Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 04:28 PM EDT

PDB ID	:	4Z0C
Title	:	Crystal structure of TLR13-ssRNA13 complex
Authors	:	Song, W.; Han, Z.; Chai, J.
Deposited on	:	2015-03-26
Resolution	:	2.30 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:

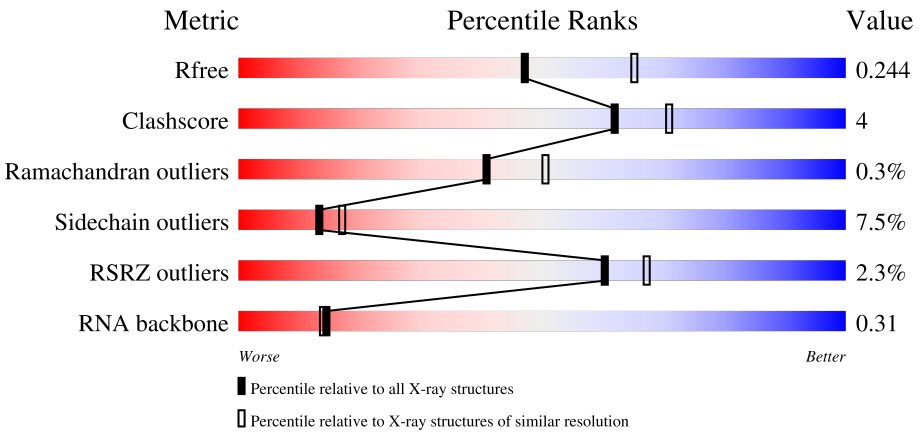
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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	709	3% 82% 16% •
1	D	709	2% 84% 14% •
2	B	13	38% 46% 15%
2	C	13	8% 54% 38% 8%

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Mol	Chain	Length	Quality of chain
3	E	2	100%
3	F	2	50% 50%
3	G	2	50% 50%
3	H	2	100%
3	I	2	50% 50%
3	J	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	915	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12821 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 Toll-like receptor 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	709	5724	3672	984	1048	20	0	0	0
1	D	709	5730	3675	987	1048	20	0	0	0

- Molecule 2 is a RNA chain called DNA (5'-R(P*AP*CP*GP*GP*AP*AP*AP*GP*AP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	13	279	125	55	86	13	0	0	0
2	C	13	279	125	55	86	13	0	0	0

- Molecule 3 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
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0

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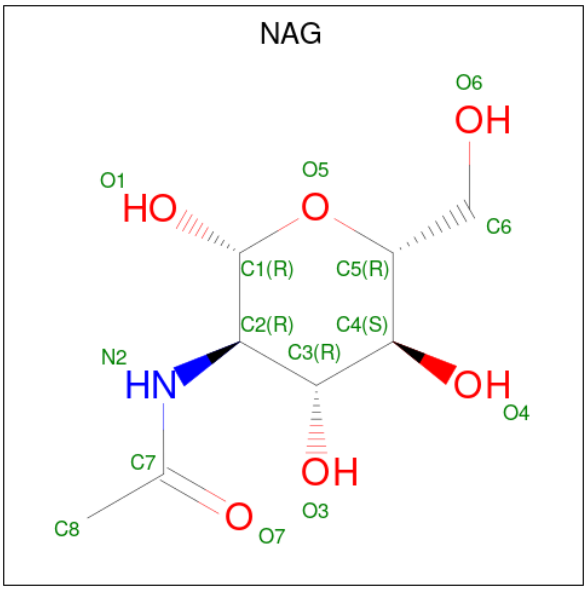
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	J	2	28	16	2	10	0	0	0

- 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
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	D	1	14	8	1	5	0	0

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

- Molecule 5 is water.

