



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:44 AM UTC

PDB ID : 4WSS / pdb_00004wss
Title : The crystal structure of hemagglutinin form A/chicken/New York/14677-13/1998 in complex with LSTa
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on : 2014-10-28
Resolution : 2.80 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:

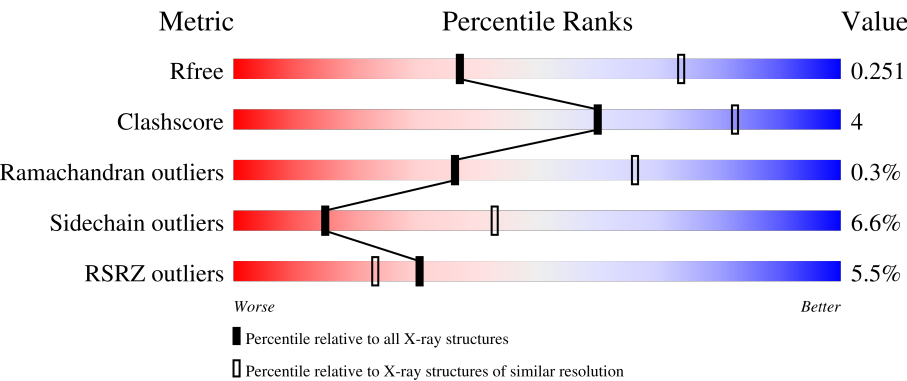
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	3% 83% 10% • 5%
1	B	514	2% 80% 11% • 6%
1	C	514	% 82% 9% • 6%
1	D	514	9% 82% 12% • •
1	E	514	% 81% 11% • 5%

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Mol	Chain	Length	Quality of chain
1	F	514	
2	G	2	
2	J	2	
3	H	3	
3	I	3	
3	K	3	

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
4	NAG	B	601	X	-	-	-
4	NAG	C	602	X	-	-	-
4	NAG	D	900	X	-	-	-
4	NAG	E	601	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23442 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3895	2446	676	754	19			
1	B	481	Total	C	N	O	S	0	0	0
			3821	2399	663	740	19			
1	C	482	Total	C	N	O	S	0	0	0
			3832	2405	667	741	19			
1	E	489	Total	C	N	O	S	0	0	0
			3886	2441	675	751	19			
1	D	493	Total	C	N	O	S	0	0	0
			3909	2458	678	754	19			
1	F	479	Total	C	N	O	S	0	0	0
			3810	2391	663	737	19			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q0A3A5
A	-2	ASP	-	expression tag	UNP Q0A3A5
A	-1	PRO	-	expression tag	UNP Q0A3A5
A	0	GLY	-	expression tag	UNP Q0A3A5
A	317	THR	UNK	conflict	UNP Q0A3A5
A	499	GLU	GLN	conflict	UNP Q0A3A5
A	504	GLY	VAL	conflict	UNP Q0A3A5
A	505	ARG	MET	conflict	UNP Q0A3A5
A	507	VAL	-	expression tag	UNP Q0A3A5
A	508	PRO	-	expression tag	UNP Q0A3A5
A	509	ARG	-	expression tag	UNP Q0A3A5
A	510	GLY	-	expression tag	UNP Q0A3A5
B	-3	ALA	-	expression tag	UNP Q0A3A5
B	-2	ASP	-	expression tag	UNP Q0A3A5
B	-1	PRO	-	expression tag	UNP Q0A3A5
B	0	GLY	-	expression tag	UNP Q0A3A5
B	317	THR	UNK	conflict	UNP Q0A3A5

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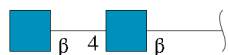
Chain	Residue	Modelled	Actual	Comment	Reference
B	499	GLU	GLN	conflict	UNP Q0A3A5
B	504	GLY	VAL	conflict	UNP Q0A3A5
B	505	ARG	MET	conflict	UNP Q0A3A5
B	507	VAL	-	expression tag	UNP Q0A3A5
B	508	PRO	-	expression tag	UNP Q0A3A5
B	509	ARG	-	expression tag	UNP Q0A3A5
B	510	GLY	-	expression tag	UNP Q0A3A5
C	-3	ALA	-	expression tag	UNP Q0A3A5
C	-2	ASP	-	expression tag	UNP Q0A3A5
C	-1	PRO	-	expression tag	UNP Q0A3A5
C	0	GLY	-	expression tag	UNP Q0A3A5
C	317	THR	UNK	conflict	UNP Q0A3A5
C	499	GLU	GLN	conflict	UNP Q0A3A5
C	504	GLY	VAL	conflict	UNP Q0A3A5
C	505	ARG	MET	conflict	UNP Q0A3A5
C	507	VAL	-	expression tag	UNP Q0A3A5
C	508	PRO	-	expression tag	UNP Q0A3A5
C	509	ARG	-	expression tag	UNP Q0A3A5
C	510	GLY	-	expression tag	UNP Q0A3A5
E	-3	ALA	-	expression tag	UNP Q0A3A5
E	-2	ASP	-	expression tag	UNP Q0A3A5
E	-1	PRO	-	expression tag	UNP Q0A3A5
E	0	GLY	-	expression tag	UNP Q0A3A5
E	317	THR	UNK	conflict	UNP Q0A3A5
E	499	GLU	GLN	conflict	UNP Q0A3A5
E	504	GLY	VAL	conflict	UNP Q0A3A5
E	505	ARG	MET	conflict	UNP Q0A3A5
E	507	VAL	-	expression tag	UNP Q0A3A5
E	508	PRO	-	expression tag	UNP Q0A3A5
E	509	ARG	-	expression tag	UNP Q0A3A5
E	510	GLY	-	expression tag	UNP Q0A3A5
D	-3	ALA	-	expression tag	UNP Q0A3A5
D	-2	ASP	-	expression tag	UNP Q0A3A5
D	-1	PRO	-	expression tag	UNP Q0A3A5
D	0	GLY	-	expression tag	UNP Q0A3A5
D	317	THR	UNK	conflict	UNP Q0A3A5
D	499	GLU	GLN	conflict	UNP Q0A3A5
D	504	GLY	VAL	conflict	UNP Q0A3A5
D	505	ARG	MET	conflict	UNP Q0A3A5
D	507	VAL	-	expression tag	UNP Q0A3A5
D	508	PRO	-	expression tag	UNP Q0A3A5
D	509	ARG	-	expression tag	UNP Q0A3A5

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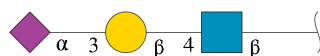
Chain	Residue	Modelled	Actual	Comment	Reference
D	510	GLY	-	expression tag	UNP Q0A3A5
F	-3	ALA	-	expression tag	UNP Q0A3A5
F	-2	ASP	-	expression tag	UNP Q0A3A5
F	-1	PRO	-	expression tag	UNP Q0A3A5
F	0	GLY	-	expression tag	UNP Q0A3A5
F	317	THR	UNK	conflict	UNP Q0A3A5
F	499	GLU	GLN	conflict	UNP Q0A3A5
F	504	GLY	VAL	conflict	UNP Q0A3A5
F	505	ARG	MET	conflict	UNP Q0A3A5
F	507	VAL	-	expression tag	UNP Q0A3A5
F	508	PRO	-	expression tag	UNP Q0A3A5
F	509	ARG	-	expression tag	UNP Q0A3A5
F	510	GLY	-	expression tag	UNP Q0A3A5

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



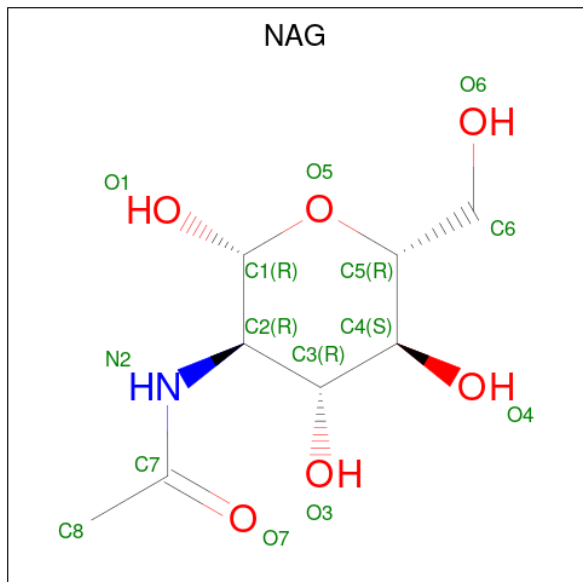
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	I	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	K	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

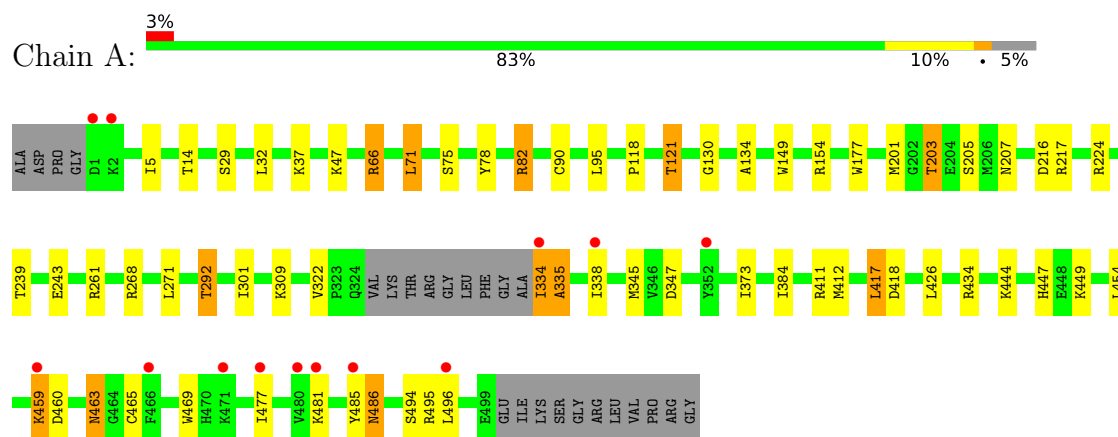


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

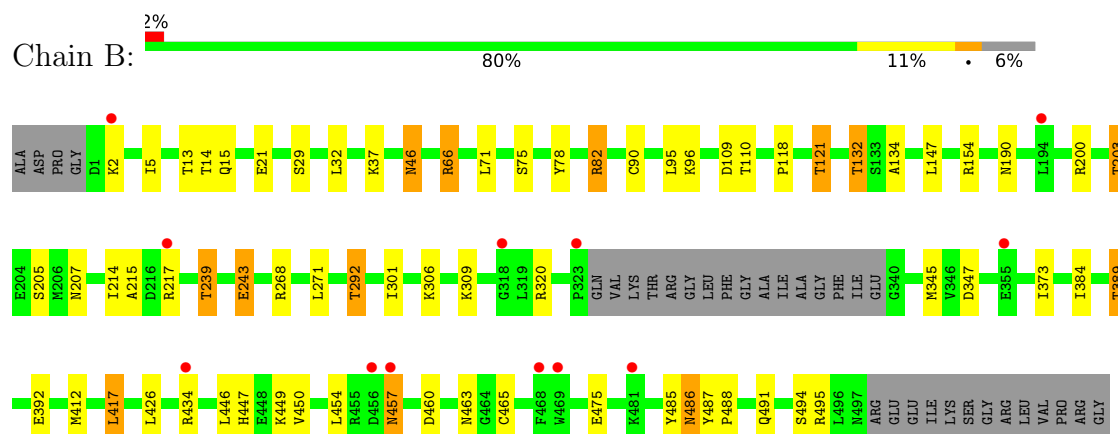
3 Residue-property plots [i](#)

