



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2025 – 10:20 AM EDT

PDB ID : 9DS2  
Title : Crystal structure of 346-54 Fab in complex with H1 HA from A/California/04/2009(H1N1)  
Authors : Lin, T.H.; Wilson, I.A.  
Deposited on : 2024-09-26  
Resolution : 3.29 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 : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

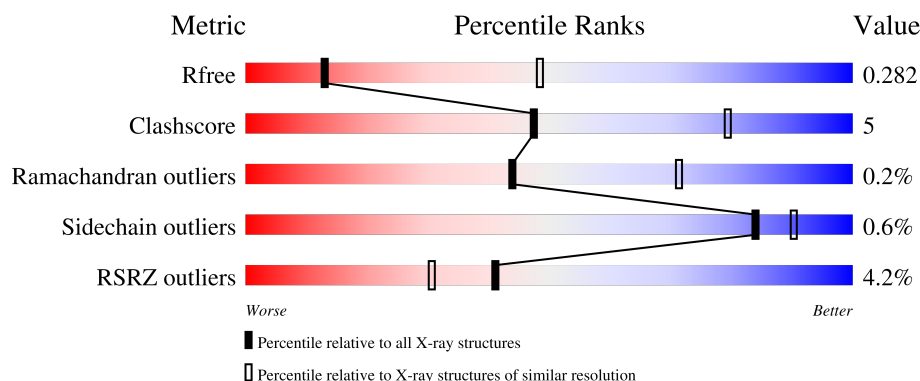
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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.










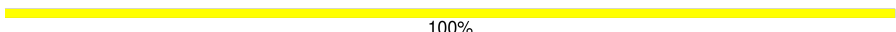
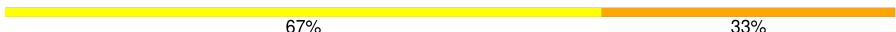
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	328	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
1	C	328	<div> <div>2%</div> <div>86%</div> <div>14%</div> </div>
1	E	328	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>..</div> </div>
2	B	175	<div> <div>%</div> <div>88%</div> <div>12%</div> </div>
2	D	175	<div> <div>%</div> <div>89%</div> <div>11%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	175	
3	G	229	
3	H	229	
3	K	229	
4	I	215	
4	J	215	
4	L	215	
5	M	2	
6	N	3	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21985 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	328	Total	C	N	O	S	0	0	0
			2559	1618	441	489	11			
1	A	328	Total	C	N	O	S	0	0	0
			2559	1618	441	489	11			
1	E	326	Total	C	N	O	S	0	0	0
			2542	1607	438	486	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	expression tag	UNP A0A5B9ZSV0
C	9	PRO	-	expression tag	UNP A0A5B9ZSV0
C	10	GLY	-	expression tag	UNP A0A5B9ZSV0
C	186	SER	UNK	conflict	UNP A0A5B9ZSV0
C	206	GLY	SER	conflict	UNP A0A5B9ZSV0
A	8	ASP	-	expression tag	UNP A0A5B9ZSV0
A	9	PRO	-	expression tag	UNP A0A5B9ZSV0
A	10	GLY	-	expression tag	UNP A0A5B9ZSV0
A	186	SER	UNK	conflict	UNP A0A5B9ZSV0
A	206	GLY	SER	conflict	UNP A0A5B9ZSV0
E	8	ASP	-	expression tag	UNP A0A5B9ZSV0
E	9	PRO	-	expression tag	UNP A0A5B9ZSV0
E	10	GLY	-	expression tag	UNP A0A5B9ZSV0
E	186	SER	UNK	conflict	UNP A0A5B9ZSV0
E	206	GLY	SER	conflict	UNP A0A5B9ZSV0

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			
2	F	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	175	SER	-	expression tag	UNP A0A6J3XB93
B	175	SER	-	expression tag	UNP A0A6J3XB93
F	175	SER	-	expression tag	UNP A0A6J3XB93

- Molecule 3 is a protein called 346-54, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	227	Total	C	N	O	S	0	0	0
			1673	1061	285	320	7			
3	H	227	Total	C	N	O	S	0	0	0
			1673	1061	285	320	7			
3	K	227	Total	C	N	O	S	0	0	0
			1673	1061	285	320	7			

- Molecule 4 is a protein called 346-54, Light chain.

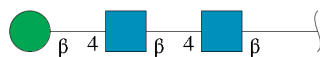
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	214	Total	C	N	O	S	0	0	0
			1641	1027	281	328	5			
4	J	214	Total	C	N	O	S	0	0	0
			1641	1027	281	328	5			
4	L	214	Total	C	N	O	S	0	0	0
			1641	1027	281	328	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



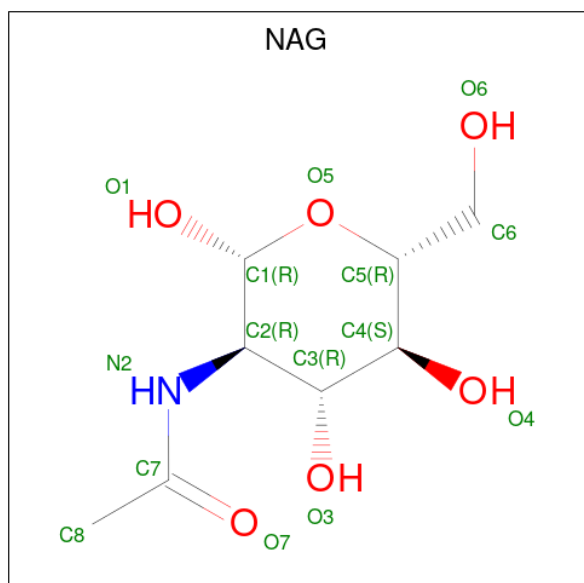
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).

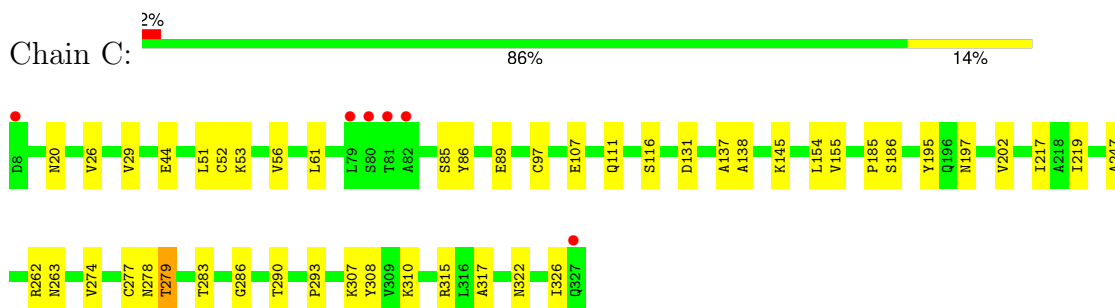


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		

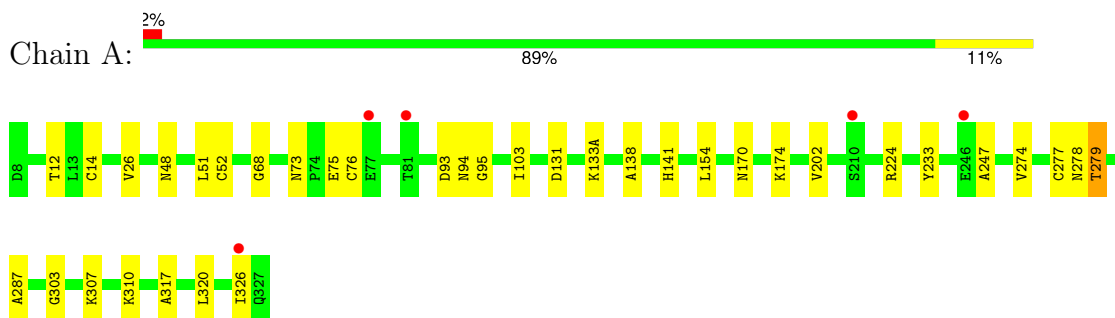
### 3 Residue-property plots [i](#)

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

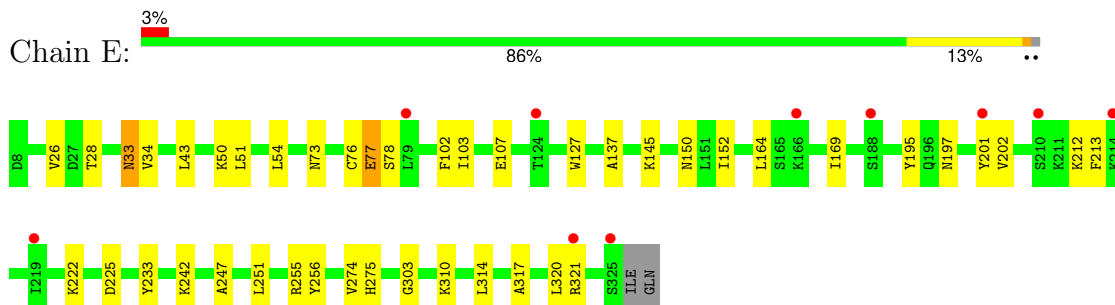
- Molecule 1: Hemagglutinin HA1 chain



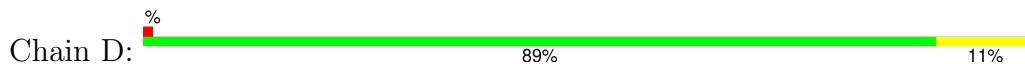
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

