Full wwPDB X-ray Structure Validation Report (i)

Aug 24, 2022 – 01:17 am BST

PDB ID	:	7QQH
Title	:	Crystal structure of MYORG (D520N) in complex with Gal-a1,4-Glc
Authors	:	Meek, R.W.; Davies, G.J.
Deposited on	:	2022-01-07
Resolution	:	2.25 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 (1)) were used in the production of this report:

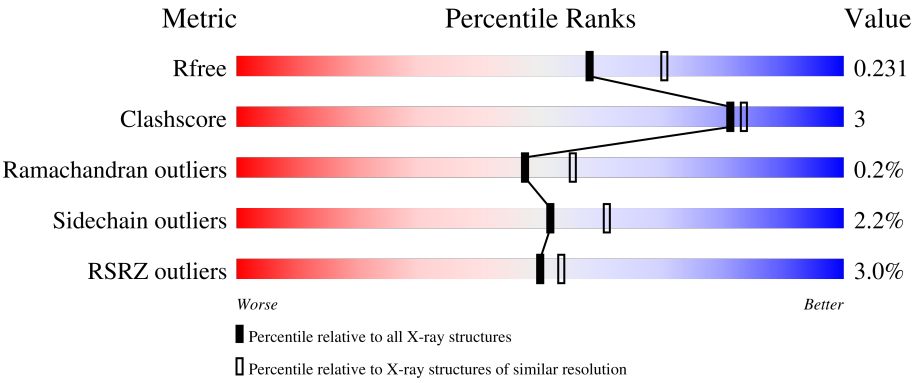
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	636	6% 90% 6% ·
1	B	636	% 89% 7% ·
1	C	636	3% 91% 6% ·
1	D	636	2% 91% 6% ·
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	100%
3	M	2	50% 50%
3	N	2	50% 50%
3	O	2	50% 50%
3	P	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20830 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 Myogenesis-regulating glycosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	1	0
			4916	3176	843	881	16			
1	B	618	Total	C	N	O	S	0	3	0
			5004	3225	870	893	16			
1	C	617	Total	C	N	O	S	0	2	0
			4933	3183	850	884	16			
1	D	618	Total	C	N	O	S	0	0	0
			4971	3208	863	884	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	-	expression tag	UNP Q6NSJ0
A	520	ASN	ASP	engineered mutation	UNP Q6NSJ0
B	79	GLY	-	expression tag	UNP Q6NSJ0
B	520	ASN	ASP	engineered mutation	UNP Q6NSJ0
C	79	GLY	-	expression tag	UNP Q6NSJ0
C	520	ASN	ASP	engineered mutation	UNP Q6NSJ0
D	79	GLY	-	expression tag	UNP Q6NSJ0
D	520	ASN	ASP	engineered mutation	UNP Q6NSJ0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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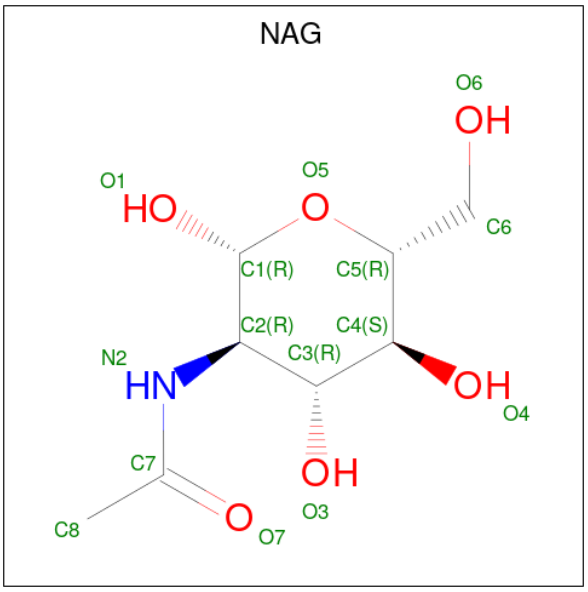
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	F	2	Total C N O 28 16 2 10	0	0	0
2	G	2	Total C N O 28 16 2 10	0	0	0
2	H	2	Total C N O 28 16 2 10	0	0	0
2	I	2	Total C N O 28 16 2 10	0	0	0
2	J	2	Total C N O 28 16 2 10	0	0	0
2	K	2	Total C N O 28 16 2 10	0	0	0
2	L	2	Total C N O 28 16 2 10	0	0	0

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

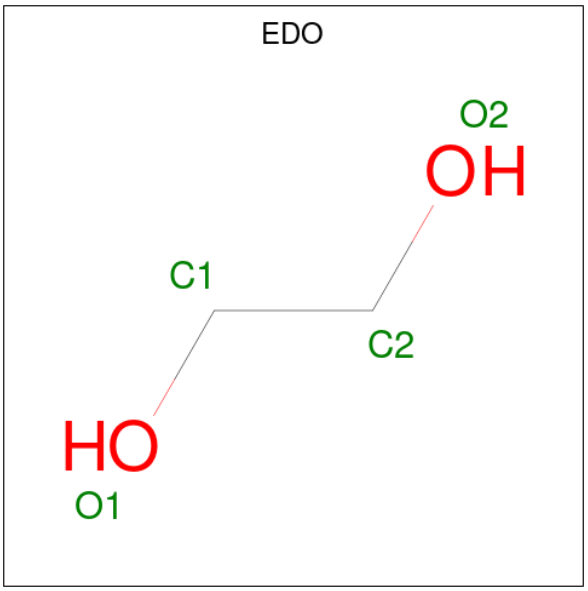
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	M	2	Total C O 23 12 11	0	0	0
3	N	2	Total C O 23 12 11	0	0	0
3	O	2	Total C O 23 12 11	0	0	0
3	P	2	Total C O 23 12 11	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



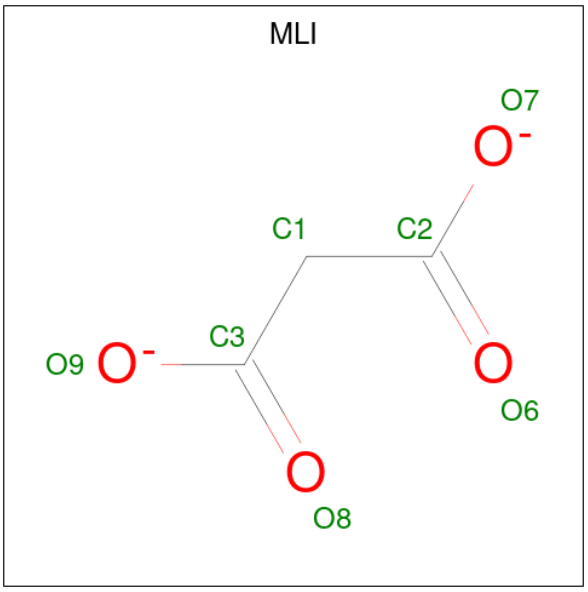
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 7 is water.

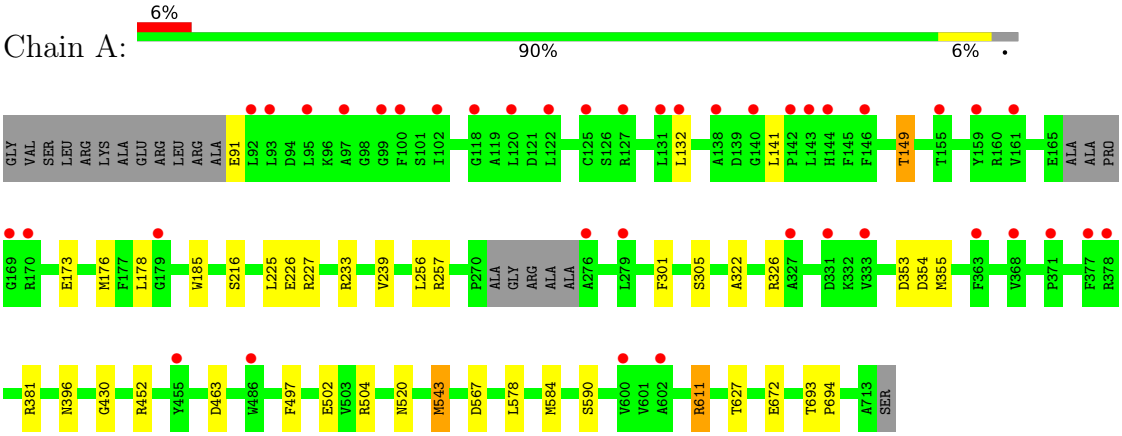
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	87	Total O 87 87	0	0
7	B	152	Total O 152 152	0	0
7	C	92	Total O 92 92	0	0
7	D	155	Total O 155 155	0	0

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.

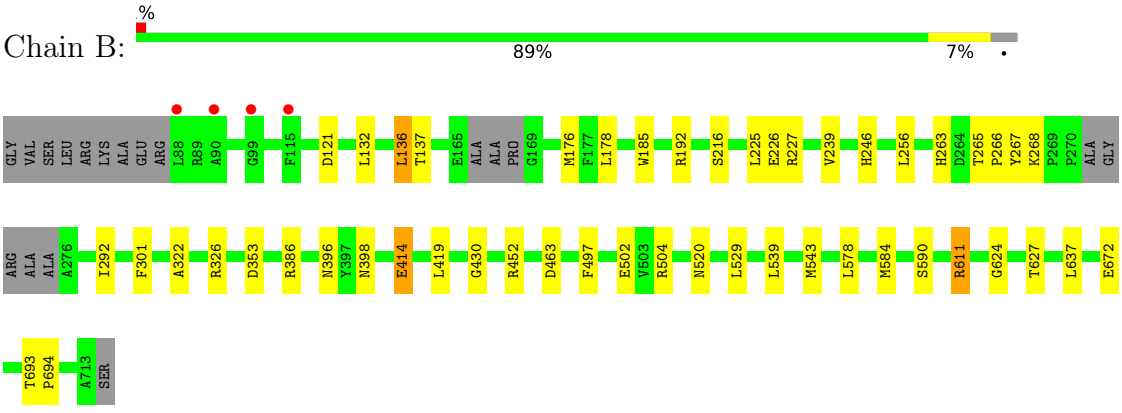
• Molecule 1: Myogenesis-regulating glycosidase

Chain A:



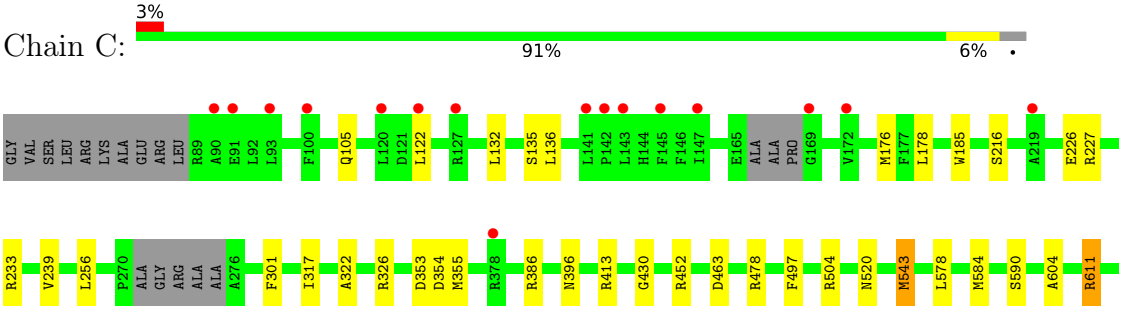
• Molecule 1: Myogenesis-regulating glycosidase

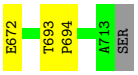
Chain B:



• Molecule 1: Myogenesis-regulating glycosidase

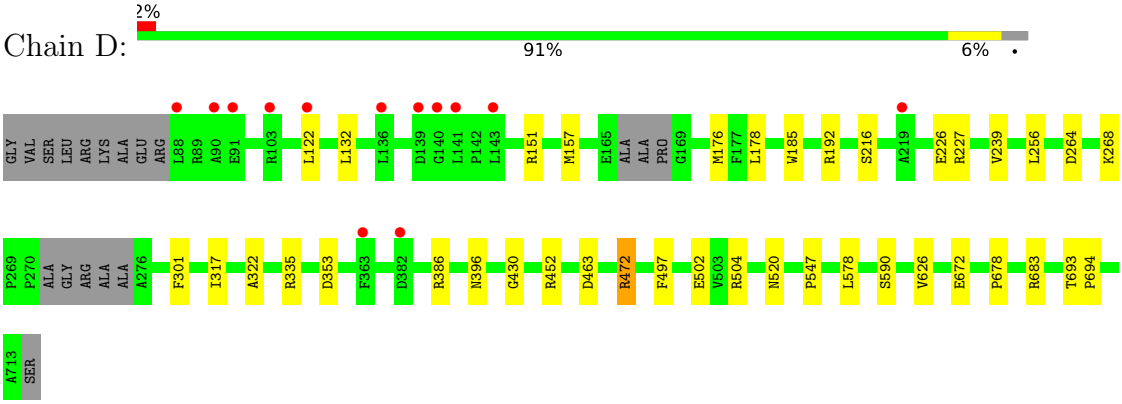
Chain C:





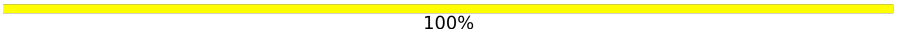
• Molecule 1: Myogenesis-regulating glycosidase

Chain D:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

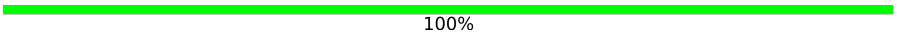


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

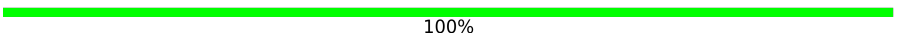
Chain J:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain M:

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

Chain N:

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

Chain O:

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

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.29Å 79.10Å 178.02Å 80.91° 79.11° 62.67°	Depositor
Resolution (Å)	64.53 – 2.25 64.53 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (64.53-2.25) 94.7 (64.53-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.227 0.217 , 0.231	Depositor DCC
R_{free} test set	7813 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20830	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, BGC, MLI, NAG, GLA

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	0.64	0/5073	0.74	0/6917
1	B	0.63	0/5158	0.75	0/7025
1	C	0.64	0/5090	0.74	0/6943
1	D	0.63	0/5125	0.75	0/6980
All	All	0.63	0/20446	0.74	0/27865

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

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	4916	0	4695	21	0
1	B	5004	0	4825	39	0
1	C	4933	0	4704	19	0
1	D	4971	0	4796	21	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
3	M	23	0	21	1	0
3	N	23	0	21	1	0
3	O	23	0	21	1	0
3	P	23	0	21	1	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
4	C	42	0	39	0	0
4	D	28	0	26	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
5	C	8	0	12	1	0
5	D	12	0	18	1	0
6	A	7	0	2	0	0
6	B	7	0	2	0	0
6	C	7	0	2	0	0
6	D	7	0	2	0	0
7	A	87	0	0	0	0
7	B	152	0	0	3	0
7	C	92	0	0	0	0
7	D	155	0	0	3	0
All	All	20830	0	19496	104	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 3.