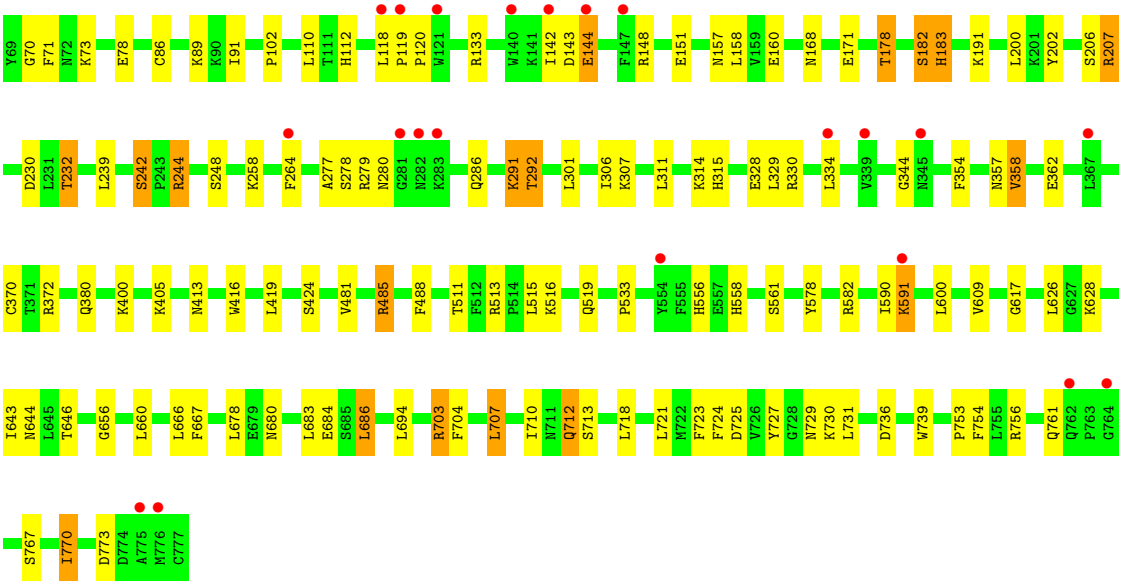
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	117	117	117	0	0
5	D	207	207	207	0	0
5	B	18	18	18	0	0
5	C	19	19	19	0	0

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.

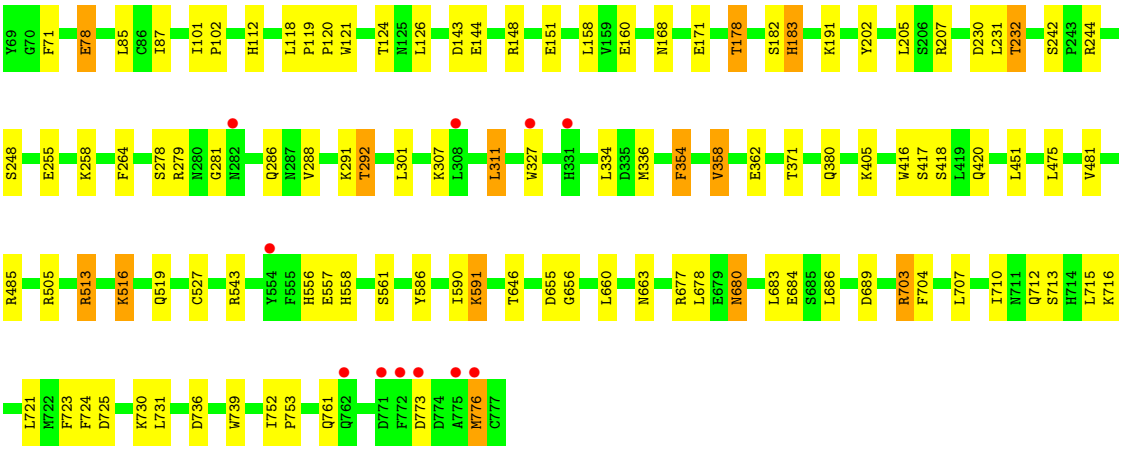
- Molecule 1: Toll-like receptor 13

Chain A:



- Molecule 1: Toll-like receptor 13

Chain D:

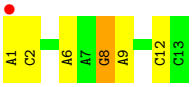


• Molecule 2: DNA (5'-R(P*AP*CP*GP*GP*AP*AP*AP*GP*AP*CP*CP*CP*C)-3')

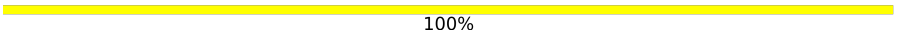
Chain B:

• Molecule 2: DNA (5'-R(P*AP*CP*GP*GP*AP*AP*AP*GP*AP*CP*CP*CP*C)-3')

Chain C:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

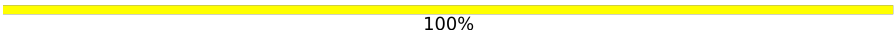
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