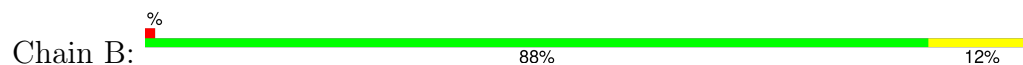


- Molecule 2: Hemagglutinin HA2 chain

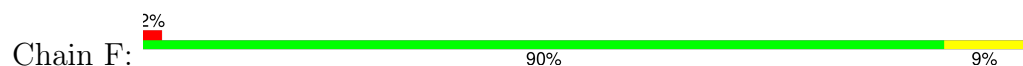




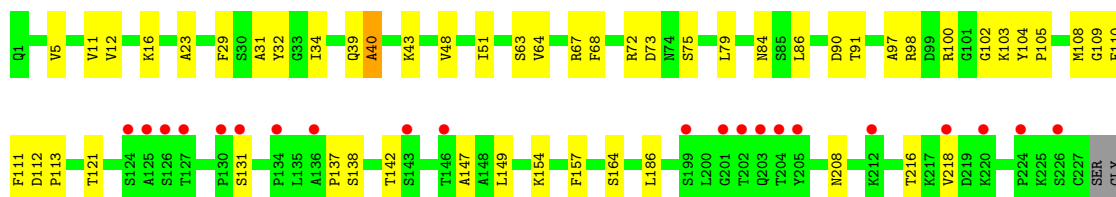
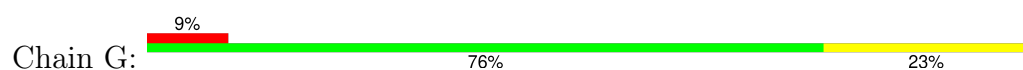
- Molecule 2: Hemagglutinin HA2 chain



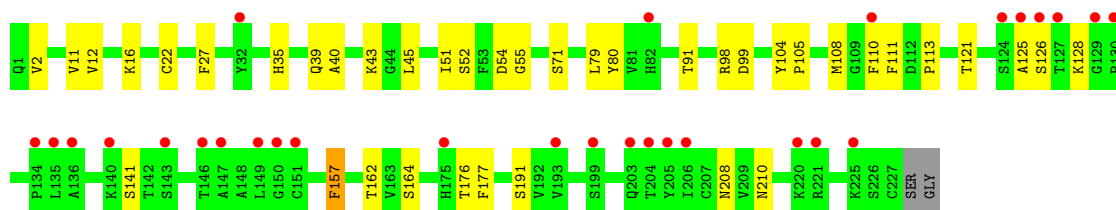
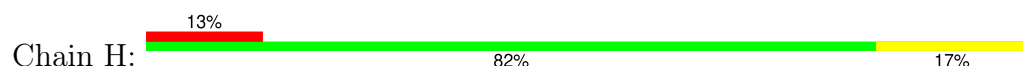
- Molecule 2: Hemagglutinin HA2 chain



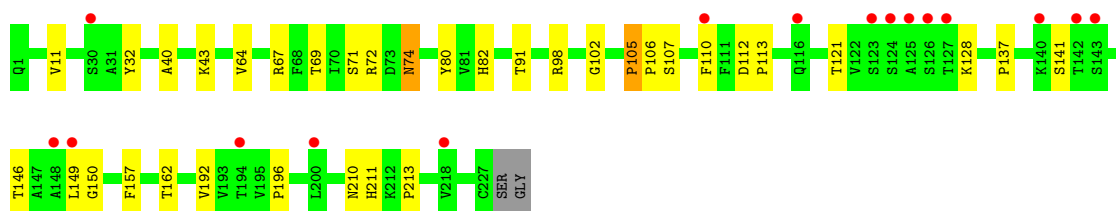
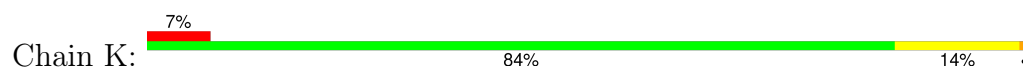
- Molecule 3: 346-54, Heavy chain



- Molecule 3: 346-54, Heavy chain

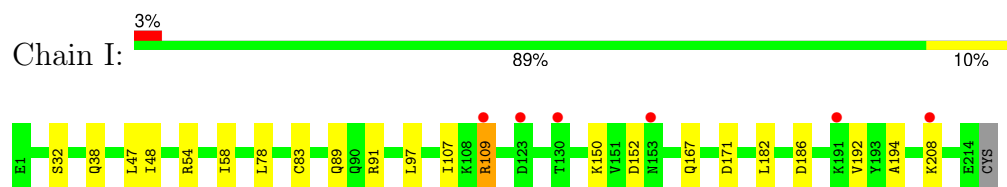


- Molecule 3: 346-54, Heavy chain

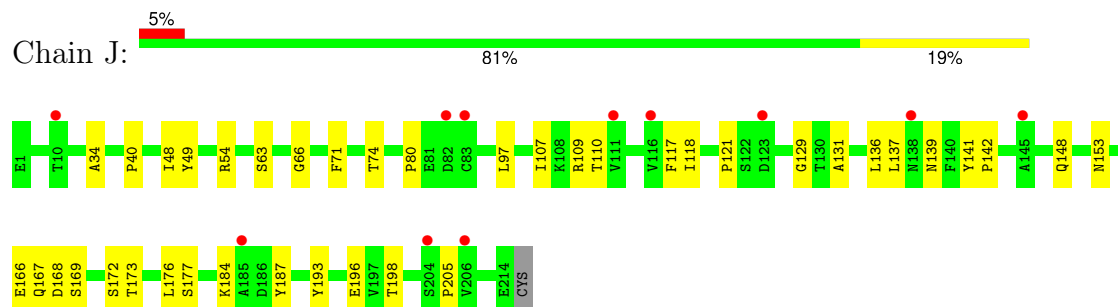




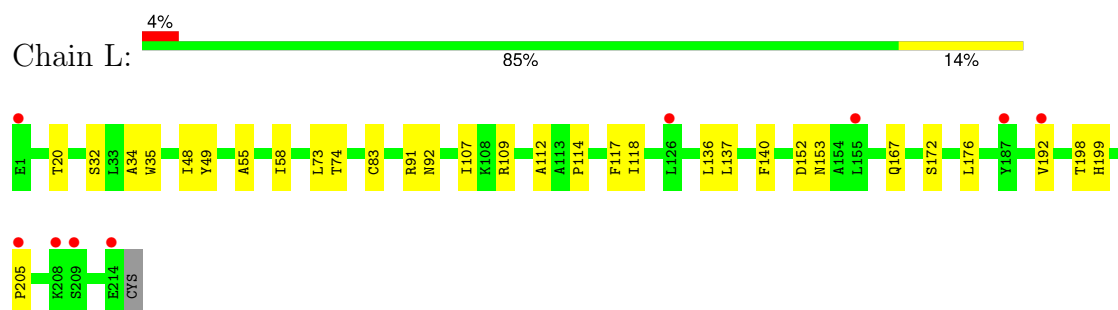
- Molecule 4: 346-54, Light chain



- Molecule 4: 346-54, Light chain



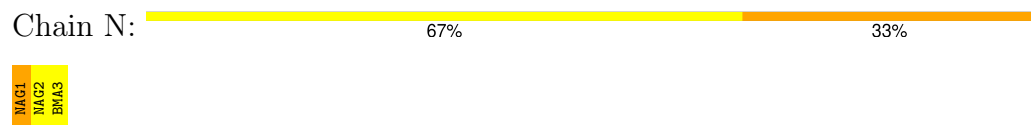
- Molecule 4: 346-54, Light chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.82Å 313.10Å 325.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.82 – 3.29 47.82 – 3.29	Depositor EDS
% Data completeness (in resolution range)	93.8 (47.82-3.29) 96.4 (47.82-3.29)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, $R_{free}$	0.244 , 0.279 0.247 , 0.282	Depositor DCC
$R_{free}$ test set	6181 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.1	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 71.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.034 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: BMA, NAG

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	0.24	0/2624	0.47	0/3567
1	C	0.26	0/2624	0.50	0/3567
1	E	0.24	0/2607	0.47	0/3544
2	B	0.24	0/1434	0.41	0/1932
2	D	0.24	0/1434	0.42	0/1932
2	F	0.24	0/1434	0.42	0/1932
3	G	0.25	0/1717	0.49	0/2338
3	H	0.25	0/1717	0.50	0/2338
3	K	0.25	0/1717	0.49	0/2338
4	I	0.25	0/1678	0.49	0/2283
4	J	0.24	0/1678	0.48	0/2283
4	L	0.24	0/1678	0.48	0/2283
All	All	0.25	0/22342	0.47	0/30337

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	2559	0	2507	26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2559	0	2504	34	0
1	E	2542	0	2487	28	0
2	B	1406	0	1325	16	0
2	D	1406	0	1325	16	0
2	F	1406	0	1325	14	0
3	G	1673	0	1608	36	0
3	H	1673	0	1610	25	0
3	K	1673	0	1608	24	0
4	I	1641	0	1599	15	0
4	J	1641	0	1599	23	0
4	L	1641	0	1599	19	0
5	M	28	0	25	0	0
6	N	39	0	34	2	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	C	28	0	26	0	0
7	D	14	0	13	0	0
7	E	14	0	13	0	0
7	F	14	0	13	1	0
All	All	21985	0	21246	237	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 237 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:278:ASN:O	1:A:279:THR:HG22	1.78	0.82
1:C:278:ASN:O	1:C:279:THR:HG22	1.79	0.82
3:H:91:THR:HG23	3:H:121:THR:HA	1.72	0.72
3:H:128:LYS:HB3	3:H:157:PHE:H	1.57	0.70
1:E:321:ARG:HH22	2:F:1:GLY:HA3	1.56	0.70

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	326/328 (99%)	308 (94%)	17 (5%)	1 (0%)	37	66
1	C	326/328 (99%)	310 (95%)	15 (5%)	1 (0%)	37	66
1	E	324/328 (99%)	309 (95%)	12 (4%)	3 (1%)	14	44
2	B	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
2	D	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
2	F	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
3	G	225/229 (98%)	212 (94%)	12 (5%)	1 (0%)	30	61
3	H	225/229 (98%)	209 (93%)	16 (7%)	0	100	100
3	K	225/229 (98%)	213 (95%)	12 (5%)	0	100	100
4	I	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
4	J	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
4	L	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	2806/2841 (99%)	2681 (96%)	119 (4%)	6 (0%)	44	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	THR
1	C	279	THR
1	E	33	ASN
1	E	34	VAL
1	E	77	GLU

