



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2021 – 10:04 AM EDT

PDB ID : 6XPR  
Title : Human antibody D2 H1-1/H3-1 H3 in complex with the influenza hemagglutinin head domain of A/Texas/50/2012(H3N2)  
Authors : McCarthy, K.R.; Harrison, S.C.; Lee, J.  
Deposited on : 2020-07-08  
Resolution : 4.09 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 : 2.18  
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) : 2.18

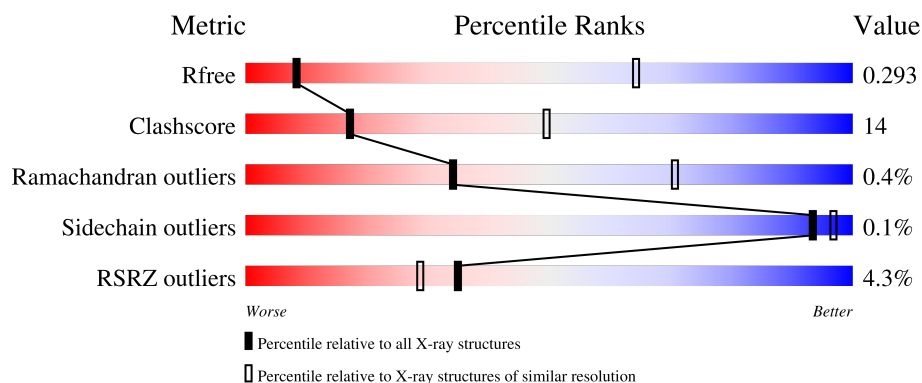
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.09 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	291	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>8%</div> </div> </div>
1	D	291	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>8%</div> </div> </div>
2	B	238	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• 5%</div> </div> </div>
2	E	238	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>7%</div> </div> </div>
3	C	214	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	214	
4	G	3	
4	H	3	
5	I	2	

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
4	BMA	H	3	-	-	-	X
6	NAG	D	401	-	-	-	X
6	NAG	D	402	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11025 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	269	Total	C	N	O	S	0	0	0
			2135	1347	378	400	10			
1	D	269	Total	C	N	O	S	0	0	0
			2135	1347	378	400	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP R4L1D1
A	321	ALA	-	expression tag	UNP R4L1D1
A	322	LEU	-	expression tag	UNP R4L1D1
A	323	GLU	-	expression tag	UNP R4L1D1
A	324	VAL	-	expression tag	UNP R4L1D1
A	325	LEU	-	expression tag	UNP R4L1D1
A	326	PHE	-	expression tag	UNP R4L1D1
A	327	GLN	-	expression tag	UNP R4L1D1
D	320	GLY	-	expression tag	UNP R4L1D1
D	321	ALA	-	expression tag	UNP R4L1D1
D	322	LEU	-	expression tag	UNP R4L1D1
D	323	GLU	-	expression tag	UNP R4L1D1
D	324	VAL	-	expression tag	UNP R4L1D1
D	325	LEU	-	expression tag	UNP R4L1D1
D	326	PHE	-	expression tag	UNP R4L1D1
D	327	GLN	-	expression tag	UNP R4L1D1

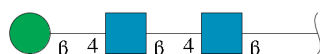
- Molecule 2 is a protein called antibody D2 H1-1/H3-1 H3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	226	Total	C	N	O	S	0	1	0
			1712	1080	297	329	6			
2	E	221	Total	C	N	O	S	0	0	0
			1667	1055	287	319	6			

- Molecule 3 is a protein called antibody D2 H1-1/H3-1 H3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1614	1009	271	329	5			
3	F	211	Total	C	N	O	S	0	0	0
			1614	1009	271	329	5			

- Molecule 4 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
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

