



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 09:56 PM UTC

PDB ID : 8BDB / pdb\_00008bdb  
Title : Ribulose-1,5-bisphosphate carboxylase/oxygenase from *Griffithsia monilis*  
Authors : Andersson, I.; Gunn, L.H.  
Deposited on : 2022-10-19  
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

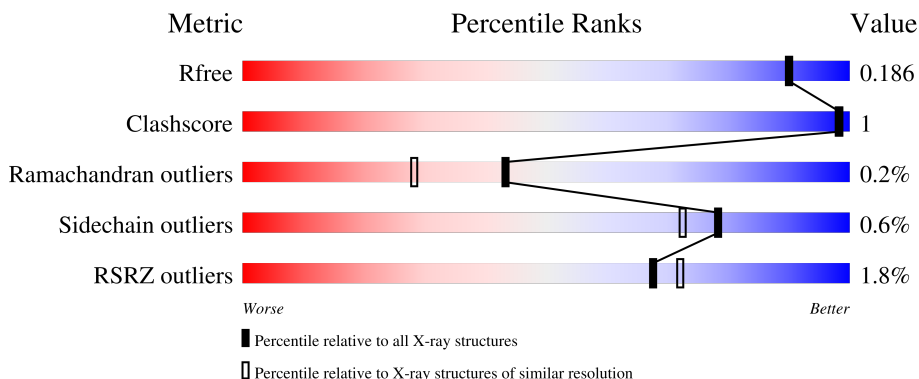
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

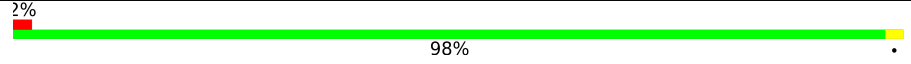
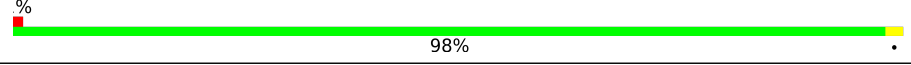
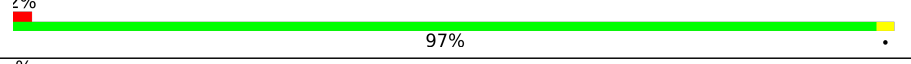
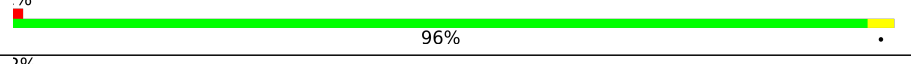
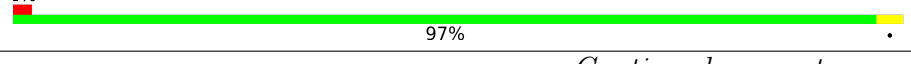
The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	480	 2% 98%
1	C	480	 % 98%
1	G	480	 2% 97%
1	K	480	 % 96%
1	O	480	 2% 97%

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Mol	Chain	Length	Quality of chain
2	B	138	 % 100%
2	D	138	 5% 99%
2	F	138	 % 99%
2	H	138	 2% 100%
2	J	138	 2% 99%
2	L	138	 3% 98%
2	N	138	 2% 100%
2	P	138	 4% 99%
3	E	480	 % 94%
3	I	480	 % 98%
3	M	480	 2% 98%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 43559 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	480	3805	2426	650	709	20	0	9	0
1	C	479	3787	2415	647	705	20	0	7	0
1	G	479	3800	2426	647	707	20	0	9	0
1	K	479	3804	2430	647	707	20	0	11	0
1	O	479	3796	2422	647	707	20	0	8	0

- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	138	1158	735	197	222	4	0	3	0
2	D	138	1149	730	196	219	4	0	1	0
2	F	138	1149	730	196	219	4	0	1	0
2	H	138	1160	736	197	223	4	0	4	0
2	J	138	1154	733	196	221	4	0	2	0
2	L	138	1149	730	196	219	4	0	1	0
2	N	138	1158	735	198	221	4	0	3	0
2	P	138	1162	739	197	222	4	0	4	0

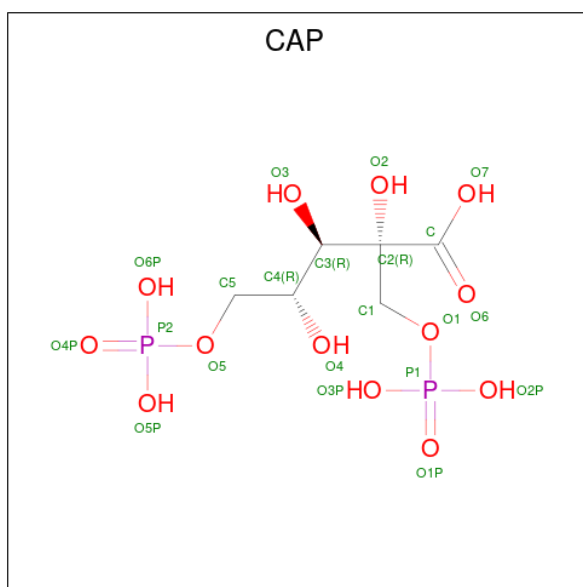
- Molecule 3 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	468	Total	C	N	O	S	0	9	0
			3703	2368	628	687	20			
3	I	479	Total	C	N	O	S	0	9	0
			3798	2421	649	708	20			
3	M	479	Total	C	N	O	S	0	11	0
			3801	2427	647	707	20			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		
4	O	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	A	1	21	6	13	2	0	0
5	C	1	21	6	13	2	0	0
5	E	1	21	6	13	2	0	0
5	G	1	21	6	13	2	0	0
5	I	1	21	6	13	2	0	0
5	K	1	21	6	13	2	0	0
5	M	1	21	6	13	2	0	0
5	O	1	21	6	13	2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 4 2 2	0	0
6	G	1	Total C O 4 2 2	0	0
6	G	1	Total C O 4 2 2	0	0
6	G	1	Total C O 4 2 2	0	0
6	G	1	Total C O 4 2 2	0	0
6	G	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0

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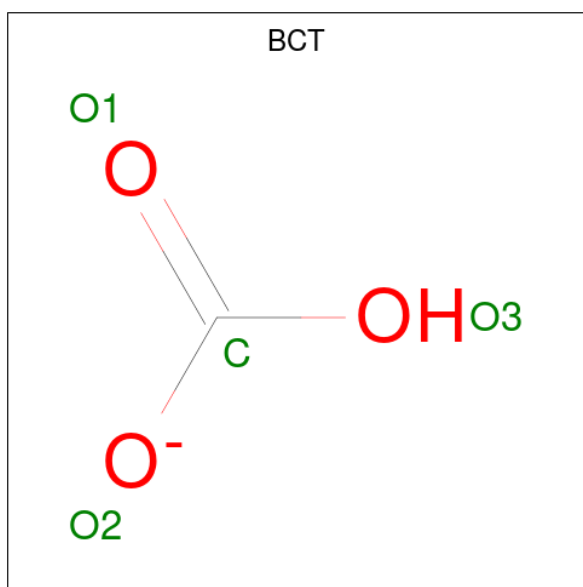
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	N	1	Total	C	O	0	0
			4	2	2		
6	N	1	Total	C	O	0	0
			4	2	2		
6	N	1	Total	C	O	0	0
			4	2	2		
6	N	1	Total	C	O	0	0
			4	2	2		
6	N	1	Total	C	O	0	0
			4	2	2		
6	N	1	Total	C	O	0	0
			4	2	2		
6	O	1	Total	C	O	0	0
			4	2	2		
6	O	1	Total	C	O	0	0
			4	2	2		
6	O	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	O	1	Total 4	C 2	O 2	0	0
6	O	1	Total 4	C 2	O 2	0	0
6	O	1	Total 4	C 2	O 2	0	0
6	O	1	Total 4	C 2	O 2	0	0
6	O	1	Total 4	C 2	O 2	0	0
6	O	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0
6	P	1	Total 4	C 2	O 2	0	0

- Molecule 7 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 1 3	0	0
7	A	1	Total C O 4 1 3	0	0
7	A	1	Total C O 4 1 3	0	0
7	A	1	Total C O 4 1 3	0	0
7	B	1	Total C O 4 1 3	0	0
7	C	1	Total C O 4 1 3	0	0
7	C	1	Total C O 4 1 3	0	0
7	D	1	Total C O 4 1 3	0	0
7	E	1	Total C O 4 1 3	0	0
7	E	1	Total C O 4 1 3	0	0
7	E	1	Total C O 4 1 3	0	0
7	E	1	Total C O 4 1 3	0	0
7	G	1	Total C O 4 1 3	0	0
7	G	1	Total C O 4 1 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C O 4 1 3	0	0
7	G	1	Total C O 4 1 3	0	0
7	G	1	Total C O 4 1 3	0	0
7	H	1	Total C O 4 1 3	0	0
7	I	1	Total C O 4 1 3	0	0
7	I	1	Total C O 4 1 3	0	0
7	I	1	Total C O 4 1 3	0	0
7	K	1	Total C O 4 1 3	0	0
7	K	1	Total C O 4 1 3	0	0
7	L	1	Total C O 4 1 3	0	0
7	M	1	Total C O 4 1 3	0	0
7	M	1	Total C O 4 1 3	0	0
7	M	1	Total C O 4 1 3	0	0
7	N	1	Total C O 4 1 3	0	0
7	O	1	Total C O 4 1 3	0	0
7	O	1	Total C O 4 1 3	0	0
7	O	1	Total C O 4 1 3	0	0

- Molecule 8 is water.

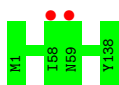
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	279	Total O 279 279	0	0
8	B	112	Total O 112 112	0	0

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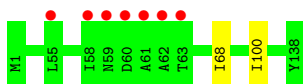
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	C	290	Total 290	O 290	0	0
8	D	109	Total 109	O 109	0	0
8	E	286	Total 286	O 286	0	0
8	F	111	Total 111	O 111	0	0
8	G	302	Total 302	O 302	0	0
8	H	113	Total 113	O 113	0	0
8	I	299	Total 299	O 299	0	0
8	J	115	Total 115	O 115	0	0
8	K	301	Total 301	O 301	0	0
8	L	113	Total 113	O 113	0	0
8	M	278	Total 278	O 278	0	0
8	N	96	Total 96	O 96	0	0
8	O	284	Total 284	O 284	0	0
8	P	106	Total 106	O 106	0	0





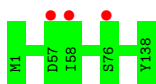
- Molecule 2: Ribulose biphosphate carboxylase small chain



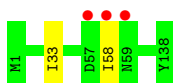
- Molecule 2: Ribulose biphosphate carboxylase small chain



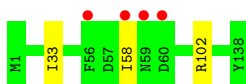
- Molecule 2: Ribulose biphosphate carboxylase small chain



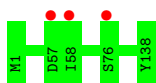
- Molecule 2: Ribulose biphosphate carboxylase small chain



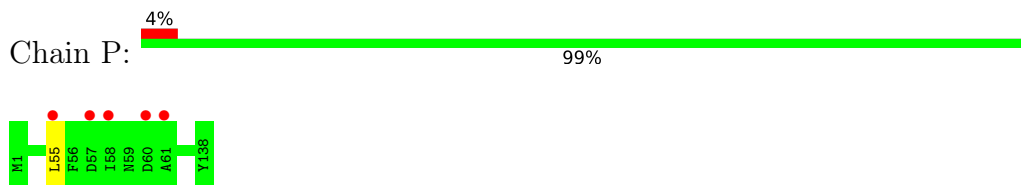
- Molecule 2: Ribulose biphosphate carboxylase small chain



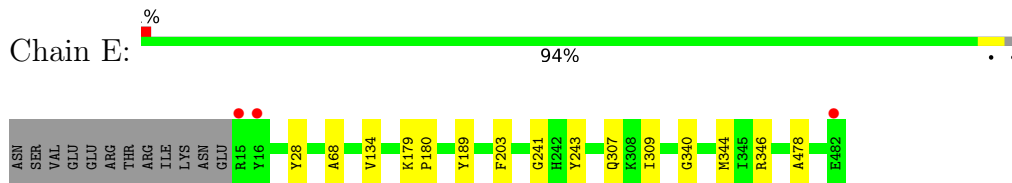
- Molecule 2: Ribulose biphosphate carboxylase small chain



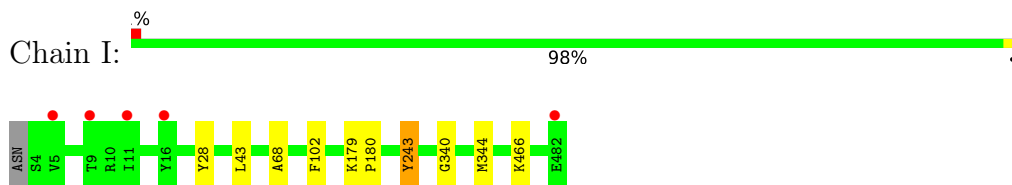
- Molecule 2: Ribulose biphosphate carboxylase small chain



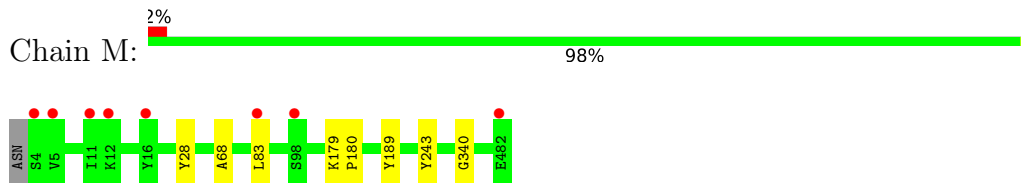
- Molecule 3: Ribulose biphosphate carboxylase large chain



- Molecule 3: Ribulose biphosphate carboxylase large chain



- Molecule 3: Ribulose biphosphate carboxylase large chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.33Å 131.93Å 196.32Å 90.00° 94.75° 90.00°	Depositor
Resolution (Å)	49.60 – 1.70 49.60 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.60-1.70) 99.2 (49.60-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.158 , 0.178 0.168 , 0.186	Depositor DCC
$R_{free}$ test set	28852 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtrriage
Anisotropy	0.266	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	43559	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, HL2, CAP, BCT, KCX, CCS

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	0.54	0/3890	0.76	0/5266
1	C	0.54	0/3864	0.77	1/5232 (0.0%)
1	G	0.55	0/3885	0.76	0/5262
1	K	0.54	0/3897	0.75	0/5278
1	O	0.53	0/3877	0.77	0/5250
2	B	0.54	0/1202	0.68	0/1630
2	D	0.51	0/1185	0.71	0/1607
2	F	0.51	0/1185	0.70	0/1607
2	H	0.54	0/1208	0.68	0/1638
2	J	0.51	0/1194	0.71	0/1619
2	L	0.53	0/1185	0.70	0/1607
2	N	0.53	0/1202	0.68	0/1630
2	P	0.52	0/1210	0.69	0/1641
3	E	0.56	0/3799	0.77	0/5148
3	I	0.56	1/3894 (0.0%)	0.78	0/5273
3	M	0.52	0/3901	0.76	0/5284
All	All	0.54	1/40578 (0.0%)	0.75	1/54972 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	243	TYR	C-O	-7.23	1.15	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	ASP	CB-CA-C	5.67	117.60	109.26

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3805	0	3760	6	0
1	C	3787	0	3743	6	0
1	G	3800	0	3762	3	0
1	K	3804	0	3765	9	0
1	O	3796	0	3755	6	0
2	B	1158	0	1089	0	0
2	D	1149	0	1085	2	0
2	F	1149	0	1085	2	0
2	H	1160	0	1090	0	0
2	J	1154	0	1087	1	0
2	L	1149	0	1085	1	0
2	N	1158	0	1091	0	0
2	P	1162	0	1096	1	0
3	E	3703	0	3662	5	0
3	I	3798	0	3754	5	0
3	M	3801	0	3762	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	A	21	0	8	0	0
5	C	21	0	8	0	0
5	E	21	0	8	0	0
5	G	21	0	8	0	0
5	I	21	0	8	0	0
5	K	21	0	8	0	0
5	M	21	0	8	0	0
5	O	21	0	8	0	0
6	A	52	0	78	1	0
6	B	24	0	36	0	0
6	C	44	0	66	0	0
6	D	24	0	36	0	0
6	E	40	0	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	20	0	30	0	0
6	G	44	0	66	0	0
6	H	28	0	42	0	0
6	I	44	0	66	0	0
6	J	24	0	36	0	0
6	K	32	0	48	0	0
6	L	32	0	48	0	0
6	M	28	0	42	0	0
6	N	28	0	42	0	0
6	O	36	0	54	0	0
6	P	32	0	48	0	0
7	A	16	0	0	0	0
7	B	4	0	0	0	0
7	C	8	0	0	0	0
7	D	4	0	0	0	0
7	E	16	0	0	0	0
7	G	20	0	0	0	0
7	H	4	0	0	0	0
7	I	12	0	0	0	0
7	K	8	0	0	0	0
7	L	4	0	0	0	0
7	M	12	0	0	0	0
7	N	4	0	0	0	0
7	O	12	0	0	0	0
8	A	279	0	0	0	0
8	B	112	0	0	0	0
8	C	290	0	0	0	0
8	D	109	0	0	0	0
8	E	286	0	0	0	0
8	F	111	0	0	0	0
8	G	302	0	0	0	0
8	H	113	0	0	0	0
8	I	299	0	0	0	0
8	J	115	0	0	0	0
8	K	301	0	0	0	0
8	L	113	0	0	0	0
8	M	278	0	0	0	0
8	N	96	0	0	0	0
8	O	284	0	0	0	0
8	P	106	0	0	0	0
All	All	43559	0	39533	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 1.

All (50) 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:A:425:VAL:HG21	1:A:455:CCS:HD2	1.80	0.62
1:A:28:TYR:CZ	1:A:68:ALA:HB2	2.39	0.58
1:C:28:TYR:CZ	1:C:68:ALA:HB2	2.39	0.58
3:I:28:TYR:CZ	3:I:68:ALA:HB2	2.39	0.57
1:A:374[A]:LEU:HD23	6:A:513:EDO:H21	1.86	0.57
1:A:425:VAL:HG21	1:A:455:CCS:CD	2.37	0.55
2:F:68:ILE:HG23	2:F:100:ILE:HD12	1.90	0.53
1:O:28:TYR:CZ	1:O:68:ALA:HB2	2.43	0.53
2:F:68:ILE:HG23	2:F:100:ILE:CD1	2.39	0.53
1:K:28:TYR:CZ	1:K:68:ALA:HB2	2.45	0.52
1:C:28:TYR:CE2	1:C:68:ALA:HB2	2.46	0.51
3:M:28:TYR:CZ	3:M:68:ALA:HB2	2.46	0.50
3:E:28:TYR:CZ	3:E:68:ALA:HB2	2.48	0.49
1:G:28:TYR:CZ	1:G:68:ALA:HB2	2.47	0.49
1:K:340:GLY:HA3	1:K:345[A]:ILE:HD11	1.95	0.48
1:G:344:MET:HA	1:G:344:MET:HE2	1.95	0.48
1:K:179:LYS:HA	1:K:180:PRO:C	2.39	0.48
3:I:28:TYR:CE2	3:I:68:ALA:HB2	2.50	0.46
1:K:307[B]:GLN:HG2	1:K:309[B]:ILE:HG22	1.98	0.46
3:I:43:LEU:HD11	3:I:102:PHE:HB3	1.97	0.46
1:C:43:LEU:HD11	1:C:102:PHE:HB3	1.98	0.46
2:L:33:ILE:HD12	2:L:58:ILE:HD13	1.98	0.46
1:K:344:MET:HA	1:K:344:MET:HE2	1.98	0.45
1:A:179:LYS:HA	1:A:180:PRO:C	2.41	0.45
1:O:179:LYS:HA	1:O:180:PRO:C	2.41	0.45
3:E:179:LYS:HA	3:E:180:PRO:C	2.41	0.45
1:O:344:MET:HA	1:O:344:MET:HE2	1.98	0.45
1:G:179:LYS:HA	1:G:180:PRO:C	2.42	0.44
1:O:175:GLY:HA2	1:O:203:PHE:O	2.17	0.44
2:D:68:ILE:HG23	2:D:100:ILE:HD12	1.99	0.44
1:C:344:MET:HA	1:C:344:MET:HE2	1.99	0.44
1:O:28:TYR:CE2	1:O:68:ALA:HB2	2.52	0.44
1:C:179:LYS:HA	1:C:180:PRO:C	2.42	0.43
1:K:455:CCS:HD2	1:K:457:PRO:HD2	2.00	0.43
3:I:179:LYS:HA	3:I:180:PRO:C	2.43	0.43
2:J:33:ILE:HD12	2:J:58:ILE:HD13	2.01	0.43
1:K:28:TYR:CE2	1:K:68:ALA:HB2	2.54	0.43
1:O:455:CCS:HD2	1:O:457:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:179:LYS:HA	3:M:180:PRO:C	2.44	0.43
3:M:28:TYR:CE2	3:M:68:ALA:HB2	2.54	0.42
1:A:28:TYR:CE2	1:A:68:ALA:HB2	2.55	0.42
3:E:307[B]:GLN:CG	3:E:309[B]:ILE:HG22	2.49	0.42
1:K:43:LEU:HD11	1:K:102:PHE:HB3	2.01	0.42
3:I:344:MET:HE2	3:I:344:MET:HA	2.00	0.41
3:E:344:MET:HE3	3:E:478:ALA:HB2	2.01	0.41
2:D:68:ILE:HG23	2:D:100:ILE:CD1	2.50	0.41
3:E:203:PHE:HA	3:E:241:GLY:O	2.21	0.41
1:C:53:ASP:HA	1:C:54:PRO:HD3	1.94	0.40
1:K:334:VAL:HG22	1:K:345[A]:ILE:HD12	2.01	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	484/480 (101%)	471 (97%)	12 (2%)	1 (0%)	43	28
1	C	481/480 (100%)	470 (98%)	10 (2%)	1 (0%)	43	28
1	G	483/480 (101%)	471 (98%)	11 (2%)	1 (0%)	43	28
1	K	485/480 (101%)	472 (97%)	12 (2%)	1 (0%)	43	28
1	O	482/480 (100%)	470 (98%)	11 (2%)	1 (0%)	43	28
2	B	139/138 (101%)	133 (96%)	6 (4%)	0	100	100
2	D	137/138 (99%)	130 (95%)	7 (5%)	0	100	100
2	F	137/138 (99%)	130 (95%)	7 (5%)	0	100	100
2	H	140/138 (101%)	133 (95%)	7 (5%)	0	100	100
2	J	138/138 (100%)	133 (96%)	5 (4%)	0	100	100
2	L	137/138 (99%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	139/138 (101%)	132 (95%)	7 (5%)	0	100	100
2	P	140/138 (101%)	133 (95%)	7 (5%)	0	100	100
3	E	473/480 (98%)	461 (98%)	11 (2%)	1 (0%)	43	28
3	I	484/480 (101%)	471 (97%)	12 (2%)	1 (0%)	43	28
3	M	485/480 (101%)	472 (97%)	12 (2%)	1 (0%)	43	28
All	All	4964/4944 (100%)	4814 (97%)	142 (3%)	8 (0%)	43	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	GLY
3	E	340	GLY
1	K	340	GLY
3	M	340	GLY
1	C	340	GLY
1	G	340	GLY
3	I	340	GLY
1	O	340	GLY

### 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	399/391 (102%)	397 (100%)	2 (0%)	81	76
1	C	396/391 (101%)	394 (100%)	2 (0%)	81	76
1	G	399/391 (102%)	395 (99%)	4 (1%)	68	58
1	K	400/391 (102%)	397 (99%)	3 (1%)	73	65
1	O	398/391 (102%)	395 (99%)	3 (1%)	73	65
2	B	129/126 (102%)	129 (100%)	0	100	100
2	D	127/126 (101%)	127 (100%)	0	100	100
2	F	127/126 (101%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	130/126 (103%)	130 (100%)	0	100	100
2	J	128/126 (102%)	128 (100%)	0	100	100
2	L	127/126 (101%)	126 (99%)	1 (1%)	73	65
2	N	129/126 (102%)	129 (100%)	0	100	100
2	P	130/126 (103%)	130 (100%)	0	100	100
3	E	389/392 (99%)	385 (99%)	4 (1%)	68	58
3	I	400/392 (102%)	397 (99%)	3 (1%)	73	65
3	M	401/392 (102%)	398 (99%)	3 (1%)	76	69
All	All	4209/4139 (102%)	4184 (99%)	25 (1%)	78	72

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	TYR
1	A	346	ARG
1	C	53	ASP
1	C	243	TYR
3	E	134	VAL
3	E	189	TYR
3	E	243	TYR
3	E	346	ARG
1	G	189	TYR
1	G	243	TYR
1	G	346	ARG
1	G	482	GLU
3	I	243	TYR
3	I	466[A]	LYS
3	I	466[B]	LYS
1	K	189	TYR
1	K	243	TYR
1	K	346	ARG
2	L	102	ARG
3	M	83	LEU
3	M	189	TYR
3	M	243	TYR
1	O	243	TYR
1	O	346	ARG
1	O	481	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	368	GLN
1	A	417	GLN
2	B	29	GLN
1	C	211	ASN
1	C	417	GLN
3	E	417	GLN
3	E	471	ASN
1	G	211	ASN
1	G	368	GLN
1	G	417	GLN
1	G	471	ASN
2	H	75	HIS
2	H	120	ASN
3	I	211	ASN
3	I	417	GLN
1	K	211	ASN
1	K	392	GLN
1	K	417	GLN
3	M	211	ASN
3	M	368	GLN
3	M	417	GLN
2	N	29	GLN
1	O	13	ASN
1	O	127	ASN
1	O	211	ASN
1	O	301	ASN
1	O	392	GLN
1	O	417	GLN
1	O	459	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](#)

21 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	HL2	M	174	3	7,8,9	0.62	0	7,10,12	0.61	0
1	HL2	A	174	1	7,8,9	0.51	0	7,10,12	0.74	0
1	HL2	G	174	1	7,8,9	0.60	0	7,10,12	0.65	0
1	HL2	O	174	1	7,8,9	0.50	0	7,10,12	0.66	0
3	HL2	I	174	3	7,8,9	0.52	0	7,10,12	0.53	0
3	KCX	I	205	3,4	10,11,12	0.70	0	6,12,14	0.44	0
1	KCX	K	205	4,1	10,11,12	2.10	1 (10%)	6,12,14	1.68	1 (16%)
1	HL2	C	174	1	7,8,9	0.49	0	7,10,12	0.58	0
1	KCX	O	205	4,1	10,11,12	2.13	1 (10%)	6,12,14	2.01	1 (16%)
1	HL2	K	174	1	7,8,9	0.51	0	7,10,12	0.57	0
3	KCX	M	205	3,4	10,11,12	0.61	0	6,12,14	0.55	0
1	KCX	C	205	4,1	10,11,12	0.53	0	6,12,14	0.56	0
1	CCS	C	455	1	8,9,10	0.91	0	7,10,12	0.92	0
1	KCX	A	205	4,1	10,11,12	2.11	1 (10%)	6,12,14	1.75	1 (16%)
1	CCS	A	455	1	8,9,10	0.92	0	7,10,12	1.17	1 (14%)
1	CCS	G	455	1	8,9,10	0.90	0	7,10,12	1.65	3 (42%)
3	KCX	E	205	3,4	10,11,12	0.62	0	6,12,14	0.48	0
1	CCS	O	455	1	8,9,10	0.91	0	7,10,12	1.65	2 (28%)
1	KCX	G	205	4,1	10,11,12	1.98	1 (10%)	6,12,14	2.03	1 (16%)
1	CCS	K	455	1	8,9,10	0.96	0	7,10,12	1.64	3 (42%)
3	HL2	E	174	3	7,8,9	0.62	0	7,10,12	0.72	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
3	HL2	M	174	3	-	1/9/10/12	-
1	HL2	A	174	1	-	1/9/10/12	-
1	HL2	G	174	1	-	1/9/10/12	-
1	HL2	O	174	1	-	1/9/10/12	-
3	HL2	I	174	3	-	1/9/10/12	-
3	KCX	I	205	3,4	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	K	205	4,1	-	0/9/10/12	-
1	HL2	C	174	1	-	1/9/10/12	-
1	KCX	O	205	4,1	-	0/9/10/12	-
1	HL2	K	174	1	-	1/9/10/12	-
3	KCX	M	205	3,4	-	0/9/10/12	-
1	KCX	C	205	4,1	-	0/9/10/12	-
1	CCS	C	455	1	-	0/6/8/10	-
1	KCX	A	205	4,1	-	0/9/10/12	-
1	CCS	A	455	1	-	0/6/8/10	-
1	CCS	G	455	1	-	1/6/8/10	-
3	KCX	E	205	3,4	-	0/9/10/12	-
1	CCS	O	455	1	-	1/6/8/10	-
1	KCX	G	205	4,1	-	0/9/10/12	-
1	CCS	K	455	1	-	1/6/8/10	-
3	HL2	E	174	3	-	1/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	205	KCX	OQ1-CX	6.42	1.33	1.21
1	K	205	KCX	OQ1-CX	6.27	1.33	1.21
1	A	205	KCX	OQ1-CX	6.27	1.33	1.21
1	G	205	KCX	OQ1-CX	5.77	1.32	1.21

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	205	KCX	OQ1-CX-NZ	-4.79	117.65	124.92
1	O	205	KCX	OQ1-CX-NZ	-4.68	117.81	124.92
1	A	205	KCX	OQ1-CX-NZ	-4.09	118.70	124.92
1	K	205	KCX	OQ1-CX-NZ	-3.94	118.94	124.92
1	O	455	CCS	OZ1-CE-CD	-2.80	115.29	122.85
1	G	455	CCS	OZ2-CE-CD	2.72	122.20	113.38
1	O	455	CCS	OZ2-CE-CD	2.66	122.00	113.38
1	K	455	CCS	OZ2-CE-CD	2.57	121.72	113.38
1	A	455	CCS	CE-CD-SG	2.55	119.81	113.18
1	K	455	CCS	OZ1-CE-CD	-2.50	116.08	122.85
1	G	455	CCS	OZ1-CE-CD	-2.40	116.37	122.85
1	K	455	CCS	CE-CD-SG	2.31	119.17	113.18
1	G	455	CCS	CE-CD-SG	2.22	118.96	113.18

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	174	HL2	O-C-CA-CB
1	C	174	HL2	O-C-CA-CB
3	E	174	HL2	O-C-CA-CB
1	G	174	HL2	O-C-CA-CB
3	I	174	HL2	O-C-CA-CB
1	K	174	HL2	O-C-CA-CB
3	M	174	HL2	O-C-CA-CB
1	O	174	HL2	O-C-CA-CB
1	K	455	CCS	CA-CB-SG-CD
1	O	455	CCS	CA-CB-SG-CD
1	G	455	CCS	CA-CB-SG-CD

