Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 09:58 PM EDT

PDB ID	:	4NM8
Title	:	Crystal structure of broadly neutralizing antibody CR8043 bound to H3 influenza hemagglutinin
Authors	:	Lee, P.S.; Wilson, I.A.
Deposited on	:	2013-11-14
Resolution	:	4.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

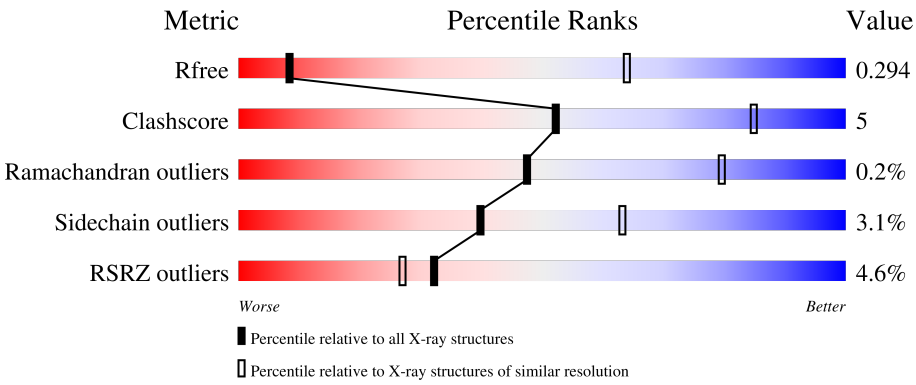
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	323	%, 89%, 9%
1	C	323	%, 90%, 8%
1	E	323	4%, 85%, 13%
2	B	176	%, 84%, 13%
2	D	176	%, 89%, 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	176	87% 10%
3	L	220	11% 78% 20%
3	M	220	10% 77% 20%
3	N	220	9% 80% 17%
4	H	230	7% 74% 18% 7%
4	I	230	3% 73% 15% 8%
4	J	230	9% 73% 18% 7%
5	G	2	100%
5	K	2	50% 50%
5	O	2	50% 50%
5	P	2	50% 50%
5	Q	2	50% 50%
5	R	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	P	2	-	-	-	X
5	NAG	R	2	-	-	-	X
6	NAG	D	201	-	-	-	X
6	NAG	E	503	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2452	1537	431	471	13	0	0	0
1	C	318	2452	1537	431	471	13	0	0	0
1	E	317	2443	1531	429	470	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Hemagglutinin HA2 Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1391	863	243	279	6	0	0	0
2	D	171	1382	858	241	277	6	0	0	0
2	F	171	1382	858	241	277	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	conflict	UNP Q91MA7
D	123	GLY	ARG	conflict	UNP Q91MA7
F	123	GLY	ARG	conflict	UNP Q91MA7

- Molecule 3 is a protein called Antibody CR8043, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	217	1685	1058	282	340	5	0	0	0
3	M	217	1685	1058	282	340	5	0	0	0
3	N	217	1685	1058	282	340	5	0	0	0

- Molecule 4 is a protein called Antibody CR8043, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	215	1621	1024	279	312	6	0	0	0
4	I	211	1601	1012	275	308	6	0	0	0
4	J	213	1613	1020	277	310	6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	217	HIS	-	expression tag	UNP Q6N089
H	218	HIS	-	expression tag	UNP Q6N089
H	219	HIS	-	expression tag	UNP Q6N089
H	220	HIS	-	expression tag	UNP Q6N089
H	221	HIS	-	expression tag	UNP Q6N089
H	222	HIS	-	expression tag	UNP Q6N089
I	217	HIS	-	expression tag	UNP Q6N089
I	218	HIS	-	expression tag	UNP Q6N089
I	219	HIS	-	expression tag	UNP Q6N089
I	220	HIS	-	expression tag	UNP Q6N089
I	221	HIS	-	expression tag	UNP Q6N089
I	222	HIS	-	expression tag	UNP Q6N089
J	217	HIS	-	expression tag	UNP Q6N089
J	218	HIS	-	expression tag	UNP Q6N089

Continued on next page...

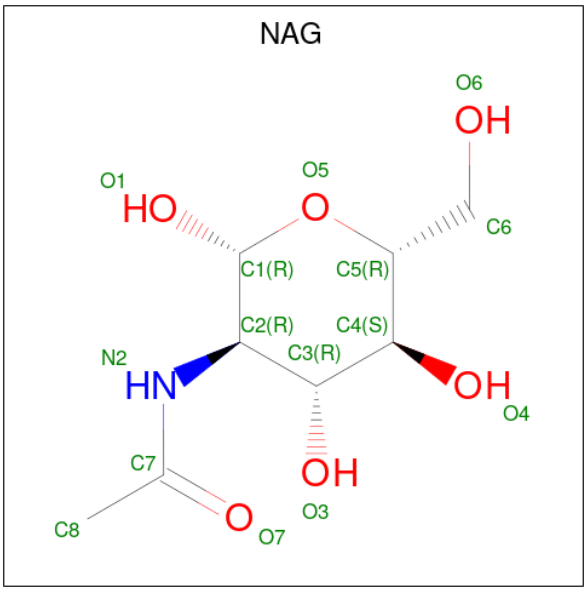
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	219	HIS	-	expression tag	UNP Q6N089
J	220	HIS	-	expression tag	UNP Q6N089
J	221	HIS	-	expression tag	UNP Q6N089
J	222	HIS	-	expression tag	UNP Q6N089

- Molecule 5 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
			Total	C	N	O			
5	G	2	28	16	2	10	0	0	0
5	K	2	28	16	2	10	0	0	0
5	O	2	28	16	2	10	0	0	0
5	P	2	28	16	2	10	0	0	0
5	Q	2	28	16	2	10	0	0	0
5	R	2	28	16	2	10	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

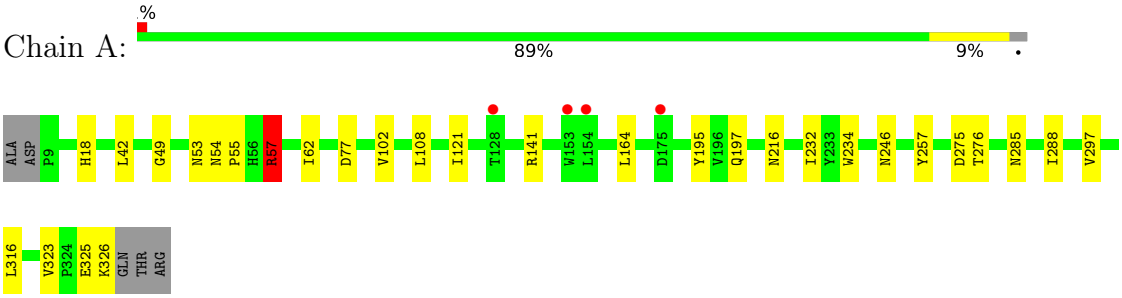


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	C	1	14	8	1	5	0	0
			Total	C	N	O		
6	C	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0
			Total	C	N	O		
6	E	1	14	8	1	5	0	0
			Total	C	N	O		
6	E	1	14	8	1	5	0	0
			Total	C	N	O		
6	E	1	14	8	1	5	0	0
			Total	C	N	O		
6	F	1	14	8	1	5	0	0

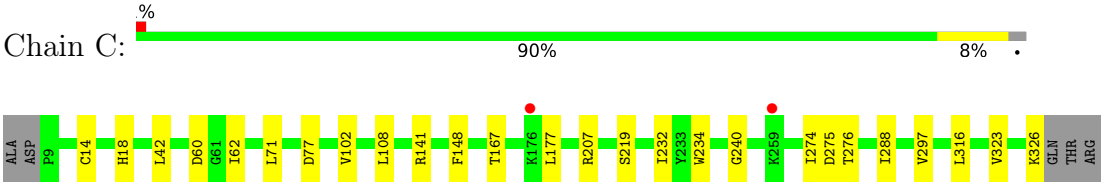
3 Residue-property plots (i)

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

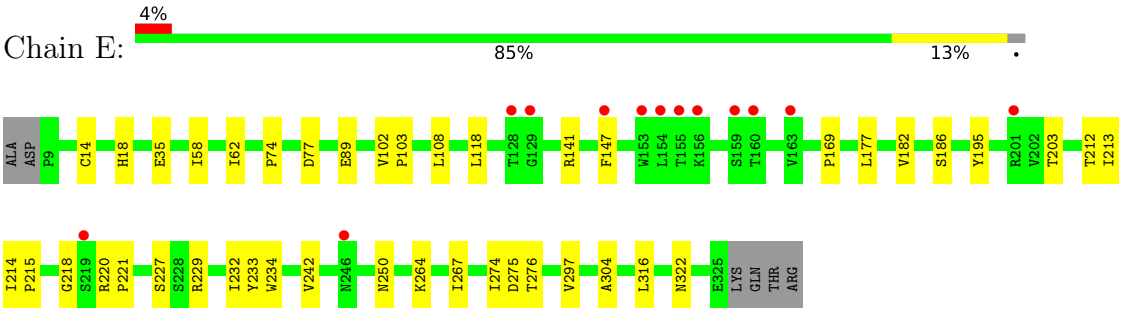
• Molecule 1: Hemagglutinin HA1 Chain



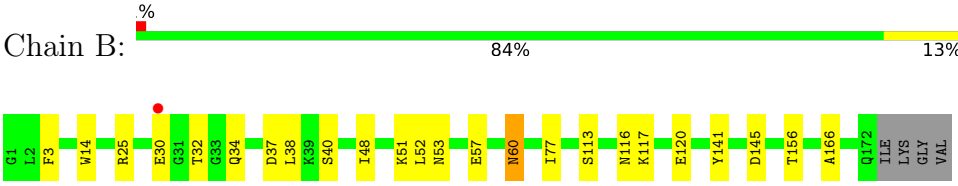
• Molecule 1: Hemagglutinin HA1 Chain



• Molecule 1: Hemagglutinin HA1 Chain

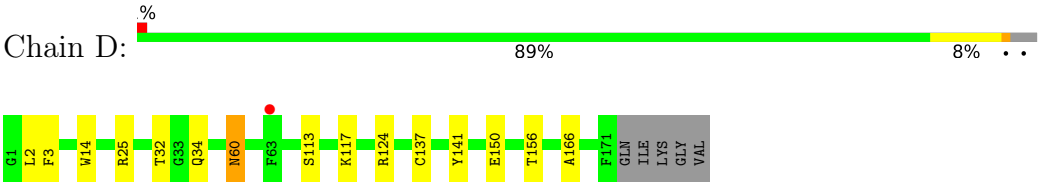


• Molecule 2: Hemagglutinin HA2 Chain



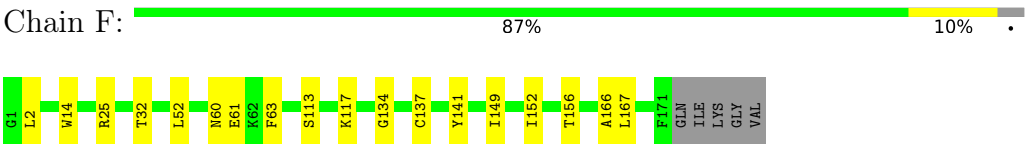
• Molecule 2: Hemagglutinin HA2 Chain

Chain D:



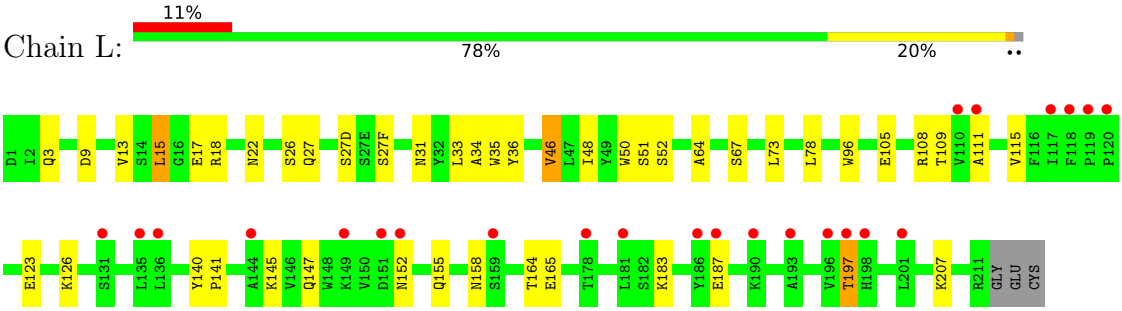
• Molecule 2: Hemagglutinin HA2 Chain

Chain F:



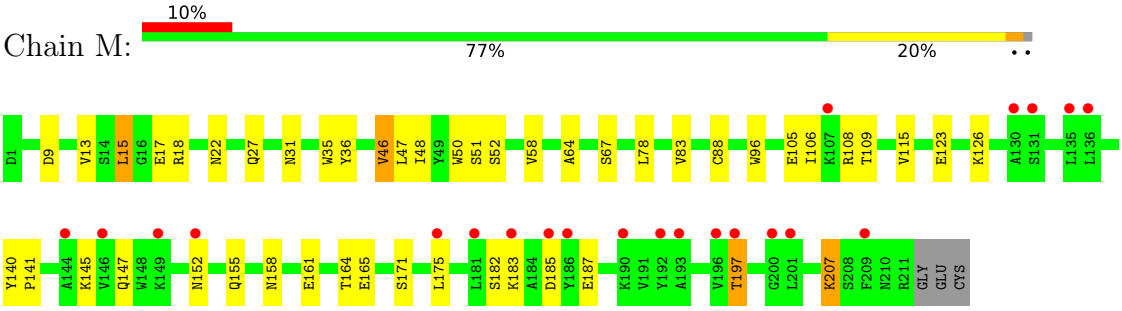
• Molecule 3: Antibody CR8043, Light Chain

Chain L:



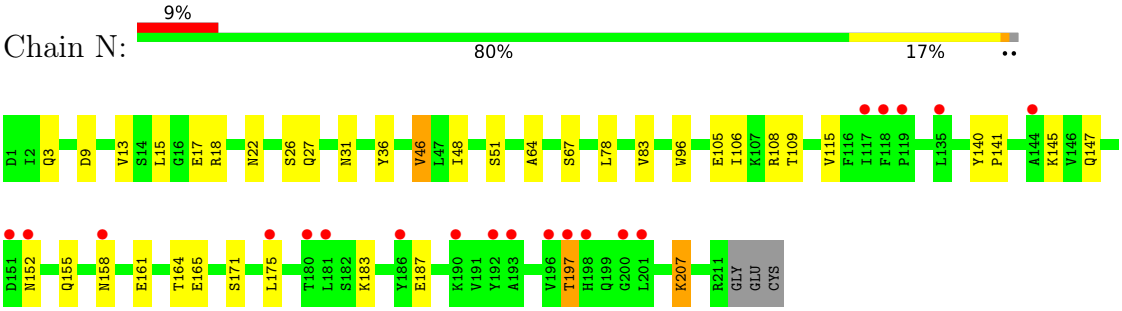
• Molecule 3: Antibody CR8043, Light Chain

Chain M:



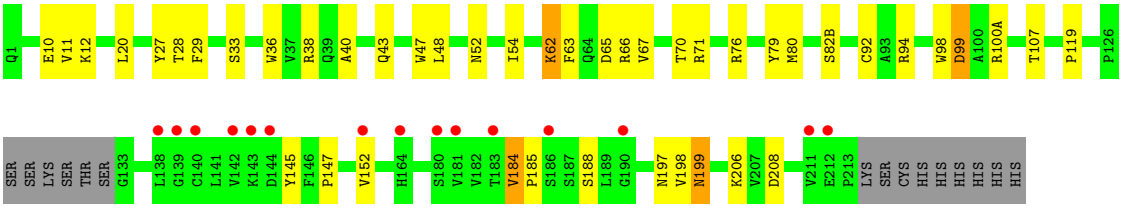
• Molecule 3: Antibody CR8043, Light Chain

Chain N:



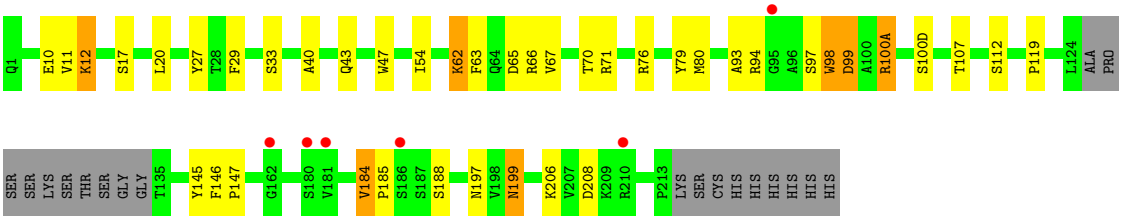
• Molecule 4: Antibody CR8043, Heavy Chain

Chain H:



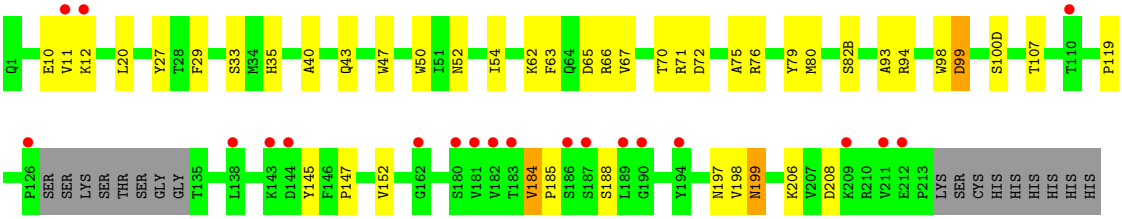
• Molecule 4: Antibody CR8043, Heavy Chain

Chain I:



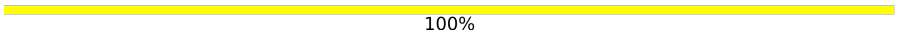
• Molecule 4: Antibody CR8043, Heavy Chain

Chain J:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	241.49Å 142.35Å 170.72Å 90.00° 133.46° 90.00°	Depositor
Resolution (Å)	43.82 – 4.00 46.73 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (43.82-4.00) 97.5 (46.73-4.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.240 , 0.292 0.241 , 0.294	Depositor DCC
R_{free} test set	1733 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	127.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h+2*l,k,-h-l 0.005 for h,-k,-h-l 0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	21672	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.36	0/2509	0.64	1/3418 (0.0%)
1	C	0.35	0/2509	0.61	0/3418
1	E	0.35	0/2500	0.63	0/3407
2	B	0.39	0/1415	0.63	1/1902 (0.1%)
2	D	0.39	0/1406	0.60	0/1890
2	F	0.37	0/1406	0.58	0/1890
3	L	0.32	0/1725	0.59	0/2347
3	M	0.31	0/1725	0.58	0/2347
3	N	0.32	0/1725	0.57	0/2347
4	H	0.34	0/1662	0.59	0/2265
4	I	0.34	0/1641	0.60	0/2236
4	J	0.32	0/1654	0.59	0/2255
All	All	0.35	0/21877	0.60	2/29722 (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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	52	LEU	CB-CG-CD2	-8.17	97.11	111.00
1	A	57	ARG	CG-CD-NE	-5.59	100.06	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2452	0	2404	15	0
1	C	2452	0	2403	15	0
1	E	2443	0	2390	26	0
2	B	1391	0	1306	19	0
2	D	1382	0	1298	21	0
2	F	1382	0	1298	18	0
3	L	1685	0	1627	22	0
3	M	1685	0	1627	23	0
3	N	1685	0	1627	20	0
4	H	1621	0	1588	29	0
4	I	1601	0	1570	28	0
4	J	1613	0	1582	28	0
5	G	28	0	25	0	0
5	K	28	0	25	1	0
5	O	28	0	25	1	0
5	P	28	0	25	1	0
5	Q	28	0	25	1	0
5	R	28	0	25	1	0
6	B	14	0	13	1	0
6	C	28	0	26	1	0
6	D	14	0	13	2	0
6	E	42	0	39	0	0
6	F	14	0	13	1	0
All	All	21672	0	20974	234	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 5.

