



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2021 – 02:11 PM EDT

PDB ID : 6X27
Title : Lon protease proteolytic domain complexed with bortezomib
Authors : Lee, C.C.; Spraggon, G.
Deposited on : 2020-05-20
Resolution : 2.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.18
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) : 2.18

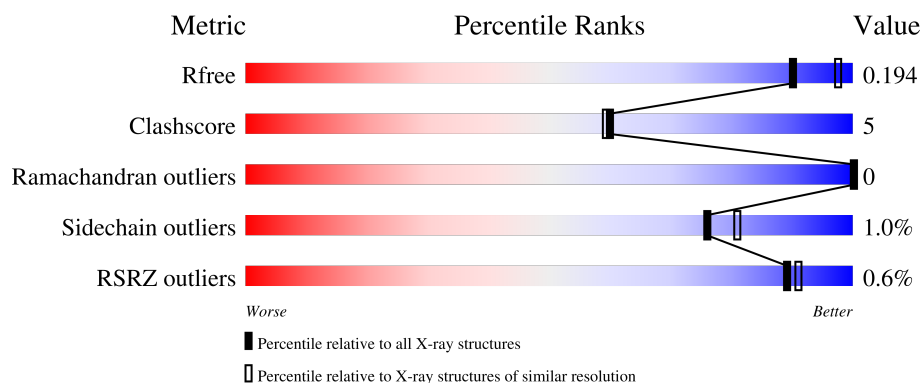
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 78%; width: 15%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 93%; width: 15%; height: 10px; background-color: grey;"></div> </div> <div>78% 7% 15%</div> </div>
1	B	218	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 77%; width: 8%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 85%; width: 15%; height: 10px; background-color: grey;"></div> </div> <div>77% 8% 15%</div> </div>
1	C	218	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 81%; width: 7%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 88%; width: 11%; height: 10px; background-color: grey;"></div> </div> <div>81% 7% 11%</div> </div>
1	D	218	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 80%; width: 5%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 85%; width: 15%; height: 10px; background-color: grey;"></div> </div> <div>80% 5% 15%</div> </div>
1	E	218	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 78%; width: 7%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 85%; width: 15%; height: 10px; background-color: grey;"></div> </div> <div>78% 7% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	218	
1	G	218	
1	H	218	
1	I	218	
1	J	218	
1	K	218	
1	L	218	

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
3	1PE	A	1002	-	-	X	-
3	1PE	F	1002	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19066 atoms, of which 16 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 Lon protease homolog, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	2	0
			1413	906	242	256	9			
1	B	185	Total	C	N	O	S	0	1	0
			1390	892	234	255	9			
1	C	194	Total	C	N	O	S	0	3	0
			1462	939	248	266	9			
1	D	185	Total	C	N	O	S	0	2	0
			1402	896	240	257	9			
1	E	185	Total	C	N	O	S	0	2	0
			1393	894	236	254	9			
1	F	185	Total	C	N	O	S	0	2	0
			1400	898	238	255	9			
1	G	184	Total	C	N	O	S	0	2	0
			1389	893	236	251	9			
1	H	193	Total	C	N	O	S	0	2	0
			1447	926	244	268	9			
1	I	186	Total	C	N	O	S	0	1	0
			1389	892	235	253	9			
1	J	186	Total	C	N	O	S	0	2	0
			1403	900	238	256	9			
1	K	186	Total	C	N	O	S	0	2	0
			1405	901	239	256	9			
1	L	194	Total	C	N	O	S	0	3	0
			1456	934	245	268	9			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	742	MET	-	initiating methionine	UNP P36776
A	743	GLY	-	expression tag	UNP P36776
A	744	SER	-	expression tag	UNP P36776
A	745	ASP	-	expression tag	UNP P36776
A	746	LYS	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
A	747	ILE	-	expression tag	UNP P36776
A	748	HIS	-	expression tag	UNP P36776
A	749	HIS	-	expression tag	UNP P36776
A	750	HIS	-	expression tag	UNP P36776
A	751	HIS	-	expression tag	UNP P36776
A	752	HIS	-	expression tag	UNP P36776
A	753	HIS	-	expression tag	UNP P36776
B	742	MET	-	initiating methionine	UNP P36776
B	743	GLY	-	expression tag	UNP P36776
B	744	SER	-	expression tag	UNP P36776
B	745	ASP	-	expression tag	UNP P36776
B	746	LYS	-	expression tag	UNP P36776
B	747	ILE	-	expression tag	UNP P36776
B	748	HIS	-	expression tag	UNP P36776
B	749	HIS	-	expression tag	UNP P36776
B	750	HIS	-	expression tag	UNP P36776
B	751	HIS	-	expression tag	UNP P36776
B	752	HIS	-	expression tag	UNP P36776
B	753	HIS	-	expression tag	UNP P36776
C	742	MET	-	initiating methionine	UNP P36776
C	743	GLY	-	expression tag	UNP P36776
C	744	SER	-	expression tag	UNP P36776
C	745	ASP	-	expression tag	UNP P36776
C	746	LYS	-	expression tag	UNP P36776
C	747	ILE	-	expression tag	UNP P36776
C	748	HIS	-	expression tag	UNP P36776
C	749	HIS	-	expression tag	UNP P36776
C	750	HIS	-	expression tag	UNP P36776
C	751	HIS	-	expression tag	UNP P36776
C	752	HIS	-	expression tag	UNP P36776
C	753	HIS	-	expression tag	UNP P36776
D	742	MET	-	initiating methionine	UNP P36776
D	743	GLY	-	expression tag	UNP P36776
D	744	SER	-	expression tag	UNP P36776
D	745	ASP	-	expression tag	UNP P36776
D	746	LYS	-	expression tag	UNP P36776
D	747	ILE	-	expression tag	UNP P36776
D	748	HIS	-	expression tag	UNP P36776
D	749	HIS	-	expression tag	UNP P36776
D	750	HIS	-	expression tag	UNP P36776
D	751	HIS	-	expression tag	UNP P36776
D	752	HIS	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
D	753	HIS	-	expression tag	UNP P36776
E	742	MET	-	initiating methionine	UNP P36776
E	743	GLY	-	expression tag	UNP P36776
E	744	SER	-	expression tag	UNP P36776
E	745	ASP	-	expression tag	UNP P36776
E	746	LYS	-	expression tag	UNP P36776
E	747	ILE	-	expression tag	UNP P36776
E	748	HIS	-	expression tag	UNP P36776
E	749	HIS	-	expression tag	UNP P36776
E	750	HIS	-	expression tag	UNP P36776
E	751	HIS	-	expression tag	UNP P36776
E	752	HIS	-	expression tag	UNP P36776
E	753	HIS	-	expression tag	UNP P36776
F	742	MET	-	initiating methionine	UNP P36776
F	743	GLY	-	expression tag	UNP P36776
F	744	SER	-	expression tag	UNP P36776
F	745	ASP	-	expression tag	UNP P36776
F	746	LYS	-	expression tag	UNP P36776
F	747	ILE	-	expression tag	UNP P36776
F	748	HIS	-	expression tag	UNP P36776
F	749	HIS	-	expression tag	UNP P36776
F	750	HIS	-	expression tag	UNP P36776
F	751	HIS	-	expression tag	UNP P36776
F	752	HIS	-	expression tag	UNP P36776
F	753	HIS	-	expression tag	UNP P36776
G	742	MET	-	initiating methionine	UNP P36776
G	743	GLY	-	expression tag	UNP P36776
G	744	SER	-	expression tag	UNP P36776
G	745	ASP	-	expression tag	UNP P36776
G	746	LYS	-	expression tag	UNP P36776
G	747	ILE	-	expression tag	UNP P36776
G	748	HIS	-	expression tag	UNP P36776
G	749	HIS	-	expression tag	UNP P36776
G	750	HIS	-	expression tag	UNP P36776
G	751	HIS	-	expression tag	UNP P36776
G	752	HIS	-	expression tag	UNP P36776
G	753	HIS	-	expression tag	UNP P36776
H	742	MET	-	initiating methionine	UNP P36776
H	743	GLY	-	expression tag	UNP P36776
H	744	SER	-	expression tag	UNP P36776
H	745	ASP	-	expression tag	UNP P36776
H	746	LYS	-	expression tag	UNP P36776

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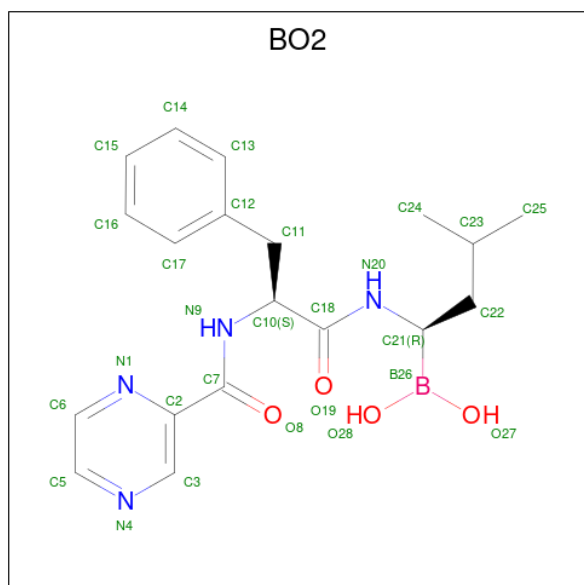
Chain	Residue	Modelled	Actual	Comment	Reference
H	747	ILE	-	expression tag	UNP P36776
H	748	HIS	-	expression tag	UNP P36776
H	749	HIS	-	expression tag	UNP P36776
H	750	HIS	-	expression tag	UNP P36776
H	751	HIS	-	expression tag	UNP P36776
H	752	HIS	-	expression tag	UNP P36776
H	753	HIS	-	expression tag	UNP P36776
I	742	MET	-	initiating methionine	UNP P36776
I	743	GLY	-	expression tag	UNP P36776
I	744	SER	-	expression tag	UNP P36776
I	745	ASP	-	expression tag	UNP P36776
I	746	LYS	-	expression tag	UNP P36776
I	747	ILE	-	expression tag	UNP P36776
I	748	HIS	-	expression tag	UNP P36776
I	749	HIS	-	expression tag	UNP P36776
I	750	HIS	-	expression tag	UNP P36776
I	751	HIS	-	expression tag	UNP P36776
I	752	HIS	-	expression tag	UNP P36776
I	753	HIS	-	expression tag	UNP P36776
J	742	MET	-	initiating methionine	UNP P36776
J	743	GLY	-	expression tag	UNP P36776
J	744	SER	-	expression tag	UNP P36776
J	745	ASP	-	expression tag	UNP P36776
J	746	LYS	-	expression tag	UNP P36776
J	747	ILE	-	expression tag	UNP P36776
J	748	HIS	-	expression tag	UNP P36776
J	749	HIS	-	expression tag	UNP P36776
J	750	HIS	-	expression tag	UNP P36776
J	751	HIS	-	expression tag	UNP P36776
J	752	HIS	-	expression tag	UNP P36776
J	753	HIS	-	expression tag	UNP P36776
K	742	MET	-	initiating methionine	UNP P36776
K	743	GLY	-	expression tag	UNP P36776
K	744	SER	-	expression tag	UNP P36776
K	745	ASP	-	expression tag	UNP P36776
K	746	LYS	-	expression tag	UNP P36776
K	747	ILE	-	expression tag	UNP P36776
K	748	HIS	-	expression tag	UNP P36776
K	749	HIS	-	expression tag	UNP P36776
K	750	HIS	-	expression tag	UNP P36776
K	751	HIS	-	expression tag	UNP P36776
K	752	HIS	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
K	753	HIS	-	expression tag	UNP P36776
L	742	MET	-	initiating methionine	UNP P36776
L	743	GLY	-	expression tag	UNP P36776
L	744	SER	-	expression tag	UNP P36776
L	745	ASP	-	expression tag	UNP P36776
L	746	LYS	-	expression tag	UNP P36776
L	747	ILE	-	expression tag	UNP P36776
L	748	HIS	-	expression tag	UNP P36776
L	749	HIS	-	expression tag	UNP P36776
L	750	HIS	-	expression tag	UNP P36776
L	751	HIS	-	expression tag	UNP P36776
L	752	HIS	-	expression tag	UNP P36776
L	753	HIS	-	expression tag	UNP P36776

- Molecule 2 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄) (labeled as "Ligand of Interest" by depositor).



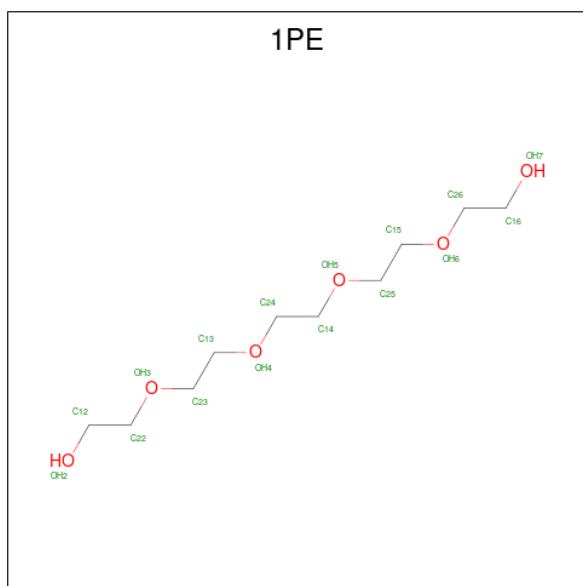
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	B	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
2	C	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	D	1	Total	B	C	N	O	0	1
			34	1	25	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	F	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	G	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	H	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	I	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	J	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	K	1	Total	B	C	N	O	0	1
			34	1	25	4	4		
2	L	1	Total	B	C	N	O	0	1
			34	1	25	4	4		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			16	10	6		
3	H	1	Total	C	O	0	0
			16	10	6		
3	I	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	L	1	Total	C	H	O	0	0
			14	3	8	3		

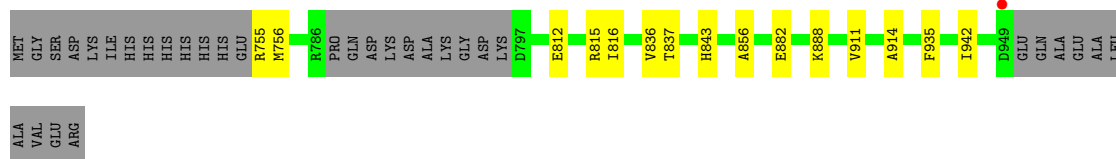
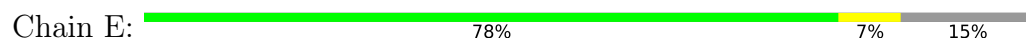
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	157	Total	O	0	0
			157	157		
5	B	125	Total	O	0	0
			125	125		
5	C	147	Total	O	0	0
			147	147		
5	D	128	Total	O	0	0
			128	128		

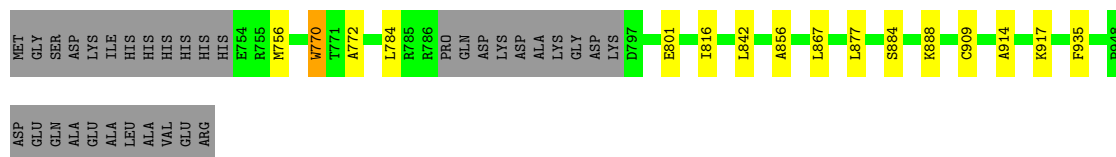
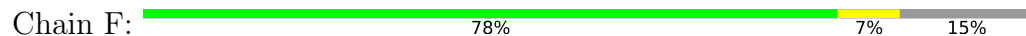
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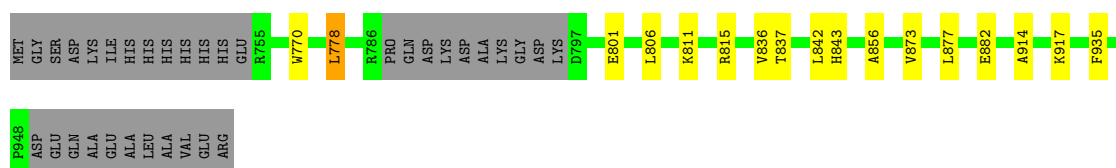
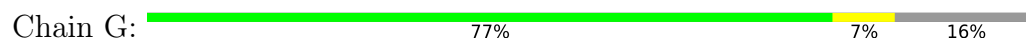
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	142	Total 142	O 142	0	0
5	F	144	Total 144	O 144	0	0
5	G	122	Total 122	O 122	0	0
5	H	121	Total 121	O 121	0	0
5	I	138	Total 138	O 138	0	0
5	J	107	Total 107	O 107	0	0
5	K	123	Total 123	O 123	0	0
5	L	137	Total 137	O 137	0	0



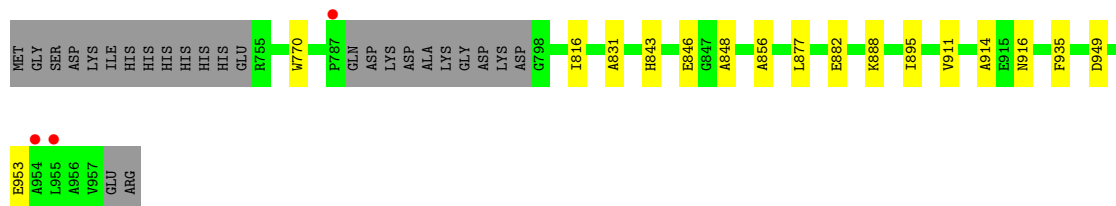
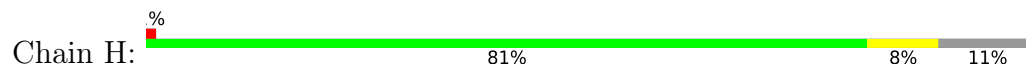
- Molecule 1: Lon protease homolog, mitochondrial



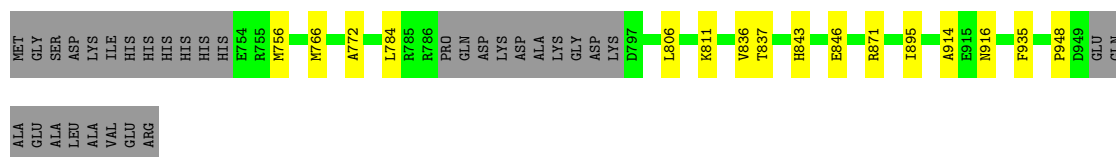
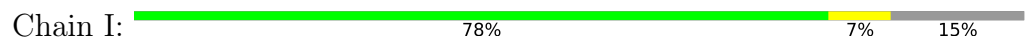
- Molecule 1: Lon protease homolog, mitochondrial




- Molecule 1: Lon protease homolog, mitochondrial

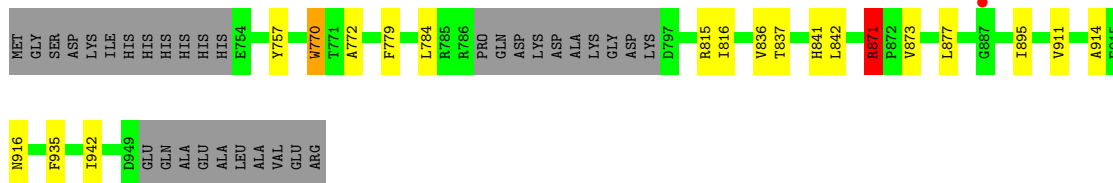


- Molecule 1: Lon protease homolog, mitochondrial




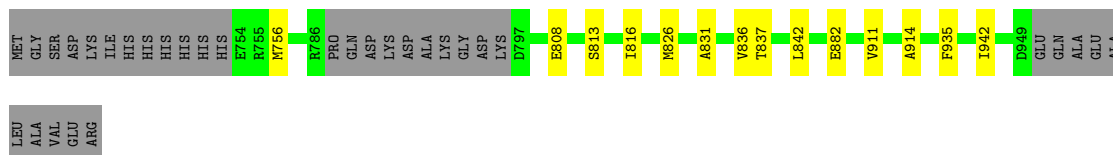
- Molecule 1: Lon protease homolog, mitochondrial

Chain J:  76% 8% 15%




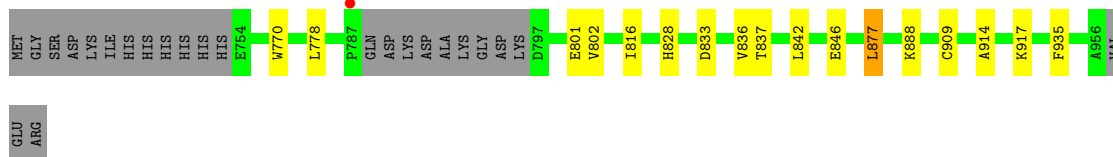
- Molecule 1: Lon protease homolog, mitochondrial

Chain K:  79% 6% 15%



- Molecule 1: Lon protease homolog, mitochondrial

Chain L:  81% 7% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	175.37Å 175.37Å 206.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.04 – 2.12 46.04 – 2.12	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.04-2.12) 100.0 (46.04-2.12)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.157 , 0.194 0.158 , 0.194	Depositor DCC
R_{free} test set	8835 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19066	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, GOL, BO2

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	0.42	0/1450	0.58	0/1968
1	B	0.40	0/1423	0.54	0/1933
1	C	0.40	0/1503	0.55	0/2043
1	D	0.40	0/1438	0.59	0/1952
1	E	0.42	0/1429	0.54	0/1941
1	F	0.44	0/1436	0.57	0/1949
1	G	0.40	0/1425	0.55	0/1934
1	H	0.41	0/1484	0.56	0/2018
1	I	0.37	0/1422	0.55	0/1932
1	J	0.41	0/1439	0.58	1/1954 (0.1%)
1	K	0.38	0/1441	0.55	0/1956
1	L	0.39	0/1497	0.55	0/2036
All	All	0.40	0/17387	0.56	1/23616 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	871	ARG	CG-CD-NE	5.62	123.61	111.80

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	1413	0	1425	15	0
1	B	1390	0	1387	14	0
1	C	1462	0	1461	12	0
1	D	1402	0	1400	7	0
1	E	1393	0	1392	15	0
1	F	1400	0	1407	20	0
1	G	1389	0	1399	17	0
1	H	1447	0	1437	13	0
1	I	1389	0	1386	12	0
1	J	1403	0	1402	15	0
1	K	1405	0	1409	10	0
1	L	1456	0	1443	11	0
2	A	34	0	14	1	0
2	B	28	0	25	0	0
2	C	34	0	14	2	0
2	D	34	0	14	0	0
2	E	34	0	14	0	0
2	F	34	0	14	3	0
2	G	34	0	14	5	0
2	H	34	0	14	1	0
2	I	34	0	14	0	0
2	J	34	0	14	0	0
2	K	34	0	14	0	0
2	L	34	0	14	0	0
3	A	16	0	22	11	0
3	B	16	0	22	2	0
3	C	16	0	22	4	0
3	F	16	0	22	14	0
3	H	16	0	22	5	0
3	I	16	0	22	2	0
4	G	6	8	8	0	0
4	L	6	8	8	0	0
5	A	157	0	0	2	0
5	B	125	0	0	3	0
5	C	147	0	0	3	0
5	D	128	0	0	0	0
5	E	142	0	0	4	0
5	F	144	0	0	3	0
5	G	122	0	0	0	0
5	H	121	0	0	5	0
5	I	138	0	0	2	0
5	J	107	0	0	0	0
5	K	123	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	137	0	0	1	0
All	All	19050	16	17275	159	0

