



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:01 AM UTC

PDB ID : 4EEF / pdb\_00004eef  
Title : Crystal structure of the designed inhibitor protein F-HB80.4 in complex with the 1918 influenza virus hemagglutinin.  
Authors : Dreyfus, C.; Wilson, I.A.  
Deposited on : 2012-03-28  
Resolution : 2.70 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

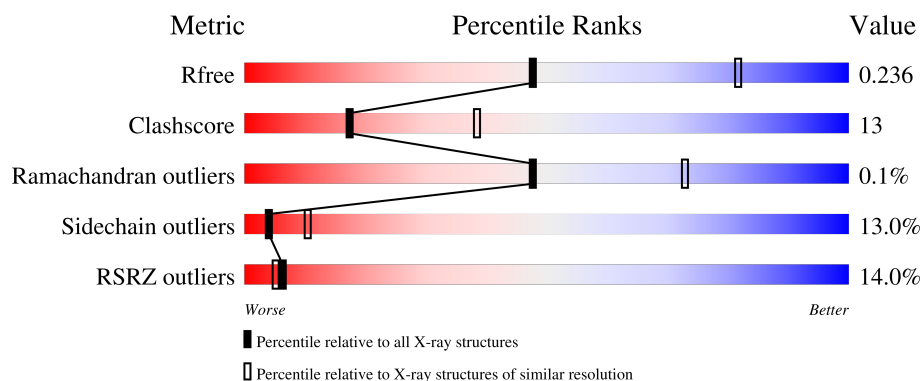
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	331	<div> <div>5%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	C	331	<div> <div>2%</div> <div>70%</div> <div>25%</div> <div>..</div> </div>
1	E	331	<div> <div>6%</div> <div>66%</div> <div>27%</div> <div>5%</div> <div>.</div> </div>
2	B	179	<div> <div>27%</div> <div>56%</div> <div>31%</div> <div>8%</div> <div>..</div> </div>
2	D	179	<div> <div>21%</div> <div>58%</div> <div>34%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	179	<div><div></div><div>27%</div><div>46%</div><div>42%</div><div>7%</div><div></div></div>
3	G	74	<div><div></div><div>28%</div><div>45%</div><div>14%</div><div></div><div>39%</div></div>
3	H	74	<div><div></div><div>15%</div><div>55%</div><div>7%</div><div></div><div>36%</div></div>
3	I	74	<div><div></div><div>24%</div><div>46%</div><div>18%</div><div></div><div>36%</div></div>
4	J	3	<div><div></div><div>33%</div><div>67%</div></div>
4	K	3	<div><div></div><div>33%</div><div>67%</div></div>
4	L	3	<div><div></div><div>33%</div><div>33%</div><div>33%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12880 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	A	325	Total	C	N	O	S	8	2	0
			2529	1594	434	490	11			
1	C	323	Total	C	N	O	S	6	1	0
			2510	1583	431	485	11			
1	E	323	Total	C	N	O	S	0	1	0
			2512	1583	432	486	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	THR	conflict	UNP Q9WFX3
A	9	PRO	ASN	conflict	UNP Q9WFX3
A	10	GLY	ALA	conflict	UNP Q9WFX3
C	8	ASP	THR	conflict	UNP Q9WFX3
C	9	PRO	ASN	conflict	UNP Q9WFX3
C	10	GLY	ALA	conflict	UNP Q9WFX3
E	8	ASP	THR	conflict	UNP Q9WFX3
E	9	PRO	ASN	conflict	UNP Q9WFX3
E	10	GLY	ALA	conflict	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1394	871	239	278	6			
2	D	173	Total	C	N	O	S	5	1	0
			1399	874	240	279	6			
2	F	171	Total	C	N	O	S	0	1	0
			1382	863	238	275	6			

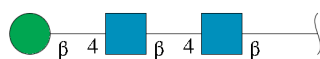
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP Q9WFX3
B	178	GLY	-	expression tag	UNP Q9WFX3
B	179	ARG	-	expression tag	UNP Q9WFX3
D	177	SER	-	expression tag	UNP Q9WFX3
D	178	GLY	-	expression tag	UNP Q9WFX3
D	179	ARG	-	expression tag	UNP Q9WFX3
F	177	SER	-	expression tag	UNP Q9WFX3
F	178	GLY	-	expression tag	UNP Q9WFX3
F	179	ARG	-	expression tag	UNP Q9WFX3

- Molecule 3 is a protein called F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	45	Total	C	N	O	0	0	0
			301	195	49	57			
3	H	47	Total	C	N	O	0	0	0
			303	195	53	55			
3	I	47	Total	C	N	O	0	0	0
			294	187	53	54			

- 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	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	13	Total	O	0	0
			13	13		

