



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:47 PM BST

PDB ID : 6P3S  
Title : Crystal structure of human Fab H5.28 in complex with influenza A H5N1  
Vietnam hemagglutinin head domain  
Authors : Dong, J.; Crowe, J.E.  
Deposited on : 2019-05-24  
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

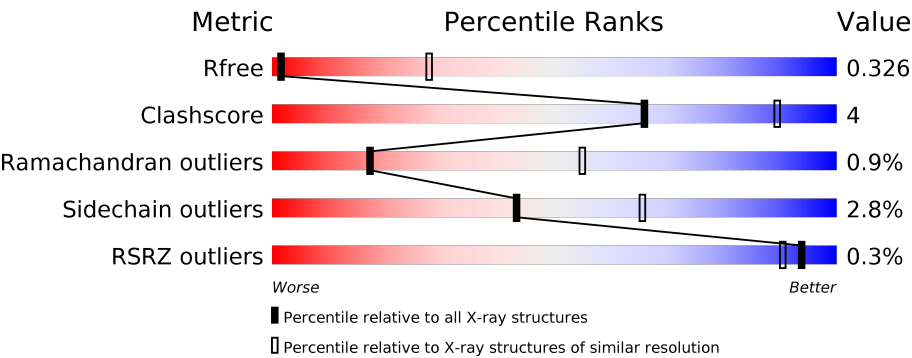
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.






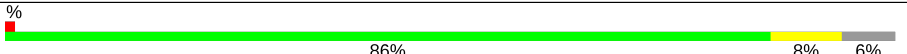





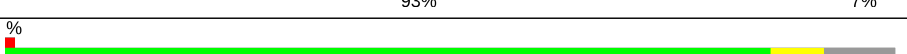




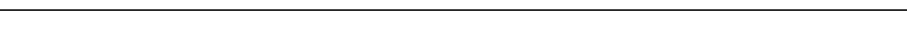




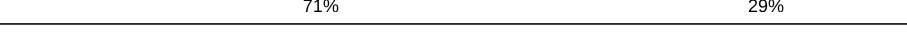

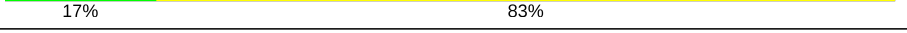

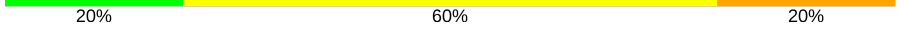

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	230	<div><div></div><div>85%12%..</div></div>
1	C	230	<div><div>%</div><div>89%6%5%</div></div>
1	F	230	<div><div></div><div>86%10%. </div></div>
1	I	230	<div><div></div><div>87%7%6%</div></div>
1	M	230	<div><div></div><div>92%6%. </div></div>
1	P	230	<div><div></div><div>90%6%. </div></div>

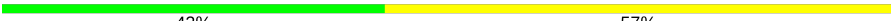
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Mol	Chain	Length	Quality of chain
1	S	230	
1	V	230	
2	B	215	
2	D	215	
2	G	215	
2	J	215	
2	N	215	
2	Q	215	
2	T	215	
2	W	215	
3	E	219	
3	H	219	
3	K	219	
3	L	219	
3	O	219	
3	R	219	
3	U	219	
3	X	219	
4	Y	7	
5	Z	7	
6	a	6	
7	b	7	
8	c	5	
9	d	7	
10	e	5	

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Mol	Chain	Length	Quality of chain
11	f	7	 43% 57%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 32097 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 Human Fab H5.28 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1472	932	258	275	7			
1	C	218	Total	C	N	O	S	0	0	0
			1301	803	237	257	4			
1	F	223	Total	C	N	O	S	0	0	0
			1436	902	258	269	7			
1	I	217	Total	C	N	O	S	0	0	0
			1364	850	248	260	6			
1	M	225	Total	C	N	O	S	0	0	0
			1432	908	260	257	7			
1	P	220	Total	C	N	O	S	0	0	0
			1313	820	241	246	6			
1	S	224	Total	C	N	O	S	0	0	0
			1393	875	256	255	7			
1	V	208	Total	C	N	O	S	0	0	0
			1236	773	225	232	6			

- Molecule 2 is a protein called Human Fab H5.28 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1477	932	254	285	6			
2	D	203	Total	C	N	O	S	0	0	0
			1211	741	228	238	4			
2	G	214	Total	C	N	O	S	0	0	0
			1363	853	243	261	6			
2	J	187	Total	C	N	O	S	0	0	0
			1097	677	201	215	4			
2	N	214	Total	C	N	O	S	0	0	0
			1295	812	233	244	6			
2	Q	202	Total	C	N	O	S	0	0	0
			1179	731	224	219	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	214	Total	C	N	O	S	0	0	0
			1280	797	240	238	5			
2	W	198	Total	C	N	O	S	0	0	0
			1121	694	212	212	3			

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	196	Total	C	N	O	S	0	0	0
			1221	777	216	223	5			
3	H	202	Total	C	N	O	S	0	0	0
			1337	849	243	240	5			
3	K	206	Total	C	N	O	S	0	0	0
			1397	883	245	264	5			
3	L	185	Total	C	N	O	S	0	0	0
			1219	772	218	226	3			
3	O	209	Total	C	N	O	S	0	0	0
			1414	895	252	262	5			
3	R	194	Total	C	N	O	S	0	0	0
			1258	792	230	231	5			
3	U	196	Total	C	N	O	S	0	0	0
			1285	811	233	236	5			
3	X	196	Total	C	N	O	S	0	0	0
			1236	778	224	229	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	269	ALA	-	expression tag	UNP Q1KHK2
E	270	ALA	-	expression tag	UNP Q1KHK2
E	271	HIS	-	expression tag	UNP Q1KHK2
E	272	HIS	-	expression tag	UNP Q1KHK2
E	273	HIS	-	expression tag	UNP Q1KHK2
E	274	HIS	-	expression tag	UNP Q1KHK2
E	275	HIS	-	expression tag	UNP Q1KHK2
E	276	HIS	-	expression tag	UNP Q1KHK2
H	269	ALA	-	expression tag	UNP Q1KHK2
H	270	ALA	-	expression tag	UNP Q1KHK2
H	271	HIS	-	expression tag	UNP Q1KHK2
H	272	HIS	-	expression tag	UNP Q1KHK2
H	273	HIS	-	expression tag	UNP Q1KHK2
H	274	HIS	-	expression tag	UNP Q1KHK2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	275	HIS	-	expression tag	UNP Q1KHK2
H	276	HIS	-	expression tag	UNP Q1KHK2
K	269	ALA	-	expression tag	UNP Q1KHK2
K	270	ALA	-	expression tag	UNP Q1KHK2
K	271	HIS	-	expression tag	UNP Q1KHK2
K	272	HIS	-	expression tag	UNP Q1KHK2
K	273	HIS	-	expression tag	UNP Q1KHK2
K	274	HIS	-	expression tag	UNP Q1KHK2
K	275	HIS	-	expression tag	UNP Q1KHK2
K	276	HIS	-	expression tag	UNP Q1KHK2
L	269	ALA	-	expression tag	UNP Q1KHK2
L	270	ALA	-	expression tag	UNP Q1KHK2
L	271	HIS	-	expression tag	UNP Q1KHK2
L	272	HIS	-	expression tag	UNP Q1KHK2
L	273	HIS	-	expression tag	UNP Q1KHK2
L	274	HIS	-	expression tag	UNP Q1KHK2
L	275	HIS	-	expression tag	UNP Q1KHK2
L	276	HIS	-	expression tag	UNP Q1KHK2
O	269	ALA	-	expression tag	UNP Q1KHK2
O	270	ALA	-	expression tag	UNP Q1KHK2
O	271	HIS	-	expression tag	UNP Q1KHK2
O	272	HIS	-	expression tag	UNP Q1KHK2
O	273	HIS	-	expression tag	UNP Q1KHK2
O	274	HIS	-	expression tag	UNP Q1KHK2
O	275	HIS	-	expression tag	UNP Q1KHK2
O	276	HIS	-	expression tag	UNP Q1KHK2
R	269	ALA	-	expression tag	UNP Q1KHK2
R	270	ALA	-	expression tag	UNP Q1KHK2
R	271	HIS	-	expression tag	UNP Q1KHK2
R	272	HIS	-	expression tag	UNP Q1KHK2
R	273	HIS	-	expression tag	UNP Q1KHK2
R	274	HIS	-	expression tag	UNP Q1KHK2
R	275	HIS	-	expression tag	UNP Q1KHK2
R	276	HIS	-	expression tag	UNP Q1KHK2
U	269	ALA	-	expression tag	UNP Q1KHK2
U	270	ALA	-	expression tag	UNP Q1KHK2
U	271	HIS	-	expression tag	UNP Q1KHK2
U	272	HIS	-	expression tag	UNP Q1KHK2
U	273	HIS	-	expression tag	UNP Q1KHK2
U	274	HIS	-	expression tag	UNP Q1KHK2
U	275	HIS	-	expression tag	UNP Q1KHK2
U	276	HIS	-	expression tag	UNP Q1KHK2

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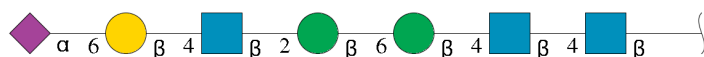
Chain	Residue	Modelled	Actual	Comment	Reference
X	269	ALA	-	expression tag	UNP Q1KHK2
X	270	ALA	-	expression tag	UNP Q1KHK2
X	271	HIS	-	expression tag	UNP Q1KHK2
X	272	HIS	-	expression tag	UNP Q1KHK2
X	273	HIS	-	expression tag	UNP Q1KHK2
X	274	HIS	-	expression tag	UNP Q1KHK2
X	275	HIS	-	expression tag	UNP Q1KHK2
X	276	HIS	-	expression tag	UNP Q1KHK2

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-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
4	Y	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-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	Z	7	Total	C	N	O	0	0	0
			95	53	4	38			

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





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	a	6	Total	C	N	O	0	0	0
			81	45	3	33			

- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.



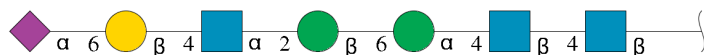
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	b	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	c	5	Total	C	N	O	0	0	0
			67	37	2	28			

- Molecule 9 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-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	d	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 10 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



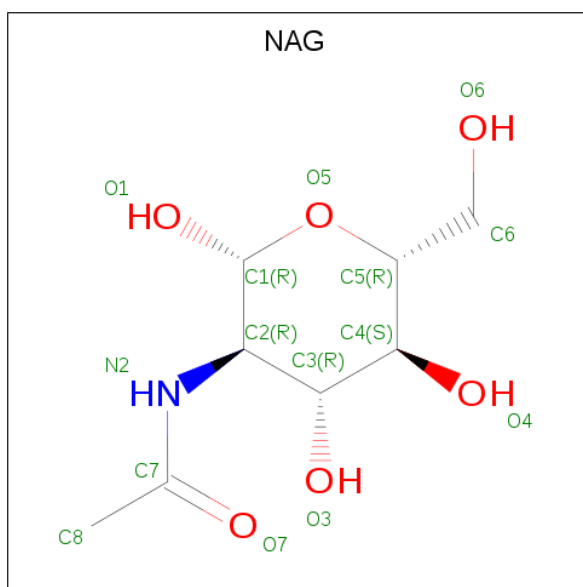
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	e	5	Total	C	N	O	0	0	0
			67	37	2	28			

- Molecule 11 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-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
11	f	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 12 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>).