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

All (159) 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)
3:H:1002:1PE:H161	5:H:1201:HOH:O	1.70	0.90
3:F:1002:1PE:H262	5:F:1202:HOH:O	1.80	0.81
1:D:756:MET:O	1:F:888:LYS:HE2	1.85	0.77
2:C:1001[A]:BO2:C17	3:C:1002:1PE:H131	2.18	0.73
3:A:1002:1PE:H232	5:A:1196:HOH:O	1.90	0.70
1:E:815[B]:ARG:NH1	5:E:1101:HOH:O	2.22	0.68
1:L:836:VAL:HG23	1:L:837:THR:HG23	1.76	0.67
1:D:877:LEU:HD23	1:D:909:CYS:SG	2.35	0.66
3:A:1002:1PE:H152	2:G:1001[A]:BO2:C13	2.26	0.66
2:F:1001[A]:BO2:C17	3:F:1002:1PE:H132	2.26	0.66
1:A:888:LYS:HE2	1:F:756:MET:O	1.97	0.65
1:F:772:ALA:HB2	3:F:1002:1PE:H261	1.78	0.65
3:I:1002:1PE:H232	5:I:1207:HOH:O	1.99	0.60
1:A:756:MET:O	1:C:888:LYS:HE2	2.01	0.60
3:B:1002:1PE:H242	5:B:1147:HOH:O	2.01	0.60
1:J:871:ARG:HG2	1:J:871:ARG:HH21	1.66	0.60
1:J:873:VAL:CG1	1:J:877:LEU:HD23	2.31	0.60
1:G:815[B]:ARG:HH11	1:L:801:GLU:HG3	1.68	0.59
1:G:836:VAL:HG23	1:G:837:THR:HG23	1.84	0.59
3:C:1002:1PE:H251	5:C:1218:HOH:O	2.04	0.57
1:B:888:LYS:NZ	5:B:1104:HOH:O	2.38	0.56
1:D:808:GLU:HB3	5:K:1149:HOH:O	2.06	0.56
1:K:836:VAL:HG23	1:K:837:THR:HG23	1.86	0.56
1:B:843:HIS:CE1	1:E:816:ILE:HD11	2.42	0.55
1:E:812:GLU:HG2	1:E:815[B]:ARG:NH1	2.21	0.55
3:A:1002:1PE:H152	2:G:1001[A]:BO2:C12	2.36	0.55
1:E:755:ARG:HG3	5:E:1235:HOH:O	2.07	0.54
1:J:873:VAL:HG11	1:J:877:LEU:HD23	1.89	0.54
1:J:914:ALA:HA	1:J:935:PHE:HB3	1.88	0.54
1:F:770:TRP:CE2	3:F:1002:1PE:H131	2.43	0.53
1:F:772:ALA:CB	3:F:1002:1PE:H261	2.37	0.53
3:F:1002:1PE:H241	1:J:772:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:ALA:HA	1:B:935:PHE:HB3	1.91	0.52
1:K:914:ALA:HA	1:K:935:PHE:HB3	1.92	0.52
1:B:888:LYS:HE2	1:I:756:MET:O	2.09	0.52
3:H:1002:1PE:H261	5:H:1196:HOH:O	2.08	0.52
1:J:871:ARG:HH21	1:J:871:ARG:CG	2.22	0.52
1:H:914:ALA:HA	1:H:935:PHE:HB3	1.93	0.51
1:E:756:MET:O	1:L:888:LYS:HE2	2.10	0.51
1:F:917:LYS:HA	1:F:935:PHE:CE1	2.46	0.51
1:C:756:MET:O	1:H:888:LYS:HE2	2.11	0.51
1:I:836:VAL:HG23	1:I:837:THR:HG23	1.92	0.50
1:D:888:LYS:NZ	1:K:756:MET:O	2.44	0.50
1:D:914:ALA:HA	1:D:935:PHE:HB3	1.94	0.50
1:C:914:ALA:HA	1:C:935:PHE:HB3	1.94	0.50
2:C:1001[A]:BO2:H17	3:C:1002:1PE:H131	1.94	0.49
1:A:914:ALA:HA	1:A:935:PHE:HB3	1.93	0.49
2:F:1001[A]:BO2:C12	3:F:1002:1PE:H132	2.43	0.49
1:B:756:MET:O	1:E:888:LYS:HE2	2.12	0.49
3:H:1002:1PE:H261	3:H:1002:1PE:H251	1.56	0.49
1:F:784:LEU:HD23	1:F:867:LEU:HG	1.93	0.48
1:A:815[B]:ARG:HG2	1:F:801:GLU:OE1	2.13	0.48
3:A:1002:1PE:H142	1:G:770:TRP:CH2	2.49	0.48
2:F:1001[A]:BO2:H112	3:F:1002:1PE:H132	1.96	0.48
1:E:843:HIS:CE1	1:L:816:ILE:HD11	2.48	0.48
1:G:770:TRP:O	2:G:1001[A]:BO2:H13	2.13	0.48
1:K:831:ALA:HB3	5:K:1104:HOH:O	2.14	0.48
1:F:877:LEU:HD23	1:F:909:CYS:SG	2.54	0.48
1:K:911:VAL:HG11	1:K:942:ILE:HG12	1.95	0.48
3:A:1002:1PE:H142	1:G:770:TRP:CZ3	2.49	0.48
1:H:846:GLU:HG2	1:K:882:GLU:OE1	2.14	0.48
2:A:1001[A]:BO2:C17	3:A:1002:1PE:H231	2.43	0.48
1:I:871:ARG:NH1	1:I:948:PRO:O	2.47	0.48
1:I:895:ILE:HG13	1:I:916:ASN:HB3	1.96	0.47
1:F:888:LYS:NZ	5:F:1102:HOH:O	2.46	0.47
3:F:1002:1PE:H251	1:J:770:TRP:CZ2	2.50	0.47
1:C:843:HIS:CE1	1:H:816:ILE:HD11	2.50	0.47
1:F:888:LYS:HE3	5:F:1172:HOH:O	2.14	0.47
3:A:1002:1PE:H262	2:G:1001[B]:BO2:C13	2.44	0.47
1:E:911:VAL:HG11	1:E:942:ILE:HG12	1.97	0.47
1:I:914:ALA:HA	1:I:935:PHE:HB3	1.97	0.47
1:J:757:TYR:HB2	1:J:779:PHE:CE1	2.49	0.47
1:H:846:GLU:CD	1:H:848:ALA:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:TRP:CE2	3:B:1002:1PE:H251	2.51	0.46
1:B:784:LEU:C	1:B:784:LEU:HD12	2.35	0.46
2:H:1001[A]:BO2:C13	3:H:1002:1PE:H231	2.44	0.46
1:E:914:ALA:HA	1:E:935:PHE:HB3	1.98	0.46
1:C:888:LYS:HE3	5:C:1178:HOH:O	2.15	0.46
1:D:843:HIS:CE1	1:F:816:ILE:HD11	2.51	0.46
1:C:782:THR:HG22	1:C:842:LEU:HD12	1.98	0.46
1:K:808:GLU:OE2	5:K:1101:HOH:O	2.20	0.46
1:B:801:GLU:OE1	1:E:815[B]:ARG:HD2	2.16	0.45
1:L:914:ALA:HA	1:L:935:PHE:HB3	1.97	0.45
1:A:784:LEU:C	1:A:784:LEU:HD12	2.37	0.45
1:E:888:LYS:HE3	5:E:1181:HOH:O	2.15	0.45
1:H:895:ILE:HG13	1:H:916:ASN:HB3	1.97	0.45
1:L:877:LEU:HD12	1:L:909:CYS:SG	2.57	0.45
1:F:784:LEU:C	1:F:784:LEU:HD12	2.36	0.45
1:I:772:ALA:HA	3:I:1002:1PE:H141	1.97	0.45
5:H:1209:HOH:O	1:K:826:MET:HE2	2.15	0.45
1:H:843:HIS:CE1	1:K:816:ILE:HD11	2.52	0.45
1:J:836:VAL:HG23	1:J:837:THR:HG23	1.99	0.44
1:L:828[A]:HIS:NE2	5:L:1101:HOH:O	2.33	0.44
1:A:846:GLU:CD	1:A:848:ALA:H	2.21	0.44
1:C:786:ARG:HD3	1:C:834:TYR:CE2	2.53	0.44
1:B:784:LEU:HD23	1:B:867:LEU:HG	2.00	0.44
3:C:1002:1PE:H132	3:C:1002:1PE:H222	1.51	0.44
1:A:770:TRP:CH2	3:A:1002:1PE:H241	2.53	0.44
1:A:786:ARG:HH21	1:A:786:ARG:HG3	1.82	0.44
1:F:772:ALA:HB2	3:F:1002:1PE:H252	1.99	0.44
1:B:882:GLU:OE2	1:I:846:GLU:HG2	2.18	0.43
1:A:843:HIS:CE1	1:C:816:ILE:HD11	2.52	0.43
1:C:930:GLY:N	5:C:1102:HOH:O	2.42	0.43
1:J:895:ILE:HG13	1:J:916:ASN:HB3	1.99	0.43
1:B:904:ARG:NH2	5:B:1106:HOH:O	2.50	0.43
1:F:877:LEU:C	1:F:877:LEU:HD13	2.38	0.43
1:G:873:VAL:HG11	1:G:877:LEU:HD23	2.00	0.43
1:F:914:ALA:HA	1:F:935:PHE:HB3	2.00	0.43
3:F:1002:1PE:H262	3:F:1002:1PE:H252	1.73	0.43
1:A:841[A]:HIS:HD2	1:A:842:LEU:N	2.16	0.42
1:H:877:LEU:HD11	1:H:911:VAL:HG23	2.01	0.42
1:E:836:VAL:HG23	1:E:837:THR:HG23	2.01	0.42
1:G:801:GLU:HG3	1:J:815[B]:ARG:HH11	1.83	0.42
1:I:784:LEU:C	1:I:784:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ARG:HG3	1:A:786:ARG:NH2	2.34	0.42
1:K:842:LEU:C	1:K:842:LEU:HD23	2.39	0.42
3:A:1002:1PE:H252	1:G:770:TRP:CE2	2.55	0.42
1:G:882:GLU:OE2	1:L:846:GLU:HG2	2.20	0.42
3:A:1002:1PE:H262	2:G:1001[A]:BO2:C17	2.50	0.42
1:L:917:LYS:HA	1:L:935:PHE:CE1	2.54	0.42
1:A:786:ARG:HD3	1:A:786:ARG:HA	1.96	0.42
1:B:816:ILE:HD11	1:I:843:HIS:CE1	2.55	0.42
1:D:841[A]:HIS:HD2	1:D:842:LEU:N	2.18	0.41
1:I:806:LEU:O	1:I:811:LYS:HE3	2.20	0.41
1:C:895:ILE:HG13	1:C:916:ASN:HB3	2.02	0.41
1:H:949:ASP:O	1:H:953:GLU:HG3	2.20	0.41
1:J:784:LEU:C	1:J:784:LEU:HD12	2.41	0.41
1:F:842:LEU:C	1:F:842:LEU:HD23	2.41	0.41
1:G:843:HIS:CE1	1:J:816:ILE:HD11	2.55	0.41
1:I:766:MET:HE3	5:I:1195:HOH:O	2.19	0.41
1:B:895:ILE:HG13	1:B:916:ASN:HB3	2.02	0.41
1:F:770:TRP:NE1	3:F:1002:1PE:H131	2.35	0.41
3:H:1002:1PE:H251	5:H:1196:HOH:O	2.20	0.41
1:I:784:LEU:HD12	1:I:784:LEU:O	2.21	0.41
1:A:770:TRP:CZ3	3:A:1002:1PE:H241	2.55	0.41
1:A:811:LYS:HE2	5:A:1162:HOH:O	2.20	0.41
1:C:846:GLU:HG2	1:H:882:GLU:OE2	2.20	0.41
1:G:842:LEU:C	1:G:842:LEU:HD23	2.41	0.41
1:H:831:ALA:HB3	5:H:1133:HOH:O	2.20	0.41
1:L:802:VAL:HA	1:L:842:LEU:O	2.20	0.41
1:C:784:LEU:HD12	1:C:784:LEU:C	2.41	0.41
1:B:846:GLU:HG2	1:E:882:GLU:OE2	2.21	0.40
1:G:806:LEU:O	1:G:811:LYS:HE3	2.21	0.40
1:G:914:ALA:HA	1:G:935:PHE:HB3	2.03	0.40
1:L:833:ASP:O	1:L:836:VAL:HG22	2.22	0.40
1:F:770:TRP:CZ2	3:F:1002:1PE:H242	2.56	0.40
1:E:756:MET:N	5:E:1102:HOH:O	2.25	0.40
1:G:917:LYS:HA	1:G:935:PHE:CE1	2.57	0.40
1:J:841[A]:HIS:HD2	1:J:842:LEU:N	2.19	0.40
1:J:911:VAL:HG11	1:J:942:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

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	184/218 (84%)	183 (100%)	1 (0%)	0	100	100
1	B	182/218 (84%)	180 (99%)	2 (1%)	0	100	100
1	C	193/218 (88%)	191 (99%)	2 (1%)	0	100	100
1	D	183/218 (84%)	182 (100%)	1 (0%)	0	100	100
1	E	183/218 (84%)	182 (100%)	1 (0%)	0	100	100
1	F	183/218 (84%)	182 (100%)	1 (0%)	0	100	100
1	G	182/218 (84%)	181 (100%)	1 (0%)	0	100	100
1	H	191/218 (88%)	189 (99%)	2 (1%)	0	100	100
1	I	183/218 (84%)	182 (100%)	1 (0%)	0	100	100
1	J	184/218 (84%)	183 (100%)	1 (0%)	0	100	100
1	K	184/218 (84%)	183 (100%)	1 (0%)	0	100	100
1	L	193/218 (88%)	192 (100%)	1 (0%)	0	100	100
All	All	2225/2616 (85%)	2210 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	148/175 (85%)	148 (100%)	0	100	100
1	B	144/175 (82%)	141 (98%)	3 (2%)	53	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	150/175 (86%)	147 (98%)	3 (2%)	55	59
1	D	146/175 (83%)	145 (99%)	1 (1%)	84	88
1	E	144/175 (82%)	144 (100%)	0	100	100
1	F	146/175 (83%)	144 (99%)	2 (1%)	67	72
1	G	144/175 (82%)	143 (99%)	1 (1%)	84	88
1	H	149/175 (85%)	148 (99%)	1 (1%)	84	88
1	I	143/175 (82%)	143 (100%)	0	100	100
1	J	145/175 (83%)	143 (99%)	2 (1%)	67	72
1	K	146/175 (83%)	145 (99%)	1 (1%)	84	88
1	L	149/175 (85%)	146 (98%)	3 (2%)	55	59
All	All	1754/2100 (84%)	1737 (99%)	17 (1%)	76	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	773	MET
1	B	813	SER
1	B	827	GLN
1	C	770	TRP
1	C	842	LEU
1	C	929	GLU
1	D	813	SER
1	F	770	TRP
1	F	884	SER
1	G	778	LEU
1	H	770	TRP
1	J	770	TRP
1	J	871	ARG
1	K	813	SER
1	L	770	TRP
1	L	778	LEU
1	L	877	LEU

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

Mol	Chain	Res	Type
1	J	827	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BO2	A	1001[B]	-	25,29,29	0.51	0	32,38,38	1.45	8 (25%)
2	BO2	H	1001[A]	-	25,29,29	0.44	0	32,38,38	2.02	7 (21%)
3	1PE	C	1002	-	15,15,15	0.73	0	14,14,14	0.49	0
2	BO2	B	1001	1	25,29,29	0.56	0	32,38,38	1.50	8 (25%)
2	BO2	J	1001[A]	-	25,29,29	0.44	0	32,38,38	1.46	7 (21%)
2	BO2	J	1001[B]	-	25,29,29	0.48	0	32,38,38	1.46	7 (21%)
2	BO2	E	1001[B]	-	25,29,29	0.49	0	32,38,38	2.27	5 (15%)
2	BO2	D	1001[B]	-	25,29,29	0.47	0	32,38,38	1.55	7 (21%)
2	BO2	E	1001[A]	-	25,29,29	0.45	0	32,38,38	2.27	5 (15%)
2	BO2	D	1001[A]	-	25,29,29	0.43	0	32,38,38	1.56	7 (21%)
2	BO2	C	1001[B]	-	25,29,29	0.54	0	32,38,38	1.51	9 (28%)
3	1PE	F	1002	-	15,15,15	0.71	0	14,14,14	0.61	0
3	1PE	B	1002	-	15,15,15	0.68	0	14,14,14	0.59	0
2	BO2	C	1001[A]	-	25,29,29	0.48	0	32,38,38	1.49	8 (25%)
2	BO2	I	1001[A]	-	25,29,29	0.54	0	32,38,38	1.43	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	G	1002	-	5,5,5	0.10	0	5,5,5	0.25	0
3	1PE	A	1002	-	15,15,15	0.70	0	14,14,14	0.70	0
2	BO2	I	1001[B]	-	25,29,29	0.56	0	32,38,38	1.43	6 (18%)
4	GOL	L	1002	-	5,5,5	0.06	0	5,5,5	0.27	0
2	BO2	L	1001[A]	-	25,29,29	0.45	0	32,38,38	1.34	5 (15%)
2	BO2	L	1001[B]	-	25,29,29	0.48	0	32,38,38	1.39	6 (18%)
2	BO2	K	1001[B]	-	25,29,29	0.52	0	32,38,38	1.38	6 (18%)
2	BO2	K	1001[A]	-	25,29,29	0.50	0	32,38,38	1.35	6 (18%)
2	BO2	G	1001[B]	-	25,29,29	0.54	0	32,38,38	2.33	6 (18%)
2	BO2	A	1001[A]	-	25,29,29	0.47	0	32,38,38	1.44	7 (21%)
2	BO2	G	1001[A]	-	25,29,29	0.51	0	32,38,38	2.32	6 (18%)
2	BO2	F	1001[B]	-	25,29,29	0.48	0	32,38,38	1.63	9 (28%)
2	BO2	F	1001[A]	-	25,29,29	0.42	0	32,38,38	1.61	8 (25%)
3	1PE	I	1002	-	15,15,15	0.74	0	14,14,14	0.52	0
3	1PE	H	1002	-	15,15,15	0.65	0	14,14,14	0.67	0
2	BO2	H	1001[B]	-	25,29,29	0.50	0	32,38,38	2.01	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BO2	A	1001[B]	-	-	4/22/28/28	0/2/2/2
2	BO2	H	1001[A]	-	-	6/22/28/28	0/2/2/2
3	1PE	C	1002	-	-	10/13/13/13	-
2	BO2	B	1001	1	-	4/22/28/28	0/2/2/2
2	BO2	J	1001[A]	-	-	4/22/28/28	0/2/2/2
2	BO2	J	1001[B]	-	-	4/22/28/28	0/2/2/2
2	BO2	E	1001[B]	-	-	6/22/28/28	0/2/2/2
2	BO2	D	1001[B]	-	-	4/22/28/28	0/2/2/2
2	BO2	E	1001[A]	-	-	6/22/28/28	0/2/2/2
2	BO2	D	1001[A]	-	-	4/22/28/28	0/2/2/2
2	BO2	C	1001[B]	-	-	4/22/28/28	0/2/2/2
3	1PE	F	1002	-	-	7/13/13/13	-
3	1PE	B	1002	-	-	7/13/13/13	-
2	BO2	C	1001[A]	-	-	4/22/28/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BO2	I	1001[A]	-	-	4/22/28/28	0/2/2/2
4	GOL	G	1002	-	-	2/4/4/4	-
3	1PE	A	1002	-	-	5/13/13/13	-
2	BO2	I	1001[B]	-	-	4/22/28/28	0/2/2/2
4	GOL	L	1002	-	-	0/4/4/4	-
2	BO2	L	1001[A]	-	-	4/22/28/28	0/2/2/2
2	BO2	L	1001[B]	-	-	4/22/28/28	0/2/2/2
2	BO2	K	1001[B]	-	-	4/22/28/28	0/2/2/2
2	BO2	K	1001[A]	-	-	4/22/28/28	0/2/2/2
2	BO2	G	1001[B]	-	-	6/22/28/28	0/2/2/2
2	BO2	A	1001[A]	-	-	4/22/28/28	0/2/2/2
2	BO2	G	1001[A]	-	-	6/22/28/28	0/2/2/2
2	BO2	F	1001[B]	-	-	4/22/28/28	0/2/2/2
2	BO2	F	1001[A]	-	-	4/22/28/28	0/2/2/2
3	1PE	I	1002	-	-	8/13/13/13	-
3	1PE	H	1002	-	-	8/13/13/13	-
2	BO2	H	1001[B]	-	-	6/22/28/28	0/2/2/2

There are no bond length outliers.

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001[A]	BO2	C21-C22-C23	-10.45	102.27	115.39
2	G	1001[B]	BO2	C21-C22-C23	-10.45	102.27	115.39
2	E	1001[A]	BO2	C21-C22-C23	-10.38	102.36	115.39
2	E	1001[B]	BO2	C21-C22-C23	-10.38	102.36	115.39
2	H	1001[A]	BO2	C21-C22-C23	-8.11	105.21	115.39
2	H	1001[B]	BO2	C21-C22-C23	-8.11	105.21	115.39
2	F	1001[A]	BO2	C18-C10-N9	-3.99	100.30	111.16
2	F	1001[B]	BO2	C18-C10-N9	-3.99	100.30	111.16
2	D	1001[A]	BO2	C18-C10-N9	-3.97	100.36	111.16
2	D	1001[B]	BO2	C18-C10-N9	-3.97	100.36	111.16
2	A	1001[A]	BO2	C18-C10-N9	-3.82	100.75	111.16
2	A	1001[B]	BO2	C18-C10-N9	-3.82	100.75	111.16
2	L	1001[A]	BO2	C18-C10-N9	-3.71	101.05	111.16
2	L	1001[B]	BO2	C18-C10-N9	-3.71	101.05	111.16
2	H	1001[A]	BO2	C18-C10-N9	-3.69	101.11	111.16
2	H	1001[B]	BO2	C18-C10-N9	-3.69	101.11	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1001[A]	BO2	C18-C10-N9	-3.69	101.12	111.16
2	K	1001[B]	BO2	C18-C10-N9	-3.69	101.12	111.16
2	J	1001[A]	BO2	C18-C10-N9	-3.47	101.72	111.16
2	J	1001[B]	BO2	C18-C10-N9	-3.47	101.72	111.16
2	B	1001	BO2	C18-C10-N9	-3.41	101.87	111.16
2	C	1001[A]	BO2	C18-C10-N9	-3.36	102.02	111.16
2	C	1001[B]	BO2	C18-C10-N9	-3.36	102.02	111.16
2	E	1001[A]	BO2	C18-C10-N9	-3.35	102.03	111.16
2	E	1001[B]	BO2	C18-C10-N9	-3.35	102.03	111.16
2	F	1001[A]	BO2	C6-N1-C2	3.30	121.21	116.93
2	F	1001[B]	BO2	C6-N1-C2	3.30	121.21	116.93
2	J	1001[A]	BO2	C6-N1-C2	3.17	121.05	116.93
2	J	1001[B]	BO2	C6-N1-C2	3.17	121.05	116.93
2	I	1001[A]	BO2	C6-N1-C2	3.13	120.99	116.93
2	I	1001[B]	BO2	C6-N1-C2	3.13	120.99	116.93
2	G	1001[A]	BO2	C2-C3-N4	-3.08	118.22	122.05
2	G	1001[B]	BO2	C2-C3-N4	-3.08	118.22	122.05
2	C	1001[A]	BO2	C6-N1-C2	3.05	120.89	116.93
2	C	1001[B]	BO2	C6-N1-C2	3.05	120.89	116.93
2	I	1001[A]	BO2	C18-C10-N9	-3.04	102.90	111.16
2	I	1001[B]	BO2	C18-C10-N9	-3.04	102.90	111.16
2	G	1001[A]	BO2	C18-C10-N9	-2.98	103.06	111.16
2	G	1001[B]	BO2	C18-C10-N9	-2.98	103.06	111.16
2	G	1001[A]	BO2	C6-N1-C2	2.97	120.79	116.93
2	G	1001[B]	BO2	C6-N1-C2	2.97	120.79	116.93
2	D	1001[A]	BO2	C6-N1-C2	2.94	120.75	116.93
2	D	1001[B]	BO2	C6-N1-C2	2.94	120.75	116.93
2	G	1001[A]	BO2	C5-N4-C3	2.85	121.78	116.85
2	G	1001[B]	BO2	C5-N4-C3	2.85	121.78	116.85
2	F	1001[A]	BO2	C5-N4-C3	2.71	121.54	116.85
2	F	1001[B]	BO2	C5-N4-C3	2.71	121.54	116.85
2	I	1001[A]	BO2	C2-C3-N4	-2.70	118.69	122.05
2	I	1001[B]	BO2	C2-C3-N4	-2.70	118.69	122.05
2	K	1001[A]	BO2	C6-N1-C2	2.66	120.38	116.93
2	K	1001[B]	BO2	C6-N1-C2	2.66	120.38	116.93
2	B	1001	BO2	C5-N4-C3	2.66	121.45	116.85
2	E	1001[A]	BO2	C2-C7-N9	2.64	120.10	115.20
2	E	1001[B]	BO2	C2-C7-N9	2.64	120.10	115.20
2	F	1001[A]	BO2	C7-C2-N1	2.62	120.57	117.48
2	F	1001[B]	BO2	C7-C2-N1	2.62	120.57	117.48
2	A	1001[A]	BO2	C7-C2-N1	2.61	120.56	117.48
2	A	1001[B]	BO2	C7-C2-N1	2.61	120.56	117.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	BO2	C6-N1-C2	2.61	120.32	116.93
2	B	1001	BO2	C2-C3-N4	-2.61	118.80	122.05
2	H	1001[A]	BO2	C6-N1-C2	2.60	120.31	116.93
2	H	1001[B]	BO2	C6-N1-C2	2.60	120.31	116.93
2	D	1001[A]	BO2	C5-N4-C3	2.60	121.34	116.85
2	D	1001[B]	BO2	C5-N4-C3	2.60	121.34	116.85
2	F	1001[A]	BO2	C11-C10-N9	2.58	116.23	110.79
2	F	1001[B]	BO2	C11-C10-N9	2.58	116.23	110.79
2	C	1001[A]	BO2	C7-C2-N1	2.57	120.52	117.48
2	C	1001[B]	BO2	C7-C2-N1	2.57	120.52	117.48
2	L	1001[A]	BO2	C6-N1-C2	2.57	120.27	116.93
2	L	1001[B]	BO2	C6-N1-C2	2.57	120.27	116.93
2	H	1001[A]	BO2	C11-C10-N9	2.57	116.20	110.79
2	H	1001[B]	BO2	C11-C10-N9	2.57	116.20	110.79
2	I	1001[A]	BO2	C5-N4-C3	2.56	121.28	116.85
2	I	1001[B]	BO2	C5-N4-C3	2.56	121.28	116.85
2	D	1001[A]	BO2	C2-C3-N4	-2.37	119.10	122.05
2	D	1001[B]	BO2	C2-C3-N4	-2.37	119.10	122.05
2	F	1001[A]	BO2	C2-C3-N4	-2.37	119.10	122.05
2	F	1001[B]	BO2	C2-C3-N4	-2.37	119.10	122.05
2	D	1001[A]	BO2	C2-C7-N9	2.37	119.60	115.20
2	D	1001[B]	BO2	C2-C7-N9	2.37	119.60	115.20
2	J	1001[A]	BO2	C5-N4-C3	2.37	120.94	116.85
2	J	1001[B]	BO2	C5-N4-C3	2.37	120.94	116.85
2	E	1001[A]	BO2	O19-C18-N20	-2.33	118.62	122.93
2	E	1001[B]	BO2	O19-C18-N20	-2.33	118.62	122.93
2	L	1001[A]	BO2	C7-C2-N1	2.33	120.23	117.48
2	L	1001[B]	BO2	C7-C2-N1	2.33	120.23	117.48
2	A	1001[A]	BO2	C6-N1-C2	2.32	119.94	116.93
2	A	1001[B]	BO2	C6-N1-C2	2.32	119.94	116.93
2	B	1001	BO2	O19-C18-N20	-2.30	118.67	122.93
2	I	1001[A]	BO2	C7-C2-N1	2.29	120.18	117.48
2	I	1001[B]	BO2	C7-C2-N1	2.29	120.18	117.48
2	J	1001[A]	BO2	C2-C7-N9	2.27	119.42	115.20
2	J	1001[B]	BO2	C2-C7-N9	2.27	119.42	115.20
2	H	1001[A]	BO2	C5-N4-C3	2.27	120.78	116.85
2	H	1001[B]	BO2	C5-N4-C3	2.27	120.78	116.85
2	A	1001[A]	BO2	C2-C7-N9	2.27	119.41	115.20
2	A	1001[B]	BO2	C2-C7-N9	2.27	119.41	115.20
2	E	1001[A]	BO2	C6-N1-C2	2.26	119.86	116.93
2	E	1001[B]	BO2	C6-N1-C2	2.26	119.86	116.93
2	C	1001[A]	BO2	O19-C18-N20	-2.24	118.78	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001[B]	BO2	O19-C18-N20	-2.24	118.78	122.93
2	F	1001[A]	BO2	C2-C7-N9	2.21	119.31	115.20
2	F	1001[B]	BO2	C2-C7-N9	2.21	119.31	115.20
2	C	1001[B]	BO2	C12-C11-C10	-2.21	107.30	113.39
2	G	1001[A]	BO2	C7-C2-N1	2.20	120.08	117.48
2	G	1001[B]	BO2	C7-C2-N1	2.20	120.08	117.48
2	J	1001[A]	BO2	C2-C3-N4	-2.20	119.31	122.05
2	J	1001[B]	BO2	C2-C3-N4	-2.20	119.31	122.05
2	K	1001[A]	BO2	C2-C7-N9	2.20	119.28	115.20
2	K	1001[B]	BO2	C2-C7-N9	2.20	119.28	115.20
2	C	1001[A]	BO2	C5-N4-C3	2.19	120.64	116.85
2	C	1001[B]	BO2	C5-N4-C3	2.19	120.64	116.85
2	B	1001	BO2	C12-C11-C10	-2.19	107.35	113.39
2	C	1001[A]	BO2	C2-C7-N9	2.18	119.25	115.20
2	C	1001[B]	BO2	C2-C7-N9	2.18	119.25	115.20
2	F	1001[A]	BO2	C3-C2-N1	-2.17	119.03	121.61
2	F	1001[B]	BO2	C3-C2-N1	-2.17	119.03	121.61
2	C	1001[A]	BO2	C10-C18-N20	2.17	121.46	116.70
2	C	1001[B]	BO2	C10-C18-N20	2.17	121.46	116.70
2	H	1001[A]	BO2	O19-C18-N20	-2.15	118.95	122.93
2	H	1001[B]	BO2	O19-C18-N20	-2.15	118.95	122.93
2	B	1001	BO2	C7-C2-N1	2.13	119.99	117.48
2	A	1001[A]	BO2	C10-C18-N20	2.13	121.36	116.70
2	A	1001[B]	BO2	C10-C18-N20	2.13	121.36	116.70
2	A	1001[A]	BO2	C5-N4-C3	2.12	120.52	116.85
2	A	1001[B]	BO2	C5-N4-C3	2.12	120.52	116.85
2	H	1001[A]	BO2	C2-C3-N4	-2.10	119.44	122.05
2	H	1001[B]	BO2	C2-C3-N4	-2.10	119.44	122.05
2	B	1001	BO2	C6-C5-N4	-2.09	119.34	121.95
2	A	1001[A]	BO2	O19-C18-N20	-2.08	119.07	122.93
2	A	1001[B]	BO2	O19-C18-N20	-2.08	119.07	122.93
2	J	1001[A]	BO2	O19-C18-N20	-2.07	119.09	122.93
2	J	1001[B]	BO2	O19-C18-N20	-2.07	119.09	122.93
2	D	1001[A]	BO2	O19-C18-N20	-2.06	119.11	122.93
2	D	1001[B]	BO2	O19-C18-N20	-2.06	119.11	122.93
2	A	1001[B]	BO2	C12-C11-C10	-2.06	107.70	113.39
2	J	1001[A]	BO2	C7-C2-N1	2.06	119.91	117.48
2	J	1001[B]	BO2	C7-C2-N1	2.06	119.91	117.48
2	K	1001[A]	BO2	C2-C3-N4	-2.05	119.50	122.05
2	K	1001[B]	BO2	C2-C3-N4	-2.05	119.50	122.05
2	L	1001[B]	BO2	C12-C11-C10	-2.05	107.74	113.39
2	L	1001[A]	BO2	C5-N4-C3	2.04	120.38	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1001[B]	BO2	C5-N4-C3	2.04	120.38	116.85
2	K	1001[A]	BO2	C5-N4-C3	2.03	120.35	116.85
2	K	1001[B]	BO2	C5-N4-C3	2.03	120.35	116.85
2	F	1001[B]	BO2	C12-C11-C10	-2.02	107.82	113.39
2	C	1001[A]	BO2	C3-C2-N1	-2.01	119.21	121.61
2	C	1001[B]	BO2	C3-C2-N1	-2.01	119.21	121.61
2	K	1001[A]	BO2	O19-C18-N20	-2.01	119.20	122.93
2	K	1001[B]	BO2	O19-C18-N20	-2.01	119.20	122.93
2	I	1001[B]	BO2	C12-C11-C10	-2.01	107.84	113.39
2	D	1001[A]	BO2	C10-C18-N20	2.01	121.11	116.70
2	D	1001[B]	BO2	C10-C18-N20	2.01	121.11	116.70
2	L	1001[A]	BO2	O19-C18-N20	-2.01	119.21	122.93
2	L	1001[B]	BO2	O19-C18-N20	-2.01	119.21	122.93

