



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 07:13 AM BST

PDB ID : 6K0V
Title : Catalytic domain of GH87 alpha-1,3-glucanase D1069A in complex with tetrasaccharides
Authors : Itoh, T.; Intuy, R.; Suyotha, W.; Hayashi, J.; Yano, S.; Makabe, K.; Wakayama, M.; Hibi, T.
Deposited on : 2019-05-07
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

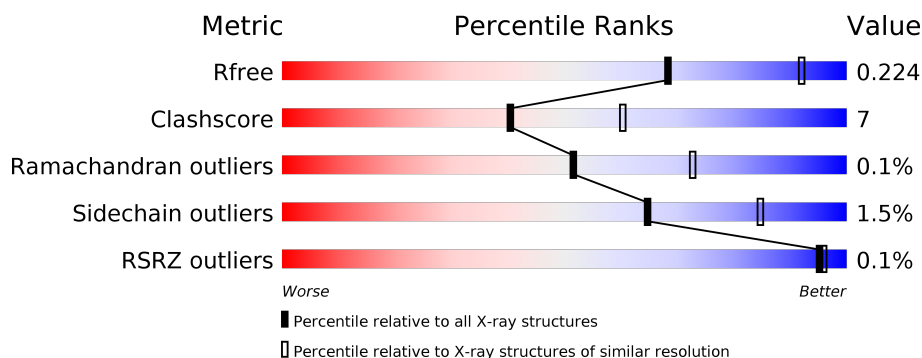
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	573	<div> <div style="width: 82%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>82% 16% ..</div>
1	B	573	<div> <div style="width: 80%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>80% 17% ..</div>
1	C	573	<div> <div style="width: 83%; background-color: green;"></div> <div style="width: 14%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>83% 14% ..</div>
1	D	573	<div> <div style="width: 77%; background-color: green;"></div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>77% 20% .</div>
2	E	3	<div> <div style="width: 100%; background-color: yellow;"></div> </div> <div>100%</div>
2	F	3	<div> <div style="width: 33%; background-color: green;"></div> <div style="width: 33%; background-color: yellow;"></div> <div style="width: 33%; background-color: orange;"></div> </div> <div>33% 33% 33%</div>

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Mol	Chain	Length	Quality of chain
2	H	3	 67% 33%
2	I	3	 33% 67%
2	K	3	 100%
3	G	3	 67% 33%
4	J	2	 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18148 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 Alpha-1,3-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4297	2709	726	852	10			
1	B	562	Total	C	N	O	S	0	2	0
			4310	2717	729	854	10			
1	C	562	Total	C	N	O	S	0	0	0
			4297	2709	726	852	10			
1	D	562	Total	C	N	O	S	0	0	0
			4297	2709	726	852	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	715	ALA	-	expression tag	UNP A0A068PS59
A	716	GLY	-	expression tag	UNP A0A068PS59
A	717	SER	-	expression tag	UNP A0A068PS59
A	718	VAL	-	expression tag	UNP A0A068PS59
A	719	ASP	-	expression tag	UNP A0A068PS59
A	1069	ALA	ASP	engineered mutation	UNP A0A068PS59
B	715	ALA	-	expression tag	UNP A0A068PS59
B	716	GLY	-	expression tag	UNP A0A068PS59
B	717	SER	-	expression tag	UNP A0A068PS59
B	718	VAL	-	expression tag	UNP A0A068PS59
B	719	ASP	-	expression tag	UNP A0A068PS59
B	1069	ALA	ASP	engineered mutation	UNP A0A068PS59
C	715	ALA	-	expression tag	UNP A0A068PS59
C	716	GLY	-	expression tag	UNP A0A068PS59
C	717	SER	-	expression tag	UNP A0A068PS59
C	718	VAL	-	expression tag	UNP A0A068PS59
C	719	ASP	-	expression tag	UNP A0A068PS59
C	1069	ALA	ASP	engineered mutation	UNP A0A068PS59
D	715	ALA	-	expression tag	UNP A0A068PS59
D	716	GLY	-	expression tag	UNP A0A068PS59
D	717	SER	-	expression tag	UNP A0A068PS59

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Chain	Residue	Modelled	Actual	Comment	Reference
D	718	VAL	-	expression tag	UNP A0A068PS59
D	719	ASP	-	expression tag	UNP A0A068PS59
D	1069	ALA	ASP	engineered mutation	UNP A0A068PS59

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			34	18	16			
2	F	3	Total	C	O	0	0	0
			34	18	16			
2	H	3	Total	C	O	0	0	0
			34	18	16			
2	I	3	Total	C	O	0	0	0
			34	18	16			
2	K	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	J	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	170	Total	O	0	0
			170	170		

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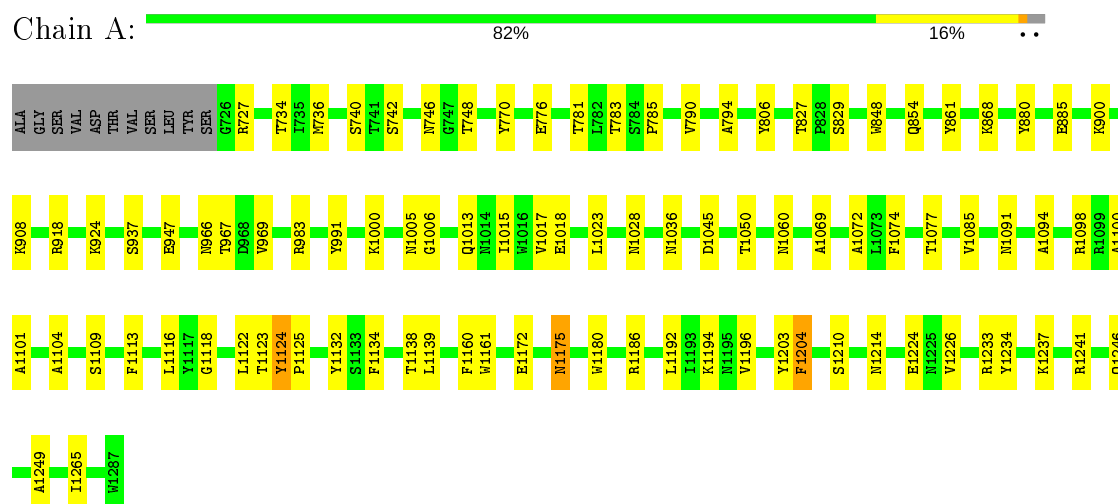
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	134	Total 134	O 134	0	0
7	C	155	Total 155	O 155	0	0
7	D	142	Total 142	O 142	0	0

