



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2019 – 07:12 PM EDT

PDB ID : 6HMW  
Title : Cholera toxin classical B-pentamer in complex with fucose  
Authors : Krengel, U.; Heim, J.B.  
Deposited on : 2018-09-13  
Resolution : 1.95 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

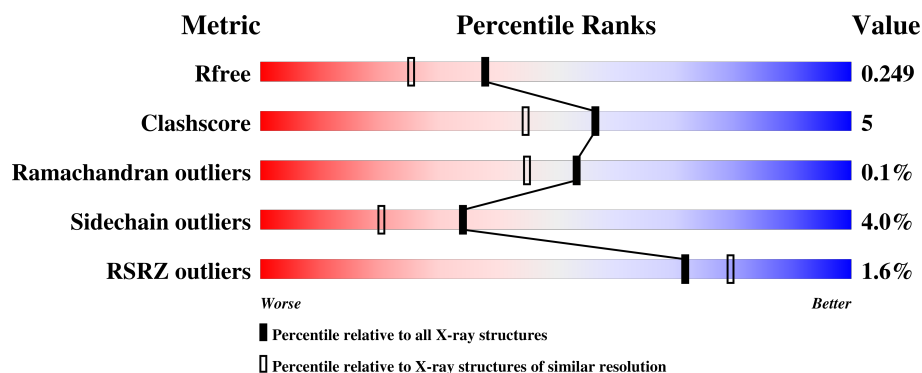
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	103	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> <span>•</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span></span> <span>84%</span> <span>14%</span> <span></span> </div> </div>
1	B	103	<div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <span>•</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span></span> <span>90%</span> <span>9%</span> <span></span> </div>
1	C	103	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <span></span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span></span> <span>90%</span> <span>10%</span> <span></span> </div> </div>
1	D	103	<div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> <span>•</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span></span> <span>90%</span> <span>8%</span> <span></span> </div>
1	E	103	<div> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <span>•</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span></span> <span>86%</span> <span>13%</span> <span></span> </div>

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Mol	Chain	Length	Quality of chain
1	F	103	<div><div></div><div>6%</div><div>82%</div><div>16%</div><div></div><div></div></div>
1	G	103	<div><div></div><div>92%</div><div>6%</div><div></div><div></div><div></div></div>
1	H	103	<div><div></div><div>83%</div><div>17%</div><div></div><div></div><div></div></div>
1	I	103	<div><div></div><div>6%</div><div>85%</div><div>13%</div><div></div><div></div></div>
1	J	103	<div><div></div><div>2%</div><div>92%</div><div>7%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8769 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cholera enterotoxin B-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	1	0
			823	516	144	158	5			
1	B	103	Total	C	N	O	S	0	2	0
			825	521	143	156	5			
1	C	103	Total	C	N	O	S	0	1	0
			820	516	143	156	5			
1	D	103	Total	C	N	O	S	0	4	0
			842	528	149	160	5			
1	E	103	Total	C	N	O	S	0	0	0
			814	511	142	156	5			
1	F	103	Total	C	N	O	S	0	0	0
			814	511	142	156	5			
1	G	102	Total	C	N	O	S	0	0	0
			805	507	140	153	5			
1	H	103	Total	C	N	O	S	0	2	0
			827	521	145	156	5			
1	I	103	Total	C	N	O	S	0	1	0
			819	516	142	156	5			
1	J	103	Total	C	N	O	S	0	2	0
			829	520	145	159	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

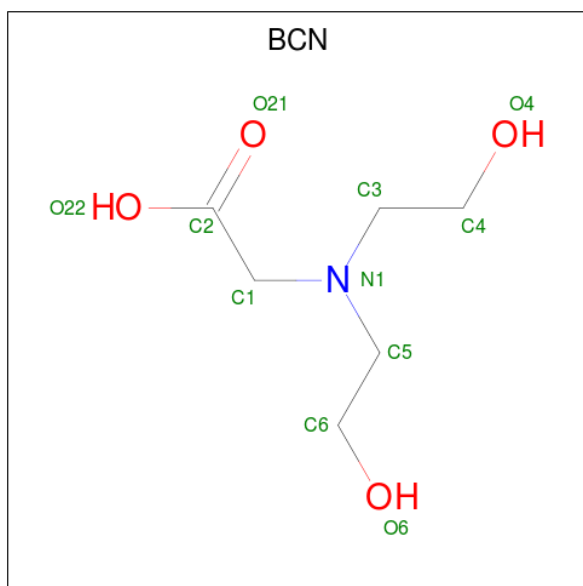
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

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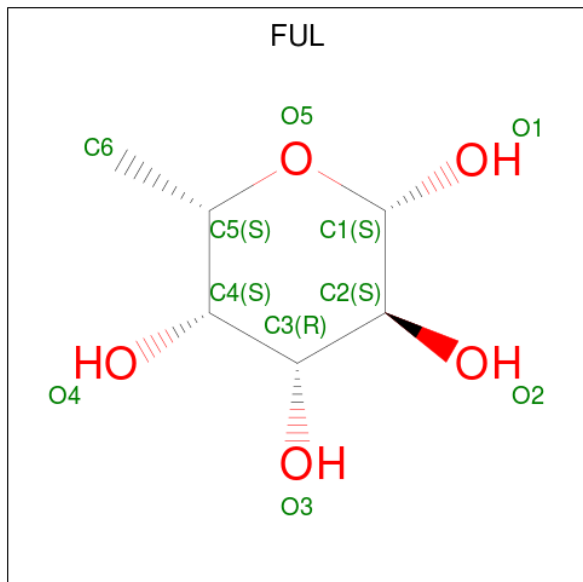
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Ca	0	0
			2	2		

- Molecule 3 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		
3	C	1	Total	C	N	O	0	0
			11	6	1	4		
3	C	1	Total	C	N	O	0	0
			11	6	1	4		
3	D	1	Total	C	N	O	0	0
			11	6	1	4		
3	D	1	Total	C	N	O	0	0
			11	6	1	4		
3	E	1	Total	C	N	O	0	0
			11	6	1	4		
3	E	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 4 is BETA-L-FUCOSE (three-letter code: FUL) (formula:  $C_6H_{12}O_5$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			11	6	5		
4	F	1	Total	C	O	0	0
			10	6	4		
4	F	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			11	6	5		
4	H	1	Total	C	O	0	0
			11	6	5		
4	I	1	Total	C	O	0	0
			11	6	5		
4	J	1	Total	C	O	0	0
			11	6	5		

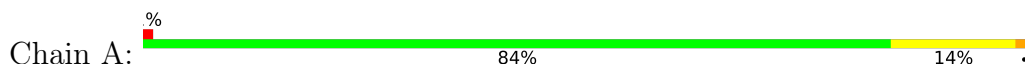
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	33	Total	O	0	0
			33	33		
5	C	33	Total	O	0	0
			33	33		
5	D	24	Total	O	0	0
			24	24		
5	E	28	Total	O	0	0
			28	28		
5	F	17	Total	O	0	0
			17	17		
5	G	30	Total	O	0	0
			30	30		
5	H	37	Total	O	0	0
			37	37		
5	I	18	Total	O	0	0
			18	18		
5	J	14	Total	O	0	0
			14	14		

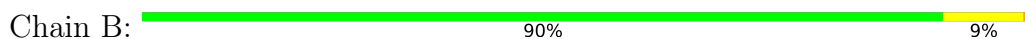
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

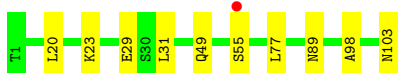
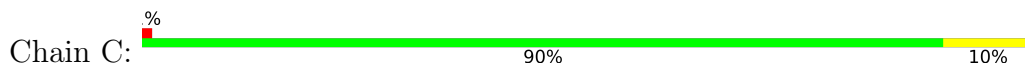
- Molecule 1: Cholera enterotoxin B-subunit



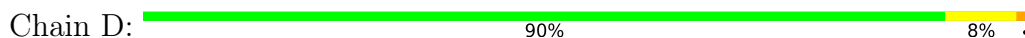
- Molecule 1: Cholera enterotoxin B-subunit



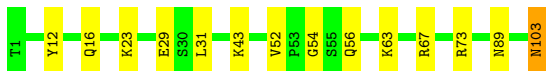
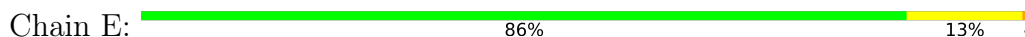
- Molecule 1: Cholera enterotoxin B-subunit



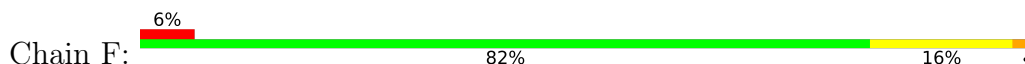
- Molecule 1: Cholera enterotoxin B-subunit



- Molecule 1: Cholera enterotoxin B-subunit



- Molecule 1: Cholera enterotoxin B-subunit

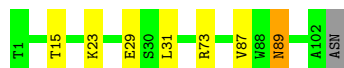






- Molecule 1: Cholera enterotoxin B-subunit

Chain G: 92% 6% ..



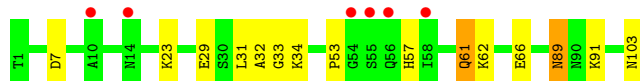
- Molecule 1: Cholera enterotoxin B-subunit

Chain H: 83% 17% .



- Molecule 1: Cholera enterotoxin B-subunit

Chain I: 6% 85% 13% .



- Molecule 1: Cholera enterotoxin B-subunit

Chain J: 2% 92% 7% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.78Å 100.54Å 93.01Å 90.00° 117.00° 90.00°	Depositor
Resolution (Å)	47.42 – 1.95 47.42 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.42-1.95) 97.6 (47.42-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.187 , 0.237 0.197 , 0.249	Depositor DCC
$R_{free}$ test set	3442 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCN, CA, FUL

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	0.75	0/837	0.87	0/1130
1	B	0.75	0/845	0.83	0/1140
1	C	0.75	0/837	0.87	0/1129
1	D	0.76	0/861	0.89	1/1158 (0.1%)
1	E	0.80	0/828	0.86	1/1118 (0.1%)
1	F	0.64	0/828	0.80	0/1118
1	G	0.80	0/819	0.85	0/1107
1	H	0.83	0/847	0.88	0/1143
1	I	0.78	2/836 (0.2%)	0.79	0/1129
1	J	0.67	0/845	0.81	0/1137
All	All	0.75	2/8383 (0.0%)	0.85	2/11309 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	J	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	29	GLU	CD-OE1	-5.85	1.19	1.25
1	I	7	ASP	CB-CG	5.03	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	D	73	ARG	NE-CZ-NH2	-6.22	117.19	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	GLN	Peptide
1	B	49	GLN	Peptide
1	C	49	GLN	Peptide
1	D	49	GLN	Peptide
1	E	67	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	823	0	824	16	0
1	B	825	0	839	15	0
1	C	820	0	828	5	0
1	D	842	0	852	14	0
1	E	814	0	816	8	0
1	F	814	0	816	14	0
1	G	805	0	810	6	0
1	H	827	0	841	18	0
1	I	819	0	828	11	0
1	J	829	0	834	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	20	0	0
3	B	22	0	20	0	0
3	C	22	0	21	0	0
3	D	22	0	21	1	0
3	E	22	0	20	4	0
4	A	11	0	12	0	0
4	B	21	0	22	0	0
4	C	21	0	22	0	0
4	D	21	0	22	0	0
4	E	21	0	22	0	0
4	F	21	0	22	2	0
4	G	21	0	22	0	0
4	H	11	0	12	0	0
4	I	11	0	12	0	0
4	J	11	0	12	0	0
5	A	27	0	0	0	0
5	B	33	0	0	0	0
5	C	33	0	0	0	0
5	D	24	0	0	1	0
5	E	28	0	0	0	0
5	F	17	0	0	1	0
5	G	30	0	0	0	0
5	H	37	0	0	3	0
5	I	18	0	0	0	0
5	J	14	0	0	0	0
All	All	8769	0	8570	92	0

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

The worst 5 of 92 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HG22	1:A:61:GLN:OE1	1.71	0.89
1:E:103:ASN:ND2	1:J:23[B]:LYS:HE2	1.89	0.88
1:J:89:ASN:HD22	1:J:89:ASN:C	1.80	0.84
1:B:23[B]:LYS:NZ	1:H:103:ASN:ND2	2.29	0.81
1:D:103[A]:ASN:HB2	3:E:201:BCN:O22	1.82	0.79

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	102/103 (99%)	98 (96%)	4 (4%)	0	100	100
1	B	103/103 (100%)	101 (98%)	2 (2%)	0	100	100
1	C	102/103 (99%)	101 (99%)	1 (1%)	0	100	100
1	D	104/103 (101%)	102 (98%)	2 (2%)	0	100	100
1	E	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	F	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	G	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
1	H	103/103 (100%)	101 (98%)	1 (1%)	1 (1%)	17	7
1	I	102/103 (99%)	100 (98%)	2 (2%)	0	100	100
1	J	102/103 (99%)	98 (96%)	4 (4%)	0	100	100
All	All	1020/1030 (99%)	995 (98%)	24 (2%)	1 (0%)	53	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	102	ALA

### 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	90/89 (101%)	86 (96%)	4 (4%)	31	17
1	B	91/89 (102%)	88 (97%)	3 (3%)	41	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	90/89 (101%)	85 (94%)	5 (6%)	23	10
1	D	92/89 (103%)	89 (97%)	3 (3%)	41	28
1	E	89/89 (100%)	83 (93%)	6 (7%)	18	6
1	F	89/89 (100%)	83 (93%)	6 (7%)	18	6
1	G	88/89 (99%)	87 (99%)	1 (1%)	76	73
1	H	91/89 (102%)	89 (98%)	2 (2%)	55	47
1	I	90/89 (101%)	86 (96%)	4 (4%)	31	17
1	J	91/89 (102%)	89 (98%)	2 (2%)	55	47
All	All	901/890 (101%)	865 (96%)	36 (4%)	34	20