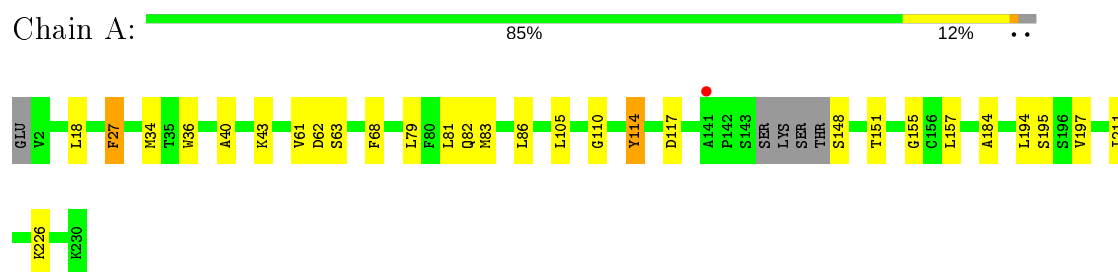


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			14	8	1	5		
12	O	1	Total	C	N	O	0	0
			14	8	1	5		
12	R	1	Total	C	N	O	0	0
			14	8	1	5		
12	U	1	Total	C	N	O	0	0
			14	8	1	5		
12	X	1	Total	C	N	O	0	0
			14	8	1	5		

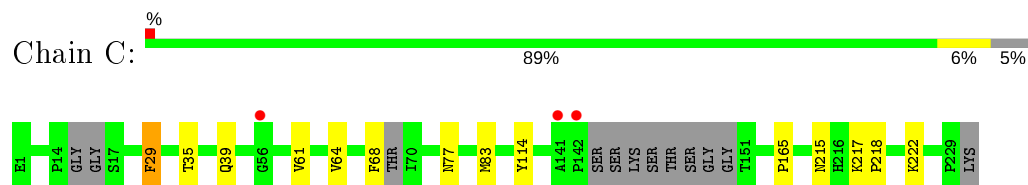
### 3 Residue-property plots [i](#)

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.

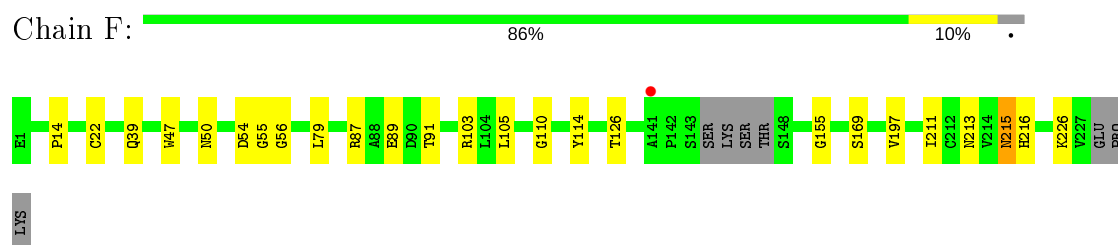
- Molecule 1: Human Fab H5.28 heavy chain



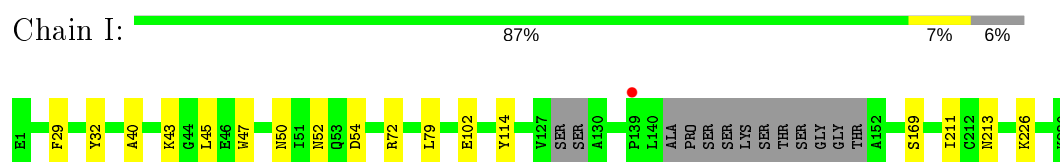
- Molecule 1: Human Fab H5.28 heavy chain



- Molecule 1: Human Fab H5.28 heavy chain



- Molecule 1: Human Fab H5.28 heavy chain



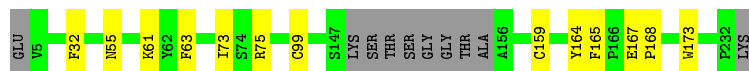
- Molecule 1: Human Fab H5.28 heavy chain





- Molecule 1: Human Fab H5.28 heavy chain

Chain P: 90% 6%



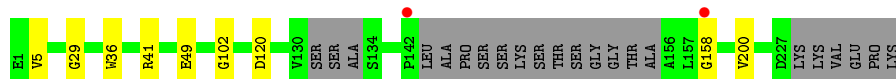
- Molecule 1: Human Fab H5.28 heavy chain

Chain S: 91% 7%



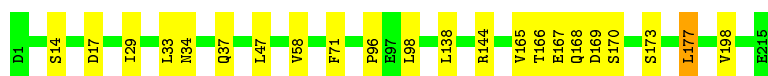
- Molecule 1: Human Fab H5.28 heavy chain

Chain V: 87% 10%



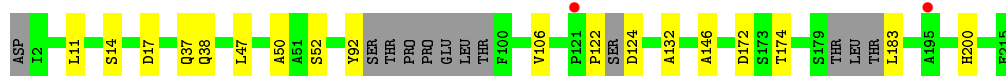
- Molecule 2: Human Fab H5.28 light chain

Chain B: 90% 10%



- Molecule 2: Human Fab H5.28 light chain

Chain D: 86% 8% 6%



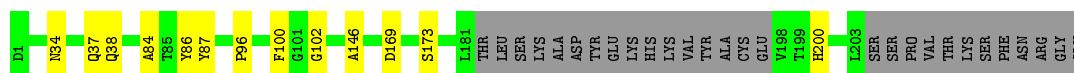
- Molecule 2: Human Fab H5.28 light chain

Chain G: 89% 10%



- Molecule 2: Human Fab H5.28 light chain

Chain J: 81% 6% 13%



- Molecule 2: Human Fab H5.28 light chain

Chain N: 94% 6%



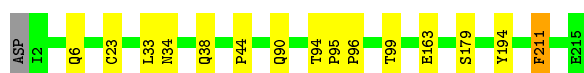
- Molecule 2: Human Fab H5.28 light chain

Chain Q: 89% 5% 6%



- Molecule 2: Human Fab H5.28 light chain

Chain T: 93% 7%



- Molecule 2: Human Fab H5.28 light chain

Chain W: 86% 6% 8%



- Molecule 3: Hemagglutinin

Chain E: 83% 6% 11%



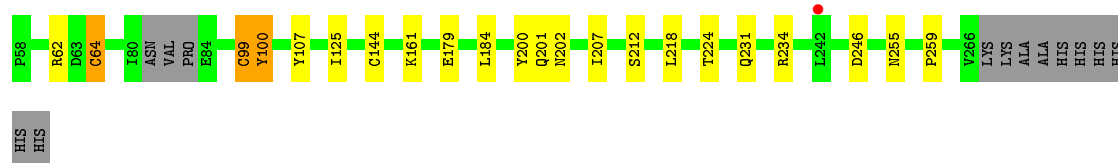
- Molecule 3: Hemagglutinin

Chain H: 87% 8% 5%



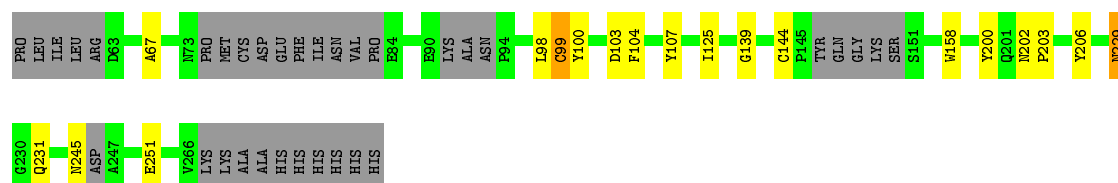
- Molecule 3: Hemagglutinin

Chain K: 84% 9% 6%



• Molecule 3: Hemagglutinin

Chain L: 76% 8% 16%



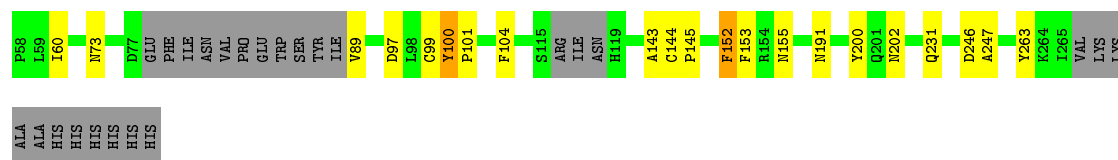
• Molecule 3: Hemagglutinin

Chain O: 86% 9% 5%



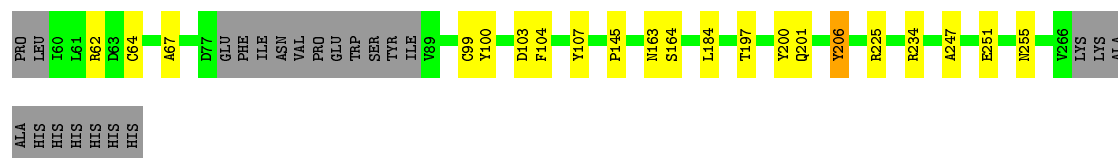
• Molecule 3: Hemagglutinin

Chain R: 79% 9% 11%



• Molecule 3: Hemagglutinin

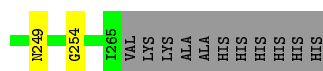
Chain U: 80% 9% 11%



• Molecule 3: Hemagglutinin

Chain X: 78% 11% 11%





- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-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 Y: 71% 29%



- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-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 Z: 14% 57% 29%



- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 17% 83%



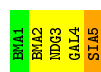
- Molecule 7: N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 29% 57% 14%



- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain c: 20% 60% 20%



- Molecule 9: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-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

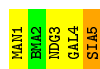


Chain d:  43% 43% 14%



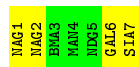
- Molecule 10: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose

Chain e:  20% 60% 20%



- Molecule 11: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-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 f:  43% 57%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.48 Å   187.22 Å   342.37 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.46 – 4.00 49.46 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.46-4.00) 100.0 (49.46-4.00)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 4.00 Å)	Xtriage
Refinement program	PHENIX (1.15.2 _3472: ???)	Depositor
R, $R_{free}$	0.281   ,   0.326 0.281   ,   0.326	Depositor DCC
$R_{free}$ test set	3660 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.0	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 106.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	32097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, GLA, NDG, SIA, GAL, 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	0.25	0/1506	0.43	0/2064
1	C	0.24	0/1325	0.45	0/1826
1	F	0.25	0/1471	0.44	0/2020
1	I	0.24	0/1395	0.43	0/1916
1	M	0.25	0/1472	0.44	0/2019
1	P	0.25	0/1344	0.43	0/1851
1	S	0.25	0/1429	0.43	0/1963
1	V	0.25	0/1267	0.43	0/1746
2	B	0.25	0/1509	0.44	0/2065
2	D	0.24	0/1230	0.42	0/1694
2	G	0.24	0/1395	0.43	0/1919
2	J	0.25	0/1118	0.46	0/1547
2	N	0.25	0/1324	0.45	0/1826
2	Q	0.24	0/1201	0.46	0/1657
2	T	0.26	0/1308	0.45	0/1807
2	W	0.24	0/1139	0.43	0/1574
3	E	0.24	0/1255	0.42	0/1736
3	H	0.24	0/1373	0.43	0/1891
3	K	0.24	0/1432	0.41	0/1968
3	L	0.24	0/1247	0.42	0/1711
3	O	0.25	0/1453	0.43	0/2004
3	R	0.24	0/1291	0.44	0/1779
3	U	0.25	0/1321	0.43	0/1818
3	X	0.24	0/1270	0.41	0/1754
All	All	0.25	0/32075	0.43	0/44155

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1472	0	1144	18	0
1	C	1301	0	860	7	0
1	F	1436	0	1090	12	0
1	I	1364	0	956	11	0
1	M	1432	0	1020	10	0
1	P	1313	0	811	4	0
1	S	1393	0	957	9	0
1	V	1236	0	750	5	0
2	B	1477	0	1244	12	0
2	D	1211	0	797	9	0
2	G	1363	0	954	11	0
2	J	1097	0	671	7	0
2	N	1295	0	826	7	0
2	Q	1179	0	718	1	0
2	T	1280	0	805	7	0
2	W	1121	0	650	9	0
3	E	1221	0	769	4	1
3	H	1337	0	963	4	0
3	K	1397	0	1099	10	2
3	L	1219	0	844	7	4
3	O	1414	0	1027	9	2
3	R	1258	0	835	9	1
3	U	1285	0	862	11	0
3	X	1236	0	763	11	4
4	Y	95	0	79	4	4
5	Z	95	0	80	2	0
6	a	81	0	64	0	0
7	b	95	0	80	0	1
8	c	67	0	55	0	2
9	d	95	0	79	0	4
10	e	67	0	55	0	2
11	f	95	0	79	0	1
12	L	14	0	13	0	0
12	O	14	0	13	0	0
12	R	14	0	13	1	0
12	U	14	0	13	2	0
12	X	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32097	0	22051	199	14

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 4.

