



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 10:06 PM JST

PDB ID : 8ZWR / pdb\_00008zwr  
Title : Structure-Based Mechanism and Specificity of Human Galactosyltransferase B3GalT5  
Authors : Lo, J.M.; Ma, C.  
Deposited on : 2024-06-13  
Resolution : 1.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

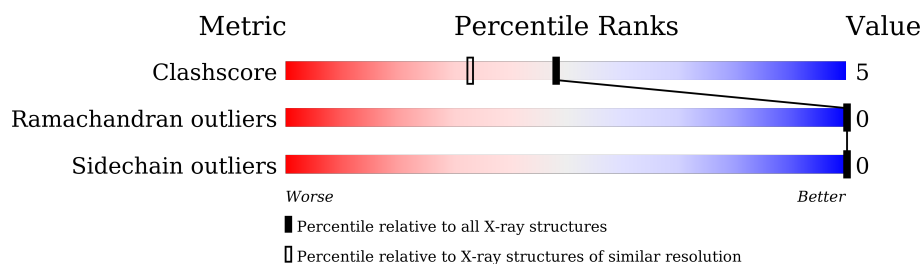
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)

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	278	
1	B	278	
2	E	2	
2	G	2	
3	F	6	
4	D	2	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5119 atoms, of which 173 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 Beta-1,3-galactosyltransferase 5.

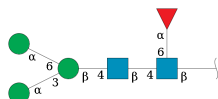
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	3	0
			2212	1437	372	390	13			
1	B	266	Total	C	N	O	S	0	0	0
			2189	1418	370	388	13			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	6	Total	C	H	N	O	0	0	0
			138	40	67	2	29			

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

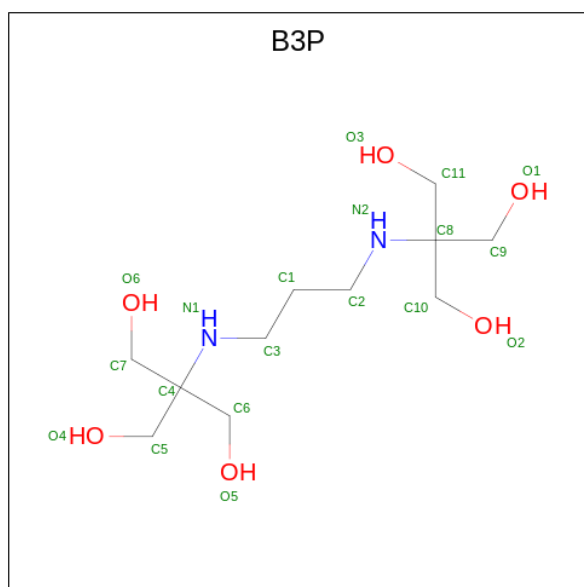


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	B	1	Total	Mn	0	0
			1	1		

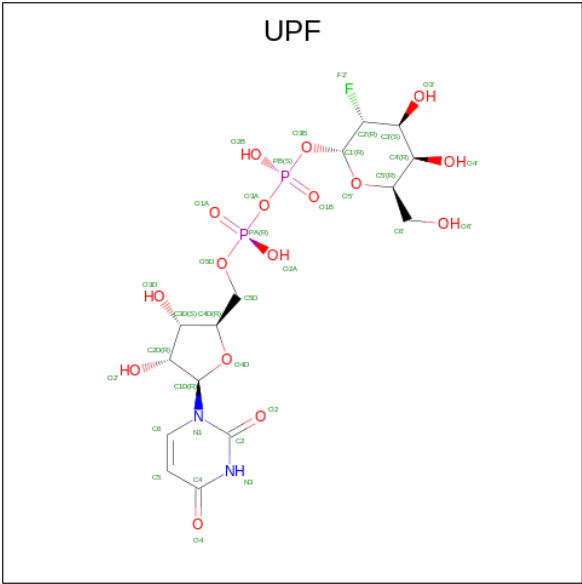
- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: C<sub>11</sub>H<sub>26</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			45	11	26	2	6		
6	B	1	Total	C	H	N	O	0	0
			45	11	26	2	6		

- Molecule 7 is URIDINE-5'-DIPHOSPHATE-2-DEOXY-2-FLUOROGALACTOSE (CCD

ID: UPF) (formula: C<sub>15</sub>H<sub>23</sub>FN<sub>2</sub>O<sub>16</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).




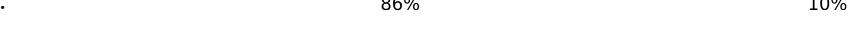
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
7	B	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		

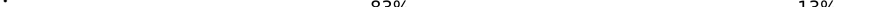


- Molecule 8 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	196	Total	O	0	0
			196	196		
8	B	86	Total	O	0	0
			86	86		



Note EDS failed to run properly.

- Chain A:  86% 10% .
- 
- | Residue | State | Percentage |
|---------|-------|------------|
| PHE     | PHE   | 0%         |
| LYS     | LYS   | 86%        |
| GLU     | GLU   | 0%         |
| GLN     | GLN   | 0%         |
| SER     | SER   | 0%         |
| PHE     | PHE   | 0%         |
| VAL     | VAL   | 0%         |
| TYR     | TYR   | 0%         |
| LYS     | LYS   | 86%        |
| LYS     | LYS   | 86%        |
| ASP     | ASP   | 0%         |
| G42     | G42   | 0%         |
| N43     | N43   | 0%         |
| K68     | K68   | 0%         |
| E72     | E72   | 0%         |
| M65     | M65   | 0%         |
| G88     | G88   | 0%         |
| K89     | K89   | 0%         |
| L133    | L133  | 0%         |
| C146    | C146  | 0%         |
| P147    | P147  | 0%         |
| K154    | K154  | 0%         |
| L171    | L171  | 0%         |
| R175    | R175  | 0%         |
| I191    | I191  | 0%         |
| R192    | R192  | 0%         |
| Q193    | Q193  | 0%         |
| P194    | P194  | 0%         |
| W198    | W198  | 0%         |
| F199    | F199  | 0%         |
| V200    | V200  | 0%         |
| V232    | V232  | 0%         |
| S233    | S233  | 86%        |
| K234    | K234  | 0%         |
| S235    | S235  | 86%        |
| V236    | V236  | 0%         |
| P237    | P237  | 0%         |
| K240    | K240  | 0%         |
| R252    | R252  | 0%         |
| P289    | P289  | 0%         |
| Q297    | Q297  | 0%         |
| N301    | N301  | 0%         |

- Chain B:  83% 13% •
- 
- 

- Chain E:  100%
- MAG1  
MAG2

- Chain G: 

- 

Chain F:  50% 50%

MAG1	MAG2	BGL3	MAN4	MAN5	FUC6
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- Molecule 4:  $\alpha$ -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1	FUC2
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## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	47.74Å 85.74Å 87.73Å 90.00° 95.52° 90.00°	Depositor
Resolution (Å)	30.71 – 1.94	Depositor
% Data completeness (in resolution range)	83.8 (30.71-1.94)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.193 , 0.216	Depositor
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.147	Xtriage
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
Total number of atoms	5119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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: MN, MAN, NAG, UPF, B3P, FUC, BMA

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	0.52	0/2282	0.73	0/3087
1	B	0.38	0/2248	0.60	0/3040
All	All	0.46	0/4530	0.67	0/6127

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	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ARG	Sidechain
1	B	209	ARG	Sidechain
1	B	303	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	2212	0	2204	18	2
1	B	2189	0	2175	31	0
2	E	28	27	25	0	0
2	G	28	27	25	1	0
3	F	71	67	61	0	0
4	D	24	0	22	0	2
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	19	26	26	0	0
6	B	19	26	26	0	0
7	A	36	0	20	0	0
7	B	36	0	20	1	0
8	A	196	0	0	4	0
8	B	86	0	0	2	0
All	All	4946	173	4604	50	2

