



# wwPDB X-ray Structure Validation Summary Report

Mar 13, 2026 – 10:08 PM UTC

PDB ID : 7PRG / pdb\_00007prg  
Title : Joint X-ray/neutron room temperature structure of perdeuterated LecB lectin in complex with perdeuterated fucose  
Authors : Gajdos, L.; Blakeley, M.P.; Haertlein, M.; Forsyth, T.V.; Devos, J.M.; Imberty, A.  
Deposited on : 2021-09-21  
Resolution : 1.85 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.

The types of validation reports are described at

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

---

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

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

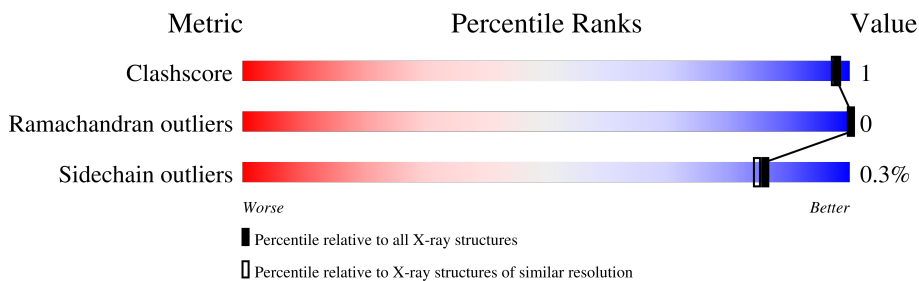
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION, NEUTRON DIFFRACTION*

The reported resolution of this entry is 1.85 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))
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	115	95% <span style="float: right;">. .</span>
1	B	115	99% <span style="float: right;">.</span>
1	C	115	97% <span style="float: right;">. .</span>
1	D	115	98% <span style="float: right;">. .</span>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8243 atoms, of which 0 are hydrogens and 4264 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.

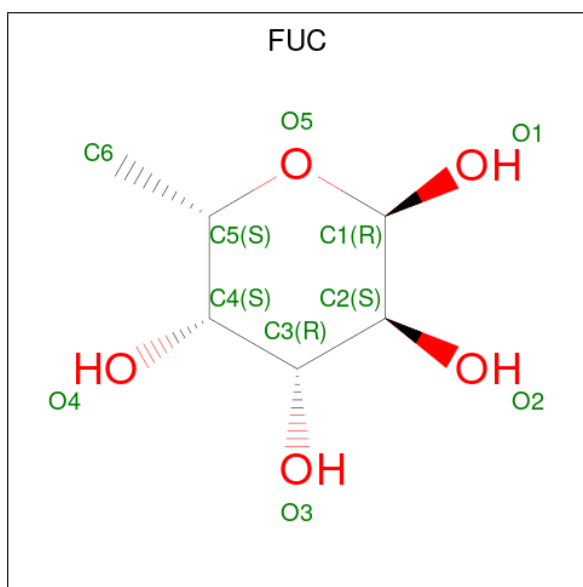
- Molecule 1 is a protein called Fucose-binding lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	D	N	O			
1	A	114	1755	543	867	155	190	0	15	0
1	B	114	1747	541	863	155	188	0	14	0
1	C	114	1758	544	870	155	189	0	16	0
1	D	114	1786	551	888	158	189	0	18	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	D	O		
3	A	1	23	6	12	5	0	0
3	B	1	23	6	12	5	0	0
3	C	1	23	6	12	5	0	0
3	D	1	23	6	12	5	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	105	Total	D	O	0	0
			315	210	105		
5	B	88	Total	D	O	0	0
			264	176	88		
5	C	84	Total	D	O	0	0
			252	168	84		
5	D	87	Total	D	O	0	0
			261	174	87		

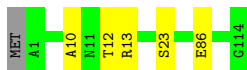
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Fucose-binding lectin