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

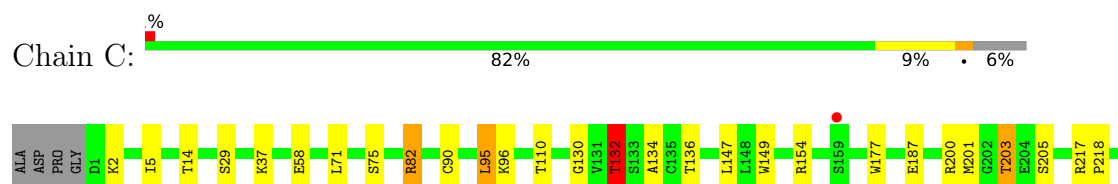
• Molecule 1: Hemagglutinin

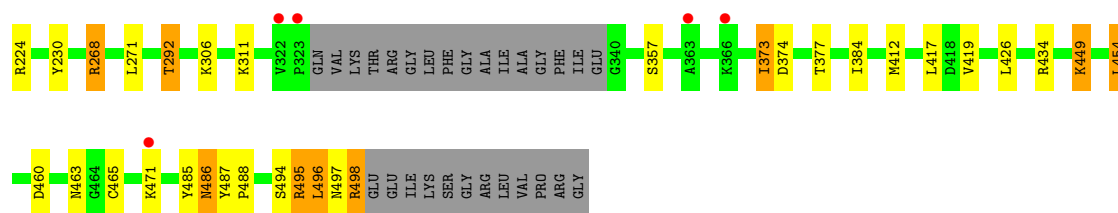


• Molecule 1: Hemagglutinin

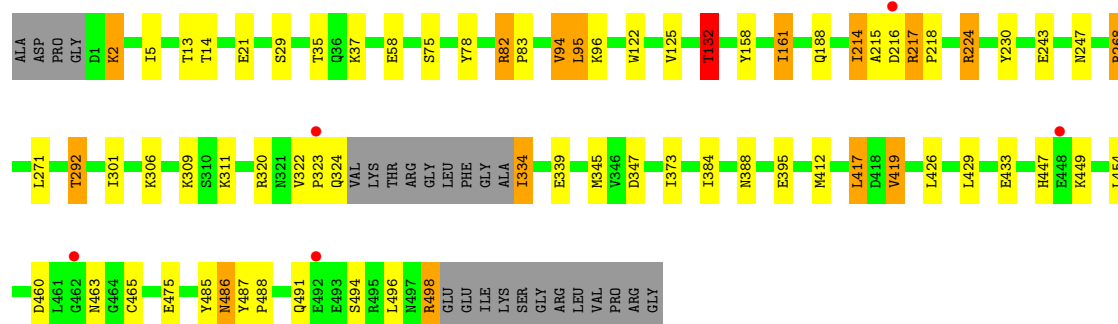
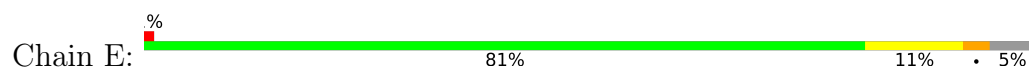


• Molecule 1: Hemagglutinin

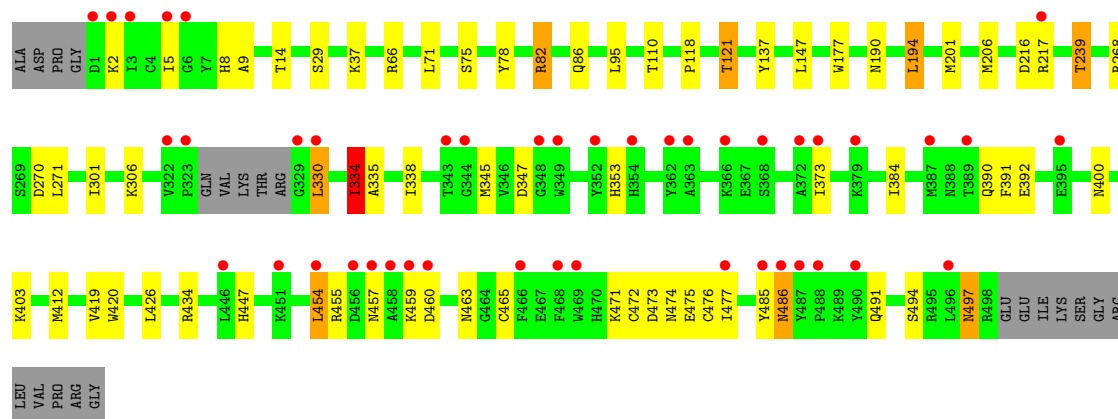
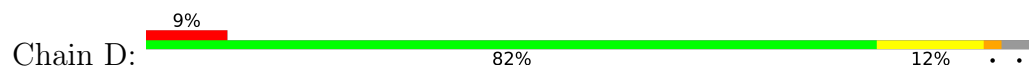




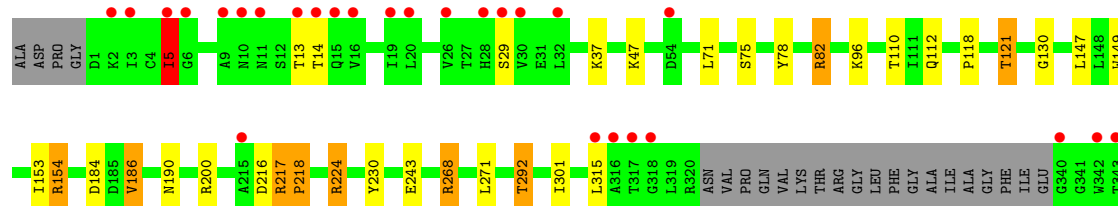
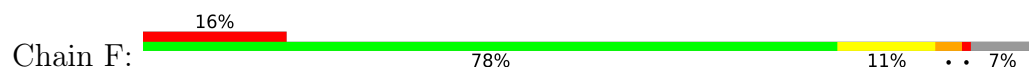
• Molecule 1: Hemagglutinin

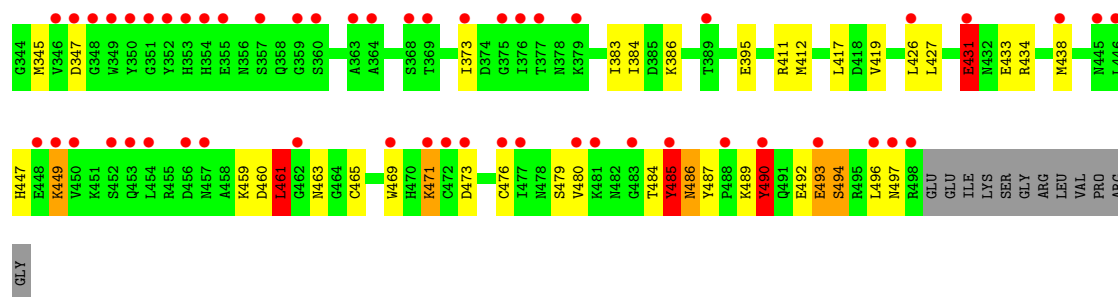


• Molecule 1: Hemagglutinin

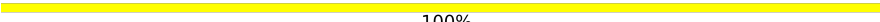


• Molecule 1: Hemagglutinin



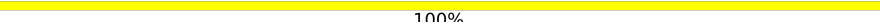


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%

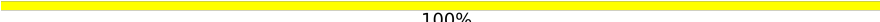
MAG1
GAL2
STA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  67% 33%