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 (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:HD12	1:B:163:VAL:HG11	1.47	0.94
1:A:234:LYS:HE3	8:A:656:HOH:O	1.84	0.77
1:A:133:LEU:HG	8:A:581:HOH:O	1.87	0.74
1:B:45:LEU:HD11	1:B:123:ASP:HB2	1.72	0.71
1:A:68:LYS:NZ	8:A:502:HOH:O	2.26	0.68
1:B:91:LEU:CD1	1:B:163:VAL:HG11	2.24	0.67
1:B:176:THR:HG22	8:B:576:HOH:O	1.99	0.62
1:B:91:LEU:C	1:B:91:LEU:HD23	2.20	0.61
1:A:232:VAL:CG2	1:A:252:ARG:HG2	2.32	0.60
1:A:232:VAL:HG21	1:A:252:ARG:HG2	1.84	0.59
1:B:176:THR:CG2	8:B:576:HOH:O	2.50	0.59
1:B:128:TYR:CZ	1:B:197:LYS:HE2	2.39	0.57
1:B:72:GLU:HG3	1:B:289:PRO:HG3	1.87	0.57
1:B:232:VAL:HG21	1:B:252:ARG:HG2	1.88	0.56
1:A:191:ILE:HD12	1:A:198[B]:TRP:HB2	1.90	0.54
1:B:45:LEU:HD11	1:B:123:ASP:CB	2.38	0.53
1:A:43:ASN:O	8:A:501:HOH:O	2.19	0.52
1:A:191:ILE:HD12	1:A:198[A]:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HE2	1:A:171:LEU:HD21	1.92	0.50
1:B:99:THR:CG2	1:B:123:ASP:HA	2.43	0.49
1:B:128:TYR:CE1	1:B:197:LYS:HE2	2.48	0.49
1:B:85:MET:HE3	1:B:88:GLY:HA2	1.94	0.48
1:B:232:VAL:CG2	1:B:252:ARG:HG2	2.45	0.46
1:B:175:ARG:CZ	1:B:175:ARG:HB3	2.46	0.45
1:B:162:ASN:HB3	1:B:281:ILE:O	2.17	0.45
1:B:278:PHE:HA	1:B:281:ILE:HG12	1.99	0.45
1:B:99:THR:HG21	1:B:123:ASP:HA	1.99	0.45
1:B:45:LEU:HD11	1:B:123:ASP:CA	2.47	0.44
1:B:154:LYS:HD3	1:B:154:LYS:C	2.38	0.44
1:B:189:PHE:CD1	1:B:209:ARG:HG2	2.53	0.44
1:B:83:GLU:HA	1:B:91:LEU:HD22	2.00	0.43
1:B:141:TRP:CD1	1:B:145:PHE:HD2	2.37	0.43
1:B:107:LYS:HA	1:B:107:LYS:HD2	1.78	0.42
1:B:125:LEU:HG	1:B:127:VAL:HG13	2.01	0.42
1:B:45:LEU:HG	1:B:122:LYS:HA	2.00	0.42
1:B:124:PHE:HA	2:G:1:NAG:H62	2.02	0.42
1:B:68:LYS:HB3	1:B:68:LYS:HE2	1.72	0.42
1:A:146:CYS:N	1:A:147:PRO:CD	2.81	0.42
1:A:297:GLN:NE2	1:A:301:ASN:OD1	2.43	0.42
1:A:175:ARG:CZ	1:A:175:ARG:HB3	2.49	0.42
1:A:85:MET:HE1	1:A:88:GLY:O	2.20	0.41
1:A:236:VAL:HG13	1:A:237:PRO:HD2	2.02	0.41
1:B:146:CYS:N	1:B:147:PRO:CD	2.83	0.41
1:A:72:GLU:HG3	1:A:289:PRO:HG3	2.03	0.41
7:B:403:UPF:H6	7:B:403:UPF:H2D	1.89	0.41
1:B:48:PRO:HD3	1:B:120:ILE:HG12	2.03	0.41
1:B:92:LYS:HB3	1:B:92:LYS:HE3	1.84	0.41
1:A:194:PRO:HA	1:A:199:PHE:CD1	2.56	0.40
1:A:154:LYS:C	1:A:154:LYS:HD3	2.42	0.40
1:A:200:VAL:HG12	1:A:240:LYS:HE2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:NE2	4:D:1:NAG:C6[1_655]	2.03	0.17
1:A:193:GLN:NE2	4:D:1:NAG:O6[1_655]	2.16	0.04

## 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	268/278 (96%)	262 (98%)	6 (2%)	0	100	100
1	B	264/278 (95%)	257 (97%)	7 (3%)	0	100	100
All	All	532/556 (96%)	519 (98%)	13 (2%)	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	247/255 (97%)	247 (100%)	0	100	100
1	B	244/255 (96%)	244 (100%)	0	100	100
All	All	491/510 (96%)	491 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

12 monosaccharides 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
4	NAG	D	1	4,1	14,14,15	0.46	0	17,19,21	0.63	0
4	FUC	D	2	4	10,10,11	0.30	0	14,14,16	1.00	1 (7%)
2	NAG	E	1	1,2	14,14,15	0.46	0	17,19,21	1.20	2 (11%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	0.83	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.46	0	17,19,21	1.04	1 (5%)
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	1.03	2 (11%)
3	BMA	F	3	3	11,11,12	0.63	0	15,15,17	0.63	0
3	MAN	F	4	3	11,11,12	0.42	0	15,15,17	0.63	0
3	MAN	F	5	3	11,11,12	0.38	0	15,15,17	0.68	0
3	FUC	F	6	3	10,10,11	0.36	0	14,14,16	0.84	2 (14%)
2	NAG	G	1	1,2	14,14,15	0.41	0	17,19,21	1.27	1 (5%)
2	NAG	G	2	2	14,14,15	0.42	0	17,19,21	1.04	1 (5%)

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
4	NAG	D	1	4,1	-	4/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	O5-C1-C2	-4.19	104.67	111.29
2	E	1	NAG	O5-C1-C2	-3.58	105.64	111.29
2	G	2	NAG	C1-O5-C5	3.34	116.71	112.19
3	F	1	NAG	C2-N2-C7	3.02	127.21	122.90
4	D	2	FUC	O5-C1-C2	-2.86	106.35	110.77
2	E	1	NAG	C2-N2-C7	2.48	126.43	122.90
3	F	2	NAG	O5-C1-C2	-2.33	107.61	111.29
2	E	2	NAG	O5-C1-C2	-2.27	107.71	111.29
3	F	2	NAG	C2-N2-C7	2.12	125.92	122.90
3	F	6	FUC	O2-C2-C3	2.10	114.35	110.14
3	F	6	FUC	O5-C1-C2	-2.09	107.55	110.77

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6

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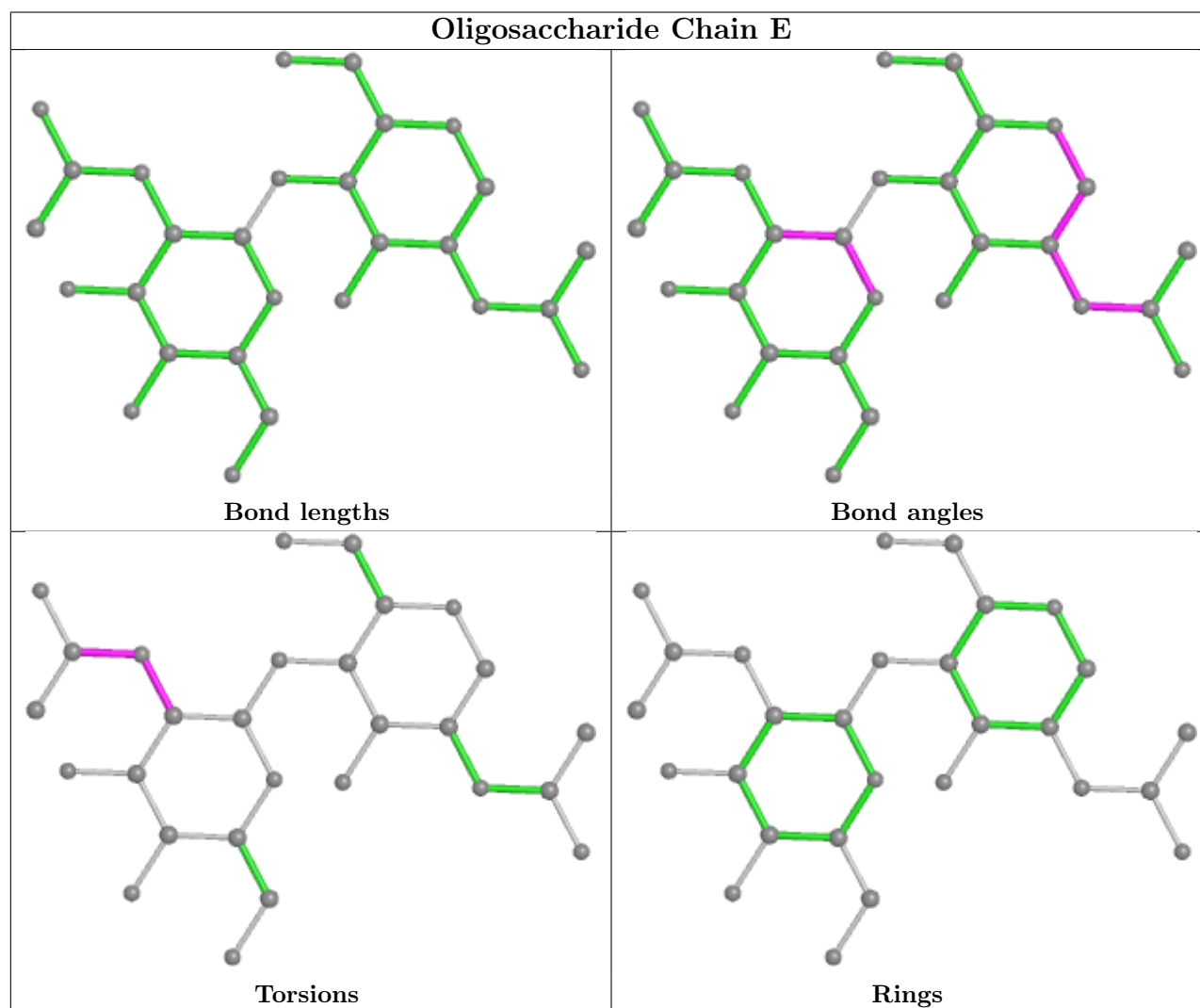
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	4	MAN	O5-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7