All (199) 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:105:GLU:OE2	3:U:234:ARG:NE	2.08	0.87
1:C:217:LYS:HG3	1:C:218:PRO:HD3	1.71	0.72
3:R:152:PHE:HD1	3:R:153:PHE:H	1.36	0.71
3:H:99:CYS:SG	3:H:100:TYR:N	2.63	0.71
1:A:155:GLY:HA3	1:A:197:VAL:HA	1.76	0.67
1:M:117:TYR:O	2:N:34:ASN:ND2	2.26	0.67
3:U:103:ASP:OD1	3:U:104:PHE:N	2.27	0.67
1:I:45:LEU:HD21	2:J:38:GLN:HE22	1.60	0.67
1:A:157:LEU:HD12	1:A:195:SER:HB3	1.78	0.66
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.77	0.66
3:L:103:ASP:OD1	3:L:104:PHE:N	2.29	0.65
3:U:99:CYS:SG	3:U:100:TYR:N	2.70	0.64
1:A:61:VAL:O	1:A:63:SER:N	2.31	0.63
1:I:102:GLU:OE2	3:K:234:ARG:NE	2.29	0.63
1:P:61:LYS:HD3	1:P:63:PHE:HE1	1.63	0.62
3:X:99:CYS:HB2	3:X:144:CYS:HA	1.82	0.62
1:P:55:ASN:O	1:P:75:ARG:NH1	2.33	0.62
1:M:55:ASN:O	1:M:75:ARG:NH1	2.33	0.61
3:O:179:GLU:OE2	3:O:179:GLU:N	2.33	0.61
1:A:184:ALA:HA	1:A:194:LEU:HB3	1.81	0.61
2:T:194:TYR:HB2	2:T:211:PHE:HE1	1.65	0.60
3:U:197:THR:HA	3:U:201:GLN:HA	1.83	0.59
1:I:169:SER:O	1:I:213:ASN:N	2.34	0.59
1:I:40:ALA:HB3	1:I:43:LYS:HB2	1.85	0.59
3:K:161:LYS:NZ	3:K:201:GLN:OE1	2.35	0.59
2:D:172:ASP:OD2	2:D:174:THR:OG1	2.17	0.58
2:B:14:SER:OG	2:B:17:ASP:OD2	2.20	0.58
2:W:29:ILE:HA	2:W:92:TYR:CE1	2.37	0.58
1:S:50:TRP:NE1	1:S:53:ASN:OD1	2.36	0.58
1:A:211:ILE:HA	1:A:226:LYS:HA	1.85	0.58
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.86	0.58
2:G:110:ARG:NH1	2:G:172:ASP:O	2.37	0.58
2:B:169:ASP:OD1	2:B:170:SER:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:99:CYS:SG	3:X:100:TYR:N	2.76	0.58
3:K:99:CYS:SG	3:K:100:TYR:N	2.78	0.57
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.86	0.57
4:Y:6:GAL:O4	4:Y:6:GAL:O6	2.14	0.57
1:V:158:GLY:HA3	1:V:200:VAL:HA	1.87	0.56
3:O:99:CYS:SG	3:O:100:TYR:N	2.79	0.56
1:F:47:TRP:NE1	1:F:50:ASN:OD1	2.37	0.56
3:X:97:ASP:OD1	3:X:97:ASP:N	2.39	0.55
1:A:68:PHE:HB3	1:A:83:MET:HA	1.89	0.55
3:H:200:TYR:O	3:H:202:ASN:N	2.39	0.54
2:T:90:GLN:HB3	2:T:99:THR:H	1.70	0.54
1:A:148:SER:N	1:A:151:THR:O	2.41	0.54
1:F:211:ILE:HA	1:F:226:LYS:HA	1.90	0.54
3:H:144:CYS:HB3	3:H:151:SER:O	2.08	0.54
3:U:225:ARG:HD3	3:U:234:ARG:HD2	1.89	0.54
1:S:55:ASN:O	1:S:75:ARG:NH1	2.40	0.54
2:D:146:ALA:HB2	2:D:200:HIS:HD2	1.73	0.54
1:C:61:VAL:HG13	1:C:64:VAL:H	1.73	0.54
1:I:114:TYR:O	2:J:34:ASN:ND2	2.41	0.53
2:D:11:LEU:HB3	2:D:106:VAL:HG22	1.89	0.52
3:R:73:ASN:ND2	3:R:97:ASP:O	2.43	0.52
2:T:6:GLN:HA	2:T:23:CYS:HA	1.90	0.52
1:P:61:LYS:NZ	1:P:73:ILE:O	2.43	0.52
2:G:88:CYS:O	2:G:101:GLY:N	2.43	0.52
1:F:54:ASP:O	1:F:56:GLY:N	2.41	0.52
2:G:33:LEU:HD11	2:G:88:CYS:HB2	1.92	0.52
3:E:200:TYR:O	3:E:202:ASN:N	2.41	0.51
2:N:66:GLY:HA3	2:N:71:PHE:HA	1.91	0.51
2:B:138:LEU:HB2	2:B:177:LEU:HD23	1.93	0.51
1:F:22:CYS:HB3	1:F:79:LEU:HB3	1.91	0.51
3:L:200:TYR:O	3:L:202:ASN:N	2.40	0.51
1:F:105:LEU:HA	1:F:110:GLY:HA3	1.93	0.51
3:X:180:ASP:OD2	3:X:243:LYS:NZ	2.30	0.51
3:K:200:TYR:O	3:K:202:ASN:N	2.39	0.51
3:L:67:ALA:HB2	3:L:107:TYR:HE1	1.75	0.51
2:W:9:SER:HA	2:W:104:THR:H	1.76	0.51
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.93	0.50
1:P:159:CYS:HB2	1:P:173:TRP:CZ2	2.46	0.50
3:E:180:ASP:O	3:E:265:ILE:N	2.42	0.50
2:D:50:ALA:O	2:D:52:SER:N	2.42	0.50
3:U:206:TYR:OH	3:U:251:GLU:OE2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:HB2	1:A:82:GLN:O	2.12	0.49
3:L:206:TYR:OH	3:L:251:GLU:OE2	2.25	0.49
1:F:91:THR:HG23	1:F:126:THR:HA	1.93	0.49
12:U:301:NAG:O3	12:U:301:NAG:O7	2.29	0.49
1:C:29:PHE:HD2	1:C:77:ASN:HA	1.78	0.49
1:A:114:TYR:O	2:B:34:ASN:ND2	2.33	0.48
1:I:72:ARG:HA	1:I:79:LEU:HA	1.95	0.48
3:K:62:ARG:O	3:K:64:CYS:N	2.44	0.48
3:L:229:ASN:ND2	3:L:229:ASN:O	2.46	0.48
1:M:158:GLY:HA2	1:M:173:TRP:HZ2	1.78	0.48
1:C:35:THR:OG1	1:C:114:TYR:OH	2.24	0.48
1:C:215:ASN:HA	1:C:222:LYS:HA	1.95	0.48
3:X:225:ARG:HD3	3:X:234:ARG:HG2	1.95	0.48
1:S:37:MET:HB3	1:S:82:LEU:HD22	1.96	0.48
2:D:14:SER:OG	2:D:17:ASP:OD2	2.32	0.47
2:W:135:VAL:HA	2:W:180:THR:HA	1.95	0.47
1:V:120:ASP:OD1	1:V:120:ASP:N	2.47	0.47
3:K:212:SER:OG	3:K:246:ASP:OD2	2.23	0.47
3:O:131:TRP:HZ3	3:O:169:ILE:HG21	1.79	0.47
1:V:5:VAL:HA	1:V:29:GLY:HA3	1.97	0.47
3:E:58:PRO:HA	3:E:88:ILE:HG12	1.96	0.47
1:F:155:GLY:HA3	1:F:197:VAL:HA	1.96	0.47
2:N:78:LEU:H	2:N:78:LEU:HD23	1.80	0.47
2:B:144:ARG:HD2	2:B:165:VAL:HG11	1.96	0.47
4:Y:7:SIA:O6	4:Y:7:SIA:O8	2.22	0.47
1:C:39:GLN:OE1	2:D:38:GLN:NE2	2.36	0.47
3:X:131:TRP:HB3	3:X:134:HIS:HB2	1.97	0.47
2:G:165:VAL:HA	2:G:177:LEU:HA	1.97	0.47
1:I:47:TRP:NE1	1:I:50:ASN:OD1	2.33	0.47
1:A:27:PHE:H	1:A:27:PHE:HD1	1.63	0.47
1:F:39:GLN:NE2	2:G:38:GLN:OE1	2.45	0.47
1:F:169:SER:O	1:F:213:ASN:N	2.36	0.46
2:B:138:LEU:HD21	2:B:198:VAL:HG11	1.97	0.46
2:G:85:THR:HA	2:G:105:LYS:HA	1.96	0.46
2:N:33:LEU:HD22	2:N:71:PHE:CG	2.50	0.46
3:L:99:CYS:HB3	3:L:144:CYS:HB2	1.72	0.46
1:M:36:TRP:NE1	1:M:56:GLN:OE1	2.49	0.46
2:W:50:ALA:O	2:W:52:SER:N	2.46	0.46
2:J:146:ALA:HB2	2:J:200:HIS:HD2	1.79	0.46
2:G:6:GLN:HA	2:G:23:CYS:HA	1.97	0.46
3:R:155:ASN:ND2	3:R:263:TYR:OH	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:25:CYS:HB3	1:S:82:LEU:HB3	1.97	0.46
2:G:37:GLN:HB3	2:G:47:LEU:HD11	1.97	0.46
3:H:71:LEU:O	3:H:153:PHE:HB3	2.16	0.46
1:M:41:ARG:O	1:M:49:GLU:N	2.43	0.46
1:A:68:PHE:CB	1:A:83:MET:HA	2.46	0.45
2:D:132:ALA:O	2:D:183:LEU:N	2.49	0.45
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.98	0.45
2:B:33:LEU:HD13	2:B:71:PHE:CD1	2.52	0.45
1:I:211:ILE:HA	1:I:226:LYS:HA	1.98	0.45
1:I:32:TYR:OH	3:K:224:THR:N	2.37	0.45
2:W:29:ILE:HA	2:W:92:TYR:CD1	2.51	0.45
3:X:166:TYR:HE2	3:X:254:GLY:HA2	1.81	0.45
2:N:33:LEU:HD11	2:N:88:CYS:SG	2.57	0.45
2:T:38:GLN:HB2	2:T:44:PRO:HB3	1.97	0.45
3:O:143:ALA:O	3:O:145:PRO:HD3	2.16	0.45
3:O:85:TRP:HA	3:O:117:ILE:HG23	1.98	0.44
3:R:246:ASP:OD1	3:R:247:ALA:N	2.39	0.44
3:E:188:HIS:HA	3:E:235:MET:HG2	1.98	0.44
3:O:110:LEU:HD12	3:O:239:TRP:CD1	2.52	0.44
3:X:211:THR:N	3:X:214:LEU:O	2.47	0.44
3:O:73:ASN:HD21	3:O:99:CYS:HB3	1.82	0.44
3:X:62:ARG:O	3:X:64:CYS:N	2.45	0.44
2:B:168:GLN:HE21	2:B:173:SER:HB3	1.82	0.44
12:R:301:NAG:O7	12:R:301:NAG:O3	2.30	0.44
1:S:155:ALA:N	1:S:203:VAL:O	2.48	0.44
1:M:172:SER:O	1:M:216:ASN:N	2.44	0.44
2:D:122:PRO:O	2:D:124:ASP:N	2.51	0.44
3:L:139:GLY:HA3	3:L:158:TRP:HB3	2.00	0.44
2:J:87:TYR:CE2	2:J:102:GLY:HA2	2.53	0.43
2:N:33:LEU:HB3	2:N:51:ALA:HB2	2.00	0.43
2:T:163:GLU:HA	2:T:179:SER:HA	2.00	0.43
3:U:67:ALA:HB2	3:U:107:TYR:CZ	2.54	0.43
3:U:163:ASN:HB3	3:U:164:SER:H	1.69	0.43
2:W:29:ILE:C	2:W:92:TYR:HE1	2.22	0.43
4:Y:6:GAL:H61	4:Y:7:SIA:H32	1.59	0.43
1:A:18:LEU:O	1:A:83:MET:N	2.50	0.43
1:F:87:ARG:HB2	1:F:89:GLU:HG2	2.00	0.43
3:K:184:LEU:O	3:K:259:PRO:HB3	2.19	0.43
3:R:200:TYR:O	3:R:202:ASN:N	2.43	0.43
2:B:166:THR:HG22	2:B:167:GLU:N	2.33	0.43
3:X:245:ASN:O	12:X:301:NAG:H82	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:1:NAG:H61	4:Y:2:NAG:H83	2.01	0.43
3:U:62:ARG:O	3:U:64:CYS:N	2.45	0.43
1:A:18:LEU:O	1:A:82:GLN:NE2	2.51	0.42
2:B:29:ILE:HD11	2:B:71:PHE:HE1	1.84	0.42
3:U:247:ALA:HB3	12:U:301:NAG:H82	2.00	0.42
1:F:215:ASN:HD22	1:F:216:HIS:N	2.16	0.42
2:W:153:ASP:N	2:W:193:VAL:O	2.52	0.42
1:I:52:ASN:O	1:I:72:ARG:NH2	2.33	0.42
1:S:117:TYR:O	2:T:34:ASN:ND2	2.47	0.42
1:V:41:ARG:O	1:V:49:GLU:N	2.39	0.42
3:K:207:ILE:HB	3:K:218:LEU:HB2	2.01	0.42
3:R:143:ALA:HB2	3:R:231:GLN:H	1.84	0.42
1:S:42:GLN:OE1	2:T:38:GLN:NE2	2.46	0.42
2:J:84:ALA:HB3	2:J:86:TYR:HE1	1.84	0.42
1:I:54:ASP:OD1	1:I:54:ASP:N	2.49	0.42
2:J:37:GLN:HB2	2:J:86:TYR:CE1	2.55	0.42
3:R:60:ILE:HA	3:R:89:VAL:O	2.20	0.41
2:W:29:ILE:C	2:W:92:TYR:CE1	2.94	0.41
1:A:36:TRP:CG	1:A:81:LEU:HD22	2.55	0.41
1:M:61:LYS:HE2	1:M:61:LYS:HB3	1.96	0.41
3:R:99:CYS:HB3	3:R:144:CYS:HB2	1.69	0.41
2:G:135:VAL:HA	2:G:180:THR:HA	2.02	0.41
1:V:36:TRP:HB2	1:V:102:GLY:O	2.21	0.41
5:Z:2:NAG:H3	5:Z:4:BMA:H62	2.02	0.41
1:F:114:TYR:O	2:G:34:ASN:ND2	2.41	0.41
2:J:169:ASP:HB3	2:J:173:SER:N	2.35	0.41
3:R:100:TYR:CD1	3:R:101:PRO:HD2	2.56	0.41
2:B:47:LEU:HA	2:B:58:VAL:HG21	2.02	0.41
2:Q:163:GLU:HA	2:Q:179:SER:HA	2.03	0.41
1:S:165:PHE:HA	1:S:166:PRO:HA	1.81	0.41
1:M:158:GLY:HA2	1:M:173:TRP:CZ2	2.55	0.41
1:A:105:LEU:HA	1:A:110:GLY:HA3	2.02	0.41
1:M:158:GLY:HA3	1:M:200:VAL:HA	2.02	0.41
2:N:53:ASN:HB3	3:O:229:ASN:H	1.85	0.41
3:K:179:GLU:OE2	3:K:179:GLU:N	2.53	0.40
1:M:55:ASN:ND2	1:M:60:GLU:H	2.19	0.40
3:U:200:TYR:CE2	3:U:255:ASN:HA	2.56	0.40
2:W:59:PRO:HB2	2:W:61:ARG:HG2	2.02	0.40
5:Z:1:NAG:H61	5:Z:2:NAG:H83	2.03	0.40
3:O:184:LEU:O	3:O:259:PRO:HB3	2.21	0.40
3:X:210:GLY:N	3:X:249:ASN:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:169:ASP:HB3	2:G:173:SER:N	2.36	0.40
1:C:68:PHE:HA	1:C:83:MET:HA	2.04	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:231:GLN:NE2	4:Y:6:GAL:O6[4_455]	1.13	1.07
3:O:231:GLN:NE2	8:c:5:SIA:O1B[3_554]	1.30	0.90
3:K:231:GLN:NE2	10:e:5:SIA:O1B[2_555]	1.30	0.90
3:E:231:GLN:NE2	11:f:7:SIA:O1A[4_454]	1.30	0.90
3:R:191:ASN:ND2	7:b:7:SIA:O9[2_555]	1.30	0.90
3:L:231:GLN:NE2	9:d:7:SIA:C1[3_544]	1.43	0.77
3:X:231:GLN:NE2	4:Y:7:SIA:C2[4_455]	1.44	0.76
3:L:231:GLN:NE2	9:d:7:SIA:O1B[3_544]	1.49	0.71
3:L:231:GLN:NE2	9:d:7:SIA:O1A[3_544]	1.64	0.56
3:O:231:GLN:NE2	8:c:5:SIA:C1[3_554]	1.71	0.49
3:X:231:GLN:NE2	4:Y:7:SIA:C1[4_455]	1.85	0.35
3:L:231:GLN:OE1	9:d:7:SIA:O8[3_544]	2.01	0.19
3:X:231:GLN:NE2	4:Y:7:SIA:O6[4_455]	2.16	0.04
3:K:100:TYR:OH	10:e:5:SIA:O9[2_555]	2.18	0.02

## 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	221/230 (96%)	202 (91%)	18 (8%)	1 (0%)	29 67
1	C	210/230 (91%)	197 (94%)	12 (6%)	1 (0%)	29 67
1	F	219/230 (95%)	201 (92%)	16 (7%)	2 (1%)	17 55
1	I	211/230 (92%)	192 (91%)	19 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	221/230 (96%)	209 (95%)	12 (5%)	0	100	100
1	P	216/230 (94%)	200 (93%)	13 (6%)	3 (1%)	11	46
1	S	220/230 (96%)	208 (94%)	12 (6%)	0	100	100
1	V	202/230 (88%)	185 (92%)	17 (8%)	0	100	100
2	B	213/215 (99%)	198 (93%)	14 (7%)	1 (0%)	29	67
2	D	195/215 (91%)	182 (93%)	13 (7%)	0	100	100
2	G	212/215 (99%)	195 (92%)	16 (8%)	1 (0%)	29	67
2	J	183/215 (85%)	167 (91%)	14 (8%)	2 (1%)	14	51
2	N	212/215 (99%)	198 (93%)	11 (5%)	3 (1%)	11	46
2	Q	196/215 (91%)	175 (89%)	16 (8%)	5 (3%)	5	34
2	T	212/215 (99%)	189 (89%)	20 (9%)	3 (1%)	11	46
2	W	192/215 (89%)	180 (94%)	11 (6%)	1 (0%)	29	67
3	E	190/219 (87%)	172 (90%)	15 (8%)	3 (2%)	9	44
3	H	198/219 (90%)	172 (87%)	22 (11%)	4 (2%)	7	40
3	K	202/219 (92%)	185 (92%)	16 (8%)	1 (0%)	29	67
3	L	175/219 (80%)	160 (91%)	11 (6%)	4 (2%)	6	37
3	O	207/219 (94%)	186 (90%)	15 (7%)	6 (3%)	4	32
3	R	188/219 (86%)	171 (91%)	16 (8%)	1 (0%)	29	67
3	U	192/219 (88%)	175 (91%)	16 (8%)	1 (0%)	29	67
3	X	192/219 (88%)	170 (88%)	19 (10%)	3 (2%)	9	44
All	All	4879/5312 (92%)	4469 (92%)	364 (8%)	46 (1%)	17	55