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	43	LYS
1	E	103	ASN
1	I	103	ASN
1	E	63	LYS
1	F	59	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	16	GLN
1	F	103	ASN
1	J	16	GLN
1	F	89	ASN
1	F	90	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 10 are monoatomic - leaving 26 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	$\# Z  > 2$
3	BCN	A	202	2	7,10,10	0.31	0	8,11,11	1.31	1 (12%)
4	FUL	A	203	-	11,11,11	0.58	0	15,16,16	0.76	0
3	BCN	A	205	2	7,10,10	0.32	0	8,11,11	1.00	0
3	BCN	B	201	2	7,10,10	0.38	0	8,11,11	0.66	0
4	FUL	B	202	1	9,10,11	0.74	0	13,14,16	1.48	3 (23%)
4	FUL	B	204	-	11,11,11	0.41	0	15,16,16	0.86	1 (6%)
3	BCN	B	205	2	7,10,10	0.31	0	8,11,11	1.14	0
4	FUL	C	201	1	9,10,11	0.73	0	13,14,16	1.53	4 (30%)
4	FUL	C	203	-	11,11,11	0.59	0	15,16,16	1.00	0
3	BCN	C	205	2	7,10,10	0.41	0	8,11,11	0.81	0
3	BCN	C	206	2	7,10,10	0.20	0	8,11,11	1.06	0
3	BCN	D	201	2	7,10,10	0.59	0	8,11,11	0.65	0
4	FUL	D	202	1	9,10,11	1.04	1 (11%)	13,14,16	1.98	4 (30%)
4	FUL	D	204	-	11,11,11	0.54	0	15,16,16	0.82	0
3	BCN	D	205	2	7,10,10	0.51	0	8,11,11	2.22	1 (12%)
3	BCN	E	201	2	7,10,10	0.33	0	8,11,11	0.88	0
4	FUL	E	202	1	9,10,11	1.23	0	13,14,16	1.70	2 (15%)
4	FUL	E	204	-	11,11,11	0.49	0	15,16,16	0.86	0
3	BCN	E	206	2	7,10,10	0.33	0	8,11,11	1.51	2 (25%)
4	FUL	F	201	1	9,10,11	0.75	0	13,14,16	1.66	3 (23%)
4	FUL	F	202	-	11,11,11	0.65	0	15,16,16	1.09	0
4	FUL	G	201	1	9,10,11	0.71	0	13,14,16	2.05	4 (30%)
4	FUL	G	202	-	11,11,11	0.71	0	15,16,16	0.73	0
4	FUL	H	201	-	11,11,11	0.63	0	15,16,16	0.94	0
4	FUL	I	201	-	11,11,11	0.58	0	15,16,16	0.93	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUL	J	201	-	11,11,11	0.64	0	15,16,16	1.11	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCN	A	202	2	-	2/8/10/10	-
4	FUL	A	203	-	-	-	0/1/1/1
3	BCN	A	205	2	-	2/8/10/10	-
3	BCN	B	201	2	-	3/8/10/10	-
4	FUL	B	202	1	-	-	0/1/1/1
4	FUL	B	204	-	-	-	0/1/1/1
3	BCN	B	205	2	-	2/8/10/10	-
4	FUL	C	201	1	-	-	0/1/1/1
4	FUL	C	203	-	-	-	0/1/1/1
3	BCN	C	205	2	-	2/8/10/10	-
3	BCN	C	206	2	-	2/8/10/10	-
3	BCN	D	201	2	-	2/8/10/10	-
4	FUL	D	202	1	-	-	0/1/1/1
4	FUL	D	204	-	-	-	0/1/1/1
3	BCN	D	205	2	-	1/8/10/10	-
3	BCN	E	201	2	-	3/8/10/10	-
4	FUL	E	202	1	-	-	0/1/1/1
4	FUL	E	204	-	-	-	0/1/1/1
3	BCN	E	206	2	-	1/8/10/10	-
4	FUL	F	201	1	-	-	0/1/1/1
4	FUL	F	202	-	-	-	0/1/1/1
4	FUL	G	201	1	-	-	0/1/1/1
4	FUL	G	202	-	-	-	0/1/1/1
4	FUL	H	201	-	-	-	0/1/1/1
4	FUL	I	201	-	-	-	0/1/1/1
4	FUL	J	201	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	202	FUL	C4-C5	2.05	1.57	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	205	BCN	C2-C1-N1	-5.75	105.29	113.48
4	F	201	FUL	O5-C1-C2	-4.13	104.43	110.79
4	D	202	FUL	O2-C2-C3	-4.13	102.10	110.16
4	E	202	FUL	C1-C2-C3	4.04	114.63	109.66
4	G	201	FUL	C1-C2-C3	3.92	114.47	109.66

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

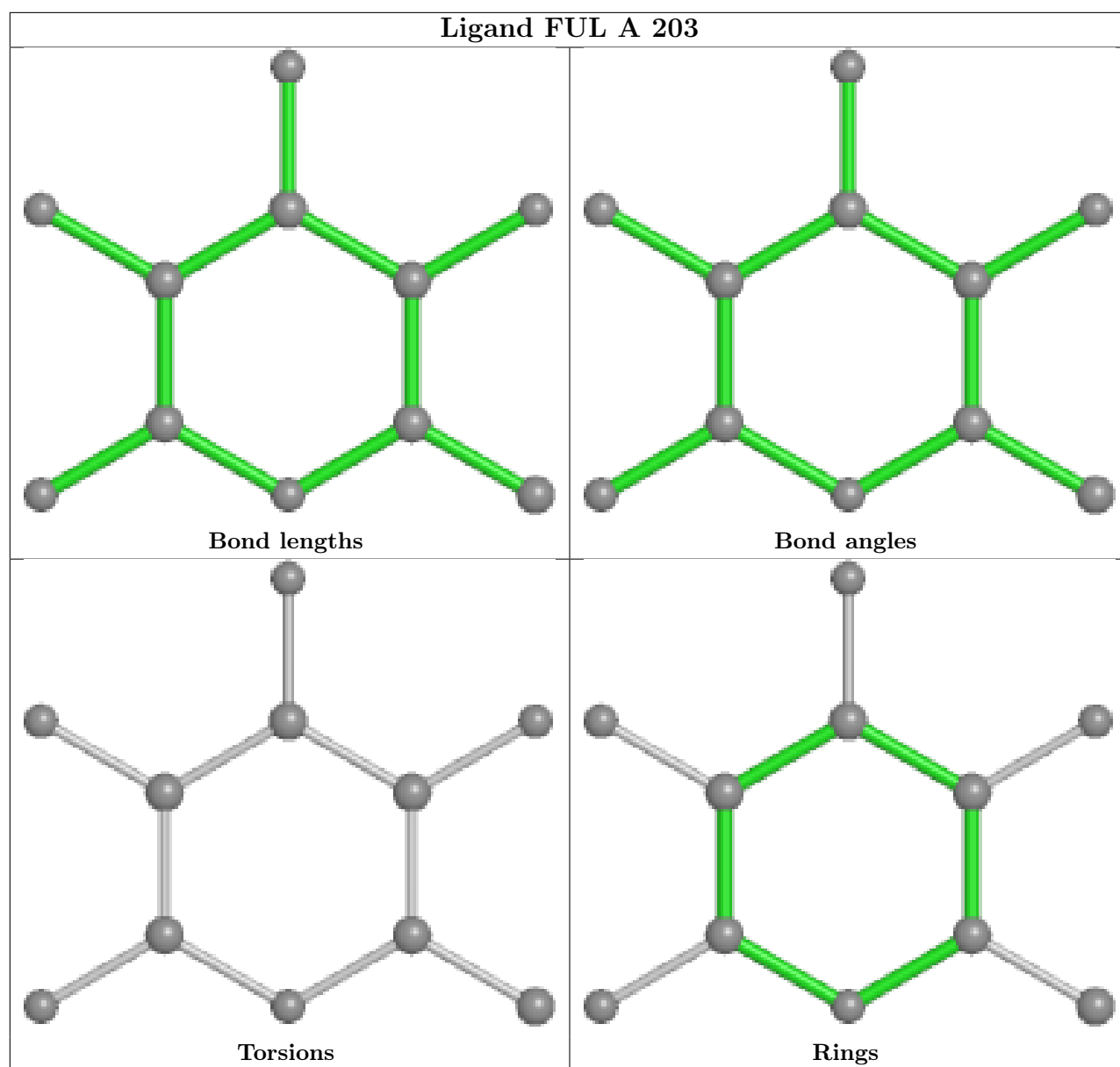
Mol	Chain	Res	Type	Atoms
3	D	205	BCN	N1-C5-C6-O6
3	C	205	BCN	C2-C1-N1-C5
3	E	201	BCN	C2-C1-N1-C5
3	C	205	BCN	C2-C1-N1-C3
3	B	205	BCN	C2-C1-N1-C5

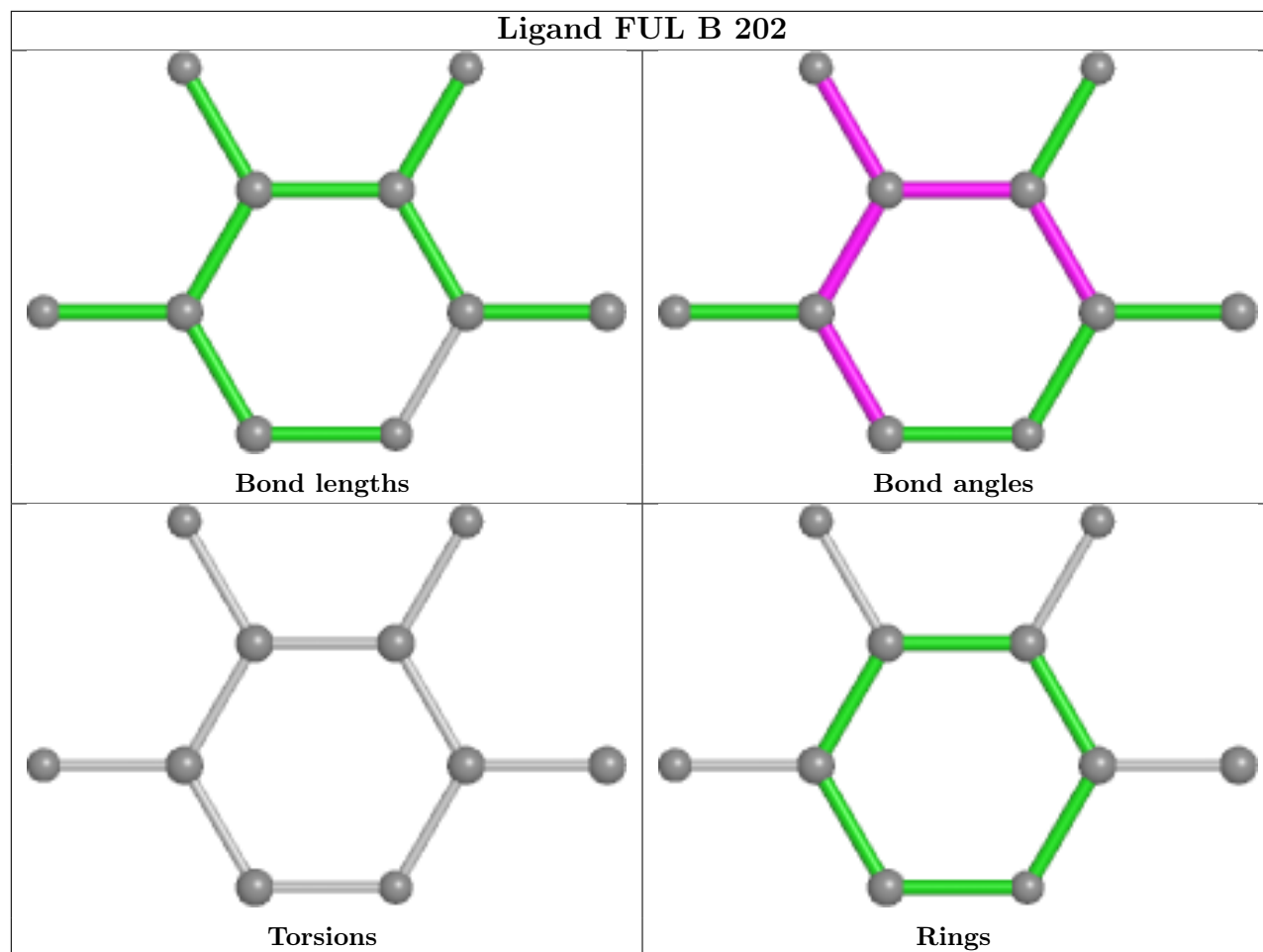
There are no ring outliers.

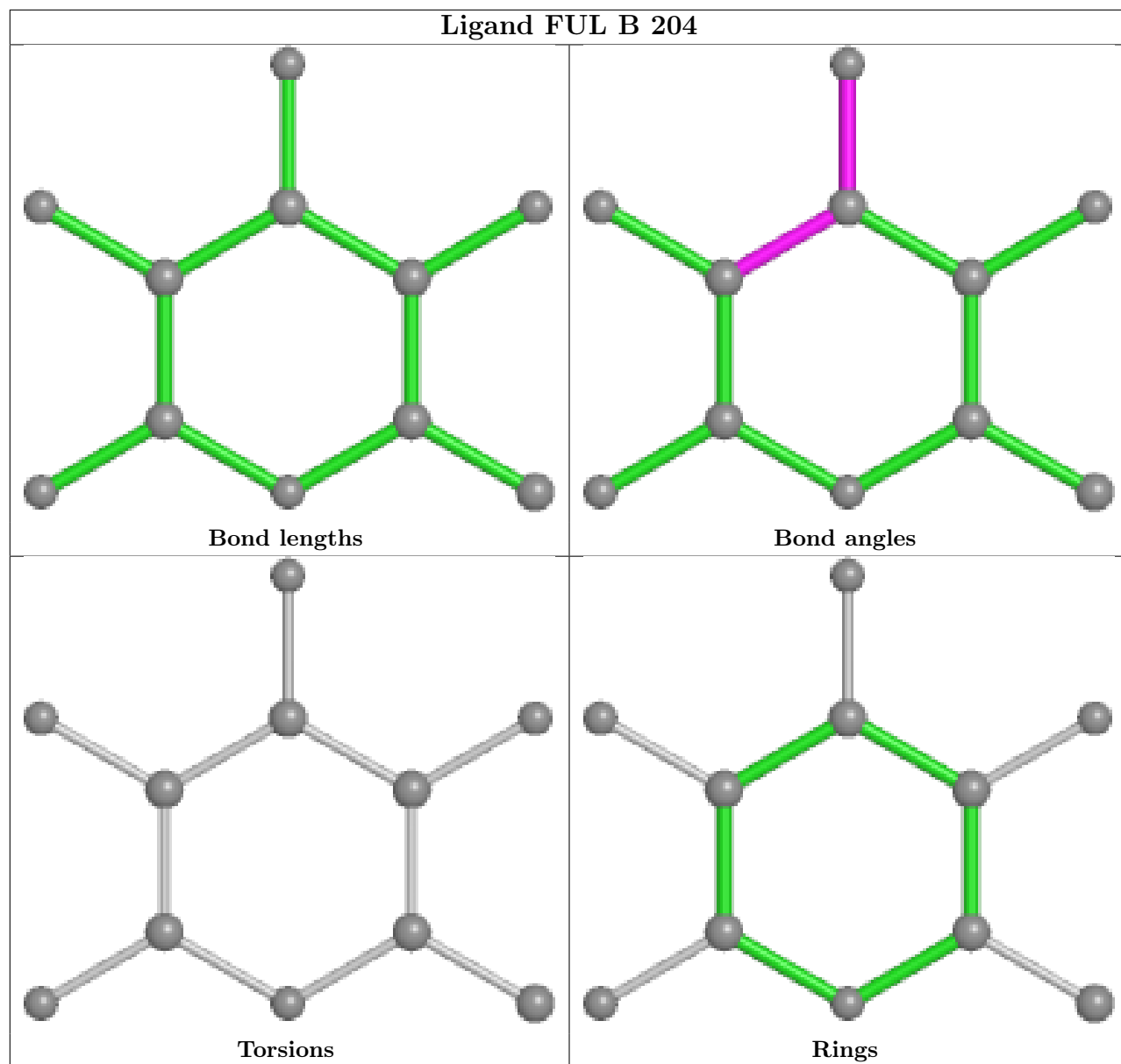
5 monomers are involved in 7 short contacts:

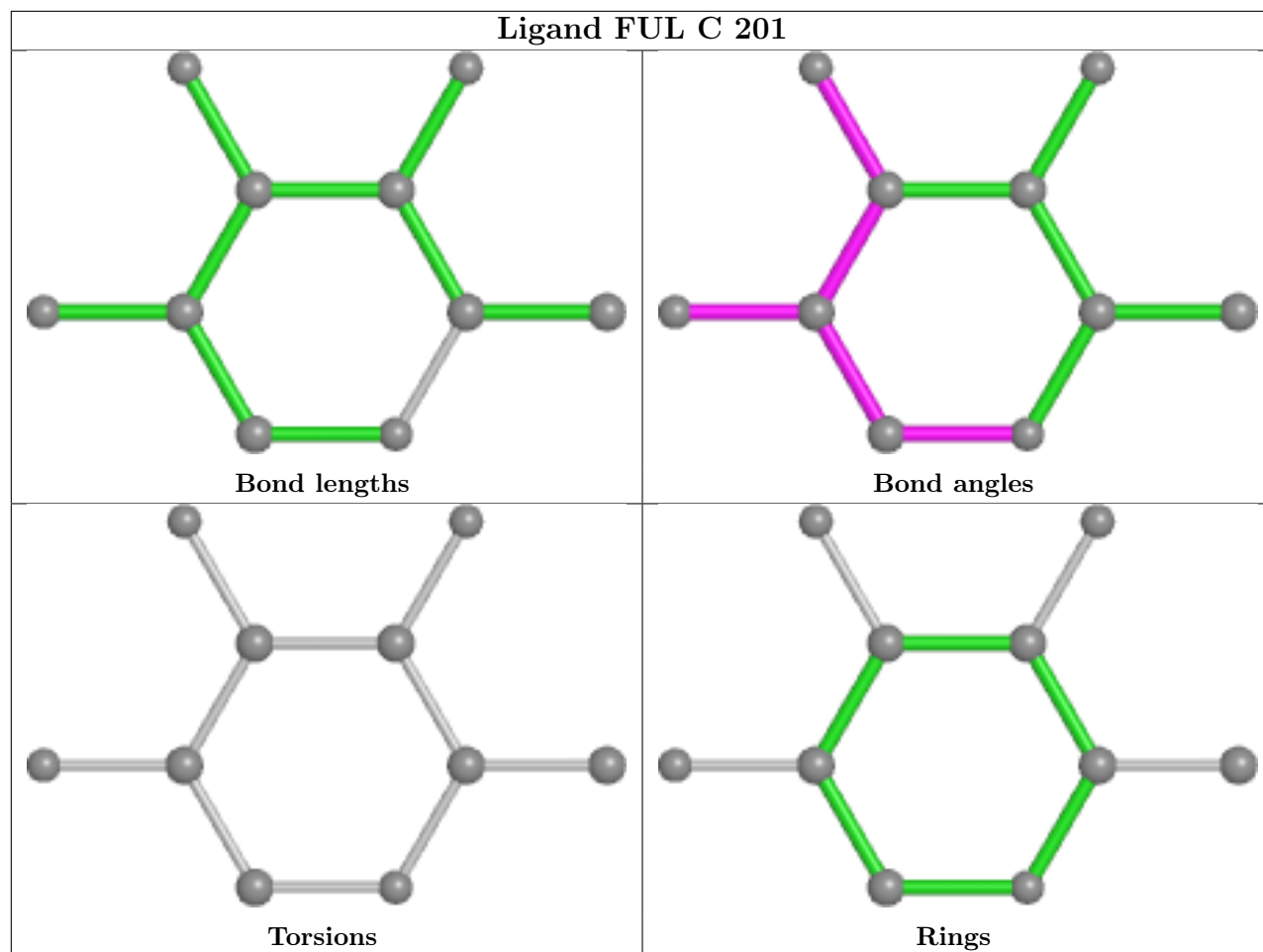
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	205	BCN	1	0
3	E	201	BCN	3	0
3	E	206	BCN	1	0
4	F	201	FUL	1	0
4	F	202	FUL	1	0

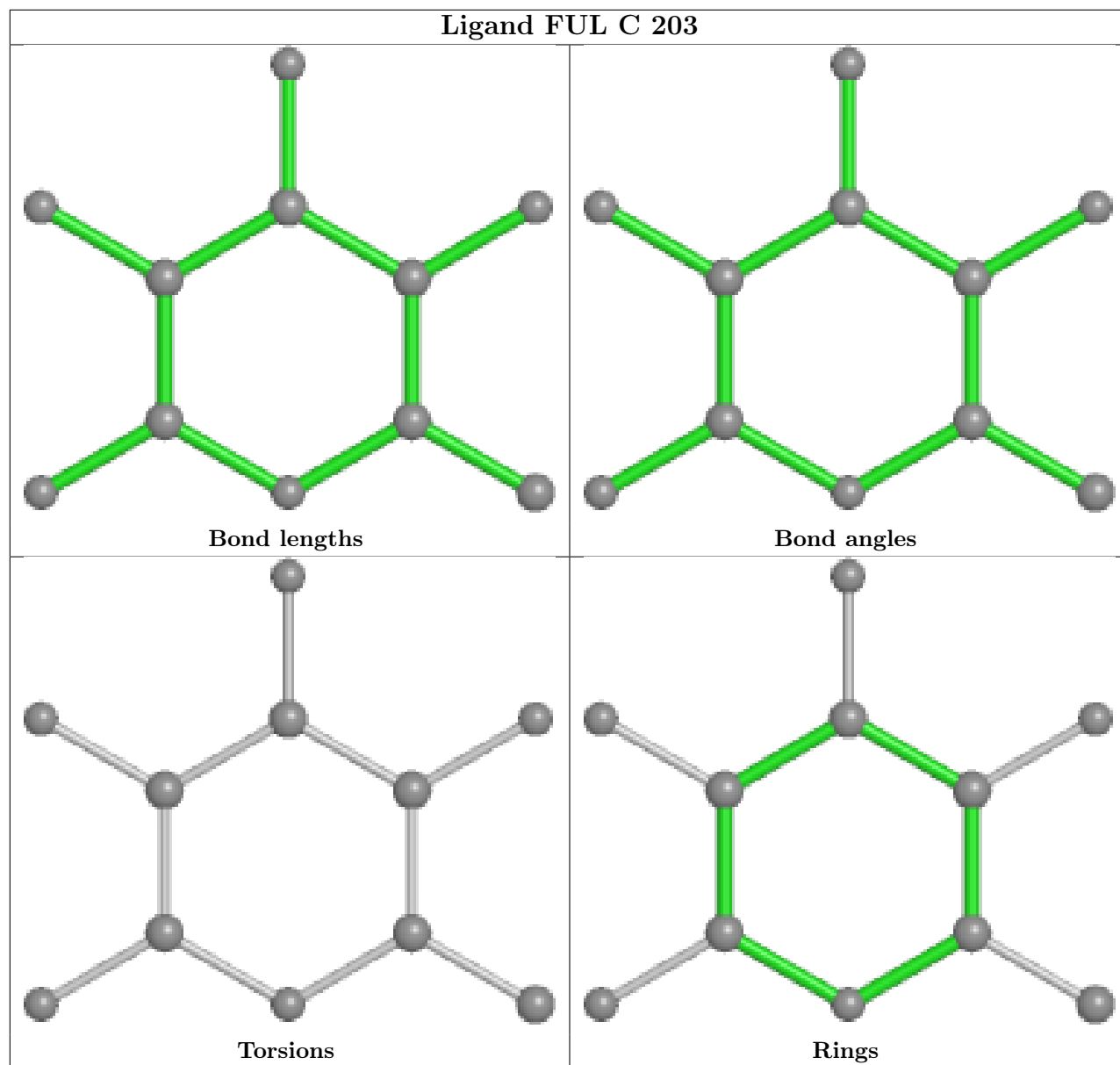
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