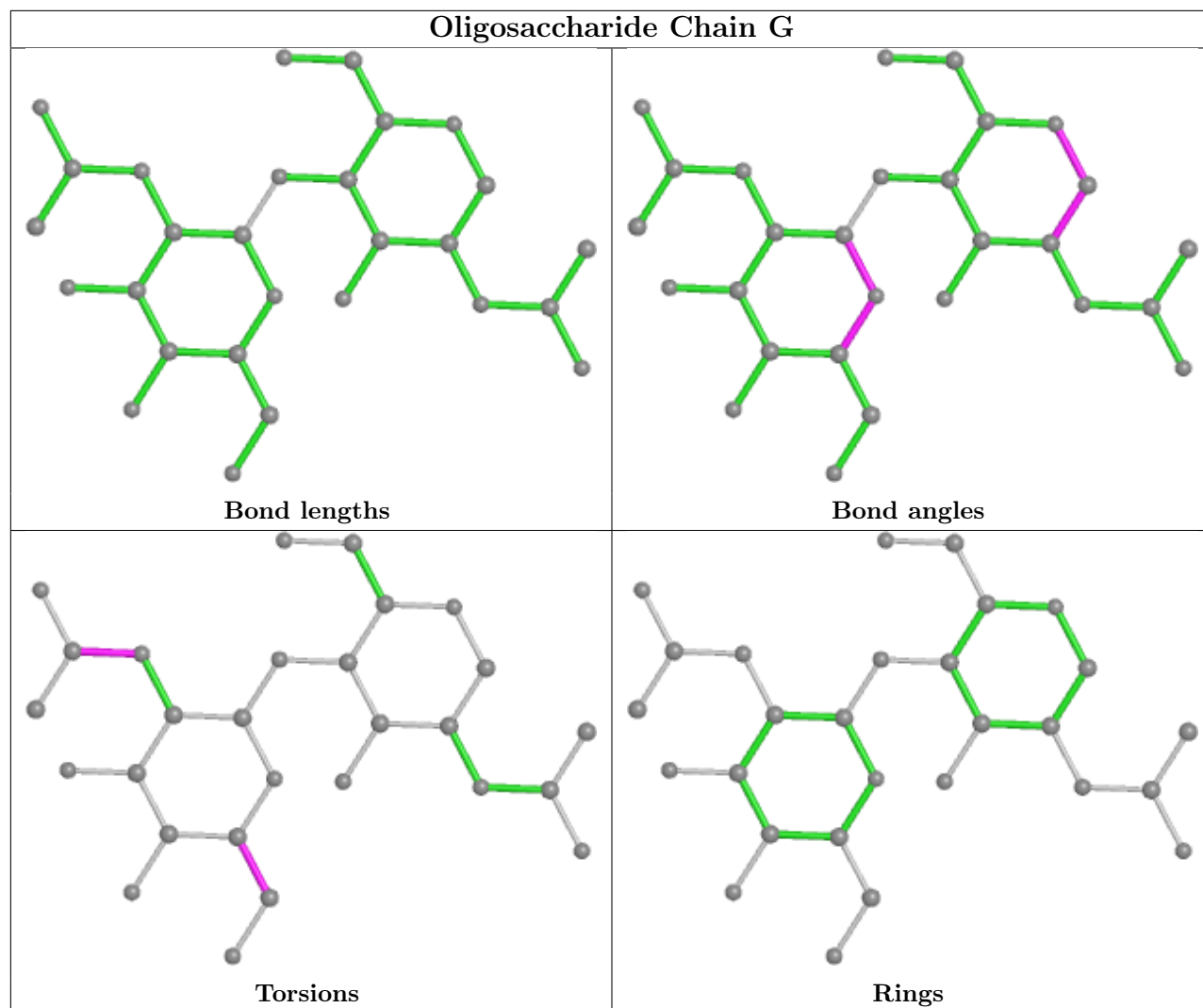
There are no ring outliers.

2 monomers are involved in 3 short contacts:

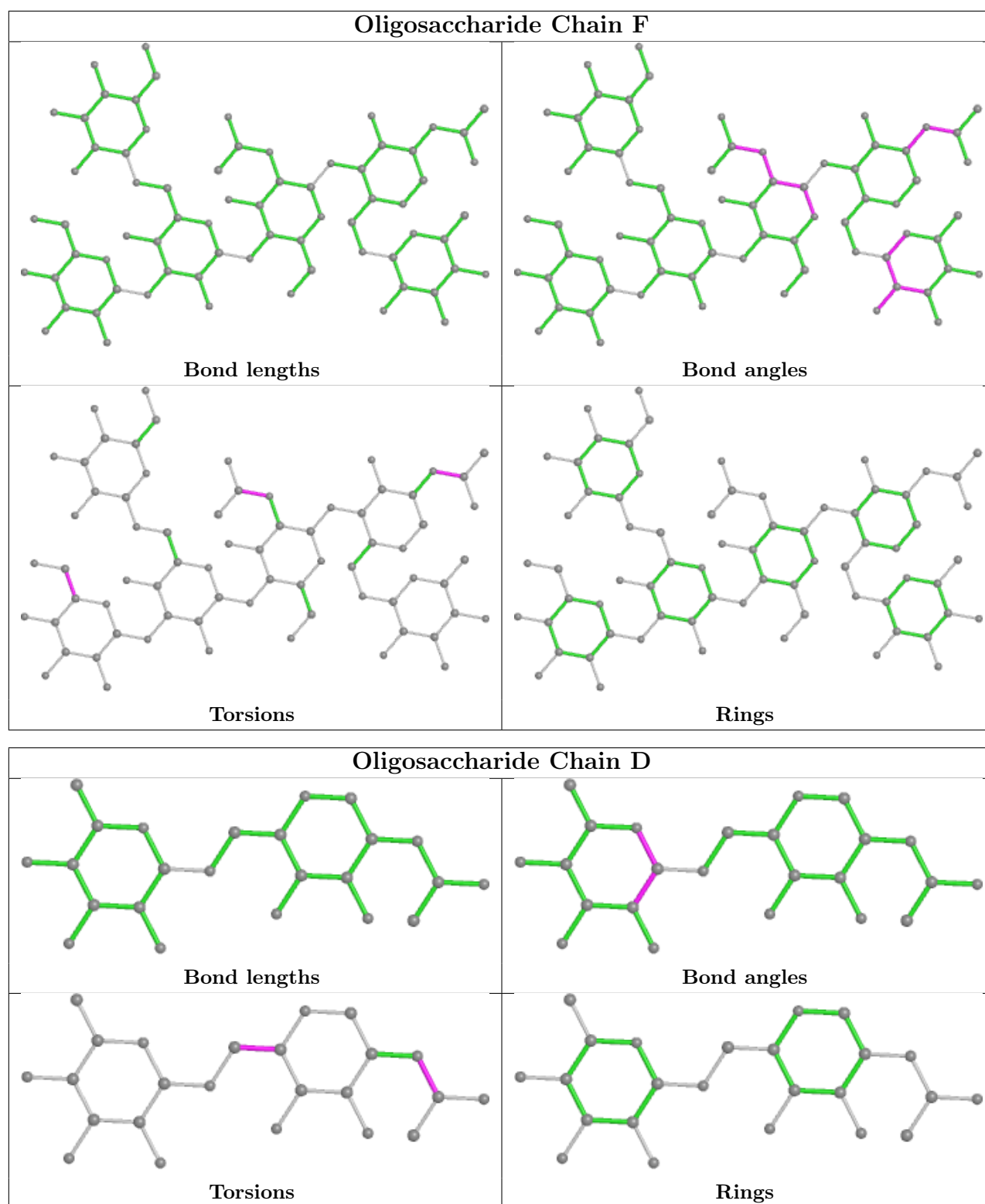
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
4	D	1	NAG	0	2