### 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	287/287 (100%)	286 (100%)	1 (0%)	91	94
1	C	287/287 (100%)	287 (100%)	0	100	100
1	E	285/287 (99%)	284 (100%)	1 (0%)	89	93
2	B	150/150 (100%)	148 (99%)	2 (1%)	65	79
2	D	150/150 (100%)	149 (99%)	1 (1%)	81	88
2	F	150/150 (100%)	149 (99%)	1 (1%)	81	88
3	G	180/190 (95%)	180 (100%)	0	100	100
3	H	180/190 (95%)	179 (99%)	1 (1%)	84	90
3	K	180/190 (95%)	178 (99%)	2 (1%)	70	82
4	I	185/187 (99%)	182 (98%)	3 (2%)	58	76
4	J	185/187 (99%)	184 (100%)	1 (0%)	86	91
4	L	185/187 (99%)	184 (100%)	1 (0%)	86	91
All	All	2404/2442 (98%)	2390 (99%)	14 (1%)	84	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	186	ASP
4	I	208	LYS
4	L	153	ASN
3	K	74	ASN
3	K	105	PRO

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

Mol	Chain	Res	Type
2	B	79	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 ⓘ

5 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$
5	NAG	M	1	5,1	14,14,15	0.65	0	17,19,21	2.23	5 (29%)
5	NAG	M	2	5	14,14,15	0.71	0	17,19,21	1.16	2 (11%)
6	NAG	N	1	6,1	14,14,15	0.68	0	17,19,21	1.54	3 (17%)
6	NAG	N	2	6	14,14,15	0.67	0	17,19,21	1.57	3 (17%)
6	BMA	N	3	6	11,11,12	0.84	0	15,15,17	1.40	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
5	NAG	M	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	3/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C2-N2-C7	6.14	131.13	122.90
6	N	1	NAG	C1-O5-C5	4.09	117.67	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C1-O5-C5	4.03	117.59	112.19
6	N	2	NAG	C2-N2-C7	3.86	128.07	122.90
6	N	3	BMA	C1-O5-C5	3.27	116.58	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C3-C2-N2-C7
6	N	2	NAG	C1-C2-N2-C7
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	M	2	NAG	O5-C5-C6-O6

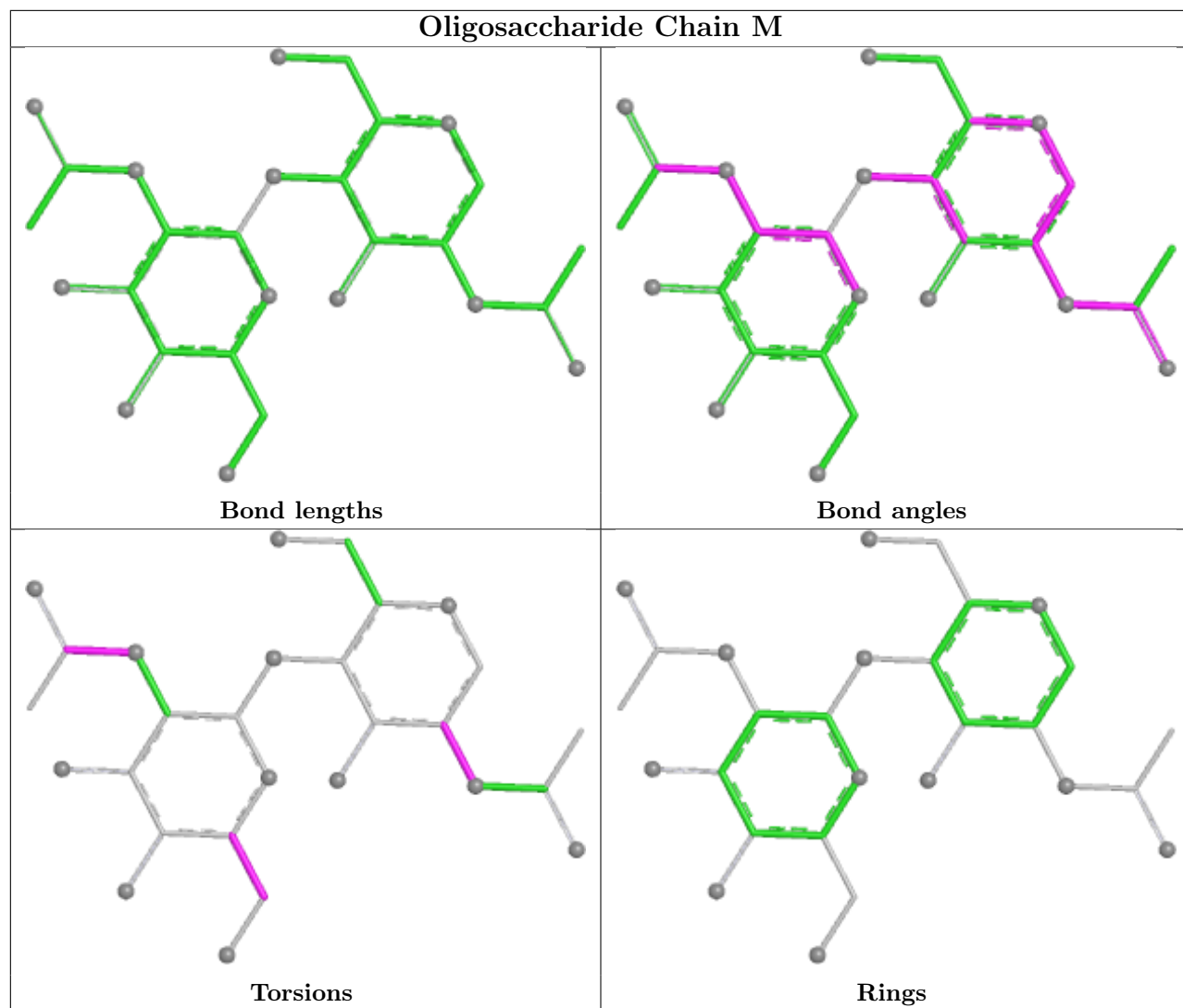
There are no ring outliers.

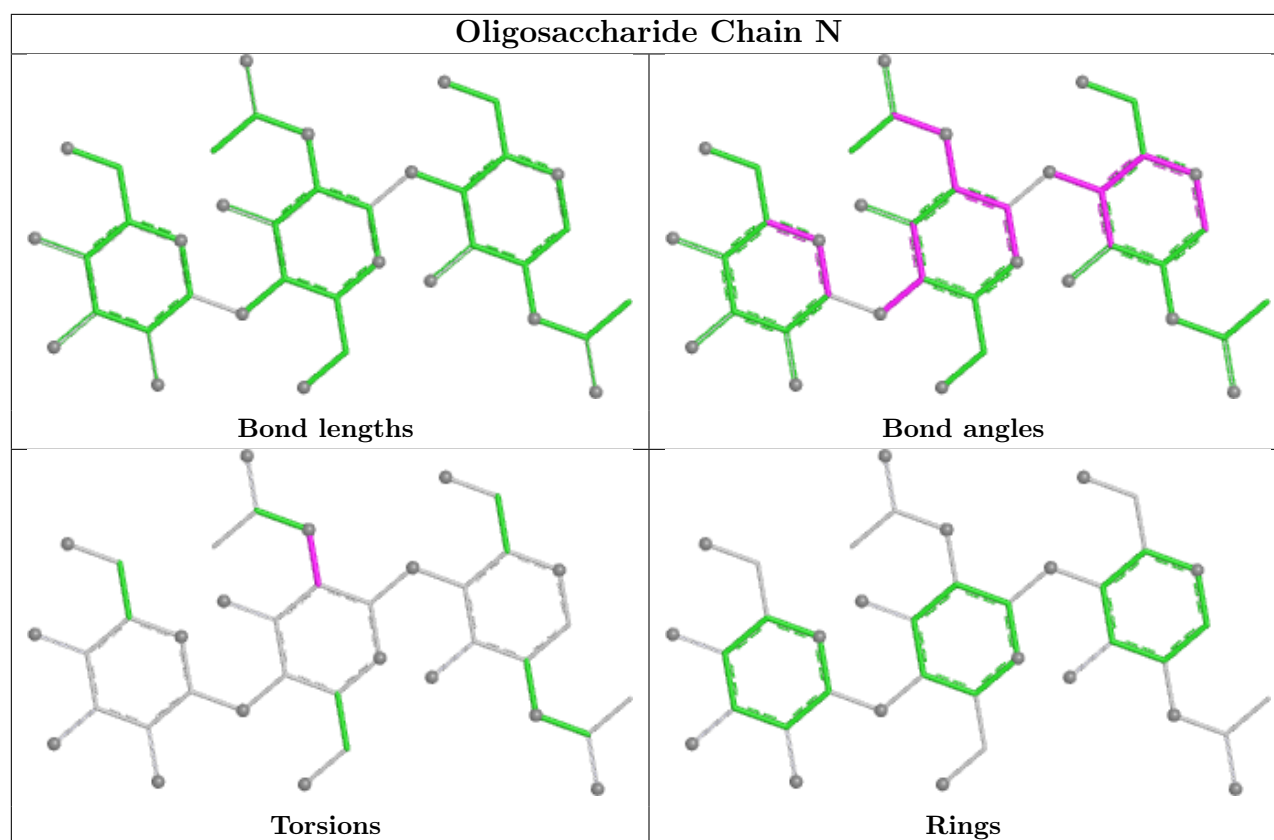
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	1	NAG	2	0

