Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2024 – 11:54 pm GMT

PDB ID	:	6GYA
Title	:	Amylase in complex with branched ligand
Authors	:	Agirre, J.; Moroz, O.; Meier, S.; Brask, J.; Munch, A.; Hoff, T.; Andersen, C.; Wilson, K.S.; Davies, G.J.
Deposited on	:	2018-06-28
Resolution	:	2.95 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:

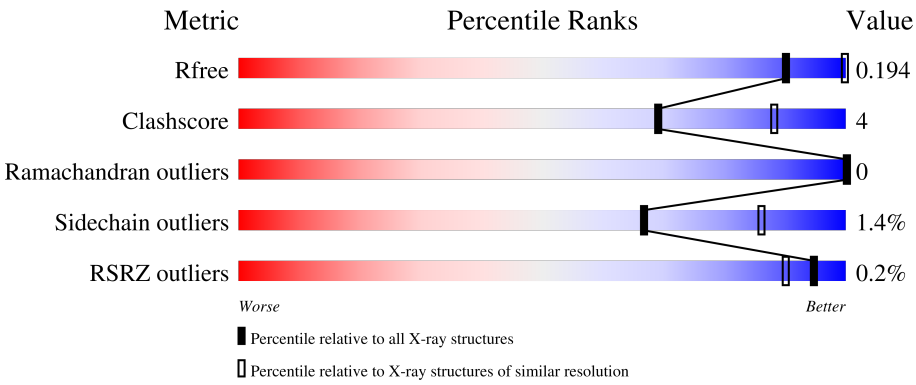
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	484	91% 8% •
1	B	484	% 90% 9% ••
1	C	484	86% 13% •
1	D	484	89% 11% •
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	G	3	100%
2	I	3	100%
2	K	3	100%
3	F	2	100%
3	H	2	100%
3	J	2	100%
3	L	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15702 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.

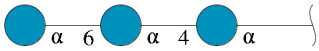
- Molecule 1 is a protein called A-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	481	3788	2390	637	745	16	0	0	0
1	B	481	3788	2390	637	745	16	0	0	0
1	C	481	3787	2390	636	745	16	0	0	0
1	D	481	3788	2390	637	745	16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP A0A3P8MUS3
A	?	-	THR	deletion	UNP A0A3P8MUS3
B	?	-	GLY	deletion	UNP A0A3P8MUS3
B	?	-	THR	deletion	UNP A0A3P8MUS3
C	?	-	GLY	deletion	UNP A0A3P8MUS3
C	?	-	THR	deletion	UNP A0A3P8MUS3
D	?	-	GLY	deletion	UNP A0A3P8MUS3
D	?	-	THR	deletion	UNP A0A3P8MUS3

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



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

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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	F	2	23	12	11	0	0	0
3	H	2	23	12	11	0	0	0
3	J	2	23	12	11	0	0	0
3	L	2	23	12	11	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	3	3	3	0	0
4	B	3	3	3	0	0
4	C	3	3	3	0	0
4	D	3	3	3	0	0

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

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

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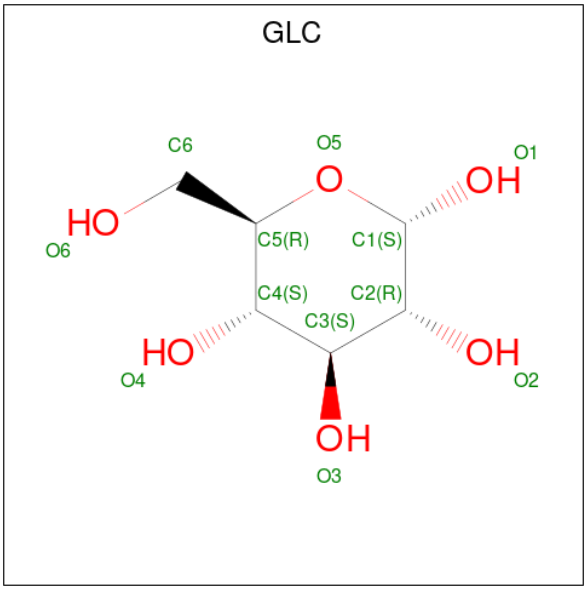
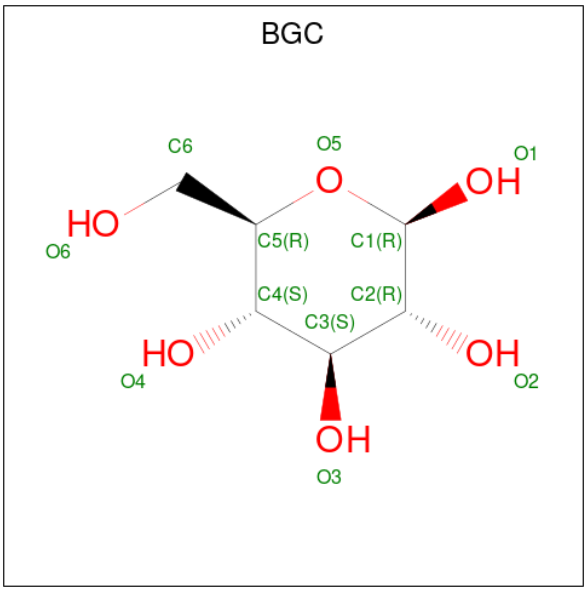
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

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



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	62	62	62	0	0
			Total	O		
8	B	52	52	52	0	0
			Total	O		
8	C	50	50	50	0	0
			Total	O		
8	D	59	59	59	0	0

3 Residue-property plots (i)

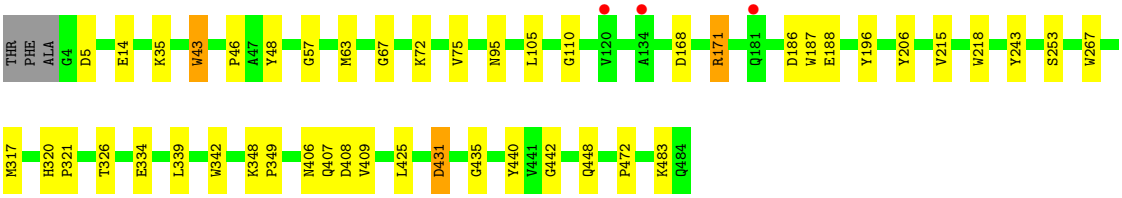
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: A-amylase

Chain A:

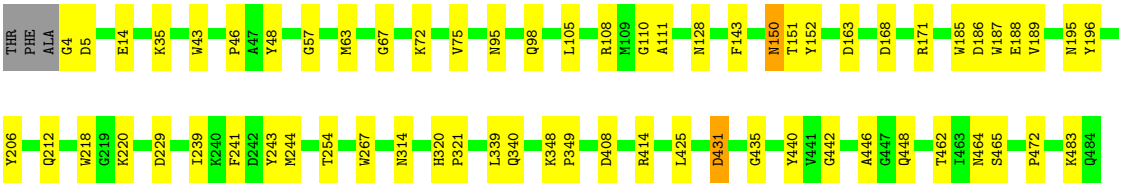
- Molecule 1: A-amylase

Chain B:



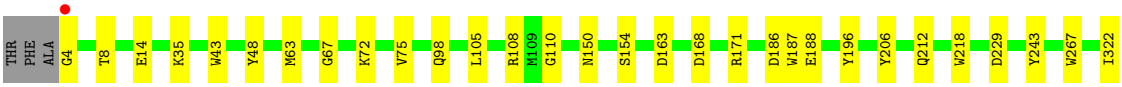
- Molecule 1: A-amylase

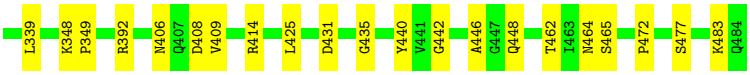
Chain C:



- Molecule 1: A-amylase

Chain D:

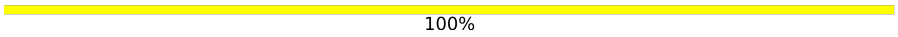




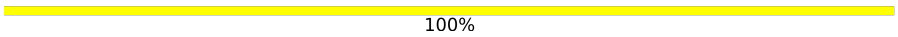
• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:

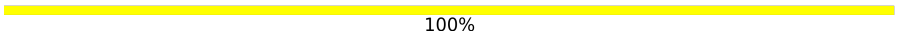
• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G: 

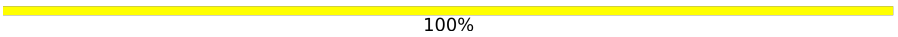
• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I: 

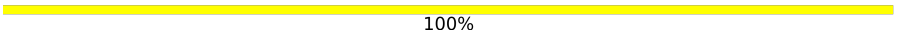
• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K: 

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

Chain F: 

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

Chain H: 

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

Chain J:

C2TG
1CTG

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

Chain L: 100%

C2TG
1CTG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	212.18Å 212.18Å 172.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.86 – 2.95 66.86 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.86-2.95) 100.0 (66.86-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.156 , 0.183 0.171 , 0.194	Depositor DCC
R_{free} test set	4492 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15702	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: BGC, NA, CA, GLC

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	0/3896	0.89	1/5299 (0.0%)
1	B	0.74	0/3896	0.90	1/5299 (0.0%)
1	C	0.74	0/3895	0.91	4/5298 (0.1%)
1	D	0.74	0/3896	0.91	3/5299 (0.1%)
All	All	0.74	0/15583	0.90	9/21195 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5	ASP	CB-CA-C	-6.70	97.01	110.40
1	A	108	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	108	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	C	414	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	108	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	462	THR	CA-CB-OG1	-5.34	97.78	109.00
1	D	414	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	462	THR	CA-CB-OG1	-5.27	97.94	109.00
1	B	253	SER	N-CA-CB	5.00	118.00	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	4	GLY	Peptide

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	3788	0	3511	21	0
1	B	3788	0	3511	25	0
1	C	3787	0	3509	36	0
1	D	3788	0	3511	26	0
2	E	34	0	30	1	0
2	G	34	0	30	0	0
2	I	34	0	30	0	0
2	K	34	0	30	0	0
3	F	23	0	21	0	0
3	H	23	0	21	0	0
3	J	23	0	21	0	0
3	L	23	0	21	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	24	0	24	0	0
6	B	12	0	12	0	0
6	C	12	0	12	0	0
7	B	12	0	12	0	0
7	C	12	0	12	1	0
7	D	12	0	12	1	0
8	A	62	0	0	1	0
8	B	52	0	0	3	0
8	C	50	0	0	4	0
8	D	59	0	0	4	0
All	All	15702	0	14330	109	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 4.