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
7	UPF	B	403	5	35,38,38	3.29	13 (37%)	51,58,58	1.49	8 (15%)
6	B3P	B	402	-	18,18,18	0.63	0	21,23,23	1.30	5 (23%)
7	UPF	A	403	5	35,38,38	3.20	11 (31%)	51,58,58	1.59	6 (11%)
6	B3P	A	402	-	18,18,18	0.74	0	21,23,23	1.05	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
7	UPF	B	403	5	-	2/22/59/59	0/3/3/3
6	B3P	B	402	-	-	4/28/28/28	-
7	UPF	A	403	5	-	3/22/59/59	0/3/3/3
6	B3P	A	402	-	-	2/28/28/28	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	403	UPF	C2'-C3'	-8.60	1.44	1.52
7	B	403	UPF	O4D-C1D	8.23	1.61	1.42
7	A	403	UPF	O4D-C1D	8.06	1.61	1.42
7	A	403	UPF	C2'-C3'	-7.46	1.46	1.52
7	B	403	UPF	O4D-C4D	-6.15	1.31	1.45
7	A	403	UPF	O4-C4	-6.05	1.12	1.24
7	B	403	UPF	O4-C4	-6.04	1.12	1.24
7	B	403	UPF	C2D-C1D	-6.02	1.34	1.53
7	A	403	UPF	O4D-C4D	-5.99	1.31	1.45
7	A	403	UPF	C2D-C1D	-5.85	1.34	1.53
7	A	403	UPF	O2-C2	-5.81	1.12	1.23
7	B	403	UPF	C2-N1	-5.42	1.29	1.38
7	A	403	UPF	C2-N1	-5.33	1.29	1.38
7	B	403	UPF	O2-C2	-5.13	1.13	1.23
7	A	403	UPF	O3D-C3D	-4.05	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	403	UPF	O3D-C3D	-4.00	1.33	1.43
7	A	403	UPF	C4-N3	-3.74	1.31	1.38
7	B	403	UPF	C4-N3	-3.55	1.32	1.38
7	A	403	UPF	F2'-C2'	-2.62	1.34	1.40
7	B	403	UPF	F2'-C2'	-2.52	1.34	1.40
7	B	403	UPF	C4'-C3'	-2.52	1.45	1.52
7	A	403	UPF	C4'-C3'	-2.19	1.46	1.52
7	B	403	UPF	C2'-C1'	2.15	1.54	1.52
7	B	403	UPF	PA-O5D	2.12	1.67	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	403	UPF	F2'-C2'-C3'	4.91	113.21	108.85
7	A	403	UPF	N3-C2-N1	4.64	121.05	114.89
7	B	403	UPF	C4-N3-C2	-4.49	120.66	126.58
7	A	403	UPF	C4-N3-C2	-4.38	120.80	126.58
7	B	403	UPF	N3-C2-N1	4.32	120.63	114.89
7	B	403	UPF	C5-C4-N3	3.48	120.04	114.84
7	A	403	UPF	C5-C4-N3	3.20	119.63	114.84
7	B	403	UPF	O4-C4-C5	-3.13	119.66	125.16
7	A	403	UPF	O4-C4-C5	-3.02	119.85	125.16
7	B	403	UPF	O3A-PB-O3B	2.86	108.25	102.48
6	B	402	B3P	C2-N2-C8	-2.47	112.57	116.08
7	B	403	UPF	O5'-C5'-C4'	2.29	113.85	109.69
6	B	402	B3P	O3-C11-C8	-2.28	107.02	111.63
7	B	403	UPF	O2-C2-N1	-2.18	119.89	122.79
7	B	403	UPF	C6'-C5'-C4'	-2.17	107.92	113.00
6	B	402	B3P	O1-C9-C8	-2.11	107.36	111.63
6	B	402	B3P	C6-C4-N1	2.08	115.28	109.03
7	A	403	UPF	O3A-PB-O3B	2.07	106.66	102.48
6	B	402	B3P	C6-C4-C5	-2.04	105.72	110.04

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	402	B3P	C5-C4-N1-C3
6	B	402	B3P	C6-C4-N1-C3
6	B	402	B3P	C7-C4-N1-C3
6	B	402	B3P	C2-C1-C3-N1
7	A	403	UPF	O5'-C5'-C6'-O6'

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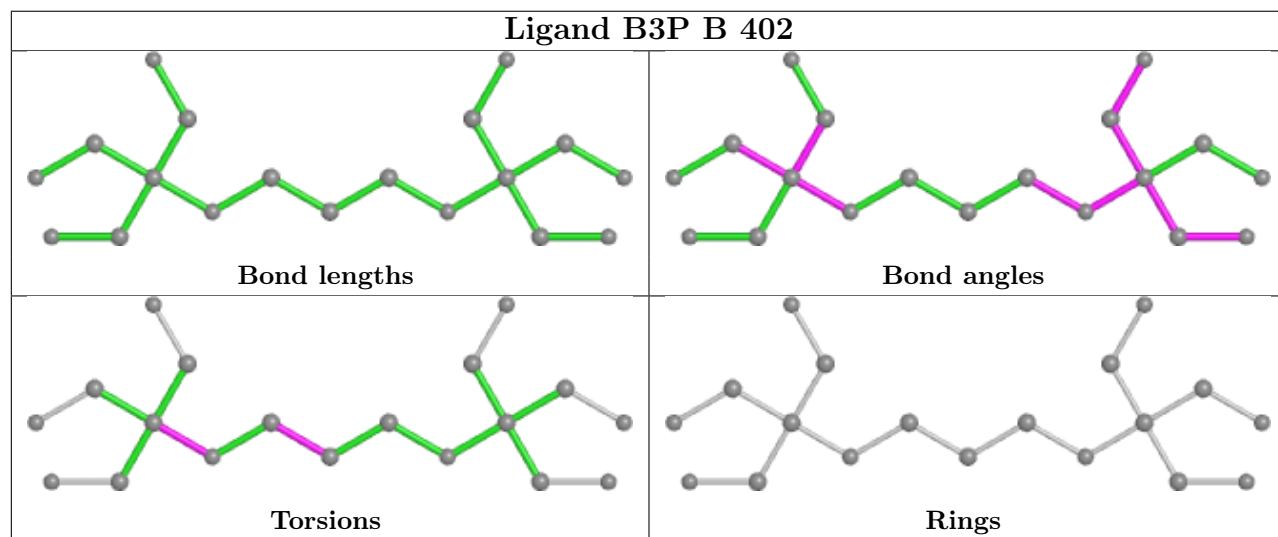
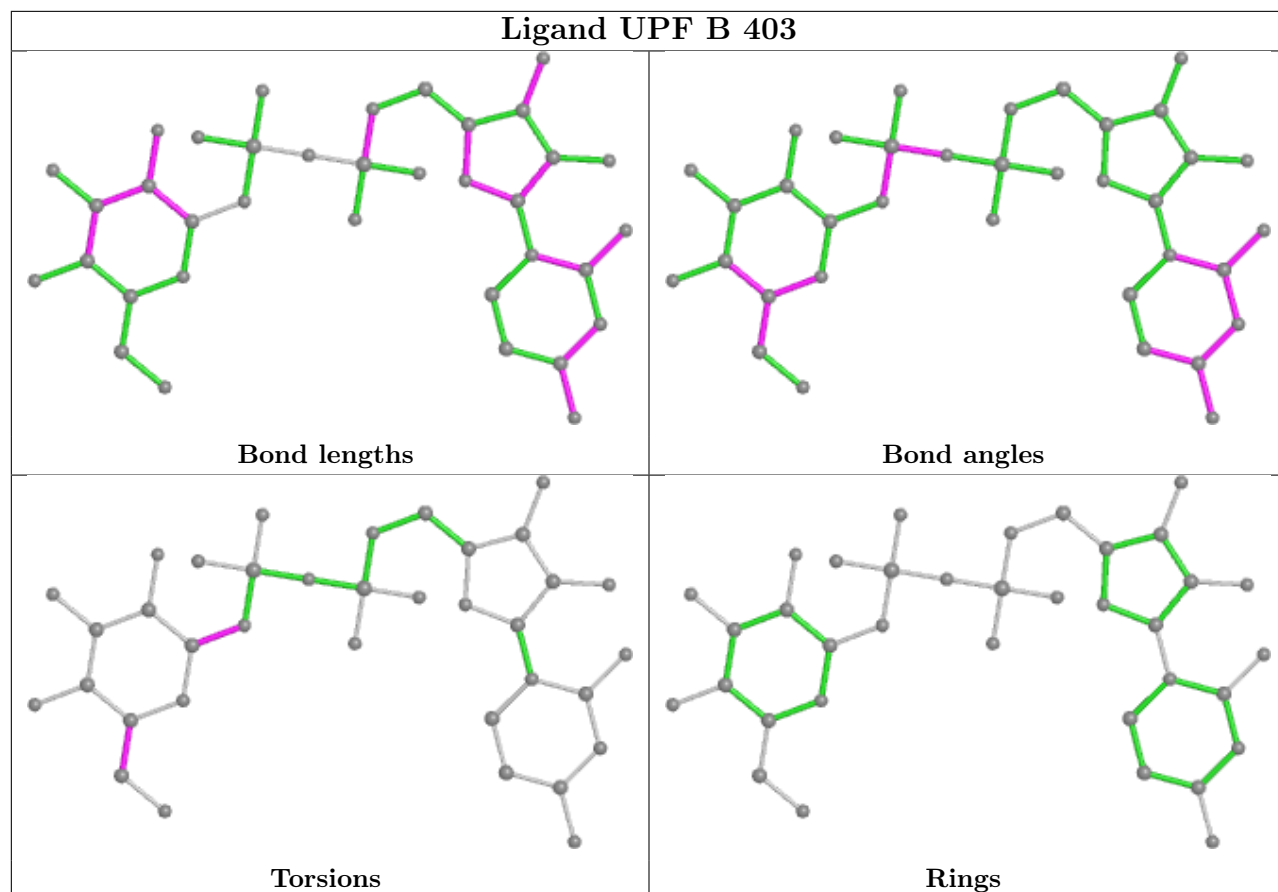
Mol	Chain	Res	Type	Atoms
7	B	403	UPF	O5'-C5'-C6'-O6'
6	A	402	B3P	C9-C8-N2-C2
6	A	402	B3P	C10-C8-N2-C2
7	A	403	UPF	O5'-C1'-O3B-PB
7	B	403	UPF	O5'-C1'-O3B-PB
7	A	403	UPF	C2D-C1D-N1-C6