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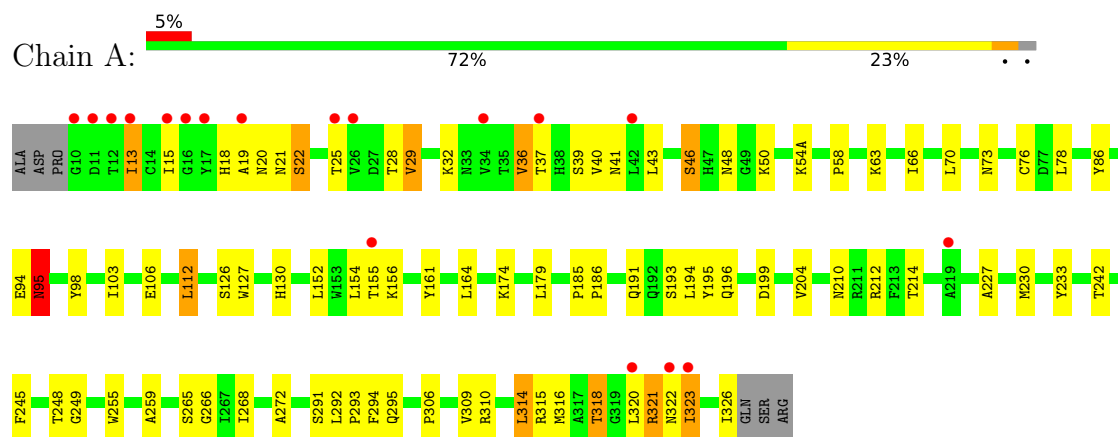
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	37	Total 37	O 37	0	0
5	D	7	Total 7	O 7	0	0
5	E	23	Total 23	O 23	0	0
5	F	9	Total 9	O 9	0	0

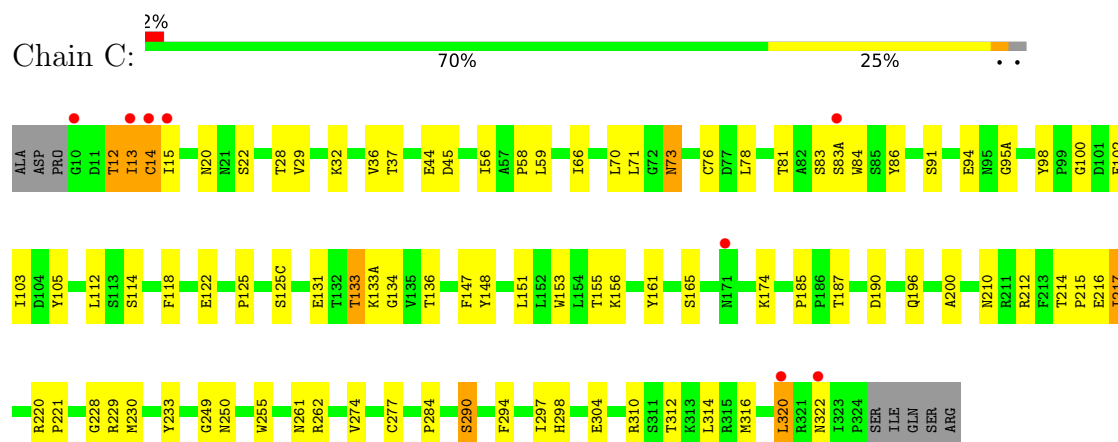
### 3 Residue-property plots [i](#)

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.