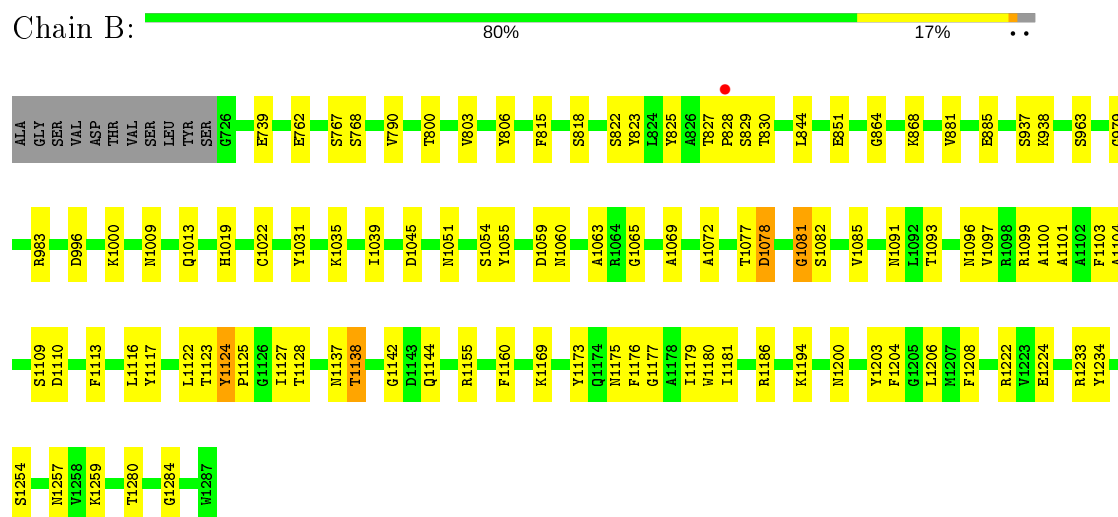
3 Residue-property plots

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.

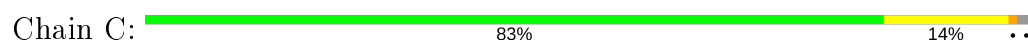
• Molecule 1: Alpha-1,3-glucanase

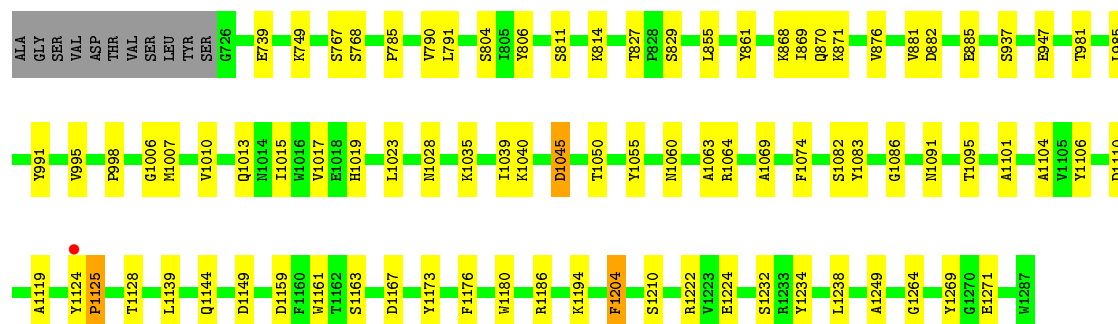


• Molecule 1: Alpha-1,3-glucanase



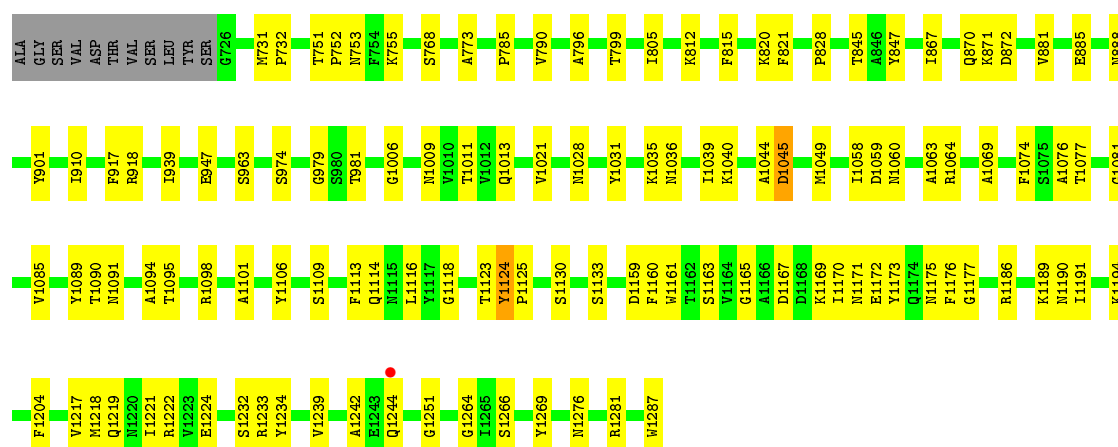
• Molecule 1: Alpha-1,3-glucanase





- Molecule 1: Alpha-1,3-glucanase

Chain D: 77% 20%



- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain E: 100%



- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain F: 33% 33% 33%



- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain H: 67% 33%

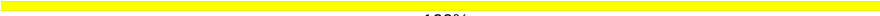


- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain I:  33% 67%

GLC1
GLC2
GLC3

- Molecule 2: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain K:  100%

GLC1
GLC2
GLC3

- Molecule 3: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain G:  67% 33%

GLC1
GLC2
GLC3

- Molecule 4: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain J:  50% 50%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.86Å 132.62Å 131.77Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	46.91 – 2.50 46.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.91-2.50) 95.3 (46.91-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.179 , 0.225 0.179 , 0.224	Depositor DCC
R_{free} test set	4409 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.227 for -h,-l,-k 0.156 for -h,l,k 0.135 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18148	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, CA, BGC, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/4397	0.59	0/5991
1	B	0.43	0/4416	0.60	0/6016
1	C	0.44	0/4397	0.62	0/5991
1	D	0.43	0/4397	0.59	0/5991
All	All	0.44	0/17607	0.60	0/23989

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4297	0	4096	63	0
1	B	4310	0	4113	59	0
1	C	4297	0	4096	57	0
1	D	4297	0	4096	67	0
2	E	34	0	30	0	0
2	F	34	0	30	1	0
2	H	34	0	30	2	0
2	I	34	0	30	0	0
2	K	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	34	0	30	0	0
4	J	23	0	21	2	0
5	A	30	0	0	0	0
5	B	25	0	0	0	0
5	C	30	0	0	1	0
5	D	30	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	170	0	0	5	0
7	B	134	0	0	4	0
7	C	155	0	0	2	0
7	D	142	0	0	2	0
All	All	18148	0	16602	247	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 7.