All (109) 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:420:HIS:HB3	8:A:643:HOH:O	1.80	0.81
1:C:464:ASN:HB3	8:C:639:HOH:O	1.82	0.78
1:D:322:ILE:HG12	8:D:653:HOH:O	1.86	0.76
1:C:464:ASN:CB	8:C:639:HOH:O	2.38	0.71
1:B:105:LEU:O	1:B:206:TYR:OH	2.10	0.69
1:C:340:GLN:HG2	8:C:645:HOH:O	1.94	0.66
1:B:35:LYS:HD3	1:B:95:ASN:O	1.96	0.65
1:D:163:ASP:OD2	1:D:186:ASP:OD1	2.16	0.63
1:C:98:GLN:NE2	1:C:229:ASP:HB3	2.16	0.61
1:A:448:GLN:NE2	1:A:483:LYS:HE2	2.17	0.59
1:B:448:GLN:NE2	1:B:483:LYS:HE2	2.18	0.59
1:C:111:ALA:HA	1:C:143:PHE:CE1	2.37	0.58
1:A:237:LYS:NZ	2:E:1:GLC:O3	2.34	0.58
1:C:35:LYS:HD3	1:C:95:ASN:O	2.05	0.56
1:A:408:ASP:HA	1:A:431:ASP:OD1	2.07	0.55
1:A:440:TYR:CZ	1:A:442:GLY:HA2	2.43	0.54
1:C:163:ASP:OD2	1:C:186:ASP:OD1	2.25	0.54
1:C:408:ASP:HA	1:C:431:ASP:OD1	2.07	0.54
1:B:408:ASP:HA	1:B:431:ASP:OD1	2.08	0.54
1:D:440:TYR:CZ	1:D:442:GLY:HA2	2.43	0.54
1:B:440:TYR:CZ	1:B:442:GLY:HA2	2.43	0.54
1:D:212:GLN:HA	1:D:243:TYR:CE1	2.43	0.54
1:D:408:ASP:HA	1:D:431:ASP:OD1	2.08	0.53
1:C:440:TYR:CZ	1:C:442:GLY:HA2	2.43	0.53
1:C:212:GLN:HA	1:C:243:TYR:CE1	2.44	0.52
1:C:314:ASN:HB3	8:C:631:HOH:O	2.09	0.52
1:C:448:GLN:NE2	1:C:483:LYS:HE3	2.25	0.52
1:B:186:ASP:OD2	8:B:601:HOH:O	2.19	0.52
1:C:220:LYS:HD3	1:C:254:THR:HB	1.92	0.52
1:D:63:MET:HE1	1:D:218:TRP:CH2	2.45	0.52
1:B:63:MET:HE1	1:B:218:TRP:CH2	2.48	0.49
1:B:72:LYS:NZ	1:B:110:GLY:O	2.46	0.49
1:D:72:LYS:NZ	1:D:110:GLY:O	2.45	0.48
1:D:348:LYS:N	1:D:349:PRO:HD2	2.29	0.48
1:B:348:LYS:N	1:B:349:PRO:HD2	2.29	0.48
1:C:72:LYS:NZ	1:C:110:GLY:O	2.46	0.48
1:C:348:LYS:N	1:C:349:PRO:HD2	2.29	0.48
1:A:63:MET:HE1	1:A:218:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:N	1:A:349:PRO:HD2	2.29	0.47
1:A:72:LYS:NZ	1:A:110:GLY:O	2.46	0.47
1:C:239:ILE:HG21	1:C:244:MET:HE2	1.97	0.47
1:D:98:GLN:OE1	1:D:229:ASP:HB3	2.15	0.47
1:D:448:GLN:NE2	1:D:483:LYS:HE3	2.29	0.47
1:D:442:GLY:HA3	8:D:644:HOH:O	2.16	0.46
1:D:4:GLY:CA	8:D:658:HOH:O	2.63	0.46
1:A:335:PRO:HA	1:A:340:GLN:OE1	2.15	0.46
1:A:187:TRP:CG	1:A:188:GLU:HA	2.51	0.46
1:D:150:ASN:OD1	1:D:154:SER:CB	2.64	0.45
1:D:168:ASP:OD2	1:D:171:ARG:NH1	2.50	0.45
1:C:267:TRP:CD2	1:C:339:LEU:HD13	2.52	0.45
1:C:150:ASN:HD22	1:C:150:ASN:N	2.15	0.45
1:D:187:TRP:CG	1:D:188:GLU:HA	2.52	0.45
1:C:168:ASP:OD2	1:C:171:ARG:NH1	2.50	0.44
1:B:105:LEU:HB3	1:B:206:TYR:OH	2.18	0.44
1:C:446:ALA:HB1	1:C:465:SER:HA	1.99	0.44
1:D:446:ALA:HB1	1:D:465:SER:HA	1.98	0.44
1:D:425:LEU:C	1:D:425:LEU:HD12	2.38	0.44
1:D:4:GLY:HA2	8:D:658:HOH:O	2.17	0.44
1:B:187:TRP:CG	1:B:188:GLU:HA	2.52	0.43
1:C:111:ALA:HA	1:C:143:PHE:CD1	2.53	0.43
1:A:320:HIS:N	1:A:321:PRO:CD	2.81	0.43
1:B:425:LEU:HD12	1:B:425:LEU:C	2.39	0.43
1:C:189:VAL:HA	1:C:241:PHE:CE1	2.53	0.43
1:A:406:ASN:HB3	1:A:409:VAL:O	2.19	0.43
1:A:435:GLY:O	1:A:472:PRO:HA	2.19	0.43
1:D:435:GLY:O	1:D:472:PRO:HA	2.19	0.43
1:C:425:LEU:HD12	1:C:425:LEU:C	2.38	0.43
1:B:67:GLY:HA2	1:B:75:VAL:O	2.19	0.42
1:B:435:GLY:O	1:B:472:PRO:HA	2.19	0.42
1:C:63:MET:HE1	1:C:218:TRP:CH2	2.54	0.42
1:A:267:TRP:CD2	1:A:339:LEU:HD13	2.54	0.42
1:D:67:GLY:HA2	1:D:75:VAL:O	2.20	0.42
1:B:168:ASP:OD2	1:B:171:ARG:NH1	2.51	0.42
1:C:128:ASN:OD1	7:C:511:BGC:H6C1	2.19	0.42
1:D:105:LEU:HB3	1:D:206:TYR:OH	2.20	0.42
1:A:168:ASP:OD2	1:A:171:ARG:NH1	2.52	0.42
1:B:320:HIS:N	1:B:321:PRO:CD	2.83	0.42
1:C:111:ALA:CA	1:C:143:PHE:CE1	3.02	0.42
1:C:187:TRP:CG	1:C:188:GLU:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:GLN:HB3	1:D:243:TYR:HE1	1.85	0.42
1:A:446:ALA:HB1	1:A:465:SER:HA	2.02	0.41
1:C:105:LEU:O	1:C:206:TYR:OH	2.24	0.41
1:A:43:TRP:CD1	1:A:43:TRP:C	2.94	0.41
1:D:267:TRP:CD2	1:D:339:LEU:HD13	2.55	0.41
1:B:5:ASP:N	8:B:610:HOH:O	2.52	0.41
1:C:67:GLY:HA2	1:C:75:VAL:O	2.20	0.41
1:C:320:HIS:N	1:C:321:PRO:CD	2.83	0.41
1:D:406:ASN:HB3	1:D:409:VAL:O	2.20	0.41
7:D:510:BGC:H6	7:D:510:BGC:HD	1.68	0.41
1:B:334:GLU:HA	1:B:342:TRP:CE3	2.56	0.41
1:B:406:ASN:HB3	1:B:409:VAL:O	2.21	0.41
1:C:435:GLY:O	1:C:472:PRO:HA	2.20	0.41
1:D:464:ASN:OD1	1:D:464:ASN:C	2.58	0.41
1:A:46:PRO:HB2	1:A:57:GLY:HA3	2.02	0.41
1:B:267:TRP:CD2	1:B:339:LEU:HD13	2.56	0.41
1:A:317:MET:HG3	1:A:326:THR:HG21	2.02	0.41
1:A:425:LEU:C	1:A:425:LEU:HD12	2.40	0.41
1:B:46:PRO:HB2	1:B:57:GLY:HA3	2.02	0.41
1:B:215:VAL:HB	1:B:243:TYR:OH	2.21	0.41
1:C:46:PRO:HB2	1:C:57:GLY:HA3	2.03	0.41
1:C:464:ASN:C	1:C:464:ASN:OD1	2.59	0.41
1:D:8:THR:OG1	1:D:392:ARG:HD3	2.21	0.41
1:B:407:GLN:HG3	8:B:613:HOH:O	2.21	0.41
1:C:187:TRP:CD2	1:C:188:GLU:HA	2.56	0.40
1:A:205:ASP:OD1	1:A:207:ASP:HB2	2.21	0.40
1:B:43:TRP:CD1	1:B:43:TRP:C	2.95	0.40
1:B:317:MET:HG3	1:B:326:THR:HG21	2.02	0.40
1:C:185:TRP:HB3	1:C:195:ASN:OD1	2.22	0.40
1:C:151:THR:HG22	1:C:152:TYR:CD2	2.56	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	479/484 (99%)	460 (96%)	19 (4%)	0	100	100
1	B	479/484 (99%)	457 (95%)	22 (5%)	0	100	100
1	C	479/484 (99%)	458 (96%)	21 (4%)	0	100	100
1	D	479/484 (99%)	459 (96%)	20 (4%)	0	100	100
All	All	1916/1936 (99%)	1834 (96%)	82 (4%)	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	400/402 (100%)	395 (99%)	5 (1%)	69	87
1	B	400/402 (100%)	394 (98%)	6 (2%)	65	85
1	C	400/402 (100%)	394 (98%)	6 (2%)	65	85
1	D	400/402 (100%)	394 (98%)	6 (2%)	65	85
All	All	1600/1608 (100%)	1577 (99%)	23 (1%)	67	86

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	43	TRP
1	A	48	TYR
1	A	196	TYR
1	A	431	ASP
1	B	14	GLU
1	B	43	TRP
1	B	48	TYR
1	B	171	ARG
1	B	196	TYR

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Mol	Chain	Res	Type
1	B	431	ASP
1	C	14	GLU
1	C	43	TRP
1	C	48	TYR
1	C	150	ASN
1	C	196	TYR
1	C	431	ASP
1	D	14	GLU
1	D	35	LYS
1	D	43	TRP
1	D	48	TYR
1	D	196	TYR
1	D	477	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	150	ASN

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)

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	1.15	0	17,17,17	1.98	8 (47%)
2	GLC	E	2	2	11,11,12	1.87	3 (27%)	15,15,17	1.94	5 (33%)
2	GLC	E	3	2	11,11,12	0.76	0	15,15,17	1.96	2 (13%)
3	GLC	F	1	3	12,12,12	1.55	3 (25%)	17,17,17	2.33	7 (41%)
3	GLC	F	2	3	11,11,12	1.39	1 (9%)	15,15,17	2.14	6 (40%)
2	GLC	G	1	2	12,12,12	0.95	0	17,17,17	1.68	6 (35%)
2	GLC	G	2	2	11,11,12	1.49	2 (18%)	15,15,17	2.21	5 (33%)
2	GLC	G	3	2	11,11,12	0.91	1 (9%)	15,15,17	1.57	5 (33%)
3	GLC	H	1	3	12,12,12	2.19	4 (33%)	17,17,17	2.91	7 (41%)
3	GLC	H	2	3	11,11,12	2.81	7 (63%)	15,15,17	3.07	9 (60%)
2	GLC	I	1	2	12,12,12	0.81	0	17,17,17	2.25	5 (29%)
2	GLC	I	2	2	11,11,12	1.33	1 (9%)	15,15,17	1.13	1 (6%)
2	GLC	I	3	2	11,11,12	1.26	1 (9%)	15,15,17	2.25	7 (46%)
3	GLC	J	1	3	12,12,12	0.41	0	17,17,17	0.48	0
3	GLC	J	2	3	11,11,12	0.23	0	15,15,17	0.62	0
2	GLC	K	1	2	12,12,12	1.41	3 (25%)	17,17,17	2.45	9 (52%)
2	GLC	K	2	2	11,11,12	0.93	0	15,15,17	1.78	6 (40%)
2	GLC	K	3	2	11,11,12	0.69	0	15,15,17	1.35	2 (13%)
3	GLC	L	1	3	12,12,12	1.08	1 (8%)	17,17,17	1.84	4 (23%)
3	GLC	L	2	3	11,11,12	1.95	4 (36%)	15,15,17	2.47	7 (46%)

