Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:17 PM UTC

PDB ID	:	5F97 / pdb_00005f97
Title	:	Blood group antigen binding adhesin BabA of Helicobacter pylori strain A730 in complex with blood group A type 1 hexasaccharide
Authors	:	Moonens, K.; Gideonsson, P.; Subedi, S.; Romao, E.; Oscarson, S.; Muyldermans, S.; Boren, T.; Remaut, H.
Deposited on	:	2015-12-09
Resolution	:	2.62 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

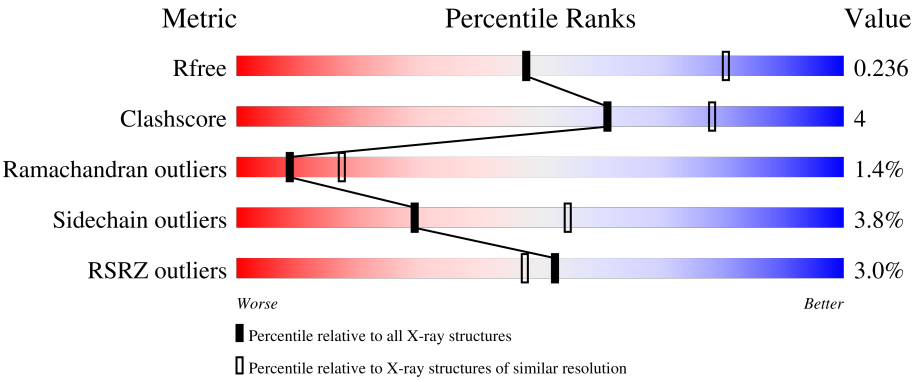
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.62 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	469	% 79% 10% • 9%
1	B	469	3% 80% 10% • 9%
1	C	469	4% 76% 12% • 9%
1	D	469	4% 82% 9% • 9%
2	E	120	2% 81% 13% • 5%

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Mol	Chain	Length	Quality of chain
2	F	120	2% 83% 9%
2	G	120	2% 85% 10% 5%
2	H	120	2% 78% 16% 6%
3	I	6	100%
3	J	6	100%
3	K	6	50% 50%
3	L	6	17% 67% 17%

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
3	BGC	I	1	X	-	-	-
3	BGC	J	1	X	-	-	-
3	BGC	K	1	X	-	-	-
3	BGC	L	1	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16664 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 Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3205	1981	547	664	13			
1	B	426	Total	C	N	O	S	0	2	0
			3205	1981	547	664	13			
1	C	426	Total	C	N	O	S	0	0	0
			3194	1974	546	661	13			
1	D	426	Total	C	N	O	S	0	2	0
			3205	1981	547	664	13			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP O52269
A	4	SER	-	expression tag	UNP O52269
A	5	TRP	-	expression tag	UNP O52269
A	6	SER	-	expression tag	UNP O52269
A	7	HIS	-	expression tag	UNP O52269
A	8	PRO	-	expression tag	UNP O52269
A	9	GLN	-	expression tag	UNP O52269
A	10	PHE	-	expression tag	UNP O52269
A	11	GLU	-	expression tag	UNP O52269
A	12	LYS	-	expression tag	UNP O52269
A	13	SER	-	expression tag	UNP O52269
A	14	GLY	-	expression tag	UNP O52269
A	15	GLY	-	expression tag	UNP O52269
A	16	GLY	-	expression tag	UNP O52269
A	17	GLY	-	expression tag	UNP O52269
A	18	GLY	-	expression tag	UNP O52269
A	19	LEU	-	expression tag	UNP O52269
A	20	VAL	-	expression tag	UNP O52269
A	21	PRO	-	expression tag	UNP O52269
A	22	ARG	-	expression tag	UNP O52269

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP O52269
A	24	SER	-	expression tag	UNP O52269
A	464	GLY	-	expression tag	UNP O52269
A	465	SER	-	expression tag	UNP O52269
A	466	HIS	-	expression tag	UNP O52269
A	467	HIS	-	expression tag	UNP O52269
A	468	HIS	-	expression tag	UNP O52269
A	469	HIS	-	expression tag	UNP O52269
A	470	HIS	-	expression tag	UNP O52269
A	471	HIS	-	expression tag	UNP O52269
B	3	ALA	-	expression tag	UNP O52269
B	4	SER	-	expression tag	UNP O52269
B	5	TRP	-	expression tag	UNP O52269
B	6	SER	-	expression tag	UNP O52269
B	7	HIS	-	expression tag	UNP O52269
B	8	PRO	-	expression tag	UNP O52269
B	9	GLN	-	expression tag	UNP O52269
B	10	PHE	-	expression tag	UNP O52269
B	11	GLU	-	expression tag	UNP O52269
B	12	LYS	-	expression tag	UNP O52269
B	13	SER	-	expression tag	UNP O52269
B	14	GLY	-	expression tag	UNP O52269
B	15	GLY	-	expression tag	UNP O52269
B	16	GLY	-	expression tag	UNP O52269
B	17	GLY	-	expression tag	UNP O52269
B	18	GLY	-	expression tag	UNP O52269
B	19	LEU	-	expression tag	UNP O52269
B	20	VAL	-	expression tag	UNP O52269
B	21	PRO	-	expression tag	UNP O52269
B	22	ARG	-	expression tag	UNP O52269
B	23	GLY	-	expression tag	UNP O52269
B	24	SER	-	expression tag	UNP O52269
B	464	GLY	-	expression tag	UNP O52269
B	465	SER	-	expression tag	UNP O52269
B	466	HIS	-	expression tag	UNP O52269
B	467	HIS	-	expression tag	UNP O52269
B	468	HIS	-	expression tag	UNP O52269
B	469	HIS	-	expression tag	UNP O52269
B	470	HIS	-	expression tag	UNP O52269
B	471	HIS	-	expression tag	UNP O52269
C	3	ALA	-	expression tag	UNP O52269
C	4	SER	-	expression tag	UNP O52269

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	TRP	-	expression tag	UNP O52269
C	6	SER	-	expression tag	UNP O52269
C	7	HIS	-	expression tag	UNP O52269
C	8	PRO	-	expression tag	UNP O52269
C	9	GLN	-	expression tag	UNP O52269
C	10	PHE	-	expression tag	UNP O52269
C	11	GLU	-	expression tag	UNP O52269
C	12	LYS	-	expression tag	UNP O52269
C	13	SER	-	expression tag	UNP O52269
C	14	GLY	-	expression tag	UNP O52269
C	15	GLY	-	expression tag	UNP O52269
C	16	GLY	-	expression tag	UNP O52269
C	17	GLY	-	expression tag	UNP O52269
C	18	GLY	-	expression tag	UNP O52269
C	19	LEU	-	expression tag	UNP O52269
C	20	VAL	-	expression tag	UNP O52269
C	21	PRO	-	expression tag	UNP O52269
C	22	ARG	-	expression tag	UNP O52269
C	23	GLY	-	expression tag	UNP O52269
C	24	SER	-	expression tag	UNP O52269
C	464	GLY	-	expression tag	UNP O52269
C	465	SER	-	expression tag	UNP O52269
C	466	HIS	-	expression tag	UNP O52269
C	467	HIS	-	expression tag	UNP O52269
C	468	HIS	-	expression tag	UNP O52269
C	469	HIS	-	expression tag	UNP O52269
C	470	HIS	-	expression tag	UNP O52269
C	471	HIS	-	expression tag	UNP O52269
D	3	ALA	-	expression tag	UNP O52269
D	4	SER	-	expression tag	UNP O52269
D	5	TRP	-	expression tag	UNP O52269
D	6	SER	-	expression tag	UNP O52269
D	7	HIS	-	expression tag	UNP O52269
D	8	PRO	-	expression tag	UNP O52269
D	9	GLN	-	expression tag	UNP O52269
D	10	PHE	-	expression tag	UNP O52269
D	11	GLU	-	expression tag	UNP O52269
D	12	LYS	-	expression tag	UNP O52269
D	13	SER	-	expression tag	UNP O52269
D	14	GLY	-	expression tag	UNP O52269
D	15	GLY	-	expression tag	UNP O52269
D	16	GLY	-	expression tag	UNP O52269

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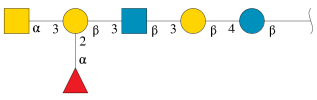
Chain	Residue	Modelled	Actual	Comment	Reference
D	17	GLY	-	expression tag	UNP O52269
D	18	GLY	-	expression tag	UNP O52269
D	19	LEU	-	expression tag	UNP O52269
D	20	VAL	-	expression tag	UNP O52269
D	21	PRO	-	expression tag	UNP O52269
D	22	ARG	-	expression tag	UNP O52269
D	23	GLY	-	expression tag	UNP O52269
D	24	SER	-	expression tag	UNP O52269
D	464	GLY	-	expression tag	UNP O52269
D	465	SER	-	expression tag	UNP O52269
D	466	HIS	-	expression tag	UNP O52269
D	467	HIS	-	expression tag	UNP O52269
D	468	HIS	-	expression tag	UNP O52269
D	469	HIS	-	expression tag	UNP O52269
D	470	HIS	-	expression tag	UNP O52269
D	471	HIS	-	expression tag	UNP O52269

- Molecule 2 is a protein called Nanbody Nb-ER19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	114	Total	C	N	O	S	0	0	0
			873	546	158	164	5			
2	F	115	Total	C	N	O	S	0	0	0
			883	552	161	165	5			
2	G	114	Total	C	N	O	S	0	0	0
			873	546	158	164	5			
2	H	113	Total	C	N	O	S	0	0	0
			863	540	155	163	5			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	K	6	Total C N O 72 40 2 30	0	0	0
3	L	6	Total C N O 72 40 2 30	0	0	0

- Molecule 4 is water.