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	94	PRO
2	J	96	PRO
3	K	125	ILE
2	N	96	PRO
3	O	80	ILE
3	O	93	ASN
3	O	94	PRO
1	P	167	GLU
1	P	168	PRO
2	Q	7	SER

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Mol	Chain	Res	Type
3	R	145	PRO
2	T	94	THR
2	T	96	PRO
3	U	145	PRO
3	X	145	PRO
2	B	96	PRO
3	E	95	VAL
3	E	125	ILE
1	F	55	GLY
2	G	96	PRO
3	H	125	ILE
2	N	99	THR
2	Q	91	SER
2	Q	145	GLU
3	H	131	TRP
3	L	99	CYS
3	O	96	ASN
2	Q	104	THR
1	C	165	PRO
2	J	100	PHE
3	L	125	ILE
2	Q	15	VAL
1	A	62	ASP
3	H	63	ASP
3	L	98	LEU
3	O	85	TRP
3	X	92	ALA
2	W	104	THR
1	P	165	PHE
3	X	203	PRO
3	H	144	CYS
2	T	95	PRO
3	L	203	PRO
2	N	142	TYR
1	F	14	PRO
3	O	207	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	103/190 (54%)	100 (97%)	3 (3%)	42	65
1	C	64/190 (34%)	63 (98%)	1 (2%)	62	79
1	F	93/190 (49%)	91 (98%)	2 (2%)	52	71
1	I	76/190 (40%)	75 (99%)	1 (1%)	69	82
1	M	77/190 (40%)	76 (99%)	1 (1%)	69	82
1	P	53/190 (28%)	50 (94%)	3 (6%)	20	49
1	S	71/190 (37%)	70 (99%)	1 (1%)	67	81
1	V	48/190 (25%)	48 (100%)	0	100	100
2	B	125/189 (66%)	123 (98%)	2 (2%)	62	79
2	D	61/189 (32%)	60 (98%)	1 (2%)	62	79
2	G	81/189 (43%)	78 (96%)	3 (4%)	34	60
2	J	46/189 (24%)	46 (100%)	0	100	100
2	N	58/189 (31%)	57 (98%)	1 (2%)	60	78
2	Q	42/189 (22%)	39 (93%)	3 (7%)	14	42
2	T	54/189 (29%)	52 (96%)	2 (4%)	34	60
2	W	33/189 (18%)	32 (97%)	1 (3%)	41	64
3	E	58/197 (29%)	56 (97%)	2 (3%)	37	61
3	H	83/197 (42%)	81 (98%)	2 (2%)	49	69
3	K	109/197 (55%)	103 (94%)	6 (6%)	21	50
3	L	72/197 (36%)	69 (96%)	3 (4%)	30	56
3	O	94/197 (48%)	94 (100%)	0	100	100
3	R	69/197 (35%)	66 (96%)	3 (4%)	29	56
3	U	73/197 (37%)	71 (97%)	2 (3%)	44	66
3	X	58/197 (29%)	53 (91%)	5 (9%)	10	37
All	All	1701/4608 (37%)	1653 (97%)	48 (3%)	43	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PHE
1	A	114	TYR
1	A	117	ASP

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Mol	Chain	Res	Type
2	B	98	LEU
2	B	177	LEU
1	C	29	PHE
2	D	92	TYR
3	E	98	LEU
3	E	104	PHE
1	F	103	ARG
1	F	215	ASN
2	G	49	TYR
2	G	88	CYS
2	G	154	ASN
3	H	100	TYR
3	H	202	ASN
1	I	29	PHE
3	K	64	CYS
3	K	99	CYS
3	K	100	TYR
3	K	107	TYR
3	K	144	CYS
3	K	255	ASN
3	L	100	TYR
3	L	229	ASN
3	L	245	ASN
1	M	56	GLN
2	N	92	TYR
1	P	32	PHE
1	P	99	CYS
1	P	164	TYR
2	Q	18	ARG
2	Q	92	TYR
2	Q	196	CYS
3	R	100	TYR
3	R	104	PHE
3	R	152	PHE
1	S	115	TYR
2	T	33	LEU
2	T	211	PHE
3	U	184	LEU
3	U	206	TYR
2	W	110	ARG
3	X	99	CYS
3	X	100	TYR

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Mol	Chain	Res	Type
3	X	107	TYR
3	X	158	TRP
3	X	173	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

51 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	Y	1	3,4	14,14,15	0.30	0	17,19,21	0.66	0
4	NAG	Y	2	4	14,14,15	0.29	0	17,19,21	1.37	2 (11%)
4	MAN	Y	3	4	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
4	MAN	Y	4	4	11,11,12	0.66	0	15,15,17	1.55	1 (6%)
4	NDG	Y	5	4	14,14,15	0.38	0	17,19,21	1.84	4 (23%)
4	GAL	Y	6	4	11,11,12	0.30	0	15,15,17	0.78	0
4	SIA	Y	7	4	17,20,21	0.38	0	21,28,31	1.04	3 (14%)
5	NAG	Z	1	3,5	14,14,15	0.33	0	17,19,21	0.62	0
5	NAG	Z	2	5	14,14,15	0.27	0	17,19,21	1.31	2 (11%)
5	BMA	Z	3	5	11,11,12	0.30	0	15,15,17	1.09	1 (6%)
5	BMA	Z	4	5	11,11,12	0.34	0	15,15,17	1.64	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	Z	5	5	14,14,15	0.32	0	17,19,21	1.22	2 (11%)
5	GAL	Z	6	5	11,11,12	0.36	0	15,15,17	1.46	2 (13%)
5	SIA	Z	7	5	17,20,21	0.33	0	21,28,31	0.76	0
6	NAG	a	1	6	14,14,15	0.35	0	17,19,21	0.80	0
6	MAN	a	2	6	11,11,12	0.28	0	15,15,17	0.96	2 (13%)
6	MAN	a	3	6	11,11,12	0.49	0	15,15,17	1.71	2 (13%)
6	NDG	a	4	6	14,14,15	0.37	0	17,19,21	1.15	2 (11%)
6	GLA	a	5	6	11,11,12	0.57	0	15,15,17	2.84	4 (26%)
6	SIA	a	6	6	17,20,21	0.31	0	21,28,31	1.07	2 (9%)
7	NAG	b	1	3,7	14,14,15	0.31	0	17,19,21	1.00	1 (5%)
7	NAG	b	2	7	14,14,15	0.46	0	17,19,21	1.64	2 (11%)
7	MAN	b	3	7	11,11,12	0.36	0	15,15,17	1.19	1 (6%)
7	MAN	b	4	7	11,11,12	0.25	0	15,15,17	0.96	1 (6%)
7	NAG	b	5	7	14,14,15	0.25	0	17,19,21	0.75	0
7	GLA	b	6	7	11,11,12	0.24	0	15,15,17	0.68	0
7	SIA	b	7	7	17,20,21	0.41	0	21,28,31	1.74	5 (23%)
8	BMA	c	1	8	11,11,12	0.25	0	15,15,17	0.68	0
8	BMA	c	2	8	11,11,12	0.37	0	15,15,17	1.64	2 (13%)
8	NDG	c	3	8	14,14,15	0.42	0	17,19,21	1.56	3 (17%)
8	GAL	c	4	8	11,11,12	0.40	0	15,15,17	1.76	2 (13%)
8	SIA	c	5	8	17,20,21	0.25	0	21,28,31	0.87	2 (9%)
9	NAG	d	1	9	14,14,15	0.29	0	17,19,21	0.76	1 (5%)
9	NAG	d	2	9	14,14,15	0.26	0	17,19,21	0.57	0
9	MAN	d	3	9	11,11,12	0.33	0	15,15,17	1.46	2 (13%)
9	BMA	d	4	9	11,11,12	0.26	0	15,15,17	0.60	0
9	NDG	d	5	9	14,14,15	0.29	0	17,19,21	0.91	0
9	GAL	d	6	9	11,11,12	0.28	0	15,15,17	1.41	1 (6%)
9	SIA	d	7	9	17,20,21	0.38	0	21,28,31	1.20	2 (9%)
10	MAN	e	1	10	11,11,12	0.31	0	15,15,17	1.20	2 (13%)
10	BMA	e	2	10	11,11,12	0.30	0	15,15,17	0.70	0
10	NDG	e	3	10	14,14,15	0.38	0	17,19,21	0.95	1 (5%)
10	GAL	e	4	10	11,11,12	0.38	0	15,15,17	1.31	2 (13%)
10	SIA	e	5	10	17,20,21	0.38	0	21,28,31	1.15	3 (14%)
11	NAG	f	1	11	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
11	NAG	f	2	11	14,14,15	0.38	0	17,19,21	0.88	2 (11%)
11	BMA	f	3	11	11,11,12	0.27	0	15,15,17	0.80	0
11	MAN	f	4	11	11,11,12	0.24	0	15,15,17	0.77	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NDG	f	5	11	14,14,15	0.33	0	17,19,21	0.88	0
11	GAL	f	6	11	11,11,12	0.30	0	15,15,17	1.67	3 (20%)
11	SIA	f	7	11	17,20,21	0.29	0	21,28,31	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Y	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	MAN	Y	3	4	-	2/2/19/22	0/1/1/1
4	MAN	Y	4	4	-	1/2/19/22	0/1/1/1
4	NDG	Y	5	4	-	3/6/23/26	0/1/1/1
4	GAL	Y	6	4	-	2/2/19/22	0/1/1/1
4	SIA	Y	7	4	-	9/14/34/38	0/1/1/1
5	NAG	Z	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	1/2/19/22	1/1/1/1
5	BMA	Z	4	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	5	5	-	3/6/23/26	0/1/1/1
5	GAL	Z	6	5	-	2/2/19/22	0/1/1/1
5	SIA	Z	7	5	-	6/14/34/38	0/1/1/1
6	NAG	a	1	6	-	2/6/23/26	0/1/1/1
6	MAN	a	2	6	-	0/2/19/22	1/1/1/1
6	MAN	a	3	6	-	0/2/19/22	0/1/1/1
6	NDG	a	4	6	-	1/6/23/26	0/1/1/1
6	GLA	a	5	6	-	2/2/19/22	0/1/1/1
6	SIA	a	6	6	-	8/14/34/38	0/1/1/1
7	NAG	b	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	1/6/23/26	0/1/1/1
7	MAN	b	3	7	-	1/2/19/22	0/1/1/1
7	MAN	b	4	7	-	1/2/19/22	1/1/1/1
7	NAG	b	5	7	-	4/6/23/26	0/1/1/1
7	GLA	b	6	7	-	2/2/19/22	0/1/1/1
7	SIA	b	7	7	-	8/14/34/38	0/1/1/1
8	BMA	c	1	8	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	c	2	8	-	0/2/19/22	1/1/1/1
8	NDG	c	3	8	-	4/6/23/26	0/1/1/1
8	GAL	c	4	8	-	1/2/19/22	0/1/1/1
8	SIA	c	5	8	-	2/14/34/38	0/1/1/1
9	NAG	d	1	9	-	2/6/23/26	0/1/1/1
9	NAG	d	2	9	-	4/6/23/26	0/1/1/1
9	MAN	d	3	9	-	2/2/19/22	0/1/1/1
9	BMA	d	4	9	-	1/2/19/22	0/1/1/1
9	NDG	d	5	9	-	3/6/23/26	0/1/1/1
9	GAL	d	6	9	-	1/2/19/22	0/1/1/1
9	SIA	d	7	9	-	7/14/34/38	0/1/1/1
10	MAN	e	1	10	-	2/2/19/22	1/1/1/1
10	BMA	e	2	10	-	0/2/19/22	0/1/1/1
10	NDG	e	3	10	-	0/6/23/26	0/1/1/1
10	GAL	e	4	10	-	0/2/19/22	0/1/1/1
10	SIA	e	5	10	-	6/14/34/38	0/1/1/1
11	NAG	f	1	11	-	0/6/23/26	0/1/1/1
11	NAG	f	2	11	-	4/6/23/26	0/1/1/1
11	BMA	f	3	11	-	0/2/19/22	0/1/1/1
11	MAN	f	4	11	-	0/2/19/22	1/1/1/1
11	NDG	f	5	11	-	2/6/23/26	0/1/1/1
11	GAL	f	6	11	-	1/2/19/22	0/1/1/1
11	SIA	f	7	11	-	2/14/34/38	0/1/1/1

