Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 06:50 am GMT

PDB ID	:	5ELF
Title	:	Cholera toxin El Tor B-pentamer in complex with A-pentasaccharide
Authors	:	Heggelund, J.E.; Burschowsky, D.; Krengel, U.
Deposited on	:	2015-11-04
Resolution	:	1.55 Å(reported)

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

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

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

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

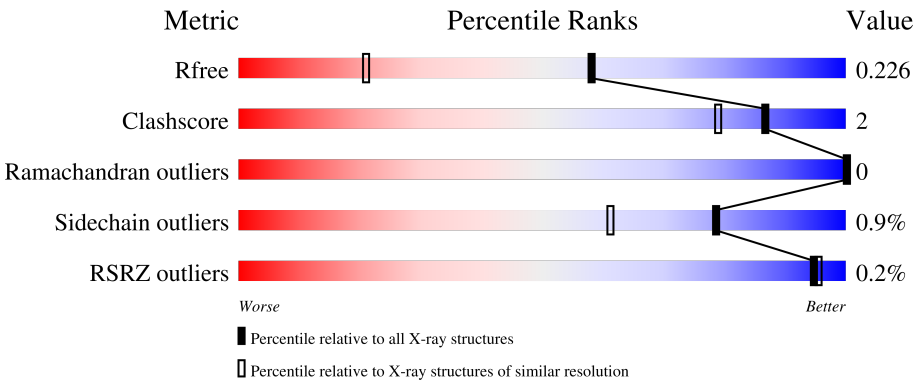
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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

Mol	Chain	Length	Quality of chain
1	A	103	99% .
1	B	103	94% 6%
1	C	103	% 97% .
1	D	103	93% 6% .
1	E	103	% 94% 6%

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Mol	Chain	Length	Quality of chain
1	F	103	99%
1	G	103	94% 6%
1	H	103	94% 6%
1	I	103	92% 6%
1	J	103	98%
2	K	5	100%
2	M	5	60% 40%
2	P	5	100%
2	Q	5	60% 40%
3	L	5	40% 60%
3	N	5	20% 80%
3	O	5	40% 60%

2 Entry composition (i)

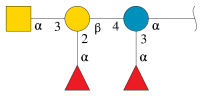
There are 9 unique types of molecules in this entry. The entry contains 10185 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cholera enterotoxin subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	103	829	525	142	157	5	0	2	0
1	B	103	828	524	141	158	5	0	2	0
1	C	103	834	531	142	156	5	0	3	0
1	D	103	836	528	145	158	5	0	2	0
1	E	103	823	521	141	156	5	0	1	0
1	F	103	823	521	141	156	5	0	1	0
1	G	103	826	522	142	157	5	0	1	0
1	H	103	817	516	140	156	5	0	0	0
1	I	103	817	516	140	156	5	0	0	0
1	J	103	829	526	142	156	5	0	2	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	K	5	57	32	1	24	0	0	0

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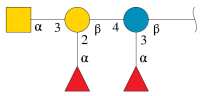
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	M	5	57	32	1	24	0	0	0
			Total	C	N	O			
2	P	5	57	32	1	24	0	0	0
			Total	C	N	O			
2	Q	5	114	64	2	48	0	5	0

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

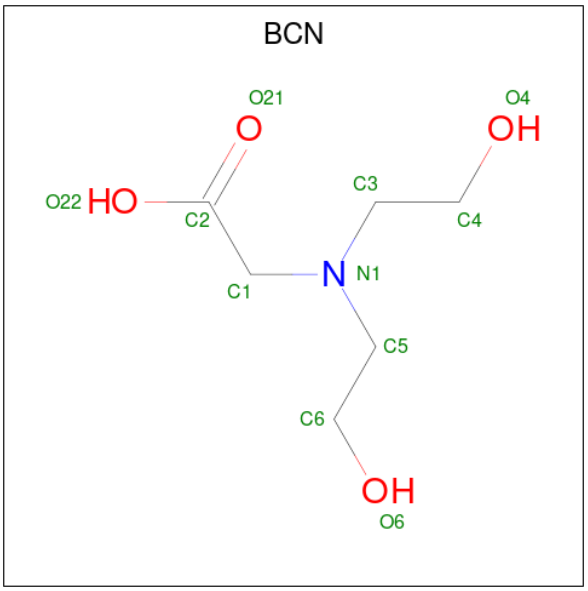


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	L	5	102	58	2	42	0	5	0
			Total	C	N	O			
3	N	5	57	32	1	24	0	0	0
			Total	C	N	O			
3	O	5	102	58	2	42	0	5	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

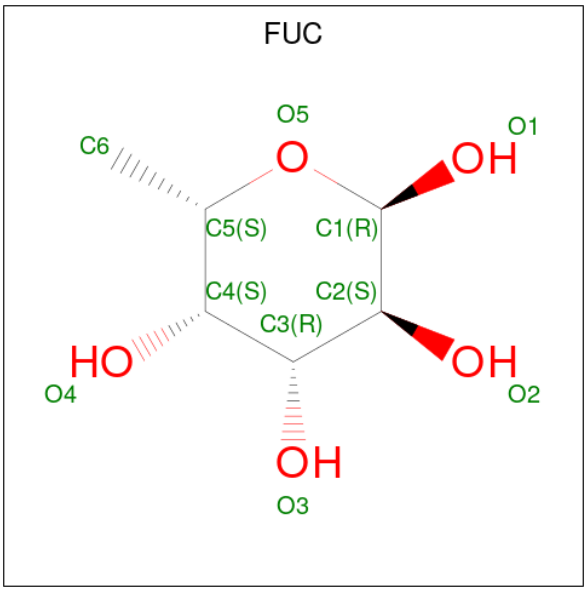
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	2	2	2	0	0
			Total	Ca		
4	B	2	2	2	0	0
			Total	Ca		
4	C	2	2	2	0	0
			Total	Ca		
4	D	2	2	2	0	0
			Total	Ca		
4	E	2	2	2	0	0

- Molecule 5 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



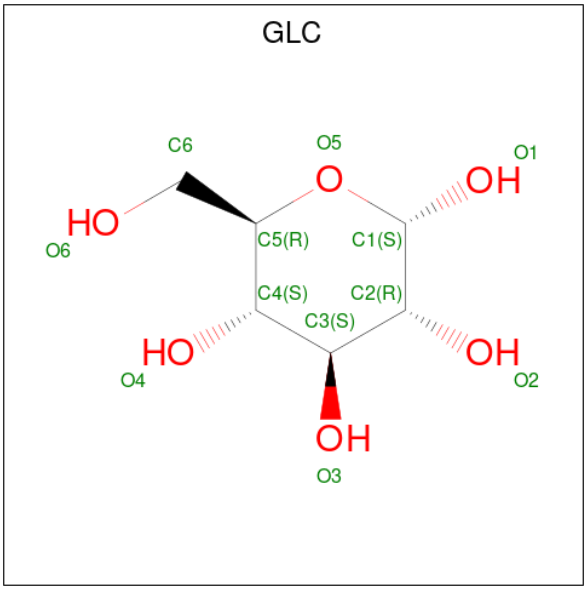
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	11	6	1	4	0	0
			Total	C	N	O		
5	A	1	11	6	1	4	0	0
			Total	C	N	O		
5	B	1	11	6	1	4	0	0
			Total	C	N	O		
5	B	1	11	6	1	4	0	0
			Total	C	N	O		
5	C	1	11	6	1	4	0	0
			Total	C	N	O		
5	C	1	11	6	1	4	0	0
			Total	C	N	O		
5	D	1	11	6	1	4	0	0
			Total	C	N	O		
5	D	1	11	6	1	4	0	0
			Total	C	N	O		
5	E	1	11	6	1	4	0	0
			Total	C	N	O		
5	E	1	11	6	1	4	0	0

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



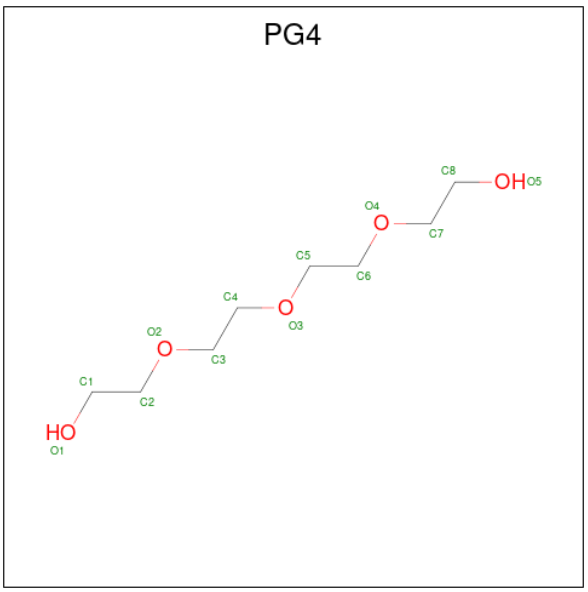
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	11	6	5	0	0
			Total	C	O		
6	H	1	11	6	5	0	0

- Molecule 7 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	12	6	6	0	1
			Total	C	O		
7	G	1	12	6	6	0	1

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	F	1	13	8	5	0	0

- Molecule 9 is water.

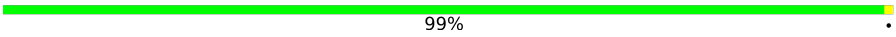
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	106	106	106	0	0
9	B	102	103	103	0	1
9	C	111	111	111	0	0
9	D	128	128	128	0	0
9	E	126	126	126	0	0
9	F	123	125	125	0	2
9	G	131	132	132	0	1
9	H	115	115	115	0	0
9	I	127	127	127	0	0
9	J	125	125	125	0	0

3 Residue-property plots (i)

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

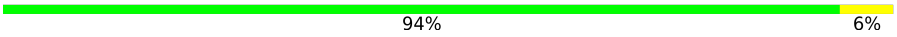
• Molecule 1: Cholera enterotoxin subunit B

Chain A:



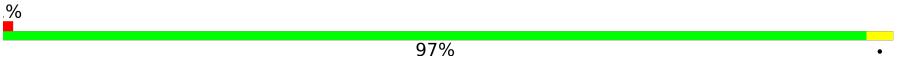
• Molecule 1: Cholera enterotoxin subunit B

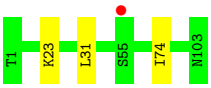
Chain B:



• Molecule 1: Cholera enterotoxin subunit B

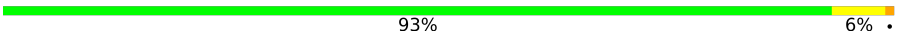
Chain C:

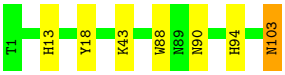




• Molecule 1: Cholera enterotoxin subunit B

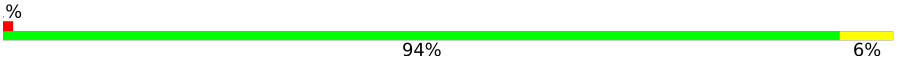
Chain D:

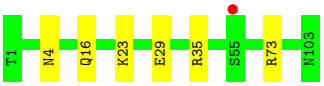




• Molecule 1: Cholera enterotoxin subunit B

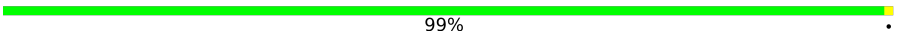
Chain E:





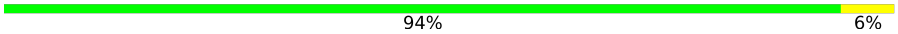
• Molecule 1: Cholera enterotoxin subunit B

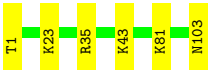
Chain F:



• Molecule 1: Cholera enterotoxin subunit B

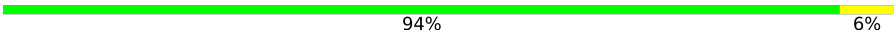
Chain G:





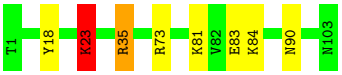
• Molecule 1: Cholera enterotoxin subunit B

Chain H:



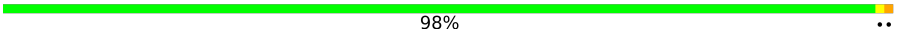
• Molecule 1: Cholera enterotoxin subunit B

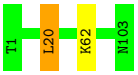
Chain I:



• Molecule 1: Cholera enterotoxin subunit B

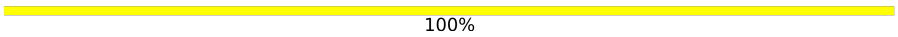
Chain J:





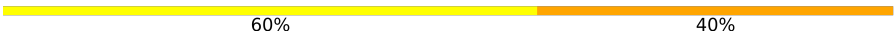
• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]alpha-D-glucopyranose

Chain K:



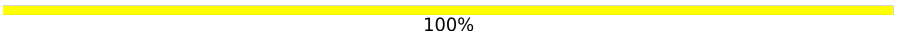
• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]alpha-D-glucopyranose

Chain M:



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

Chain P:



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

Chain Q:

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

Chain L:

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

Chain N:

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

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.63Å 84.72Å 195.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 1.55 45.55 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.92-1.55) 99.6 (45.55-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.220 0.189 , 0.226	Depositor DCC
R_{free} test set	7664 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10185	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A2G, BCN, GLC, BGC, PG4, GAL, CA, FUC

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	0.75	0/849	0.80	0/1145
1	B	0.71	0/848	0.81	3/1144 (0.3%)
1	C	0.75	0/857	0.77	0/1155
1	D	0.75	0/851	0.85	0/1148
1	E	0.79	0/840	0.89	3/1133 (0.3%)
1	F	0.82	0/840	0.85	1/1133 (0.1%)
1	G	0.80	0/840	0.86	1/1133 (0.1%)
1	H	0.83	0/831	0.84	0/1122
1	I	0.80	0/831	0.88	3/1122 (0.3%)
1	J	0.83	0/849	0.86	1/1144 (0.1%)
All	All	0.78	0/8436	0.84	12/11379 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	35	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	J	20	LEU	CA-CB-CG	-5.58	102.46	115.30
1	E	35	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	I	35	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	35	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	70	ASP	CB-CG-OD1	5.36	123.12	118.30
1	E	73	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	I	73	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	73	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	I	23	LYS	CD-CE-NZ	5.08	123.38	111.70
1	B	73	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	F	22	ASP	CB-CG-OD1	5.00	122.80	118.30

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	829	0	844	1	0
1	B	828	0	840	7	0
1	C	834	0	860	3	0
1	D	836	0	841	5	0
1	E	823	0	836	2	0
1	F	823	0	836	0	0
1	G	826	0	835	4	0
1	H	817	0	823	4	0
1	I	817	0	823	7	0
1	J	829	0	849	1	0
2	K	57	0	50	0	0
2	M	57	0	50	2	0
2	P	57	0	50	0	0
2	Q	114	0	100	2	0
3	L	102	0	85	6	0
3	N	57	0	50	0	0
3	O	102	0	86	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
5	C	22	0	20	0	0
5	D	22	0	20	0	0
5	E	22	0	20	0	0
6	B	11	0	12	1	0
6	H	11	0	12	0	0
7	D	12	0	5	3	0
7	G	12	0	6	0	0
8	F	13	0	18	0	0
9	A	106	0	0	1	0
9	B	103	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	111	0	0	1	0
9	D	128	0	0	3	0
9	E	126	0	0	1	0
9	F	125	0	0	0	0
9	G	132	0	0	1	0
9	H	115	0	0	2	0
9	I	127	0	0	2	0
9	J	125	0	0	0	0
All	All	10185	0	9011	38	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (38) 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:A:16[B]:GLN:OE1	9:A:301:HOH:O	1.56	1.22
9:D:301:HOH:O	3:L:4[A]:A2G:O6	1.53	1.21
1:B:103:ASN:HD21	1:I:23:LYS:CE	2.12	0.61
1:H:35:ARG:NH1	9:H:301:HOH:O	2.33	0.61
1:D:103:ASN:O	1:G:43:LYS:NZ	2.30	0.59
2:Q:1[A]:GLC:O6	2:Q:3[A]:FUC:H3	2.02	0.59
1:H:103:ASN:ND2	9:H:304:HOH:O	2.39	0.55
1:D:13[B]:HIS:NE2	9:D:302:HOH:O	2.18	0.54
1:B:102:ALA:O	1:B:103:ASN:HB2	2.08	0.54
1:D:18:TYR:CE2	3:L:4[B]:A2G:H8A	2.44	0.53
1:E:16:GLN:NE2	2:M:4:A2G:HN2	2.08	0.52
1:B:103:ASN:HD21	1:I:23:LYS:HE2	1.75	0.50
1:I:35:ARG:NH1	9:I:302:HOH:O	2.43	0.50
1:G:23[B]:LYS:NZ	9:G:304:HOH:O	2.47	0.47
1:B:94:HIS:CD2	6:B:203:FUC:H4	2.50	0.46
1:I:83:GLU:HG2	1:I:84:LYS:HG3	1.98	0.46
7:D:210[B]:GLC:H5	3:L:3[B]:FUC:H5	1.98	0.46
1:B:102:ALA:O	1:B:103:ASN:CB	2.65	0.45
1:H:4:ASN:HD22	1:H:6:THR:H	1.63	0.45
3:O:4[B]:A2G:H8A	3:O:4[B]:A2G:O3	2.17	0.44
9:B:374:HOH:O	1:I:81:LYS:HD2	2.18	0.44
7:D:210[B]:GLC:C5	3:L:3[B]:FUC:H5	2.48	0.44
1:B:103:ASN:HD21	1:I:23:LYS:HE3	1.82	0.43
1:D:94:HIS:CD2	3:L:5[A]:FUC:H4	2.53	0.43
1:C:74[A]:ILE:HD13	9:D:410:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2:GAL:H3	2:M:4:A2G:C5	2.48	0.43
1:C:31:LEU:C	1:C:31:LEU:HD12	2.39	0.42
1:J:62[A]:LYS:HA	1:J:62[A]:LYS:HD3	1.76	0.42
1:C:23[A]:LYS:NZ	9:C:301:HOH:O	2.10	0.42
1:G:1:THR:HB	1:H:92:THR:O	2.19	0.42
1:I:90:ASN:HB2	9:I:350:HOH:O	2.19	0.42
1:G:81:LYS:HE2	1:G:103:ASN:ND2	2.35	0.42
1:E:23:LYS:NZ	9:E:303:HOH:O	2.47	0.42
1:B:81:LYS:HD2	1:B:103:ASN:HB2	2.02	0.41
1:D:88:TRP:HB3	1:D:90:ASN:OD1	2.21	0.41
2:Q:1[A]:GLC:HO6	2:Q:3[A]:FUC:H3	1.86	0.41
3:O:1[B]:BGC:O2	3:O:5[B]:FUC:C1	2.69	0.40
7:D:210[B]:GLC:H62	3:L:2[B]:GAL:C1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/103 (100%)	102 (99%)	1 (1%)	0	100	100
1	B	103/103 (100%)	101 (98%)	2 (2%)	0	100	100
1	C	104/103 (101%)	103 (99%)	1 (1%)	0	100	100
1	D	103/103 (100%)	102 (99%)	1 (1%)	0	100	100
1	E	102/103 (99%)	101 (99%)	1 (1%)	0	100	100
1	F	102/103 (99%)	101 (99%)	1 (1%)	0	100	100
1	G	102/103 (99%)	101 (99%)	1 (1%)	0	100	100
1	H	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	I	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	J	103/103 (100%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1024/1030 (99%)	1010 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/89 (102%)	91 (100%)	0	100	100
1	B	91/89 (102%)	91 (100%)	0	100	100
1	C	92/89 (103%)	92 (100%)	0	100	100
1	D	91/89 (102%)	89 (98%)	2 (2%)	52	23
1	E	90/89 (101%)	88 (98%)	2 (2%)	52	23
1	F	90/89 (101%)	90 (100%)	0	100	100
1	G	90/89 (101%)	90 (100%)	0	100	100
1	H	89/89 (100%)	88 (99%)	1 (1%)	73	53
1	I	89/89 (100%)	87 (98%)	2 (2%)	52	23
1	J	91/89 (102%)	90 (99%)	1 (1%)	73	53
All	All	904/890 (102%)	896 (99%)	8 (1%)	78	61

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	43	LYS
1	D	103	ASN
1	E	4	ASN
1	E	29	GLU
1	H	89	ASN
1	I	18	TYR
1	I	23	LYS
1	J	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	14	ASN
1	D	16	GLN
1	E	4	ASN
1	F	94	HIS
1	G	14	ASN
1	G	103	ASN
1	H	4	ASN
1	H	16	GLN
1	H	89	ASN
1	I	3	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

