



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 05:47 AM BST

PDB ID : 6B3M  
Title : The crystal structure of a broadly-reactive human anti-hemagglutinin stalk antibody (70-1F02) in complex with H5 hemagglutinin  
Authors : Shore, D.A.; Yang, H.; Stevens, J.  
Deposited on : 2017-09-22  
Resolution : 3.92 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

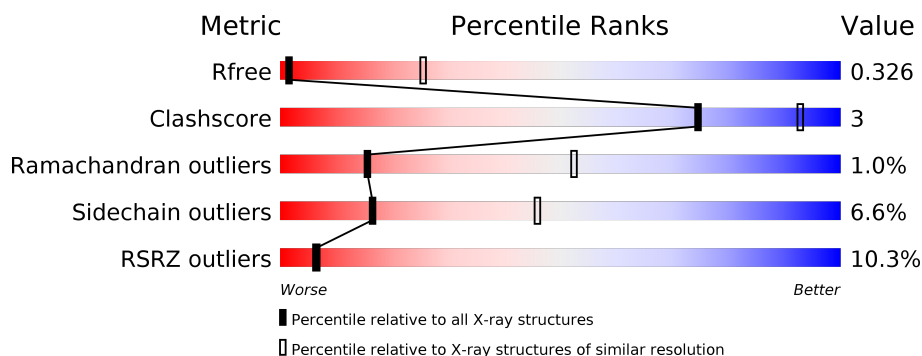
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.92 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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>6%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	E	330	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	G	330	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div> </div>
1	K	330	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	Q	330	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	S	330	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	181	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>
2	F	181	<div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
2	H	181	<div> <div>6%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
2	L	181	<div> <div>7%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
2	R	181	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
2	T	181	<div> <div>%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
3	C	221	<div> <div>8%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
3	I	221	<div> <div>25%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
3	M	221	<div> <div>19%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
3	O	221	<div> <div>9%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
3	V	221	<div> <div>10%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
3	Y	221	<div> <div>29%</div> <div>82%</div> <div>12%</div> <div>• •</div> </div>
4	D	215	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
4	J	215	<div> <div>38%</div> <div>93%</div> <div>7%</div> </div>
4	N	215	<div> <div>10%</div> <div>91%</div> <div>8%</div> </div>
4	P	215	<div> <div>%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
4	U	215	<div> <div>47%</div> <div>92%</div> <div>8%</div> </div>
4	W	215	<div> <div>8%</div> <div>89%</div> <div>10%</div> </div>
5	X	4	<div> <div>100%</div> </div>
5	k	4	<div> <div>100%</div> </div>
5	o	4	<div> <div>100%</div> </div>
5	p	4	<div> <div>100%</div> </div>
6	Z	3	<div> <div>67%</div> <div>33%</div> </div>
7	a	2	<div> <div>50%</div> <div>50%</div> </div>
7	b	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
7	c	2	 100%
7	d	2	 100%
7	e	2	 100%
7	f	2	 100%
7	h	2	 100%
7	m	2	 100%
7	n	2	 100%
8	g	5	 100%
9	i	5	 100%
9	l	5	 20%  80%
10	j	4	 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
10	NAG	j	1	-	-	-	X
10	NAG	j	2	-	-	-	X
10	MAN	j	3	-	-	-	X
10	BMA	j	4	-	-	-	X
11	NAG	F	201	X	-	-	X
11	NAG	G	401	X	-	-	-
11	NAG	K	401	-	-	-	X
11	NAG	Q	401	-	-	-	X
5	MAN	X	4	-	-	-	X
5	MAN	k	3	-	-	-	X
5	MAN	k	4	-	-	-	X
5	MAN	o	3	-	-	-	X
5	NAG	p	2	-	-	-	X
5	MAN	p	3	-	-	-	X
5	MAN	p	4	-	-	-	X
6	NAG	Z	1	X	-	-	-
6	NAG	Z	2	-	-	-	X
7	NAG	a	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	b	1	X	-	-	-
7	NAG	b	2	-	-	-	X
7	NAG	e	1	X	-	-	X
7	NAG	f	1	X	-	-	-
7	NAG	f	2	-	-	-	X
7	NAG	h	2	-	-	-	X
7	NAG	m	2	-	-	-	X
7	NAG	n	1	-	-	-	X
7	NAG	n	2	-	-	-	X
9	NAG	i	2	-	-	-	X
9	MAN	i	4	-	-	-	X
9	BMA	i	5	X	-	-	X
9	NAG	l	1	X	-	-	-
9	NAG	l	2	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 44024 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	E	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	G	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	K	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	Q	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			
1	S	321	Total	C	N	O	S	0	0	0
			2549	1611	440	483	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	H	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	L	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	R	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	T	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	GLU	LYS	conflict	UNP A0A182DWE1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	147	GLU	LYS	conflict	UNP A0A182DWE1
H	147	GLU	LYS	conflict	UNP A0A182DWE1
L	147	GLU	LYS	conflict	UNP A0A182DWE1
R	147	GLU	LYS	conflict	UNP A0A182DWE1
T	147	GLU	LYS	conflict	UNP A0A182DWE1

- Molecule 3 is a protein called 70-1F02 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	I	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	M	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	O	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	V	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			
3	Y	214	Total	C	N	O	S	0	0	0
			1596	1006	270	313	7			

- Molecule 4 is a protein called 70-1F02 Fab Light Chain.

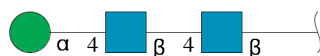
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	213	Total	C	N	O	S	0	0	0
			1626	1016	278	327	5			
4	U	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	J	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	D	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	W	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	N	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-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
5	X	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	k	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	o	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	p	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

- Molecule 7 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
7	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

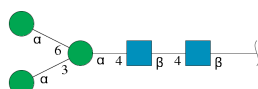
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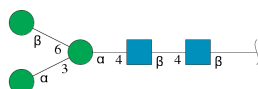
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	h	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	m	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	n	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



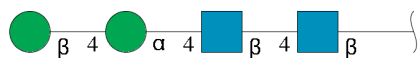
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	g	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



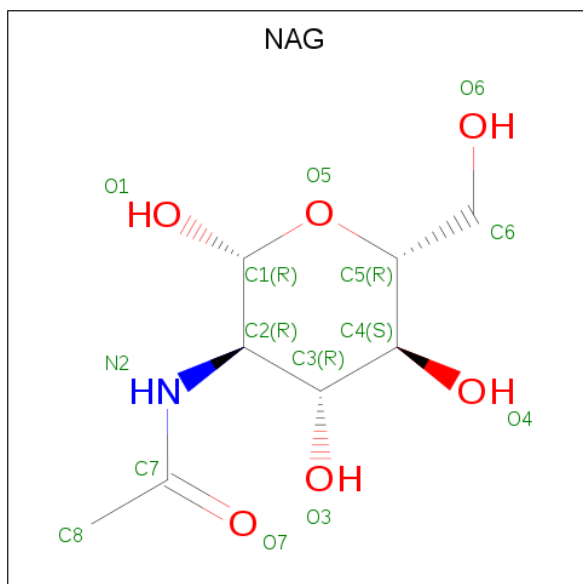
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	i	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	l	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-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
10	j	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 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>).