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	5	GLA	C1-O5-C5	6.57	121.09	112.19
6	a	5	GLA	C1-C2-C3	6.35	117.47	109.67
7	b	2	NAG	C1-O5-C5	5.96	120.26	112.19
8	c	4	GAL	C1-O5-C5	5.04	119.02	112.19
4	Y	4	MAN	O2-C2-C3	5.04	120.23	110.14
8	c	2	BMA	C1-O5-C5	4.87	118.80	112.19
5	Z	4	BMA	C1-O5-C5	4.80	118.69	112.19
7	b	7	SIA	C6-O6-C2	4.76	121.52	111.34
6	a	3	MAN	C1-O5-C5	4.64	118.48	112.19
6	a	5	GLA	O5-C1-C2	4.40	117.56	110.77
4	Y	2	NAG	C1-O5-C5	4.21	117.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	2	NAG	C1-O5-C5	4.14	117.81	112.19
9	d	7	SIA	C6-O6-C2	3.98	119.86	111.34
5	Z	6	GAL	C1-O5-C5	3.95	117.54	112.19
7	b	3	MAN	O5-C5-C6	3.85	113.24	107.20
4	Y	5	NDG	C2-N2-C7	3.83	128.35	122.90
8	c	3	NDG	C3-C4-C5	3.81	117.04	110.24
8	c	3	NDG	O5-C1-C2	-3.81	105.27	111.29
9	d	3	MAN	C1-O5-C5	3.79	117.33	112.19
4	Y	5	NDG	C1-O5-C5	3.77	117.30	112.19
6	a	5	GLA	O5-C5-C6	3.75	113.08	107.20
8	c	4	GAL	C1-C2-C3	3.71	114.22	109.67
4	Y	5	NDG	C1-C2-N2	3.58	116.61	110.49
9	d	6	GAL	O5-C5-C6	3.58	112.81	107.20
10	e	4	GAL	O5-C5-C6	3.51	112.70	107.20
7	b	7	SIA	C4-C3-C2	3.47	116.03	109.81
6	a	4	NDG	O5-C1-C2	-3.47	105.80	111.29
5	Z	4	BMA	O5-C5-C6	3.46	112.63	107.20
6	a	6	SIA	C6-O6-C2	3.38	118.57	111.34
11	f	6	GAL	C1-O5-C5	3.33	116.71	112.19
4	Y	2	NAG	O5-C5-C6	3.25	112.31	107.20
5	Z	3	BMA	C1-O5-C5	3.23	116.57	112.19
10	e	5	SIA	C6-O6-C2	3.20	118.20	111.34
10	e	1	MAN	O5-C5-C6	3.17	112.17	107.20
5	Z	6	GAL	C1-C2-C3	3.14	113.53	109.67
8	c	2	BMA	O5-C5-C6	3.14	112.13	107.20
11	f	6	GAL	O5-C1-C2	-3.13	105.94	110.77
4	Y	7	SIA	C3-C2-C1	-2.97	105.44	111.93
7	b	7	SIA	C4-C5-C6	2.90	116.43	109.10
6	a	3	MAN	C3-C4-C5	2.71	115.08	110.24
5	Z	2	NAG	O5-C5-C6	2.69	111.42	107.20
9	d	3	MAN	O5-C5-C6	2.60	111.28	107.20
10	e	1	MAN	C1-O5-C5	2.59	115.71	112.19
7	b	4	MAN	C1-O5-C5	2.59	115.70	112.19
7	b	1	NAG	O5-C5-C6	2.56	111.21	107.20
8	c	5	SIA	C3-C2-C1	-2.54	106.38	111.93
10	e	4	GAL	C1-C2-C3	2.51	112.76	109.67
6	a	2	MAN	C1-O5-C5	2.51	115.59	112.19
5	Z	5	NAG	O5-C1-C2	-2.47	107.38	111.29
4	Y	5	NDG	C3-C4-C5	2.47	114.65	110.24
10	e	5	SIA	C8-C7-C6	2.41	117.61	113.03
10	e	3	NDG	C1-O5-C5	2.37	115.41	112.19
7	b	7	SIA	O6-C2-C3	2.37	114.03	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	7	SIA	C8-C7-C6	2.36	117.51	113.03
10	e	5	SIA	C4-C5-N5	-2.30	105.83	110.38
4	Y	7	SIA	C6-O6-C2	2.30	116.25	111.34
6	a	4	NDG	C3-C4-C5	2.26	114.27	110.24
9	d	7	SIA	C4-C3-C2	2.23	113.80	109.81
6	a	6	SIA	C4-C5-C6	2.22	114.70	109.10
11	f	1	NAG	C4-C3-C2	2.21	114.26	111.02
4	Y	3	MAN	O5-C5-C6	2.19	110.64	107.20
11	f	6	GAL	O2-C2-C1	2.17	113.59	109.15
6	a	2	MAN	O5-C5-C6	2.14	110.56	107.20
8	c	5	SIA	C6-O6-C2	2.11	115.86	111.34
4	Y	7	SIA	C3-C4-C5	-2.10	108.93	111.46
11	f	2	NAG	C4-C3-C2	2.09	114.09	111.02
7	b	2	NAG	C4-C3-C2	2.09	114.08	111.02
9	d	1	NAG	O5-C1-C2	-2.08	108.00	111.29
8	c	3	NDG	C4-C3-C2	2.01	113.97	111.02
5	Z	5	NAG	C2-N2-C7	2.01	125.77	122.90
11	f	2	NAG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	f	7	SIA	C11-C10-N5-C5
11	f	7	SIA	O10-C10-N5-C5
9	d	5	NDG	C3-C2-N2-C7
9	d	5	NDG	C8-C7-N2-C2
9	d	5	NDG	O7-C7-N2-C2
5	Z	7	SIA	O6-C6-C7-O7
4	Y	5	NDG	C1-C2-N2-C7
4	Y	5	NDG	C8-C7-N2-C2
4	Y	5	NDG	O7-C7-N2-C2
11	f	2	NAG	C3-C2-N2-C7
11	f	2	NAG	C8-C7-N2-C2
11	f	2	NAG	O7-C7-N2-C2
10	e	5	SIA	C5-C6-C7-C8
10	e	5	SIA	C5-C6-C7-O7
10	e	5	SIA	O6-C6-C7-C8
9	d	7	SIA	C6-C5-N5-C10
9	d	7	SIA	C5-C6-C7-C8
9	d	7	SIA	C5-C6-C7-O7
9	d	7	SIA	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	d	7	SIA	C11-C10-N5-C5
9	d	7	SIA	O10-C10-N5-C5
4	Y	7	SIA	C5-C6-C7-C8
4	Y	7	SIA	C5-C6-C7-O7
4	Y	7	SIA	O6-C6-C7-C8
4	Y	7	SIA	O6-C6-C7-O7
6	a	6	SIA	C6-C7-C8-O8
6	a	6	SIA	O7-C7-C8-O8
6	a	6	SIA	C11-C10-N5-C5
6	a	6	SIA	O10-C10-N5-C5
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
7	b	7	SIA	C5-C6-C7-C8
7	b	7	SIA	C5-C6-C7-O7
7	b	7	SIA	O6-C6-C7-C8
7	b	7	SIA	O6-C6-C7-O7
7	b	7	SIA	C6-C7-C8-C9
7	b	7	SIA	C6-C7-C8-O8
7	b	7	SIA	O7-C7-C8-C9
7	b	7	SIA	O7-C7-C8-O8
5	Z	6	GAL	C4-C5-C6-O6
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
4	Y	6	GAL	C4-C5-C6-O6
7	b	6	GLA	C4-C5-C6-O6
10	e	1	MAN	O5-C5-C6-O6
4	Y	2	NAG	C8-C7-N2-C2
8	c	3	NDG	C4-C5-C6-O6
5	Z	6	GAL	O5-C5-C6-O6
8	c	1	BMA	O5-C5-C6-O6
10	e	1	MAN	C4-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
8	c	3	NDG	O5-C5-C6-O6
4	Y	6	GAL	O5-C5-C6-O6
9	d	2	NAG	C8-C7-N2-C2
9	d	2	NAG	O7-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
6	a	5	GLA	O5-C5-C6-O6
5	Z	2	NAG	C1-C2-N2-C7
6	a	6	SIA	O7-C7-C8-C9
6	a	6	SIA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	Y	3	MAN	C4-C5-C6-O6
7	b	6	GLA	O5-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
5	Z	7	SIA	C11-C10-N5-C5
9	d	1	NAG	C8-C7-N2-C2
9	d	1	NAG	O7-C7-N2-C2
8	c	5	SIA	C11-C10-N5-C5
8	c	5	SIA	O10-C10-N5-C5
11	f	5	NDG	C8-C7-N2-C2
11	f	5	NDG	O7-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
8	c	3	NDG	C8-C7-N2-C2
8	c	3	NDG	O7-C7-N2-C2
6	a	1	NAG	C4-C5-C6-O6
6	a	5	GLA	C4-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
8	c	1	BMA	C4-C5-C6-O6
4	Y	3	MAN	O5-C5-C6-O6
9	d	4	BMA	O5-C5-C6-O6
9	d	6	GAL	O5-C5-C6-O6
5	Z	7	SIA	O10-C10-N5-C5
7	b	5	NAG	C8-C7-N2-C2
4	Y	7	SIA	C11-C10-N5-C5
6	a	4	NDG	O5-C5-C6-O6
9	d	3	MAN	O5-C5-C6-O6
7	b	5	NAG	O7-C7-N2-C2
5	Z	5	NAG	O5-C5-C6-O6
4	Y	7	SIA	O10-C10-N5-C5
8	c	4	GAL	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
4	Y	4	MAN	O5-C5-C6-O6
7	b	5	NAG	O5-C5-C6-O6
7	b	3	MAN	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	b	4	MAN	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
11	f	2	NAG	O5-C5-C6-O6
7	b	5	NAG	C3-C2-N2-C7
10	e	5	SIA	O7-C7-C8-C9
9	d	3	MAN	C4-C5-C6-O6
4	Y	7	SIA	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
10	e	5	SIA	O7-C7-C8-O8
5	Z	7	SIA	C5-C6-C7-O7
5	Z	7	SIA	O6-C6-C7-C8
9	d	7	SIA	O6-C6-C7-O7
4	Y	7	SIA	C6-C7-C8-C9
11	f	6	GAL	C4-C5-C6-O6
6	a	6	SIA	C6-C5-N5-C10
5	Z	5	NAG	C3-C2-N2-C7
6	a	6	SIA	C4-C5-N5-C10
4	Y	7	SIA	O7-C7-C8-O8
5	Z	7	SIA	C4-C5-N5-C10
10	e	5	SIA	C6-C7-C8-O8
5	Z	5	NAG	C1-C2-N2-C7