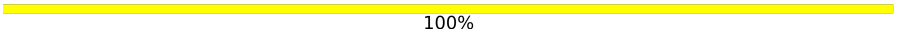
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.55Å 115.21Å 167.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 2.30 45.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (45.90-2.30) 92.4 (45.90-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.191 , 0.244 0.193 , 0.244	Depositor DCC
R_{free} test set	4489 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.989	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12821	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: NAG

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	0.41	0/5845	0.61	1/7918 (0.0%)
1	D	0.45	0/5851	0.62	0/7925
2	B	0.68	0/312	1.21	1/484 (0.2%)
2	C	0.61	0/312	1.35	1/484 (0.2%)
All	All	0.45	0/12320	0.67	3/16811 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	8	G	O4'-C1'-N9	6.81	113.65	108.20
2	B	2	C	P-O3'-C3'	5.72	126.56	119.70
1	A	70	GLY	N-CA-C	-5.37	99.68	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5724	0	5782	61	0
1	D	5730	0	5789	46	0
2	B	279	0	144	3	0
2	C	279	0	144	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	1	0
3	I	28	0	25	1	0
3	J	28	0	25	0	0
4	A	126	0	117	4	0
4	D	154	0	143	1	0
5	A	117	0	0	3	0
5	B	18	0	0	0	0
5	C	19	0	0	0	0
5	D	207	0	0	6	0
All	All	12821	0	12269	108	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 (108) 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:279:ARG:NH1	5:A:1001:HOH:O	2.11	0.82
1:D:689:ASP:OD1	1:D:716:LYS:NZ	2.13	0.81
1:D:148:ARG:NH1	1:D:171:GLU:HG2	1.97	0.80
1:A:556:HIS:CD2	1:A:558:HIS:H	2.01	0.78
4:D:917:NAG:O4	5:D:1001:HOH:O	2.04	0.75
1:D:230:ASP:OD1	1:D:232:THR:HG22	1.86	0.75
1:D:334:LEU:HG	1:D:358:VAL:HG22	1.76	0.66
1:A:328:GLU:HG3	1:A:330:ARG:NH1	2.10	0.65
1:A:230:ASP:OD1	1:A:232:THR:HG22	1.96	0.65
1:A:582:ARG:NH1	5:A:1005:HOH:O	2.30	0.63
1:A:120:PRO:HD3	1:A:143:ASP:OD2	2.00	0.61
1:D:590:ILE:HG23	1:D:591:LYS:HD2	1.81	0.60
1:A:328:GLU:HG3	1:A:330:ARG:HH12	1.65	0.59
1:A:644:ASN:OD1	4:A:914:NAG:N2	2.36	0.58
1:D:286:GLN:HG2	1:D:307:LYS:HD3	1.85	0.58
1:A:556:HIS:HD2	1:A:558:HIS:H	1.48	0.58
1:D:556:HIS:CD2	1:D:558:HIS:H	2.22	0.57
1:A:712:GLN:HG3	1:A:739:TRP:CD2	2.39	0.57
1:A:357:ASN:HD21	4:A:909:NAG:C1	2.18	0.56
1:D:712:GLN:HG3	1:D:739:TRP:CD2	2.41	0.56
1:A:334:LEU:HG	1:A:358:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:O	1:A:292:THR:HG21	2.08	0.54
1:A:286:GLN:HG2	1:A:307:LYS:HD3	1.90	0.53
1:A:291:LYS:HB2	1:A:315:HIS:CD2	2.44	0.53
1:A:686:LEU:HD13	1:A:707:LEU:HD11	1.91	0.53
1:D:78:GLU:OE1	1:D:677:ARG:NH2	2.30	0.52
1:A:703:ARG:HD2	1:A:727:TYR:HD2	1.74	0.52
1:D:776:MET:SD	1:D:776:MET:N	2.74	0.52
1:A:207:ARG:NH1	2:B:13:C:O2	2.44	0.51
1:A:148:ARG:NH2	1:A:171:GLU:HG2	2.25	0.51
1:A:707:LEU:HB2	1:A:729:ASN:OD1	2.10	0.51
1:A:667:PHE:HB3	1:A:694:LEU:HD21	1.91	0.51
1:D:663:ASN:ND2	5:D:1010:HOH:O	2.37	0.50
1:A:144:GLU:HG2	1:A:168:ASN:O	2.12	0.50
1:A:178:THR:HB	1:A:202:TYR:HB2	1.94	0.50
1:A:628:LYS:HE2	2:B:5:A:N6	2.27	0.50
1:D:264:PHE:O	1:D:292:THR:HG21	2.11	0.50
1:D:513:ARG:HH21	1:D:516:LYS:NZ	2.11	0.48
1:A:277:ALA:O	1:A:280:ASN:ND2	2.41	0.48
1:A:329:LEU:HD22	1:A:357:ASN:HB2	1.94	0.48
1:D:160:GLU:HA	1:D:183:HIS:O	2.14	0.48
1:D:721:LEU:HD21	1:D:724:PHE:HB2	1.95	0.48