All (104) 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:173:GLU:OE2	1:A:257:ARG:HD2	1.85	0.76
1:B:246:HIS:NE2	1:B:265[B]:THR:CG2	2.53	0.71
1:A:584:MET:O	1:A:611:ARG:NH2	2.25	0.70
1:B:584:MET:O	1:B:611:ARG:NH2	2.25	0.69
1:C:584:MET:O	1:C:611:ARG:NH2	2.25	0.69
1:B:246:HIS:NE2	1:B:265[B]:THR:HG21	2.14	0.63
1:B:121:ASP:OD1	1:B:136:LEU:HD11	2.01	0.61
1:B:226:GLU:HG2	1:B:301:PHE:CE1	2.37	0.59
1:B:246:HIS:NE2	1:B:265[B]:THR:HG23	2.17	0.59
1:D:226:GLU:HG2	1:D:301:PHE:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD12	1:A:225:LEU:C	2.24	0.58
1:C:226:GLU:HG2	1:C:301:PHE:CE1	2.39	0.57
1:A:226:GLU:HG2	1:A:301:PHE:CE1	2.39	0.57
1:B:225:LEU:C	1:B:225:LEU:HD12	2.25	0.56
1:D:268:LYS:NZ	7:D:905:HOH:O	2.38	0.56
1:B:539:LEU:O	1:B:543:MET:HG2	2.06	0.56
1:D:678:PRO:O	1:D:694:PRO:HB3	2.06	0.56
1:C:317:ILE:HD13	5:C:806:EDO:O2	2.07	0.55
1:B:246:HIS:CE1	1:B:265[B]:THR:HG21	2.43	0.54
1:C:543:MET:CE	1:C:543:MET:HA	2.38	0.54
1:A:543:MET:HA	1:A:543:MET:CE	2.39	0.53
1:B:624:GLY:O	1:B:627:THR:HG22	2.09	0.53
1:C:543:MET:HA	1:C:543:MET:HE2	1.91	0.53
1:B:543:MET:HA	1:B:543:MET:CE	2.39	0.52
1:A:178:LEU:HG	1:A:185:TRP:CD1	2.45	0.51
1:C:227:ARG:HB3	1:C:239:VAL:HB	1.92	0.51
1:B:178:LEU:HG	1:B:185:TRP:CD1	2.45	0.51
1:C:178:LEU:HG	1:C:185:TRP:CD1	2.46	0.51
1:D:264:ASP:OD1	1:D:472:ARG:NH2	2.43	0.51
3:P:1:BGC:H6C2	3:P:2:GLA:H5	1.93	0.51
1:D:547:PRO:HG3	1:D:626:VAL:HG11	1.94	0.49
1:D:178:LEU:HG	1:D:185:TRP:CD1	2.47	0.49
1:B:398:ASN:HD22	2:H:1:NAG:H83	1.77	0.49
1:A:578:LEU:C	1:A:578:LEU:HD23	2.33	0.49
1:B:246:HIS:NE2	1:B:265[A]:THR:CG2	2.75	0.49
1:B:578:LEU:C	1:B:578:LEU:HD23	2.33	0.49
1:C:578:LEU:C	1:C:578:LEU:HD23	2.33	0.48
1:B:265[B]:THR:HG22	1:B:267:TYR:H	1.78	0.48
1:D:396:ASN:HA	1:D:430:GLY:HA3	1.95	0.48
1:D:578:LEU:C	1:D:578:LEU:HD23	2.33	0.48
1:A:396:ASN:HA	1:A:430:GLY:HA3	1.95	0.48
1:B:136:LEU:HD12	1:B:137:THR:O	2.13	0.48
1:B:265[B]:THR:CG2	1:B:267:TYR:HD2	2.27	0.48
1:D:227:ARG:HB3	1:D:239:VAL:HB	1.96	0.48
1:A:543:MET:HA	1:A:543:MET:HE2	1.96	0.48
1:B:396:ASN:HA	1:B:430:GLY:HA3	1.96	0.47
1:D:683:ARG:NE	7:D:901:HOH:O	2.27	0.47
1:B:227:ARG:HB3	1:B:239:VAL:HB	1.95	0.47
1:B:452:ARG:HD2	1:B:497:PHE:CE1	2.49	0.47
1:A:227:ARG:HB3	1:A:239:VAL:HB	1.96	0.47
1:A:141:LEU:HD12	1:A:141:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:SER:HA	1:A:627[B]:THR:HG23	1.96	0.47
1:C:396:ASN:HA	1:C:430:GLY:HA3	1.96	0.47
1:A:463:ASP:OD1	1:A:504:ARG:HD3	2.15	0.46
1:C:463:ASP:OD1	1:C:504:ARG:HD3	2.16	0.46
1:B:463:ASP:OD1	1:B:504:ARG:HD3	2.16	0.46
1:C:452:ARG:HD2	1:C:497:PHE:CE1	2.51	0.46
1:A:452:ARG:HD2	1:A:497:PHE:CE1	2.51	0.46
1:C:135:SER:C	1:C:136:LEU:HD22	2.36	0.46
1:D:176:MET:CE	1:D:256:LEU:HD12	2.46	0.46
1:B:263:HIS:O	1:B:265[A]:THR:HG23	2.16	0.45
1:B:322:ALA:HB3	1:B:590:SER:HB3	1.98	0.45
1:D:463:ASP:OD1	1:D:504:ARG:HD3	2.16	0.45
1:D:452:ARG:HD2	1:D:497:PHE:CE1	2.50	0.45
1:A:176:MET:CE	1:A:256:LEU:HD12	2.47	0.45
1:D:322:ALA:HB3	1:D:590:SER:HB3	1.98	0.44
1:B:265[B]:THR:CG2	1:B:266:PRO:HD2	2.46	0.44
1:D:317:ILE:HD13	5:D:803:EDO:O2	2.17	0.44
1:B:226:GLU:HG2	1:B:301:PHE:CZ	2.53	0.44
1:C:176:MET:CE	1:C:256:LEU:HD12	2.48	0.44
1:C:322:ALA:HB3	1:C:590:SER:HB3	1.99	0.44
1:C:693:THR:HA	1:C:694:PRO:C	2.38	0.43
1:A:322:ALA:HB3	1:A:590:SER:HB3	1.98	0.43
1:B:693:THR:HA	1:B:694:PRO:C	2.38	0.43
1:B:176:MET:CE	1:B:256:LEU:HD12	2.48	0.43
1:D:151:ARG:HD3	1:D:157:MET:CE	2.48	0.43
1:D:693:THR:HA	1:D:694:PRO:C	2.39	0.43
1:B:543:MET:HA	1:B:543:MET:HE2	2.00	0.43
3:N:1:BGC:H6C2	3:N:2:GLA:H5	2.01	0.42
1:B:268:LYS:NZ	7:B:902:HOH:O	2.42	0.42
1:D:226:GLU:HG2	1:D:301:PHE:CZ	2.54	0.42
1:B:414:GLU:OE2	1:B:419:LEU:HB2	2.20	0.42
1:D:452:ARG:HD2	1:D:497:PHE:CD1	2.54	0.42
3:O:1:BGC:H6C2	3:O:2:GLA:H5	2.02	0.42
1:A:693:THR:HA	1:A:694:PRO:C	2.39	0.42
1:D:176:MET:HE2	1:D:256:LEU:HD12	2.01	0.42
1:D:192:ARG:NH1	7:D:915:HOH:O	2.53	0.42
1:A:354:ASP:HA	1:A:355:MET:HA	1.83	0.41
3:M:1:BGC:H6C2	3:M:2:GLA:H5	2.00	0.41
1:B:265[B]:THR:HG21	1:B:267:TYR:HD2	1.84	0.41
1:A:91:GLU:CG	1:A:149:THR:HG21	2.51	0.41
1:C:226:GLU:HG2	1:C:301:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:HG2	1:A:301:PHE:CZ	2.55	0.41
1:A:452:ARG:HD2	1:A:497:PHE:CD1	2.55	0.41
1:B:192:ARG:NH1	7:B:910:HOH:O	2.54	0.41
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.94	0.41
1:B:452:ARG:HD2	1:B:497:PHE:CD1	2.55	0.41
1:B:292:ILE:HD12	1:B:292:ILE:HA	1.92	0.41
1:C:354:ASP:HA	1:C:355:MET:HA	1.83	0.41
1:B:192:ARG:NH2	7:B:908:HOH:O	2.53	0.40
1:B:192:ARG:HG3	1:B:529:LEU:HD11	2.03	0.40
1:B:246:HIS:NE2	1:B:265[A]:THR:HG21	2.36	0.40
1:C:452:ARG:HD2	1:C:497:PHE:CD1	2.57	0.40
1:C:578:LEU:HD11	1:C:604:ALA:HB2	2.04	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	610/636 (96%)	589 (97%)	20 (3%)	1 (0%)	47	55
1	B	615/636 (97%)	592 (96%)	22 (4%)	1 (0%)	47	55
1	C	613/636 (96%)	589 (96%)	23 (4%)	1 (0%)	47	55
1	D	612/636 (96%)	588 (96%)	23 (4%)	1 (0%)	47	55
All	All	2450/2544 (96%)	2358 (96%)	88 (4%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
1	B	520	ASN
1	C	520	ASN

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Mol	Chain	Res	Type
1	D	520	ASN

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	506/533 (95%)	494 (98%)	12 (2%)	49	58
1	B	521/533 (98%)	511 (98%)	10 (2%)	57	66
1	C	508/533 (95%)	495 (97%)	13 (3%)	46	55
1	D	516/533 (97%)	507 (98%)	9 (2%)	60	71
All	All	2051/2132 (96%)	2007 (98%)	44 (2%)	52	62

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	149	THR
1	A	216	SER
1	A	233	ARG
1	A	326	ARG
1	A	353	ASP
1	A	381	ARG
1	A	502	GLU
1	A	543	MET
1	A	567	ASP
1	A	611	ARG
1	A	672	GLU
1	B	132	LEU
1	B	136	LEU
1	B	216	SER
1	B	326	ARG
1	B	353	ASP
1	B	386	ARG
1	B	414	GLU
1	B	502	GLU

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Mol	Chain	Res	Type
1	B	611	ARG
1	B	672	GLU
1	C	105	GLN
1	C	122	LEU
1	C	132	LEU
1	C	216	SER
1	C	233	ARG
1	C	326	ARG
1	C	353	ASP
1	C	386	ARG
1	C	413	ARG
1	C	478	ARG
1	C	543	MET
1	C	611	ARG
1	C	672	GLU
1	D	122	LEU
1	D	132	LEU
1	D	216	SER
1	D	335	ARG
1	D	353	ASP
1	D	386	ARG
1	D	472	ARG
1	D	502	GLU
1	D	672	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	561	GLN
1	C	338	GLN
1	C	561	GLN
1	D	338	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)

24 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	NAG	E	1	2,1	14,14,15	0.37	0	17,19,21	1.09	2 (11%)
2	NAG	E	2	2	14,14,15	0.27	0	17,19,21	1.13	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.51	0	17,19,21	0.91	1 (5%)
2	NAG	F	2	2	14,14,15	0.45	0	17,19,21	0.95	0
2	NAG	G	1	2,1	14,14,15	0.32	0	17,19,21	0.87	0
2	NAG	G	2	2	14,14,15	0.38	0	17,19,21	0.74	0
2	NAG	H	1	2,1	14,14,15	0.52	0	17,19,21	1.49	4 (23%)
2	NAG	H	2	2	14,14,15	0.44	0	17,19,21	1.38	3 (17%)
2	NAG	I	1	2,1	14,14,15	0.37	0	17,19,21	0.95	1 (5%)
2	NAG	I	2	2	14,14,15	0.30	0	17,19,21	0.87	0
2	NAG	J	1	2,1	14,14,15	0.30	0	17,19,21	1.09	1 (5%)
2	NAG	J	2	2	14,14,15	0.26	0	17,19,21	0.82	0
2	NAG	K	1	2,1	14,14,15	0.35	0	17,19,21	1.38	2 (11%)
2	NAG	K	2	2	14,14,15	0.34	0	17,19,21	0.99	0
2	NAG	L	1	2,1	14,14,15	0.46	0	17,19,21	0.54	0
2	NAG	L	2	2	14,14,15	0.26	0	17,19,21	0.72	0
3	BGC	M	1	3	12,12,12	0.42	0	17,17,17	0.73	0
3	GLA	M	2	3	11,11,12	0.30	0	15,15,17	1.21	1 (6%)
3	BGC	N	1	3	12,12,12	0.46	0	17,17,17	0.70	0
3	GLA	N	2	3	11,11,12	0.50	0	15,15,17	1.19	1 (6%)
3	BGC	O	1	3	12,12,12	0.53	0	17,17,17	0.85	0
3	GLA	O	2	3	11,11,12	0.57	0	15,15,17	1.14	1 (6%)
3	BGC	P	1	3	12,12,12	0.48	0	17,17,17	0.70	0
3	GLA	P	2	3	11,11,12	0.46	0	15,15,17	1.20	1 (6%)

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	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
3	BGC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLA	M	2	3	-	0/2/19/22	0/1/1/1
3	BGC	N	1	3	-	0/2/22/22	0/1/1/1
3	GLA	N	2	3	-	0/2/19/22	0/1/1/1
3	BGC	O	1	3	-	0/2/22/22	0/1/1/1
3	GLA	O	2	3	-	0/2/19/22	0/1/1/1
3	BGC	P	1	3	-	0/2/22/22	0/1/1/1
3	GLA	P	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	2	GLA	C1-O5-C5	3.91	117.49	112.19
3	M	2	GLA	C1-O5-C5	3.64	117.13	112.19
3	N	2	GLA	C1-O5-C5	3.56	117.02	112.19
2	K	1	NAG	C1-C2-N2	3.18	115.92	110.49
2	E	2	NAG	O5-C5-C6	3.03	111.96	107.20
3	O	2	GLA	C1-O5-C5	3.03	116.30	112.19
2	H	1	NAG	O5-C1-C2	-2.99	106.56	111.29
2	H	2	NAG	C2-N2-C7	2.92	127.07	122.90
2	F	1	NAG	C1-C2-N2	-2.91	105.52	110.49
2	E	1	NAG	O5-C1-C2	-2.82	106.83	111.29
2	H	1	NAG	C8-C7-N2	2.82	120.87	116.10
2	J	1	NAG	O3-C3-C4	-2.60	104.34	110.35
2	H	1	NAG	C1-O5-C5	2.48	115.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	NAG	O5-C5-C6	2.48	111.09	107.20
2	H	2	NAG	O5-C5-C6	2.39	110.95	107.20
2	H	1	NAG	C4-C3-C2	-2.37	107.55	111.02
2	K	1	NAG	C4-C3-C2	-2.32	107.61	111.02
2	E	1	NAG	C1-C2-N2	2.14	114.15	110.49
2	H	2	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6

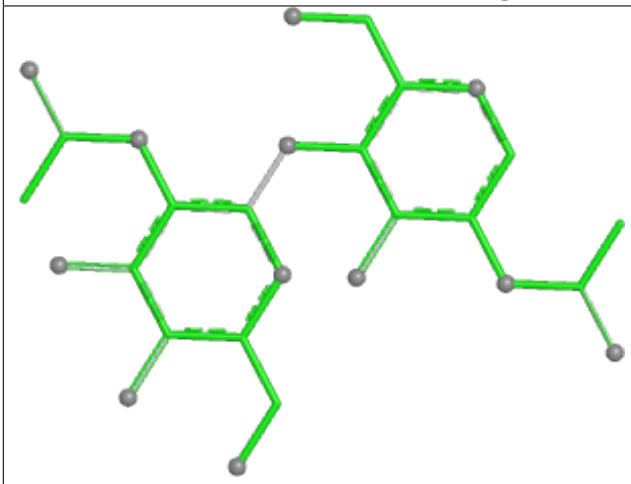
There are no ring outliers.