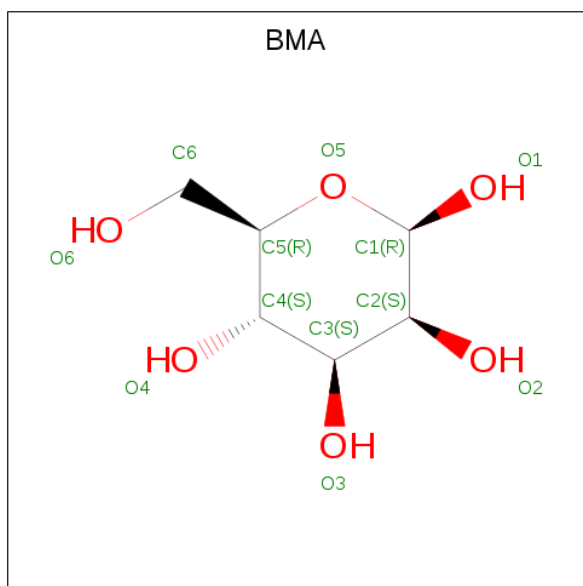
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	F	1	Total	C	N	O	0	0
			14	8	1	5		
11	G	1	Total	C	N	O	0	0
			14	8	1	5		
11	G	1	Total	C	N	O	0	0
			14	8	1	5		
11	K	1	Total	C	N	O	0	0
			14	8	1	5		
11	K	1	Total	C	N	O	0	0
			14	8	1	5		
11	Q	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	S	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

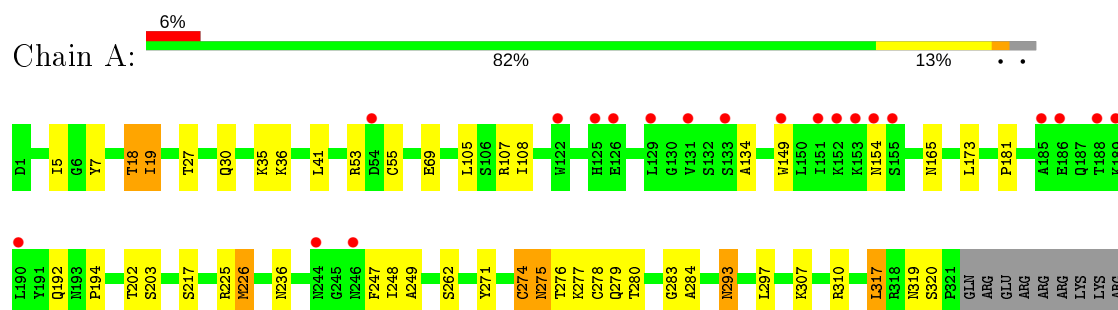


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			11	6	5		

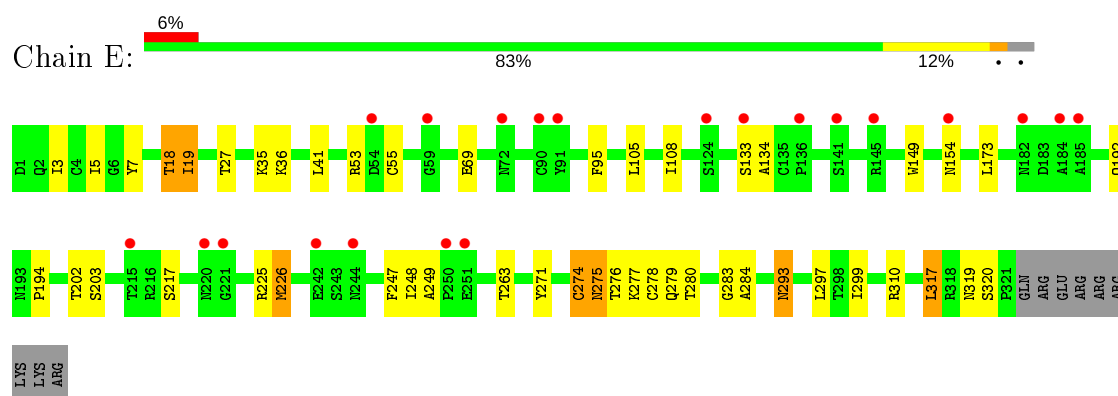
### 3 Residue-property plots [i](#)

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

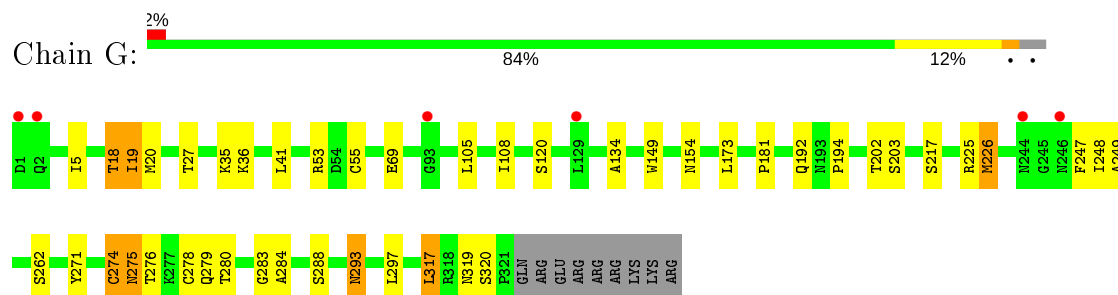
#### • Molecule 1: Hemagglutinin HA1



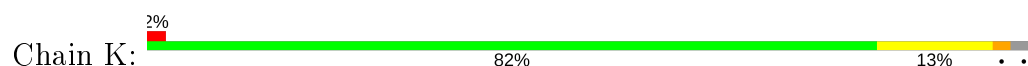
#### • Molecule 1: Hemagglutinin HA1



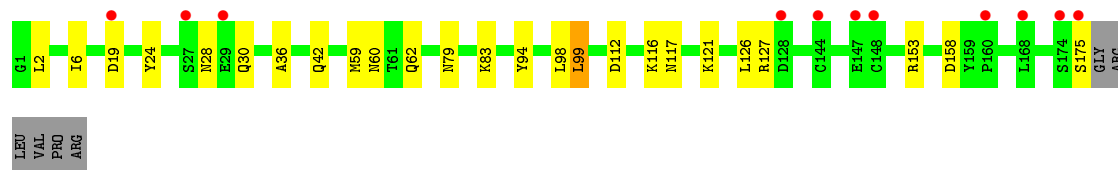
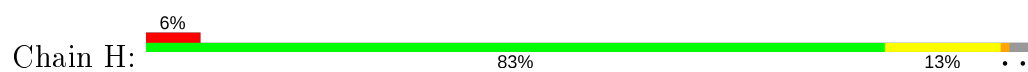
#### • Molecule 1: Hemagglutinin HA1



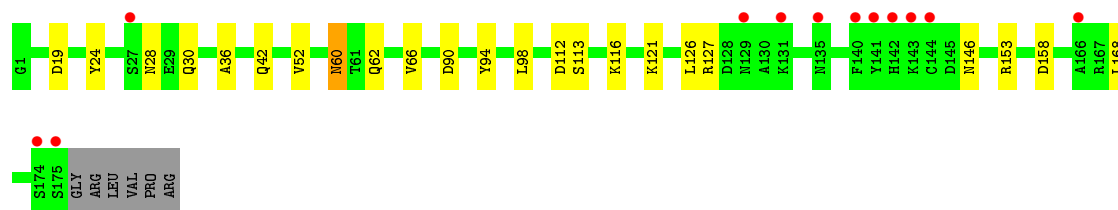
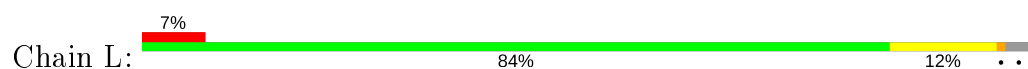
#### • Molecule 1: Hemagglutinin HA1



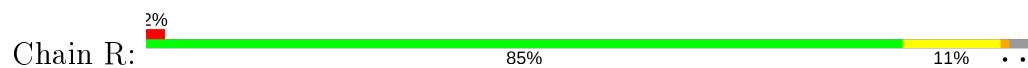




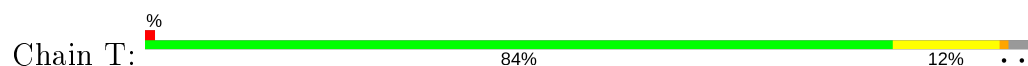
- Molecule 2: Hemagglutinin HA2



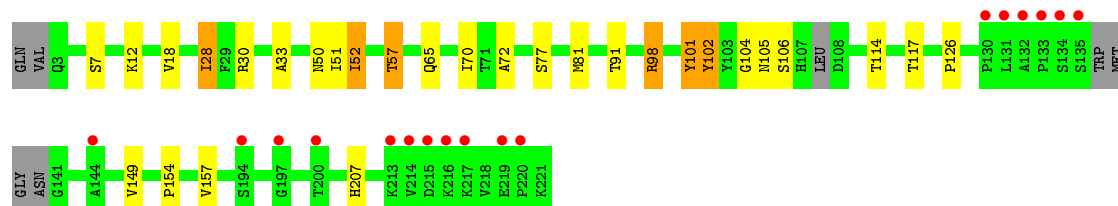
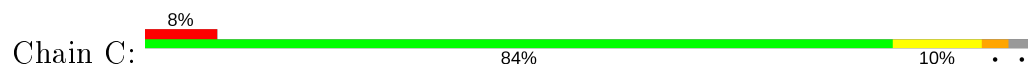
- Molecule 2: Hemagglutinin HA2