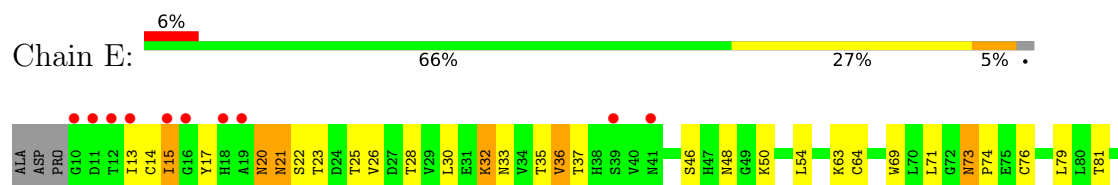
- Molecule 1: Hemagglutinin HA1 chain

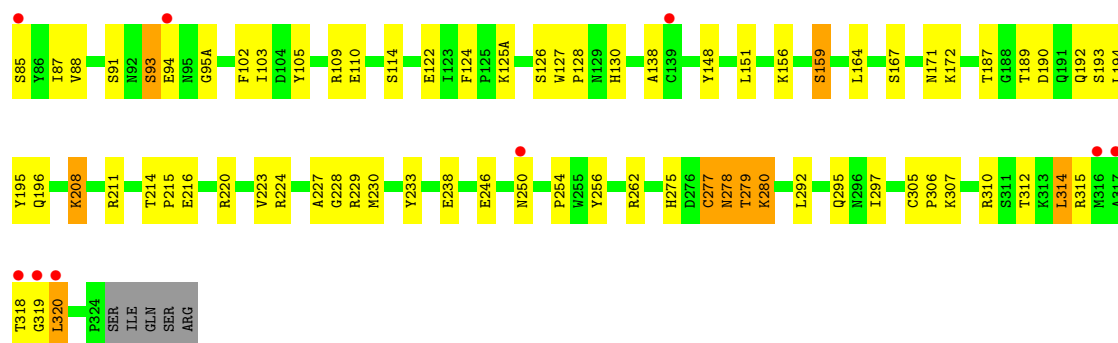


- Molecule 1: Hemagglutinin HA1 chain

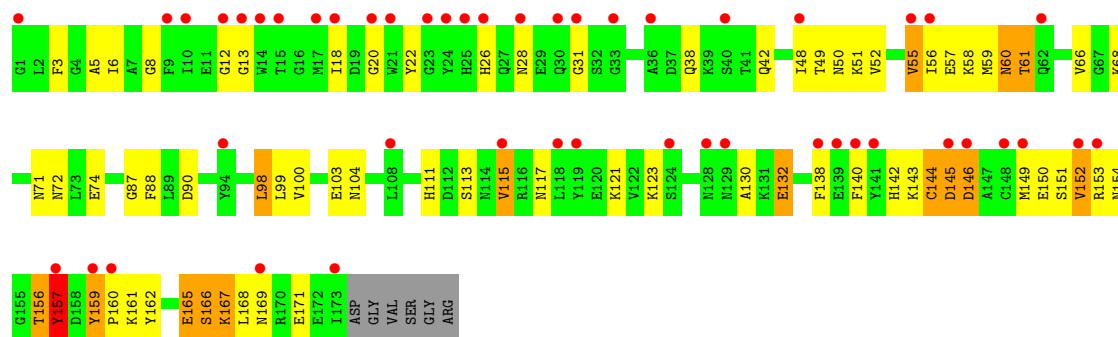


- Molecule 1: Hemagglutinin HA1 chain

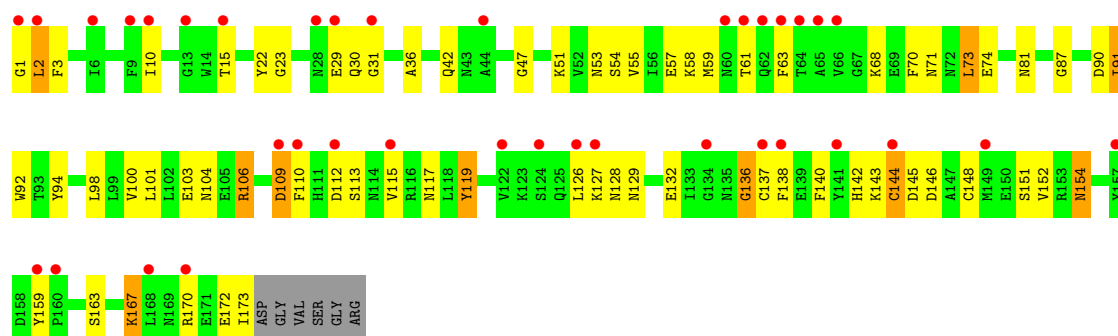




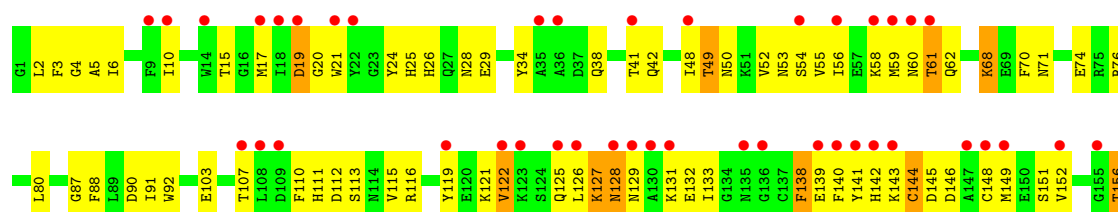
• Molecule 2: Hemagglutinin HA2 chain



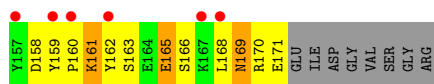
• Molecule 2: Hemagglutinin HA2 chain



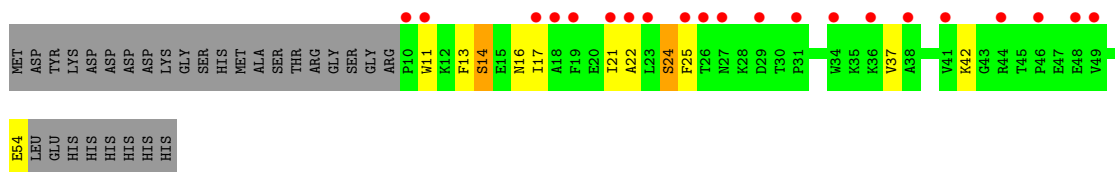
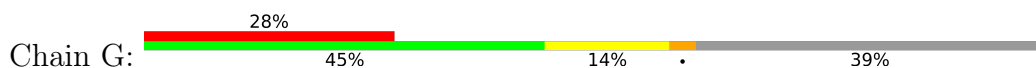
• Molecule 2: Hemagglutinin HA2 chain



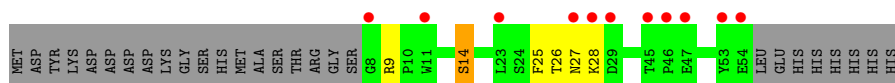




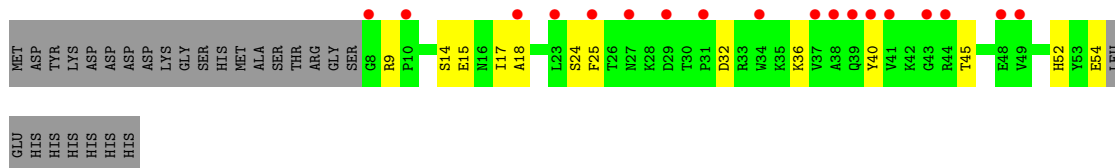
- Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN



- Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN



- Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN



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



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



- Molecule 4: 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	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.33Å 126.15Å 243.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 2.70 43.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.1 (43.67-2.70) 90.1 (43.67-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.09 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.229 , 0.285 0.232 , 0.236	Depositor DCC
$R_{free}$ test set	2953 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.0	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	0.92	EDS
Total number of atoms	12880	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.62	0/2596	1.00	10/3536 (0.3%)
1	C	0.62	0/2577	1.01	8/3510 (0.2%)
1	E	0.58	0/2576	0.97	8/3509 (0.2%)
2	B	0.51	0/1421	1.01	5/1913 (0.3%)
2	D	0.49	0/1429	0.93	4/1924 (0.2%)
2	F	0.48	0/1412	0.96	3/1901 (0.2%)
3	G	0.53	0/308	1.16	2/421 (0.5%)
3	H	0.40	0/309	1.06	1/423 (0.2%)
3	I	0.40	0/299	1.12	2/409 (0.5%)
All	All	0.56	0/12927	0.99	43/17546 (0.2%)

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
2	B	0	1
2	F	0	2
3	G	0	1
3	H	0	3
3	I	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	45	THR	CA-C-N	7.78	129.57	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	45	THR	C-N-CA	7.78	129.57	119.84
2	F	163	SER	N-CA-C	7.75	121.84	112.38
2	B	31	GLY	N-CA-C	7.09	120.52	111.09
1	A	272	ALA	CA-C-N	7.00	126.92	119.85

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	ASN	Peptide
2	B	157	TYR	Peptide
2	F	144	CYS	Peptide
2	F	168	LEU	Peptide
3	G	42	LYS	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	2529	0	2453	49	0
1	C	2510	0	2435	53	0
1	E	2512	0	2431	78	0
2	B	1394	0	1312	63	0
2	D	1399	0	1318	53	0
2	F	1382	0	1300	79	0
3	G	301	0	212	9	0
3	H	303	0	217	1	0
3	I	294	0	203	8	0
4	J	39	0	34	0	0
4	K	39	0	34	0	0
4	L	39	0	34	1	0
5	A	50	0	0	0	0
5	B	13	0	0	0	0
5	C	37	0	0	1	0
5	D	7	0	0	0	0
5	E	23	0	0	3	0
5	F	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12880	0	11983	309	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 13.

The worst 5 of 309 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:E:307:LYS:CD	2:F:59:MET:HE1	1.58	1.31
1:E:307:LYS:HD2	2:F:59:MET:CE	1.70	1.19
2:D:70:PHE:HA	2:D:74:GLU:OE1	1.51	1.10
1:E:307:LYS:CD	2:F:59:MET:CE	2.25	1.10
3:G:14:SER:HA	3:G:17:ILE:HD12	1.32	1.10

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	325/331 (98%)	316 (97%)	9 (3%)	0	100	100
1	C	322/331 (97%)	314 (98%)	8 (2%)	0	100	100
1	E	322/331 (97%)	309 (96%)	13 (4%)	0	100	100
2	B	171/179 (96%)	160 (94%)	11 (6%)	0	100	100
2	D	172/179 (96%)	162 (94%)	10 (6%)	0	100	100
2	F	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
3	G	43/74 (58%)	39 (91%)	4 (9%)	0	100	100
3	H	45/74 (61%)	41 (91%)	3 (7%)	1 (2%)	5	14
3	I	45/74 (61%)	40 (89%)	5 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1615/1752 (92%)	1538 (95%)	76 (5%)	1 (0%)	48 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	26	THR

### 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	282/285 (99%)	253 (90%)	29 (10%)	7 18
1	C	279/285 (98%)	252 (90%)	27 (10%)	8 20
1	E	279/285 (98%)	246 (88%)	33 (12%)	5 13
2	B	148/152 (97%)	123 (83%)	25 (17%)	2 6
2	D	149/152 (98%)	124 (83%)	25 (17%)	2 6
2	F	147/152 (97%)	122 (83%)	25 (17%)	2 6
3	G	18/66 (27%)	13 (72%)	5 (28%)	0 1
3	H	17/66 (26%)	16 (94%)	1 (6%)	18 42
3	I	15/66 (23%)	13 (87%)	2 (13%)	4 10
All	All	1334/1509 (88%)	1162 (87%)	172 (13%)	4 10

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	36	VAL
2	F	41	THR
1	E	93	SER
1	E	275	HIS
2	F	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	ASN
1	E	250	ASN
1	E	60	GLN
2	F	53	ASN
1	C	171	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 ⓘ