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	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
3	GLC	F	1	3	-	1/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	2/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	2/2/19/22	0/1/1/1
3	GLC	H	1	3	-	1/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	2	2	-	1/2/19/22	0/1/1/1
2	GLC	I	3	2	-	2/2/19/22	0/1/1/1
3	GLC	J	1	3	-	1/2/22/22	0/1/1/1
3	GLC	J	2	3	-	1/2/19/22	0/1/1/1
2	GLC	K	1	2	-	1/2/22/22	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
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	2/2/19/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	GLC	C2-C3	5.01	1.59	1.52
3	H	2	GLC	O5-C1	4.76	1.51	1.43
3	H	1	GLC	C4-C3	4.00	1.62	1.52
2	E	2	GLC	C2-C3	3.58	1.57	1.52
3	L	2	GLC	C2-C3	3.40	1.57	1.52
2	G	2	GLC	C2-C3	3.39	1.57	1.52
3	H	1	GLC	C4-C5	3.30	1.60	1.53
3	H	1	GLC	O4-C4	3.28	1.50	1.43
3	H	2	GLC	O5-C5	3.16	1.49	1.43
3	F	1	GLC	C4-C5	3.12	1.59	1.53
3	H	2	GLC	C4-C5	2.85	1.59	1.53
3	F	2	GLC	C1-C2	2.80	1.58	1.52
3	L	2	GLC	C4-C3	2.75	1.59	1.52
3	L	2	GLC	O5-C1	2.75	1.48	1.43
2	K	1	GLC	C1-C2	2.75	1.58	1.52
2	I	3	GLC	C1-C2	2.58	1.58	1.52
3	L	2	GLC	C4-C5	2.47	1.58	1.53
3	H	2	GLC	O4-C4	2.46	1.48	1.43
3	F	1	GLC	O4-C4	2.45	1.48	1.43
2	E	2	GLC	O5-C5	2.42	1.48	1.43
2	G	2	GLC	O4-C4	2.38	1.48	1.43
2	I	2	GLC	C1-C2	2.36	1.57	1.52
2	G	3	GLC	C2-C3	2.34	1.56	1.52
3	H	2	GLC	C4-C3	2.26	1.58	1.52
2	E	2	GLC	O3-C3	2.24	1.48	1.43
3	F	1	GLC	C1-C2	2.23	1.57	1.52
2	K	1	GLC	O3-C3	2.23	1.48	1.43
2	K	1	GLC	C4-C5	2.21	1.57	1.53
3	L	1	GLC	C4-C5	2.19	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	GLC	C1-C2	2.12	1.57	1.52
3	H	1	GLC	C1-C2	2.01	1.57	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	GLC	O5-C5-C6	6.81	117.88	107.20
2	I	1	GLC	O2-C2-C3	-6.66	94.96	110.35
3	H	1	GLC	O4-C4-C3	6.44	125.23	110.35
2	K	1	GLC	O2-C2-C3	-6.14	96.15	110.35
3	H	1	GLC	O3-C3-C4	5.71	123.56	110.35
2	G	2	GLC	O2-C2-C3	5.33	120.81	110.14
2	E	3	GLC	O2-C2-C1	5.24	119.88	109.15
3	F	1	GLC	O4-C4-C5	5.07	121.88	109.30
3	H	1	GLC	O5-C5-C6	4.86	118.51	106.44
2	I	3	GLC	O5-C5-C6	4.76	114.67	107.20
3	L	1	GLC	O4-C4-C5	4.27	119.89	109.30
2	I	3	GLC	O4-C4-C3	-4.20	100.64	110.35
3	H	2	GLC	O3-C3-C2	4.18	118.00	109.99
3	H	1	GLC	O1-C1-C2	4.13	120.66	109.03
3	L	2	GLC	O3-C3-C4	3.88	119.33	110.35
3	H	2	GLC	O5-C1-C2	-3.87	104.79	110.77
2	E	1	GLC	O4-C4-C3	-3.83	101.48	110.35
3	F	1	GLC	C6-C5-C4	3.81	121.93	113.00
3	L	2	GLC	C1-O5-C5	3.80	117.35	112.19
3	F	1	GLC	O2-C2-C1	3.80	117.98	109.16
3	L	2	GLC	O5-C5-C6	3.80	113.16	107.20
2	E	2	GLC	O4-C4-C3	3.80	119.13	110.35
3	H	2	GLC	C1-O5-C5	3.77	117.30	112.19
2	K	1	GLC	O4-C4-C3	-3.66	101.89	110.35
2	K	1	GLC	O1-C1-C2	3.64	119.29	109.03
3	H	2	GLC	O4-C4-C5	3.61	118.27	109.30
3	L	2	GLC	O4-C4-C3	3.52	118.48	110.35
3	L	1	GLC	O5-C5-C6	3.51	115.15	106.44
3	H	2	GLC	C6-C5-C4	-3.49	104.83	113.00
2	I	1	GLC	C6-C5-C4	-3.47	104.88	113.00
3	F	2	GLC	O2-C2-C1	3.38	116.08	109.15
2	E	3	GLC	O5-C1-C2	-3.38	105.55	110.77
3	F	1	GLC	O1-C1-C2	3.37	118.53	109.03
2	K	3	GLC	O2-C2-C1	3.24	115.79	109.15
3	F	2	GLC	C2-C3-C4	-3.24	105.29	110.89
2	G	2	GLC	O4-C4-C3	3.15	117.63	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	GLC	C1-C2-C3	3.12	113.50	109.67
3	F	2	GLC	C1-O5-C5	2.95	116.18	112.19
2	K	2	GLC	O2-C2-C3	2.94	116.03	110.14
2	E	1	GLC	O2-C2-C1	-2.90	102.42	109.16
2	K	1	GLC	O5-C5-C6	2.87	113.57	106.44
2	K	2	GLC	O2-C2-C1	-2.87	103.29	109.15
2	G	1	GLC	O5-C1-C2	-2.83	105.24	110.28
2	E	2	GLC	C2-C3-C4	-2.82	106.01	110.89
2	E	1	GLC	O2-C2-C3	-2.82	103.83	110.35
3	H	1	GLC	C6-C5-C4	2.82	119.60	113.00
2	G	2	GLC	O3-C3-C2	2.77	115.30	109.99
2	G	3	GLC	O2-C2-C3	2.76	115.67	110.14
3	F	2	GLC	O5-C1-C2	-2.76	106.51	110.77
2	I	3	GLC	O2-C2-C3	-2.75	104.63	110.14
3	F	1	GLC	O2-C2-C3	-2.73	104.03	110.35
3	H	2	GLC	C1-C2-C3	2.71	113.00	109.67
2	I	3	GLC	O3-C3-C4	-2.70	104.11	110.35
2	I	1	GLC	O5-C5-C6	2.68	113.11	106.44
3	L	2	GLC	O2-C2-C1	2.68	114.63	109.15
2	E	1	GLC	O3-C3-C2	2.64	116.46	110.35
3	L	2	GLC	O5-C1-C2	-2.64	106.70	110.77
2	K	2	GLC	C2-C3-C4	-2.63	106.35	110.89
2	I	1	GLC	O4-C4-C3	-2.61	104.31	110.35
2	I	3	GLC	O4-C4-C5	-2.59	102.85	109.30
2	E	2	GLC	C1-C2-C3	2.59	112.86	109.67
3	F	2	GLC	O3-C3-C4	2.58	116.32	110.35
2	I	2	GLC	C2-C3-C4	-2.58	106.43	110.89
2	E	2	GLC	C6-C5-C4	-2.57	106.99	113.00
2	G	1	GLC	O4-C4-C3	-2.53	104.51	110.35
2	G	1	GLC	C6-C5-C4	-2.49	107.17	113.00
3	L	2	GLC	O4-C4-C5	2.48	115.45	109.30
2	K	1	GLC	O4-C4-C5	2.48	115.45	109.30
2	K	1	GLC	O2-C2-C1	2.46	114.87	109.16
3	H	1	GLC	O3-C3-C2	-2.46	104.66	110.35
2	G	3	GLC	O3-C3-C2	2.45	114.68	109.99
2	E	2	GLC	O5-C5-C6	2.43	111.02	107.20
2	G	2	GLC	O2-C2-C1	-2.41	104.23	109.15
3	L	1	GLC	O3-C3-C2	2.38	115.84	110.35
2	I	3	GLC	C3-C4-C5	2.35	114.43	110.24
3	F	1	GLC	O5-C5-C6	-2.33	100.65	106.44
2	G	2	GLC	O3-C3-C4	-2.32	105.00	110.35
2	E	1	GLC	C6-C5-C4	-2.26	107.70	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	GLC	O4-C4-C5	2.24	114.87	109.30
3	F	1	GLC	O3-C3-C2	-2.23	105.20	110.35
2	K	2	GLC	O3-C3-C4	-2.22	105.21	110.35
3	H	2	GLC	O4-C4-C3	2.22	115.48	110.35
2	G	1	GLC	C4-C3-C2	-2.21	106.97	110.82
2	I	1	GLC	O3-C3-C2	2.19	115.41	110.35
2	I	3	GLC	O2-C2-C1	2.18	113.61	109.15
2	K	2	GLC	O4-C4-C5	-2.16	103.92	109.30
2	K	3	GLC	O5-C5-C6	2.16	110.59	107.20
2	K	1	GLC	C6-C5-C4	-2.14	108.00	113.00
2	G	3	GLC	C1-O5-C5	2.13	115.08	112.19
2	K	1	GLC	O3-C3-C2	2.13	115.26	110.35
2	E	1	GLC	O1-C1-C2	2.13	115.02	109.03
2	G	1	GLC	O1-C1-C2	2.09	114.93	109.03
3	H	1	GLC	O2-C2-C1	2.09	114.01	109.16
3	L	1	GLC	C4-C3-C2	-2.09	107.18	110.82
2	E	1	GLC	O5-C1-C2	-2.08	106.57	110.28
3	H	2	GLC	C2-C3-C4	-2.06	107.33	110.89
2	G	3	GLC	C6-C5-C4	2.06	117.82	113.00
2	G	3	GLC	O5-C5-C6	-2.05	103.99	107.20
2	G	1	GLC	O5-C5-C6	2.04	111.51	106.44
2	K	2	GLC	O5-C5-C6	-2.01	104.06	107.20
2	K	1	GLC	C4-C3-C2	-2.00	107.33	110.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	GLC	O5-C5-C6-O6
2	I	3	GLC	O5-C5-C6-O6
2	I	3	GLC	C4-C5-C6-O6
3	L	2	GLC	C4-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
3	H	1	GLC	C4-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6
2	K	1	GLC	O5-C5-C6-O6
2	G	3	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
3	L	2	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	2	GLC	O5-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6