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1001[A]	BO2	C21-C22-C23-C24
2	E	1001[A]	BO2	C21-C22-C23-C25
2	E	1001[B]	BO2	C21-C22-C23-C24
2	E	1001[B]	BO2	C21-C22-C23-C25
2	G	1001[A]	BO2	C21-C22-C23-C24
2	G	1001[A]	BO2	C21-C22-C23-C25
2	G	1001[B]	BO2	C21-C22-C23-C24
2	G	1001[B]	BO2	C21-C22-C23-C25
2	H	1001[A]	BO2	C21-C22-C23-C24
2	H	1001[A]	BO2	C21-C22-C23-C25
2	H	1001[B]	BO2	C21-C22-C23-C24
2	H	1001[B]	BO2	C21-C22-C23-C25
3	C	1002	1PE	C13-C23-OH3-C22
3	F	1002	1PE	C25-C15-OH6-C26
3	H	1002	1PE	C25-C15-OH6-C26
2	C	1001[A]	BO2	N1-C2-C7-O8
2	C	1001[B]	BO2	N1-C2-C7-O8
2	A	1001[A]	BO2	N1-C2-C7-O8
2	A	1001[B]	BO2	N1-C2-C7-O8
2	B	1001	BO2	N1-C2-C7-O8
2	K	1001[A]	BO2	N1-C2-C7-O8
2	K	1001[B]	BO2	N1-C2-C7-O8
2	A	1001[A]	BO2	N1-C2-C7-N9
2	A	1001[B]	BO2	N1-C2-C7-N9

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Mol	Chain	Res	Type	Atoms
2	C	1001[A]	BO2	N1-C2-C7-N9
2	C	1001[B]	BO2	N1-C2-C7-N9
2	J	1001[A]	BO2	N1-C2-C7-O8
2	J	1001[B]	BO2	N1-C2-C7-O8
2	E	1001[A]	BO2	N1-C2-C7-O8
2	E	1001[B]	BO2	N1-C2-C7-O8
2	H	1001[A]	BO2	N1-C2-C7-O8
2	H	1001[B]	BO2	N1-C2-C7-O8
2	I	1001[A]	BO2	N1-C2-C7-O8
2	I	1001[B]	BO2	N1-C2-C7-O8
2	L	1001[A]	BO2	N1-C2-C7-O8
2	L	1001[B]	BO2	N1-C2-C7-O8
2	B	1001	BO2	N1-C2-C7-N9
2	E	1001[A]	BO2	N1-C2-C7-N9
2	E	1001[B]	BO2	N1-C2-C7-N9
2	H	1001[A]	BO2	N1-C2-C7-N9
2	H	1001[B]	BO2	N1-C2-C7-N9
2	J	1001[A]	BO2	N1-C2-C7-N9
2	J	1001[B]	BO2	N1-C2-C7-N9
2	K	1001[A]	BO2	N1-C2-C7-N9
2	K	1001[B]	BO2	N1-C2-C7-N9
2	D	1001[A]	BO2	N1-C2-C7-O8
2	D	1001[B]	BO2	N1-C2-C7-O8
3	A	1002	1PE	OH4-C13-C23-OH3
3	C	1002	1PE	OH6-C15-C25-OH5
2	G	1001[A]	BO2	N1-C2-C7-N9
2	G	1001[B]	BO2	N1-C2-C7-N9
2	I	1001[A]	BO2	N1-C2-C7-N9
2	I	1001[B]	BO2	N1-C2-C7-N9
2	L	1001[A]	BO2	N1-C2-C7-N9
2	L	1001[B]	BO2	N1-C2-C7-N9
3	H	1002	1PE	OH4-C13-C23-OH3
2	G	1001[A]	BO2	N1-C2-C7-O8
2	G	1001[B]	BO2	N1-C2-C7-O8
3	H	1002	1PE	OH6-C15-C25-OH5
3	I	1002	1PE	OH6-C15-C25-OH5
2	D	1001[A]	BO2	N1-C2-C7-N9
2	D	1001[B]	BO2	N1-C2-C7-N9
2	F	1001[A]	BO2	N1-C2-C7-N9
2	F	1001[B]	BO2	N1-C2-C7-N9
2	F	1001[A]	BO2	N1-C2-C7-O8
2	F	1001[B]	BO2	N1-C2-C7-O8

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Mol	Chain	Res	Type	Atoms
3	H	1002	1PE	OH5-C14-C24-OH4
2	A	1001[A]	BO2	C3-C2-C7-O8
2	A	1001[B]	BO2	C3-C2-C7-O8
2	B	1001	BO2	C3-C2-C7-O8
2	C	1001[A]	BO2	C3-C2-C7-O8
2	C	1001[B]	BO2	C3-C2-C7-O8
2	D	1001[A]	BO2	C3-C2-C7-O8
2	D	1001[B]	BO2	C3-C2-C7-O8
2	E	1001[A]	BO2	C3-C2-C7-O8
2	E	1001[B]	BO2	C3-C2-C7-O8
2	F	1001[A]	BO2	C3-C2-C7-O8
2	F	1001[B]	BO2	C3-C2-C7-O8
2	G	1001[A]	BO2	C3-C2-C7-O8
2	G	1001[B]	BO2	C3-C2-C7-O8
2	H	1001[A]	BO2	C3-C2-C7-O8
2	H	1001[B]	BO2	C3-C2-C7-O8
2	I	1001[A]	BO2	C3-C2-C7-O8
2	I	1001[B]	BO2	C3-C2-C7-O8
2	J	1001[A]	BO2	C3-C2-C7-O8
2	J	1001[B]	BO2	C3-C2-C7-O8
2	K	1001[A]	BO2	C3-C2-C7-O8
2	K	1001[B]	BO2	C3-C2-C7-O8
2	L	1001[A]	BO2	C3-C2-C7-O8
2	L	1001[B]	BO2	C3-C2-C7-O8
3	F	1002	1PE	OH5-C14-C24-OH4
3	A	1002	1PE	C12-C22-OH3-C23
3	B	1002	1PE	OH6-C15-C25-OH5
3	B	1002	1PE	OH4-C13-C23-OH3
3	H	1002	1PE	OH7-C16-C26-OH6
3	I	1002	1PE	OH2-C12-C22-OH3
3	I	1002	1PE	OH7-C16-C26-OH6
3	C	1002	1PE	OH4-C13-C23-OH3
2	A	1001[A]	BO2	C3-C2-C7-N9
2	A	1001[B]	BO2	C3-C2-C7-N9
2	B	1001	BO2	C3-C2-C7-N9
2	C	1001[A]	BO2	C3-C2-C7-N9
2	C	1001[B]	BO2	C3-C2-C7-N9
2	D	1001[A]	BO2	C3-C2-C7-N9
2	D	1001[B]	BO2	C3-C2-C7-N9
2	E	1001[A]	BO2	C3-C2-C7-N9
2	E	1001[B]	BO2	C3-C2-C7-N9
2	F	1001[A]	BO2	C3-C2-C7-N9

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Mol	Chain	Res	Type	Atoms
2	F	1001[B]	BO2	C3-C2-C7-N9
2	G	1001[A]	BO2	C3-C2-C7-N9
2	G	1001[B]	BO2	C3-C2-C7-N9
2	H	1001[A]	BO2	C3-C2-C7-N9
2	H	1001[B]	BO2	C3-C2-C7-N9
2	I	1001[A]	BO2	C3-C2-C7-N9
2	I	1001[B]	BO2	C3-C2-C7-N9
2	J	1001[A]	BO2	C3-C2-C7-N9
2	J	1001[B]	BO2	C3-C2-C7-N9
2	K	1001[A]	BO2	C3-C2-C7-N9
2	K	1001[B]	BO2	C3-C2-C7-N9
2	L	1001[A]	BO2	C3-C2-C7-N9
2	L	1001[B]	BO2	C3-C2-C7-N9
3	A	1002	1PE	OH7-C16-C26-OH6
3	B	1002	1PE	OH7-C16-C26-OH6
3	C	1002	1PE	OH2-C12-C22-OH3
3	H	1002	1PE	OH2-C12-C22-OH3
3	B	1002	1PE	OH5-C14-C24-OH4
3	I	1002	1PE	OH4-C13-C23-OH3
3	F	1002	1PE	OH2-C12-C22-OH3
3	C	1002	1PE	OH5-C14-C24-OH4
3	F	1002	1PE	OH7-C16-C26-OH6
3	C	1002	1PE	C25-C15-OH6-C26
3	A	1002	1PE	OH2-C12-C22-OH3
3	C	1002	1PE	OH7-C16-C26-OH6
3	C	1002	1PE	C15-C25-OH5-C14
3	B	1002	1PE	C23-C13-OH4-C24
3	F	1002	1PE	OH6-C15-C25-OH5
4	G	1002	GOL	O1-C1-C2-O2
3	C	1002	1PE	C14-C24-OH4-C13
3	I	1002	1PE	OH5-C14-C24-OH4
3	B	1002	1PE	C16-C26-OH6-C15
3	F	1002	1PE	C12-C22-OH3-C23
3	A	1002	1PE	C13-C23-OH3-C22
3	H	1002	1PE	C13-C23-OH3-C22
3	H	1002	1PE	C24-C14-OH5-C25
3	C	1002	1PE	C24-C14-OH5-C25
3	I	1002	1PE	C23-C13-OH4-C24
4	G	1002	GOL	O1-C1-C2-C3
3	I	1002	1PE	C15-C25-OH5-C14
3	F	1002	1PE	C23-C13-OH4-C24
3	I	1002	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
3	B	1002	1PE	C24-C14-OH5-C25

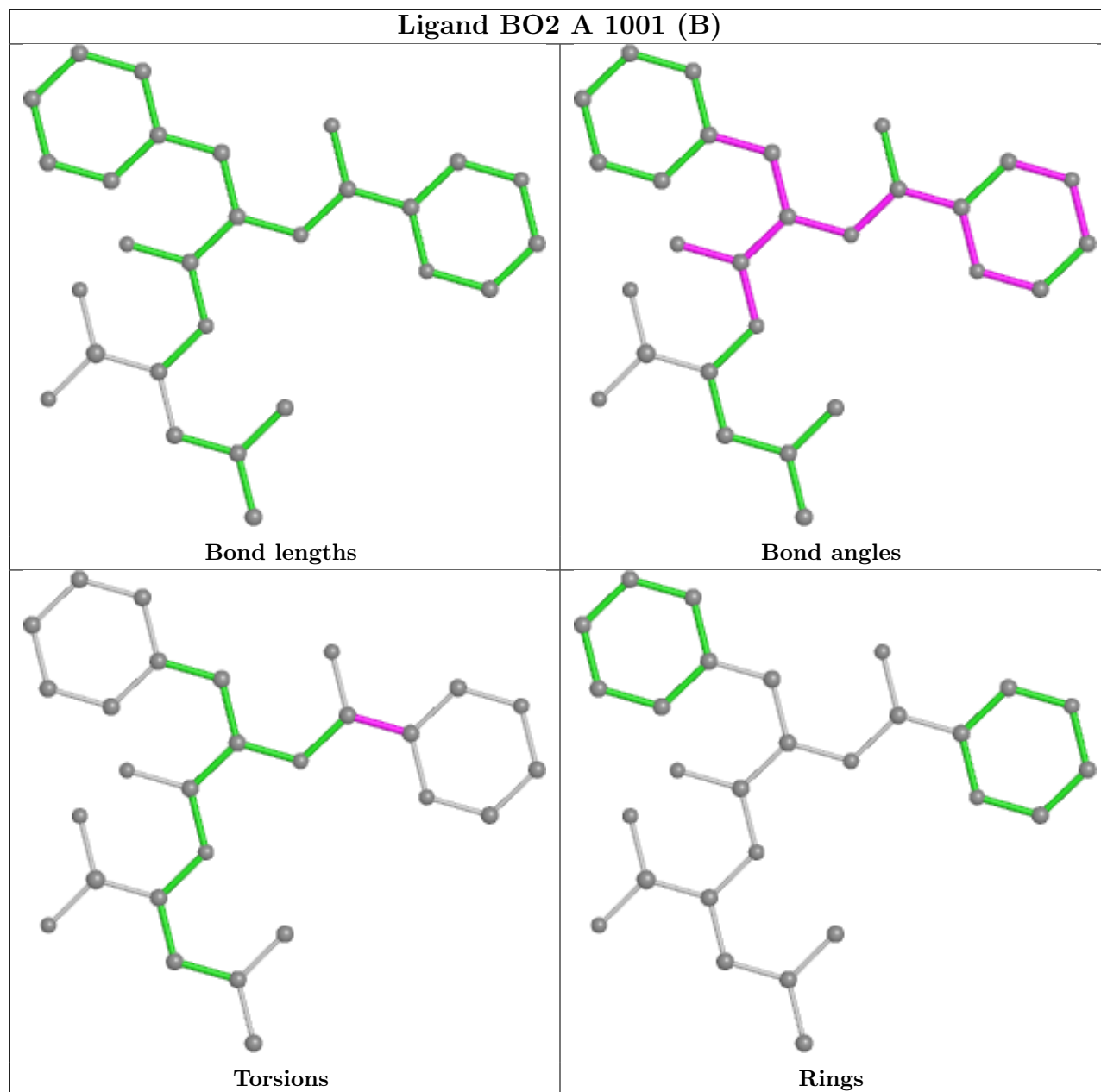
There are no ring outliers.

12 monomers are involved in 39 short contacts:

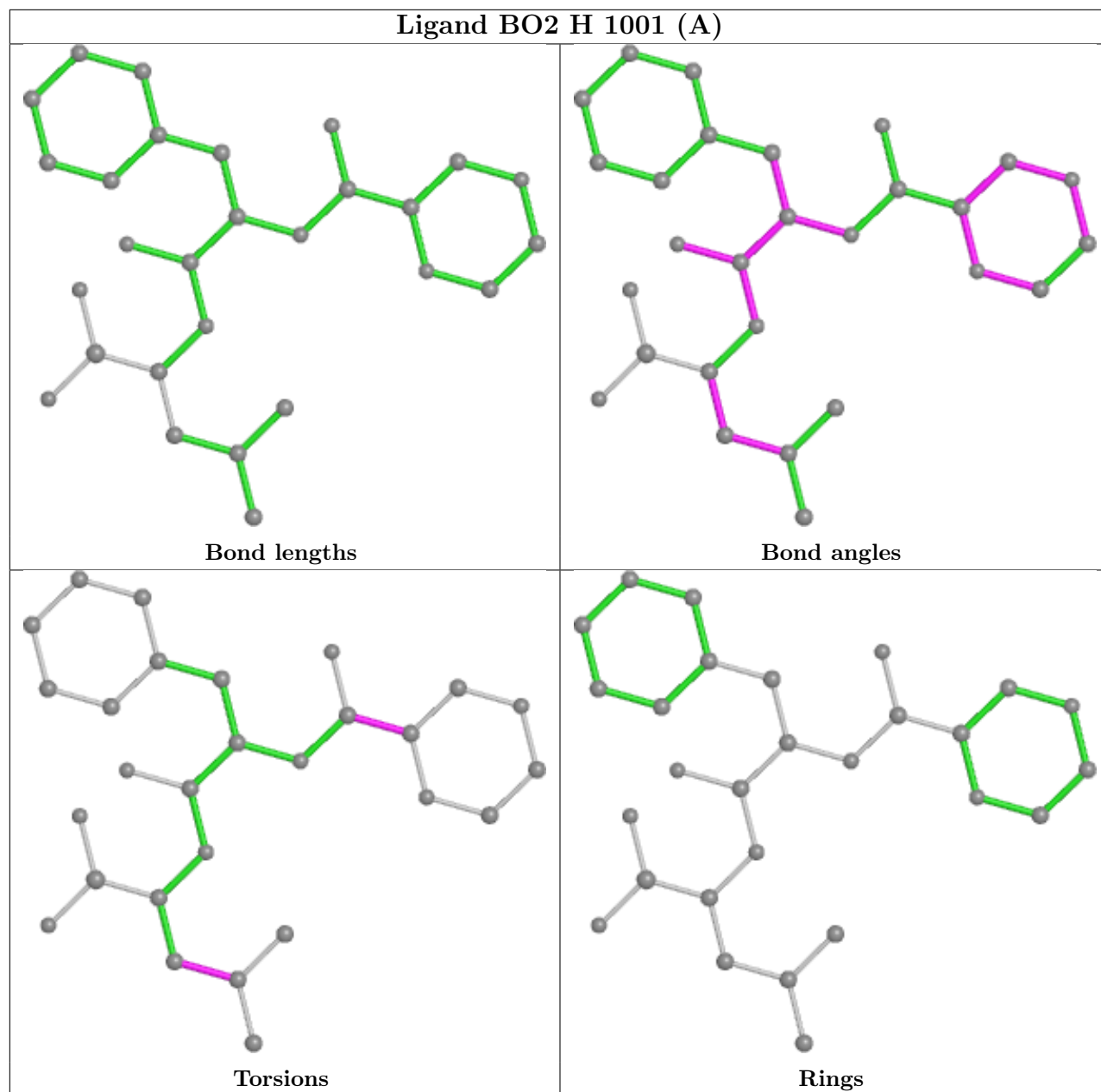
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1001[A]	BO2	1	0
3	C	1002	1PE	4	0
3	F	1002	1PE	14	0
3	B	1002	1PE	2	0
2	C	1001[A]	BO2	2	0
3	A	1002	1PE	11	0
2	G	1001[B]	BO2	1	0
2	A	1001[A]	BO2	1	0
2	G	1001[A]	BO2	4	0
2	F	1001[A]	BO2	3	0
3	I	1002	1PE	2	0
3	H	1002	1PE	5	0

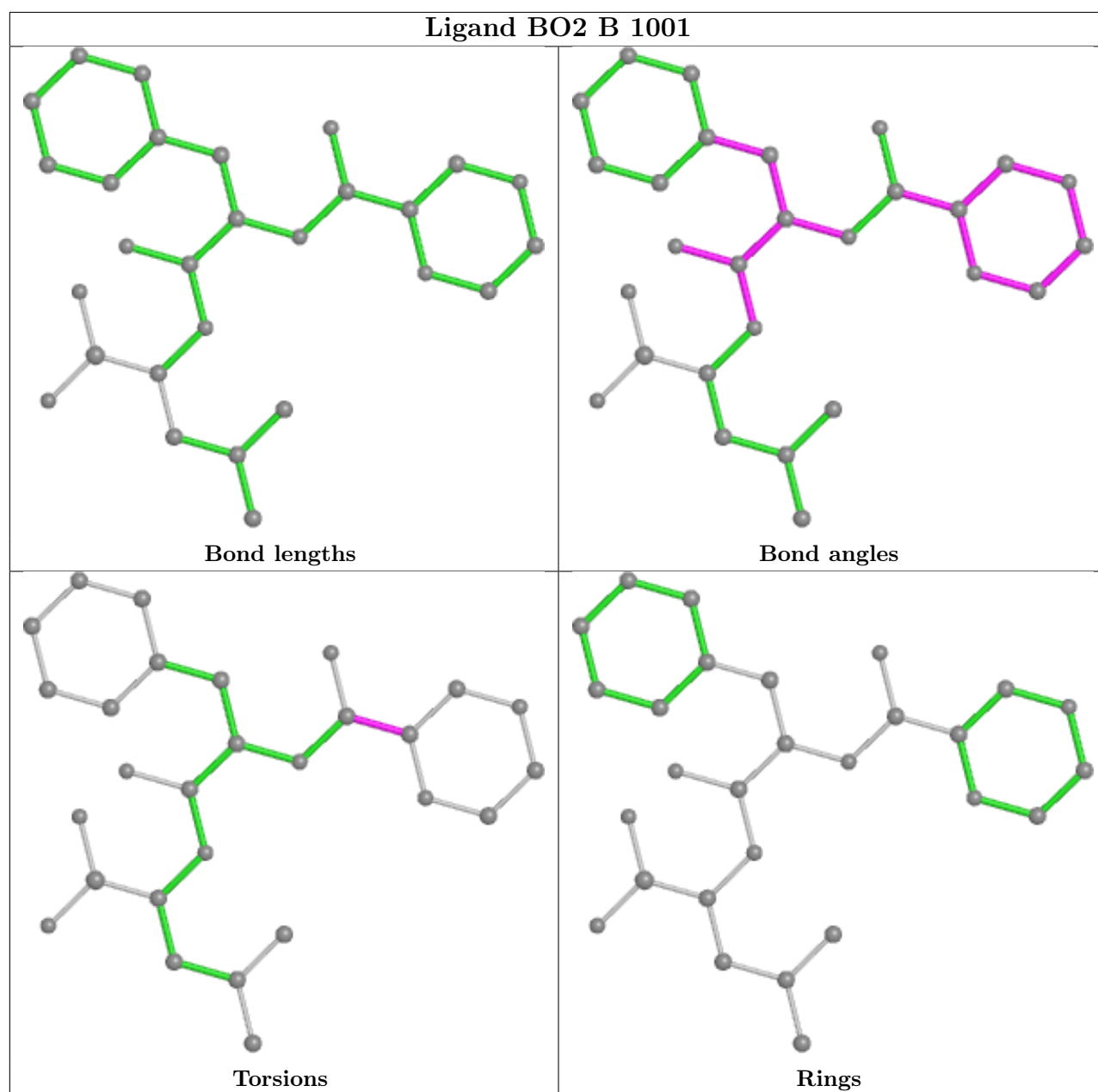
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 BO2 A 1001 (B)