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	455	CCS	2	0
1	O	455	CCS	1	0
1	K	455	CCS	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 8 are monoatomic - leaving 172 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	EDO	K	506	-	3,3,3	0.42	0	2,2,2	0.48	0
6	EDO	L	206	-	3,3,3	0.52	0	2,2,2	0.14	0
6	EDO	G	513	-	3,3,3	0.40	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCT	A	519	-	3,3,3	0.50	0	2,3,3	0.64	0
6	EDO	G	512	-	3,3,3	0.58	0	2,2,2	0.19	0
6	EDO	H	206	-	3,3,3	0.32	0	2,2,2	0.66	0
6	EDO	E	512	-	3,3,3	0.43	0	2,2,2	0.30	0
6	EDO	G	511	-	3,3,3	0.37	0	2,2,2	0.48	0
6	EDO	B	206	-	3,3,3	0.36	0	2,2,2	0.51	0
6	EDO	D	202	-	3,3,3	0.40	0	2,2,2	0.30	0
6	EDO	E	504	-	3,3,3	0.49	0	2,2,2	0.23	0
6	EDO	K	509	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	A	512	-	3,3,3	0.32	0	2,2,2	0.53	0
5	CAP	E	502	4	18,20,20	0.84	0	23,31,31	1.27	2 (8%)
6	EDO	I	503	-	3,3,3	0.48	0	2,2,2	0.29	0
6	EDO	M	507	-	3,3,3	0.38	0	2,2,2	0.36	0
7	BCT	O	514	-	3,3,3	0.58	0	2,3,3	0.49	0
6	EDO	M	505	-	3,3,3	0.48	0	2,2,2	0.31	0
6	EDO	K	508	-	3,3,3	0.38	0	2,2,2	0.42	0
6	EDO	P	204	-	3,3,3	0.37	0	2,2,2	0.42	0
6	EDO	B	204	-	3,3,3	0.50	0	2,2,2	0.14	0
6	EDO	I	507	-	3,3,3	0.41	0	2,2,2	0.11	0
6	EDO	K	510	-	3,3,3	0.45	0	2,2,2	0.09	0
7	BCT	H	208	-	3,3,3	0.58	0	2,3,3	0.63	0
6	EDO	O	511	-	3,3,3	0.32	0	2,2,2	0.44	0
6	EDO	N	202	-	3,3,3	0.35	0	2,2,2	0.28	0
6	EDO	E	503	-	3,3,3	0.57	0	2,2,2	0.24	0
6	EDO	C	512	-	3,3,3	0.38	0	2,2,2	0.37	0
6	EDO	F	205	-	3,3,3	0.38	0	2,2,2	0.60	0
6	EDO	N	203	-	3,3,3	0.48	0	2,2,2	0.31	0
6	EDO	H	204	-	3,3,3	0.42	0	2,2,2	0.29	0
6	EDO	C	513	-	3,3,3	0.43	0	2,2,2	0.47	0
6	EDO	J	204	-	3,3,3	0.47	0	2,2,2	0.20	0
6	EDO	K	503	-	3,3,3	0.39	0	2,2,2	0.58	0
6	EDO	A	504	-	3,3,3	0.41	0	2,2,2	0.42	0
6	EDO	G	507	-	3,3,3	0.43	0	2,2,2	0.23	0
6	EDO	J	202	-	3,3,3	0.46	0	2,2,2	0.18	0
6	EDO	M	508	-	3,3,3	0.39	0	2,2,2	0.42	0
6	EDO	A	505	-	3,3,3	0.35	0	2,2,2	0.47	0
6	EDO	D	201	-	3,3,3	0.42	0	2,2,2	0.31	0
7	BCT	A	516	-	3,3,3	1.35	0	2,3,3	0.61	0
7	BCT	E	513	-	3,3,3	0.64	0	2,3,3	0.46	0
6	EDO	M	506	-	3,3,3	0.43	0	2,2,2	0.41	0
6	EDO	I	508	-	3,3,3	0.47	0	2,2,2	0.04	0
6	EDO	L	207	-	3,3,3	0.41	0	2,2,2	0.41	0
6	EDO	J	203	-	3,3,3	0.46	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	D	205	-	3,3,3	0.37	0	2,2,2	0.37	0
6	EDO	N	205	-	3,3,3	0.35	0	2,2,2	0.57	0
6	EDO	G	506	-	3,3,3	0.40	0	2,2,2	0.43	0
6	EDO	A	513	-	3,3,3	0.41	0	2,2,2	0.26	0
6	EDO	L	205	-	3,3,3	0.36	0	2,2,2	0.61	0
7	BCT	E	515	-	3,3,3	1.52	1 (33%)	2,3,3	0.35	0
6	EDO	F	201	-	3,3,3	0.46	0	2,2,2	0.23	0
6	EDO	A	510	-	3,3,3	0.40	0	2,2,2	0.40	0
7	BCT	M	511	-	3,3,3	1.44	1 (33%)	2,3,3	0.69	0
6	EDO	G	510	-	3,3,3	0.38	0	2,2,2	0.37	0
6	EDO	N	206	-	3,3,3	0.46	0	2,2,2	0.32	0
7	BCT	I	515	-	3,3,3	1.54	1 (33%)	2,3,3	0.28	0
6	EDO	J	205	-	3,3,3	0.38	0	2,2,2	0.42	0
7	BCT	N	208	-	3,3,3	1.51	1 (33%)	2,3,3	0.26	0
7	BCT	K	511	-	3,3,3	0.62	0	2,3,3	0.99	0
6	EDO	I	510	-	3,3,3	0.44	0	2,2,2	0.43	0
7	BCT	I	516	-	3,3,3	0.57	0	2,3,3	0.54	0
6	EDO	G	505	-	3,3,3	0.38	0	2,2,2	0.39	0
6	EDO	E	505	-	3,3,3	0.41	0	2,2,2	0.49	0
6	EDO	C	506	-	3,3,3	0.45	0	2,2,2	0.11	0
6	EDO	P	208	-	3,3,3	0.33	0	2,2,2	0.46	0
6	EDO	A	506	-	3,3,3	0.40	0	2,2,2	0.43	0
6	EDO	O	503	-	3,3,3	0.47	0	2,2,2	0.28	0
6	EDO	D	203	-	3,3,3	0.49	0	2,2,2	0.22	0
6	EDO	D	204	-	3,3,3	0.44	0	2,2,2	0.24	0
5	CAP	O	502	4	18,20,20	0.79	0	23,31,31	1.47	2 (8%)
6	EDO	E	509	-	3,3,3	0.52	0	2,2,2	0.13	0
6	EDO	J	206	-	3,3,3	0.34	0	2,2,2	0.59	0
5	CAP	C	502	4	18,20,20	0.80	0	23,31,31	0.99	1 (4%)
6	EDO	L	204	-	3,3,3	0.50	0	2,2,2	0.04	0
6	EDO	E	508	-	3,3,3	0.43	0	2,2,2	0.44	0
7	BCT	E	514	-	3,3,3	0.53	0	2,3,3	0.85	0
7	BCT	C	514	-	3,3,3	0.53	0	2,3,3	0.49	0
7	BCT	G	515	-	3,3,3	1.51	1 (33%)	2,3,3	0.19	0
7	BCT	M	510	-	3,3,3	1.50	1 (33%)	2,3,3	0.30	0
6	EDO	A	514	-	3,3,3	0.27	0	2,2,2	0.39	0
6	EDO	D	206	-	3,3,3	0.38	0	2,2,2	0.63	0
6	EDO	P	203	-	3,3,3	0.41	0	2,2,2	0.30	0
6	EDO	E	511	-	3,3,3	0.41	0	2,2,2	0.40	0
7	BCT	B	207	-	3,3,3	0.56	0	2,3,3	0.57	0
6	EDO	I	505	-	3,3,3	0.40	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	F	204	-	3,3,3	0.30	0	2,2,2	0.45	0
6	EDO	N	207	-	3,3,3	0.36	0	2,2,2	0.35	0
6	EDO	A	515	-	3,3,3	0.43	0	2,2,2	0.42	0
6	EDO	P	206	-	3,3,3	0.44	0	2,2,2	0.30	0
6	EDO	E	507	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	I	509	-	3,3,3	0.43	0	2,2,2	0.42	0
6	EDO	L	202	-	3,3,3	0.37	0	2,2,2	0.48	0
6	EDO	B	202	-	3,3,3	0.36	0	2,2,2	0.32	0
6	EDO	P	205	-	3,3,3	0.38	0	2,2,2	0.25	0
6	EDO	P	202	-	3,3,3	0.42	0	2,2,2	0.30	0
6	EDO	O	505	-	3,3,3	0.45	0	2,2,2	0.33	0
7	BCT	M	512	-	3,3,3	0.53	0	2,3,3	0.64	0
6	EDO	L	203	-	3,3,3	0.31	0	2,2,2	0.39	0
7	BCT	A	517	-	3,3,3	0.52	0	2,3,3	0.55	0
6	EDO	K	504	-	3,3,3	0.43	0	2,2,2	0.48	0
7	BCT	O	513	-	3,3,3	0.57	0	2,3,3	0.61	0
6	EDO	B	203	-	3,3,3	0.45	0	2,2,2	0.35	0
7	BCT	G	514	-	3,3,3	0.66	0	2,3,3	0.20	0
6	EDO	A	509	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	O	510	-	3,3,3	0.45	0	2,2,2	0.21	0
5	CAP	K	502	4	18,20,20	0.78	0	23,31,31	1.33	2 (8%)
6	EDO	I	513	-	3,3,3	0.48	0	2,2,2	0.10	0
6	EDO	K	507	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	N	204	-	3,3,3	0.44	0	2,2,2	0.31	0
6	EDO	L	208	-	3,3,3	0.38	0	2,2,2	0.47	0
6	EDO	B	201	-	3,3,3	0.50	0	2,2,2	0.22	0
6	EDO	I	511	-	3,3,3	0.46	0	2,2,2	0.36	0
6	EDO	M	503	-	3,3,3	0.45	0	2,2,2	0.29	0
6	EDO	C	505	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	M	509	-	3,3,3	0.41	0	2,2,2	0.19	0
7	BCT	O	512	-	3,3,3	0.61	0	2,3,3	0.76	0
5	CAP	M	502	4	18,20,20	0.77	0	23,31,31	0.95	0
6	EDO	O	504	-	3,3,3	0.36	0	2,2,2	0.51	0
6	EDO	O	509	-	3,3,3	0.39	0	2,2,2	0.45	0
6	EDO	G	504	-	3,3,3	0.38	0	2,2,2	0.46	0
6	EDO	O	508	-	3,3,3	0.39	0	2,2,2	0.40	0
6	EDO	K	505	-	3,3,3	0.37	0	2,2,2	0.43	0
6	EDO	F	203	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	M	504	-	3,3,3	0.38	0	2,2,2	0.54	0
7	BCT	G	516	-	3,3,3	0.57	0	2,3,3	0.62	0
6	EDO	A	508	-	3,3,3	0.49	0	2,2,2	0.32	0
6	EDO	E	510	-	3,3,3	0.37	0	2,2,2	0.46	0
6	EDO	A	503	-	3,3,3	0.47	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	C	504	-	3,3,3	0.42	0	2,2,2	0.41	0
6	EDO	I	506	-	3,3,3	0.48	0	2,2,2	0.25	0
7	BCT	A	518	-	3,3,3	1.48	1 (33%)	2,3,3	0.47	0
6	EDO	G	503	-	3,3,3	0.41	0	2,2,2	0.17	0
7	BCT	C	515	-	3,3,3	1.50	1 (33%)	2,3,3	0.32	0
6	EDO	C	510	-	3,3,3	0.42	0	2,2,2	0.40	0
7	BCT	G	518	-	3,3,3	1.49	1 (33%)	2,3,3	0.17	0
6	EDO	C	509	-	3,3,3	0.41	0	2,2,2	0.46	0
6	EDO	O	506	-	3,3,3	0.42	0	2,2,2	0.42	0
7	BCT	K	512	-	3,3,3	0.54	0	2,3,3	0.68	0
5	CAP	A	502	4	18,20,20	0.79	0	23,31,31	1.43	2 (8%)
6	EDO	A	511	-	3,3,3	0.41	0	2,2,2	0.37	0
6	EDO	H	205	-	3,3,3	0.37	0	2,2,2	0.26	0
7	BCT	E	516	-	3,3,3	1.50	1 (33%)	2,3,3	0.32	0
6	EDO	C	508	-	3,3,3	0.42	0	2,2,2	0.38	0
7	BCT	D	207	-	3,3,3	0.56	0	2,3,3	0.52	0
6	EDO	H	202	-	3,3,3	0.45	0	2,2,2	0.15	0
6	EDO	E	506	-	3,3,3	0.38	0	2,2,2	0.48	0
5	CAP	I	502	4	18,20,20	0.74	0	23,31,31	0.98	0
6	EDO	O	507	-	3,3,3	0.37	0	2,2,2	0.44	0
6	EDO	L	201	-	3,3,3	0.48	0	2,2,2	0.19	0
6	EDO	C	503	-	3,3,3	0.41	0	2,2,2	0.25	0
7	BCT	L	209	-	3,3,3	1.51	1 (33%)	2,3,3	0.19	0
6	EDO	P	207	-	3,3,3	0.34	0	2,2,2	0.56	0
6	EDO	H	203	-	3,3,3	0.50	0	2,2,2	0.13	0
6	EDO	I	504	-	3,3,3	0.41	0	2,2,2	0.28	0
6	EDO	A	507	-	3,3,3	0.35	0	2,2,2	0.44	0
6	EDO	P	201	-	3,3,3	0.39	0	2,2,2	0.25	0
6	EDO	C	511	-	3,3,3	0.51	0	2,2,2	0.28	0
6	EDO	J	201	-	3,3,3	0.44	0	2,2,2	0.32	0
6	EDO	H	201	-	3,3,3	0.43	0	2,2,2	0.28	0
6	EDO	C	507	-	3,3,3	0.41	0	2,2,2	0.42	0
6	EDO	G	509	-	3,3,3	0.51	0	2,2,2	0.20	0
6	EDO	N	201	-	3,3,3	0.43	0	2,2,2	0.26	0
5	CAP	G	502	4	18,20,20	0.76	0	23,31,31	0.87	0
6	EDO	B	205	-	3,3,3	0.36	0	2,2,2	0.45	0
6	EDO	H	207	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	I	512	-	3,3,3	0.50	0	2,2,2	0.25	0
6	EDO	G	508	-	3,3,3	0.56	0	2,2,2	0.08	0
7	BCT	G	517	-	3,3,3	1.50	1 (33%)	2,3,3	0.38	0
6	EDO	F	202	-	3,3,3	0.51	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCT	I	514	-	3,3,3	0.55	0	2,3,3	0.57	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	EDO	K	506	-	-	0/1/1/1	-
6	EDO	L	206	-	-	1/1/1/1	-
6	EDO	G	513	-	-	1/1/1/1	-
6	EDO	G	512	-	-	0/1/1/1	-
6	EDO	H	206	-	-	0/1/1/1	-
6	EDO	E	512	-	-	0/1/1/1	-
6	EDO	G	511	-	-	0/1/1/1	-
6	EDO	B	206	-	-	0/1/1/1	-
6	EDO	D	202	-	-	0/1/1/1	-
6	EDO	E	504	-	-	0/1/1/1	-
6	EDO	K	509	-	-	1/1/1/1	-
6	EDO	A	512	-	-	0/1/1/1	-
5	CAP	E	502	4	-	9/29/29/29	-
6	EDO	I	503	-	-	0/1/1/1	-
6	EDO	M	507	-	-	0/1/1/1	-
6	EDO	M	505	-	-	0/1/1/1	-
6	EDO	K	508	-	-	0/1/1/1	-
6	EDO	P	204	-	-	0/1/1/1	-
6	EDO	B	204	-	-	0/1/1/1	-
6	EDO	I	507	-	-	1/1/1/1	-
6	EDO	K	510	-	-	1/1/1/1	-
6	EDO	O	511	-	-	1/1/1/1	-
6	EDO	N	202	-	-	0/1/1/1	-
6	EDO	E	503	-	-	0/1/1/1	-
6	EDO	C	512	-	-	0/1/1/1	-
6	EDO	F	205	-	-	0/1/1/1	-
6	EDO	N	203	-	-	0/1/1/1	-
6	EDO	H	204	-	-	0/1/1/1	-
6	EDO	C	513	-	-	1/1/1/1	-
6	EDO	J	204	-	-	0/1/1/1	-
6	EDO	K	503	-	-	0/1/1/1	-
6	EDO	A	504	-	-	0/1/1/1	-
6	EDO	G	507	-	-	0/1/1/1	-
6	EDO	J	202	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	M	508	-	-	0/1/1/1	-
6	EDO	A	505	-	-	0/1/1/1	-
6	EDO	D	201	-	-	0/1/1/1	-
6	EDO	M	506	-	-	0/1/1/1	-
6	EDO	I	508	-	-	1/1/1/1	-
6	EDO	L	207	-	-	0/1/1/1	-
6	EDO	J	203	-	-	0/1/1/1	-
6	EDO	D	205	-	-	0/1/1/1	-
6	EDO	N	205	-	-	0/1/1/1	-
6	EDO	G	506	-	-	1/1/1/1	-
6	EDO	A	513	-	-	0/1/1/1	-
6	EDO	L	205	-	-	0/1/1/1	-
6	EDO	F	201	-	-	0/1/1/1	-
6	EDO	A	510	-	-	1/1/1/1	-
6	EDO	G	510	-	-	0/1/1/1	-
6	EDO	N	206	-	-	0/1/1/1	-
6	EDO	J	205	-	-	1/1/1/1	-
6	EDO	I	510	-	-	0/1/1/1	-
6	EDO	G	505	-	-	1/1/1/1	-
6	EDO	E	505	-	-	0/1/1/1	-
6	EDO	C	506	-	-	1/1/1/1	-
6	EDO	P	208	-	-	1/1/1/1	-
6	EDO	A	506	-	-	0/1/1/1	-
6	EDO	O	503	-	-	0/1/1/1	-
6	EDO	D	203	-	-	0/1/1/1	-
6	EDO	D	204	-	-	0/1/1/1	-
5	CAP	O	502	4	-	9/29/29/29	-
6	EDO	E	509	-	-	0/1/1/1	-
6	EDO	J	206	-	-	0/1/1/1	-
5	CAP	C	502	4	-	7/29/29/29	-
6	EDO	L	204	-	-	0/1/1/1	-
6	EDO	E	508	-	-	0/1/1/1	-
6	EDO	A	514	-	-	1/1/1/1	-
6	EDO	D	206	-	-	0/1/1/1	-
6	EDO	P	203	-	-	0/1/1/1	-
6	EDO	E	511	-	-	1/1/1/1	-
6	EDO	I	505	-	-	0/1/1/1	-
6	EDO	F	204	-	-	0/1/1/1	-
6	EDO	N	207	-	-	1/1/1/1	-
6	EDO	A	515	-	-	0/1/1/1	-
6	EDO	P	206	-	-	1/1/1/1	-
6	EDO	E	507	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	I	509	-	-	1/1/1/1	-
6	EDO	L	202	-	-	0/1/1/1	-
6	EDO	B	202	-	-	0/1/1/1	-
6	EDO	P	205	-	-	1/1/1/1	-
6	EDO	P	202	-	-	0/1/1/1	-
6	EDO	O	505	-	-	1/1/1/1	-
6	EDO	L	203	-	-	0/1/1/1	-
6	EDO	K	504	-	-	0/1/1/1	-
6	EDO	B	203	-	-	0/1/1/1	-
6	EDO	A	509	-	-	1/1/1/1	-
6	EDO	O	510	-	-	0/1/1/1	-
5	CAP	K	502	4	-	8/29/29/29	-
6	EDO	I	513	-	-	1/1/1/1	-
6	EDO	K	507	-	-	1/1/1/1	-
6	EDO	N	204	-	-	0/1/1/1	-
6	EDO	L	208	-	-	1/1/1/1	-
6	EDO	B	201	-	-	0/1/1/1	-
6	EDO	I	511	-	-	0/1/1/1	-
6	EDO	M	503	-	-	0/1/1/1	-
6	EDO	C	505	-	-	0/1/1/1	-
6	EDO	M	509	-	-	1/1/1/1	-
5	CAP	M	502	4	-	7/29/29/29	-
6	EDO	O	504	-	-	0/1/1/1	-
6	EDO	O	509	-	-	1/1/1/1	-
6	EDO	G	504	-	-	0/1/1/1	-
6	EDO	O	508	-	-	0/1/1/1	-
6	EDO	K	505	-	-	1/1/1/1	-
6	EDO	F	203	-	-	0/1/1/1	-
6	EDO	M	504	-	-	0/1/1/1	-
6	EDO	A	508	-	-	0/1/1/1	-
6	EDO	E	510	-	-	0/1/1/1	-
6	EDO	A	503	-	-	0/1/1/1	-
6	EDO	C	504	-	-	0/1/1/1	-
6	EDO	I	506	-	-	0/1/1/1	-
6	EDO	G	503	-	-	0/1/1/1	-
6	EDO	C	510	-	-	0/1/1/1	-
6	EDO	C	509	-	-	0/1/1/1	-
6	EDO	O	506	-	-	0/1/1/1	-
5	CAP	A	502	4	-	9/29/29/29	-
6	EDO	A	511	-	-	0/1/1/1	-
6	EDO	H	205	-	-	1/1/1/1	-
6	EDO	C	508	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	H	202	-	-	0/1/1/1	-
6	EDO	E	506	-	-	0/1/1/1	-
5	CAP	I	502	4	-	7/29/29/29	-
6	EDO	O	507	-	-	1/1/1/1	-
6	EDO	L	201	-	-	0/1/1/1	-
6	EDO	C	503	-	-	0/1/1/1	-
6	EDO	P	207	-	-	0/1/1/1	-
6	EDO	H	203	-	-	0/1/1/1	-
6	EDO	I	504	-	-	0/1/1/1	-
6	EDO	A	507	-	-	0/1/1/1	-
6	EDO	P	201	-	-	0/1/1/1	-
6	EDO	C	511	-	-	1/1/1/1	-
6	EDO	J	201	-	-	0/1/1/1	-
6	EDO	H	201	-	-	0/1/1/1	-
6	EDO	C	507	-	-	1/1/1/1	-
6	EDO	G	509	-	-	0/1/1/1	-
6	EDO	N	201	-	-	0/1/1/1	-
5	CAP	G	502	4	-	7/29/29/29	-
6	EDO	B	205	-	-	1/1/1/1	-
6	EDO	H	207	-	-	0/1/1/1	-
6	EDO	I	512	-	-	1/1/1/1	-
6	EDO	G	508	-	-	0/1/1/1	-
6	EDO	F	202	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	515	BCT	O1-C	2.28	1.33	1.25
7	N	208	BCT	O1-C	2.25	1.33	1.25
7	E	516	BCT	O1-C	2.25	1.33	1.25
7	M	510	BCT	O1-C	2.24	1.33	1.25
7	G	515	BCT	O1-C	2.24	1.33	1.25
7	L	209	BCT	O1-C	2.23	1.33	1.25
7	G	517	BCT	O1-C	2.23	1.33	1.25
7	C	515	BCT	O1-C	2.22	1.33	1.25
7	A	518	BCT	O1-C	2.21	1.33	1.25
7	M	511	BCT	O1-C	2.16	1.33	1.25
7	I	515	BCT	O1-C	2.16	1.33	1.25
7	G	518	BCT	O1-C	2.15	1.33	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	502	CAP	O7-C-C2	4.52	121.63	114.06
5	A	502	CAP	O7-C-C2	4.26	121.19	114.06
5	E	502	CAP	O7-C-C2	4.19	121.07	114.06
5	K	502	CAP	O7-C-C2	4.13	120.97	114.06
5	O	502	CAP	O6-C-C2	-3.29	116.19	122.32
5	A	502	CAP	O6-C-C2	-3.20	116.36	122.32
5	E	502	CAP	O6-C-C2	-2.93	116.86	122.32
5	K	502	CAP	O6-C-C2	-2.51	117.65	122.32
5	C	502	CAP	O7-C-C2	2.32	117.94	114.06

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	CAP	O6-C-C2-O2
5	A	502	CAP	C2-C3-C4-O4
5	A	502	CAP	O3-C3-C4-O4
5	C	502	CAP	O6-C-C2-C1
5	C	502	CAP	O7-C-C2-C1
5	C	502	CAP	O6-C-C2-O2
5	C	502	CAP	O7-C-C2-O2
5	C	502	CAP	O3-C3-C4-O4
5	E	502	CAP	O6-C-C2-O2
5	E	502	CAP	O3-C3-C4-O4
5	G	502	CAP	O6-C-C2-C1
5	G	502	CAP	O7-C-C2-C1
5	G	502	CAP	O6-C-C2-O2
5	G	502	CAP	O7-C-C2-O2
5	G	502	CAP	C2-C3-C4-O4
5	G	502	CAP	O3-C3-C4-O4
5	I	502	CAP	O6-C-C2-C1
5	I	502	CAP	O7-C-C2-C1
5	I	502	CAP	O6-C-C2-O2
5	I	502	CAP	O7-C-C2-O2
5	I	502	CAP	O3-C3-C4-O4
5	K	502	CAP	O7-C-C2-C1
5	K	502	CAP	O6-C-C2-O2
5	K	502	CAP	O3-C3-C4-O4
5	M	502	CAP	O6-C-C2-C1
5	M	502	CAP	O7-C-C2-C1
5	M	502	CAP	O6-C-C2-O2
5	M	502	CAP	O7-C-C2-O2
5	M	502	CAP	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	M	502	CAP	O3-C3-C4-O4
5	O	502	CAP	O6-C-C2-O2
5	O	502	CAP	O3-C3-C4-O4
5	A	502	CAP	O7-C-C2-C1
5	E	502	CAP	O7-C-C2-C1
5	O	502	CAP	O7-C-C2-C1
6	A	510	EDO	O1-C1-C2-O2
6	B	205	EDO	O1-C1-C2-O2
6	G	506	EDO	O1-C1-C2-O2
6	G	513	EDO	O1-C1-C2-O2
6	O	509	EDO	O1-C1-C2-O2
5	A	502	CAP	O7-C-C2-O2
5	K	502	CAP	O7-C-C2-O2
5	O	502	CAP	O7-C-C2-O2
5	C	502	CAP	C2-C3-C4-O4
5	I	502	CAP	C2-C3-C4-O4
5	K	502	CAP	C2-C3-C4-O4
6	I	512	EDO	O1-C1-C2-O2
6	K	505	EDO	O1-C1-C2-O2
5	K	502	CAP	O6-C-C2-C1
6	I	508	EDO	O1-C1-C2-O2
6	P	208	EDO	O1-C1-C2-O2
5	A	502	CAP	O6-C-C2-C1
5	E	502	CAP	O6-C-C2-C1
5	O	502	CAP	O6-C-C2-C1
5	E	502	CAP	O7-C-C2-O2
5	A	502	CAP	O2-C2-C3-C4
5	C	502	CAP	O2-C2-C3-C4
5	E	502	CAP	O2-C2-C3-C4
5	G	502	CAP	O2-C2-C3-C4
5	I	502	CAP	O2-C2-C3-C4
5	K	502	CAP	O2-C2-C3-C4
5	M	502	CAP	O2-C2-C3-C4
5	O	502	CAP	O2-C2-C3-C4
5	A	502	CAP	O7-C-C2-C3
5	E	502	CAP	O7-C-C2-C3
5	K	502	CAP	O7-C-C2-C3
5	O	502	CAP	O7-C-C2-C3
6	C	506	EDO	O1-C1-C2-O2
6	C	511	EDO	O1-C1-C2-O2
6	C	513	EDO	O1-C1-C2-O2
6	K	509	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	L	208	EDO	O1-C1-C2-O2
6	M	509	EDO	O1-C1-C2-O2
6	A	514	EDO	O1-C1-C2-O2
6	E	511	EDO	O1-C1-C2-O2
6	I	513	EDO	O1-C1-C2-O2
6	K	507	EDO	O1-C1-C2-O2
5	E	502	CAP	C2-C3-C4-O4
6	I	507	EDO	O1-C1-C2-O2
6	J	205	EDO	O1-C1-C2-O2
6	P	205	EDO	O1-C1-C2-O2
5	A	502	CAP	O6-C-C2-C3
5	E	502	CAP	O6-C-C2-C3
5	O	502	CAP	O6-C-C2-C3
6	A	509	EDO	O1-C1-C2-O2
6	C	507	EDO	O1-C1-C2-O2
6	H	205	EDO	O1-C1-C2-O2
6	L	206	EDO	O1-C1-C2-O2
6	N	207	EDO	O1-C1-C2-O2
6	O	511	EDO	O1-C1-C2-O2
6	E	507	EDO	O1-C1-C2-O2
6	I	509	EDO	O1-C1-C2-O2
6	K	510	EDO	O1-C1-C2-O2
6	O	507	EDO	O1-C1-C2-O2
6	P	206	EDO	O1-C1-C2-O2
5	O	502	CAP	C2-C3-C4-O4
6	G	505	EDO	O1-C1-C2-O2
6	O	505	EDO	O1-C1-C2-O2

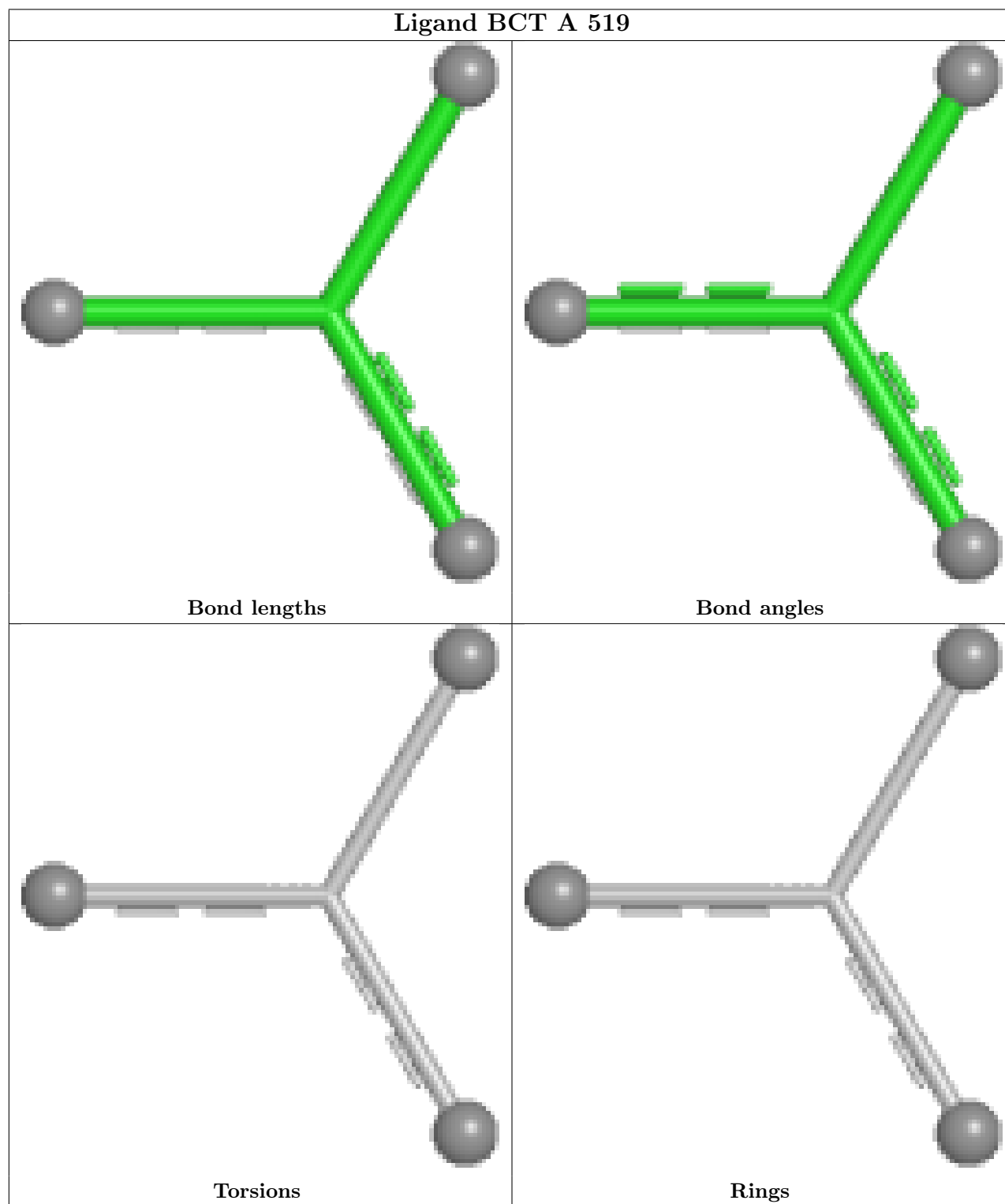
There are no ring outliers.

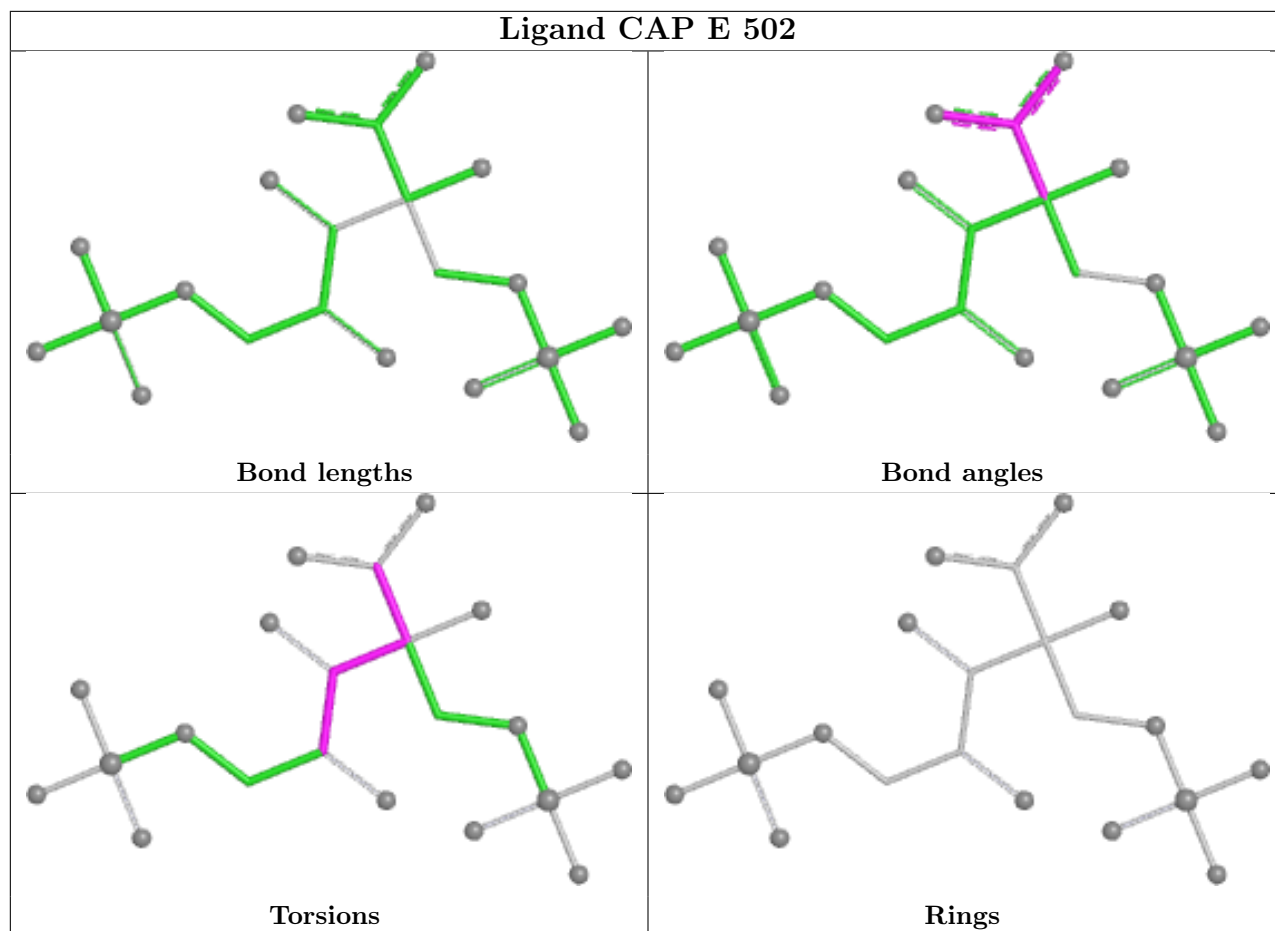
1 monomer is involved in 1 short contact:

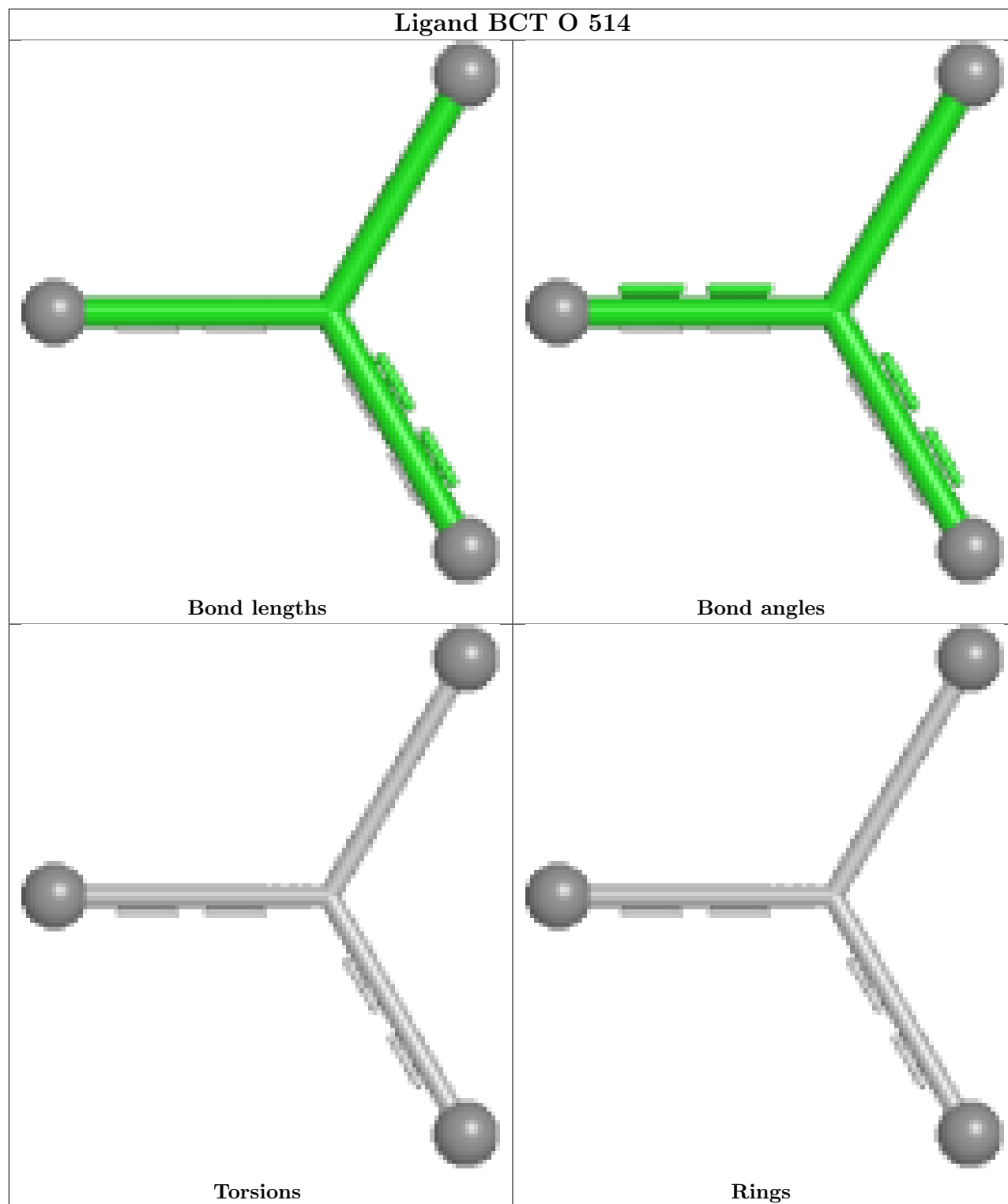
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	513	EDO	1	0

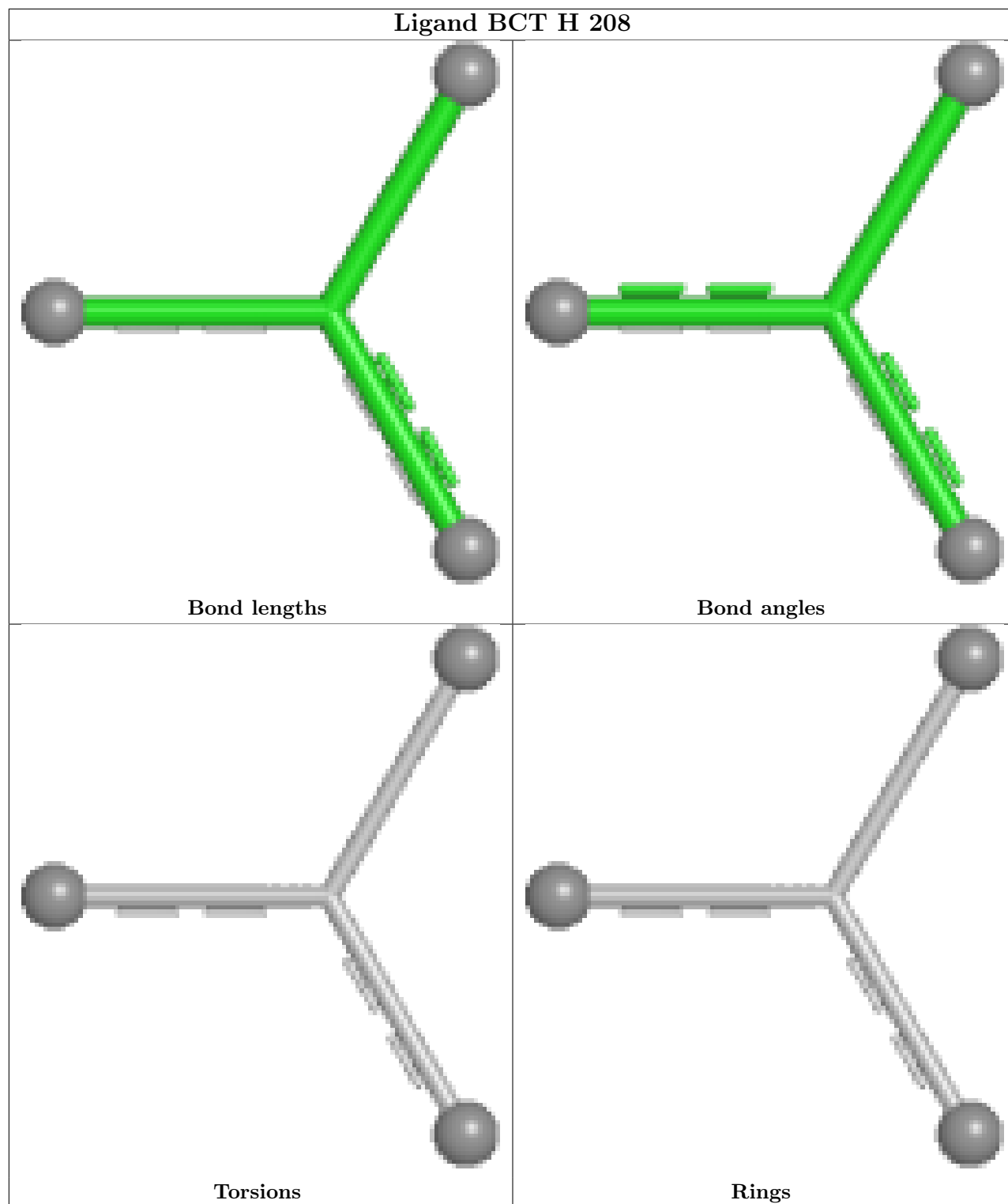
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

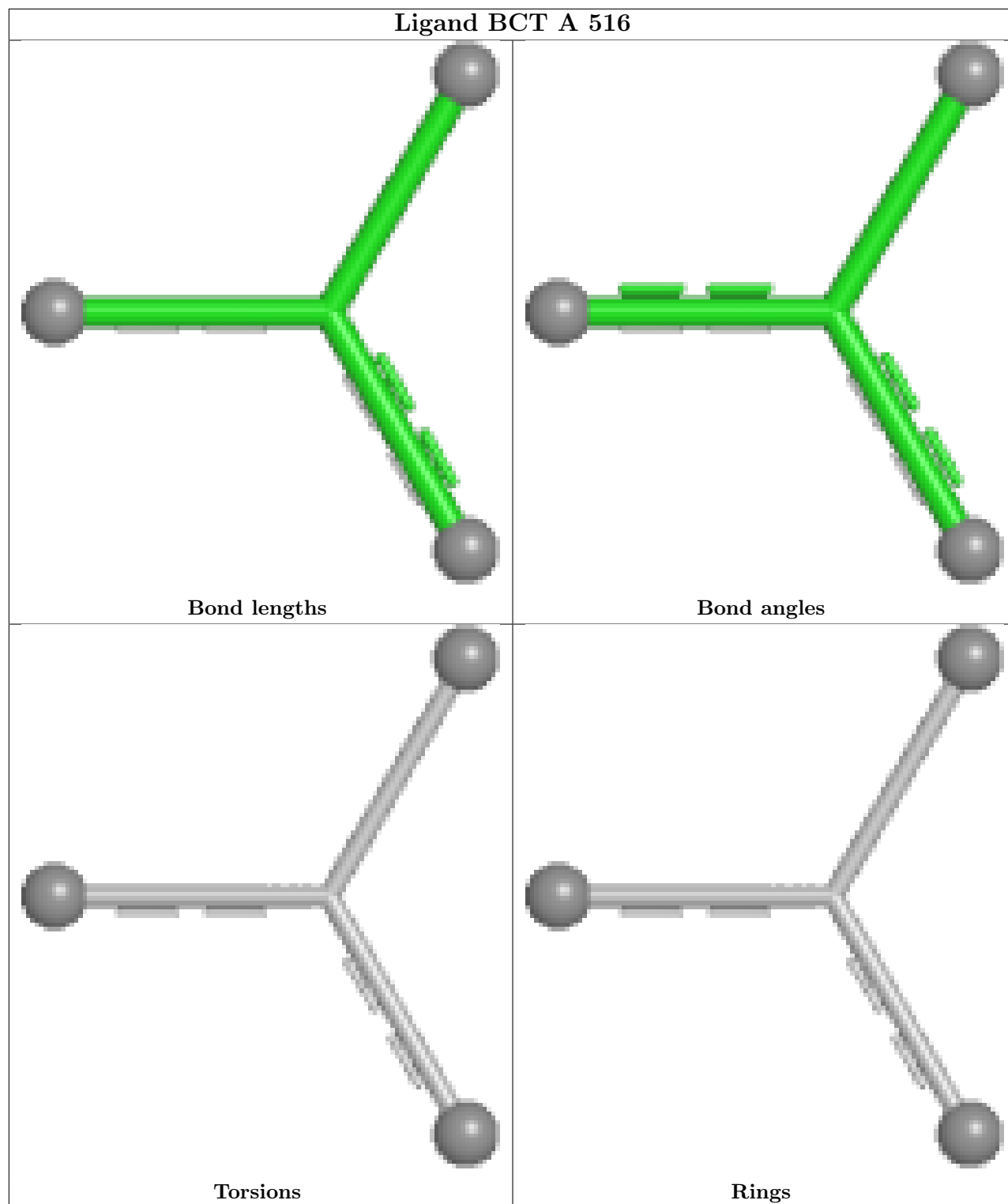
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