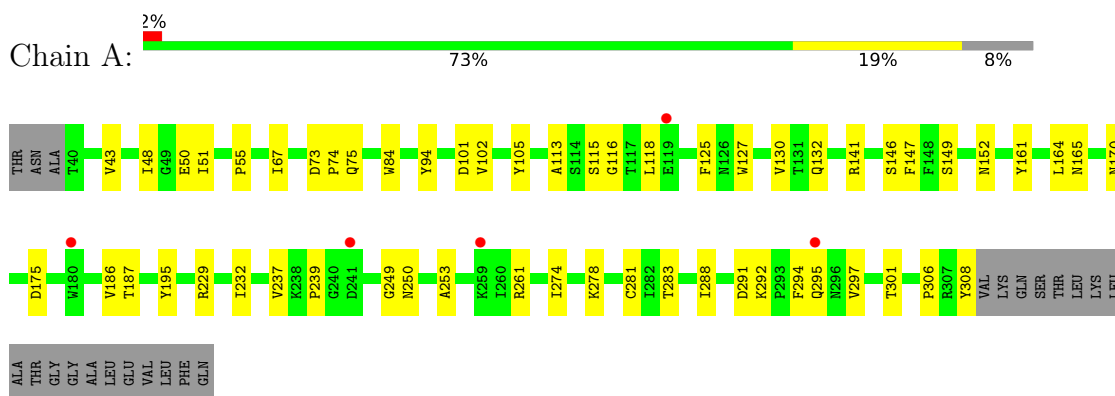


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

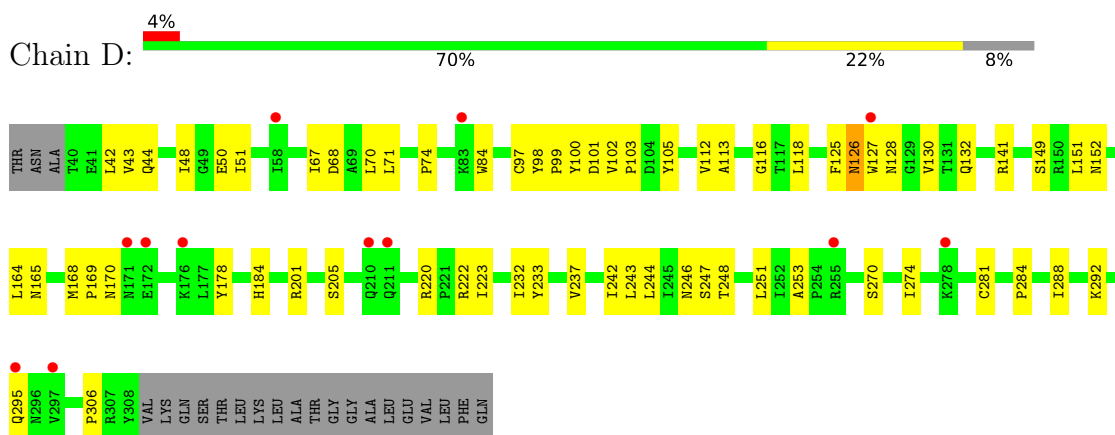
### 3 Residue-property plots [i](#)

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.

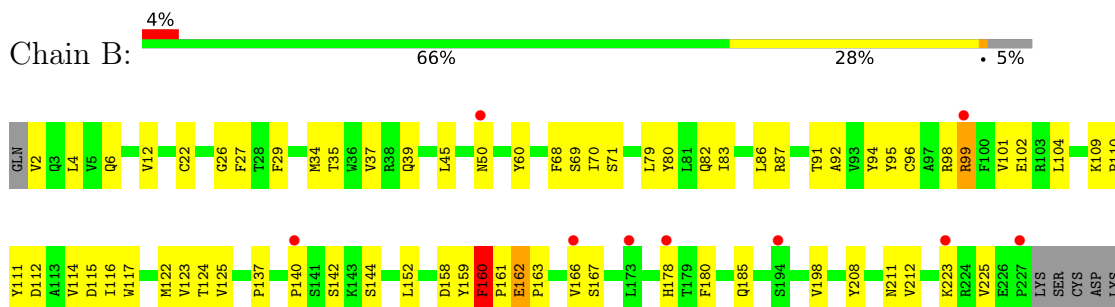
#### • Molecule 1: Hemagglutinin



#### • Molecule 1: Hemagglutinin



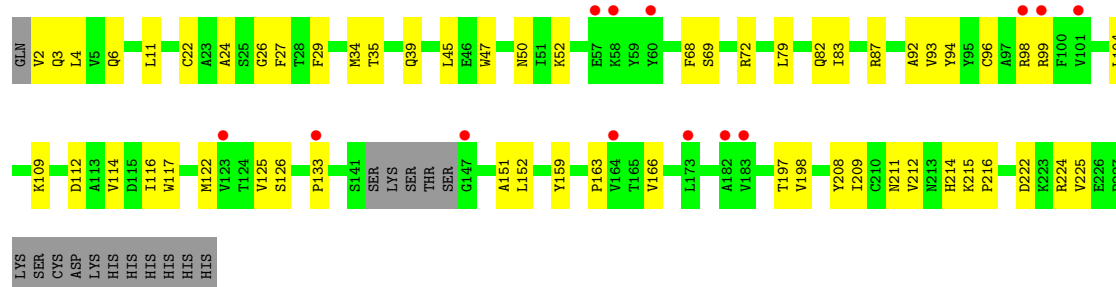
#### • Molecule 2: antibody D2 H1-1/H3-1 H3 heavy chain