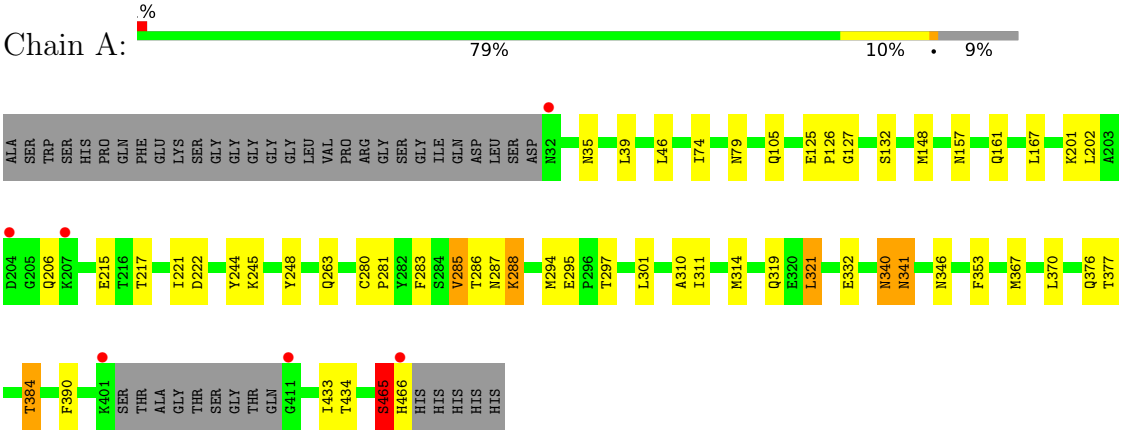
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	23	Total O 23 23	0	0
4	B	14	Total O 14 14	0	0
4	C	12	Total O 12 12	0	0
4	D	9	Total O 9 9	0	0
4	E	5	Total O 5 5	0	0
4	F	2	Total O 2 2	0	0
4	G	8	Total O 8 8	0	0
4	H	2	Total O 2 2	0	0

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.

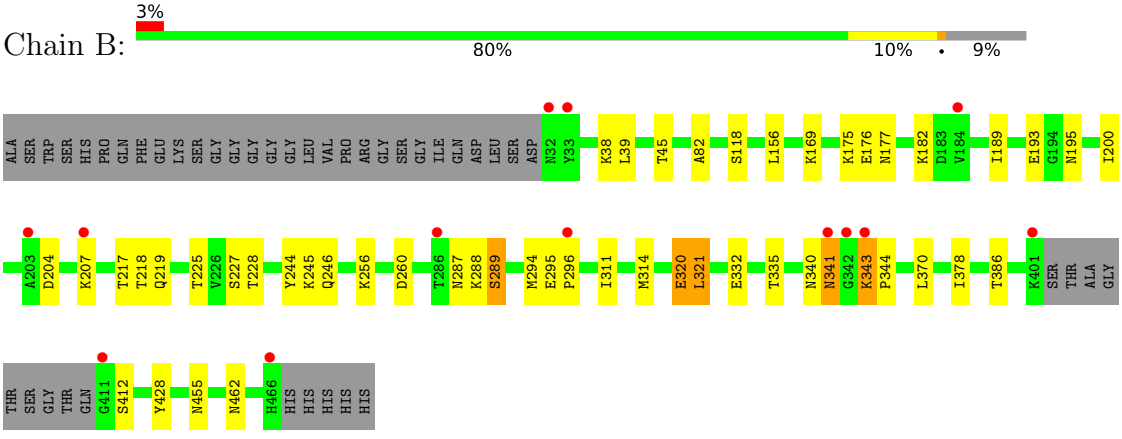
• Molecule 1: Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen

Chain A:



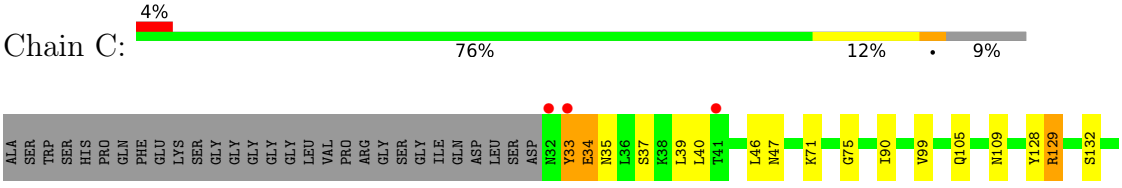
• Molecule 1: Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen

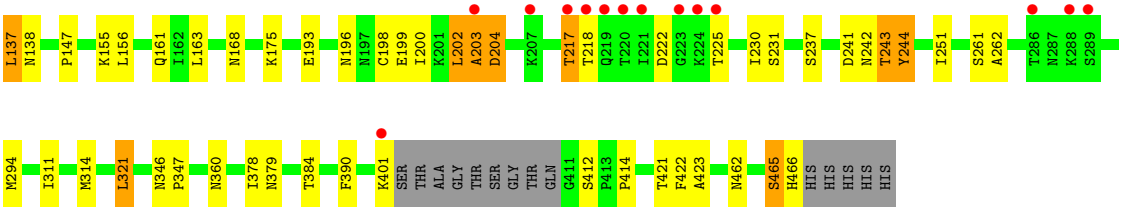
Chain B:



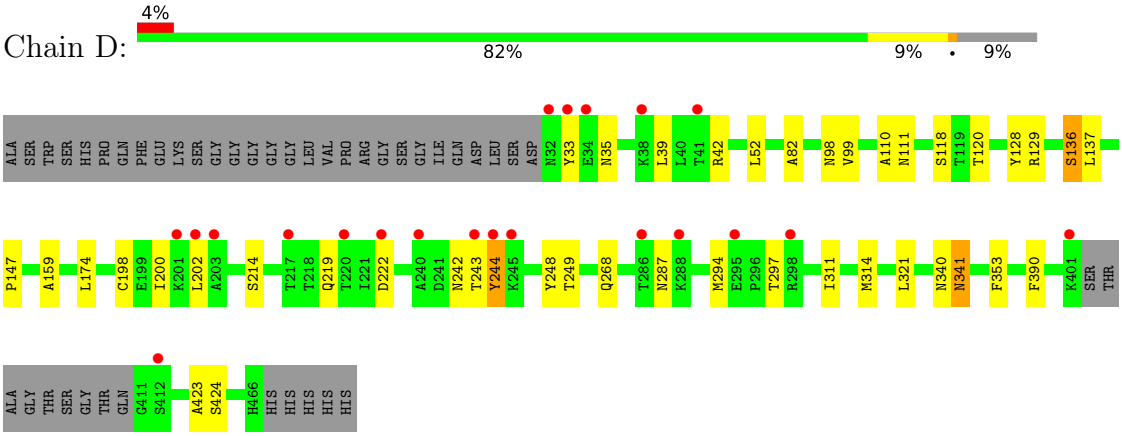
• Molecule 1: Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen

Chain C:

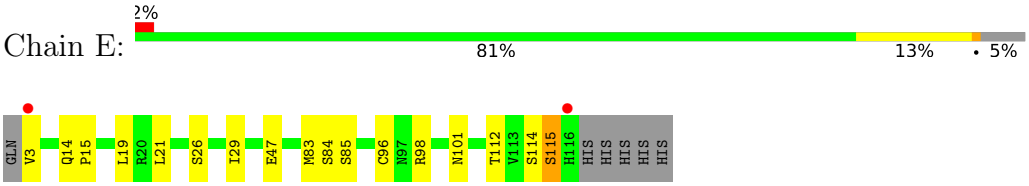




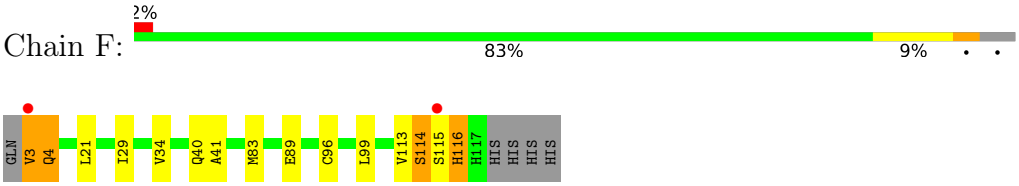
• Molecule 1: Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen



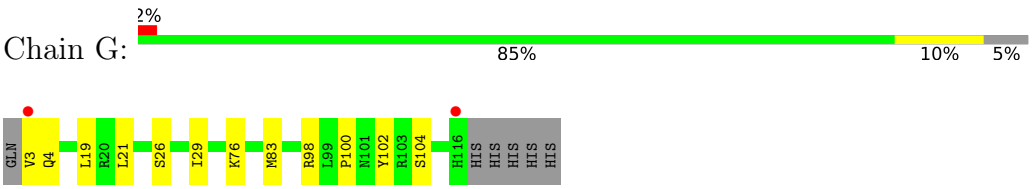
• Molecule 2: Nanbody Nb-ER19



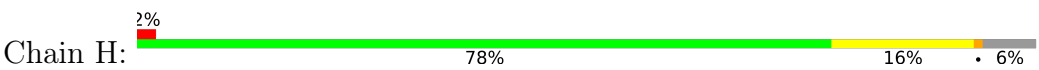
• Molecule 2: Nanbody Nb-ER19



• Molecule 2: Nanbody Nb-ER19

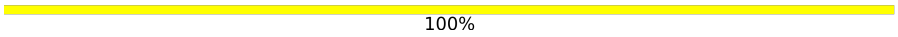


• Molecule 2: Nanbody Nb-ER19



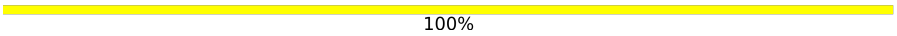
• Molecule 3: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain I:



• Molecule 3: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain J:

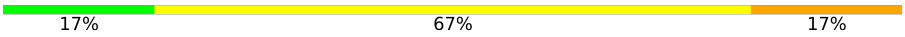


• Molecule 3: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:

• Molecule 3: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.90Å 134.91Å 123.80Å 90.00° 102.52° 90.00°	Depositor
Resolution (Å)	67.46 – 2.62 67.46 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.46-2.62) 99.8 (67.46-2.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.188 , 0.237 0.193 , 0.236	Depositor DCC
R_{free} test set	4878 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16664	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7827e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, BGC, FUC, NAG, A2G

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	1.03	3/3261 (0.1%)	1.08	4/4433 (0.1%)
1	B	1.00	0/3261	1.06	1/4433 (0.0%)
1	C	0.87	0/3244	0.97	1/4410 (0.0%)
1	D	0.87	0/3261	1.00	2/4433 (0.0%)
2	E	0.88	0/893	0.99	0/1210
2	F	0.89	0/904	1.06	3/1225 (0.2%)
2	G	0.94	0/893	1.04	1/1210 (0.1%)
2	H	1.01	1/882 (0.1%)	1.10	4/1195 (0.3%)
All	All	0.94	4/16599 (0.0%)	1.03	16/22549 (0.1%)

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
1	B	0	1
1	D	0	1
2	F	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	PRO	CA-C	-5.56	1.47	1.53
1	A	346	ASN	CA-C	5.38	1.59	1.52
1	A	376	GLN	C-O	-5.24	1.17	1.24
2	H	40	GLN	N-CA	-5.13	1.40	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	4	GLN	N-CA-C	11.18	124.16	108.74
2	F	4	GLN	N-CA-C	8.39	121.09	109.18
2	G	4	GLN	N-CA-C	6.63	118.84	108.96
1	A	79	ASN	N-CA-C	5.97	120.43	113.20
2	F	34	VAL	N-CA-C	-5.97	101.88	109.58
2	H	14	GLN	CA-C-N	-5.86	113.66	119.93
2	H	14	GLN	C-N-CA	-5.86	113.66	119.93
1	B	455	ASN	N-CA-C	5.81	117.69	111.36
1	A	35	ASN	N-CA-C	5.74	117.69	109.14
1	C	99	VAL	CB-CA-C	-5.45	104.79	112.14
1	A	167	LEU	N-CA-C	-5.43	105.52	111.82
1	D	136	SER	N-CA-C	5.36	122.21	110.80
1	A	248	TYR	N-CA-C	5.20	117.09	109.24
2	H	34	VAL	N-CA-C	-5.20	102.88	109.58
1	D	248	TYR	N-CA-C	5.05	117.06	109.23
2	F	29	ILE	CB-CA-C	-5.05	105.25	112.22

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	ILE	Peptide
1	B	341	ASN	Peptide
1	D	341	ASN	Peptide
2	F	3	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3205	0	3106	27	0
1	B	3205	0	3106	21	0
1	C	3194	0	3094	37	0
1	D	3205	0	3106	21	0
2	E	873	0	852	8	0
2	F	883	0	859	7	0
2	G	873	0	852	5	0
2	H	863	0	845	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	72	0	62	0	0
3	J	72	0	61	0	0
3	K	72	0	62	4	0
3	L	72	0	62	2	0
4	A	23	0	0	0	0
4	B	14	0	0	0	0
4	C	12	0	0	0	0
4	D	9	0	0	0	0
4	E	5	0	0	0	0
4	F	2	0	0	0	0
4	G	8	0	0	0	0
4	H	2	0	0	0	0
All	All	16664	0	16067	137	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 4.

All (137) 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:D:242:ASN:O	1:D:244:TYR:N	2.01	0.92
2:E:3:VAL:N	2:E:26:SER:HG	1.70	0.90
3:L:1:BGC:H6C1	3:L:2:GAL:C1	2.03	0.88
1:A:201:LYS:O	1:A:206:GLN:O	1.91	0.87
1:A:311:ILE:HA	1:A:314:MET:HE3	1.62	0.81
1:B:311:ILE:HA	1:B:314:MET:HE3	1.68	0.75
3:K:3:NAG:H81	3:K:5:FUC:H3	1.75	0.68
2:E:21:LEU:HG	2:E:83:MET:HE2	1.78	0.64
3:K:3:NAG:C8	3:K:5:FUC:H3	2.27	0.63
1:C:75:GLY:HA2	1:C:175:LYS:HE3	1.79	0.63
2:H:19:LEU:HB2	2:H:83:MET:HE3	1.82	0.62
1:B:175:LYS:HE3	1:B:176:GLU:OE2	2.00	0.62
2:G:3:VAL:N	2:G:26:SER:HG	1.97	0.60
1:D:52:LEU:CD1	2:H:45:LEU:HD11	2.33	0.58
2:F:114:SER:OG	2:F:115:SER:CB	2.52	0.58
1:C:311:ILE:HA	1:C:314:MET:HE3	1.85	0.57
1:D:294:MET:HE3	1:D:294:MET:HA	1.87	0.56
2:F:40:GLN:NE2	2:F:41:ALA:O	2.38	0.56
2:G:21:LEU:HG	2:G:83:MET:HE2	1.87	0.56
2:G:19:LEU:HB2	2:G:83:MET:HE3	1.88	0.54
1:D:340:ASN:O	1:D:341:ASN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:SER:OG	2:F:115:SER:HB2	2.08	0.54
1:A:281:PRO:HG2	1:A:301:LEU:HD12	1.90	0.53
1:D:118:SER:O	1:D:136:SER:HA	2.08	0.53
1:D:82:ALA:HB1	1:D:321:LEU:HD21	1.89	0.53
1:B:320[A]:GLU:HB3	1:B:370:LEU:HD13	1.91	0.53
1:D:128:TYR:O	1:D:129:ARG:C	2.52	0.52
1:C:137:LEU:HD23	1:C:138:ASN:N	2.24	0.52
1:D:33:TYR:OH	1:D:42:ARG:NH1	2.43	0.51
1:C:218:THR:HB	1:C:225:THR:HG22	1.90	0.51
1:C:242:ASN:O	1:C:243:THR:C	2.53	0.51
2:E:3:VAL:O	2:E:3:VAL:HG23	2.10	0.51
3:K:3:NAG:H82	3:K:5:FUC:H5	1.92	0.51
1:B:343:LYS:HG2	1:B:344:PRO:N	2.26	0.51
1:A:321:LEU:C	1:A:321:LEU:HD23	2.36	0.50
1:A:263:GLN:HE22	1:A:319:GLN:HG2	1.75	0.50
2:G:102:TYR:CE2	2:G:104:SER:HB2	2.47	0.50
1:C:109:ASN:HB3	1:C:196:ASN:OD1	2.13	0.49
1:C:168:ASN:HA	1:C:414:PRO:O	2.13	0.49
2:E:3:VAL:N	2:E:26:SER:OG	2.40	0.49
1:B:412:SER:O	1:B:428:TYR:OH	2.26	0.48
1:B:321:LEU:C	1:B:321:LEU:HD23	2.38	0.48
2:G:98:ARG:HG3	2:G:100:PRO:O	2.13	0.48
1:C:401:LYS:HA	1:C:401:LYS:HE2	1.95	0.48
1:A:294:MET:HE3	1:A:295:GLU:H	1.77	0.48
1:B:82:ALA:HB1	1:B:321:LEU:HD21	1.95	0.48
1:C:242:ASN:O	1:C:244:TYR:O	2.32	0.48
1:C:465:SER:O	1:C:466:HIS:HB2	2.13	0.48
1:C:346:ASN:OD1	1:C:346:ASN:C	2.57	0.48
1:B:288:LYS:HG2	1:B:289:SER:O	2.14	0.48
1:B:217:THR:CG2	1:B:228:THR:HB	2.44	0.48
1:B:217:THR:HG23	1:B:228:THR:HB	1.96	0.48
1:B:244:TYR:C	1:B:246:GLN:H	2.22	0.47
3:L:1:BGC:C6	3:L:2:GAL:C1	2.83	0.47
2:H:18:SER:HA	2:H:83:MET:O	2.14	0.47
1:A:310:ALA:HB1	1:A:377:THR:HG22	1.96	0.47
1:A:148:MET:HE3	1:A:281:PRO:HG3	1.97	0.47
1:B:156:LEU:C	1:B:156:LEU:HD23	2.39	0.47
2:E:19:LEU:HB2	2:E:83:MET:HE3	1.97	0.47
2:F:21:LEU:HG	2:F:83:MET:HE2	1.97	0.47
1:C:40:LEU:HD13	1:C:47:ASN:OD1	2.15	0.47
1:D:137:LEU:HD23	1:D:147:PRO:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:SER:O	1:A:466:HIS:HB2	2.15	0.46
2:E:98:ARG:O	2:E:101:ASN:HA	2.16	0.46
1:A:244:TYR:O	1:A:245:LYS:C	2.58	0.46
1:C:198:CYS:HB2	1:C:251:ILE:CG1	2.46	0.46
1:C:90:ILE:HG23	1:C:163:LEU:HD22	1.98	0.45
1:D:353:PHE:CD1	1:D:353:PHE:C	2.94	0.45
1:A:294:MET:HE1	1:A:390:PHE:HD2	1.80	0.45
1:B:118:SER:OG	1:B:195:ASN:HA	2.16	0.45
1:B:314:MET:HE1	1:B:378:ILE:HD13	1.96	0.45
1:C:35:ASN:C	1:C:35:ASN:OD1	2.59	0.45
1:A:201:LYS:O	1:A:202:LEU:HB2	2.15	0.45
2:H:14:GLN:O	2:H:15:PRO:C	2.57	0.45
1:A:125:GLU:OE2	1:A:157:ASN:ND2	2.39	0.45
1:B:169:LYS:NZ	1:B:260:ASP:OD2	2.49	0.45
2:E:84:SER:O	2:E:85:SER:C	2.59	0.45
1:B:38:LYS:N	1:B:38:LYS:HD3	2.31	0.44
1:D:159:ALA:HA	1:D:268:GLN:OE1	2.17	0.44
1:C:198:CYS:HB2	1:C:251:ILE:HD11	1.99	0.44
1:A:127:GLY:HA3	1:A:132:SER:O	2.18	0.44
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.99	0.44
1:D:52:LEU:HD11	2:H:45:LEU:HD11	2.00	0.44
1:B:294:MET:HE3	1:B:294:MET:HA	2.00	0.43
1:A:215:GLU:OE1	2:H:44:LYS:HE2	2.18	0.43
1:D:294:MET:HE1	1:D:390:PHE:HD2	1.83	0.43
1:C:314:MET:SD	1:C:378:ILE:HB	2.58	0.43
2:H:98:ARG:HG3	2:H:100:PRO:O	2.18	0.43
1:A:280:CYS:N	1:A:281:PRO:CD	2.81	0.43
1:A:353:PHE:CD1	1:A:353:PHE:C	2.96	0.43
1:C:294:MET:HE1	1:C:390:PHE:HD2	1.84	0.43
1:C:321:LEU:C	1:C:321:LEU:HD23	2.43	0.43
1:D:174:LEU:N	1:D:174:LEU:HD12	2.33	0.43
2:E:15:PRO:HD3	2:E:115:SER:HA	2.01	0.43
1:C:202:LEU:O	1:C:203:ALA:C	2.61	0.43
1:C:360:ASN:OD1	1:C:360:ASN:C	2.62	0.42
1:D:200:ILE:HD12	1:D:200:ILE:N	2.34	0.42
1:A:283:PHE:CD2	1:A:283:PHE:C	2.94	0.42
1:B:244:TYR:C	1:B:246:GLN:N	2.77	0.42
1:C:199:GLU:HB2	3:K:6:A2G:O3	2.19	0.42
1:C:422:PHE:O	1:C:423:ALA:HB3	2.18	0.42
1:C:161:GLN:NE2	1:C:161:GLN:HA	2.34	0.42
1:C:33:TYR:O	1:C:34:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HD23	1:C:156:LEU:O	2.20	0.42
1:C:200:ILE:HG12	1:C:230:ILE:HD11	2.01	0.42
1:B:343:LYS:HG3	1:B:344:PRO:HD2	2.01	0.42
1:C:346:ASN:HA	1:C:347:PRO:HD3	1.89	0.42
2:F:113:VAL:O	2:F:114:SER:HB2	2.20	0.42
1:A:287:ASN:O	1:A:288:LYS:HG2	2.19	0.42
1:A:340:ASN:O	1:A:341:ASN:CB	2.68	0.42
1:C:261:SER:O	1:C:262:ALA:C	2.62	0.42
1:C:421:THR:O	1:C:422:PHE:C	2.62	0.42
1:A:157:ASN:O	1:A:161:GLN:HG2	2.20	0.42
1:A:285:VAL:O	1:A:297:THR:HG23	2.20	0.41
1:C:203:ALA:O	1:C:204:ASP:HB3	2.20	0.41
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.88	0.41
1:D:98:ASN:HB3	1:D:424:SER:O	2.20	0.41
1:D:294:MET:HE1	1:D:390:PHE:CD2	2.56	0.41
2:F:3:VAL:HG12	2:F:4:GLN:HB3	2.01	0.41
1:A:433:ILE:O	1:A:434:THR:C	2.63	0.41
1:D:311:ILE:HA	1:D:314:MET:HE3	2.03	0.41
1:C:379:ASN:OD1	1:C:379:ASN:C	2.64	0.41
1:D:35:ASN:OD1	1:D:35:ASN:C	2.63	0.41
1:C:33:TYR:HB3	1:C:39:LEU:CD2	2.51	0.41
1:D:198:CYS:SG	1:D:249:THR:HB	2.61	0.41
1:A:201:LYS:O	1:A:202:LEU:CB	2.69	0.41
1:A:384:THR:HG21	1:B:335:THR:HA	2.03	0.41
1:C:465:SER:O	1:C:466:HIS:CB	2.67	0.41
2:H:25:ALA:O	2:H:77:ASN:HB3	2.21	0.41
1:D:99:VAL:O	1:D:423:ALA:HA	2.20	0.41
1:C:105:GLN:HG3	1:C:147:PRO:HA	2.04	0.40
2:F:115:SER:O	2:F:116:HIS:HB2	2.20	0.40
1:B:295:GLU:HA	1:B:296:PRO:HA	1.96	0.40
1:C:128:TYR:O	1:C:129:ARG:C	2.64	0.40
1:C:156:LEU:HD23	1:C:156:LEU:C	2.46	0.40
1:A:74:ILE:CG2	1:A:367:MET:HE1	2.51	0.40
2:H:98:ARG:O	2:H:101:ASN:HA	2.22	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	424/469 (90%)	402 (95%)	18 (4%)	4 (1%)	14 28
1	B	424/469 (90%)	399 (94%)	21 (5%)	4 (1%)	14 28
1	C	422/469 (90%)	386 (92%)	26 (6%)	10 (2%)	4 8
1	D	424/469 (90%)	386 (91%)	32 (8%)	6 (1%)	9 17
2	E	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	14 28
2	F	113/120 (94%)	107 (95%)	3 (3%)	3 (3%)	4 6
2	G	112/120 (93%)	111 (99%)	1 (1%)	0	100 100
2	H	111/120 (92%)	104 (94%)	6 (5%)	1 (1%)	14 28
All	All	2142/2356 (91%)	2003 (94%)	110 (5%)	29 (1%)	9 17

