Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 02:21 pm GMT

PDB ID	:	5ELD
Title	:	Cholera toxin classical B-pentamer in complex with A Lewis-y
Authors	:	Heggelund, J.E.; Burschowsky, D.; Krengel, U.
Deposited on	:	2015-11-04
Resolution	:	1.40 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:

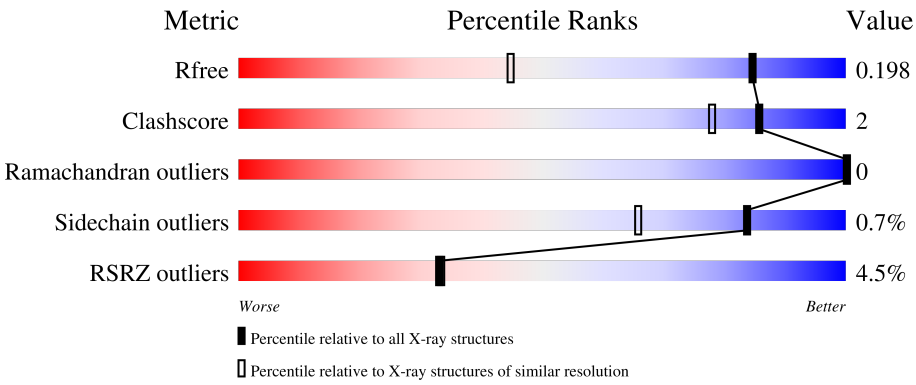
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	7% 95% 5%
1	B	103	10% 94% 6%
1	C	103	93% 7%
1	D	103	5% 96% .
1	E	103	. % 94% 6%

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Mol	Chain	Length	Quality of chain
2	F	5	20% 80%
2	G	5	20% 80%
2	H	5	60% 40%
2	I	5	20% 80%

2 Entry composition (i)

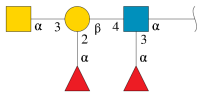
There are 9 unique types of molecules in this entry. The entry contains 5418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 B subunit.

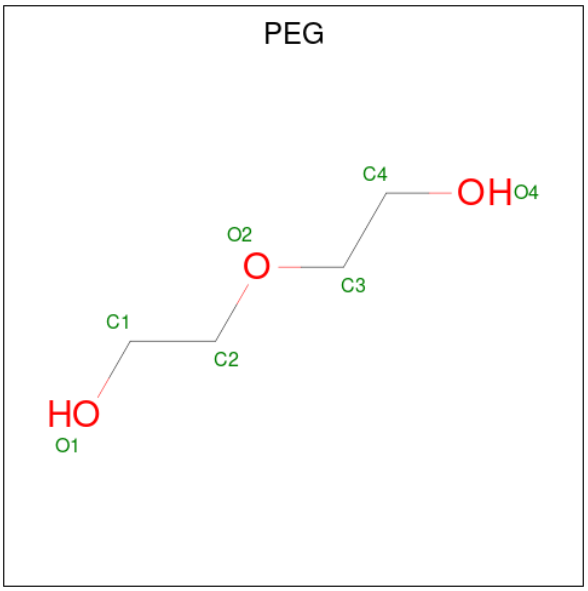
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	103	857	544	147	159	7	0	8	0
1	B	103	879	559	149	164	7	0	12	0
1	C	103	864	549	145	163	7	0	9	0
1	D	103	842	532	147	156	7	0	5	0
1	E	103	841	533	146	156	6	0	5	0

- 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)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



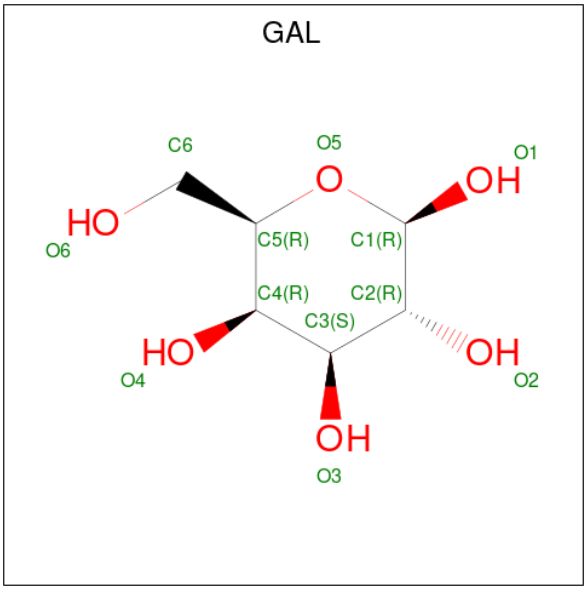
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	5	120	68	4	48	0	5	0
2	G	5	120	68	4	48	0	5	0
2	H	5	120	68	4	48	0	5	0
2	I	5	60	34	2	24	0	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
			Total	C	O		
3	D	1	7	4	3	0	0

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	12	6	6	0	0
			Total	C	O		
4	C	1	12	6	6	0	0

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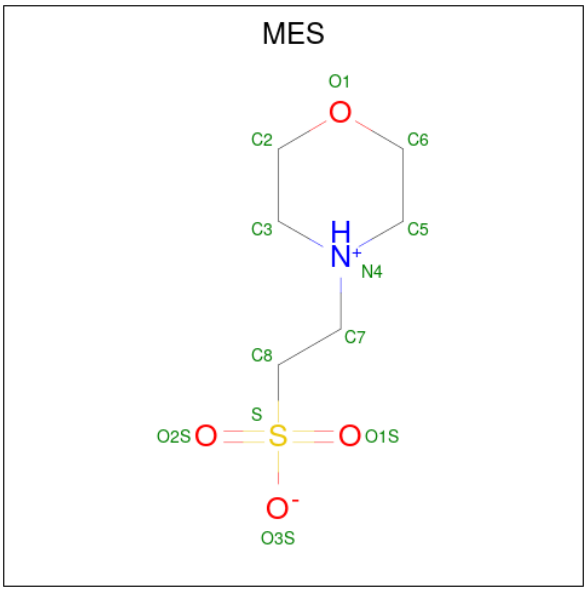
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	E	1	12	6	6	0	1

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

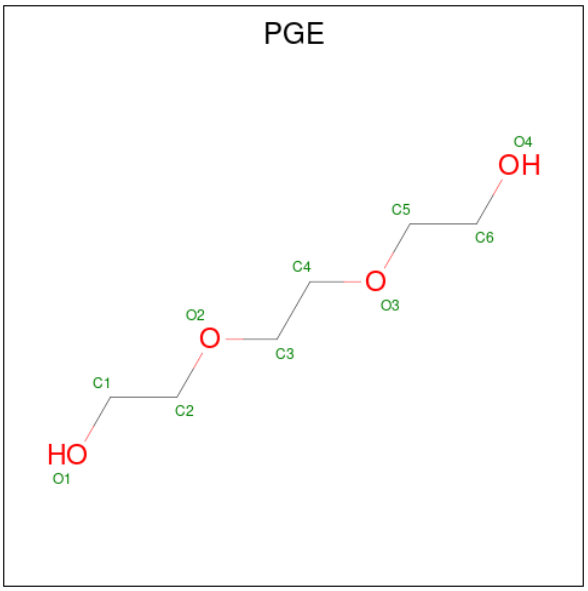
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	B	1	1	1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



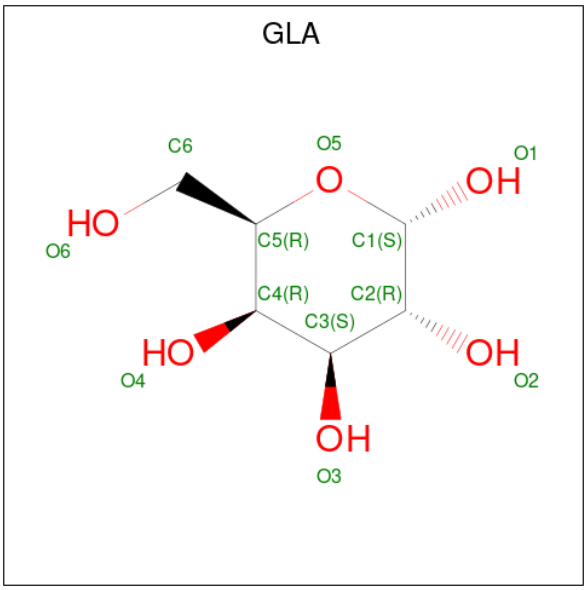
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	C	1	12	6	1	4	1	6	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 10 6 4	0	0
7	D	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0

- Molecule 8 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 12 6 6	0	1

- Molecule 9 is water.