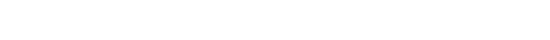
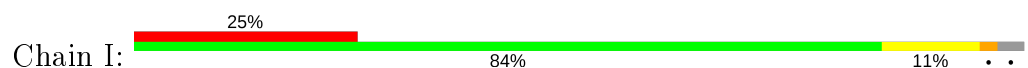
- Molecule 2: Hemagglutinin HA2

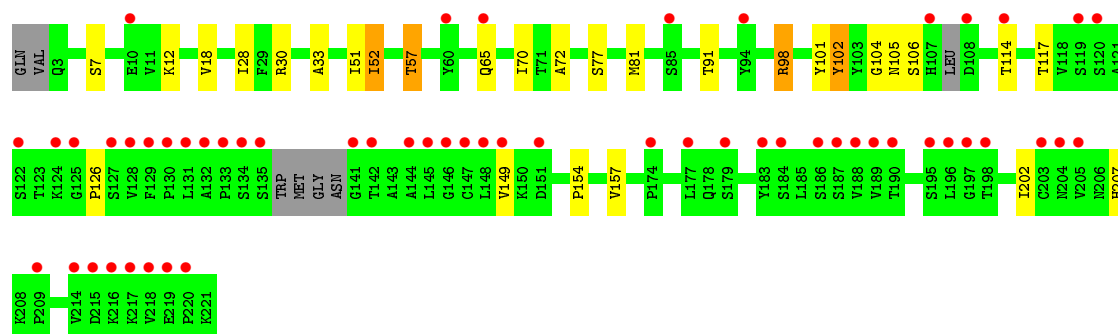


- Molecule 3: 70-1F02 Fab Heavy Chain

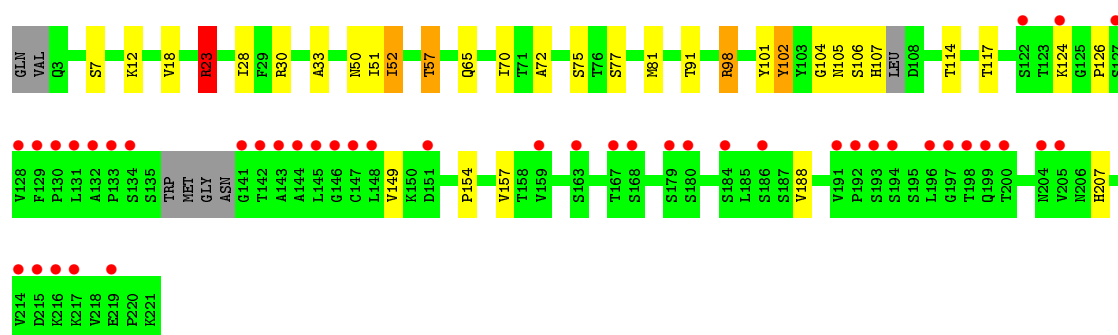
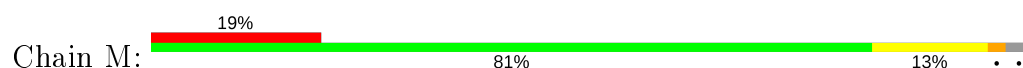


- Molecule 3: 70-1F02 Fab Heavy Chain

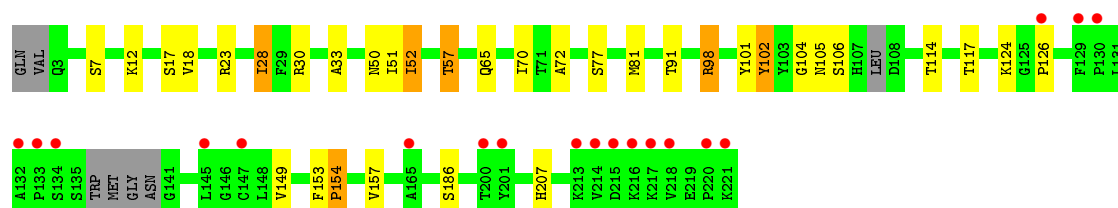
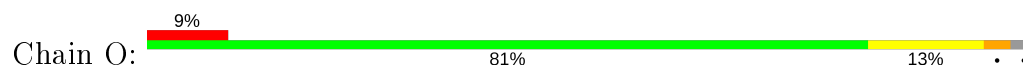




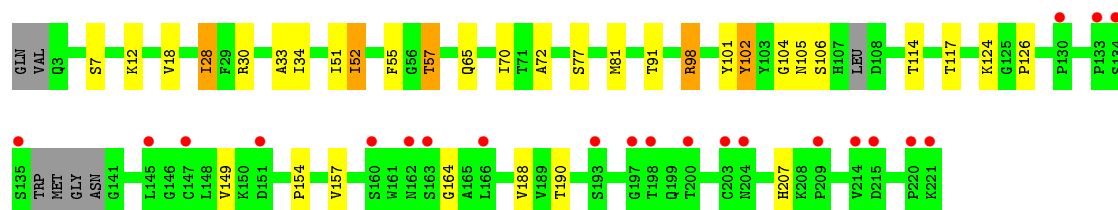
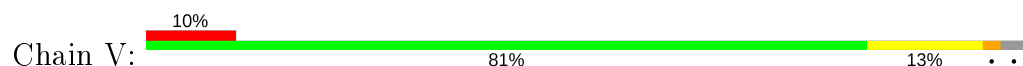
• Molecule 3: 70-1F02 Fab Heavy Chain



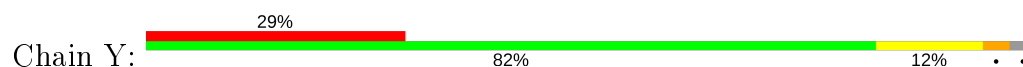
• Molecule 3: 70-1F02 Fab Heavy Chain

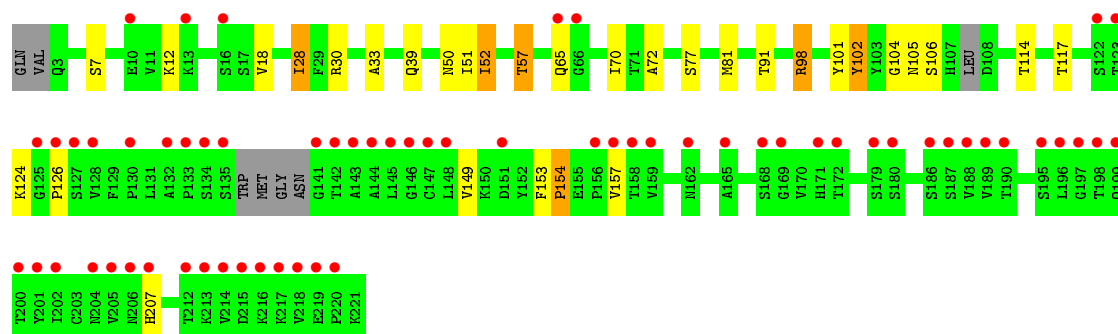


• Molecule 3: 70-1F02 Fab Heavy Chain

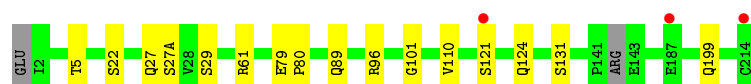


• Molecule 3: 70-1F02 Fab Heavy Chain

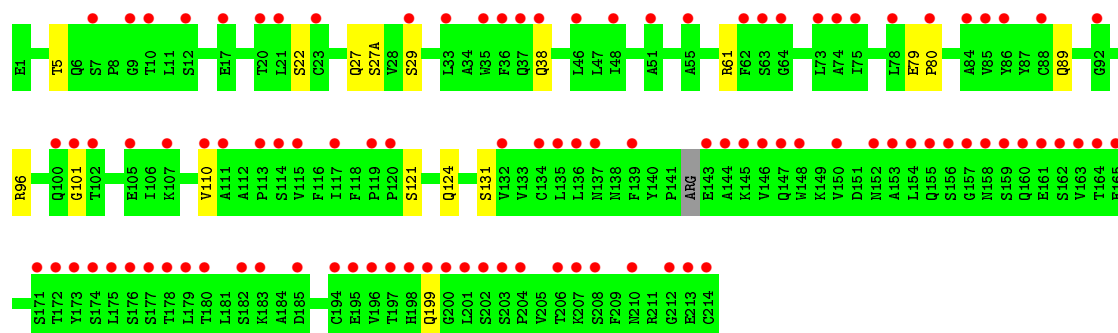
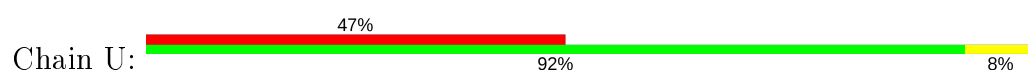




