



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 09:56 AM BST

PDB ID : 4KTH  
Title : Structure of A/Hubei/1/2010 H5 HA  
Authors : Shore, D.A.; Yang, H.; Carney, P.J.; Chang, J.C.; Stevens, J.  
Deposited on : 2013-05-20  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

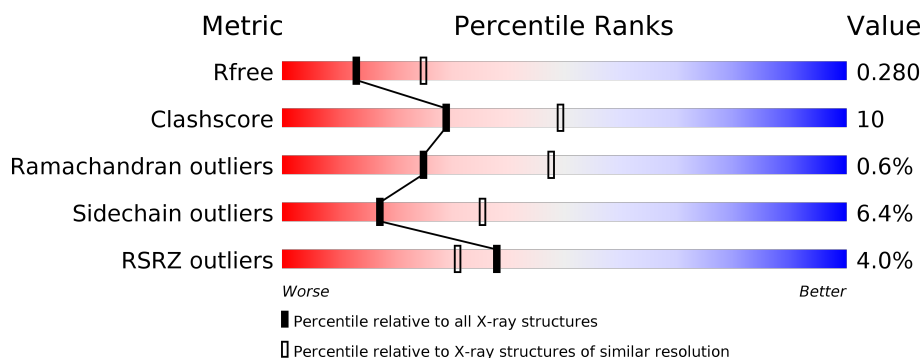
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.





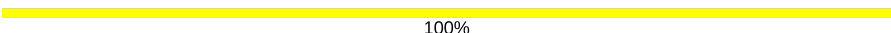
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	330	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	330	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	E	330	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>
2	B	181	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>• 9%</div> </div> </div>
2	D	181	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 6%</div> </div> </div>
2	F	181	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>• 10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 50% 50%
3	H	2	 50% 50%
3	I	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	I	1	X	-	-	-
4	NAG	A	406	X	-	-	-
4	NAG	E	402	X	-	-	-
4	NAG	F	201	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11987 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	322	Total	C	N	O	S	0	0	0
			2553	1617	441	482	13			
1	E	321	Total	C	N	O	S	0	0	0
			2546	1612	440	481	13			
1	C	321	Total	C	N	O	S	0	0	0
			2546	1612	440	481	13			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP G2U0T8
A	-2	ASP	-	expression tag	UNP G2U0T8
A	-1	PRO	-	expression tag	UNP G2U0T8
A	0	GLY	-	expression tag	UNP G2U0T8
A	325	THR	ARG	conflict	UNP G2U0T8
E	-3	ALA	-	expression tag	UNP G2U0T8
E	-2	ASP	-	expression tag	UNP G2U0T8
E	-1	PRO	-	expression tag	UNP G2U0T8
E	0	GLY	-	expression tag	UNP G2U0T8
E	325	THR	ARG	conflict	UNP G2U0T8
C	-3	ALA	-	expression tag	UNP G2U0T8
C	-2	ASP	-	expression tag	UNP G2U0T8
C	-1	PRO	-	expression tag	UNP G2U0T8
C	0	GLY	-	expression tag	UNP G2U0T8
C	325	THR	ARG	conflict	UNP G2U0T8

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1352	836	236	272	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	163	Total	C	N	O	S	0	0	0
			1338	827	234	269	8			
2	D	170	Total	C	N	O	S	0	0	0
			1384	858	241	277	8			

There are 18 discrepancies between the modelled and reference sequences:

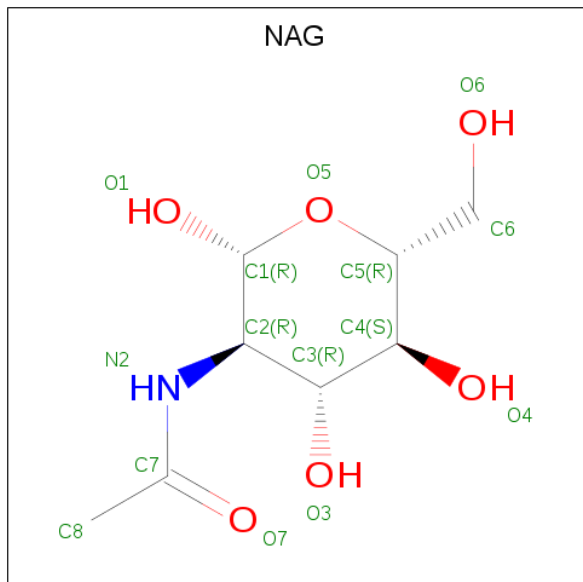
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	GLY	conflict	UNP G2U0T8
B	176	GLY	VAL	conflict	UNP G2U0T8
B	177	ARG	LYS	conflict	UNP G2U0T8
B	179	VAL	-	expression tag	UNP G2U0T8
B	180	PRO	-	expression tag	UNP G2U0T8
B	181	ARG	-	expression tag	UNP G2U0T8
F	175	SER	GLY	conflict	UNP G2U0T8
F	176	GLY	VAL	conflict	UNP G2U0T8
F	177	ARG	LYS	conflict	UNP G2U0T8
F	179	VAL	-	expression tag	UNP G2U0T8
F	180	PRO	-	expression tag	UNP G2U0T8
F	181	ARG	-	expression tag	UNP G2U0T8
D	175	SER	GLY	conflict	UNP G2U0T8
D	176	GLY	VAL	conflict	UNP G2U0T8
D	177	ARG	LYS	conflict	UNP G2U0T8
D	179	VAL	-	expression tag	UNP G2U0T8
D	180	PRO	-	expression tag	UNP G2U0T8
D	181	ARG	-	expression tag	UNP G2U0T8