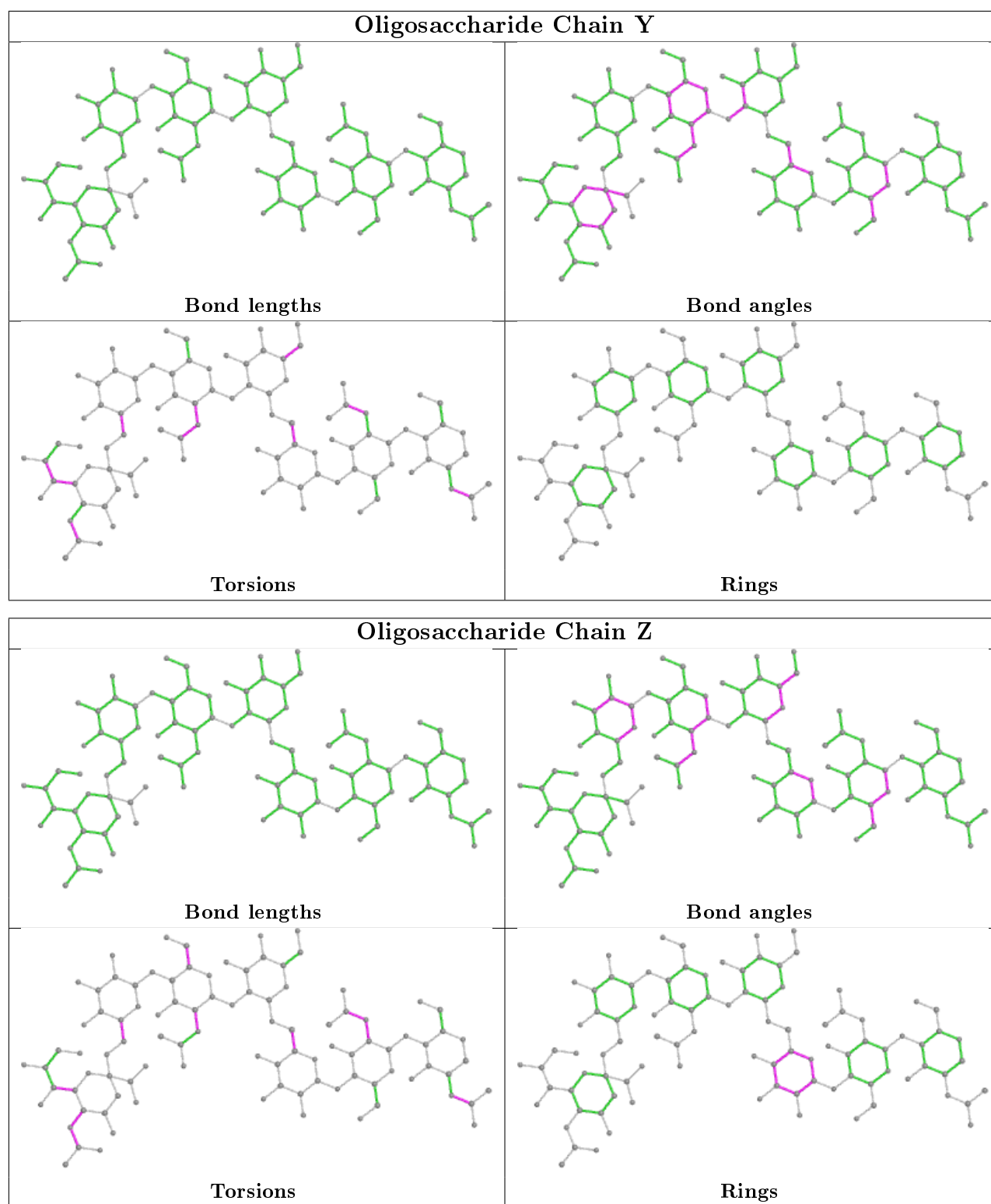
All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	3	BMA	C1-C2-C3-C4-C5-O5
11	f	4	MAN	C1-C2-C3-C4-C5-O5
8	c	2	BMA	C1-C2-C3-C4-C5-O5
10	e	1	MAN	C1-C2-C3-C4-C5-O5
6	a	2	MAN	C1-C2-C3-C4-C5-O5
7	b	4	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	f	7	SIA	0	1
4	Y	2	NAG	1	0
5	Z	2	NAG	2	0
10	e	5	SIA	0	2
9	d	7	SIA	0	4
8	c	5	SIA	0	2
4	Y	7	SIA	2	3
5	Z	1	NAG	1	0
5	Z	4	BMA	1	0
4	Y	1	NAG	1	0
4	Y	6	GAL	2	1
7	b	7	SIA	0	1

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](#)

5 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	$\# Z  > 2$
12	NAG	O	301	3	14,14,15	0.30	0	17,19,21	0.58	0
12	NAG	L	306	-	14,14,15	0.26	0	17,19,21	0.96	0
12	NAG	X	301	3	14,14,15	0.22	0	17,19,21	0.44	0
12	NAG	U	301	3	14,14,15	0.39	0	17,19,21	0.42	0
12	NAG	R	301	3	14,14,15	0.35	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	O	301	3	-	0/6/23/26	0/1/1/1
12	NAG	L	306	-	-	0/6/23/26	0/1/1/1
12	NAG	X	301	3	-	2/6/23/26	0/1/1/1
12	NAG	U	301	3	-	4/6/23/26	0/1/1/1
12	NAG	R	301	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	U	301	NAG	C4-C5-C6-O6
12	U	301	NAG	O5-C5-C6-O6
12	U	301	NAG	C1-C2-N2-C7
12	R	301	NAG	C1-C2-N2-C7
12	X	301	NAG	O5-C5-C6-O6
12	R	301	NAG	O5-C5-C6-O6
12	R	301	NAG	C4-C5-C6-O6
12	X	301	NAG	C4-C5-C6-O6
12	U	301	NAG	C3-C2-N2-C7
12	R	301	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	X	301	NAG	1	0
12	U	301	NAG	2	0
12	R	301	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	225/230 (97%)	-0.49	1 (0%) 92 87	36, 61, 122, 163	0
1	C	218/230 (94%)	-0.29	3 (1%) 75 65	59, 121, 178, 200	0
1	F	223/230 (96%)	-0.45	1 (0%) 92 87	36, 70, 143, 176	0
1	I	217/230 (94%)	-0.35	1 (0%) 91 85	46, 113, 161, 179	0
1	M	225/230 (97%)	-0.46	1 (0%) 92 87	43, 82, 128, 151	0
1	P	220/230 (95%)	-0.21	0 100 100	64, 109, 149, 172	0
1	S	224/230 (97%)	-0.43	0 100 100	46, 92, 150, 182	0
1	V	208/230 (90%)	-0.23	2 (0%) 82 74	57, 108, 158, 201	0
2	B	215/215 (100%)	-0.49	0 100 100	39, 64, 126, 159	0
2	D	203/215 (94%)	-0.38	2 (0%) 82 74	59, 107, 178, 210	0
2	G	214/215 (99%)	-0.53	1 (0%) 91 85	38, 64, 136, 183	0
2	J	187/215 (86%)	-0.45	0 100 100	50, 90, 160, 187	0
2	N	214/215 (99%)	-0.42	0 100 100	39, 84, 135, 158	0
2	Q	202/215 (93%)	-0.35	0 100 100	56, 103, 151, 185	0
2	T	214/215 (99%)	-0.48	0 100 100	54, 87, 144, 177	0
2	W	198/215 (92%)	-0.26	2 (1%) 82 74	63, 104, 164, 189	0
3	E	196/219 (89%)	-0.40	1 (0%) 91 85	57, 95, 138, 167	0
3	H	202/219 (92%)	-0.51	0 100 100	37, 79, 122, 147	0
3	K	206/219 (94%)	-0.38	1 (0%) 91 85	47, 81, 132, 152	0
3	L	185/219 (84%)	-0.52	0 100 100	51, 85, 137, 160	0
3	O	209/219 (95%)	-0.59	0 100 100	35, 60, 118, 143	0
3	R	194/219 (88%)	-0.49	0 100 100	68, 92, 136, 156	0
3	U	196/219 (89%)	-0.61	0 100 100	40, 70, 125, 175	0
3	X	196/219 (89%)	-0.43	0 100 100	65, 96, 147, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4991/5312 (93%)	-0.42	16 (0%) 94 90	35, 89, 150, 210	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	PRO	3.1
3	E	245	ASN	3.0
3	K	242	LEU	2.9
1	I	139	PRO	2.9
1	V	158	GLY	2.7
2	W	158	SER	2.6
2	D	121	PRO	2.5
2	D	195	ALA	2.4
1	C	56	GLY	2.4
2	G	194	TYR	2.4
2	W	118	PHE	2.2
1	C	141	ALA	2.2
1	F	141	ALA	2.1
1	V	142	PRO	2.1
1	M	132	SER	2.1
1	A	141	ALA	2.1

## 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
6	NAG	a	1	14/15	0.48	0.34	129,139,148,148	0
7	MAN	b	3	11/12	0.64	0.33	169,183,186,187	0
10	MAN	e	1	11/12	0.66	0.27	150,153,161,164	0
4	MAN	Y	3	11/12	0.71	0.23	140,153,163,163	0
7	MAN	b	4	11/12	0.72	0.32	151,167,171,172	0
10	BMA	e	2	11/12	0.72	0.28	141,155,158,160	0