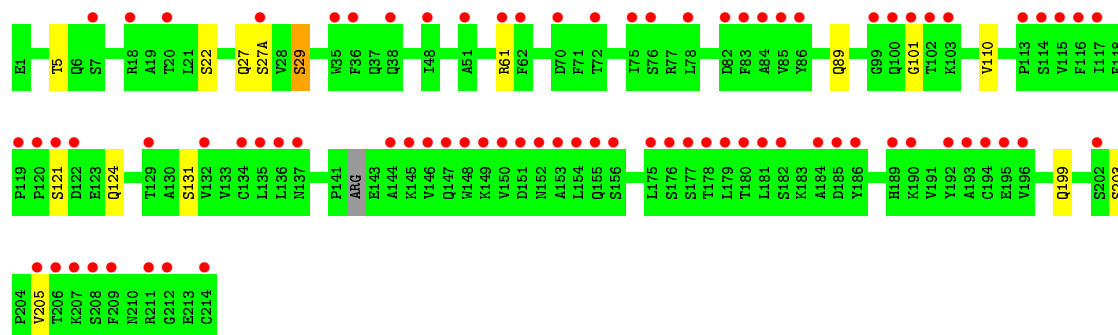
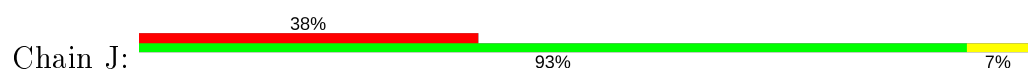
• Molecule 4: 70-1F02 Fab Light Chain



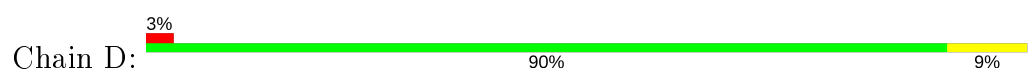
• Molecule 4: 70-1F02 Fab Light Chain



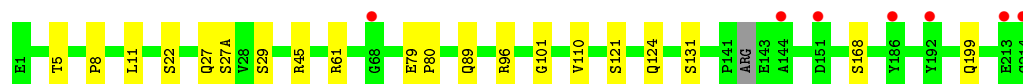
• Molecule 4: 70-1F02 Fab Light Chain



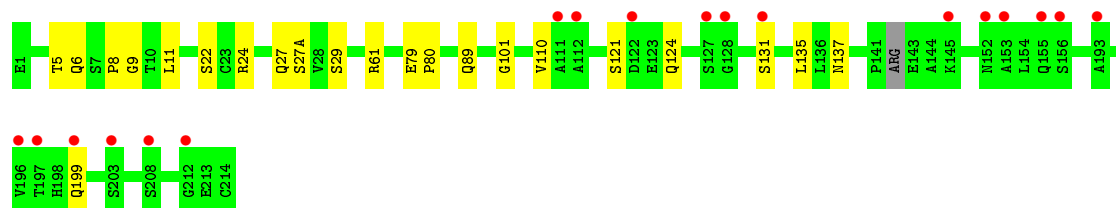
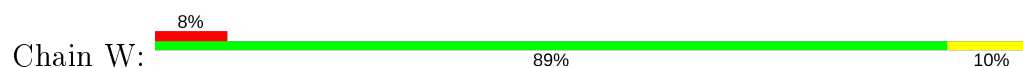
• Molecule 4: 70-1F02 Fab Light Chain



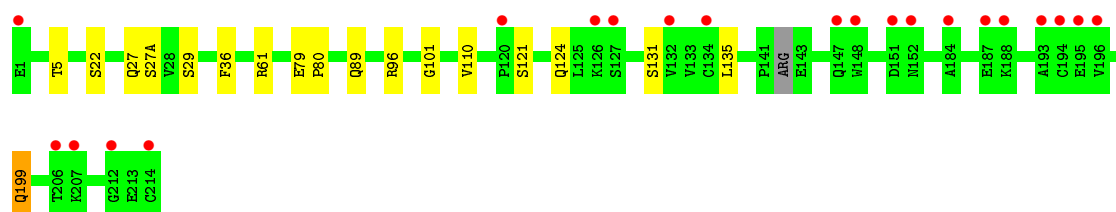




- Molecule 4: 70-1F02 Fab Light Chain



- Molecule 4: 70-1F02 Fab Light Chain



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%

MAG1  
MAG2  
MAN3  
MAN4

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

Chain Z:  67% 33%

MAG1  
MAG2  
MAN3

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%MAG1  
MAG2


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  100%MAG1  
MAG2

- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%MAG1  
MAG2  
MAN3  
MAN4  
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%MAG1  
MAG2  
MAN3  
MAN4  
MAN5

- Molecule 9:  $\alpha$ -D-mannopyranose-(1-3)-[ $\beta$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain l:  20% 80%

MAG1	MAG2	MAG3	MAG4	EMJ45
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- Molecule 10:  $\beta$ -D-mannopyranose-(1-4)- $\alpha$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain j:  100%

MAG1	MAG2	MAG3	EMJ44
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.58Å 205.37Å 222.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.92 49.49 – 3.92	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.01-3.92) 93.8 (49.49-3.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.286 , 0.329 0.285 , 0.326	Depositor DCC
$R_{free}$ test set	3422 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	44024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.56	0/2611	0.71	2/3546 (0.1%)
1	E	0.53	0/2611	0.69	1/3546 (0.0%)
1	G	0.55	0/2611	0.73	0/3546
1	K	0.53	0/2611	0.72	0/3546
1	Q	0.57	1/2611 (0.0%)	0.73	1/3546 (0.0%)
1	S	0.53	0/2611	0.70	0/3546
2	B	0.66	0/1439	0.72	0/1934
2	F	0.69	0/1443	0.75	0/1939
2	H	0.65	0/1443	0.73	0/1939
2	L	0.65	0/1443	0.71	0/1939
2	R	0.64	0/1443	0.72	1/1939 (0.1%)
2	T	0.67	0/1443	0.73	0/1939
3	C	0.57	0/1634	0.71	0/2224
3	I	0.52	0/1634	0.68	0/2224
3	M	0.61	2/1634 (0.1%)	0.84	5/2224 (0.2%)
3	O	0.58	0/1634	0.72	1/2224 (0.0%)
3	V	0.56	0/1634	0.70	0/2224
3	Y	0.53	0/1634	0.68	0/2224
4	D	0.50	0/1668	0.67	1/2261 (0.0%)
4	J	0.48	0/1668	0.64	0/2261
4	N	0.53	0/1668	0.66	0/2261
4	P	0.51	0/1659	0.68	0/2249
4	U	0.48	0/1668	0.63	0/2261
4	W	0.50	0/1668	0.65	0/2261
All	All	0.56	3/44123 (0.0%)	0.71	12/59803 (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	1
2	F	0	1
2	R	0	1
2	T	0	1
3	M	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	23	ARG	CZ-NH1	-7.07	1.23	1.33
1	Q	301	GLU	CG-CD	5.63	1.60	1.51
3	M	23	ARG	CD-NE	5.06	1.55	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	23	ARG	NE-CZ-NH1	-20.07	110.26	120.30
3	O	23	ARG	NE-CZ-NH2	-7.31	116.65	120.30
4	D	45	ARG	NE-CZ-NH1	6.22	123.41	120.30
3	M	23	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
1	Q	266	LYS	CD-CE-NZ	5.66	124.72	111.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	68	ARG	Peptide
2	F	68	ARG	Peptide
3	M	23	ARG	Sidechain
2	R	68	ARG	Peptide
2	T	68	ARG	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2549	0	2493	19	0
1	E	2549	0	2493	16	0
1	G	2549	0	2493	15	0
1	K	2549	0	2494	20	0
1	Q	2549	0	2495	19	0
1	S	2549	0	2495	23	0
2	B	1412	0	1317	11	0
2	F	1416	0	1318	6	0
2	H	1416	0	1320	12	0
2	L	1416	0	1320	14	0
2	R	1416	0	1319	8	0
2	T	1416	0	1320	11	0
3	C	1596	0	1557	15	0
3	I	1596	0	1557	14	0
3	M	1596	0	1550	15	0
3	O	1596	0	1555	17	0
3	V	1596	0	1557	23	0
3	Y	1596	0	1556	16	0
4	D	1635	0	1582	6	0
4	J	1635	0	1582	7	0
4	N	1635	0	1582	7	0
4	P	1626	0	1573	5	0
4	U	1635	0	1582	6	0
4	W	1635	0	1582	13	0
5	X	50	0	41	0	0
5	k	50	0	41	0	0
5	o	50	0	43	0	0
5	p	50	0	43	0	0
6	Z	39	0	34	3	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	d	28	0	25	0	0
7	e	28	0	25	0	0
7	f	28	0	25	0	0
7	h	28	0	25	0	0
7	m	28	0	25	0	0
7	n	28	0	25	0	0
8	g	61	0	50	0	0
9	i	61	0	49	0	0
9	l	61	0	51	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	j	50	0	39	0	0
11	A	14	0	13	0	0
11	E	14	0	13	0	0
11	F	14	0	13	0	0
11	G	28	0	26	0	0
11	K	28	0	26	0	0
11	Q	14	0	13	1	0
11	S	14	0	13	0	0
12	C	11	0	10	0	0
All	All	44024	0	42435	264	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 3.