- Molecule 3 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	E	13	Total	O	0	0
			13	13		

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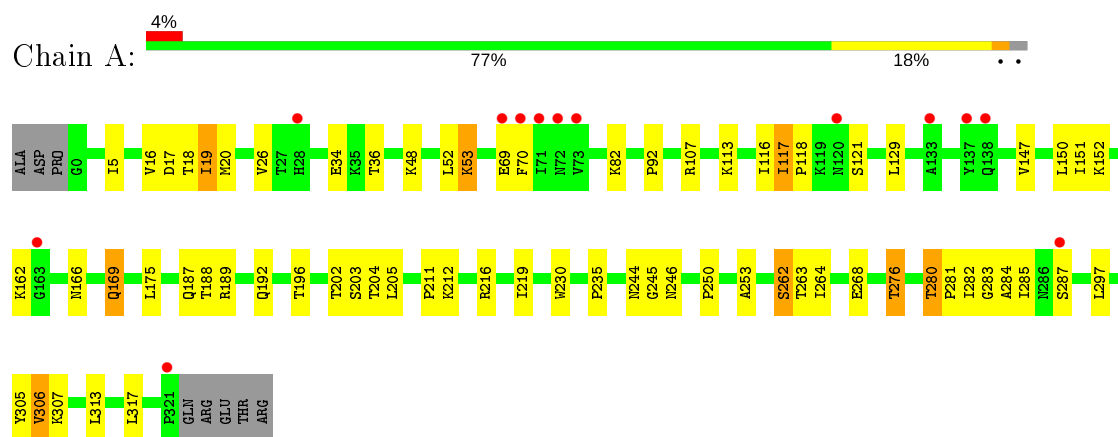
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	7	Total 7	O 7	0	0
5	C	17	Total 17	O 17	0	0
5	F	6	Total 6	O 6	0	0
5	D	6	Total 6	O 6	0	0

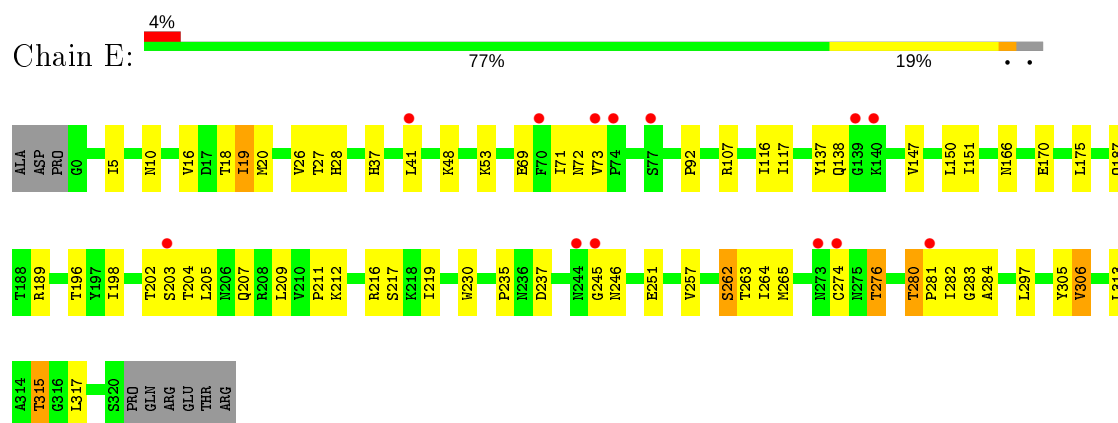
### 3 Residue-property plots [i](#)

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.