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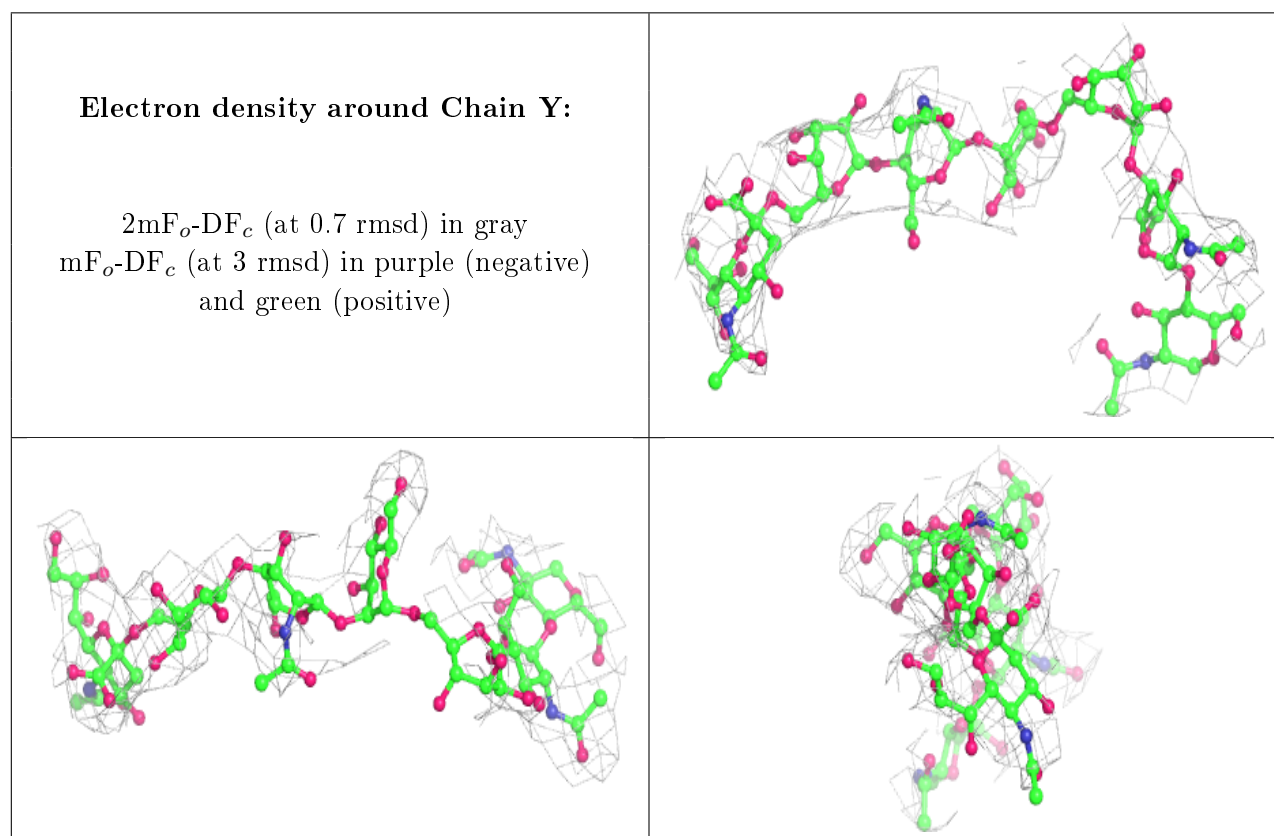
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	d	2	14/15	0.75	0.15	120,145,156,157	0
9	NAG	d	1	14/15	0.75	0.27	138,149,158,160	0
7	NAG	b	2	14/15	0.77	0.29	163,172,178,182	0
8	BMA	c	1	11/12	0.77	0.26	129,155,160,162	0
10	NDG	e	3	14/15	0.80	0.35	107,130,149,150	0
5	BMA	Z	3	11/12	0.80	0.23	153,157,159,161	0
7	NAG	b	1	14/15	0.81	0.25	142,156,163,167	0
4	NAG	Y	2	14/15	0.82	0.23	115,141,152,155	0
6	MAN	a	2	11/12	0.82	0.17	119,122,125,129	0
6	GLA	a	5	11/12	0.84	0.34	109,128,145,150	0
10	GAL	e	4	11/12	0.84	0.31	101,115,136,136	0
5	GAL	Z	6	11/12	0.85	0.27	90,109,117,123	0
4	MAN	Y	4	11/12	0.85	0.19	130,141,147,151	0
5	NAG	Z	1	14/15	0.85	0.28	152,162,176,177	0
5	NAG	Z	2	14/15	0.85	0.14	104,141,148,153	0
11	NAG	f	2	14/15	0.85	0.24	119,141,149,150	0
7	SIA	b	7	20/21	0.85	0.50	115,135,147,155	0
4	NDG	Y	5	14/15	0.86	0.35	143,145,157,161	0
9	BMA	d	4	11/12	0.86	0.18	103,113,120,122	0
11	BMA	f	3	11/12	0.87	0.17	134,146,151,154	0
6	NDG	a	4	14/15	0.88	0.31	118,129,137,139	0
8	GAL	c	4	11/12	0.88	0.26	99,112,121,124	0
7	GLA	b	6	11/12	0.89	0.20	103,118,127,129	0
5	NAG	Z	5	14/15	0.89	0.40	113,128,152,155	0
6	MAN	a	3	11/12	0.89	0.26	135,142,147,148	0
4	SIA	Y	7	20/21	0.89	0.50	110,144,159,159	0
11	NDG	f	5	14/15	0.89	0.23	119,144,156,158	0
4	GAL	Y	6	11/12	0.89	0.38	141,146,156,161	0
5	SIA	Z	7	20/21	0.89	0.41	61,75,105,105	0
4	NAG	Y	1	14/15	0.90	0.16	135,146,152,152	0
5	BMA	Z	4	11/12	0.90	0.25	141,155,158,159	0
11	MAN	f	4	11/12	0.90	0.16	149,154,158,159	0
9	MAN	d	3	11/12	0.90	0.20	128,148,153,154	0
11	NAG	f	1	14/15	0.90	0.22	114,124,133,135	0
6	SIA	a	6	20/21	0.91	0.38	85,101,111,124	0
10	SIA	e	5	20/21	0.91	0.31	64,75,107,108	0
7	NAG	b	5	14/15	0.91	0.30	90,128,136,140	0
8	SIA	c	5	20/21	0.91	0.34	55,109,134,136	0
8	NDG	c	3	14/15	0.91	0.21	111,128,136,141	0
8	BMA	c	2	11/12	0.92	0.12	127,136,139,139	0
9	GAL	d	6	11/12	0.93	0.17	94,100,112,115	0
11	SIA	f	7	20/21	0.93	0.25	86,103,124,126	0

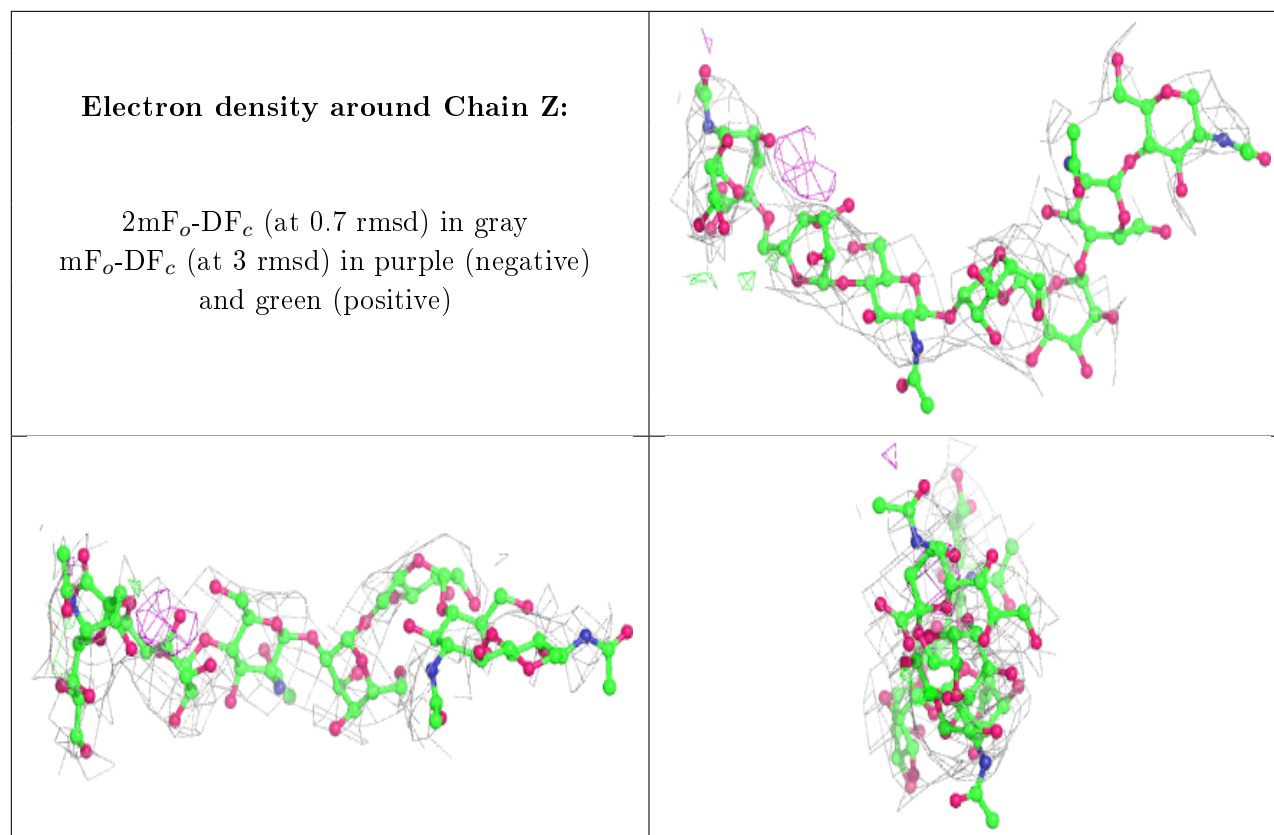
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NDG	d	5	14/15	0.93	0.20	113,124,128,133	0
9	SIA	d	7	20/21	0.93	0.28	45,99,124,125	0
11	GAL	f	6	11/12	0.94	0.14	105,112,114,117	0

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(Å <sup>2</sup> )	Q<0.9
12	NAG	L	306	14/15	0.65	0.30	148,153,160,161	0
12	NAG	O	301	14/15	0.77	0.26	34,65,73,75	0
12	NAG	X	301	14/15	0.80	0.23	88,114,119,124	0
12	NAG	U	301	14/15	0.80	0.26	92,108,117,126	0
12	NAG	R	301	14/15	0.81	0.22	80,114,118,121	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.