



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:04 PM UTC

PDB ID : 4BH1 / pdb_00004bh1
Title : H5 (tyTy) Influenza Virus Haemagglutinin in Complex with Avian Receptor Analogue 3'-SLN
Authors : Xiong, X.; Coombs, P.J.; Martin, S.R.; Liu, J.; Xiao, H.; McCauley, J.W.; Locher, K.; Walker, P.A.; Collins, P.J.; Kawaoka, Y.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2013-03-29
Resolution : 2.15 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

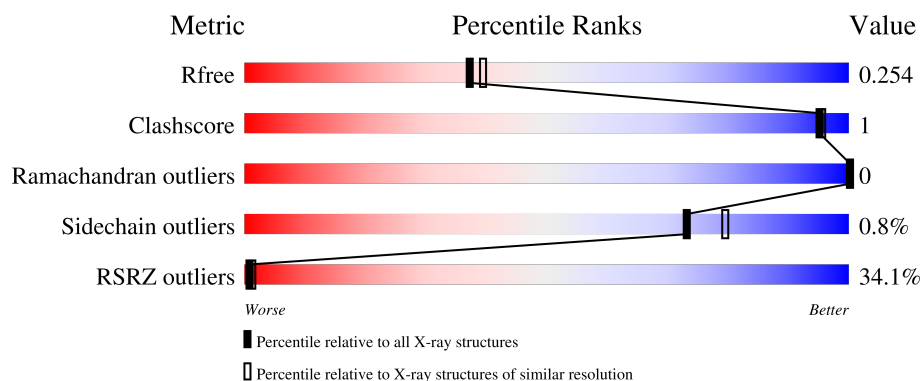
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	326	17% 94% • •
1	C	326	17% 94% • •
1	E	326	19% 94% • •
2	B	166	60% 86% • 13%

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Mol	Chain	Length	Quality of chain
2	D	166	 57% 84% 12%
2	F	166	 65% 83% 13%
3	G	3	 33% 67%
3	H	3	 100%
3	I	3	 33% 67%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11980 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	319	Total	C	N	O	S	0	0	0
			2526	1592	439	481	14			
1	C	319	Total	C	N	O	S	0	0	0
			2519	1587	439	479	14			
1	E	319	Total	C	N	O	S	0	0	0
			2519	1587	439	479	14			

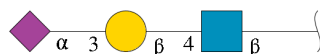
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ARG	-	expression tag	UNP Q207Z6
A	324	GLU	-	expression tag	UNP Q207Z6
A	325	THR	-	expression tag	UNP Q207Z6
A	326	ARG	-	expression tag	UNP Q207Z6
C	323	ARG	-	expression tag	UNP Q207Z6
C	324	GLU	-	expression tag	UNP Q207Z6
C	325	THR	-	expression tag	UNP Q207Z6
C	326	ARG	-	expression tag	UNP Q207Z6
E	323	ARG	-	expression tag	UNP Q207Z6
E	324	GLU	-	expression tag	UNP Q207Z6
E	325	THR	-	expression tag	UNP Q207Z6
E	326	ARG	-	expression tag	UNP Q207Z6

- Molecule 2 is a protein called HEMAGGLUTININ.

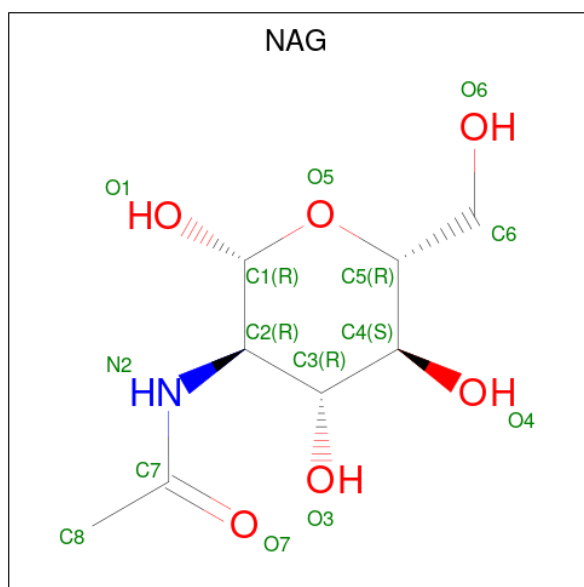
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1129	697	200	224	8			
2	D	146	Total	C	N	O	S	0	0	0
			1130	698	201	223	8			
2	F	145	Total	C	N	O	S	0	0	0
			1129	697	200	224	8			

- 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.



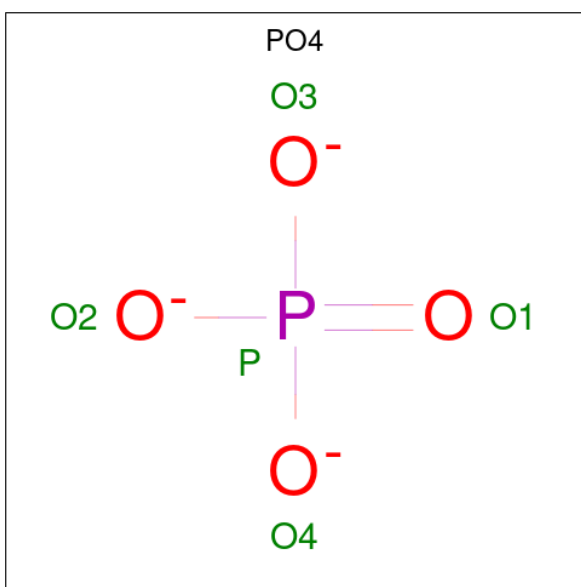
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	H	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	I	3	Total	C	N	O	0	0	0
			46	25	2	19			

- 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	A	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		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		

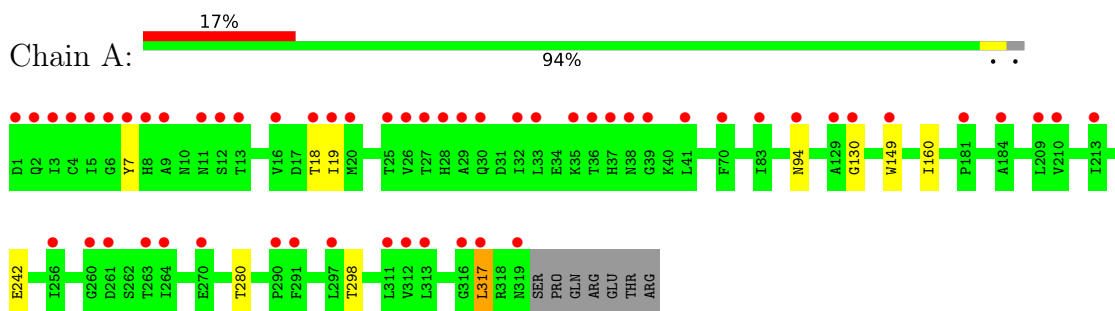
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	266	Total	O	0	0
			266	266		
6	B	36	Total	O	0	0
			36	36		
6	C	243	Total	O	0	0
			243	243		
6	D	35	Total	O	0	0
			35	35		
6	E	218	Total	O	0	0
			218	218		
6	F	30	Total	O	0	0
			30	30		

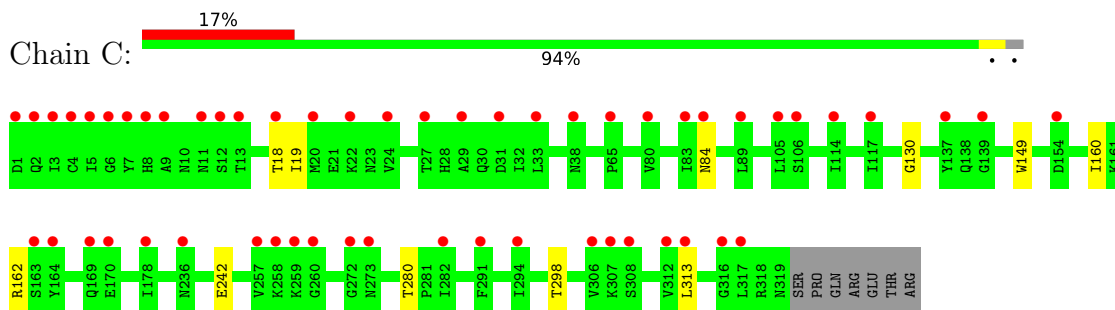
3 Residue-property plots [i](#)

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.