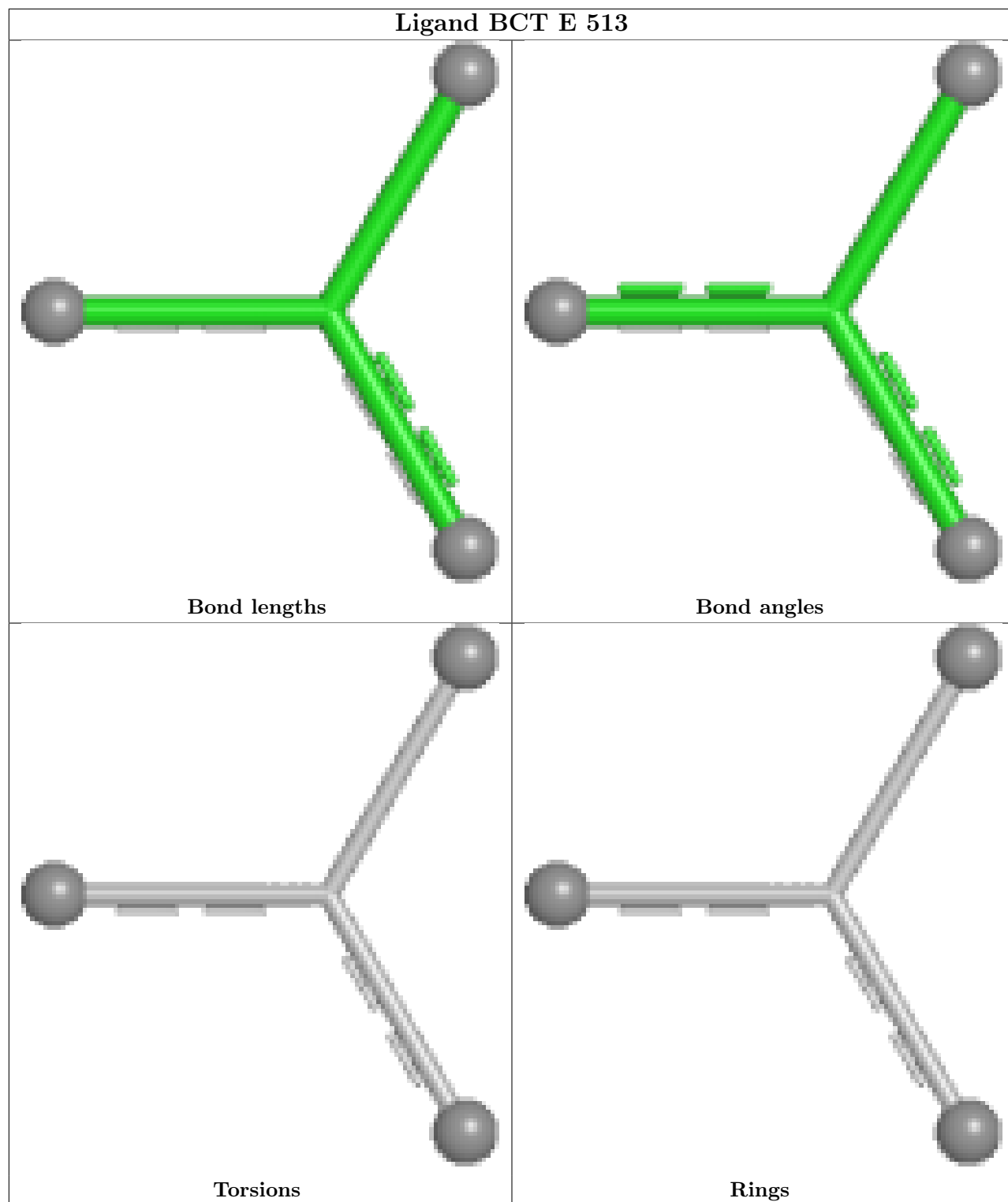


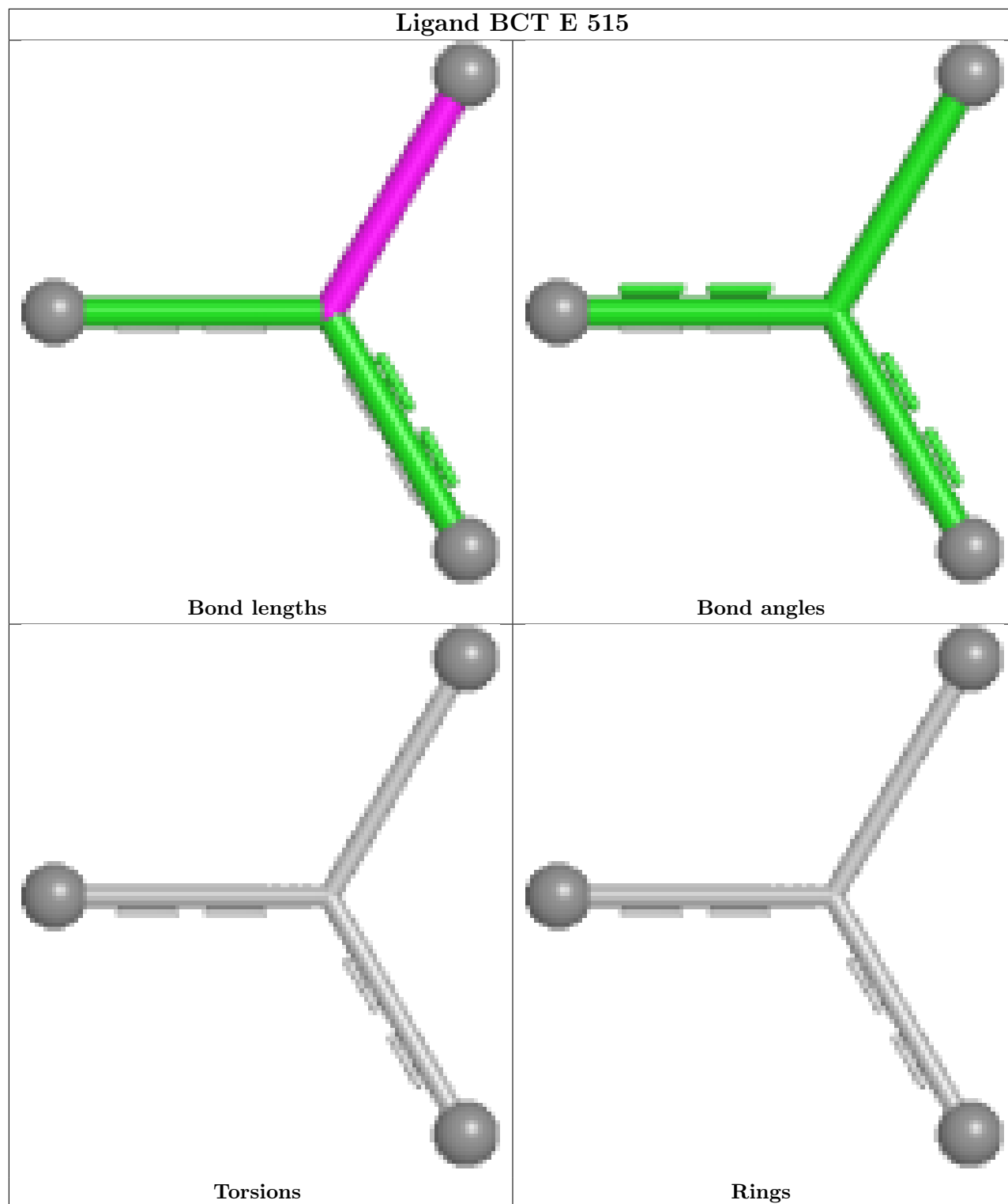


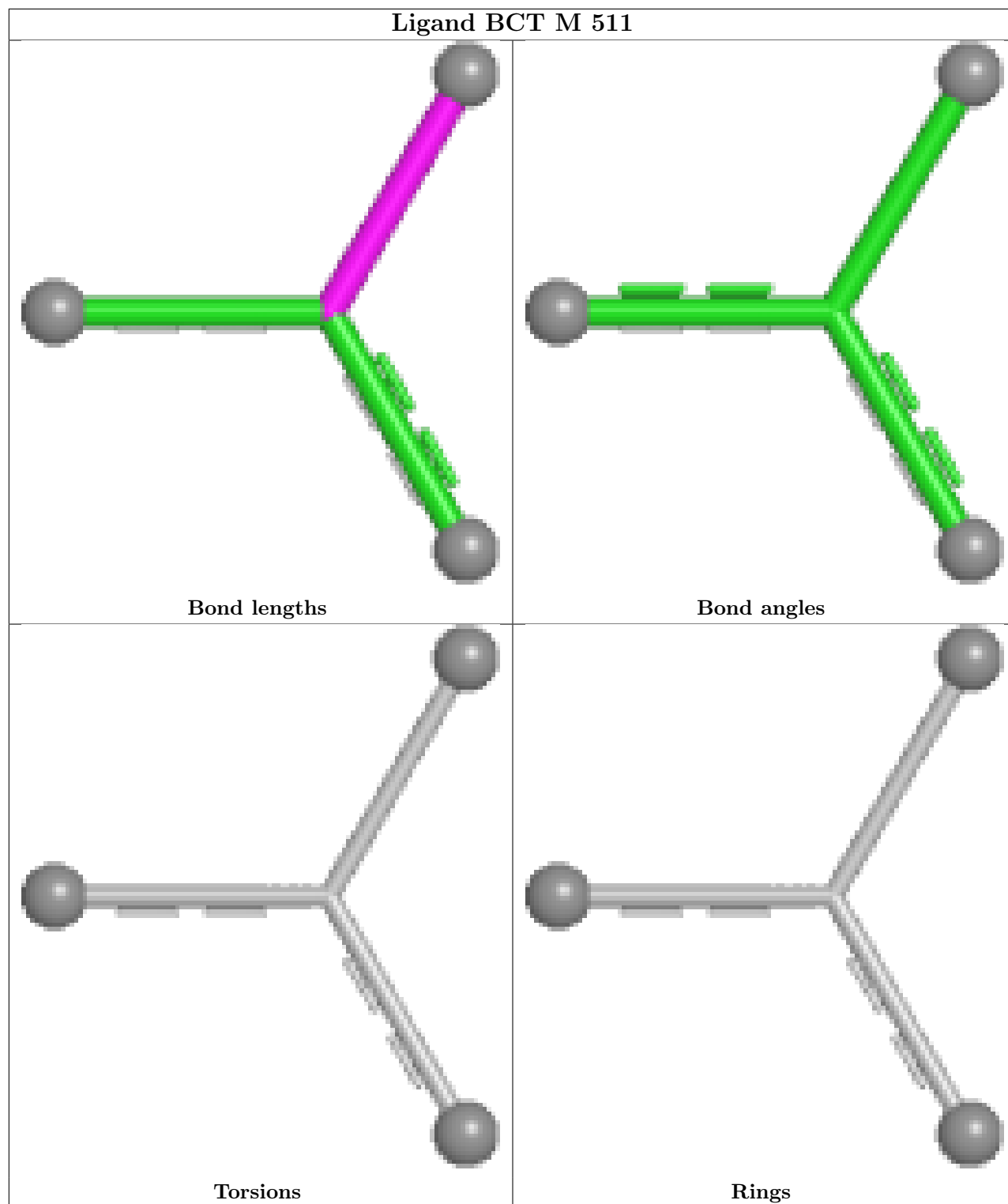


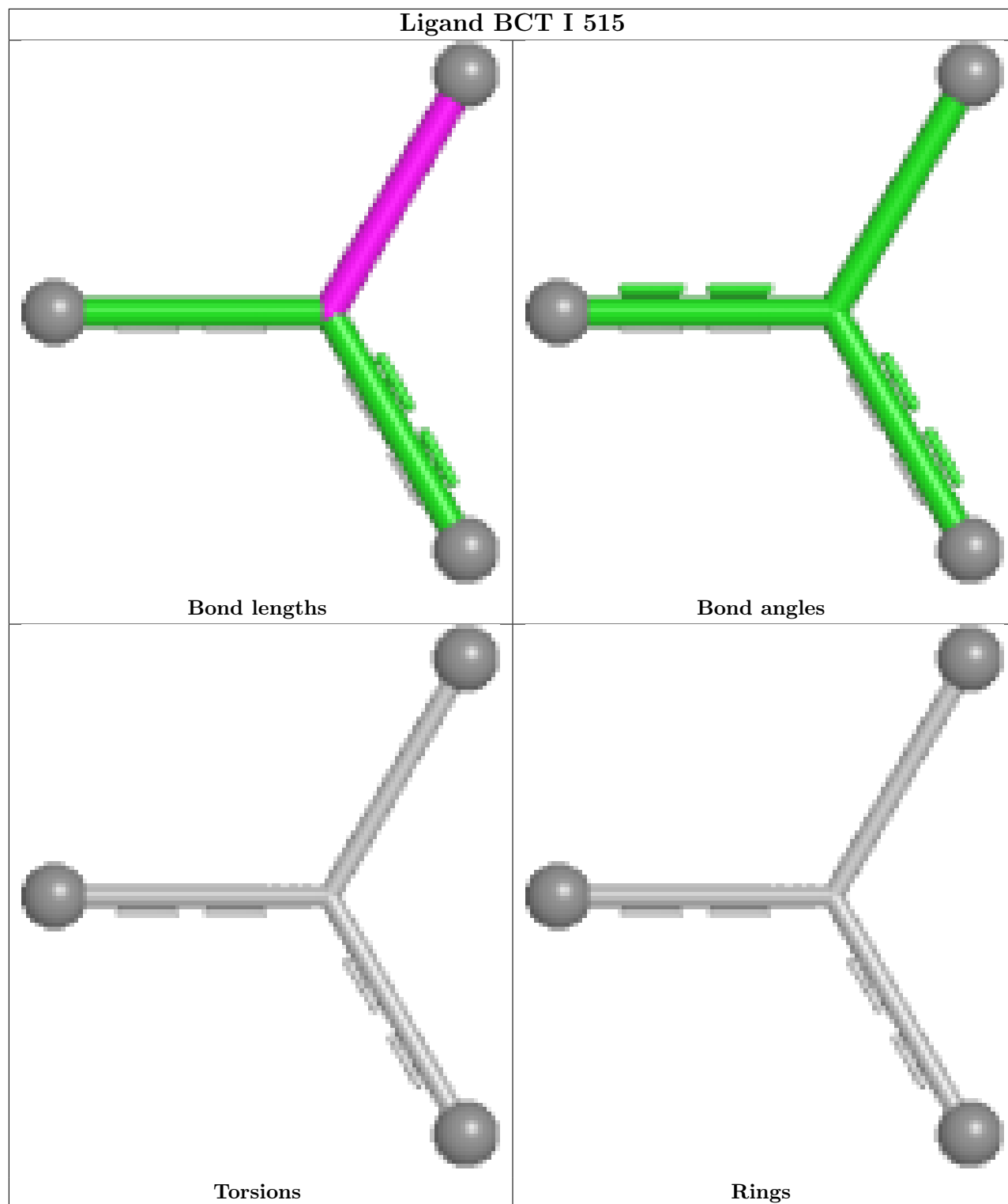


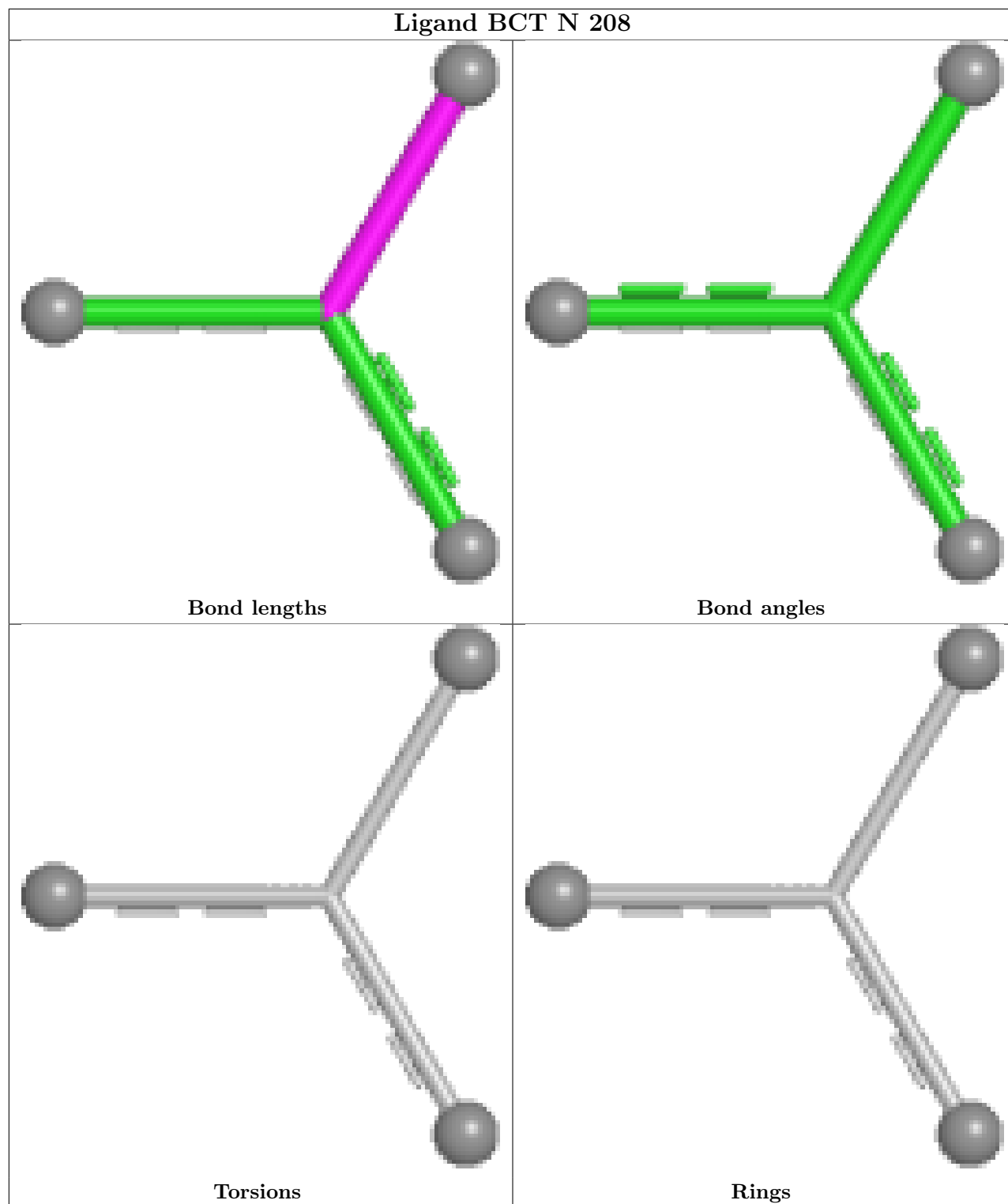




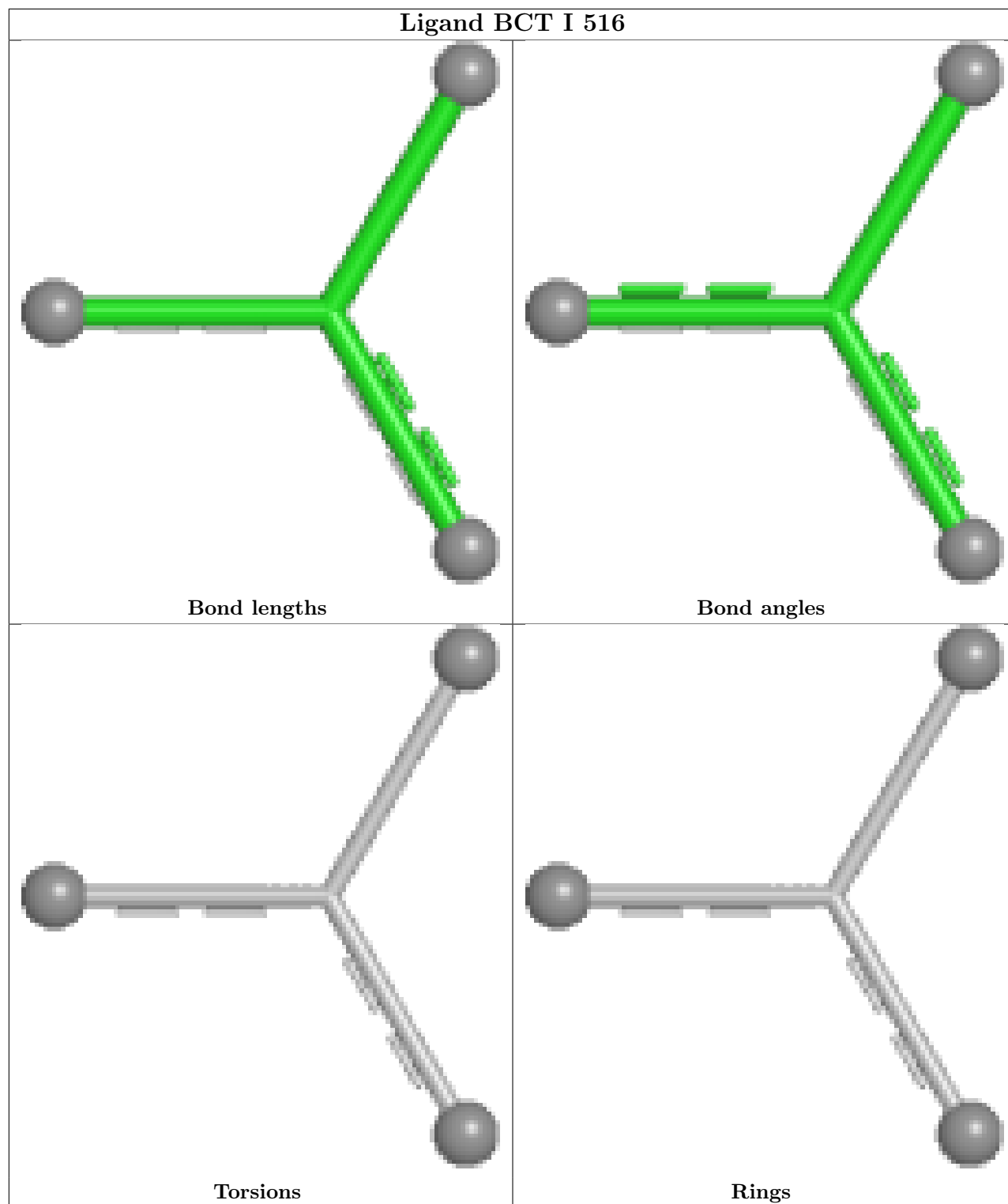


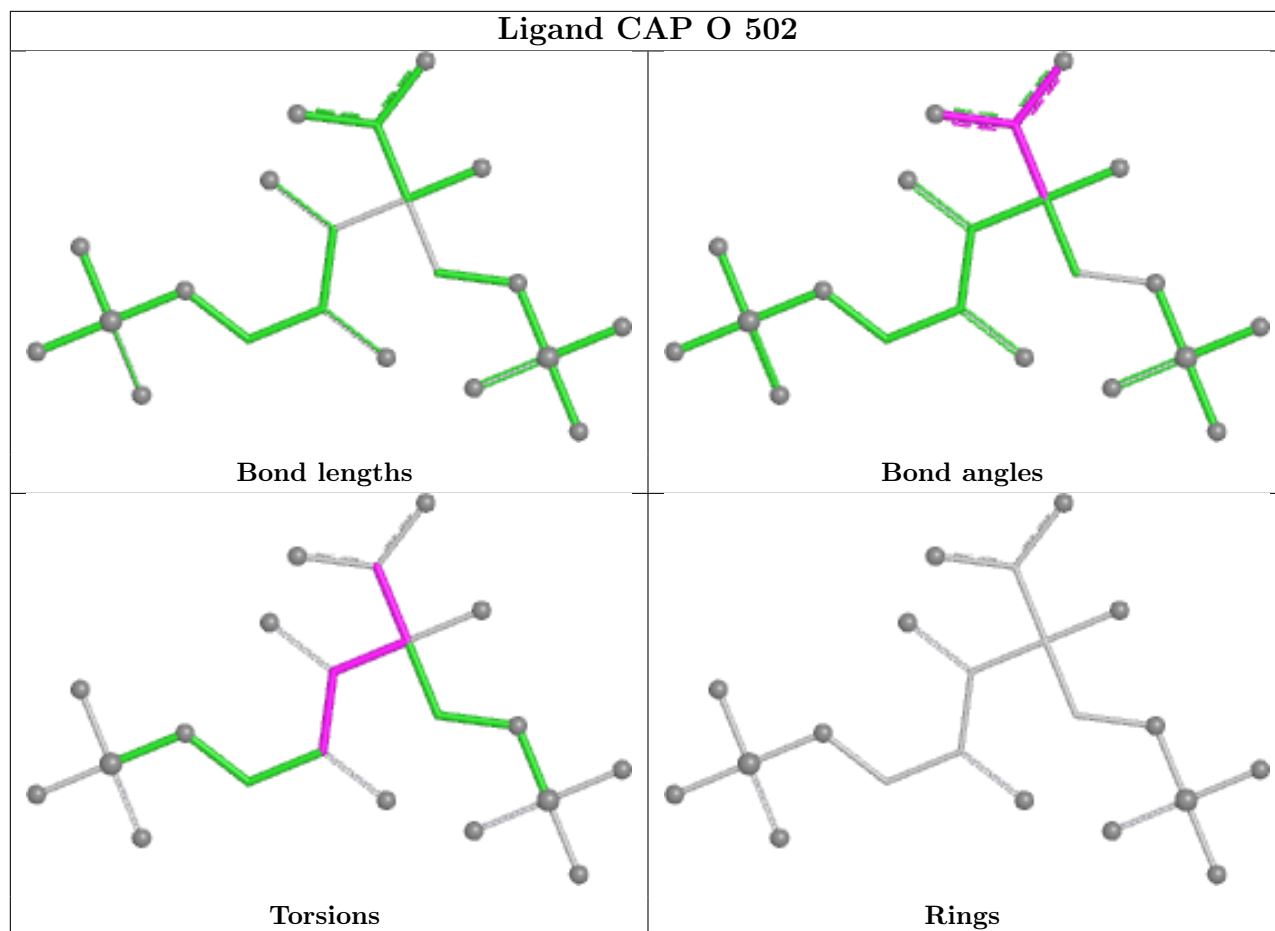


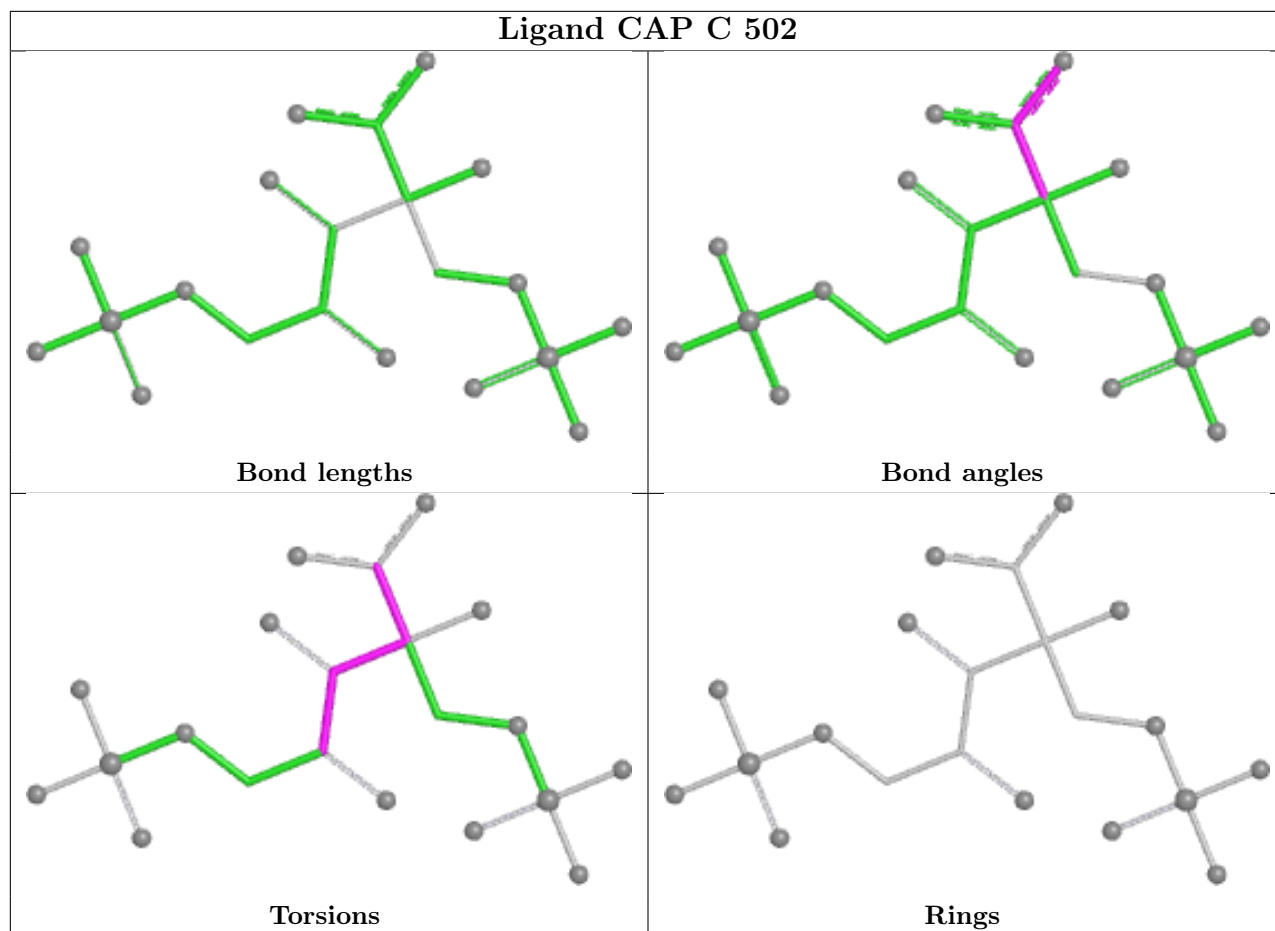


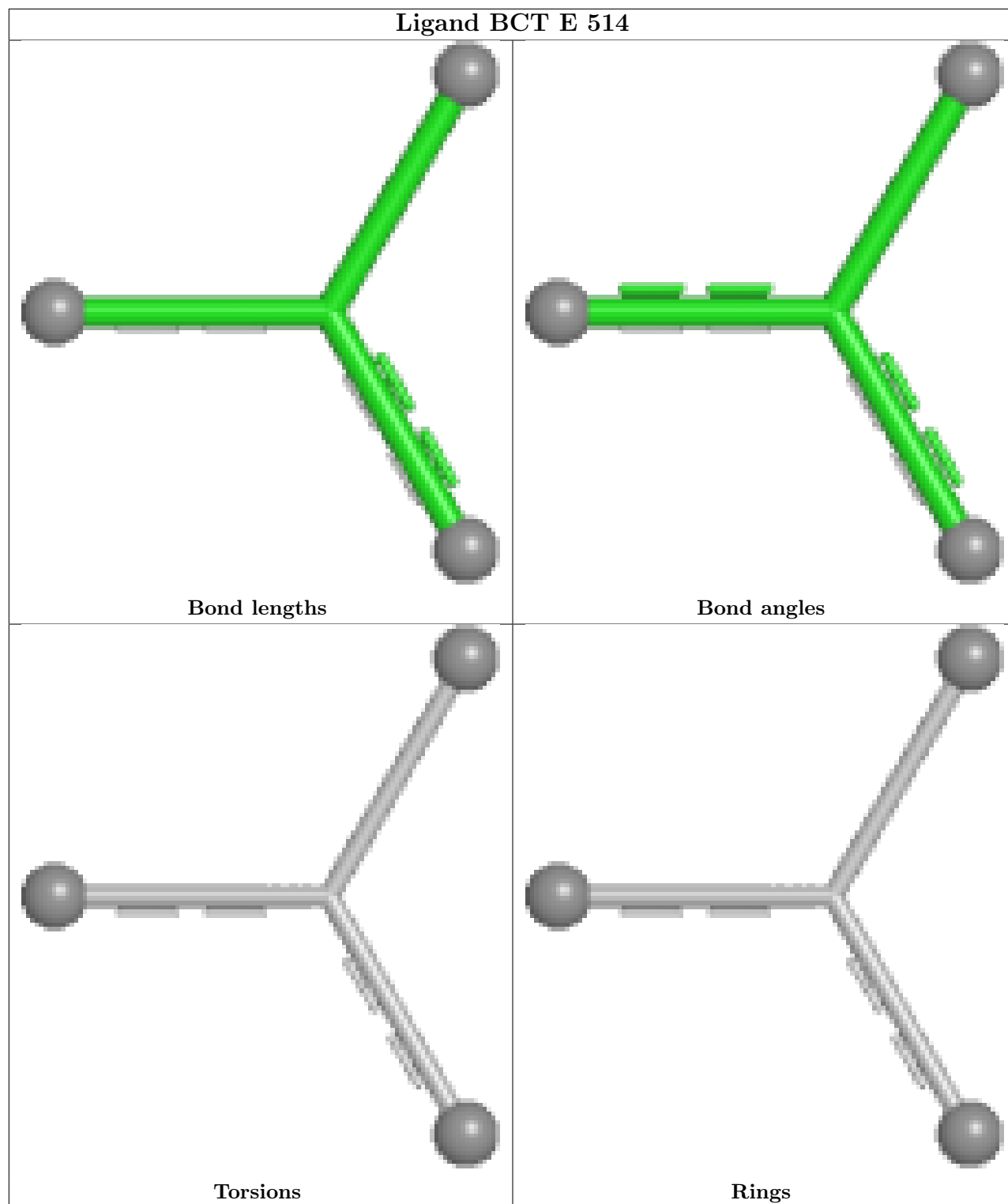


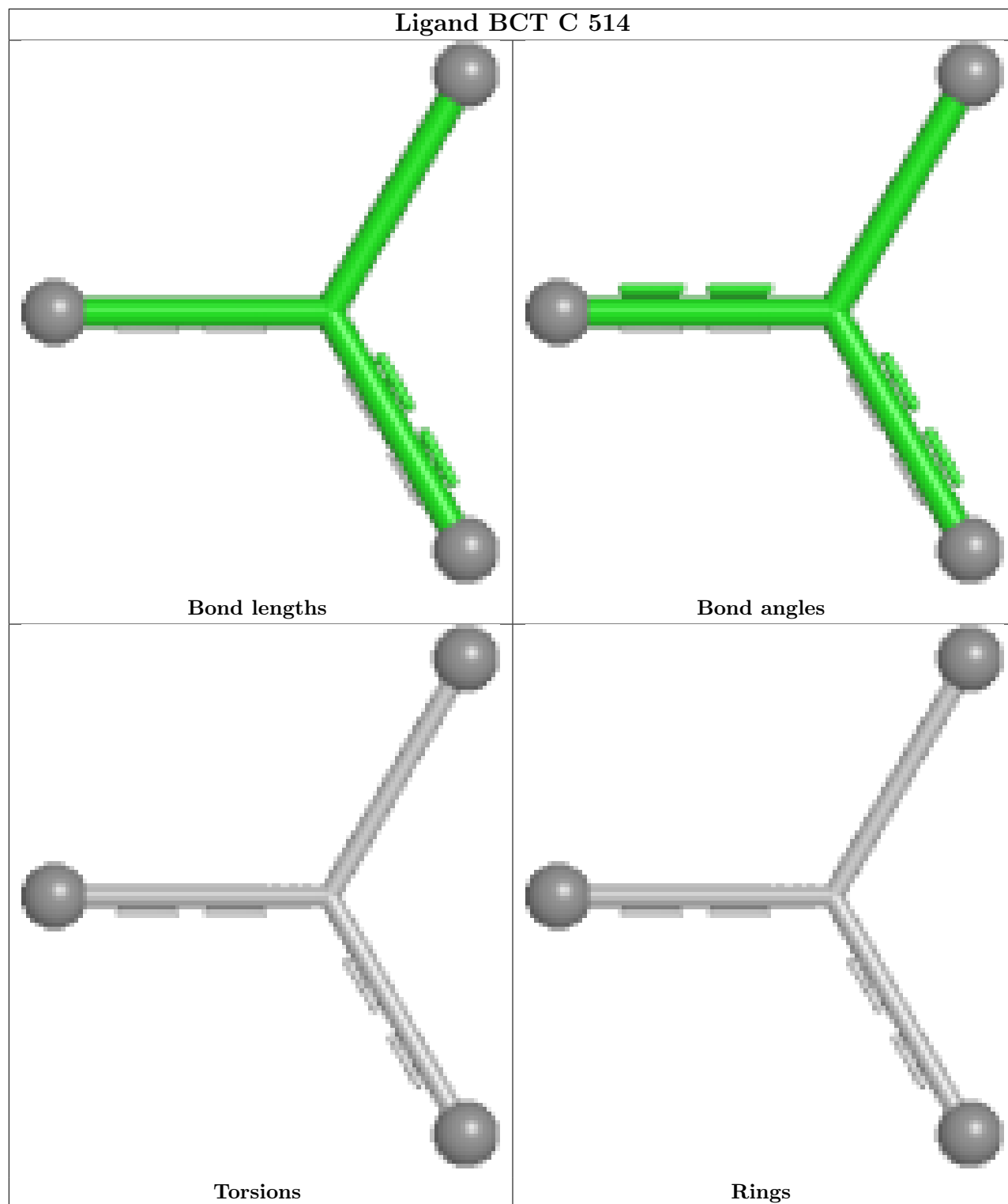


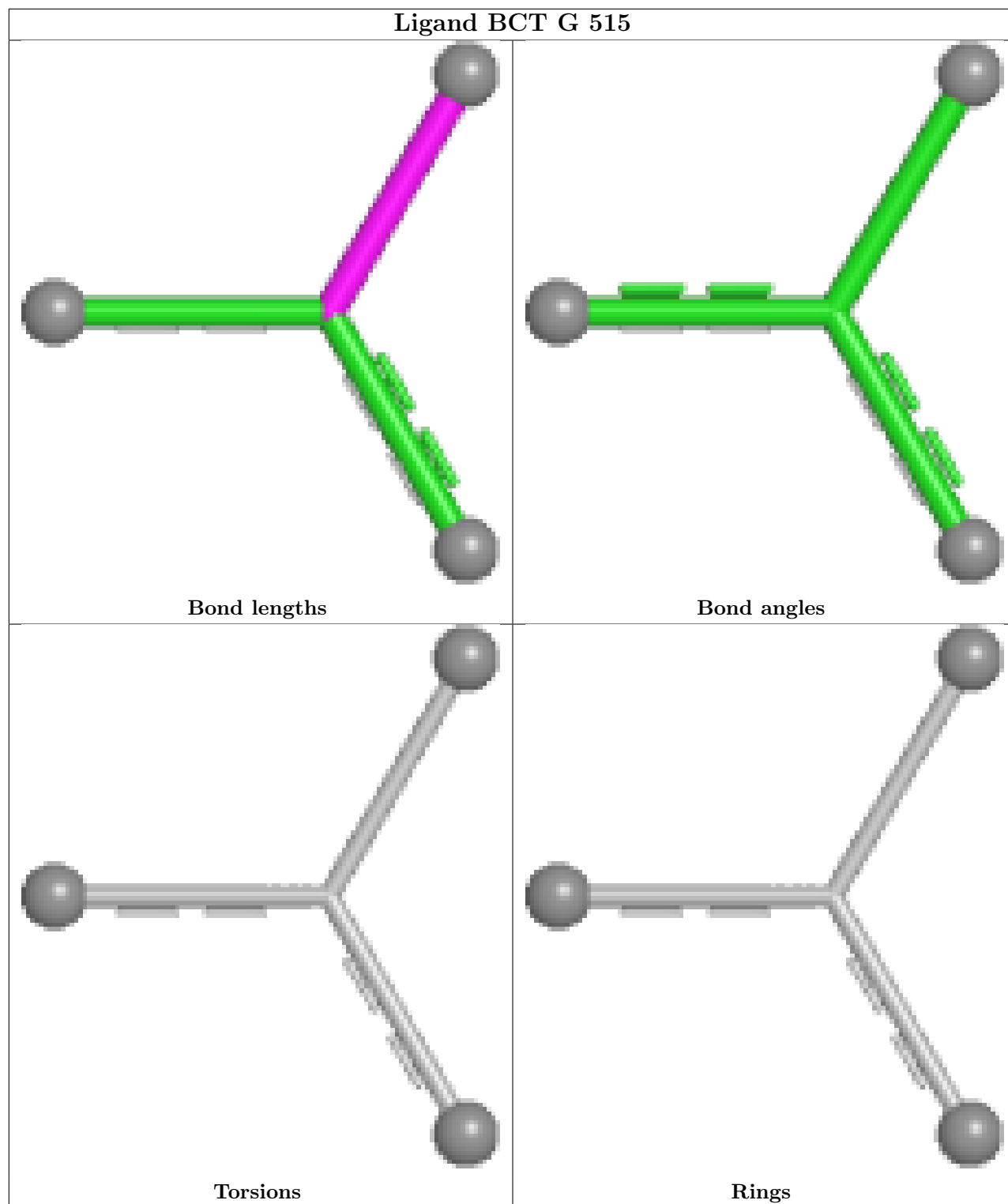


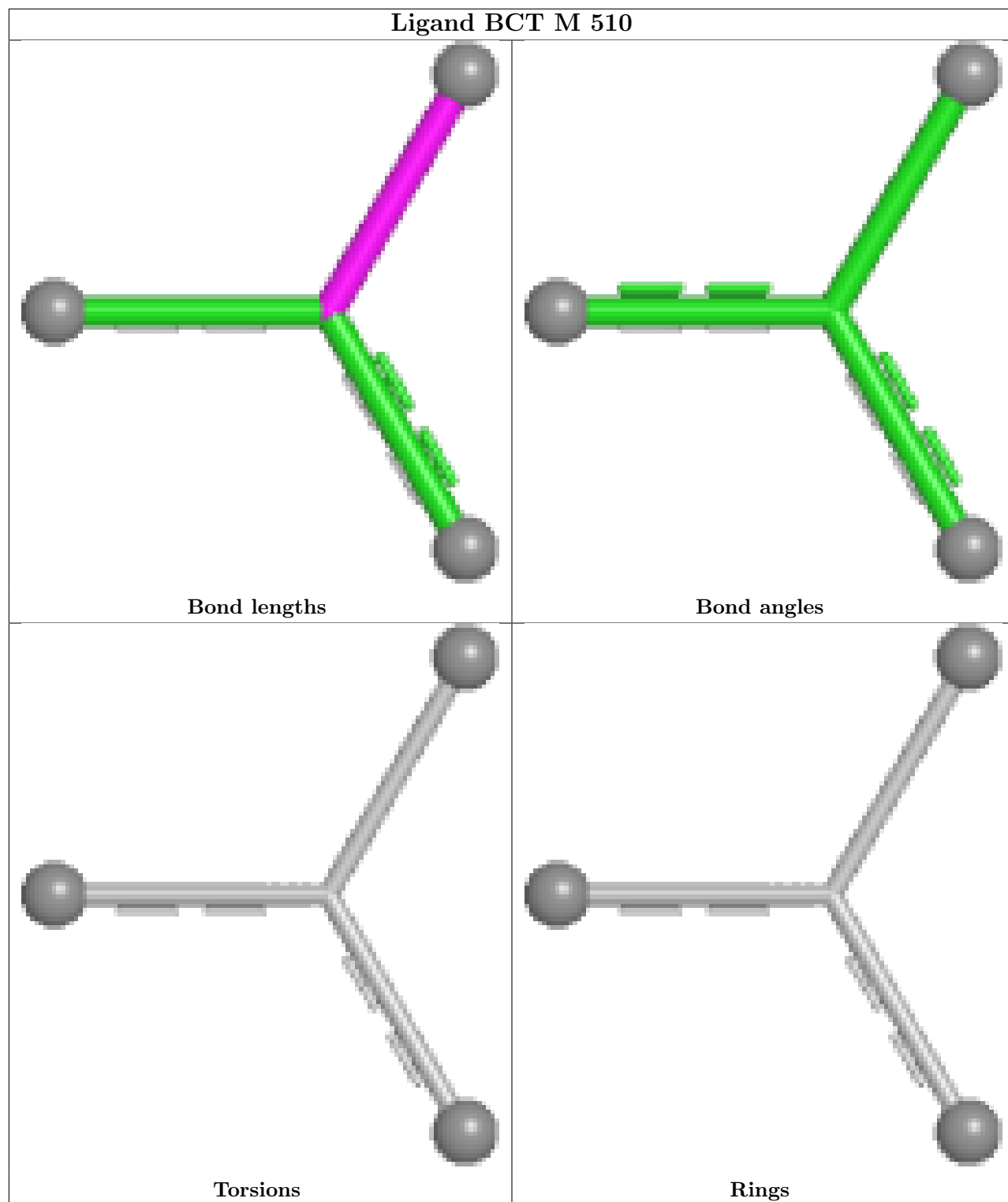


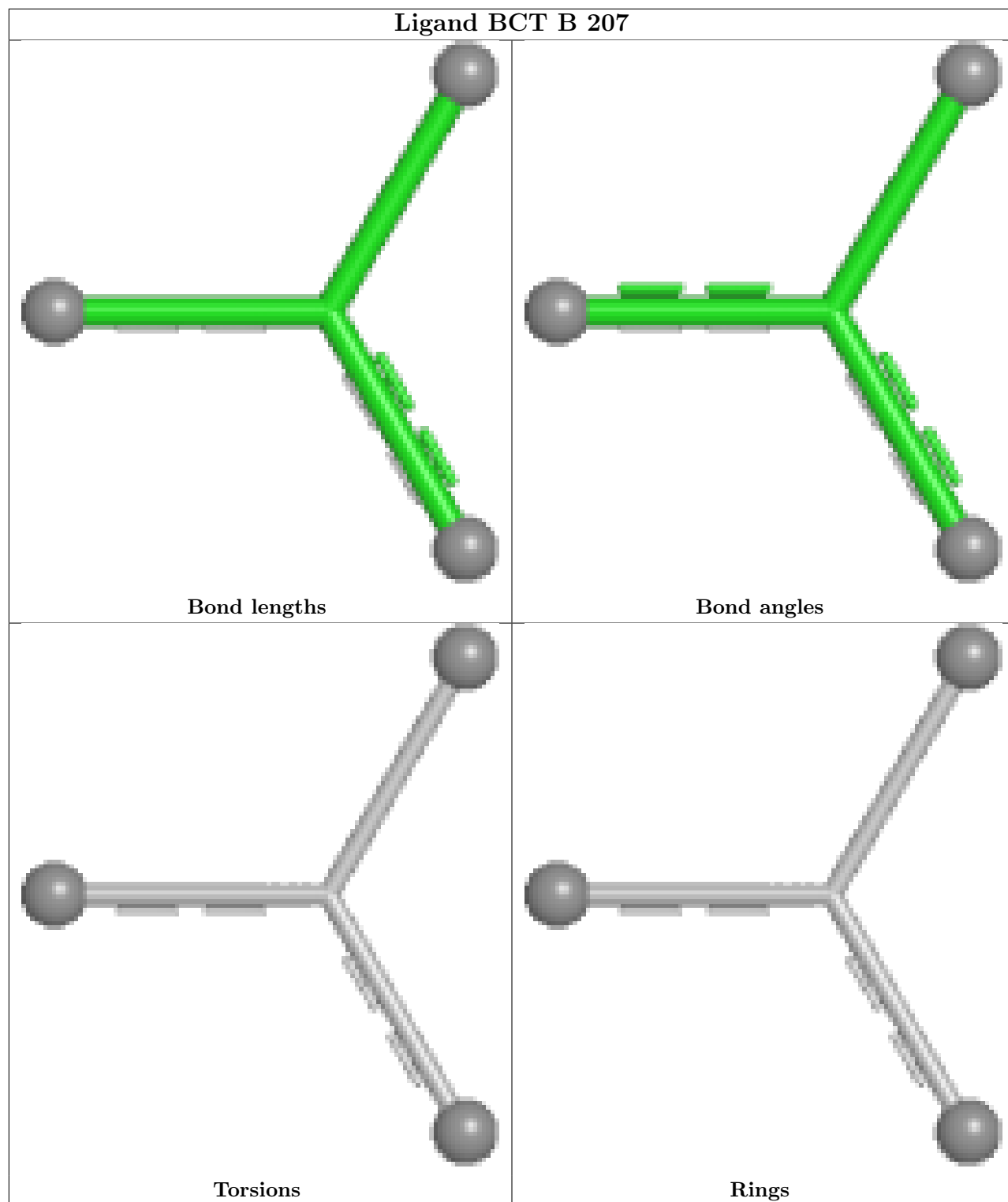


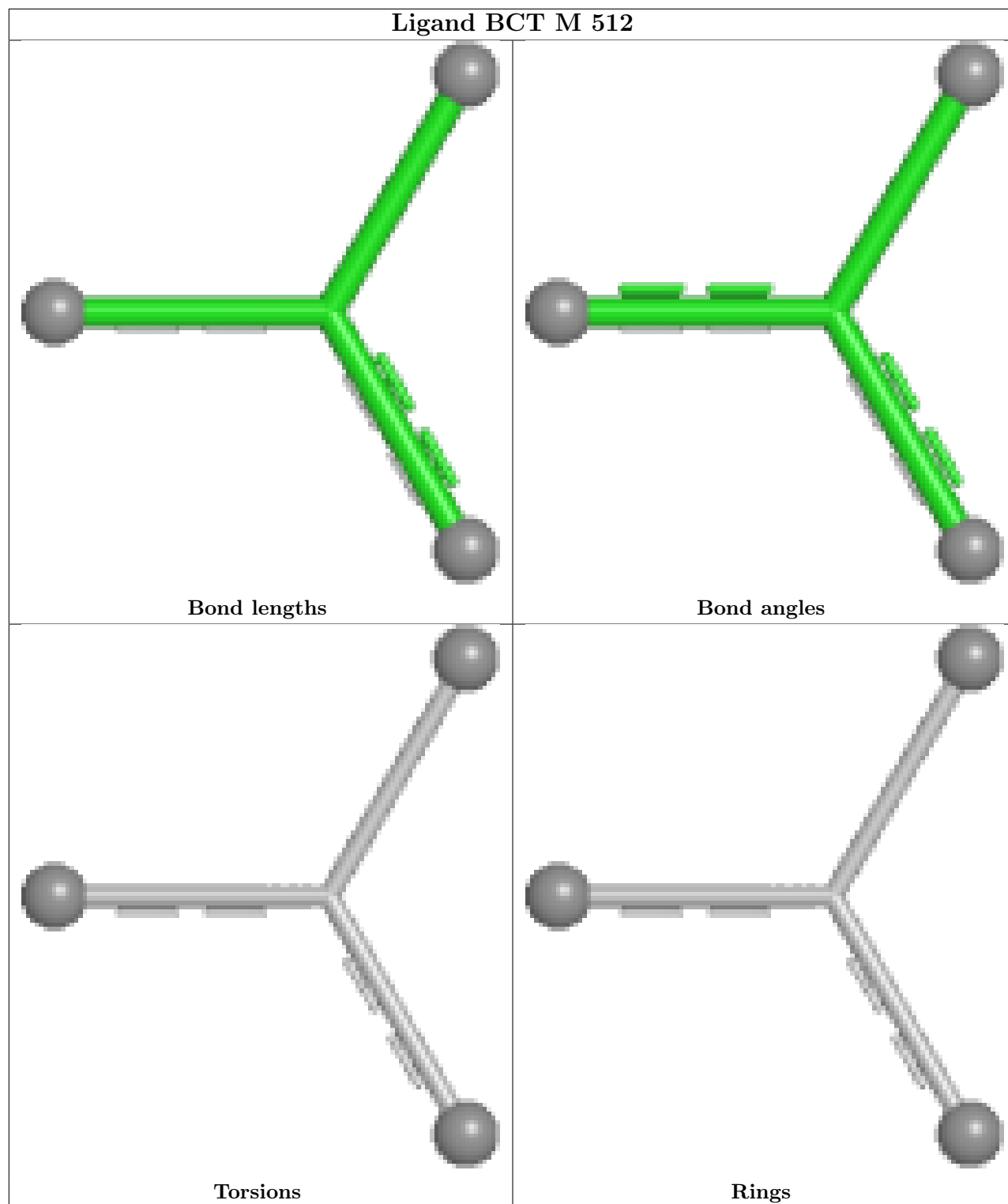


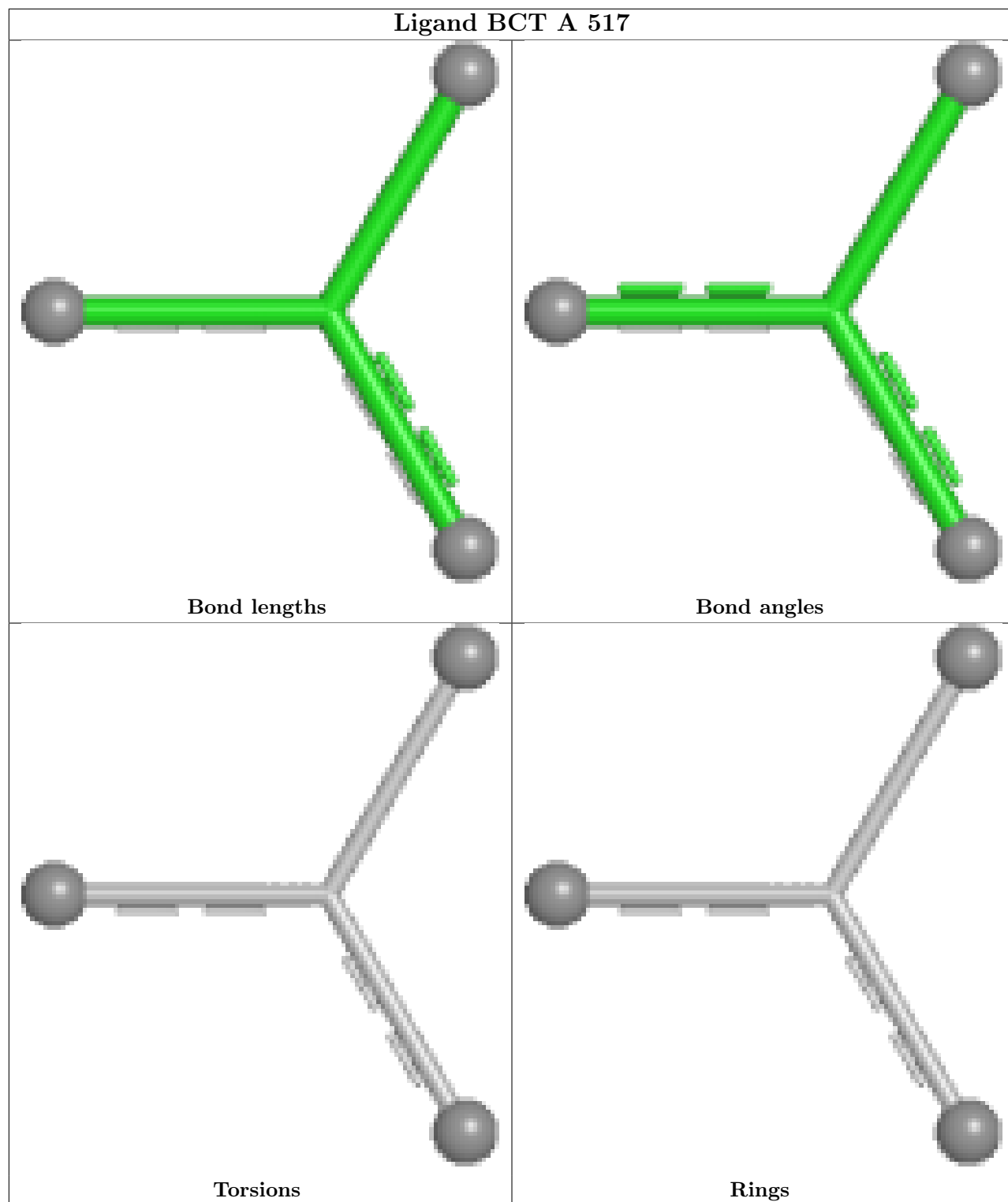


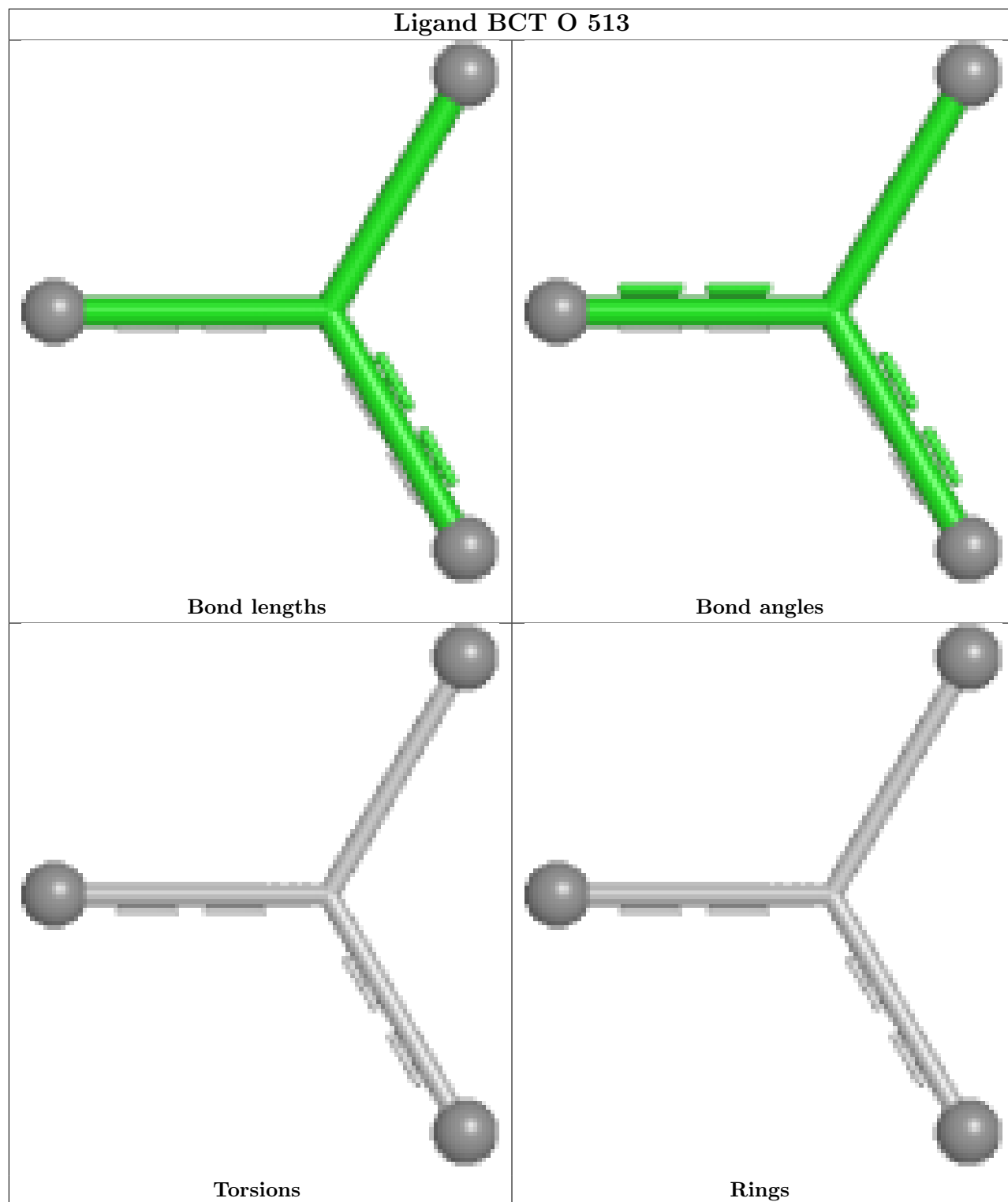


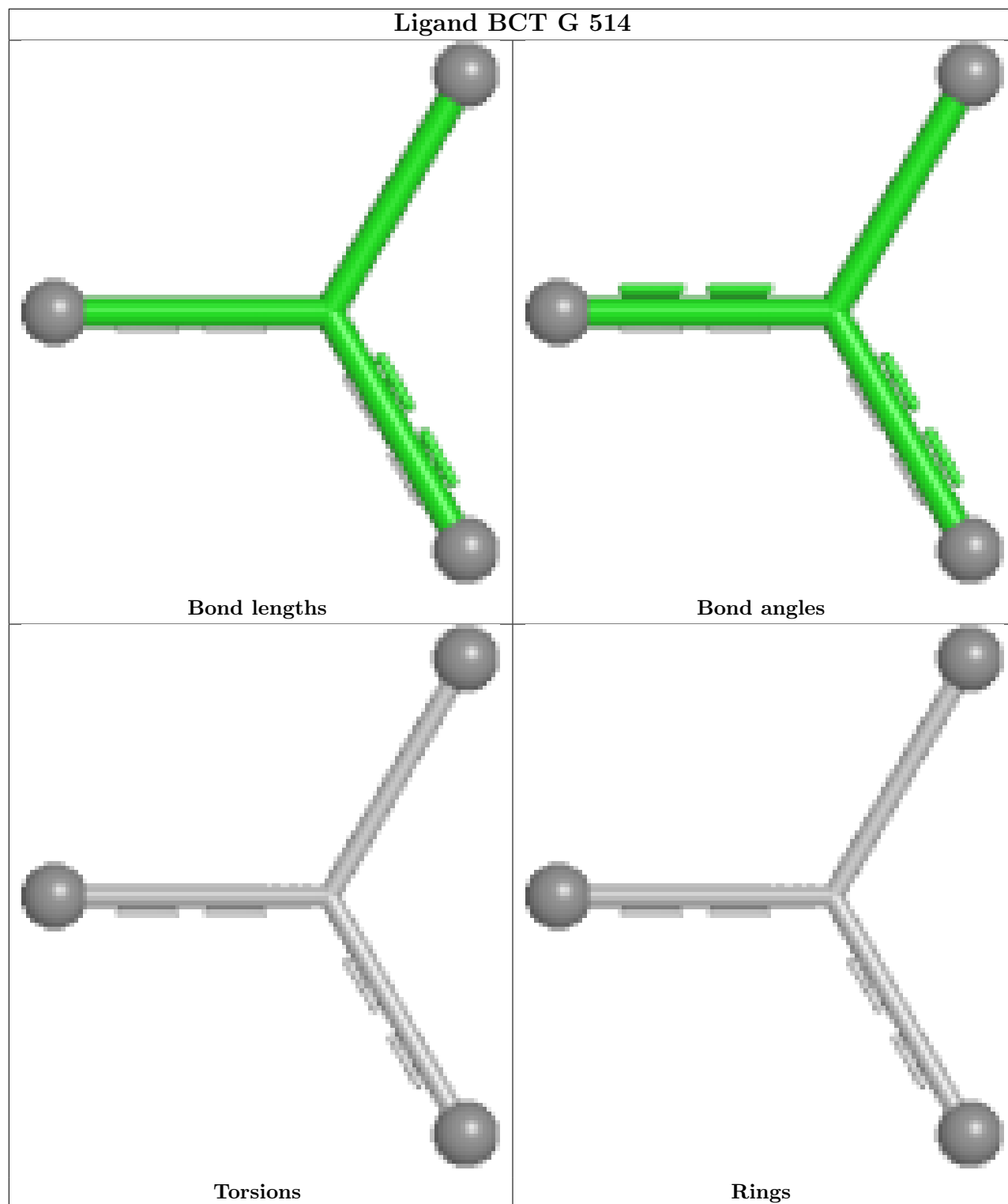


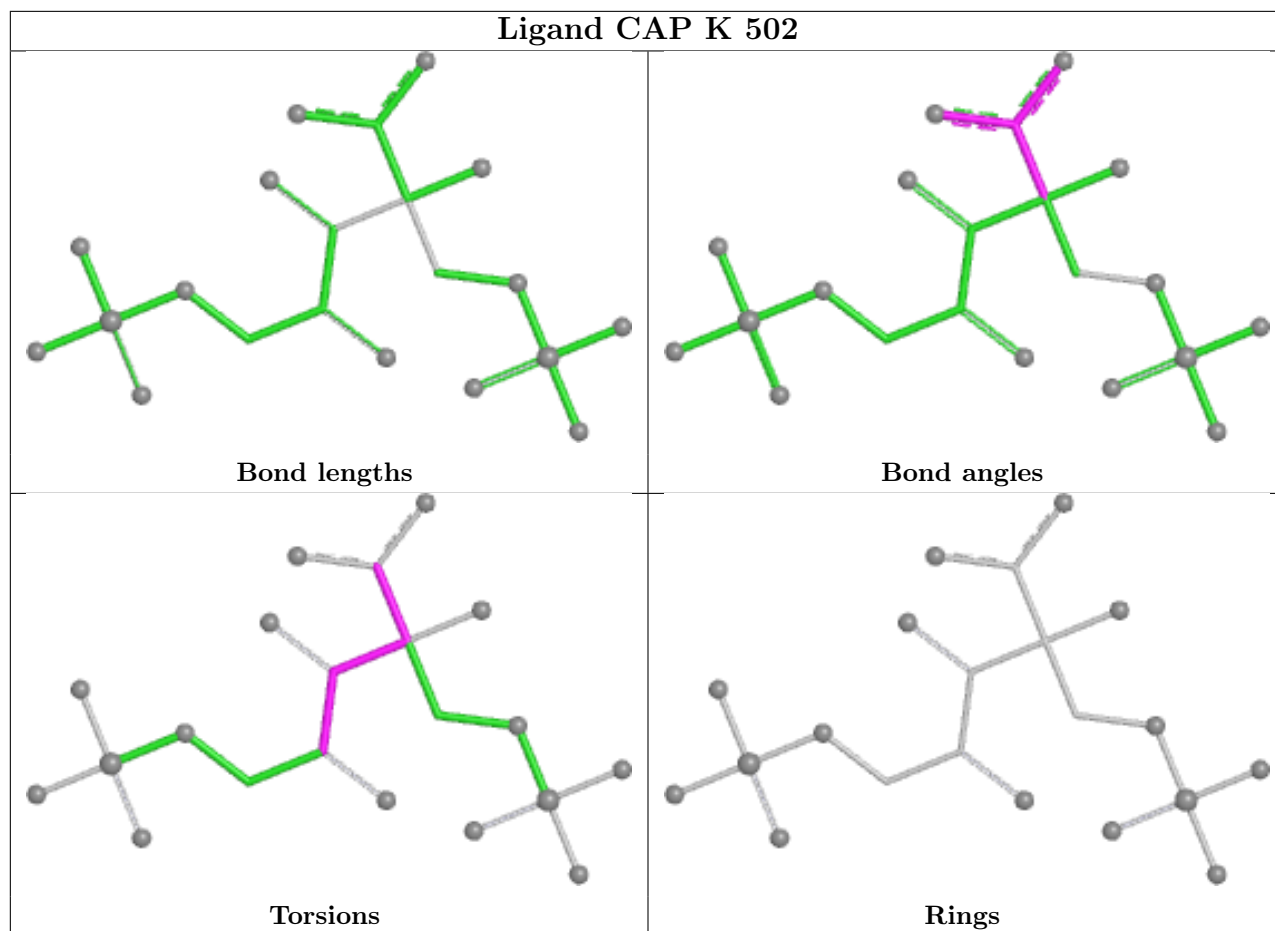


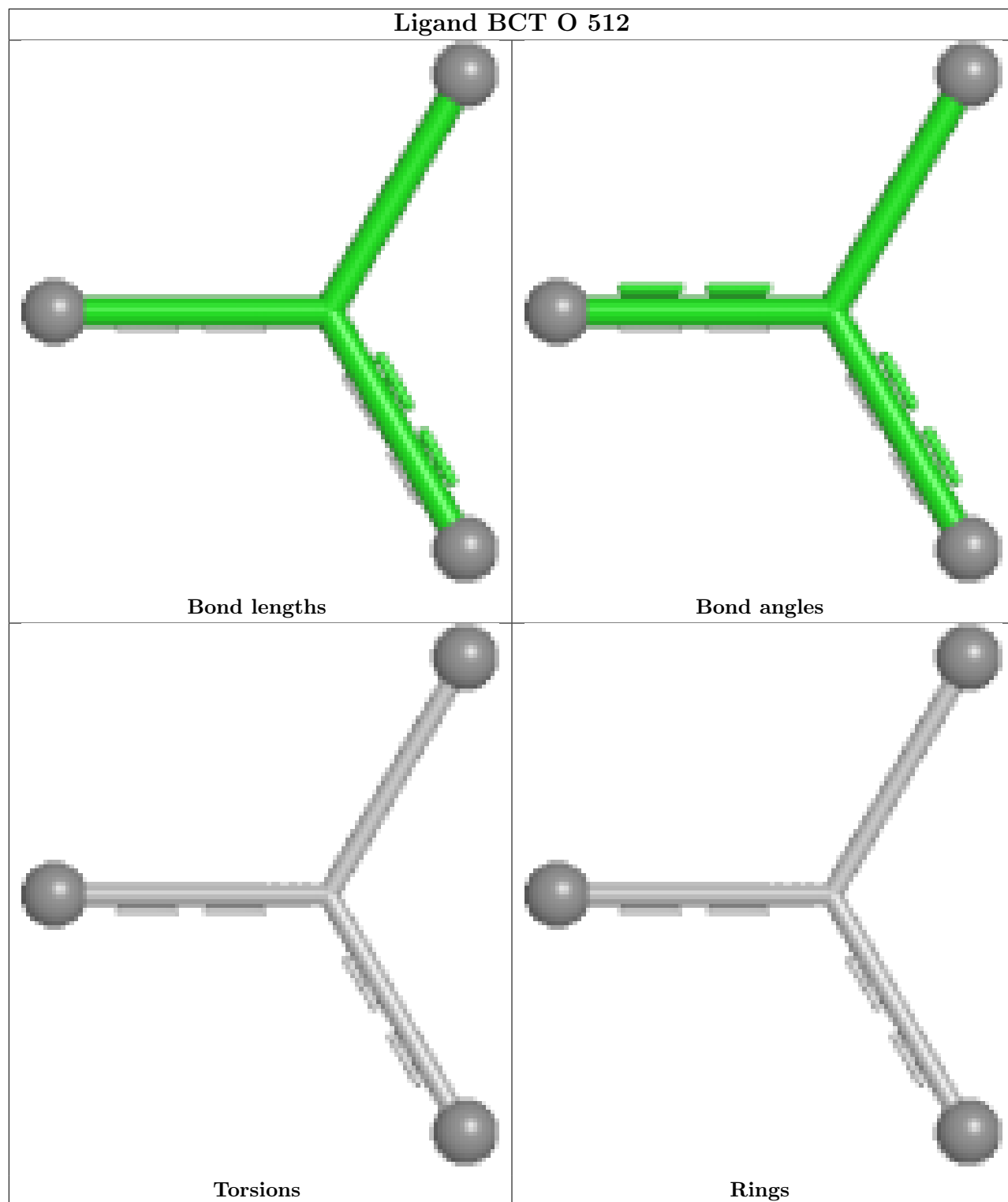


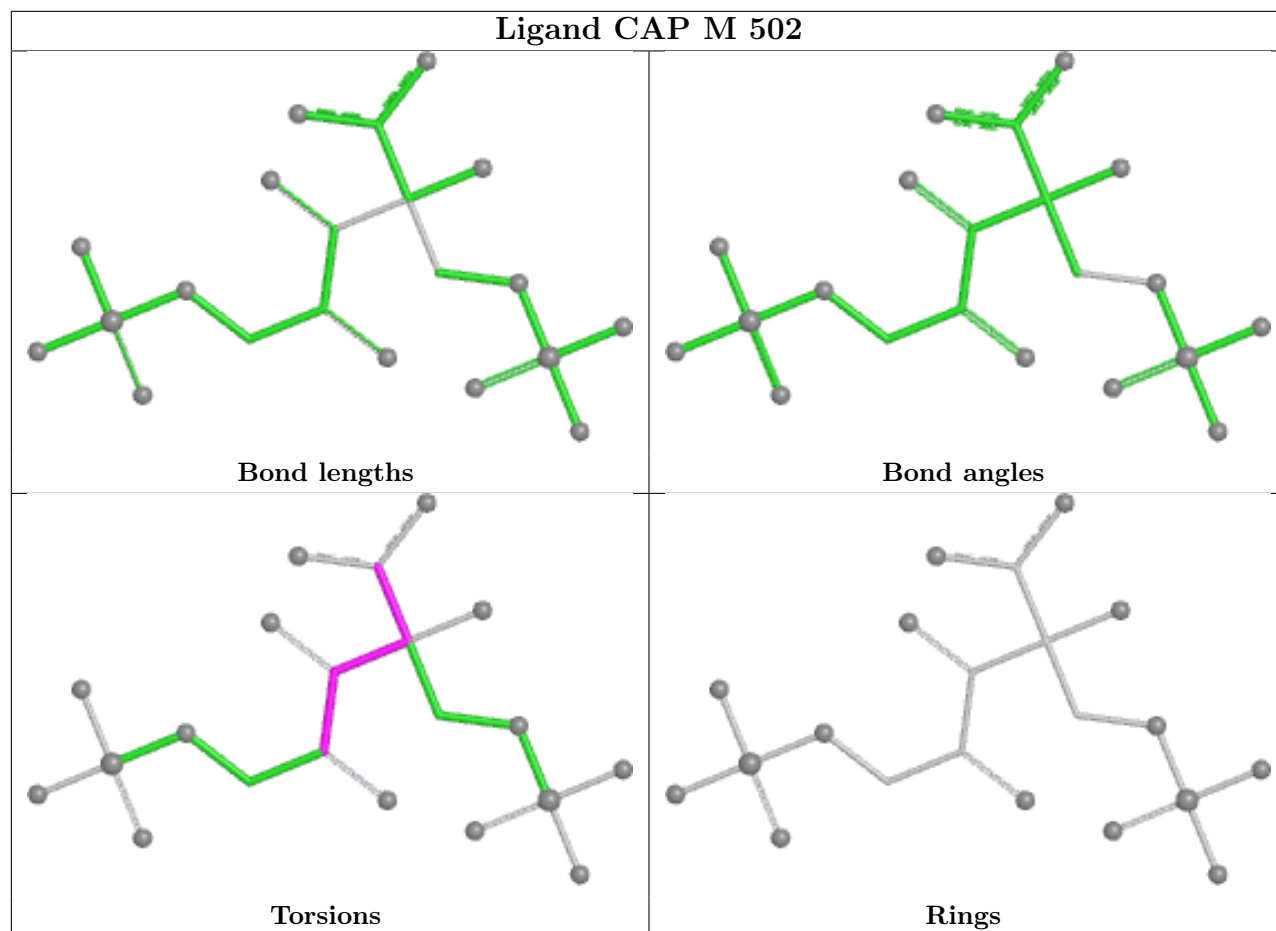


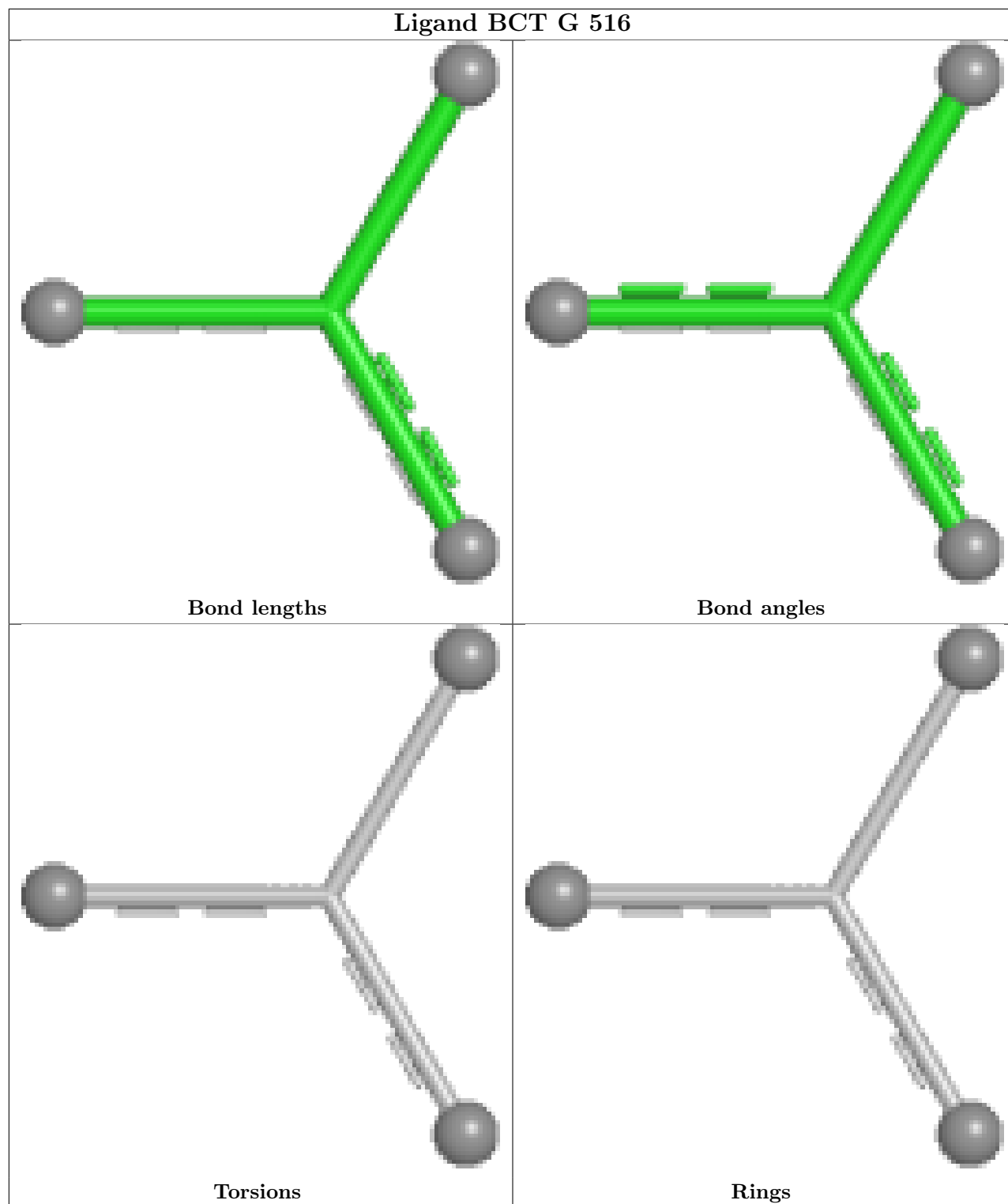


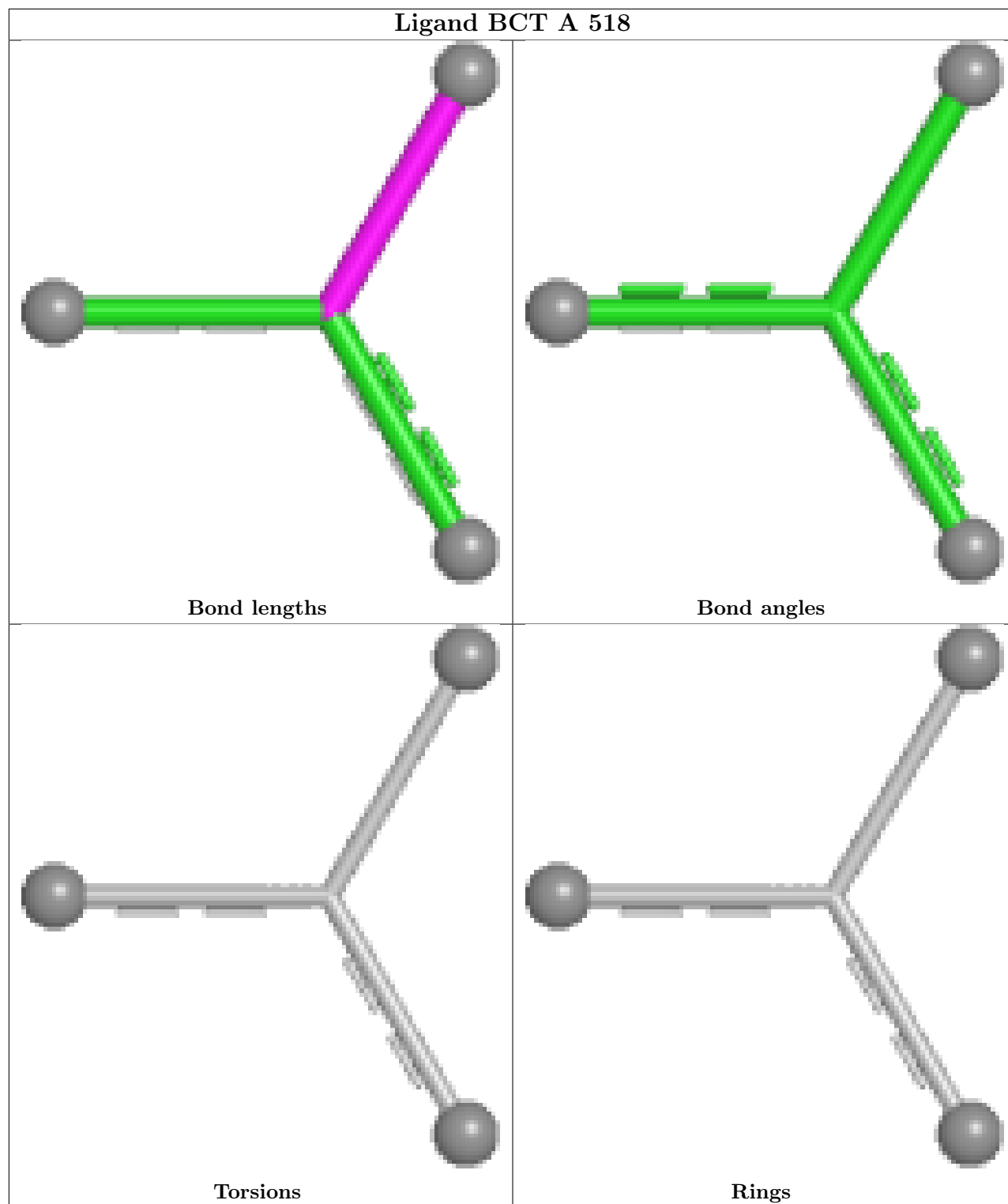


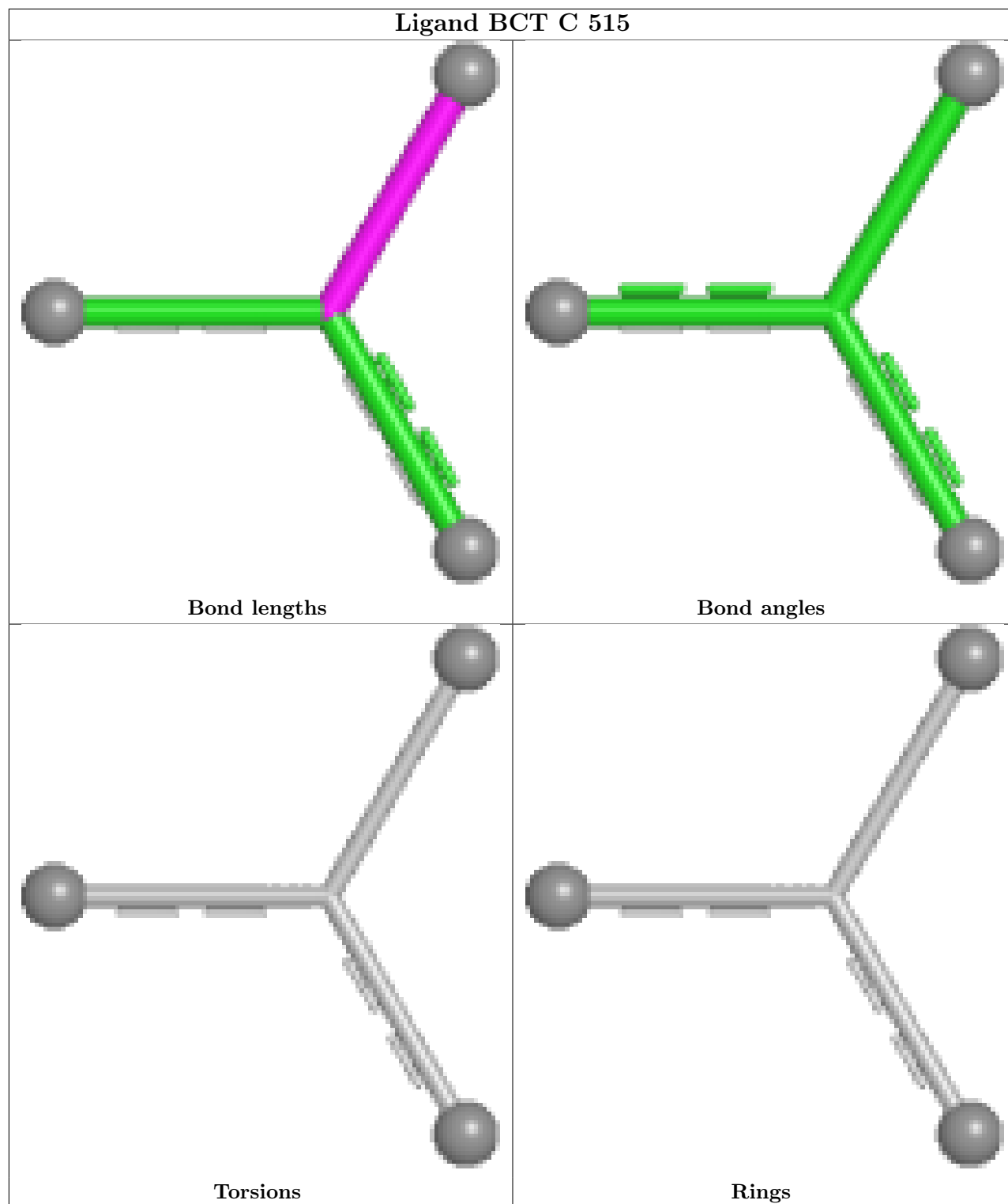


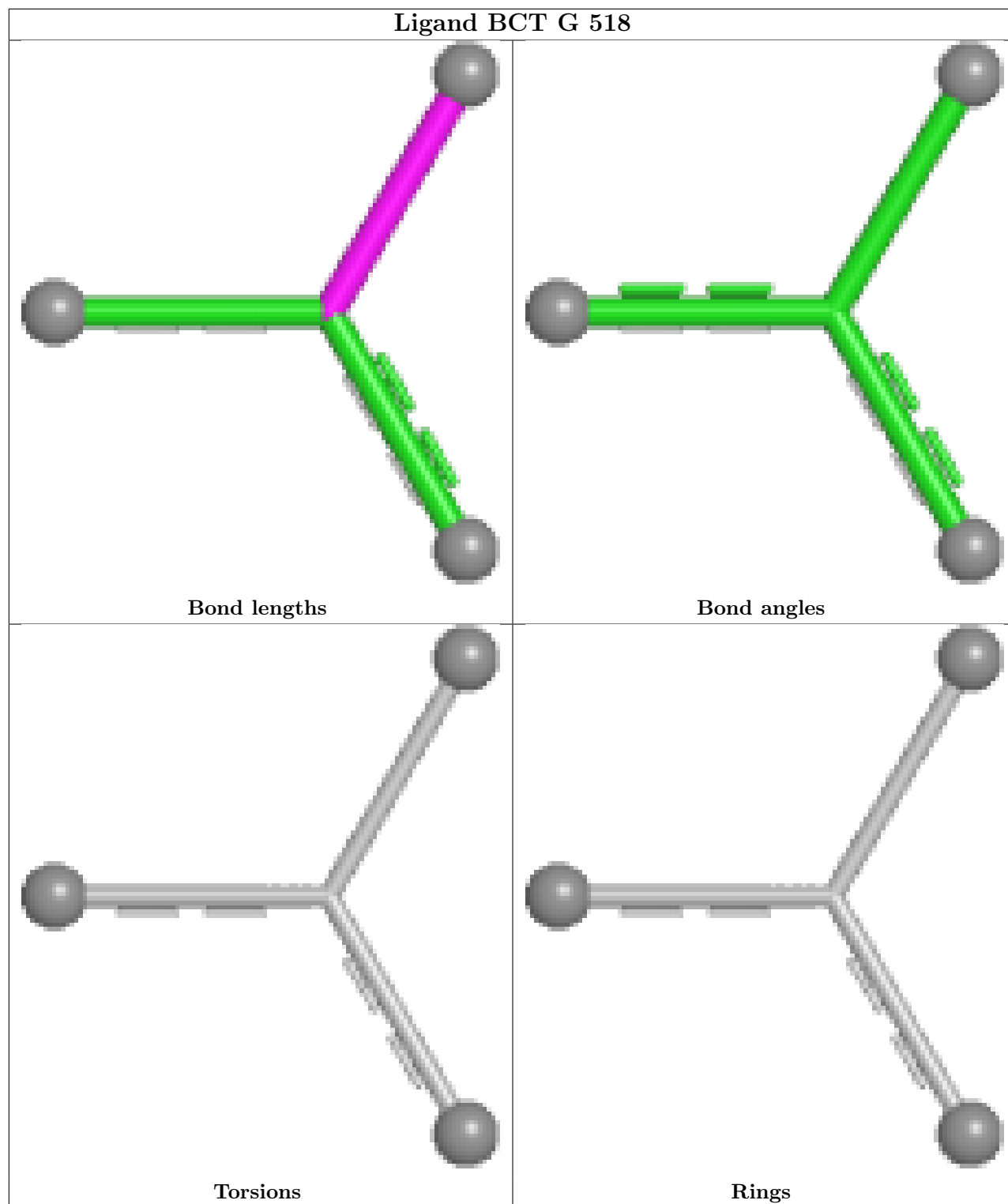


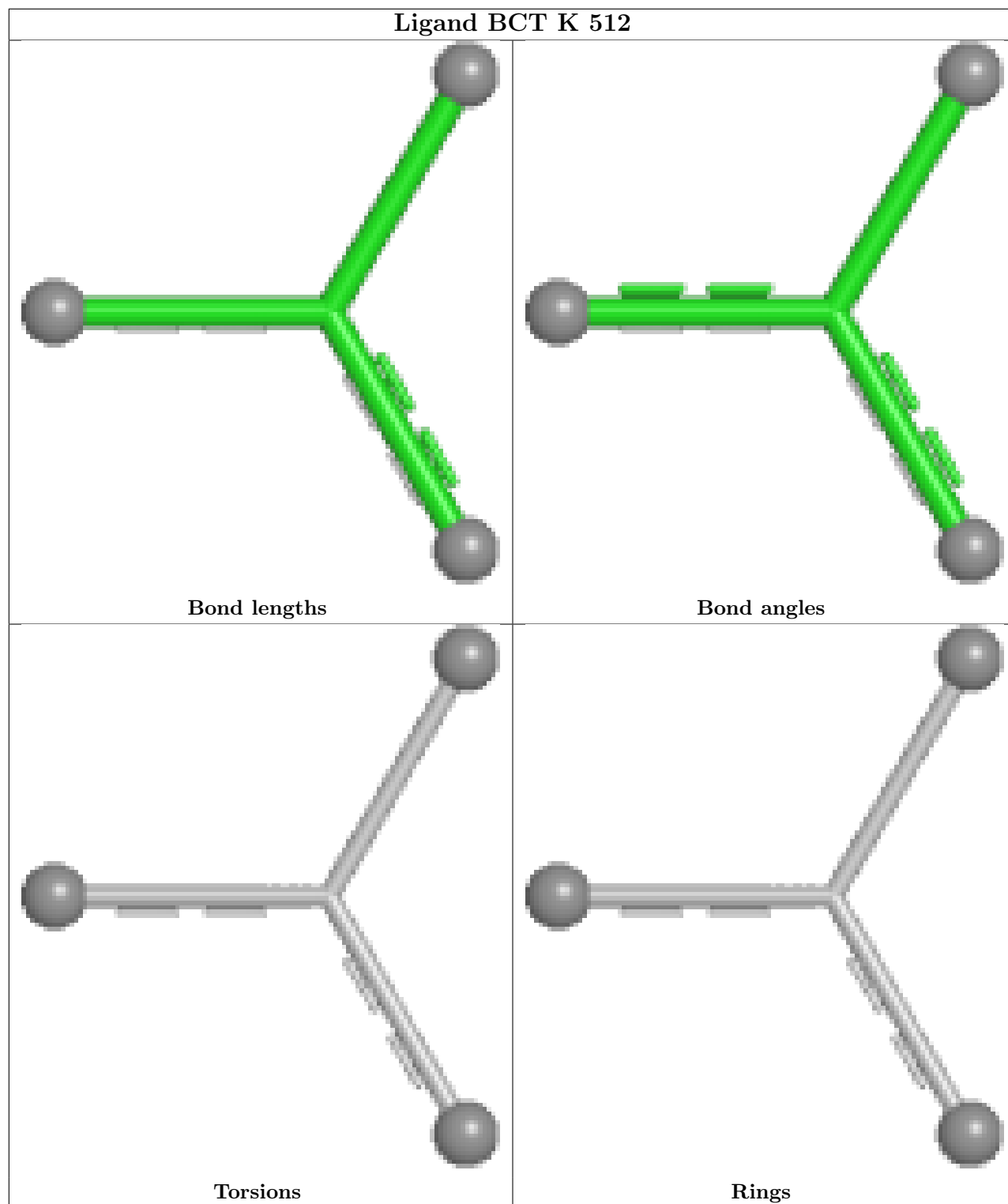


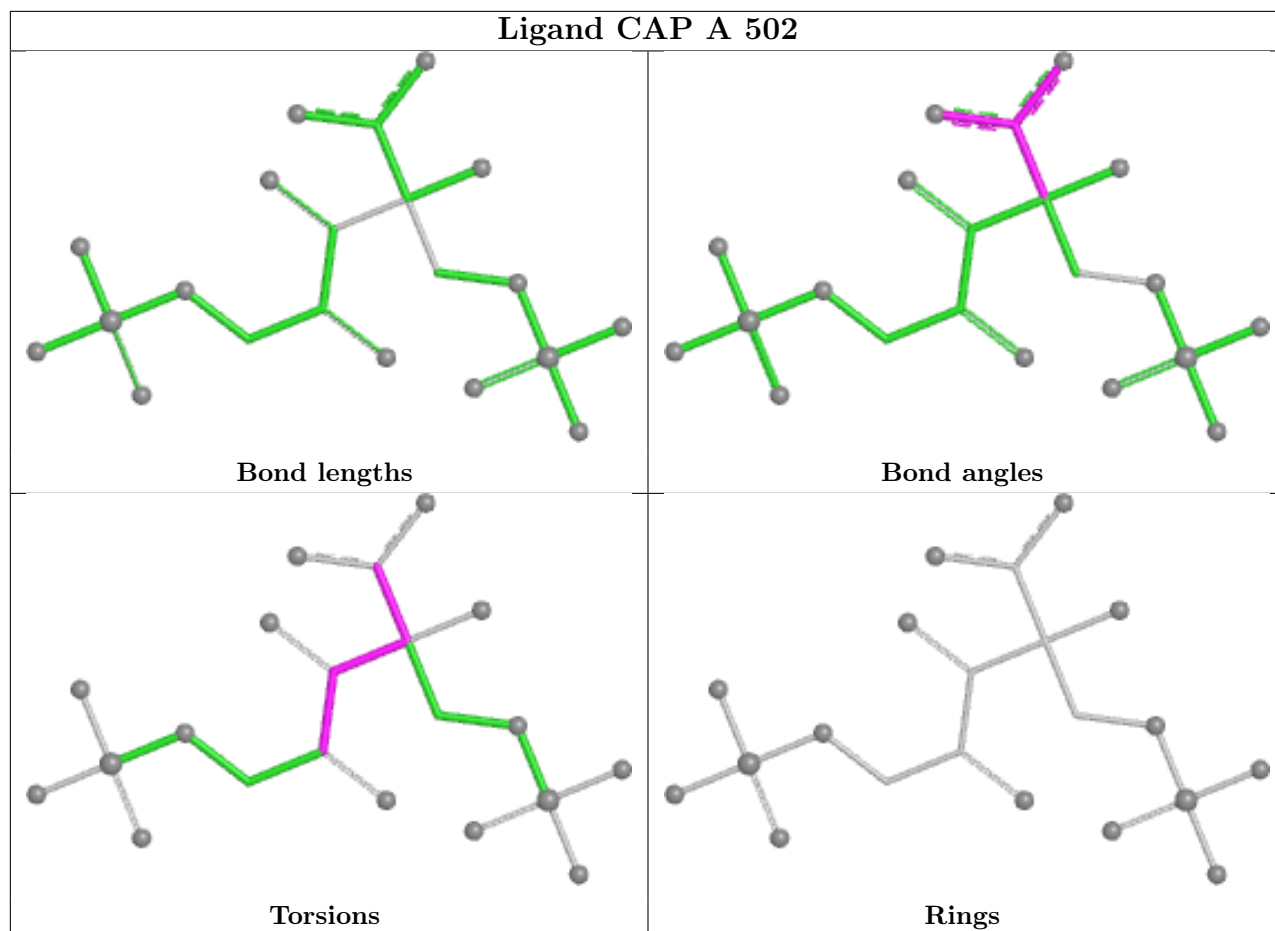


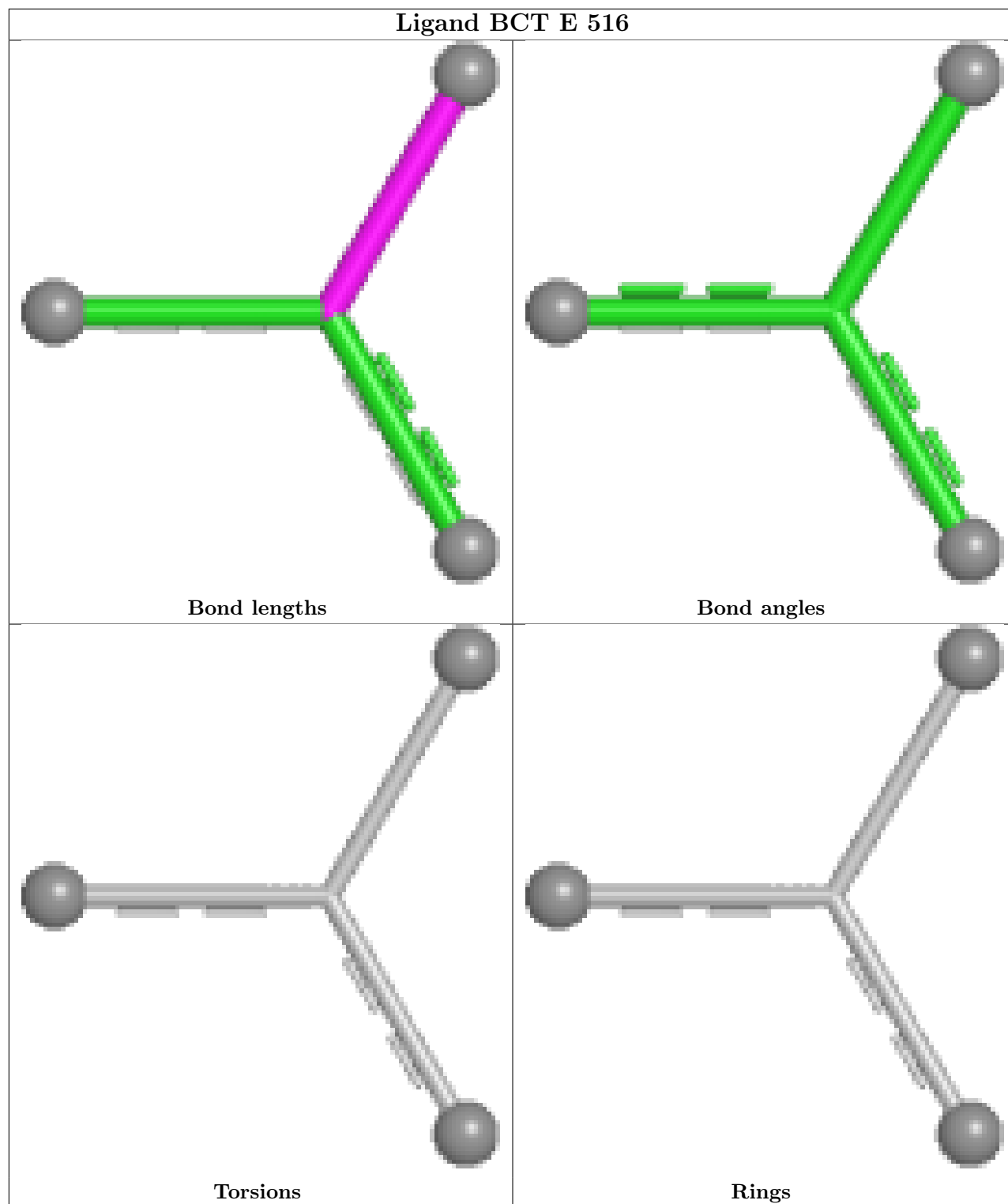


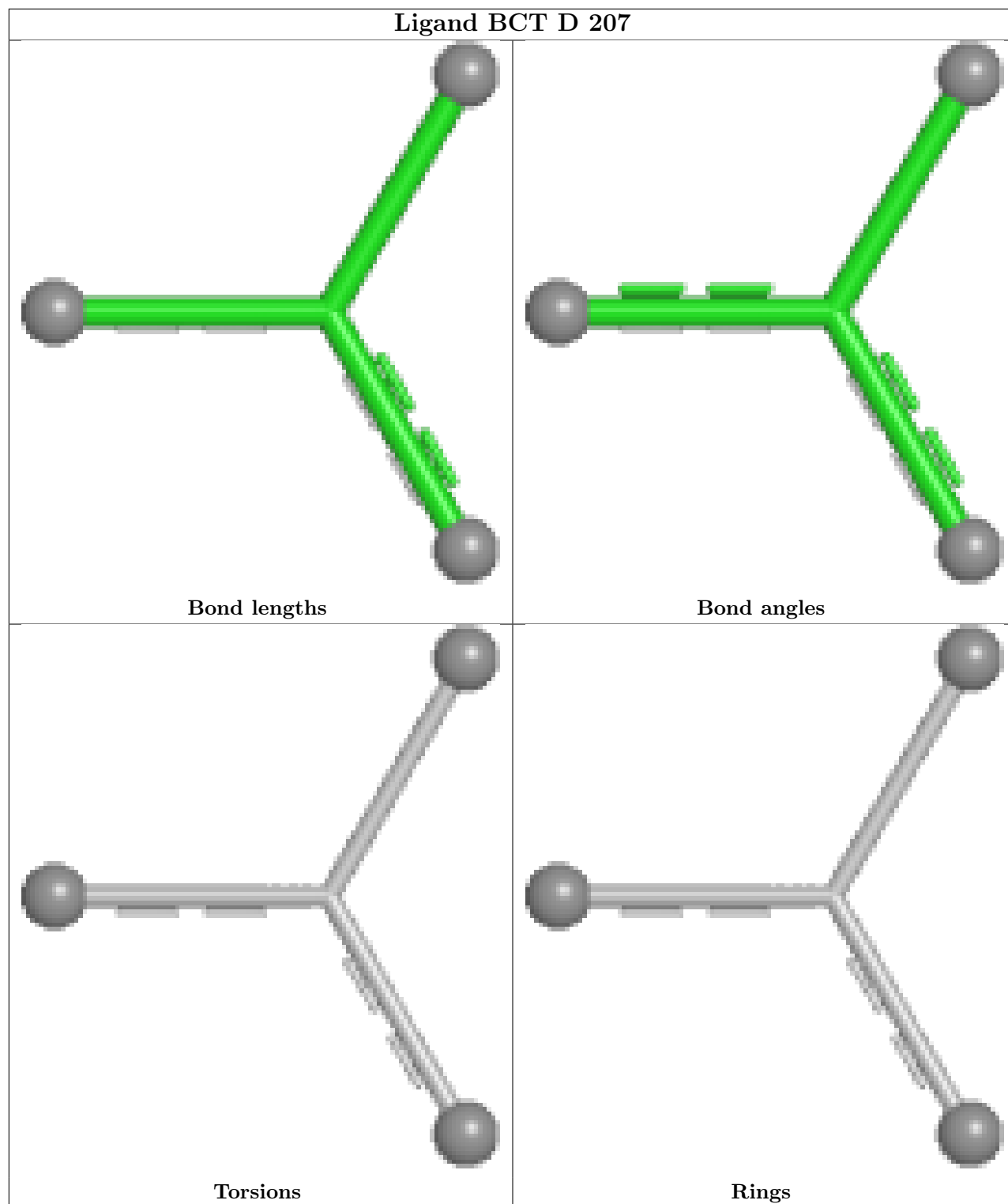


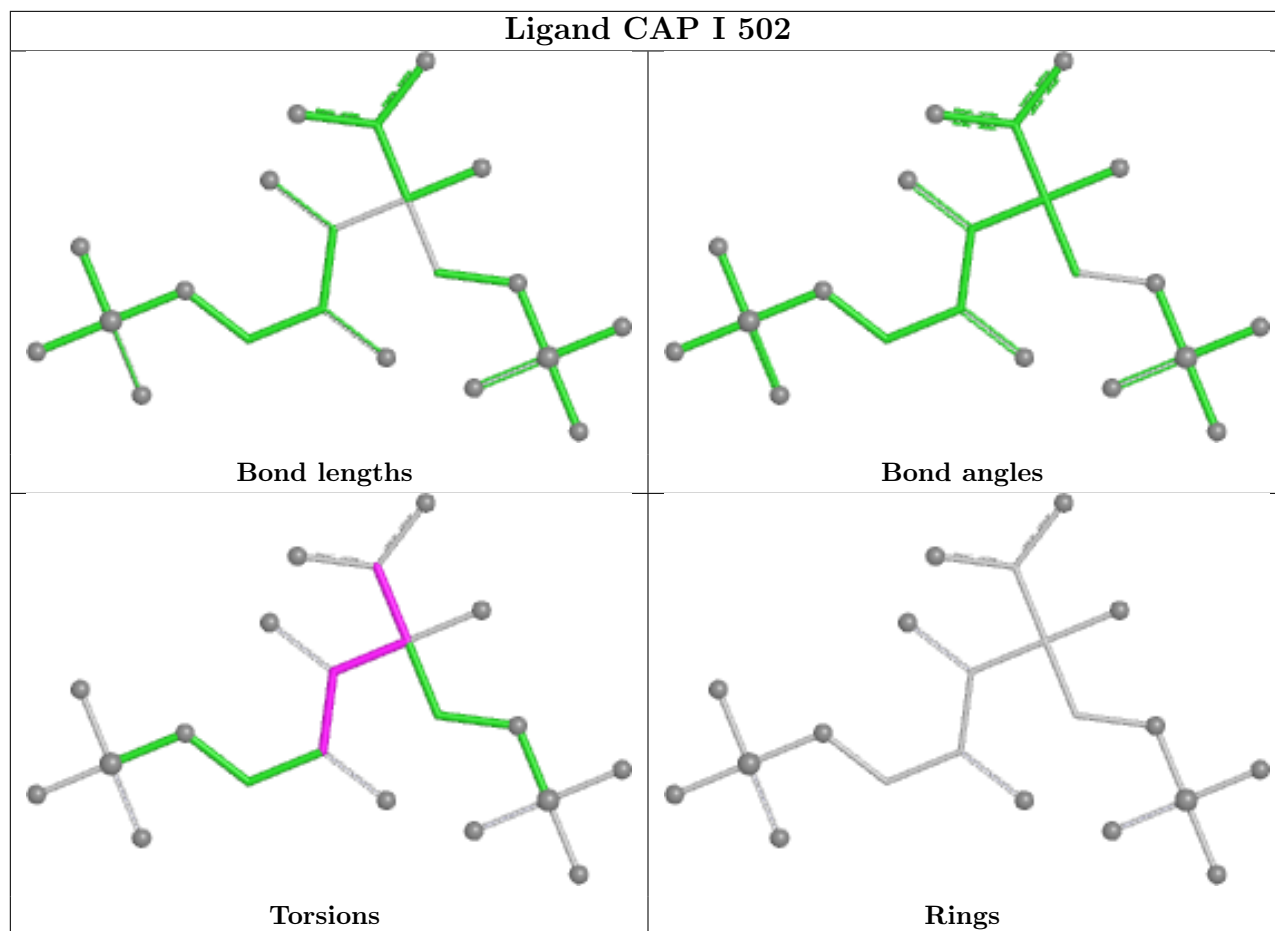


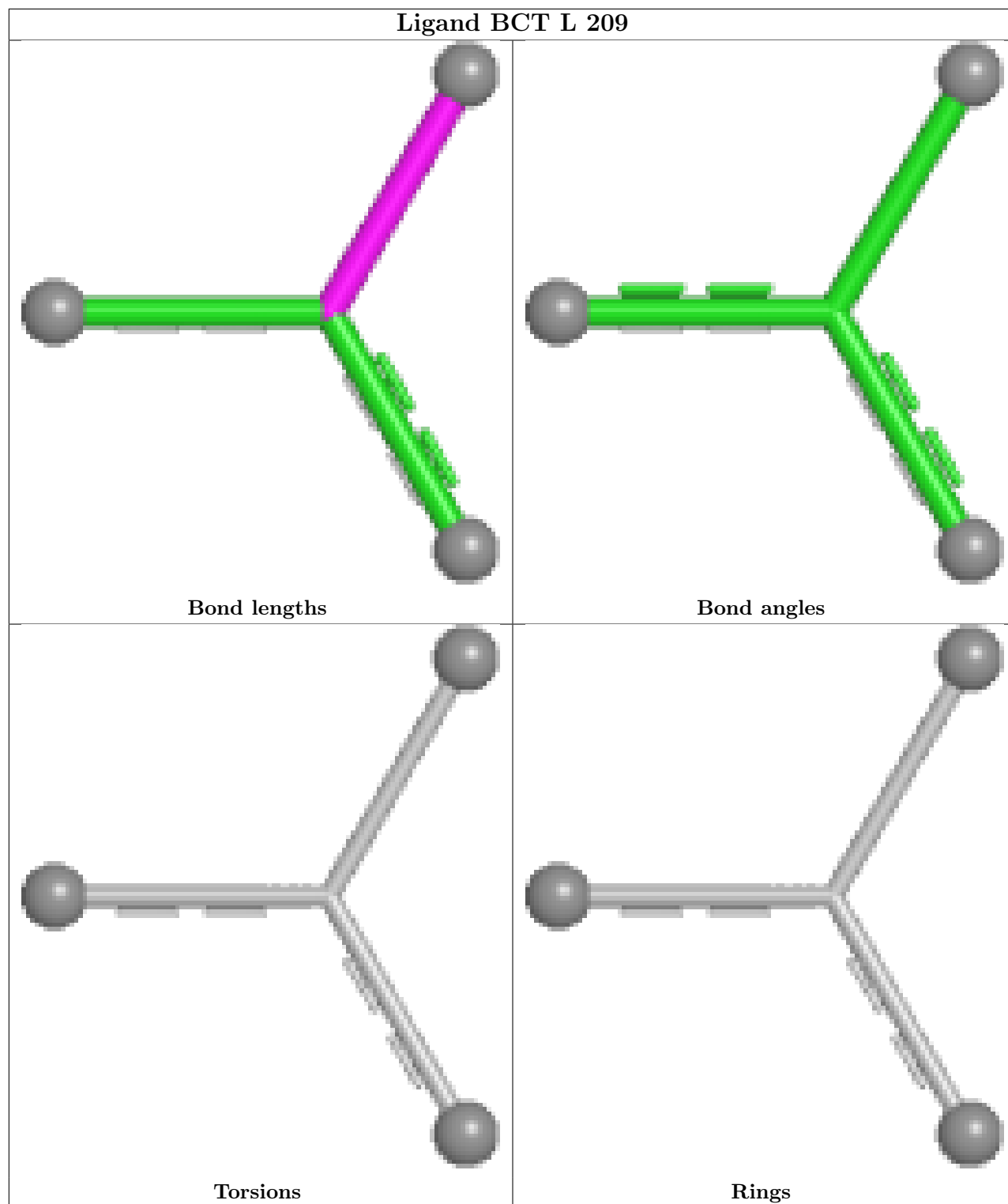


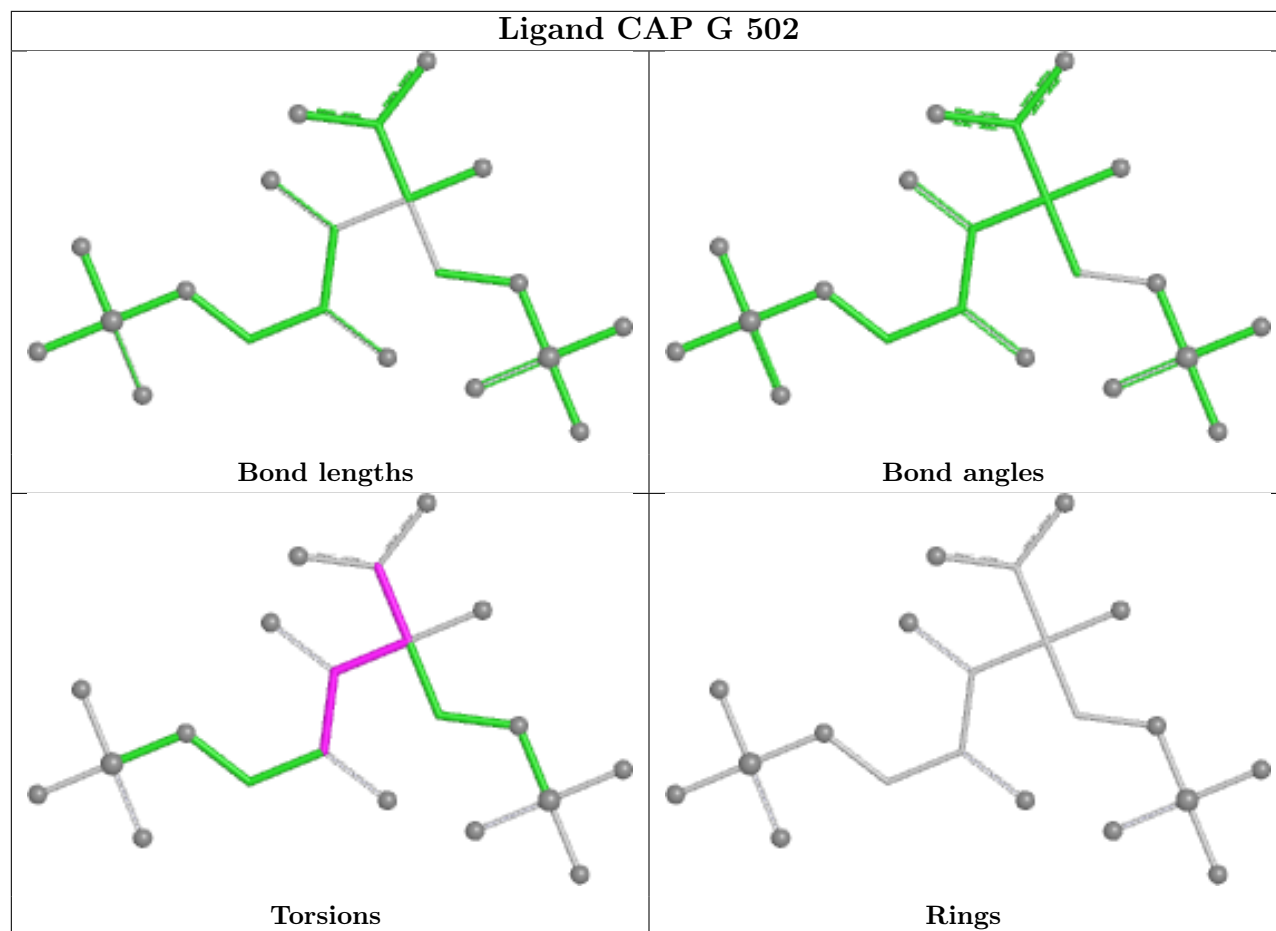


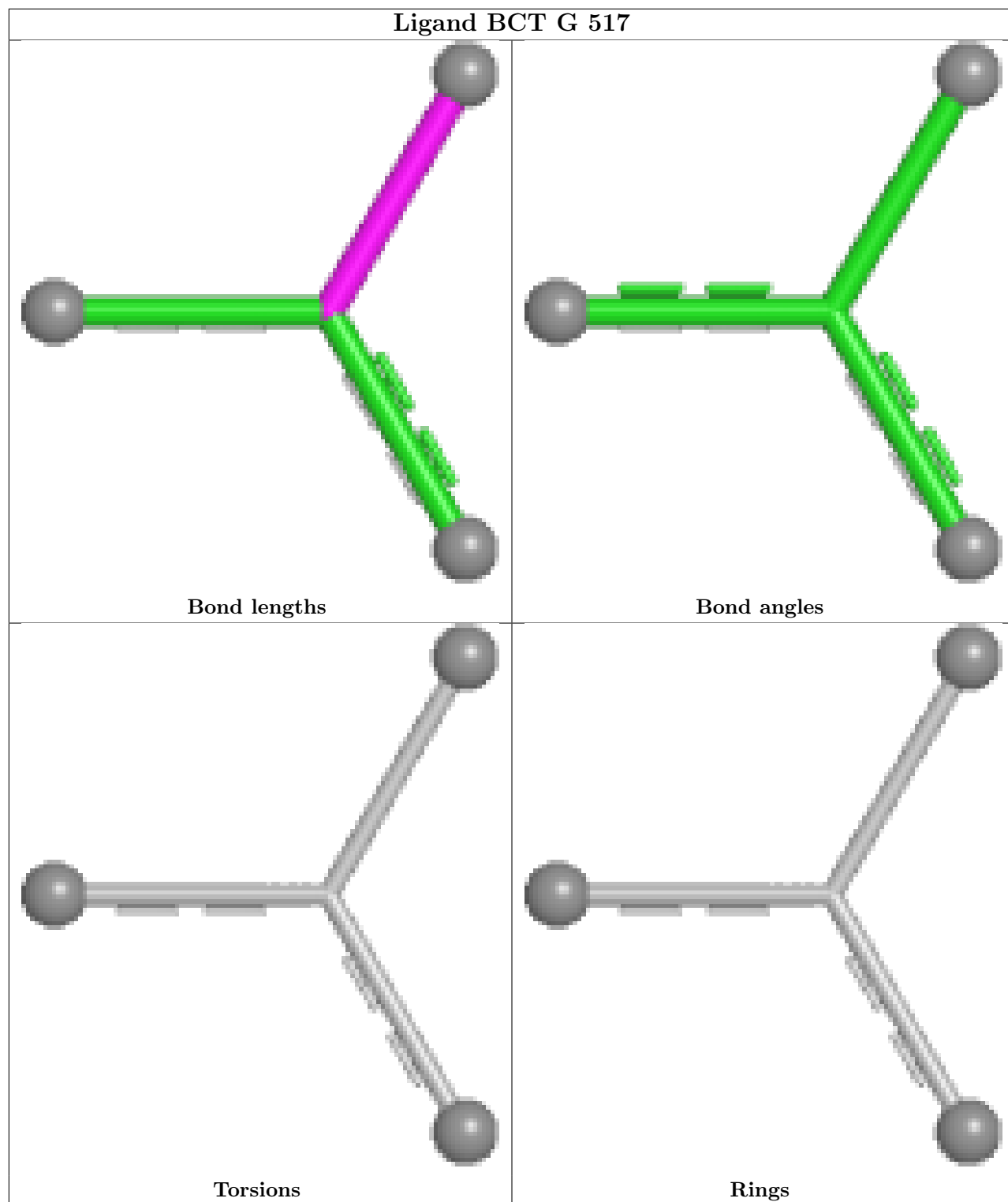


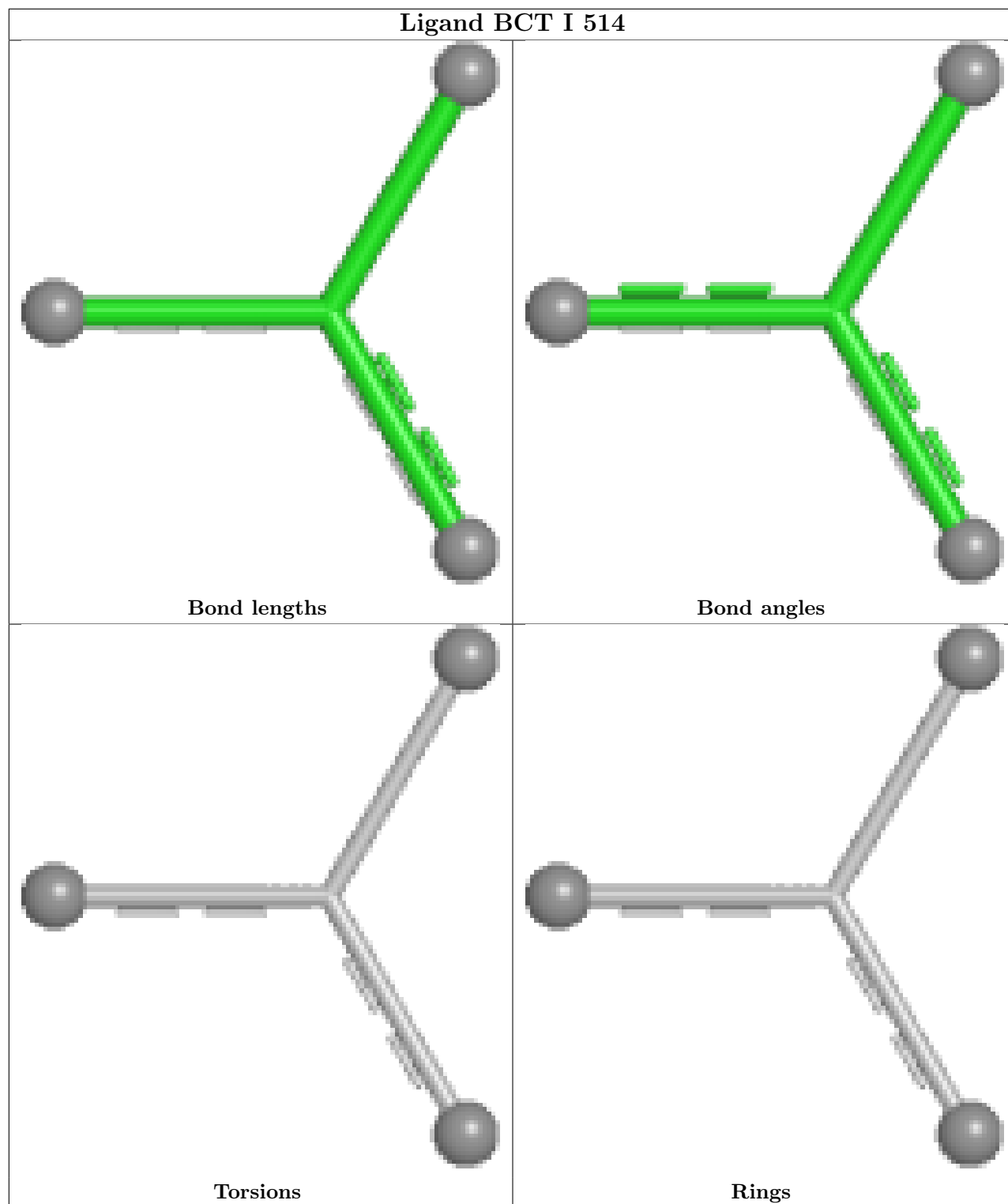












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	477/480 (99%)	-0.24	12 (2%) 58 62	8, 16, 31, 61	9 (1%)
1	C	476/480 (99%)	-0.32	6 (1%) 75 79	8, 15, 30, 54	7 (1%)
1	G	476/480 (99%)	-0.43	9 (1%) 66 71	7, 14, 25, 59	9 (1%)
1	K	476/480 (99%)	-0.43	7 (1%) 72 76	7, 14, 27, 50	11 (2%)
1	O	476/480 (99%)	-0.30	8 (1%) 69 73	8, 16, 30, 67	8 (1%)
2	B	138/138 (100%)	-0.10	2 (1%) 73 77	10, 18, 34, 52	3 (2%)
2	D	138/138 (100%)	-0.04	7 (5%) 33 37	11, 18, 34, 57	1 (0%)
2	F	138/138 (100%)	-0.12	2 (1%) 73 77	11, 18, 33, 54	1 (0%)
2	H	138/138 (100%)	-0.29	3 (2%) 62 66	9, 15, 28, 46	4 (2%)
2	J	138/138 (100%)	-0.25	3 (2%) 62 66	10, 16, 30, 52	2 (1%)
2	L	138/138 (100%)	-0.20	4 (2%) 53 58	10, 17, 32, 50	1 (0%)
2	N	138/138 (100%)	0.03	3 (2%) 62 66	11, 19, 32, 52	3 (2%)
2	P	138/138 (100%)	-0.02	5 (3%) 46 50	12, 18, 35, 53	4 (2%)
3	E	466/480 (97%)	-0.30	3 (0%) 85 88	7, 16, 27, 56	9 (1%)
3	I	477/480 (99%)	-0.34	5 (1%) 79 82	8, 15, 26, 54	9 (1%)
3	M	477/480 (99%)	-0.18	8 (1%) 69 73	7, 18, 31, 57	10 (2%)
All	All	4905/4944 (99%)	-0.28	87 (1%) 67 72	7, 16, 30, 67	91 (1%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	481	VAL	5.5
3	E	16	TYR	5.3
2	P	58	ILE	4.6
1	A	3	ASN	4.5
1	A	5	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	11[A]	ILE	4.3
1	A	4	SER	4.3
2	N	58	ILE	4.1
1	A	9	THR	3.9
3	I	11[A]	ILE	3.9
1	G	9	THR	3.8
2	J	58	ILE	3.7
1	G	11[A]	ILE	3.6
2	D	58	ILE	3.6
2	B	58	ILE	3.6
2	N	76	SER	3.6
1	C	11[A]	ILE	3.5
2	H	76	SER	3.5
1	G	5	VAL	3.5
1	K	11[A]	ILE	3.5
1	O	482	GLU	3.5
3	M	11[A]	ILE	3.4
1	O	11[A]	ILE	3.4
2	L	58	ILE	3.3
1	C	481	VAL	3.2
1	O	5	VAL	3.1
1	C	13	ASN	3.1
1	A	16	TYR	2.9
1	C	16	TYR	2.9
2	F	58	ILE	2.9
1	A	7	GLU	2.9
2	N	57	ASP	2.8
3	E	482	GLU	2.8
1	A	466	LYS	2.8
1	G	16	TYR	2.7
2	P	57	ASP	2.7
2	D	63	THR	2.7
3	I	5	VAL	2.7
1	A	8	ARG	2.7
1	K	5	VAL	2.7
2	P	55[A]	LEU	2.6
3	I	482	GLU	2.6
1	G	13	ASN	2.5
3	M	16	TYR	2.5
3	I	9	THR	2.5
3	M	98	SER	2.5
2	D	60	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	481	VAL	2.4
2	H	58	ILE	2.4
2	L	59	ASN	2.4
1	A	482	GLU	2.4
1	O	16	TYR	2.4