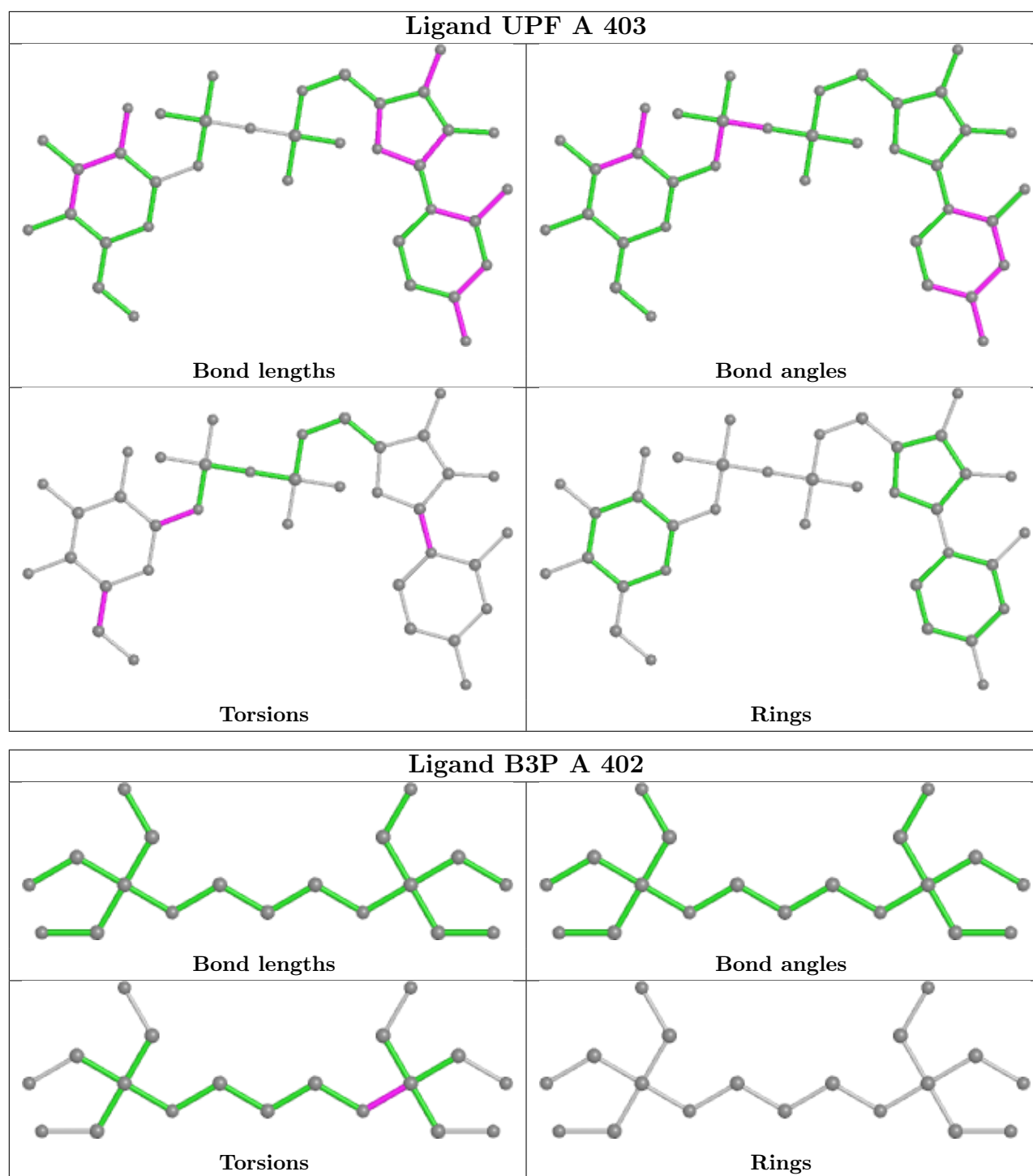
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	403	UPF	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

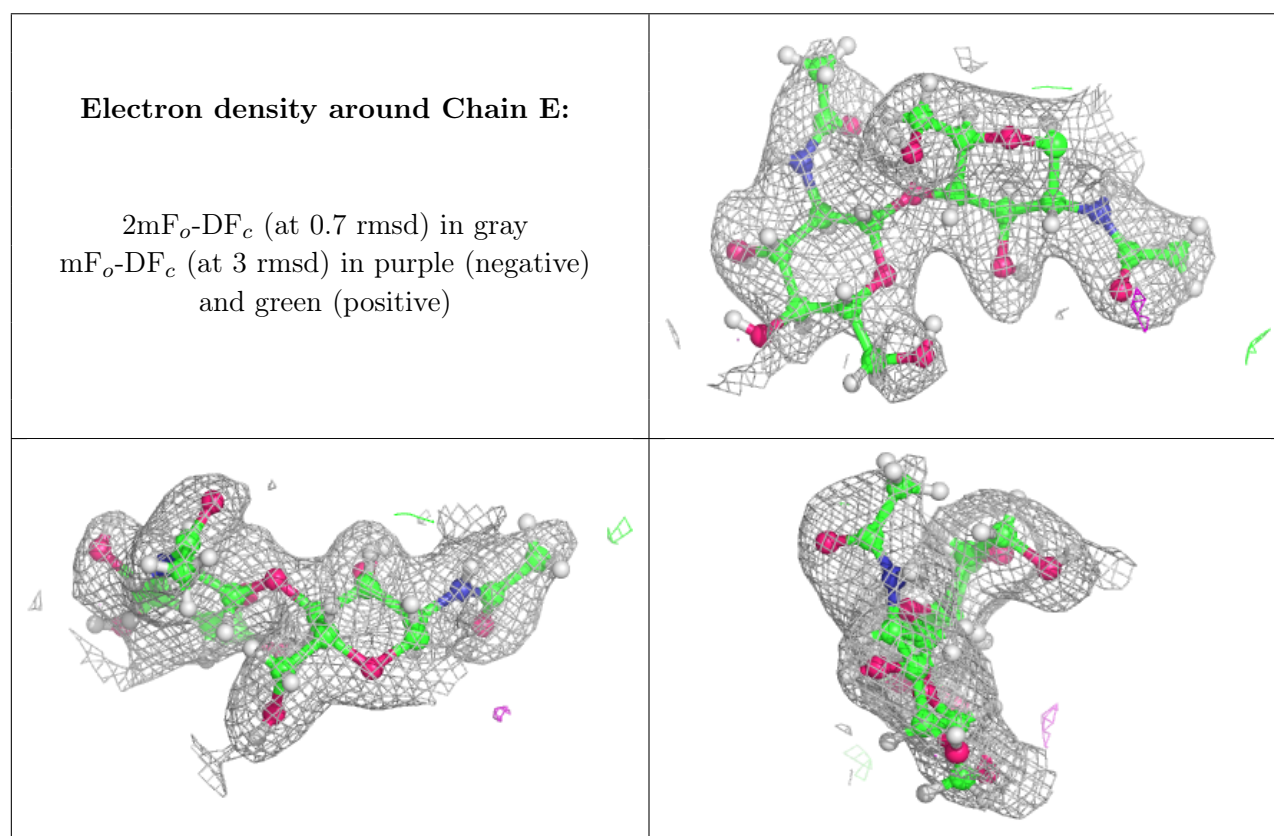
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

