



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 07:42 PM EDT

PDB ID : 7RTH
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

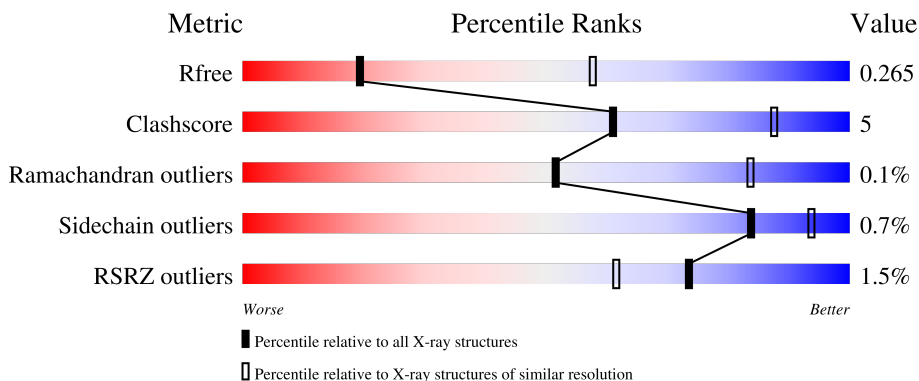
1 Overall quality at a glance i

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.
















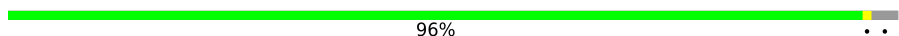
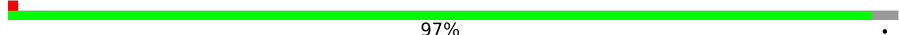
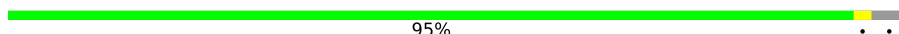
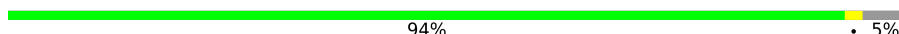
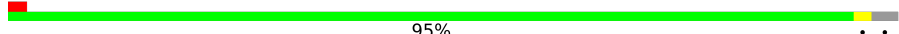
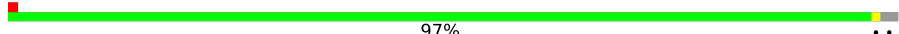

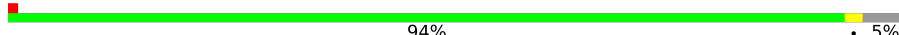
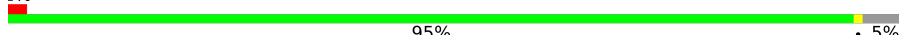
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	
1	C	215	
1	E	215	
1	G	215	
1	I	215	

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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	 10% 80% 8% 11%
2	D	239	 87% 8% 5%
2	F	239	 85% 9% 6%
2	H	239	 85% 10% 6%
2	J	239	 2% 83% 11% 5%
2	L	239	 80% 13% 7%
2	N	239	 5% 85% 7% 8%
2	P	239	 2% 79% 12% 9%
2	R	239	 2% 83% 7% 9%
3	a	129	 96%
3	c	129	 97%
3	e	129	 95%
3	g	129	 94% 5%
3	i	129	 2% 95% 5%
3	k	129	 97%
3	m	129	 2% 92% 6%
3	o	129	 94% 5%
3	q	129	 2% 95% 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	e	203	-	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	Total 1533	C 959	N 258	O 312	S 4	0	0	0
1	C	204	Total 1554	C 970	N 262	O 318	S 4	0	0	0
1	E	209	Total 1587	C 989	N 268	O 326	S 4	0	0	0
1	G	209	Total 1587	C 989	N 268	O 326	S 4	0	0	0
1	I	203	Total 1548	C 967	N 261	O 316	S 4	0	0	0
1	K	210	Total 1601	C 999	N 270	O 327	S 5	0	0	0
1	M	207	Total 1574	C 982	N 266	O 322	S 4	0	0	0
1	O	202	Total 1535	C 960	N 257	O 314	S 4	0	0	0
1	Q	203	Total 1548	C 967	N 261	O 316	S 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	Total 1625	C 1039	N 268	O 313	S 5	0	0	0
2	D	228	Total 1729	C 1100	N 286	O 338	S 5	0	0	0
2	F	225	Total 1712	C 1091	N 283	O 332	S 6	0	0	0
2	H	225	Total 1715	C 1093	N 283	O 334	S 5	0	0	0
2	J	226	Total 1718	C 1094	N 284	O 335	S 5	0	0	0

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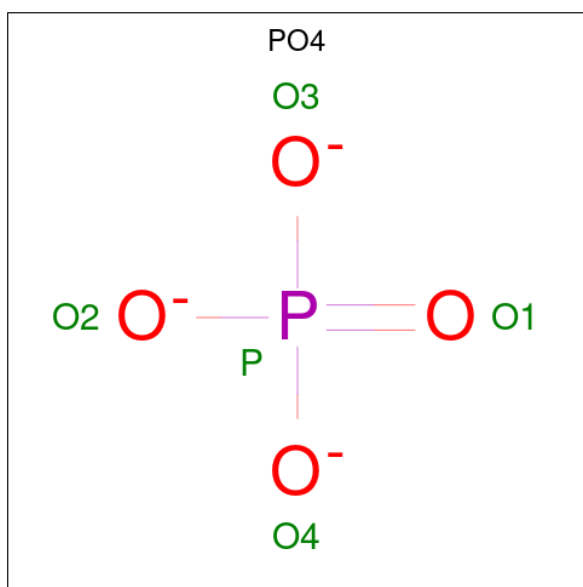
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	223	Total	C	N	O	S	0	0	0
			1700	1085	281	329	5			
2	N	221	Total	C	N	O	S	0	0	0
			1682	1073	277	327	5			
2	P	218	Total	C	N	O	S	0	0	0
			1667	1067	275	320	5			
2	R	217	Total	C	N	O	S	0	0	0
			1663	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 (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

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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 (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

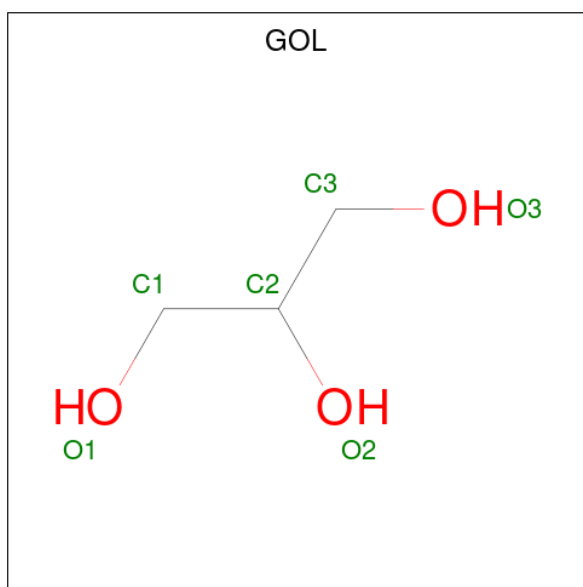
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	C	2	Total	Cl	0	0
			2	2		
5	D	2	Total	Cl	0	0
			2	2		
5	E	2	Total	Cl	0	0
			2	2		

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

- Molecule 6 is GLYCEROL (three-letter code: 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 (three-letter code: 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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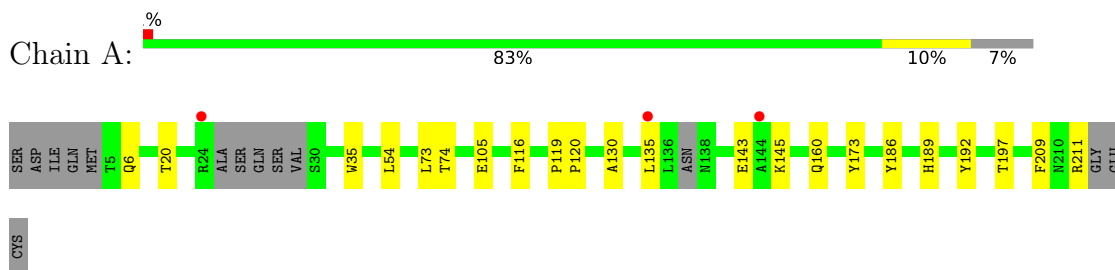
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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8	K	12	Total O 12 12	0	0
8	L	8	Total O 8 8	0	0
8	M	5	Total O 5 5	0	0
8	N	4	Total O 4 4	0	0
8	O	3	Total O 3 3	0	0
8	P	8	Total O 8 8	0	0
8	Q	10	Total O 10 10	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

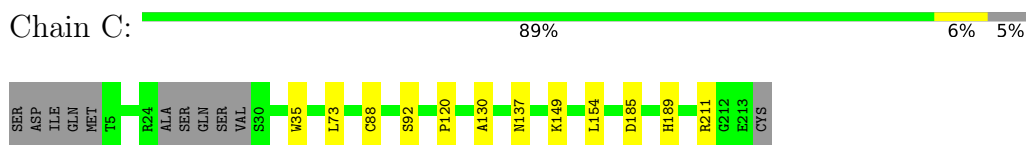
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

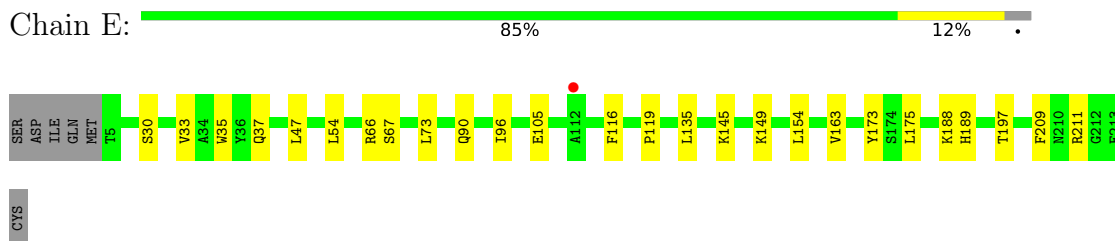
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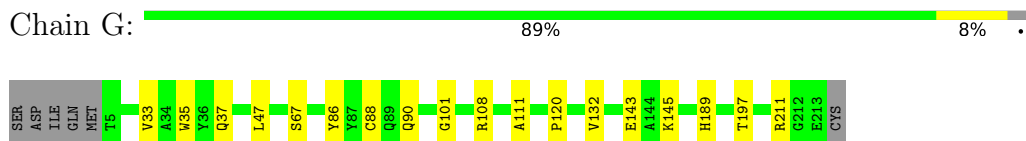
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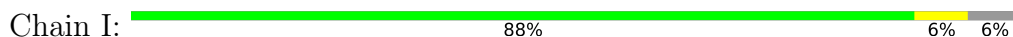
- Molecule 1: Fragment Antigen-Binding Light Chain



- Molecule 1: Fragment Antigen-Binding Light Chain

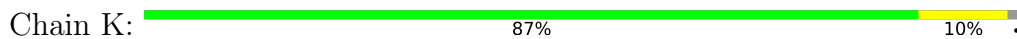


- Molecule 1: Fragment Antigen-Binding Light Chain

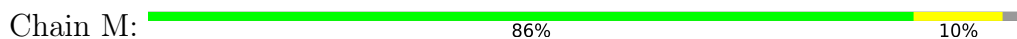




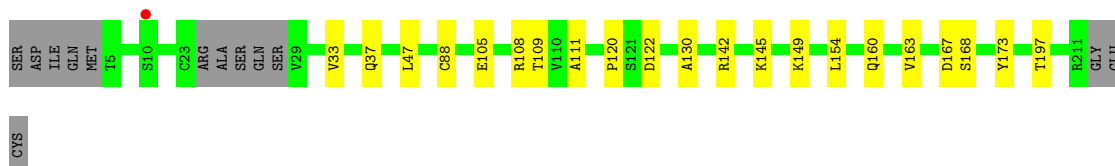
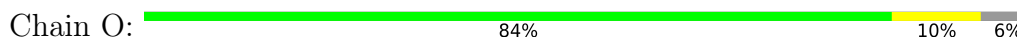
● Molecule 1: Fragment Antigen-Binding Light Chain



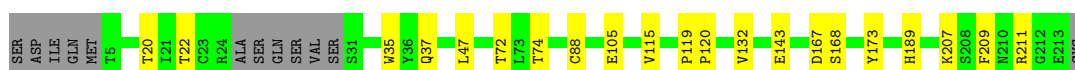
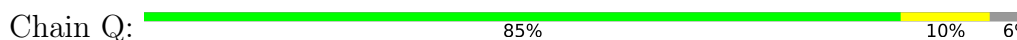
● Molecule 1: Fragment Antigen-Binding Light Chain



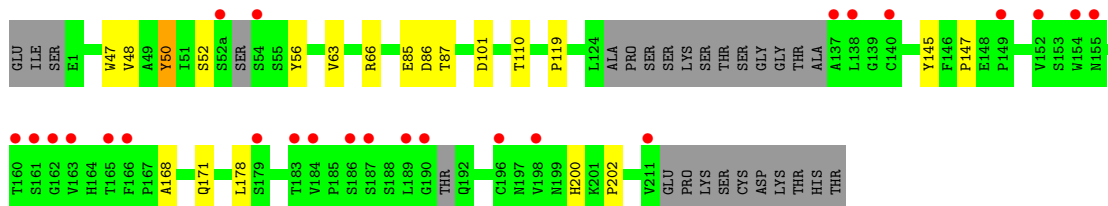
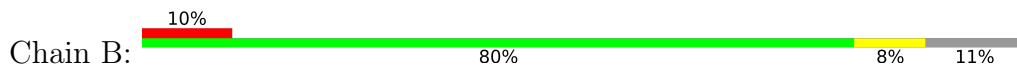
● Molecule 1: Fragment Antigen-Binding Light Chain



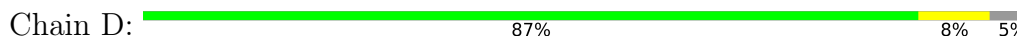
● Molecule 1: Fragment Antigen-Binding Light Chain



● Molecule 2: Fragment Antigen-Binding Heavy Chain

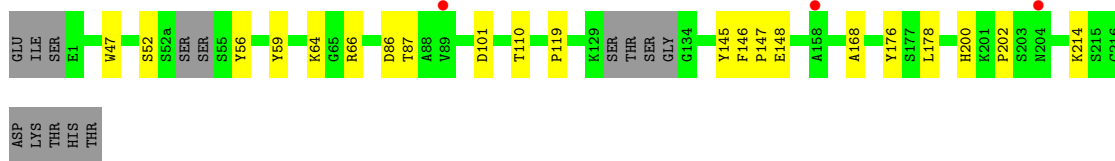
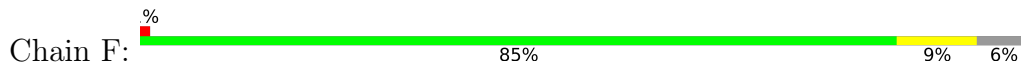


● Molecule 2: Fragment Antigen-Binding Heavy Chain

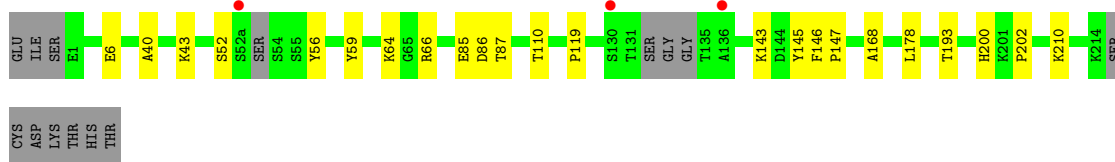
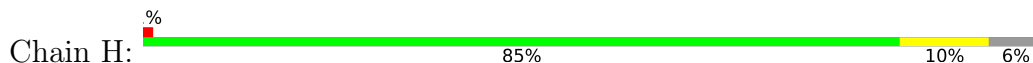




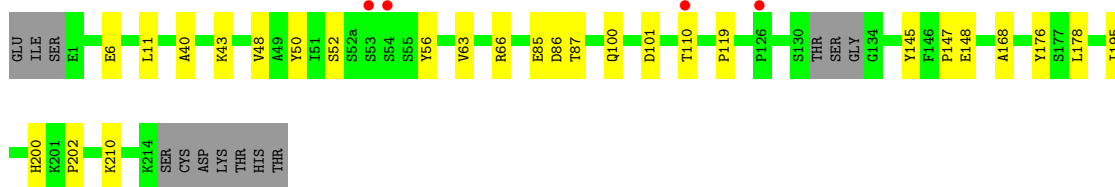
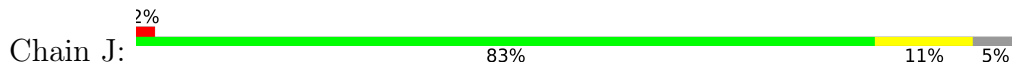
● Molecule 2: Fragment Antigen-Binding Heavy Chain



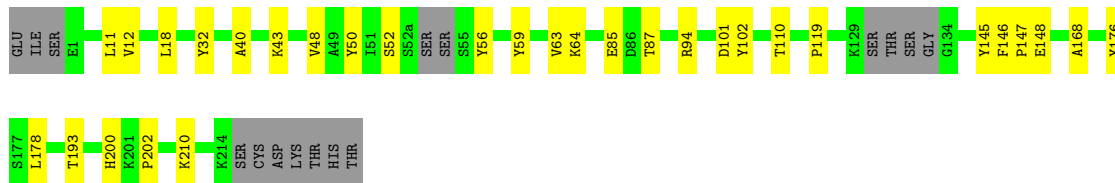
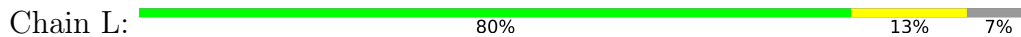
● Molecule 2: Fragment Antigen-Binding Heavy Chain



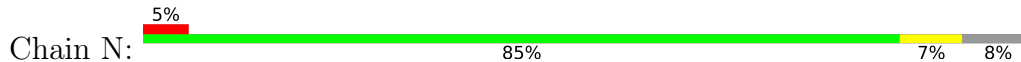
● Molecule 2: Fragment Antigen-Binding Heavy Chain

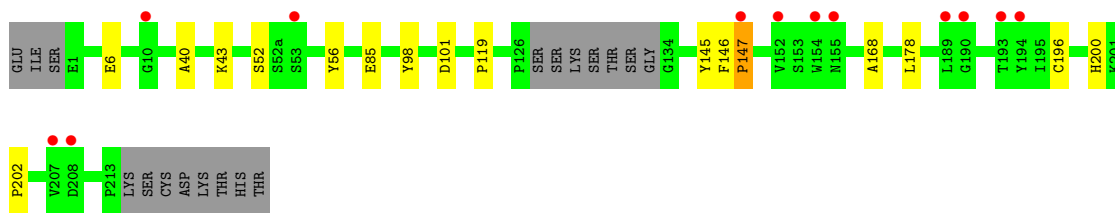


● Molecule 2: Fragment Antigen-Binding Heavy Chain

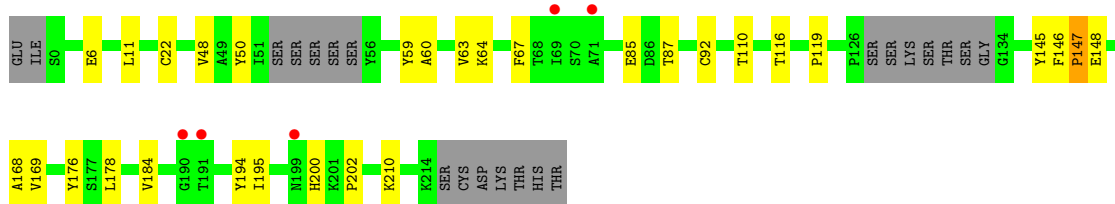
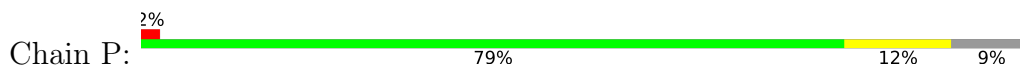


● Molecule 2: Fragment Antigen-Binding Heavy Chain

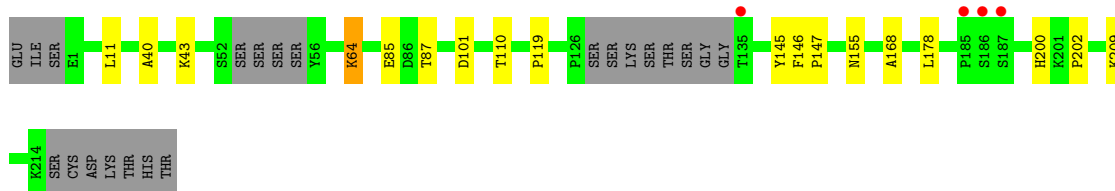
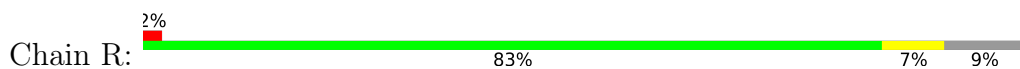




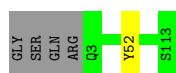
● Molecule 2: Fragment Antigen-Binding Heavy Chain



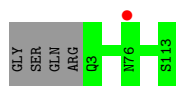
● Molecule 2: Fragment Antigen-Binding Heavy Chain



● Molecule 3: Nanobody



● Molecule 3: Nanobody

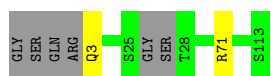


● Molecule 3: Nanobody




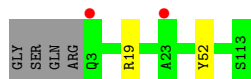
- Molecule 3: Nanobody

Chain g:  94% • 5%



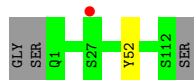
- Molecule 3: Nanobody

Chain i:  95% • •




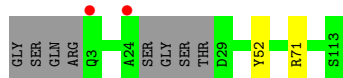
- Molecule 3: Nanobody

Chain k:  97% • •



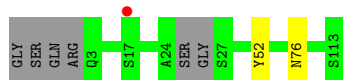
- Molecule 3: Nanobody

Chain m:  92% • 6%



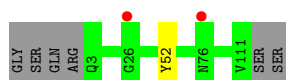
- Molecule 3: Nanobody

Chain o:  94% • 5%



- Molecule 3: Nanobody

Chain q:  95% • 5%



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 – 3.19 111.35 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.0 (90.91-3.19) 97.0 (111.35-3.19)	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 (5.12%)	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 , 52.7	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, PO4, GOL, 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	0.25	0/1563	0.43	0/2118
1	C	0.25	0/1585	0.44	0/2149
1	E	0.25	0/1619	0.43	0/2197
1	G	0.24	0/1619	0.44	0/2197
1	I	0.25	0/1579	0.43	0/2141
1	K	0.24	0/1632	0.44	0/2212
1	M	0.25	0/1606	0.44	0/2180
1	O	0.25	0/1566	0.43	0/2125
1	Q	0.24	0/1579	0.43	0/2141
2	B	0.24	0/1670	0.44	0/2276
2	D	0.24	0/1778	0.44	0/2426
2	F	0.25	0/1760	0.44	0/2400
2	H	0.26	0/1763	0.45	0/2405
2	J	0.25	0/1767	0.44	0/2411
2	L	0.24	0/1748	0.44	0/2384
2	N	0.25	0/1731	0.44	0/2365
2	P	0.24	0/1715	0.44	0/2341
2	R	0.24	0/1711	0.44	0/2336
3	a	0.24	0/999	0.41	0/1351
3	c	0.24	0/999	0.42	0/1351
3	e	0.25	0/981	0.43	0/1329
3	g	0.26	0/977	0.43	0/1321
3	i	0.25	0/988	0.43	0/1337
3	k	0.24	0/1012	0.43	0/1369
3	m	0.25	0/964	0.43	0/1303
3	o	0.25	0/988	0.42	0/1335
3	q	0.24	0/975	0.42	0/1321
All	All	0.25	0/38874	0.44	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	13	0
1	G	1587	0	1551	12	0
1	I	1548	0	1513	8	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	10	0
2	D	1729	0	1657	11	0
2	F	1712	0	1641	11	0
2	H	1715	0	1645	13	0
2	J	1718	0	1647	15	0
2	L	1700	0	1631	17	0
2	N	1682	0	1606	9	0
2	P	1667	0	1598	19	0
2	R	1663	0	1595	12	0
3	a	967	0	923	0	0
3	c	977	0	940	0	0
3	e	959	0	923	0	0
3	g	956	0	919	0	0
3	i	966	0	928	0	0
3	k	980	0	942	0	0
3	m	943	0	907	0	0
3	o	957	0	914	0	0
3	q	953	0	918	0	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	0	0
4	c	10	0	0	0	0
4	e	15	0	0	0	0
4	g	10	0	0	0	0
4	i	15	0	0	0	0
4	m	10	0	0	0	0
4	o	15	0	0	0	0
4	q	5	0	0	0	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	0	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	0	0
6	c	6	0	8	0	0
6	k	6	0	8	0	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	0	0
7	N	7	0	10	1	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	212	0

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

All (212) 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
2:H:143:LYS:NZ	8:H:401:HOH:O	2.21	0.67
2:H:168:ALA:HB2	2:H:178:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:168:ALA:HB2	2:P:178:LEU:HD23	1.76	0.67
1:Q:22:THR:HG22	1:Q:72:THR:HG22	1.77	0.66
1:A:189:HIS:O	1:A:211:ARG:NH1	2.29	0.65
2:N:168:ALA:HB2	2:N:178:LEU:HD23	1.78	0.65
2:P:195:ILE:HG12	2:P:210:LYS:HG2	1.79	0.65
1:G:88:CYS:SG	6:G:306:GOL:O2	2.53	0.65
2:L:168:ALA:HB2	2:L:178:LEU:HD23	1.79	0.64
2:F:168:ALA:HB2	2:F:178:LEU:HD23	1.79	0.64
2:L:48:VAL:HG13	2:L:63:VAL:HG21	1.80	0.64
1:K:117:ILE:HG22	1:K:207:LYS:HE3	1.80	0.63
2:H:87:THR:HG23	2:H:110:THR:HA	1.81	0.62
1:M:189:HIS:O	1:M:211:ARG:NH1	2.32	0.62
1:G:120:PRO:HD3	1:G:132:VAL:HG22	1.82	0.61
2:B:168:ALA:HB2	2:B:178:LEU:HD23	1.81	0.61
2:B:48:VAL:HG13	2:B:63:VAL:HG21	1.81	0.61
1:M:117:ILE:HG22	1:M:207:LYS:HE3	1.83	0.61
2:B:52:SER:HB2	2:B:56:TYR:HB2	1.82	0.60
1:A:160:GLN:OE1	2:B:171:GLN:NE2	2.35	0.59
1:Q:189:HIS:O	1:Q:211:ARG:NH1	2.34	0.59
2:J:168:ALA:HB2	2:J:178:LEU:HD23	1.84	0.58
2:R:87:THR:HG23	2:R:110:THR:HA	1.84	0.58
2:R:168:ALA:HB2	2:R:178:LEU:HD23	1.85	0.58
1:K:189:HIS:O	1:K:211:ARG:NH1	2.37	0.58
2:J:48:VAL:HG13	2:J:63:VAL:HG21	1.86	0.58
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.85	0.57
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.36	0.57
2:J:52:SER:HB2	2:J:56:TYR:HB2	1.87	0.57
2:D:87:THR:HG23	2:D:110:THR:HA	1.85	0.57
1:A:143:GLU:N	1:A:143:GLU:OE1	2.37	0.57
2:N:98:TYR:HD1	7:N:303:PEG:H11	1.70	0.56
1:A:105:GLU:OE1	1:A:173:TYR:OH	2.23	0.56
2:J:11:LEU:HD21	2:J:147:PRO:HG3	1.88	0.56
2:D:12:VAL:HG11	2:D:18:LEU:HB2	1.88	0.55
2:P:48:VAL:HG13	2:P:63:VAL:HG21	1.89	0.54
1:G:67:SER:OG	1:I:185:ASP:OD2	2.23	0.54
1:C:185:ASP:OD2	1:E:67:SER:OG	2.22	0.54
2:L:52:SER:HB2	2:L:56:TYR:HB2	1.89	0.54
2:L:193:THR:HB	2:L:210:LYS:HE3	1.89	0.54
2:L:87:THR:HG23	2:L:110:THR:HA	1.89	0.54
2:F:52:SER:HB2	2:F:56:TYR:HB2	1.90	0.54
1:G:33:VAL:HG22	1:G:90:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:85:GLU:OE1	2:P:85:GLU:N	2.40	0.54
2:B:85:GLU:N	2:B:85:GLU:OE1	2.40	0.54
2:N:85:GLU:N	2:N:85:GLU:OE1	2.40	0.54
2:H:59:TYR:HB2	2:H:64:LYS:HD2	1.89	0.53
1:O:105:GLU:OE1	1:O:173:TYR:OH	2.20	0.53
2:J:100:GLN:NE2	4:J:302:PO4:O3	2.42	0.53
2:J:195:ILE:HG22	2:J:210:LYS:HG2	1.91	0.53
2:N:200:HIS:CD2	2:N:202:PRO:HD2	2.44	0.53
2:R:85:GLU:OE1	2:R:85:GLU:N	2.40	0.53
2:L:200:HIS:CD2	2:L:202:PRO:HD2	2.45	0.52
2:N:52:SER:HB2	2:N:56:TYR:HB2	1.92	0.52
1:C:149:LYS:HG2	1:C:154:LEU:HD23	1.92	0.52
2:D:85:GLU:OE1	2:D:85:GLU:N	2.41	0.52
2:L:85:GLU:N	2:L:85:GLU:OE1	2.42	0.52
1:O:142:ARG:HE	1:O:163:VAL:HG11	1.75	0.51
1:G:143:GLU:OE1	1:G:143:GLU:N	2.42	0.51
1:M:105:GLU:OE1	1:M:173:TYR:OH	2.24	0.51
1:K:149:LYS:HG2	1:K:154:LEU:HD23	1.93	0.51
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.92	0.51
2:H:85:GLU:OE1	2:H:85:GLU:N	2.43	0.50
2:J:85:GLU:N	2:J:85:GLU:OE1	2.44	0.50
2:J:87:THR:HG23	2:J:110:THR:HA	1.91	0.50
1:K:185:ASP:OD2	1:M:67:SER:OG	2.25	0.50
2:R:200:HIS:CD2	2:R:202:PRO:HD2	2.46	0.50
1:I:37:GLN:HB2	1:I:47:LEU:HD11	1.92	0.50
2:P:168:ALA:HA	2:P:178:LEU:HB3	1.93	0.50
2:J:200:HIS:CD2	2:J:202:PRO:HD2	2.46	0.50
1:K:92:SER:OG	1:K:93:SER:N	2.44	0.50
1:M:30:SER:HB2	1:M:90:GLN:NE2	2.27	0.50
1:K:89:GLN:HE21	1:K:96:ILE:HG23	1.76	0.49
2:L:40:ALA:HB3	2:L:43:LYS:HB2	1.94	0.49
2:H:200:HIS:CD2	2:H:202:PRO:HD2	2.48	0.49
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.48	0.49
2:F:200:HIS:CD2	2:F:202:PRO:HD2	2.48	0.49
1:C:120:PRO:HG3	1:C:130:ALA:HB1	1.94	0.48
2:J:66:ARG:NH1	2:J:86:ASP:OD2	2.43	0.48
1:O:108:ARG:HG2	1:O:109:THR:H	1.78	0.48
2:R:168:ALA:HA	2:R:178:LEU:HB3	1.95	0.48
1:K:116:PHE:HA	1:K:207:LYS:HE2	1.96	0.48
1:E:189:HIS:O	1:E:211:ARG:NH1	2.46	0.48
2:F:87:THR:HG23	2:F:110:THR:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:ARG:NH1	2:F:86:ASP:OD2	2.37	0.47
2:F:119:PRO:HB3	2:F:145:TYR:HB3	1.95	0.47
1:K:105:GLU:OE1	1:K:173:TYR:OH	2.29	0.47
1:Q:143:GLU:OE1	1:Q:143:GLU:N	2.45	0.47
1:E:145:LYS:HB3	1:E:197:THR:HB	1.97	0.47
1:K:22:THR:HG22	1:K:72:THR:HG22	1.95	0.47
1:M:108:ARG:HH12	1:M:111:ALA:HB2	1.78	0.47
2:D:159:LEU:HD21	2:D:182:VAL:HG21	1.96	0.47
1:A:116:PHE:HB2	1:A:135:LEU:HB3	1.97	0.47
1:C:137:ASN:ND2	4:C:301:PO4:O4	2.47	0.47
2:D:66:ARG:NH1	2:D:86:ASP:OD2	2.41	0.47
1:G:101:GLY:H	6:G:306:GOL:H2	1.80	0.47
1:Q:37:GLN:HB2	1:Q:47:LEU:HD11	1.96	0.47
2:R:155:ASN:ND2	4:R:301:PO4:O4	2.34	0.47
1:E:33:VAL:HG22	1:E:90:GLN:HG2	1.96	0.47
1:E:149:LYS:HG2	1:E:154:LEU:HD23	1.95	0.47
2:F:59:TYR:HB2	2:F:64:LYS:HG3	1.96	0.47
1:O:33:VAL:HG21	1:O:88:CYS:HB2	1.97	0.47
2:B:66:ARG:NH1	2:B:86:ASP:OD2	2.48	0.47
2:B:87:THR:HG23	2:B:110:THR:HA	1.96	0.47
2:P:63:VAL:O	2:P:67:PHE:HB2	2.15	0.47
1:A:120:PRO:HG3	1:A:130:ALA:HB1	1.95	0.46
1:G:108:ARG:HH12	1:G:111:ALA:HB2	1.80	0.46
2:P:200:HIS:CD2	2:P:202:PRO:HD2	2.50	0.46
2:L:32:TYR:CD1	2:L:94:ARG:HD3	2.50	0.46
2:D:200:HIS:CD2	2:D:202:PRO:HD2	2.50	0.46
2:H:193:THR:HB	2:H:210:LYS:HD2	1.98	0.46
1:G:86:TYR:O	6:G:306:GOL:O1	2.34	0.46
1:O:145:LYS:HB3	1:O:197:THR:HB	1.97	0.46
1:M:149:LYS:HG2	1:M:154:LEU:HD23	1.98	0.46
1:Q:20:THR:HG22	1:Q:74:THR:HG23	1.98	0.46
1:Q:167:ASP:OD1	1:Q:168:SER:N	2.48	0.46
1:M:61:ARG:N	4:M:302:PO4:O2	2.48	0.46
1:M:145:LYS:HB3	1:M:197:THR:HB	1.97	0.46
2:D:168:ALA:HB2	2:D:178:LEU:HD23	1.98	0.46
1:I:108:ARG:HD3	1:I:109:THR:O	2.16	0.45
1:C:35:TRP:CD2	1:C:73:LEU:HB2	2.50	0.45
2:P:116:THR:HG22	2:P:147:PRO:HD3	1.99	0.45
2:R:11:LEU:HD23	2:R:110:THR:HB	1.97	0.45
2:P:119:PRO:HB3	2:P:145:TYR:HB3	1.99	0.45
2:R:40:ALA:HB3	2:R:43:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:O	1:A:192:TYR:OH	2.34	0.45
2:J:168:ALA:HA	2:J:178:LEU:HB3	1.98	0.45
2:L:168:ALA:HA	2:L:178:LEU:HB3	1.99	0.45
1:Q:105:GLU:OE1	1:Q:173:TYR:OH	2.21	0.45
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.99	0.45
1:A:145:LYS:HB2	1:A:197:THR:HB	1.99	0.45
1:E:119:PRO:HB3	1:E:209:PHE:CE2	2.52	0.45
1:E:105:GLU:OE1	1:E:173:TYR:OH	2.28	0.45
2:H:52:SER:HB2	2:H:56:TYR:HB2	1.99	0.45
2:J:6:GLU:N	2:J:6:GLU:OE1	2.50	0.45
2:P:60:ALA:O	2:P:64:LYS:HG3	2.17	0.45
1:M:89:GLN:HE21	1:M:96:ILE:HG23	1.82	0.44
2:R:119:PRO:HB3	2:R:145:TYR:HB3	1.99	0.44
1:C:189:HIS:O	1:C:211:ARG:NH1	2.49	0.44
1:I:189:HIS:O	1:I:211:ARG:NH1	2.45	0.44
2:L:12:VAL:HG11	2:L:18:LEU:HB2	2.00	0.44
2:R:146:PHE:HA	2:R:147:PRO:HA	1.79	0.44
2:B:47:TRP:HZ2	2:B:50:TYR:HB3	1.82	0.44
1:I:116:PHE:HB2	1:I:135:LEU:HB3	2.00	0.44
1:E:30:SER:OG	1:E:66:ARG:NH2	2.50	0.44
1:K:185:ASP:OD1	1:K:188:LYS:NZ	2.50	0.44
1:M:119:PRO:HB3	1:M:209:PHE:CE2	2.53	0.44
2:L:119:PRO:HB3	2:L:145:TYR:HB3	1.99	0.44
2:N:146:PHE:HA	2:N:147:PRO:HA	1.79	0.44
2:P:59:TYR:HB2	2:P:64:LYS:HG2	1.99	0.44
1:O:149:LYS:HG2	1:O:154:LEU:HD23	1.99	0.44
2:H:146:PHE:HA	2:H:147:PRO:HA	1.79	0.43
1:K:35:TRP:CZ3	1:K:88:CYS:HB3	2.52	0.43
2:N:6:GLU:OE1	2:N:6:GLU:N	2.51	0.43
2:B:200:HIS:CD2	2:B:202:PRO:HD2	2.53	0.43
2:L:59:TYR:HB2	2:L:64:LYS:HD2	2.00	0.43
1:G:35:TRP:CZ3	1:G:88:CYS:HB3	2.53	0.43
1:E:116:PHE:HB2	1:E:135:LEU:HB3	2.01	0.43
1:E:163:VAL:HG22	1:E:175:LEU:HD12	2.01	0.43
1:K:132:VAL:HB	1:K:179:LEU:HB3	1.99	0.43
1:M:35:TRP:CE2	1:M:73:LEU:HB2	2.54	0.43
1:E:35:TRP:CD2	1:E:73:LEU:HB2	2.54	0.43
2:L:146:PHE:HA	2:L:147:PRO:HA	1.79	0.43
1:Q:119:PRO:HB3	1:Q:209:PHE:CE2	2.54	0.43
2:D:119:PRO:HB3	2:D:145:TYR:HB3	2.01	0.42
1:I:35:TRP:CD2	1:I:73:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:40:ALA:HB3	2:N:43:LYS:HD2	2.01	0.42
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.54	0.42
1:E:96:ILE:HB	2:F:47:TRP:CG	2.54	0.42
1:K:20:THR:HG22	1:K:74:THR:HG23	2.02	0.42
1:G:189:HIS:O	1:G:211:ARG:NH1	2.48	0.42
2:P:87:THR:HG23	2:P:110:THR:HA	2.01	0.42
2:D:206:LYS:HE2	2:D:206:LYS:HB3	1.89	0.42
2:H:6:GLU:N	2:H:6:GLU:OE1	2.53	0.42
2:N:119:PRO:HB3	2:N:145:TYR:HB3	2.02	0.42
1:Q:35:TRP:CZ3	1:Q:88:CYS:HB3	2.54	0.42
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.02	0.42
2:L:11:LEU:HD11	2:L:146:PHE:CE2	2.55	0.42
1:O:108:ARG:HH22	1:O:111:ALA:HB2	1.84	0.42
2:L:148:GLU:HG2	2:L:176:TYR:CE2	2.54	0.41
1:Q:115:VAL:O	1:Q:207:LYS:NZ	2.49	0.41
4:E:304:PO4:O4	2:F:214:LYS:NZ	2.53	0.41
2:J:119:PRO:HB3	2:J:145:TYR:HB3	2.03	0.41
2:P:184:VAL:HG11	2:P:194:TYR:CE1	2.56	0.41
2:J:40:ALA:HB3	2:J:43:LYS:HB2	2.01	0.41
1:G:145:LYS:HB2	1:G:197:THR:HB	2.02	0.41
2:R:209:LYS:HD2	2:R:209:LYS:HA	1.98	0.41
2:F:146:PHE:HA	2:F:147:PRO:HA	1.83	0.41
2:H:40:ALA:HB3	2:H:43:LYS:HB2	2.03	0.41
1:I:23:CYS:HB2	1:I:35:TRP:CH2	2.56	0.41
1:A:6:GLN:OE1	1:A:6:GLN:N	2.51	0.41
1:A:20:THR:HG22	1:A:74:THR:HG23	2.02	0.41
2:D:11:LEU:HD21	2:D:147:PRO:HG3	2.03	0.41
2:D:168:ALA:HA	2:D:178:LEU:HB3	2.03	0.41
2:J:148:GLU:HG2	2:J:176:TYR:CE2	2.56	0.41
1:O:122:ASP:OD1	1:O:122:ASP:N	2.52	0.41
2:P:11:LEU:HD11	2:P:146:PHE:HE2	1.85	0.41
1:Q:120:PRO:HD3	1:Q:132:VAL:HG22	2.03	0.41
2:R:64:LYS:HD3	2:R:64:LYS:HA	1.82	0.41
1:M:35:TRP:CD2	1:M:73:LEU:HB2	2.56	0.41
1:O:167:ASP:OD1	1:O:168:SER:N	2.54	0.41
2:P:6:GLU:HA	2:P:22:CYS:HA	2.03	0.40
1:I:35:TRP:CE2	1:I:73:LEU:HB2	2.56	0.40
2:L:101:ASP:OD1	2:L:102:TYR:N	2.53	0.40
1:O:37:GLN:HB2	1:O:47:LEU:HD11	2.03	0.40
2:F:148:GLU:HG2	2:F:176:TYR:CE2	2.56	0.40
1:O:120:PRO:HG3	1:O:130:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:GLU:HB3	2:P:92:CYS:SG	2.62	0.40
2:P:148:GLU:HG2	2:P:176:TYR:CE2	2.55	0.40
1:A:35:TRP:CD2	1:A:73:LEU:HB2	2.57	0.40
2:P:6:GLU:N	2:P:6:GLU:OE1	2.55	0.40

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%)	29	67
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%)	29	67
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%)	29	67
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%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	212/239 (89%)	200 (94%)	11 (5%)	1 (0%)	29	67
2	R	211/239 (88%)	200 (95%)	10 (5%)	1 (0%)	29	67
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%)	51	83

All (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
2	P	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%)	177 (99%)	1 (1%)	86	94
1	C	180/190 (95%)	180 (100%)	0	100	100
1	E	184/190 (97%)	182 (99%)	2 (1%)	73	88
1	G	184/190 (97%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	179/190 (94%)	177 (99%)	2 (1%)	73	88
1	K	186/190 (98%)	186 (100%)	0	100	100
1	M	183/190 (96%)	183 (100%)	0	100	100
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%)	175 (99%)	2 (1%)	73	88
2	D	189/200 (94%)	188 (100%)	1 (0%)	88	95
2	F	187/200 (94%)	186 (100%)	1 (0%)	88	95
2	H	188/200 (94%)	188 (100%)	0	100	100
2	J	188/200 (94%)	186 (99%)	2 (1%)	73	88
2	L	185/200 (92%)	184 (100%)	1 (0%)	88	95
2	N	183/200 (92%)	181 (99%)	2 (1%)	73	88
2	P	180/200 (90%)	179 (99%)	1 (1%)	86	94
2	R	180/200 (90%)	179 (99%)	1 (1%)	86	94
3	a	103/105 (98%)	102 (99%)	1 (1%)	76	90
3	c	103/105 (98%)	103 (100%)	0	100	100
3	e	101/105 (96%)	99 (98%)	2 (2%)	55	80
3	g	101/105 (96%)	99 (98%)	2 (2%)	55	80
3	i	102/105 (97%)	100 (98%)	2 (2%)	55	80
3	k	104/105 (99%)	103 (99%)	1 (1%)	76	90
3	m	99/105 (94%)	97 (98%)	2 (2%)	55	80
3	o	102/105 (97%)	100 (98%)	2 (2%)	55	80
3	q	100/105 (95%)	99 (99%)	1 (1%)	76	90
All	All	4203/4455 (94%)	4174 (99%)	29 (1%)	84	94

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
2	B	50	TYR
2	B	101	ASP
2	D	50	TYR
1	E	54	LEU
1	E	188	LYS

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Mol	Chain	Res	Type
2	F	101	ASP
1	I	54	LEU
1	I	108	ARG
2	J	50	TYR
2	J	101	ASP
2	L	50	TYR
2	N	101	ASP
2	N	196	CYS
2	P	50	TYR
2	R	101	ASP
3	a	52	TYR
3	e	52	TYR
3	e	71	ARG
3	g	3	GLN
3	g	71	ARG
3	i	19	ARG
3	i	52	TYR
3	k	52	TYR
3	m	52	TYR
3	m	71	ARG
3	o	52	TYR
3	o	76	ASN
3	q	52	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
2	B	171	GLN
2	J	100	GLN
3	o	76	ASN
3	o	100(g)	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 monosaccharides 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
6	GOL	I	306	-	5,5,5	0.91	0	5,5,5	1.00	0
4	PO4	g	202	-	4,4,4	0.91	0	6,6,6	0.51	0
6	GOL	G	306	-	5,5,5	0.92	0	5,5,5	0.99	0
4	PO4	i	201	-	4,4,4	0.94	0	6,6,6	0.43	0
4	PO4	g	201	-	4,4,4	0.93	0	6,6,6	0.41	0
4	PO4	m	202	-	4,4,4	0.93	0	6,6,6	0.42	0
4	PO4	K	301	-	4,4,4	0.94	0	6,6,6	0.43	0
4	PO4	i	203	-	4,4,4	0.94	0	6,6,6	0.43	0
7	PEG	F	302	-	6,6,6	0.49	0	5,5,5	0.29	0
6	GOL	B	304	-	5,5,5	0.09	0	5,5,5	0.37	0
4	PO4	I	301	-	4,4,4	0.93	0	6,6,6	0.43	0
4	PO4	a	201	-	4,4,4	0.93	0	6,6,6	0.42	0
4	PO4	J	301	-	4,4,4	0.92	0	6,6,6	0.42	0
6	GOL	C	308	-	5,5,5	0.90	0	5,5,5	1.00	0
4	PO4	E	303	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	G	303	-	4,4,4	0.91	0	6,6,6	0.43	0
6	GOL	L	303	-	5,5,5	0.90	0	5,5,5	0.99	0
4	PO4	R	301	-	4,4,4	0.93	0	6,6,6	0.43	0
4	PO4	Q	301	-	4,4,4	0.92	0	6,6,6	0.44	0
4	PO4	I	302	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	o	202	-	4,4,4	0.89	0	6,6,6	0.49	0
4	PO4	I	304	-	4,4,4	0.95	0	6,6,6	0.41	0
7	PEG	H	303	-	6,6,6	0.48	0	5,5,5	0.24	0
6	GOL	k	201	-	5,5,5	0.90	0	5,5,5	1.01	0
4	PO4	O	301	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	B	301	-	4,4,4	0.92	0	6,6,6	0.41	0
4	PO4	e	202	-	4,4,4	0.94	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEG	N	303	-	6,6,6	0.48	0	5,5,5	0.26	0
4	PO4	L	301	-	4,4,4	0.92	0	6,6,6	0.44	0
4	PO4	C	303	-	4,4,4	0.91	0	6,6,6	0.44	0
4	PO4	D	301	-	4,4,4	0.94	0	6,6,6	0.39	0
4	PO4	c	202	-	4,4,4	0.93	0	6,6,6	0.40	0
4	PO4	M	303	-	4,4,4	0.93	0	6,6,6	0.46	0
6	GOL	c	203	-	5,5,5	0.92	0	5,5,5	0.98	0
4	PO4	m	201	-	4,4,4	0.93	0	6,6,6	0.42	0
4	PO4	G	301	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	o	203	-	4,4,4	0.93	0	6,6,6	0.46	0
4	PO4	M	302	-	4,4,4	0.93	0	6,6,6	0.44	0
4	PO4	O	302	-	4,4,4	0.92	0	6,6,6	0.41	0
4	PO4	e	203	-	4,4,4	2.97	4 (100%)	6,6,6	0.44	0
4	PO4	G	302	-	4,4,4	0.92	0	6,6,6	0.42	0
4	PO4	H	301	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	q	201	-	4,4,4	0.95	0	6,6,6	0.38	0
6	GOL	G	307	-	5,5,5	0.78	0	5,5,5	1.10	0
4	PO4	D	302	-	4,4,4	0.92	0	6,6,6	0.42	0
4	PO4	C	305	-	4,4,4	0.92	0	6,6,6	0.42	0
4	PO4	E	301	-	4,4,4	0.91	0	6,6,6	0.43	0
4	PO4	C	301	-	4,4,4	0.97	0	6,6,6	0.45	0
4	PO4	o	201	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	a	202	-	4,4,4	0.94	0	6,6,6	0.50	0
4	PO4	E	302	-	4,4,4	0.92	0	6,6,6	0.44	0
4	PO4	i	202	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	I	303	-	4,4,4	0.94	0	6,6,6	0.41	0
6	GOL	E	307	-	5,5,5	0.92	0	5,5,5	0.96	0
4	PO4	C	304	-	4,4,4	0.92	0	6,6,6	0.43	0
4	PO4	M	301	-	4,4,4	0.92	0	6,6,6	0.41	0
4	PO4	C	302	-	4,4,4	0.91	0	6,6,6	0.42	0
4	PO4	c	201	-	4,4,4	0.96	0	6,6,6	0.44	0
4	PO4	K	302	-	4,4,4	0.92	0	6,6,6	0.42	0
4	PO4	J	302	-	4,4,4	0.91	0	6,6,6	0.44	0
4	PO4	E	304	-	4,4,4	0.92	0	6,6,6	0.34	0
4	PO4	e	201	-	4,4,4	0.91	0	6,6,6	0.49	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	I	306	-	-	0/4/4/4	-
6	GOL	B	304	-	-	0/4/4/4	-
6	GOL	c	203	-	-	2/4/4/4	-
6	GOL	L	303	-	-	0/4/4/4	-
7	PEG	N	303	-	-	1/4/4/4	-
6	GOL	G	306	-	-	0/4/4/4	-
6	GOL	E	307	-	-	1/4/4/4	-
7	PEG	F	302	-	-	2/4/4/4	-
7	PEG	H	303	-	-	2/4/4/4	-
6	GOL	k	201	-	-	2/4/4/4	-
6	GOL	G	307	-	-	2/4/4/4	-
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	4.53	1.61	1.50
4	e	203	PO4	P-O2	2.29	1.61	1.54
4	e	203	PO4	P-O3	2.27	1.61	1.54
4	e	203	PO4	P-O4	-2.08	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

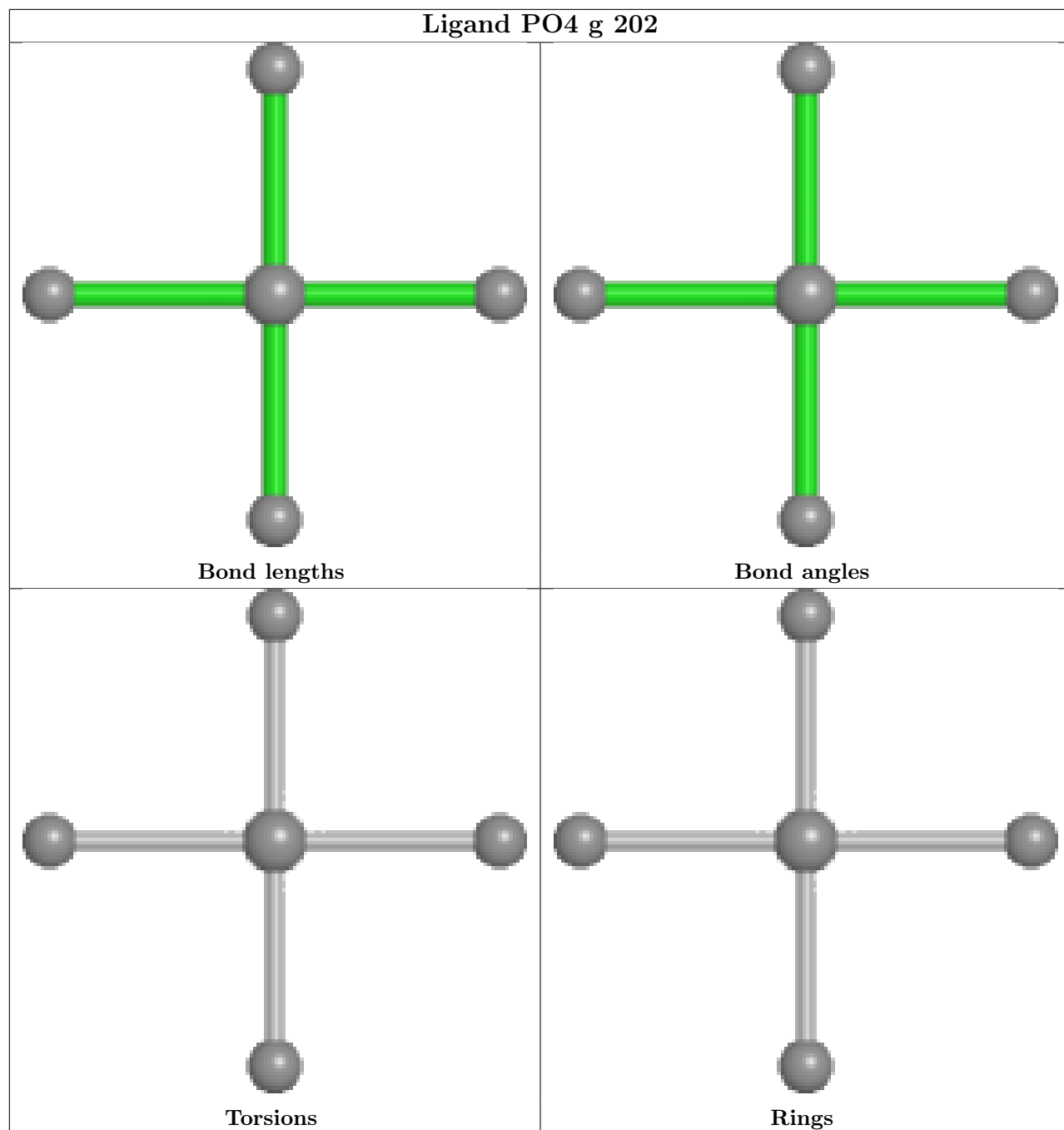
Mol	Chain	Res	Type	Atoms
6	k	201	GOL	O1-C1-C2-C3
6	c	203	GOL	O1-C1-C2-C3
6	k	201	GOL	O1-C1-C2-O2
7	H	303	PEG	O1-C1-C2-O2
7	H	303	PEG	C1-C2-O2-C3
7	F	302	PEG	C4-C3-O2-C2
6	G	307	GOL	O1-C1-C2-O2
7	N	303	PEG	C1-C2-O2-C3
7	F	302	PEG	C1-C2-O2-C3
6	c	203	GOL	O1-C1-C2-O2
6	E	307	GOL	O1-C1-C2-O2
6	G	307	GOL	O2-C2-C3-O3

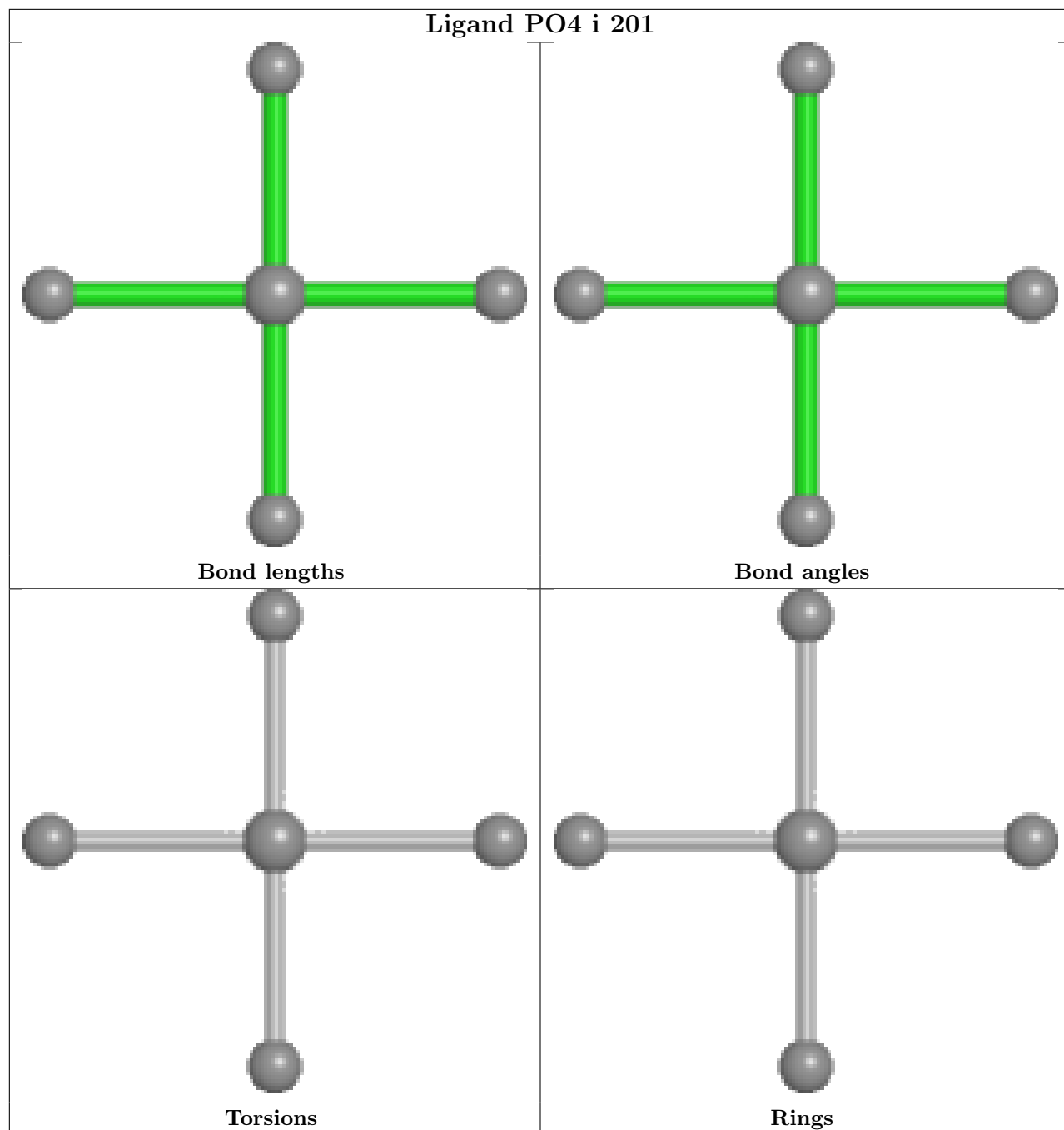
There are no ring outliers.