1	A	481	VAL	2.4
1	G	4	SER	2.4
2	D	55	LEU	2.3
1	K	16	TYR	2.3
3	I	16	TYR	2.3
2	J	57	ASP	2.3
3	M	12	LYS	2.3
2	D	61	ALA	2.3
2	D	59	ASN	2.3
1	K	482	GLU	2.3
1	A	12	LYS	2.3
1	K	13	ASN	2.3
1	G	482	GLU	2.2
1	O	8	ARG	2.2
2	H	57	ASP	2.2
2	D	62	ALA	2.2
1	G	14	GLU	2.2
2	B	59	ASN	2.2
1	K	98	SER	2.2
3	M	4	SER	2.2
3	M	83	LEU	2.2
1	O	12	LYS	2.2
2	J	59	ASN	2.2
3	E	15	ARG	2.1
1	C	12	LYS	2.1
3	M	482	GLU	2.1
2	L	56	PHE	2.1
3	M	5	VAL	2.1
2	P	61	ALA	2.0
1	C	97	THR	2.0
2	F	63	THR	2.0
1	K	12	LYS	2.0
1	O	13	ASN	2.0
2	L	60	ASP	2.0
2	P	60	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CCS	O	455	10/11	0.93	0.12	24,27,41,41	0
1	CCS	C	455	10/11	0.94	0.12	23,27,41,42	0
1	CCS	G	455	10/11	0.94	0.12	18,21,35,37	0
1	CCS	K	455	10/11	0.94	0.11	19,23,37,38	0
1	CCS	A	455	10/11	0.94	0.13	19,23,35,37	0
1	KCX	C	205	12/13	0.96	0.05	12,12,13,13	0
1	KCX	K	205	12/13	0.96	0.06	11,11,12,12	0
1	KCX	A	205	12/13	0.96	0.06	13,14,15,16	0
1	KCX	O	205	12/13	0.96	0.05	12,13,13,14	0
1	KCX	G	205	12/13	0.96	0.05	11,12,12,13	0
1	HL2	C	174	9/10	0.97	0.05	12,13,14,14	0
3	HL2	M	174	9/10	0.97	0.05	15,15,16,16	0
3	KCX	M	205	12/13	0.97	0.05	13,14,16,16	0
1	HL2	O	174	9/10	0.97	0.05	13,14,14,14	0
3	HL2	E	174	9/10	0.97	0.05	14,14,15,15	0
3	KCX	E	205	12/13	0.97	0.05	12,12,13,13	0
3	HL2	I	174	9/10	0.98	0.04	13,13,14,14	0
3	KCX	I	205	12/13	0.98	0.04	12,12,13,13	0
1	HL2	K	174	9/10	0.98	0.04	12,12,13,13	0
1	HL2	A	174	9/10	0.98	0.04	12,13,14,14	0
1	HL2	G	174	9/10	0.98	0.04	11,12,12,12	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	C	513	4/4	0.58	0.30	32,33,33,36	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	O	511	4/4	0.69	0.21	28,29,30,32	4
7	BCT	B	207	4/4	0.73	0.16	50,52,52,52	0
7	BCT	N	208	4/4	0.77	0.15	61,63,63,63	0
7	BCT	O	513	4/4	0.77	0.14	42,43,44,45	0
7	BCT	A	519	4/4	0.78	0.15	44,46,46,47	0
6	EDO	I	510	4/4	0.78	0.19	44,46,47,47	0
6	EDO	E	510	4/4	0.79	0.21	43,44,45,47	0
7	BCT	C	515	4/4	0.79	0.13	39,41,42,43	0
7	BCT	L	209	4/4	0.79	0.14	53,54,55,55	0
7	BCT	A	517	4/4	0.79	0.13	43,44,45,46	0
6	EDO	A	515	4/4	0.79	0.17	52,52,52,53	0
7	BCT	O	514	4/4	0.79	0.14	50,51,51,52	0
6	EDO	P	208	4/4	0.80	0.19	29,29,30,32	4
7	BCT	K	512	4/4	0.80	0.11	47,48,48,49	0
6	EDO	A	514	4/4	0.80	0.19	45,47,48,49	0
6	EDO	L	208	4/4	0.81	0.17	34,35,35,37	0
6	EDO	N	207	4/4	0.81	0.18	29,31,31,32	4
7	BCT	E	515	4/4	0.81	0.15	37,44,44,45	0
7	BCT	E	516	4/4	0.81	0.12	51,53,53,54	0
7	BCT	I	515	4/4	0.81	0.15	34,36,36,37	0
7	BCT	I	516	4/4	0.82	0.15	50,53,53,54	0
7	BCT	E	514	4/4	0.82	0.16	51,52,54,54	0
7	BCT	G	518	4/4	0.82	0.13	52,52,53,54	0
7	BCT	M	512	4/4	0.82	0.12	39,39,40,42	0
7	BCT	H	208	4/4	0.82	0.14	48,49,49,51	0
7	BCT	I	514	4/4	0.82	0.13	40,43,43,45	0
6	EDO	C	511	4/4	0.82	0.14	26,29,29,31	0
7	BCT	A	518	4/4	0.83	0.17	38,45,46,46	0
6	EDO	H	205	4/4	0.83	0.16	32,34,34,37	0
6	EDO	K	510	4/4	0.84	0.16	32,35,36,37	0
6	EDO	G	511	4/4	0.84	0.14	38,38,39,39	0
6	EDO	G	512	4/4	0.84	0.15	26,28,28,29	0
7	BCT	G	514	4/4	0.84	0.13	37,38,39,40	0
7	BCT	G	516	4/4	0.84	0.14	39,44,46,47	0
6	EDO	A	513	4/4	0.84	0.20	27,28,29,30	0
7	BCT	C	514	4/4	0.84	0.12	43,47,47,48	0
6	EDO	A	511	4/4	0.84	0.15	35,39,39,41	0
7	BCT	A	516	4/4	0.85	0.13	35,36,36,38	0
7	BCT	D	207	4/4	0.85	0.10	48,49,50,51	0
7	BCT	G	515	4/4	0.85	0.13	51,52,53,53	0
6	EDO	K	507	4/4	0.86	0.16	43,43,43,44	0
6	EDO	O	509	4/4	0.86	0.15	38,40,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	BCT	M	511	4/4	0.86	0.14	34,39,40,42	0
6	EDO	O	510	4/4	0.86	0.16	41,44,45,47	0
6	EDO	K	509	4/4	0.86	0.13	28,31,33,36	0
