



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:47 AM BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

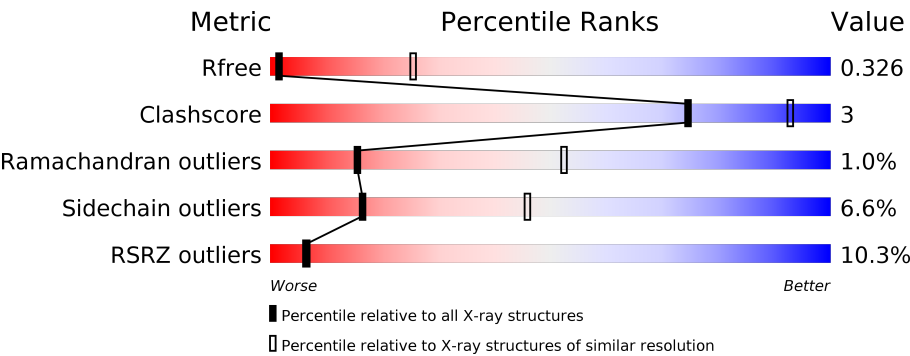
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	<div><div>6%</div><div><div></div><div>82%</div><div>13%</div><div></div><div></div></div><div></div></div>
1	E	330	<div><div>6%</div><div><div></div><div>83%</div><div>12%</div><div></div><div></div></div><div></div></div>
1	G	330	<div><div>2%</div><div><div></div><div>84%</div><div>12%</div><div></div><div></div></div><div></div></div>
1	K	330	<div><div>2%</div><div><div></div><div>82%</div><div>13%</div><div></div><div></div></div><div></div></div>
1	Q	330	<div><div>2%</div><div><div></div><div>82%</div><div>13%</div><div></div><div></div></div><div></div></div>
1	S	330	<div><div>7%</div><div><div></div><div>82%</div><div>14%</div><div></div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	181	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>
2	F	181	<div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
2	H	181	<div> <div>6%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
2	L	181	<div> <div>7%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
2	R	181	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
2	T	181	<div> <div>0%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
3	C	221	<div> <div>8%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
3	I	221	<div> <div>25%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
3	M	221	<div> <div>19%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
3	O	221	<div> <div>9%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
3	V	221	<div> <div>10%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
3	Y	221	<div> <div>29%</div> <div>82%</div> <div>12%</div> <div>• •</div> </div>
4	D	215	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
4	J	215	<div> <div>38%</div> <div>93%</div> <div>7%</div> </div>
4	N	215	<div> <div>10%</div> <div>91%</div> <div>8%</div> </div>
4	P	215	<div> <div>0%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
4	U	215	<div> <div>47%</div> <div>92%</div> <div>8%</div> </div>
4	W	215	<div> <div>8%</div> <div>89%</div> <div>10%</div> </div>
5	X	4	<div> <div>100%</div> </div>
5	k	4	<div> <div>100%</div> </div>
5	o	4	<div> <div>100%</div> </div>
5	p	4	<div> <div>100%</div> </div>
6	Z	3	<div> <div>67%</div> <div>33%</div> </div>
7	a	2	<div> <div>50%</div> <div>50%</div> </div>
7	b	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
7	c	2	 100%
7	d	2	 100%
7	e	2	 100%
7	f	2	 100%
7	h	2	 100%
7	m	2	 100%
7	n	2	 100%
8	g	5	 100%
9	i	5	 100%
9	l	5	 20%  80%
10	j	4	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	j	1	-	-	-	X
10	NAG	j	2	-	-	-	X
10	MAN	j	3	-	-	-	X
10	BMA	j	4	-	-	-	X
11	NAG	F	201	X	-	-	X
11	NAG	G	401	X	-	-	-
11	NAG	K	401	-	-	-	X
11	NAG	Q	401	-	-	-	X
5	MAN	X	4	-	-	-	X
5	MAN	k	3	-	-	-	X
5	MAN	k	4	-	-	-	X
5	MAN	o	3	-	-	-	X
5	NAG	p	2	-	-	-	X
5	MAN	p	3	-	-	-	X
5	MAN	p	4	-	-	-	X
6	NAG	Z	1	X	-	-	-
6	NAG	Z	2	-	-	-	X
7	NAG	a	2	-	-	-	X

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

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 44024 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

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

- Molecule 2 is a protein called Hemagglutinin HA2.

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

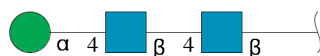
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	213	Total	C	N	O	S	0	0	0
			1626	1016	278	327	5			
4	U	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	J	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	D	214	Total	C	N	O	S	0	0	0
			1635	1021	279	330	5			
4	W	214	Total	C	N	O	S	0	0	0
			1635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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	X	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	k	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	o	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	p	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



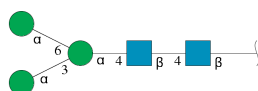
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

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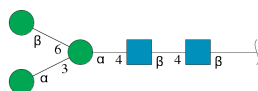
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	h	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	m	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	n	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



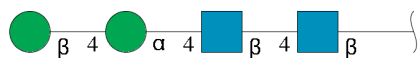
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	g	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



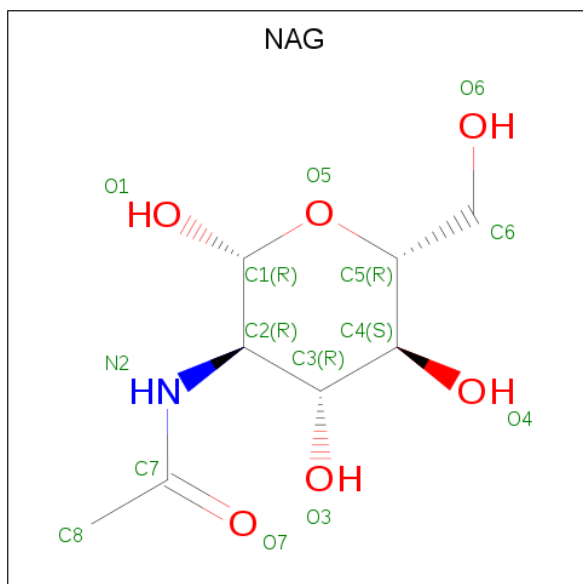
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	i	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	l	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	j	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



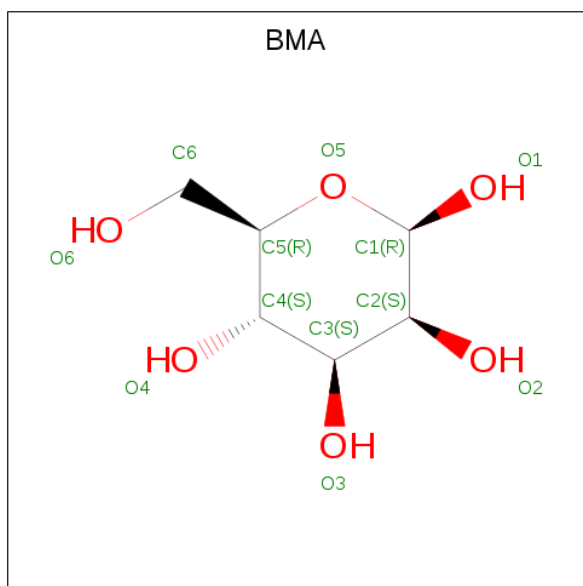
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	F	1	Total	C	N	O	0	0
			14	8	1	5		
11	G	1	Total	C	N	O	0	0
			14	8	1	5		
11	G	1	Total	C	N	O	0	0
			14	8	1	5		
11	K	1	Total	C	N	O	0	0
			14	8	1	5		
11	K	1	Total	C	N	O	0	0
			14	8	1	5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

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

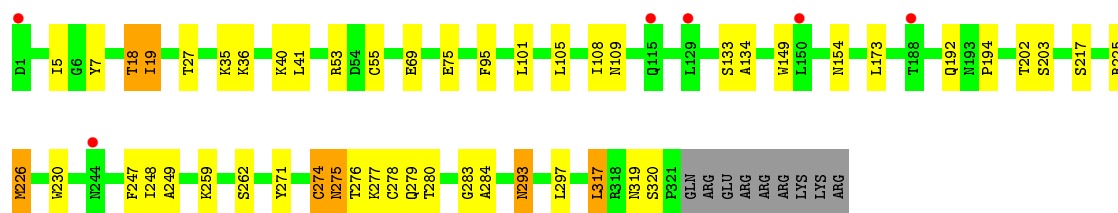
- Molecule 12 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



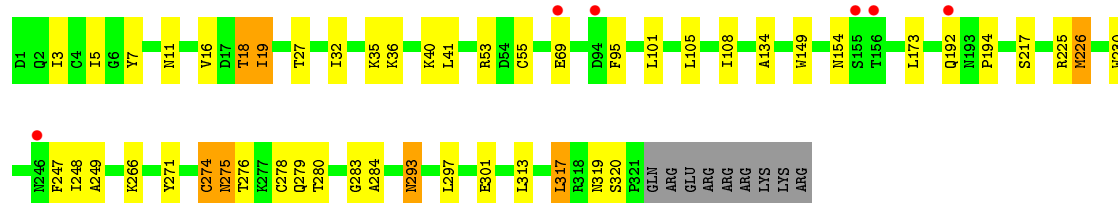
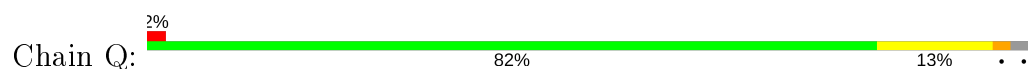
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 1: Hemagglutinin HA1

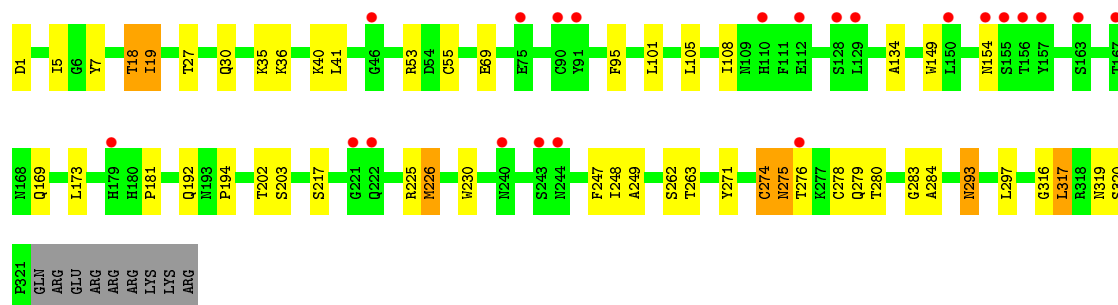
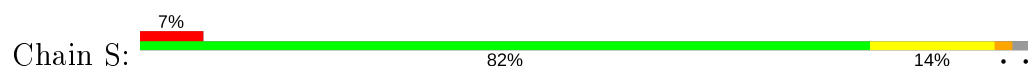




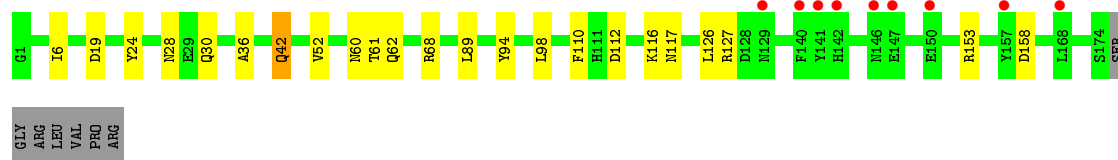
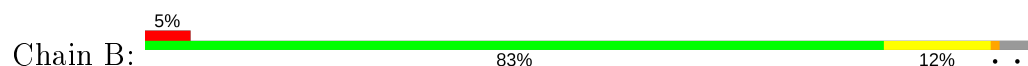
- Molecule 1: Hemagglutinin HA1



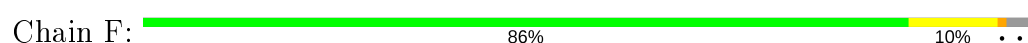
- Molecule 1: Hemagglutinin HA1



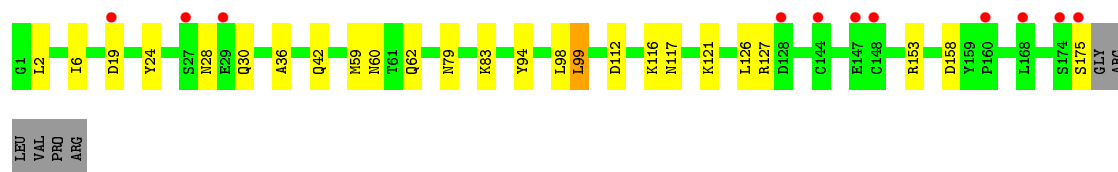
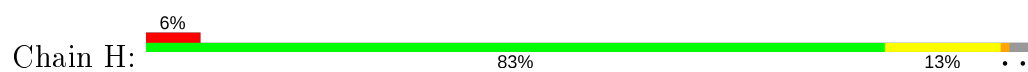
- Molecule 2: Hemagglutinin HA2



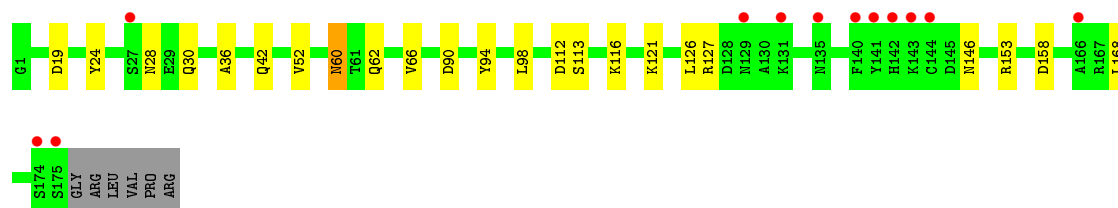
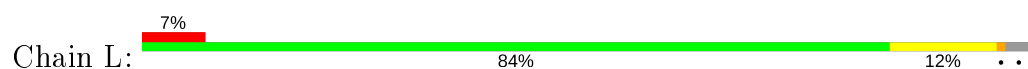
- Molecule 2: Hemagglutinin HA2



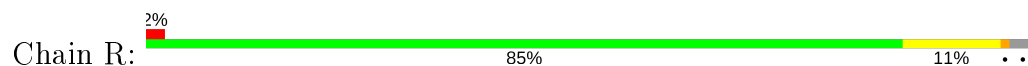
- Molecule 2: Hemagglutinin HA2



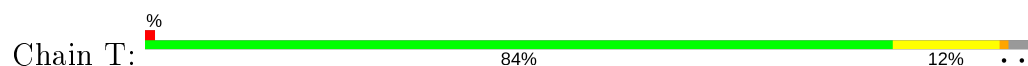
• Molecule 2: Hemagglutinin HA2



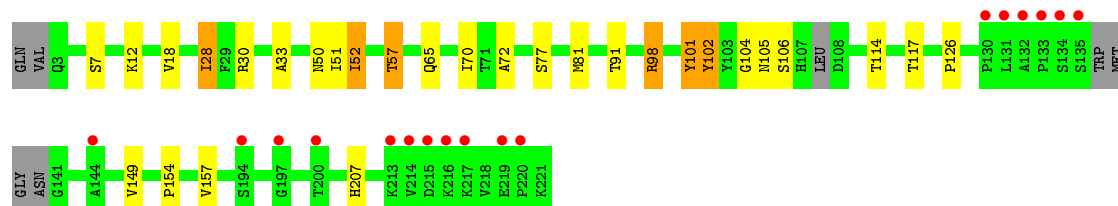
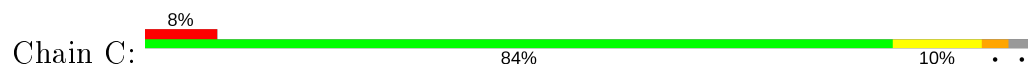
• Molecule 2: Hemagglutinin HA2