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ASP
1	A	340	ASN
1	A	341	ASN
1	B	341	ASN
1	C	204	ASP
1	D	243	THR
1	D	287	ASN
2	F	114	SER
1	A	465	SER
1	C	34	GLU
1	C	222	ASP
1	D	222	ASP
1	D	244	TYR
2	E	115	SER
2	F	116	HIS
1	C	203	ALA
1	C	241	ASP

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Mol	Chain	Res	Type
1	C	243	THR
2	F	89	GLU
1	B	287	ASN
1	C	217	THR
1	C	244	TYR
1	D	110	ALA
1	B	245	LYS
1	C	237	SER
1	D	214	SER
1	C	465	SER
1	B	343	LYS
2	H	58	PRO

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	353/384 (92%)	342 (97%)	11 (3%)	35	61
1	B	353/384 (92%)	331 (94%)	22 (6%)	16	35
1	C	351/384 (91%)	335 (95%)	16 (5%)	24	47
1	D	353/384 (92%)	347 (98%)	6 (2%)	53	76
2	E	93/99 (94%)	87 (94%)	6 (6%)	15	33
2	F	94/99 (95%)	92 (98%)	2 (2%)	47	72
2	G	93/99 (94%)	91 (98%)	2 (2%)	45	70
2	H	92/99 (93%)	89 (97%)	3 (3%)	33	59
All	All	1782/1932 (92%)	1714 (96%)	68 (4%)	29	54

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	46	LEU
1	A	105	GLN

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Mol	Chain	Res	Type
1	A	217	THR
1	A	285	VAL
1	A	286	THR
1	A	288	LYS
1	A	321	LEU
1	A	332	GLU
1	A	384	THR
1	A	465	SER
1	B	39	LEU
1	B	45	THR
1	B	177	ASN
1	B	182	LYS
1	B	189	ILE
1	B	193	GLU
1	B	200	ILE
1	B	204	ASP
1	B	207	LYS
1	B	218	THR
1	B	219	GLN
1	B	225	THR
1	B	227	SER
1	B	256	LYS
1	B	289	SER
1	B	320[A]	GLU
1	B	320[B]	GLU
1	B	321	LEU
1	B	332	GLU
1	B	340	ASN
1	B	386	THR
1	B	462	ASN
1	C	33	TYR
1	C	37	SER
1	C	46	LEU
1	C	71	LYS
1	C	129	ARG
1	C	132	SER
1	C	137	LEU
1	C	155	LYS
1	C	193	GLU
1	C	202	LEU
1	C	217	THR
1	C	231	SER

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Mol	Chain	Res	Type
1	C	321	LEU
1	C	384	THR
1	C	412	SER
1	C	462	ASN
1	D	39	LEU
1	D	111	ASN
1	D	120	THR
1	D	202	LEU
1	D	219	GLN
1	D	297	THR
2	E	14	GLN
2	E	29	ILE
2	E	47	GLU
2	E	96	CYS
2	E	112	THR
2	E	114	SER
2	F	96	CYS
2	F	99	LEU
2	G	29	ILE
2	G	76	LYS
2	H	23	CYS
2	H	26	SER
2	H	28	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	124	ASN
1	A	157	ASN
1	A	161	GLN
1	A	197	ASN
1	A	253	ASN
1	A	263	GLN
1	A	277	ASN
1	A	293	GLN
1	A	355	GLN
1	A	373	GLN
1	A	431	GLN
1	B	123	ASN
1	B	124	ASN
1	B	157	ASN

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Mol	Chain	Res	Type
1	B	161	GLN
1	B	168	ASN
1	B	177	ASN
1	B	324	GLN
1	B	341	ASN
1	B	364	GLN
1	C	124	ASN
1	C	157	ASN
1	C	161	GLN
1	C	274	ASN
1	C	312	GLN
1	C	324	GLN
1	C	369	ASN
1	C	373	GLN
1	D	124	ASN
1	D	178	ASN
1	D	263	GLN
1	D	277	ASN
1	D	364	GLN
1	D	373	GLN
2	E	40	GLN
2	G	14	GLN
2	G	40	GLN
2	G	55	GLN
2	G	116	HIS