6	EDO	B	205	4/4	0.86	0.15	34,36,36,39	0
6	EDO	F	205	4/4	0.86	0.17	35,37,38,40	0
6	EDO	L	207	4/4	0.87	0.13	36,38,39,40	0
6	EDO	G	513	4/4	0.87	0.12	29,32,34,38	0
6	EDO	A	509	4/4	0.87	0.15	41,43,44,45	0
6	EDO	O	507	4/4	0.87	0.13	39,40,40,41	0
6	EDO	G	506	4/4	0.87	0.15	31,35,36,37	0
6	EDO	I	513	4/4	0.87	0.13	41,42,42,42	0
6	EDO	J	205	4/4	0.87	0.13	32,33,34,35	0
6	EDO	P	205	4/4	0.87	0.16	45,45,46,46	0
6	EDO	P	206	4/4	0.87	0.15	45,45,45,45	0
6	EDO	G	508	4/4	0.87	0.14	26,30,31,32	0
7	BCT	O	512	4/4	0.87	0.12	38,39,41,42	0
6	EDO	A	512	4/4	0.87	0.14	38,39,40,42	0
6	EDO	C	510	4/4	0.87	0.15	27,30,31,34	0
7	BCT	M	510	4/4	0.88	0.09	42,44,45,46	0
6	EDO	G	507	4/4	0.88	0.16	34,35,36,37	0
6	EDO	A	510	4/4	0.88	0.14	36,38,39,40	0
6	EDO	I	507	4/4	0.88	0.14	38,41,41,43	0
7	BCT	K	511	4/4	0.88	0.11	35,35,36,37	0
6	EDO	E	506	4/4	0.88	0.12	31,33,33,34	0
6	EDO	E	508	4/4	0.88	0.13	38,39,40,41	0
6	EDO	E	511	4/4	0.89	0.12	33,36,38,41	0
6	EDO	M	506	4/4	0.89	0.13	30,34,36,38	0
6	EDO	I	509	4/4	0.89	0.13	32,35,36,37	0
6	EDO	D	205	4/4	0.89	0.14	38,39,39,41	0
6	EDO	I	512	4/4	0.89	0.13	26,30,32,35	0
6	EDO	A	506	4/4	0.89	0.11	35,37,38,39	0
7	BCT	E	513	4/4	0.89	0.10	39,39,39,40	0
6	EDO	L	205	4/4	0.90	0.14	31,32,33,34	0
6	EDO	L	206	4/4	0.90	0.15	32,36,38,40	0
6	EDO	E	509	4/4	0.90	0.11	24,27,27,29	0
6	EDO	K	505	4/4	0.90	0.13	30,33,35,36	0
7	BCT	G	517	4/4	0.90	0.09	35,37,38,39	0
6	EDO	C	505	4/4	0.90	0.12	32,35,35,38	0
6	EDO	P	207	4/4	0.90	0.17	30,32,34,34	0
6	EDO	N	206	4/4	0.90	0.11	29,30,30,30	0
6	EDO	I	506	4/4	0.90	0.12	40,42,42,44	0
6	EDO	C	507	4/4	0.90	0.13	28,31,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	M	509	4/4	0.91	0.13	36,38,38,39	0
6	EDO	A	508	4/4	0.91	0.11	29,31,31,32	0
6	EDO	C	509	4/4	0.91	0.13	37,38,39,39	0
6	EDO	D	206	4/4	0.91	0.14	31,33,33,34	0
6	EDO	K	506	4/4	0.91	0.10	25,26,27,27	0
6	EDO	M	507	4/4	0.91	0.10	33,35,36,37	0
6	EDO	C	508	4/4	0.92	0.10	28,30,31,32	0
6	EDO	N	205	4/4	0.92	0.12	29,31,31,33	0
6	EDO	I	511	4/4	0.92	0.11	22,23,23,23	4
6	EDO	H	204	4/4	0.92	0.10	25,27,27,27	0
6	EDO	O	506	4/4	0.92	0.11	42,42,43,44	0
6	EDO	C	506	4/4	0.92	0.12	31,34,35,36	0
6	EDO	E	507	4/4	0.92	0.11	33,34,34,35	0
6	EDO	C	504	4/4	0.92	0.08	22,22,23,24	0
6	EDO	I	508	4/4	0.92	0.10	33,34,34,37	0
6	EDO	G	505	4/4	0.92	0.10	32,32,32,34	0
6	EDO	M	508	4/4	0.92	0.09	23,25,25,26	0
6	EDO	O	505	4/4	0.93	0.09	30,31,31,31	0
6	EDO	A	507	4/4	0.93	0.10	23,24,25,26	0
6	EDO	H	206	4/4	0.93	0.10	31,31,32,34	0
6	EDO	J	206	4/4	0.93	0.10	29,29,30,30	0
6	EDO	K	503	4/4	0.93	0.09	22,22,23,23	0
6	EDO	B	206	4/4	0.93	0.14	27,28,29,30	0
6	EDO	P	204	4/4	0.93	0.11	22,22,23,24	0
6	EDO	A	505	4/4	0.94	0.09	21,21,21,22	0
6	EDO	B	202	4/4	0.94	0.10	21,22,22,23	0
6	EDO	O	508	4/4	0.94	0.09	32,33,33,33	0
6	EDO	G	509	4/4	0.94	0.09	29,29,30,30	0
6	EDO	M	505	4/4	0.94	0.11	28,29,30,31	0
6	EDO	K	504	4/4	0.94	0.09	18,19,19,19	4
6	EDO	I	504	4/4	0.94	0.09	25,26,26,26	0
6	EDO	E	505	4/4	0.95	0.08	23,23,24,24	0
6	EDO	K	508	4/4	0.95	0.09	34,35,37,38	0
6	EDO	J	201	4/4	0.95	0.09	19,20,21,21	0
6	EDO	D	202	4/4	0.95	0.09	19,21,21,22	0
6	EDO	C	512	4/4	0.95	0.10	22,25,25,27	0
6	EDO	A	504	4/4	0.95	0.07	21,21,21,21	0
6	EDO	H	207	4/4	0.95	0.09	20,20,21,21	0
6	EDO	E	503	4/4	0.95	0.07	17,18,18,18	0
6	EDO	M	504	4/4	0.95	0.07	25,25,25,25	0
6	EDO	I	505	4/4	0.95	0.08	22,23,24,24	0
6	EDO	G	510	4/4	0.96	0.08	22,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	N	202	4/4	0.96	0.08	20,21,21,21	0
6	EDO	N	203	4/4	0.96	0.06	18,19,19,19	0
6	EDO	N	204	4/4	0.96	0.07	21,21,21,21	0