All (234) 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)
4:I:11:VAL:HG21	4:I:147:PRO:HG3	1.45	0.95
4:H:11:VAL:HG21	4:H:147:PRO:HG3	1.49	0.94
3:N:108:ARG:NH1	3:N:109:THR:O	2.10	0.84
4:J:11:VAL:HG21	4:J:147:PRO:HG3	1.59	0.82
3:L:108:ARG:NH1	3:L:109:THR:O	2.14	0.80
4:H:33:SER:HB3	4:H:98:TRP:HA	1.63	0.79
3:M:108:ARG:NH1	3:M:109:THR:O	2.16	0.78
3:N:13:VAL:HG23	3:N:78:LEU:HD22	1.66	0.78
4:J:199:ASN:HD21	4:J:206:LYS:HE3	1.50	0.76
3:M:13:VAL:HG23	3:M:78:LEU:HD22	1.67	0.74
4:J:33:SER:HB3	4:J:98:TRP:HA	1.69	0.74
4:J:29:PHE:HB2	4:J:76:ARG:HG2	1.72	0.70
2:D:32:THR:HG21	4:I:54:ILE:HD13	1.73	0.69
4:I:199:ASN:HD21	4:I:206:LYS:HE3	1.58	0.69
2:F:32:THR:HG21	4:J:54:ILE:HD13	1.73	0.69
4:H:199:ASN:HD21	4:H:206:LYS:HE3	1.57	0.68
3:L:13:VAL:HG23	3:L:78:LEU:HD22	1.73	0.68
4:I:29:PHE:HB2	4:I:76:ARG:HG2	1.77	0.67
4:I:33:SER:HB3	4:I:98:TRP:HA	1.76	0.67
3:N:96:TRP:HB2	4:J:47:TRP:CG	2.31	0.65
4:H:99:ASP:OD2	4:H:100(A):ARG:HB2	1.96	0.65
1:E:169:PRO:HA	1:E:242:VAL:HG12	1.78	0.64
4:J:63:PHE:O	4:J:67:VAL:HG12	1.98	0.64
1:C:297:VAL:HA	5:Q:1:NAG:H82	1.81	0.63
4:J:52:ASN:HD21	4:J:98:TRP:HZ3	1.46	0.62
4:H:63:PHE:O	4:H:67:VAL:HG12	1.99	0.62
3:L:36:TYR:CE2	3:L:46:VAL:HG13	2.33	0.62
3:L:96:TRP:HB2	4:H:47:TRP:CG	2.35	0.62
2:D:156:THR:HG21	6:D:201:NAG:H82	1.82	0.61
1:E:275:ASP:OD1	1:E:276:THR:N	2.29	0.61
1:E:141:ARG:NH2	1:E:147:PHE:O	2.33	0.61
1:A:275:ASP:OD1	1:A:276:THR:N	2.32	0.61
3:M:108:ARG:HD2	3:M:171:SER:HB2	1.81	0.61
4:I:184:VAL:HG22	4:I:185:PRO:HD2	1.83	0.61
1:A:297:VAL:HA	5:O:1:NAG:H82	1.82	0.61
2:B:32:THR:HG21	4:H:54:ILE:HD13	1.82	0.60
4:I:63:PHE:O	4:I:67:VAL:HG12	2.01	0.60
4:J:70:THR:HB	4:J:79:TYR:HB2	1.84	0.59
4:H:70:THR:HB	4:H:79:TYR:HB2	1.84	0.58
1:C:207:ARG:NH1	1:C:240:GLY:O	2.36	0.58
1:E:297:VAL:HA	5:R:1:NAG:H82	1.86	0.57
3:N:155:GLN:HE21	3:N:158:ASN:HD21	1.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:33:SER:CB	4:J:98:TRP:HA	2.34	0.57
2:D:113:SER:OG	2:D:117:LYS:HE2	2.04	0.57
3:L:164:THR:HG22	3:L:165:GLU:O	2.05	0.56
3:N:96:TRP:HB2	4:J:47:TRP:CD1	2.40	0.56
1:C:275:ASP:OD1	1:C:276:THR:N	2.34	0.56
3:N:145:LYS:HB3	3:N:197:THR:OG1	2.05	0.56
4:J:50:TRP:CH2	4:J:99:ASP:HA	2.41	0.56
2:F:25:ARG:NE	4:J:98:TRP:HZ2	2.03	0.56
4:J:184:VAL:HG22	4:J:185:PRO:HD2	1.88	0.56
4:H:184:VAL:HG22	4:H:185:PRO:HD2	1.87	0.56
2:F:141:TYR:O	2:F:166:ALA:HA	2.06	0.55
2:D:14:TRP:HB3	2:D:25:ARG:NH2	2.22	0.55
4:J:40:ALA:HB3	4:J:43:GLN:HG3	1.88	0.55
4:H:20:LEU:HD22	4:H:107:THR:HG21	1.89	0.55
3:N:36:TYR:CE2	3:N:46:VAL:HG13	2.42	0.55
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.38	0.55
1:A:108:LEU:HB2	1:A:234:TRP:CZ3	2.41	0.54
4:H:33:SER:CB	4:H:98:TRP:HA	2.33	0.54
3:M:161:GLU:HG2	3:M:175:LEU:HD21	1.88	0.54
4:I:99:ASP:OD1	4:I:100(A):ARG:HB2	2.08	0.54
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.90	0.54
4:I:70:THR:HB	4:I:79:TYR:HB2	1.89	0.54
2:B:32:THR:HG21	4:H:54:ILE:CD1	2.38	0.53
2:B:113:SER:OG	2:B:117:LYS:HE2	2.07	0.53
3:M:155:GLN:HE21	3:M:158:ASN:HD21	1.56	0.53
4:I:20:LEU:HD22	4:I:107:THR:HG21	1.90	0.53
3:L:31:ASN:ND2	3:L:67:SER:HA	2.24	0.53
2:D:32:THR:HG21	4:I:54:ILE:CD1	2.39	0.52
2:B:38:LEU:HD13	3:L:27(F):SER:O	2.10	0.52
3:N:48:ILE:HG21	3:N:64:ALA:HB3	1.90	0.52
4:J:197:ASN:ND2	4:J:208:ASP:OD2	2.28	0.52
3:L:48:ILE:HG21	3:L:64:ALA:HB3	1.92	0.52
3:L:183:LYS:O	3:L:187:GLU:HG2	2.10	0.52
2:D:124:ARG:HD3	2:F:134:GLY:HA2	1.90	0.51
3:N:164:THR:HG22	3:N:165:GLU:O	2.10	0.51
4:H:29:PHE:HB2	4:H:76:ARG:HG2	1.93	0.51
3:M:36:TYR:CE2	3:M:46:VAL:HG13	2.45	0.51
2:D:34:GLN:NE2	4:I:99:ASP:OD2	2.44	0.51
3:L:115:VAL:HB	3:L:207:LYS:HD3	1.92	0.51
2:B:156:THR:HG21	6:B:201:NAG:H82	1.93	0.51
3:M:96:TRP:HB2	4:I:47:TRP:CG	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:108:ARG:HD2	3:N:171:SER:HB2	1.93	0.51
4:H:36:TRP:CH2	4:H:92:CYS:HB3	2.46	0.50
4:H:52:ASN:HD21	4:H:98:TRP:HZ3	1.60	0.50
3:M:164:THR:HG22	3:M:165:GLU:O	2.12	0.50
4:H:197:ASN:ND2	4:H:208:ASP:OD2	2.35	0.50
3:M:115:VAL:HB	3:M:207:LYS:HD3	1.94	0.49
3:M:31:ASN:ND2	3:M:67:SER:HA	2.27	0.49
3:M:145:LYS:HB3	3:M:197:THR:OG1	2.11	0.49
2:D:3:PHE:CE1	2:D:113:SER:HB2	2.46	0.49
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.94	0.49
3:L:123:GLU:HA	3:L:126:LYS:NZ	2.27	0.49
4:I:29:PHE:CB	4:I:76:ARG:HG2	2.42	0.49
1:C:167:THR:HB	6:C:504:NAG:H62	1.94	0.49
2:D:25:ARG:HD3	4:I:98:TRP:HZ2	1.77	0.48
2:D:141:TYR:O	2:D:166:ALA:HA	2.13	0.48
1:E:186:SER:HA	1:E:218:GLY:O	2.13	0.48
4:H:152:VAL:HG22	4:H:198:VAL:HG22	1.95	0.48
2:B:37:ASP:OD2	2:B:40:SER:OG	2.22	0.48
4:I:197:ASN:ND2	4:I:208:ASP:OD2	2.37	0.48
4:I:112:SER:HB3	4:I:146:PHE:CZ	2.49	0.48
4:I:11:VAL:CG2	4:I:147:PRO:HG3	2.32	0.48
2:F:60:ASN:H	2:F:60:ASN:HD22	1.62	0.48
4:H:82(B):SER:O	4:H:82(B):SER:OG	2.32	0.48
2:B:60:ASN:HD22	2:B:60:ASN:N	2.12	0.47
1:A:57:ARG:HH11	1:A:57:ARG:HG3	1.79	0.47
3:L:3:GLN:HB2	3:L:26:SER:HB3	1.95	0.47
2:D:60:ASN:N	2:D:60:ASN:HD22	2.12	0.47
1:E:89:GLU:HG3	1:E:267:ILE:HD11	1.95	0.47
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.95	0.47
3:M:183:LYS:O	3:M:187:GLU:HG2	2.15	0.47
3:N:115:VAL:HB	3:N:207:LYS:HD3	1.97	0.47
4:J:119:PRO:HB3	4:J:145:TYR:HB3	1.97	0.47
1:E:182:VAL:HG21	1:E:213:ILE:HG21	1.95	0.47
4:I:40:ALA:HB3	4:I:43:GLN:HG3	1.96	0.47
4:I:119:PRO:HB3	4:I:145:TYR:HB3	1.97	0.46
2:B:14:TRP:HB3	2:B:25:ARG:NH2	2.29	0.46
4:J:152:VAL:HG22	4:J:198:VAL:HG22	1.98	0.46
1:C:177:LEU:HD11	1:C:234:TRP:HB2	1.97	0.46
4:I:93:ALA:HB1	4:I:100(D):SER:OG	2.16	0.46
1:C:77:ASP:OD2	1:C:141:ARG:NH1	2.44	0.46
2:F:149:ILE:HA	2:F:152:ILE:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:38:ARG:HD3	4:H:48:LEU:HD21	1.97	0.46
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.51	0.46
2:B:25:ARG:NE	4:H:98:TRP:HZ2	2.14	0.45
3:N:183:LYS:O	3:N:187:GLU:HG2	2.15	0.45
1:A:326:LYS:HB3	4:H:28:THR:HB	1.98	0.45
3:M:182:SER:OG	3:M:185:ASP:OD1	2.34	0.45
1:A:216:ASN:ND2	1:E:212:THR:HB	2.32	0.45
2:D:150:GLU:HG3	6:D:201:NAG:O5	2.17	0.45
1:E:316:LEU:HD23	2:F:52:LEU:HD13	1.98	0.45
3:M:15:LEU:HD22	3:M:15:LEU:HA	1.81	0.45
4:I:62:LYS:H	4:I:62:LYS:HG3	1.53	0.45
3:L:140:TYR:CG	3:L:141:PRO:HA	2.52	0.45
3:L:145:LYS:HB3	3:L:197:THR:OG1	2.16	0.45
3:N:161:GLU:HG2	3:N:175:LEU:HD21	1.98	0.45
4:J:20:LEU:HD22	4:J:107:THR:HG21	1.99	0.45
4:J:65:ASP:OD1	4:J:66:ARG:HG3	2.15	0.45
1:C:108:LEU:HB2	1:C:234:TRP:CZ3	2.52	0.45
4:I:97:SER:OG	4:I:98:TRP:O	2.33	0.45
1:A:121:ILE:HD13	1:A:257:TYR:CE2	2.53	0.44
2:D:14:TRP:CD1	2:D:25:ARG:CZ	3.00	0.44
2:F:113:SER:OG	2:F:117:LYS:HE2	2.17	0.44
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.99	0.44
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.17	0.44
2:B:116:ASN:O	2:B:120:GLU:HG3	2.17	0.44
4:H:65:ASP:OD1	4:H:66:ARG:HG3	2.17	0.44
3:M:48:ILE:HG21	3:M:64:ALA:HB3	1.99	0.44
2:D:3:PHE:HZ	2:F:2:LEU:HB3	1.81	0.44
1:E:220:ARG:N	1:E:227:SER:OG	2.49	0.44
3:L:27(D):SER:OG	3:L:27(F):SER:HB3	2.17	0.44
1:E:304:ALA:HA	2:F:61:GLU:HA	1.99	0.44
3:M:96:TRP:HB2	4:I:47:TRP:CD1	2.52	0.44
3:M:140:TYR:CG	3:M:141:PRO:HA	2.53	0.44
4:I:33:SER:CB	4:I:98:TRP:HA	2.46	0.44
3:N:3:GLN:HB2	3:N:26:SER:HB3	2.00	0.44
1:C:60:ASP:HB2	1:C:274:ILE:HD11	2.00	0.44
2:B:48:ILE:HA	2:B:51:LYS:HG2	2.00	0.43
1:C:42:LEU:HD11	1:C:316:LEU:HB2	1.98	0.43
2:B:141:TYR:O	2:B:166:ALA:HA	2.18	0.43
1:C:219:SER:HG	5:K:1:NAG:HN2	1.61	0.43
1:E:220:ARG:HD3	1:E:229:ARG:HG2	1.99	0.43
5:P:1:NAG:H61	5:P:2:NAG:C7	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:TRP:CG	2:D:25:ARG:CZ	3.01	0.43
4:H:27:TYR:CE1	4:H:94:ARG:HD2	2.53	0.43
1:A:54:ASN:HD22	1:A:55:PRO:HA	1.82	0.43
3:L:96:TRP:HB2	4:H:47:TRP:CD1	2.52	0.43
3:N:83:VAL:CG2	3:N:106:ILE:HG13	2.48	0.43
4:J:27:TYR:CE1	4:J:94:ARG:HD2	2.54	0.43
2:B:3:PHE:CZ	2:D:2:LEU:HB3	2.53	0.43
1:E:14:CYS:HA	2:F:137:CYS:HA	2.01	0.43
1:C:288:ILE:HG21	1:C:297:VAL:HG21	2.01	0.43
2:F:14:TRP:CG	2:F:25:ARG:NH2	2.87	0.43
2:F:156:THR:HG21	6:F:201:NAG:HN2	1.83	0.43
3:L:35:TRP:CE2	3:L:73:LEU:HB2	2.53	0.43
1:E:35:GLU:OE2	1:E:322:ASN:ND2	2.45	0.43
4:I:27:TYR:CE1	4:I:94:ARG:HD2	2.54	0.43
1:A:42:LEU:HD11	1:A:316:LEU:HB2	2.01	0.42
2:B:77:ILE:HD13	2:B:77:ILE:HA	1.80	0.42
3:N:96:TRP:HH2	4:J:100(D):SER:HB2	1.83	0.42
2:F:14:TRP:CD1	2:F:25:ARG:CZ	3.03	0.42
2:F:167:LEU:HD23	2:F:167:LEU:HA	1.88	0.42
3:M:31:ASN:HD21	3:M:67:SER:HA	1.85	0.42
4:J:52:ASN:ND2	4:J:98:TRP:CE3	2.87	0.42
2:D:14:TRP:CZ2	2:D:25:ARG:HD2	2.54	0.42
1:E:108:LEU:HB2	1:E:234:TRP:CZ3	2.54	0.42
1:A:288:ILE:HG21	1:A:297:VAL:HG21	2.01	0.42
1:C:14:CYS:HA	2:D:137:CYS:HA	2.00	0.42
2:F:14:TRP:CZ2	2:F:25:ARG:HD2	2.54	0.42
3:L:50:TRP:C	3:L:52:SER:H	2.22	0.42
2:B:3:PHE:CE1	2:B:113:SER:HB2	2.55	0.42
4:H:40:ALA:HB3	4:H:43:GLN:HG3	2.01	0.42
2:B:53:ASN:O	2:B:57:GLU:HB2	2.20	0.42
1:C:71:LEU:O	1:C:148:PHE:HB3	2.19	0.42
1:A:164:LEU:O	1:A:246:ASN:HA	2.20	0.42
3:L:15:LEU:HD22	3:L:15:LEU:HA	1.77	0.42
4:J:52:ASN:ND2	4:J:98:TRP:CZ3	2.86	0.42
1:E:195:TYR:CZ	1:E:250:ASN:HA	2.55	0.41
4:H:52:ASN:ND2	4:H:98:TRP:CZ3	2.87	0.41
3:N:31:ASN:ND2	3:N:67:SER:HA	2.34	0.41
2:D:3:PHE:CZ	2:F:2:LEU:HB3	2.55	0.41
3:M:50:TRP:C	3:M:52:SER:H	2.24	0.41
2:D:14:TRP:HB3	2:D:25:ARG:HH21	1.84	0.41
4:I:12:LYS:HD2	4:I:17:SER:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:108:ARG:HH12	3:L:111:ALA:HB2	1.85	0.41
2:B:34:GLN:NE2	4:H:99:ASP:OD1	2.53	0.41
1:E:74:PRO:HA	1:E:77:ASP:OD2	2.21	0.41
1:E:220:ARG:HB3	1:E:221:PRO:HD2	2.03	0.41
1:E:58:ILE:HG21	1:E:274:ILE:HD12	2.03	0.41
3:L:33:LEU:HD13	3:L:34:ALA:N	2.36	0.41
3:M:123:GLU:HA	3:M:126:LYS:NZ	2.36	0.41
2:B:3:PHE:HZ	2:D:2:LEU:HB3	1.85	0.41
1:C:60:ASP:HB2	1:C:274:ILE:CD1	2.50	0.41
1:E:177:LEU:HD11	1:E:234:TRP:HB2	2.03	0.41
1:E:264:LYS:HD3	2:F:63:PHE:CZ	2.56	0.41
3:L:155:GLN:HE21	3:L:158:ASN:HD21	1.68	0.41
3:M:47:LEU:HA	3:M:58:VAL:HG21	2.02	0.41
3:N:96:TRP:CZ2	4:J:35:HIS:CE1	3.09	0.41
1:E:103:PRO:HG2	1:E:233:TYR:CE1	2.56	0.41
4:I:65:ASP:OD1	4:I:66:ARG:HG3	2.20	0.41
3:N:140:TYR:CG	3:N:141:PRO:HA	2.56	0.41
1:E:203:THR:HG23	1:E:212:THR:HG22	2.02	0.40
4:H:62:LYS:H	4:H:62:LYS:HG3	1.55	0.40
3:N:83:VAL:HG21	3:N:106:ILE:HG13	2.03	0.40
4:J:93:ALA:HB1	4:J:100(D):SER:OG	2.22	0.40
1:E:214:ILE:HA	1:E:215:PRO:HD3	1.94	0.40
3:M:83:VAL:CG2	3:M:106:ILE:HG13	2.51	0.40
4:J:82(B):SER:O	4:J:82(B):SER:OG	2.34	0.40
1:A:195:TYR:O	1:A:197:GLN:N	2.47	0.40
1:E:118:LEU:HD23	1:E:118:LEU:HA	1.89	0.40
4:J:72:ASP:HB3	4:J:75:ALA:HB3	2.03	0.40
1:A:49:GLY:HA2	1:A:285:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/323 (98%)	308 (98%)	7 (2%)	1 (0%)	41	75
1	C	316/323 (98%)	309 (98%)	6 (2%)	1 (0%)	41	75
1	E	315/323 (98%)	307 (98%)	7 (2%)	1 (0%)	41	75
2	B	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
2	D	169/176 (96%)	162 (96%)	7 (4%)	0	100	100
2	F	169/176 (96%)	162 (96%)	7 (4%)	0	100	100
3	L	215/220 (98%)	209 (97%)	5 (2%)	1 (0%)	29	67
3	M	215/220 (98%)	210 (98%)	4 (2%)	1 (0%)	29	67
3	N	215/220 (98%)	210 (98%)	4 (2%)	1 (0%)	29	67
4	H	211/230 (92%)	207 (98%)	4 (2%)	0	100	100
4	I	207/230 (90%)	203 (98%)	4 (2%)	0	100	100
4	J	209/230 (91%)	204 (98%)	5 (2%)	0	100	100
All	All	2727/2847 (96%)	2654 (97%)	67 (2%)	6 (0%)	47	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
3	L	51	SER
3	M	51	SER
3	N	51	SER