Chain A:  95%



- Molecule 1: Fucose-binding lectin

Chain B:  99%



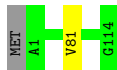
- Molecule 1: Fucose-binding lectin

Chain C:  97%



- Molecule 1: Fucose-binding lectin

Chain D:  98%



## 4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.90Å 73.87Å 55.00Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	27.41 – 1.85	Depositor
% Data completeness (in resolution range)	96.2 (27.41-1.85)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 1.85Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.104 , 0.142	Depositor
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtrriage
Anisotropy	0.169	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for l,-k,h	Xtrriage
Total number of atoms	8243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FUC, CA

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	0.66	0/951	0.70	0/1301
1	B	0.63	0/957	0.69	0/1309
1	C	0.60	0/961	0.66	0/1314
1	D	0.58	0/975	0.64	0/1333
All	All	0.62	0/3844	0.67	0/5257

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1755	0	806	3	0
1	B	1747	0	799	0	0
1	C	1758	0	800	2	0
1	D	1786	0	809	1	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
3	A	23	0	9	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	9	0	0
3	C	23	0	9	0	0
3	D	23	0	8	0	0
4	B	5	0	0	0	0
5	A	315	0	0	1	0
5	B	264	0	0	1	0
5	C	252	0	0	1	0
5	D	261	0	0	0	0
All	All	8243	0	3249	5	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (5) 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:C:72:ARG:NE	5:C:301:HOH:O	2.32	0.62
1:A:23[A]:SER:OG	5:A:301:HOH:O	2.16	0.61
1:A:10:ALA:O	1:A:12[A]:THR:HG23	2.01	0.55
1:A:13[B]:ARG:HD2	5:B:383:HOH:O	2.04	0.52
1:C:81[B]:VAL:HG21	1:D:81[B]:VAL:HG11	1.87	0.46

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/115 (110%)	123 (97%)	4 (3%)	0	100	100
1	B	126/115 (110%)	122 (97%)	4 (3%)	0	100	100
1	C	128/115 (111%)	122 (95%)	6 (5%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	130/115 (113%)	127 (98%)	3 (2%)	0	100	100
All	All	511/460 (111%)	494 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/94 (114%)	105 (98%)	2 (2%)	50	38
1	B	107/94 (114%)	107 (100%)	0	100	100
1	C	108/94 (115%)	108 (100%)	0	100	100
1	D	110/94 (117%)	110 (100%)	0	100	100
All	All	432/376 (115%)	430 (100%)	2 (0%)	86	77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86[A]	GLU
1	A	86[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	110	ASN
1	D	21	ASN
1	D	110	ASN
1	D	47	ASN
1	C	21	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	FUC	C	203	2	11,11,11	1.30	1 (9%)	16,16,16	0.90	0
3	FUC	D	201	2	11,11,11	1.21	0	16,16,16	1.25	1 (6%)
3	FUC	B	203	2	11,11,11	0.98	1 (9%)	16,16,16	1.15	1 (6%)
3	FUC	A	203	2	11,11,11	0.90	0	16,16,16	1.00	1 (6%)
4	SO4	B	204	-	4,4,4	0.37	0	6,6,6	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	C	203	2	-	-	0/1/1/1
3	FUC	D	201	2	-	-	0/1/1/1
3	FUC	A	203	2	-	-	0/1/1/1
3	FUC	B	203	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	203	FUC	O5-C1	2.76	1.49	1.42
3	B	203	FUC	O5-C1	2.66	1.49	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	FUC	O5-C1-C2	-3.22	104.63	110.30
3	B	203	FUC	O2-C2-C1	2.48	114.98	109.25
3	A	203	FUC	O4-C4-C3	-2.24	105.09	110.38