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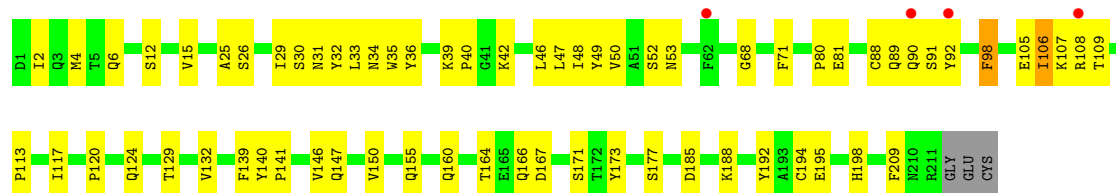
- Molecule 2: antibody D2 H1-1/H3-1 H3 heavy chain

Chain E: 5% 69% 24% 7%



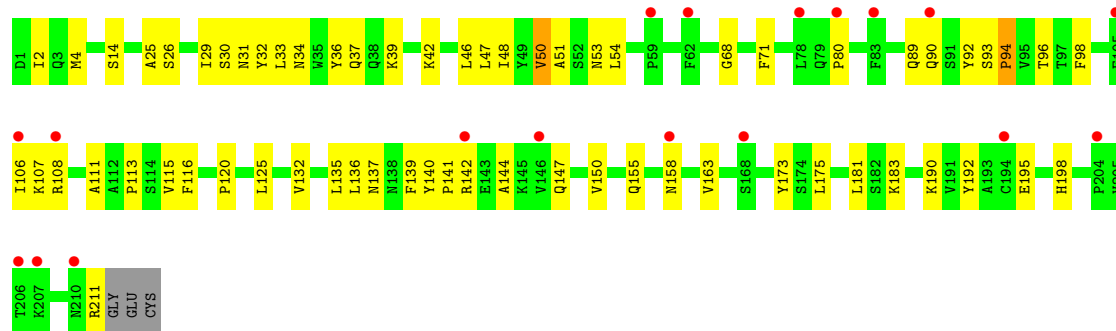
- Molecule 3: antibody D2 H1-1/H3-1 H3 light chain

Chain C: 2% 67% 30% ..



- Molecule 3: antibody D2 H1-1/H3-1 H3 light chain

Chain F: 8% 69% 29% ..



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

Chain G: 33% 33% 33%






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

Chain H:  100%

MAG1  
MAG2  
EMJ3

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

Chain I:  50% 50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.49Å 204.49Å 132.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 4.09 49.12 – 4.09	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.12-4.09) 98.6 (49.12-4.09)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.252 , 0.298 0.253 , 0.293	Depositor DCC
$R_{free}$ test set	1240 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.7	Xtriage
Anisotropy	0.790	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.139 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	11025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: 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	0.25	0/2189	0.47	0/2975
1	D	0.25	0/2189	0.46	0/2975
2	B	0.27	0/1753	0.53	0/2384
2	E	0.26	0/1707	0.50	0/2322
3	C	0.32	0/1648	0.57	1/2238 (0.0%)
3	F	0.31	0/1648	0.52	0/2238
All	All	0.28	0/11134	0.50	1/15132 (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
2	B	0	2
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	106	ILE	CG1-CB-CG2	-6.09	98.00	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	160	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	B	162	GLU	Peptide
3	C	98	PHE	Peptide

## 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	2135	0	2079	40	0
1	D	2135	0	2079	49	0
2	B	1712	0	1687	60	0
2	E	1667	0	1639	41	0
3	C	1614	0	1573	73	0
3	F	1614	0	1573	58	0
4	G	39	0	34	1	0
4	H	39	0	34	0	0
5	I	28	0	25	1	0
6	A	14	0	13	1	0
6	D	28	0	26	0	0
All	All	11025	0	10762	302	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 14.

The worst 5 of 302 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:295:GLN:HB2	1:A:306:PRO:HG2	1.58	0.85
3:F:2:ILE:HG23	3:F:26:SER:HB3	1.57	0.85
3:C:4:MET:HE3	3:C:25:ALA:HB2	1.58	0.84
3:F:94:PRO:HG2	3:F:96:THR:HG23	1.61	0.83
2:B:185:GLN:HA	3:C:160:GLN:HE22	1.44	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/291 (92%)	250 (94%)	17 (6%)	0	100	100
1	D	267/291 (92%)	250 (94%)	17 (6%)	0	100	100
2	B	225/238 (94%)	205 (91%)	17 (8%)	3 (1%)	12	47
2	E	217/238 (91%)	199 (92%)	17 (8%)	1 (0%)	29	67
3	C	209/214 (98%)	188 (90%)	21 (10%)	0	100	100
3	F	209/214 (98%)	187 (90%)	20 (10%)	2 (1%)	15	52
All	All	1394/1486 (94%)	1279 (92%)	109 (8%)	6 (0%)	34	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	163	PRO
2	B	160	PHE
2	B	99	ARG
3	F	94	PRO
3	F	50	VAL