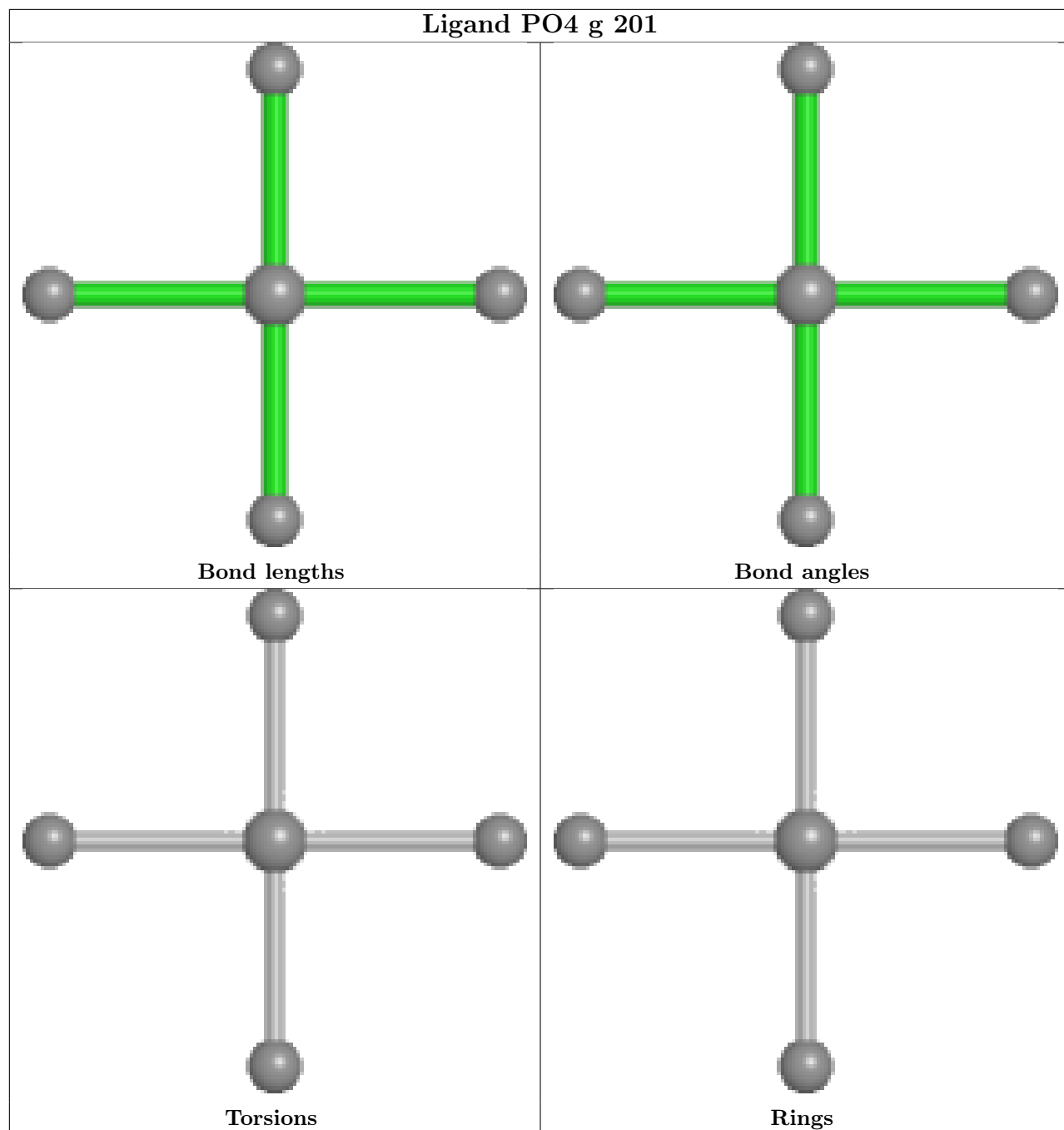
7 monomers are involved in 9 short contacts:

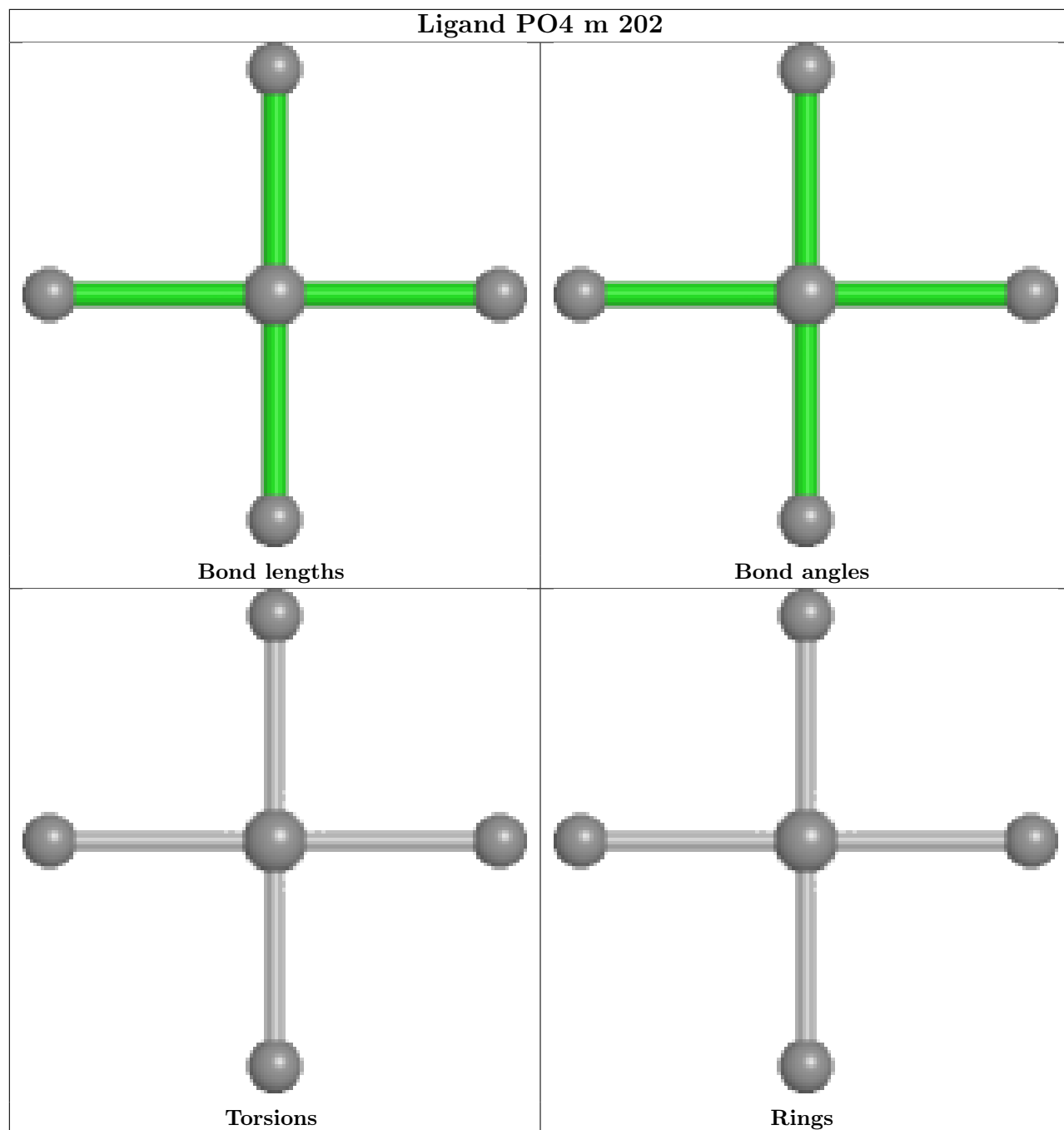
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	306	GOL	3	0
4	R	301	PO4	1	0
7	N	303	PEG	1	0
4	M	302	PO4	1	0
4	C	301	PO4	1	0
4	J	302	PO4	1	0
4	E	304	PO4	1	0

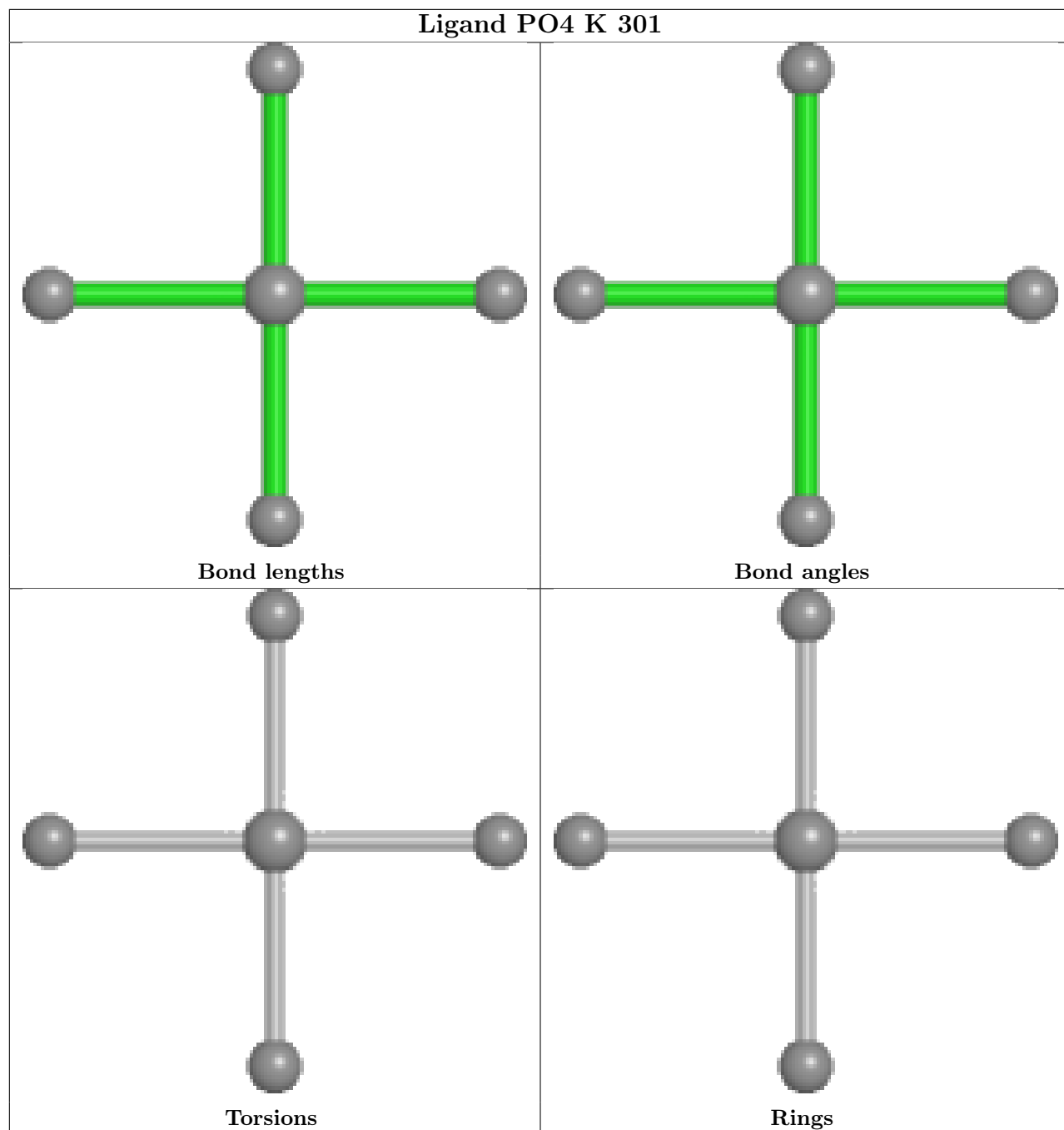
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