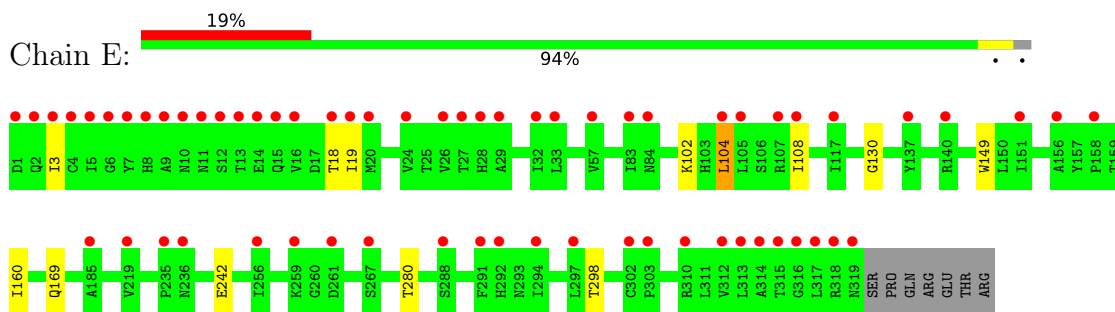
• Molecule 1: HEMAGGLUTININ



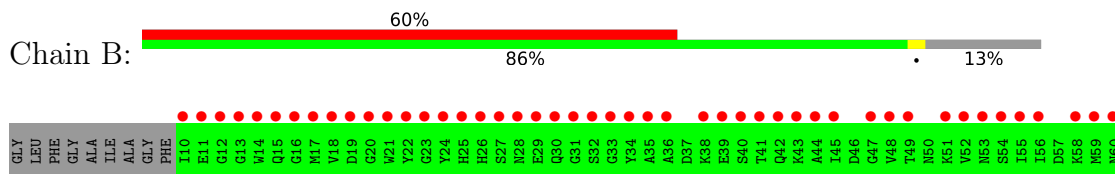
• Molecule 1: HEMAGGLUTININ

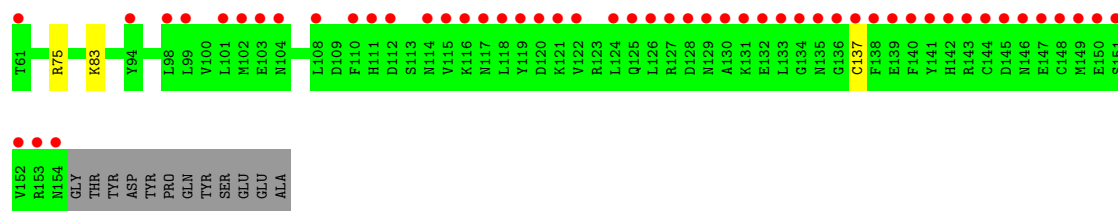


• Molecule 1: HEMAGGLUTININ

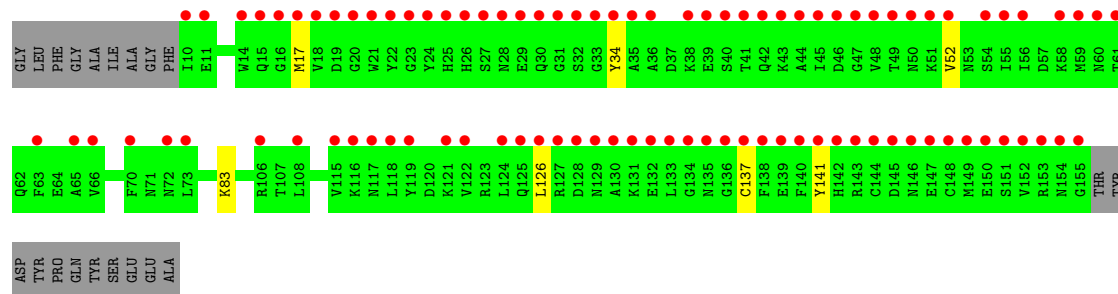
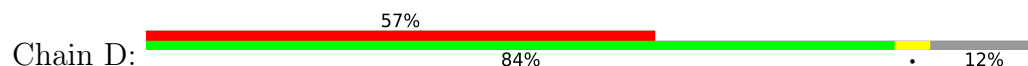


• Molecule 2: HEMAGGLUTININ

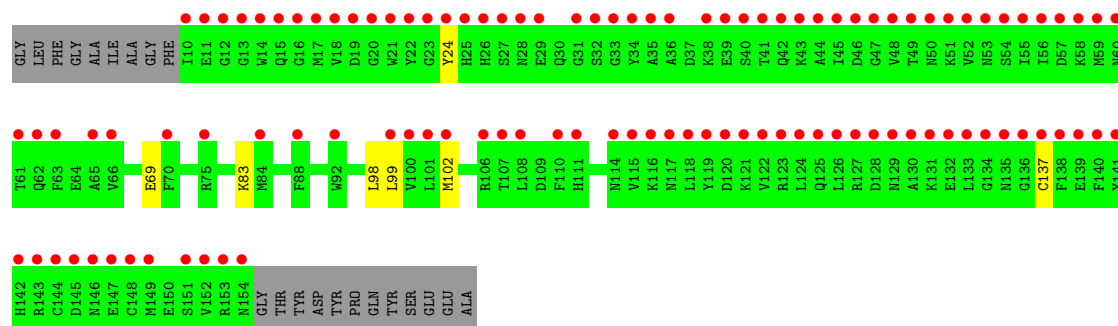
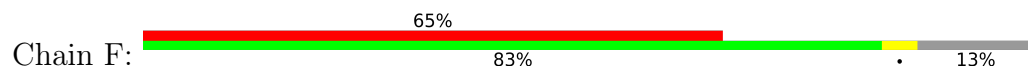




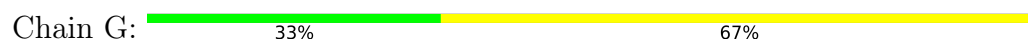
• Molecule 2: HEMAGGLUTININ



• Molecule 2: HEMAGGLUTININ



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



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



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

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.86Å 228.29Å 71.92Å 90.00° 113.71° 90.00°	Depositor
Resolution (Å)	62.48 – 2.15 62.48 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.0 (62.48-2.15) 97.8 (62.48-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.224 0.261 , 0.254	Depositor DCC
R_{free} test set	5489 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11980	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PO4, GAL, SIA

