



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2021 – 12:22 PM EDT

PDB ID : 4FQR  
Title : Crystal structure of broadly neutralizing antibody C05 bound to H3 influenza hemagglutinin  
Authors : Ekiert, D.C.; Wilson, I.A.  
Deposited on : 2012-06-25  
Resolution : 4.10 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

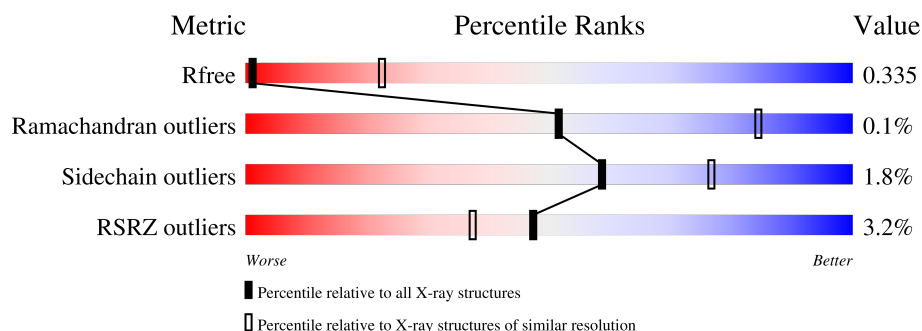
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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)
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	323	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>
1	C	323	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>
1	E	323	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
1	G	323	<div> <div>3%</div> <div>98%</div> <div>..</div> </div>
1	I	323	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>
1	K	323	<div> <div>%</div> <div>97%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	323	8% 97% ..
1	O	323	7% 97% ..
1	Q	323	5% 98% ..
1	S	323	7% 97% ..
1	U	323	2% 97% ..
1	W	323	5% 97% ..
2	B	174	2% 98% ..
2	D	174	4% 98% ..
2	F	174	5% 98% ..
2	H	174	2% 98% ..
2	J	174	3% 98% ..
2	L	174	5% 98% ..
2	N	174	9% 98% ..
2	P	174	5% 98% ..
2	R	174	% 98% ..
2	T	174	5% 98% ..
2	V	174	% 98% ..
2	X	174	3% 98% ..
3	a	241	% 96% ..
3	c	241	% 97% ..
3	e	241	7% 96% ..
3	g	241	3% 96% ..
3	i	241	% 96% ..
3	k	241	6% 96% ..
3	m	241	6% 97% ..

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Mol	Chain	Length	Quality of chain
3	o	241	
3	q	241	
3	s	241	
3	u	241	
3	w	241	
4	b	214	
4	d	214	
4	f	214	
4	h	214	
4	j	214	
4	l	214	
4	n	214	
4	p	214	
4	r	214	
4	t	214	
4	v	214	
4	x	214	
5	0	4	
5	2	4	
5	4	4	
5	6	4	
5	8	4	
5	AA	4	
5	CA	4	
5	EA	4	

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Mol	Chain	Length	Quality of chain
5	GA	4	
5	IA	4	
5	Y	4	
5	y	4	
6	1	2	
6	3	2	
6	5	2	
6	7	2	
6	9	2	
6	BA	2	
6	DA	2	
6	FA	2	
6	HA	2	
6	JA	2	
6	Z	2	
6	z	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
5	NAG	6	2	-	-	-	X
5	NAG	AA	2	-	-	-	X
5	MAN	AA	4	-	-	-	X
5	NAG	Y	1	-	-	-	X
6	NAG	3	2	-	-	-	X
6	NAG	7	2	-	-	-	X
7	NAG	A	601	-	-	-	X
7	NAG	C	501	-	-	-	X
7	NAG	E	601	-	-	-	X
7	NAG	F	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	G	502	-	-	-	X
7	NAG	M	502	-	-	-	X
7	NAG	O	501	-	-	-	X
7	NAG	Q	502	-	-	-	X
7	NAG	R	201	-	-	-	X
7	NAG	S	501	-	-	-	X
7	NAG	S	502	-	-	-	X
7	NAG	T	201	-	-	-	X
7	NAG	U	502	-	-	-	X
7	NAG	V	201	-	-	-	X
7	NAG	W	601	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 90792 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	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	C	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	E	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	G	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	I	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	K	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	M	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	O	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	Q	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	S	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	U	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	W	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7
G	7	ALA	-	expression tag	UNP Q91MA7
G	8	ASP	-	expression tag	UNP Q91MA7
G	9	PRO	-	expression tag	UNP Q91MA7
G	10	GLY	-	expression tag	UNP Q91MA7
I	7	ALA	-	expression tag	UNP Q91MA7
I	8	ASP	-	expression tag	UNP Q91MA7
I	9	PRO	-	expression tag	UNP Q91MA7
I	10	GLY	-	expression tag	UNP Q91MA7
K	7	ALA	-	expression tag	UNP Q91MA7
K	8	ASP	-	expression tag	UNP Q91MA7
K	9	PRO	-	expression tag	UNP Q91MA7
K	10	GLY	-	expression tag	UNP Q91MA7
M	7	ALA	-	expression tag	UNP Q91MA7
M	8	ASP	-	expression tag	UNP Q91MA7
M	9	PRO	-	expression tag	UNP Q91MA7
M	10	GLY	-	expression tag	UNP Q91MA7
O	7	ALA	-	expression tag	UNP Q91MA7
O	8	ASP	-	expression tag	UNP Q91MA7
O	9	PRO	-	expression tag	UNP Q91MA7
O	10	GLY	-	expression tag	UNP Q91MA7
Q	7	ALA	-	expression tag	UNP Q91MA7
Q	8	ASP	-	expression tag	UNP Q91MA7
Q	9	PRO	-	expression tag	UNP Q91MA7
Q	10	GLY	-	expression tag	UNP Q91MA7
S	7	ALA	-	expression tag	UNP Q91MA7
S	8	ASP	-	expression tag	UNP Q91MA7
S	9	PRO	-	expression tag	UNP Q91MA7
S	10	GLY	-	expression tag	UNP Q91MA7
U	7	ALA	-	expression tag	UNP Q91MA7
U	8	ASP	-	expression tag	UNP Q91MA7
U	9	PRO	-	expression tag	UNP Q91MA7
U	10	GLY	-	expression tag	UNP Q91MA7
W	7	ALA	-	expression tag	UNP Q91MA7
W	8	ASP	-	expression tag	UNP Q91MA7
W	9	PRO	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
W	10	GLY	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	D	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	F	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	H	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	J	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	L	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	N	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	P	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	R	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	T	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	V	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	X	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
D	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
F	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
H	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
J	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
L	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
N	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
P	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
R	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
T	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
V	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
X	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is a protein called Broadly neutralizing antibody C05, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	c	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	e	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	g	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	i	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	k	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	m	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	o	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	q	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	s	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	u	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	w	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			

- Molecule 4 is a protein called Broadly neutralizing antibody C05, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	b	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	d	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	f	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	h	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	l	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	n	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	p	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	r	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	t	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	v	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	x	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
5	Y	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	y	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	0	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	2	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	4	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	6	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	8	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	AA	4	Total	C	N	O	0	0	0
			50	28	2	20			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	CA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	EA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	GA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	IA	4	Total	C	N	O	0	0	0
			50	28	2	20			