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







## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	C	401	1	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
7	NAG	B	201	2	14,14,15	0.72	0	17,19,21	0.84	0
7	NAG	D	201	2	14,14,15	0.69	0	17,19,21	1.26	1 (5%)
7	NAG	E	401	1	14,14,15	0.70	0	17,19,21	1.00	1 (5%)
7	NAG	F	201	2	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
7	NAG	C	402	1	14,14,15	0.73	0	17,19,21	0.87	0
7	NAG	A	401	1	14,14,15	0.67	0	17,19,21	0.85	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	NAG	C	401	1	-	0/6/23/26	0/1/1/1
7	NAG	B	201	2	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2	-	2/6/23/26	0/1/1/1
7	NAG	E	401	1	-	2/6/23/26	0/1/1/1
7	NAG	F	201	2	-	0/6/23/26	0/1/1/1
7	NAG	C	402	1	-	1/6/23/26	0/1/1/1
7	NAG	A	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	201	NAG	C2-N2-C7	3.41	127.47	122.90
7	E	401	NAG	C1-O5-C5	2.49	115.52	112.19
7	C	401	NAG	O5-C1-C2	-2.24	107.83	111.29
7	F	201	NAG	O5-C1-C2	-2.09	108.06	111.29

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	NAG	C8-C7-N2-C2
7	A	401	NAG	O7-C7-N2-C2
7	E	401	NAG	C8-C7-N2-C2
7	E	401	NAG	O7-C7-N2-C2
7	C	402	NAG	O5-C5-C6-O6

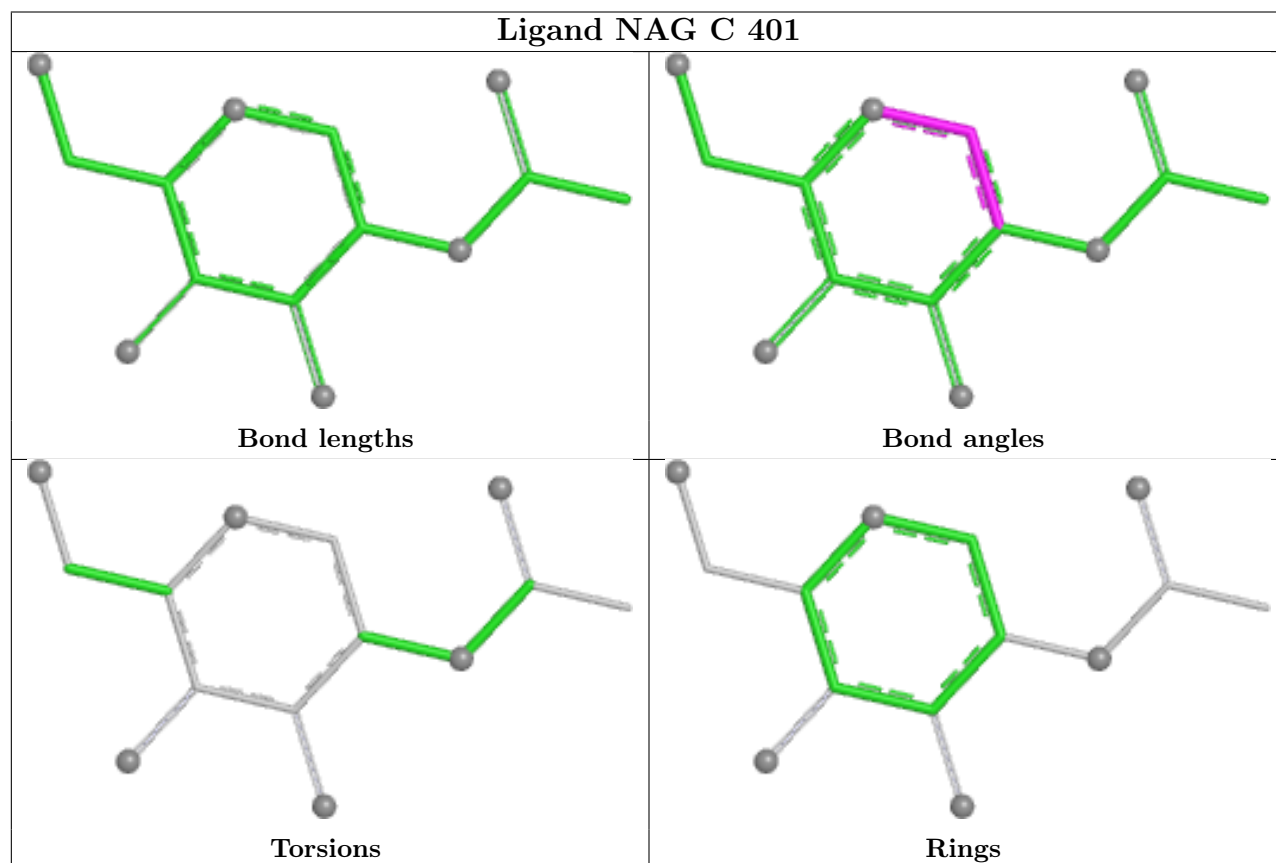
There are no ring outliers.

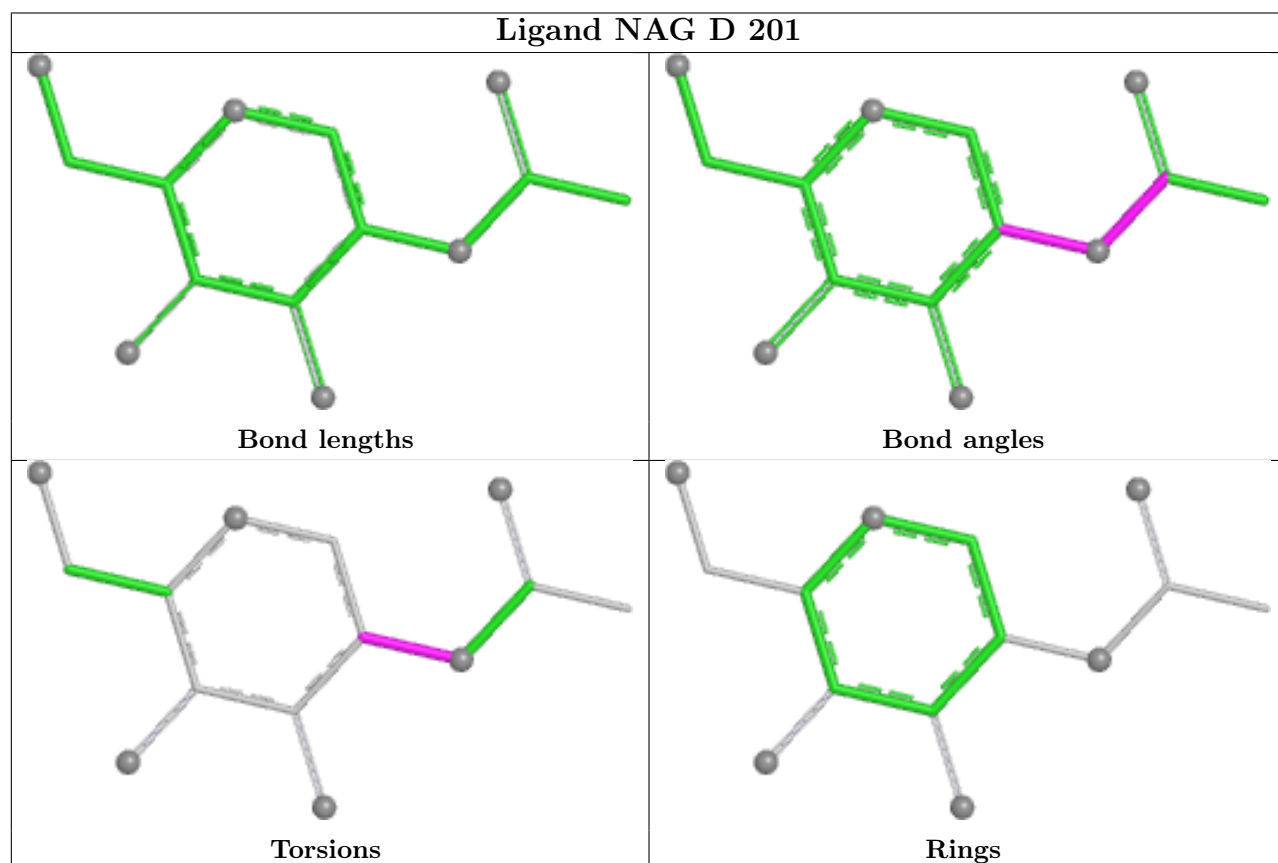
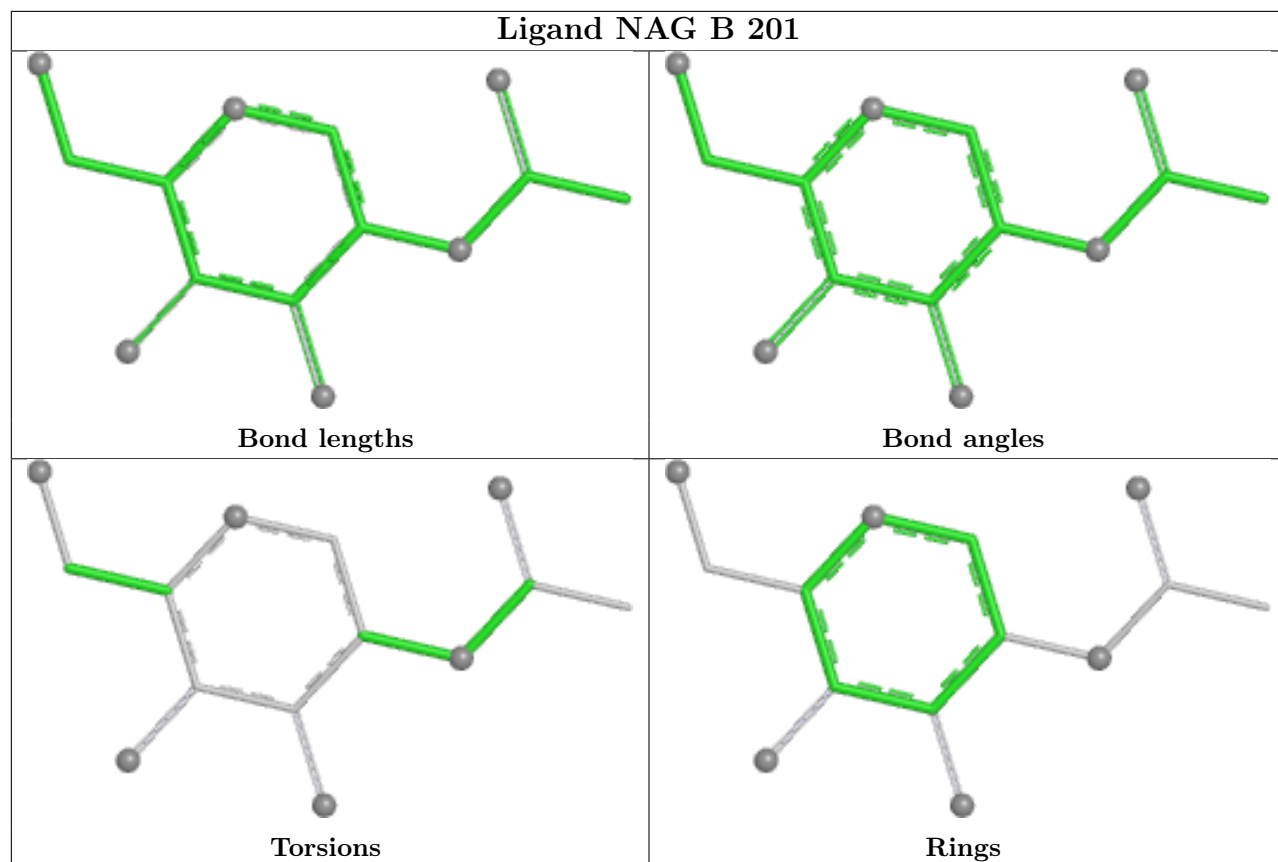
1 monomer is involved in 1 short contact:

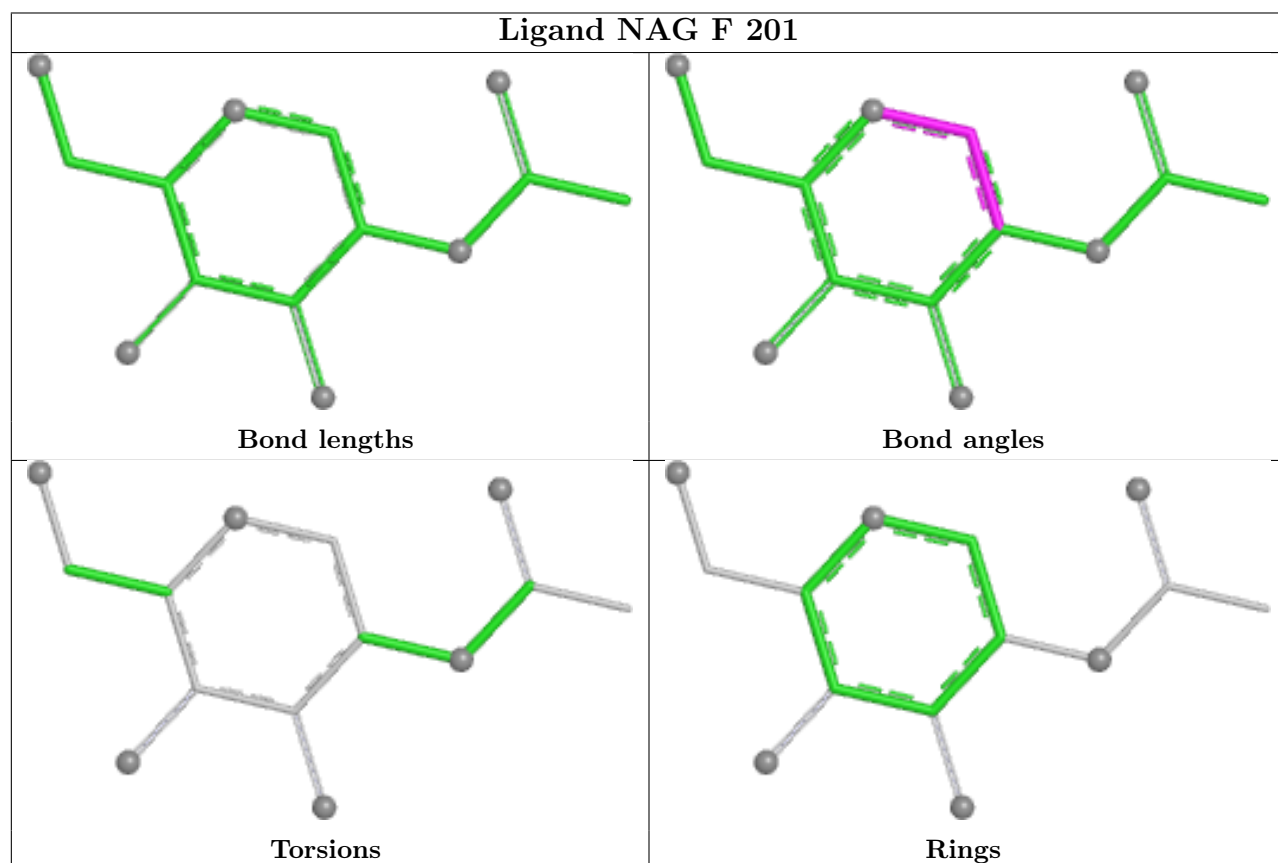
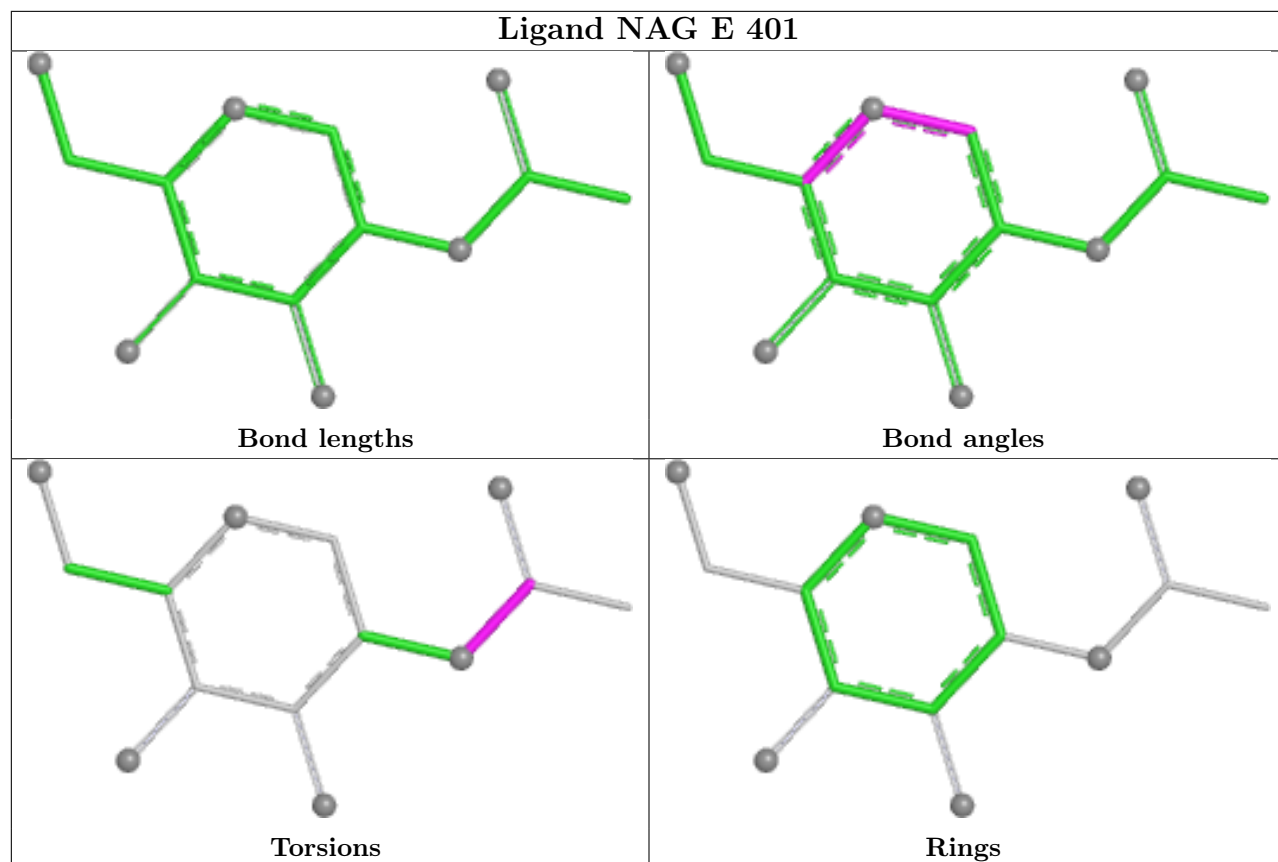
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	201	NAG	1	0