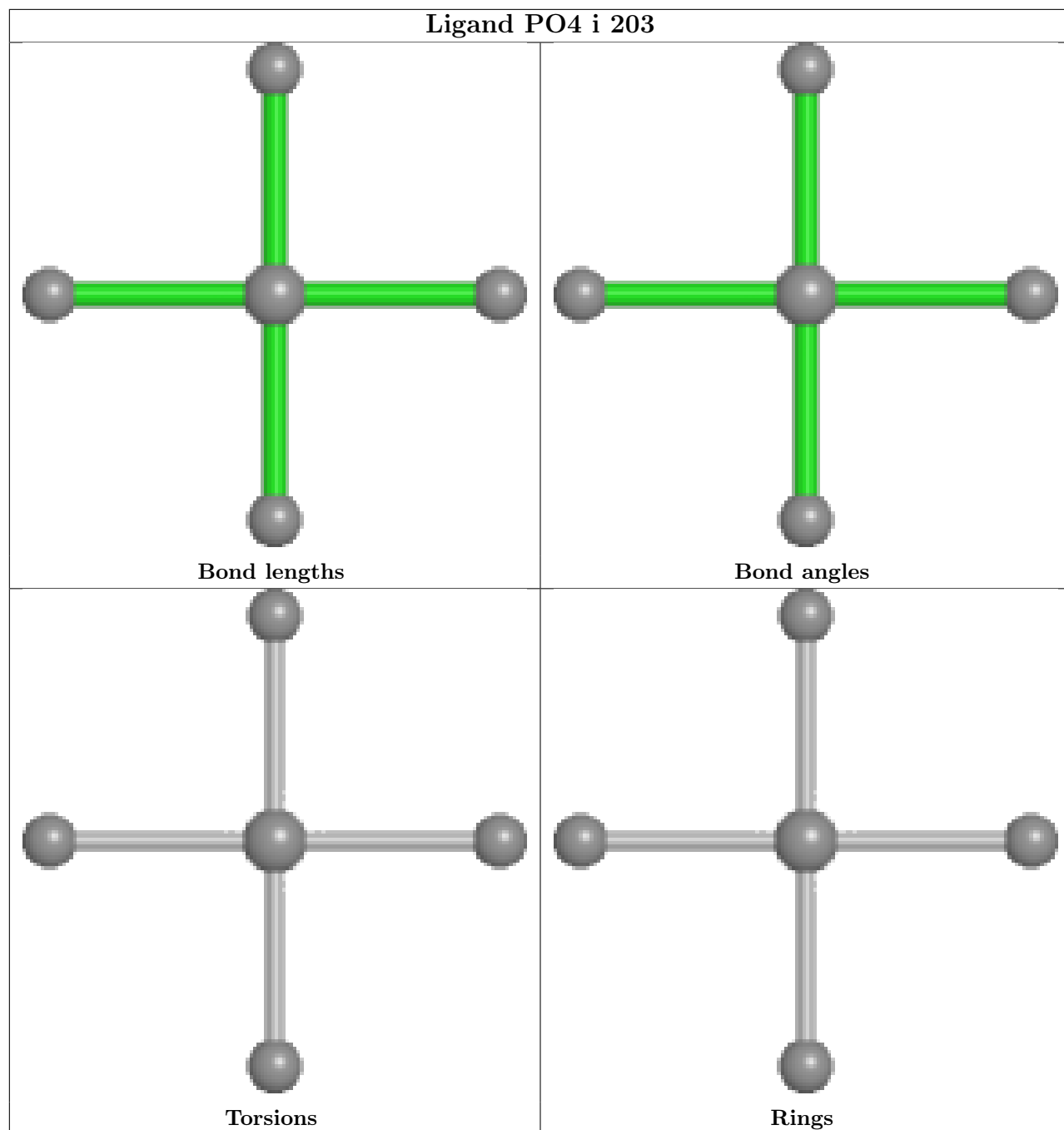


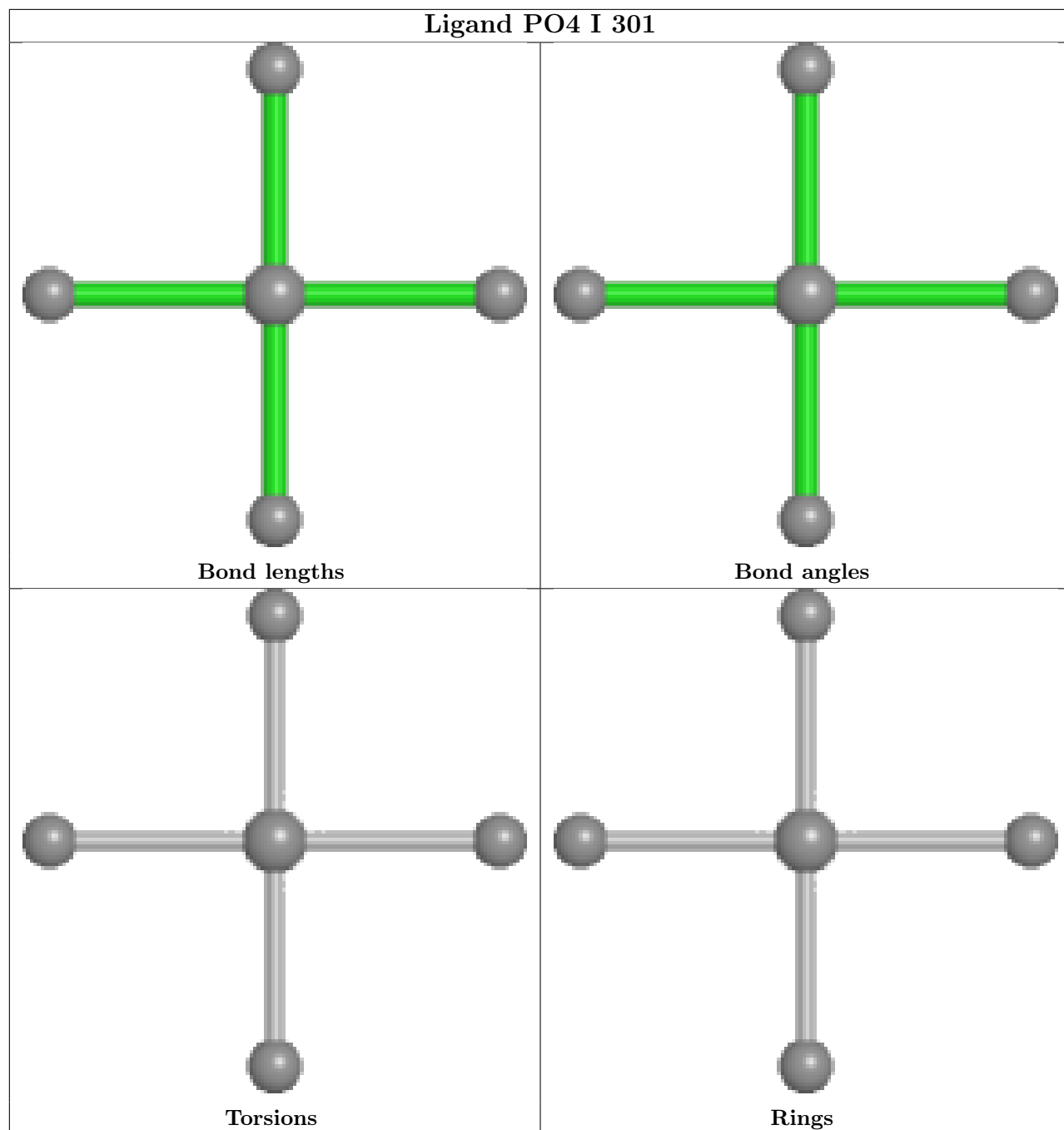


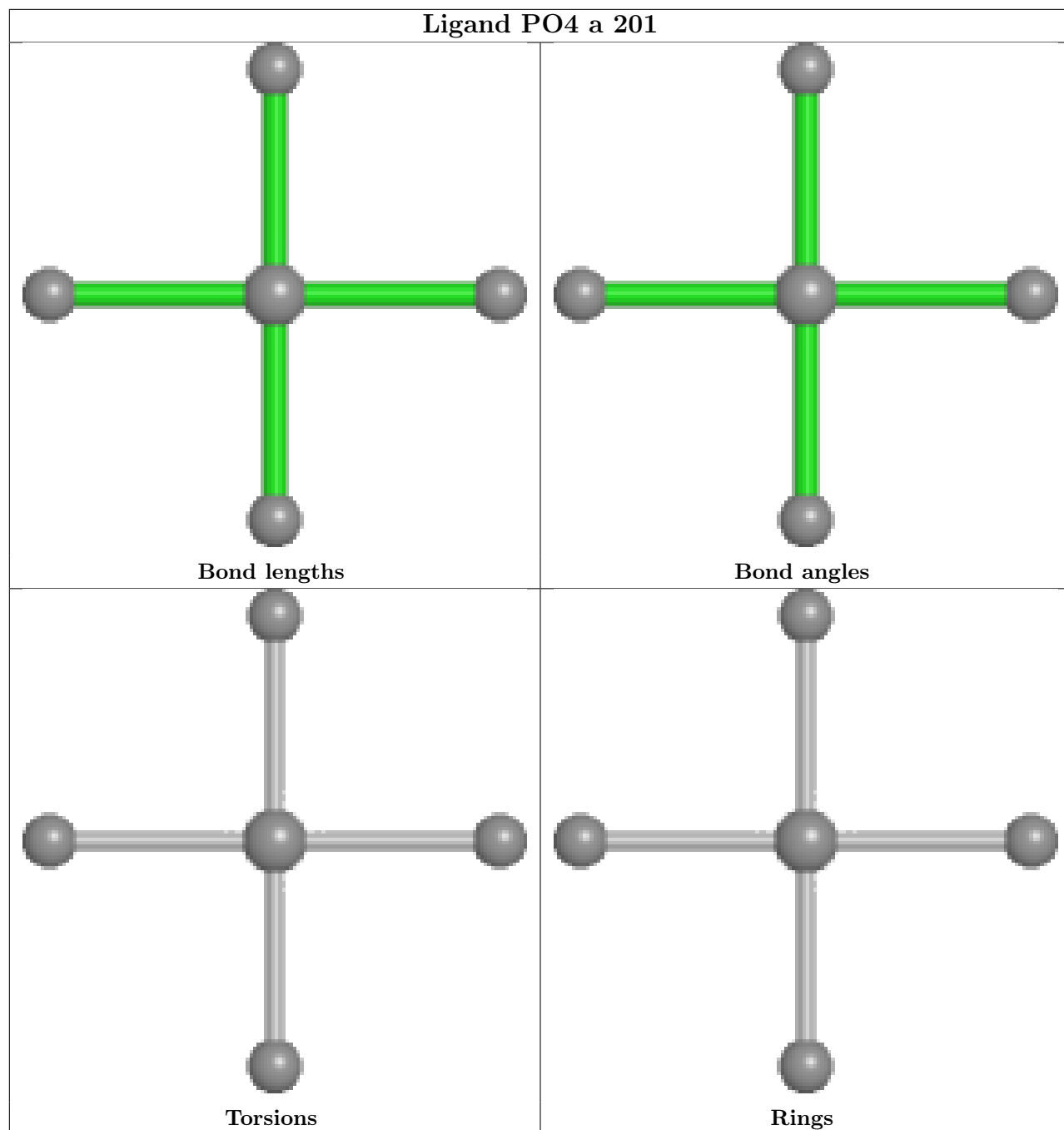


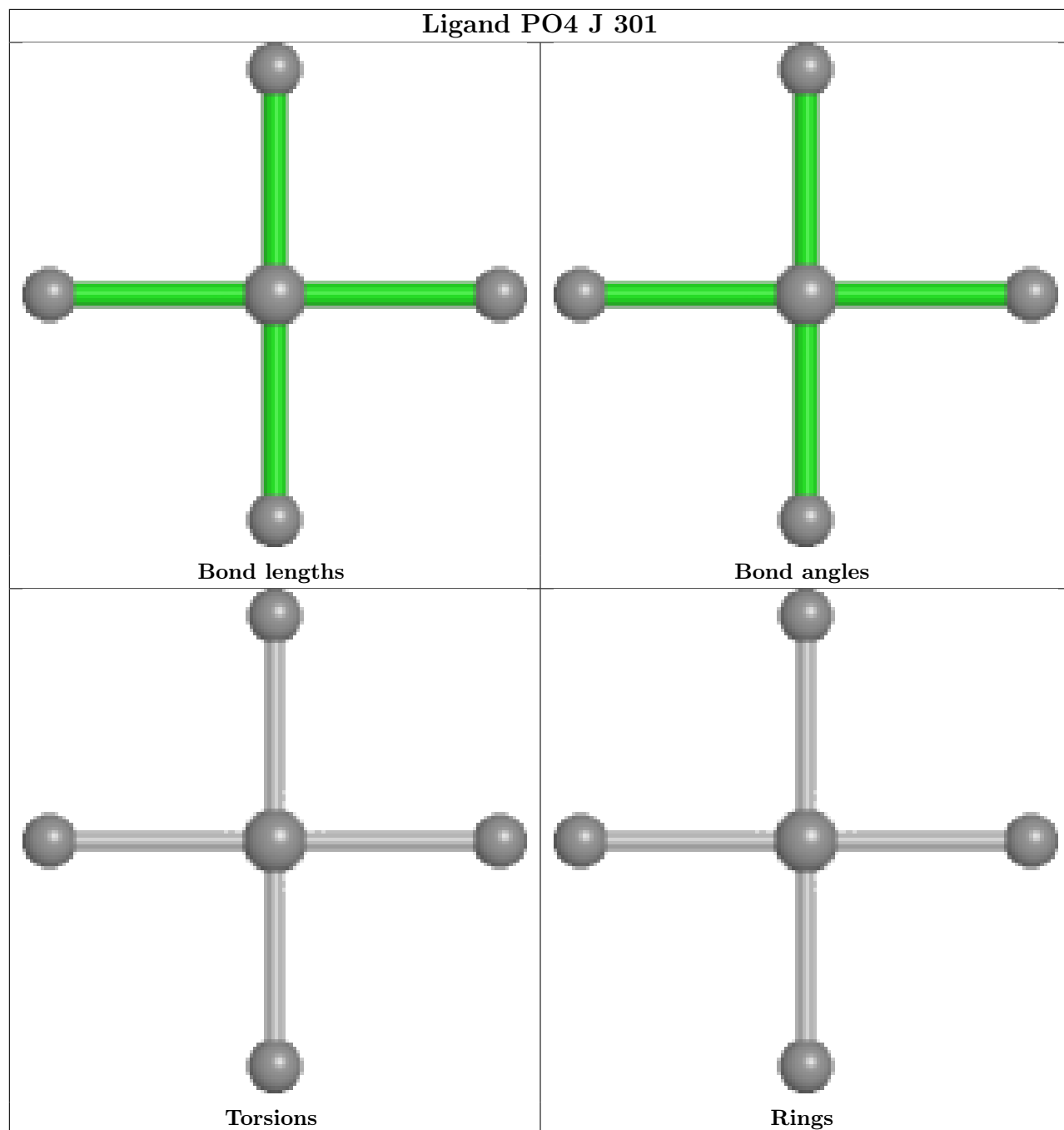


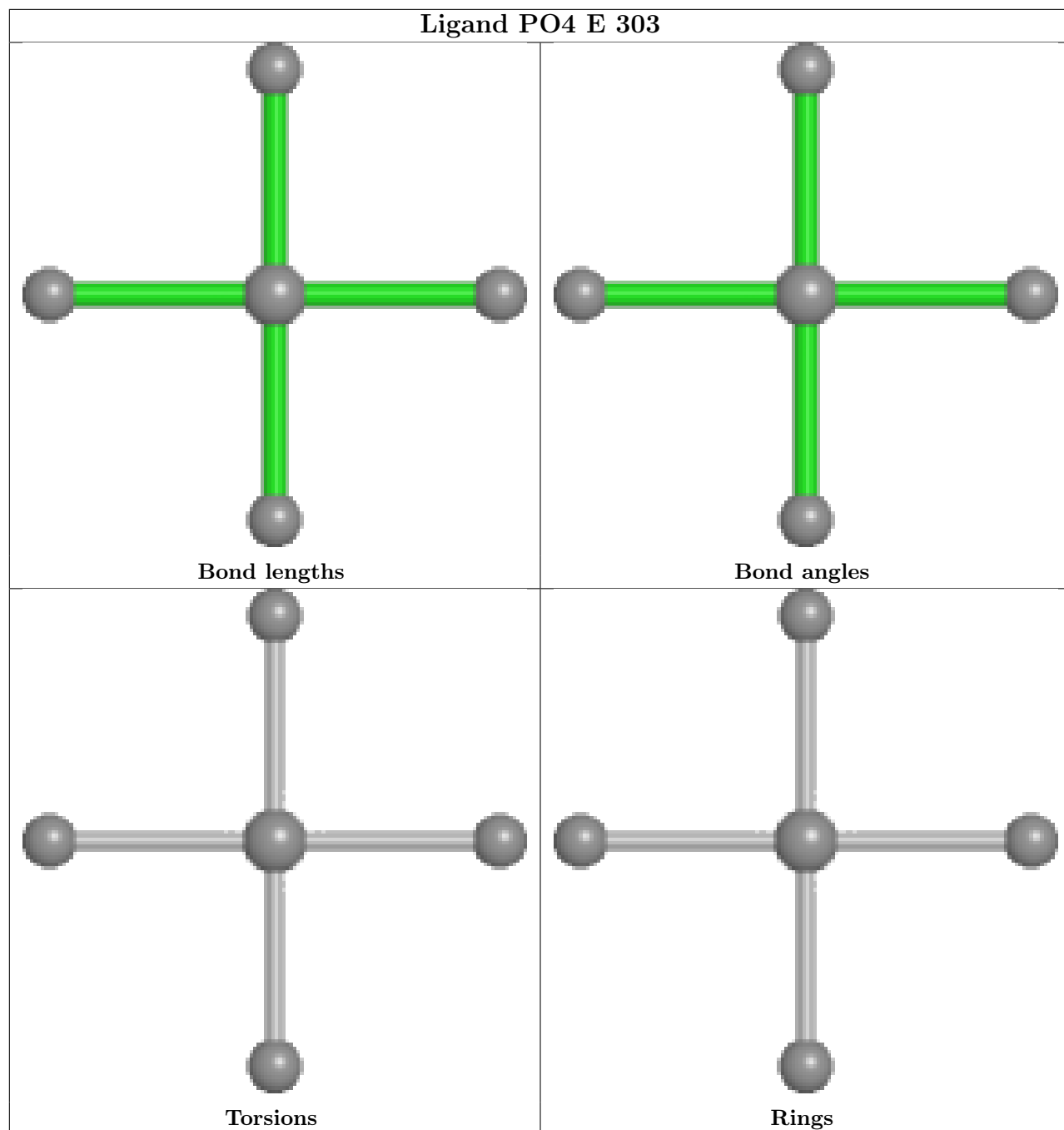


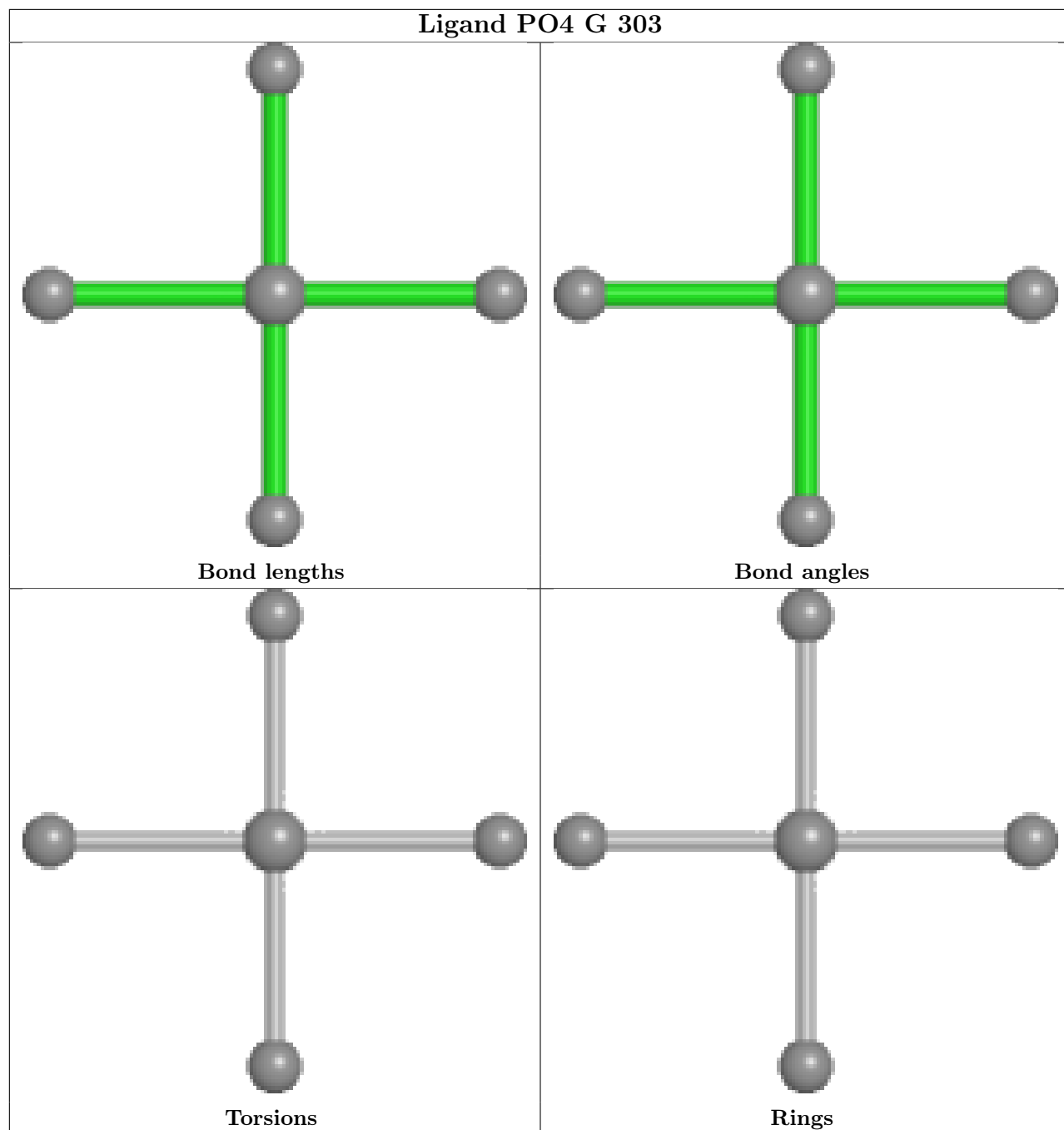


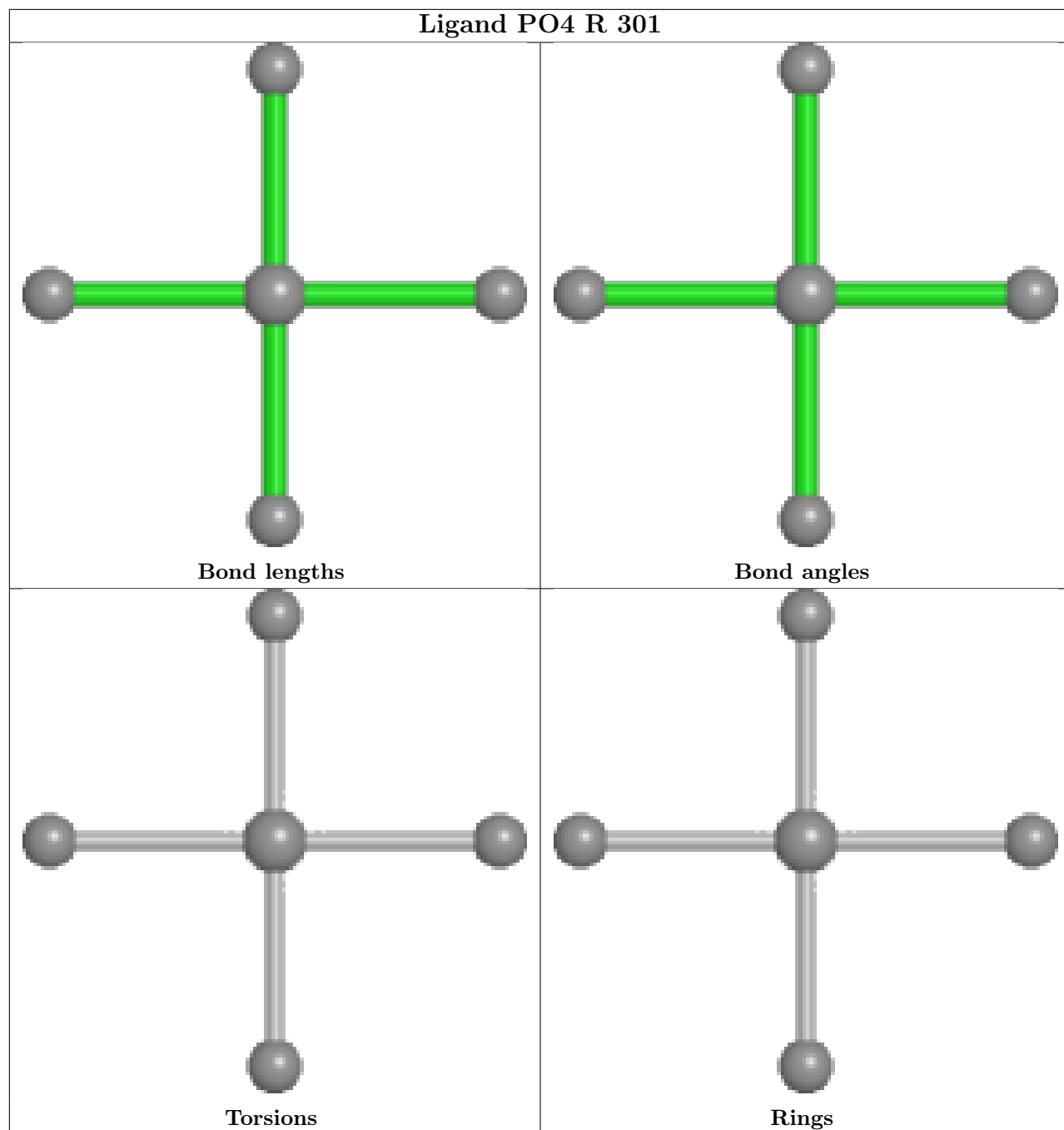


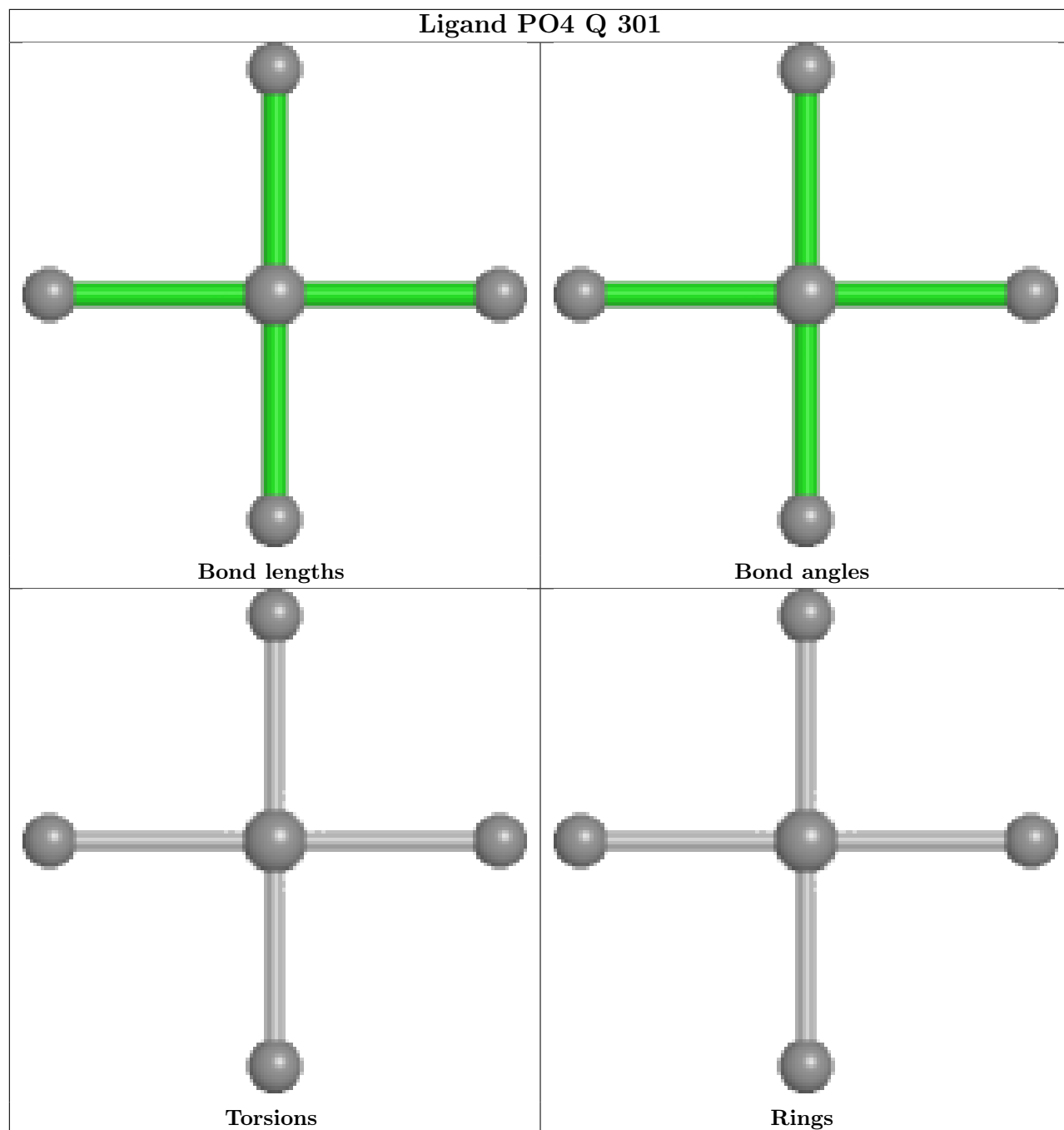


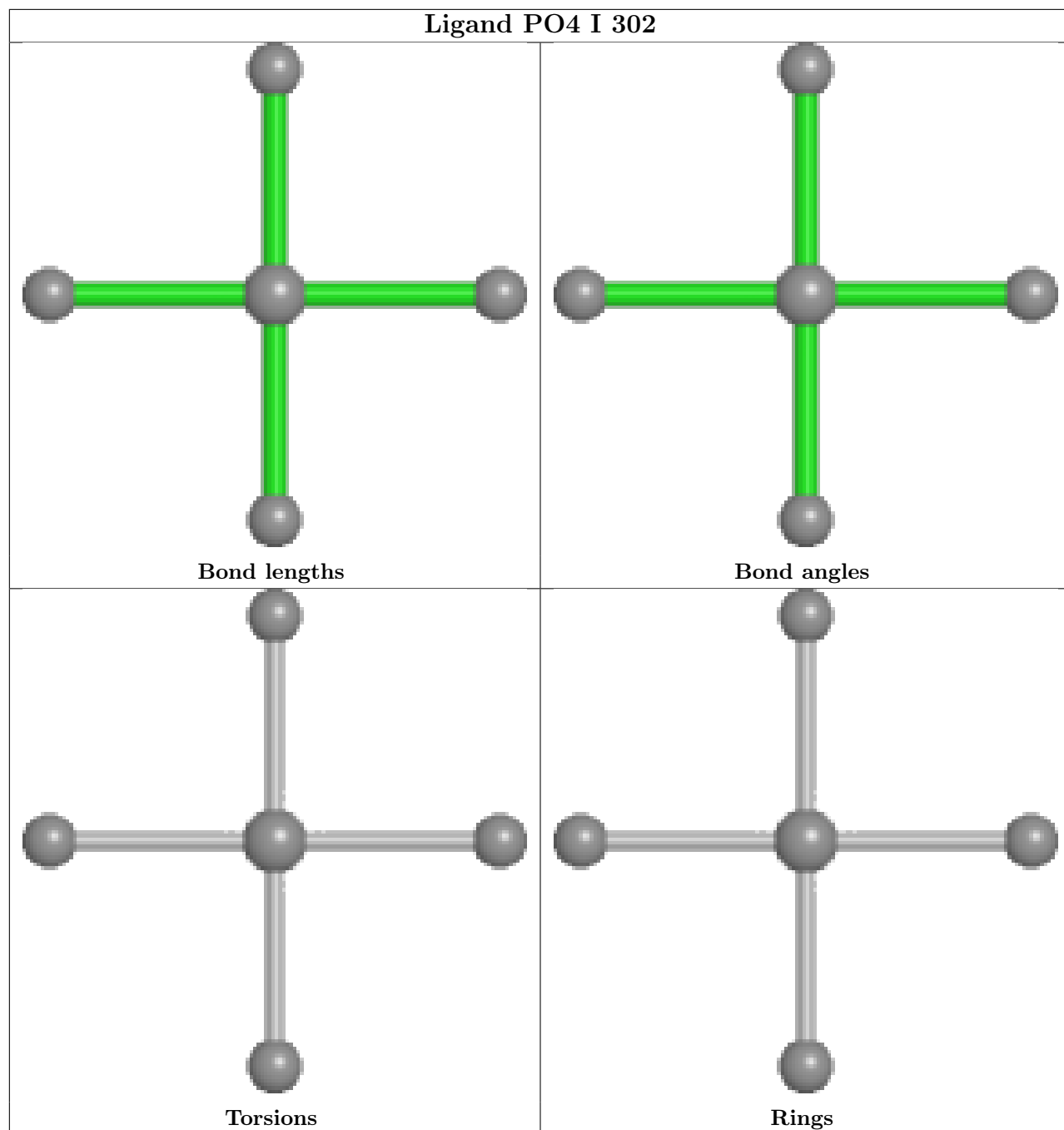


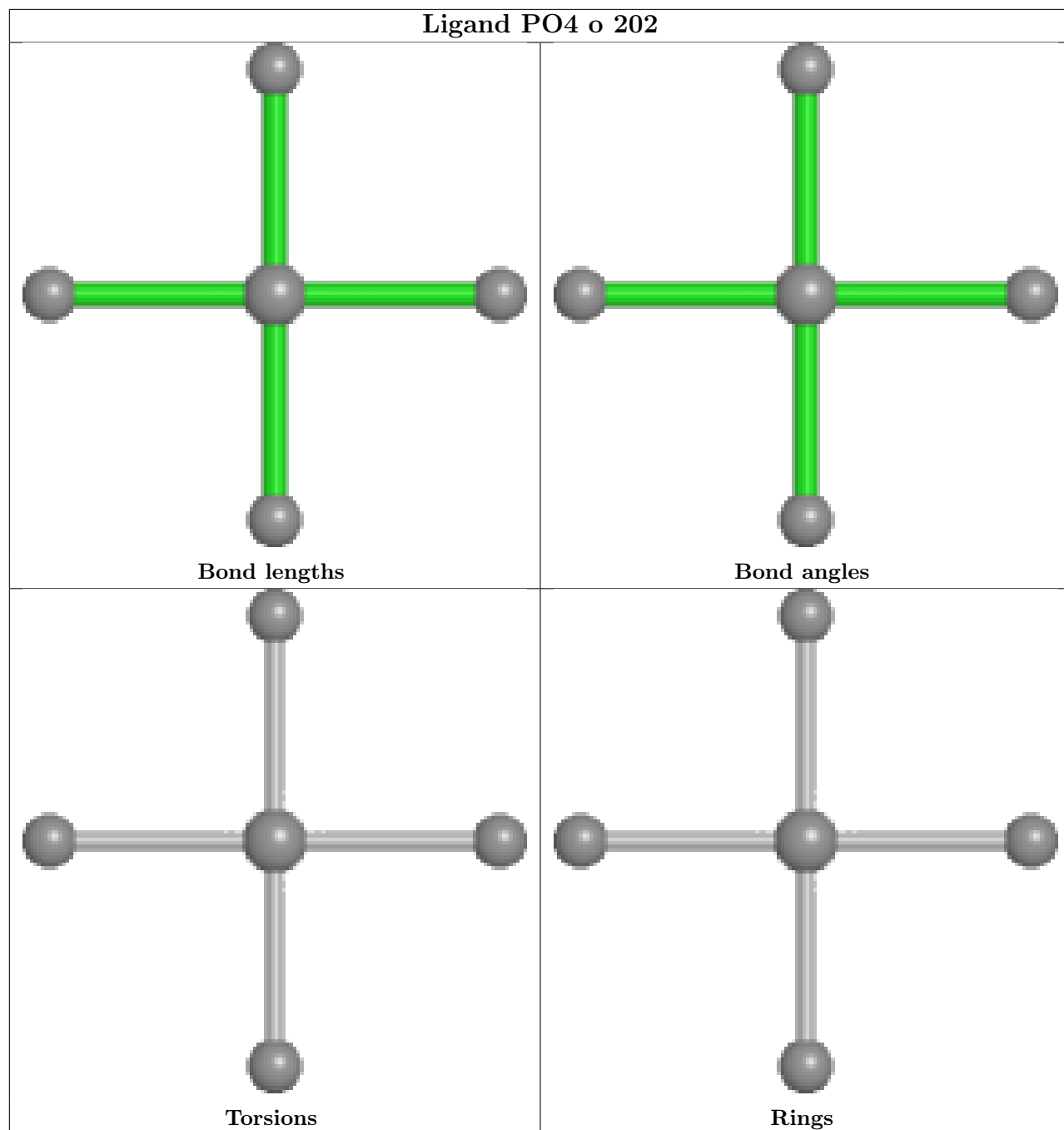


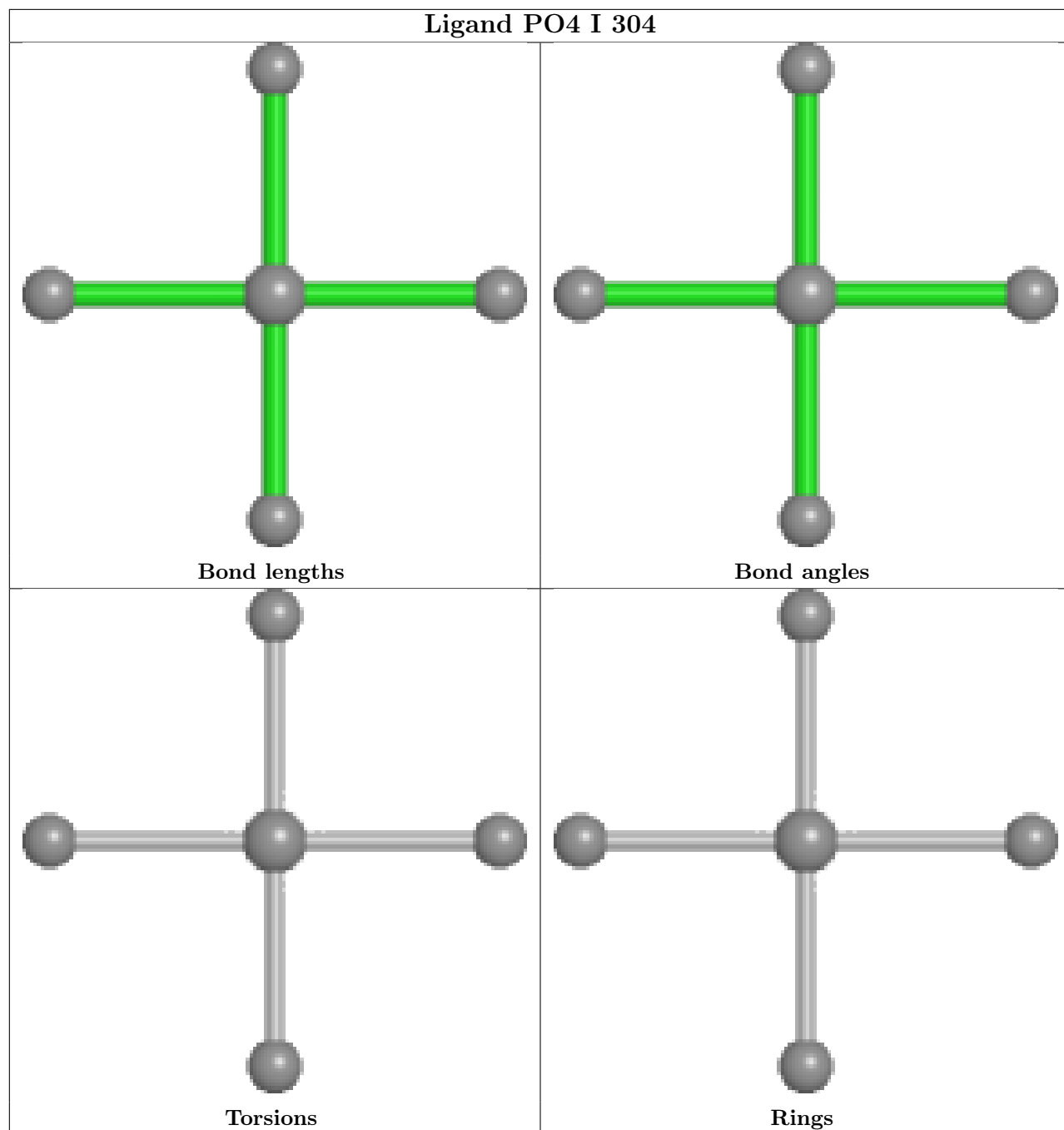


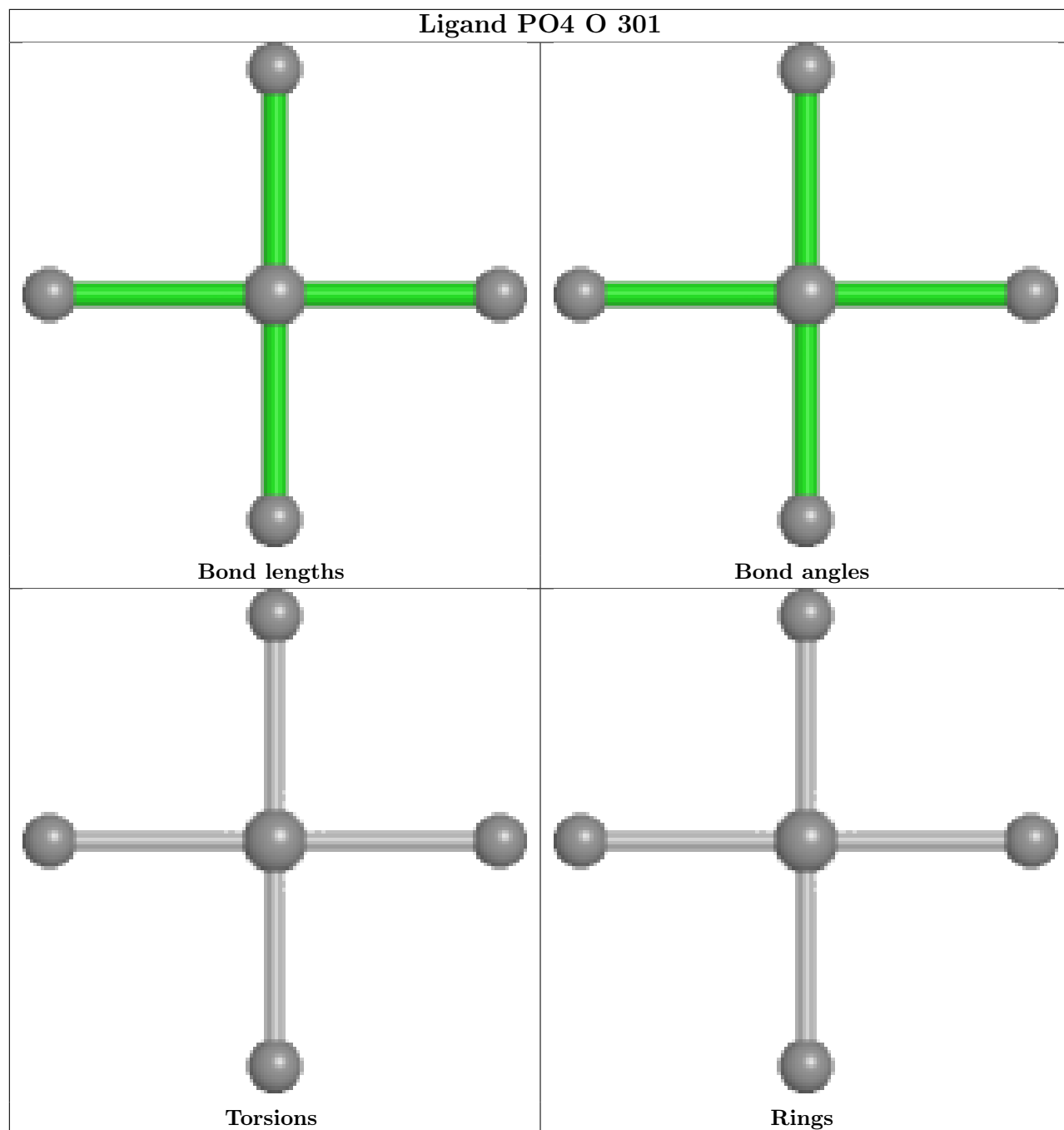


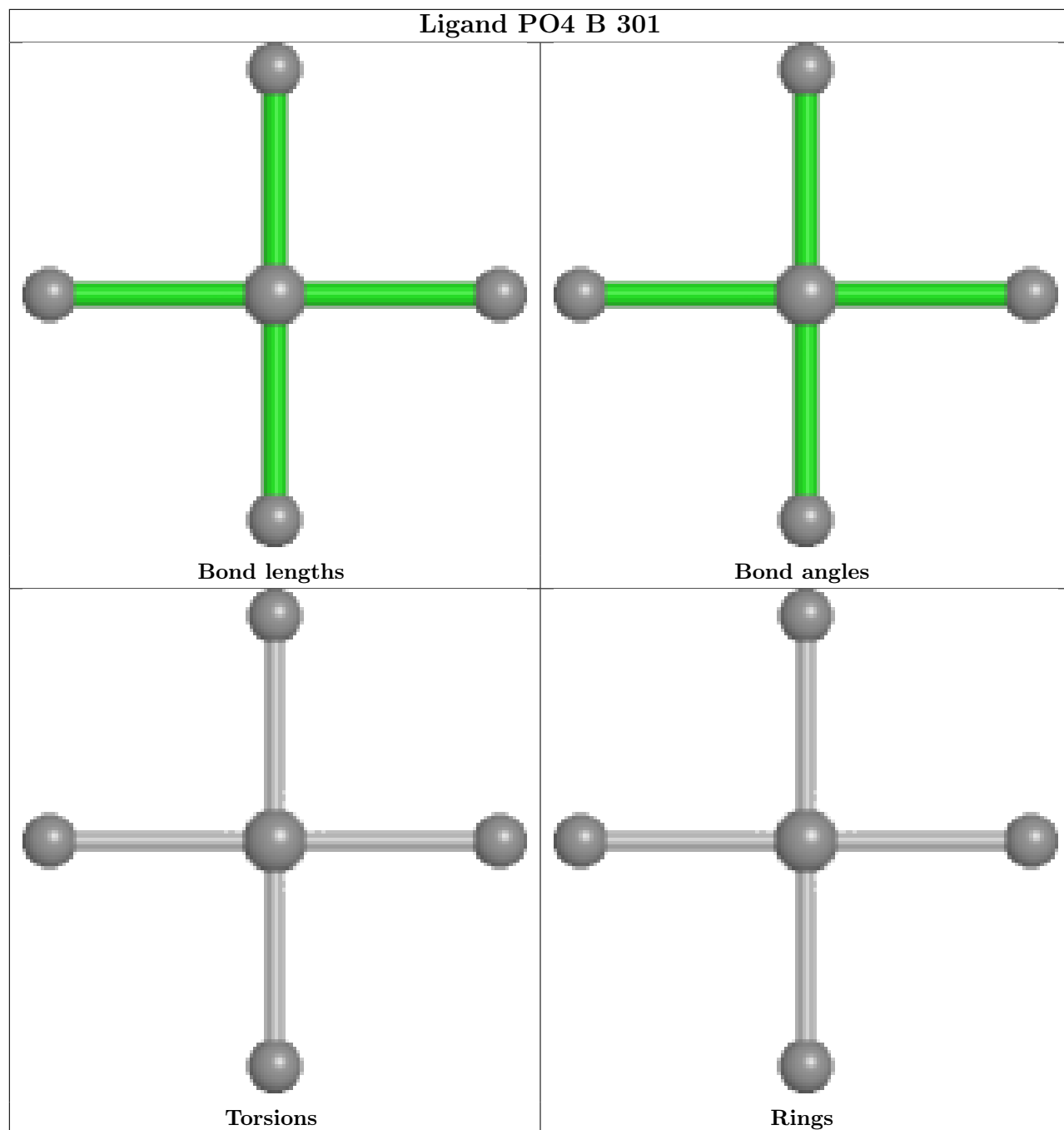


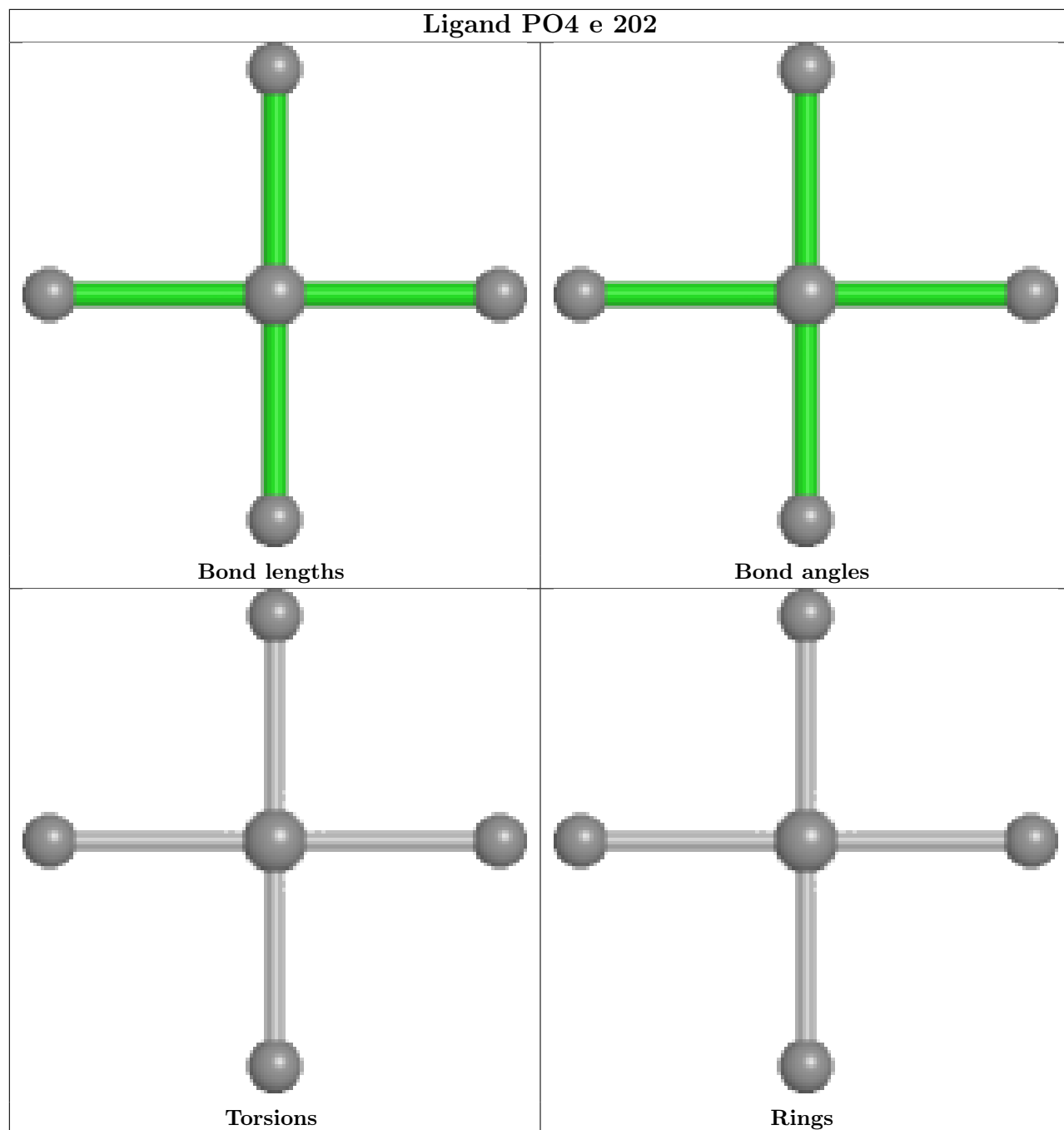


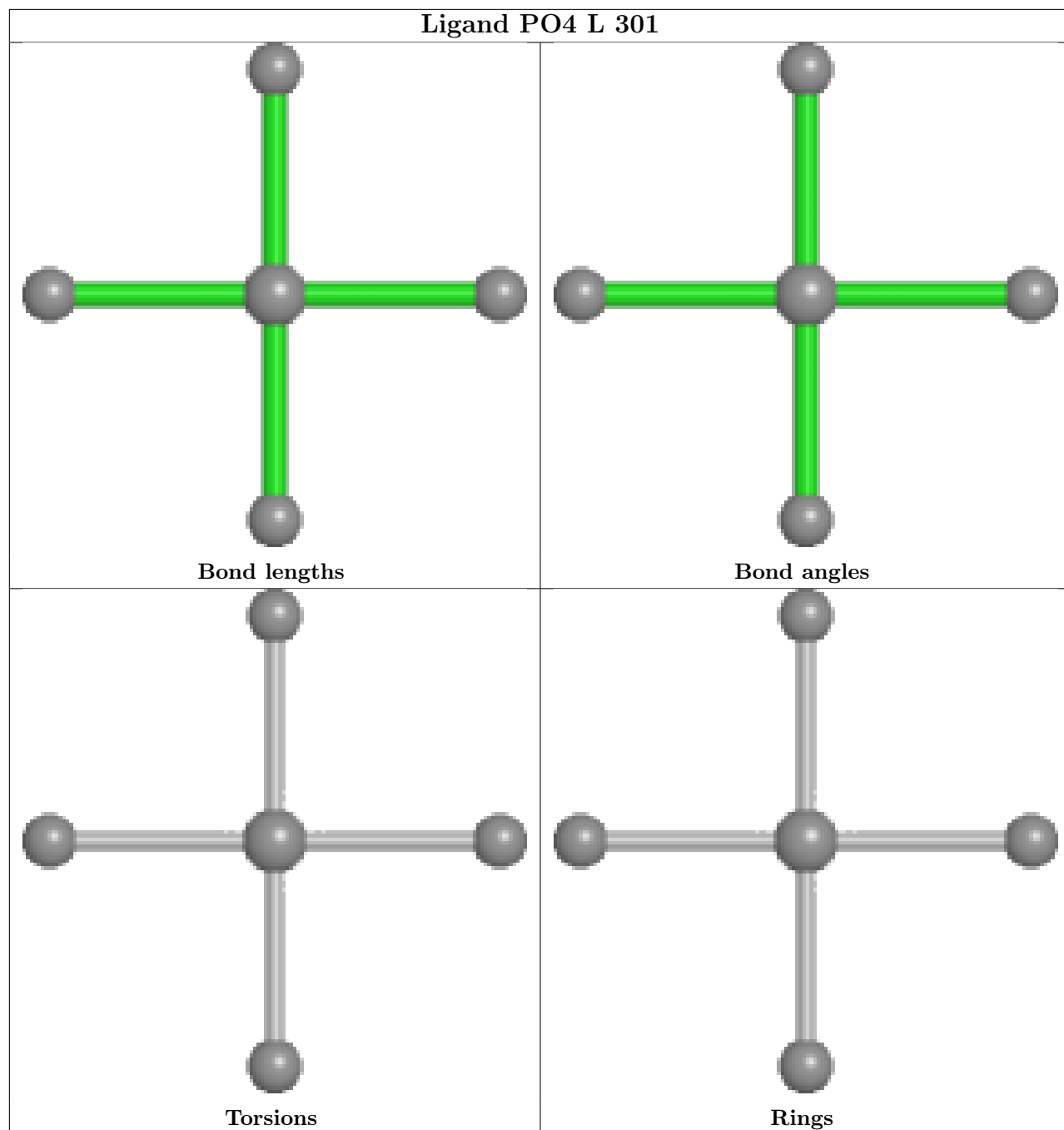


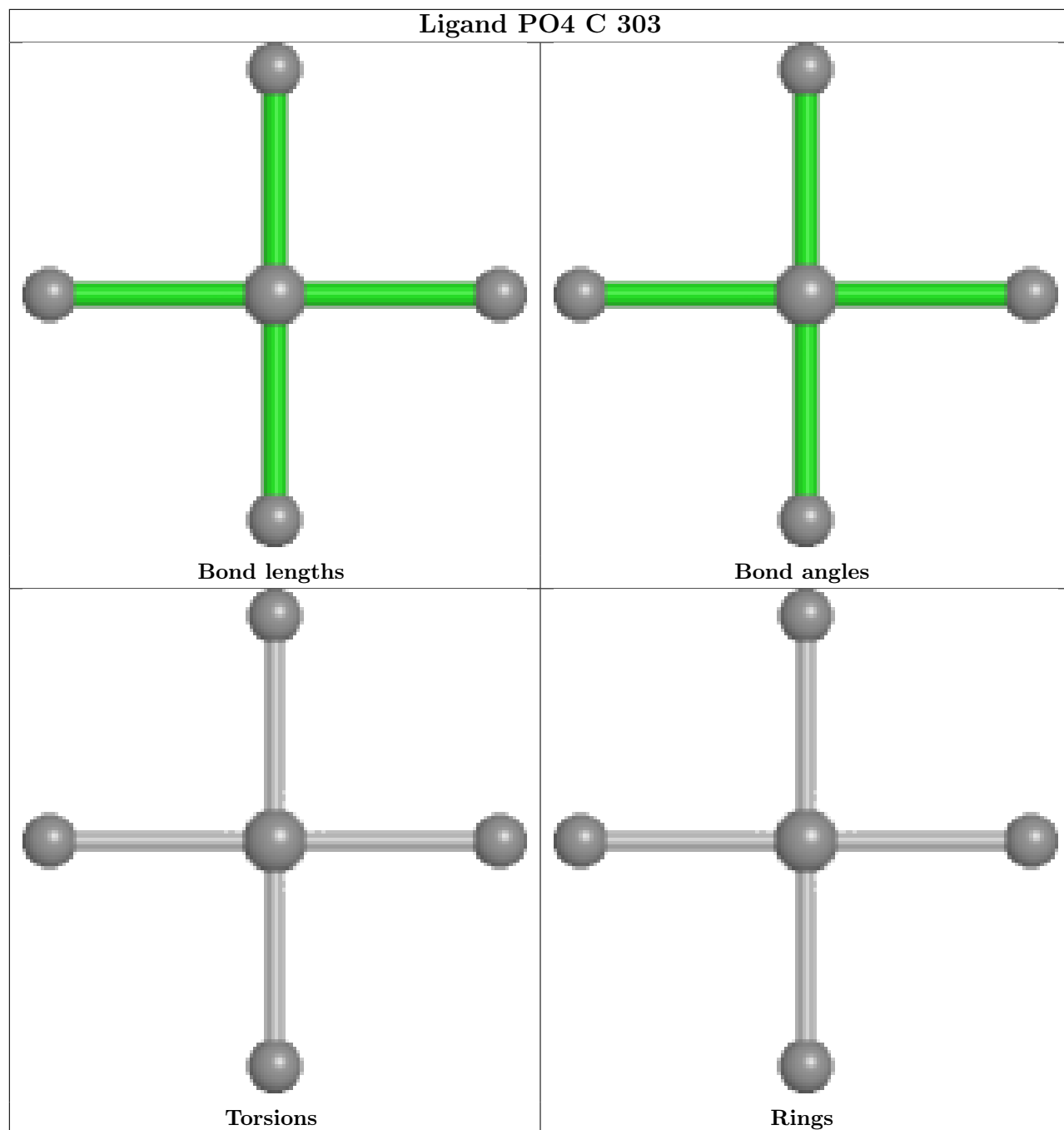


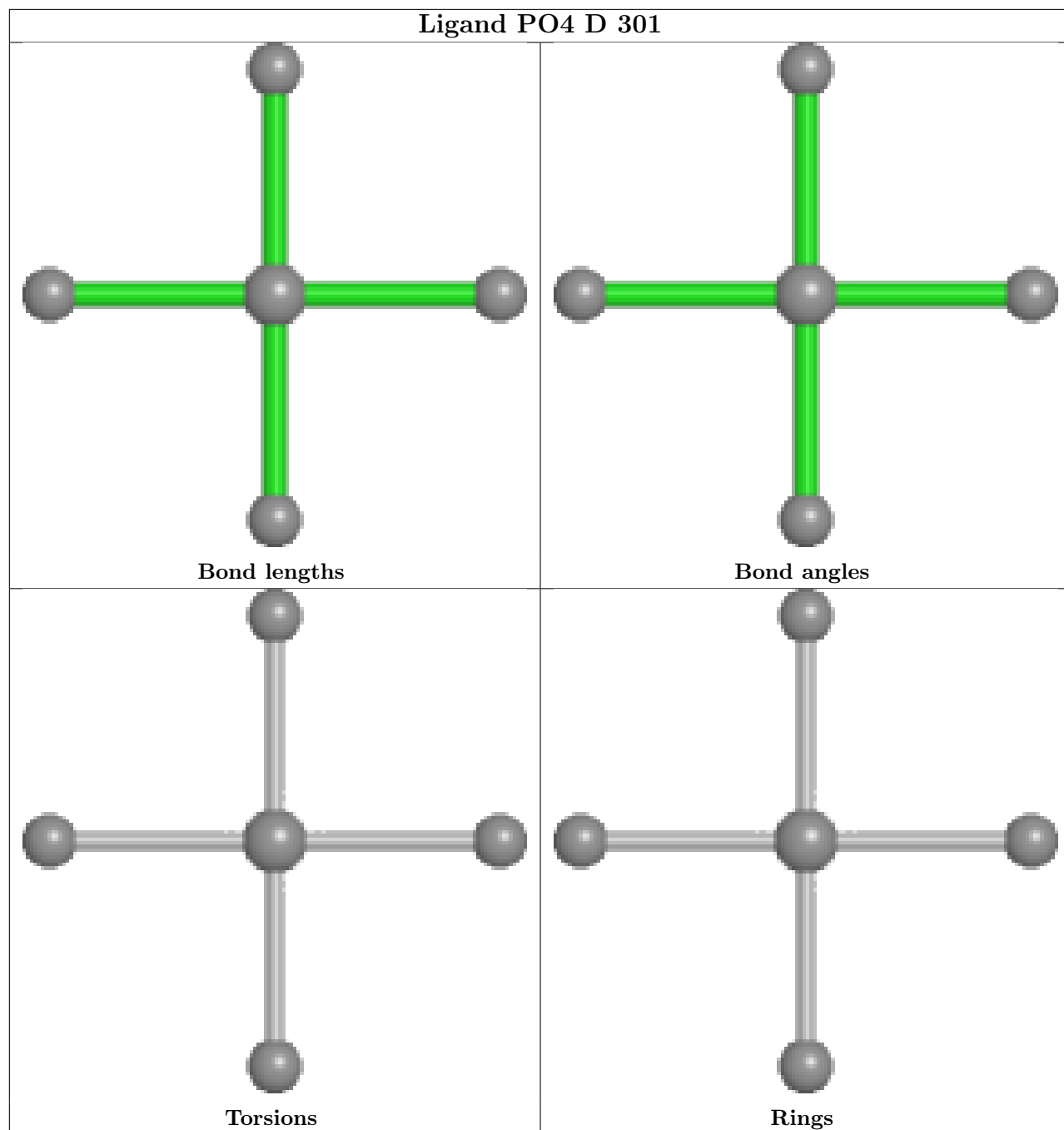


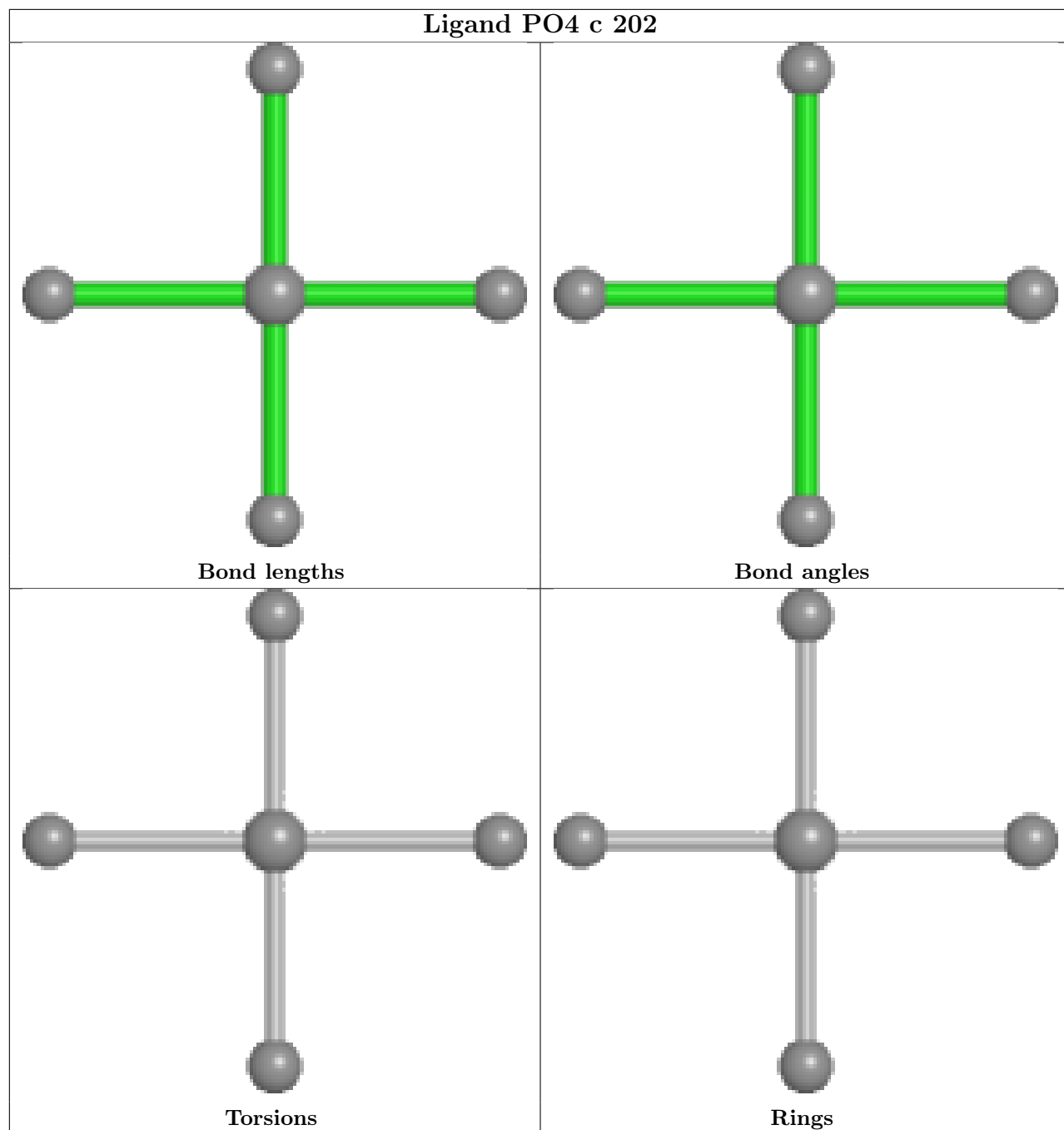


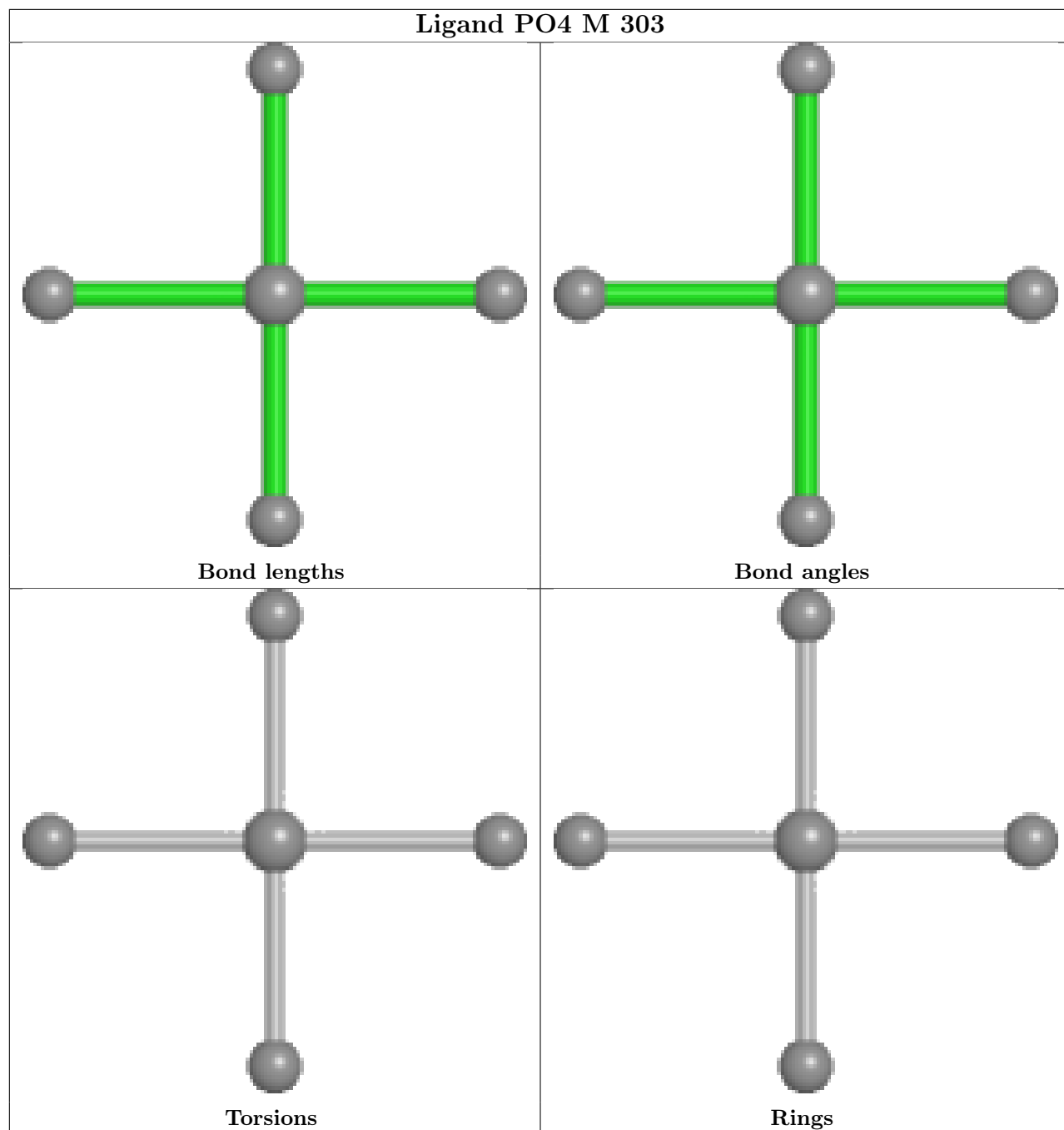


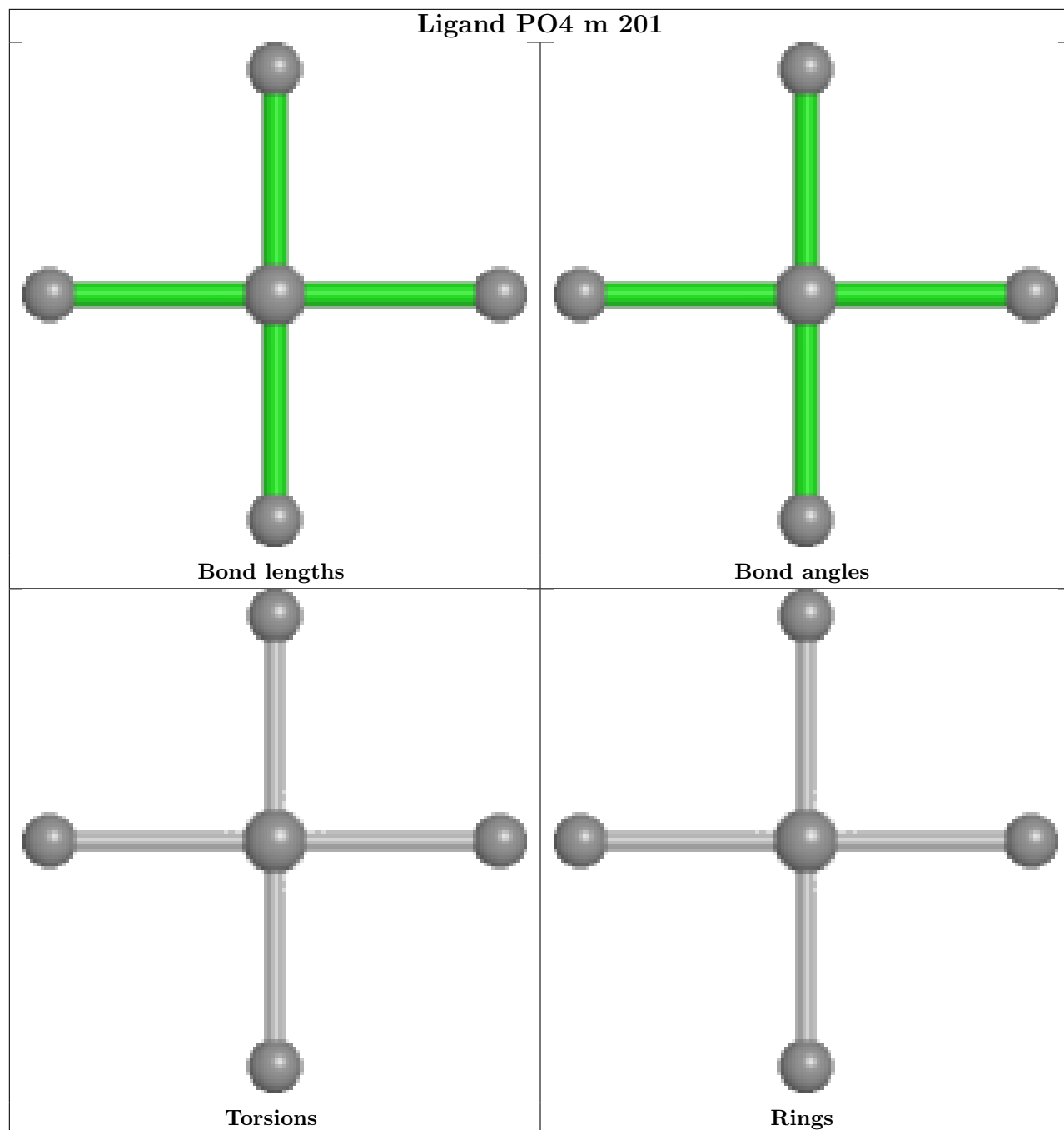


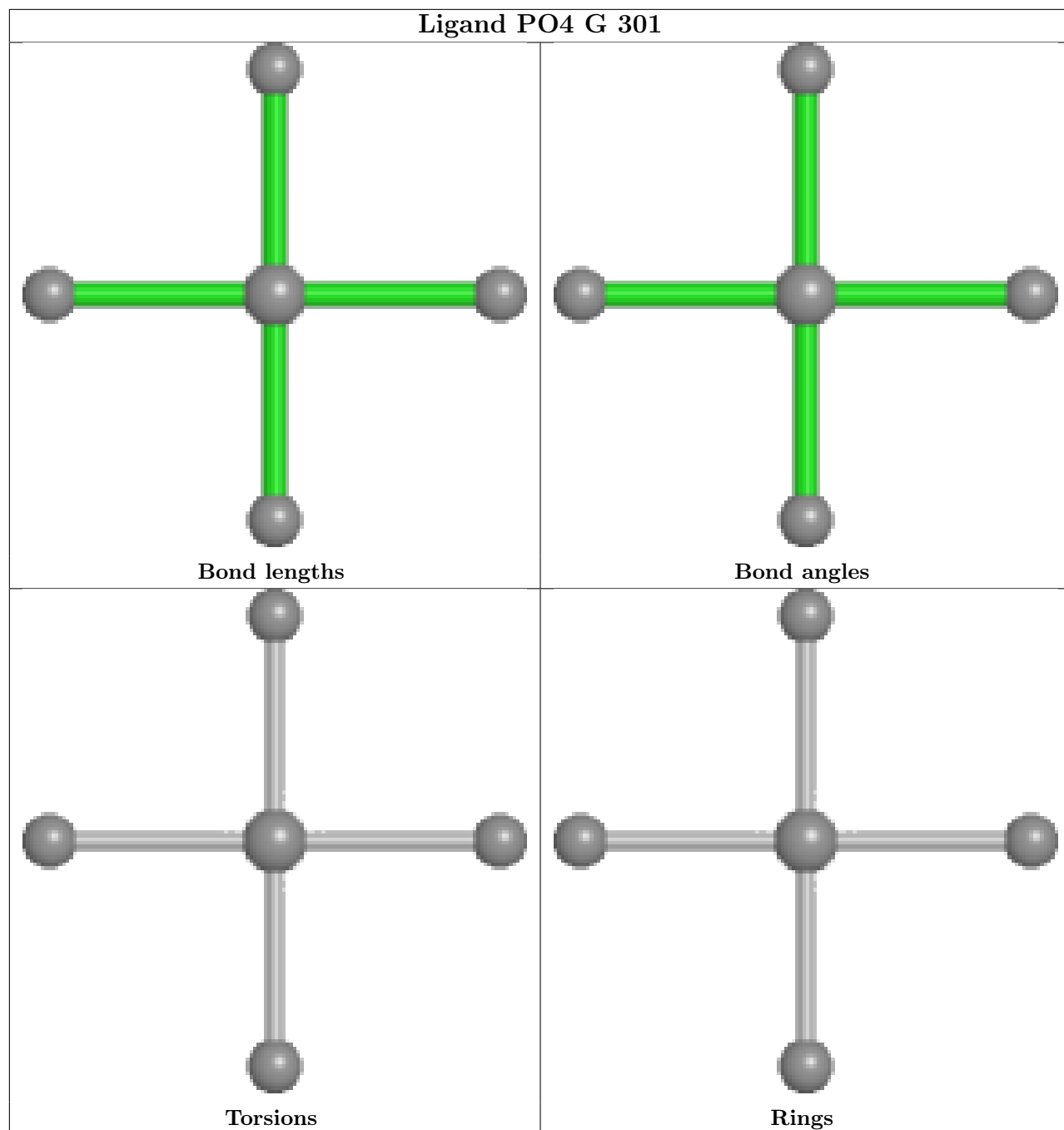


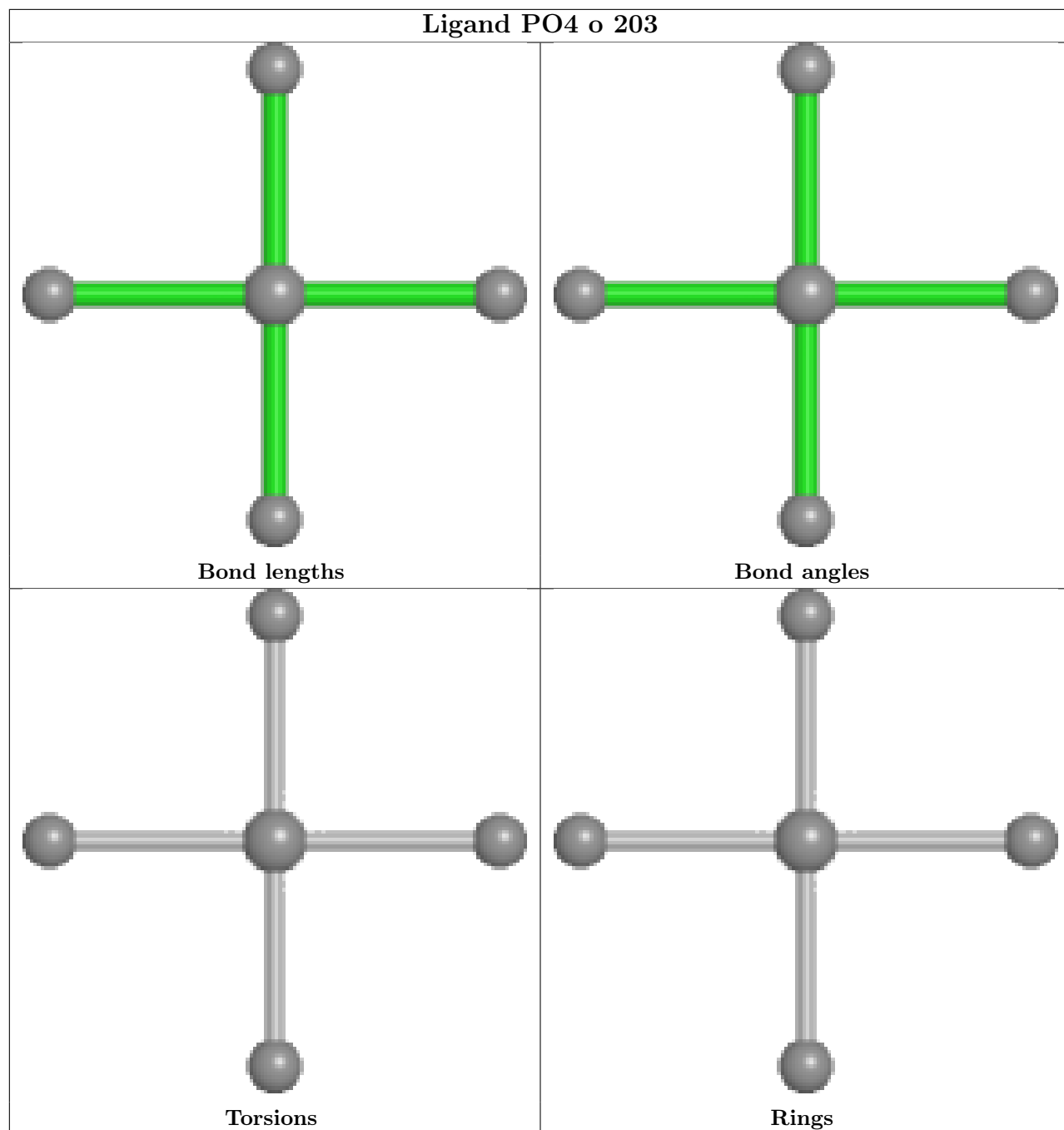


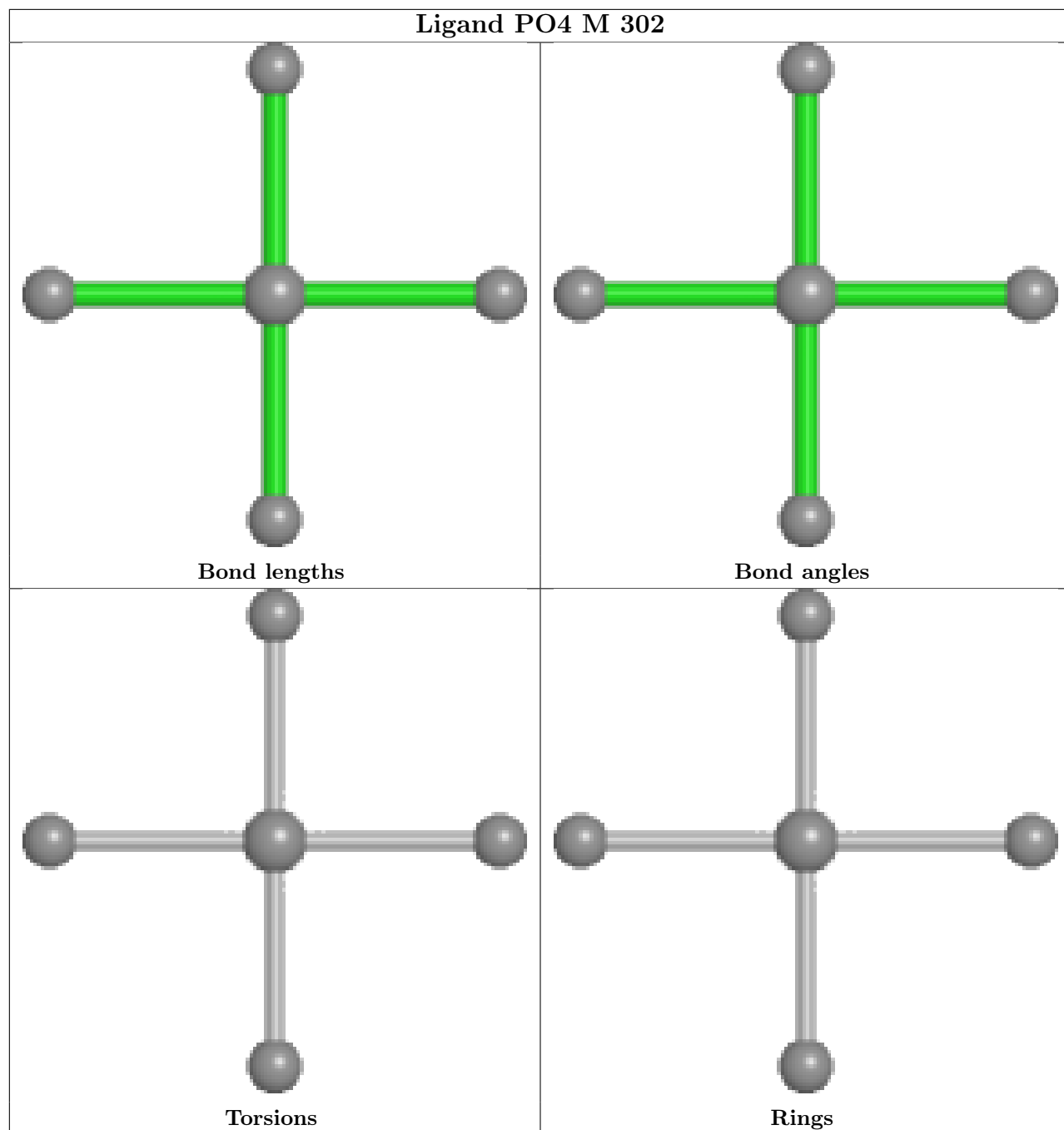


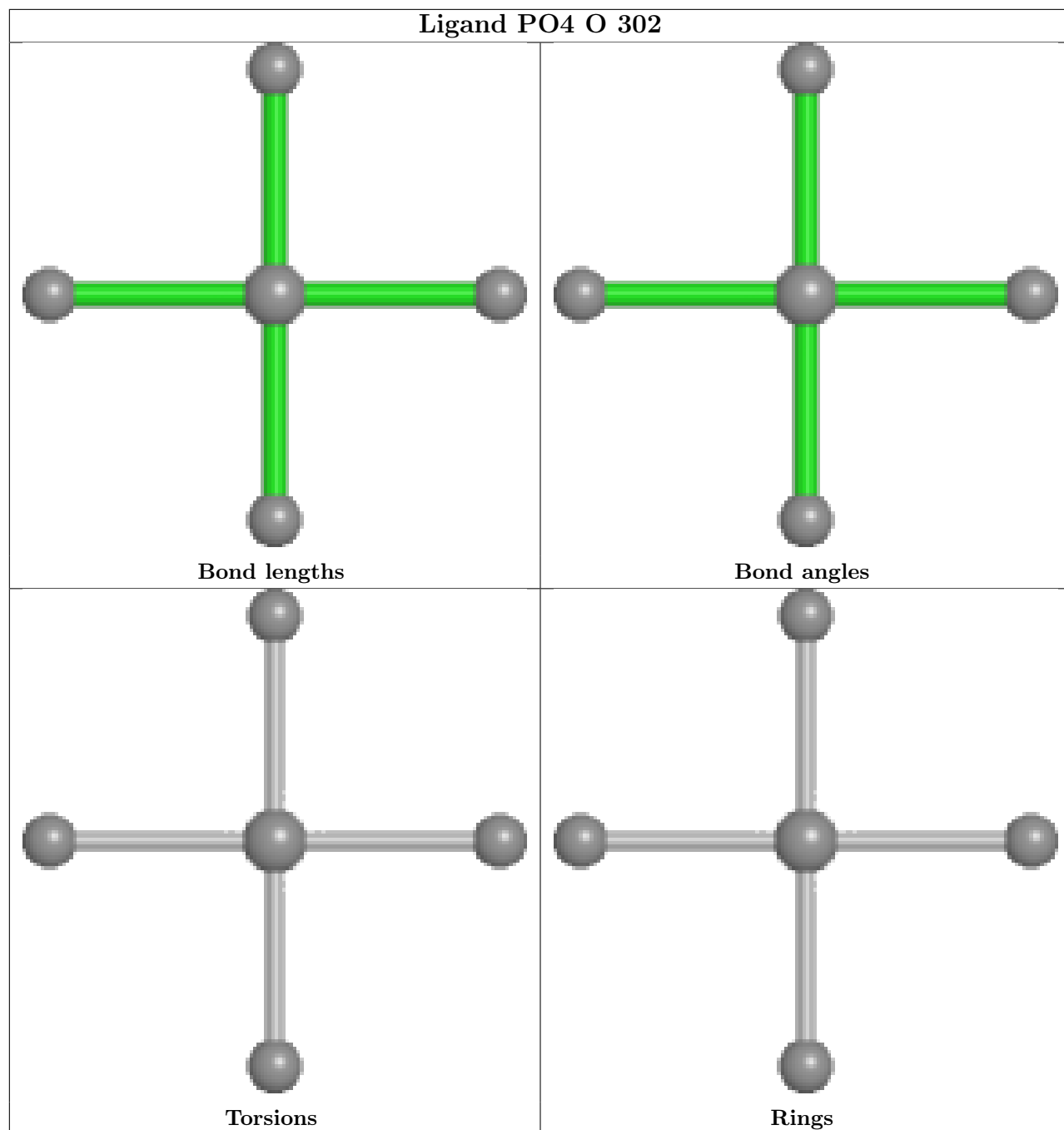


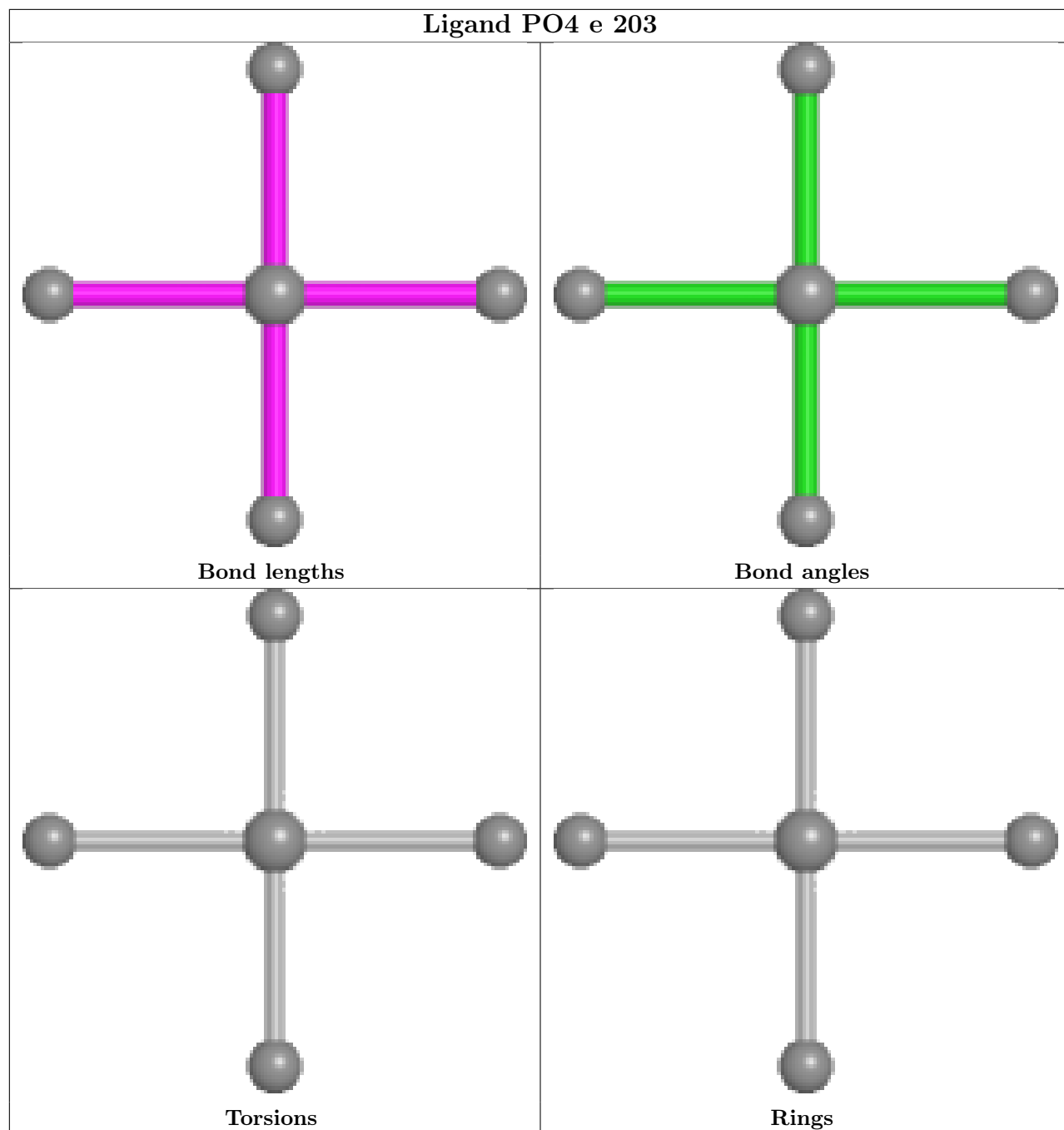


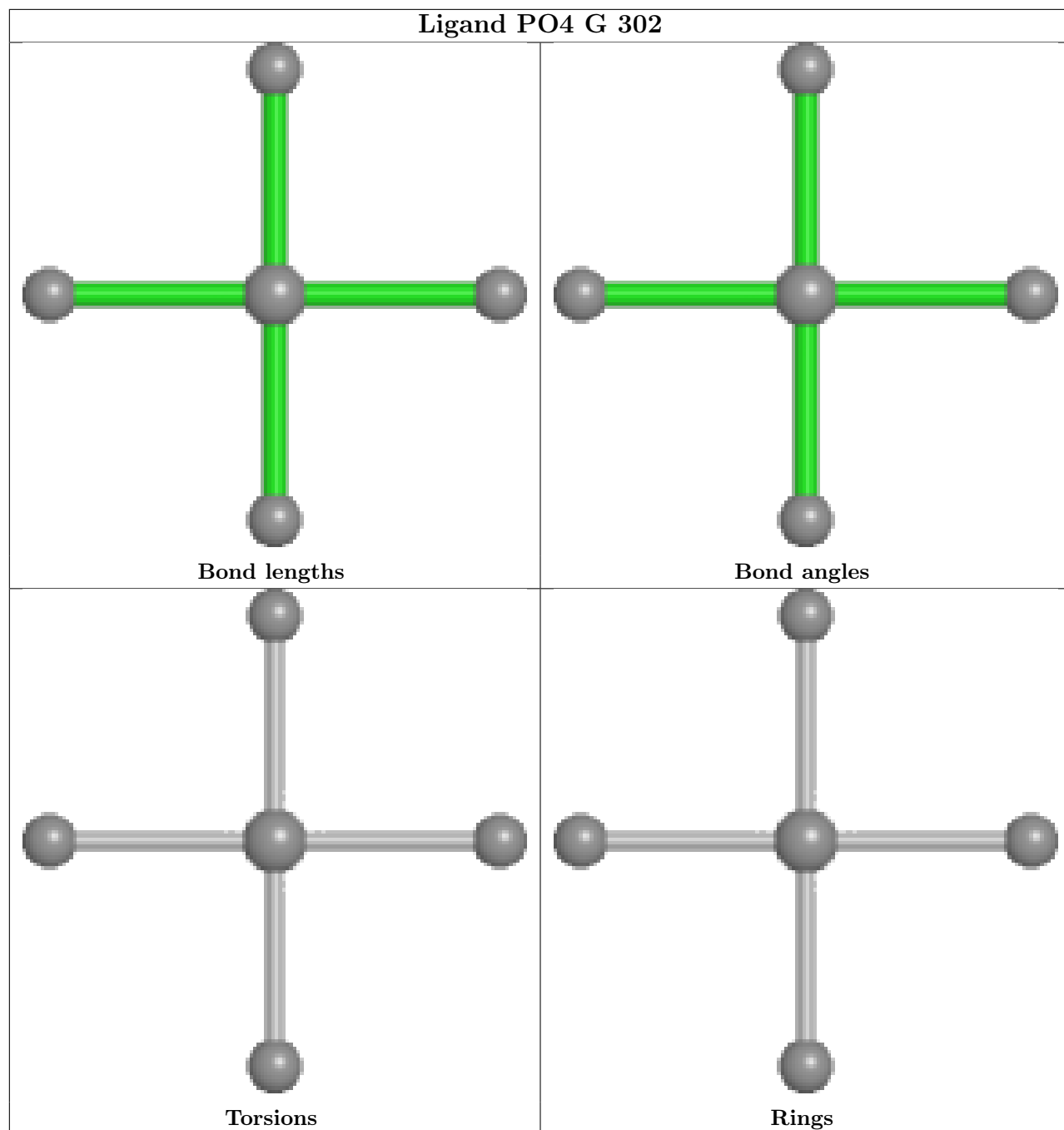


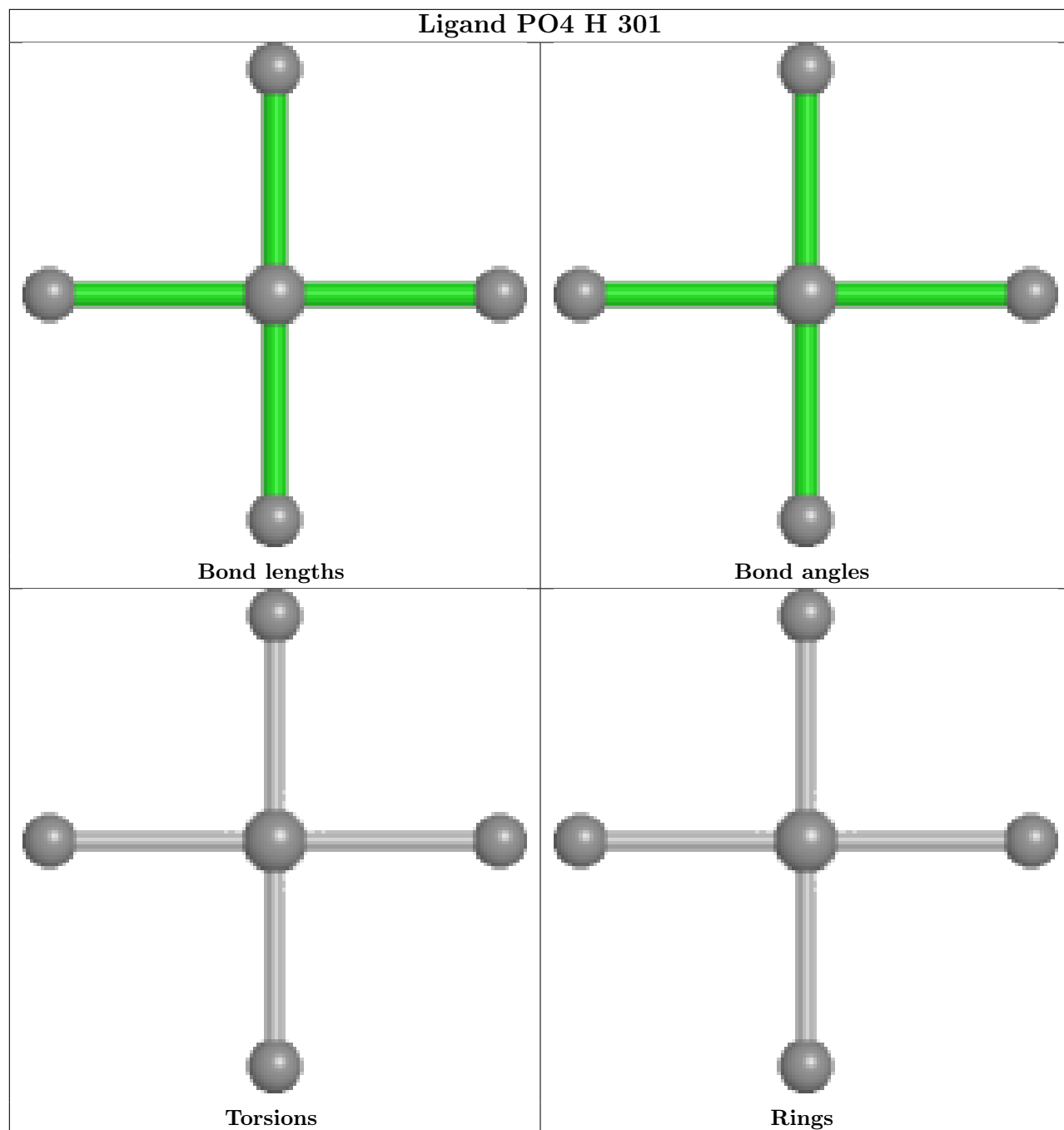


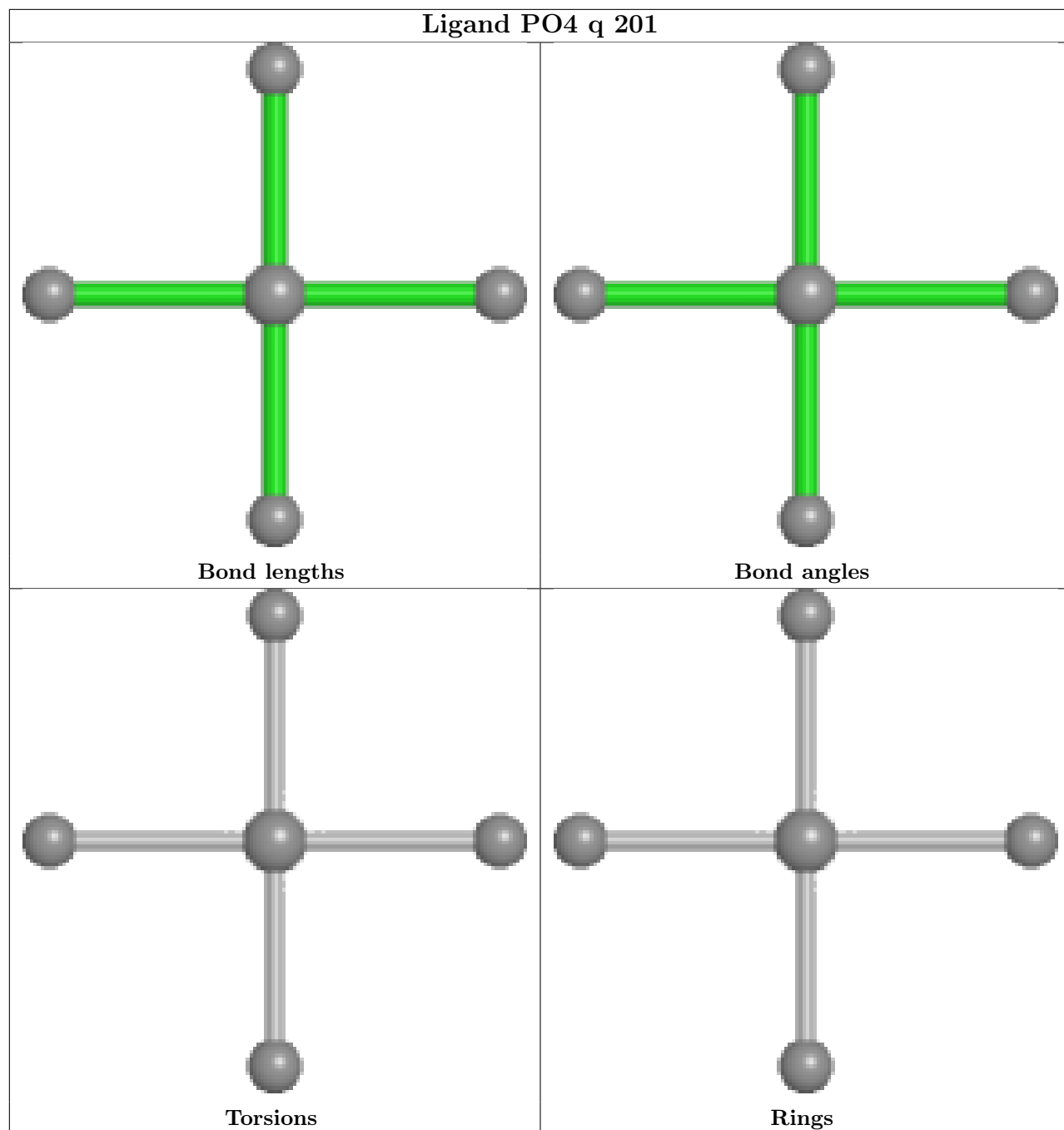


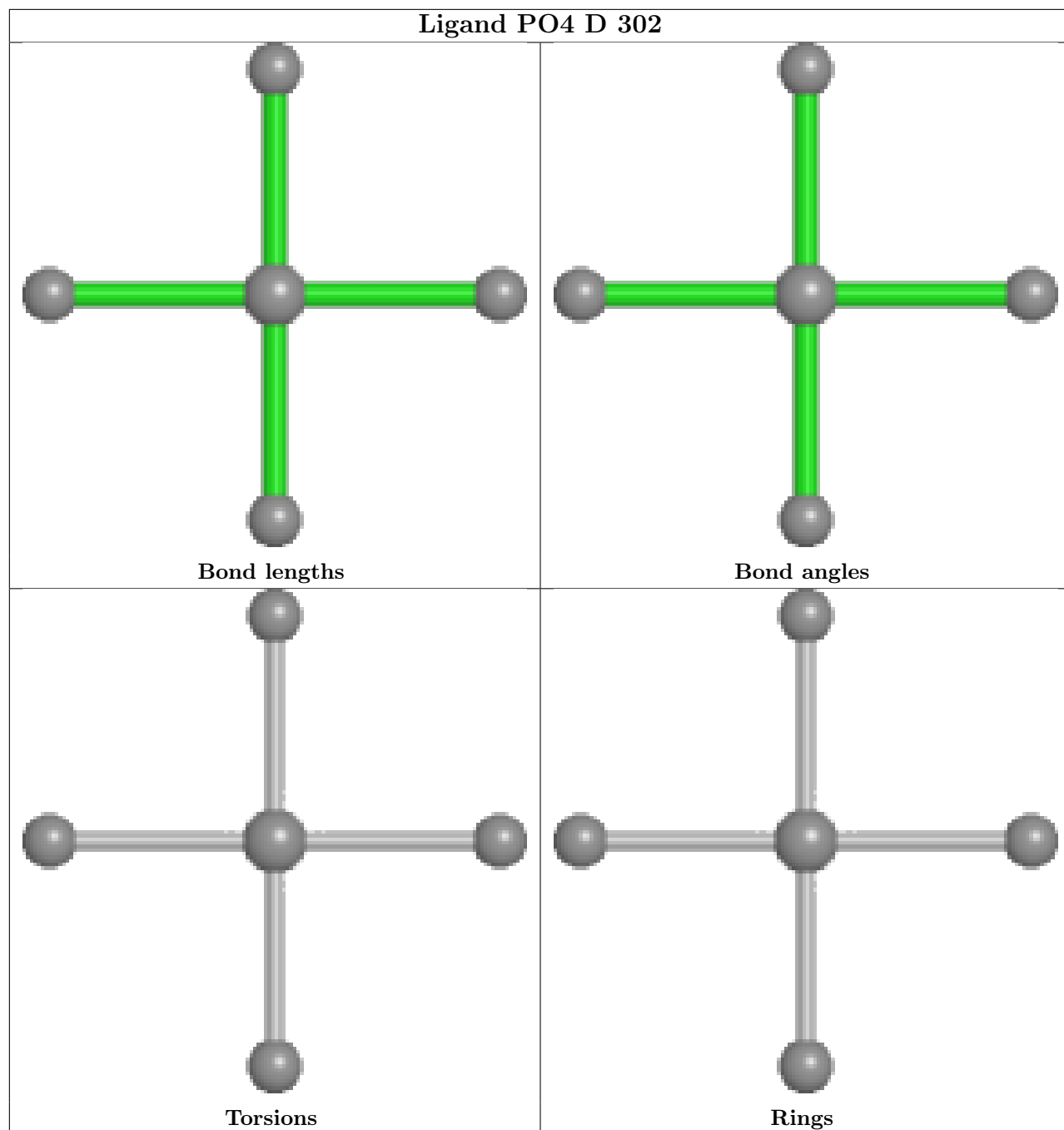


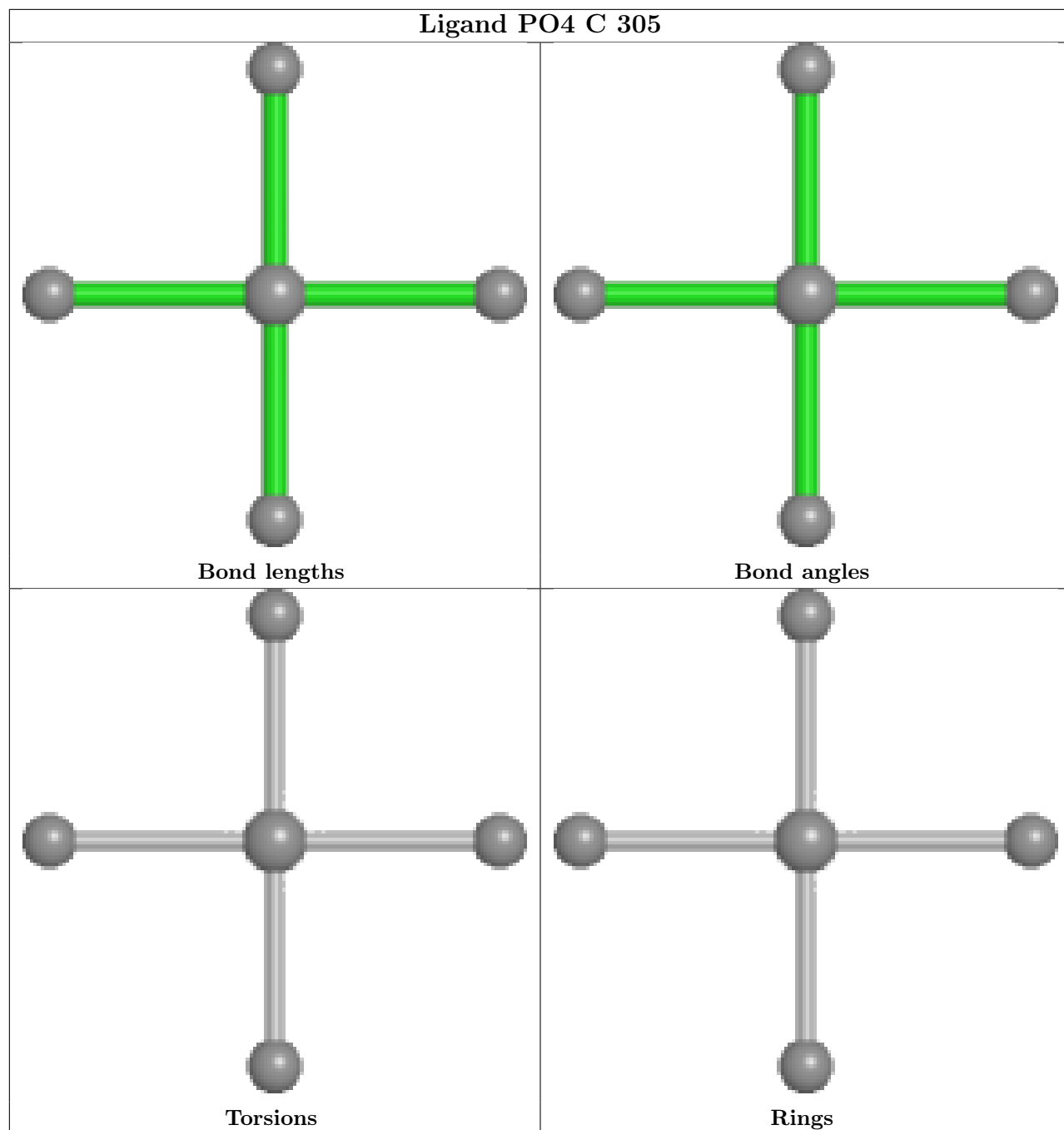


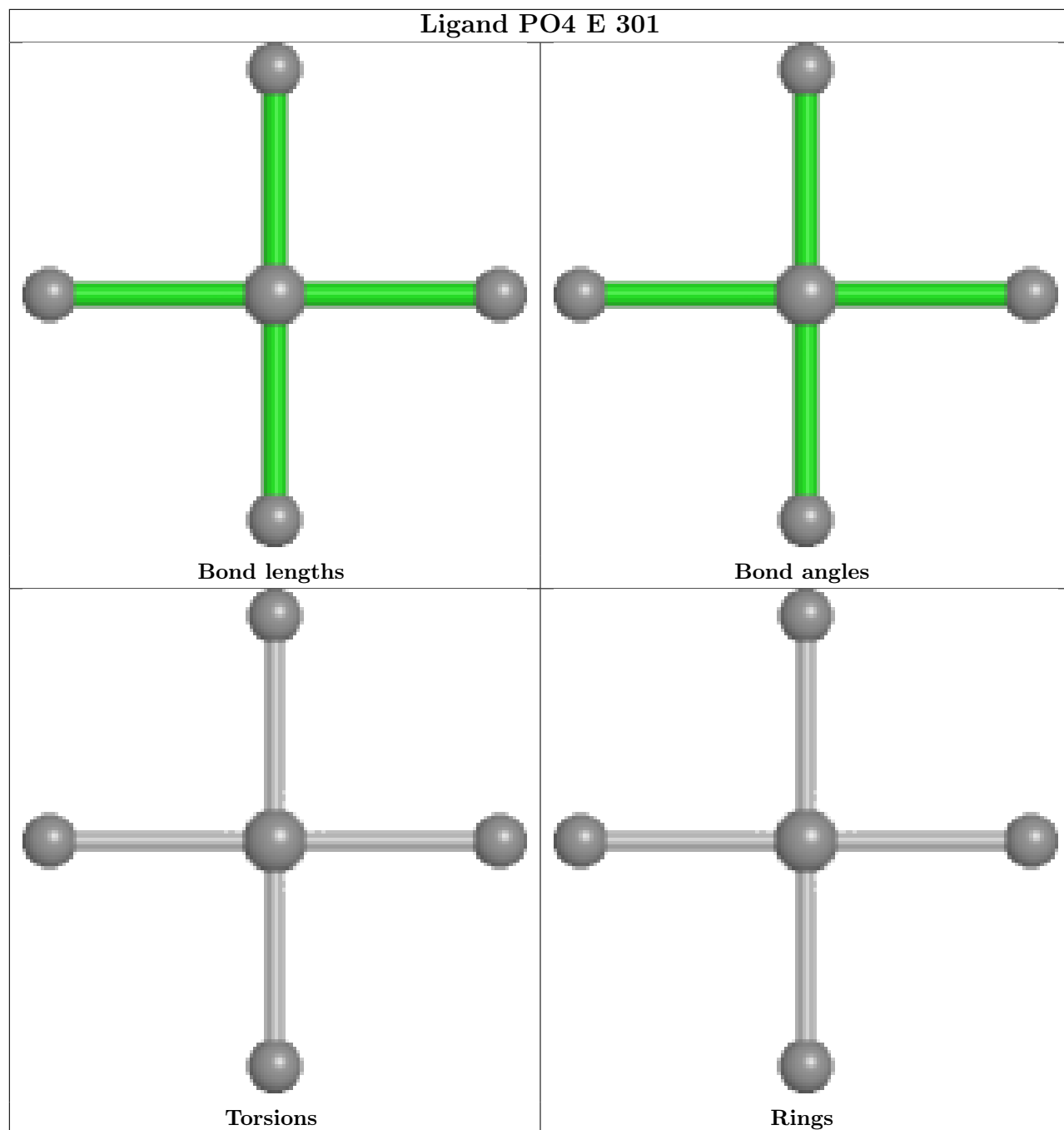


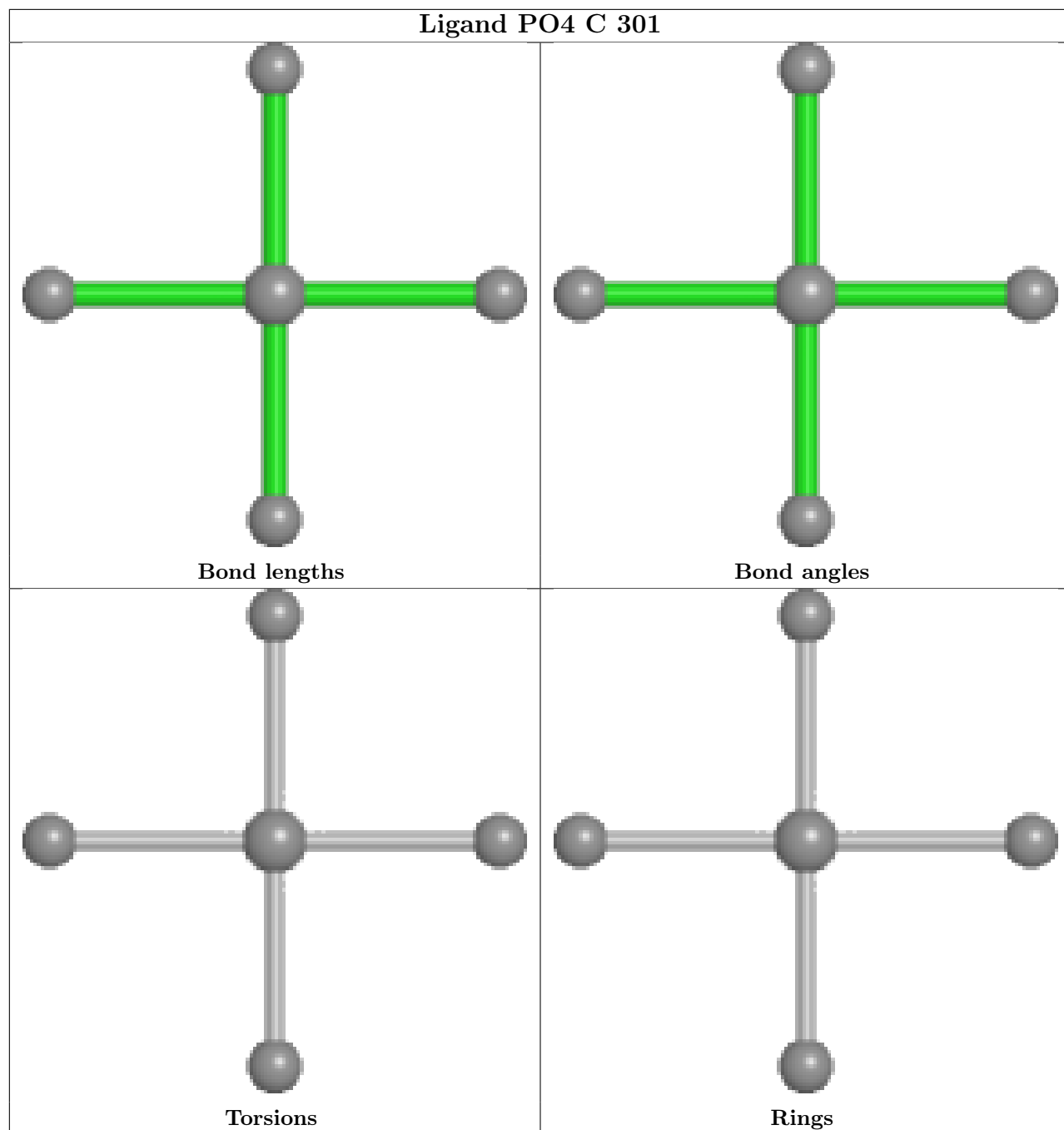


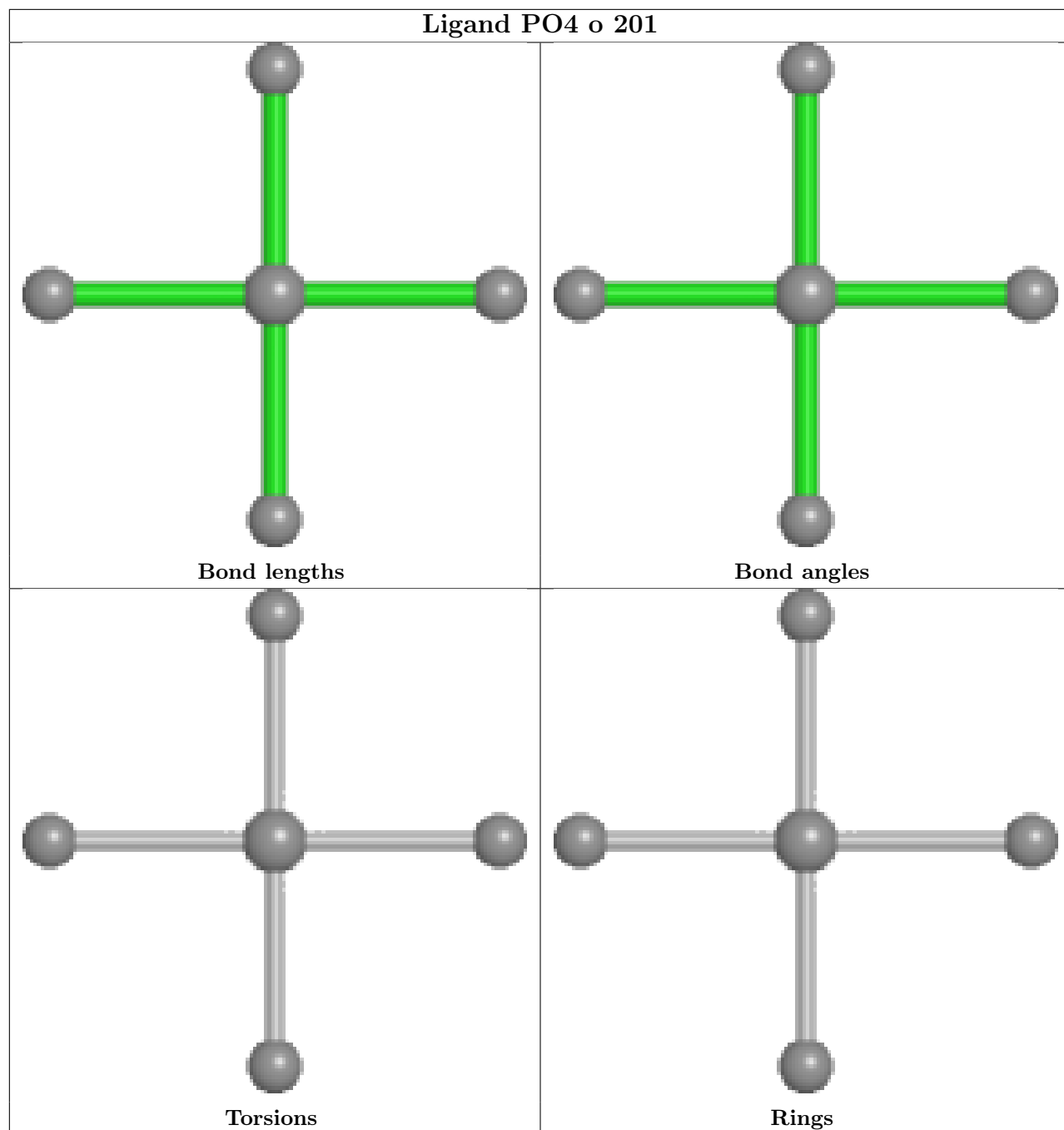


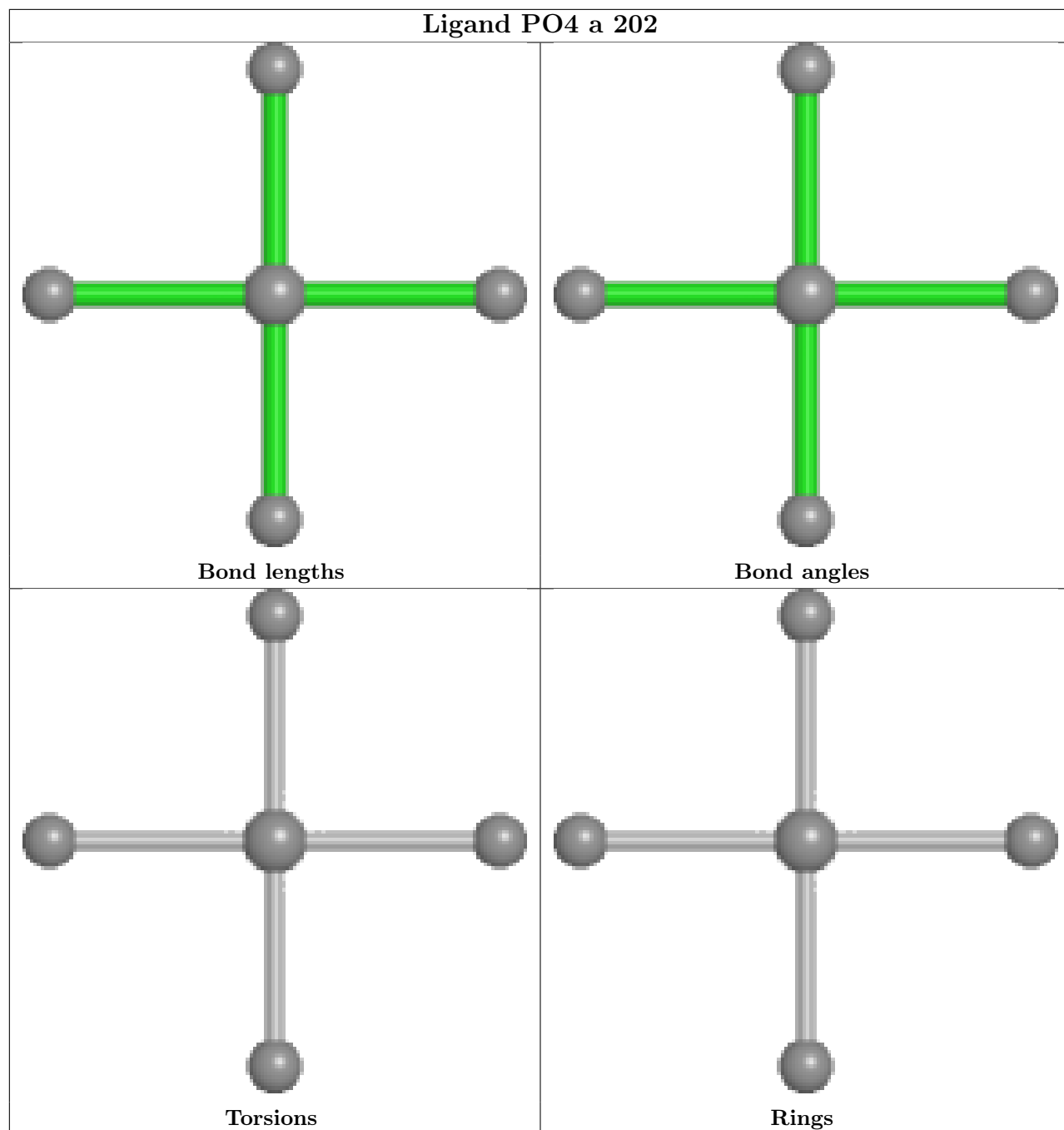


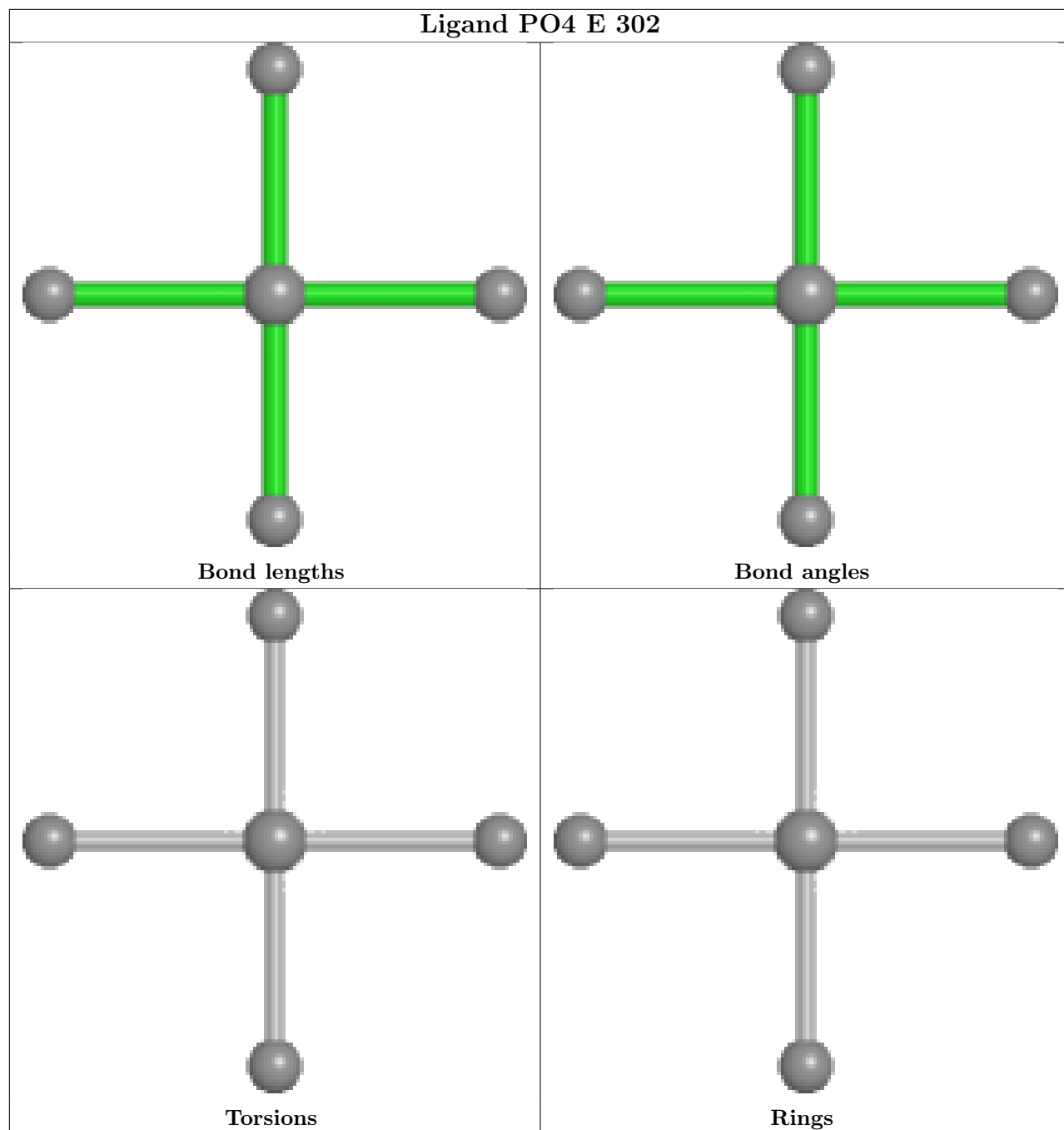


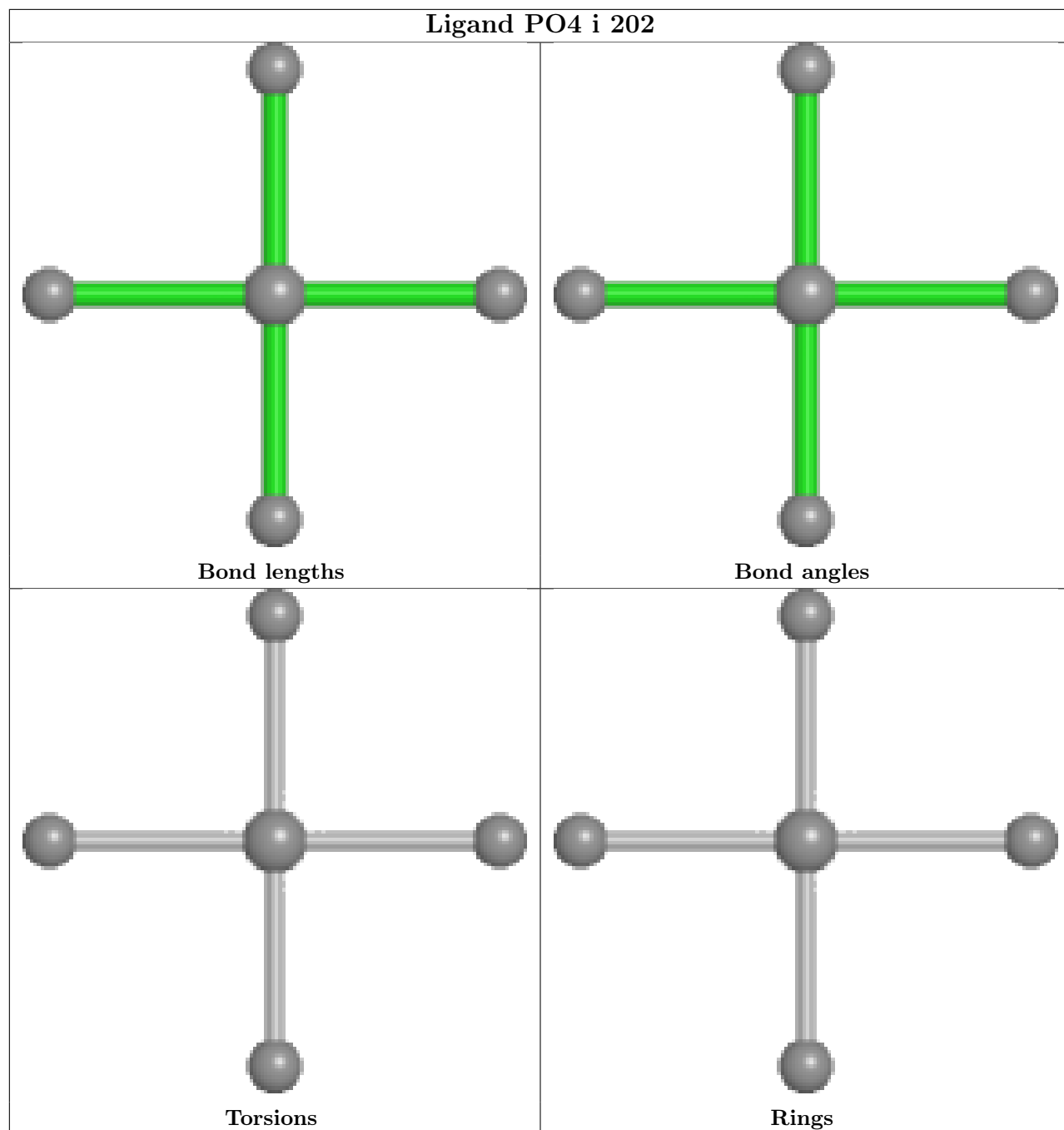


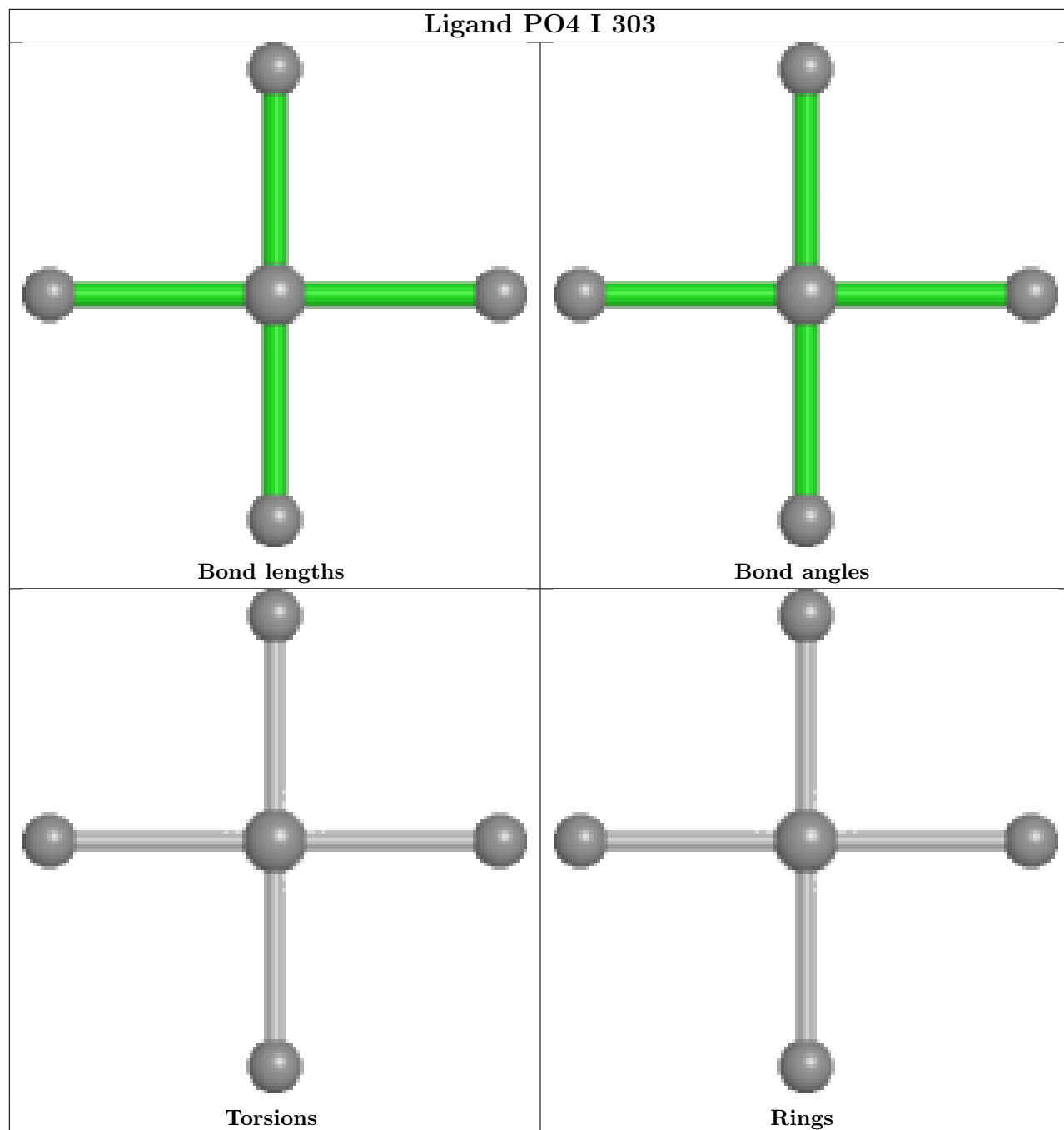


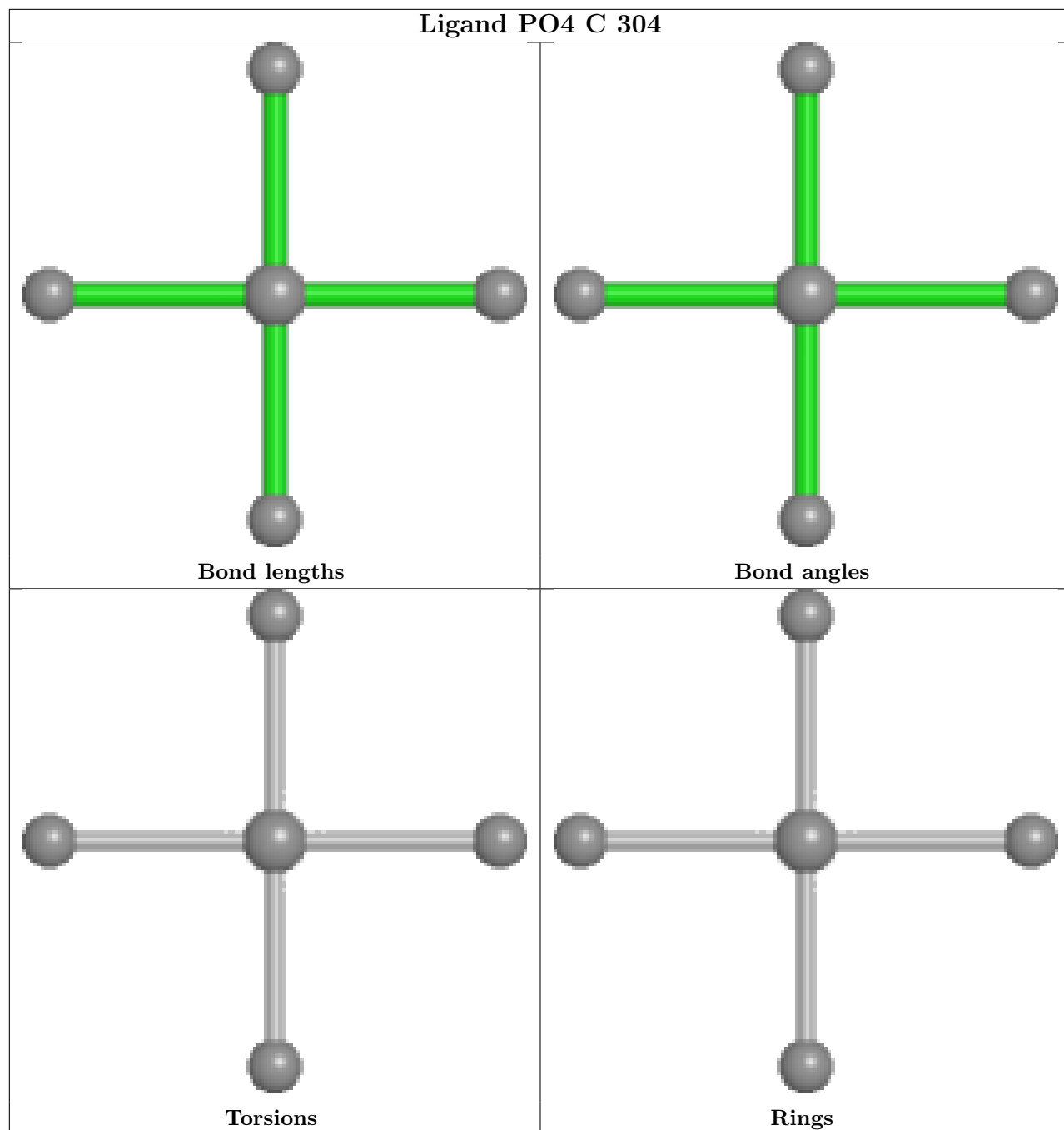


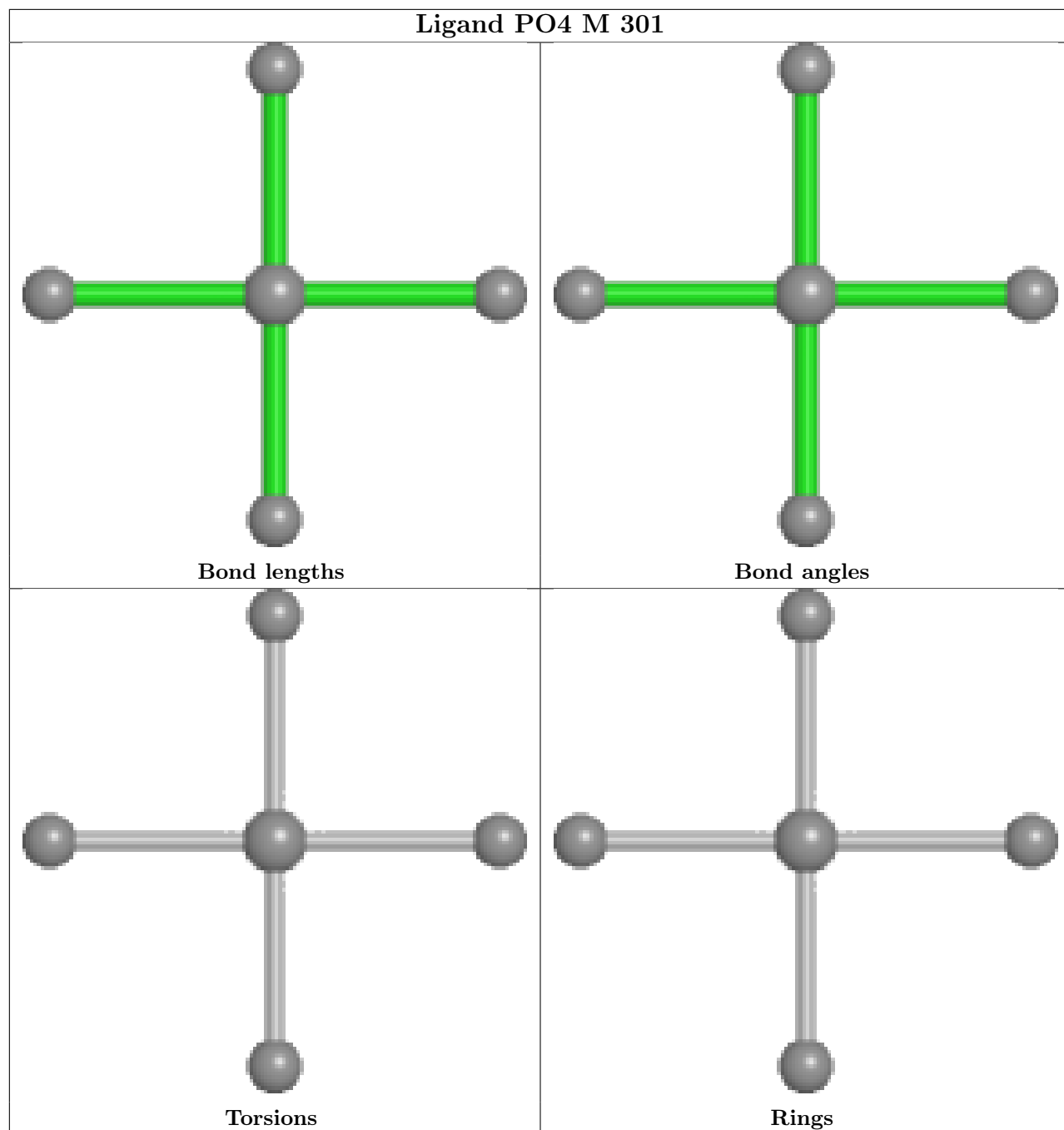


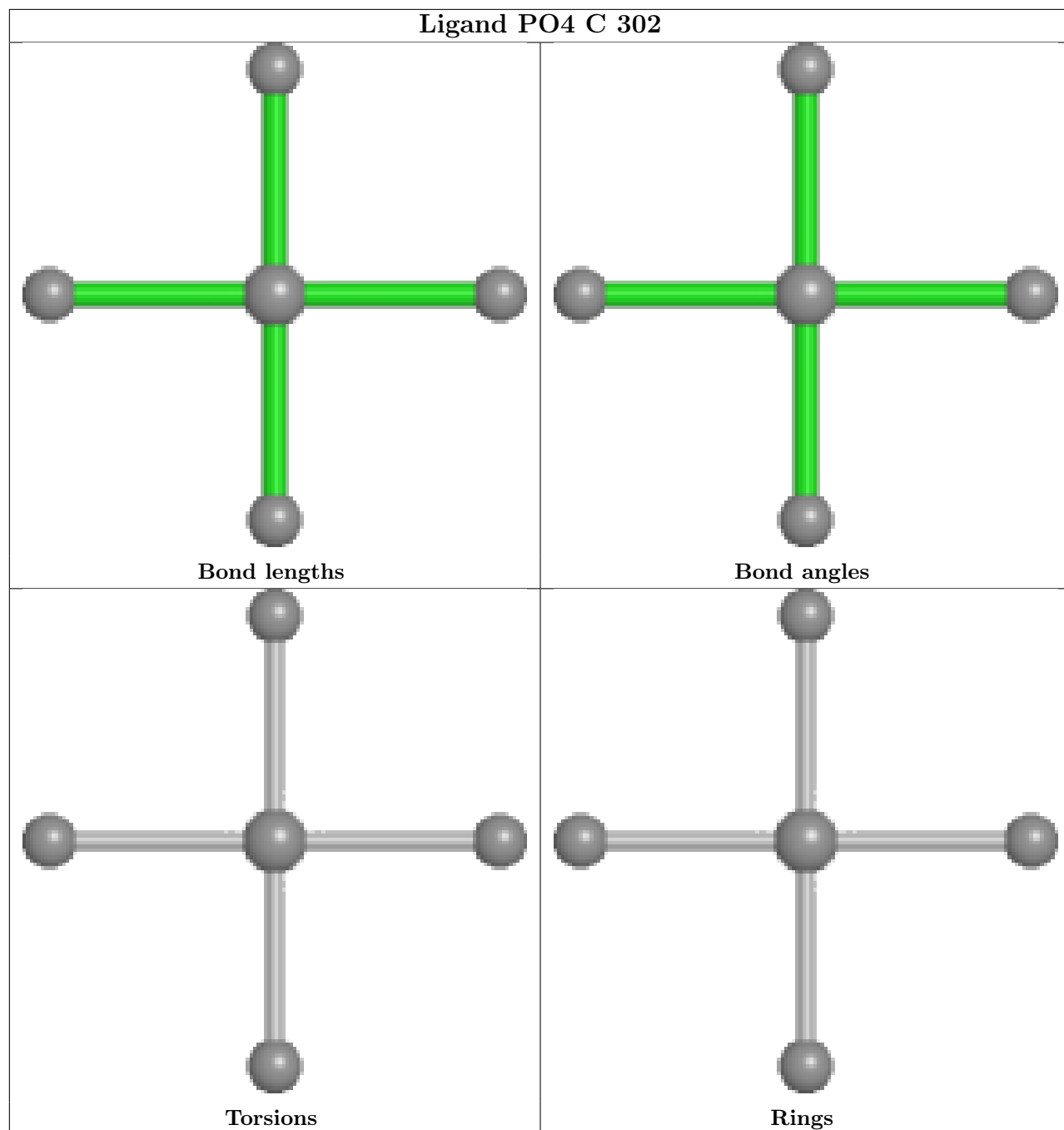


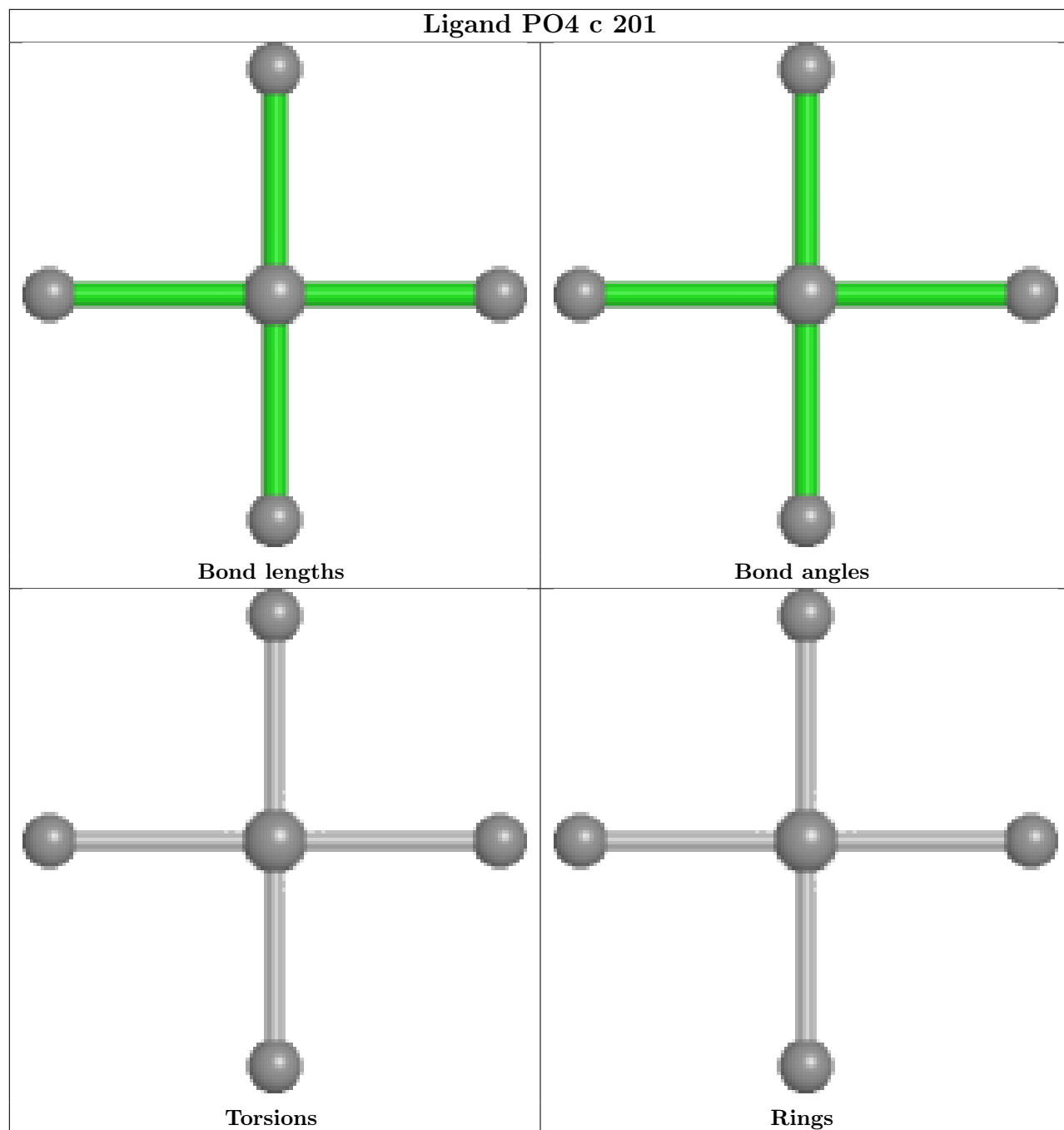


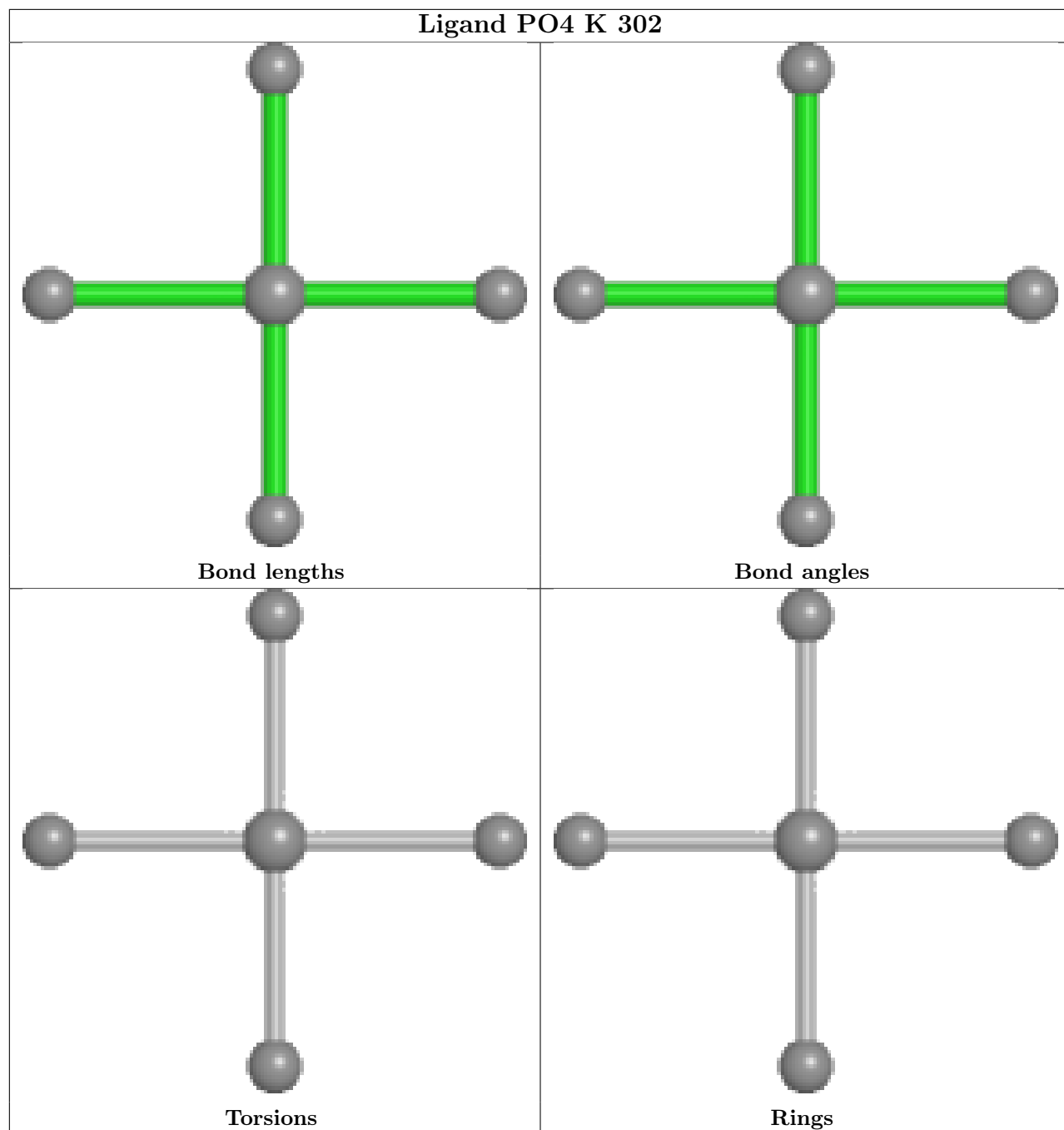


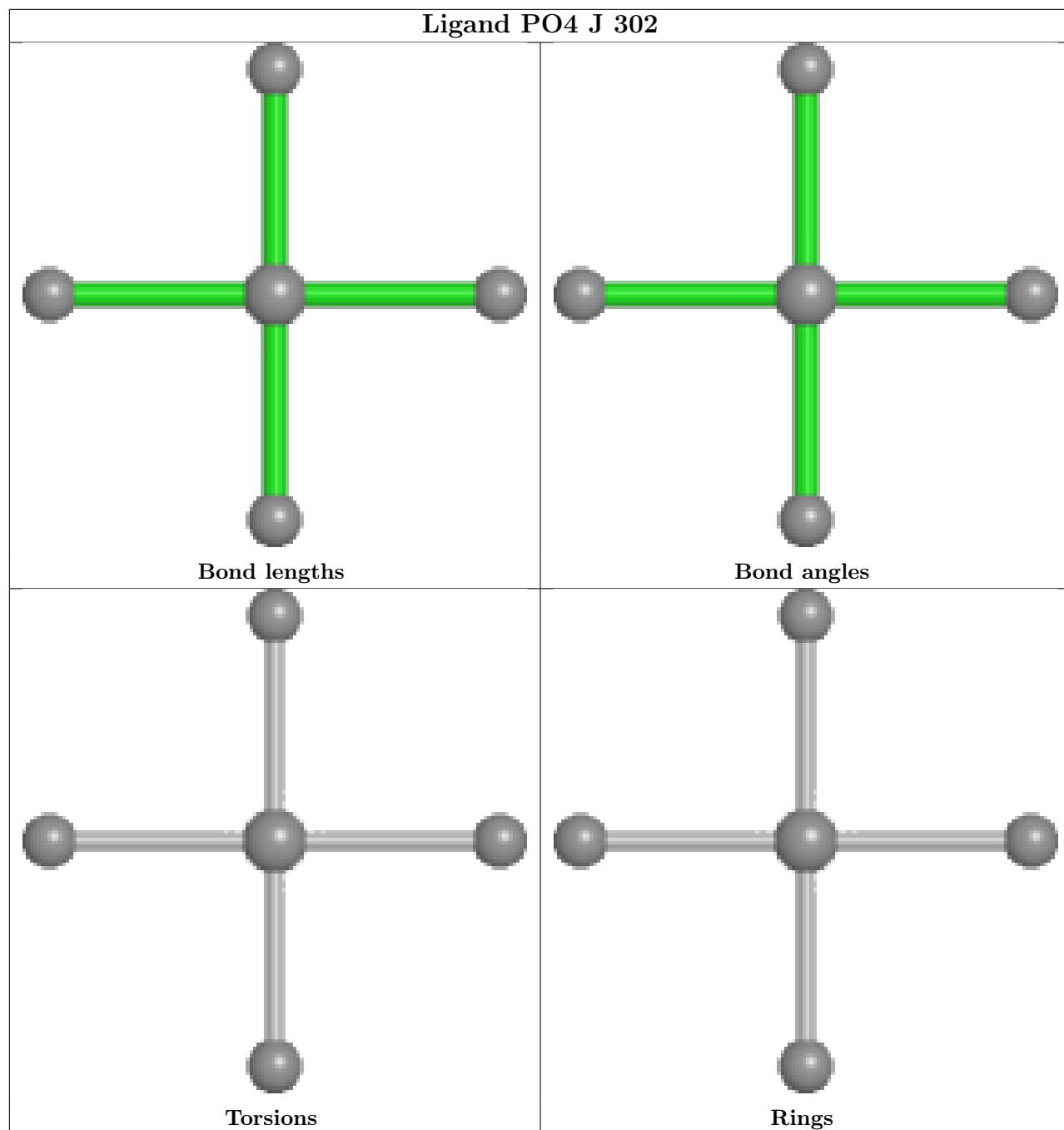


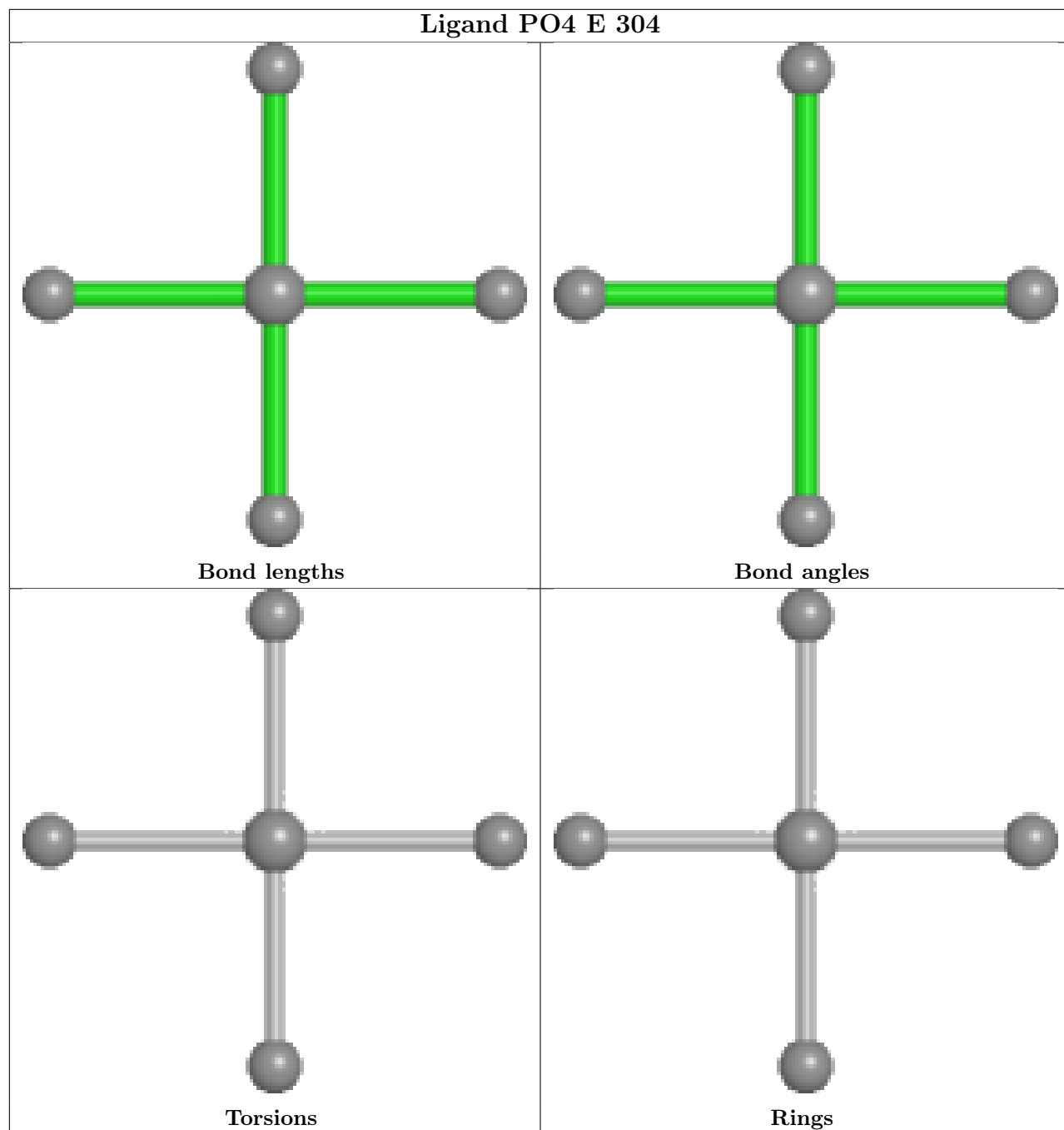


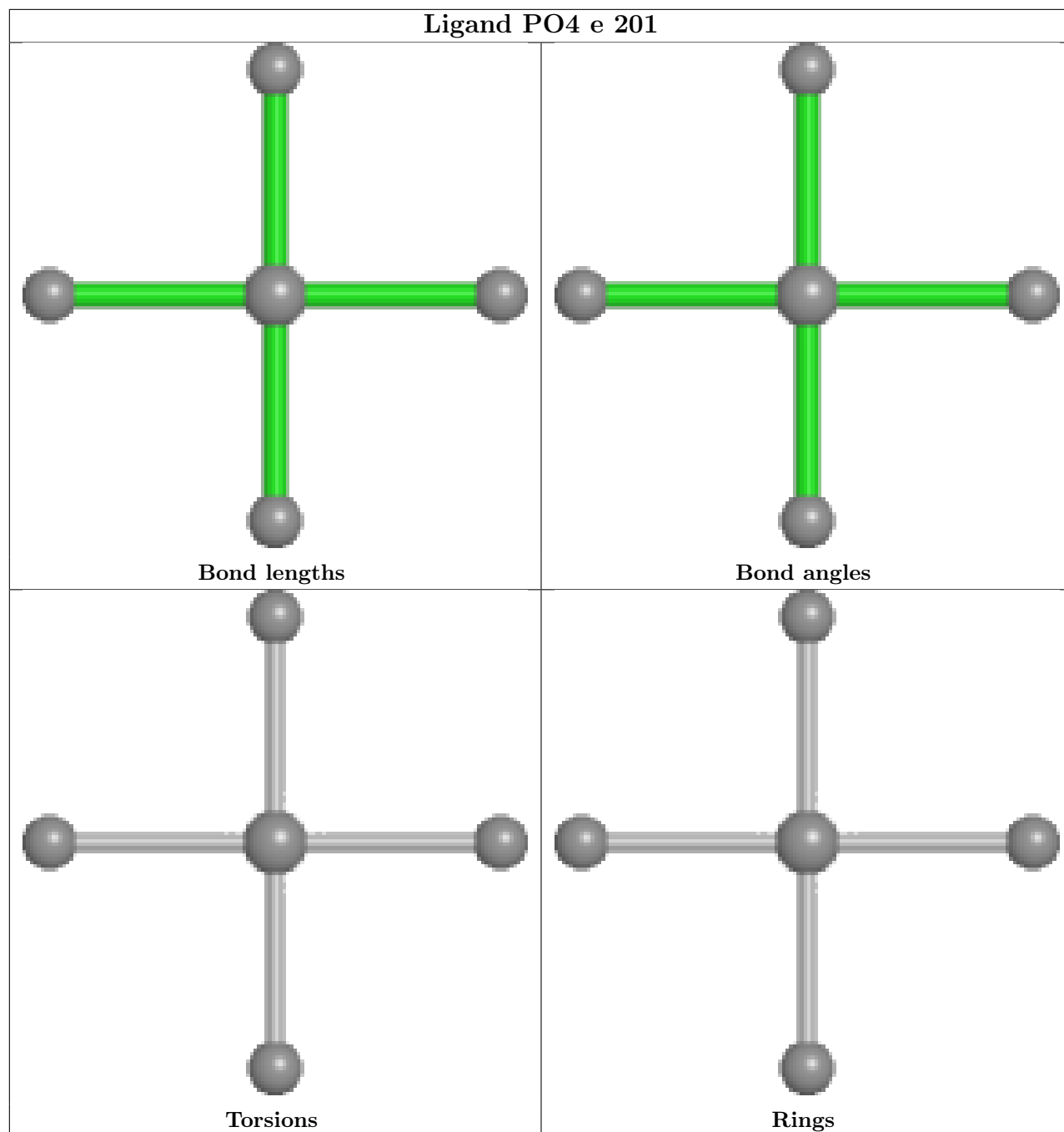












5.7 Other polymers [i](#)

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%)	0.28	3 (1%) 73 61	58, 105, 150, 198	0
1	C	204/215 (94%)	-0.30	0 100 100	30, 49, 87, 138	0
1	E	209/215 (97%)	-0.22	1 (0%) 91 86	34, 55, 91, 143	0
1	G	209/215 (97%)	-0.43	0 100 100	25, 49, 81, 151	0
1	I	203/215 (94%)	-0.25	0 100 100	29, 50, 95, 122	0
1	K	210/215 (97%)	-0.37	0 100 100	37, 58, 111, 139	0
1	M	207/215 (96%)	-0.21	1 (0%) 91 86	39, 71, 112, 161	0
1	O	202/215 (93%)	-0.02	1 (0%) 91 86	61, 80, 123, 152	0
1	Q	203/215 (94%)	-0.29	0 100 100	46, 78, 108, 144	0
2	B	212/239 (88%)	0.39	25 (11%) 4 2	47, 92, 161, 195	0
2	D	228/239 (95%)	-0.20	1 (0%) 92 89	30, 59, 99, 133	0
2	F	225/239 (94%)	0.02	3 (1%) 77 65	36, 72, 106, 142	0
2	H	225/239 (94%)	-0.15	3 (1%) 77 65	32, 57, 99, 142	0
2	J	226/239 (94%)	0.04	4 (1%) 68 55	39, 77, 112, 197	0
2	L	223/239 (93%)	-0.15	0 100 100	44, 77, 111, 152	0
2	N	221/239 (92%)	0.24	12 (5%) 25 14	42, 97, 160, 216	0
2	P	218/239 (91%)	0.20	5 (2%) 60 47	68, 110, 140, 153	0
2	R	217/239 (90%)	-0.08	4 (1%) 68 55	54, 92, 121, 150	0
3	a	125/129 (96%)	-0.01	0 100 100	48, 81, 125, 193	0
3	c	125/129 (96%)	-0.11	1 (0%) 86 78	35, 56, 90, 169	0
3	e	124/129 (96%)	-0.11	0 100 100	33, 54, 85, 112	0
3	g	123/129 (95%)	-0.22	0 100 100	25, 54, 86, 108	0
3	i	125/129 (96%)	-0.09	2 (1%) 72 59	45, 77, 124, 149	0
3	k	126/129 (97%)	-0.08	1 (0%) 86 78	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%)	-0.12	2 (1%) 70 57	34, 64, 112, 146	0
3	o	123/129 (95%)	0.21	1 (0%) 86 78	86, 115, 150, 217	0
3	q	123/129 (95%)	0.15	2 (1%) 72 59	67, 103, 140, 177	0
All	All	4958/5247 (94%)	-0.07	72 (1%) 73 61	25, 73, 131, 217	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	54	SER	4.9
2	B	54	SER	4.7
2	B	160	THR	4.4
2	N	154	TRP	4.4
2	B	162	GLY	4.4
2	B	140	CYS	4.4
2	N	152	VAL	4.1
2	B	196	CYS	4.0
2	B	163	VAL	3.9
2	B	154	TRP	3.7
2	N	53	SER	3.6
2	J	53	SER	3.6
2	B	211	VAL	3.5
2	N	194	TYR	3.4
2	N	190	GLY	3.3
2	B	198	VAL	3.3
3	q	26	GLY	3.2
2	B	189	LEU	3.2
2	P	69	ILE	3.2
2	N	193	THR	3.1
2	N	189	LEU	3.0
3	o	17	SER	2.9
2	B	165	THR	2.8
2	F	204	ASN	2.8
2	D	132	SER	2.8
3	m	3	GLN	2.7
2	F	158	ALA	2.7
2	N	147	PRO	2.7
3	k	27	SER	2.7
1	A	135	LEU	2.7
2	P	71	ALA	2.7
3	c	76	ASN	2.6
2	B	179	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	161	SER	2.6
2	B	149	PRO	2.6
3	m	24	ALA	2.5
2	N	155	ASN	2.5
1	O	10	SER	2.5
2	N	208	ASP	2.5
2	B	190	GLY	2.5
2	B	186	SER	2.5
2	R	135	THR	2.4
1	A	144	ALA	2.4
2	N	207	VAL	2.4
2	B	184	VAL	2.4
2	P	199	ASN	2.4
2	B	155	ASN	2.3
2	B	52(a)	SER	2.3
2	B	138	LEU	2.3
2	B	183	THR	2.3