48 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	GLC	K	1	2	12,12,12	0.99	1 (8%)	17,17,17	1.35	3 (17%)
2	GAL	K	2	2	11,11,12	1.01	1 (9%)	15,15,17	1.73	1 (6%)
2	FUC	K	3	2	10,10,11	1.15	1 (10%)	14,14,16	0.88	1 (7%)
2	A2G	K	4	2	14,14,15	1.50	3 (21%)	17,19,21	2.11	4 (23%)
2	FUC	K	5	2	10,10,11	1.48	1 (10%)	14,14,16	1.25	2 (14%)
3	BGC	L	1[A]	3	12,12,12	0.84	1 (8%)	17,17,17	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GAL	L	2[A]	3	11,11,12	1.69	3 (27%)	15,15,17	2.15	5 (33%)
3	GAL	L	2[B]	7,3	11,11,12	1.10	1 (9%)	15,15,17	1.44	2 (13%)
3	FUC	L	3[A]	3	10,10,11	0.94	0	14,14,16	0.77	0
3	FUC	L	3[B]	3	10,10,11	0.91	0	14,14,16	0.95	0
3	A2G	L	4[A]	3	14,14,15	0.87	1 (7%)	17,19,21	1.42	1 (5%)
3	A2G	L	4[B]	3	14,14,15	1.22	2 (14%)	17,19,21	1.34	2 (11%)
3	FUC	L	5[A]	3	10,10,11	1.26	1 (10%)	14,14,16	0.64	0
3	FUC	L	5[B]	7	10,10,11	0.81	0	14,14,16	0.93	0
2	GLC	M	1	2	12,12,12	0.65	0	17,17,17	1.25	2 (11%)
2	GAL	M	2	2	11,11,12	1.07	1 (9%)	15,15,17	1.07	1 (6%)
2	FUC	M	3	2	10,10,11	1.04	0	14,14,16	1.15	2 (14%)
2	A2G	M	4	2	14,14,15	1.73	4 (28%)	17,19,21	3.04	6 (35%)
2	FUC	M	5	2	10,10,11	1.49	2 (20%)	14,14,16	1.25	2 (14%)
3	BGC	N	1	3	12,12,12	1.46	4 (33%)	17,17,17	1.29	2 (11%)
3	GAL	N	2	3	11,11,12	1.38	2 (18%)	15,15,17	1.65	2 (13%)
3	FUC	N	3	3	10,10,11	0.76	0	14,14,16	0.84	0
3	A2G	N	4	3	14,14,15	1.42	2 (14%)	17,19,21	1.49	2 (11%)
3	FUC	N	5	3	10,10,11	2.20	5 (50%)	14,14,16	0.53	0
3	BGC	O	1[B]	3	12,12,12	0.90	0	17,17,17	1.64	1 (5%)
3	GAL	O	2[A]	7,3	11,11,12	1.29	1 (9%)	15,15,17	1.22	0
3	GAL	O	2[B]	3	11,11,12	1.25	1 (9%)	15,15,17	1.12	1 (6%)
3	FUC	O	3[A]	3	10,10,11	1.00	0	14,14,16	0.99	0
3	FUC	O	3[B]	3	10,10,11	0.75	0	14,14,16	1.21	1 (7%)
3	A2G	O	4[A]	3	14,14,15	1.51	4 (28%)	17,19,21	1.43	2 (11%)
3	A2G	O	4[B]	3	14,14,15	1.91	1 (7%)	17,19,21	2.42	4 (23%)
3	FUC	O	5[A]	7	10,10,11	1.36	2 (20%)	14,14,16	1.28	3 (21%)
3	FUC	O	5[B]	3	10,10,11	1.70	3 (30%)	14,14,16	1.65	2 (14%)
2	GLC	P	1	2	12,12,12	1.16	2 (16%)	17,17,17	1.34	3 (17%)
2	GAL	P	2	2	11,11,12	0.95	1 (9%)	15,15,17	1.69	3 (20%)
2	FUC	P	3	2	10,10,11	0.85	0	14,14,16	1.07	1 (7%)
2	A2G	P	4	2	14,14,15	1.47	2 (14%)	17,19,21	1.63	1 (5%)
2	FUC	P	5	2	10,10,11	1.38	2 (20%)	14,14,16	0.88	1 (7%)
2	GLC	Q	1[A]	2	12,12,12	0.99	1 (8%)	17,17,17	1.10	1 (5%)
2	GLC	Q	1[B]	2	12,12,12	0.90	0	17,17,17	1.82	3 (17%)
2	GAL	Q	2[A]	2	11,11,12	1.13	1 (9%)	15,15,17	1.51	4 (26%)
2	GAL	Q	2[B]	2	11,11,12	1.13	1 (9%)	15,15,17	1.05	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FUC	Q	3[A]	2	10,10,11	1.17	1 (10%)	14,14,16	1.50	2 (14%)
2	FUC	Q	3[B]	2	10,10,11	1.66	1 (10%)	14,14,16	1.44	3 (21%)
2	A2G	Q	4[A]	2	14,14,15	1.65	3 (21%)	17,19,21	1.79	3 (17%)
2	A2G	Q	4[B]	2	14,14,15	1.10	1 (7%)	17,19,21	1.68	5 (29%)
2	FUC	Q	5[A]	2	10,10,11	1.13	1 (10%)	14,14,16	0.90	0
2	FUC	Q	5[B]	2	10,10,11	0.67	0	14,14,16	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GAL	K	2	2	-	1/2/19/22	0/1/1/1
2	FUC	K	3	2	-	-	0/1/1/1
2	A2G	K	4	2	-	2/6/23/26	0/1/1/1
2	FUC	K	5	2	-	-	0/1/1/1
3	BGC	L	1[A]	3	-	0/2/22/22	0/1/1/1
3	GAL	L	2[A]	3	-	1/2/19/22	0/1/1/1
3	GAL	L	2[B]	7,3	-	0/2/19/22	0/1/1/1
3	FUC	L	3[A]	3	-	-	0/1/1/1
3	FUC	L	3[B]	3	-	-	0/1/1/1
3	A2G	L	4[A]	3	-	2/6/23/26	0/1/1/1
3	A2G	L	4[B]	3	-	0/6/23/26	0/1/1/1
3	FUC	L	5[A]	3	-	-	0/1/1/1
3	FUC	L	5[B]	7	-	-	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GAL	M	2	2	-	0/2/19/22	0/1/1/1
2	FUC	M	3	2	-	-	0/1/1/1
2	A2G	M	4	2	-	4/6/23/26	0/1/1/1
2	FUC	M	5	2	-	-	0/1/1/1
3	BGC	N	1	3	-	0/2/22/22	0/1/1/1
3	GAL	N	2	3	-	1/2/19/22	0/1/1/1
3	FUC	N	3	3	-	-	0/1/1/1
3	A2G	N	4	3	-	0/6/23/26	0/1/1/1
3	FUC	N	5	3	-	-	0/1/1/1
3	BGC	O	1[B]	3	-	0/2/22/22	0/1/1/1
3	GAL	O	2[A]	7,3	-	0/2/19/22	0/1/1/1
3	GAL	O	2[B]	3	-	1/2/19/22	0/1/1/1
3	FUC	O	3[A]	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	O	3[B]	3	-	-	0/1/1/1
3	A2G	O	4[A]	3	-	2/6/23/26	0/1/1/1
3	A2G	O	4[B]	3	-	2/6/23/26	0/1/1/1
3	FUC	O	5[A]	7	-	-	0/1/1/1
3	FUC	O	5[B]	3	-	-	0/1/1/1
2	GLC	P	1	2	-	0/2/22/22	0/1/1/1
2	GAL	P	2	2	-	0/2/19/22	0/1/1/1
2	FUC	P	3	2	-	-	0/1/1/1
2	A2G	P	4	2	-	2/6/23/26	0/1/1/1
2	FUC	P	5	2	-	-	0/1/1/1
2	GLC	Q	1[A]	2	-	2/2/22/22	0/1/1/1
2	GLC	Q	1[B]	2	-	0/2/22/22	0/1/1/1
2	GAL	Q	2[A]	2	-	1/2/19/22	0/1/1/1
2	GAL	Q	2[B]	2	-	0/2/19/22	0/1/1/1
2	FUC	Q	3[A]	2	-	-	0/1/1/1
2	FUC	Q	3[B]	2	-	-	0/1/1/1
2	A2G	Q	4[A]	2	-	0/6/23/26	0/1/1/1
2	A2G	Q	4[B]	2	-	2/6/23/26	0/1/1/1
2	FUC	Q	5[A]	2	-	-	0/1/1/1
2	FUC	Q	5[B]	2	-	-	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	4[B]	A2G	O3-C3	6.11	1.57	1.43
2	Q	3[B]	FUC	O5-C1	-4.77	1.36	1.43
2	M	4	A2G	C1-C2	4.27	1.58	1.52
2	P	4	A2G	O5-C5	3.87	1.51	1.43
3	L	5[A]	FUC	O4-C4	3.56	1.51	1.43
3	N	5	FUC	C2-C3	3.54	1.57	1.52
3	O	2[A]	GAL	C2-C3	3.47	1.57	1.52
3	N	4	A2G	O5-C1	3.47	1.49	1.43
3	L	2[A]	GAL	C2-C3	3.35	1.57	1.52
2	Q	4[A]	A2G	O5-C1	3.29	1.49	1.43
3	N	5	FUC	O3-C3	3.25	1.50	1.43
3	O	5[A]	FUC	O4-C4	3.14	1.50	1.43
3	L	2[A]	GAL	O5-C5	3.06	1.49	1.43
3	N	5	FUC	O5-C1	2.95	1.48	1.43
3	N	2	GAL	O3-C3	2.87	1.49	1.43
3	N	5	FUC	C4-C5	2.86	1.59	1.52
3	O	5[B]	FUC	O5-C1	-2.84	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	4[A]	A2G	C4-C5	2.83	1.59	1.53
2	M	4	A2G	C2-N2	2.82	1.51	1.46
3	L	4[B]	A2G	O4-C4	2.80	1.49	1.43
2	K	5	FUC	C2-C3	-2.80	1.48	1.52
2	K	4	A2G	O5-C5	2.74	1.49	1.43
3	O	5[B]	FUC	C2-C3	-2.74	1.48	1.52
2	P	5	FUC	O3-C3	2.74	1.49	1.43
2	Q	4[A]	A2G	C1-C2	2.73	1.56	1.52
3	O	5[B]	FUC	O4-C4	2.69	1.49	1.43
3	O	4[A]	A2G	O5-C5	2.69	1.48	1.43
2	P	4	A2G	C3-C2	2.62	1.58	1.52
2	M	4	A2G	C8-C7	2.61	1.56	1.50
2	K	3	FUC	O5-C1	2.56	1.47	1.43
2	K	4	A2G	C8-C7	2.56	1.55	1.50
2	Q	2[B]	GAL	O5-C1	-2.54	1.39	1.43
2	M	2	GAL	O3-C3	2.54	1.49	1.43
3	O	2[B]	GAL	C4-C5	-2.53	1.47	1.53
2	P	1	GLC	O1-C1	2.50	1.47	1.39
2	M	5	FUC	O4-C4	-2.47	1.37	1.43
3	L	4[B]	A2G	C8-C7	2.43	1.55	1.50
2	Q	3[A]	FUC	O4-C4	2.40	1.48	1.43
2	Q	2[A]	GAL	O5-C1	-2.35	1.40	1.43
3	N	1	BGC	O5-C1	2.34	1.48	1.42
3	O	4[A]	A2G	O3-C3	2.30	1.48	1.43
3	N	1	BGC	C4-C5	2.30	1.57	1.53
3	N	1	BGC	O3-C3	2.29	1.48	1.43
2	Q	1[A]	GLC	O1-C1	2.29	1.46	1.39
2	Q	4[A]	A2G	O5-C5	2.28	1.48	1.43
2	K	1	GLC	O3-C3	-2.25	1.37	1.43
3	O	5[A]	FUC	C2-C3	-2.25	1.49	1.52
3	L	2[A]	GAL	O4-C4	2.24	1.48	1.43
2	P	5	FUC	C6-C5	2.21	1.56	1.51
2	K	4	A2G	O5-C1	2.15	1.47	1.43
3	L	1[A]	BGC	C4-C5	2.14	1.57	1.53
2	P	1	GLC	C3-C2	2.14	1.57	1.52
2	P	2	GAL	O3-C3	2.14	1.48	1.43
3	N	2	GAL	O2-C2	-2.11	1.38	1.43
3	O	4[A]	A2G	O5-C1	2.10	1.47	1.43
3	L	2[B]	GAL	O4-C4	2.09	1.47	1.43
2	K	2	GAL	O5-C1	-2.06	1.40	1.43
2	Q	4[B]	A2G	C8-C7	2.06	1.54	1.50
2	Q	5[A]	FUC	C2-C3	-2.06	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	BGC	C3-C2	2.04	1.57	1.52
2	M	4	A2G	O5-C5	2.03	1.47	1.43
2	M	5	FUC	C1-C2	2.01	1.56	1.52
3	L	4[A]	A2G	C8-C7	2.01	1.54	1.50
3	N	4	A2G	C8-C7	2.01	1.54	1.50
3	N	5	FUC	O4-C4	2.01	1.47	1.43