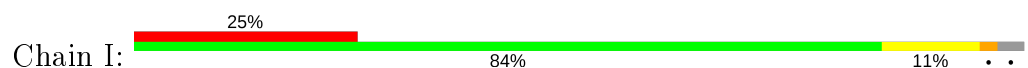
• Molecule 2: Hemagglutinin HA2

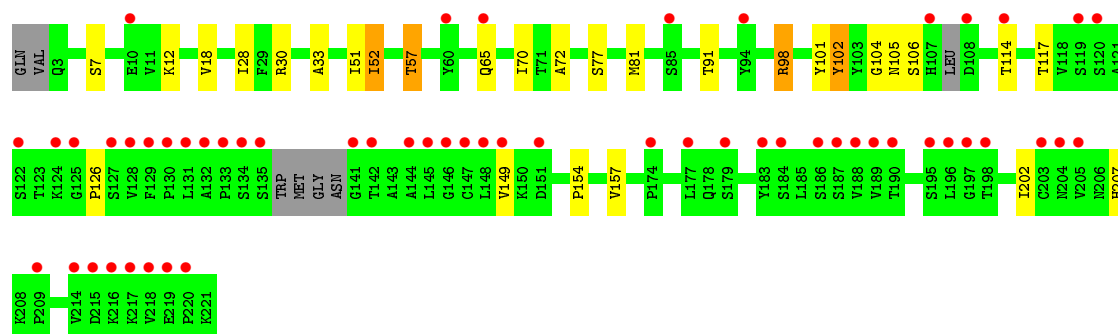


• Molecule 3: 70-1F02 Fab Heavy Chain

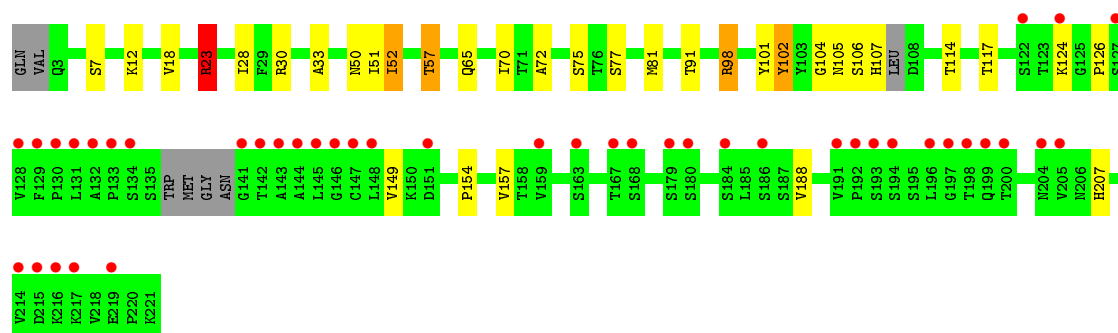
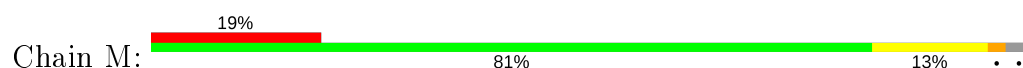


• Molecule 3: 70-1F02 Fab Heavy Chain

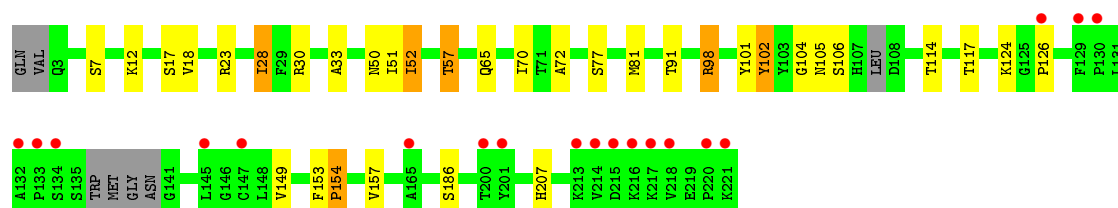
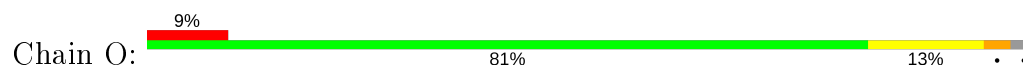




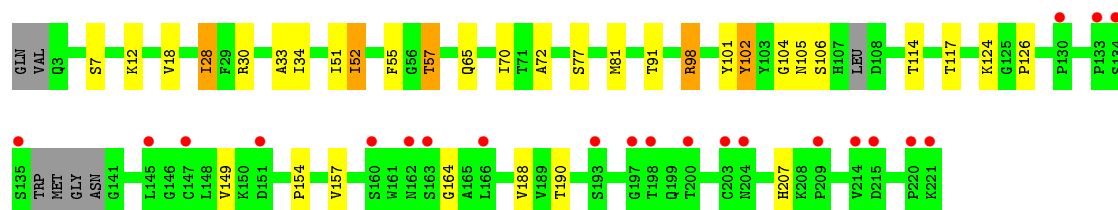
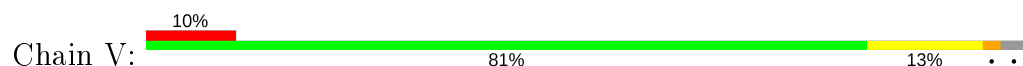
• Molecule 3: 70-1F02 Fab Heavy Chain



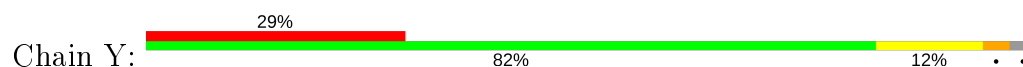
• Molecule 3: 70-1F02 Fab Heavy Chain

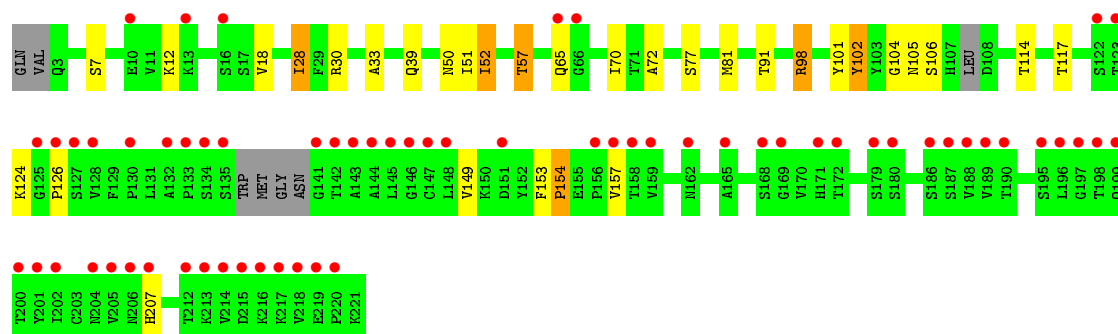


• Molecule 3: 70-1F02 Fab Heavy Chain

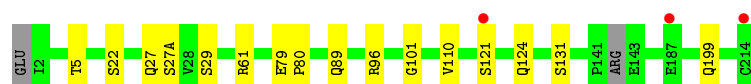


• Molecule 3: 70-1F02 Fab Heavy Chain

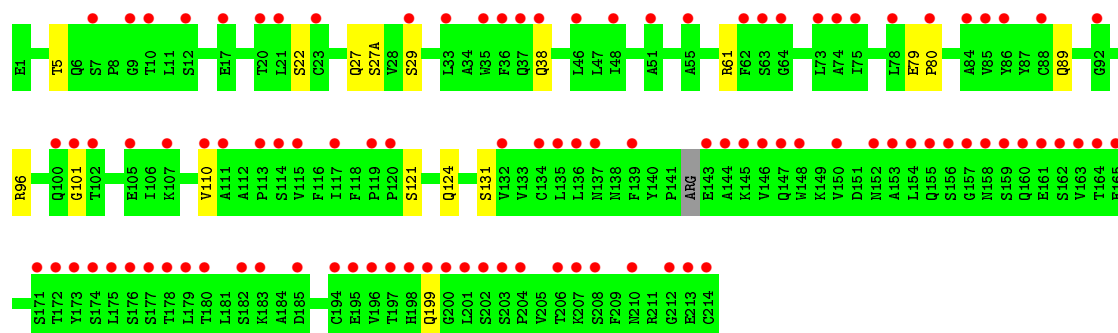
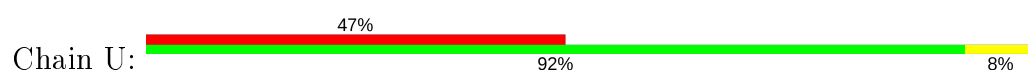




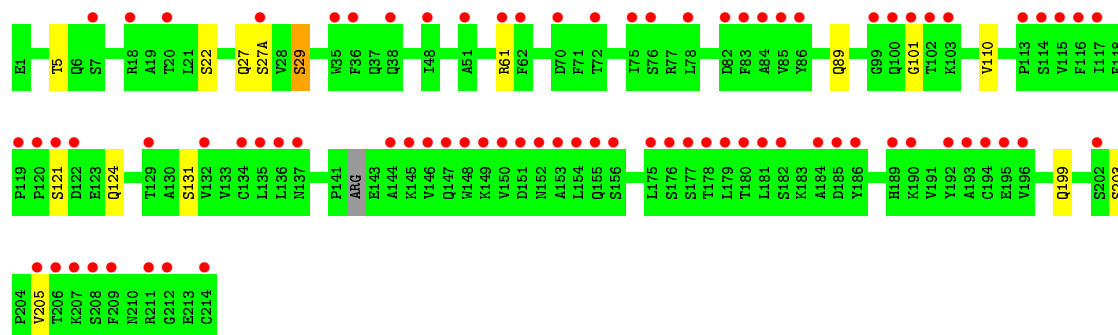
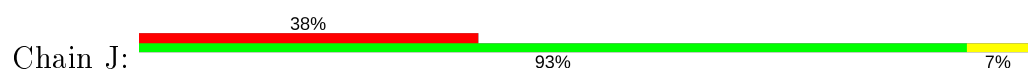
• Molecule 4: 70-1F02 Fab Light Chain



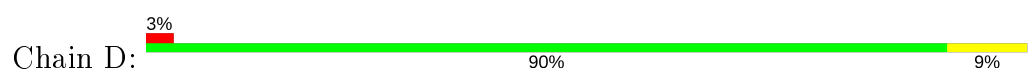
• Molecule 4: 70-1F02 Fab Light Chain

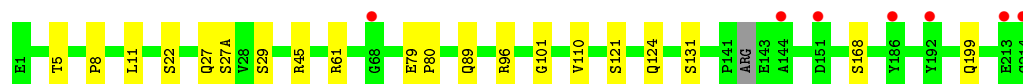


• Molecule 4: 70-1F02 Fab Light Chain

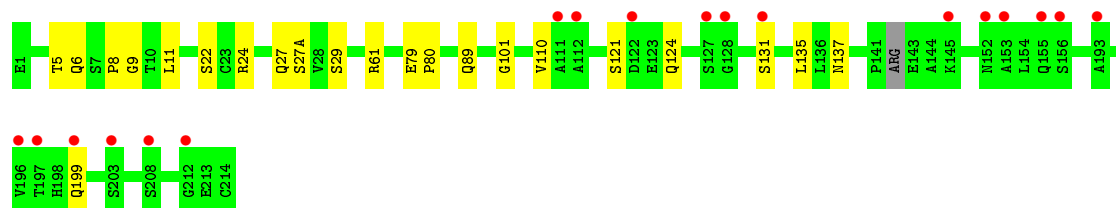
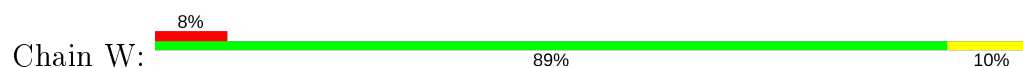


• Molecule 4: 70-1F02 Fab Light Chain

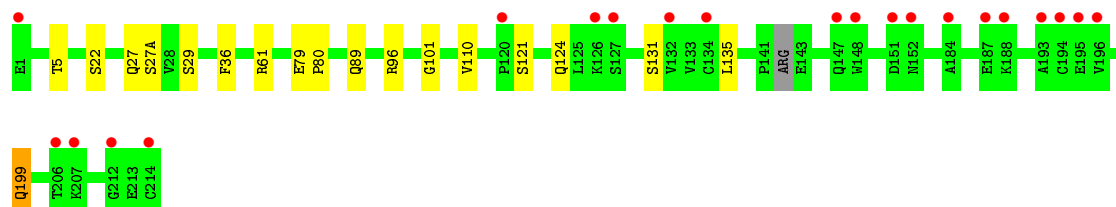




- Molecule 4: 70-1F02 Fab Light Chain



- Molecule 4: 70-1F02 Fab Light Chain



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



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



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



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

Chain p:  100%

MAG1
MAG2
MAN3
MAN4

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

Chain Z:  67% 33%

MAG1
MAG2
MAN3

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

Chain a:  50% 50%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain d:  100%

MAG1
MAG2

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

Chain e:  100%

MAG1
MAG2


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

Chain f:  100%MAG1
MAG2

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

Chain h:  100%MAG1
MAG2


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

Chain m:  100%MAG1
MAG2

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

Chain n:  100%MAG1
MAG2

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

Chain g:  100%MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain i:  100%MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain l:  20% 80%

MAG1	MAG2	MAG3	MAG4	EMJ45
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- Molecule 10: β -D-mannopyranose-(1-4)- α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain j:  100%

MAG1	MAG2	MAG3	EMJ44
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4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
2	R	0	1
2	T	0	1
3	M	0	1
All	All	0	5

All (3) bond length outliers are listed below:

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

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	23	ARG	NE-CZ-NH1	-20.07	110.26	120.30
3	O	23	ARG	NE-CZ-NH2	-7.31	116.65	120.30
4	D	45	ARG	NE-CZ-NH1	6.22	123.41	120.30
3	M	23	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
1	Q	266	LYS	CD-CE-NZ	5.66	124.72	111.70
3	M	23	ARG	CG-CD-NE	5.66	123.68	111.80
3	M	23	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	310	ARG	NE-CZ-NH1	5.49	123.05	120.30
3	M	23	ARG	CD-NE-CZ	5.44	131.21	123.60
1	A	107	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	R	68	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	310	ARG	NE-CZ-NH1	5.11	122.85	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	n	28	0	25	0	0
8	g	61	0	50	0	0
9	i	61	0	49	0	0
9	l	61	0	51	0	0
10	j	50	0	39	0	0
11	A	14	0	13	0	0
11	E	14	0	13	0	0
11	F	14	0	13	0	0
11	G	28	0	26	0	0
11	K	28	0	26	0	0
11	Q	14	0	13	1	0
11	S	14	0	13	0	0
12	C	11	0	10	0	0
All	All	44024	0	42435	264	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (264) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:169:GLN:NE2	4:J:203:SER:O	2.25	0.70
1:A:236:ASN:HA	6:Z:1:NAG:H81	1.73	0.69
1:S:169:GLN:NE2	4:J:205:VAL:HG23	2.10	0.67
2:L:52:VAL:HG11	3:O:28:ILE:HG21	1.76	0.66
1:S:169:GLN:NE2	4:J:205:VAL:CG2	2.61	0.64
3:M:50:ASN:HD21	4:N:96:ARG:NH1	1.97	0.63
3:I:30:ARG:HB3	3:I:77:SER:HB2	1.81	0.62
1:Q:276:THR:HG21	1:Q:284:ALA:HB1	1.81	0.62
3:V:30:ARG:HB3	3:V:77:SER:HB2	1.82	0.62
1:K:279:GLN:NE2	1:K:283:GLY:O	2.33	0.62
3:O:30:ARG:HB3	3:O:77:SER:HB2	1.82	0.61
1:A:279:GLN:NE2	1:A:283:GLY:O	2.33	0.61
1:S:276:THR:HG21	1:S:284:ALA:HB1	1.82	0.61
1:E:279:GLN:NE2	1:E:283:GLY:O	2.33	0.61
3:C:30:ARG:HB3	3:C:77:SER:HB2	1.82	0.60
1:Q:279:GLN:NE2	1:Q:283:GLY:O	2.34	0.60
1:K:276:THR:HG21	1:K:284:ALA:HB1	1.82	0.60
1:E:276:THR:HG21	1:E:284:ALA:HB1	1.82	0.60
1:G:279:GLN:NE2	1:G:283:GLY:O	2.33	0.60
1:S:279:GLN:NE2	1:S:283:GLY:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:THR:HG21	1:A:284:ALA:HB1	1.83	0.59
3:M:30:ARG:HB3	3:M:77:SER:HB2	1.82	0.59
3:O:50:ASN:HD21	4:P:96:ARG:NH1	2.00	0.59
1:G:276:THR:HG21	1:G:284:ALA:HB1	1.83	0.58
3:Y:30:ARG:HB3	3:Y:77:SER:HB2	1.83	0.58
3:M:52:ILE:HD11	3:M:57:THR:HG23	1.88	0.56
3:V:104:GLY:C	3:V:105:ASN:HD22	2.10	0.55
4:N:27:GLN:C	4:N:27(A):SER:N	2.61	0.55
1:A:7:TYR:CZ	2:B:6:ILE:HG23	2.42	0.55
4:W:110:VAL:HG21	4:W:199:GLN:HE22	1.70	0.54
2:B:52:VAL:HG11	3:C:28:ILE:HG21	1.89	0.54
3:O:52:ILE:HD11	3:O:57:THR:HG23	1.90	0.54
3:Y:52:ILE:HD11	3:Y:57:THR:HG23	1.89	0.54
4:P:27:GLN:C	4:P:27(A):SER:N	2.61	0.54
4:U:27:GLN:C	4:U:27(A):SER:N	2.62	0.54
4:J:27:GLN:C	4:J:27(A):SER:N	2.61	0.54
4:W:27:GLN:C	4:W:27(A):SER:N	2.61	0.53
4:D:27:GLN:C	4:D:27(A):SER:N	2.61	0.53
3:V:190:THR:HG21	4:W:137:ASN:ND2	2.24	0.53
3:C:52:ILE:HD11	3:C:57:THR:HG23	1.90	0.53
3:I:52:ILE:HD11	3:I:57:THR:HG23	1.90	0.53
1:S:7:TYR:CZ	2:T:6:ILE:HG23	2.43	0.53
3:I:104:GLY:C	3:I:105:ASN:HD22	2.10	0.52
4:D:110:VAL:HG21	4:D:199:GLN:HE22	1.74	0.52
1:E:7:TYR:CZ	2:F:6:ILE:HG23	2.45	0.52
3:V:52:ILE:HD11	3:V:57:THR:HG23	1.91	0.51
4:N:110:VAL:HG21	4:N:199:GLN:HE22	1.76	0.51
2:L:30:GLN:NE2	2:L:146:ASN:ND2	2.59	0.51
3:I:202:ILE:HD13	3:V:164:GLY:HA3	1.91	0.51
1:Q:3:ILE:HD11	2:R:149:MET:SD	2.50	0.51
3:Y:50:ASN:HD21	4:U:96:ARG:NH1	2.09	0.51
1:K:109:ASN:ND2	4:W:6:GLN:O	2.44	0.51
1:K:109:ASN:OD1	4:W:8:PRO:HA	2.11	0.50
1:A:165:ASN:OD1	6:Z:1:NAG:C7	2.59	0.50
3:O:104:GLY:C	3:O:105:ASN:HD22	2.15	0.50
2:T:20:GLY:HA2	3:V:55:PHE:CZ	2.46	0.50
2:H:94:TYR:CZ	2:H:98:LEU:HD11	2.47	0.50
2:R:94:TYR:CZ	2:R:98:LEU:HD11	2.47	0.49
1:S:149:TRP:HA	1:S:248:ILE:HG22	1.94	0.49
4:U:110:VAL:HG21	4:U:199:GLN:HE22	1.77	0.49
3:M:104:GLY:C	3:M:105:ASN:HD22	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:N	1:A:317:LEU:HD13	2.27	0.49
1:E:149:TRP:HA	1:E:248:ILE:HG22	1.95	0.49
1:G:317:LEU:HD13	1:G:317:LEU:N	2.28	0.49
2:L:94:TYR:CZ	2:L:98:LEU:HD11	2.47	0.49
3:C:12:LYS:HG3	3:C:18:VAL:HG22	1.94	0.49
1:K:317:LEU:HD13	1:K:317:LEU:N	2.28	0.49
1:Q:35:LYS:HA	1:Q:293:ASN:HD21	1.77	0.49
2:F:19:ASP:HB2	2:F:36:ALA:HB3	1.95	0.49
1:E:317:LEU:HD13	1:E:317:LEU:N	2.28	0.49
2:F:24:TYR:CE1	2:F:153:ARG:HG2	2.47	0.49
2:H:19:ASP:HB2	2:H:36:ALA:HB3	1.94	0.49
1:S:105:LEU:HA	1:S:108:ILE:HD11	1.95	0.49
1:G:35:LYS:HA	1:G:293:ASN:HD21	1.78	0.49
1:S:317:LEU:HD13	1:S:317:LEU:N	2.27	0.49
1:S:30:GLN:OE1	3:V:28:ILE:HG22	2.12	0.48
1:E:105:LEU:HA	1:E:108:ILE:HD11	1.95	0.48
2:H:6:ILE:HG23	1:K:7:TYR:CZ	2.48	0.48
1:K:105:LEU:HA	1:K:108:ILE:HD11	1.94	0.48
1:K:35:LYS:HA	1:K:293:ASN:HD21	1.77	0.48
2:L:30:GLN:NE2	2:L:146:ASN:HD22	2.12	0.48
1:E:35:LYS:HA	1:E:293:ASN:HD21	1.77	0.48
1:G:105:LEU:HA	1:G:108:ILE:HD11	1.95	0.48
1:G:247:PHE:CE2	1:G:249:ALA:HB2	2.48	0.48
1:Q:317:LEU:HD13	1:Q:317:LEU:N	2.28	0.48
1:A:247:PHE:CE2	1:A:249:ALA:HB2	2.49	0.48
4:J:110:VAL:HG21	4:J:199:GLN:HE22	1.79	0.48
1:K:149:TRP:HA	1:K:248:ILE:HG22	1.95	0.48
1:G:149:TRP:HA	1:G:248:ILE:HG22	1.95	0.48
1:A:149:TRP:HA	1:A:248:ILE:HG22	1.96	0.48
1:Q:149:TRP:HA	1:Q:248:ILE:HG22	1.95	0.48
1:S:35:LYS:HA	1:S:293:ASN:HD21	1.78	0.48
1:Q:105:LEU:HA	1:Q:108:ILE:HD11	1.96	0.47
1:Q:247:PHE:CE2	1:Q:249:ALA:HB2	2.48	0.47
1:A:35:LYS:HA	1:A:293:ASN:HD21	1.78	0.47
2:B:94:TYR:CZ	2:B:98:LEU:HD11	2.49	0.47
2:F:94:TYR:CZ	2:F:98:LEU:HD11	2.50	0.47
4:P:110:VAL:HG21	4:P:199:GLN:HE22	1.78	0.47
3:Y:104:GLY:C	3:Y:105:ASN:HD22	2.17	0.47
1:K:247:PHE:CE2	1:K:249:ALA:HB2	2.49	0.47
2:H:79:ASN:HD21	2:L:66:VAL:HG21	1.80	0.47
1:S:247:PHE:CE2	1:S:249:ALA:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:12:LYS:HG3	3:I:18:VAL:HG22	1.96	0.47
2:B:24:TYR:CE1	2:B:153:ARG:HG2	2.49	0.47
1:G:5:ILE:N	1:G:5:ILE:HD12	2.30	0.47
1:S:5:ILE:N	1:S:5:ILE:HD12	2.29	0.47
2:T:94:TYR:CZ	2:T:98:LEU:HD11	2.49	0.47
3:V:12:LYS:HG3	3:V:18:VAL:HG22	1.97	0.47
2:B:94:TYR:CD1	2:H:59:MET:HG3	2.49	0.46
1:A:105:LEU:HA	1:A:108:ILE:HD11	1.96	0.46
1:E:247:PHE:CE2	1:E:249:ALA:HB2	2.49	0.46
3:Y:39:GLN:NE2	4:U:38:GLN:OE1	2.46	0.46
2:T:24:TYR:CE1	2:T:153:ARG:HG2	2.51	0.46
3:M:12:LYS:HG3	3:M:18:VAL:HG22	1.97	0.46
1:S:274:CYS:SG	1:S:275:ASN:N	2.89	0.46
2:R:19:ASP:HB2	2:R:36:ALA:HB3	1.97	0.46
1:A:274:CYS:SG	1:A:275:ASN:N	2.89	0.46
1:E:274:CYS:SG	1:E:275:ASN:N	2.89	0.46
1:K:5:ILE:N	1:K:5:ILE:HD12	2.31	0.46
2:T:18:VAL:O	3:V:57:THR:HG21	2.16	0.46
3:C:104:GLY:C	3:C:105:ASN:HD22	2.16	0.46
3:C:50:ASN:HD21	4:D:96:ARG:NH1	2.14	0.46
3:C:30:ARG:HH12	3:C:72:ALA:HB1	1.81	0.46
1:E:5:ILE:HD12	1:E:5:ILE:N	2.31	0.45
3:O:30:ARG:HH12	3:O:72:ALA:HB1	1.81	0.45
1:A:236:ASN:OD1	6:Z:1:NAG:C7	2.64	0.45
3:I:70:ILE:HG22	3:I:81:MET:HA	1.98	0.45
3:M:188:VAL:HG21	4:N:135:LEU:HD22	1.97	0.45
3:V:30:ARG:HH12	3:V:72:ALA:HB1	1.81	0.45
3:Y:12:LYS:HG3	3:Y:18:VAL:HG22	1.97	0.45
1:G:274:CYS:SG	1:G:275:ASN:N	2.89	0.45
1:K:274:CYS:SG	1:K:275:ASN:N	2.89	0.45
1:Q:274:CYS:SG	1:Q:275:ASN:N	2.89	0.45
1:Q:7:TYR:CZ	2:R:6:ILE:HG23	2.52	0.45
3:V:102:TYR:O	3:V:102:TYR:CD2	2.70	0.45
3:Y:102:TYR:O	3:Y:102:TYR:CD2	2.70	0.45
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.99	0.45
2:H:175:SER:O	2:L:168:LEU:HD11	2.16	0.45
3:M:102:TYR:CD2	3:M:102:TYR:O	2.70	0.45
1:S:169:GLN:NE2	4:J:205:VAL:HG22	2.31	0.45
3:C:7:SER:O	3:C:114:THR:HG22	2.16	0.45
3:M:70:ILE:HG22	3:M:81:MET:HA	1.99	0.45
3:O:7:SER:O	3:O:114:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:188:VAL:HG21	4:W:135:LEU:CD2	2.46	0.45
3:V:70:ILE:HG22	3:V:81:MET:HA	1.98	0.45
3:I:7:SER:O	3:I:114:THR:HG22	2.17	0.45
2:L:24:TYR:CE1	2:L:153:ARG:HG2	2.52	0.45
2:R:24:TYR:CE1	2:R:153:ARG:HG2	2.51	0.45
3:O:12:LYS:HG3	3:O:18:VAL:HG22	1.98	0.45
3:Y:7:SER:O	3:Y:114:THR:HG22	2.17	0.45
1:E:3:ILE:HD11	2:F:149:MET:HG2	1.99	0.44
3:M:7:SER:O	3:M:114:THR:HG22	2.16	0.44
1:E:226:MET:CE	1:E:248:ILE:HG21	2.48	0.44
2:B:61:THR:HG22	2:L:90:ASP:OD1	2.18	0.44
1:K:226:MET:CE	1:K:248:ILE:HG21	2.47	0.44
1:Q:5:ILE:N	1:Q:5:ILE:HD12	2.32	0.44
3:Y:70:ILE:HG22	3:Y:81:MET:HA	1.99	0.44
3:I:102:TYR:O	3:I:102:TYR:CD2	2.70	0.44
3:O:102:TYR:CD2	3:O:102:TYR:O	2.71	0.44
1:S:226:MET:CE	1:S:248:ILE:HG21	2.47	0.44
3:Y:30:ARG:HH12	3:Y:72:ALA:HB1	1.81	0.44
1:Q:11:ASN:HD21	11:Q:401:NAG:C7	2.31	0.44
3:V:7:SER:O	3:V:114:THR:HG22	2.17	0.44
1:A:5:ILE:HD12	1:A:5:ILE:N	2.32	0.44
2:T:19:ASP:HB2	2:T:36:ALA:HB3	1.98	0.44
3:C:70:ILE:HG22	3:C:81:MET:HA	1.99	0.44
3:I:126:PRO:HB2	3:I:149:VAL:HG13	2.00	0.44
2:R:52:VAL:HG11	3:Y:28:ILE:HG21	2.00	0.44
1:G:293:ASN:HD22	1:G:293:ASN:N	2.16	0.43
3:O:70:ILE:HG22	3:O:81:MET:HA	2.00	0.43
3:I:30:ARG:HH12	3:I:72:ALA:HB1	1.83	0.43
2:L:52:VAL:HG11	3:O:28:ILE:CG2	2.47	0.43
2:H:83:LYS:HE2	2:L:66:VAL:HG23	2.01	0.43
1:Q:226:MET:CE	1:Q:248:ILE:HG21	2.48	0.43
2:B:42:GLN:NE2	3:C:101:TYR:HB2	2.34	0.43
1:A:226:MET:CE	1:A:248:ILE:HG21	2.48	0.43
2:H:2:LEU:O	2:L:113:SER:OG	2.37	0.43
2:H:175:SER:C	2:L:168:LEU:HD11	2.39	0.43
3:I:202:ILE:HG21	3:V:164:GLY:O	2.19	0.43
3:I:91:THR:HG23	3:I:117:THR:HA	2.01	0.43
2:L:19:ASP:HB2	2:L:36:ALA:HB3	2.00	0.43
3:V:126:PRO:HB2	3:V:149:VAL:HG13	2.01	0.43
1:A:18:THR:OG1	1:A:19:ILE:N	2.52	0.43
1:K:18:THR:OG1	1:K:19:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HB2	2:B:89:LEU:HD11	2.01	0.42
3:C:102:TYR:O	3:C:102:TYR:CD2	2.71	0.42
3:C:91:THR:HG23	3:C:117:THR:HA	2.01	0.42
1:E:293:ASN:N	1:E:293:ASN:HD22	2.17	0.42
3:M:107:HIS:HB2	4:N:36:PHE:CE1	2.55	0.42
4:W:110:VAL:HG21	4:W:199:GLN:NE2	2.34	0.42
1:Q:293:ASN:HD22	1:Q:293:ASN:N	2.17	0.42
1:S:18:THR:OG1	1:S:19:ILE:N	2.53	0.42
2:H:24:TYR:CE1	2:H:153:ARG:HG2	2.53	0.42
3:M:102:TYR:CG	3:M:102:TYR:O	2.72	0.42
3:O:126:PRO:HB2	3:O:149:VAL:HG13	2.00	0.42
1:Q:18:THR:OG1	1:Q:19:ILE:N	2.52	0.42
3:V:33:ALA:O	3:V:98:ARG:O	2.38	0.42
1:S:293:ASN:HD22	1:S:293:ASN:N	2.17	0.42
4:U:124:GLN:HE22	4:U:131:SER:CB	2.33	0.42
3:V:34:ILE:N	3:V:34:ILE:HD12	2.35	0.42
2:T:20:GLY:HA2	3:V:55:PHE:CE1	2.54	0.42
3:Y:126:PRO:HB2	3:Y:149:VAL:HG13	2.01	0.42
1:A:293:ASN:N	1:A:293:ASN:HD22	2.17	0.42
1:A:30:GLN:OE1	3:C:28:ILE:HG22	2.20	0.42
3:O:17:SER:OG	2:R:143:LYS:NZ	2.30	0.42
4:U:79:GLU:HB3	4:U:80:PRO:HD2	2.02	0.42
1:E:18:THR:OG1	1:E:19:ILE:N	2.53	0.42
3:O:153:PHE:HA	3:O:154:PRO:HA	1.91	0.42
3:M:126:PRO:HB2	3:M:149:VAL:HG13	2.02	0.42
3:M:30:ARG:HH12	3:M:72:ALA:HB1	1.84	0.42
4:D:124:GLN:HE22	4:D:131:SER:CB	2.33	0.41
4:J:124:GLN:HE22	4:J:131:SER:CB	2.33	0.41
3:O:91:THR:HG23	3:O:117:THR:HA	2.01	0.41
1:G:226:MET:CE	1:G:248:ILE:HG21	2.50	0.41
1:K:293:ASN:N	1:K:293:ASN:HD22	2.16	0.41
4:N:79:GLU:HB3	4:N:80:PRO:HD2	2.02	0.41
4:N:124:GLN:HE22	4:N:131:SER:CB	2.33	0.41
1:S:1:ASP:OD1	2:T:28:ASN:HB2	2.19	0.41
3:Y:153:PHE:HA	3:Y:154:PRO:HA	1.92	0.41
1:G:18:THR:OG1	1:G:19:ILE:N	2.52	0.41
4:P:124:GLN:HE22	4:P:131:SER:CB	2.33	0.41
3:Y:102:TYR:O	3:Y:102:TYR:CG	2.73	0.41
1:S:316:GLY:O	2:T:111:HIS:CD2	2.74	0.41
4:W:124:GLN:HE22	4:W:131:SER:CB	2.33	0.41
4:W:79:GLU:HB3	4:W:80:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:THR:HG22	1:A:203:SER:N	2.35	0.41
2:T:42:GLN:HE21	3:V:102:TYR:HD2	1.68	0.41
3:V:91:THR:HG23	3:V:117:THR:HA	2.01	0.41
3:Y:33:ALA:O	3:Y:98:ARG:O	2.38	0.41
3:I:33:ALA:O	3:I:98:ARG:O	2.38	0.41
3:M:33:ALA:O	3:M:98:ARG:O	2.39	0.41
3:M:91:THR:HG23	3:M:117:THR:HA	2.03	0.41
4:P:79:GLU:HB3	4:P:80:PRO:HD2	2.03	0.41
3:V:188:VAL:HG11	4:W:135:LEU:HD22	2.02	0.41
4:D:8:PRO:HG2	4:D:11:LEU:HG	2.03	0.41
3:I:102:TYR:O	3:I:102:TYR:CG	2.73	0.41
3:O:33:ALA:O	3:O:98:ARG:O	2.39	0.41
3:Y:91:THR:HG23	3:Y:117:THR:HA	2.02	0.41
2:B:110:PHE:CE1	1:G:20:MET:HE1	2.55	0.41
4:D:79:GLU:HB3	4:D:80:PRO:HD2	2.03	0.41
3:V:102:TYR:O	3:V:102:TYR:CG	2.73	0.41
3:C:126:PRO:HB2	3:C:149:VAL:HG13	2.02	0.41
3:C:33:ALA:O	3:C:98:ARG:O	2.38	0.41
2:H:19:ASP:HB2	2:H:36:ALA:CB	2.51	0.41
1:K:101:LEU:HD13	1:K:230:TRP:CE3	2.55	0.41
1:K:202:THR:HG22	1:K:203:SER:N	2.36	0.41
2:F:19:ASP:HB2	2:F:36:ALA:CB	2.51	0.40
1:K:259:LYS:HE3	4:W:24:ARG:CG	2.51	0.40
1:Q:32:ILE:HD11	1:Q:313:LEU:HD22	2.03	0.40
1:S:101:LEU:HD13	1:S:230:TRP:CE3	2.56	0.40
1:S:263:THR:HG21	2:T:67:GLY:H	1.86	0.40
4:W:8:PRO:HG2	4:W:11:LEU:HG	2.04	0.40
1:E:263:THR:HG22	1:E:299:ILE:CD1	2.52	0.40
1:G:202:THR:HG22	1:G:203:SER:N	2.36	0.40
1:G:293:ASN:HD22	1:G:293:ASN:H	1.69	0.40
1:Q:101:LEU:HD13	1:Q:230:TRP:CE3	2.57	0.40
1:Q:293:ASN:HD22	1:Q:293:ASN:H	1.69	0.40
1:K:75:GLU:OE2	4:W:9:GLY:N	2.55	0.40
1:E:202:THR:HG22	1:E:203:SER:N	2.36	0.40
1:K:293:ASN:H	1:K:293:ASN:HD22	1.69	0.40
2:L:52:VAL:CG1	3:O:28:ILE:HG21	2.47	0.40
2:B:98:LEU:HD13	2:H:99:LEU:HD11	2.04	0.40
1:S:202:THR:HG22	1:S:203:SER:N	2.36	0.40
1:Q:16:VAL:CG1	2:R:104:ASN:ND2	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/330 (97%)	282 (88%)	33 (10%)	4 (1%)	12	48
1	E	319/330 (97%)	283 (89%)	32 (10%)	4 (1%)	12	48
1	G	319/330 (97%)	283 (89%)	32 (10%)	4 (1%)	12	48
1	K	319/330 (97%)	283 (89%)	31 (10%)	5 (2%)	9	44
1	Q	319/330 (97%)	283 (89%)	33 (10%)	3 (1%)	17	54
1	S	319/330 (97%)	284 (89%)	31 (10%)	4 (1%)	12	48
2	B	172/181 (95%)	159 (92%)	12 (7%)	1 (1%)	25	63
2	F	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	H	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	L	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	R	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
2	T	173/181 (96%)	159 (92%)	13 (8%)	1 (1%)	25	63
3	C	210/221 (95%)	181 (86%)	26 (12%)	3 (1%)	11	46
3	I	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
3	M	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
3	O	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
3	V	210/221 (95%)	183 (87%)	24 (11%)	3 (1%)	11	46
3	Y	210/221 (95%)	182 (87%)	25 (12%)	3 (1%)	11	46
4	D	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	29	67
4	J	208/215 (97%)	198 (95%)	8 (4%)	2 (1%)	15	52
4	N	208/215 (97%)	199 (96%)	8 (4%)	1 (0%)	29	67
4	P	207/215 (96%)	198 (96%)	8 (4%)	1 (0%)	29	67
4	U	208/215 (97%)	199 (96%)	8 (4%)	1 (0%)	29	67
4	W	208/215 (97%)	200 (96%)	7 (3%)	1 (0%)	29	67
All	All	5458/5682 (96%)	4938 (90%)	465 (8%)	55 (1%)	15	52

