



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2025 – 12:24 AM JST

PDB ID : 8X2D / pdb\_00008x2d  
Title : Crystal structure of H5 hemagglutinin from swan-infecting H5N8 influenza virus complexed with avian receptor analog LSTc  
Authors : Jin, X.Y.; Han, P.; Song, H.; Qi, J.X.  
Deposited on : 2023-11-09  
Resolution : 2.48 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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

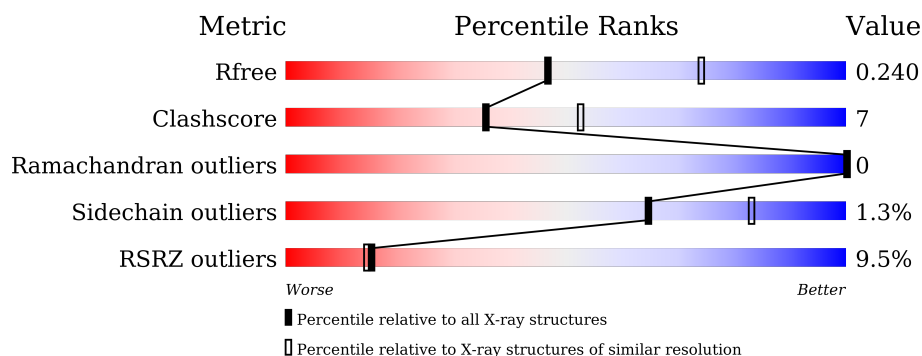
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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.



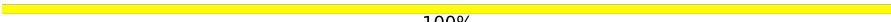
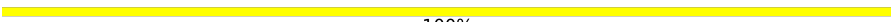
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

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	506	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div></div> </div> <div></div> </div>
1	B	506	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div></div> </div> <div></div> </div>
1	C	506	<div> <div>15%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div></div> </div> <div></div> </div>
2	D	4	<div> <div></div> <div> <div>25%</div> <div>50%</div> <div>25%</div> </div> <div></div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	3	 100%
4	H	3	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12327 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3921	2470	680	749	22			
1	B	490	Total	C	N	O	S	0	0	0
			3921	2470	680	749	22			
1	C	490	Total	C	N	O	S	0	0	0
			3921	2470	680	749	22			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
A	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
A	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5
B	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
B	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
B	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5
C	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
C	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
C	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			57	31	2	24			

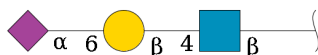
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



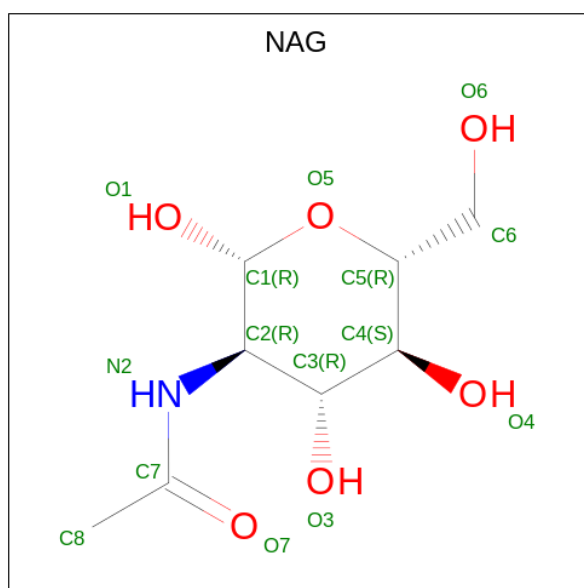
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			46	25	2	19			
4	H	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

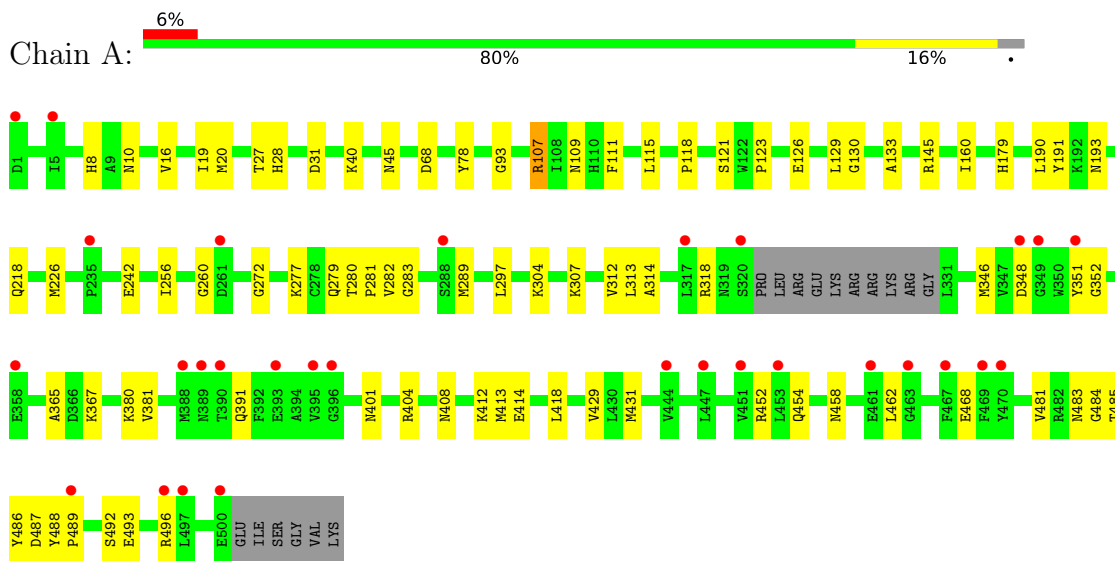
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	97	Total	O	0	0
			97	97		
6	C	55	Total	O	0	0
			55	55		