The worst 5 of 264 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:S:169:GLN:NE2	4:J:203:SER:O	2.25	0.70
1:A:236:ASN:HA	6:Z:1:NAG:H81	1.73	0.69
1:S:169:GLN:NE2	4:J:205:VAL:HG23	2.10	0.67
2:L:52:VAL:HG11	3:O:28:ILE:HG21	1.76	0.66
1:S:169:GLN:NE2	4:J:205:VAL:CG2	2.61	0.64

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	319/330 (97%)	282 (88%)	33 (10%)	4 (1%)	12 48
1	E	319/330 (97%)	283 (89%)	32 (10%)	4 (1%)	12 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	319/330 (97%)	283 (89%)	32 (10%)	4 (1%)	12	48
1	K	319/330 (97%)	283 (89%)	31 (10%)	5 (2%)	9	44
1	Q	319/330 (97%)	283 (89%)	33 (10%)	3 (1%)	17	54
1	S	319/330 (97%)	284 (89%)	31 (10%)	4 (1%)	12	48
2	B	172/181 (95%)	159 (92%)	12 (7%)	1 (1%)	25	63
2	F	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	H	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	L	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	R	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	T	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
3	C	210/221 (95%)	181 (86%)	26 (12%)	3 (1%)	11	46
3	I	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
3	M	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
3	O	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
3	V	210/221 (95%)	183 (87%)	24 (11%)	3 (1%)	11	46
3	Y	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
4	D	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	29	67
4	J	208/215 (97%)	198 (95%)	8 (4%)	2 (1%)	15	52
4	N	208/215 (97%)	199 (96%)	8 (4%)	1 (0%)	29	67
4	P	207/215 (96%)	198 (96%)	8 (4%)	1 (0%)	29	67
4	U	208/215 (97%)	199 (96%)	8 (4%)	1 (0%)	29	67
4	W	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	29	67
All	All	5458/5682 (96%)	4938 (90%)	465 (8%)	55 (1%)	15	52

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	65	GLN
3	I	65	GLN
3	M	65	GLN
3	O	65	GLN
3	V	65	GLN

### 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	289/298 (97%)	264 (91%)	25 (9%)	10	37
1	E	289/298 (97%)	264 (91%)	25 (9%)	10	37
1	G	289/298 (97%)	263 (91%)	26 (9%)	9	35
1	K	289/298 (97%)	263 (91%)	26 (9%)	9	35
1	Q	289/298 (97%)	264 (91%)	25 (9%)	10	37
1	S	289/298 (97%)	263 (91%)	26 (9%)	9	35
2	B	149/155 (96%)	139 (93%)	10 (7%)	16	45
2	F	149/155 (96%)	138 (93%)	11 (7%)	13	42
2	H	149/155 (96%)	137 (92%)	12 (8%)	11	40
2	L	149/155 (96%)	139 (93%)	10 (7%)	16	45
2	R	149/155 (96%)	139 (93%)	10 (7%)	16	45
2	T	149/155 (96%)	139 (93%)	10 (7%)	16	45
3	C	177/183 (97%)	168 (95%)	9 (5%)	24	53
3	I	177/183 (97%)	168 (95%)	9 (5%)	24	53
3	M	177/183 (97%)	165 (93%)	12 (7%)	16	45
3	O	177/183 (97%)	166 (94%)	11 (6%)	18	47
3	V	177/183 (97%)	167 (94%)	10 (6%)	21	50
3	Y	177/183 (97%)	167 (94%)	10 (6%)	21	50
4	D	183/185 (99%)	176 (96%)	7 (4%)	33	59
4	J	183/185 (99%)	177 (97%)	6 (3%)	38	63
4	N	183/185 (99%)	176 (96%)	7 (4%)	33	59
4	P	182/185 (98%)	176 (97%)	6 (3%)	38	63
4	U	183/185 (99%)	177 (97%)	6 (3%)	38	63
4	W	183/185 (99%)	177 (97%)	6 (3%)	38	63
All	All	4787/4926 (97%)	4472 (93%)	315 (7%)	16	46

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	271	TYR
3	O	51	ILE
4	J	29	SER
1	K	278	CYS
2	L	121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	178	GLN
2	R	117	ASN
4	W	155	GLN
4	P	124	GLN
1	Q	11	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 ⓘ