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	65	GLN
3	I	65	GLN
3	M	65	GLN
3	O	65	GLN
3	V	65	GLN
3	Y	65	GLN
2	B	60	ASN
3	C	207	HIS
2	F	60	ASN
2	H	60	ASN
3	I	207	HIS
2	L	60	ASN
3	M	207	HIS
3	O	207	HIS
4	P	101	GLY
2	R	60	ASN
1	S	154	ASN
2	T	60	ASN
3	V	207	HIS
3	Y	207	HIS
4	U	101	GLY
4	J	101	GLY
4	D	101	GLY
4	W	101	GLY
4	N	101	GLY
1	A	154	ASN
1	A	194	PRO
1	E	154	ASN
1	E	194	PRO
1	G	154	ASN
1	G	194	PRO
1	K	154	ASN
1	K	194	PRO
1	Q	154	ASN
1	Q	194	PRO
1	S	194	PRO
1	A	134	ALA
1	E	134	ALA
1	G	134	ALA
1	K	134	ALA
1	Q	134	ALA
1	S	134	ALA

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Mol	Chain	Res	Type
3	O	154	PRO
4	J	29	SER
1	A	262	SER
3	C	154	PRO
1	E	133	SER
1	G	262	SER
1	K	133	SER
1	K	262	SER
1	S	262	SER
3	I	154	PRO
3	Y	154	PRO
3	V	154	PRO
3	M	154	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/298 (97%)	264 (91%)	25 (9%)	10	37
1	E	289/298 (97%)	264 (91%)	25 (9%)	10	37
1	G	289/298 (97%)	263 (91%)	26 (9%)	9	35
1	K	289/298 (97%)	263 (91%)	26 (9%)	9	35
1	Q	289/298 (97%)	264 (91%)	25 (9%)	10	37
1	S	289/298 (97%)	263 (91%)	26 (9%)	9	35
2	B	149/155 (96%)	139 (93%)	10 (7%)	16	45
2	F	149/155 (96%)	138 (93%)	11 (7%)	13	42
2	H	149/155 (96%)	137 (92%)	12 (8%)	11	40
2	L	149/155 (96%)	139 (93%)	10 (7%)	16	45
2	R	149/155 (96%)	139 (93%)	10 (7%)	16	45
2	T	149/155 (96%)	139 (93%)	10 (7%)	16	45
3	C	177/183 (97%)	168 (95%)	9 (5%)	24	53
3	I	177/183 (97%)	168 (95%)	9 (5%)	24	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	177/183 (97%)	165 (93%)	12 (7%)	16	45
3	O	177/183 (97%)	166 (94%)	11 (6%)	18	47
3	V	177/183 (97%)	167 (94%)	10 (6%)	21	50
3	Y	177/183 (97%)	167 (94%)	10 (6%)	21	50
4	D	183/185 (99%)	176 (96%)	7 (4%)	33	59
4	J	183/185 (99%)	177 (97%)	6 (3%)	38	63
4	N	183/185 (99%)	176 (96%)	7 (4%)	33	59
4	P	182/185 (98%)	176 (97%)	6 (3%)	38	63
4	U	183/185 (99%)	177 (97%)	6 (3%)	38	63
4	W	183/185 (99%)	177 (97%)	6 (3%)	38	63
All	All	4787/4926 (97%)	4472 (93%)	315 (7%)	16	46

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	19	ILE
1	A	27	THR
1	A	36	LYS
1	A	41	LEU
1	A	53	ARG
1	A	55	CYS
1	A	69	GLU
1	A	173	LEU
1	A	181	PRO
1	A	192	GLN
1	A	217	SER
1	A	225	ARG
1	A	226	MET
1	A	271	TYR
1	A	274	CYS
1	A	275	ASN
1	A	277	LYS
1	A	278	CYS
1	A	280	THR
1	A	293	ASN
1	A	297	LEU
1	A	317	LEU

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Mol	Chain	Res	Type
1	A	319	ASN
1	A	320	SER
2	B	28	ASN
2	B	30	GLN
2	B	42	GLN
2	B	62	GLN
2	B	112	ASP
2	B	116	LYS
2	B	117	ASN
2	B	126	LEU
2	B	127	ARG
2	B	158	ASP
3	C	28	ILE
3	C	51	ILE
3	C	52	ILE
3	C	57	THR
3	C	98	ARG
3	C	101	TYR
3	C	102	TYR
3	C	106	SER
3	C	157	VAL
1	E	18	THR
1	E	19	ILE
1	E	27	THR
1	E	36	LYS
1	E	41	LEU
1	E	53	ARG
1	E	55	CYS
1	E	69	GLU
1	E	95	PHE
1	E	173	LEU
1	E	192	GLN
1	E	217	SER
1	E	225	ARG
1	E	226	MET
1	E	271	TYR
1	E	274	CYS
1	E	275	ASN
1	E	277	LYS
1	E	278	CYS
1	E	280	THR
1	E	293	ASN

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Mol	Chain	Res	Type
1	E	297	LEU
1	E	317	LEU
1	E	319	ASN
1	E	320	SER
2	F	28	ASN
2	F	30	GLN
2	F	42	GLN
2	F	60	ASN
2	F	62	GLN
2	F	112	ASP
2	F	116	LYS
2	F	117	ASN
2	F	126	LEU
2	F	127	ARG
2	F	158	ASP
1	G	18	THR
1	G	19	ILE
1	G	27	THR
1	G	36	LYS
1	G	41	LEU
1	G	53	ARG
1	G	55	CYS
1	G	69	GLU
1	G	120	SER
1	G	173	LEU
1	G	181	PRO
1	G	192	GLN
1	G	217	SER
1	G	225	ARG
1	G	226	MET
1	G	271	TYR
1	G	274	CYS
1	G	275	ASN
1	G	278	CYS
1	G	280	THR
1	G	288	SER
1	G	293	ASN
1	G	297	LEU
1	G	317	LEU
1	G	319	ASN
1	G	320	SER
2	H	28	ASN

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Mol	Chain	Res	Type
2	H	30	GLN
2	H	42	GLN
2	H	62	GLN
2	H	99	LEU
2	H	112	ASP
2	H	116	LYS
2	H	117	ASN
2	H	121	LYS
2	H	126	LEU
2	H	127	ARG
2	H	158	ASP
3	I	28	ILE
3	I	51	ILE
3	I	52	ILE
3	I	57	THR
3	I	98	ARG
3	I	101	TYR
3	I	102	TYR
3	I	106	SER
3	I	157	VAL
1	K	18	THR
1	K	19	ILE
1	K	27	THR
1	K	36	LYS
1	K	40	LYS
1	K	41	LEU
1	K	53	ARG
1	K	55	CYS
1	K	69	GLU
1	K	95	PHE
1	K	173	LEU
1	K	192	GLN
1	K	217	SER
1	K	225	ARG
1	K	226	MET
1	K	271	TYR
1	K	274	CYS
1	K	275	ASN
1	K	277	LYS
1	K	278	CYS
1	K	280	THR
1	K	293	ASN

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Mol	Chain	Res	Type
1	K	297	LEU
1	K	317	LEU
1	K	319	ASN
1	K	320	SER
2	L	28	ASN
2	L	42	GLN
2	L	60	ASN
2	L	62	GLN
2	L	112	ASP
2	L	116	LYS
2	L	121	LYS
2	L	126	LEU
2	L	127	ARG
2	L	158	ASP
3	M	23	ARG
3	M	28	ILE
3	M	51	ILE
3	M	52	ILE
3	M	57	THR
3	M	75	SER
3	M	98	ARG
3	M	101	TYR
3	M	102	TYR
3	M	106	SER
3	M	124	LYS
3	M	157	VAL
3	O	28	ILE
3	O	51	ILE
3	O	52	ILE
3	O	57	THR
3	O	98	ARG
3	O	101	TYR
3	O	102	TYR
3	O	106	SER
3	O	124	LYS
3	O	157	VAL
3	O	186	SER
4	P	5	THR
4	P	22	SER
4	P	29	SER
4	P	61	ARG
4	P	89	GLN

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Mol	Chain	Res	Type
4	P	121	SER
1	Q	18	THR
1	Q	19	ILE
1	Q	27	THR
1	Q	36	LYS
1	Q	40	LYS
1	Q	41	LEU
1	Q	53	ARG
1	Q	55	CYS
1	Q	69	GLU
1	Q	95	PHE
1	Q	173	LEU
1	Q	192	GLN
1	Q	217	SER
1	Q	225	ARG
1	Q	226	MET
1	Q	271	TYR
1	Q	274	CYS
1	Q	275	ASN
1	Q	278	CYS
1	Q	280	THR
1	Q	293	ASN
1	Q	297	LEU
1	Q	317	LEU
1	Q	319	ASN
1	Q	320	SER
2	R	28	ASN
2	R	30	GLN
2	R	42	GLN
2	R	60	ASN
2	R	62	GLN
2	R	112	ASP
2	R	116	LYS
2	R	126	LEU
2	R	127	ARG
2	R	158	ASP
1	S	18	THR
1	S	19	ILE
1	S	27	THR
1	S	36	LYS
1	S	40	LYS
1	S	41	LEU

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Mol	Chain	Res	Type
1	S	53	ARG
1	S	55	CYS
1	S	69	GLU
1	S	95	PHE
1	S	173	LEU
1	S	181	PRO
1	S	192	GLN
1	S	217	SER
1	S	225	ARG
1	S	226	MET
1	S	271	TYR
1	S	274	CYS
1	S	275	ASN
1	S	278	CYS
1	S	280	THR
1	S	293	ASN
1	S	297	LEU
1	S	317	LEU
1	S	319	ASN
1	S	320	SER
2	T	28	ASN
2	T	30	GLN
2	T	42	GLN
2	T	62	GLN
2	T	112	ASP
2	T	116	LYS
2	T	117	ASN
2	T	126	LEU
2	T	127	ARG
2	T	158	ASP
3	V	28	ILE
3	V	51	ILE
3	V	52	ILE
3	V	57	THR
3	V	98	ARG
3	V	101	TYR
3	V	102	TYR
3	V	106	SER
3	V	124	LYS
3	V	157	VAL
3	Y	28	ILE
3	Y	51	ILE

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Mol	Chain	Res	Type
3	Y	52	ILE
3	Y	57	THR
3	Y	98	ARG
3	Y	101	TYR
3	Y	102	TYR
3	Y	106	SER
3	Y	124	LYS
3	Y	157	VAL
4	U	5	THR
4	U	22	SER
4	U	29	SER
4	U	61	ARG
4	U	89	GLN
4	U	121	SER
4	J	5	THR
4	J	22	SER
4	J	29	SER
4	J	61	ARG
4	J	89	GLN
4	J	121	SER
4	D	5	THR
4	D	22	SER
4	D	29	SER
4	D	61	ARG
4	D	89	GLN
4	D	121	SER
4	D	168	SER
4	W	5	THR
4	W	22	SER
4	W	29	SER
4	W	61	ARG
4	W	89	GLN
4	W	121	SER
4	N	5	THR
4	N	22	SER
4	N	29	SER
4	N	61	ARG
4	N	89	GLN
4	N	121	SER
4	N	199	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	138	GLN
1	A	293	ASN
1	A	319	ASN
2	B	42	GLN
2	B	79	ASN
2	B	95	ASN
2	B	117	ASN
2	B	135	ASN
3	C	39	GLN
3	C	50	ASN
3	C	178	GLN
1	E	15	GLN
1	E	109	ASN
1	E	138	GLN
1	E	192	GLN
1	E	293	ASN
1	E	319	ASN
2	F	135	ASN
1	G	15	GLN
1	G	138	GLN
1	G	293	ASN
1	G	319	ASN
2	H	79	ASN
2	H	95	ASN
2	H	117	ASN
2	H	135	ASN
3	I	39	GLN
3	I	105	ASN
3	I	178	GLN
1	K	138	GLN
1	K	293	ASN
1	K	319	ASN
2	L	30	GLN
2	L	42	GLN
2	L	95	ASN
2	L	135	ASN
3	M	39	GLN
3	M	50	ASN
3	M	178	GLN
3	O	50	ASN
3	O	107	HIS
3	O	178	GLN