1:A:71:PHE:CZ	1:A:102:PRO:HD3	2.48	0.48
1:A:191:LYS:HB3	1:A:191:LYS:HE3	1.71	0.47
1:D:380:GLN:HA	1:D:405:LYS:O	2.14	0.47
1:A:133:ARG:HA	1:A:157:ASN:HB3	1.95	0.47
1:D:417:SER:O	1:D:420:GLN:NE2	2.47	0.47
1:D:505:ARG:HG2	1:D:527:CYS:HB2	1.96	0.47
1:D:120:PRO:HD3	1:D:143:ASP:OD2	2.15	0.47
1:A:400:LYS:HG3	1:A:424:SER:HB3	1.97	0.47
1:D:591:LYS:HA	1:D:591:LYS:HE2	1.96	0.47
1:A:485:ARG:HA	1:A:511:THR:HA	1.98	0.47
1:A:591:LYS:HA	1:A:591:LYS:HE2	1.97	0.46
1:A:182:SER:HA	1:A:206:SER:O	2.15	0.46
1:A:160:GLU:HA	1:A:183:HIS:O	2.15	0.46
1:D:543:ARG:NH1	5:D:1007:HOH:O	2.35	0.45
1:A:723:PHE:CZ	1:A:753:PRO:HG3	2.51	0.45
1:D:87:ILE:HD13	3:H:1:NAG:H82	1.97	0.45
1:A:590:ILE:HG23	1:A:591:LYS:HD2	1.99	0.45
1:D:232:THR:HA	1:D:255:GLU:O	2.16	0.45
1:A:242:SER:O	1:A:244:ARG:HG2	2.17	0.45
1:D:703:ARG:HD3	1:D:725:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:SER:HA	1:D:420:GLN:HE22	1.82	0.45
1:A:704:PHE:CE2	2:B:8:G:H2'	2.51	0.45
1:A:600:LEU:HB2	1:A:626:LEU:HD23	1.98	0.44
1:A:301:LEU:HD13	1:A:306:ILE:HG21	1.99	0.44
1:D:101:ILE:HG13	1:D:126:LEU:HD21	1.98	0.44
1:A:578:TYR:HB2	1:A:609:VAL:O	2.17	0.44
1:A:357:ASN:HD21	4:A:909:NAG:C2	2.31	0.44
1:D:336:MET:HE1	1:D:354:PHE:HZ	1.83	0.44
1:D:178:THR:HB	1:D:202:TYR:HB2	1.99	0.43
1:D:202:TYR:HB3	5:D:1186:HOH:O	2.18	0.43
1:D:557:GLU:HG3	1:D:586:TYR:CD1	2.54	0.43
1:A:344:GLY:HA2	1:A:370:CYS:O	2.19	0.43
1:D:191:LYS:HB3	1:D:191:LYS:HE3	1.75	0.43
1:A:590:ILE:HD12	1:A:617:GLY:HA3	2.01	0.43
1:A:118:LEU:HA	1:A:119:PRO:HD2	1.86	0.43
1:D:168:ASN:ND2	5:D:1030:HOH:O	2.50	0.42
1:D:279:ARG:HH22	3:I:1:NAG:H62	1.84	0.42
1:A:86:CYS:HB2	1:A:110:LEU:HD23	2.01	0.42
1:D:281:GLY:H	1:D:327:TRP:HZ3	1.65	0.42
1:A:73:LYS:HG2	1:A:91:ILE:HG12	2.01	0.42
1:D:118:LEU:HA	1:D:119:PRO:HD2	1.93	0.42
1:A:721:LEU:HD21	1:A:724:PHE:HB2	2.02	0.42
1:D:655:ASP:OD1	1:D:655:ASP:N	2.53	0.42
1:D:723:PHE:CZ	1:D:753:PRO:HG3	2.55	0.42
1:A:516:LYS:HD2	1:A:516:LYS:HA	1.84	0.42
1:D:85:LEU:HD21	2:C:6:A:N3	2.35	0.42
1:D:752:ILE:HA	1:D:753:PRO:HD2	1.86	0.42
1:D:451:LEU:HD12	1:D:475:LEU:HD21	2.02	0.41
1:A:533:PRO:HG3	1:A:556:HIS:CE1	2.55	0.41
1:D:288:VAL:HG11	1:D:311:LEU:HD13	2.01	0.41
1:A:230:ASP:CG	1:A:232:THR:HG22	2.41	0.41
1:A:703:ARG:HD3	1:A:725:ASP:OD2	2.20	0.41
1:A:756:ARG:CZ	1:A:770:ILE:HD11	2.50	0.41
1:D:586:TYR:HB3	5:D:1005:HOH:O	2.20	0.41
1:A:119:PRO:HA	1:A:120:PRO:HD3	1.92	0.41
1:D:71:PHE:CZ	1:D:102:PRO:HD3	2.55	0.41
1:D:121:TRP:HB3	1:D:124:THR:OG1	2.21	0.41
1:A:89:LYS:HE3	1:A:754:PHE:CE1	2.57	0.40
1:A:142:ILE:HG13	4:A:904:NAG:H81	2.03	0.40
1:A:372:ARG:NH2	3:G:1:NAG:O7	2.55	0.40
1:A:488:PHE:HB3	1:A:515:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LEU:HB2	1:D:231:LEU:HD23	2.03	0.40
1:A:380:GLN:HA	1:A:405:LYS:O	2.22	0.40
1:A:666:LEU:HD12	5:A:1068:HOH:O	2.22	0.40
1:D:680:ASN:HA	1:D:704:PHE:O	2.21	0.40
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.96	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	707/709 (100%)	657 (93%)	48 (7%)	2 (0%)	41	50
1	D	707/709 (100%)	650 (92%)	55 (8%)	2 (0%)	41	50
All	All	1414/1418 (100%)	1307 (92%)	103 (7%)	4 (0%)	41	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	773	ASP
1	A	656	GLY
1	D	656	GLY
1	A	773	ASP