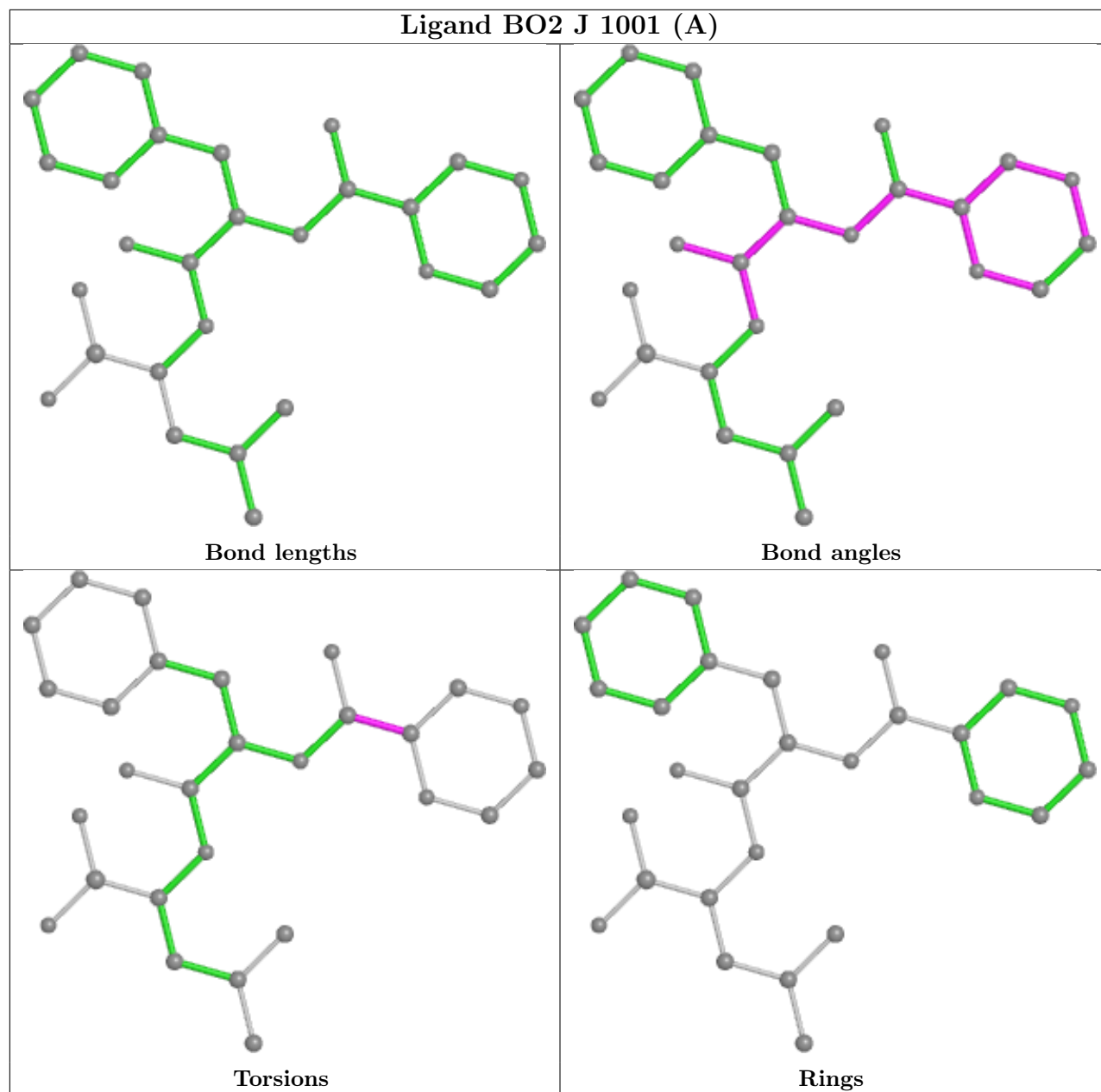


Ligand BO2 H 1001 (A)

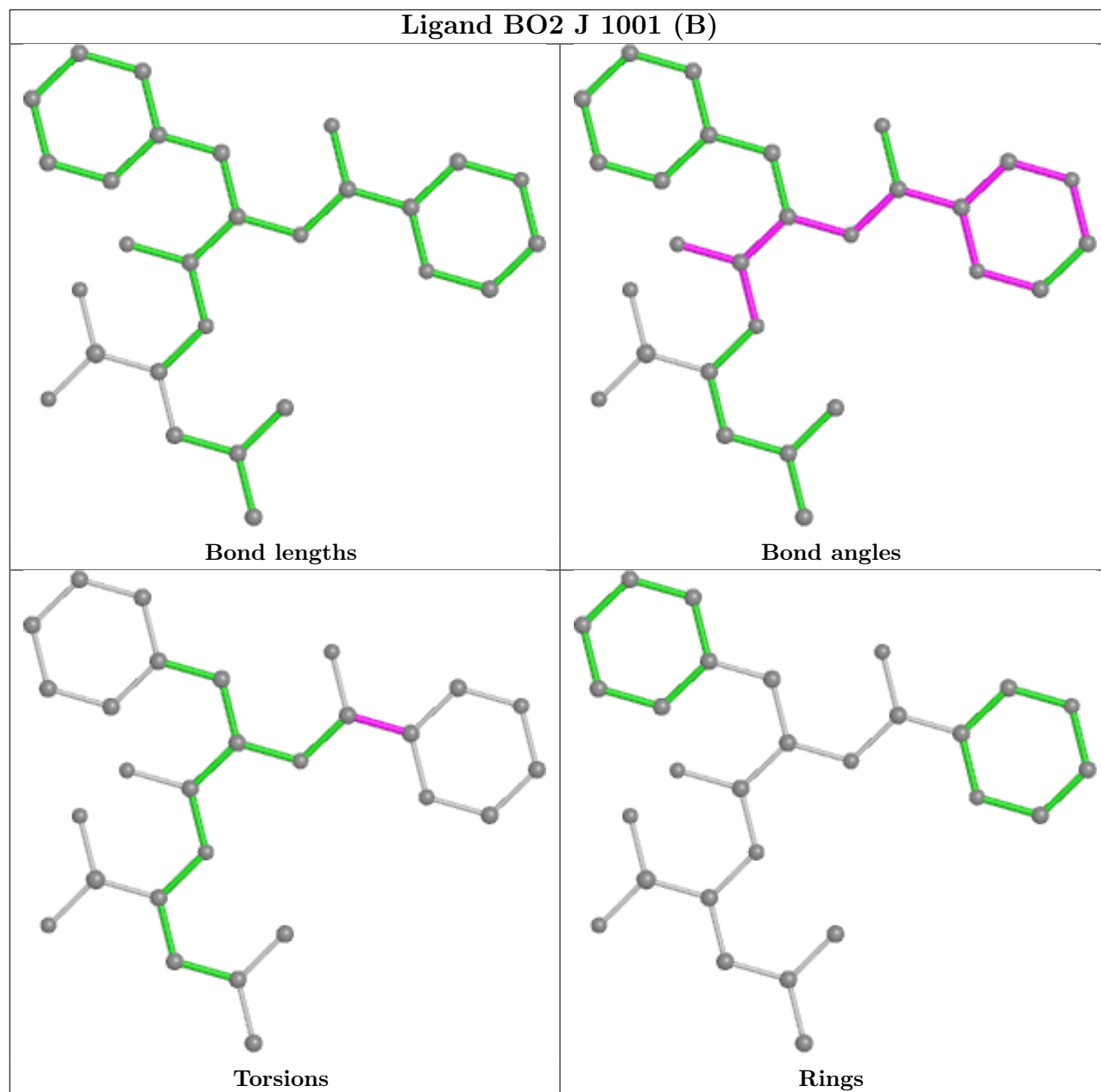




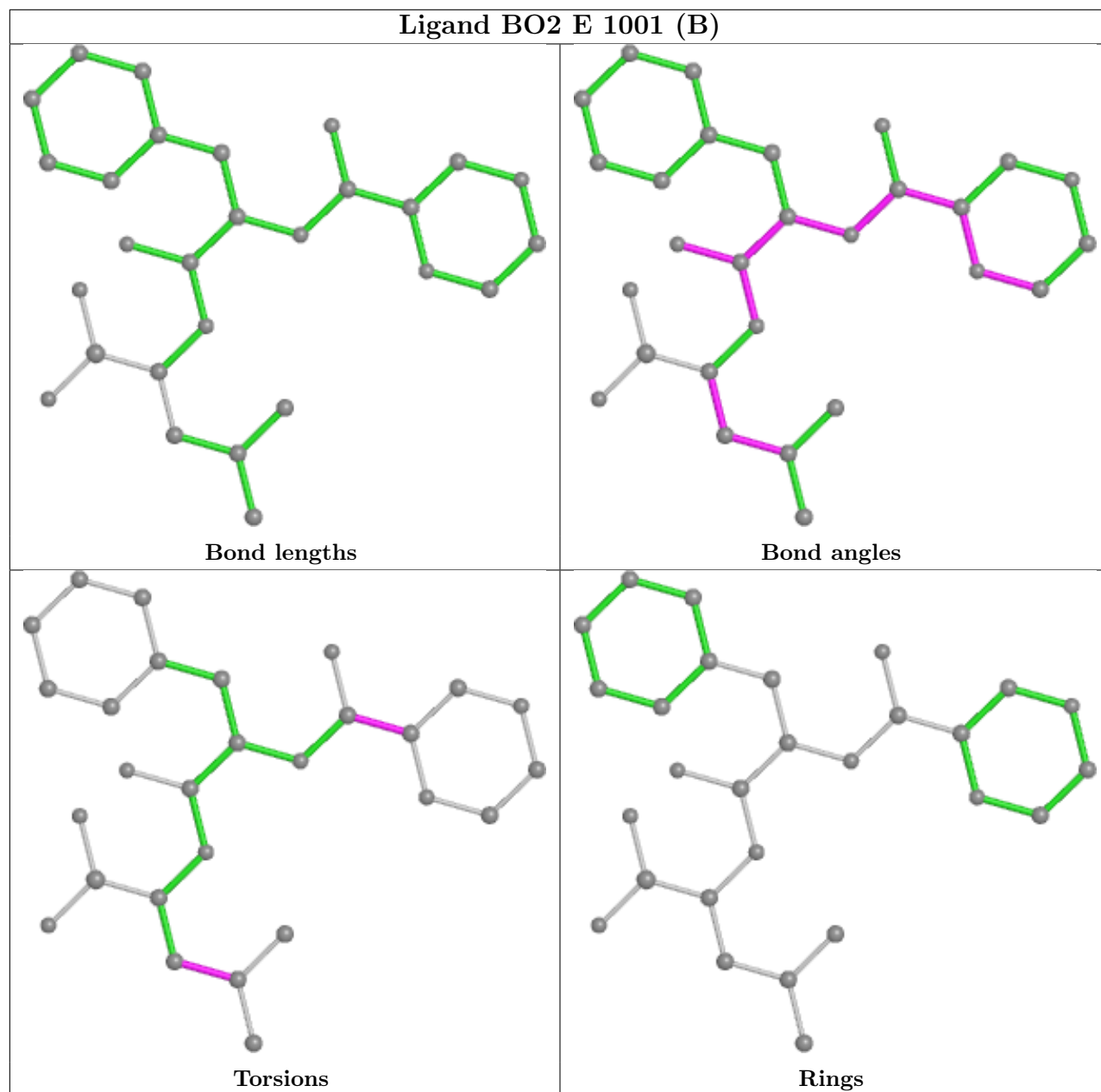
Ligand BO2 J 1001 (A)



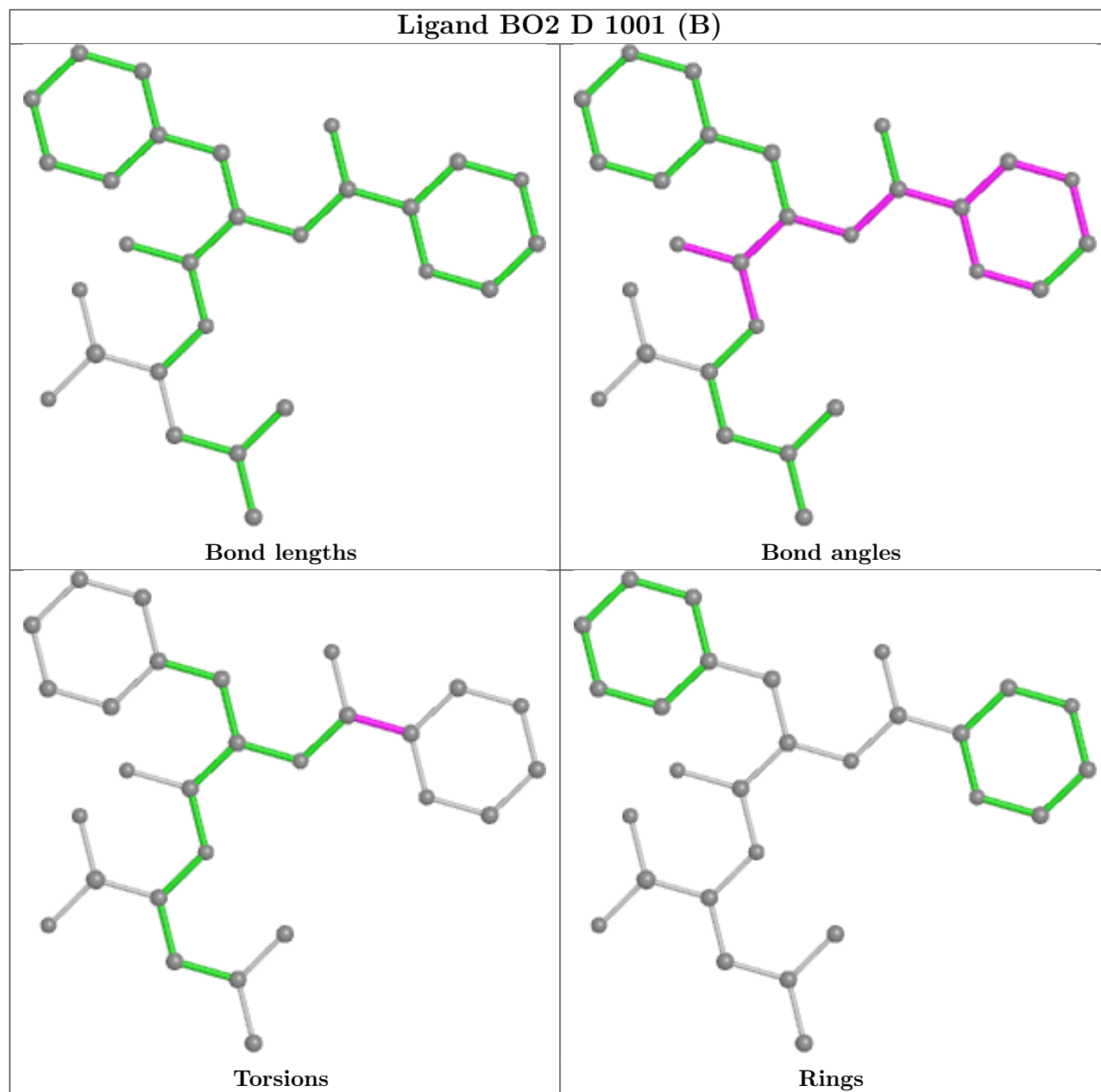
Ligand BO2 J 1001 (B)



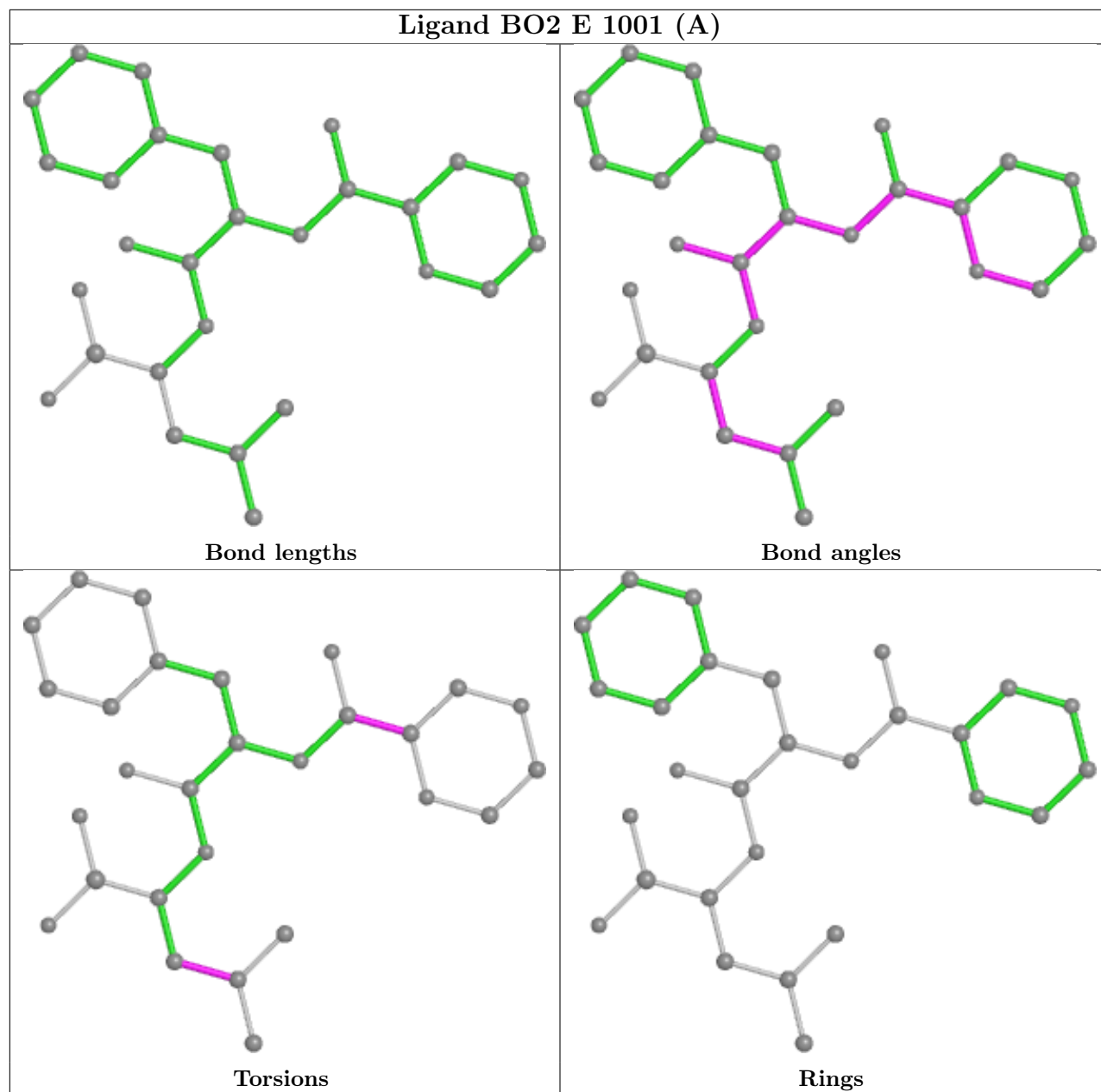
Ligand BO2 E 1001 (B)



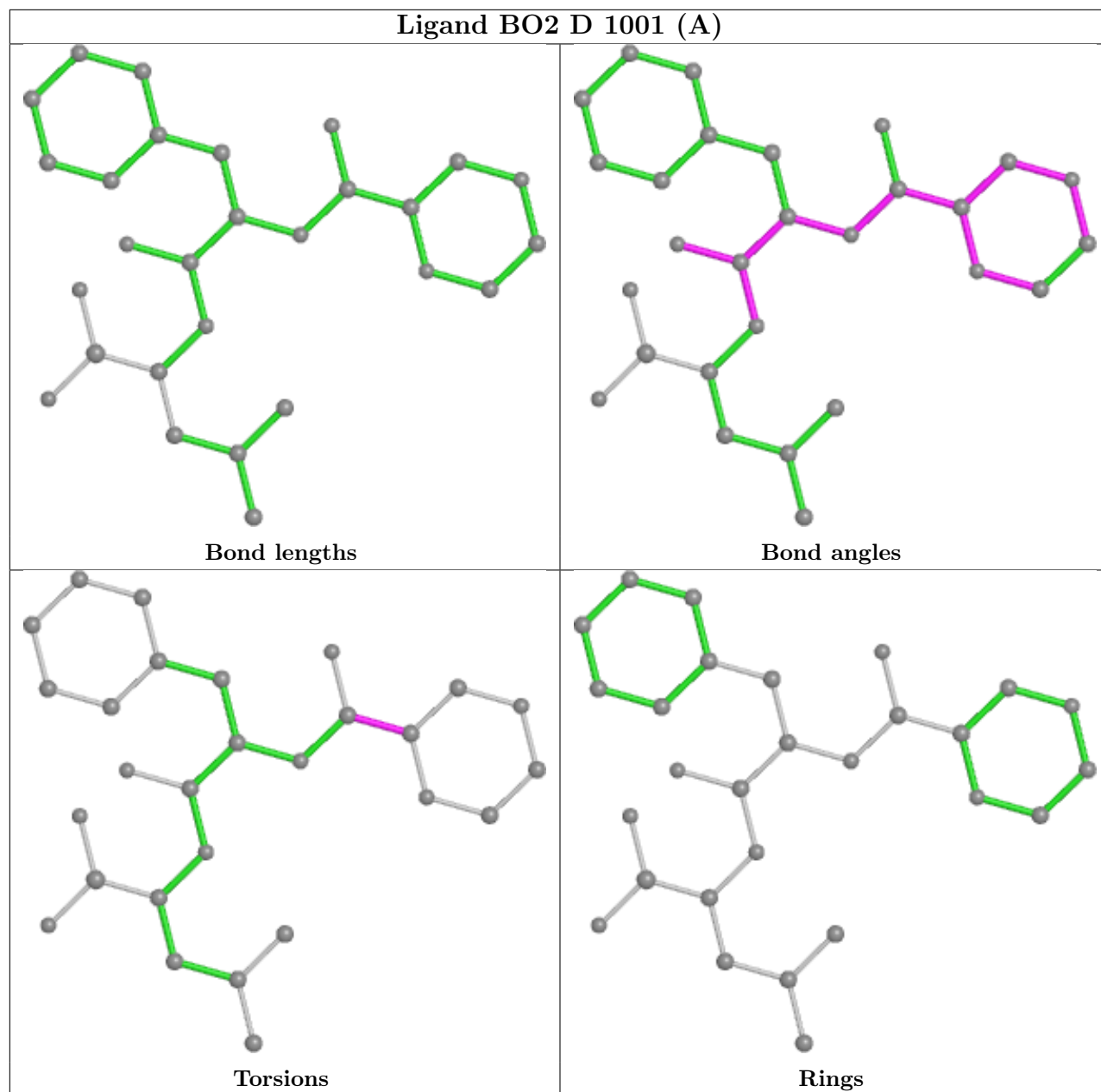
Ligand BO2 D 1001 (B)



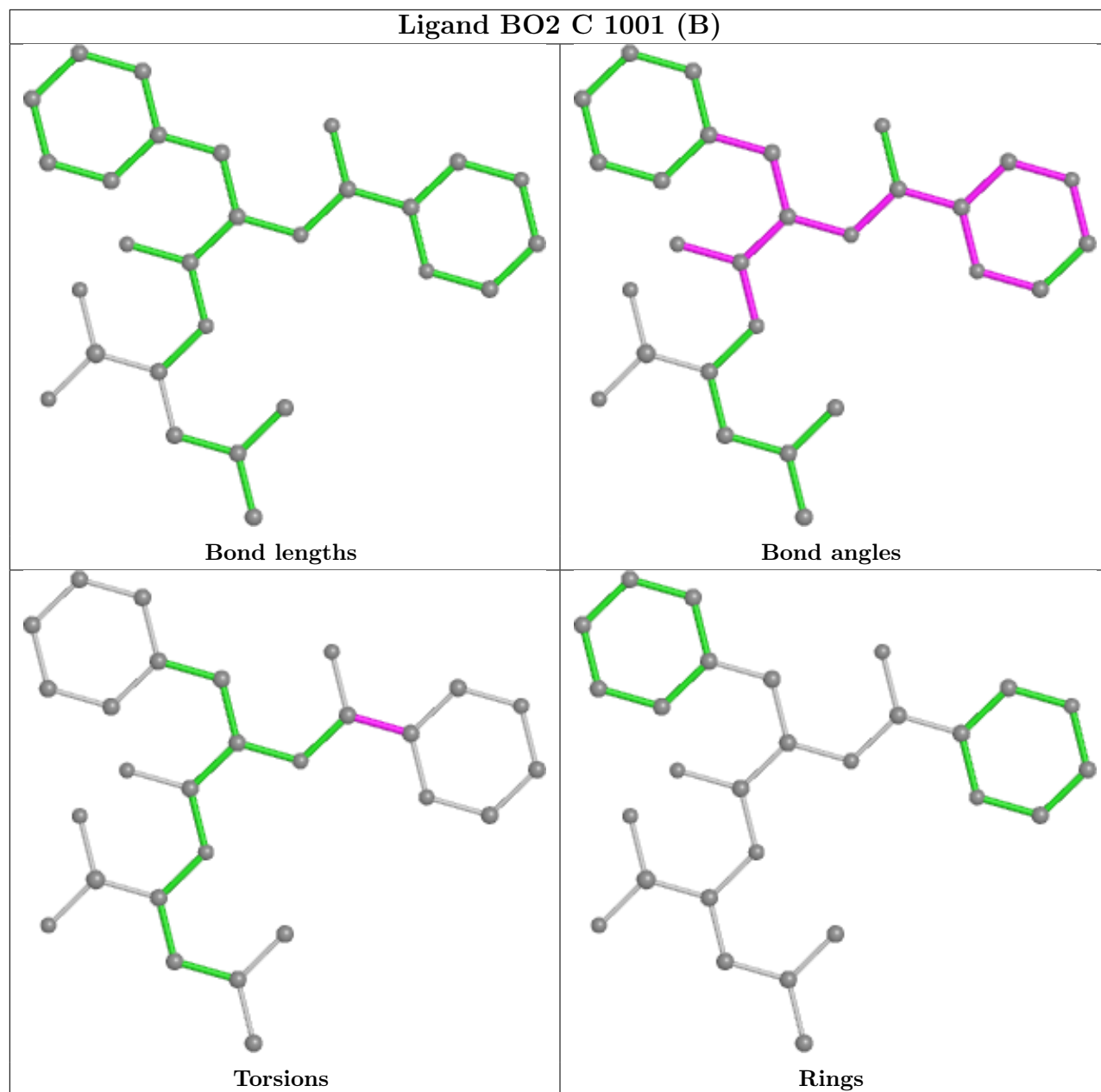
Ligand BO2 E 1001 (A)