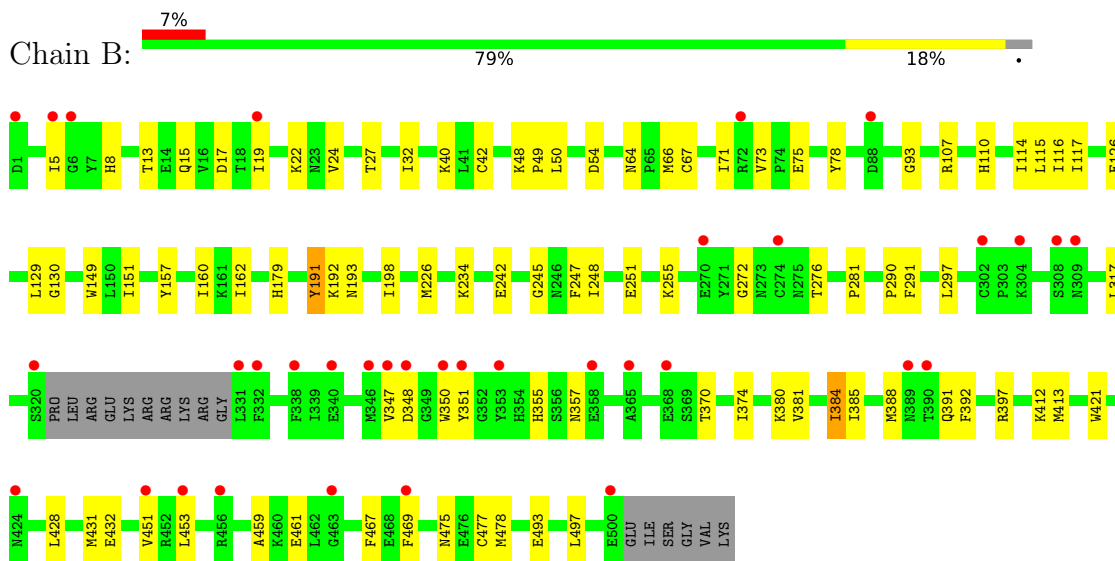
### 3 Residue-property plots [i](#)

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.

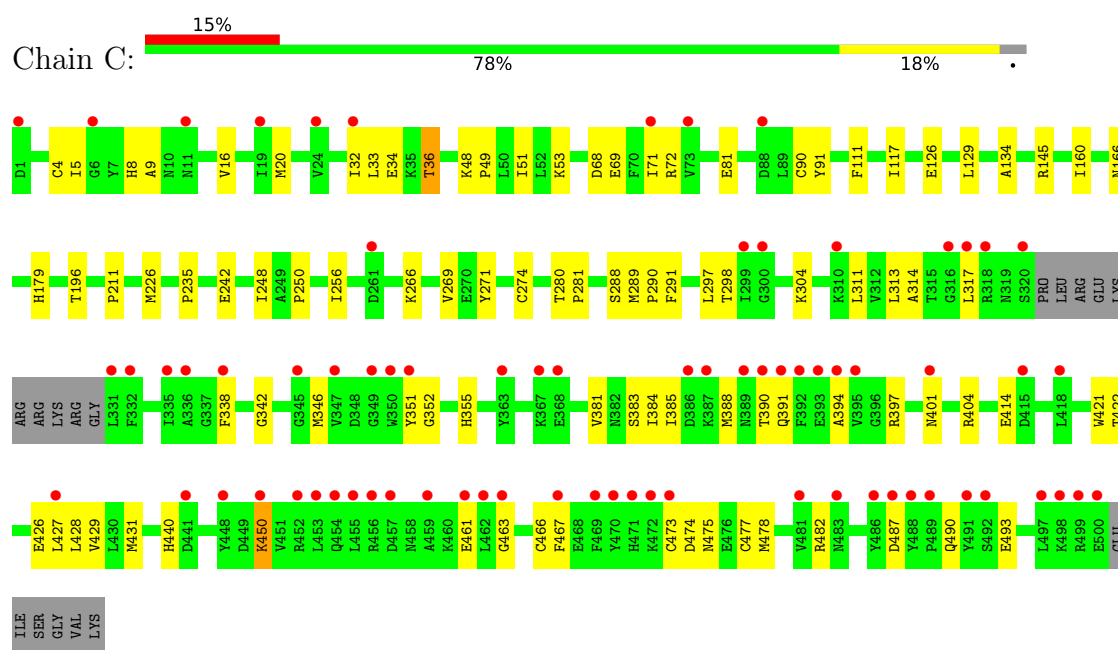
#### • Molecule 1: Hemagglutinin



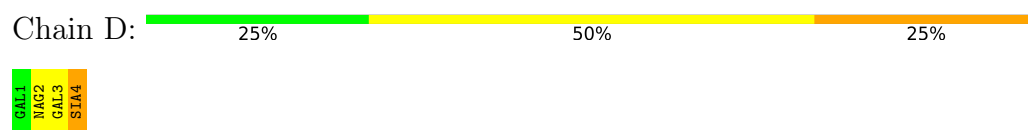
#### • Molecule 1: Hemagglutinin



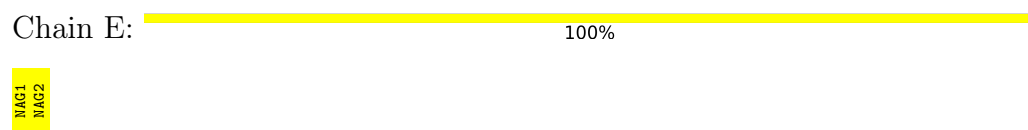
#### • Molecule 1: Hemagglutinin



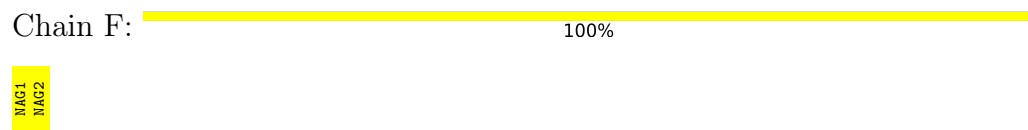
- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



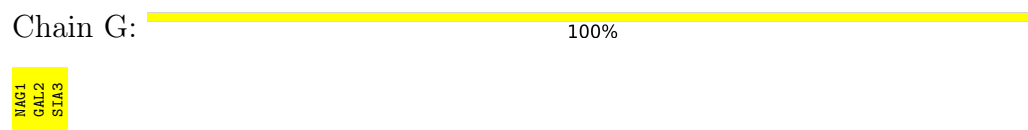
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

100%

MAG1  
GAL2  
SIA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.68Å 107.03Å 134.33Å 90.00° 100.47° 90.00°	Depositor
Resolution (Å)	49.63 – 2.48 49.63 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.63-2.48) 92.2 (49.63-2.48)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.234 , 0.252 0.234 , 0.240	Depositor DCC
$R_{free}$ test set	76660 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: SIA, NAG, GAL

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	0.44	0/4010	0.61	0/5431
1	B	0.41	0/4010	0.59	1/5431 (0.0%)
1	C	0.35	0/4010	0.52	0/5431
All	All	0.40	0/12030	0.57	1/16293 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	VAL	N-CA-CB	-5.01	105.44	112.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3921	0	3787	60	0
1	B	3921	0	3787	60	0
1	C	3921	0	3788	59	0
2	D	57	0	49	6	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	G	46	0	40	0	0
4	H	46	0	40	0	0
5	A	42	0	39	1	0
5	B	14	0	13	0	0
5	C	28	0	26	0	0
6	A	123	0	0	2	0
6	B	97	0	0	0	0
6	C	55	0	0	0	0
All	All	12327	0	11619	171	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 7.