9 monomers are involved in 5 short contacts:

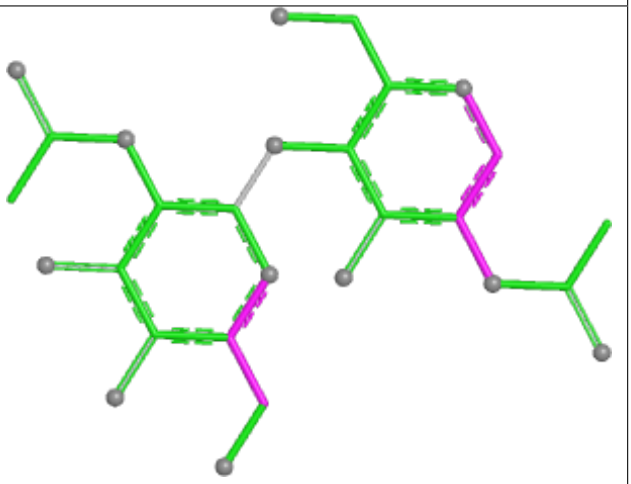
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	BGC	1	0
3	M	1	BGC	1	0
3	P	2	GLA	1	0
3	M	2	GLA	1	0
2	H	1	NAG	1	0
3	O	2	GLA	1	0
3	N	2	GLA	1	0
3	P	1	BGC	1	0
3	N	1	BGC	1	0