5.3.2 Protein sidechains (i)

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	279/283 (99%)	275 (99%)	4 (1%)	67	81
1	C	279/283 (99%)	276 (99%)	3 (1%)	73	85
1	E	278/283 (98%)	277 (100%)	1 (0%)	91	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	146/149 (98%)	145 (99%)	1 (1%)	84	90
2	D	145/149 (97%)	144 (99%)	1 (1%)	84	90
2	F	145/149 (97%)	145 (100%)	0	100	100
3	L	192/194 (99%)	181 (94%)	11 (6%)	20	49
3	M	192/194 (99%)	180 (94%)	12 (6%)	18	46
3	N	192/194 (99%)	180 (94%)	12 (6%)	18	46
4	H	178/193 (92%)	169 (95%)	9 (5%)	24	52
4	I	177/193 (92%)	166 (94%)	11 (6%)	18	46
4	J	178/193 (92%)	169 (95%)	9 (5%)	24	52
All	All	2381/2457 (97%)	2307 (97%)	74 (3%)	40	63

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	53	ASN
1	A	323	VAL
1	A	325	GLU
2	B	60	ASN
1	C	18	HIS
1	C	323	VAL
1	C	326	LYS
2	D	60	ASN
1	E	18	HIS
3	L	9	ASP
3	L	15	LEU
3	L	17	GLU
3	L	18	ARG
3	L	22	ASN
3	L	27	GLN
3	L	46	VAL
3	L	105	GLU
3	L	147	GLN
3	L	152	ASN
3	L	197	THR
4	H	10	GLU
4	H	12	LYS
4	H	62	LYS
4	H	71	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	80	MET
4	H	99	ASP
4	H	184	VAL
4	H	188	SER
4	H	199	ASN
3	M	9	ASP
3	M	15	LEU
3	M	17	GLU
3	M	18	ARG
3	M	22	ASN
3	M	27	GLN
3	M	46	VAL
3	M	105	GLU
3	M	147	GLN
3	M	152	ASN
3	M	197	THR
3	M	207	LYS
4	I	10	GLU
4	I	12	LYS
4	I	62	LYS
4	I	71	ARG
4	I	80	MET
4	I	98	TRP
4	I	99	ASP
4	I	100(A)	ARG
4	I	184	VAL
4	I	188	SER
4	I	199	ASN
3	N	9	ASP
3	N	15	LEU
3	N	17	GLU
3	N	18	ARG
3	N	22	ASN
3	N	27	GLN
3	N	46	VAL
3	N	105	GLU
3	N	147	GLN
3	N	152	ASN
3	N	197	THR
3	N	207	LYS
4	J	10	GLU
4	J	12	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	J	62	LYS
4	J	71	ARG
4	J	80	MET
4	J	99	ASP
4	J	184	VAL
4	J	188	SER
4	J	199	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	54	ASN
1	A	171	ASN
2	B	53	ASN
2	B	60	ASN
2	B	125	GLN
1	C	18	HIS
1	C	54	ASN
1	C	171	ASN
2	D	53	ASN
2	D	60	ASN
2	D	125	GLN
1	E	54	ASN
1	E	211	GLN
1	E	216	ASN
2	F	27	GLN
2	F	53	ASN
2	F	60	ASN
2	F	125	GLN
3	L	155	GLN
4	H	58	GLN
4	H	199	ASN
3	M	155	GLN
4	I	58	GLN
4	I	199	ASN
3	N	155	GLN
4	J	199	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

12 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	G	1	1,5	14,14,15	0.52	0	17,19,21	1.05	2 (11%)
5	NAG	G	2	5	14,14,15	0.63	0	17,19,21	1.14	1 (5%)
5	NAG	K	1	1,5	14,14,15	0.58	0	17,19,21	0.83	0
5	NAG	K	2	5	14,14,15	0.62	0	17,19,21	1.03	0
5	NAG	O	1	1,5	14,14,15	0.55	0	17,19,21	1.00	1 (5%)
5	NAG	O	2	5	14,14,15	0.57	0	17,19,21	0.90	0
5	NAG	P	1	1,5	14,14,15	0.61	0	17,19,21	0.84	1 (5%)
5	NAG	P	2	5	14,14,15	0.54	0	17,19,21	0.81	0
5	NAG	Q	1	1,5	14,14,15	0.55	0	17,19,21	0.74	0
5	NAG	Q	2	5	14,14,15	0.55	0	17,19,21	0.90	0
5	NAG	R	1	1,5	14,14,15	0.57	0	17,19,21	0.75	0
5	NAG	R	2	5	14,14,15	0.52	0	17,19,21	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	1	NAG	C1-O5-C5	3.03	116.29	112.19
5	G	1	NAG	C2-N2-C7	-2.70	119.06	122.90
5	G	1	NAG	C1-O5-C5	2.52	115.60	112.19
5	G	2	NAG	O5-C1-C2	-2.05	108.06	111.29
5	P	1	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1	NAG	1	0
5	O	1	NAG	1	0