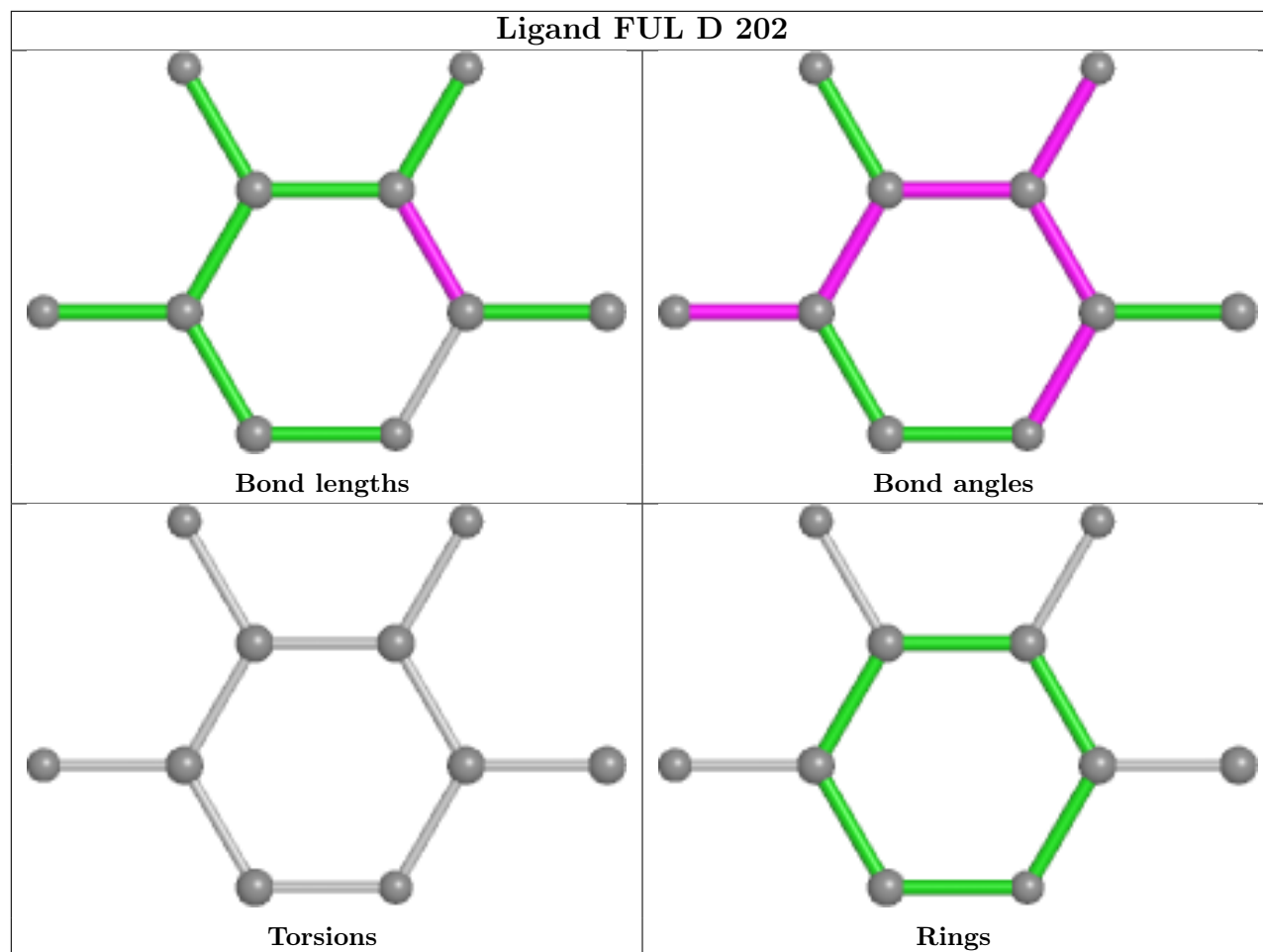




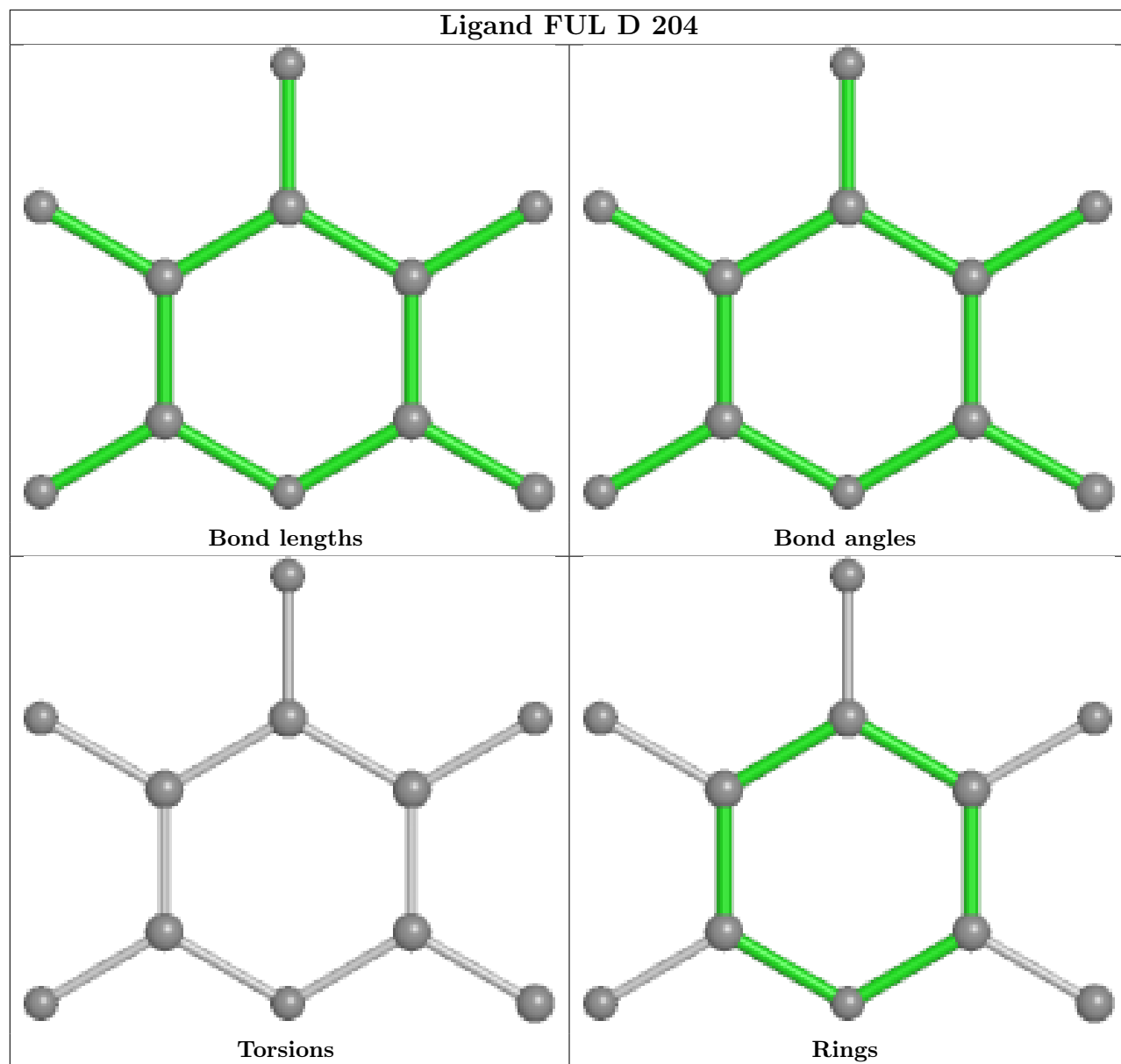


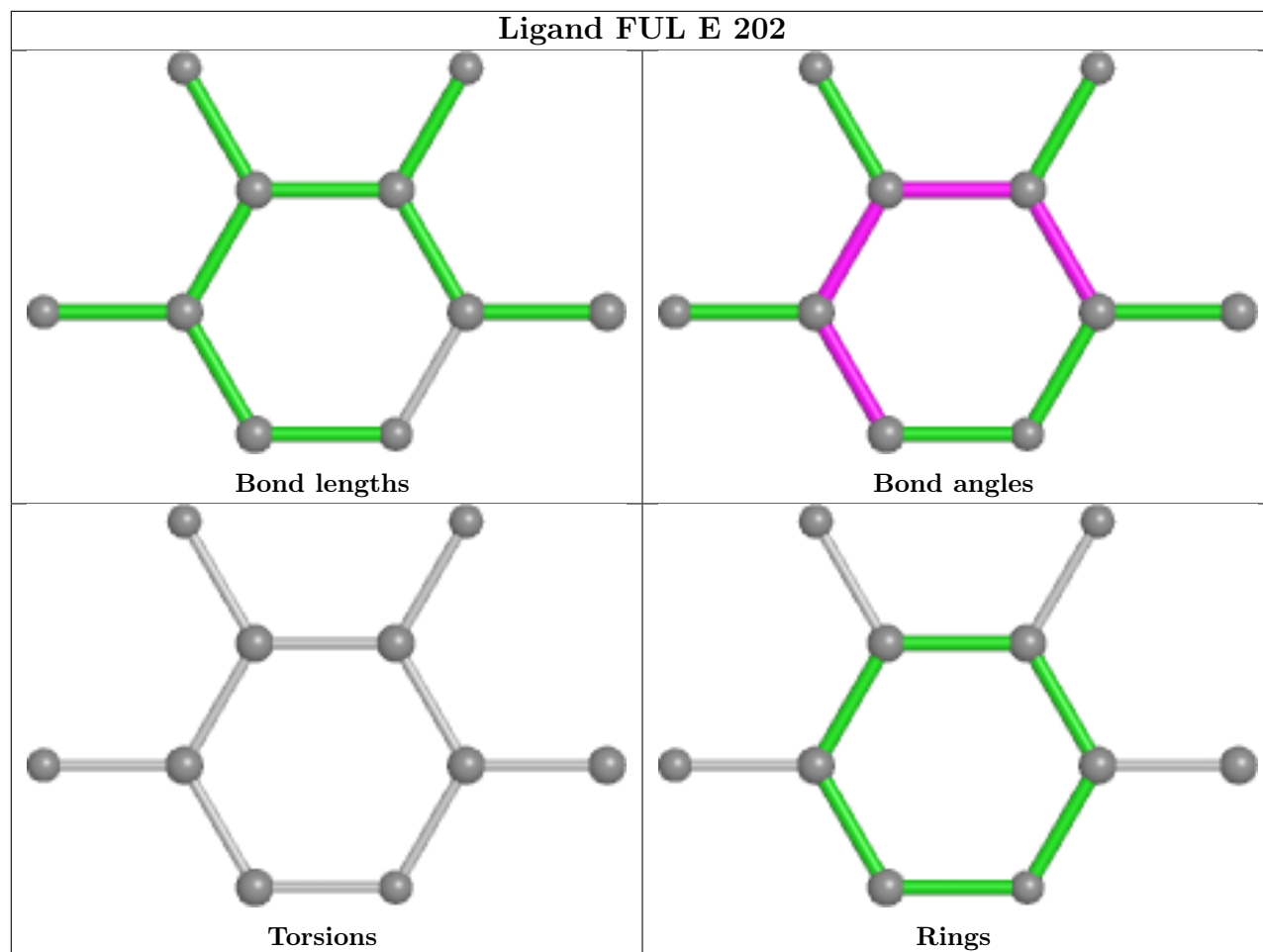




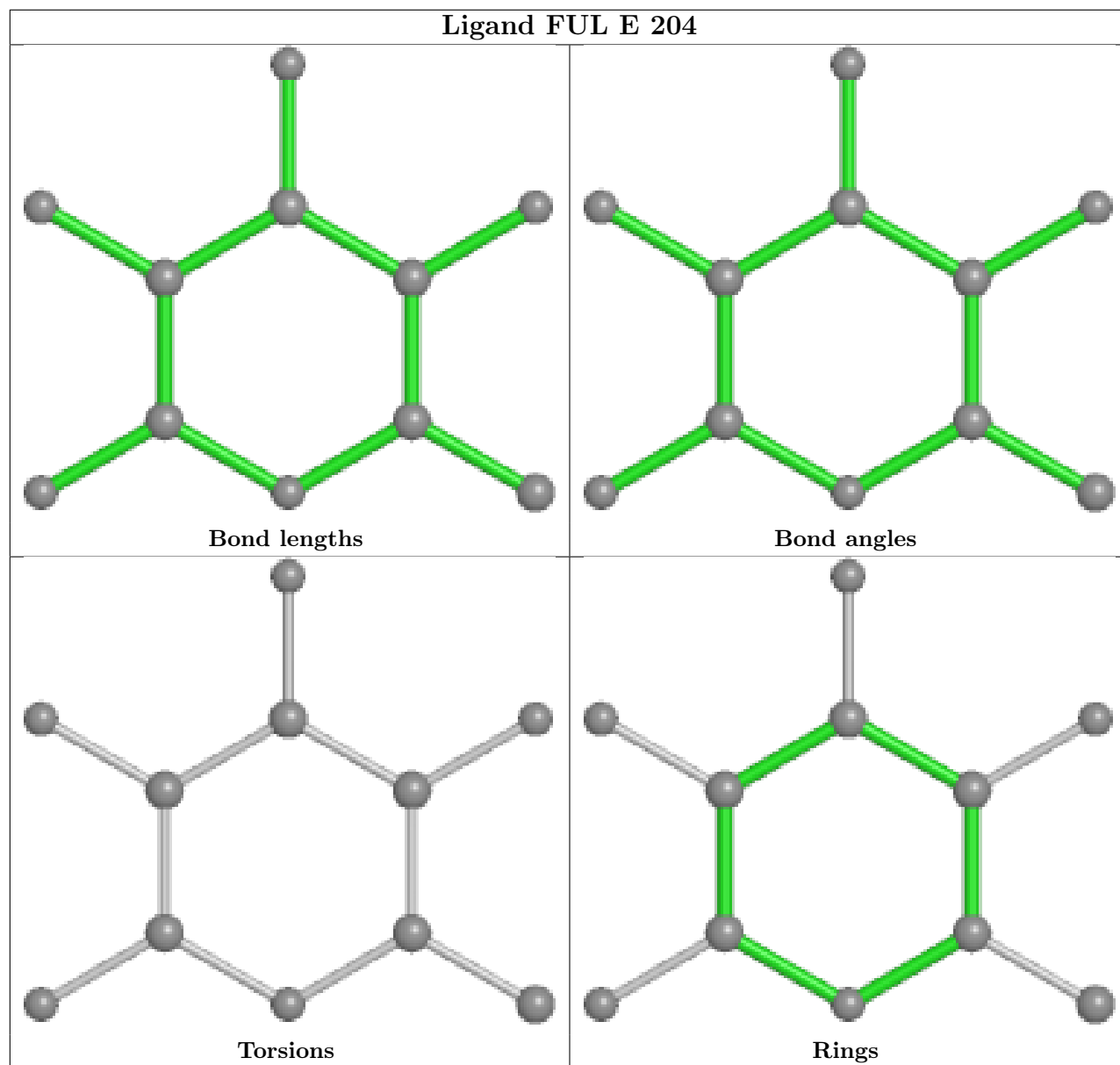


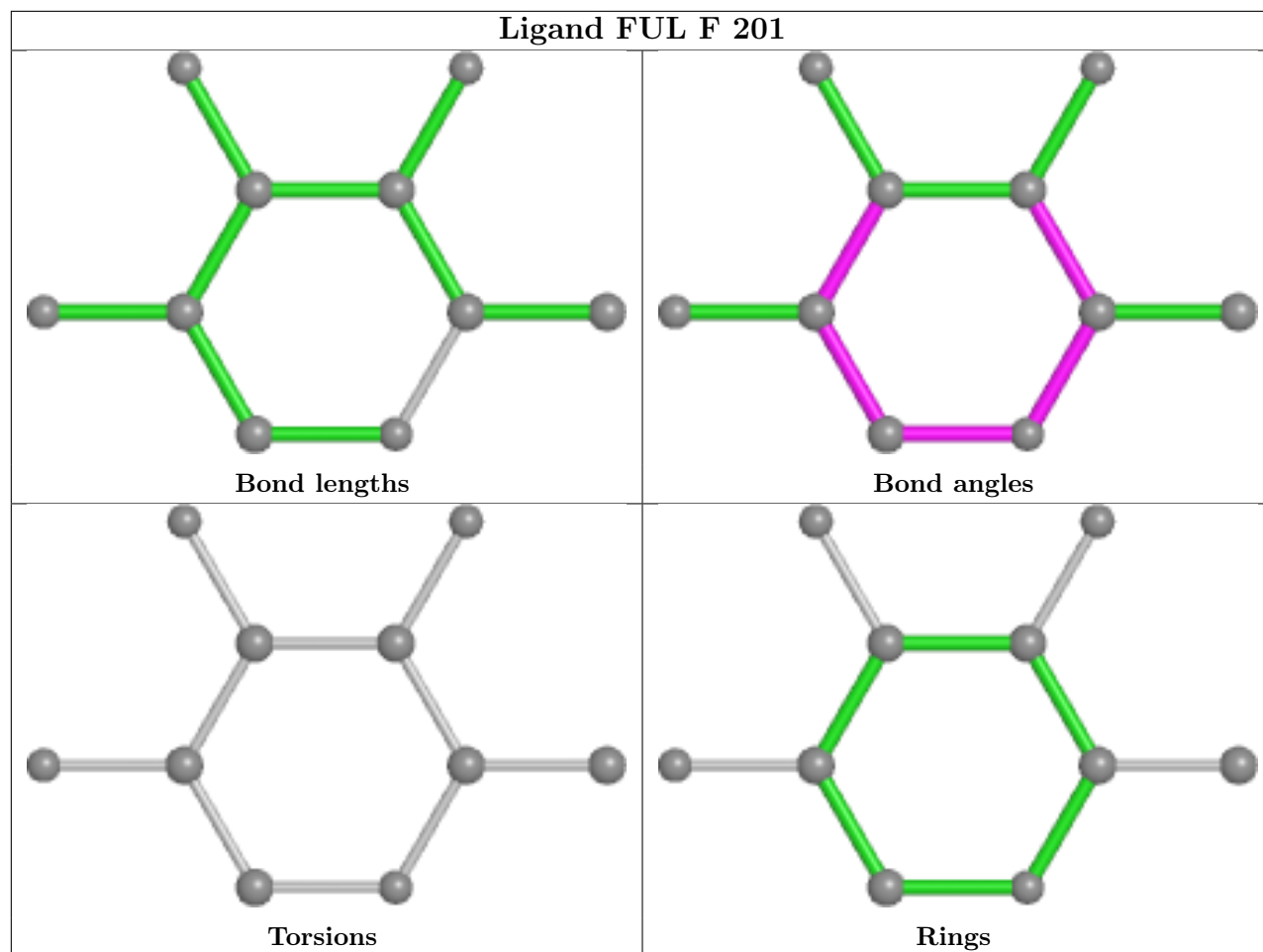


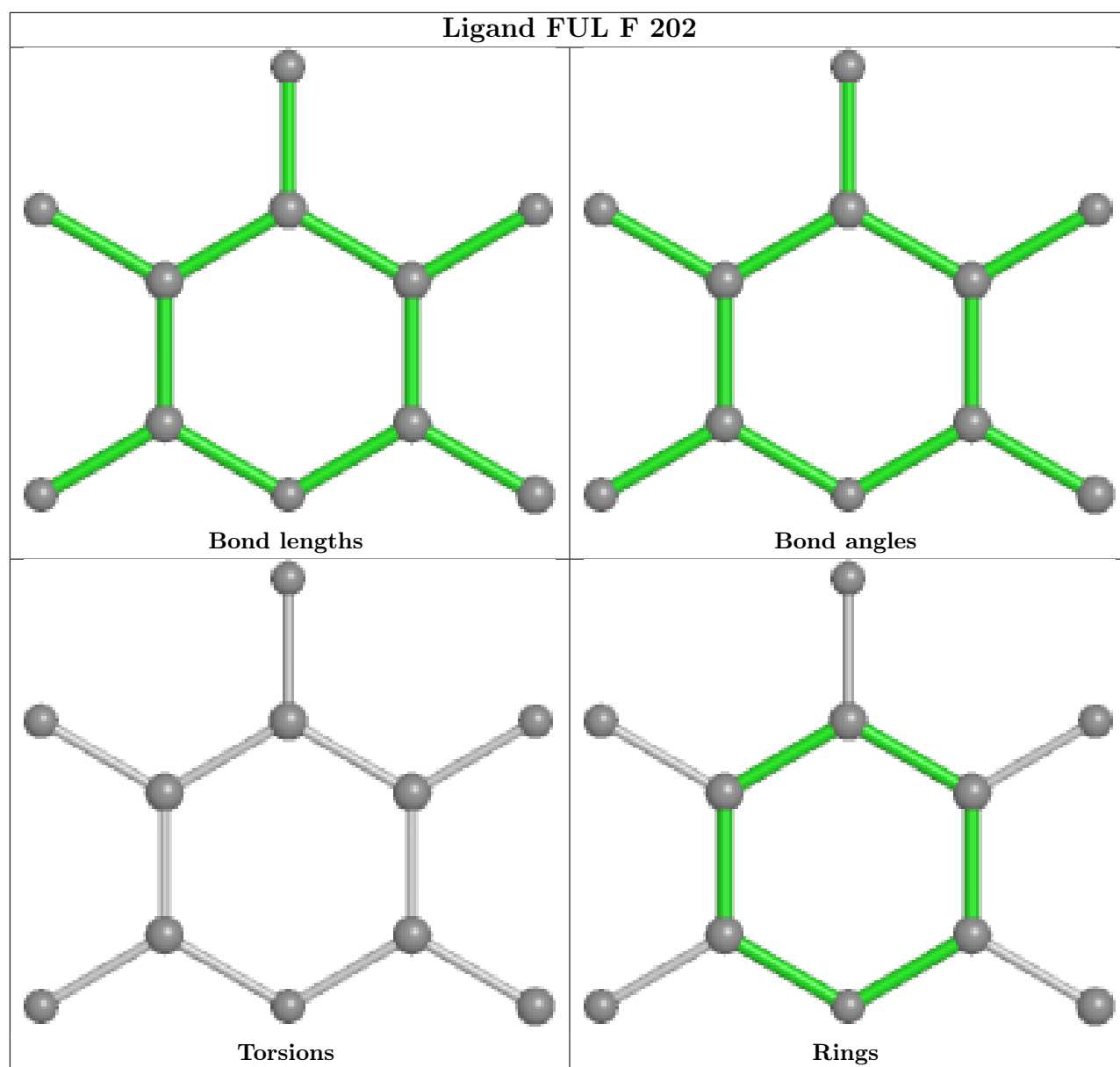


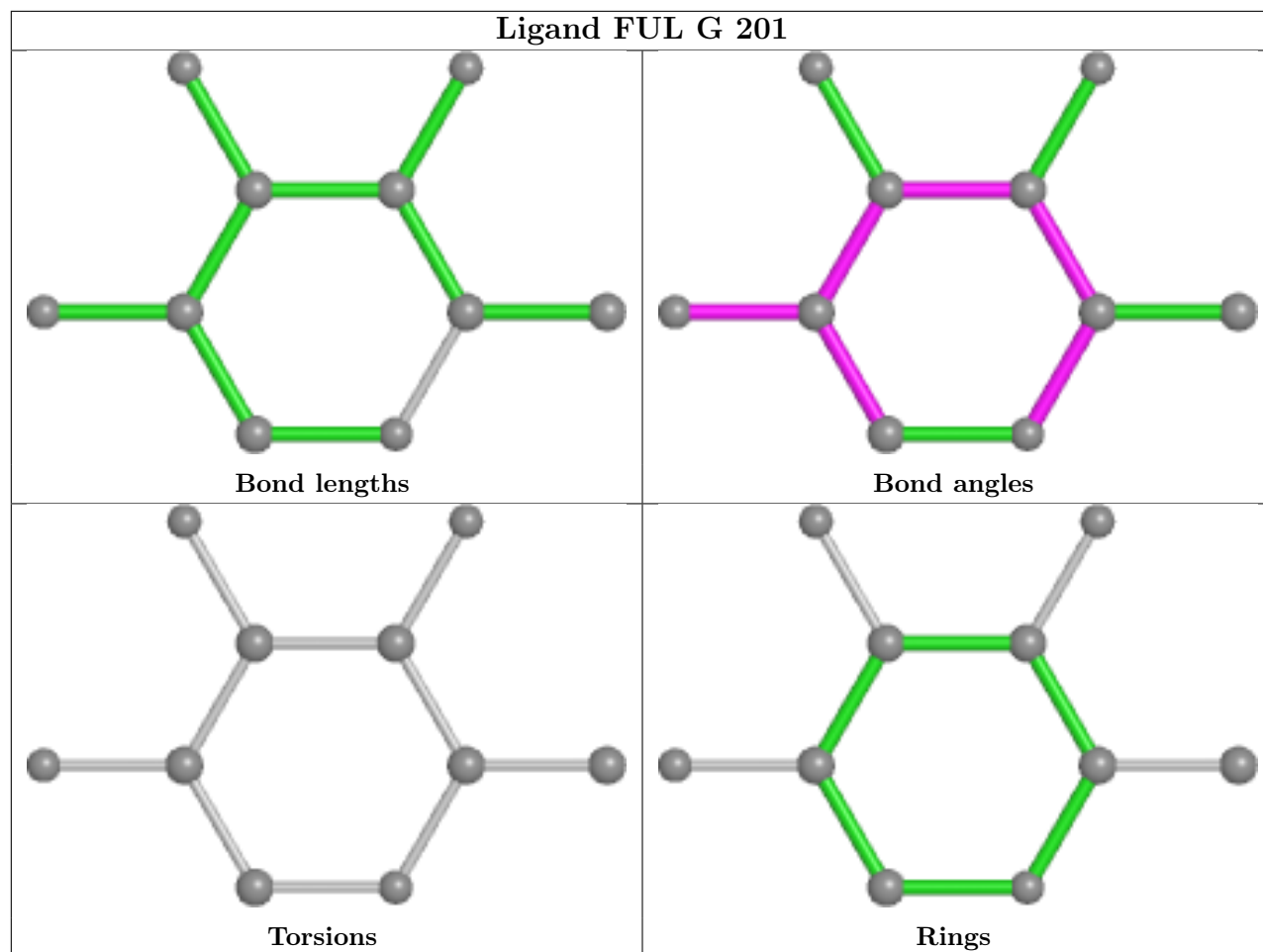


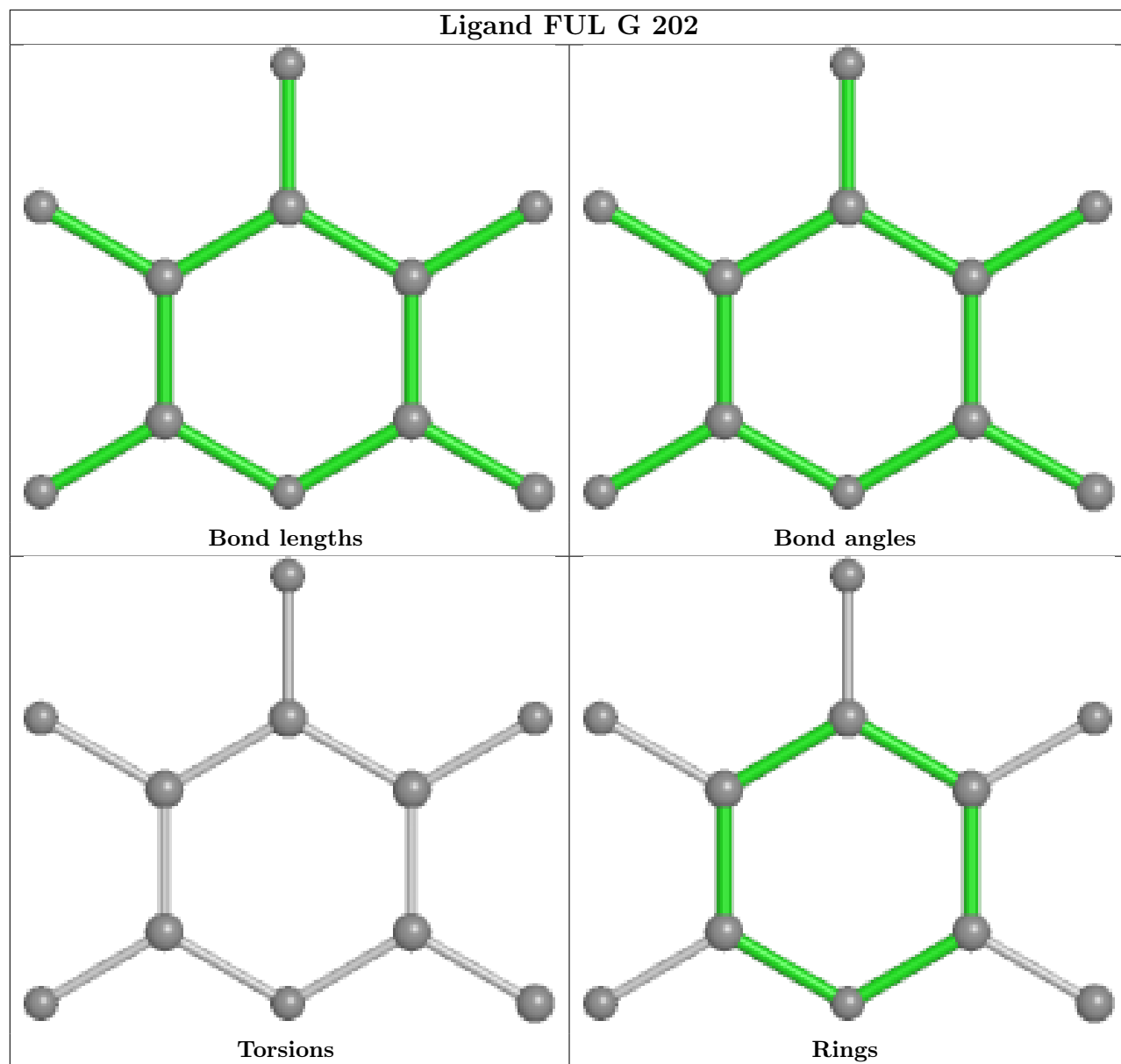
## Ligand FUL E 204

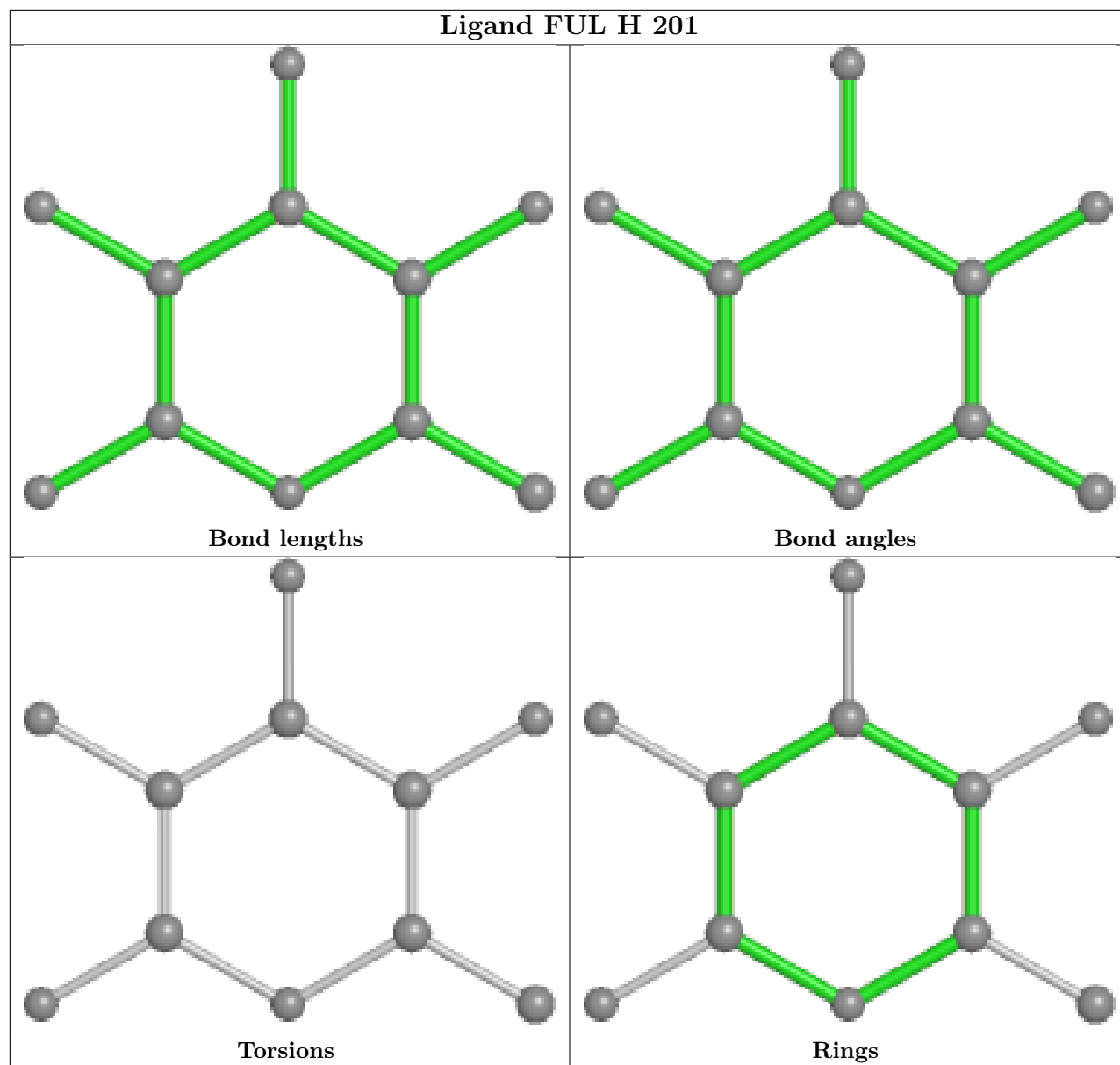




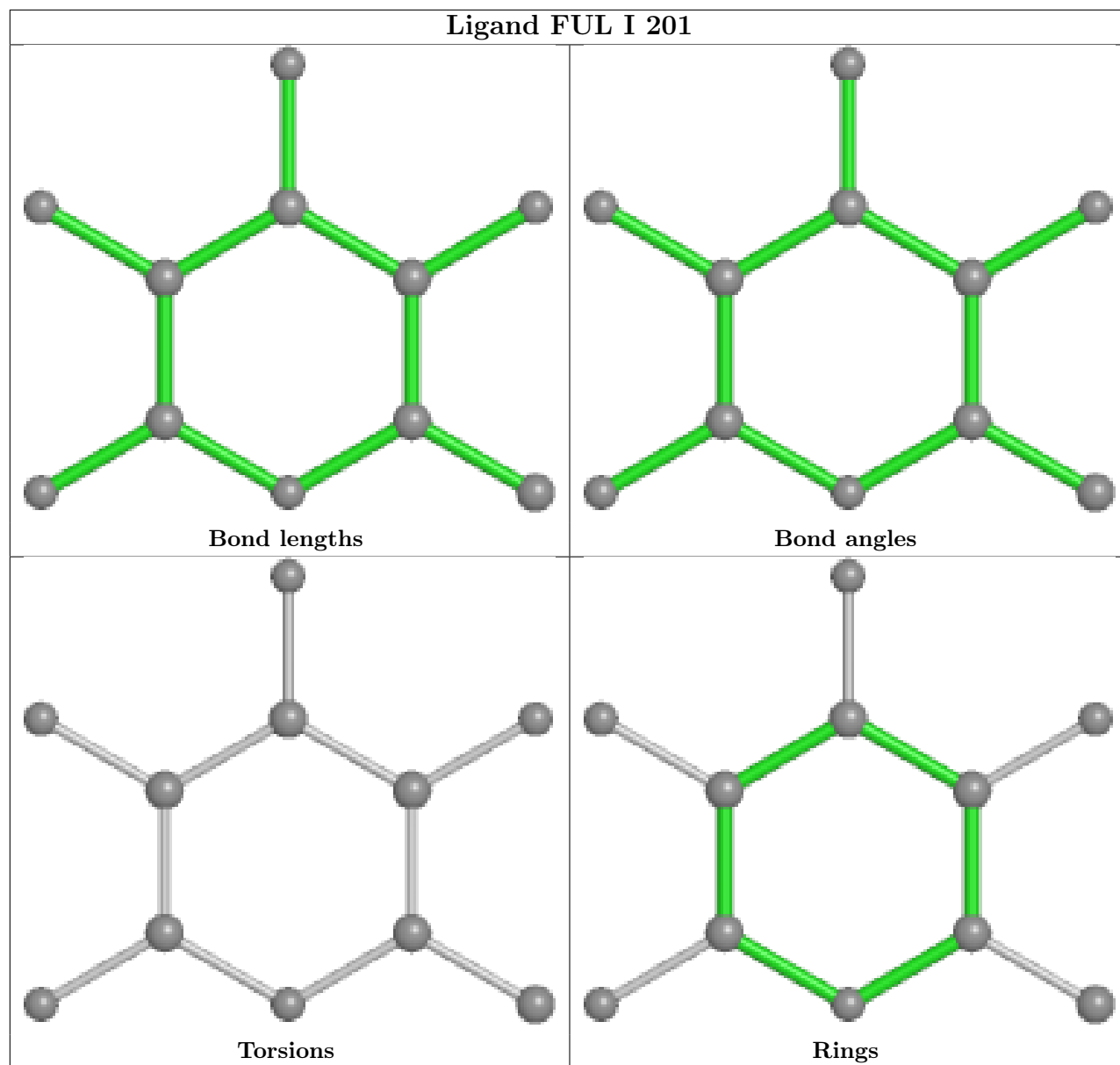


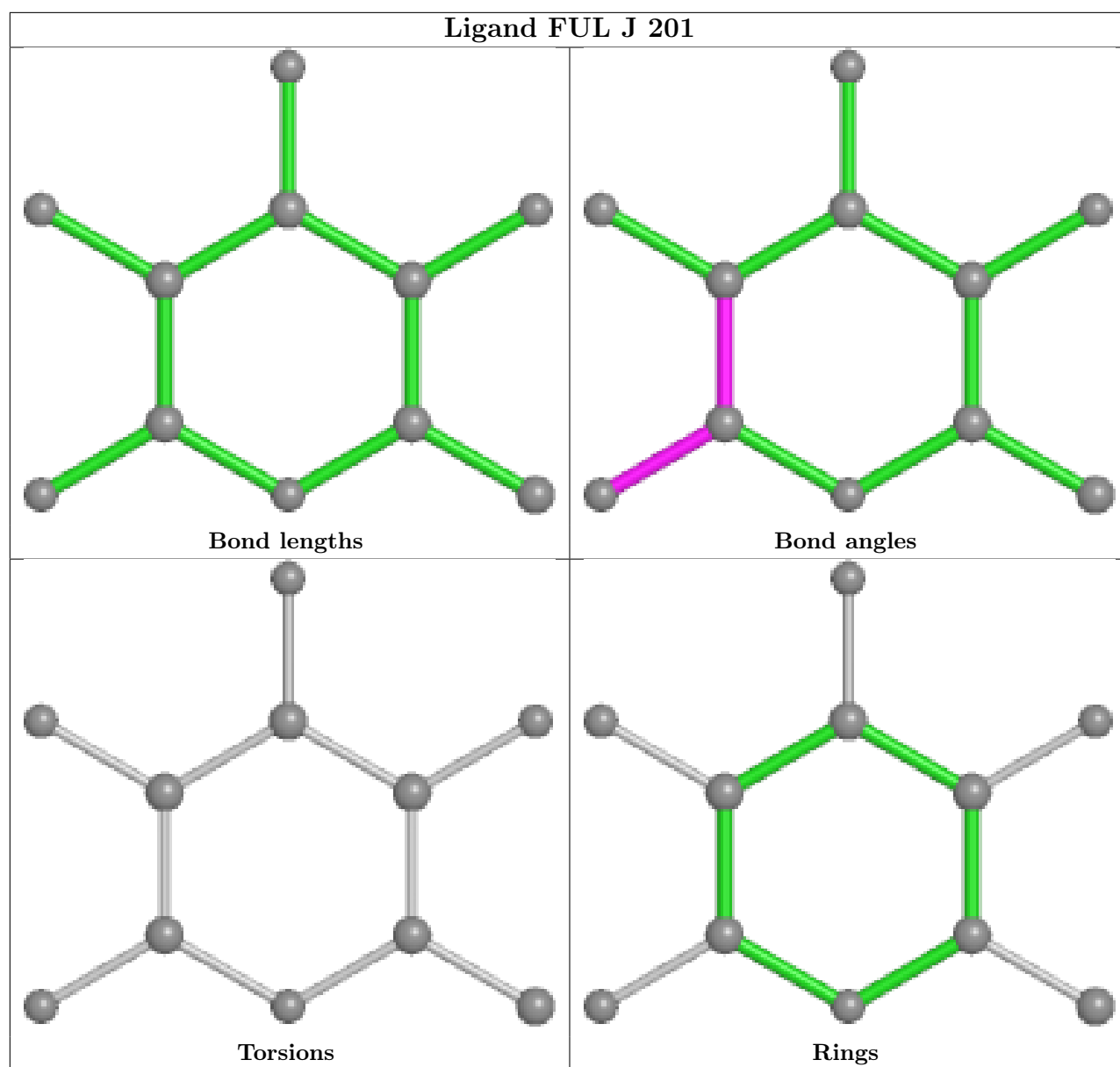












## 5.7 Other polymers [i](#)

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, 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	103/103 (100%)	-0.38	1 (0%) 82 87	19, 26, 38, 50	0
1	B	103/103 (100%)	-0.33	0 100 100	19, 27, 40, 52	0
1	C	103/103 (100%)	-0.33	1 (0%) 82 87	19, 26, 41, 52	0
1	D	103/103 (100%)	-0.31	0 100 100	21, 29, 43, 56	0
1	E	103/103 (100%)	-0.42	0 100 100	21, 27, 37, 47	0
1	F	103/103 (100%)	0.11	6 (5%) 23 32	25, 38, 57, 62	0
1	G	102/103 (99%)	-0.31	0 100 100	19, 27, 42, 48	0
1	H	103/103 (100%)	-0.33	0 100 100	20, 26, 41, 51	0
1	I	103/103 (100%)	0.08	6 (5%) 23 32	22, 36, 62, 79	0
1	J	103/103 (100%)	0.01	2 (1%) 66 75	23, 38, 52, 65	0