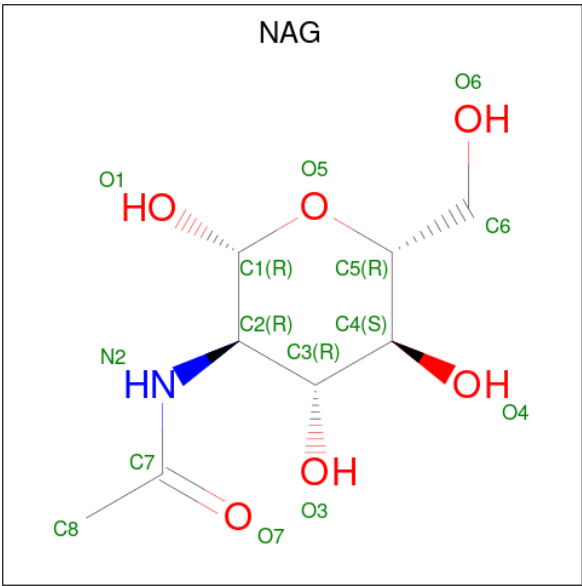
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	1	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	3	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	5	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	7	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	9	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	BA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	DA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	FA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	HA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	JA	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 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
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			14	8	1	5		
7	M	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		
7	O	1	Total	C	N	O	0	0
			14	8	1	5		
7	O	1	Total	C	N	O	0	0
			14	8	1	5		
7	P	1	Total	C	N	O	0	0
			14	8	1	5		
7	Q	1	Total	C	N	O	0	0
			14	8	1	5		
7	Q	1	Total	C	N	O	0	0
			14	8	1	5		
7	R	1	Total	C	N	O	0	0
			14	8	1	5		
7	S	1	Total	C	N	O	0	0
			14	8	1	5		
7	S	1	Total	C	N	O	0	0
			14	8	1	5		
7	T	1	Total	C	N	O	0	0
			14	8	1	5		
7	U	1	Total	C	N	O	0	0
			14	8	1	5		
7	U	1	Total	C	N	O	0	0
			14	8	1	5		
7	V	1	Total	C	N	O	0	0
			14	8	1	5		
7	W	1	Total	C	N	O	0	0
			14	8	1	5		
7	X	1	Total	C	N	O	0	0
			14	8	1	5		

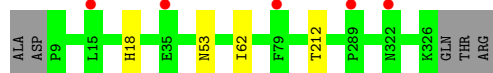
### 3 Residue-property plots [i](#)

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 HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



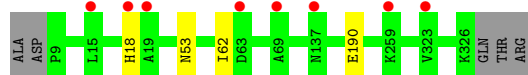
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



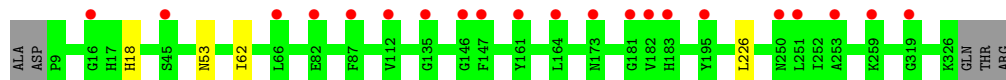
- Molecule 1: Hemagglutinin HA1 chain



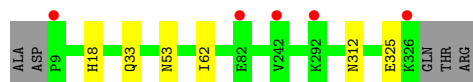
- Molecule 1: Hemagglutinin HA1 chain



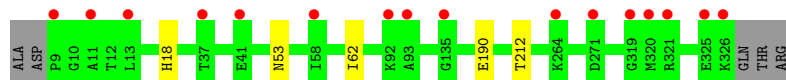
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

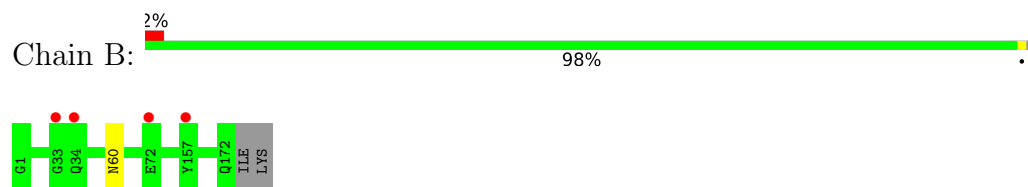


- Molecule 1: Hemagglutinin HA1 chain

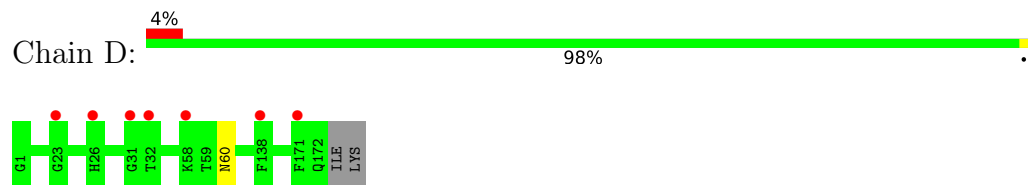




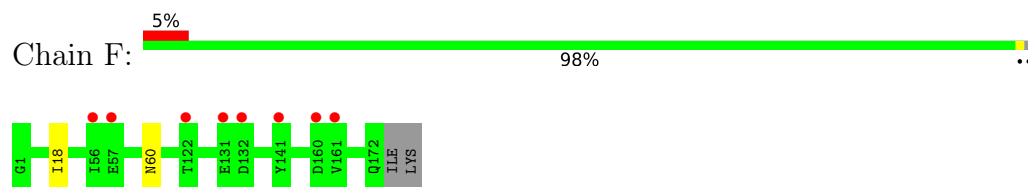
## ● Molecule 2: Hemagglutinin HA2 chain



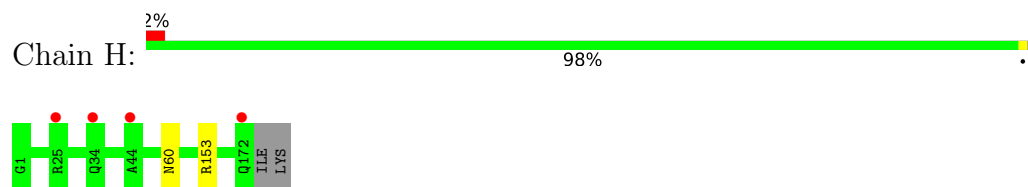
## ● Molecule 2: Hemagglutinin HA2 chain



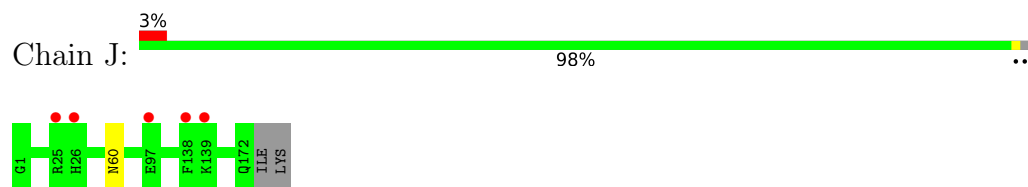
## ● Molecule 2: Hemagglutinin HA2 chain



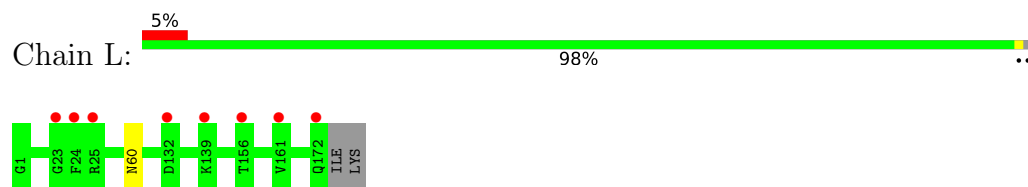
## ● Molecule 2: Hemagglutinin HA2 chain