The worst 5 of 247 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:B:1138:THR:O	1:B:1186[B]:ARG:NH1	1.85	1.10
1:A:1124:TYR:HH	1:A:1161:TRP:HE1	1.03	1.00
1:C:1124:TYR:HH	1:C:1180:TRP:HZ3	1.11	0.93
1:C:1161:TRP:HH2	4:J:2:GLC:H3	1.37	0.89
1:A:790:VAL:HB	1:A:885:GLU:HG3	1.58	0.84

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	560/573 (98%)	527 (94%)	33 (6%)	0	100	100
1	B	562/573 (98%)	526 (94%)	34 (6%)	2 (0%)	34	54
1	C	560/573 (98%)	522 (93%)	38 (7%)	0	100	100
1	D	560/573 (98%)	525 (94%)	34 (6%)	1 (0%)	47	68
All	All	2242/2292 (98%)	2100 (94%)	139 (6%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1078	ASP
1	D	974	SER
1	B	1081	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/461 (98%)	446 (99%)	6 (1%)	69	87
1	B	454/461 (98%)	446 (98%)	8 (2%)	59	81
1	C	452/461 (98%)	446 (99%)	6 (1%)	69	87
1	D	452/461 (98%)	445 (98%)	7 (2%)	65	85
All	All	1810/1844 (98%)	1783 (98%)	27 (2%)	65	85

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1138	THR
1	C	937	SER
1	D	1204	PHE
1	B	1222	ARG
1	A	1175	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1013	GLN
1	C	1137	ASN
1	B	1137	ASN
1	B	919	GLN
1	C	919	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	E	1	2	12,12,12	1.37	2 (16%)	17,17,17	1.87	4 (23%)
2	GLC	E	2	2	11,11,12	0.73	0	15,15,17	1.20	2 (13%)
2	GLC	E	3	2	11,11,12	0.62	0	15,15,17	1.21	2 (13%)
2	GLC	F	1	2	12,12,12	0.96	1 (8%)	17,17,17	1.20	3 (17%)
2	GLC	F	2	2	11,11,12	0.59	0	15,15,17	1.42	3 (20%)
2	GLC	F	3	2	11,11,12	0.67	0	15,15,17	0.93	0
3	BGC	G	1	3	12,12,12	0.55	0	17,17,17	0.87	0
3	GLC	G	2	3	11,11,12	0.67	0	15,15,17	0.73	0
3	GLC	G	3	3	11,11,12	0.70	0	15,15,17	0.92	1 (6%)
2	GLC	H	1	2	12,12,12	0.88	1 (8%)	17,17,17	2.20	6 (35%)
2	GLC	H	2	2	11,11,12	0.53	0	15,15,17	1.23	2 (13%)
2	GLC	H	3	2	11,11,12	0.66	0	15,15,17	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	I	1	2	12,12,12	1.01	1 (8%)	17,17,17	2.29	6 (35%)
2	GLC	I	2	2	11,11,12	0.62	0	15,15,17	0.76	0
2	GLC	I	3	2	11,11,12	0.58	0	15,15,17	1.23	2 (13%)
4	GLC	J	1	4	12,12,12	0.91	1 (8%)	17,17,17	2.09	5 (29%)
4	GLC	J	2	4	11,11,12	1.44	2 (18%)	15,15,17	2.86	6 (40%)
2	GLC	K	1	2	12,12,12	0.79	0	17,17,17	1.84	5 (29%)
2	GLC	K	2	2	11,11,12	0.53	0	15,15,17	1.02	2 (13%)
2	GLC	K	3	2	11,11,12	0.62	0	15,15,17	1.14	2 (13%)

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	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	0/2/19/22	0/1/1/1
3	BGC	G	1	3	-	2/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	G	3	3	-	2/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	1/2/19/22	0/1/1/1
4	GLC	J	1	4	-	0/2/22/22	0/1/1/1
4	GLC	J	2	4	-	0/2/19/22	0/1/1/1
2	GLC	K	1	2	-	2/2/22/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	GLC	C2-C3	3.30	1.57	1.52
2	E	1	GLC	O5-C1	-2.72	1.36	1.42
4	J	1	GLC	O5-C5	-2.50	1.38	1.44
4	J	2	GLC	O5-C1	-2.37	1.39	1.43
2	H	1	GLC	O5-C5	-2.29	1.38	1.44

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	GLC	O3-C3-C2	6.77	122.95	109.99
4	J	2	GLC	C1-C2-C3	6.15	117.23	109.67
2	I	1	GLC	O3-C3-C4	-4.65	99.59	110.35
2	I	1	GLC	C4-C3-C2	-4.35	103.23	110.82
4	J	1	GLC	C4-C3-C2	-4.26	103.39	110.82

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	GLC	O5-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	K	1	GLC	C4-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6

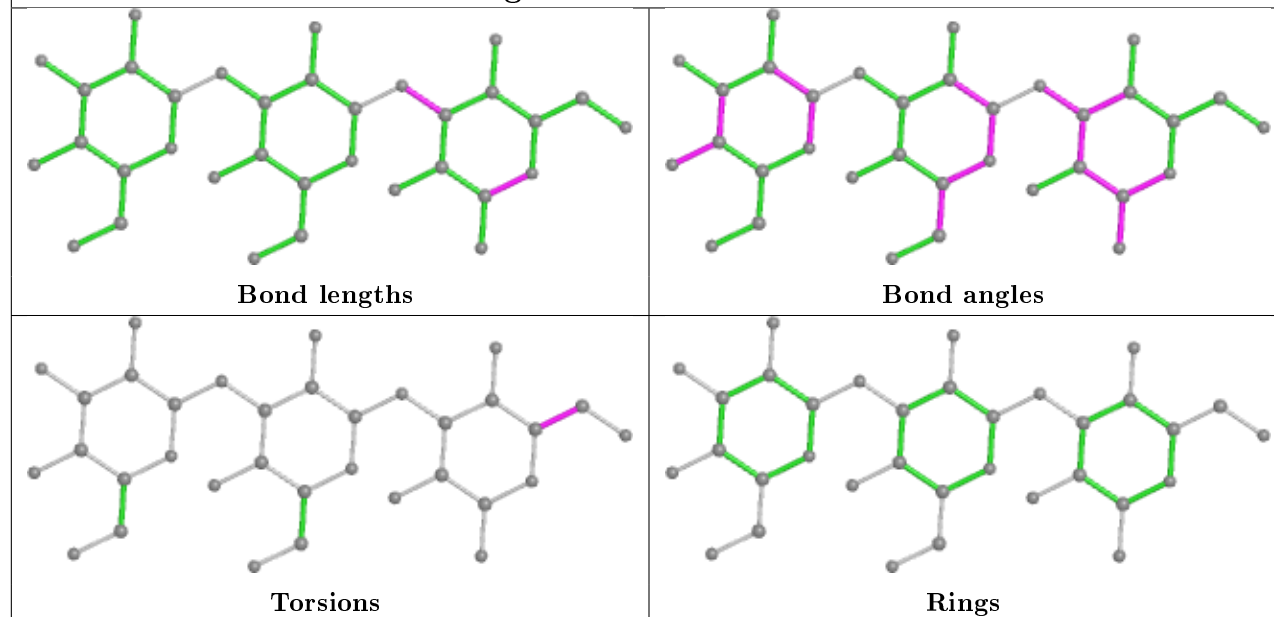
There are no ring outliers.