The worst 5 of 171 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:190:LEU:HD11	2:D:2:NAG:H83	1.64	0.78
1:C:401:ASN:OD1	1:C:404:ARG:NH1	2.17	0.77
1:A:280:THR:HB	1:A:283:GLY:O	1.89	0.73
1:A:190:LEU:CD1	2:D:2:NAG:H83	2.22	0.70
1:B:412:LYS:NZ	1:C:414:GLU:OE2	2.24	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	486/506 (96%)	470 (97%)	16 (3%)	0	100	100
1	B	486/506 (96%)	474 (98%)	12 (2%)	0	100	100
1	C	486/506 (96%)	471 (97%)	15 (3%)	0	100	100
All	All	1458/1518 (96%)	1415 (97%)	43 (3%)	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	432/446 (97%)	429 (99%)	3 (1%)	81	92
1	B	432/446 (97%)	423 (98%)	9 (2%)	48	72
1	C	432/446 (97%)	427 (99%)	5 (1%)	67	84
All	All	1296/1338 (97%)	1279 (99%)	17 (1%)	65	83

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	274	CYS
1	C	473	CYS
1	B	162	ILE
1	B	191	TYR
1	B	348	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	475	ASN
1	C	189	ASN
1	C	454	GLN
1	C	440	HIS

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Mol	Chain	Res	Type
1	A	458	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 ⓘ

14 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	$\# Z  > 2$
2	GAL	D	1	2	12,12,12	0.17	0	17,17,17	0.37	0
2	NAG	D	2	2	14,14,15	0.38	0	17,19,21	1.02	0
2	GAL	D	3	2	11,11,12	0.77	0	15,15,17	1.12	1 (6%)
2	SIA	D	4	2	20,20,21	1.93	2 (10%)	24,28,31	1.85	6 (25%)
3	NAG	E	1	1,3	14,14,15	2.01	3 (21%)	17,19,21	1.72	5 (29%)
3	NAG	E	2	3	14,14,15	1.96	4 (28%)	17,19,21	0.95	0
3	NAG	F	1	1,3	14,14,15	2.01	4 (28%)	17,19,21	1.29	2 (11%)
3	NAG	F	2	3	14,14,15	2.43	4 (28%)	17,19,21	1.88	5 (29%)
4	NAG	G	1	4	15,15,15	1.87	5 (33%)	21,21,21	2.96	12 (57%)
4	GAL	G	2	4	11,11,12	1.70	3 (27%)	15,15,17	2.10	5 (33%)
4	SIA	G	3	4	20,20,21	1.81	4 (20%)	24,28,31	2.76	13 (54%)
4	NAG	H	1	4	15,15,15	1.76	3 (20%)	21,21,21	2.77	12 (57%)
4	GAL	H	2	4	11,11,12	1.67	2 (18%)	15,15,17	1.83	3 (20%)
4	SIA	H	3	4	20,20,21	1.64	3 (15%)	24,28,31	2.52	8 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	D	1	2	-	0/2/22/22	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	GAL	D	3	2	-	0/2/19/22	0/1/1/1
2	SIA	D	4	2	-	3/18/34/38	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
4	NAG	G	1	4	-	4/6/26/26	0/1/1/1
4	GAL	G	2	4	-	0/2/19/22	0/1/1/1
4	SIA	G	3	4	-	0/18/34/38	0/1/1/1
4	NAG	H	1	4	-	2/6/26/26	0/1/1/1
4	GAL	H	2	4	-	0/2/19/22	0/1/1/1
4	SIA	H	3	4	-	0/18/34/38	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	SIA	C2-C1	7.29	1.58	1.52
3	F	2	NAG	O5-C1	5.94	1.53	1.43
4	G	3	SIA	O6-C2	4.98	1.50	1.43
4	H	3	SIA	O6-C2	4.79	1.50	1.43
3	F	1	NAG	O5-C1	4.59	1.51	1.43

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C8-C7-N2	7.05	128.04	116.10
4	H	1	NAG	C1-C2-N2	-6.26	103.47	110.73
4	H	3	SIA	C6-C5-N5	-6.02	100.91	110.91
4	G	3	SIA	C6-C5-N5	-5.19	102.28	110.91
4	H	1	NAG	C8-C7-N2	5.19	124.89	116.10

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

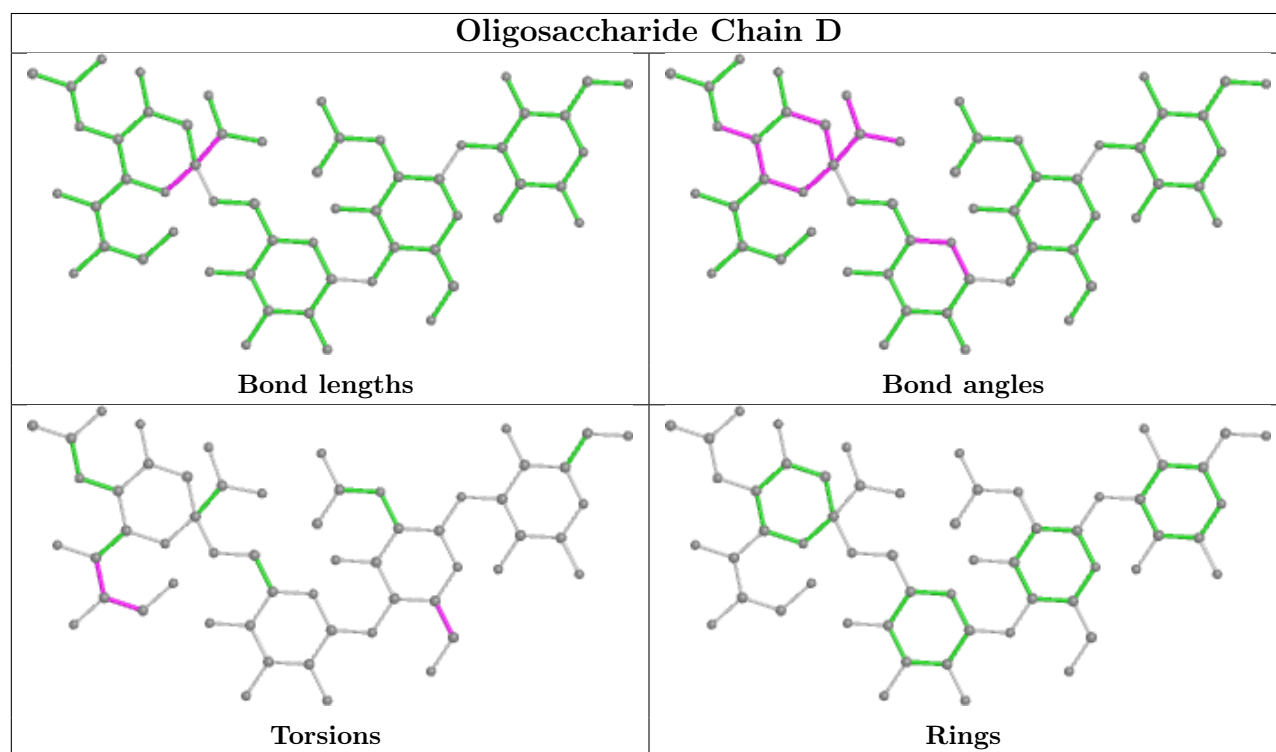
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2

There are no ring outliers.