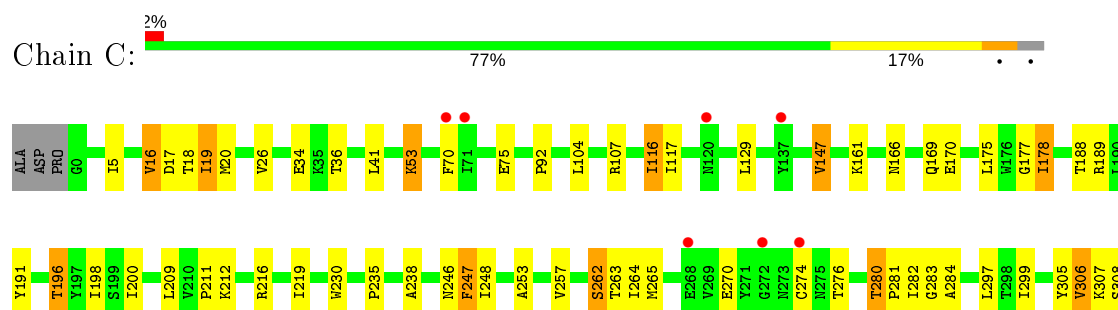
#### • Molecule 1: Hemagglutinin

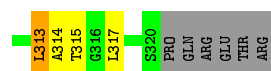


#### • Molecule 1: Hemagglutinin

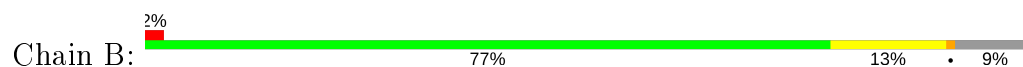


#### • Molecule 1: Hemagglutinin

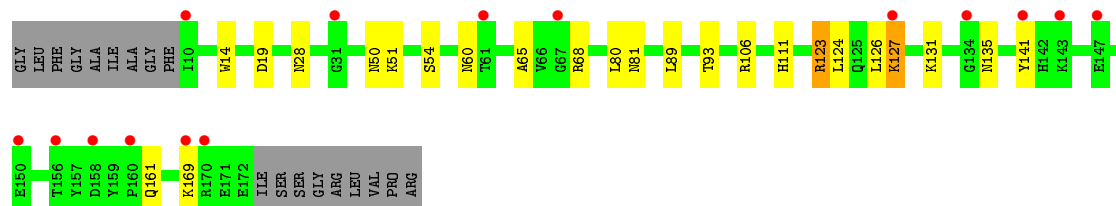
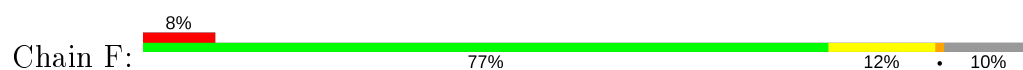




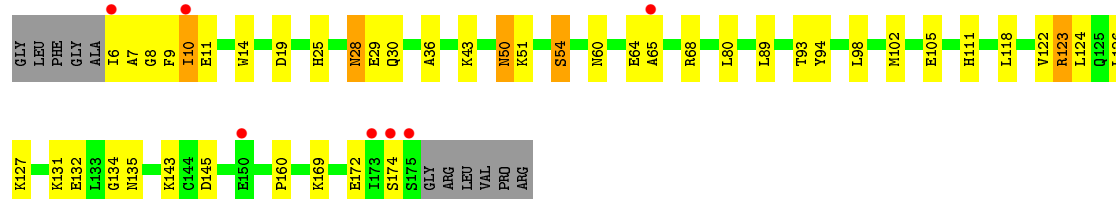
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



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

Chain I:

100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.12Å 101.58Å 124.93Å 90.00° 121.66° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.77 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.60) 99.2 (49.77-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.234 , 0.266 0.254 , 0.280	Depositor DCC
$R_{free}$ test set	2876 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 30.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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:  
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	0.49	0/2617	0.56	0/3557
1	C	0.49	0/2609	0.55	0/3545
1	E	0.48	0/2609	0.54	0/3545
2	B	0.49	2/1377 (0.1%)	0.52	0/1851
2	D	0.48	0/1410	0.53	0/1895
2	F	0.49	1/1363 (0.1%)	0.57	0/1832
All	All	0.49	3/11985 (0.0%)	0.55	0/16225

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	14	TRP	CD2-CE2	5.50	1.48	1.41
2	B	21	TRP	CD2-CE2	5.14	1.47	1.41
2	B	14	TRP	CD2-CE2	5.05	1.47	1.41

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	2553	0	2491	50	0
1	C	2546	0	2485	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2546	0	2486	44	0
2	B	1352	0	1256	19	0
2	D	1384	0	1286	63	0
2	F	1338	0	1239	47	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	A	28	0	26	0	0
4	C	42	0	39	1	0
4	E	28	0	26	0	0
4	F	14	0	13	0	0
5	A	23	0	0	1	0
5	B	7	0	0	2	0
5	C	17	0	0	1	0
5	D	6	0	0	3	0
5	E	13	0	0	1	0
5	F	6	0	0	0	0
All	All	11987	0	11422	225	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 10.

The worst 5 of 225 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)
2:F:123:ARG:NH1	2:F:124:LEU:CD1	1.72	1.51
2:F:123:ARG:NH1	2:F:124:LEU:HD11	1.20	1.46
2:F:127:LYS:HZ3	2:D:132:GLU:N	1.33	1.25
2:F:123:ARG:NH2	2:D:132:GLU:OE1	1.74	1.20
2:F:127:LYS:NZ	2:D:132:GLU:N	1.94	1.14

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	320/330 (97%)	300 (94%)	18 (6%)	2 (1%)	25	47
1	C	319/330 (97%)	301 (94%)	17 (5%)	1 (0%)	41	64
1	E	319/330 (97%)	294 (92%)	23 (7%)	2 (1%)	25	47
2	B	163/181 (90%)	160 (98%)	3 (2%)	0	100	100
2	D	168/181 (93%)	162 (96%)	4 (2%)	2 (1%)	13	27
2	F	161/181 (89%)	158 (98%)	2 (1%)	1 (1%)	25	47
All	All	1450/1533 (95%)	1375 (95%)	67 (5%)	8 (1%)	25	47

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	E	53	LYS
1	C	53	LYS
1	A	245	GLY
2	F	127	LYS