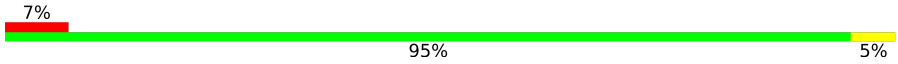
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	122	122	122	0	0
			Total	O		
9	B	114	114	114	0	0
			Total	O		
9	C	127	127	127	0	0
			Total	O		
9	D	128	128	128	0	0
			Total	O		
9	E	119	119	119	0	0

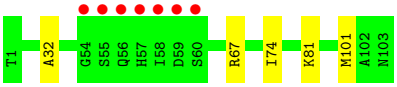
3 Residue-property plots (i)

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 B subunit

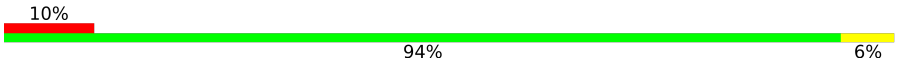
Chain A:

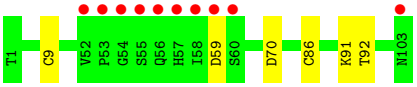




• Molecule 1: Cholera enterotoxin B subunit

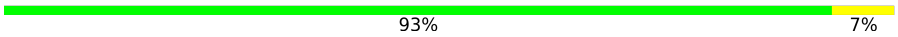
Chain B:

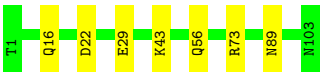




• Molecule 1: Cholera enterotoxin B subunit

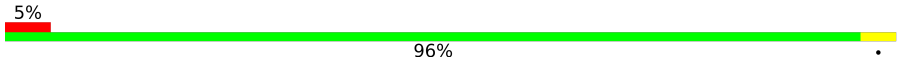
Chain C:

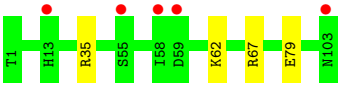




• Molecule 1: Cholera enterotoxin B subunit

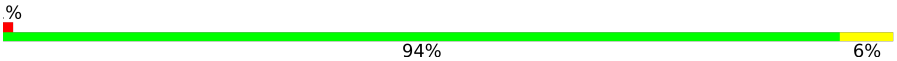
Chain D:





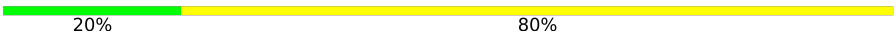
• Molecule 1: Cholera enterotoxin B subunit

Chain E:



• 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)]2-acetamido-2-deoxy-alpha-D-glucopyran

ose

Chain F: 

• 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)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain G:

• 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)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain H:

• 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)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.70Å 69.81Å 134.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 1.40 48.48 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.48-1.40) 99.1 (48.48-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.171 , 0.193 0.178 , 0.198	Depositor DCC
R_{free} test set	6438 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5418	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: GLA, MES, PGE, GAL, PEG, NDG, FUC, NA, A2G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.73	0/895	0.97	2/1205 (0.2%)
1	B	0.75	0/923	0.83	0/1243
1	C	0.67	0/907	0.78	2/1224 (0.2%)
1	D	0.75	1/871 (0.1%)	0.81	1/1172 (0.1%)
1	E	0.70	0/870	0.85	1/1170 (0.1%)
All	All	0.72	1/4466 (0.0%)	0.85	6/6014 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	79	GLU	CD-OE1	-5.61	1.19	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101[A]	MET	CG-SD-CE	-10.77	82.97	100.20
1	A	101[B]	MET	CG-SD-CE	-10.77	82.97	100.20
1	E	35	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	22	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	D	35	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	73	ARG	NE-CZ-NH1	5.35	122.97	120.30

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	857	0	894	3	0
1	B	879	0	924	5	0
1	C	864	0	883	3	0
1	D	842	0	870	3	0
1	E	841	0	874	4	0
2	F	120	0	100	0	0
2	G	120	0	100	5	0
2	H	120	0	100	1	0
2	I	60	0	50	0	0
3	A	7	0	10	0	0
3	D	7	0	10	0	0
4	A	12	0	12	0	0
4	C	12	0	12	1	0
4	E	12	0	12	0	0
5	B	1	0	0	0	0
6	C	12	0	9	0	0
7	C	10	0	14	0	0
7	D	10	0	14	0	0
7	E	10	0	14	0	0
8	E	12	0	12	0	0
9	A	122	0	0	0	0
9	B	114	0	0	1	0
9	C	127	0	0	2	0
9	D	128	0	0	1	0
9	E	119	0	0	1	0
All	All	5418	0	4914	21	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 (21) 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:67[B]:ARG:NH2	9:D:301:HOH:O	1.58	1.29
1:B:92[B]:THR:O	9:B:301:HOH:O	1.77	1.02
2:G:3[A]:FUC:O2	2:G:4[A]:A2G:H3	1.62	0.96
1:D:67[B]:ARG:NH1	1:E:70:ASP:OD1	2.08	0.84
1:C:56[B]:GLN:NE2	4:C:203:GAL:O1	2.22	0.73
1:B:91[B]:LYS:HD2	1:B:91[B]:LYS:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2[A]:GAL:H3	2:G:4[A]:A2G:C5	2.23	0.68
1:A:67[B]:ARG:NH1	1:B:70:ASP:OD1	2.26	0.68
2:G:3[A]:FUC:O2	2:G:4[A]:A2G:C3	2.42	0.66
1:E:81[A]:LYS:HG2	9:E:319:HOH:O	2.08	0.54
1:C:16:GLN:NE2	1:C:89:ASN:HD22	2.09	0.51
1:B:9[B]:CYS:SG	1:B:86:CYS:SG	3.08	0.48
1:C:43:LYS:NZ	9:C:303:HOH:O	2.43	0.47
2:G:2[A]:GAL:C3	2:G:4[A]:A2G:C5	2.93	0.46
1:B:91[B]:LYS:HD2	1:B:91[B]:LYS:C	2.36	0.46
1:A:74[B]:ILE:HD12	9:C:425:HOH:O	2.17	0.45
1:E:59:ASP:HA	1:E:62:LYS:HG2	1.99	0.45
2:H:2[B]:GAL:H3	2:H:4[B]:A2G:C5	2.51	0.41
1:D:62[B]:LYS:HB2	1:D:62[B]:LYS:HE3	1.80	0.41
1:A:32:ALA:HB1	1:E:12:TYR:CZ	2.56	0.40
2:G:1[A]:NDG:H6C1	2:G:2[A]: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	109/103 (106%)	107 (98%)	2 (2%)	0	100	100
1	B	113/103 (110%)	110 (97%)	3 (3%)	0	100	100
1	C	110/103 (107%)	109 (99%)	1 (1%)	0	100	100
1	D	106/103 (103%)	105 (99%)	1 (1%)	0	100	100
1	E	106/103 (103%)	104 (98%)	2 (2%)	0	100	100
All	All	544/515 (106%)	535 (98%)	9 (2%)	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	97/89 (109%)	95 (98%)	2 (2%)	53	21
1	B	101/89 (114%)	100 (99%)	1 (1%)	76	53
1	C	98/89 (110%)	96 (98%)	2 (2%)	55	23
1	D	94/89 (106%)	94 (100%)	0	100	100
1	E	94/89 (106%)	94 (100%)	0	100	100
All	All	484/445 (109%)	479 (99%)	5 (1%)	84	53