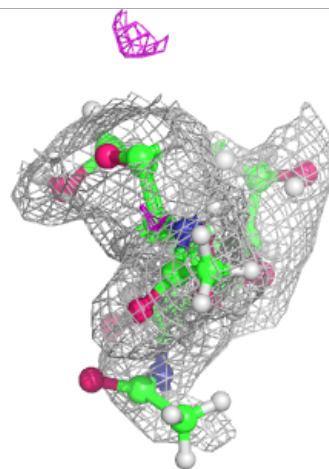
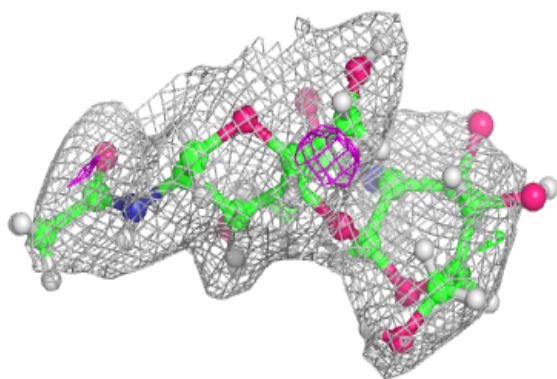
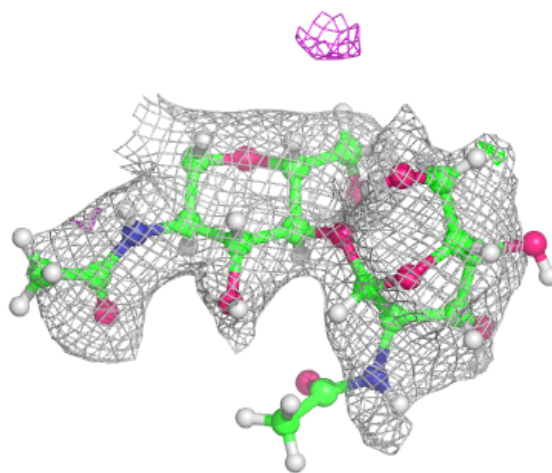
EDS failed to run properly - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain G:**

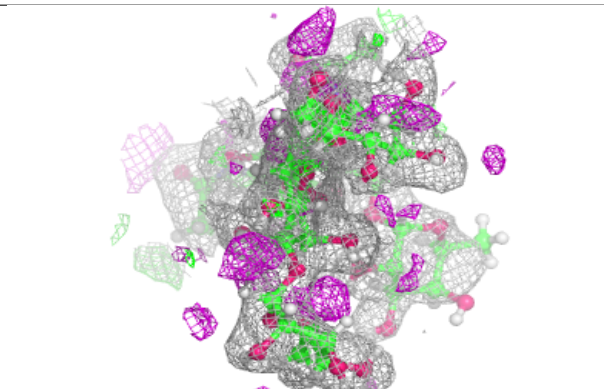
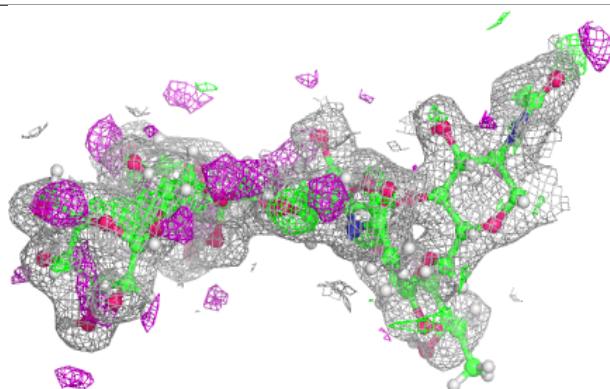
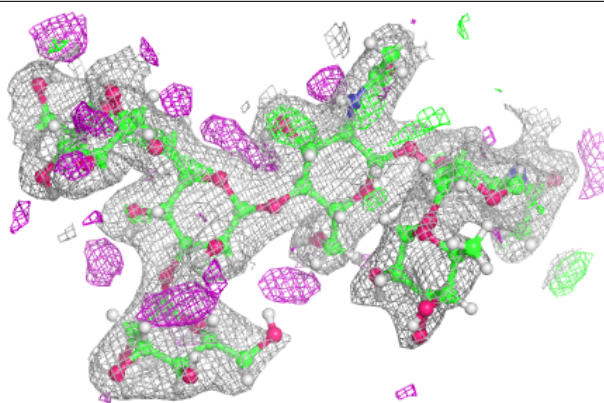
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



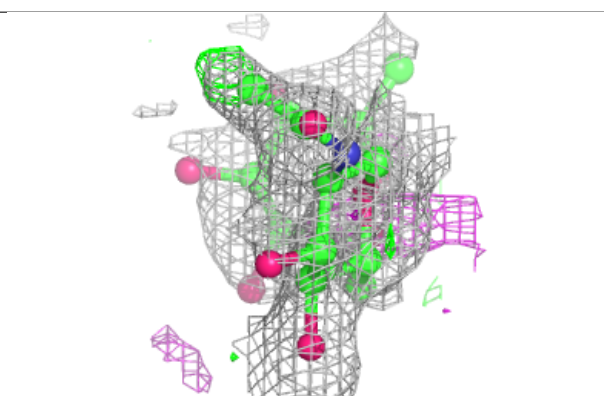
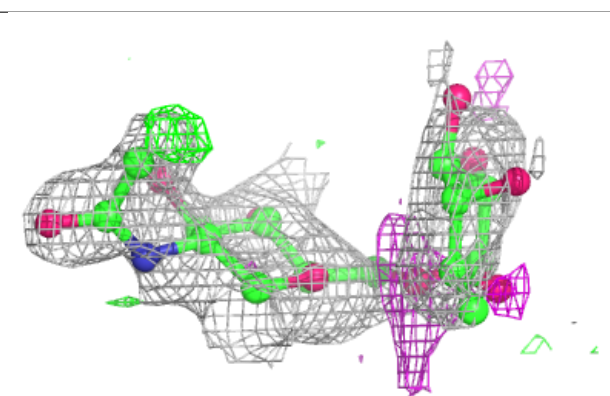
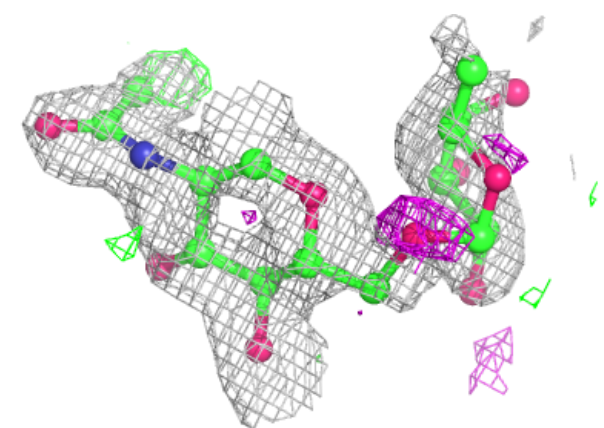