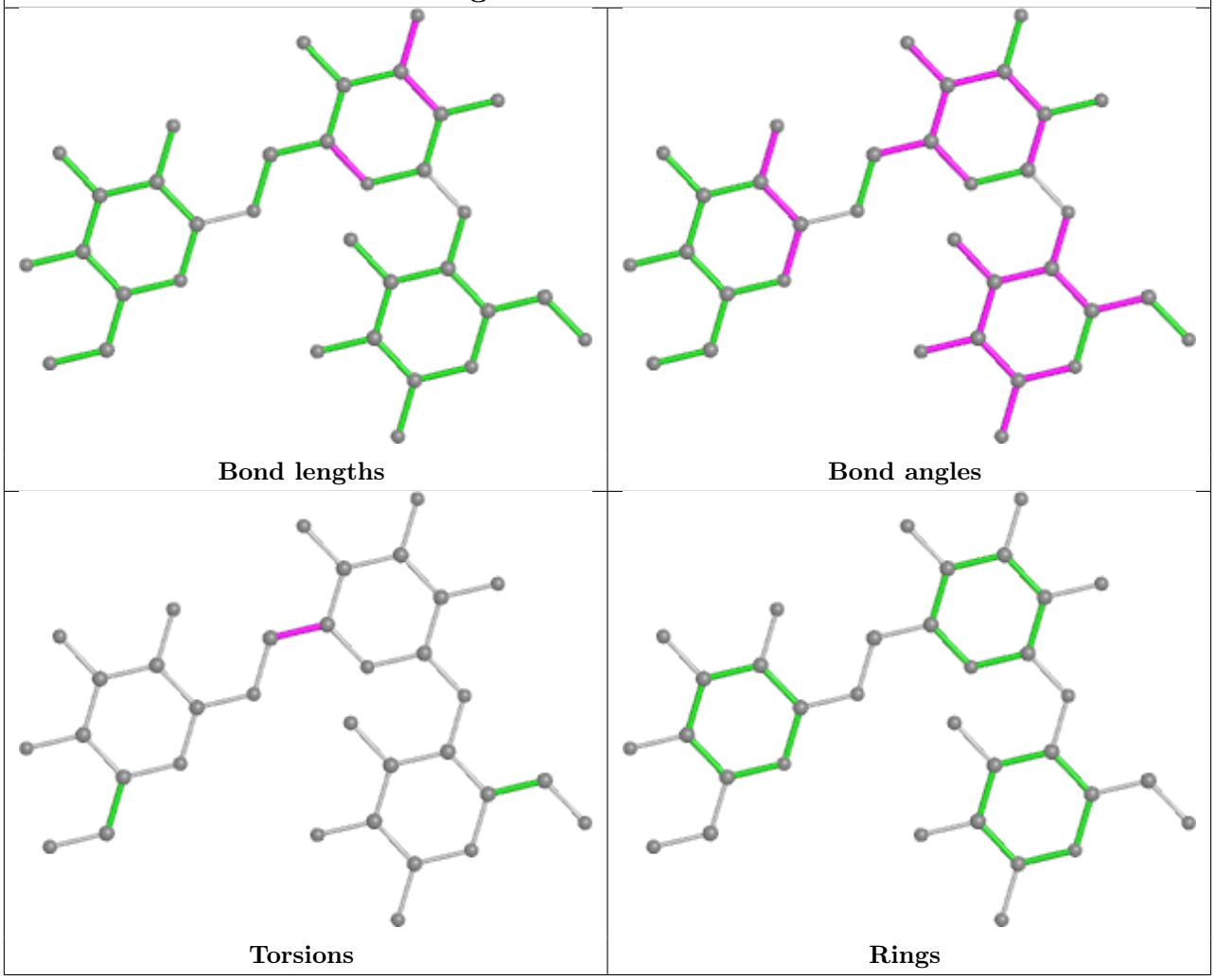
There are no ring outliers.

1 monomer is involved in 1 short contact:

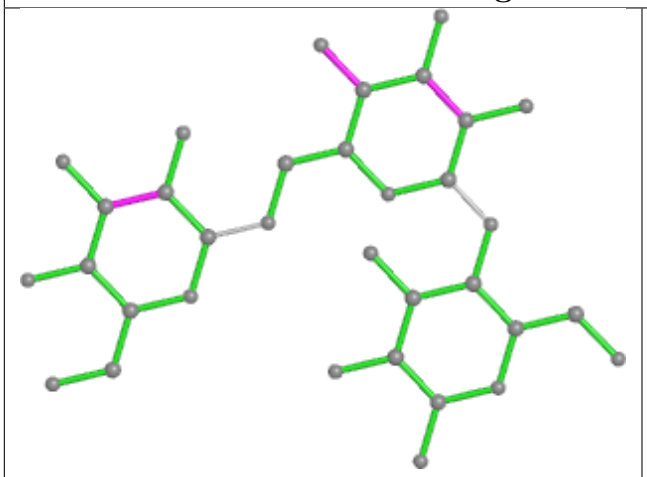
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	GLC	1	0