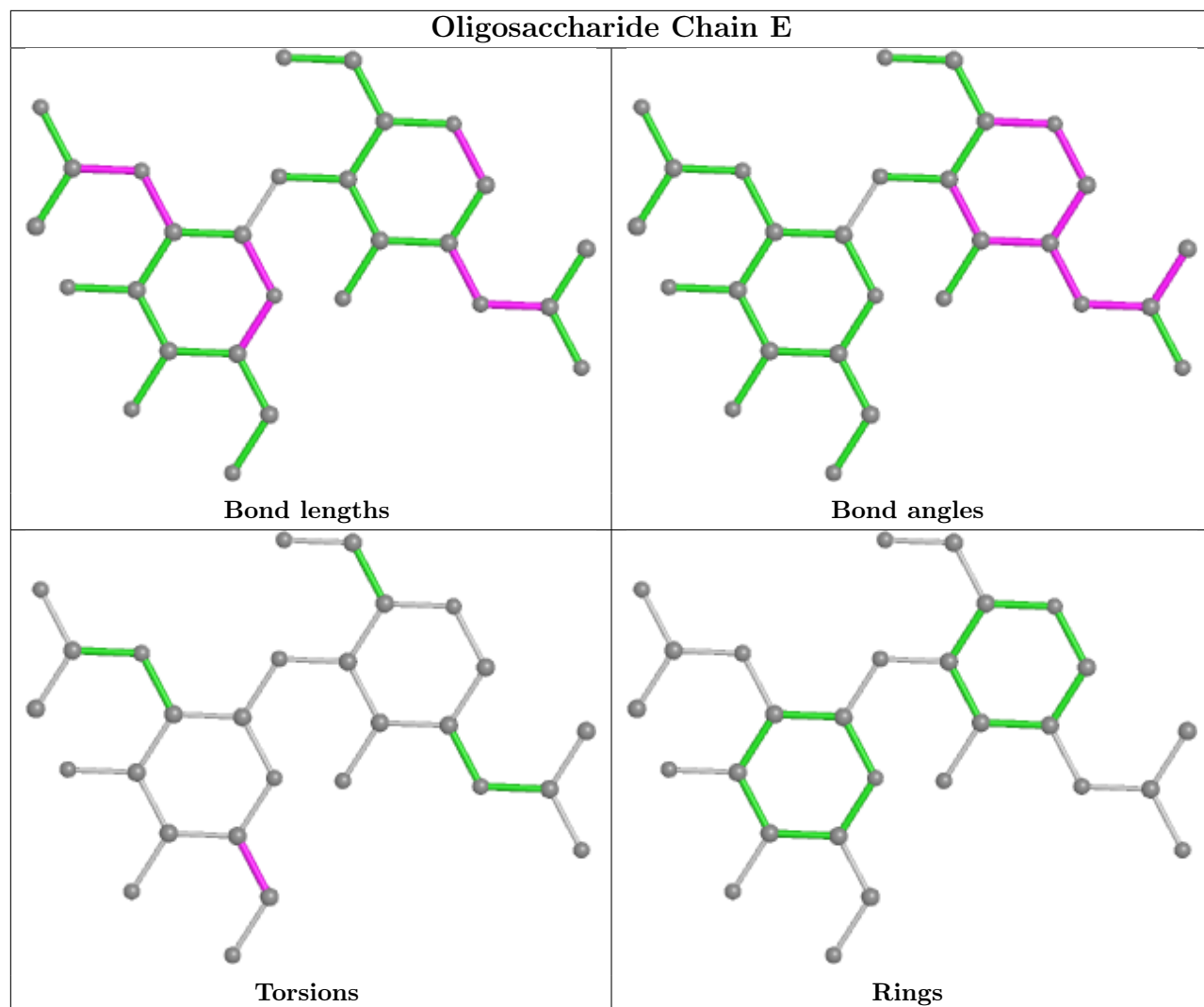
2 monomers are involved in 6 short contacts:

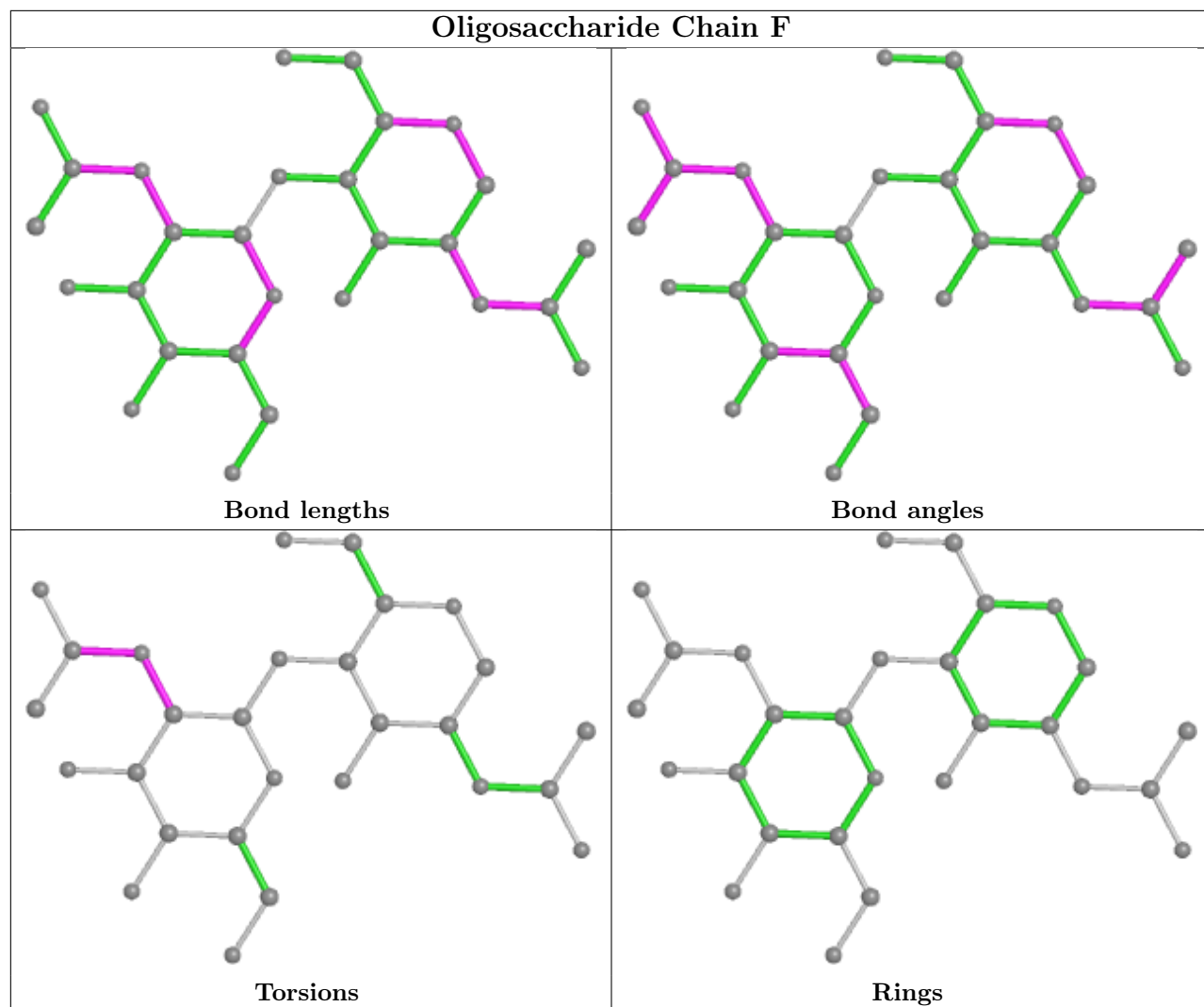
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	2	0
2	D	4	SIA	4	0