### 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	286/293 (98%)	269 (94%)	17 (6%)	19	39
1	C	285/293 (97%)	262 (92%)	23 (8%)	11	23
1	E	285/293 (97%)	269 (94%)	16 (6%)	21	42
2	B	145/155 (94%)	139 (96%)	6 (4%)	30	56
2	D	147/155 (95%)	137 (93%)	10 (7%)	16	32
2	F	143/155 (92%)	133 (93%)	10 (7%)	15	30
All	All	1291/1344 (96%)	1209 (94%)	82 (6%)	17	35

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	SER
1	C	104	LEU
2	D	54	SER
2	B	60	ASN
1	C	19	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	142	HIS
1	C	220	ASN
2	D	95	ASN
1	C	28	HIS
1	E	109	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 ⓘ

6 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	$\# Z  > 2$
3	NAG	G	1	1,3	14,14,15	0.59	0	17,19,21	0.91	0
3	NAG	G	2	3	14,14,15	0.56	0	17,19,21	0.70	0
3	NAG	H	1	1,3	14,14,15	0.70	0	17,19,21	1.39	3 (17%)
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	1	3,2	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
3	NAG	I	2	3	14,14,15	0.68	0	17,19,21	1.26	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,2	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	O5-C1-C2	-3.69	105.47	111.29
3	I	2	NAG	C4-C3-C2	3.43	116.04	111.02
3	I	2	NAG	O5-C5-C6	2.63	111.33	107.20
3	H	1	NAG	C3-C4-C5	2.54	114.78	110.24
3	I	1	NAG	O5-C1-C2	-2.42	107.47	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	1	NAG	C1

5 of 11 torsion outliers are listed below:

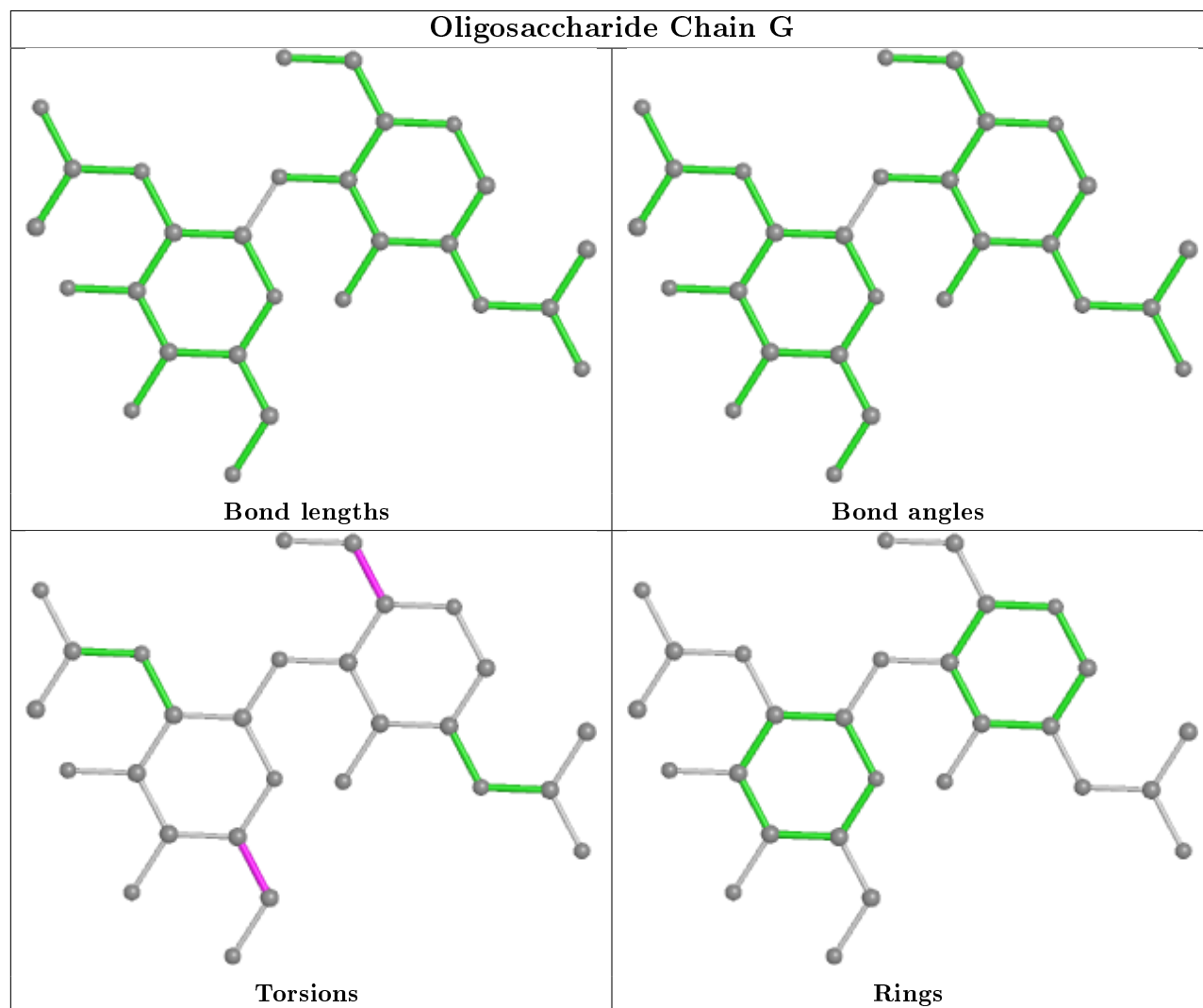
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6