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

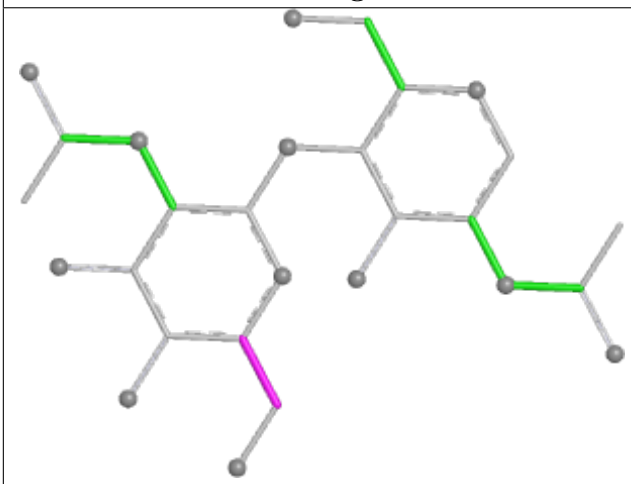
Oligosaccharide Chain E



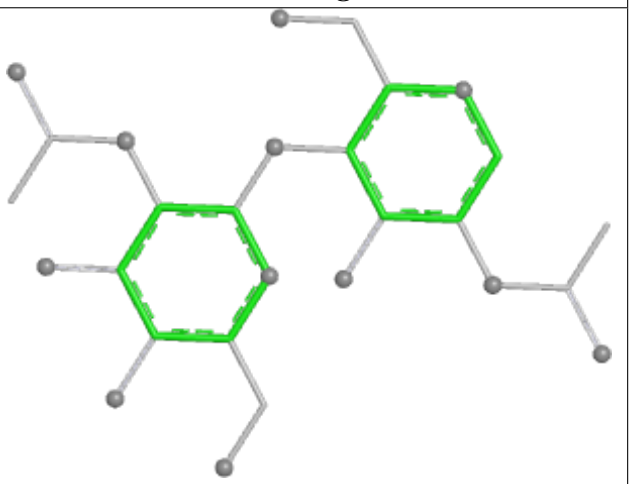
Bond lengths



Bond angles

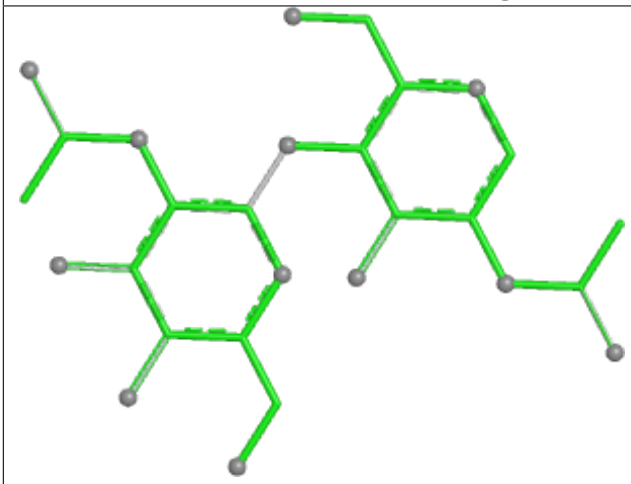


Torsions

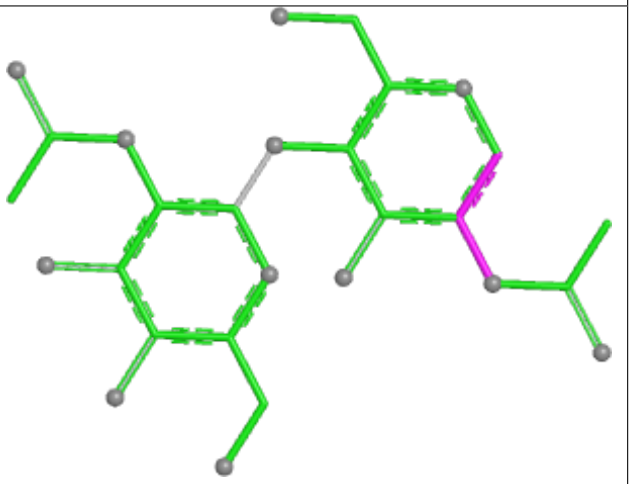


Rings

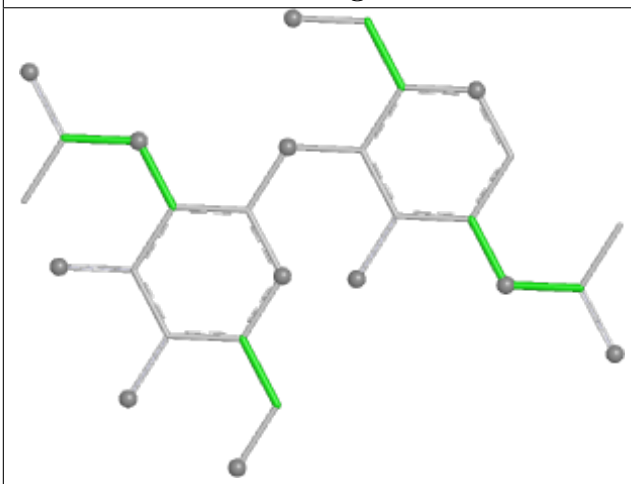
Oligosaccharide Chain F



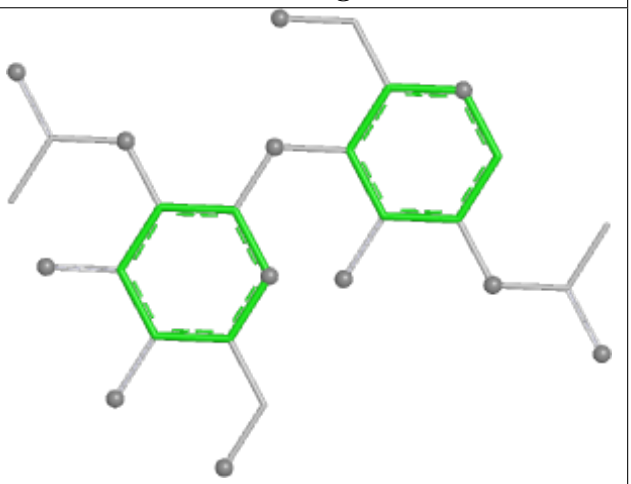
Bond lengths



Bond angles

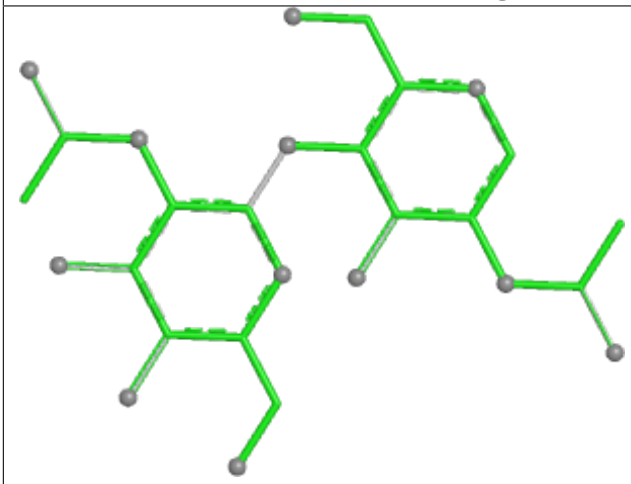


Torsions

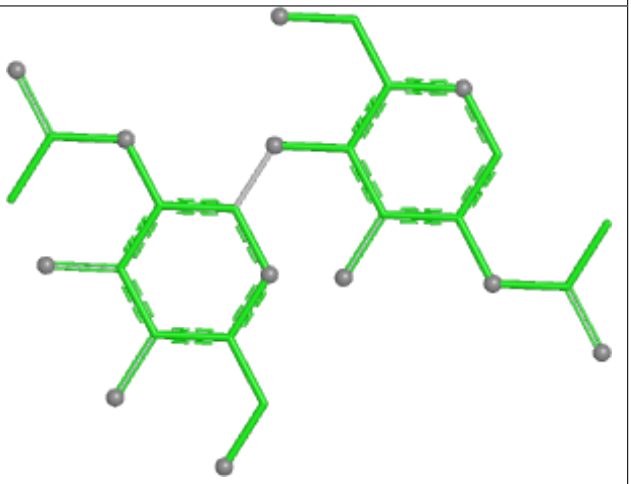


Rings

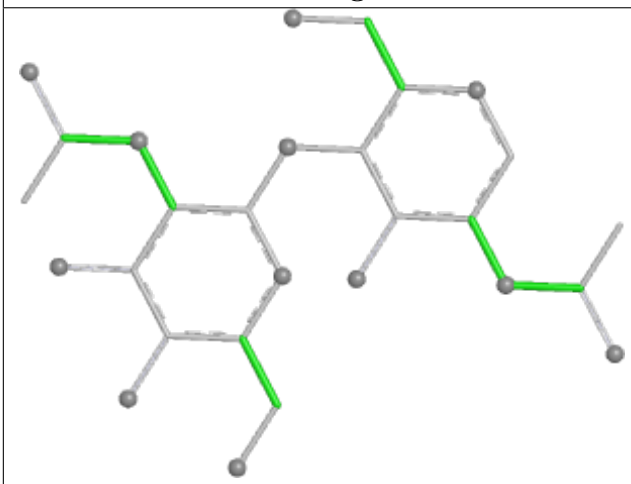
Oligosaccharide Chain G



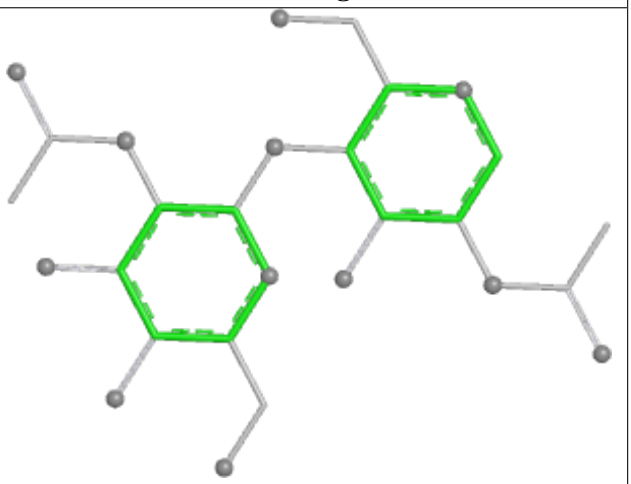
Bond lengths



Bond angles

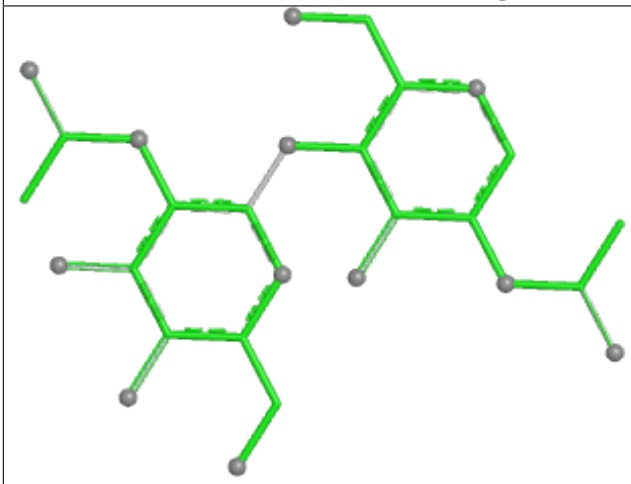


Torsions

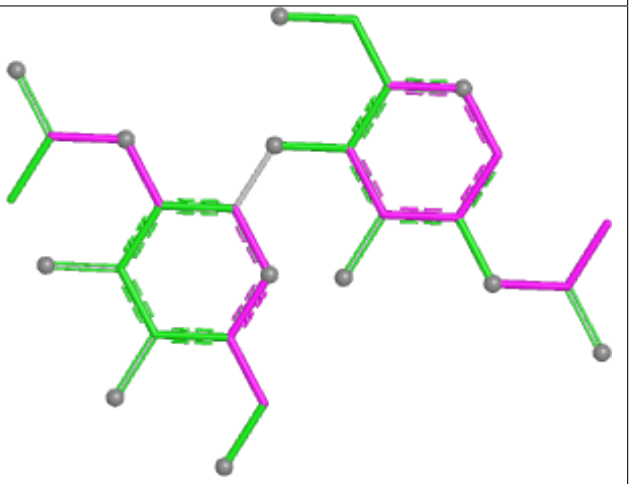


Rings

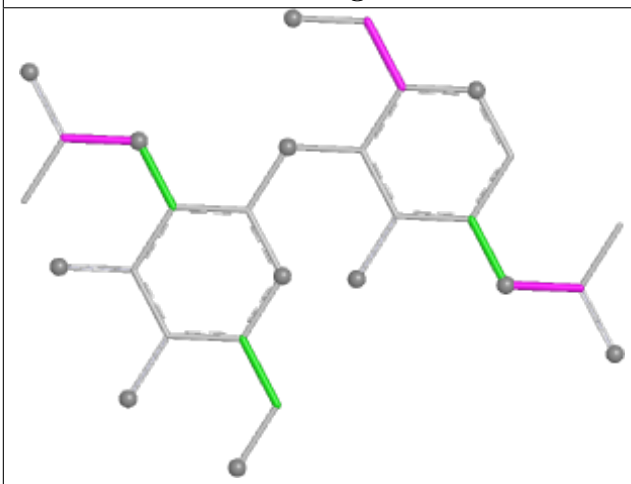
Oligosaccharide Chain H



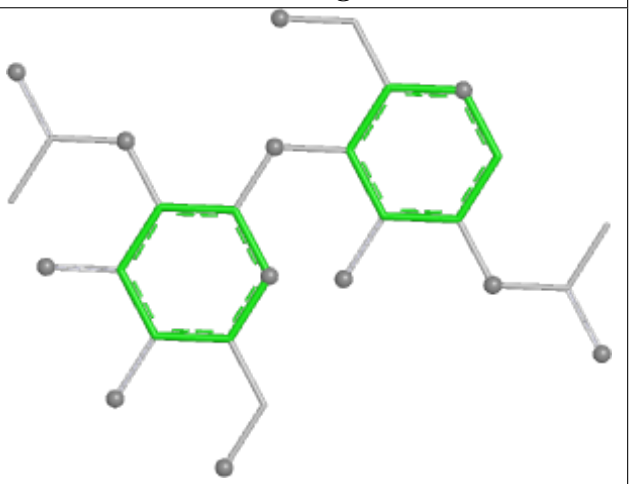
Bond lengths



Bond angles

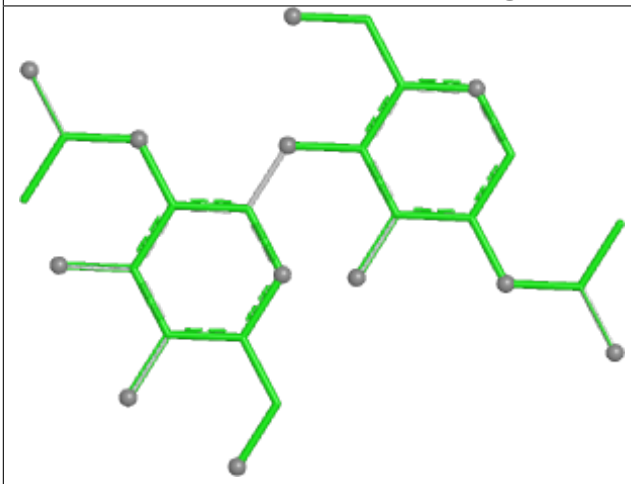


Torsions

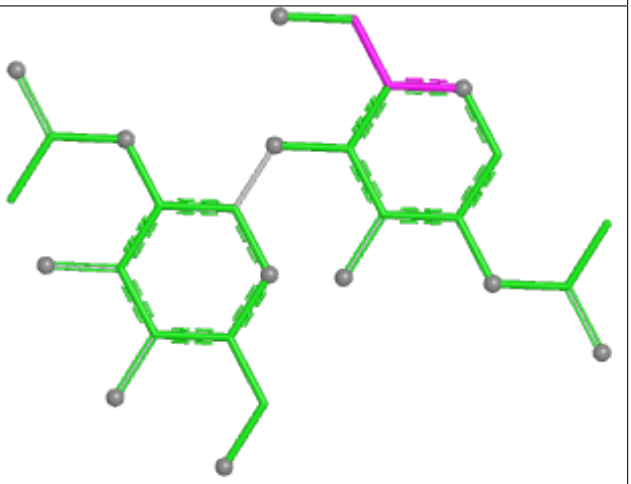


Rings

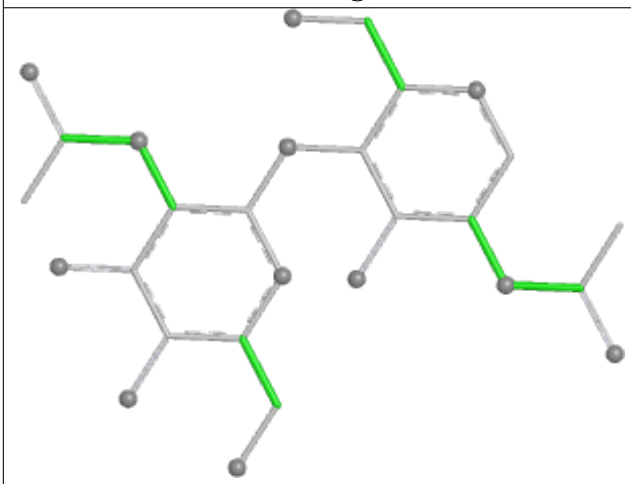
Oligosaccharide Chain I



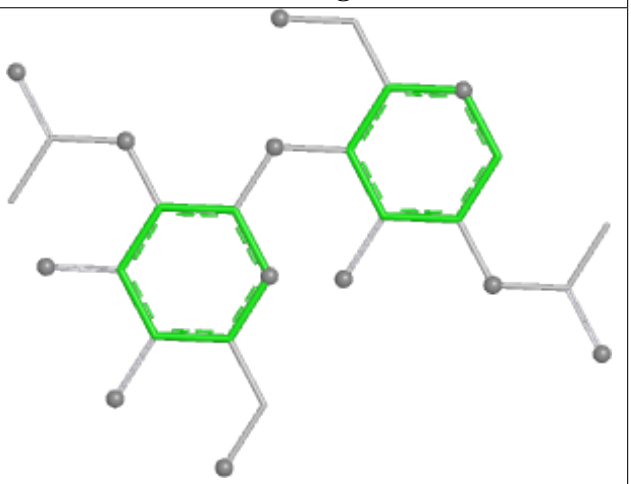
Bond lengths



Bond angles

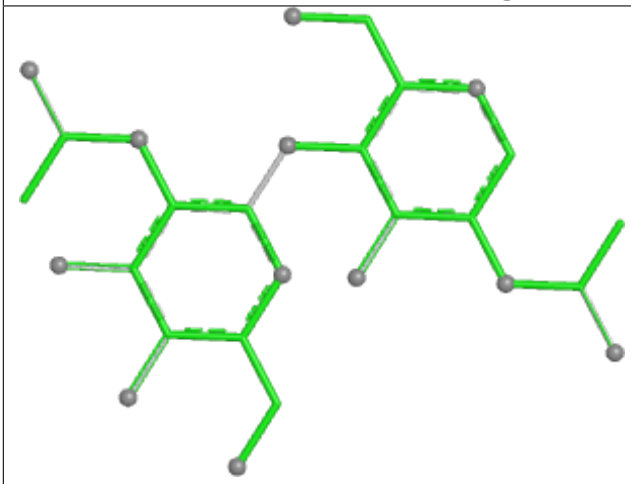


Torsions

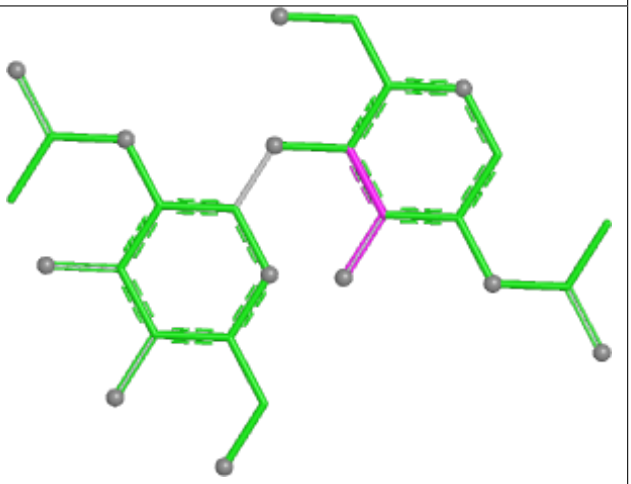


Rings

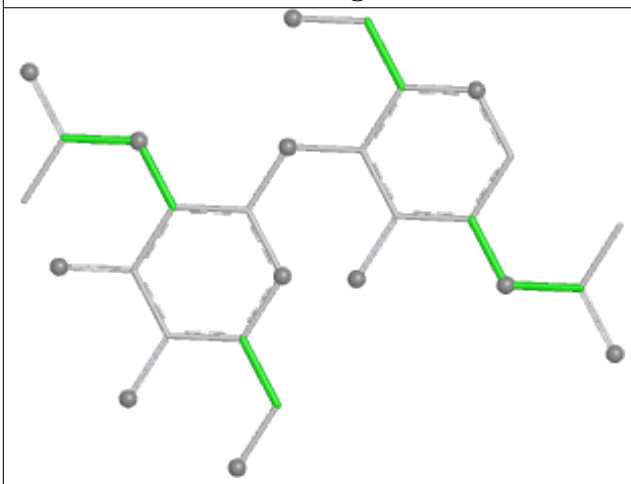
Oligosaccharide Chain J



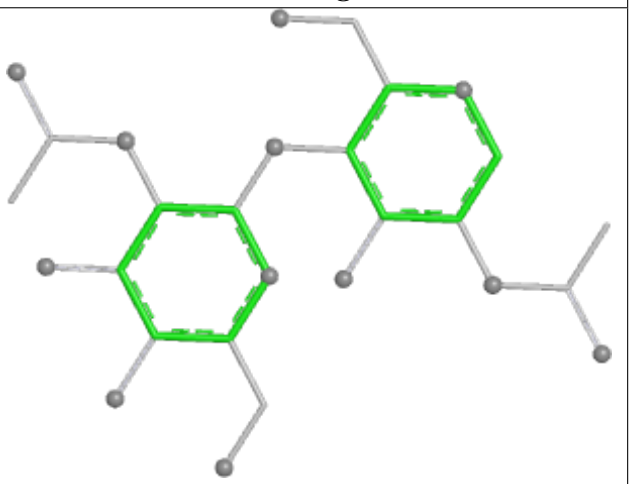
Bond lengths



Bond angles

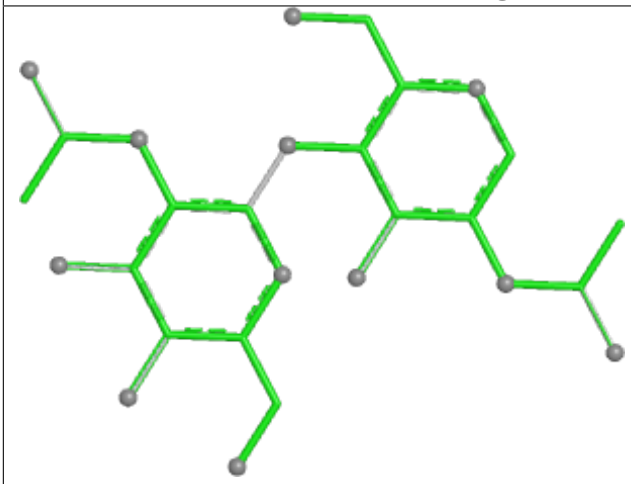


Torsions

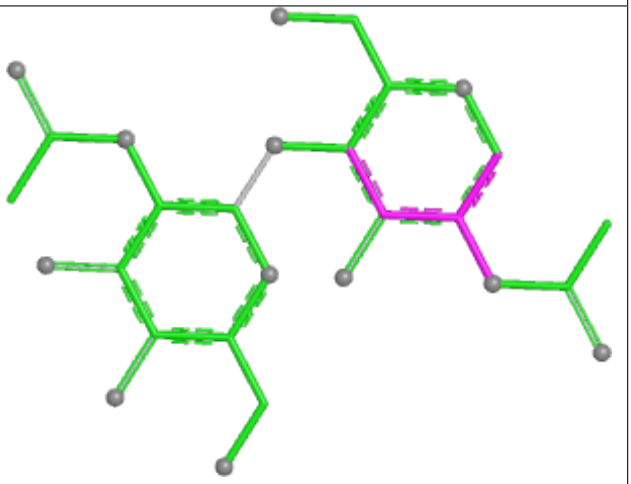


Rings

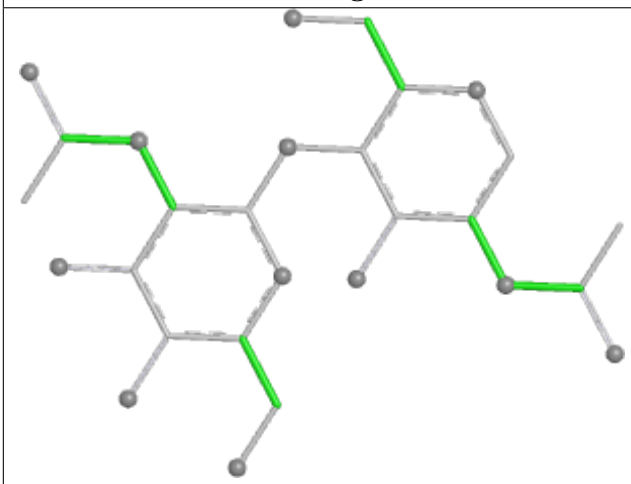
Oligosaccharide Chain K



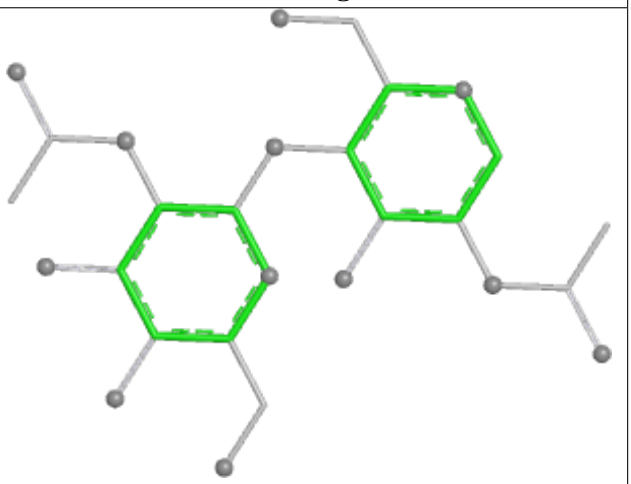
Bond lengths



Bond angles

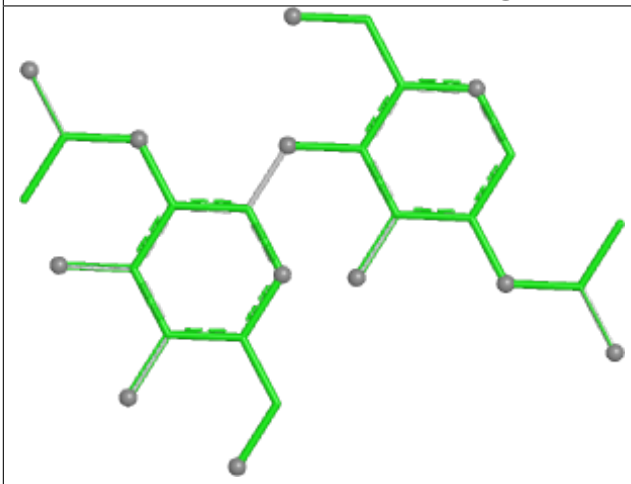


Torsions

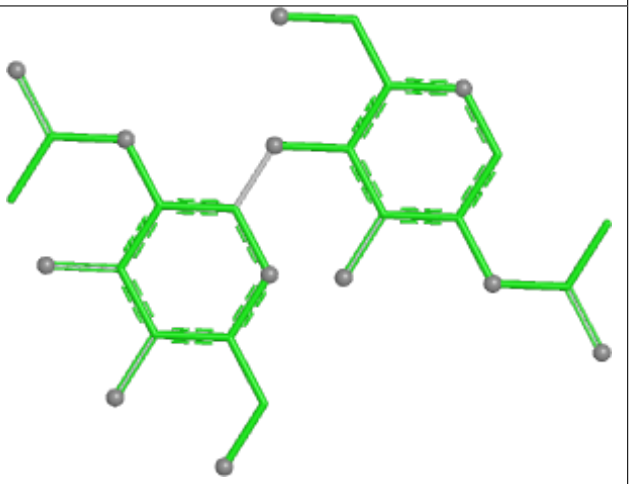


Rings

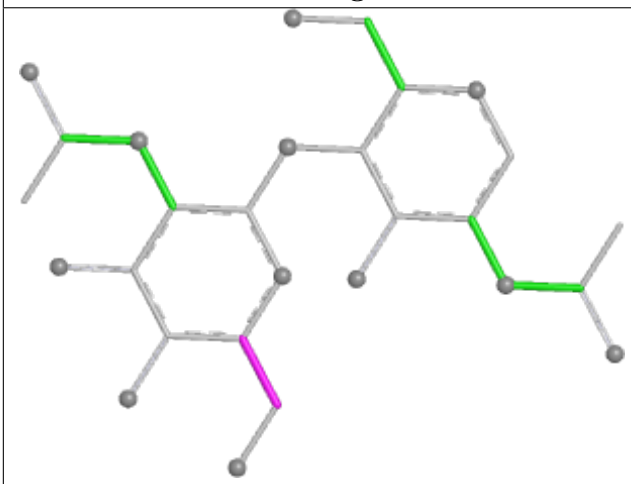
Oligosaccharide Chain L



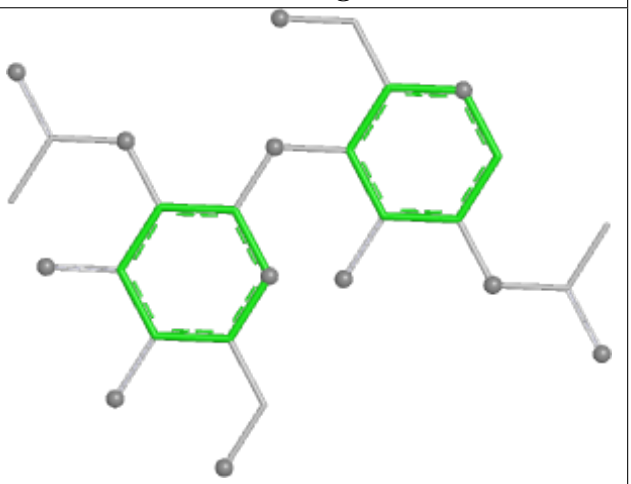
Bond lengths



Bond angles

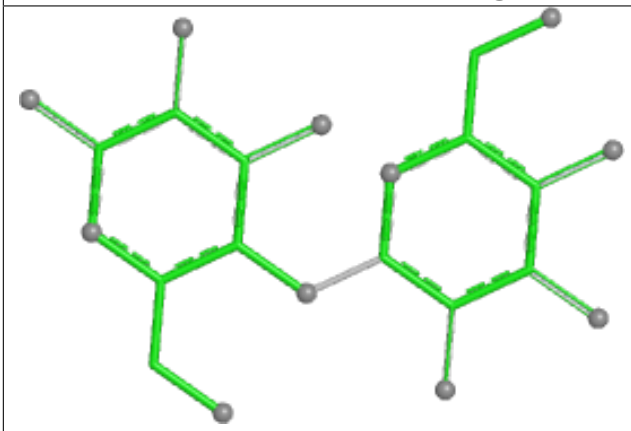


Torsions

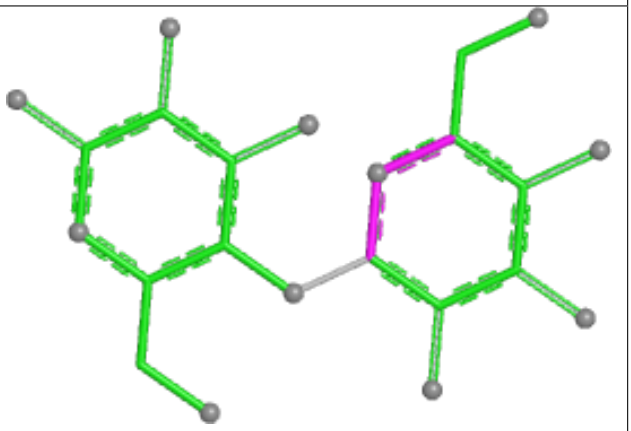


Rings

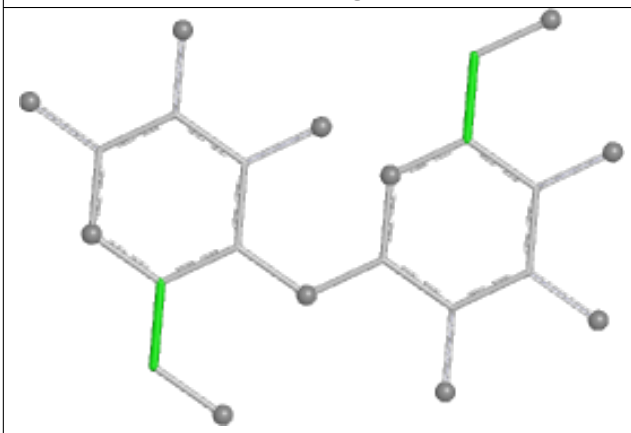
Oligosaccharide Chain M



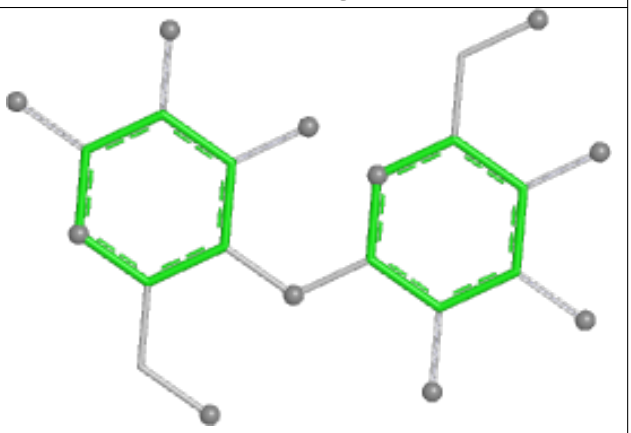
Bond lengths



Bond angles

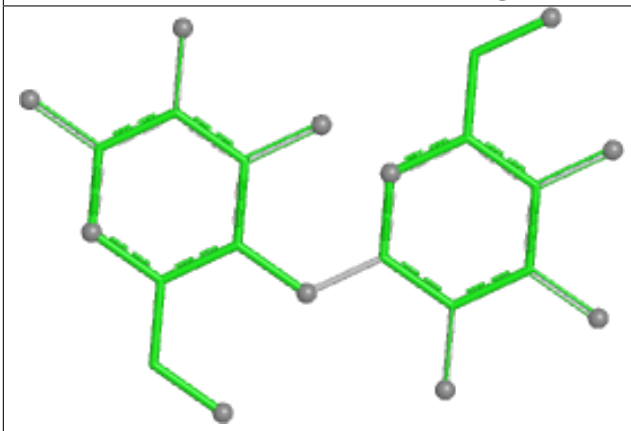


Torsions

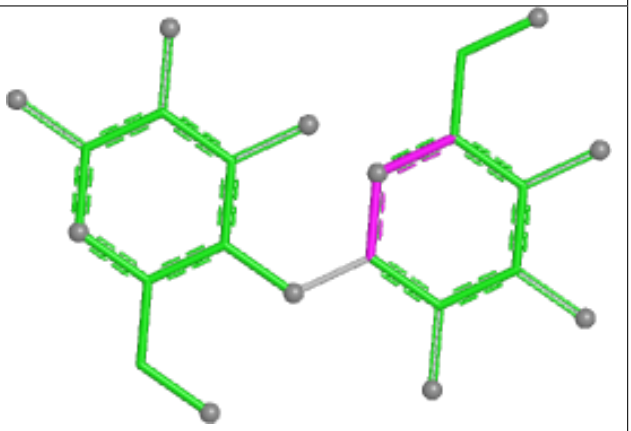


Rings

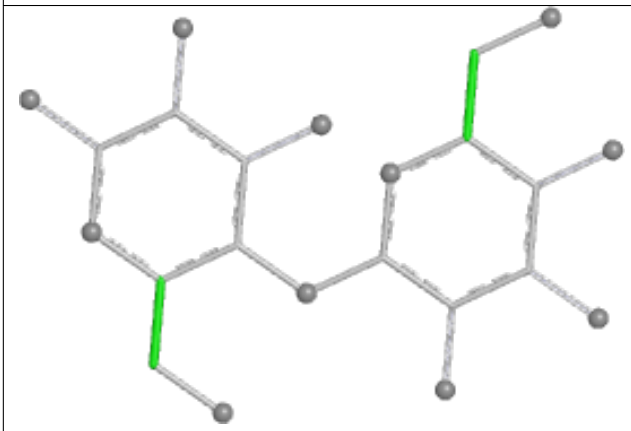
Oligosaccharide Chain N



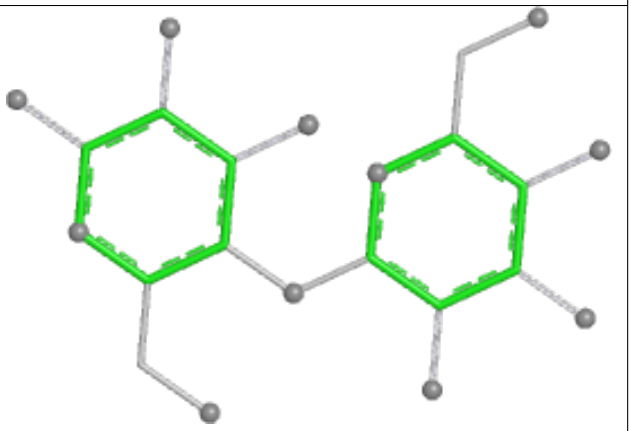
Bond lengths



Bond angles

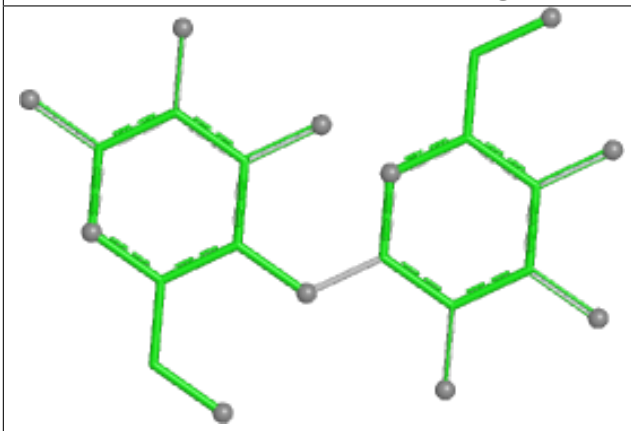


Torsions

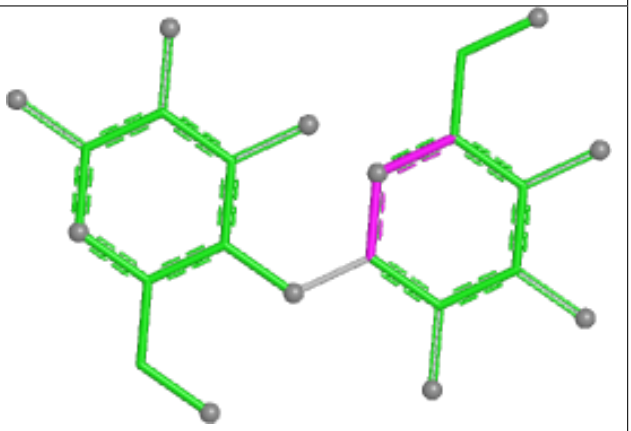


Rings

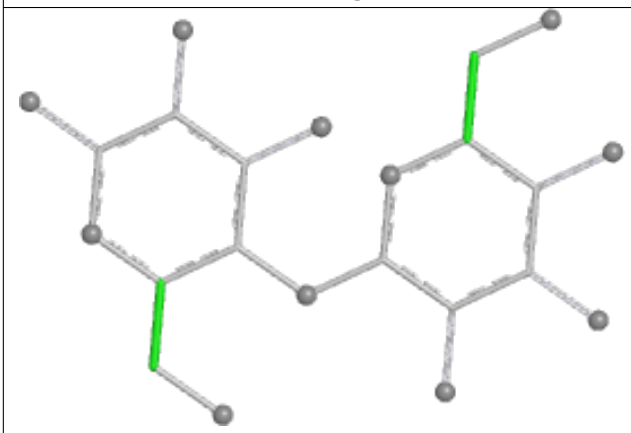
Oligosaccharide Chain O



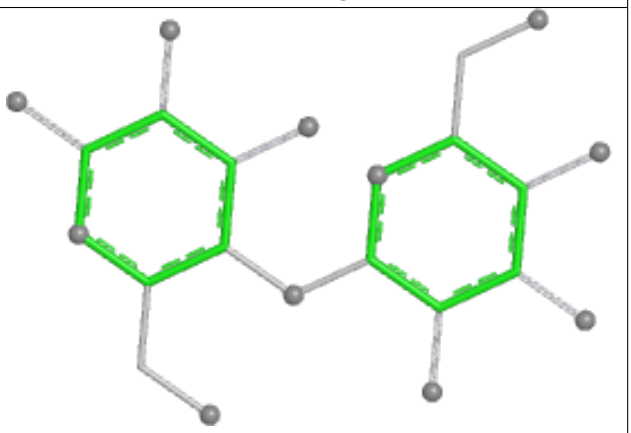
Bond lengths



Bond angles

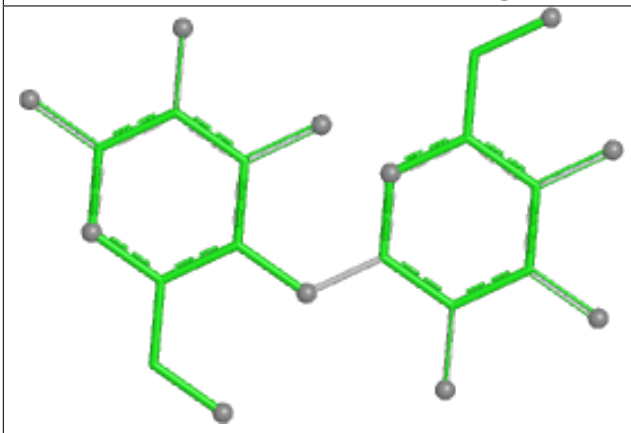


Torsions

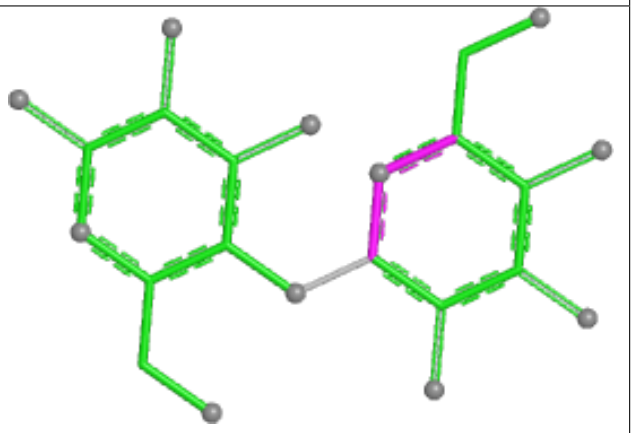


Rings