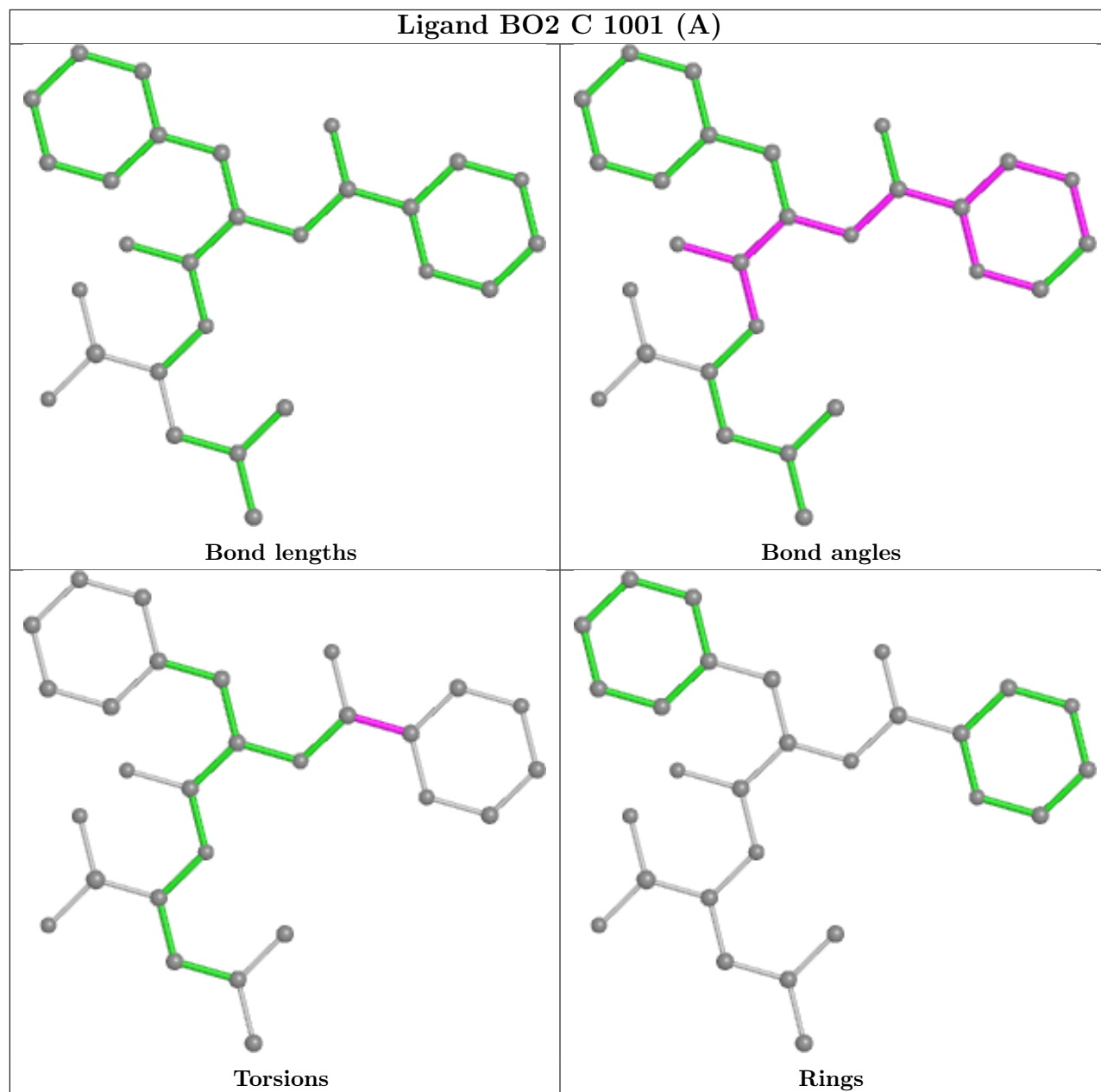
Ligand BO2 D 1001 (A)



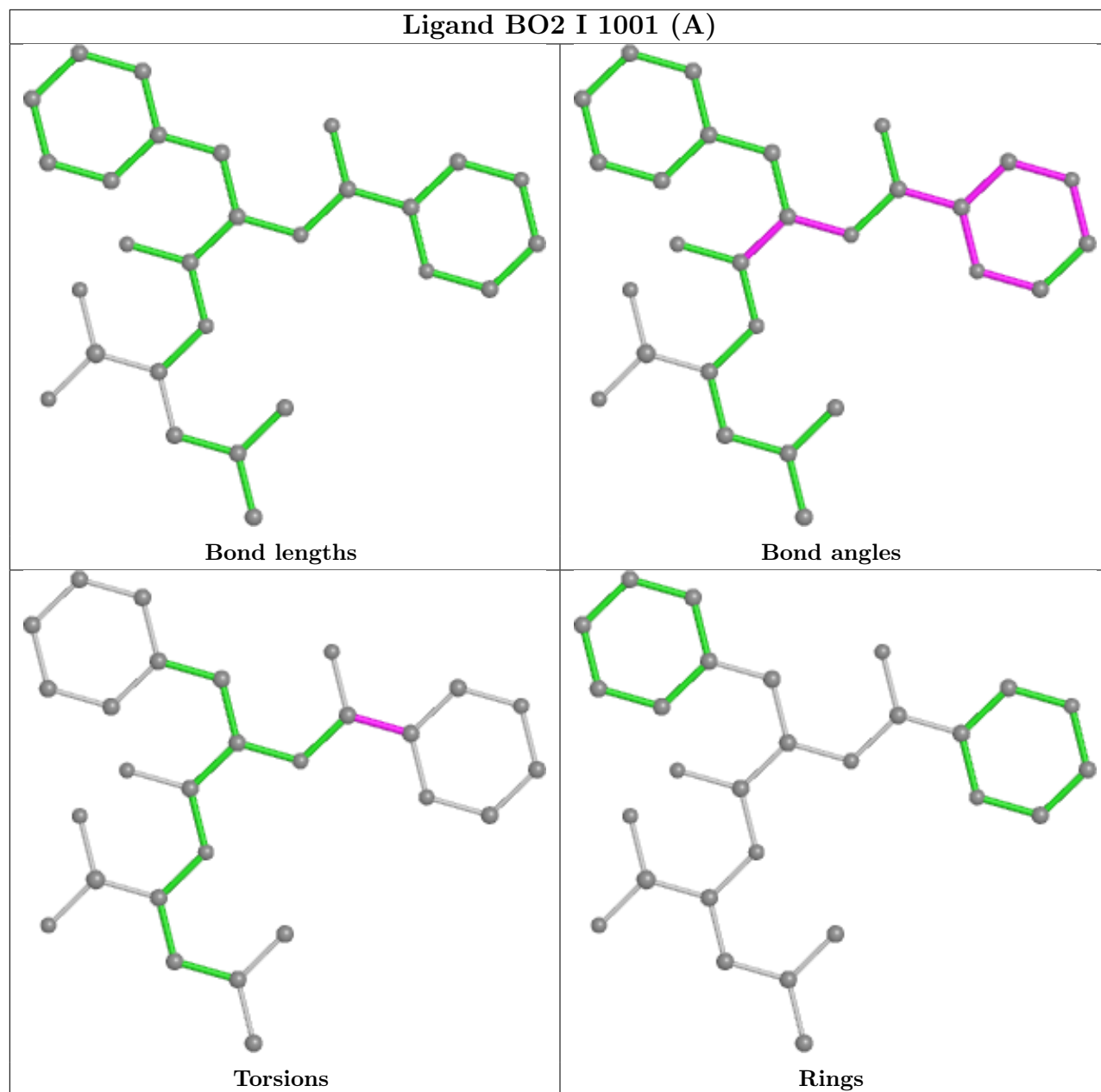
Ligand BO2 C 1001 (B)



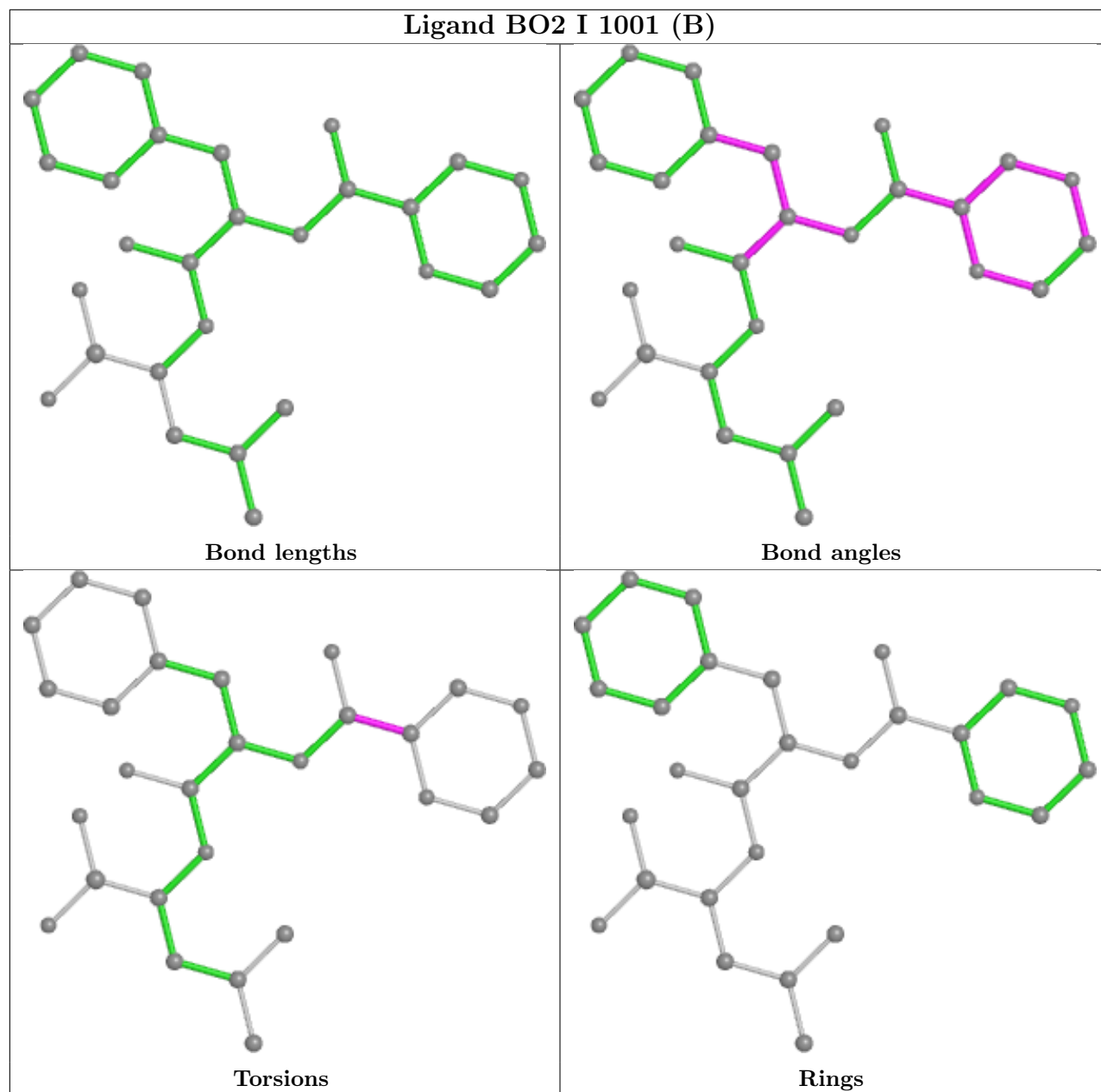
Ligand BO2 C 1001 (A)



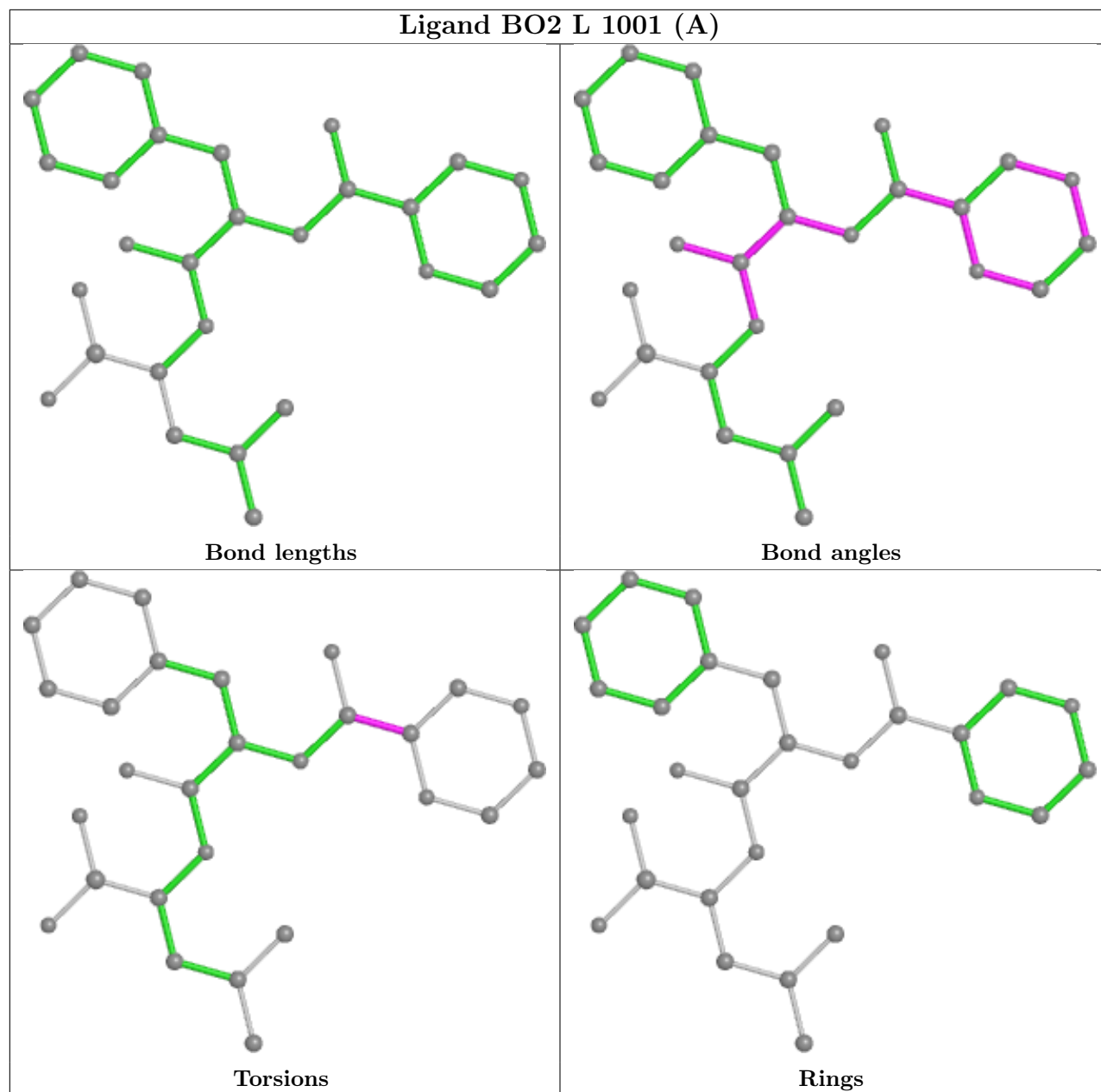
Ligand BO2 I 1001 (A)



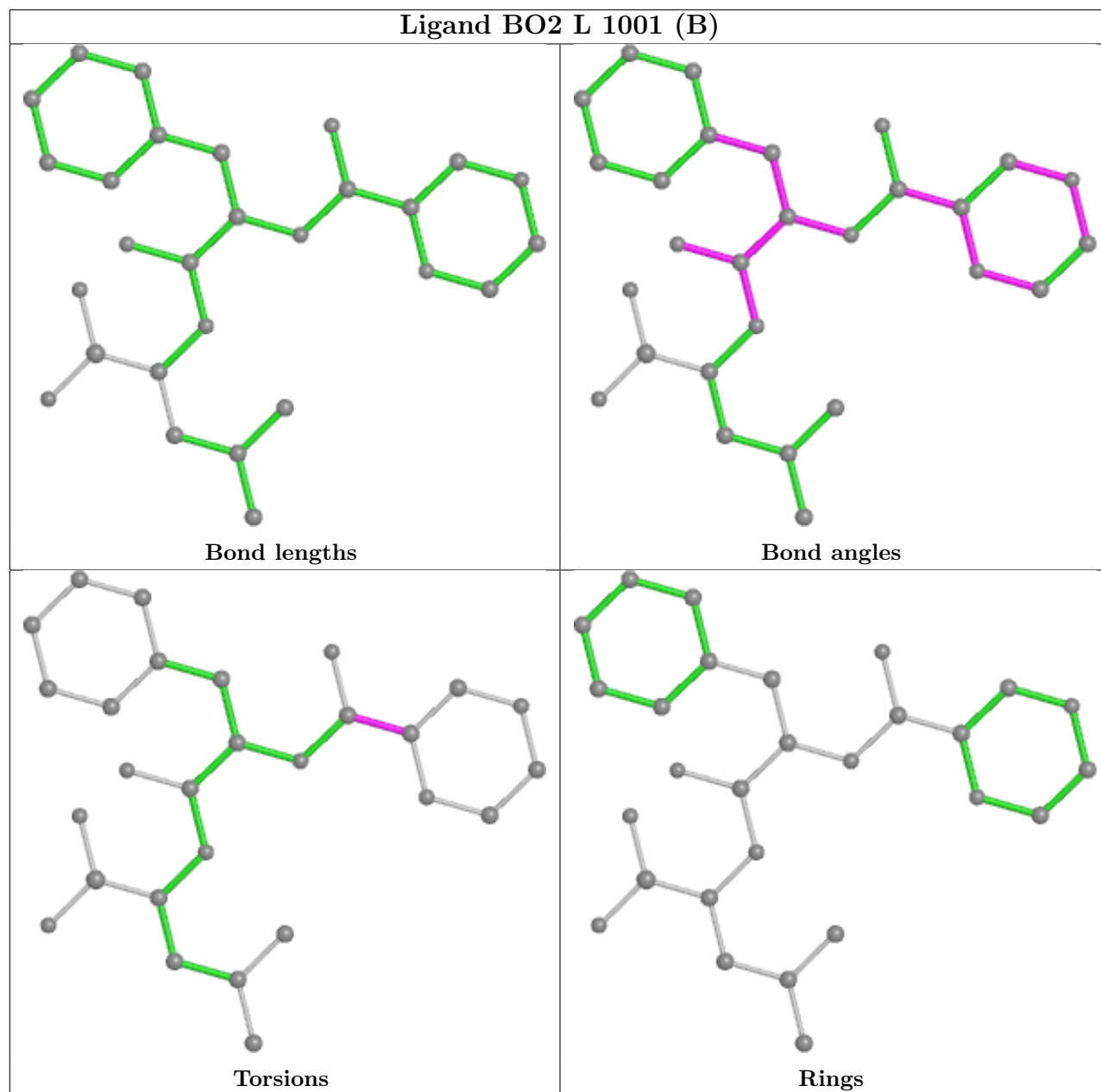
Ligand BO2 I 1001 (B)



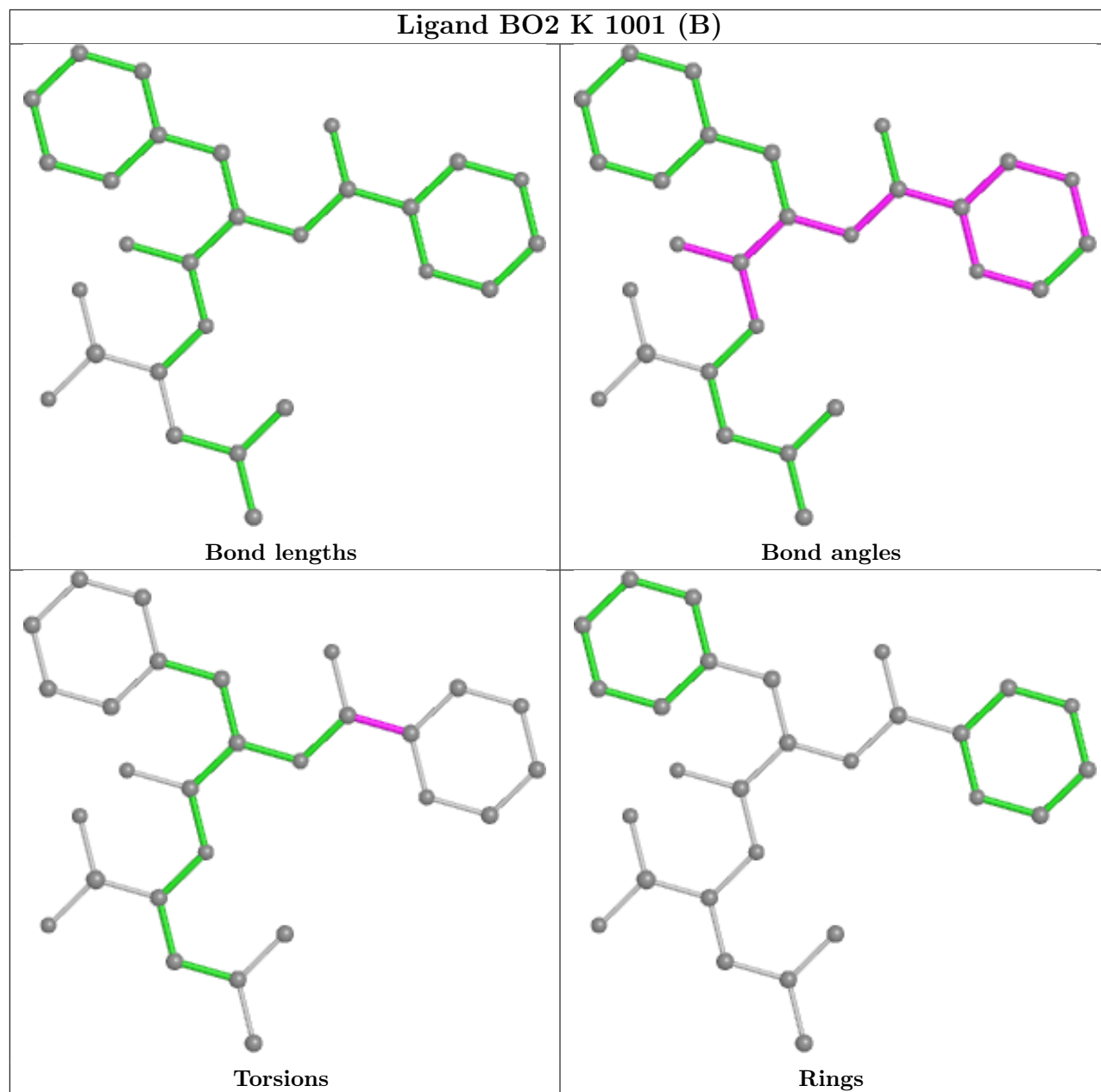
Ligand BO2 L 1001 (A)



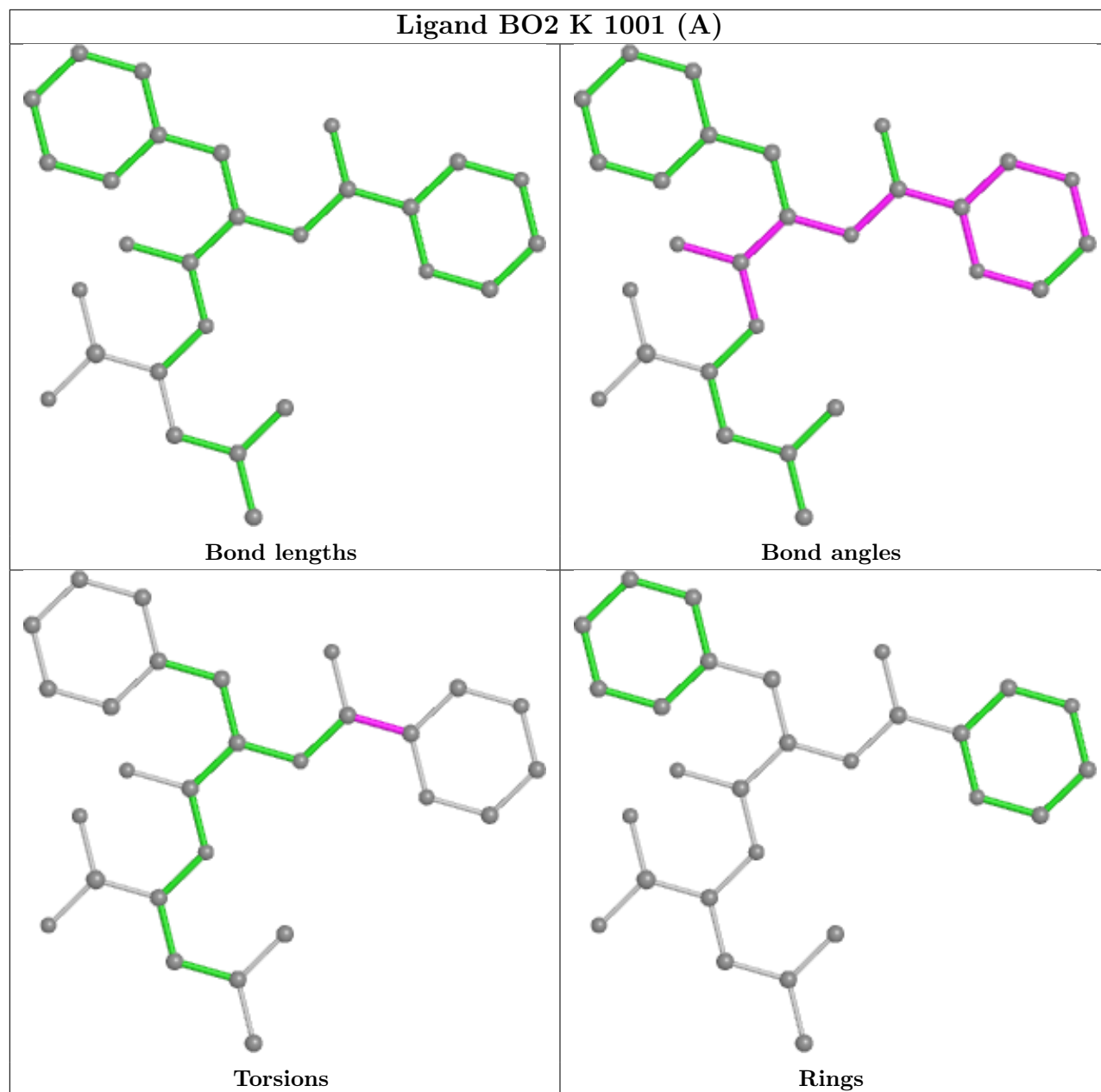
Ligand BO2 L 1001 (B)