MAG1
GAL2
STA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
GAL2
STA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.97Å 134.78Å 122.62Å 90.00° 112.20° 90.00°	Depositor
Resolution (Å)	45.20 – 2.80 45.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.20-2.80) 98.4 (45.20-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.220 , 0.254 0.221 , 0.251	Depositor DCC
R_{free} test set	4650 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 22.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23442	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.83	0/3983	0.90	1/5397 (0.0%)
1	B	0.82	0/3908	0.91	7/5297 (0.1%)
1	C	0.82	0/3919	0.89	3/5311 (0.1%)
1	D	0.84	1/3998 (0.0%)	0.93	5/5417 (0.1%)
1	E	0.83	0/3974	0.92	7/5385 (0.1%)
1	F	0.85	4/3896 (0.1%)	0.95	11/5278 (0.2%)
All	All	0.83	5/23678 (0.0%)	0.92	34/32085 (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	D	0	1
1	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	485	TYR	N-CA	6.94	1.55	1.46
1	F	431	GLU	CA-C	6.68	1.61	1.52
1	F	485	TYR	CA-C	6.45	1.61	1.52
1	F	218	PRO	CA-C	5.20	1.56	1.52
1	D	194	LEU	CA-CB	5.07	1.60	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	485	TYR	N-CA-C	9.87	131.82	110.80
1	F	5	ILE	CB-CA-C	8.32	123.23	110.83
1	F	112	GLN	CB-CA-C	-7.55	98.07	110.14
1	F	431	GLU	CB-CA-C	7.47	125.60	109.99
1	F	484	THR	N-CA-C	7.34	121.09	108.02
1	B	46	ASN	CB-CA-C	-7.20	99.50	111.23
1	B	109	ASP	N-CA-CB	6.96	119.84	110.59
1	F	492	GLU	N-CA-C	6.90	118.59	111.14
1	F	153	ILE	CB-CA-C	6.70	120.85	111.34
1	D	335	ALA	N-CA-C	6.56	124.25	113.89
1	C	5	ILE	CB-CG1-CD1	6.54	127.53	113.80
1	D	384	ILE	CA-CB-CG1	6.42	121.32	110.40
1	C	132	THR	CB-CA-C	-6.31	96.51	109.94
1	E	161	ILE	CB-CA-C	-6.26	101.18	110.82
1	F	461	LEU	CA-CB-CG	6.09	137.62	116.30
1	F	489	LYS	N-CA-C	6.04	123.67	110.80
1	D	384	ILE	CB-CA-C	-6.04	104.15	111.88
1	E	13	THR	CB-CA-C	5.74	120.52	110.64
1	E	214	ILE	CA-CB-CG1	5.56	119.86	110.40
1	F	473	ASP	N-CA-CB	-5.56	102.73	110.29
1	E	132	THR	CB-CA-C	-5.42	97.53	109.56
1	D	239	THR	CB-CA-C	5.36	119.96	109.35
1	E	419	VAL	N-CA-CB	5.36	118.62	110.58
1	B	66	ARG	CG-CD-NE	5.31	123.68	112.00
1	B	239	THR	CB-CA-C	5.25	119.75	109.35
1	A	243	GLU	CB-CA-C	-5.24	98.73	109.38
1	E	2	LYS	N-CA-C	5.20	116.98	109.07
1	F	490	TYR	N-CA-C	5.19	117.53	110.88
1	D	497	ASN	N-CA-C	5.18	121.84	110.80
1	E	94	VAL	CB-CA-C	5.15	118.29	110.62
1	B	2	LYS	N-CA-C	5.12	116.86	109.07
1	B	132	THR	CB-CA-C	-5.11	98.21	109.56
1	B	457	ASN	CB-CA-C	5.07	119.74	110.36
1	C	2	LYS	N-CA-C	5.02	116.70	109.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	334	ILE	Peptide
1	E	323	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3895	0	3753	34	0
1	B	3821	0	3680	29	0
1	C	3832	0	3693	36	0
1	D	3909	0	3770	33	2
1	E	3886	0	3746	40	0
1	F	3810	0	3672	45	0
2	G	28	0	25	0	0
2	J	28	0	25	0	0
3	H	45	0	38	4	0
3	I	45	0	38	1	0
3	K	45	0	38	0	0
4	B	28	0	26	1	0
4	C	28	0	26	1	0
4	D	14	0	13	0	0
4	E	28	0	26	2	0
All	All	23442	0	22569	199	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ASN:ND2	1:D:485:TYR:OH	1.98	0.96
1:B:457:ASN:ND2	1:B:485:TYR:OH	1.98	0.96
1:D:473:ASP:O	1:D:476:CYS:SG	2.24	0.96
1:E:2:LYS:NZ	1:E:334:ILE:O	1.98	0.95
1:F:469:TRP:CD1	1:F:494:SER:OG	2.20	0.95
1:F:469:TRP:CG	1:F:494:SER:HG	1.85	0.94
1:A:207:ASN:OD1	1:C:217:ARG:NH1	2.00	0.94
1:F:476:CYS:SG	1:F:485:TYR:OH	2.29	0.89
1:E:268:ARG:HB3	1:E:268:ARG:NH1	1.87	0.88
1:D:476:CYS:SG	1:D:477:ILE:N	2.46	0.88
1:A:463:ASN:O	1:A:463:ASN:OD1	1.99	0.79
1:C:311:LYS:O	4:C:602:NAG:H82	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:GLN:HE22	1:E:247:ASN:HD21	1.33	0.77
1:F:469:TRP:CD1	1:F:494:SER:HG	1.97	0.76
1:E:122:TRP:HE3	1:E:161:ILE:CG2	1.99	0.75
1:D:474:ASN:HA	1:D:477:ILE:HG12	1.67	0.74
1:F:490:TYR:O	1:F:493:GLU:OE1	2.05	0.73
1:B:118:PRO:O	1:B:121:THR:HG23	1.90	0.72
1:D:118:PRO:O	1:D:121:THR:HG23	1.90	0.72
1:A:118:PRO:O	1:A:121:THR:HG23	1.90	0.71
1:F:118:PRO:O	1:F:121:THR:HG23	1.90	0.71
1:E:268:ARG:HB3	1:E:268:ARG:HH11	1.54	0.71
1:E:311:LYS:HB3	4:E:601:NAG:H82	1.72	0.70
1:B:203:THR:HG22	1:B:205:SER:H	1.57	0.69
1:D:334:ILE:HD11	1:D:353:HIS:CE1	2.27	0.69
1:A:203:THR:HG22	1:A:205:SER:H	1.58	0.69
1:F:493:GLU:H	1:F:493:GLU:CD	2.01	0.68
1:D:334:ILE:HD11	1:D:353:HIS:NE2	2.09	0.67
1:C:203:THR:HG22	1:C:205:SER:H	1.61	0.65
1:E:122:TRP:CE3	1:E:161:ILE:CG2	2.80	0.64
1:F:427:LEU:O	1:F:431:GLU:HG3	1.97	0.64
1:C:373:ILE:O	1:C:377:THR:HG22	1.98	0.64
1:D:306:LYS:HD3	1:D:390:GLN:HA	1.80	0.64
1:B:446:LEU:O	1:B:450:VAL:HG12	1.96	0.64
1:A:207:ASN:CG	1:C:217:ARG:NH1	2.57	0.63
1:F:480:VAL:HG22	1:F:485:TYR:CE2	2.34	0.62
1:B:154:ARG:NH1	1:B:190:ASN:OD1	2.32	0.62
1:F:82:ARG:NH2	1:F:271:LEU:O	2.32	0.62
1:C:132:THR:CG2	3:H:3:SIA:O1B	2.49	0.61
1:E:82:ARG:NH2	1:E:271:LEU:O	2.33	0.61
1:A:216:ASP:N	1:B:243:GLU:OE1	2.26	0.60
1:F:383:ILE:HD11	1:F:431:GLU:OE2	2.01	0.60
1:D:306:LYS:HE3	1:D:391:PHE:H	1.66	0.60
1:E:5:ILE:HG13	1:E:447:HIS:HA	1.84	0.60
1:A:82:ARG:NH2	1:A:271:LEU:O	2.34	0.60
1:B:5:ILE:HG13	1:B:447:HIS:HA	1.85	0.59
1:E:388:ASN:O	1:E:388:ASN:OD1	2.21	0.59
1:D:5:ILE:HG13	1:D:447:HIS:HA	1.84	0.59
1:D:82:ARG:NH2	1:D:271:LEU:O	2.35	0.59
1:A:66:ARG:CZ	1:A:66:ARG:HB3	2.33	0.59
1:E:96:LYS:HG3	1:E:230:TYR:CE1	2.38	0.59
1:A:5:ILE:HG13	1:A:447:HIS:HA	1.85	0.58
1:F:315:LEU:HD11	1:F:431:GLU:CD	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ARG:NH2	1:B:271:LEU:O	2.37	0.58
1:C:82:ARG:NH2	1:C:271:LEU:O	2.35	0.58
1:A:459:LYS:HE2	1:A:469:TRP:CZ2	2.40	0.57
1:D:400:ASN:O	1:D:403:LYS:HE3	2.03	0.57
1:C:96:LYS:HG3	1:C:230:TYR:CE1	2.40	0.56
1:D:334:ILE:HD11	1:D:353:HIS:CD2	2.39	0.56
1:B:15:GLN:OE1	4:B:601:NAG:H82	2.06	0.55
1:C:357:SER:OG	1:C:471:LYS:HE2	2.07	0.55
1:E:14:THR:HG21	1:E:29:SER:OG	2.07	0.55
1:A:418:ASP:HB3	1:B:389:THR:HG21	1.89	0.55
1:D:2:LYS:NZ	1:D:334:ILE:O	2.39	0.55
1:F:471:LYS:HD3	1:F:471:LYS:H	1.72	0.55
1:F:431:GLU:OE1	1:F:431:GLU:C	2.50	0.54
1:A:14:THR:HG21	1:A:29:SER:OG	2.08	0.54
1:E:460:ASP:O	1:E:465:CYS:O	2.26	0.54
1:D:472:CYS:C	1:D:476:CYS:SG	2.91	0.53
1:E:83:PRO:HA	1:E:268:ARG:HH12	1.73	0.53
1:F:14:THR:HG21	1:F:29:SER:OG	2.08	0.53
1:B:14:THR:HG21	1:B:29:SER:OG	2.08	0.53
1:F:75:SER:HB2	1:F:110:THR:HG22	1.91	0.53
1:A:177:TRP:CD2	1:A:201:MET:HE2	2.43	0.53
1:F:154:ARG:NH2	1:F:190:ASN:OD1	2.34	0.53
1:E:433:GLU:OE2	1:F:434:ARG:NH2	2.42	0.53
1:C:460:ASP:O	1:C:465:CYS:O	2.27	0.52
1:F:96:LYS:HG3	1:F:230:TYR:CE1	2.44	0.52
1:C:14:THR:HG21	1:C:29:SER:OG	2.09	0.52
1:B:460:ASP:O	1:B:465:CYS:O	2.26	0.52
1:D:460:ASP:O	1:D:465:CYS:O	2.27	0.52
1:F:292:THR:HG21	1:F:384:ILE:HG12	1.92	0.52
1:D:14:THR:HG21	1:D:29:SER:OG	2.10	0.51
1:F:469:TRP:CG	1:F:494:SER:OG	2.48	0.51
1:A:460:ASP:O	1:A:465:CYS:O	2.27	0.51
1:F:383:ILE:CD1	1:F:431:GLU:OE2	2.59	0.51
1:D:75:SER:HB2	1:D:110:THR:HG22	1.92	0.51
1:C:132:THR:HG23	3:H:3:SIA:O1B	2.11	0.50
1:C:75:SER:HB2	1:C:110:THR:HG22	1.92	0.50
1:D:8:HIS:CD2	1:D:9:ALA:O	2.65	0.50
1:B:292:THR:HG21	1:B:384:ILE:HG12	1.93	0.50
1:A:292:THR:HG21	1:A:384:ILE:HG12	1.92	0.50
1:A:334:ILE:O	1:A:335:ALA:HB3	2.12	0.50
1:A:463:ASN:OD1	1:A:463:ASN:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:THR:HG21	1:C:384:ILE:HG12	1.93	0.49
1:D:177:TRP:CD2	1:D:201:MET:HE2	2.47	0.49
1:E:454:LEU:HD23	1:E:485:TYR:CE2	2.48	0.49
1:E:215:ALA:HA	1:F:200:ARG:HD3	1.94	0.49
1:F:493:GLU:OE1	1:F:493:GLU:N	2.45	0.49
1:F:460:ASP:O	1:F:465:CYS:O	2.30	0.49
1:E:292:THR:HG21	1:E:384:ILE:HG12	1.95	0.48
1:C:132:THR:HG22	3:H:3:SIA:O1B	2.14	0.48
1:E:125:VAL:HG11	1:E:161:ILE:HD11	1.95	0.48
1:B:75:SER:HB2	1:B:110:THR:HG22	1.95	0.48
1:C:177:TRP:CD2	1:C:201:MET:HE2	2.48	0.48
1:A:434:ARG:HH22	1:C:434:ARG:CG	2.27	0.48
1:A:477:ILE:HG23	1:A:481:LYS:HZ2	1.79	0.48
1:C:217:ARG:HB2	1:C:218:PRO:HD2	1.97	0.47
1:F:493:GLU:CD	1:F:493:GLU:N	2.69	0.47
1:E:158:TYR:CE2	1:E:161:ILE:HD12	2.50	0.47
1:A:454:LEU:HD23	1:A:485:TYR:CE2	2.50	0.47
1:B:454:LEU:HD23	1:B:485:TYR:CE2	2.49	0.47
1:C:187:GLU:OE2	3:H:3:SIA:H92	2.15	0.47
1:E:243:GLU:OE1	1:D:216:ASP:N	2.42	0.47
1:F:216:ASP:HB2	1:F:224:ARG:HH11	1.79	0.47
1:E:216:ASP:HB2	1:E:224:ARG:HH11	1.79	0.46
1:D:8:HIS:CD2	1:D:9:ALA:N	2.84	0.46
1:B:215:ALA:HB2	1:C:200:ARG:HD3	1.98	0.46
1:A:71:LEU:HD12	1:D:270:ASP:HB2	1.98	0.45
1:B:345:MET:O	1:B:347:ASP:N	2.48	0.45
1:E:21:GLU:OE1	1:E:320:ARG:NH2	2.48	0.45
1:B:214:ILE:O	1:C:200:ARG:HD3	2.16	0.45
1:F:345:MET:O	1:F:347:ASP:N	2.48	0.45
1:D:330:LEU:HD22	1:D:330:LEU:H	1.81	0.45
1:D:345:MET:O	1:D:347:ASP:N	2.48	0.45
1:F:268:ARG:HE	1:F:268:ARG:HB3	1.63	0.45
1:A:411:ARG:HD2	1:B:392:GLU:O	2.17	0.45
1:C:449:LYS:HD3	1:C:449:LYS:HA	1.85	0.45
1:E:78:TYR:CD2	1:E:301:ILE:HD11	2.52	0.45
1:C:495:ARG:HA	1:C:498:ARG:NH1	2.32	0.45
1:A:78:TYR:CD2	1:A:301:ILE:HD11	2.52	0.45
1:D:78:TYR:CD2	1:D:301:ILE:HD11	2.52	0.44
1:F:217:ARG:HB2	1:F:218:PRO:HD2	1.99	0.44
1:A:130:GLY:HA3	1:A:149:TRP:HB3	1.99	0.44
1:E:58:GLU:HG2	1:E:95:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:TYR:CD2	1:B:301:ILE:HD11	2.52	0.44
1:C:374:ASP:HA	1:C:377:THR:HG22	2.00	0.44
1:E:388:ASN:OD1	1:E:388:ASN:C	2.60	0.44
1:D:474:ASN:O	1:D:477:ILE:HG13	2.18	0.44
1:F:449:LYS:HA	1:F:449:LYS:HD3	1.72	0.44
1:F:485:TYR:O	1:F:486:ASN:CB	2.66	0.44
1:A:434:ARG:CG	1:B:434:ARG:HH22	2.31	0.44
1:C:454:LEU:HD12	1:C:485:TYR:CE2	2.52	0.44
1:A:309:LYS:HE3	1:A:417:LEU:HD13	2.00	0.43
1:D:454:LEU:HD12	1:D:485:TYR:CE2	2.53	0.43
1:F:479:SER:OG	1:F:485:TYR:CE1	2.71	0.43
1:F:485:TYR:O	1:F:486:ASN:HB3	2.18	0.43
1:B:21:GLU:OE1	1:B:320:ARG:NH2	2.49	0.43
1:F:184:ASP:OD1	1:F:186:VAL:HG13	2.18	0.43
1:A:345:MET:O	1:A:347:ASP:N	2.50	0.43
1:A:459:LYS:HE2	1:A:469:TRP:CH2	2.54	0.43
1:F:78:TYR:CD2	1:F:301:ILE:HD11	2.53	0.43
1:A:434:ARG:HH22	1:C:434:ARG:HG2	1.82	0.43
1:E:429:LEU:HD11	1:F:386:LYS:HE3	2.00	0.43
1:D:434:ARG:NH1	1:F:433:GLU:OE1	2.52	0.43
1:A:217:ARG:NH1	1:B:207:ASN:OD1	2.44	0.42
1:E:388:ASN:O	1:E:388:ASN:CG	2.62	0.42
1:F:47:LYS:HA	1:F:47:LYS:HD3	1.90	0.42
1:E:35:THR:HG21	4:E:601:NAG:O7	2.19	0.42
1:E:306:LYS:HB2	1:E:306:LYS:HE2	1.92	0.42
1:E:485:TYR:O	1:E:486:ASN:CB	2.68	0.42
1:F:490:TYR:O	1:F:493:GLU:CD	2.63	0.42
1:E:345:MET:O	1:E:347:ASP:N	2.49	0.42
1:C:58:GLU:HG2	1:C:95:LEU:HD12	2.00	0.41
1:C:485:TYR:O	1:C:486:ASN:CB	2.67	0.41
1:F:460:ASP:C	1:F:461:LEU:HD23	2.45	0.41
1:E:158:TYR:CE2	1:E:161:ILE:CD1	3.03	0.41
1:E:496:LEU:C	1:E:498:ARG:H	2.28	0.41
1:E:217:ARG:HB2	1:E:218:PRO:HD2	2.02	0.41
1:F:130:GLY:HA3	1:F:149:TRP:HB3	2.02	0.41
1:A:477:ILE:HG23	1:A:481:LYS:NZ	2.35	0.41
1:A:90:CYS:HB2	1:A:134:ALA:O	2.21	0.41
1:C:90:CYS:HB2	1:C:134:ALA:O	2.21	0.41
1:A:216:ASP:OD2	1:A:224:ARG:NH2	2.52	0.41
1:D:306:LYS:HE2	1:D:420:TRP:CG	2.55	0.41
1:A:485:TYR:O	1:A:486:ASN:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:GLN:HB2	1:E:339:GLU:O	2.19	0.41
1:D:334:ILE:HG21	1:D:334:ILE:HD13	1.85	0.41
1:B:200:ARG:HB2	1:B:243:GLU:HG3	2.02	0.41
1:E:485:TYR:O	1:E:486:ASN:HB3	2.21	0.41
1:F:5:ILE:HG21	1:F:447:HIS:HA	2.03	0.41
1:B:306:LYS:HB2	1:B:306:LYS:HE2	1.91	0.41
1:B:309:LYS:HE3	1:B:417:LEU:HD13	2.02	0.41
1:B:485:TYR:O	1:B:486:ASN:CB	2.68	0.41
1:C:306:LYS:HB2	1:C:306:LYS:HE2	1.92	0.41
1:E:132:THR:CG2	3:I:3:SIA:O1A	2.69	0.41
1:C:485:TYR:O	1:C:486:ASN:HB3	2.20	0.41
1:E:487:TYR:N	1:E:488:PRO:HD2	2.36	0.41
1:D:485:TYR:O	1:D:486:ASN:CB	2.68	0.41
1:B:487:TYR:N	1:B:488:PRO:HD2	2.36	0.40
1:C:268:ARG:HE	1:C:268:ARG:HB3	1.60	0.40
1:C:374:ASP:HA	1:C:377:THR:CG2	2.51	0.40
1:C:487:TYR:N	1:C:488:PRO:HD2	2.37	0.40
1:D:392:GLU:O	1:F:411:ARG:HD2	2.21	0.40
1:B:90:CYS:HB2	1:B:134:ALA:O	2.21	0.40
1:F:487:TYR:CD2	1:F:487:TYR:C	2.96	0.40
1:C:130:GLY:HA3	1:C:149:TRP:HB3	2.03	0.40
1:C:496:LEU:C	1:C:498:ARG:H	2.28	0.40
1:E:309:LYS:HE3	1:E:417:LEU:HD13	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:OH	1:D:137:TYR:OH[2_555]	1.91	0.29
1:D:137:TYR:CZ	1:D:137:TYR:OH[2_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/514 (95%)	465 (96%)	19 (4%)	2 (0%)	30	60
1	B	477/514 (93%)	457 (96%)	19 (4%)	1 (0%)	43	72
1	C	478/514 (93%)	457 (96%)	19 (4%)	2 (0%)	30	60
1	D	489/514 (95%)	468 (96%)	19 (4%)	2 (0%)	30	60
1	E	485/514 (94%)	464 (96%)	20 (4%)	1 (0%)	43	72
1	F	475/514 (92%)	451 (95%)	22 (5%)	2 (0%)	30	60
All	All	2890/3084 (94%)	2762 (96%)	118 (4%)	10 (0%)	36	66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	486	ASN
1	A	486	ASN
1	B	486	ASN
1	C	486	ASN
1	D	486	ASN
1	D	497	ASN
1	F	486	ASN
1	F	497	ASN
1	A	335	ALA
1	C	497	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/443 (96%)	397 (93%)	29 (7%)	14	42
1	B	419/443 (95%)	390 (93%)	29 (7%)	14	41
1	C	420/443 (95%)	396 (94%)	24 (6%)	18	49
1	D	426/443 (96%)	397 (93%)	29 (7%)	14	42
1	E	425/443 (96%)	400 (94%)	25 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	417/443 (94%)	385 (92%)	32 (8%)	12	36
All	All	2533/2658 (95%)	2365 (93%)	168 (7%)	15	43