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	0.45	0/2586	0.64	0/3515
1	C	0.45	0/2579	0.64	0/3506
1	E	0.44	0/2579	0.64	0/3506
2	B	0.41	0/1149	0.70	0/1551
2	D	0.42	0/1150	0.69	0/1552
2	F	0.42	0/1149	0.70	0/1551
All	All	0.44	0/11192	0.66	0/15181

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2526	0	2460	7	0
1	C	2519	0	2447	7	0
1	E	2519	0	2447	8	1
2	B	1129	0	1007	1	0
2	D	1130	0	1008	2	0
2	F	1129	0	1007	4	0
3	G	46	0	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	46	0	40	0	0
3	I	46	0	40	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
5	A	10	0	0	0	0
5	C	5	0	0	0	0
5	E	5	0	0	0	0
6	A	266	0	0	2	1
6	B	36	0	0	0	0
6	C	243	0	0	3	0
6	D	35	0	0	0	0
6	E	218	0	0	0	0
6	F	30	0	0	0	0
All	All	11980	0	10535	26	1

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 1.

All (26) 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)
2:F:98:LEU:HG	2:F:102:MET:HE2	1.79	0.65
2:F:99:LEU:HA	2:F:102:MET:HE3	1.80	0.62
1:C:162:ARG:HD2	6:C:2149:HOH:O	2.03	0.58
1:C:84:ASN:ND2	6:C:2069:HOH:O	2.36	0.57
1:A:7:TYR:HB2	1:A:317:LEU:CD2	2.43	0.48
1:A:130:GLY:HA3	1:A:149:TRP:HB3	1.96	0.47
1:E:130:GLY:HA3	1:E:149:TRP:HB3	1.95	0.47
1:C:130:GLY:HA3	1:C:149:TRP:HB3	1.97	0.47
1:E:280:THR:HG22	1:E:298:THR:HG22	1.98	0.46
1:A:280:THR:HG22	1:A:298:THR:HG22	1.98	0.45
1:E:160:ILE:O	1:E:242:GLU:HA	2.17	0.45
1:A:94:ASN:ND2	6:A:2077:HOH:O	2.45	0.45
1:C:313:LEU:HD13	2:D:52:VAL:HG12	1.98	0.45
1:A:160:ILE:O	1:A:242:GLU:HA	2.17	0.44
1:C:160:ILE:O	1:C:242:GLU:HA	2.17	0.44
2:D:17:MET:HG3	2:D:34:TYR:HB3	1.99	0.44
1:A:18:THR:HG22	1:A:19:ILE:N	2.33	0.43
1:C:280:THR:HG22	1:C:298:THR:HG22	1.98	0.43
1:E:18:THR:HG22	1:E:19:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:LYS:NZ	2:F:69:GLU:OE1	2.46	0.43
1:E:3:ILE:HD11	2:F:24:TYR:HB3	2.01	0.42
1:E:104:LEU:C	1:E:104:LEU:HD13	2.45	0.42
1:A:94:ASN:HB2	6:A:2078:HOH:O	2.20	0.41
1:C:18:THR:HG22	1:C:19:ILE:N	2.34	0.41
2:B:75:ARG:HG3	6:C:2090:HOH:O	2.20	0.41
1:E:104:LEU:HD13	1:E:108:ILE:HD12	2.02	0.41

All (1) 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:E:169:GLN:NE2	6:A:2135:HOH:O[1_655]	2.09	0.11

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	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
1	C	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
1	E	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
2	B	143/166 (86%)	137 (96%)	6 (4%)	0	100	100
2	D	144/166 (87%)	137 (95%)	7 (5%)	0	100	100
2	F	143/166 (86%)	137 (96%)	6 (4%)	0	100	100
All	All	1381/1476 (94%)	1338 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	284/292 (97%)	283 (100%)	1 (0%)	84	89
1	C	282/292 (97%)	282 (100%)	0	100	100
1	E	282/292 (97%)	281 (100%)	1 (0%)	84	89
2	B	113/141 (80%)	111 (98%)	2 (2%)	51	58
2	D	112/141 (79%)	108 (96%)	4 (4%)	31	31
2	F	113/141 (80%)	111 (98%)	2 (2%)	51	58
All	All	1186/1299 (91%)	1176 (99%)	10 (1%)	73	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	LEU
2	B	83	LYS
2	B	137	CYS
2	D	83	LYS
2	D	126	LEU
2	D	137	CYS
2	D	141	TYR
1	E	104	LEU
2	F	83	LYS
2	F	137	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	103	HIS
1	A	138	GLN
1	A	169	GLN
2	B	125	GLN
1	C	72	ASN
2	D	15	GLN

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Mol	Chain	Res	Type
1	E	72	ASN
1	E	169	GLN
1	E	222	GLN
2	F	15	GLN
2	F	125	GLN
2	F	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	NAG	G	1	3	15,15,15	0.38	0	21,21,21	1.37	4 (19%)
3	GAL	G	2	3	11,11,12	0.41	0	15,15,17	0.88	0
3	SIA	G	3	3	20,20,21	0.73	0	21,28,31	1.51	4 (19%)
3	NAG	H	1	3	15,15,15	0.45	0	21,21,21	1.24	2 (9%)
3	GAL	H	2	3	11,11,12	0.33	0	15,15,17	1.07	2 (13%)
3	SIA	H	3	3	20,20,21	0.70	0	21,28,31	1.19	2 (9%)
3	NAG	I	1	3	15,15,15	0.40	0	21,21,21	1.27	2 (9%)
3	GAL	I	2	3	11,11,12	0.26	0	15,15,17	0.77	0
3	SIA	I	3	3	20,20,21	0.63	0	21,28,31	1.11	2 (9%)

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-C2-N2	-4.25	105.80	110.73
3	G	3	SIA	O6-C2-C1	3.62	114.55	107.72
3	G	1	NAG	C1-C2-N2	-3.61	106.55	110.73
3	I	1	NAG	C1-C2-N2	-3.52	106.65	110.73
3	G	3	SIA	C6-C5-N5	-2.77	106.48	110.91
3	G	3	SIA	O1B-C1-C2	2.75	119.85	112.71
3	G	1	NAG	C3-C2-N2	-2.65	105.74	110.62
3	H	3	SIA	C6-C5-N5	-2.60	106.75	110.91
3	I	1	NAG	C3-C2-N2	-2.60	105.83	110.62
3	G	1	NAG	O5-C1-C2	2.52	112.05	109.52
3	I	3	SIA	C4-C5-N5	-2.47	105.56	110.44
3	H	3	SIA	O1B-C1-C2	2.45	119.07	112.71
3	I	3	SIA	C6-C5-N5	-2.35	107.16	110.91
3	H	2	GAL	C1-C2-C3	2.28	112.97	109.64
3	G	1	NAG	C1-C2-C3	2.25	113.61	110.54
3	H	1	NAG	C3-C2-N2	-2.18	106.60	110.62
3	H	2	GAL	C1-O5-C5	2.09	114.99	112.19
3	G	3	SIA	O1A-C1-C2	-2.05	118.42	122.85

There are no chirality outliers.