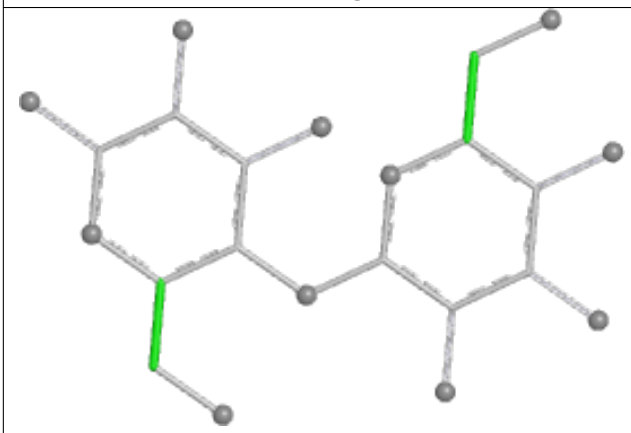
Oligosaccharide Chain P



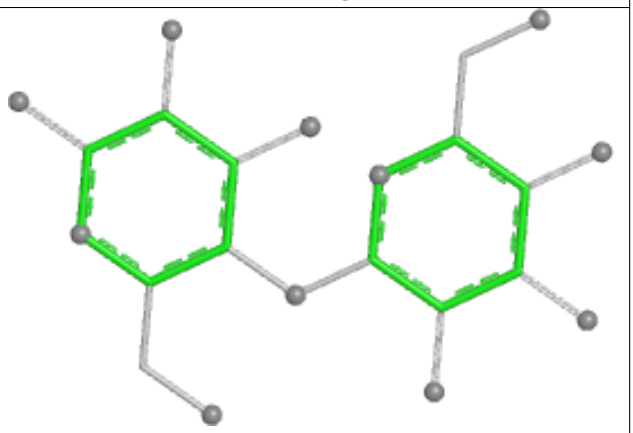
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	D	806	-	3,3,3	0.08	0	2,2,2	0.25	0
5	EDO	C	804	-	3,3,3	0.09	0	2,2,2	0.11	0
5	EDO	B	804	-	3,3,3	0.15	0	2,2,2	0.24	0
6	MLI	D	805	-	6,6,6	1.12	0	7,7,7	1.64	1 (14%)
5	EDO	D	804	-	3,3,3	0.17	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MLI	B	805	-	6,6,6	1.35	0	7,7,7	1.53	1 (14%)
5	EDO	C	806	-	3,3,3	0.04	0	2,2,2	0.11	0
4	NAG	C	802	1	14,14,15	0.51	0	17,19,21	1.20	2 (11%)
5	EDO	A	803	-	3,3,3	0.04	0	2,2,2	0.32	0
4	NAG	D	801	1	14,14,15	0.63	0	17,19,21	0.97	1 (5%)
4	NAG	D	802	1	14,14,15	0.58	0	17,19,21	1.19	2 (11%)
4	NAG	C	803	1	14,14,15	0.66	0	17,19,21	1.32	1 (5%)
4	NAG	B	801	1	14,14,15	0.46	0	17,19,21	1.17	1 (5%)
4	NAG	B	802	1	14,14,15	0.55	0	17,19,21	0.97	0
4	NAG	C	801	1	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
5	EDO	D	803	-	3,3,3	0.11	0	2,2,2	0.20	0
4	NAG	A	802	1	14,14,15	0.37	0	17,19,21	1.10	0
4	NAG	A	804	1	14,14,15	0.48	0	17,19,21	0.77	0
5	EDO	B	803	-	3,3,3	0.07	0	2,2,2	0.36	0
6	MLI	A	805	-	6,6,6	1.28	0	7,7,7	1.39	0
4	NAG	A	801	1	14,14,15	0.37	0	17,19,21	1.17	2 (11%)
6	MLI	C	805	-	6,6,6	1.41	0	7,7,7	1.62	2 (28%)
5	EDO	A	806	-	3,3,3	0.12	0	2,2,2	0.34	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
5	EDO	D	806	-	-	1/1/1/1	-
5	EDO	C	804	-	-	1/1/1/1	-
5	EDO	B	804	-	-	1/1/1/1	-
6	MLI	D	805	-	-	0/4/4/4	-
5	EDO	D	804	-	-	0/1/1/1	-
6	MLI	B	805	-	-	0/4/4/4	-
5	EDO	C	806	-	-	0/1/1/1	-
4	NAG	C	802	1	-	0/6/23/26	0/1/1/1
5	EDO	A	803	-	-	1/1/1/1	-
4	NAG	D	801	1	-	0/6/23/26	0/1/1/1
4	NAG	D	802	1	-	0/6/23/26	0/1/1/1
4	NAG	C	803	1	-	0/6/23/26	0/1/1/1
4	NAG	B	801	1	-	0/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	NAG	C	801	1	-	0/6/23/26	0/1/1/1
5	EDO	D	803	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	802	1	-	0/6/23/26	0/1/1/1
4	NAG	A	804	1	-	0/6/23/26	0/1/1/1
5	EDO	B	803	-	-	1/1/1/1	-
6	MLI	A	805	-	-	0/4/4/4	-
4	NAG	A	801	1	-	2/6/23/26	0/1/1/1
6	MLI	C	805	-	-	2/4/4/4	-
5	EDO	A	806	-	-	1/1/1/1	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	803	NAG	C1-C2-N2	-3.66	104.24	110.49
4	C	802	NAG	O5-C5-C6	3.40	112.53	107.20
4	D	802	NAG	C1-O5-C5	3.28	116.64	112.19
4	A	801	NAG	O5-C5-C6	2.92	111.78	107.20
6	C	805	MLI	O7-C2-C1	2.73	123.25	114.54
6	D	805	MLI	O7-C2-C1	2.50	122.51	114.54
4	C	801	NAG	O4-C4-C5	2.31	115.03	109.30
4	C	802	NAG	C1-O5-C5	2.29	115.30	112.19
4	D	802	NAG	O5-C1-C2	-2.28	107.68	111.29
4	B	801	NAG	C3-C4-C5	-2.25	106.22	110.24
4	D	801	NAG	O4-C4-C5	2.19	114.73	109.30
6	B	805	MLI	O9-C3-C1	2.06	121.11	114.54
4	A	801	NAG	C3-C4-C5	-2.04	106.59	110.24
6	C	805	MLI	O7-C2-O6	-2.03	118.23	123.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	806	EDO	O1-C1-C2-O2
4	A	801	NAG	C4-C5-C6-O6