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81[A]	LYS
1	A	81[B]	LYS
1	B	59	ASP
1	C	29[A]	GLU
1	C	29[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	16	GLN
1	D	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)

35 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	NDG	F	1[A]	2	15,15,15	0.91	0	21,21,21	1.16	3 (14%)
2	NDG	F	1[B]	2	15,15,15	0.68	0	21,21,21	1.24	2 (9%)
2	GAL	F	2[A]	2	11,11,12	1.07	1 (9%)	15,15,17	1.12	1 (6%)
2	GAL	F	2[B]	2	11,11,12	1.07	2 (18%)	15,15,17	0.83	0
2	FUC	F	3[A]	2	10,10,11	1.20	0	14,14,16	0.77	0
2	FUC	F	3[B]	2	10,10,11	1.07	1 (10%)	14,14,16	0.90	0
2	A2G	F	4[A]	2	14,14,15	1.19	1 (7%)	17,19,21	1.35	2 (11%)
2	A2G	F	4[B]	2	14,14,15	1.43	2 (14%)	17,19,21	1.37	3 (17%)
2	FUC	F	5[A]	2	10,10,11	0.92	0	14,14,16	0.61	0
2	FUC	F	5[B]	2	10,10,11	0.84	0	14,14,16	1.02	0
2	NDG	G	1[A]	2	15,15,15	0.72	0	21,21,21	1.35	4 (19%)
2	NDG	G	1[B]	2	15,15,15	0.69	0	21,21,21	1.16	1 (4%)
2	GAL	G	2[A]	2	11,11,12	0.42	0	15,15,17	1.00	0
2	GAL	G	2[B]	2	11,11,12	1.42	3 (27%)	15,15,17	0.92	1 (6%)
2	FUC	G	3[A]	2	10,10,11	0.58	0	14,14,16	1.06	1 (7%)
2	FUC	G	3[B]	2	10,10,11	0.73	0	14,14,16	0.88	1 (7%)
2	A2G	G	4[A]	2	14,14,15	0.74	0	17,19,21	1.21	2 (11%)
2	A2G	G	4[B]	2	14,14,15	1.38	2 (14%)	17,19,21	1.40	3 (17%)
2	FUC	G	5[A]	2	10,10,11	0.60	0	14,14,16	0.79	0
2	FUC	G	5[B]	2	10,10,11	1.08	0	14,14,16	0.83	0
2	NDG	H	1[A]	2	15,15,15	1.15	3 (20%)	21,21,21	1.32	3 (14%)
2	NDG	H	1[B]	2	15,15,15	1.05	1 (6%)	21,21,21	1.38	3 (14%)
2	GAL	H	2[A]	2	11,11,12	0.72	0	15,15,17	1.58	3 (20%)
2	GAL	H	2[B]	2	11,11,12	0.72	0	15,15,17	0.73	0
2	FUC	H	3[A]	2	10,10,11	1.15	1 (10%)	14,14,16	0.94	0
2	FUC	H	3[B]	2	10,10,11	0.64	0	14,14,16	1.08	1 (7%)
2	A2G	H	4[A]	2	14,14,15	1.03	1 (7%)	17,19,21	1.61	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A2G	H	4[B]	2	14,14,15	0.96	0	17,19,21	0.98	0
2	FUC	H	5[A]	2	10,10,11	1.06	1 (10%)	14,14,16	0.82	0
2	FUC	H	5[B]	2	10,10,11	1.05	1 (10%)	14,14,16	1.21	1 (7%)
2	NDG	I	1	2	15,15,15	0.72	0	21,21,21	0.95	0
2	GAL	I	2	2	11,11,12	0.87	0	15,15,17	1.47	4 (26%)
2	FUC	I	3	2	10,10,11	0.73	0	14,14,16	1.25	1 (7%)
2	A2G	I	4	2	14,14,15	1.39	3 (21%)	17,19,21	2.23	2 (11%)
2	FUC	I	5	2	10,10,11	1.12	1 (10%)	14,14,16	1.08	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	NDG	F	1[A]	2	-	0/6/26/26	0/1/1/1
2	NDG	F	1[B]	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2[A]	2	-	0/2/19/22	0/1/1/1
2	GAL	F	2[B]	2	-	1/2/19/22	0/1/1/1
2	FUC	F	3[A]	2	-	-	0/1/1/1
2	FUC	F	3[B]	2	-	-	0/1/1/1
2	A2G	F	4[A]	2	-	2/6/23/26	0/1/1/1
2	A2G	F	4[B]	2	-	2/6/23/26	0/1/1/1
2	FUC	F	5[A]	2	-	-	0/1/1/1
2	FUC	F	5[B]	2	-	-	0/1/1/1
2	NDG	G	1[A]	2	-	3/6/26/26	0/1/1/1
2	NDG	G	1[B]	2	-	0/6/26/26	0/1/1/1
2	GAL	G	2[A]	2	-	1/2/19/22	0/1/1/1
2	GAL	G	2[B]	2	-	0/2/19/22	0/1/1/1
2	FUC	G	3[A]	2	-	-	0/1/1/1
2	FUC	G	3[B]	2	-	-	0/1/1/1
2	A2G	G	4[A]	2	-	0/6/23/26	0/1/1/1
2	A2G	G	4[B]	2	-	2/6/23/26	0/1/1/1
2	FUC	G	5[A]	2	-	-	0/1/1/1
2	FUC	G	5[B]	2	-	-	0/1/1/1
2	NDG	H	1[A]	2	-	0/6/26/26	0/1/1/1
2	NDG	H	1[B]	2	-	0/6/26/26	0/1/1/1
2	GAL	H	2[A]	2	-	1/2/19/22	0/1/1/1
2	GAL	H	2[B]	2	-	0/2/19/22	0/1/1/1
2	FUC	H	3[A]	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	H	3[B]	2	-	-	0/1/1/1
2	A2G	H	4[A]	2	-	0/6/23/26	0/1/1/1
2	A2G	H	4[B]	2	-	0/6/23/26	0/1/1/1
2	FUC	H	5[A]	2	-	-	0/1/1/1
2	FUC	H	5[B]	2	-	-	0/1/1/1
2	NDG	I	1	2	-	0/6/26/26	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	FUC	I	3	2	-	-	0/1/1/1
2	A2G	I	4	2	-	0/6/23/26	0/1/1/1
2	FUC	I	5	2	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4[B]	A2G	C1-C2	3.20	1.57	1.52
2	F	4[B]	A2G	O4-C4	3.07	1.50	1.43
2	I	5	FUC	O5-C1	-2.86	1.39	1.43
2	I	4	A2G	O5-C5	2.75	1.49	1.43
2	H	1[B]	NDG	C1-C2	-2.71	1.49	1.52
2	I	4	A2G	C1-C2	2.69	1.56	1.52
2	F	4[B]	A2G	C4-C5	2.61	1.58	1.53
2	G	4[B]	A2G	O5-C5	2.55	1.48	1.43
2	F	2[A]	GAL	O5-C1	-2.44	1.39	1.43
2	G	2[B]	GAL	O5-C1	-2.44	1.39	1.43
2	F	4[A]	A2G	C1-C2	-2.40	1.48	1.52
2	F	2[B]	GAL	C2-C3	2.30	1.55	1.52
2	H	1[A]	NDG	C2-N2	2.29	1.49	1.45
2	H	5[B]	FUC	O4-C4	2.29	1.48	1.43
2	G	2[B]	GAL	O2-C2	2.29	1.48	1.43
2	F	3[B]	FUC	O5-C1	2.28	1.47	1.43
2	H	1[A]	NDG	O5-C1	2.15	1.48	1.42
2	H	4[A]	A2G	C2-N2	2.15	1.50	1.46
2	I	4	A2G	C8-C7	2.15	1.55	1.50
2	F	2[B]	GAL	O5-C1	-2.15	1.40	1.43
2	H	3[A]	FUC	O2-C2	2.07	1.47	1.43
2	G	2[B]	GAL	C2-C3	2.05	1.55	1.52
2	H	5[A]	FUC	O5-C1	-2.04	1.40	1.43
2	H	1[A]	NDG	O5-C5	-2.02	1.39	1.44