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Mol	Chain	Res	Type
4	P	89	GLN
4	P	124	GLN
4	P	155	GLN
4	P	199	GLN
4	P	210	ASN
1	Q	11	ASN
1	Q	15	GLN
1	Q	293	ASN
1	Q	319	ASN
2	R	42	GLN
2	R	117	ASN
2	R	135	ASN
1	S	138	GLN
1	S	293	ASN
1	S	319	ASN
2	T	42	GLN
2	T	117	ASN
2	T	135	ASN
3	V	39	GLN
3	V	105	ASN
3	V	178	GLN
3	Y	39	GLN
3	Y	50	ASN
3	Y	178	GLN
4	U	38	GLN
4	U	124	GLN
4	U	199	GLN
4	U	210	ASN
4	J	27	GLN
4	J	38	GLN
4	J	124	GLN
4	J	155	GLN
4	J	199	GLN
4	J	210	ASN
4	D	27	GLN
4	D	38	GLN
4	D	124	GLN
4	D	155	GLN
4	D	199	GLN
4	D	210	ASN
4	W	27	GLN
4	W	38	GLN

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Mol	Chain	Res	Type
4	W	124	GLN
4	W	137	ASN
4	W	155	GLN
4	W	199	GLN
4	W	210	ASN
4	N	38	GLN
4	N	124	GLN
4	N	155	GLN
4	N	199	GLN
4	N	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

56 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	X	1	1,5	14,14,15	0.99	2 (14%)	17,19,21	1.43	3 (17%)
5	NAG	X	2	5	14,14,15	0.79	0	17,19,21	2.15	6 (35%)
5	MAN	X	3	5	11,11,12	0.87	0	15,15,17	1.90	2 (13%)
5	MAN	X	4	5	11,11,12	0.72	0	15,15,17	1.99	6 (40%)
6	NAG	Z	1	1,6	14,14,15	1.16	1 (7%)	17,19,21	2.61	8 (47%)
6	NAG	Z	2	6	14,14,15	0.67	0	17,19,21	1.13	1 (5%)
6	MAN	Z	3	6	11,11,12	0.78	0	15,15,17	2.31	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	a	1	1,7	14,14,15	0.81	0	17,19,21	0.95	0
7	NAG	a	2	7	14,14,15	0.88	0	17,19,21	1.69	4 (23%)
7	NAG	b	1	2,7	14,14,15	1.08	2 (14%)	17,19,21	1.28	1 (5%)
7	NAG	b	2	7	14,14,15	0.81	1 (7%)	17,19,21	1.41	4 (23%)
7	NAG	c	1	1,7	14,14,15	0.52	0	17,19,21	2.09	4 (23%)
7	NAG	c	2	7	14,14,15	0.73	0	17,19,21	1.38	2 (11%)
7	NAG	d	1	1,7	14,14,15	1.29	2 (14%)	17,19,21	1.69	2 (11%)
7	NAG	d	2	7	14,14,15	0.70	0	17,19,21	1.34	2 (11%)
7	NAG	e	1	1,7	14,14,15	1.58	2 (14%)	17,19,21	1.86	4 (23%)
7	NAG	e	2	7	14,14,15	0.82	1 (7%)	17,19,21	2.04	5 (29%)
7	NAG	f	1	1,7	14,14,15	0.82	0	17,19,21	1.53	2 (11%)
7	NAG	f	2	7	14,14,15	0.45	0	17,19,21	1.40	2 (11%)
8	NAG	g	1	1,8	14,14,15	0.90	0	17,19,21	1.81	4 (23%)
8	NAG	g	2	8	14,14,15	0.49	0	17,19,21	1.94	5 (29%)
8	MAN	g	3	8	11,11,12	1.19	1 (9%)	15,15,17	2.46	6 (40%)
8	MAN	g	4	8	11,11,12	0.69	0	15,15,17	1.46	2 (13%)
8	MAN	g	5	8	11,11,12	1.12	2 (18%)	15,15,17	3.56	4 (26%)
7	NAG	h	1	1,7	14,14,15	1.87	4 (28%)	17,19,21	1.98	4 (23%)
7	NAG	h	2	7	14,14,15	1.30	2 (14%)	17,19,21	1.97	3 (17%)
9	NAG	i	1	1,9	14,14,15	0.72	0	17,19,21	1.95	5 (29%)
9	NAG	i	2	9	14,14,15	0.63	0	17,19,21	1.88	5 (29%)
9	MAN	i	3	9	11,11,12	1.49	2 (18%)	15,15,17	2.56	6 (40%)
9	MAN	i	4	9	11,11,12	0.77	0	15,15,17	1.66	4 (26%)
9	BMA	i	5	9	11,11,12	2.11	3 (27%)	15,15,17	3.23	6 (40%)
10	NAG	j	1	1,10	14,14,15	1.77	4 (28%)	17,19,21	1.74	4 (23%)
10	NAG	j	2	10	14,14,15	0.65	0	17,19,21	1.71	3 (17%)
10	MAN	j	3	10	11,11,12	0.97	0	15,15,17	3.11	7 (46%)
10	BMA	j	4	10	11,11,12	1.04	0	15,15,17	1.58	3 (20%)
5	NAG	k	1	1,5	14,14,15	0.68	0	17,19,21	2.89	8 (47%)
5	NAG	k	2	5	14,14,15	0.42	0	17,19,21	1.42	4 (23%)
5	MAN	k	3	5	11,11,12	1.46	3 (27%)	15,15,17	3.41	10 (66%)
5	MAN	k	4	5	11,11,12	1.13	2 (18%)	15,15,17	3.17	6 (40%)
9	NAG	l	1	1,9	14,14,15	1.36	2 (14%)	17,19,21	2.19	4 (23%)
9	NAG	l	2	9	14,14,15	0.86	0	17,19,21	1.84	5 (29%)
9	MAN	l	3	9	11,11,12	1.48	2 (18%)	15,15,17	1.68	3 (20%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	X	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	MAN	X	3	5	-	2/2/19/22	0/1/1/1
5	MAN	X	4	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	1/1/5/7	1/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
6	MAN	Z	3	6	-	0/2/19/22	0/1/1/1
7	NAG	a	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	NAG	b	1	2,7	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	b	2	7	-	1/6/23/26	0/1/1/1
7	NAG	c	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1
7	NAG	d	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	NAG	e	1	1,7	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	p	4	5	-	0/2/19/22	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	1	NAG	O5-C1	-4.98	1.35	1.43
7	h	1	NAG	O5-C1	-4.66	1.36	1.43
9	i	5	BMA	O5-C1	-4.37	1.36	1.43
7	e	1	NAG	C1-C2	4.16	1.58	1.52
5	o	1	NAG	O5-C1	-4.16	1.37	1.43
9	i	5	BMA	C4-C5	3.88	1.61	1.53
7	d	1	NAG	C1-C2	3.70	1.57	1.52
7	h	1	NAG	O4-C4	3.39	1.51	1.43
9	l	3	MAN	O2-C2	3.28	1.50	1.43
9	i	3	MAN	C2-C3	3.21	1.57	1.52
7	e	1	NAG	C3-C2	2.95	1.58	1.52
7	h	2	NAG	C1-C2	2.87	1.56	1.52
9	l	1	NAG	C1-C2	2.84	1.56	1.52
6	Z	1	NAG	C2-N2	-2.78	1.41	1.46
7	b	1	NAG	C1-C2	2.68	1.56	1.52
5	o	1	NAG	O4-C4	2.59	1.49	1.43
7	h	1	NAG	C4-C5	2.57	1.58	1.53
10	j	1	NAG	C1-C2	2.55	1.56	1.52
9	i	3	MAN	C6-C5	2.45	1.60	1.51
7	h	1	NAG	O5-C5	2.42	1.48	1.43
9	l	1	NAG	O4-C4	2.40	1.48	1.43
8	g	5	MAN	O5-C1	-2.38	1.39	1.43
5	k	4	MAN	C2-C3	2.37	1.56	1.52
9	l	4	MAN	C2-C3	2.34	1.56	1.52
5	k	4	MAN	O5-C1	2.31	1.47	1.43
8	g	3	MAN	C2-C3	2.28	1.55	1.52
10	j	1	NAG	O4-C4	2.27	1.48	1.43
5	k	3	MAN	C4-C5	2.26	1.57	1.53
9	i	5	BMA	C4-C3	2.21	1.58	1.52
7	h	2	NAG	C2-N2	2.21	1.50	1.46
5	k	3	MAN	O3-C3	2.21	1.48	1.43
5	X	1	NAG	O4-C4	2.19	1.48	1.43
9	l	3	MAN	C1-C2	2.14	1.57	1.52
7	b	2	NAG	C1-C2	2.13	1.55	1.52
5	k	3	MAN	O5-C5	2.10	1.47	1.43
7	d	1	NAG	O5-C1	-2.09	1.40	1.43
7	e	2	NAG	C1-C2	2.05	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	1	NAG	O4-C4	2.04	1.47	1.43
10	j	1	NAG	C4-C5	2.04	1.57	1.53
5	X	1	NAG	C4-C5	2.02	1.57	1.53
8	g	5	MAN	C2-C3	2.01	1.55	1.52