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

24 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	$\#\|Z\| > 2$
3	BGC	I	1	3	12,12,12	0.63	0	17,17,17	1.88	3 (17%)
3	GAL	I	2	3	11,11,12	0.73	0	15,15,17	1.42	2 (13%)
3	NAG	I	3	3	14,14,15	0.87	1 (7%)	17,19,21	2.54	10 (58%)
3	GAL	I	4	3	11,11,12	0.69	0	15,15,17	1.59	3 (20%)
3	FUC	I	5	3	10,10,11	0.85	0	14,14,16	1.31	1 (7%)
3	A2G	I	6	3	14,14,15	0.62	0	17,19,21	1.37	2 (11%)
3	BGC	J	1	3	12,12,12	0.70	0	17,17,17	2.15	5 (29%)
3	GAL	J	2	3	11,11,12	0.66	0	15,15,17	1.15	1 (6%)
3	NAG	J	3	3	14,14,15	0.65	0	17,19,21	1.58	4 (23%)
3	GAL	J	4	3	11,11,12	0.71	0	15,15,17	1.61	3 (20%)
3	FUC	J	5	3	10,10,11	0.82	0	14,14,16	1.05	1 (7%)
3	A2G	J	6	3	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
3	BGC	K	1	3	12,12,12	0.65	0	17,17,17	1.36	3 (17%)
3	GAL	K	2	3	11,11,12	0.68	0	15,15,17	1.32	1 (6%)
3	NAG	K	3	3	14,14,15	0.63	0	17,19,21	2.50	6 (35%)
3	GAL	K	4	3	11,11,12	0.64	0	15,15,17	1.22	2 (13%)
3	FUC	K	5	3	10,10,11	0.70	0	14,14,16	1.51	3 (21%)
3	A2G	K	6	3	14,14,15	0.42	0	17,19,21	1.71	3 (17%)
3	BGC	L	1	3	12,12,12	0.46	0	17,17,17	0.53	0
3	GAL	L	2	3	11,11,12	0.68	0	15,15,17	1.22	1 (6%)
3	NAG	L	3	3	14,14,15	0.67	0	17,19,21	1.21	1 (5%)
3	GAL	L	4	3	11,11,12	0.87	0	15,15,17	1.47	3 (20%)
3	FUC	L	5	3	10,10,11	0.64	0	14,14,16	0.85	0
3	A2G	L	6	3	14,14,15	0.39	0	17,19,21	1.38	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	I	1	3	1/1/5/5	0/2/22/22	0/1/1/1
3	GAL	I	2	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	3	3	-	2/6/23/26	0/1/1/1
3	GAL	I	4	3	-	0/2/19/22	0/1/1/1
3	FUC	I	5	3	-	-	0/1/1/1
3	A2G	I	6	3	-	4/6/23/26	0/1/1/1
3	BGC	J	1	3	1/1/5/5	1/2/22/22	0/1/1/1
3	GAL	J	2	3	-	2/2/19/22	0/1/1/1
3	NAG	J	3	3	-	0/6/23/26	0/1/1/1
3	GAL	J	4	3	-	1/2/19/22	0/1/1/1
3	FUC	J	5	3	-	-	0/1/1/1
3	A2G	J	6	3	-	4/6/23/26	0/1/1/1
3	BGC	K	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	GAL	K	2	3	-	0/2/19/22	0/1/1/1
3	NAG	K	3	3	-	4/6/23/26	0/1/1/1
3	GAL	K	4	3	-	1/2/19/22	0/1/1/1
3	FUC	K	5	3	-	-	0/1/1/1
3	A2G	K	6	3	-	4/6/23/26	0/1/1/1
3	BGC	L	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	GAL	L	2	3	-	2/2/19/22	0/1/1/1
3	NAG	L	3	3	-	0/6/23/26	0/1/1/1
3	GAL	L	4	3	-	2/2/19/22	0/1/1/1
3	FUC	L	5	3	-	-	0/1/1/1
3	A2G	L	6	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	NAG	C1-C2	2.10	1.55	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3	NAG	C1-O5-C5	5.73	119.86	112.19
3	K	3	NAG	C2-N2-C7	5.01	129.61	122.90
3	I	3	NAG	C1-C2-N2	4.89	118.14	110.43
3	K	3	NAG	C1-O5-C5	4.51	118.24	112.19
3	K	6	A2G	C1-C2-N2	-4.43	103.46	110.43
3	K	3	NAG	O7-C7-C8	-4.37	114.26	122.05
3	J	1	BGC	O1-C1-C2	4.28	121.41	108.98
3	I	1	BGC	O1-C1-C2	4.24	121.29	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	4	GAL	C1-C2-C3	4.19	115.75	109.64
3	J	1	BGC	O1-C1-O5	4.10	122.58	110.41
3	I	1	BGC	O5-C1-C2	3.78	116.94	110.30
3	K	3	NAG	C8-C7-N2	3.76	122.35	116.12
3	K	6	A2G	C2-N2-C7	3.69	127.85	122.90
3	I	1	BGC	O1-C1-O5	3.58	121.03	110.41
3	L	4	GAL	C1-C2-C3	3.56	114.83	109.64
3	K	2	GAL	C1-C2-C3	3.54	114.80	109.64
3	K	5	FUC	C1-C2-C3	3.52	114.77	109.64
3	J	1	BGC	O5-C5-C4	3.45	115.92	109.70
3	J	4	GAL	C1-C2-C3	3.29	114.44	109.64
3	I	2	GAL	C1-C2-C3	-3.18	105.01	109.64
3	J	4	GAL	O5-C5-C6	3.16	113.81	107.66
3	I	6	A2G	C8-C7-N2	3.15	121.34	116.12
3	L	6	A2G	C1-O5-C5	3.14	116.40	112.19
3	J	1	BGC	C1-O5-C5	3.04	119.53	113.65
3	J	1	BGC	O5-C1-C2	3.02	115.61	110.30
3	K	1	BGC	O4-C4-C5	3.00	116.70	109.32
3	L	6	A2G	C8-C7-N2	2.97	121.04	116.12
3	J	6	A2G	O5-C1-C2	-2.96	106.71	111.29
3	J	3	NAG	C1-C2-N2	2.93	115.06	110.43
3	I	3	NAG	O7-C7-C8	-2.88	116.93	122.05
3	J	2	GAL	C2-C3-C4	-2.74	106.05	110.86
3	I	5	FUC	C2-C3-C4	-2.71	106.09	110.86
3	K	5	FUC	C3-C4-C5	2.67	113.87	109.81
3	K	4	GAL	C1-O5-C5	2.65	115.74	112.19
3	J	3	NAG	C4-C3-C2	-2.65	107.14	111.02
3	K	1	BGC	C3-C4-C5	-2.64	105.44	110.23
3	K	3	NAG	O3-C3-C2	-2.61	103.98	109.40
3	I	3	NAG	O7-C7-N2	2.60	126.58	121.98
3	J	4	GAL	C3-C4-C5	-2.51	105.68	110.23
3	J	5	FUC	C1-C2-C3	2.49	113.27	109.64
3	J	6	A2G	O7-C7-N2	-2.48	117.59	121.98
3	I	3	NAG	C2-N2-C7	2.46	126.19	122.90
3	L	4	GAL	O5-C5-C4	-2.42	104.94	110.83
3	I	2	GAL	C2-C3-C4	-2.34	106.74	110.86
3	K	3	NAG	O5-C5-C6	2.33	112.19	107.66
3	I	3	NAG	C4-C3-C2	2.29	114.38	111.02
3	I	4	GAL	O6-C6-C5	-2.28	103.58	111.33
3	L	2	GAL	O3-C3-C4	2.27	115.73	110.38
3	L	4	GAL	O5-C5-C6	2.23	112.01	107.66
3	K	5	FUC	O5-C5-C6	2.22	112.23	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	1	BGC	C1-C2-C3	2.22	114.89	110.36
3	K	6	A2G	C3-C4-C5	2.16	114.15	110.23
3	I	6	A2G	O5-C1-C2	-2.15	107.97	111.29
3	K	4	GAL	C3-C4-C5	-2.14	106.35	110.23
3	I	3	NAG	O3-C3-C4	-2.13	105.36	110.38
3	I	3	NAG	O5-C5-C4	2.11	115.97	110.83
3	J	3	NAG	O5-C5-C6	2.11	111.77	107.66
3	I	3	NAG	O4-C4-C3	-2.11	105.41	110.38
3	I	3	NAG	C3-C4-C5	2.10	114.04	110.23
3	J	3	NAG	O7-C7-N2	2.10	125.68	121.98
3	I	4	GAL	O3-C3-C2	-2.04	105.88	110.05
3	L	3	NAG	C1-C2-N2	2.04	113.64	110.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	1	BGC	C1
3	J	1	BGC	C1
3	K	1	BGC	C1
3	L	1	BGC	C1

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	3	NAG	O5-C5-C6-O6
3	L	4	GAL	O5-C5-C6-O6
3	I	3	NAG	O5-C5-C6-O6
3	L	2	GAL	O5-C5-C6-O6
3	I	2	GAL	O5-C5-C6-O6
3	K	1	BGC	O5-C5-C6-O6
3	K	3	NAG	C4-C5-C6-O6
3	K	1	BGC	C4-C5-C6-O6
3	K	6	A2G	C4-C5-C6-O6
3	I	6	A2G	C4-C5-C6-O6
3	L	4	GAL	C4-C5-C6-O6
3	I	3	NAG	C4-C5-C6-O6
3	K	6	A2G	O5-C5-C6-O6
3	I	2	GAL	C4-C5-C6-O6
3	L	2	GAL	C4-C5-C6-O6
3	L	1	BGC	O5-C5-C6-O6
3	I	6	A2G	O7-C7-N2-C2
3	I	6	A2G	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	J	6	A2G	O7-C7-N2-C2
3	J	6	A2G	C8-C7-N2-C2
3	K	3	NAG	C8-C7-N2-C2
3	K	3	NAG	O7-C7-N2-C2
3	L	6	A2G	O7-C7-N2-C2
3	L	6	A2G	C8-C7-N2-C2
3	I	6	A2G	O5-C5-C6-O6
3	L	1	BGC	C4-C5-C6-O6
3	L	6	A2G	O5-C5-C6-O6
3	J	2	GAL	O5-C5-C6-O6
3	J	1	BGC	O5-C5-C6-O6
3	J	2	GAL	C4-C5-C6-O6
3	K	4	GAL	O5-C5-C6-O6
3	J	6	A2G	C4-C5-C6-O6
3	L	6	A2G	C4-C5-C6-O6
3	K	6	A2G	C3-C2-N2-C7
3	J	6	A2G	C1-C2-N2-C7
3	K	6	A2G	C1-C2-N2-C7
3	J	4	GAL	C4-C5-C6-O6

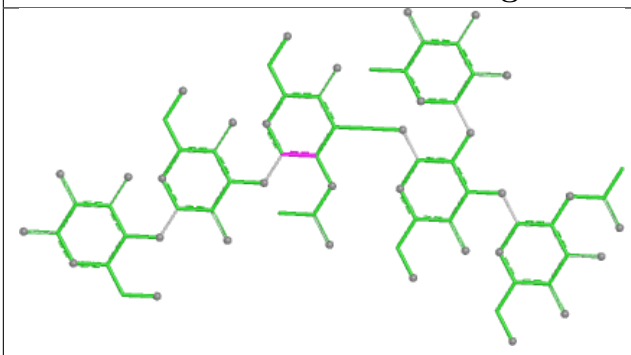
There are no ring outliers.