3 monomers are involved in 5 short contacts:

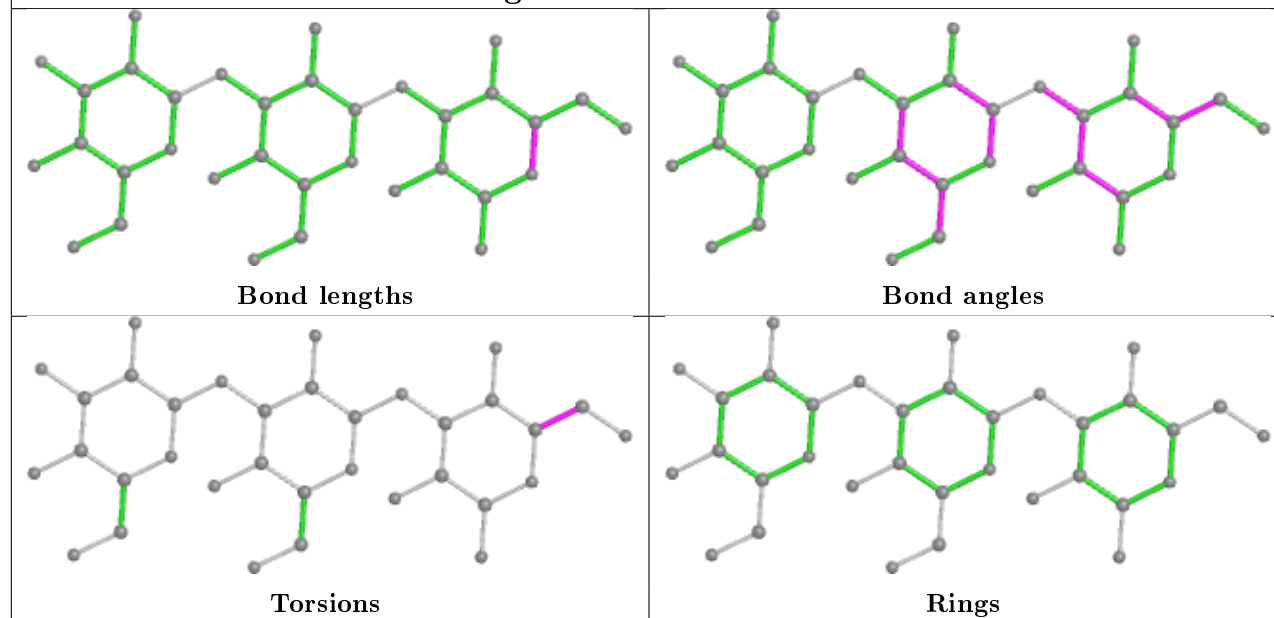
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	GLC	2	0
2	F	1	GLC	1	0
4	J	2	GLC	2	0

