



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2021 – 02:50 PM EST

PDB ID : 5BKQ  
Title : Crystallographic structure of a cubic form of STMV grown from nitrate  
Authors : McPherson, A.  
Deposited on : 2021-03-21  
Resolution : 3.19 Å(reported)

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

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.24  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.24

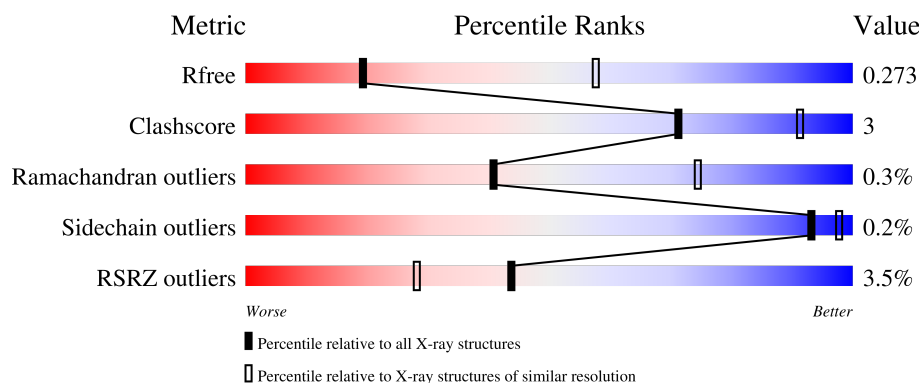
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	159	
1	B	159	
1	C	159	
1	D	159	
1	E	159	

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Mol	Chain	Length	Quality of chain
1	F	159	
1	G	159	
1	GG	159	
1	H	159	
1	HH	159	
1	I	159	
1	II	159	
1	J	159	
1	JJ	159	
1	K	159	
1	KK	159	
1	L	159	
1	M	159	
1	N	159	
1	O	159	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NO3	B	306	-	-	-	X
2	NO3	B	307	-	-	X	-
2	NO3	B	312	-	-	-	X
2	NO3	D	302	-	-	-	X
2	NO3	E	405	-	-	X	-
2	NO3	G	501	-	-	-	X
2	NO3	GG	205	-	-	-	X
2	NO3	GG	206	-	-	X	-
2	NO3	H	504	-	-	X	-
2	NO3	H	507	-	-	-	X
2	NO3	H	508	-	-	X	-
2	NO3	HH	302	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NO3	HH	304	-	-	-	X
2	NO3	I	604	-	-	-	X
2	NO3	I	606	-	-	-	X
2	NO3	II	204	-	-	-	X
2	NO3	J	902	-	-	-	X
2	NO3	J	905	-	-	-	X
2	NO3	K	1504	-	-	-	X
2	NO3	L	508	-	-	-	X
2	NO3	M	504	-	-	-	X
2	NO3	M	505	-	-	-	X
2	NO3	M	507	-	-	X	X
2	NO3	N	1305	-	-	-	X
2	NO3	N	1309	-	-	-	X
2	NO3	O	301	-	-	-	X
3	MG	II	203	-	-	-	X
3	MG	JJ	203	-	-	-	X



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48091 atoms, of which 22720 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 Coat protein.

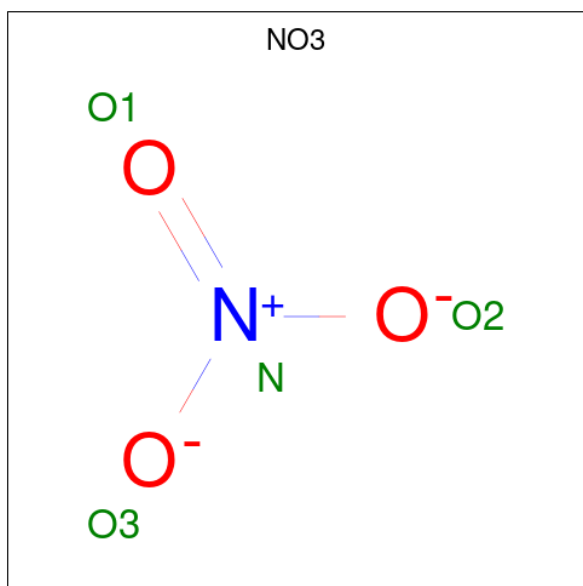
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	150	Total 2323	C 741	H 1145	N 210	O 220	S 7	0	13	0
1	B	151	Total 2273	C 736	H 1097	N 211	O 222	S 7	1	12	0
1	C	151	Total 2304	C 741	H 1119	N 213	O 224	S 7	2	22	0
1	D	151	Total 2312	C 741	H 1129	N 212	O 223	S 7	2	21	0
1	E	149	Total 2276	C 731	H 1112	N 206	O 220	S 7	0	19	0
1	F	144	Total 2298	C 723	H 1152	N 202	O 214	S 7	19	17	0
1	G	155	Total 2336	C 765	H 1119	N 218	O 227	S 7	2	15	0
1	H	145	Total 2306	C 729	H 1152	N 203	O 215	S 7	0	19	0
1	I	156	Total 2348	C 764	H 1130	N 219	O 228	S 7	1	13	0
1	J	147	Total 2302	C 732	H 1138	N 205	O 220	S 7	2	15	0
1	K	146	Total 2341	C 736	H 1170	N 209	O 220	S 6	16	15	0
1	L	151	Total 2407	C 767	H 1187	N 216	O 229	S 8	14	14	0
1	M	150	Total 2375	C 757	H 1170	N 214	O 227	S 7	1	11	0
1	N	150	Total 2365	C 752	H 1167	N 211	O 226	S 9	15	13	0
1	O	149	Total 2285	C 729	H 1123	N 205	O 221	S 7	0	23	0
1	GG	145	Total 2245	C 710	H 1116	N 200	O 212	S 7	0	19	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HH	144	Total	C	H	N	O	S	1	16	0
			2283	719	1145	200	212	7			
1	II	142	Total	C	H	N	O	S	2	16	0
			2235	709	1113	199	206	8			
1	JJ	144	Total	C	H	N	O	S	0	16	0
			2230	703	1112	199	210	6			
1	KK	144	Total	C	H	N	O	S	0	14	0
			2247	707	1124	199	210	7			

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 4	N 1	O 3	0	0
2	F	1	Total 4	N 1	O 3	0	0
2	G	1	Total 4	N 1	O 3	0	0
2	G	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	H	1	Total 4	N 1	O 3	0	0
2	I	1	Total 4	N 1	O 3	0	0
2	I	1	Total 4	N 1	O 3	0	0
2	I	1	Total 4	N 1	O 3	0	0
2	I	1	Total 4	N 1	O 3	0	0
2	I	1	Total 4	N 1	O 3	0	0
2	I	1	Total 4	N 1	O 3	0	0
2	J	1	Total 4	N 1	O 3	0	0
2	J	1	Total 4	N 1	O 3	0	0
2	J	1	Total 4	N 1	O 3	0	0
2	J	1	Total 4	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	N	O	0	0
			4	1	3		
2	K	1	Total	N	O	0	0
			4	1	3		
2	K	1	Total	N	O	0	0
			4	1	3		
2	K	1	Total	N	O	0	0
			4	1	3		
2	K	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	L	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		
2	M	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	N	1	Total 4	N 1	O 3	0	0
2	O	1	Total 4	N 1	O 3	0	0
2	O	1	Total 4	N 1	O 3	0	0
2	O	1	Total 4	N 1	O 3	0	0
2	O	1	Total 4	N 1	O 3	0	0
2	GG	1	Total 4	N 1	O 3	0	0
2	GG	1	Total 4	N 1	O 3	0	0
2	GG	1	Total 4	N 1	O 3	0	0
2	GG	1	Total 4	N 1	O 3	0	0
2	GG	1	Total 4	N 1	O 3	0	0
2	GG	1	Total 4	N 1	O 3	0	0
2	HH	1	Total 4	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	HH	1	Total N O 4 1 3	0	0
2	HH	1	Total N O 4 1 3	0	0
2	HH	1	Total N O 4 1 3	0	0
2	II	1	Total N O 4 1 3	0	0
2	II	1	Total N O 4 1 3	0	0
2	II	1	Total N O 4 1 3	0	0
2	II	1	Total N O 4 1 3	0	0
2	JJ	1	Total N O 4 1 3	0	0
2	JJ	1	Total N O 4 1 3	0	0
2	KK	1	Total N O 4 1 3	0	0
2	KK	1	Total N O 4 1 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0
3	O	1	Total Mg 1 1	0	0
3	II	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	JJ	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total 92	O 92	0	0
4	B	54	Total 54	O 54	0	0
4	C	55	Total 55	O 55	0	0
4	D	81	Total 81	O 81	0	0
4	E	73	Total 73	O 73	0	0
4	F	63	Total 63	O 63	0	0
4	G	87	Total 87	O 87	0	0
4	H	77	Total 77	O 77	0	0
4	I	118	Total 118	O 118	0	0
4	J	93	Total 93	O 93	0	0
4	K	96	Total 96	O 96	0	0
4	L	108	Total 108	O 108	0	0
4	M	55	Total 55	O 55	0	0
4	N	54	Total 54	O 54	0	0
4	O	116	Total 116	O 116	0	0
4	GG	54	Total 54	O 54	0	0
4	HH	115	Total 115	O 115	0	0
4	II	58	Total 58	O 58	0	0

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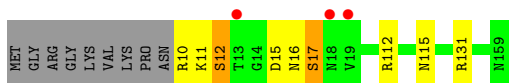
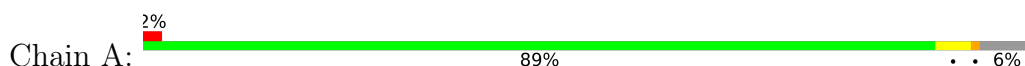
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	JJ	41	Total 41	O 41	0	0
4	KK	93	Total 93	O 93	0	0

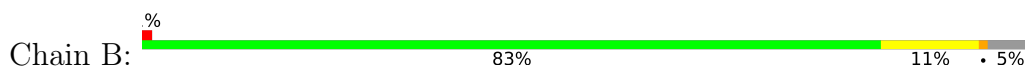
### 3 Residue-property plots [i](#)

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

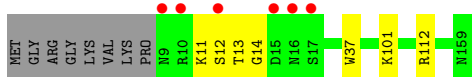
- Molecule 1: Coat protein



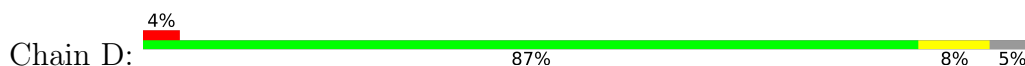
- Molecule 1: Coat protein



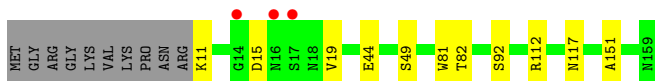
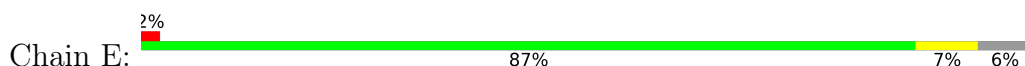
- Molecule 1: Coat protein




- Molecule 1: Coat protein

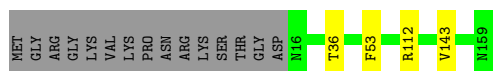


- Molecule 1: Coat protein




- Molecule 1: Coat protein

Chain F:  88% 9%




• Molecule 1: Coat protein

Chain G:  88% 9%

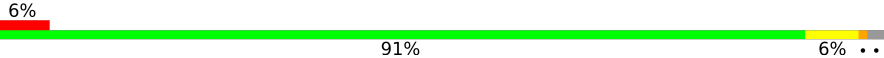


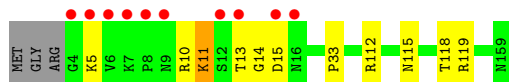
• Molecule 1: Coat protein

Chain H:  84% 8% 9%




• Molecule 1: Coat protein

Chain I:  91% 6%




• Molecule 1: Coat protein

Chain J:  86% 7% 8%




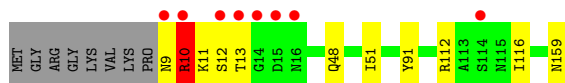
• Molecule 1: Coat protein

Chain K:  87% 5% 8%

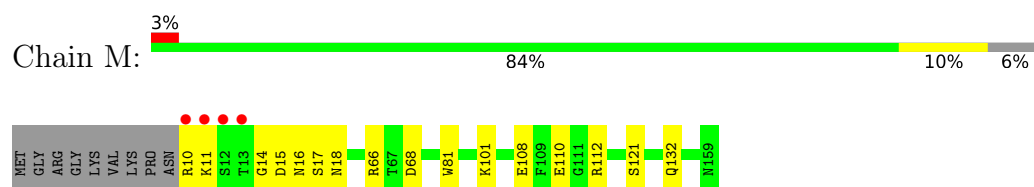


• Molecule 1: Coat protein

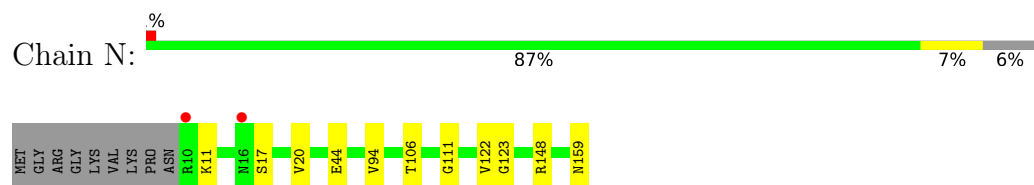
Chain L:  88% 6% 5%



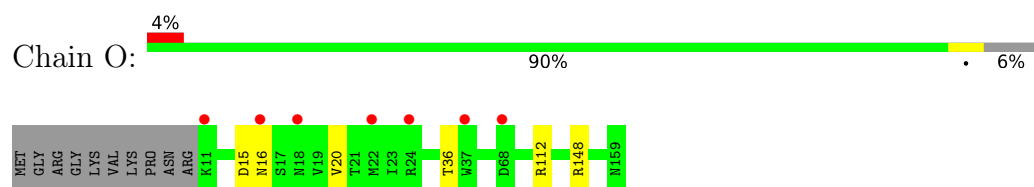
- Molecule 1: Coat protein



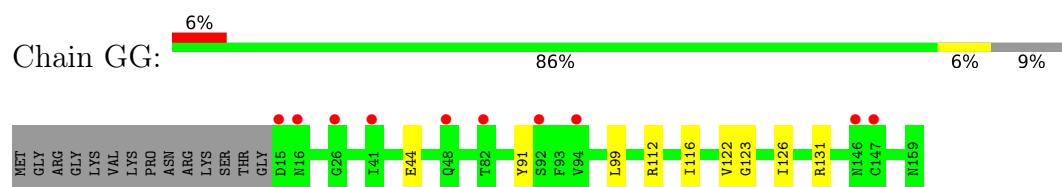
- Molecule 1: Coat protein



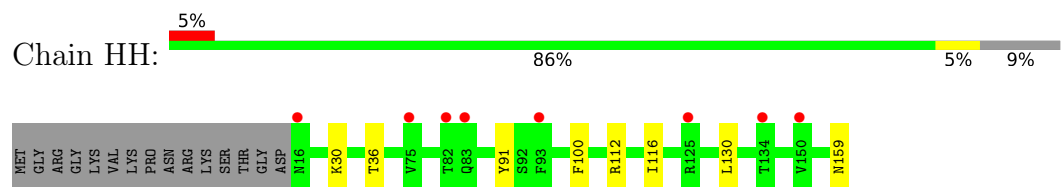
- Molecule 1: Coat protein



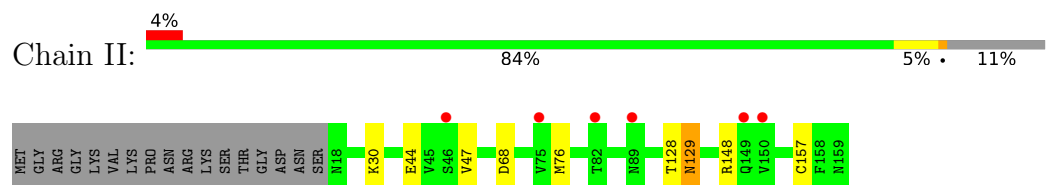
- Molecule 1: Coat protein



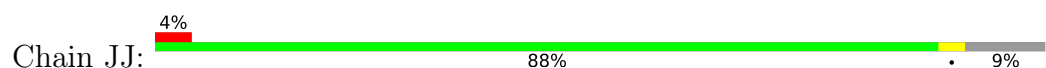
- Molecule 1: Coat protein

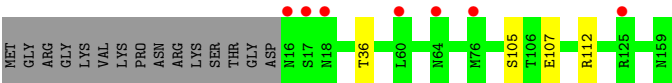


- Molecule 1: Coat protein

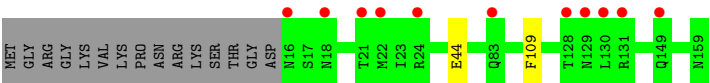
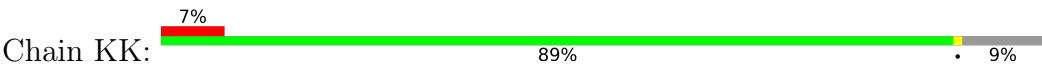


- Molecule 1: Coat protein





● Molecule 1: Coat protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.05Å 234.05Å 234.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.00 – 3.19 104.67 – 3.19	Depositor EDS
% Data completeness (in resolution range)	64.2 (75.00-3.19) 53.8 (104.67-3.19)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.261 , 0.273 0.242 , 0.273	Depositor DCC
$R_{free}$ test set	2302 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	48091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: NO3, MG

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	0.26	0/1226	0.53	0/1667
1	B	0.27	0/1215	0.54	0/1652
1	C	0.26	0/1228	0.53	0/1670
1	D	0.26	0/1245	0.52	0/1694
1	E	0.26	0/1218	0.51	0/1657
1	F	0.26	0/1222	0.53	0/1665
1	G	0.26	0/1279	0.53	0/1739
1	GG	0.25	0/1172	0.52	0/1596
1	H	0.27	0/1218	0.53	0/1660
1	HH	0.25	0/1202	0.52	0/1638
1	I	0.25	0/1257	0.54	0/1708
1	II	0.25	0/1197	0.53	0/1628
1	J	0.26	0/1223	0.52	0/1664
1	JJ	0.26	0/1142	0.52	0/1556
1	K	0.26	0/1256	0.52	0/1711
1	KK	0.25	0/1177	0.52	0/1602
1	L	0.26	0/1303	0.54	0/1771
1	M	0.27	0/1275	0.53	0/1732
1	N	0.26	0/1286	0.52	0/1748
1	O	0.26	0/1192	0.53	0/1622
All	All	0.26	0/24533	0.53	0/33380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1178	1145	1149	6	0
1	B	1176	1097	1150	18	0
1	C	1185	1119	1119	5	1
1	D	1183	1129	1117	12	4
1	E	1164	1112	1107	10	0
1	F	1146	1152	1085	5	0
1	G	1217	1119	1180	18	0
1	GG	1129	1116	1052	6	0
1	H	1154	1152	1106	9	1
1	HH	1138	1145	1097	6	0
1	I	1218	1130	1192	8	0
1	II	1122	1113	1088	13	0
1	J	1164	1138	1130	9	0
1	JJ	1118	1112	1079	7	0
1	K	1171	1170	1114	6	0
1	KK	1123	1124	1075	1	0
1	L	1220	1187	1199	10	0
1	M	1205	1170	1201	14	0
1	N	1198	1167	1164	10	0
1	O	1162	1123	1104	6	0
2	A	16	0	0	0	0
2	B	48	0	0	3	1
2	C	16	0	0	1	0
2	D	8	0	0	1	0
2	E	24	0	0	4	0
2	F	8	0	0	0	0
2	G	8	0	0	0	0
2	GG	24	0	0	0	4
2	H	28	0	0	5	0
2	HH	16	0	0	0	0
2	I	24	0	0	1	0
2	II	16	0	0	0	0
2	J	20	0	0	0	0
2	JJ	8	0	0	0	0
2	K	16	0	0	0	0
2	KK	8	0	0	0	0
2	L	32	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	36	0	0	4	0
2	N	36	0	0	0	0
2	O	16	0	0	0	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	II	1	0	0	0	0
3	JJ	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
4	A	92	0	0	0	1
4	B	54	0	0	0	0
4	C	55	0	0	0	0
4	D	81	0	0	1	0
4	E	73	0	0	1	0
4	F	63	0	0	0	0
4	G	87	0	0	1	0
4	GG	54	0	0	1	0
4	H	77	0	0	2	2
4	HH	115	0	0	0	0
4	I	118	0	0	0	0
4	II	58	0	0	2	1
4	J	93	0	0	2	1
4	JJ	41	0	0	0	0
4	K	96	0	0	2	0
4	KK	93	0	0	0	0
4	L	108	0	0	3	1
4	M	55	0	0	0	0
4	N	54	0	0	1	0
4	O	116	0	0	1	0
All	All	25371	22720	22508	164	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 164 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:G:13:THR:HG23	1:G:16:ASN:HA	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:ASN:O	1:L:10:ARG:HB3	1.76	0.86
1:L:10:ARG:HG3	1:L:11:LYS:N	1.91	0.85
1:M:14:GLY:HA2	1:M:15:ASP:HB2	1.61	0.83
1:O:148:ARG:NH2	4:O:401:HOH:O	2.12	0.81

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ARG:O	2:GG:206:NO3:N[12_665]	1.30	0.90
1:D:112:ARG:O	2:GG:206:NO3:O2[12_665]	1.64	0.56
1:D:112:ARG:O	2:GG:206:NO3:O3[12_665]	1.86	0.34
1:D:112:ARG:O	2:GG:206:NO3:O1[12_665]	1.95	0.25
4:H:628:HOH:O	4:H:628:HOH:O[4_565]	1.98	0.22

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	153/159 (96%)	142 (93%)	10 (6%)	1 (1%)	22	61
1	B	151/159 (95%)	132 (87%)	17 (11%)	2 (1%)	12	47
1	C	153/159 (96%)	138 (90%)	15 (10%)	0	100	100
1	D	155/159 (98%)	137 (88%)	18 (12%)	0	100	100
1	E	152/159 (96%)	141 (93%)	11 (7%)	0	100	100
1	F	152/159 (96%)	142 (93%)	10 (7%)	0	100	100
1	G	159/159 (100%)	145 (91%)	13 (8%)	1 (1%)	25	64
1	GG	146/159 (92%)	130 (89%)	16 (11%)	0	100	100
1	H	152/159 (96%)	138 (91%)	13 (9%)	1 (1%)	22	61
1	HH	150/159 (94%)	137 (91%)	13 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	12	47
1	II	148/159 (93%)	138 (93%)	9 (6%)	1 (1%)	22	61
1	J	152/159 (96%)	140 (92%)	12 (8%)	0	100	100
1	JJ	142/159 (89%)	133 (94%)	9 (6%)	0	100	100
1	K	156/159 (98%)	147 (94%)	9 (6%)	0	100	100
1	KK	146/159 (92%)	136 (93%)	9 (6%)	1 (1%)	22	61
1	L	163/159 (102%)	147 (90%)	15 (9%)	1 (1%)	25	64
1	M	159/159 (100%)	146 (92%)	13 (8%)	0	100	100
1	N	161/159 (101%)	150 (93%)	11 (7%)	0	100	100
1	O	149/159 (94%)	134 (90%)	15 (10%)	0	100	100
All	All	3056/3180 (96%)	2797 (92%)	249 (8%)	10 (0%)	41	74

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	G	12	SER
1	L	10	ARG
1	II	129	ASN
1	KK	109	PHE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	138/140 (99%)	137 (99%)	1 (1%)	84	94
1	B	136/140 (97%)	136 (100%)	0	100	100
1	C	138/140 (99%)	138 (100%)	0	100	100
1	D	140/140 (100%)	140 (100%)	0	100	100
1	E	137/140 (98%)	137 (100%)	0	100	100
1	F	138/140 (99%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	144/140 (103%)	143 (99%)	1 (1%)	84	94
1	GG	131/140 (94%)	131 (100%)	0	100	100
1	H	138/140 (99%)	138 (100%)	0	100	100
1	HH	136/140 (97%)	136 (100%)	0	100	100
1	I	141/140 (101%)	141 (100%)	0	100	100
1	II	134/140 (96%)	134 (100%)	0	100	100
1	J	137/140 (98%)	137 (100%)	0	100	100
1	JJ	128/140 (91%)	128 (100%)	0	100	100
1	K	141/140 (101%)	141 (100%)	0	100	100
1	KK	132/140 (94%)	132 (100%)	0	100	100
1	L	148/140 (106%)	146 (99%)	2 (1%)	67	86
1	M	144/140 (103%)	144 (100%)	0	100	100
1	N	146/140 (104%)	145 (99%)	1 (1%)	84	94
1	O	134/140 (96%)	134 (100%)	0	100	100
All	All	2761/2800 (99%)	2756 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	G	159	ASN
1	L	10	ARG
1	L	159	ASN
1	N	159	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 9 are monoatomic - leaving 102 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	$\# Z  > 2$
2	NO3	E	402	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	F	602	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	B	306	-	1,3,3	0.62	0	0,3,3	-	-
2	NO3	M	510	-	1,3,3	0.67	0	0,3,3	-	-
2	NO3	I	606	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	H	502	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	B	303	-	1,3,3	0.60	0	0,3,3	-	-
2	NO3	N	1302	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	O	301	-	1,3,3	0.58	0	0,3,3	-	-
2	NO3	F	601	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	E	406	-	1,3,3	0.61	0	0,3,3	-	-
2	NO3	M	502	-	1,3,3	0.59	0	0,3,3	-	-
2	NO3	GG	202	-	1,3,3	0.61	0	0,3,3	-	-
2	NO3	G	501	-	1,3,3	0.68	0	0,3,3	-	-
2	NO3	A	805	-	1,3,3	0.58	0	0,3,3	-	-
2	NO3	L	501	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	I	605	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	KK	202	-	1,3,3	0.62	0	0,3,3	-	-
2	NO3	B	302	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	C	302	-	1,3,3	0.67	0	0,3,3	-	-
2	NO3	D	301	-	1,3,3	0.62	0	0,3,3	-	-
2	NO3	C	301	-	1,3,3	0.66	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NO3	N	1304	-	1,3,3	0.68	0	0,3,3	-	-
2	NO3	J	905	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	GG	204	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	N	1301	-	1,3,3	0.59	0	0,3,3	-	-
2	NO3	GG	203	-	1,3,3	0.67	0	0,3,3	-	-
2	NO3	GG	205	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	II	201	-	1,3,3	0.61	0	0,3,3	-	-
2	NO3	M	504	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	M	505	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	I	602	-	1,3,3	0.69	0	0,3,3	-	-
2	NO3	M	506	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	J	904	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	I	604	-	1,3,3	0.62	0	0,3,3	-	-
2	NO3	N	1307	-	1,3,3	0.62	0	0,3,3	-	-
2	NO3	E	401	-	1,3,3	0.67	0	0,3,3	-	-
2	NO3	N	1305	-	1,3,3	0.67	0	0,3,3	-	-
2	NO3	E	403	-	1,3,3	0.69	0	0,3,3	-	-
2	NO3	H	507	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	B	308	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	L	502	-	1,3,3	0.61	0	0,3,3	-	-
2	NO3	A	801	-	1,3,3	0.67	0	0,3,3	-	-
2	NO3	J	903	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	H	506	-	1,3,3	0.67	0	0,3,3	-	-
2	NO3	L	503	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	B	301	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	N	1309	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	HH	302	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	L	507	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	N	1303	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	HH	301	-	1,3,3	0.68	0	0,3,3	-	-
2	NO3	GG	201	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	B	312	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	H	505	-	1,3,3	0.60	0	0,3,3	-	-
2	NO3	KK	201	-	1,3,3	0.56	0	0,3,3	-	-
2	NO3	L	506	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	B	304	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	GG	206	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	H	508	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	O	303	-	1,3,3	0.59	0	0,3,3	-	-
2	NO3	J	902	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	II	205	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	JJ	201	-	1,3,3	0.75	0	0,3,3	-	-
2	NO3	JJ	202	-	1,3,3	0.66	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NO3	HH	303	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	C	303	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	N	1306	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	J	901	-	1,3,3	0.71	0	0,3,3	-	-
2	NO3	N	1308	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	B	310	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	B	311	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	E	404	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	G	502	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	M	501	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	A	802	-	1,3,3	0.68	0	0,3,3	-	-
2	NO3	HH	304	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	M	508	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	K	1503	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	K	1504	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	II	204	-	1,3,3	0.61	0	0,3,3	-	-
2	NO3	B	307	-	1,3,3	0.56	0	0,3,3	-	-
2	NO3	H	504	-	1,3,3	0.60	0	0,3,3	-	-
2	NO3	A	804	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	II	202	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	M	507	-	1,3,3	0.59	0	0,3,3	-	-
2	NO3	O	305	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	B	309	-	1,3,3	0.65	0	0,3,3	-	-
2	NO3	B	305	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	C	304	-	1,3,3	0.62	0	0,3,3	-	-
2	NO3	H	501	-	1,3,3	0.60	0	0,3,3	-	-
2	NO3	K	1501	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	I	603	-	1,3,3	0.61	0	0,3,3	-	-
2	NO3	I	601	-	1,3,3	0.56	0	0,3,3	-	-
2	NO3	K	1505	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	D	302	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	L	504	-	1,3,3	0.66	0	0,3,3	-	-
2	NO3	M	509	-	1,3,3	0.62	0	0,3,3	-	-
2	NO3	O	304	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	L	505	-	1,3,3	0.63	0	0,3,3	-	-
2	NO3	L	508	-	1,3,3	0.64	0	0,3,3	-	-
2	NO3	E	405	-	1,3,3	0.61	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

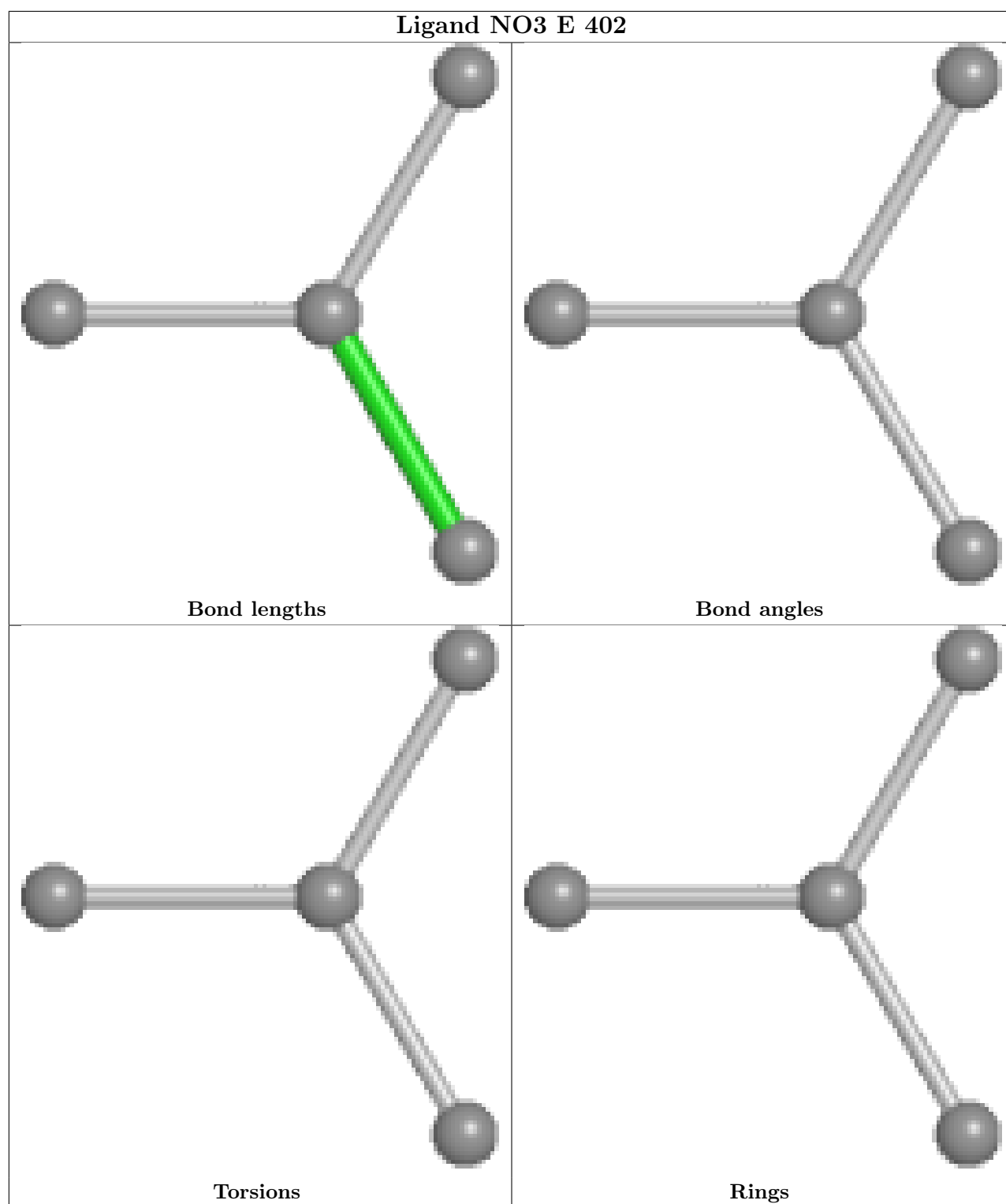
There are no ring outliers.

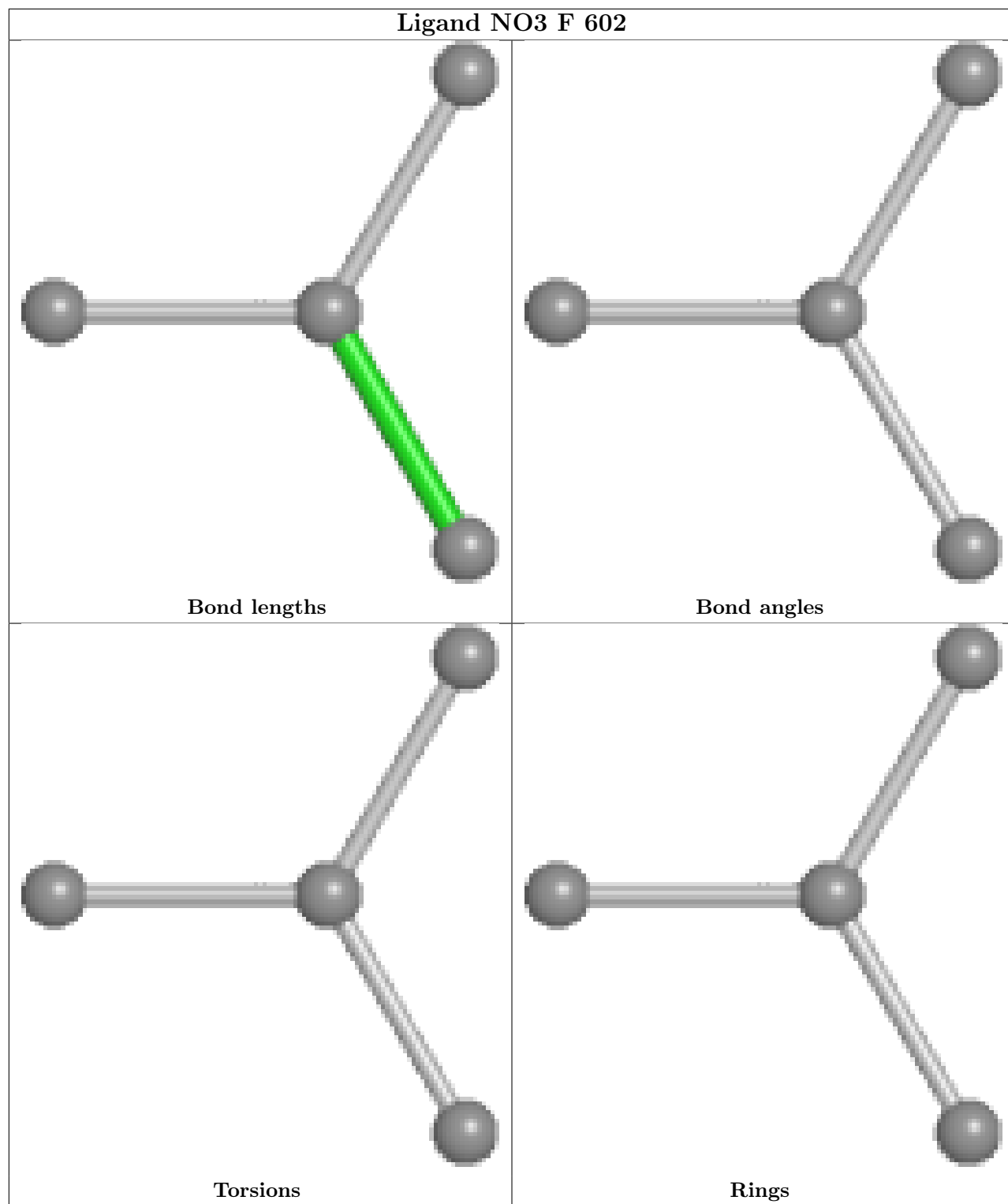
18 monomers are involved in 26 short contacts:

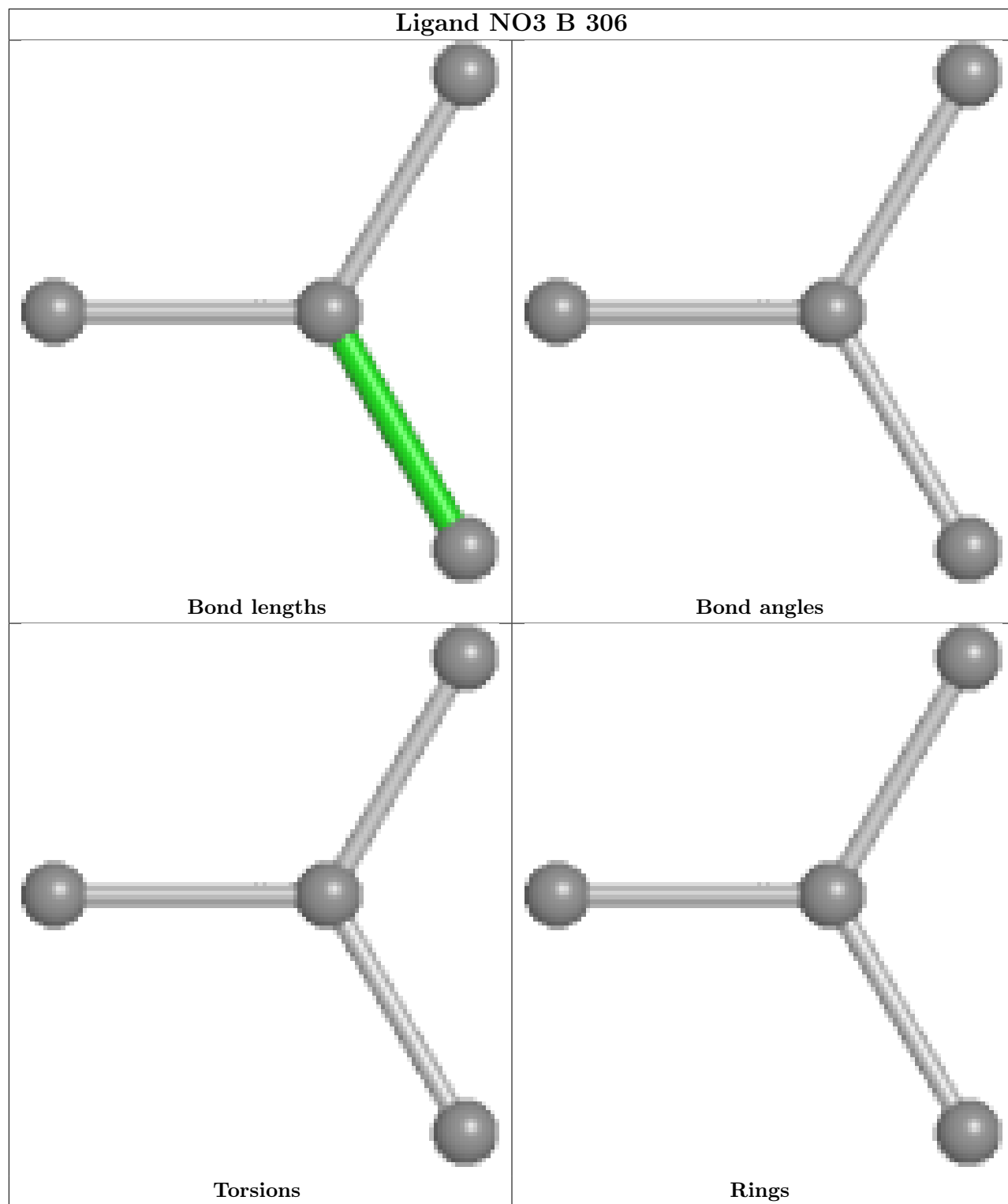
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	406	NO3	1	0
2	M	502	NO3	1	0
2	C	302	NO3	1	0
2	D	301	NO3	1	0
2	E	401	NO3	1	0
2	B	308	NO3	1	0
2	H	506	NO3	1	0
2	L	507	NO3	1	0
2	GG	206	NO3	0	4
2	H	508	NO3	2	0
2	M	508	NO3	1	0
2	B	307	NO3	1	1
2	H	504	NO3	2	0
2	M	507	NO3	2	0
2	B	305	NO3	1	0
2	I	601	NO3	1	0
2	L	504	NO3	1	0
2	E	405	NO3	2	0

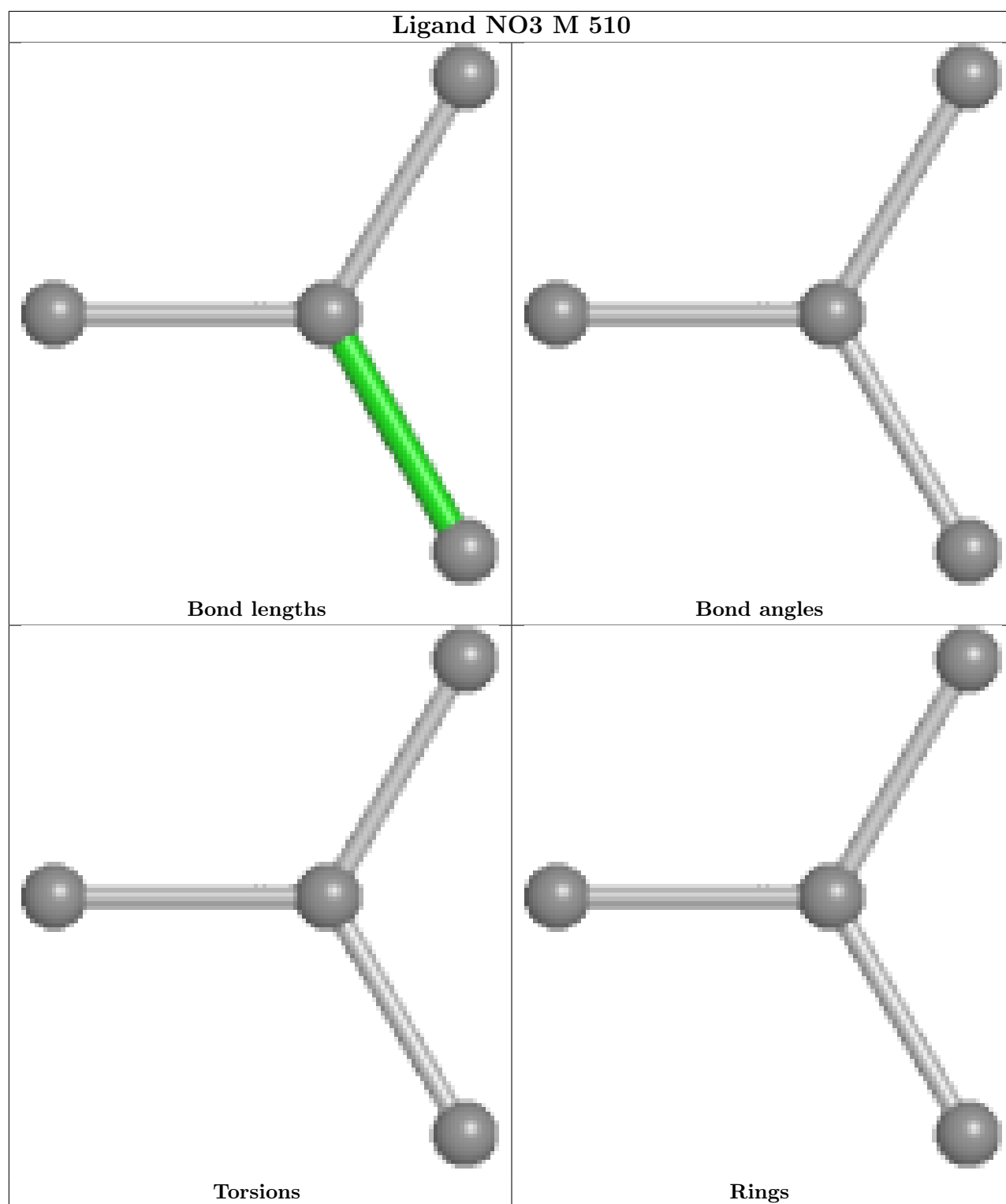
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