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	4	A2G	O5-C5-C6	7.57	119.07	107.20
2	H	2[A]	GAL	O5-C5-C6	-4.11	100.77	107.20
2	H	1[B]	NDG	C1-O5-C5	-3.41	107.22	113.66
2	I	2	GAL	O5-C5-C6	3.18	112.19	107.20
2	G	1[A]	NDG	C1-O5-C5	-3.16	107.70	113.66
2	I	3	FUC	C1-C2-C3	3.15	113.54	109.67
2	H	1[B]	NDG	O6-C6-C5	-3.08	100.73	111.29
2	H	2[A]	GAL	C3-C4-C5	-2.98	104.92	110.24
2	H	1[A]	NDG	C1-O5-C5	2.95	119.23	113.66
2	I	4	A2G	C6-C5-C4	-2.81	106.43	113.00
2	H	1[B]	NDG	C1-C2-N2	-2.79	107.49	110.73
2	G	4[A]	A2G	C4-C3-C2	-2.79	106.93	111.02
2	H	4[A]	A2G	O5-C1-C2	-2.77	106.91	111.29
2	H	4[A]	A2G	C1-O5-C5	2.73	115.90	112.19
2	H	5[B]	FUC	C6-C5-C4	-2.68	108.12	113.07
2	I	2	GAL	C1-O5-C5	2.60	115.71	112.19
2	G	4[B]	A2G	C1-O5-C5	-2.57	108.70	112.19
2	F	4[B]	A2G	O5-C1-C2	-2.57	107.23	111.29
2	H	1[A]	NDG	O6-C6-C5	-2.52	102.65	111.29
2	G	4[B]	A2G	O5-C5-C6	2.51	111.13	107.20
2	H	4[A]	A2G	O5-C5-C6	2.51	111.13	107.20
2	F	1[B]	NDG	C1-C2-N2	-2.44	107.90	110.73
2	F	1[B]	NDG	O1-C1-O5	-2.44	103.07	110.38
2	G	4[B]	A2G	C3-C4-C5	-2.43	105.90	110.24
2	F	4[A]	A2G	C2-N2-C7	-2.43	119.44	122.90
2	F	2[A]	GAL	O3-C3-C4	2.43	115.96	110.35
2	F	1[A]	NDG	O5-C5-C6	2.42	112.44	106.44
2	G	1[A]	NDG	O6-C6-C5	-2.41	103.02	111.29
2	F	4[B]	A2G	O5-C5-C4	2.40	116.67	110.83
2	G	1[A]	NDG	O5-C1-C2	-2.39	107.12	109.52
2	F	4[B]	A2G	O4-C4-C5	2.37	115.18	109.30
2	H	2[A]	GAL	O6-C6-C5	-2.36	103.21	111.29
2	H	4[A]	A2G	O7-C7-N2	2.33	126.24	121.95
2	F	4[A]	A2G	C3-C4-C5	-2.25	106.23	110.24
2	G	3[A]	FUC	C2-C3-C4	-2.20	107.09	110.89
2	G	3[B]	FUC	O5-C5-C4	2.14	113.36	109.52
2	F	1[A]	NDG	C1-C2-N2	-2.14	108.25	110.73
2	G	1[B]	NDG	C1-C2-N2	-2.14	108.25	110.73
2	F	1[A]	NDG	O5-C1-C2	-2.14	107.37	109.52
2	I	2	GAL	O6-C6-C5	-2.10	104.08	111.29
2	I	2	GAL	C6-C5-C4	-2.09	108.12	113.00
2	H	1[A]	NDG	C1-C2-C3	2.08	113.38	110.54
2	G	4[A]	A2G	C6-C5-C4	-2.08	108.13	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	3[B]	FUC	C1-C2-C3	2.05	112.19	109.67
2	G	1[A]	NDG	O3-C3-C4	-2.01	105.69	110.35
2	G	2[B]	GAL	C3-C4-C5	-2.00	106.67	110.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	4[B]	A2G	O5-C5-C6-O6
2	G	1[A]	NDG	O5-C5-C6-O6
2	G	4[B]	A2G	C4-C5-C6-O6
2	F	4[B]	A2G	C4-C5-C6-O6
2	G	1[A]	NDG	C4-C5-C6-O6
2	G	4[B]	A2G	O5-C5-C6-O6
2	F	4[A]	A2G	O5-C5-C6-O6
2	G	2[A]	GAL	O5-C5-C6-O6
2	H	2[A]	GAL	O5-C5-C6-O6
2	F	2[B]	GAL	O5-C5-C6-O6
2	F	4[A]	A2G	C4-C5-C6-O6
2	G	1[A]	NDG	C3-C2-N2-C7

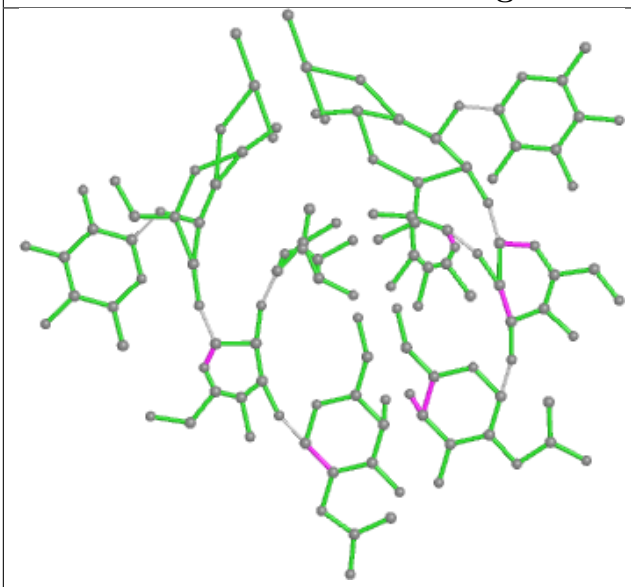
There are no ring outliers.