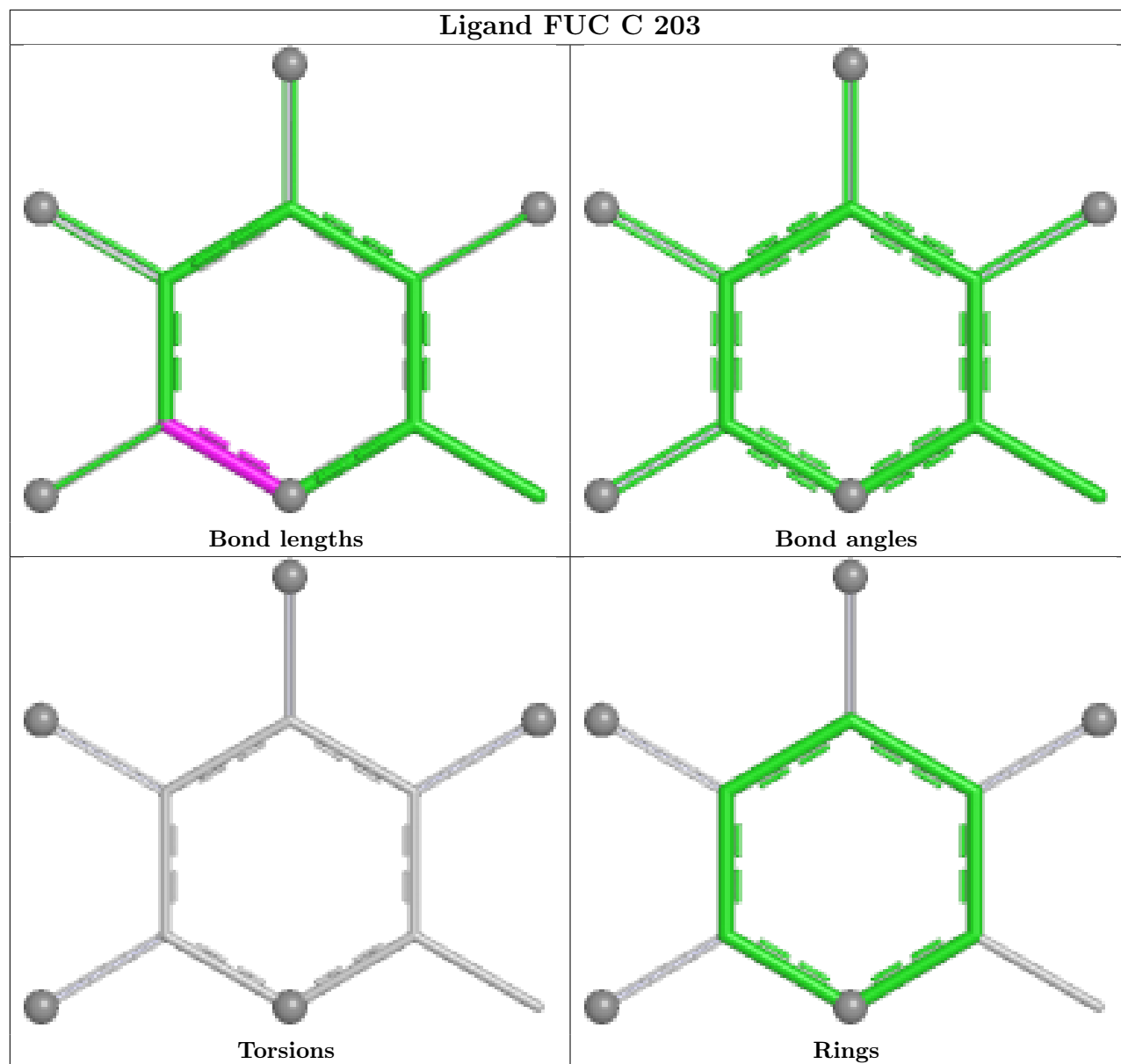
There are no chirality outliers.