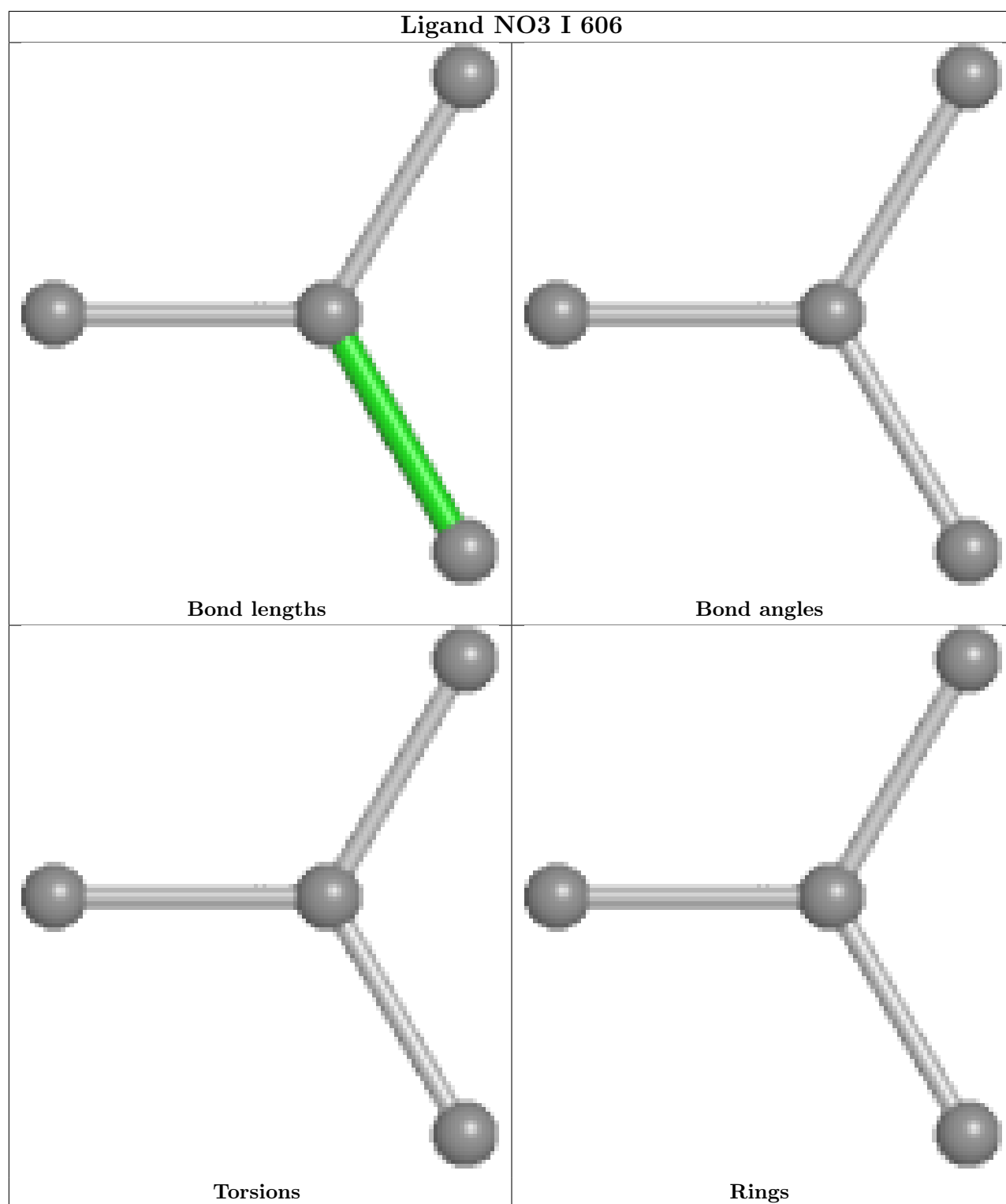


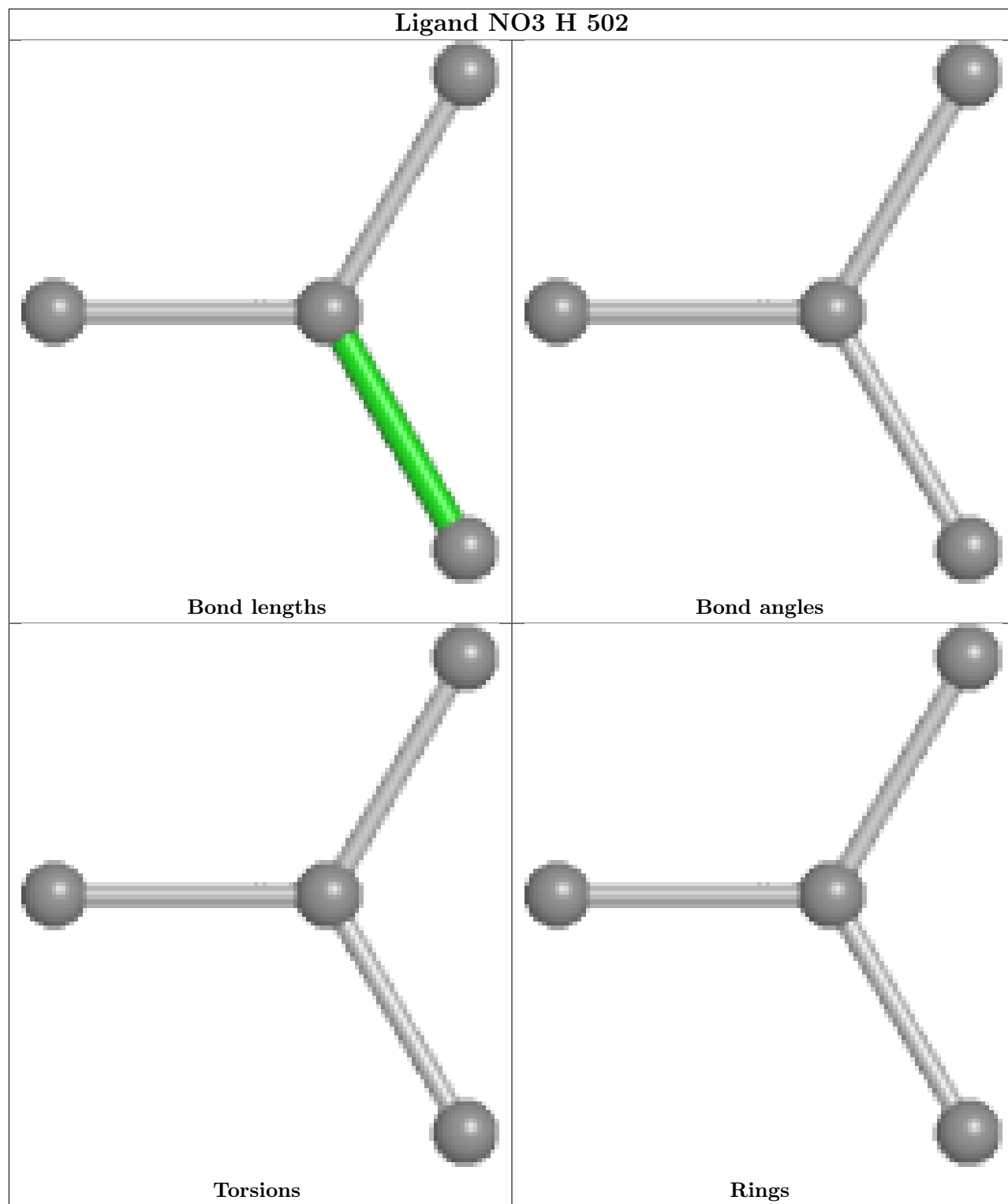


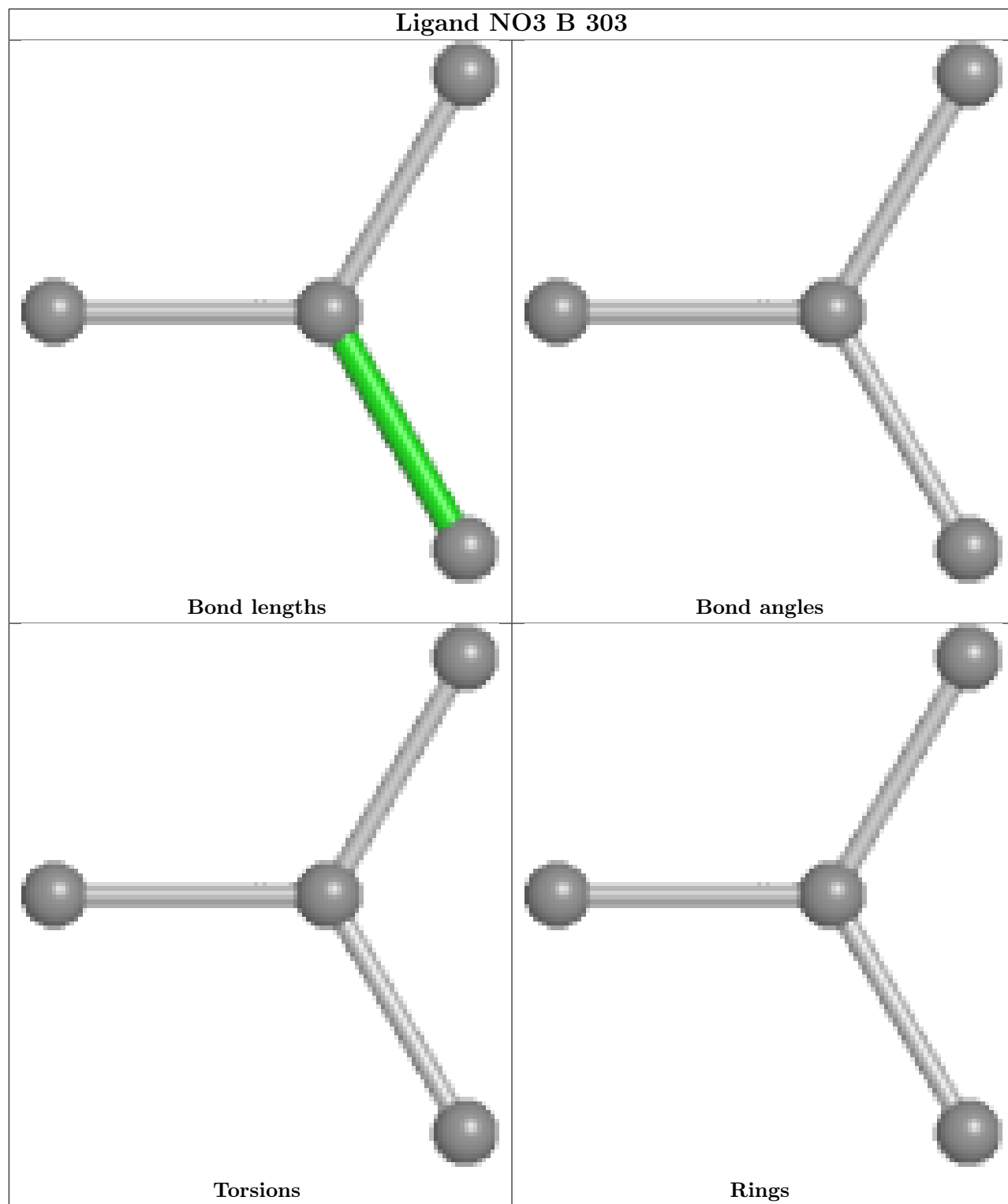


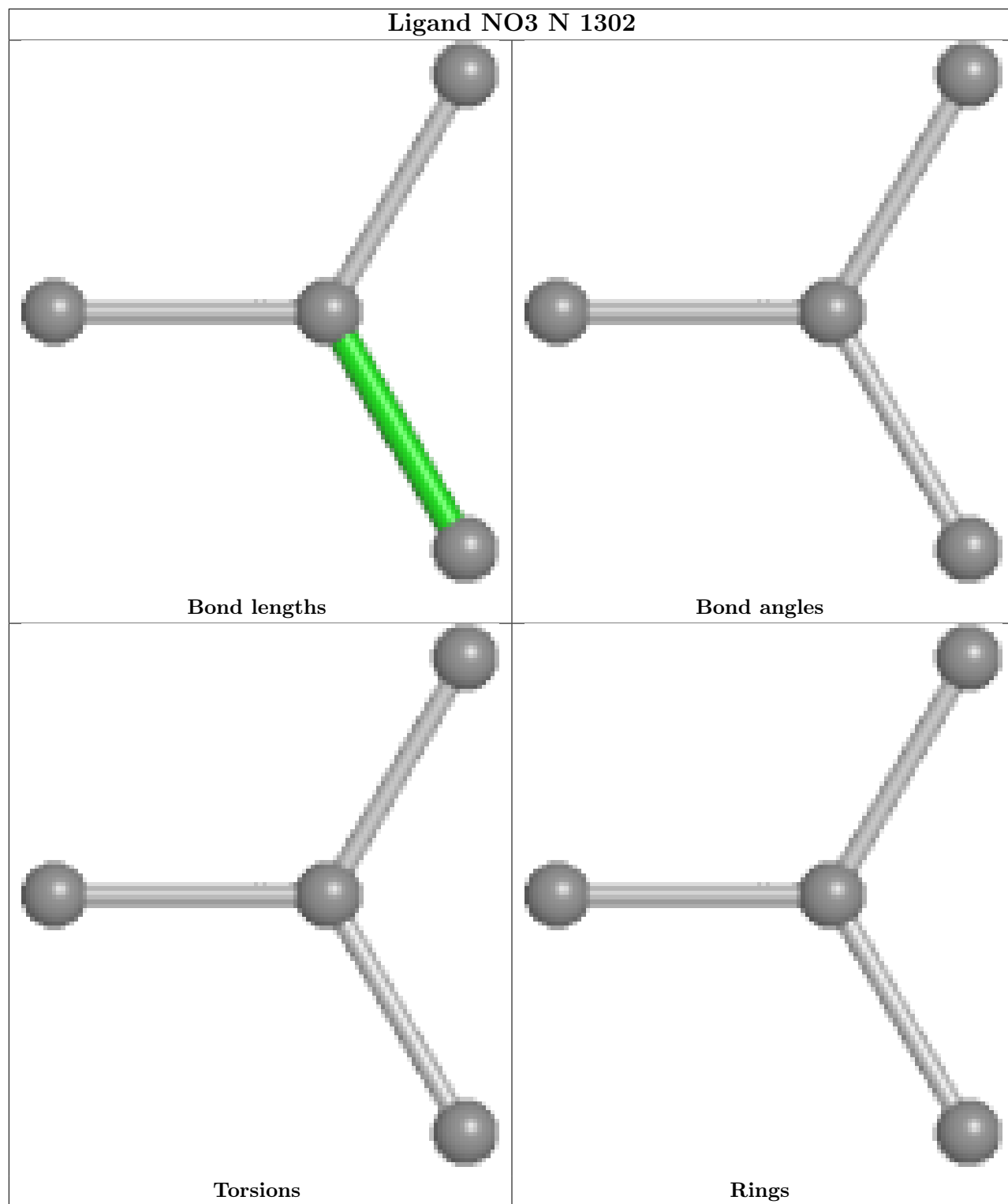




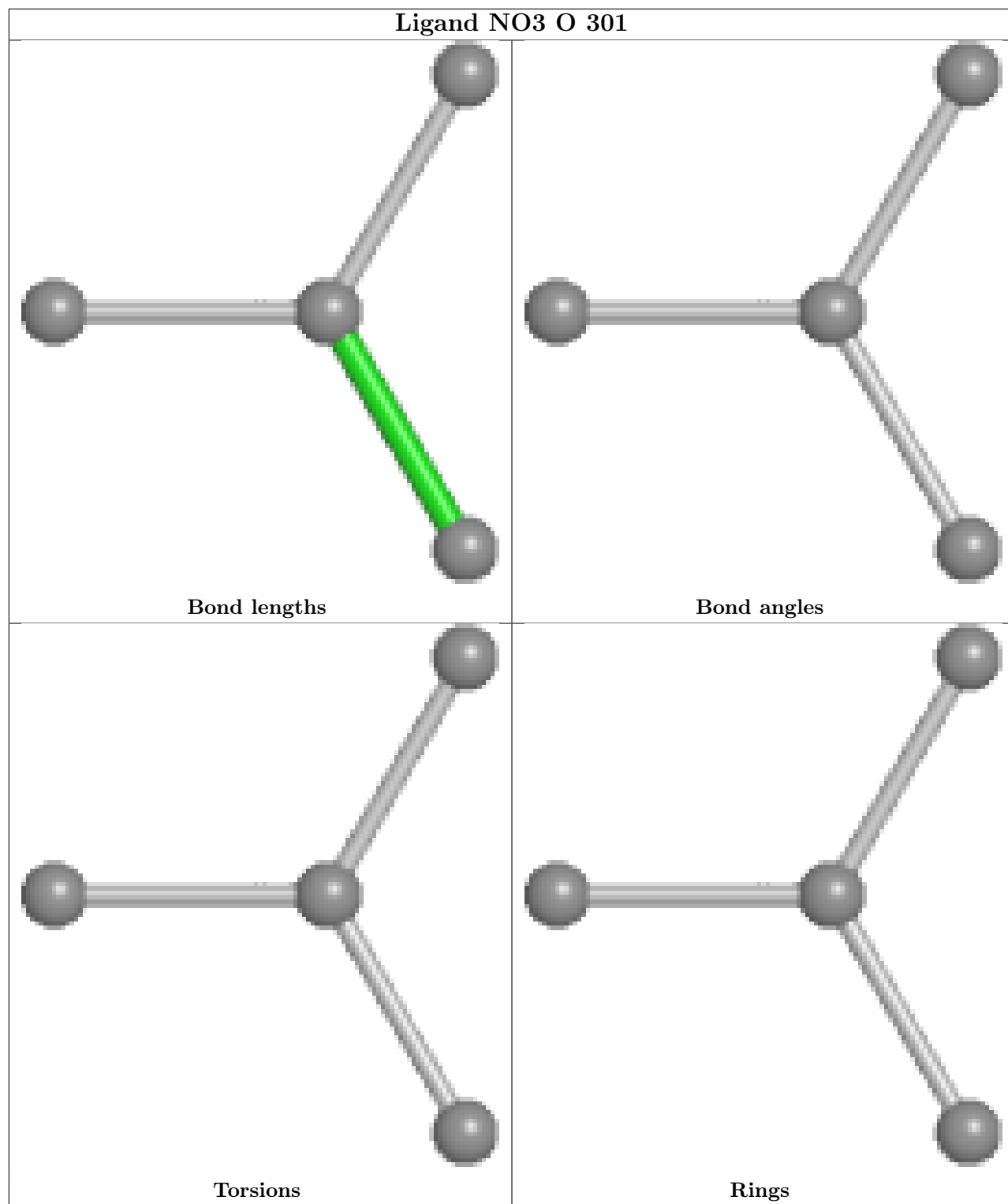


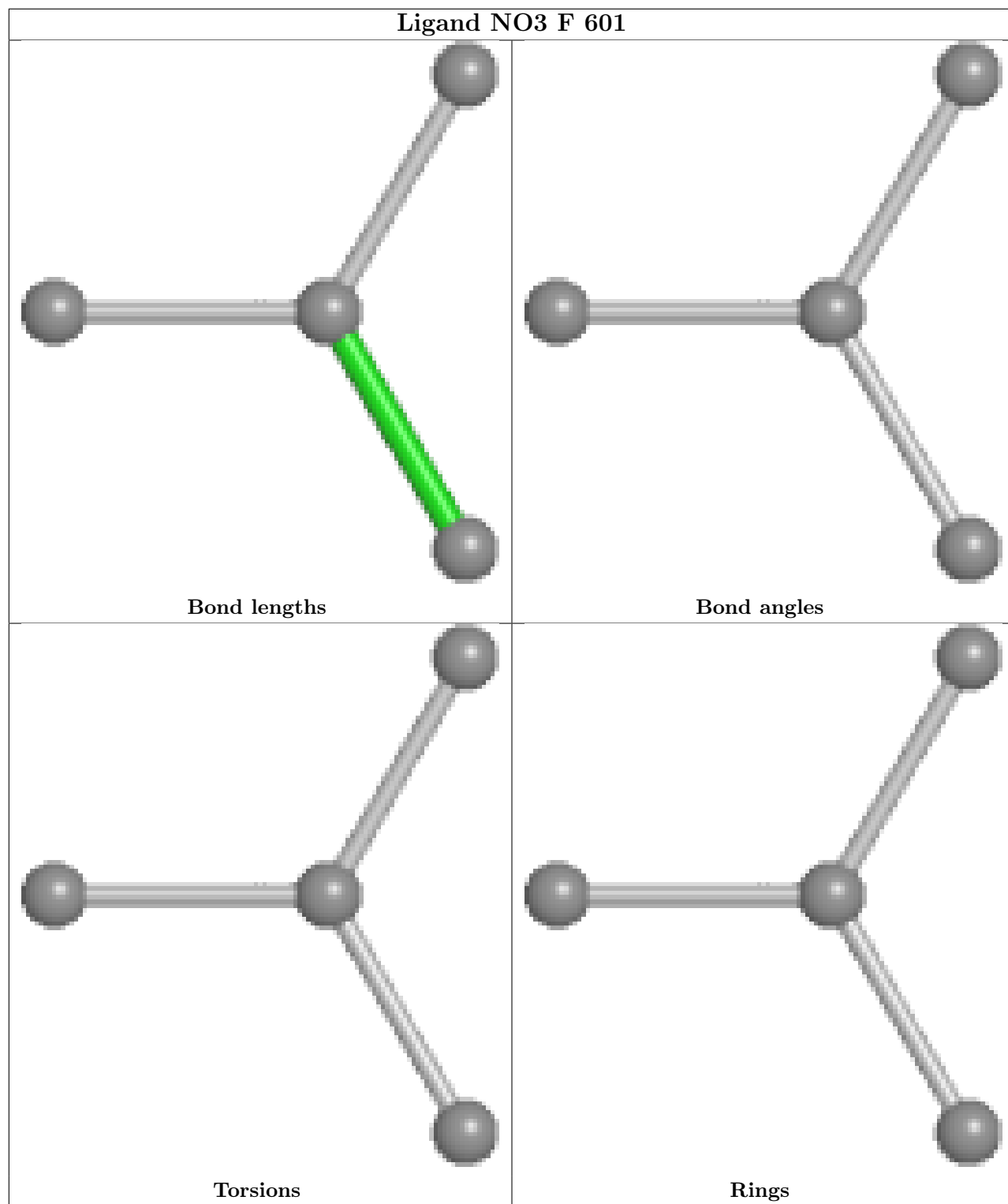


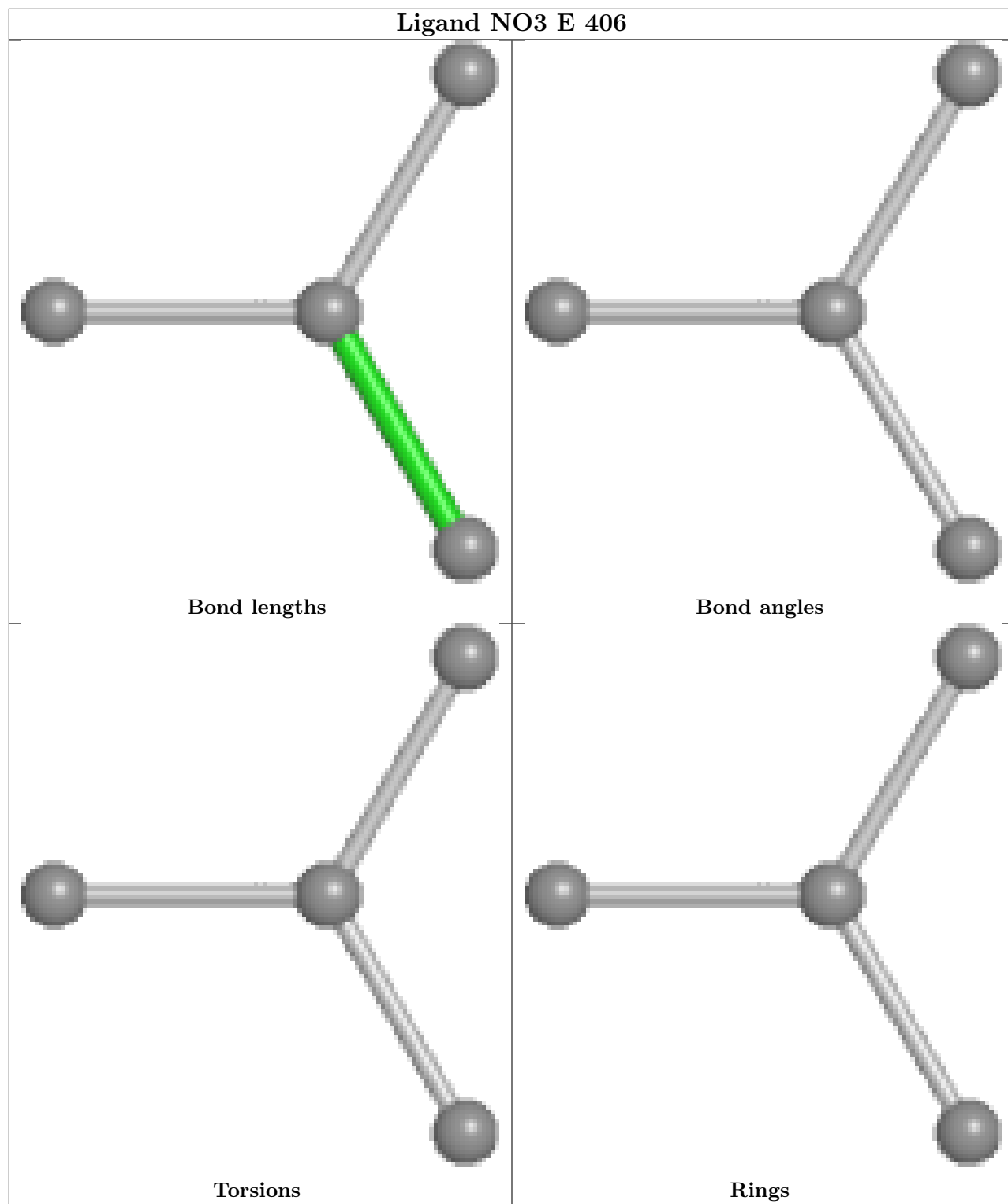


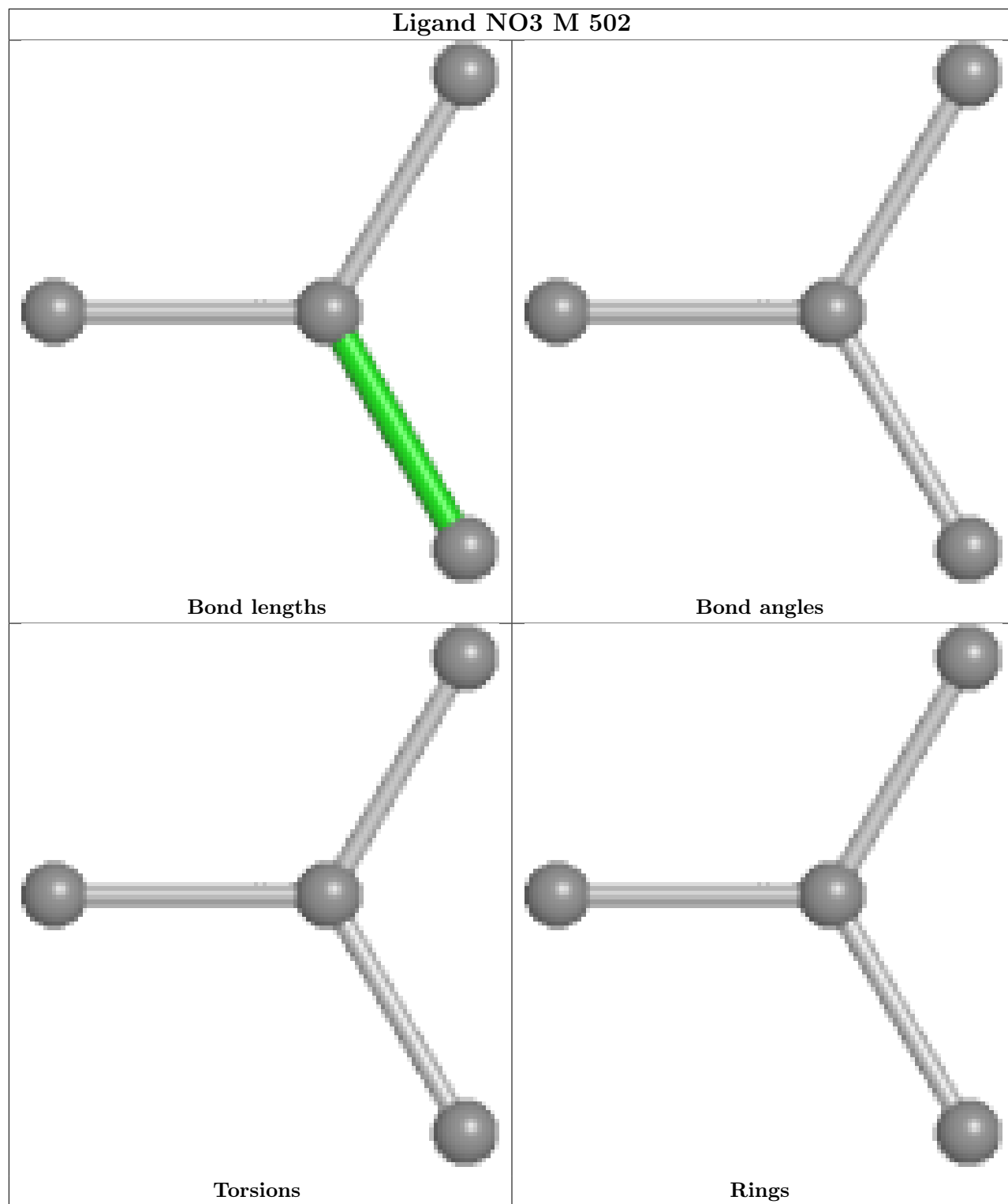


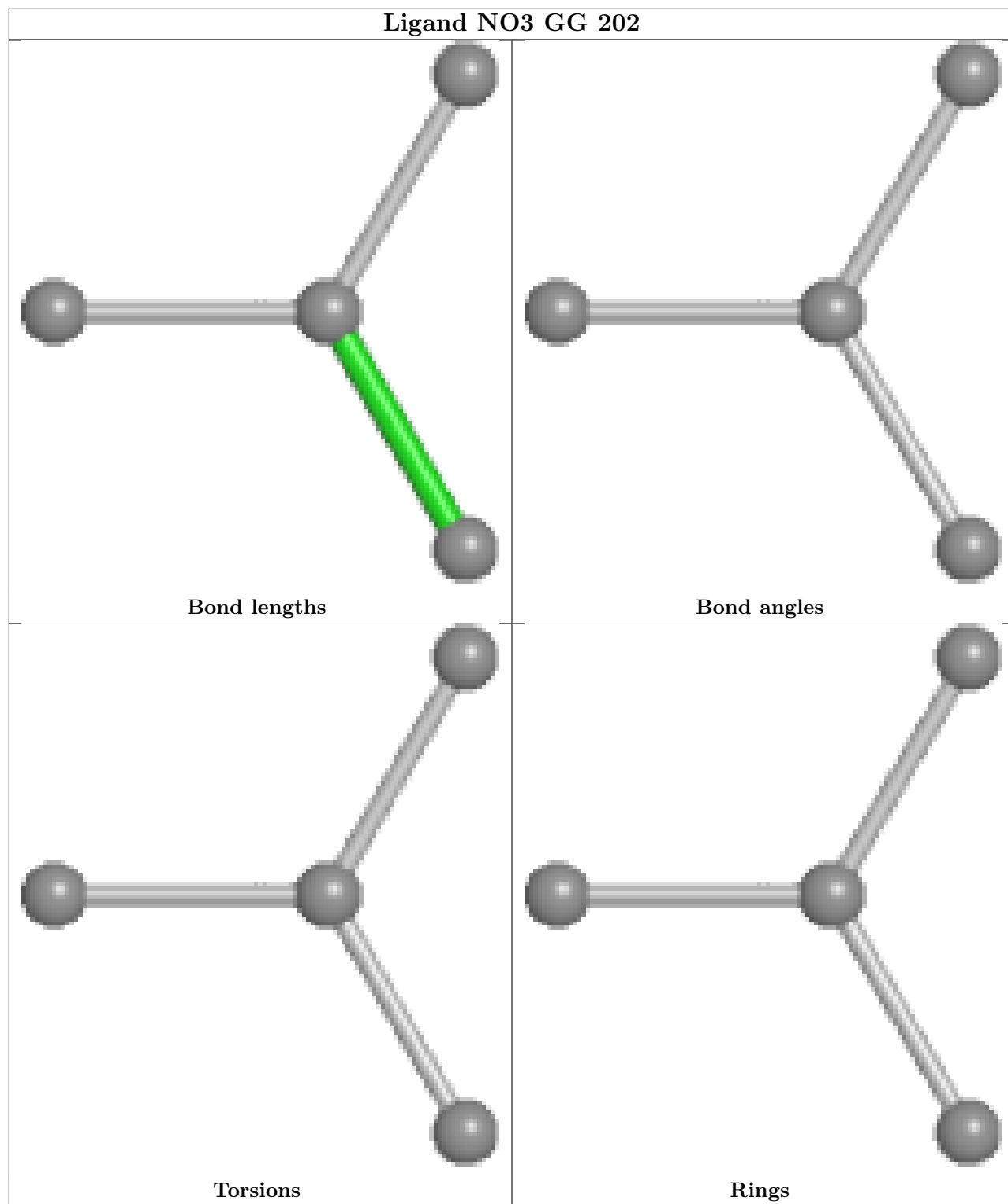


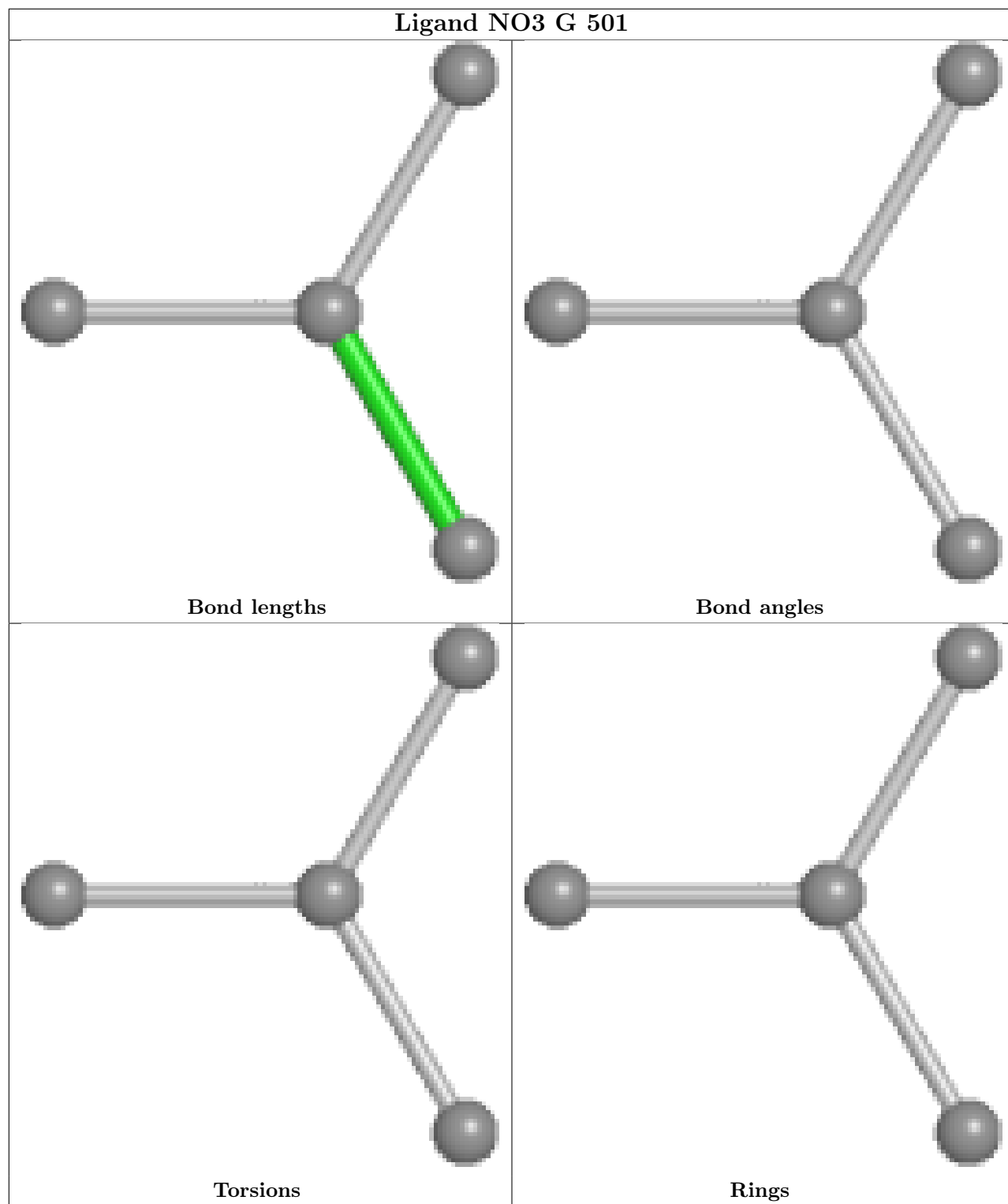


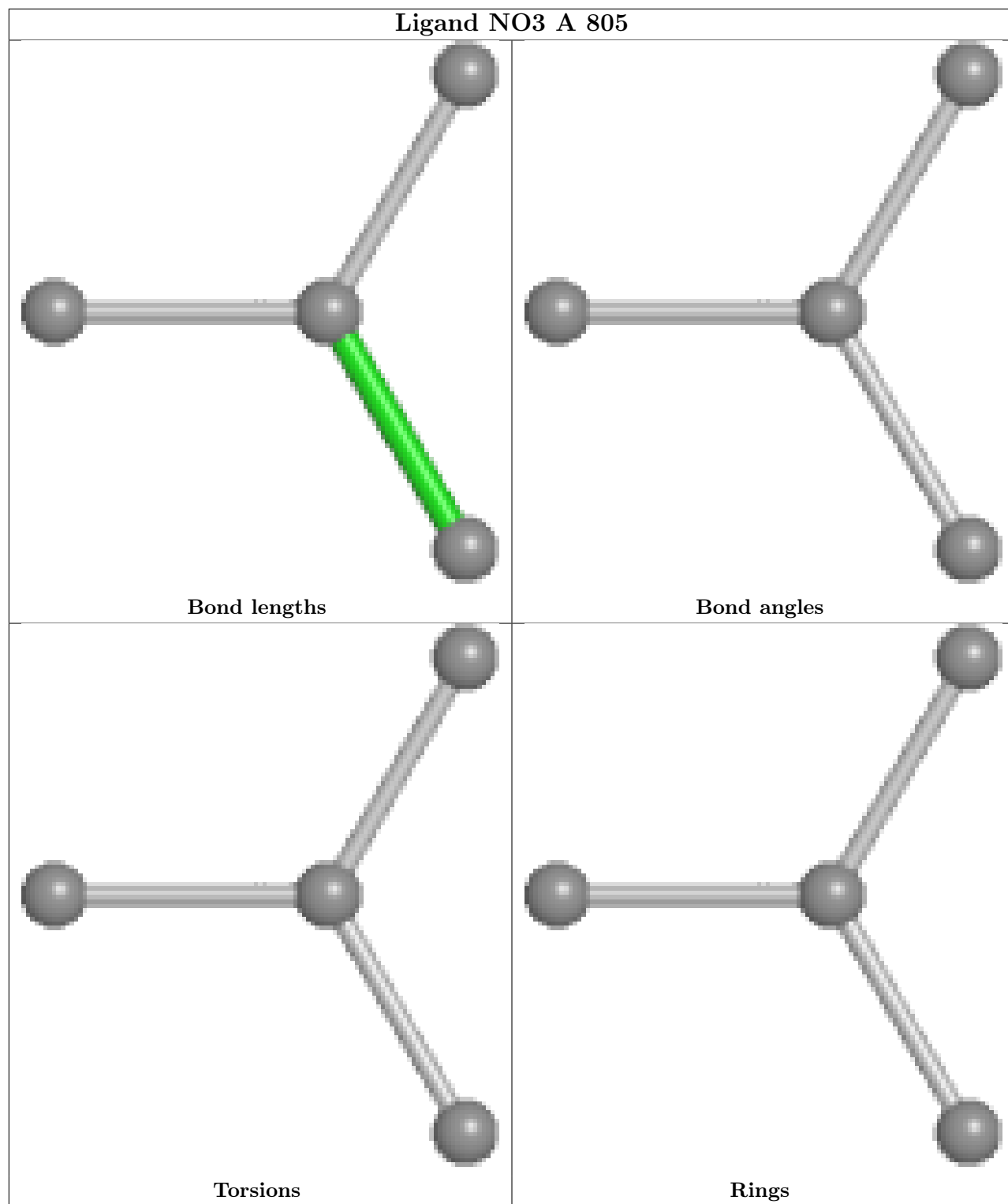


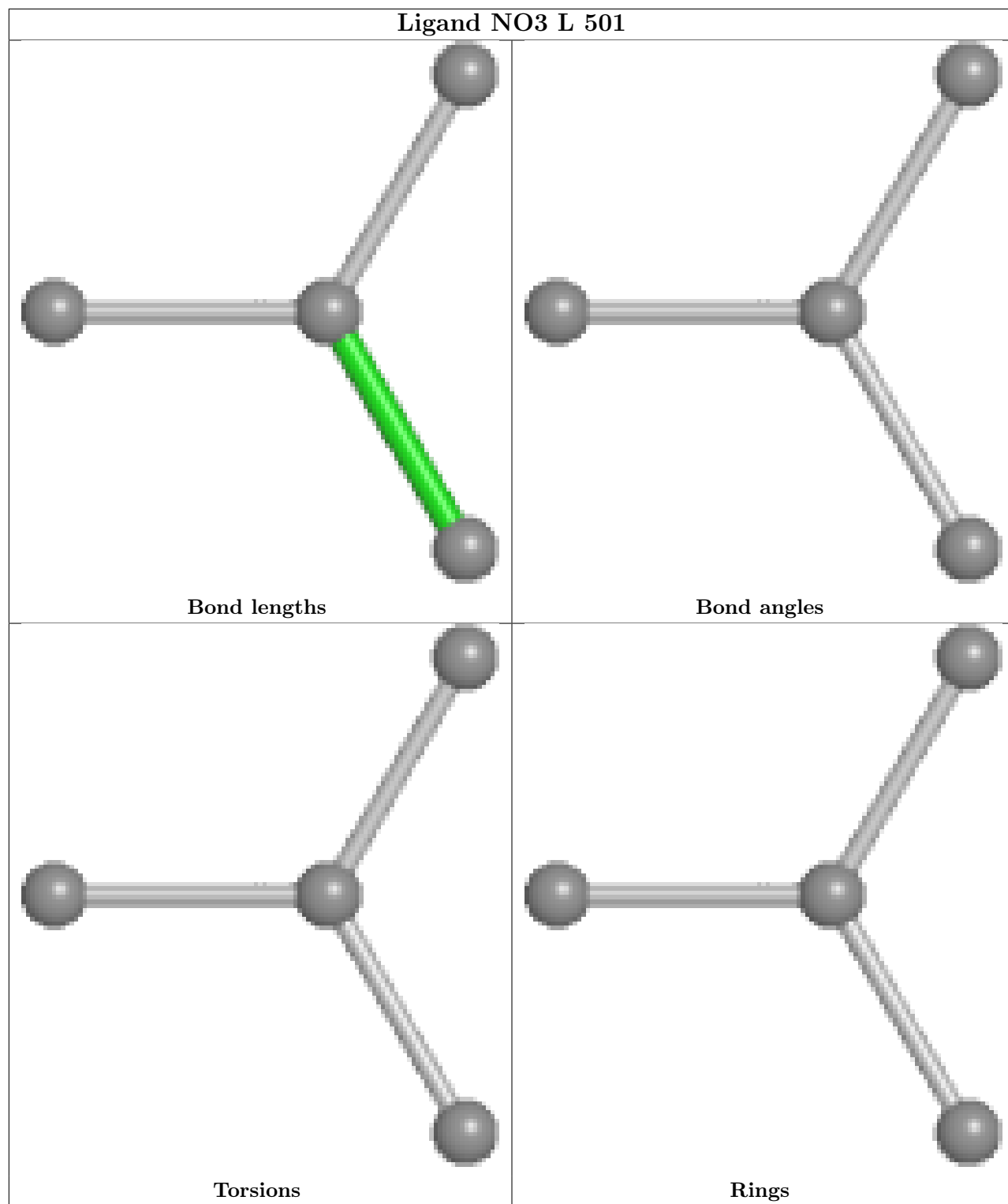




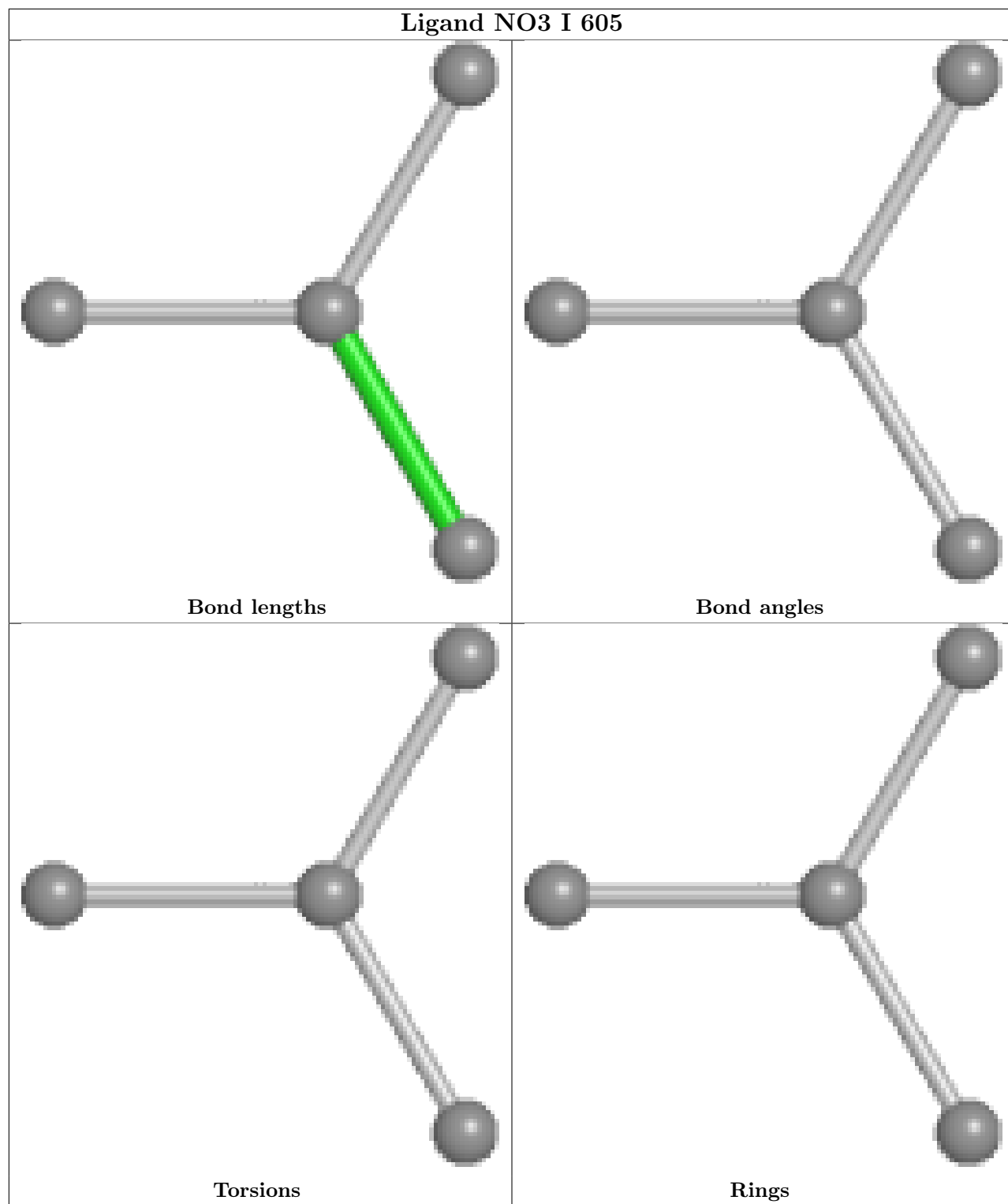


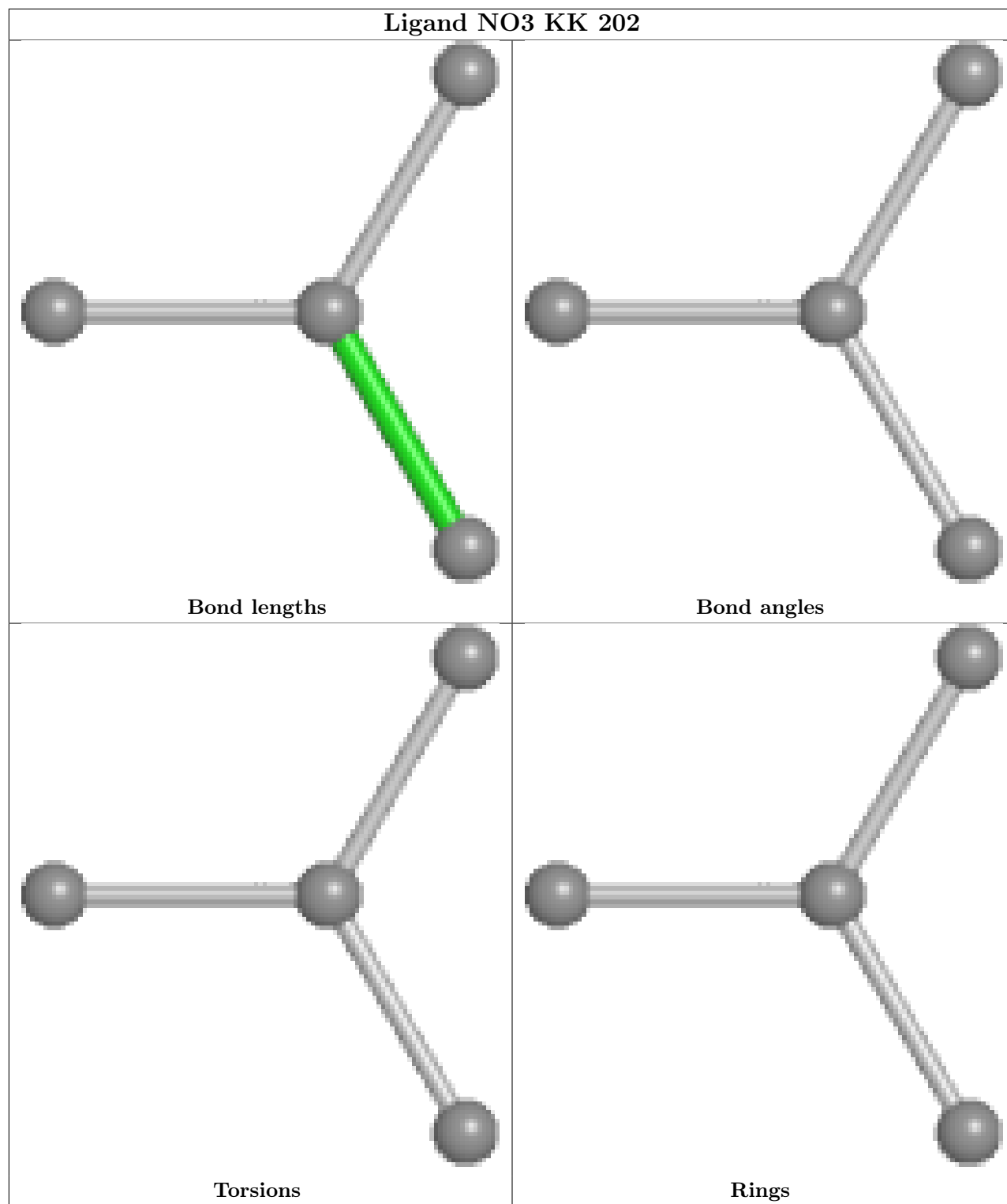


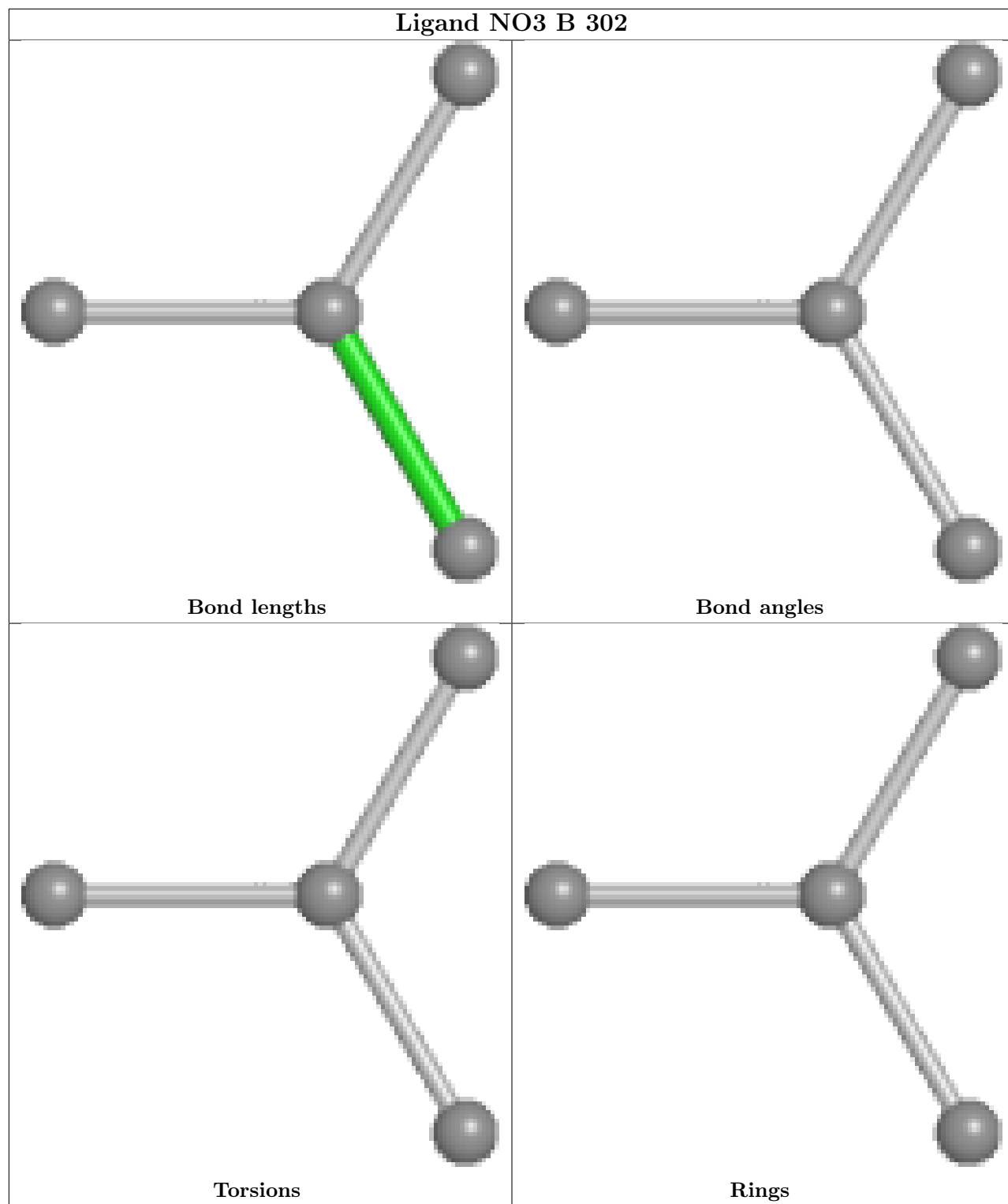


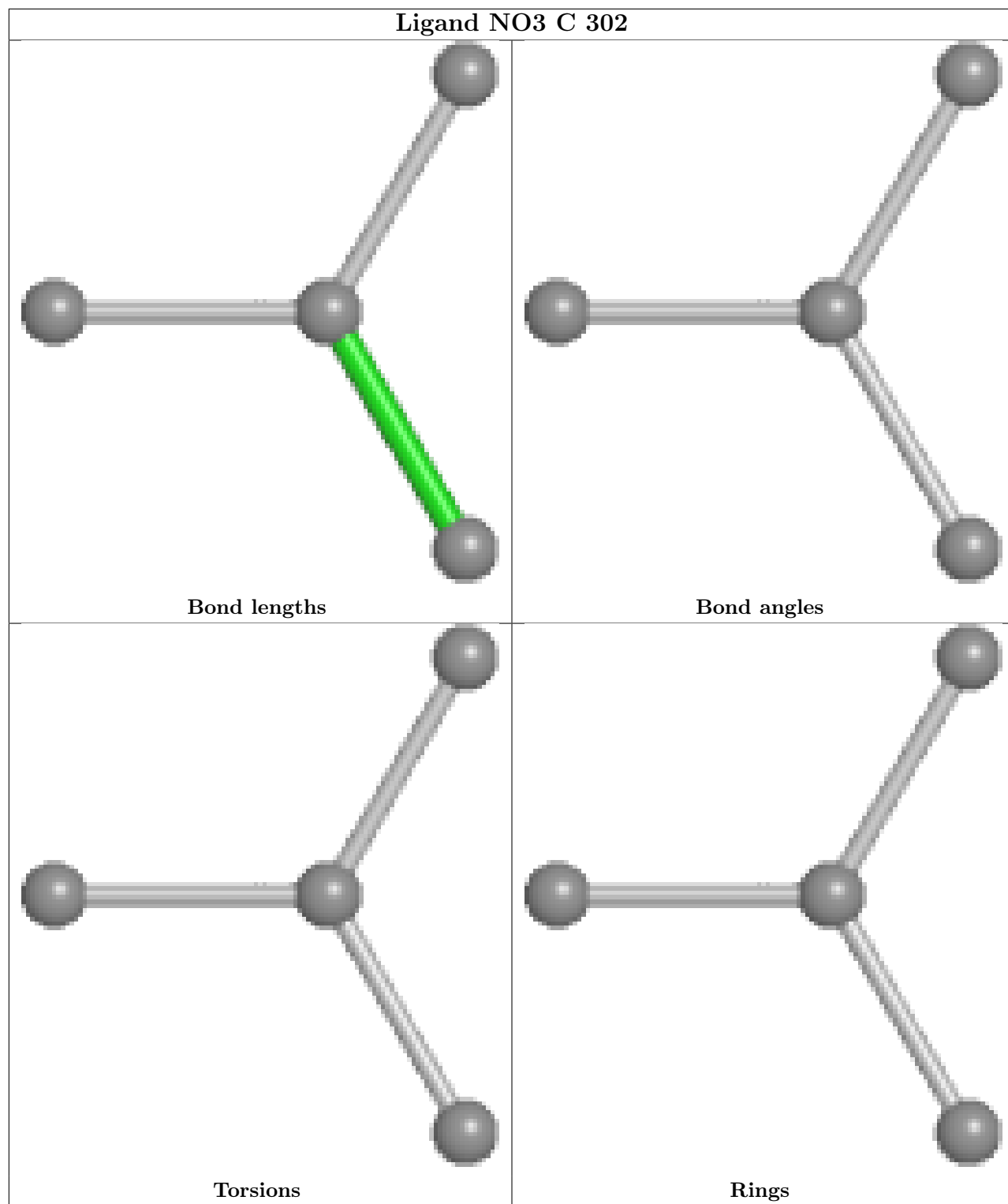


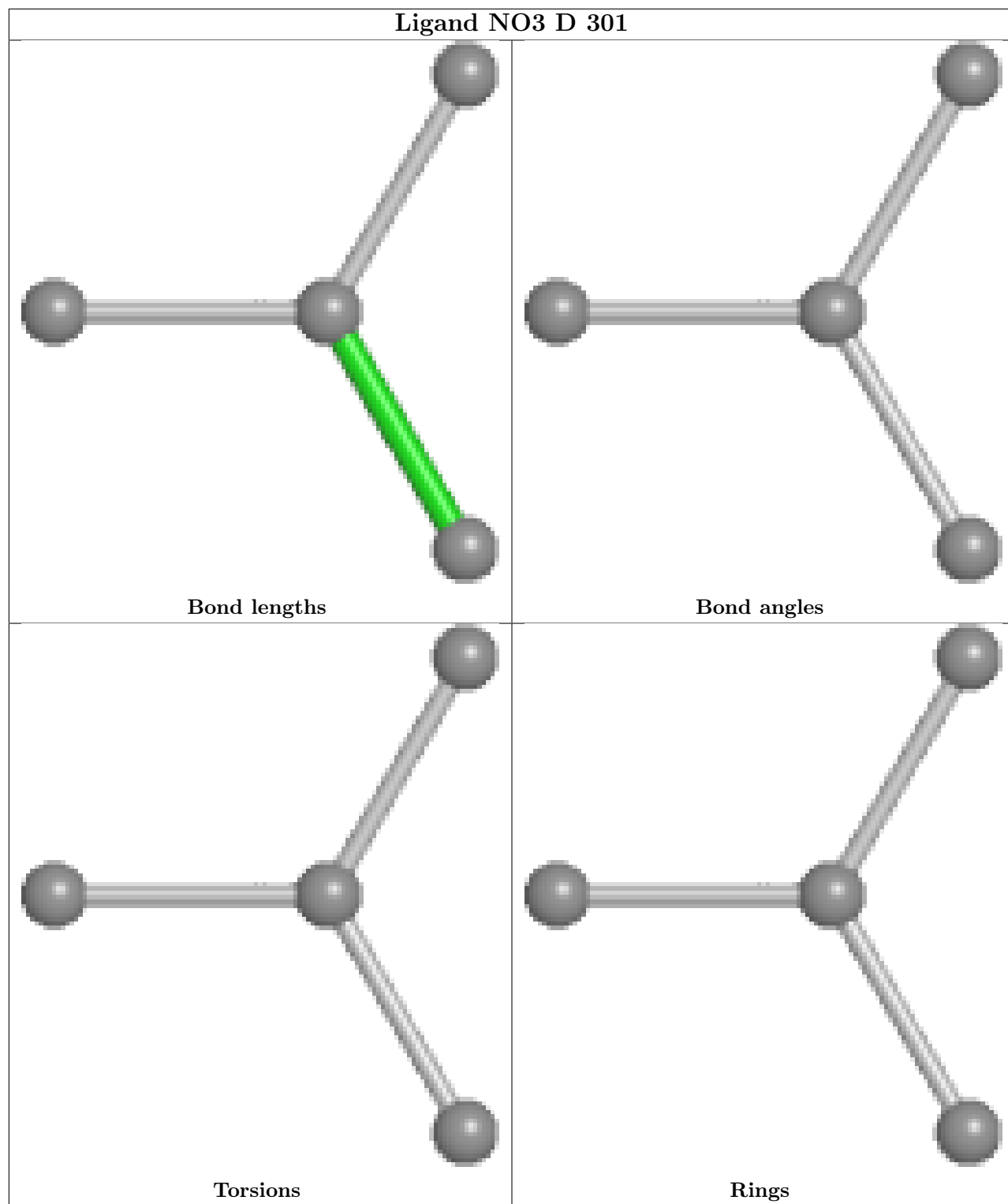


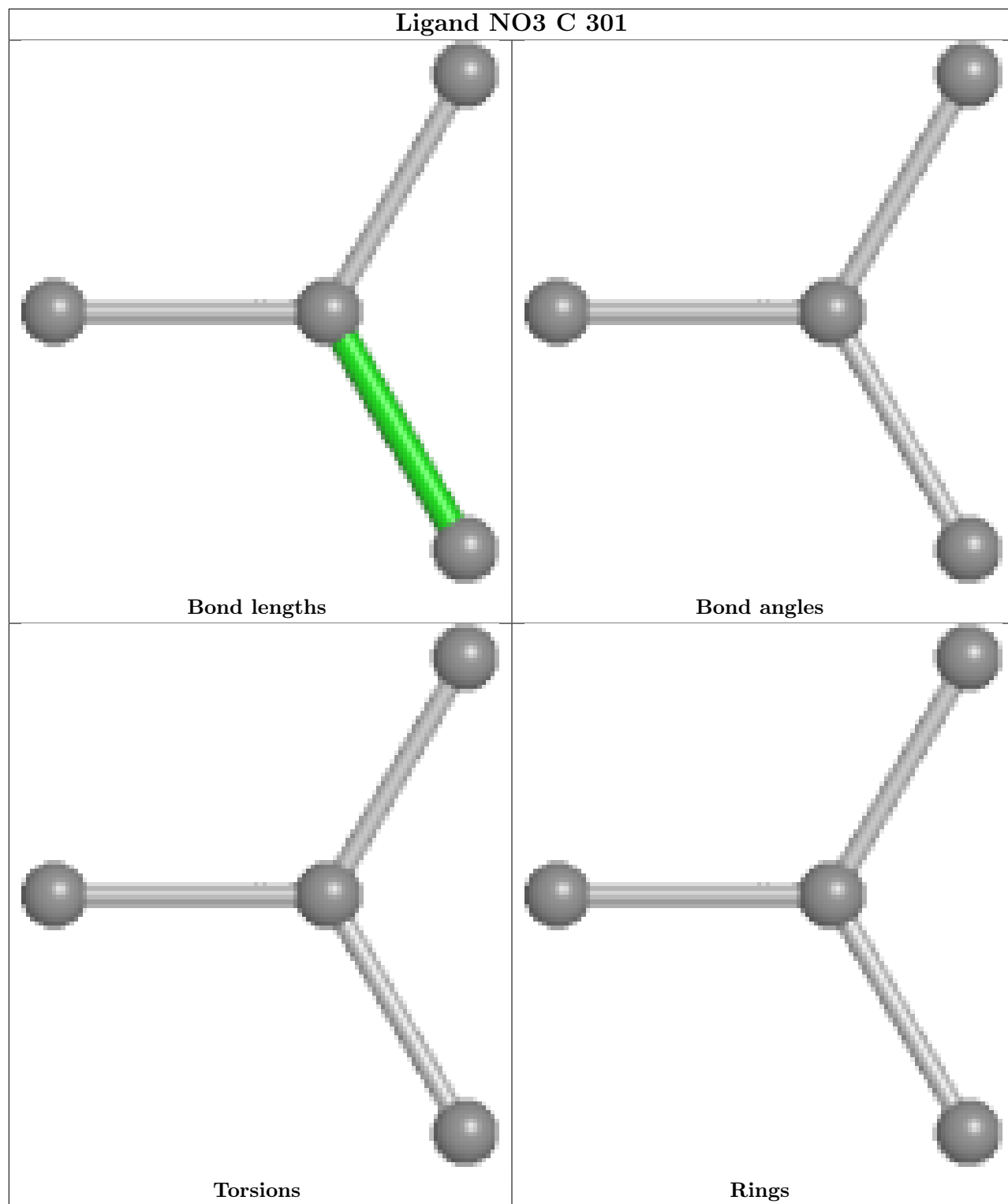


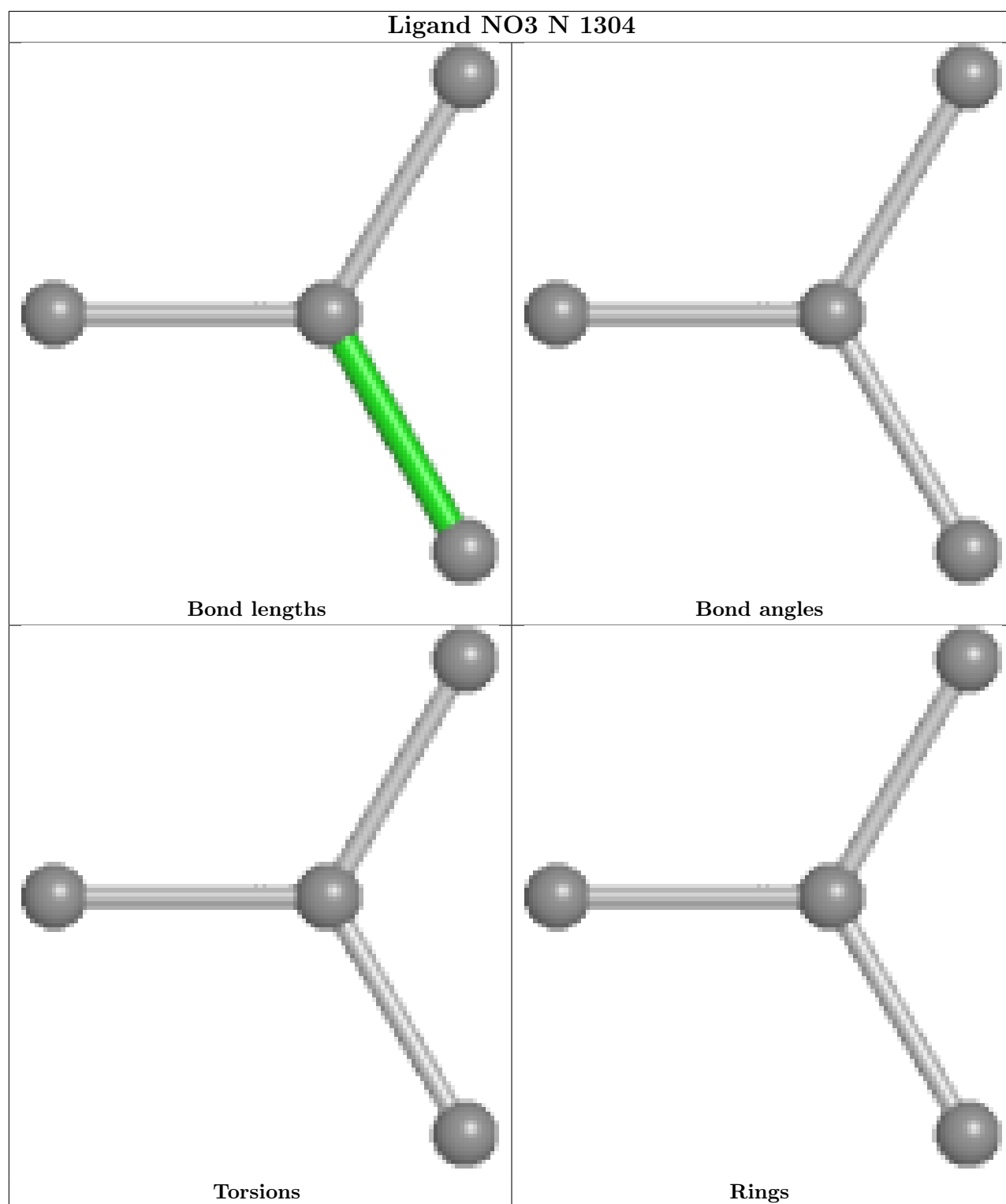


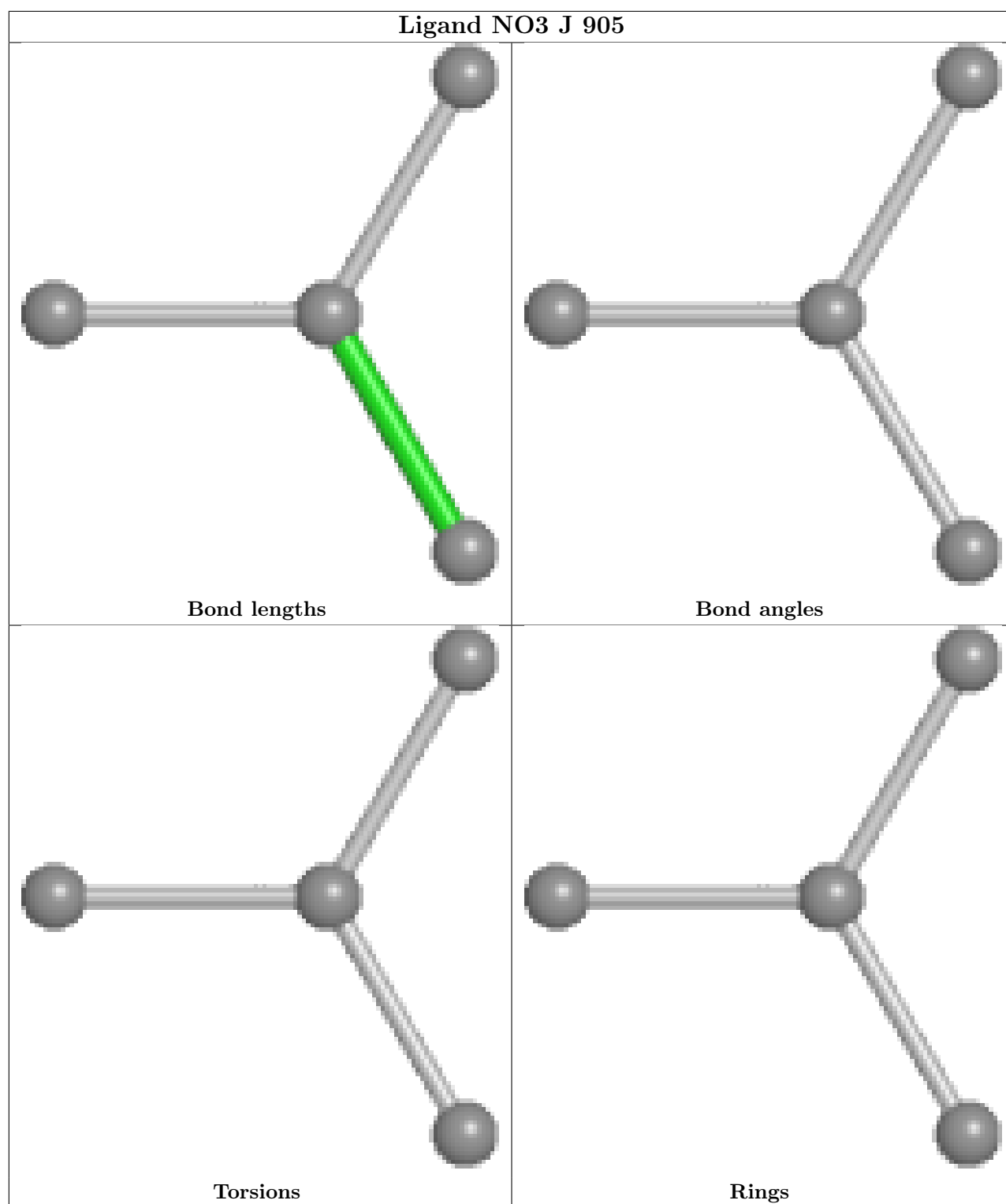




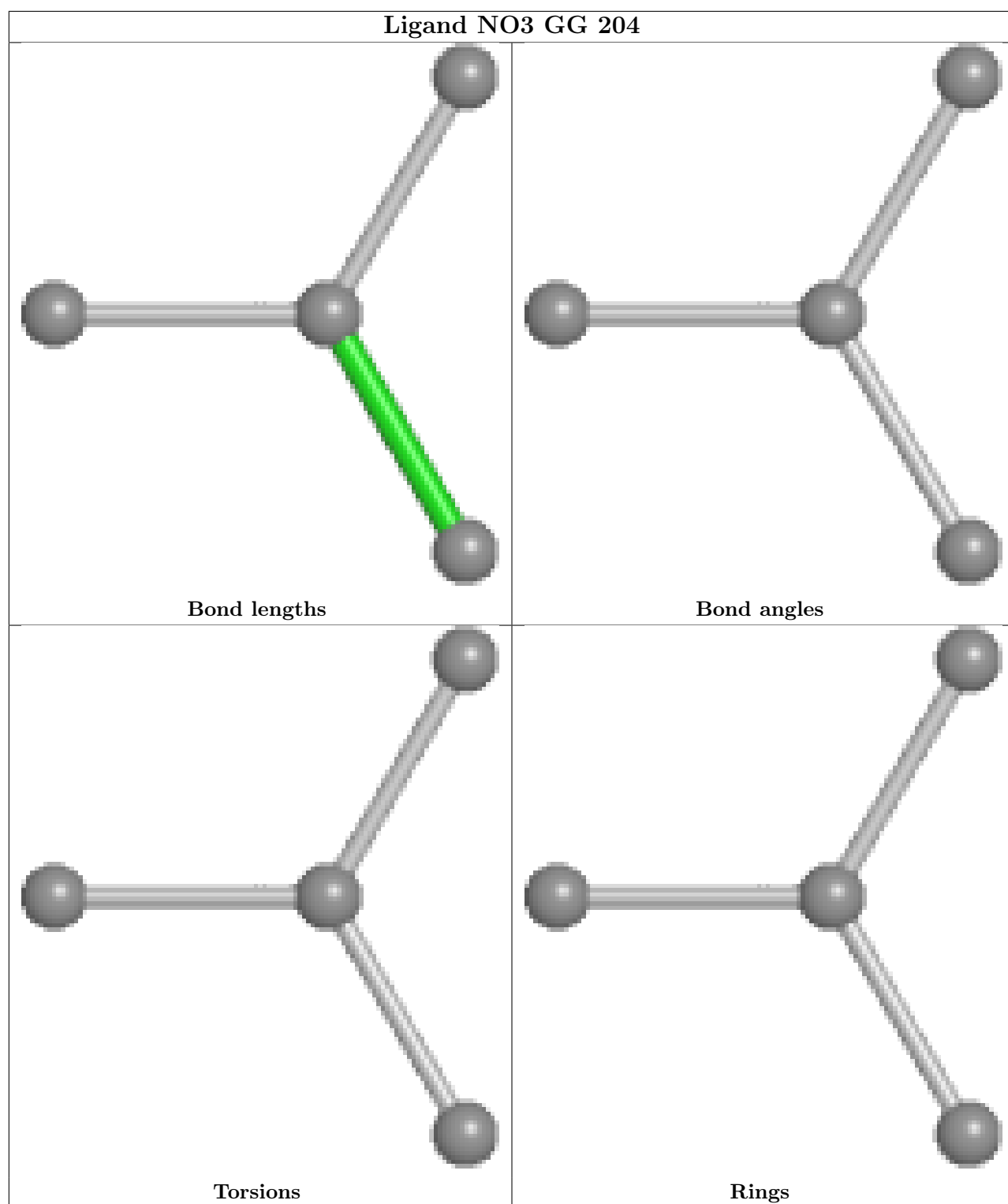


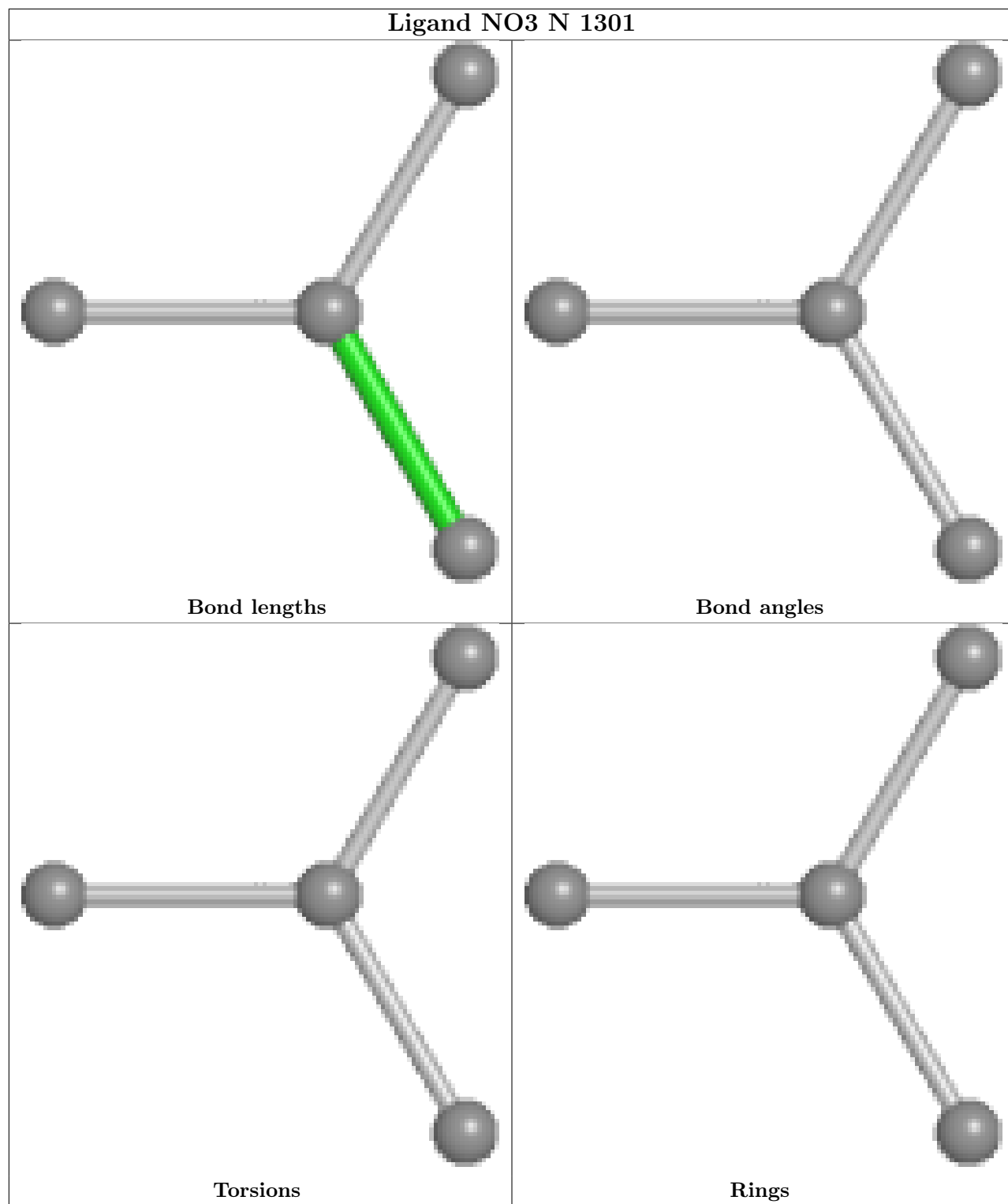


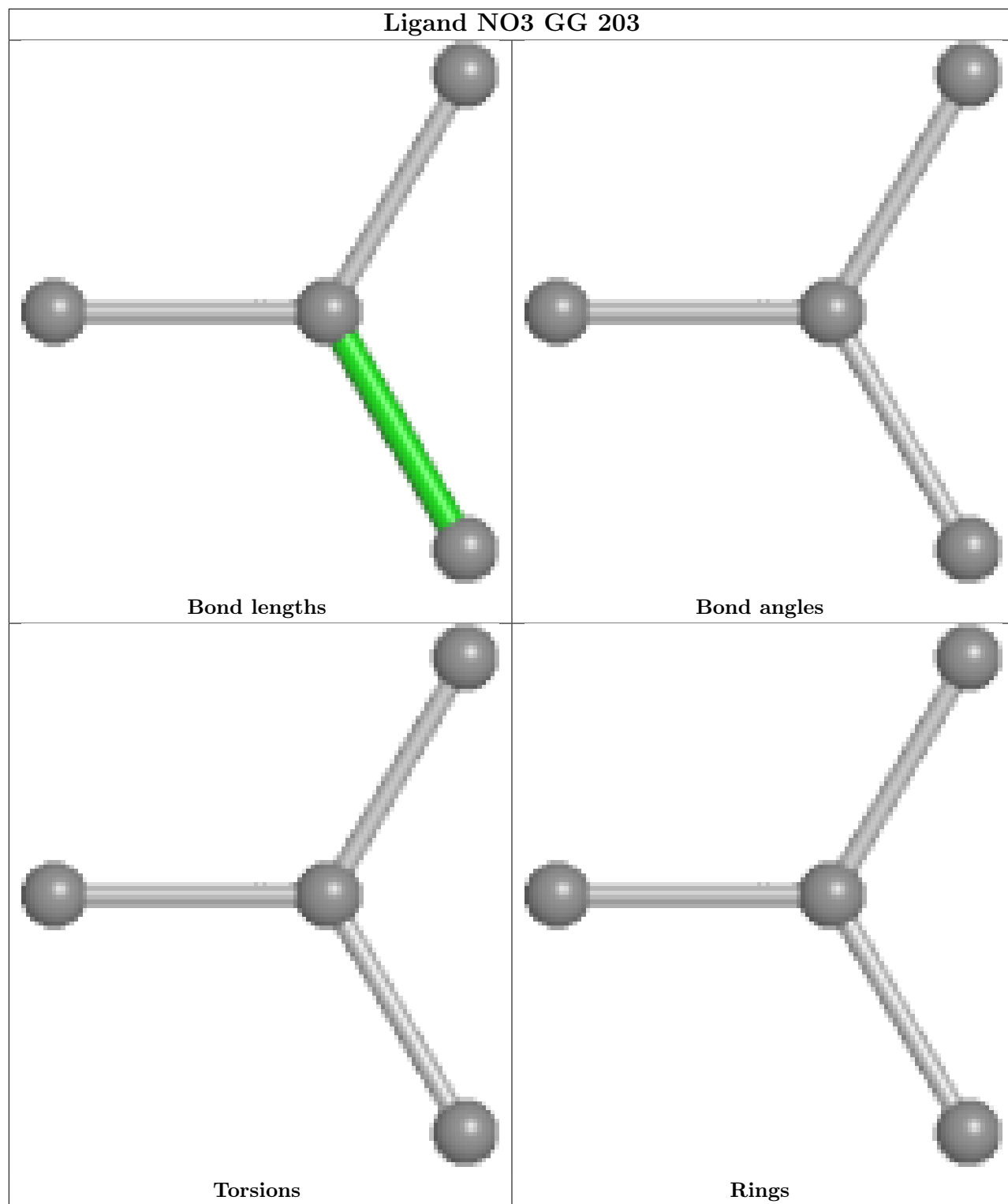


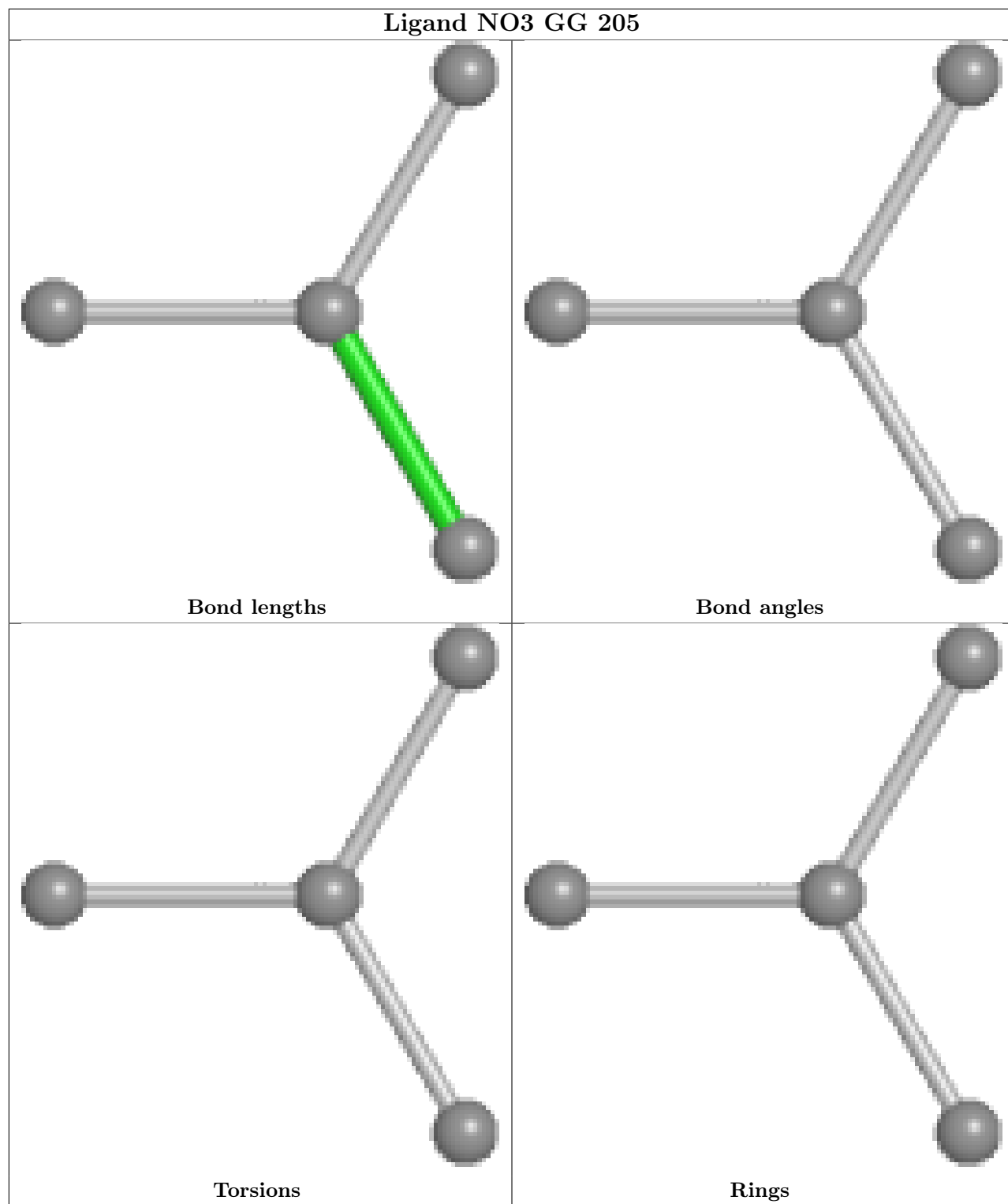


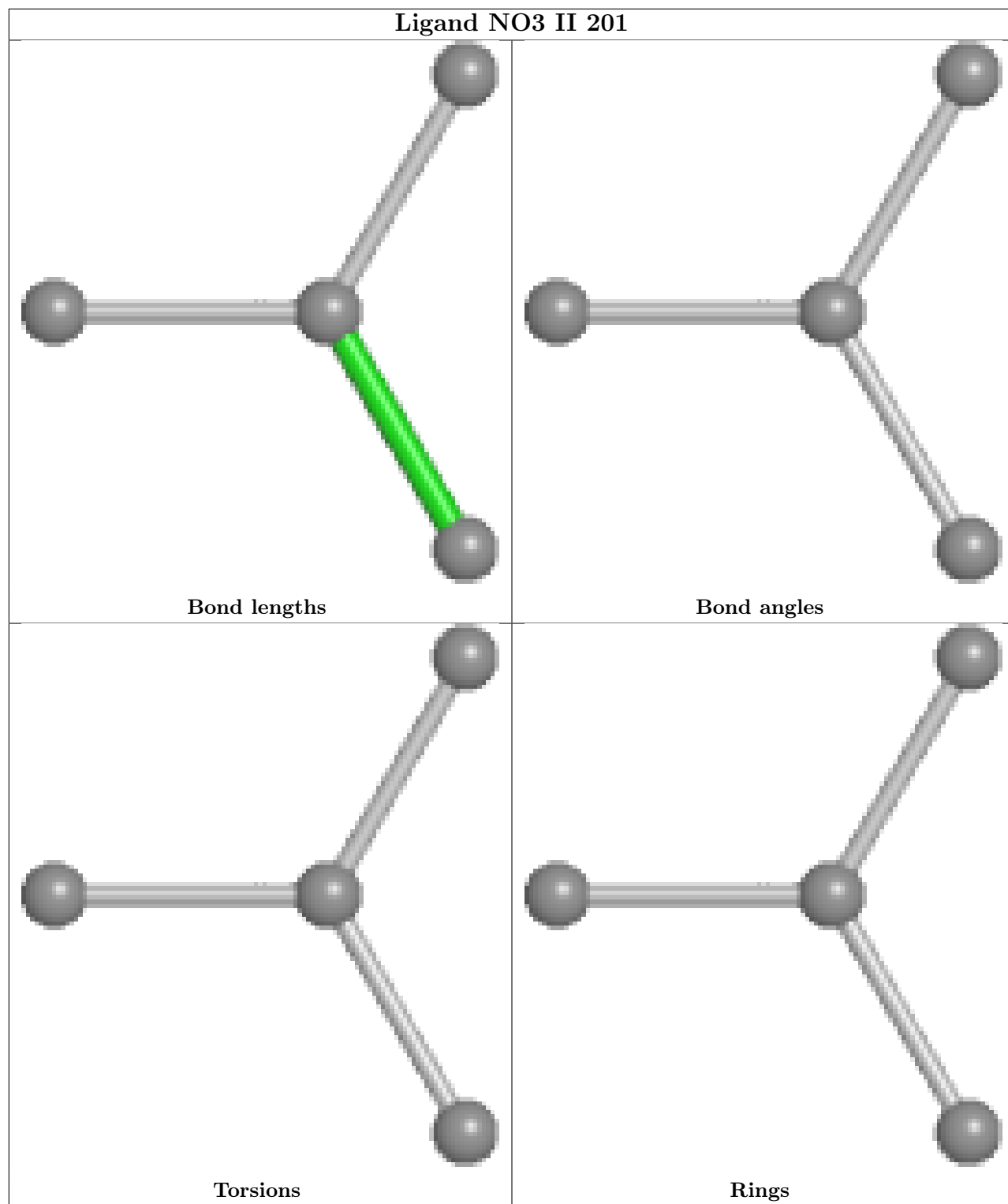


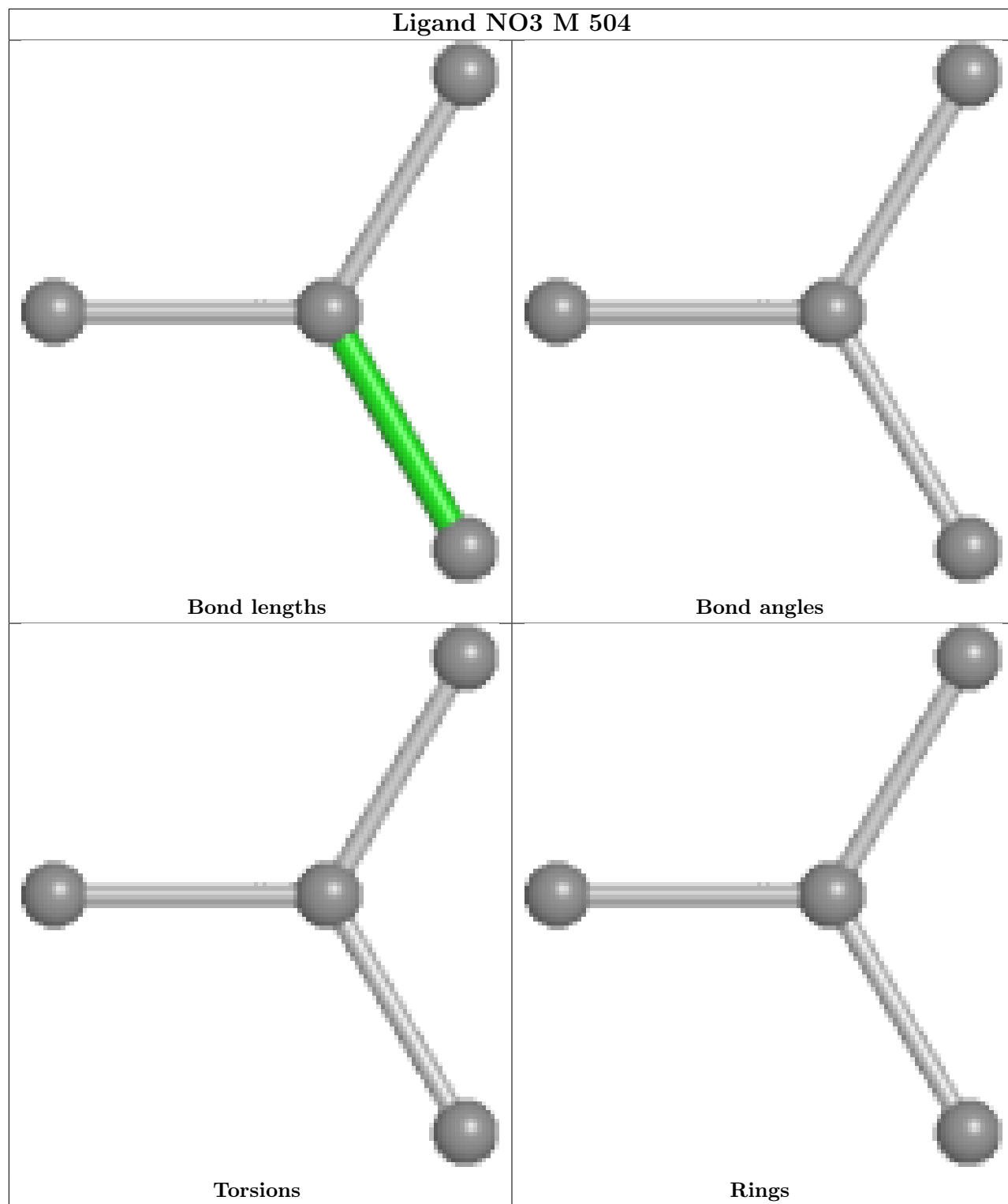


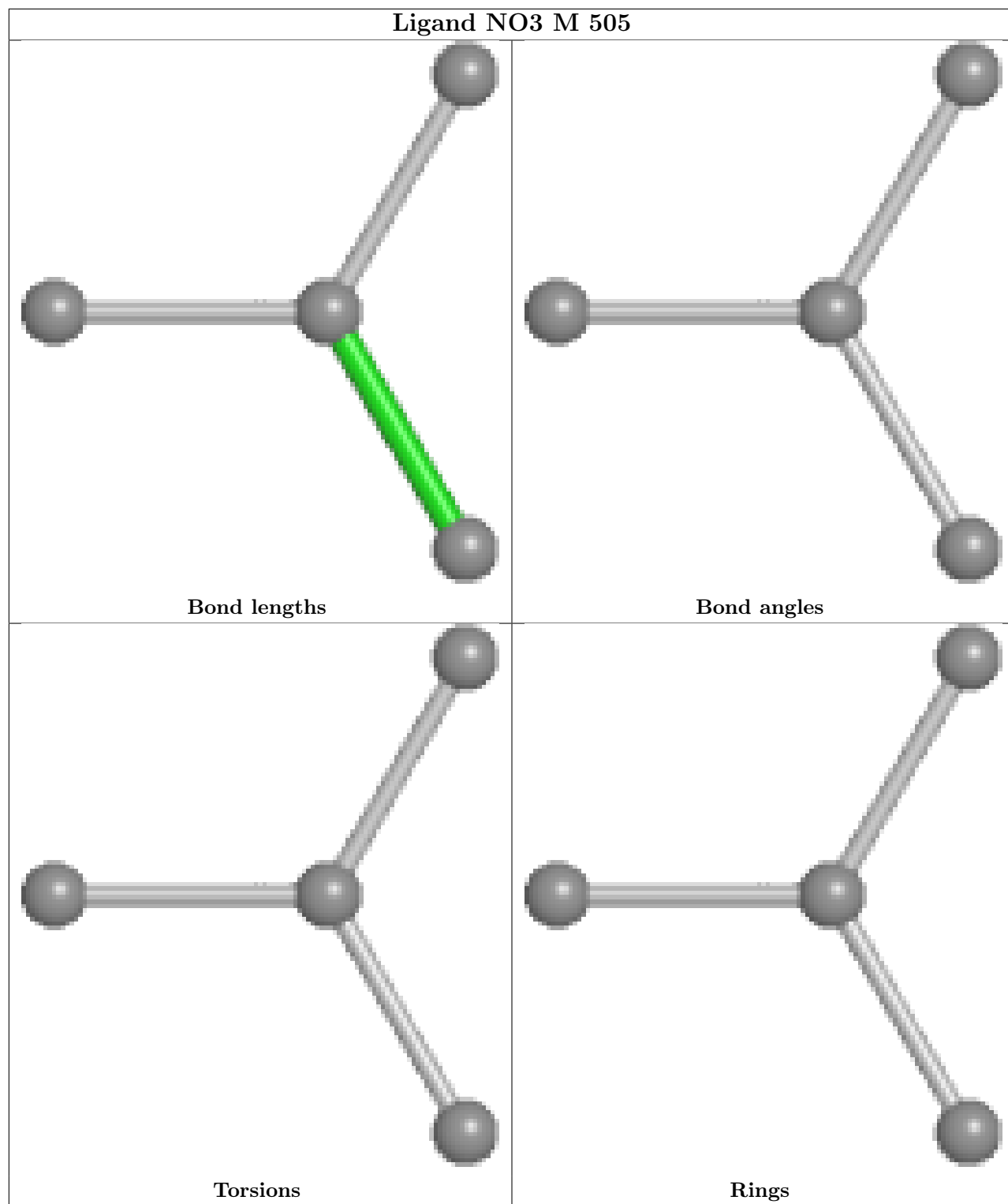


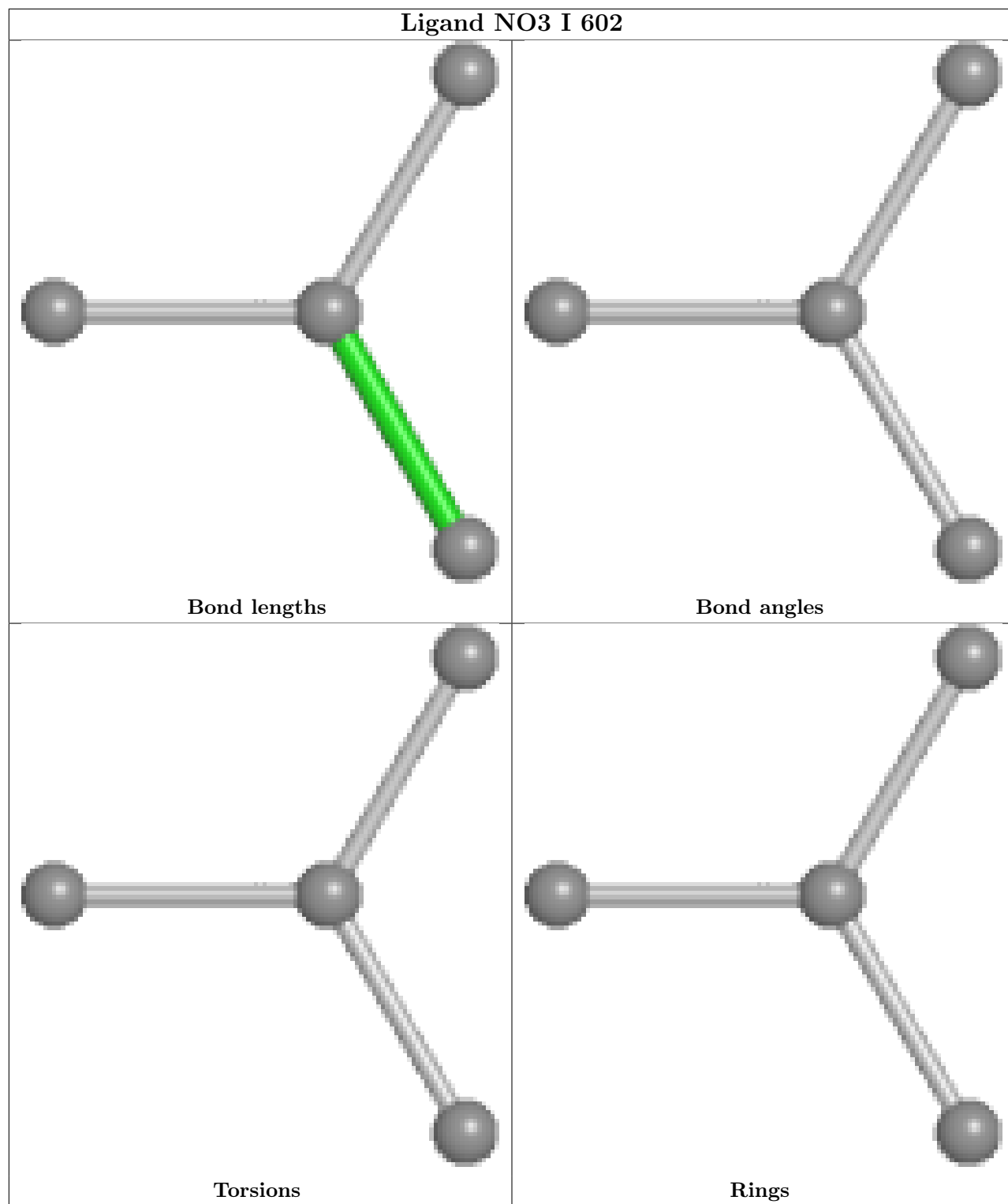




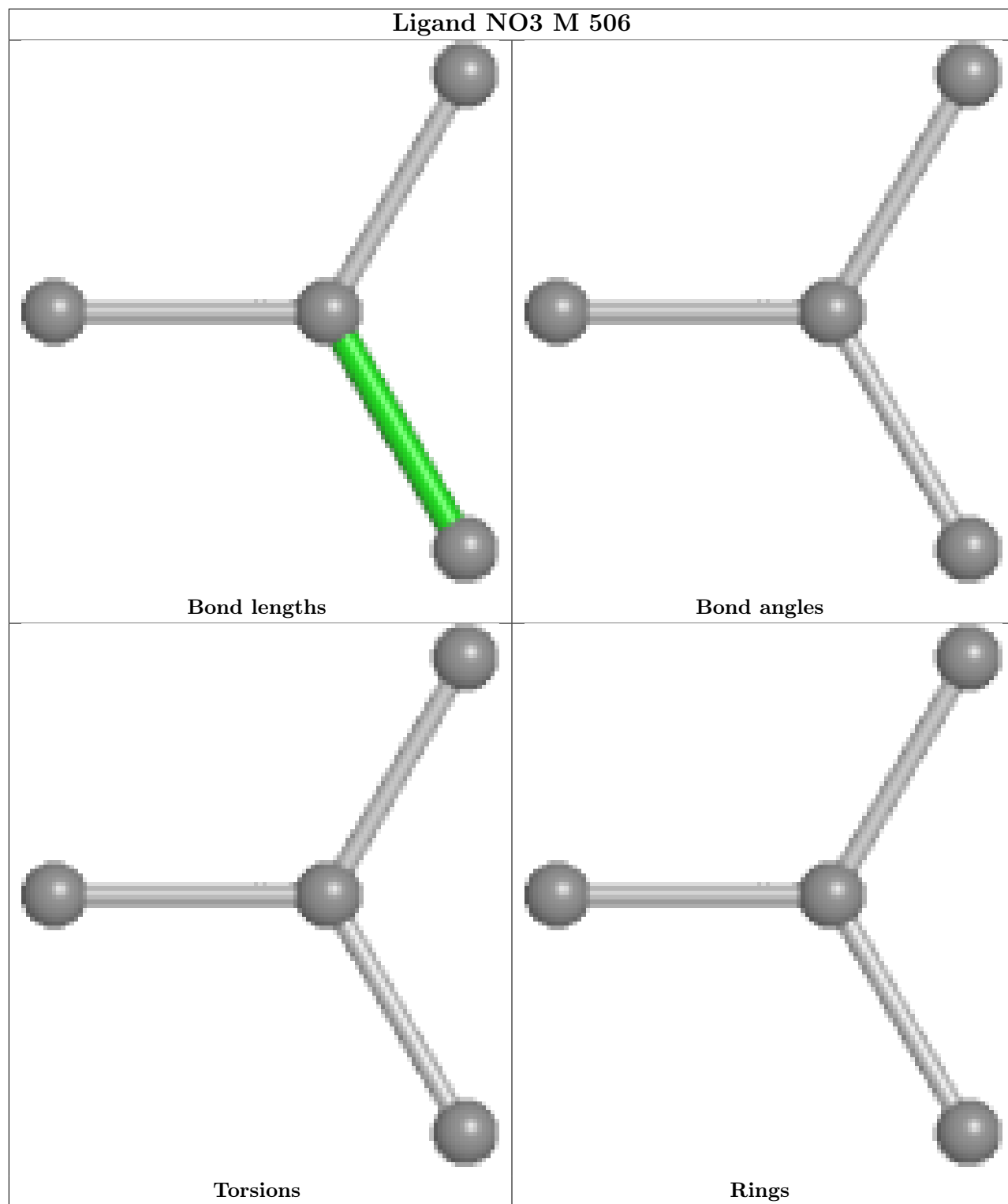


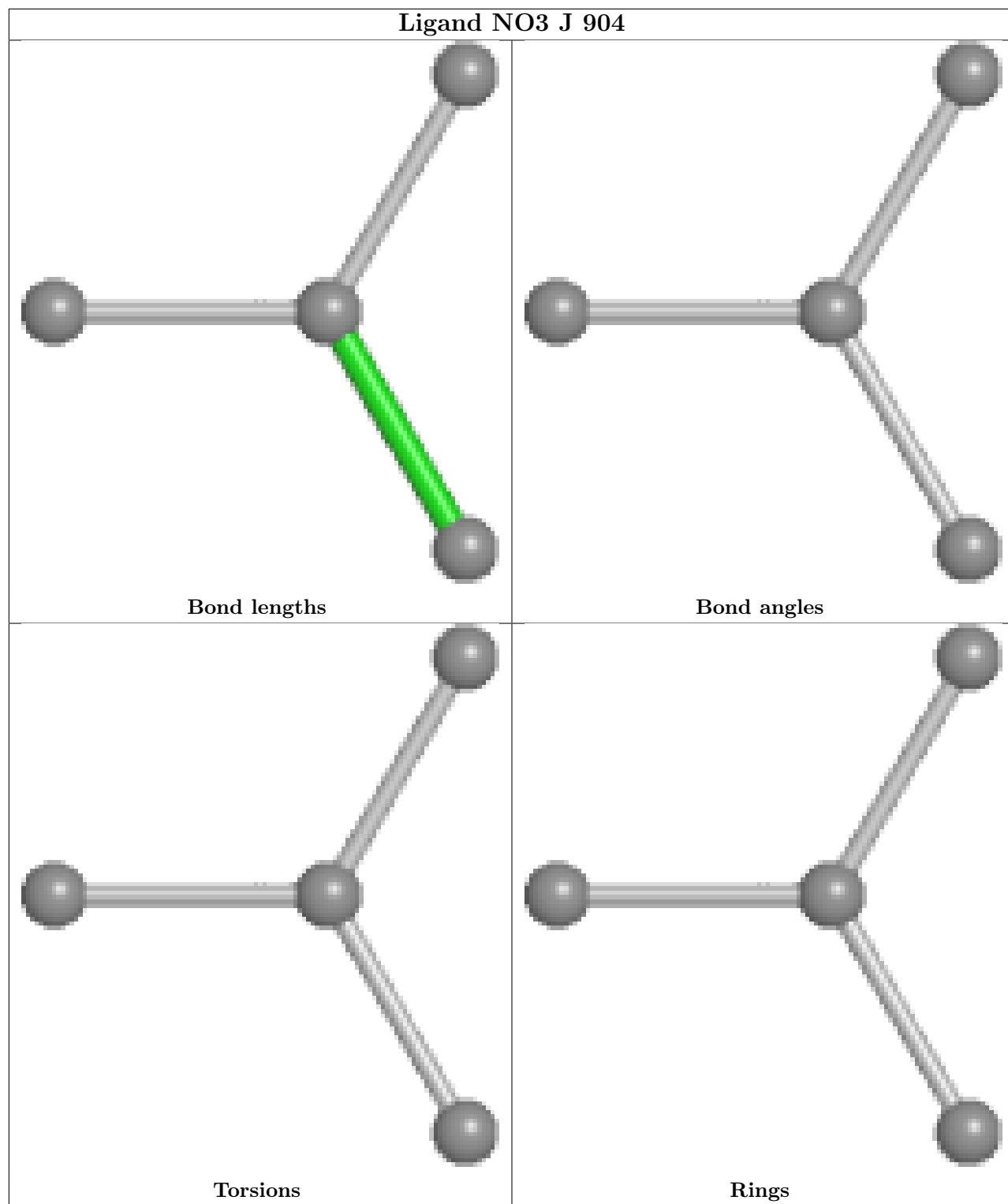


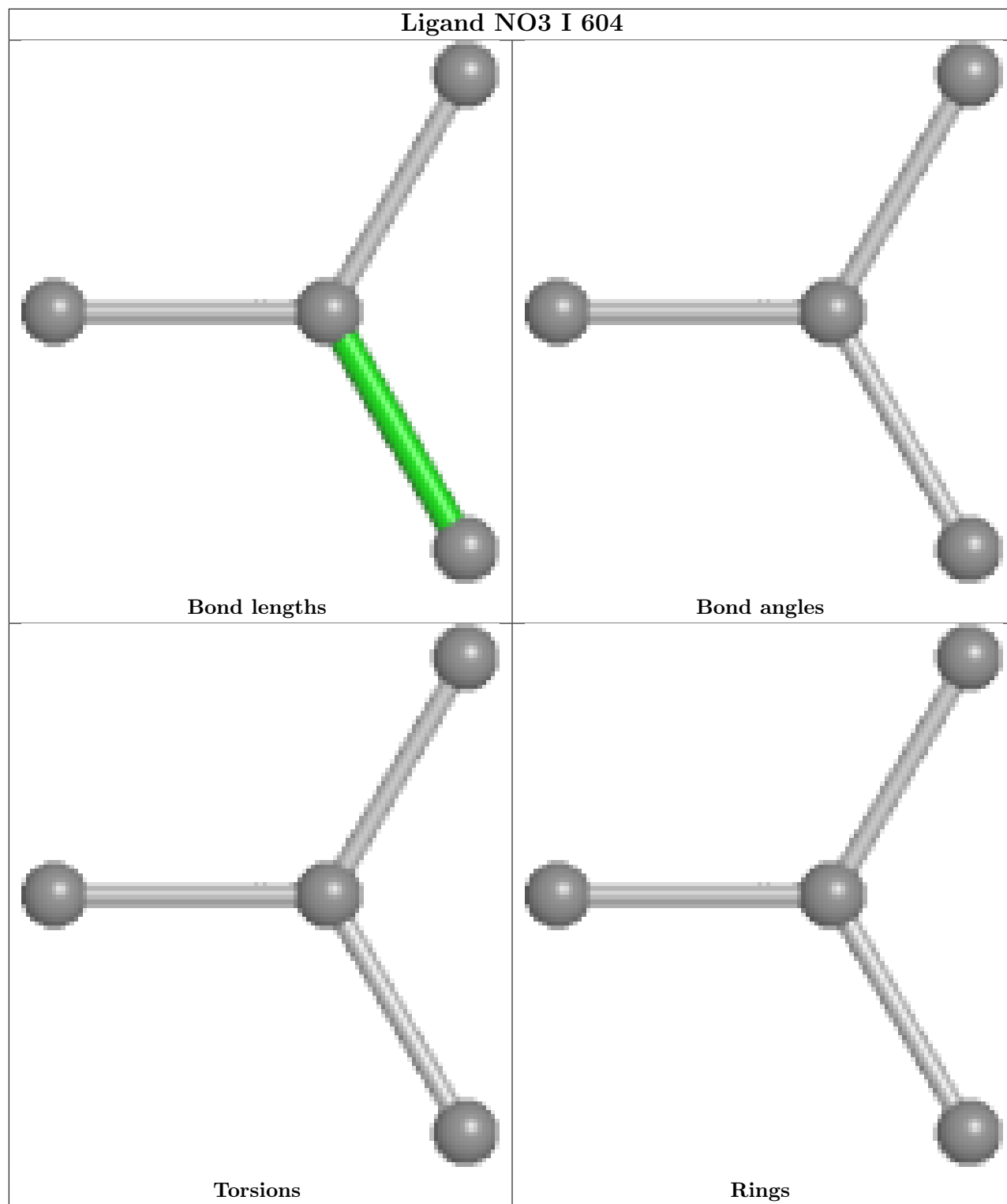


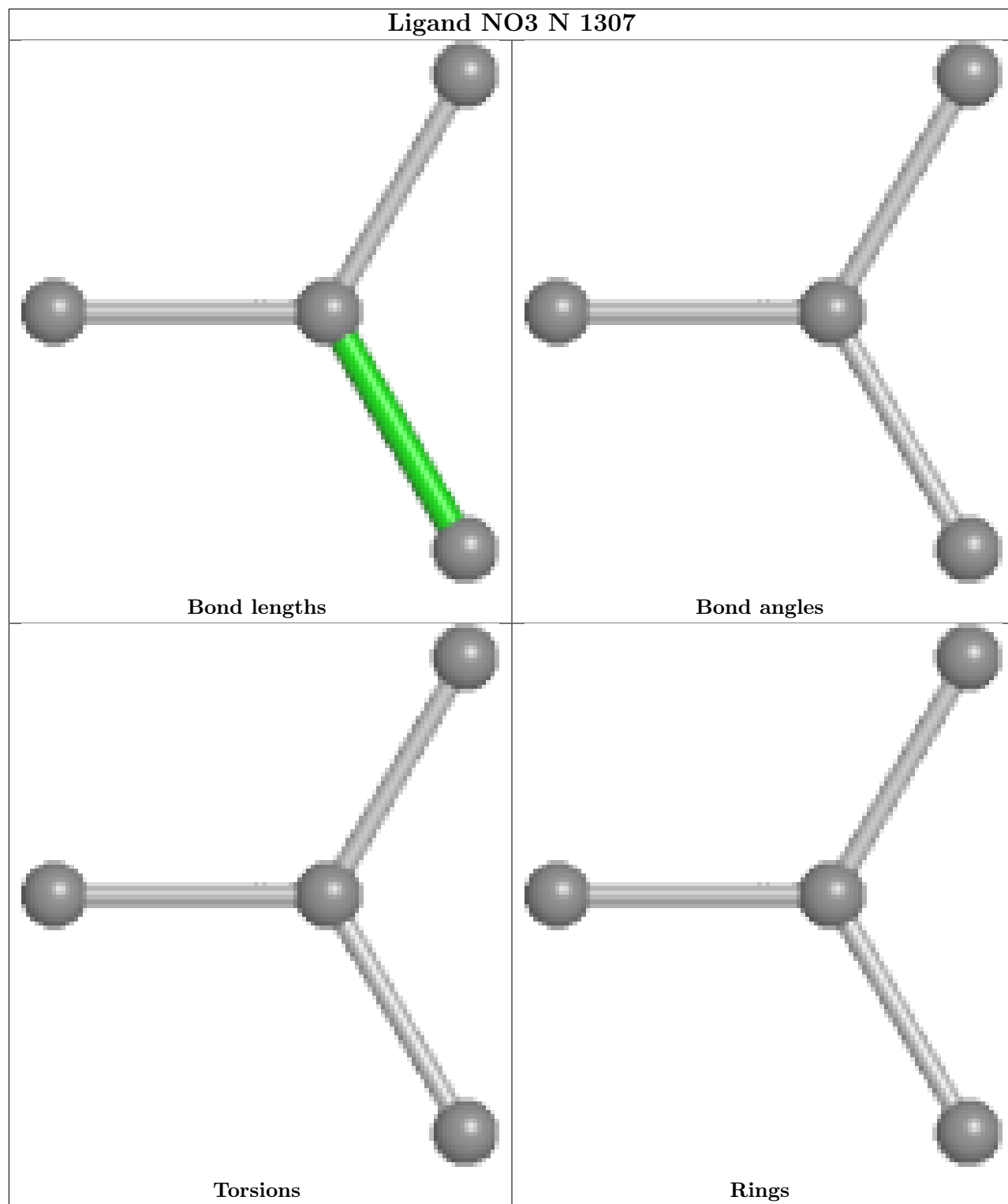


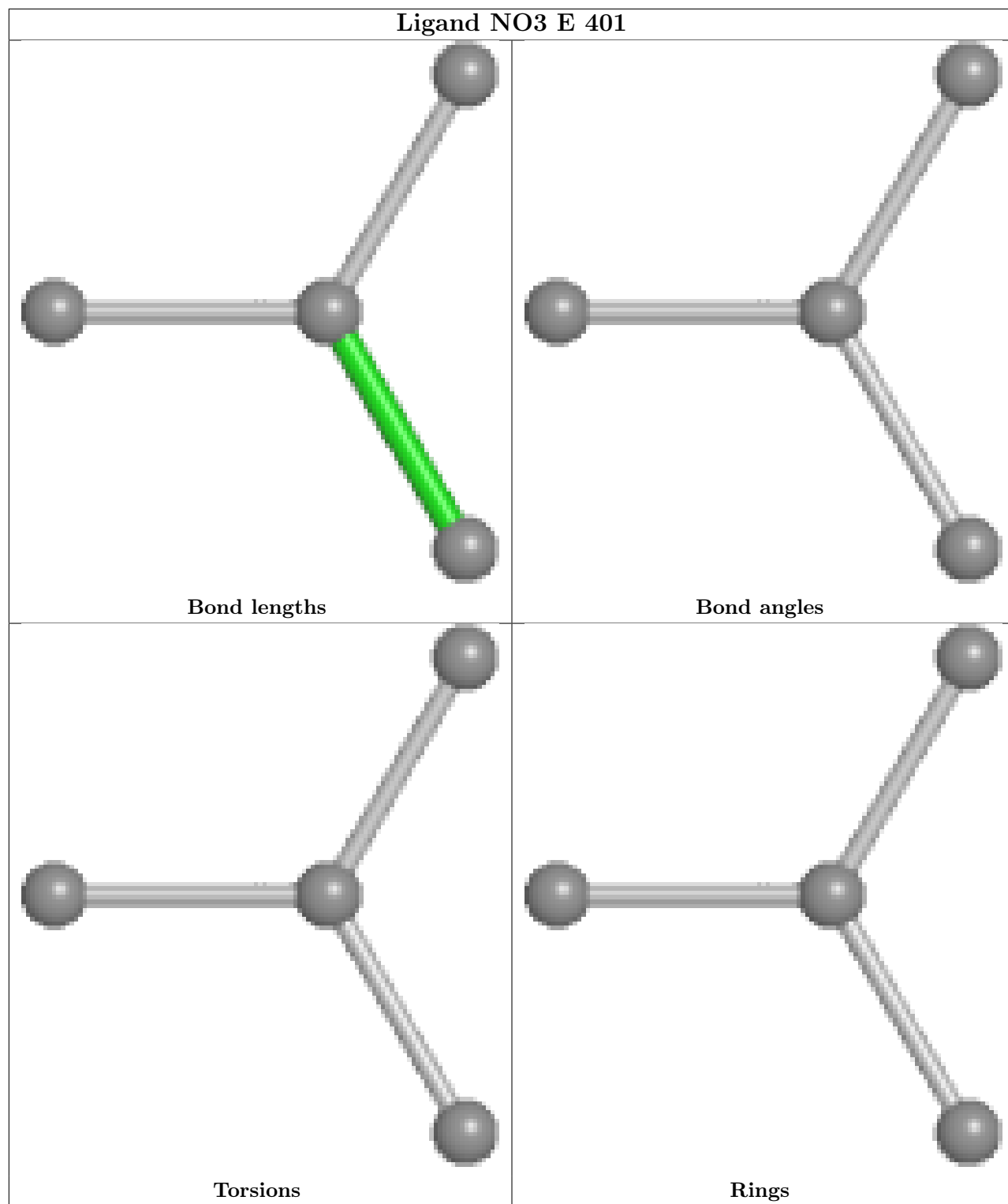


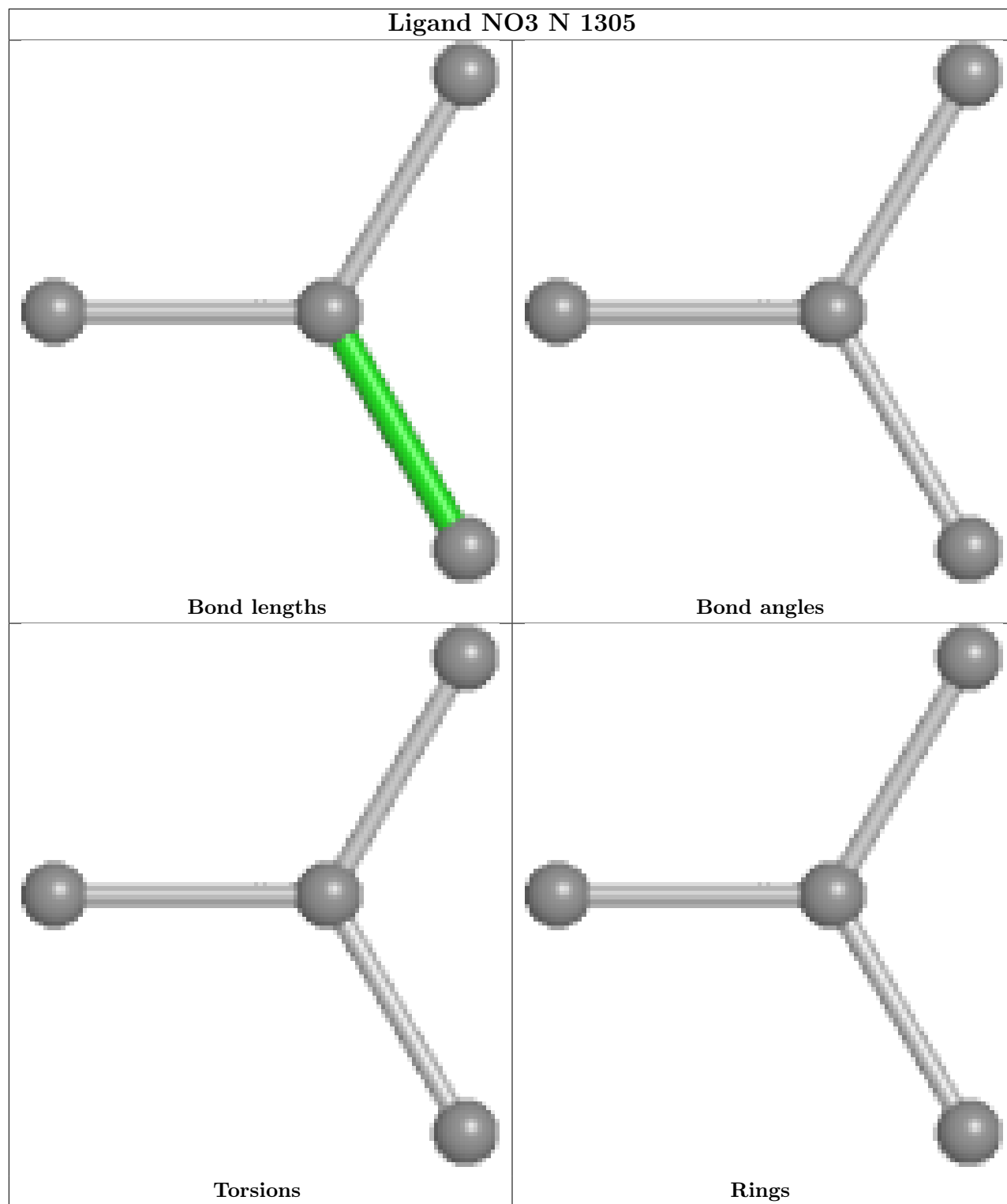


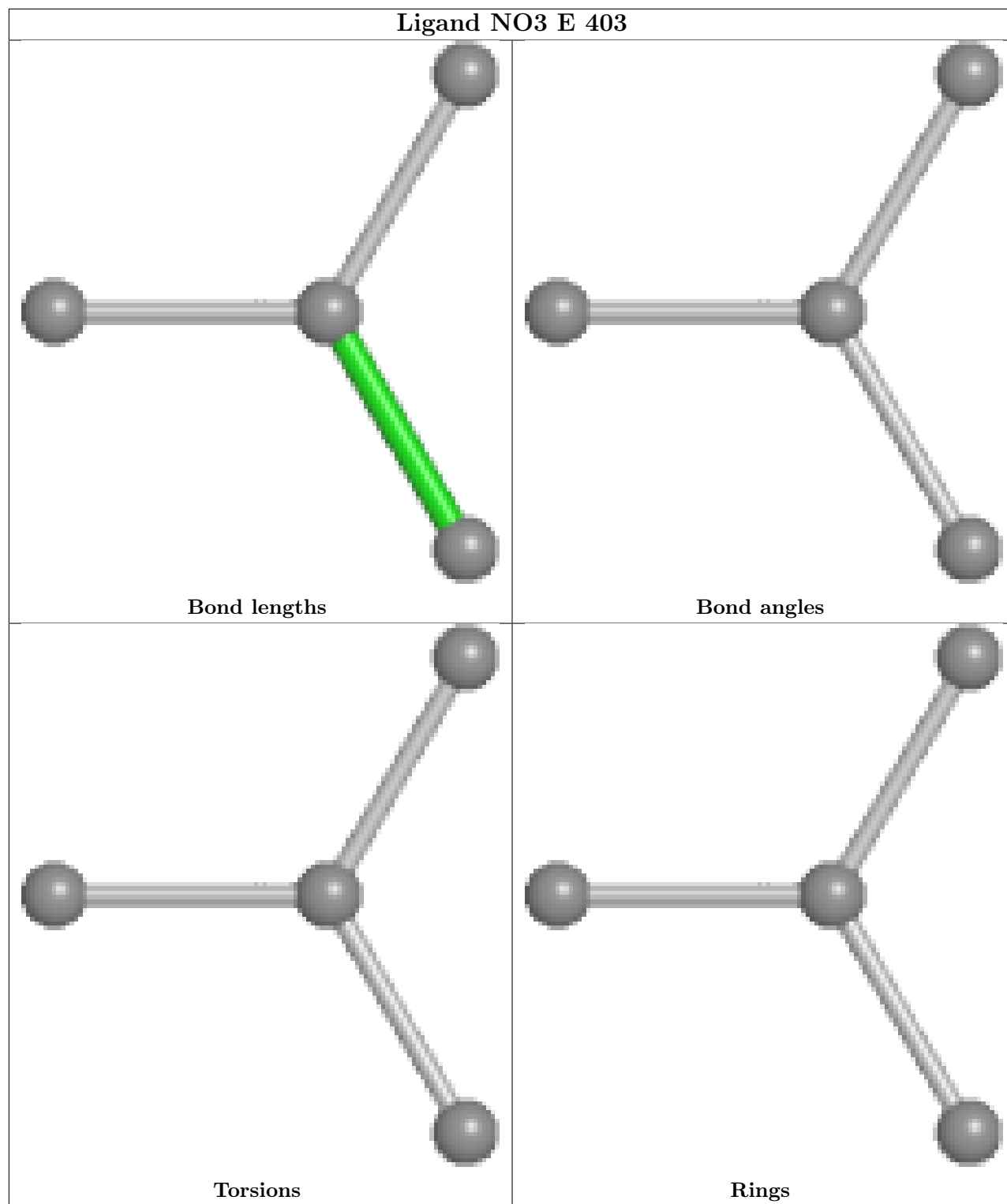


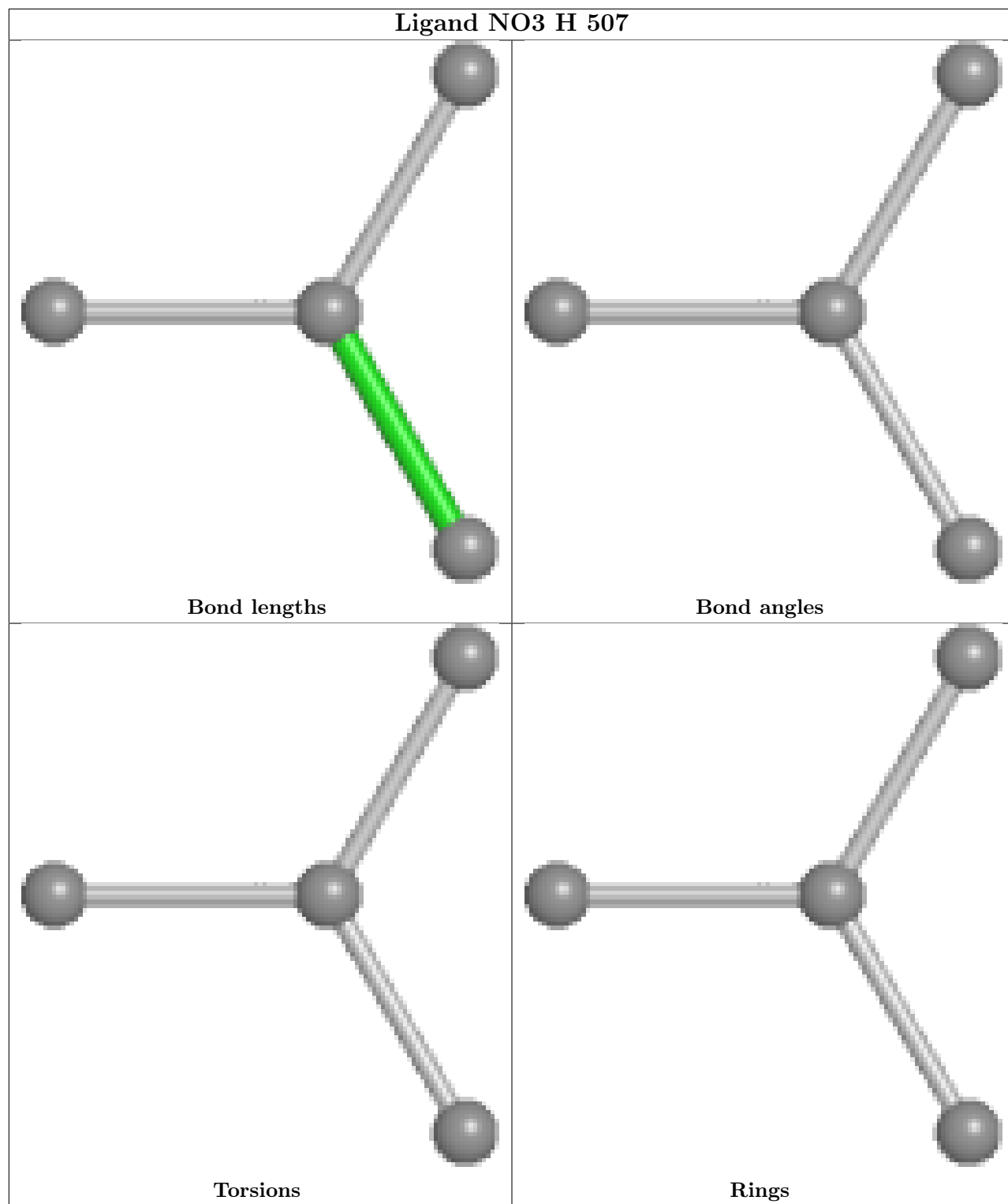




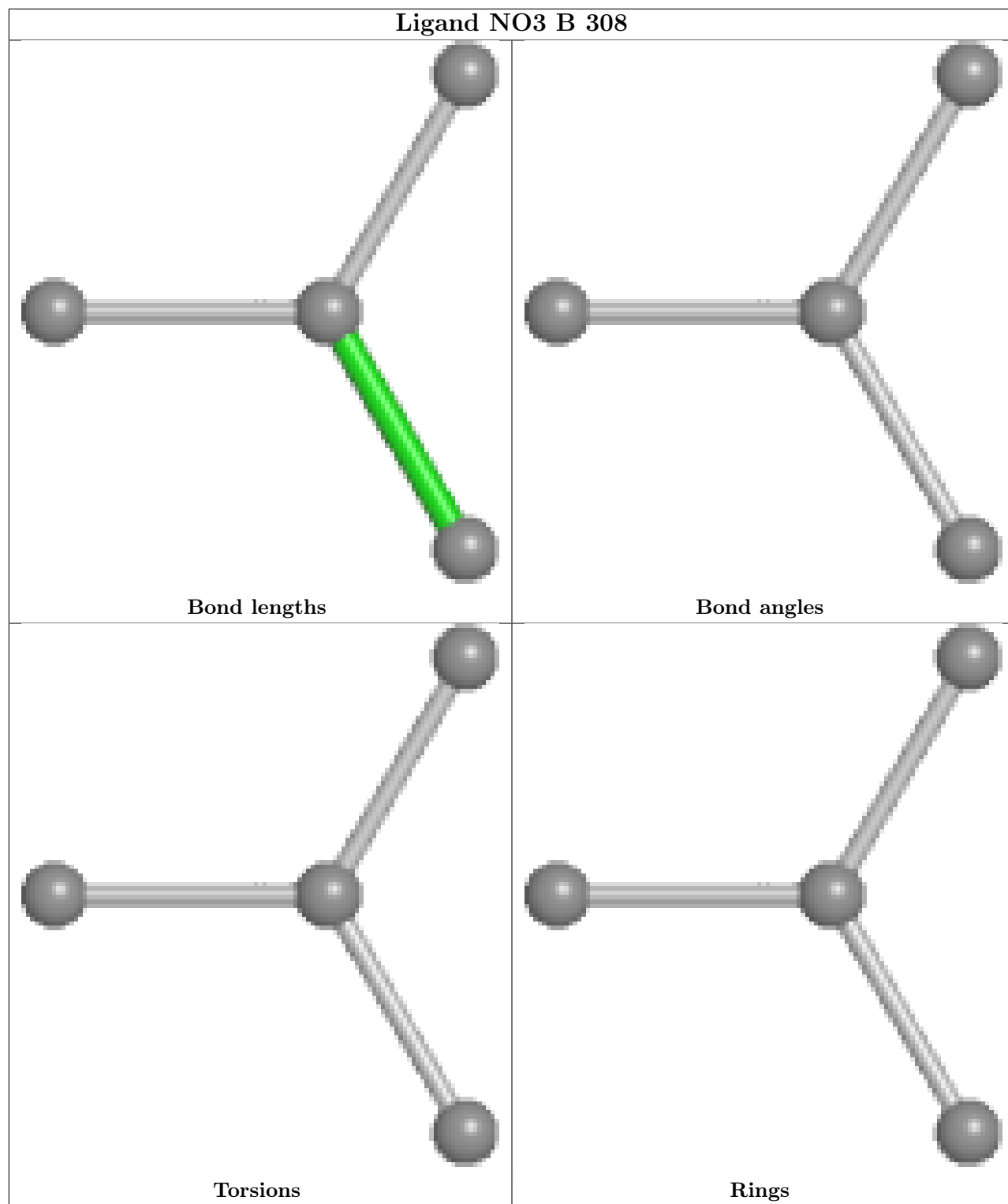


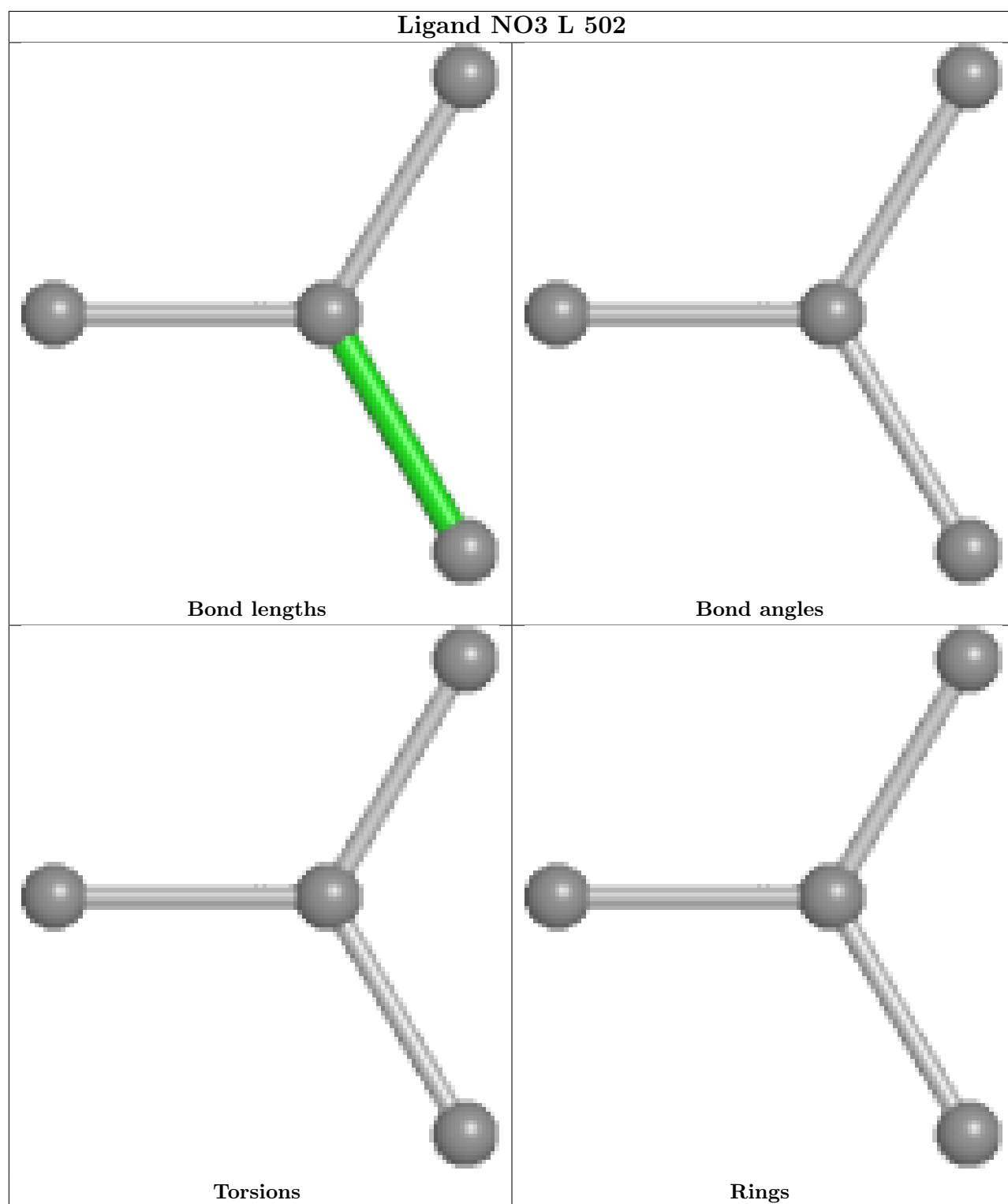


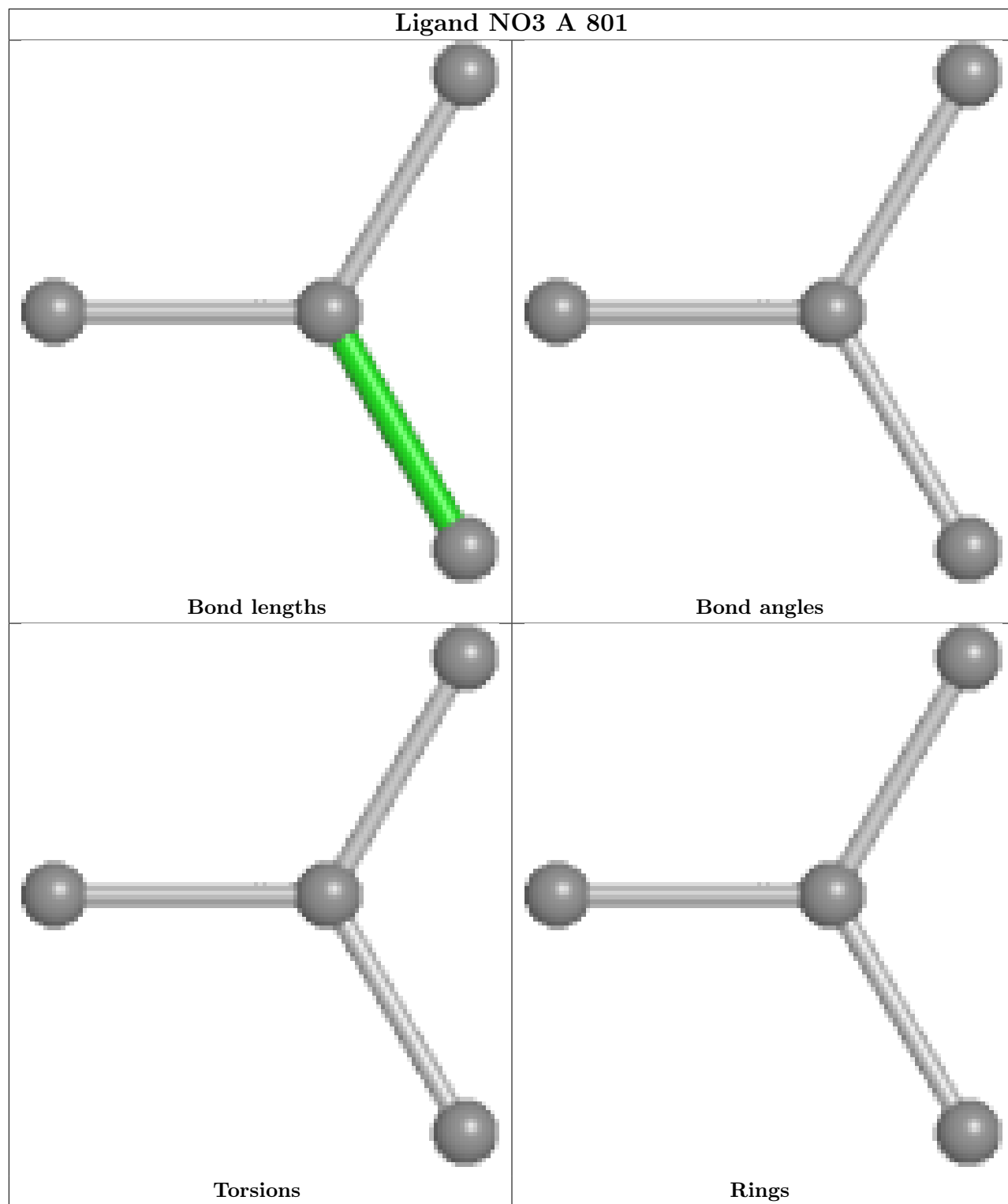


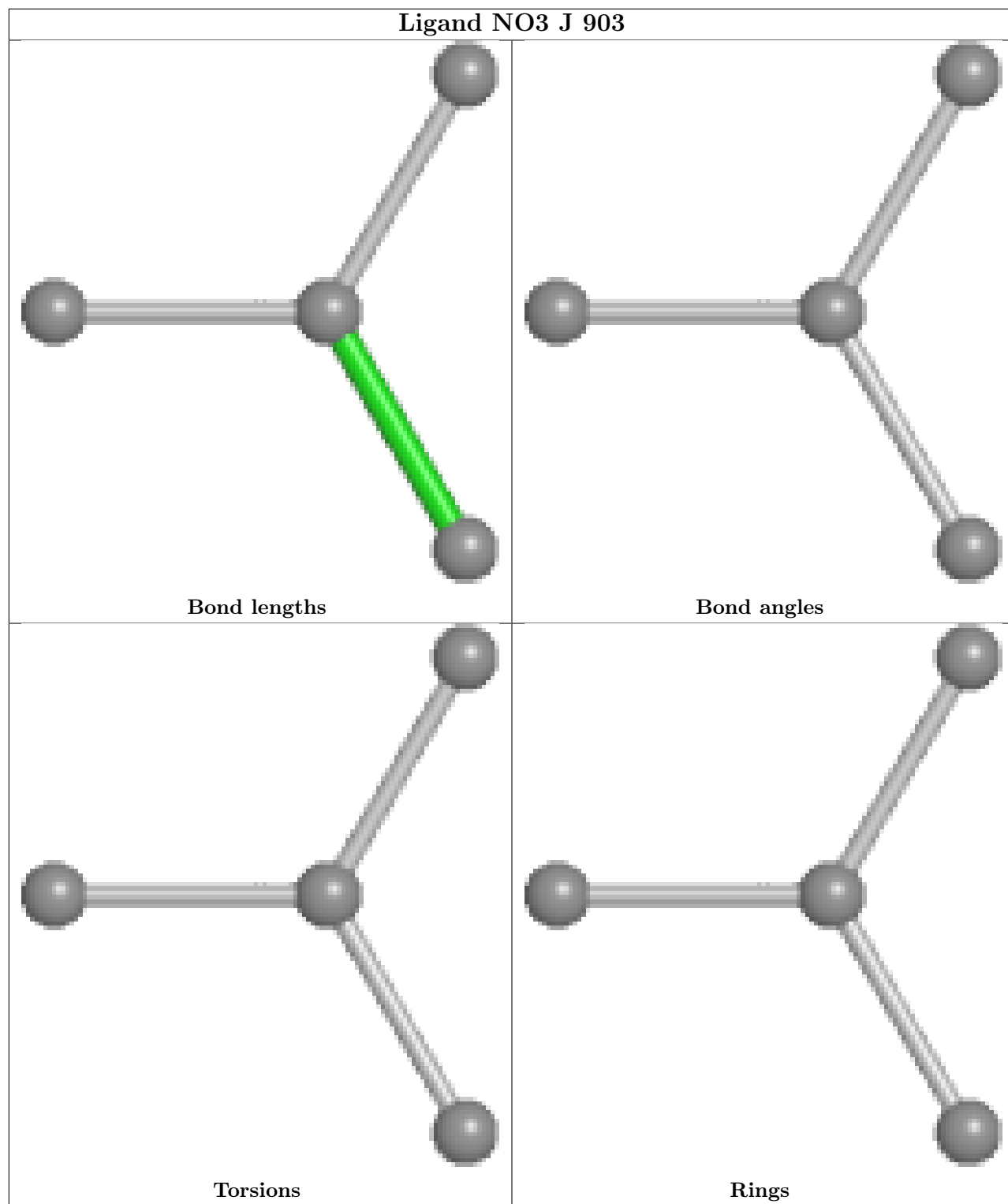


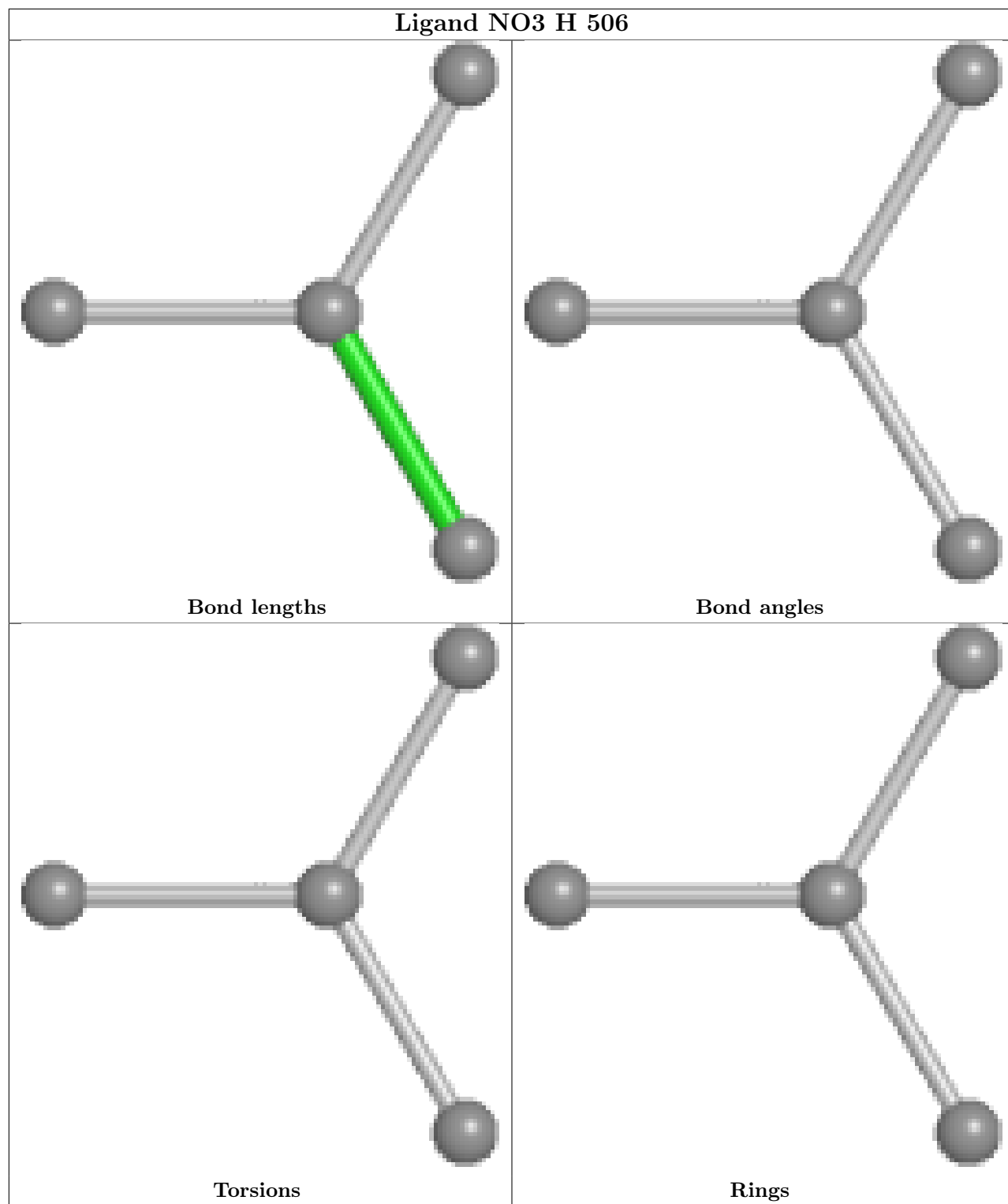


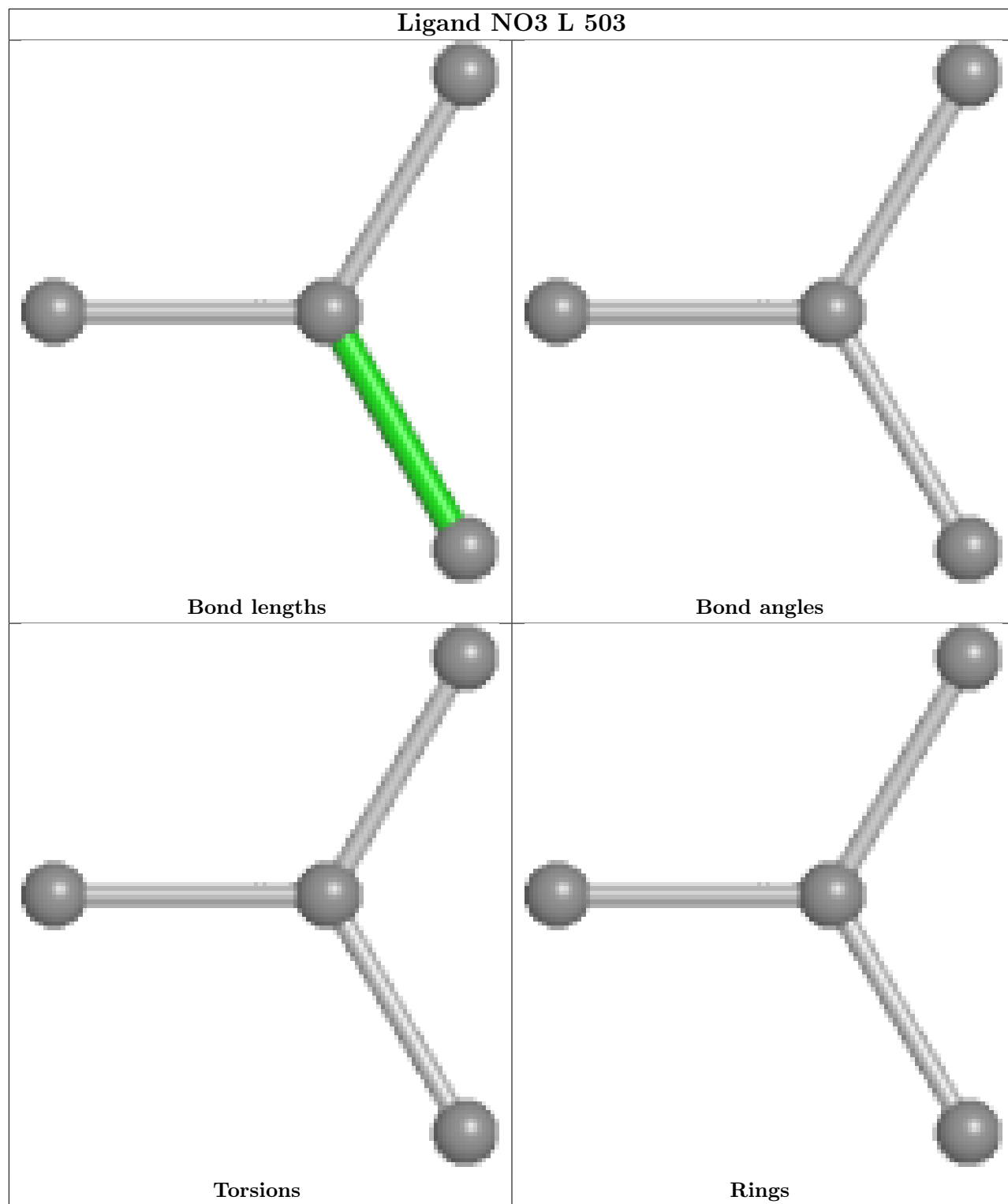


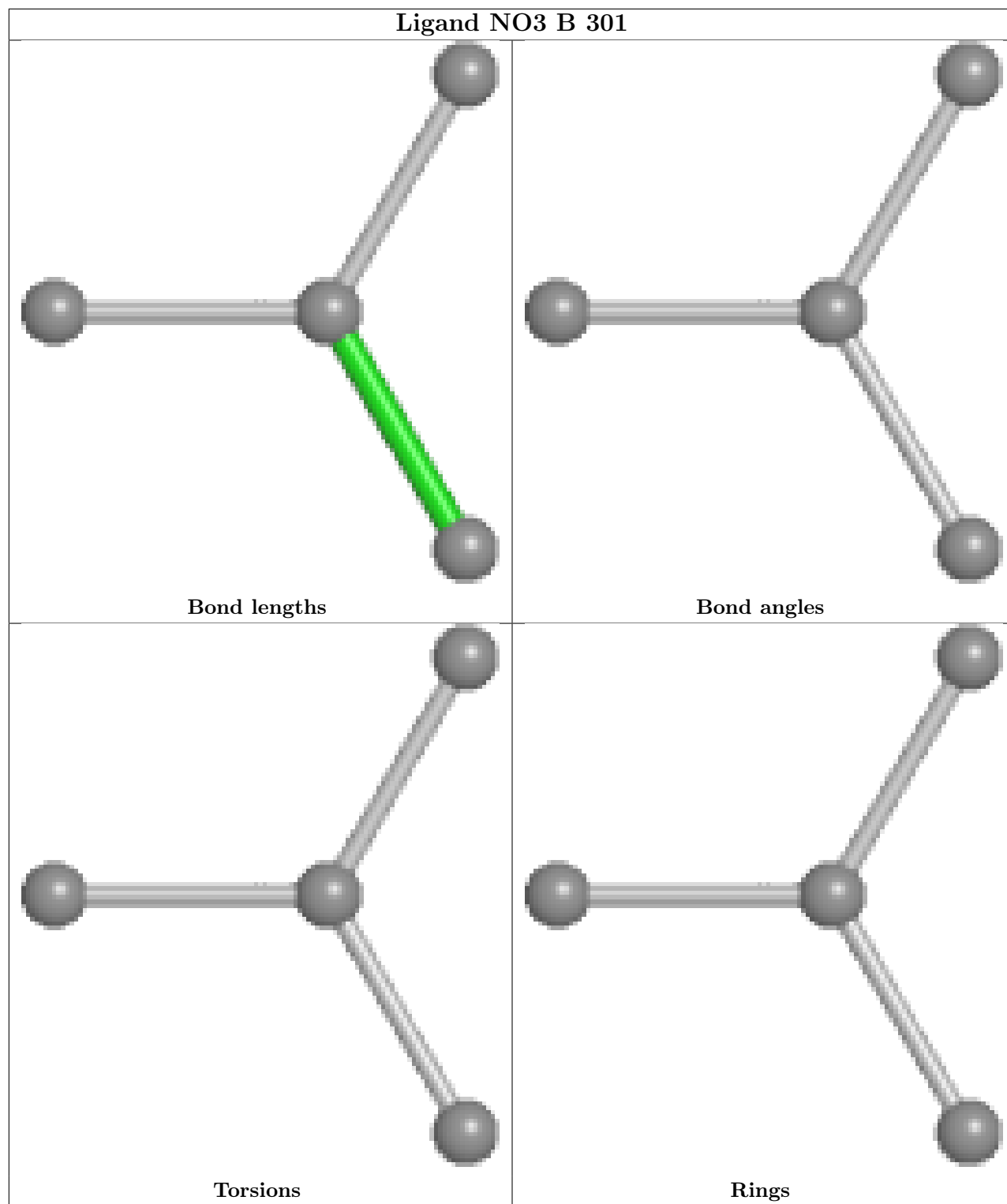


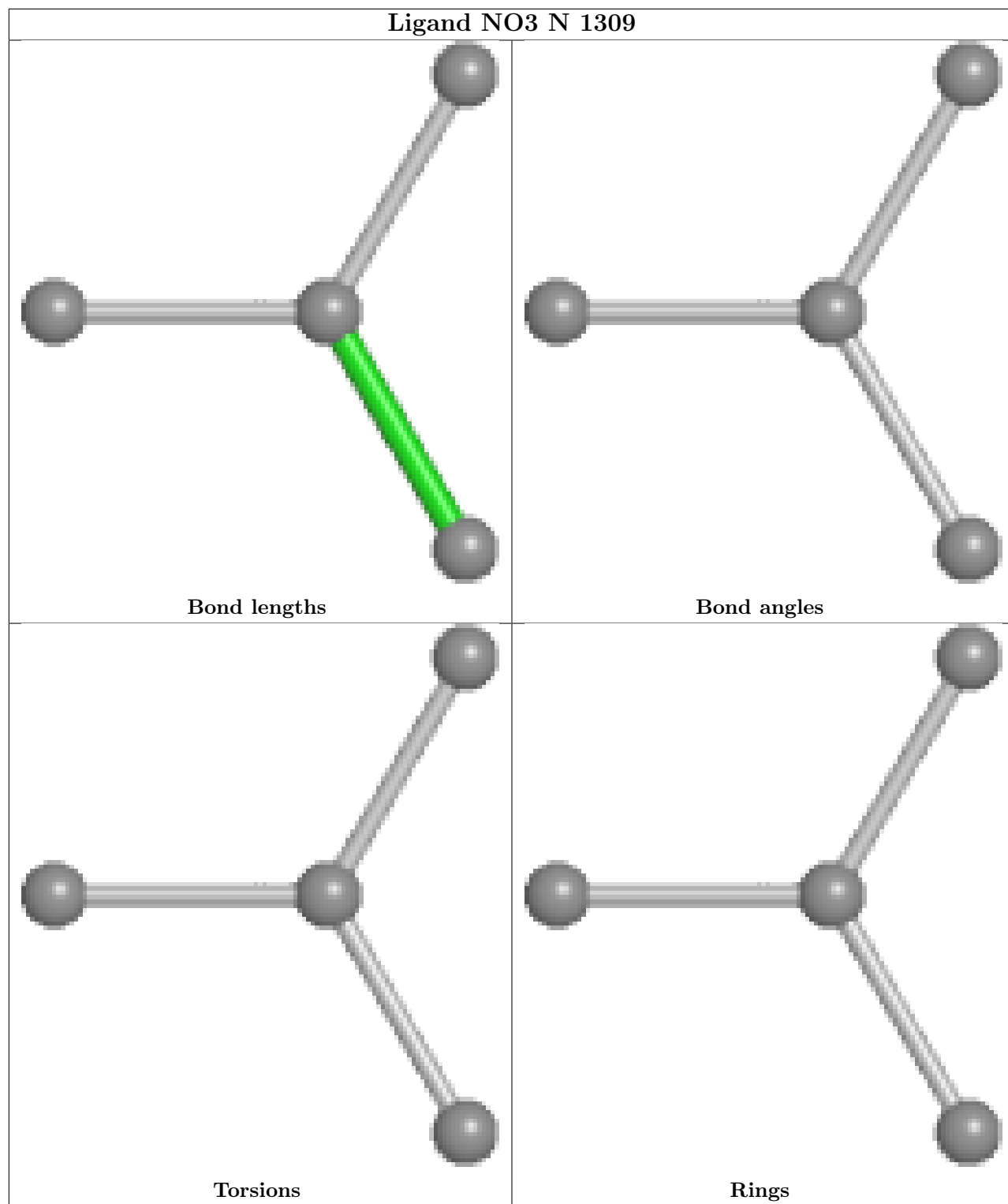




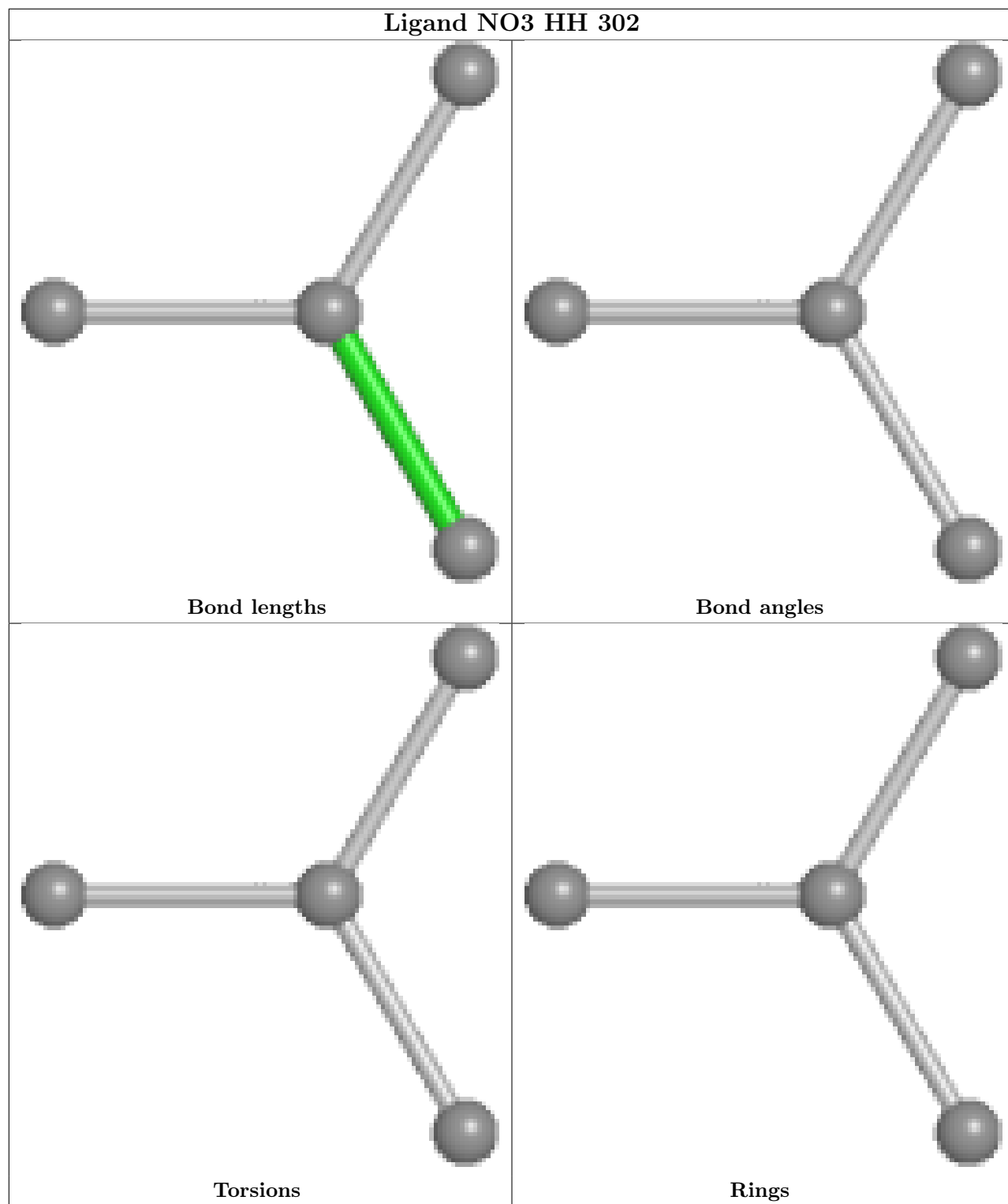


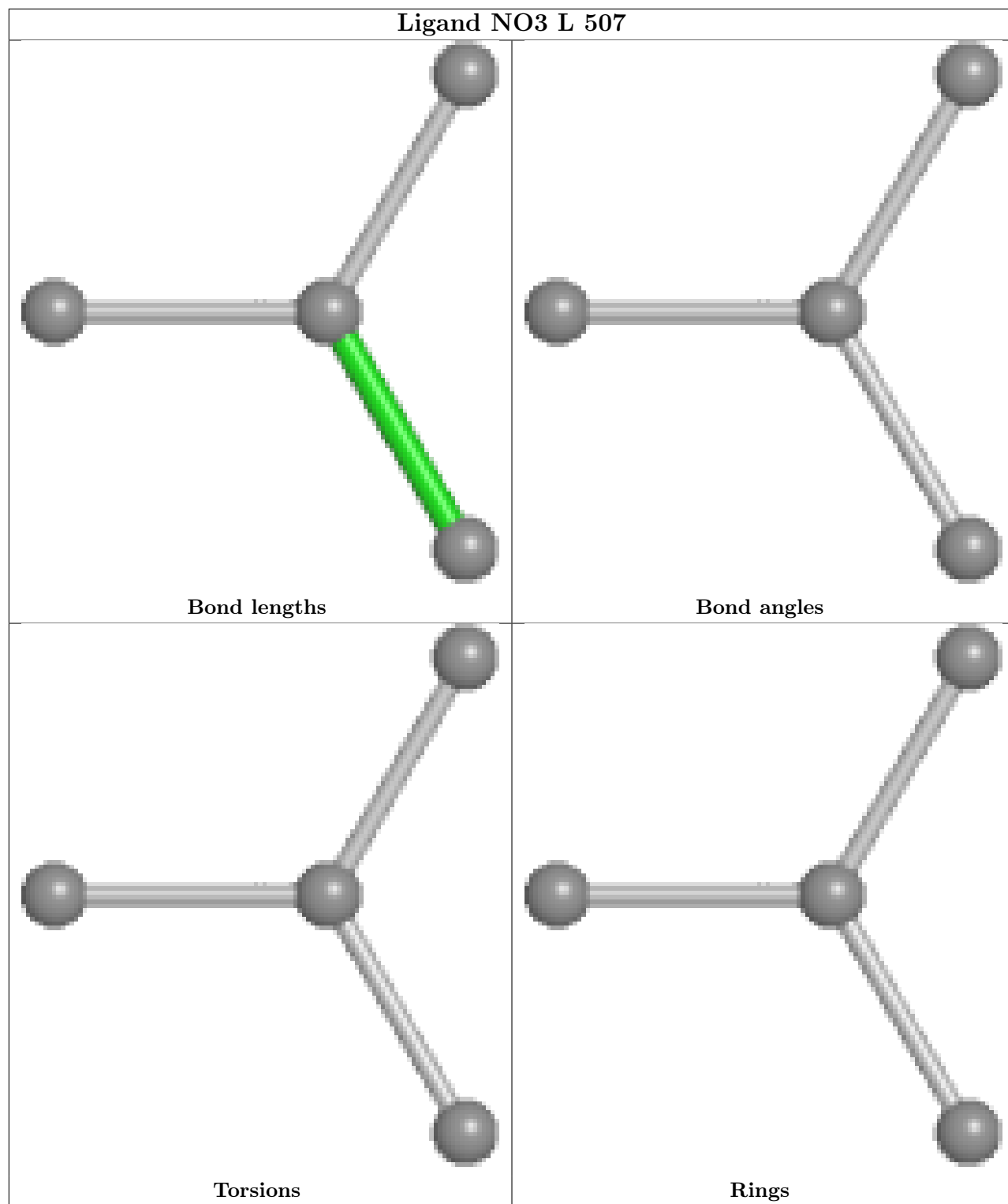


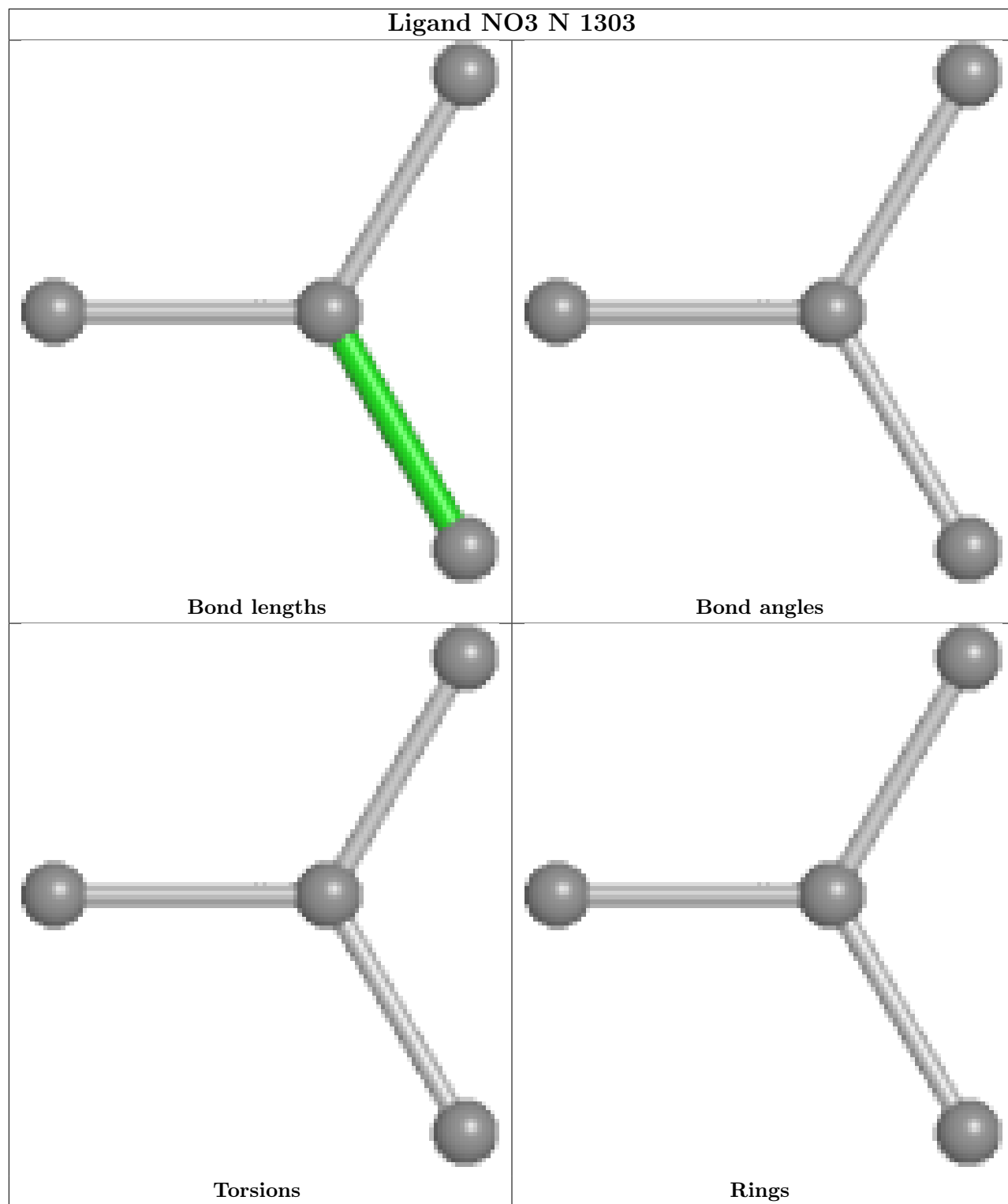


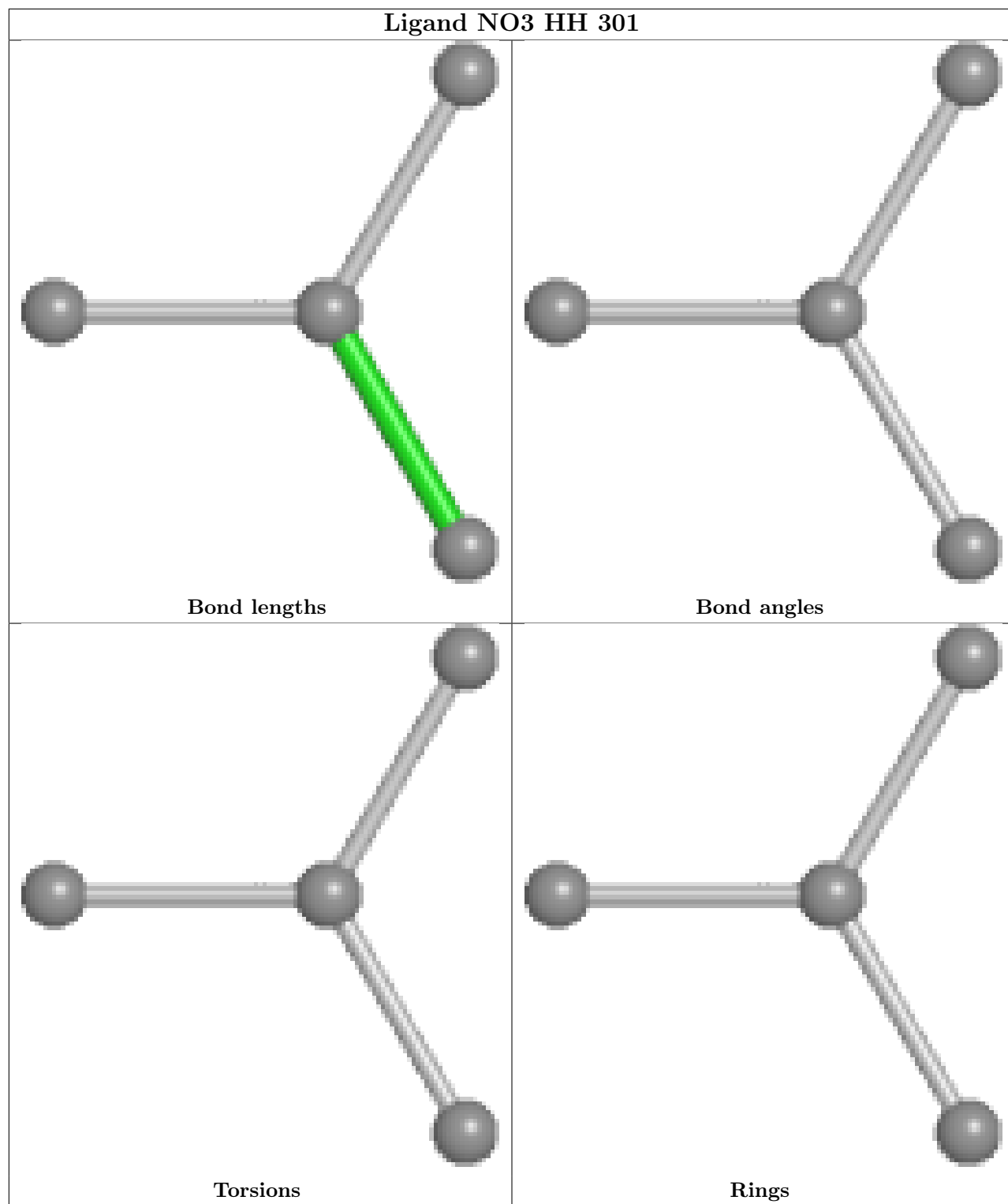


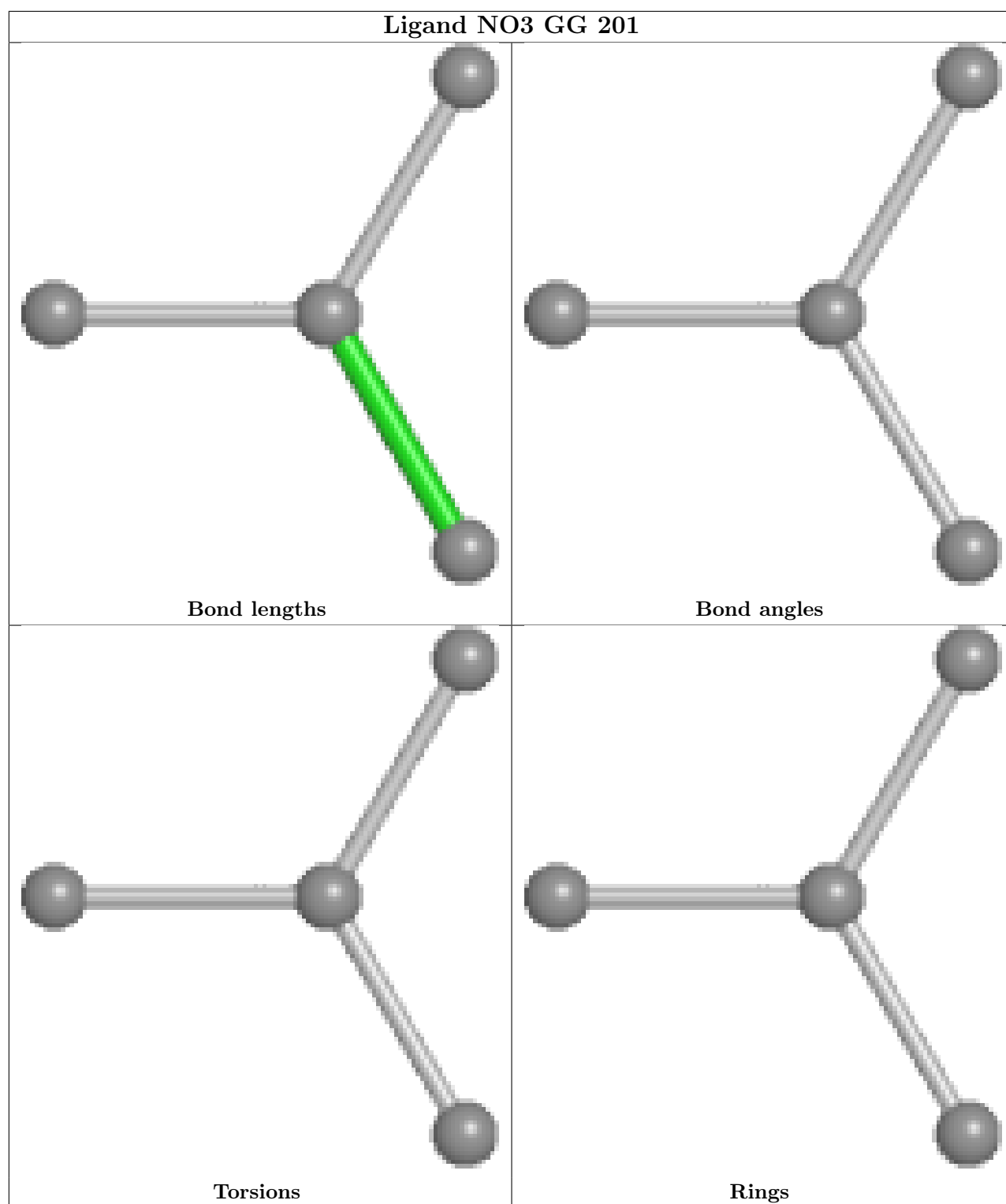


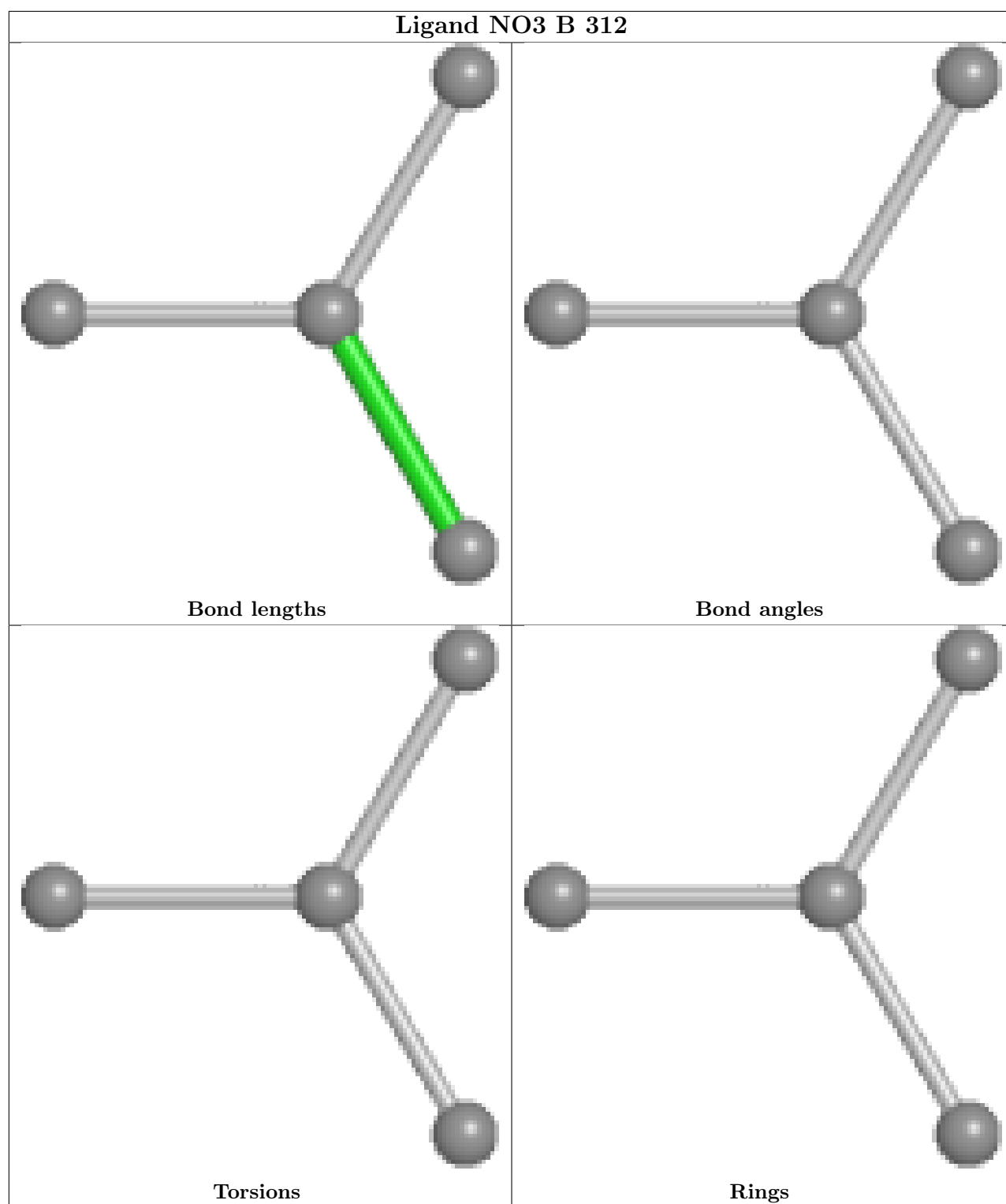


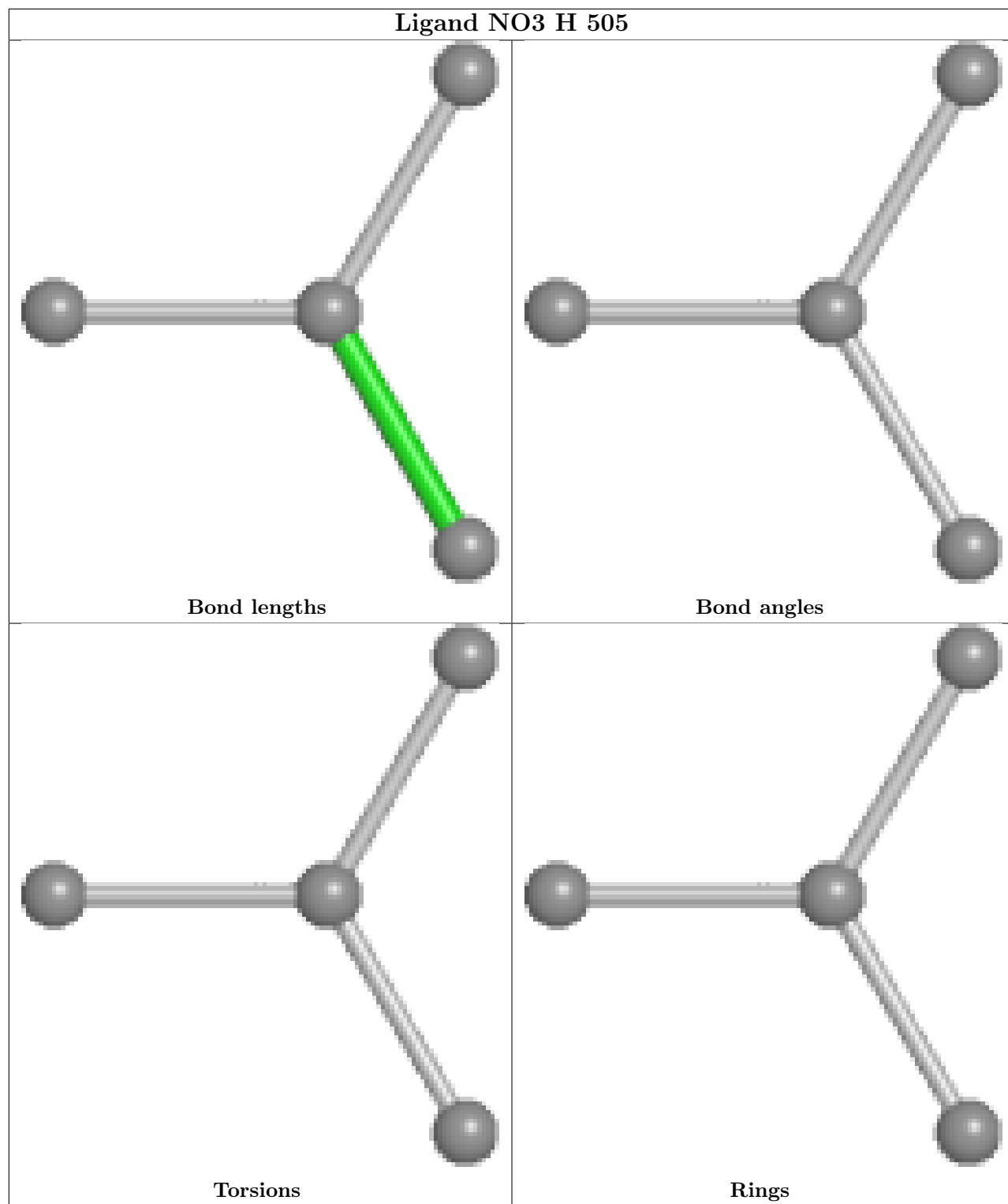


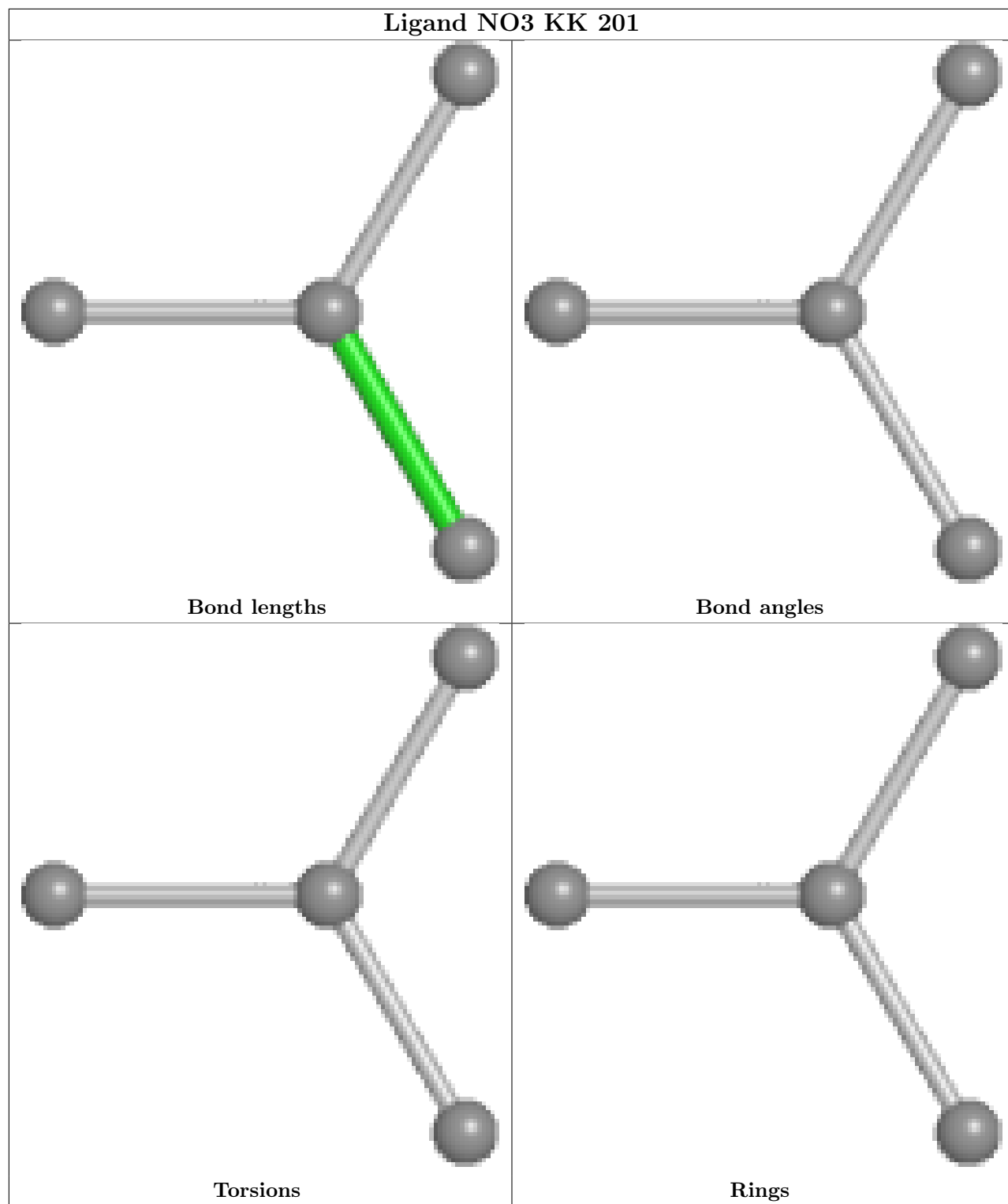




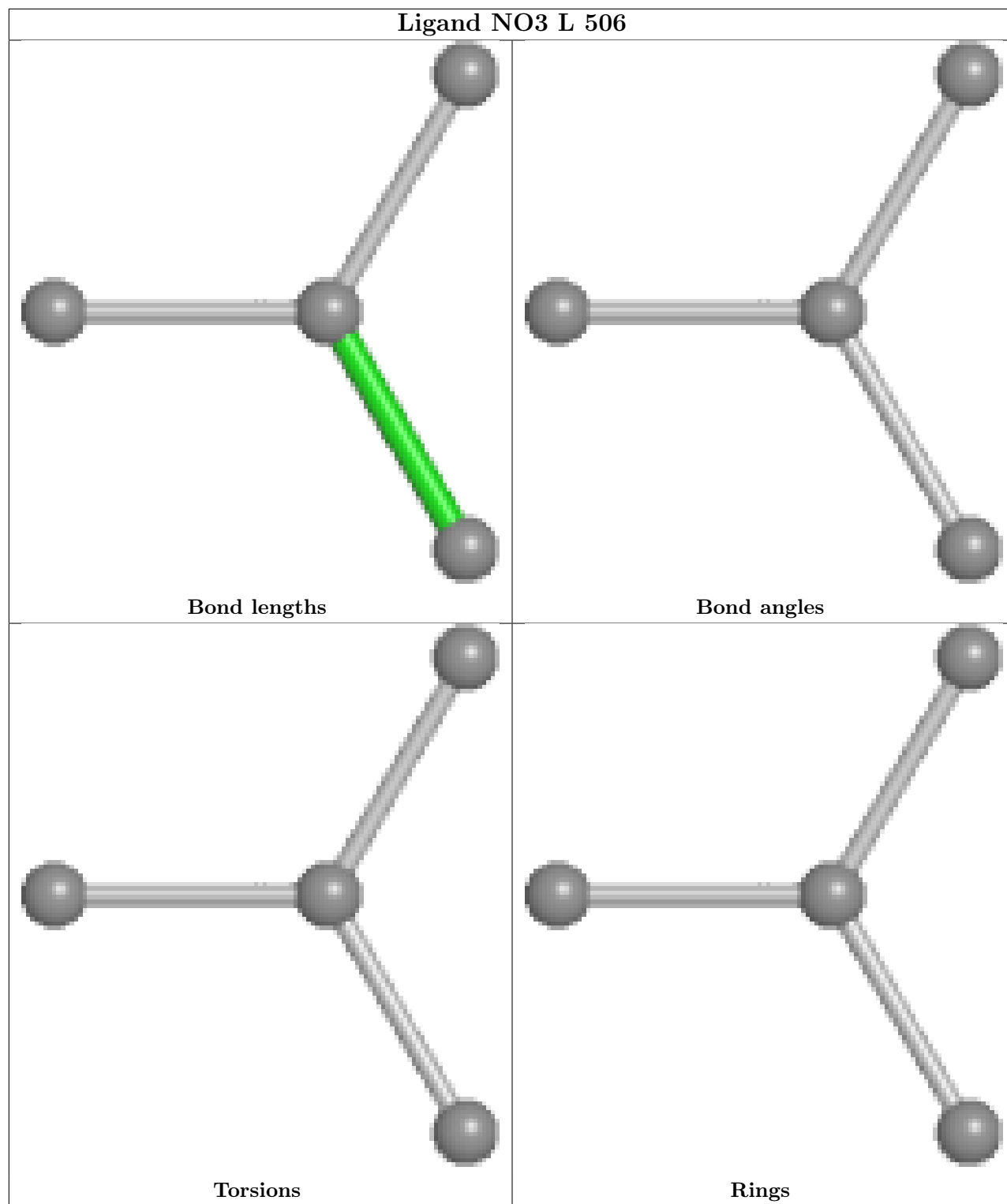


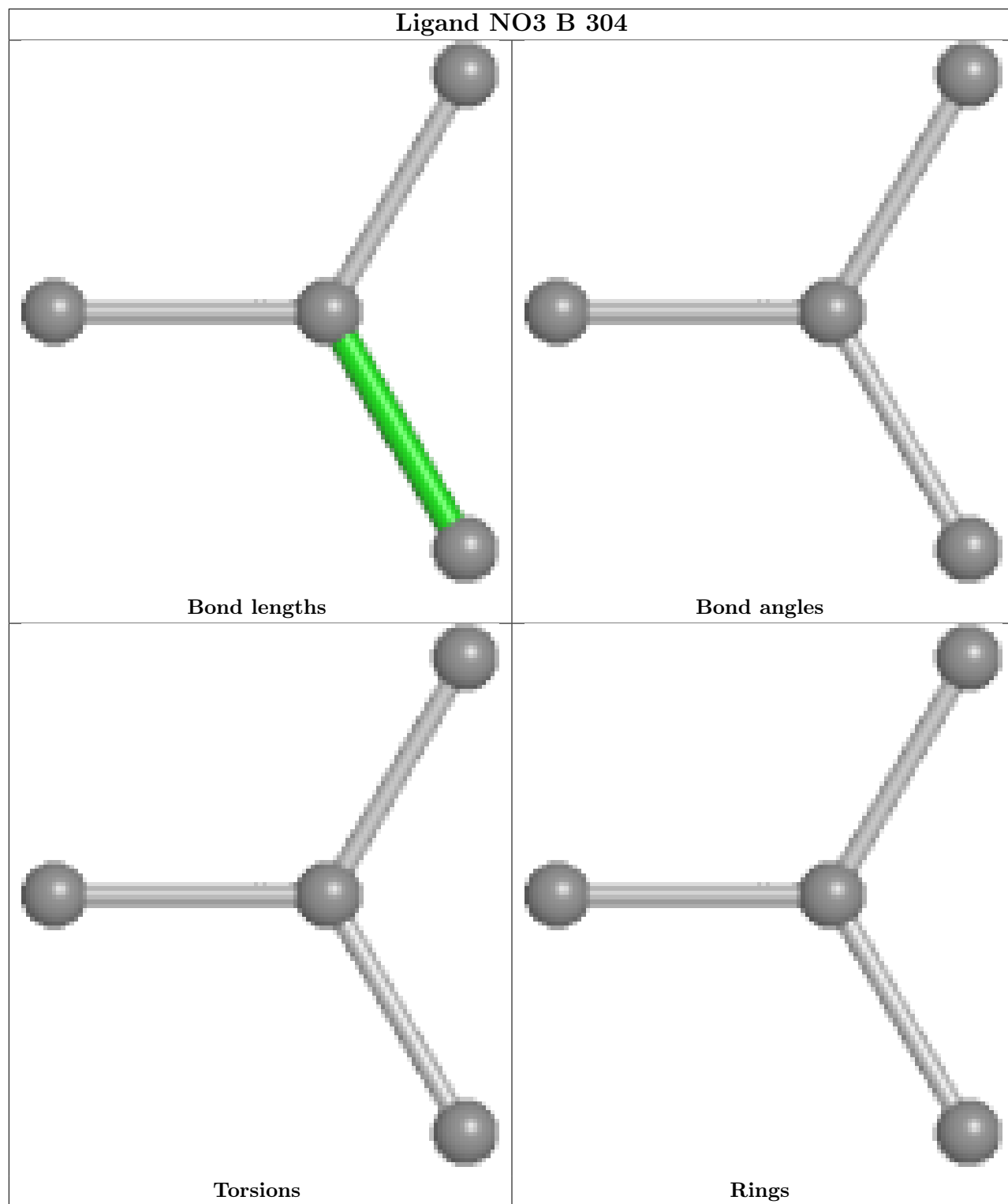


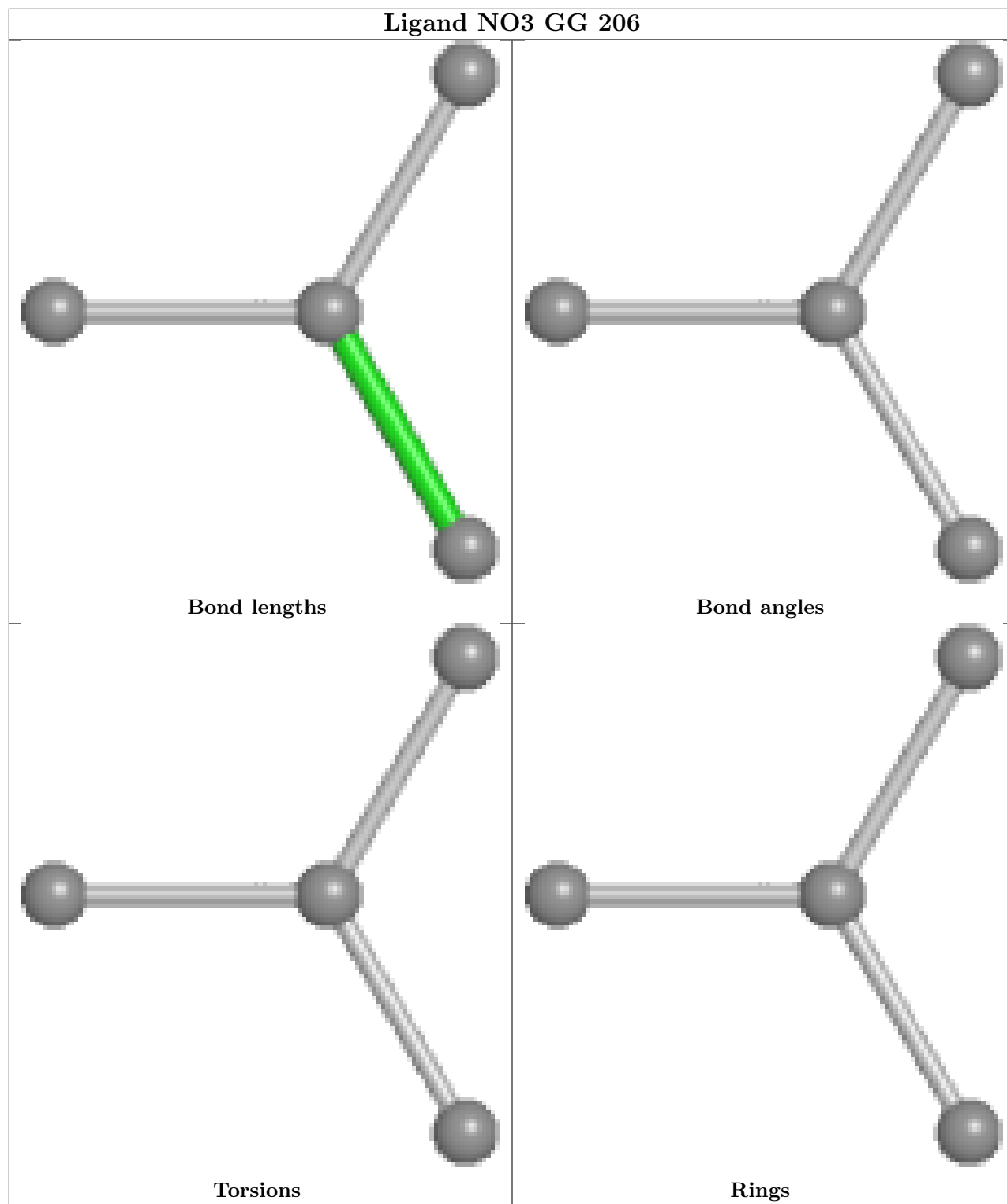


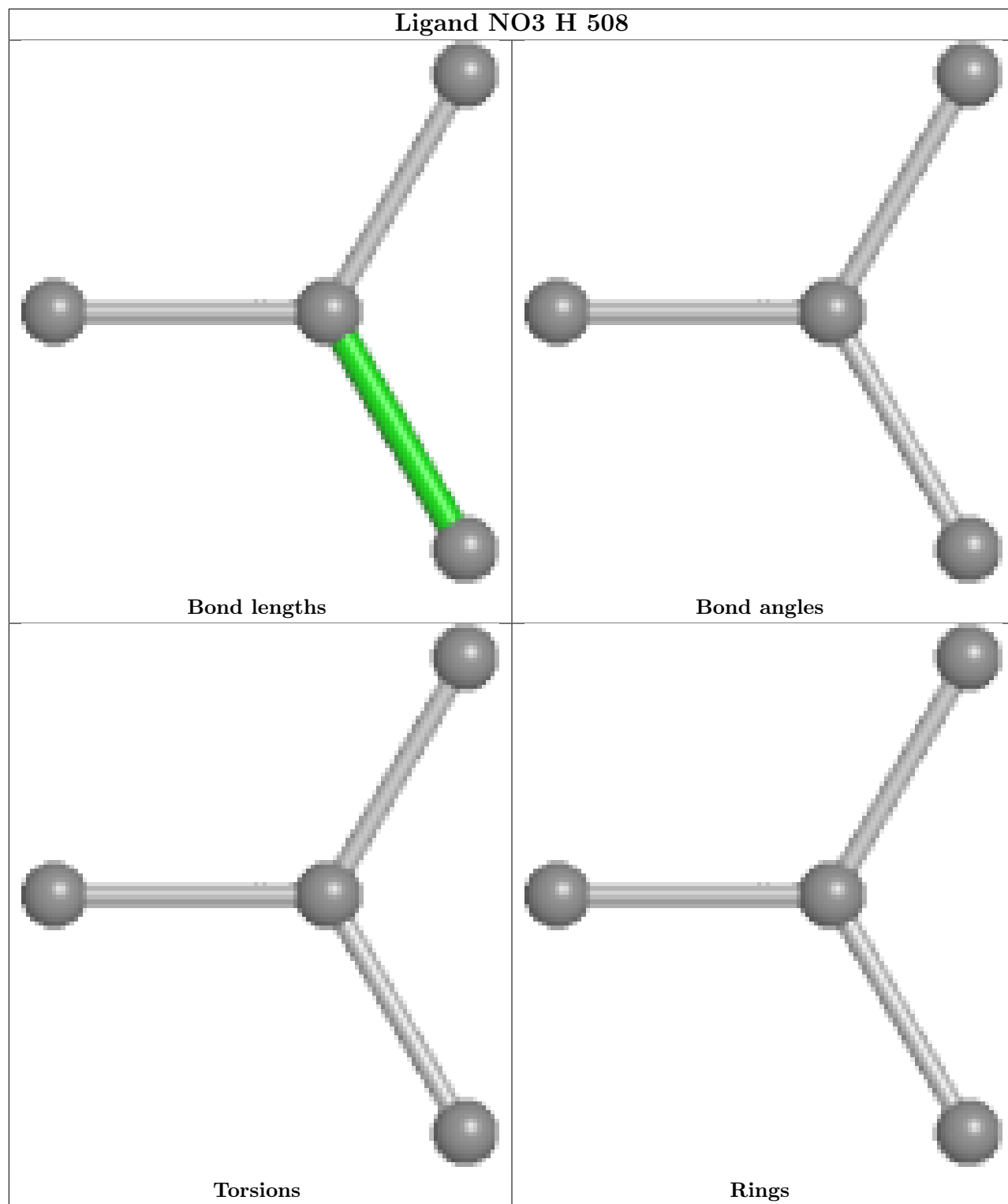


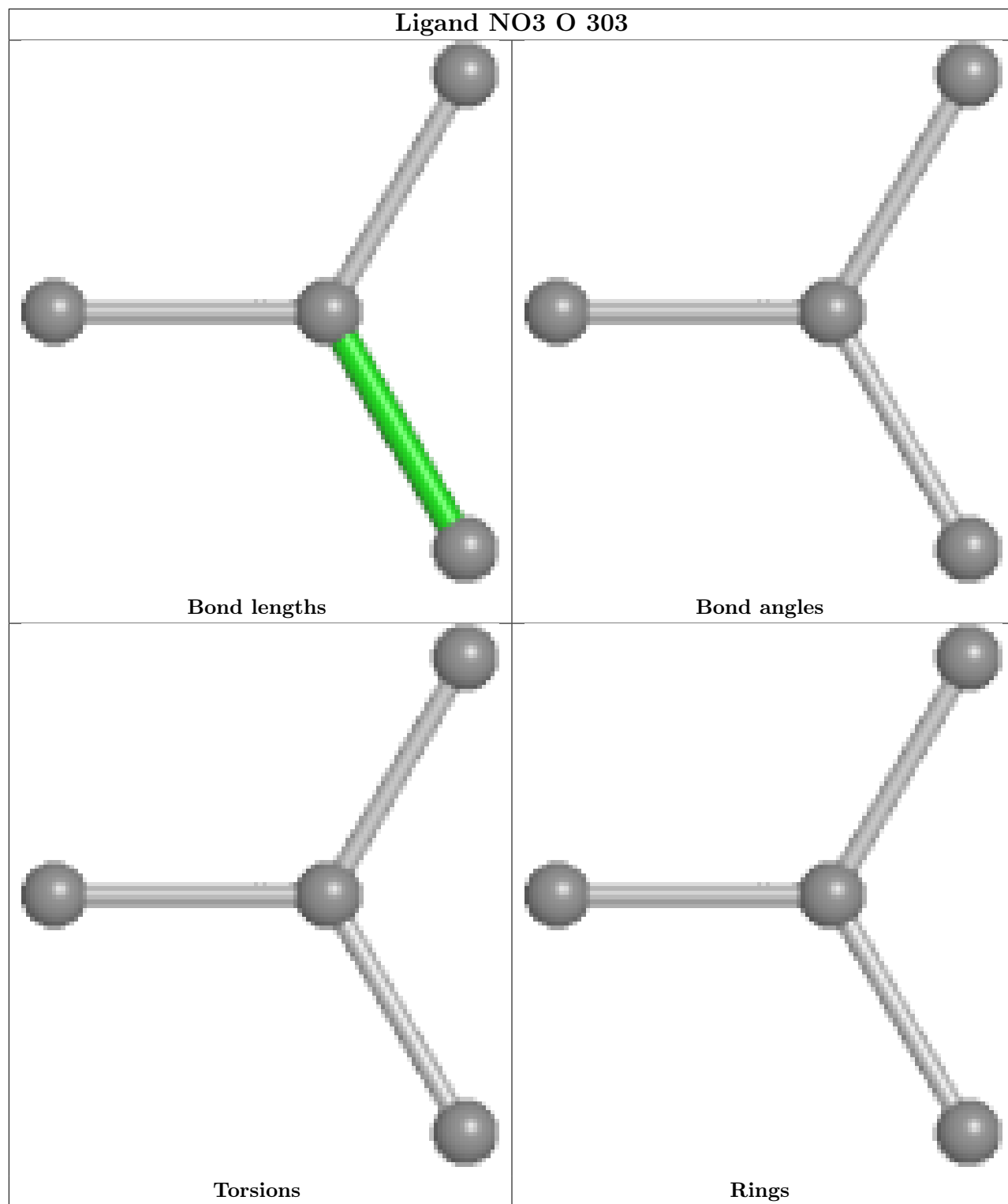


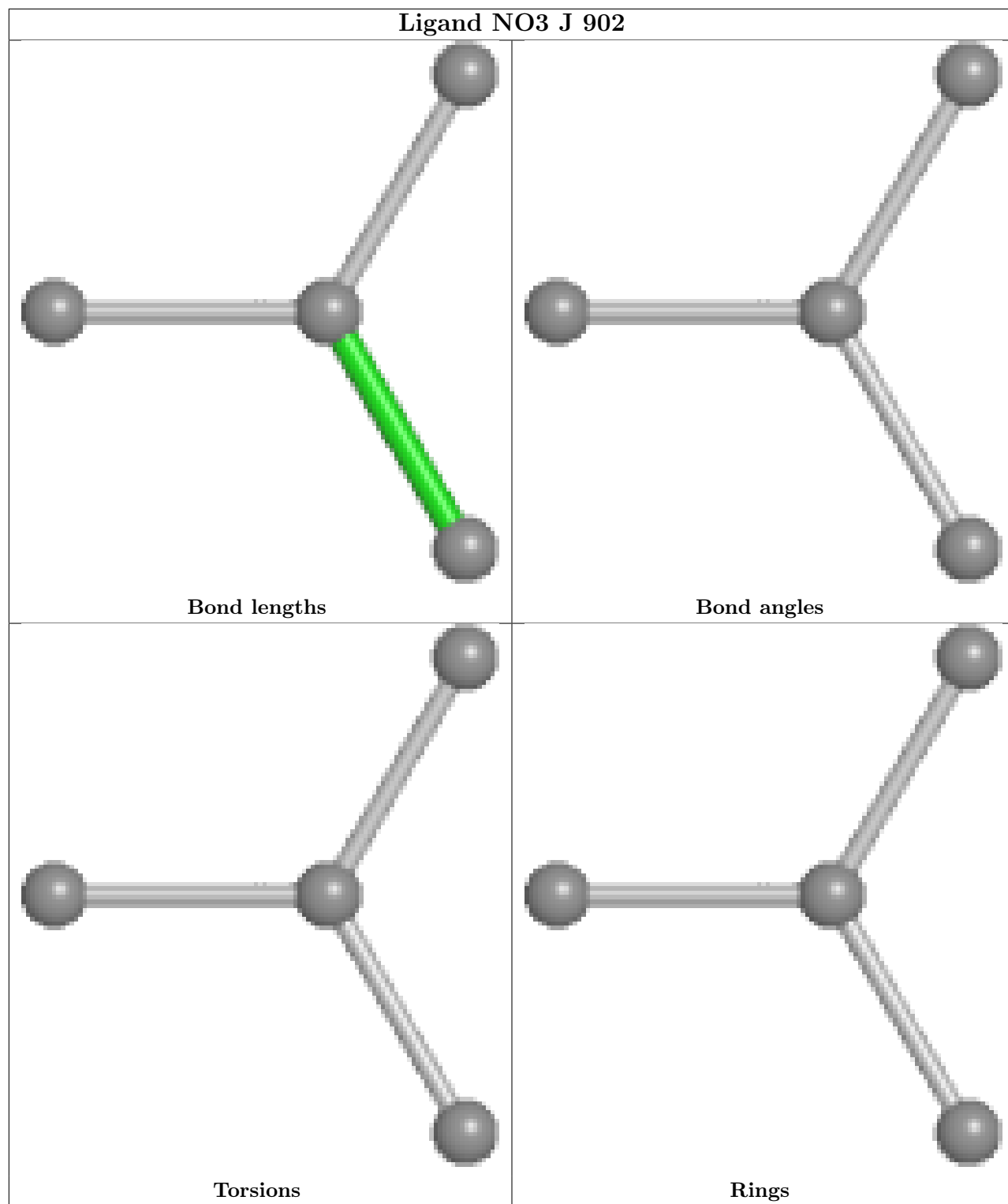


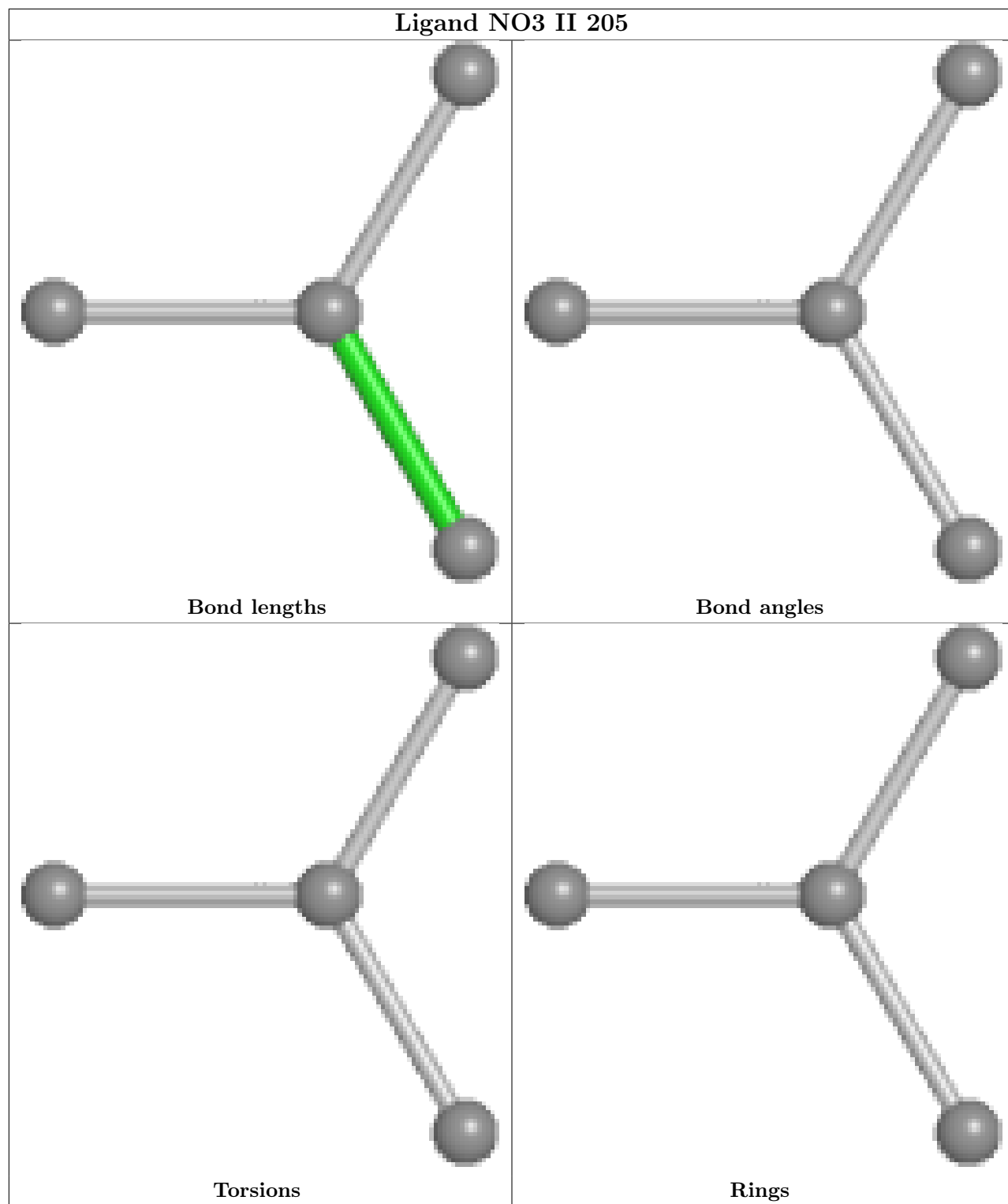


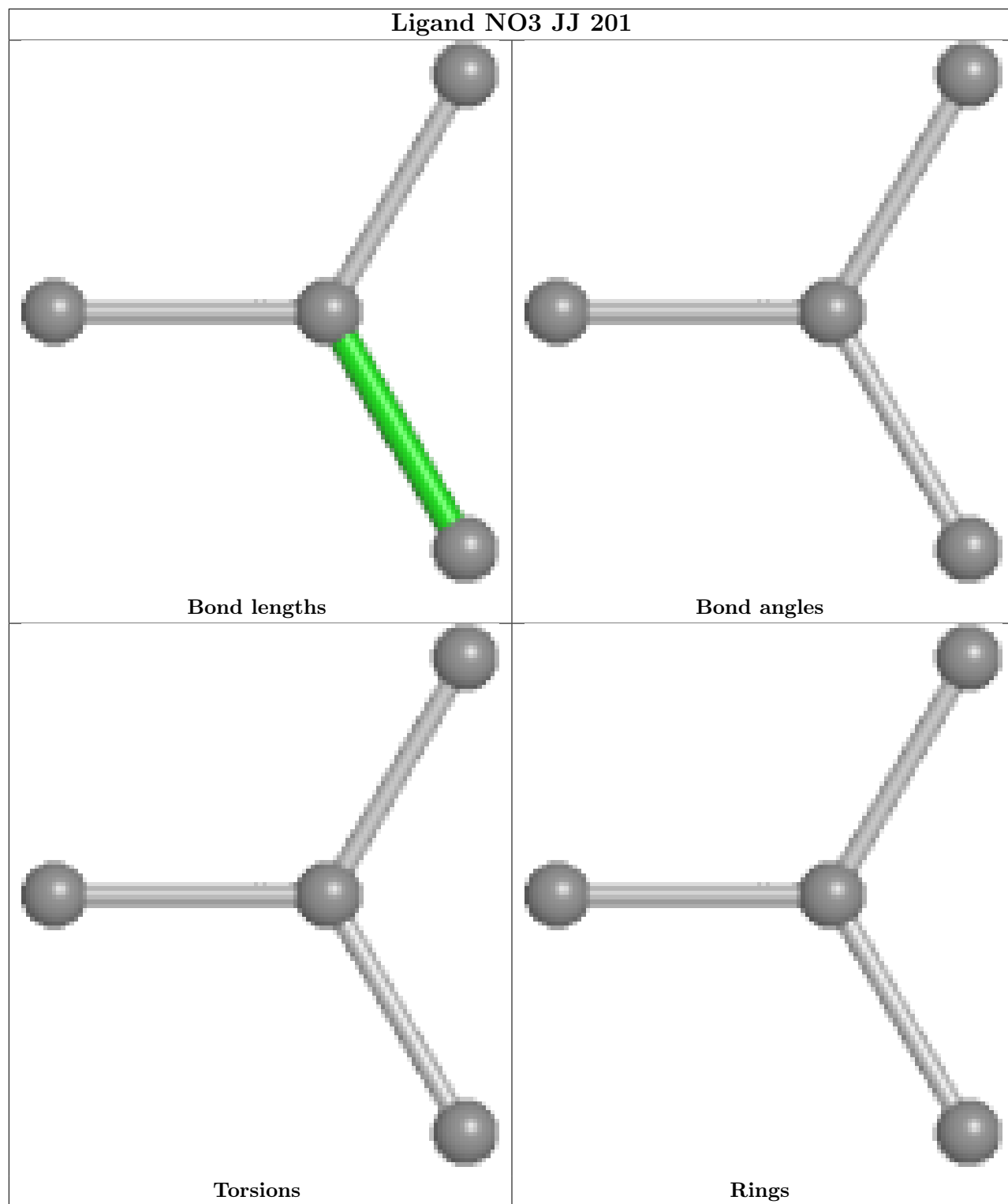




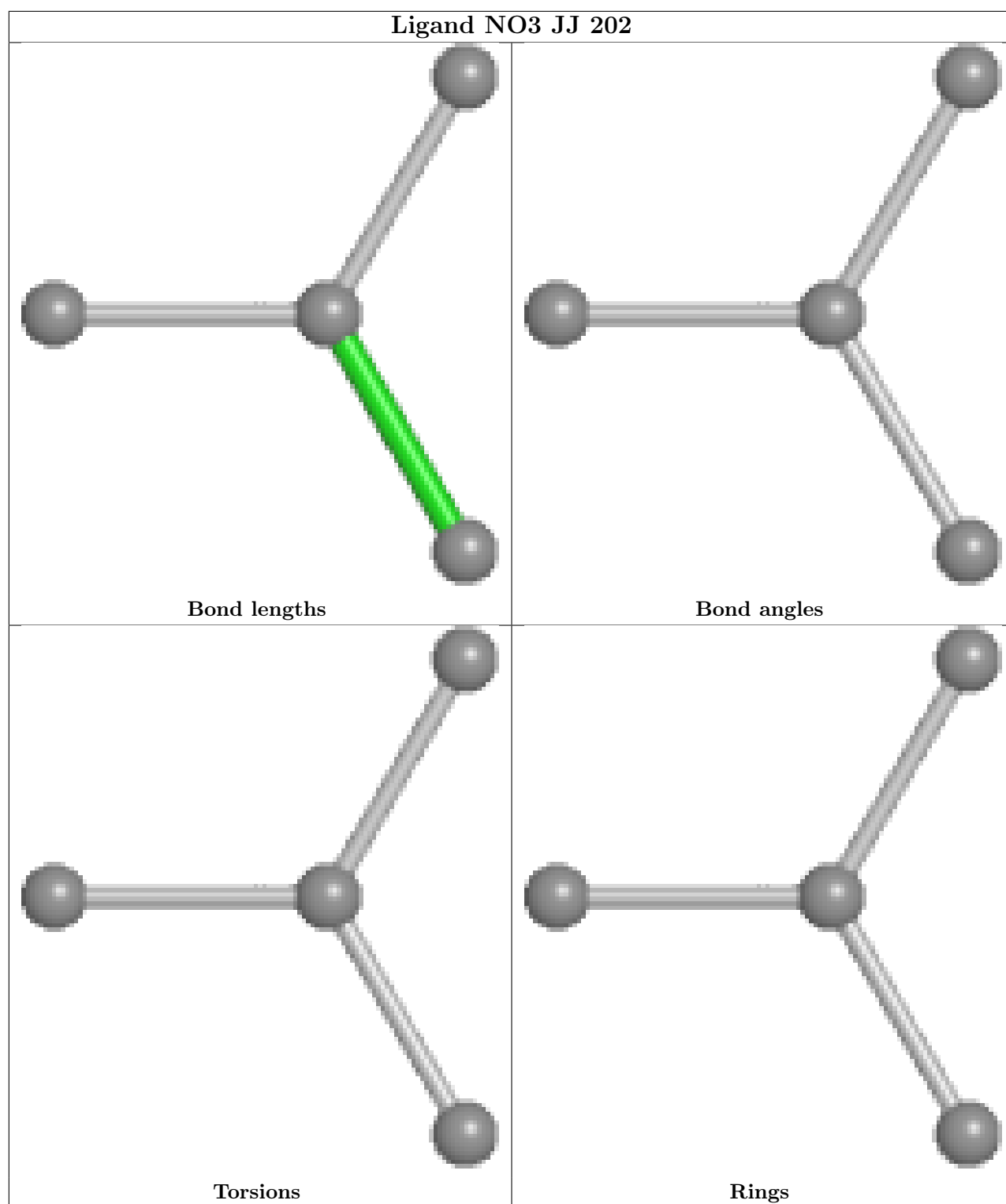


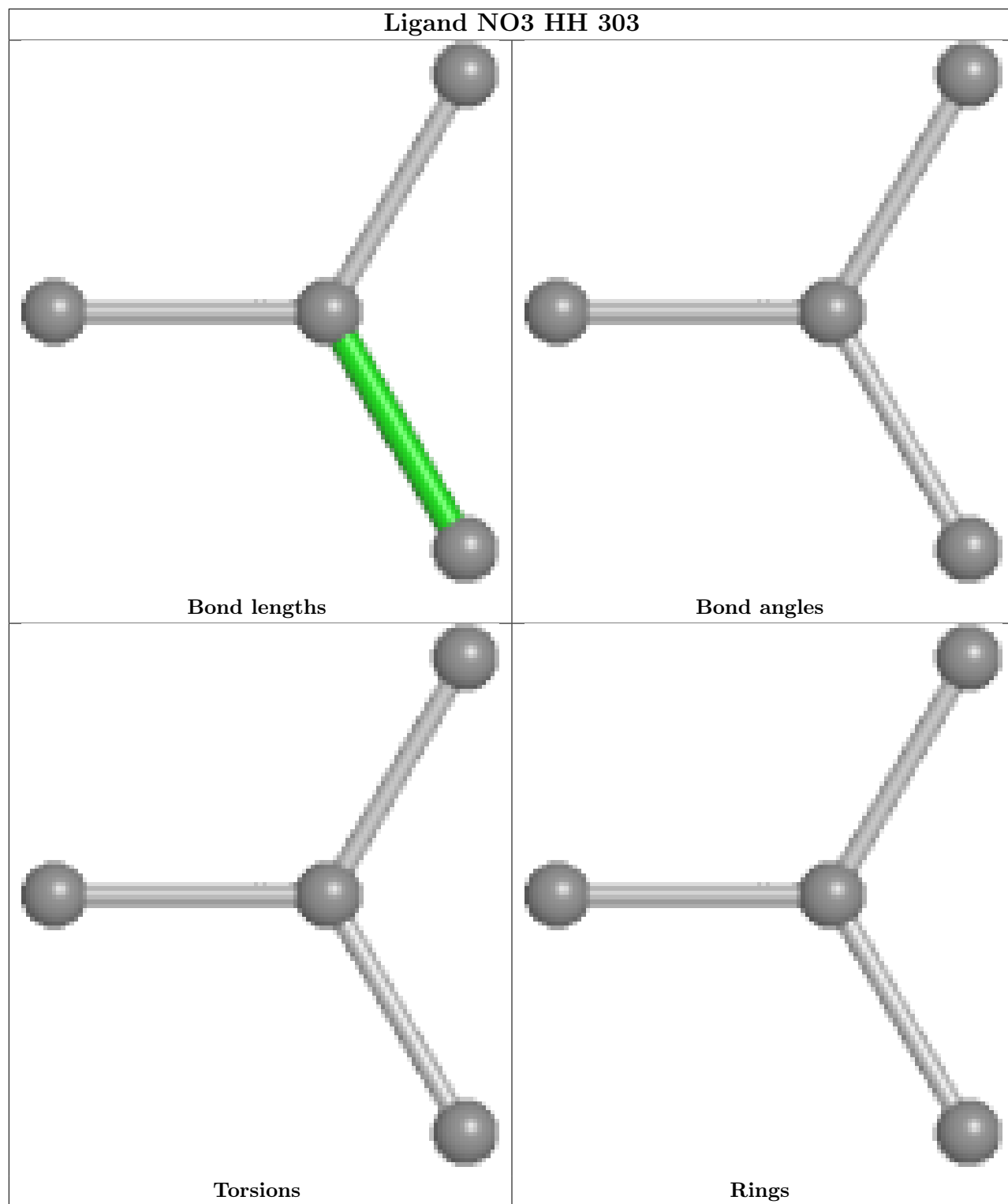