All	All	1029/1030 (99%)	-0.22	16 (1%) 72 79	19, 30, 50, 79	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	55	SER	5.1
1	I	14	ASN	3.7
1	I	56	GLN	3.7
1	J	13	HIS	2.9
1	I	58	ILE	2.9

### 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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FUL	F	201	10/11	0.86	0.22	50,53,56,58	0
4	FUL	D	202	10/11	0.87	0.21	42,44,47,47	0
4	FUL	E	202	10/11	0.87	0.23	39,42,44,46	0
4	FUL	F	202	11/11	0.88	0.15	36,42,45,46	0
4	FUL	C	201	10/11	0.90	0.25	45,47,49,51	0
3	BCN	D	205	11/11	0.90	0.13	29,31,34,34	0
3	BCN	C	206	11/11	0.92	0.14	26,28,33,37	0
4	FUL	B	202	10/11	0.92	0.20	42,45,48,49	0
3	BCN	D	201	11/11	0.92	0.12	25,30,34,37	0
4	FUL	J	201	11/11	0.93	0.12	33,33,35,35	0
4	FUL	G	201	10/11	0.94	0.15	31,33,35,36	0
3	BCN	E	206	11/11	0.94	0.10	30,34,39,43	0
3	BCN	C	205	11/11	0.94	0.12	22,25,27,29	0
4	FUL	C	203	11/11	0.95	0.07	25,26,26,27	0
4	FUL	D	204	11/11	0.95	0.07	32,34,37,37	0
4	FUL	A	203	11/11	0.95	0.08	24,27,29,32	0
3	BCN	E	201	11/11	0.95	0.10	25,31,33,35	0
4	FUL	I	201	11/11	0.95	0.09	34,36,37,44	0
4	FUL	G	202	11/11	0.96	0.08	24,24,26,29	0
4	FUL	H	201	11/11	0.96	0.07	27,28,30,31	0
3	BCN	A	205	11/11	0.96	0.09	23,26,28,28	0
4	FUL	E	204	11/11	0.96	0.07	28,31,34,36	0
3	BCN	B	201	11/11	0.96	0.10	24,29,31,31	0