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	4	A2G	C2-N2-C7	10.61	138.01	122.90
3	L	2[A]	GAL	O5-C5-C6	6.51	117.41	107.20
3	O	4[B]	A2G	C4-C3-C2	-6.15	102.01	111.02
3	O	1[B]	BGC	C1-O5-C5	-5.93	102.47	113.66
2	P	4	A2G	O5-C5-C6	5.48	115.80	107.20
3	N	2	GAL	O5-C5-C6	-5.29	98.91	107.20
2	K	4	A2G	C1-O5-C5	5.28	119.34	112.19
3	O	4[B]	A2G	C2-N2-C7	-5.25	115.42	122.90
2	K	2	GAL	O5-C5-C6	-5.08	99.23	107.20
2	Q	1[B]	GLC	O5-C5-C6	-4.98	94.06	106.44
2	Q	4[A]	A2G	O5-C5-C6	4.76	114.66	107.20
2	K	4	A2G	O5-C5-C6	-4.69	99.85	107.20
2	P	2	GAL	O5-C5-C6	4.34	114.01	107.20
3	N	4	A2G	C1-O5-C5	3.98	117.58	112.19
3	O	5[B]	FUC	C1-O5-C5	-3.86	104.02	112.78
3	O	4[A]	A2G	O5-C1-C2	-3.61	105.59	111.29
2	Q	3[A]	FUC	C3-C4-C5	-3.53	104.27	109.77
3	O	4[B]	A2G	O3-C3-C4	3.36	118.12	110.35
3	L	4[A]	A2G	C1-O5-C5	3.32	116.69	112.19
3	L	4[B]	A2G	C4-C3-C2	-3.28	106.21	111.02
2	Q	4[B]	A2G	C2-N2-C7	-3.19	118.36	122.90
3	O	4[A]	A2G	C2-N2-C7	-3.18	118.37	122.90
3	L	2[A]	GAL	C6-C5-C4	-3.16	105.59	113.00
2	Q	4[A]	A2G	C1-C2-N2	3.09	115.77	110.49
2	M	4	A2G	O5-C5-C6	-3.09	102.37	107.20
3	L	2[B]	GAL	C3-C4-C5	-3.06	104.78	110.24
2	Q	4[B]	A2G	O5-C1-C2	-3.03	106.50	111.29
3	L	1[A]	BGC	O6-C6-C5	-2.91	101.30	111.29
2	K	4	A2G	C2-N2-C7	2.88	127.00	122.90
2	Q	2[A]	GAL	O2-C2-C3	-2.80	104.54	110.14
2	Q	3[B]	FUC	C6-C5-C4	-2.79	107.91	113.07
2	M	4	A2G	C1-C2-N2	2.77	115.23	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	2[B]	GAL	O3-C3-C2	-2.77	104.70	109.99
2	Q	1[A]	GLC	O3-C3-C4	-2.76	103.97	110.35
2	Q	1[B]	GLC	O6-C6-C5	-2.70	102.02	111.29
2	M	4	A2G	C4-C3-C2	-2.70	107.06	111.02
2	Q	4[B]	A2G	C1-O5-C5	-2.70	108.53	112.19
2	K	1	GLC	O3-C3-C4	-2.70	104.11	110.35
3	O	4[B]	A2G	C1-O5-C5	-2.70	108.54	112.19
2	M	2	GAL	O6-C6-C5	-2.69	102.07	111.29
3	L	4[B]	A2G	C3-C4-C5	-2.67	105.47	110.24
2	M	5	FUC	O4-C4-C5	2.65	115.55	109.67
3	N	4	A2G	C3-C4-C5	-2.63	105.55	110.24
3	O	2[B]	GAL	C3-C4-C5	-2.61	105.58	110.24
3	O	3[B]	FUC	O5-C1-C2	-2.59	106.77	110.77
2	P	2	GAL	O5-C1-C2	2.57	114.73	110.77
2	Q	1[B]	GLC	O5-C5-C4	2.48	114.20	109.69
2	P	1	GLC	O5-C1-C2	-2.48	105.86	110.28
3	O	5[B]	FUC	C2-C3-C4	-2.48	106.61	110.89
3	N	1	BGC	O6-C6-C5	-2.47	102.81	111.29
2	Q	4[B]	A2G	O5-C5-C6	2.47	111.07	107.20
2	Q	3[A]	FUC	C6-C5-C4	-2.47	108.52	113.07
2	Q	2[A]	GAL	O6-C6-C5	-2.46	102.87	111.29
2	P	1	GLC	O1-C1-C2	2.44	115.90	109.03
2	K	5	FUC	O2-C2-C1	-2.43	104.17	109.15
2	Q	2[A]	GAL	C1-C2-C3	2.41	112.63	109.67
3	O	5[A]	FUC	C1-O5-C5	2.40	118.23	112.78
3	N	1	BGC	C1-O5-C5	-2.39	109.15	113.66
2	Q	4[A]	A2G	C4-C3-C2	-2.38	107.53	111.02
2	K	5	FUC	C1-C2-C3	2.37	112.58	109.67
2	Q	4[B]	A2G	C1-C2-N2	2.33	114.46	110.49
2	M	5	FUC	O4-C4-C3	-2.31	105.01	110.35
2	P	3	FUC	O2-C2-C3	-2.27	105.60	110.14
2	M	4	A2G	O5-C1-C2	-2.26	107.72	111.29
3	L	2[A]	GAL	O6-C6-C5	-2.24	103.60	111.29
2	K	3	FUC	C3-C4-C5	-2.23	106.30	109.77
3	O	5[A]	FUC	C6-C5-C4	-2.22	108.97	113.07
2	K	1	GLC	O3-C3-C2	-2.21	105.25	110.35
2	Q	3[B]	FUC	C3-C4-C5	2.19	113.19	109.77
2	M	1	GLC	O4-C4-C3	-2.18	105.31	110.35
2	Q	2[A]	GAL	C6-C5-C4	-2.17	107.91	113.00
2	P	5	FUC	O5-C5-C6	2.17	112.00	107.33
2	K	1	GLC	C1-O5-C5	2.15	117.72	113.66
2	Q	2[B]	GAL	C3-C4-C5	-2.14	106.42	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	5[A]	FUC	C1-C2-C3	2.13	112.29	109.67
2	M	1	GLC	O6-C6-C5	-2.13	103.98	111.29
2	M	3	FUC	O3-C3-C4	-2.13	105.43	110.35
2	M	4	A2G	C8-C7-N2	2.13	119.70	116.10
3	L	1[A]	BGC	O3-C3-C4	-2.10	105.50	110.35
2	P	2	GAL	O2-C2-C1	-2.09	104.88	109.15
3	N	2	GAL	O4-C4-C3	-2.06	105.58	110.35
3	L	2[A]	GAL	C3-C4-C5	-2.06	106.57	110.24
3	L	2[A]	GAL	C1-C2-C3	2.04	112.18	109.67
2	Q	3[B]	FUC	O5-C1-C2	-2.04	107.62	110.77
2	M	3	FUC	O3-C3-C2	-2.03	106.10	109.99
2	K	4	A2G	O6-C6-C5	-2.03	104.33	111.29
2	Q	2[B]	GAL	O5-C5-C6	2.03	110.38	107.20
2	P	1	GLC	O3-C3-C4	-2.00	105.72	110.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	4	A2G	C3-C2-N2-C7
2	Q	4[B]	A2G	O5-C5-C6-O6
3	O	4[A]	A2G	C4-C5-C6-O6
2	Q	1[A]	GLC	O5-C5-C6-O6
2	K	4	A2G	O7-C7-N2-C2
2	K	4	A2G	C8-C7-N2-C2
2	M	4	A2G	O7-C7-N2-C2
2	M	4	A2G	C8-C7-N2-C2
3	O	4[B]	A2G	O7-C7-N2-C2
3	O	4[B]	A2G	C8-C7-N2-C2
2	P	4	A2G	O5-C5-C6-O6
3	L	4[A]	A2G	O5-C5-C6-O6
2	Q	4[B]	A2G	C4-C5-C6-O6
3	O	4[A]	A2G	O5-C5-C6-O6
3	L	2[A]	GAL	O5-C5-C6-O6
2	Q	1[A]	GLC	C4-C5-C6-O6
2	Q	2[A]	GAL	O5-C5-C6-O6
3	N	2	GAL	O5-C5-C6-O6
2	M	4	A2G	O5-C5-C6-O6
2	K	2	GAL	O5-C5-C6-O6
3	O	2[B]	GAL	O5-C5-C6-O6
3	L	4[A]	A2G	C4-C5-C6-O6
2	P	4	A2G	C4-C5-C6-O6