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

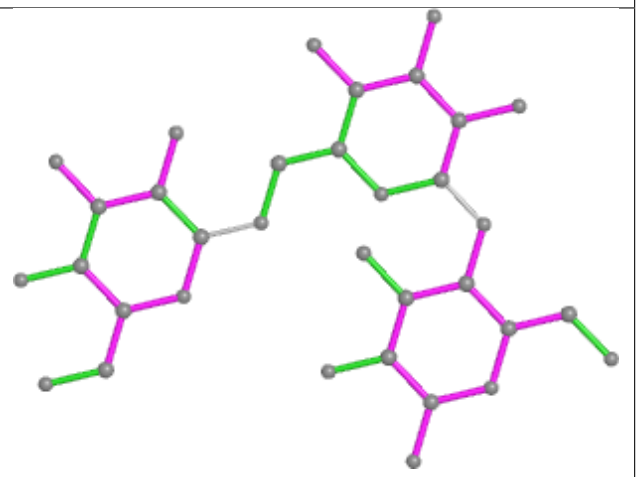
Oligosaccharide Chain E



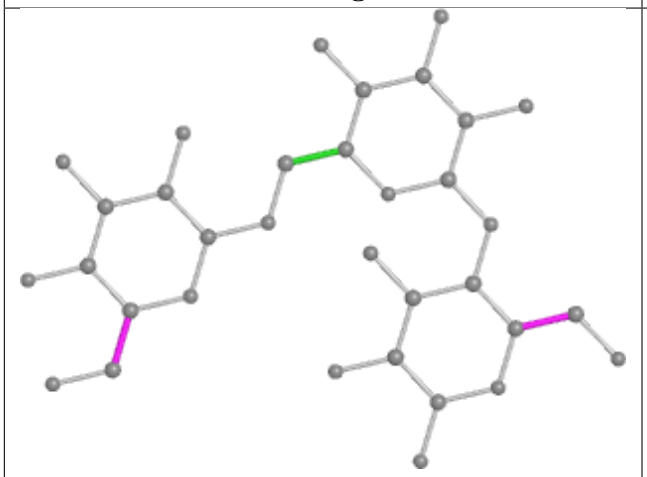
Oligosaccharide Chain G



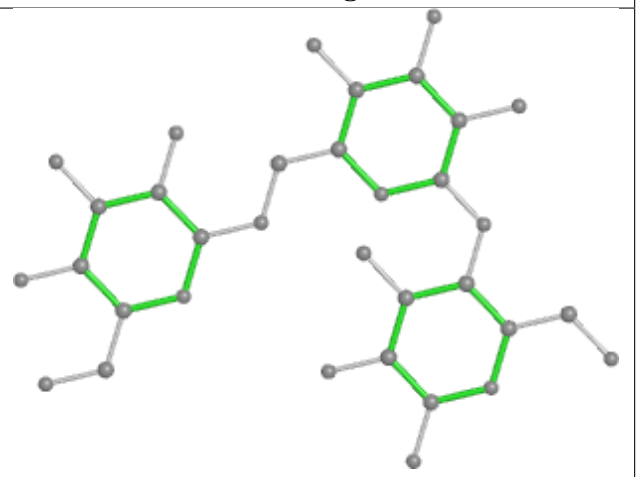
Bond lengths



Bond angles

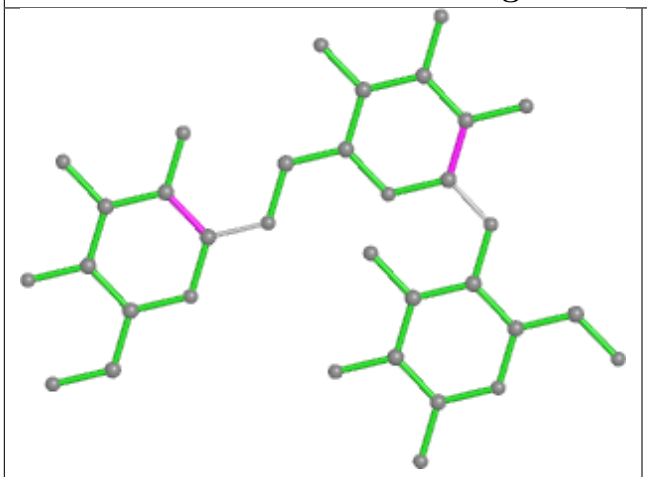


Torsions

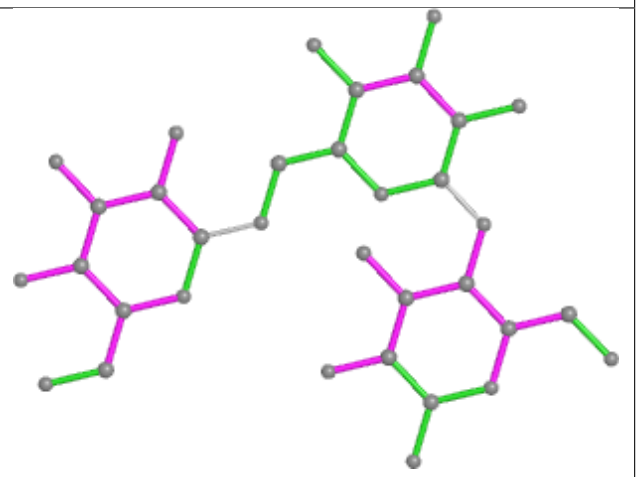


Rings

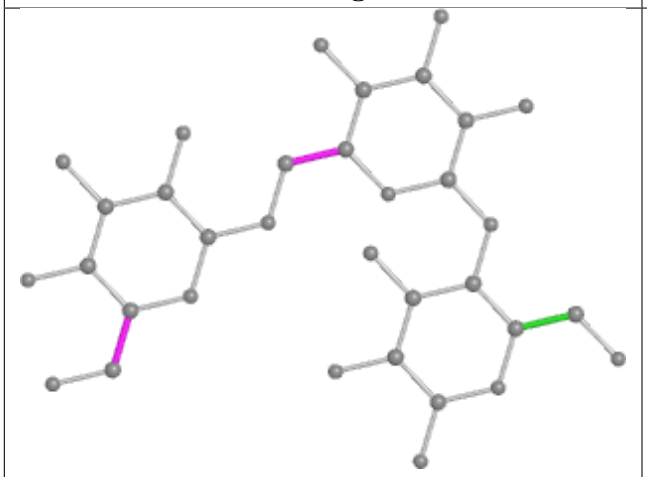
Oligosaccharide Chain I



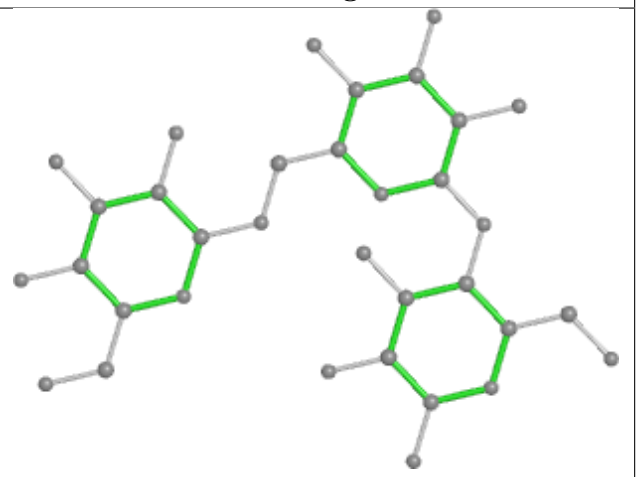
Bond lengths



Bond angles

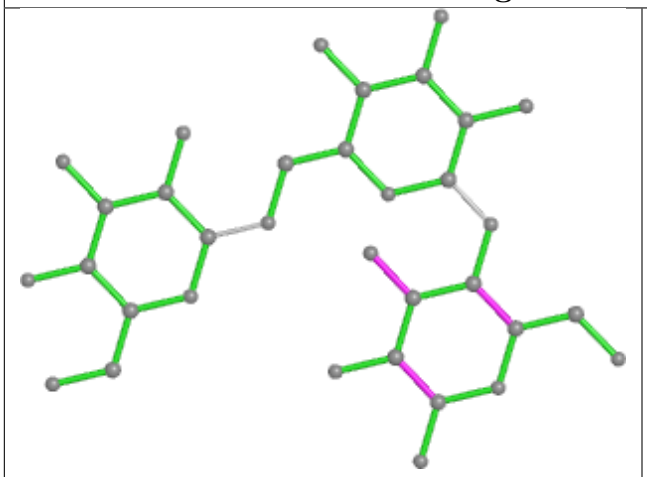


Torsions

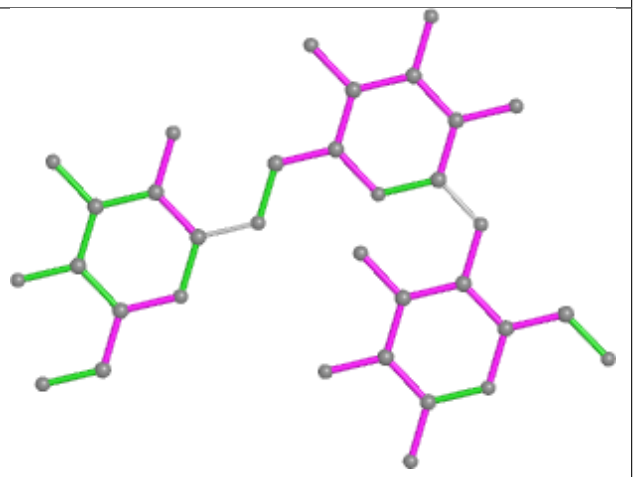


Rings

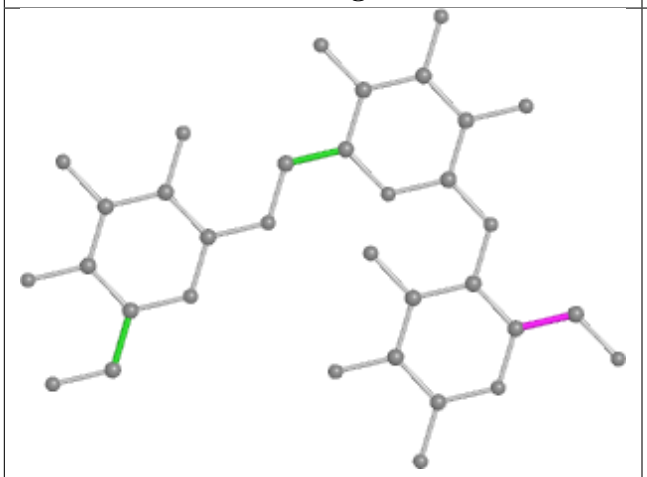
Oligosaccharide Chain K



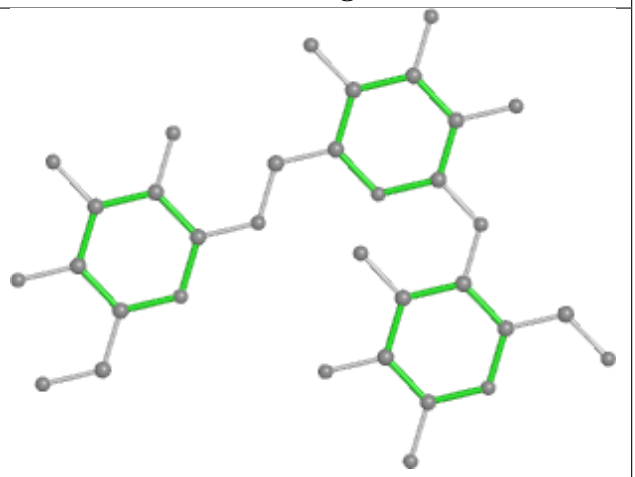
Bond lengths



Bond angles

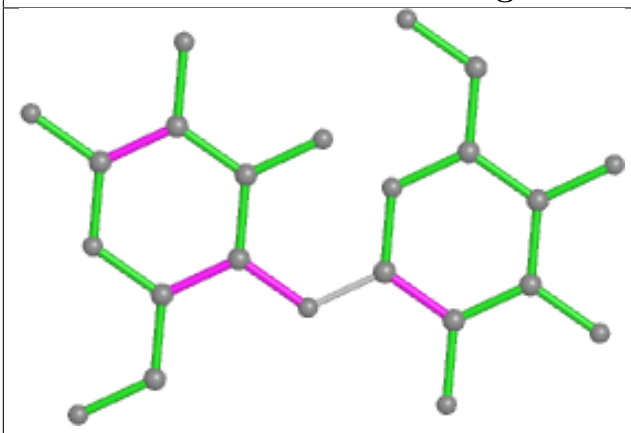


Torsions

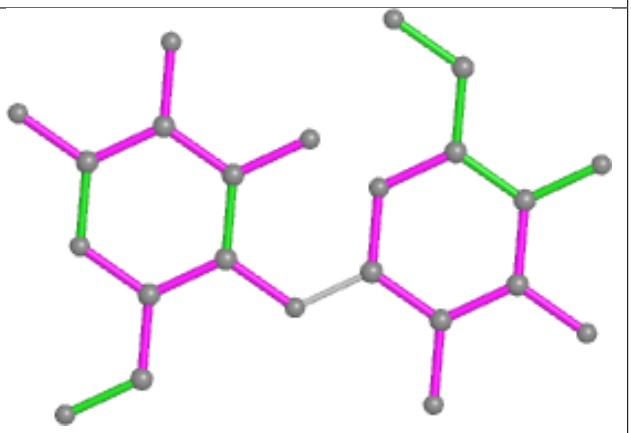


Rings

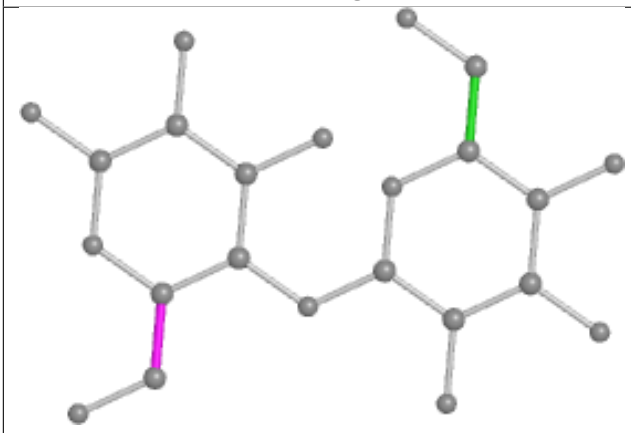
Oligosaccharide Chain F



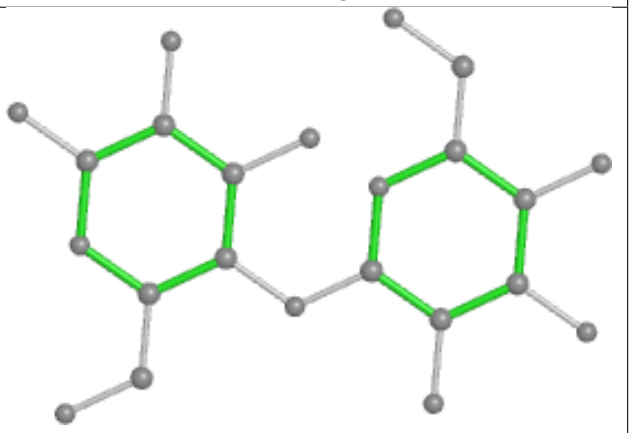
Bond lengths



Bond angles

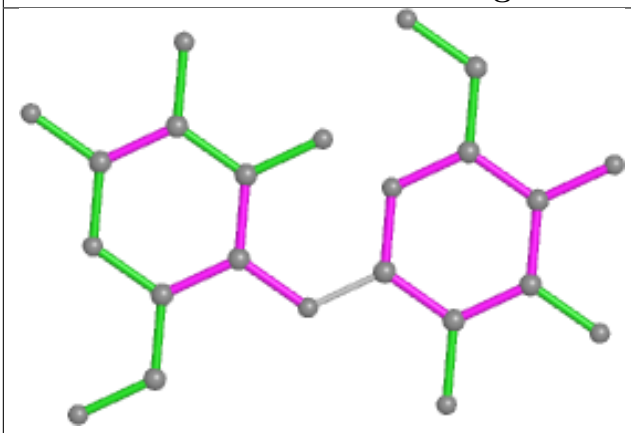


Torsions

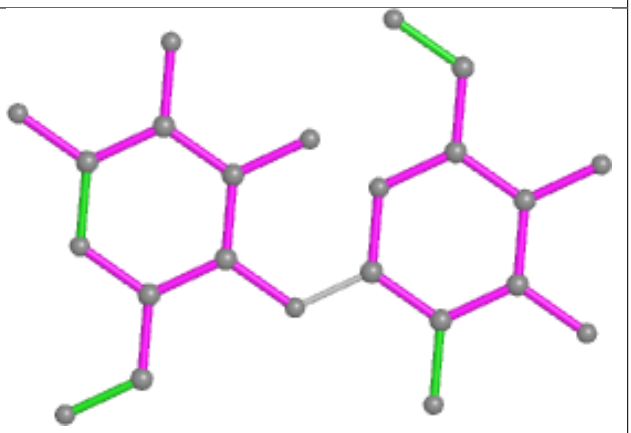


Rings

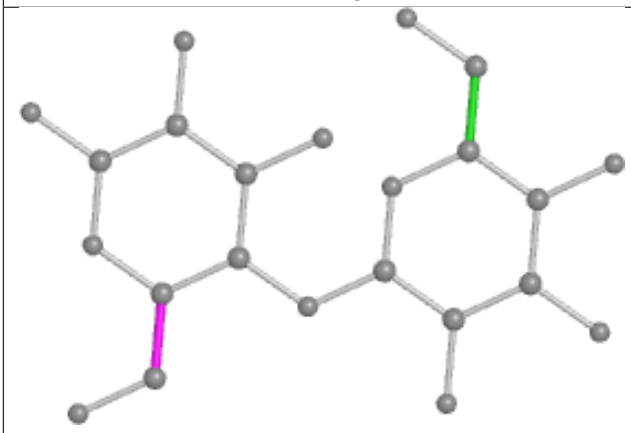
Oligosaccharide Chain H



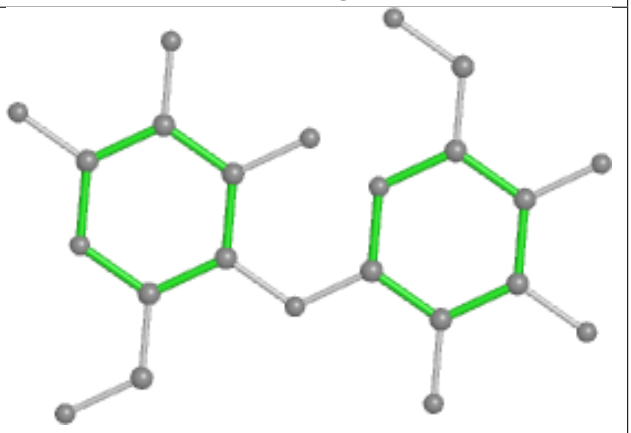
Bond lengths



Bond angles

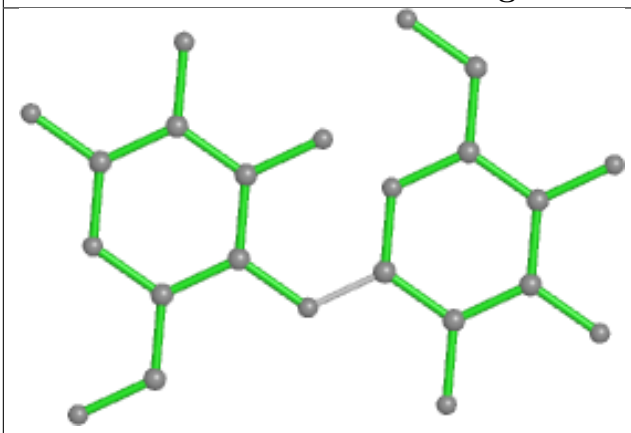


Torsions

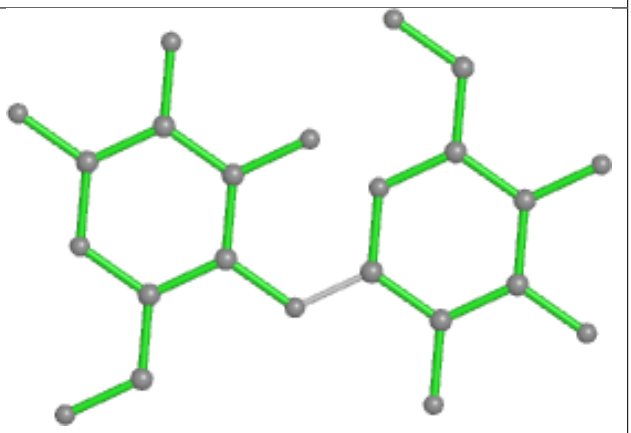


Rings

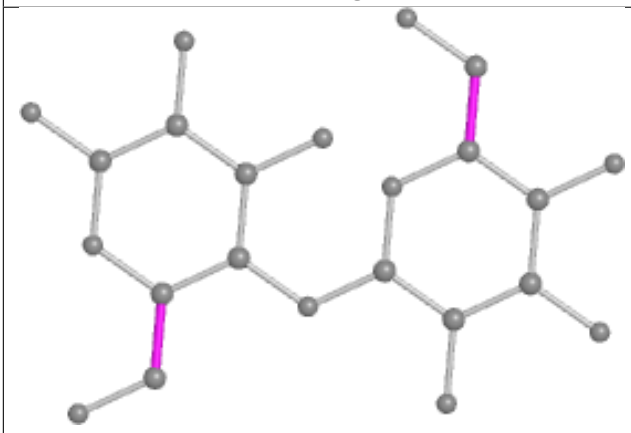
Oligosaccharide Chain J



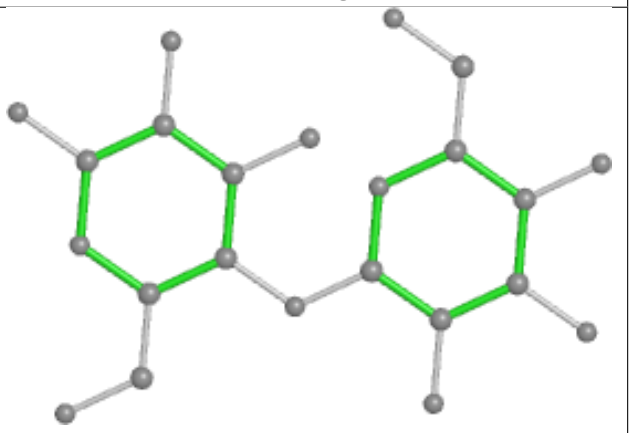
Bond lengths



Bond angles

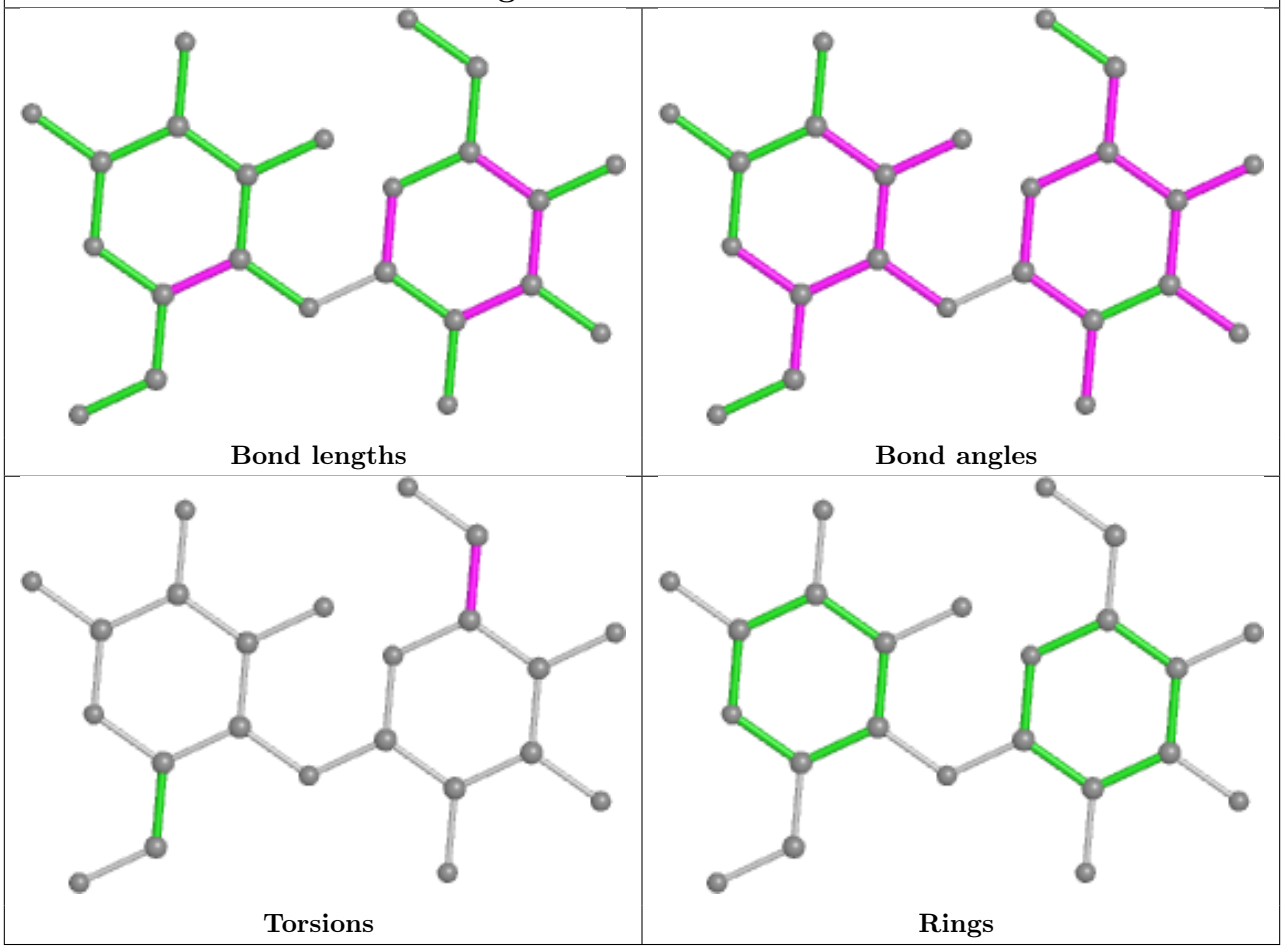


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 16 are monoatomic - leaving 7 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	BGC	B	511	-	12,12,12	1.57	2 (16%)	17,17,17	1.41	4 (23%)
6	GLC	B	510	-	12,12,12	1.32	1 (8%)	17,17,17	1.33	3 (17%)
6	GLC	C	510	-	12,12,12	1.30	1 (8%)	17,17,17	2.13	4 (23%)
7	BGC	D	510	-	12,12,12	0.43	0	17,17,17	0.63	0
6	GLC	A	508	-	12,12,12	1.80	3 (25%)	17,17,17	1.66	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BGC	C	511	-	12,12,12	3.56	10 (83%)	17,17,17	3.49	9 (52%)
6	GLC	A	511	-	12,12,12	1.68	2 (16%)	17,17,17	2.63	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BGC	B	511	-	-	2/2/22/22	0/1/1/1