4	A	801	NAG	O5-C5-C6-O6
5	A	803	EDO	O1-C1-C2-O2
6	C	805	MLI	C2-C1-C3-O9
6	C	805	MLI	C2-C1-C3-O8
5	D	806	EDO	O1-C1-C2-O2
5	B	803	EDO	O1-C1-C2-O2
5	B	804	EDO	O1-C1-C2-O2
5	C	804	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	806	EDO	1	0
5	D	803	EDO	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	615/636 (96%)	0.58	40 (6%)	18	20	46, 63, 89, 112	0
1	B	618/636 (97%)	0.32	4 (0%)	89	89	28, 43, 66, 89	0
1	C	617/636 (97%)	0.35	16 (2%)	56	59	42, 56, 81, 92	0
1	D	618/636 (97%)	0.33	13 (2%)	63	66	30, 47, 69, 85	0
All	All	2468/2544 (97%)	0.39	73 (2%)	50	53	28, 53, 79, 112	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	7.3
1	B	88	LEU	5.2
1	A	95	LEU	4.7
1	D	88	LEU	4.7
1	A	97	ALA	4.7
1	B	90	ALA	4.6
1	A	92	LEU	4.5
1	D	90	ALA	4.3
1	A	138	ALA	4.1
1	A	125	CYS	4.1
1	C	219	ALA	4.0
1	A	377	PHE	3.8
1	A	100	PHE	3.7
1	A	118	GLY	3.7
1	C	141	LEU	3.6
1	A	363	PHE	3.5
1	A	93	LEU	3.3
1	A	276	ALA	3.2
1	A	170	ARG	3.2
1	C	100	PHE	3.1
1	A	132	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	90	ALA	3.1
1	A	142	PRO	3.0
1	D	219	ALA	3.0
1	A	455	TYR	3.0
1	A	122	LEU	2.9
1	A	146	PHE	2.9
1	A	159	TYR	2.9
1	C	120	LEU	2.8
1	A	144	HIS	2.8
1	D	141	LEU	2.8
1	D	382	ASP	2.7
1	C	91	GLU	2.7
1	A	99	GLY	2.7
1	A	279	LEU	2.7
1	C	142	PRO	2.6
1	A	179	GLY	2.6
1	A	327	ALA	2.6
1	A	161	VAL	2.5
1	C	93	LEU	2.5
1	D	363	PHE	2.5
1	C	122	LEU	2.5
1	A	378	ARG	2.4
1	D	140	GLY	2.4
1	A	333	VAL	2.4
1	A	131	LEU	2.4
1	C	169	GLY	2.4
1	C	143	LEU	2.4
1	D	91	GLU	2.3
1	A	102	ILE	2.3
1	A	127	ARG	2.3
1	A	169	GLY	2.3
1	D	103	ARG	2.3
1	A	143	LEU	2.2
1	D	143	LEU	2.2
1	A	368	VAL	2.2
1	A	140	GLY	2.2
1	A	331	ASP	2.2
1	A	600	VAL	2.2
1	C	145	PHE	2.2
1	A	155	THR	2.2
1	A	486	TRP	2.2
1	A	371	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	99	GLY	2.1
1	C	172	VAL	2.1
1	C	127	ARG	2.1
1	C	147	ILE	2.1
1	B	115	PHE	2.1
1	A	602	ALA	2.0
1	C	378	ARG	2.0
1	D	122	LEU	2.0
1	D	136	LEU	2.0
1	D	139	ASP	2.0

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, 95^{th} 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	NAG	H	1	14/15	0.82	0.18	68,72,75,75	0
2	NAG	H	2	14/15	0.82	0.22	73,81,84,84	0
2	NAG	G	2	14/15	0.86	0.22	69,72,77,79	0
2	NAG	E	2	14/15	0.87	0.12	64,72,76,77	0
2	NAG	E	1	14/15	0.87	0.14	63,67,72,72	0
2	NAG	J	2	14/15	0.87	0.23	77,80,84,84	0
2	NAG	J	1	14/15	0.88	0.17	65,66,71,74	0
2	NAG	L	2	14/15	0.88	0.28	72,77,82,85	0
2	NAG	F	2	14/15	0.89	0.14	45,51,57,57	0
2	NAG	K	1	14/15	0.91	0.14	45,47,51,51	0
2	NAG	L	1	14/15	0.91	0.15	59,62,67,69	0
2	NAG	I	2	14/15	0.91	0.12	60,65,68,69	0
2	NAG	I	1	14/15	0.92	0.14	56,59,62,63	0
3	BGC	M	1	12/12	0.92	0.13	46,46,49,51	0
3	GLA	P	2	11/12	0.93	0.13	34,36,37,37	0
2	NAG	F	1	14/15	0.94	0.15	45,47,54,55	0
3	GLA	M	2	11/12	0.94	0.14	45,46,47,48	0
3	GLA	O	2	11/12	0.94	0.12	38,40,41,44	0