6 monomers are involved in 6 short contacts:

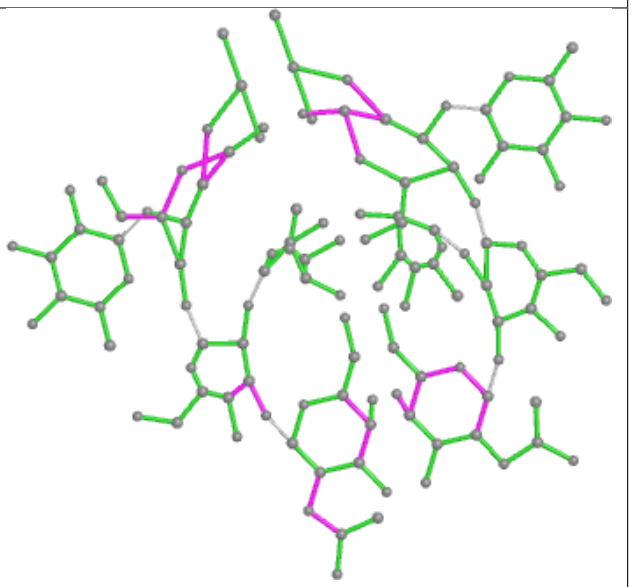
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	4[B]	A2G	1	0
2	G	2[A]	GAL	3	0
2	H	2[B]	GAL	1	0
2	G	3[A]	FUC	2	0
2	G	1[A]	NDG	1	0
2	G	4[A]	A2G	4	0