**Electron density around Chain F:**

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

**Electron density around Chain D:**

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



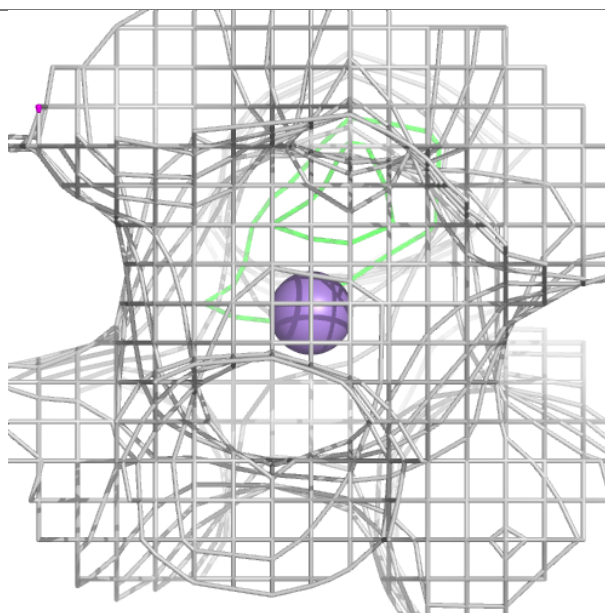
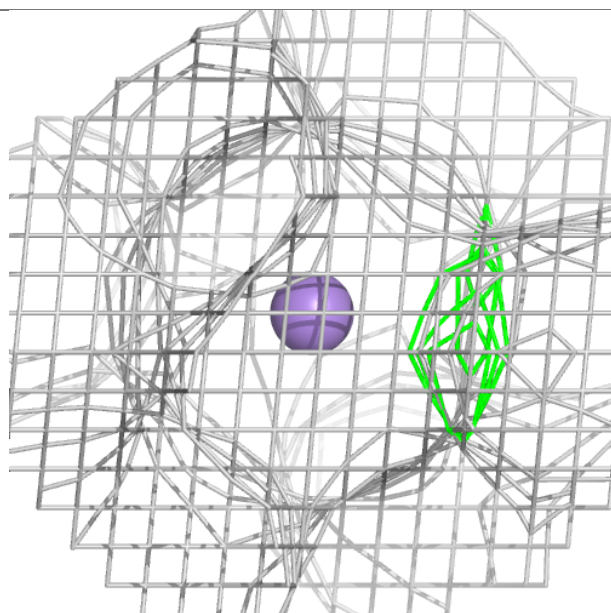
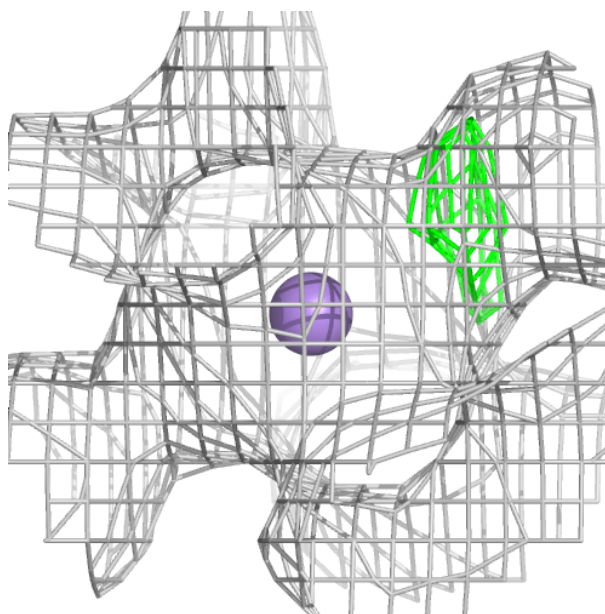
## 6.4 Ligands ⓘ

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

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.

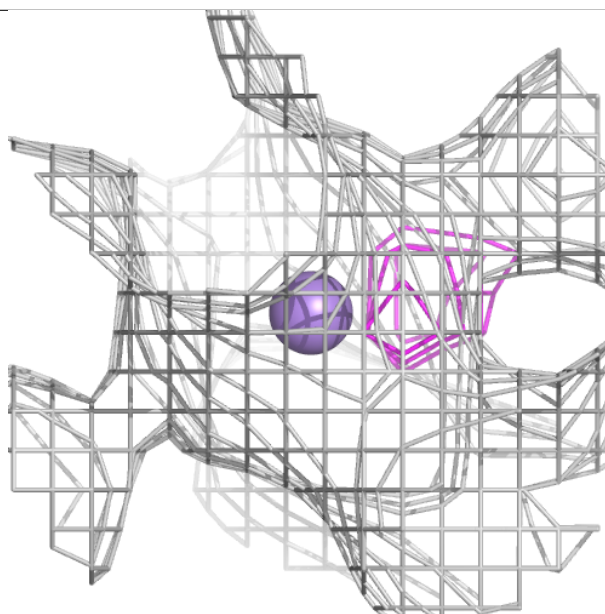
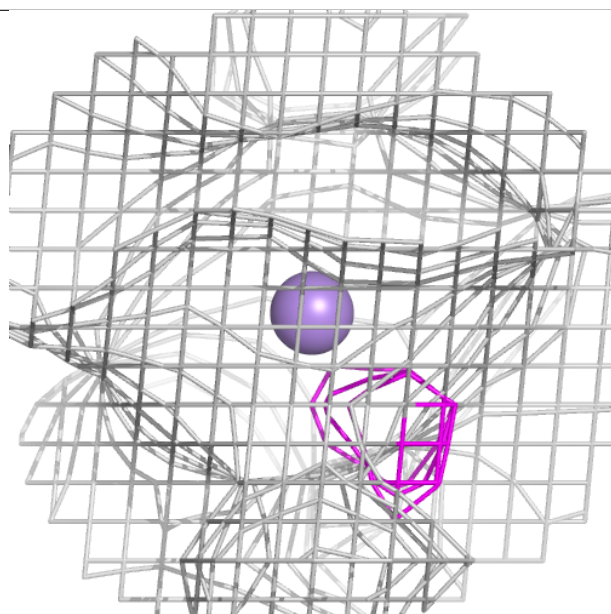
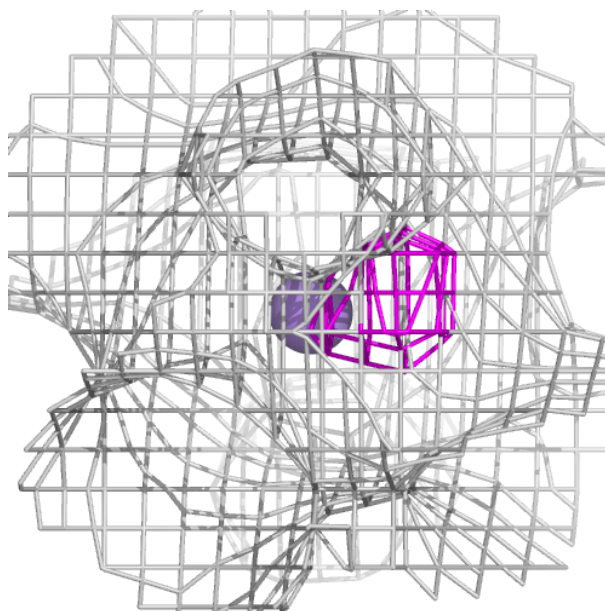
**Electron density around MN A 401:**

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



**Electron density around MN B 401:**

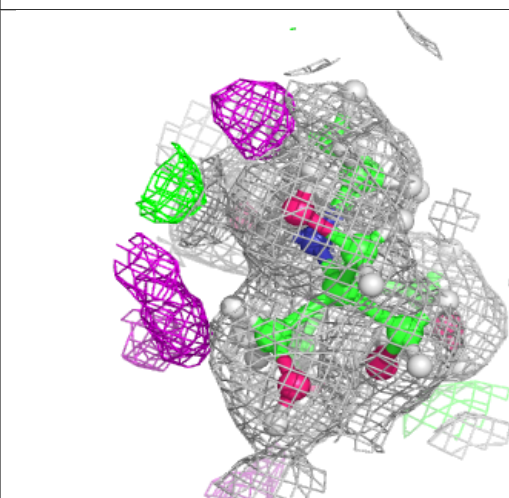
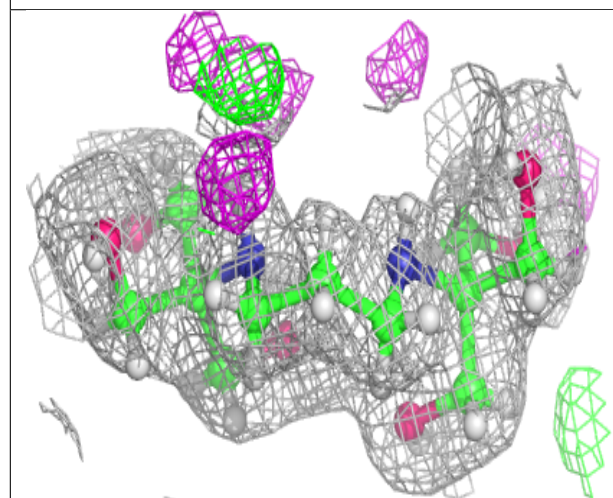
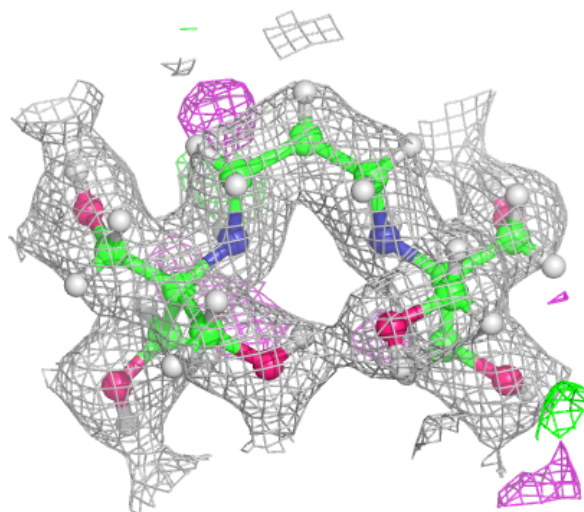
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