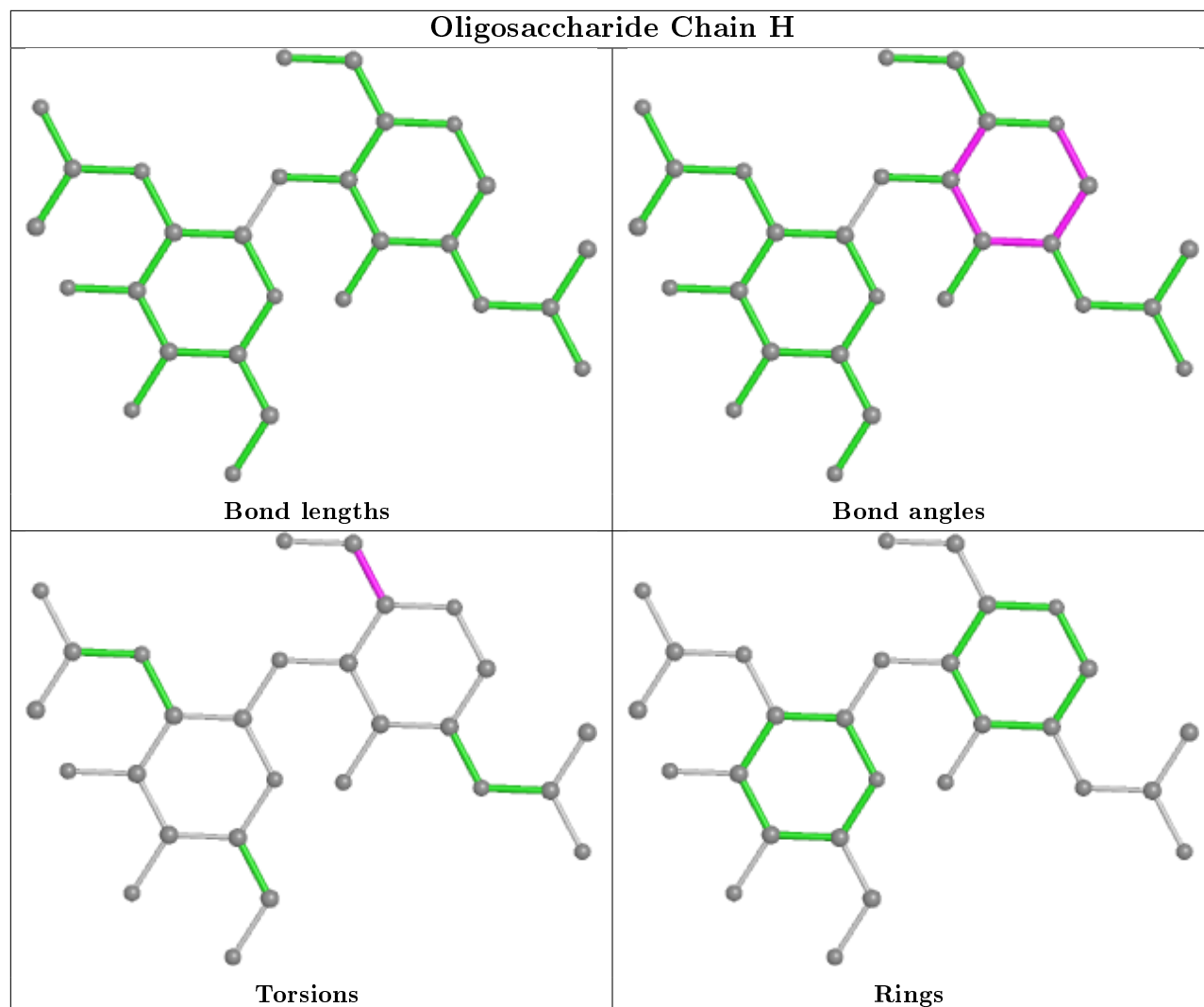
There are no ring outliers.