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	5	MAN	C1-O5-C5	-12.38	95.41	112.19
5	k	4	MAN	C1-O5-C5	8.79	124.11	112.19
10	j	3	MAN	O5-C5-C6	8.13	119.95	107.20
5	p	1	NAG	C1-O5-C5	8.07	123.13	112.19
5	o	4	MAN	C1-O5-C5	7.84	122.81	112.19
9	i	5	BMA	C1-O5-C5	-7.81	101.61	112.19
5	k	3	MAN	O5-C5-C6	7.42	118.84	107.20
6	Z	1	NAG	C1-C2-N2	-7.28	98.05	110.49
6	Z	3	MAN	C1-C2-C3	7.08	118.37	109.67
5	k	1	NAG	C1-O5-C5	6.93	121.58	112.19
8	g	3	MAN	C1-C2-C3	6.86	118.09	109.67
9	i	5	BMA	O5-C5-C4	6.71	127.16	110.83
7	m	1	NAG	C1-O5-C5	6.35	120.80	112.19
10	j	3	MAN	C1-C2-C3	5.89	116.91	109.67
7	h	2	NAG	C2-N2-C7	5.86	131.25	122.90
5	k	4	MAN	C1-C2-C3	5.79	116.78	109.67
9	i	3	MAN	C1-C2-C3	5.74	116.72	109.67
9	l	1	NAG	C1-C2-N2	5.47	119.83	110.49
5	k	1	NAG	O5-C1-C2	5.22	119.53	111.29
7	d	1	NAG	C1-O5-C5	5.17	119.19	112.19
7	n	2	NAG	C1-O5-C5	5.07	119.06	112.19
5	k	3	MAN	C6-C5-C4	-5.06	101.16	113.00
5	X	3	MAN	C1-C2-C3	5.05	115.88	109.67
7	e	1	NAG	C4-C3-C2	4.99	118.33	111.02
5	k	3	MAN	C1-C2-C3	4.80	115.57	109.67
7	c	1	NAG	C3-C4-C5	4.71	118.64	110.24
7	h	1	NAG	C1-O5-C5	4.71	118.57	112.19
7	e	2	NAG	O5-C5-C6	4.65	114.49	107.20
5	o	4	MAN	O5-C1-C2	4.65	117.95	110.77
5	X	3	MAN	O6-C6-C5	-4.63	95.40	111.29
5	X	2	NAG	C1-C2-N2	-4.63	102.58	110.49
7	c	1	NAG	C1-O5-C5	4.55	118.36	112.19
8	g	1	NAG	C1-O5-C5	4.53	118.34	112.19
5	k	3	MAN	C1-O5-C5	4.52	118.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	m	2	NAG	C1-C2-N2	-4.44	102.90	110.49
9	i	1	NAG	O5-C5-C6	4.43	114.15	107.20
9	l	4	MAN	C2-C3-C4	4.42	118.55	110.89
9	l	2	NAG	C4-C3-C2	4.39	117.44	111.02
9	l	1	NAG	C1-O5-C5	4.38	118.12	112.19
5	k	1	NAG	C3-C4-C5	4.33	117.97	110.24
9	i	2	NAG	C4-C3-C2	4.31	117.33	111.02
7	f	2	NAG	C1-C2-N2	-4.26	103.22	110.49
10	j	1	NAG	O5-C1-C2	-4.26	104.57	111.29
5	X	4	MAN	C1-O5-C5	4.25	117.95	112.19
9	i	3	MAN	C6-C5-C4	4.24	122.94	113.00
9	i	3	MAN	C2-C3-C4	4.23	118.21	110.89
9	l	4	MAN	C1-C2-C3	4.21	114.84	109.67
7	h	2	NAG	O5-C5-C6	4.18	113.76	107.20
5	o	2	NAG	C1-O5-C5	4.13	117.79	112.19
9	i	5	BMA	O4-C4-C3	-4.08	100.92	110.35
7	h	1	NAG	O5-C5-C4	4.07	120.74	110.83
5	k	3	MAN	O6-C6-C5	-4.05	97.38	111.29
7	d	2	NAG	C4-C3-C2	4.05	116.95	111.02
6	Z	1	NAG	O7-C7-C8	4.04	129.57	122.06
10	j	1	NAG	C3-C4-C5	4.02	117.41	110.24
10	j	2	NAG	C1-C2-N2	-3.94	103.75	110.49
8	g	5	MAN	O5-C5-C4	-3.93	101.27	110.83
9	l	3	MAN	O2-C2-C1	3.93	117.19	109.15
8	g	2	NAG	C4-C3-C2	3.92	116.76	111.02
7	f	1	NAG	C1-O5-C5	3.90	117.47	112.19
6	Z	1	NAG	C8-C7-N2	-3.85	109.58	116.10
7	a	2	NAG	C1-O5-C5	3.84	117.40	112.19
5	o	3	MAN	O5-C5-C6	3.84	113.22	107.20
10	j	4	BMA	C6-C5-C4	-3.74	104.24	113.00
5	k	1	NAG	O4-C4-C3	-3.71	101.76	110.35
5	o	1	NAG	O5-C1-C2	-3.71	105.43	111.29
7	n	1	NAG	C4-C3-C2	3.67	116.39	111.02
5	X	2	NAG	O4-C4-C5	3.66	118.39	109.30
5	o	2	NAG	C4-C3-C2	3.66	116.38	111.02
7	e	2	NAG	C2-N2-C7	3.63	128.08	122.90
10	j	3	MAN	O4-C4-C5	-3.63	100.28	109.30
5	o	1	NAG	C3-C4-C5	3.62	116.70	110.24
7	n	1	NAG	C2-N2-C7	3.59	128.01	122.90
8	g	4	MAN	C1-C2-C3	3.57	114.06	109.67
9	i	1	NAG	C2-N2-C7	3.55	127.96	122.90
7	a	2	NAG	C2-N2-C7	3.53	127.93	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	o	3	MAN	C1-C2-C3	3.43	113.88	109.67
5	k	4	MAN	O5-C5-C6	3.41	112.56	107.20
7	m	2	NAG	C4-C3-C2	3.41	116.02	111.02
5	X	2	NAG	O4-C4-C3	-3.41	102.47	110.35
9	i	2	NAG	C3-C4-C5	3.38	116.26	110.24
8	g	2	NAG	C1-C2-N2	-3.36	104.74	110.49
9	l	2	NAG	O4-C4-C5	3.33	117.55	109.30
9	l	1	NAG	C4-C3-C2	3.32	115.88	111.02
7	c	2	NAG	C3-C4-C5	3.30	116.12	110.24
9	i	1	NAG	O5-C1-C2	3.28	116.47	111.29
5	X	1	NAG	C3-C4-C5	3.28	116.08	110.24
7	b	2	NAG	O5-C5-C6	3.26	112.31	107.20
5	k	1	NAG	O5-C5-C6	-3.20	102.19	107.20
5	X	2	NAG	C2-N2-C7	3.18	127.43	122.90
8	g	2	NAG	O4-C4-C5	3.16	117.14	109.30
9	i	4	MAN	C1-C2-C3	3.15	113.54	109.67
9	l	3	MAN	O5-C5-C6	-3.13	102.30	107.20
6	Z	2	NAG	C4-C3-C2	3.12	115.58	111.02
7	e	2	NAG	O5-C1-C2	3.08	116.16	111.29
8	g	1	NAG	C2-N2-C7	-3.08	118.52	122.90
10	j	2	NAG	C1-O5-C5	-3.08	108.02	112.19
10	j	3	MAN	O5-C5-C4	-3.08	103.34	110.83
7	b	2	NAG	C4-C3-C2	3.06	115.50	111.02
5	k	3	MAN	C3-C4-C5	3.05	115.68	110.24
6	Z	3	MAN	C1-O5-C5	3.04	116.32	112.19
5	p	3	MAN	C1-C2-C3	3.00	113.35	109.67
9	i	5	BMA	O6-C6-C5	3.00	121.58	111.29
9	i	4	MAN	C1-O5-C5	3.00	116.25	112.19
5	o	1	NAG	C8-C7-N2	-2.99	111.04	116.10
9	i	2	NAG	C1-C2-N2	-2.97	105.42	110.49
7	m	2	NAG	O5-C5-C6	2.96	111.84	107.20
9	l	4	MAN	O5-C5-C6	2.95	111.83	107.20
8	g	5	MAN	O5-C5-C6	2.95	111.82	107.20
8	g	3	MAN	C1-O5-C5	2.94	116.17	112.19
5	k	2	NAG	O5-C5-C6	2.91	111.77	107.20
9	i	4	MAN	O5-C5-C6	2.91	111.76	107.20
5	p	2	NAG	C1-O5-C5	2.84	116.03	112.19
8	g	1	NAG	O5-C1-C2	-2.83	106.82	111.29
7	h	1	NAG	C2-N2-C7	2.83	126.93	122.90
7	e	1	NAG	O5-C5-C4	-2.79	104.04	110.83
5	X	2	NAG	O3-C3-C2	2.75	115.16	109.47
9	i	5	BMA	C1-C2-C3	2.72	113.01	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	4	MAN	O2-C2-C1	-2.72	103.59	109.15
7	e	2	NAG	O5-C5-C4	-2.67	104.34	110.83
8	g	3	MAN	O5-C5-C4	-2.67	104.34	110.83
7	c	1	NAG	O5-C5-C6	2.66	111.37	107.20
7	h	2	NAG	C1-C2-N2	2.66	115.03	110.49
9	i	3	MAN	O5-C5-C4	-2.65	104.37	110.83
10	j	4	BMA	C3-C4-C5	2.65	114.96	110.24
6	Z	3	MAN	C2-C3-C4	2.64	115.46	110.89
5	k	2	NAG	C3-C4-C5	2.63	114.94	110.24
7	n	1	NAG	C3-C4-C5	2.63	114.92	110.24
10	j	1	NAG	O4-C4-C3	-2.63	104.28	110.35
8	g	3	MAN	C2-C3-C4	2.62	115.43	110.89
5	k	1	NAG	O5-C5-C4	2.61	117.17	110.83
7	b	1	NAG	C2-N2-C7	2.61	126.61	122.90
5	k	1	NAG	C2-N2-C7	2.60	126.61	122.90
9	l	2	NAG	C1-C2-N2	-2.60	106.04	110.49
8	g	2	NAG	O3-C3-C2	-2.60	104.09	109.47
7	h	1	NAG	O5-C5-C6	-2.57	103.18	107.20
10	j	1	NAG	O5-C5-C4	2.56	117.05	110.83
9	i	3	MAN	O2-C2-C1	-2.54	103.96	109.15
7	c	2	NAG	C1-C2-N2	-2.53	106.16	110.49
5	p	4	MAN	C1-O5-C5	2.53	115.62	112.19
9	l	4	MAN	C1-O5-C5	2.51	115.59	112.19
7	f	1	NAG	O5-C1-C2	2.50	115.24	111.29
7	b	2	NAG	C1-C2-N2	-2.50	106.21	110.49
10	j	2	NAG	C2-N2-C7	2.50	126.47	122.90
8	g	4	MAN	C1-O5-C5	2.47	115.55	112.19
6	Z	1	NAG	O3-C3-C4	2.47	116.07	110.35
7	n	1	NAG	C1-O5-C5	2.47	115.54	112.19
10	j	3	MAN	O4-C4-C3	2.47	116.05	110.35
7	d	1	NAG	O4-C4-C3	-2.46	104.67	110.35
5	o	1	NAG	C1-C2-N2	-2.46	106.29	110.49
5	X	4	MAN	O2-C2-C3	2.45	115.04	110.14
8	g	3	MAN	O6-C6-C5	2.45	119.68	111.29
7	n	1	NAG	O3-C3-C4	-2.45	104.70	110.35
8	g	1	NAG	O4-C4-C3	-2.44	104.71	110.35
9	i	2	NAG	O7-C7-C8	-2.44	117.53	122.06
5	X	1	NAG	C2-N2-C7	2.43	126.37	122.90
7	c	1	NAG	C2-N2-C7	2.43	126.37	122.90
7	e	2	NAG	C4-C3-C2	2.43	114.58	111.02
7	m	2	NAG	C1-O5-C5	2.42	115.47	112.19
7	n	1	NAG	O5-C1-C2	-2.40	107.51	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	1	NAG	C2-N2-C7	2.38	126.30	122.90
5	o	2	NAG	C2-N2-C7	2.38	126.29	122.90
5	X	4	MAN	O5-C5-C6	2.37	110.92	107.20
8	g	5	MAN	C1-C2-C3	2.33	112.53	109.67
5	p	2	NAG	C2-N2-C7	2.32	126.21	122.90
5	p	4	MAN	O5-C1-C2	-2.32	107.19	110.77
7	a	2	NAG	C1-C2-N2	-2.32	106.52	110.49
9	i	4	MAN	O5-C1-C2	2.31	114.34	110.77
9	i	1	NAG	C1-C2-N2	-2.31	106.54	110.49
6	Z	1	NAG	C2-N2-C7	-2.29	119.64	122.90
8	g	3	MAN	O5-C5-C6	2.29	110.79	107.20
5	X	1	NAG	O5-C5-C4	2.28	116.37	110.83
9	l	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	k	4	MAN	C3-C4-C5	-2.26	106.21	110.24
5	k	4	MAN	O5-C1-C2	2.24	114.24	110.77
5	k	3	MAN	O5-C5-C4	-2.24	105.37	110.83
9	l	3	MAN	C3-C4-C5	2.24	114.24	110.24
5	k	1	NAG	C1-C2-N2	-2.23	106.68	110.49
6	Z	1	NAG	O3-C3-C2	-2.23	104.86	109.47
5	X	2	NAG	O3-C3-C4	-2.23	105.20	110.35
5	p	2	NAG	O4-C4-C5	2.23	114.82	109.30
6	Z	3	MAN	O5-C5-C6	2.22	110.68	107.20
10	j	4	BMA	C1-C2-C3	2.20	112.37	109.67
9	i	5	BMA	O5-C5-C6	2.17	110.60	107.20
6	Z	1	NAG	O5-C5-C6	2.15	110.58	107.20
5	p	3	MAN	O5-C5-C6	2.15	110.58	107.20
5	k	4	MAN	C6-C5-C4	-2.15	107.97	113.00
7	e	1	NAG	C1-C2-N2	2.15	114.16	110.49
7	f	2	NAG	O5-C5-C6	2.13	110.55	107.20
5	k	3	MAN	O3-C3-C2	-2.12	105.93	109.99
7	d	2	NAG	O5-C5-C6	2.12	110.52	107.20
8	g	2	NAG	C2-N2-C7	-2.12	119.89	122.90
7	e	1	NAG	C6-C5-C4	2.10	117.92	113.00
5	o	3	MAN	O5-C5-C4	-2.09	105.73	110.83
10	j	3	MAN	O5-C1-C2	2.09	114.00	110.77
7	b	2	NAG	C3-C4-C5	2.09	113.97	110.24
10	j	3	MAN	C3-C4-C5	2.09	113.97	110.24
9	l	4	MAN	C3-C4-C5	2.08	113.96	110.24
5	k	2	NAG	C1-C2-N2	-2.08	106.94	110.49
5	k	3	MAN	C2-C3-C4	2.07	114.47	110.89
5	k	2	NAG	O4-C4-C5	-2.06	104.19	109.30
6	Z	1	NAG	C1-O5-C5	2.05	114.97	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	2	NAG	O7-C7-N2	2.05	125.72	121.95
7	a	2	NAG	O3-C3-C2	2.04	113.69	109.47
9	i	1	NAG	O4-C4-C3	-2.03	105.64	110.35
5	o	2	NAG	C3-C4-C5	2.03	113.86	110.24
7	m	2	NAG	C2-N2-C7	2.02	125.78	122.90
9	i	3	MAN	O5-C1-C2	-2.02	107.66	110.77
9	i	2	NAG	O4-C4-C3	-2.01	105.70	110.35
5	k	3	MAN	O3-C3-C4	2.01	114.99	110.35
5	X	4	MAN	O5-C5-C4	-2.01	105.94	110.83
5	X	4	MAN	O3-C3-C2	2.00	113.83	109.99

All (6) chirality outliers are listed below:

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

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	c	2	NAG	O5-C5-C6-O6
9	l	2	NAG	O5-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
5	X	4	MAN	C4-C5-C6-O6
8	g	4	MAN	O5-C5-C6-O6
5	X	3	MAN	O5-C5-C6-O6
8	g	2	NAG	O5-C5-C6-O6
5	k	4	MAN	O5-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
7	c	2	NAG	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
5	p	3	MAN	O5-C5-C6-O6
9	l	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	i	4	MAN	C4-C5-C6-O6
5	X	4	MAN	O5-C5-C6-O6
9	i	1	NAG	C1-C2-N2-C7
7	m	2	NAG	O5-C5-C6-O6
5	o	3	MAN	C4-C5-C6-O6
10	j	3	MAN	C4-C5-C6-O6
7	m	2	NAG	C4-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6
8	g	5	MAN	C4-C5-C6-O6
5	p	3	MAN	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
9	l	1	NAG	C4-C5-C6-O6
10	j	3	MAN	O5-C5-C6-O6
8	g	4	MAN	C4-C5-C6-O6
8	g	2	NAG	C4-C5-C6-O6
5	o	3	MAN	O5-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
7	d	1	NAG	O5-C5-C6-O6
5	X	3	MAN	C4-C5-C6-O6
9	i	4	MAN	O5-C5-C6-O6
7	h	2	NAG	C1-C2-N2-C7
9	l	1	NAG	O5-C5-C6-O6
9	i	5	BMA	O5-C5-C6-O6
10	j	2	NAG	C4-C5-C6-O6
10	j	2	NAG	O5-C5-C6-O6
5	k	4	MAN	C4-C5-C6-O6
7	n	1	NAG	C4-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
7	c	1	NAG	C1-C2-N2-C7
7	e	1	NAG	C1-C2-N2-C7
10	j	4	BMA	O5-C5-C6-O6
5	o	4	MAN	O5-C5-C6-O6
9	l	3	MAN	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
5	o	2	NAG	C4-C5-C6-O6
5	o	1	NAG	C3-C2-N2-C7
7	h	1	NAG	C3-C2-N2-C7
5	o	1	NAG	C4-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
5	X	2	NAG	C1-C2-N2-C7

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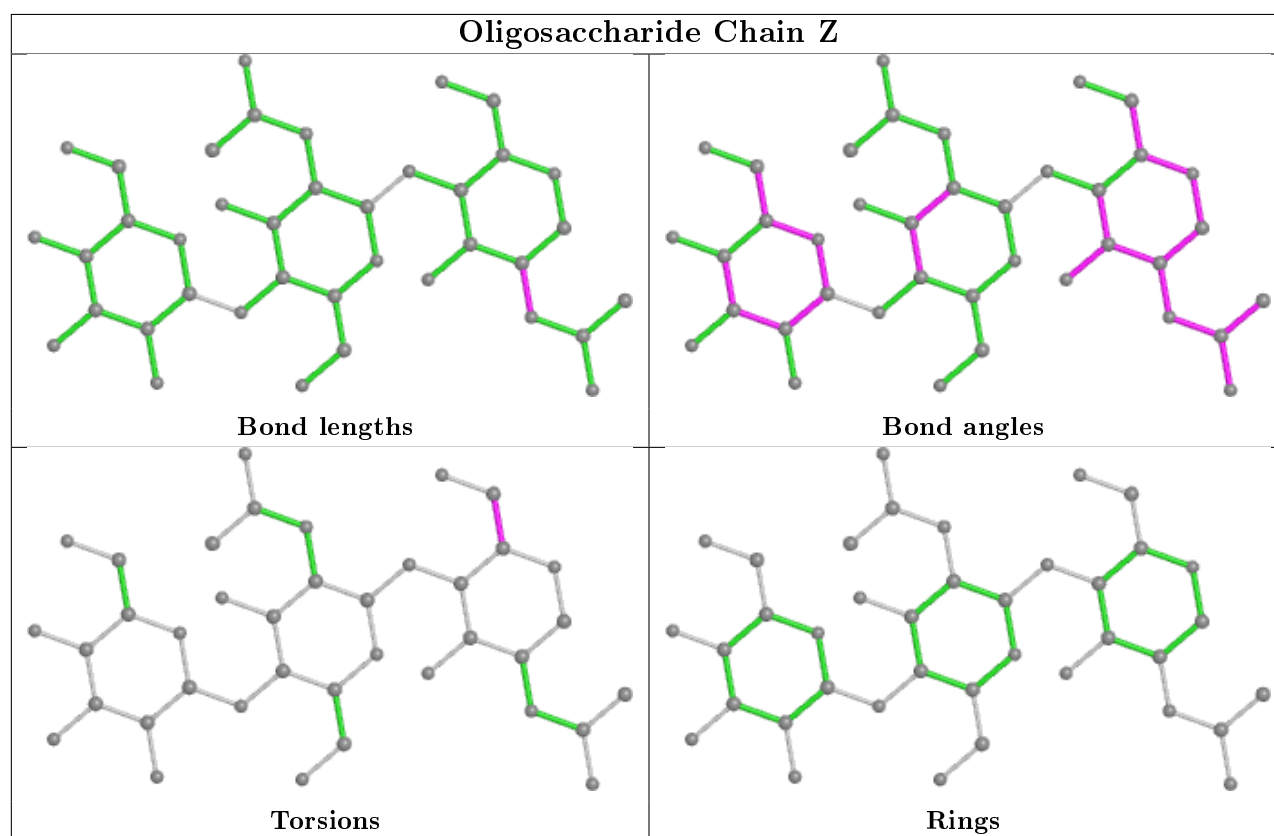
Mol	Chain	Res	Type	Atoms
8	g	5	MAN	O5-C5-C6-O6
5	X	2	NAG	C3-C2-N2-C7
9	i	1	NAG	C3-C2-N2-C7
7	m	1	NAG	O5-C5-C6-O6
7	e	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	K	401	1	14,14,15	1.35	3 (21%)	17,19,21	1.96	5 (29%)
11	NAG	Q	401	-	14,14,15	0.55	0	17,19,21	1.82	3 (17%)
12	BMA	C	301	-	11,11,12	0.56	0	15,15,17	2.05	2 (13%)
11	NAG	E	401	1	14,14,15	0.90	1 (7%)	17,19,21	1.92	3 (17%)
11	NAG	F	201	2	14,14,15	1.04	1 (7%)	17,19,21	1.66	3 (17%)
11	NAG	K	409	1	14,14,15	0.85	0	17,19,21	1.83	3 (17%)
11	NAG	G	401	1	14,14,15	0.83	0	17,19,21	1.08	1 (5%)
11	NAG	S	409	1	14,14,15	1.10	1 (7%)	17,19,21	1.48	2 (11%)
11	NAG	A	401	1	14,14,15	1.59	3 (21%)	17,19,21	2.41	6 (35%)
11	NAG	G	402	1	14,14,15	0.92	0	17,19,21	2.41	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	K	401	1	-	2/6/23/26	0/1/1/1
11	NAG	Q	401	-	-	2/6/23/26	0/1/1/1
12	BMA	C	301	-	-	2/2/19/22	0/1/1/1
11	NAG	E	401	1	-	0/6/23/26	0/1/1/1
11	NAG	F	201	2	1/1/5/7	2/6/23/26	0/1/1/1
11	NAG	K	409	1	-	0/6/23/26	0/1/1/1
11	NAG	G	401	1	1/1/5/7	2/6/23/26	0/1/1/1
11	NAG	S	409	1	-	2/6/23/26	0/1/1/1
11	NAG	A	401	1	-	2/6/23/26	0/1/1/1
11	NAG	G	402	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	401	NAG	C1-C2	4.28	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	201	NAG	C1-C2	3.37	1.57	1.52
11	A	401	NAG	C2-N2	2.84	1.51	1.46
11	K	401	NAG	C2-N2	2.74	1.51	1.46
11	K	401	NAG	C1-C2	2.64	1.56	1.52
11	E	401	NAG	C1-C2	2.53	1.56	1.52
11	K	401	NAG	C3-C2	2.39	1.57	1.52
11	A	401	NAG	C3-C2	2.15	1.57	1.52
11	S	409	NAG	C1-C2	2.09	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	402	NAG	C1-O5-C5	7.37	122.18	112.19
11	E	401	NAG	C1-O5-C5	5.79	120.03	112.19
11	K	401	NAG	C2-N2-C7	5.70	131.02	122.90
11	K	409	NAG	C1-O5-C5	5.57	119.74	112.19
11	A	401	NAG	C2-N2-C7	5.50	130.74	122.90
12	C	301	BMA	C1-O5-C5	5.45	119.58	112.19
11	Q	401	NAG	C4-C3-C2	4.68	117.88	111.02
11	F	201	NAG	O5-C1-C2	4.67	118.66	111.29
11	A	401	NAG	C1-O5-C5	4.57	118.39	112.19
12	C	301	BMA	C1-C2-C3	4.52	115.22	109.67
11	S	409	NAG	C1-C2-N2	-3.68	104.21	110.49
11	G	401	NAG	C1-O5-C5	3.64	117.13	112.19
11	G	402	NAG	O5-C1-C2	3.58	116.94	111.29
11	Q	401	NAG	C3-C4-C5	3.56	116.59	110.24
11	G	402	NAG	C1-C2-N2	-3.37	104.72	110.49
11	F	201	NAG	O5-C5-C6	3.17	112.17	107.20
11	A	401	NAG	O5-C1-C2	3.00	116.03	111.29
11	A	401	NAG	C4-C3-C2	2.91	115.28	111.02
11	A	401	NAG	C1-C2-N2	2.90	115.44	110.49
11	G	402	NAG	C2-N2-C7	2.88	127.00	122.90
11	S	409	NAG	C2-N2-C7	2.70	126.75	122.90
11	K	401	NAG	C4-C3-C2	2.56	114.77	111.02
11	K	401	NAG	O3-C3-C2	2.48	114.60	109.47
11	Q	401	NAG	O5-C1-C2	-2.47	107.39	111.29
11	E	401	NAG	O5-C5-C4	2.43	116.73	110.83
11	G	402	NAG	C3-C4-C5	2.40	114.52	110.24
11	E	401	NAG	O5-C5-C6	-2.35	103.52	107.20
11	A	401	NAG	O5-C5-C4	-2.35	105.12	110.83
11	K	401	NAG	C3-C4-C5	2.30	114.35	110.24
11	K	409	NAG	C1-C2-N2	-2.28	106.59	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	409	NAG	O4-C4-C5	2.16	114.66	109.30
11	F	201	NAG	C3-C4-C5	-2.13	106.44	110.24
11	K	401	NAG	O7-C7-C8	-2.13	118.10	122.06