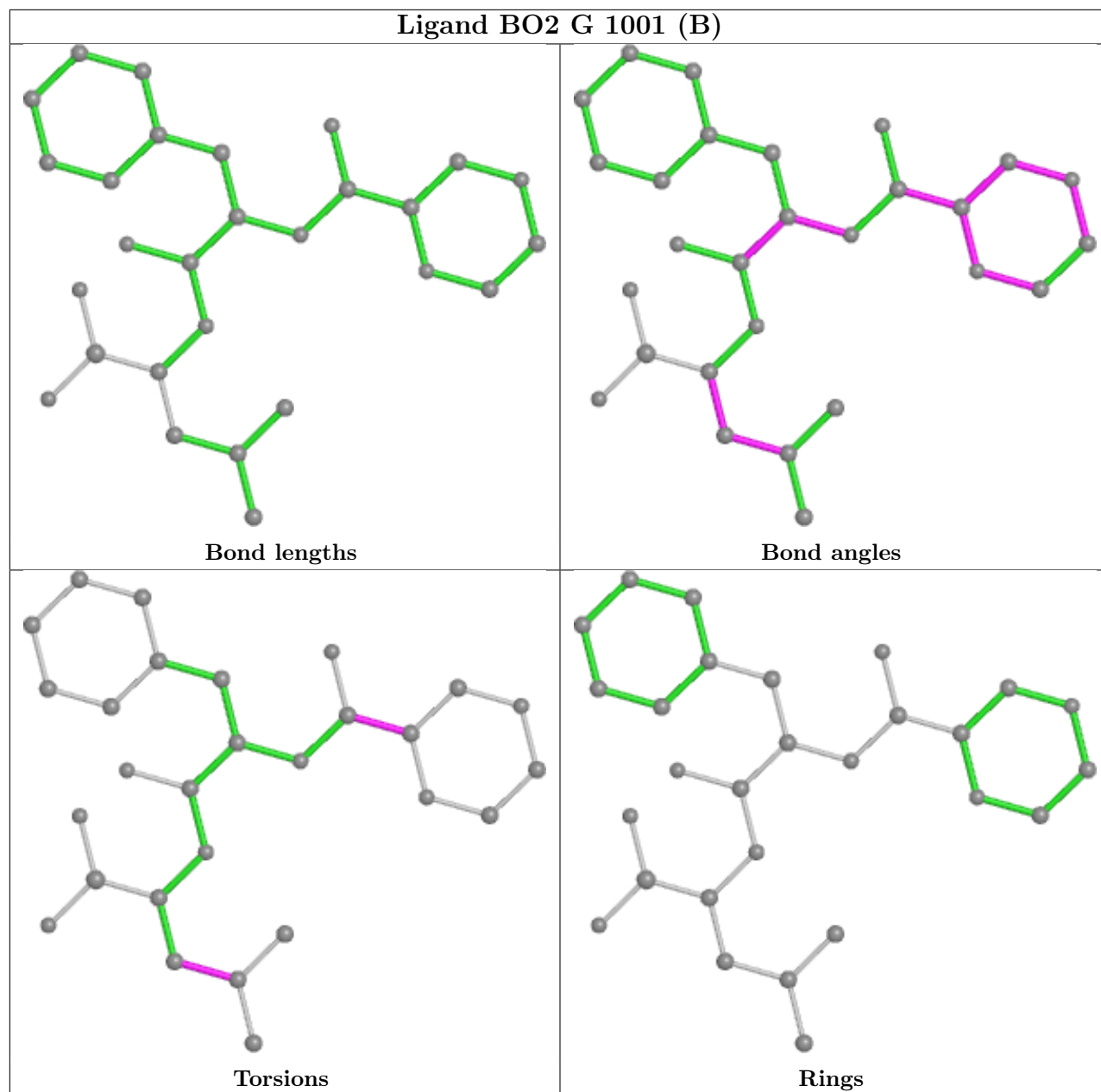
Ligand BO2 K 1001 (B)



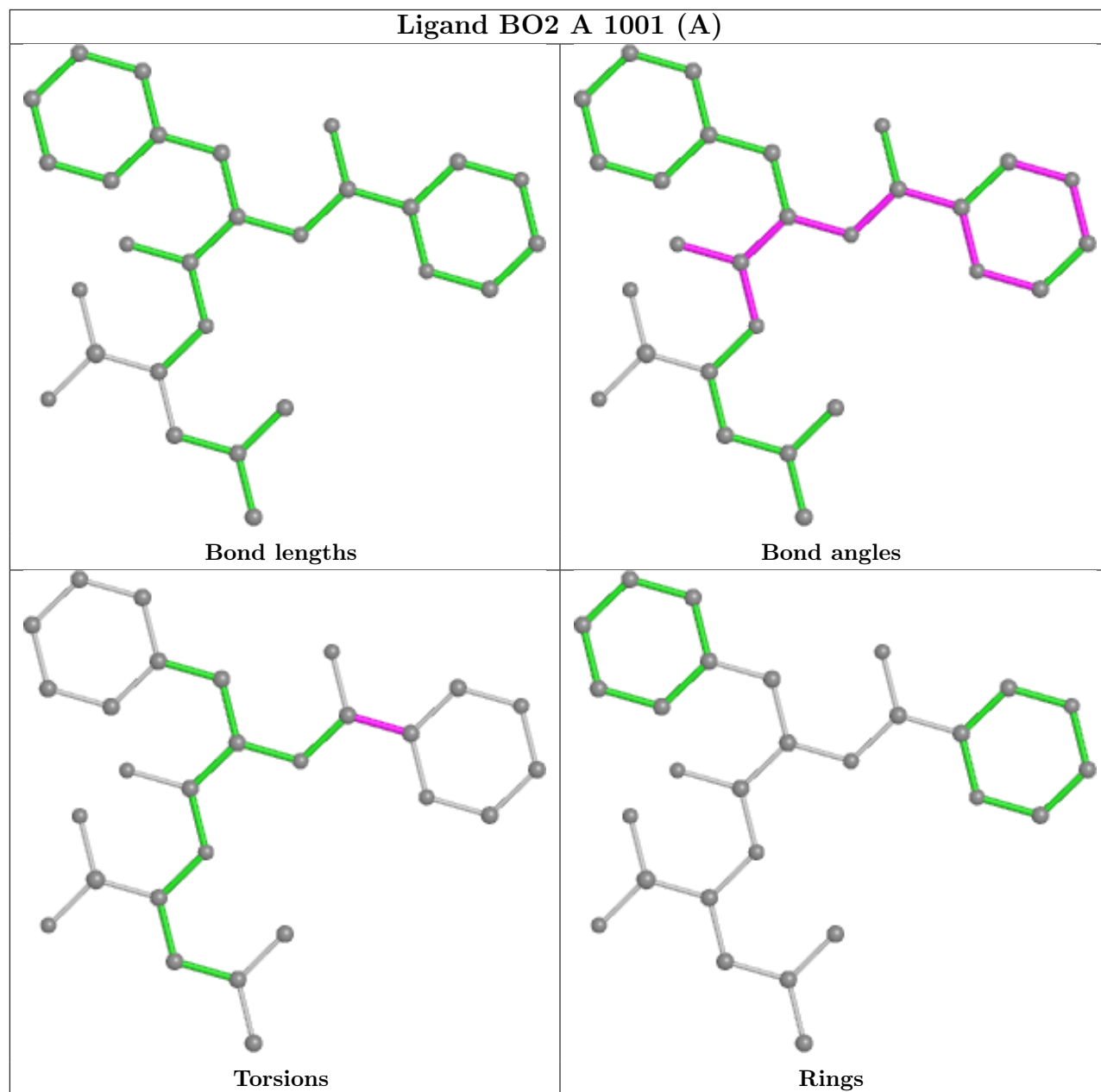
Ligand BO2 K 1001 (A)



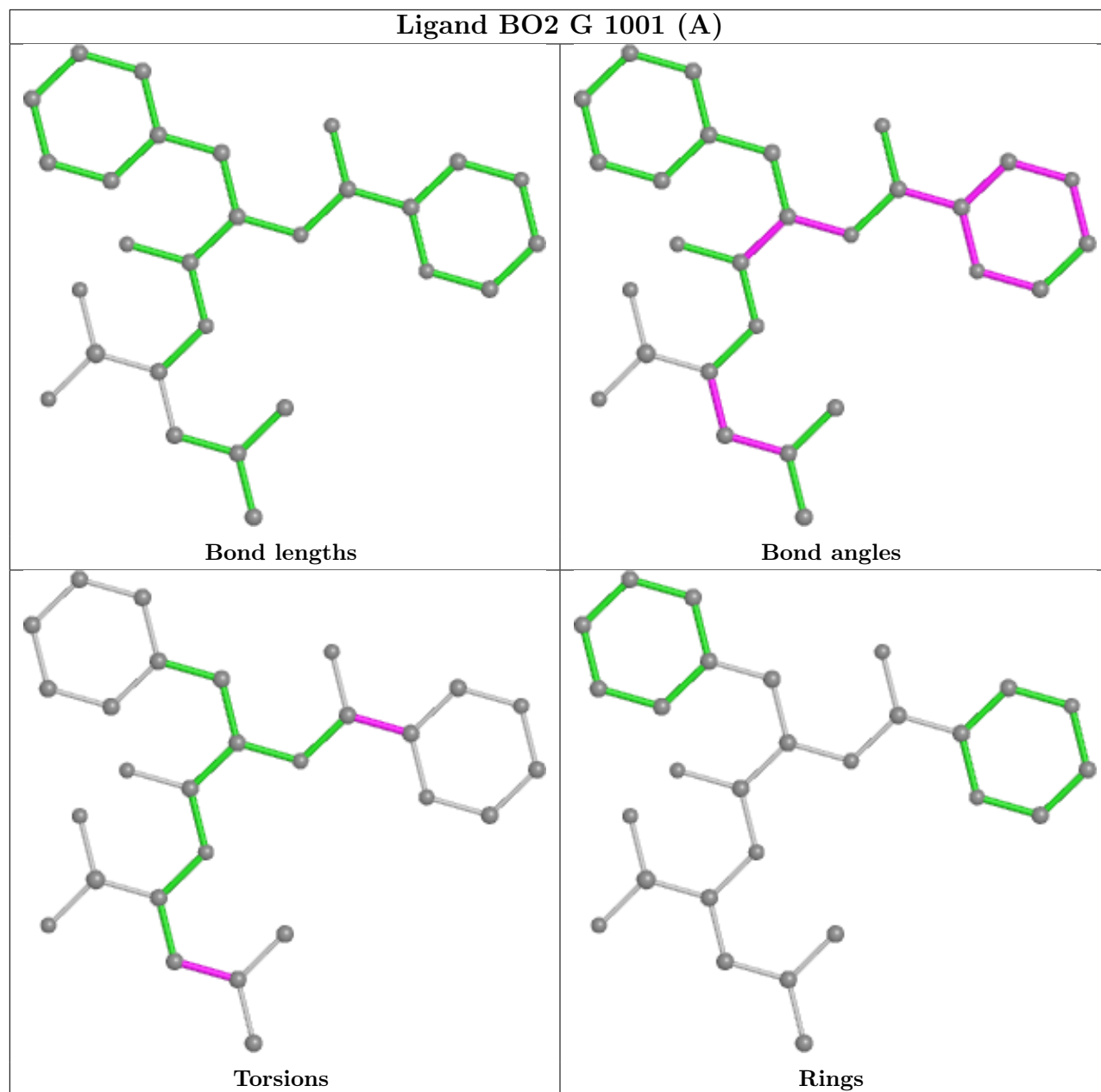
Ligand BO2 G 1001 (B)



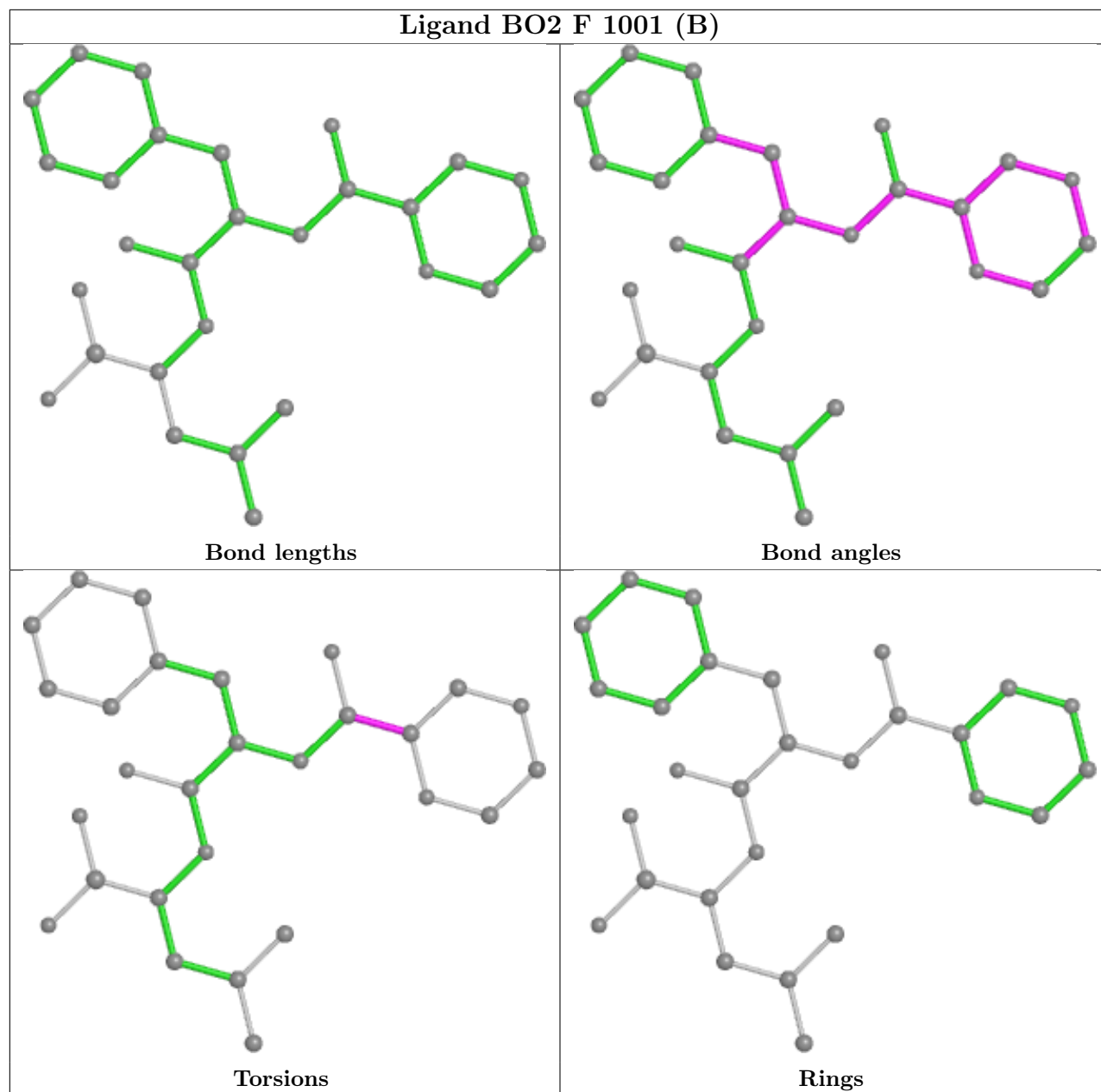
Ligand BO2 A 1001 (A)



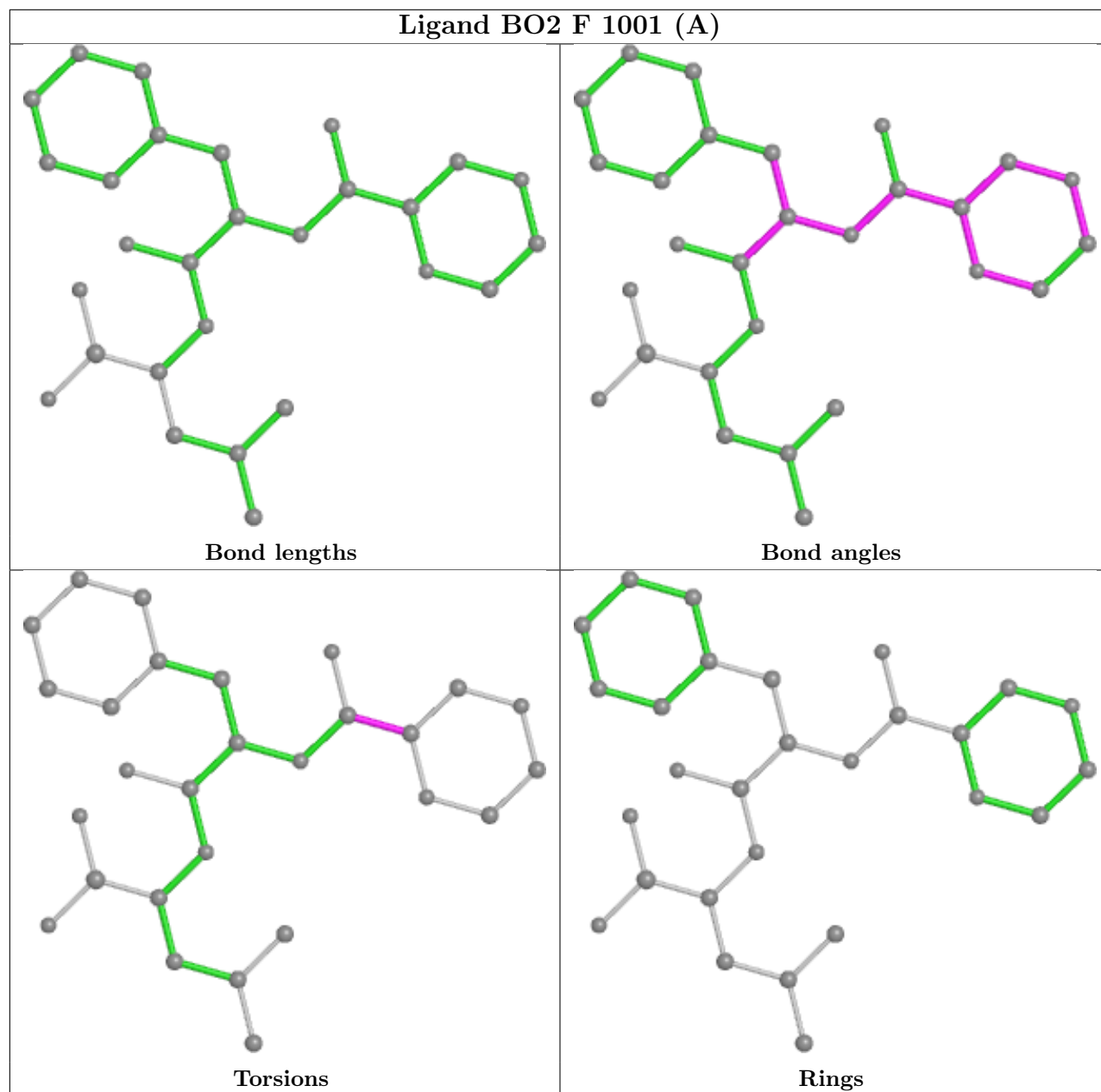
Ligand BO2 G 1001 (A)

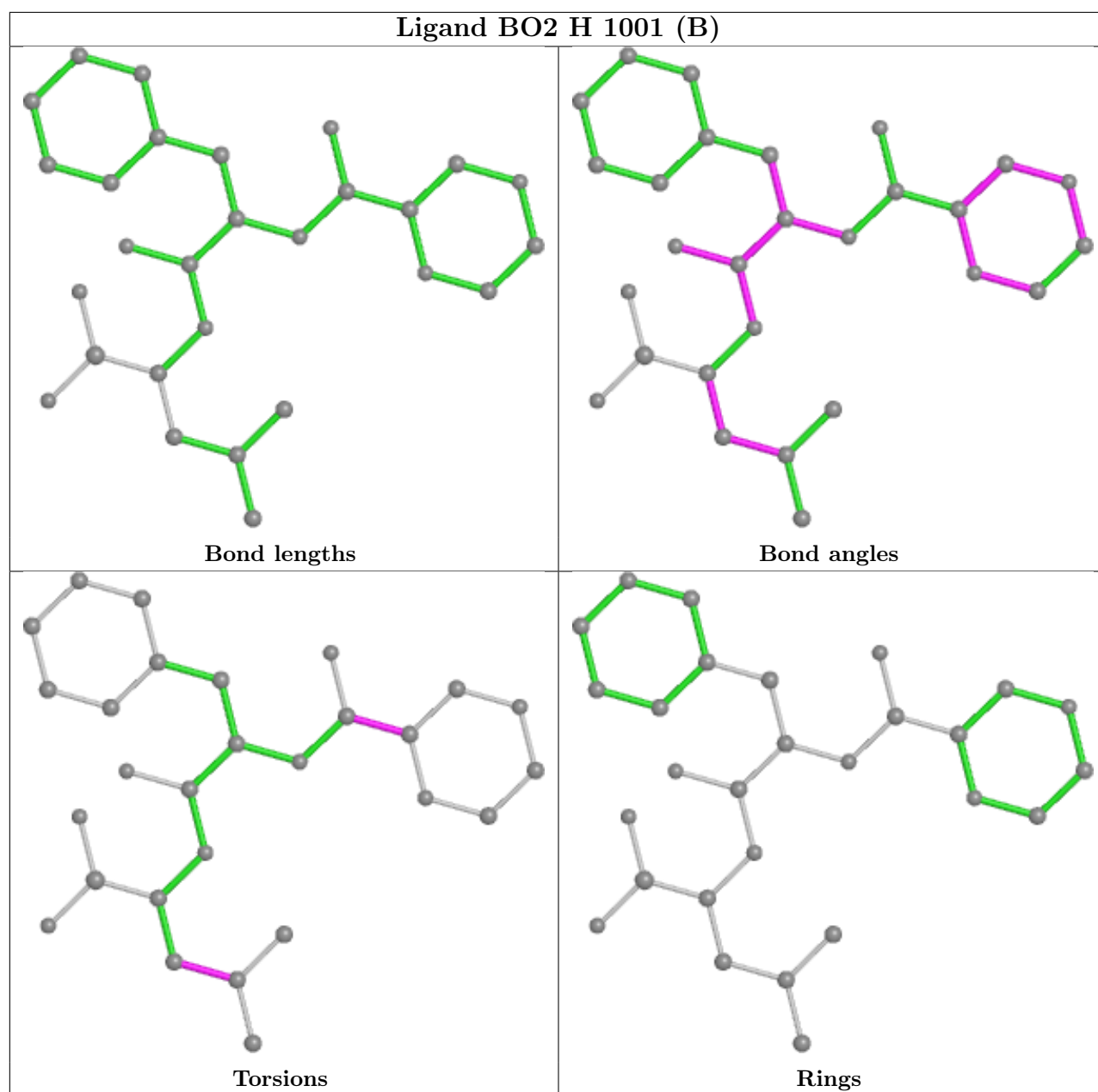


Ligand BO2 F 1001 (B)



Ligand BO2 F 1001 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	186/218 (85%)	-0.52	2 (1%) 80 84	12, 19, 42, 86	0
1	B	185/218 (84%)	-0.44	1 (0%) 91 92	13, 22, 47, 76	0
1	C	194/218 (88%)	-0.46	3 (1%) 73 77	13, 21, 50, 78	0
1	D	185/218 (84%)	-0.59	1 (0%) 91 92	13, 21, 41, 66	0
1	E	185/218 (84%)	-0.56	1 (0%) 91 92	12, 20, 42, 69	0
1	F	185/218 (84%)	-0.47	0 100 100	12, 20, 42, 83	0
1	G	184/218 (84%)	-0.60	0 100 100	13, 22, 42, 70	0
1	H	193/218 (88%)	-0.54	3 (1%) 72 76	14, 21, 57, 90	0
1	I	186/218 (85%)	-0.63	0 100 100	14, 22, 42, 75	0
1	J	186/218 (85%)	-0.56	1 (0%) 91 92	14, 23, 50, 75	0
1	K	186/218 (85%)	-0.65	0 100 100	14, 22, 45, 77	0
1	L	194/218 (88%)	-0.48	1 (0%) 91 92	13, 21, 48, 74	0
All	All	2249/2616 (85%)	-0.54	13 (0%) 89 91	12, 21, 47, 90	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	955	LEU	3.8
1	B	831	ALA	3.3
1	H	954	ALA	3.1
1	A	787	PRO	2.9
1	C	929	GLU	2.7
1	A	786	ARG	2.6
1	L	787	PRO	2.5
1	J	887	GLY	2.5
1	H	787	PRO	2.5
1	C	955	LEU	2.2
1	E	949	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	954	ALA	2.2
1	D	929	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	L	1002	6/6	0.74	0.31	76,91,100,107	0
4	GOL	G	1002	6/6	0.90	0.23	51,63,75,76	0
2	BO2	G	1001[B]	28/28	0.92	0.14	5,18,29,32	6
2	BO2	L	1001[A]	28/28	0.92	0.14	14,19,28,33	6
2	BO2	L	1001[B]	28/28	0.92	0.14	5,19,28,33	6
3	1PE	C	1002	16/16	0.92	0.16	26,35,50,56	0
2	BO2	B	1001	28/28	0.92	0.11	13,23,31,32	0
2	BO2	G	1001[A]	28/28	0.92	0.14	12,21,29,32	6
2	BO2	C	1001[B]	28/28	0.93	0.14	3,18,27,32	6
2	BO2	H	1001[A]	28/28	0.93	0.12	10,21,29,34	6
2	BO2	H	1001[B]	28/28	0.93	0.12	7,20,29,34	6
2	BO2	J	1001[A]	28/28	0.93	0.11	12,23,30,32	6
2	BO2	J	1001[B]	28/28	0.93	0.11	6,22,30,32	6
2	BO2	K	1001[A]	28/28	0.93	0.14	14,21,26,31	6
2	BO2	K	1001[B]	28/28	0.93	0.14	6,20,26,31	6
2	BO2	E	1001[A]	28/28	0.93	0.14	11,20,30,31	6
2	BO2	E	1001[B]	28/28	0.93	0.14	6,20,30,31	6
2	BO2	F	1001[A]	28/28	0.93	0.13	12,19,27,32	6
2	BO2	F	1001[B]	28/28	0.93	0.13	6,18,27,32	6
2	BO2	C	1001[A]	28/28	0.93	0.14	10,20,27,32	6
2	BO2	D	1001[B]	28/28	0.94	0.11	3,21,30,30	6

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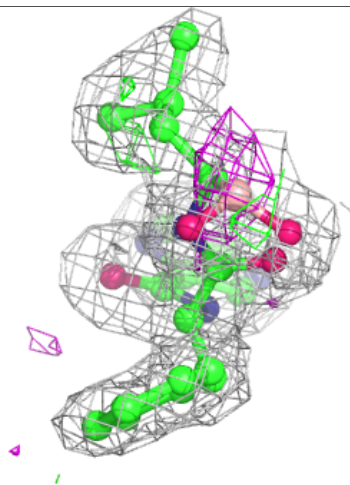
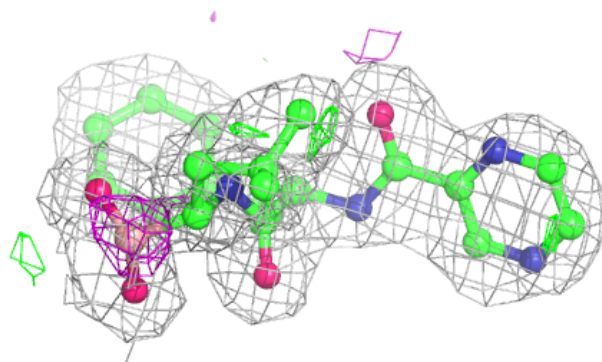
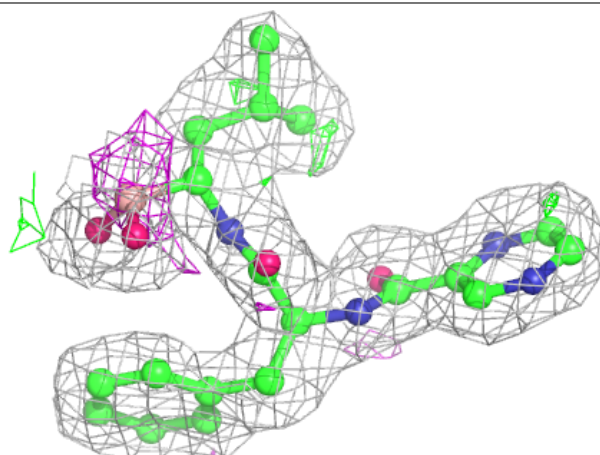
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BO2	I	1001[A]	28/28	0.94	0.12	13,21,30,33	6
2	BO2	I	1001[B]	28/28	0.94	0.12	7,21,30,33	6
3	1PE	A	1002	16/16	0.94	0.13	19,28,50,56	0
2	BO2	A	1001[B]	28/28	0.94	0.12	6,19,32,33	6
3	1PE	F	1002	16/16	0.94	0.13	15,36,49,49	0
3	1PE	H	1002	16/16	0.94	0.12	18,29,50,53	0
2	BO2	A	1001[A]	28/28	0.94	0.12	8,19,32,33	6
2	BO2	D	1001[A]	28/28	0.94	0.11	11,21,30,30	6
3	1PE	B	1002	16/16	0.95	0.12	22,33,47,48	0
3	1PE	I	1002	16/16	0.95	0.10	25,32,46,56	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.