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	37	LYS
1	A	47	LYS
1	A	66	ARG
1	A	71	LEU
1	A	75	SER
1	A	82	ARG
1	A	95	LEU
1	A	121	THR
1	A	154	ARG
1	A	203	THR
1	A	239	THR
1	A	261	ARG
1	A	268	ARG
1	A	292	THR
1	A	322	VAL
1	A	334	ILE
1	A	338	ILE
1	A	373	ILE
1	A	412	MET
1	A	417	LEU
1	A	426	LEU
1	A	444	LYS
1	A	449	LYS
1	A	459	LYS
1	A	463	ASN
1	A	494	SER
1	A	495	ARG
1	A	496	LEU
1	B	13	THR
1	B	32	LEU
1	B	37	LYS
1	B	46	ASN
1	B	66	ARG
1	B	71	LEU
1	B	82	ARG

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Mol	Chain	Res	Type
1	B	95	LEU
1	B	96	LYS
1	B	121	THR
1	B	132	THR
1	B	147	LEU
1	B	203	THR
1	B	217	ARG
1	B	239	THR
1	B	243	GLU
1	B	268	ARG
1	B	292	THR
1	B	373	ILE
1	B	389	THR
1	B	412	MET
1	B	417	LEU
1	B	426	LEU
1	B	449	LYS
1	B	463	ASN
1	B	475	GLU
1	B	491	GLN
1	B	494	SER
1	B	495	ARG
1	C	37	LYS
1	C	71	LEU
1	C	82	ARG
1	C	95	LEU
1	C	132	THR
1	C	136	THR
1	C	147	LEU
1	C	154	ARG
1	C	203	THR
1	C	224	ARG
1	C	268	ARG
1	C	292	THR
1	C	373	ILE
1	C	412	MET
1	C	417	LEU
1	C	419	VAL
1	C	426	LEU
1	C	449	LYS
1	C	454	LEU
1	C	463	ASN

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Mol	Chain	Res	Type
1	C	494	SER
1	C	495	ARG
1	C	496	LEU
1	C	498	ARG
1	E	37	LYS
1	E	75	SER
1	E	82	ARG
1	E	94	VAL
1	E	95	LEU
1	E	132	THR
1	E	214	ILE
1	E	217	ARG
1	E	224	ARG
1	E	268	ARG
1	E	292	THR
1	E	322	VAL
1	E	334	ILE
1	E	373	ILE
1	E	395	GLU
1	E	412	MET
1	E	417	LEU
1	E	419	VAL
1	E	426	LEU
1	E	449	LYS
1	E	463	ASN
1	E	475	GLU
1	E	491	GLN
1	E	494	SER
1	E	498	ARG
1	D	37	LYS
1	D	66	ARG
1	D	71	LEU
1	D	82	ARG
1	D	86	GLN
1	D	95	LEU
1	D	121	THR
1	D	147	LEU
1	D	190	ASN
1	D	194	LEU
1	D	206	MET
1	D	217	ARG
1	D	239	THR

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Mol	Chain	Res	Type
1	D	268	ARG
1	D	330	LEU
1	D	334	ILE
1	D	338	ILE
1	D	373	ILE
1	D	412	MET
1	D	419	VAL
1	D	426	LEU
1	D	454	LEU
1	D	455	ARG
1	D	459	LYS
1	D	463	ASN
1	D	471	LYS
1	D	475	GLU
1	D	491	GLN
1	D	494	SER
1	F	5	ILE
1	F	13	THR
1	F	37	LYS
1	F	71	LEU
1	F	82	ARG
1	F	121	THR
1	F	147	LEU
1	F	154	ARG
1	F	186	VAL
1	F	217	ARG
1	F	224	ARG
1	F	243	GLU
1	F	268	ARG
1	F	292	THR
1	F	373	ILE
1	F	395	GLU
1	F	412	MET
1	F	417	LEU
1	F	419	VAL
1	F	426	LEU
1	F	431	GLU
1	F	438	MET
1	F	449	LYS
1	F	459	LYS
1	F	461	LEU
1	F	463	ASN

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Mol	Chain	Res	Type
1	F	471	LYS
1	F	485	TYR
1	F	490	TYR
1	F	493	GLU
1	F	494	SER
1	F	496	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	87	ASN
1	A	370	GLN
1	A	463	ASN
1	A	486	ASN
1	B	8	HIS
1	B	87	ASN
1	B	353	HIS
1	B	457	ASN
1	B	478	ASN
1	B	486	ASN
1	C	15	GLN
1	C	171	GLN
1	C	241	ASN
1	C	353	HIS
1	C	486	ASN
1	E	15	GLN
1	E	241	ASN
1	E	247	ASN
1	E	453	GLN
1	E	486	ASN
1	D	8	HIS
1	D	15	GLN
1	D	171	GLN
1	D	190	ASN
1	D	457	ASN
1	D	486	ASN
1	D	497	ASN
1	F	8	HIS
1	F	15	GLN
1	F	23	ASN
1	F	87	ASN

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Mol	Chain	Res	Type
1	F	112	GLN
1	F	241	ASN
1	F	288	ASN
1	F	353	HIS
1	F	354	HIS
1	F	478	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	601	1	14,14,15	0.72	0	17,19,21	1.40	2 (11%)
3	NAG	H	1	3	14,14,15	0.73	0	17,19,21	1.35	2 (11%)
3	NAG	K	1	3	14,14,15	0.92	1 (7%)	17,19,21	2.07	7 (41%)
4	NAG	E	601	1	14,14,15	1.62	2 (14%)	17,19,21	3.07	12 (70%)
3	NAG	I	1	3	14,14,15	0.91	1 (7%)	17,19,21	1.89	5 (29%)
2	NAG	J	1	2,1	14,14,15	0.60	0	17,19,21	1.66	3 (17%)
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	1.25	2 (11%)
4	NAG	B	602	1	14,14,15	1.10	1 (7%)	17,19,21	1.98	5 (29%)
4	NAG	E	602	1	14,14,15	0.58	0	17,19,21	1.89	2 (11%)
4	NAG	D	900	1	14,14,15	0.85	0	17,19,21	1.61	2 (11%)
3	GAL	K	2	3	11,11,12	0.77	0	15,15,17	2.18	5 (33%)
2	NAG	J	2	2	14,14,15	0.68	0	17,19,21	1.27	2 (11%)
4	NAG	B	601	1	14,14,15	0.44	0	17,19,21	1.57	4 (23%)
3	GAL	I	2	3	11,11,12	0.86	0	15,15,17	1.81	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	602	1	14,14,15	1.09	1 (7%)	17,19,21	2.18	6 (35%)
3	GAL	H	2	3	11,11,12	0.86	0	15,15,17	1.65	3 (20%)
2	NAG	G	1	2,1	14,14,15	0.91	1 (7%)	17,19,21	1.33	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
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3	-	2/6/23/26	0/1/1/1
4	NAG	E	601	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	I	1	3	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	E	602	1	-	1/6/23/26	0/1/1/1
4	NAG	D	900	1	1/1/5/7	2/6/23/26	0/1/1/1
3	GAL	K	2	3	-	2/2/19/22	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	1/1/5/7	1/6/23/26	0/1/1/1
3	GAL	I	2	3	-	0/2/19/22	0/1/1/1
4	NAG	C	602	1	1/1/5/7	2/6/23/26	0/1/1/1
3	GAL	H	2	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	601	NAG	C1-C2	4.96	1.59	1.52
4	B	602	NAG	C1-C2	2.90	1.56	1.52
3	I	1	NAG	C1-C2	2.72	1.56	1.52
2	G	1	NAG	C1-C2	2.61	1.55	1.52
4	C	602	NAG	C1-C2	2.40	1.55	1.52
4	E	601	NAG	C3-C2	2.31	1.57	1.52
3	K	1	NAG	C3-C2	2.19	1.57	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	NAG	C1-O5-C5	5.92	120.12	112.19
4	E	601	NAG	O5-C5-C4	-5.09	98.44	110.83
4	E	601	NAG	C3-C4-C5	-5.04	101.08	110.23
3	K	2	GAL	O3-C3-C2	-4.45	100.97	110.05
4	C	602	NAG	O5-C5-C4	-4.33	100.28	110.83
4	E	601	NAG	O5-C5-C6	4.31	116.05	107.66
2	J	1	NAG	O5-C1-C2	-4.21	104.78	111.29
3	K	2	GAL	O2-C2-C3	-4.15	101.55	110.15
4	E	601	NAG	C1-O5-C5	4.10	117.68	112.19
3	I	1	NAG	O5-C1-C2	4.05	117.56	111.29
3	K	1	NAG	C4-C3-C2	3.93	116.78	111.02
4	D	900	NAG	O5-C1-C2	-3.82	105.37	111.29
4	C	602	NAG	O5-C1-C2	-3.58	105.75	111.29
4	C	602	NAG	C1-C2-N2	3.53	115.99	110.43
3	H	2	GAL	O3-C3-C2	-3.47	102.97	110.05
4	C	602	NAG	C8-C7-N2	3.46	121.85	116.12
4	B	602	NAG	C4-C3-C2	3.45	116.08	111.02
2	J	1	NAG	C1-C2-N2	3.45	115.87	110.43
4	E	601	NAG	C1-C2-N2	3.43	115.83	110.43
4	E	601	NAG	C6-C5-C4	3.38	121.31	113.02
4	B	602	NAG	C2-N2-C7	3.37	127.42	122.90
3	I	2	GAL	O3-C3-C2	-3.36	103.20	110.05
4	E	601	NAG	O4-C4-C5	3.23	117.29	109.32
3	I	1	NAG	O5-C5-C6	3.19	113.88	107.66
4	B	602	NAG	C1-C2-N2	3.19	115.46	110.43
4	C	602	NAG	O7-C7-C8	-3.17	116.42	122.05
4	B	601	NAG	C1-O5-C5	3.16	116.43	112.19
4	C	601	NAG	C1-O5-C5	3.14	116.39	112.19
3	H	1	NAG	O4-C4-C3	-3.05	103.20	110.38
4	E	601	NAG	O7-C7-C8	-3.03	116.66	122.05
4	B	602	NAG	O7-C7-C8	-3.00	116.71	122.05
3	H	2	GAL	O5-C1-C2	-2.93	103.79	110.79
3	K	1	NAG	C1-O5-C5	2.88	116.05	112.19
3	K	2	GAL	O4-C4-C5	2.87	116.39	109.32
3	K	2	GAL	O5-C1-C2	-2.85	104.00	110.79
4	B	601	NAG	O5-C5-C6	2.84	113.19	107.66
3	K	1	NAG	O5-C1-C2	2.82	115.65	111.29
2	G	1	NAG	C1-C2-N2	2.79	114.83	110.43
4	D	900	NAG	C4-C3-C2	2.76	115.07	111.02
4	E	601	NAG	O3-C3-C2	2.75	115.11	109.40
3	I	1	NAG	C1-O5-C5	2.72	115.83	112.19
3	I	2	GAL	O5-C5-C6	2.71	112.94	107.66
2	J	2	NAG	C1-C2-N2	2.69	114.68	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	NAG	O4-C4-C3	2.67	116.68	110.38
3	K	1	NAG	O7-C7-C8	-2.65	117.34	122.05
3	K	1	NAG	O3-C3-C2	2.62	114.85	109.40
2	G	1	NAG	C4-C3-C2	2.62	114.86	111.02
3	I	2	GAL	O5-C1-C2	-2.55	104.70	110.79
3	K	2	GAL	O2-C2-C1	2.55	115.06	109.22
4	E	602	NAG	O5-C1-C2	2.52	115.19	111.29
4	C	602	NAG	C6-C5-C4	2.49	119.13	113.02
2	G	2	NAG	C3-C4-C5	-2.48	105.73	110.23
4	B	601	NAG	O7-C7-C8	-2.43	117.73	122.05
3	H	1	NAG	C4-C3-C2	2.37	114.49	111.02
2	G	2	NAG	O4-C4-C5	2.32	115.03	109.32
4	E	601	NAG	O3-C3-C4	2.30	115.79	110.38
3	I	1	NAG	O4-C4-C5	2.26	114.90	109.32
3	H	2	GAL	O2-C2-C3	-2.25	105.48	110.15
3	K	1	NAG	O4-C4-C5	2.25	114.87	109.32
2	J	1	NAG	O7-C7-C8	-2.25	118.05	122.05
3	I	2	GAL	O3-C3-C4	-2.24	105.09	110.38
3	I	1	NAG	O3-C3-C2	2.24	114.05	109.40
2	J	2	NAG	C3-C4-C5	-2.23	106.19	110.23
4	C	601	NAG	O3-C3-C2	2.23	114.03	109.40
3	I	2	GAL	C1-C2-C3	-2.19	106.45	109.64
4	B	601	NAG	C6-C5-C4	-2.15	107.75	113.02
3	K	1	NAG	O4-C4-C3	-2.12	105.37	110.38
4	B	602	NAG	O4-C4-C3	2.12	115.38	110.38
4	E	601	NAG	C8-C7-N2	2.05	119.52	116.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	601	NAG	C1
4	C	602	NAG	C1
4	E	601	NAG	C1
4	D	900	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C4-C5-C6-O6
4	E	601	NAG	O5-C5-C6-O6
4	C	602	NAG	C4-C5-C6-O6
4	C	602	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
4	D	900	NAG	O5-C5-C6-O6
3	K	2	GAL	C4-C5-C6-O6
4	D	900	NAG	C4-C5-C6-O6
4	E	601	NAG	C4-C5-C6-O6
3	K	2	GAL	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	E	602	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	601	NAG	2	0
4	B	601	NAG	1	0
4	C	602	NAG	1	0