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

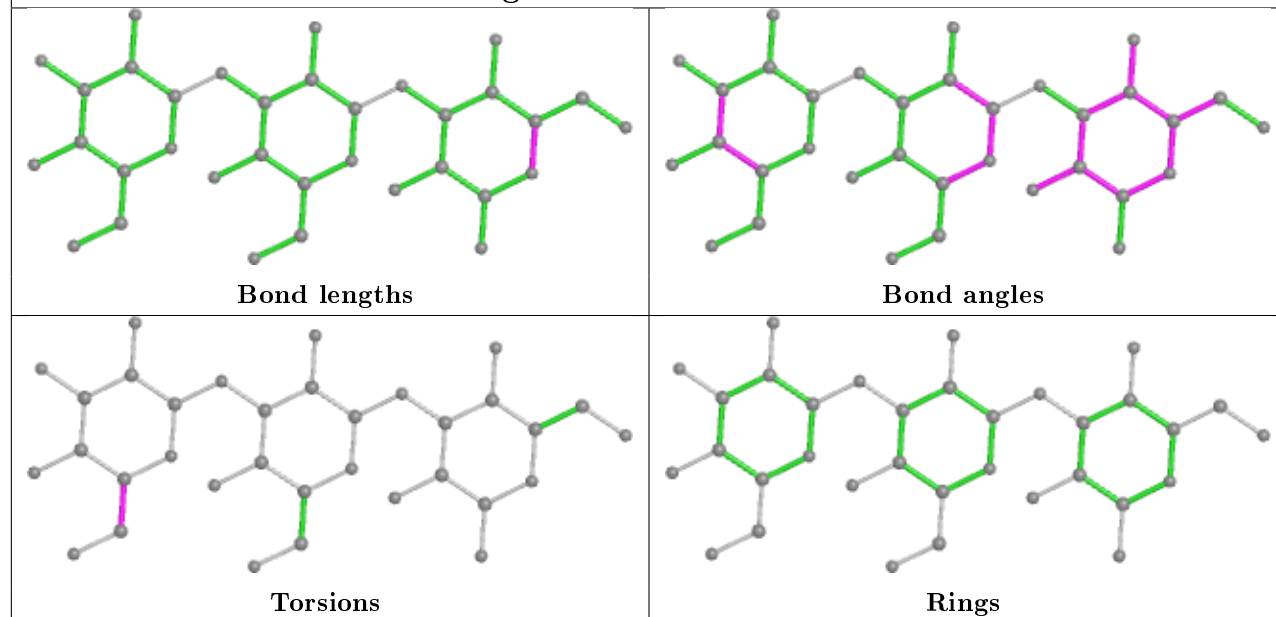
Oligosaccharide Chain E



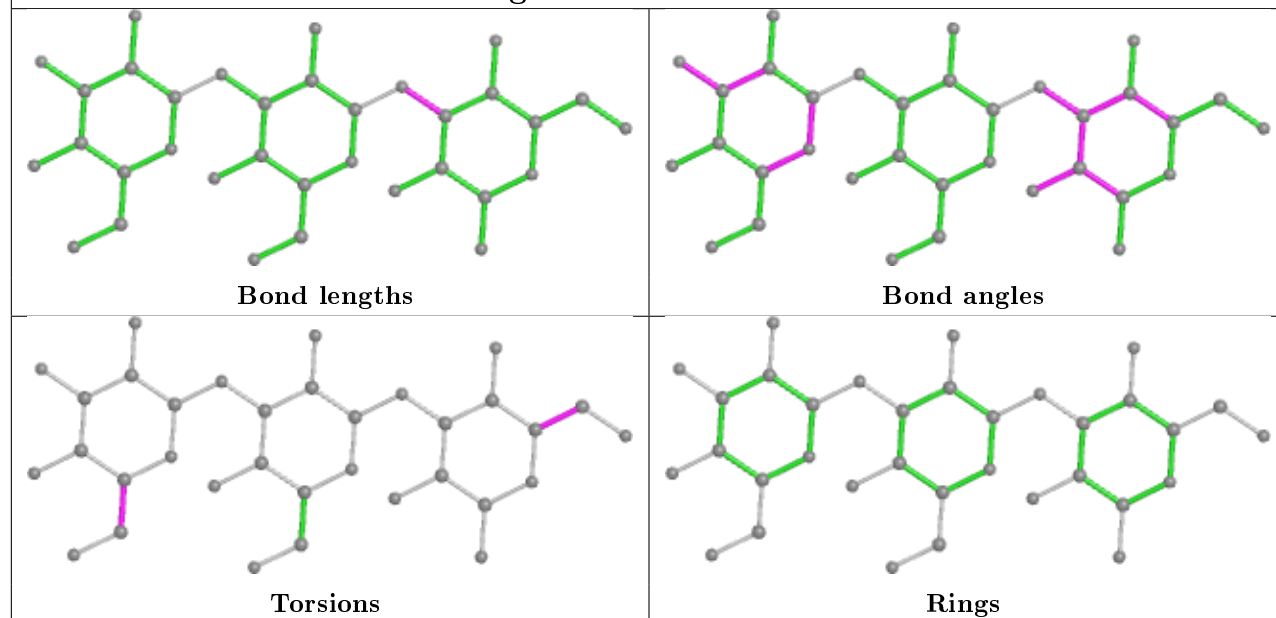
Oligosaccharide Chain F



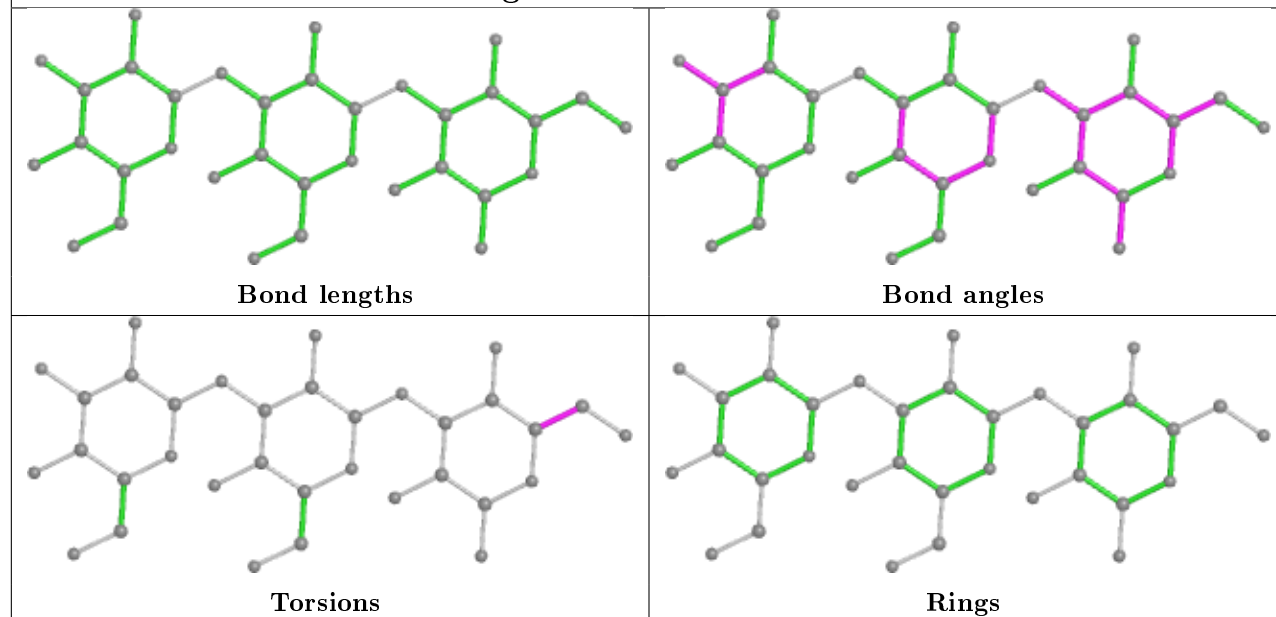
Oligosaccharide Chain H



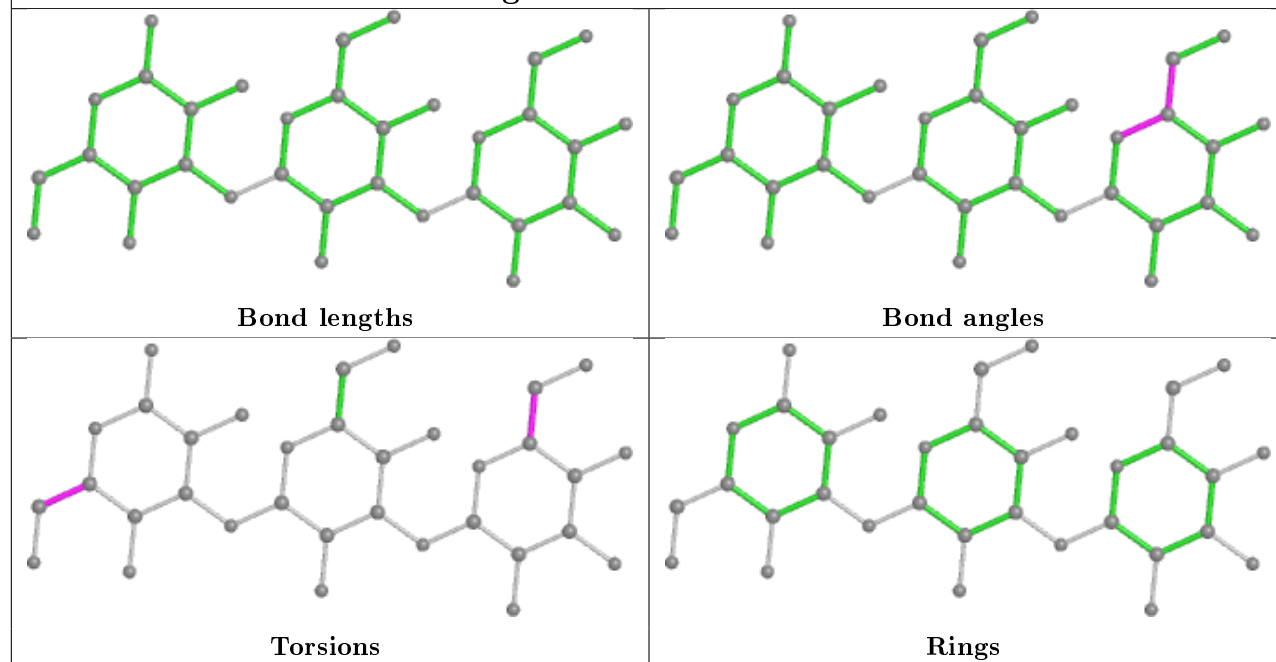
Oligosaccharide Chain I

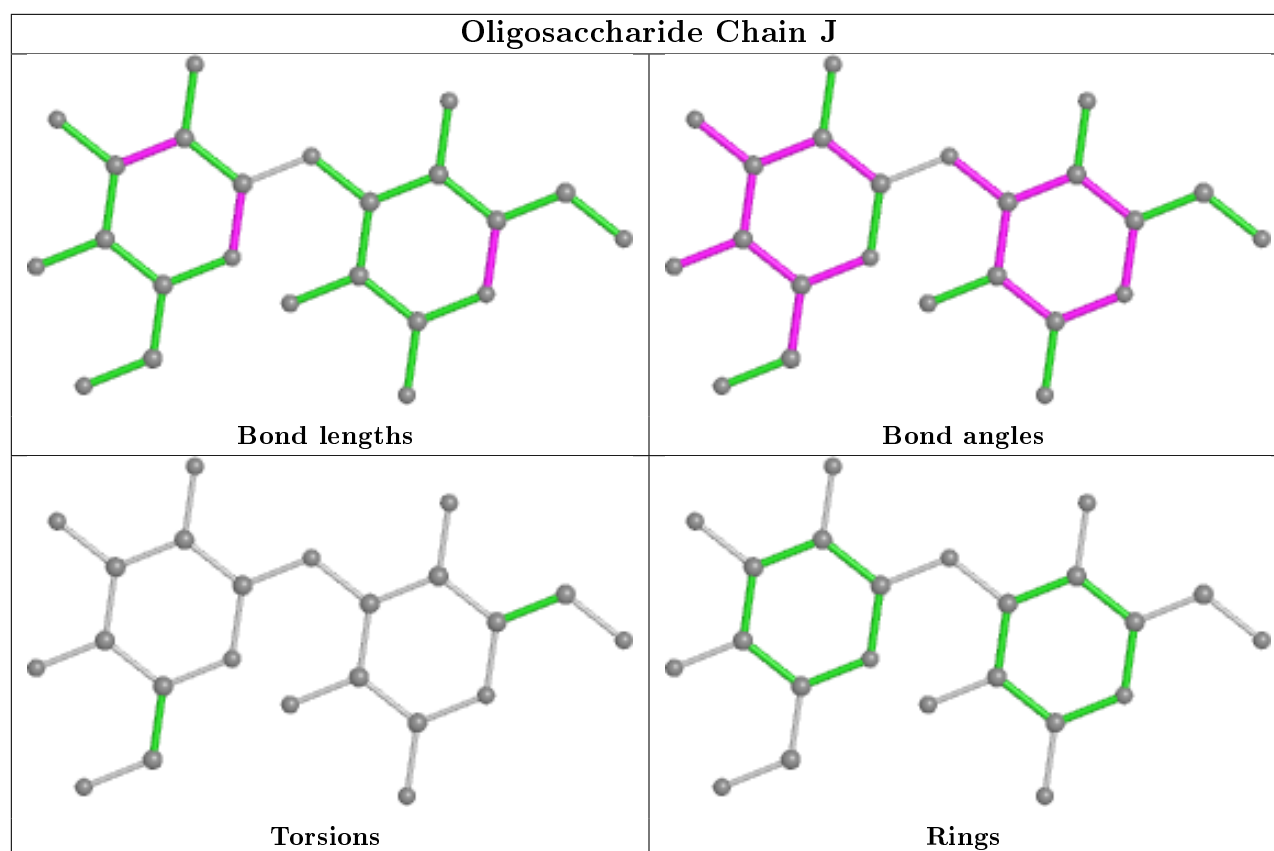


Oligosaccharide Chain K



Oligosaccharide Chain G





5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	$\# Z > 2$
5	SO4	D	2002	-	4,4,4	0.14	0	6,6,6	0.14	0
5	SO4	D	2005	-	4,4,4	0.16	0	6,6,6	0.14	0
5	SO4	C	2003	-	4,4,4	0.15	0	6,6,6	0.14	0
5	SO4	D	2004	-	4,4,4	0.22	0	6,6,6	0.21	0
5	SO4	C	2005	-	4,4,4	0.22	0	6,6,6	0.17	0
5	SO4	C	2006	-	4,4,4	0.22	0	6,6,6	0.27	0
5	SO4	C	2001	-	4,4,4	0.19	0	6,6,6	0.51	0
5	SO4	D	2001	-	4,4,4	0.12	0	6,6,6	0.27	0
5	SO4	B	2004	-	4,4,4	0.16	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	C	2004	-	4,4,4	0.24	0	6,6,6	0.16	0
5	SO4	B	2003	-	4,4,4	0.28	0	6,6,6	0.18	0
5	SO4	A	2001	-	4,4,4	0.11	0	6,6,6	0.31	0
5	SO4	B	2002	-	4,4,4	0.24	0	6,6,6	0.26	0
5	SO4	B	2001	-	4,4,4	0.12	0	6,6,6	0.29	0
5	SO4	B	2005	-	4,4,4	0.14	0	6,6,6	0.23	0
5	SO4	A	2004	-	4,4,4	0.26	0	6,6,6	0.34	0
5	SO4	A	2003	-	4,4,4	0.19	0	6,6,6	0.16	0
5	SO4	D	2003	-	4,4,4	0.15	0	6,6,6	0.19	0
5	SO4	A	2005	-	4,4,4	0.19	0	6,6,6	0.17	0
5	SO4	C	2002	-	4,4,4	0.18	0	6,6,6	0.22	0
5	SO4	A	2002	-	4,4,4	0.22	0	6,6,6	0.19	0
5	SO4	A	2006	-	4,4,4	0.16	0	6,6,6	0.18	0
5	SO4	D	2006	-	4,4,4	0.17	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2002	SO4	1	0