3	BCN	B	205	11/11	0.96	0.07	25,27,28,31	0
4	FUL	B	204	11/11	0.97	0.09	28,33,36,39	0
3	BCN	A	202	11/11	0.97	0.10	25,29,33,35	0
2	CA	E	203	1/1	0.98	0.12	30,30,30,30	0
2	CA	E	205	1/1	0.98	0.04	28,28,28,28	0
2	CA	D	206	1/1	0.99	0.05	26,26,26,26	0
2	CA	A	204	1/1	0.99	0.05	23,23,23,23	0
2	CA	D	203	1/1	0.99	0.07	27,27,27,27	0
2	CA	B	203	1/1	0.99	0.05	23,23,23,23	0

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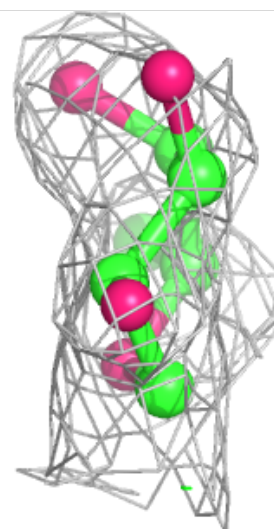
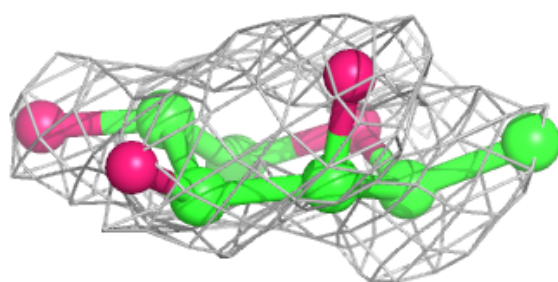
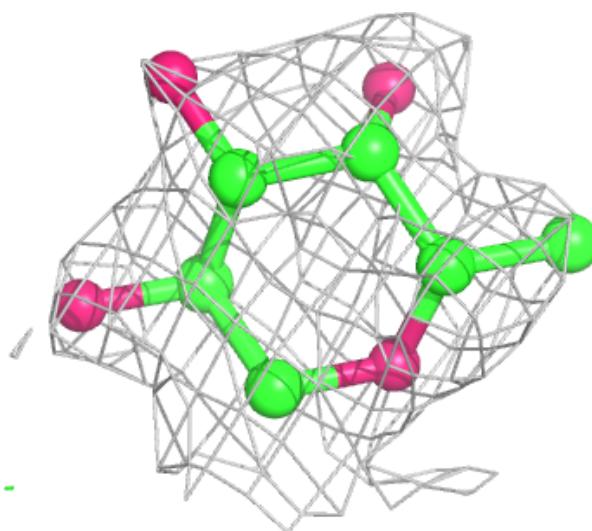
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	C	202	1/1	0.99	0.06	25,25,25,25	0
2	CA	A	201	1/1	0.99	0.08	25,25,25,25	0
2	CA	B	206	1/1	1.00	0.07	22,22,22,22	0
2	CA	C	204	1/1	1.00	0.07	22,22,22,22	0

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.

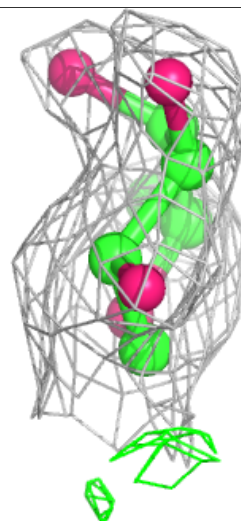
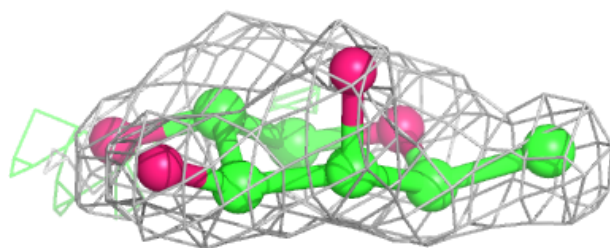
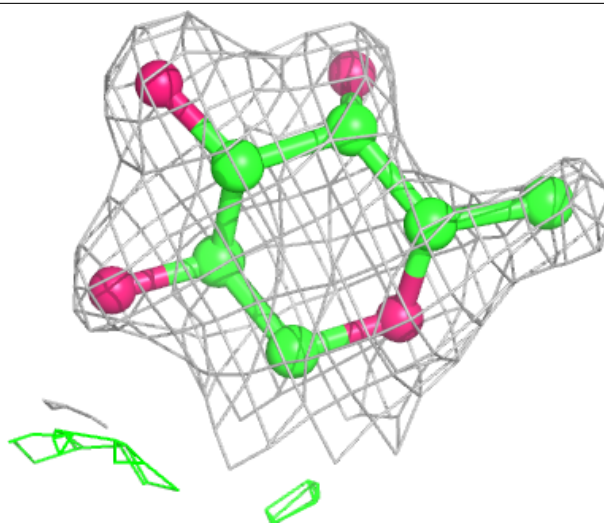
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mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



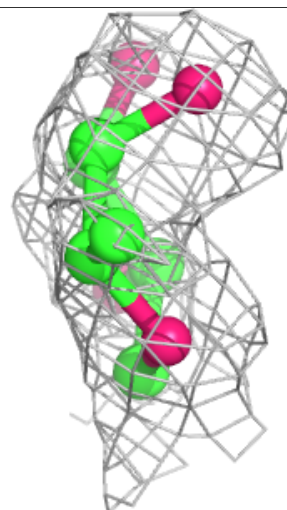
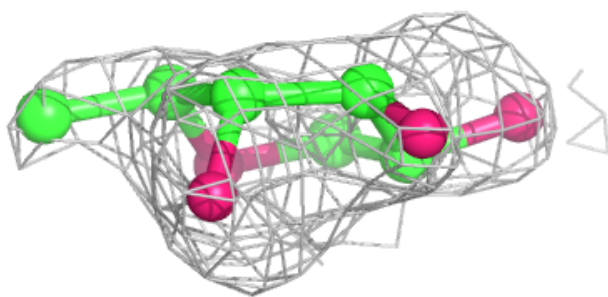
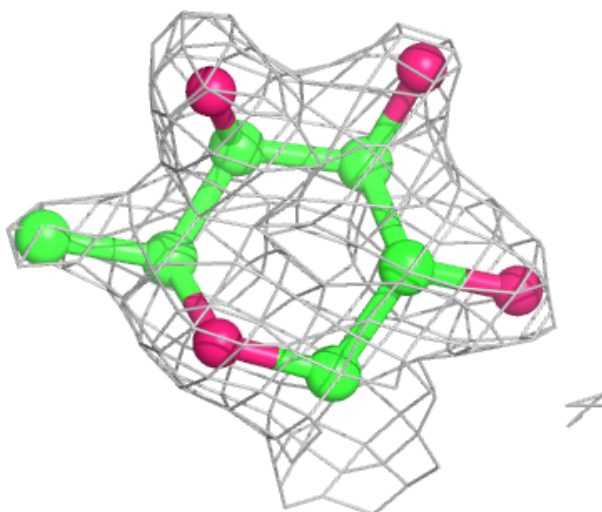
**Electron density around FUL D 202:**