## ● Molecule 2: Hemagglutinin HA2 chain

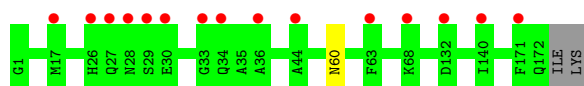


## ● Molecule 2: Hemagglutinin HA2 chain

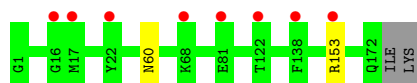


## ● Molecule 2: Hemagglutinin HA2 chain

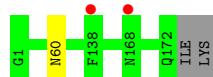




- Molecule 2: Hemagglutinin HA2 chain



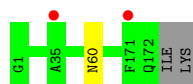
- Molecule 2: Hemagglutinin HA2 chain



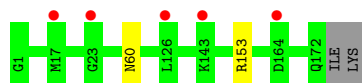
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



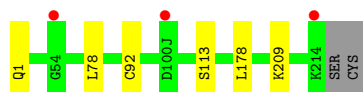
- Molecule 2: Hemagglutinin HA2 chain



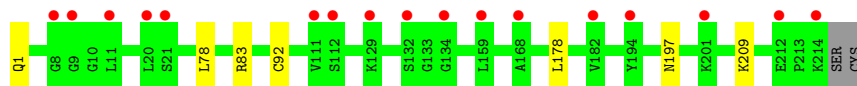
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



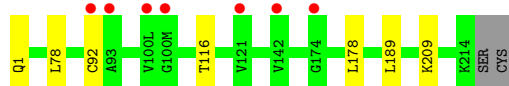
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



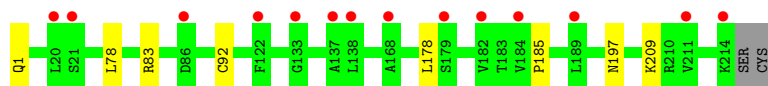
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



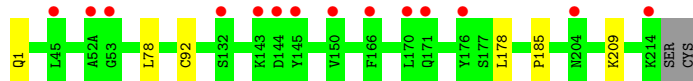
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



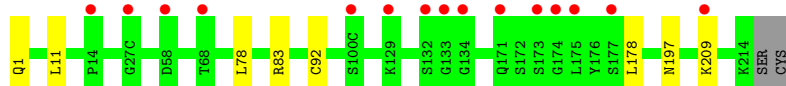
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



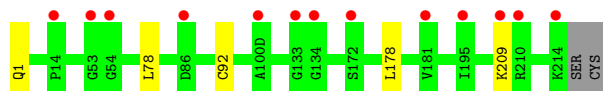
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



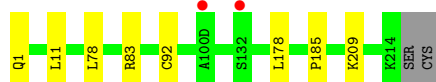
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



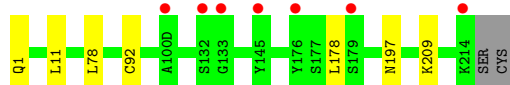
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain

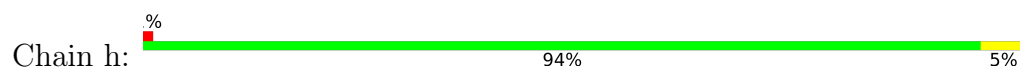


- Molecule 4: Broadly neutralizing antibody C05, light chain

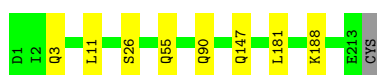




- Molecule 4: Broadly neutralizing antibody C05, light chain



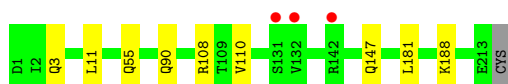
- Molecule 4: Broadly neutralizing antibody C05, light chain



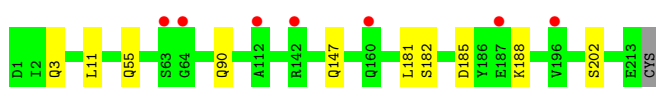
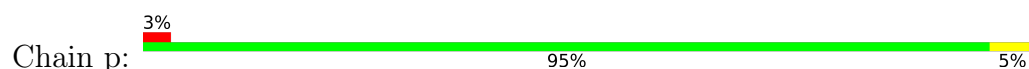
- Molecule 4: Broadly neutralizing antibody C05, light chain



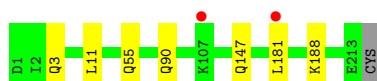
- Molecule 4: Broadly neutralizing antibody C05, light chain



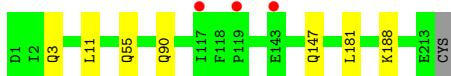
- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



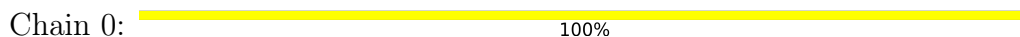
- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-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-(1-6)-beta-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-(1-6)-beta-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-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4: 25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6: 25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8: 100%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA: 25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA: 25% 75%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA: 100%



- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:  25% 75%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:  50% 50%

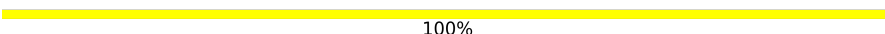
NAG1  
NAG2  
BMA3  
MAN4

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

Chain Z:  100%

NAG1  
NAG2

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

Chain z:  100%

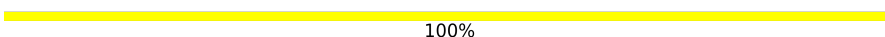
NAG1  
NAG2

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

Chain 1:  50% 50%

NAG1  
NAG2

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

Chain 3:  100%

NAG1  
NAG2

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

Chain 5:  50% 50%





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

Chain 7:  50% 50%



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

Chain 9:  50% 50%



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

Chain BA:  50% 50%



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

Chain DA:  100%



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

Chain FA:  50% 50%



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

Chain HA:  50% 50%



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

Chain JA: 

  
MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.02Å 158.62Å 178.50Å 89.95° 85.44° 84.37°	Depositor
Resolution (Å)	49.07 – 4.10 49.07 – 4.10	Depositor EDS
% Data completeness (in resolution range)	73.9 (49.07-4.10) 58.9 (49.07-4.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 4.14Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.309 , 0.334 0.312 , 0.335	Depositor DCC
$R_{free}$ test set	4527 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.6	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 8.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	90792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1185e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PCA, MAN, NAG, BMA