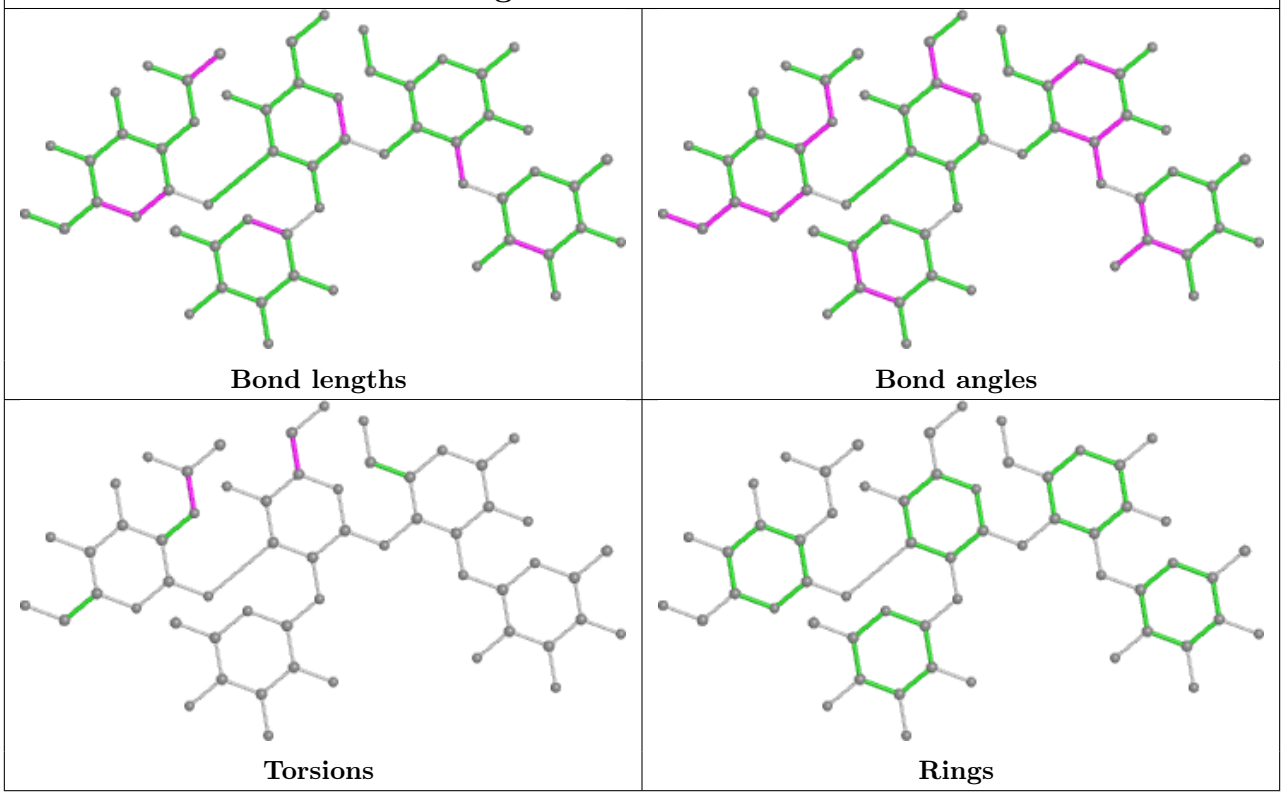
There are no ring outliers.

12 monomers are involved in 12 short contacts:

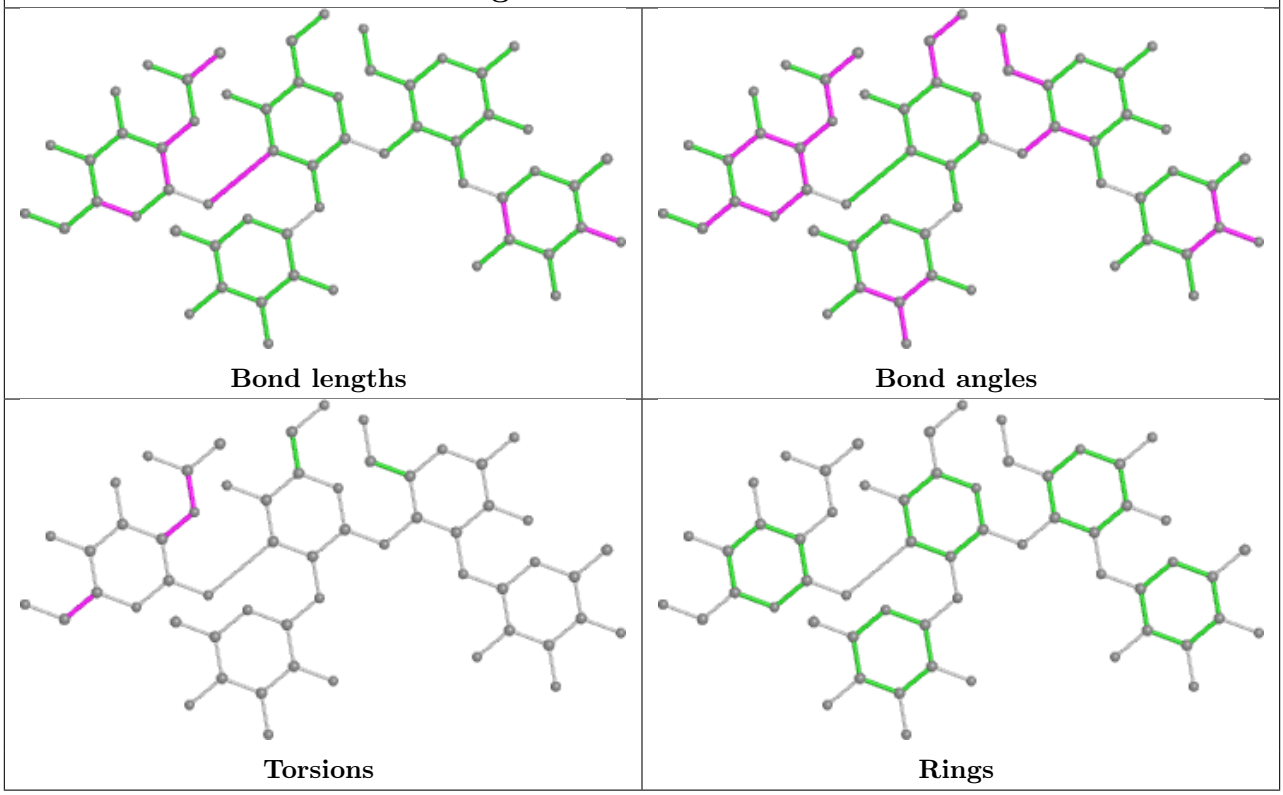
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	3[A]	FUC	2	0
3	O	4[B]	A2G	1	0
3	L	5[A]	FUC	1	0
3	L	2[B]	GAL	1	0
3	L	3[B]	FUC	2	0
2	Q	1[A]	GLC	2	0
2	M	4	A2G	2	0
3	L	4[A]	A2G	1	0
3	L	4[B]	A2G	1	0
3	O	5[B]	FUC	1	0
2	M	2	GAL	1	0
3	O	1[B]	BGC	1	0