5 monomers are involved in 6 short contacts:

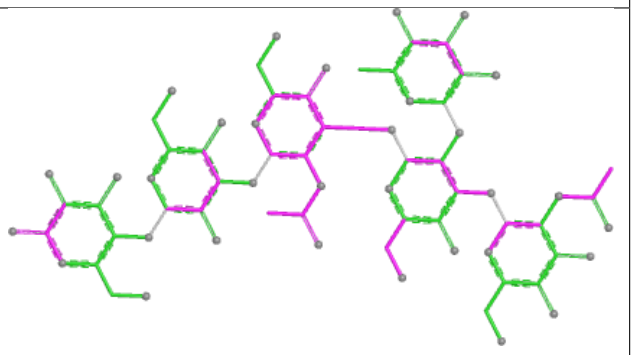
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	6	A2G	1	0
3	K	5	FUC	3	0
3	L	2	GAL	2	0
3	K	3	NAG	3	0
3	L	1	BGC	2	0

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

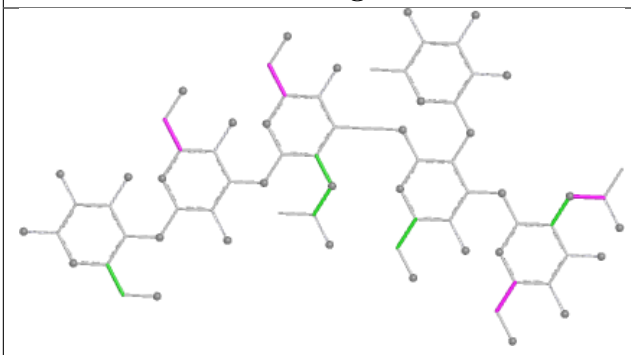
Oligosaccharide Chain I



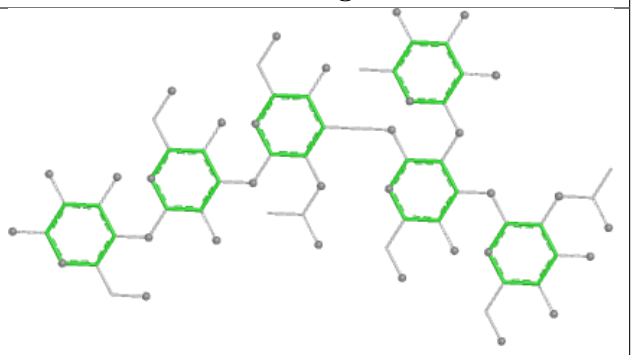
Bond lengths



Bond angles

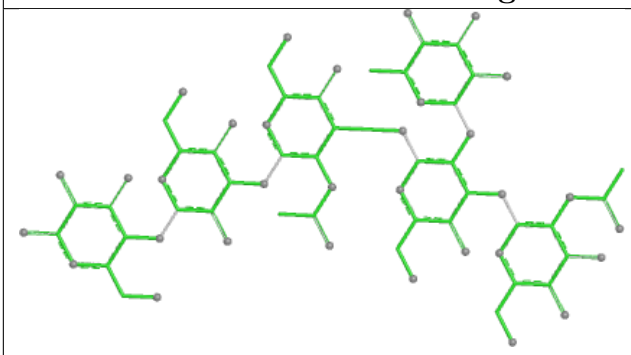


Torsions

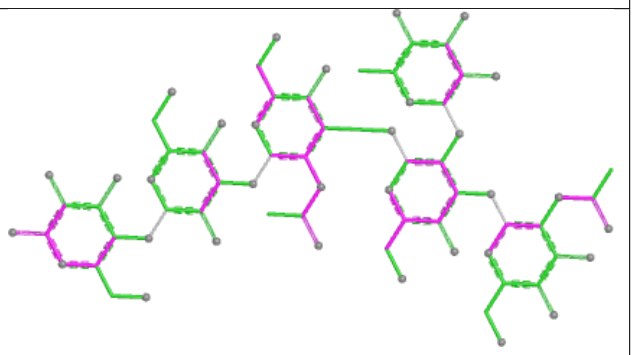


Rings

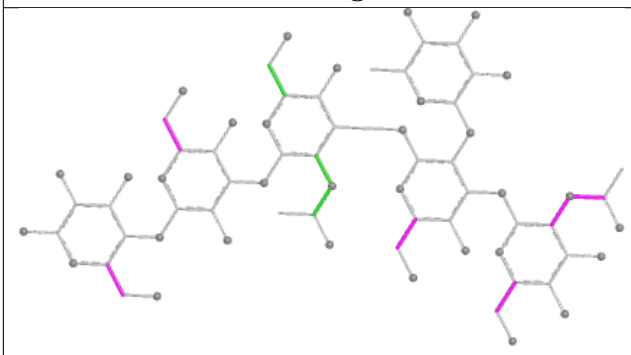
Oligosaccharide Chain J



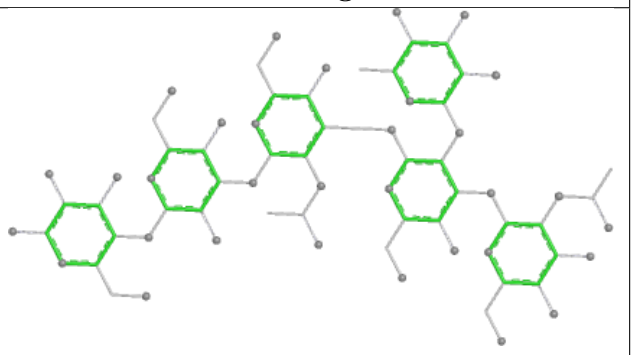
Bond lengths



Bond angles

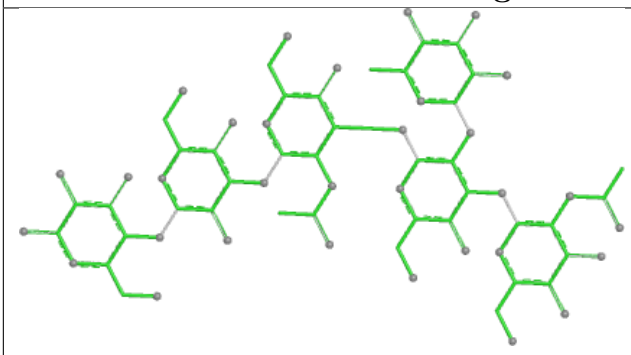


Torsions

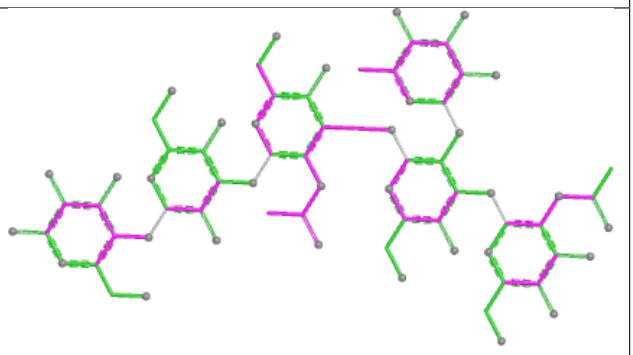


Rings

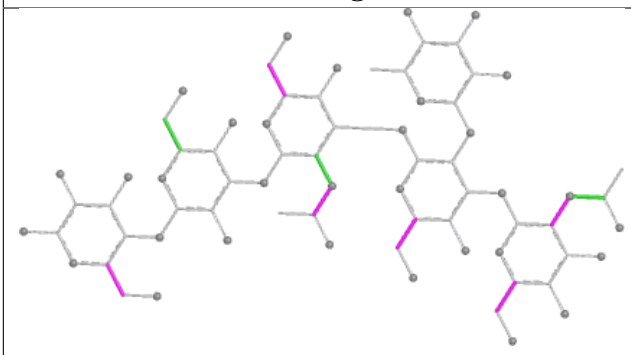
Oligosaccharide Chain K



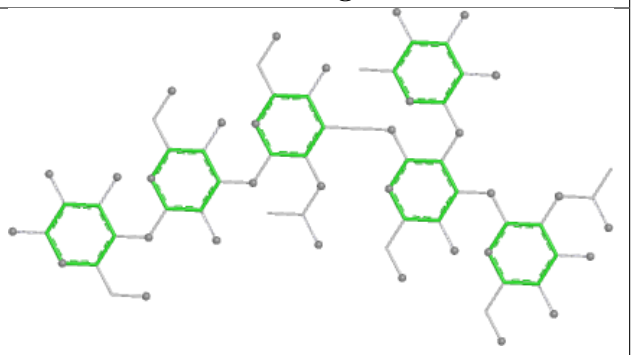
Bond lengths



Bond angles

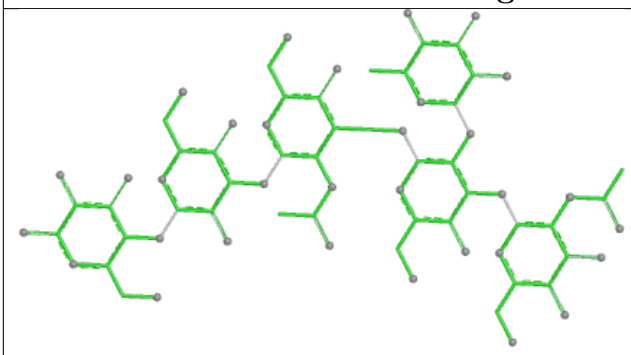


Torsions

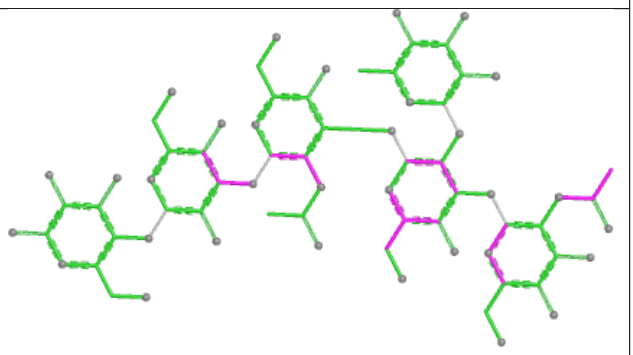


Rings

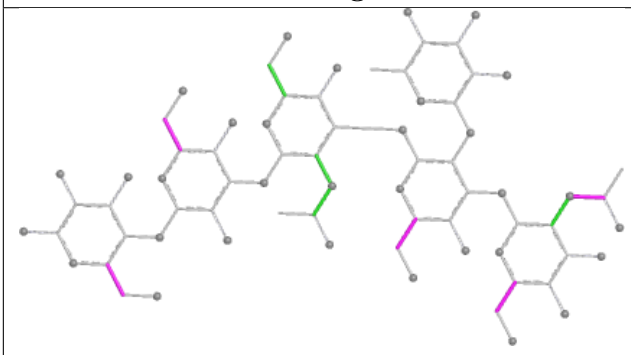
Oligosaccharide Chain L



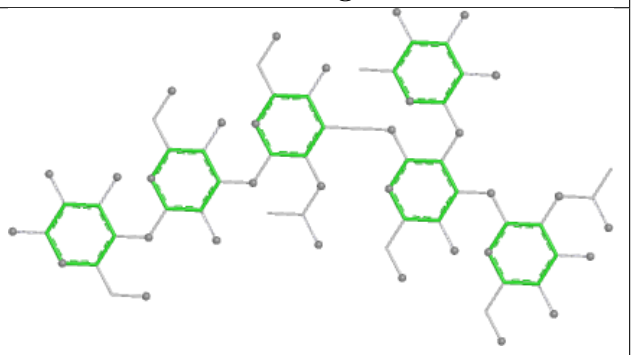
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	426/469 (90%)	-0.30	6 (1%)	73	70	28, 52, 94, 133	2 (0%)
1	B	426/469 (90%)	-0.28	13 (3%)	51	46	27, 55, 106, 133	2 (0%)
1	C	426/469 (90%)	-0.06	17 (3%)	42	37	41, 65, 120, 146	0
1	D	426/469 (90%)	-0.01	21 (4%)	35	29	33, 66, 123, 144	2 (0%)
2	E	114/120 (95%)	-0.37	2 (1%)	67	63	40, 59, 83, 126	0
2	F	115/120 (95%)	-0.27	2 (1%)	69	65	44, 64, 92, 115	0
2	G	114/120 (95%)	-0.43	2 (1%)	67	63	39, 53, 72, 91	0
2	H	113/120 (94%)	-0.40	2 (1%)	67	63	38, 52, 67, 99	0
All	All	2160/2356 (91%)	-0.21	65 (3%)	52	47	27, 58, 110, 146	6 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	3	VAL	6.8
2	F	3	VAL	6.2
2	E	116	HIS	5.5
1	D	202	LEU	5.4
1	D	401	LYS	5.4
2	H	3	VAL	4.9
1	B	401	LYS	4.5
1	B	342	GLY	4.5
1	A	32	ASN	4.2
2	E	3	VAL	4.2
1	C	221	ILE	3.9
1	B	296	PRO	3.9
1	D	286	THR	3.9
1	A	401	LYS	3.8
1	B	32	ASN	3.4
1	D	33	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	220	THR	3.3
1	C	203	ALA	3.3