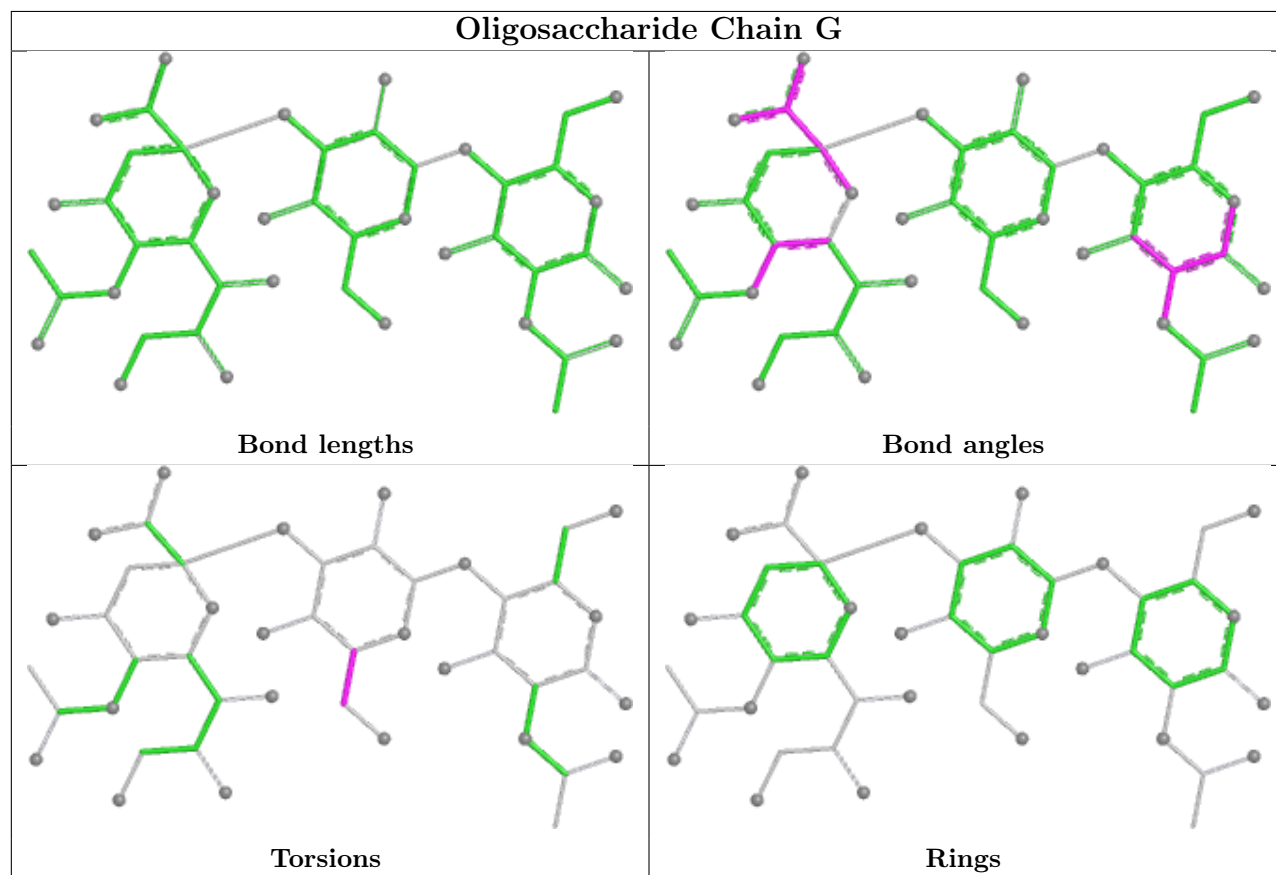
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	GAL	C4-C5-C6-O6
3	G	2	GAL	C4-C5-C6-O6

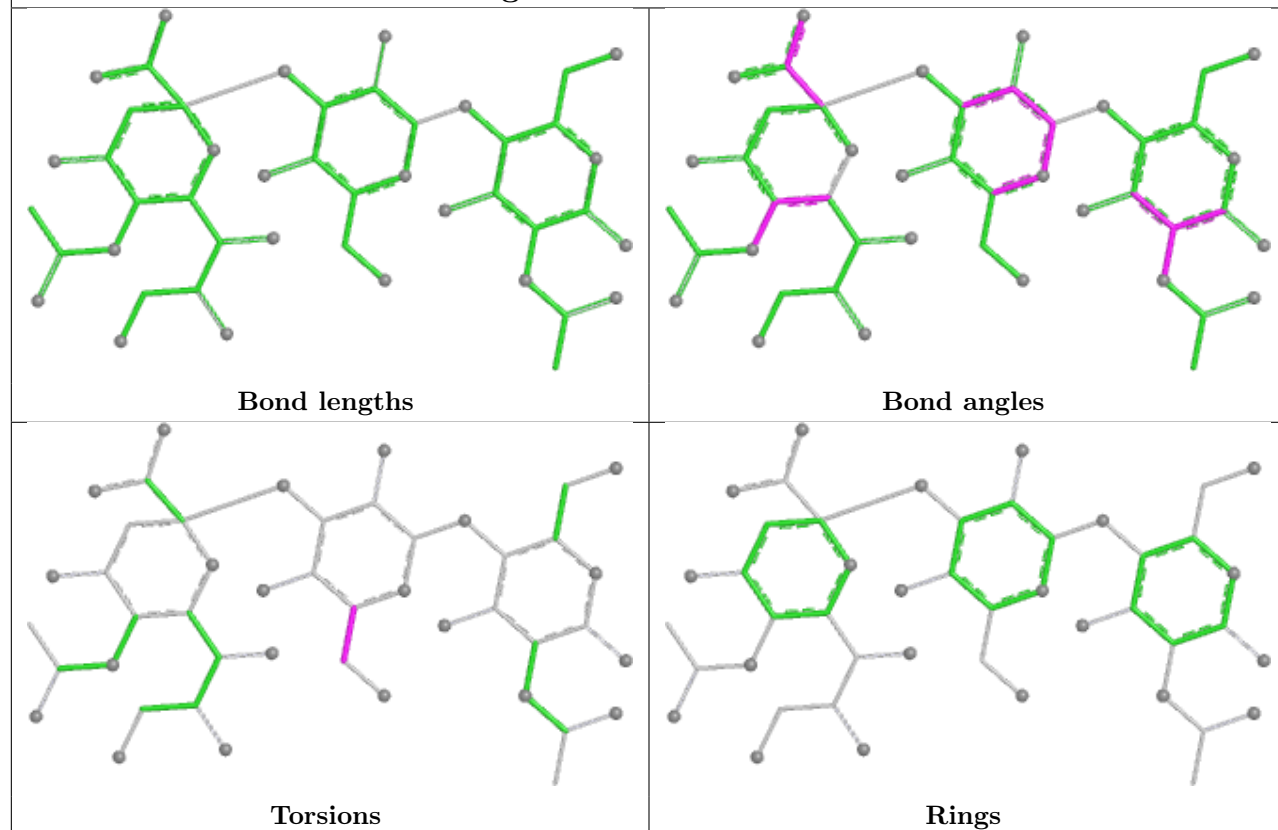
There are no ring outliers.

No monomer is involved in short contacts.