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

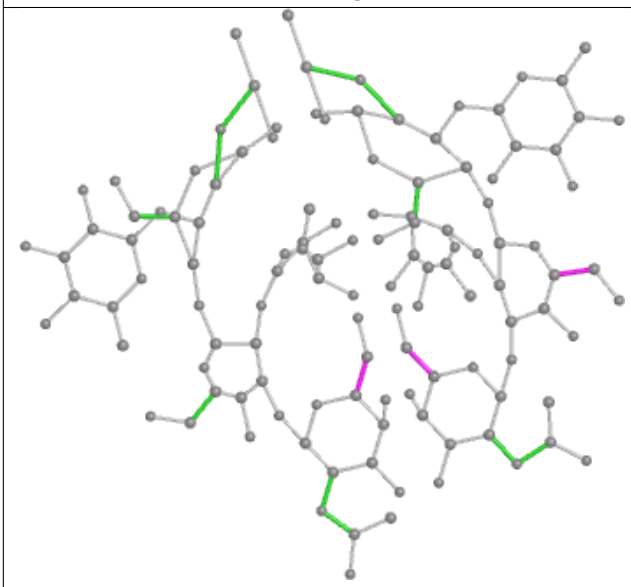
Oligosaccharide Chain F



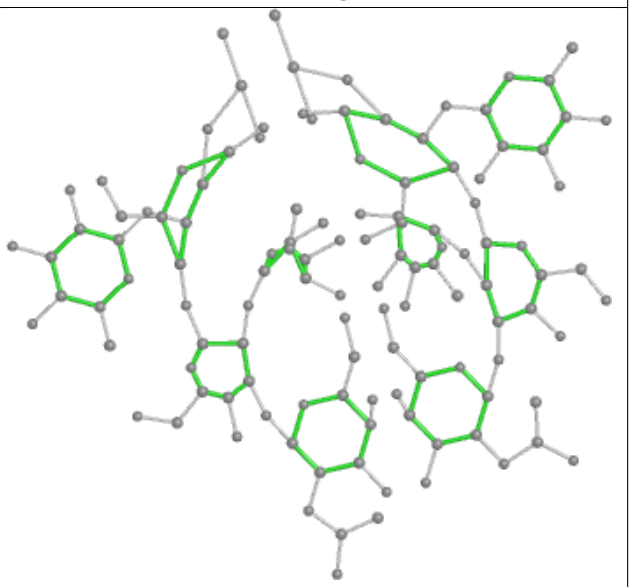
Bond lengths



Bond angles

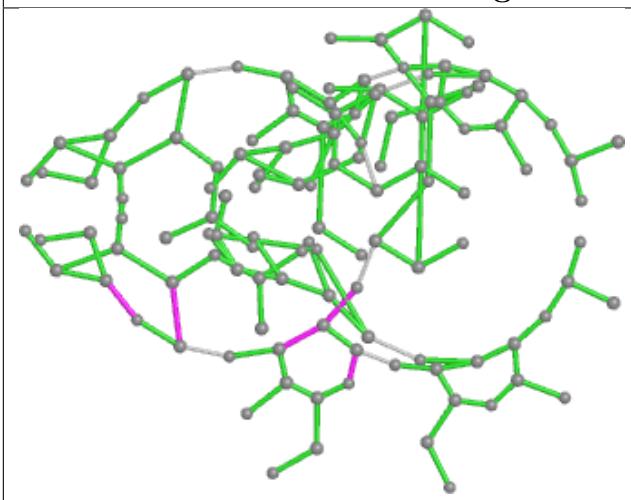


Torsions

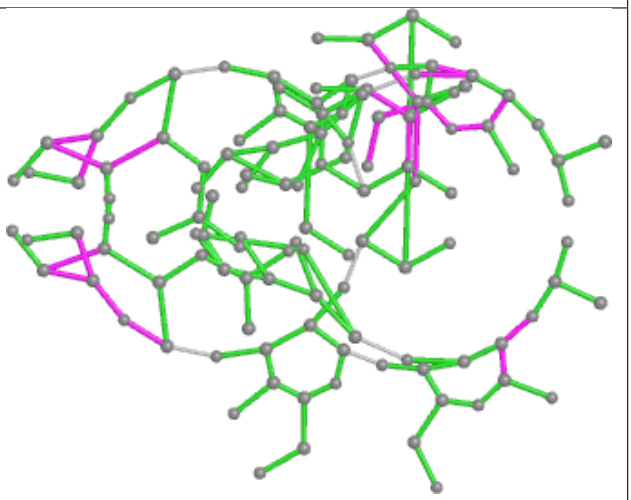


Rings

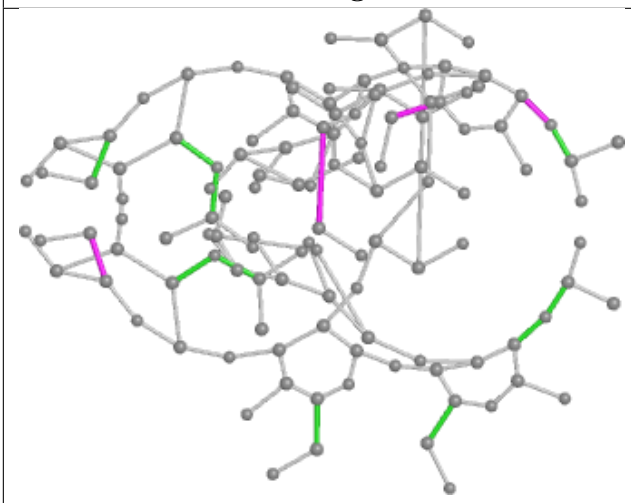
Oligosaccharide Chain G



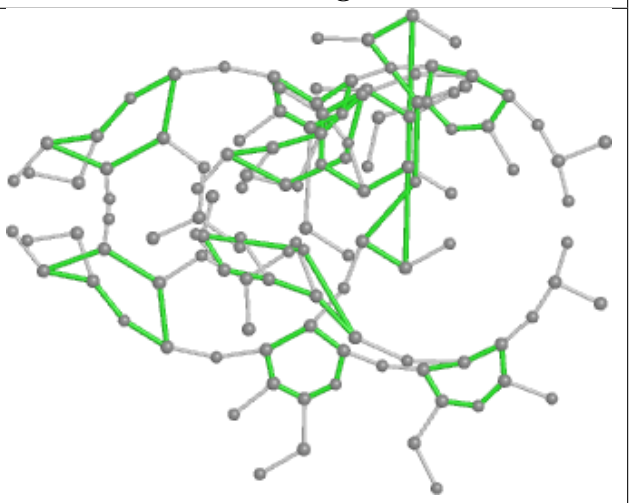
Bond lengths



Bond angles

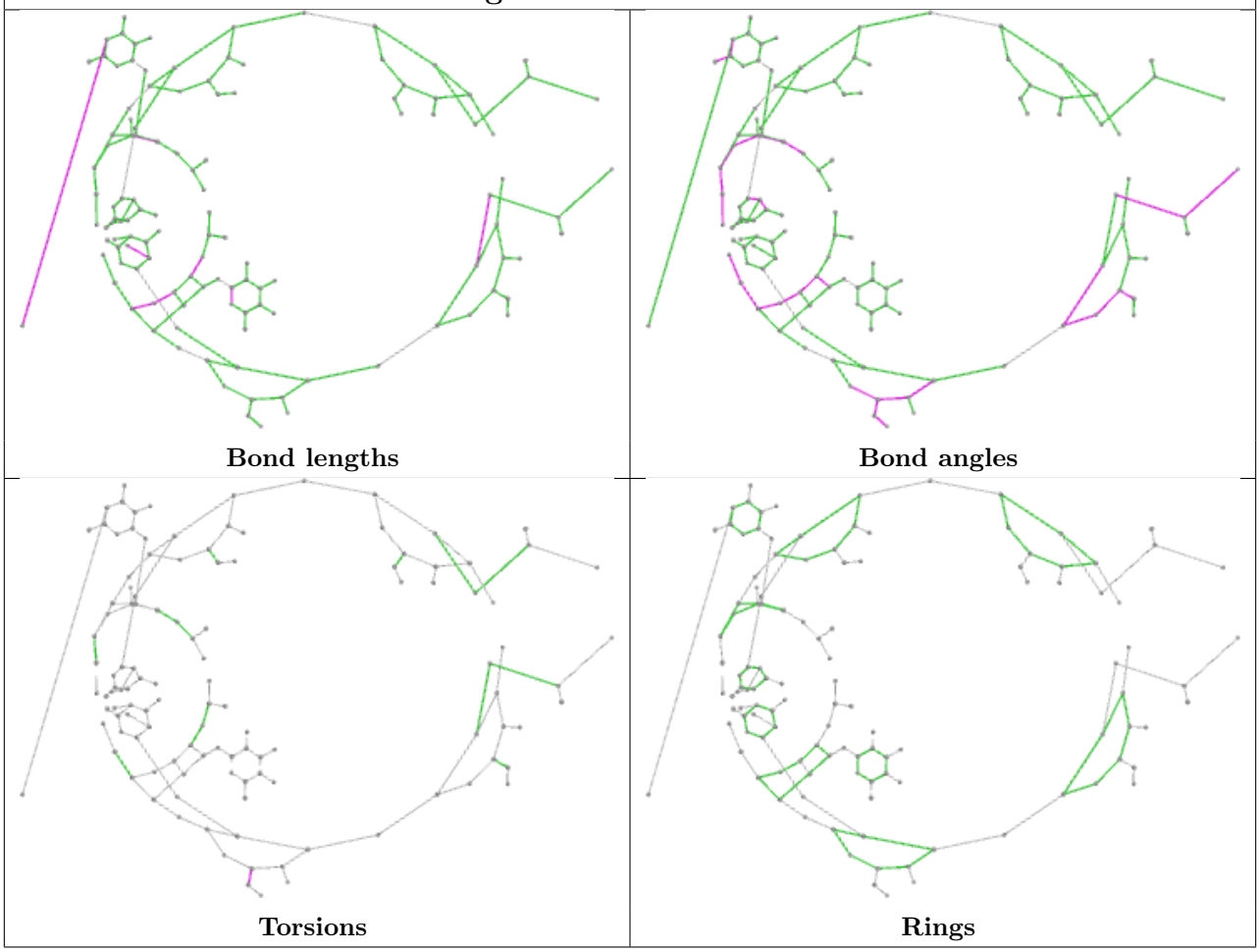


Torsions

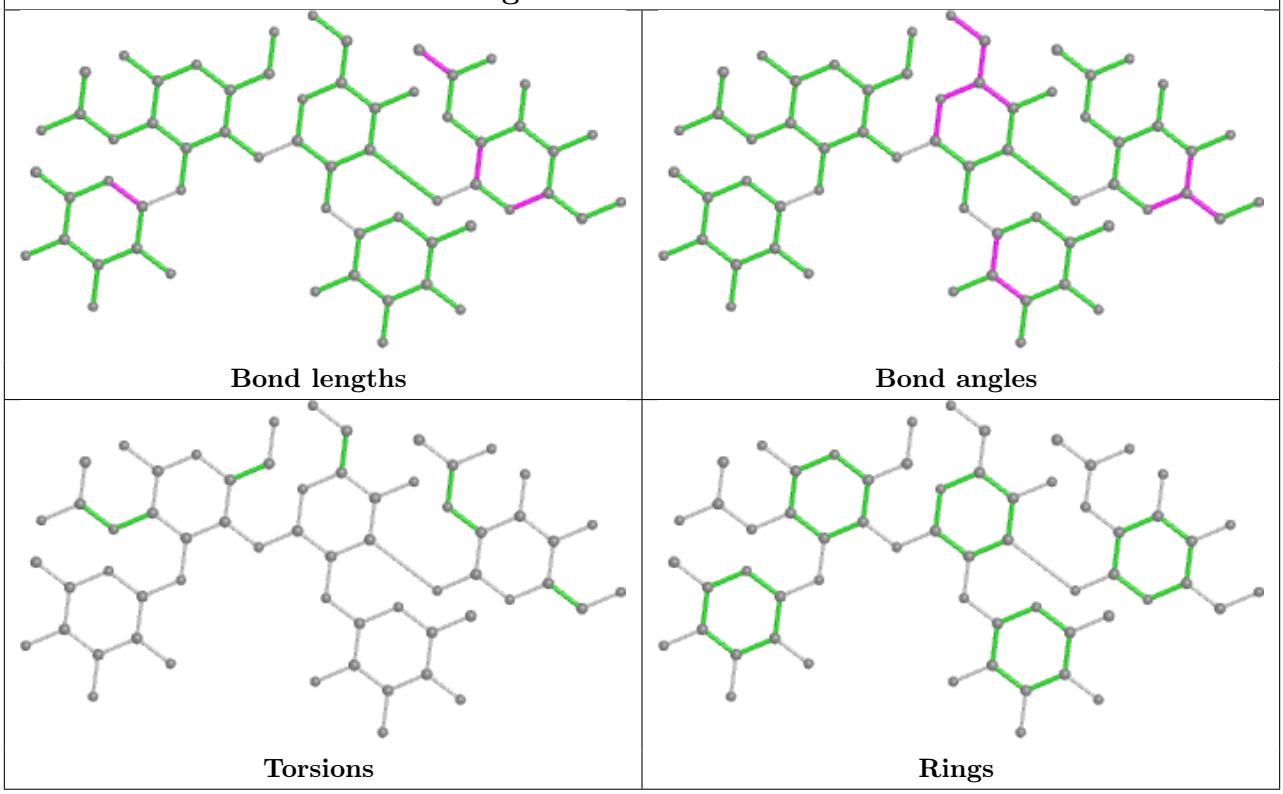


Rings

Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#\|Z\| > 2$
3	PEG	D	201	-	6,6,6	0.49	0	5,5,5	0.32	0
7	PGE	D	202	-	9,9,9	0.53	0	8,8,8	0.37	0
8	GLA	E	203[B]	-	12,12,12	1.13	1 (8%)	17,17,17	1.00	1 (5%)
4	GAL	E	202[A]	-	12,12,12	0.65	0	17,17,17	0.98	0
7	PGE	E	201	-	9,9,9	0.42	0	8,8,8	0.40	0
4	GAL	A	202	-	12,12,12	1.05	1 (8%)	17,17,17	0.72	0
3	PEG	A	201	-	6,6,6	0.39	0	5,5,5	0.34	0
7	PGE	C	202	-	9,9,9	0.42	0	8,8,8	0.32	0
6	MES	C	201	-	12,12,12	6.06	2 (16%)	14,16,16	3.35	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GAL	C	203	-	12,12,12	1.21	1 (8%)	17,17,17	0.87	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
3	PEG	D	201	-	-	0/4/4/4	-
7	PGE	D	202	-	-	0/7/7/7	-
8	GLA	E	203[B]	-	-	0/2/22/22	0/1/1/1
4	GAL	E	202[A]	-	-	0/2/22/22	0/1/1/1
7	PGE	E	201	-	-	0/7/7/7	-
4	GAL	A	202	-	-	0/2/22/22	0/1/1/1
3	PEG	A	201	-	-	1/4/4/4	-
7	PGE	C	202	-	-	1/7/7/7	-
6	MES	C	201	-	-	5/6/14/14	0/1/1/1
4	GAL	C	203	-	-	0/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	201	MES	C7-C8	-18.03	1.03	1.52
6	C	201	MES	C8-S	-10.43	1.62	1.77
4	A	202	GAL	O3-C3	2.47	1.48	1.43
8	E	203[B]	GLA	O2-C2	2.41	1.48	1.43
4	C	203	GAL	O2-C2	2.03	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	201	MES	O3S-S-C8	9.13	120.53	105.77
6	C	201	MES	C2-C3-N4	4.42	116.80	110.10
6	C	201	MES	O3S-S-O2S	-3.57	102.56	111.27
6	C	201	MES	C6-C5-N4	3.16	114.89	110.10
6	C	201	MES	O1-C6-C5	2.80	117.97	111.80
6	C	201	MES	C6-O1-C2	2.58	118.49	109.89
8	E	203[B]	GLA	C1-O5-C5	2.51	118.39	113.66
6	C	201	MES	O2S-S-O1S	-2.46	105.42	113.95