56 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	X	1	1,5	14,14,15	0.99	2 (14%)	17,19,21	1.43	3 (17%)
5	NAG	X	2	5	14,14,15	0.79	0	17,19,21	2.15	6 (35%)
5	MAN	X	3	5	11,11,12	0.87	0	15,15,17	1.90	2 (13%)
5	MAN	X	4	5	11,11,12	0.72	0	15,15,17	1.99	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	Z	1	1,6	14,14,15	1.16	1 (7%)	17,19,21	2.61	8 (47%)
6	NAG	Z	2	6	14,14,15	0.67	0	17,19,21	1.13	1 (5%)
6	MAN	Z	3	6	11,11,12	0.78	0	15,15,17	2.31	4 (26%)
7	NAG	a	1	1,7	14,14,15	0.81	0	17,19,21	0.95	0
7	NAG	a	2	7	14,14,15	0.88	0	17,19,21	1.69	4 (23%)
7	NAG	b	1	2,7	14,14,15	1.08	2 (14%)	17,19,21	1.28	1 (5%)
7	NAG	b	2	7	14,14,15	0.81	1 (7%)	17,19,21	1.41	4 (23%)
7	NAG	c	1	1,7	14,14,15	0.52	0	17,19,21	2.09	4 (23%)
7	NAG	c	2	7	14,14,15	0.73	0	17,19,21	1.38	2 (11%)
7	NAG	d	1	1,7	14,14,15	1.29	2 (14%)	17,19,21	1.69	2 (11%)
7	NAG	d	2	7	14,14,15	0.70	0	17,19,21	1.34	2 (11%)
7	NAG	e	1	1,7	14,14,15	1.58	2 (14%)	17,19,21	1.86	4 (23%)
7	NAG	e	2	7	14,14,15	0.82	1 (7%)	17,19,21	2.04	5 (29%)
7	NAG	f	1	1,7	14,14,15	0.82	0	17,19,21	1.53	2 (11%)
7	NAG	f	2	7	14,14,15	0.45	0	17,19,21	1.40	2 (11%)
8	NAG	g	1	1,8	14,14,15	0.90	0	17,19,21	1.81	4 (23%)
8	NAG	g	2	8	14,14,15	0.49	0	17,19,21	1.94	5 (29%)
8	MAN	g	3	8	11,11,12	1.19	1 (9%)	15,15,17	2.46	6 (40%)
8	MAN	g	4	8	11,11,12	0.69	0	15,15,17	1.46	2 (13%)
8	MAN	g	5	8	11,11,12	1.12	2 (18%)	15,15,17	3.56	4 (26%)
7	NAG	h	1	1,7	14,14,15	1.87	4 (28%)	17,19,21	1.98	4 (23%)
7	NAG	h	2	7	14,14,15	1.30	2 (14%)	17,19,21	1.97	3 (17%)
9	NAG	i	1	1,9	14,14,15	0.72	0	17,19,21	1.95	5 (29%)
9	NAG	i	2	9	14,14,15	0.63	0	17,19,21	1.88	5 (29%)
9	MAN	i	3	9	11,11,12	1.49	2 (18%)	15,15,17	2.56	6 (40%)
9	MAN	i	4	9	11,11,12	0.77	0	15,15,17	1.66	4 (26%)
9	BMA	i	5	9	11,11,12	2.11	3 (27%)	15,15,17	3.23	6 (40%)
10	NAG	j	1	1,10	14,14,15	1.77	4 (28%)	17,19,21	1.74	4 (23%)
10	NAG	j	2	10	14,14,15	0.65	0	17,19,21	1.71	3 (17%)
10	MAN	j	3	10	11,11,12	0.97	0	15,15,17	3.11	7 (46%)
10	BMA	j	4	10	11,11,12	1.04	0	15,15,17	1.58	3 (20%)
5	NAG	k	1	1,5	14,14,15	0.68	0	17,19,21	2.89	8 (47%)
5	NAG	k	2	5	14,14,15	0.42	0	17,19,21	1.42	4 (23%)
5	MAN	k	3	5	11,11,12	1.46	3 (27%)	15,15,17	3.41	10 (66%)
5	MAN	k	4	5	11,11,12	1.13	2 (18%)	15,15,17	3.17	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	l	1	1,9	14,14,15	1.36	2 (14%)	17,19,21	2.19	4 (23%)
9	NAG	l	2	9	14,14,15	0.86	0	17,19,21	1.84	5 (29%)
9	MAN	l	3	9	11,11,12	1.48	2 (18%)	15,15,17	1.68	3 (20%)
9	MAN	l	4	9	11,11,12	0.99	1 (9%)	15,15,17	2.08	5 (33%)
9	BMA	l	5	9	11,11,12	0.41	0	15,15,17	0.89	0
7	NAG	m	1	1,7	14,14,15	0.46	0	17,19,21	1.82	1 (5%)
7	NAG	m	2	7	14,14,15	0.86	0	17,19,21	1.84	5 (29%)
7	NAG	n	1	2,7	14,14,15	0.84	0	17,19,21	1.97	6 (35%)
7	NAG	n	2	7	14,14,15	0.67	0	17,19,21	1.48	1 (5%)
5	NAG	o	1	1,5	14,14,15	1.50	2 (14%)	17,19,21	1.83	4 (23%)
5	NAG	o	2	5	14,14,15	0.81	0	17,19,21	1.67	4 (23%)
5	MAN	o	3	5	11,11,12	0.92	0	15,15,17	1.65	3 (20%)
5	MAN	o	4	5	11,11,12	0.81	0	15,15,17	2.50	2 (13%)
5	NAG	p	1	1,5	14,14,15	0.67	0	17,19,21	2.20	1 (5%)
5	NAG	p	2	5	14,14,15	0.75	0	17,19,21	1.28	3 (17%)
5	MAN	p	3	5	11,11,12	0.72	0	15,15,17	1.16	2 (13%)
5	MAN	p	4	5	11,11,12	0.40	0	15,15,17	1.04	2 (13%)

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	X	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	MAN	X	3	5	-	2/2/19/22	0/1/1/1
5	MAN	X	4	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	1/1/5/7	1/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
6	MAN	Z	3	6	-	0/2/19/22	0/1/1/1
7	NAG	a	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	NAG	b	1	2,7	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	b	2	7	-	1/6/23/26	0/1/1/1
7	NAG	c	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	d	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	NAG	e	1	1,7	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
7	NAG	f	1	1,7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	0/6/23/26	0/1/1/1
8	NAG	g	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
8	MAN	g	3	8	-	0/2/19/22	0/1/1/1
8	MAN	g	4	8	-	2/2/19/22	0/1/1/1
8	MAN	g	5	8	-	2/2/19/22	0/1/1/1
7	NAG	h	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	h	2	7	-	1/6/23/26	0/1/1/1
9	NAG	i	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	i	2	9	-	0/6/23/26	0/1/1/1
9	MAN	i	3	9	-	0/2/19/22	0/1/1/1
9	MAN	i	4	9	-	2/2/19/22	0/1/1/1
9	BMA	i	5	9	1/1/4/5	1/2/19/22	0/1/1/1
10	NAG	j	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	j	2	10	-	2/6/23/26	0/1/1/1
10	MAN	j	3	10	-	2/2/19/22	0/1/1/1
10	BMA	j	4	10	-	1/2/19/22	0/1/1/1
5	NAG	k	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
5	MAN	k	3	5	-	0/2/19/22	0/1/1/1
5	MAN	k	4	5	-	2/2/19/22	0/1/1/1
9	NAG	l	1	1,9	1/1/5/7	2/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	MAN	l	3	9	-	1/2/19/22	0/1/1/1
9	MAN	l	4	9	-	0/2/19/22	0/1/1/1
9	BMA	l	5	9	-	0/2/19/22	0/1/1/1
7	NAG	m	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	m	2	7	-	2/6/23/26	0/1/1/1
7	NAG	n	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	n	2	7	-	0/6/23/26	0/1/1/1
5	NAG	o	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	2/6/23/26	0/1/1/1
5	MAN	o	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	o	4	5	-	1/2/19/22	0/1/1/1
5	NAG	p	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	0/6/23/26	0/1/1/1
5	MAN	p	3	5	-	2/2/19/22	0/1/1/1
5	MAN	p	4	5	-	0/2/19/22	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	1	NAG	O5-C1	-4.98	1.35	1.43
7	h	1	NAG	O5-C1	-4.66	1.36	1.43
9	i	5	BMA	O5-C1	-4.37	1.36	1.43
7	e	1	NAG	C1-C2	4.16	1.58	1.52
5	o	1	NAG	O5-C1	-4.16	1.37	1.43

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	5	MAN	C1-O5-C5	-12.38	95.41	112.19
5	k	4	MAN	C1-O5-C5	8.79	124.11	112.19
10	j	3	MAN	O5-C5-C6	8.13	119.95	107.20
5	p	1	NAG	C1-O5-C5	8.07	123.13	112.19
5	o	4	MAN	C1-O5-C5	7.84	122.81	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	b	1	NAG	C1
6	Z	1	NAG	C1
9	i	5	BMA	C5
7	f	1	NAG	C1
9	l	1	NAG	C1

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	c	2	NAG	O5-C5-C6-O6
9	l	2	NAG	O5-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6