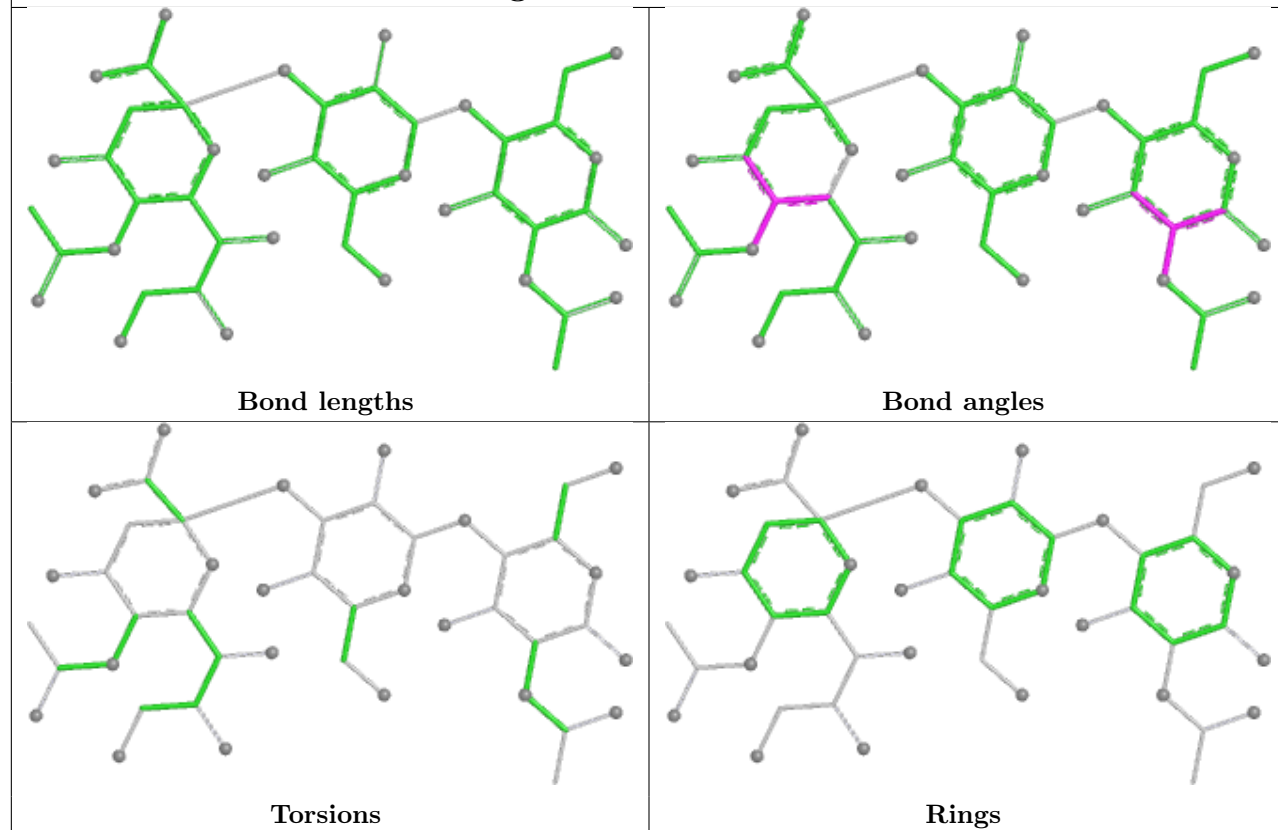
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry

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$
5	PO4	E	1324	-	4,4,4	1.00	0	6,6,6	0.56	0
5	PO4	C	1324	-	4,4,4	0.99	0	6,6,6	0.53	0
5	PO4	A	1325	-	4,4,4	0.82	0	6,6,6	0.60	0
4	NAG	A	1320	1	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
4	NAG	E	1320	1	14,14,15	0.37	0	17,19,21	1.06	1 (5%)
4	NAG	C	1320	1	14,14,15	0.55	0	17,19,21	1.38	3 (17%)
5	PO4	A	1324	-	4,4,4	0.92	0	6,6,6	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1320	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1320	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1320	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1320	NAG	C1-O5-C5	3.70	117.14	112.19
4	A	1320	NAG	C1-O5-C5	3.54	116.93	112.19
4	E	1320	NAG	C1-O5-C5	2.61	115.68	112.19
4	C	1320	NAG	C1-C2-N2	2.25	113.98	110.43
4	A	1320	NAG	C3-C4-C5	-2.09	106.44	110.23
4	C	1320	NAG	C3-C4-C5	-2.03	106.55	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1320	NAG	C4-C5-C6-O6
4	A	1320	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	319/326 (97%)	1.32	56 (17%) 4 4	23, 38, 124, 285	0
1	C	319/326 (97%)	1.34	55 (17%) 4 4	22, 40, 101, 147	0
1	E	319/326 (97%)	1.37	63 (19%) 3 4	24, 41, 129, 233	0
2	B	145/166 (87%)	3.07	99 (68%) 0 0	25, 172, 220, 245	0
2	D	146/166 (87%)	3.06	94 (64%) 0 0	29, 126, 188, 208	0
2	F	145/166 (87%)	3.13	108 (74%) 0 0	24, 166, 204, 226	0
All	All	1393/1476 (94%)	1.89	475 (34%) 1 1	22, 47, 193, 285	0