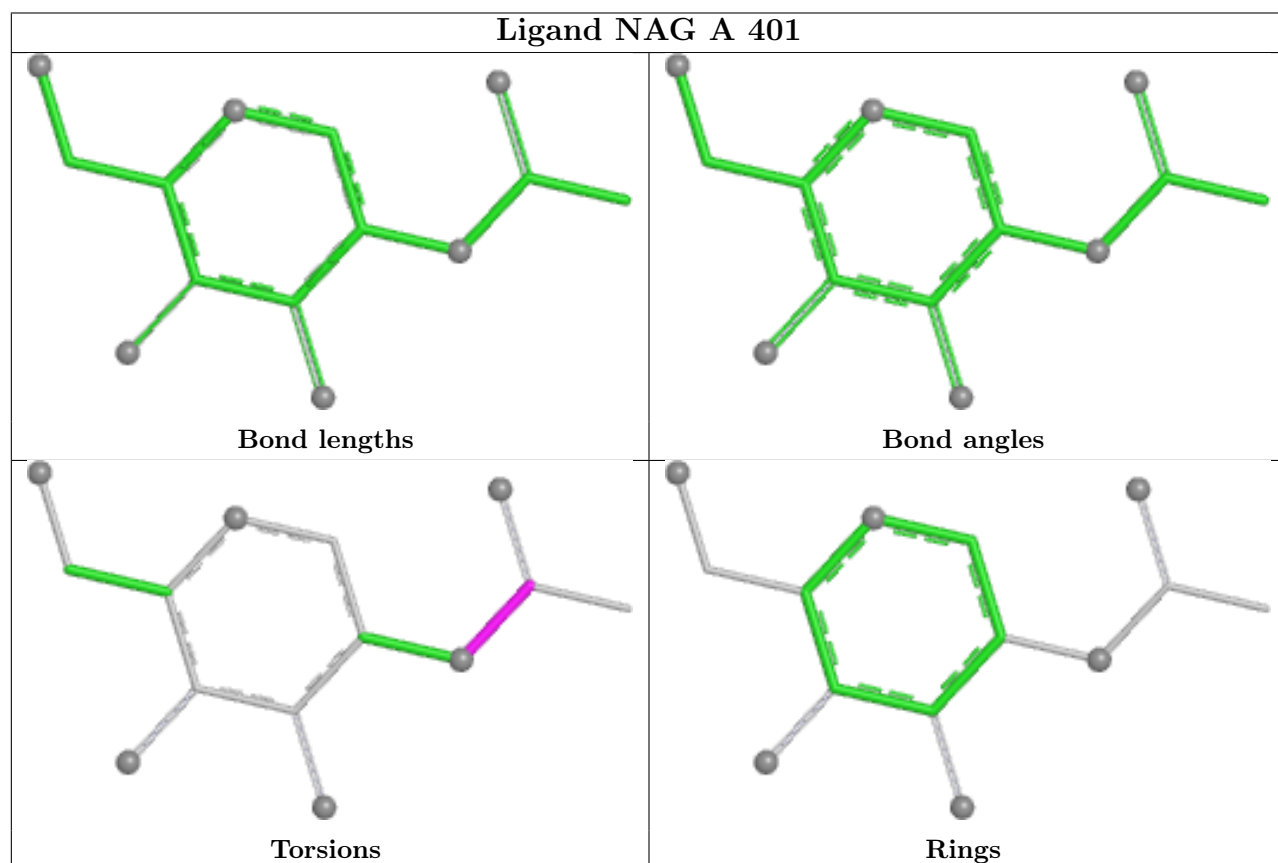
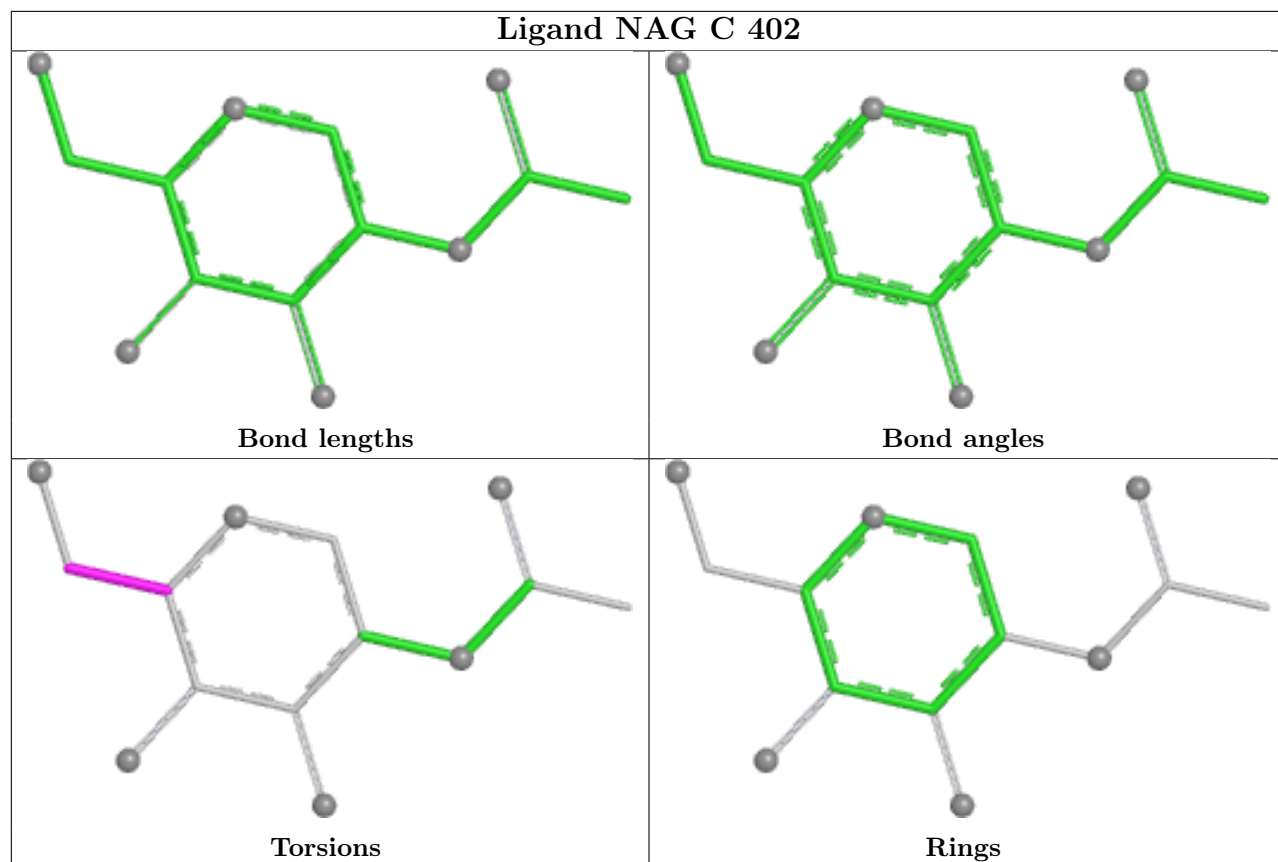
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	328/328 (100%)	0.05	5 (1%) 71 58	61, 108, 140, 176	0
1	C	328/328 (100%)	-0.07	6 (1%) 67 53	63, 90, 120, 176	0
1	E	326/328 (99%)	0.17	10 (3%) 51 38	72, 122, 154, 167	0
2	B	175/175 (100%)	-0.17	2 (1%) 77 66	53, 85, 127, 168	0
2	D	175/175 (100%)	-0.12	1 (0%) 85 78	57, 82, 119, 160	0
2	F	175/175 (100%)	-0.02	3 (1%) 69 55	65, 90, 122, 169	0
3	G	227/229 (99%)	0.57	21 (9%) 16 15	66, 98, 141, 170	0
3	H	227/229 (99%)	0.69	29 (12%) 9 9	70, 112, 172, 193	0
3	K	227/229 (99%)	0.57	16 (7%) 24 20	80, 124, 185, 193	0
4	I	214/215 (99%)	0.21	6 (2%) 55 40	66, 88, 134, 159	0
4	J	214/215 (99%)	0.58	11 (5%) 34 27	77, 128, 148, 156	0
4	L	214/215 (99%)	0.32	9 (4%) 41 31	81, 122, 180, 191	0
All	All	2830/2841 (99%)	0.23	119 (4%) 41 31	53, 104, 163, 193	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	125	ALA	5.4
3	H	127	THR	5.1
3	K	127	THR	5.0
3	H	126	SER	4.9
3	G	126	SER	4.6

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

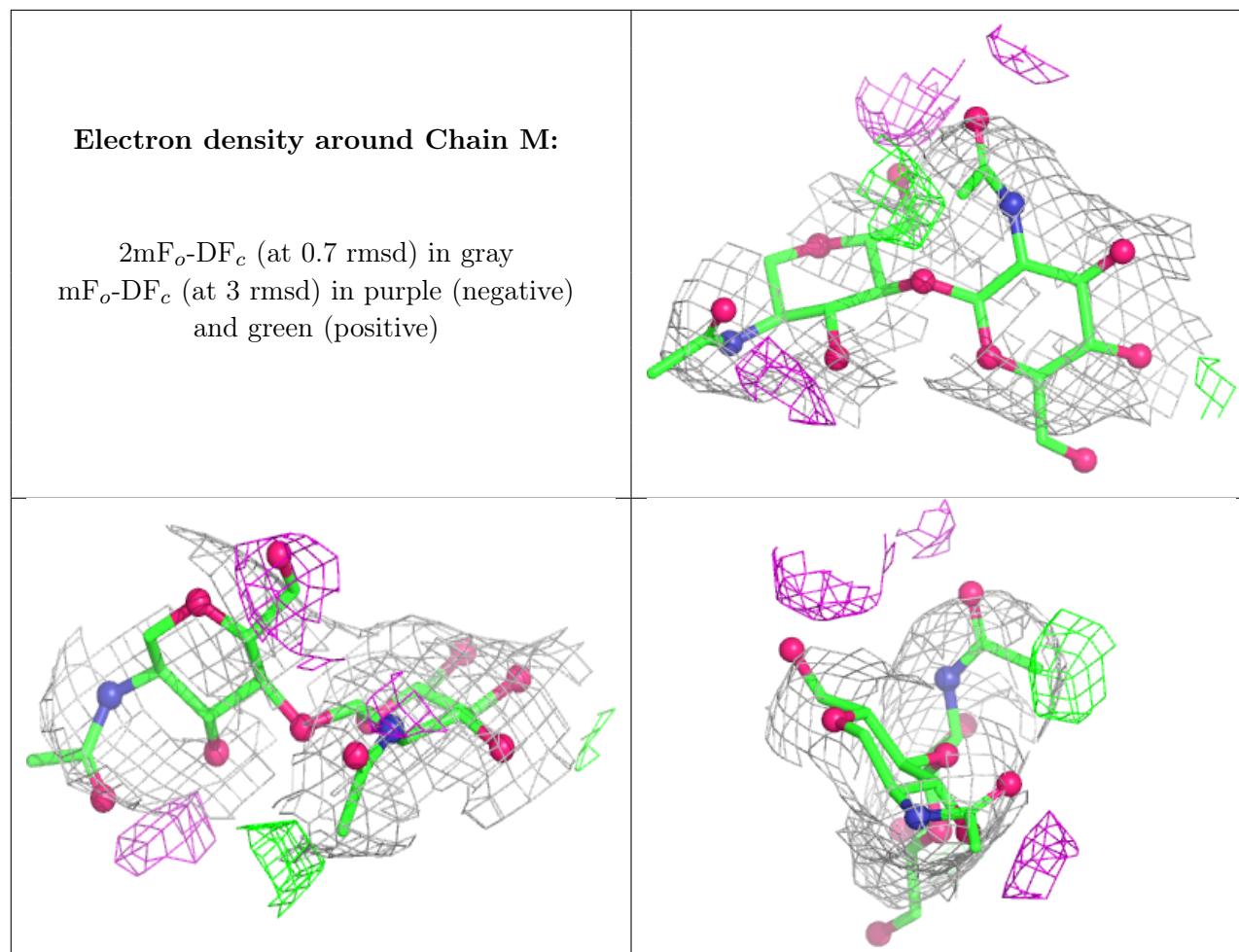
There are no non-standard protein/DNA/RNA residues in this entry.