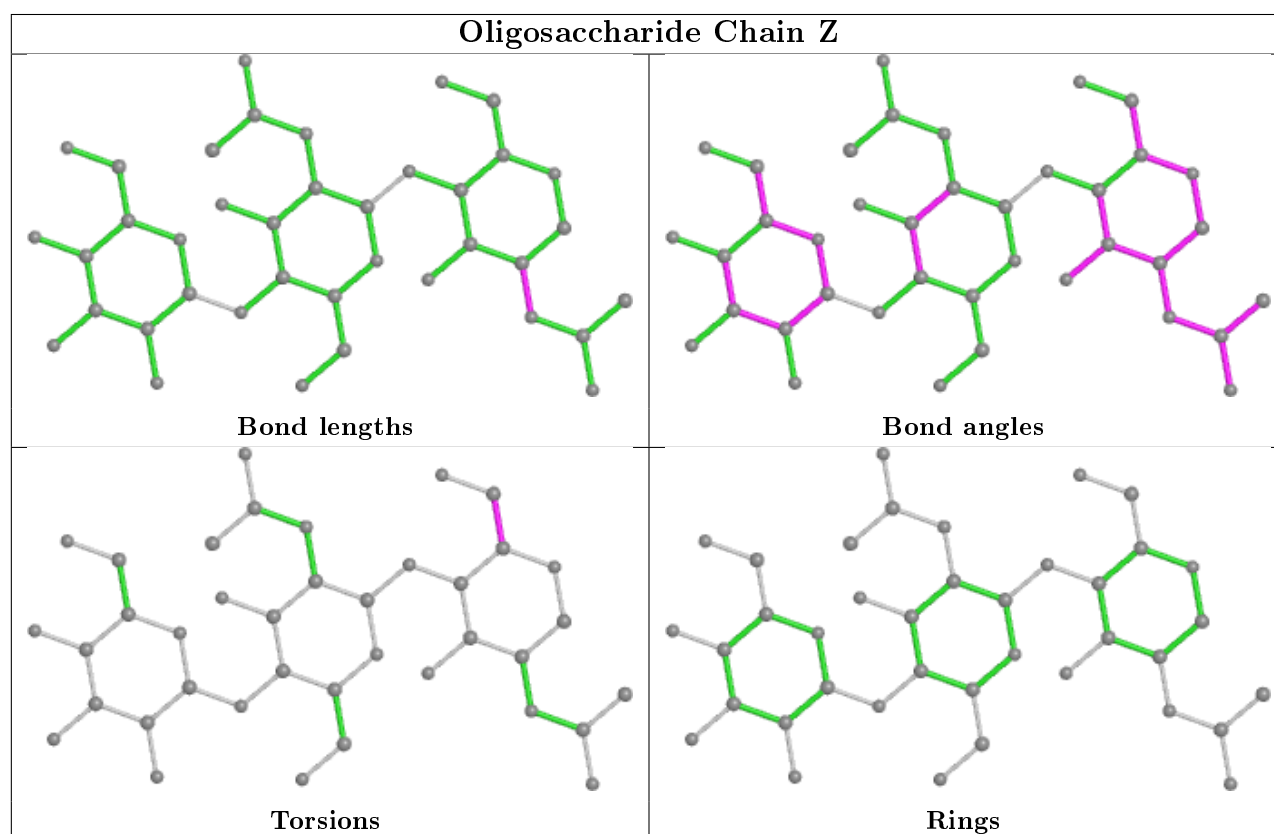


There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	3	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](#)

10 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	$\# Z  > 2$
11	NAG	K	401	1	14,14,15	1.35	3 (21%)	17,19,21	1.96	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	Q	401	-	14,14,15	0.55	0	17,19,21	1.82	3 (17%)
12	BMA	C	301	-	11,11,12	0.56	0	15,15,17	2.05	2 (13%)
11	NAG	E	401	1	14,14,15	0.90	1 (7%)	17,19,21	1.92	3 (17%)
11	NAG	F	201	2	14,14,15	1.04	1 (7%)	17,19,21	1.66	3 (17%)
11	NAG	K	409	1	14,14,15	0.85	0	17,19,21	1.83	3 (17%)
11	NAG	G	401	1	14,14,15	0.83	0	17,19,21	1.08	1 (5%)
11	NAG	S	409	1	14,14,15	1.10	1 (7%)	17,19,21	1.48	2 (11%)
11	NAG	A	401	1	14,14,15	1.59	3 (21%)	17,19,21	2.41	6 (35%)
11	NAG	G	402	1	14,14,15	0.92	0	17,19,21	2.41	5 (29%)

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
11	NAG	K	401	1	-	2/6/23/26	0/1/1/1
11	NAG	Q	401	-	-	2/6/23/26	0/1/1/1
12	BMA	C	301	-	-	2/2/19/22	0/1/1/1
11	NAG	E	401	1	-	0/6/23/26	0/1/1/1
11	NAG	F	201	2	1/1/5/7	2/6/23/26	0/1/1/1
11	NAG	K	409	1	-	0/6/23/26	0/1/1/1
11	NAG	G	401	1	1/1/5/7	2/6/23/26	0/1/1/1
11	NAG	S	409	1	-	2/6/23/26	0/1/1/1
11	NAG	A	401	1	-	2/6/23/26	0/1/1/1
11	NAG	G	402	1	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	401	NAG	C1-C2	4.28	1.58	1.52
11	F	201	NAG	C1-C2	3.37	1.57	1.52
11	A	401	NAG	C2-N2	2.84	1.51	1.46
11	K	401	NAG	C2-N2	2.74	1.51	1.46
11	K	401	NAG	C1-C2	2.64	1.56	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
11	G	402	NAG	C1-O5-C5	7.37	122.18	112.19
11	E	401	NAG	C1-O5-C5	5.79	120.03	112.19
11	K	401	NAG	C2-N2-C7	5.70	131.02	122.90
11	K	409	NAG	C1-O5-C5	5.57	119.74	112.19
11	A	401	NAG	C2-N2-C7	5.50	130.74	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	F	201	NAG	C1
11	G	401	NAG	C1

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	301	BMA	O5-C5-C6-O6
12	C	301	BMA	C4-C5-C6-O6
11	G	401	NAG	O5-C5-C6-O6
11	G	402	NAG	C4-C5-C6-O6
11	G	402	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Q	401	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	P	1
4	J	1
4	D	1
4	W	1
4	N	1

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Mol	Chain	Number of breaks
4	U	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	27:GLN	C	27(A):SER	N	2.62
1	P	27:GLN	C	27(A):SER	N	2.61
1	J	27:GLN	C	27(A):SER	N	2.61
1	D	27:GLN	C	27(A):SER	N	2.61
1	W	27:GLN	C	27(A):SER	N	2.61

## 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	321/330 (97%)	0.41	20 (6%) 20 17	1, 43, 128, 182	0
1	E	321/330 (97%)	0.53	21 (6%) 18 15	1, 56, 147, 233	0
1	G	321/330 (97%)	0.24	6 (1%) 66 58	1, 38, 98, 145	0
1	K	321/330 (97%)	0.18	6 (1%) 66 58	1, 28, 91, 189	0
1	Q	321/330 (97%)	0.11	6 (1%) 66 58	1, 31, 107, 145	0
1	S	321/330 (97%)	0.52	22 (6%) 16 13	1, 52, 111, 147	0
2	B	174/181 (96%)	0.20	9 (5%) 27 24	1, 13, 112, 137	0
2	F	175/181 (96%)	-0.07	0 100 100	1, 10, 104, 172	0
2	H	175/181 (96%)	0.24	11 (6%) 20 16	1, 37, 138, 210	0
2	L	175/181 (96%)	0.25	12 (6%) 16 13	1, 27, 138, 185	0
2	R	175/181 (96%)	0.06	4 (2%) 60 51	1, 20, 112, 164	0
2	T	175/181 (96%)	0.08	2 (1%) 80 73	1, 13, 115, 164	0
3	C	214/221 (96%)	0.42	17 (7%) 12 11	1, 31, 145, 197	0
3	I	214/221 (96%)	1.47	56 (26%) 0 0	11, 115, 242, 317	0
3	M	214/221 (96%)	1.06	43 (20%) 1 1	1, 64, 214, 295	0
3	O	214/221 (96%)	0.51	19 (8%) 9 8	1, 37, 120, 166	0
3	V	214/221 (96%)	0.79	22 (10%) 6 6	1, 63, 144, 180	0
3	Y	214/221 (96%)	1.68	63 (29%) 0 0	1, 97, 270, 367	0
4	D	214/215 (99%)	0.40	7 (3%) 46 37	1, 48, 131, 162	0
4	J	214/215 (99%)	1.91	81 (37%) 0 0	59, 137, 196, 270	0
4	N	214/215 (99%)	0.68	21 (9%) 7 7	1, 40, 173, 230	0
4	P	213/215 (99%)	0.22	3 (1%) 75 66	1, 44, 83, 111	0
4	U	214/215 (99%)	2.37	102 (47%) 0 0	60, 167, 283, 360	0
4	W	214/215 (99%)	0.59	18 (8%) 11 10	1, 42, 149, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5542/5682 (97%)	0.61	571 (10%) 6 6	1, 48, 178, 367	0

The worst 5 of 571 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	214	VAL	12.0
4	U	136	LEU	11.3
3	I	134	SER	10.8
4	J	134	CYS	8.6
4	U	214	CYS	8.3

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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.