All (475) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	138	PHE	12.2
2	D	140	PHE	9.5
2	F	138	PHE	9.1
2	B	21	TRP	8.5
2	B	138	PHE	8.2
2	F	141	TYR	7.8
2	B	141	TYR	7.7
2	B	122	VAL	7.5
2	D	126	LEU	7.4
2	B	10	ILE	7.3
2	B	55	ILE	7.3
2	F	55	ILE	7.3
2	F	152	VAL	7.3
2	D	136	GLY	7.2
2	B	136	GLY	7.2
2	D	127	ARG	7.2
2	F	122	VAL	7.2
2	B	52	VAL	7.0
2	B	56	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
2	D	141	TYR	6.8
2	D	52	VAL	6.8
2	B	51	LYS	6.8
2	D	48	VAL	6.7
1	A	3	ILE	6.7
2	B	59	MET	6.6
2	D	61	THR	6.6
2	F	22	TYR	6.6
2	F	56	ILE	6.6
2	B	140	PHE	6.5
2	F	48	VAL	6.4
2	F	51	LYS	6.4
1	A	39	GLY	6.4
2	F	140	PHE	6.3
1	E	3	ILE	6.3
2	F	52	VAL	6.3
2	F	133	LEU	6.3
1	A	5	ILE	6.3
2	D	119	TYR	6.3
2	B	48	VAL	6.3
2	F	126	LEU	6.3
2	F	118	LEU	6.2
2	F	47	GLY	6.1
2	F	21	TRP	6.0
2	B	34	TYR	6.0
2	B	126	LEU	6.0
2	B	152	VAL	6.0
2	B	23	GLY	5.9
2	B	14	TRP	5.8
2	B	118	LEU	5.7
2	D	145	ASP	5.6
2	F	124	LEU	5.6
2	D	34	TYR	5.6
2	D	51	LYS	5.6
2	D	21	TRP	5.5
2	F	132	GLU	5.5
2	D	45	ILE	5.4
1	E	4	CYS	5.4
2	B	124	LEU	5.4
2	B	24	TYR	5.4
2	F	49	THR	5.4
2	D	28	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
2	F	10	ILE	5.4
2	D	30	GLN	5.3
1	E	317	LEU	5.3
2	D	131	LYS	5.2
2	D	35	ALA	5.2
2	D	55	ILE	5.2
2	F	45	ILE	5.2
2	D	59	MET	5.2
2	F	25	HIS	5.2
2	B	45	ILE	5.1
2	F	14	TRP	5.1
2	D	133	LEU	5.0
2	B	137	CYS	5.0
2	F	148	CYS	5.0
2	B	133	LEU	5.0
2	D	122	VAL	4.9
1	A	6	GLY	4.9
2	D	58	LYS	4.9
2	D	155	GLY	4.9
1	E	7	TYR	4.9
2	D	142	HIS	4.8
2	B	27	SER	4.8
2	F	142	HIS	4.7
2	D	128	ASP	4.7
1	A	4	CYS	4.7
2	D	27	SER	4.6
2	D	32	SER	4.6
2	D	130	ALA	4.6
2	D	125	GLN	4.6
2	F	136	GLY	4.5
2	D	26	HIS	4.5
2	F	137	CYS	4.5
1	E	12	SER	4.4
2	B	22	TYR	4.4
2	D	153	ARG	4.4
2	F	12	GLY	4.4
1	A	38	ASN	4.4
2	B	25	HIS	4.4
2	F	115	VAL	4.4
2	F	27	SER	4.4
2	D	16	GLY	4.3
2	D	118	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	32	ILE	4.3
2	F	16	GLY	4.3
2	F	33	GLY	4.3
2	B	58	LYS	4.3
2	B	142	HIS	4.2
2	F	110	PHE	4.2
2	D	134	GLY	4.2
1	E	26	VAL	4.2
2	D	152	VAL	4.2
2	B	16	GLY	4.2
2	B	33	GLY	4.2
2	D	132	GLU	4.2
1	E	20	MET	4.2
1	E	9	ALA	4.2
1	A	33	LEU	4.1
1	E	19	ILE	4.1
2	D	56	ILE	4.1
2	F	17	MET	4.1
2	B	132	GLU	4.1
2	D	154	ASN	4.1
2	B	35	ALA	4.1
2	B	44	ALA	4.1
1	C	5	ILE	4.1
2	D	144	CYS	4.1
1	C	6	GLY	4.1
2	F	119	TYR	4.1
2	F	129	ASN	4.0
2	D	36	ALA	4.0
2	F	34	TYR	4.0
2	D	143	ARG	4.0
2	F	32	SER	4.0
2	D	47	GLY	4.0
2	B	17	MET	4.0
1	A	37	HIS	4.0
2	D	129	ASN	3.9
2	B	131	LYS	3.9
1	C	3	ILE	3.9
1	C	20	MET	3.9
2	F	130	ALA	3.9
2	F	40	SER	3.9
2	F	61	THR	3.9
2	B	139	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	119	TYR	3.9
2	D	22	TYR	3.9
2	D	24	TYR	3.9
2	D	137	CYS	3.9
1	E	2	GLN	3.9
1	E	11	ASN	3.9
2	B	143	ARG	3.9
1	A	7	TYR	3.8
2	B	12	GLY	3.8
2	F	13	GLY	3.8
2	F	31	GLY	3.8
1	E	24	VAL	3.8
1	E	6	GLY	3.8
1	C	4	CYS	3.8
1	A	316	GLY	3.8
1	A	2	GLN	3.8
1	E	5	ILE	3.7
2	D	10	ILE	3.7
2	D	14	TRP	3.7
2	D	150	GLU	3.7
2	F	28	ASN	3.7
2	B	61	THR	3.7
1	E	104	LEU	3.7
2	F	116	LYS	3.7
2	D	18	VAL	3.7
2	F	128	ASP	3.7
2	F	23	GLY	3.6
2	F	18	VAL	3.6
2	F	127	ARG	3.6
2	F	131	LYS	3.6
2	B	125	GLN	3.6
1	E	29	ALA	3.6
2	B	20	GLY	3.6
2	B	11	GLU	3.6
2	F	58	LYS	3.6
2	F	44	ALA	3.6
2	D	33	GLY	3.6
2	F	144	CYS	3.6
1	C	294	ILE	3.5
2	F	11	GLU	3.5
2	F	38	LYS	3.5
2	D	148	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	49	THR	3.5
2	B	13	GLY	3.5
1	E	1	ASP	3.5
2	F	139	GLU	3.5
2	B	115	VAL	3.5
1	C	2	GLN	3.5
2	D	135	ASN	3.5
1	A	11	ASN	3.5
1	A	83	ILE	3.4
2	D	124	LEU	3.4
2	F	24	TYR	3.4
2	B	128	ASP	3.4
2	B	26	HIS	3.3
2	F	60	ASN	3.3
2	D	41	THR	3.3
2	B	43	LYS	3.3
2	B	31	GLY	3.3
2	B	32	SER	3.3
2	D	20	GLY	3.3
2	D	66	VAL	3.3
2	B	146	ASN	3.3
2	F	15	GLN	3.3
1	A	213	ILE	3.3
2	F	111	HIS	3.3
2	B	110	PHE	3.3
2	B	135	ASN	3.3
1	C	170	GLU	3.3
1	E	315	THR	3.3
2	B	18	VAL	3.3
1	C	282	ILE	3.3
2	B	29	GLU	3.3
2	B	117	ASN	3.3
2	D	29	GLU	3.3
2	F	120	ASP	3.3
2	F	123	ARG	3.2
1	A	30	GLN	3.2
2	F	26	HIS	3.2
2	F	147	GLU	3.2
2	D	117	ASN	3.2
1	A	264	ILE	3.2
1	A	317	LEU	3.2
1	A	8	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	135	ASN	3.2
1	C	317	LEU	3.2
2	B	153	ARG	3.2
2	F	41	THR	3.2
1	A	26	VAL	3.1
2	F	65	ALA	3.1