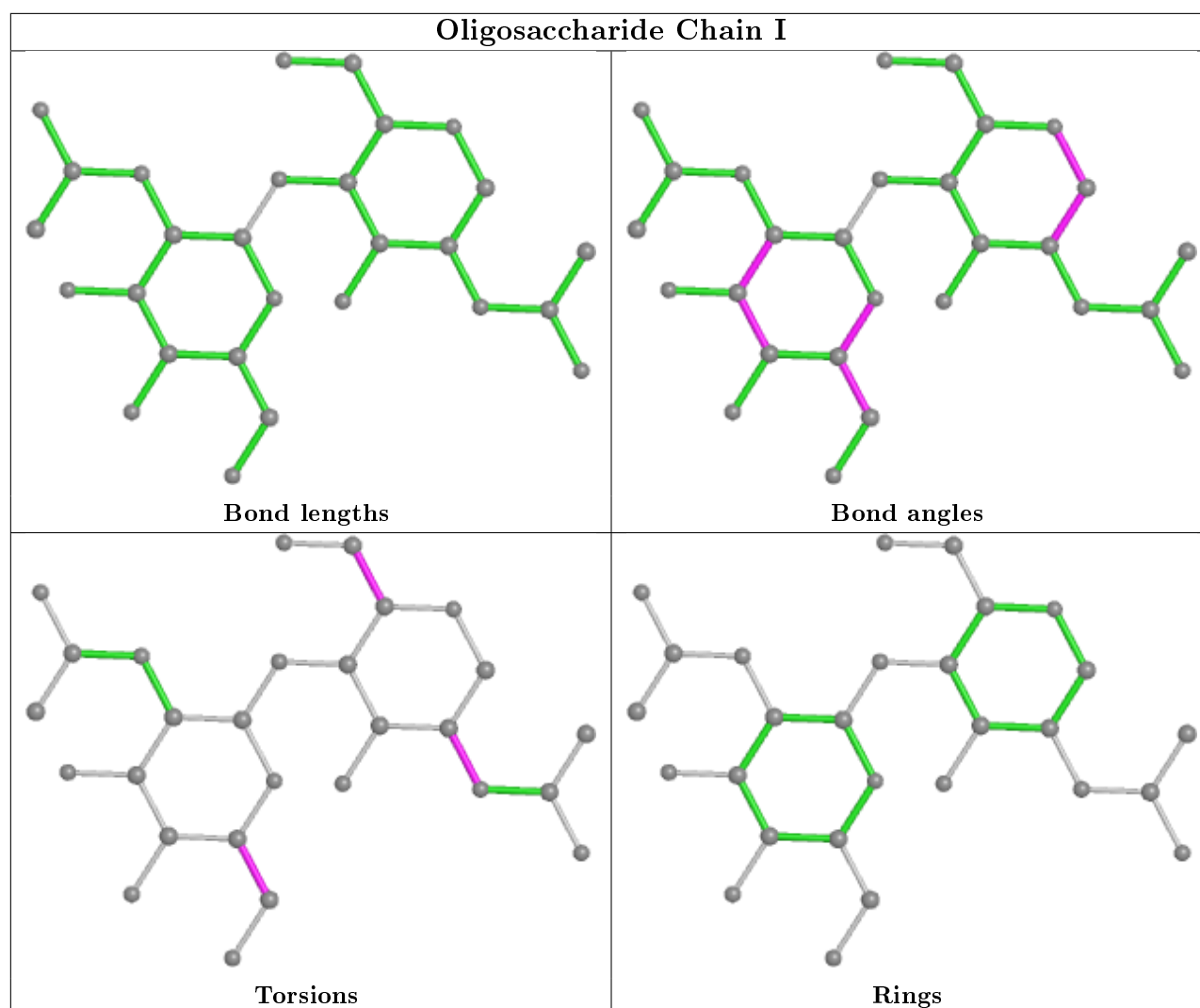
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	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 oligosaccharide.







## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
4	NAG	C	403	1	14,14,15	0.69	1 (7%)	17,19,21	2.01	2 (11%)
4	NAG	E	402	1	14,14,15	0.80	0	17,19,21	1.44	2 (11%)
4	NAG	C	402	1	14,14,15	0.62	0	17,19,21	1.64	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	401	1	14,14,15	0.65	0	17,19,21	1.14	2 (11%)
4	NAG	C	401	1	14,14,15	0.54	0	17,19,21	1.11	1 (5%)
4	NAG	F	201	2	14,14,15	0.63	0	17,19,21	1.03	1 (5%)
4	NAG	E	401	1	14,14,15	0.51	0	17,19,21	1.30	1 (5%)
4	NAG	A	406	1	14,14,15	0.75	0	17,19,21	1.25	2 (11%)

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	C	403	1	-	2/6/23/26	0/1/1/1
4	NAG	E	402	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	F	201	2	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	406	1	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	NAG	C1-C2	2.20	1.55	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	NAG	C1-O5-C5	6.83	121.44	112.19
4	C	402	NAG	C1-O5-C5	5.32	119.40	112.19
4	E	401	NAG	C1-O5-C5	4.39	118.14	112.19
4	E	402	NAG	C4-C3-C2	4.05	116.96	111.02
4	C	403	NAG	O5-C1-C2	3.97	117.56	111.29

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	402	NAG	C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
4	F	201	NAG	C1
4	A	406	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	NAG	O5-C5-C6-O6
4	C	403	NAG	O5-C5-C6-O6
4	F	201	NAG	C4-C5-C6-O6
4	E	402	NAG	O5-C5-C6-O6
4	E	402	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
4	C	401	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	322/330 (97%)	0.06	13 (4%) 38 31	19, 32, 59, 126	0
1	C	321/330 (97%)	0.19	7 (2%) 62 56	30, 52, 87, 160	0
1	E	321/330 (97%)	0.36	13 (4%) 38 31	33, 55, 90, 166	0
2	B	165/181 (91%)	0.04	4 (2%) 59 53	13, 32, 59, 86	0
2	D	170/181 (93%)	0.49	7 (4%) 37 30	24, 57, 95, 159	0
2	F	163/181 (90%)	0.63	15 (9%) 9 6	28, 54, 105, 136	0
All	All	1462/1533 (95%)	0.26	59 (4%) 38 31	13, 47, 87, 166	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	173	ILE	8.3
1	E	70	PHE	8.2
1	A	70	PHE	8.0
1	C	70	PHE	6.0
1	E	245	GLY	5.2