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

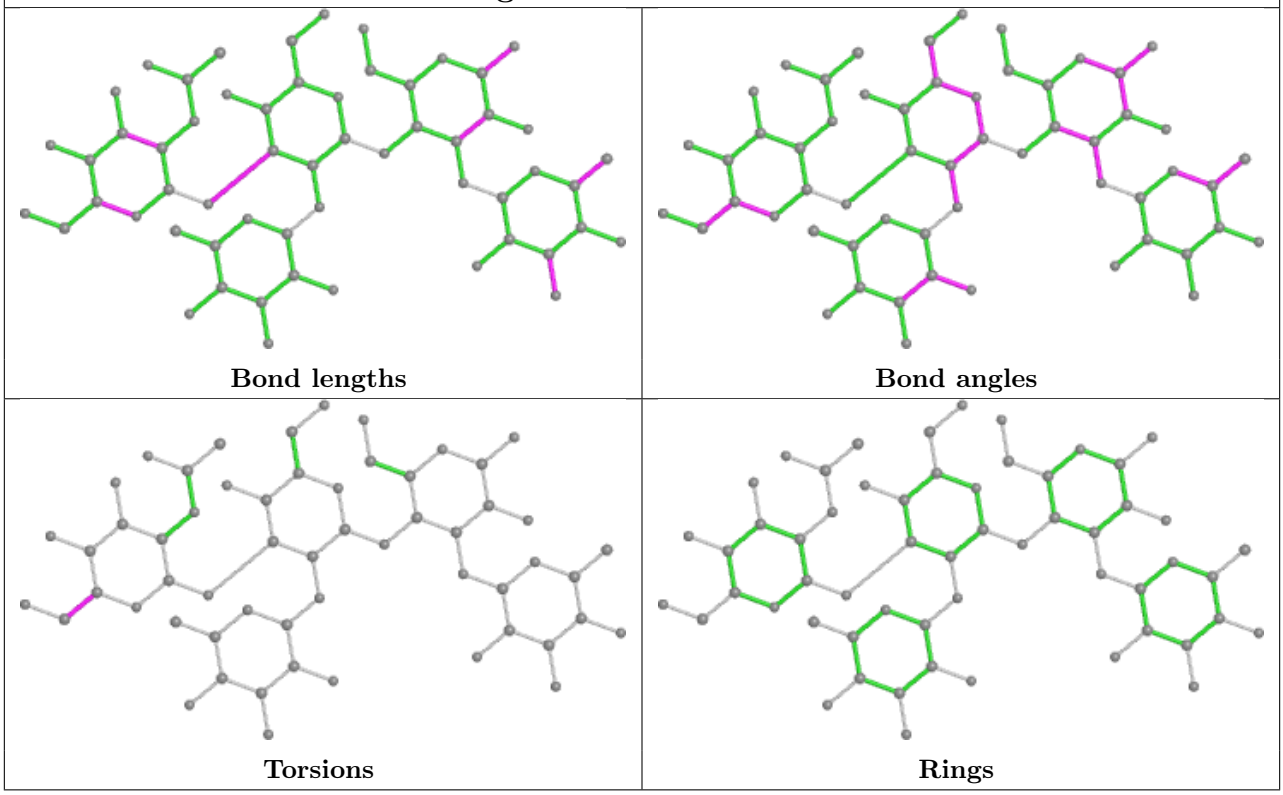
Oligosaccharide Chain K



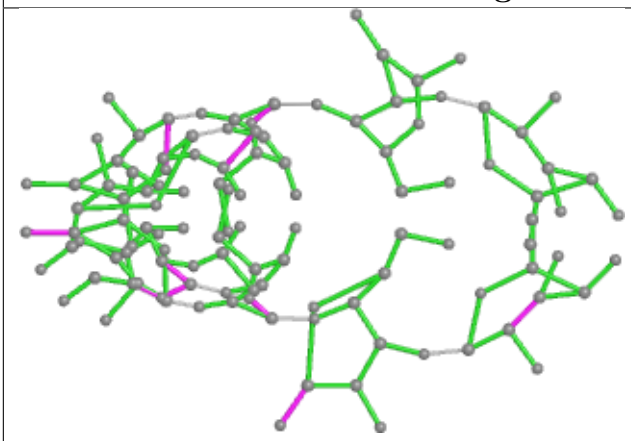
Oligosaccharide Chain M



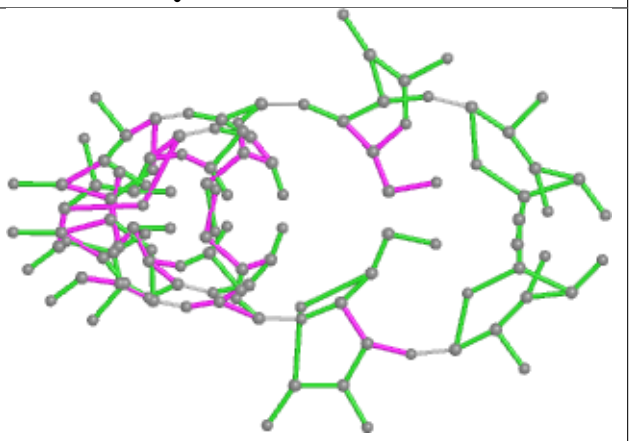
Oligosaccharide Chain P



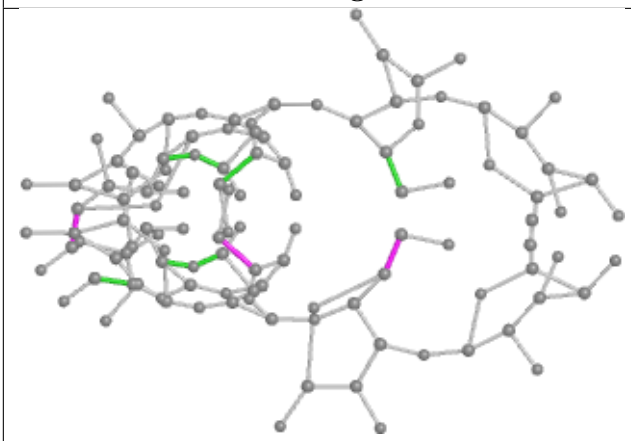
Oligosaccharide Chain Q



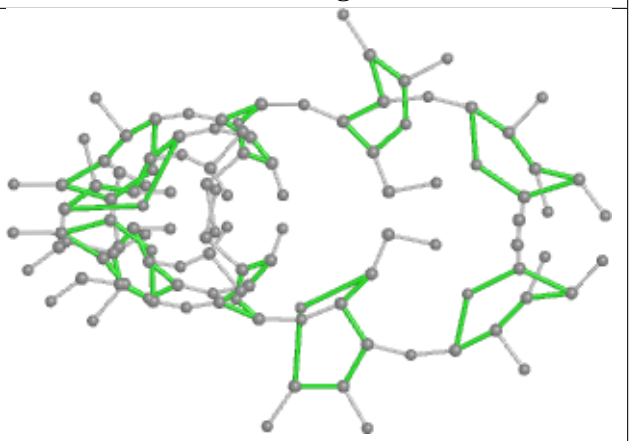
Bond lengths



Bond angles

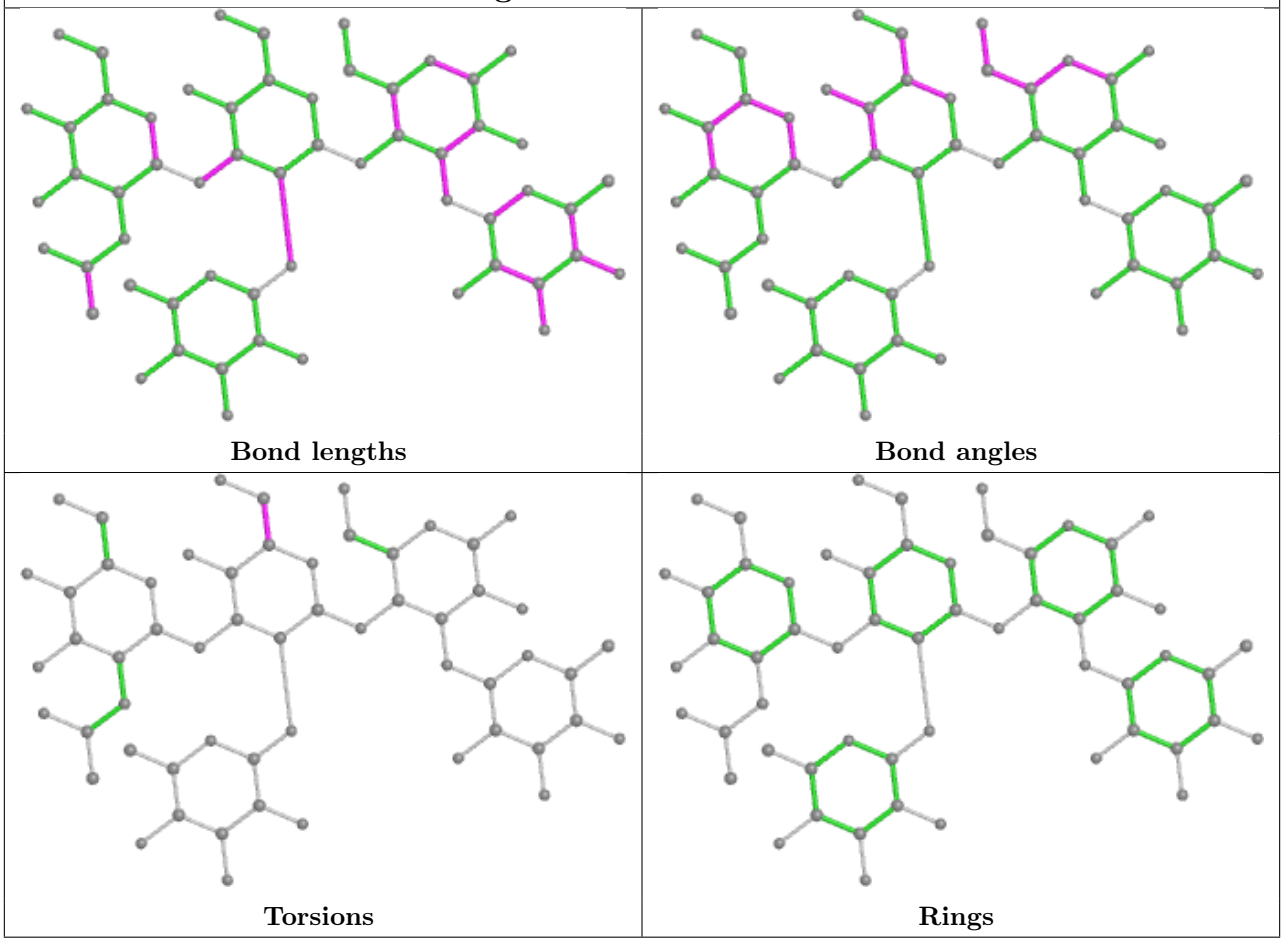


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 for Mogul analysis.

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	$\#\|Z\| > 2$
7	GLC	D	210[B]	3	12,12,12	0.85	0	17,17,17	1.28	3 (17%)
5	BCN	E	203	4	10,10,10	0.83	0	11,11,11	2.37	5 (45%)
5	BCN	A	204	4	10,10,10	0.61	0	11,11,11	2.41	4 (36%)
5	BCN	E	201	4	10,10,10	0.74	0	11,11,11	2.41	6 (54%)
5	BCN	B	204	4	10,10,10	0.79	0	11,11,11	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FUC	B	203	-	11,11,11	1.03	0	15,16,16	1.45	4 (26%)
8	PG4	F	201	-	12,12,12	0.32	0	11,11,11	0.43	0
5	BCN	D	203	4	10,10,10	0.78	0	11,11,11	1.04	1 (9%)
5	BCN	B	201	4	10,10,10	1.09	1 (10%)	11,11,11	2.73	5 (45%)
5	BCN	C	203	4	10,10,10	0.79	0	11,11,11	1.10	1 (9%)
5	BCN	D	202	4	10,10,10	0.91	1 (10%)	11,11,11	0.80	0
6	FUC	H	201	-	11,11,11	0.88	0	15,16,16	1.37	2 (13%)
5	BCN	C	202	4	10,10,10	0.85	0	11,11,11	0.69	0
7	GLC	G	206[A]	3	12,12,12	1.66	3 (25%)	17,17,17	1.03	1 (5%)
5	BCN	A	202	4	10,10,10	0.86	0	11,11,11	0.85	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
7	GLC	D	210[B]	3	-	0/2/22/22	0/1/1/1
5	BCN	E	203	4	-	7/10/10/10	-
5	BCN	A	204	4	-	4/10/10/10	-
5	BCN	E	201	4	-	3/10/10/10	-
5	BCN	B	204	4	-	1/10/10/10	-
8	PG4	F	201	-	-	4/10/10/10	-
6	FUC	B	203	-	-	-	0/1/1/1
5	BCN	D	203	4	-	1/10/10/10	-
6	FUC	H	201	-	-	-	0/1/1/1
5	BCN	B	201	4	-	6/10/10/10	-
5	BCN	C	203	4	-	2/10/10/10	-
5	BCN	D	202	4	-	0/10/10/10	-
7	GLC	G	206[A]	3	-	0/2/22/22	0/1/1/1
5	BCN	C	202	4	-	1/10/10/10	-
5	BCN	A	202	4	-	2/10/10/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	206[A]	GLC	C4-C3	3.35	1.60	1.52
5	B	201	BCN	C1-N1	3.02	1.53	1.47
7	G	206[A]	GLC	O2-C2	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	202	BCN	O22-C2	-2.20	1.23	1.30
7	G	206[A]	GLC	O1-C1	2.00	1.46	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	201	BCN	C1-N1-C3	5.55	125.45	111.94
5	E	203	BCN	C5-N1-C3	4.78	122.81	111.44
5	A	204	BCN	C1-N1-C3	4.62	123.17	111.94
5	B	201	BCN	C2-C1-N1	4.51	128.35	113.63
5	A	204	BCN	C2-C1-N1	4.22	127.40	113.63
5	E	201	BCN	C1-N1-C3	4.16	122.07	111.94
5	B	201	BCN	C5-N1-C3	3.47	119.69	111.44
5	E	201	BCN	C5-N1-C3	3.24	119.14	111.44
5	E	201	BCN	C2-C1-N1	3.23	124.17	113.63
7	D	210[B]	GLC	C1-O5-C5	-3.15	107.72	113.66
6	B	203	FUC	O2-C2-C1	3.06	116.25	109.16
5	A	204	BCN	C5-N1-C3	3.02	118.63	111.44
5	E	201	BCN	C6-C5-N1	2.91	123.86	113.40
7	G	206[A]	GLC	O3-C3-C4	-2.91	103.63	110.35
5	E	203	BCN	C4-C3-N1	2.79	123.42	113.40
5	E	201	BCN	C1-N1-C5	2.78	118.70	111.94
6	H	201	FUC	O4-C4-C3	-2.71	104.09	110.35
6	B	203	FUC	O4-C4-C5	2.57	115.37	109.67
5	A	204	BCN	C1-N1-C5	2.57	118.18	111.94
5	E	203	BCN	C1-N1-C5	2.50	118.01	111.94
5	E	201	BCN	C4-C3-N1	2.47	122.28	113.40
5	E	203	BCN	O21-C2-C1	-2.46	112.51	122.31
5	B	201	BCN	O6-C6-C5	-2.30	101.65	111.19
7	D	210[B]	GLC	O5-C5-C6	2.29	112.12	106.44
6	B	203	FUC	O4-C4-C3	-2.22	105.22	110.35
5	E	203	BCN	O22-C2-O21	2.18	128.72	123.30
5	B	201	BCN	C4-C3-N1	2.16	121.15	113.40
5	D	203	BCN	C1-N1-C3	-2.15	106.71	111.94
6	B	203	FUC	C4-C3-C2	-2.12	107.12	110.82
7	D	210[B]	GLC	O6-C6-C5	-2.05	104.25	111.29
6	H	201	FUC	O2-C2-C3	-2.04	105.64	110.35
5	C	203	BCN	O21-C2-C1	-2.03	114.22	122.31