All (2) chirality outliers are listed below:

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

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	301	BMA	O5-C5-C6-O6
12	C	301	BMA	C4-C5-C6-O6
11	G	401	NAG	O5-C5-C6-O6
11	G	402	NAG	C4-C5-C6-O6
11	G	402	NAG	O5-C5-C6-O6
11	Q	401	NAG	O5-C5-C6-O6
11	K	401	NAG	O5-C5-C6-O6
11	Q	401	NAG	C4-C5-C6-O6
11	S	409	NAG	O5-C5-C6-O6
11	G	401	NAG	C4-C5-C6-O6
11	F	201	NAG	O5-C5-C6-O6
11	A	401	NAG	C4-C5-C6-O6
11	K	401	NAG	C4-C5-C6-O6
11	A	401	NAG	O5-C5-C6-O6
11	S	409	NAG	C4-C5-C6-O6
11	F	201	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	321/330 (97%)	0.41	20 (6%) 20 17	1, 43, 128, 182	0
1	E	321/330 (97%)	0.53	21 (6%) 18 15	1, 56, 147, 233	0
1	G	321/330 (97%)	0.24	6 (1%) 66 58	1, 38, 98, 145	0
1	K	321/330 (97%)	0.18	6 (1%) 66 58	1, 28, 91, 189	0
1	Q	321/330 (97%)	0.11	6 (1%) 66 58	1, 31, 107, 145	0
1	S	321/330 (97%)	0.52	22 (6%) 16 13	1, 52, 111, 147	0
2	B	174/181 (96%)	0.20	9 (5%) 27 24	1, 13, 112, 137	0
2	F	175/181 (96%)	-0.07	0 100 100	1, 10, 104, 172	0
2	H	175/181 (96%)	0.24	11 (6%) 20 16	1, 37, 138, 210	0
2	L	175/181 (96%)	0.25	12 (6%) 16 13	1, 27, 138, 185	0
2	R	175/181 (96%)	0.06	4 (2%) 60 51	1, 20, 112, 164	0
2	T	175/181 (96%)	0.08	2 (1%) 80 73	1, 13, 115, 164	0
3	C	214/221 (96%)	0.42	17 (7%) 12 11	1, 31, 145, 197	0
3	I	214/221 (96%)	1.47	56 (26%) 0 0	11, 115, 242, 317	0
3	M	214/221 (96%)	1.06	43 (20%) 1 1	1, 64, 214, 295	0
3	O	214/221 (96%)	0.51	19 (8%) 9 8	1, 37, 120, 166	0
3	V	214/221 (96%)	0.79	22 (10%) 6 6	1, 63, 144, 180	0
3	Y	214/221 (96%)	1.68	63 (29%) 0 0	1, 97, 270, 367	0
4	D	214/215 (99%)	0.40	7 (3%) 46 37	1, 48, 131, 162	0
4	J	214/215 (99%)	1.91	81 (37%) 0 0	59, 137, 196, 270	0
4	N	214/215 (99%)	0.68	21 (9%) 7 7	1, 40, 173, 230	0
4	P	213/215 (99%)	0.22	3 (1%) 75 66	1, 44, 83, 111	0
4	U	214/215 (99%)	2.37	102 (47%) 0 0	60, 167, 283, 360	0
4	W	214/215 (99%)	0.59	18 (8%) 11 10	1, 42, 149, 189	0

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

All (571) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	214	VAL	12.0
4	U	136	LEU	11.3
3	I	134	SER	10.8
4	J	134	CYS	8.6
4	U	214	CYS	8.3
3	Y	200	THR	8.1
4	J	120	PRO	7.6
3	Y	179	SER	7.4
4	J	116	PHE	7.4
3	Y	215	ASP	7.2
3	Y	133	PRO	7.2
3	M	215	ASP	7.1
4	J	119	PRO	7.0
3	I	130	PRO	6.7
4	J	117	ILE	6.6
4	U	143	GLU	6.6
3	Y	190	THR	6.6
4	U	144	ALA	6.5
4	U	113	PRO	6.5
4	U	174	SER	6.5
4	U	147	GLN	6.5
4	U	197	THR	6.5
3	I	204	ASN	6.5
4	J	152	ASN	6.4
3	C	130	PRO	6.4
3	I	205	VAL	6.1
3	Y	187	SER	6.1
4	U	213	GLU	6.1
3	Y	180	SER	6.0
3	O	130	PRO	5.8
3	V	135	SER	5.8
4	U	157	GLY	5.8
3	Y	127	SER	5.7
1	E	154	ASN	5.7
3	Y	188	VAL	5.7
4	U	212	GLY	5.6
4	U	177	SER	5.6

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Mol	Chain	Res	Type	RSRZ
4	U	175	LEU	5.5
4	U	173	TYR	5.5
4	J	115	VAL	5.4
3	Y	132	ALA	5.4
4	U	182	SER	5.4
3	Y	212	THR	5.4
4	J	147	GLN	5.3
3	M	214	VAL	5.3
4	U	146	VAL	5.2
3	V	130	PRO	5.2
3	M	180	SER	5.2
4	U	178	THR	5.2
4	U	134	CYS	5.2
3	Y	151	ASP	5.1
4	J	100	GLN	5.1
4	J	102	THR	5.1
3	I	187	SER	5.0
3	Y	197	GLY	5.0
4	U	115	VAL	5.0
4	U	135	LEU	5.0
4	N	214	CYS	5.0
3	Y	217	LYS	5.0
3	Y	198	THR	5.0
3	Y	201	TYR	5.0
4	U	155	GLN	5.0
2	L	141	TYR	5.0
3	C	134	SER	4.9
4	J	137	ASN	4.9
4	J	206	THR	4.9
3	Y	135	SER	4.9
3	I	217	LYS	4.8
4	J	114	SER	4.8
4	U	204	PRO	4.8
4	J	192	TYR	4.8
3	I	190	THR	4.8
3	V	134	SER	4.7
4	U	148	TRP	4.7
1	A	154	ASN	4.7
3	Y	205	VAL	4.7
4	J	101	GLY	4.7
4	J	132	VAL	4.7
3	O	215	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
3	M	197	GLY	4.6
3	M	130	PRO	4.5
4	J	76	SER	4.5
4	U	62	PHE	4.5
1	A	126	GLU	4.5
3	Y	126	PRO	4.5
3	I	135	SER	4.4
4	J	136	LEU	4.4
4	J	153	ALA	4.4
1	A	151	ILE	4.4
3	M	219	GLU	4.4
3	V	200	THR	4.4
4	W	152	ASN	4.4
1	E	221	GLY	4.4
3	I	141	GLY	4.3
4	J	86	TYR	4.3
3	C	132	ALA	4.3
4	W	111	ALA	4.2
3	I	188	VAL	4.2
3	Y	134	SER	4.2
4	U	161	GLU	4.2
4	U	200	GLY	4.2
3	I	146	GLY	4.2
4	U	63	SER	4.2
4	U	158	ASN	4.2
3	Y	147	CYS	4.2
4	N	194	CYS	4.2
4	U	117	ILE	4.2
2	H	175	SER	4.2
4	J	99	GLY	4.2
4	U	162	SER	4.2
1	A	155	SER	4.1
4	J	178	THR	4.1
4	U	180	THR	4.0
3	I	197	GLY	4.0
4	J	84	ALA	4.0
3	Y	144	ALA	4.0
4	W	197	THR	4.0
1	G	1	ASP	4.0
4	W	131	SER	4.0
4	J	179	LEU	3.9
4	U	35	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
4	U	206	THR	3.9
3	I	142	THR	3.9
4	U	12	SER	3.9
3	M	128	VAL	3.9
4	U	154	LEU	3.8
3	Y	199	GLN	3.8
4	U	102	THR	3.8
4	J	82	ASP	3.8
4	U	194	CYS	3.8
3	M	216	LYS	3.8
3	Y	219	GLU	3.8
4	U	114	SER	3.8
4	J	177	SER	3.8
4	U	137	ASN	3.8
4	N	206	THR	3.8
3	I	119	SER	3.7
3	I	216	LYS	3.7
3	I	209	PRO	3.7
3	I	215	ASP	3.7
4	U	207	LYS	3.7
3	M	127	SER	3.7
3	V	160	SER	3.7
2	B	141	TYR	3.7
3	C	135	SER	3.7
3	M	132	ALA	3.7
4	U	208	SER	3.7
3	I	145	LEU	3.7
3	M	141	GLY	3.6
4	J	176	SER	3.6
4	U	156	SER	3.6
3	I	214	VAL	3.6
2	B	168	LEU	3.6
3	I	196	LEU	3.6
3	O	217	LYS	3.6
2	L	175	SER	3.6
3	Y	122	SER	3.6
4	U	132	VAL	3.6
3	V	214	VAL	3.6
3	Y	172	THR	3.6
1	G	93	GLY	3.5
3	Y	169	GLY	3.5
3	M	191	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
4	J	154	LEU	3.5
3	I	148	LEU	3.5
3	I	131	LEU	3.5
3	O	221	LYS	3.5
4	U	195	GLU	3.5
4	J	189	HIS	3.5
4	N	120	PRO	3.4
3	I	120	SER	3.4
4	J	208	SER	3.4
3	I	219	GLU	3.4
4	U	153	ALA	3.4
4	U	20	THR	3.4
3	C	133	PRO	3.4
3	V	147	CYS	3.4
3	Y	143	ALA	3.4
4	J	156	SER	3.4
4	U	196	VAL	3.4
4	J	38	GLN	3.4
3	I	203	CYS	3.4
3	I	124	LYS	3.4
4	D	214	CYS	3.4
4	U	37	GLN	3.3
3	M	200	THR	3.3
3	O	200	THR	3.3
1	E	90	CYS	3.3
4	J	155	GLN	3.3
4	J	146	VAL	3.3
3	I	195	SER	3.3
4	J	121	SER	3.3
4	U	107	LYS	3.3
4	J	144	ALA	3.3
1	A	152	LYS	3.2
4	J	62	PHE	3.2
4	P	121	SER	3.2
3	Y	216	LYS	3.2
3	Y	10	GLU	3.2
4	U	120	PRO	3.2
4	J	148	TRP	3.2
3	I	122	SER	3.2
4	U	119	PRO	3.2
4	N	148	TRP	3.2
4	J	75	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	1	ASP	3.2
4	U	183	LYS	3.2
1	E	133	SER	3.1
2	H	19	ASP	3.1
3	M	192	PRO	3.1
3	M	131	LEU	3.1
4	U	9	GLY	3.1
3	Y	202	ILE	3.1
1	A	149	TRP	3.1
4	P	214	CYS	3.1
3	I	179	SER	3.1
1	S	90	CYS	3.1
3	I	220	PRO	3.1
3	M	147	CYS	3.1
1	A	188	THR	3.1
1	E	136	PRO	3.1
4	J	186	TYR	3.1
1	A	131	VAL	3.1
4	W	212	GLY	3.1
3	Y	195	SER	3.1
4	N	184	ALA	3.1
4	J	207	LYS	3.1
4	U	171	SER	3.1
3	C	219	GLU	3.1
4	W	208	SER	3.1
4	J	18	ARG	3.1
3	I	125	GLY	3.1
3	M	124	LYS	3.1
3	Y	146	GLY	3.1
3	Y	206	ASN	3.1
4	U	145	LYS	3.1
2	T	175	SER	3.1
3	I	107	HIS	3.0
2	H	29	GLU	3.0
4	J	135	LEU	3.0
4	U	139	PHE	3.0
3	Y	171	HIS	3.0
4	U	176	SER	3.0
3	I	151	ASP	3.0
3	Y	162	ASN	3.0
4	N	151	ASP	3.0
3	Y	156	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
4	U	202	SER	3.0
4	U	105	GLU	3.0
3	C	215	ASP	3.0
4	U	198	HIS	3.0
4	U	164	THR	3.0
3	M	151	ASP	3.0
3	C	194	SER	3.0
4	J	51	ALA	3.0
3	I	189	VAL	3.0
4	U	210	ASN	3.0
3	M	129	PHE	2.9
1	E	182	ASN	2.9
3	I	128	VAL	2.9
4	U	86	TYR	2.9
2	L	135	ASN	2.9
2	B	140	PHE	2.9
3	I	147	CYS	2.9
4	U	179	LEU	2.9
1	A	54	ASP	2.9
3	M	148	LEU	2.9
1	S	167	THR	2.9
3	I	129	PHE	2.9
4	U	17	GLU	2.9
2	L	27	SER	2.9
3	Y	157	VAL	2.9
4	U	199	GLN	2.9
4	J	78	LEU	2.9
3	O	214	VAL	2.9
3	C	217	LYS	2.9
4	U	38	GLN	2.9
3	M	159	VAL	2.8
4	N	1	GLU	2.8
3	M	196	LEU	2.8
3	M	167	THR	2.8
4	N	134	CYS	2.8
2	B	146	ASN	2.8
4	J	149	LYS	2.8
4	J	214	CYS	2.8
3	C	214	VAL	2.8
4	U	10	THR	2.8
4	W	196	VAL	2.8
2	H	27	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	M	186	SER	2.8
4	J	209	PHE	2.8
4	N	126	LYS	2.8
3	O	213	LYS	2.8
3	Y	196	LEU	2.8
4	U	64	GLY	2.8
2	L	142	HIS	2.8
4	N	152	ASN	2.8
3	Y	186	SER	2.8
4	J	113	PRO	2.8
4	N	212	GLY	2.8
1	E	220	ASN	2.8
3	M	146	GLY	2.8
1	A	129	LEU	2.8
3	C	131	LEU	2.8
3	C	220	PRO	2.7
3	Y	141	GLY	2.7
2	B	129	ASN	2.7
3	Y	145	LEU	2.7
4	J	85	VAL	2.7
4	J	195	GLU	2.7
3	I	218	VAL	2.7
4	N	187	GLU	2.7
1	S	112	GLU	2.7
1	Q	156	THR	2.7
3	I	184	SER	2.7
1	S	46	GLY	2.7
4	U	74	ALA	2.7
2	T	27	SER	2.7
3	C	216	LYS	2.7
2	L	174	SER	2.7
1	E	54	ASP	2.7
4	J	83	PHE	2.7
1	S	91	TYR	2.7
3	Y	13	LYS	2.7
3	M	144	ALA	2.6
3	M	133	PRO	2.6
4	N	195	GLU	2.6
4	W	127	SER	2.6
3	M	163	SER	2.6
1	E	215	THR	2.6
4	U	85	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
4	J	35	TRP	2.6
3	M	122	SER	2.6
4	U	152	ASN	2.6
1	S	128	SER	2.6
4	J	205	VAL	2.6
3	Y	148	LEU	2.6
4	W	128	GLY	2.6
3	V	204	ASN	2.6
4	J	185	ASP	2.6
3	V	215	ASP	2.6
3	Y	213	LYS	2.6
2	L	140	PHE	2.6
1	A	185	ALA	2.6
1	K	244	ASN	2.6
1	K	129	LEU	2.6
3	I	133	PRO	2.6
4	U	88	CYS	2.6
4	J	151	ASP	2.6
3	V	221	LYS	2.6
4	D	192	TYR	2.6
4	J	194	CYS	2.5
3	Y	128	VAL	2.5
3	O	134	SER	2.5
4	U	73	LEU	2.5
4	U	111	ALA	2.5
4	J	181	LEU	2.5
3	M	193	SER	2.5
4	U	165	GLU	2.5
4	J	182	SER	2.5
1	K	150	LEU	2.5
3	V	198	THR	2.5
1	A	133	SER	2.5
3	V	197	GLY	2.5
3	Y	125	GLY	2.5
4	W	112	ALA	2.5
3	Y	168	SER	2.5
1	A	189	LYS	2.5
4	U	51	ALA	2.5
4	J	175	LEU	2.5
1	S	221	GLY	2.5
4	U	29	SER	2.5
4	U	101	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	Y	159	VAL	2.5
4	J	122	ASP	2.5
4	W	155	GLN	2.5
1	E	59	GLY	2.5
3	Y	207	HIS	2.5
4	J	184	ALA	2.5
1	S	276	THR	2.5
2	B	147	GLU	2.5
2	L	131	LYS	2.5
2	H	160	PRO	2.4
1	E	124	SER	2.4
4	N	188	LYS	2.4
3	V	151	ASP	2.4
3	I	144	ALA	2.4
3	I	186	SER	2.4
3	Y	142	THR	2.4
3	O	165	ALA	2.4
2	H	144	CYS	2.4
4	U	23	CYS	2.4
2	R	146	ASN	2.4
3	I	127	SER	2.4
4	U	75	ILE	2.4
1	Q	69	GLU	2.4
3	O	220	PRO	2.4
4	J	202	SER	2.4
1	A	153	LYS	2.4
2	R	29	GLU	2.4
4	J	212	GLY	2.4
3	C	213	LYS	2.4
3	Y	218	VAL	2.4
4	J	20	THR	2.4
4	U	160	GLN	2.4
1	K	188	THR	2.4
3	M	184	SER	2.4
3	Y	66	GLY	2.4
3	I	132	ALA	2.4
3	Y	165	ALA	2.4
1	S	240	ASN	2.4
3	Y	204	ASN	2.4
4	N	196	VAL	2.4
4	U	33	LEU	2.4
4	J	180	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	149	VAL	2.4
3	O	145	LEU	2.4
1	A	190	LEU	2.4
1	S	243	SER	2.4
1	G	2	GLN	2.3
4	D	151	ASP	2.3
4	U	92	GLY	2.3
3	V	162	ASN	2.3
1	Q	155	SER	2.3
4	P	187	GLU	2.3
3	V	163	SER	2.3
2	L	129	ASN	2.3
3	M	134	SER	2.3
1	E	184	ALA	2.3
4	W	145	LYS	2.3
4	J	211	ARG	2.3
1	A	244	ASN	2.3
4	U	36	PHE	2.3
4	U	80	PRO	2.3
3	V	203	CYS	2.3
4	J	61	ARG	2.3
4	U	78	LEU	2.3
3	M	143	ALA	2.3
4	N	147	GLN	2.3
3	Y	158	THR	2.3
1	A	125	HIS	2.3
2	H	174	SER	2.3
4	W	203	SER	2.3
3	M	198	THR	2.3
1	A	122	TRP	2.3
1	G	129	LEU	2.3
1	E	185	ALA	2.3
3	Y	123	THR	2.3
4	J	145	LYS	2.3
4	J	190	LYS	2.3
4	W	156	SER	2.3
4	W	193	ALA	2.3
3	Y	189	VAL	2.3
1	E	91	TYR	2.3
1	S	222	GLN	2.2
2	B	142	HIS	2.3
4	J	150	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	94	ASP	2.2
1	K	115	GLN	2.2
3	I	10	GLU	2.2
3	I	174	PRO	2.2
3	M	194	SER	2.2
4	D	68	GLY	2.2
4	N	207	LYS	2.2
2	L	144	CYS	2.2
3	C	144	ALA	2.2
3	O	147	CYS	2.2
3	V	133	PRO	2.2
1	A	246	ASN	2.2
4	U	201	LEU	2.2
4	U	159	SER	2.2
3	O	201	TYR	2.2
3	M	204	ASN	2.2
3	M	205	VAL	2.2
4	N	132	VAL	2.2
4	J	129	THR	2.2
3	O	218	VAL	2.2
3	O	132	ALA	2.2
4	W	153	ALA	2.2
4	J	27(A)	SER	2.2
4	U	46	LEU	2.2
4	J	36	PHE	2.2
1	S	150	LEU	2.2
4	J	48	ILE	2.2
3	M	217	LYS	2.2
3	I	183	TYR	2.2
2	R	143	LYS	2.2
4	J	7	SER	2.2
1	G	244	ASN	2.2
3	I	114	THR	2.2
4	J	72	THR	2.2
2	H	148	CYS	2.2
3	O	129	PHE	2.2
3	Y	16	SER	2.2
3	O	133	PRO	2.2
4	U	163	VAL	2.2
1	E	141	SER	2.2
3	O	216	LYS	2.2
3	V	209	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	244	ASN	2.2
4	U	185	ASP	2.2
1	E	145	ARG	2.2
3	I	65	GLN	2.1
3	O	126	PRO	2.1
3	M	145	LEU	2.1
4	U	172	THR	2.1
4	U	55	ALA	2.1
4	J	70	ASP	2.1
1	Q	192	GLN	2.1
3	M	199	GLN	2.1
4	U	100	GLN	2.1
1	S	157	TYR	2.1
3	I	60	TYR	2.1
4	U	48	ILE	2.1
2	R	145	ASP	2.1
3	Y	65	GLN	2.1
3	I	94	TYR	2.1
3	V	145	LEU	2.1
3	V	166	LEU	2.1
3	Y	130	PRO	2.1
1	S	75	GLU	2.1
2	H	147	GLU	2.1
3	I	177	LEU	2.1
4	U	7	SER	2.1
4	W	122	ASP	2.1
4	D	186	TYR	2.1
1	E	242	GLU	2.1
4	D	213	GLU	2.1
3	M	168	SER	2.1
4	U	203	SER	2.1
1	E	244	ASN	2.1
3	C	197	GLY	2.1
3	I	108	ASP	2.1
1	E	250	PRO	2.1
1	G	246	ASN	2.1
1	S	154	ASN	2.1
4	U	21	LEU	2.1
4	D	144	ALA	2.1
1	S	163	SER	2.1
1	Q	246	ASN	2.1
2	H	168	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	143	LYS	2.1
1	S	129	LEU	2.1
2	B	150	GLU	2.1
4	U	150	VAL	2.1
2	B	157	TYR	2.1
4	N	127	SER	2.0
1	S	155	SER	2.0
2	L	166	ALA	2.0
1	S	156	THR	2.0
4	U	110	VAL	2.0
4	J	196	VAL	2.0
1	E	251	GLU	2.0
4	J	103	LYS	2.0
1	A	186	GLU	2.0
1	S	179	HIS	2.0
3	V	193	SER	2.0
3	Y	220	PRO	2.0
2	H	128	ASP	2.0
4	W	199	GLN	2.0
1	E	72	ASN	2.0
4	J	193	ALA	2.0
3	V	220	PRO	2.0
1	S	110	HIS	2.0
3	C	200	THR	2.0
3	I	198	THR	2.0
3	M	142	THR	2.0
4	U	84	ALA	2.0
4	N	193	ALA	2.0
3	I	85	SER	2.0
3	M	179	SER	2.0