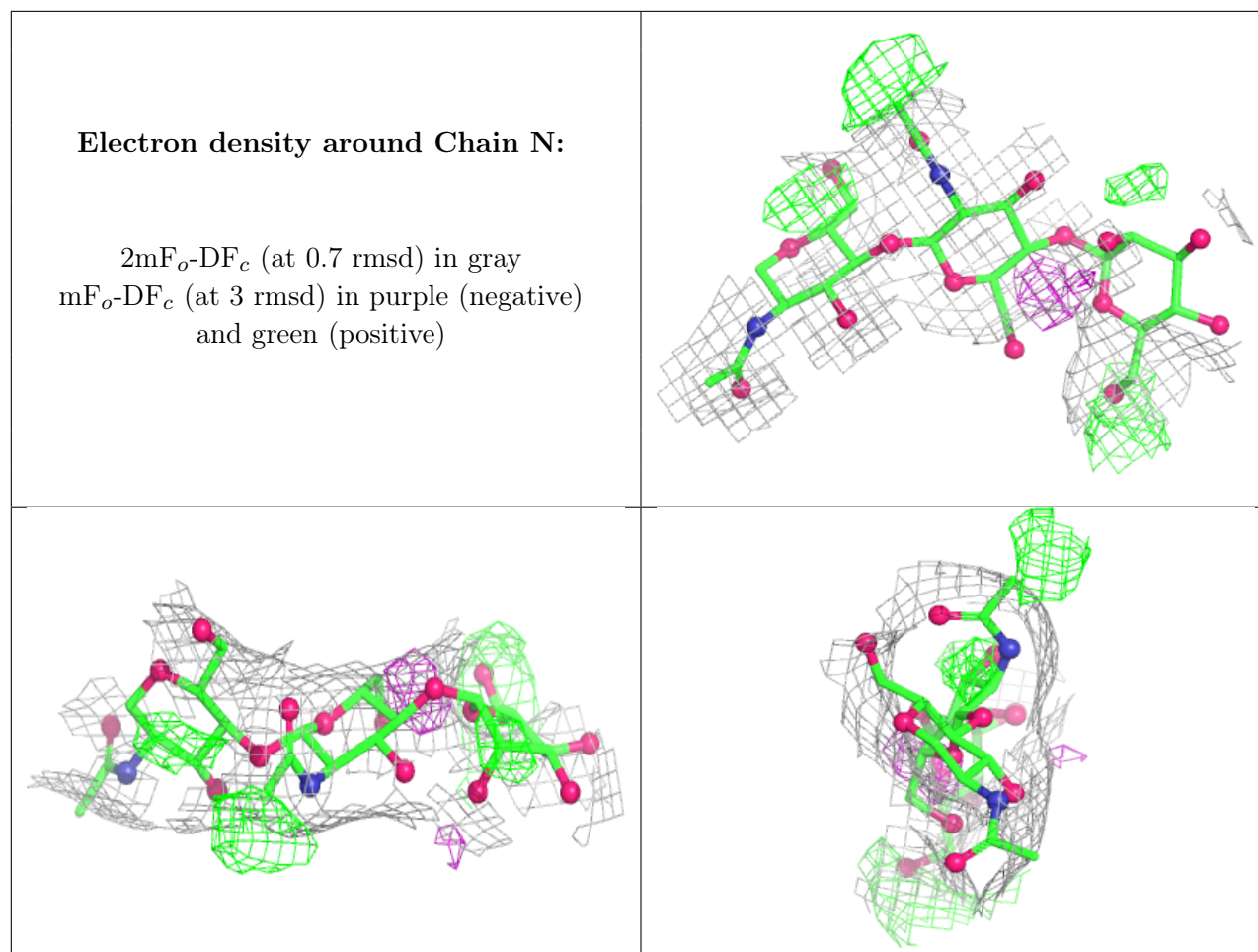
### 6.3 Carbohydrates [i](#)

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
6	BMA	N	3	11/12	0.43	0.18	114,146,172,182	0
5	NAG	M	2	14/15	0.56	0.15	115,141,157,166	0
6	NAG	N	2	14/15	0.71	0.16	121,137,172,176	0
5	NAG	M	1	14/15	0.81	0.14	119,142,151,152	0
6	NAG	N	1	14/15	0.89	0.11	98,118,139,152	0

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.





## 6.4 Ligands ⓘ

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

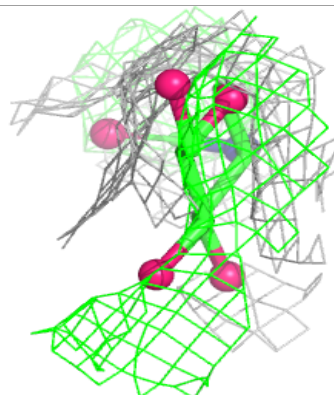
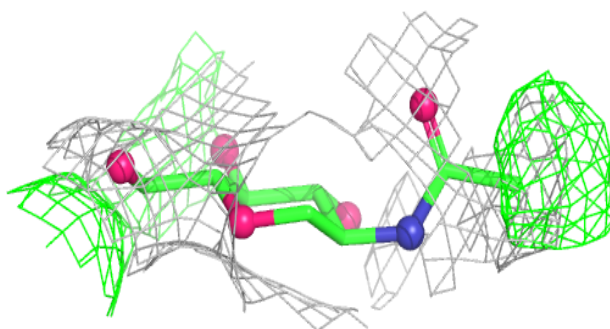
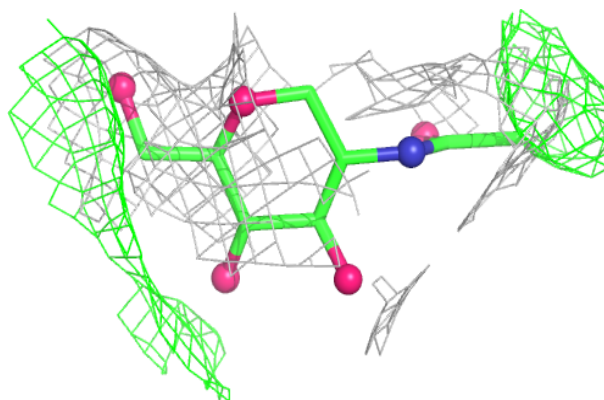
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	D	201	14/15	0.24	0.19	117,151,160,162	0
7	NAG	E	401	14/15	0.44	0.18	127,135,153,159	0
7	NAG	A	401	14/15	0.68	0.11	110,140,148,149	0
7	NAG	C	401	14/15	0.68	0.15	118,159,175,175	0
7	NAG	F	201	14/15	0.71	0.15	96,126,146,151	0
7	NAG	B	201	14/15	0.75	0.15	121,137,156,157	0
7	NAG	C	402	14/15	0.80	0.11	106,123,133,136	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

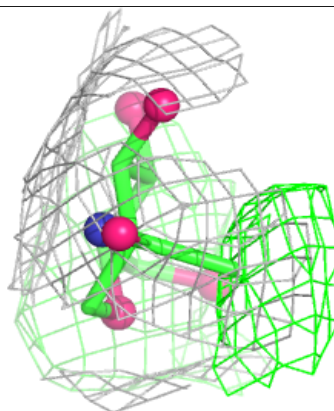
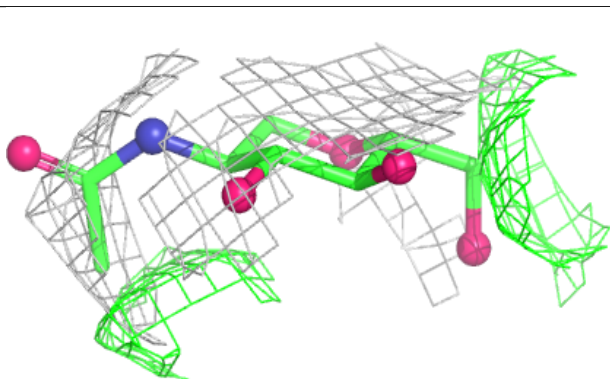
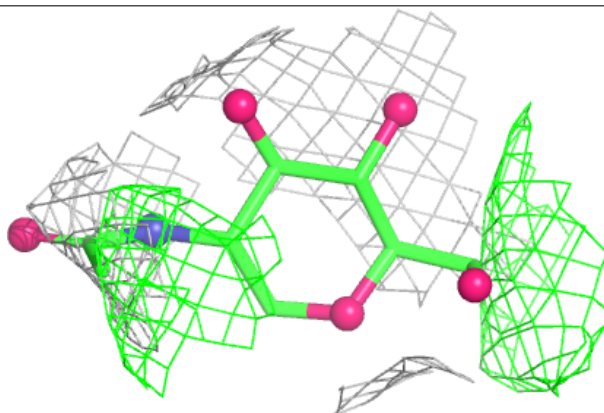
**Electron density around NAG D 201:**