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	204	BCN	C4-C3-N1-C1
5	E	203	BCN	C2-C1-N1-C3
5	E	203	BCN	C6-C5-N1-C1
5	E	203	BCN	N1-C1-C2-O21
5	E	203	BCN	N1-C1-C2-O22
5	B	201	BCN	C4-C3-N1-C1
5	E	201	BCN	C4-C3-N1-C1
5	B	201	BCN	N1-C1-C2-O21
5	A	204	BCN	N1-C3-C4-O4
5	B	201	BCN	N1-C1-C2-O22
5	B	201	BCN	C2-C1-N1-C5
5	E	203	BCN	C4-C3-N1-C5
5	A	202	BCN	N1-C5-C6-O6
8	F	201	PG4	C3-C4-O3-C5
5	C	203	BCN	C2-C1-N1-C3
8	F	201	PG4	O3-C5-C6-O4
5	C	203	BCN	C2-C1-N1-C5
8	F	201	PG4	O1-C1-C2-O2
5	E	201	BCN	C2-C1-N1-C5
8	F	201	PG4	C5-C6-O4-C7
5	A	204	BCN	C2-C1-N1-C5
5	A	202	BCN	N1-C3-C4-O4
5	A	204	BCN	C6-C5-N1-C3
5	B	201	BCN	C2-C1-N1-C3
5	E	203	BCN	C2-C1-N1-C5
5	B	201	BCN	C6-C5-N1-C1
5	E	203	BCN	C4-C3-N1-C1
5	E	201	BCN	C6-C5-N1-C3
5	D	203	BCN	C2-C1-N1-C3
5	B	204	BCN	C2-C1-N1-C3
5	C	202	BCN	C2-C1-N1-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	210[B]	GLC	3	0
6	B	203	FUC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	103/103 (100%)	-0.29	0	100	100	13, 20, 33, 38	0
1	B	103/103 (100%)	-0.29	0	100	100	13, 23, 35, 51	0
1	C	103/103 (100%)	-0.37	1 (0%)	82	86	12, 18, 30, 44	0
1	D	103/103 (100%)	-0.36	0	100	100	12, 17, 30, 43	0
1	E	103/103 (100%)	-0.32	1 (0%)	82	86	12, 18, 31, 44	0
1	F	103/103 (100%)	-0.56	0	100	100	12, 15, 24, 39	0
1	G	103/103 (100%)	-0.48	0	100	100	12, 16, 29, 45	0
1	H	103/103 (100%)	-0.31	0	100	100	12, 18, 31, 44	0
1	I	103/103 (100%)	-0.42	0	100	100	12, 16, 29, 34	0
1	J	103/103 (100%)	-0.47	0	100	100	11, 15, 25, 43	0
All	All	1030/1030 (100%)	-0.39	2 (0%)	95	95	11, 18, 32, 51	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	55	SER	3.7
1	C	55	SER	2.2

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	M	3	10/11	0.68	0.21	37,40,43,43	10
2	A2G	K	4	14/15	0.70	0.23	43,47,57,60	14
2	A2G	M	4	14/15	0.73	0.23	34,39,42,43	14
2	GAL	M	2	11/12	0.82	0.28	37,40,43,47	11
3	A2G	N	4	14/15	0.83	0.20	33,38,42,44	0
3	A2G	O	4[A]	14/15	0.83	0.18	26,29,33,38	14
3	A2G	O	4[B]	14/15	0.83	0.18	19,21,24,27	14
2	GLC	M	1	12/12	0.84	0.28	31,38,43,44	12
2	GLC	K	1	12/12	0.85	0.15	28,36,40,40	12
2	FUC	K	3	10/11	0.85	0.13	35,39,41,45	10
2	GAL	K	2	11/12	0.86	0.17	37,39,40,41	11
3	FUC	N	3	10/11	0.88	0.13	26,30,32,33	0
2	FUC	Q	3[A]	10/11	0.89	0.14	20,23,23,24	10
2	FUC	Q	3[B]	10/11	0.89	0.14	19,21,22,22	10
2	FUC	M	5	10/11	0.89	0.11	22,26,27,28	10
2	A2G	Q	4[A]	14/15	0.90	0.14	24,27,29,30	14
2	A2G	Q	4[B]	14/15	0.90	0.14	20,21,22,22	14
3	BGC	N	1	12/12	0.91	0.14	22,27,33,34	0
2	FUC	K	5	10/11	0.92	0.09	23,27,29,30	10
3	FUC	N	5	10/11	0.92	0.09	18,22,24,25	0
2	FUC	P	3	10/11	0.93	0.08	26,30,35,36	0
2	A2G	P	4	14/15	0.93	0.09	24,27,33,35	0
3	A2G	L	4[B]	14/15	0.94	0.09	17,17,19,19	14
2	GLC	P	1	12/12	0.94	0.11	16,26,35,36	0
3	GAL	N	2	11/12	0.94	0.13	23,26,30,30	0
3	A2G	L	4[A]	14/15	0.94	0.09	18,19,21,21	14
2	GAL	Q	2[B]	11/12	0.95	0.08	18,19,20,20	11
2	FUC	Q	5[A]	10/11	0.95	0.08	14,15,17,17	10
3	BGC	O	1[B]	12/12	0.95	0.10	13,14,14,17	12
2	FUC	Q	5[B]	10/11	0.95	0.08	13,14,15,16	10
2	GAL	Q	2[A]	11/12	0.95	0.08	20,21,21,23	11
2	GAL	P	2	11/12	0.96	0.05	18,20,22,24	0
3	BGC	L	1[A]	12/12	0.96	0.09	14,16,17,18	12
3	FUC	L	5[A]	10/11	0.96	0.07	11,13,13,14	10
3	FUC	L	5[B]	10/11	0.96	0.07	13,14,15,15	10
3	FUC	L	3[A]	10/11	0.97	0.07	16,17,17,18	10
3	FUC	L	3[B]	10/11	0.97	0.07	14,15,16,16	10
2	FUC	P	5	10/11	0.97	0.06	14,15,16,17	0
2	GLC	Q	1[A]	12/12	0.97	0.09	19,23,26,31	12
2	GLC	Q	1[B]	12/12	0.97	0.09	15,16,17,17	12
3	GAL	L	2[A]	11/12	0.97	0.07	16,17,17,19	11

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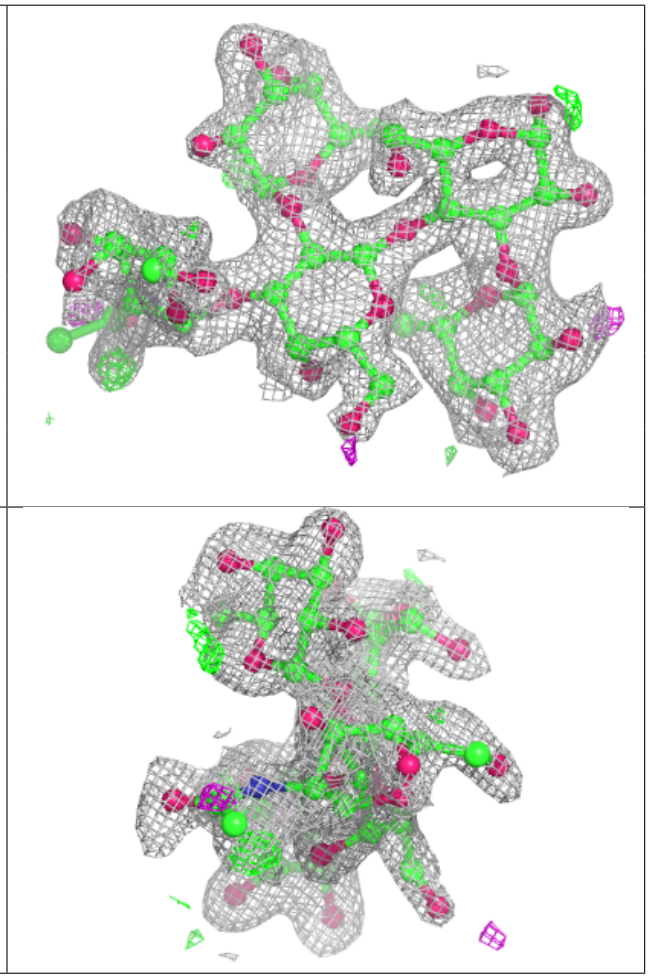
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GAL	L	2[B]	11/12	0.97	0.07	14,14,15,15	11
3	FUC	O	3[A]	10/11	0.98	0.06	14,14,15,15	10
3	FUC	O	3[B]	10/11	0.98	0.06	11,11,12,12	10
3	GAL	O	2[A]	11/12	0.98	0.07	16,18,19,21	11
3	GAL	O	2[B]	11/12	0.98	0.07	11,13,13,15	11
3	FUC	O	5[A]	10/11	0.98	0.06	11,12,12,13	10
3	FUC	O	5[B]	10/11	0.98	0.06	12,13,13,14	10

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.