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

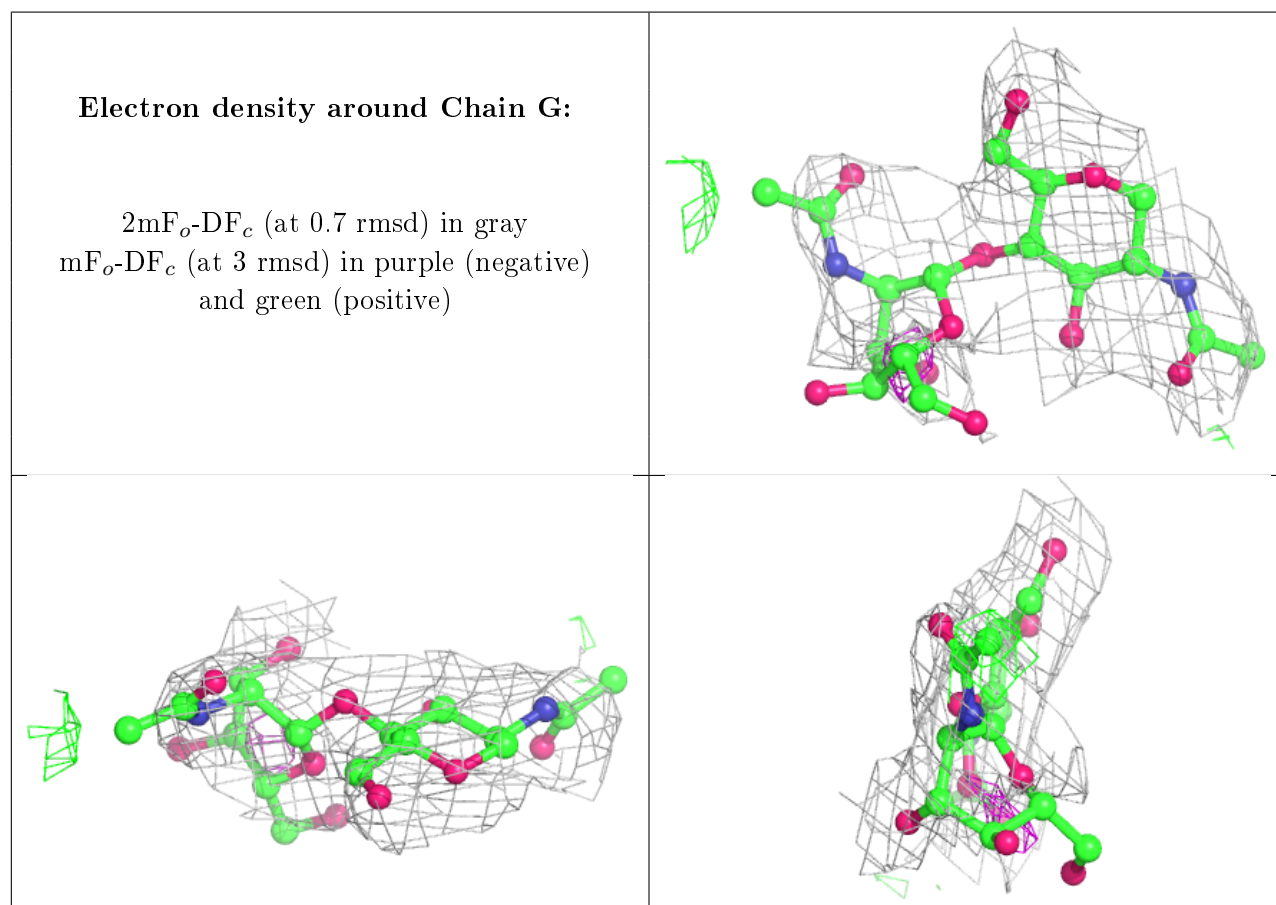
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

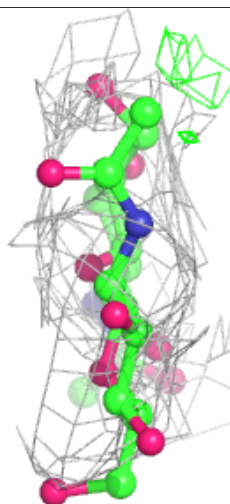
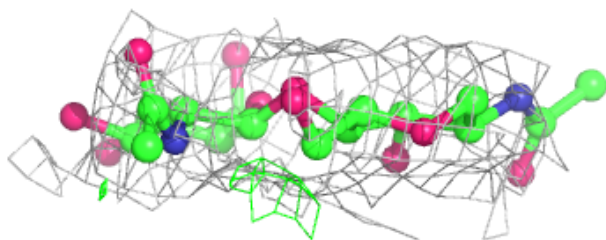
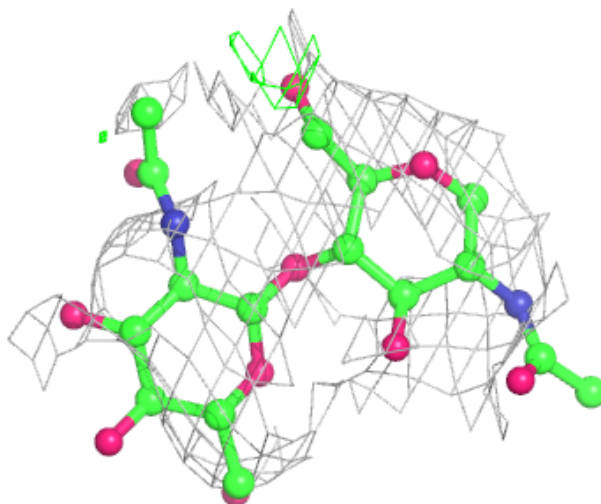
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	G	2	14/15	0.63	0.33	106,130,149,154	0
3	NAG	H	2	14/15	0.72	0.27	124,141,167,175	0
3	NAG	I	2	14/15	0.76	0.32	88,128,151,160	0
3	NAG	H	1	14/15	0.82	0.21	68,101,118,130	0
3	NAG	I	1	14/15	0.83	0.38	99,119,137,160	0
3	NAG	G	1	14/15	0.89	0.13	63,72,81,107	0