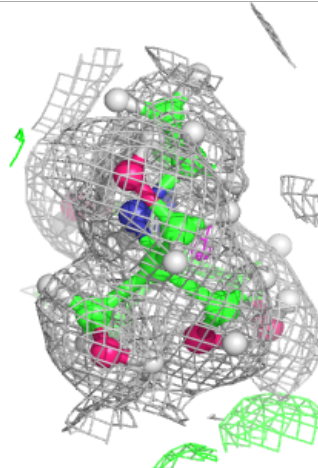
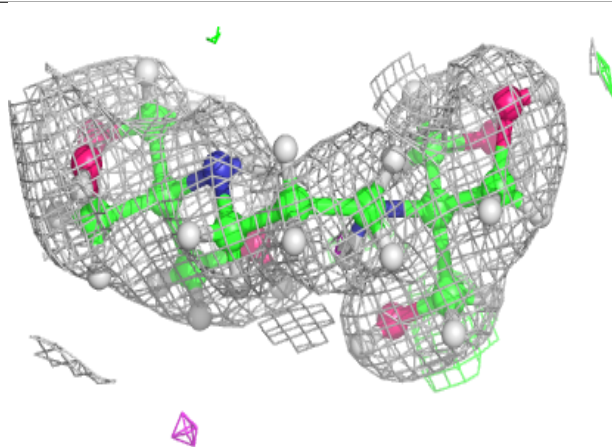
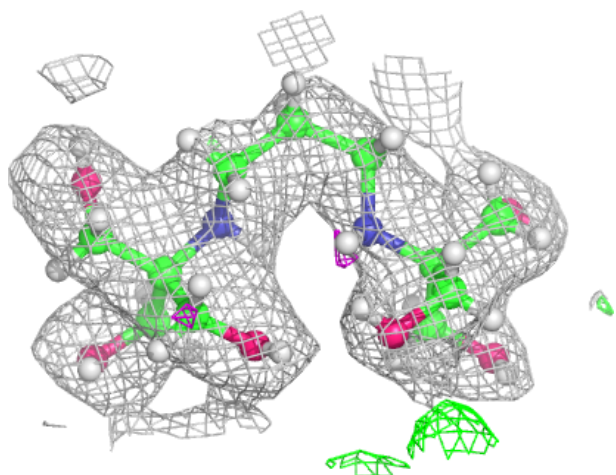
**Electron density around B3P A 402:**

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



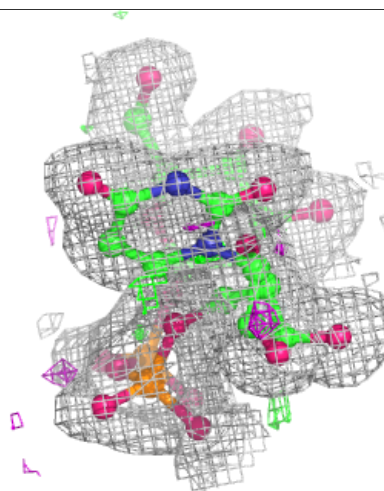
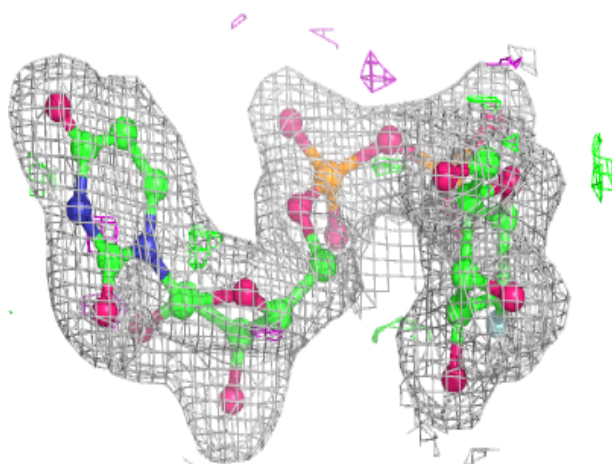
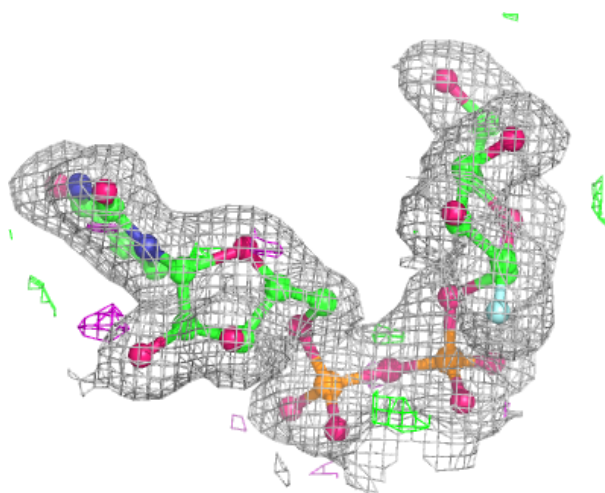
**Electron density around B3P B 402:**

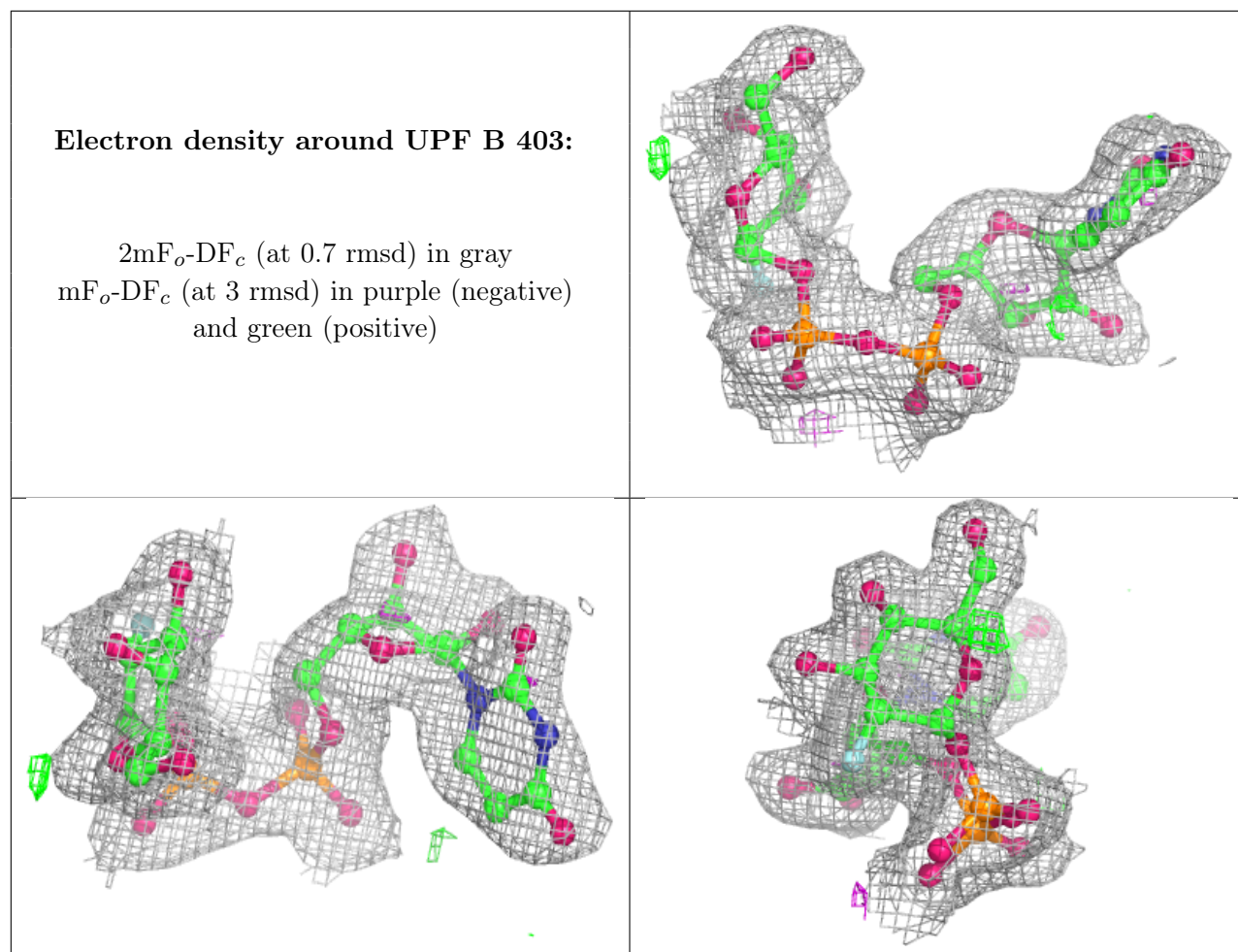
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UPF A 403:**

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





## 6.5 Other polymers [i](#)

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