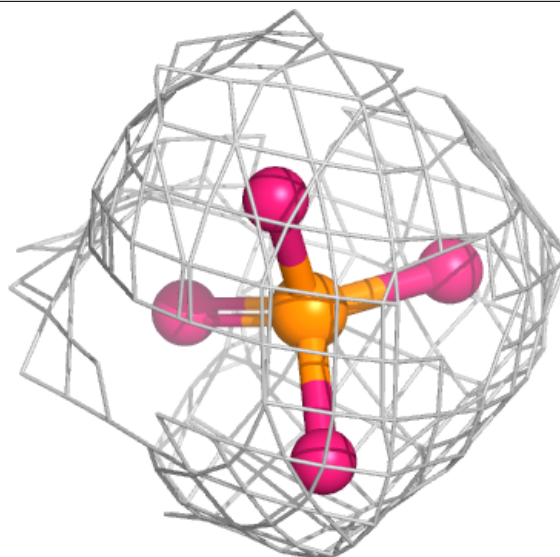
Electron density around PO4 K 301:

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



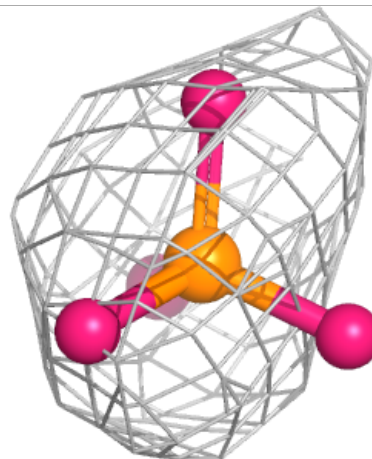
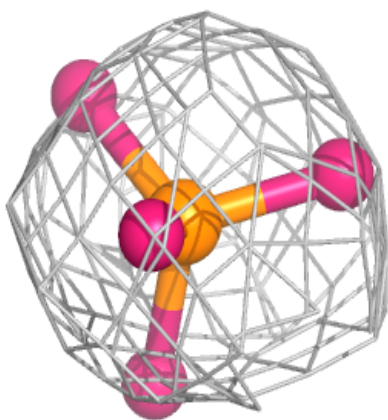
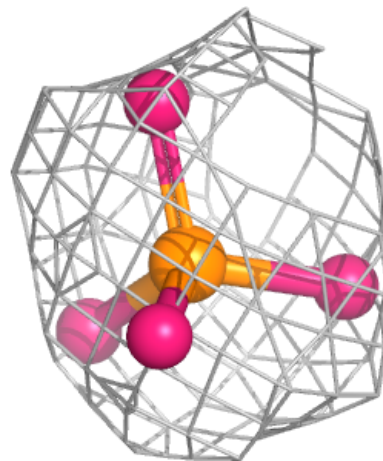
Electron density around PO4 R 301:

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



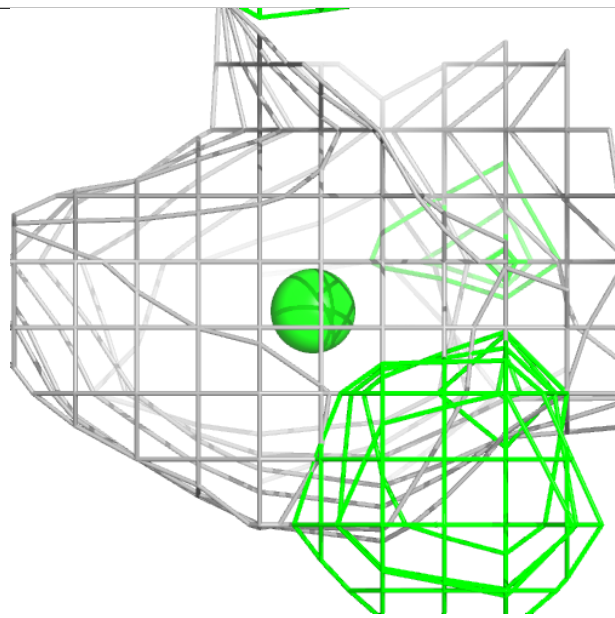
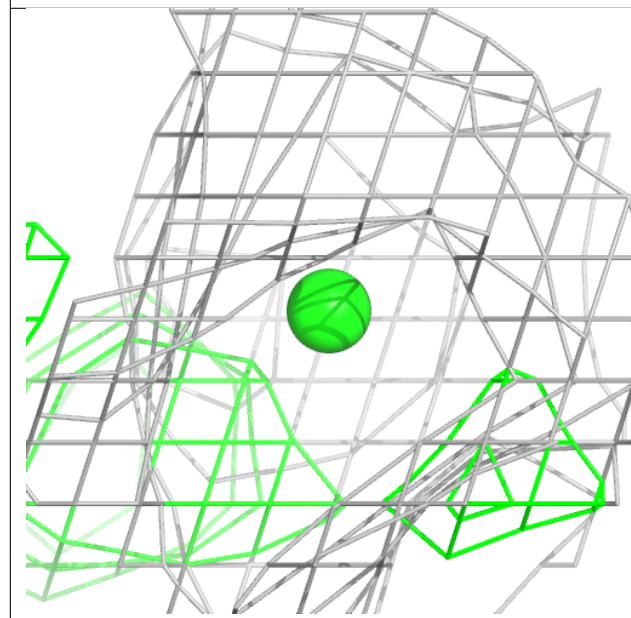
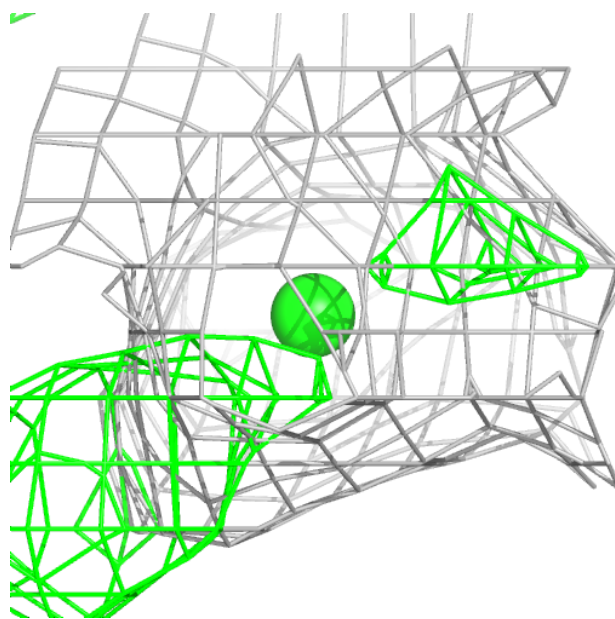
Electron density around PO4 E 303:

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



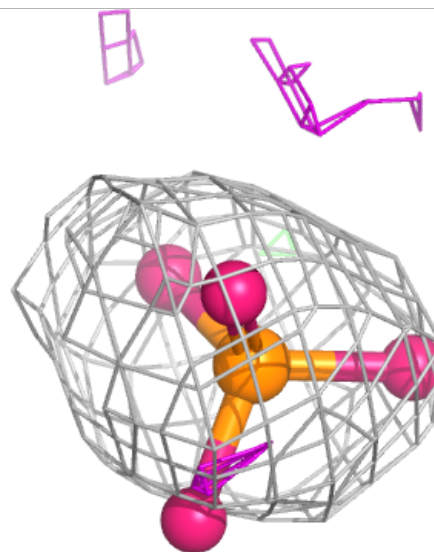
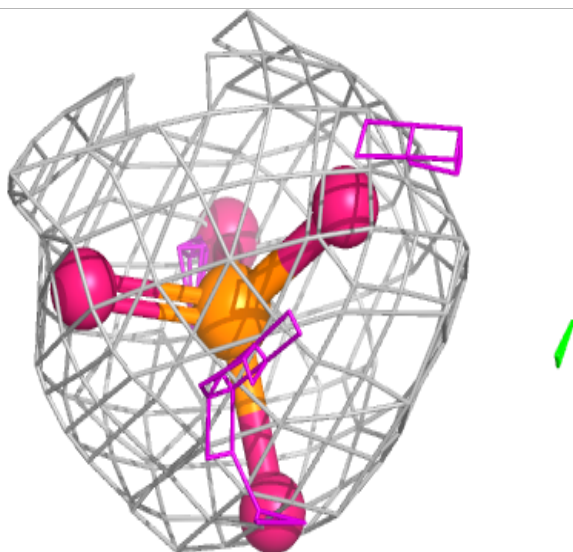
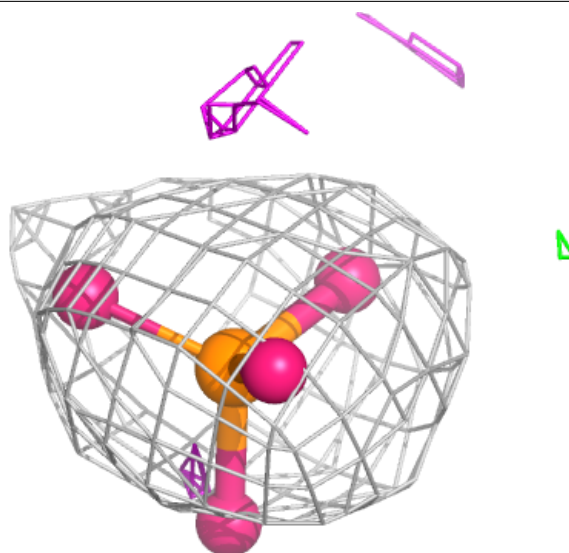
Electron density around CL K 304:

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



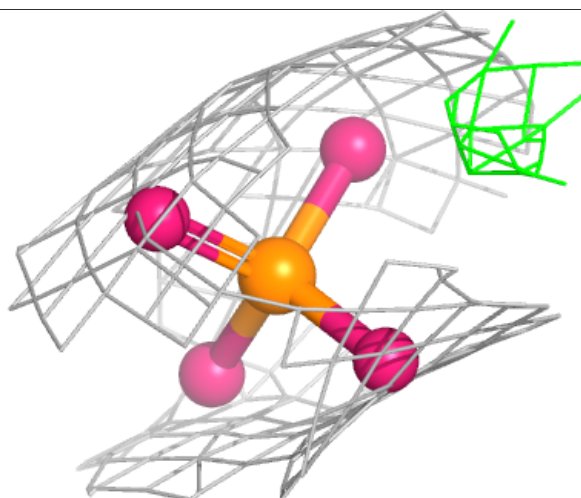
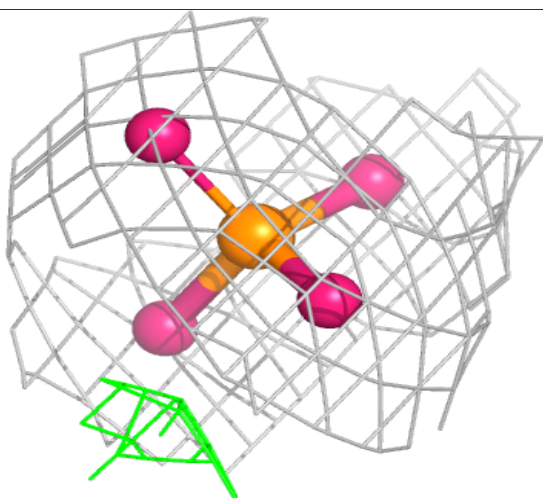
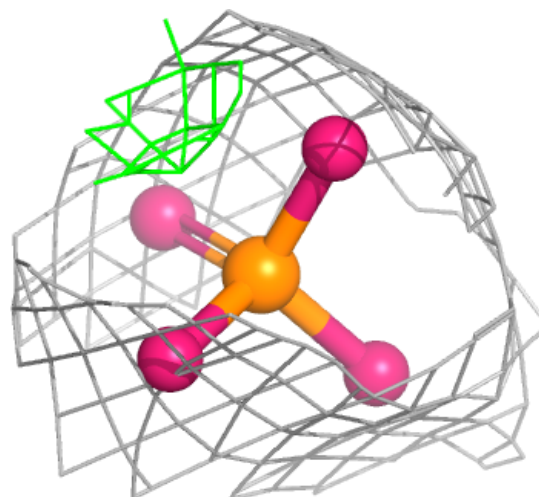
Electron density around PO4 J 302:

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



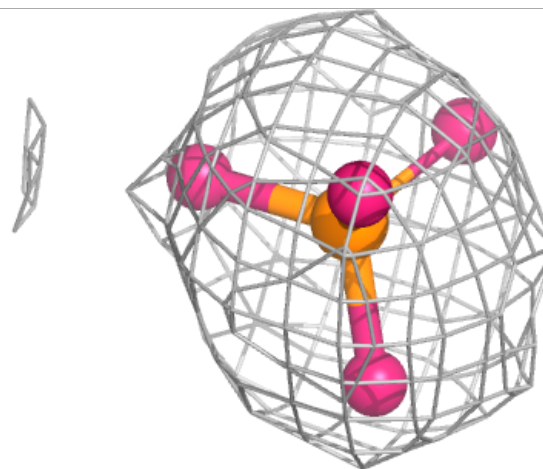
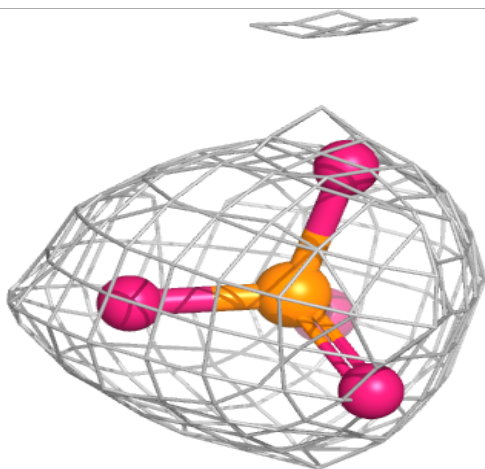
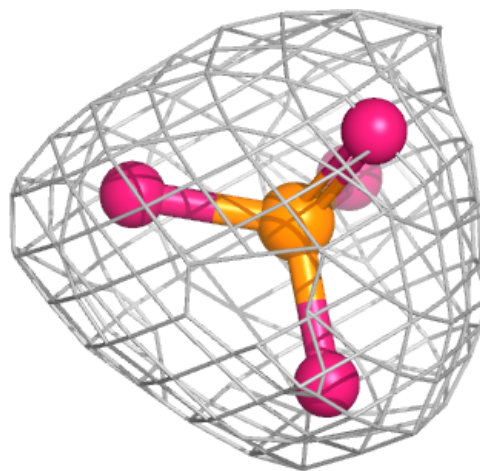
Electron density around PO4 o 201:

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



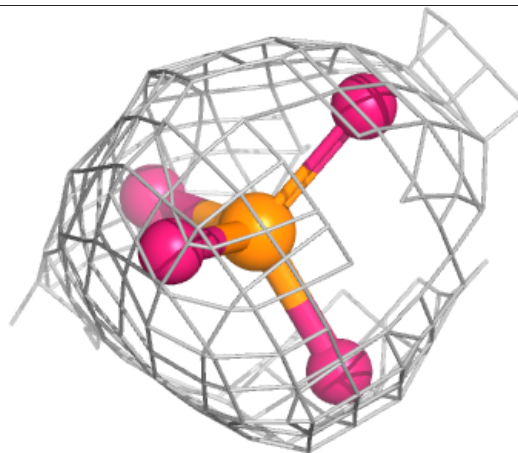
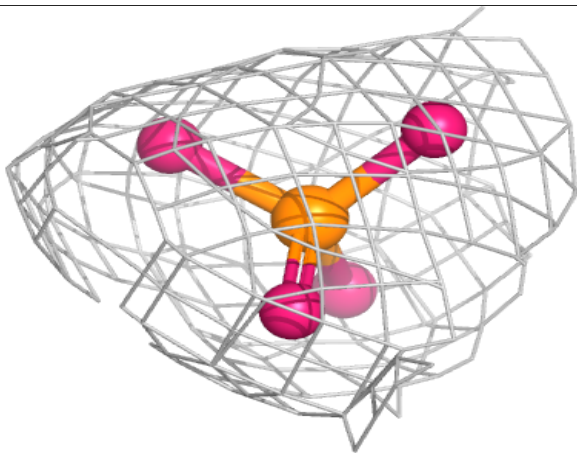
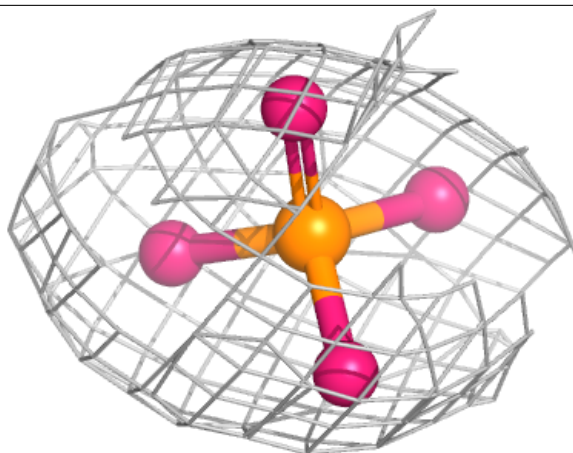
Electron density around PO4 O 302:

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



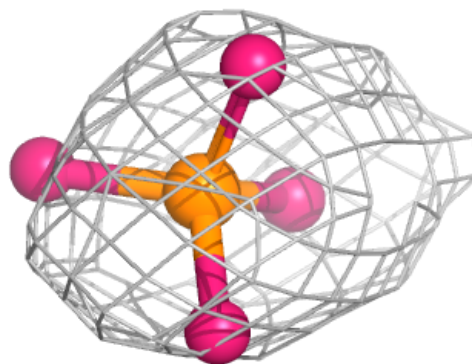
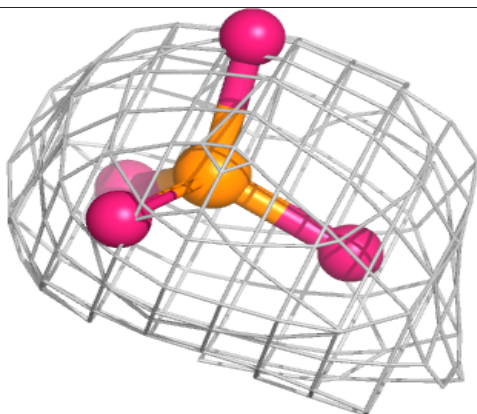
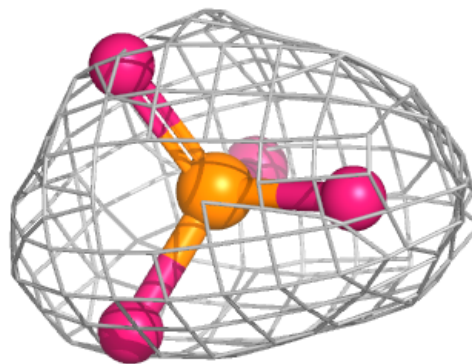
Electron density around PO4 m 201:

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



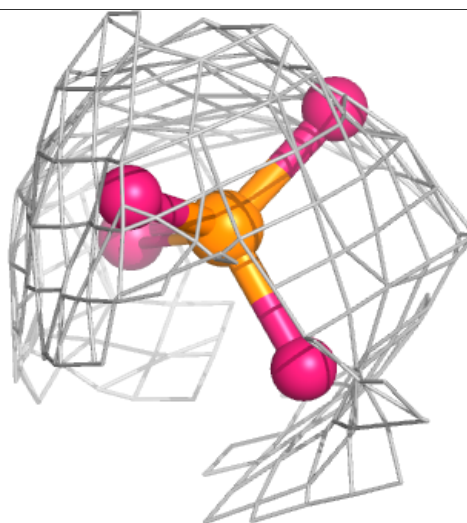
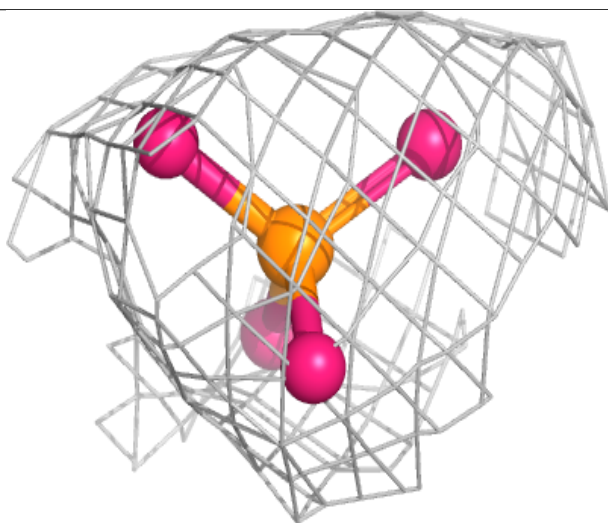
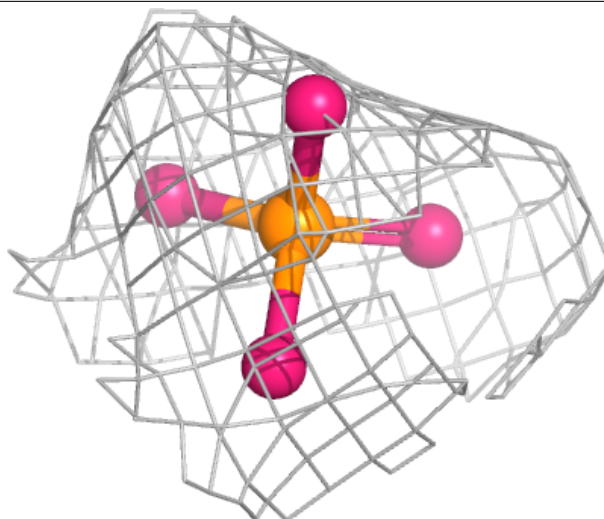
Electron density around PO4 C 304:

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



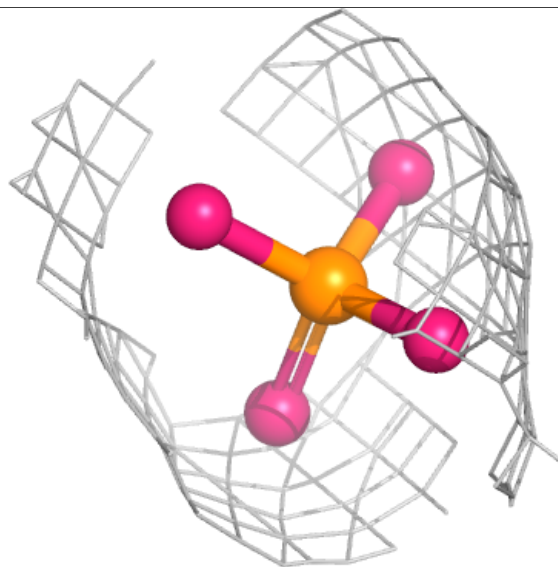
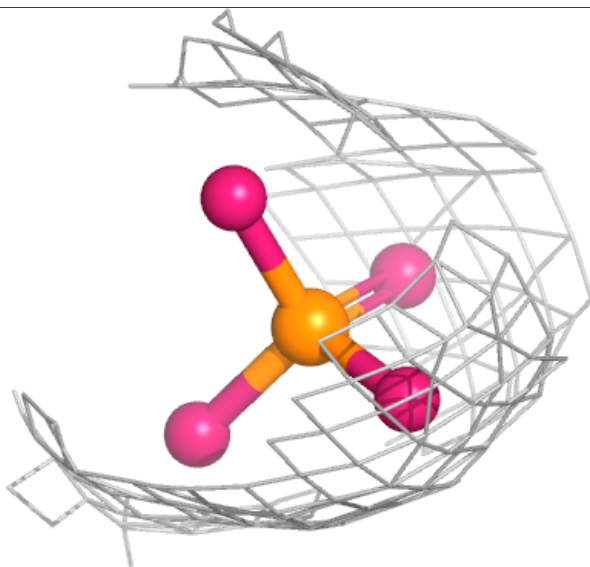
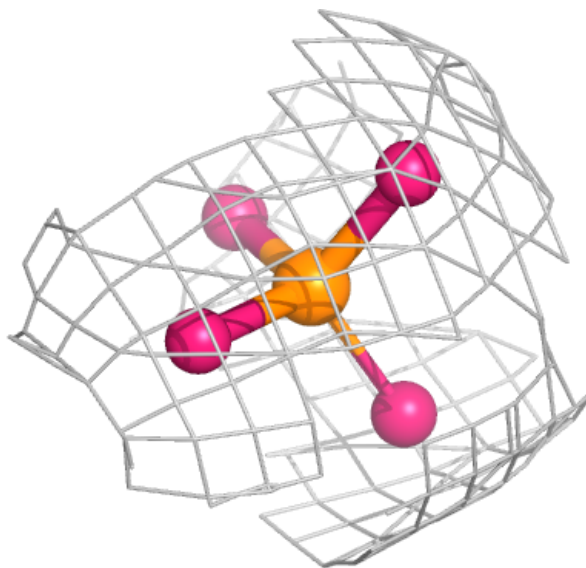
Electron density around PO4 C 303:

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



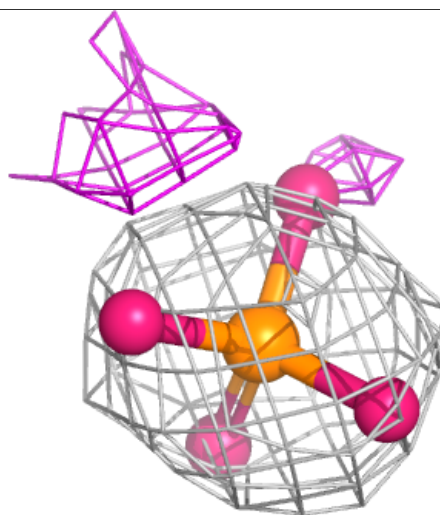
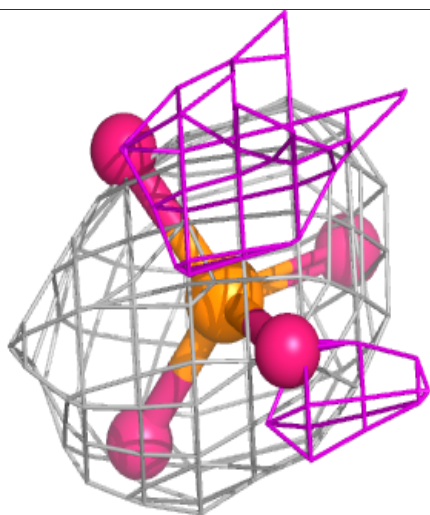
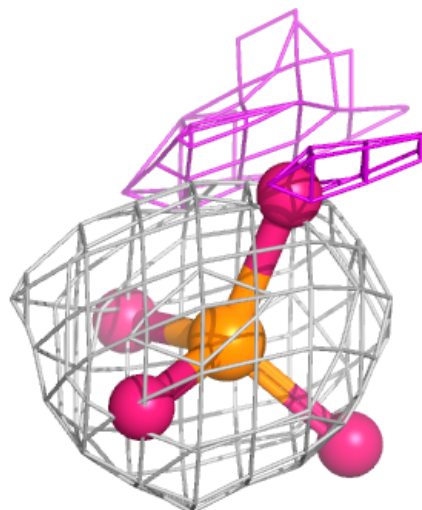
Electron density around PO4 o 203:

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



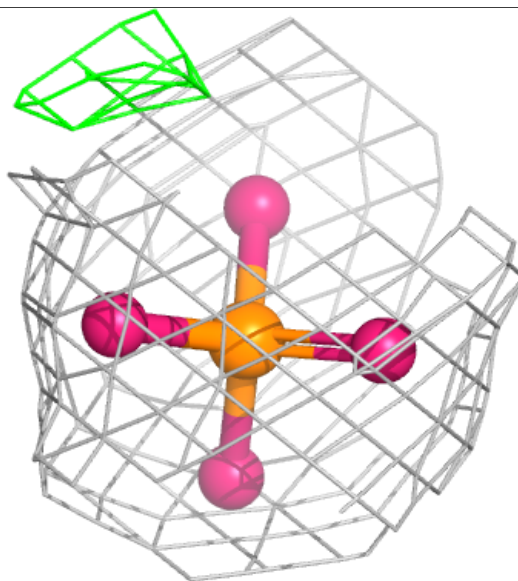
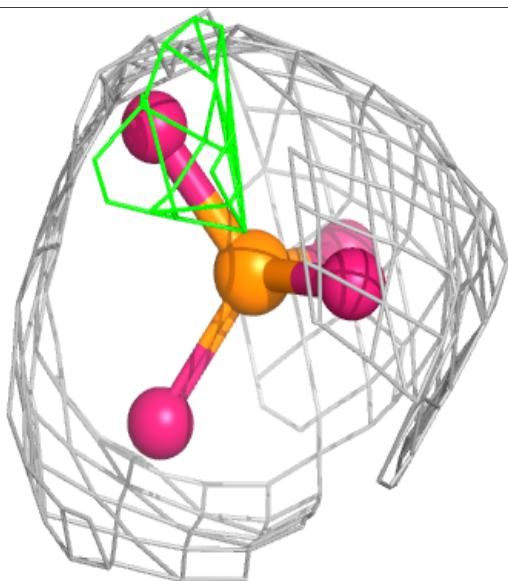
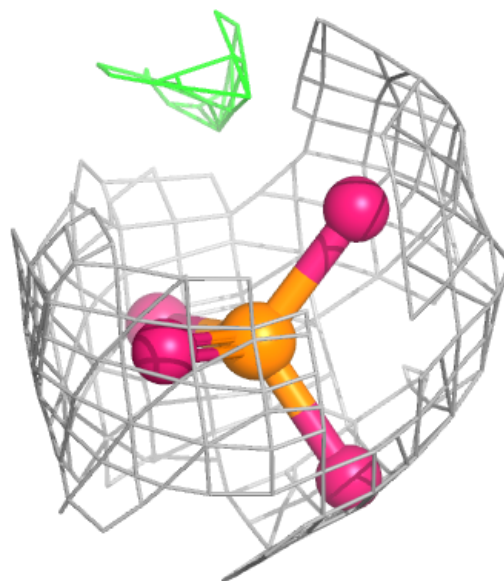
Electron density around PO4 I 302:

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



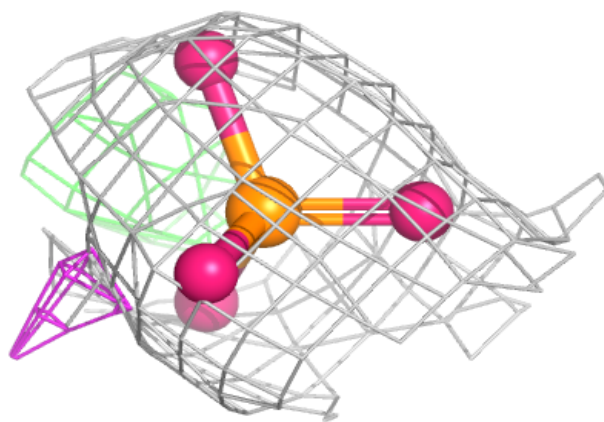
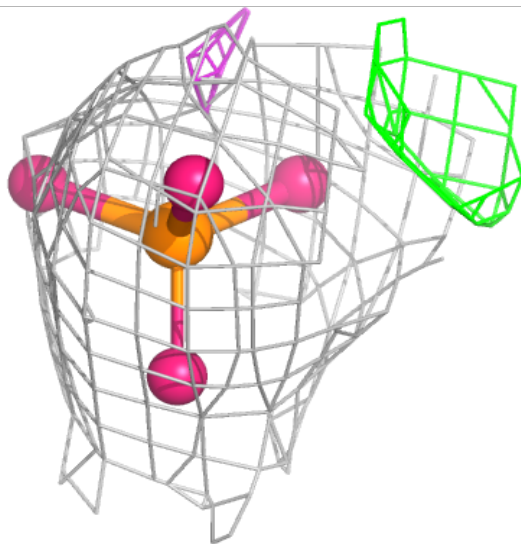
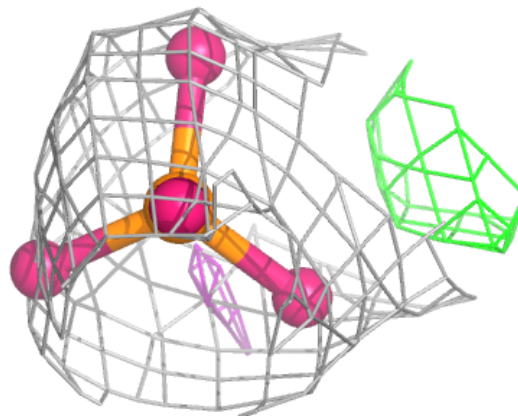
Electron density around PO4 i 201:

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



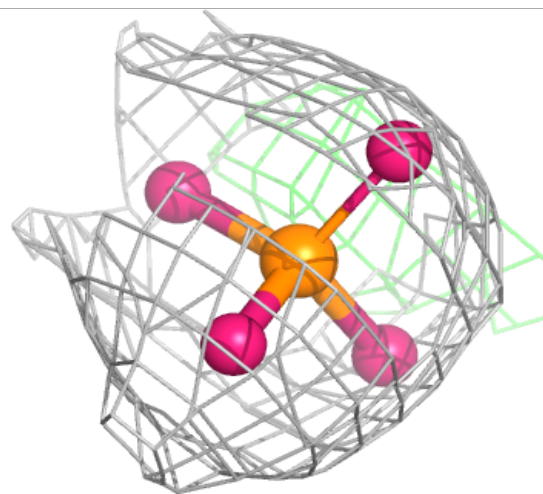
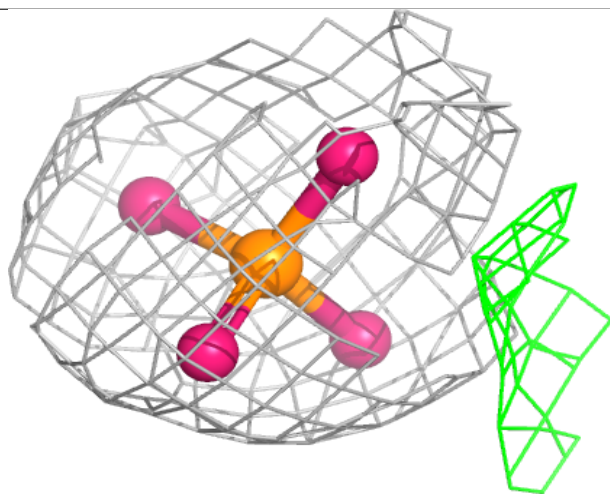
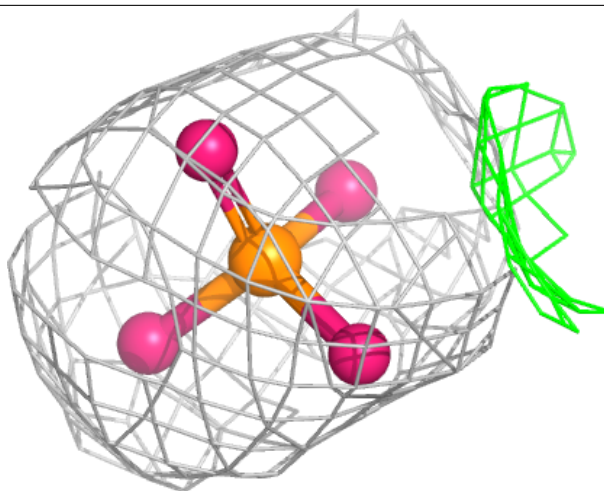
Electron density around PO4 e 203:

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



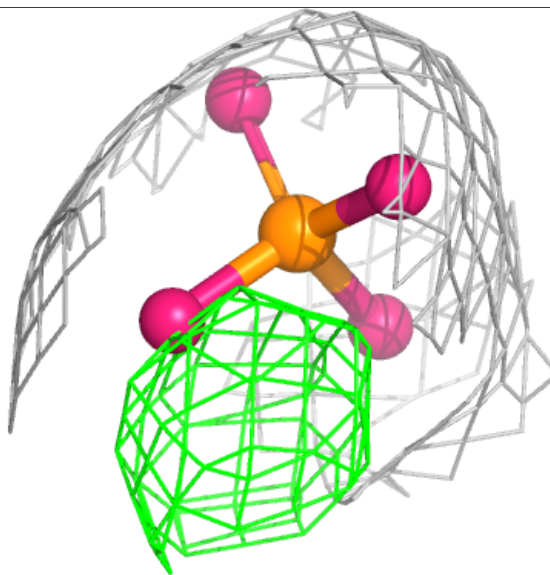
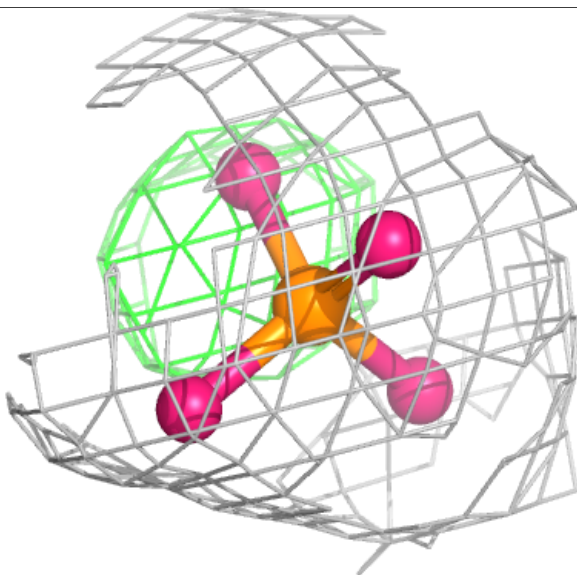
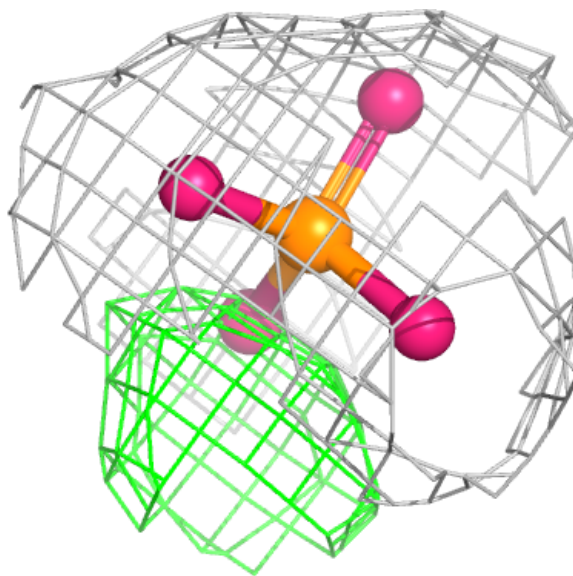
Electron density around PO4 B 301:

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



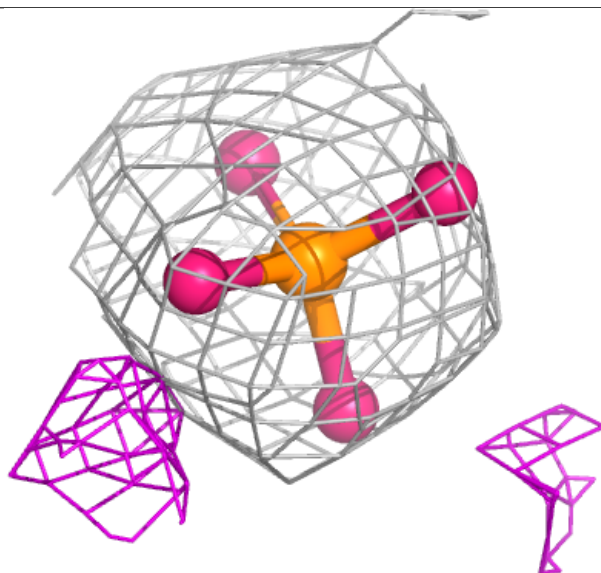
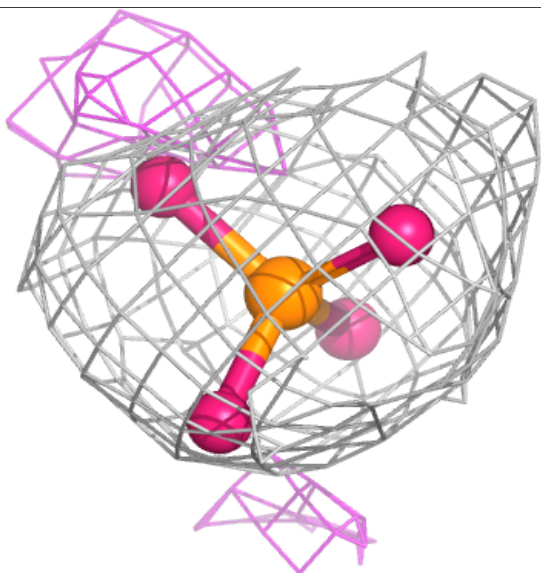
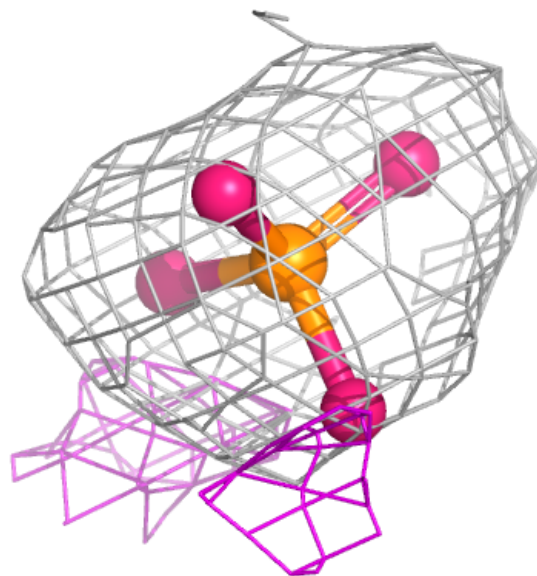
Electron density around PO4 m 202:

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



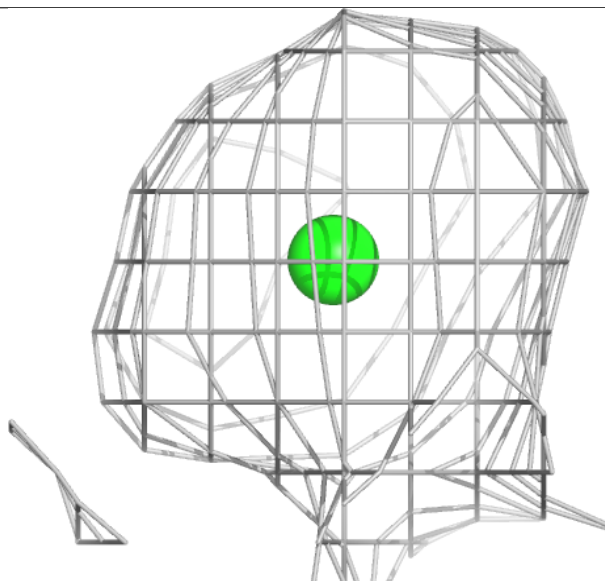
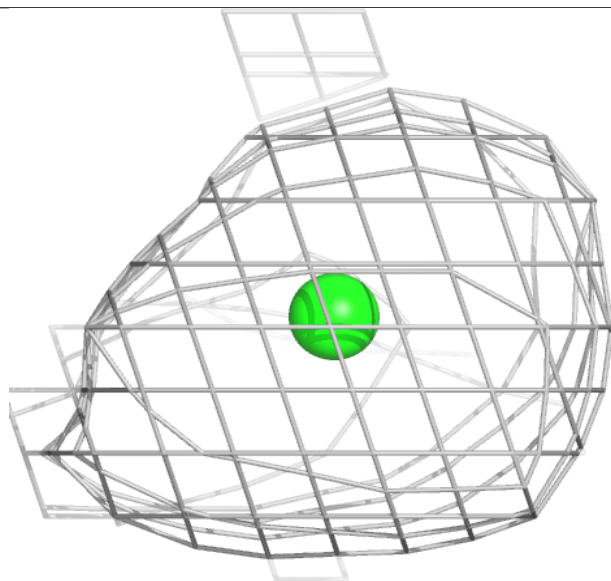
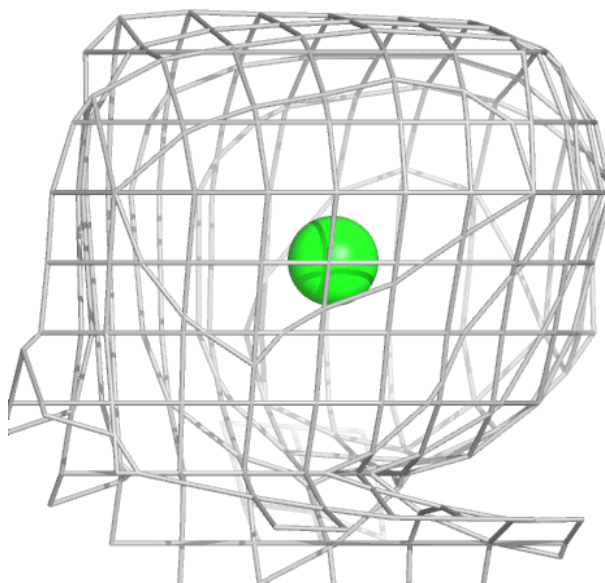
Electron density around PO4 C 305:

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



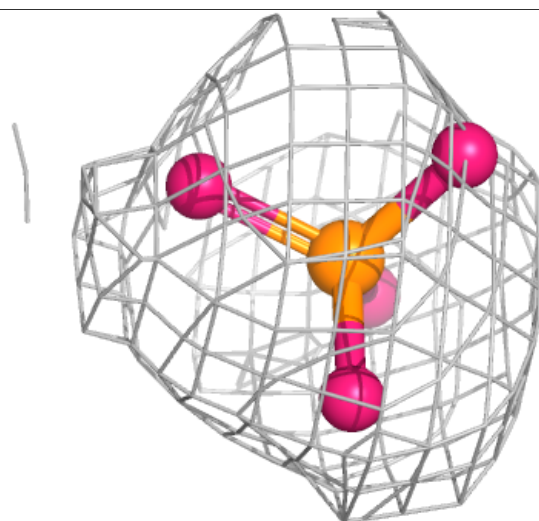
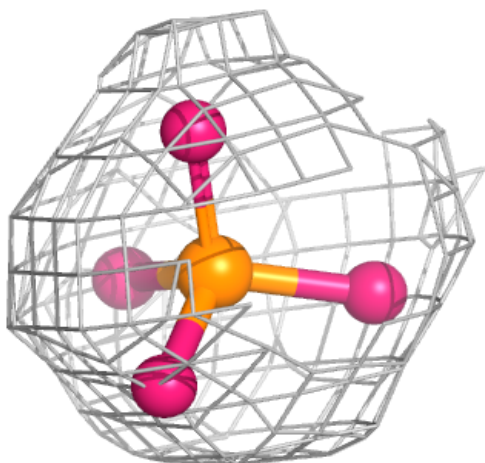
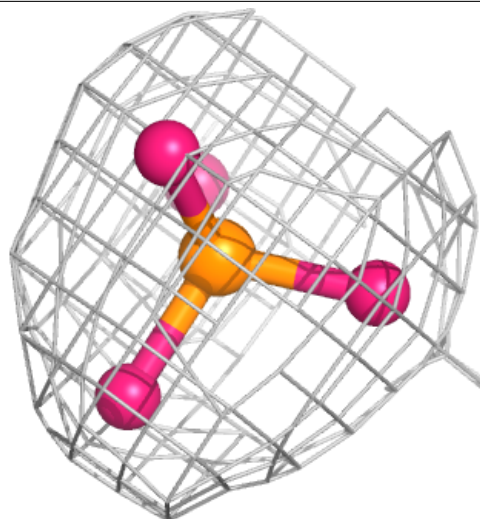
Electron density around CL R 302:

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



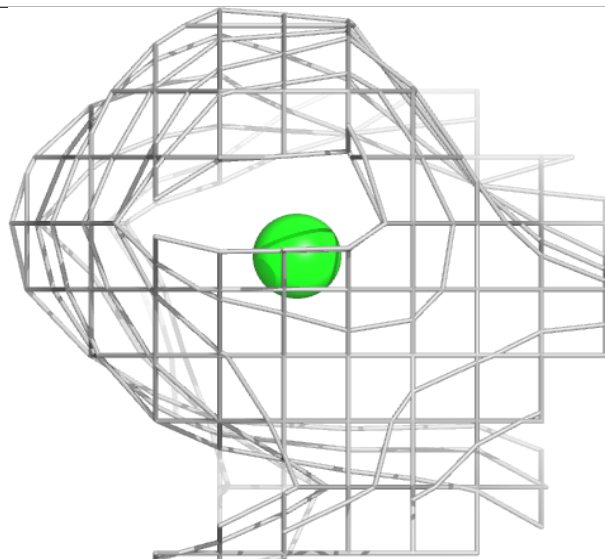
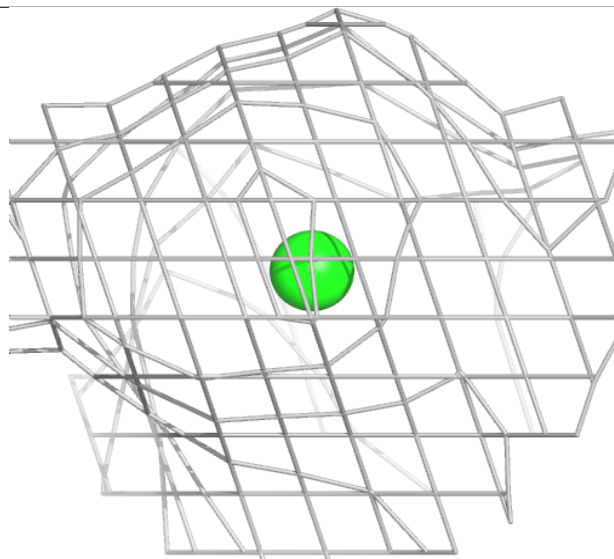
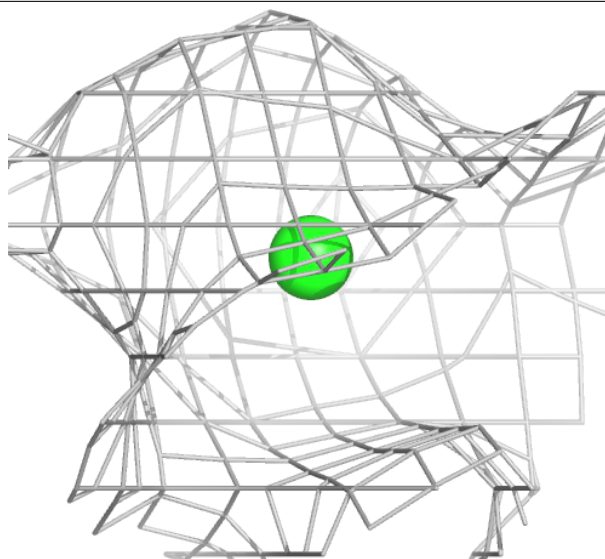
Electron density around PO4 M 303:

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



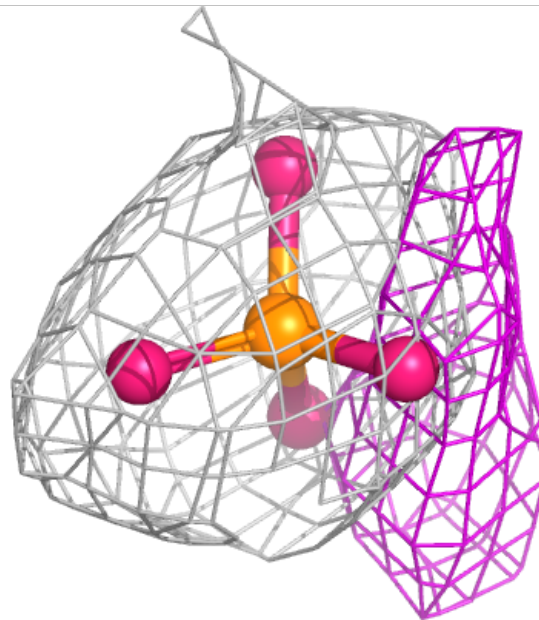
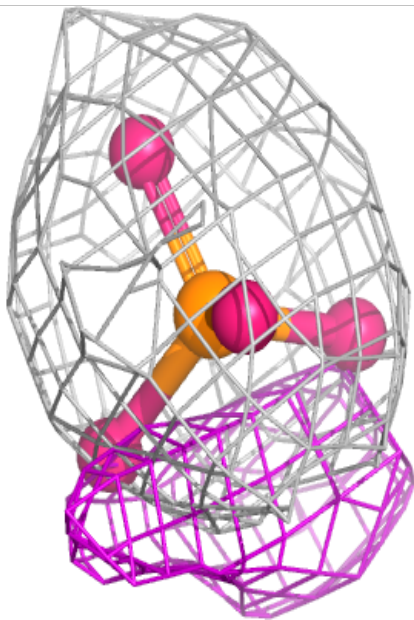
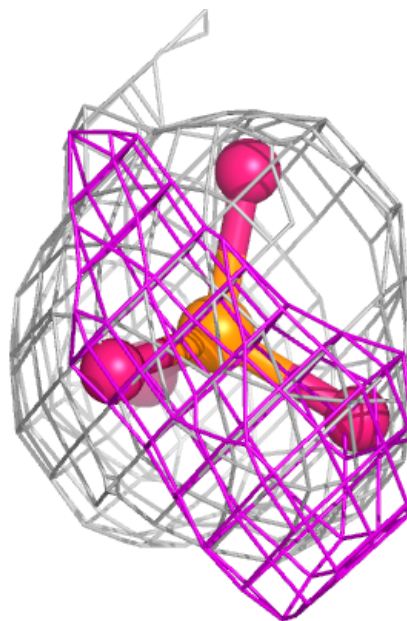
Electron density around CL G 304:

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



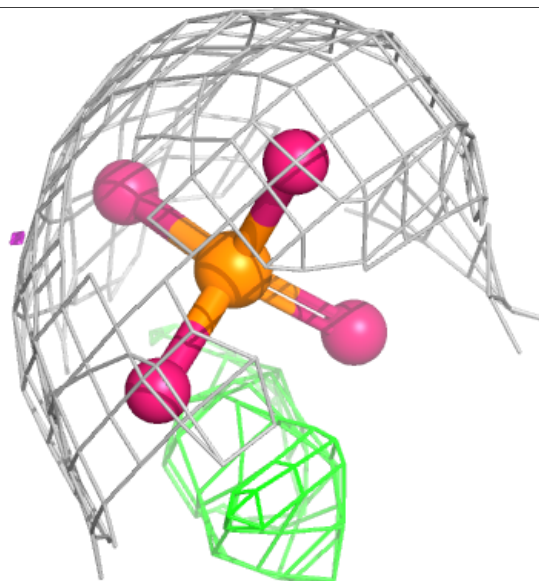
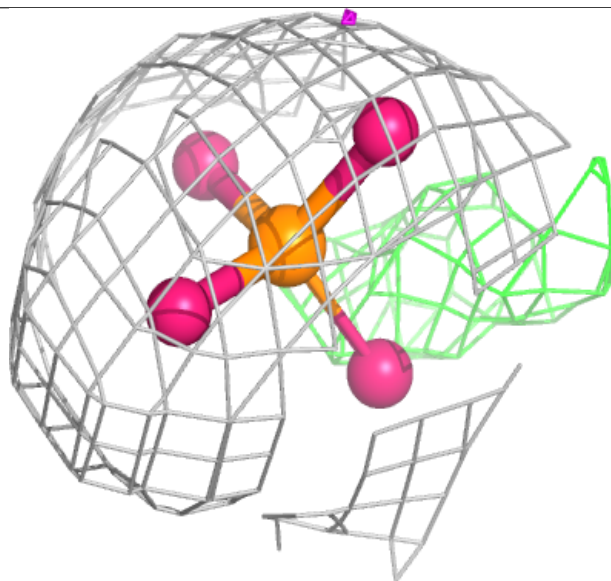
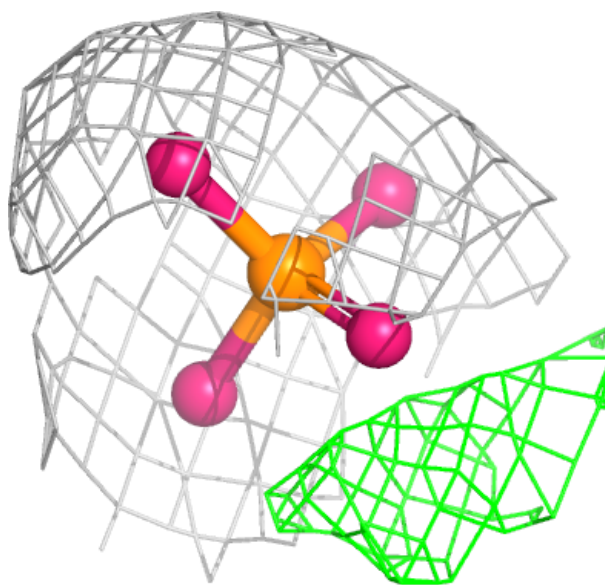
Electron density around PO4 I 304:

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



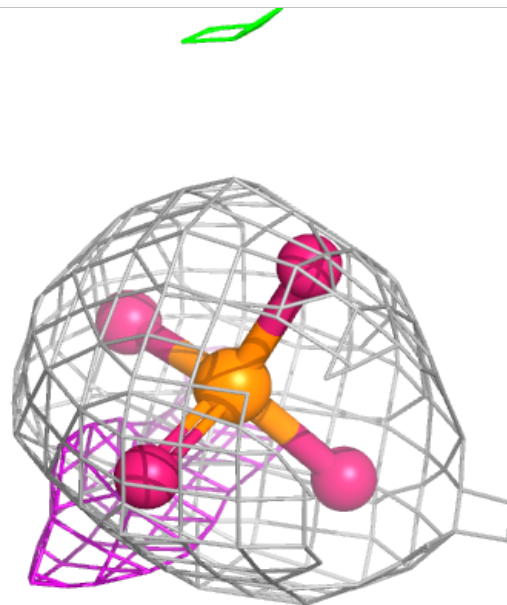
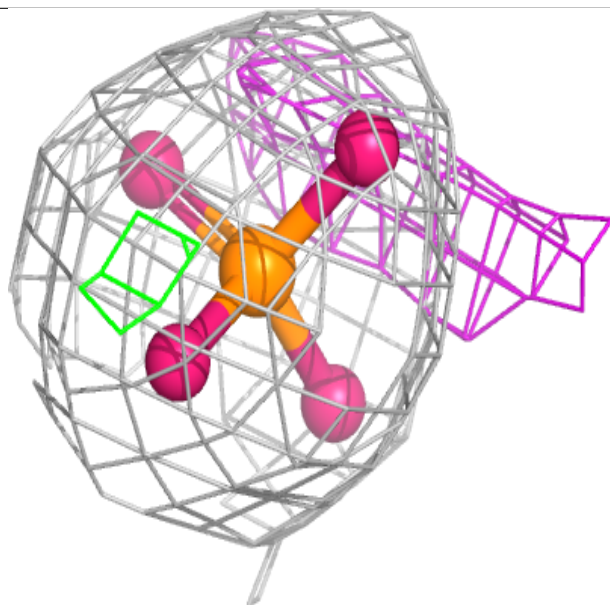
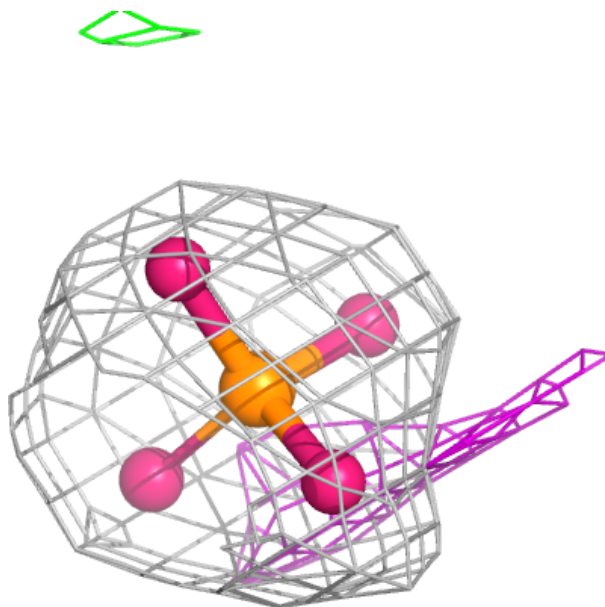
Electron density around PO4 i 203:

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



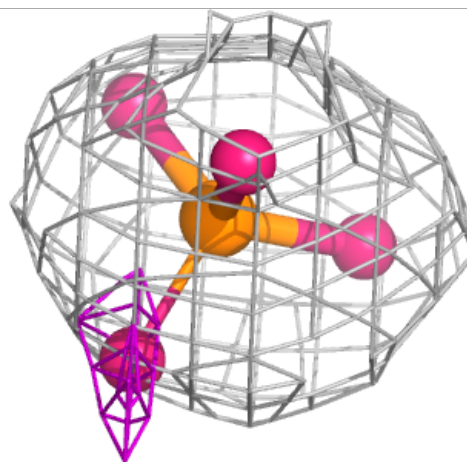
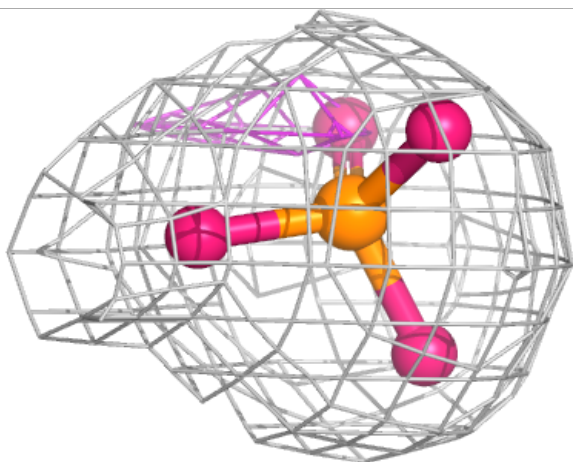
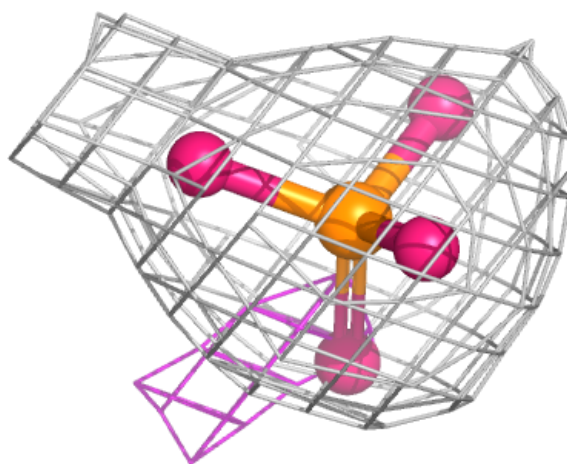
Electron density around PO4 G 301:

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



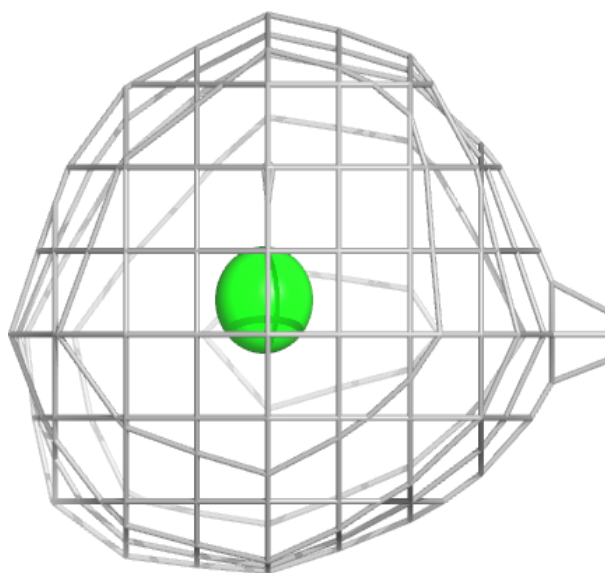
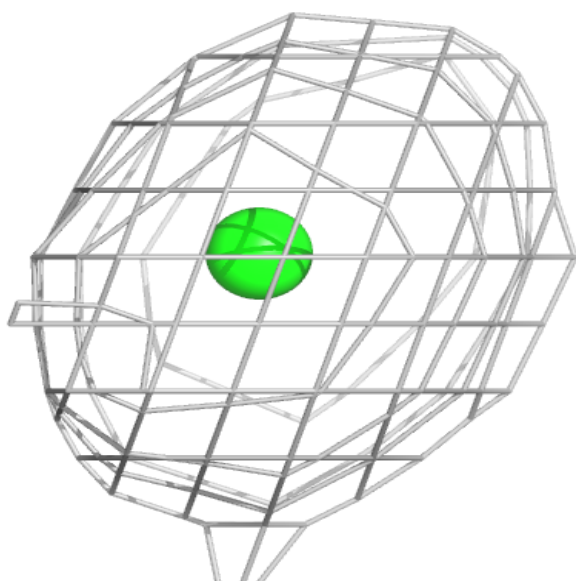
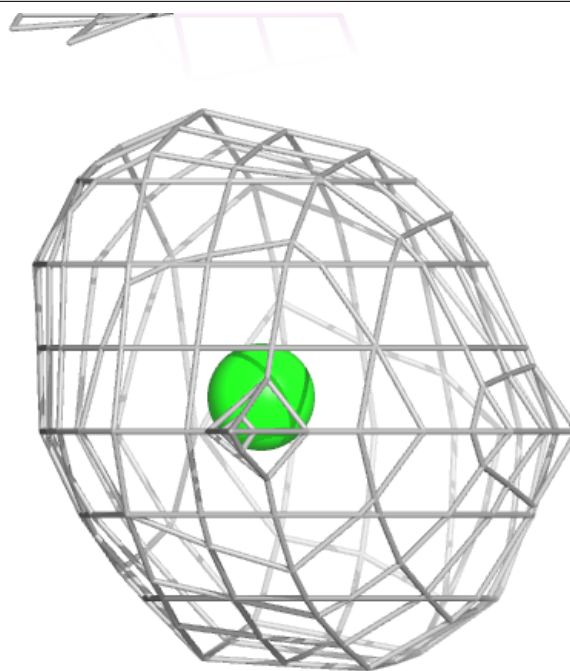
Electron density around PO4 D 301:

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



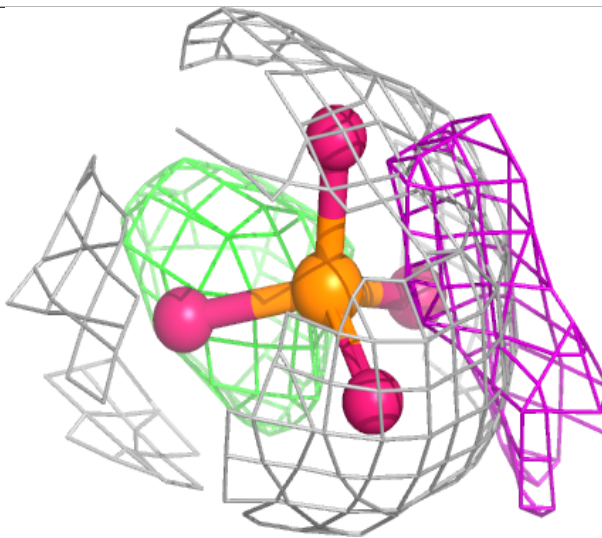
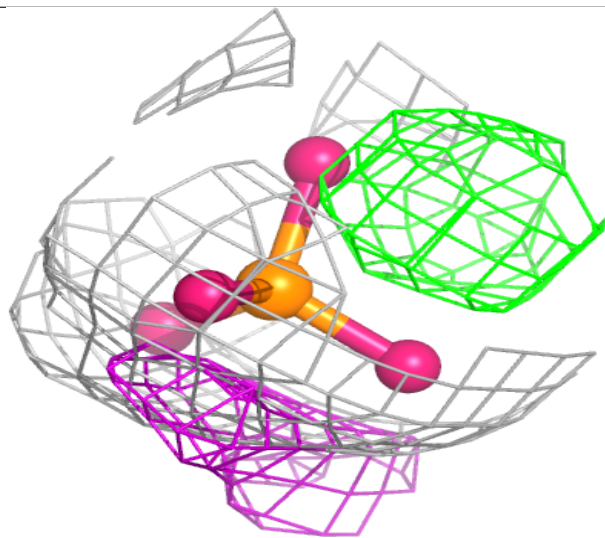
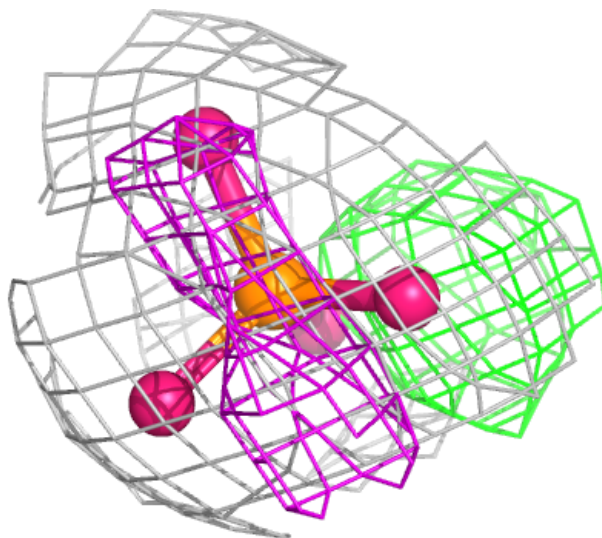
Electron density around CL M 304:

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



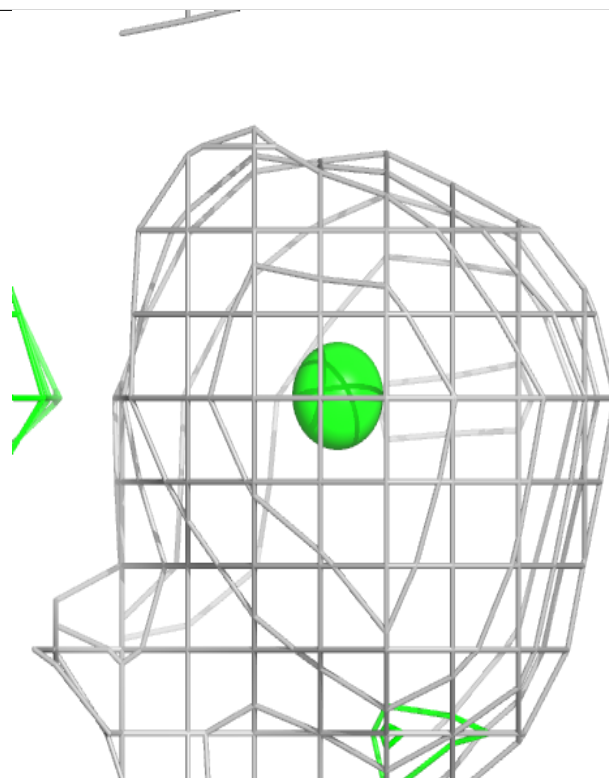
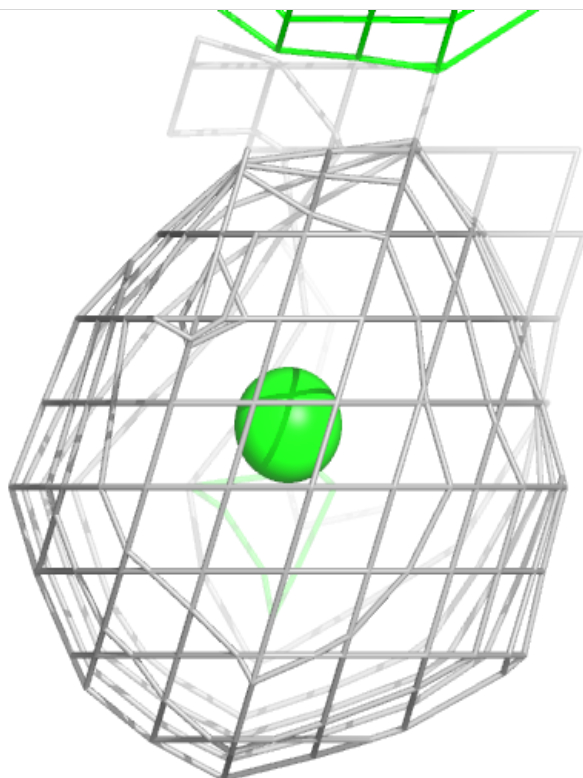
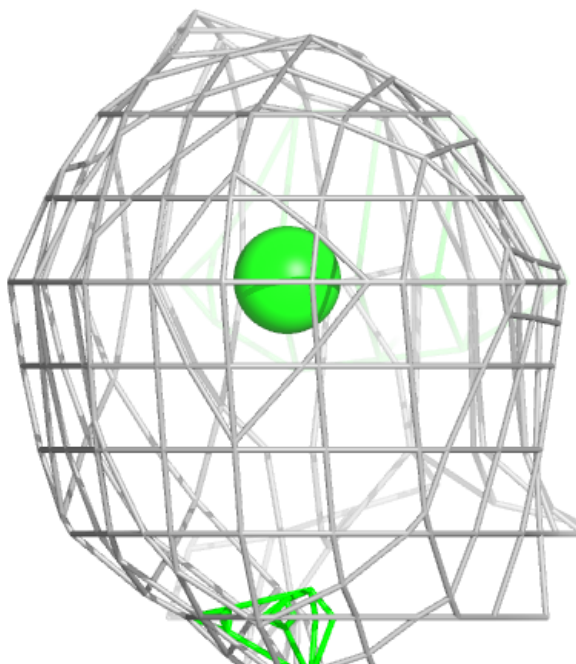
Electron density around PO4 e 202:

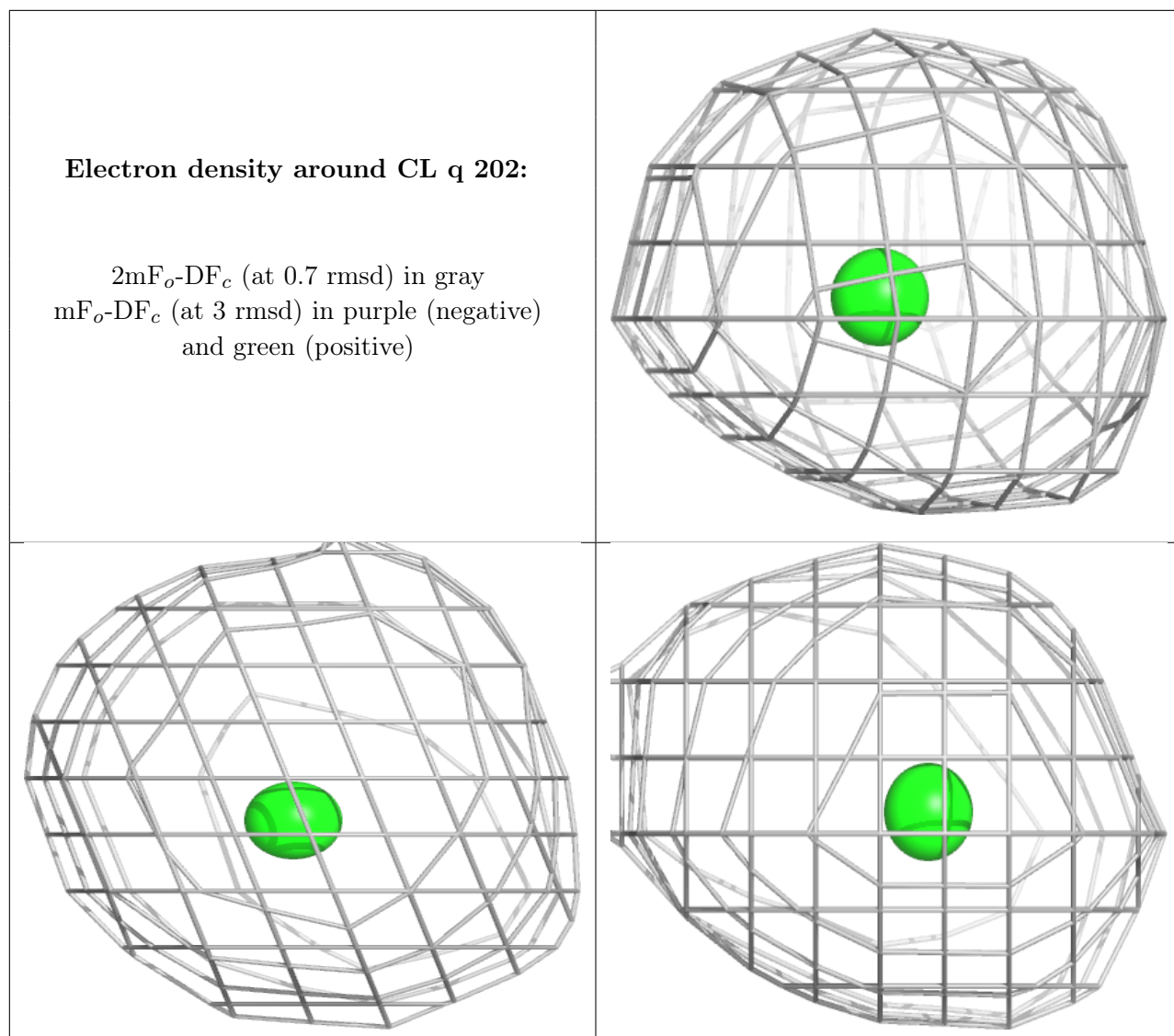
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

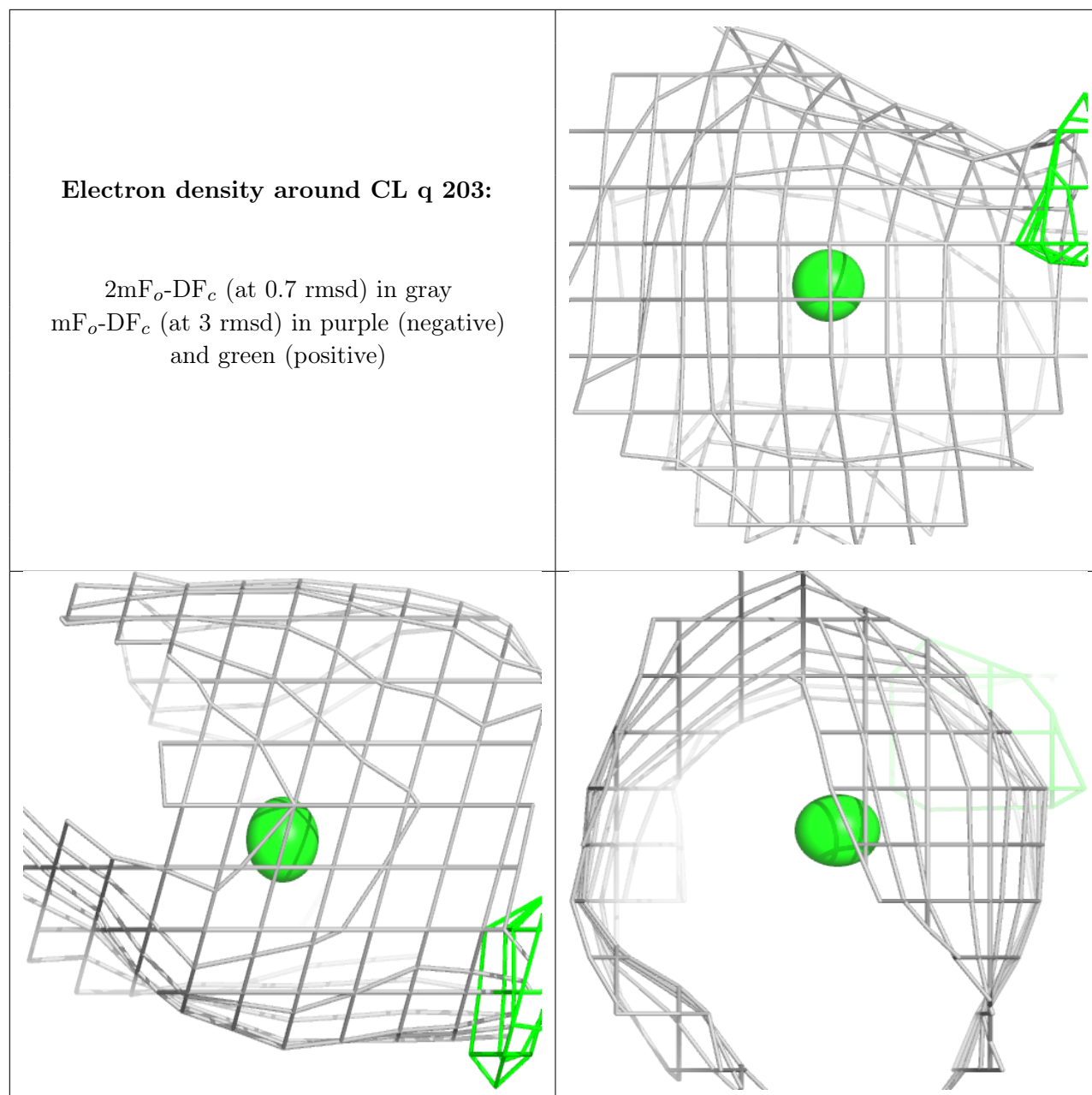


Electron density around CL C 307:

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

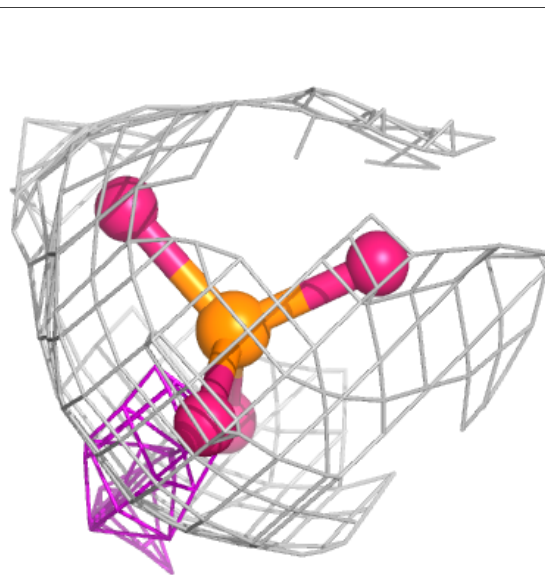
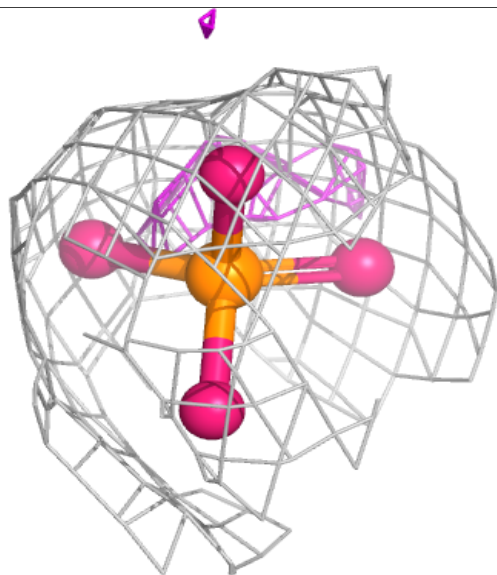
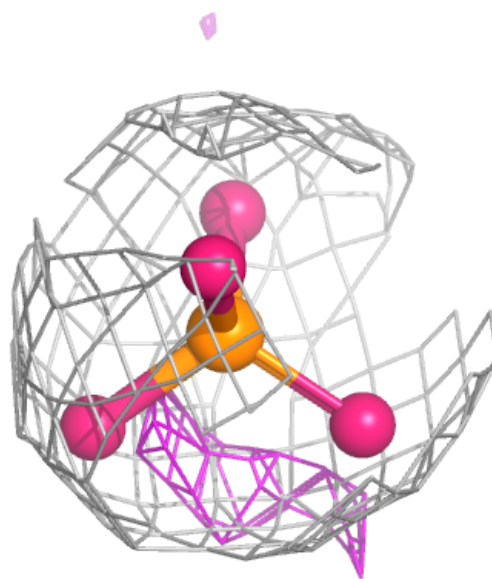






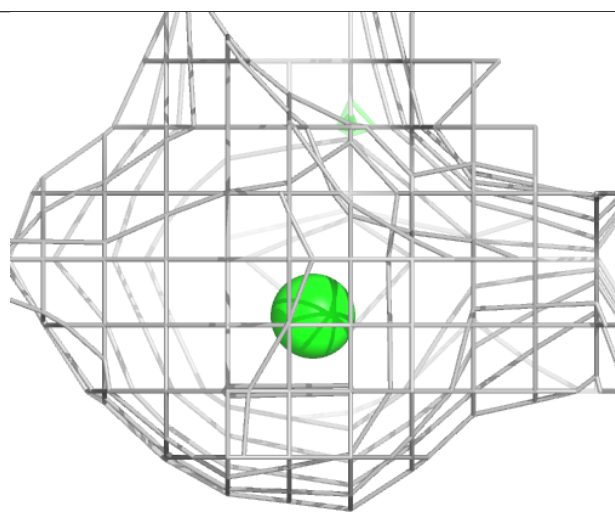
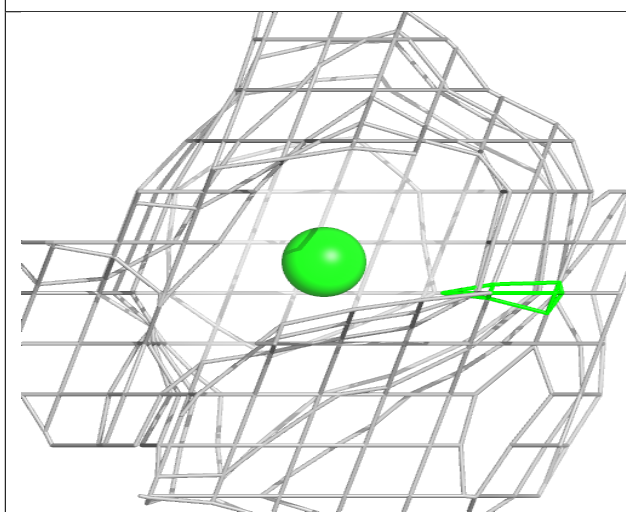
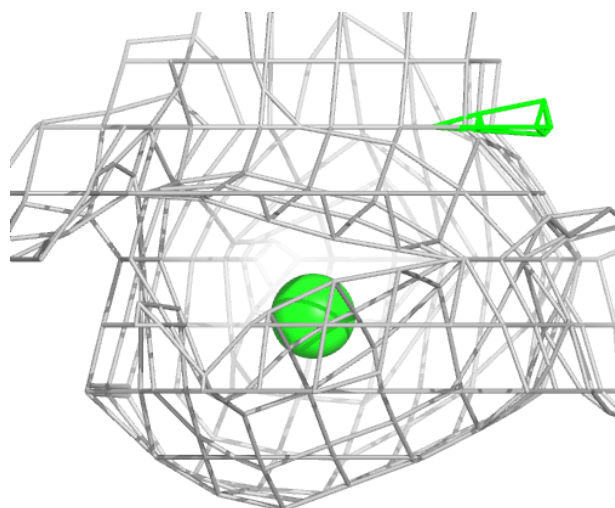
Electron density around PO4 a 202:

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



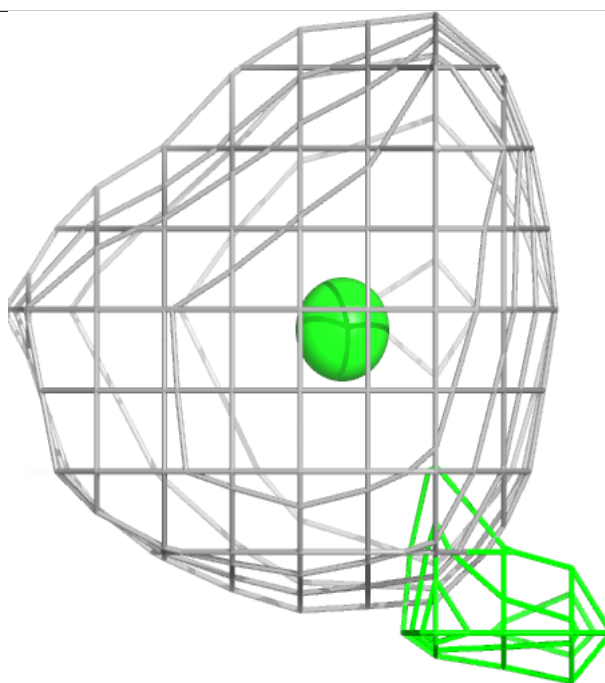
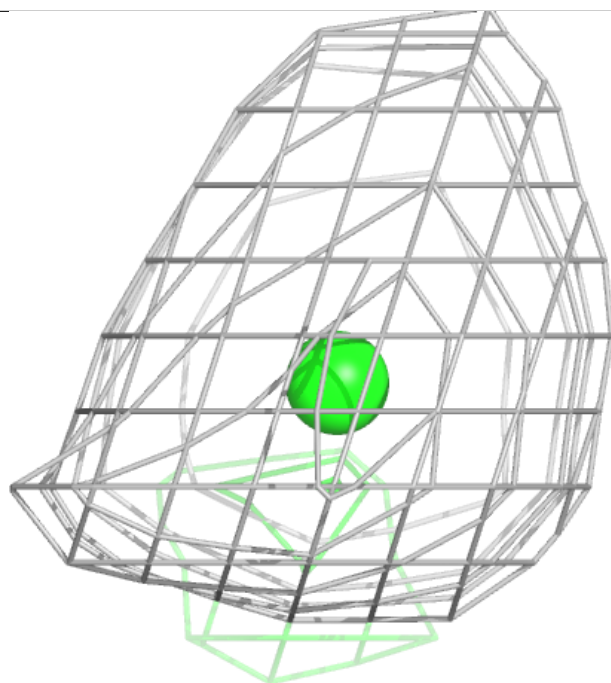
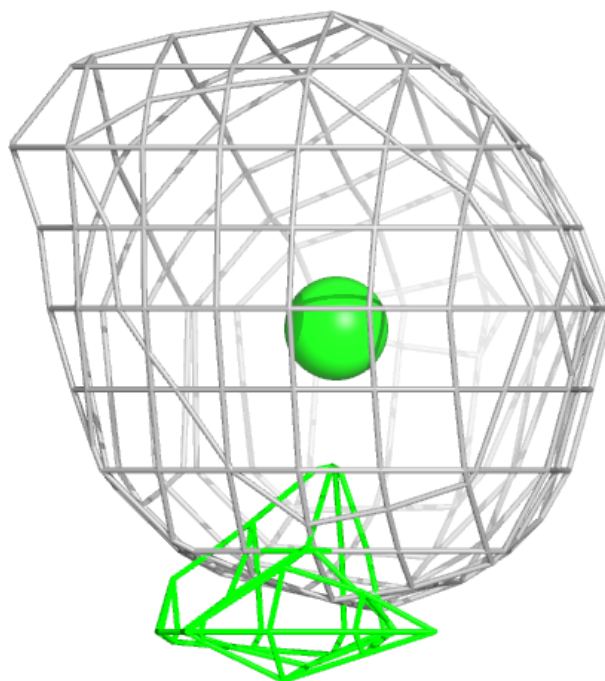
Electron density around CL C 306:

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



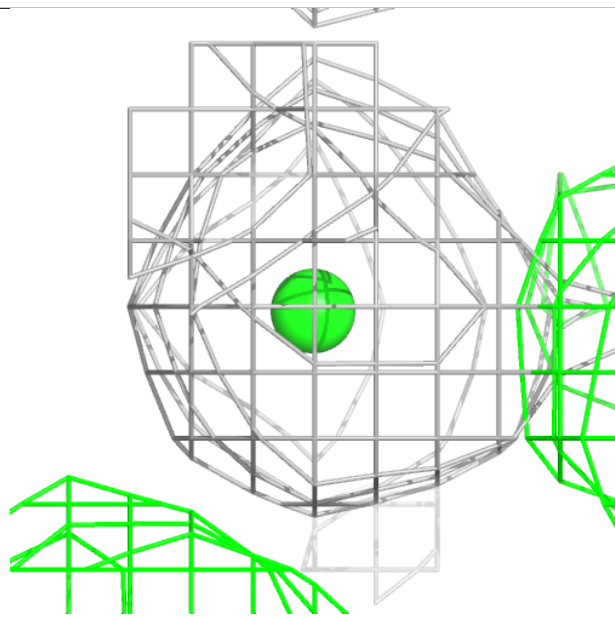
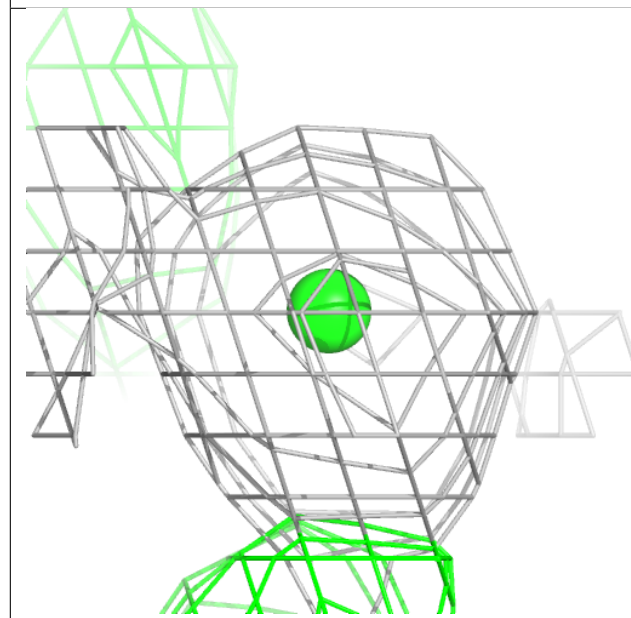
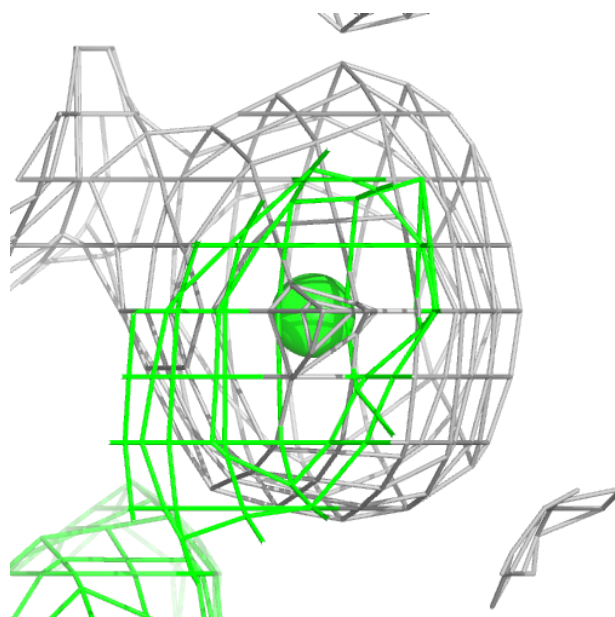
Electron density around CL P 301:

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



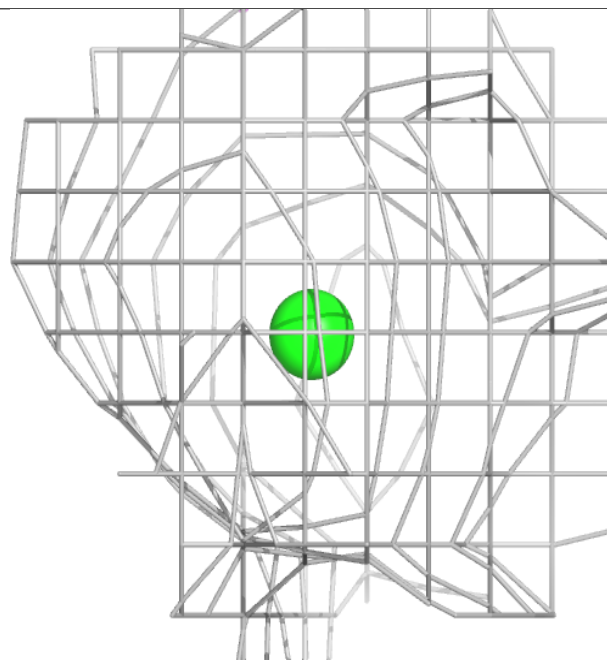
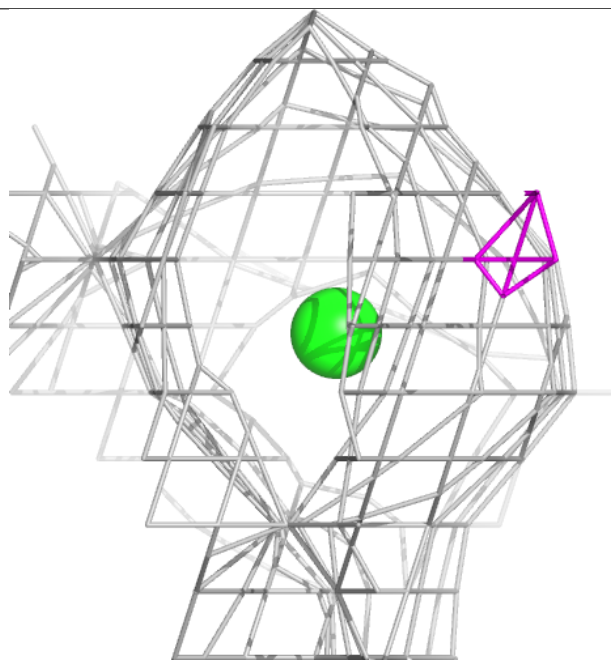
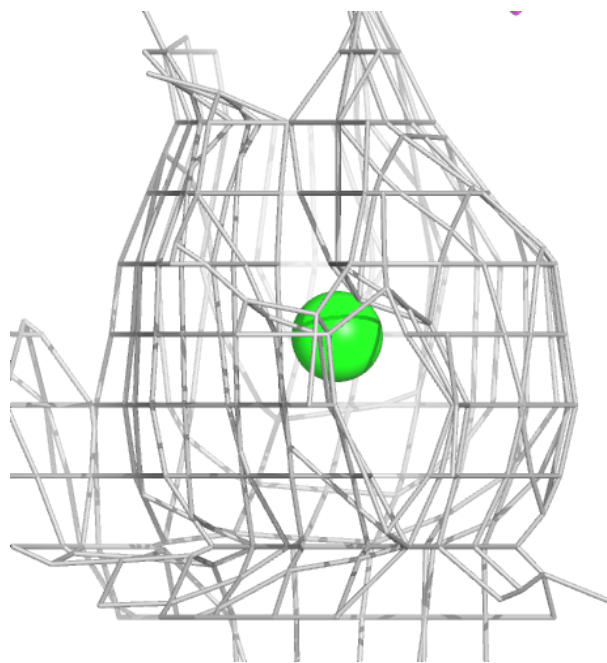
Electron density around CL H 302:

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



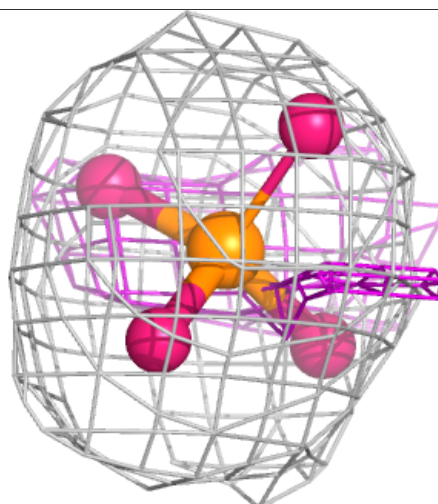
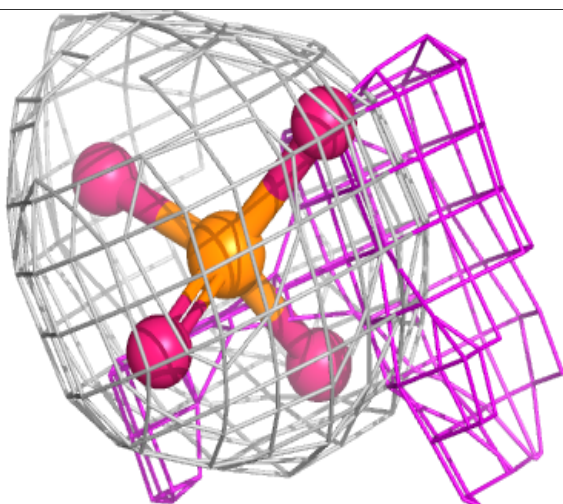
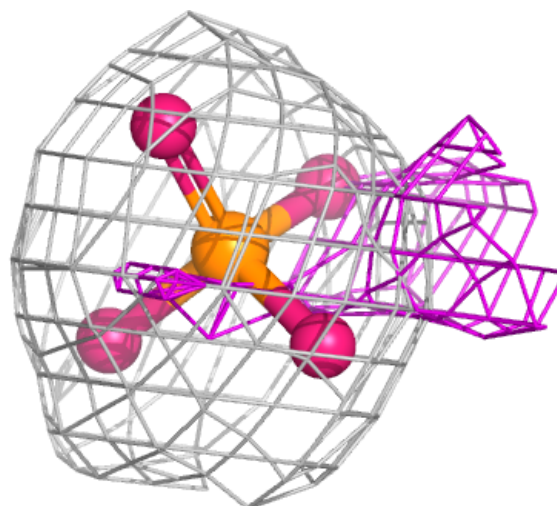
Electron density around CL E 306:

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



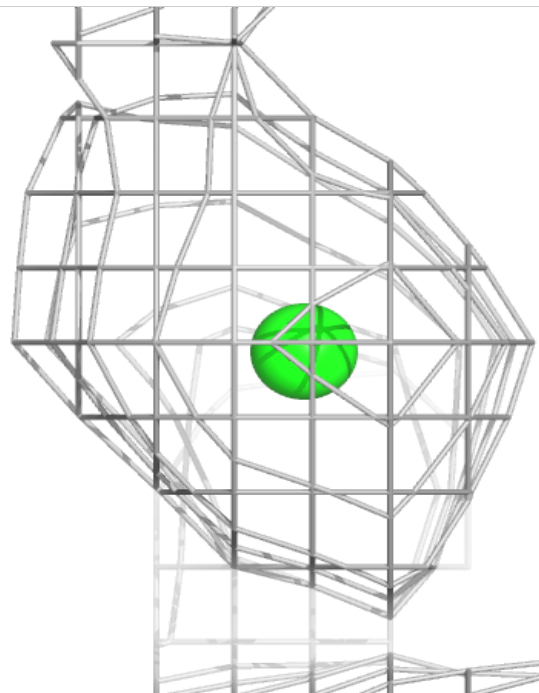
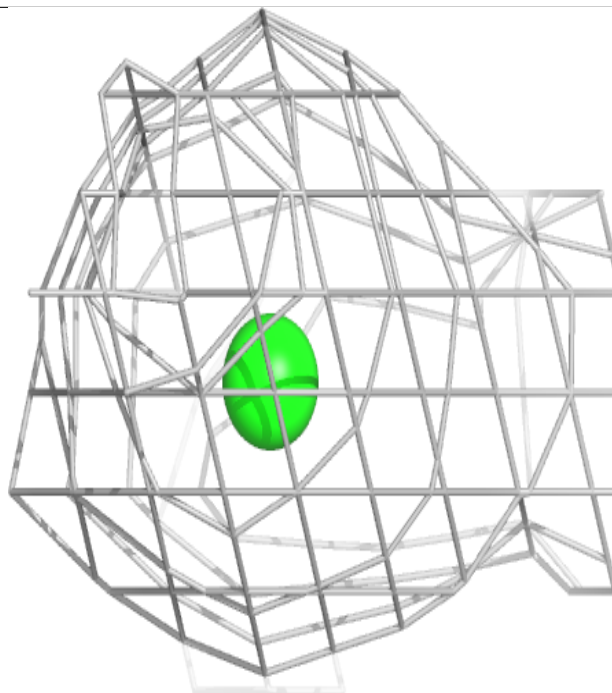
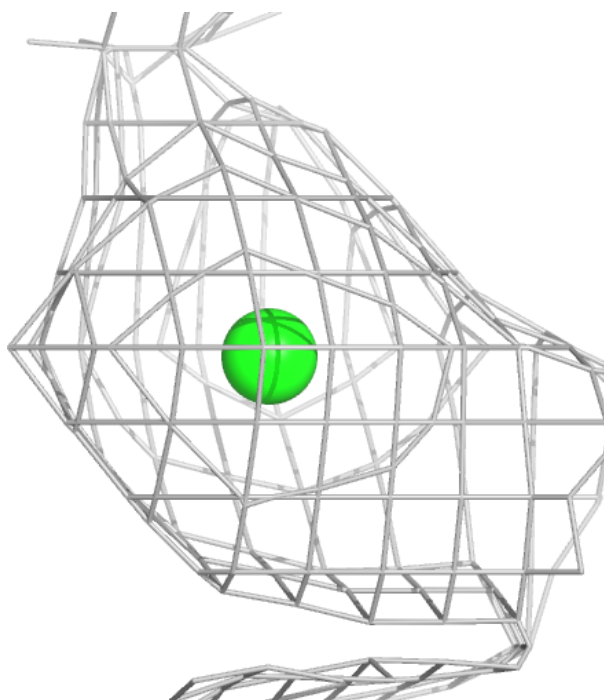
Electron density around PO4 C 301:

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



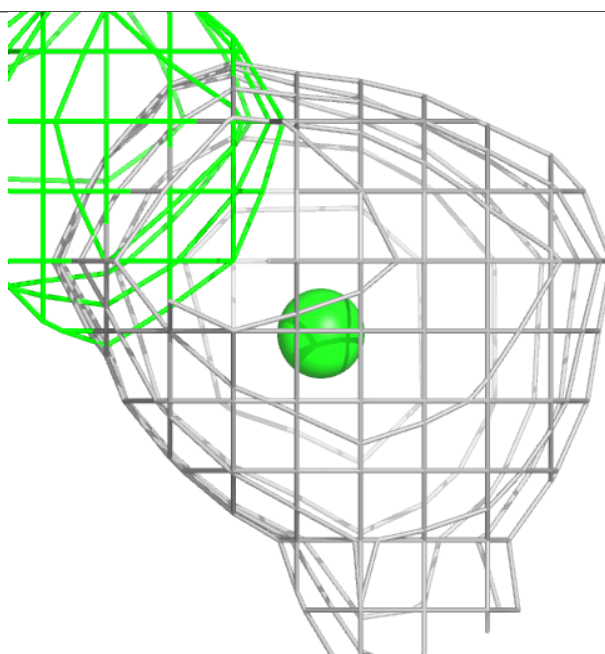
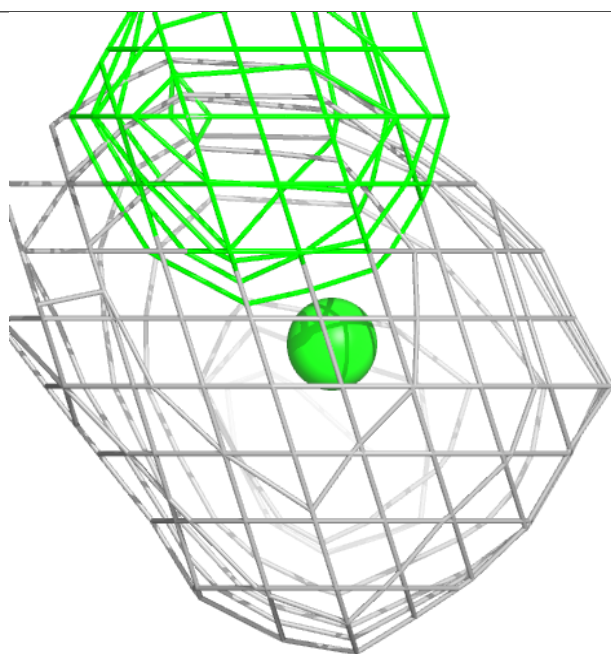
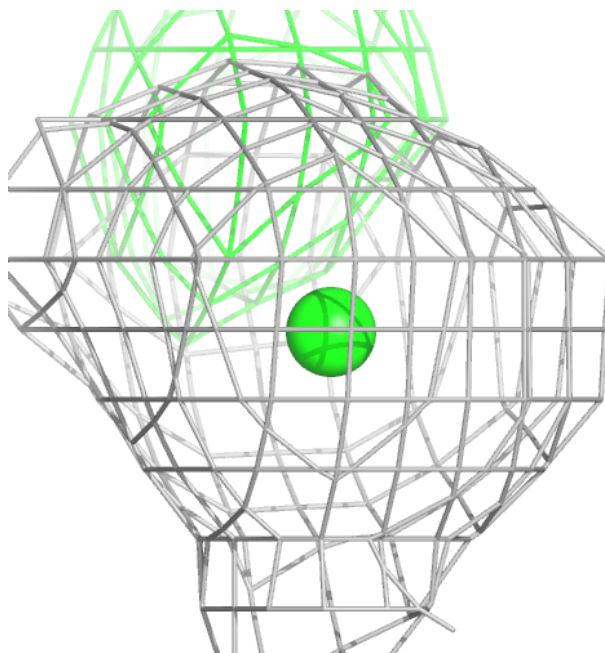
Electron density around CL R 303:

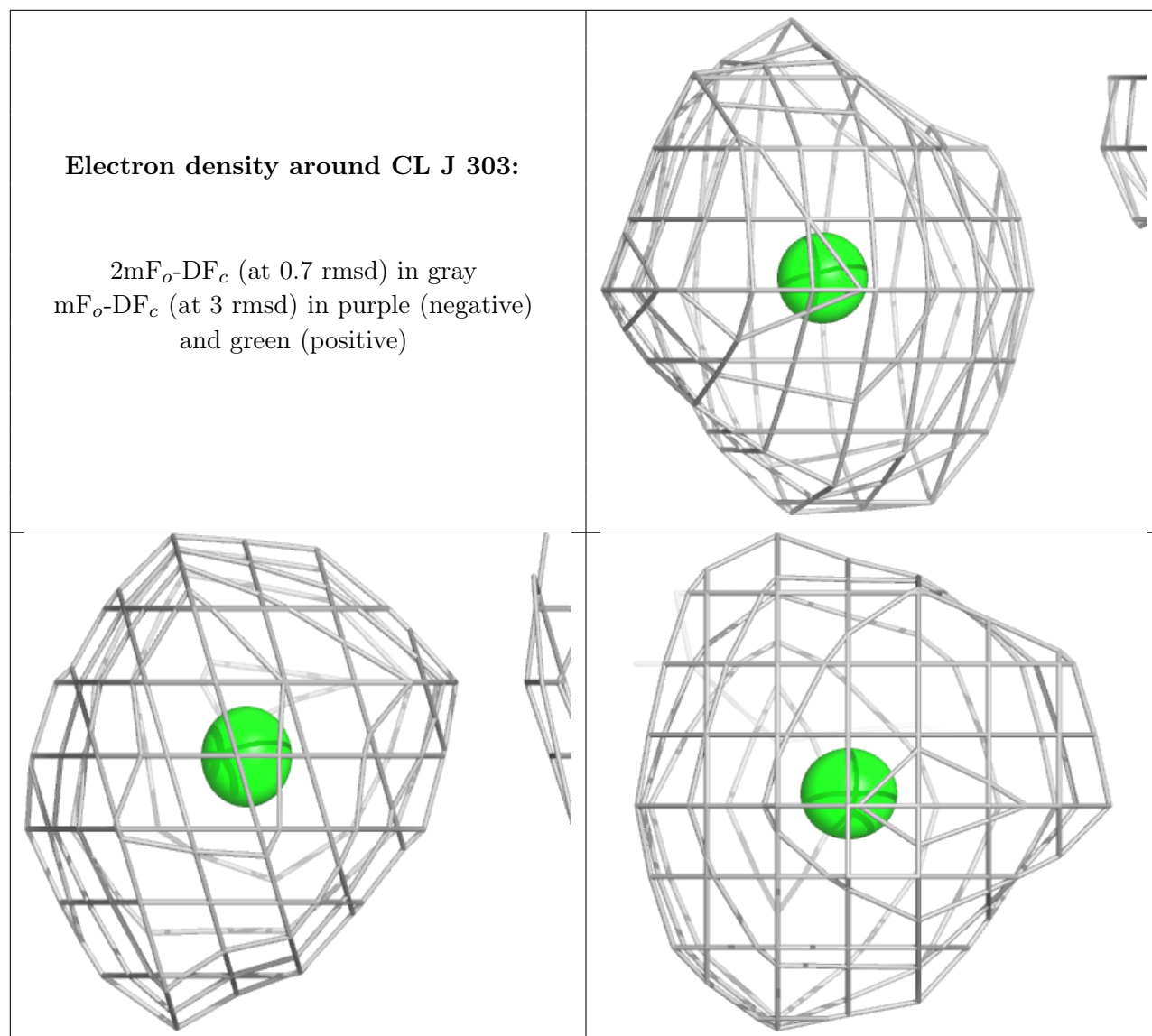
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL g 203:

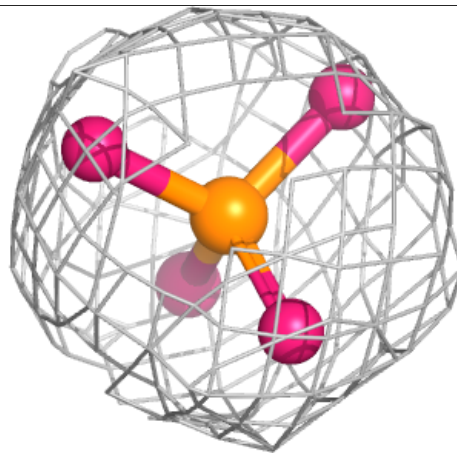
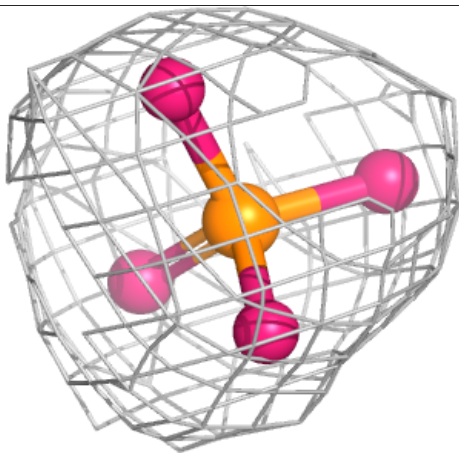
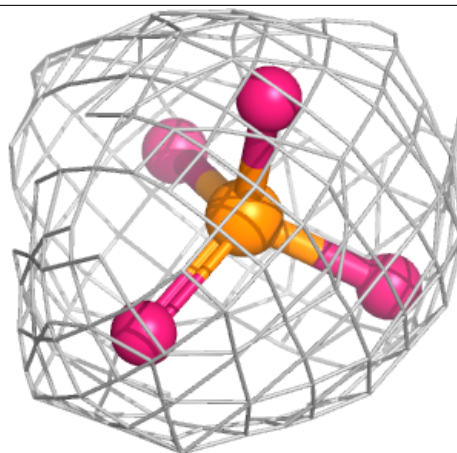
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





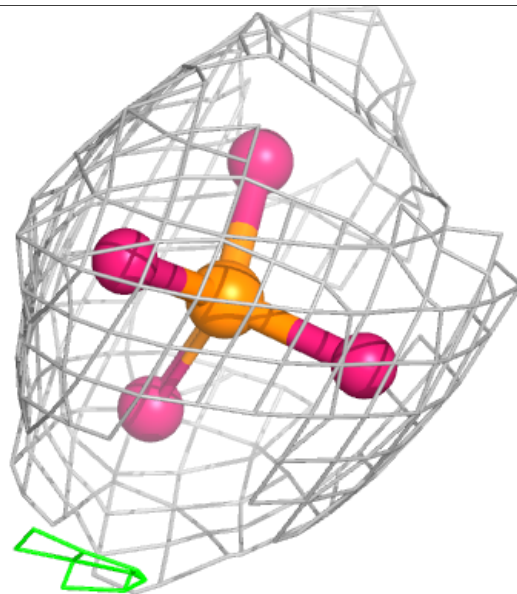
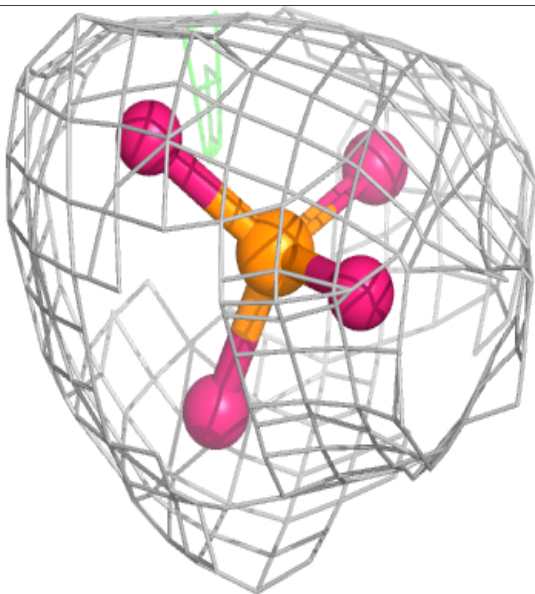
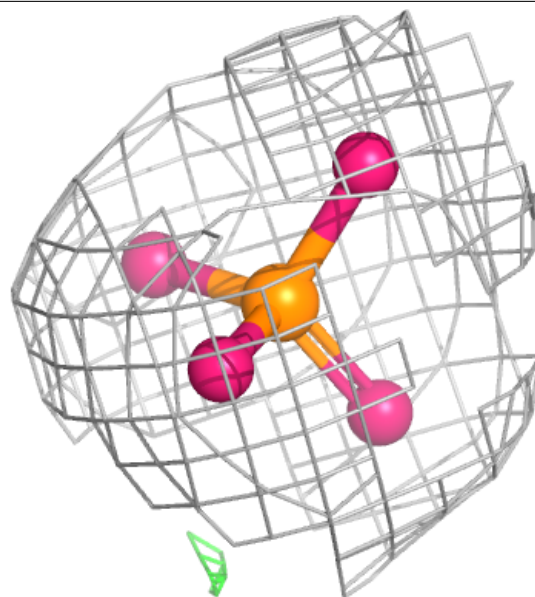
Electron density around PO4 L 301:

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



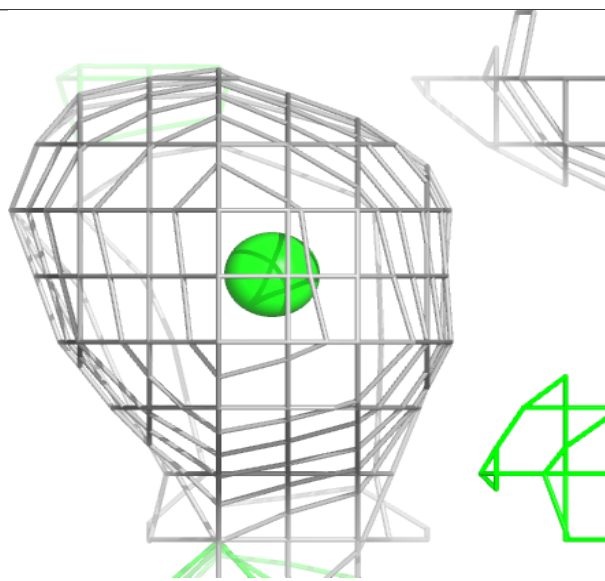
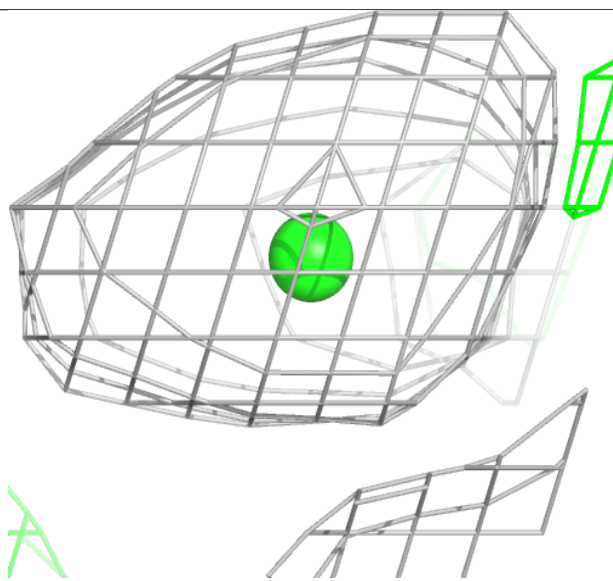
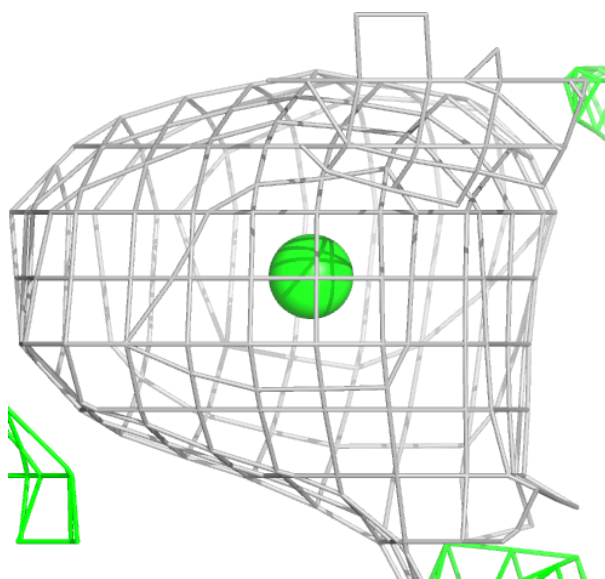
Electron density around PO4 I 303:

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



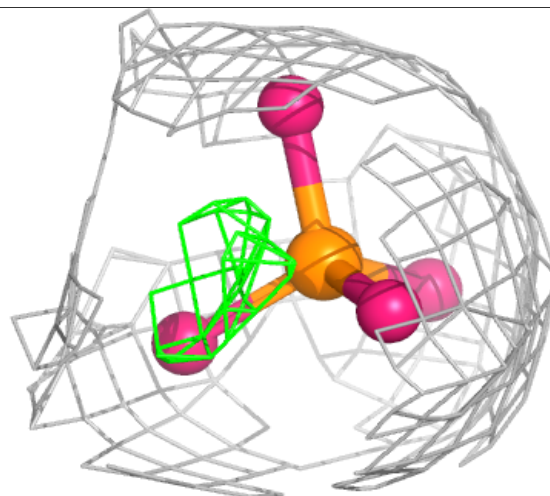
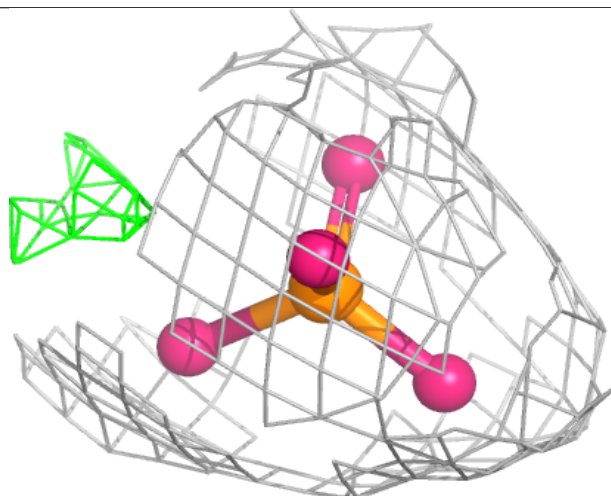
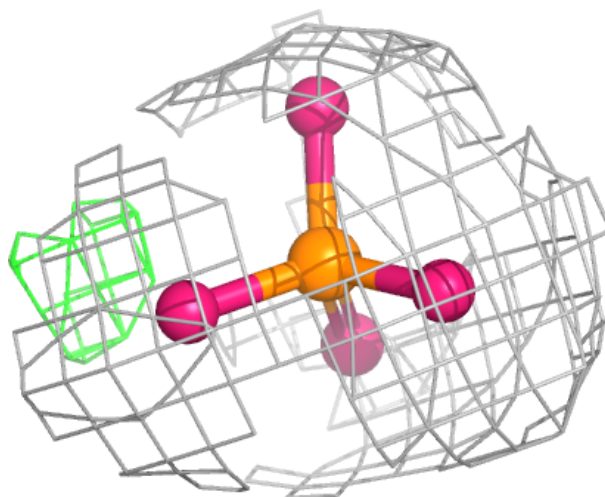
Electron density around CL N 302:

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



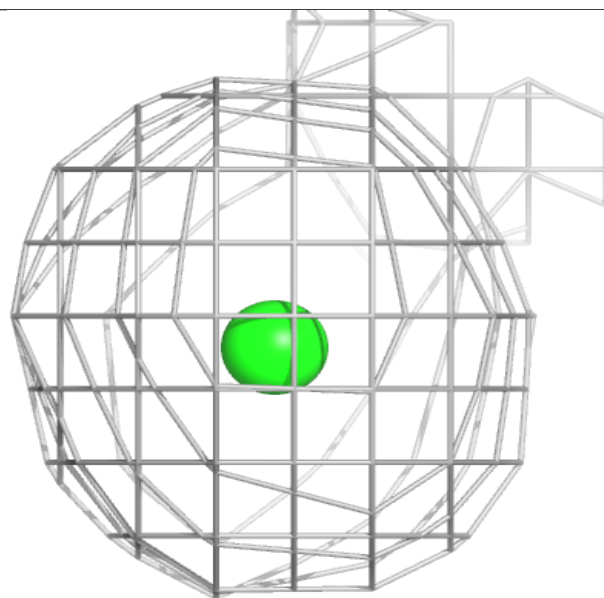
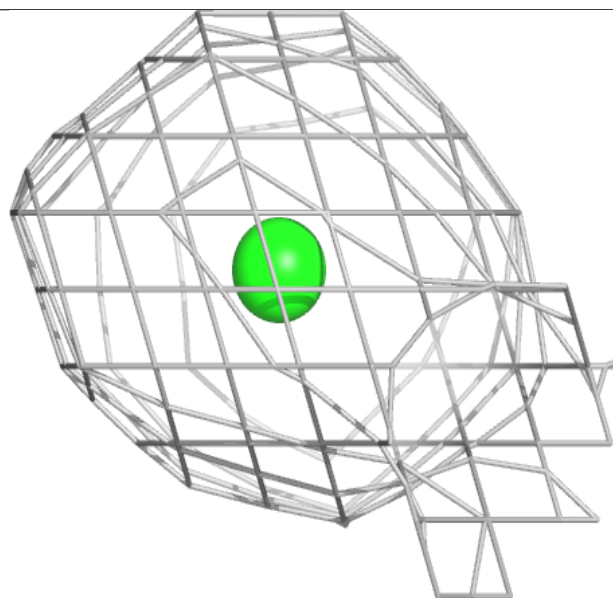
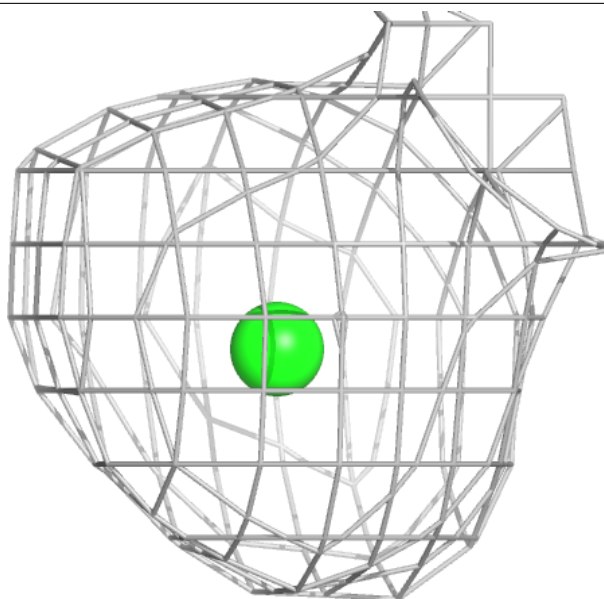
Electron density around PO4 q 201:

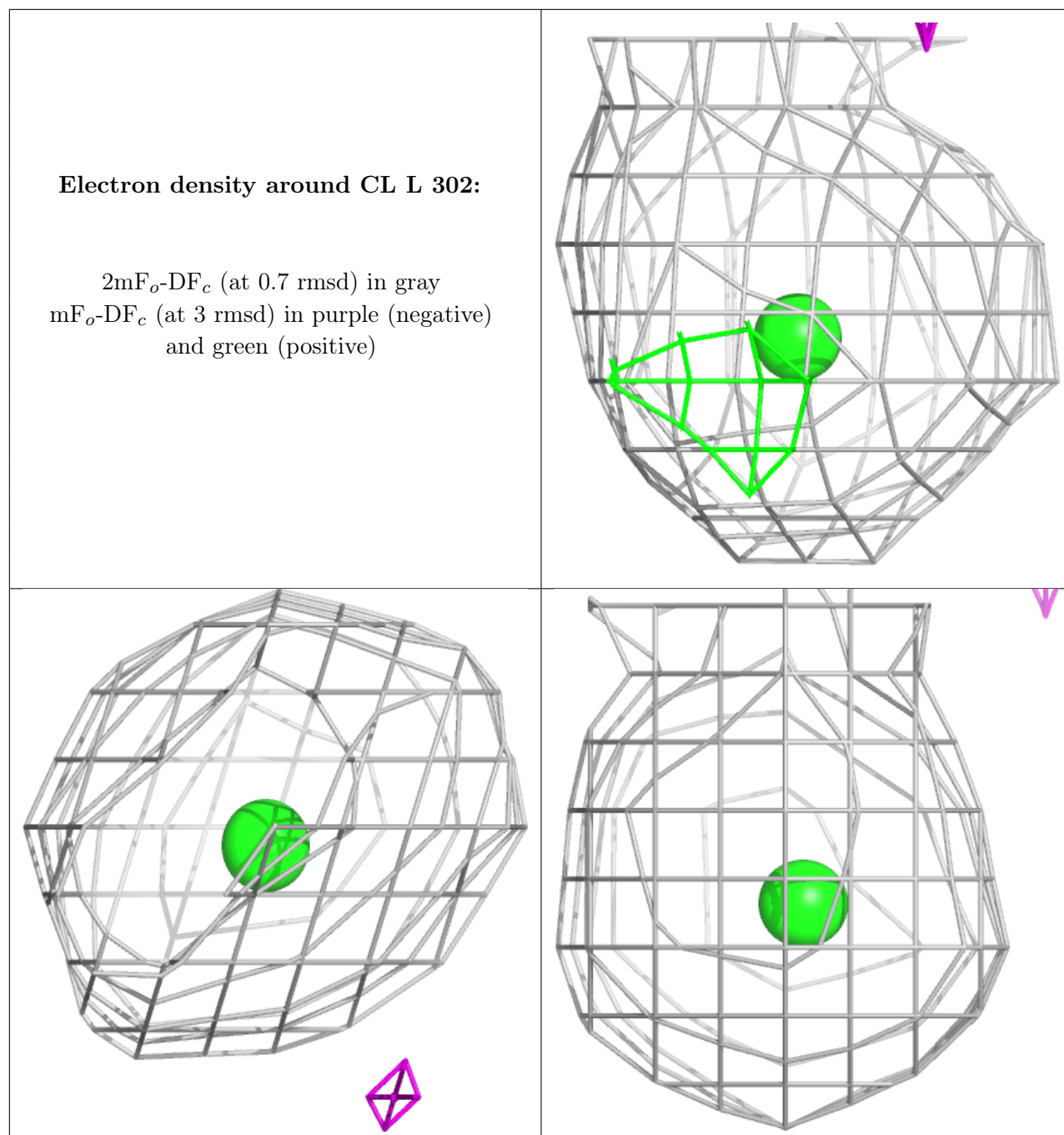
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL e 204:

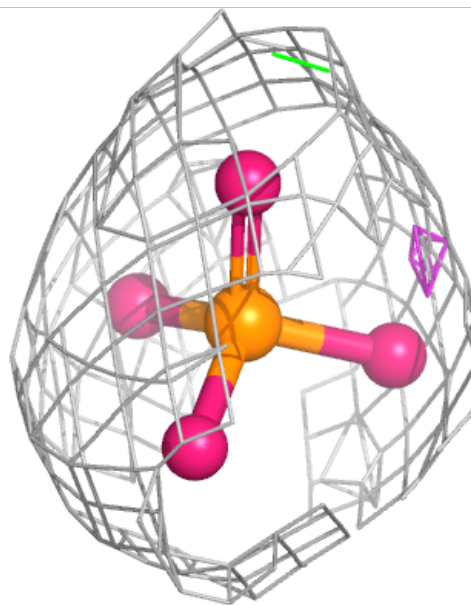
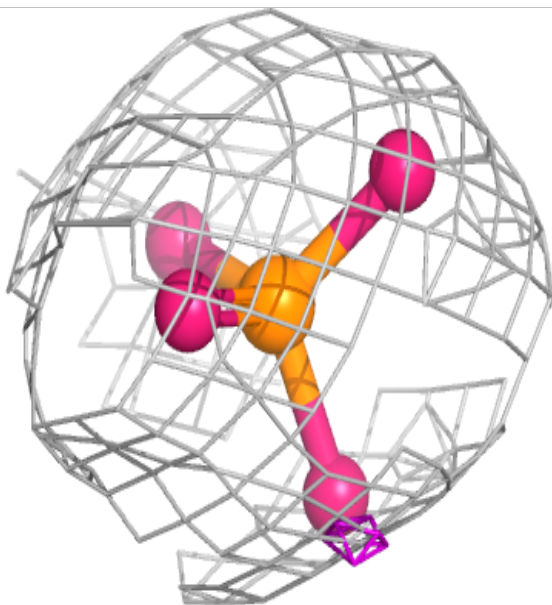
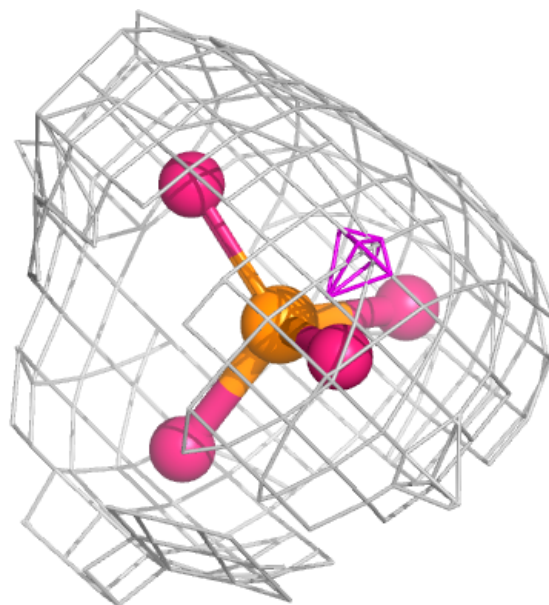
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