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

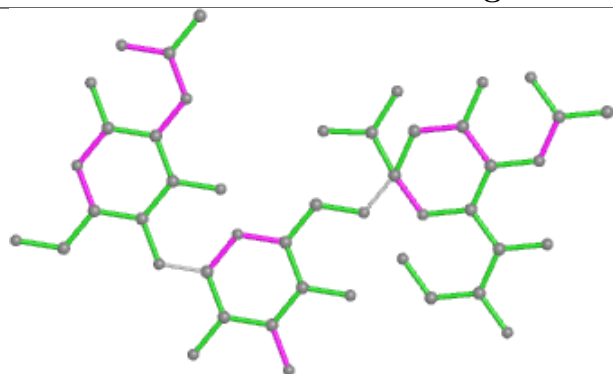




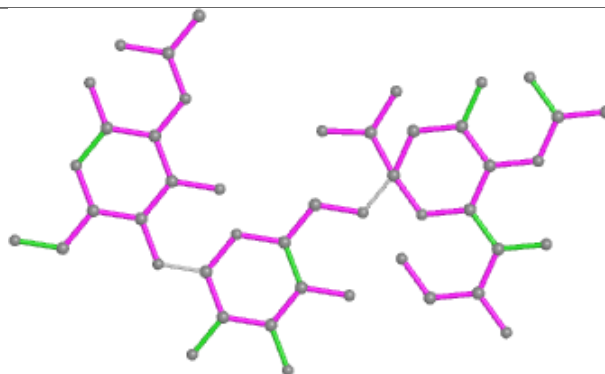




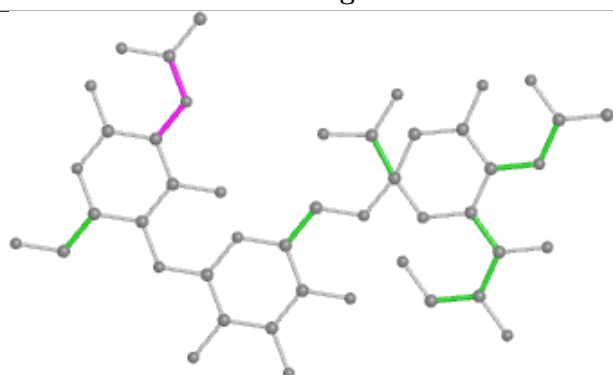
## Oligosaccharide Chain G



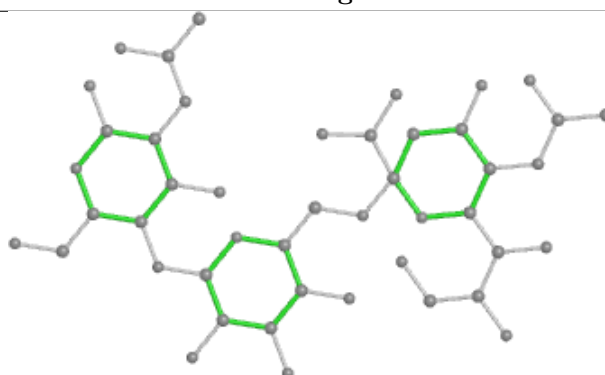
Bond lengths



Bond angles

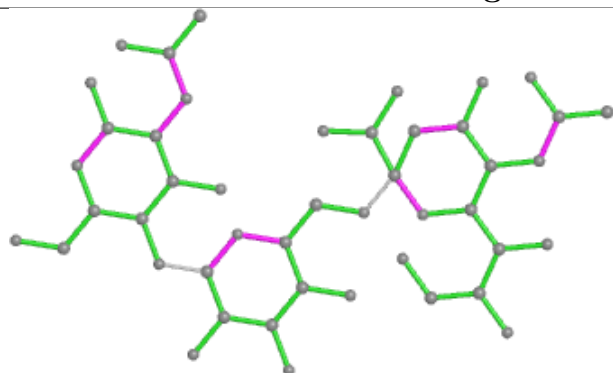


Torsions

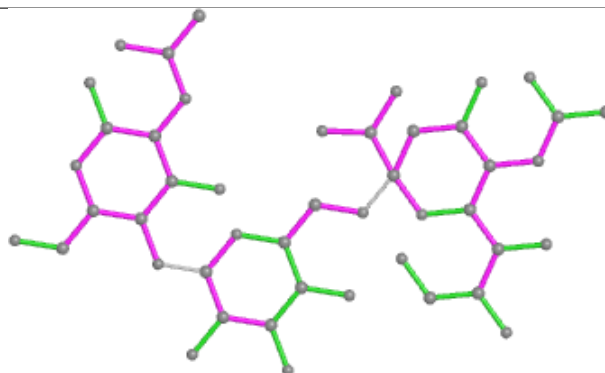


Rings

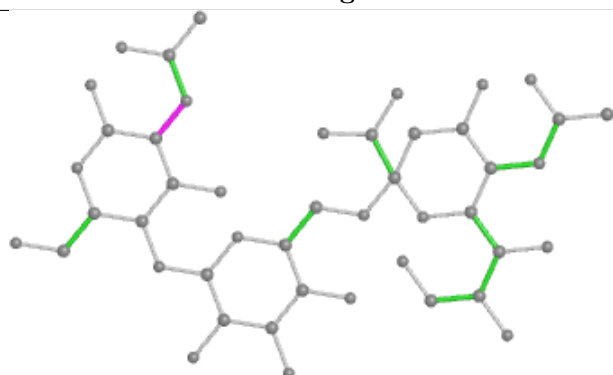
## Oligosaccharide Chain H



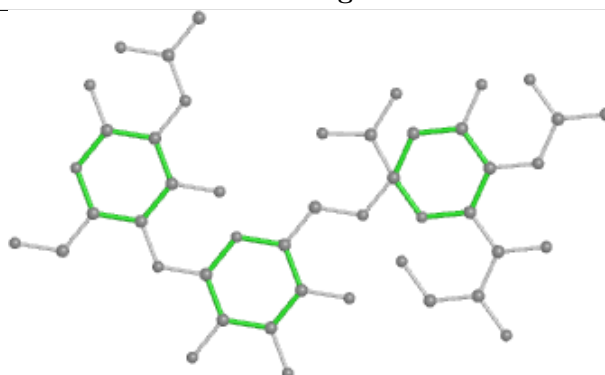
Bond lengths



Bond angles



Torsions



Rings

## 5.6 Ligand geometry

6 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
5	NAG	A	602	1	14,14,15	2.06	4 (28%)	17,19,21	0.99	1 (5%)
5	NAG	C	601	1	14,14,15	2.00	4 (28%)	17,19,21	0.89	0
5	NAG	C	602	1	14,14,15	2.04	4 (28%)	17,19,21	1.19	3 (17%)
5	NAG	A	601	1	14,14,15	2.10	4 (28%)	17,19,21	1.30	2 (11%)
5	NAG	B	601	1	14,14,15	2.11	4 (28%)	17,19,21	1.27	3 (17%)
5	NAG	A	603	1	14,14,15	2.06	4 (28%)	17,19,21	1.20	3 (17%)

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	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	1/6/23/26	0/1/1/1
5	NAG	B	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	603	1	-	2/6/23/26	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	O5-C1	5.13	1.51	1.43
5	B	601	NAG	O5-C1	4.83	1.51	1.43