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, 95th 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.

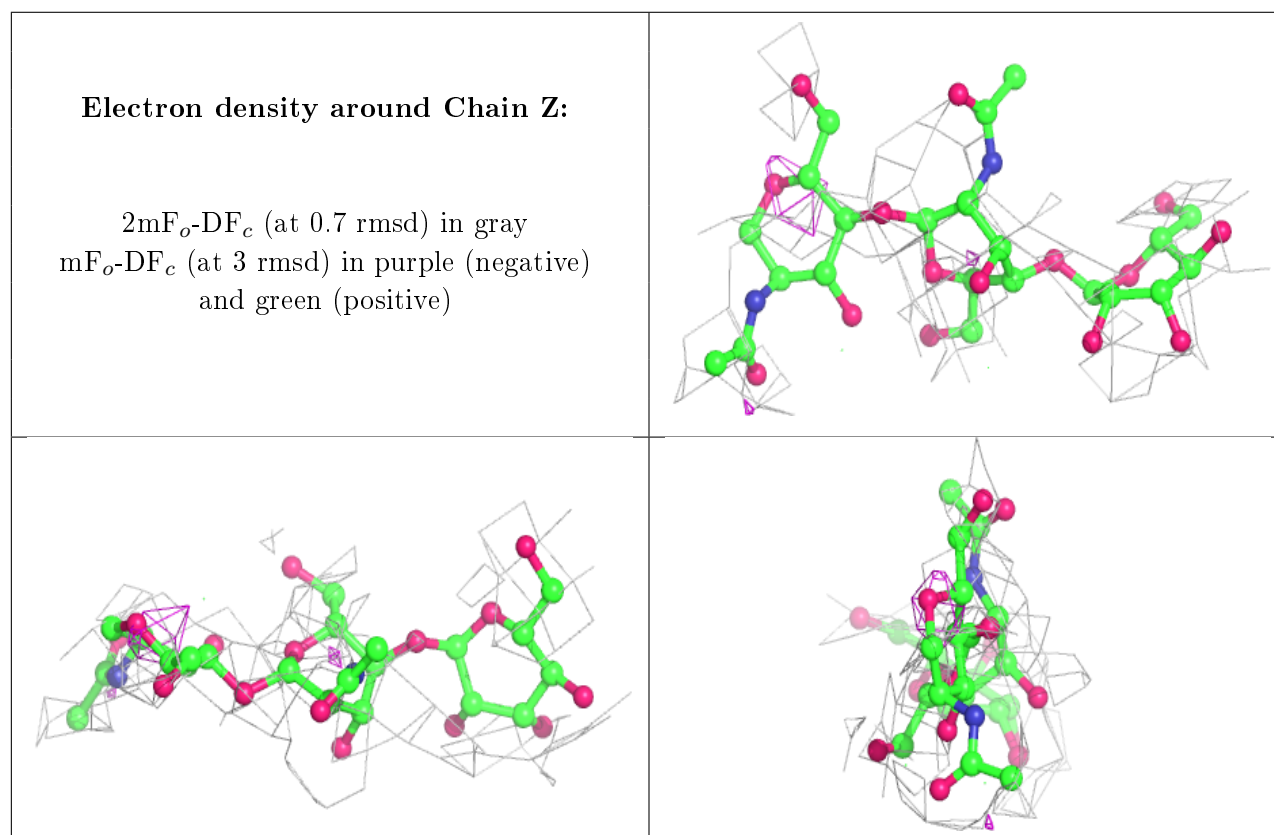
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	p	4	11/12	0.25	0.42	144,166,175,180	0
9	BMA	i	5	11/12	0.30	0.58	141,159,196,214	0
5	MAN	p	3	11/12	0.41	0.43	192,209,219,224	0
5	MAN	k	3	11/12	0.43	0.49	112,143,181,190	0
6	NAG	Z	2	14/15	0.45	0.41	119,137,149,152	0
9	MAN	i	3	11/12	0.55	0.35	87,116,171,202	0
7	NAG	a	2	14/15	0.55	0.51	76,93,102,103	0
5	NAG	p	2	14/15	0.56	0.54	143,181,207,212	0
10	BMA	j	4	11/12	0.57	0.73	154,187,199,204	0
5	MAN	k	4	11/12	0.59	0.42	68,100,120,125	0
9	NAG	i	2	14/15	0.60	0.46	101,113,121,135	0
9	MAN	i	4	11/12	0.61	0.50	90,136,150,174	0
6	NAG	Z	1	14/15	0.62	0.36	83,104,122,138	0
7	NAG	f	1	14/15	0.63	0.38	99,114,121,131	0
7	NAG	n	1	14/15	0.66	0.49	97,118,127,128	0
7	NAG	e	1	14/15	0.66	0.46	52,74,79,80	0
7	NAG	m	2	14/15	0.67	0.50	68,77,89,91	0
10	MAN	j	3	11/12	0.67	0.52	142,151,171,179	0
7	NAG	f	2	14/15	0.67	0.42	128,138,151,171	0
7	NAG	h	2	14/15	0.70	0.49	59,75,80,80	0
6	MAN	Z	3	11/12	0.72	0.30	97,107,115,117	0
10	NAG	j	1	14/15	0.73	0.55	76,106,129,136	0
7	NAG	n	2	14/15	0.73	0.52	82,116,122,125	0
9	NAG	l	2	14/15	0.73	0.43	57,74,83,85	0
5	MAN	o	3	11/12	0.73	0.44	60,87,97,105	0
5	NAG	k	2	14/15	0.74	0.35	82,110,131,138	0
7	NAG	b	2	14/15	0.75	0.54	95,101,108,116	0
5	MAN	o	4	11/12	0.75	0.38	64,84,92,93	0
9	MAN	l	3	11/12	0.76	0.34	54,74,80,84	0
10	NAG	j	2	14/15	0.77	0.66	90,115,129,133	0
7	NAG	a	1	14/15	0.77	0.34	20,42,61,73	0
5	NAG	X	2	14/15	0.77	0.38	30,71,85,86	0
5	MAN	X	4	11/12	0.78	0.48	66,73,88,95	0
5	NAG	p	1	14/15	0.79	0.34	75,81,101,134	0
7	NAG	e	2	14/15	0.80	0.34	53,63,69,70	0
7	NAG	b	1	14/15	0.80	0.41	58,72,83,93	0
5	NAG	X	1	14/15	0.80	0.44	38,48,59,61	0
5	NAG	k	1	14/15	0.81	0.37	69,83,93,97	0
9	NAG	l	1	14/15	0.81	0.34	39,47,66,75	0
8	MAN	g	4	11/12	0.81	0.30	76,83,96,104	0
7	NAG	d	2	14/15	0.82	0.32	32,36,42,44	0
9	BMA	l	5	11/12	0.82	0.35	74,80,92,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MAN	l	4	11/12	0.84	0.38	60,73,77,81	0
8	MAN	g	5	11/12	0.84	0.37	61,68,79,80	0
8	MAN	g	3	11/12	0.84	0.30	64,75,83,84	0
5	MAN	X	3	11/12	0.84	0.29	40,52,71,76	0
9	NAG	i	1	14/15	0.84	0.29	37,63,87,103	0
5	NAG	o	2	14/15	0.84	0.46	67,79,90,101	0
8	NAG	g	1	14/15	0.85	0.29	48,52,59,62	0
8	NAG	g	2	14/15	0.86	0.32	44,54,61,70	0
7	NAG	h	1	14/15	0.87	0.24	19,40,48,56	0
7	NAG	c	2	14/15	0.87	0.25	41,56,61,64	0
5	NAG	o	1	14/15	0.87	0.34	44,56,66,67	0
7	NAG	c	1	14/15	0.89	0.25	32,40,43,47	0
7	NAG	m	1	14/15	0.89	0.28	21,28,35,50	0
7	NAG	d	1	14/15	0.93	0.23	20,29,33,36	0

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
11	NAG	Q	401	14/15	0.53	0.57	91,97,112,116	0
11	NAG	F	201	14/15	0.73	0.46	65,85,92,97	0
11	NAG	K	401	14/15	0.74	0.48	32,48,55,57	0
11	NAG	G	402	14/15	0.77	0.35	25,35,39,40	0
11	NAG	A	401	14/15	0.80	0.35	34,44,48,50	0
11	NAG	G	401	14/15	0.82	0.31	41,63,75,78	0
11	NAG	S	409	14/15	0.82	0.32	18,23,28,31	0
11	NAG	K	409	14/15	0.83	0.34	16,21,39,42	0
12	BMA	C	301	11/12	0.84	0.32	25,30,35,38	0
11	NAG	E	401	14/15	0.86	0.30	24,29,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.