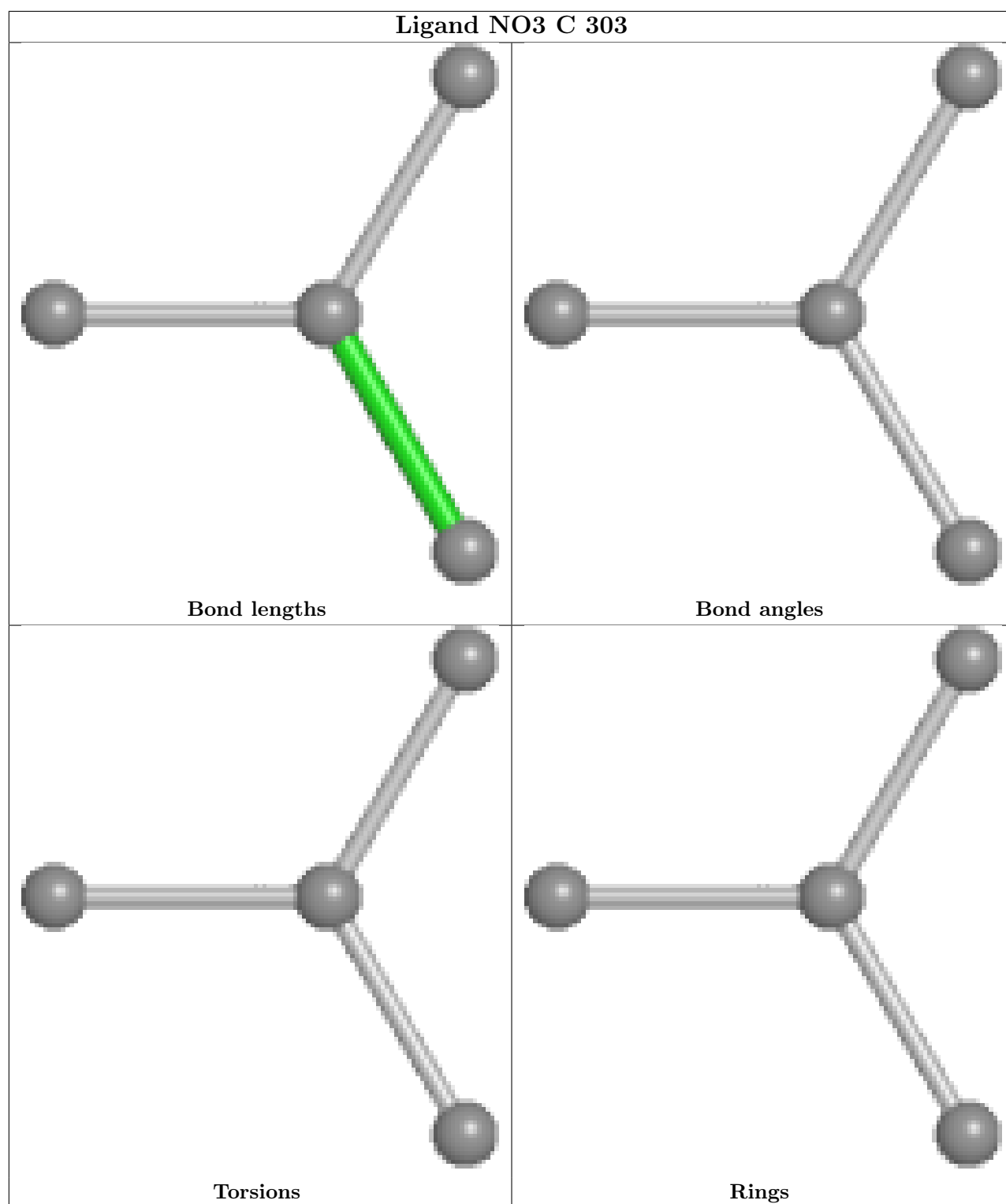


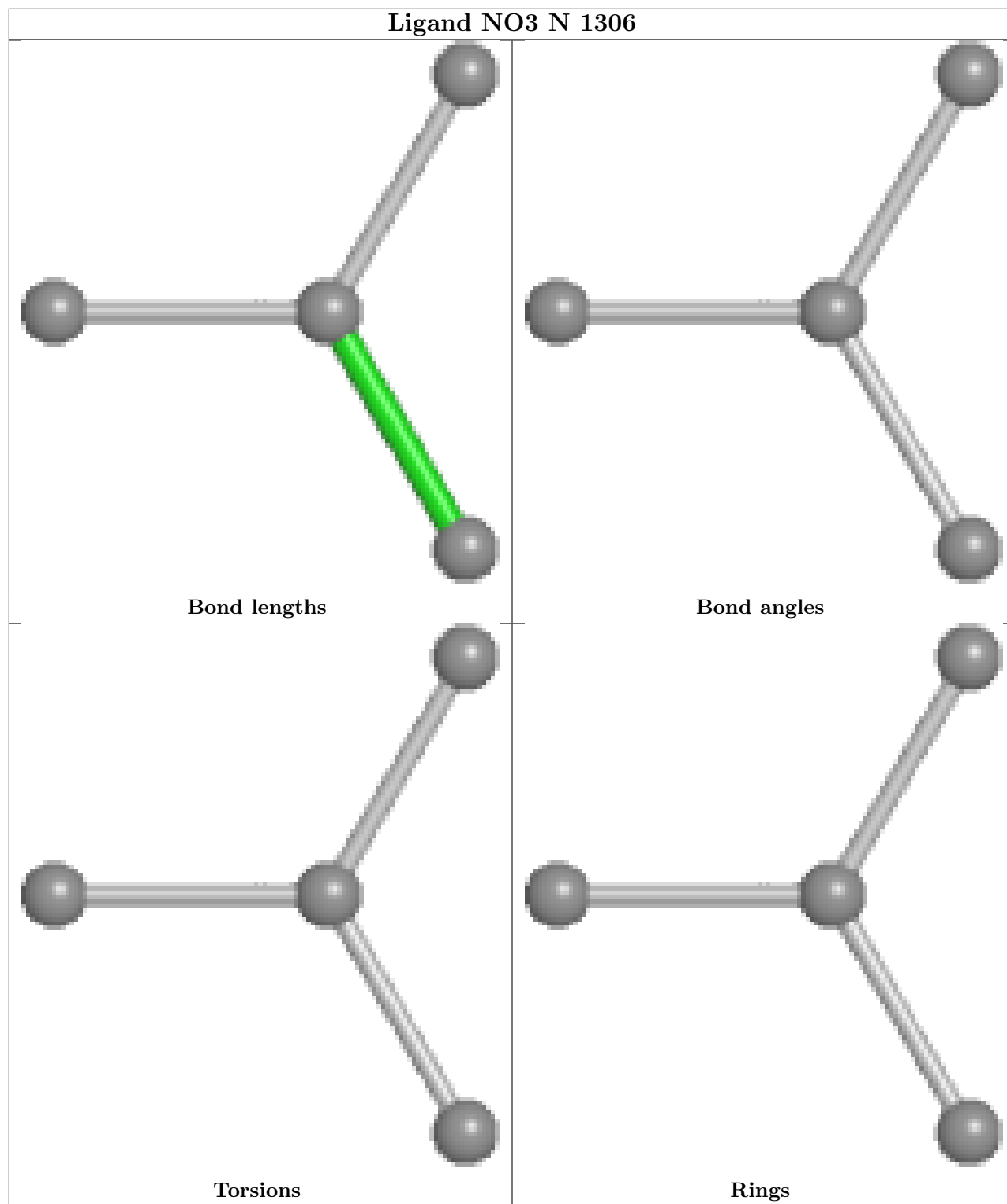




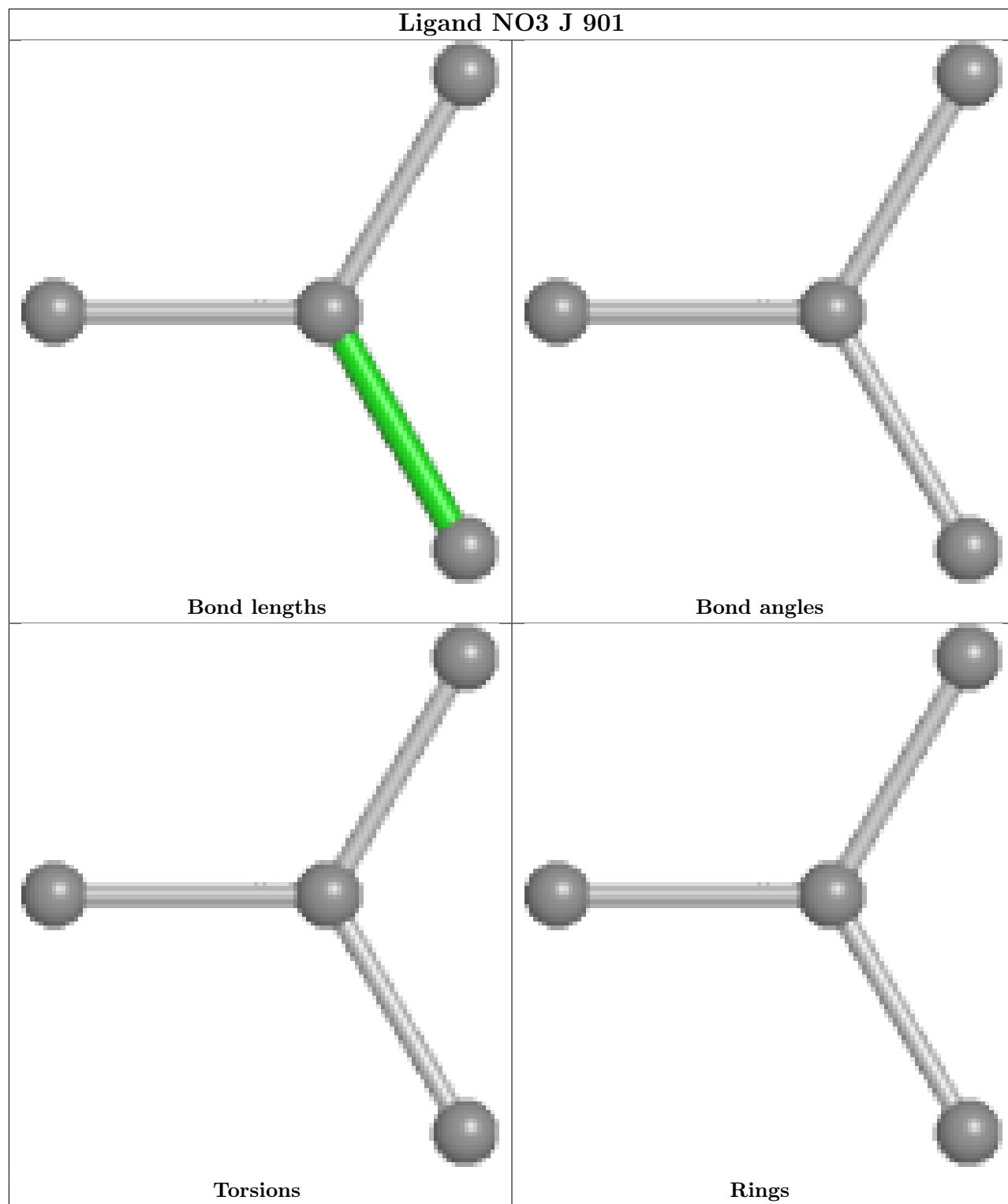


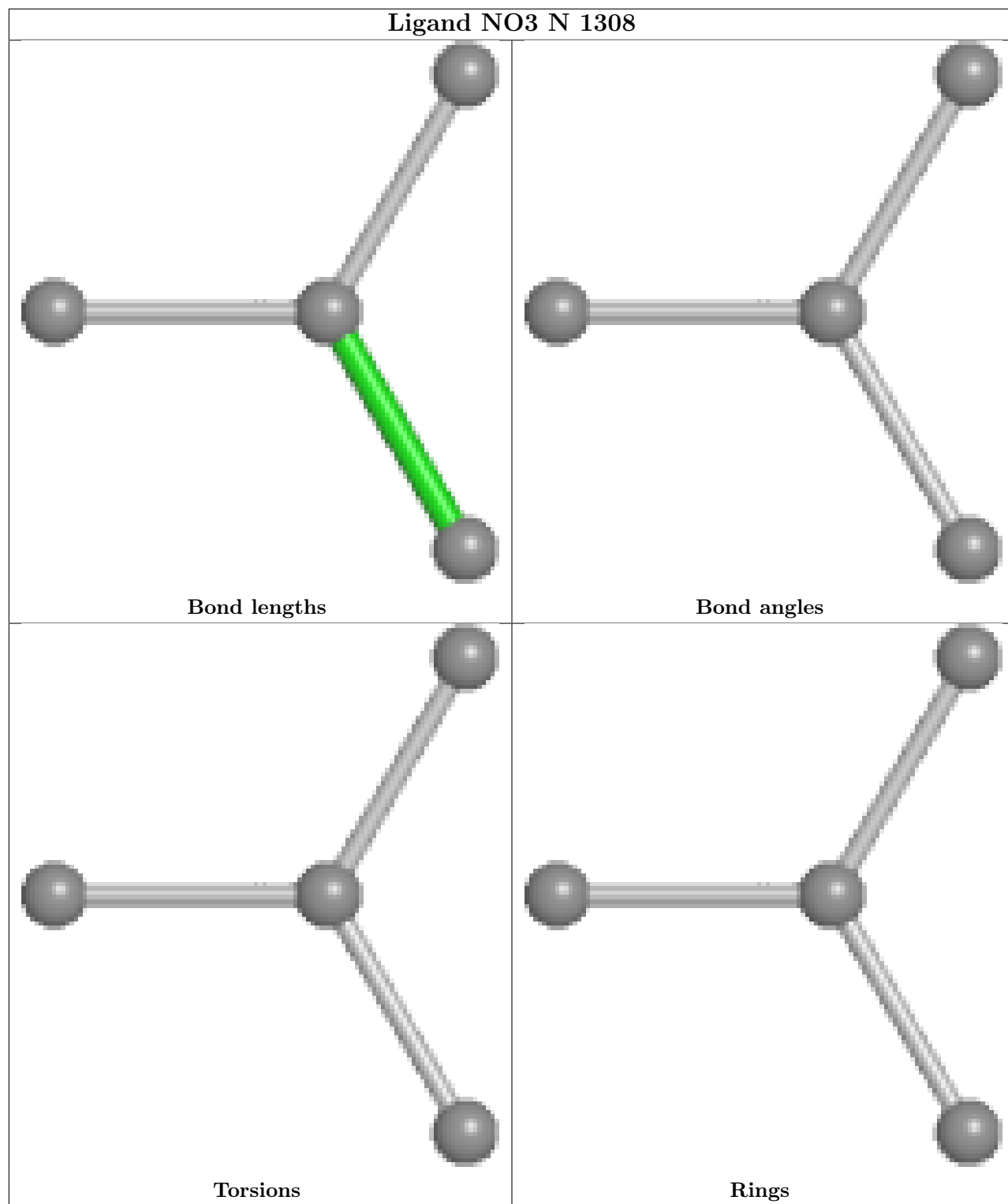


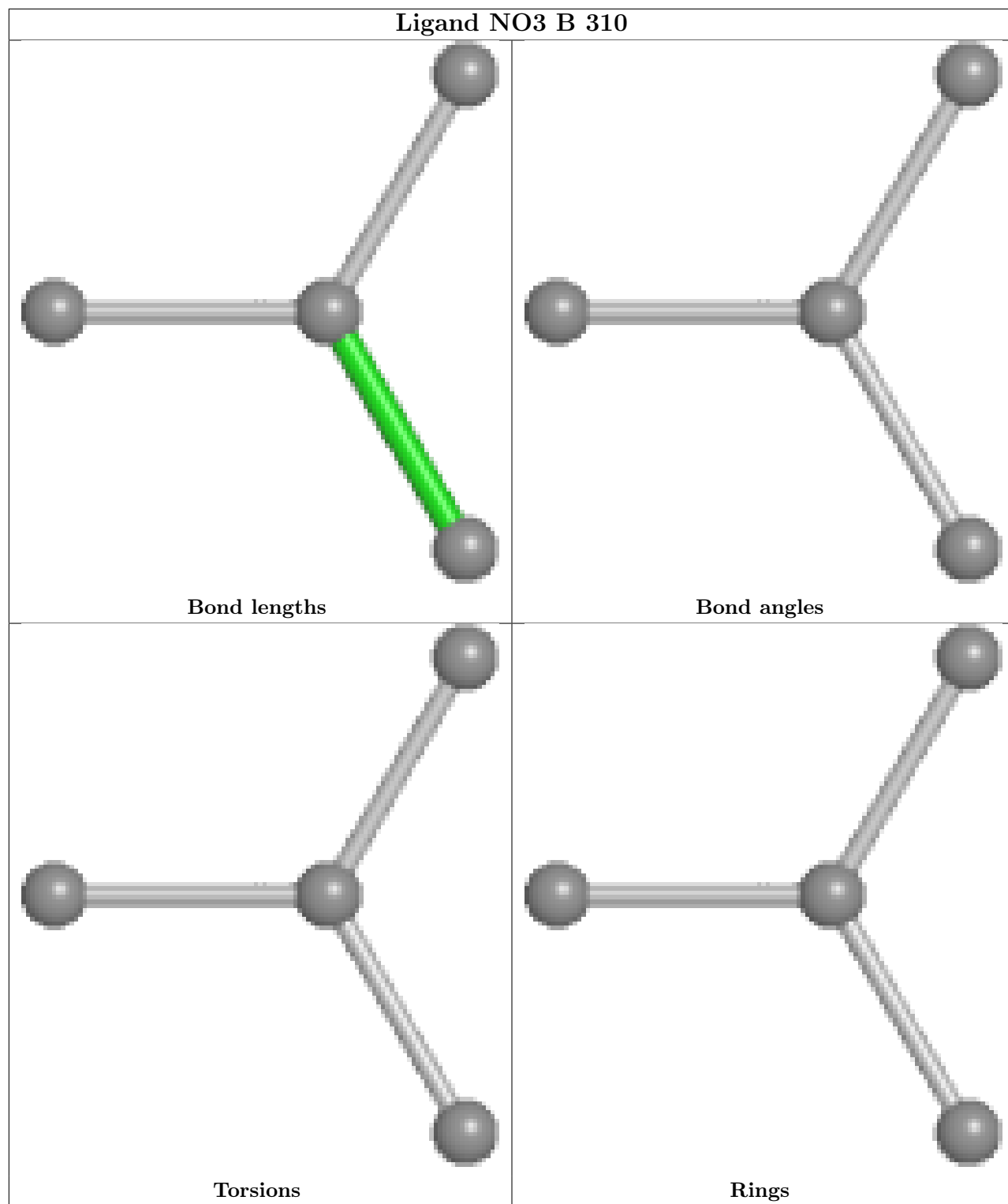


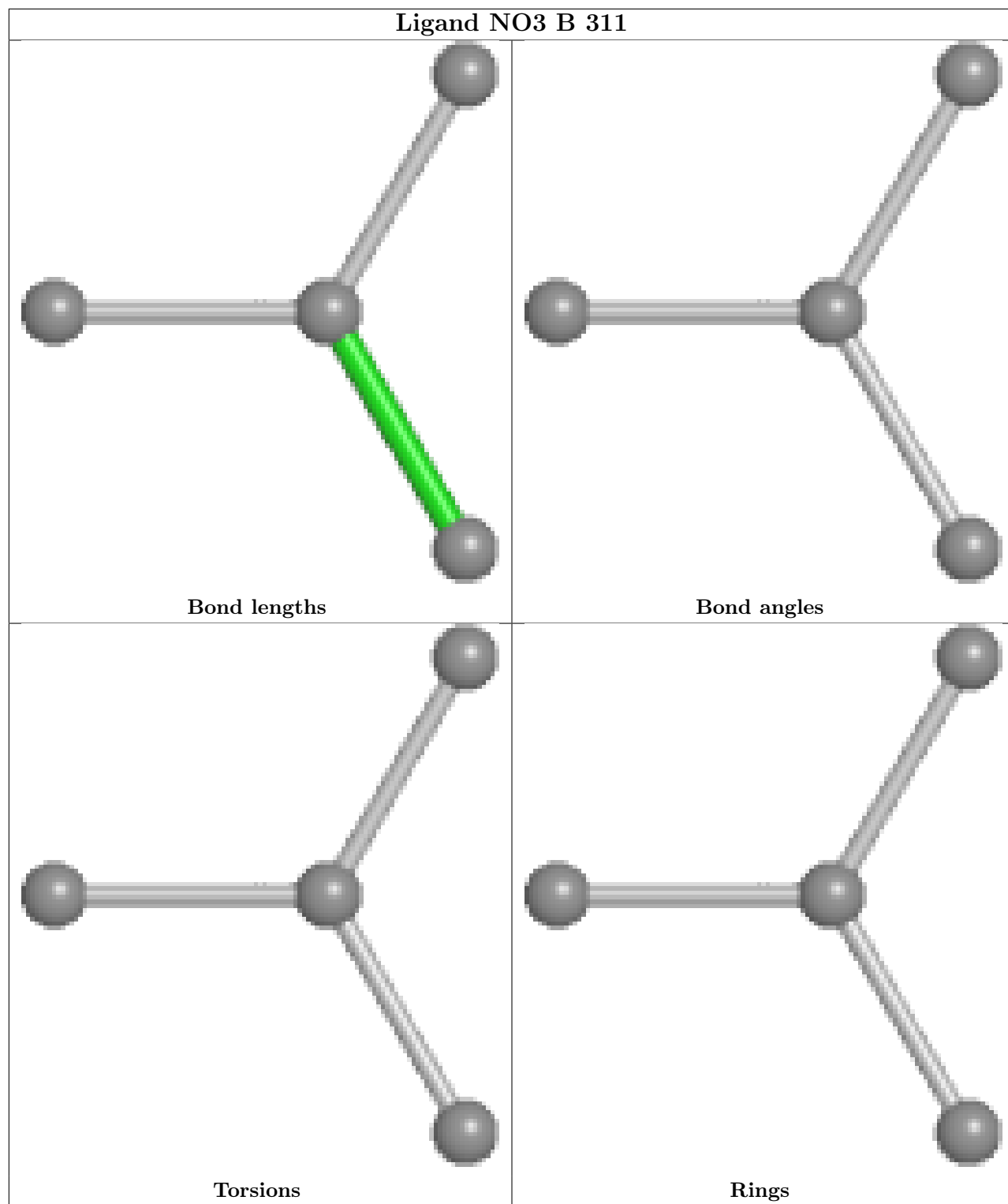


## Ligand NO3 J 901

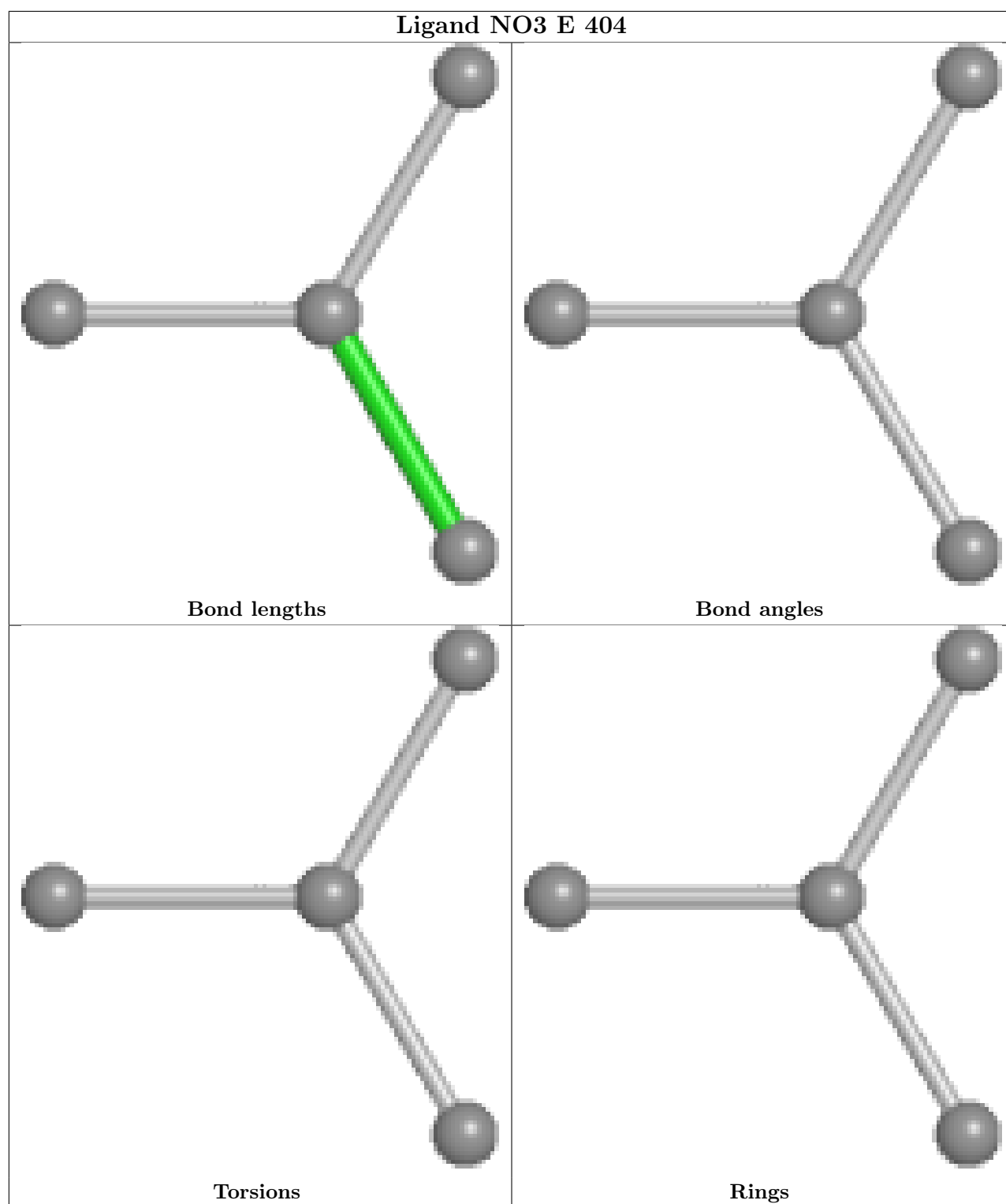


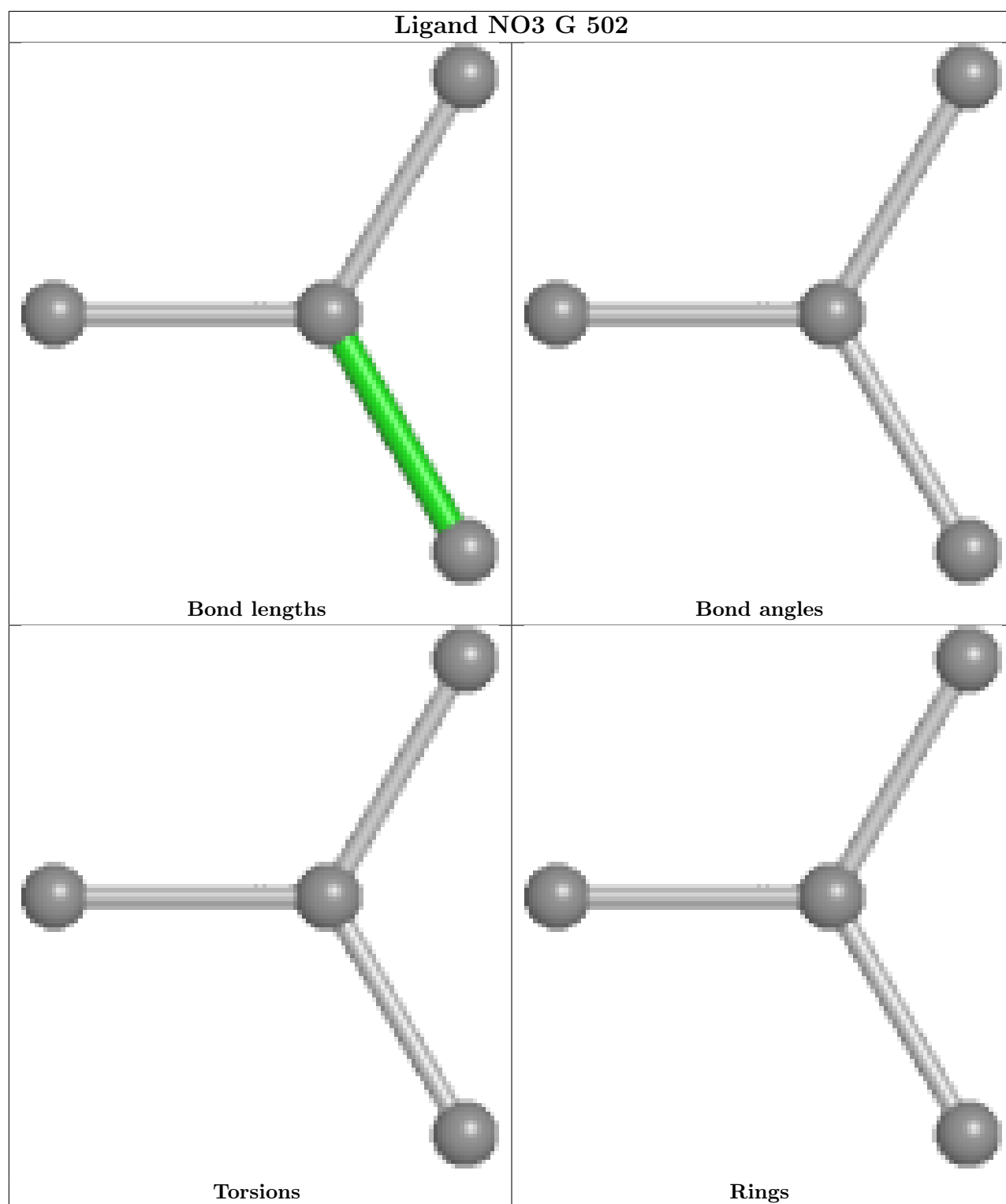


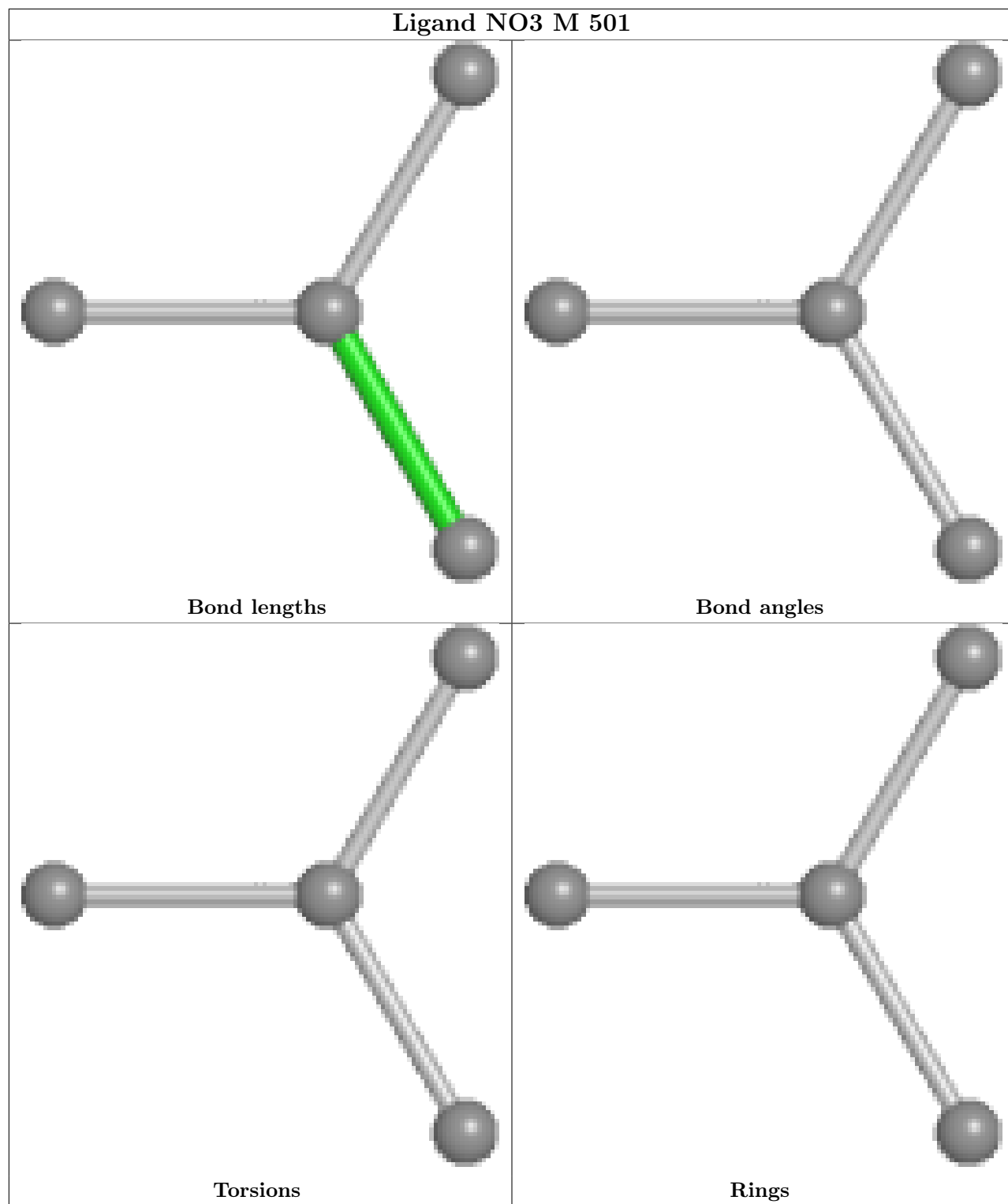


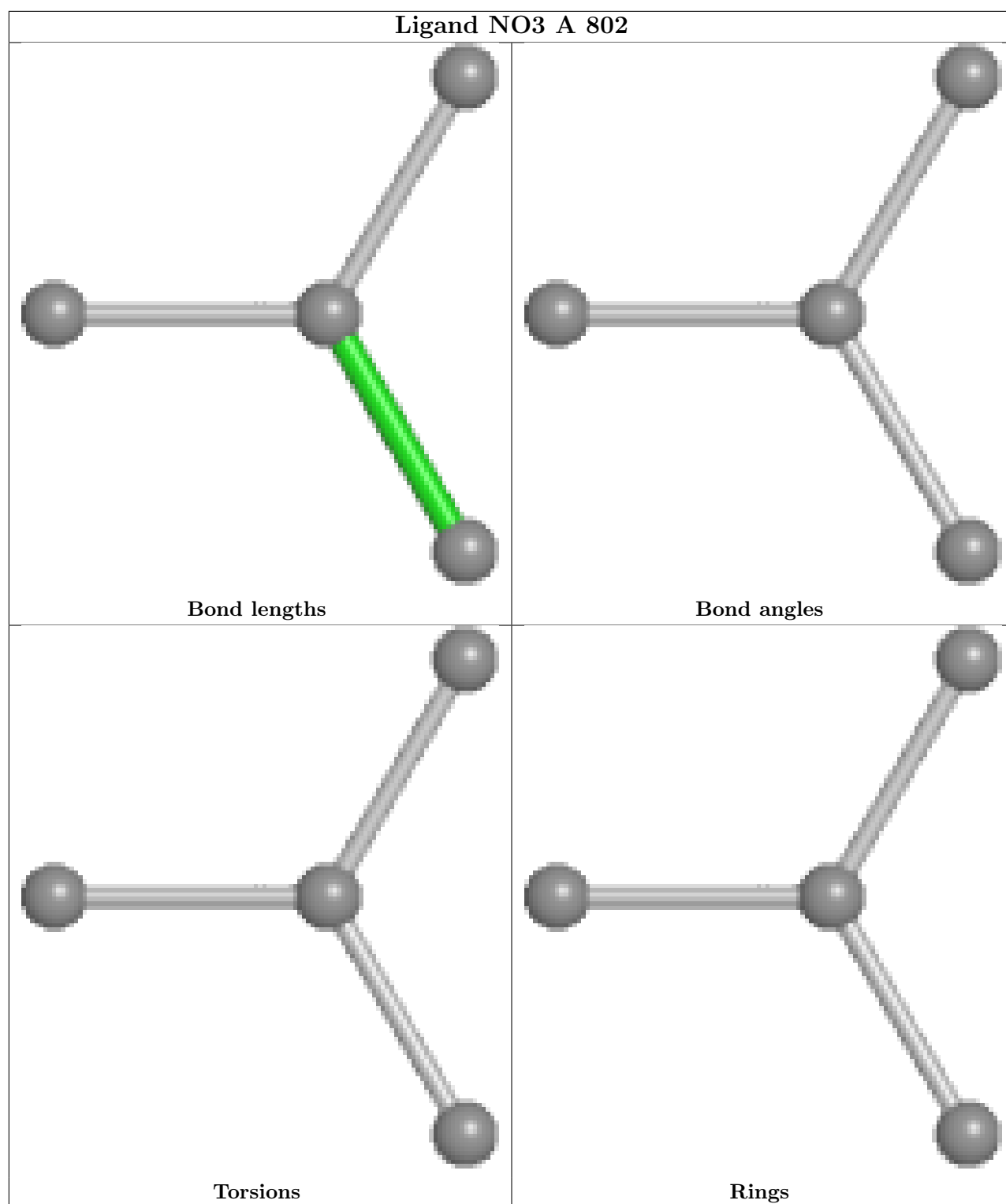


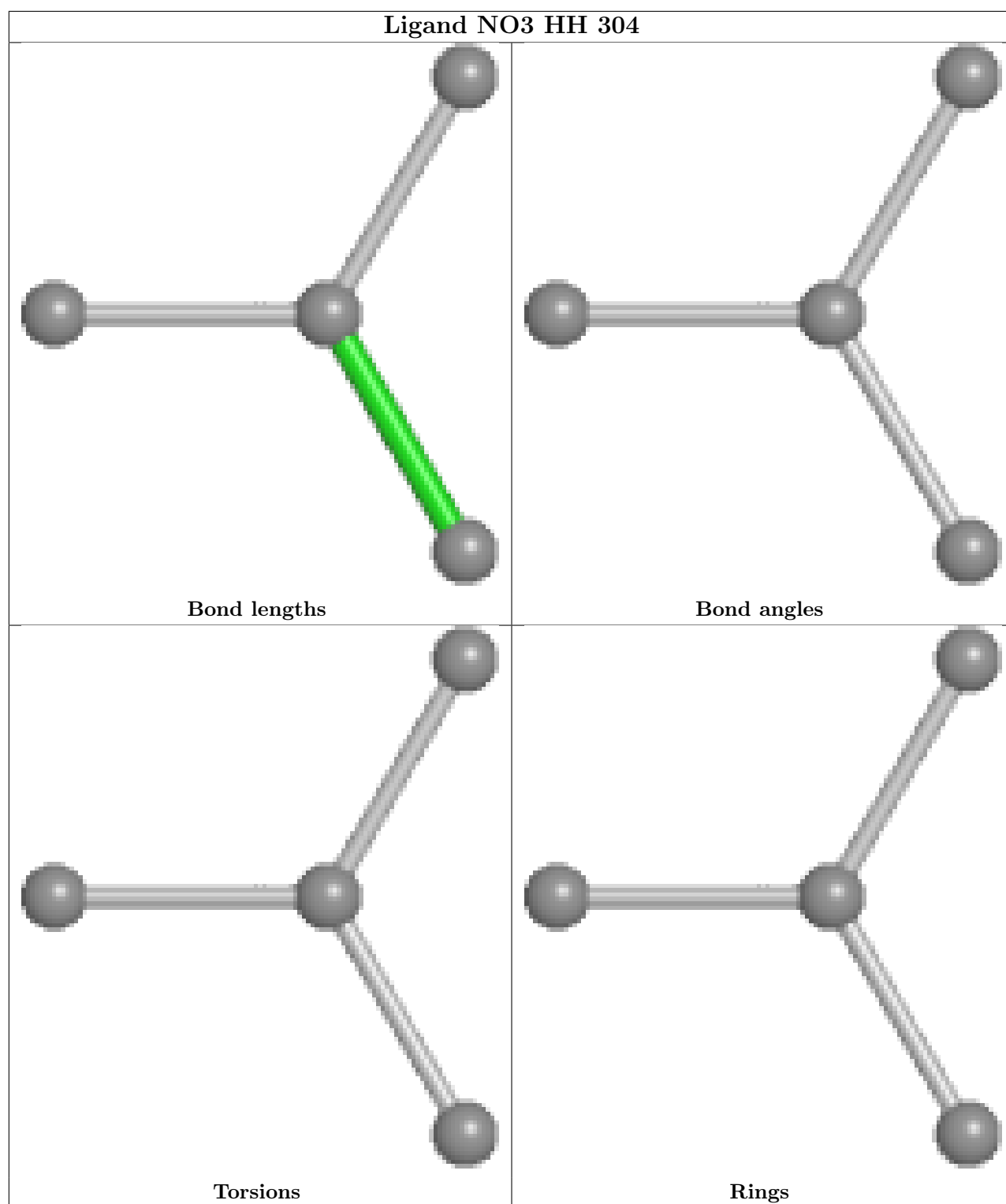


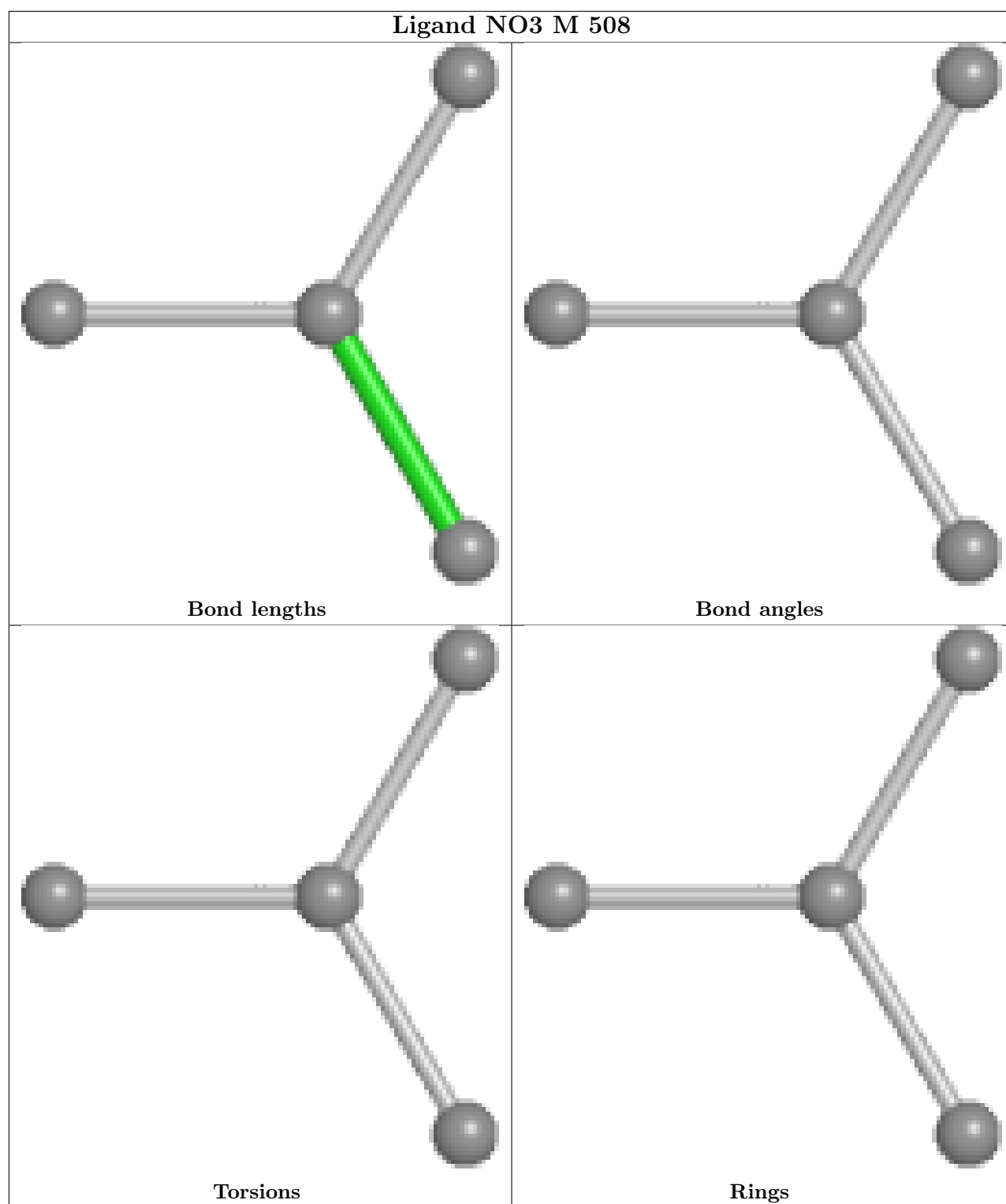


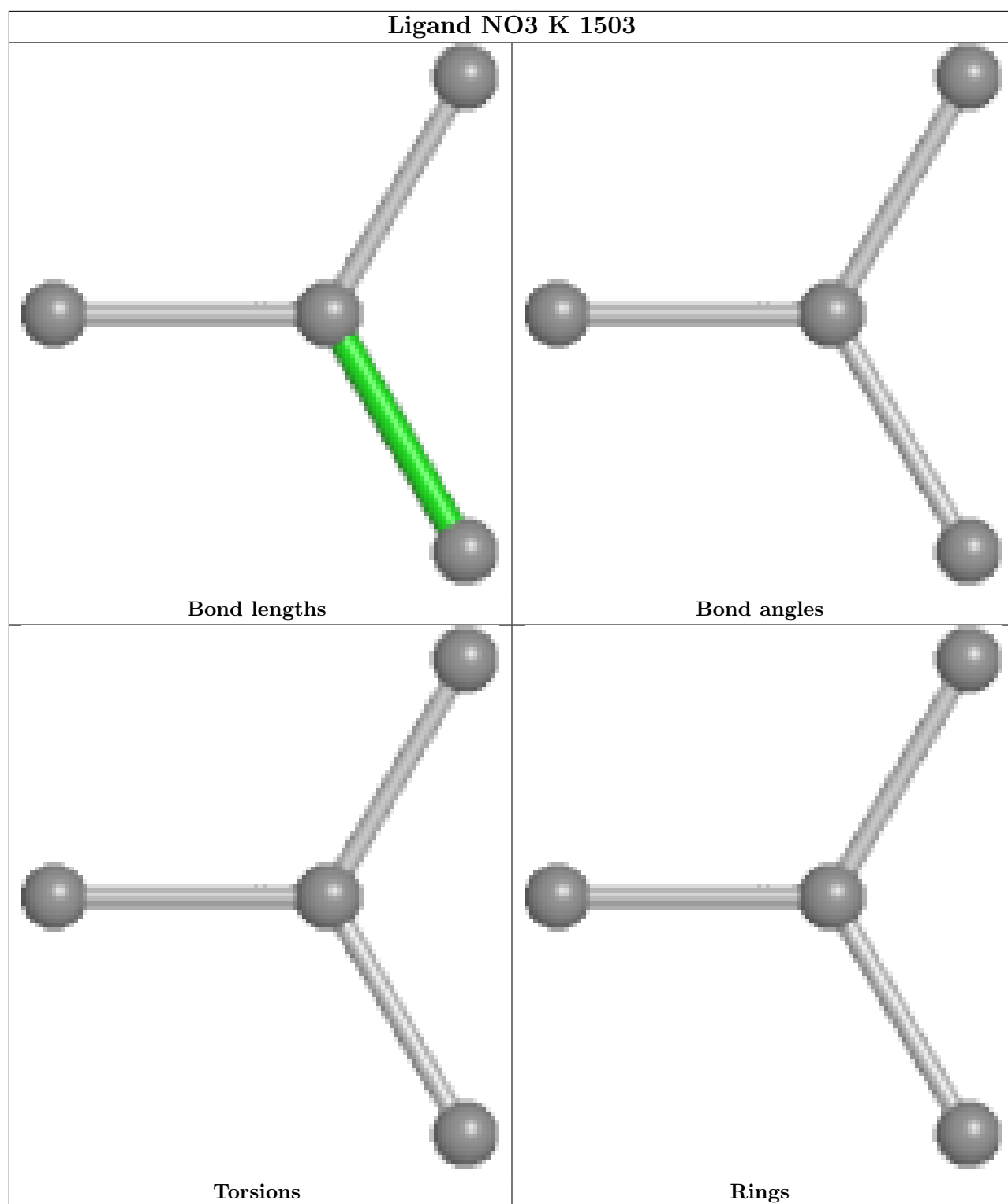


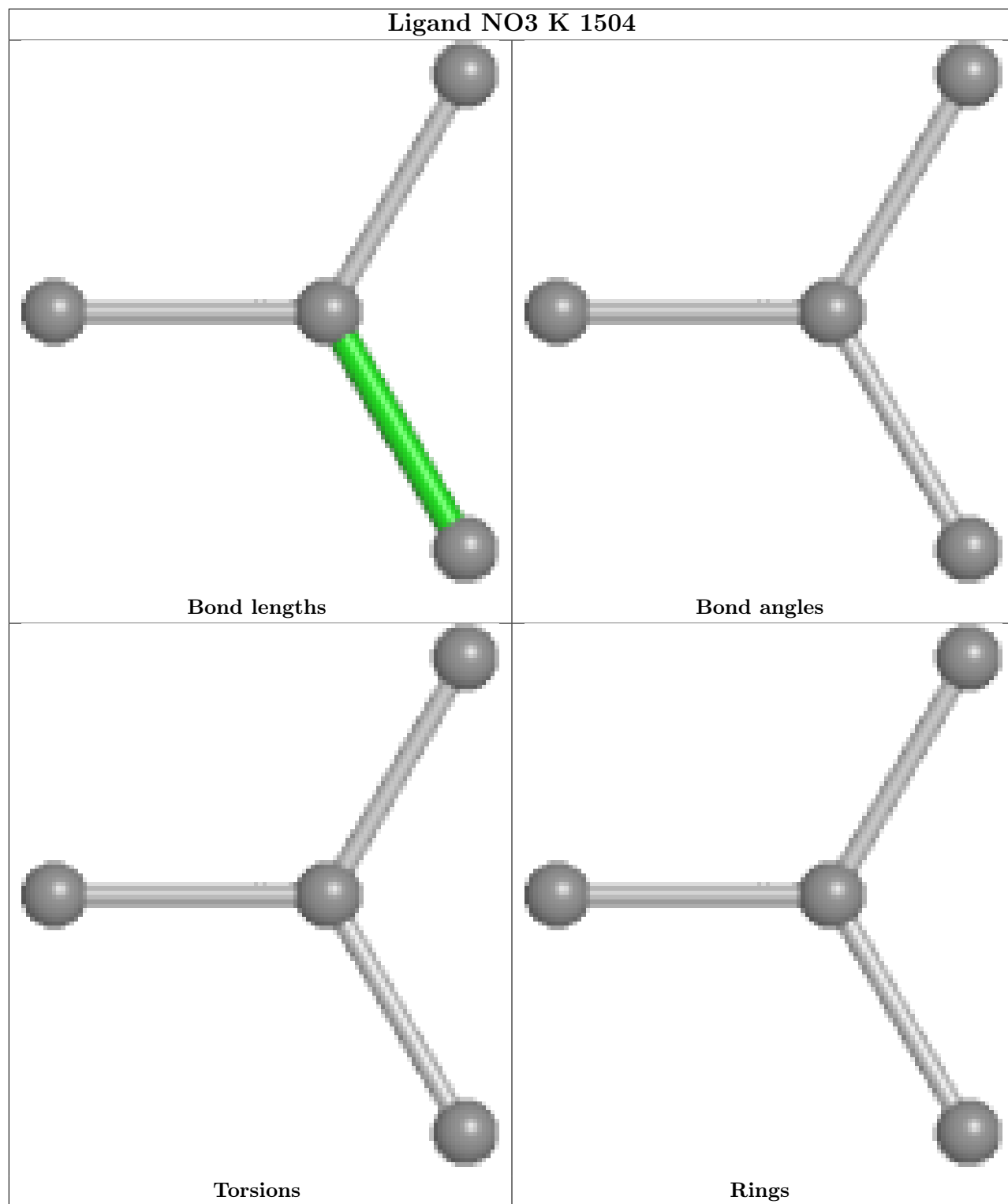




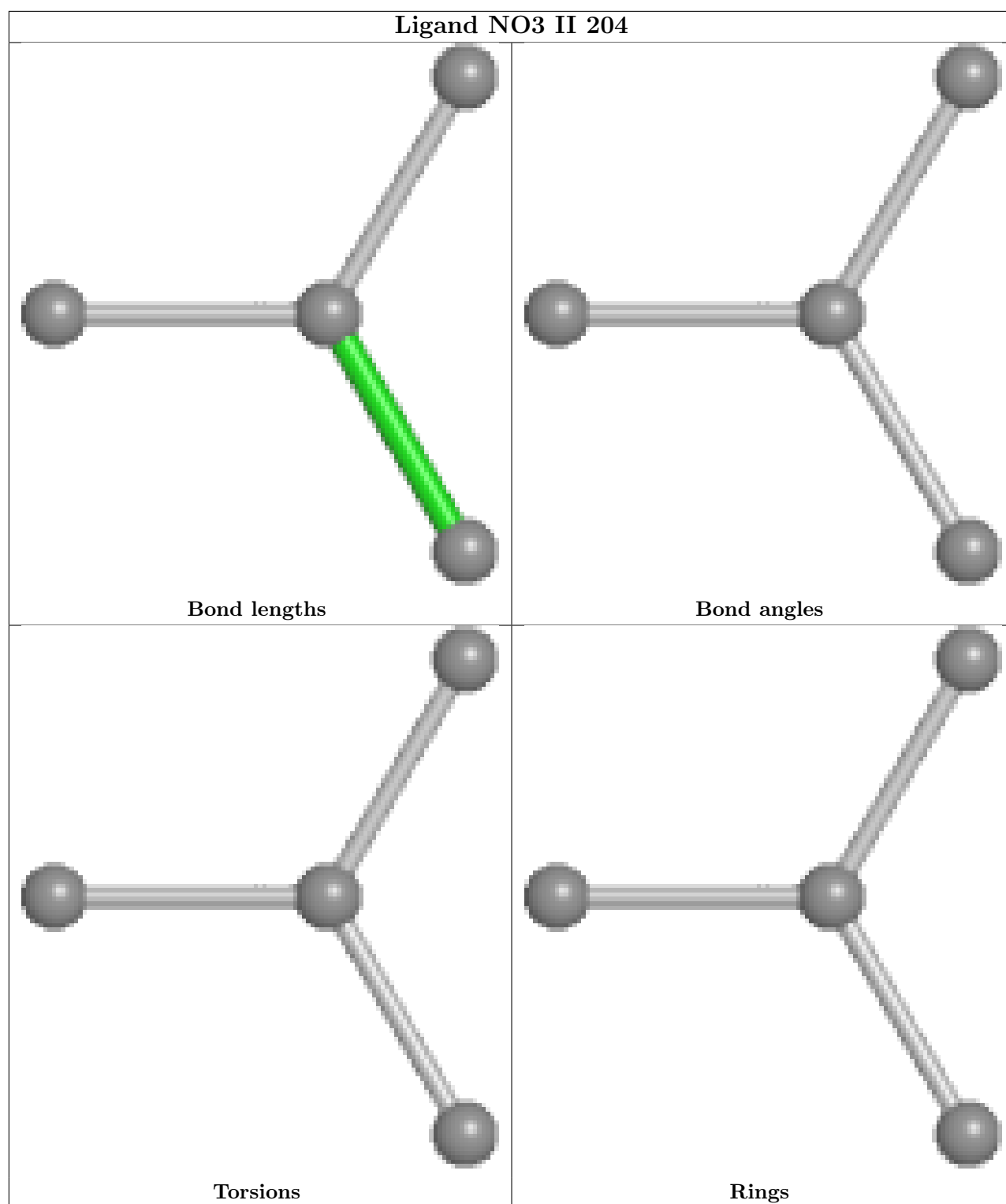


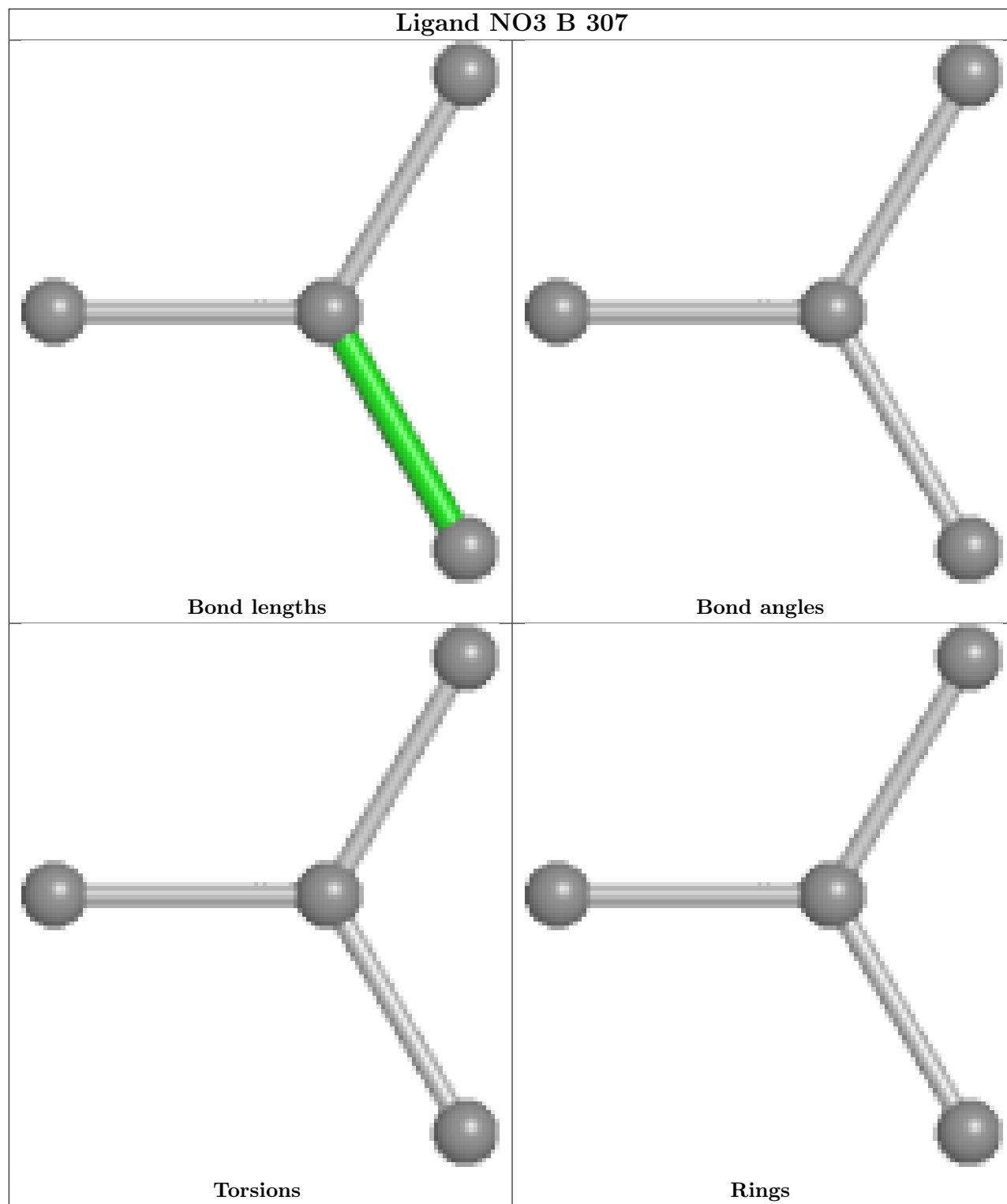


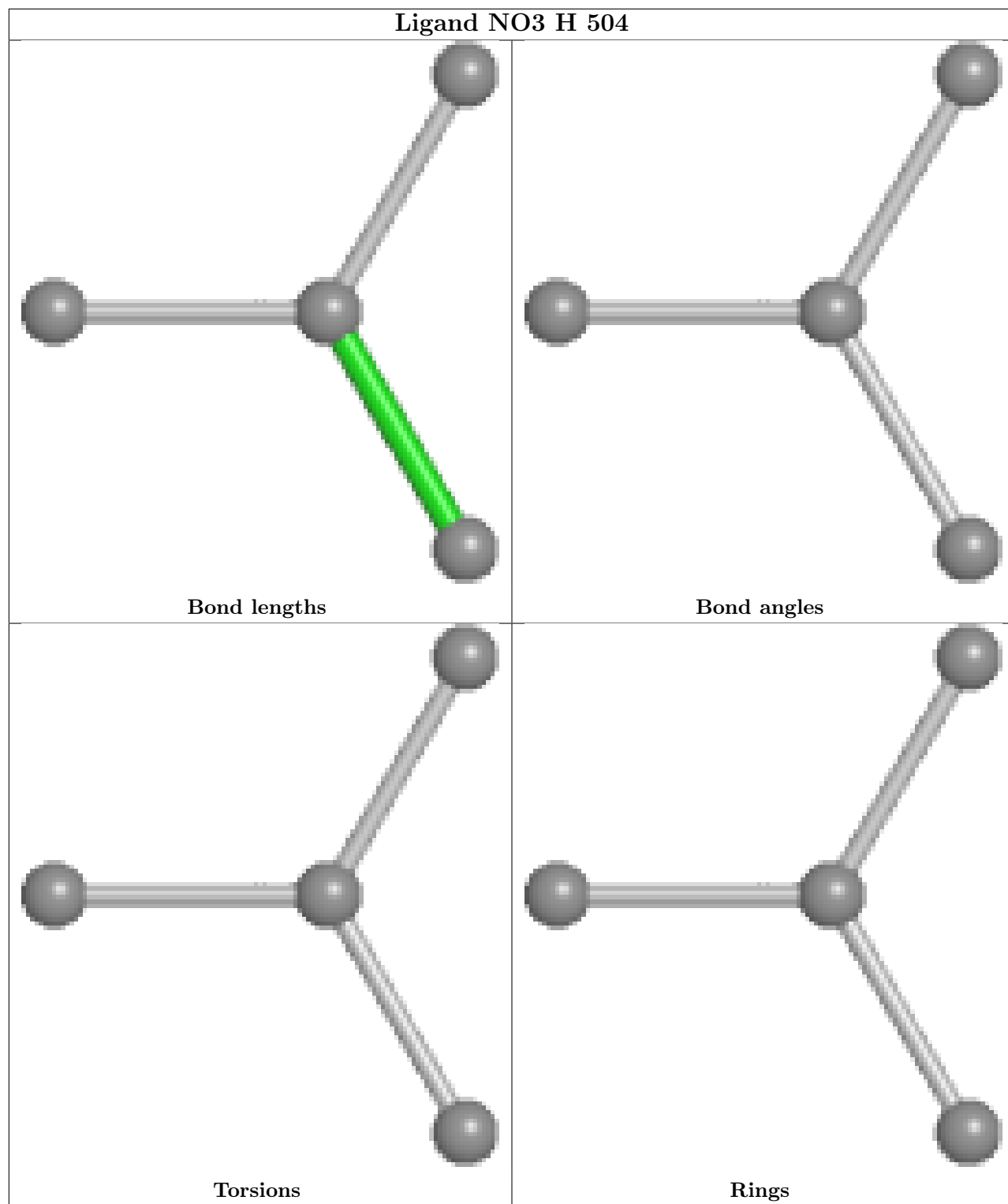


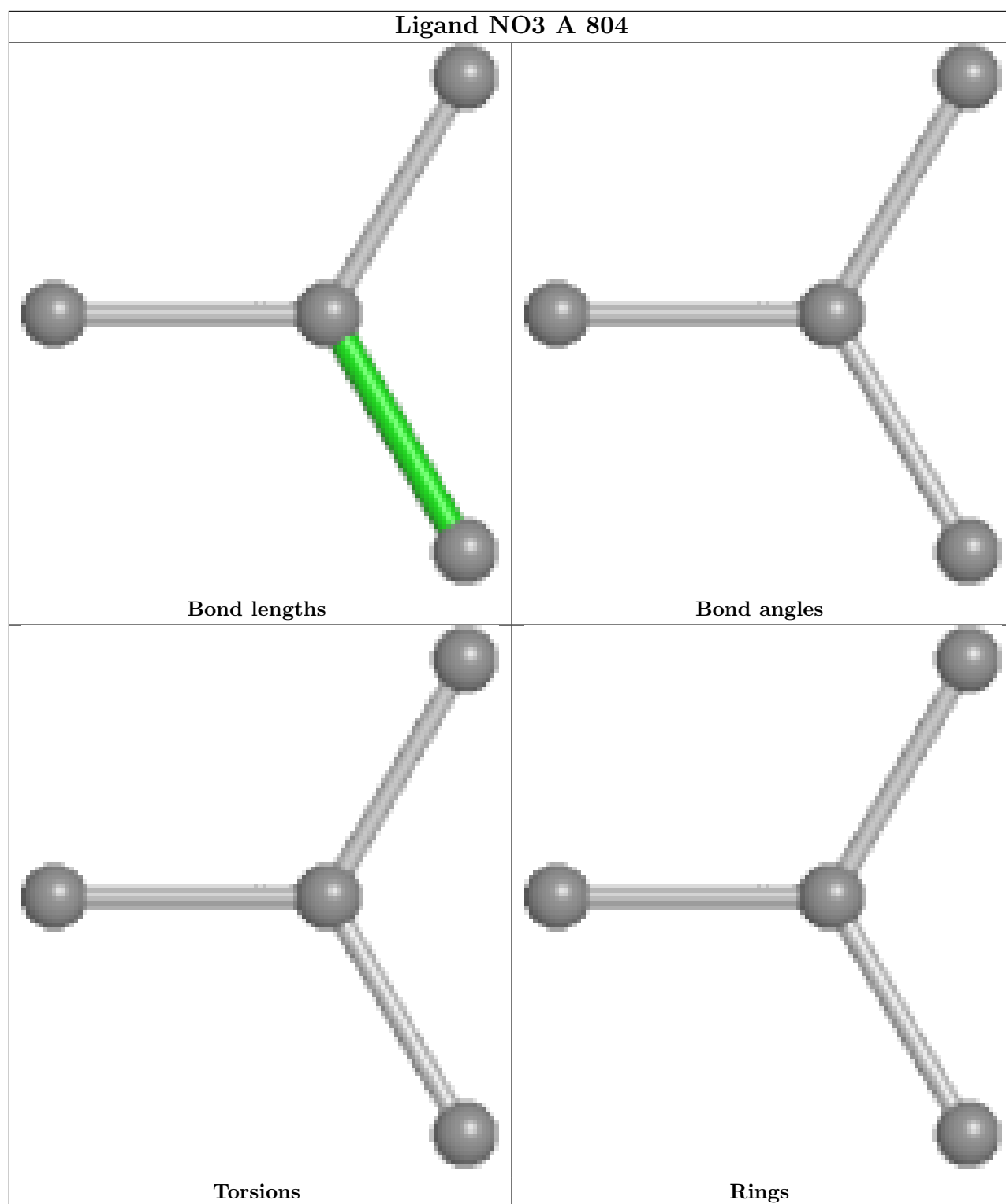


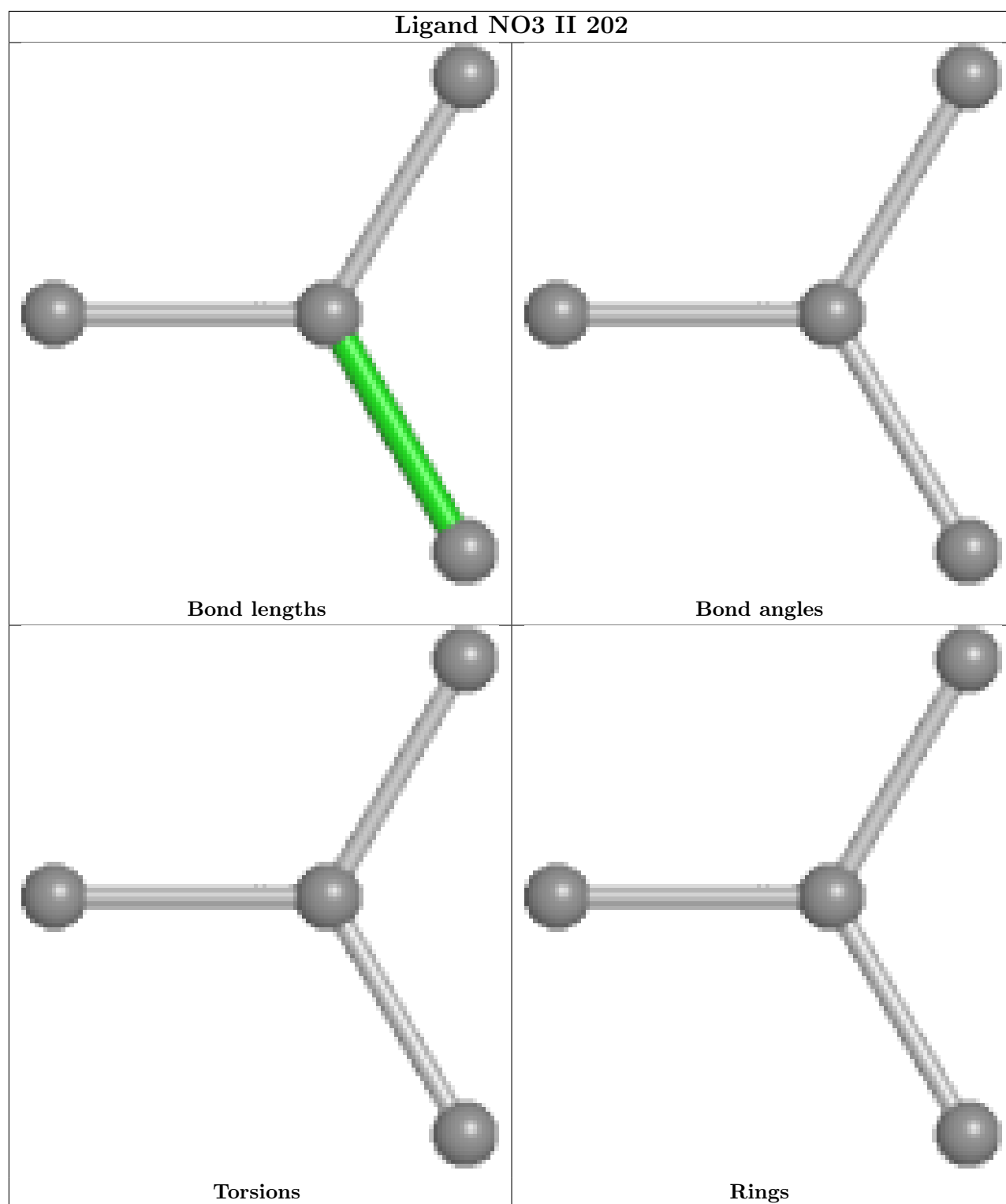


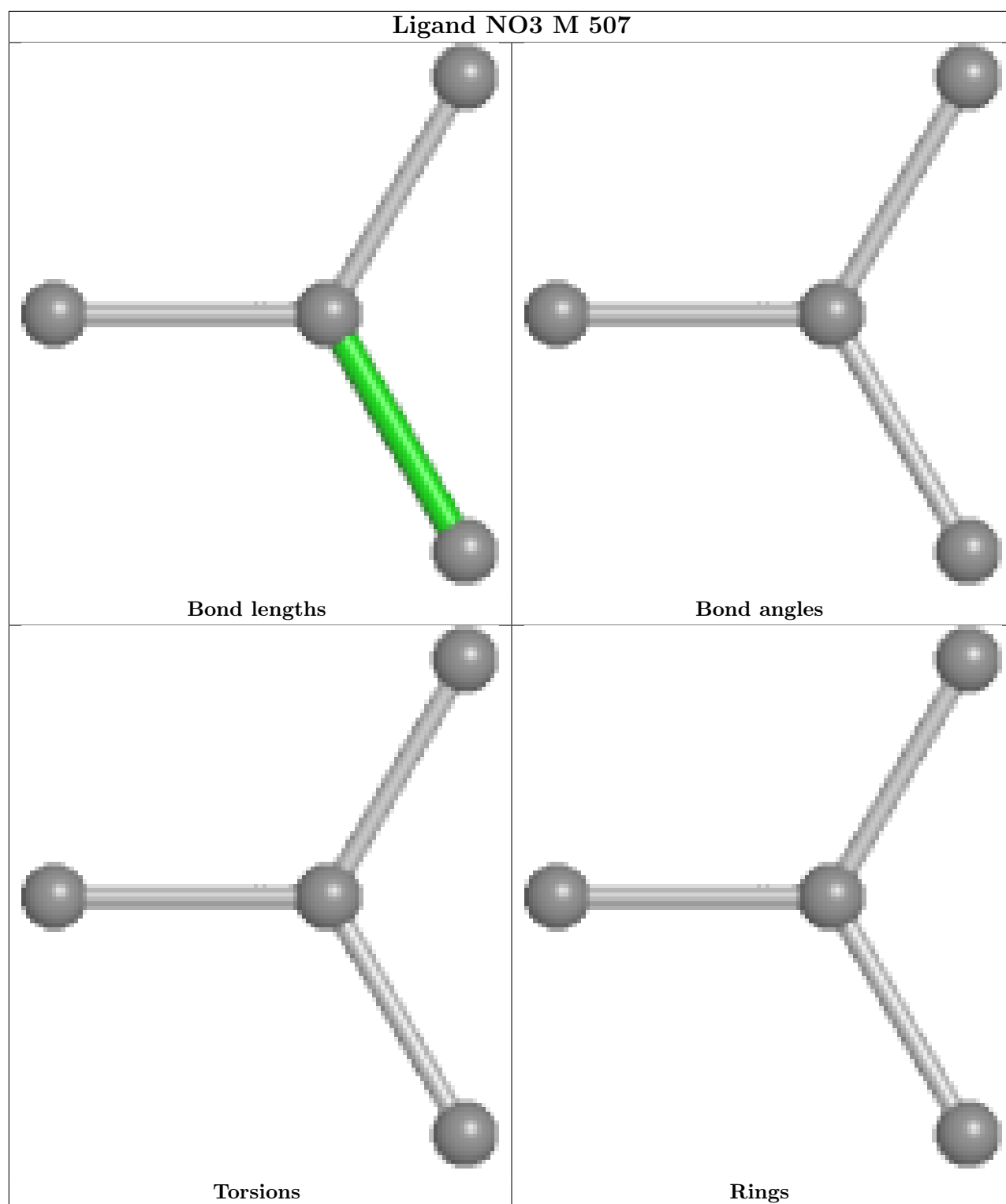


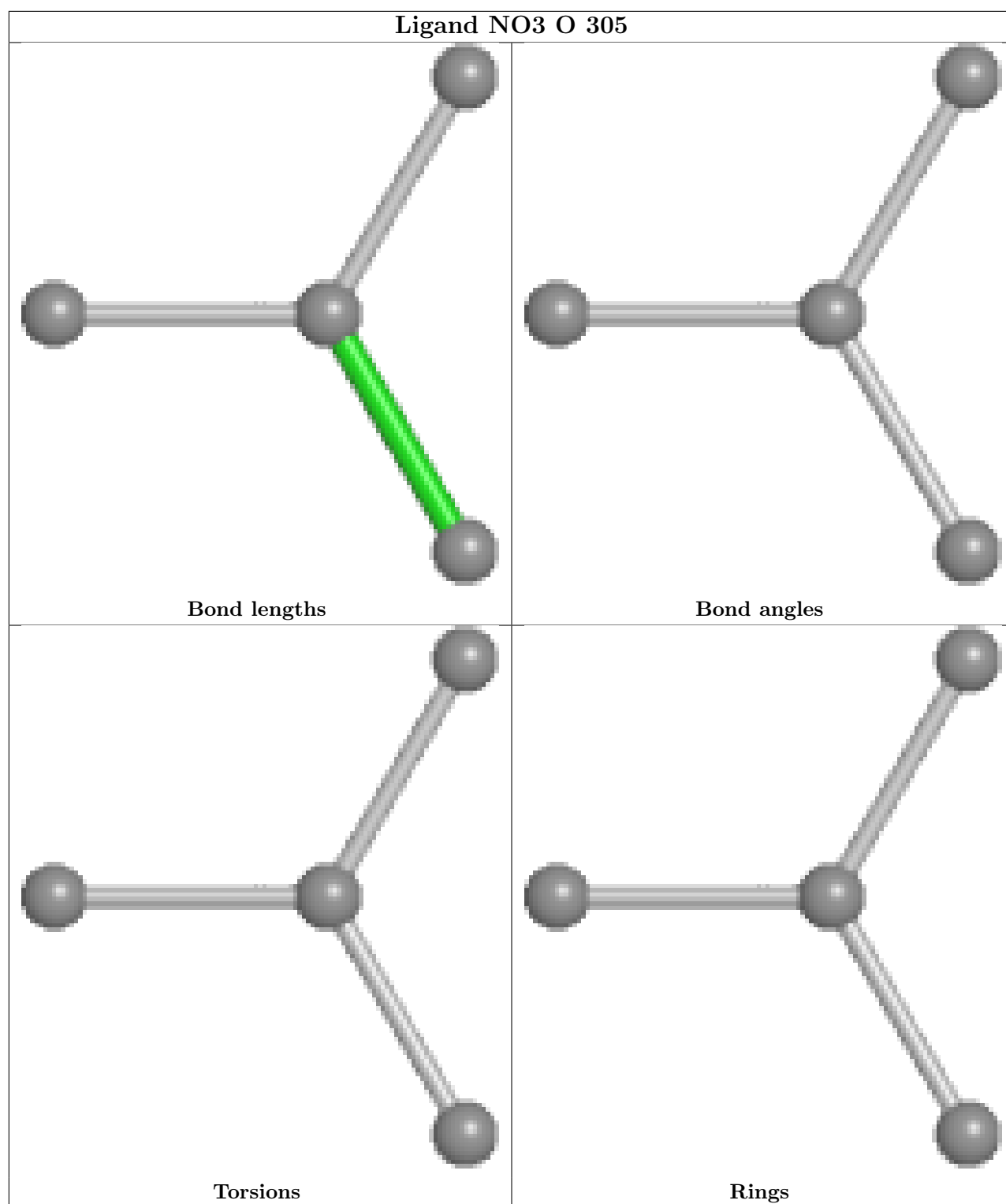


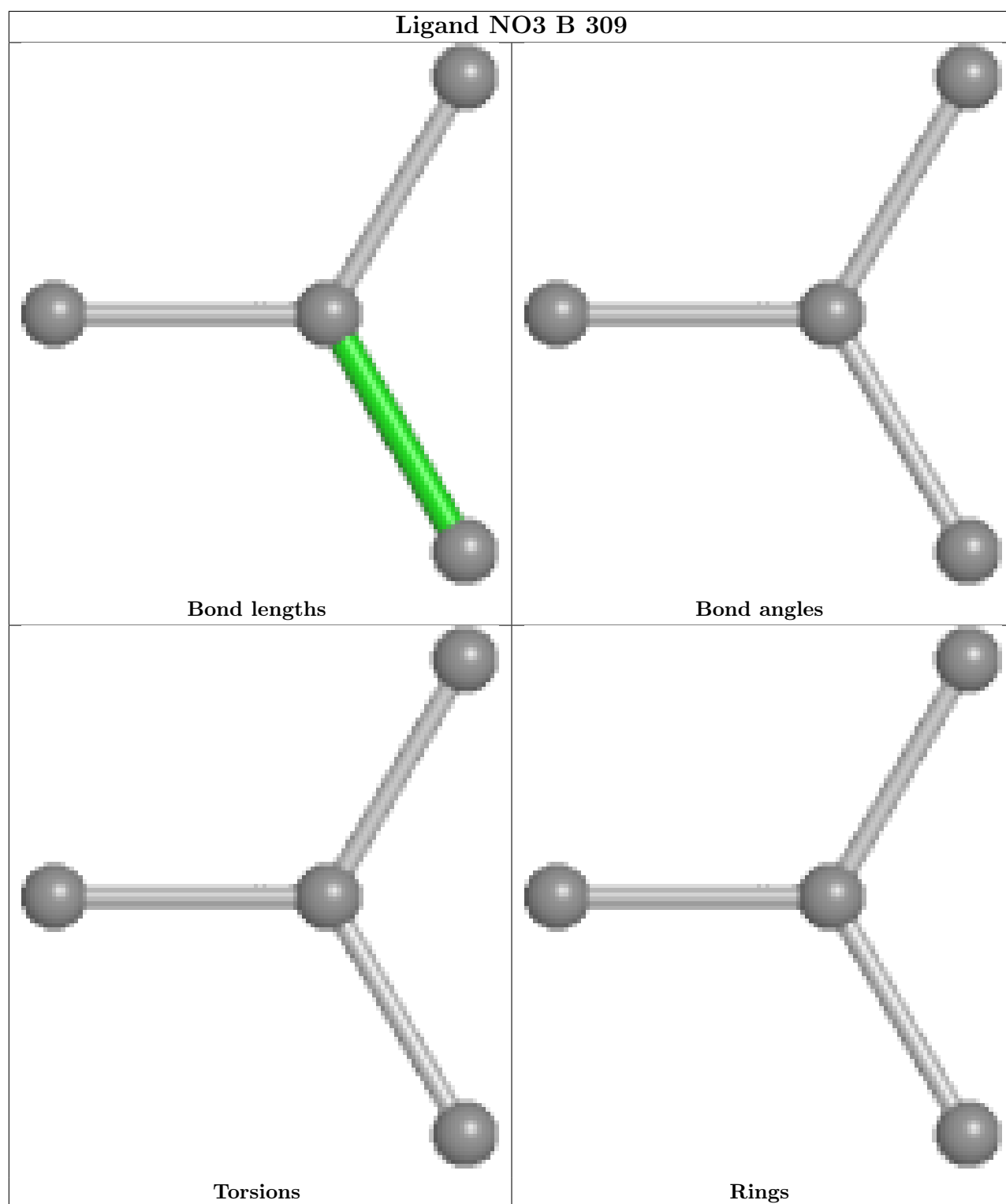




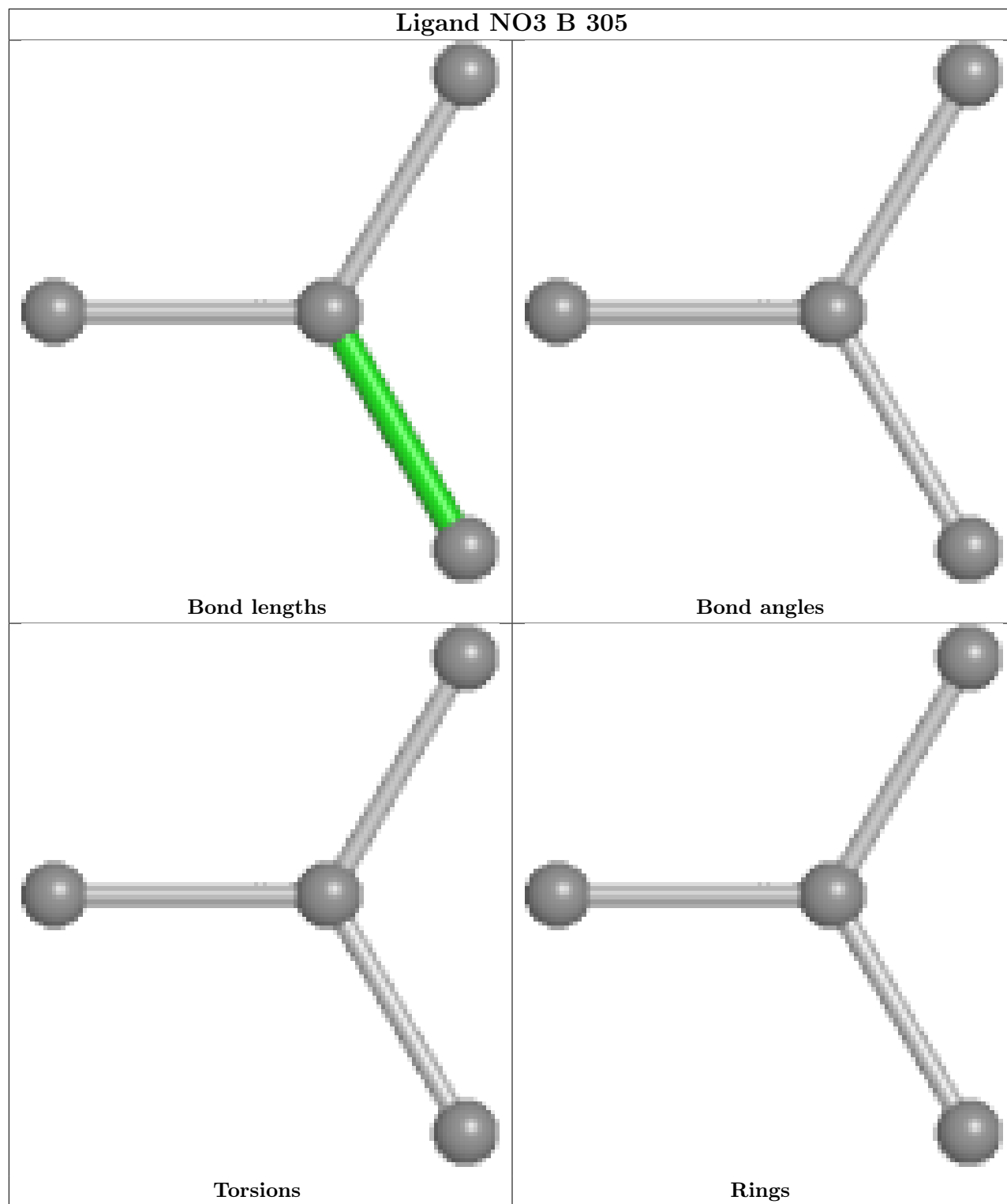


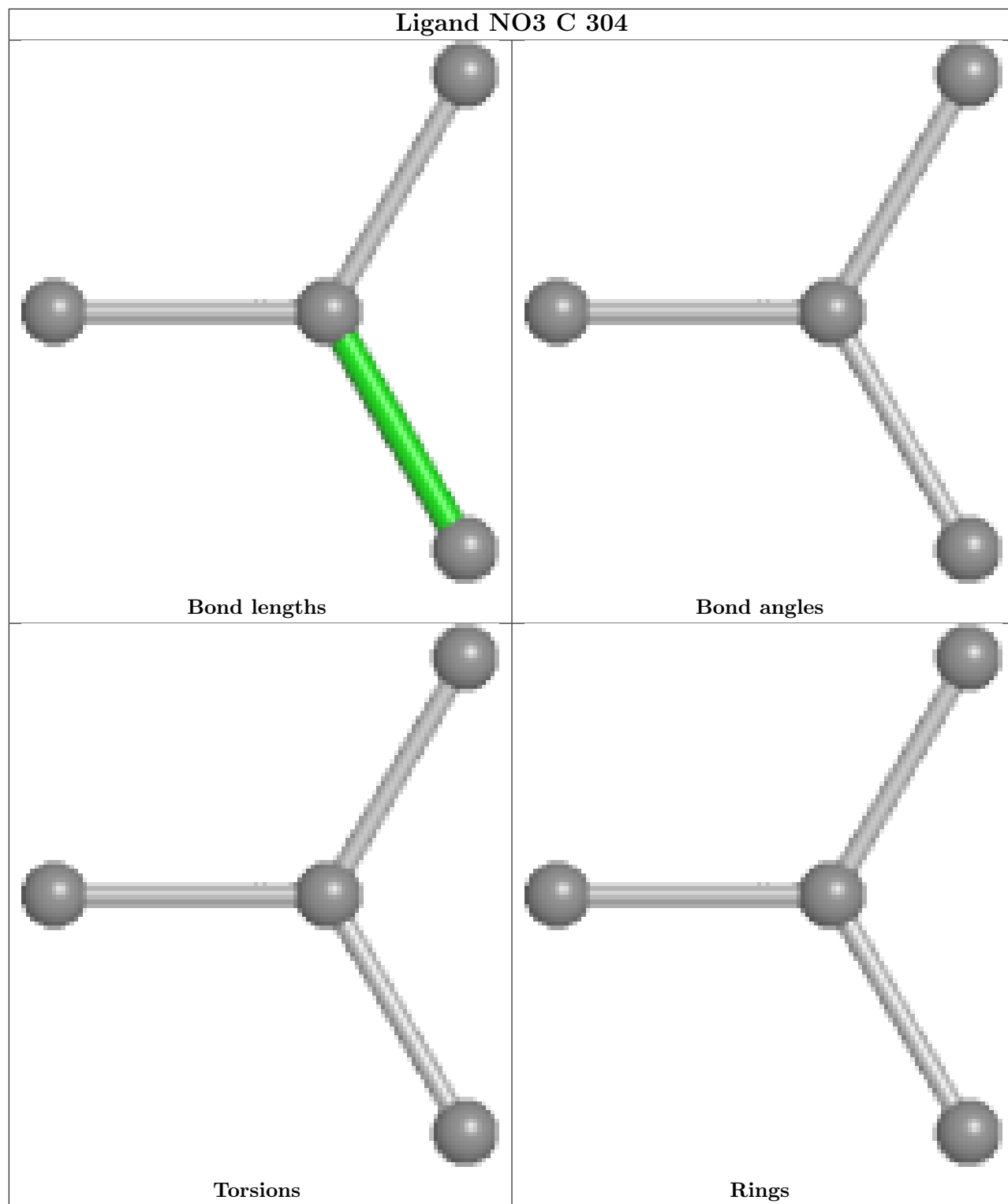


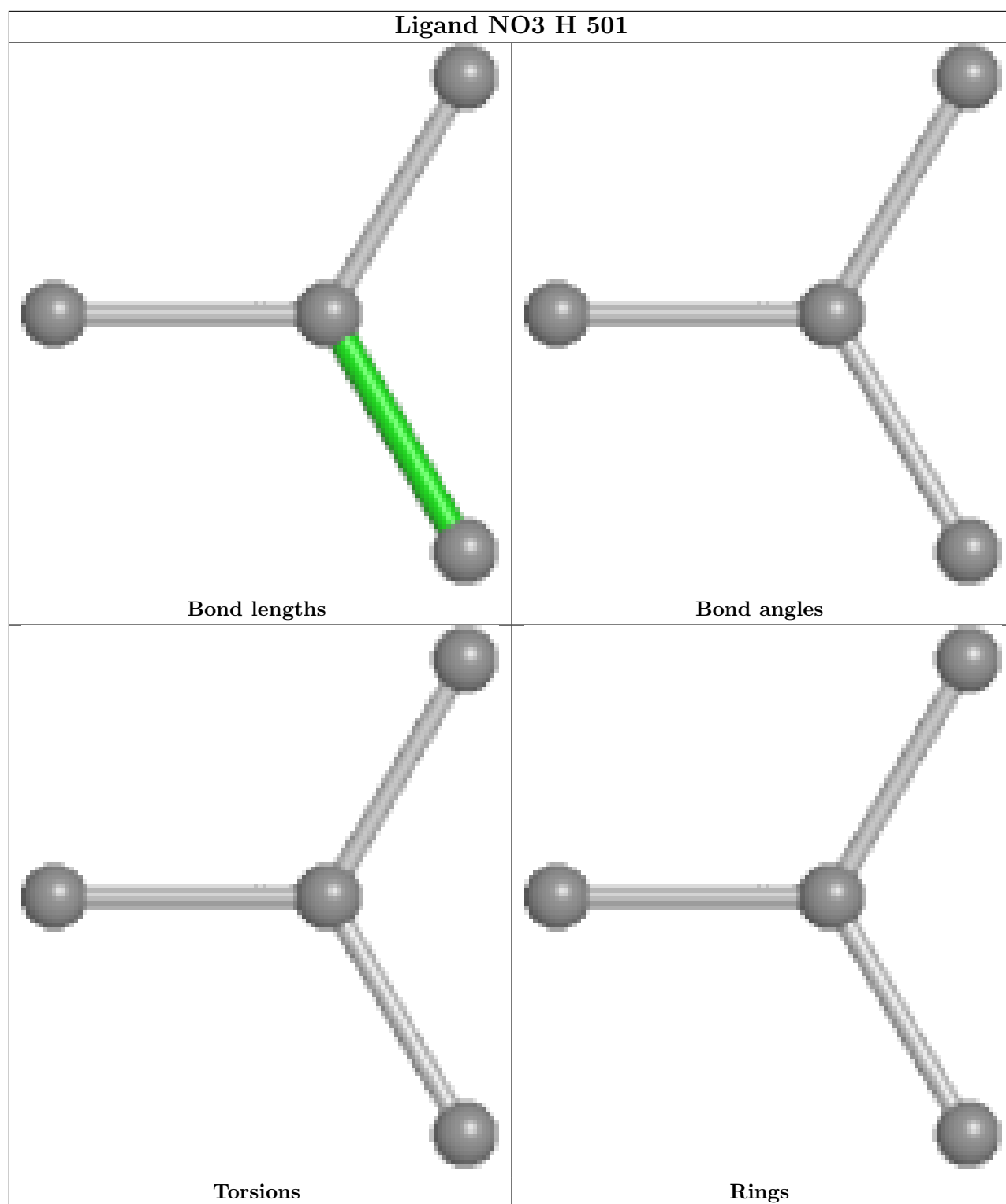


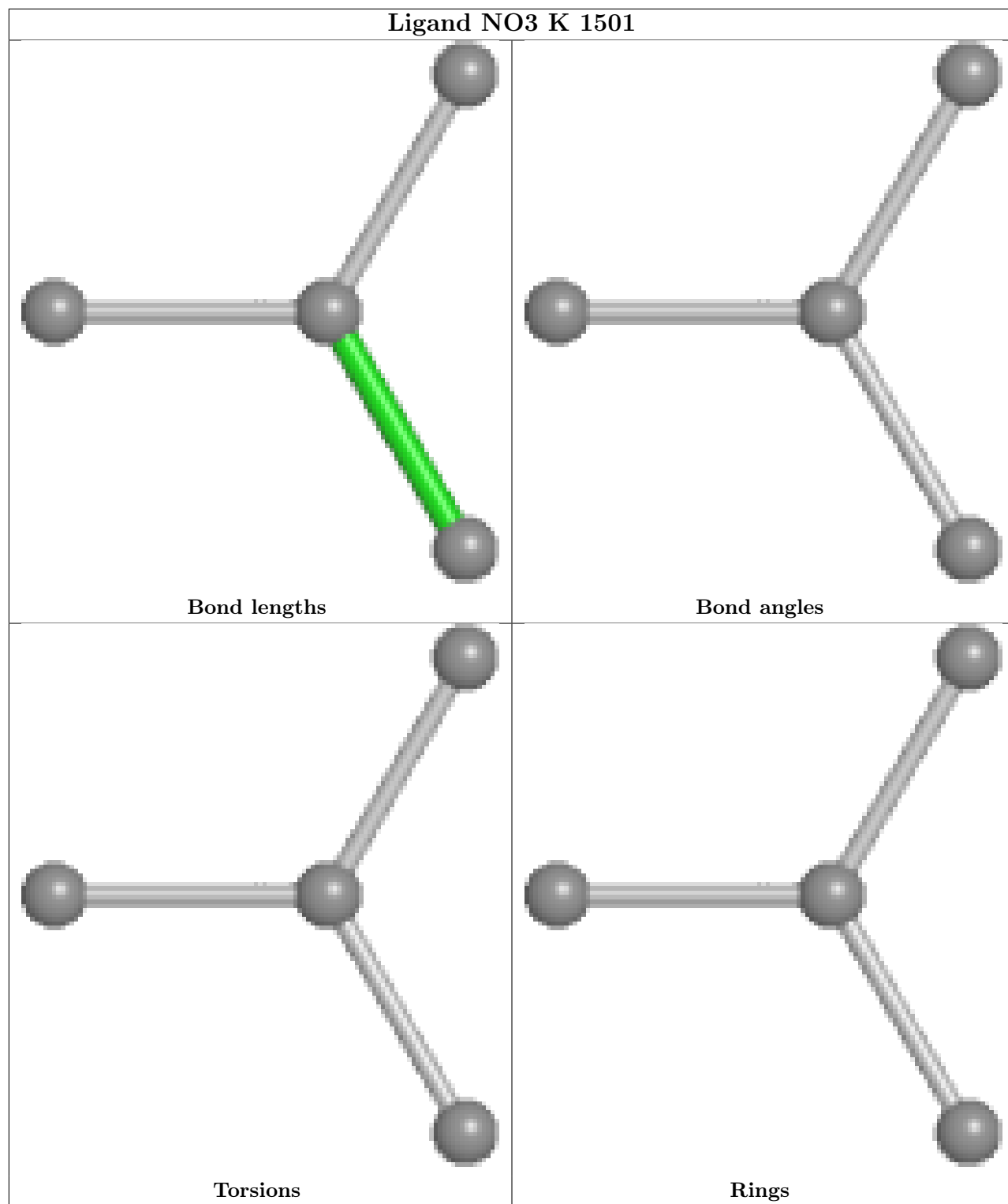


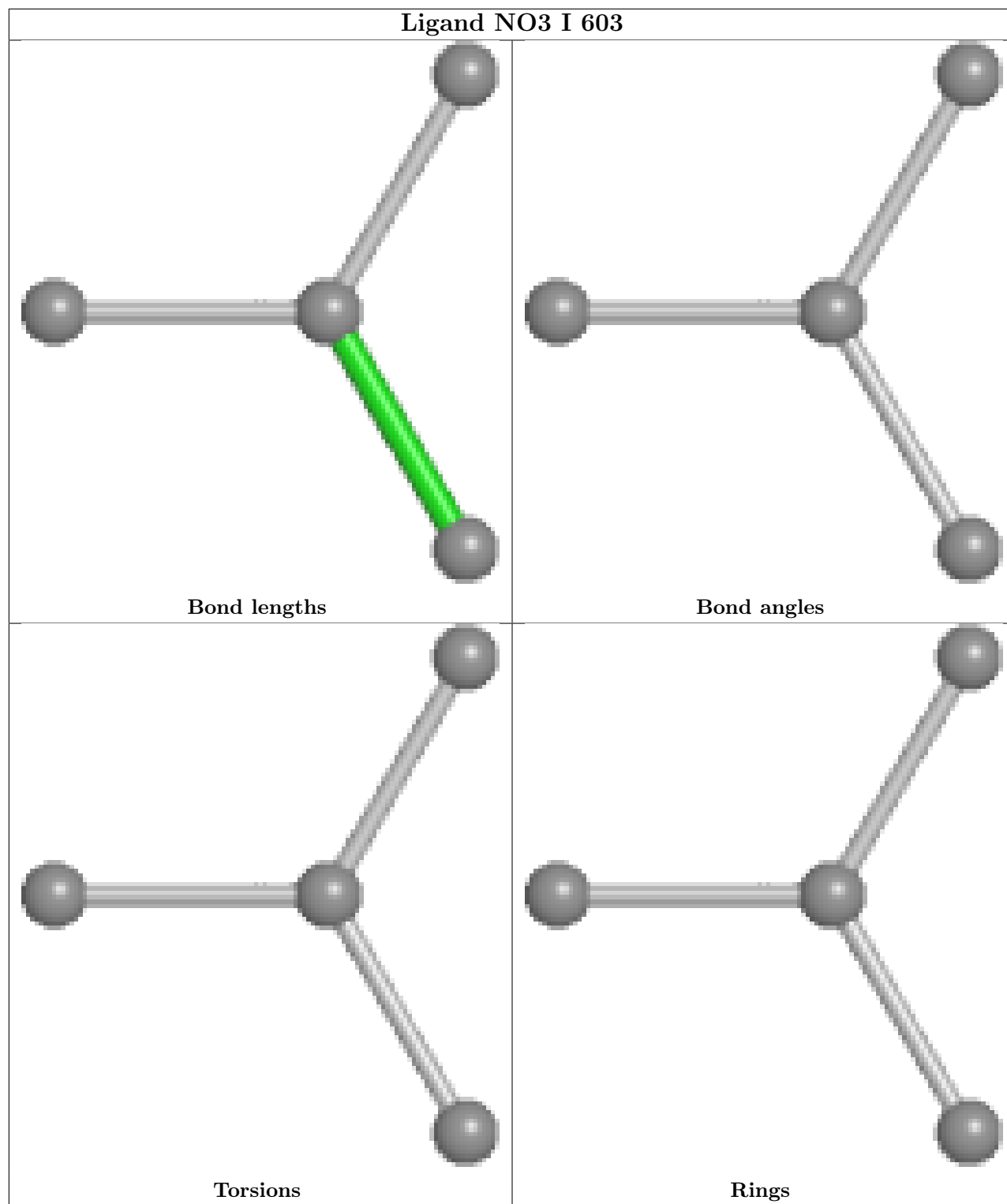


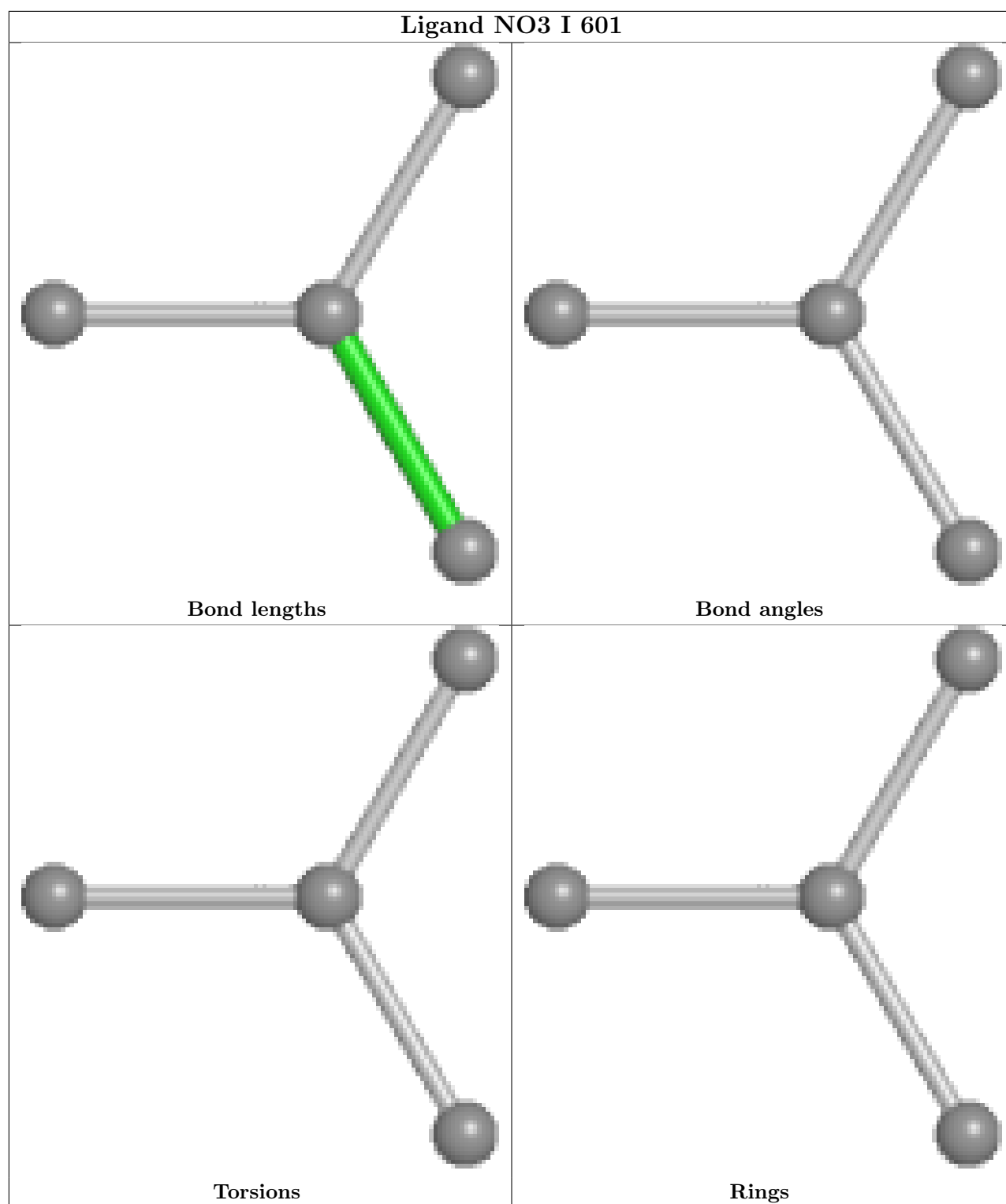


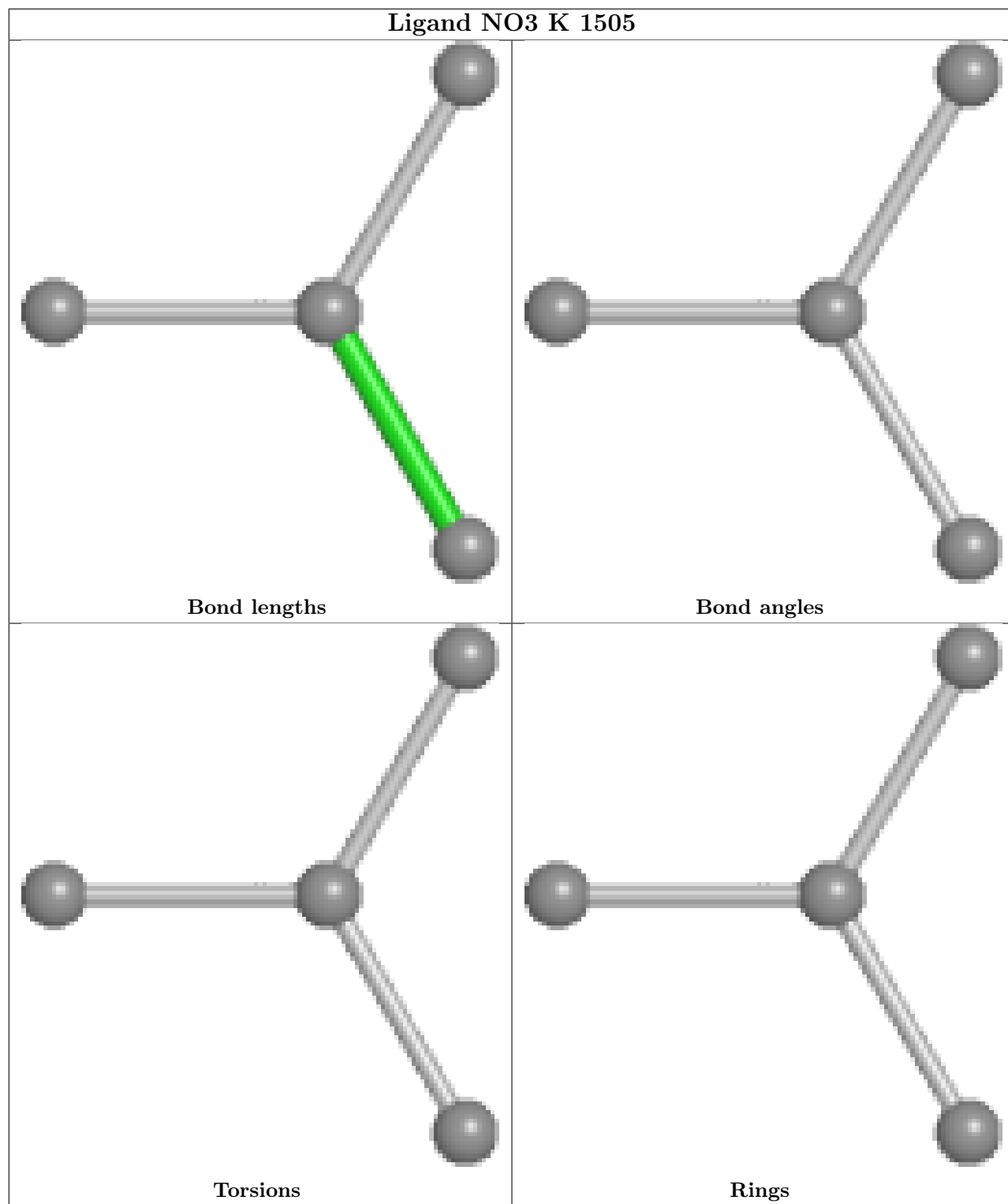


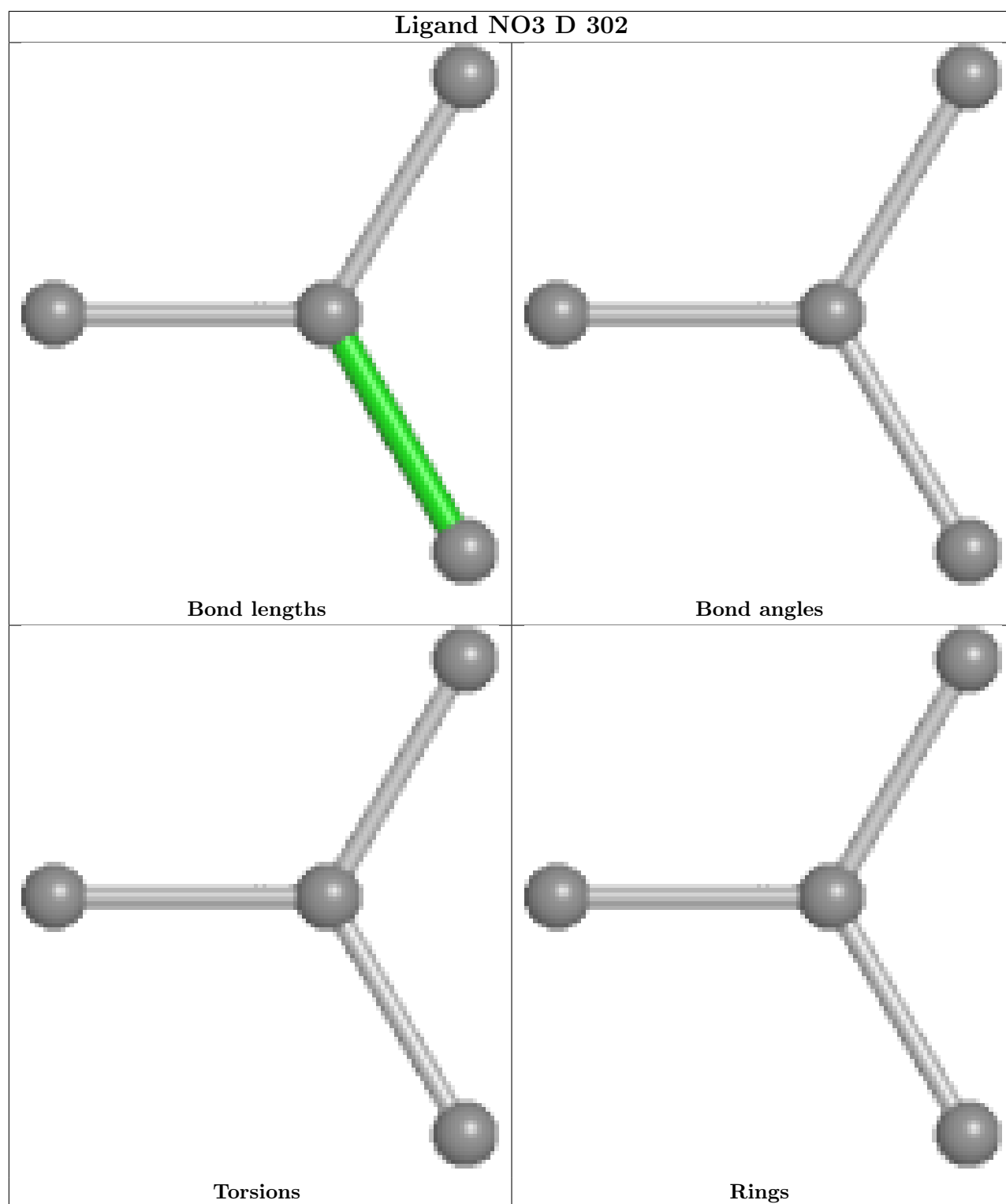




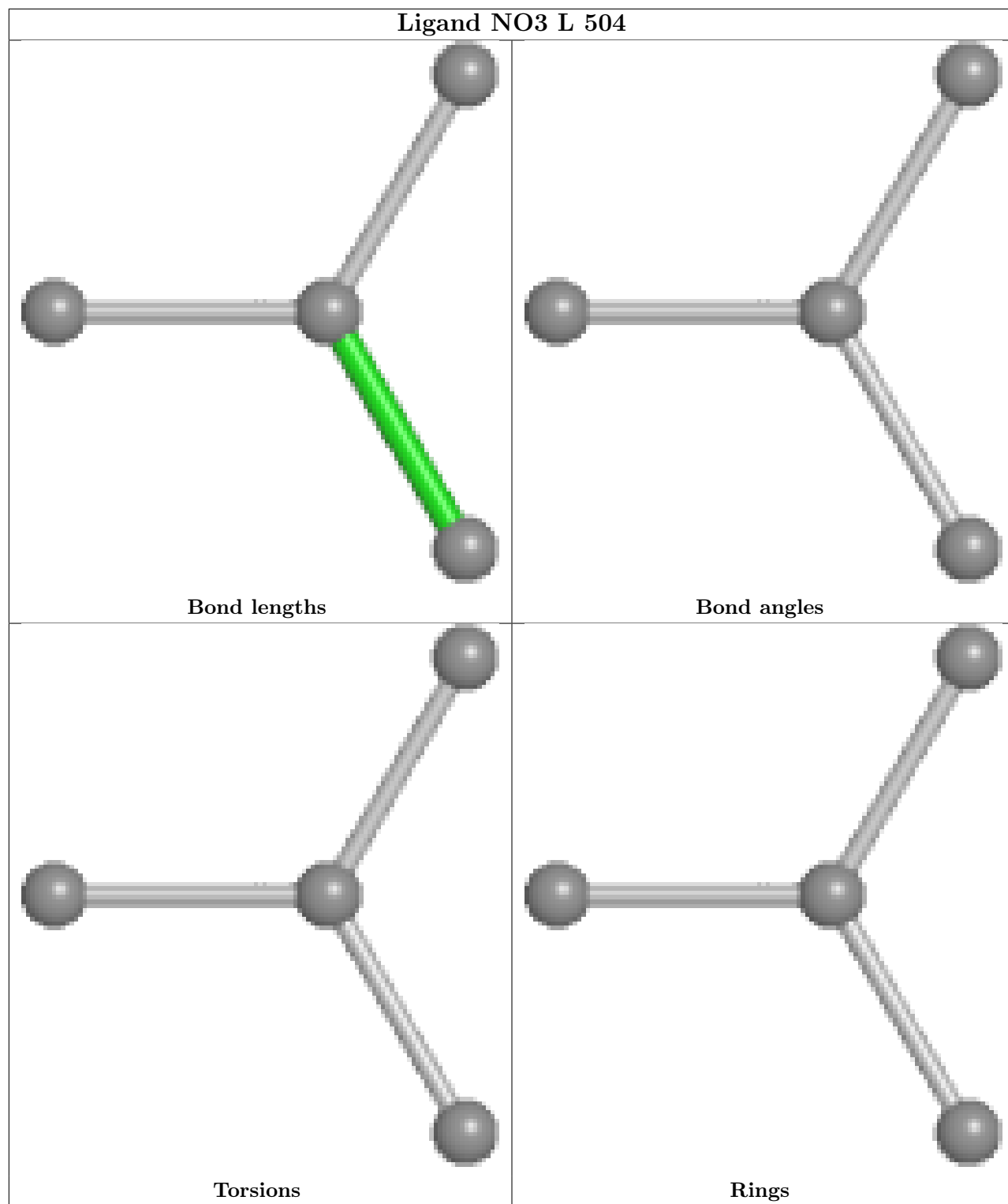


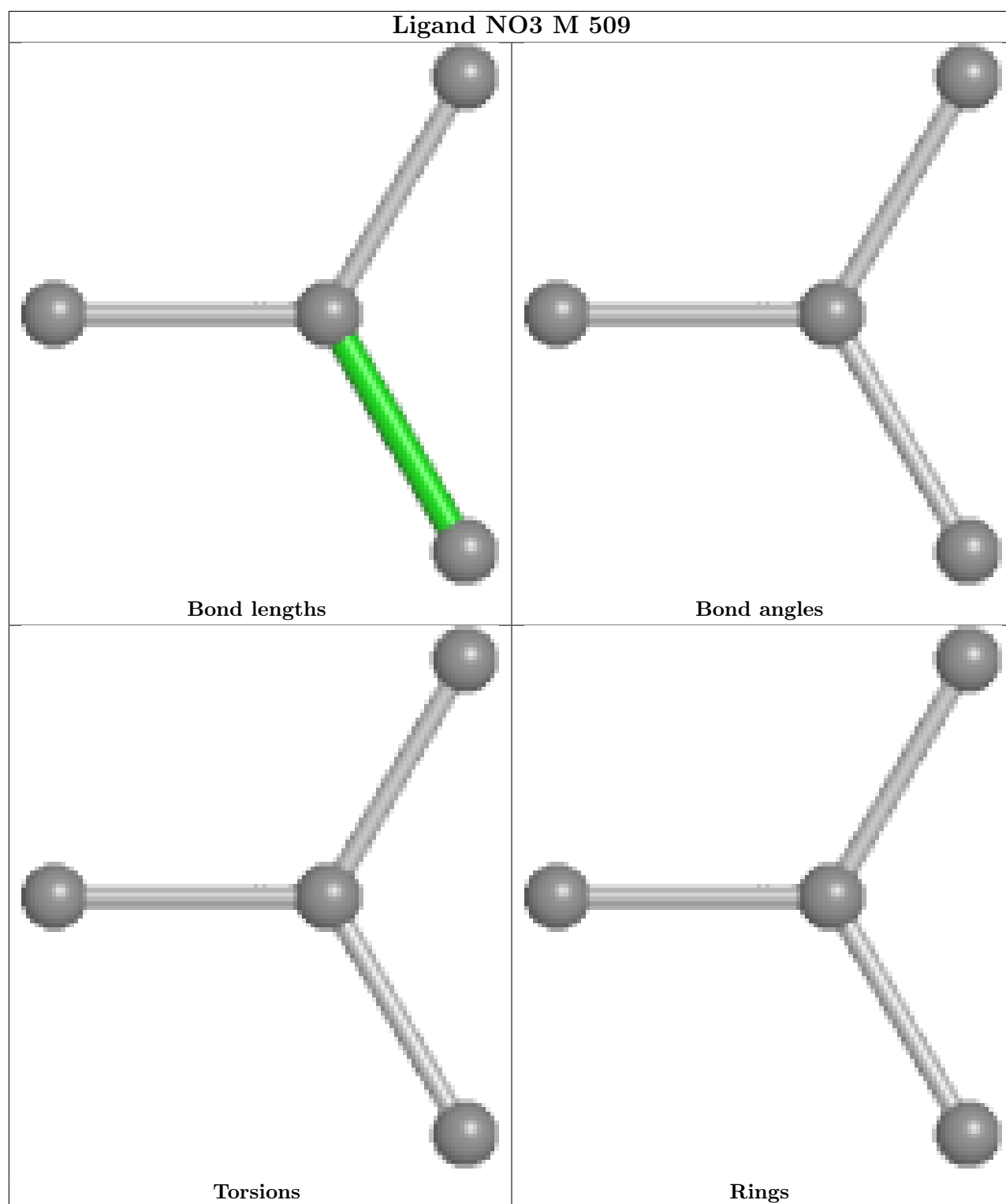


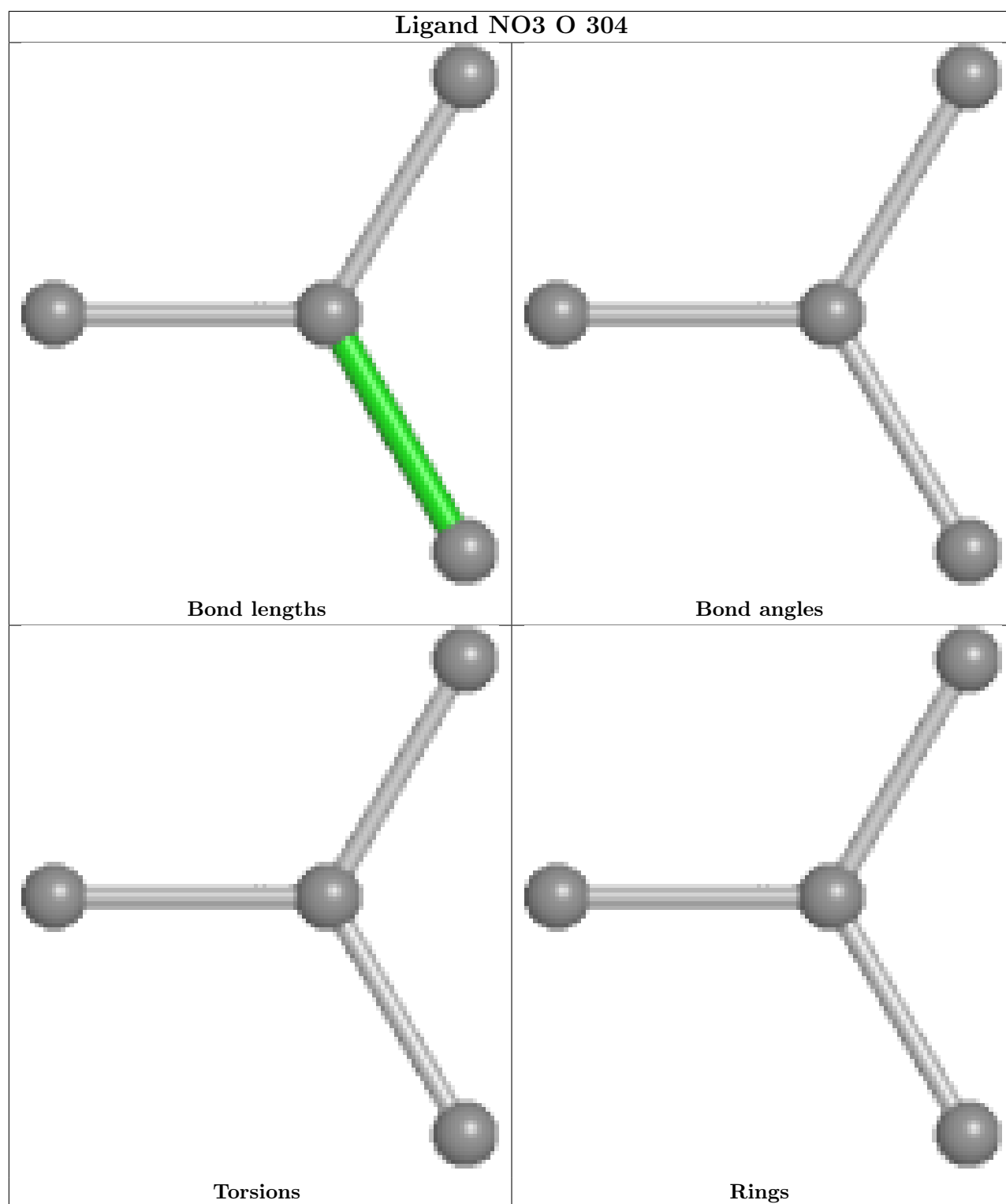


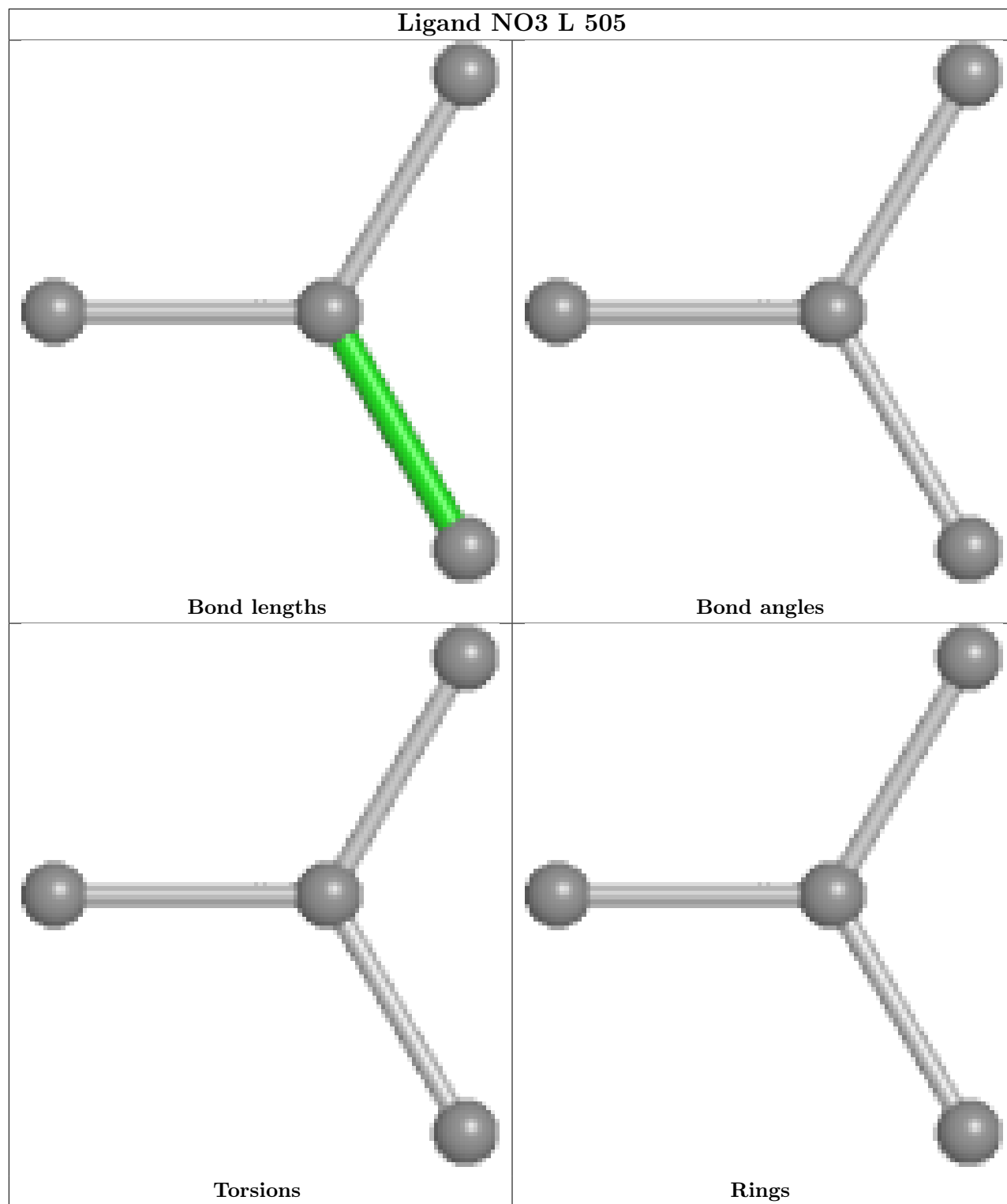


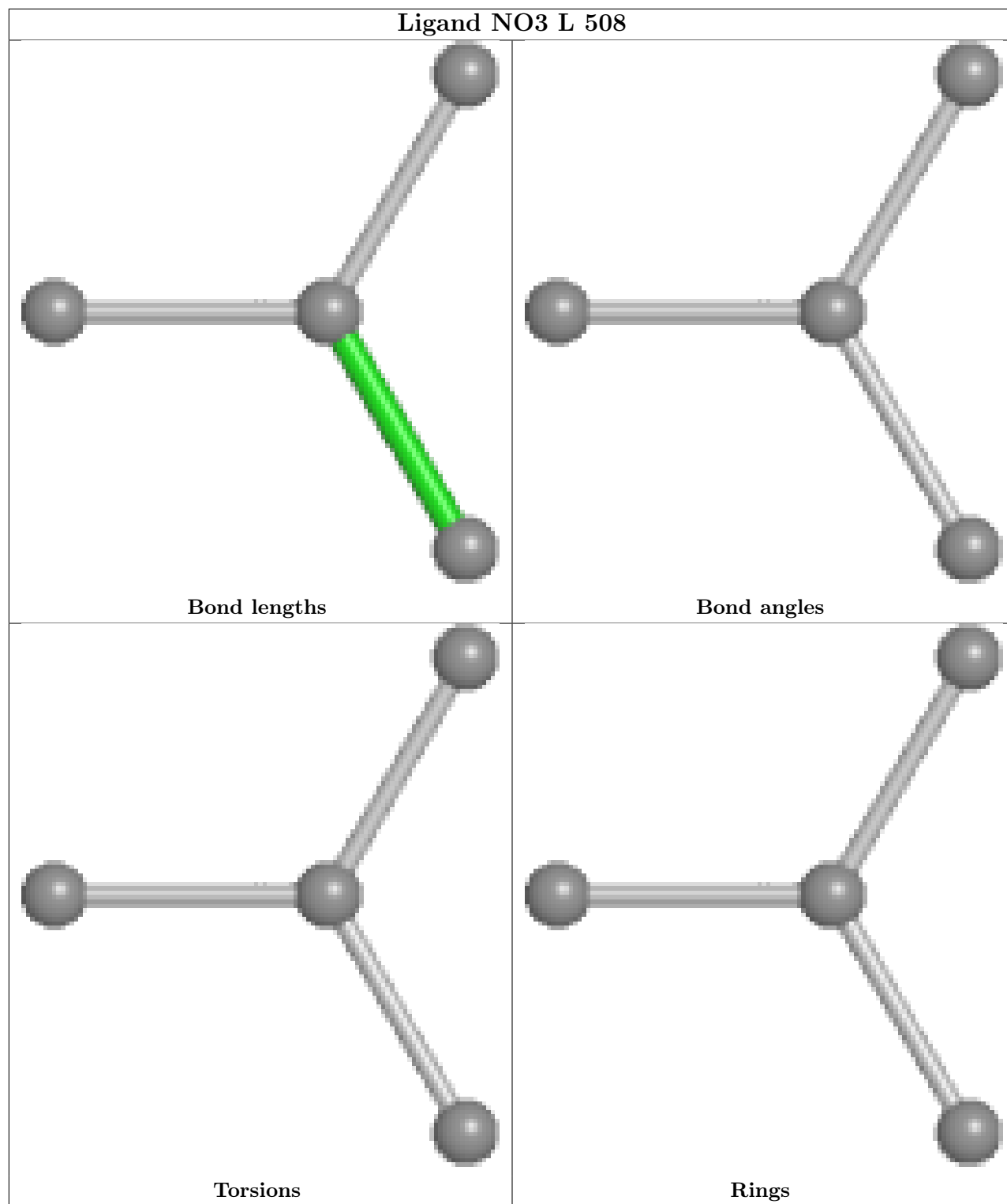


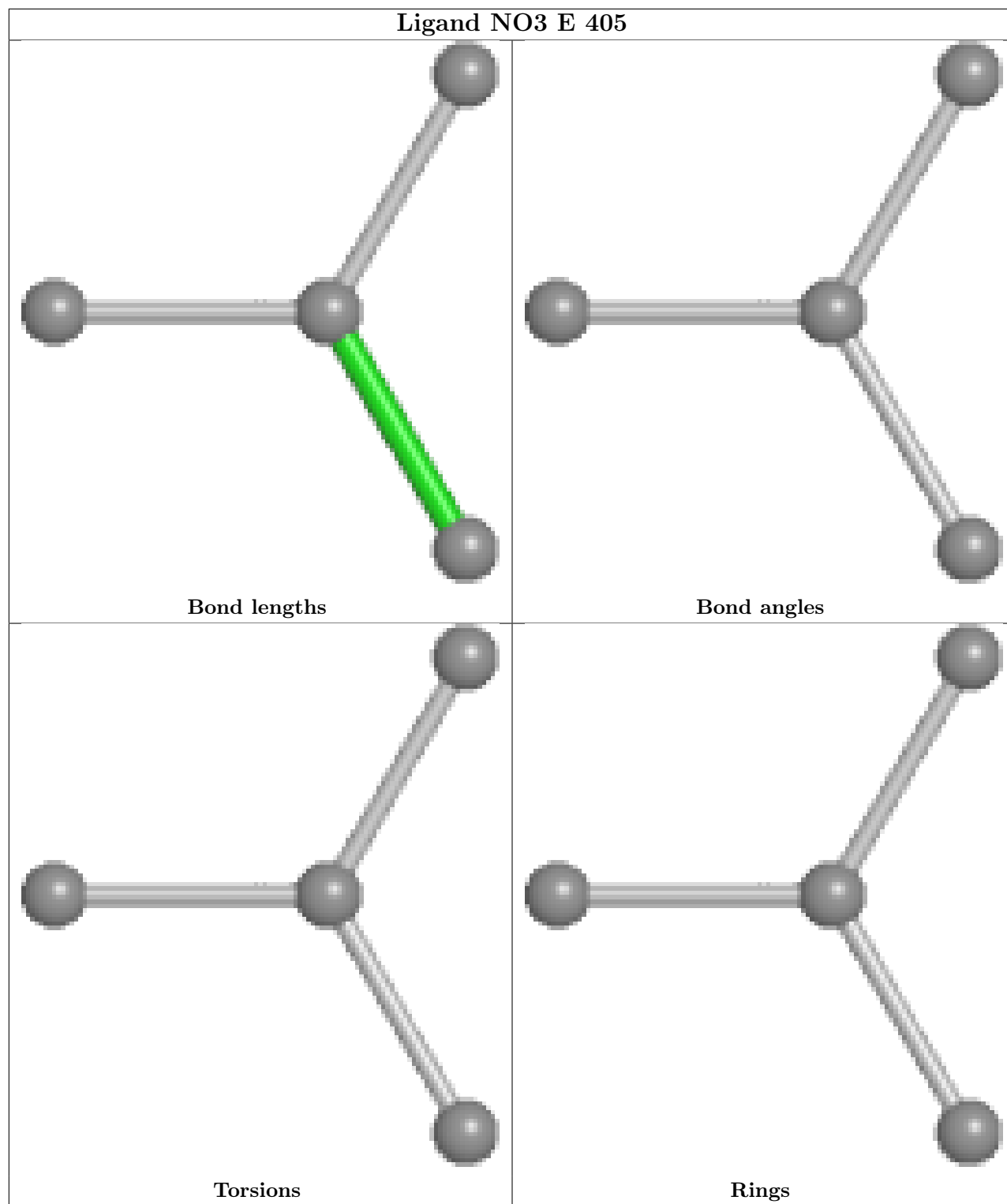












## 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	150/159 (94%)	0.11	3 (2%) 65 51	28, 44, 65, 80	0
1	B	151/159 (94%)	0.14	2 (1%) 77 65	32, 44, 62, 74	2 (1%)
1	C	151/159 (94%)	0.20	6 (3%) 38 25	34, 42, 59, 91	2 (1%)
1	D	151/159 (94%)	0.31	7 (4%) 32 20	34, 49, 70, 78	0
1	E	149/159 (93%)	0.22	3 (2%) 65 51	34, 47, 69, 87	2 (1%)
1	F	144/159 (90%)	0.08	0 100 100	33, 43, 61, 83	1 (0%)
1	G	155/159 (97%)	0.35	3 (1%) 66 53	34, 47, 64, 77	4 (2%)
1	GG	145/159 (91%)	0.78	10 (6%) 16 9	50, 74, 100, 130	1 (0%)
1	H	145/159 (91%)	0.00	1 (0%) 87 81	31, 42, 59, 75	4 (2%)
1	HH	144/159 (90%)	0.77	8 (5%) 24 13	53, 71, 102, 121	2 (1%)
1	I	156/159 (98%)	0.19	10 (6%) 19 11	30, 40, 49, 59	1 (0%)
1	II	142/159 (89%)	0.77	6 (4%) 36 23	61, 74, 94, 115	0
1	J	147/159 (92%)	0.17	5 (3%) 45 29	28, 39, 52, 64	2 (1%)
1	JJ	144/159 (90%)	0.79	7 (4%) 29 17	66, 80, 103, 166	3 (2%)
1	K	146/159 (91%)	0.36	2 (1%) 75 63	29, 44, 60, 66	2 (1%)
1	KK	144/159 (90%)	0.69	11 (7%) 13 7	64, 82, 102, 122	0
1	L	151/159 (94%)	0.58	8 (5%) 26 14	35, 49, 87, 141	0
1	M	150/159 (94%)	0.27	4 (2%) 54 39	36, 49, 84, 113	0