1	A	204	ASP	3.2
1	C	286	THR	3.1
1	D	203	ALA	3.1
2	F	115	SER	3.1
1	B	411	GLY	3.0
1	D	201	LYS	3.0
1	C	32	ASN	3.0
1	C	217	THR	2.9
1	B	343	LYS	2.8
1	A	411	GLY	2.8
1	B	33	TYR	2.8
1	C	33	TYR	2.8
1	D	32	ASN	2.7
1	C	401	LYS	2.7
1	D	220	THR	2.7
1	D	34	GLU	2.7
1	B	207	LYS	2.7
1	A	466	HIS	2.6
1	B	286	THR	2.6
1	D	240	ALA	2.6
2	G	116	HIS	2.6
1	C	207	LYS	2.5
1	C	223	GLY	2.5
1	D	288	LYS	2.5
1	C	219	GLN	2.4
1	D	412	SER	2.4
1	D	243	THR	2.3
1	B	466	HIS	2.3
1	B	341	ASN	2.3
1	C	41	THR	2.3
1	C	288	LYS	2.3
1	D	41	THR	2.3
1	D	298	ARG	2.3
1	B	203	ALA	2.2
1	C	218	THR	2.2
1	D	244	TYR	2.2
1	A	207	LYS	2.2
1	D	38	LYS	2.2
1	D	245	LYS	2.2
1	C	289	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	295	GLU	2.1
1	C	224	LYS	2.1
1	D	217	THR	2.0
1	D	222	ASP	2.0
1	C	225	THR	2.0
1	B	184	VAL	2.0
2	H	103	ARG	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, 95^{th} 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
3	BGC	L	1	12/12	0.18	0.17	97,113,118,119	0
3	GAL	L	2	11/12	0.32	0.19	101,113,119,119	0
3	BGC	I	1	12/12	0.43	0.14	89,101,107,111	0
3	BGC	J	1	12/12	0.43	0.15	105,116,124,124	0
3	GAL	I	2	11/12	0.45	0.17	72,101,111,118	0
3	BGC	K	1	12/12	0.45	0.15	102,115,128,129	0
3	GAL	K	2	11/12	0.47	0.15	88,106,114,120	0
3	GAL	J	2	11/12	0.65	0.13	76,89,97,102	0
3	GAL	L	4	11/12	0.69	0.15	62,75,78,78	0
3	GAL	K	4	11/12	0.73	0.15	58,70,74,74	0
3	A2G	L	6	14/15	0.74	0.15	66,72,77,80	0
3	NAG	K	3	14/15	0.78	0.12	50,70,77,82	0
3	A2G	J	6	14/15	0.78	0.12	61,67,71,72	0
3	A2G	K	6	14/15	0.79	0.14	58,65,79,80	0
3	A2G	I	6	14/15	0.82	0.13	41,48,51,53	0
3	GAL	J	4	11/12	0.85	0.10	57,67,71,72	0
3	NAG	L	3	14/15	0.86	0.12	68,81,89,89	0
3	FUC	L	5	10/11	0.87	0.10	59,64,68,70	0
3	FUC	K	5	10/11	0.89	0.10	58,64,69,73	0
3	GAL	I	4	11/12	0.89	0.09	48,50,51,53	0
3	NAG	J	3	14/15	0.92	0.08	54,64,68,68	0

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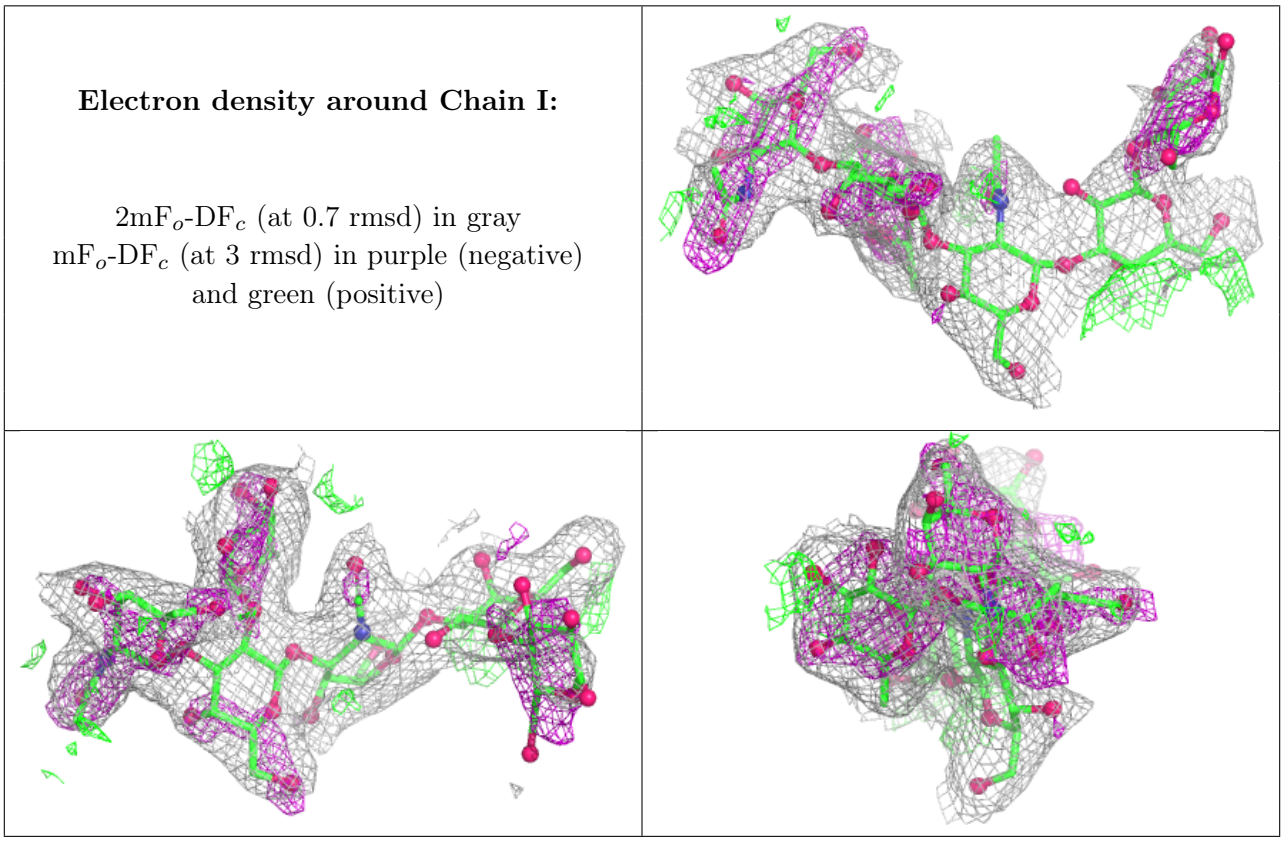
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	I	5	10/11	0.92	0.10	35,41,46,46	0
3	NAG	I	3	14/15	0.92	0.09	55,58,66,67	0
3	FUC	J	5	10/11	0.93	0.08	40,48,50,52	0