5	C	2006	SO4	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	562/573 (98%)	-0.20	0 100 100	21, 32, 46, 61	0
1	B	562/573 (98%)	-0.14	1 (0%) 95 95	26, 36, 50, 73	0
1	C	562/573 (98%)	-0.21	1 (0%) 95 95	23, 33, 46, 67	0
1	D	562/573 (98%)	-0.18	1 (0%) 95 95	26, 35, 51, 67	0
All	All	2248/2292 (98%)	-0.18	3 (0%) 95 96	21, 34, 49, 73	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	828	PRO	2.7
1	D	1244	GLN	2.5
1	C	1124	TYR	2.3

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
4	GLC	J	2	11/12	0.64	0.29	63,65,70,73	0
2	GLC	I	1	12/12	0.85	0.24	52,63,68,72	0
4	GLC	J	1	12/12	0.90	0.16	46,58,62,65	0
2	GLC	H	2	11/12	0.91	0.14	47,60,66,66	0

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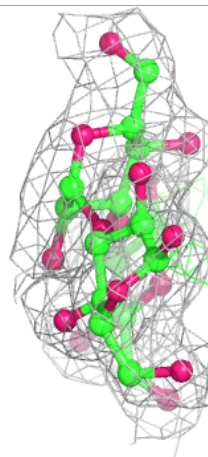
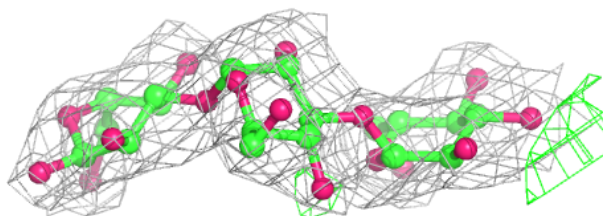
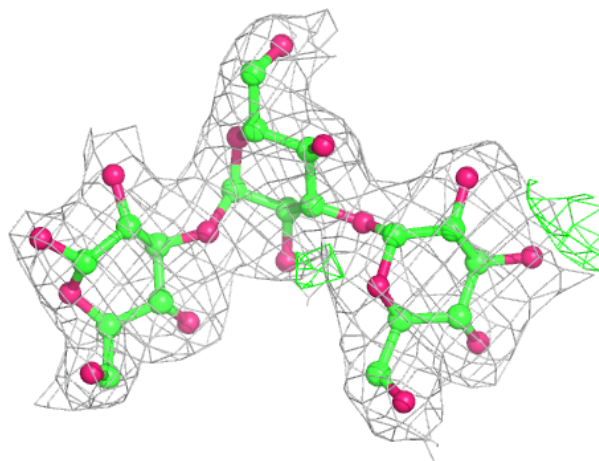
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	K	1	12/12	0.91	0.18	51,59,66,67	0
2	GLC	H	1	12/12	0.92	0.17	47,62,68,69	0
2	GLC	K	3	11/12	0.94	0.13	40,45,49,51	0
2	GLC	I	2	11/12	0.94	0.12	44,50,59,60	0
3	BGC	G	1	12/12	0.94	0.16	45,52,57,59	0
2	GLC	I	3	11/12	0.94	0.13	46,53,60,62	0
2	GLC	H	3	11/12	0.94	0.13	51,59,61,63	0
2	GLC	F	1	12/12	0.94	0.13	36,50,54,61	0
2	GLC	E	3	11/12	0.95	0.12	30,35,39,39	0
2	GLC	E	1	12/12	0.95	0.17	37,40,46,47	0
2	GLC	F	3	11/12	0.96	0.13	35,39,43,44	0
2	GLC	F	2	11/12	0.96	0.10	35,39,45,45	0
3	GLC	G	3	11/12	0.97	0.14	34,40,45,45	0
2	GLC	E	2	11/12	0.97	0.12	31,34,40,46	0
2	GLC	K	2	11/12	0.97	0.10	37,45,50,53	0
3	GLC	G	2	11/12	0.98	0.15	39,43,45,49	0