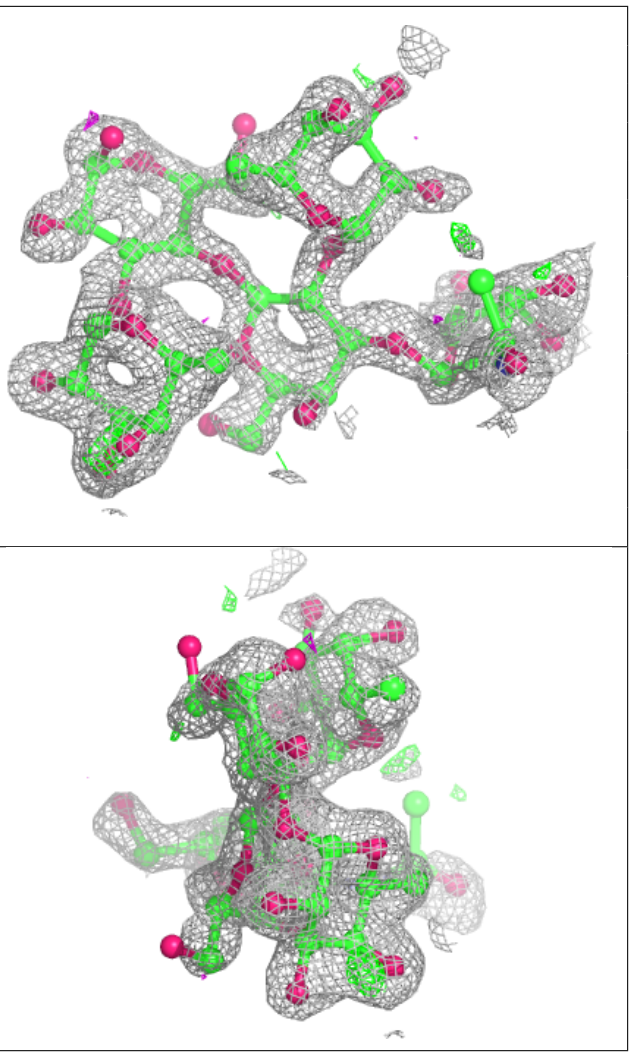
Electron density around Chain K:

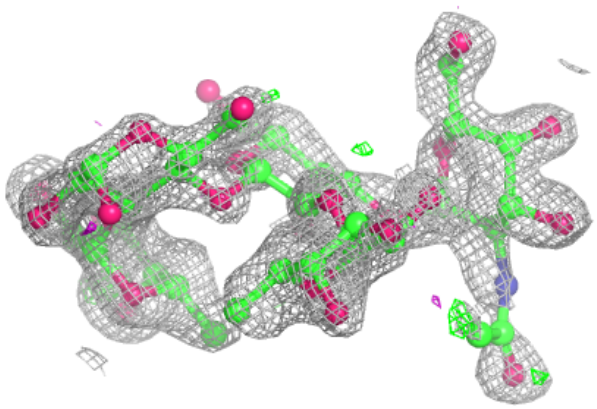
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain M:

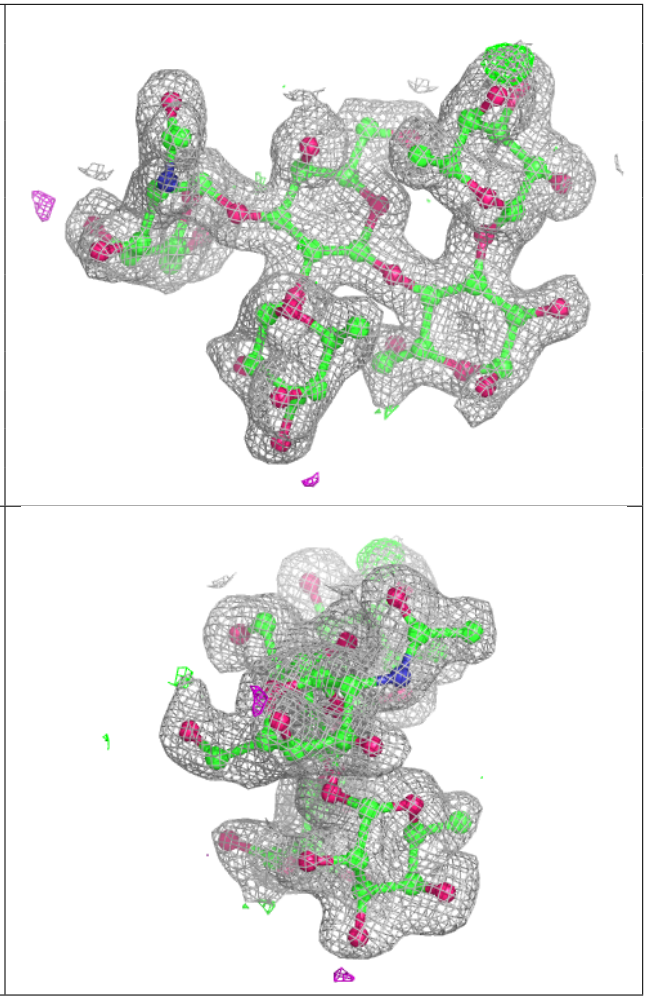
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





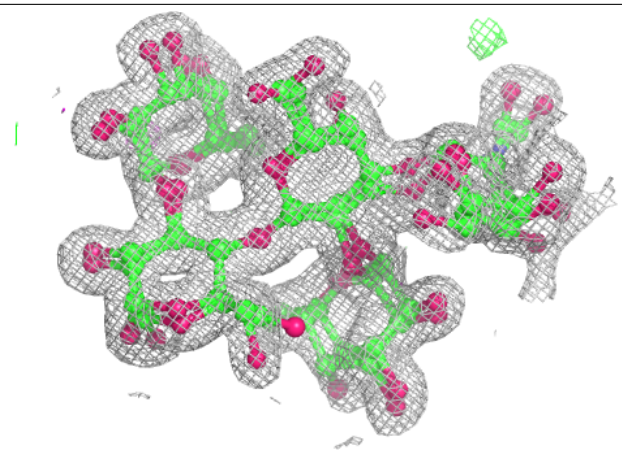
Electron density around Chain P:

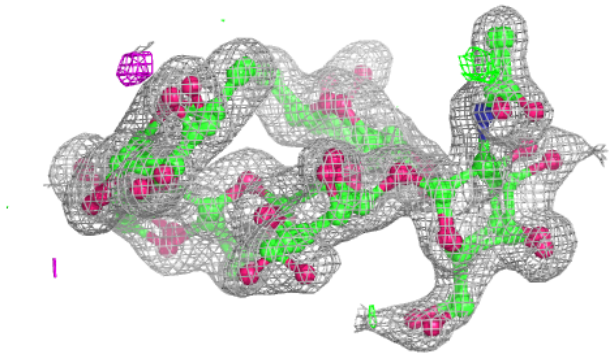
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

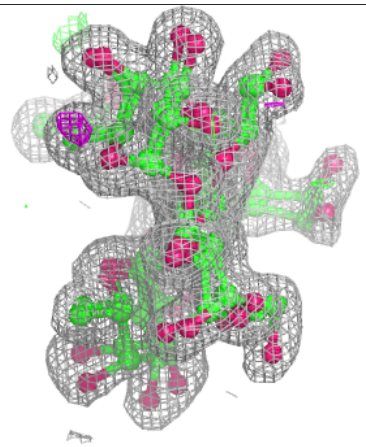


Electron density around Chain Q:

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

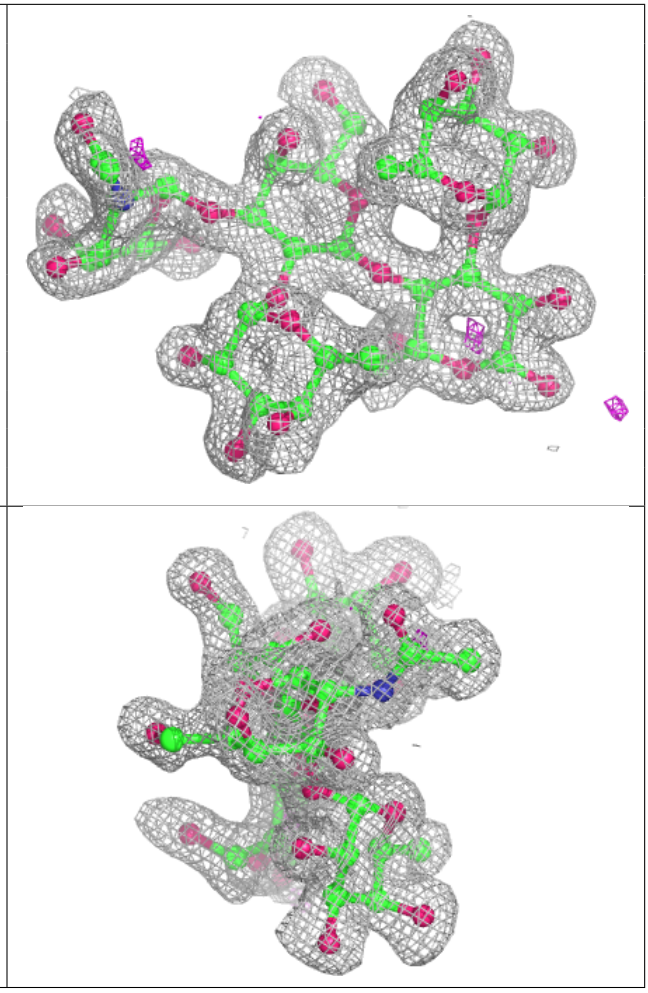






Electron density around Chain N:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	FUC	B	203	11/11	0.72	0.17	39,46,50,52	0
6	FUC	H	201	11/11	0.75	0.17	31,39,42,44	0
5	BCN	B	201	11/11	0.90	0.10	19,24,30,32	0
5	BCN	B	204	11/11	0.92	0.09	20,24,28,29	0
8	PG4	F	201	13/13	0.92	0.10	29,35,41,45	0
5	BCN	A	204	11/11	0.93	0.11	18,23,26,28	0
5	BCN	A	202	11/11	0.94	0.08	18,21,25,26	0
5	BCN	C	202	11/11	0.94	0.12	17,22,25,26	0
5	BCN	E	203	11/11	0.94	0.10	17,23,26,27	0
5	BCN	D	202	11/11	0.95	0.10	16,23,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GLC	G	206[A]	12/12	0.95	0.09	14,15,15,17	12
5	BCN	E	201	11/11	0.95	0.11	17,19,23,24	0
5	BCN	C	203	11/11	0.96	0.10	16,22,25,26	0
7	GLC	D	210[B]	12/12	0.96	0.08	15,17,18,19	12
5	BCN	D	203	11/11	0.97	0.10	17,22,27,27	0
4	CA	A	203	1/1	0.99	0.04	15,15,15,15	0
4	CA	D	201	1/1	0.99	0.04	14,14,14,14	0
4	CA	D	204	1/1	0.99	0.05	15,15,15,15	0
4	CA	C	201	1/1	1.00	0.05	15,15,15,15	0
4	CA	C	204	1/1	1.00	0.04	16,16,16,16	0
4	CA	A	201	1/1	1.00	0.04	13,13,13,13	0
4	CA	B	202	1/1	1.00	0.04	15,15,15,15	0
4	CA	E	202	1/1	1.00	0.05	14,14,14,14	0
4	CA	E	204	1/1	1.00	0.03	14,14,14,14	0
4	CA	B	205	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.