6	EDO	J	203	4/4	0.96	0.06	18,19,20,20	0
6	EDO	L	203	4/4	0.96	0.07	18,19,20,20	0
6	EDO	L	204	4/4	0.96	0.06	21,21,22,22	0
6	EDO	O	504	4/4	0.96	0.07	22,24,24,25	0
6	EDO	J	204	4/4	0.96	0.06	17,17,17,17	0
6	EDO	F	204	4/4	0.96	0.07	19,19,19,19	0
6	EDO	B	201	4/4	0.96	0.07	16,17,17,17	0
6	EDO	G	503	4/4	0.96	0.07	16,16,16,17	0
6	EDO	B	204	4/4	0.96	0.07	21,21,21,22	0
6	EDO	E	504	4/4	0.96	0.06	14,14,15,15	0
6	EDO	D	204	4/4	0.96	0.06	20,20,21,21	0
6	EDO	C	503	4/4	0.96	0.06	14,14,15,15	0
6	EDO	E	512	4/4	0.96	0.10	22,23,24,24	0
6	EDO	B	203	4/4	0.97	0.07	17,17,17,18	0
6	EDO	M	503	4/4	0.97	0.05	16,16,16,17	0
6	EDO	L	201	4/4	0.97	0.05	17,17,17,17	0
6	EDO	I	503	4/4	0.97	0.05	14,14,15,15	0
6	EDO	H	203	4/4	0.97	0.06	19,20,20,21	0
6	EDO	F	202	4/4	0.97	0.06	16,16,17,17	0
6	EDO	P	202	4/4	0.97	0.05	18,18,18,18	0
6	EDO	P	203	4/4	0.97	0.06	21,22,22,22	0
6	EDO	O	503	4/4	0.97	0.05	16,16,16,16	0
6	EDO	F	203	4/4	0.97	0.06	18,18,19,19	0
6	EDO	G	504	4/4	0.97	0.06	20,20,20,20	0
6	EDO	N	201	4/4	0.98	0.05	16,16,16,17	0
5	CAP	M	502	21/21	0.98	0.05	16,17,18,19	0
6	EDO	A	503	4/4	0.98	0.05	14,14,14,14	0
6	EDO	P	201	4/4	0.98	0.05	15,16,16,16	0
6	EDO	F	201	4/4	0.98	0.05	13,14,14,14	0
4	MG	A	501	1/1	0.98	0.03	16,16,16,16	0
6	EDO	D	201	4/4	0.98	0.04	15,16,16,16	0
4	MG	M	501	1/1	0.98	0.03	16,16,16,16	0
4	MG	O	501	1/1	0.98	0.03	15,15,15,15	0
6	EDO	J	202	4/4	0.98	0.04	15,15,16,16	0
5	CAP	A	502	21/21	0.98	0.04	15,16,16,17	0
5	CAP	E	502	21/21	0.98	0.05	14,15,16,16	0
6	EDO	L	202	4/4	0.98	0.04	13,13,13,14	0
6	EDO	H	201	4/4	0.98	0.04	13,14,14,14	0
5	CAP	K	502	21/21	0.99	0.04	12,13,13,13	0

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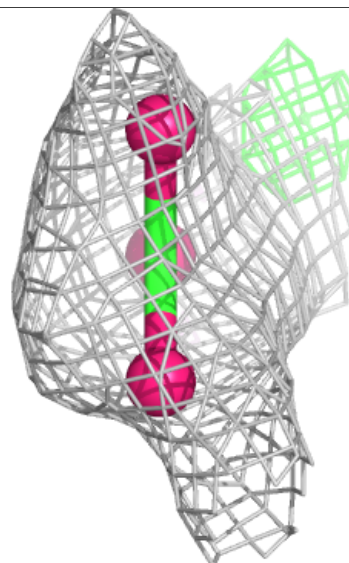
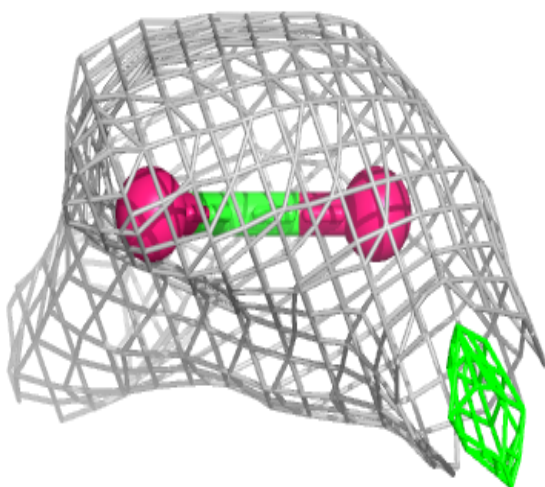
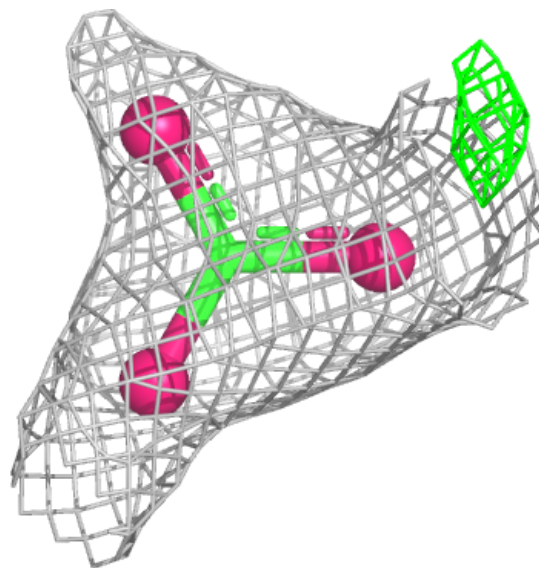
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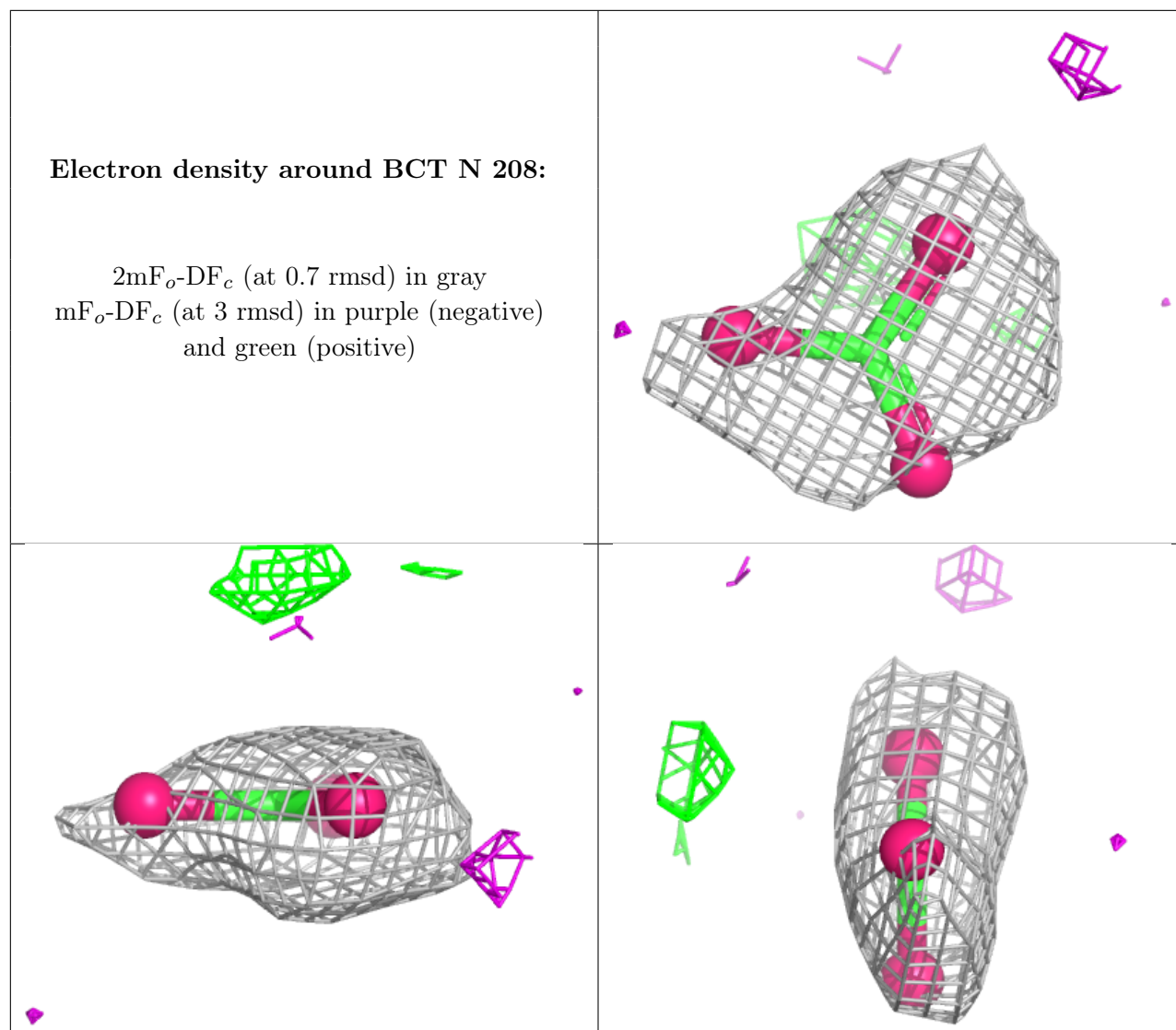
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	C	501	1/1	0.99	0.02	15,15,15,15	0
5	CAP	O	502	21/21	0.99	0.04	14,15,15,16	0
4	MG	E	501	1/1	0.99	0.03	14,14,14,14	0
4	MG	G	501	1/1	0.99	0.02	14,14,14,14	0
5	CAP	C	502	21/21	0.99	0.04	14,15,16,16	0
4	MG	K	501	1/1	0.99	0.04	13,13,13,13	0
5	CAP	G	502	21/21	0.99	0.04	12,13,13,13	0
6	EDO	D	203	4/4	0.99	0.04	16,16,16,16	0
6	EDO	H	202	4/4	0.99	0.03	16,16,16,16	0
5	CAP	I	502	21/21	0.99	0.04	14,15,15,16	0
4	MG	I	501	1/1	1.00	0.02	14,14,14,14	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 BCT B 207:**

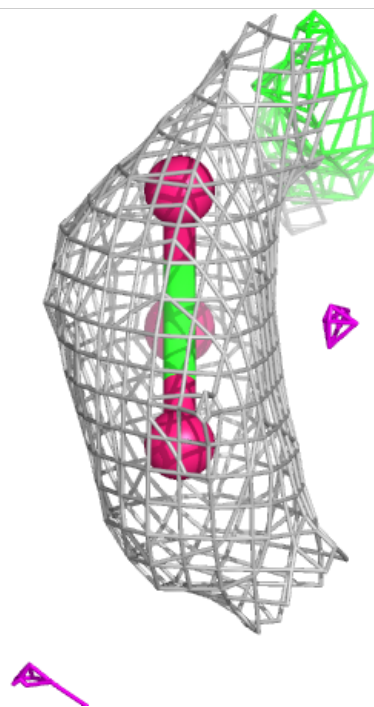
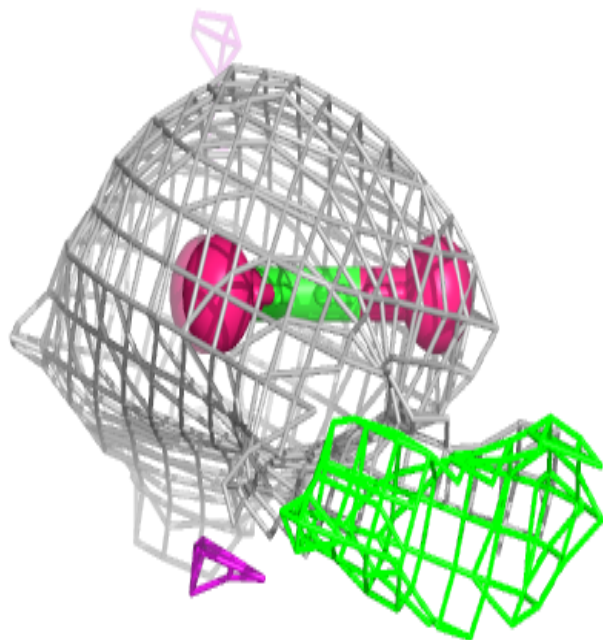
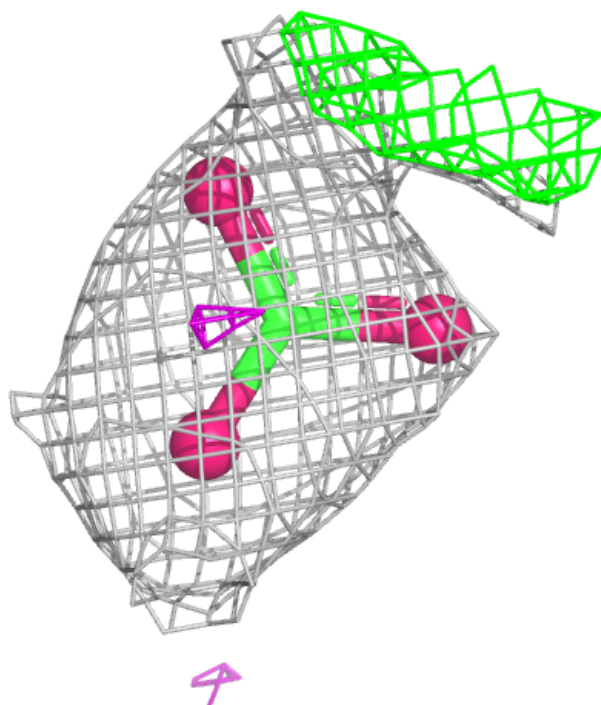
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

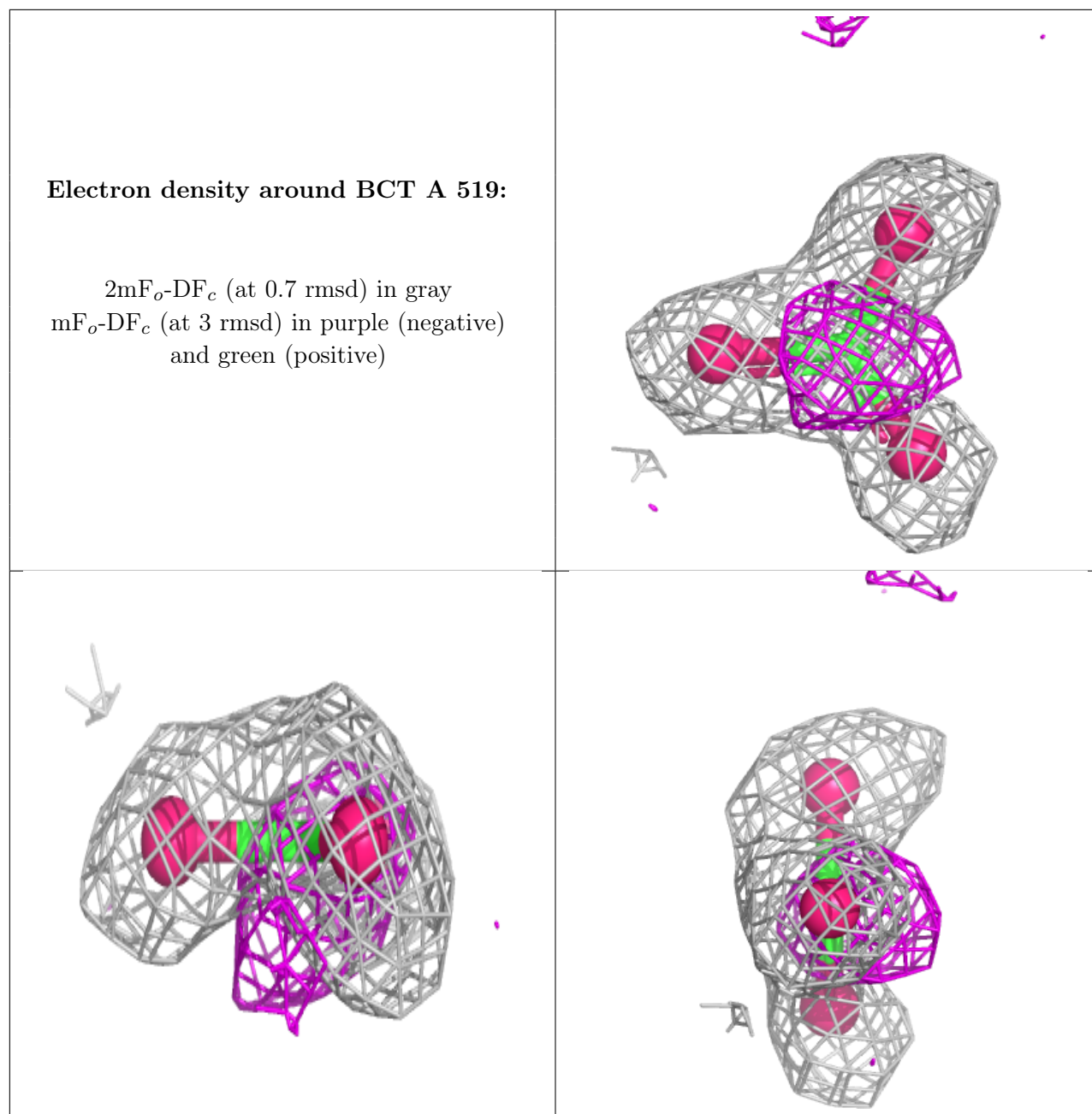




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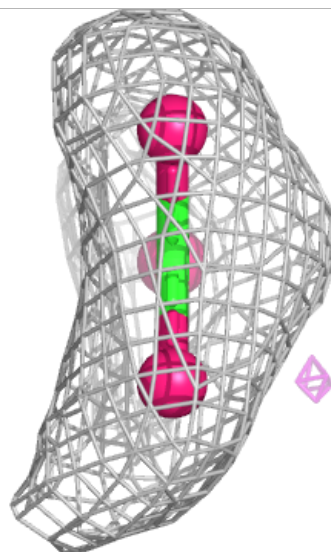
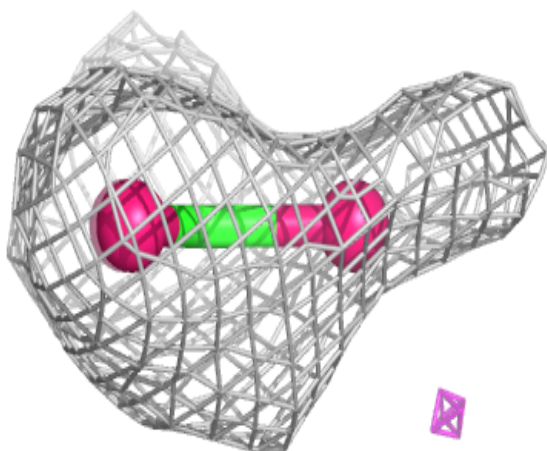
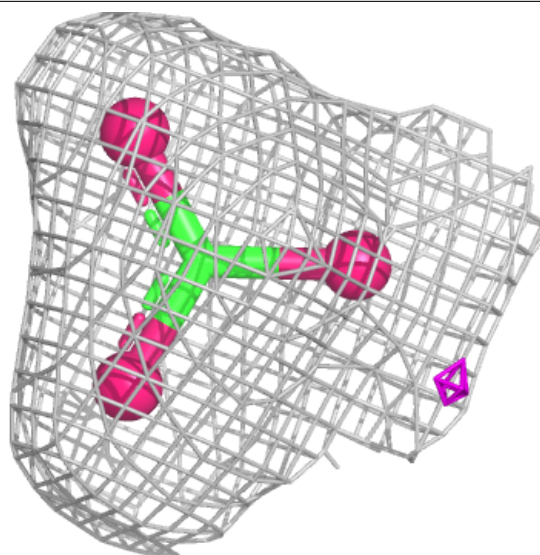
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





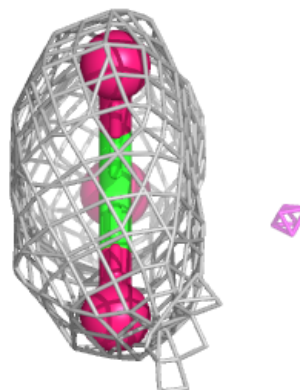
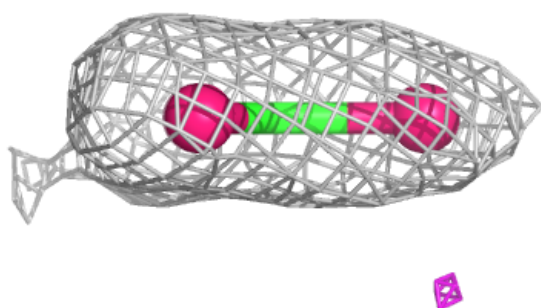
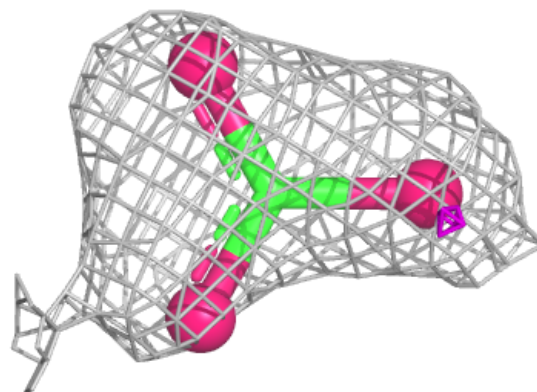
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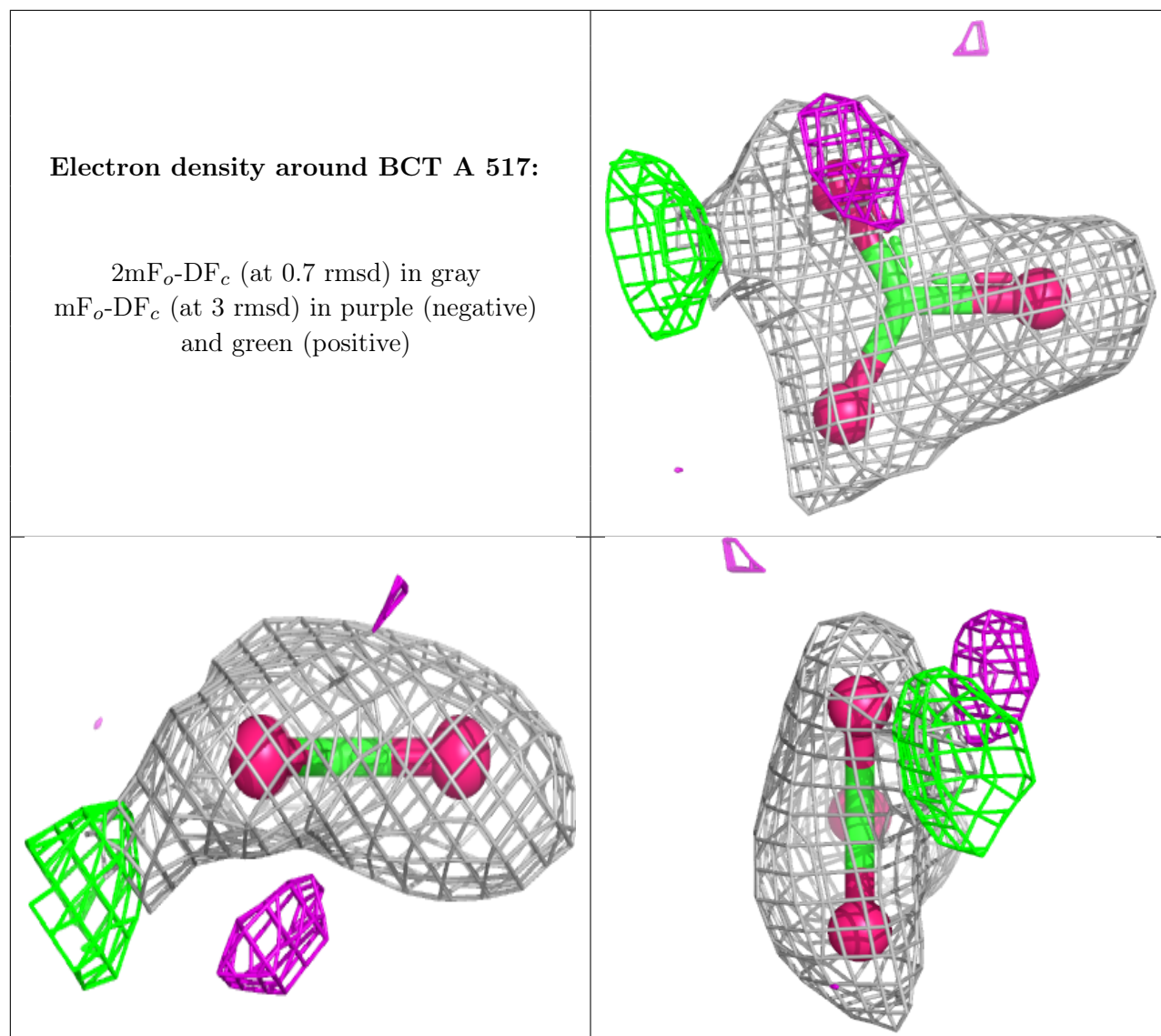
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

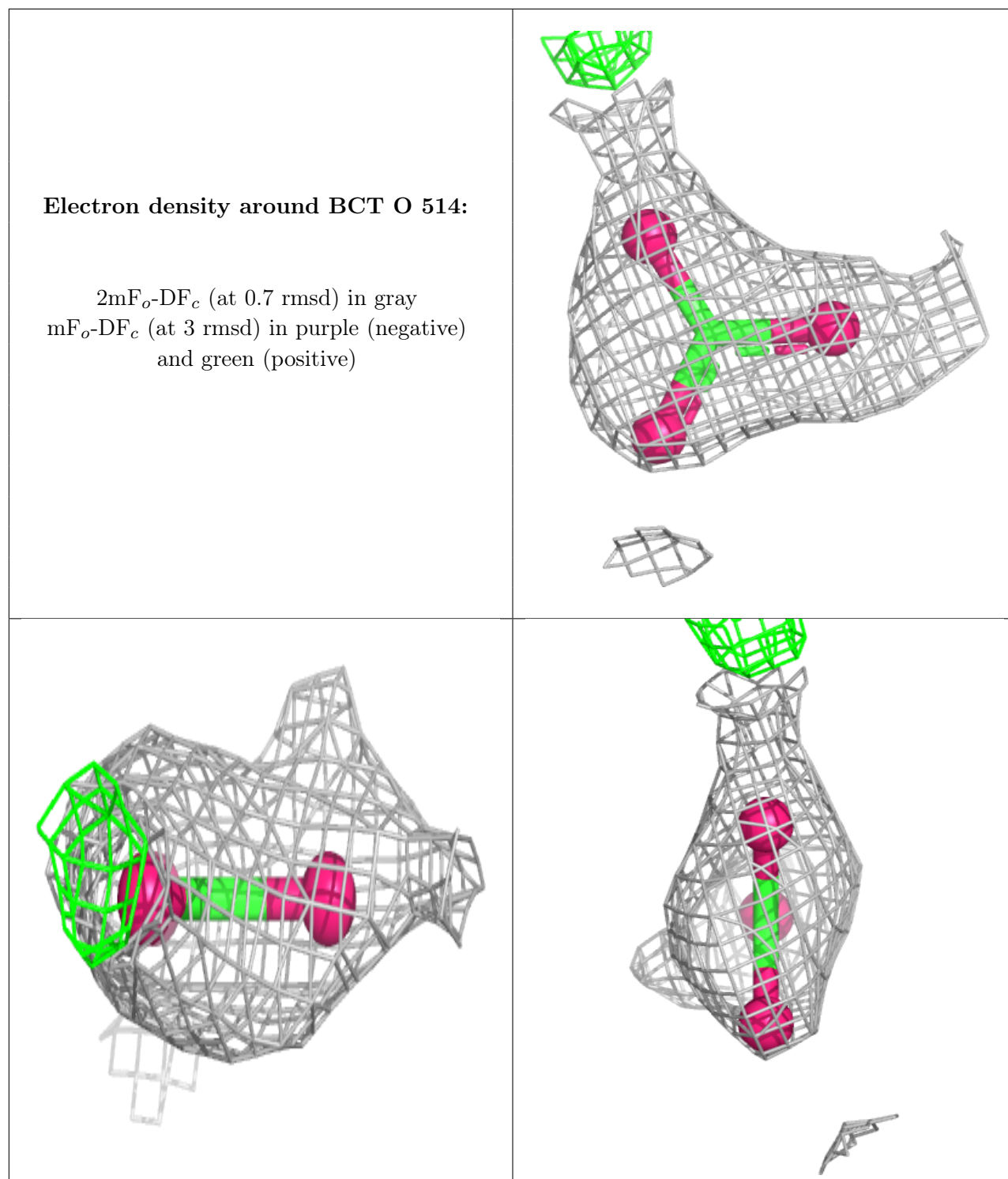


**Electron density around BCT L 209:**

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and green (positive)

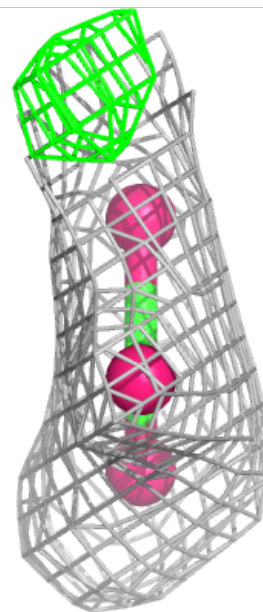
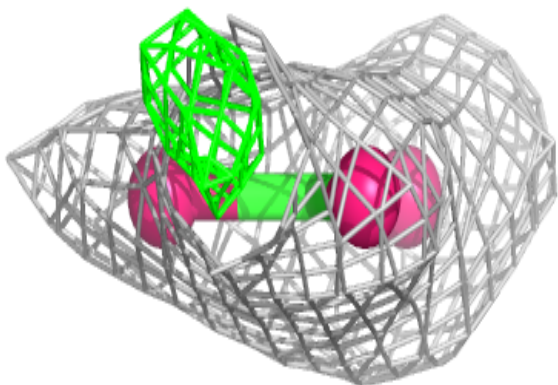
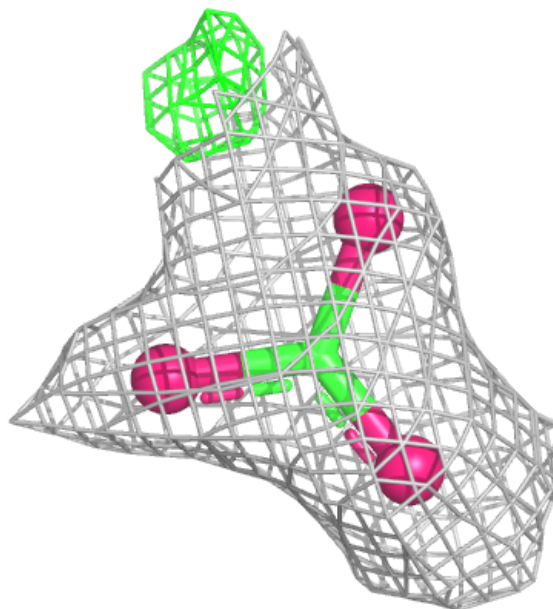