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	0.42	0/2612	0.66	0/3558
1	C	0.39	0/2612	0.65	1/3558 (0.0%)
1	E	0.38	1/2612 (0.0%)	0.65	0/3558
1	G	0.39	0/2612	0.66	0/3558
1	I	0.48	2/2612 (0.1%)	0.69	2/3558 (0.1%)
1	K	0.39	0/2612	0.64	1/3558 (0.0%)
1	M	0.42	0/2612	0.68	2/3558 (0.1%)
1	O	0.41	1/2612 (0.0%)	0.65	1/3558 (0.0%)
1	Q	0.40	0/2612	0.66	0/3558
1	S	0.38	0/2612	0.66	1/3558 (0.0%)
1	U	0.44	1/2612 (0.0%)	0.68	1/3558 (0.0%)
1	W	0.42	1/2612 (0.0%)	0.65	1/3558 (0.0%)
2	B	0.37	0/1470	0.63	0/1975
2	D	0.36	0/1470	0.64	0/1975
2	F	0.41	0/1470	0.66	0/1975
2	H	0.37	0/1470	0.64	1/1975 (0.1%)
2	J	0.37	0/1470	0.63	0/1975
2	L	0.39	0/1470	0.64	0/1975
2	N	0.35	0/1470	0.63	0/1975
2	P	0.38	0/1470	0.63	1/1975 (0.1%)
2	R	0.36	0/1470	0.64	0/1975
2	T	0.36	0/1470	0.63	0/1975
2	V	0.37	0/1470	0.65	0/1975
2	X	0.36	0/1470	0.63	1/1975 (0.1%)
3	a	0.48	1/1837 (0.1%)	0.75	2/2500 (0.1%)
3	c	0.41	0/1837	0.68	0/2500
3	e	0.43	0/1837	0.71	0/2500
3	g	0.46	1/1837 (0.1%)	0.71	1/2500 (0.0%)
3	i	0.53	0/1837	0.79	1/2500 (0.0%)
3	k	0.42	0/1837	0.69	0/2500
3	m	0.41	0/1837	0.69	0/2500
3	o	0.43	0/1837	0.71	1/2500 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	q	0.43	0/1837	0.69	0/2500
3	s	0.42	0/1837	0.69	0/2500
3	u	0.41	0/1837	0.70	1/2500 (0.0%)
3	w	0.42	0/1837	0.69	1/2500 (0.0%)
4	b	0.45	0/1682	0.67	0/2280
4	d	0.50	1/1682 (0.1%)	0.72	0/2280
4	f	0.40	0/1682	0.66	0/2280
4	h	0.51	1/1682 (0.1%)	0.71	0/2280
4	j	0.44	0/1682	0.69	0/2280
4	l	0.44	0/1682	0.68	0/2280
4	n	0.48	1/1682 (0.1%)	0.69	0/2280
4	p	0.51	0/1682	0.78	4/2280 (0.2%)
4	r	0.39	0/1682	0.66	0/2280
4	t	0.37	0/1682	0.64	0/2280
4	v	0.48	1/1682 (0.1%)	0.70	0/2280
4	x	0.40	0/1682	0.66	0/2280
All	All	0.42	12/91212 (0.0%)	0.67	24/123756 (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	F	0	1
3	k	0	1
3	m	0	1
3	u	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	190	GLU	CG-CD	-11.09	1.35	1.51
1	W	190	GLU	CB-CG	-7.77	1.37	1.52
3	a	100(D)	ALA	CA-CB	-7.11	1.37	1.52
3	g	116	THR	CB-CG2	-7.02	1.29	1.52
4	n	110	VAL	CB-CG2	-6.42	1.39	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	185	ASP	CB-CG-OD2	10.08	127.37	118.30
3	i	58	ASP	CB-CG-OD1	-8.49	110.66	118.30
1	M	20	VAL	N-CA-C	-8.49	88.08	111.00
4	p	185	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	I	190	GLU	OE1-CD-OE2	7.20	131.93	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	18	ILE	Mainchain
3	k	185	PRO	Mainchain
3	m	185	PRO	Mainchain
3	u	185	PRO	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	C	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	E	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	G	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	I	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	K	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	M	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	O	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	S	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	U	328/323 (102%)	323 (98%)	4 (1%)	1 (0%)	41	75
1	W	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
2	B	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	D	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	F	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	H	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	J	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	L	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	N	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	P	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	R	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	T	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	V	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	X	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
3	a	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	c	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	e	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	g	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	i	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	k	241/241 (100%)	235 (98%)	6 (2%)	0	100	100
3	m	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	o	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	q	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	s	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	u	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	w	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
4	b	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	d	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	f	212/214 (99%)	209 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	h	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	j	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	l	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	n	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	p	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	r	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	t	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	v	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	x	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	11496/11424 (101%)	11268 (98%)	216 (2%)	12 (0%)	51	84

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
1	G	62	ILE
1	I	62	ILE

### 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	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	C	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	E	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	G	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	I	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	K	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	M	291/283 (103%)	289 (99%)	2 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	Q	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	S	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	U	291/283 (103%)	289 (99%)	2 (1%)	84	90
1	W	291/283 (103%)	289 (99%)	2 (1%)	84	90
2	B	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	D	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	F	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	H	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	J	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	L	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	N	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	P	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	R	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	T	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	V	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	X	153/148 (103%)	152 (99%)	1 (1%)	84	90
3	a	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	c	202/200 (101%)	197 (98%)	5 (2%)	47	68
3	e	202/200 (101%)	196 (97%)	6 (3%)	41	64
3	g	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	i	202/200 (101%)	197 (98%)	5 (2%)	47	68
3	k	202/200 (101%)	196 (97%)	6 (3%)	41	64
3	m	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	o	202/200 (101%)	196 (97%)	6 (3%)	41	64
3	q	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	s	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	u	202/200 (101%)	197 (98%)	5 (2%)	47	68
3	w	202/200 (101%)	197 (98%)	5 (2%)	47	68
4	b	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	d	187/187 (100%)	180 (96%)	7 (4%)	34	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	f	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	h	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	j	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	l	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	n	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	p	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	r	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	t	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	v	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	x	187/187 (100%)	180 (96%)	7 (4%)	34	59
All	All	9996/9816 (102%)	9818 (98%)	178 (2%)	59	77

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	n	90	GLN
3	s	78	LEU
3	o	78	LEU
4	p	181	LEU
4	t	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	53	ASN
4	f	199	GLN
3	u	192	GLN
2	X	125	GLN
4	d	55	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PCA	u	1	3	7,8,9	2.19	2 (28%)	9,10,12	2.32	5 (55%)
3	PCA	i	1	3	7,8,9	2.24	2 (28%)	9,10,12	2.23	5 (55%)
3	PCA	a	1	3	7,8,9	2.29	2 (28%)	9,10,12	2.30	5 (55%)
3	PCA	s	1	3	7,8,9	2.30	2 (28%)	9,10,12	2.32	5 (55%)
3	PCA	g	1	3	7,8,9	2.09	2 (28%)	9,10,12	2.34	5 (55%)
3	PCA	e	1	3	7,8,9	2.18	2 (28%)	9,10,12	2.31	5 (55%)
3	PCA	o	1	3	7,8,9	2.19	2 (28%)	9,10,12	2.25	5 (55%)
3	PCA	m	1	3	7,8,9	2.14	2 (28%)	9,10,12	2.12	5 (55%)
3	PCA	q	1	3	7,8,9	2.11	2 (28%)	9,10,12	2.24	5 (55%)
3	PCA	k	1	3	7,8,9	2.15	2 (28%)	9,10,12	2.36	5 (55%)
3	PCA	w	1	3	7,8,9	2.19	2 (28%)	9,10,12	2.27	5 (55%)
3	PCA	c	1	3	7,8,9	2.20	2 (28%)	9,10,12	2.33	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	u	1	3	-	0/0/11/13	0/1/1/1
3	PCA	i	1	3	-	0/0/11/13	0/1/1/1
3	PCA	a	1	3	-	0/0/11/13	0/1/1/1
3	PCA	s	1	3	-	0/0/11/13	0/1/1/1
3	PCA	g	1	3	-	0/0/11/13	0/1/1/1
3	PCA	e	1	3	-	0/0/11/13	0/1/1/1
3	PCA	o	1	3	-	0/0/11/13	0/1/1/1
3	PCA	m	1	3	-	0/0/11/13	0/1/1/1
3	PCA	q	1	3	-	0/0/11/13	0/1/1/1
3	PCA	k	1	3	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	w	1	3	-	0/0/11/13	0/1/1/1
3	PCA	c	1	3	-	0/0/11/13	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1	PCA	CD-N	4.80	1.47	1.34
3	s	1	PCA	CD-N	4.78	1.47	1.34
3	i	1	PCA	CD-N	4.77	1.47	1.34
3	c	1	PCA	CD-N	4.75	1.47	1.34
3	u	1	PCA	CD-N	4.73	1.47	1.34