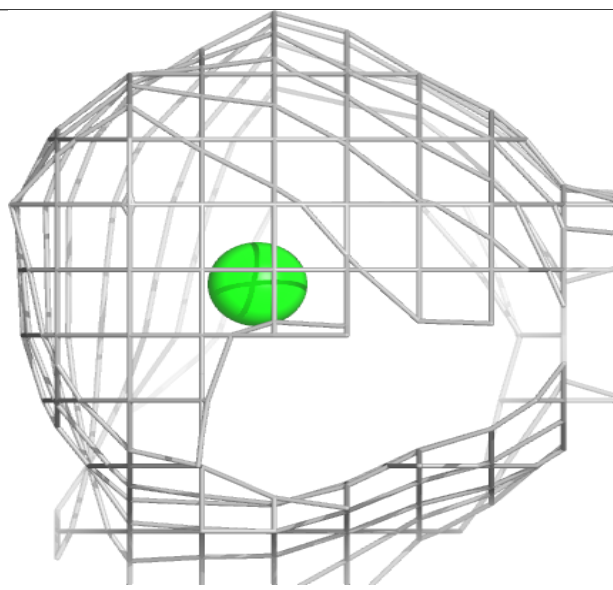
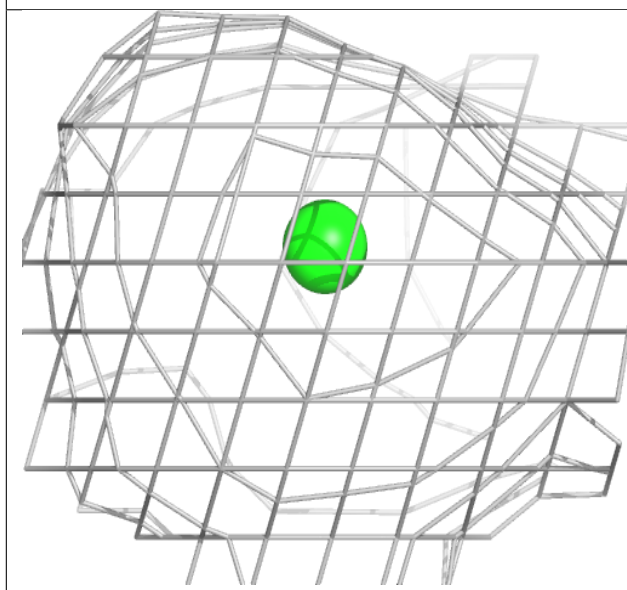
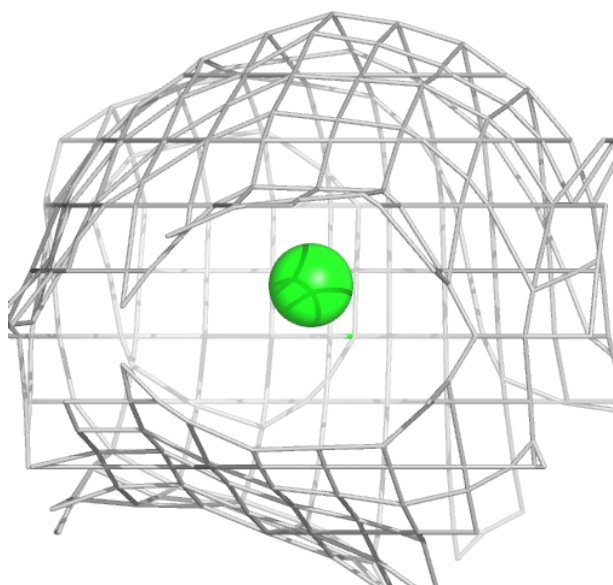
Electron density around PO4 g 202:

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



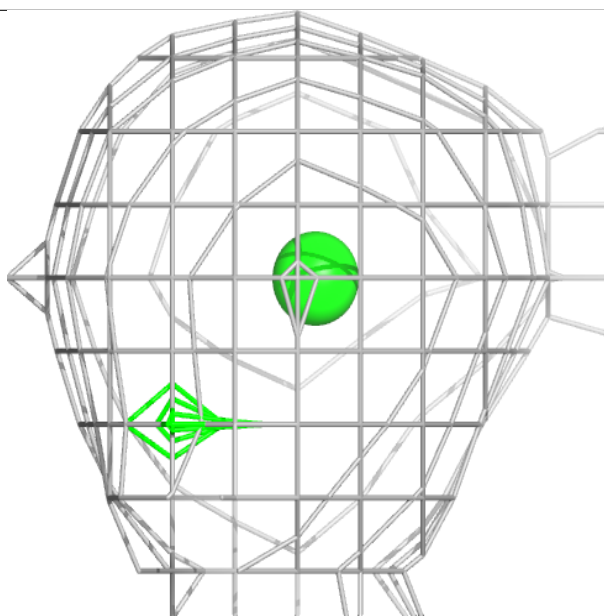
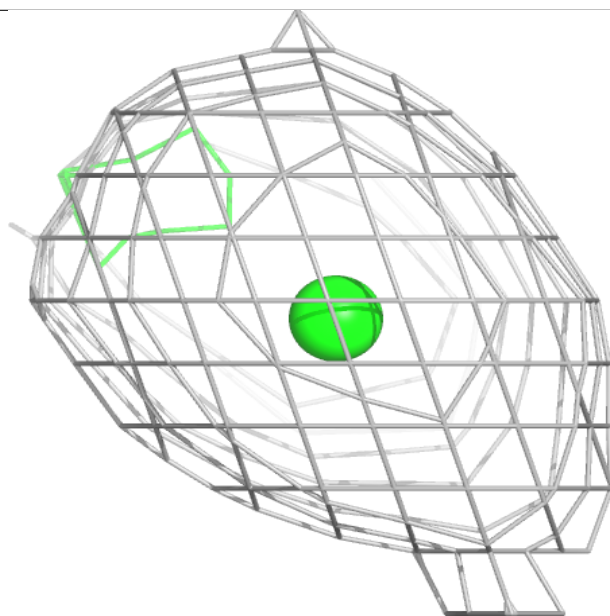
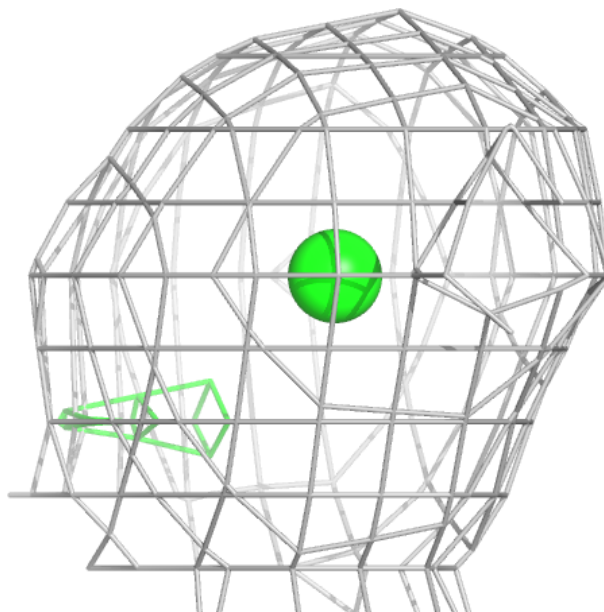
Electron density around CL B 302:

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



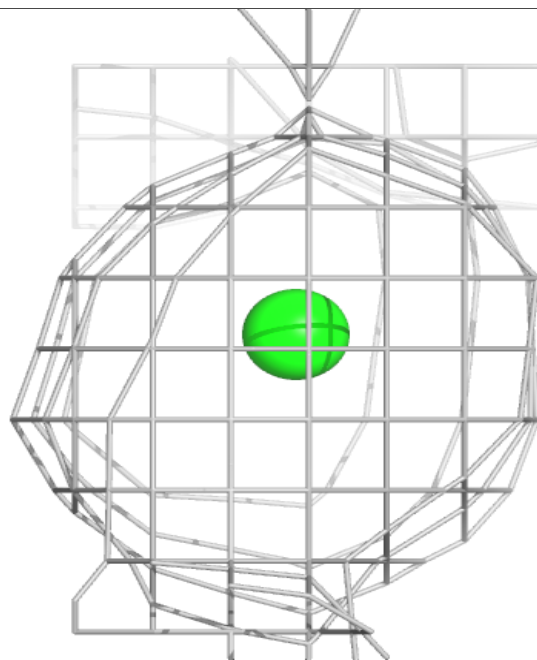
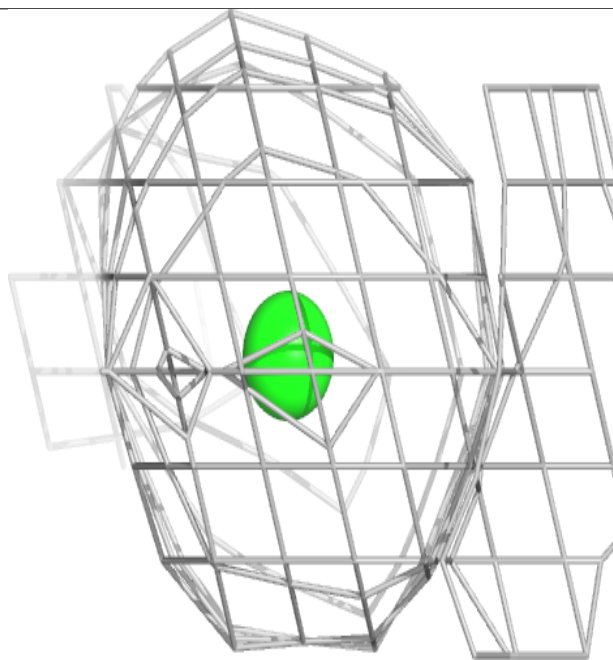
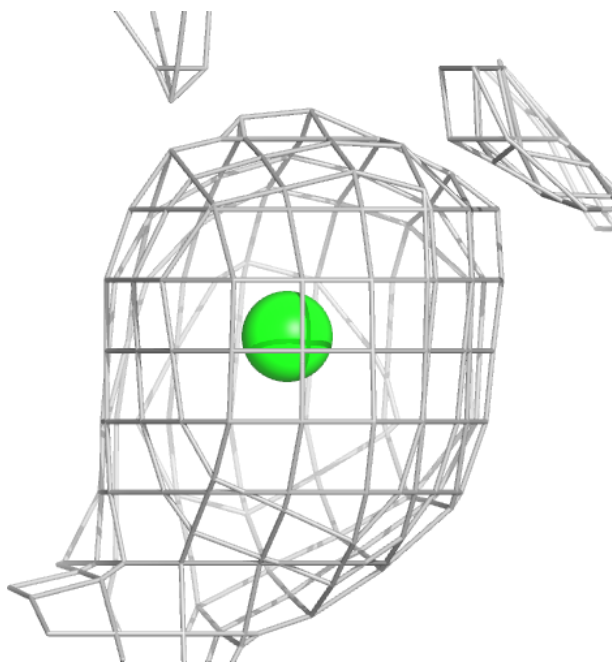
Electron density around CL D 303:

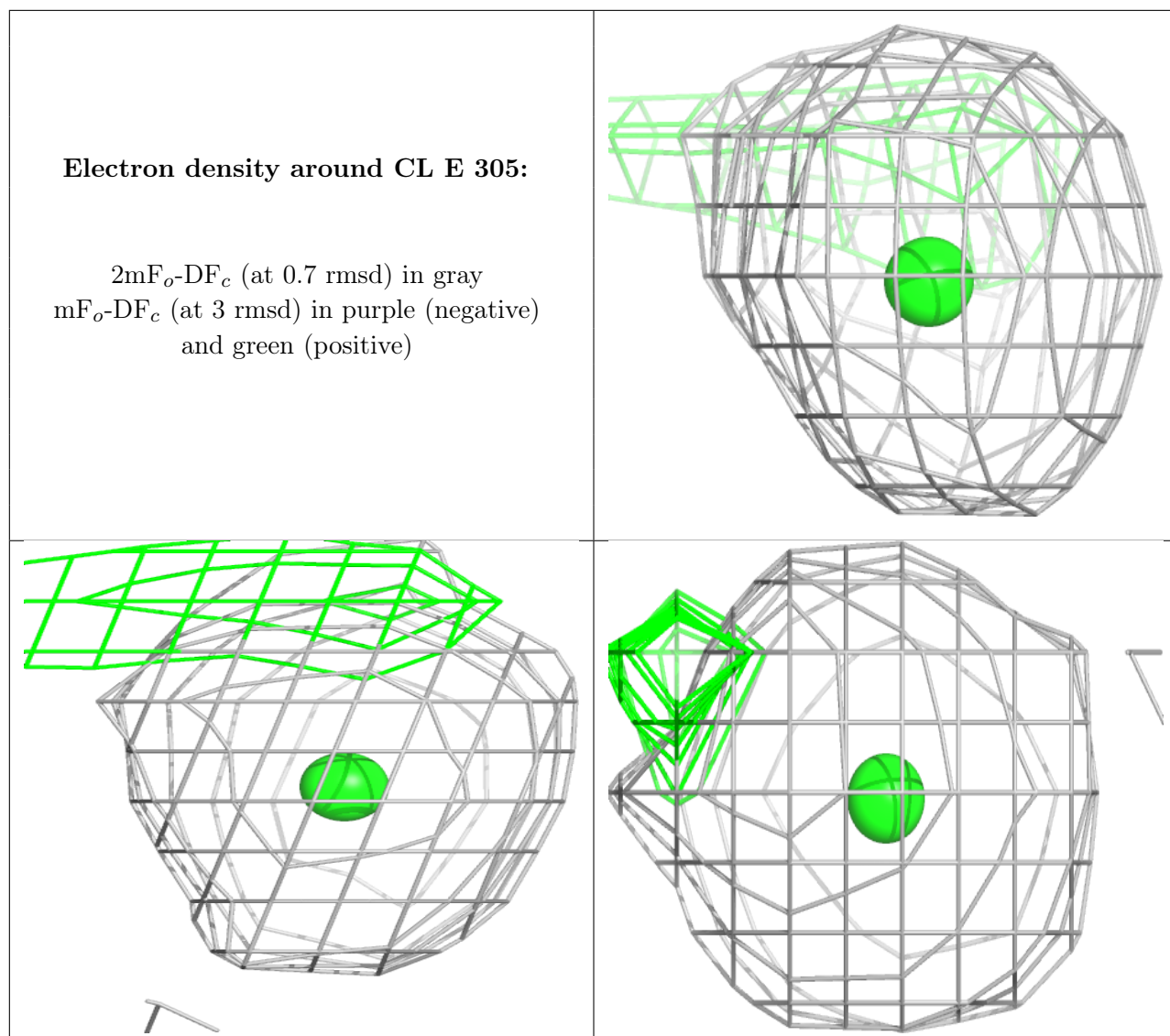
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL D 304:

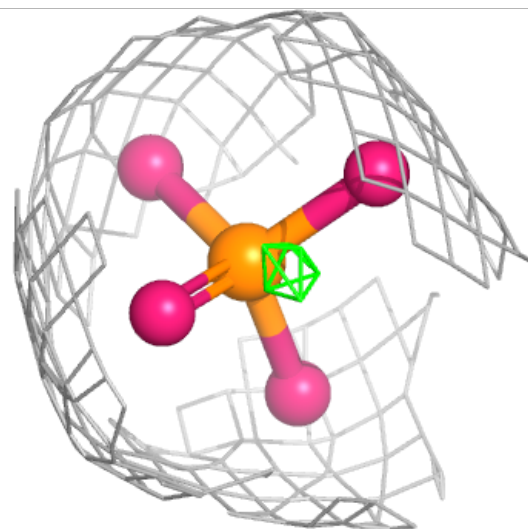
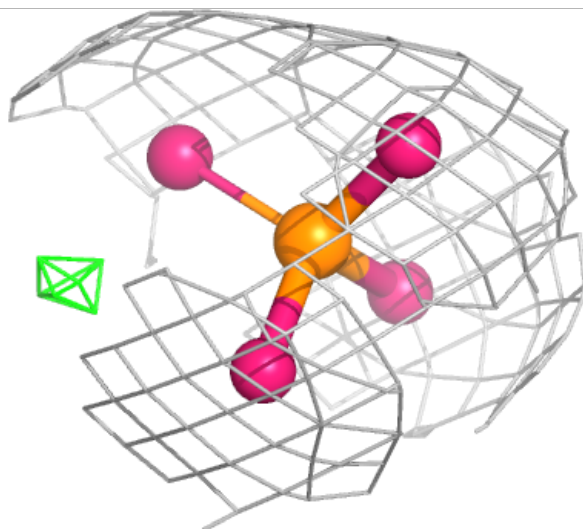
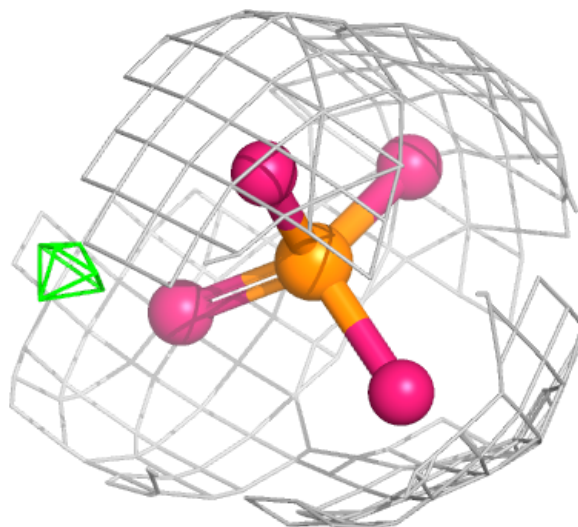
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





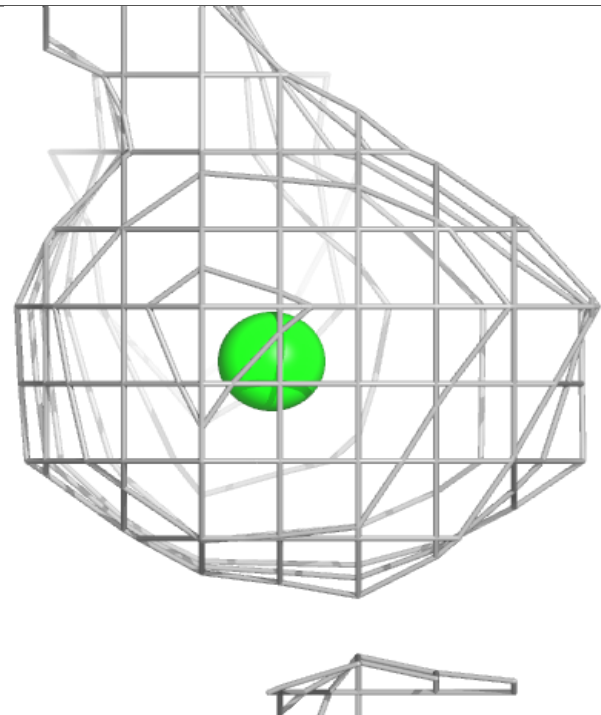
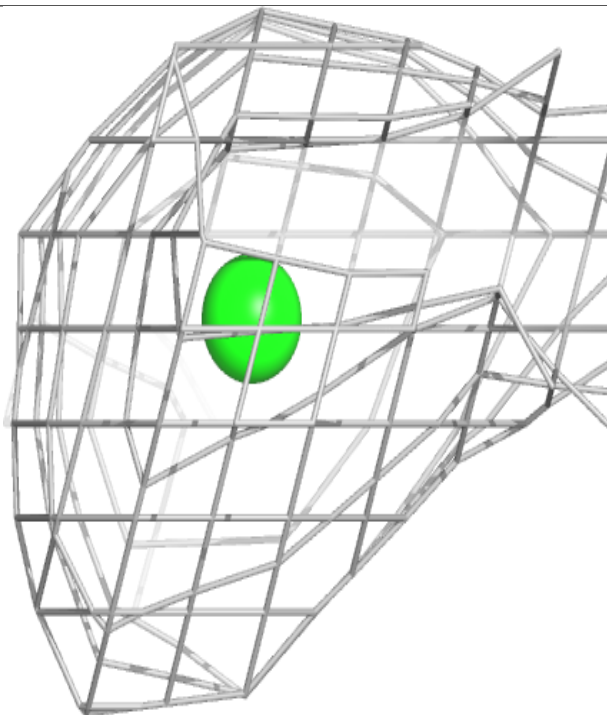
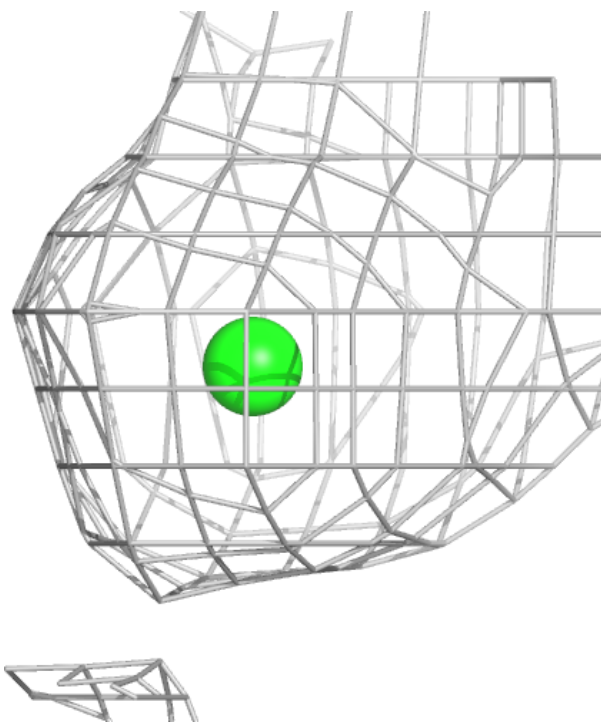
Electron density around PO4 c 201:

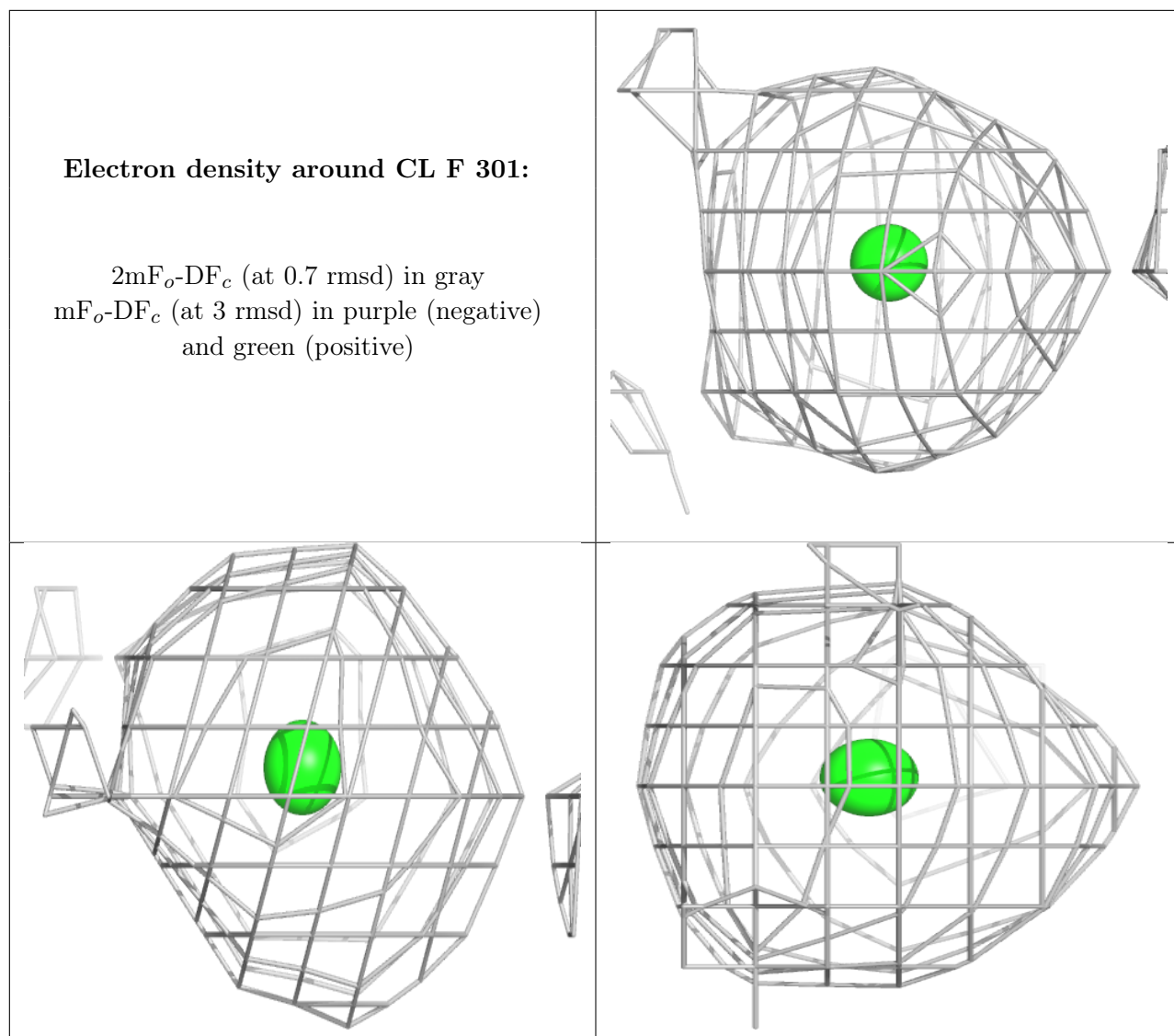
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL B 303:

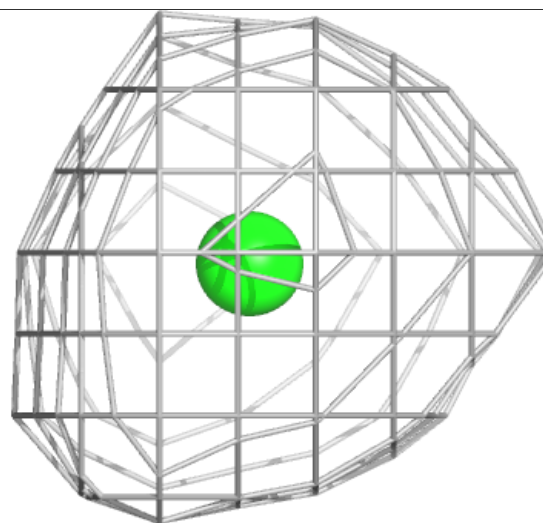
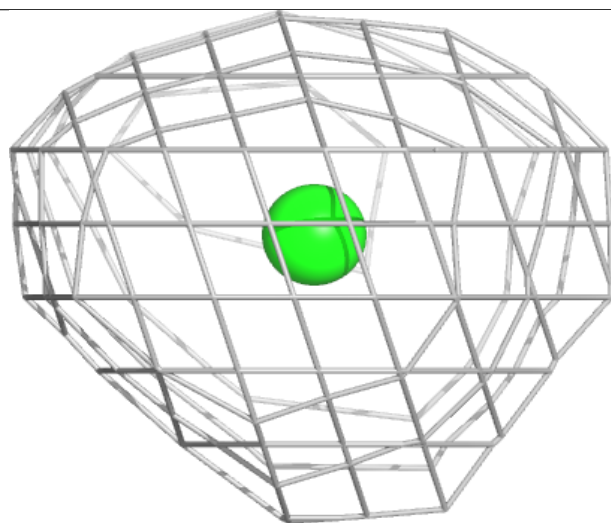
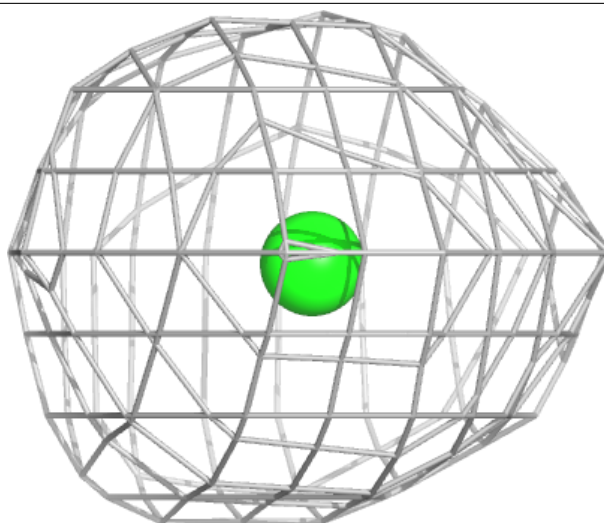
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





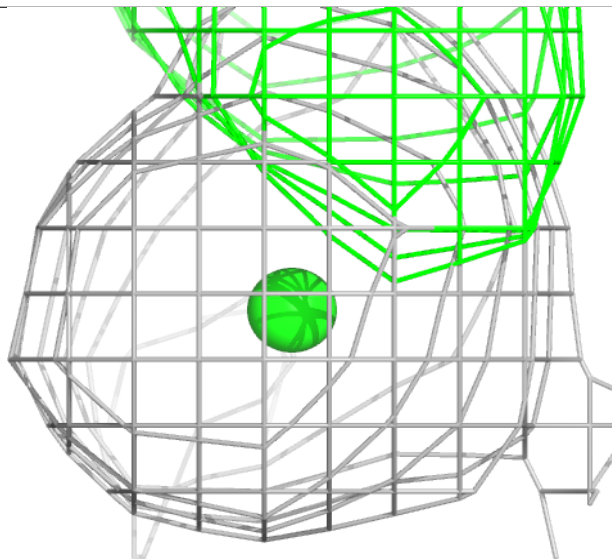
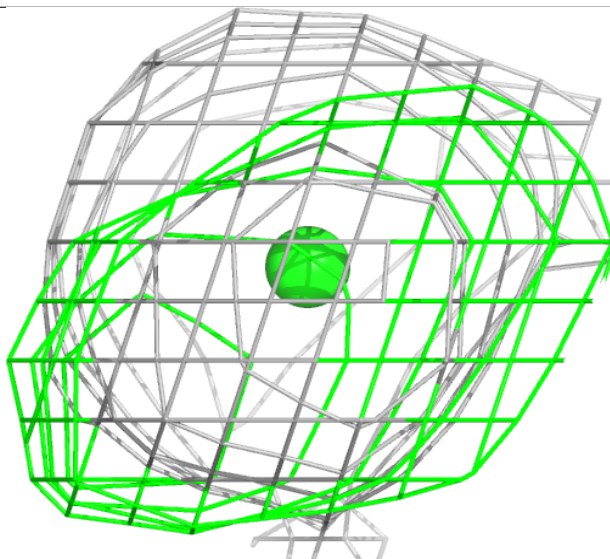
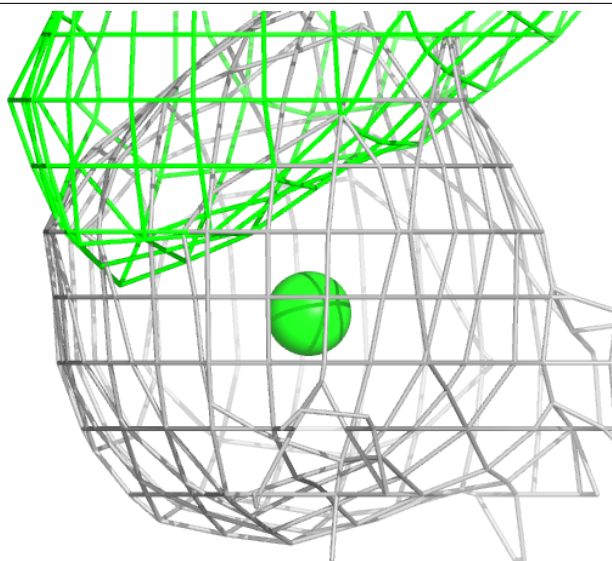
Electron density around CL R 304:

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



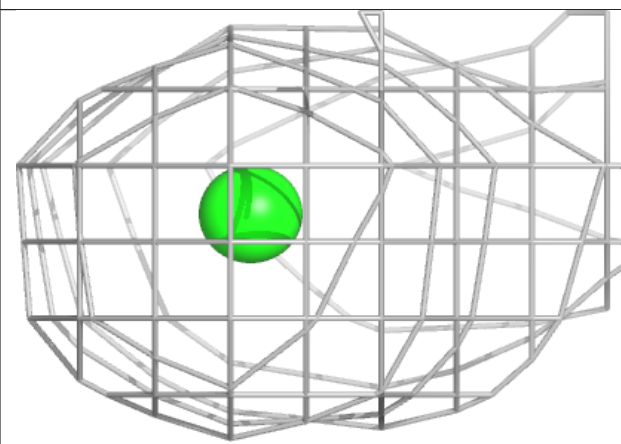
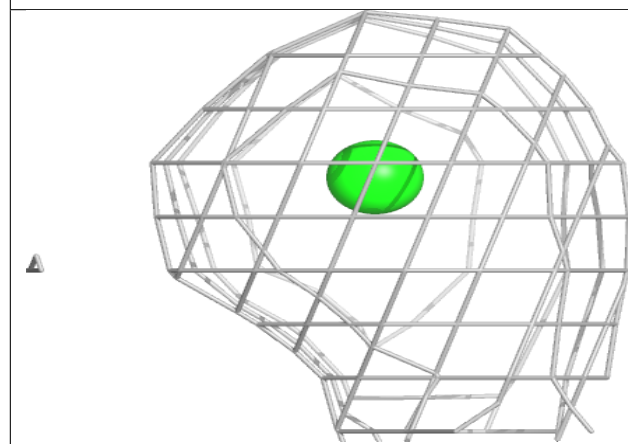
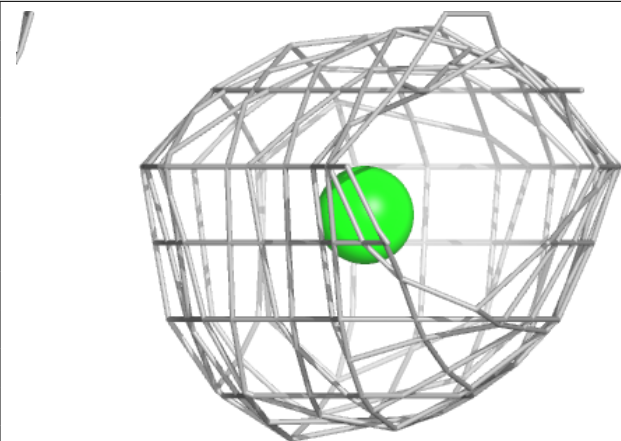
Electron density around CL N 301:

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



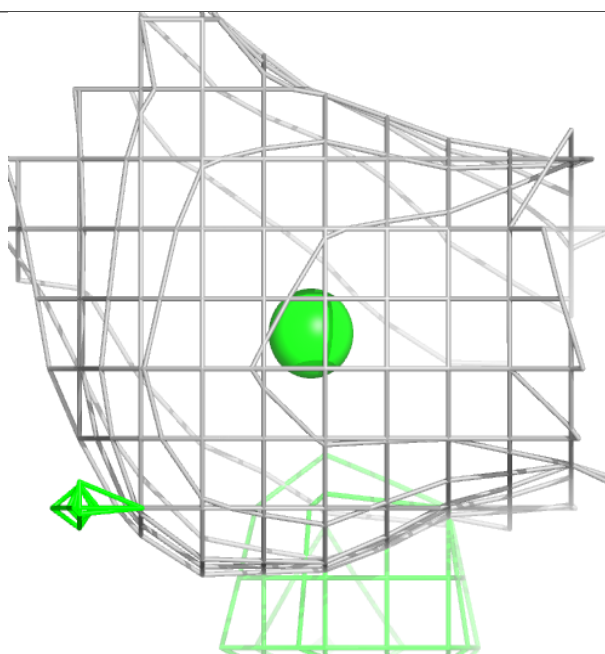
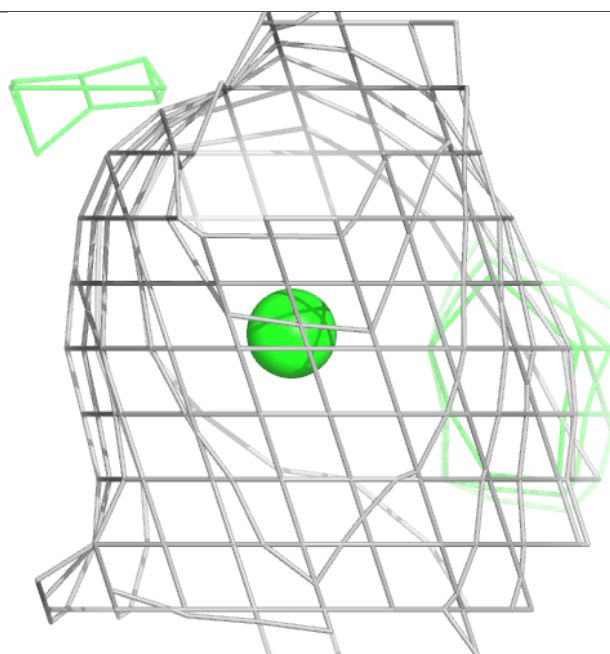
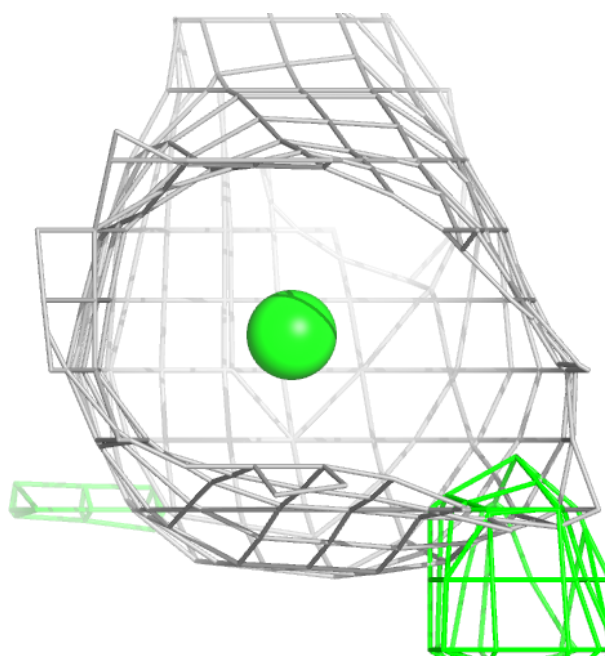
Electron density around CL K 303:

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



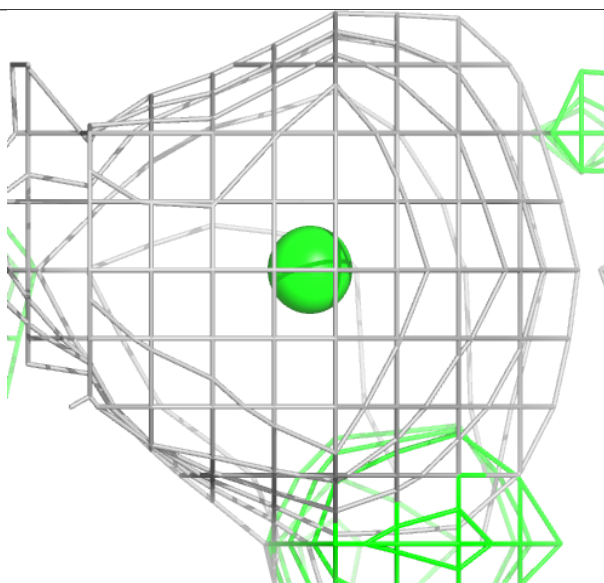
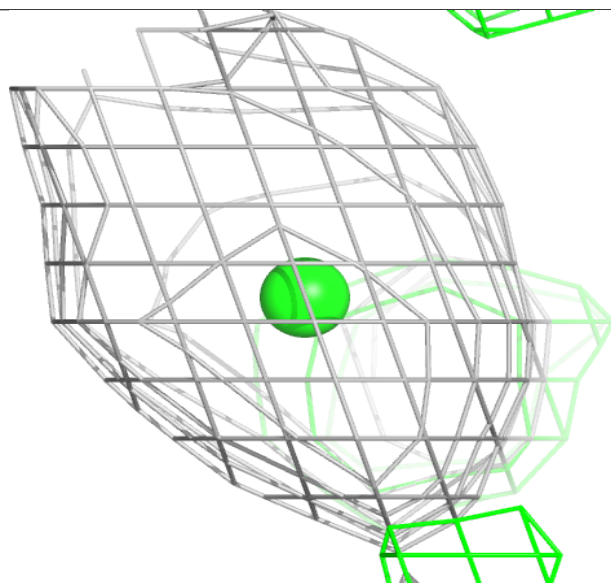
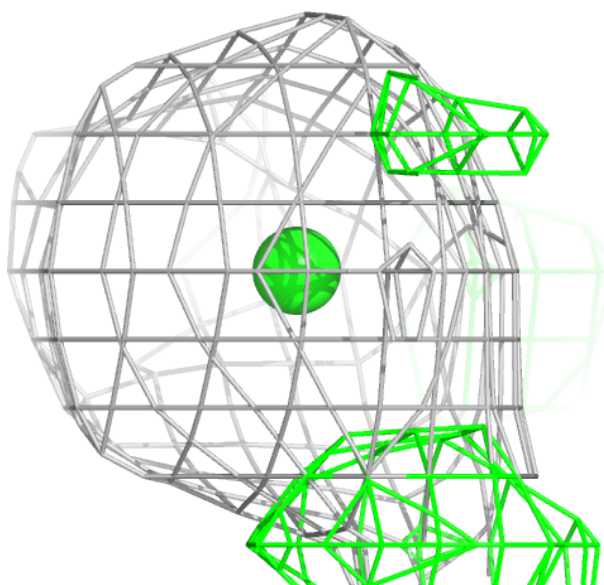
Electron density around CL g 204:

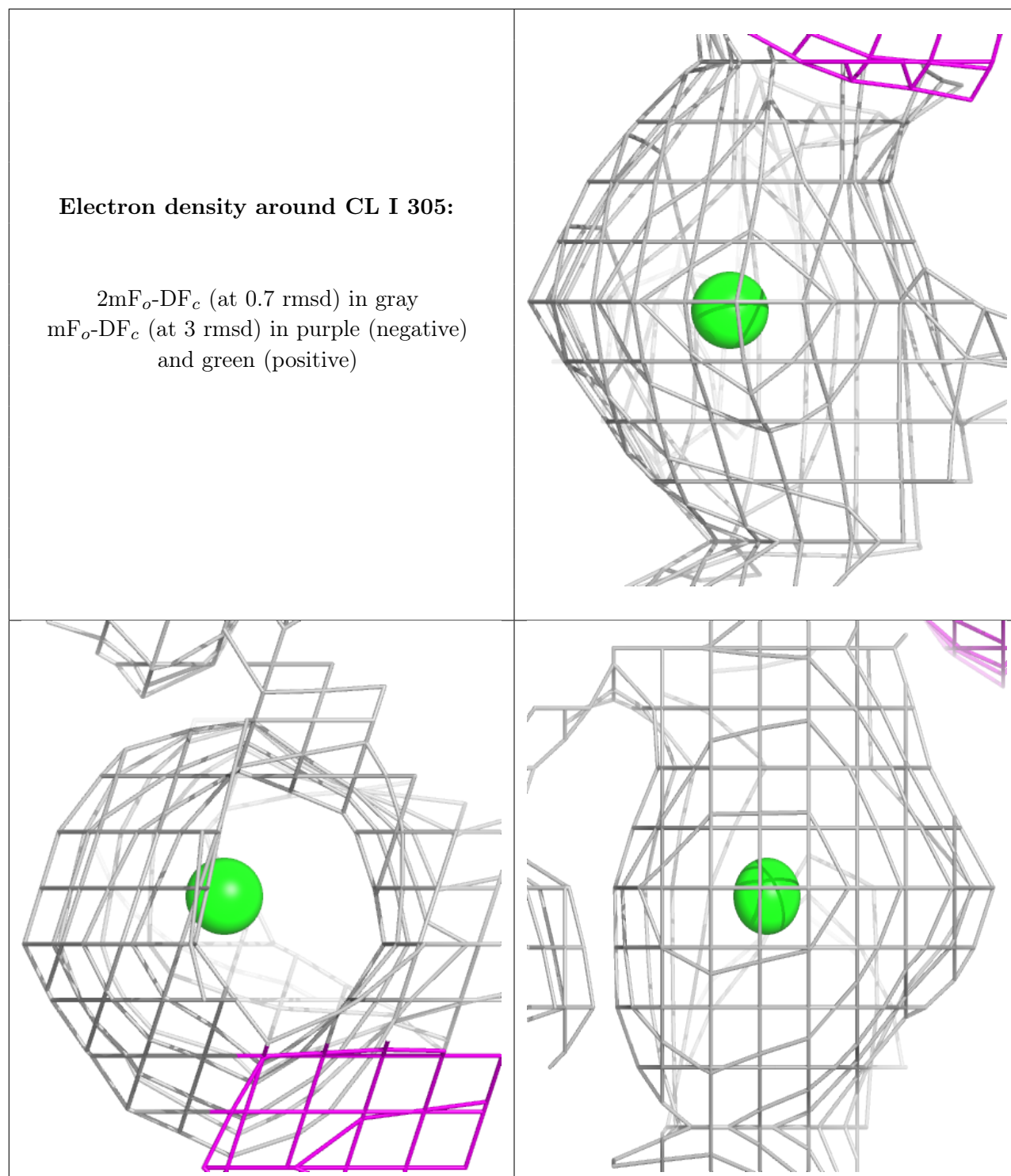
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL G 305:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.