9 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	J	1	1,4	14,14,15	0.48	0	17,19,21	2.21	4 (23%)
4	NAG	J	2	4	14,14,15	0.60	0	17,19,21	1.74	3 (17%)
4	BMA	J	3	4	11,11,12	0.59	0	15,15,17	0.80	0
4	NAG	K	1	1,4	14,14,15	0.71	0	17,19,21	2.32	5 (29%)
4	NAG	K	2	4	14,14,15	0.73	1 (7%)	17,19,21	1.54	2 (11%)
4	BMA	K	3	4	11,11,12	0.66	0	15,15,17	0.87	0
4	NAG	L	1	1,4	14,14,15	0.48	0	17,19,21	1.69	4 (23%)
4	NAG	L	2	4	14,14,15	0.72	0	17,19,21	1.33	2 (11%)
4	BMA	L	3	4	11,11,12	0.60	0	15,15,17	0.65	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
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	NAG	O5-C1	-2.09	1.40	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C1-O5-C5	7.11	121.72	112.19
4	K	1	NAG	C1-O5-C5	6.85	121.37	112.19
4	J	2	NAG	C1-O5-C5	4.75	118.55	112.19
4	L	1	NAG	O5-C5-C6	4.73	116.86	107.66
4	L	2	NAG	C2-N2-C7	-3.95	117.61	122.90

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

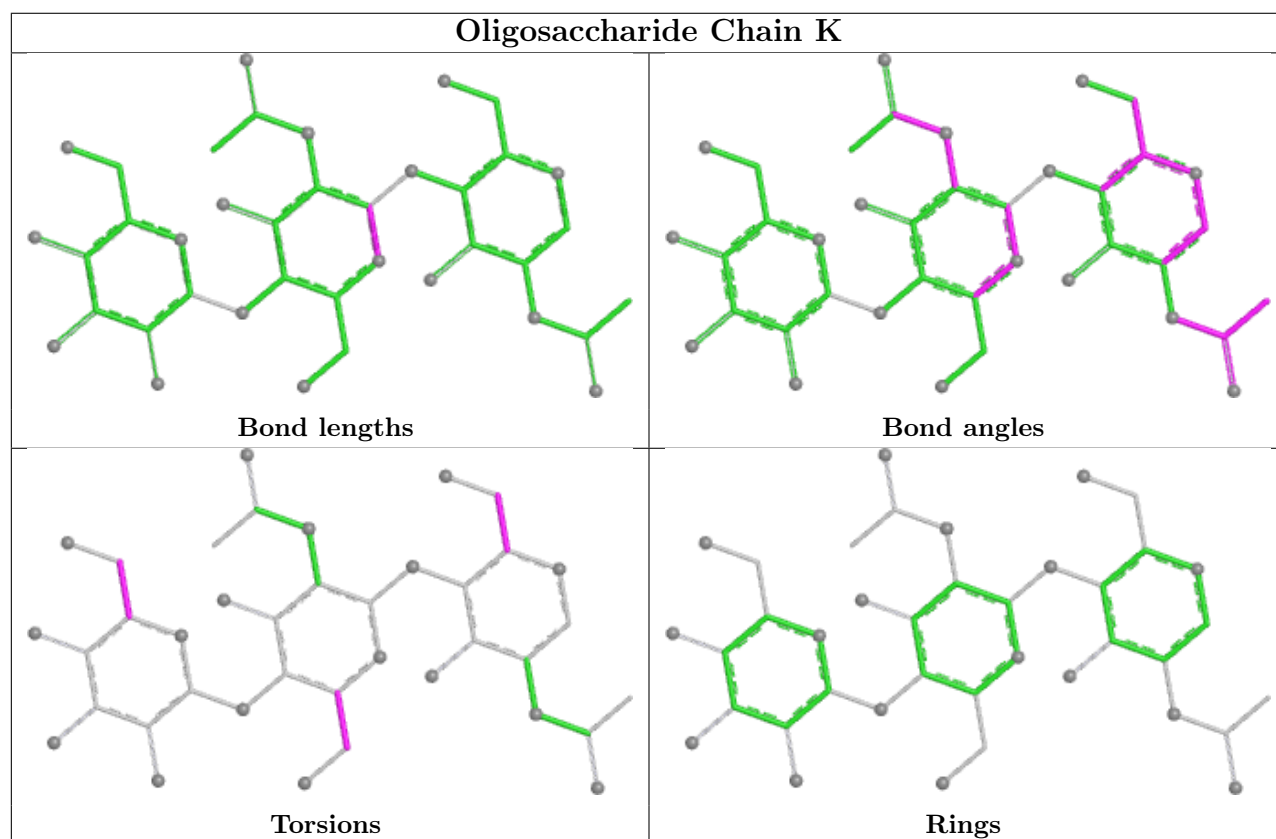
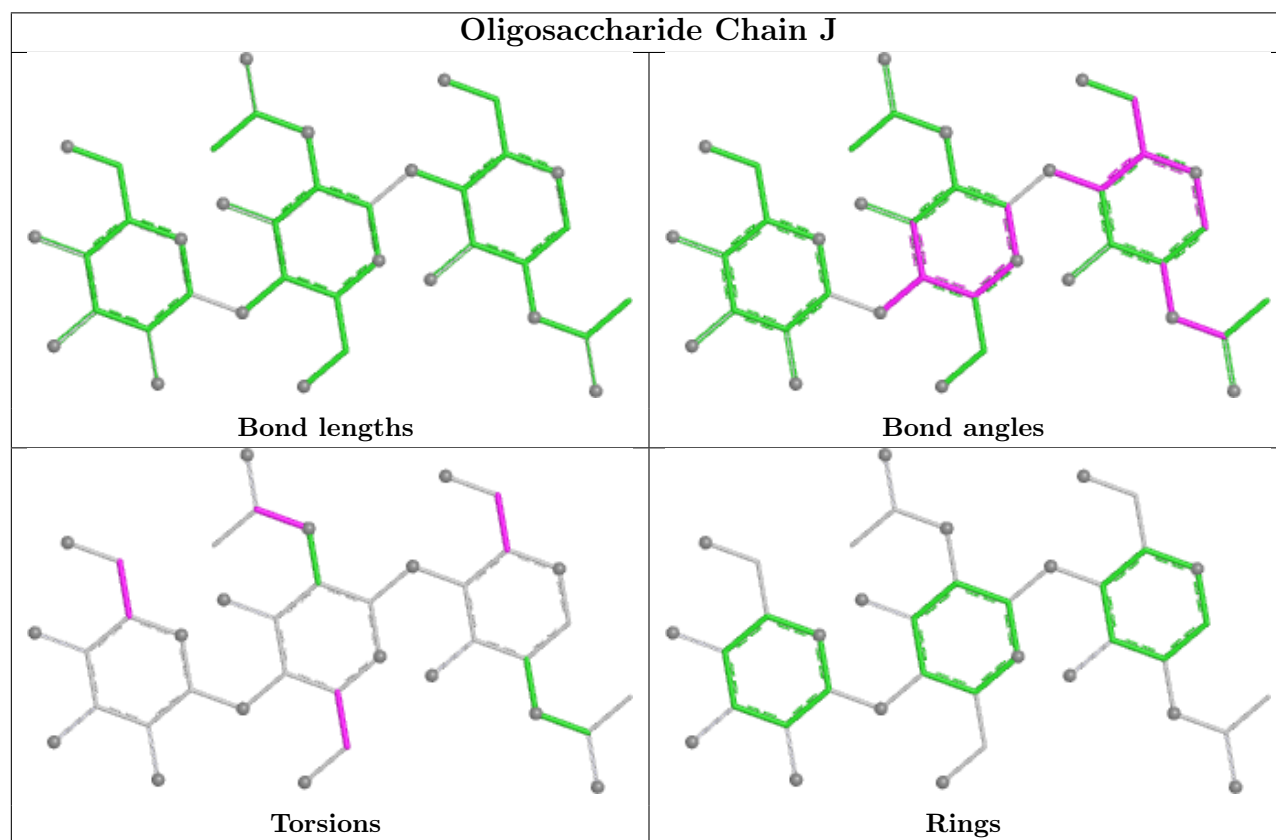
Mol	Chain	Res	Type	Atoms
4	K	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O5-C5-C6-O6