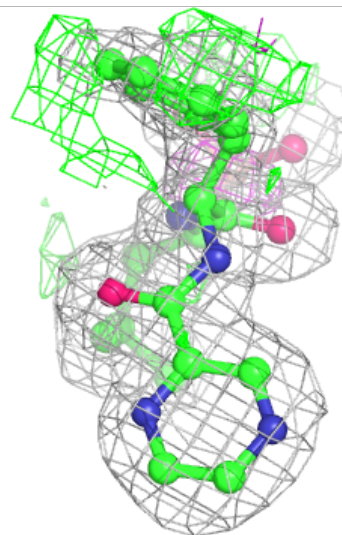
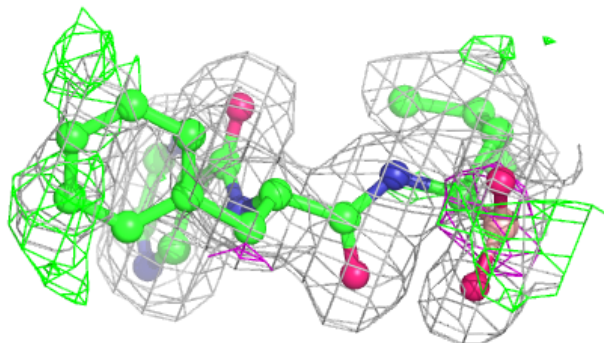
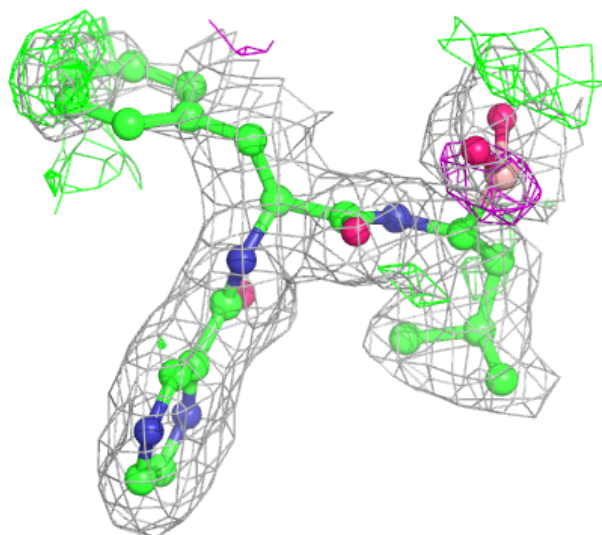
Electron density around BO2 G 1001 (B):

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



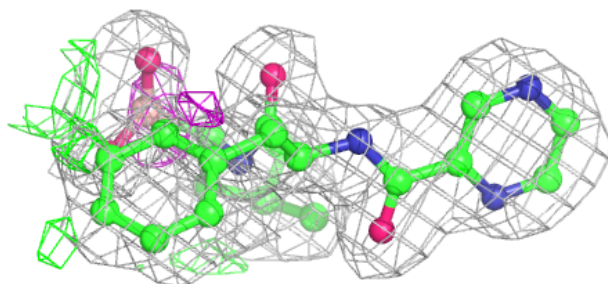
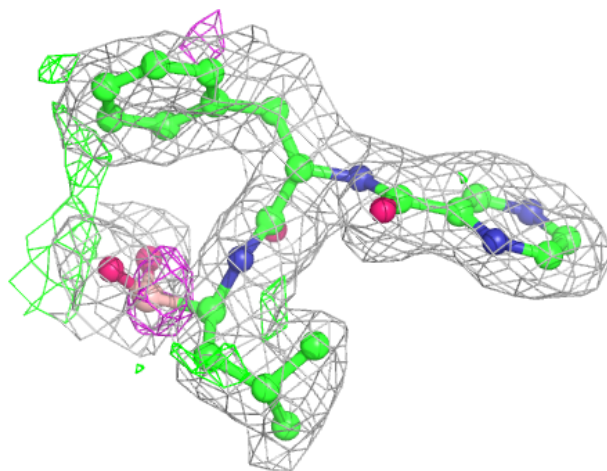
Electron density around BO2 L 1001 (A):

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



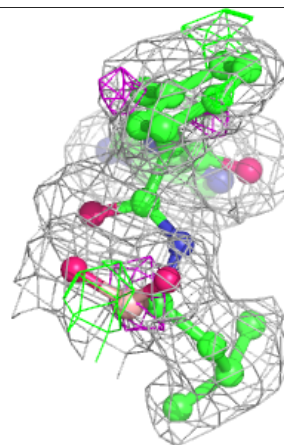
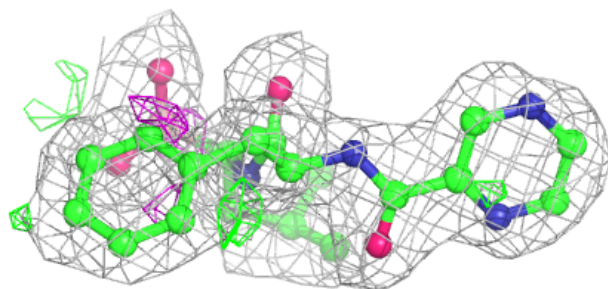
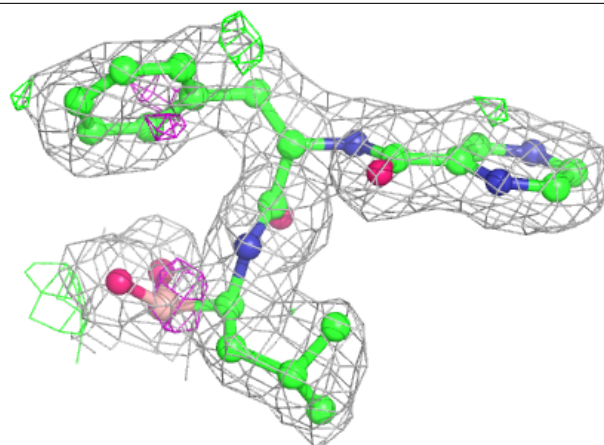
Electron density around BO2 L 1001 (B):

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



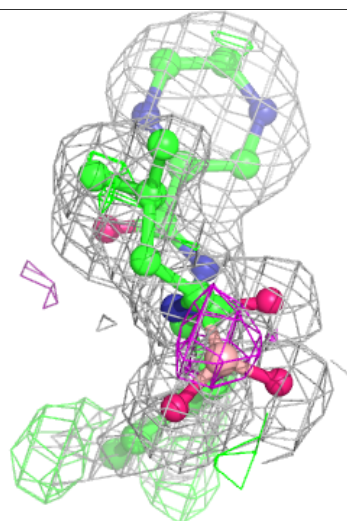
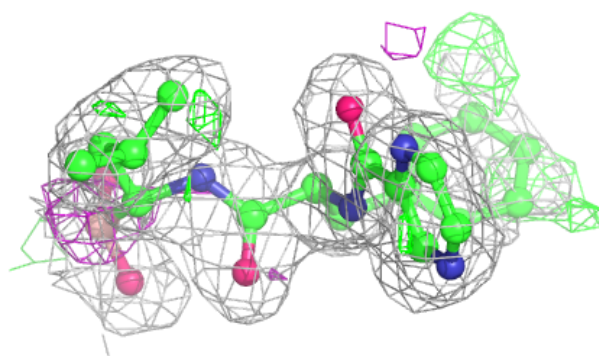
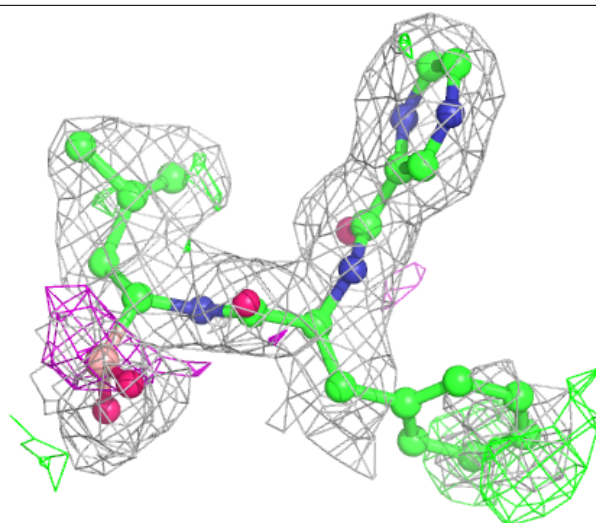
Electron density around BO2 B 1001:

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



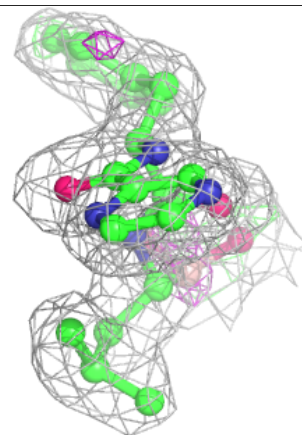
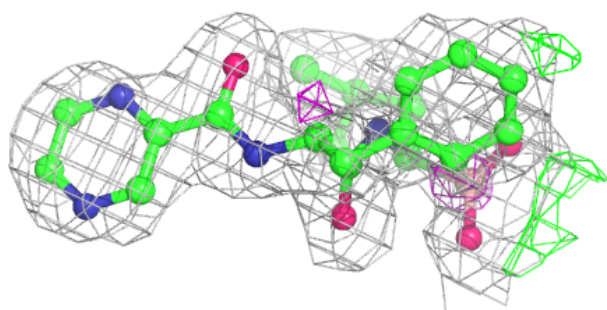
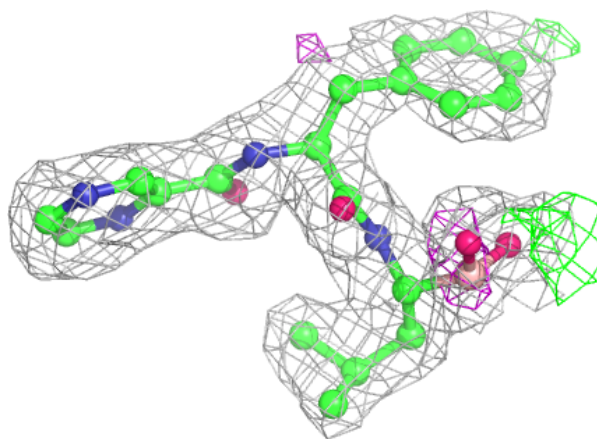
Electron density around BO2 G 1001 (A):

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



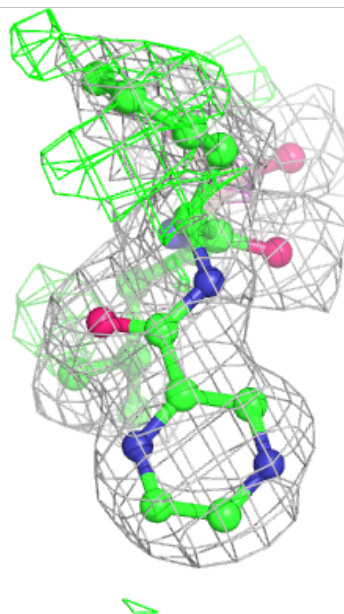
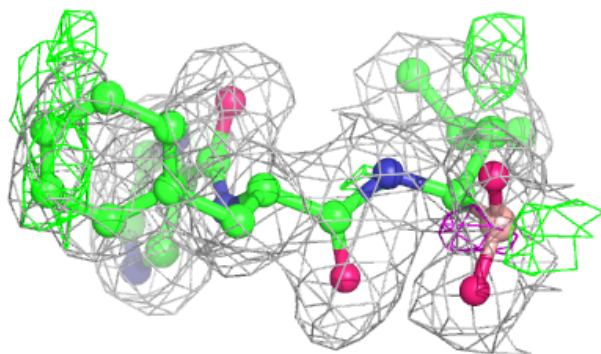
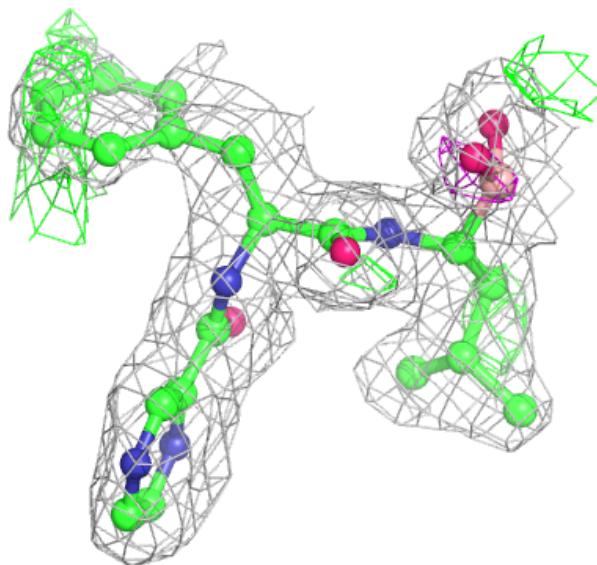
Electron density around BO2 C 1001 (B):

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



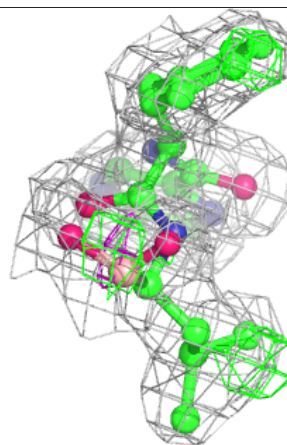
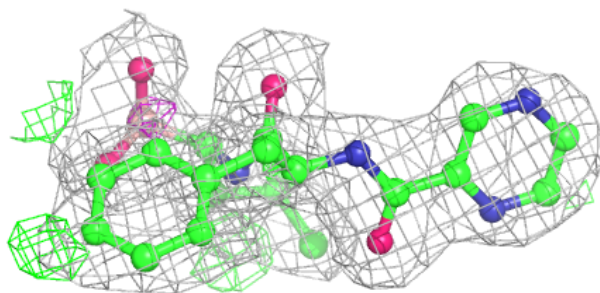
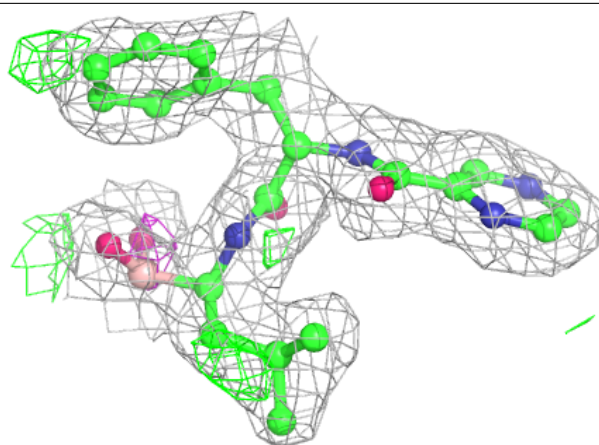
Electron density around BO2 H 1001 (A):

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



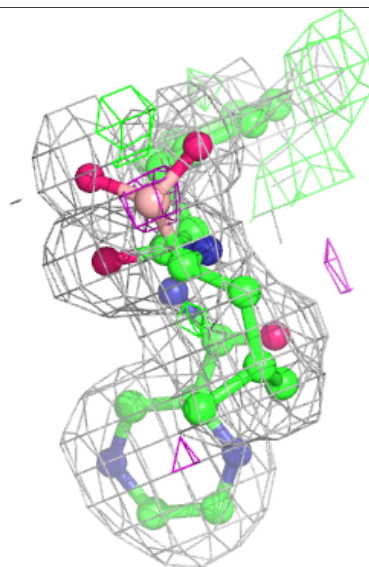
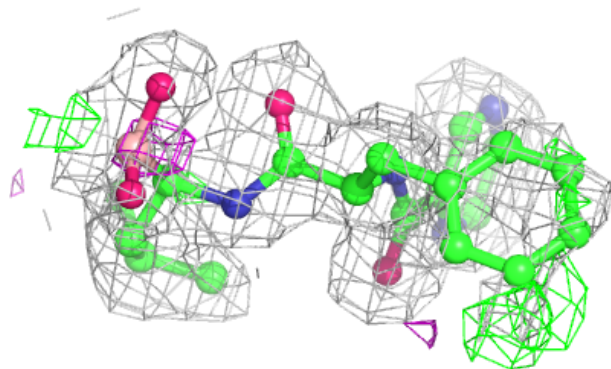
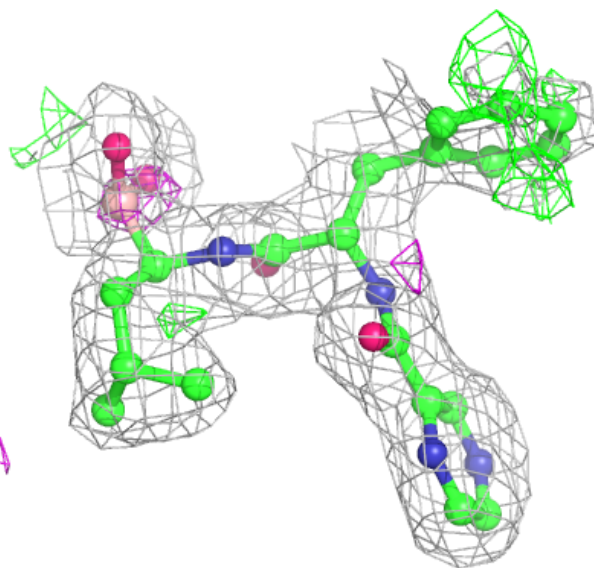
Electron density around BO2 H 1001 (B):

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



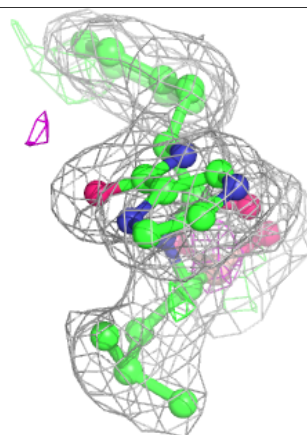
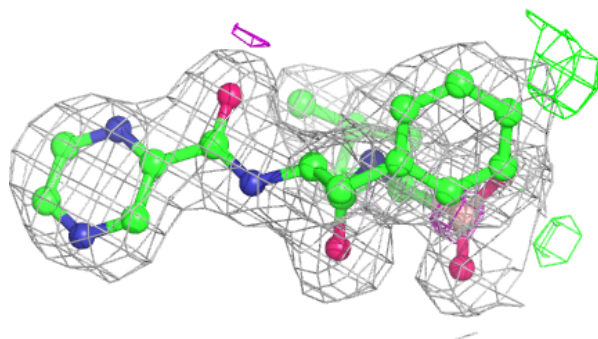
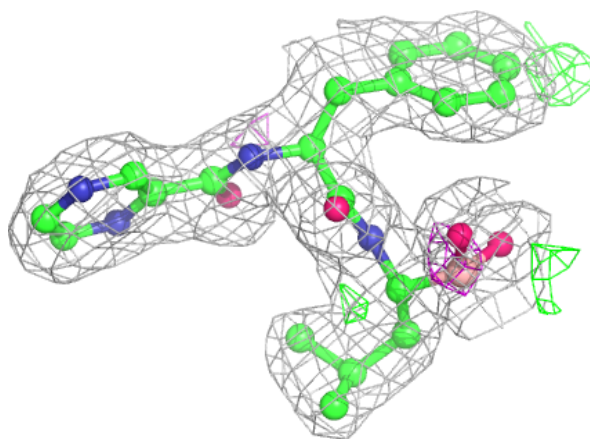
Electron density around BO2 J 1001 (A):

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



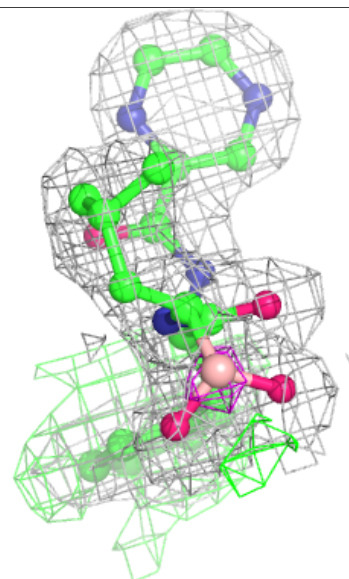
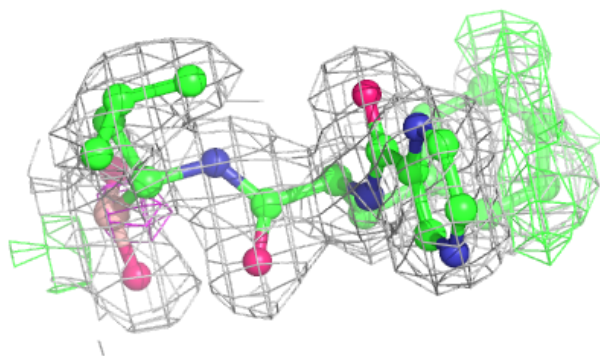
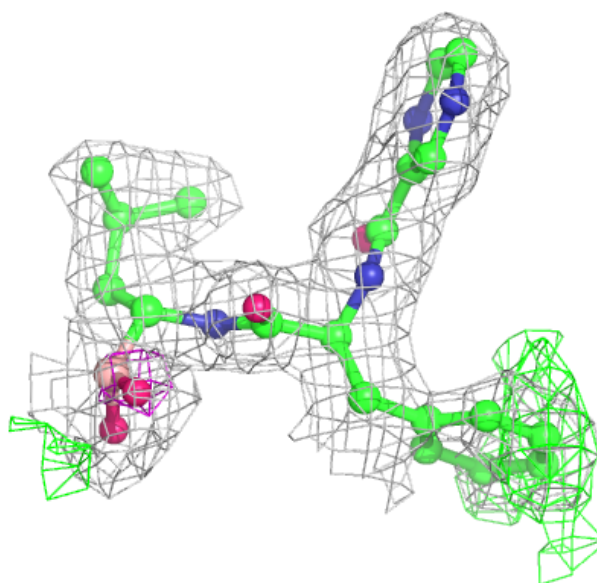
Electron density around BO2 J 1001 (B):