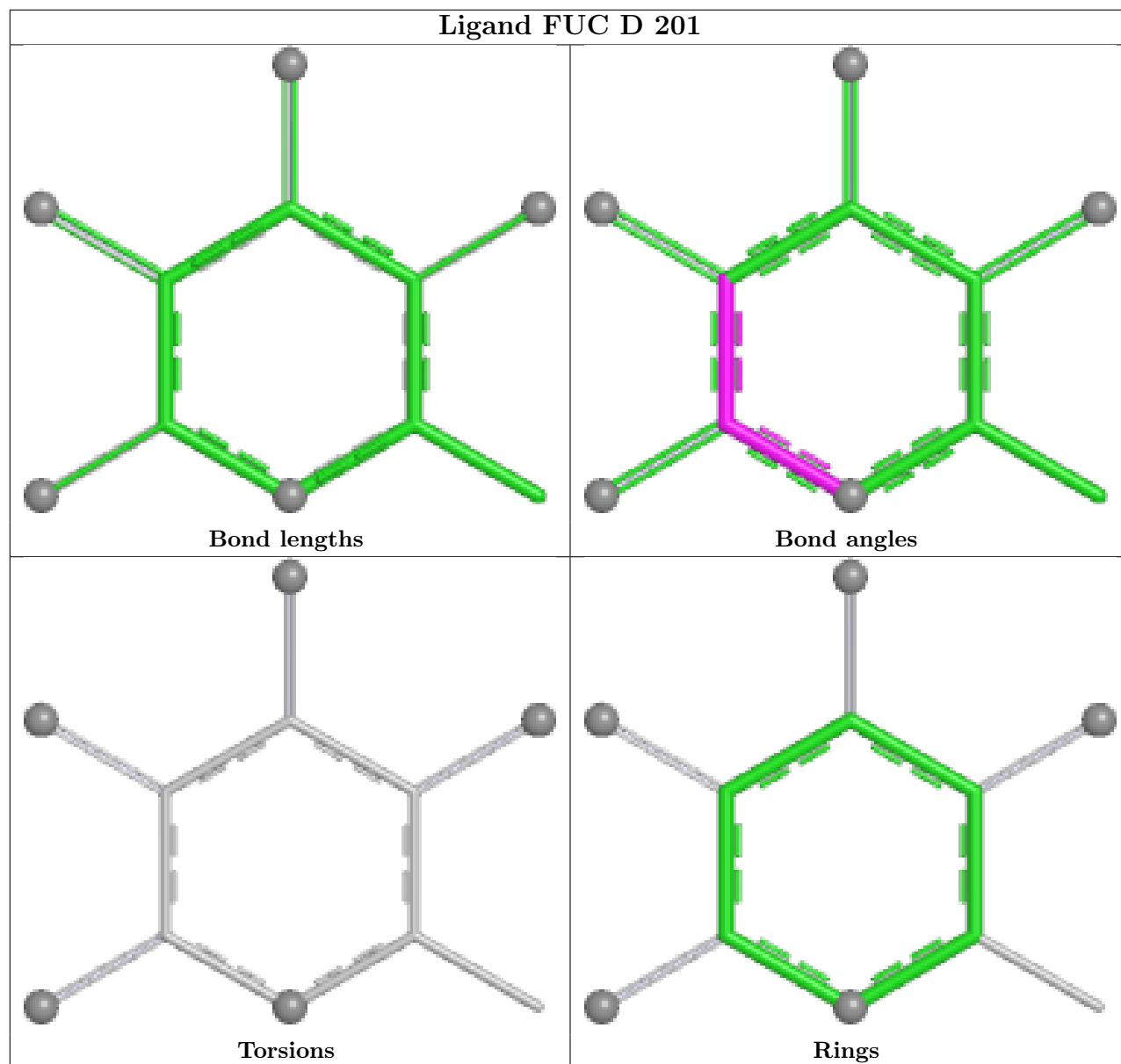
There are no torsion outliers.