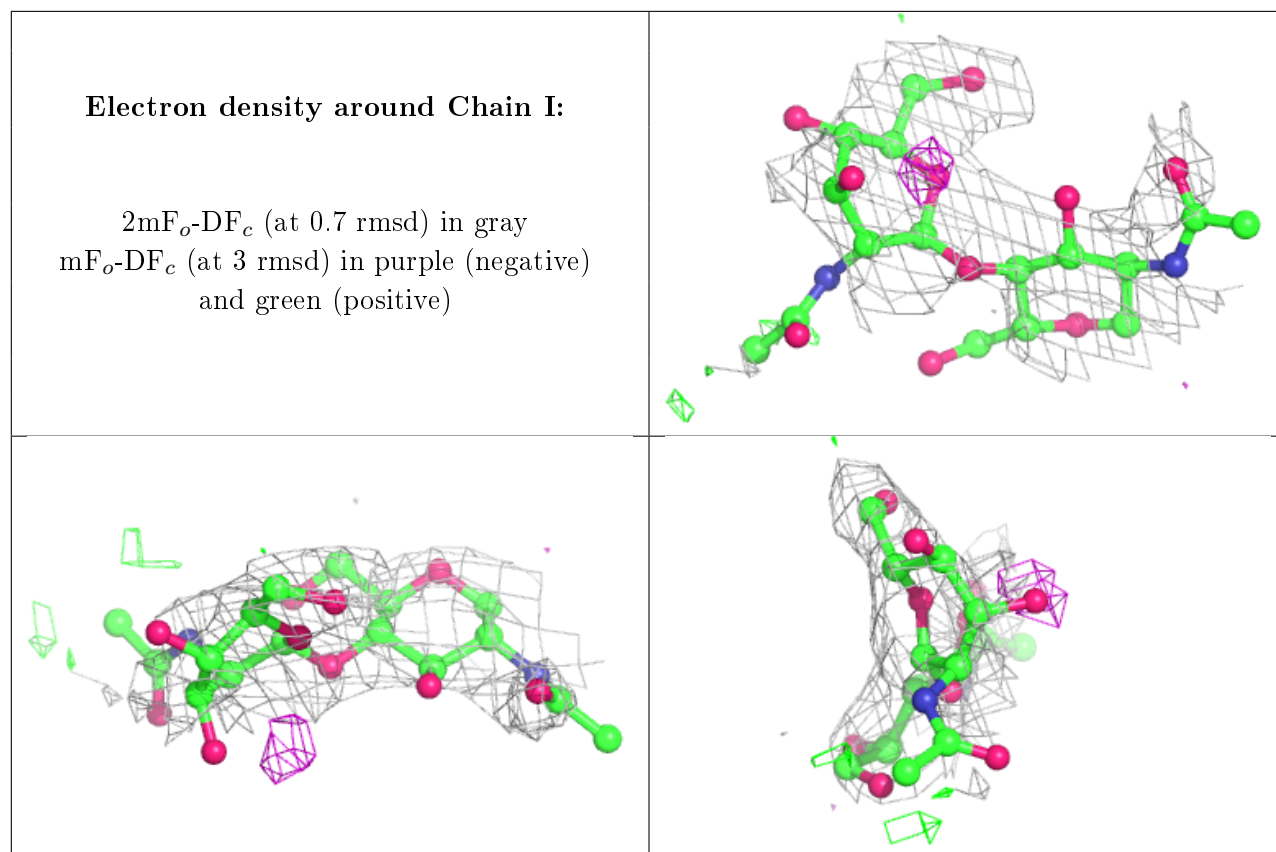
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain H:**

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





## 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	406	14/15	0.61	0.22	99,114,125,125	0
4	NAG	F	201	14/15	0.64	0.35	97,111,122,123	0
4	NAG	C	402	14/15	0.65	0.19	86,100,113,115	0
4	NAG	C	403	14/15	0.68	0.35	85,96,115,117	0
4	NAG	E	401	14/15	0.79	0.25	86,91,97,98	0
4	NAG	A	401	14/15	0.81	0.20	103,118,126,129	0
4	NAG	C	401	14/15	0.86	0.17	61,66,68,69	0
4	NAG	E	402	14/15	0.86	0.18	68,80,86,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.