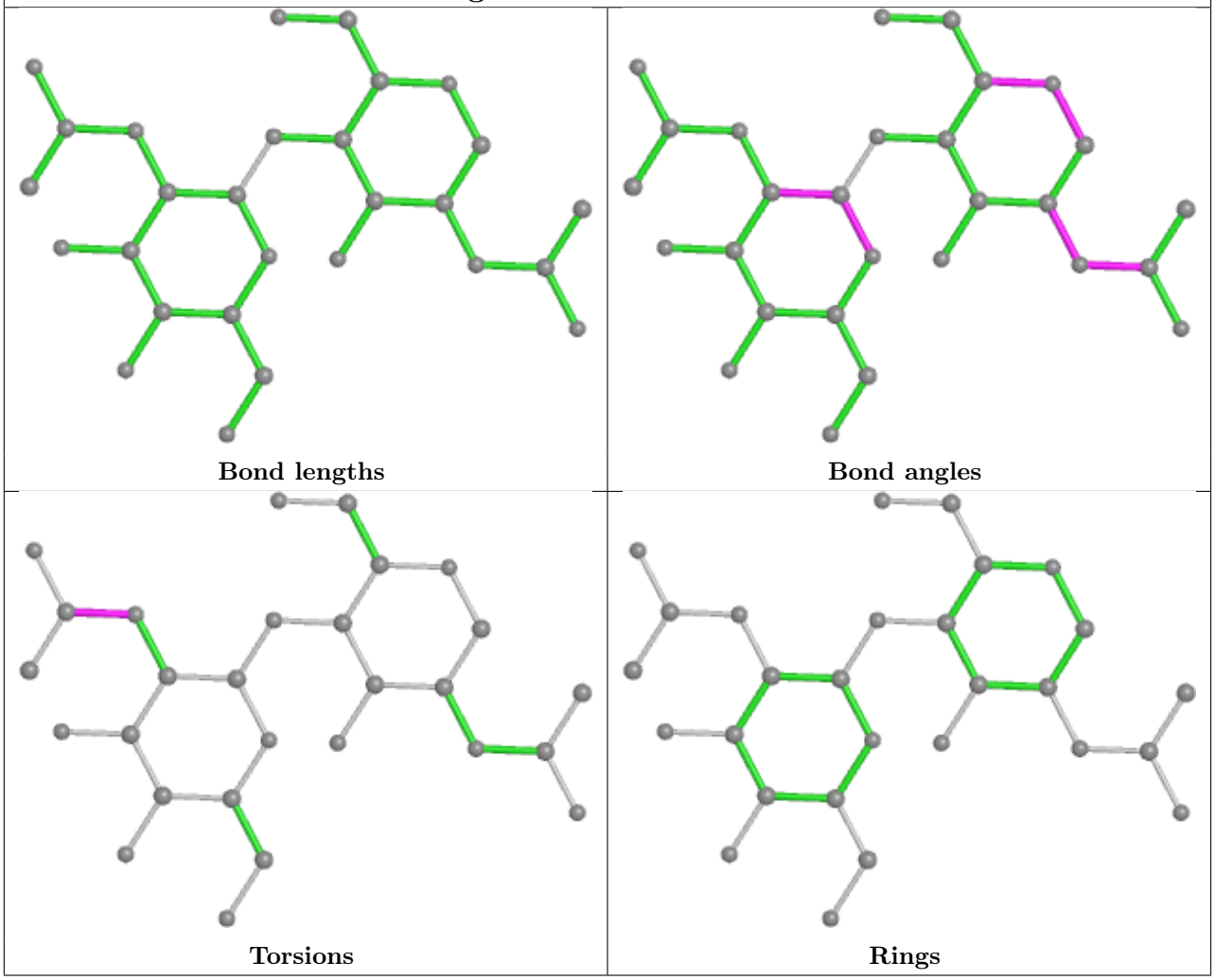
Continued on next page...

Continued from previous page...

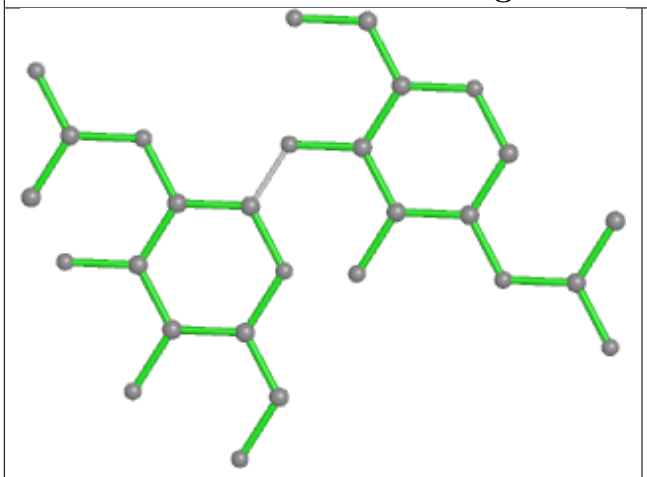
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
5	P	1	NAG	1	0
5	P	2	NAG	1	0
5	Q	1	NAG	1	0