5	A	603	NAG	O5-C1	4.80	1.51	1.43
5	C	602	NAG	O5-C1	4.72	1.51	1.43
5	C	601	NAG	O5-C1	4.55	1.51	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C6-C5-C4	-2.83	106.37	113.00
5	B	601	NAG	C8-C7-N2	2.66	120.60	116.10
5	A	601	NAG	O5-C5-C6	2.56	111.22	107.20
5	C	602	NAG	C1-C2-N2	-2.26	106.62	110.49
5	C	602	NAG	C8-C7-N2	2.26	119.93	116.10

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	NAG	C4-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	B	601	NAG	C4-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	C	602	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	NAG	1	0

## 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	490/506 (96%)	0.64	30 (6%) 28 26	36, 60, 103, 136	0
1	B	490/506 (96%)	0.73	35 (7%) 23 22	41, 72, 100, 123	0
1	C	490/506 (96%)	0.99	74 (15%) 6 6	31, 75, 155, 177	0
All	All	1470/1518 (96%)	0.79	139 (9%) 15 14	31, 69, 119, 177	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	ASP	5.9
1	C	331	LEU	5.1
1	C	455	LEU	5.1
1	B	331	LEU	5.1
1	C	453	LEU	5.1

### 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.

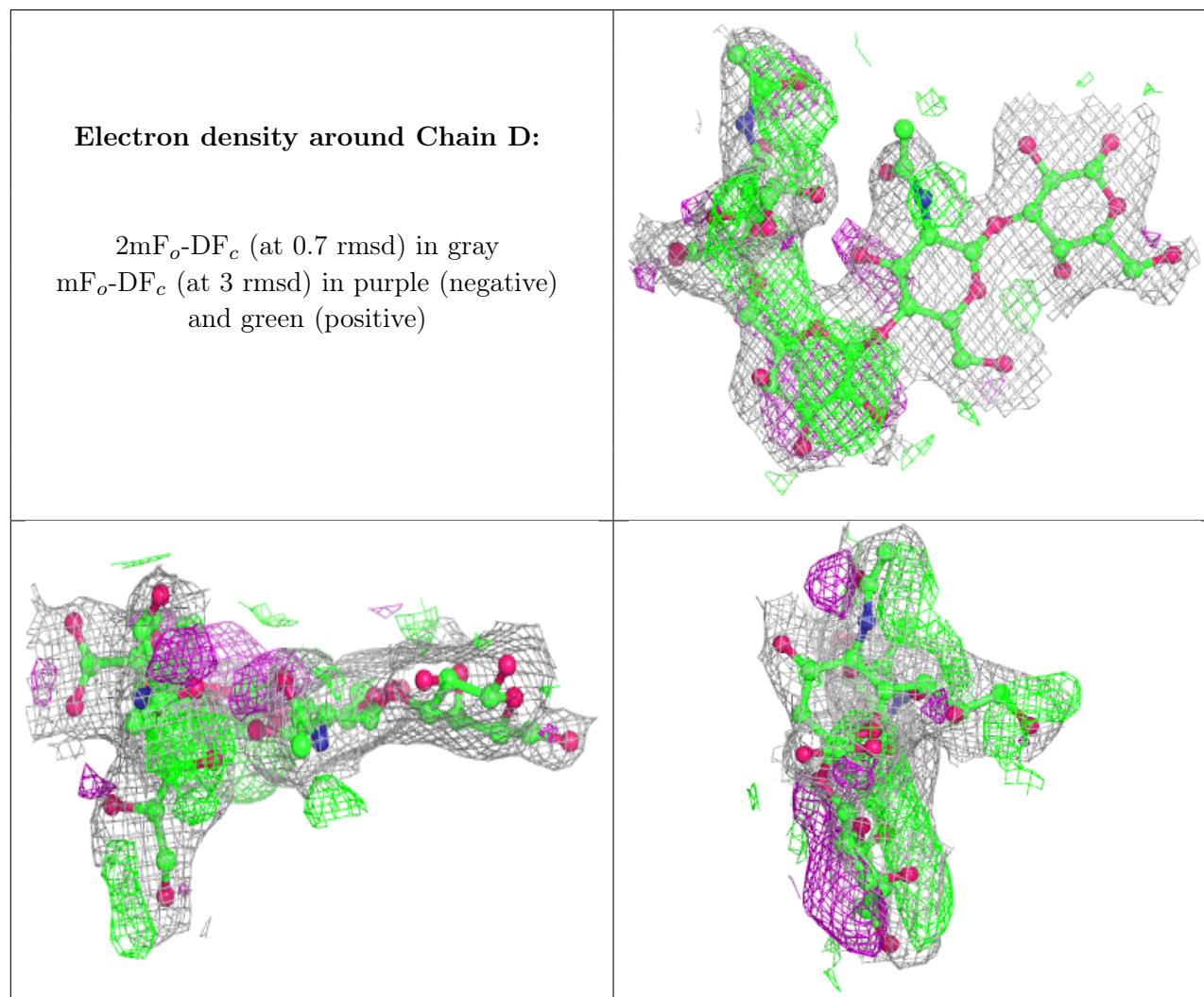
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	F	2	14/15	0.33	0.18	112,117,122,122	0
2	GAL	D	3	11/12	0.41	0.29	57,63,69,69	0
4	NAG	G	1	15/15	0.48	0.24	70,79,89,89	0