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	MES	C8-C7-N4-C5
6	C	201	MES	C7-C8-S-O2S
6	C	201	MES	C7-C8-S-O3S
3	A	201	PEG	O1-C1-C2-O2
7	C	202	PGE	O1-C1-C2-O2
6	C	201	MES	C7-C8-S-O1S
6	C	201	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	203	GAL	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%)	0.05	7 (6%)	17	15	8, 13, 34, 49	0
1	B	103/103 (100%)	0.44	10 (9%)	7	7	7, 11, 48, 79	0
1	C	103/103 (100%)	-0.12	0	100	100	9, 14, 23, 30	0
1	D	103/103 (100%)	0.05	5 (4%)	29	29	9, 14, 30, 39	0
1	E	103/103 (100%)	-0.27	1 (0%)	82	80	9, 15, 24, 35	0
All	All	515/515 (100%)	0.03	23 (4%)	33	33	7, 14, 31, 79	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	GLY	11.9
1	B	57	HIS	6.9
1	B	58	ILE	6.6
1	B	55	SER	6.2
1	A	55	SER	5.5
1	A	58	ILE	5.3
1	B	56	GLN	5.0
1	B	60	SER	4.0
1	A	59	ASP	3.9
1	D	55	SER	3.5
1	B	59	ASP	3.5
1	D	58	ILE	3.3
1	A	57	HIS	3.1
1	B	53	PRO	2.9
1	A	54	GLY	2.8
1	E	103	ASN	2.7
1	D	13	HIS	2.7
1	D	59	ASP	2.7
1	A	60	SER	2.7
1	A	56	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	103	ASN	2.5
1	D	103	ASN	2.2
1	B	52	VAL	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	A2G	G	4[A]	14/15	0.70	0.30	31,32,34,34	14
2	A2G	G	4[B]	14/15	0.70	0.30	36,39,45,45	14
2	A2G	I	4	14/15	0.71	0.29	39,42,56,57	14
2	FUC	I	3	10/11	0.78	0.17	24,27,30,33	10
2	GAL	G	2[A]	11/12	0.87	0.12	24,27,27,30	11
2	GAL	G	2[B]	11/12	0.87	0.12	22,24,27,34	11
2	FUC	G	3[A]	10/11	0.88	0.13	22,22,23,23	10
2	FUC	G	3[B]	10/11	0.88	0.13	21,24,25,27	10
2	GAL	I	2	11/12	0.89	0.10	25,29,31,34	11
2	NDG	I	1	15/15	0.90	0.08	18,22,28,30	15
2	NDG	G	1[A]	15/15	0.93	0.11	21,22,23,24	15
2	NDG	G	1[B]	15/15	0.93	0.11	14,17,21,24	15
2	NDG	H	1[A]	15/15	0.94	0.10	12,14,16,17	15
2	NDG	H	1[B]	15/15	0.94	0.10	18,20,22,23	15
2	A2G	H	4[A]	14/15	0.95	0.12	12,13,14,14	14
2	A2G	H	4[B]	14/15	0.95	0.12	20,20,21,21	14
2	A2G	F	4[A]	14/15	0.95	0.09	12,14,15,16	14
2	A2G	F	4[B]	14/15	0.95	0.09	13,16,17,18	14
2	FUC	F	3[A]	10/11	0.95	0.08	13,14,16,16	10
2	FUC	F	3[B]	10/11	0.95	0.08	16,17,17,19	10
2	FUC	G	5[A]	10/11	0.96	0.09	17,19,19,19	10
2	FUC	G	5[B]	10/11	0.96	0.09	11,12,13,13	10
2	FUC	F	5[A]	10/11	0.96	0.07	11,12,12,12	10
2	FUC	F	5[B]	10/11	0.96	0.07	15,16,16,17	10
2	FUC	H	3[A]	10/11	0.96	0.10	10,10,11,11	10

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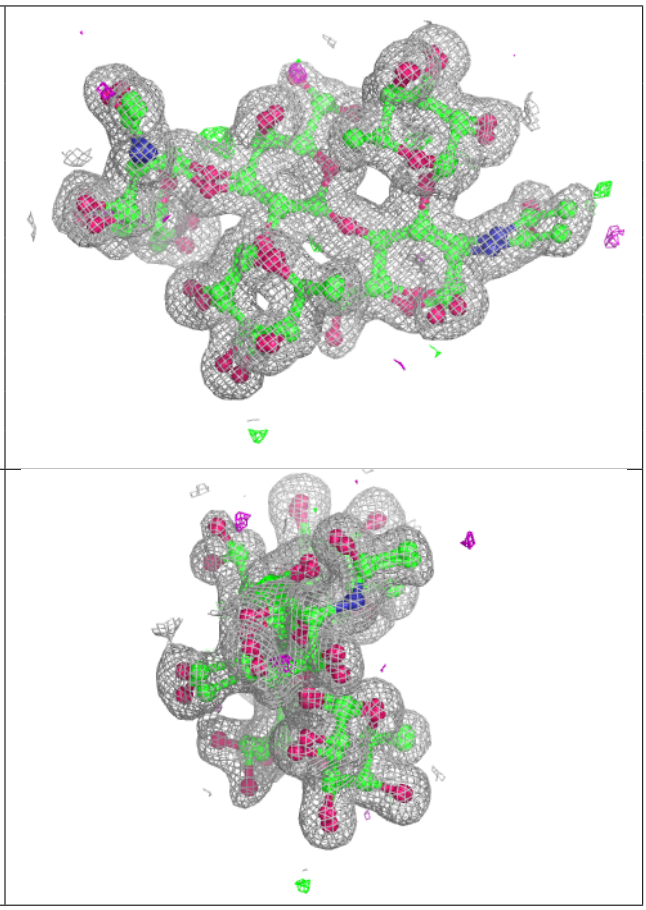
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	H	3[B]	10/11	0.96	0.10	16,16,17,17	10
2	FUC	I	5	10/11	0.96	0.07	16,17,19,20	10
2	NDG	F	1[B]	15/15	0.97	0.09	15,16,19,19	15
2	FUC	H	5[A]	10/11	0.97	0.07	12,13,13,13	10
2	FUC	H	5[B]	10/11	0.97	0.07	17,18,19,19	10
2	GAL	H	2[A]	11/12	0.97	0.07	10,12,12,14	11
2	GAL	H	2[B]	11/12	0.97	0.07	16,18,18,19	11
2	GAL	F	2[A]	11/12	0.97	0.07	12,13,14,14	11
2	GAL	F	2[B]	11/12	0.97	0.07	14,15,15,16	11
2	NDG	F	1[A]	15/15	0.97	0.09	12,14,15,17	15

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.