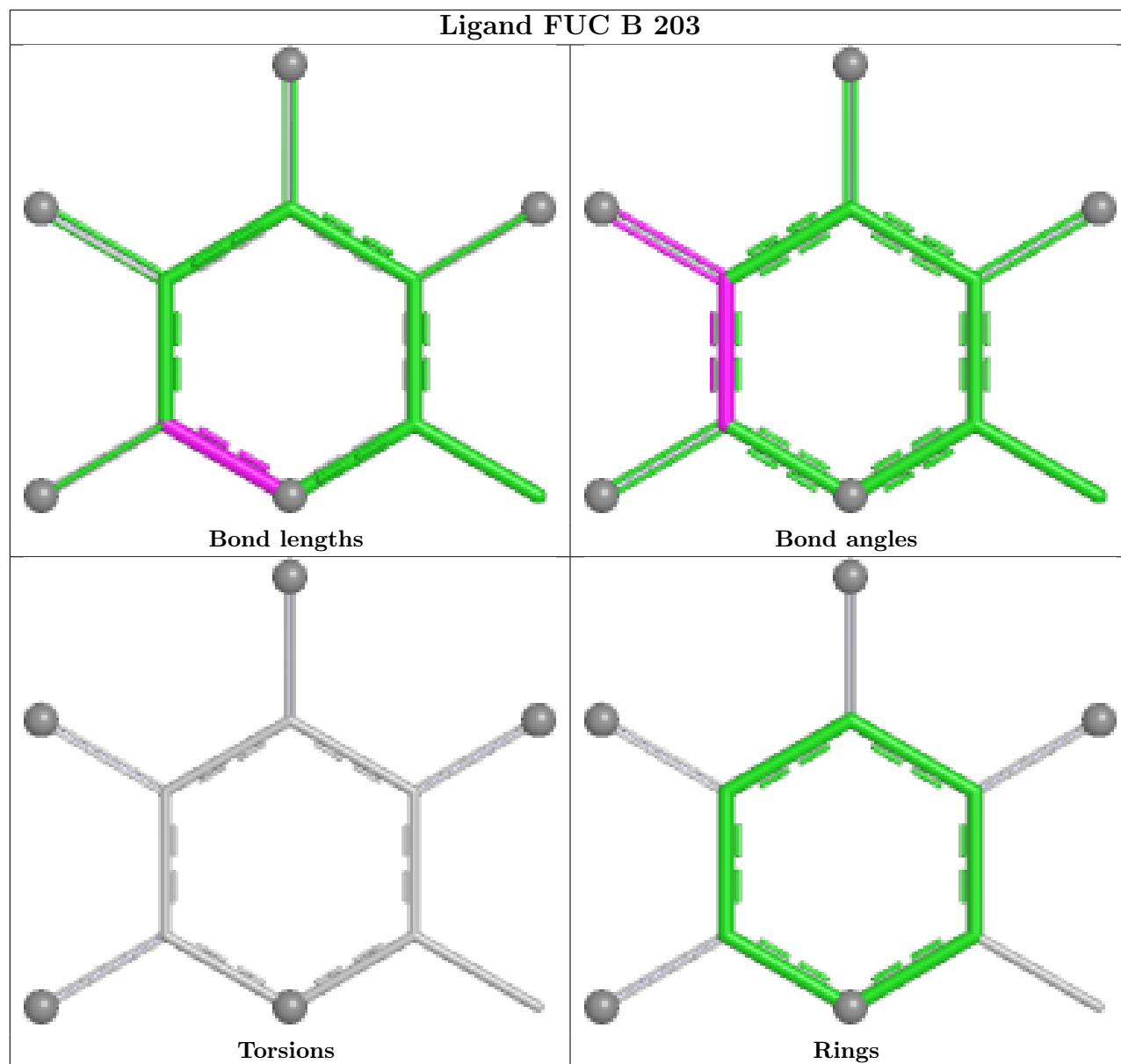
There are no ring outliers.