2	J	110	THR	2.3
2	P	190	GLY	2.3
2	B	152	VAL	2.3
2	H	136	ALA	2.3
1	E	112	ALA	2.2
2	R	186	SER	2.2
2	B	187	SER	2.2
2	R	185	PRO	2.2
2	B	137	ALA	2.1
3	q	76	ASN	2.1
2	H	130	SER	2.1
2	P	191	THR	2.1
2	R	187	SER	2.1
2	B	166	PHE	2.1
1	M	28	SER	2.1
2	H	52(a)	SER	2.1
2	N	10	GLY	2.1
3	i	3	GLN	2.0
2	J	126	PRO	2.0
2	F	89	VAL	2.0
3	i	23	ALA	2.0
1	A	24	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	GOL	G	307	6/6	0.77	0.23	93,96,97,100	0
4	PO4	o	201	5/5	0.80	0.21	156,157,158,160	0
6	GOL	k	201	6/6	0.80	0.27	59,67,70,70	0
4	PO4	K	302	5/5	0.82	0.26	116,116,117,120	0
4	PO4	i	202	5/5	0.84	0.18	119,120,121,121	0
4	PO4	o	202	5/5	0.86	0.15	125,126,127,129	0
4	PO4	E	304	5/5	0.86	0.18	147,149,151,152	0
6	GOL	c	203	6/6	0.86	0.21	71,75,81,87	0
4	PO4	D	302	5/5	0.86	0.35	128,131,132,134	0
4	PO4	C	303	5/5	0.87	0.18	109,112,115,116	0
4	PO4	G	303	5/5	0.87	0.27	132,134,135,136	0
5	CL	C	307	1/1	0.87	0.14	47,47,47,47	0
4	PO4	H	301	5/5	0.88	0.17	115,119,121,121	0
4	PO4	I	301	5/5	0.89	0.16	118,120,121,122	0
6	GOL	B	304	6/6	0.89	0.16	63,66,68,68	0
4	PO4	m	201	5/5	0.89	0.30	97,97,98,100	0
4	PO4	C	304	5/5	0.89	0.46	98,105,109,110	0
4	PO4	g	201	5/5	0.89	0.36	92,96,102,106	0
4	PO4	J	301	5/5	0.90	0.24	112,114,116,118	0
5	CL	K	304	1/1	0.90	0.24	76,76,76,76	0
5	CL	R	302	1/1	0.90	0.13	54,54,54,54	0
4	PO4	K	301	5/5	0.90	0.55	140,140,142,143	0
6	GOL	G	306	6/6	0.90	0.24	45,54,56,58	0
4	PO4	G	302	5/5	0.90	0.34	103,104,105,110	0
4	PO4	O	301	5/5	0.90	0.28	102,103,104,108	0
4	PO4	a	201	5/5	0.90	0.23	138,138,139,140	0
4	PO4	Q	301	5/5	0.91	0.24	122,125,125,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	o	203	5/5	0.91	0.18	69,70,75,80	0
4	PO4	J	302	5/5	0.91	0.40	95,99,103,106	0
4	PO4	m	202	5/5	0.91	0.18	59,69,72,81	0
4	PO4	E	301	5/5	0.91	0.37	102,105,106,108	0
7	PEG	F	302	7/7	0.91	0.20	34,42,61,61	0
4	PO4	E	302	5/5	0.92	0.27	118,118,121,123	0
4	PO4	e	201	5/5	0.92	0.43	106,109,110,113	0
4	PO4	R	301	5/5	0.92	0.19	102,106,107,109	0
7	PEG	N	303	7/7	0.92	0.21	61,65,67,68	0
5	CL	q	202	1/1	0.93	0.14	58,58,58,58	0
4	PO4	e	202	5/5	0.93	0.20	17,34,44,50	0
6	GOL	E	307	6/6	0.93	0.33	47,59,64,65	0
4	PO4	e	203	5/5	0.93	0.28	67,76,78,79	0
4	PO4	B	301	5/5	0.93	0.16	66,71,79,81	0
4	PO4	M	302	5/5	0.93	0.16	107,107,109,113	0
5	CL	G	304	1/1	0.93	0.09	61,61,61,61	0
4	PO4	E	303	5/5	0.93	0.39	123,125,126,127	0
4	PO4	O	302	5/5	0.93	0.20	94,95,99,101	0
4	PO4	c	202	5/5	0.94	0.21	73,74,76,85	0
5	CL	H	302	1/1	0.94	0.08	37,37,37,37	0
4	PO4	C	302	5/5	0.94	0.28	101,102,103,107	0
6	GOL	L	303	6/6	0.94	0.24	38,55,59,66	0
5	CL	M	304	1/1	0.94	0.12	53,53,53,53	0
5	CL	C	306	1/1	0.94	0.12	42,42,42,42	0
4	PO4	M	301	5/5	0.94	0.18	88,88,94,96	0
7	PEG	H	303	7/7	0.94	0.19	28,41,50,51	0
5	CL	E	306	1/1	0.94	0.12	41,41,41,41	0
5	CL	N	302	1/1	0.95	0.12	38,38,38,38	0
5	CL	P	301	1/1	0.95	0.18	66,66,66,66	0
4	PO4	I	302	5/5	0.95	0.52	103,103,105,108	0
5	CL	e	204	1/1	0.95	0.10	42,42,42,42	0
5	CL	J	303	1/1	0.95	0.12	45,45,45,45	0
5	CL	q	203	1/1	0.95	0.17	66,66,66,66	0
4	PO4	C	305	5/5	0.95	0.27	77,80,80,84	0
4	PO4	i	203	5/5	0.95	0.17	40,45,51,57	0
5	CL	G	305	1/1	0.96	0.18	29,29,29,29	0
6	GOL	I	306	6/6	0.96	0.15	51,53,55,55	0
4	PO4	M	303	5/5	0.96	0.21	88,88,93,94	0
4	PO4	i	201	5/5	0.96	0.18	82,84,90,91	0
5	CL	D	304	1/1	0.96	0.14	42,42,42,42	0
5	CL	E	305	1/1	0.96	0.12	31,31,31,31	0
4	PO4	D	301	5/5	0.96	0.22	62,64,71,81	0

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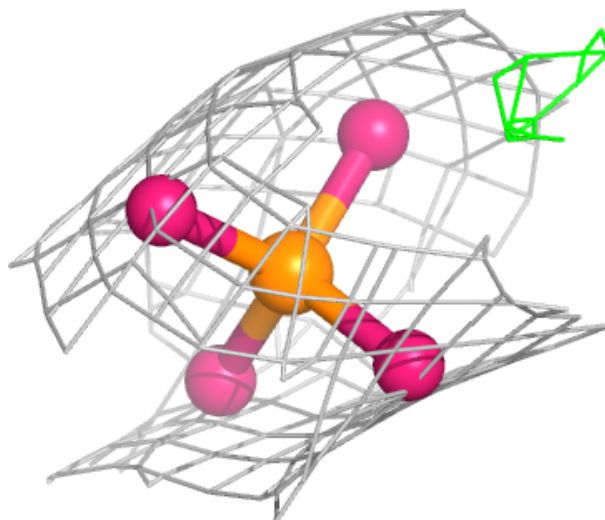
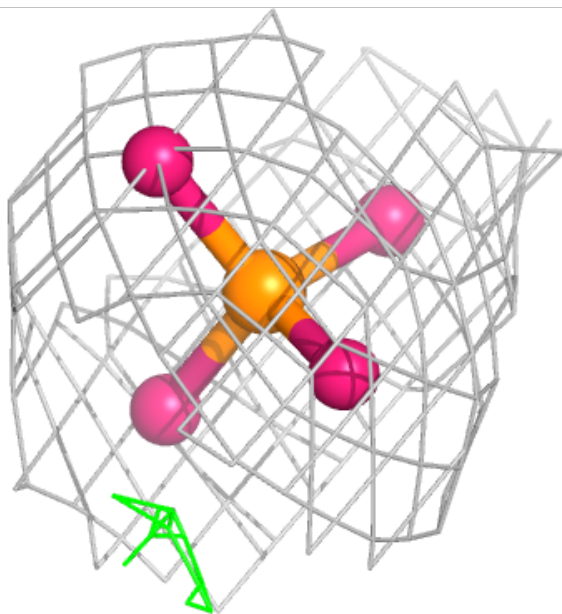
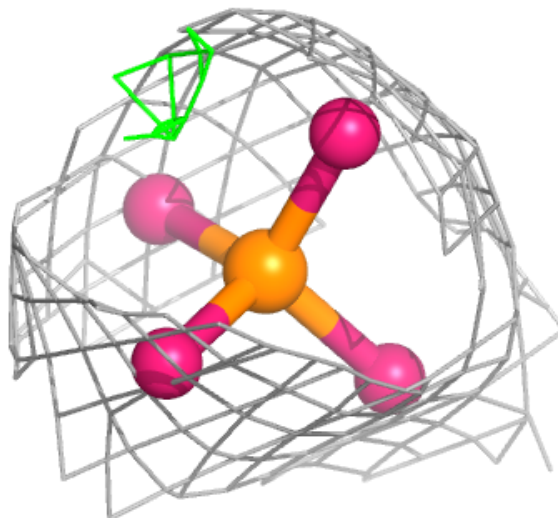
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	B	302	1/1	0.96	0.16	53,53,53,53	0
4	PO4	C	301	5/5	0.97	0.26	35,37,43,48	0
5	CL	N	301	1/1	0.97	0.17	40,40,40,40	0
5	CL	F	301	1/1	0.97	0.10	20,20,20,20	0
4	PO4	I	304	5/5	0.97	0.29	48,53,66,68	0
4	PO4	a	202	5/5	0.97	0.19	33,39,47,48	0
5	CL	D	303	1/1	0.97	0.16	27,27,27,27	0
5	CL	g	203	1/1	0.97	0.18	33,33,33,33	0
5	CL	I	305	1/1	0.97	0.14	42,42,42,42	0
4	PO4	G	301	5/5	0.97	0.23	60,60,63,65	0
4	PO4	q	201	5/5	0.97	0.12	26,37,49,50	0
4	PO4	L	301	5/5	0.98	0.18	48,50,53,60	0
5	CL	K	303	1/1	0.98	0.10	41,41,41,41	0
4	PO4	I	303	5/5	0.98	0.14	41,44,48,51	0
6	GOL	C	308	6/6	0.98	0.17	12,31,40,42	0
5	CL	R	303	1/1	0.98	0.08	55,55,55,55	0
4	PO4	g	202	5/5	0.98	0.17	16,16,19,31	0
4	PO4	c	201	5/5	0.98	0.18	9,18,26,33	0
5	CL	L	302	1/1	0.99	0.08	45,45,45,45	0
5	CL	g	204	1/1	0.99	0.15	29,29,29,29	0
5	CL	R	304	1/1	0.99	0.08	33,33,33,33	0
5	CL	B	303	1/1	0.99	0.15	55,55,55,55	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.