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

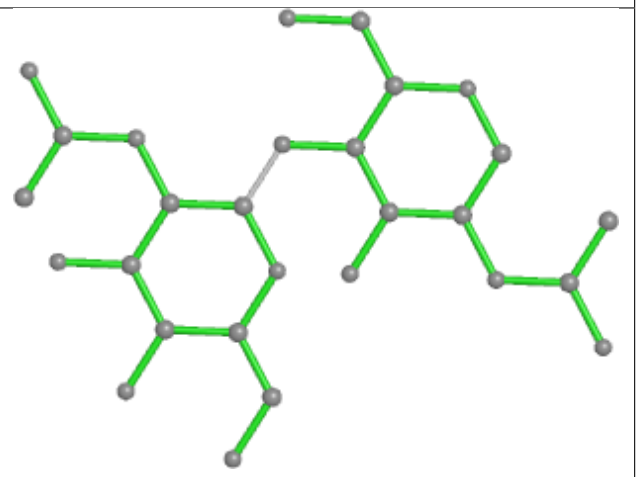
Oligosaccharide Chain G



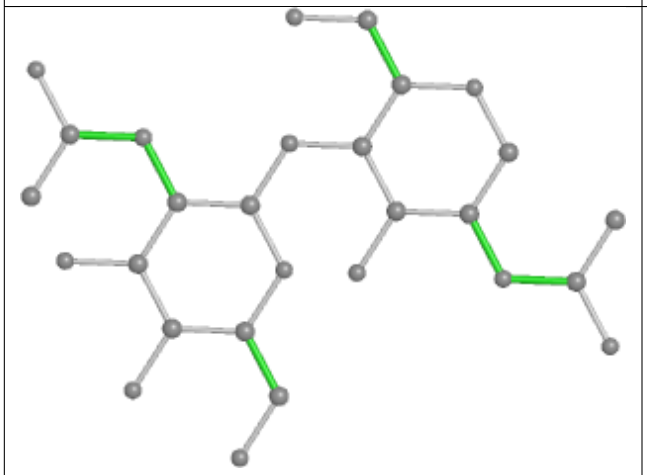
Oligosaccharide Chain K



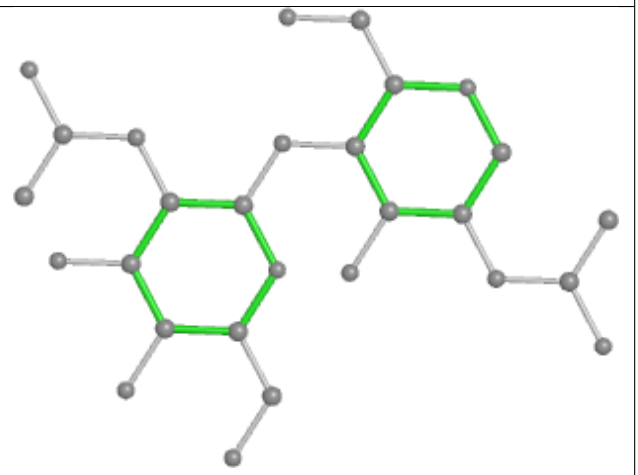
Bond lengths



Bond angles

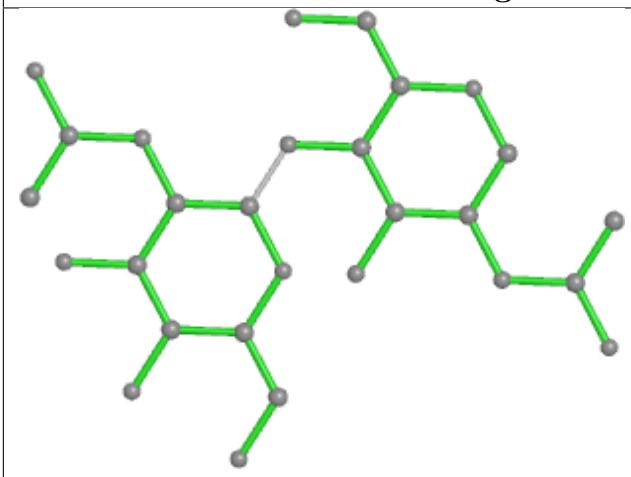


Torsions

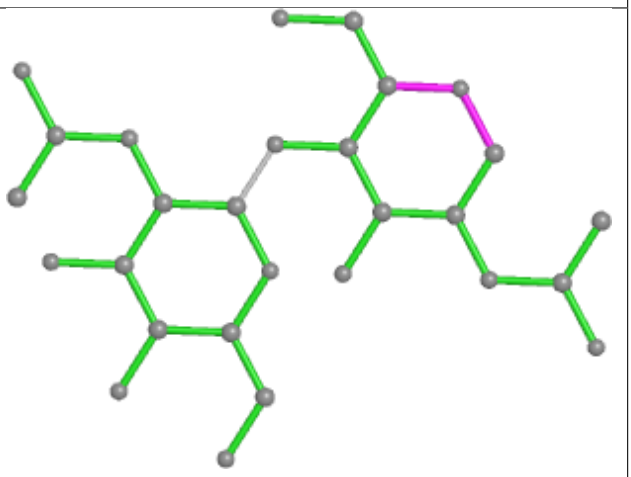


Rings

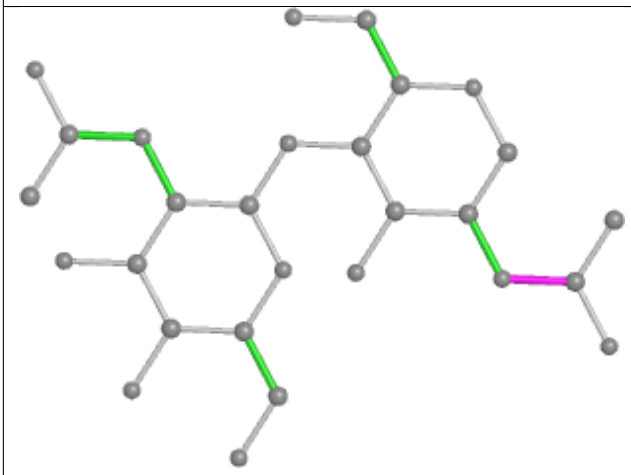
Oligosaccharide Chain O



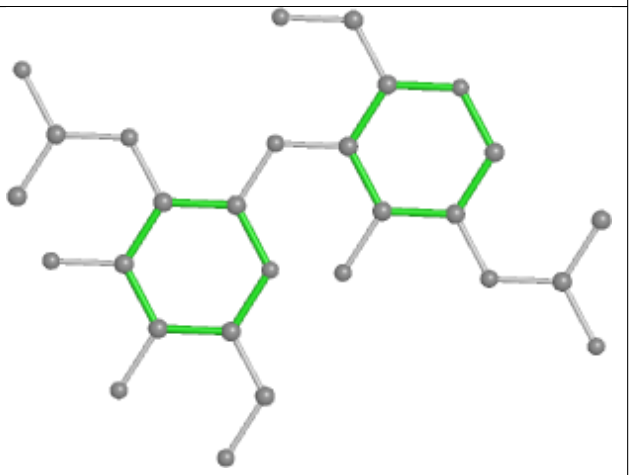
Bond lengths



Bond angles

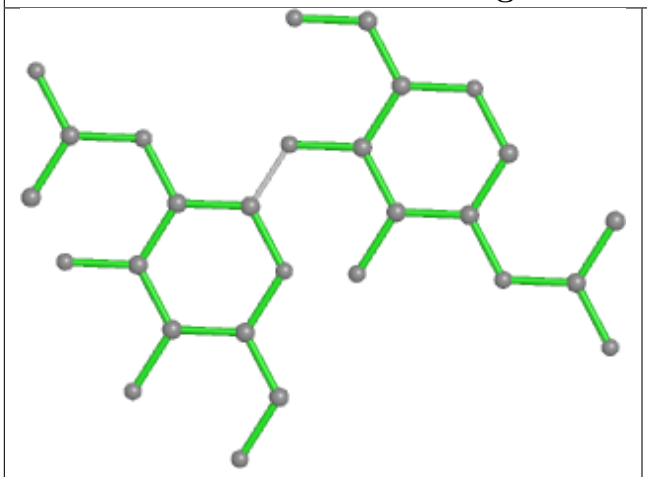


Torsions

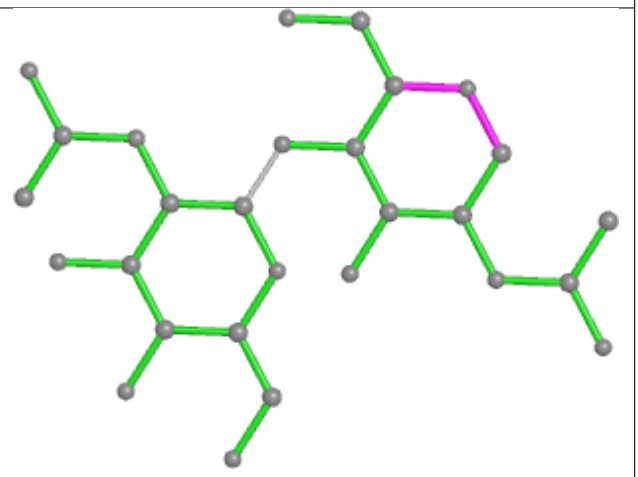


Rings

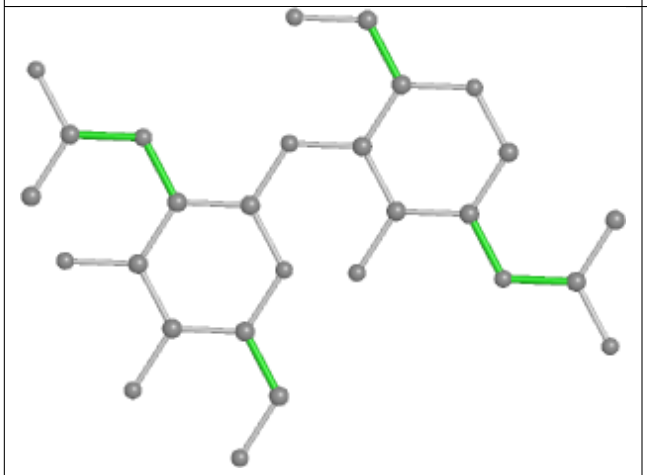
Oligosaccharide Chain P



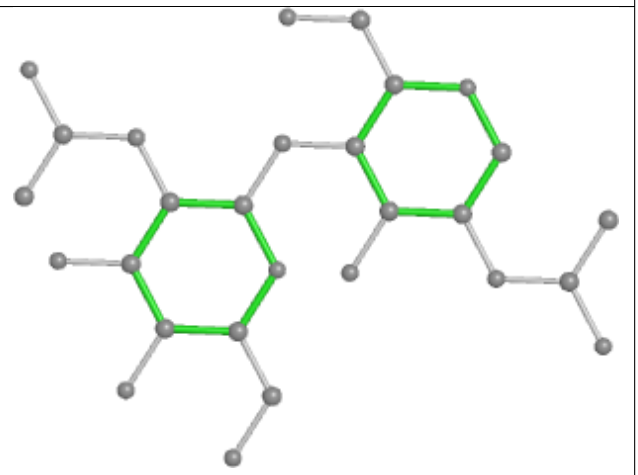
Bond lengths



Bond angles

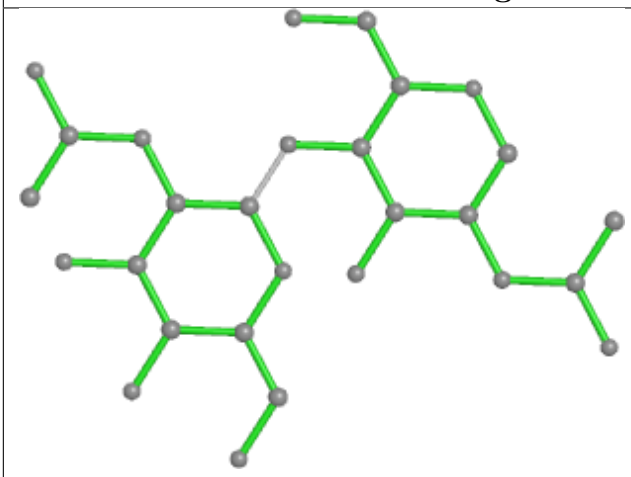


Torsions

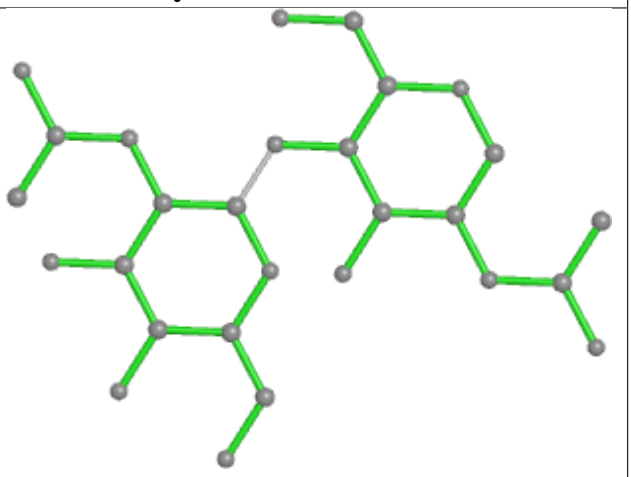


Rings

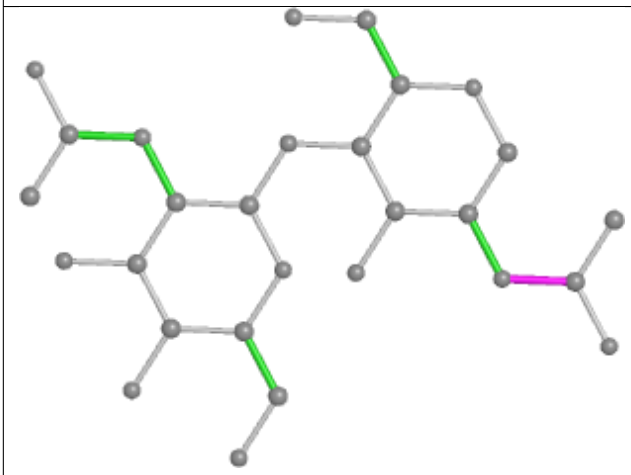
Oligosaccharide Chain Q



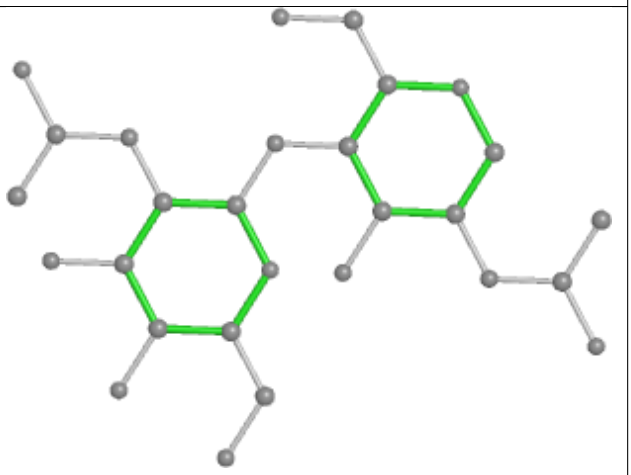
Bond lengths



Bond angles

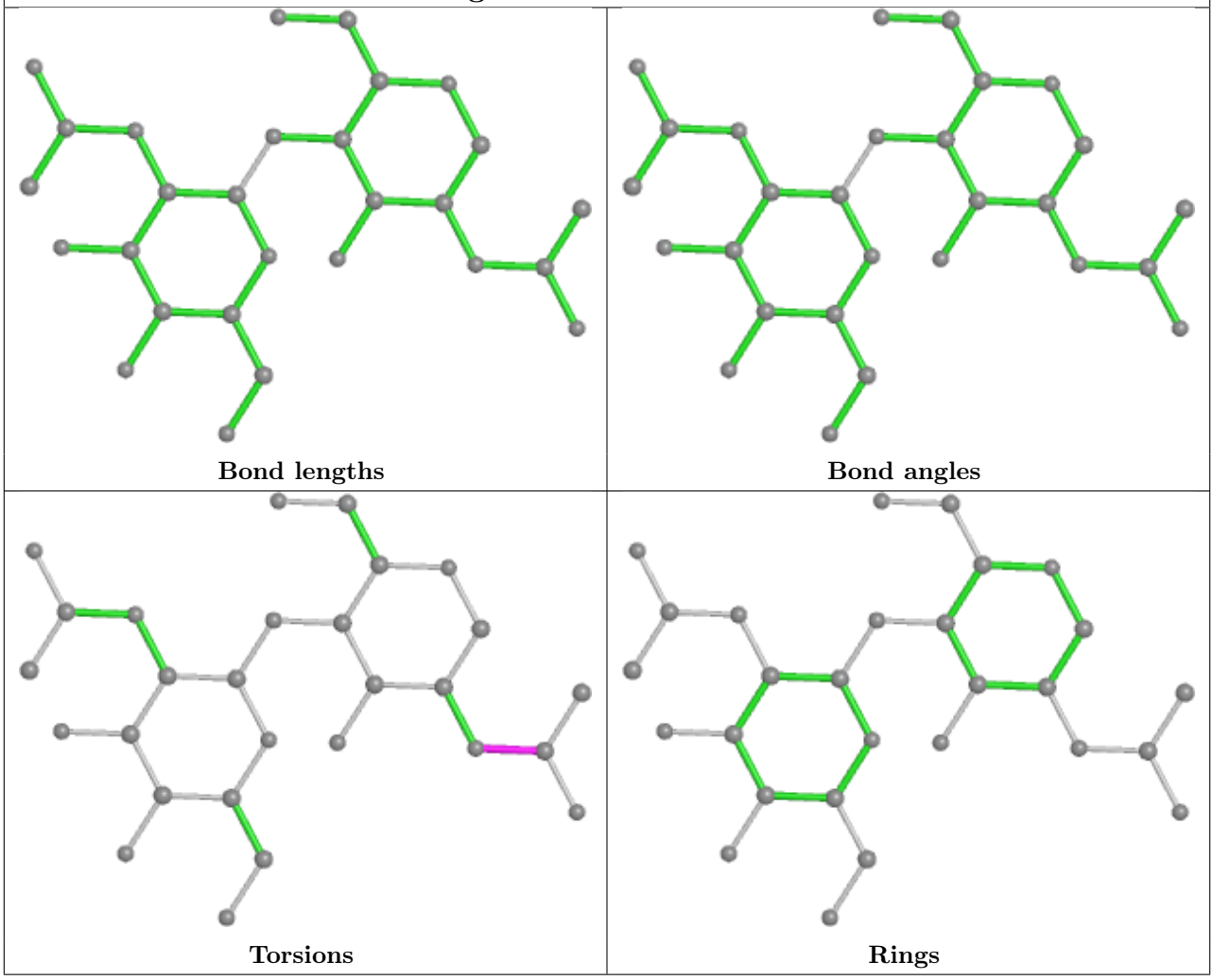


Torsions



Rings

Oligosaccharide Chain R



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
6	NAG	D	201	2	14,14,15	0.55	0	17,19,21	1.71	3 (17%)
6	NAG	B	201	2	14,14,15	0.54	0	17,19,21	1.32	2 (11%)
6	NAG	C	504	1	14,14,15	0.56	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	F	201	2	14,14,15	0.54	0	17,19,21	1.49	3 (17%)
6	NAG	E	502	1	14,14,15	0.50	0	17,19,21	1.27	1 (5%)
6	NAG	E	503	1	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
6	NAG	C	501	1	14,14,15	0.50	0	17,19,21	0.88	1 (5%)
6	NAG	E	501	1	14,14,15	0.46	0	17,19,21	1.08	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	201	2	-	2/6/23/26	0/1/1/1
6	NAG	B	201	2	-	2/6/23/26	0/1/1/1
6	NAG	C	504	1	-	0/6/23/26	0/1/1/1
6	NAG	F	201	2	-	2/6/23/26	0/1/1/1
6	NAG	E	502	1	-	0/6/23/26	0/1/1/1
6	NAG	E	503	1	-	0/6/23/26	0/1/1/1
6	NAG	C	501	1	-	0/6/23/26	0/1/1/1
6	NAG	E	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	201	NAG	O5-C5-C6	4.80	114.72	107.20
6	E	502	NAG	C1-O5-C5	4.49	118.28	112.19
6	F	201	NAG	C1-O5-C5	4.44	118.20	112.19
6	B	201	NAG	C1-O5-C5	4.03	117.65	112.19
6	E	501	NAG	C1-O5-C5	3.29	116.65	112.19
6	D	201	NAG	C1-O5-C5	3.24	116.58	112.19
6	D	201	NAG	C6-C5-C4	-2.94	106.11	113.00
6	E	503	NAG	C1-O5-C5	2.70	115.85	112.19
6	C	501	NAG	C1-O5-C5	2.31	115.32	112.19
6	C	504	NAG	C1-O5-C5	2.21	115.19	112.19
6	F	201	NAG	C1-C2-N2	2.19	114.23	110.49
6	F	201	NAG	C2-N2-C7	-2.10	119.92	122.90
6	B	201	NAG	O5-C5-C6	2.04	110.41	107.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	201	NAG	C8-C7-N2-C2
6	F	201	NAG	O7-C7-N2-C2
6	B	201	NAG	C8-C7-N2-C2
6	D	201	NAG	C8-C7-N2-C2
6	B	201	NAG	O7-C7-N2-C2
6	D	201	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	201	NAG	2	0
6	B	201	NAG	1	0
6	C	504	NAG	1	0
6	F	201	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	318/323 (98%)	0.18	4 (1%)	77	68	20, 55, 110, 160	0
1	C	318/323 (98%)	0.07	2 (0%)	89	84	18, 51, 106, 132	0
1	E	317/323 (98%)	0.24	13 (4%)	37	30	19, 58, 136, 168	0
2	B	172/176 (97%)	0.08	1 (0%)	89	84	18, 34, 90, 135	0
2	D	171/176 (97%)	0.02	1 (0%)	89	84	18, 33, 88, 129	0
2	F	171/176 (97%)	0.05	0	100	100	18, 36, 95, 161	0
3	L	217/220 (98%)	0.59	24 (11%)	5	5	20, 81, 162, 203	0
3	M	217/220 (98%)	0.54	22 (10%)	7	7	22, 79, 154, 177	0