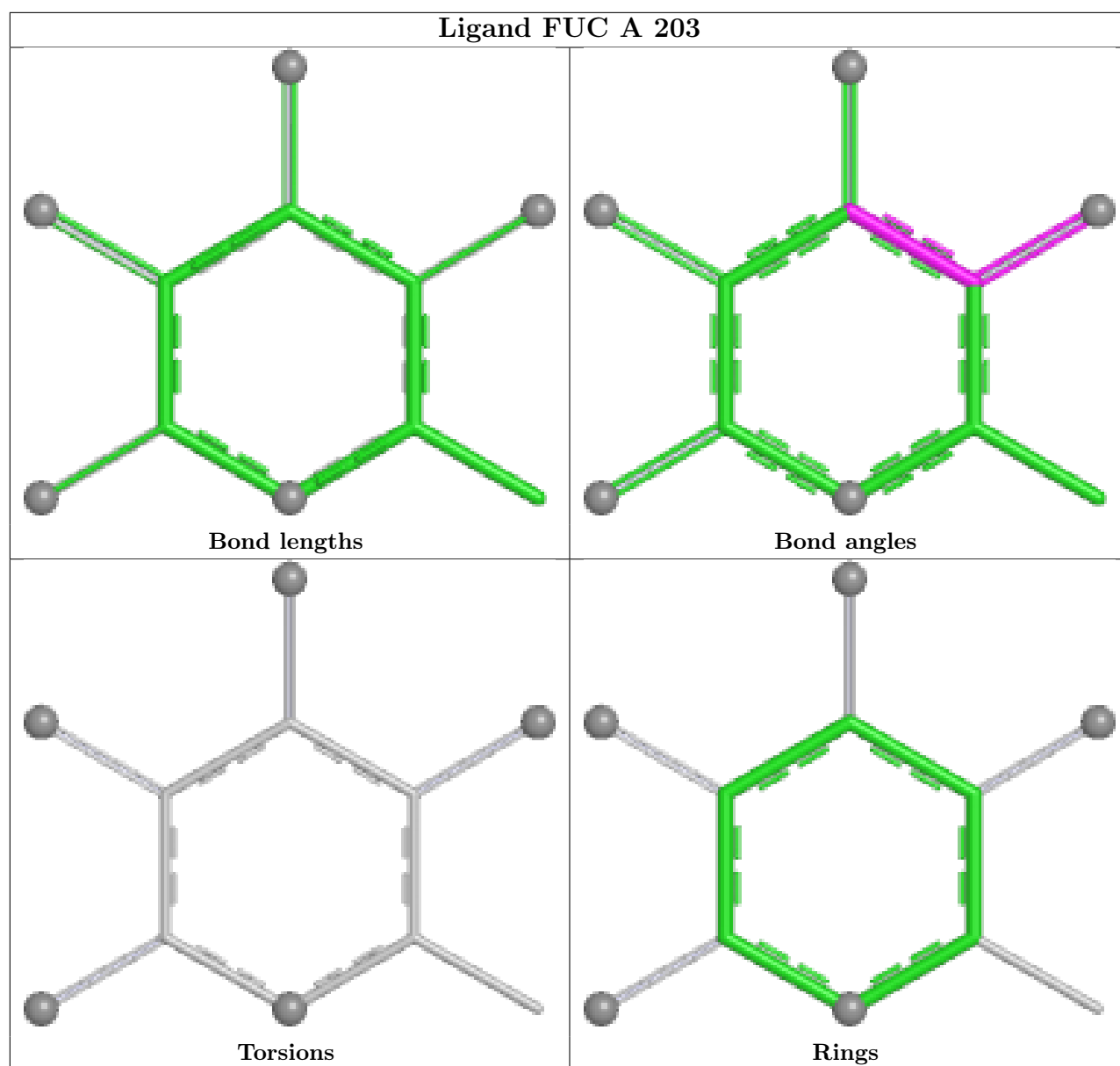
No monomer is involved in short contacts.

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









## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.