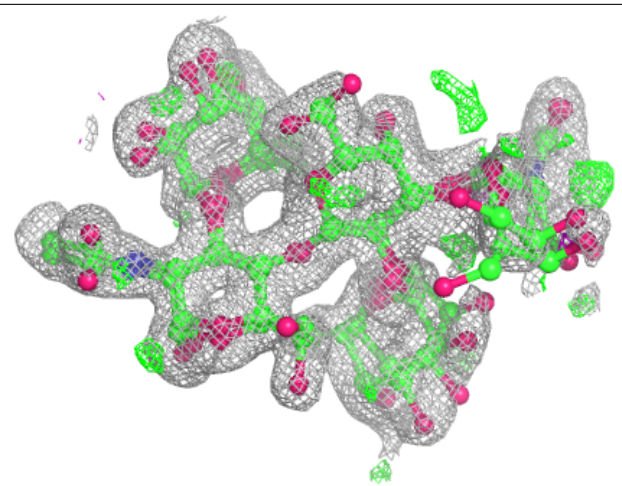
Electron density around Chain F:

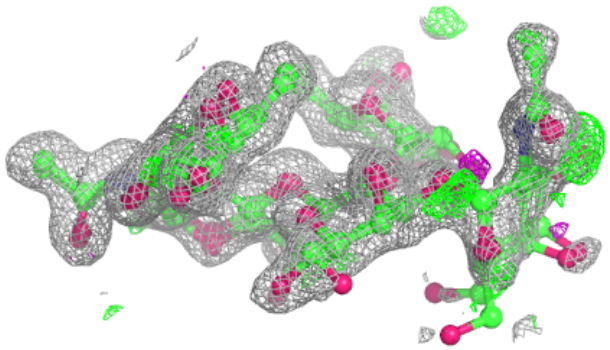
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

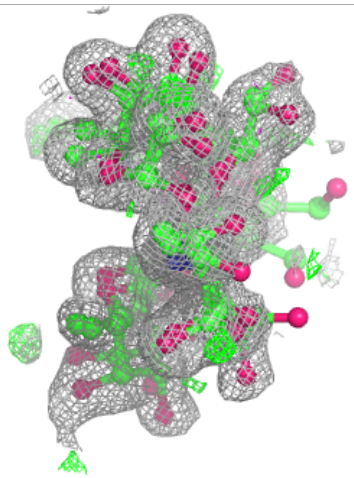


Electron density around Chain G:

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

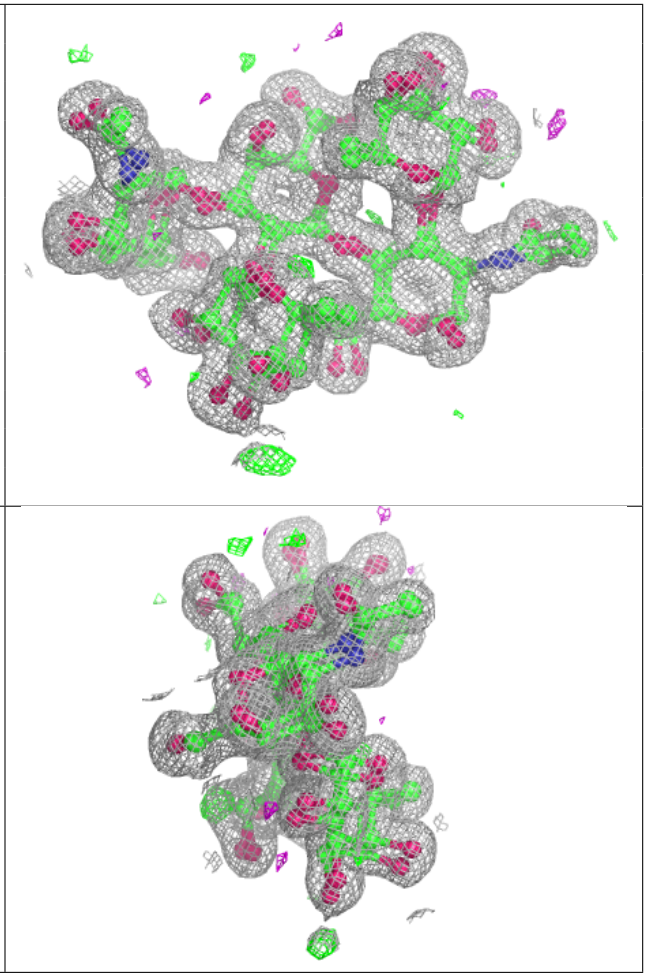






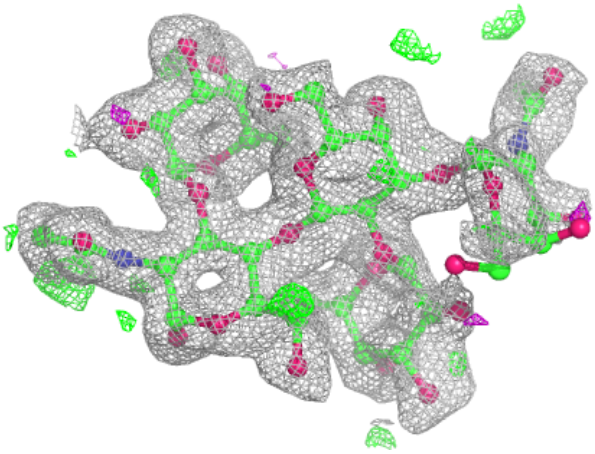
Electron density around Chain H:

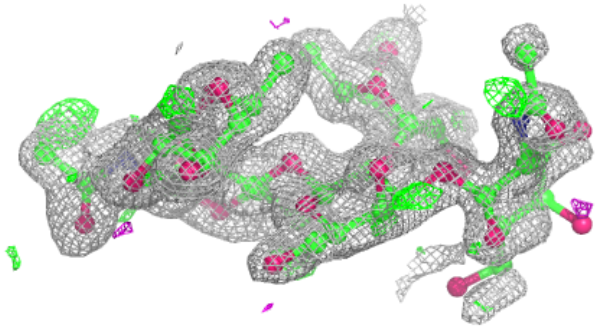
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

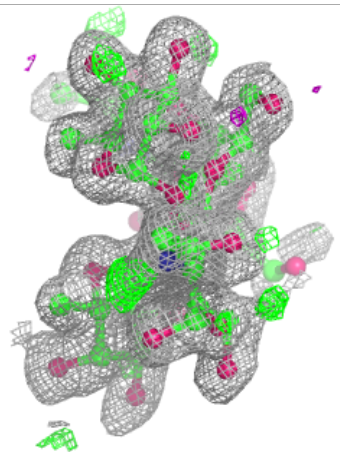


Electron density around Chain I:

$2mF_o$-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
7	PGE	D	202	10/10	0.67	0.20	36,40,44,44	0
3	PEG	A	201	7/7	0.70	0.14	38,40,43,44	0
4	GAL	A	202	12/12	0.73	0.17	26,28,31,34	12
3	PEG	D	201	7/7	0.73	0.14	44,44,49,53	0
4	GAL	C	203	12/12	0.74	0.26	19,27,31,34	12
7	PGE	E	201	10/10	0.75	0.19	37,42,46,50	0
7	PGE	C	202	10/10	0.80	0.19	35,40,44,48	0
6	MES	C	201	12/12	0.89	0.10	24,27,64,65	6
4	GAL	E	202[A]	12/12	0.90	0.12	18,19,20,20	12
8	GLA	E	203[B]	12/12	0.91	0.11	16,18,19,19	12
5	NA	B	201	1/1	0.99	0.07	11,11,11,11	1

6.5 Other polymers (i)

There are no such residues in this entry.