1	N	150/159 (94%)	0.27	2 (1%) 77 65	35, 49, 93, 136	0
1	O	149/159 (93%)	0.58	7 (4%) 31 19	39, 56, 89, 122	3 (2%)
All	All	2964/3180 (93%)	0.38	105 (3%) 44 28	28, 49, 88, 166	29 (0%)

The worst 5 of 105 RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	I	6	VAL	6.3
1	I	4	GLY	6.0
1	J	15	ASP	5.9
1	L	9	ASN	5.5
1	L	14	GLY	5.4

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NO3	K	1504	4/4	-0.16	0.68	145,148,151,151	0
2	NO3	L	508	4/4	0.03	0.45	115,116,116,116	4
2	NO3	HH	303	4/4	0.06	0.39	132,133,133,134	4
2	NO3	B	311	4/4	0.17	0.34	124,126,129,130	0
2	NO3	K	1505	4/4	0.43	0.32	112,113,114,114	0
2	NO3	KK	202	4/4	0.47	0.36	107,109,110,111	0
2	NO3	I	604	4/4	0.48	0.61	89,90,91,92	0
2	NO3	H	507	4/4	0.55	0.49	98,99,101,102	0
2	NO3	H	508	4/4	0.61	0.31	110,116,117,119	0
2	NO3	II	202	4/4	0.64	0.29	101,102,104,105	0
2	NO3	D	302	4/4	0.64	0.79	108,108,110,110	0
2	NO3	N	1309	4/4	0.66	0.62	70,77,78,83	0
2	NO3	GG	205	4/4	0.67	0.44	113,115,115,117	0
2	NO3	L	507	4/4	0.67	0.20	109,113,115,115	0
2	NO3	N	1305	4/4	0.69	0.44	81,83,83,85	0
2	NO3	M	506	4/4	0.69	0.29	92,92,98,99	0
2	NO3	M	510	4/4	0.70	0.34	84,86,92,95	0
3	MG	JJ	203	1/1	0.70	0.93	89,89,89,89	0
2	NO3	G	502	4/4	0.71	0.33	50,52,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	II	203	1/1	0.72	0.56	78,78,78,78	0
2	NO3	KK	201	4/4	0.72	0.23	112,113,114,114	0
2	NO3	I	606	4/4	0.73	0.55	122,125,125,127	0
2	NO3	O	301	4/4	0.74	0.77	85,87,88,90	0
2	NO3	GG	204	4/4	0.74	0.38	75,78,79,80	0
2	NO3	M	507	4/4	0.74	0.49	79,84,84,86	0
2	NO3	B	312	4/4	0.75	0.56	95,98,100,104	0
2	NO3	II	204	4/4	0.75	0.79	101,102,102,103	0
2	NO3	L	504	4/4	0.76	0.40	94,97,98,99	0
2	NO3	HH	302	4/4	0.77	0.41	85,86,88,92	0
2	NO3	L	506	4/4	0.78	0.25	53,53,53,53	4
2	NO3	JJ	202	4/4	0.78	0.33	77,77,78,78	0
2	NO3	J	905	4/4	0.78	0.43	83,85,86,86	0
2	NO3	J	902	4/4	0.79	0.49	36,42,42,46	0
2	NO3	O	304	4/4	0.79	0.30	84,87,89,95	0
2	NO3	GG	203	4/4	0.79	0.33	69,69,70,71	0
2	NO3	L	505	4/4	0.79	0.23	101,101,101,101	4
2	NO3	G	501	4/4	0.79	0.52	57,57,69,70	0
2	NO3	B	308	4/4	0.79	0.23	77,83,85,85	0
2	NO3	B	306	4/4	0.79	0.49	63,64,66,71	0
2	NO3	HH	304	4/4	0.80	0.40	98,99,99,99	0
2	NO3	N	1308	4/4	0.80	0.39	56,64,65,66	0
2	NO3	M	504	4/4	0.80	0.41	60,64,65,68	0
2	NO3	M	505	4/4	0.80	0.49	54,55,55,57	0
2	NO3	B	310	4/4	0.81	0.25	81,84,85,91	0
2	NO3	A	804	4/4	0.81	0.30	82,85,89,92	0
2	NO3	O	305	4/4	0.82	0.37	73,75,77,79	0
2	NO3	H	506	4/4	0.82	0.25	77,80,83,84	0
2	NO3	H	505	4/4	0.83	0.54	101,102,105,108	0
2	NO3	E	406	4/4	0.84	0.52	85,86,87,89	0
2	NO3	E	402	4/4	0.84	0.20	49,53,57,57	0
2	NO3	H	504	4/4	0.85	0.52	96,97,97,98	0
2	NO3	E	403	4/4	0.85	0.36	51,51,54,58	0
2	NO3	J	901	4/4	0.86	0.29	38,41,44,45	0
2	NO3	D	301	4/4	0.86	0.21	43,45,46,48	0
2	NO3	M	508	4/4	0.86	0.48	51,53,53,53	4