6	GLC	B	510	-	-	2/2/22/22	0/1/1/1
6	GLC	C	510	-	-	0/2/22/22	0/1/1/1
7	BGC	D	510	-	-	1/2/22/22	0/1/1/1
6	GLC	A	508	-	-	0/2/22/22	0/1/1/1
7	BGC	C	511	-	-	1/2/22/22	0/1/1/1
6	GLC	A	511	-	-	1/2/22/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	511	BGC	C4-C3	6.14	1.68	1.52
7	C	511	BGC	O4-C4	4.99	1.54	1.43
7	C	511	BGC	C4-C5	4.34	1.62	1.53
7	C	511	BGC	O5-C1	4.31	1.53	1.42
6	A	511	GLC	O5-C1	3.96	1.52	1.42
7	C	511	BGC	O2-C2	3.60	1.51	1.43
7	C	511	BGC	O5-C5	3.50	1.52	1.44
6	A	508	GLC	C4-C3	3.08	1.60	1.52
6	A	511	GLC	O1-C1	2.86	1.48	1.39
7	C	511	BGC	C6-C5	2.79	1.61	1.51
6	B	510	GLC	C4-C3	2.77	1.59	1.52
6	A	508	GLC	O4-C4	2.53	1.48	1.43
7	C	511	BGC	C3-C2	2.42	1.58	1.52
6	C	510	GLC	C1-C2	2.41	1.58	1.52
6	A	508	GLC	C4-C5	2.39	1.58	1.53
7	B	511	BGC	O2-C2	2.26	1.48	1.43
7	C	511	BGC	O3-C3	2.21	1.48	1.43
7	C	511	BGC	C1-C2	2.07	1.57	1.52
7	B	511	BGC	C4-C3	2.07	1.57	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	511	BGC	O3-C3-C4	6.37	125.08	110.35
6	A	511	GLC	O1-C1-O5	6.27	129.21	110.38
7	C	511	BGC	O5-C1-C2	6.24	121.42	110.28
7	C	511	BGC	O4-C4-C3	6.22	124.72	110.35
7	C	511	BGC	O5-C5-C6	6.17	121.77	106.44
6	C	510	GLC	O5-C5-C6	6.01	121.38	106.44
6	A	511	GLC	C6-C5-C4	-5.68	99.71	113.00
6	A	508	GLC	O4-C4-C3	4.16	119.96	110.35
7	C	511	BGC	C4-C3-C2	3.89	117.61	110.82
6	A	511	GLC	O4-C4-C3	-3.75	101.69	110.35
6	A	508	GLC	O5-C5-C6	3.71	115.65	106.44
6	B	510	GLC	O4-C4-C3	3.39	118.19	110.35
7	C	511	BGC	O1-C1-O5	3.33	120.36	110.38
6	C	510	GLC	O2-C2-C3	-3.25	102.85	110.35
6	C	510	GLC	O2-C2-C1	3.24	116.68	109.16
6	A	508	GLC	O1-C1-C2	2.79	116.89	109.03
7	C	511	BGC	O3-C3-C2	-2.74	104.02	110.35
6	B	510	GLC	C6-C5-C4	-2.74	106.59	113.00
6	A	511	GLC	O3-C3-C4	-2.53	104.50	110.35
6	C	510	GLC	O1-C1-C2	2.46	115.96	109.03
7	B	511	BGC	C1-O5-C5	2.38	118.16	113.66
7	C	511	BGC	C1-C2-C3	-2.36	105.42	110.31
7	C	511	BGC	O1-C1-C2	-2.36	102.39	109.03
7	B	511	BGC	C4-C3-C2	2.25	114.76	110.82
6	A	511	GLC	O1-C1-C2	-2.16	102.94	109.03
7	B	511	BGC	C1-C2-C3	-2.12	105.92	110.31
6	B	510	GLC	O6-C6-C5	-2.01	104.40	111.29
6	A	511	GLC	O5-C1-C2	-2.01	106.70	110.28
7	B	511	BGC	O5-C5-C6	2.00	111.42	106.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	510	GLC	O5-C5-C6-O6