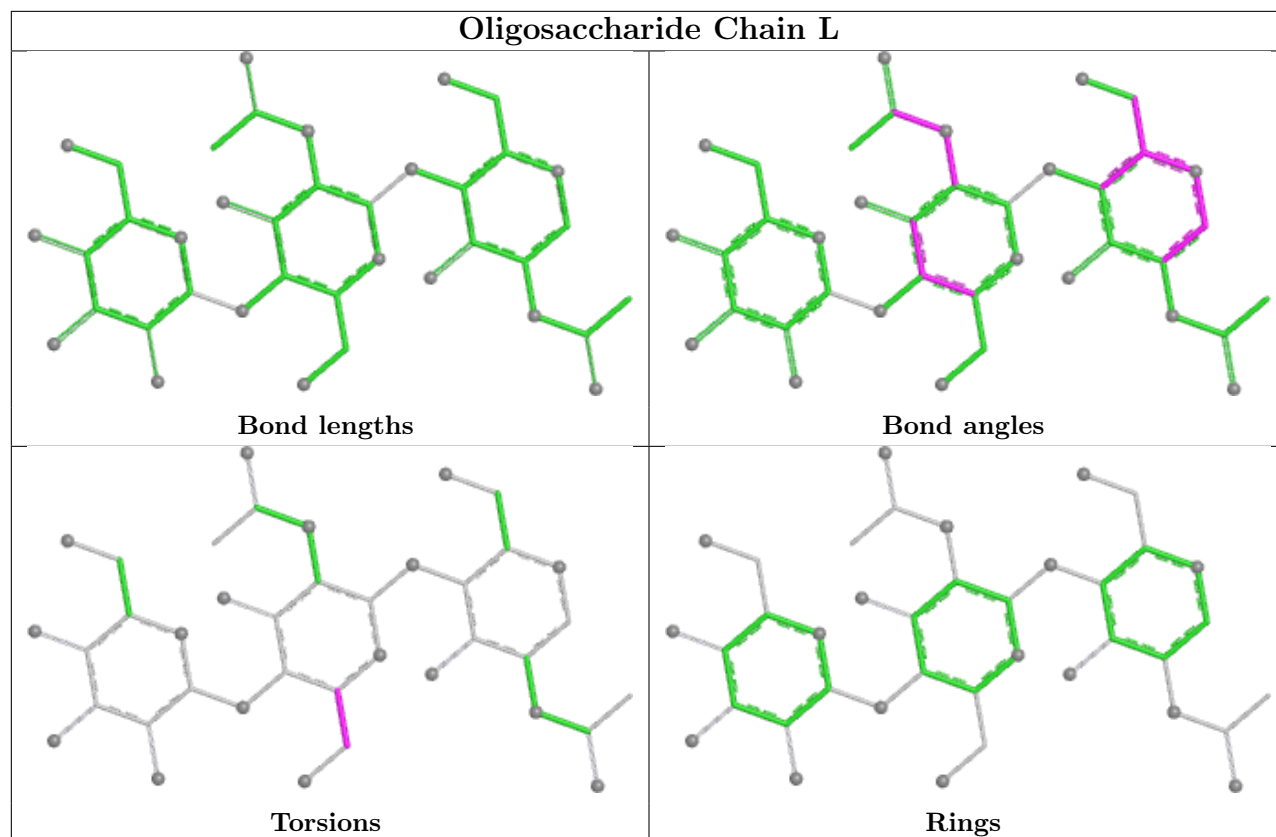
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	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](#)