1	A	32	ILE	3.1
2	F	108	LEU	3.1
2	B	38	LYS	3.1
2	D	31	GLY	3.1
2	B	28	ASN	3.1
1	E	288	SER	3.1
1	A	36	THR	3.1
1	A	9	ALA	3.1
2	D	115	VAL	3.1
1	C	83	ILE	3.1
1	C	9	ALA	3.1
1	E	313	LEU	3.1
2	B	47	GLY	3.0
2	F	134	GLY	3.0
2	D	49	THR	3.0
2	F	36	ALA	3.0
1	A	16	VAL	3.0
2	D	42	GLN	3.0
1	C	105	LEU	3.0
1	E	140	ARG	3.0
2	B	127	ARG	3.0
1	E	13	THR	3.0
2	D	17	MET	3.0
2	B	30	GLN	3.0
2	B	148	CYS	3.0
1	C	236	ASN	3.0
1	A	291	PHE	3.0
2	F	143	ARG	2.9
2	B	54	SER	2.9
2	B	53	ASN	2.9
1	A	19	ILE	2.9
2	D	149	MET	2.9
2	B	151	SER	2.9
1	C	84	ASN	2.9
2	F	50	ASN	2.9
1	A	1	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	15	GLN	2.9
2	B	40	SER	2.9
1	E	319	ASN	2.9
2	D	146	ASN	2.9
2	B	36	ALA	2.9
1	A	313	LEU	2.9
1	C	80	VAL	2.9
1	E	18	THR	2.9
2	D	40	SER	2.9
2	D	60	ASN	2.9
1	A	297	LEU	2.8
2	B	147	GLU	2.8
1	C	164	TYR	2.8
2	D	65	ALA	2.8
1	A	13	THR	2.8
1	A	210	VAL	2.8
1	A	130	GLY	2.8
1	A	184	ALA	2.8
2	D	121	LYS	2.8
1	E	84	ASN	2.8
2	F	151	SER	2.8
2	D	11	GLU	2.8
1	E	291	PHE	2.8
2	F	20	GLY	2.8
1	C	7	TYR	2.8
2	B	99	LEU	2.8
2	F	121	LYS	2.8
1	A	20	MET	2.7
1	E	8	HIS	2.7
2	B	102	MET	2.7
2	F	57	ASP	2.7
2	F	35	ALA	2.7
1	A	311	LEU	2.7
2	B	98	LEU	2.7
2	F	107	THR	2.7
1	E	158	PRO	2.7
2	F	153	ARG	2.7
1	C	257	VAL	2.7
2	F	125	GLN	2.7
2	F	102	MET	2.7
2	B	108	LEU	2.7
2	B	94	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	72	ASN	2.7
1	A	270	GLU	2.7
2	F	66	VAL	2.7
1	A	260	GLY	2.7
2	D	44	ALA	2.7
2	B	42	GLN	2.6
2	D	50	ASN	2.6
2	F	100	VAL	2.6
1	C	316	GLY	2.6
2	D	23	GLY	2.6
2	B	111	HIS	2.6
1	C	13	THR	2.6
2	B	129	ASN	2.6
2	F	146	ASN	2.6
1	C	313	LEU	2.6
1	C	1	ASP	2.6
1	C	22	LYS	2.6
1	E	83	ILE	2.6
2	B	149	MET	2.6
1	A	290	PRO	2.6
2	B	121	LYS	2.6
2	F	43	LYS	2.6
1	A	70	PHE	2.6
2	B	19	ASP	2.6
2	D	70	PHE	2.6
1	E	310	ARG	2.6
1	C	137	TYR	2.6
2	F	62	GLN	2.6
1	C	27	THR	2.6
2	B	130	ALA	2.6
2	B	39	GLU	2.5
1	A	94	ASN	2.5
2	F	53	ASN	2.5
1	A	29	ALA	2.5
1	E	27	THR	2.5
2	F	70	PHE	2.5
1	C	306	VAL	2.5
1	E	117	ILE	2.5
1	C	11	ASN	2.5
1	E	156	ALA	2.5
2	D	151	SER	2.5
2	F	39	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	219	VAL	2.5
2	B	114	ASN	2.5
2	B	154	ASN	2.5
2	D	19	ASP	2.5
2	F	145	ASP	2.5
1	E	185	ALA	2.5
1	C	139	GLY	2.5
1	C	169	GLN	2.4
2	B	145	ASP	2.4
1	C	308	SER	2.4
1	C	307	LYS	2.4
1	A	319	ASN	2.4
2	F	154	ASN	2.4
1	E	151	ILE	2.4
1	E	294	ILE	2.4
1	E	316	GLY	2.4
1	C	273	ASN	2.4
2	D	139	GLU	2.4
2	F	29	GLU	2.4
1	E	16	VAL	2.4
1	E	302	CYS	2.4
2	B	144	CYS	2.4
2	D	116	LYS	2.4
1	A	28	HIS	2.4
2	D	108	LEU	2.4
1	C	272	GLY	2.4
1	E	236	ASN	2.4
2	B	60	ASN	2.4
2	F	114	ASN	2.4
1	A	312	VAL	2.4
1	E	108	ILE	2.4
1	C	259	LYS	2.4
1	A	27	THR	2.4
2	F	92	TRP	2.4
2	F	99	LEU	2.3
2	F	59	MET	2.3
1	C	24	VAL	2.3
2	B	103	GLU	2.3
1	E	33	LEU	2.3
1	A	35	LYS	2.3
2	F	149	MET	2.3
1	C	114	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	312	VAL	2.3
2	F	42	GLN	2.3
1	E	10	ASN	2.3
1	A	129	ALA	2.3
1	C	31	ASP	2.3
1	E	137	TYR	2.3
1	E	14	GLU	2.3
2	D	25	HIS	2.3
2	D	63	PHE	2.3
2	D	147	GLU	2.3
2	F	63	PHE	2.3
1	E	57	VAL	2.3
2	D	38	LYS	2.3
1	C	89	LEU	2.3
2	B	101	LEU	2.3
2	D	15	GLN	2.2
2	D	106	ARG	2.2
2	D	43	LYS	2.2
1	C	106	SER	2.2
1	E	267	SER	2.2
1	C	291	PHE	2.2
1	A	18	THR	2.2
1	A	256	ILE	2.2
1	E	256	ILE	2.2
2	B	134	GLY	2.2
1	E	314	ALA	2.2
1	E	318	ARG	2.2
1	E	259	LYS	2.2
1	A	25	THR	2.2
1	A	261	ASP	2.2
1	E	261	ASP	2.2
2	D	39	GLU	2.2
1	C	33	LEU	2.2
2	D	73	LEU	2.2
2	D	54	SER	2.2
2	F	75	ARG	2.2
1	A	149	TRP	2.2
2	F	46	ASP	2.2
1	C	312	VAL	2.1
1	E	107	ARG	2.1
2	F	101	LEU	2.1
1	C	38	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	84	MET	2.1
2	B	120	ASP	2.1
2	D	46	ASP	2.1
1	E	235	PRO	2.1
1	E	15	GLN	2.1
1	C	8	HIS	2.1
1	C	163	SER	2.1
2	F	54	SER	2.1
2	F	117	ASN	2.1
1	C	154	ASP	2.1
2	F	19	ASP	2.1
1	C	65	PRO	2.1
1	E	303	PRO	2.1
1	E	28	HIS	2.1
1	E	292	HIS	2.1
2	F	106	ARG	2.1
1	E	105	LEU	2.1
2	B	41	THR	2.1
1	C	117	ILE	2.1
1	C	178	ILE	2.1
2	B	116	LYS	2.1
2	F	88	PHE	2.1
1	A	12	SER	2.1
1	C	29	ALA	2.1
2	B	150	GLU	2.0
1	A	41	LEU	2.0
1	C	258	LYS	2.0
1	C	260	GLY	2.0
1	C	12	SER	2.0
2	B	104	ASN	2.0
1	A	209	LEU	2.0
1	E	297	LEU	2.0
2	B	112	ASP	2.0
1	A	181	PRO	2.0
1	A	263	THR	2.0
1	C	18	THR	2.0