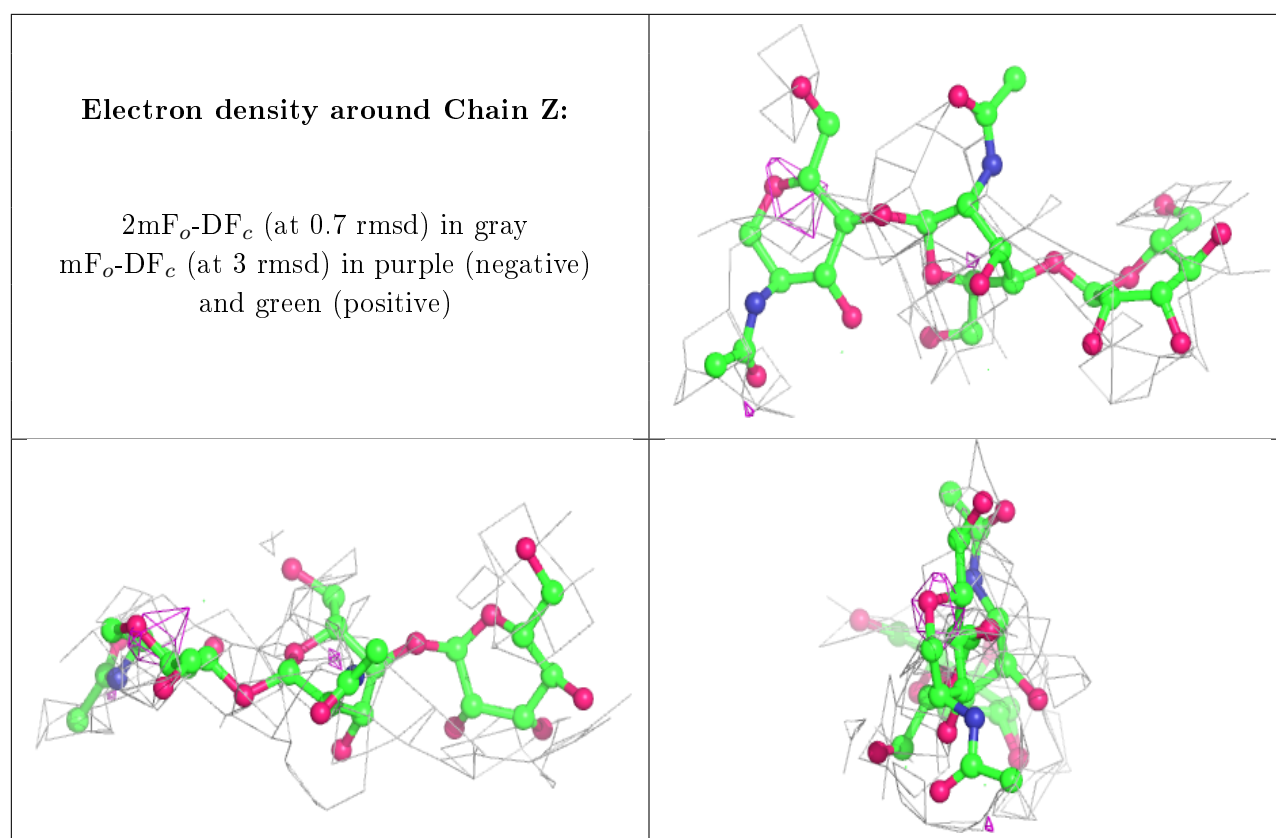
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	p	4	11/12	0.25	0.42	144,166,175,180	0
9	BMA	i	5	11/12	0.30	0.58	141,159,196,214	0
5	MAN	p	3	11/12	0.41	0.43	192,209,219,224	0
5	MAN	k	3	11/12	0.43	0.49	112,143,181,190	0
6	NAG	Z	2	14/15	0.45	0.41	119,137,149,152	0
9	MAN	i	3	11/12	0.55	0.35	87,116,171,202	0
7	NAG	a	2	14/15	0.55	0.51	76,93,102,103	0
5	NAG	p	2	14/15	0.56	0.54	143,181,207,212	0
10	BMA	j	4	11/12	0.57	0.73	154,187,199,204	0
5	MAN	k	4	11/12	0.59	0.42	68,100,120,125	0
9	NAG	i	2	14/15	0.60	0.46	101,113,121,135	0
9	MAN	i	4	11/12	0.61	0.50	90,136,150,174	0
6	NAG	Z	1	14/15	0.62	0.36	83,104,122,138	0
7	NAG	f	1	14/15	0.63	0.38	99,114,121,131	0
7	NAG	n	1	14/15	0.66	0.49	97,118,127,128	0
7	NAG	e	1	14/15	0.66	0.46	52,74,79,80	0
7	NAG	m	2	14/15	0.67	0.50	68,77,89,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MAN	j	3	11/12	0.67	0.52	142,151,171,179	0
7	NAG	f	2	14/15	0.67	0.42	128,138,151,171	0
7	NAG	h	2	14/15	0.70	0.49	59,75,80,80	0
6	MAN	Z	3	11/12	0.72	0.30	97,107,115,117	0
10	NAG	j	1	14/15	0.73	0.55	76,106,129,136	0
7	NAG	n	2	14/15	0.73	0.52	82,116,122,125	0
9	NAG	l	2	14/15	0.73	0.43	57,74,83,85	0
5	MAN	o	3	11/12	0.73	0.44	60,87,97,105	0
5	NAG	k	2	14/15	0.74	0.35	82,110,131,138	0
7	NAG	b	2	14/15	0.75	0.54	95,101,108,116	0
5	MAN	o	4	11/12	0.75	0.38	64,84,92,93	0
9	MAN	l	3	11/12	0.76	0.34	54,74,80,84	0
10	NAG	j	2	14/15	0.77	0.66	90,115,129,133	0
7	NAG	a	1	14/15	0.77	0.34	20,42,61,73	0
5	NAG	X	2	14/15	0.77	0.38	30,71,85,86	0
5	MAN	X	4	11/12	0.78	0.48	66,73,88,95	0
5	NAG	p	1	14/15	0.79	0.34	75,81,101,134	0
7	NAG	e	2	14/15	0.80	0.34	53,63,69,70	0
7	NAG	b	1	14/15	0.80	0.41	58,72,83,93	0
5	NAG	X	1	14/15	0.80	0.44	38,48,59,61	0
5	NAG	k	1	14/15	0.81	0.37	69,83,93,97	0
9	NAG	l	1	14/15	0.81	0.34	39,47,66,75	0
8	MAN	g	4	11/12	0.81	0.30	76,83,96,104	0
7	NAG	d	2	14/15	0.82	0.32	32,36,42,44	0
9	BMA	l	5	11/12	0.82	0.35	74,80,92,98	0
9	MAN	l	4	11/12	0.84	0.38	60,73,77,81	0
8	MAN	g	5	11/12	0.84	0.37	61,68,79,80	0
8	MAN	g	3	11/12	0.84	0.30	64,75,83,84	0
5	MAN	X	3	11/12	0.84	0.29	40,52,71,76	0
9	NAG	i	1	14/15	0.84	0.29	37,63,87,103	0
5	NAG	o	2	14/15	0.84	0.46	67,79,90,101	0
8	NAG	g	1	14/15	0.85	0.29	48,52,59,62	0
8	NAG	g	2	14/15	0.86	0.32	44,54,61,70	0
7	NAG	h	1	14/15	0.87	0.24	19,40,48,56	0
7	NAG	c	2	14/15	0.87	0.25	41,56,61,64	0
5	NAG	o	1	14/15	0.87	0.34	44,56,66,67	0
7	NAG	c	1	14/15	0.89	0.25	32,40,43,47	0
7	NAG	m	1	14/15	0.89	0.28	21,28,35,50	0
7	NAG	d	1	14/15	0.93	0.23	20,29,33,36	0

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



## 6.4 Ligands [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
11	NAG	Q	401	14/15	0.53	0.57	91,97,112,116	0
11	NAG	F	201	14/15	0.73	0.46	65,85,92,97	0
11	NAG	K	401	14/15	0.74	0.48	32,48,55,57	0
11	NAG	G	402	14/15	0.77	0.35	25,35,39,40	0
11	NAG	A	401	14/15	0.80	0.35	34,44,48,50	0
11	NAG	G	401	14/15	0.82	0.31	41,63,75,78	0
11	NAG	S	409	14/15	0.82	0.32	18,23,28,31	0
11	NAG	K	409	14/15	0.83	0.34	16,21,39,42	0
12	BMA	C	301	11/12	0.84	0.32	25,30,35,38	0
11	NAG	E	401	14/15	0.86	0.30	24,29,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.