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	1	PCA	CB-CA-C	-3.91	107.32	112.70
3	s	1	PCA	CB-CA-C	-3.91	107.32	112.70
3	o	1	PCA	CB-CA-C	-3.59	107.76	112.70
3	a	1	PCA	CB-CA-C	-3.58	107.77	112.70
3	w	1	PCA	CB-CA-C	-3.55	107.81	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

72 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	0	1	1,5	14,14,15	0.53	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	0	2	5	14,14,15	0.59	0	17,19,21	0.82	1 (5%)
5	BMA	0	3	5	11,11,12	0.75	0	15,15,17	1.00	1 (6%)
5	MAN	0	4	5	11,11,12	0.68	0	15,15,17	0.82	1 (6%)
6	NAG	1	1	6,1	14,14,15	0.59	0	17,19,21	0.66	0
6	NAG	1	2	6	14,14,15	0.47	0	17,19,21	0.89	1 (5%)
5	NAG	2	1	1,5	14,14,15	0.63	0	17,19,21	0.99	0
5	NAG	2	2	5	14,14,15	0.56	0	17,19,21	0.80	0
5	BMA	2	3	5	11,11,12	0.76	0	15,15,17	1.18	1 (6%)
5	MAN	2	4	5	11,11,12	0.60	0	15,15,17	0.83	1 (6%)
6	NAG	3	1	6,1	14,14,15	0.51	0	17,19,21	0.86	1 (5%)
6	NAG	3	2	6	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
5	NAG	4	1	1,5	14,14,15	0.52	0	17,19,21	0.86	0
5	NAG	4	2	5	14,14,15	0.54	0	17,19,21	0.80	1 (5%)
5	BMA	4	3	5	11,11,12	0.72	0	15,15,17	1.05	1 (6%)
5	MAN	4	4	5	11,11,12	0.64	0	15,15,17	0.90	1 (6%)
6	NAG	5	1	6,1	14,14,15	0.59	0	17,19,21	0.68	0
6	NAG	5	2	6	14,14,15	0.51	0	17,19,21	0.78	1 (5%)
5	NAG	6	1	1,5	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
5	NAG	6	2	5	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
5	BMA	6	3	5	11,11,12	0.77	0	15,15,17	1.02	1 (6%)
5	MAN	6	4	5	11,11,12	0.62	0	15,15,17	0.69	0
6	NAG	7	1	6,1	14,14,15	0.57	0	17,19,21	0.60	0
6	NAG	7	2	6	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
5	NAG	8	1	1,5	14,14,15	0.46	0	17,19,21	1.19	1 (5%)
5	NAG	8	2	5	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
5	BMA	8	3	5	11,11,12	0.70	0	15,15,17	1.02	1 (6%)
5	MAN	8	4	5	11,11,12	0.64	0	15,15,17	0.99	1 (6%)
6	NAG	9	1	6,1	14,14,15	0.58	0	17,19,21	0.74	0
6	NAG	9	2	6	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
5	NAG	AA	1	1,5	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
5	NAG	AA	2	5	14,14,15	0.57	0	17,19,21	0.82	0
5	BMA	AA	3	5	11,11,12	0.83	0	15,15,17	1.01	1 (6%)
5	MAN	AA	4	5	11,11,12	0.63	0	15,15,17	0.97	1 (6%)
6	NAG	BA	1	6,1	14,14,15	0.56	0	17,19,21	0.71	0
6	NAG	BA	2	6	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
5	NAG	CA	1	1,5	14,14,15	0.51	0	17,19,21	0.93	0
5	NAG	CA	2	5	14,14,15	0.55	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	CA	3	5	11,11,12	0.79	0	15,15,17	1.04	1 (6%)
5	MAN	CA	4	5	11,11,12	0.63	0	15,15,17	0.82	1 (6%)
6	NAG	DA	1	6,1	14,14,15	0.60	0	17,19,21	0.86	1 (5%)
6	NAG	DA	2	6	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
5	NAG	EA	1	1,5	14,14,15	0.46	0	17,19,21	0.98	1 (5%)
5	NAG	EA	2	5	14,14,15	0.54	0	17,19,21	1.06	2 (11%)
5	BMA	EA	3	5	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
5	MAN	EA	4	5	11,11,12	0.63	0	15,15,17	0.75	1 (6%)
6	NAG	FA	1	6,1	14,14,15	0.58	0	17,19,21	0.75	1 (5%)
6	NAG	FA	2	6	14,14,15	0.55	0	17,19,21	0.76	0
5	NAG	GA	1	1,5	14,14,15	0.55	0	17,19,21	1.10	0
5	NAG	GA	2	5	14,14,15	0.56	0	17,19,21	1.01	1 (5%)
5	BMA	GA	3	5	11,11,12	0.79	0	15,15,17	0.96	1 (6%)
5	MAN	GA	4	5	11,11,12	0.63	0	15,15,17	0.77	1 (6%)
6	NAG	HA	1	6,1	14,14,15	0.53	0	17,19,21	0.75	0
6	NAG	HA	2	6	14,14,15	0.52	0	17,19,21	0.84	1 (5%)
5	NAG	IA	1	1,5	14,14,15	0.48	0	17,19,21	0.98	0
5	NAG	IA	2	5	14,14,15	0.57	0	17,19,21	0.66	0
5	BMA	IA	3	5	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
5	MAN	IA	4	5	11,11,12	0.59	0	15,15,17	0.81	1 (6%)
6	NAG	JA	1	6,1	14,14,15	0.58	0	17,19,21	0.59	0
6	NAG	JA	2	6	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
5	NAG	Y	1	1,5	14,14,15	0.50	0	17,19,21	1.11	1 (5%)
5	NAG	Y	2	5	14,14,15	0.65	0	17,19,21	1.21	2 (11%)
5	BMA	Y	3	5	11,11,12	0.75	0	15,15,17	1.29	3 (20%)
5	MAN	Y	4	5	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	Z	1	6,1	14,14,15	0.55	0	17,19,21	0.55	0
6	NAG	Z	2	6	14,14,15	0.48	0	17,19,21	0.70	0
5	NAG	y	1	1,5	14,14,15	0.53	0	17,19,21	0.85	0
5	NAG	y	2	5	14,14,15	0.55	0	17,19,21	0.69	0
5	BMA	y	3	5	11,11,12	0.71	0	15,15,17	1.29	2 (13%)
5	MAN	y	4	5	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	z	1	6,1	14,14,15	0.61	0	17,19,21	0.79	1 (5%)
6	NAG	z	2	6	14,14,15	0.45	0	17,19,21	0.91	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
5	NAG	0	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	BMA	0	3	5	-	0/2/19/22	0/1/1/1
5	MAN	0	4	5	-	1/2/19/22	0/1/1/1
6	NAG	1	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	1	2	6	-	0/6/23/26	0/1/1/1
5	NAG	2	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	2	2	5	-	0/6/23/26	0/1/1/1
5	BMA	2	3	5	-	0/2/19/22	0/1/1/1
5	MAN	2	4	5	-	2/2/19/22	0/1/1/1
6	NAG	3	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	3	2	6	-	0/6/23/26	0/1/1/1
5	NAG	4	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	4	2	5	-	0/6/23/26	0/1/1/1
5	BMA	4	3	5	-	0/2/19/22	0/1/1/1
5	MAN	4	4	5	-	0/2/19/22	0/1/1/1
6	NAG	5	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	5	2	6	-	0/6/23/26	0/1/1/1
5	NAG	6	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	6	2	5	-	0/6/23/26	0/1/1/1
5	BMA	6	3	5	-	0/2/19/22	0/1/1/1
5	MAN	6	4	5	-	0/2/19/22	0/1/1/1
6	NAG	7	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	7	2	6	-	0/6/23/26	0/1/1/1
5	NAG	8	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	8	2	5	-	0/6/23/26	0/1/1/1
5	BMA	8	3	5	-	0/2/19/22	0/1/1/1
5	MAN	8	4	5	-	2/2/19/22	0/1/1/1
6	NAG	9	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	9	2	6	-	0/6/23/26	0/1/1/1
5	NAG	AA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	AA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	AA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	BA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	BA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	CA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	CA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	CA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	CA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	DA	1	6,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	DA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	EA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	EA	2	5	-	2/6/23/26	0/1/1/1
5	BMA	EA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	EA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	FA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	FA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	GA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	GA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	GA	3	5	-	1/2/19/22	0/1/1/1
5	MAN	GA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	HA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	HA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	IA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	IA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	IA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	IA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	JA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	JA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	Y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
5	NAG	y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	y	4	5	-	0/2/19/22	0/1/1/1
6	NAG	z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	z	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	3	BMA	C1-C2-C3	3.68	114.19	109.67
5	2	3	BMA	C1-C2-C3	3.51	113.99	109.67
5	Y	2	NAG	O5-C5-C6	3.33	112.43	107.20
5	EA	3	BMA	C1-C2-C3	3.31	113.73	109.67
6	3	2	NAG	C1-O5-C5	3.30	116.67	112.19