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.

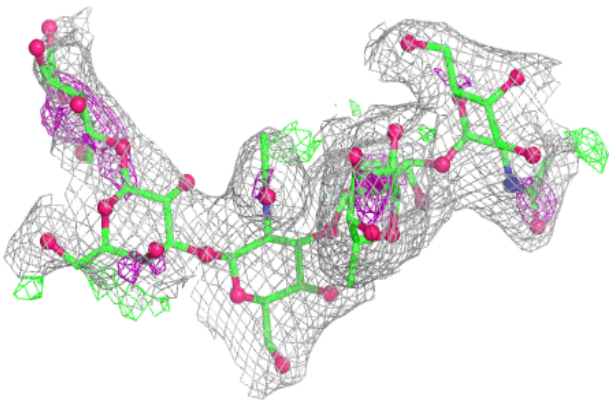
Electron density around Chain I:

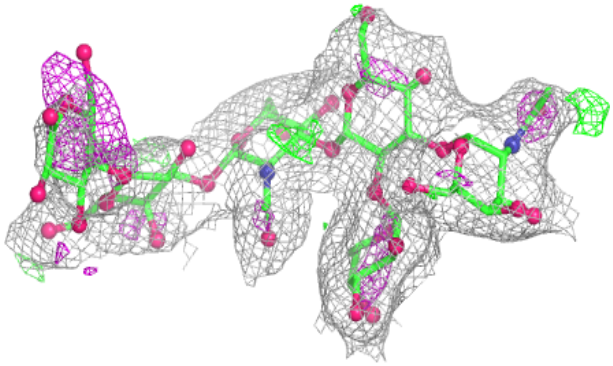
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

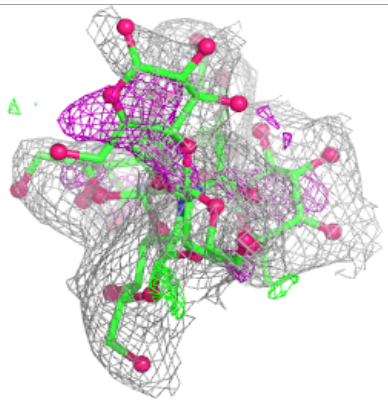


Electron density around Chain J:

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

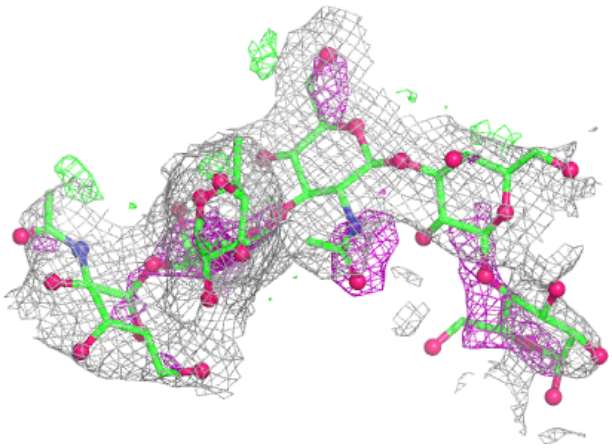


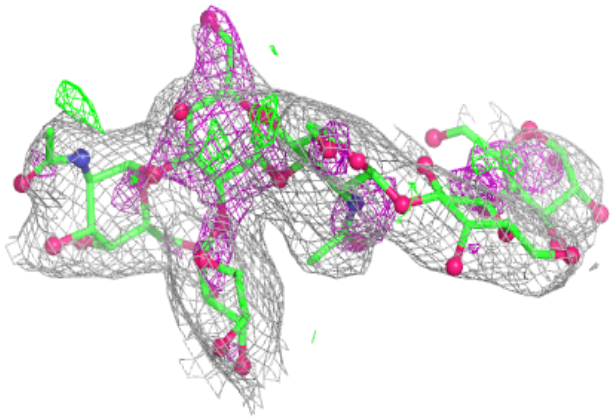


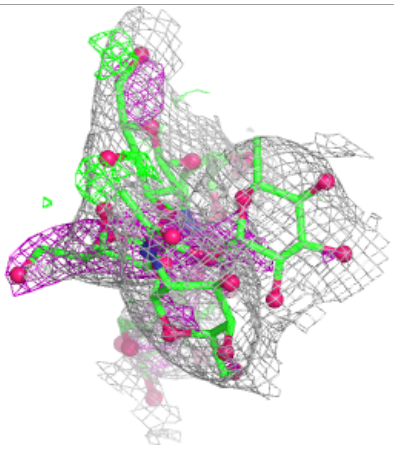


Electron density around Chain K:

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

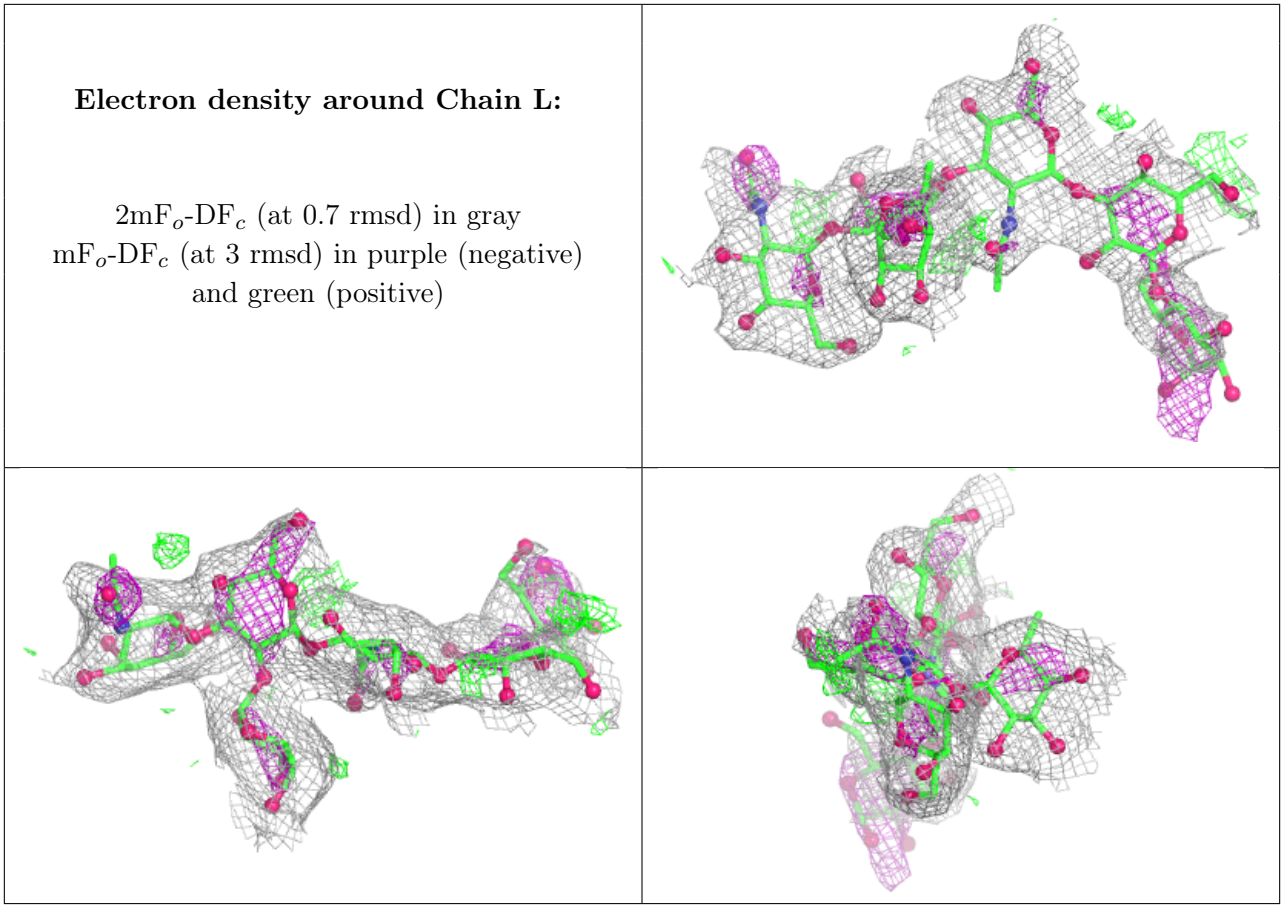






Electron density around Chain L:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.