5.5 Carbohydrates [i](#)

13 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	$\# Z > 2$
2	NAG	G	1	2,1	14,14,15	0.91	1 (7%)	17,19,21	1.33	2 (11%)
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	1.25	2 (11%)
3	NAG	H	1	3	14,14,15	0.73	0	17,19,21	1.35	2 (11%)
3	GAL	H	2	3	11,11,12	0.86	0	15,15,17	1.65	3 (20%)
3	SIA	H	3	3	20,20,21	0.88	1 (5%)	21,28,31	1.20	3 (14%)
3	NAG	I	1	3	14,14,15	0.91	1 (7%)	17,19,21	1.89	5 (29%)
3	GAL	I	2	3	11,11,12	0.86	0	15,15,17	1.81	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIA	I	3	3	20,20,21	1.10	3 (15%)	21,28,31	1.68	6 (28%)
2	NAG	J	1	2,1	14,14,15	0.60	0	17,19,21	1.66	3 (17%)
2	NAG	J	2	2	14,14,15	0.68	0	17,19,21	1.27	2 (11%)
3	NAG	K	1	3	14,14,15	0.92	1 (7%)	17,19,21	2.07	7 (41%)
3	GAL	K	2	3	11,11,12	0.77	0	15,15,17	2.18	5 (33%)
3	SIA	K	3	3	20,20,21	0.84	0	21,28,31	1.47	5 (23%)

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
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3	-	0/6/23/26	0/1/1/1
3	GAL	H	2	3	-	0/2/19/22	0/1/1/1
3	SIA	H	3	3	-	2/18/34/38	0/1/1/1
3	NAG	I	1	3	-	2/6/23/26	0/1/1/1
3	GAL	I	2	3	-	0/2/19/22	0/1/1/1
3	SIA	I	3	3	-	1/18/34/38	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3	-	2/6/23/26	0/1/1/1
3	GAL	K	2	3	-	2/2/19/22	0/1/1/1
3	SIA	K	3	3	-	0/18/34/38	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C1-C2	2.72	1.56	1.52
2	G	1	NAG	C1-C2	2.61	1.55	1.52
3	I	3	SIA	C5-N5	-2.52	1.41	1.45
3	I	3	SIA	O1B-C1	-2.25	1.23	1.30
3	K	1	NAG	C3-C2	2.19	1.57	1.52
3	H	3	SIA	O1A-C1	2.09	1.28	1.22
3	I	3	SIA	C3-C2	2.02	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	GAL	O3-C3-C2	-4.45	100.97	110.05
2	J	1	NAG	O5-C1-C2	-4.21	104.78	111.29
3	K	2	GAL	O2-C2-C3	-4.15	101.55	110.15
3	I	1	NAG	O5-C1-C2	4.05	117.56	111.29
3	K	1	NAG	C4-C3-C2	3.93	116.78	111.02
3	H	2	GAL	O3-C3-C2	-3.47	102.97	110.05
2	J	1	NAG	C1-C2-N2	3.45	115.87	110.43
3	I	2	GAL	O3-C3-C2	-3.36	103.20	110.05
3	I	1	NAG	O5-C5-C6	3.19	113.88	107.66
3	K	3	SIA	O1B-C1-C2	3.09	120.74	112.71
3	I	3	SIA	O4-C4-C3	3.06	117.47	109.86
3	H	1	NAG	O4-C4-C3	-3.05	103.20	110.38
3	I	3	SIA	O1B-C1-C2	3.00	120.51	112.71
3	I	3	SIA	C9-C8-C7	-2.95	106.15	112.17
3	H	2	GAL	O5-C1-C2	-2.93	103.79	110.79
3	K	1	NAG	C1-O5-C5	2.88	116.05	112.19
3	K	2	GAL	O4-C4-C5	2.87	116.39	109.32
3	K	2	GAL	O5-C1-C2	-2.85	104.00	110.79
3	K	3	SIA	C6-C5-N5	-2.83	106.39	110.91
3	K	1	NAG	O5-C1-C2	2.82	115.65	111.29
2	G	1	NAG	C1-C2-N2	2.79	114.83	110.43
3	I	1	NAG	C1-O5-C5	2.72	115.83	112.19
3	I	2	GAL	O5-C5-C6	2.71	112.94	107.66
2	J	2	NAG	C1-C2-N2	2.69	114.68	110.43
3	K	1	NAG	O7-C7-C8	-2.65	117.34	122.05
3	H	3	SIA	C9-C8-C7	-2.64	106.79	112.17
3	I	3	SIA	O6-C2-C3	-2.63	107.02	110.56
3	K	1	NAG	O3-C3-C2	2.62	114.85	109.40
2	G	1	NAG	C4-C3-C2	2.62	114.86	111.02
3	K	3	SIA	O1A-C1-C2	-2.56	117.32	122.85
3	I	2	GAL	O5-C1-C2	-2.55	104.70	110.79
3	K	2	GAL	O2-C2-C1	2.55	115.06	109.22
3	H	3	SIA	O6-C2-C1	-2.53	102.95	107.72
2	G	2	NAG	C3-C4-C5	-2.48	105.73	110.23
3	H	1	NAG	C4-C3-C2	2.37	114.49	111.02
2	G	2	NAG	O4-C4-C5	2.32	115.03	109.32
3	I	1	NAG	O4-C4-C5	2.26	114.90	109.32
3	H	2	GAL	O2-C2-C3	-2.25	105.48	110.15
3	K	1	NAG	O4-C4-C5	2.25	114.87	109.32
3	K	3	SIA	O9-C9-C8	-2.25	106.43	111.16
2	J	1	NAG	O7-C7-C8	-2.25	118.05	122.05
3	I	2	GAL	O3-C3-C4	-2.24	105.09	110.38
3	I	1	NAG	O3-C3-C2	2.24	114.05	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	SIA	O6-C2-C3	2.23	113.56	110.56
2	J	2	NAG	C3-C4-C5	-2.23	106.19	110.23
3	I	2	GAL	C1-C2-C3	-2.19	106.45	109.64
3	K	1	NAG	O4-C4-C3	-2.12	105.37	110.38
3	I	3	SIA	C4-C5-N5	-2.09	106.32	110.44
3	I	3	SIA	O1A-C1-C2	-2.09	118.34	122.85
3	K	3	SIA	O6-C2-C3	-2.08	107.77	110.56

There are no chirality outliers.

All (10) torsion outliers are listed below:

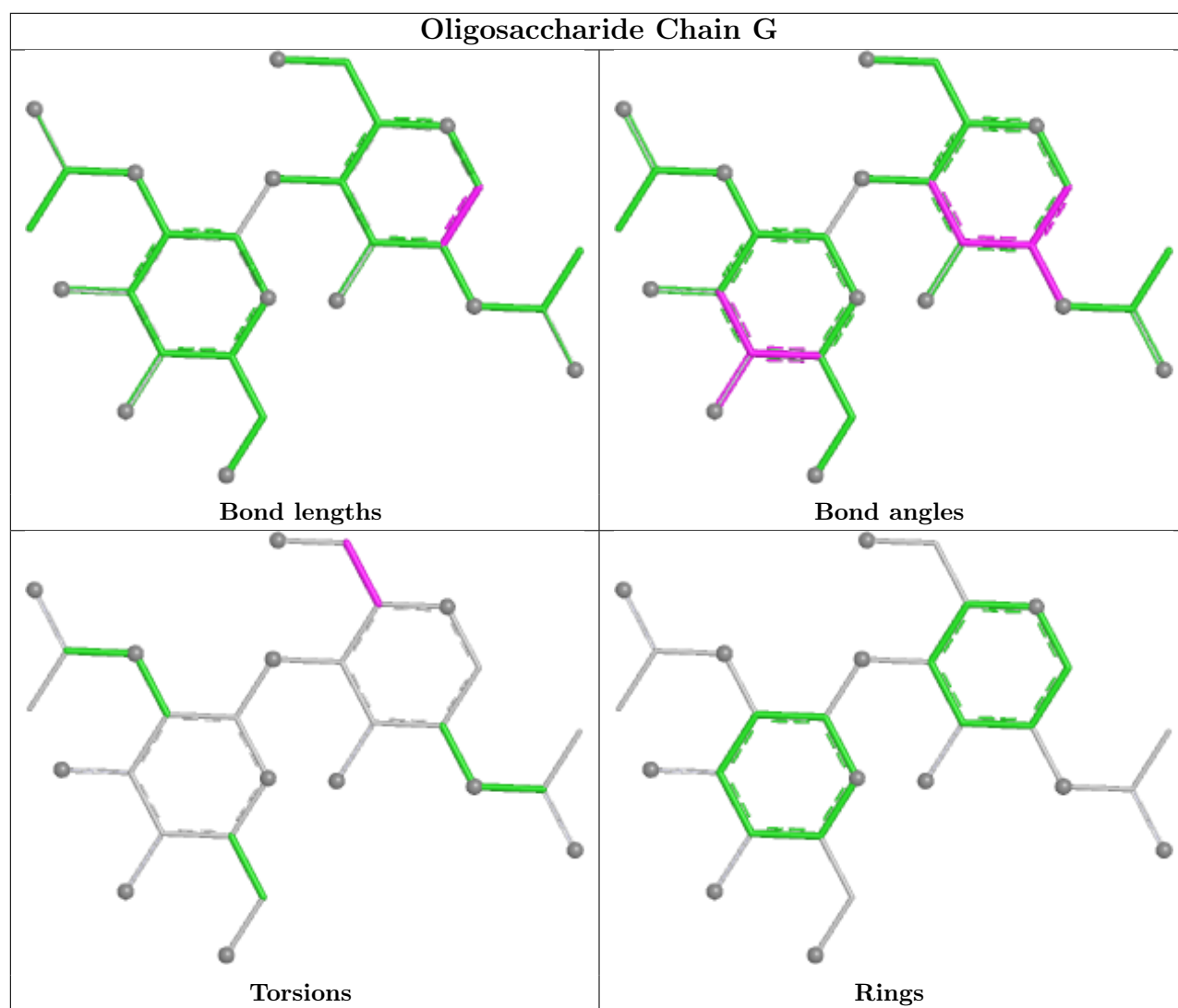
Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	2	GAL	C4-C5-C6-O6
3	K	2	GAL	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	H	3	SIA	O8-C8-C9-O9
2	G	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	3	SIA	O1A-C1-C2-O6
3	H	3	SIA	C7-C8-C9-O9