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

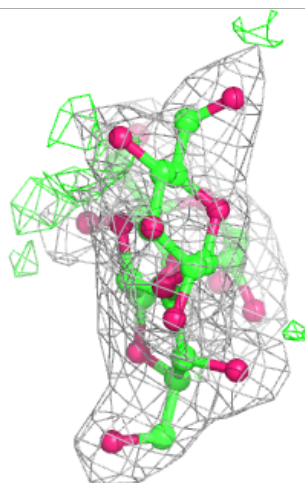
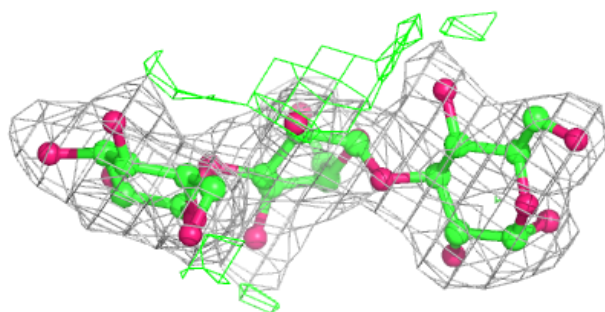
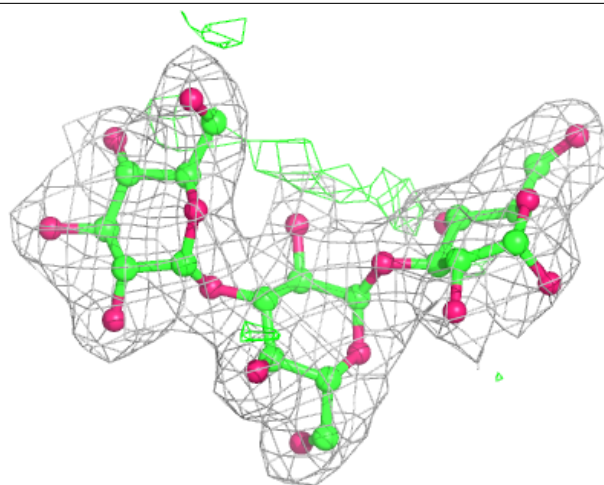
Electron density around Chain E:

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



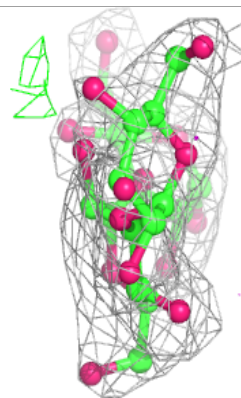
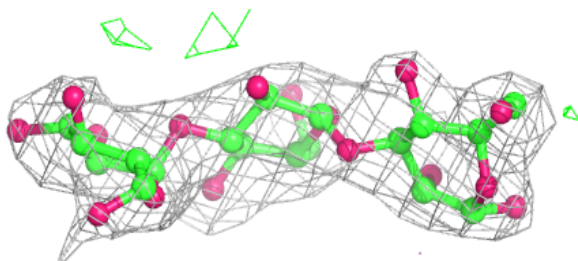
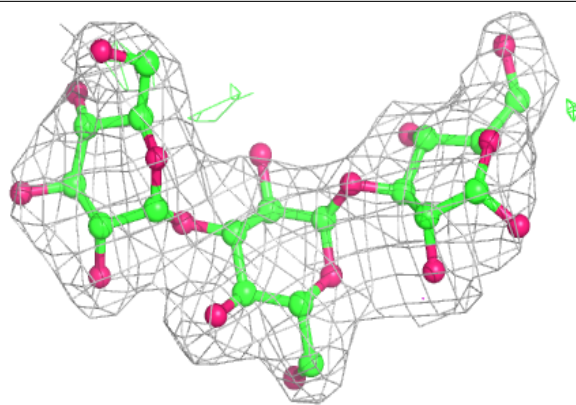
Electron density around Chain F:

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



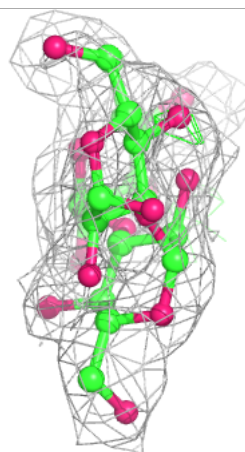
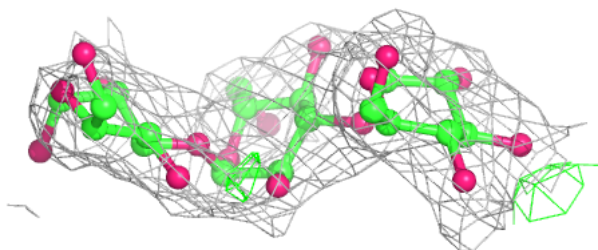
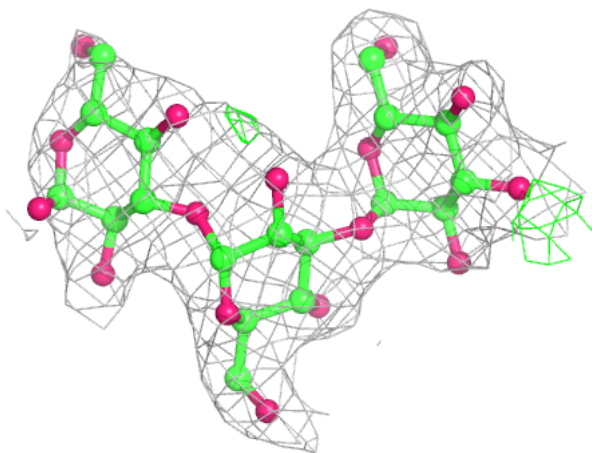
Electron density around Chain H:

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



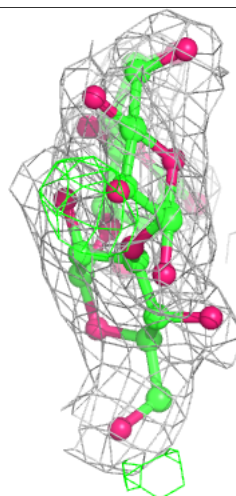
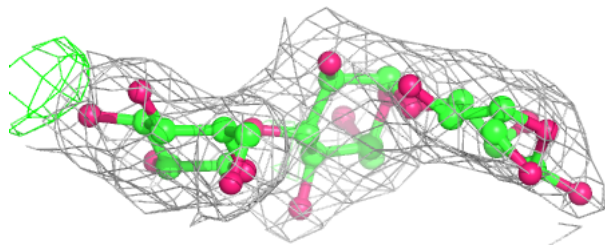
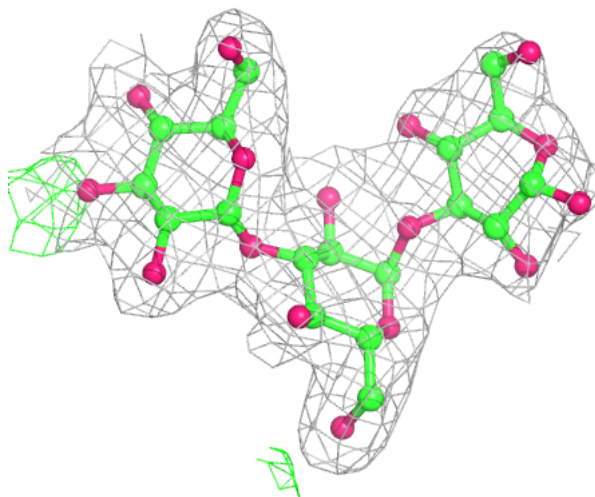
Electron density around Chain I:

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



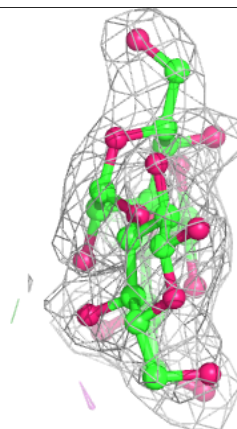
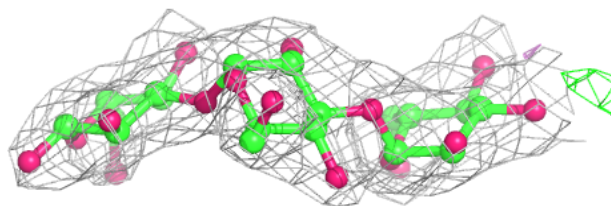
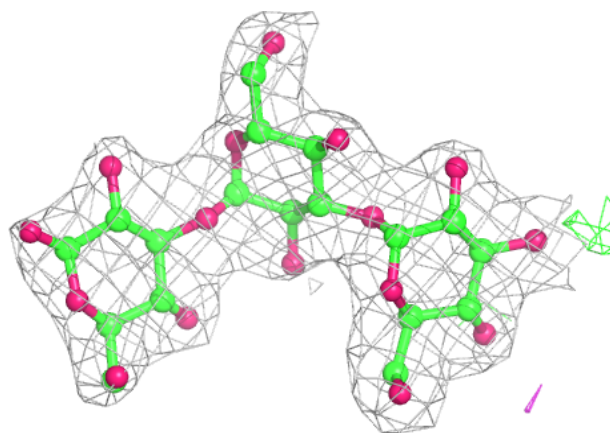
Electron density around Chain K:

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

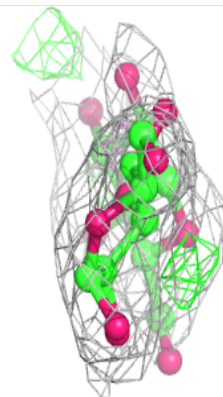
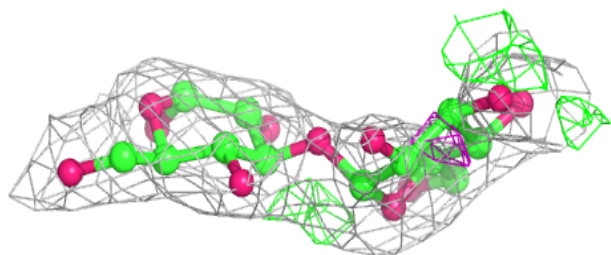
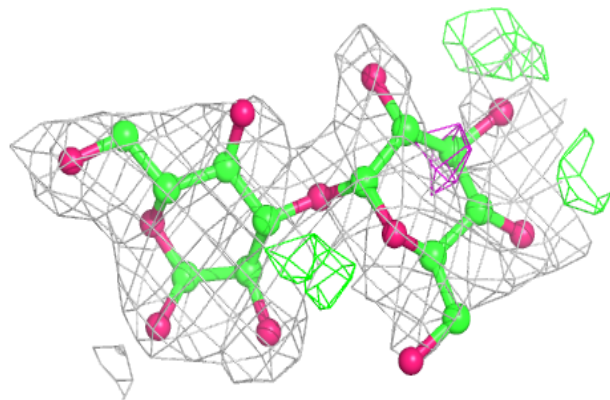


Electron density around Chain G:

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

**Electron density around Chain J:**

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



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(\AA^2)	Q<0.9
5	SO4	A	2003	5/5	0.79	0.35	75,85,93,103	0
5	SO4	A	2005	5/5	0.86	0.22	69,77,93,97	0
5	SO4	B	2002	5/5	0.90	0.35	66,75,77,95	0
5	SO4	C	2005	5/5	0.92	0.16	57,64,86,88	0
5	SO4	D	2003	5/5	0.93	0.22	67,81,83,88	0
5	SO4	B	2005	5/5	0.94	0.12	62,65,81,82	0
5	SO4	B	2004	5/5	0.94	0.22	75,83,92,97	0
5	SO4	B	2003	5/5	0.94	0.12	43,51,66,79	0
5	SO4	C	2006	5/5	0.94	0.17	54,54,59,61	0
5	SO4	D	2004	5/5	0.95	0.19	46,57,70,77	0
5	SO4	D	2005	5/5	0.95	0.10	73,74,86,87	0
5	SO4	C	2004	5/5	0.95	0.17	50,51,56,61	0
5	SO4	A	2002	5/5	0.95	0.13	61,64,76,85	0
5	SO4	D	2006	5/5	0.95	0.12	51,57,65,69	0
5	SO4	A	2004	5/5	0.96	0.17	49,50,61,62	0
5	SO4	C	2002	5/5	0.96	0.10	56,58,65,73	0
5	SO4	D	2002	5/5	0.96	0.22	69,70,75,80	0
5	SO4	A	2006	5/5	0.96	0.12	54,65,67,72	0
5	SO4	C	2003	5/5	0.96	0.12	67,69,76,79	0
5	SO4	A	2001	5/5	0.98	0.12	42,42,50,54	0
6	CA	D	2007	1/1	0.99	0.10	31,31,31,31	0
5	SO4	D	2001	5/5	0.99	0.13	31,33,38,52	0
6	CA	B	2006	1/1	0.99	0.14	26,26,26,26	0
5	SO4	C	2001	5/5	0.99	0.13	35,35,46,46	0
5	SO4	B	2001	5/5	0.99	0.10	38,39,44,51	0
6	CA	A	2007	1/1	1.00	0.15	21,21,21,21	0
6	CA	C	2007	1/1	1.00	0.14	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.