7	B	511	BGC	O5-C5-C6-O6
6	B	510	GLC	C4-C5-C6-O6
7	B	511	BGC	C4-C5-C6-O6
7	C	511	BGC	O5-C5-C6-O6
7	D	510	BGC	O5-C5-C6-O6
6	A	511	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	510	BGC	1	0
7	C	511	BGC	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	481/484 (99%)	-0.16	0	100	100	40, 54, 79, 104	0
1	B	481/484 (99%)	-0.09	3 (0%)	89	78	41, 57, 88, 104	0
1	C	481/484 (99%)	-0.06	0	100	100	43, 63, 85, 96	0
1	D	481/484 (99%)	-0.05	1 (0%)	95	90	43, 63, 84, 107	0
All	All	1924/1936 (99%)	-0.09	4 (0%)	95	90	40, 60, 85, 107	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	GLY	2.3
1	B	181	GLN	2.2
1	B	120	VAL	2.1
1	B	134	ALA	2.1

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
3	GLC	H	2	11/12	0.77	0.20	86,106,124,125	0
3	GLC	L	2	11/12	0.77	0.25	76,114,136,155	0
3	GLC	H	1	12/12	0.78	0.25	79,115,126,131	0

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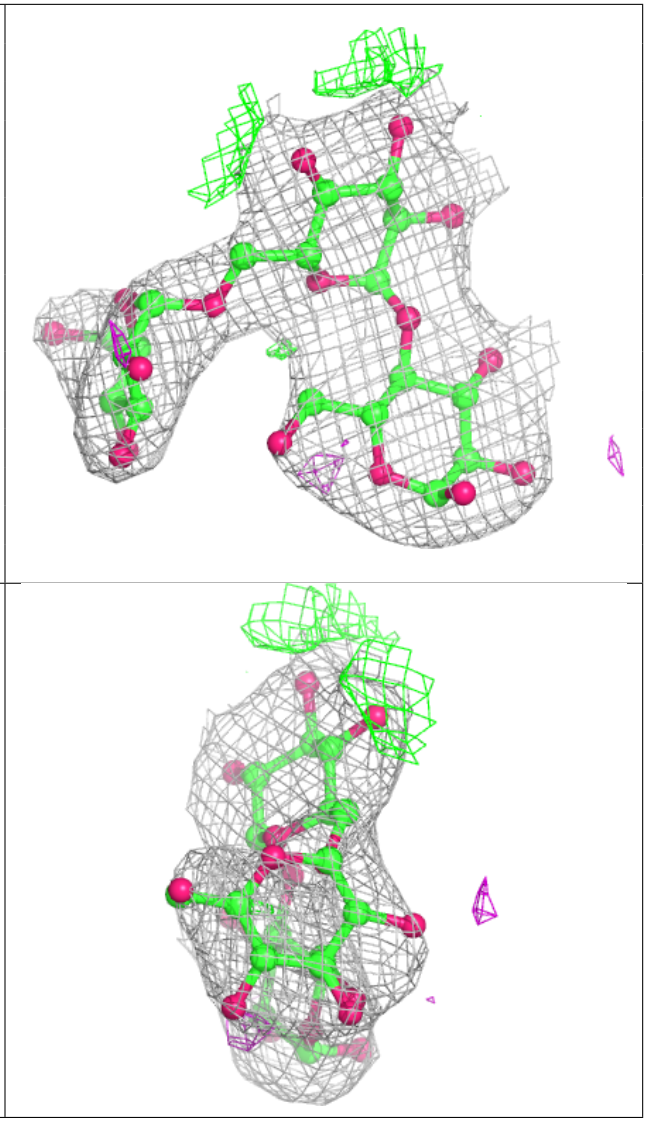
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	J	2	11/12	0.81	0.32	76,102,118,129	0
3	GLC	F	1	12/12	0.81	0.24	88,118,135,152	0
3	GLC	F	2	11/12	0.82	0.20	83,108,143,147	0
3	GLC	J	1	12/12	0.82	0.20	88,123,135,138	0
2	GLC	G	3	11/12	0.87	0.33	84,106,128,156	0
3	GLC	L	1	12/12	0.90	0.17	73,109,125,148	0
2	GLC	E	3	11/12	0.91	0.22	78,96,113,122	0
2	GLC	I	3	11/12	0.93	0.16	63,71,76,85	0
2	GLC	K	3	11/12	0.94	0.17	78,81,88,95	0
2	GLC	G	1	12/12	0.94	0.13	56,70,76,77	0
2	GLC	G	2	11/12	0.94	0.16	47,74,95,104	0
2	GLC	K	1	12/12	0.95	0.16	50,61,69,83	0
2	GLC	I	1	12/12	0.96	0.15	49,61,65,96	0
2	GLC	E	1	12/12	0.96	0.16	57,69,75,87	0
2	GLC	E	2	11/12	0.96	0.15	58,71,88,99	0
2	GLC	K	2	11/12	0.97	0.16	56,62,73,78	0
2	GLC	I	2	11/12	0.97	0.16	60,65,68,68	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.

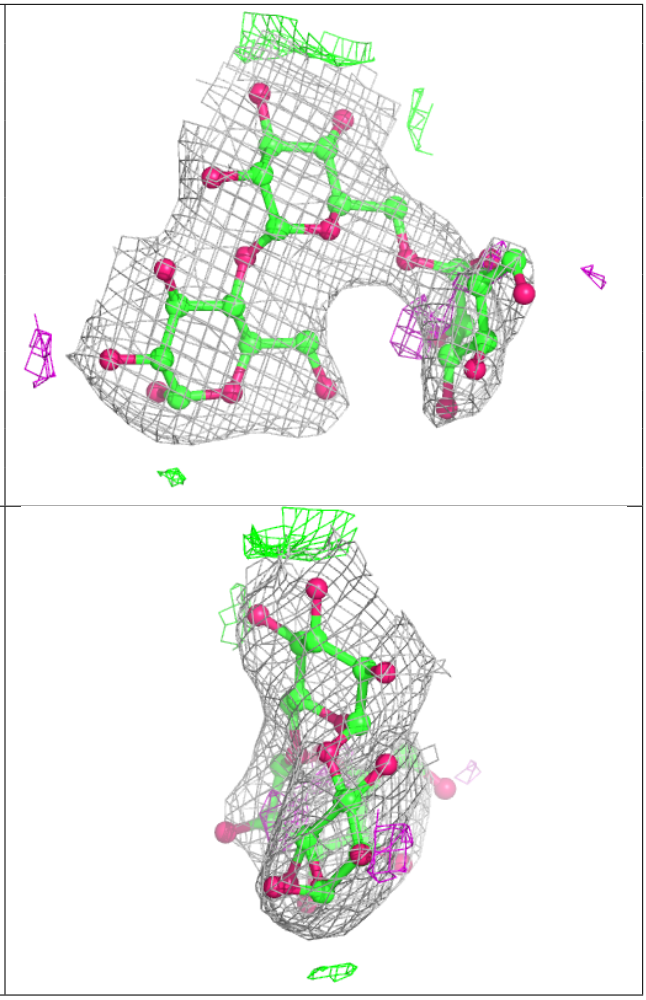
Electron density around Chain E:

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



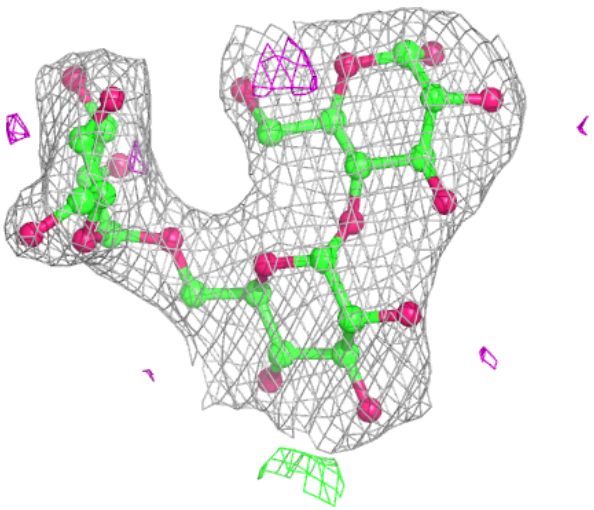
Electron density around Chain G:

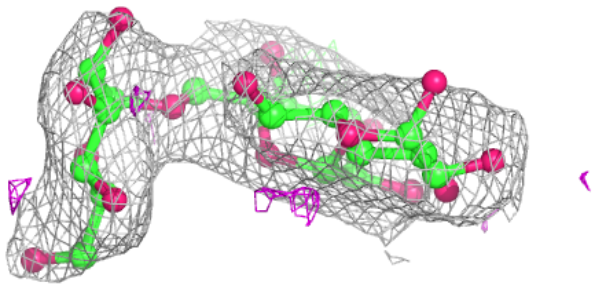
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

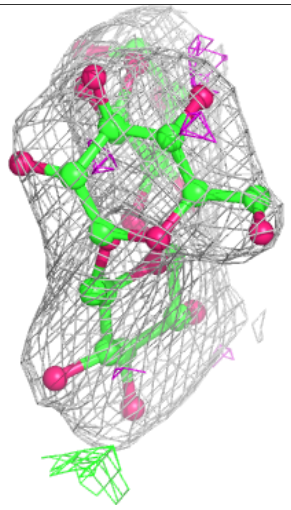


Electron density around Chain I:

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

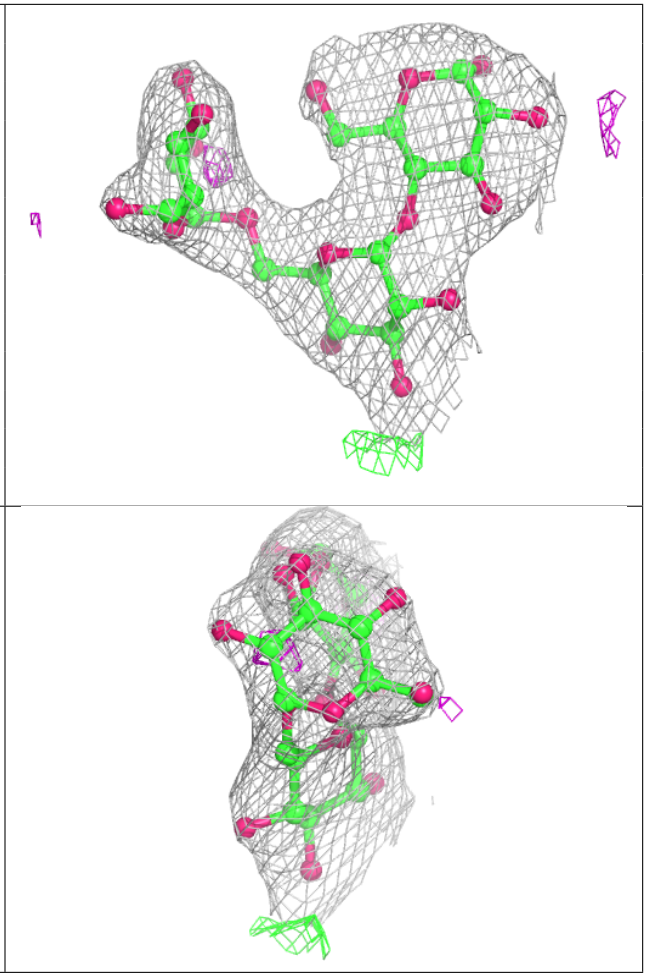






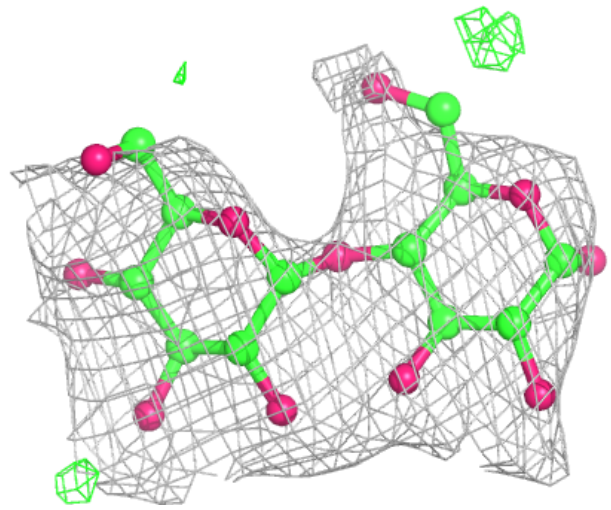
Electron density around Chain K:

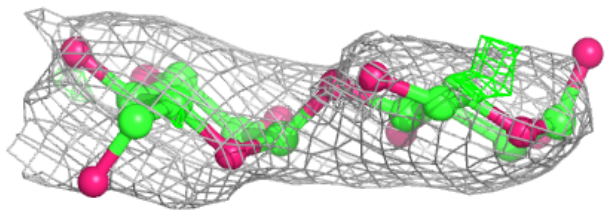
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

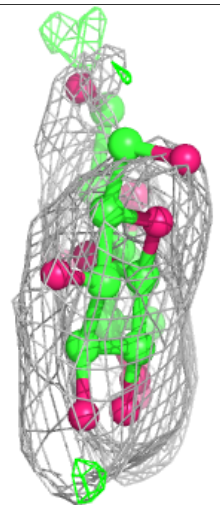


Electron density around Chain F:

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

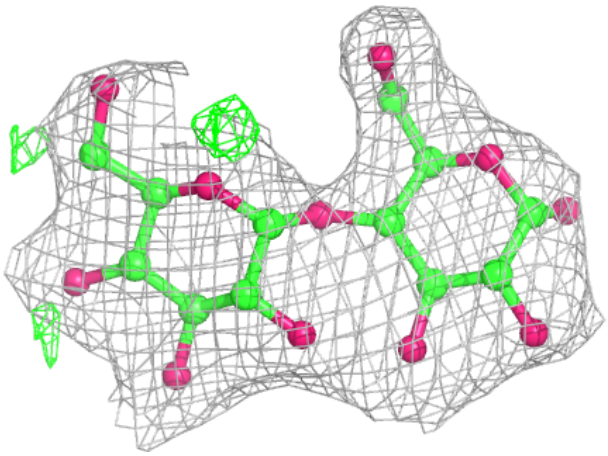


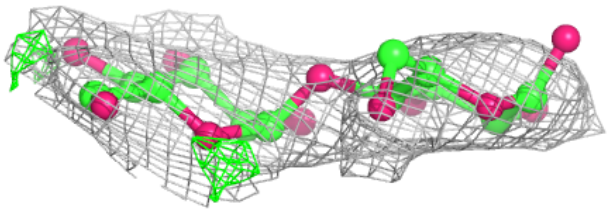


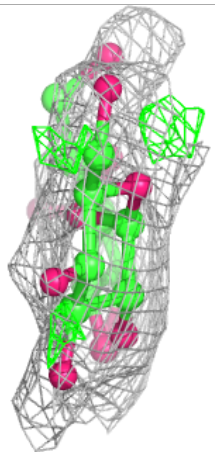


Electron density around Chain H:

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

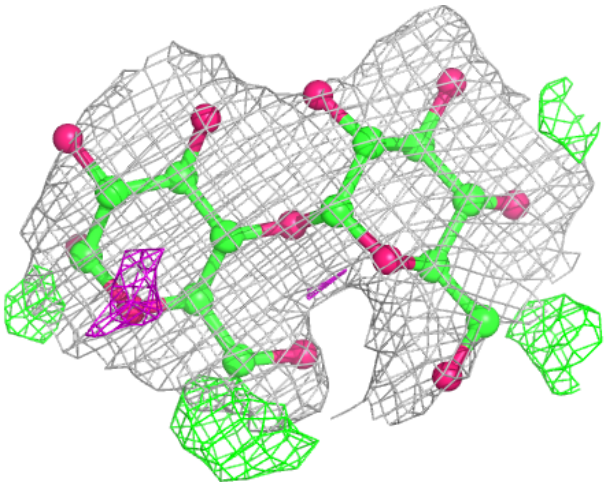


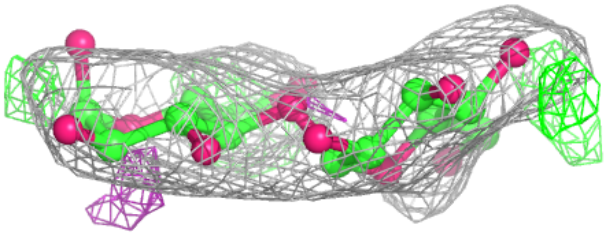


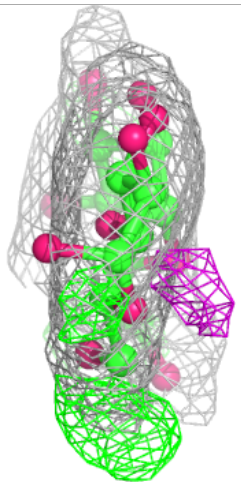


Electron density around Chain J:

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

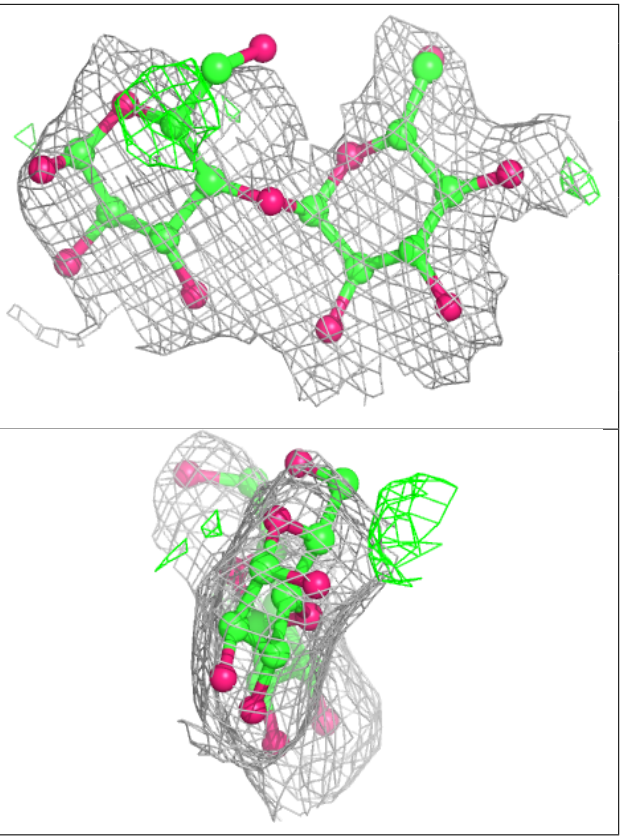






Electron density around Chain L:

$2mF_o$-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
5	NA	C	502	1/1	0.68	0.14	64,64,64,64	0
6	GLC	A	508	12/12	0.75	0.36	81,116,124,137	0
4	CA	B	503	1/1	0.76	0.09	71,71,71,71	0
7	BGC	C	511	12/12	0.76	0.19	44,63,75,75	0
7	BGC	D	510	12/12	0.76	0.22	38,53,68,68	0
7	BGC	B	511	12/12	0.79	0.34	72,102,115,116	0
6	GLC	A	511	12/12	0.81	0.24	76,103,125,125	0
6	GLC	C	510	12/12	0.83	0.36	79,115,139,144	0
5	NA	B	502	1/1	0.85	0.20	74,74,74,74	0
6	GLC	B	510	12/12	0.85	0.28	77,108,124,143	0
5	NA	A	502	1/1	0.89	0.14	59,59,59,59	0
5	NA	D	502	1/1	0.93	0.21	60,60,60,60	0
4	CA	D	503	1/1	0.95	0.07	71,71,71,71	0
4	CA	B	501	1/1	0.96	0.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	C	503	1/1	0.97	0.05	65,65,65,65	0
4	CA	C	504	1/1	0.97	0.12	54,54,54,54	0
4	CA	D	504	1/1	0.98	0.13	57,57,57,57	0
4	CA	C	501	1/1	0.98	0.08	59,59,59,59	0
4	CA	D	501	1/1	0.98	0.08	58,58,58,58	0
4	CA	A	503	1/1	0.98	0.07	62,62,62,62	0
4	CA	B	504	1/1	0.99	0.16	53,53,53,53	0
4	CA	A	501	1/1	0.99	0.07	54,54,54,54	0
4	CA	A	504	1/1	0.99	0.17	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.