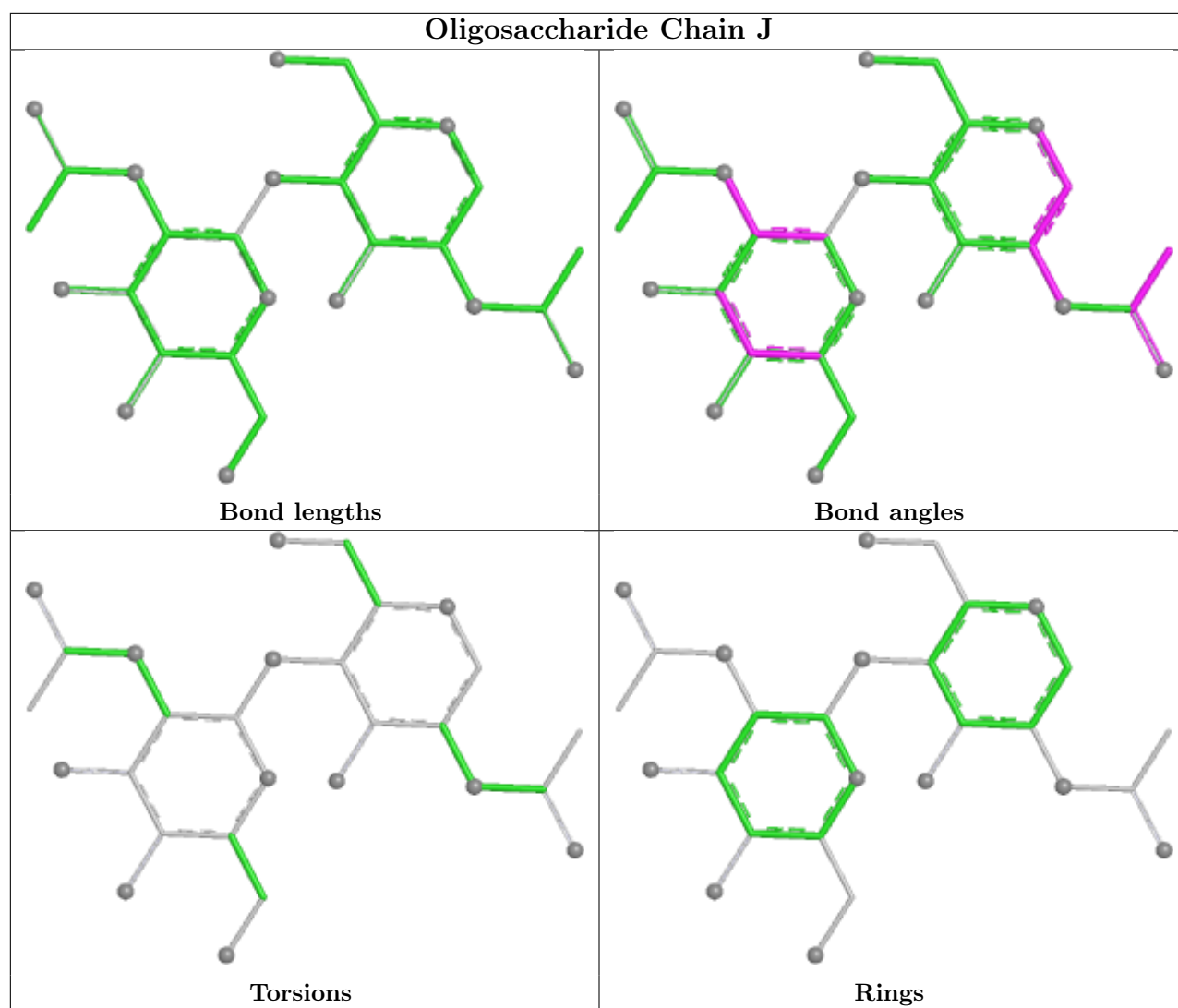
There are no ring outliers.

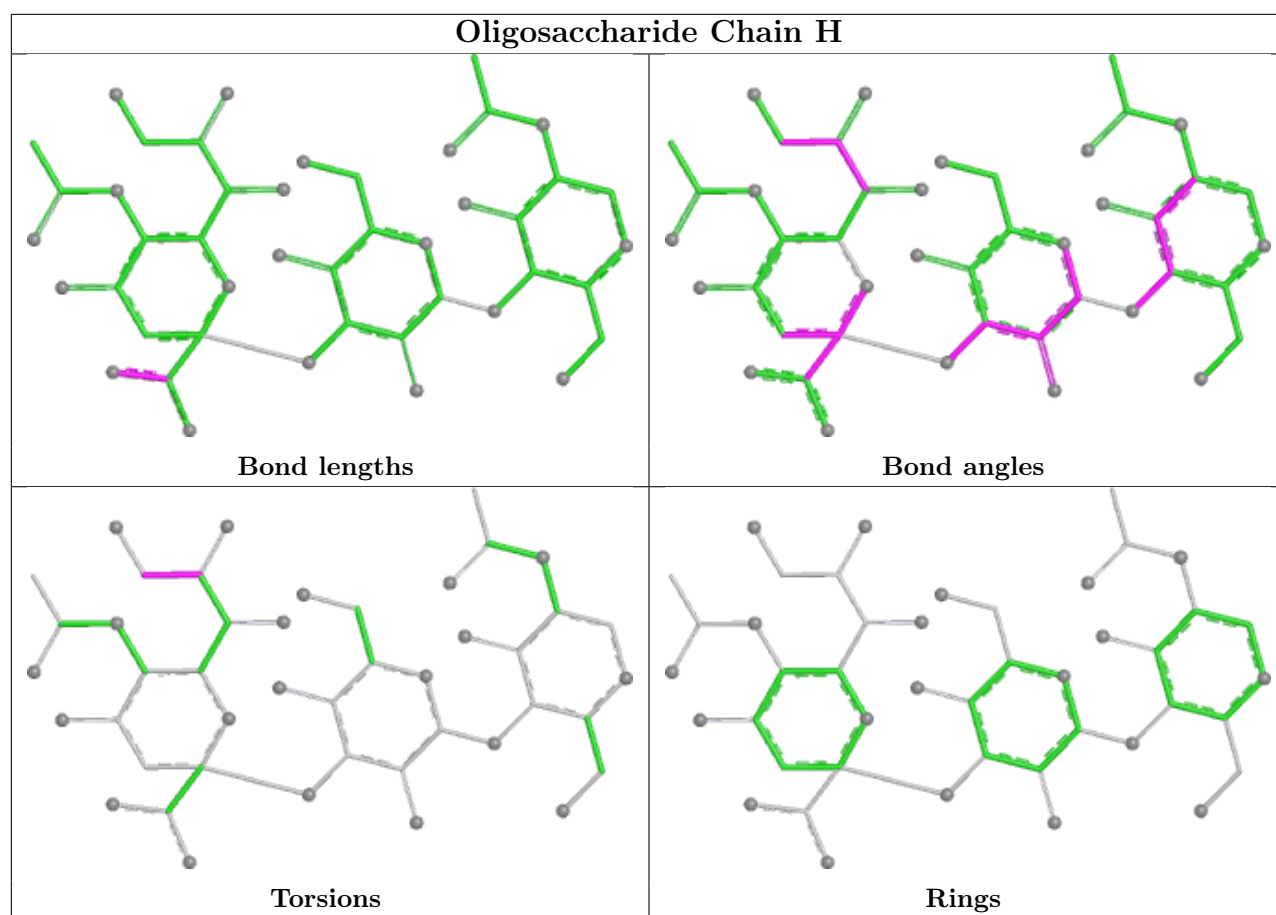
2 monomers are involved in 5 short contacts:

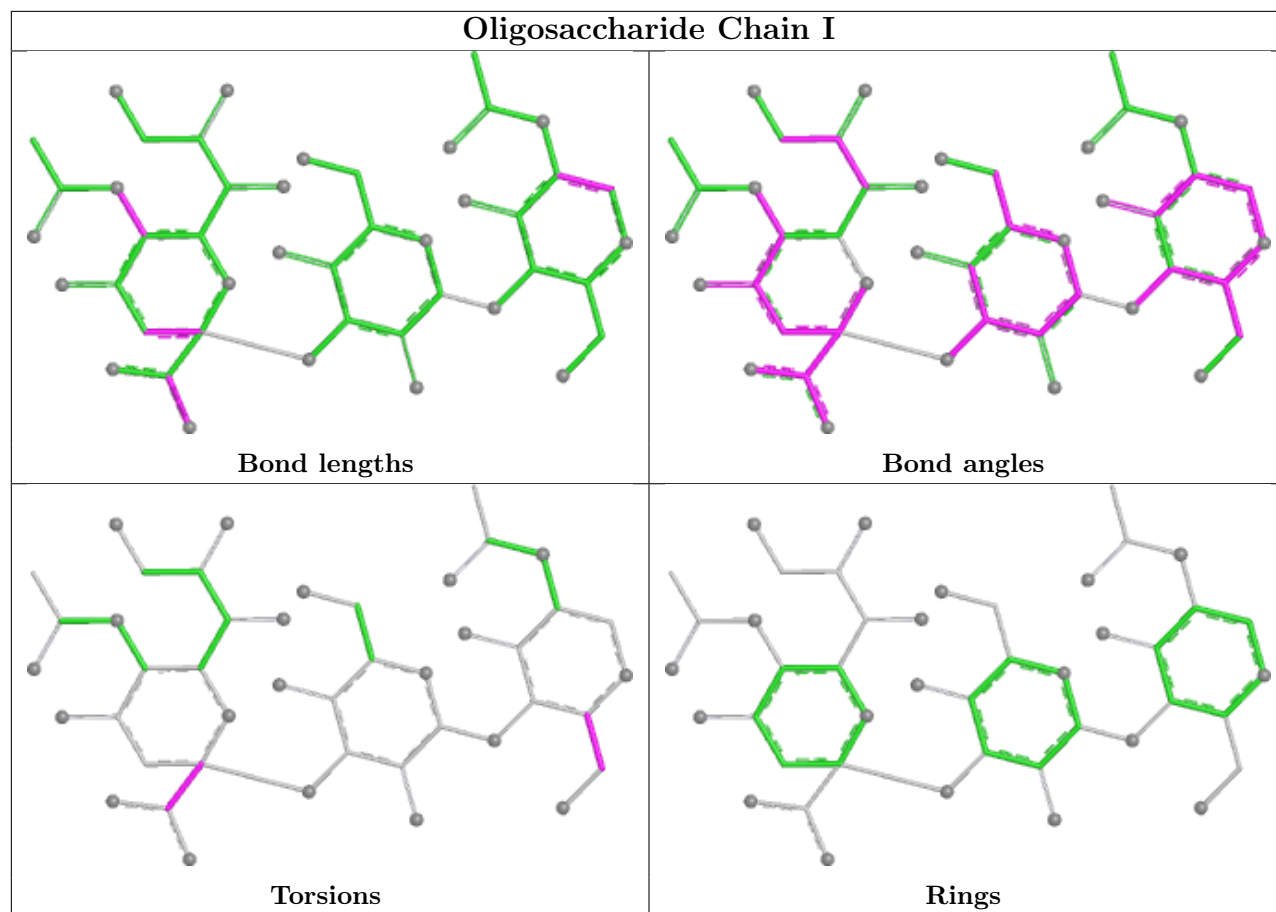
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	SIA	1	0
3	H	3	SIA	4	0