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



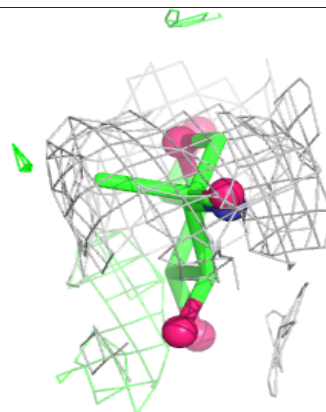
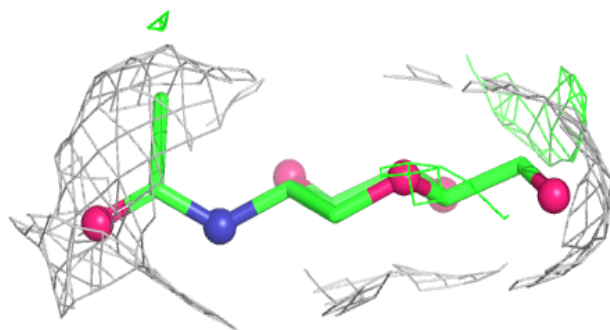
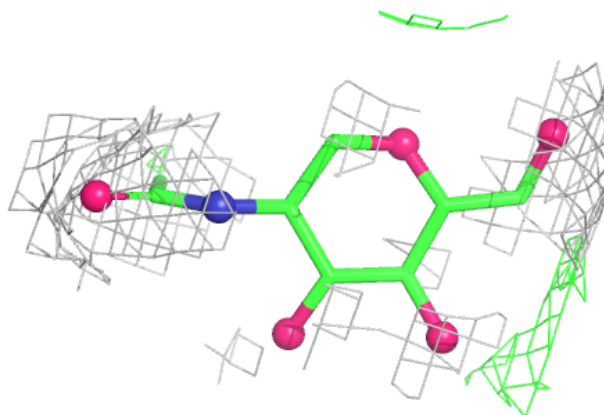
**Electron density around NAG E 401:**

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

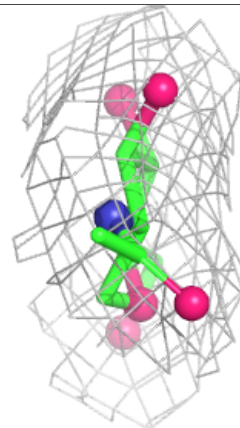
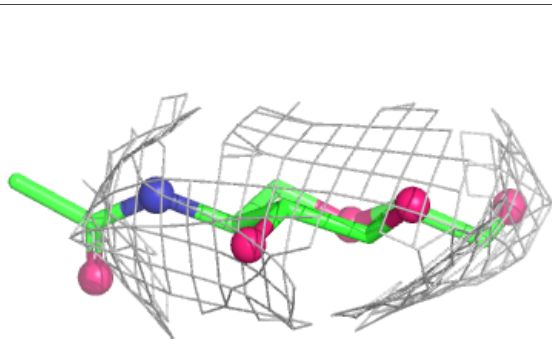
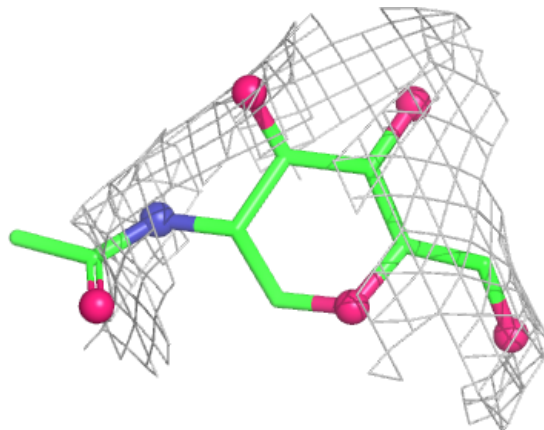


**Electron density around NAG A 401:**

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

**Electron density around NAG C 401:**

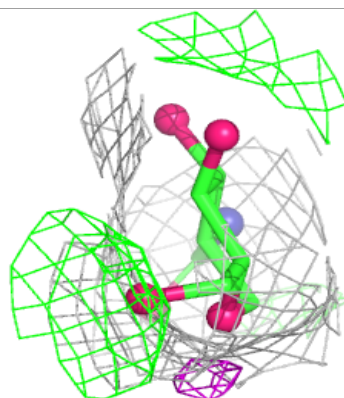
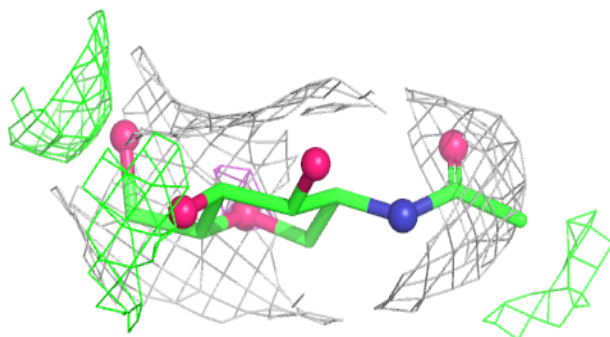
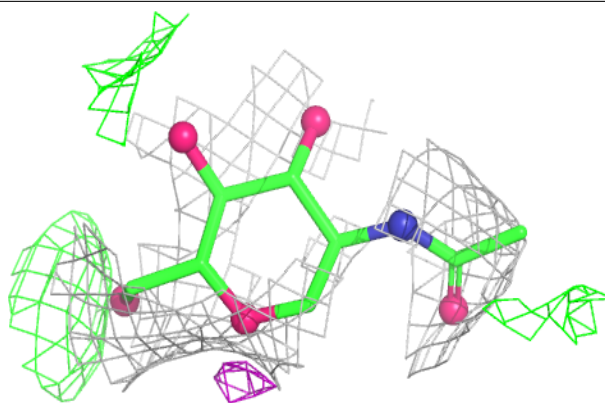
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



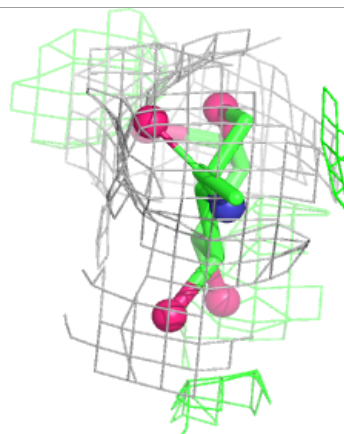
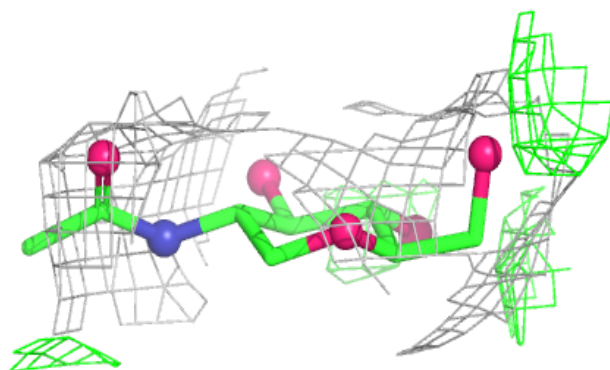
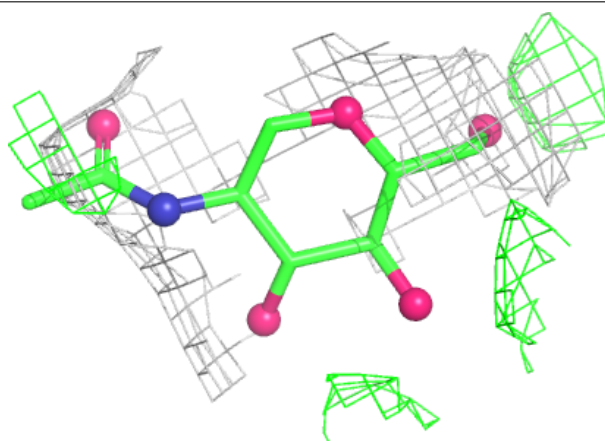


**Electron density around NAG F 201:**

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

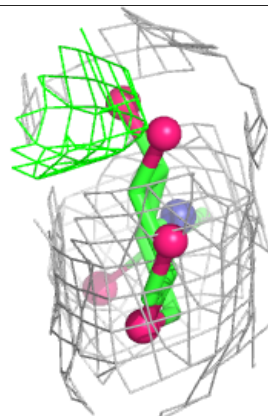
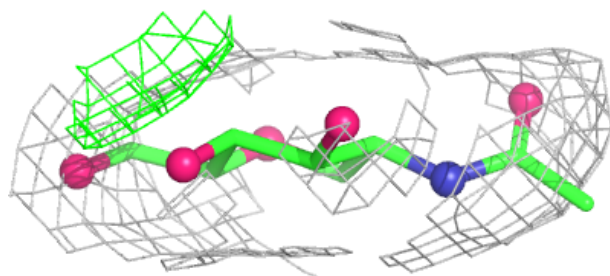
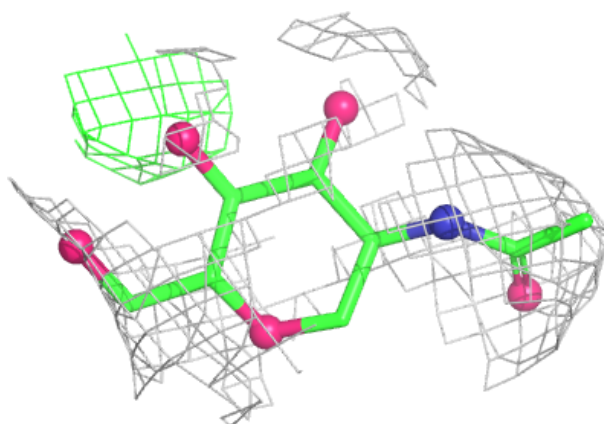
**Electron density around NAG B 201:**

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



**Electron density around NAG C 402:**

$2mF_o-DF_c$  (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.