2	NO3	E	405	4/4	0.86	0.56	114,115,120,125	0
2	NO3	N	1304	4/4	0.86	0.38	38,42,43,45	0
2	NO3	I	602	4/4	0.86	0.32	42,51,51,60	0
2	NO3	B	309	4/4	0.86	0.29	80,81,82,82	0
2	NO3	B	302	4/4	0.86	0.44	52,54,54,56	0
2	NO3	GG	201	4/4	0.87	0.18	83,83,83,85	0

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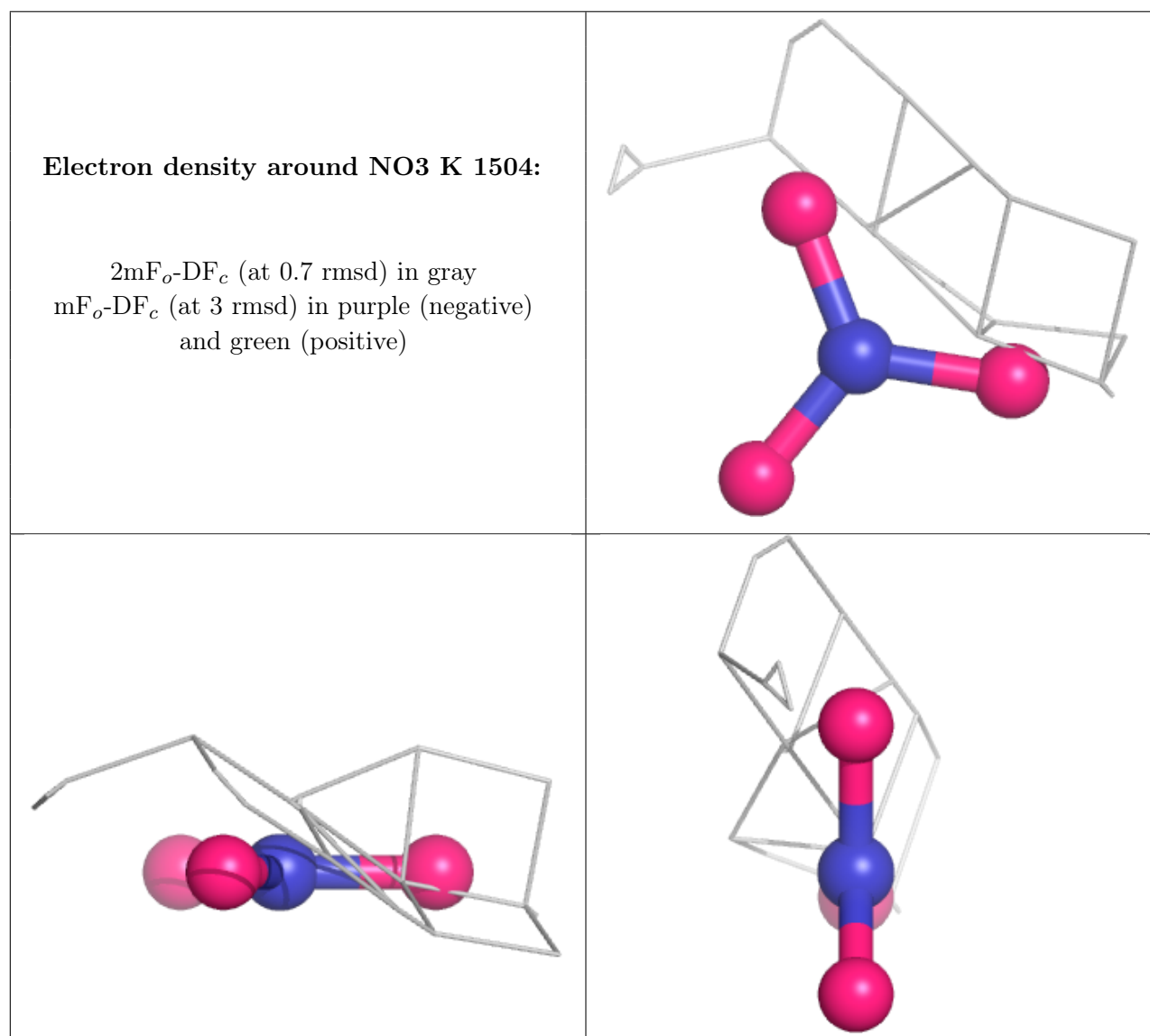
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NO3	C	302	4/4	0.87	0.43	37,40,41,43	0
2	NO3	C	304	4/4	0.87	0.27	72,80,81,88	0
2	NO3	B	305	4/4	0.87	0.29	50,57,59,59	0
2	NO3	L	502	4/4	0.87	0.21	56,57,59,65	0
2	NO3	M	502	4/4	0.87	0.23	64,64,65,66	0
2	NO3	C	301	4/4	0.87	0.38	46,49,50,56	0
2	NO3	B	304	4/4	0.88	0.33	42,42,45,48	0
2	NO3	N	1302	4/4	0.88	0.31	59,60,65,77	0
2	NO3	JJ	201	4/4	0.88	0.63	71,80,82,96	0
2	NO3	II	201	4/4	0.88	0.27	90,91,91,92	0
2	NO3	K	1503	4/4	0.89	0.59	62,63,63,65	0
2	NO3	K	1501	4/4	0.89	0.22	68,69,73,75	0
2	NO3	GG	206	4/4	0.89	0.43	128,130,131,132	0
2	NO3	L	501	4/4	0.90	0.30	45,45,45,49	0
2	NO3	J	904	4/4	0.91	0.40	79,82,84,85	0
2	NO3	A	805	4/4	0.91	0.60	71,71,71,71	0
3	MG	O	302	1/1	0.91	0.48	46,46,46,46	0
2	NO3	F	602	4/4	0.91	0.18	43,44,45,47	0
2	NO3	HH	301	4/4	0.91	0.16	51,61,74,98	0
2	NO3	I	601	4/4	0.92	0.58	70,73,74,76	0
2	NO3	M	509	4/4	0.92	0.40	71,73,74,75	0
2	NO3	H	502	4/4	0.92	0.82	62,65,67,75	0
2	NO3	E	401	4/4	0.92	0.46	55,64,65,74	0
2	NO3	B	301	4/4	0.92	0.36	42,48,50,52	0
2	NO3	B	307	4/4	0.93	0.57	116,118,118,118	0
2	NO3	N	1306	4/4	0.93	0.29	61,62,62,63	0
2	NO3	GG	202	4/4	0.93	0.19	83,83,83,84	0
2	NO3	A	802	4/4	0.93	0.41	54,59,61,61	0
2	NO3	F	601	4/4	0.93	0.43	38,38,39,43	0
2	NO3	I	605	4/4	0.93	0.40	45,46,47,48	0
2	NO3	E	404	4/4	0.93	0.44	65,77,79,84	0
2	NO3	N	1303	4/4	0.94	0.61	44,46,47,48	0
2	NO3	J	903	4/4	0.94	0.21	38,39,40,40	0
2	NO3	A	801	4/4	0.94	0.25	46,47,47,48	0
3	MG	M	503	1/1	0.94	0.44	52,52,52,52	0
2	NO3	M	501	4/4	0.94	0.15	55,57,58,60	0
2	NO3	N	1307	4/4	0.94	0.61	59,60,61,63	0
2	NO3	C	303	4/4	0.94	0.15	43,43,44,45	0
2	NO3	N	1301	4/4	0.95	0.19	43,45,48,48	0
2	NO3	II	205	4/4	0.95	0.34	118,118,118,118	4
2	NO3	O	303	4/4	0.95	0.49	60,60,61,63	0
2	NO3	I	603	4/4	0.95	0.48	84,85,85,88	0

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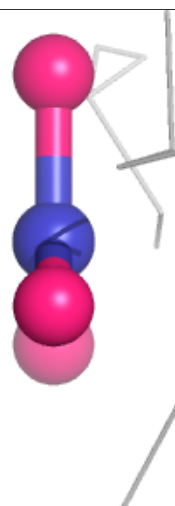
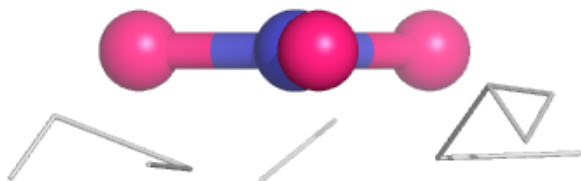
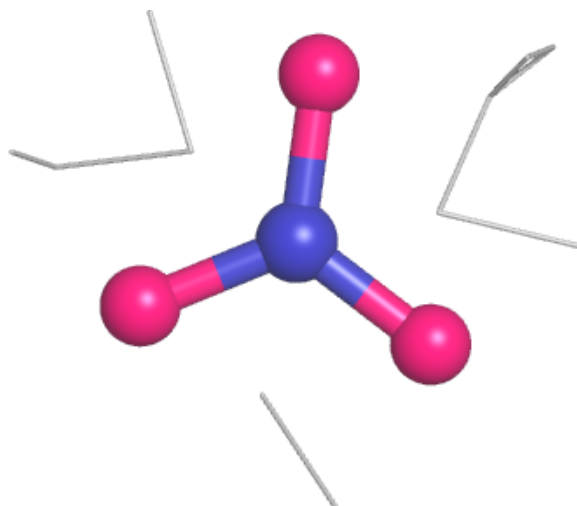
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NO3	L	503	4/4	0.95	0.20	53,54,56,60	0
3	MG	A	803	1/1	0.96	0.26	63,63,63,63	0
3	MG	H	503	1/1	0.96	0.18	52,52,52,52	0
2	NO3	H	501	4/4	0.96	0.23	43,45,49,58	0
2	NO3	B	303	4/4	0.97	0.20	40,42,44,46	0
3	MG	K	1502	1/1	0.97	0.43	48,48,48,48	0
3	MG	F	603	1/1	0.97	0.28	53,53,53,53	0
3	MG	G	503	1/1	0.98	0.18	57,57,57,57	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.