### 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	241/258 (93%)	241 (100%)	0	100	100
1	D	241/258 (93%)	240 (100%)	1 (0%)	91	94
2	B	189/200 (94%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	183/200 (92%)	183 (100%)	0	100	100
3	C	186/188 (99%)	186 (100%)	0	100	100
3	F	186/188 (99%)	186 (100%)	0	100	100
All	All	1226/1292 (95%)	1225 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	126	ASN

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

Mol	Chain	Res	Type
1	D	246	ASN
2	E	6	GLN
3	F	124	GLN
3	F	90	GLN
3	C	38	GLN

### 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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	1	1,4	14,14,15	0.48	0	17,19,21	0.76	1 (5%)
4	NAG	G	2	4	14,14,15	0.53	0	17,19,21	1.32	1 (5%)
4	BMA	G	3	4	11,11,12	0.66	0	15,15,17	0.93	0
4	NAG	H	1	1,4	14,14,15	0.22	0	17,19,21	0.59	0
4	NAG	H	2	4	14,14,15	0.38	0	17,19,21	0.46	0
4	BMA	H	3	4	11,11,12	0.71	0	15,15,17	0.71	0
5	NAG	I	1	5,1	14,14,15	0.26	0	17,19,21	0.60	1 (5%)
5	NAG	I	2	5	14,14,15	0.56	0	17,19,21	1.23	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	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(°)
4	G	2	NAG	C2-N2-C7	4.59	129.44	122.90
5	I	2	NAG	C2-N2-C7	4.27	128.98	122.90
4	G	1	NAG	C1-O5-C5	2.10	115.03	112.19
5	I	1	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

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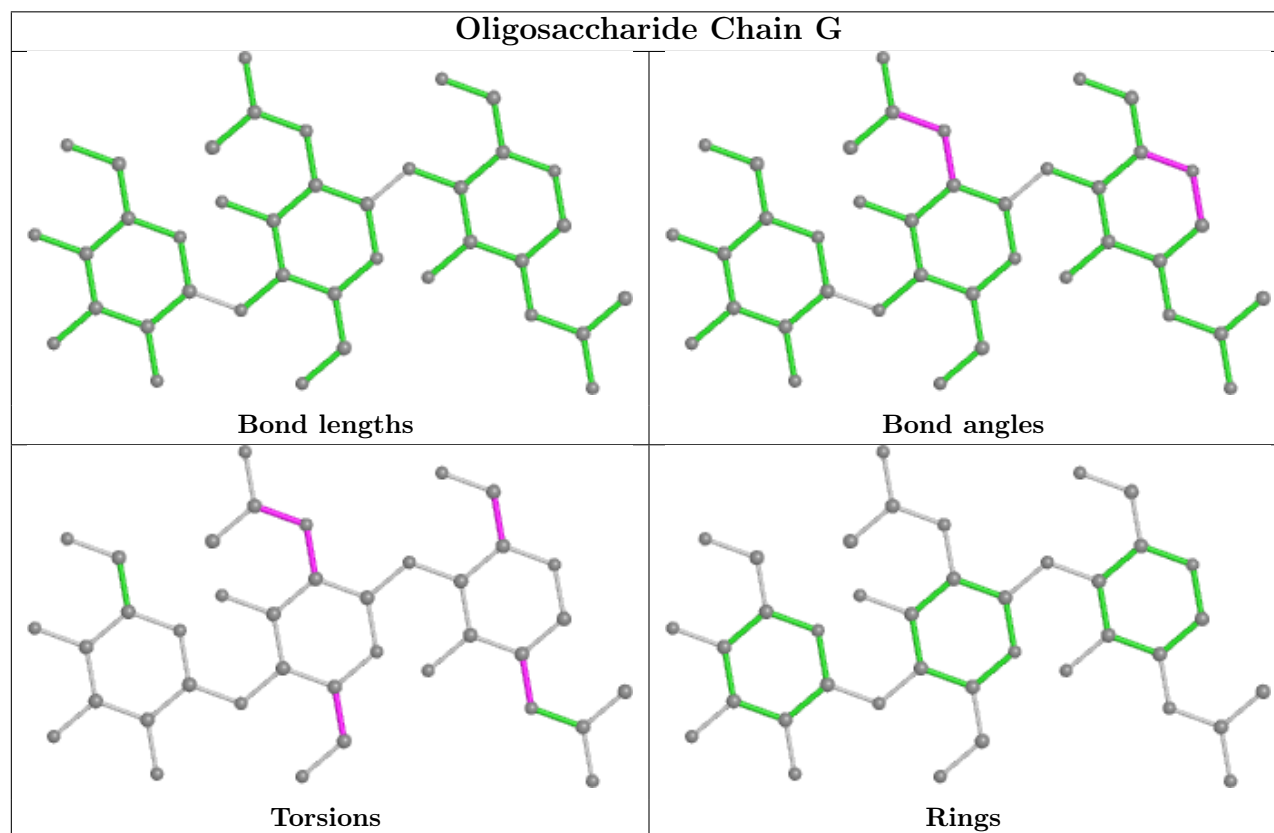
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2

There are no ring outliers.