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



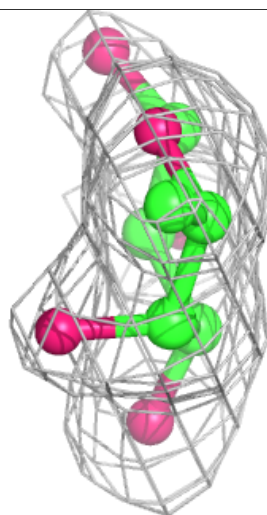
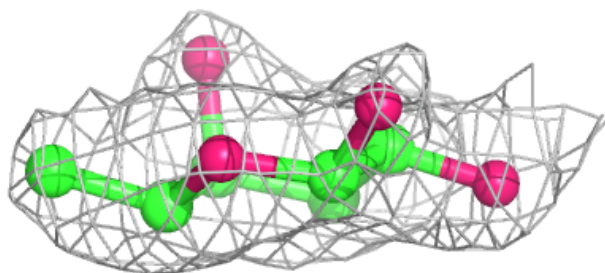
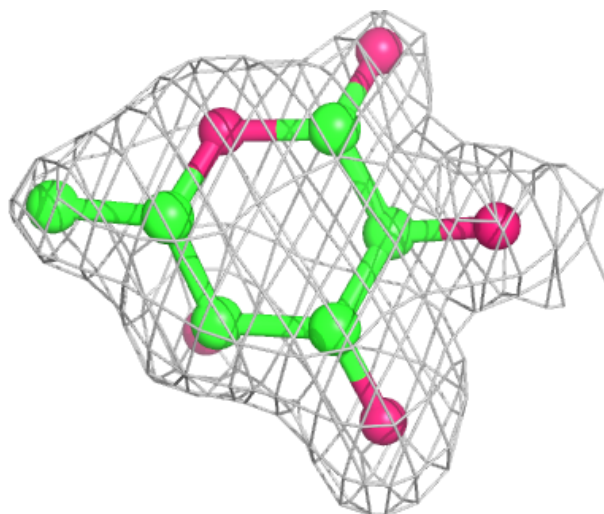
**Electron density around FUL E 202:**

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



**Electron density around FUL F 202:**

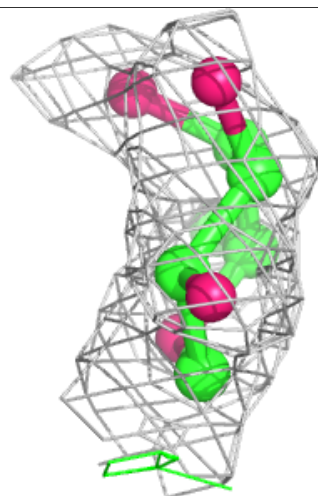
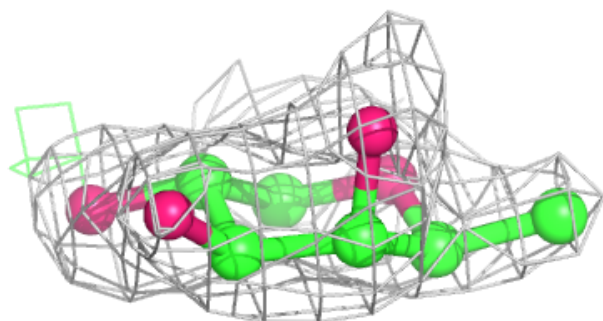
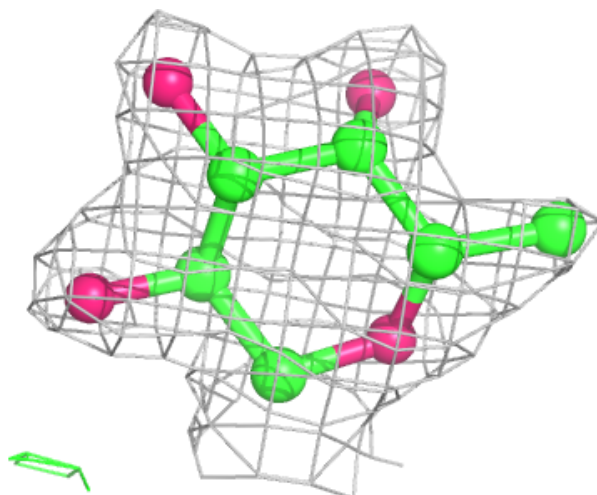
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





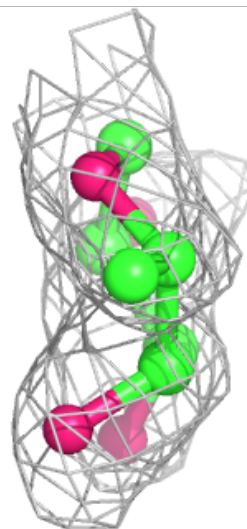
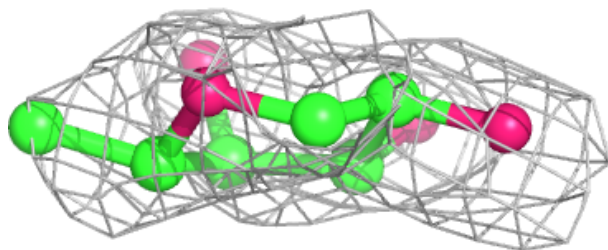
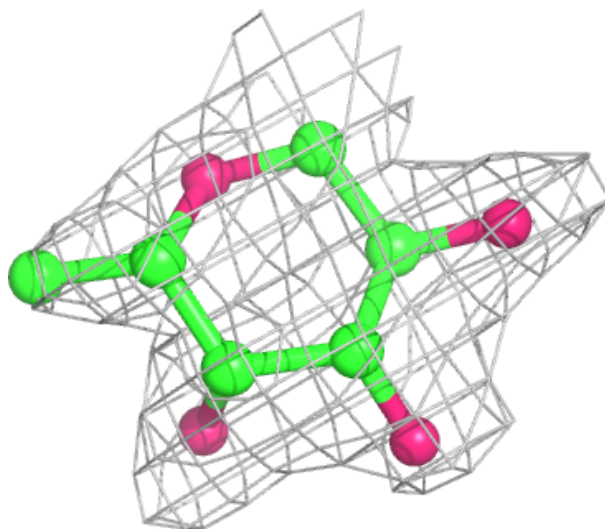
**Electron density around FUL C 201:**

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



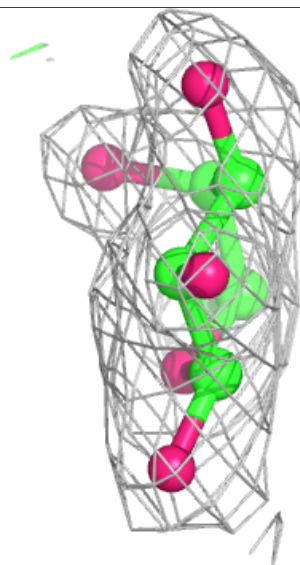
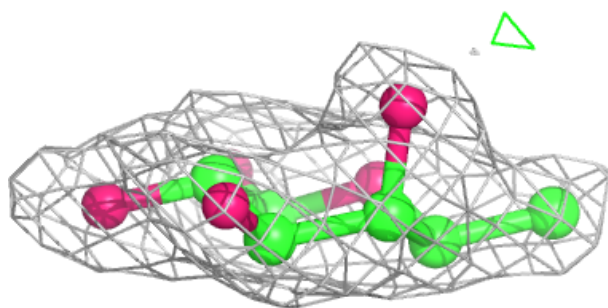
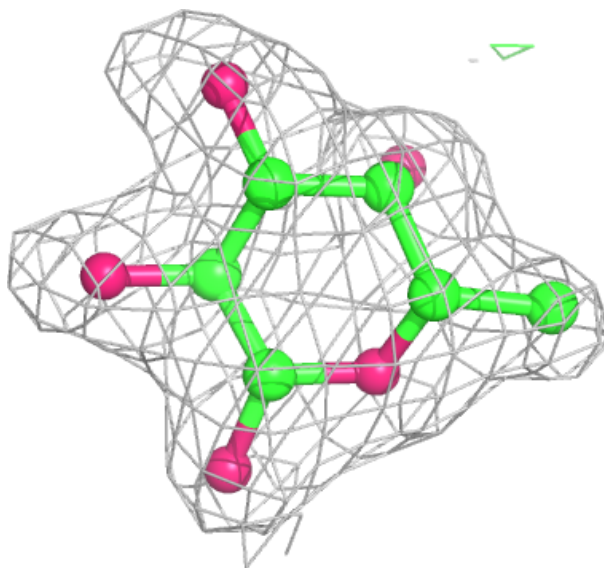
**Electron density around FUL B 202:**

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)



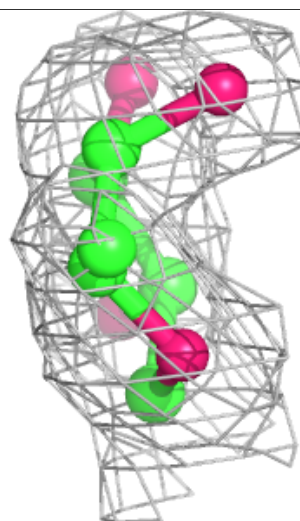
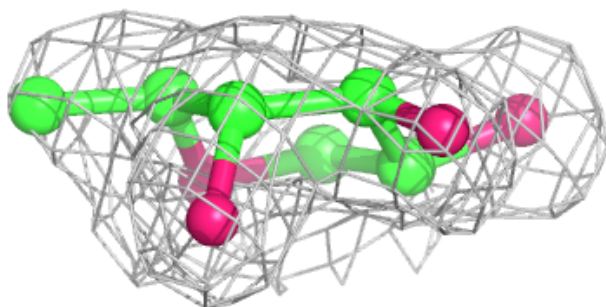
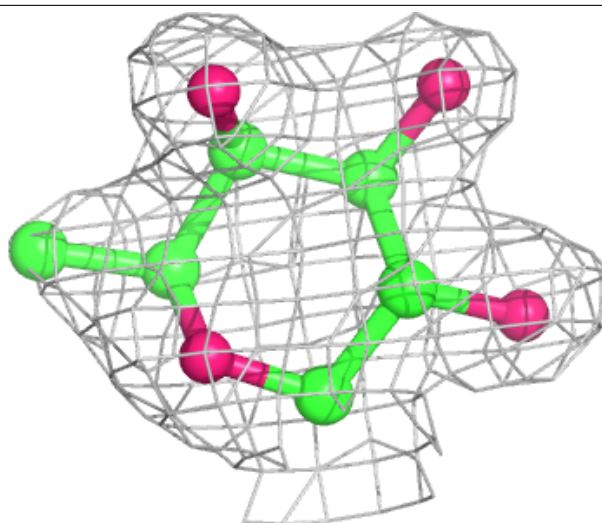
**Electron density around FUL J 201:**

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



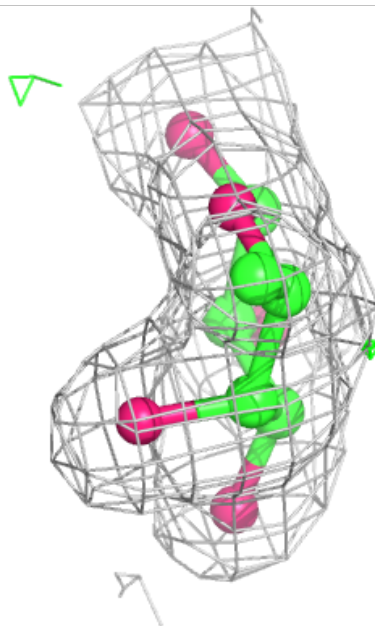
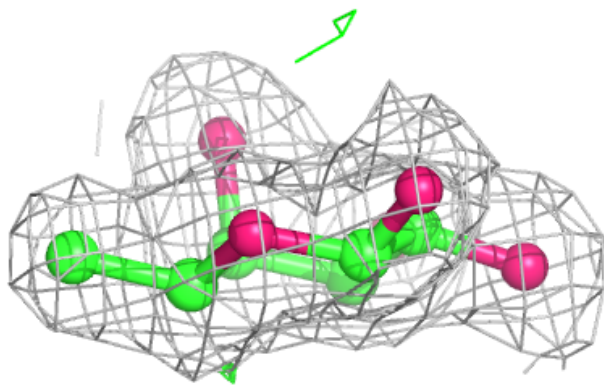
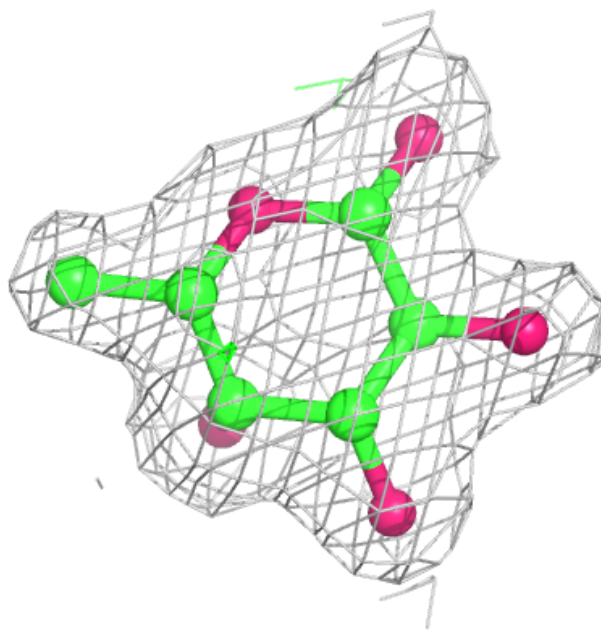
**Electron density around FUL G 201:**

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



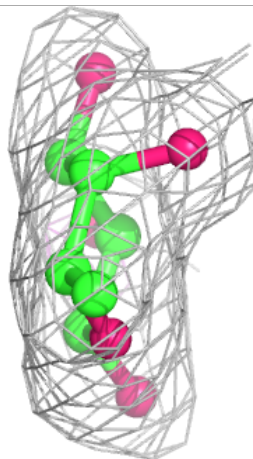
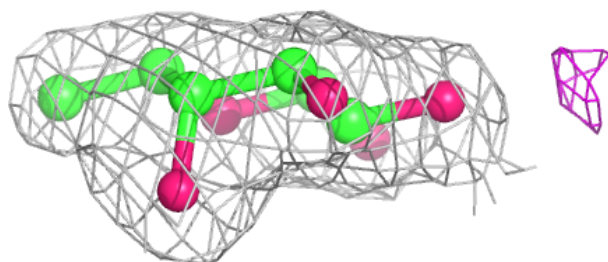
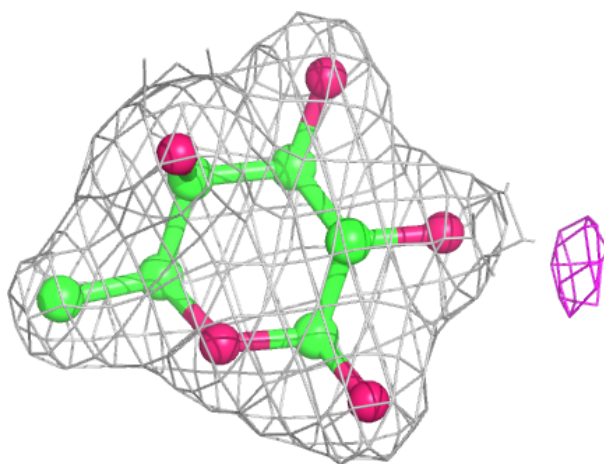
**Electron density around FUL C 203:**