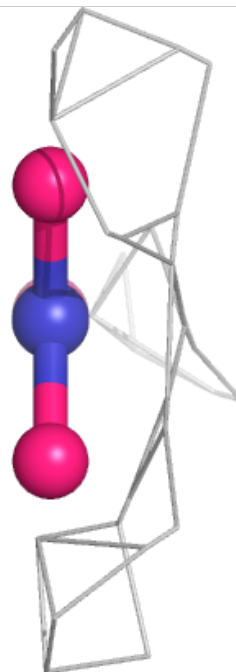
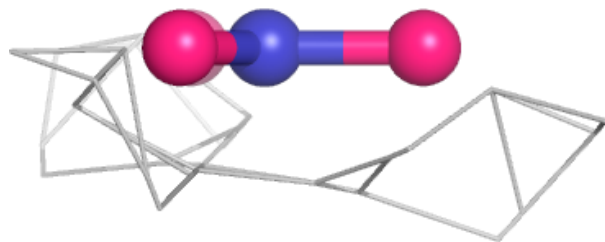
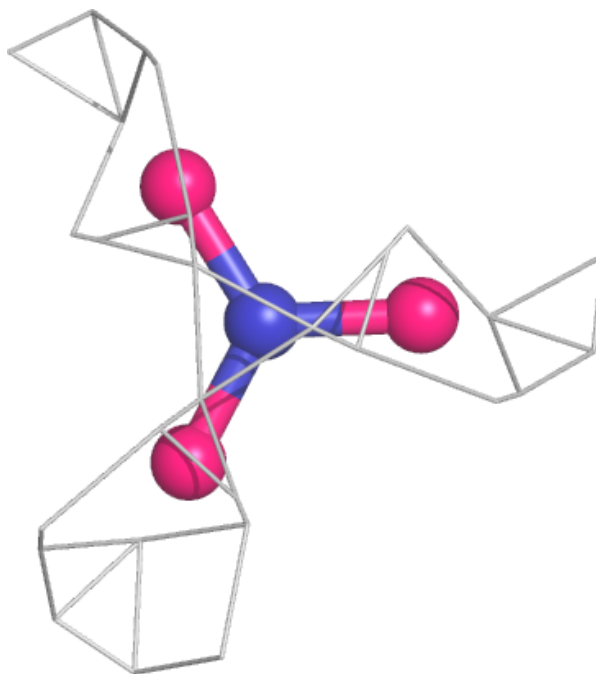
**Electron density around NO3 L 508:**

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



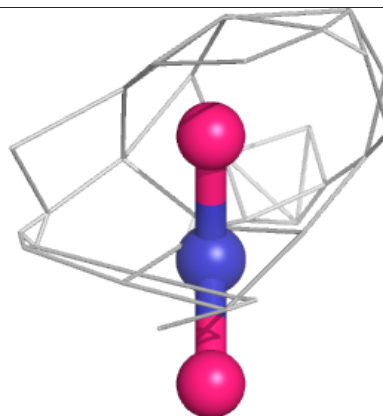
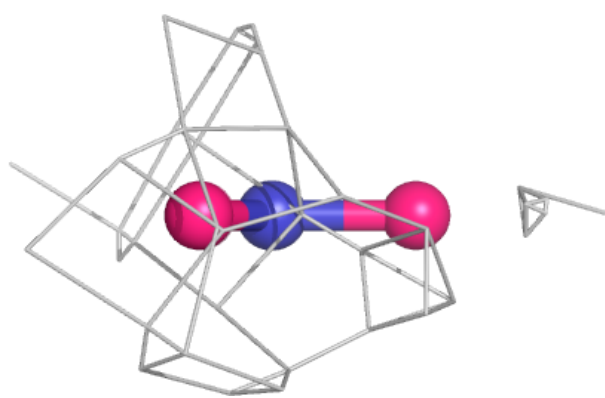
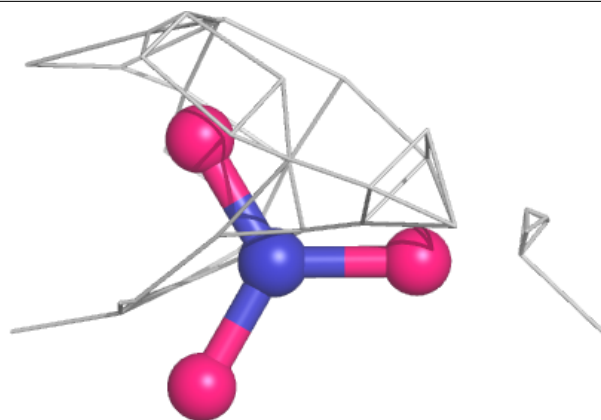
**Electron density around NO3 HH 303:**

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



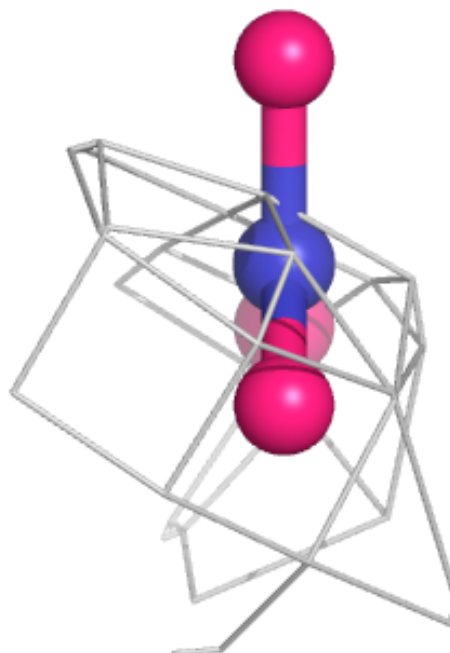
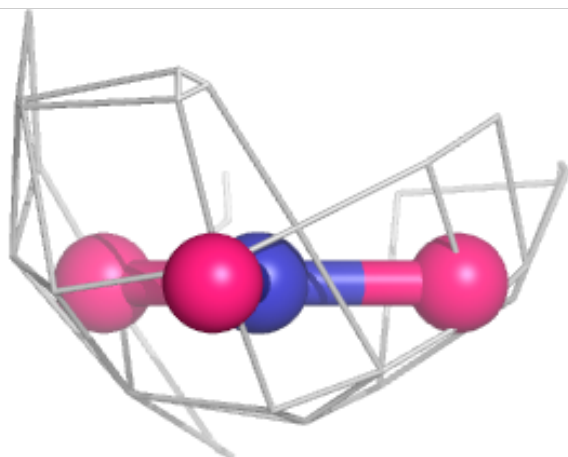
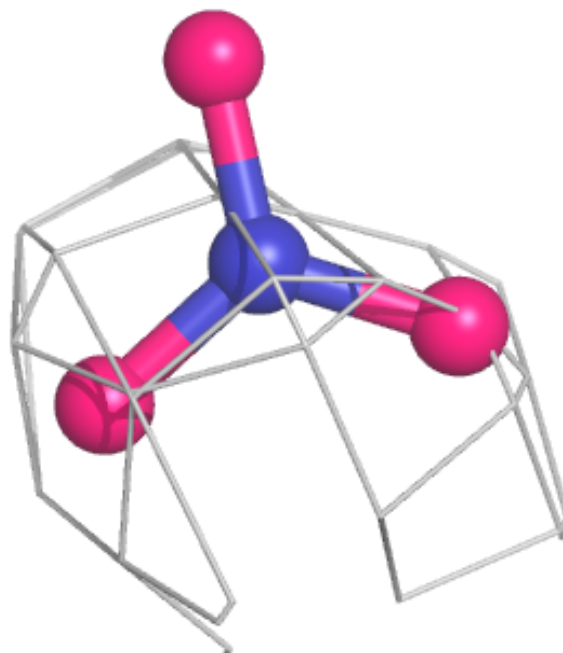
**Electron density around NO3 B 311:**

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



**Electron density around NO3 K 1505:**

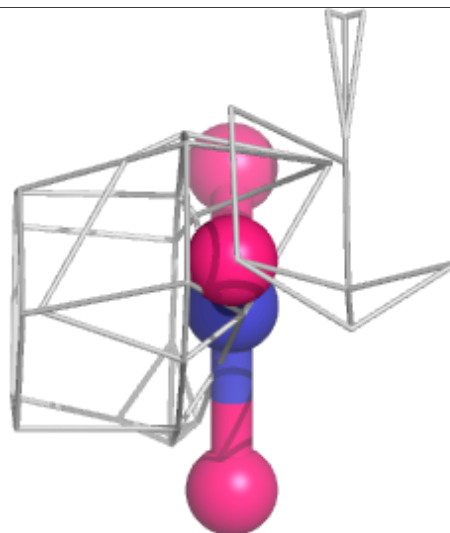
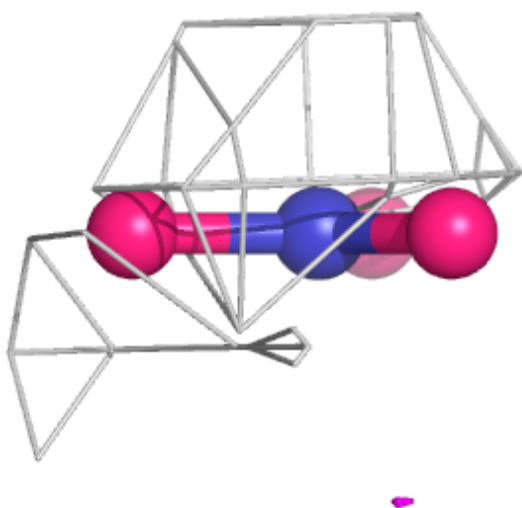
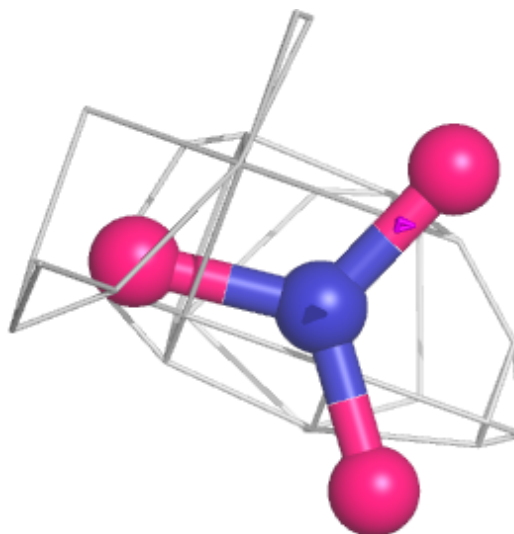
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





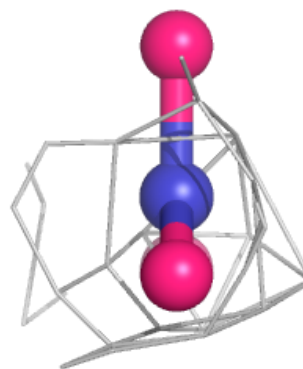
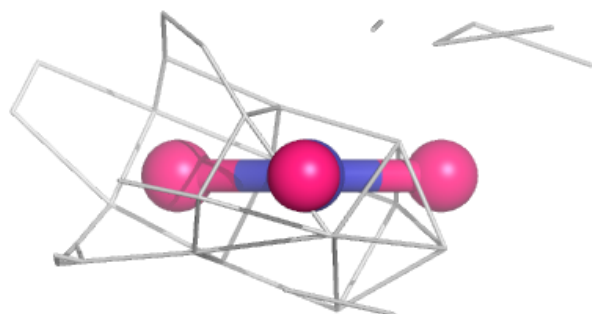
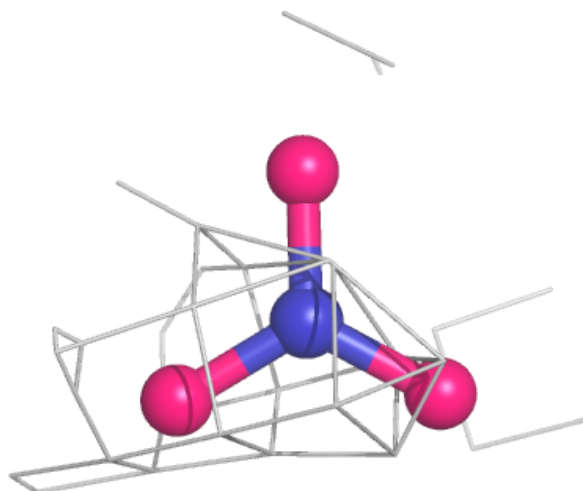
**Electron density around NO3 KK 202:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



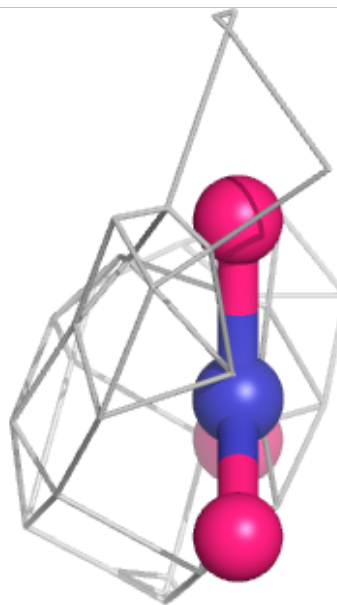
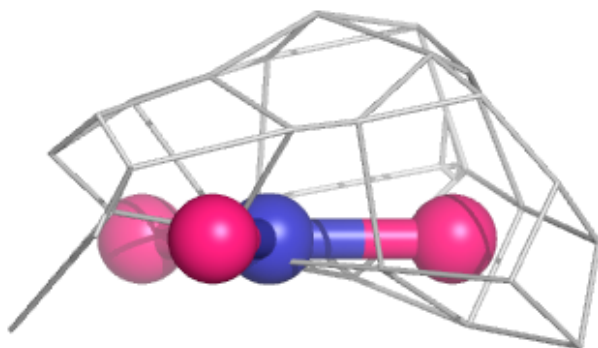
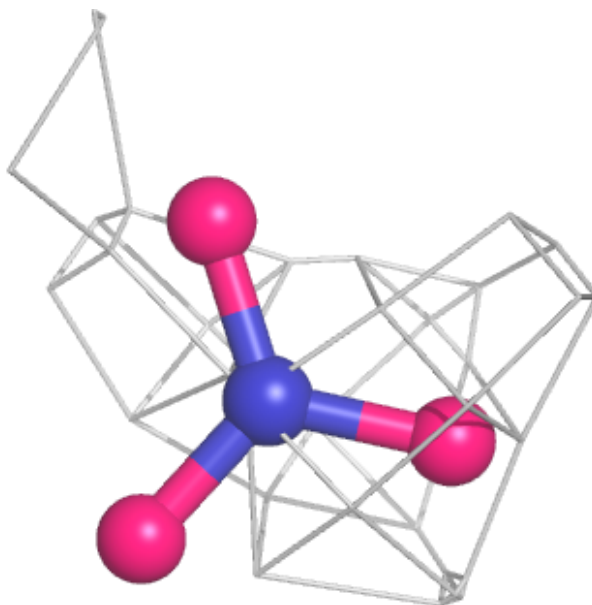
**Electron density around NO3 I 604:**

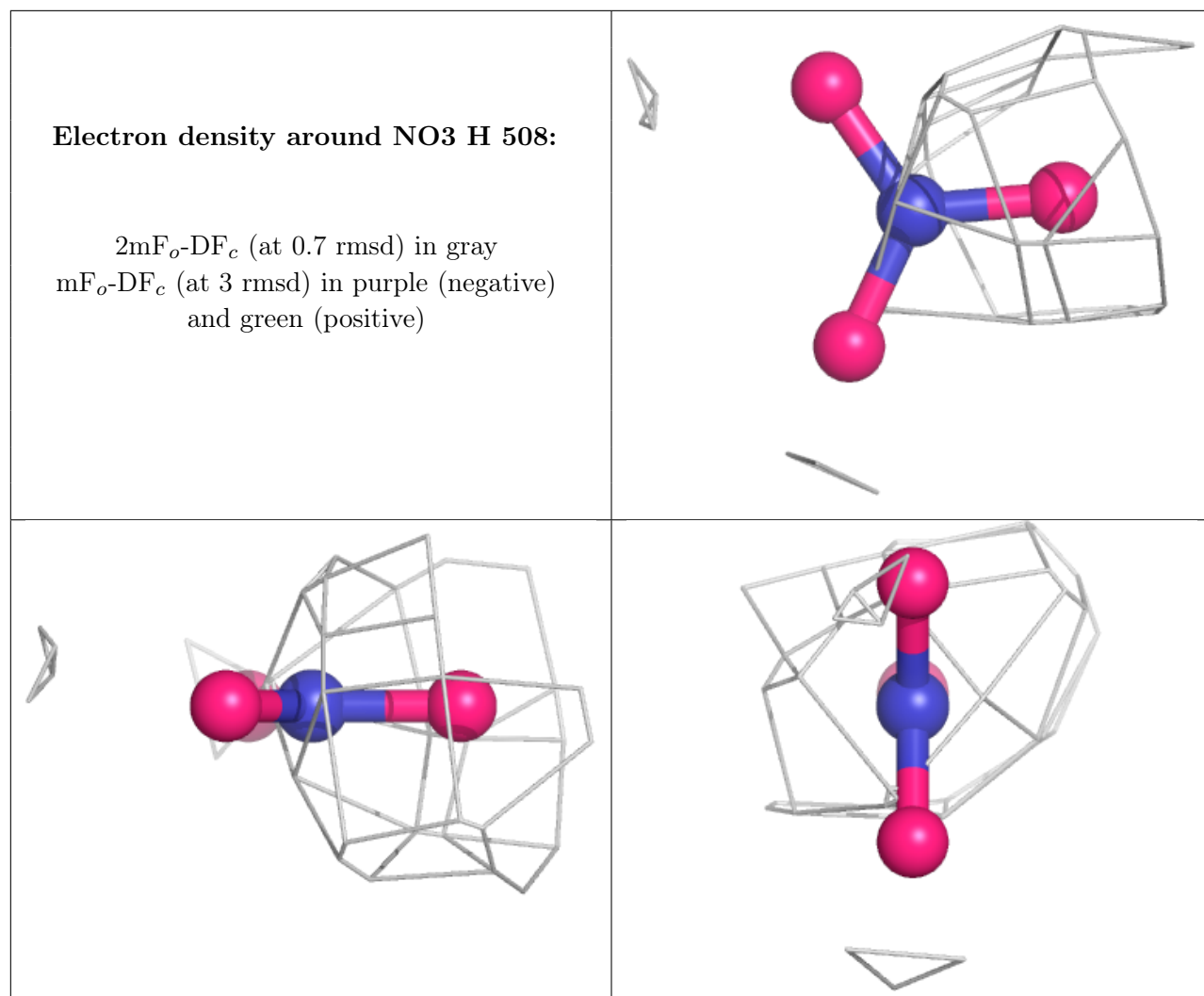
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NO3 H 507:**

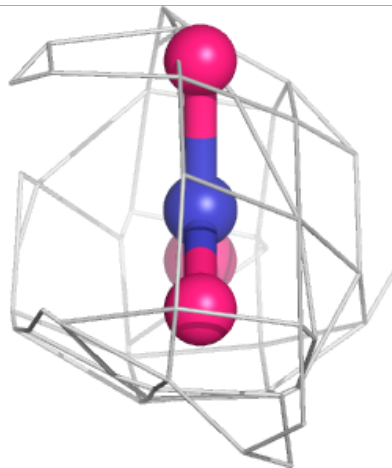
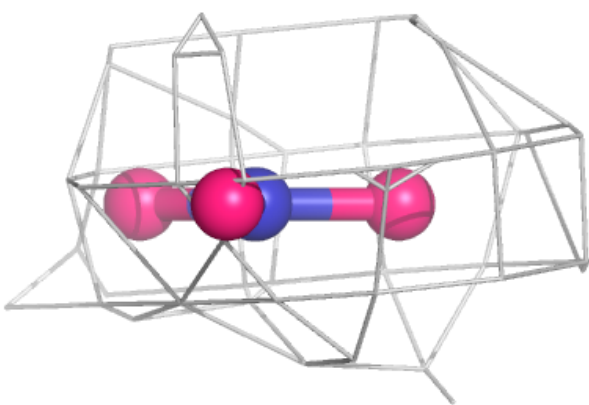
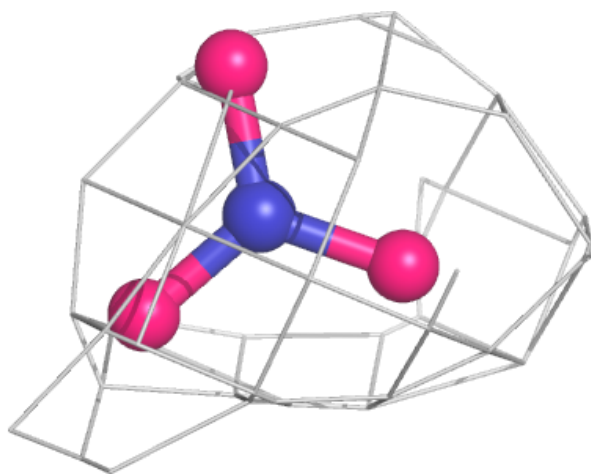
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





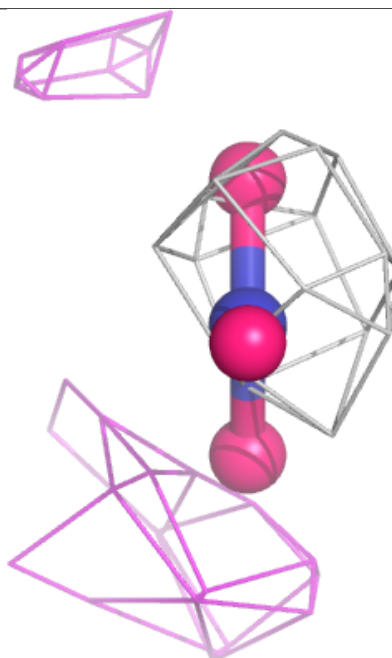
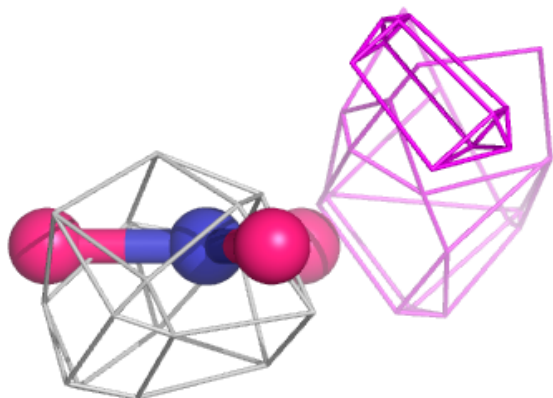
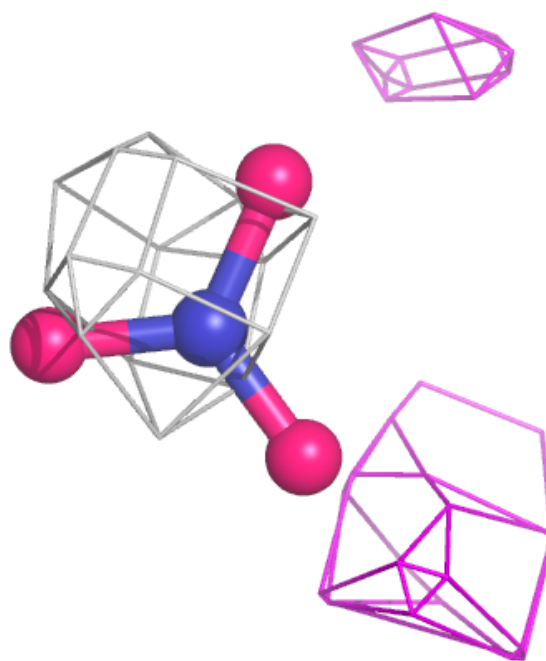
**Electron density around NO3 II 202:**

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



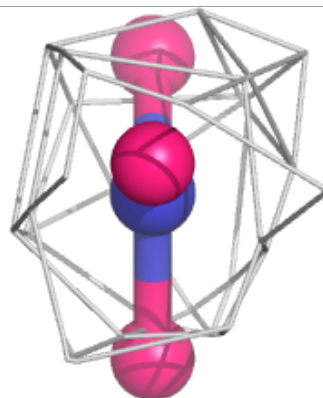
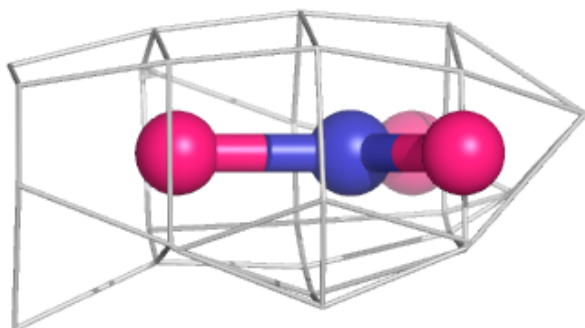
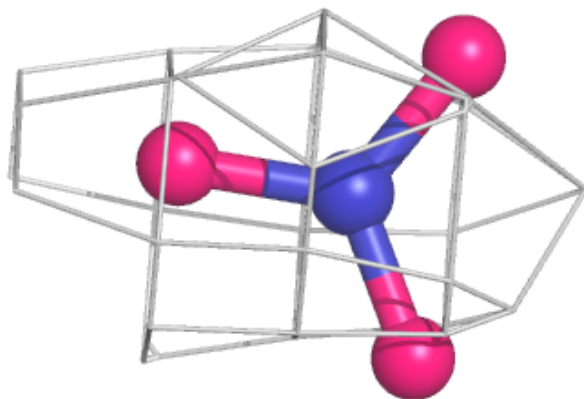
**Electron density around NO3 D 302:**

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



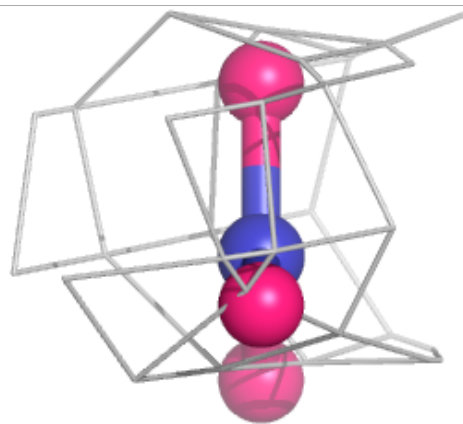
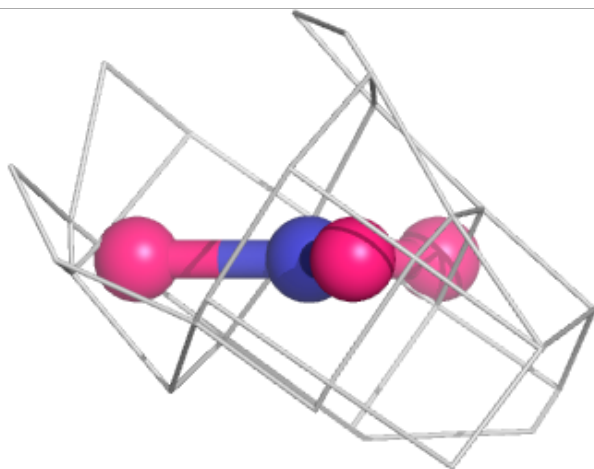
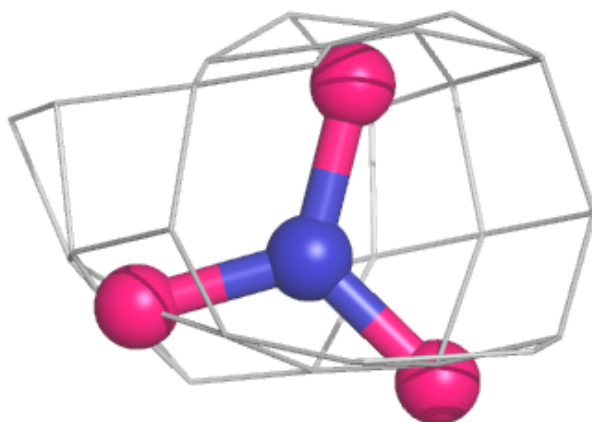
**Electron density around NO3 N 1309:**

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



**Electron density around NO3 GG 205:**

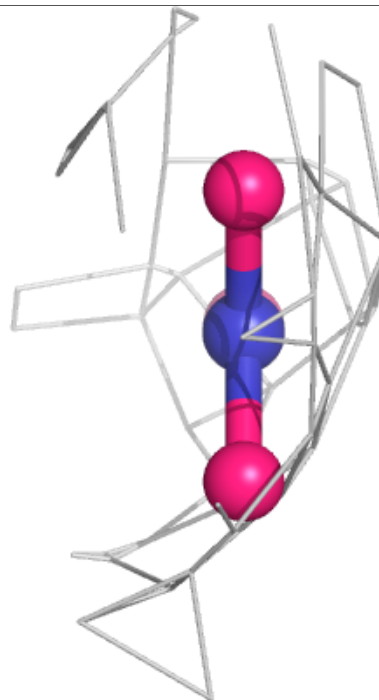
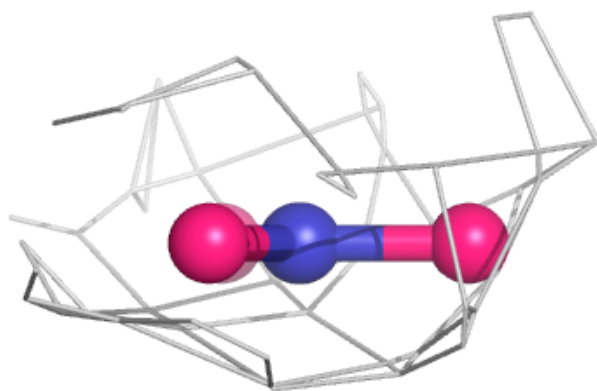
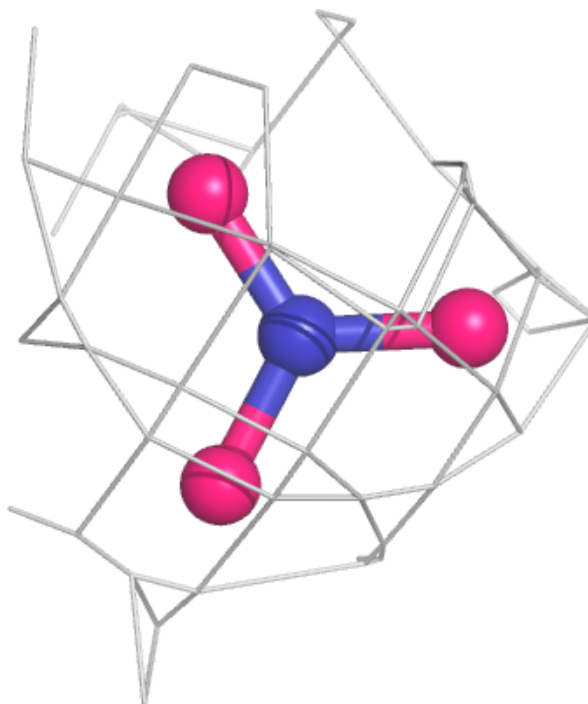
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





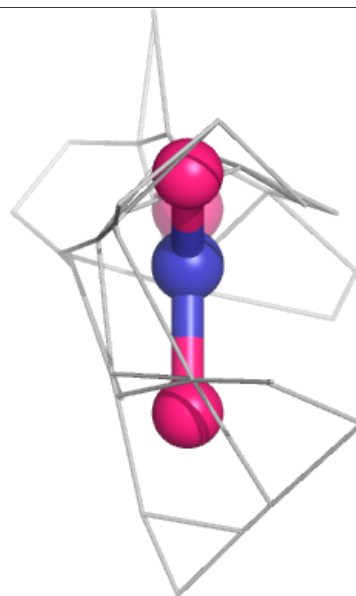
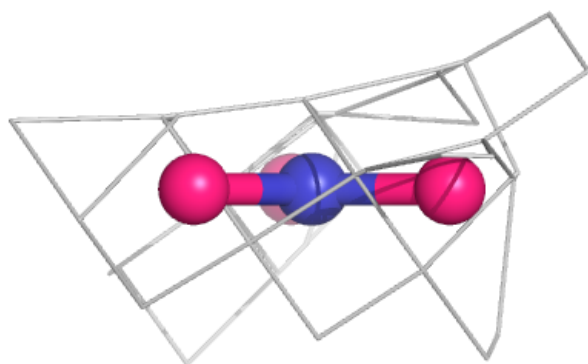
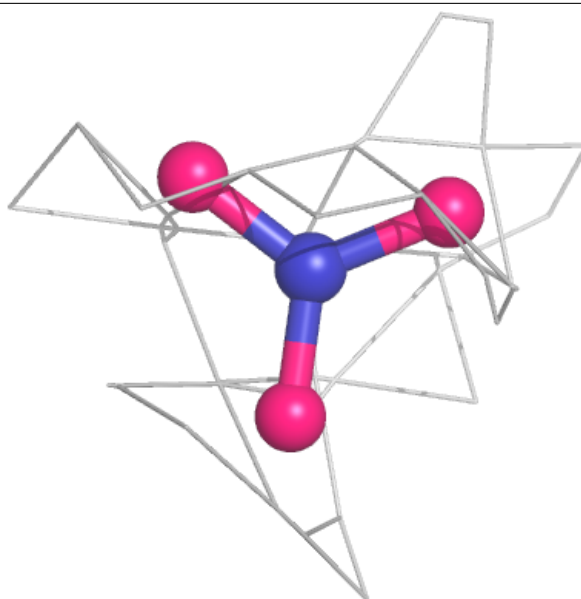
**Electron density around NO3 L 507:**

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



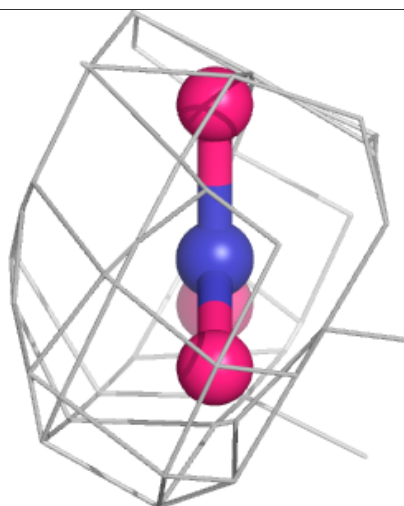
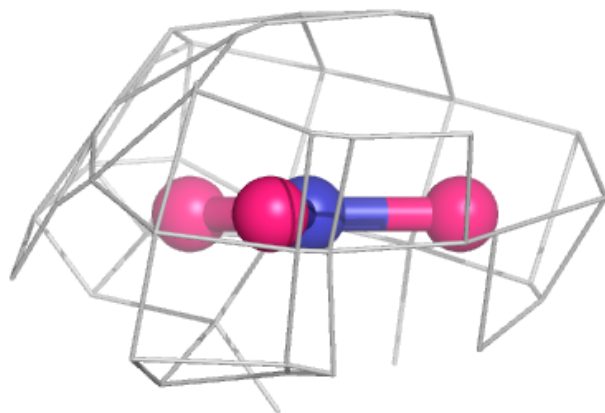
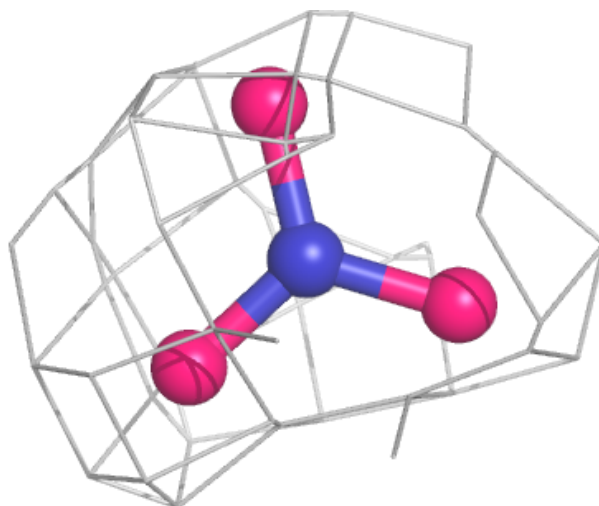
**Electron density around NO3 N 1305:**

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



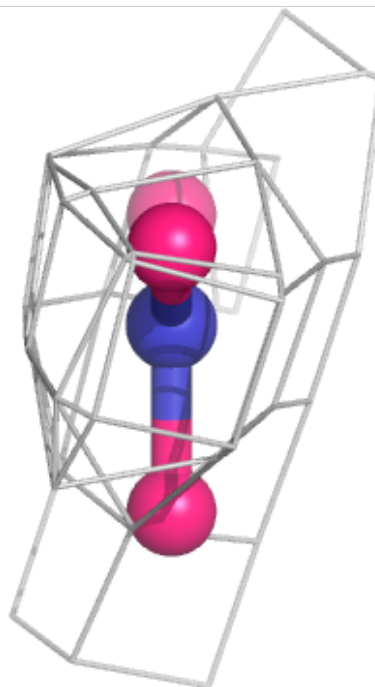
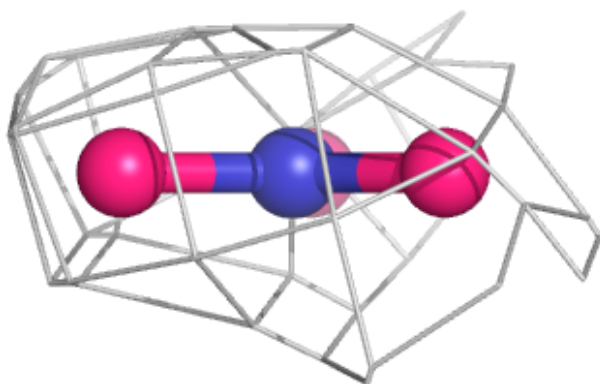
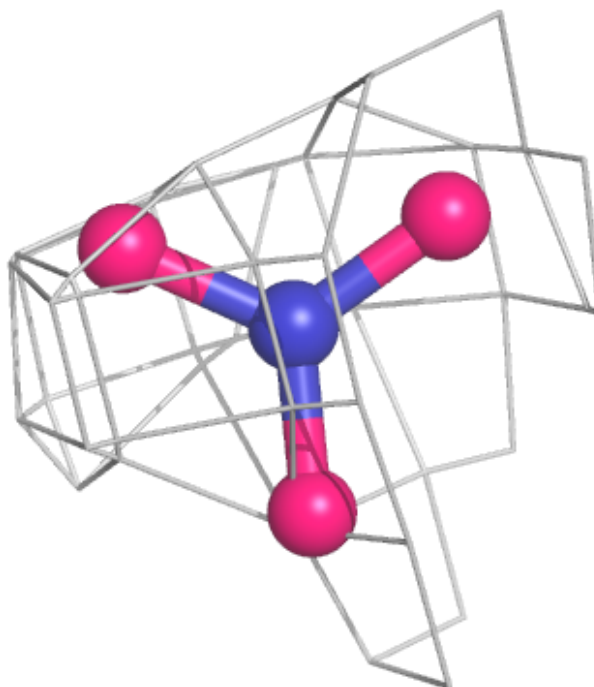
**Electron density around NO3 M 506:**

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



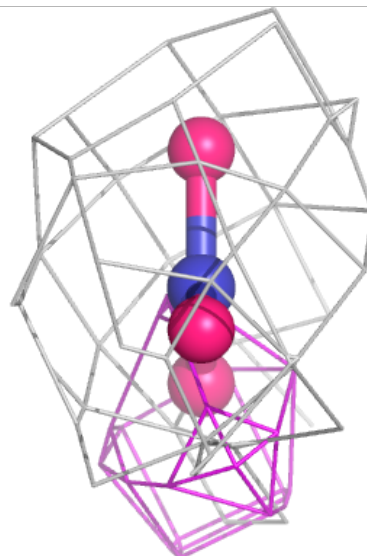
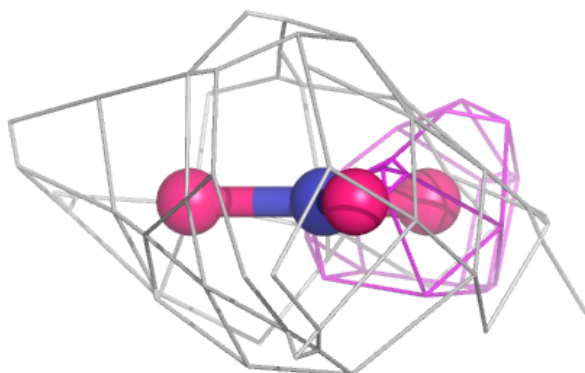
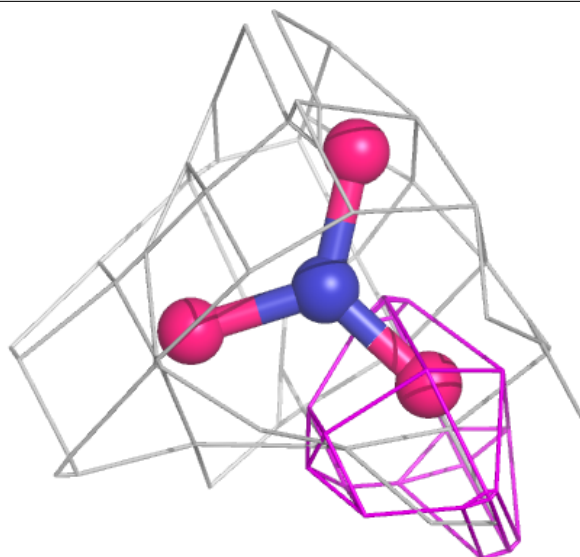
**Electron density around NO3 M 510:**

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



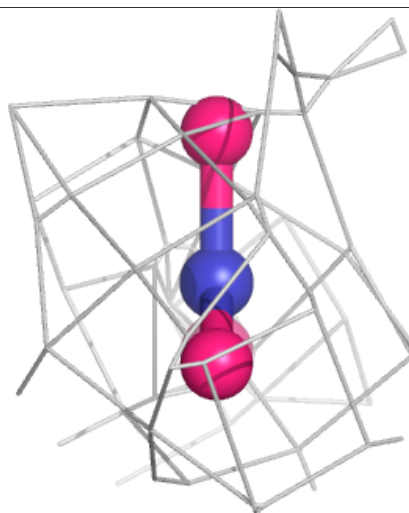
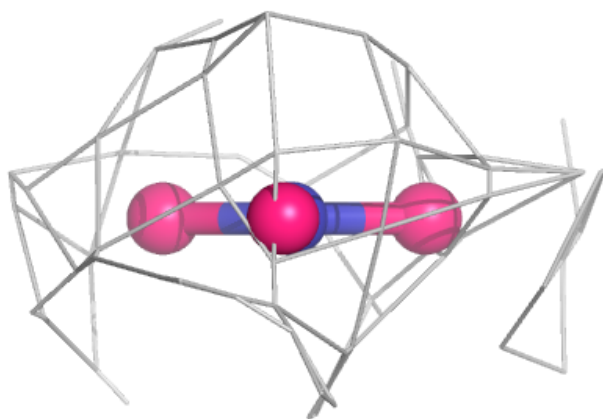
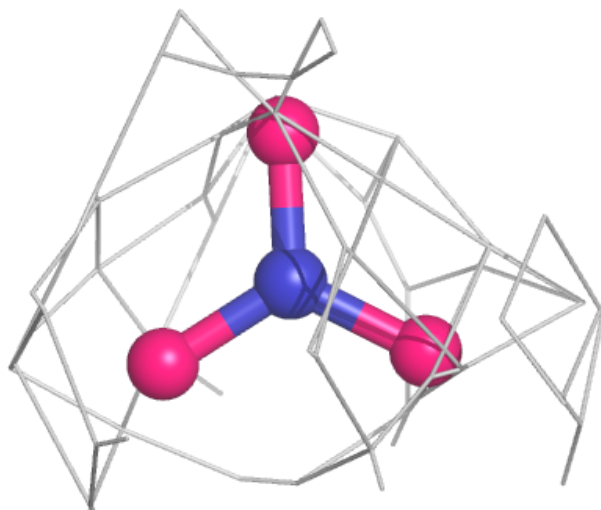
**Electron density around NO3 G 502:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



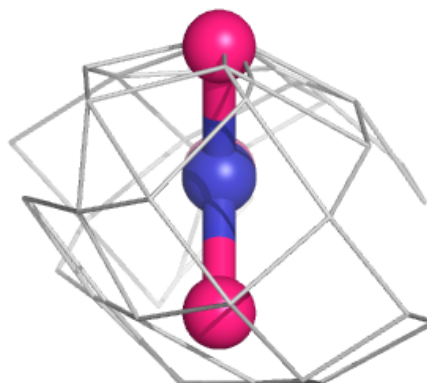
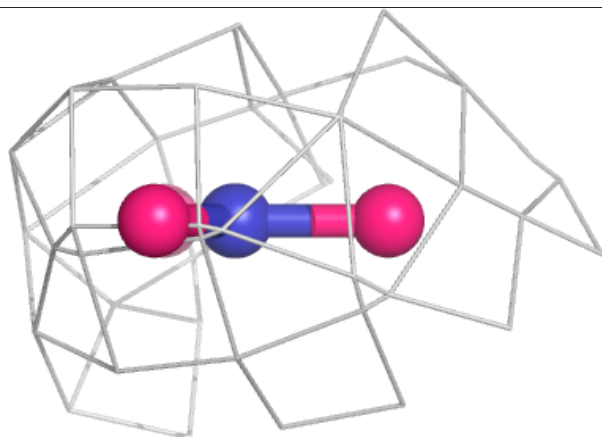
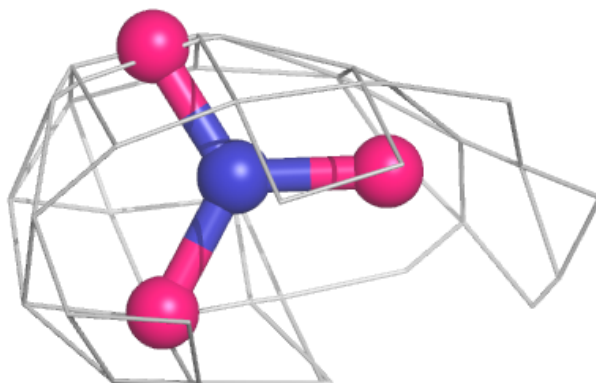
**Electron density around NO3 KK 201:**

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



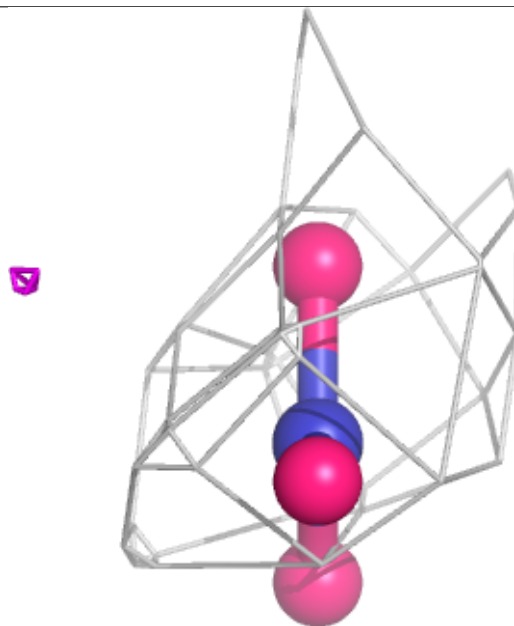
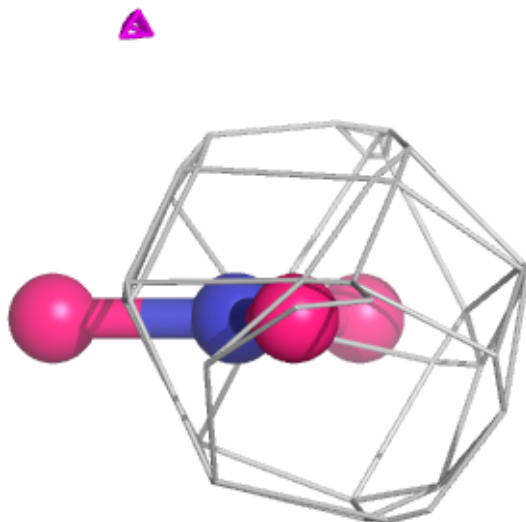
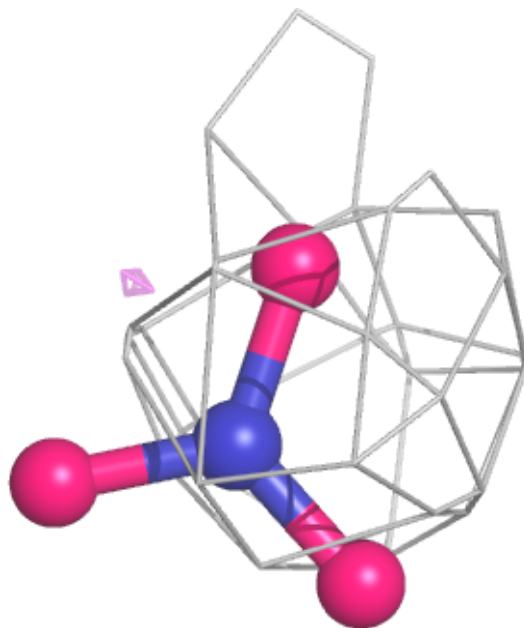
**Electron density around NO3 I 606:**

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



**Electron density around NO3 O 301:**

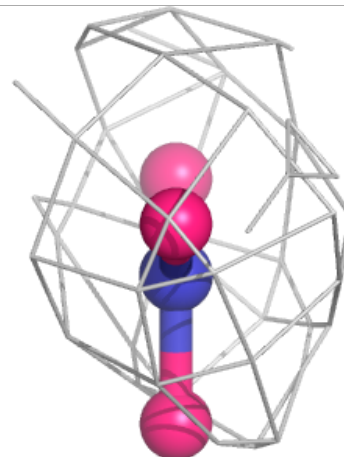
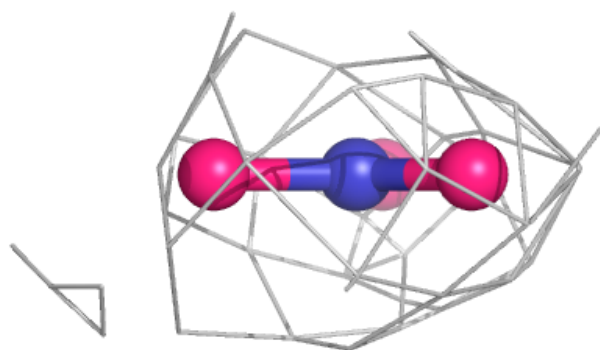
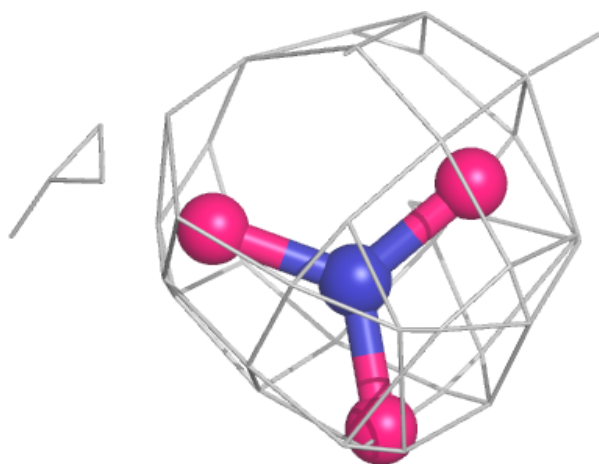
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





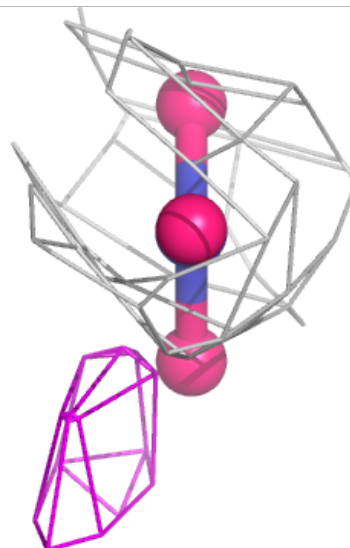
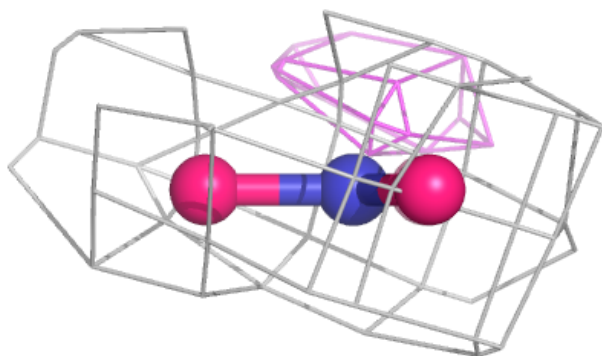
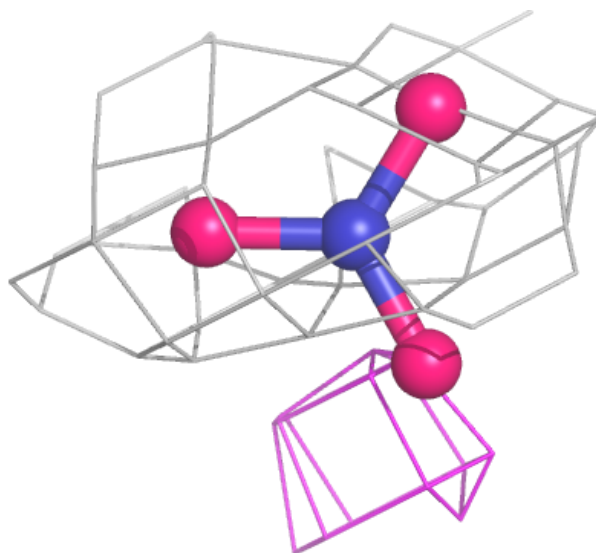
**Electron density around NO3 GG 204:**

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



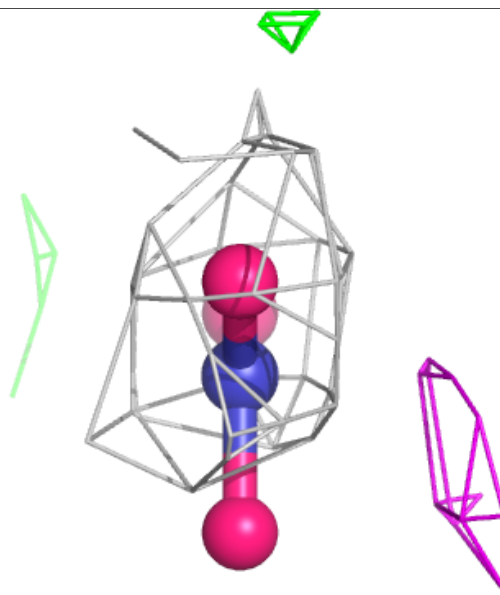
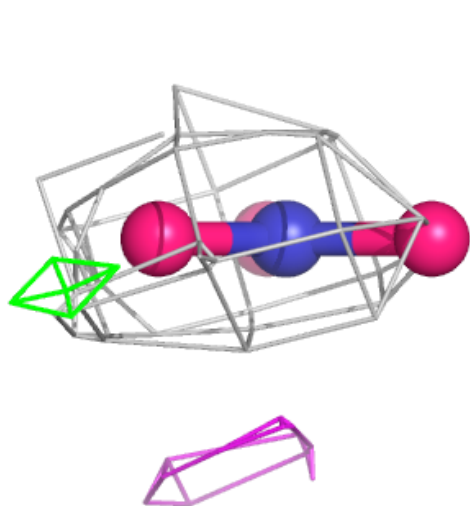
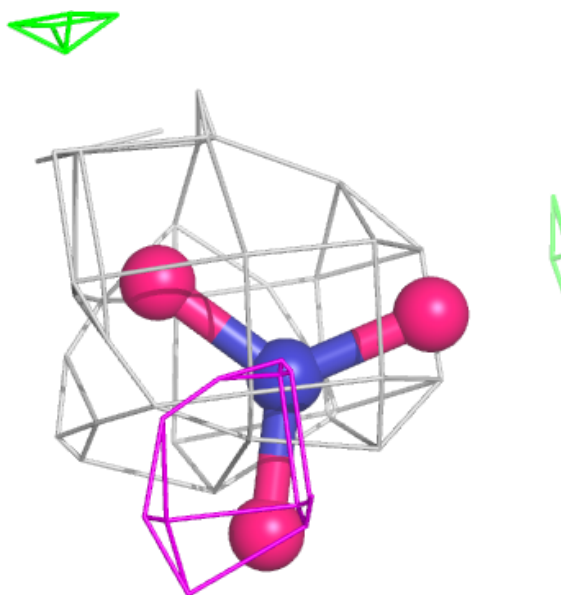
**Electron density around NO3 M 507:**

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



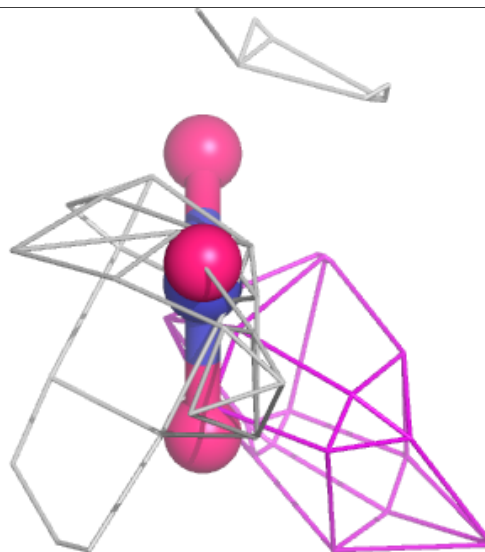
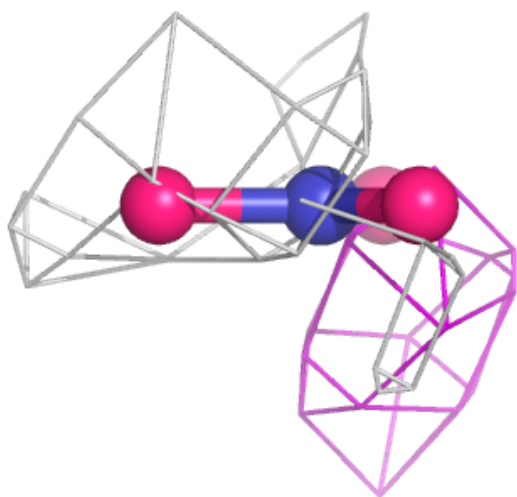
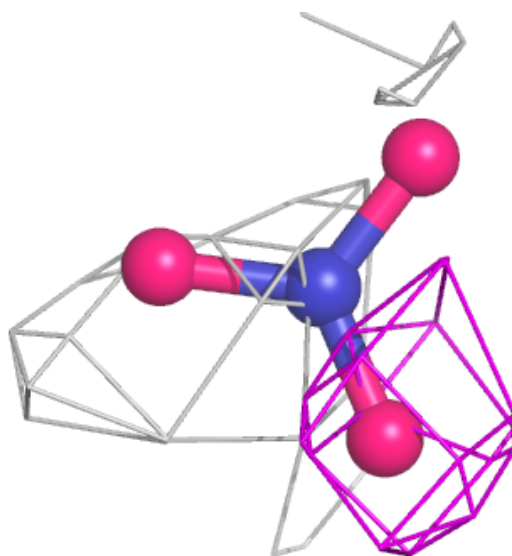
**Electron density around NO3 B 312:**

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



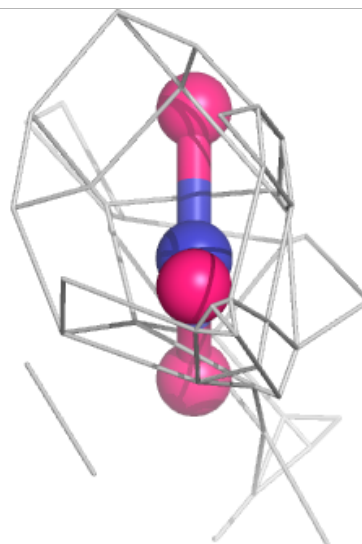
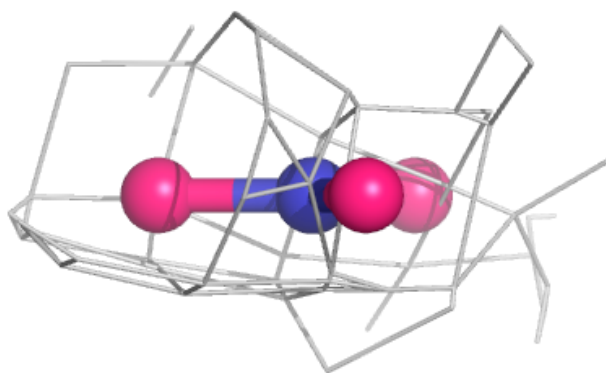
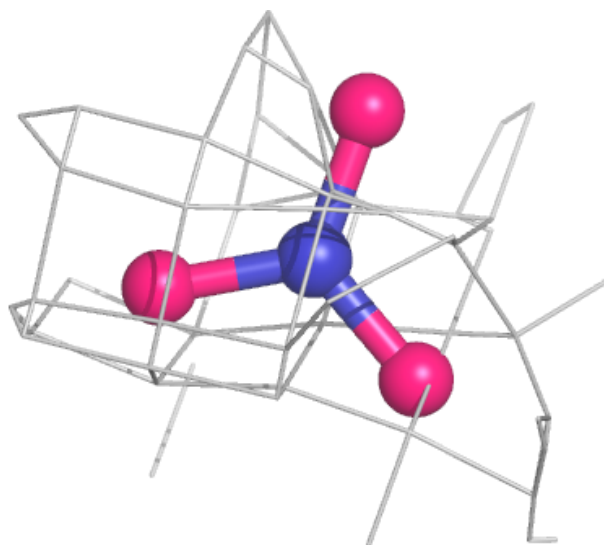
**Electron density around NO3 II 204:**

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



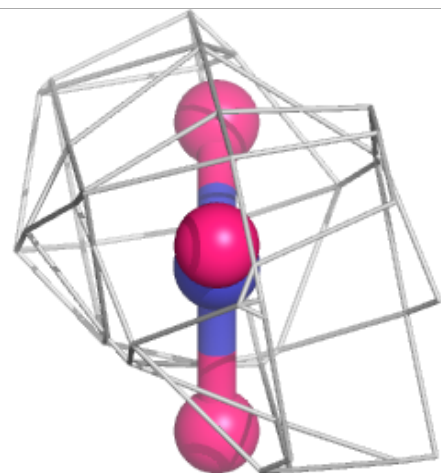
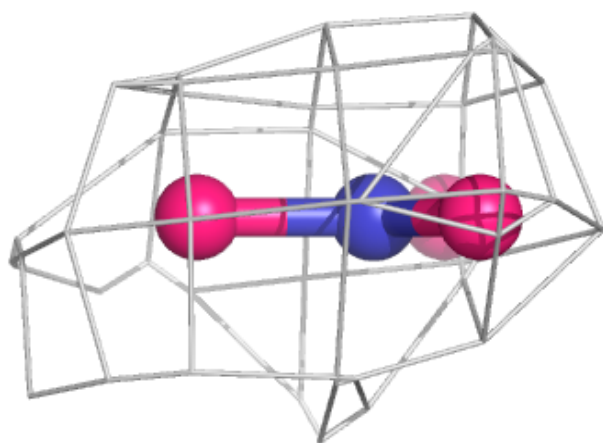
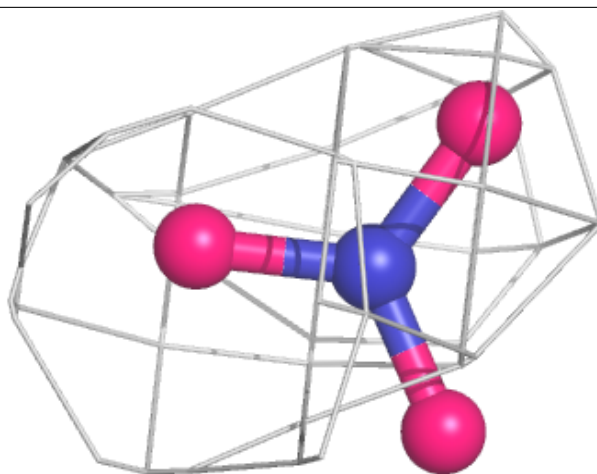
**Electron density around NO3 L 504:**

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



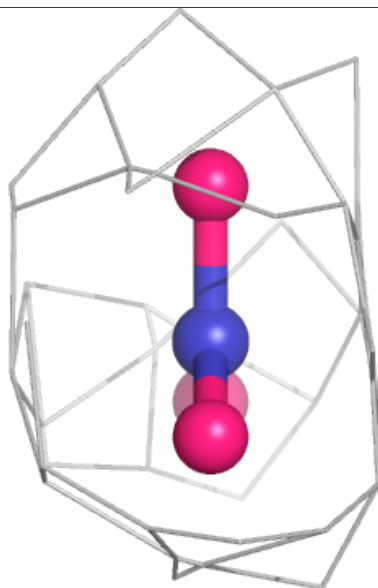
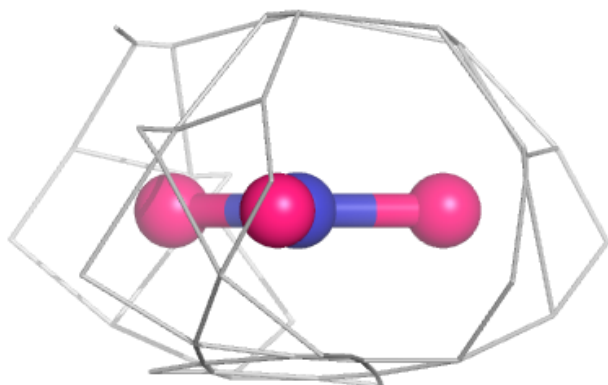
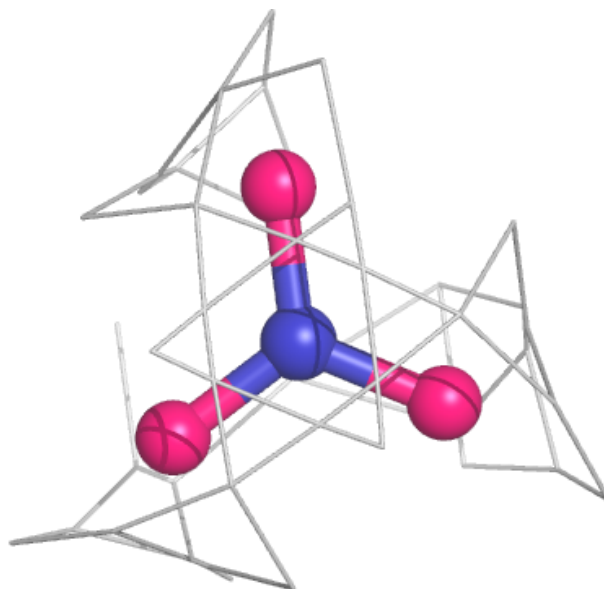
**Electron density around NO3 HH 302:**

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



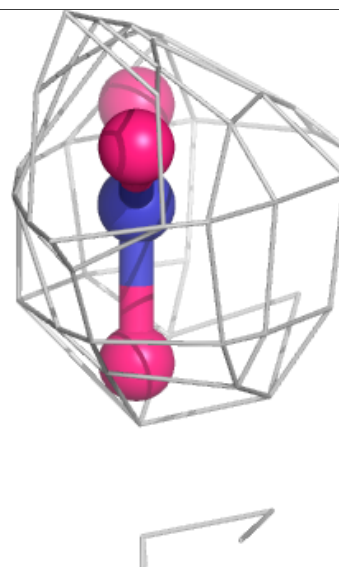
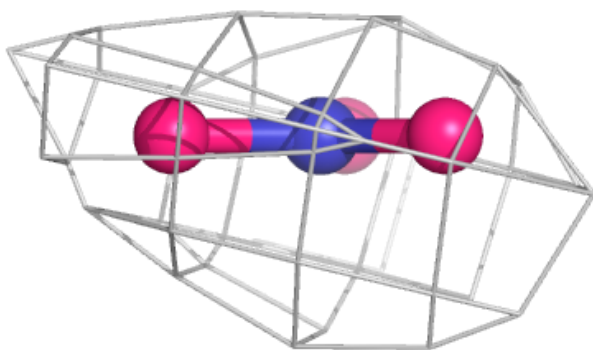
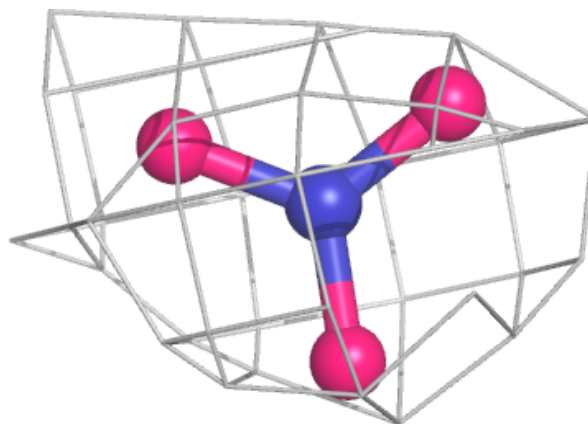
**Electron density around NO3 L 506:**

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



**Electron density around NO3 JJ 202:**

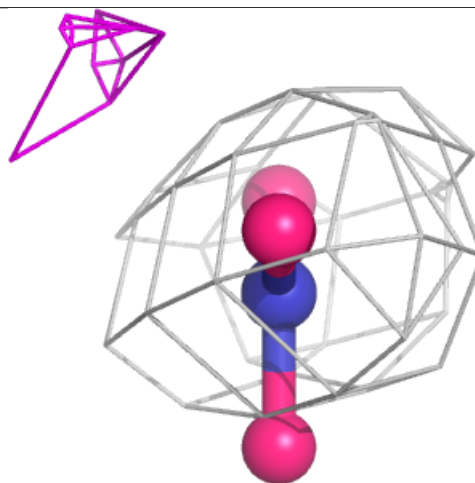
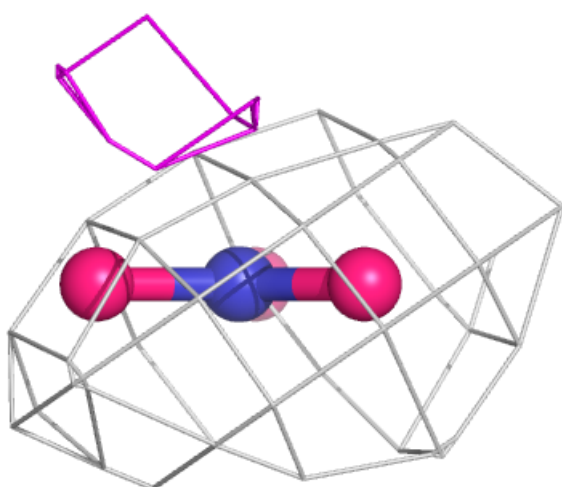
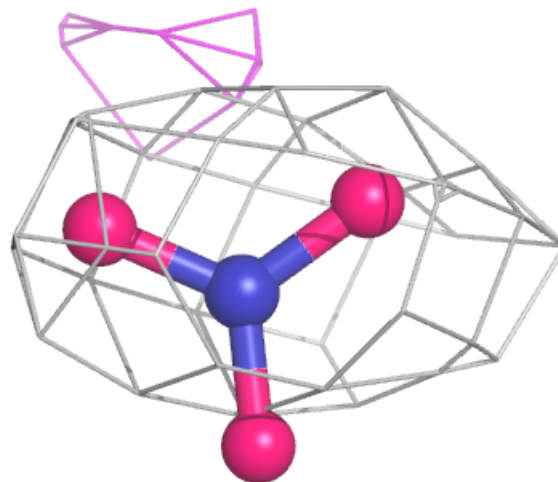
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





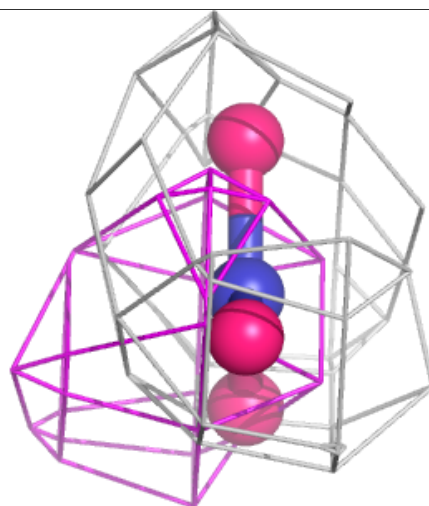
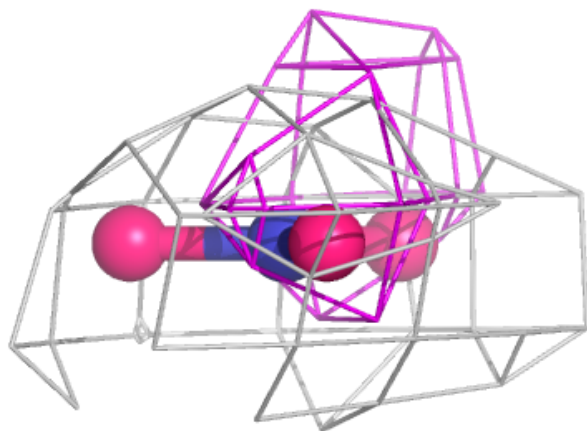
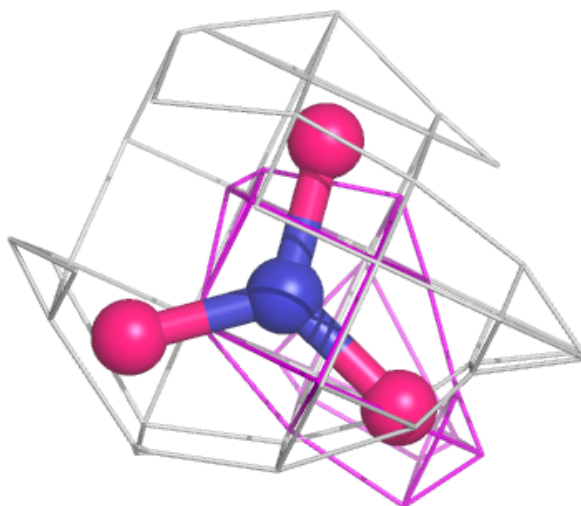
**Electron density around NO3 J 905:**

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



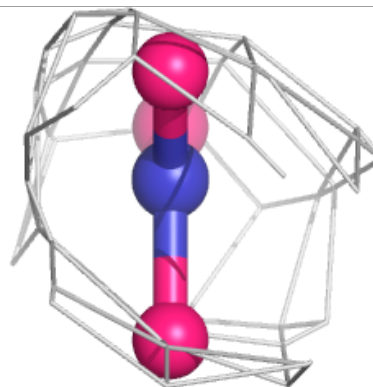
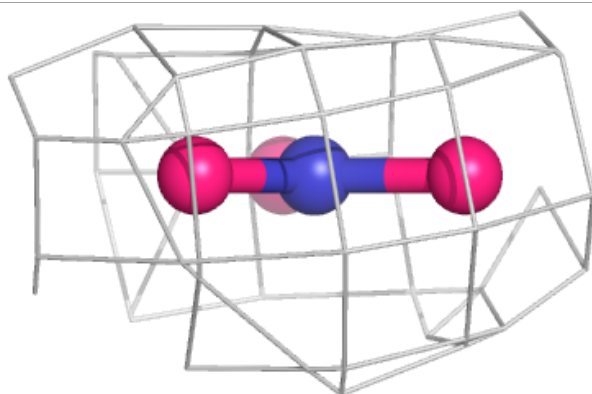
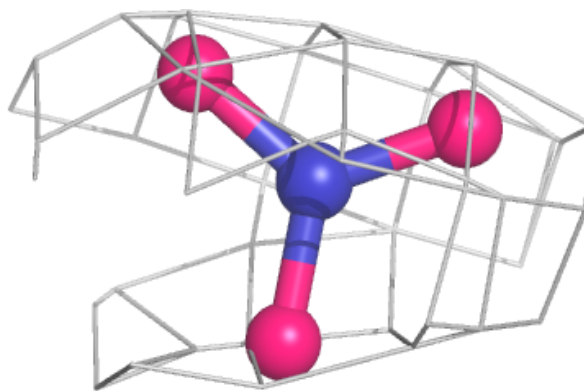
**Electron density around NO3 J 902:**

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

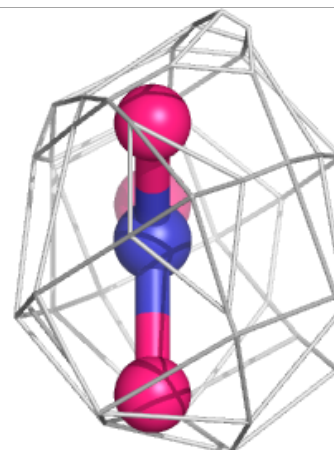
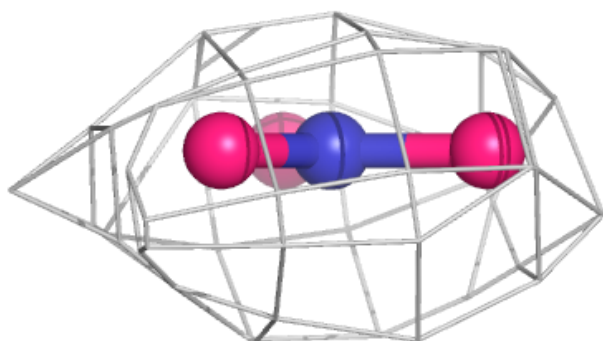
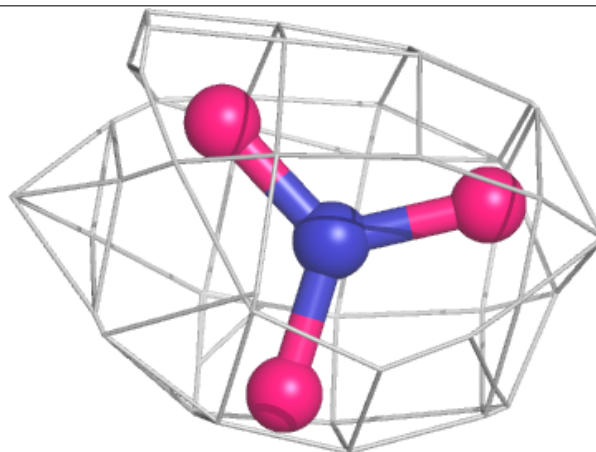


**Electron density around NO3 O 304:**

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

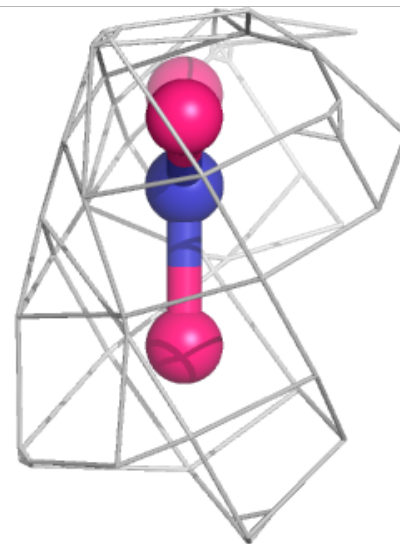
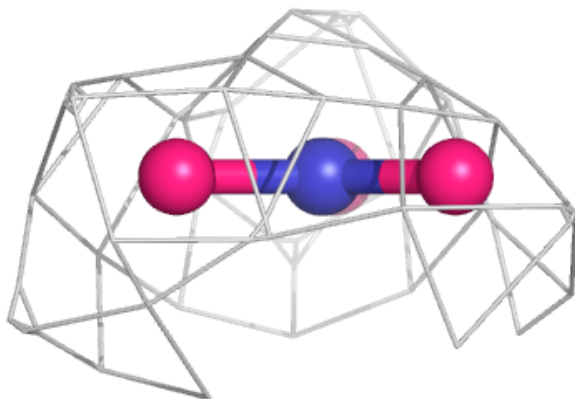
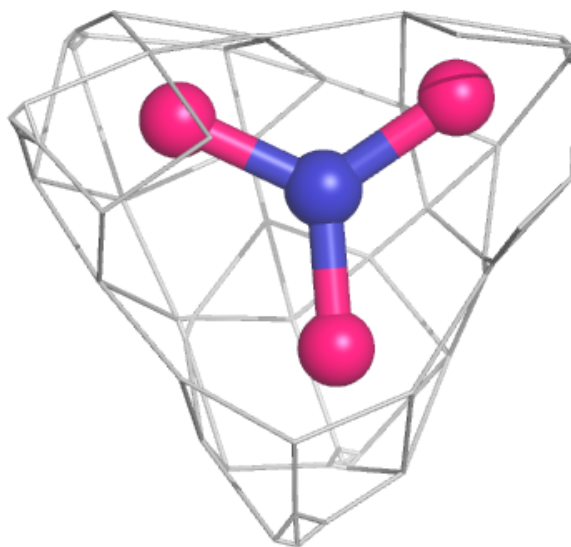
**Electron density around NO3 GG 203:**

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



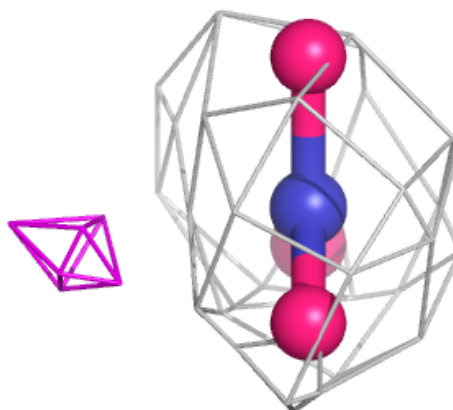
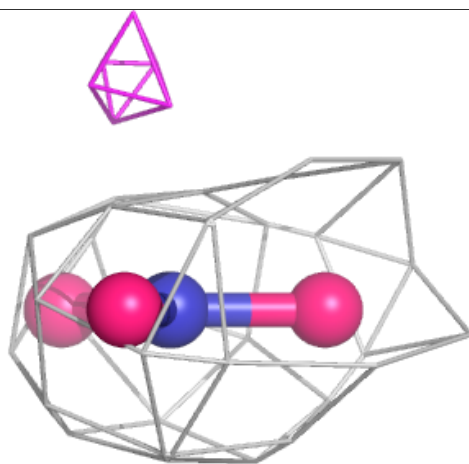
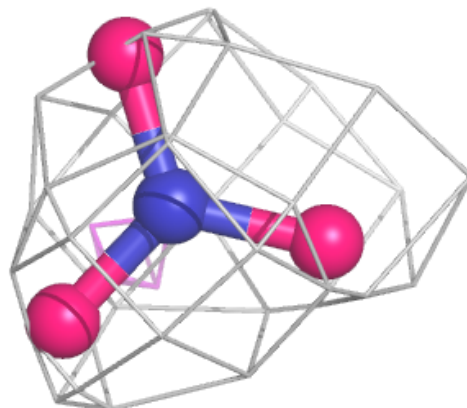
**Electron density around NO3 L 505:**

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



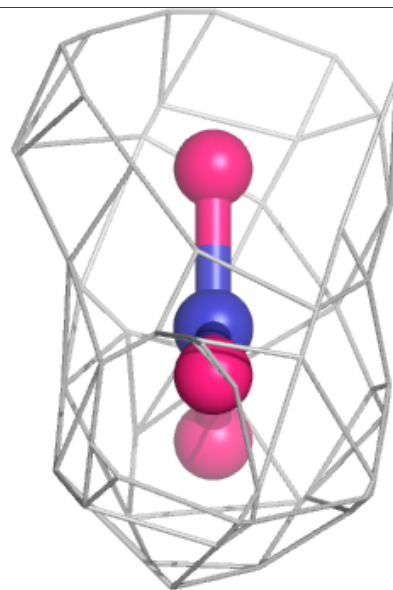
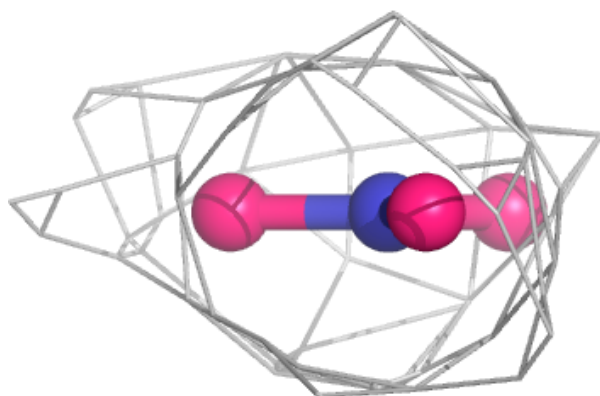
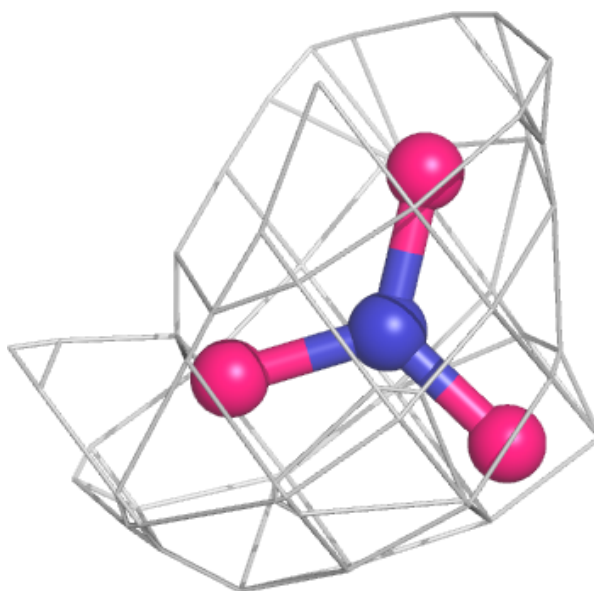
**Electron density around NO3 G 501:**

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



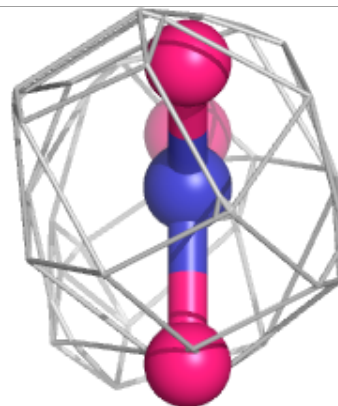
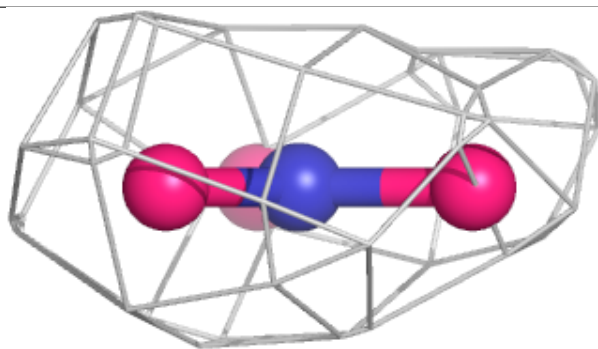
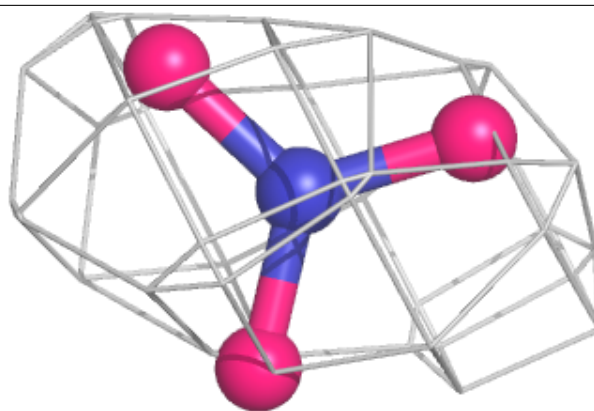
**Electron density around NO3 B 308:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

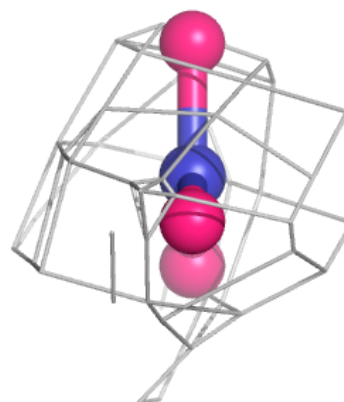
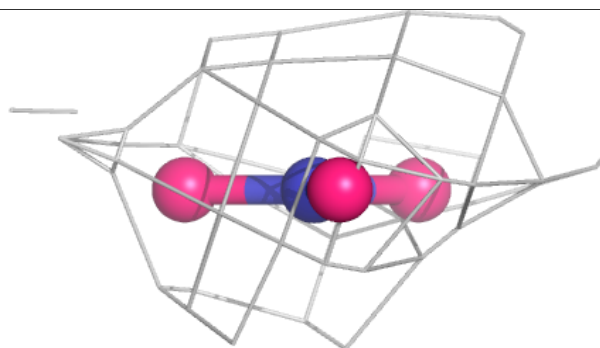
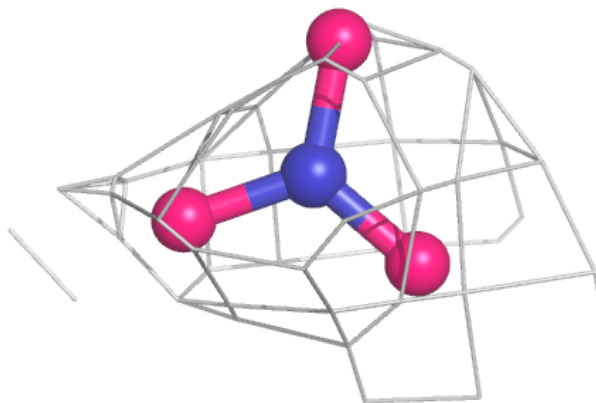


**Electron density around NO3 B 306:**

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

**Electron density around NO3 HH 304:**

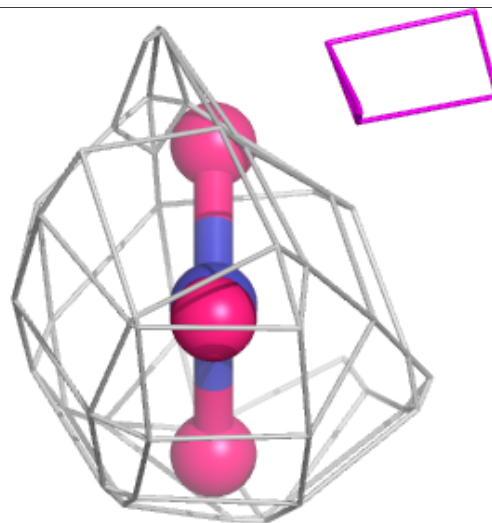
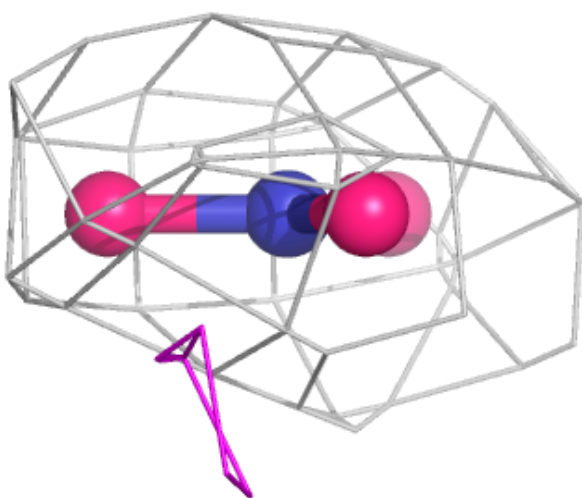
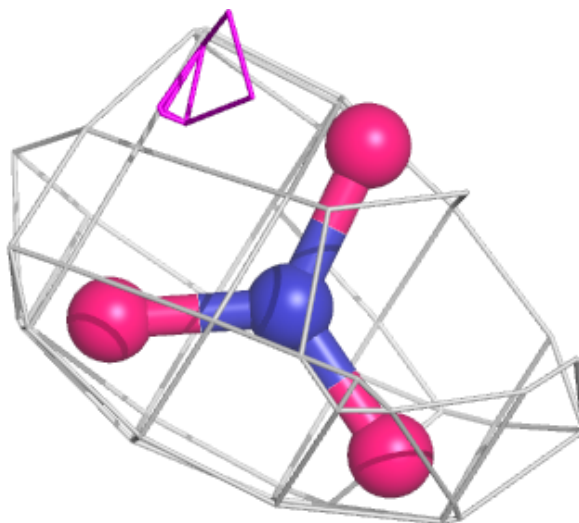
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around NO3 N 1308:**

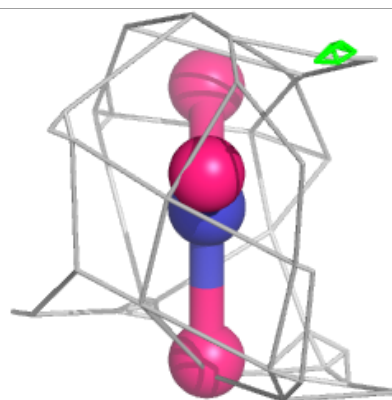
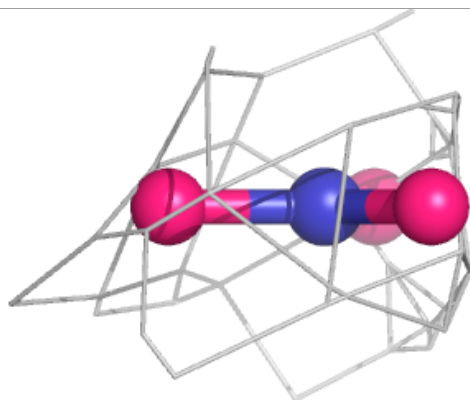
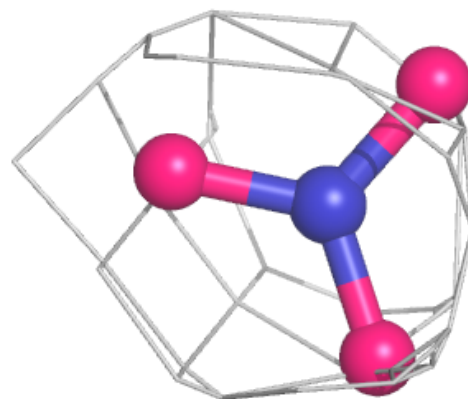
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