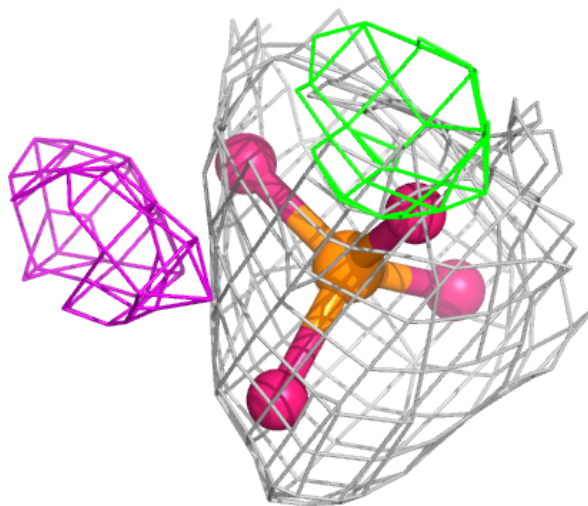
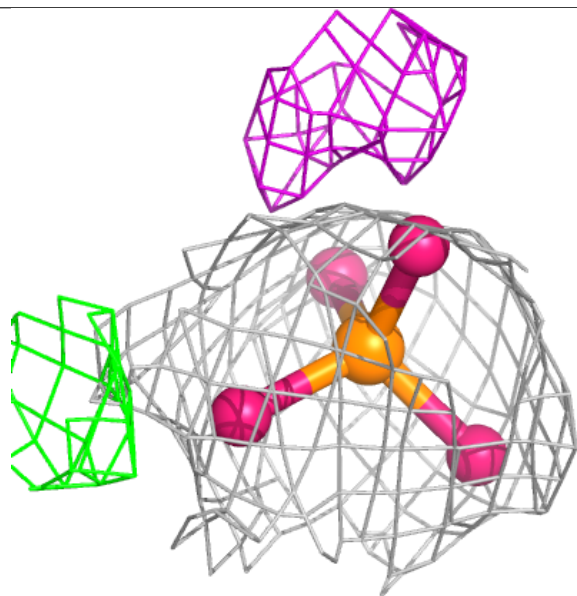
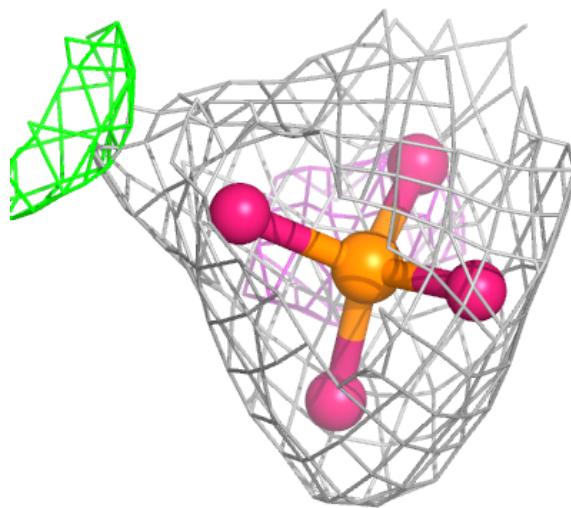
Electron density around PO4 o 201:

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



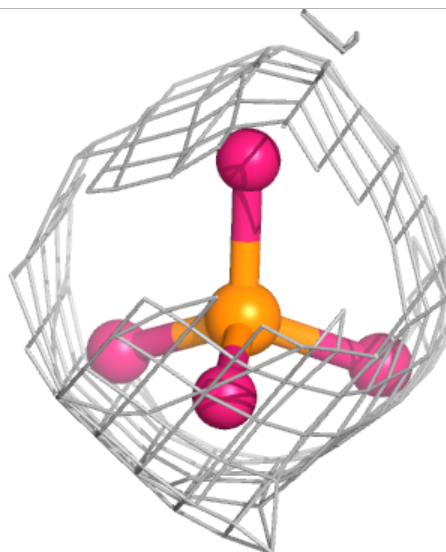
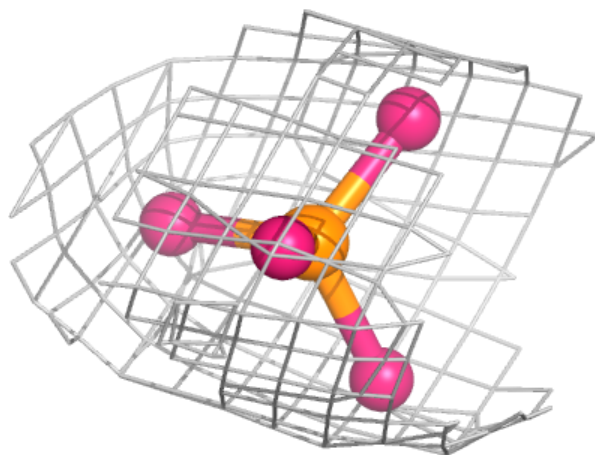
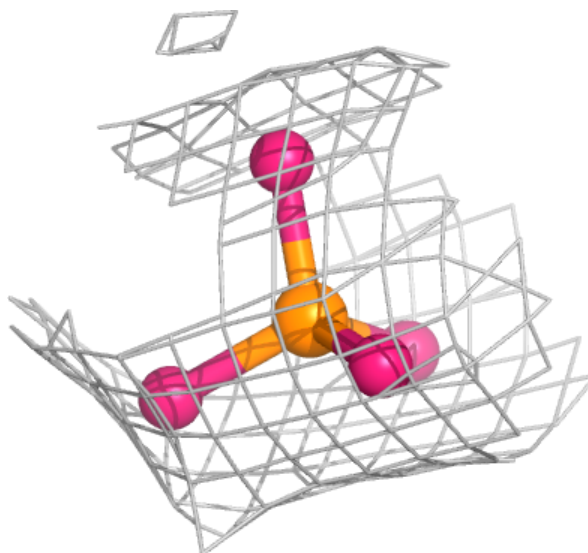
Electron density around PO4 K 302:

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



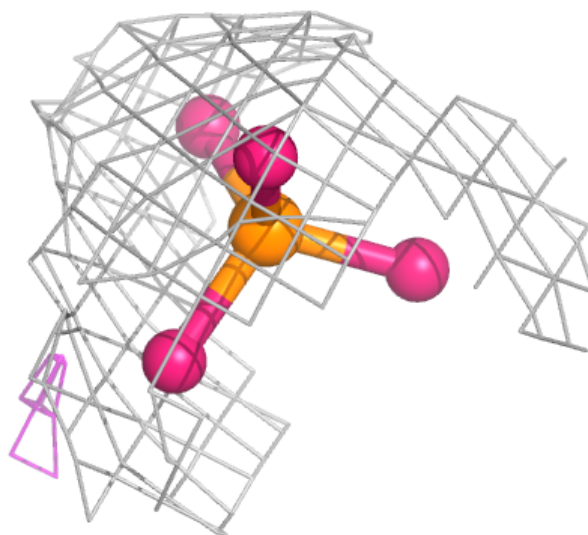
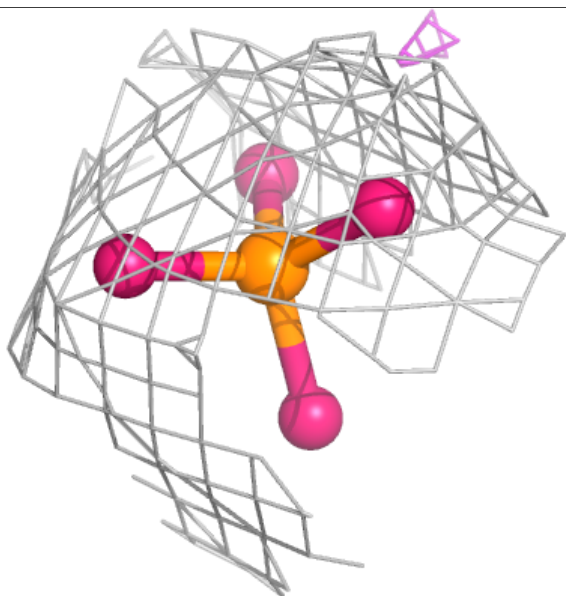
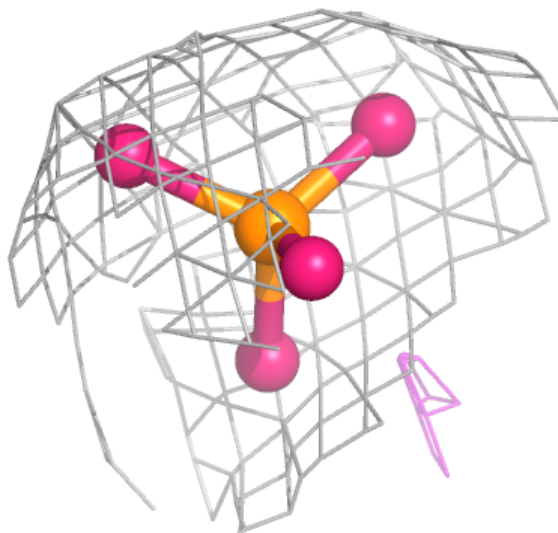
Electron density around PO4 i 202:

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



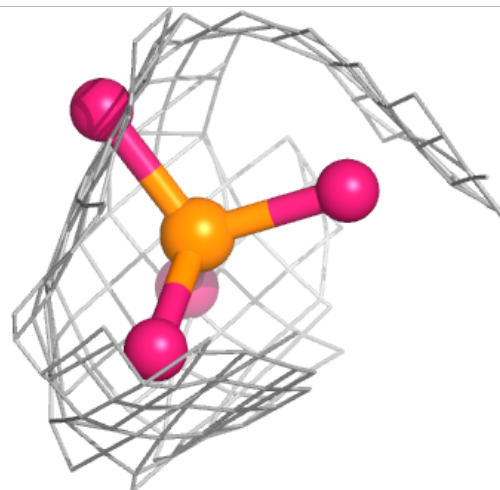
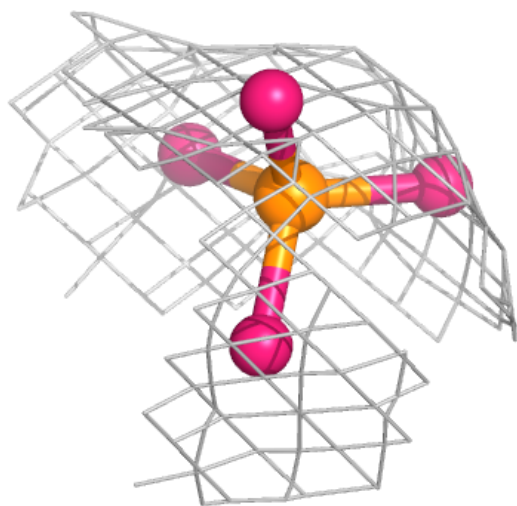
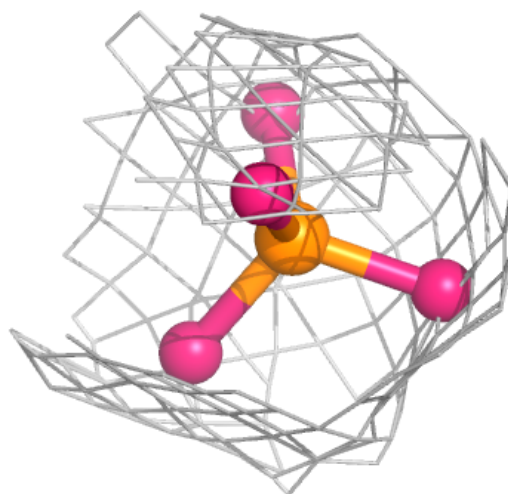
Electron density around PO4 o 202:

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



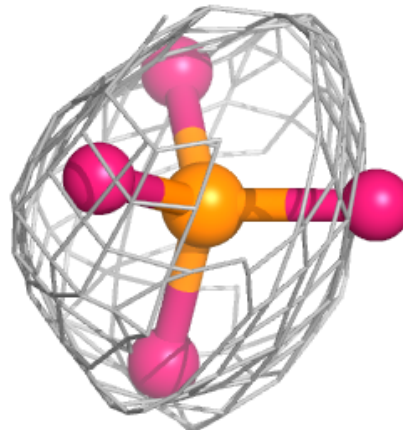
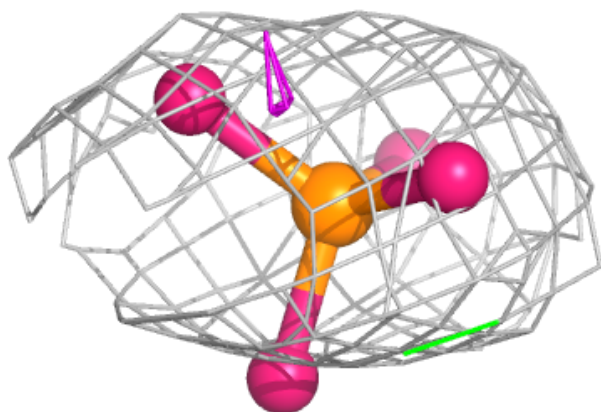
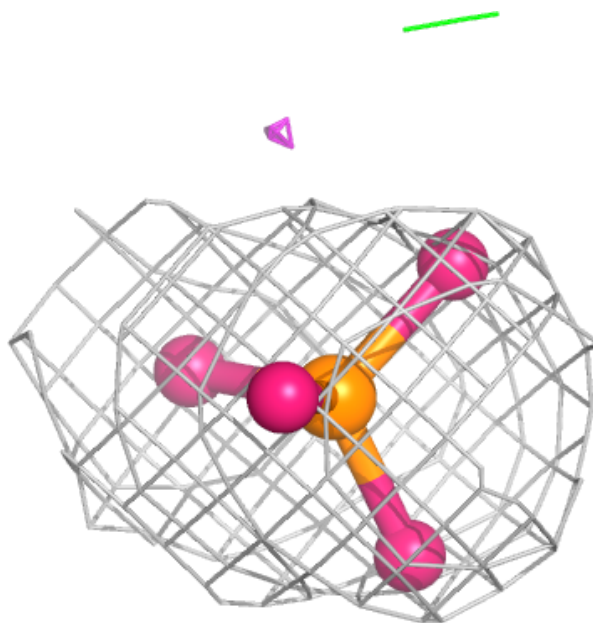
Electron density around PO4 E 304:

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



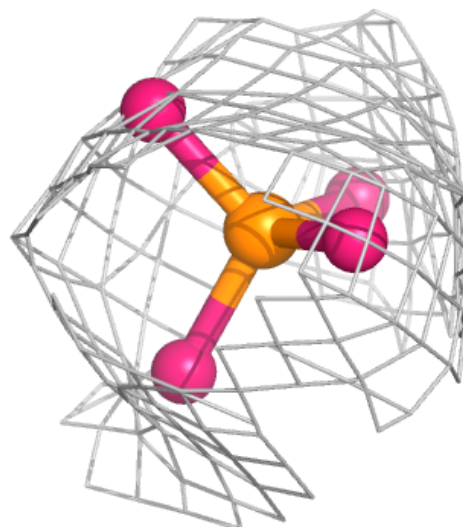
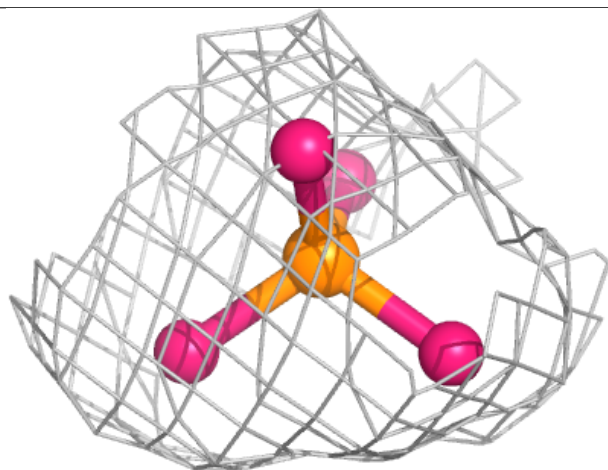
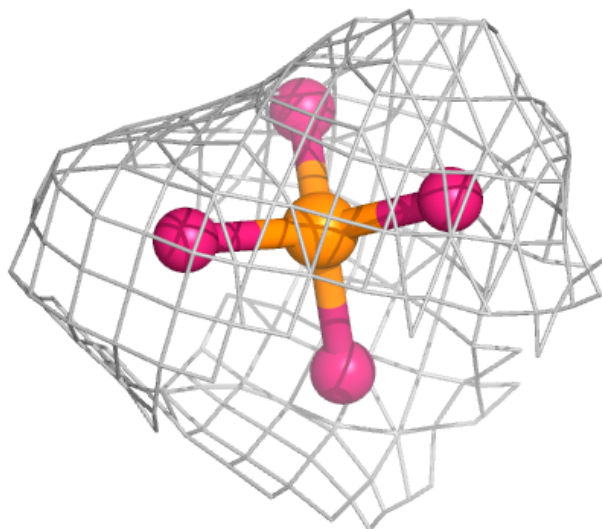
Electron density around PO4 D 302:

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



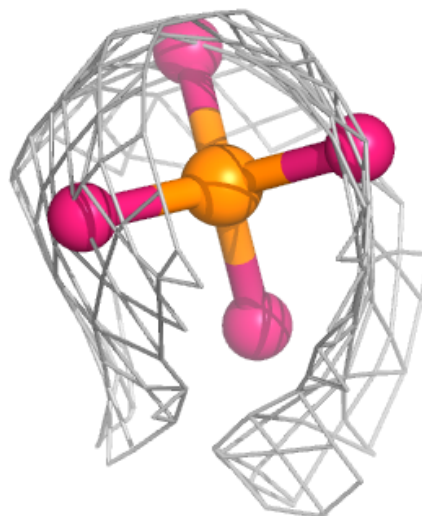
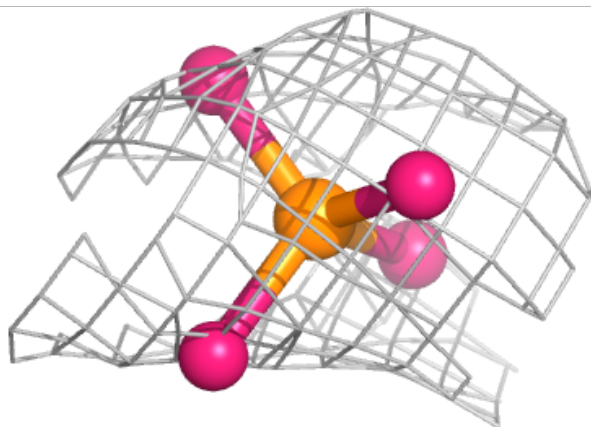
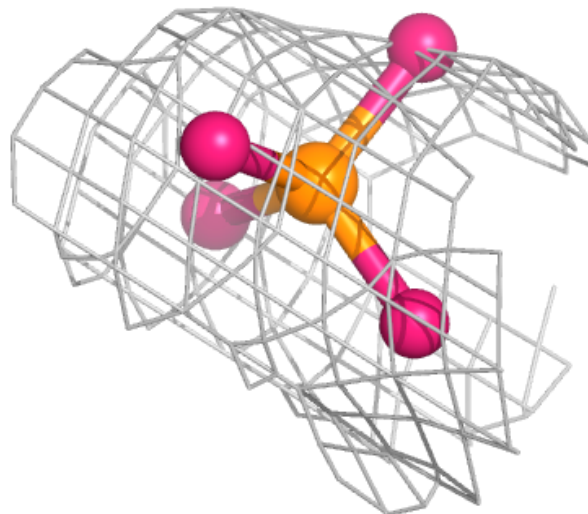
Electron density around PO4 C 303:

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



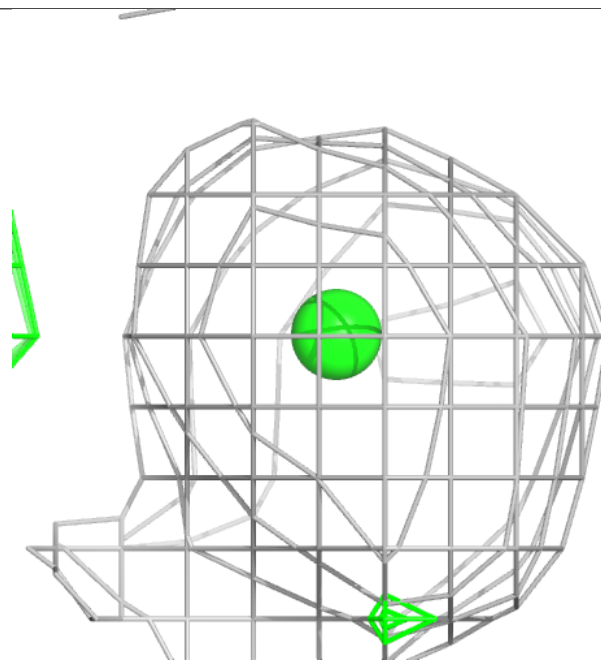
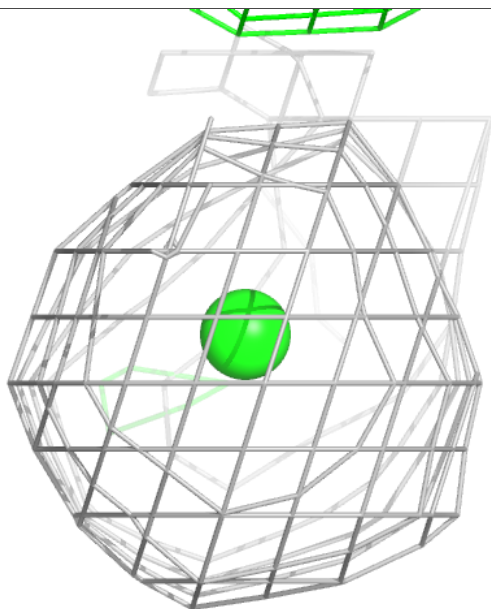
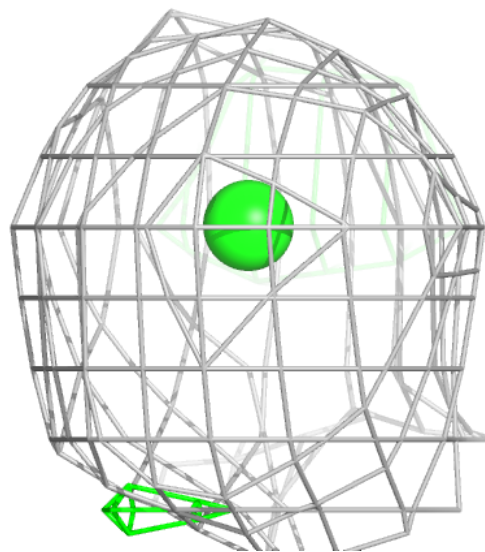
Electron density around PO4 G 303:

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



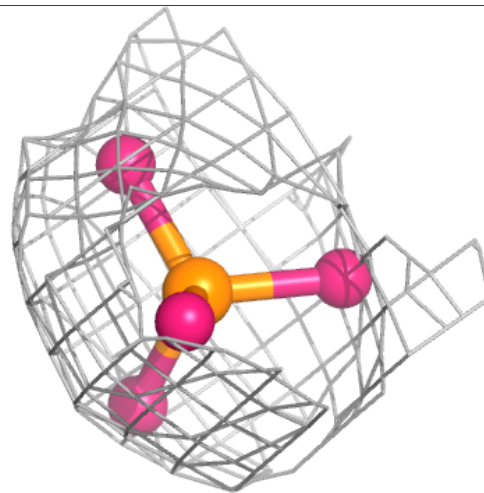
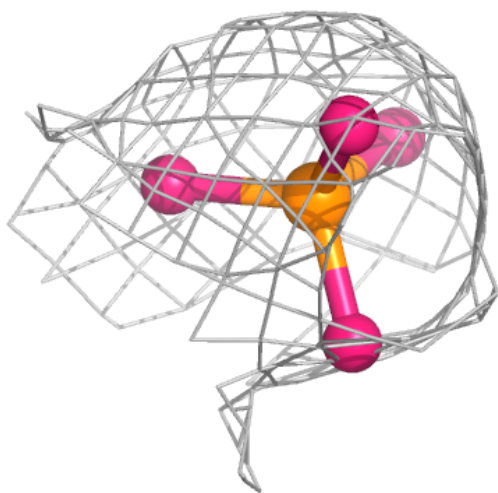
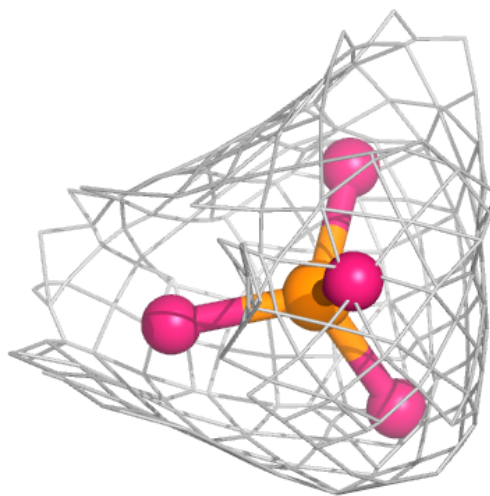
Electron density around CL C 307:

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



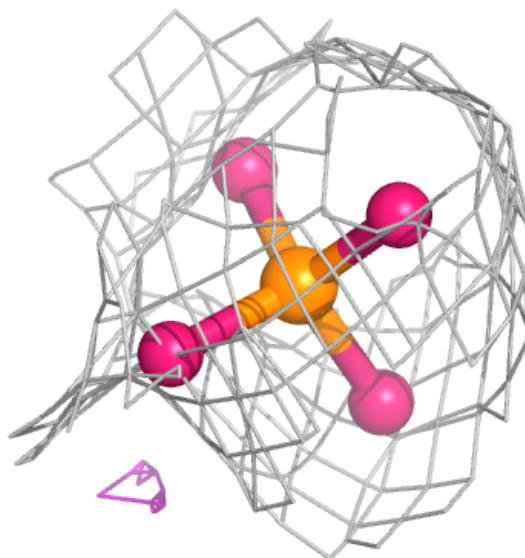
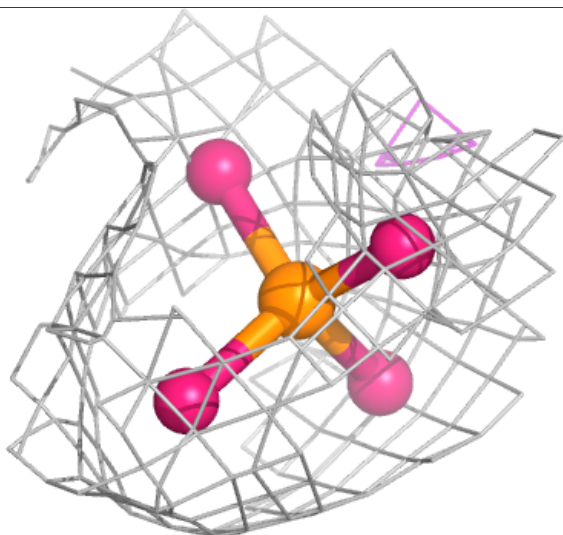
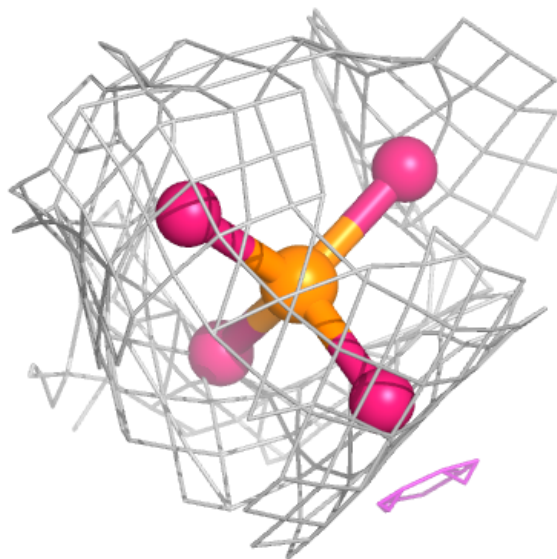
Electron density around PO4 H 301:

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



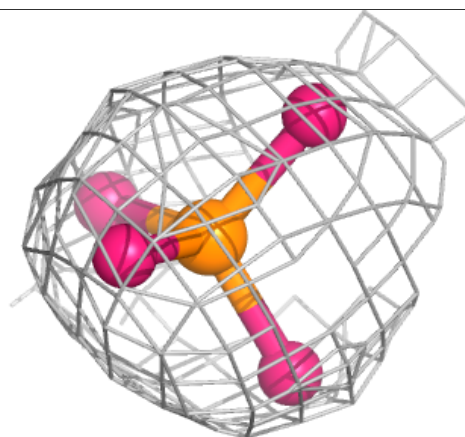
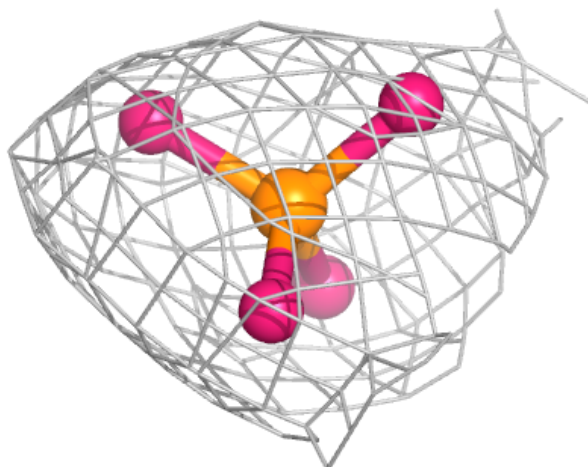
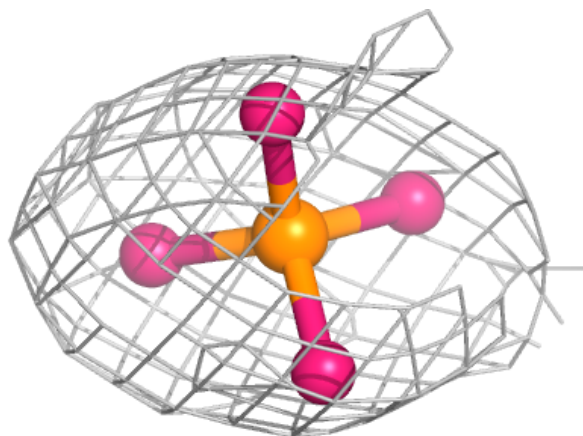
Electron density around PO4 I 301:

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



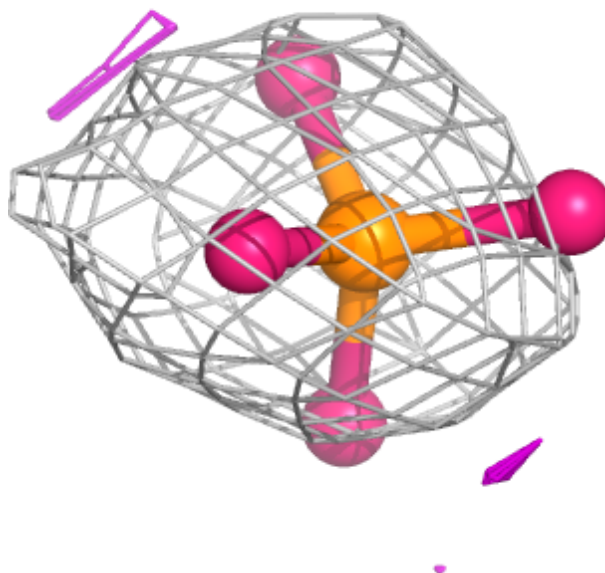
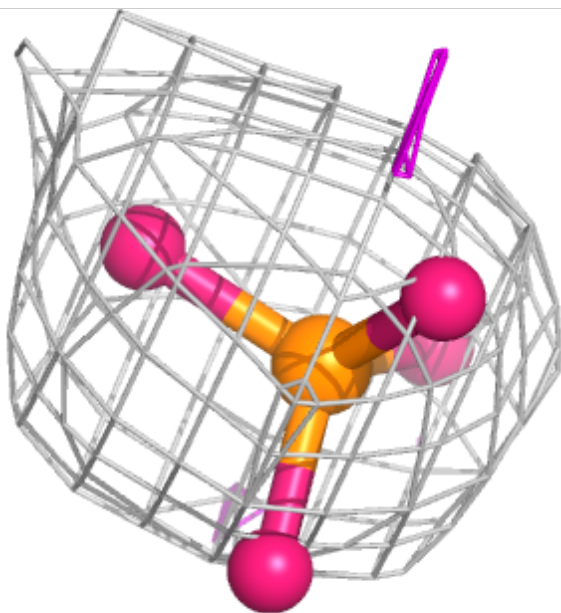
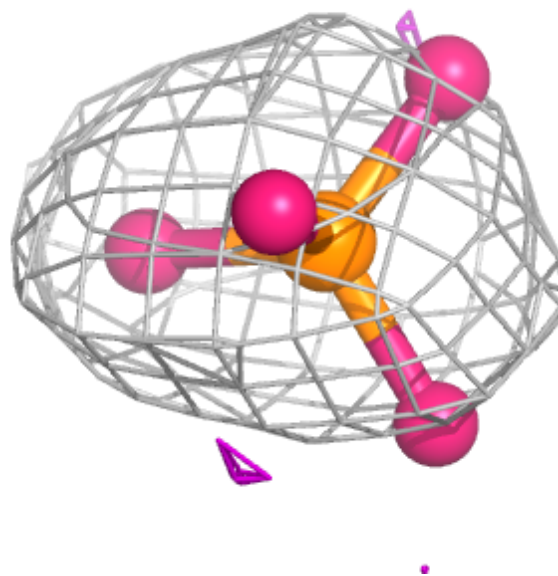
Electron density around PO4 m 201:

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



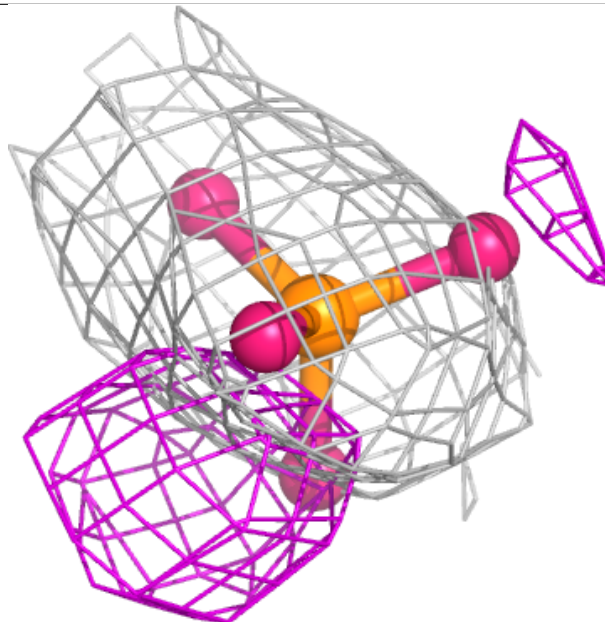
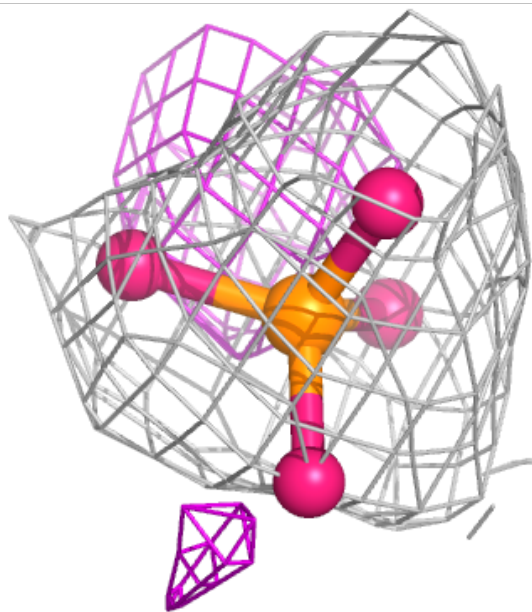
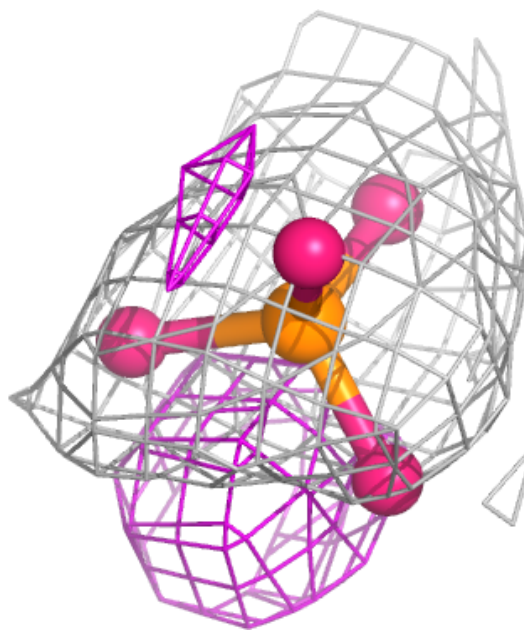
Electron density around PO4 C 304:

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



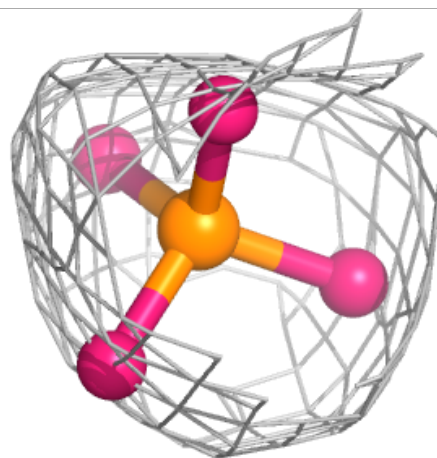
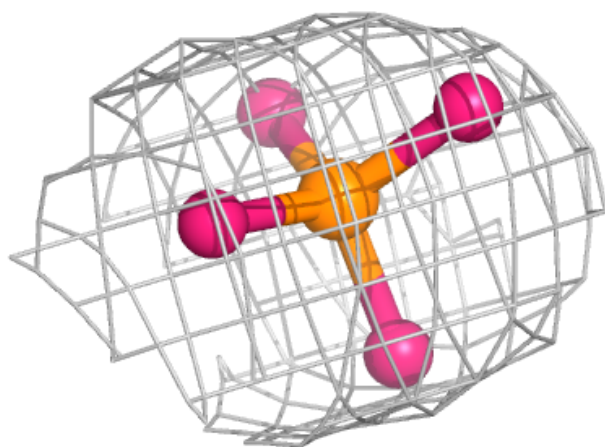
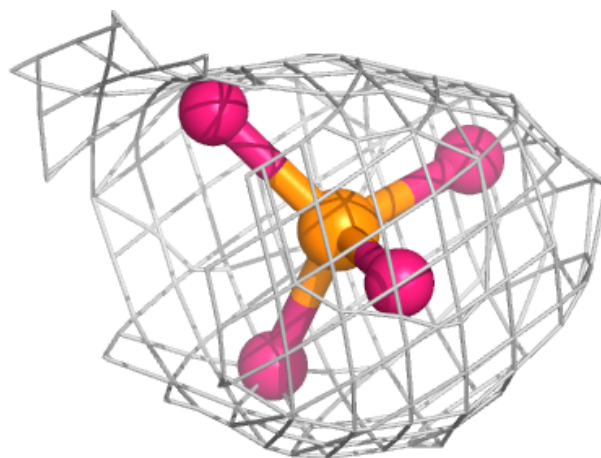
Electron density around PO4 g 201:

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



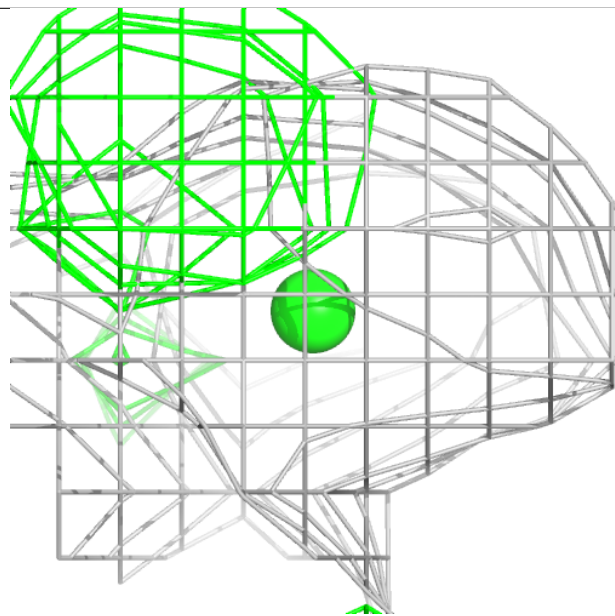
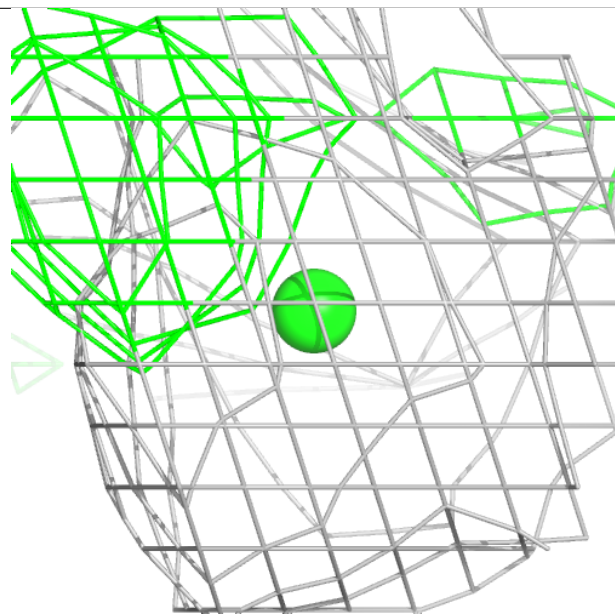
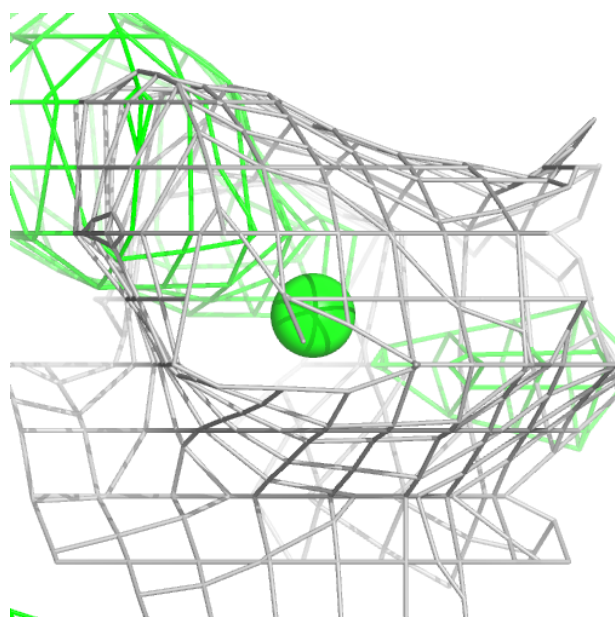
Electron density around PO4 J 301:

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



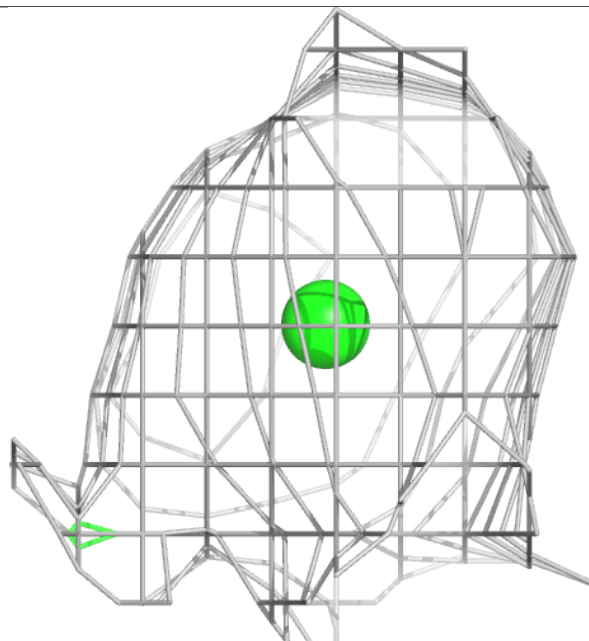
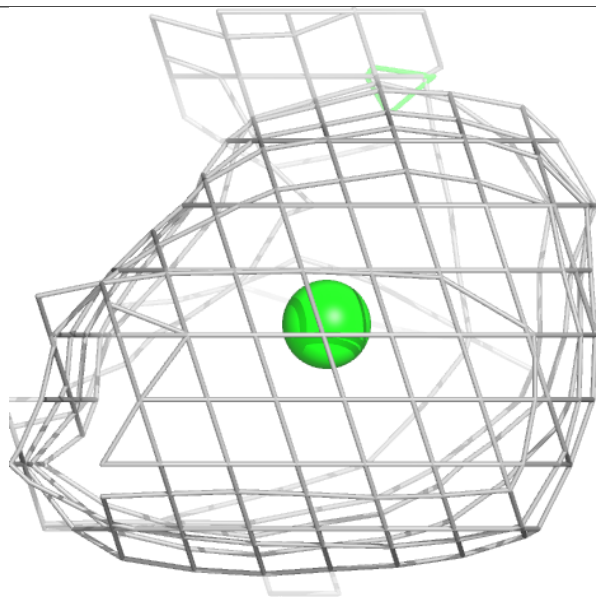
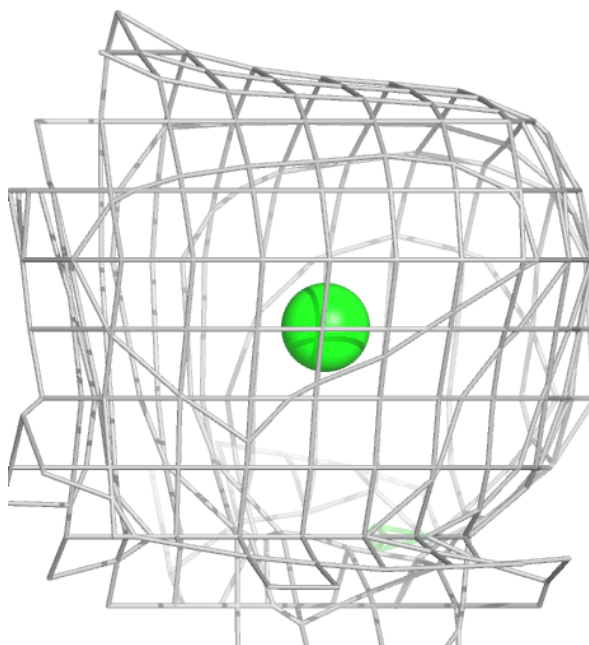
Electron density around CL K 304:

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



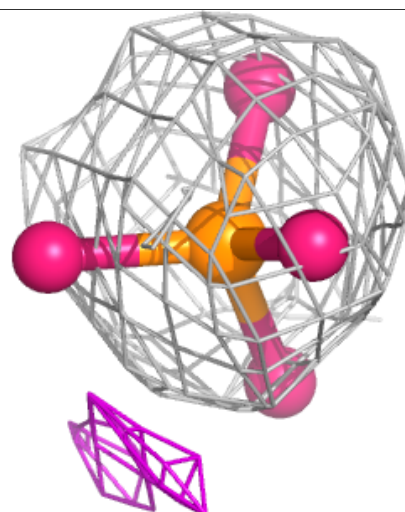
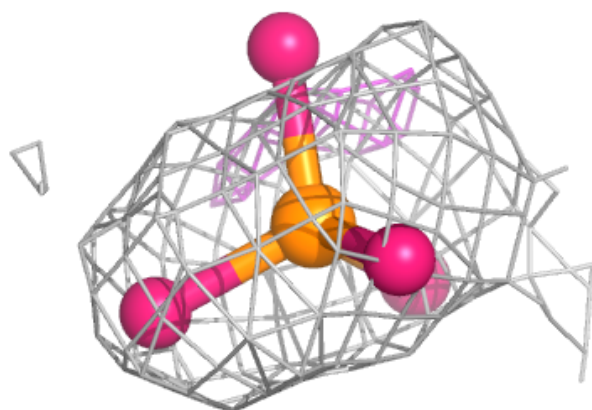
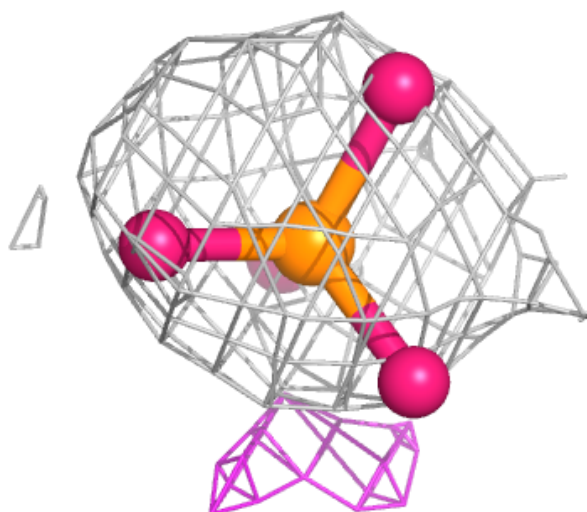
Electron density around CL R 302:

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



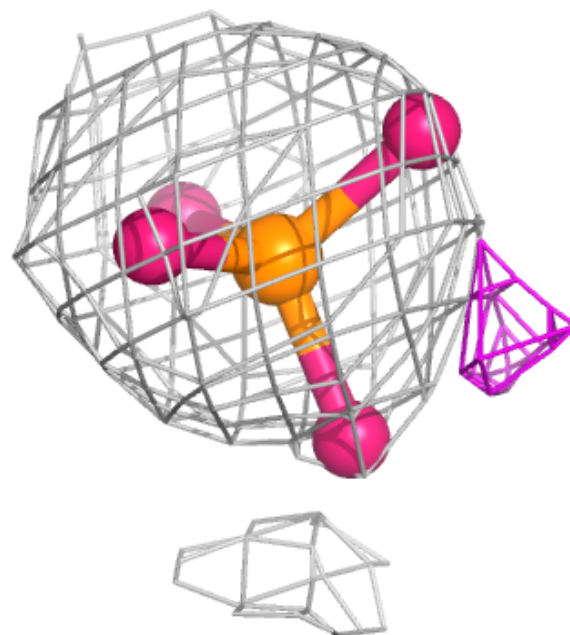
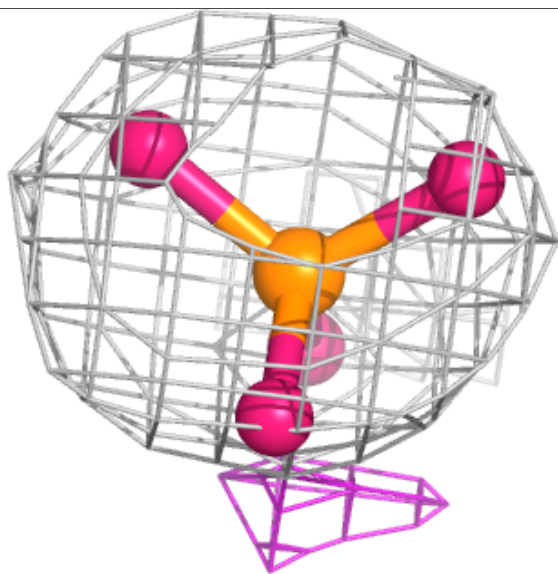
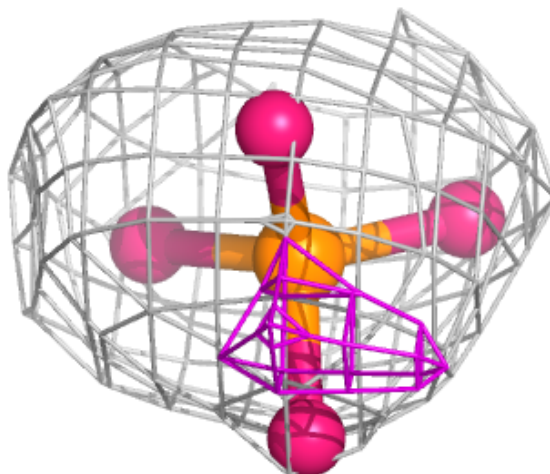
Electron density around PO4 K 301:

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



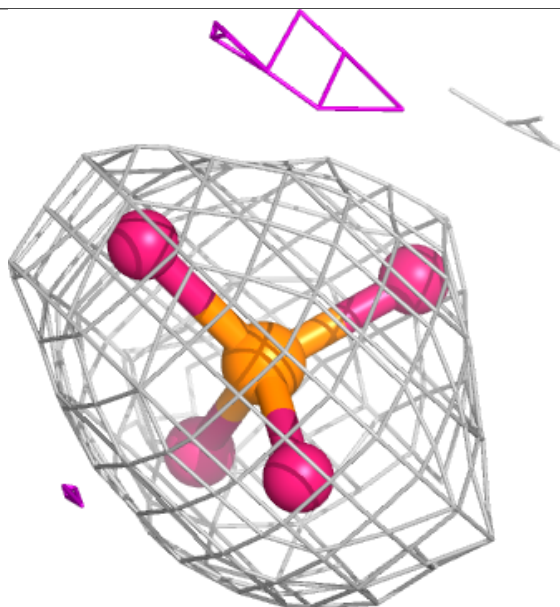
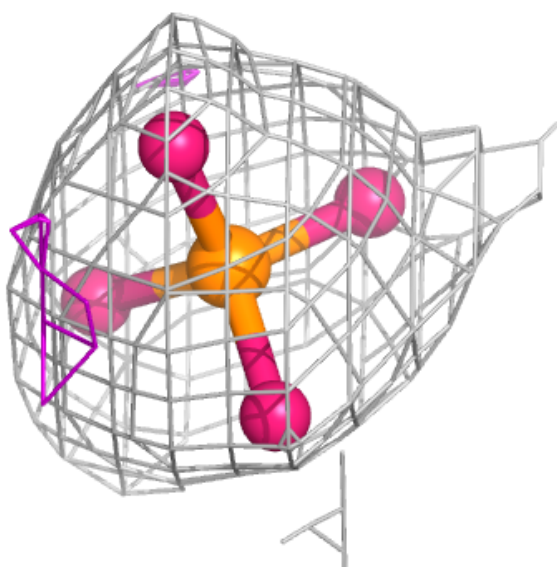
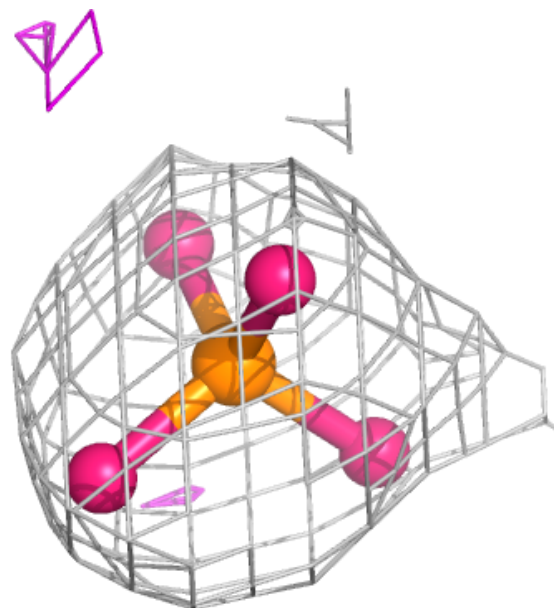
Electron density around PO4 G 302:

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



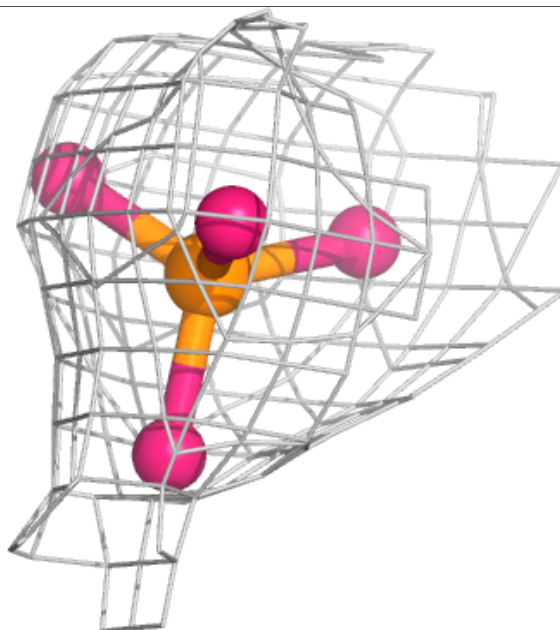
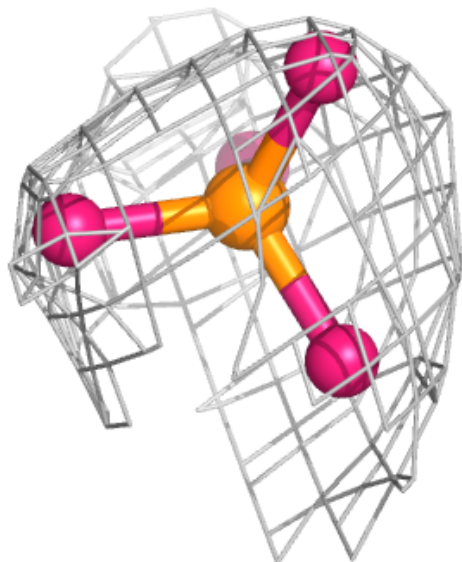
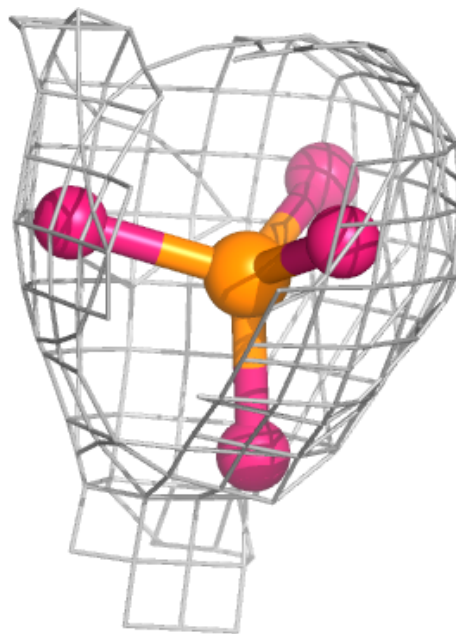
Electron density around PO4 O 301:

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



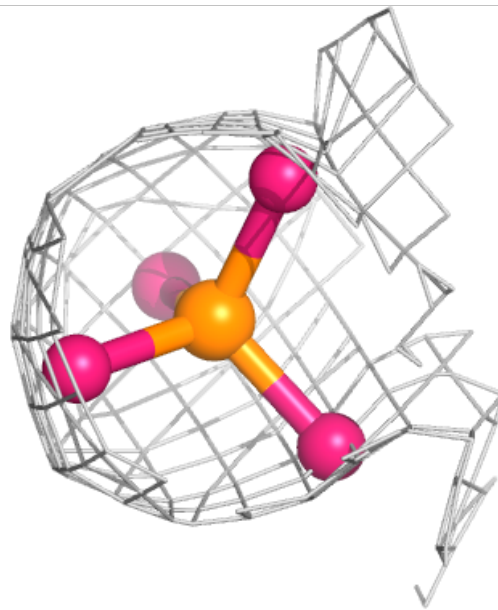
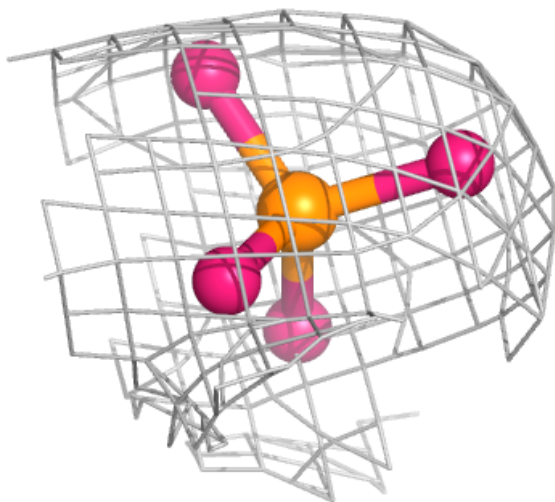
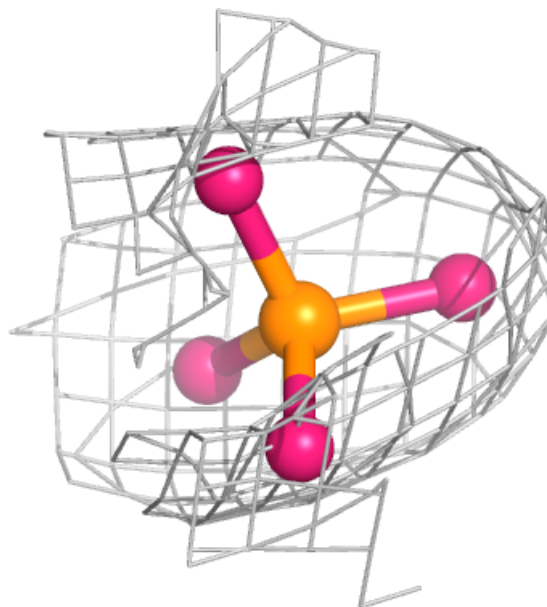
Electron density around PO4 a 201:

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



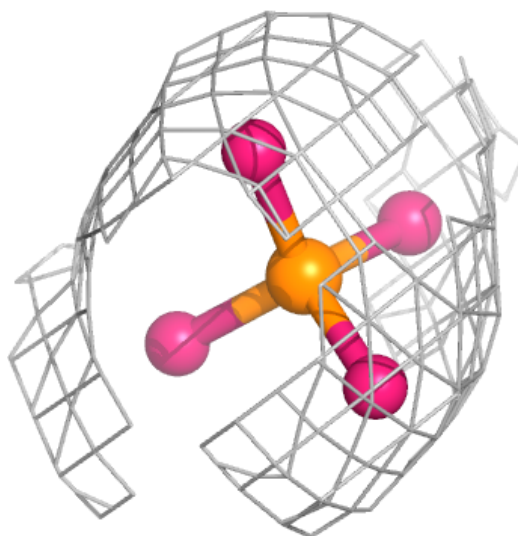
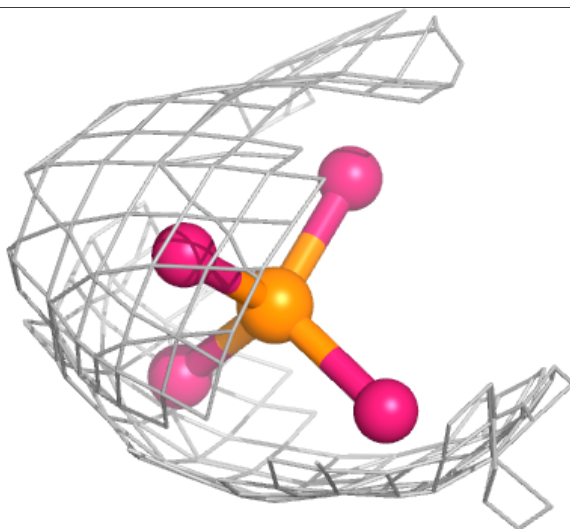
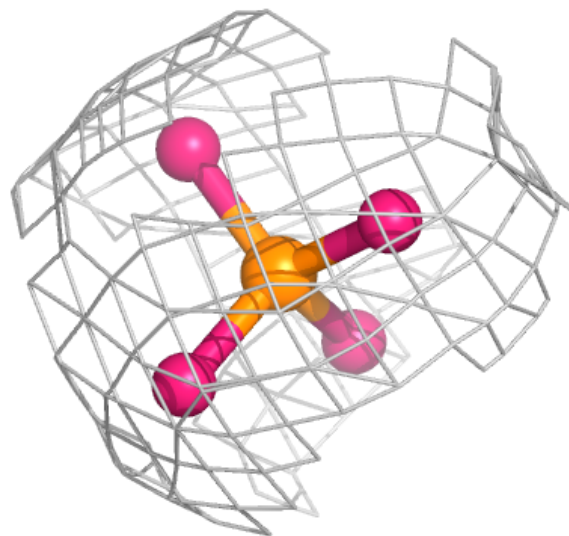
Electron density around PO4 Q 301:

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



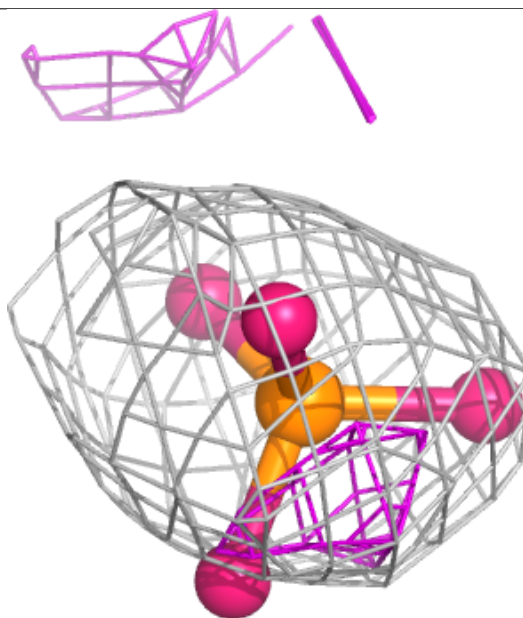
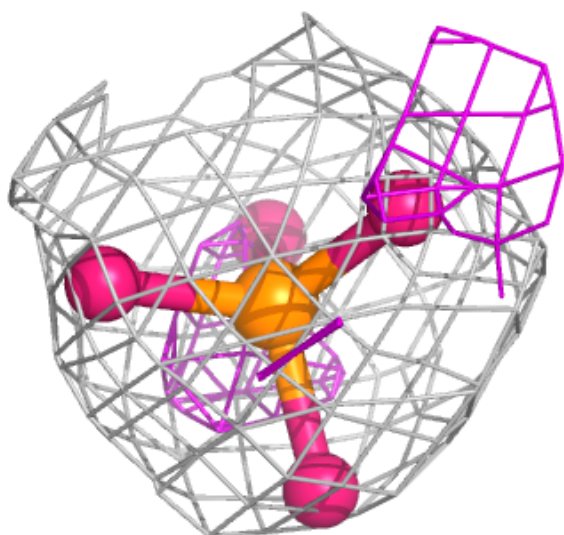
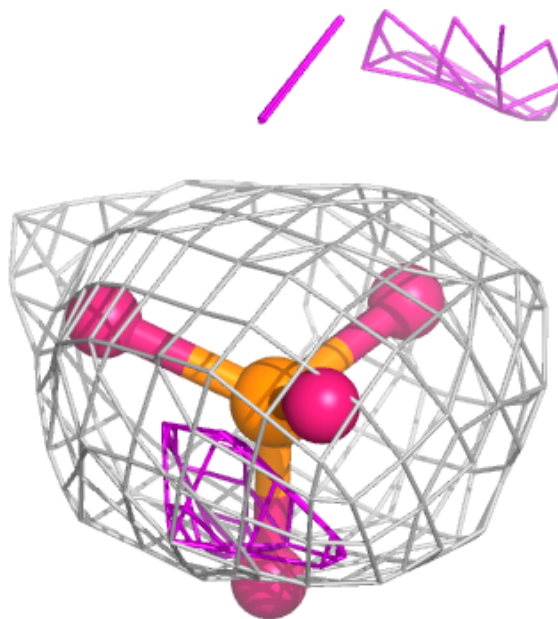
Electron density around PO4 o 203:

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



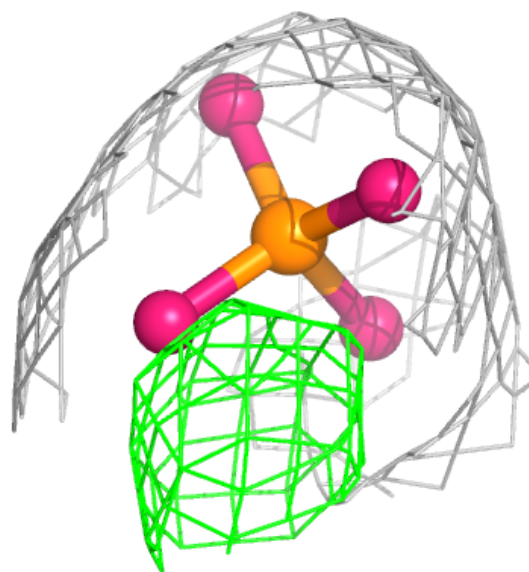
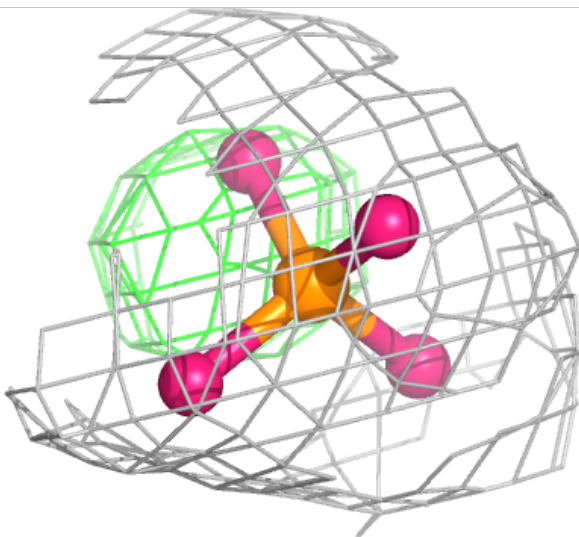
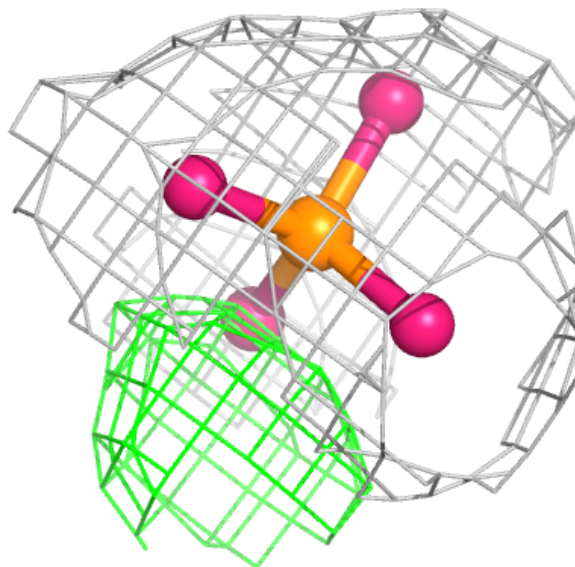
Electron density around PO4 J 302:

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



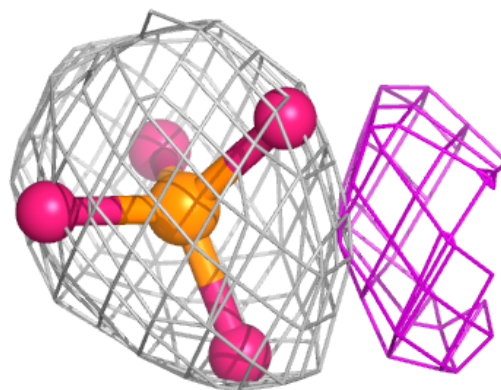
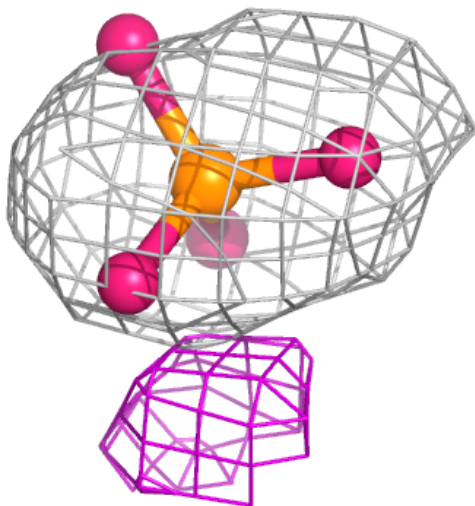
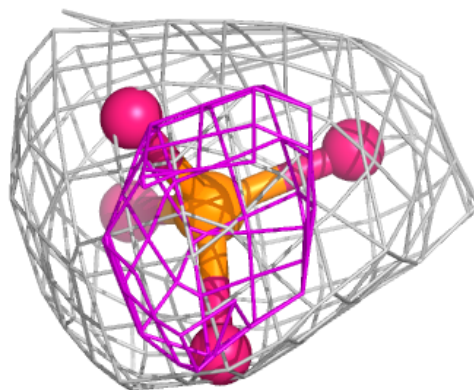
Electron density around PO4 m 202:

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



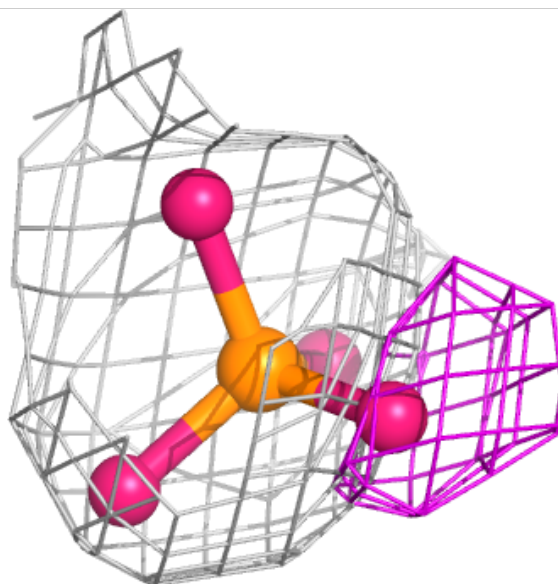
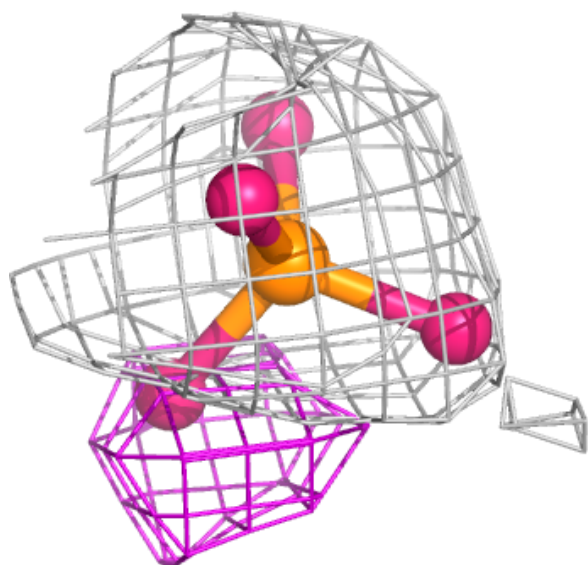
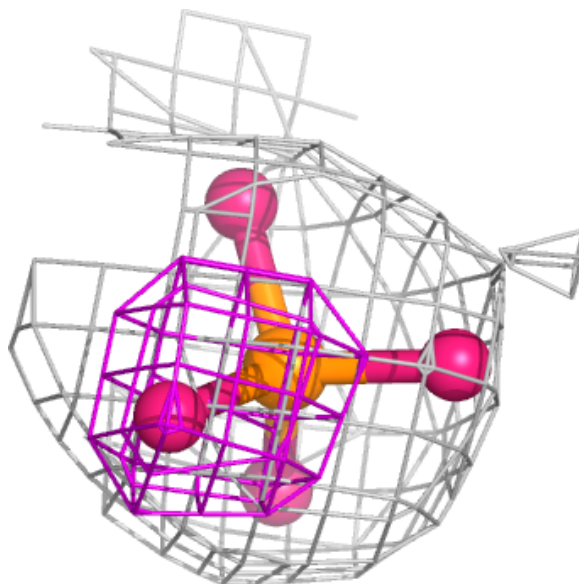
Electron density around PO4 E 301:

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



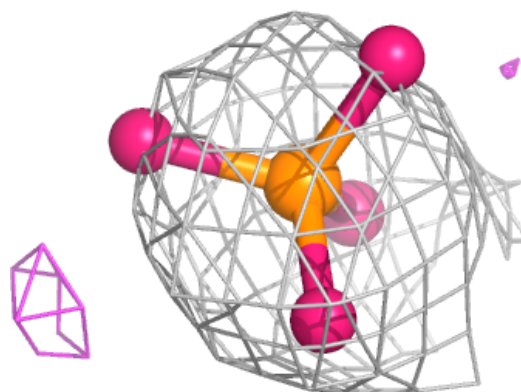
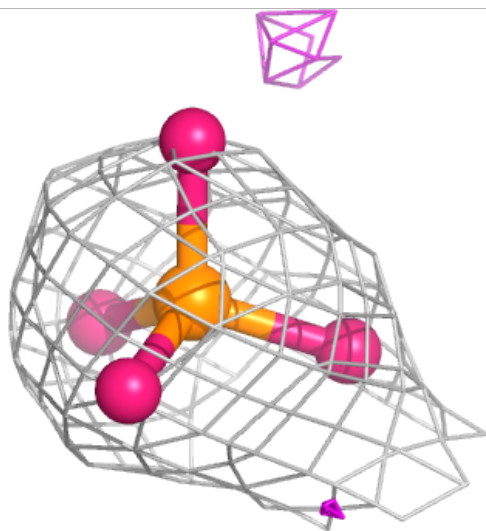
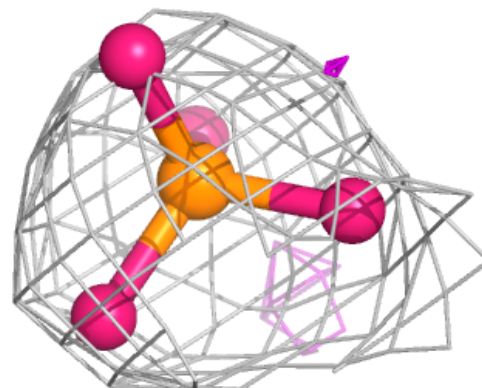
Electron density around PO4 E 302:

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



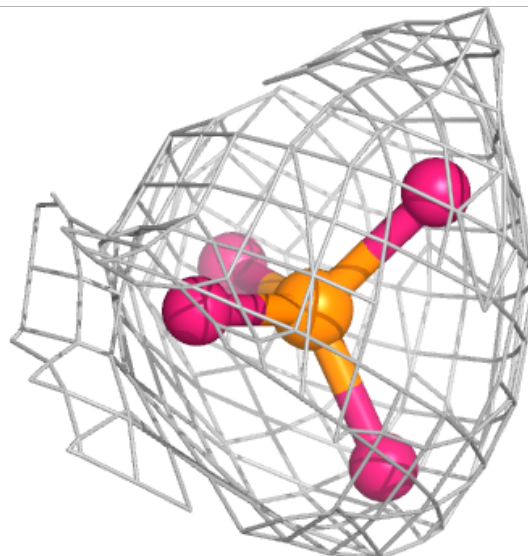
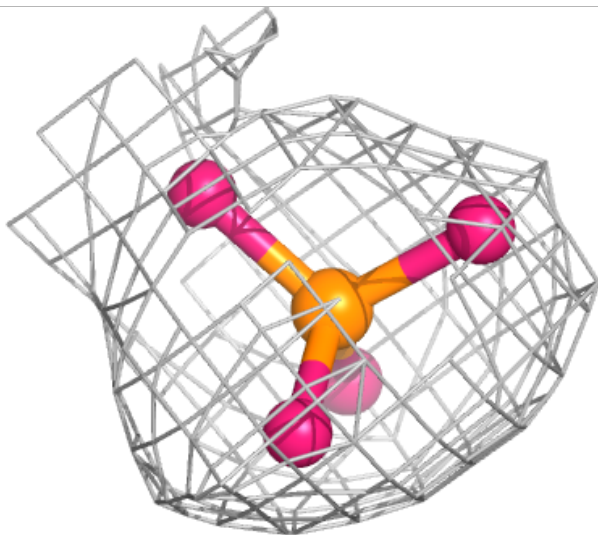
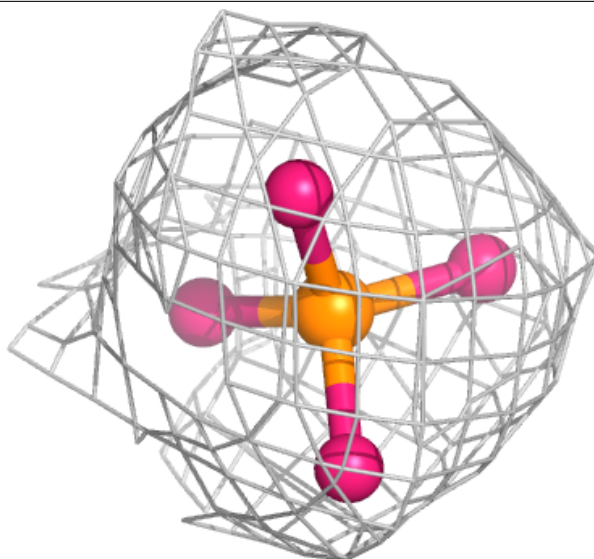
Electron density around PO4 e 201:

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



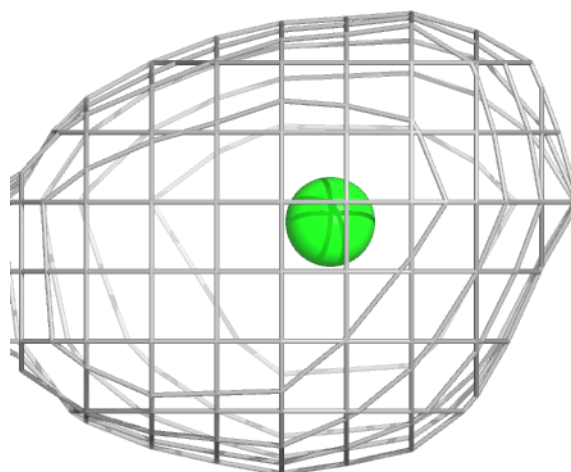
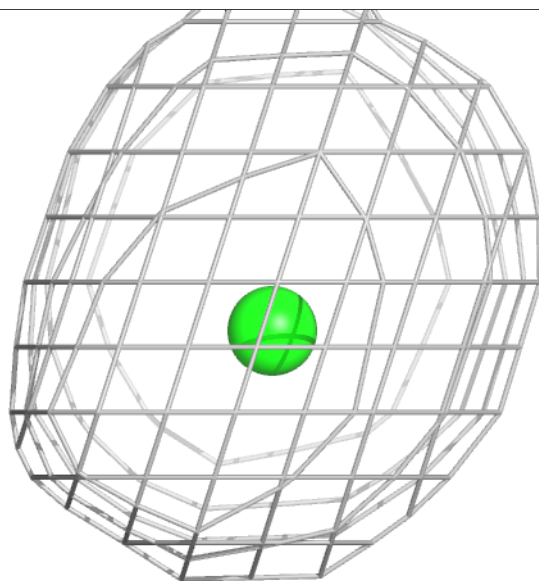
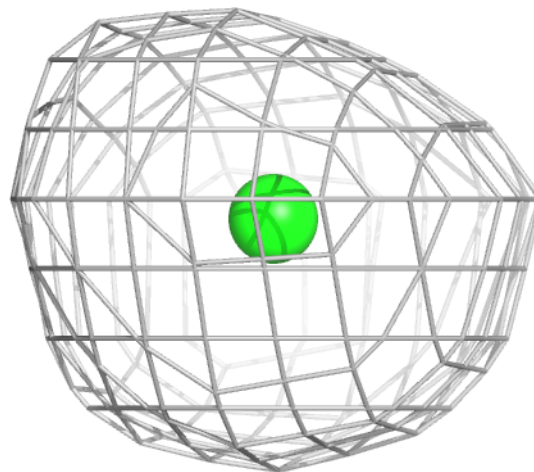
Electron density around PO4 R 301:

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



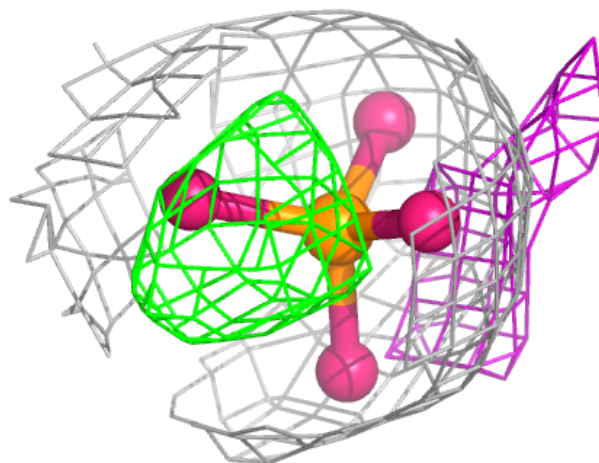
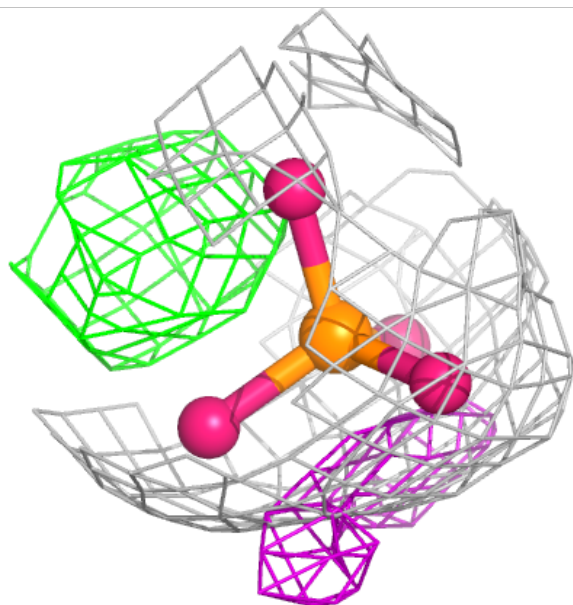
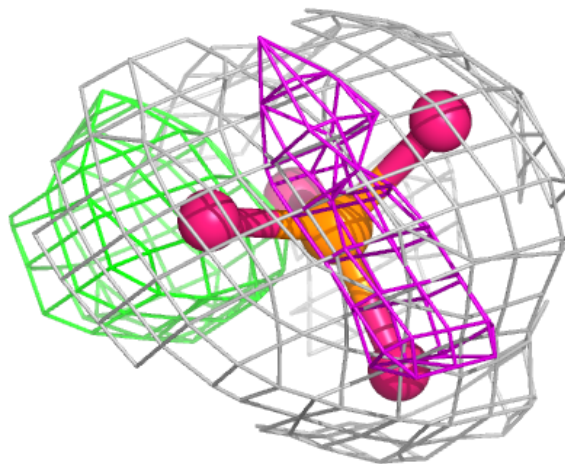
Electron density around CL q 202:

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



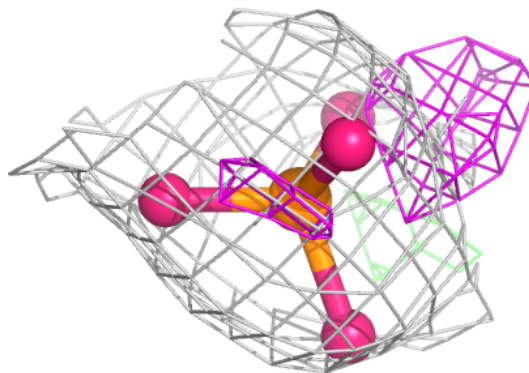
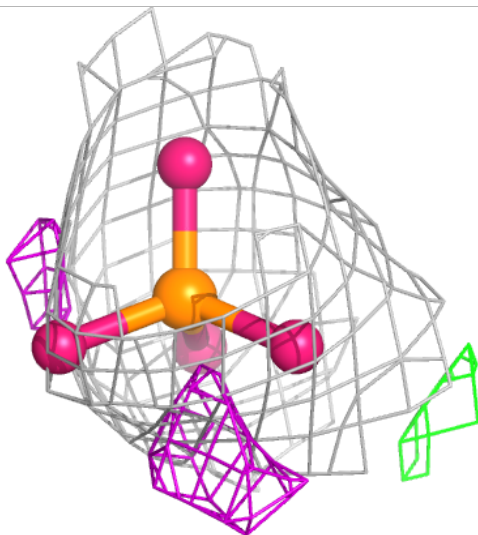
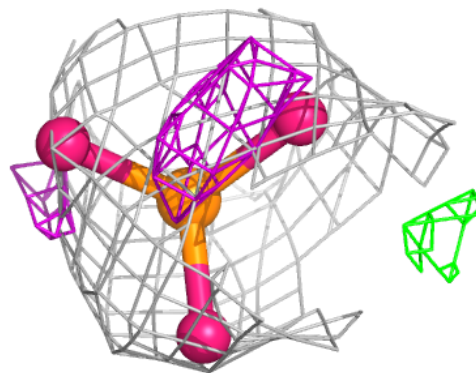
Electron density around PO4 e 202:

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



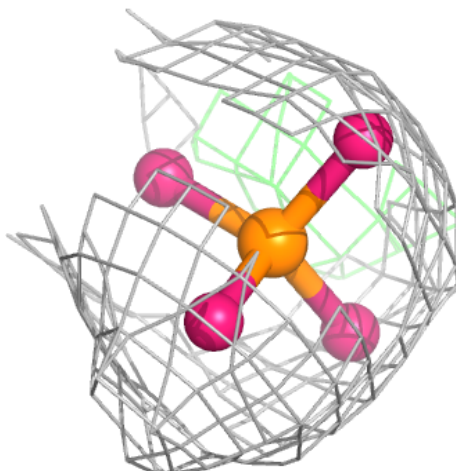
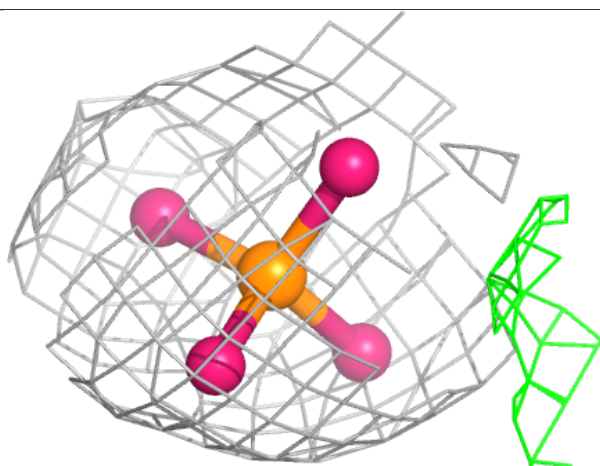
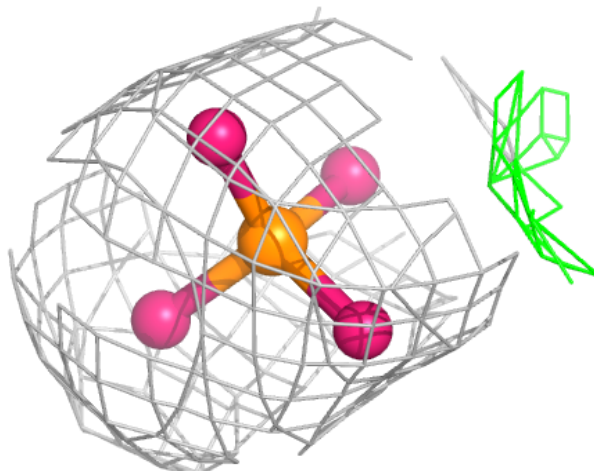
Electron density around PO4 e 203:

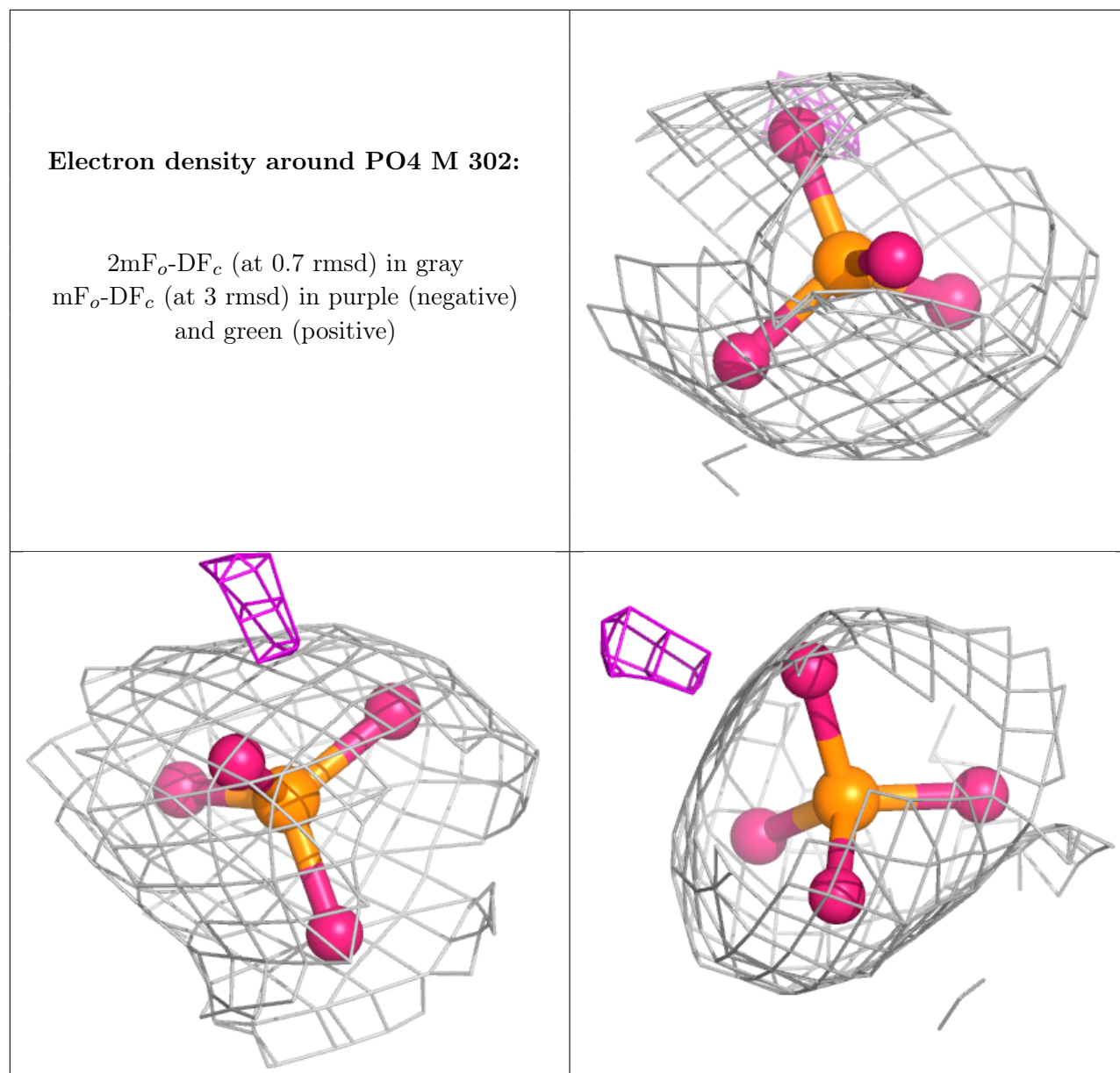
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PO4 B 301:

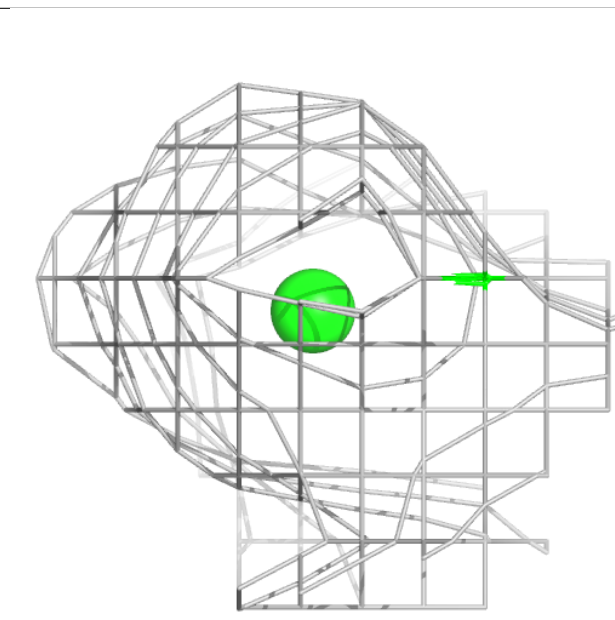
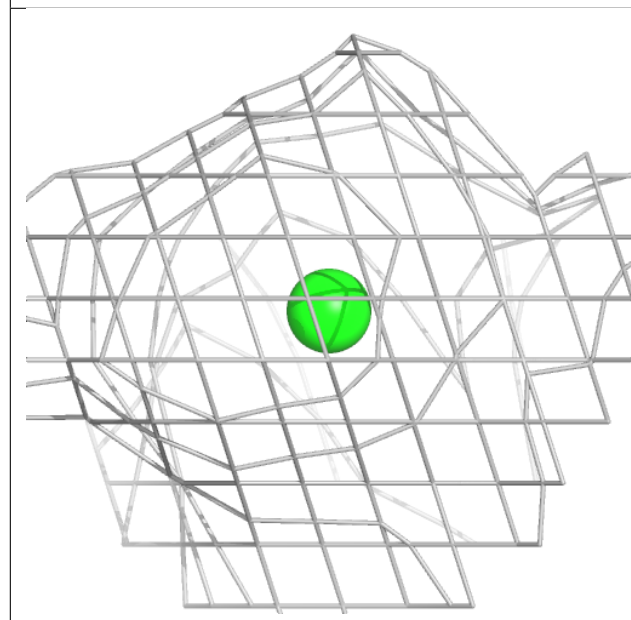
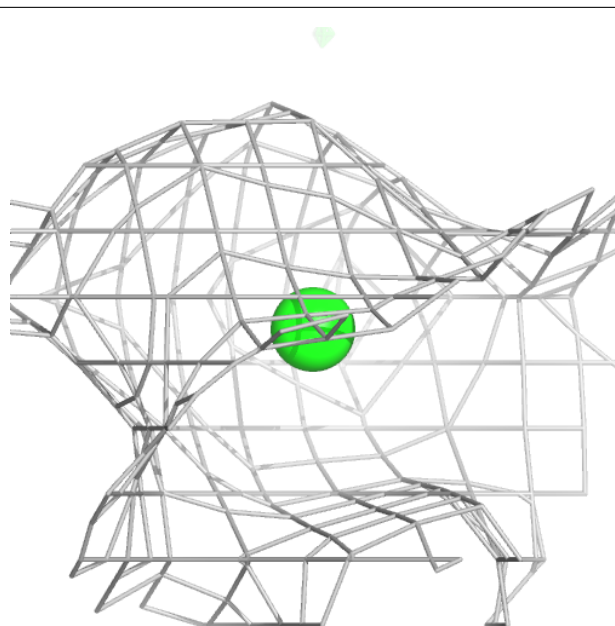
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





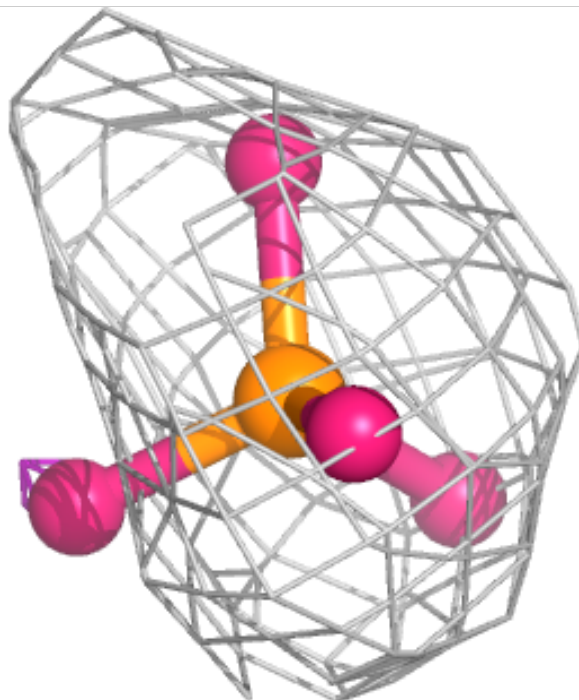
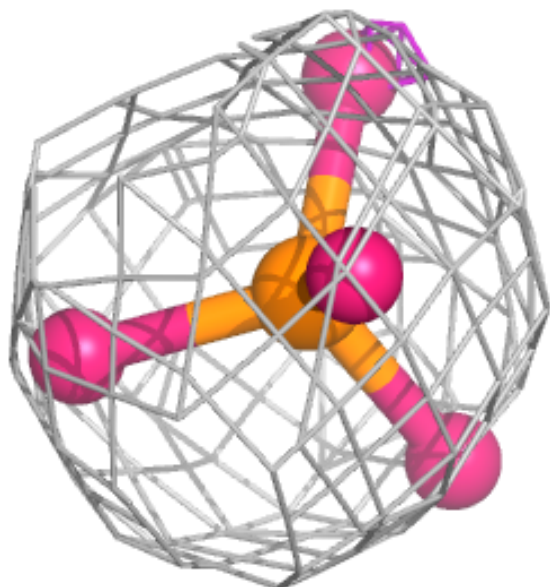
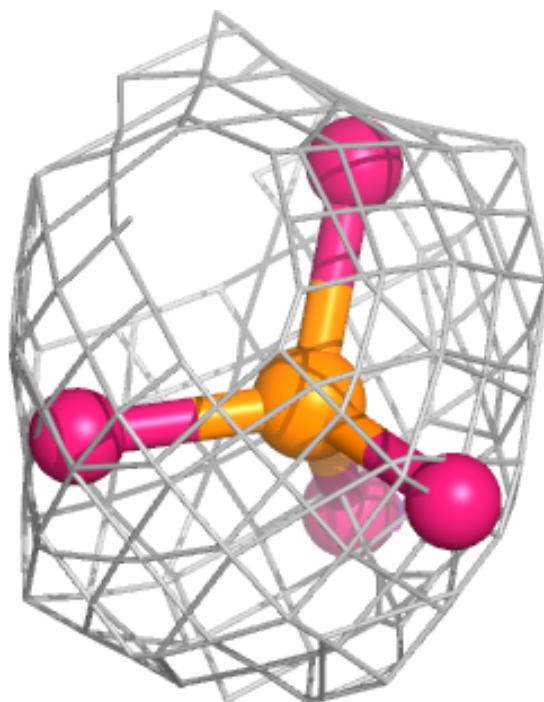
Electron density around CL G 304:

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



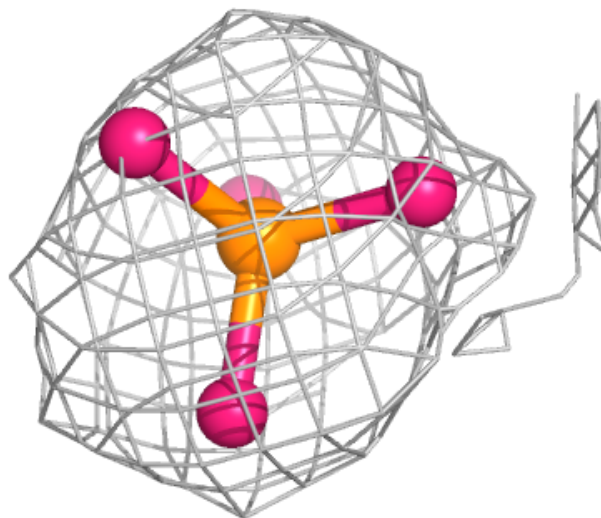
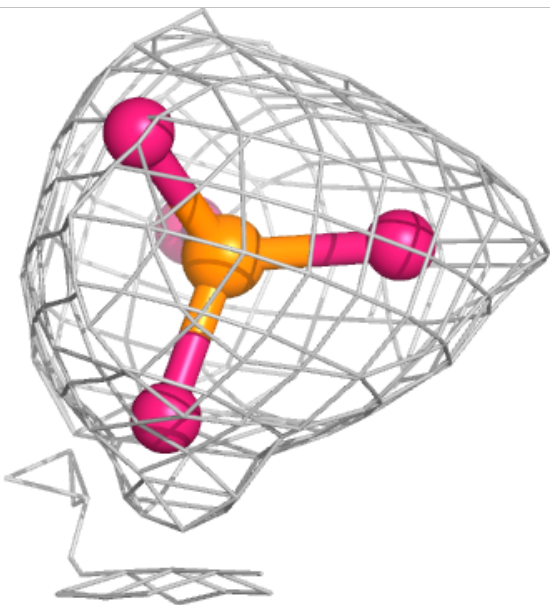
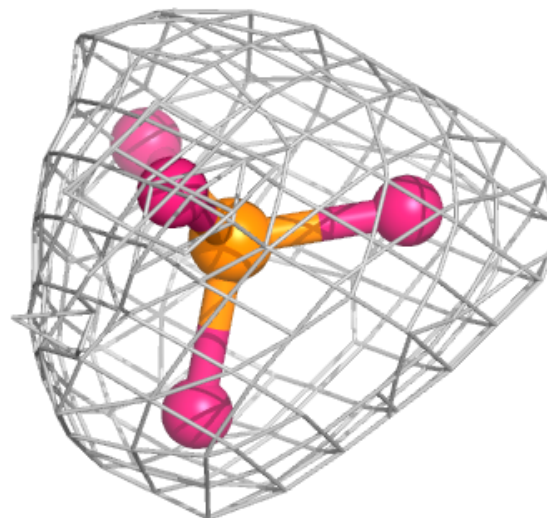
Electron density around PO4 E 303:

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



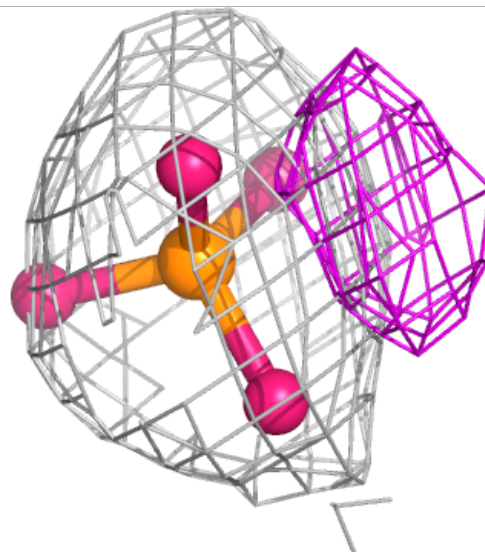
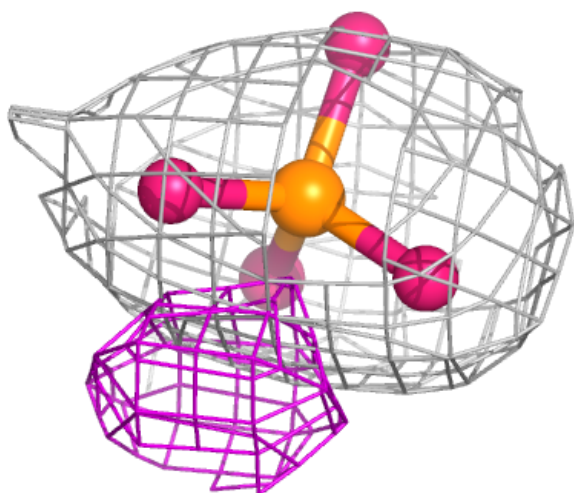
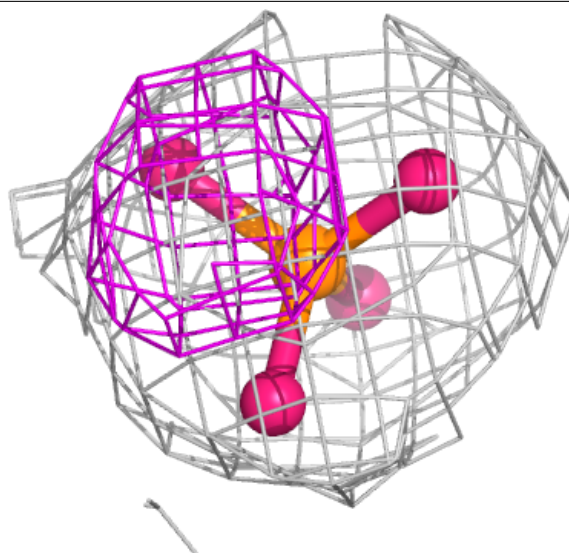
Electron density around PO4 O 302:

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



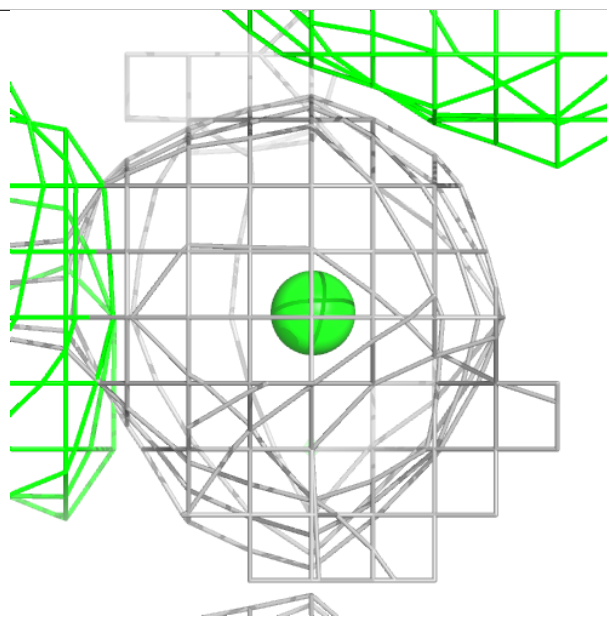
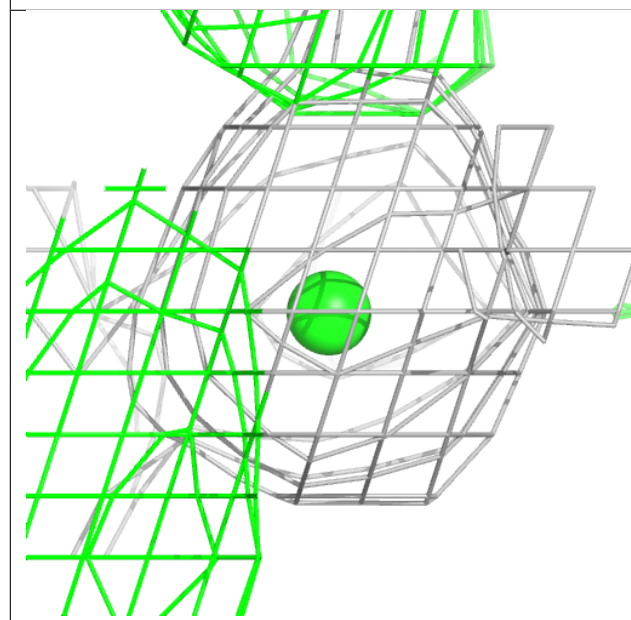
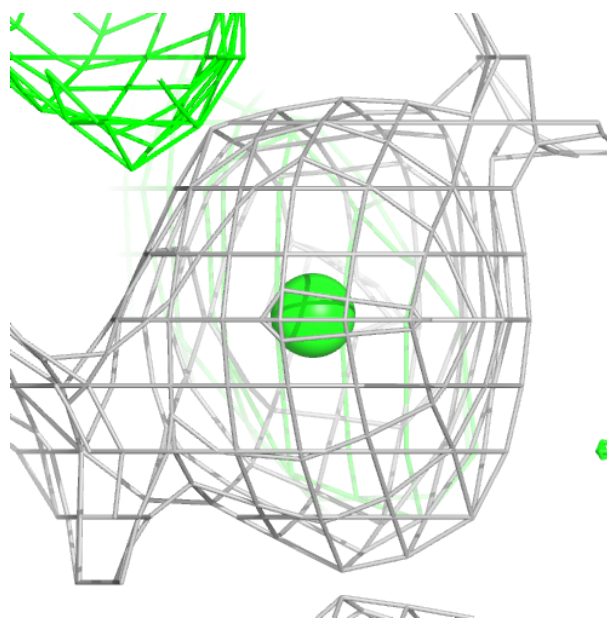
Electron density around PO4 c 202:

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



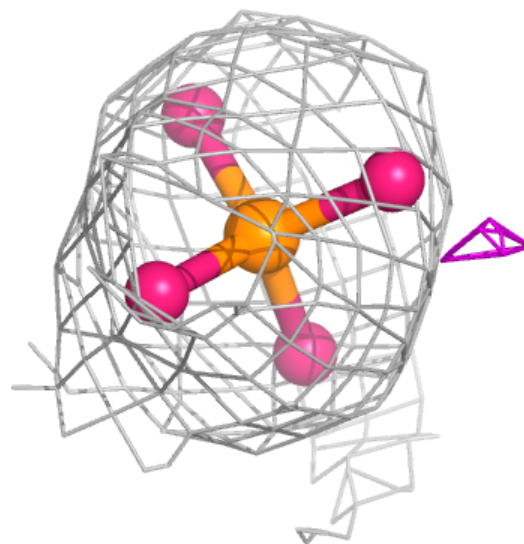
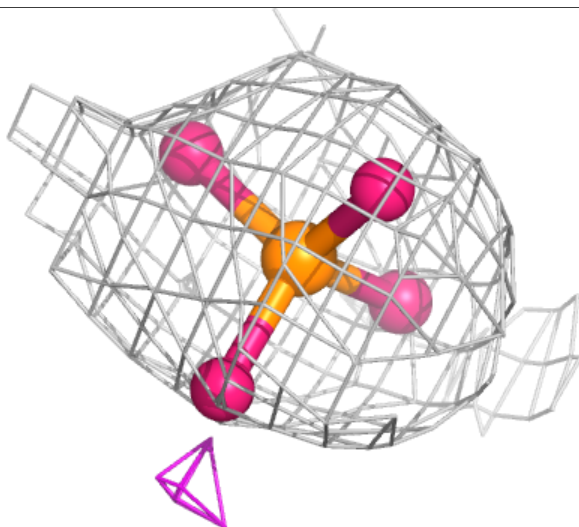
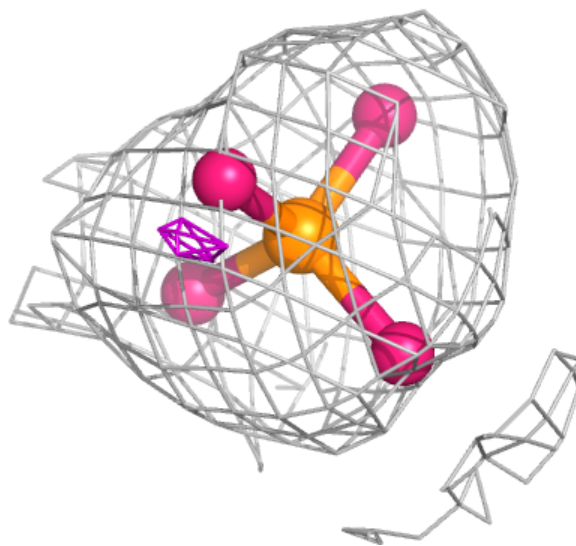
Electron density around CL H 302:

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



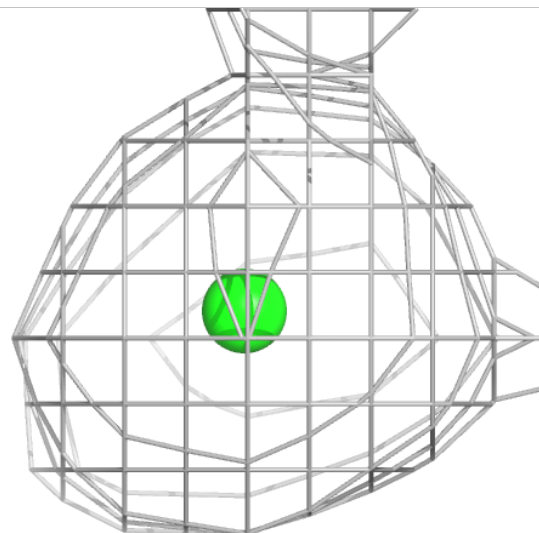
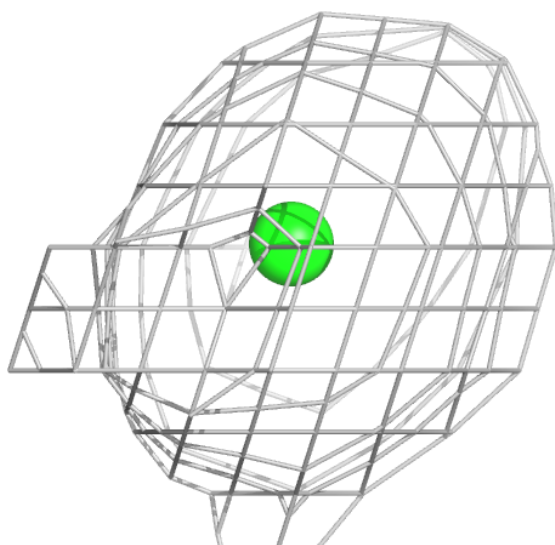
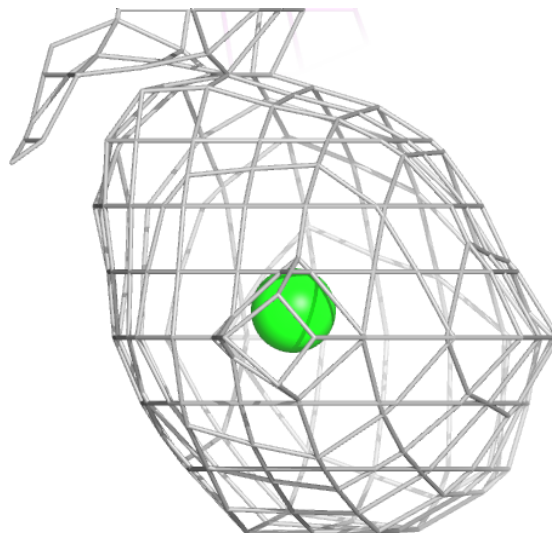
Electron density around PO4 C 302:

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



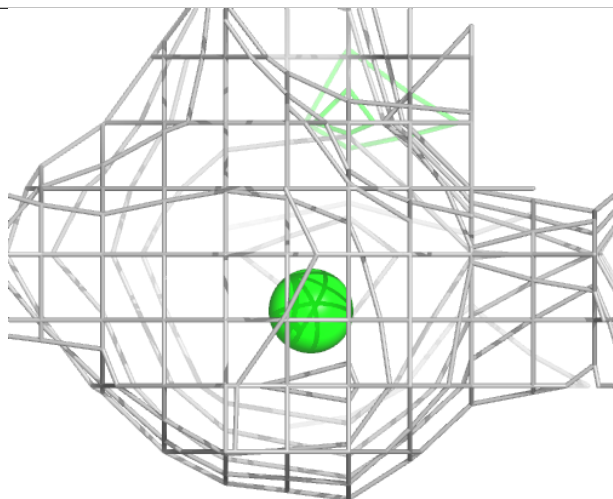
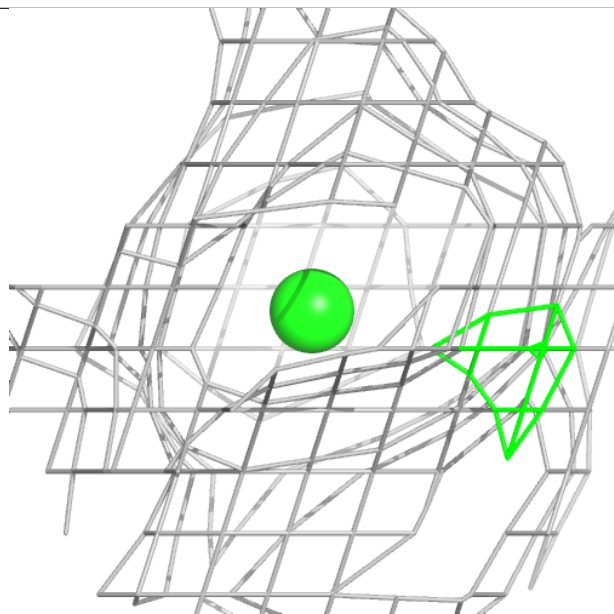
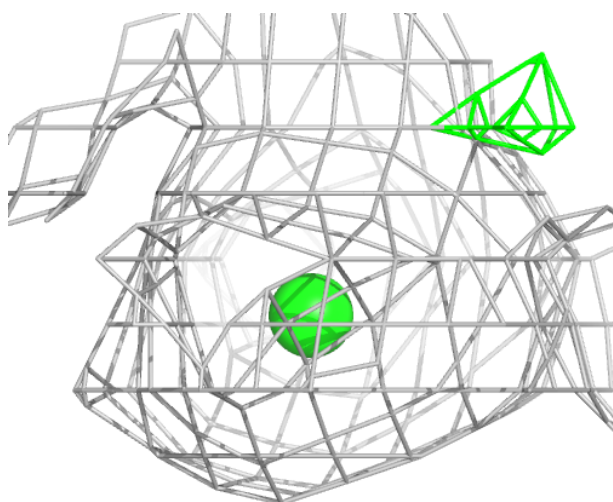
Electron density around CL M 304:

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



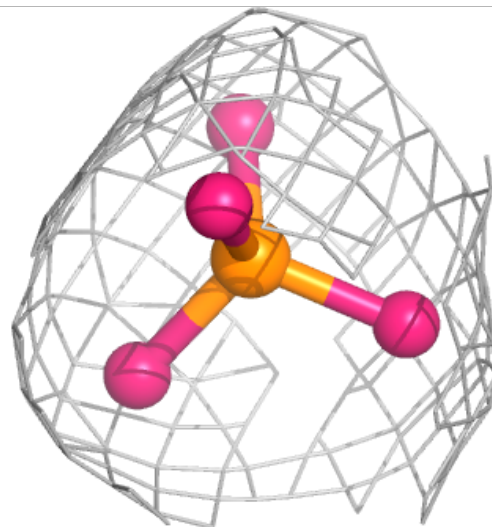
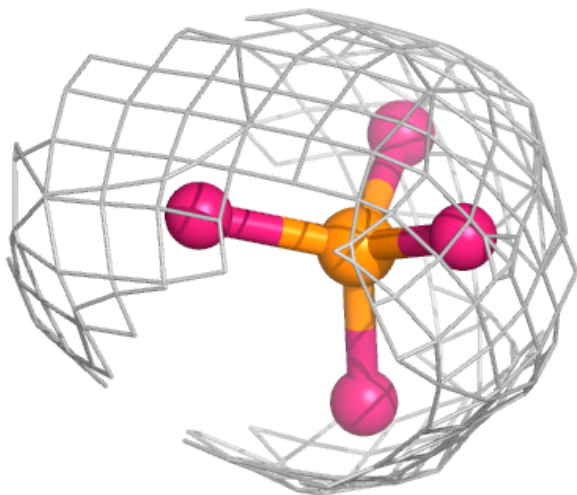
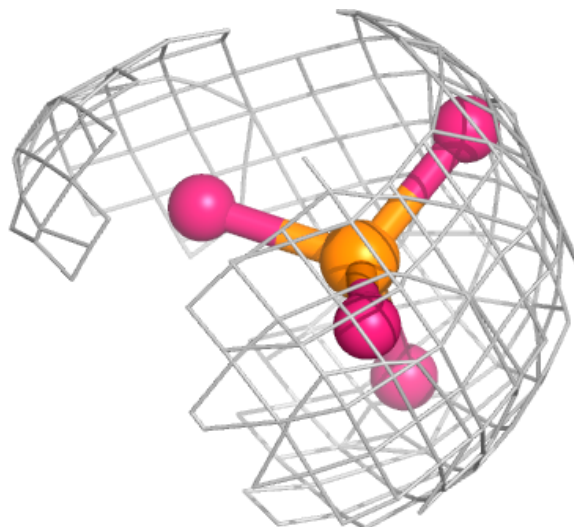
Electron density around CL C 306:

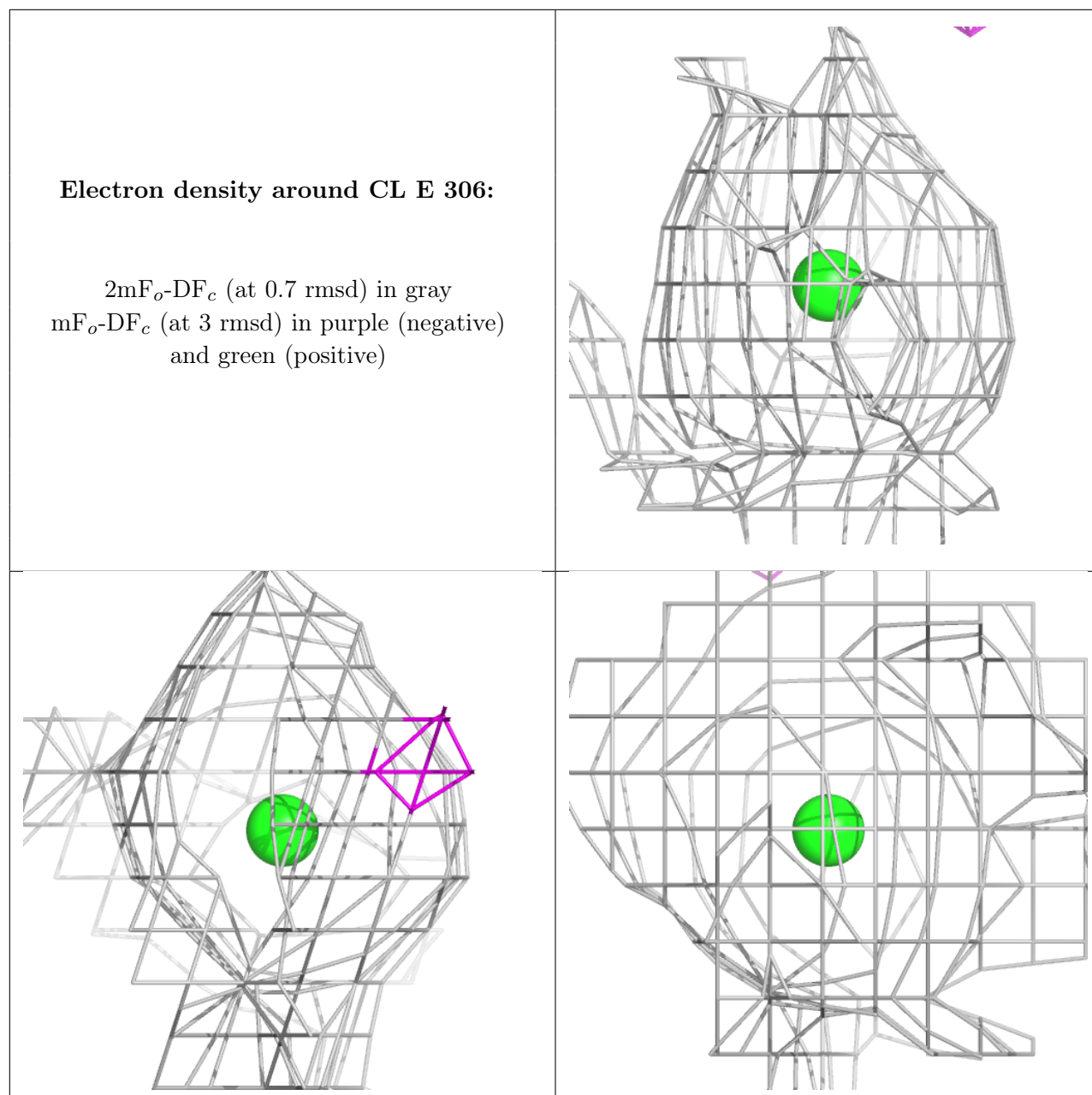
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PO4 M 301:

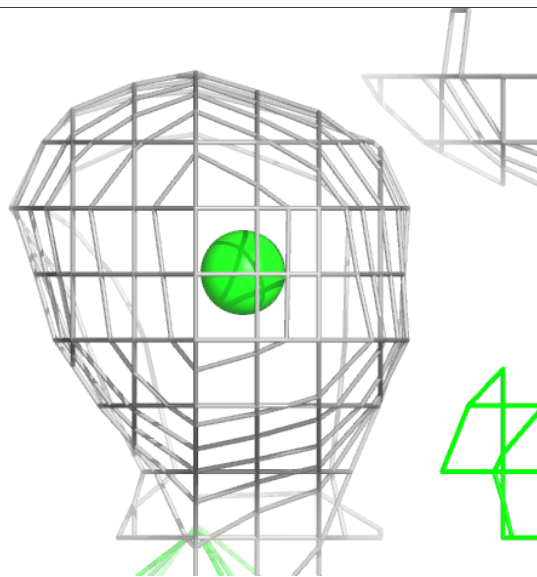
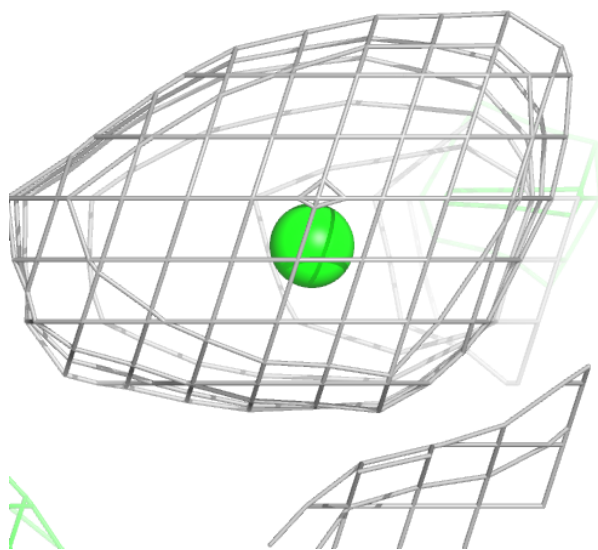
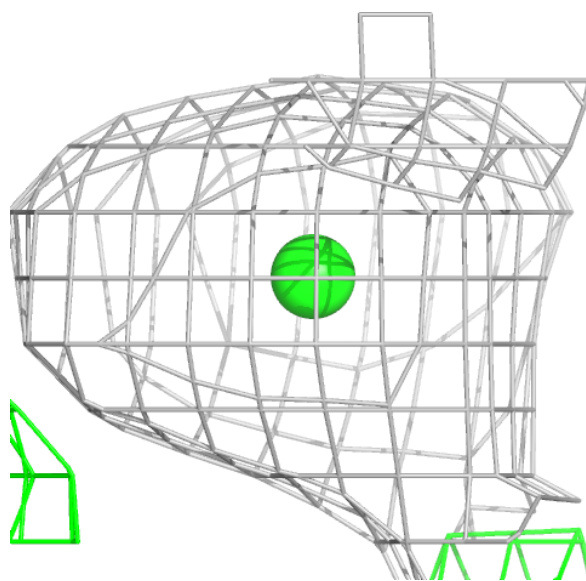
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





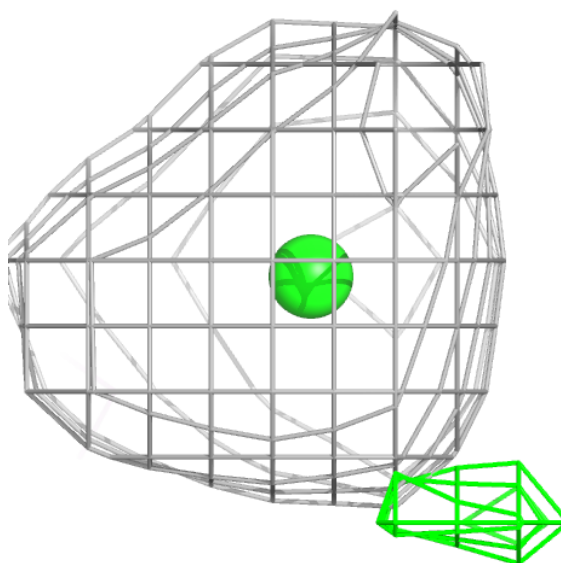
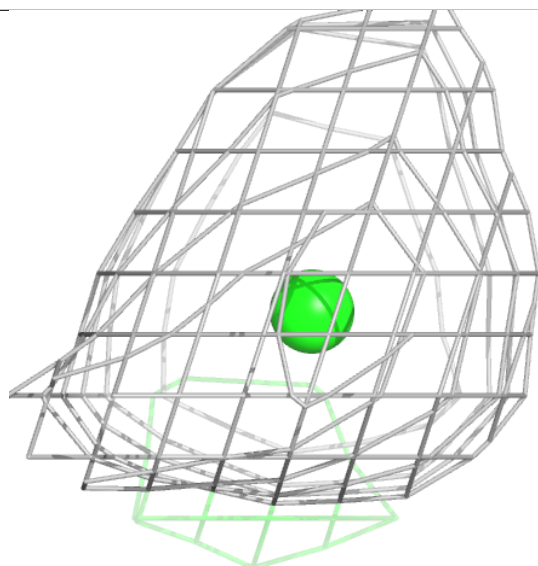
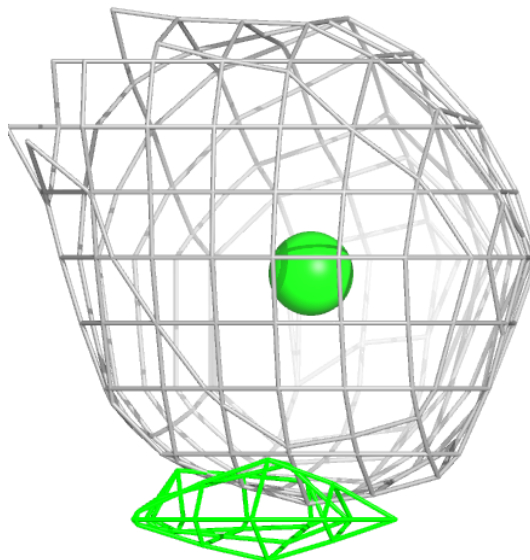
Electron density around CL N 302:

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



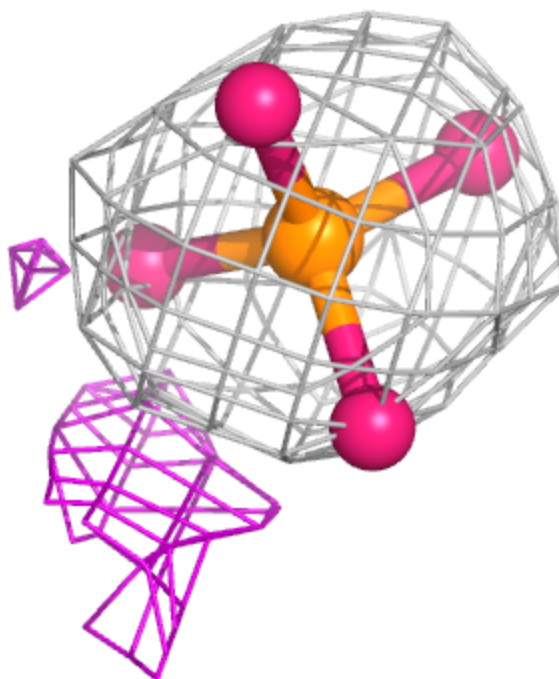
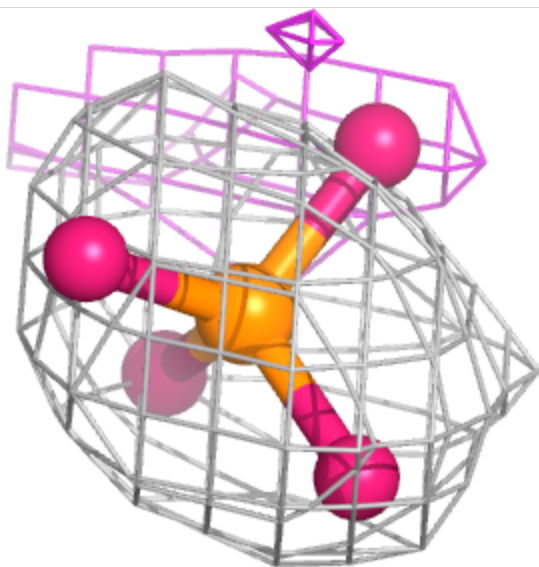
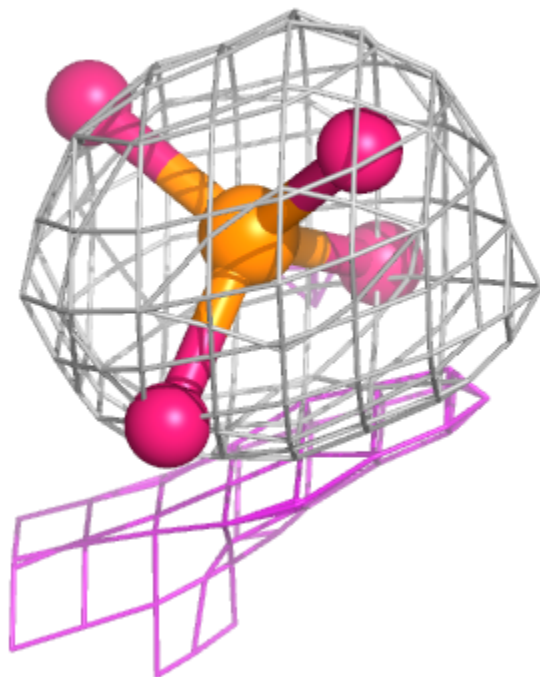
Electron density around CL P 301:

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



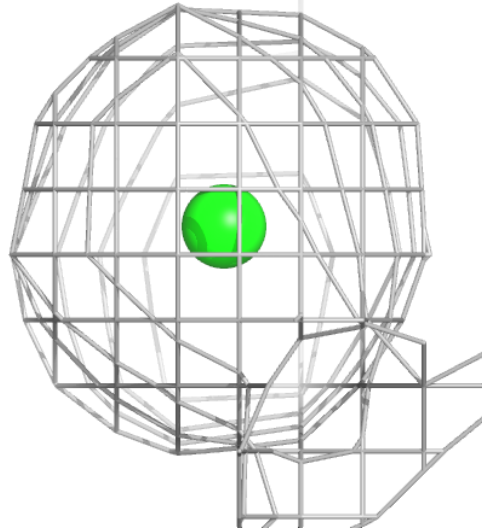
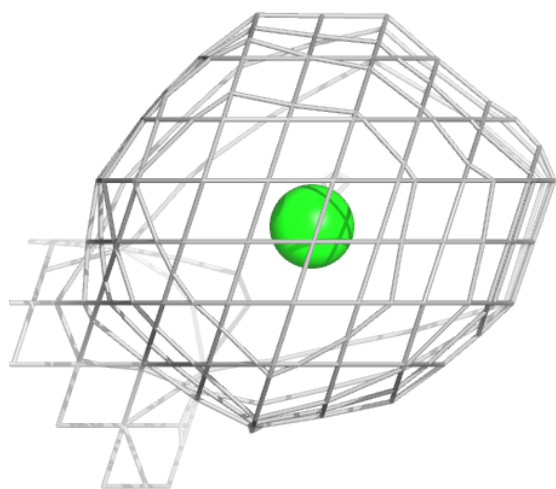
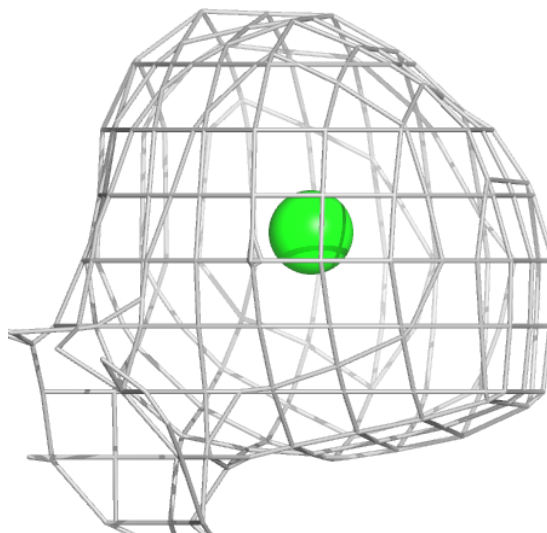
Electron density around PO4 I 302:

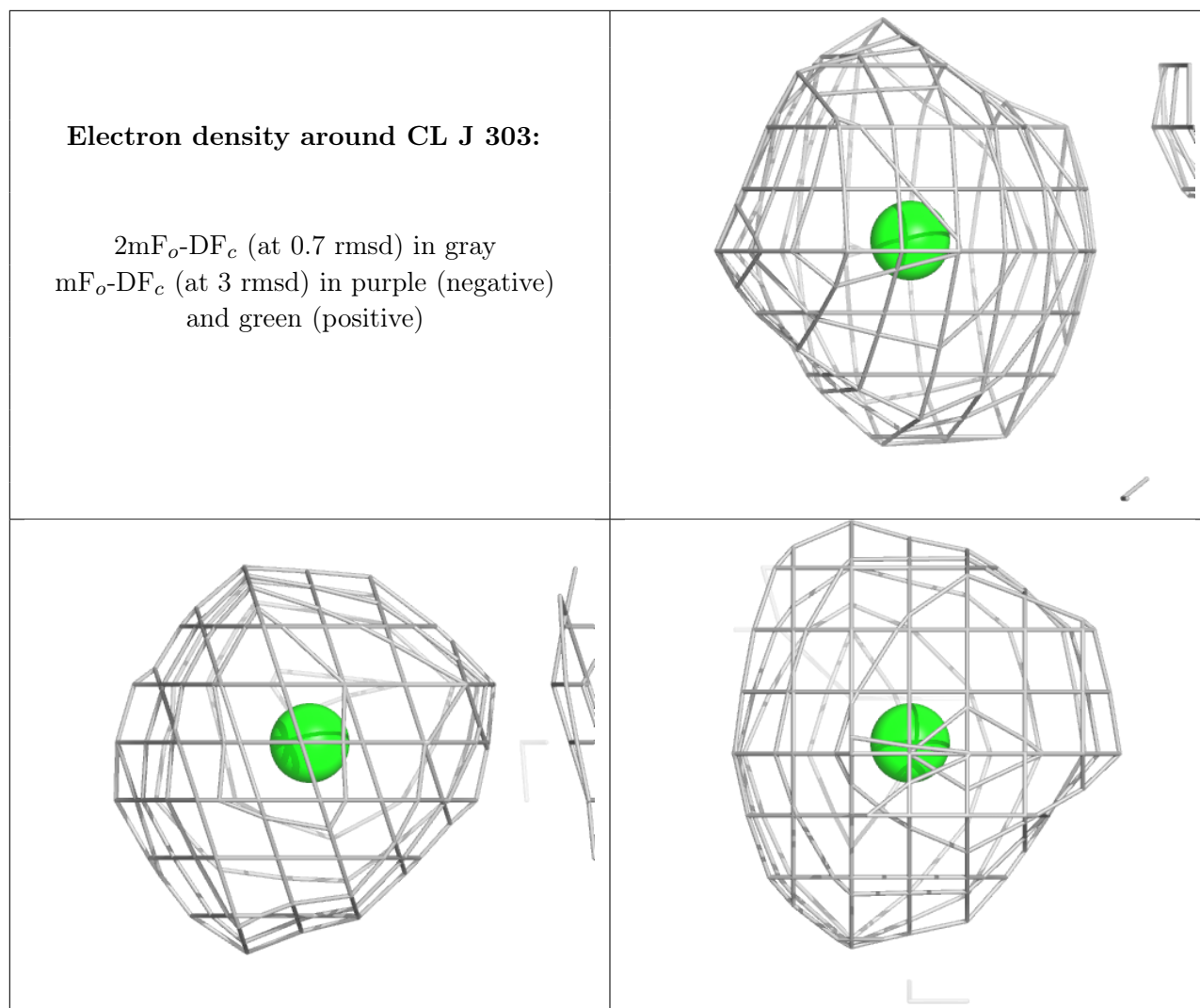
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

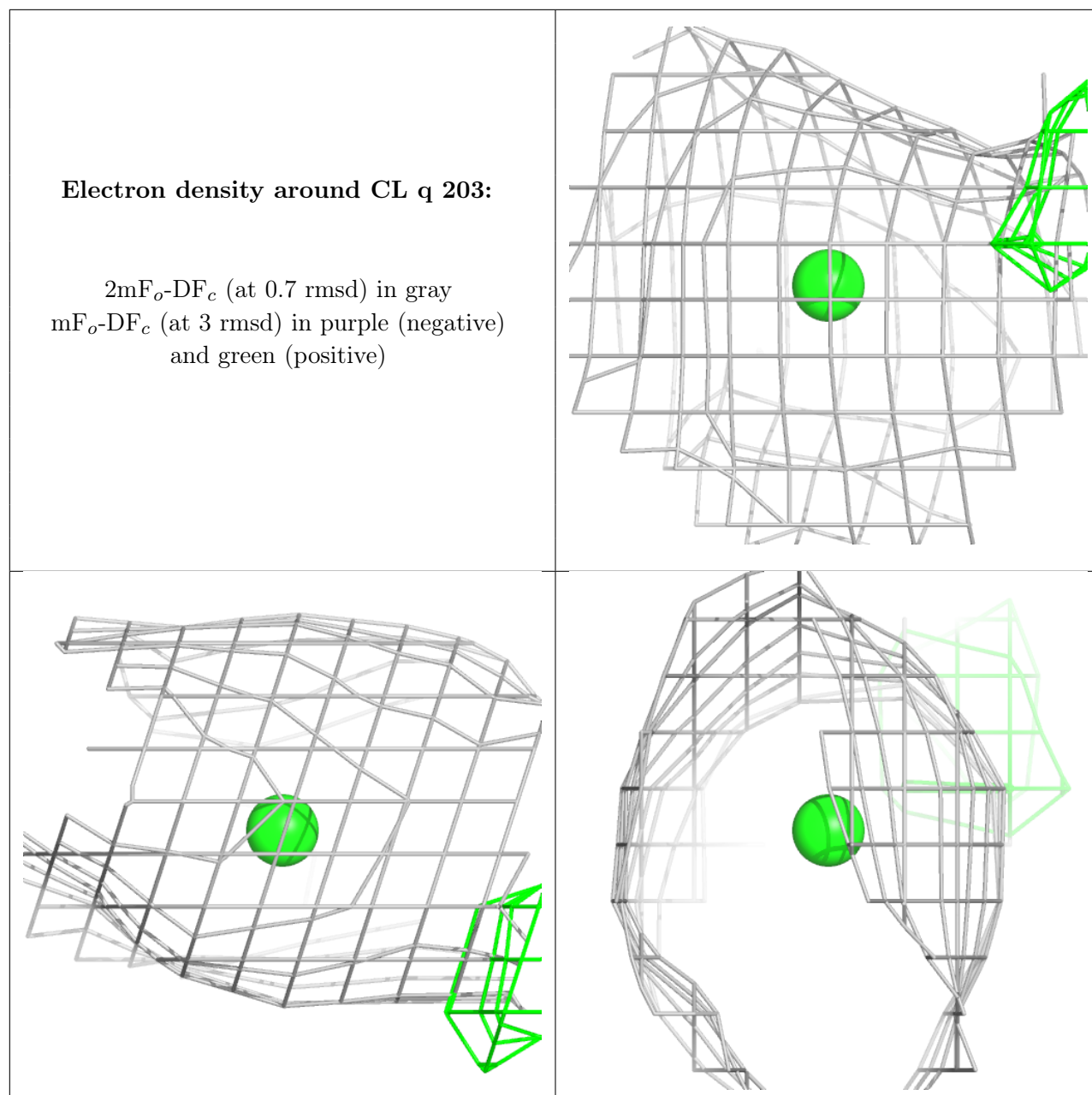


Electron density around CL e 204:

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

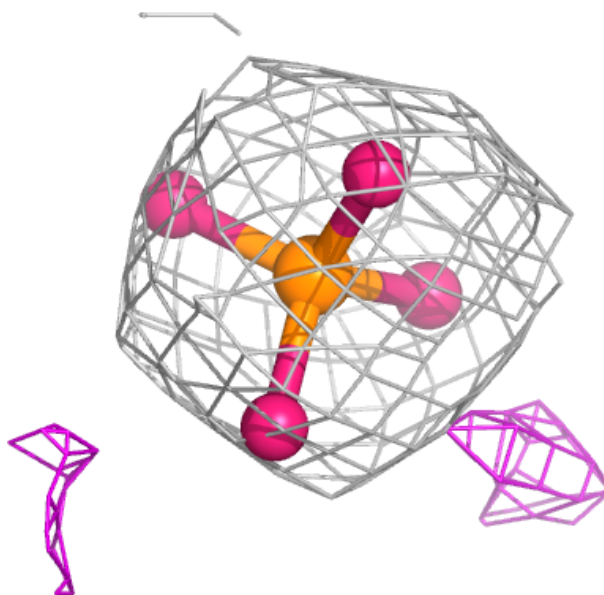
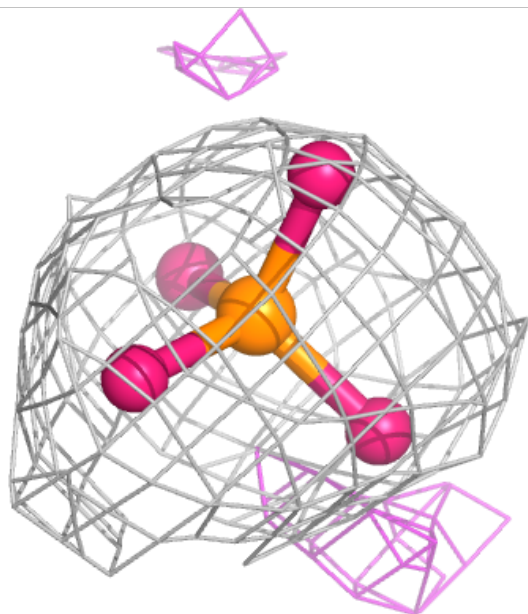
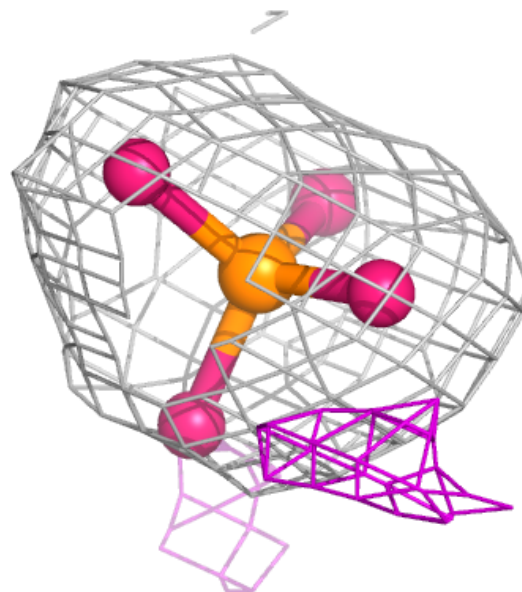






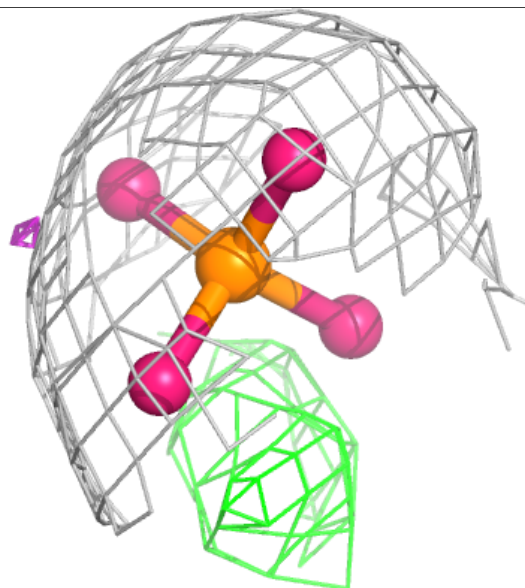
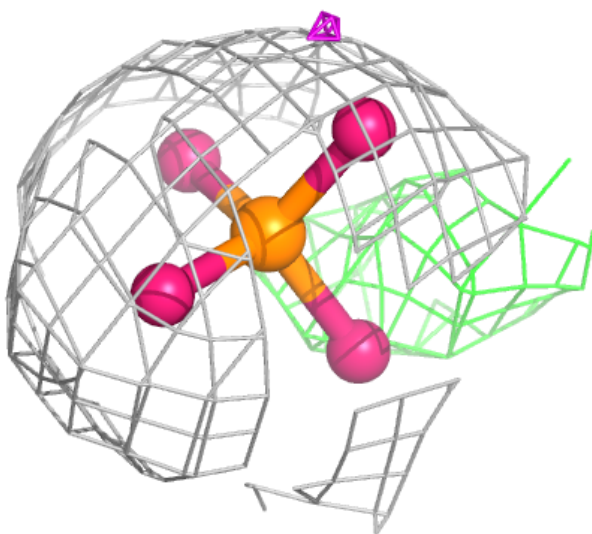
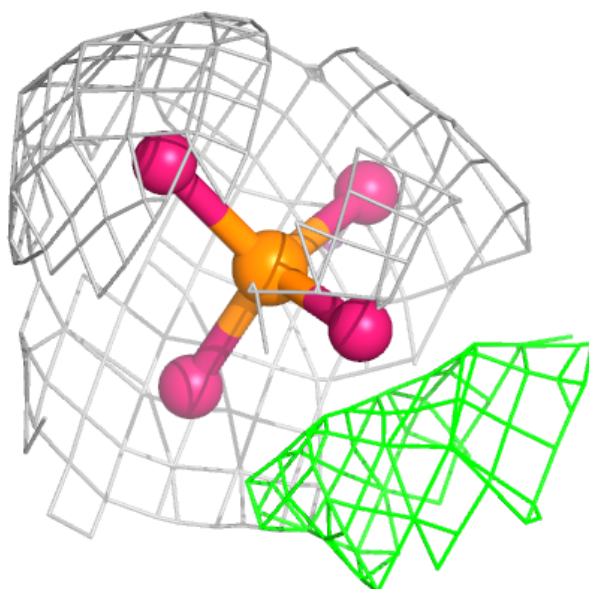
Electron density around PO4 C 305:

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



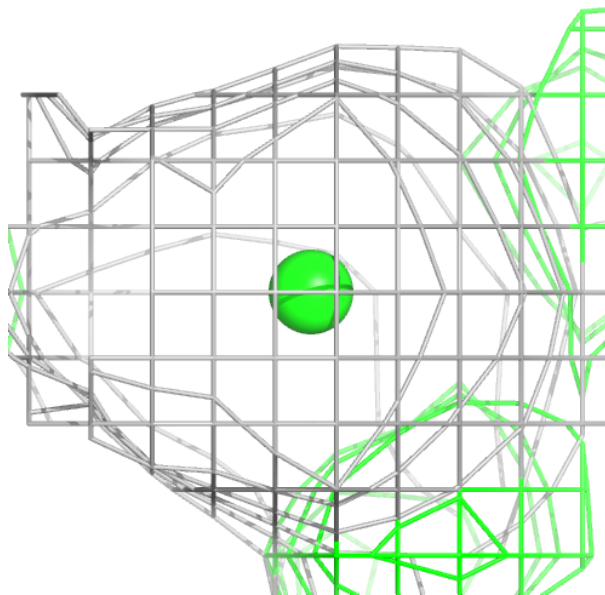
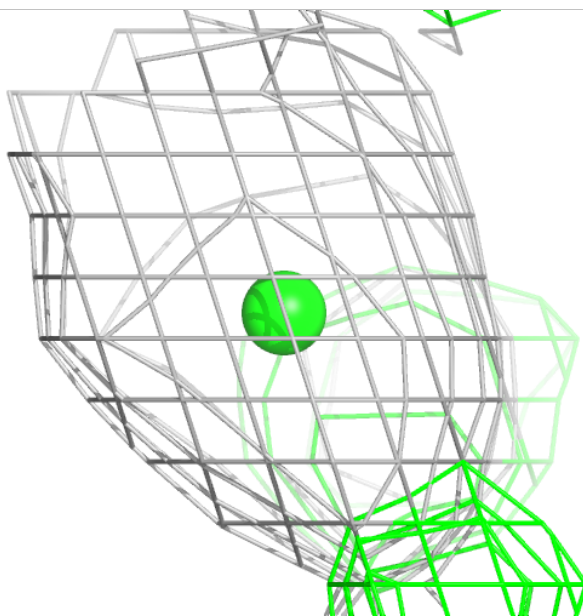
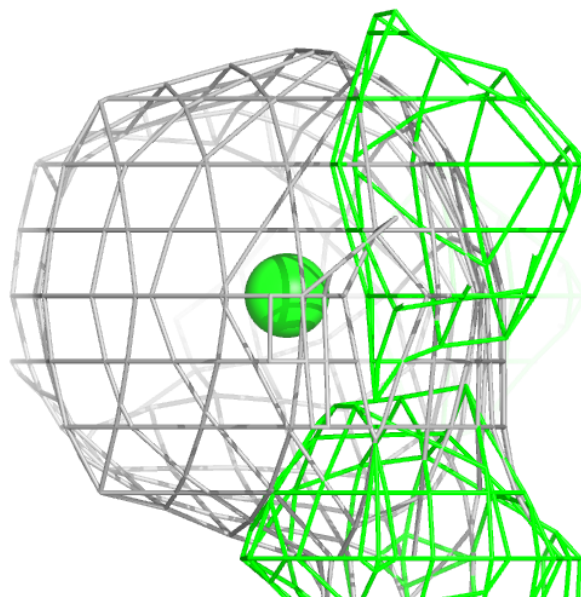
Electron density around PO4 i 203:

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



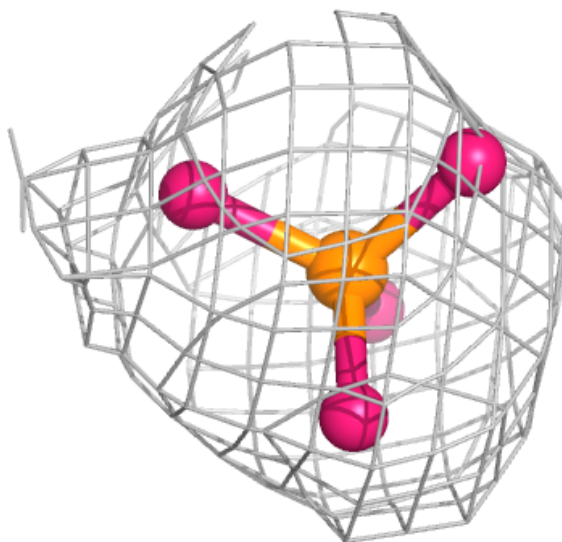
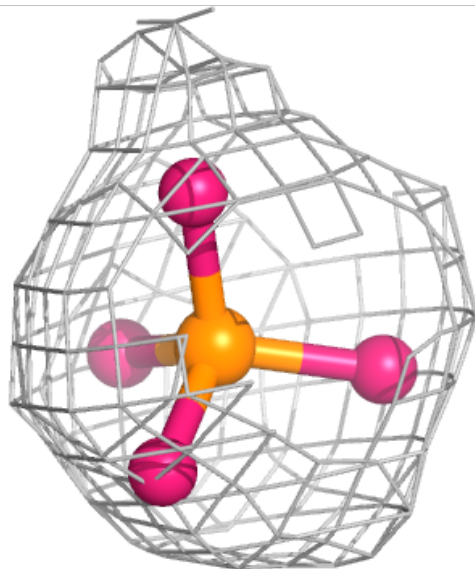
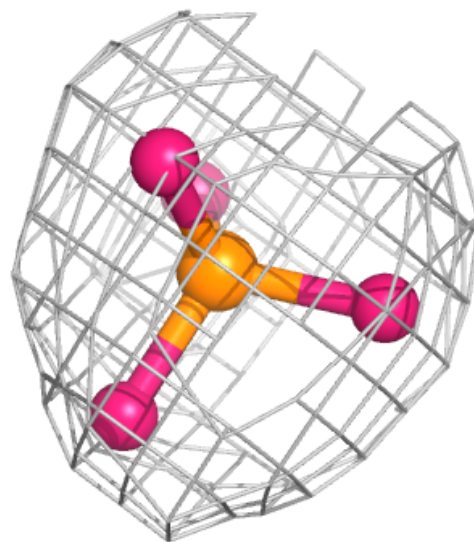
Electron density around CL G 305:

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



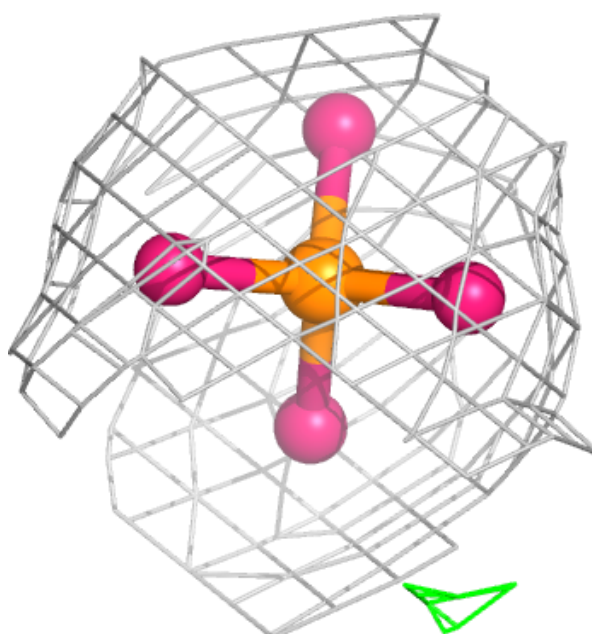
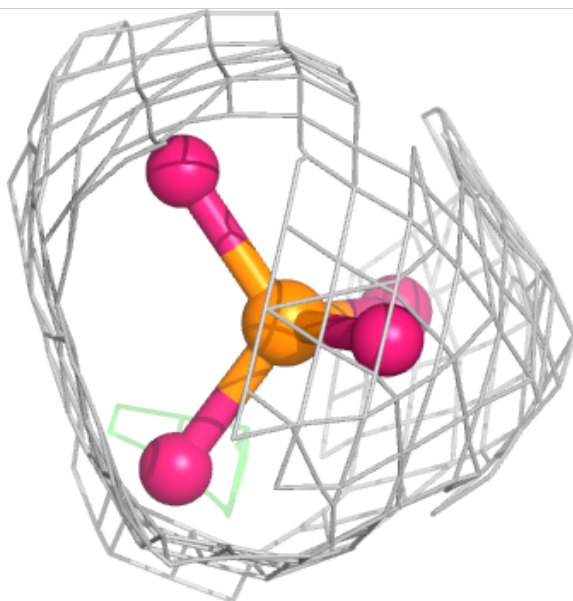
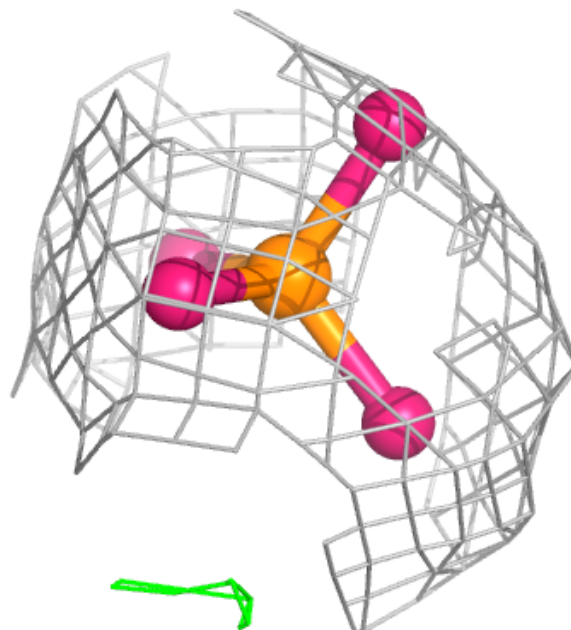
Electron density around PO4 M 303:

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



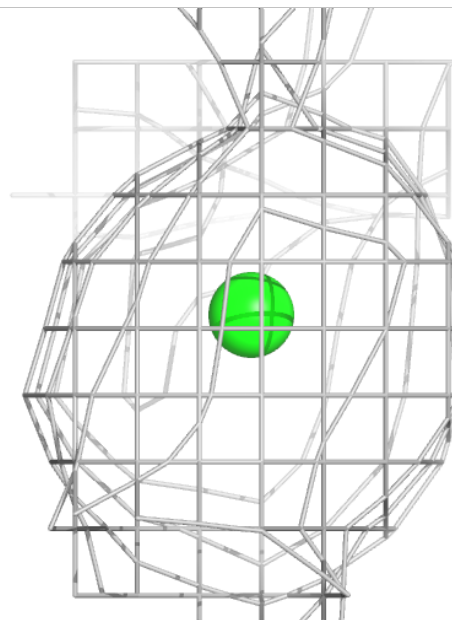
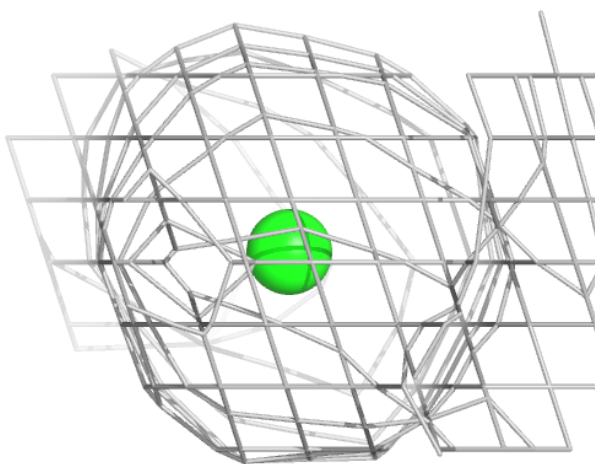
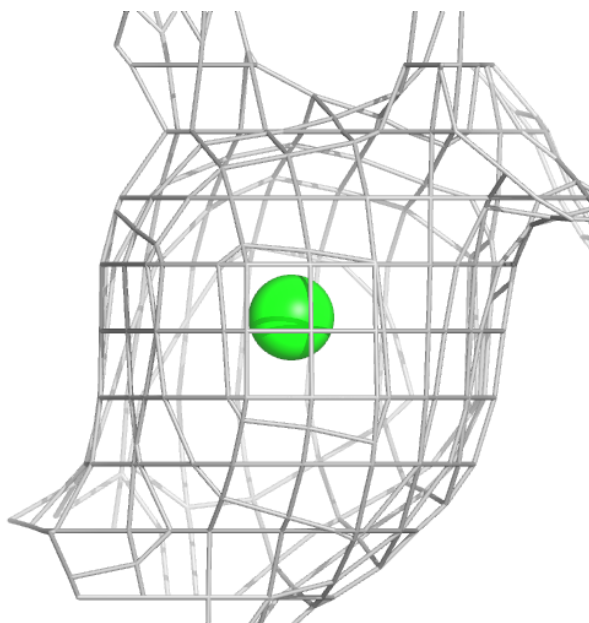
Electron density around PO4 i 201:

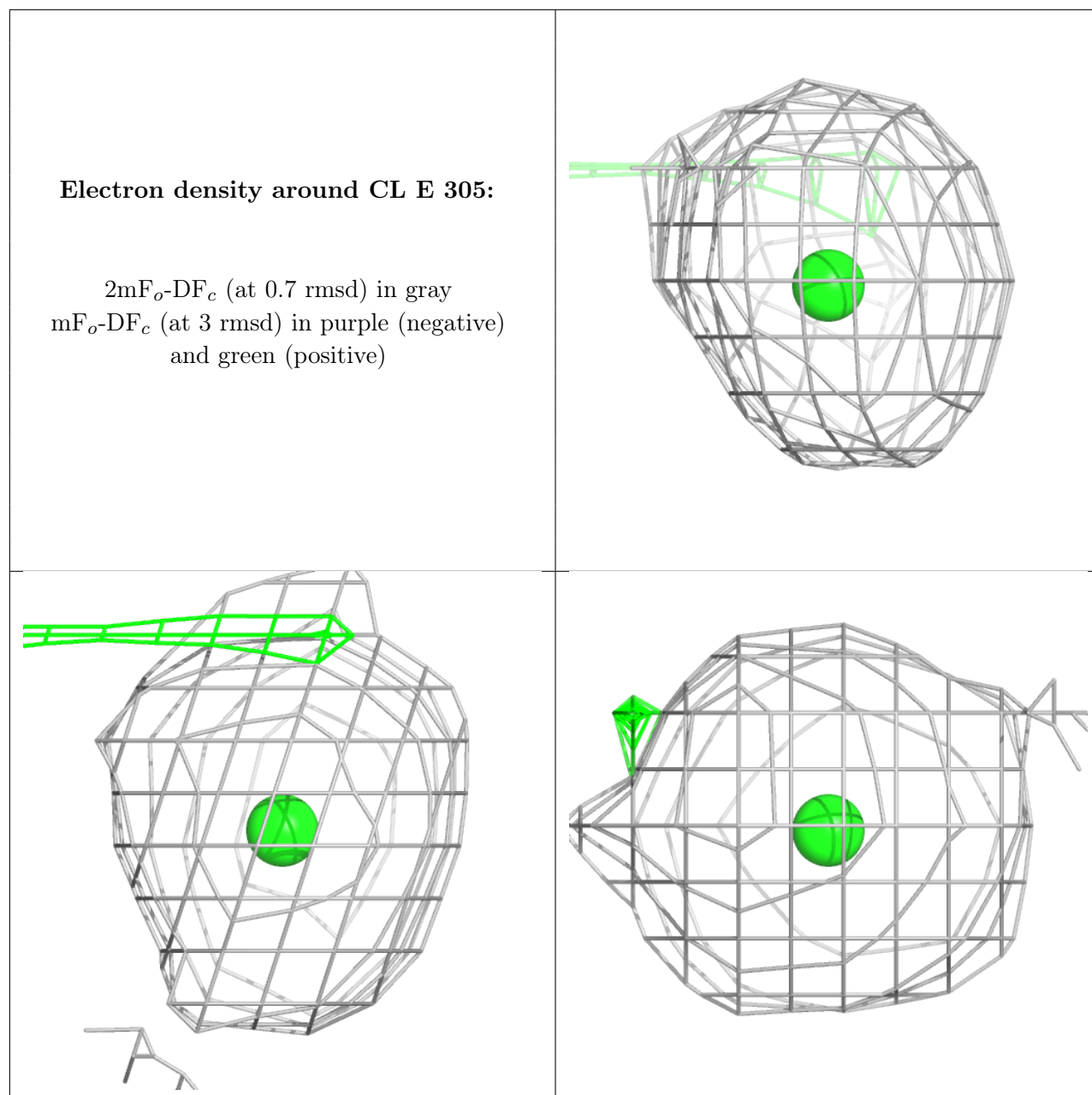
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL D 304:

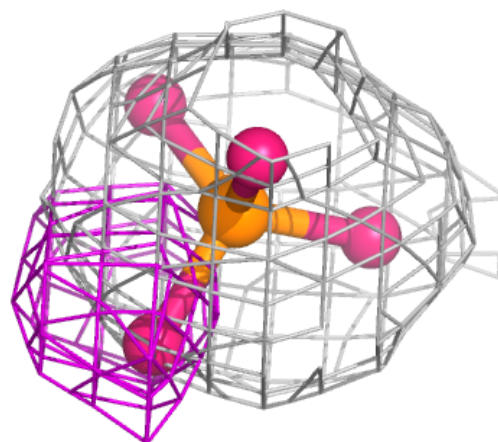
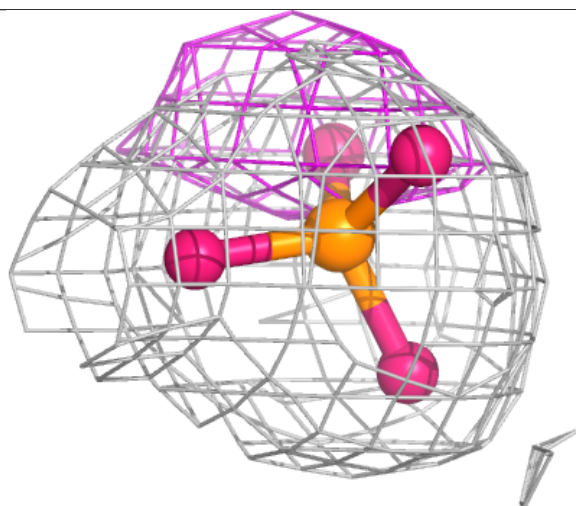
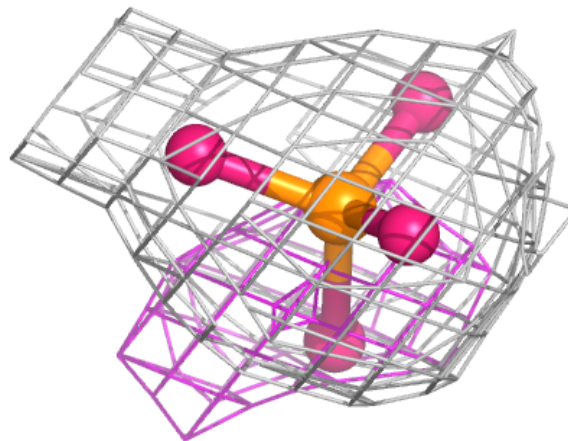
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





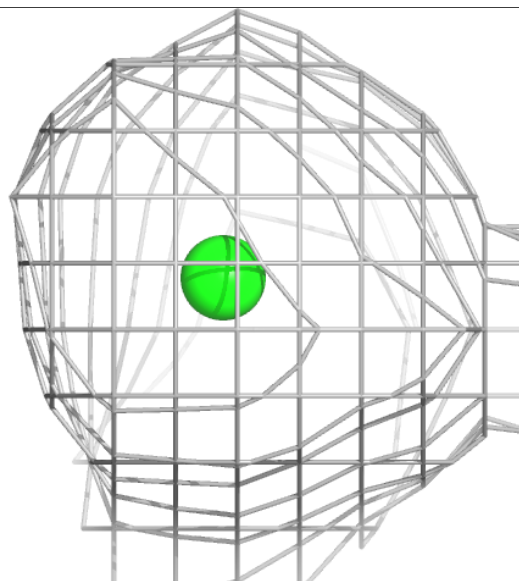
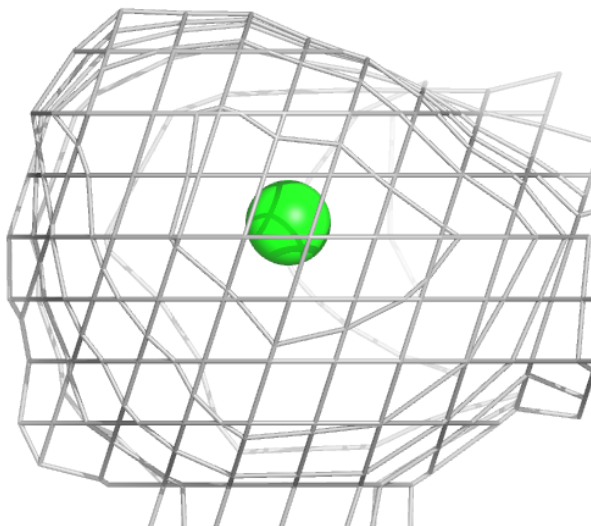
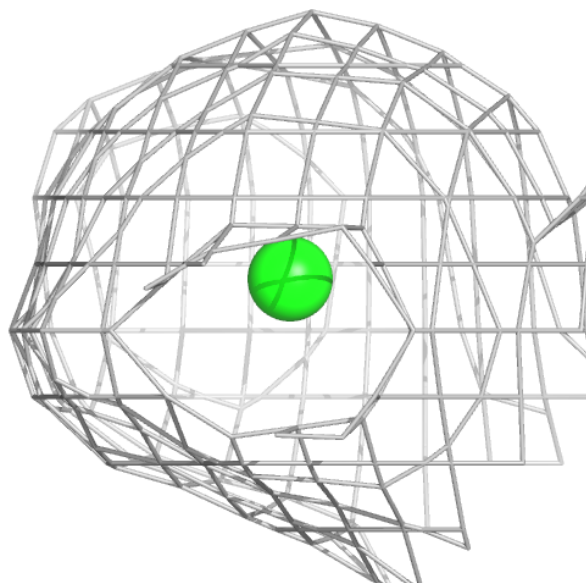
Electron density around PO4 D 301:

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



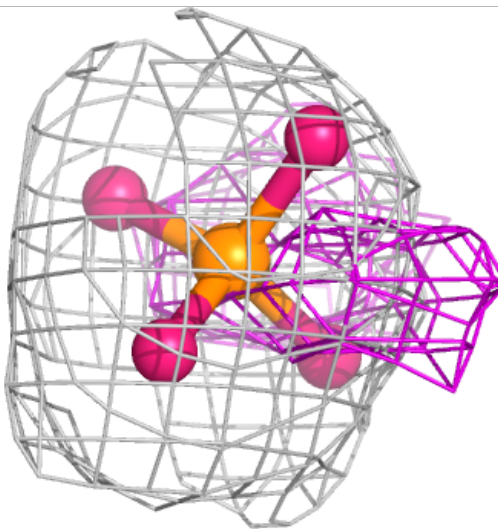
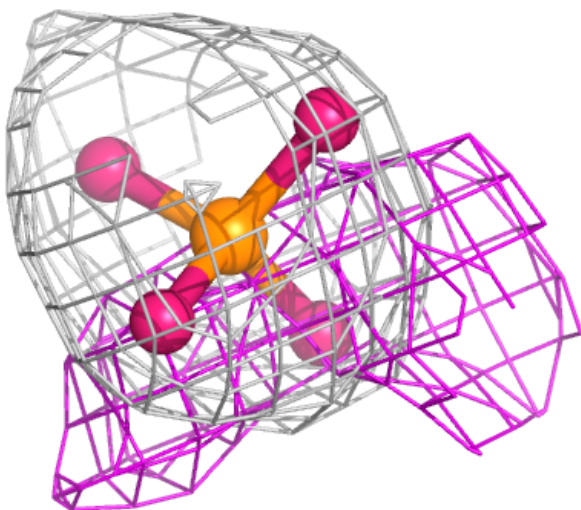
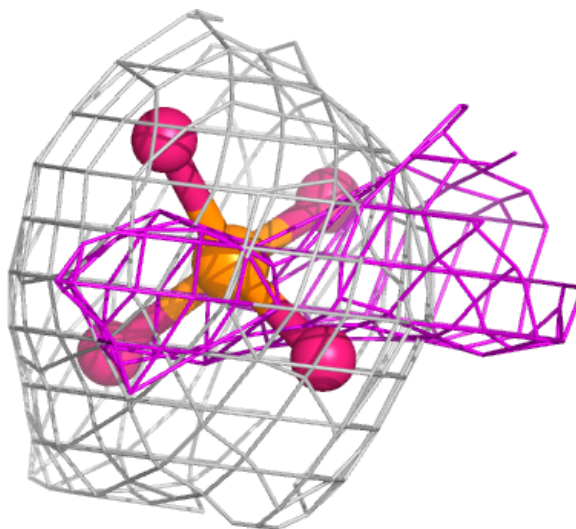
Electron density around CL B 302:

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



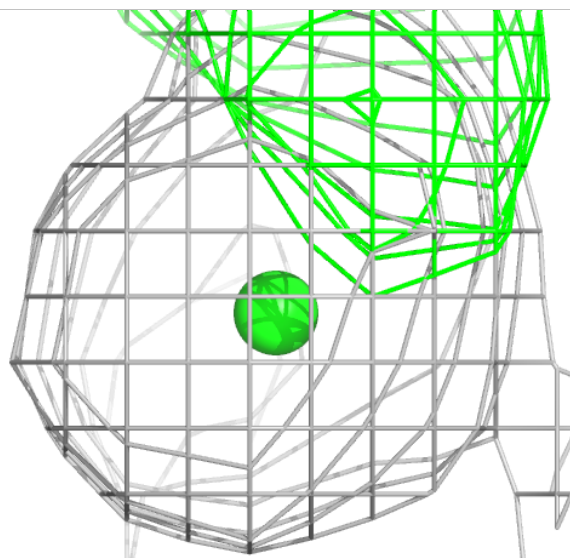
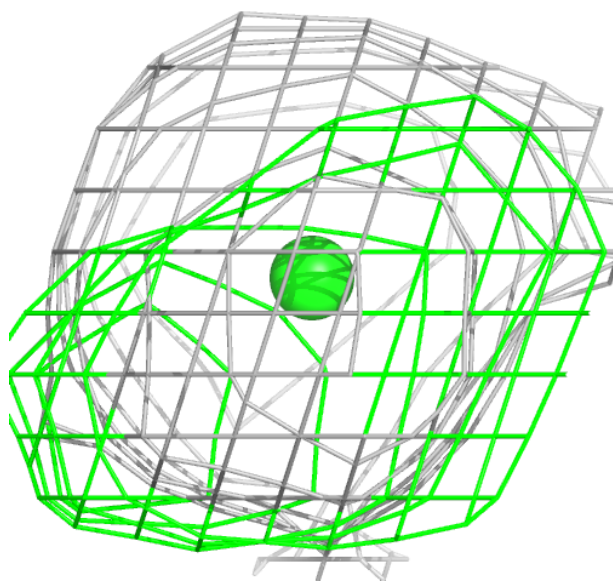
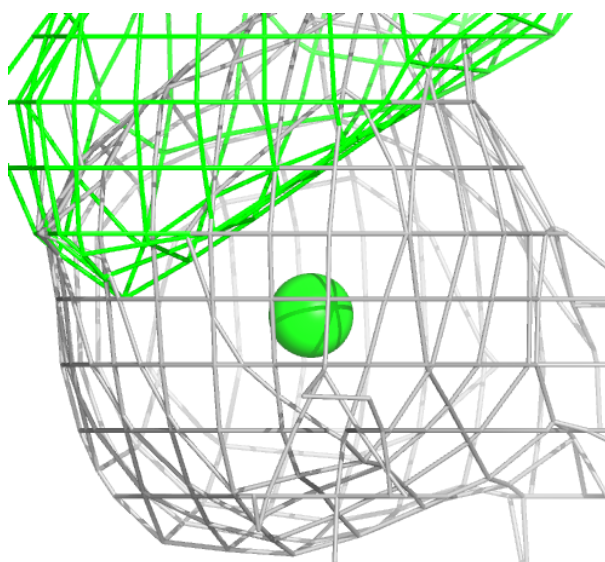
Electron density around PO4 C 301:

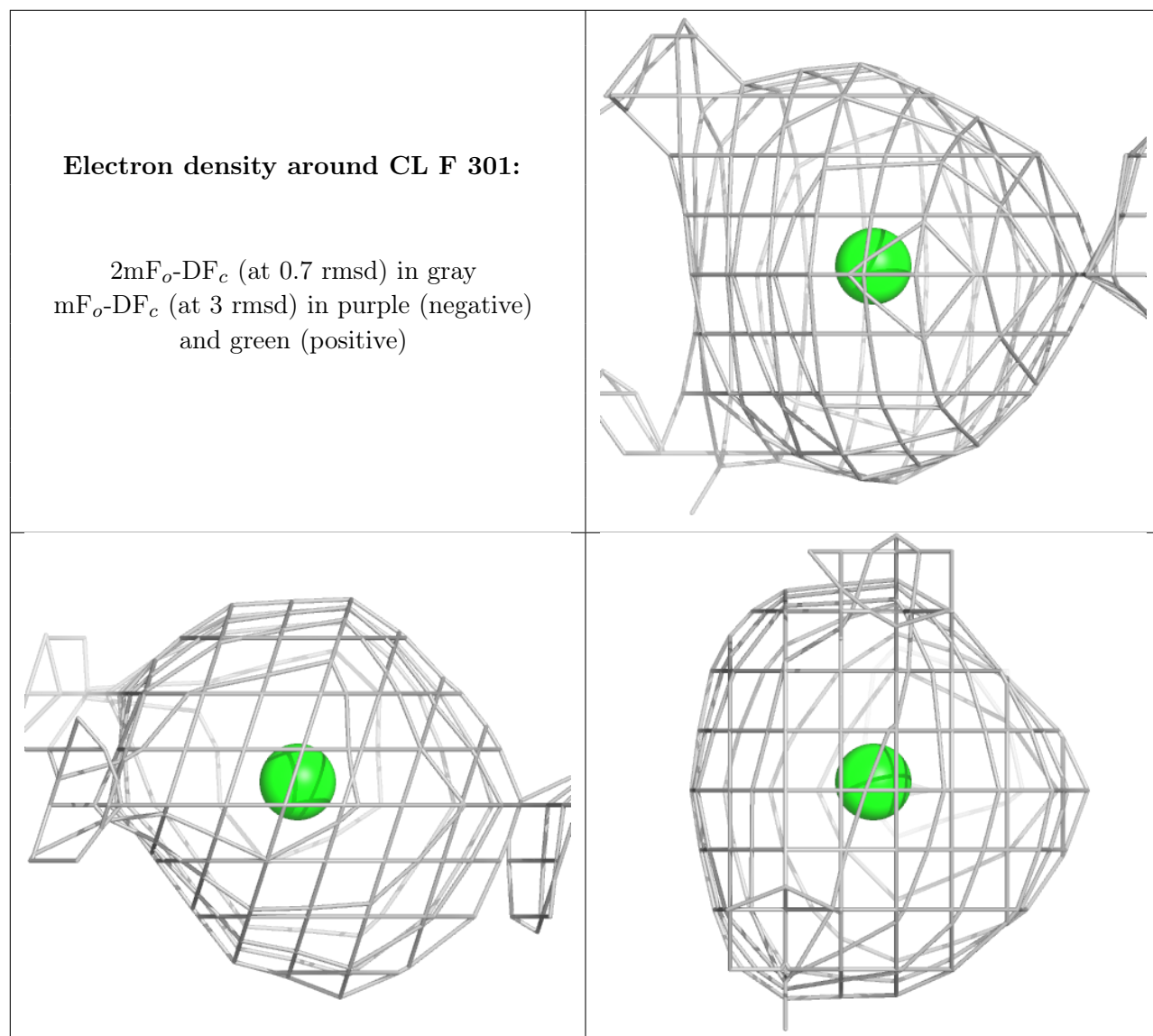
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL N 301:

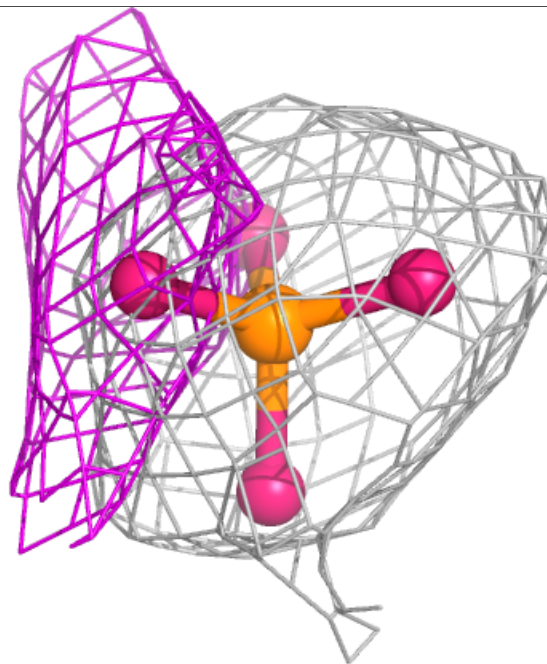
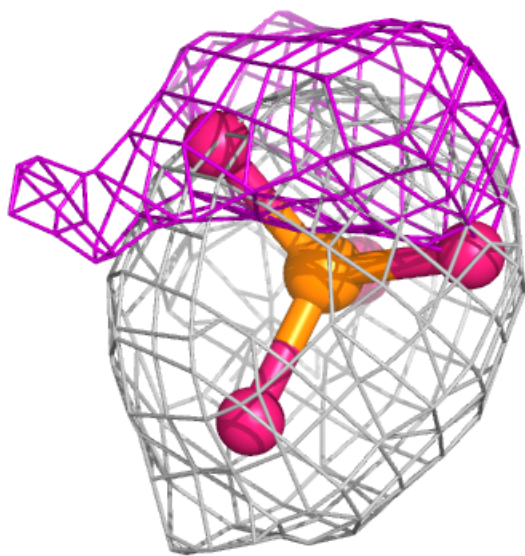
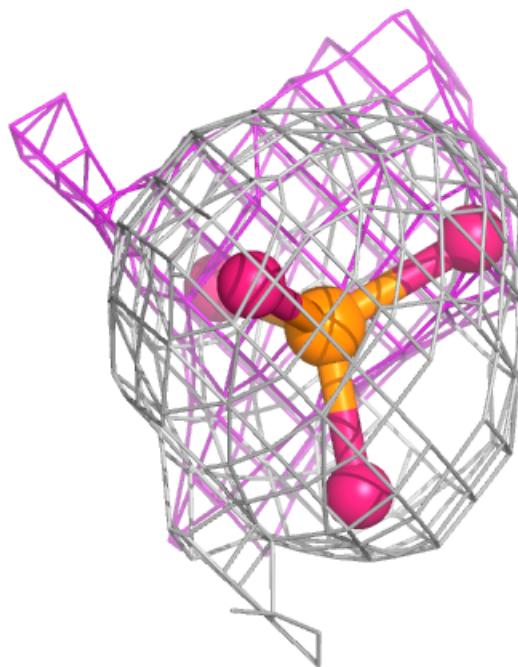
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





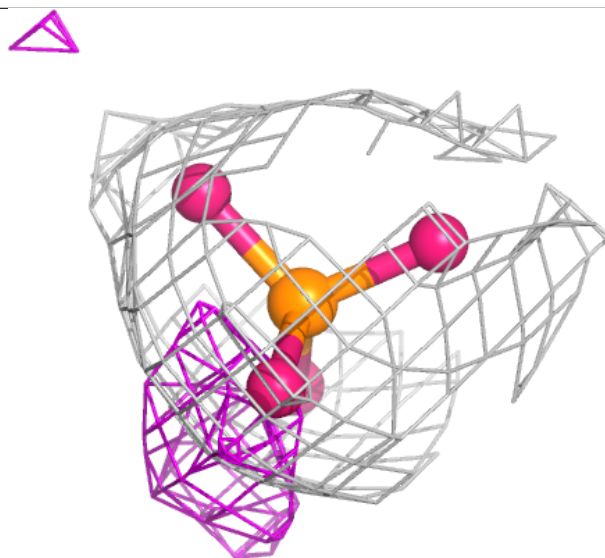
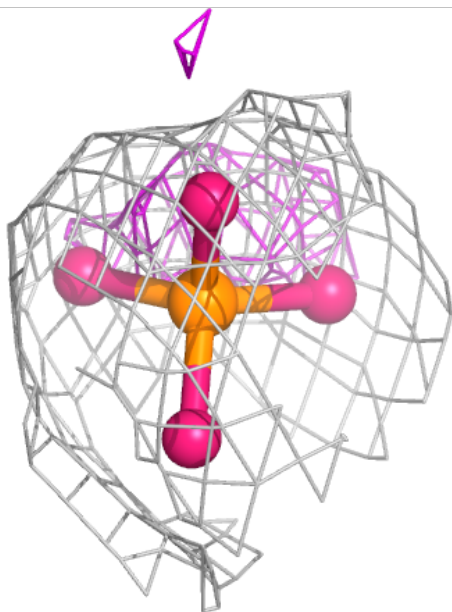
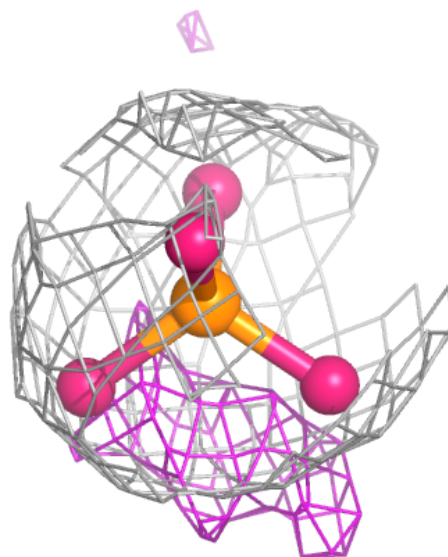
Electron density around PO4 I 304:

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



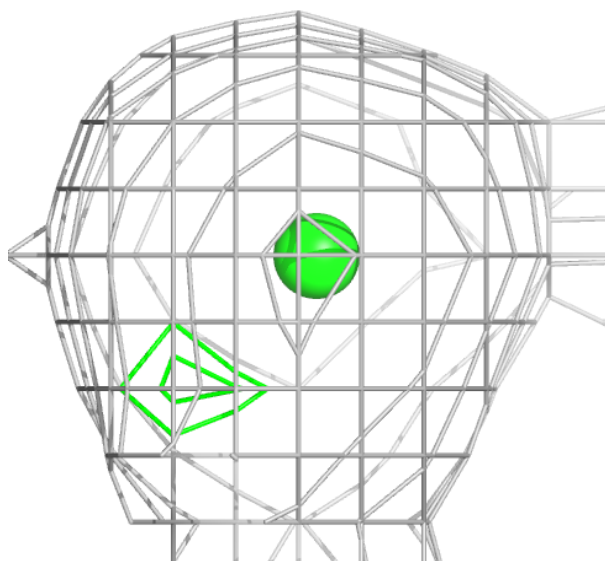
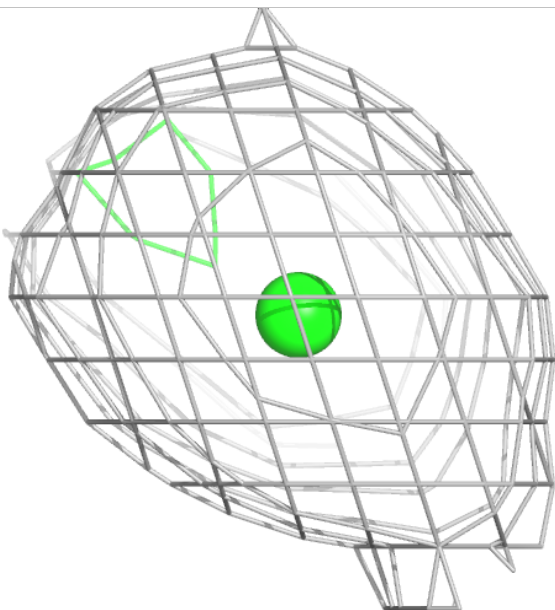
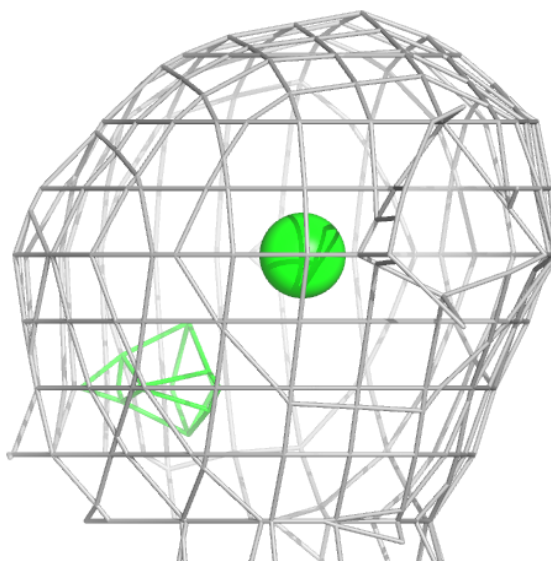
Electron density around PO4 a 202:

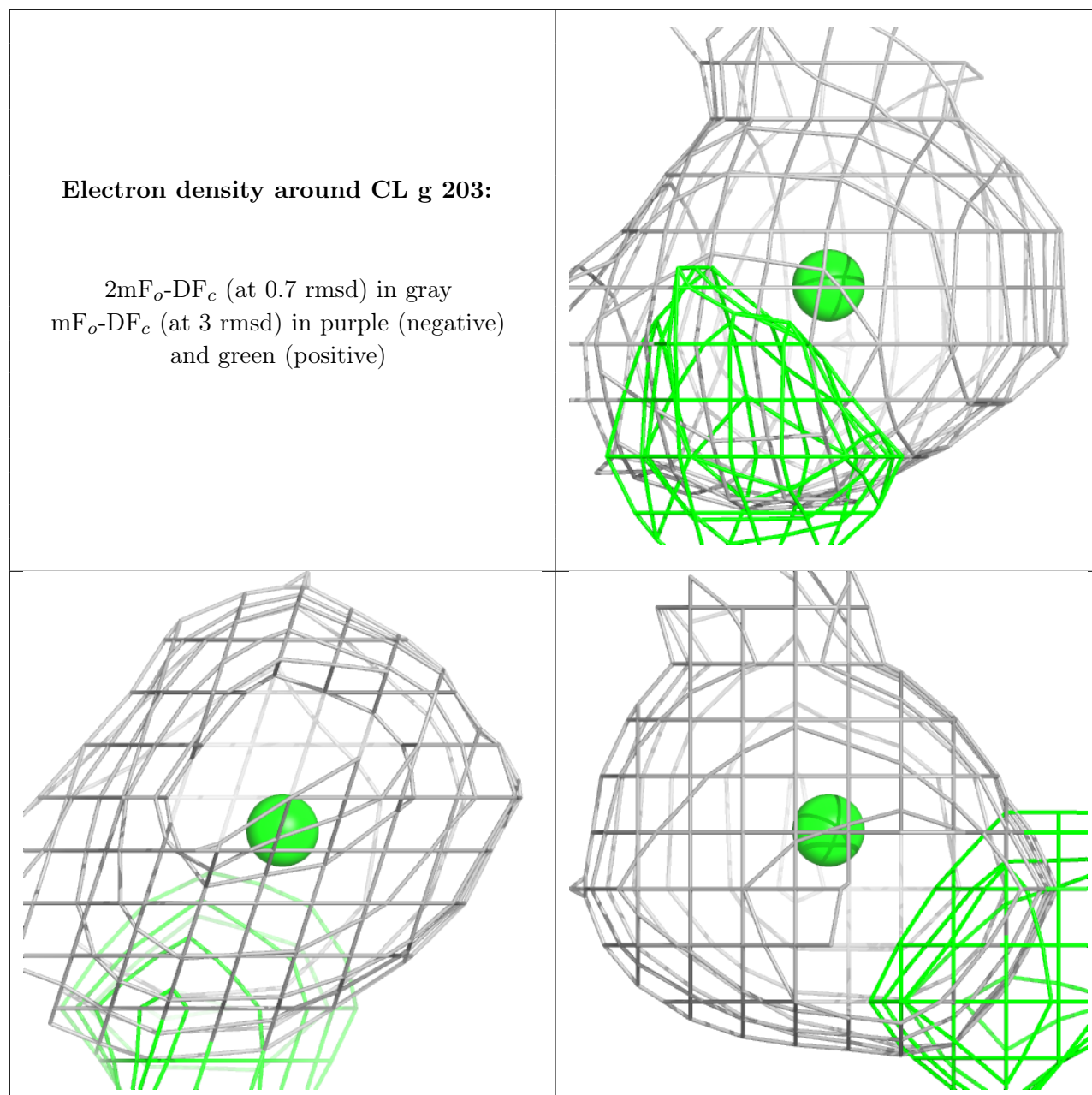
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL D 303:

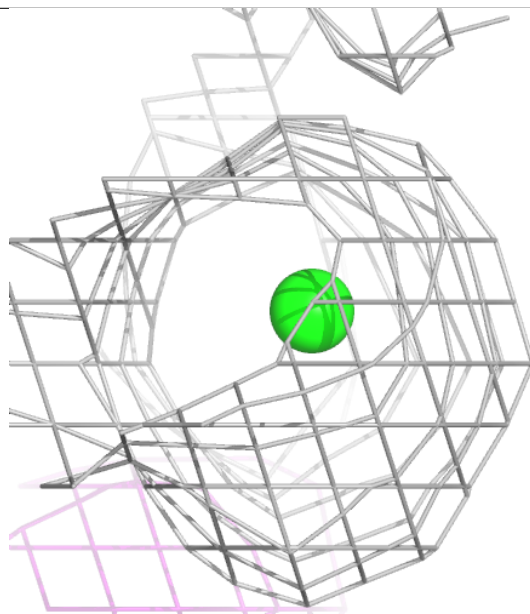
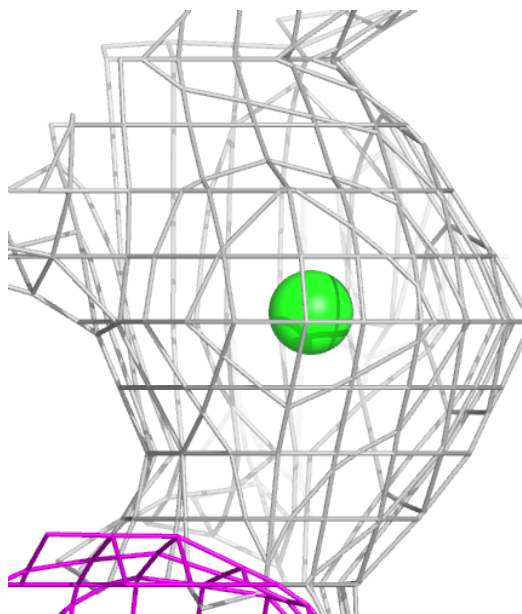
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





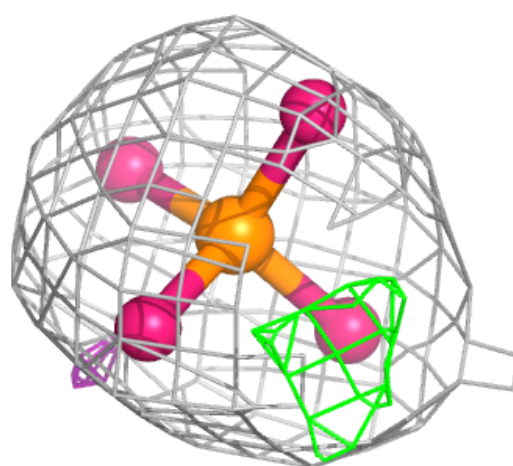
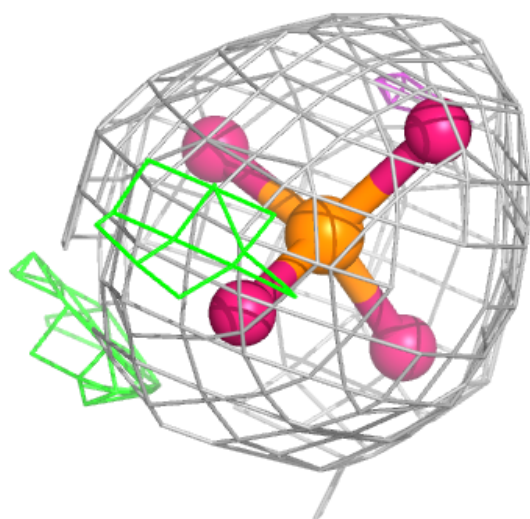
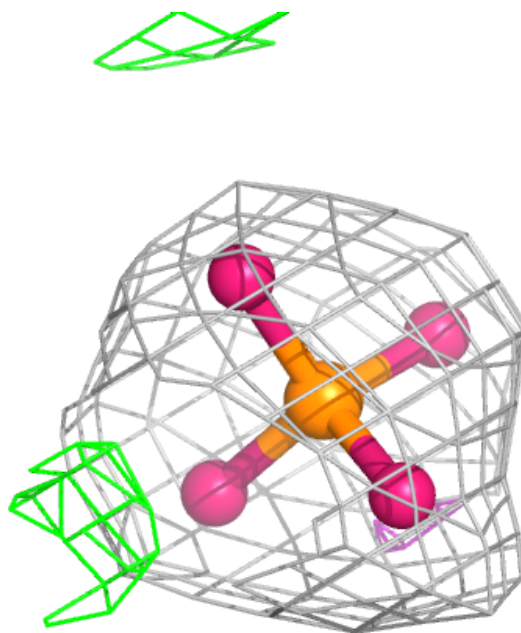
Electron density around CL I 305:

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



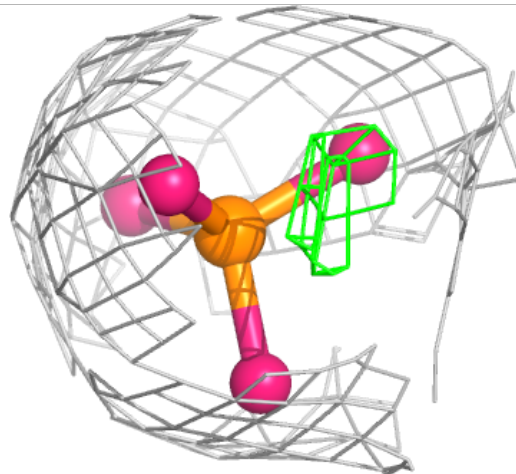
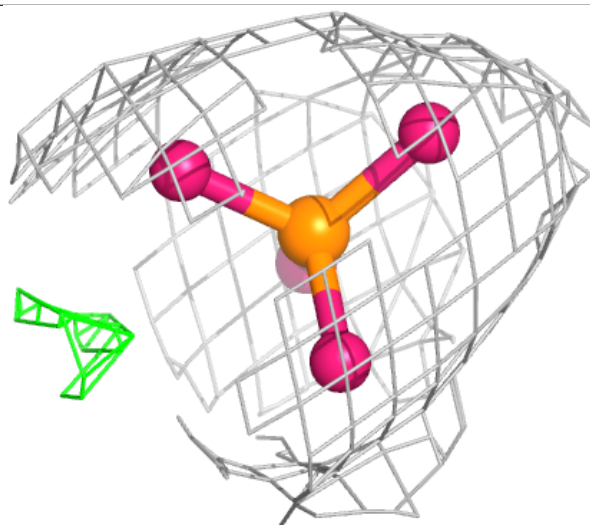
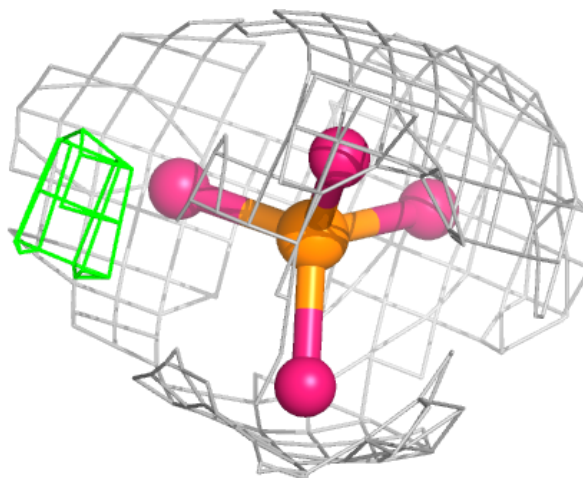
Electron density around PO4 G 301:

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



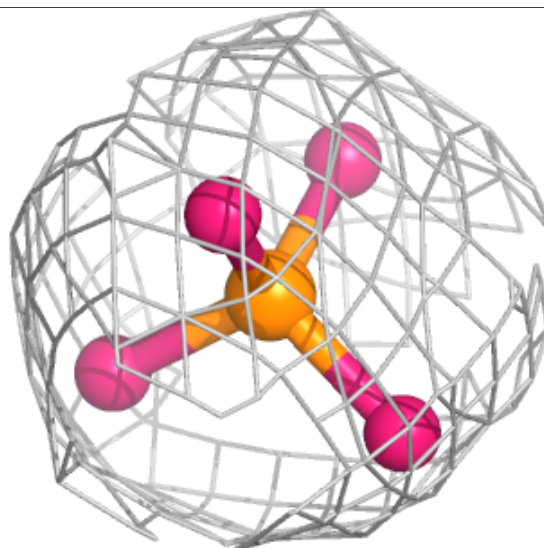
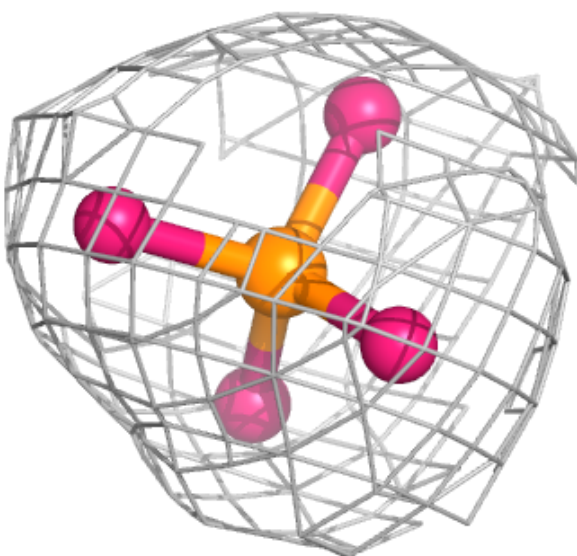
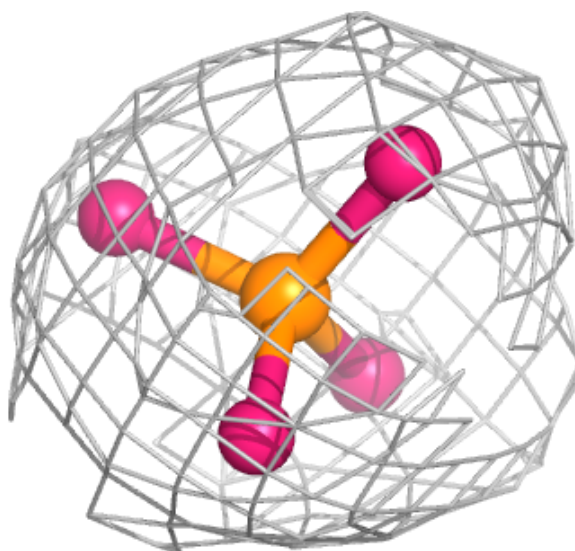
Electron density around PO4 q 201:

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



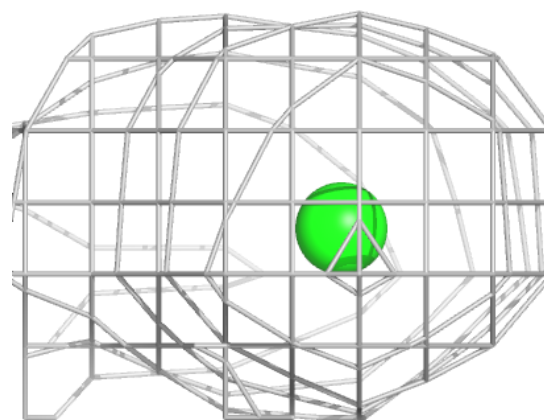
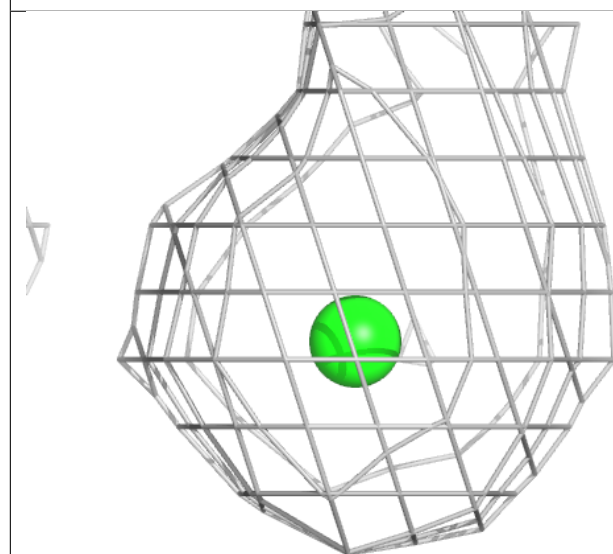
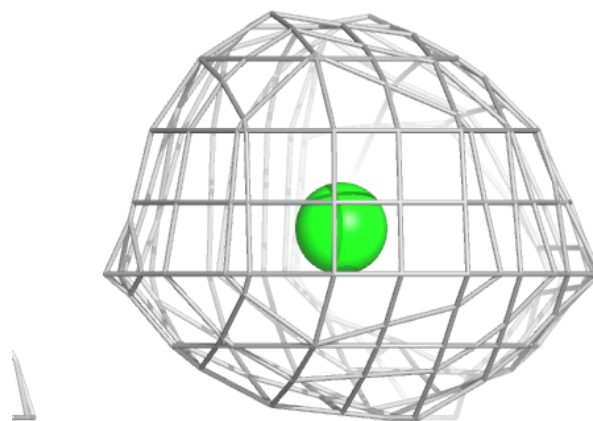
Electron density around PO4 L 301:

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



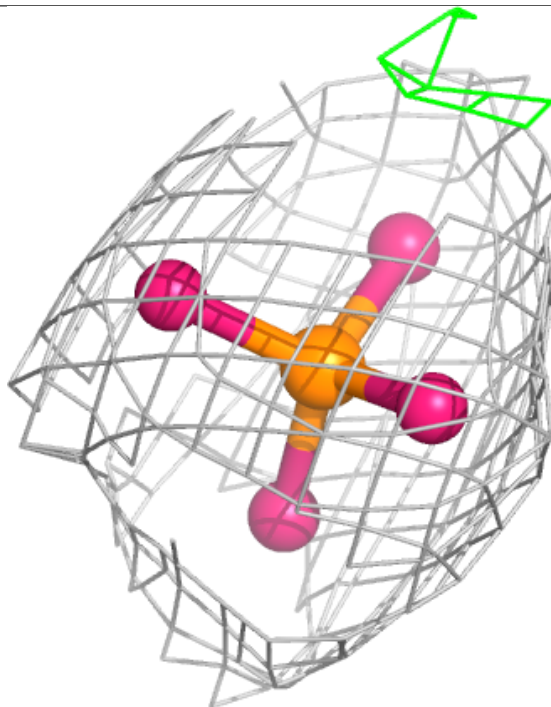
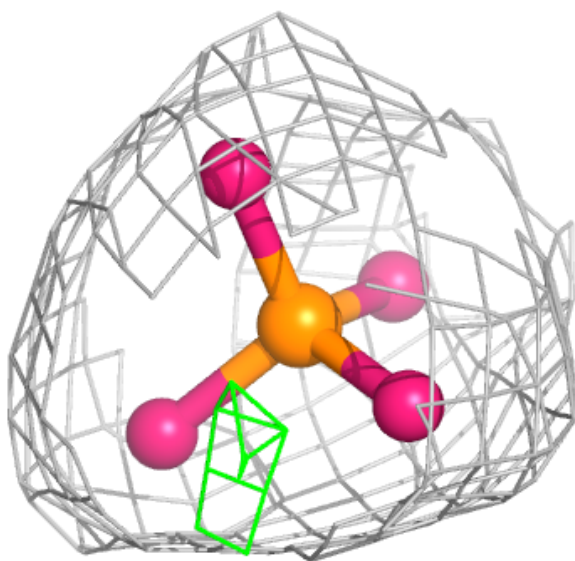
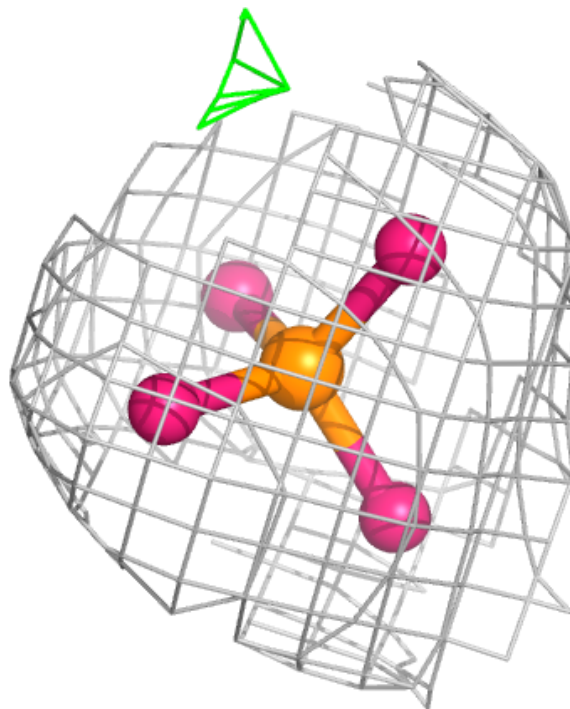
Electron density around CL K 303:

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



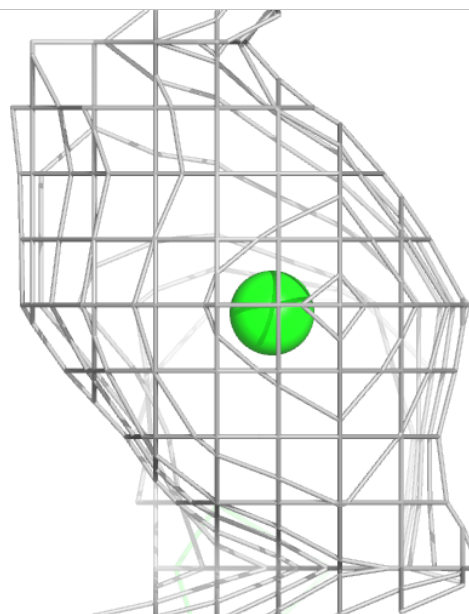
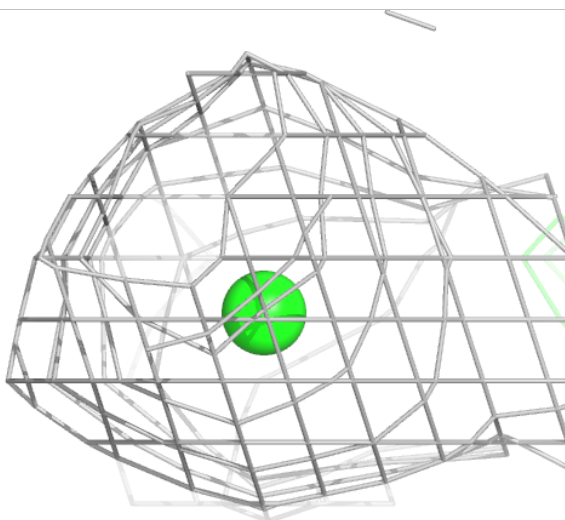
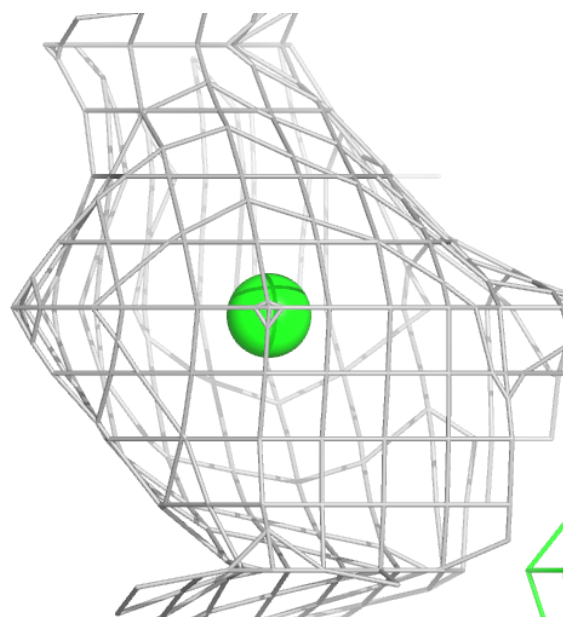
Electron density around PO4 I 303:

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



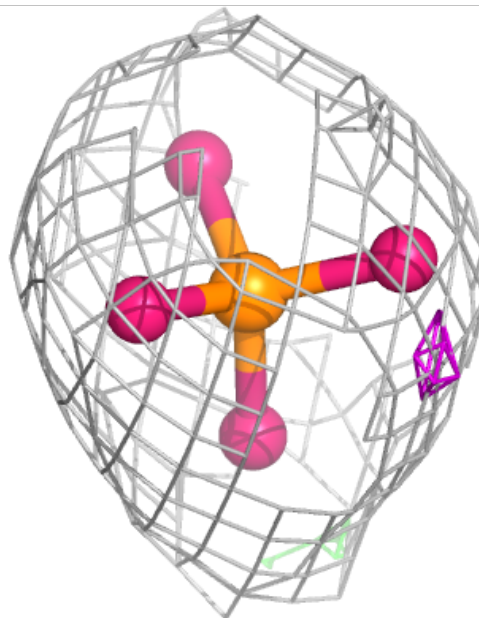
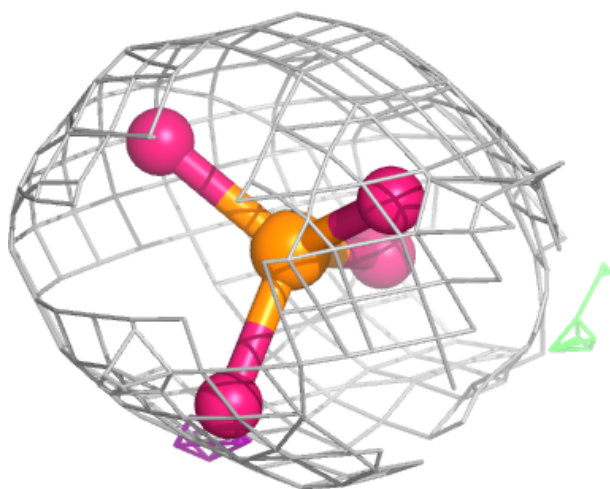
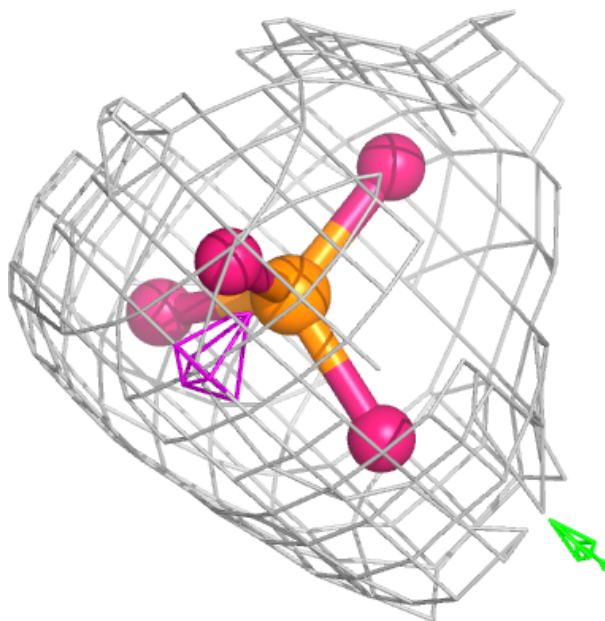
Electron density around CL R 303:

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



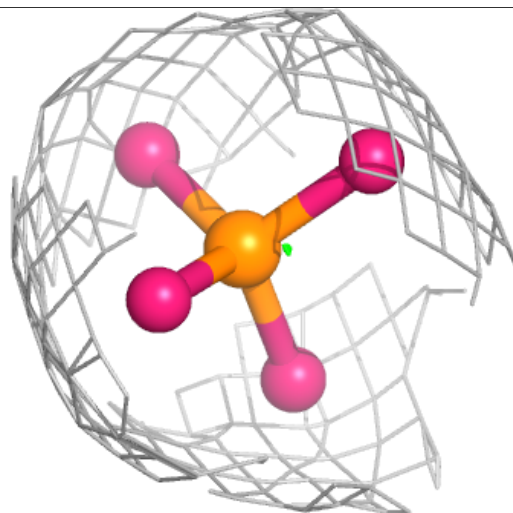
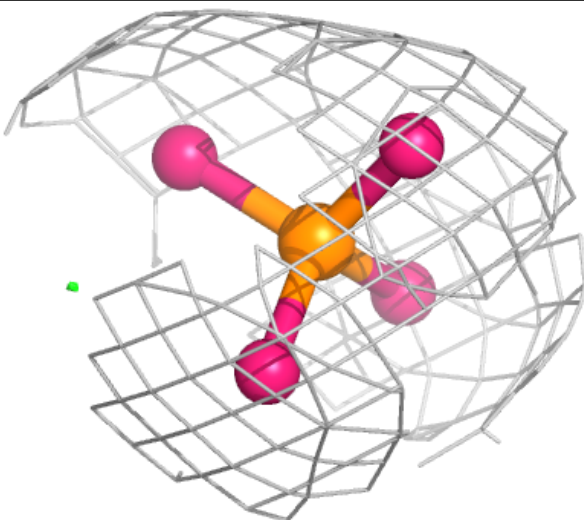
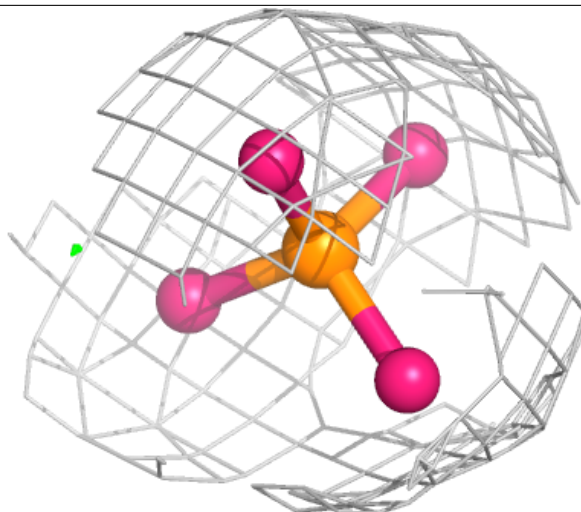
Electron density around PO4 g 202:

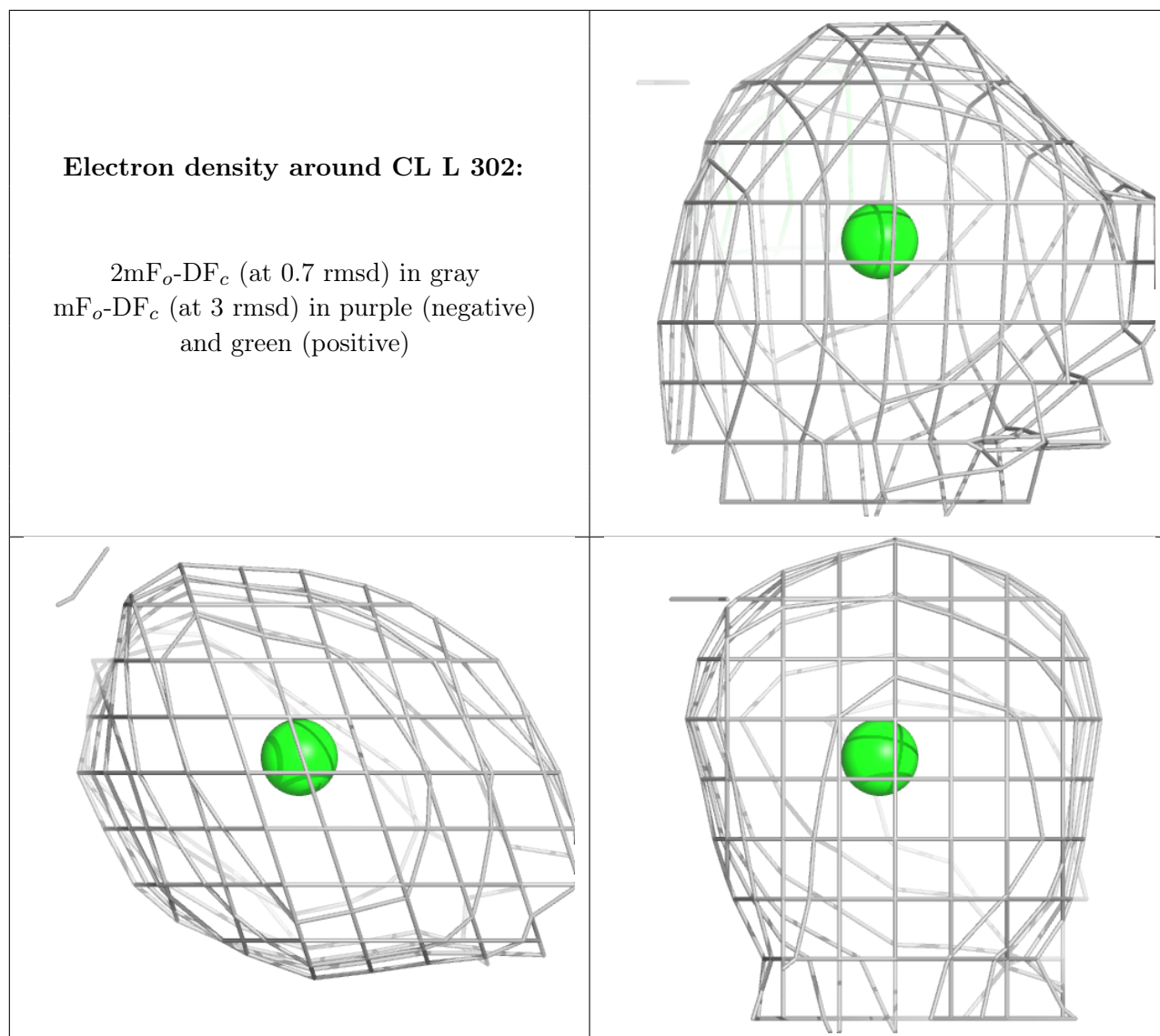
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PO4 c 201:

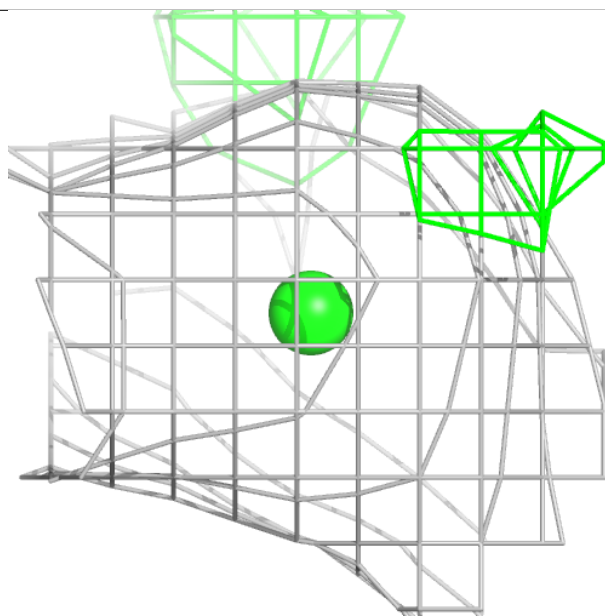
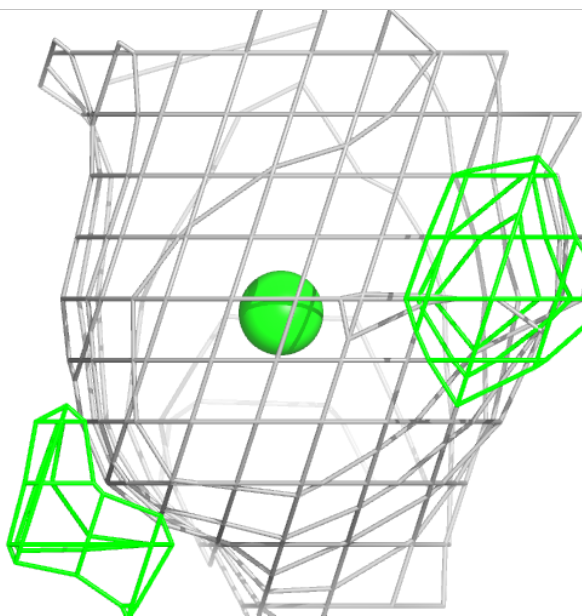
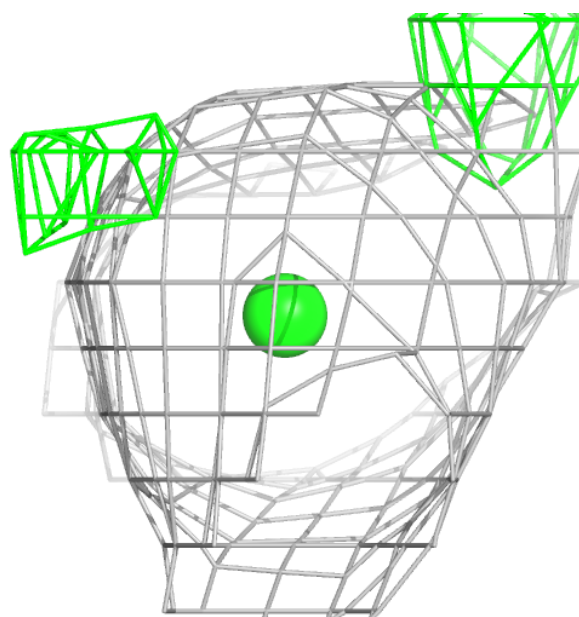
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





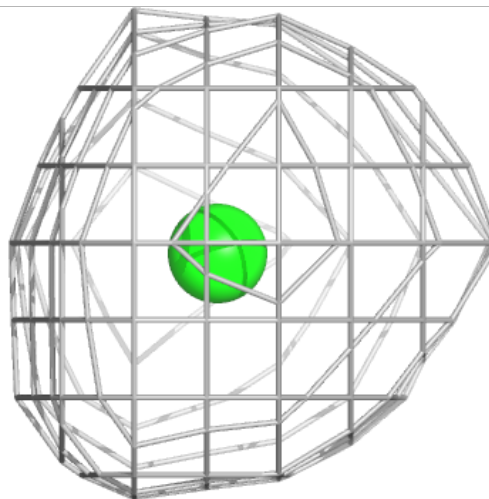
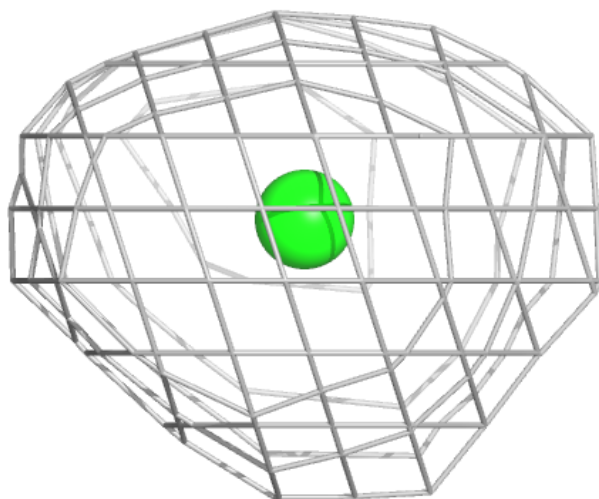
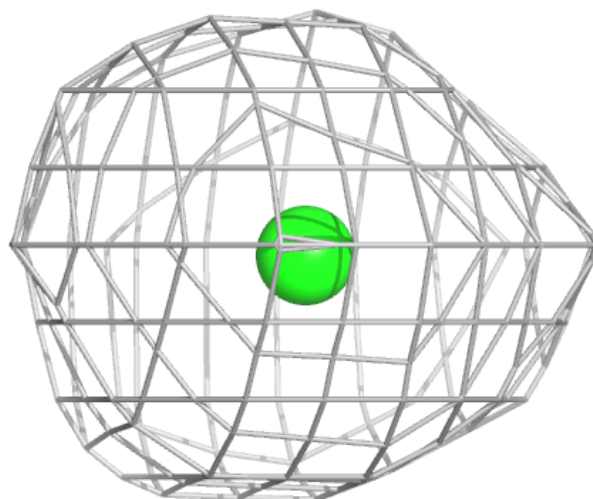
Electron density around CL g 204:

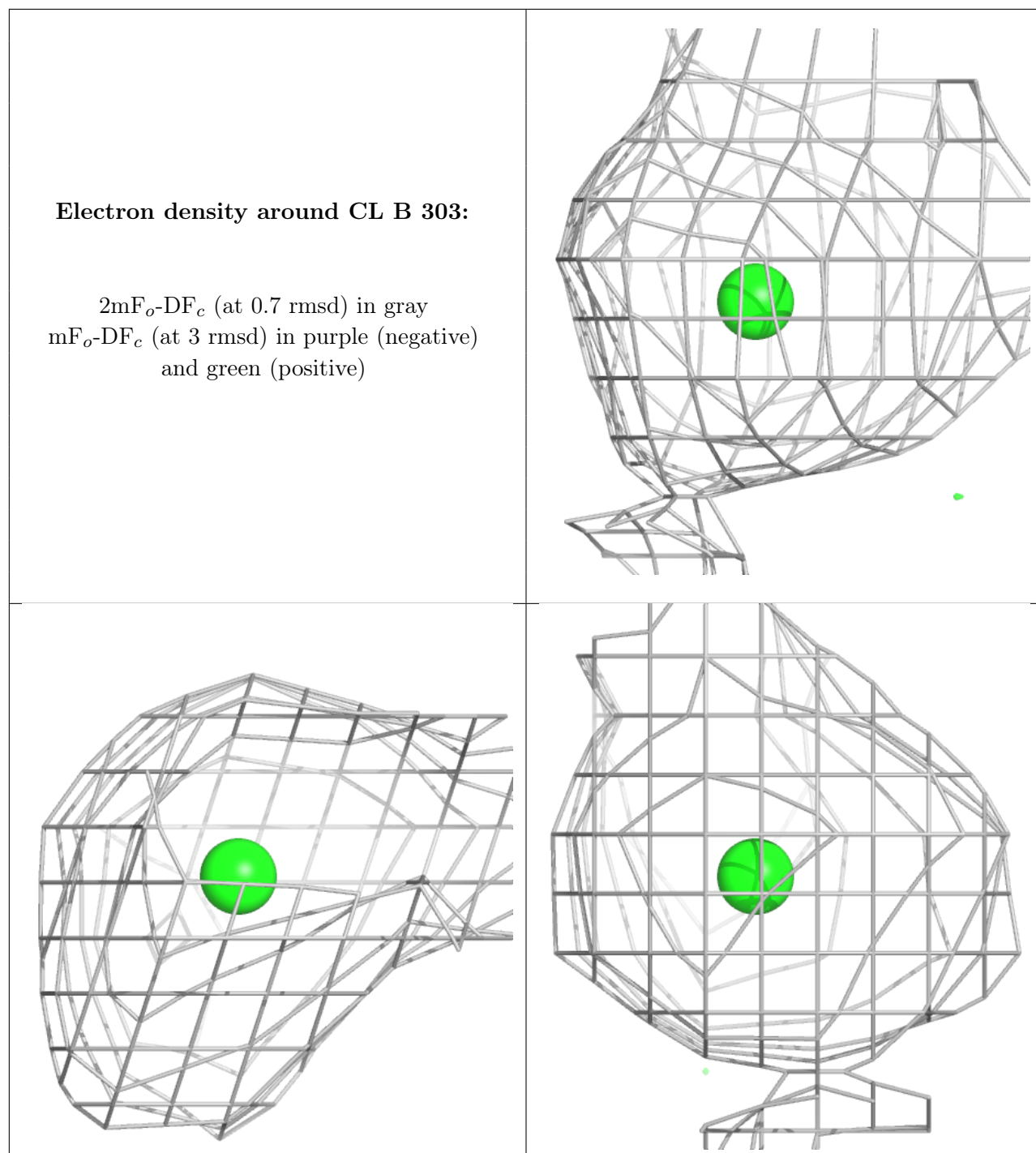
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.