There are no ligands in this entry.

## 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	325/331 (98%)	0.13	18 (5%)	30 27	25, 53, 103, 161	2 (0%)
1	C	323/331 (97%)	0.18	8 (2%)	58 55	23, 58, 97, 120	1 (0%)
1	E	323/331 (97%)	0.32	19 (5%)	28 25	34, 62, 106, 155	1 (0%)
2	B	173/179 (96%)	1.29	48 (27%)	1 1	36, 105, 151, 174	0
2	D	173/179 (96%)	1.13	37 (21%)	2 2	28, 102, 129, 153	1 (0%)
2	F	171/179 (95%)	1.40	48 (28%)	1 1	28, 119, 172, 183	1 (0%)
3	G	45/74 (60%)	2.06	21 (46%)	0 0	63, 121, 145, 159	0
3	H	47/74 (63%)	1.26	11 (23%)	2 2	100, 125, 158, 186	0
3	I	47/74 (63%)	1.70	18 (38%)	1 0	111, 156, 179, 208	0
All	All	1627/1752 (92%)	0.67	228 (14%)	6 5	23, 74, 153, 208	6 (0%)

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	18	ALA	6.7
1	A	15	ILE	5.2
1	A	34	VAL	4.7
3	G	17	ILE	4.6
2	B	25	HIS	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.

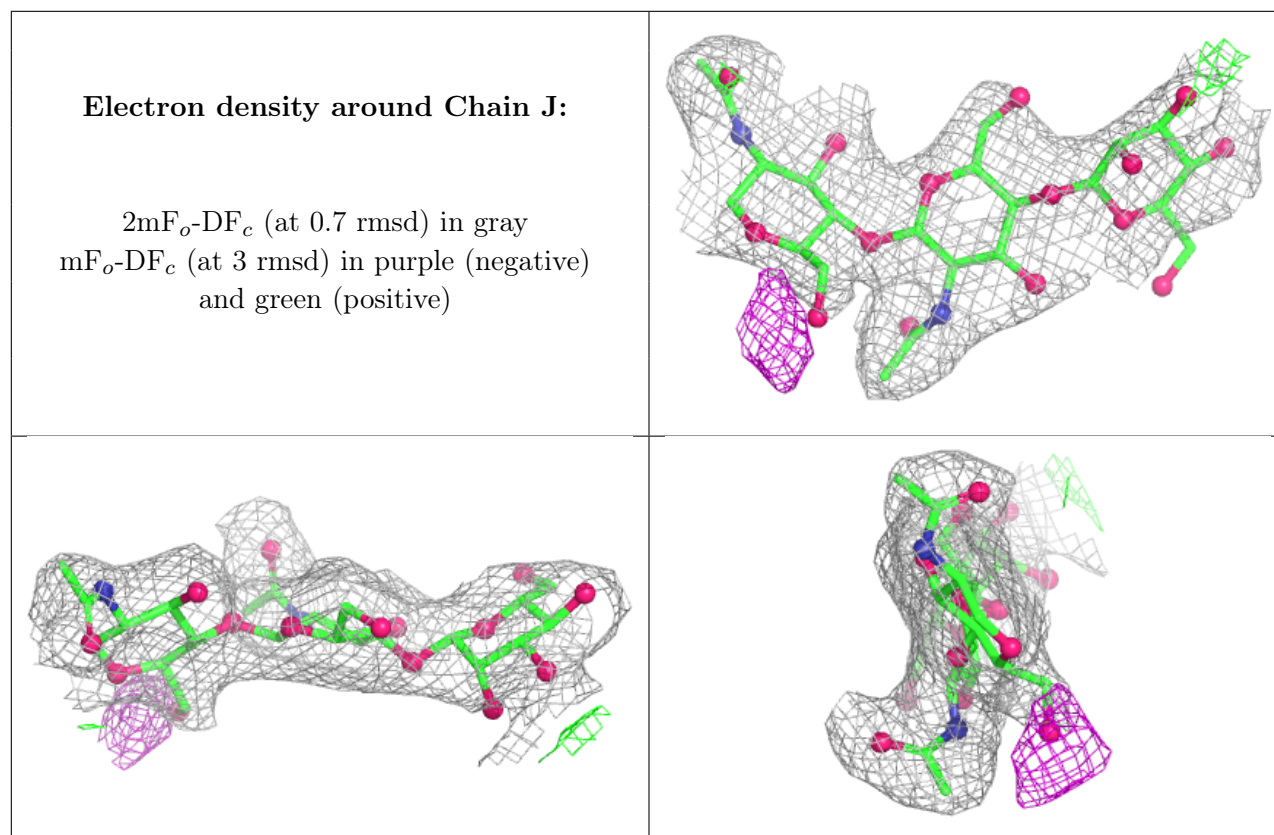
### 6.3 Carbohydrates [i](#)