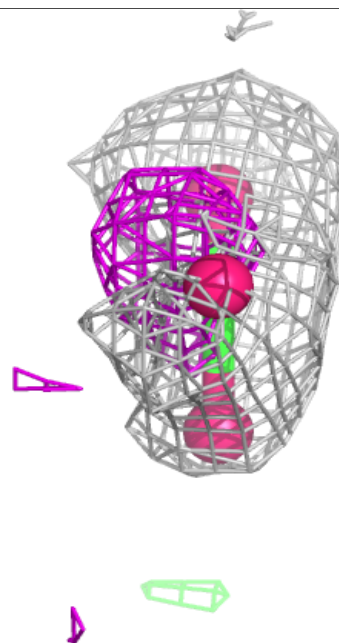
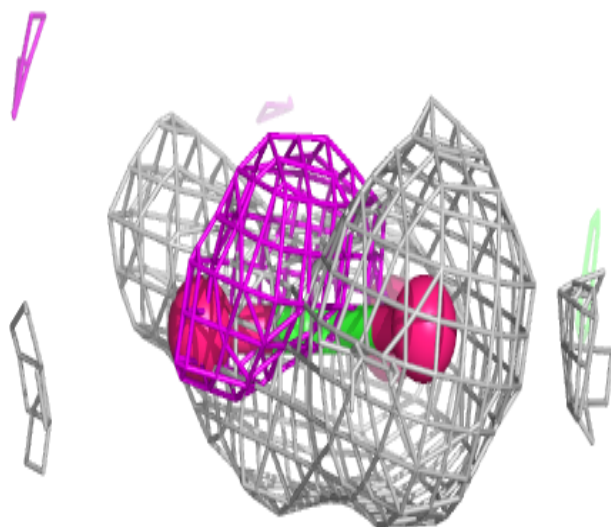
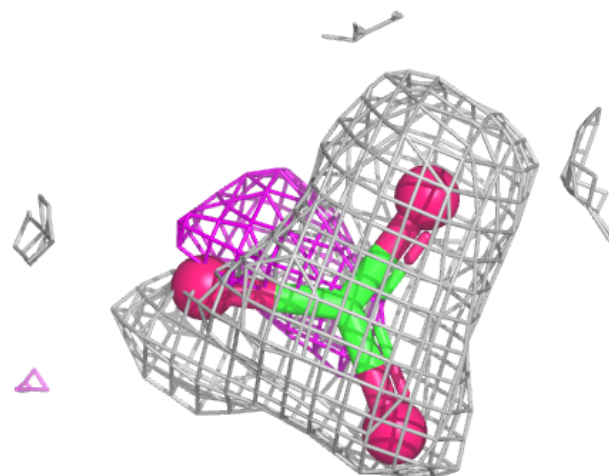
**Electron density around BCT K 512:**

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



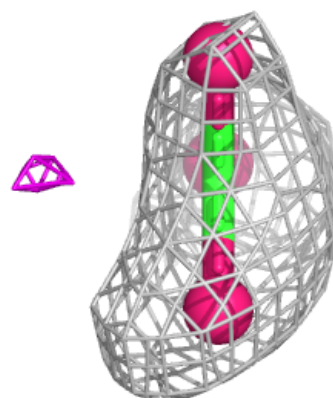
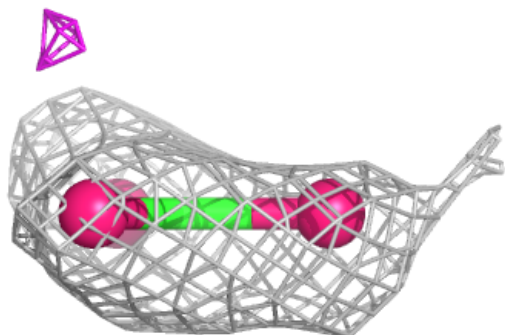
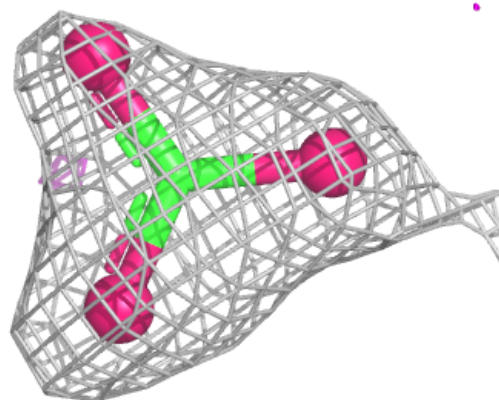
**Electron density around BCT E 515:**

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

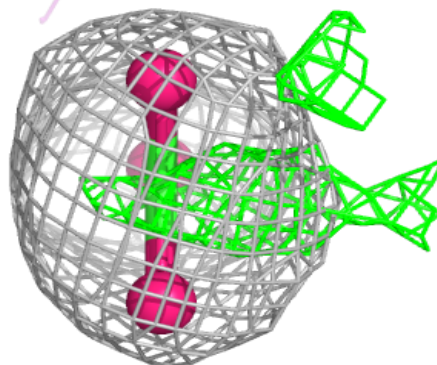
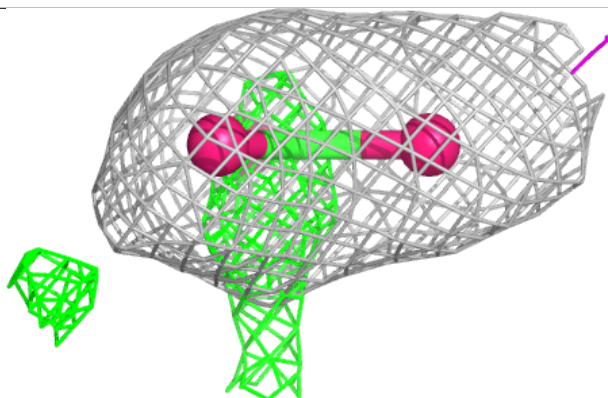
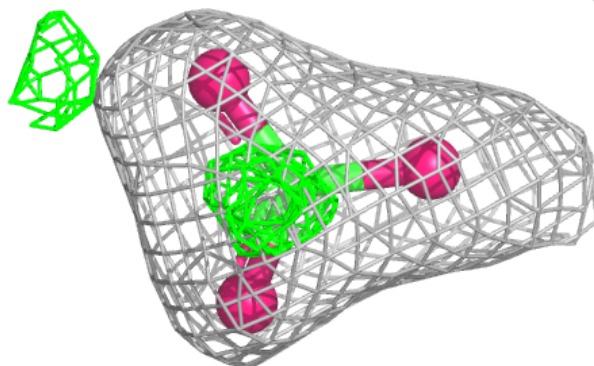


**Electron density around BCT E 516:**

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and green (positive)

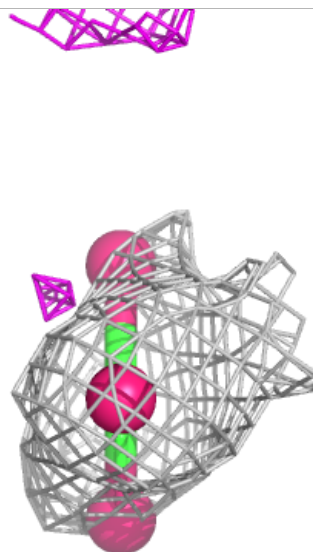
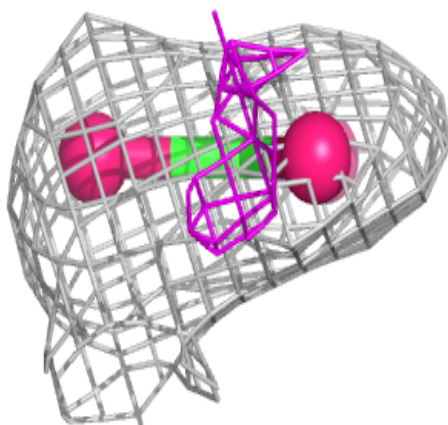
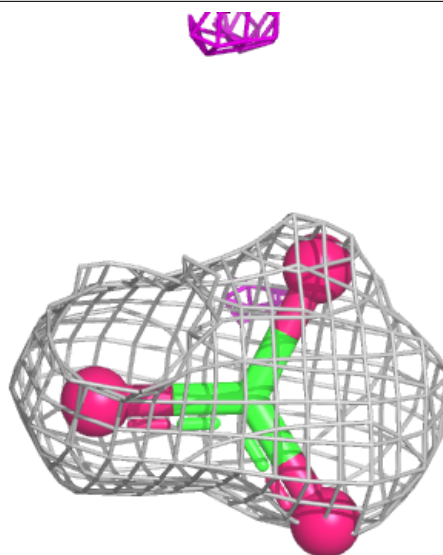
**Electron density around BCT I 515:**

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and green (positive)



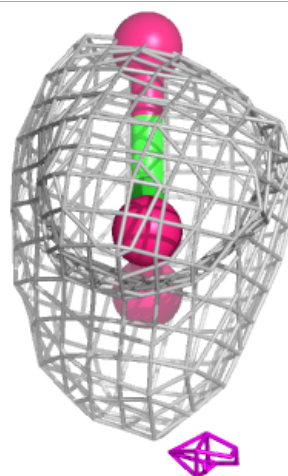
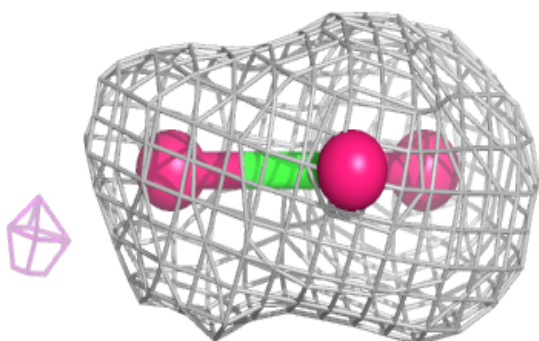
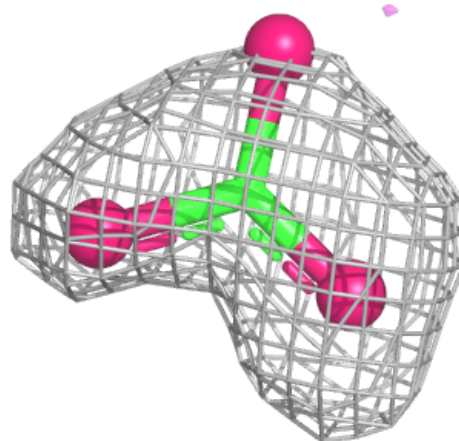
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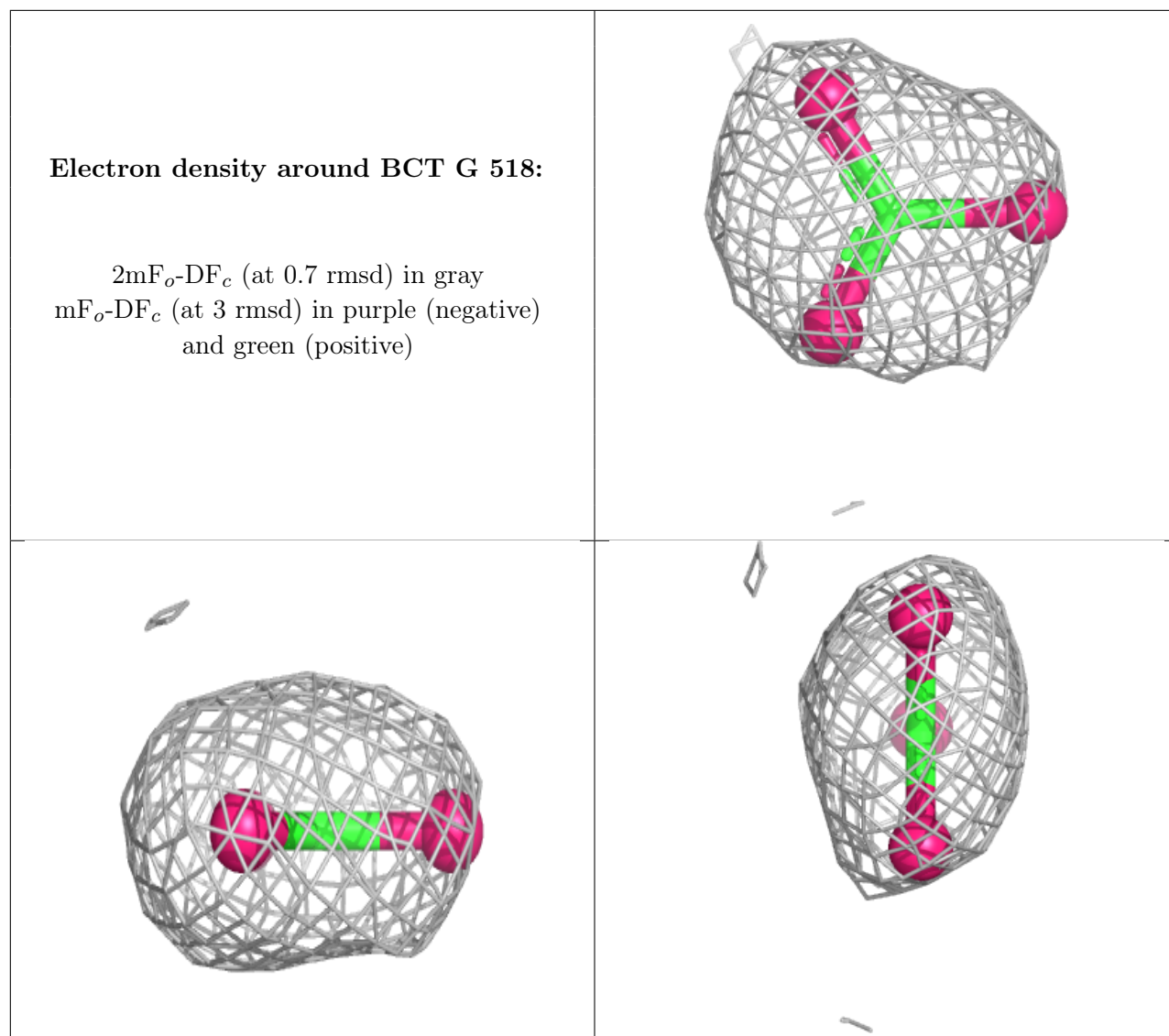
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and green (positive)



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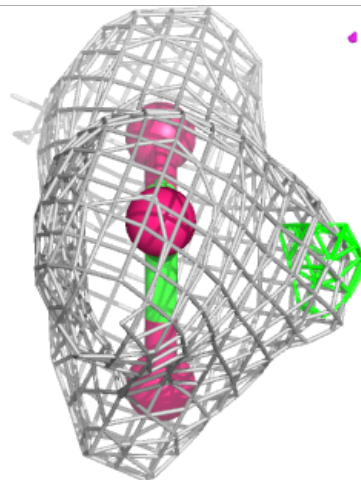
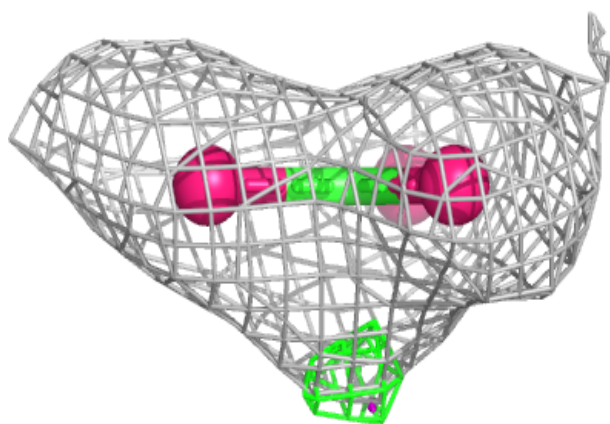
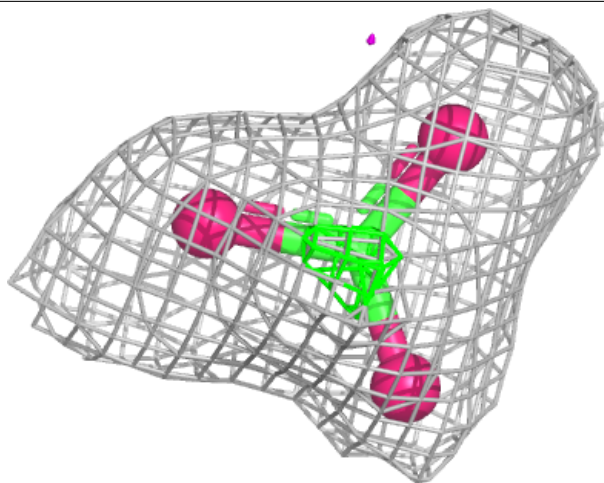
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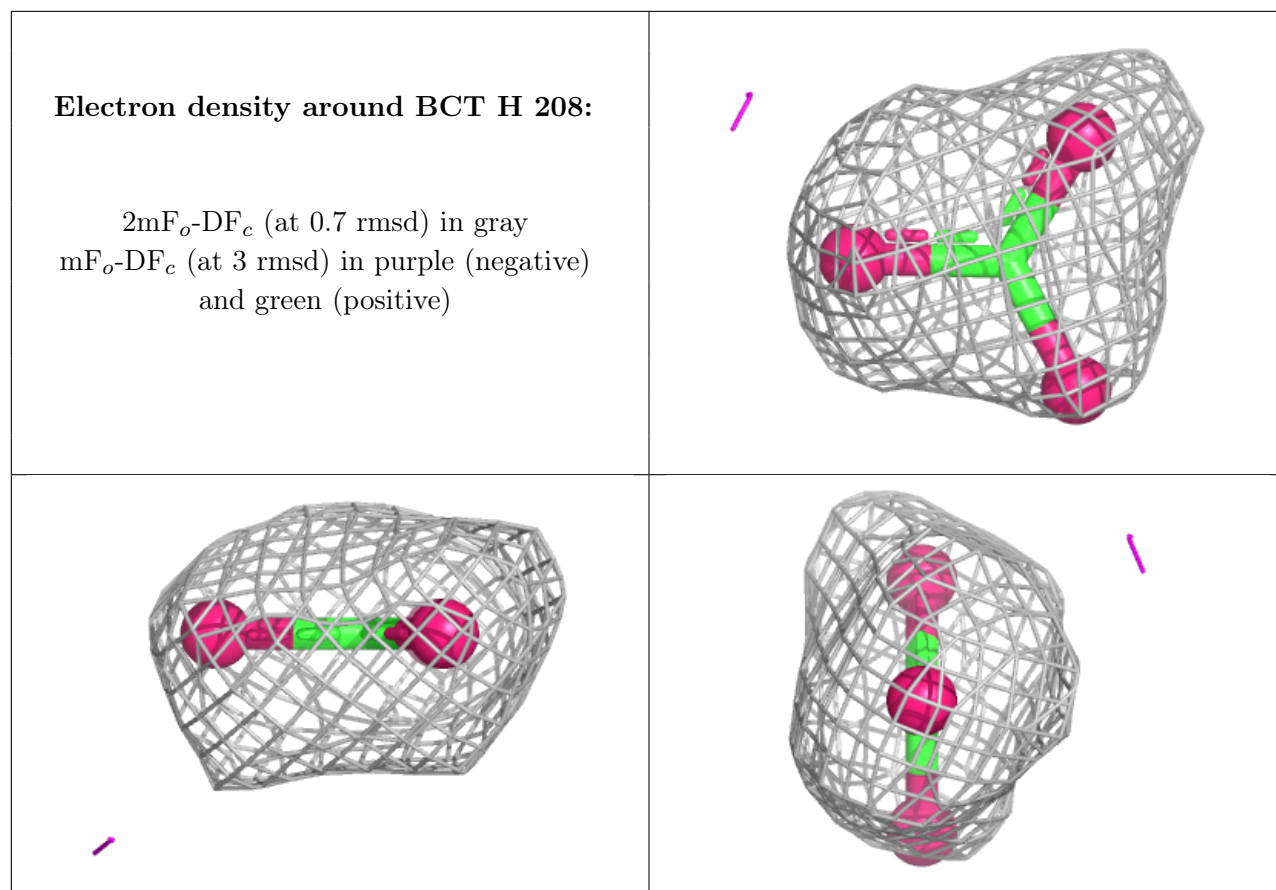




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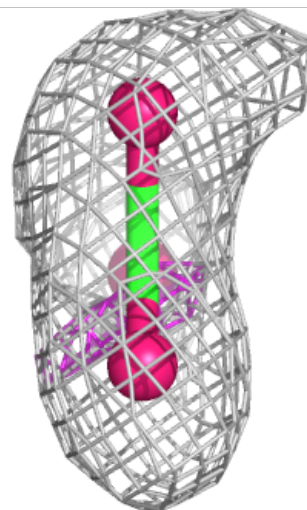
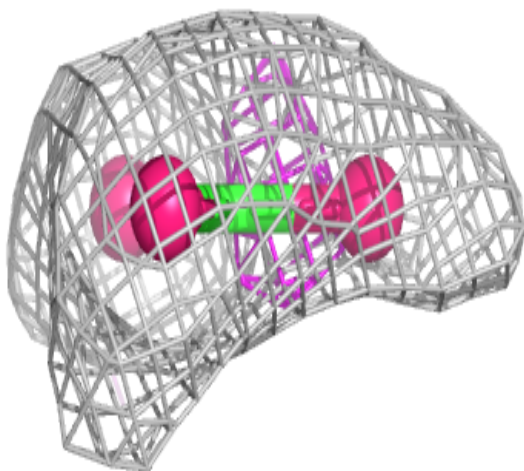
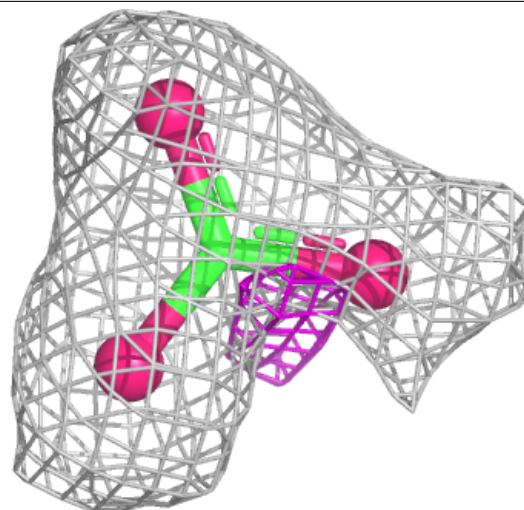
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and green (positive)

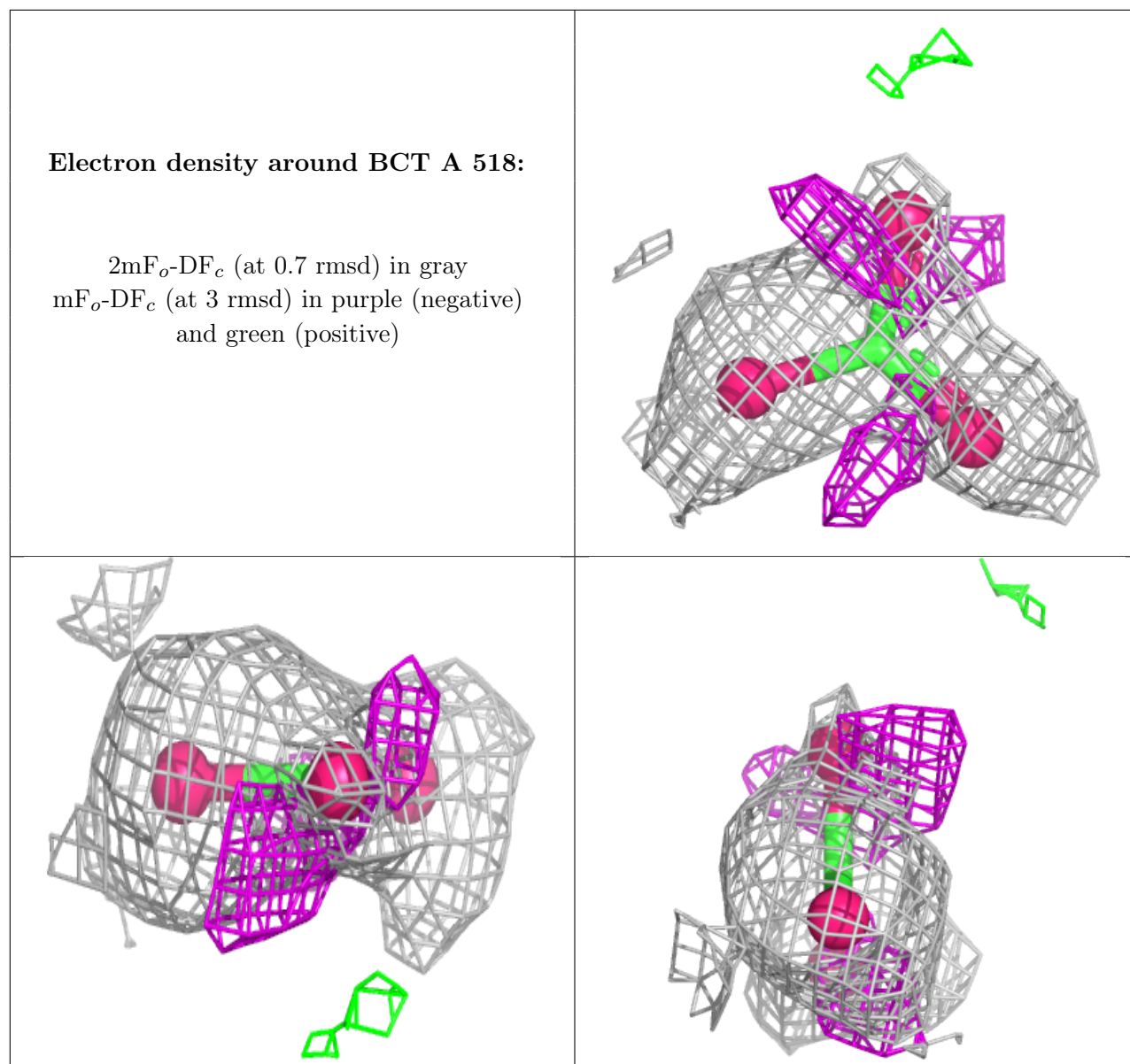


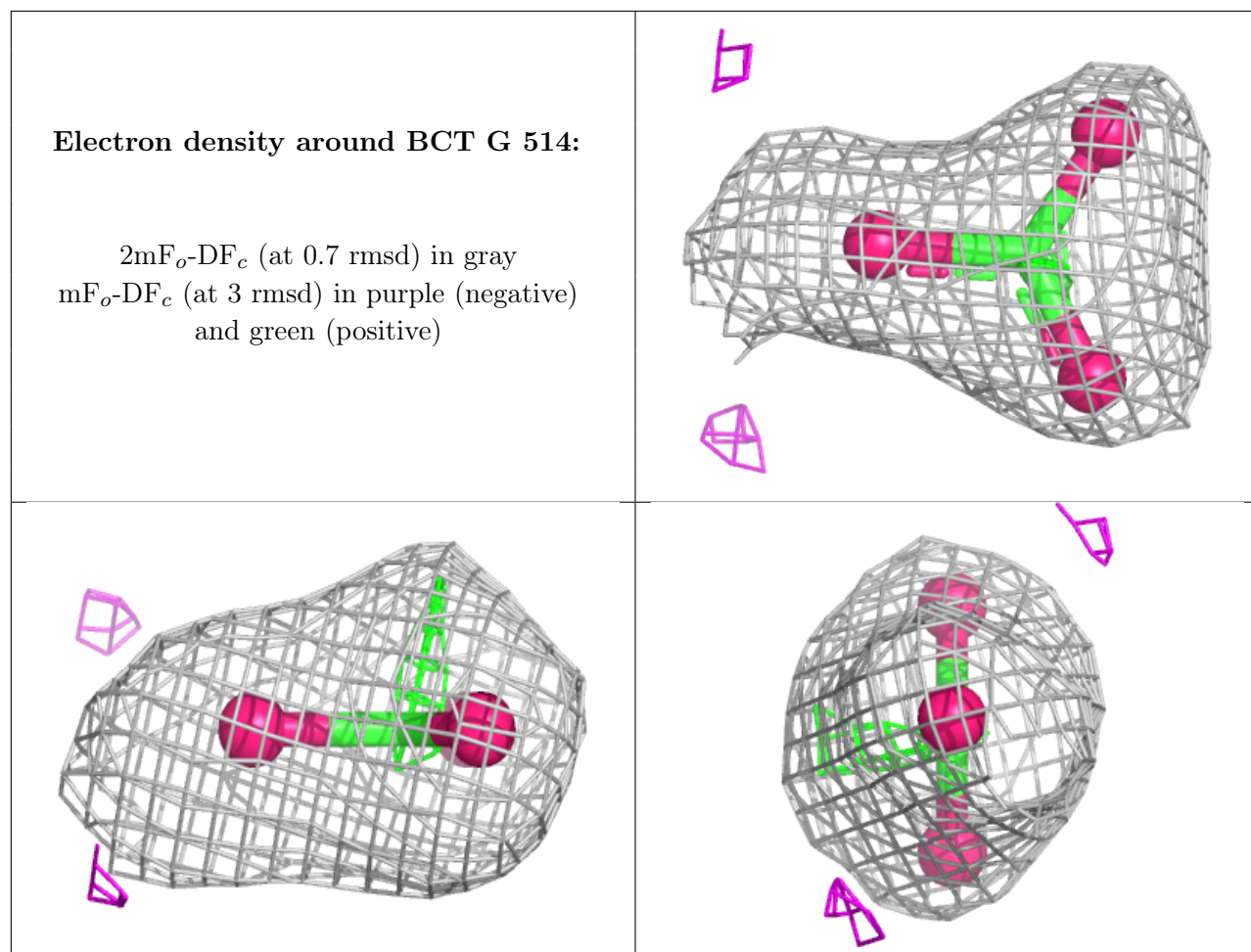


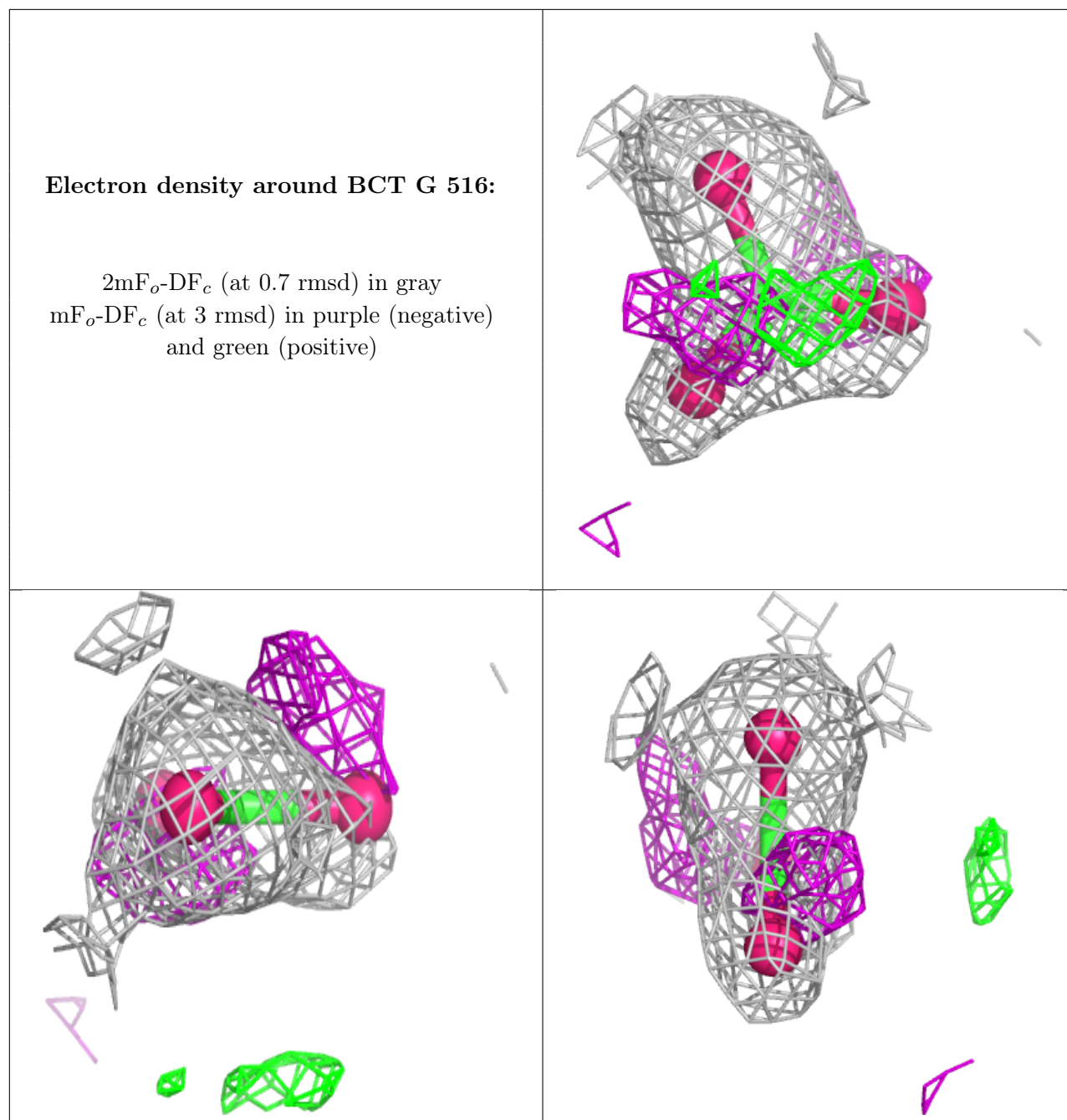
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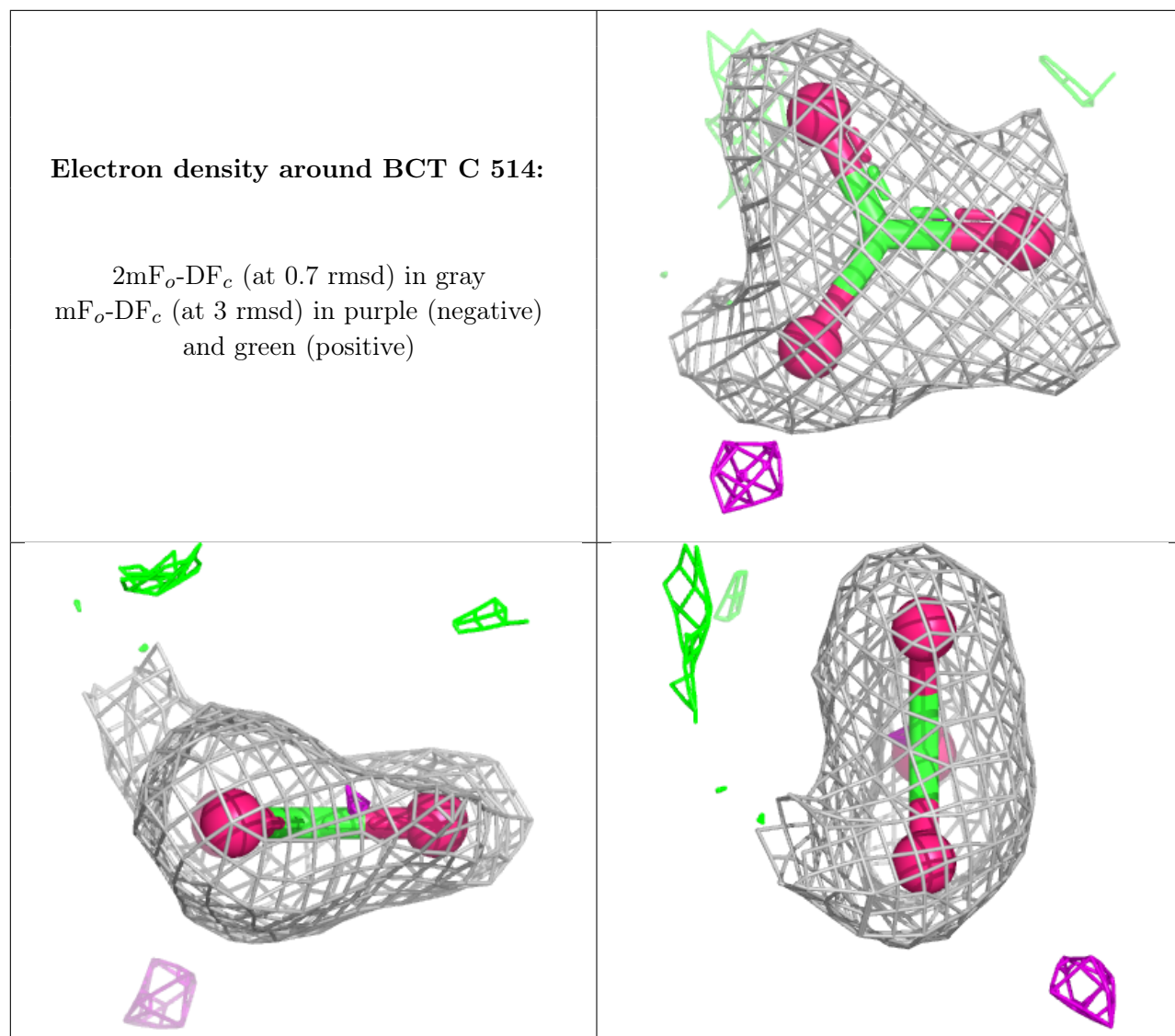
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and green (positive)