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*Continued from previous page...*

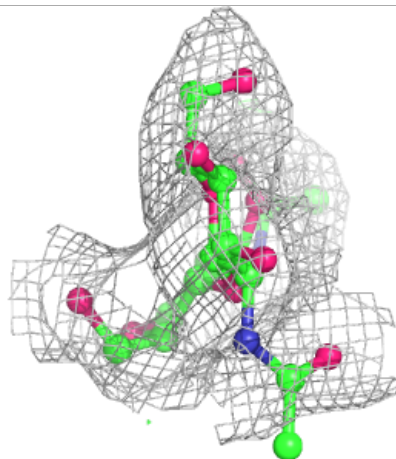
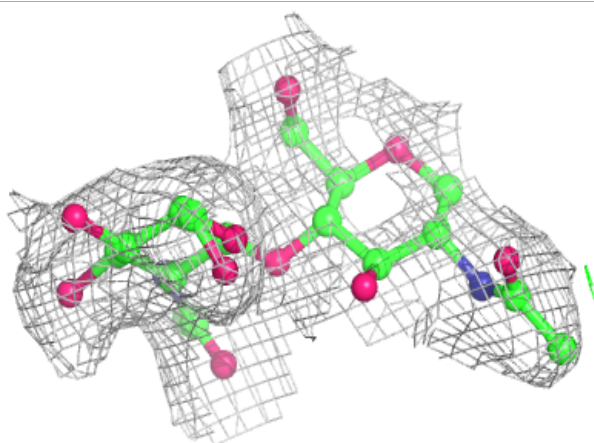
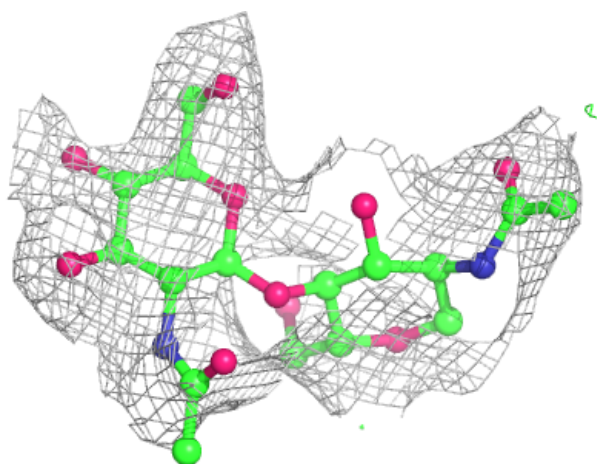
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	H	1	15/15	0.51	0.19	81,96,99,104	0
4	GAL	G	2	11/12	0.63	0.24	68,73,83,91	0
4	GAL	H	2	11/12	0.68	0.15	76,87,92,92	0
3	NAG	E	2	14/15	0.70	0.13	88,95,102,102	0
2	NAG	D	2	14/15	0.73	0.20	67,72,76,78	0
2	SIA	D	4	20/21	0.76	0.19	44,57,65,67	0
2	GAL	D	1	12/12	0.77	0.17	63,78,83,87	0
3	NAG	F	1	14/15	0.79	0.13	81,98,105,112	0
3	NAG	E	1	14/15	0.85	0.10	60,75,87,93	0
4	SIA	G	3	20/21	0.88	0.12	33,54,65,70	0
4	SIA	H	3	20/21	0.89	0.12	54,62,74,77	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.



**Electron density around Chain E:**

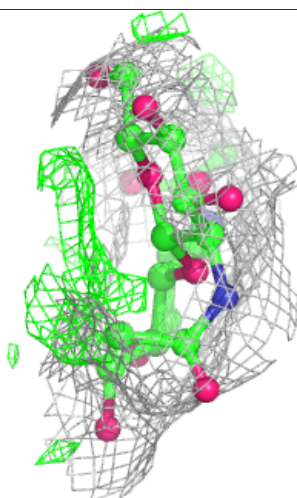
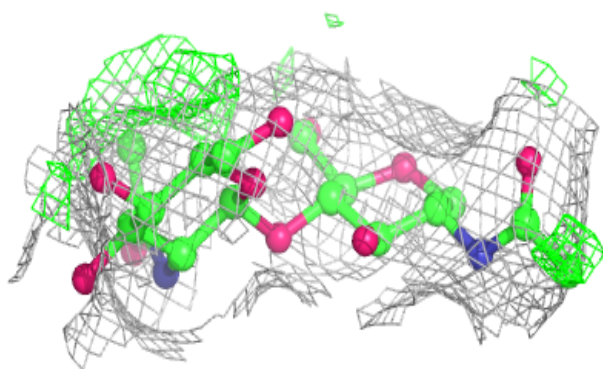
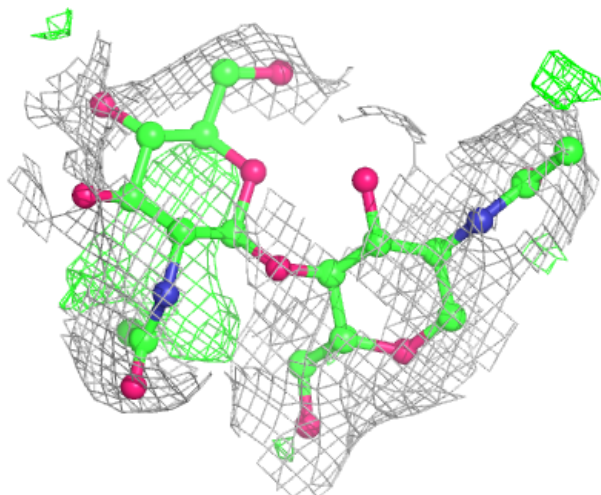
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