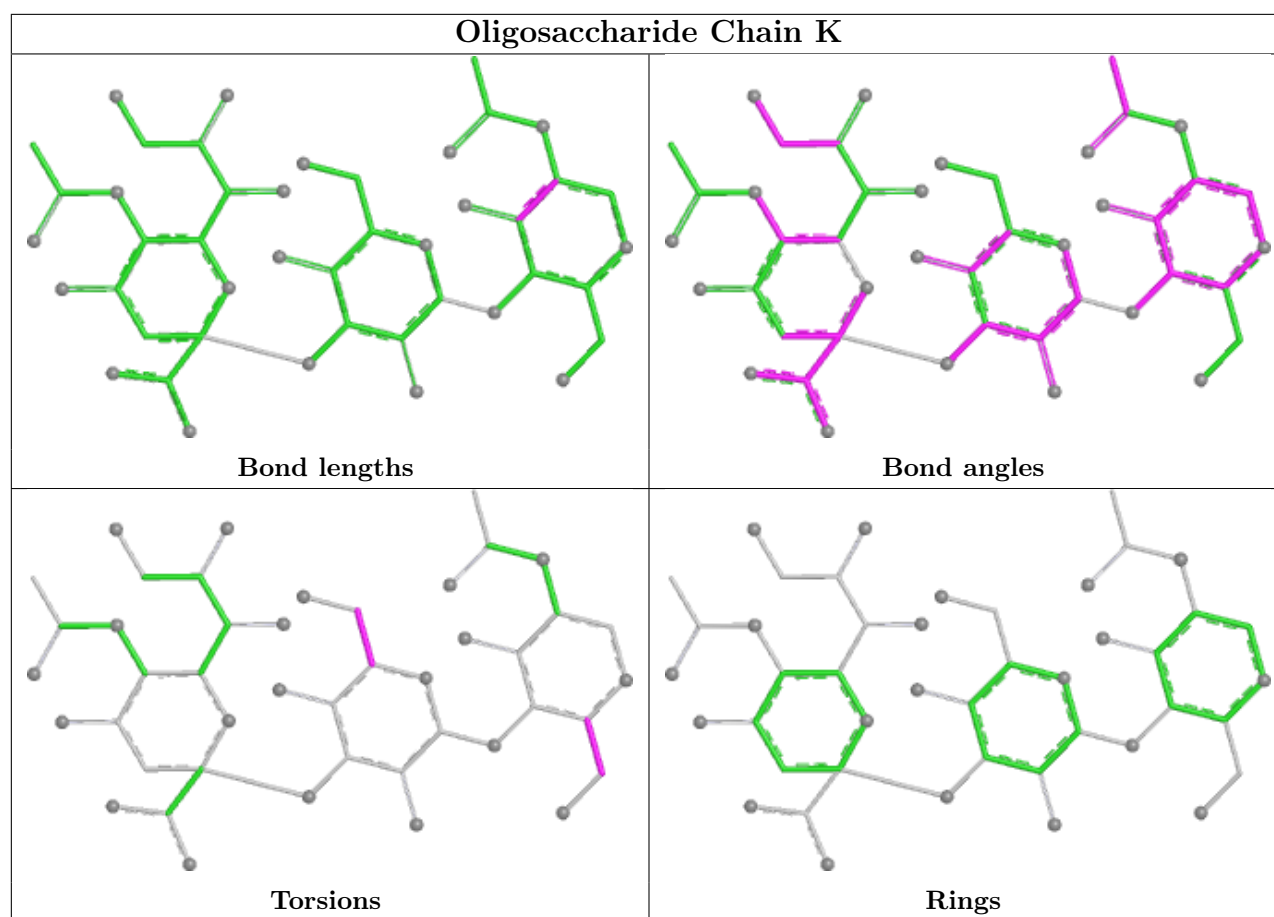
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
4	NAG	C	601	1	14,14,15	0.72	0	17,19,21	1.40	2 (11%)
4	NAG	E	601	1	14,14,15	1.62	2 (14%)	17,19,21	3.07	12 (70%)
4	NAG	E	602	1	14,14,15	0.58	0	17,19,21	1.89	2 (11%)
4	NAG	B	602	1	14,14,15	1.10	1 (7%)	17,19,21	1.98	5 (29%)
4	NAG	D	900	1	14,14,15	0.85	0	17,19,21	1.61	2 (11%)
4	NAG	B	601	1	14,14,15	0.44	0	17,19,21	1.57	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	602	1	14,14,15	1.09	1 (7%)	17,19,21	2.18	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	E	602	1	-	1/6/23/26	0/1/1/1
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	D	900	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	B	601	1	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	C	602	1	1/1/5/7	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	601	NAG	C1-C2	4.96	1.59	1.52
4	B	602	NAG	C1-C2	2.90	1.56	1.52
4	C	602	NAG	C1-C2	2.40	1.55	1.52
4	E	601	NAG	C3-C2	2.31	1.57	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	NAG	C1-O5-C5	5.92	120.12	112.19
4	E	601	NAG	O5-C5-C4	-5.09	98.44	110.83
4	E	601	NAG	C3-C4-C5	-5.04	101.08	110.23
4	C	602	NAG	O5-C5-C4	-4.33	100.28	110.83
4	E	601	NAG	O5-C5-C6	4.31	116.05	107.66
4	E	601	NAG	C1-O5-C5	4.10	117.68	112.19
4	D	900	NAG	O5-C1-C2	-3.82	105.37	111.29
4	C	602	NAG	O5-C1-C2	-3.58	105.75	111.29
4	C	602	NAG	C1-C2-N2	3.53	115.99	110.43
4	C	602	NAG	C8-C7-N2	3.46	121.85	116.12
4	B	602	NAG	C4-C3-C2	3.45	116.08	111.02
4	E	601	NAG	C1-C2-N2	3.43	115.83	110.43
4	E	601	NAG	C6-C5-C4	3.38	121.31	113.02
4	B	602	NAG	C2-N2-C7	3.37	127.42	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	NAG	O4-C4-C5	3.23	117.29	109.32
4	B	602	NAG	C1-C2-N2	3.19	115.46	110.43
4	C	602	NAG	O7-C7-C8	-3.17	116.42	122.05
4	B	601	NAG	C1-O5-C5	3.16	116.43	112.19
4	C	601	NAG	C1-O5-C5	3.14	116.39	112.19
4	E	601	NAG	O7-C7-C8	-3.03	116.66	122.05
4	B	602	NAG	O7-C7-C8	-3.00	116.71	122.05
4	B	601	NAG	O5-C5-C6	2.84	113.19	107.66
4	D	900	NAG	C4-C3-C2	2.76	115.07	111.02
4	E	601	NAG	O3-C3-C2	2.75	115.11	109.40
4	E	601	NAG	O4-C4-C3	2.67	116.68	110.38
4	E	602	NAG	O5-C1-C2	2.52	115.19	111.29
4	C	602	NAG	C6-C5-C4	2.49	119.13	113.02
4	B	601	NAG	O7-C7-C8	-2.43	117.73	122.05
4	E	601	NAG	O3-C3-C4	2.30	115.79	110.38
4	C	601	NAG	O3-C3-C2	2.23	114.03	109.40
4	B	601	NAG	C6-C5-C4	-2.15	107.75	113.02
4	B	602	NAG	O4-C4-C3	2.12	115.38	110.38
4	E	601	NAG	C8-C7-N2	2.05	119.52	116.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	601	NAG	C1
4	C	602	NAG	C1
4	E	601	NAG	C1
4	D	900	NAG	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	601	NAG	O5-C5-C6-O6
4	C	602	NAG	C4-C5-C6-O6
4	C	602	NAG	O5-C5-C6-O6
4	D	900	NAG	O5-C5-C6-O6
4	D	900	NAG	C4-C5-C6-O6
4	E	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	E	602	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	601	NAG	2	0
4	B	601	NAG	1	0
4	C	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	490/514 (95%)	0.10	13 (2%) 56 46	33, 52, 101, 128	0
1	B	481/514 (93%)	0.17	12 (2%) 58 48	34, 56, 115, 140	0
1	C	482/514 (93%)	0.02	6 (1%) 76 68	35, 52, 98, 133	0
1	D	493/514 (95%)	0.32	44 (8%) 15 11	32, 55, 160, 224	0
1	E	489/514 (95%)	0.03	5 (1%) 79 72	36, 54, 76, 99	0
1	F	479/514 (93%)	0.60	80 (16%) 4 3	36, 58, 164, 200	0
All	All	2914/3084 (94%)	0.20	160 (5%) 30 23	32, 54, 130, 224	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	480	VAL	5.1
1	F	349	TRP	4.9
1	F	353	HIS	4.6
1	A	496	LEU	4.6
1	F	354	HIS	4.5
1	F	316	ALA	4.4
1	A	481	LYS	4.3
1	D	330	LEU	4.2
1	F	9	ALA	4.1
1	F	496	LEU	4.1
1	F	357	SER	4.0
1	E	462	GLY	4.0
1	F	3	ILE	4.0
1	F	376	ILE	4.0
1	B	469	TRP	3.9
1	D	368	SER	3.9
1	F	472	CYS	3.7
1	F	13	THR	3.6
1	F	348	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	3	ILE	3.6
1	F	318	GLY	3.6
1	F	448	GLU	3.6
1	B	355	GLU	3.5
1	F	360	SER	3.5
1	D	468	PHE	3.4
1	B	217	ARG	3.4
1	D	451	LYS	3.4
1	F	452	SER	3.4
1	B	318	GLY	3.3
1	F	350	TYR	3.3
1	D	352	TYR	3.3
1	D	363	ALA	3.2
1	F	340	GLY	3.2
1	D	323	PRO	3.2
1	F	5	ILE	3.1
1	F	352	TYR	3.1
1	F	317	THR	3.1
1	F	6	GLY	3.1
1	F	497	ASN	3.1
1	A	477	ILE	3.1
1	F	19	ILE	3.1
1	D	490	TYR	3.0
1	A	334	ILE	3.0
1	F	373	ILE	3.0
1	D	354	HIS	3.0
1	F	445	ASN	3.0
1	F	476	CYS	3.0
1	D	2	LYS	3.0
1	D	459	LYS	3.0
1	D	329	GLY	2.9
1	F	431	GLU	2.9
1	B	2	LYS	2.9
1	F	477	ILE	2.9
1	B	481	LYS	2.9
1	F	343	THR	2.9
1	B	457	ASN	2.9
1	A	2	LYS	2.8
1	F	368	SER	2.8
1	E	323	PRO	2.8
1	D	322	VAL	2.8
1	F	16	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	342	TRP	2.7
1	B	468	PHE	2.7
1	F	483	GLY	2.7
1	D	496	LEU	2.7
1	F	315	LEU	2.7
1	F	11	ASN	2.7
1	F	450	VAL	2.7
1	F	10	ASN	2.7
1	D	477	ILE	2.6
1	F	446	LEU	2.7
1	F	379	LYS	2.6
1	F	363	ALA	2.6
1	F	469	TRP	2.6
1	F	449	LYS	2.6
1	F	14	THR	2.6
1	F	30	VAL	2.6
1	F	347	ASP	2.6
1	F	215	ALA	2.6
1	F	29	SER	2.6
1	F	375	GLY	2.6
1	D	458	ALA	2.6
1	C	323	PRO	2.6
1	C	471	LYS	2.6
1	D	488	PRO	2.6
1	F	2	LYS	2.6
1	F	369	THR	2.6
1	F	359	GLY	2.5
1	A	485	TYR	2.5
1	D	5	ILE	2.5
1	F	26	VAL	2.5
1	D	456	ASP	2.5
1	B	323	PRO	2.5
1	F	454	LEU	2.5
1	F	351	GLY	2.5
1	F	355	GLU	2.5
1	F	490	TYR	2.5
1	F	498	ARG	2.5
1	E	448	GLU	2.4
1	F	389	THR	2.4
1	F	28	HIS	2.4
1	A	480	VAL	2.4
1	A	352	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	426	LEU	2.4
1	D	373	ILE	2.4
1	B	456	ASP	2.4
1	D	217	ARG	2.4
1	F	364	ALA	2.4
1	F	453	GLN	2.4
1	D	485	TYR	2.4
1	B	194	LEU	2.4
1	F	462	GLY	2.3
1	F	471	LYS	2.3
1	F	481	LYS	2.3
1	D	487	TYR	2.3
1	D	6	GLY	2.3
1	F	54	ASP	2.3
1	F	20	LEU	2.3
1	B	434	ARG	2.3
1	D	362	TYR	2.3
1	F	485	TYR	2.3
1	D	344	GLY	2.3
1	D	349	TRP	2.3
1	D	469	TRP	2.3
1	F	377	THR	2.3
1	F	473	ASP	2.2
1	D	389	THR	2.2
1	D	466	PHE	2.2
1	D	366	LYS	2.2
1	D	486	ASN	2.2
1	F	32	LEU	2.2
1	D	1	ASP	2.2
1	C	159	SER	2.2
1	D	446	LEU	2.2
1	D	372	ALA	2.2
1	D	454	LEU	2.2
1	F	15	GLN	2.1
1	E	216	ASP	2.1
1	C	363	ALA	2.1
1	C	366	LYS	2.1
1	A	1	ASP	2.1
1	F	456	ASP	2.1
1	F	346	VAL	2.1
1	A	459	LYS	2.1
1	F	488	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	457	ASN	2.1
1	A	466	PHE	2.1
1	D	348	GLY	2.1
1	D	460	ASP	2.1
1	E	492	GLU	2.1
1	A	471	LYS	2.0
1	D	379	LYS	2.0
1	F	438	MET	2.0
1	D	457	ASN	2.0
1	A	338	ILE	2.0
1	D	343	THR	2.0
1	D	395	GLU	2.0
1	F	493	GLU	2.0
1	D	387	MET	2.0
1	C	322	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
4	NAG	D	900	14/15	0.50	0.19	101,115,122,126	0
3	NAG	I	1	14/15	0.58	0.15	85,102,118,127	0
3	NAG	K	1	14/15	0.59	0.15	87,98,110,110	0
2	NAG	G	2	14/15	0.61	0.11	86,101,109,110	0
4	NAG	E	602	14/15	0.62	0.13	97,114,122,122	0
3	NAG	H	1	14/15	0.62	0.15	73,94,107,113	0
4	NAG	C	601	14/15	0.64	0.13	104,117,132,133	0
2	NAG	J	2	14/15	0.72	0.12	88,109,115,115	0
4	NAG	B	602	14/15	0.72	0.13	68,75,78,81	0
4	NAG	E	601	14/15	0.72	0.13	55,85,93,97	0
4	NAG	B	601	14/15	0.73	0.11	106,117,129,130	0
4	NAG	C	602	14/15	0.74	0.14	57,80,94,100	0
2	NAG	J	1	14/15	0.84	0.11	82,87,99,100	0
2	NAG	G	1	14/15	0.86	0.09	68,84,92,94	0
3	GAL	K	2	11/12	0.89	0.09	57,65,74,77	0
3	GAL	I	2	11/12	0.91	0.09	59,65,74,76	0
3	GAL	H	2	11/12	0.93	0.07	53,57,65,66	0