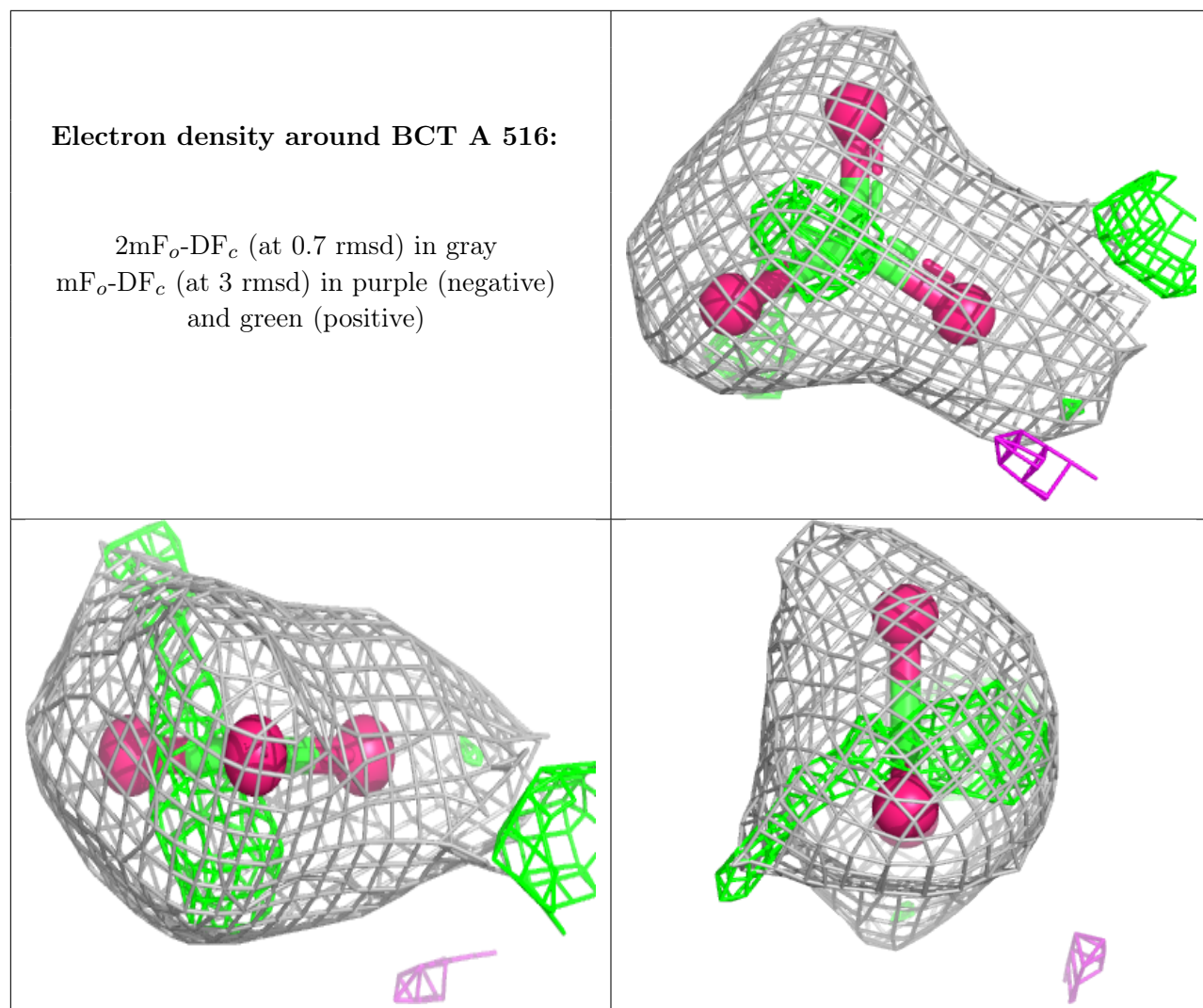


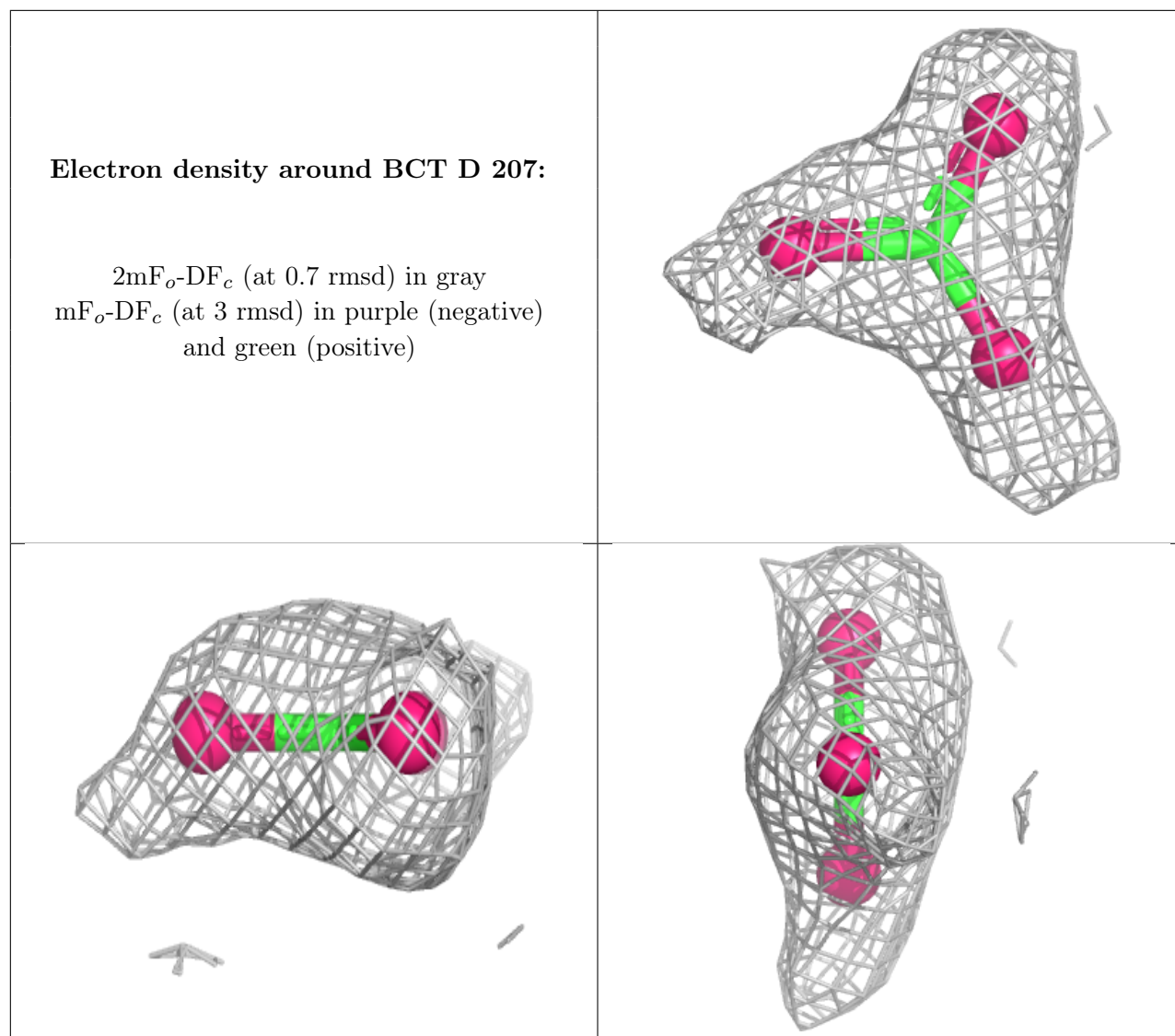






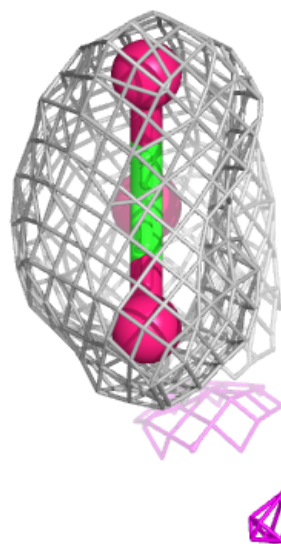
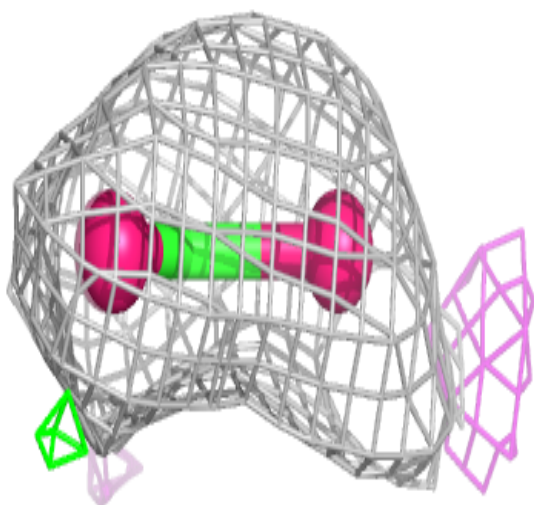
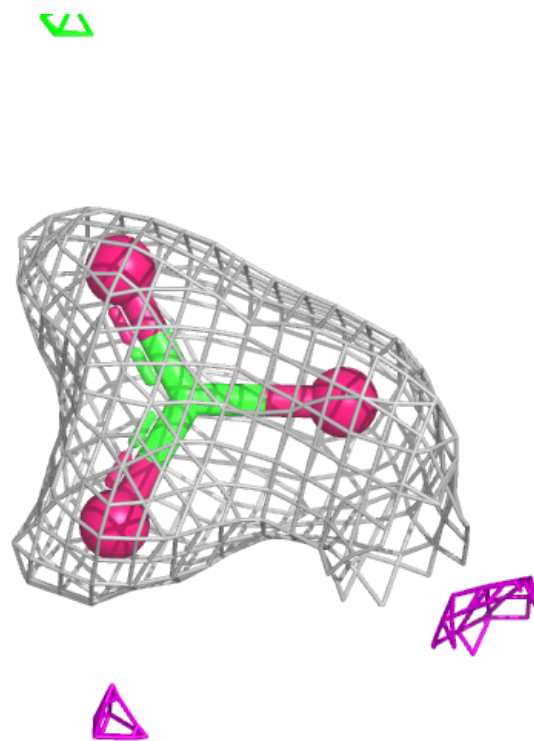






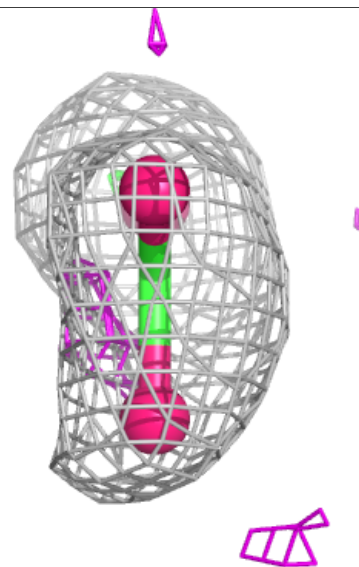
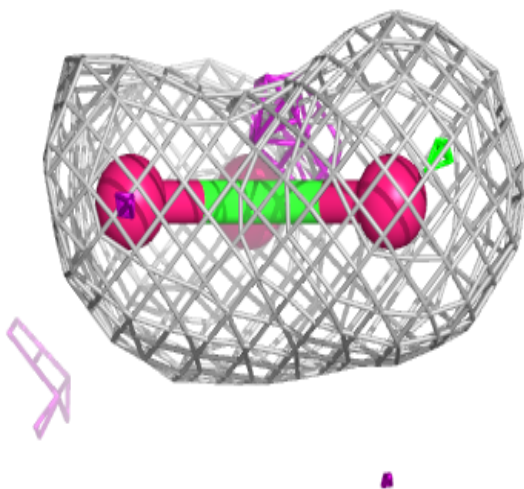
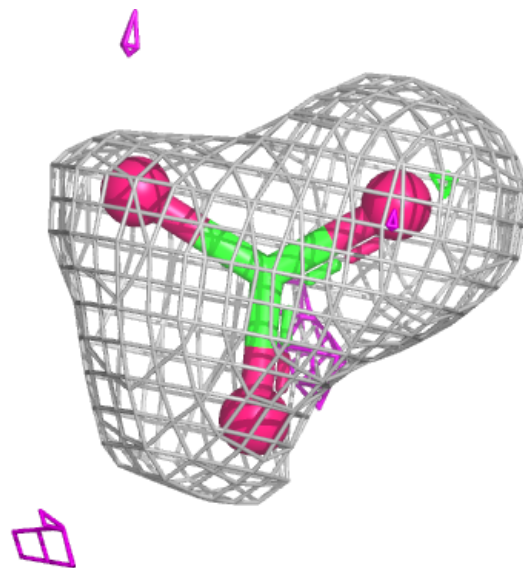
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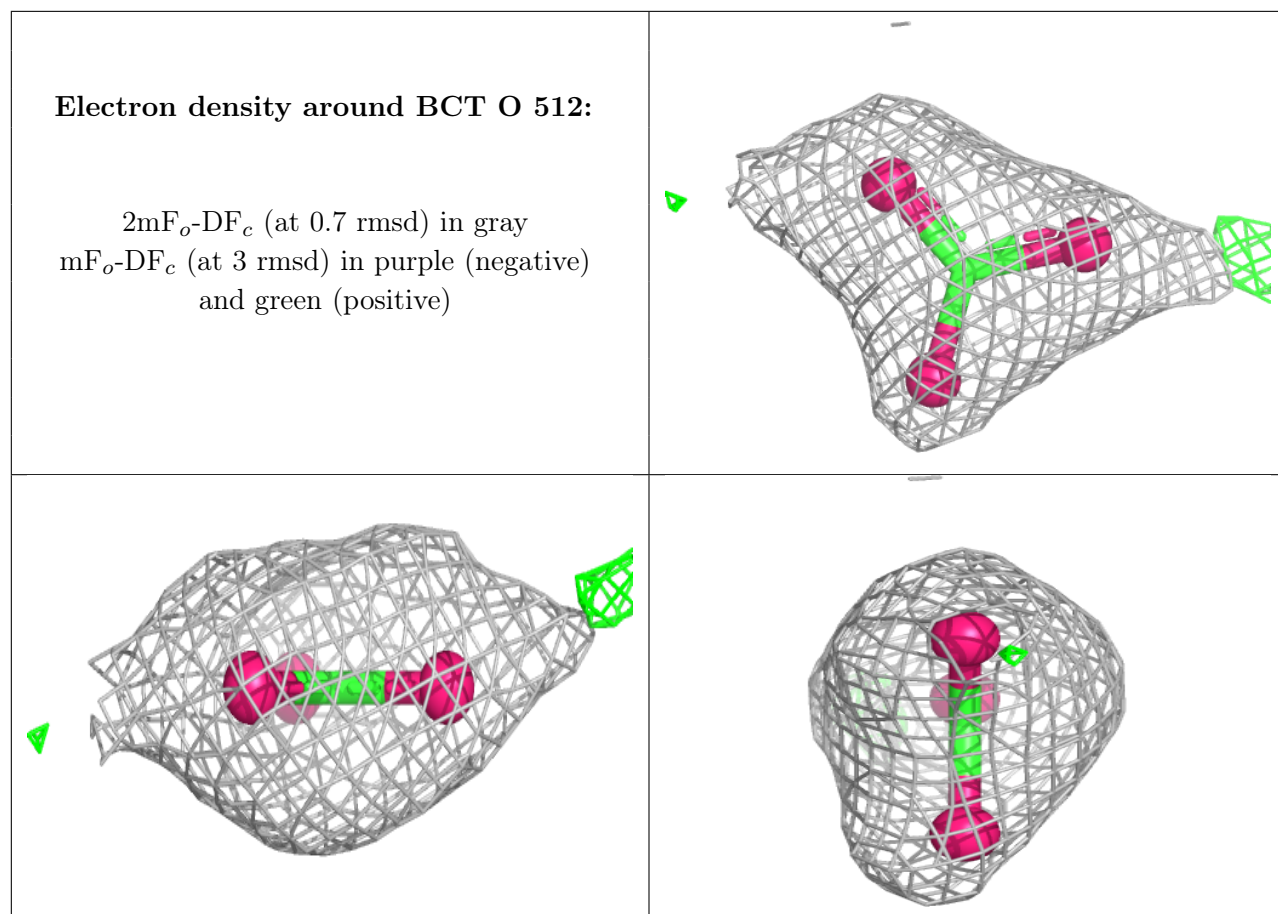
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

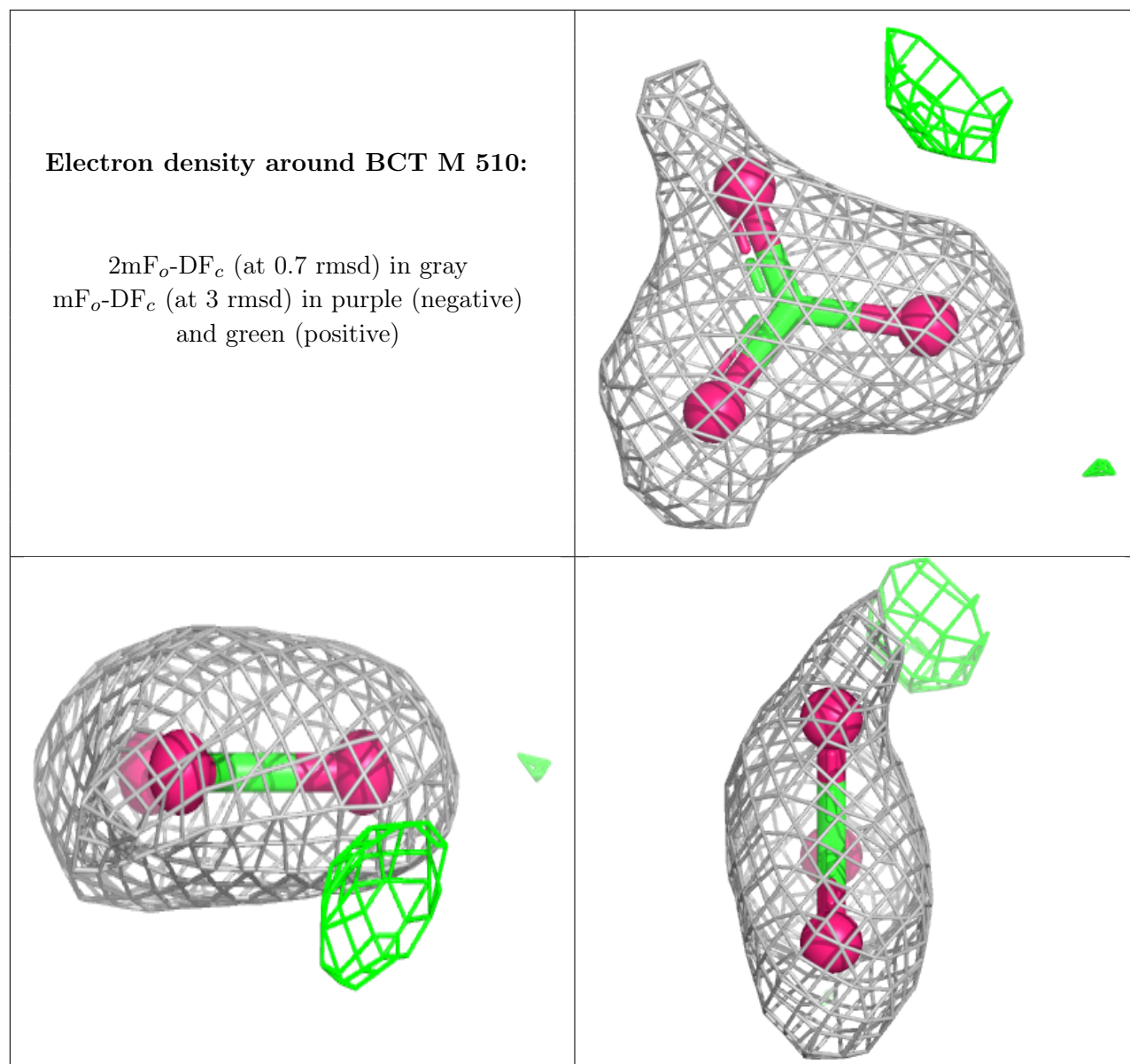


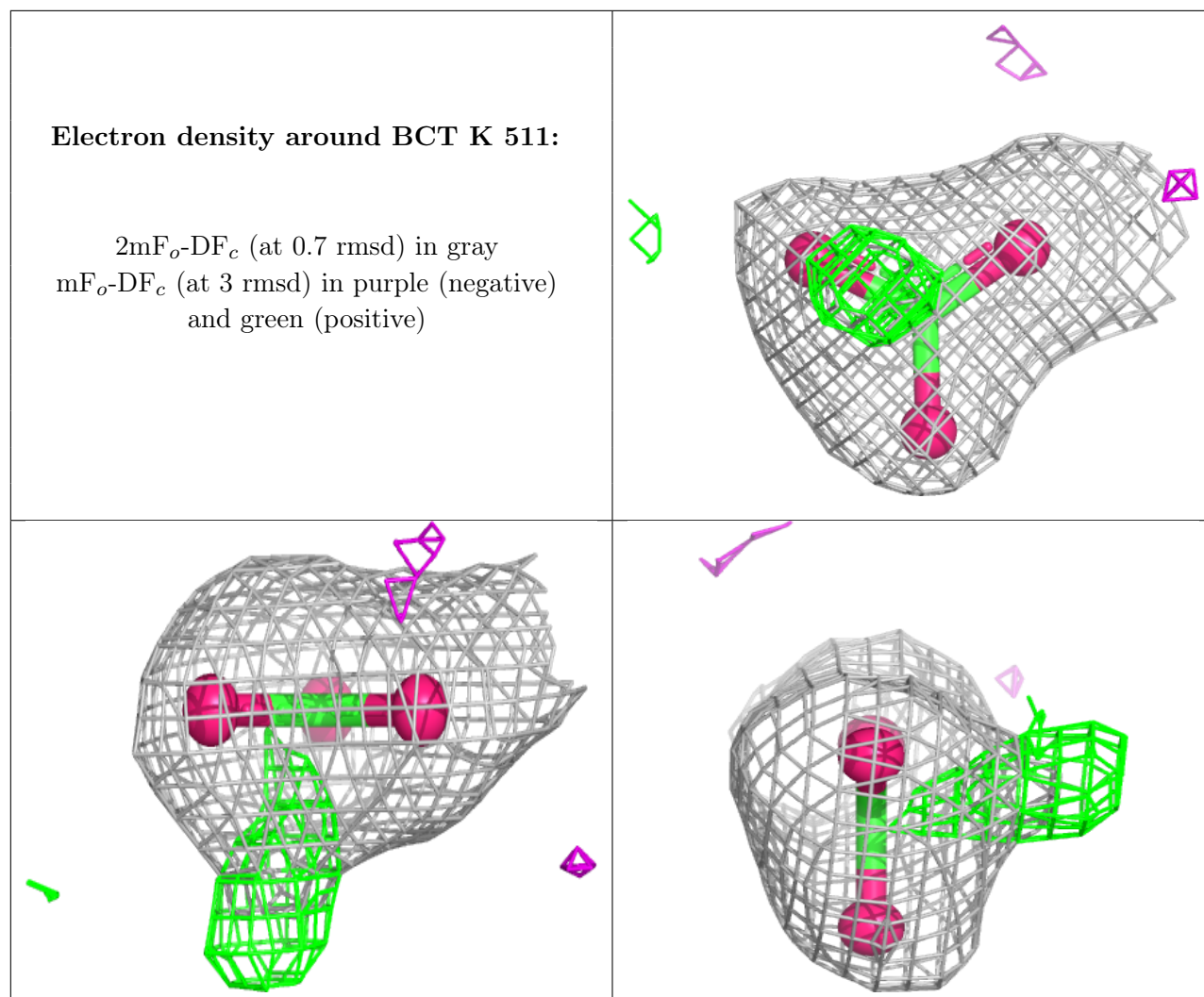
**Electron density around BCT M 511:**

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



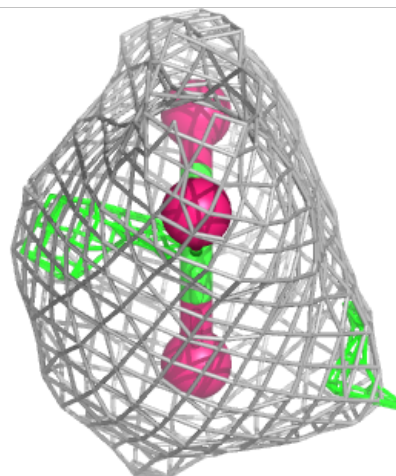
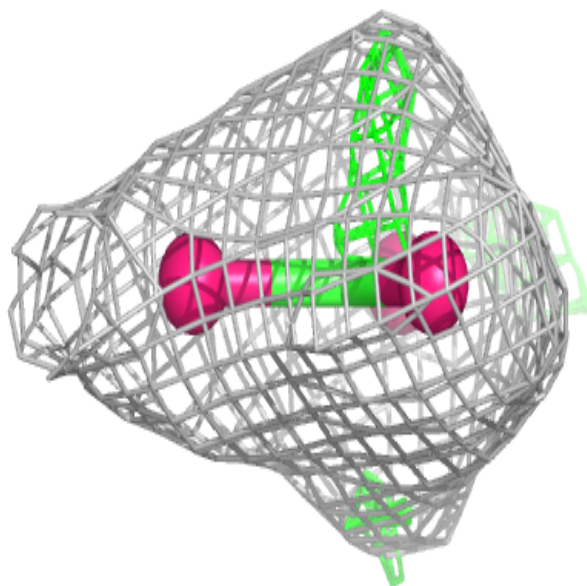
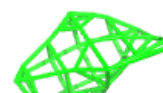
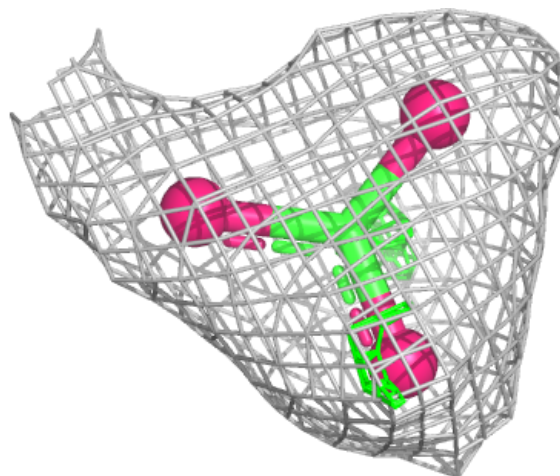


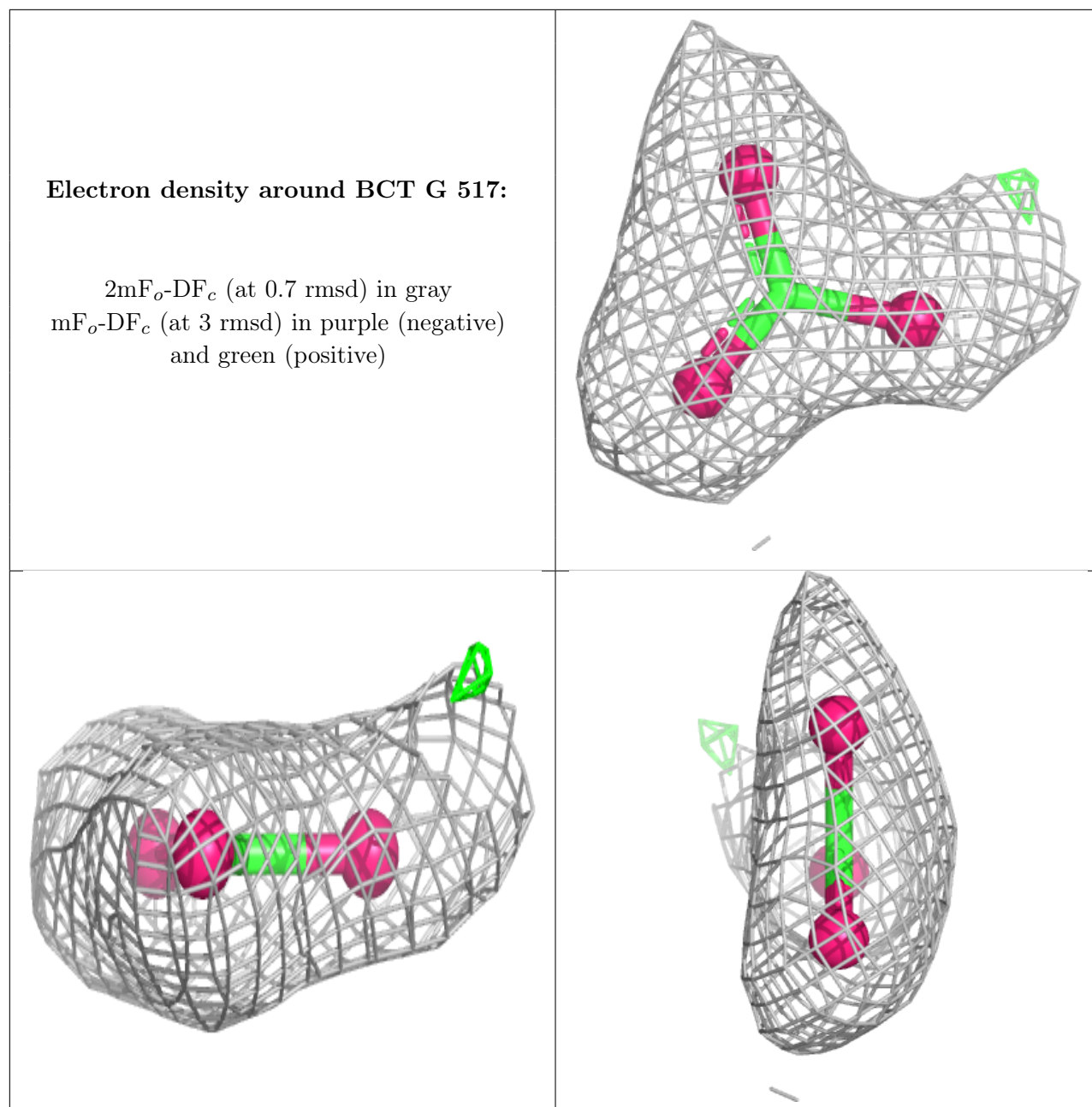




**Electron density around BCT E 513:**

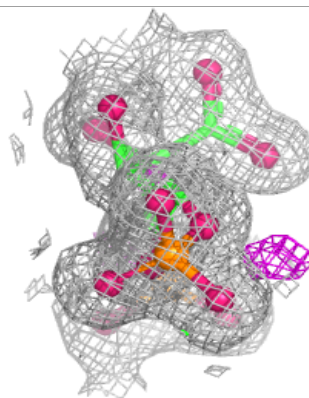
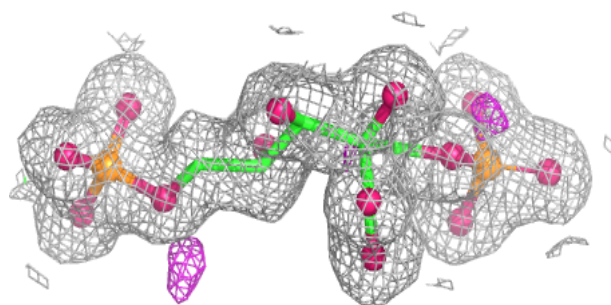
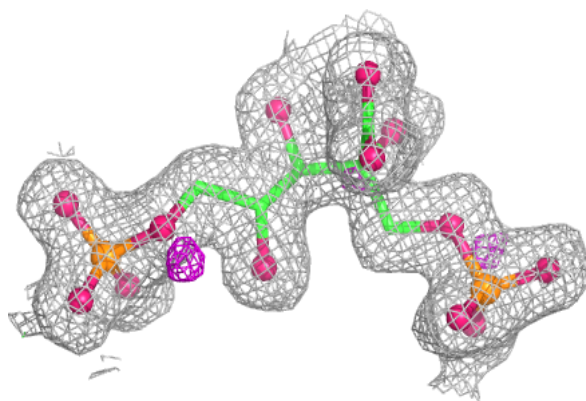
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



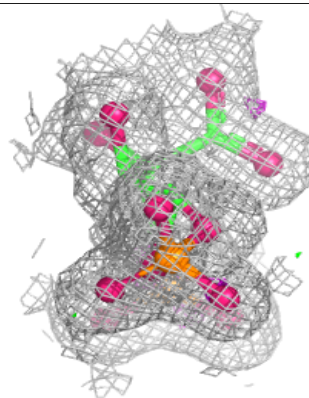
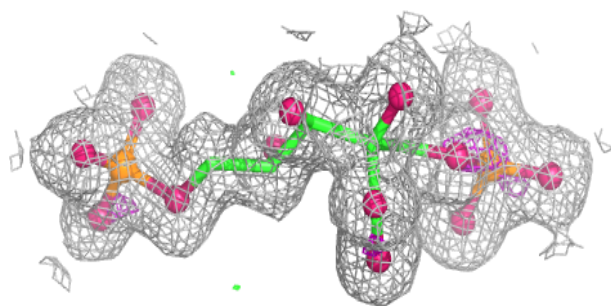
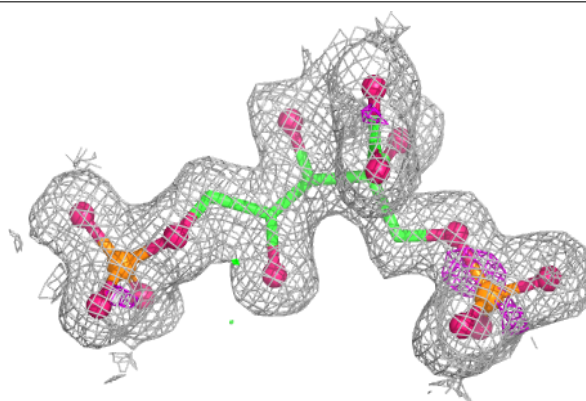


**Electron density around CAP M 502:**

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

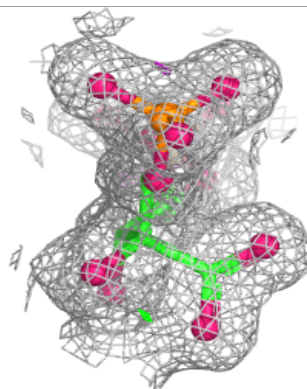
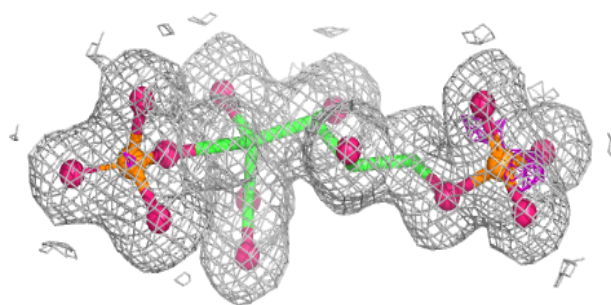
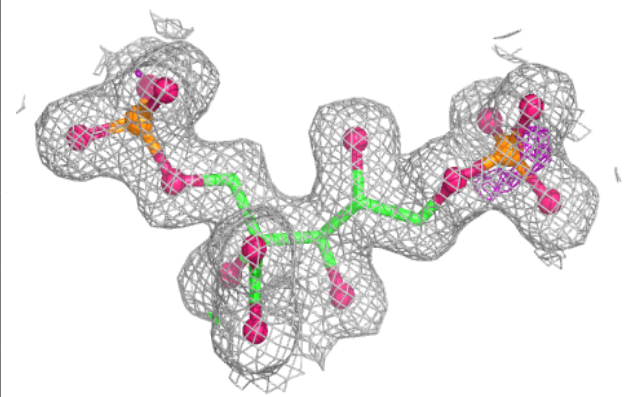
**Electron density around CAP A 502:**

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

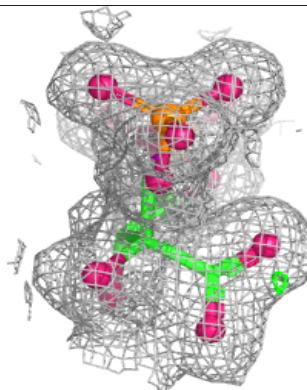
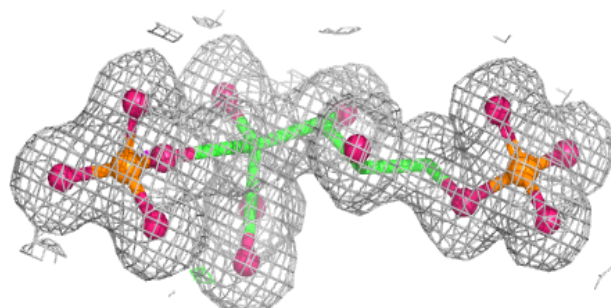
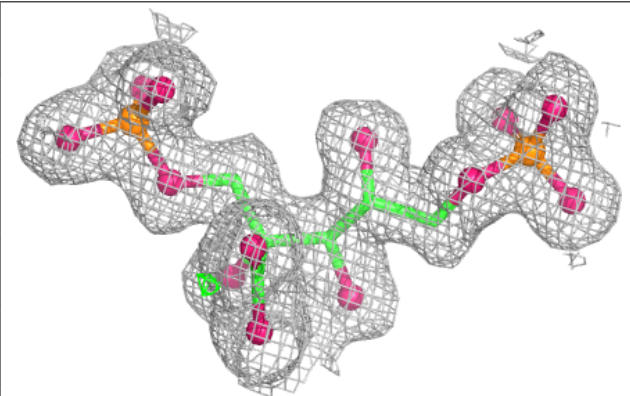


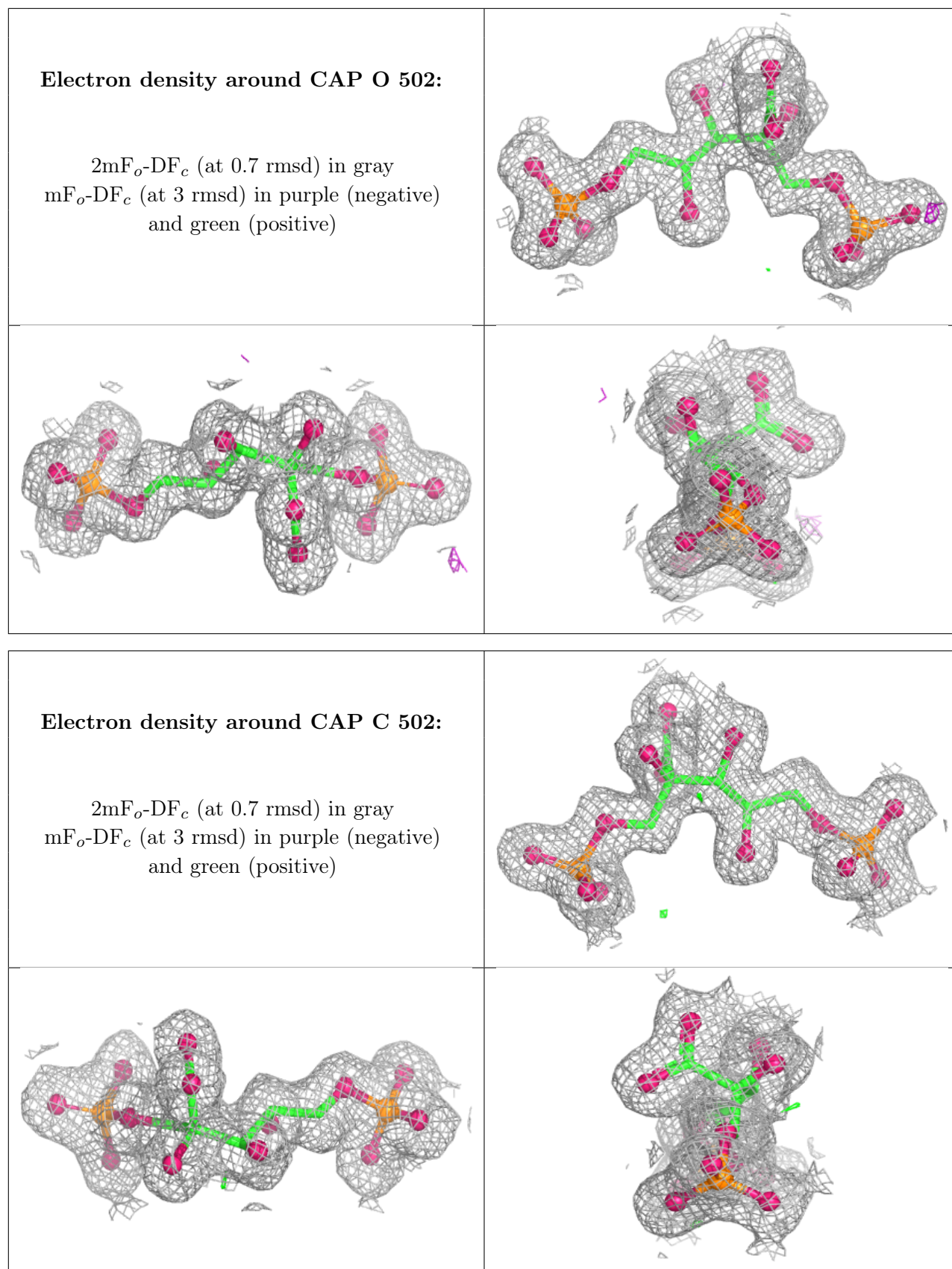
**Electron density around CAP E 502:**

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

**Electron density around CAP K 502:**

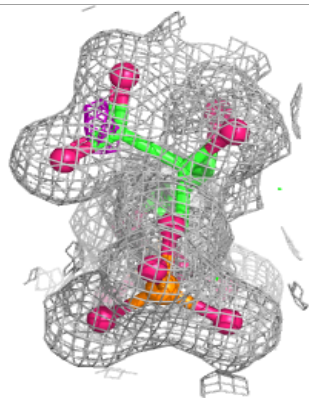
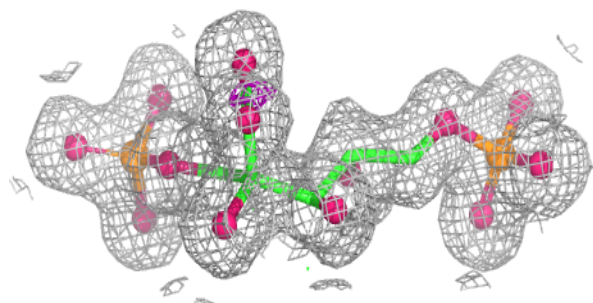
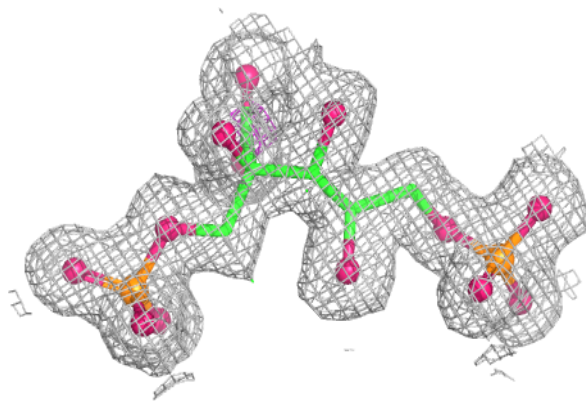
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



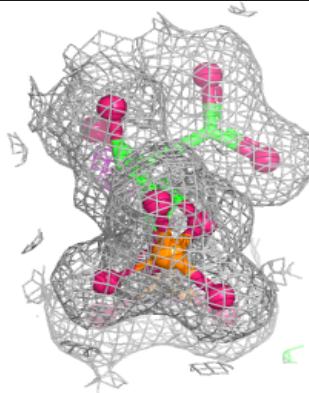
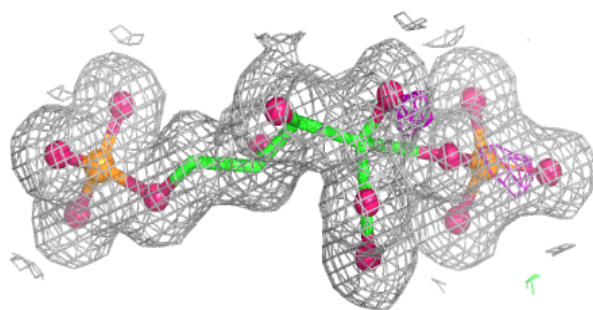
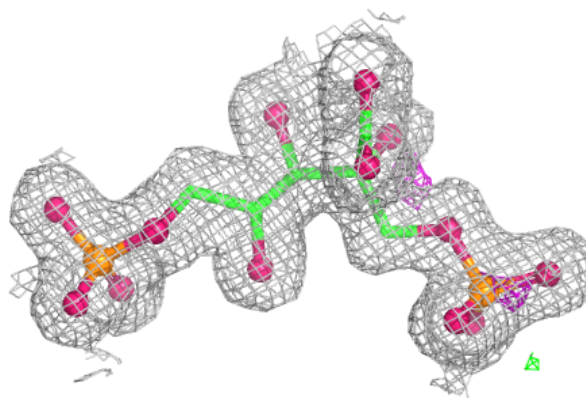


**Electron density around CAP G 502:**

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

**Electron density around CAP I 502:**

$2mF_o-DF_c$  (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.