3	N	217/220 (98%)	0.55	20 (9%)	9	8	22, 85, 165, 211	0
4	H	215/230 (93%)	0.37	15 (6%)	16	13	22, 76, 162, 203	0
4	I	211/230 (91%)	0.31	6 (2%)	53	42	25, 68, 153, 188	0
4	J	213/230 (92%)	0.47	20 (9%)	8	8	24, 78, 175, 209	0
All	All	2757/2847 (96%)	0.29	128 (4%)	32	27	18, 56, 150, 211	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	197	THR	5.8
3	L	144	ALA	5.2
4	J	183	THR	5.1
4	H	144	ASP	4.8
3	N	193	ALA	4.7
3	M	181	LEU	4.7
3	N	197	THR	4.6
3	N	117	ILE	4.3
3	M	197	THR	4.1
4	H	143	LYS	4.1
3	N	181	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	149	LYS	3.8
3	N	201	LEU	3.7
4	J	186	SER	3.7
4	H	180	SER	3.6
3	L	201	LEU	3.5
4	J	12	LYS	3.4
4	I	180	SER	3.4
3	M	201	LEU	3.4
3	L	196	VAL	3.3
3	L	159	SER	3.3
3	L	187	GLU	3.3
4	J	209	LYS	3.2
3	M	107	LYS	3.2
4	J	182	VAL	3.2
4	J	138	LEU	3.2
4	H	139	GLY	3.1
3	M	196	VAL	3.1
3	L	119	PRO	3.1
1	E	153	TRP	3.0
3	N	151	ASP	3.0
3	L	136	LEU	2.9
3	L	181	LEU	2.9
4	H	183	THR	2.9
4	H	212	GLU	2.9
4	J	162	GLY	2.9
3	M	186	TYR	2.8
4	H	138	LEU	2.8
3	N	152	ASN	2.8
4	H	190	GLY	2.8
4	H	211	VAL	2.8
4	J	144	ASP	2.7
3	M	209	PHE	2.7
3	M	146	VAL	2.7
3	N	196	VAL	2.7
3	M	130	ALA	2.7
3	M	144	ALA	2.7
3	M	185	ASP	2.7
3	N	144	ALA	2.7
1	A	154	LEU	2.7
1	E	159	SER	2.7
3	M	193	ALA	2.7
4	J	211	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	110	VAL	2.6
4	H	181	VAL	2.6
1	E	160	THR	2.6
3	N	192	TYR	2.6
3	L	152	ASN	2.6
4	J	194	TYR	2.6
3	L	151	ASP	2.6
3	L	198	HIS	2.5
4	I	95	GLY	2.5
1	E	154	LEU	2.5
3	L	193	ALA	2.5
3	L	135	LEU	2.5
3	M	149	LYS	2.5
3	L	118	PHE	2.5
4	H	142	VAL	2.5
4	I	181	VAL	2.5
1	E	219	SER	2.5
3	M	175	LEU	2.5
3	M	183	LYS	2.5
1	E	246	ASN	2.5
3	L	117	ILE	2.4
3	N	186	TYR	2.4
4	I	210	ARG	2.4
3	M	152	ASN	2.4
4	H	186	SER	2.4
3	M	131	SER	2.4
1	A	128	THR	2.4
3	N	180	THR	2.3
4	J	11	VAL	2.3
4	I	186	SER	2.3
3	M	190	LYS	2.3
1	A	153	TRP	2.3
4	J	180	SER	2.3
4	J	110	THR	2.3
4	J	190	GLY	2.3
4	J	189	LEU	2.3
3	M	192	TYR	2.3
3	N	135	LEU	2.3
3	N	158	ASN	2.3
3	N	175	LEU	2.3
1	C	259	LYS	2.3
1	E	147	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	156	LYS	2.3
4	J	181	VAL	2.3
1	E	128	THR	2.2
4	H	152	VAL	2.2
3	M	200	GLY	2.2
1	E	155	THR	2.2
1	E	201	ARG	2.2
3	N	118	PHE	2.2
3	L	120	PRO	2.2
3	L	131	SER	2.2
3	N	200	GLY	2.2
1	C	176	LYS	2.2
3	M	136	LEU	2.2
4	I	162	GLY	2.2
4	H	140	CYS	2.2
3	L	186	TYR	2.2
4	J	187	SER	2.2
2	D	63	PHE	2.2
1	A	175	ASP	2.2
3	M	135	LEU	2.1
4	J	126	PRO	2.1
1	E	129	GLY	2.1
3	N	190	LYS	2.1
4	J	143	LYS	2.1
3	N	198	HIS	2.1
4	H	164	HIS	2.1
3	L	190	LYS	2.1
3	N	119	PRO	2.1
3	L	111	ALA	2.1
1	E	163	VAL	2.1
4	J	212	GLU	2.1
3	L	178	THR	2.0
2	B	30	GLU	2.0

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

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

6.3 Carbohydrates (i)

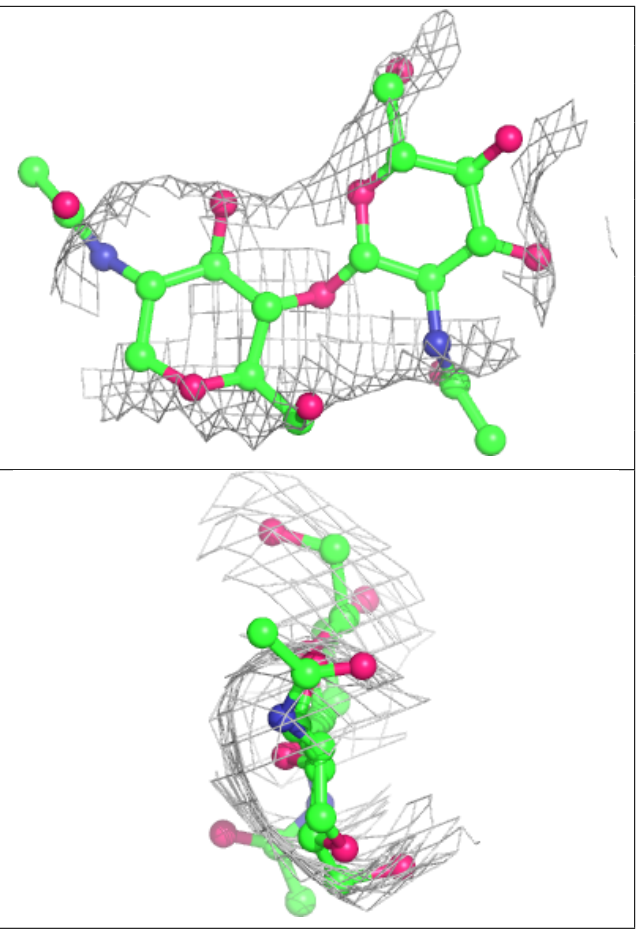
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	R	2	14/15	0.57	0.42	101,107,112,112	0
5	NAG	P	2	14/15	0.60	0.63	119,131,133,134	0
5	NAG	P	1	14/15	0.70	0.27	80,92,97,99	0
5	NAG	O	2	14/15	0.73	0.34	90,96,101,101	0
5	NAG	Q	2	14/15	0.74	0.34	89,95,101,101	0
5	NAG	R	1	14/15	0.77	0.29	49,59,64,65	0
5	NAG	G	2	14/15	0.78	0.27	102,111,115,115	0
5	NAG	Q	1	14/15	0.79	0.30	45,55,60,61	0
5	NAG	O	1	14/15	0.79	0.23	36,46,51,51	0
5	NAG	K	1	14/15	0.83	0.32	101,113,116,117	0
5	NAG	K	2	14/15	0.83	0.30	114,127,130,130	0
5	NAG	G	1	14/15	0.86	0.26	59,71,75,76	0