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



**Electron density around FUL D 204:**

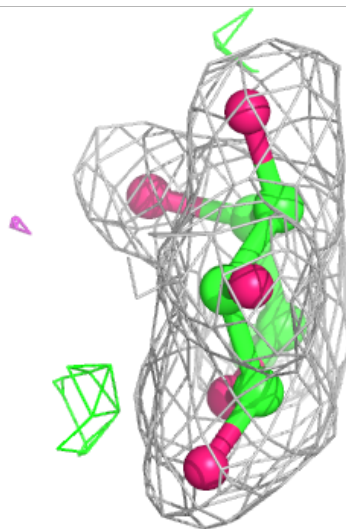
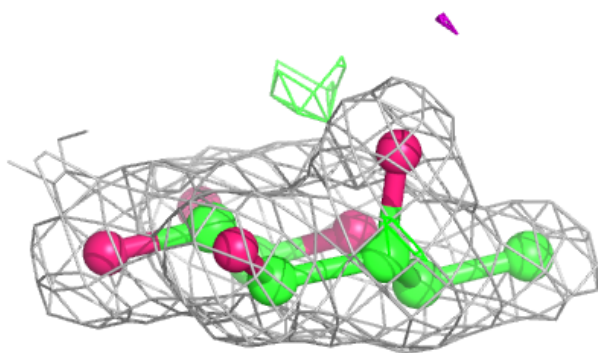
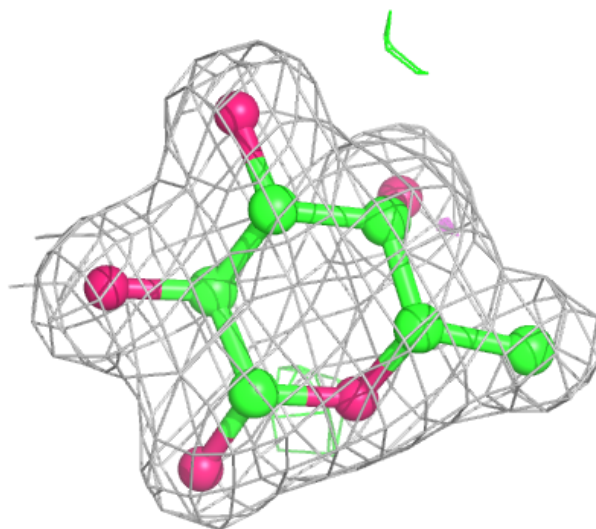
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





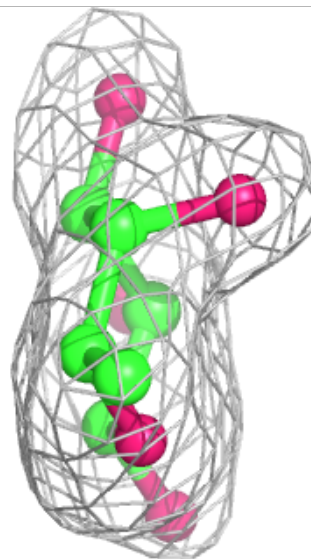
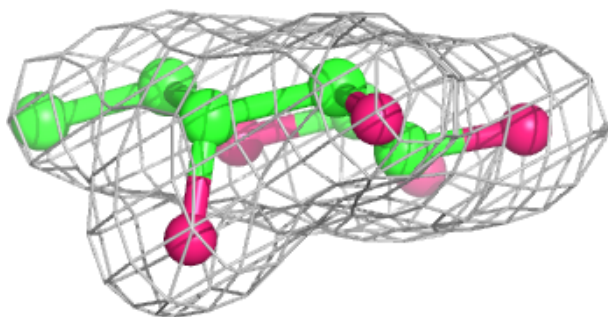
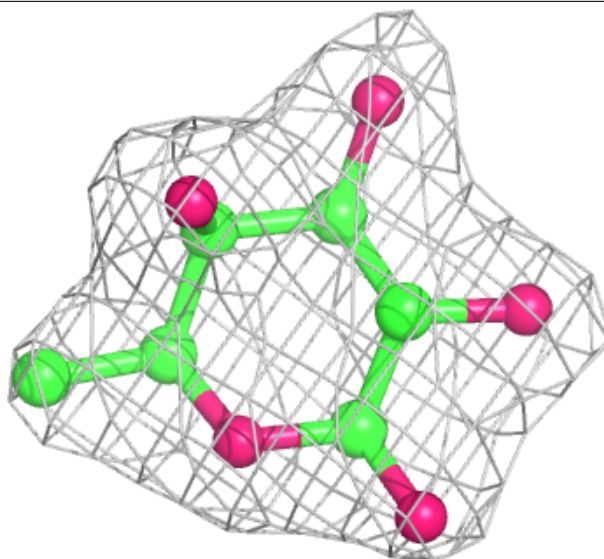
**Electron density around FUL A 203:**

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



**Electron density around FUL I 201:**

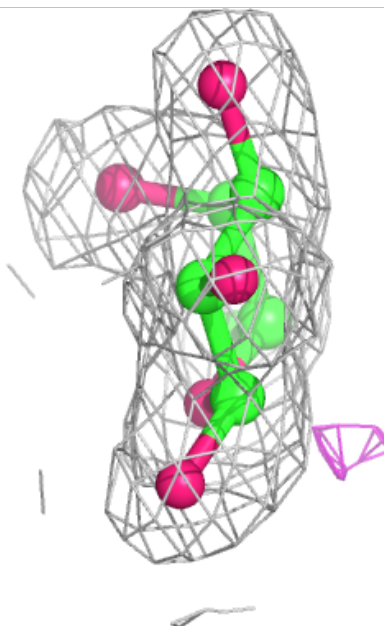
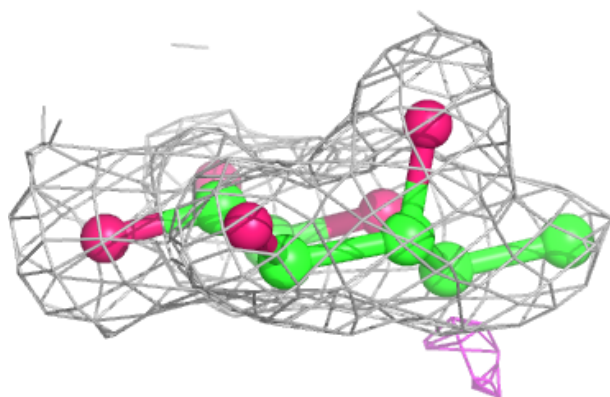
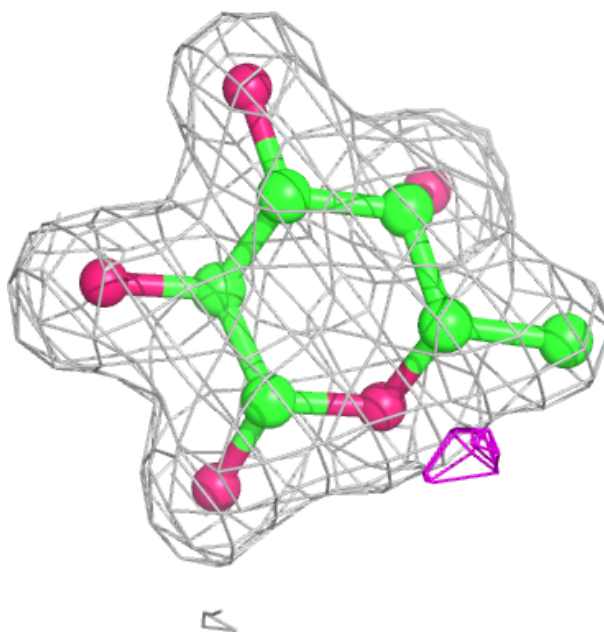
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





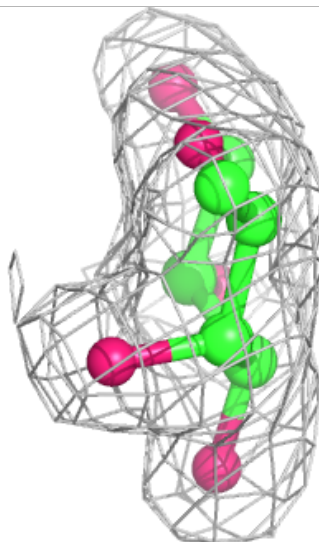
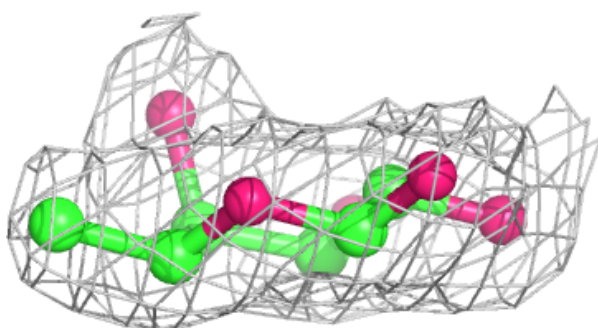
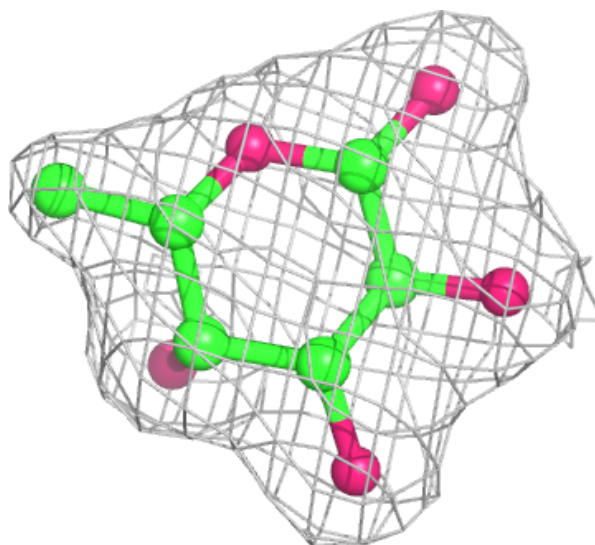
**Electron density around FUL G 202:**

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



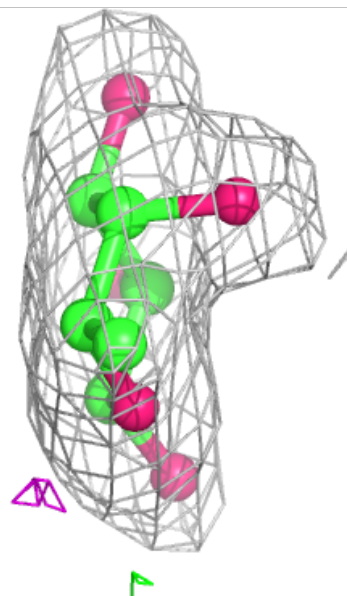
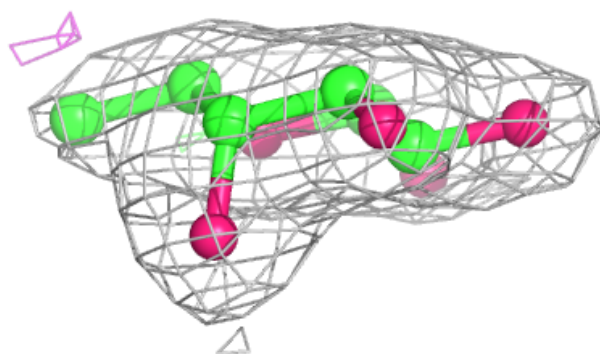
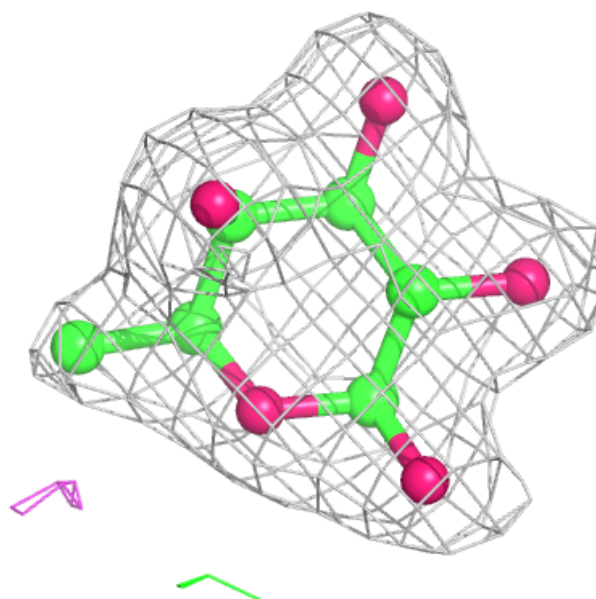
**Electron density around FUL H 201:**

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



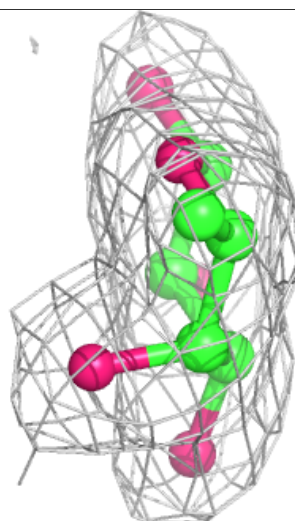
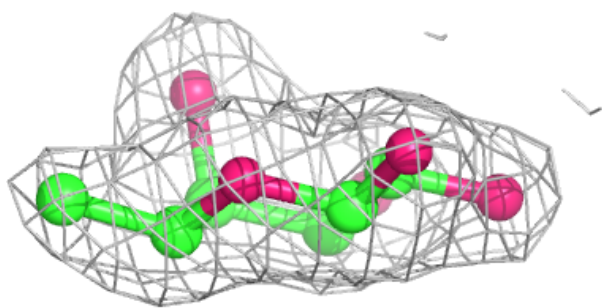
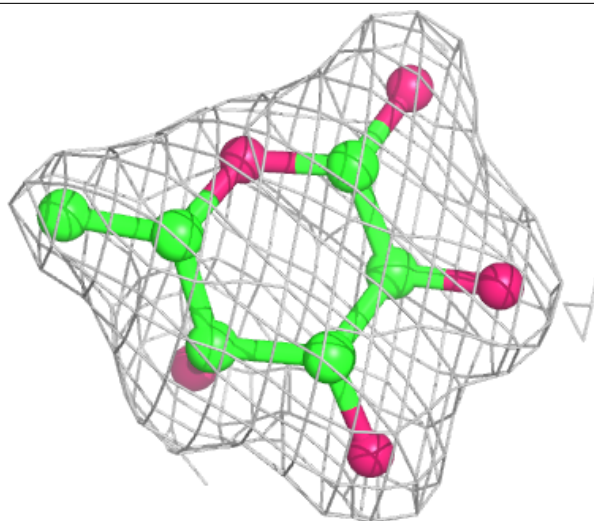
**Electron density around FUL E 204:**

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



**Electron density around FUL B 204:**

$2mF_o-DF_c$  (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.