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



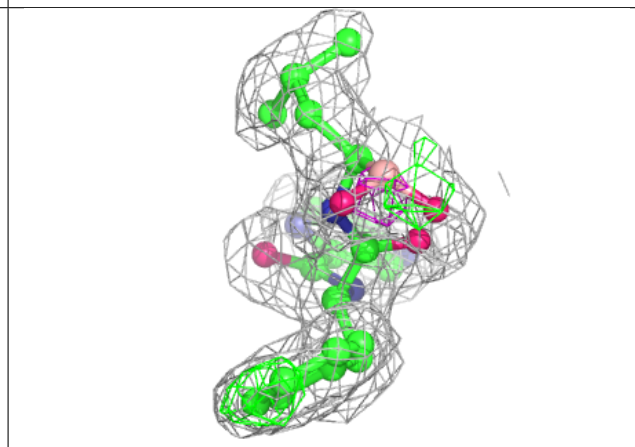
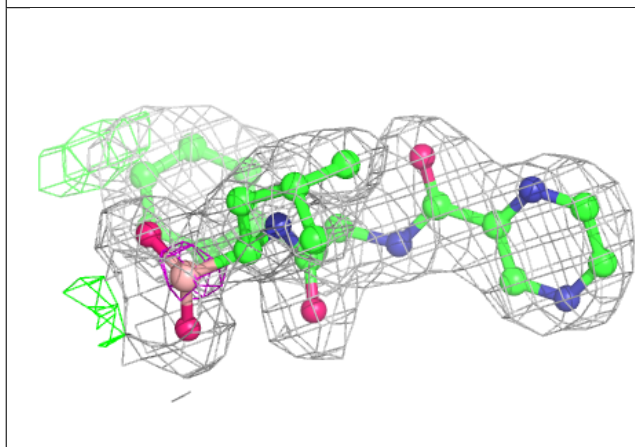
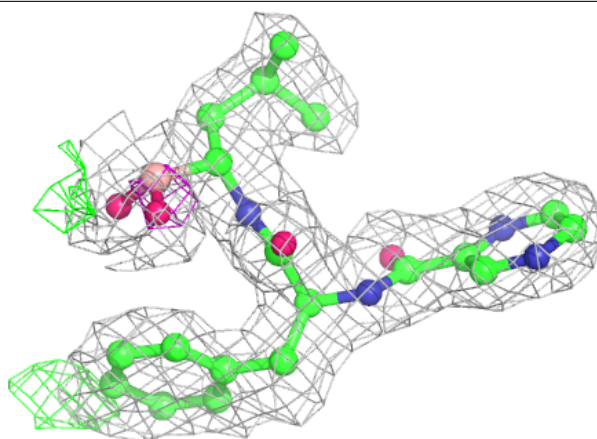
Electron density around BO2 K 1001 (A):

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



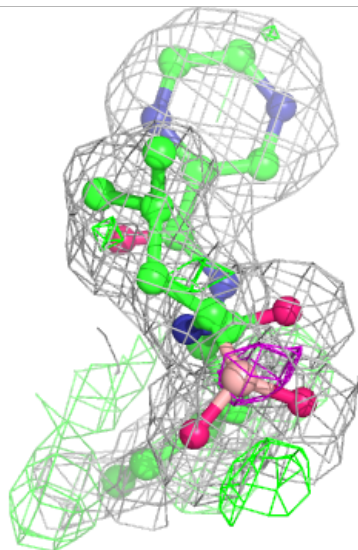
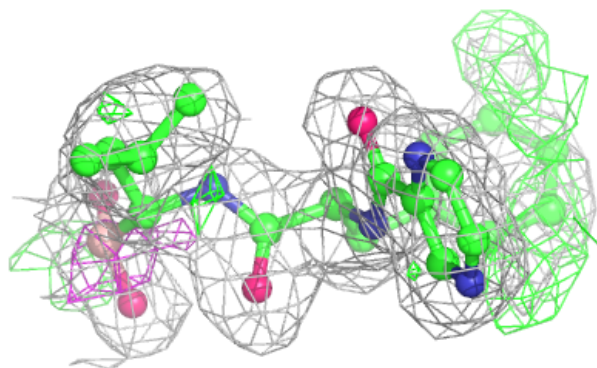
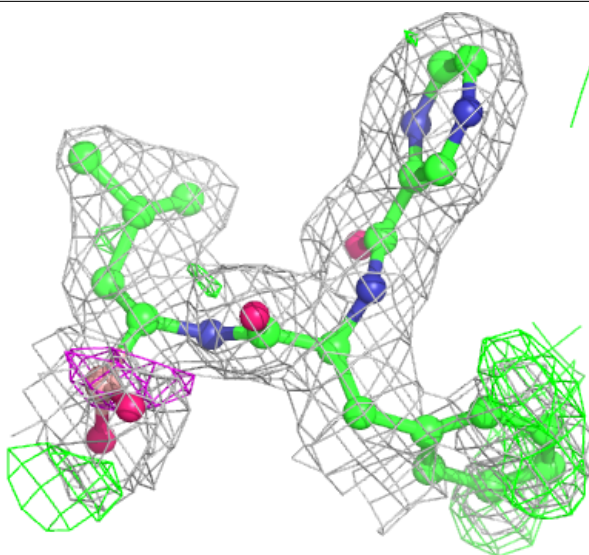
Electron density around BO2 K 1001 (B):

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



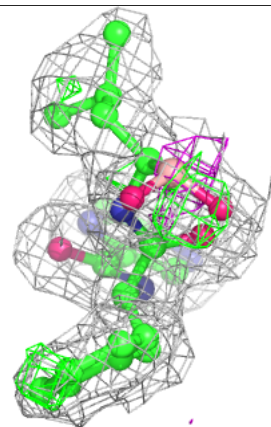
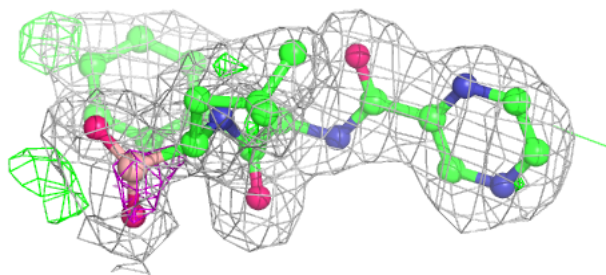
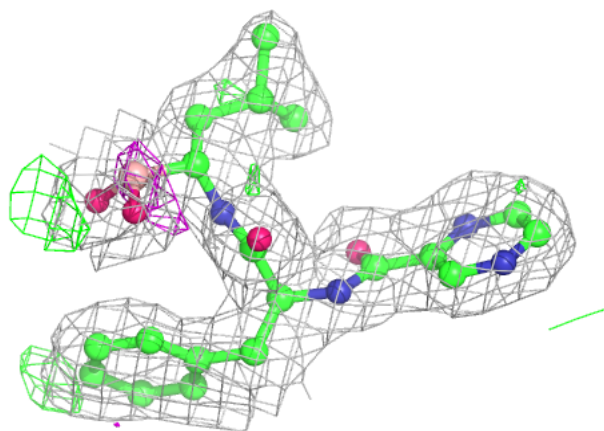
Electron density around BO2 E 1001 (A):

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



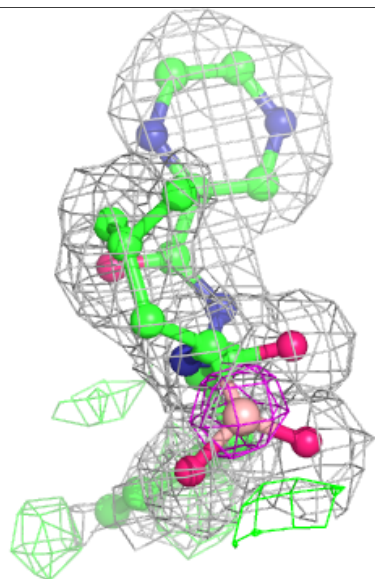
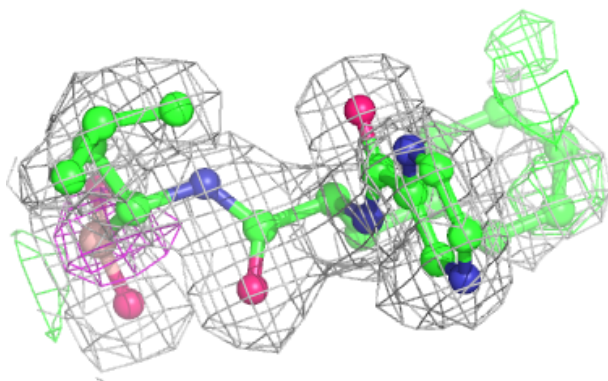
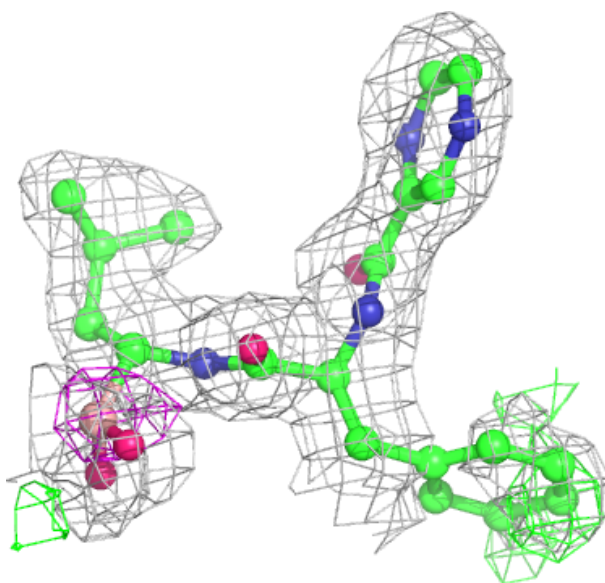
Electron density around BO2 E 1001 (B):

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



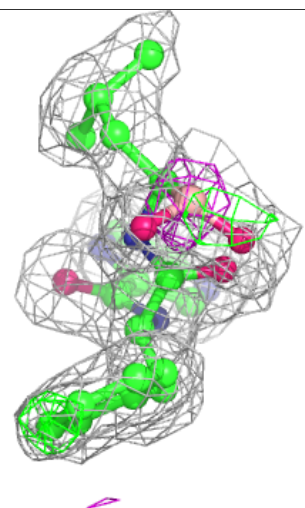
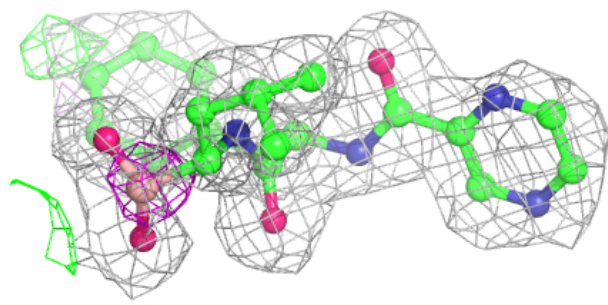
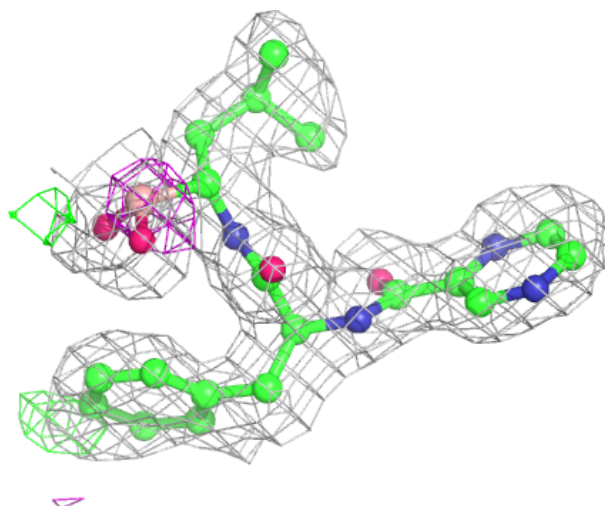
Electron density around BO2 F 1001 (A):

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



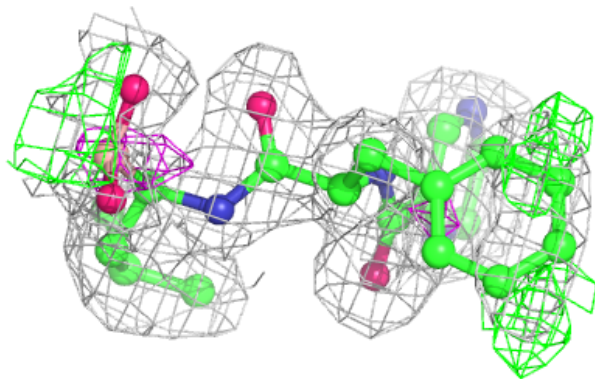
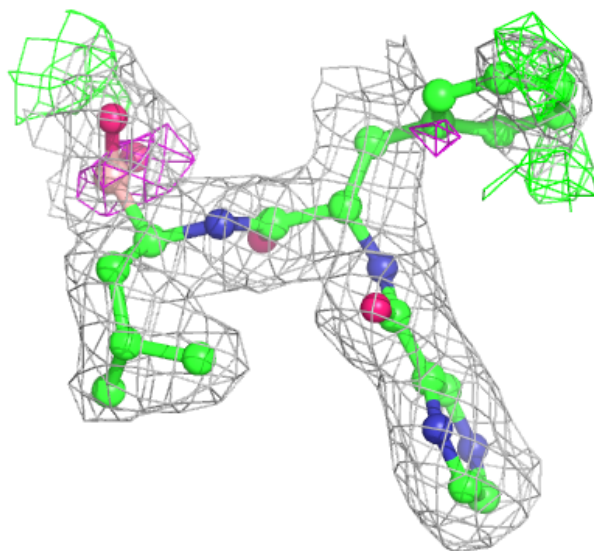
Electron density around BO2 F 1001 (B):

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



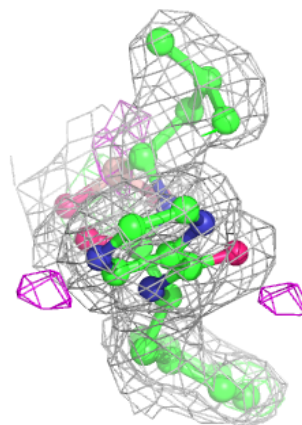
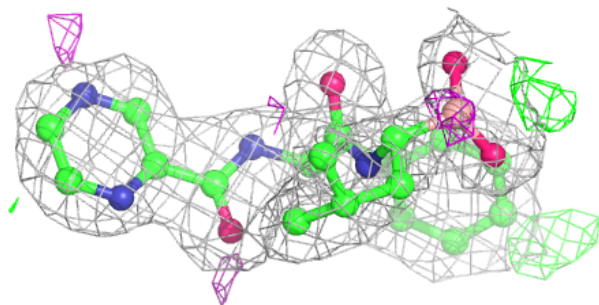
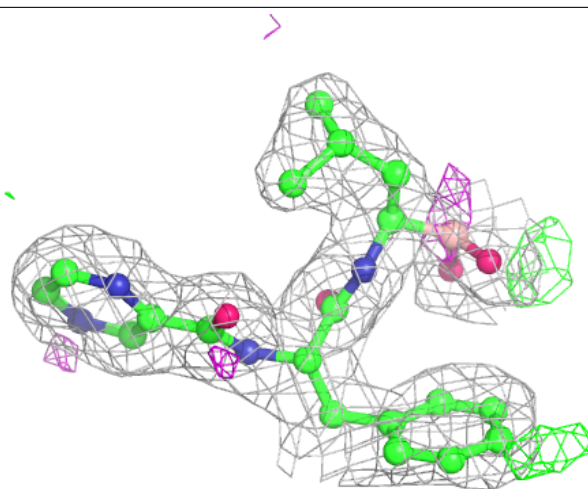
Electron density around BO2 C 1001 (A):

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and green (positive)



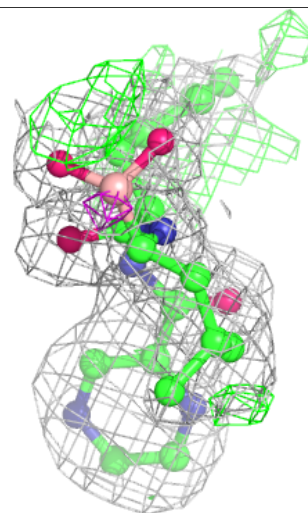
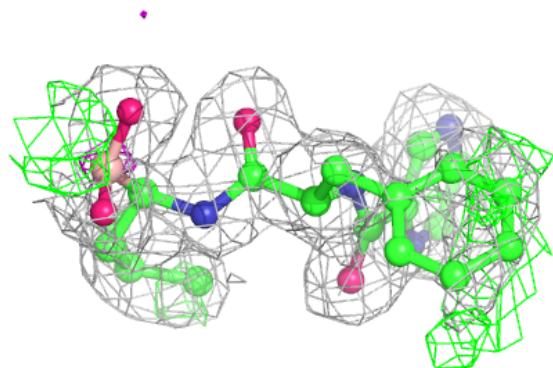
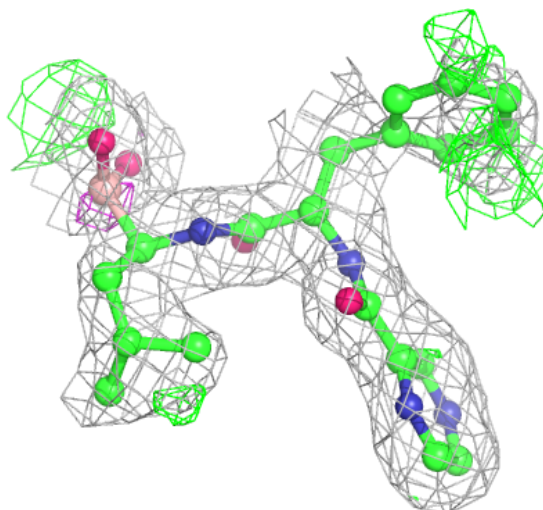
Electron density around BO2 D 1001 (B):

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



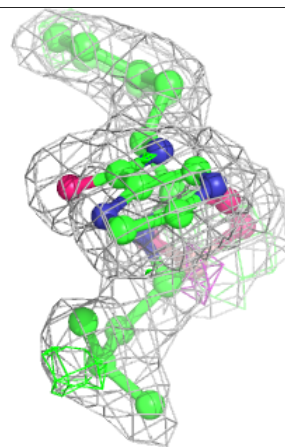
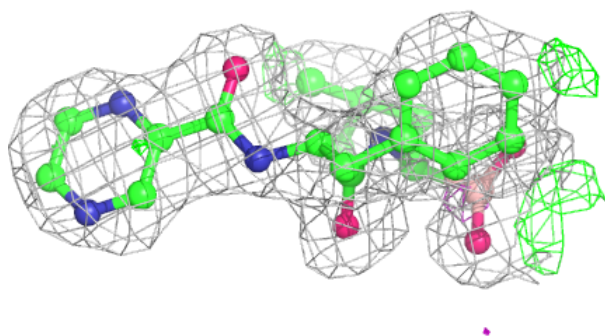
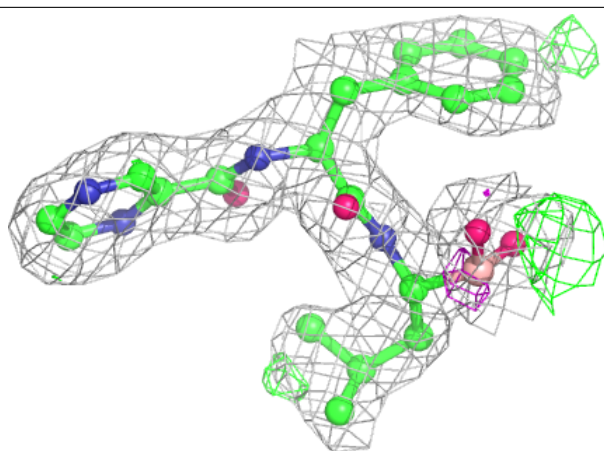
Electron density around BO2 I 1001 (A):

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



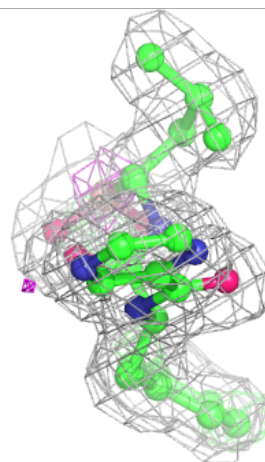
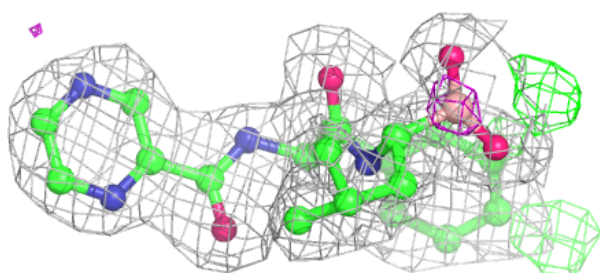
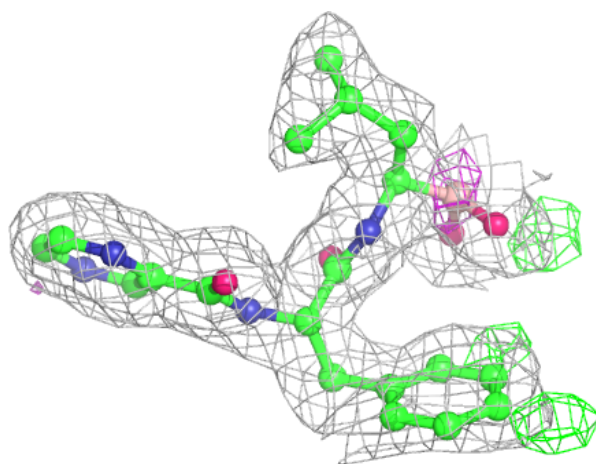
Electron density around BO2 I 1001 (B):

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



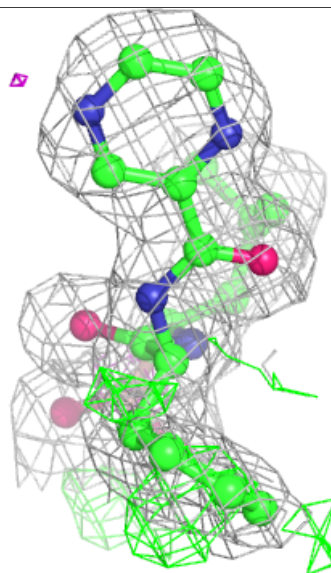
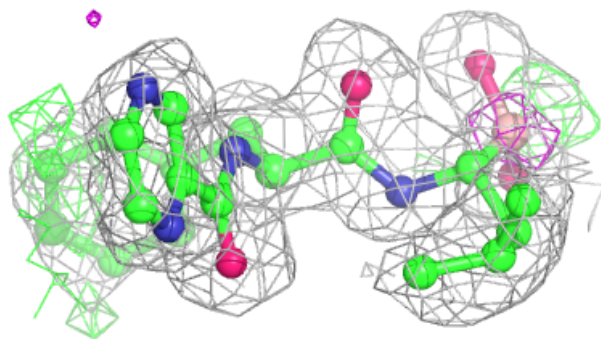
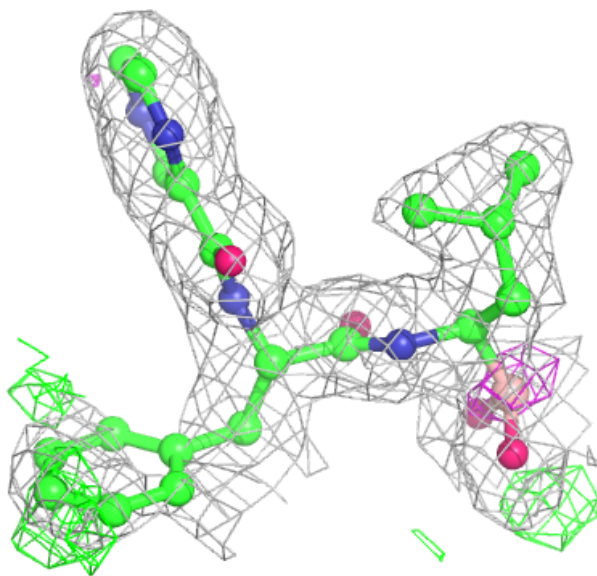
Electron density around BO2 A 1001 (B):

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



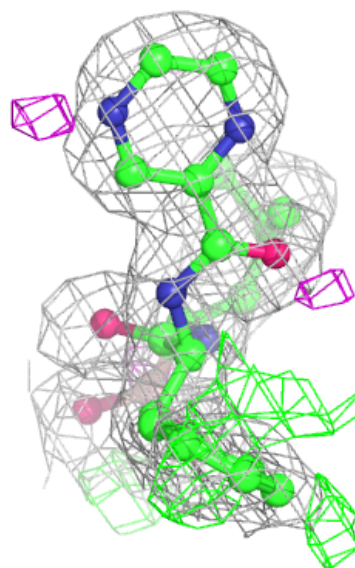
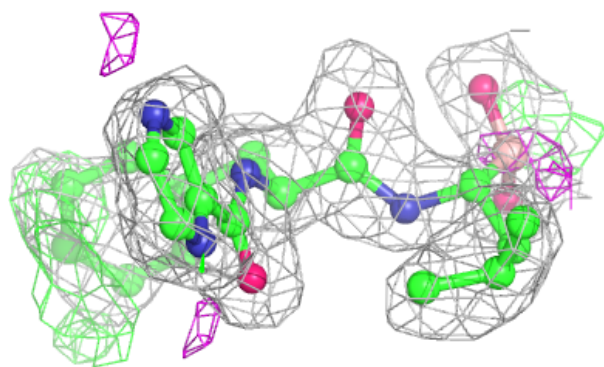
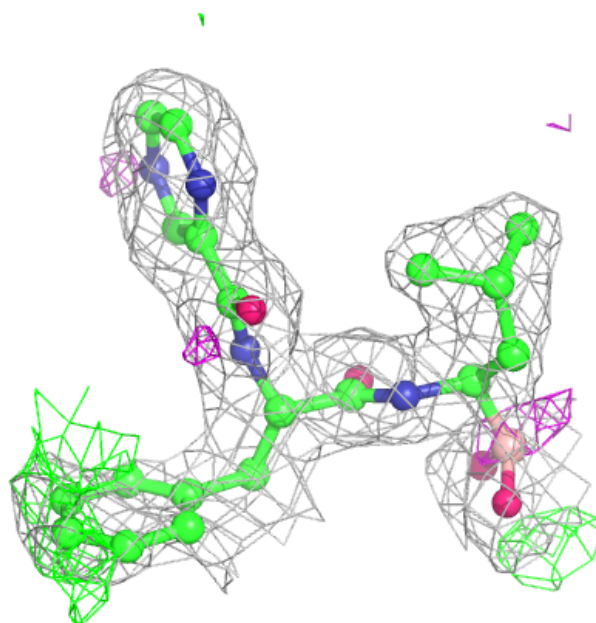
Electron density around BO2 A 1001 (A):

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 BO2 D 1001 (A):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.