6.3 Carbohydrates

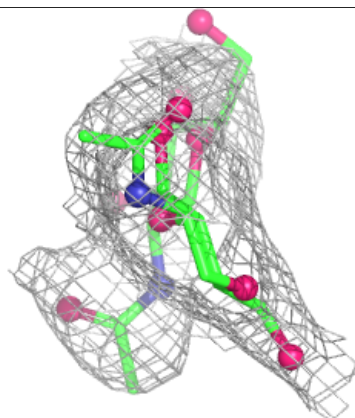
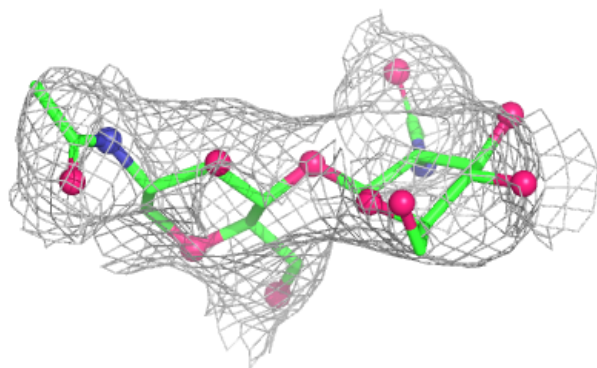
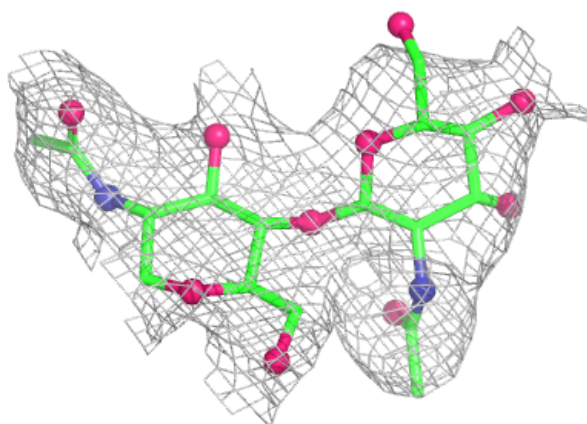
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	I	1	14/15	0.58	0.15	85,102,118,127	0
3	NAG	K	1	14/15	0.59	0.15	87,98,110,110	0
2	NAG	G	2	14/15	0.61	0.11	86,101,109,110	0
3	NAG	H	1	14/15	0.62	0.15	73,94,107,113	0
2	NAG	J	2	14/15	0.72	0.12	88,109,115,115	0
2	NAG	J	1	14/15	0.84	0.11	82,87,99,100	0
2	NAG	G	1	14/15	0.86	0.09	68,84,92,94	0
3	GAL	K	2	11/12	0.89	0.09	57,65,74,77	0
3	GAL	I	2	11/12	0.91	0.09	59,65,74,76	0
3	GAL	H	2	11/12	0.93	0.07	53,57,65,66	0
3	SIA	H	3	20/21	0.93	0.09	38,45,57,65	0
3	SIA	I	3	20/21	0.94	0.10	42,46,53,55	0
3	SIA	K	3	20/21	0.94	0.09	49,52,64,67	0

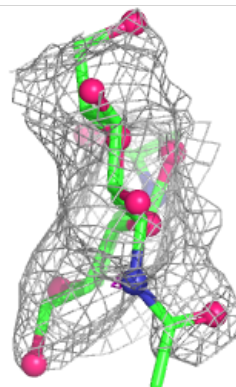
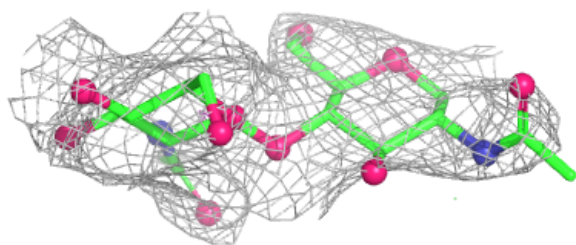
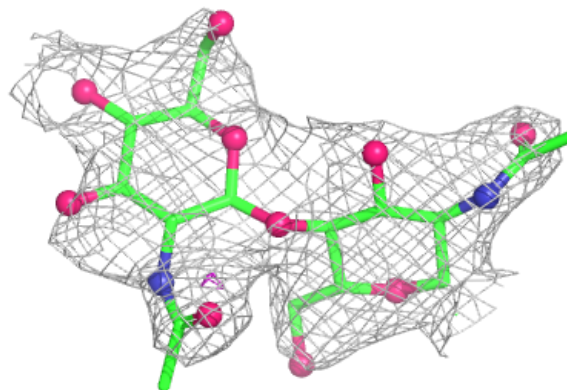
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

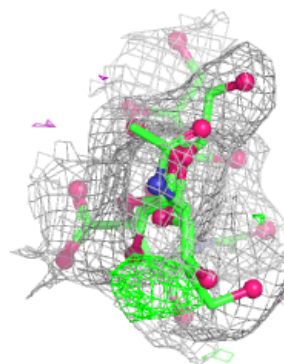
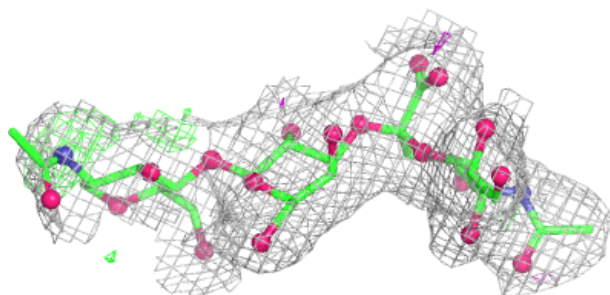
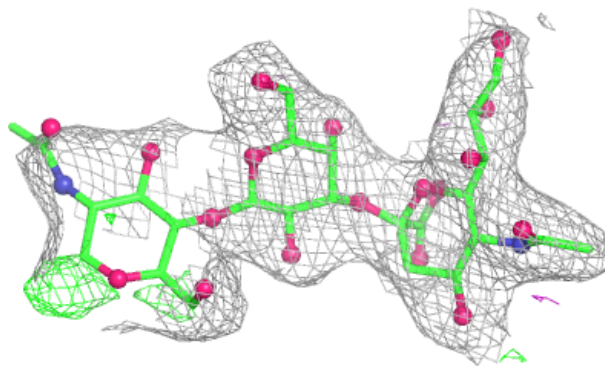
**Electron density around Chain J:**

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

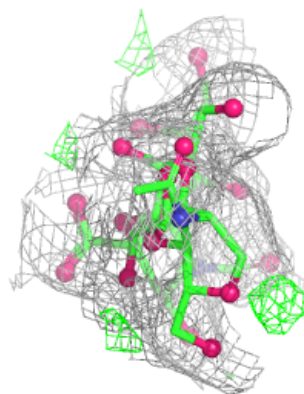
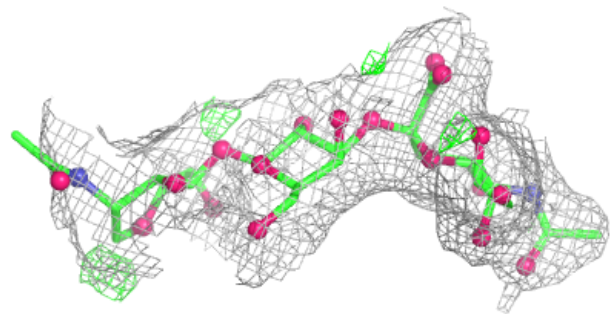
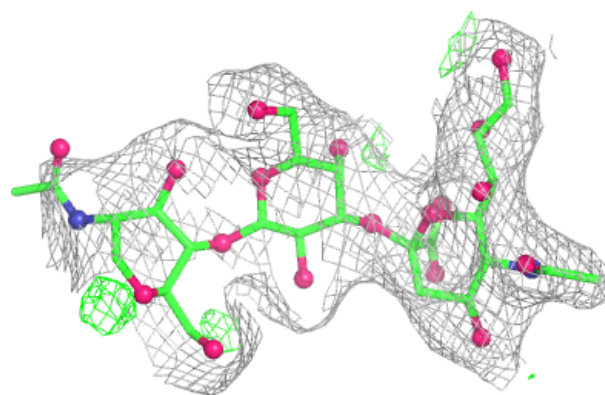


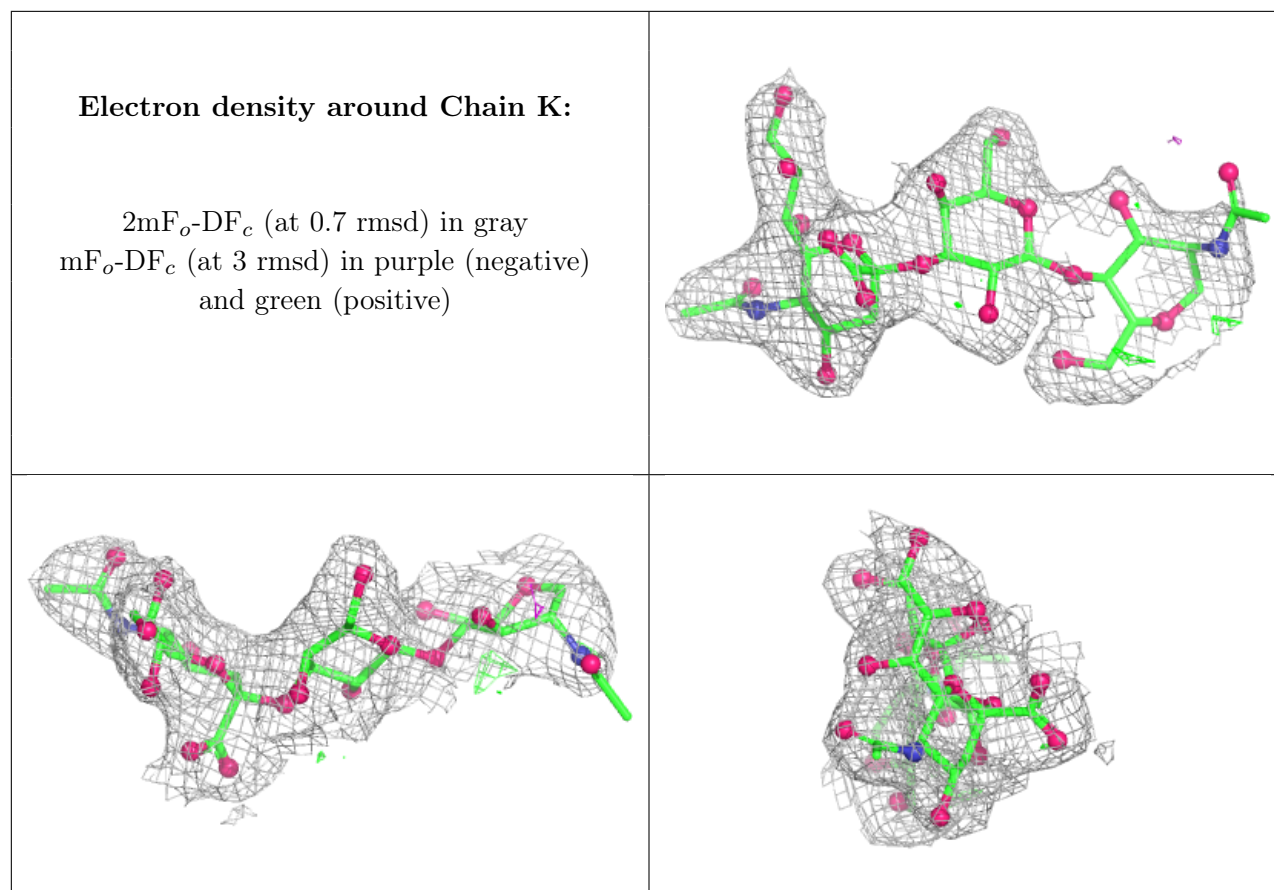
Electron density around Chain H:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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
4	NAG	D	900	14/15	0.50	0.19	101,115,122,126	0
4	NAG	E	602	14/15	0.62	0.13	97,114,122,122	0
4	NAG	C	601	14/15	0.64	0.13	104,117,132,133	0
4	NAG	B	602	14/15	0.72	0.13	68,75,78,81	0
4	NAG	E	601	14/15	0.72	0.13	55,85,93,97	0
4	NAG	B	601	14/15	0.73	0.11	106,117,129,130	0
4	NAG	C	602	14/15	0.74	0.14	57,80,94,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.