There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	8	4	MAN	C4-C5-C6-O6
5	EA	2	NAG	C4-C5-C6-O6
5	EA	2	NAG	O5-C5-C6-O6
5	AA	4	MAN	C4-C5-C6-O6
5	CA	4	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

30 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
7	NAG	Q	501	1	14,14,15	0.44	0	17,19,21	1.05	1 (5%)
7	NAG	A	601	1	14,14,15	1.56	2 (14%)	17,19,21	4.27	9 (52%)
7	NAG	S	501	1	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
7	NAG	S	502	1	14,14,15	0.52	0	17,19,21	1.57	3 (17%)
7	NAG	G	501	1	14,14,15	0.40	0	17,19,21	1.07	1 (5%)
7	NAG	I	501	1	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
7	NAG	D	201	2	14,14,15	0.53	0	17,19,21	1.20	1 (5%)
7	NAG	T	201	2	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
7	NAG	Q	502	1	14,14,15	0.57	0	17,19,21	1.50	2 (11%)
7	NAG	M	502	1	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
7	NAG	C	501	1	14,14,15	0.46	0	17,19,21	1.16	2 (11%)
7	NAG	O	501	1	14,14,15	0.52	0	17,19,21	0.85	0
7	NAG	H	201	2	14,14,15	0.58	0	17,19,21	0.92	1 (5%)
7	NAG	U	501	1	14,14,15	0.49	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	K	601	1	14,14,15	0.48	0	17,19,21	1.59	2 (11%)
7	NAG	L	201	2	14,14,15	0.56	0	17,19,21	0.91	0
7	NAG	M	501	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)
7	NAG	N	201	2	14,14,15	0.56	0	17,19,21	1.16	1 (5%)
7	NAG	R	201	2	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
7	NAG	X	201	2	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
7	NAG	O	502	1	14,14,15	0.50	0	17,19,21	1.42	3 (17%)
7	NAG	U	502	1	14,14,15	0.47	0	17,19,21	1.50	2 (11%)
7	NAG	P	201	2	14,14,15	0.57	0	17,19,21	0.93	0
7	NAG	B	201	2	14,14,15	0.62	0	17,19,21	0.86	1 (5%)
7	NAG	J	201	2	14,14,15	0.52	0	17,19,21	1.22	1 (5%)
7	NAG	W	601	1	14,14,15	0.54	0	17,19,21	1.58	4 (23%)
7	NAG	F	201	2	14,14,15	0.51	0	17,19,21	1.05	1 (5%)
7	NAG	G	502	1	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
7	NAG	E	601	1	14,14,15	0.47	0	17,19,21	1.40	2 (11%)
7	NAG	V	201	2	14,14,15	0.56	0	17,19,21	0.88	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
7	NAG	Q	501	1	-	0/6/23/26	0/1/1/1
7	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	NAG	S	501	1	-	0/6/23/26	0/1/1/1
7	NAG	S	502	1	-	0/6/23/26	0/1/1/1
7	NAG	G	501	1	-	0/6/23/26	0/1/1/1
7	NAG	I	501	1	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2	-	0/6/23/26	0/1/1/1
7	NAG	T	201	2	-	0/6/23/26	0/1/1/1
7	NAG	Q	502	1	-	0/6/23/26	0/1/1/1
7	NAG	M	502	1	-	0/6/23/26	0/1/1/1
7	NAG	C	501	1	-	2/6/23/26	0/1/1/1
7	NAG	O	501	1	-	0/6/23/26	0/1/1/1
7	NAG	H	201	2	-	0/6/23/26	0/1/1/1
7	NAG	U	501	1	-	0/6/23/26	0/1/1/1
7	NAG	K	601	1	-	0/6/23/26	0/1/1/1
7	NAG	L	201	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	M	501	1	-	0/6/23/26	0/1/1/1
7	NAG	N	201	2	-	0/6/23/26	0/1/1/1
7	NAG	R	201	2	-	0/6/23/26	0/1/1/1
7	NAG	X	201	2	-	0/6/23/26	0/1/1/1
7	NAG	O	502	1	-	0/6/23/26	0/1/1/1
7	NAG	U	502	1	-	0/6/23/26	0/1/1/1
7	NAG	P	201	2	-	0/6/23/26	0/1/1/1
7	NAG	B	201	2	-	0/6/23/26	0/1/1/1
7	NAG	J	201	2	-	0/6/23/26	0/1/1/1
7	NAG	W	601	1	-	0/6/23/26	0/1/1/1
7	NAG	F	201	2	-	0/6/23/26	0/1/1/1
7	NAG	G	502	1	-	0/6/23/26	0/1/1/1
7	NAG	E	601	1	-	0/6/23/26	0/1/1/1
7	NAG	V	201	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	601	NAG	C2-N2	-4.00	1.39	1.46
7	A	601	NAG	C8-C7	-3.49	1.43	1.50