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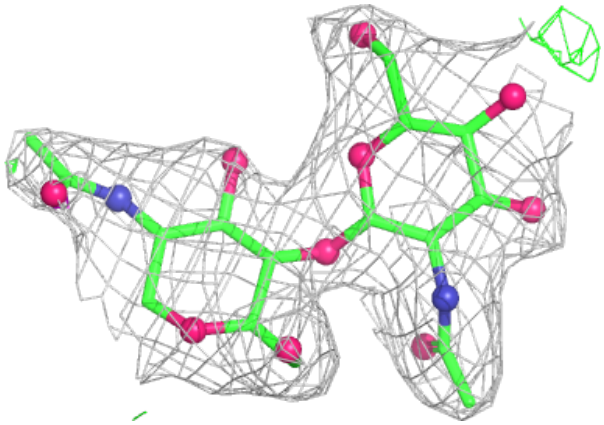
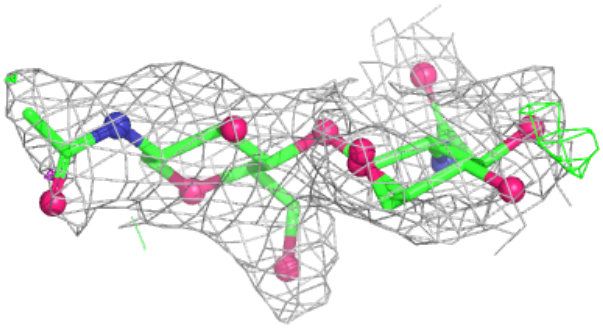
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	P	1	12/12	0.94	0.13	33,34,38,41	0
2	NAG	K	2	14/15	0.94	0.11	43,49,56,56	0
3	BGC	O	1	12/12	0.95	0.16	39,40,42,44	0
3	BGC	N	1	12/12	0.96	0.19	32,33,35,35	0
3	GLA	N	2	11/12	0.96	0.14	32,33,35,36	0
2	NAG	G	1	14/15	0.96	0.11	56,59,64,65	0

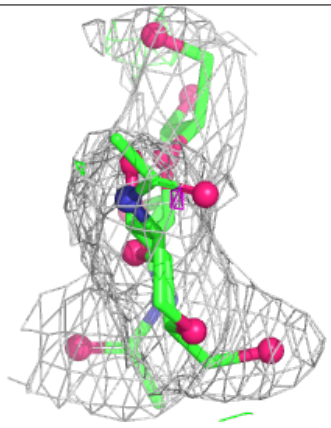
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

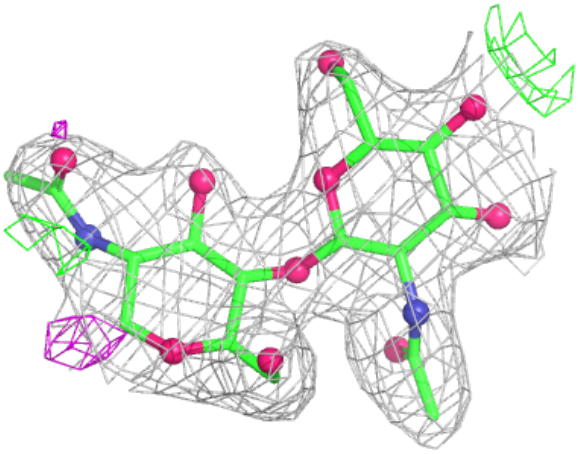


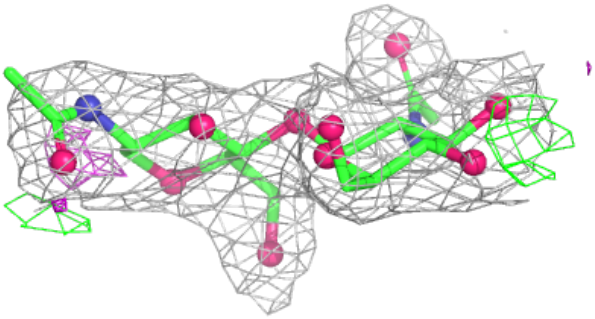


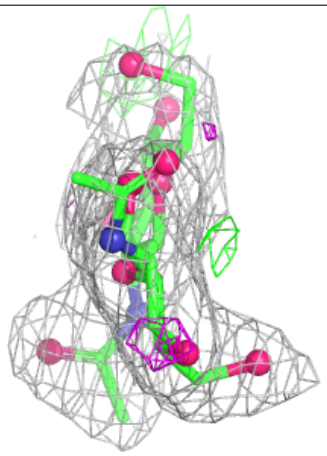


Electron density around Chain F:

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

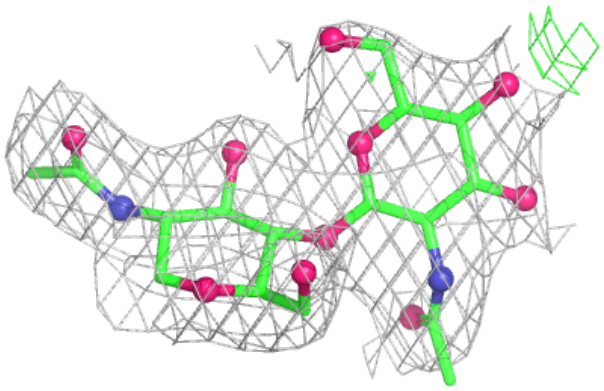


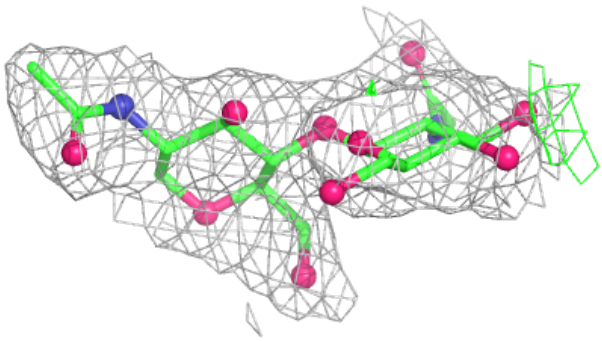


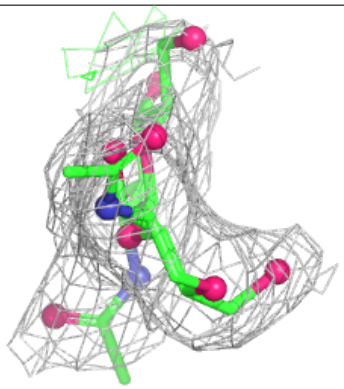


Electron density around Chain G:

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

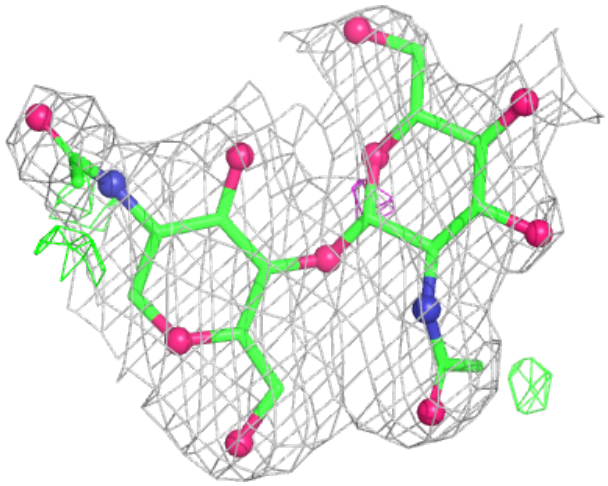


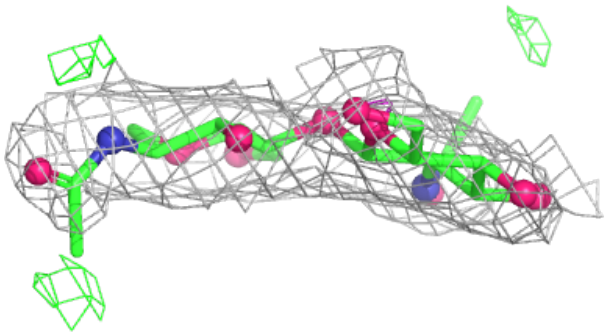


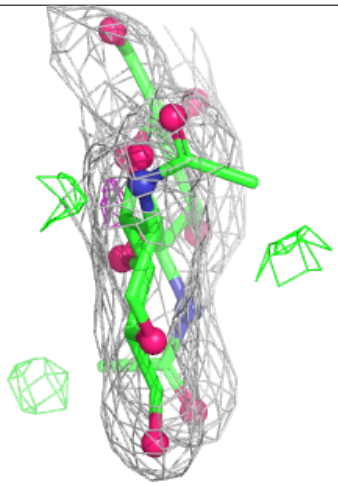


Electron density around Chain H:

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

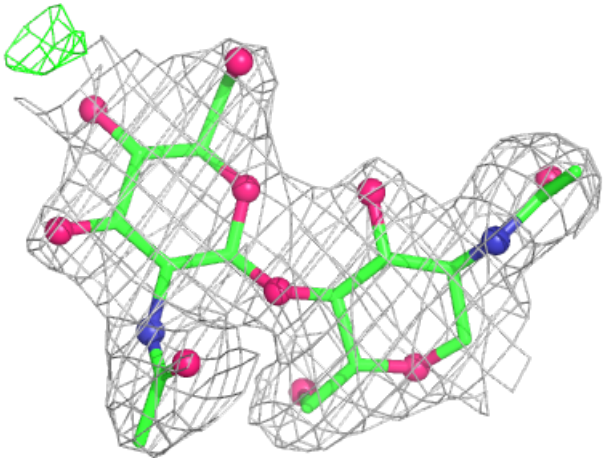


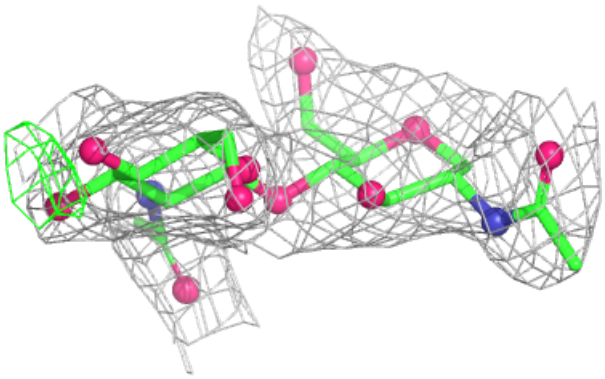


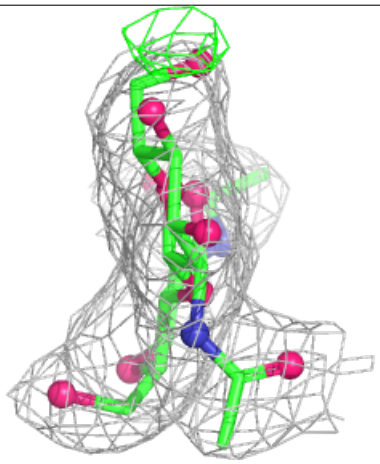


Electron density around Chain I:

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

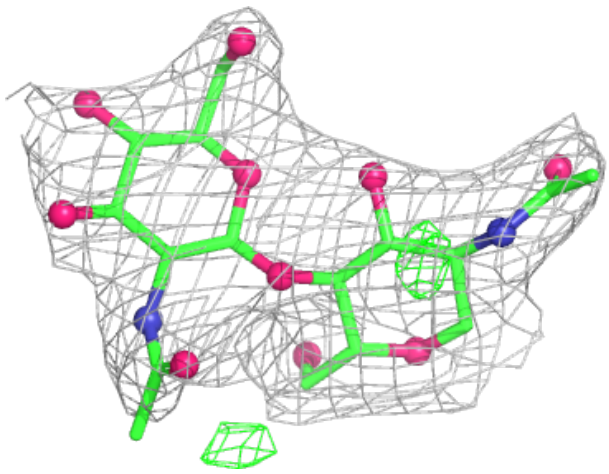


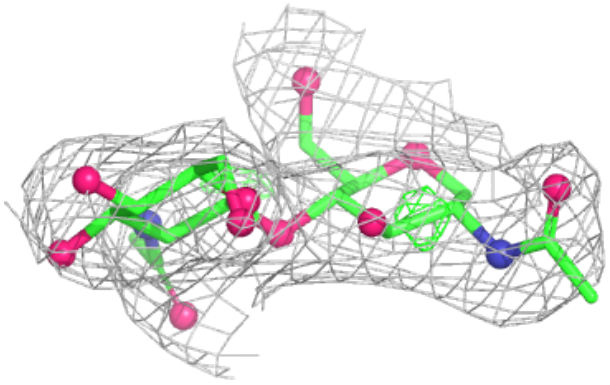


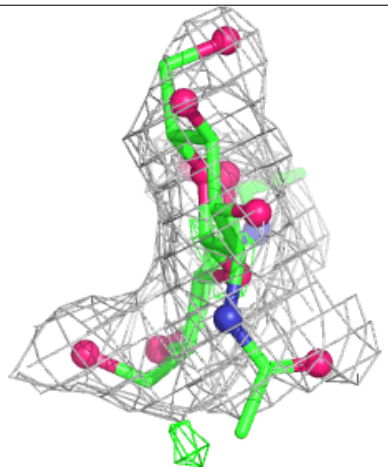


Electron density around Chain J:

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

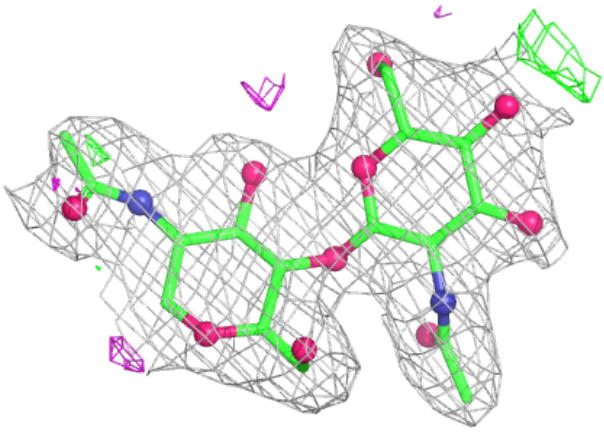


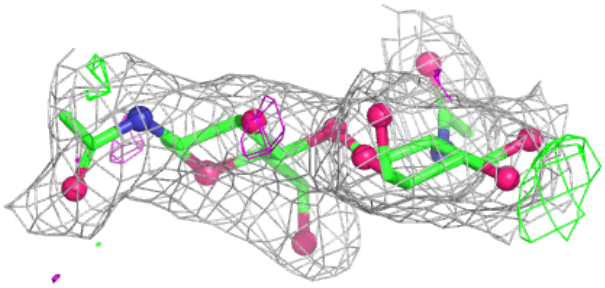




Electron density around Chain K:

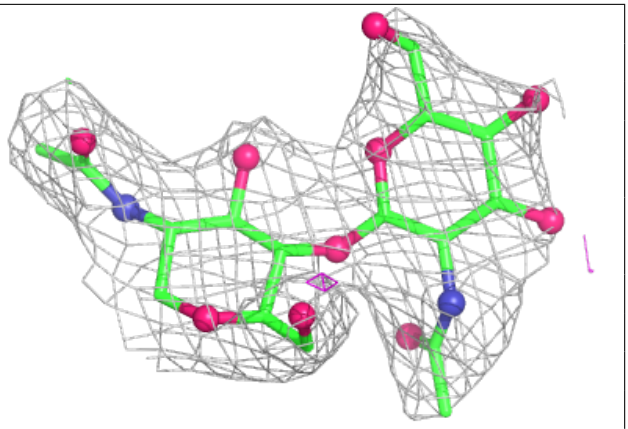
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

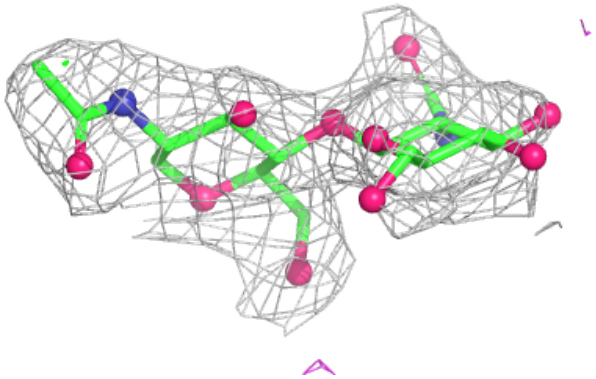


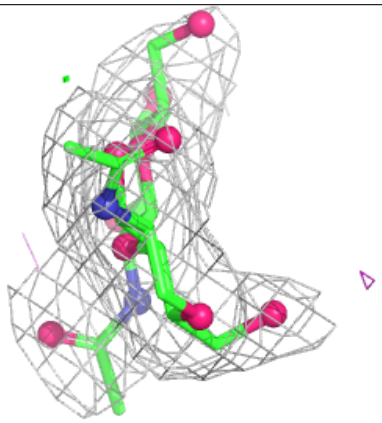


Electron density around Chain L:

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

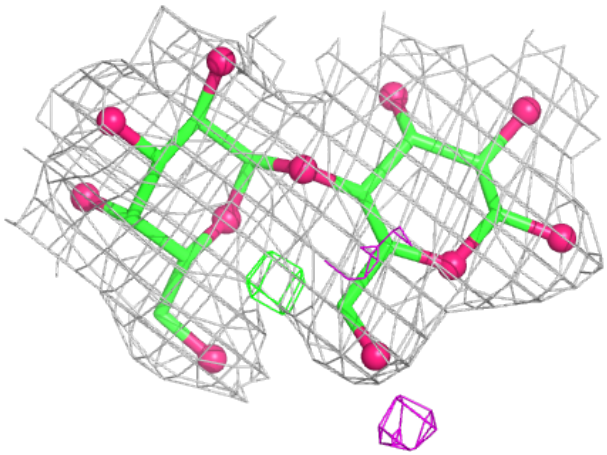


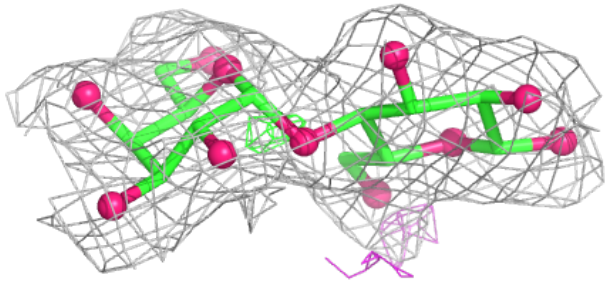


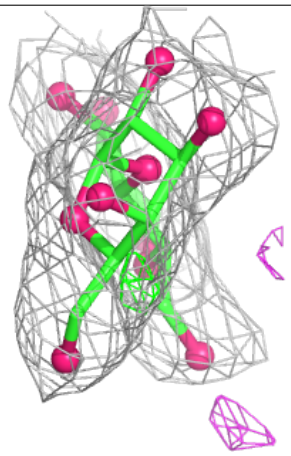


Electron density around Chain M:

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

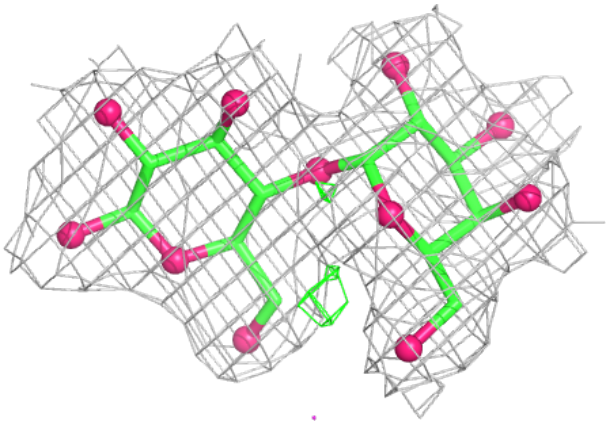


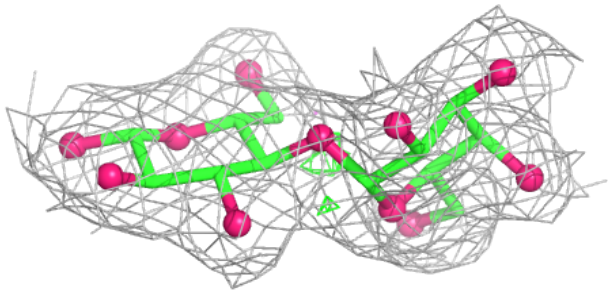


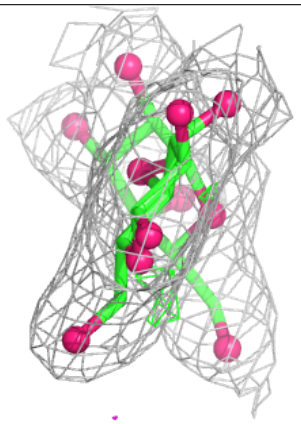


Electron density around Chain N:

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

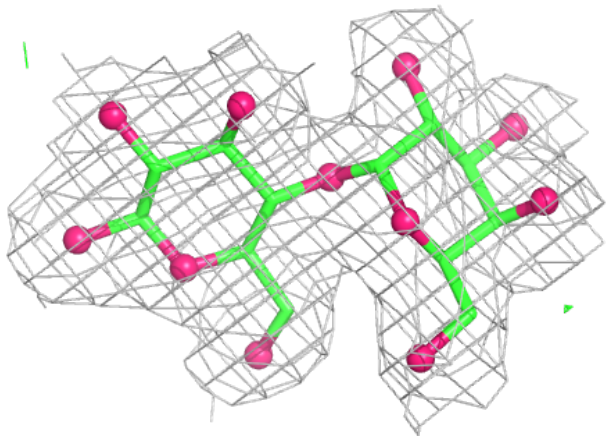


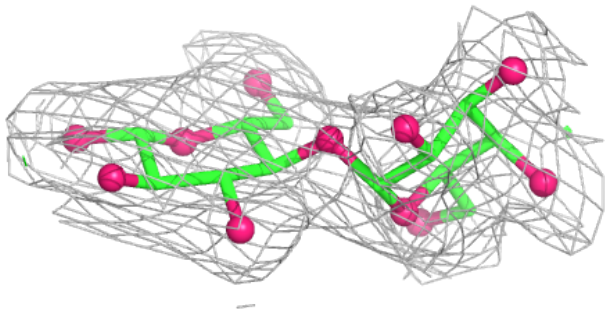


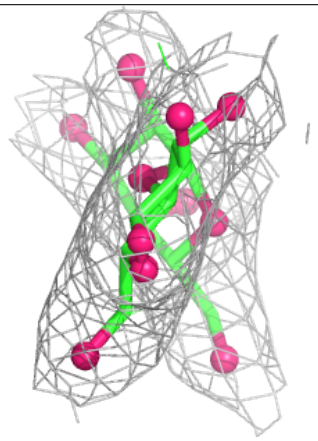


Electron density around Chain O:

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

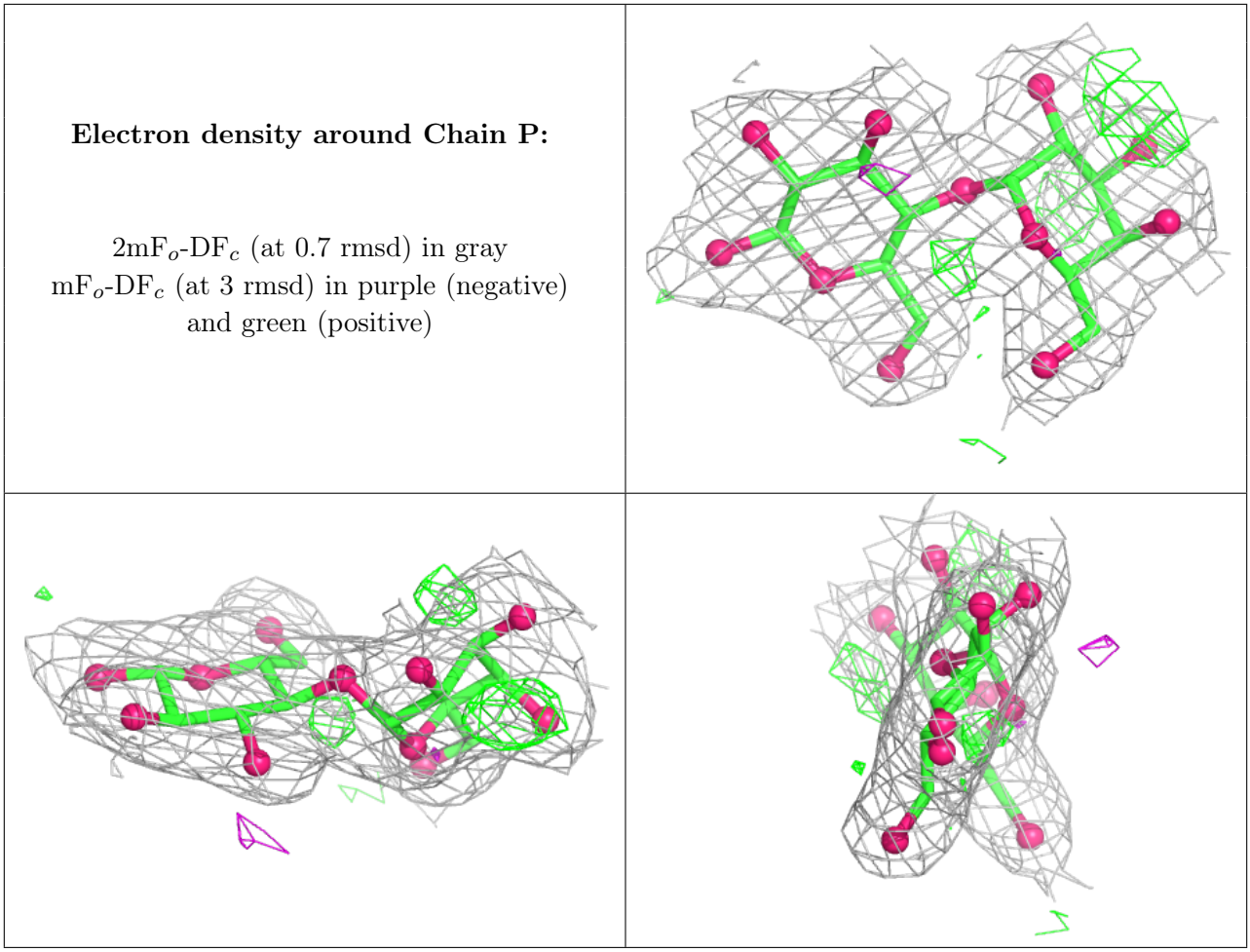






Electron density around Chain P:

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



6.4 Ligands

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, 95^{th} 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	NAG	C	803	14/15	0.75	0.21	70,75,82,83	0
4	NAG	A	801	14/15	0.81	0.21	70,71,75,77	0
4	NAG	A	804	14/15	0.83	0.17	83,86,89,92	0
5	EDO	A	806	4/4	0.83	0.29	82,83,83,84	0
4	NAG	D	802	14/15	0.84	0.16	64,66,69,70	0
5	EDO	D	804	4/4	0.84	0.23	53,54,54,55	0
5	EDO	D	803	4/4	0.85	0.24	61,61,61,62	0
4	NAG	C	801	14/15	0.86	0.15	59,60,63,64	0
4	NAG	B	802	14/15	0.86	0.12	56,58,61,61	0
4	NAG	C	802	14/15	0.87	0.11	70,72,74,75	0
5	EDO	C	806	4/4	0.89	0.17	67,67,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	802	14/15	0.91	0.19	72,75,78,78	0
6	MLI	A	805	7/7	0.91	0.25	71,72,74,74	0
4	NAG	B	801	14/15	0.92	0.13	46,48,53,54	0
4	NAG	D	801	14/15	0.92	0.11	47,49,51,53	0
6	MLI	C	805	7/7	0.92	0.24	56,58,59,61	0
6	MLI	B	805	7/7	0.94	0.12	41,42,46,46	0
5	EDO	D	806	4/4	0.96	0.17	33,33,34,34	0
5	EDO	A	803	4/4	0.96	0.12	43,45,45,46	0
5	EDO	B	803	4/4	0.96	0.20	53,54,54,55	0
5	EDO	C	804	4/4	0.96	0.16	41,41,41,41	0
6	MLI	D	805	7/7	0.97	0.14	41,42,45,48	0
5	EDO	B	804	4/4	0.99	0.17	30,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.