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

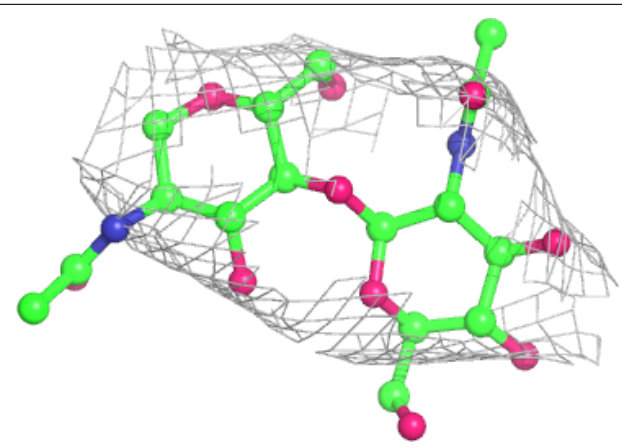
Electron density around Chain G:

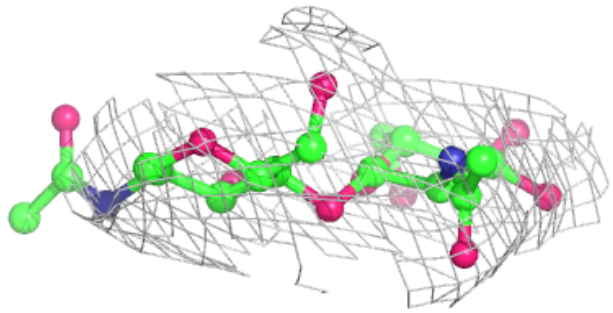
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

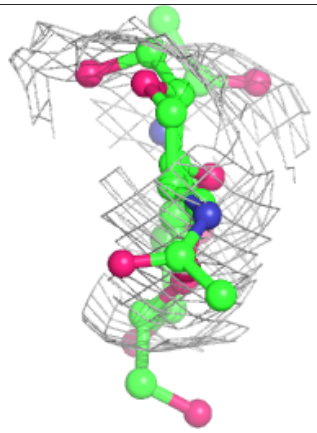


Electron density around Chain K:

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

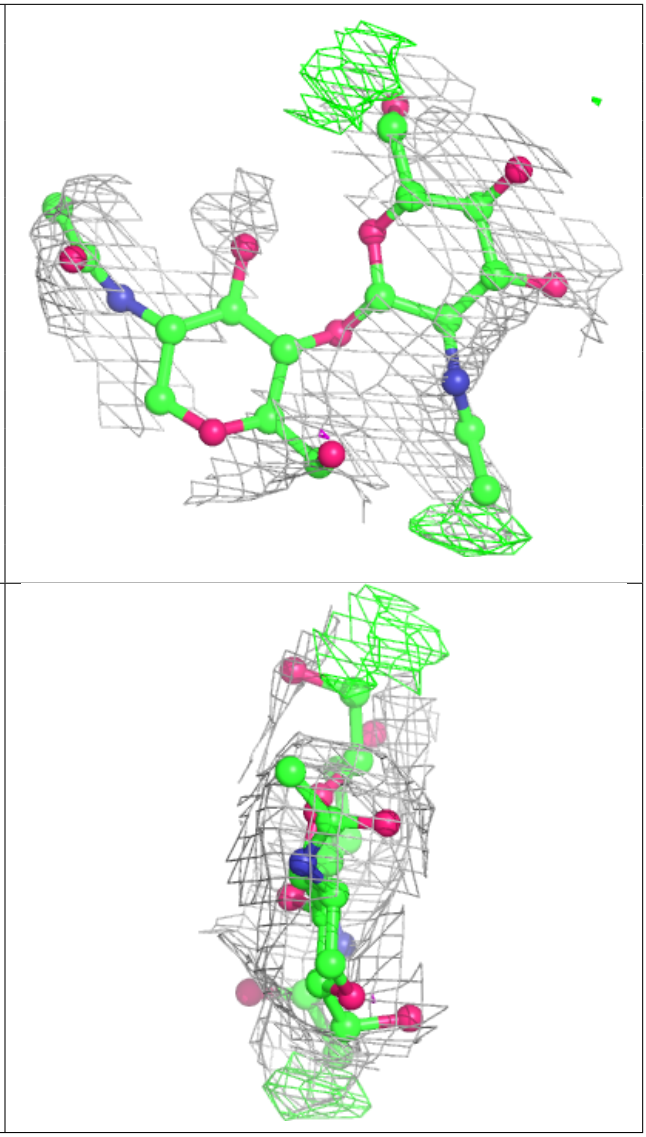






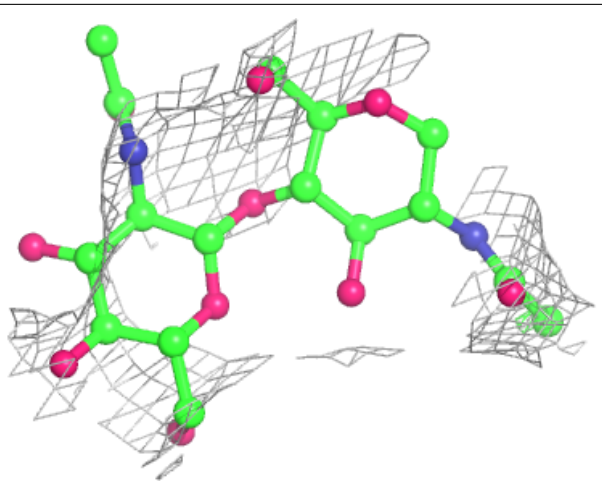
Electron density around Chain O:

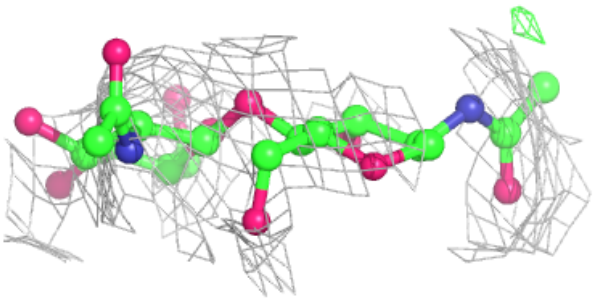
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

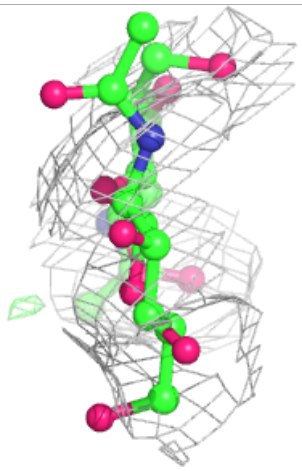


Electron density around Chain P:

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

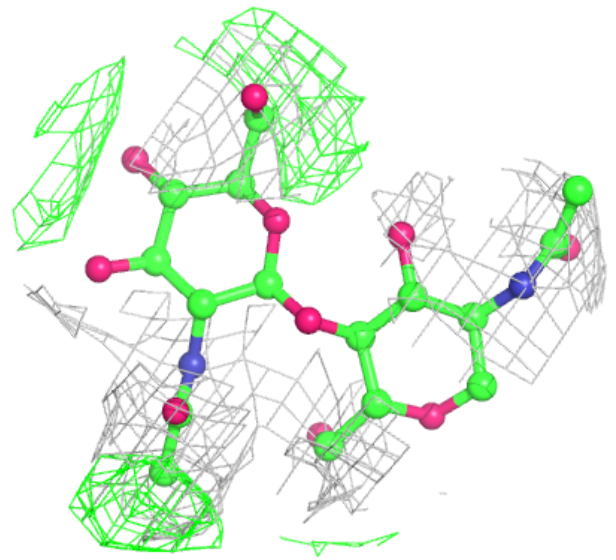


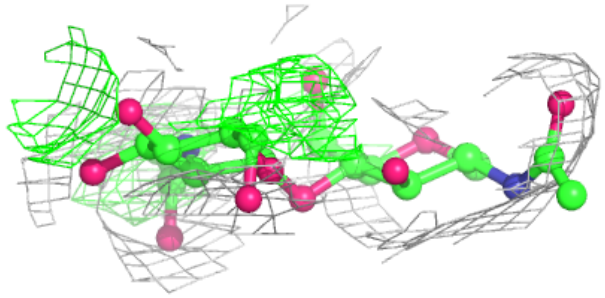


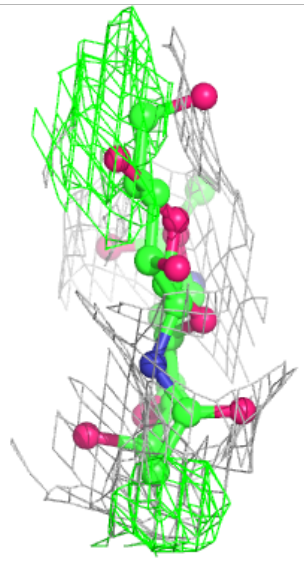


Electron density around Chain Q:

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

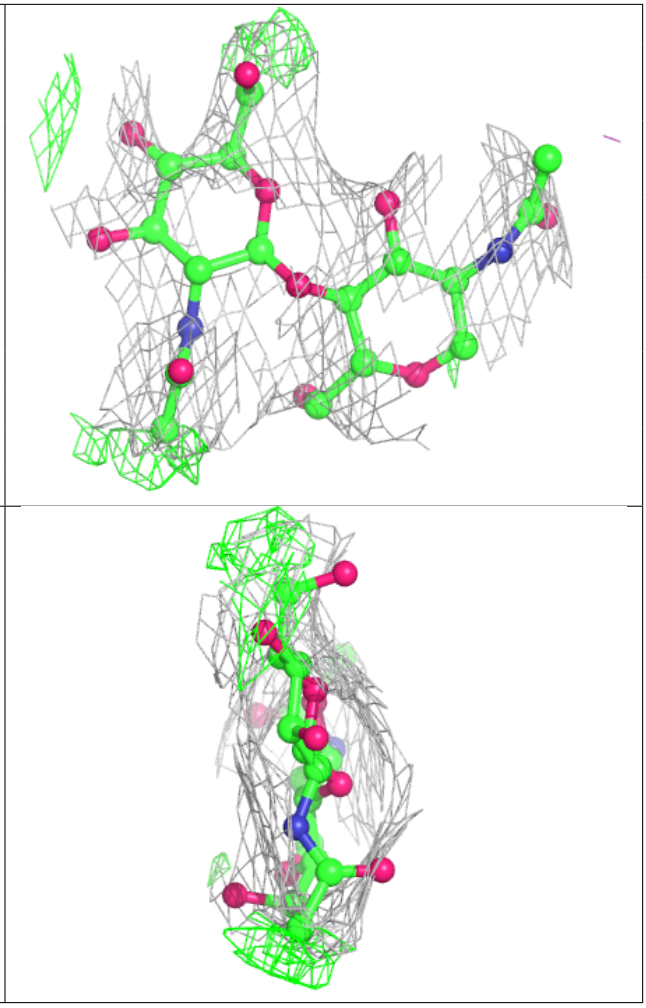






Electron density around Chain R:

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



6.4 Ligands (i)

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(Å^2)	Q<0.9
6	NAG	E	503	14/15	0.62	0.42	95,108,111,112	0
6	NAG	C	504	14/15	0.68	0.37	83,96,99,101	0
6	NAG	D	201	14/15	0.70	0.40	93,104,110,111	0
6	NAG	E	502	14/15	0.73	0.34	67,80,85,87	0
6	NAG	F	201	14/15	0.80	0.32	92,103,109,111	0
6	NAG	C	501	14/15	0.81	0.31	81,93,97,98	0
6	NAG	B	201	14/15	0.82	0.25	80,91,96,98	0
6	NAG	E	501	14/15	0.83	0.30	70,81,86,87	0

6.5 Other polymers (i)

There are no such residues in this entry.