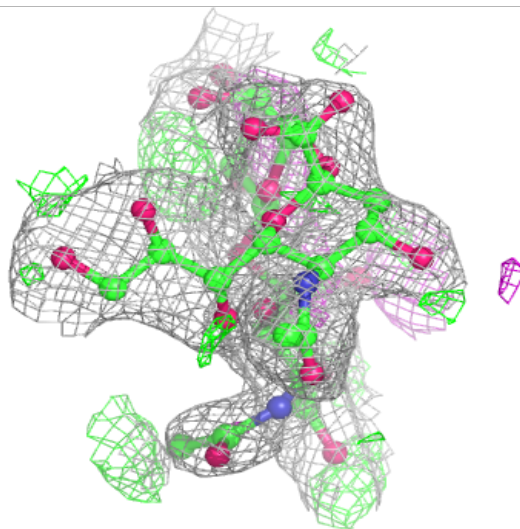
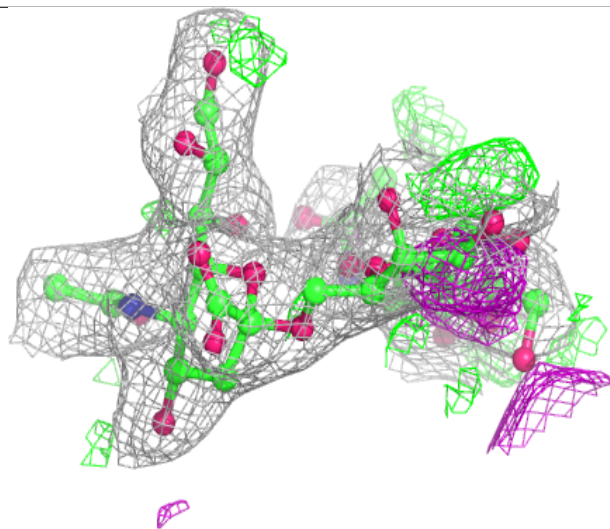
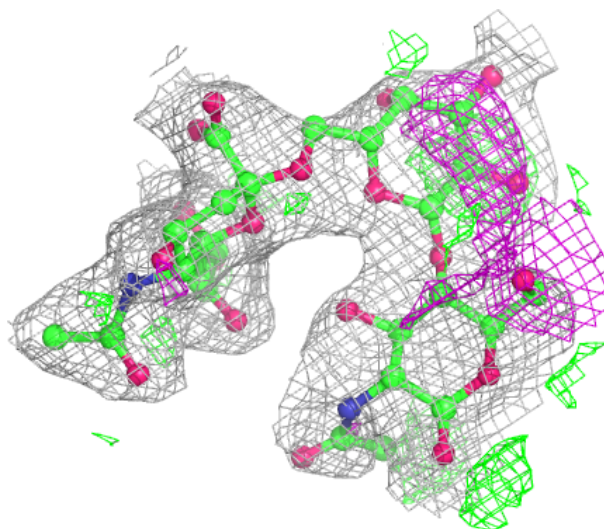
**Electron density around Chain F:**

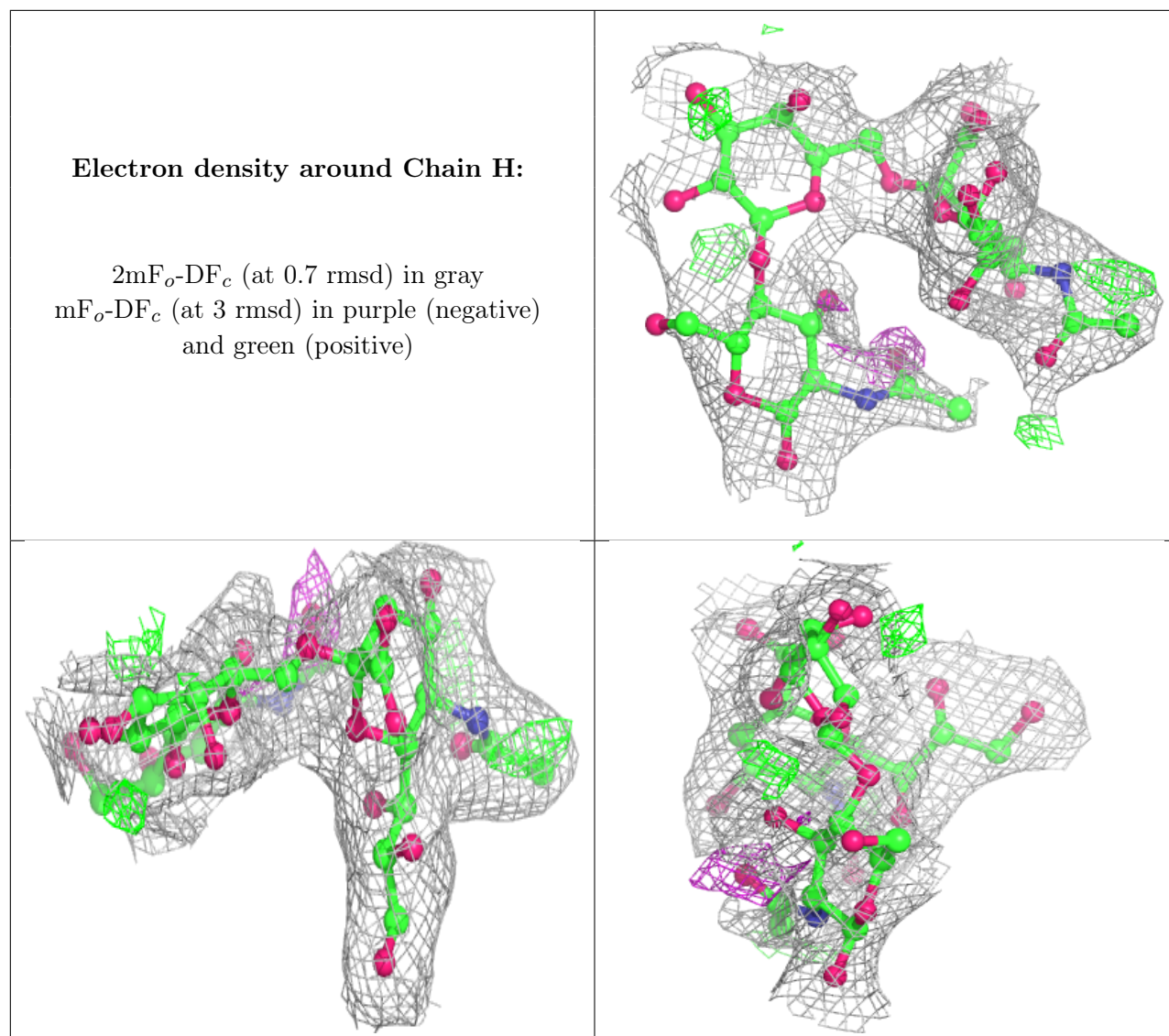
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 6.4 Ligands ⓘ

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
5	NAG	A	603	14/15	0.56	0.17	82,95,100,103	0
5	NAG	A	602	14/15	0.68	0.17	86,93,98,102	0
5	NAG	C	602	14/15	0.71	0.16	105,111,113,116	0
5	NAG	B	601	14/15	0.75	0.18	99,104,109,109	0
5	NAG	C	601	14/15	0.76	0.13	66,82,90,92	0
5	NAG	A	601	14/15	0.83	0.13	70,77,90,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.