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.

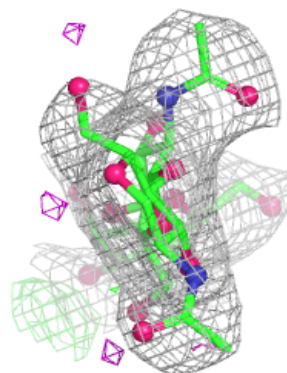
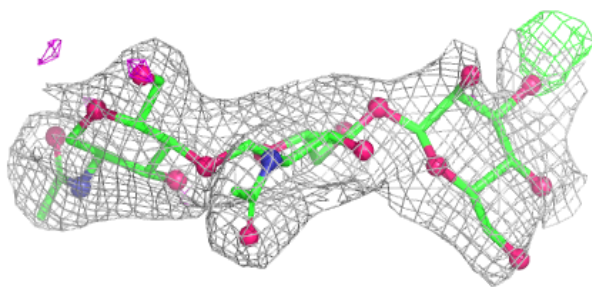
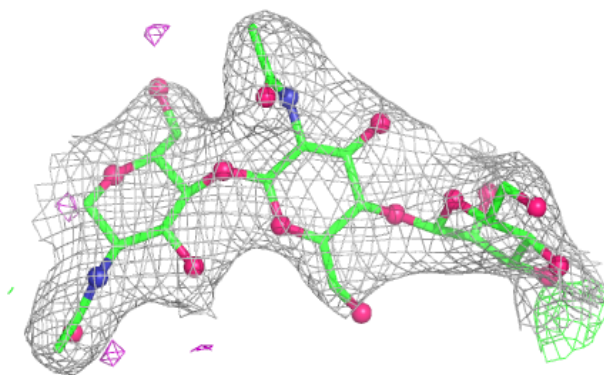
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	J	3	11/12	0.55	0.15	89,94,107,110	0
4	BMA	K	3	11/12	0.58	0.16	98,102,104,105	0
4	BMA	L	3	11/12	0.61	0.12	97,99,109,109	0
4	NAG	L	2	14/15	0.81	0.13	72,78,85,92	0
4	NAG	K	2	14/15	0.88	0.09	67,76,88,95	0
4	NAG	J	2	14/15	0.89	0.09	51,65,82,82	0
4	NAG	J	1	14/15	0.89	0.11	48,60,67,72	0
4	NAG	L	1	14/15	0.90	0.10	38,50,64,74	0
4	NAG	K	1	14/15	0.92	0.10	27,47,62,74	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.

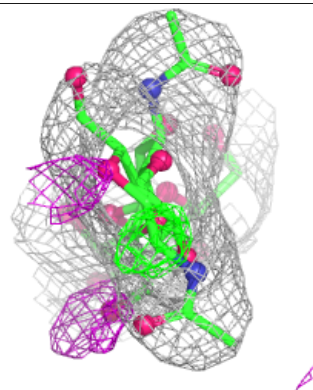
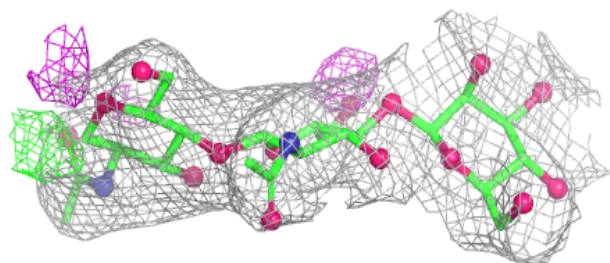
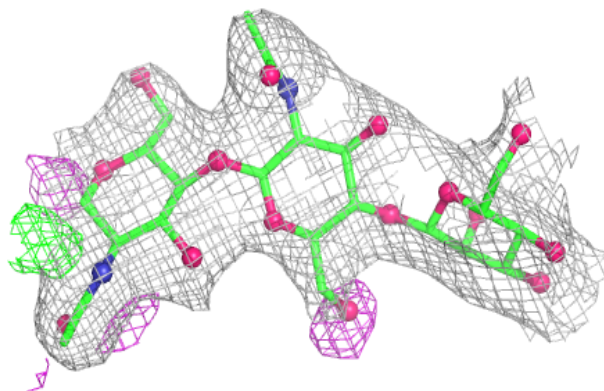


**Electron density around Chain K:**

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

**Electron density around Chain L:**

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



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.