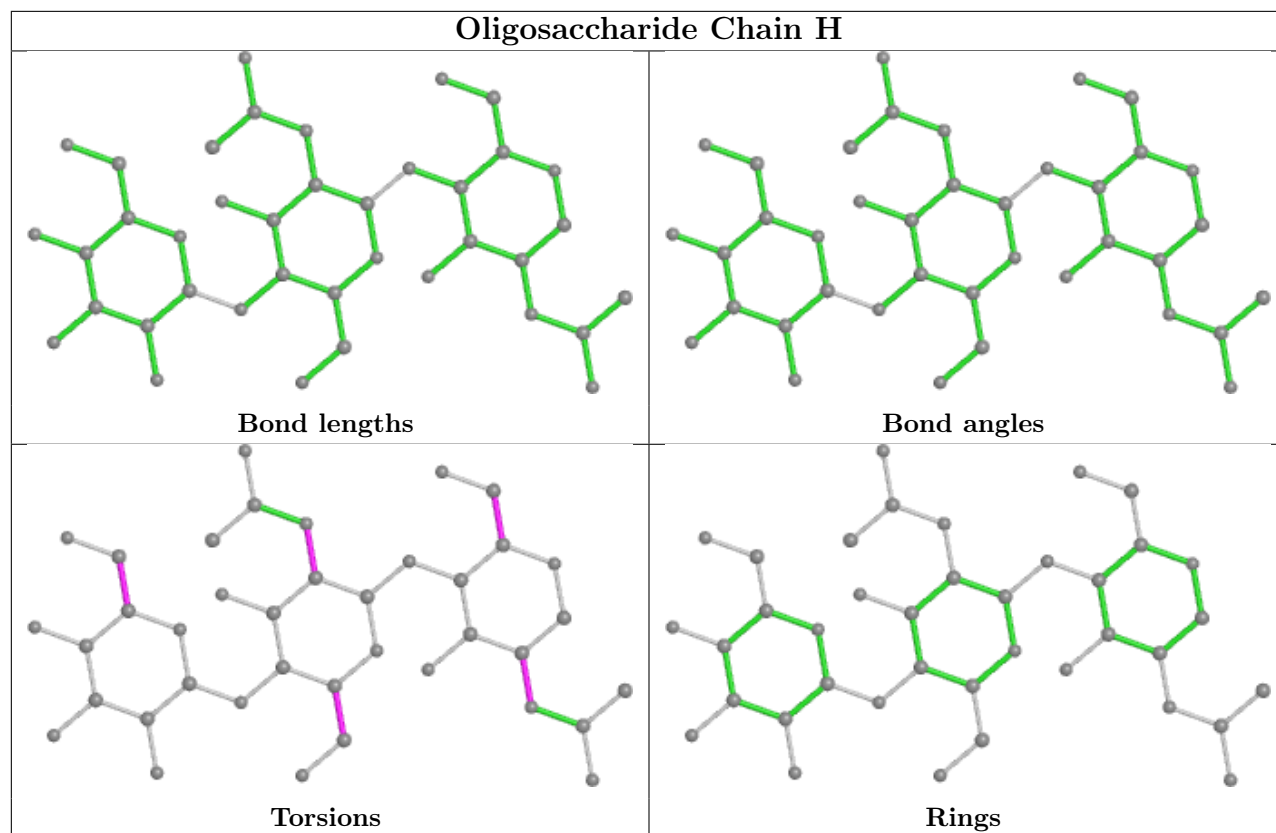
2 monomers are involved in 2 short contacts:

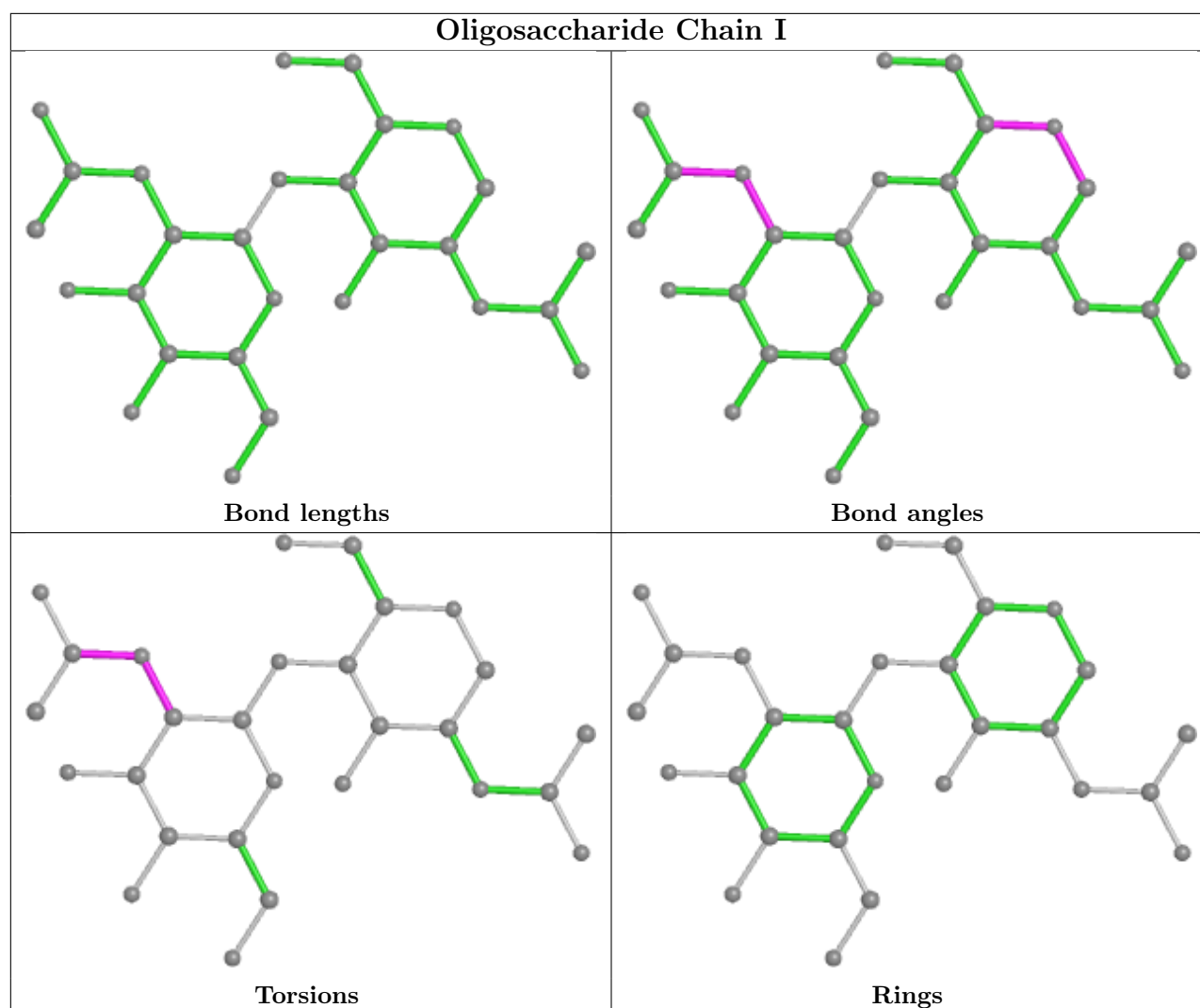
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	1	0
4	G	2	NAG	1	0

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](#)

3 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	$\# Z  > 2$
6	NAG	D	402	1	14,14,15	0.32	0	17,19,21	0.49	0
6	NAG	A	401	1	14,14,15	0.30	0	17,19,21	0.59	0
6	NAG	D	401	1	14,14,15	0.19	0	17,19,21	0.93	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	402	1	-	0/6/23/26	0/1/1/1
6	NAG	A	401	1	-	1/6/23/26	0/1/1/1
6	NAG	D	401	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	401	NAG	C2-N2-C7	2.73	126.79	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	401	NAG	C3-C2-N2-C7
6	D	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C3-C2-N2-C7
6	D	401	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
6	A	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	269/291 (92%)	0.40	5 (1%) 66 58	72, 110, 136, 161	0
1	D	269/291 (92%)	0.55	12 (4%) 33 27	77, 124, 156, 168	0
2	B	226/238 (94%)	0.42	9 (3%) 38 30	82, 129, 156, 172	0
2	E	221/238 (92%)	0.51	13 (5%) 22 18	84, 139, 176, 191	0
3	C	211/214 (98%)	0.49	4 (1%) 66 58	72, 125, 159, 176	0
3	F	211/214 (98%)	0.68	18 (8%) 10 10	117, 159, 187, 213	0
All	All	1407/1486 (94%)	0.50	61 (4%) 35 29	72, 129, 172, 213	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	142	ARG	4.5
3	F	80	PRO	4.4
1	D	210	GLN	4.4
3	F	194	CYS	3.6
1	D	172	GLU	3.5