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	NAG	O5-C1-C2	-8.70	97.54	111.29
7	A	601	NAG	C2-N2-C7	-7.89	111.67	122.90
7	A	601	NAG	C4-C3-C2	-7.71	99.72	111.02
7	A	601	NAG	C8-C7-N2	-5.86	106.18	116.10
7	A	601	NAG	C3-C4-C5	-4.89	101.51	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	NAG	C8-C7-N2-C2
7	A	601	NAG	O7-C7-N2-C2
7	C	501	NAG	C8-C7-N2-C2
7	C	501	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	318/323 (98%)	0.22	7 (2%) 62 52	33, 40, 68, 127	0
1	C	318/323 (98%)	0.15	5 (1%) 72 62	24, 43, 70, 106	0
1	E	318/323 (98%)	0.19	9 (2%) 53 42	30, 41, 77, 116	0
1	G	318/323 (98%)	0.08	9 (2%) 53 42	21, 33, 78, 132	0
1	I	318/323 (98%)	0.24	8 (2%) 57 47	25, 42, 64, 102	0
1	K	318/323 (98%)	0.05	3 (0%) 84 77	29, 42, 61, 112	0
1	M	318/323 (98%)	0.52	25 (7%) 12 11	58, 70, 100, 141	0
1	O	318/323 (98%)	0.42	22 (6%) 16 13	38, 61, 90, 116	0
1	Q	318/323 (98%)	0.22	16 (5%) 28 24	40, 49, 72, 115	0
1	S	318/323 (98%)	0.40	21 (6%) 18 15	43, 60, 76, 109	0
1	U	318/323 (98%)	0.13	5 (1%) 72 62	33, 42, 74, 121	0
1	W	318/323 (98%)	0.23	16 (5%) 28 24	31, 38, 91, 159	0
2	B	172/174 (98%)	0.03	4 (2%) 60 51	34, 61, 97, 111	0
2	D	172/174 (98%)	0.27	7 (4%) 37 30	40, 58, 81, 85	0
2	F	172/174 (98%)	0.18	8 (4%) 31 26	46, 61, 92, 97	0
2	H	172/174 (98%)	0.15	4 (2%) 60 51	15, 74, 123, 133	0
2	J	172/174 (98%)	0.22	5 (2%) 51 41	39, 61, 89, 96	0
2	L	172/174 (98%)	0.19	8 (4%) 31 26	23, 54, 94, 102	0
2	N	172/174 (98%)	0.34	15 (8%) 10 9	40, 87, 125, 133	0
2	P	172/174 (98%)	0.30	8 (4%) 31 26	40, 81, 115, 128	0
2	R	172/174 (98%)	0.04	2 (1%) 79 70	33, 61, 100, 111	0
2	T	172/174 (98%)	0.22	8 (4%) 31 26	43, 70, 121, 136	0
2	V	172/174 (98%)	0.01	2 (1%) 79 70	35, 57, 102, 115	0
2	X	172/174 (98%)	0.14	5 (2%) 51 41	36, 76, 130, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	a	238/241 (98%)	-0.02	2 (0%) 86 79	23, 37, 62, 74	0
3	c	238/241 (98%)	0.06	3 (1%) 77 68	26, 36, 54, 59	0
3	e	238/241 (98%)	0.30	17 (7%) 16 13	45, 66, 75, 83	0
3	g	238/241 (98%)	0.17	7 (2%) 51 41	18, 39, 95, 107	0
3	i	238/241 (98%)	0.08	2 (0%) 86 79	23, 30, 59, 70	0
3	k	238/241 (98%)	0.25	14 (5%) 22 18	50, 65, 91, 107	0
3	m	238/241 (98%)	0.14	14 (5%) 22 18	39, 47, 73, 86	0
3	o	238/241 (98%)	0.39	15 (6%) 20 16	70, 85, 107, 124	0
3	q	238/241 (98%)	0.18	8 (3%) 45 36	38, 54, 81, 91	0
3	s	238/241 (98%)	0.34	13 (5%) 25 21	63, 81, 100, 126	0
3	u	238/241 (98%)	0.02	2 (0%) 86 79	42, 57, 74, 86	0
3	w	238/241 (98%)	0.14	7 (2%) 51 41	28, 47, 83, 97	0
4	b	213/214 (99%)	-0.08	0 100 100	17, 28, 62, 66	0
4	d	213/214 (99%)	-0.08	0 100 100	23, 39, 67, 73	0
4	f	213/214 (99%)	-0.13	1 (0%) 91 85	44, 54, 86, 97	0
4	h	213/214 (99%)	0.05	3 (1%) 75 65	20, 33, 85, 91	0
4	j	213/214 (99%)	-0.05	0 100 100	23, 31, 66, 80	0
4	l	213/214 (99%)	-0.02	6 (2%) 53 42	54, 79, 103, 107	0
4	n	213/214 (99%)	0.04	3 (1%) 75 65	33, 44, 55, 62	0
4	p	213/214 (99%)	0.10	7 (3%) 46 37	70, 79, 105, 111	0
4	r	213/214 (99%)	-0.07	2 (0%) 84 77	33, 53, 68, 73	0
4	t	213/214 (99%)	-0.09	3 (1%) 75 65	47, 68, 105, 115	0
4	v	213/214 (99%)	-0.01	4 (1%) 66 58	34, 48, 84, 93	0
4	x	213/214 (99%)	0.03	2 (0%) 84 77	25, 41, 54, 59	0
All	All	11292/11424 (98%)	0.15	357 (3%) 47 37	15, 51, 98, 159	0

The worst 5 of 357 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	o	133	GLY	7.9
1	Q	10	GLY	7.6
1	W	326	LYS	7.0
3	w	132	SER	7.0
2	N	27	GLN	6.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PCA	o	1	8/9	0.77	0.26	77,78,79,79	0
3	PCA	i	1	8/9	0.82	0.34	32,32,33,33	0
3	PCA	e	1	8/9	0.86	0.29	54,56,59,62	0
3	PCA	u	1	8/9	0.86	0.30	54,55,56,56	0
3	PCA	q	1	8/9	0.87	0.24	57,57,58,58	0
3	PCA	c	1	8/9	0.88	0.25	36,37,38,39	0
3	PCA	a	1	8/9	0.90	0.21	36,36,37,38	0
3	PCA	k	1	8/9	0.90	0.20	50,52,54,57	0
3	PCA	s	1	8/9	0.90	0.18	63,64,64,64	0
3	PCA	m	1	8/9	0.90	0.17	40,41,41,41	0
3	PCA	w	1	8/9	0.91	0.17	27,27,27,29	0
3	PCA	g	1	8/9	0.94	0.17	35,36,38,38	0