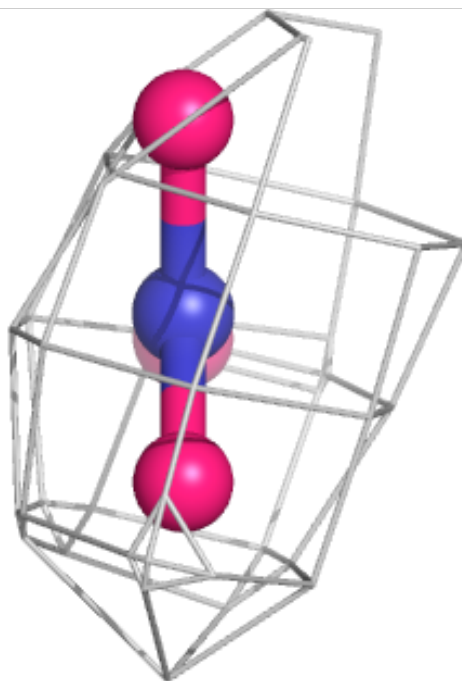
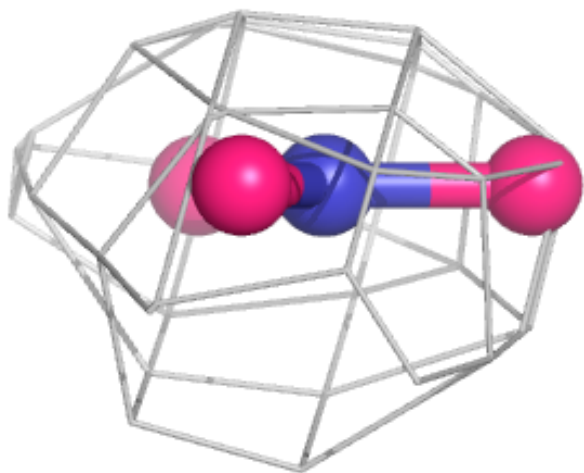
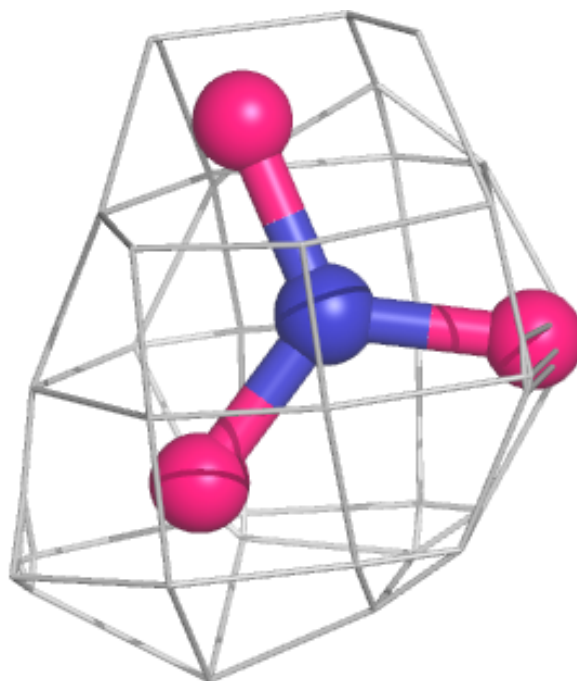
**Electron density around NO3 M 504:**

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



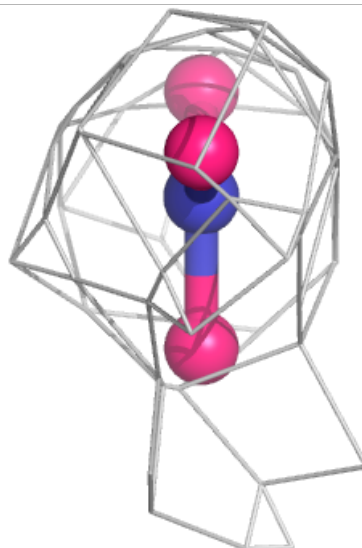
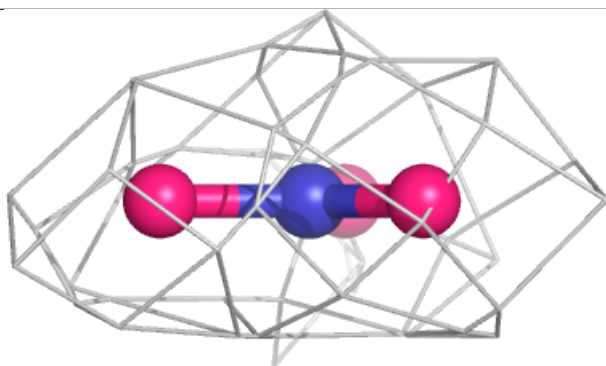
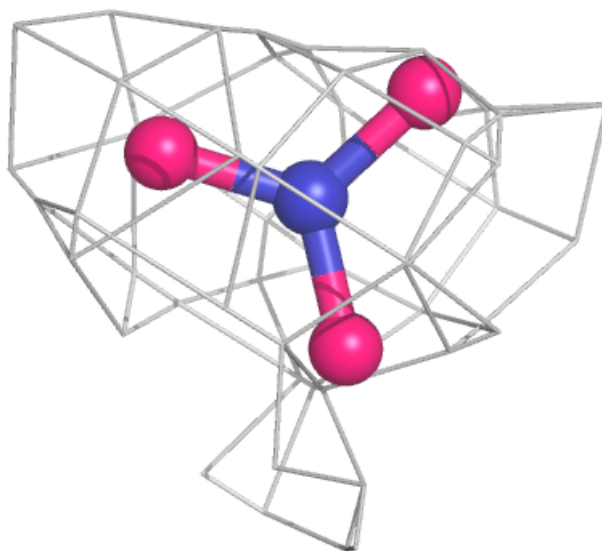
**Electron density around NO3 M 505:**

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



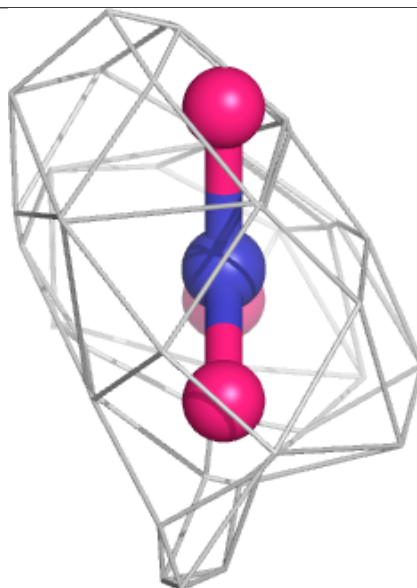
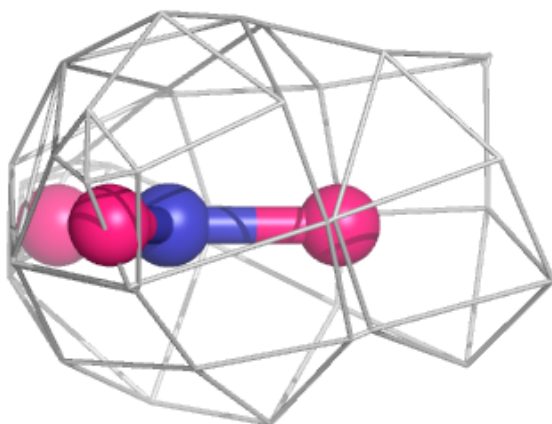
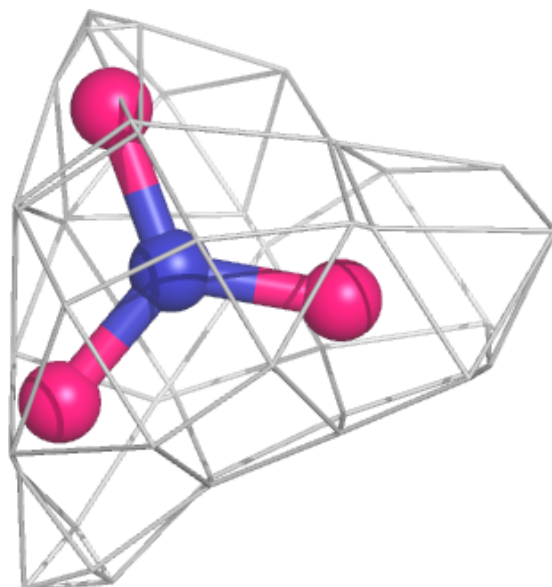
**Electron density around NO3 B 310:**

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



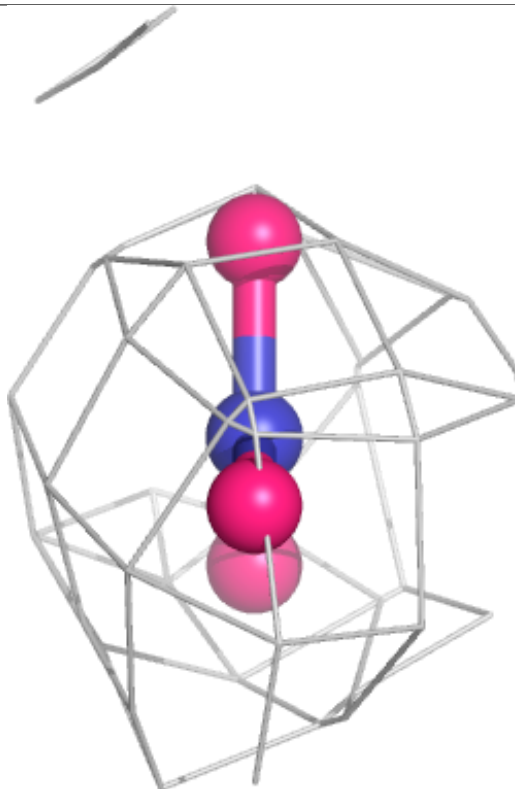
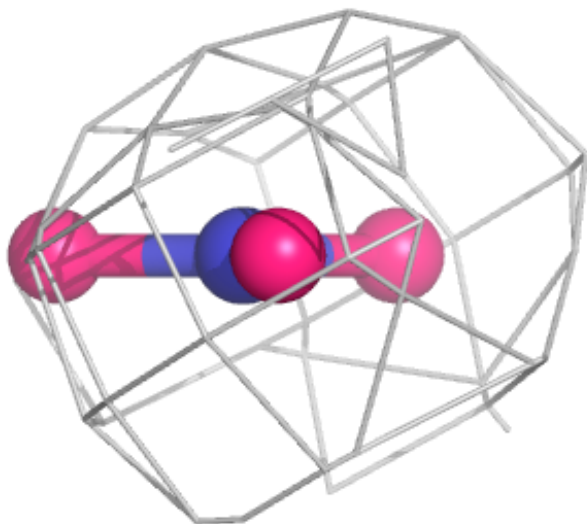
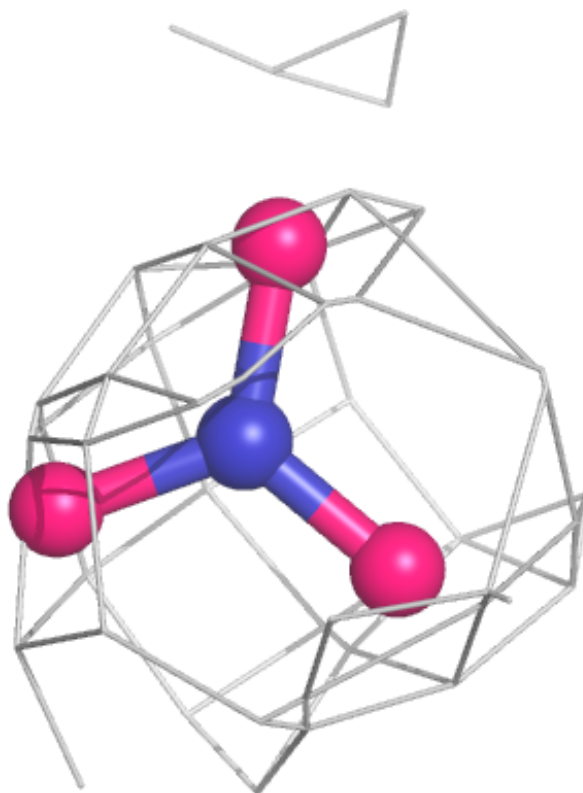
**Electron density around NO3 A 804:**

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



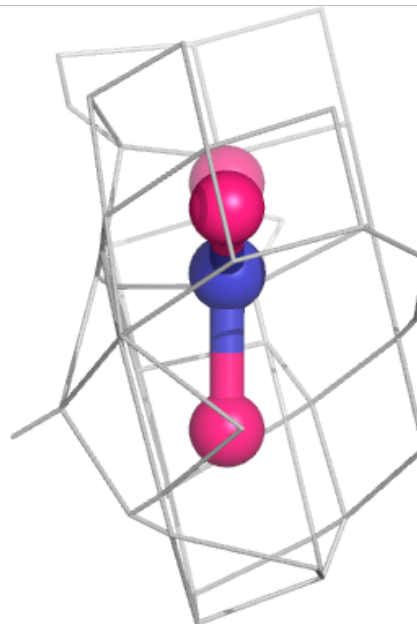
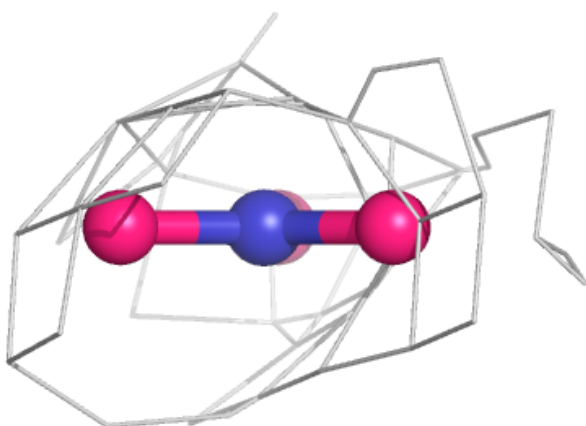
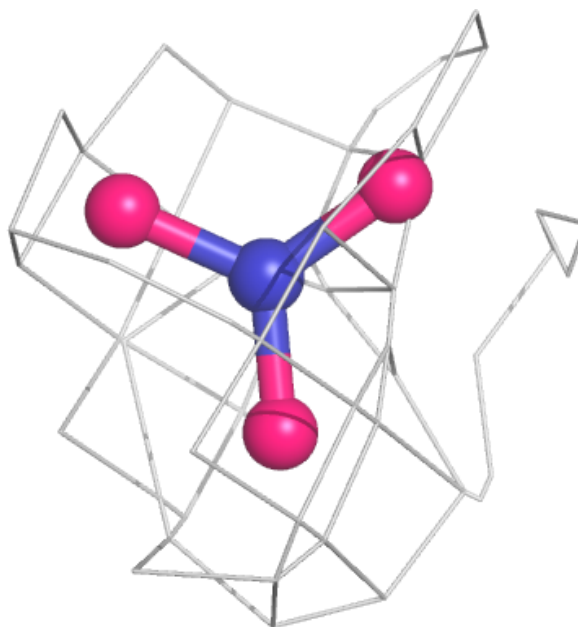
**Electron density around NO3 O 305:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



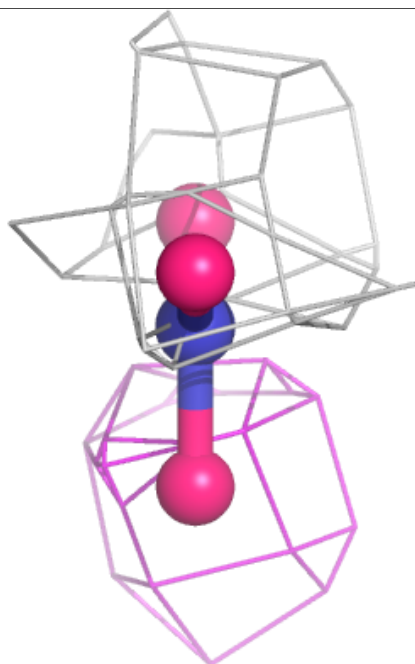
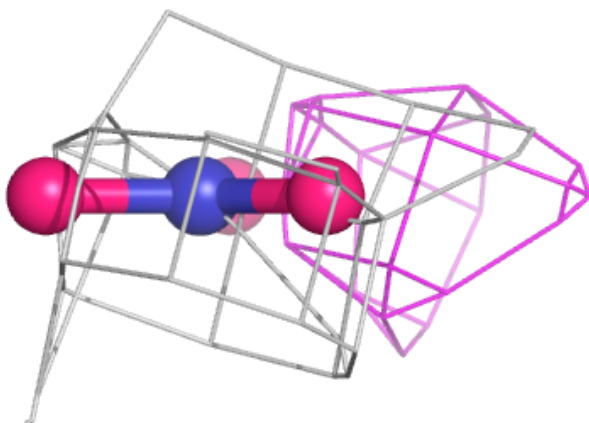
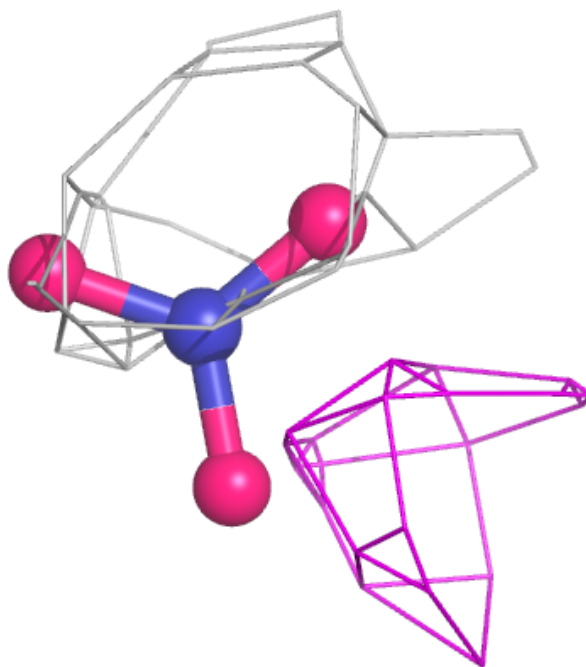
**Electron density around NO3 H 506:**

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



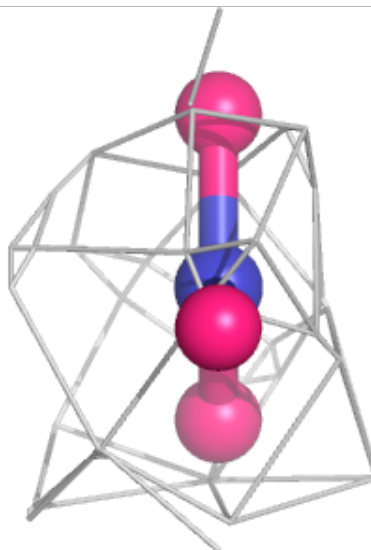
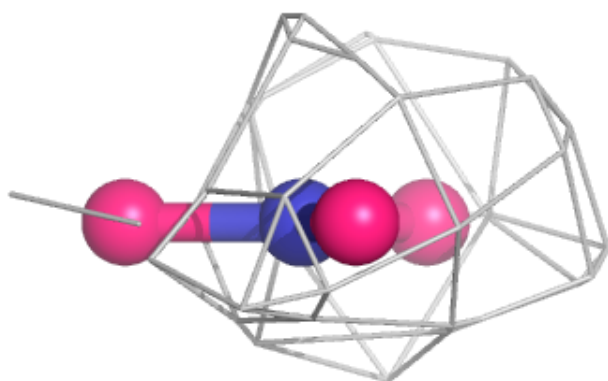
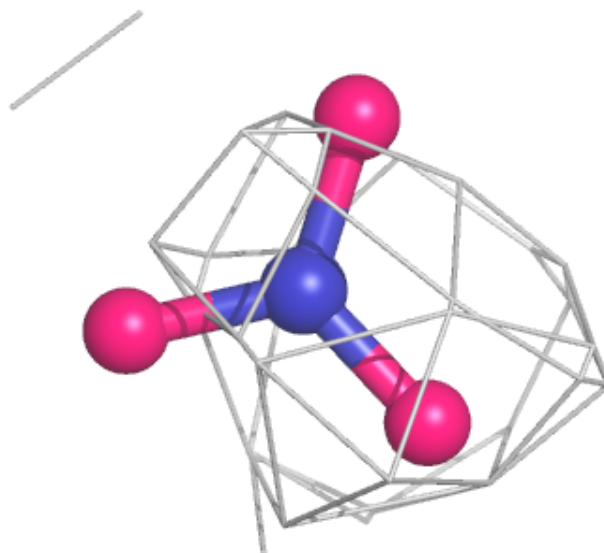
**Electron density around NO3 H 505:**

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



**Electron density around NO3 E 406:**

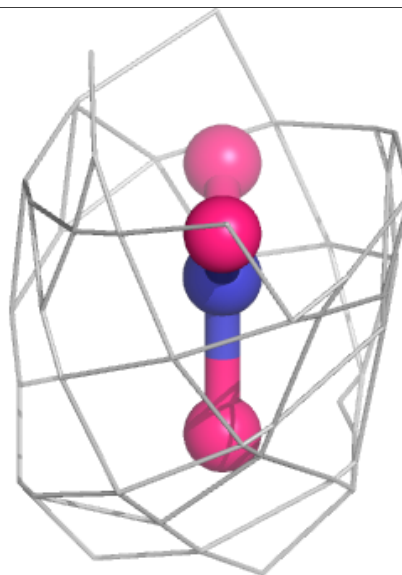
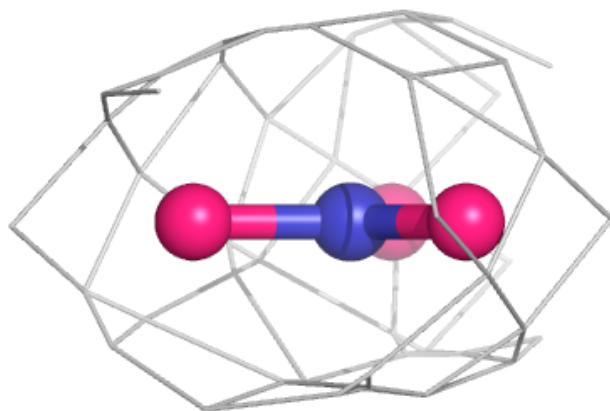
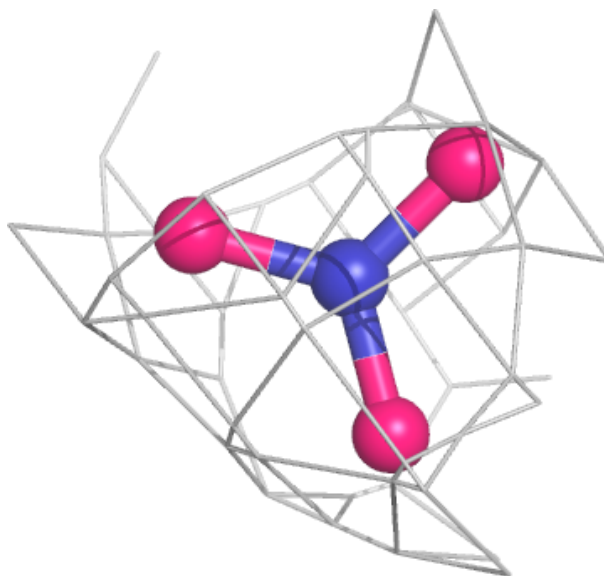
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





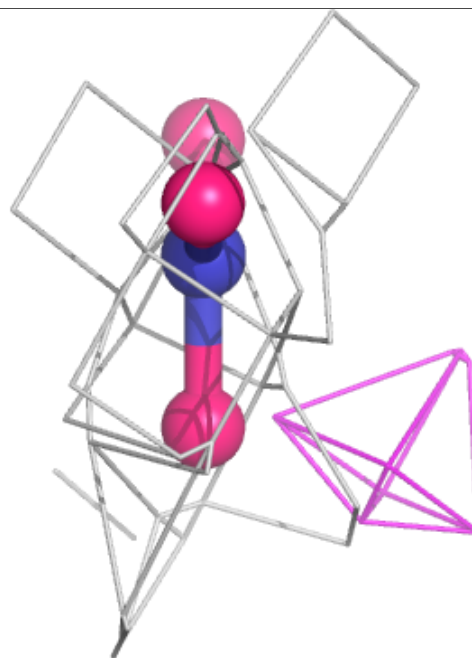
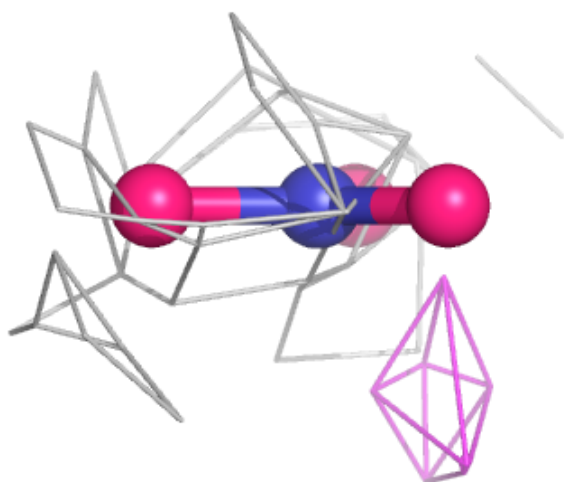
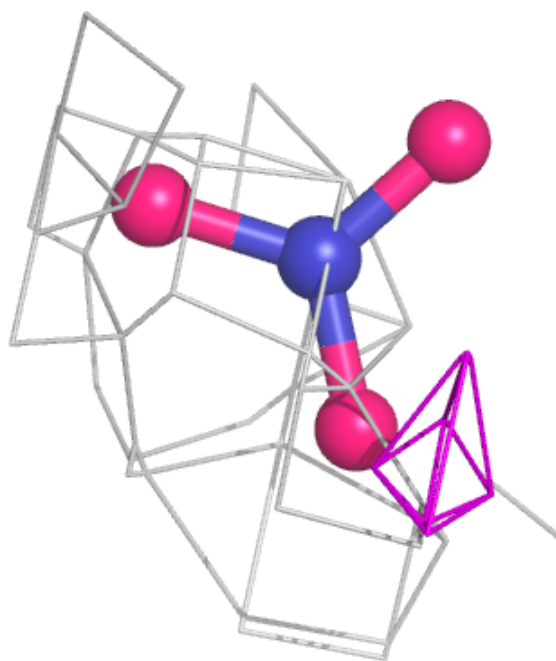
**Electron density around NO3 E 402:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



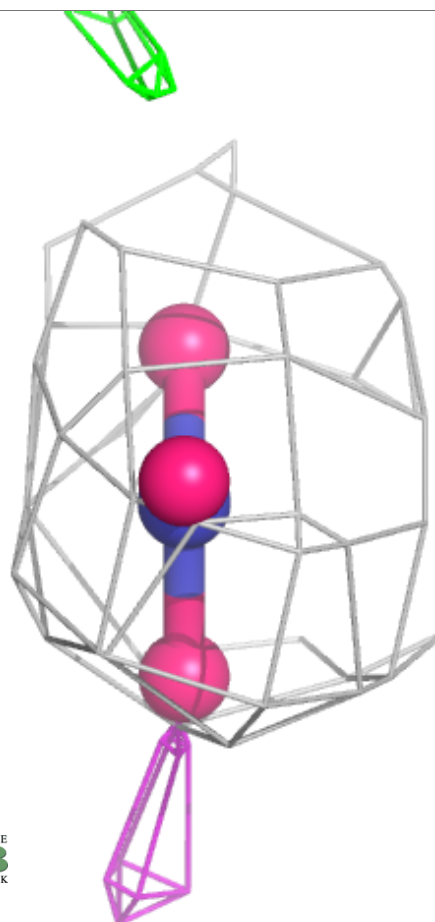
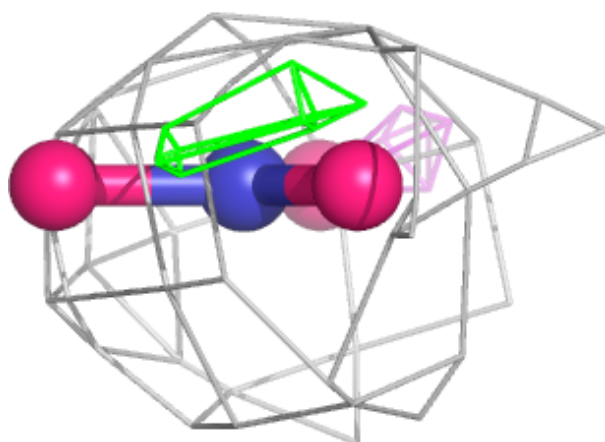
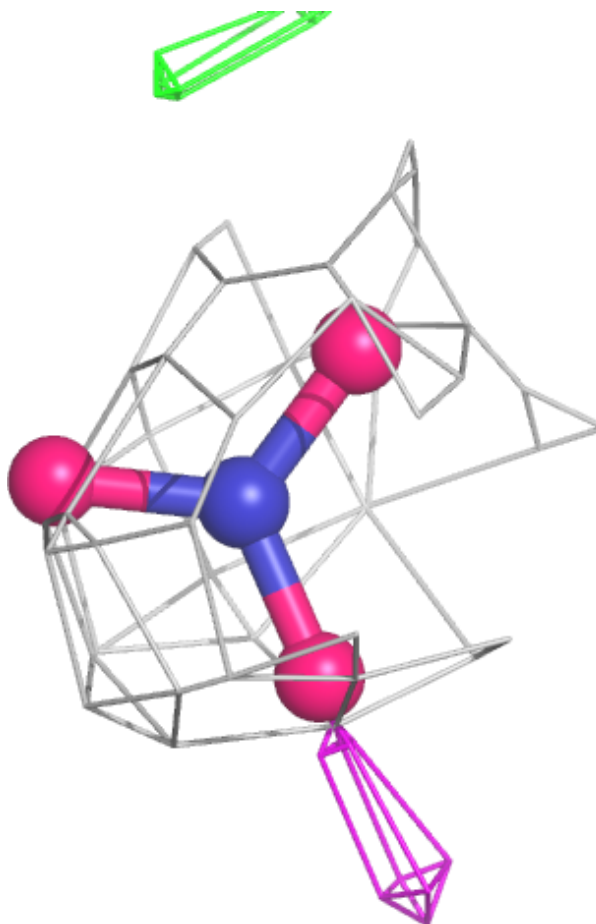
**Electron density around NO3 H 504:**

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



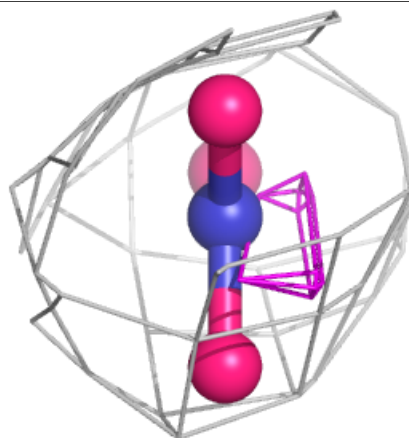
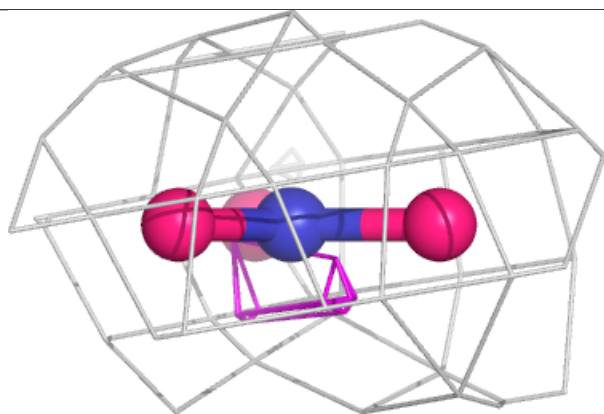
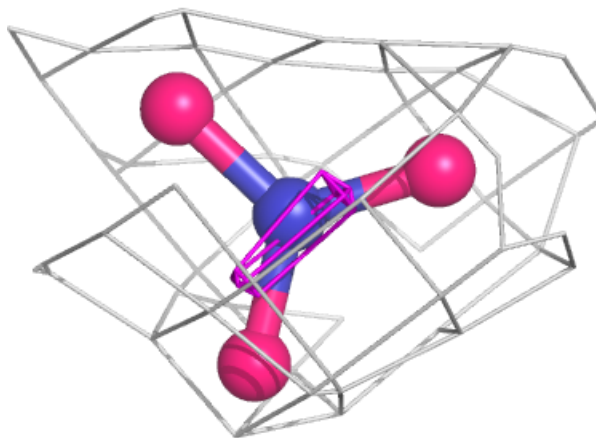
**Electron density around NO3 E 403:**

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



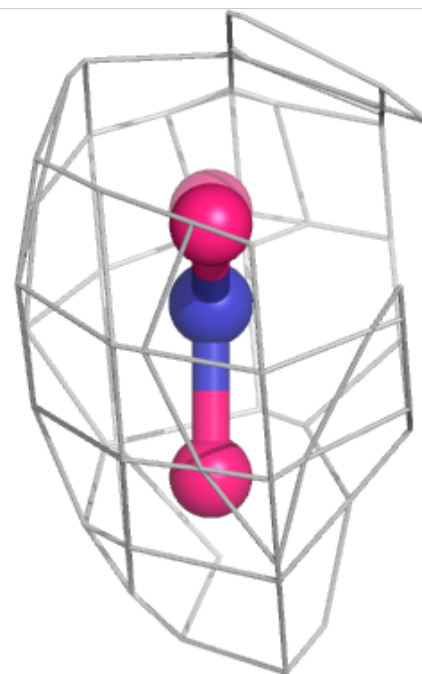
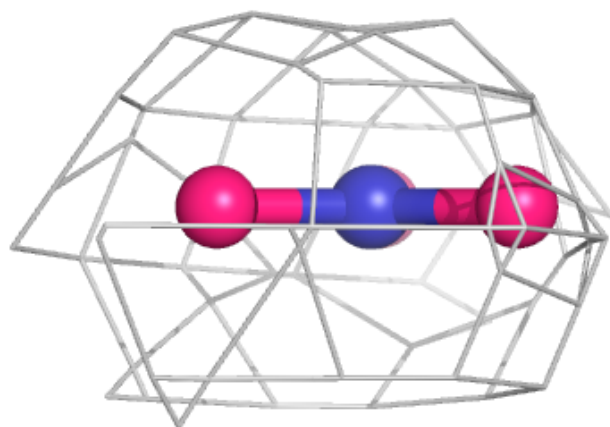
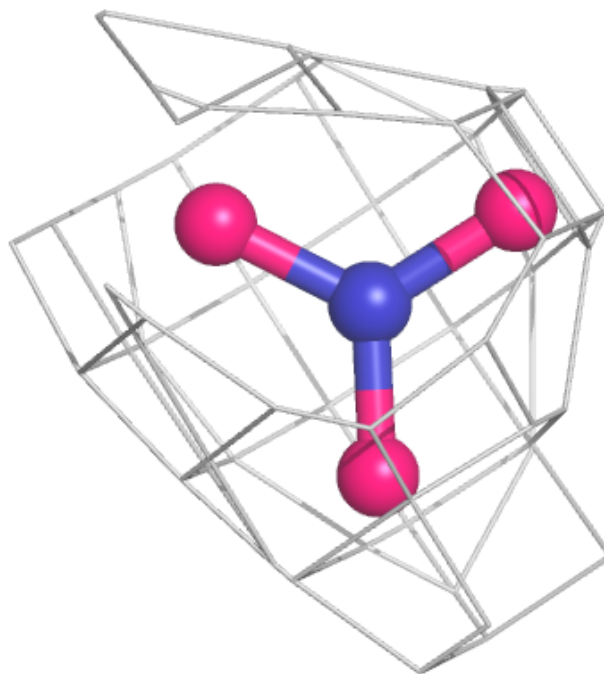
**Electron density around NO3 J 901:**

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



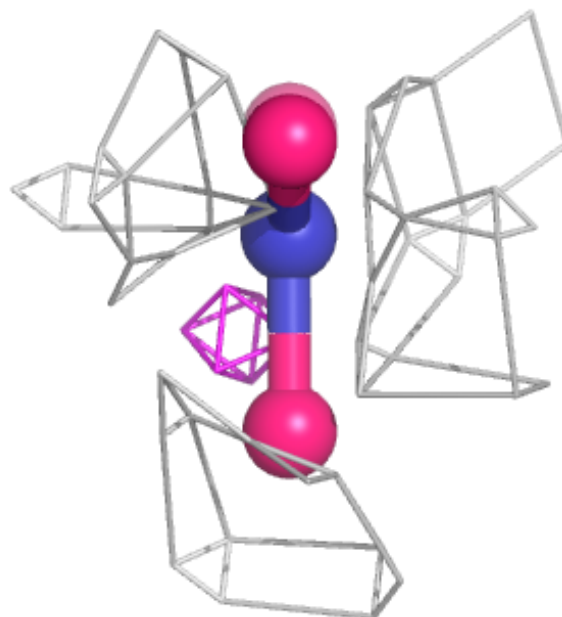
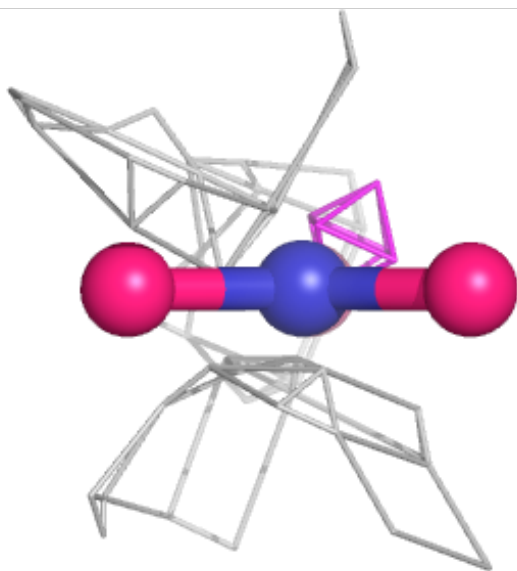
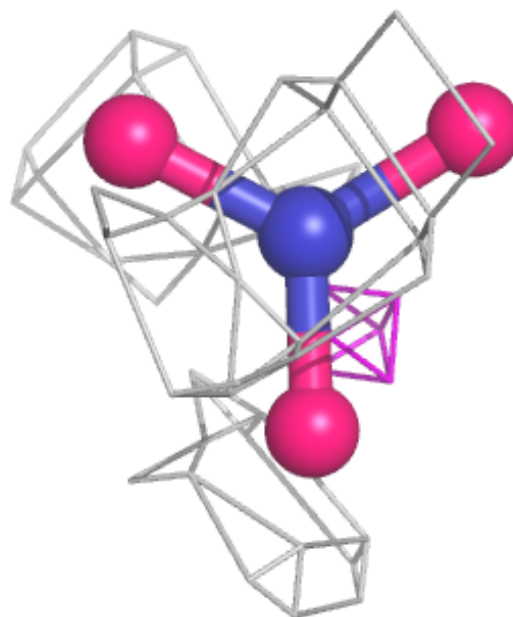
**Electron density around NO3 D 301:**

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



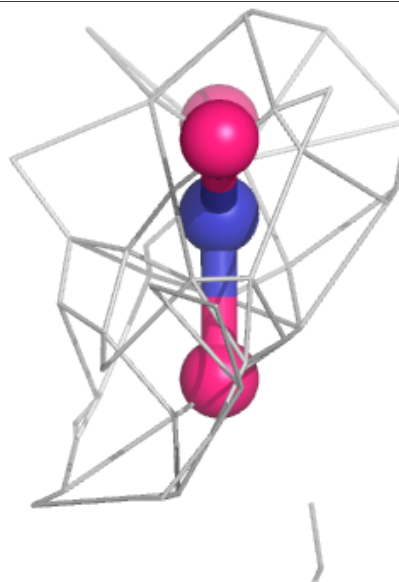
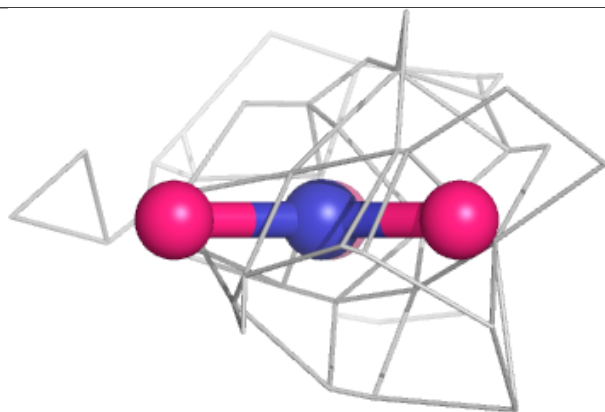
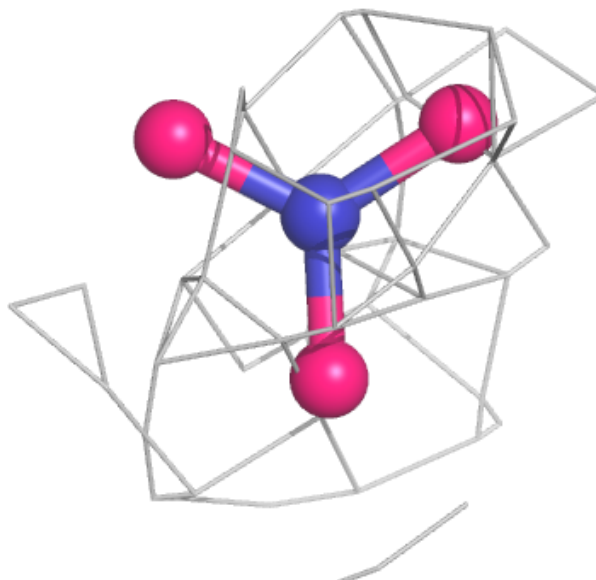
**Electron density around NO3 M 508:**

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



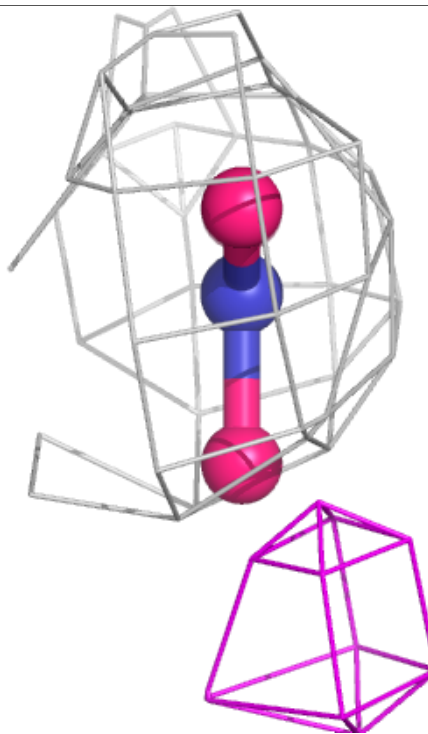
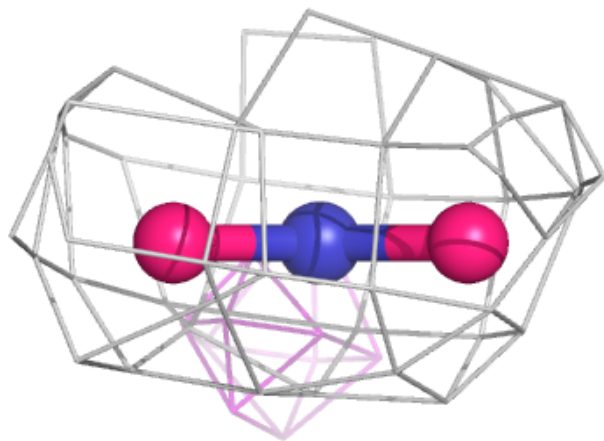
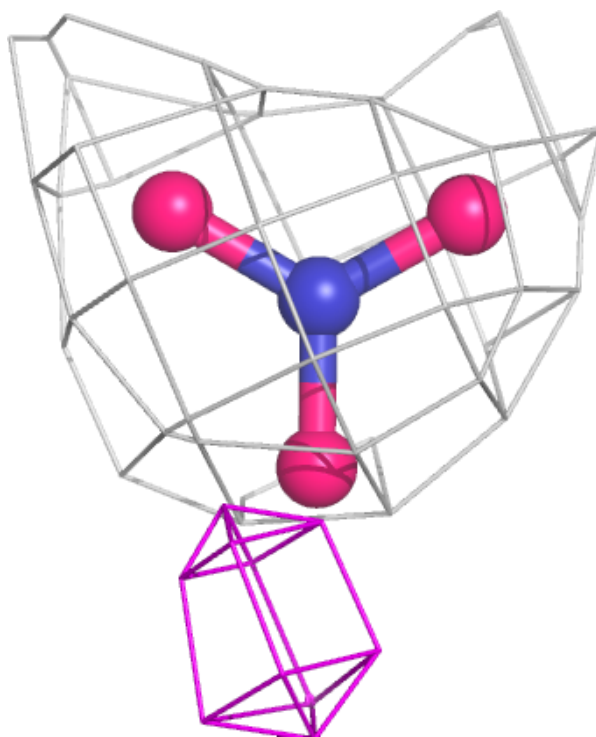
**Electron density around NO3 E 405:**

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



**Electron density around NO3 N 1304:**

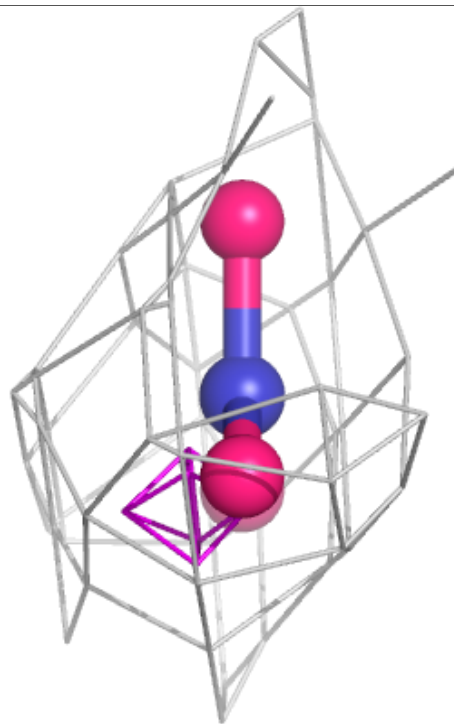
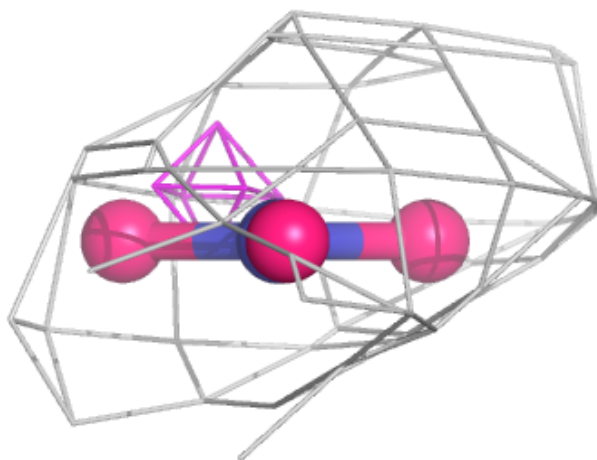
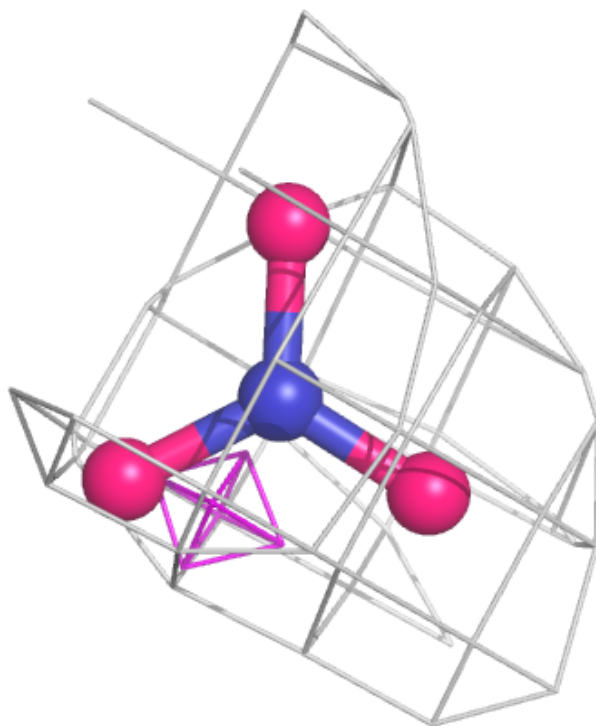
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





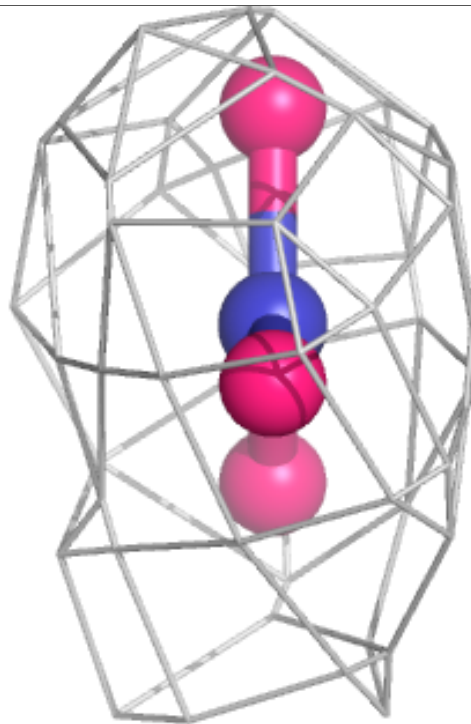
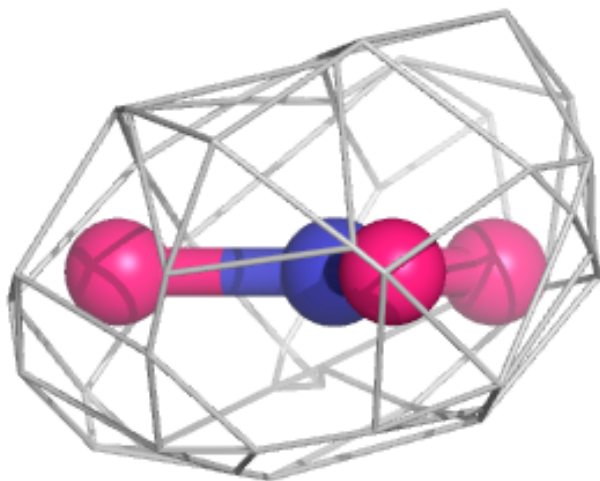
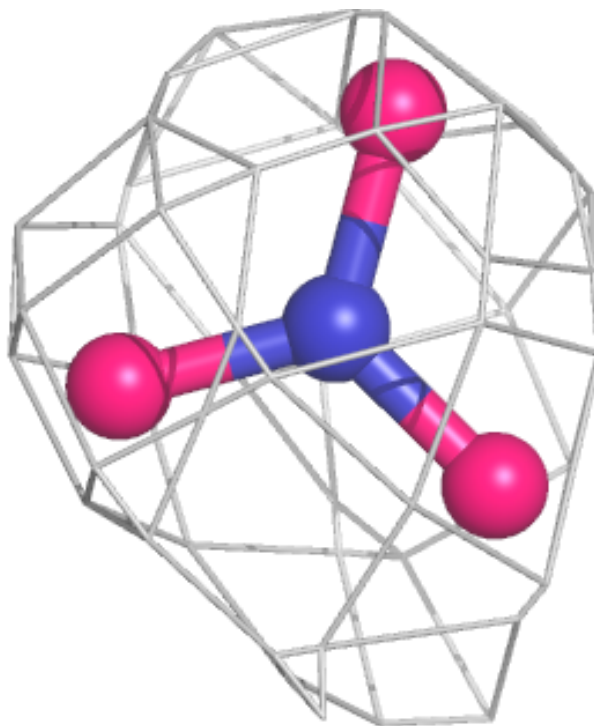
**Electron density around NO3 I 602:**

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



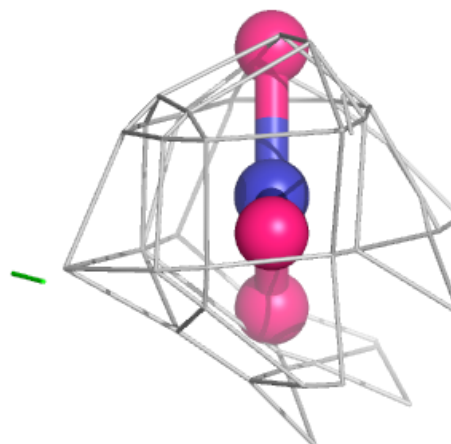
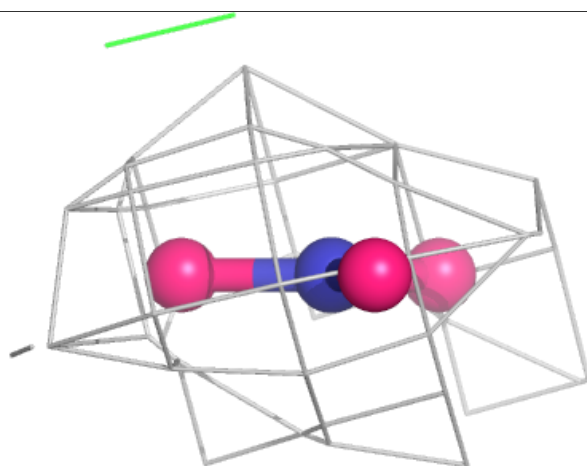
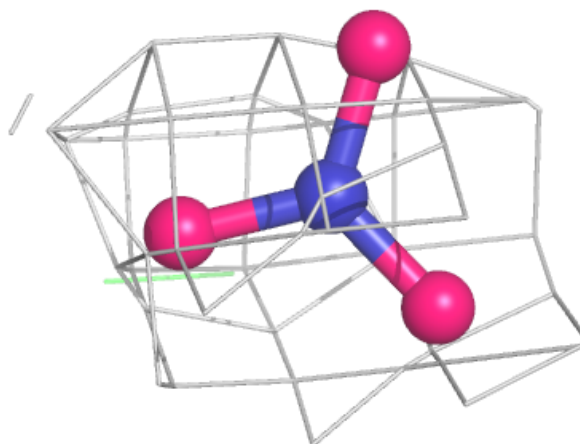
**Electron density around NO3 B 309:**

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



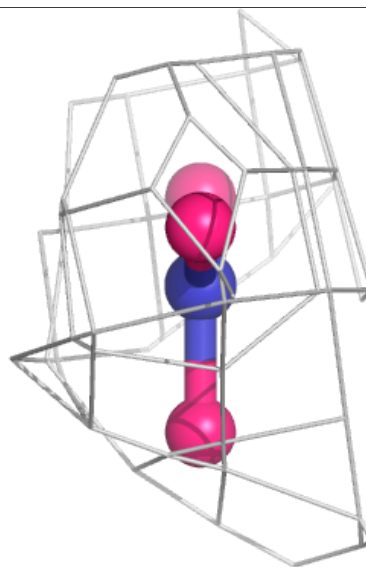
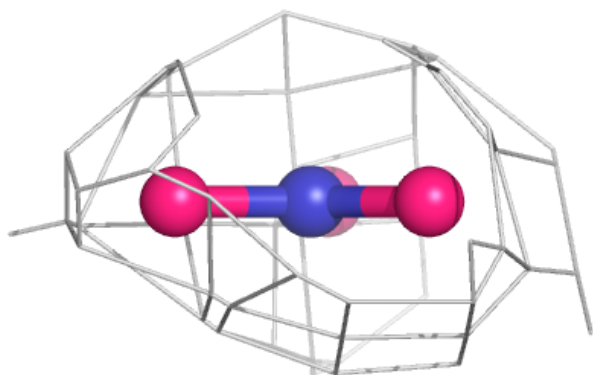
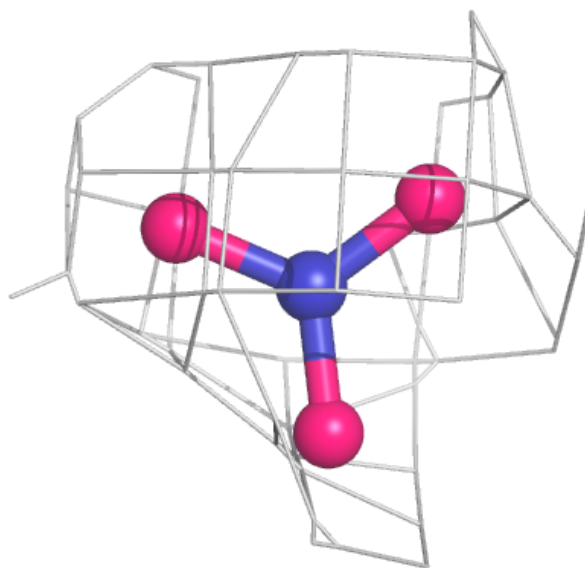
**Electron density around NO3 B 302:**

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



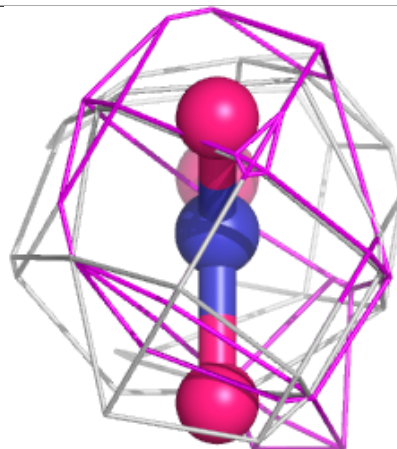
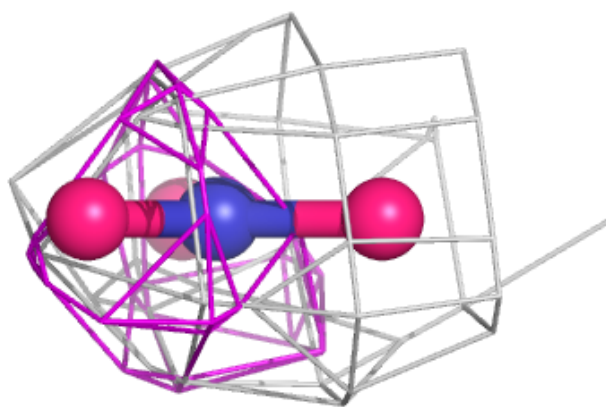
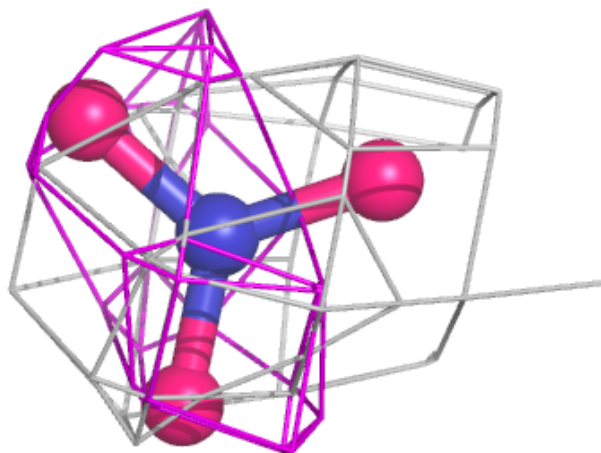
**Electron density around NO3 GG 201:**

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



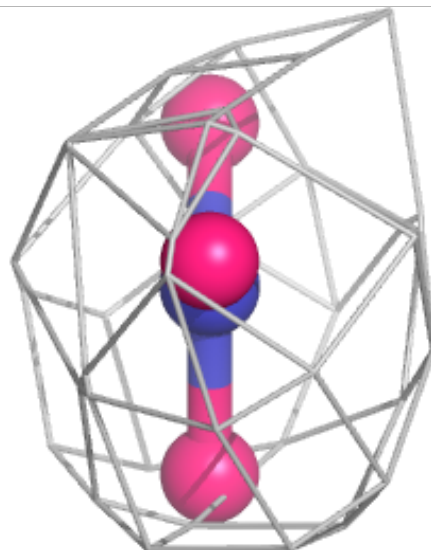
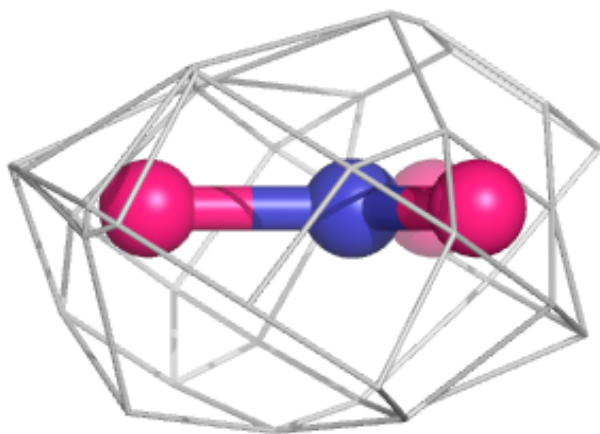
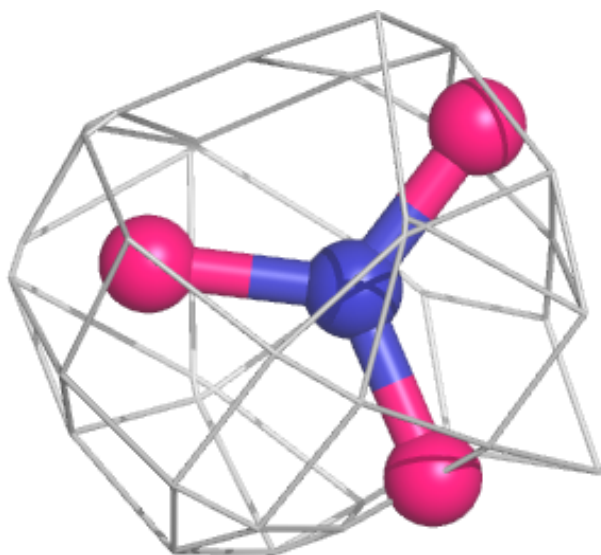
**Electron density around NO3 C 302:**

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



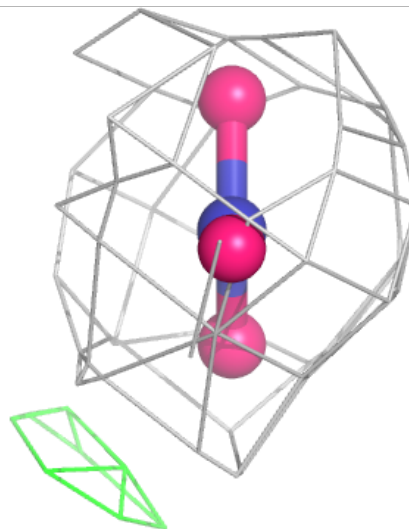
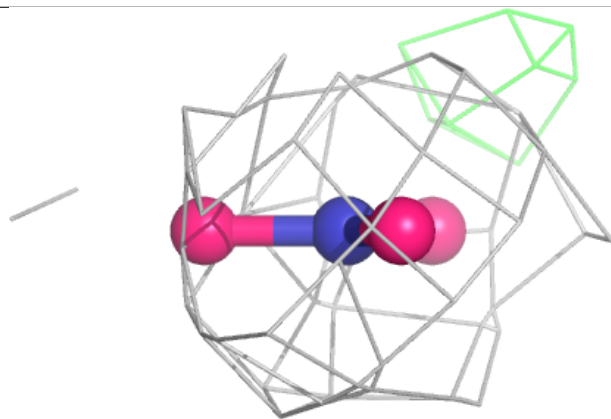
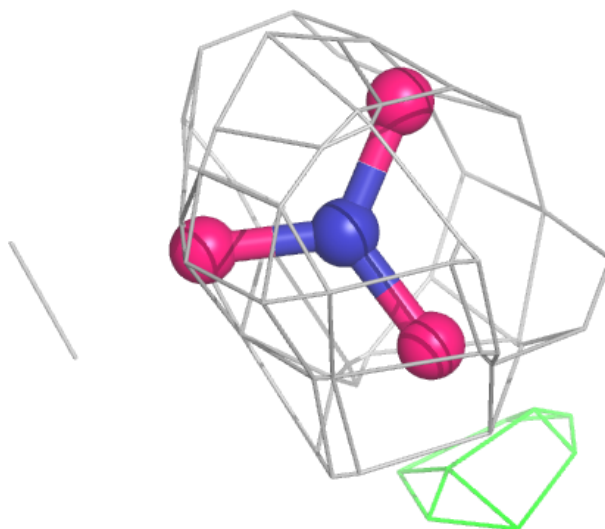
**Electron density around NO3 C 304:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



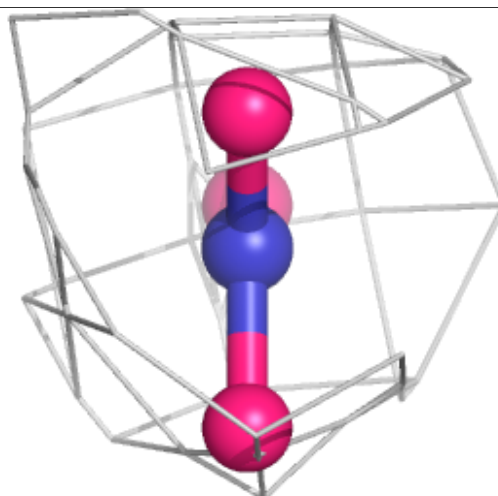
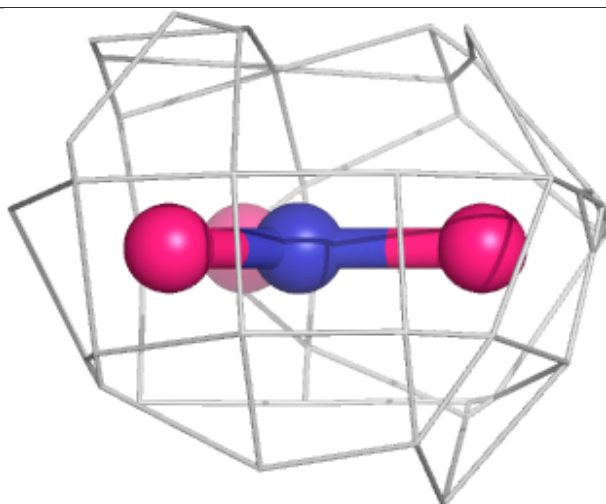
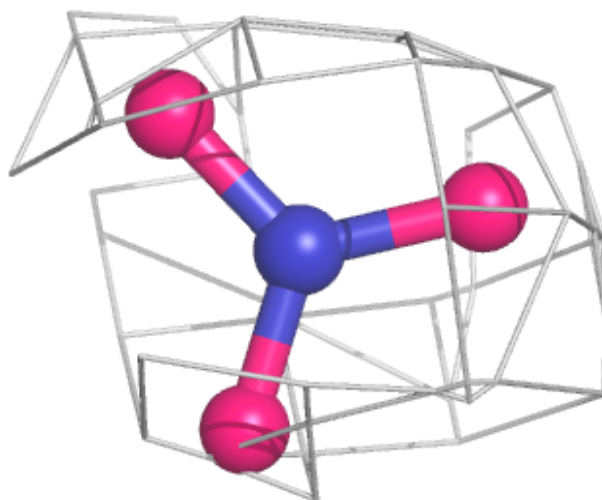
**Electron density around NO3 B 305:**

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



**Electron density around NO3 L 502:**

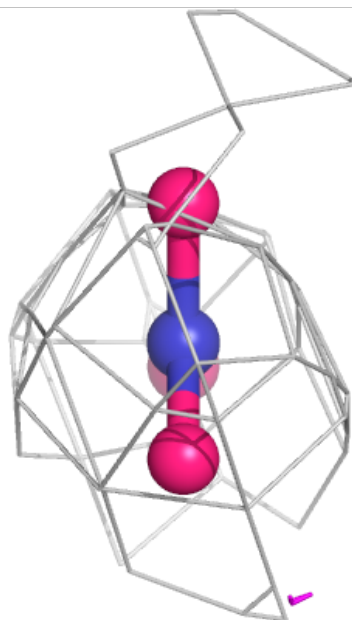
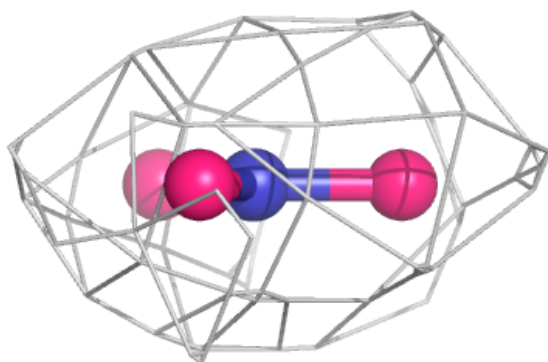
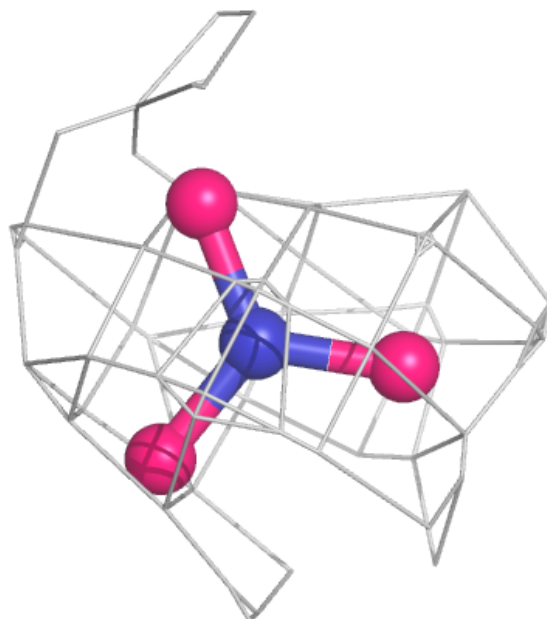
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





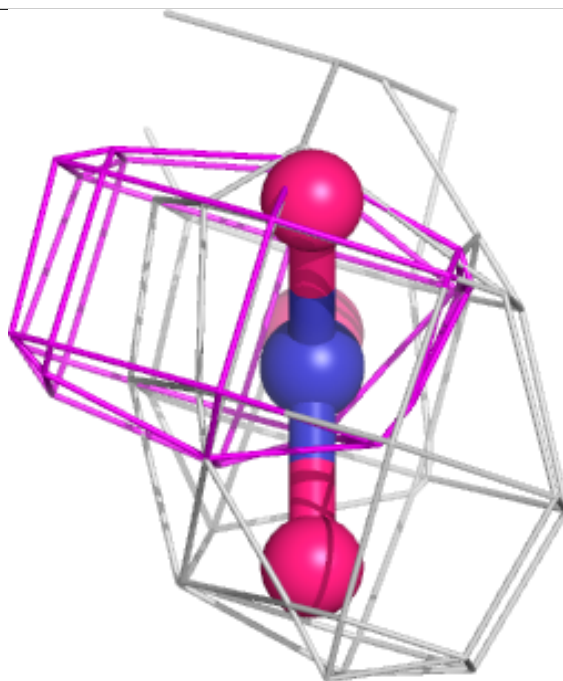
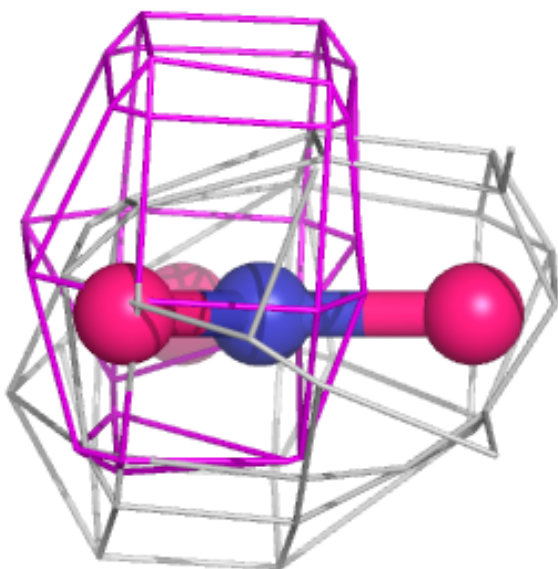
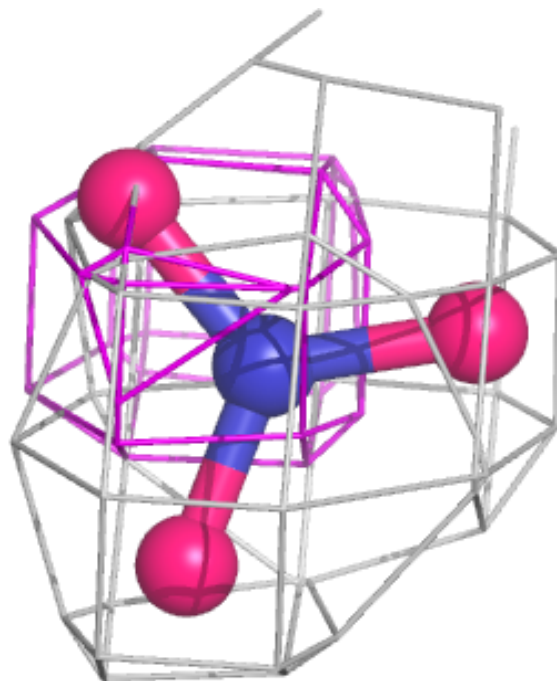
**Electron density around NO3 M 502:**

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



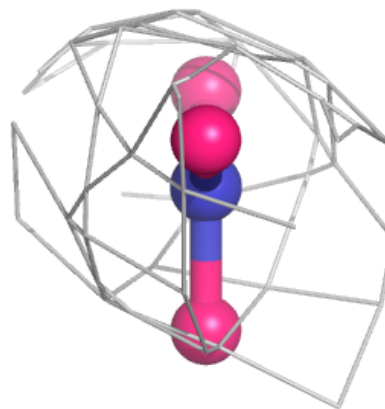
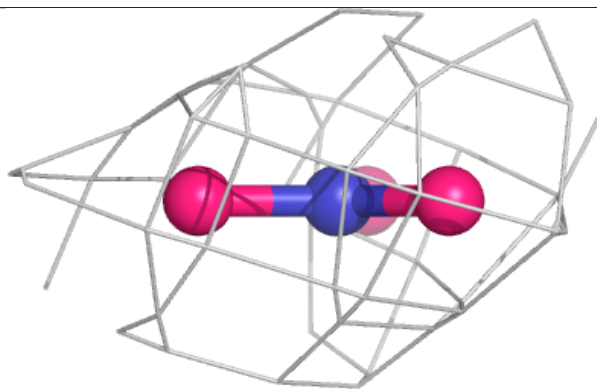
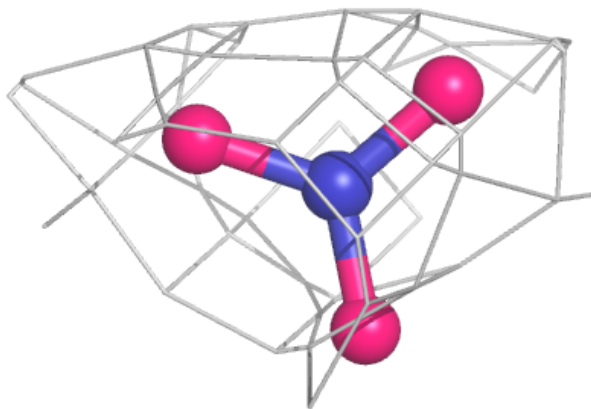
**Electron density around NO3 C 301:**

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



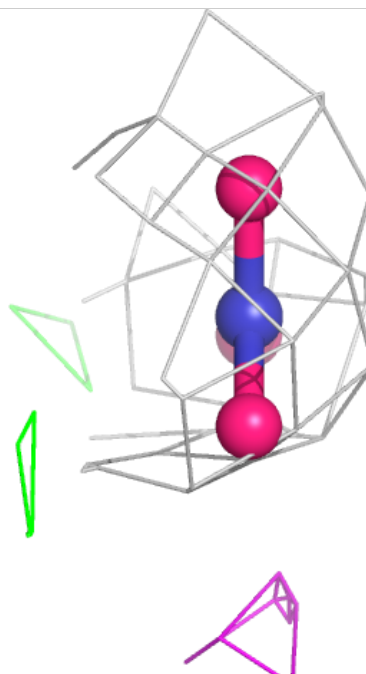
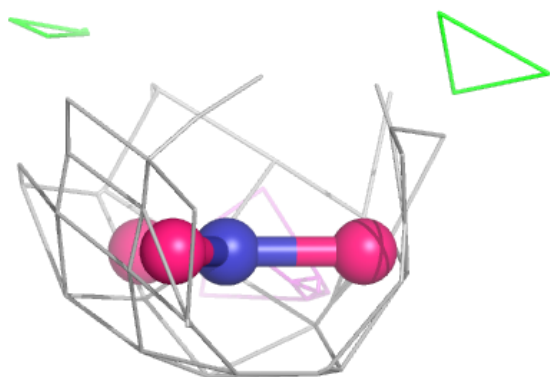
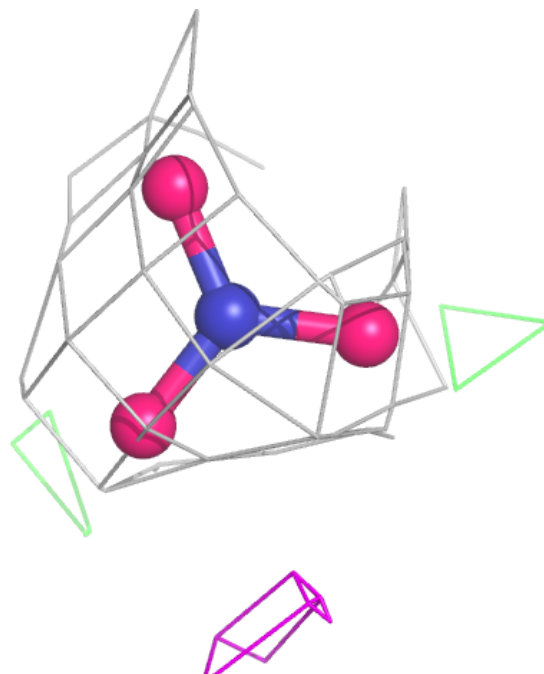
**Electron density around NO3 B 304:**

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



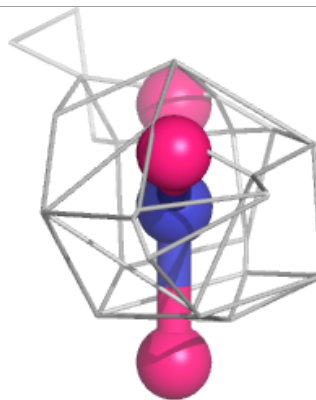
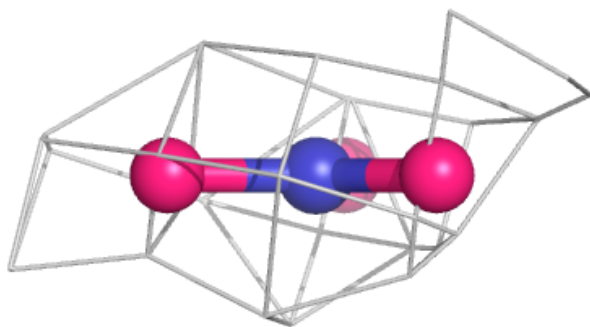
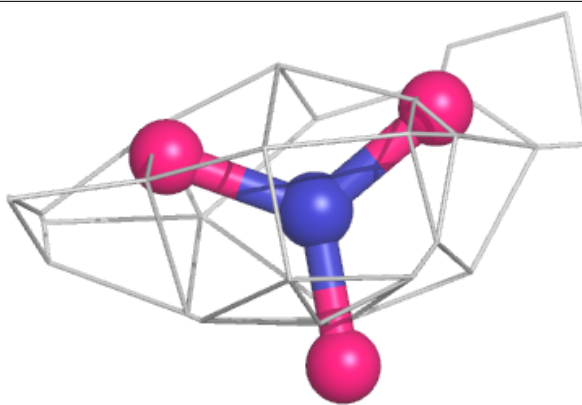
**Electron density around NO3 N 1302:**

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



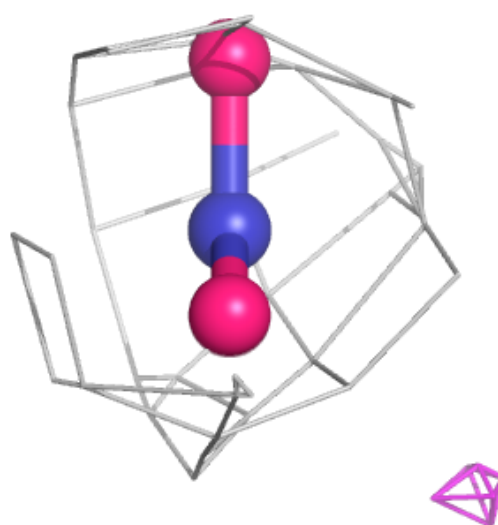
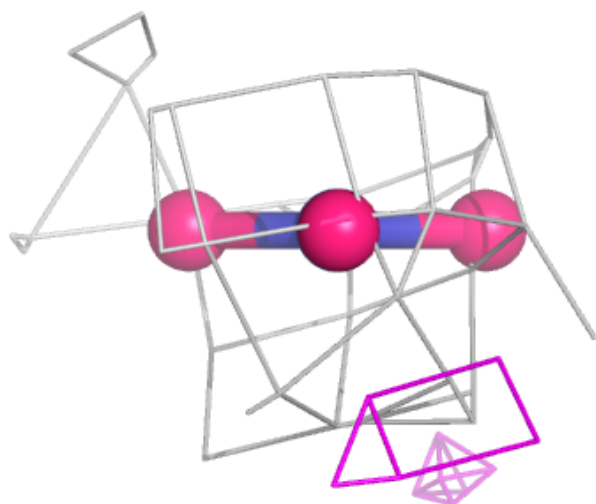
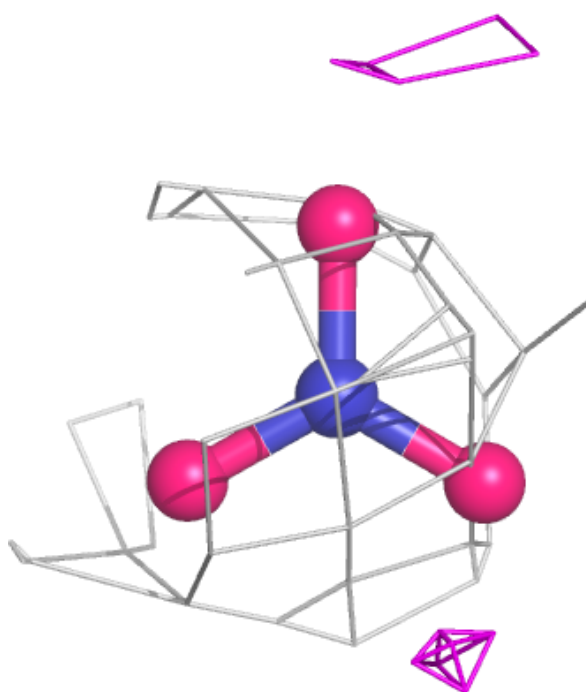
**Electron density around NO3 JJ 201:**

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



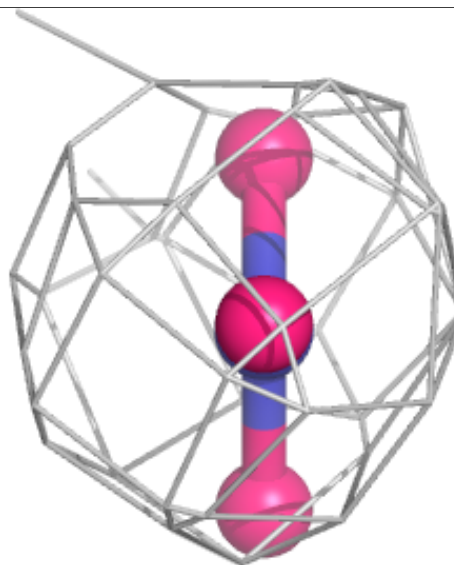
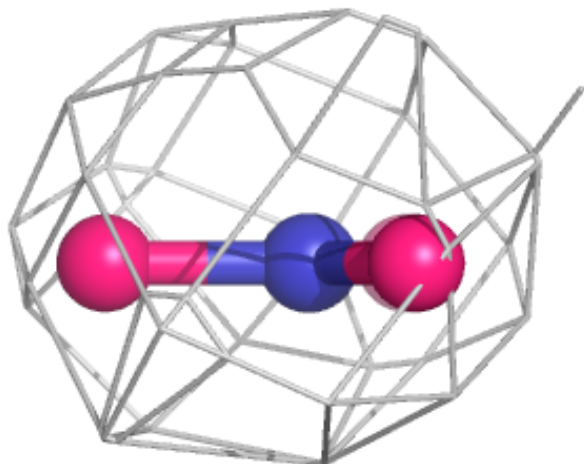
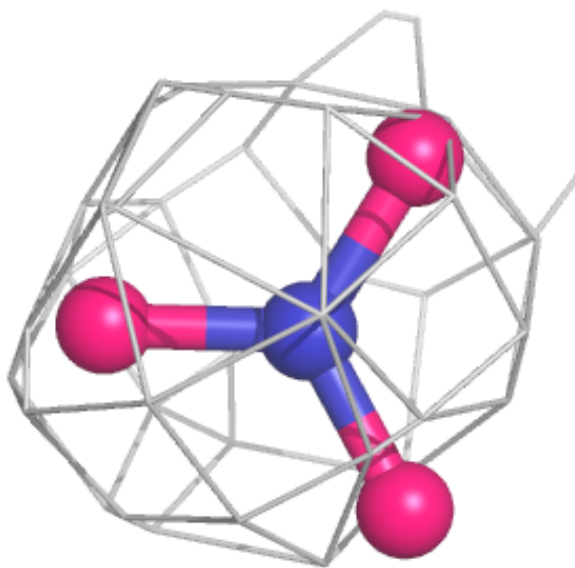
**Electron density around NO3 II 201:**