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

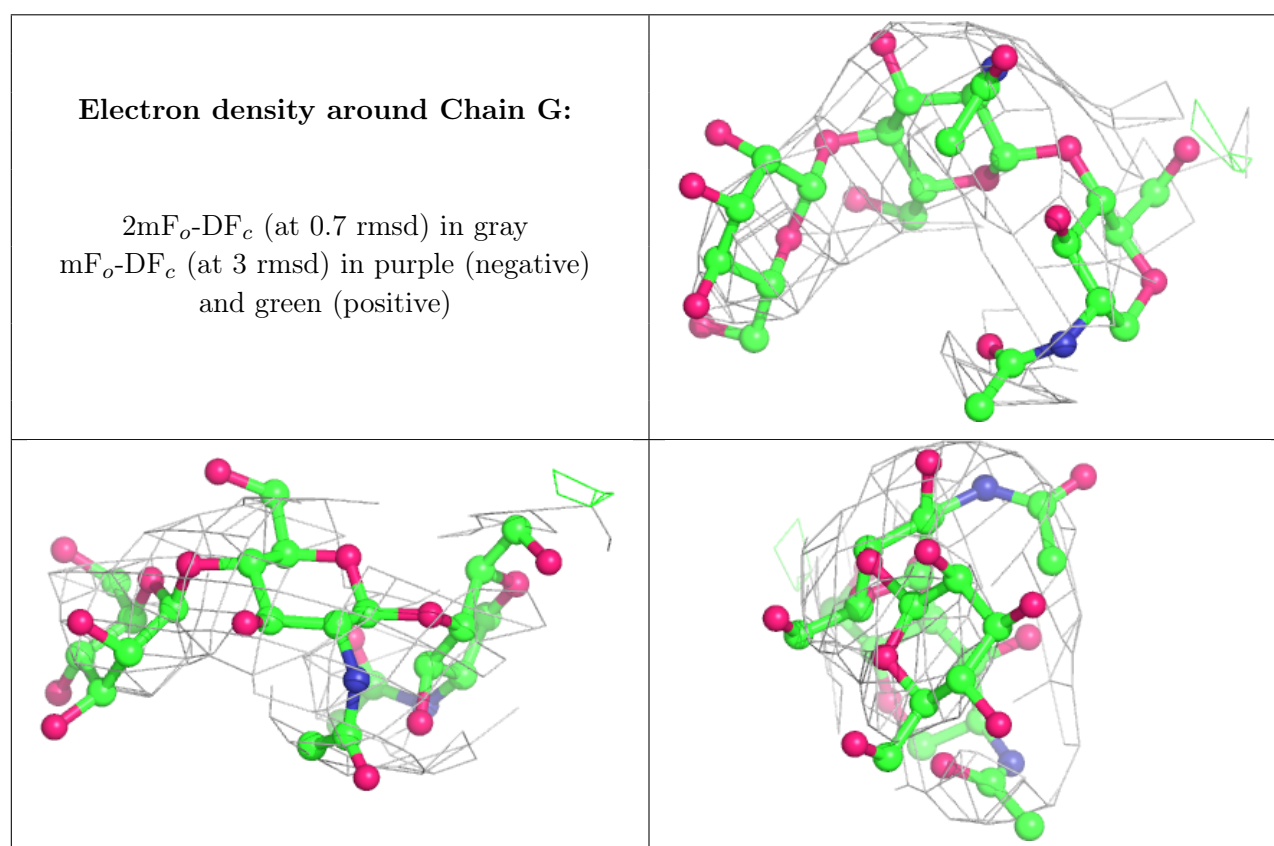
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

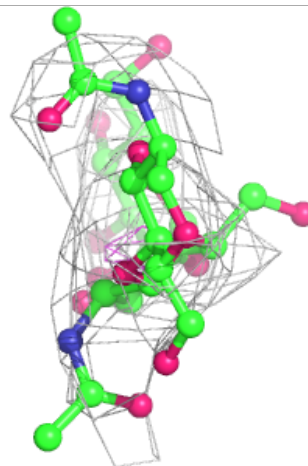
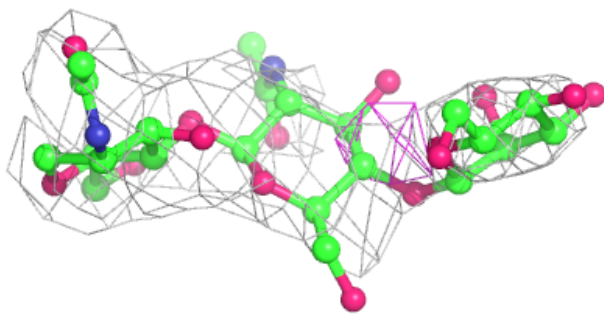
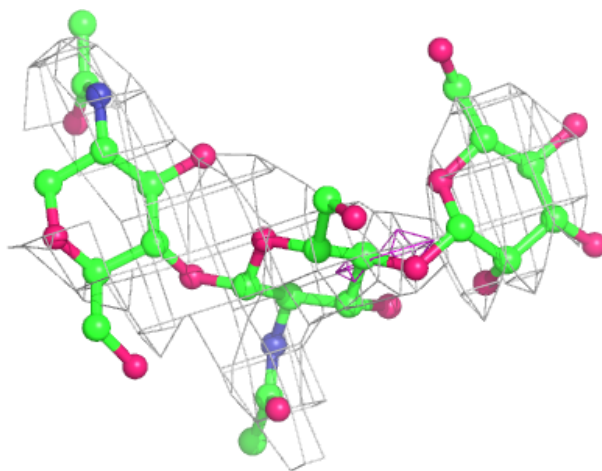
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	I	2	14/15	0.75	0.35	80,175,198,204	0
4	BMA	H	3	11/12	0.77	0.75	152,178,201,208	0
4	NAG	H	2	14/15	0.80	0.64	146,172,203,210	0
5	NAG	I	1	14/15	0.87	0.25	80,139,173,183	0
4	BMA	G	3	11/12	0.87	0.66	177,220,231,238	0
4	NAG	G	2	14/15	0.89	0.33	161,183,212,228	0
4	NAG	G	1	14/15	0.89	0.25	118,155,178,185	0
4	NAG	H	1	14/15	0.92	0.41	113,170,184,186	0