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

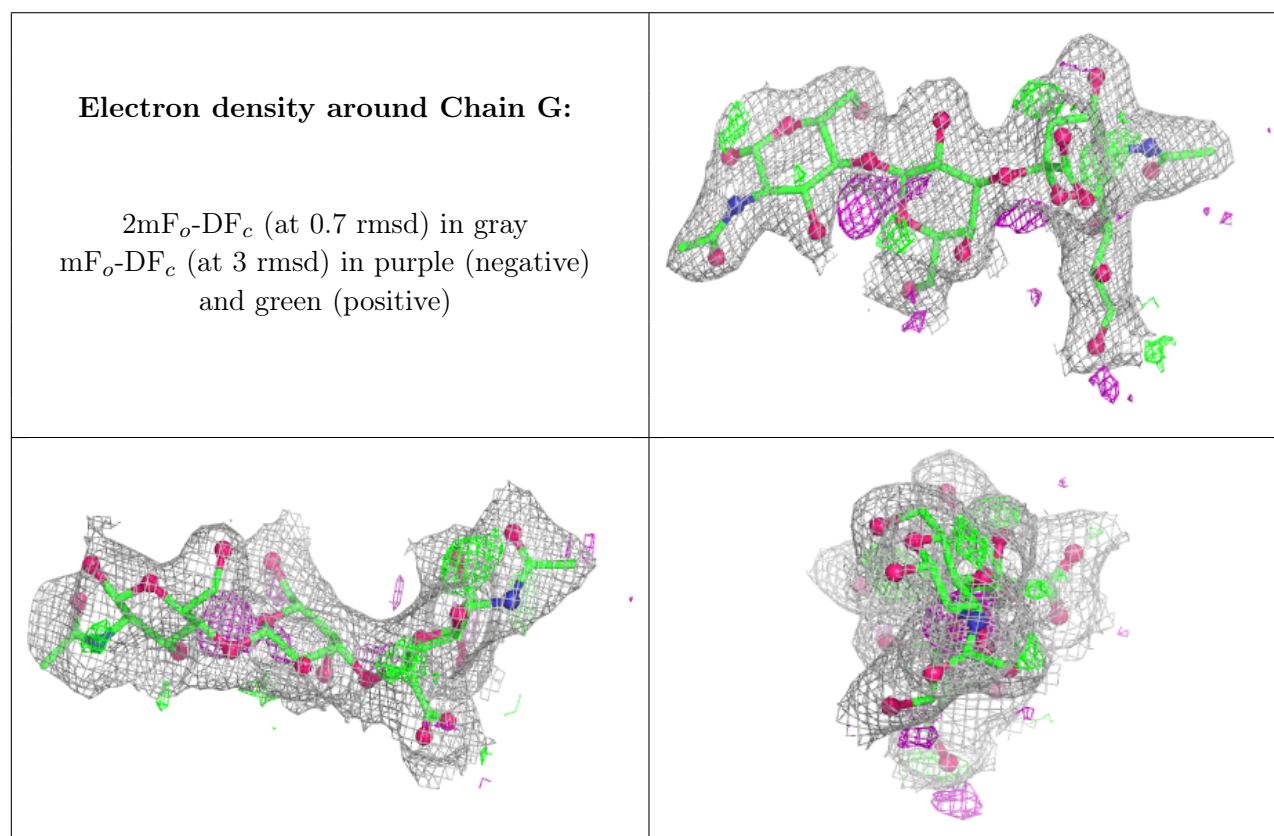
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

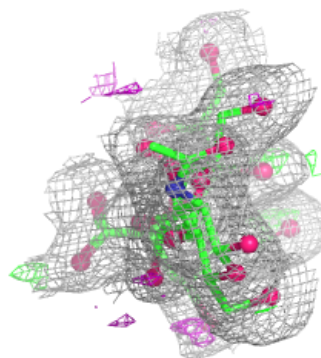
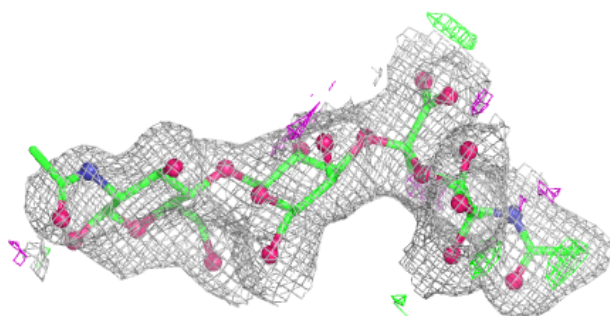
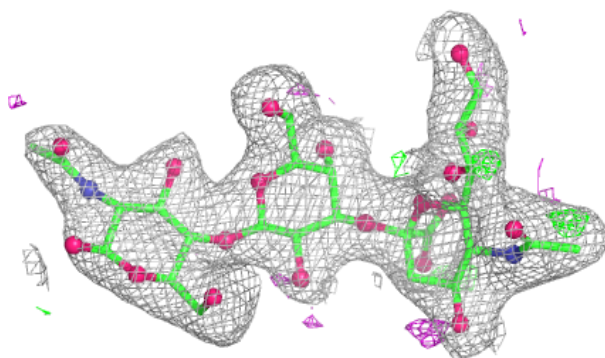
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	1	15/15	0.77	0.14	46,56,64,66	0
3	NAG	I	1	15/15	0.78	0.14	62,73,76,78	0
3	NAG	H	1	15/15	0.84	0.13	43,56,66,68	0
3	GAL	G	2	11/12	0.86	0.12	30,36,37,40	0
3	GAL	H	2	11/12	0.88	0.10	28,32,34,36	0
3	SIA	H	3	20/21	0.89	0.10	23,25,29,30	0
3	SIA	G	3	20/21	0.89	0.10	26,31,33,34	0
3	SIA	I	3	20/21	0.90	0.10	34,40,46,46	0
3	GAL	I	2	11/12	0.91	0.08	47,50,54,56	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.

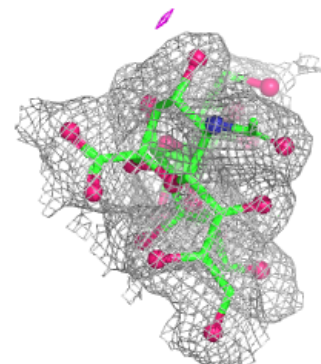
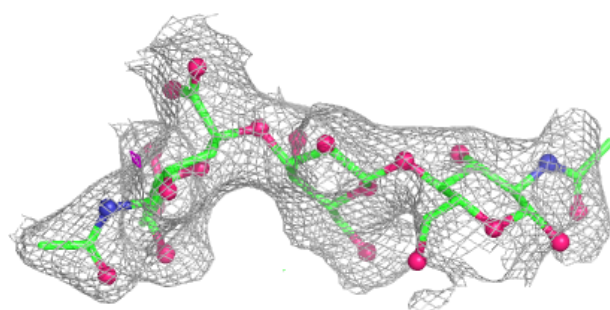
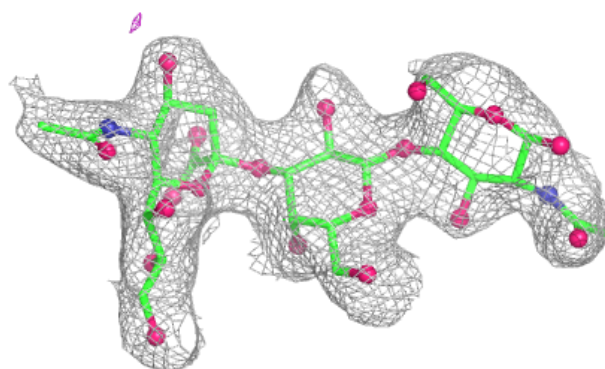


Electron density around Chain H:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
5	PO4	A	1325	5/5	0.66	0.20	66,71,78,80	0
5	PO4	C	1324	5/5	0.67	0.20	53,65,67,67	0
5	PO4	E	1324	5/5	0.68	0.15	64,71,74,75	0
4	NAG	C	1320	14/15	0.80	0.12	37,40,47,49	0
5	PO4	A	1324	5/5	0.82	0.17	63,63,67,68	0
4	NAG	E	1320	14/15	0.84	0.12	35,37,46,50	0
4	NAG	A	1320	14/15	0.89	0.09	36,39,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.