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



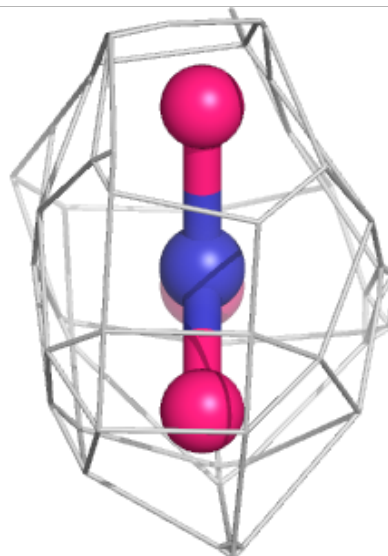
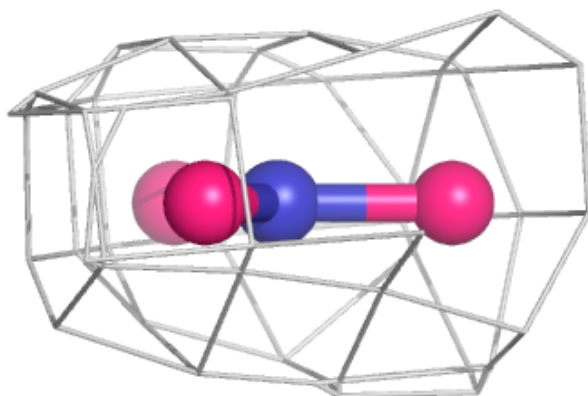
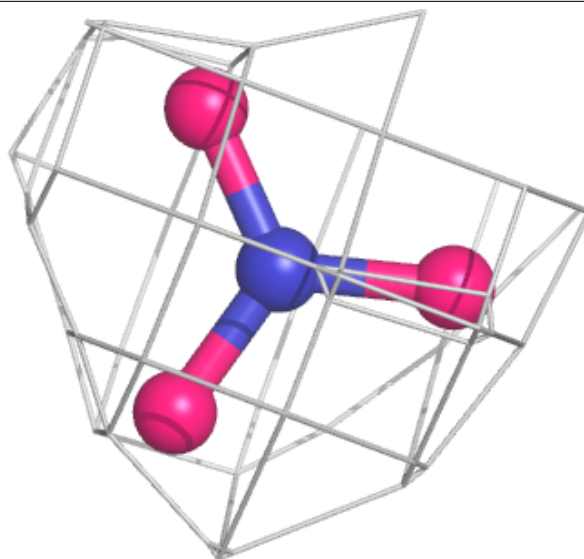
**Electron density around NO3 K 1503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NO3 K 1501:**

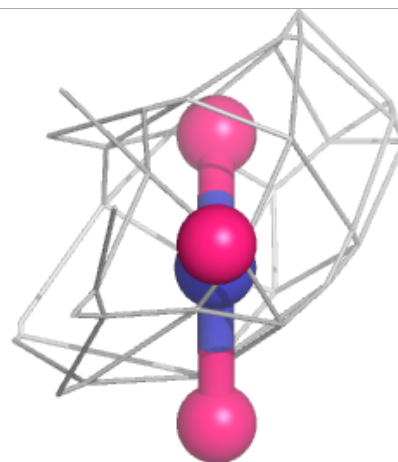
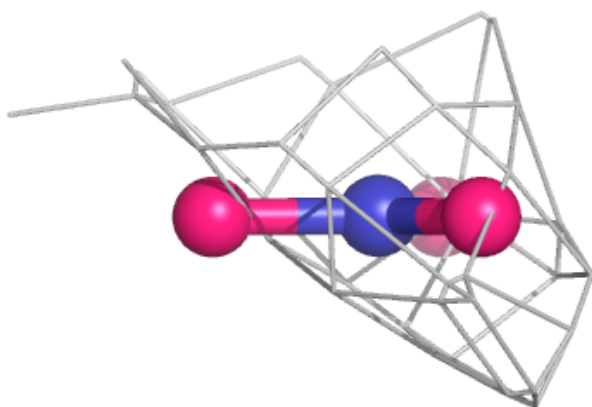
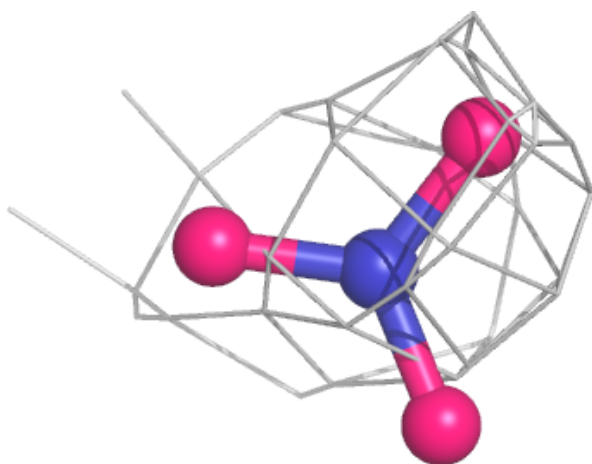
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





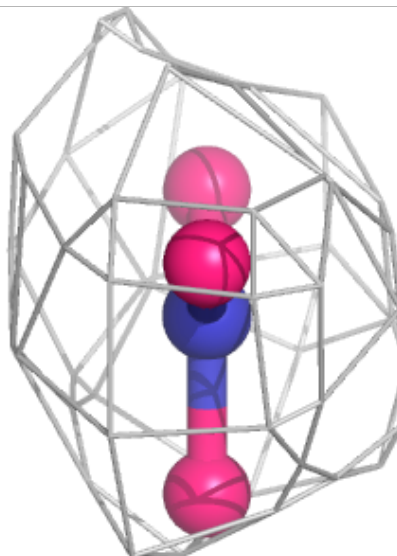
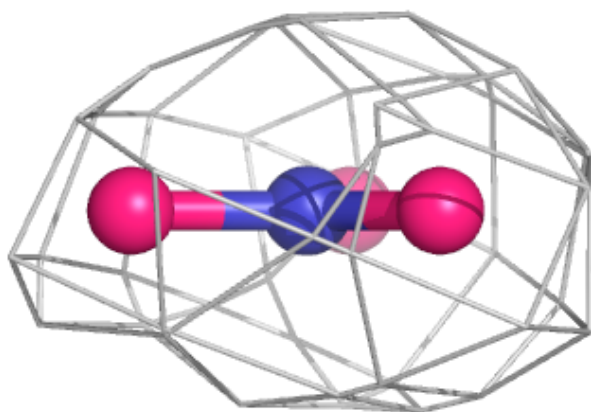
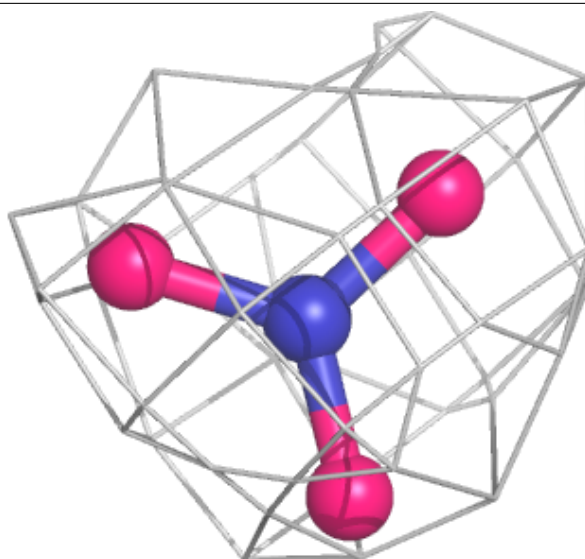
**Electron density around NO3 GG 206:**

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



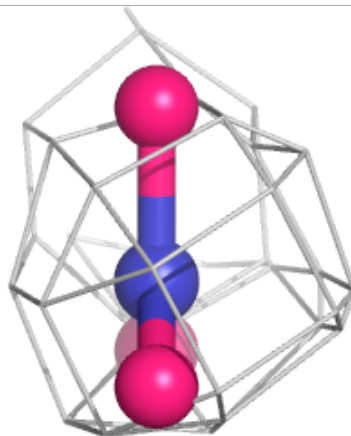
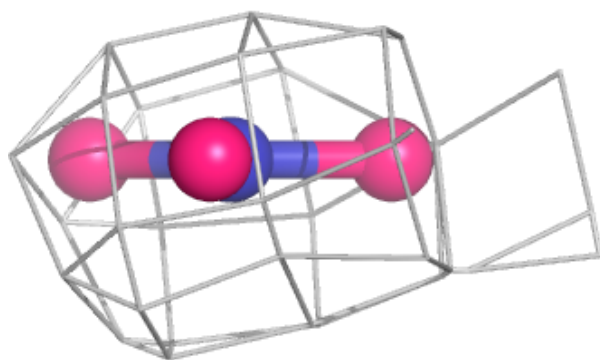
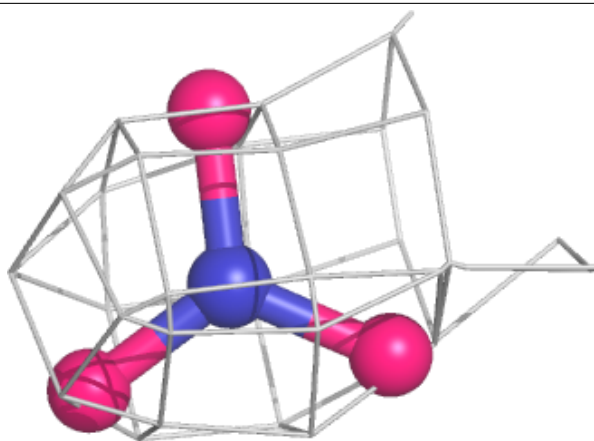
**Electron density around NO3 L 501:**

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



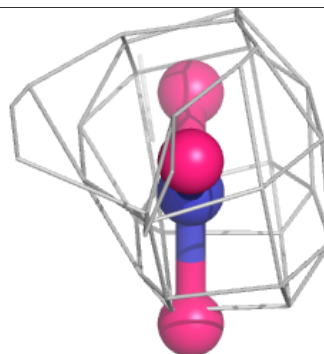
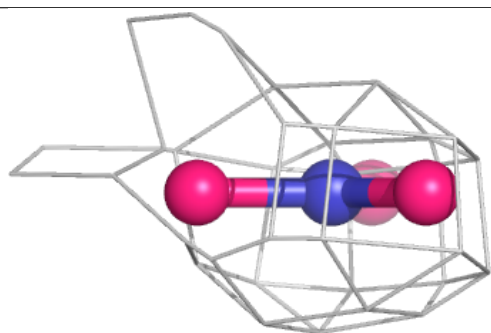
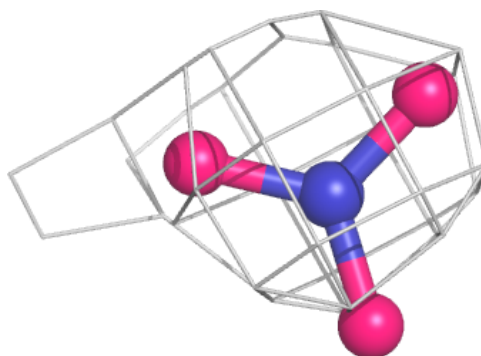
**Electron density around NO3 J 904:**

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



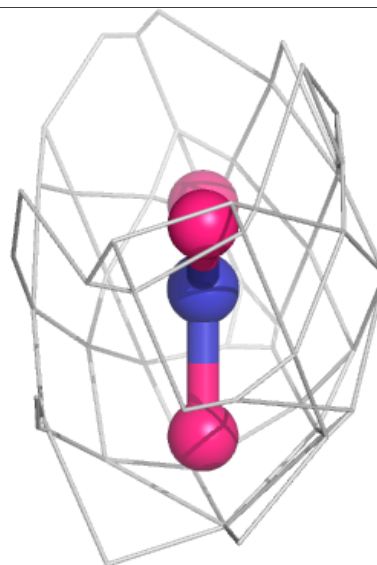
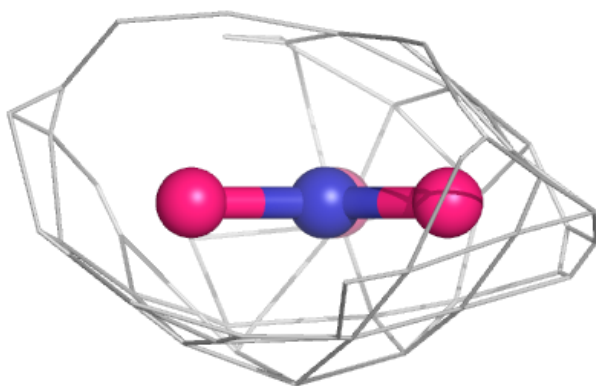
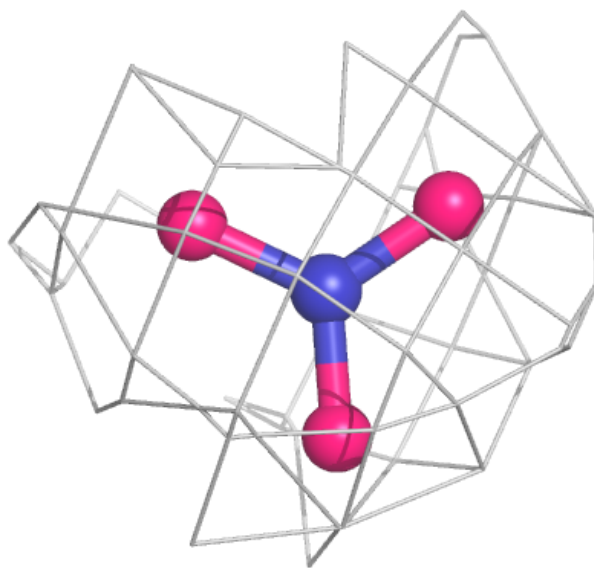
**Electron density around NO3 A 805:**

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



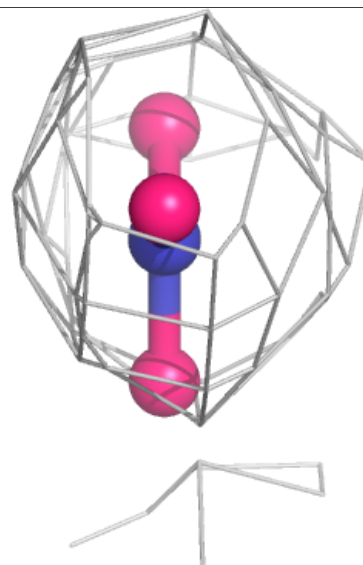
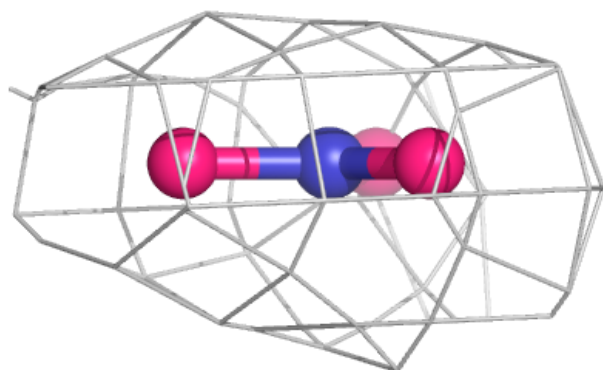
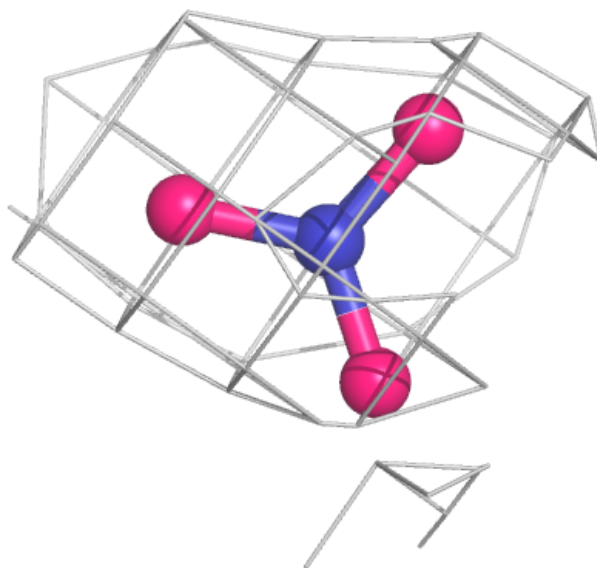
**Electron density around NO3 F 602:**

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



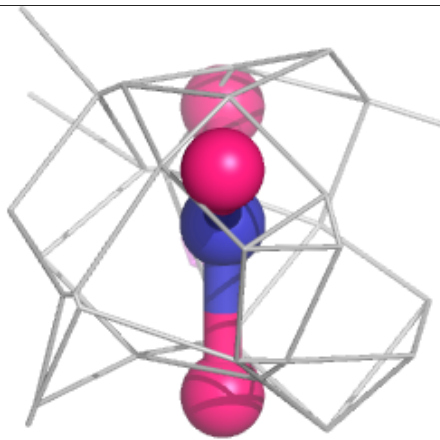
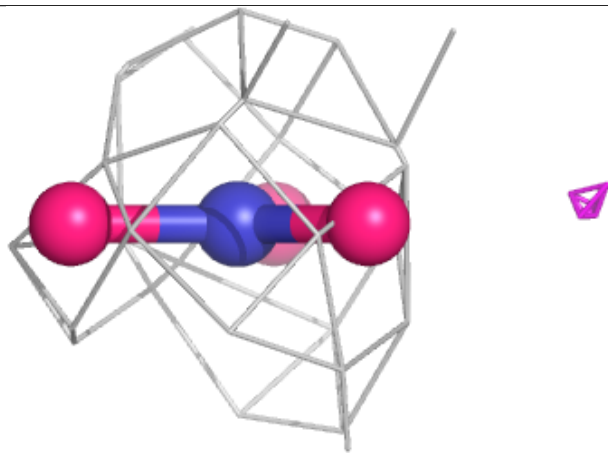
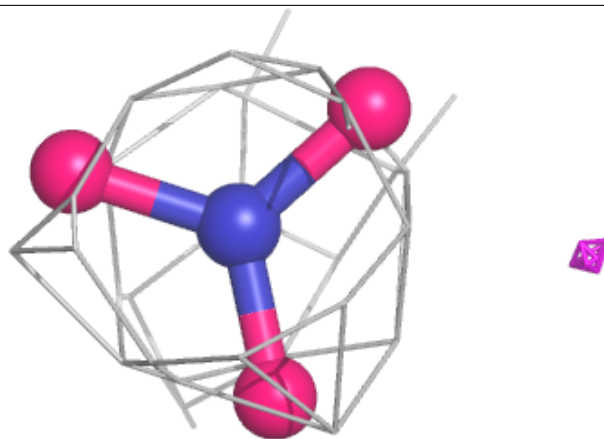
**Electron density around NO3 HH 301:**

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



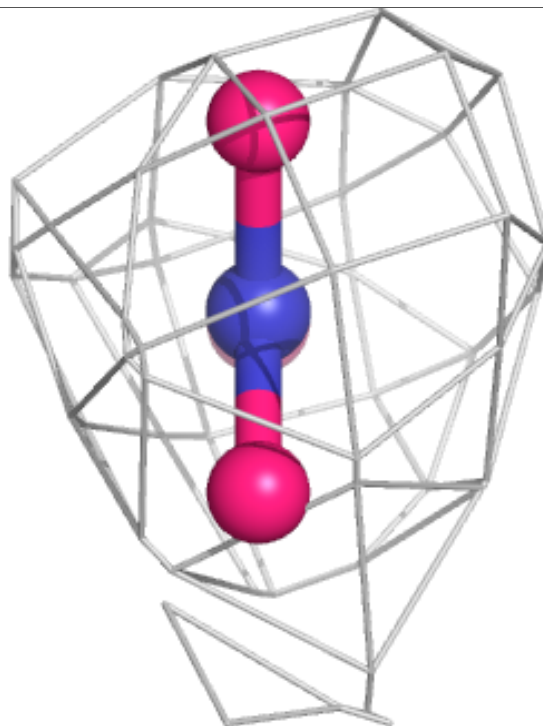
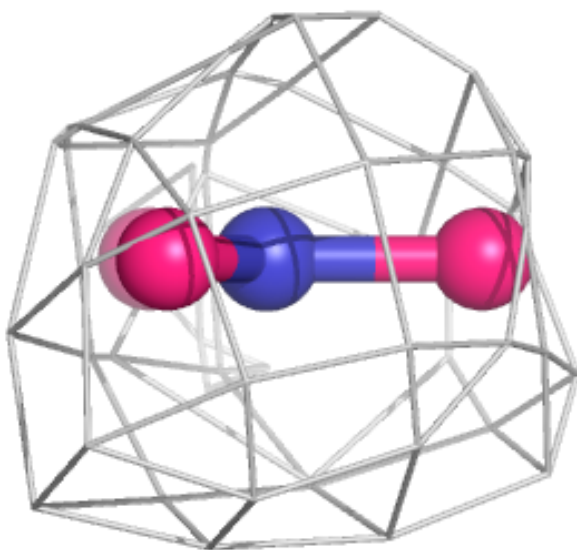
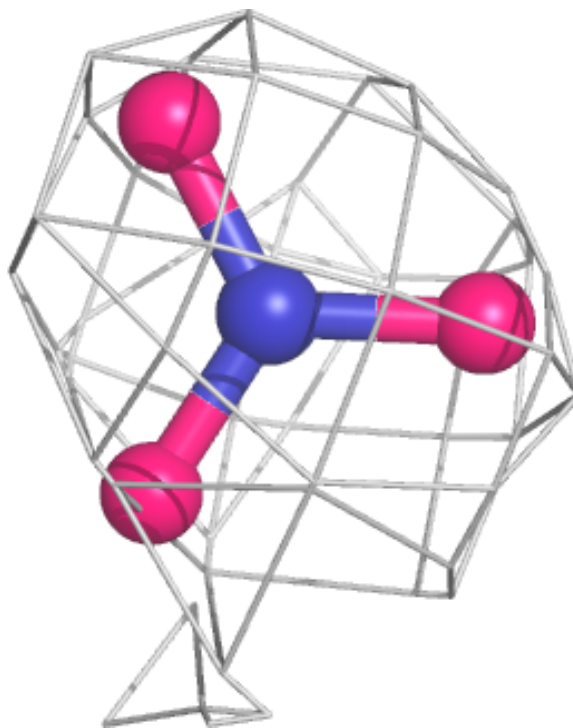
**Electron density around NO3 I 601:**

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



**Electron density around NO3 M 509:**

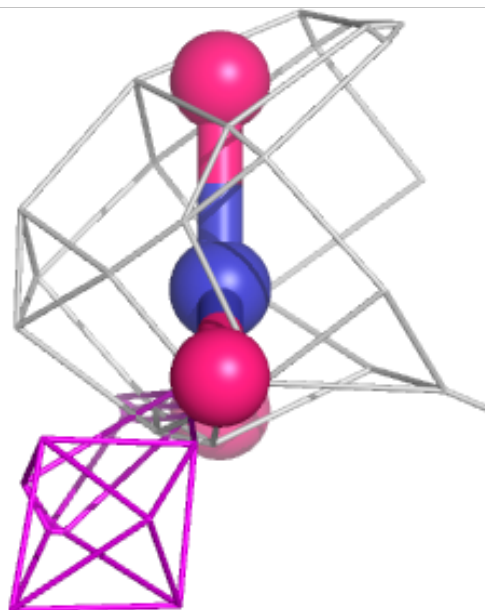
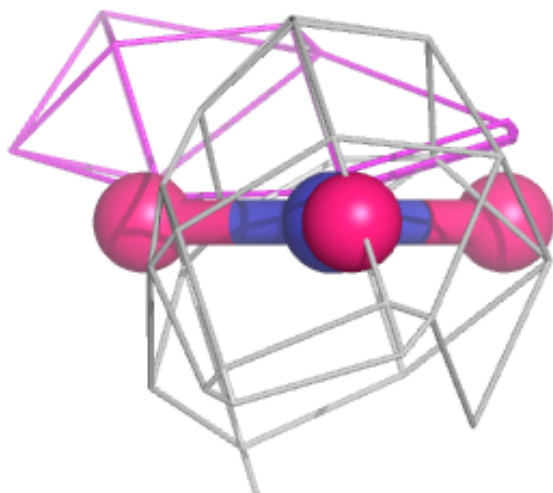
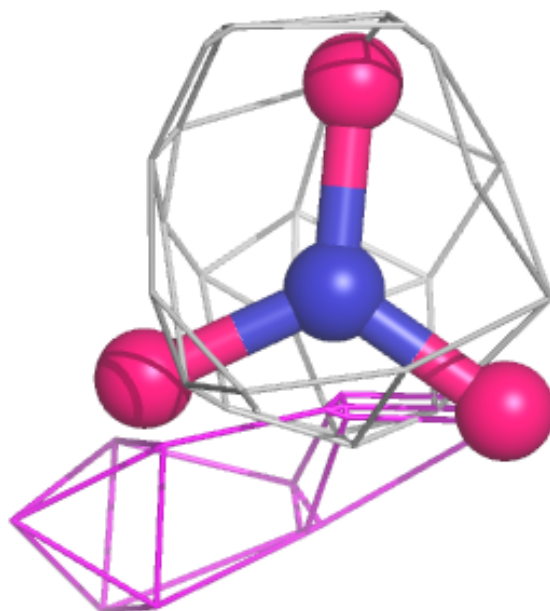
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





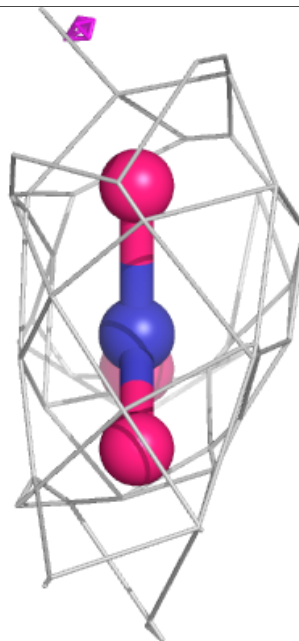
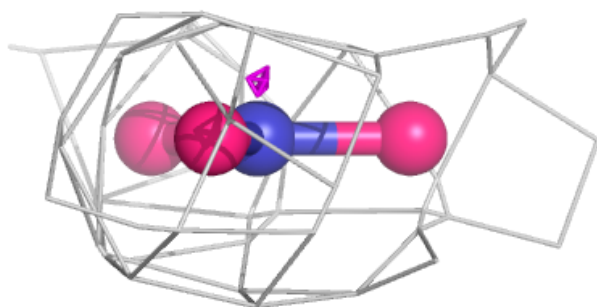
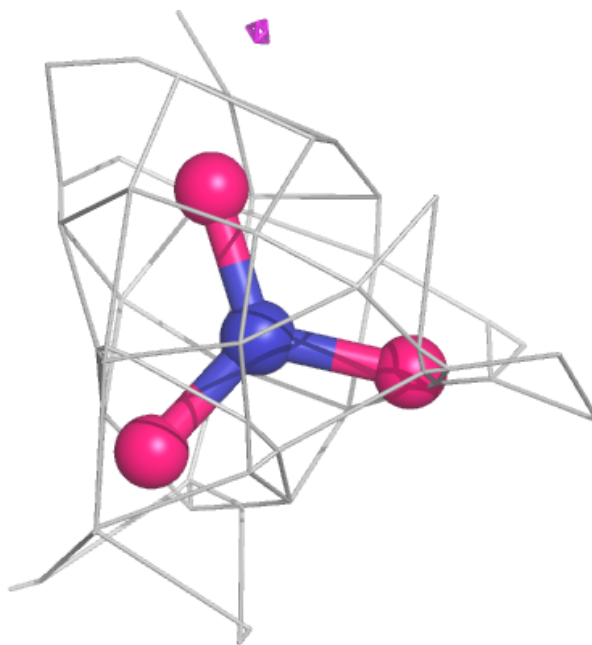
**Electron density around NO3 H 502:**

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



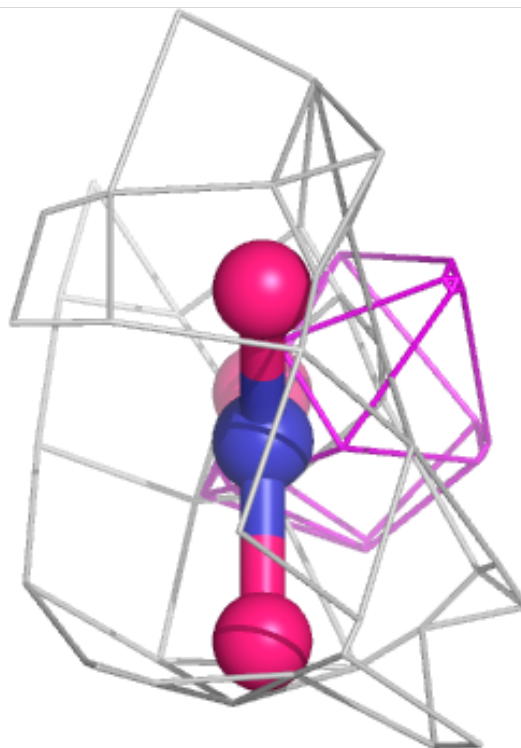
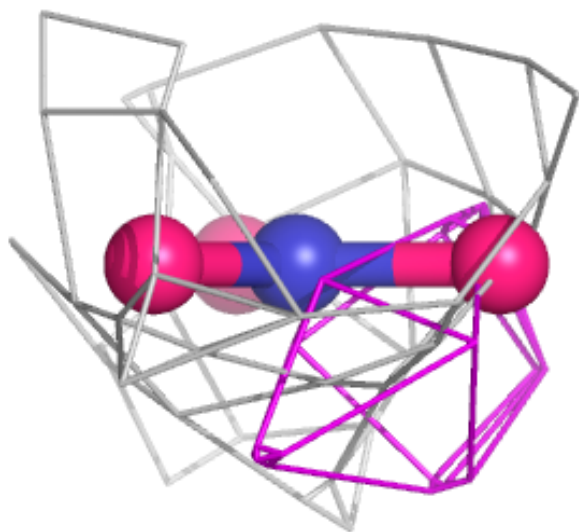
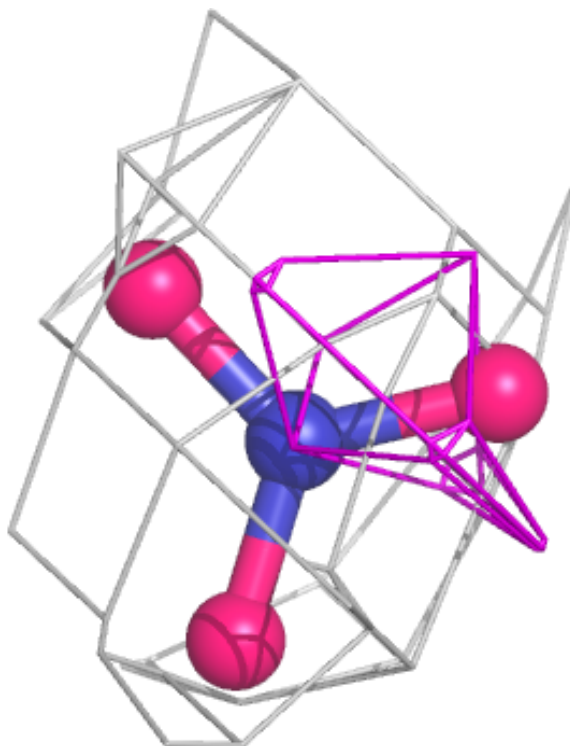
**Electron density around NO3 E 401:**

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



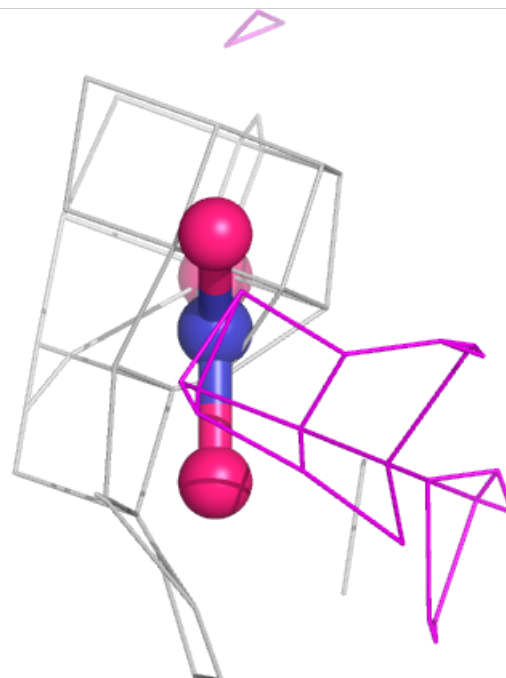
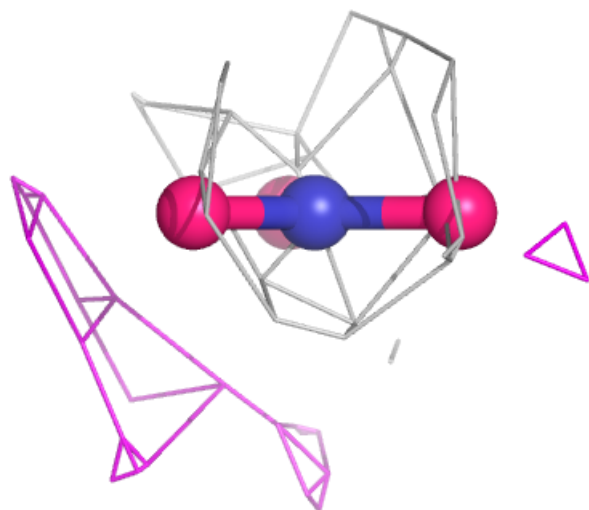
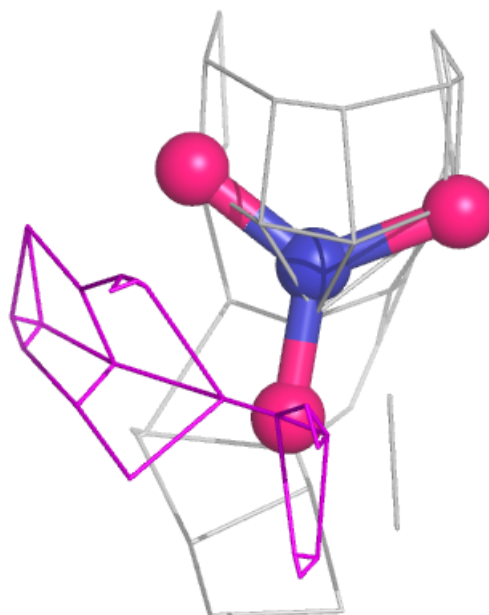
**Electron density around NO3 B 301:**

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



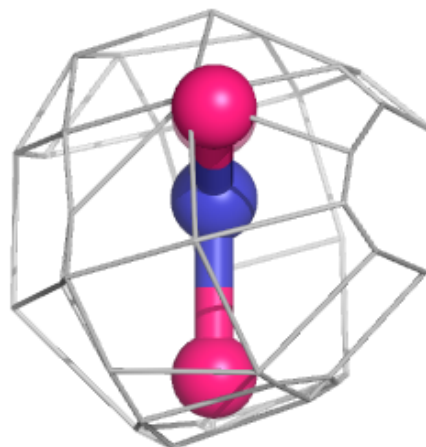
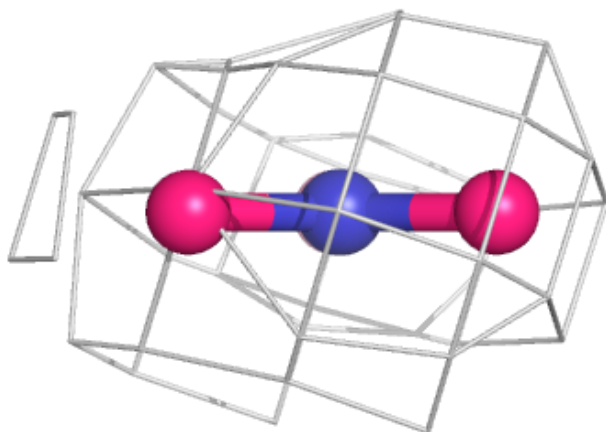
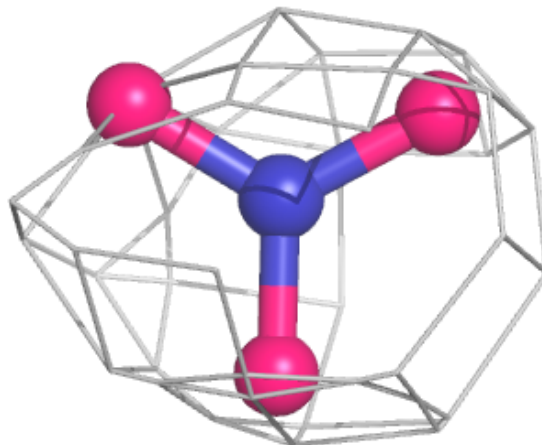
**Electron density around NO3 B 307:**

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



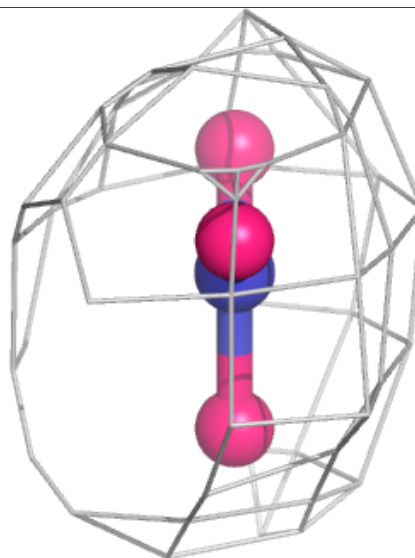
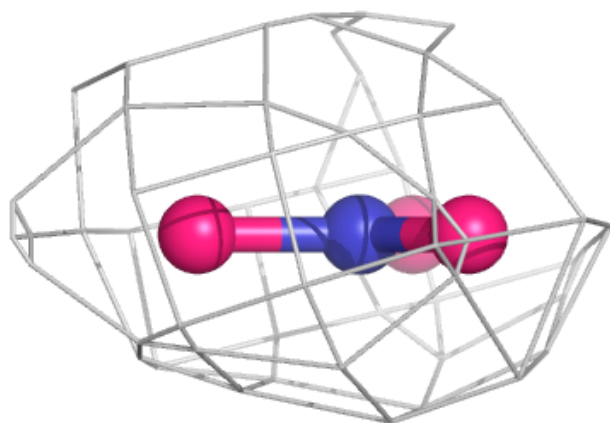
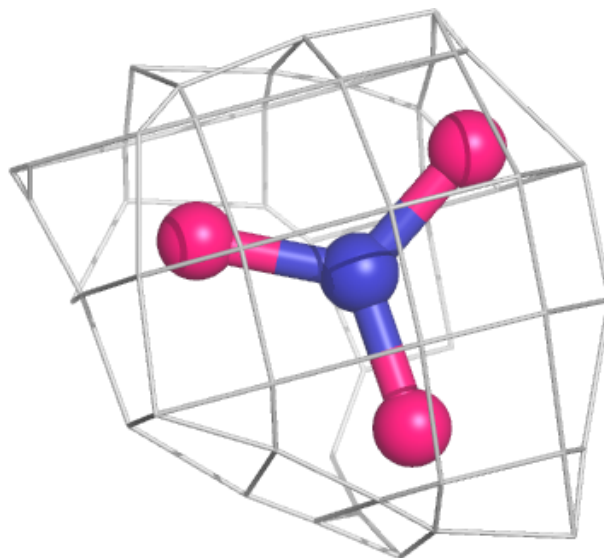
**Electron density around NO3 N 1306:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



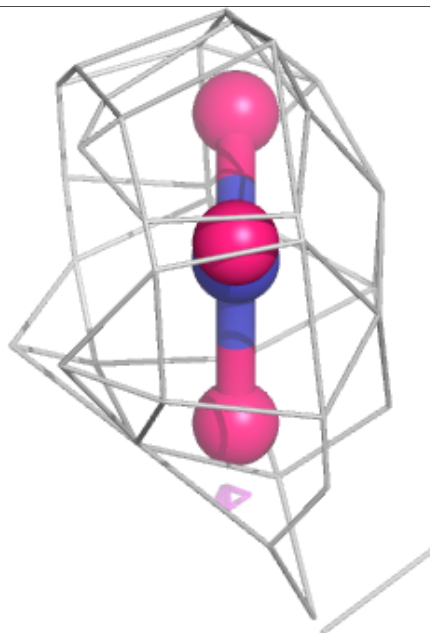
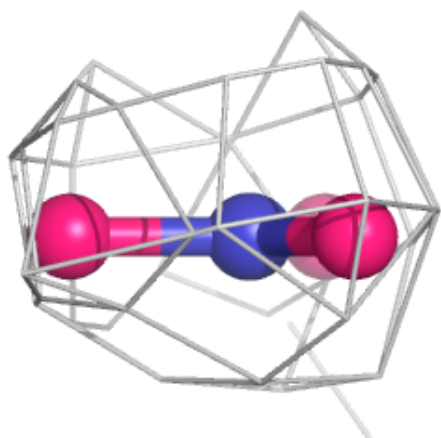
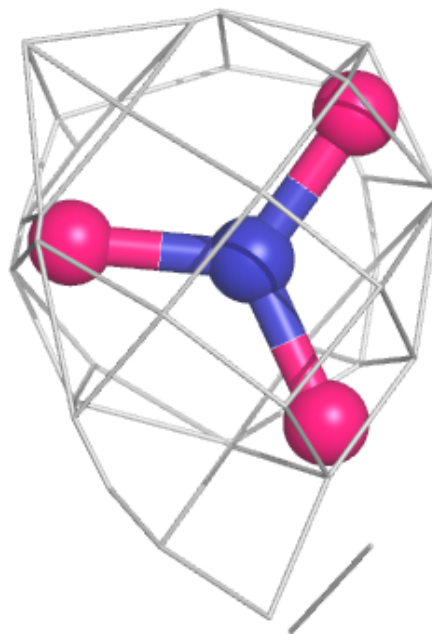
**Electron density around NO3 GG 202:**

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



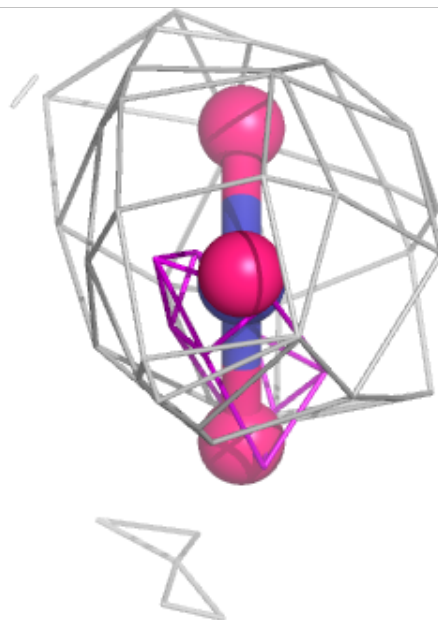
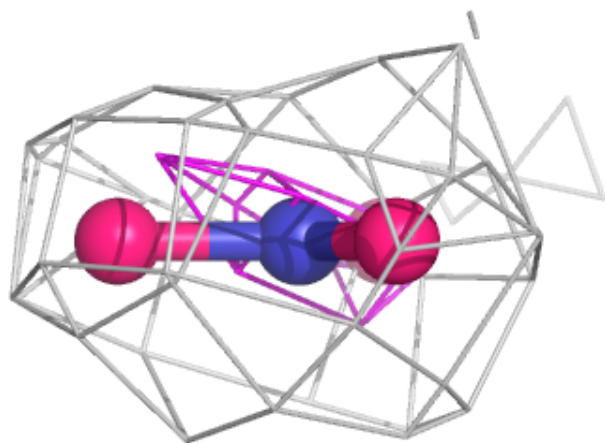
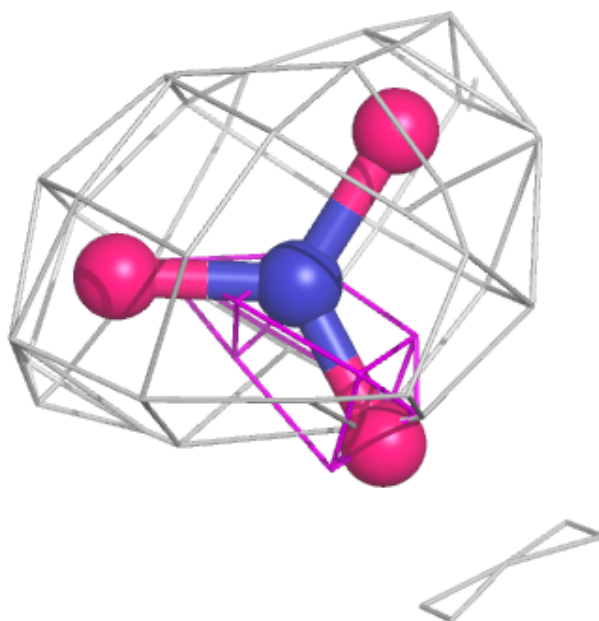
**Electron density around NO3 A 802:**

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



**Electron density around NO3 F 601:**

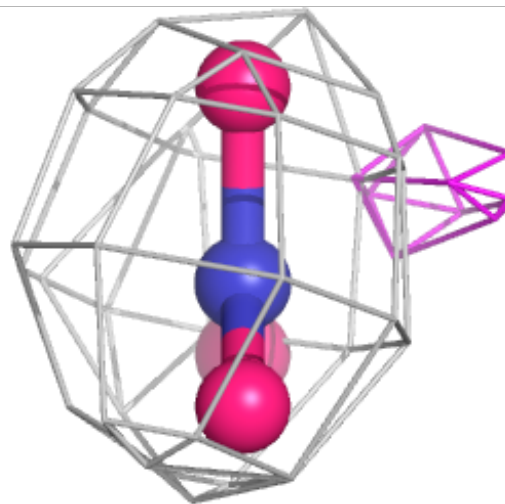
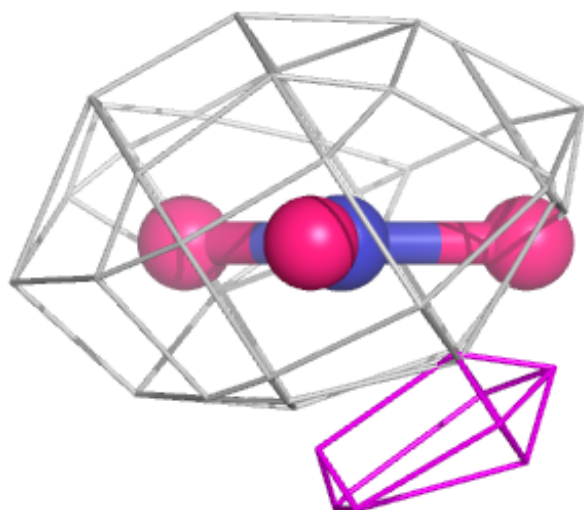
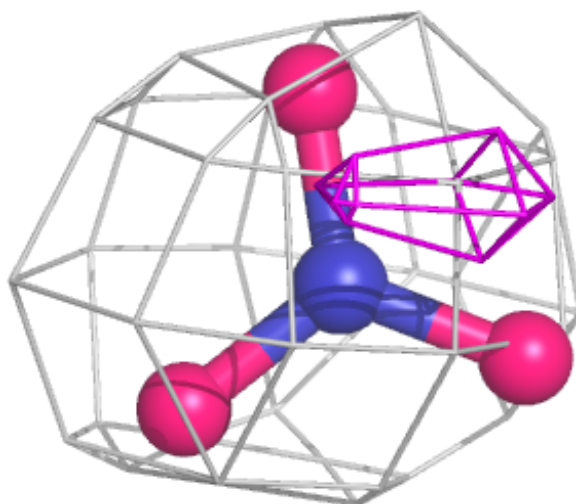
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





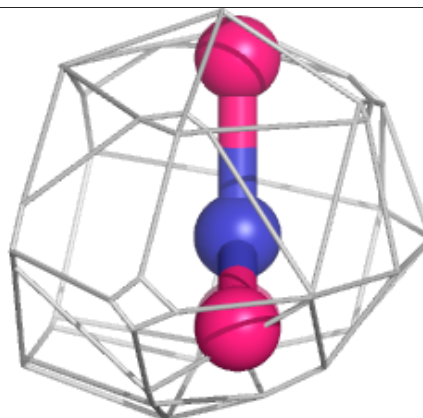
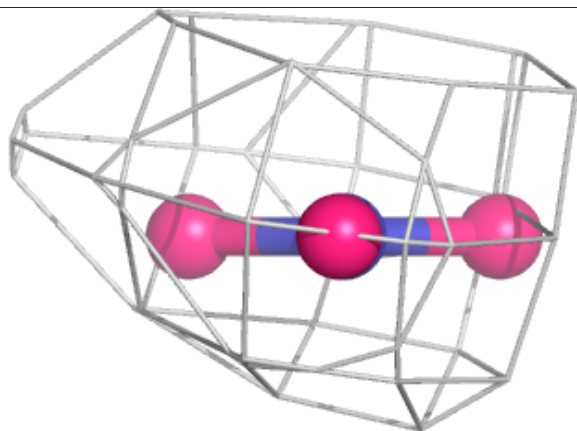
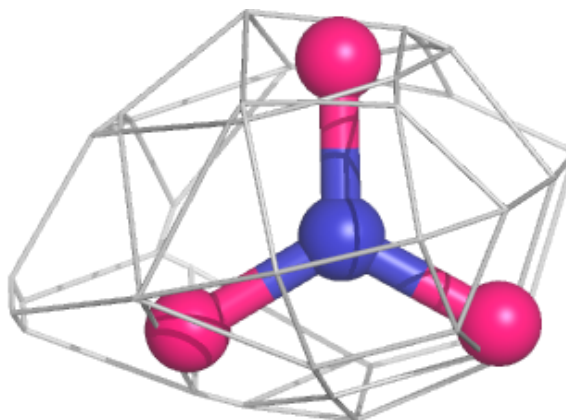
**Electron density around NO3 I 605:**

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



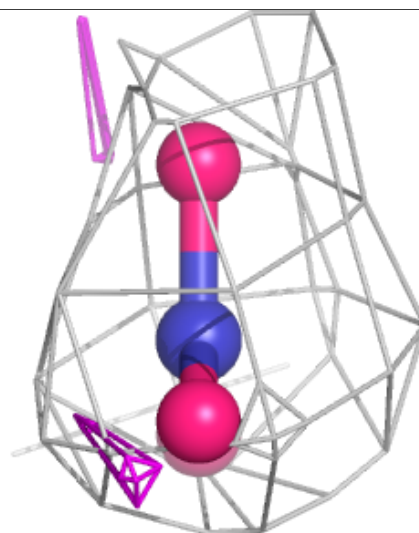
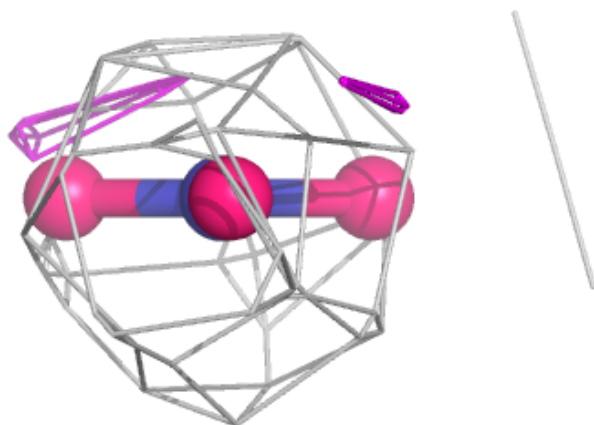
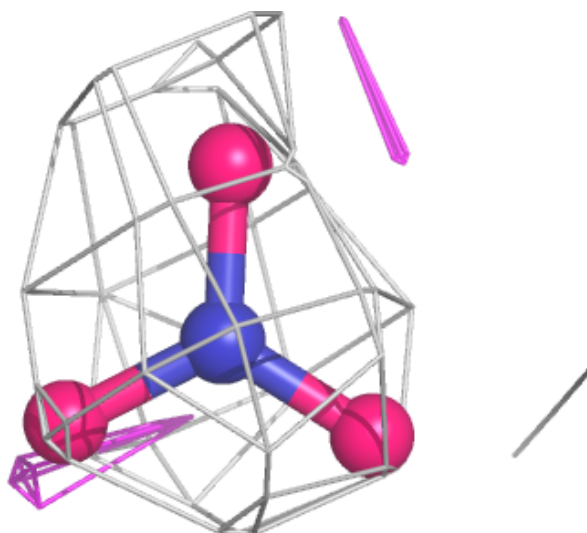
**Electron density around NO3 E 404:**

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



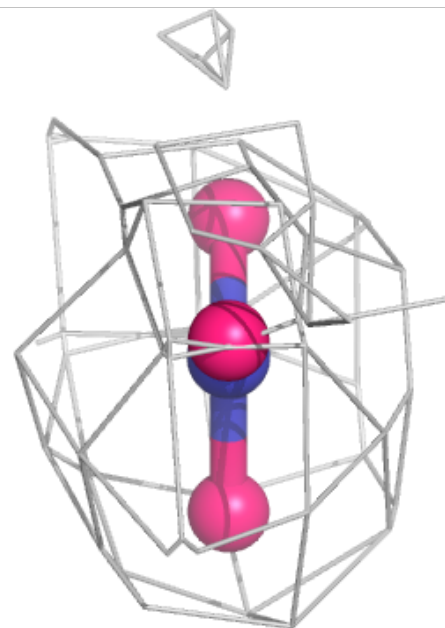
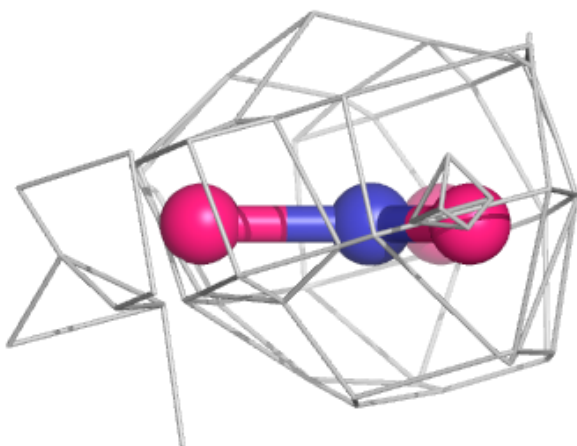
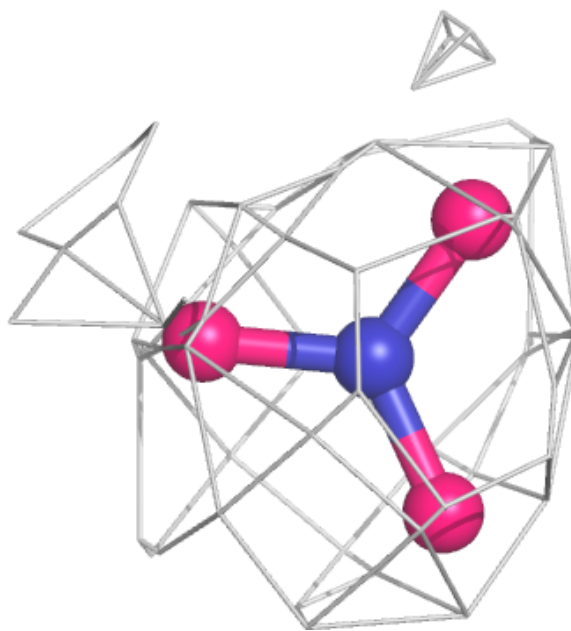
**Electron density around NO3 N 1303:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



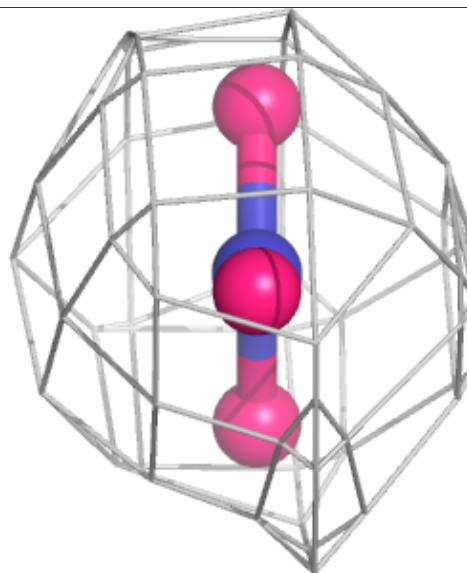
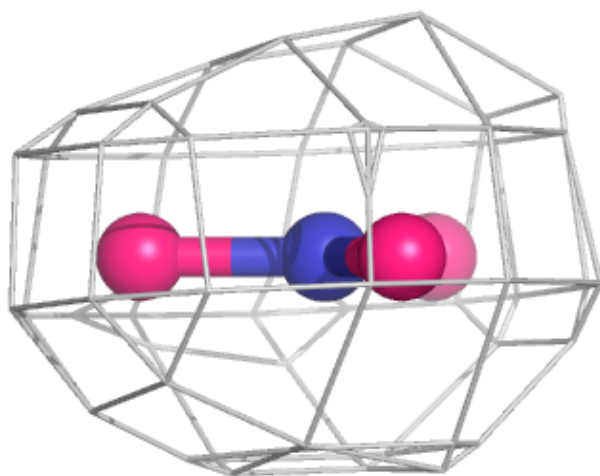
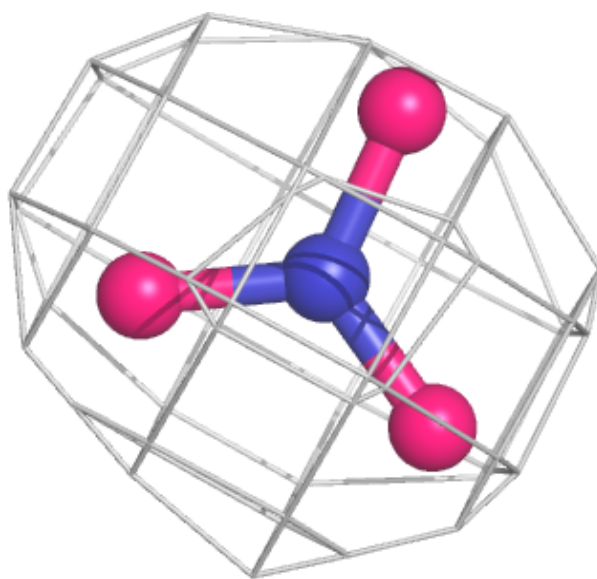
**Electron density around NO3 J 903:**

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



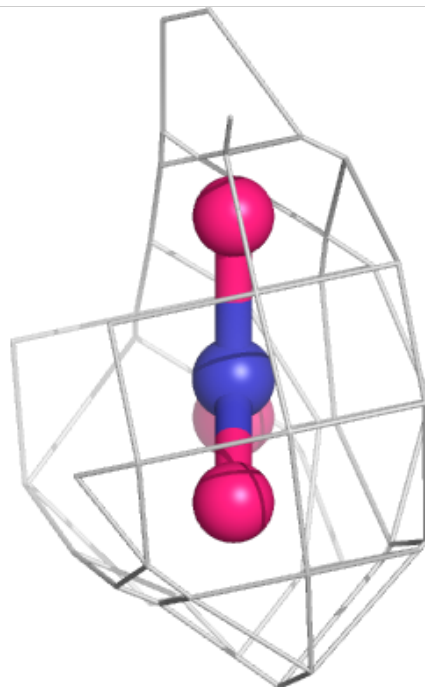
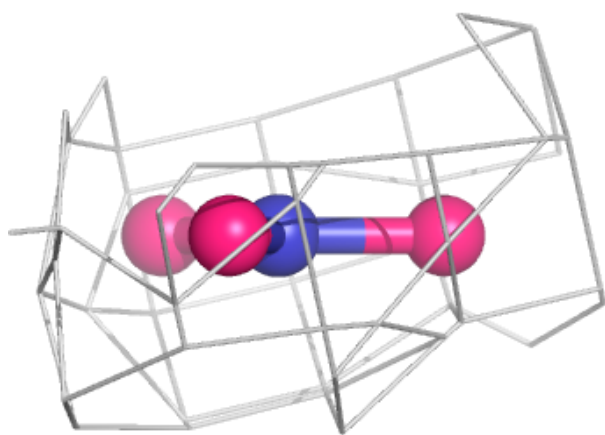
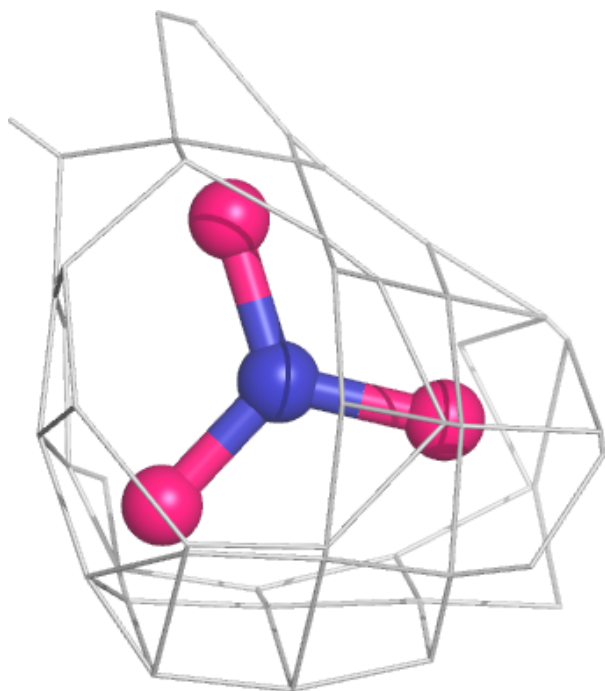
**Electron density around NO3 A 801:**

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



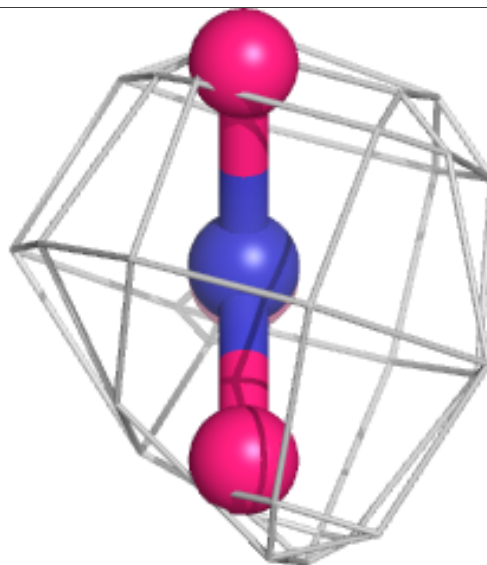
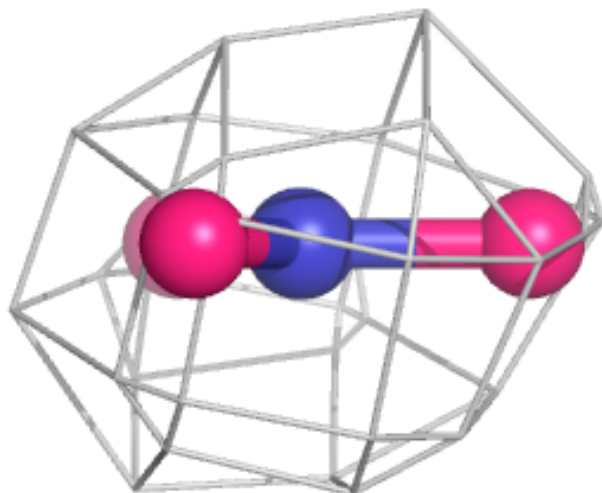
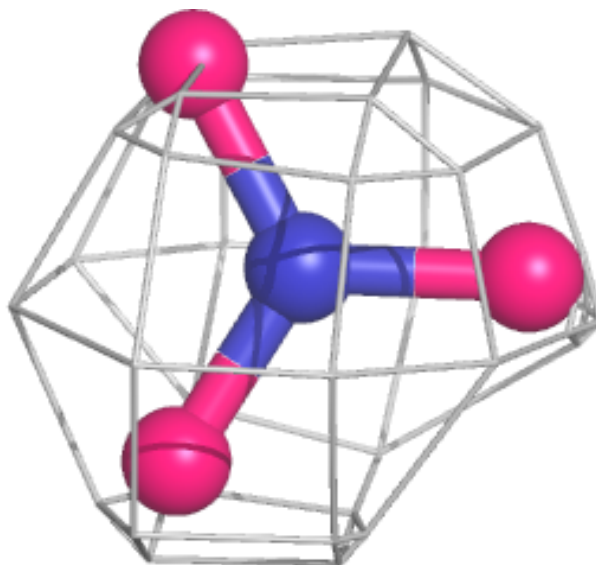
**Electron density around NO3 M 501:**

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



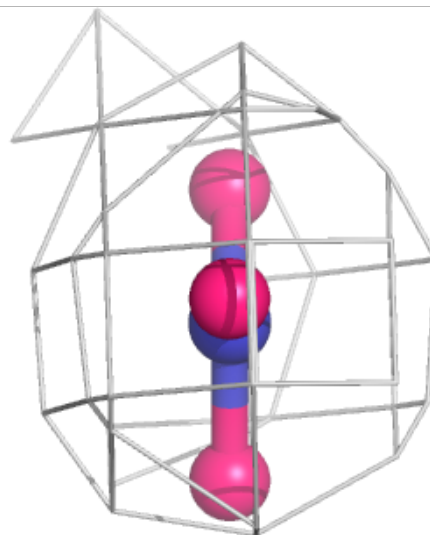
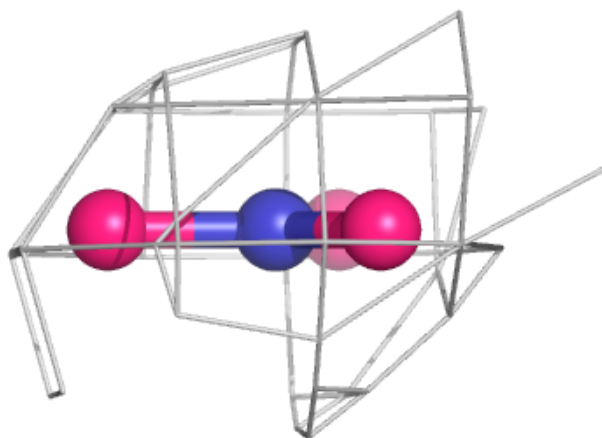
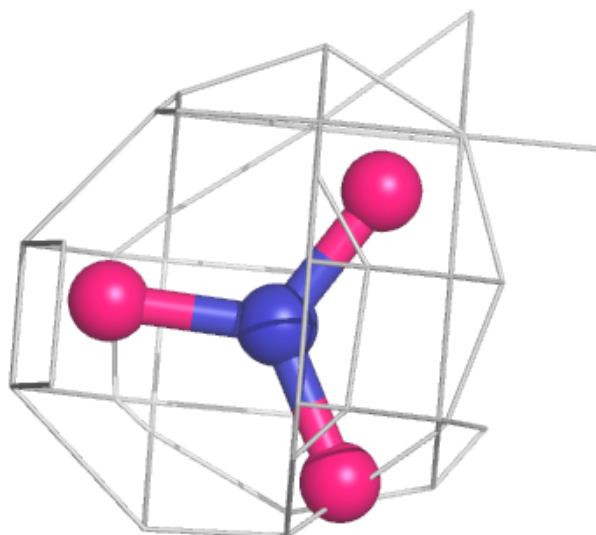
**Electron density around NO3 N 1307:**

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



**Electron density around NO3 C 303:**

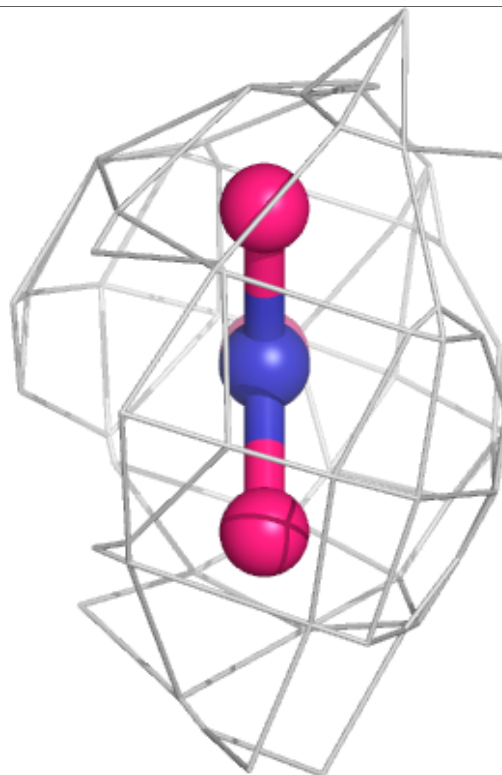
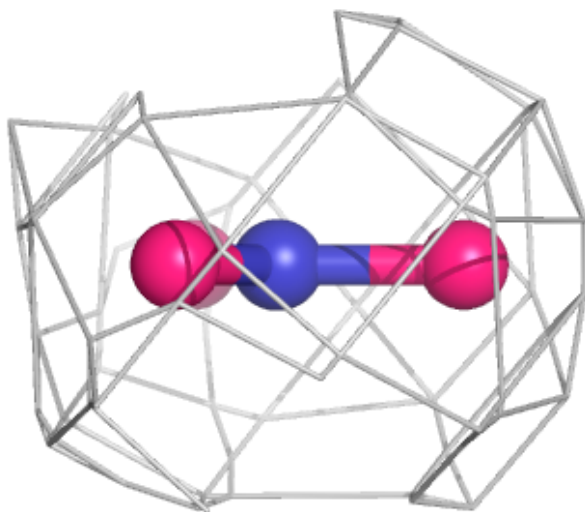
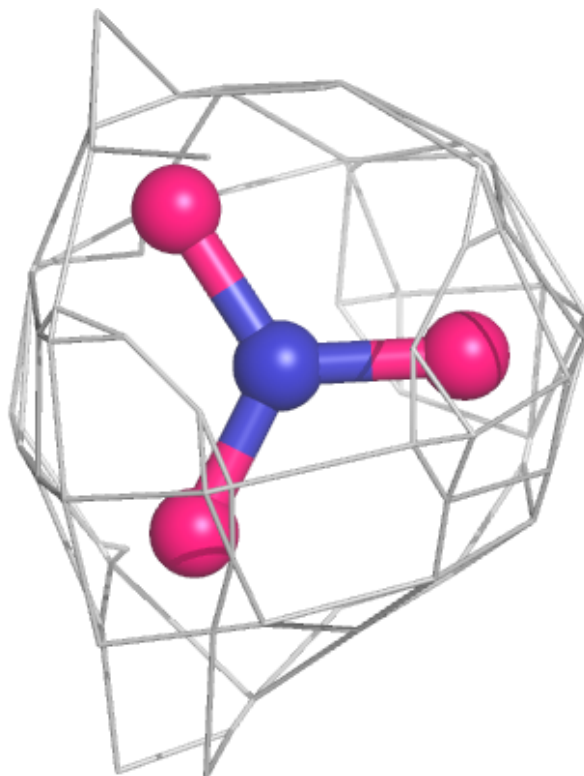
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





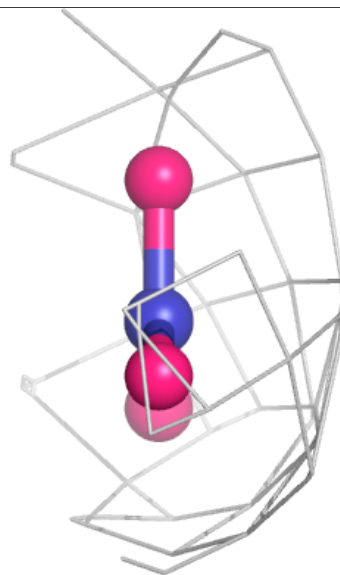
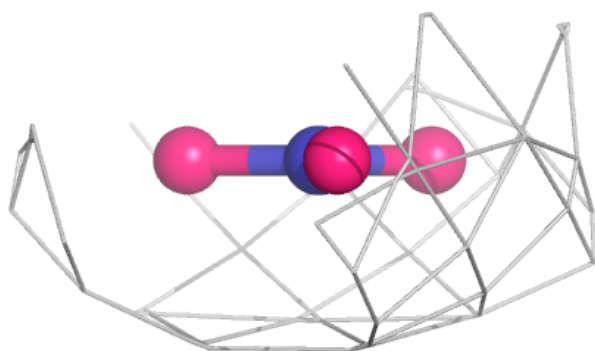
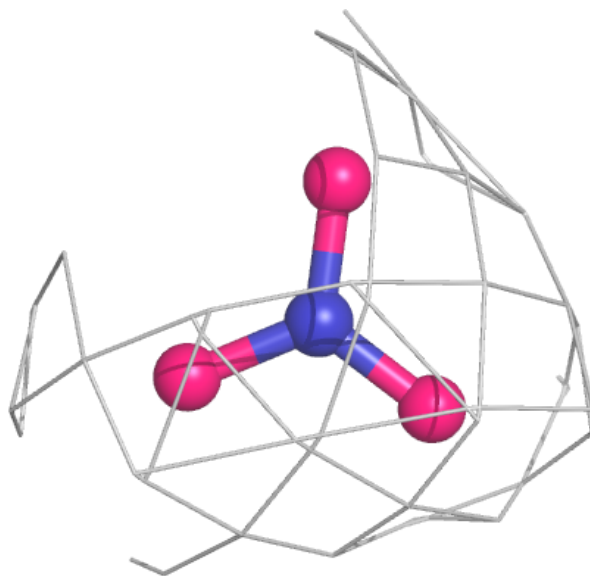
**Electron density around NO3 N 1301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



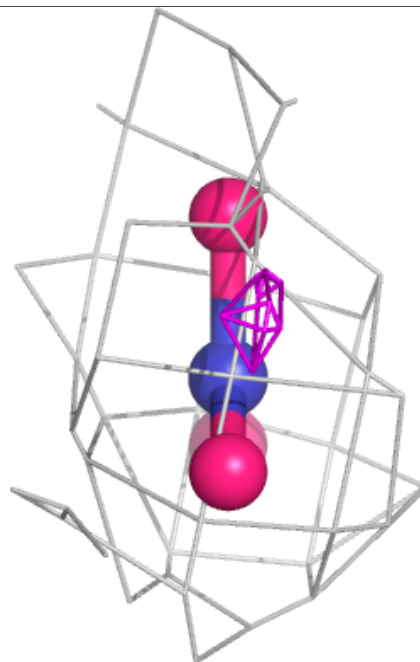
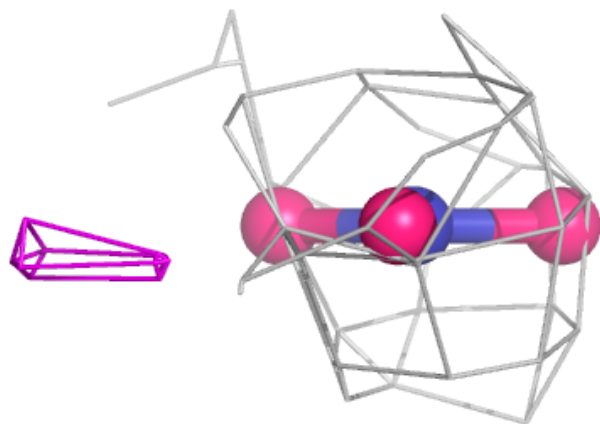
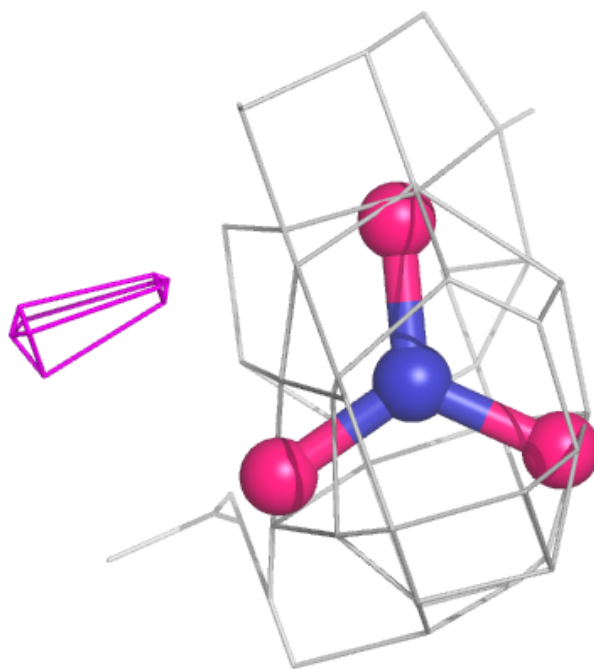
**Electron density around NO3 II 205:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



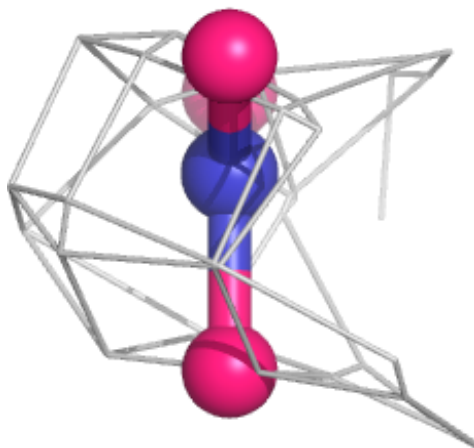
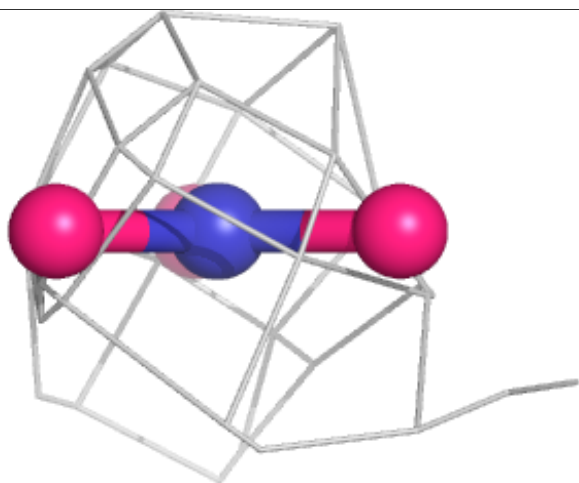
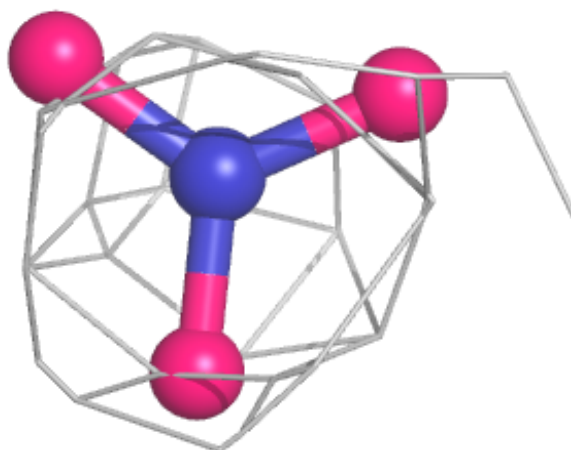
**Electron density around NO3 O 303:**

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



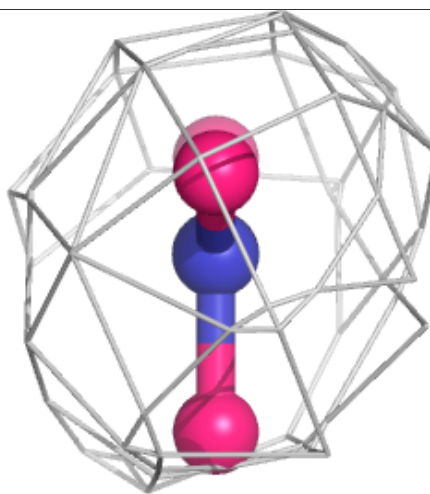
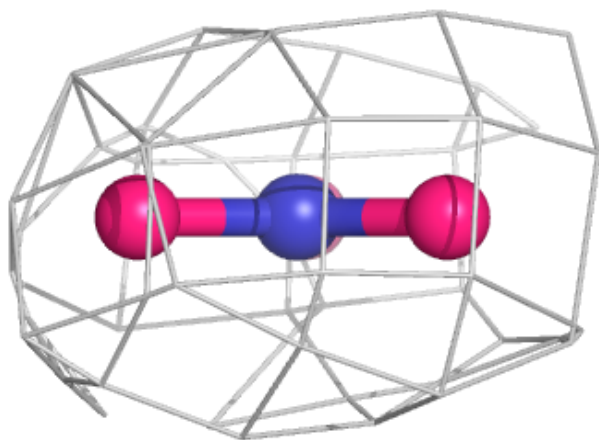
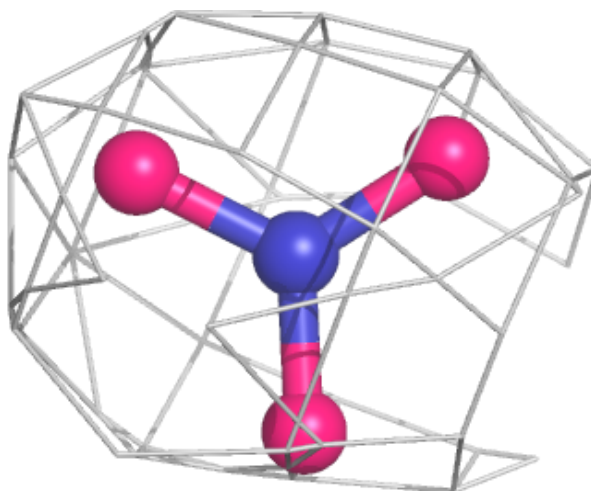
**Electron density around NO3 I 603:**

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



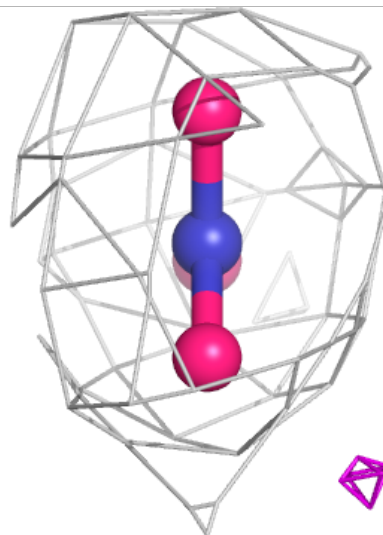
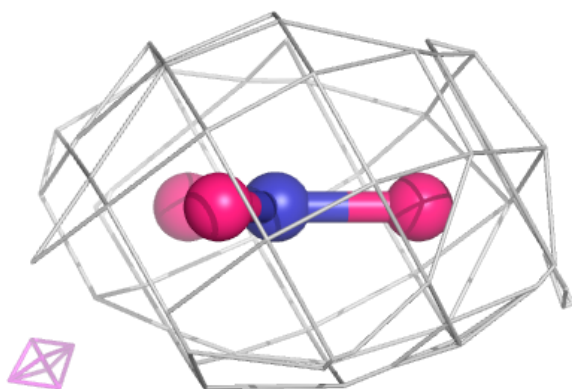
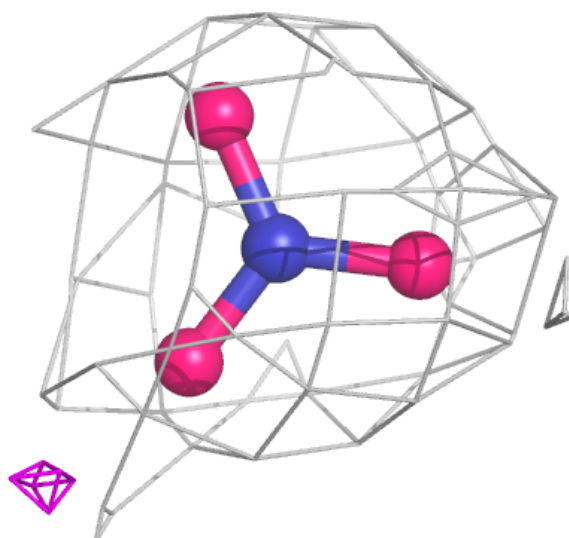
**Electron density around NO3 L 503:**

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



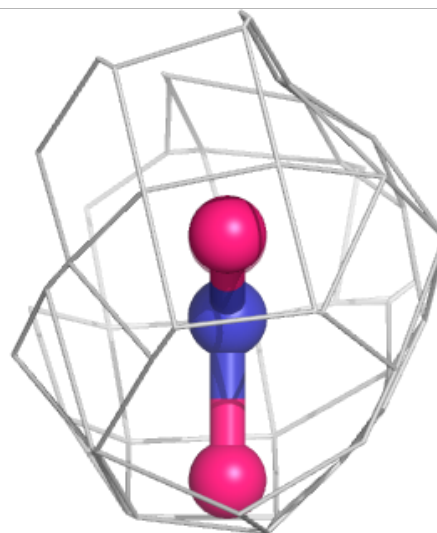
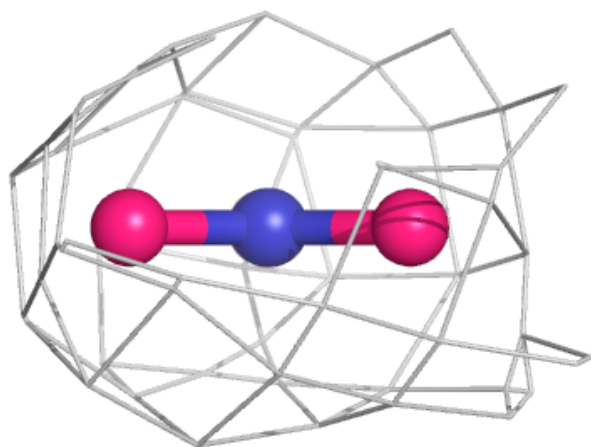
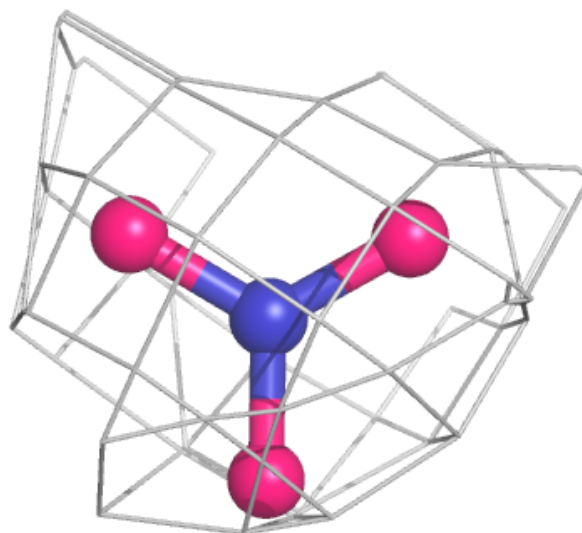
**Electron density around NO3 H 501:**

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



**Electron density around NO3 B 303:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.