## 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	AA	4	11/12	0.45	0.53	78,81,81,82	0
5	BMA	AA	3	11/12	0.46	0.38	66,70,72,75	0
5	BMA	8	3	11/12	0.47	0.31	78,82,85,86	0
5	BMA	GA	3	11/12	0.54	0.31	62,67,72,72	0
5	BMA	0	3	11/12	0.60	0.26	64,68,72,73	0
6	NAG	7	2	14/15	0.61	0.41	54,62,69,69	0
5	MAN	8	4	11/12	0.68	0.35	88,92,93,93	0
6	NAG	1	2	14/15	0.70	0.33	75,83,89,90	0
5	BMA	CA	3	11/12	0.70	0.27	82,87,91,92	0
5	BMA	EA	3	11/12	0.71	0.27	72,75,77,79	0
5	BMA	IA	3	11/12	0.71	0.27	68,73,76,76	0
5	NAG	6	2	14/15	0.72	0.50	51,60,69,71	0
5	MAN	6	4	11/12	0.72	0.34	84,87,89,90	0
5	NAG	Y	1	14/15	0.72	0.40	45,48,60,61	0
5	BMA	4	3	11/12	0.72	0.26	65,69,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	BA	1	14/15	0.72	0.36	71,77,82,84	0
5	MAN	CA	4	11/12	0.73	0.30	92,96,98,98	0
5	NAG	IA	1	14/15	0.73	0.32	39,46,56,57	0
5	MAN	Y	4	11/12	0.73	0.40	78,80,84,84	0
5	MAN	2	4	11/12	0.74	0.30	62,65,66,67	0
5	BMA	y	3	11/12	0.74	0.23	44,48,51,53	0
5	MAN	4	4	11/12	0.74	0.33	75,78,80,80	0
6	NAG	FA	2	14/15	0.74	0.26	70,80,86,87	0
6	NAG	3	2	14/15	0.76	0.54	49,58,66,66	0
5	BMA	2	3	11/12	0.76	0.24	51,55,58,60	0
6	NAG	9	1	14/15	0.76	0.36	70,73,76,76	0
5	MAN	IA	4	11/12	0.76	0.26	78,81,84,84	0
5	NAG	IA	2	14/15	0.76	0.32	43,52,61,63	0
5	BMA	Y	3	11/12	0.77	0.22	70,74,78,78	0
6	NAG	9	2	14/15	0.77	0.30	70,79,89,89	0
6	NAG	5	2	14/15	0.77	0.24	62,74,81,82	0
5	BMA	6	3	11/12	0.77	0.23	75,79,82,83	0
5	NAG	8	2	14/15	0.78	0.22	66,69,71,74	0
6	NAG	1	1	14/15	0.78	0.24	60,66,70,74	0
5	NAG	Y	2	14/15	0.79	0.28	45,54,65,65	0
5	NAG	EA	2	14/15	0.79	0.38	52,58,68,69	0
6	NAG	FA	1	14/15	0.79	0.29	59,63,67,70	0
6	NAG	Z	2	14/15	0.79	0.36	51,59,65,65	0
6	NAG	BA	2	14/15	0.80	0.31	82,93,102,102	0
5	NAG	6	1	14/15	0.80	0.27	49,56,67,67	0
5	NAG	AA	2	14/15	0.80	0.41	47,52,59,62	0
6	NAG	5	1	14/15	0.81	0.39	50,57,61,63	0
6	NAG	Z	1	14/15	0.82	0.25	37,40,44,49	0
6	NAG	DA	2	14/15	0.82	0.36	59,67,73,73	0
5	NAG	CA	2	14/15	0.82	0.42	57,66,77,78	0
6	NAG	z	2	14/15	0.82	0.26	45,52,59,60	0
6	NAG	HA	1	14/15	0.82	0.53	42,44,47,47	0
6	NAG	z	1	14/15	0.83	0.33	43,45,49,50	0
5	NAG	y	2	14/15	0.83	0.21	32,34,37,40	0
5	MAN	0	4	11/12	0.83	0.27	76,78,80,81	0
5	MAN	GA	4	11/12	0.83	0.24	74,78,81,82	0
5	NAG	GA	2	14/15	0.84	0.27	44,46,55,58	0
5	MAN	EA	4	11/12	0.84	0.29	81,83,84,84	0
6	NAG	7	1	14/15	0.84	0.30	40,47,50,53	0
6	NAG	JA	2	14/15	0.84	0.28	67,78,86,87	0
6	NAG	DA	1	14/15	0.85	0.33	46,50,54,57	0
6	NAG	JA	1	14/15	0.85	0.26	53,60,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	EA	1	14/15	0.85	0.19	53,58,69,69	0
5	NAG	CA	1	14/15	0.86	0.23	54,60,70,71	0
6	NAG	3	1	14/15	0.86	0.21	37,42,47,49	0
5	NAG	0	1	14/15	0.87	0.28	40,46,56,56	0
5	NAG	0	2	14/15	0.88	0.25	46,50,58,60	0
6	NAG	HA	2	14/15	0.88	0.32	48,56,62,63	0
5	NAG	4	2	14/15	0.89	0.23	42,50,60,62	0
5	MAN	y	4	11/12	0.90	0.20	56,59,60,61	0
5	NAG	8	1	14/15	0.91	0.26	66,67,68,68	0
5	NAG	2	2	14/15	0.91	0.21	30,37,45,47	0
5	NAG	AA	1	14/15	0.91	0.19	43,49,57,58	0
5	NAG	GA	1	14/15	0.93	0.17	41,43,48,48	0
5	NAG	2	1	14/15	0.93	0.25	26,32,41,42	0
5	NAG	y	1	14/15	0.94	0.24	30,32,34,34	0
5	NAG	4	1	14/15	0.95	0.25	40,47,57,58	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	R	201	14/15	0.35	0.60	100,111,117,117	0
7	NAG	M	502	14/15	0.40	0.58	75,76,77,78	0
7	NAG	E	601	14/15	0.43	0.43	59,64,66,67	0
7	NAG	U	502	14/15	0.45	0.61	46,48,50,51	0
7	NAG	G	502	14/15	0.49	0.70	42,47,49,51	0
7	NAG	Q	502	14/15	0.49	0.65	61,67,70,71	0
7	NAG	N	201	14/15	0.52	0.34	109,114,121,122	0
7	NAG	P	201	14/15	0.55	0.37	96,101,106,107	0
7	NAG	A	601	14/15	0.55	0.46	38,44,45,46	0
7	NAG	W	601	14/15	0.55	0.40	45,51,52,54	0
7	NAG	S	502	14/15	0.57	0.42	65,69,74,75	0
7	NAG	T	201	14/15	0.59	0.47	93,100,105,107	0
7	NAG	O	502	14/15	0.61	0.37	74,78,81,83	0
7	NAG	K	601	14/15	0.63	0.34	58,64,66,68	0
7	NAG	L	201	14/15	0.63	0.38	81,89,95,96	0
7	NAG	V	201	14/15	0.64	0.58	83,85,91,93	0
7	NAG	O	501	14/15	0.64	0.63	90,98,105,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	X	201	14/15	0.66	0.34	119,129,138,140	0
7	NAG	J	201	14/15	0.67	0.39	73,75,79,80	0
7	NAG	I	501	14/15	0.68	0.36	66,74,81,84	0
7	NAG	H	201	14/15	0.69	0.33	115,125,133,134	0
7	NAG	D	201	14/15	0.71	0.38	73,75,77,78	0
7	NAG	S	501	14/15	0.72	0.48	71,78,84,87	0
7	NAG	C	501	14/15	0.74	0.42	66,69,74,76	0
7	NAG	B	201	14/15	0.75	0.27	80,89,94,96	0
7	NAG	F	201	14/15	0.76	0.45	88,93,99,100	0
7	NAG	G	501	14/15	0.78	0.30	68,75,84,87	0
7	NAG	M	501	14/15	0.84	0.23	89,92,96,98	0
7	NAG	U	501	14/15	0.84	0.26	66,70,75,78	0
7	NAG	Q	501	14/15	0.85	0.24	66,74,80,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.