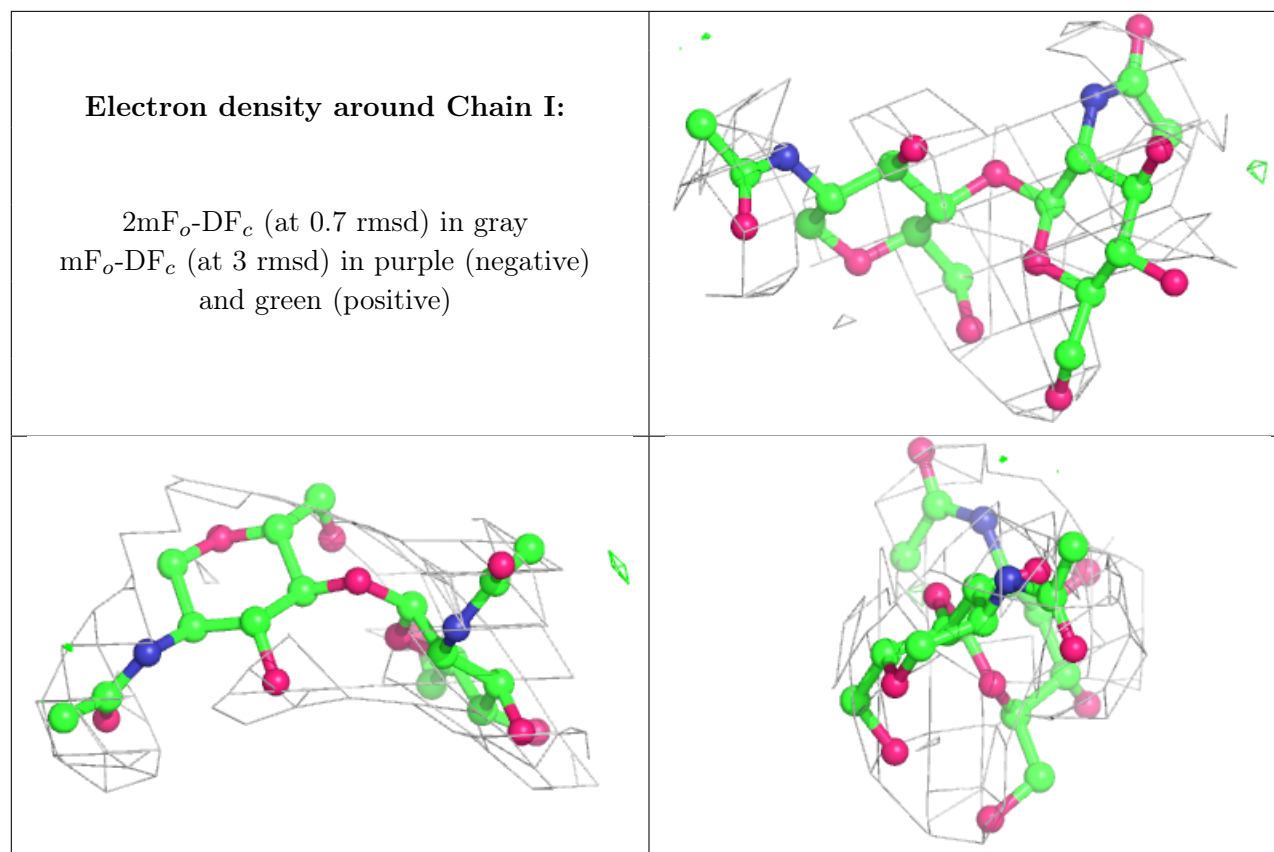
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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
6	NAG	D	402	14/15	0.65	0.43	97,150,172,176	0
6	NAG	A	401	14/15	0.76	0.28	100,161,177,179	0
6	NAG	D	401	14/15	0.80	0.64	123,159,184,213	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.