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	662/663 (100%)	610 (92%)	52 (8%)	12	15
1	D	663/663 (100%)	615 (93%)	48 (7%)	14	18
All	All	1325/1326 (100%)	1225 (92%)	100 (8%)	13	17

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	112	HIS
1	A	144	GLU
1	A	151	GLU
1	A	158	LEU
1	A	178	THR
1	A	182	SER
1	A	183	HIS
1	A	207	ARG
1	A	232	THR
1	A	239	LEU
1	A	242	SER
1	A	244	ARG
1	A	248	SER
1	A	258	LYS
1	A	278	SER
1	A	291	LYS
1	A	292	THR
1	A	311	LEU
1	A	314	LYS
1	A	354	PHE
1	A	358	VAL
1	A	362	GLU
1	A	413	ASN
1	A	416	TRP
1	A	419	LEU
1	A	481	VAL
1	A	485	ARG
1	A	513	ARG
1	A	519	GLN
1	A	561	SER
1	A	591	LYS
1	A	643	ILE
1	A	646	THR
1	A	660	LEU

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Mol	Chain	Res	Type
1	A	678	LEU
1	A	680	ASN
1	A	683	LEU
1	A	684	GLU
1	A	686	LEU
1	A	703	ARG
1	A	707	LEU
1	A	710	ILE
1	A	712	GLN
1	A	713	SER
1	A	718	LEU
1	A	730	LYS
1	A	731	LEU
1	A	736	ASP
1	A	761	GLN
1	A	767	SER
1	A	770	ILE
1	D	78	GLU
1	D	112	HIS
1	D	144	GLU
1	D	151	GLU
1	D	158	LEU
1	D	178	THR
1	D	182	SER
1	D	183	HIS
1	D	207	ARG
1	D	232	THR
1	D	242	SER
1	D	244	ARG
1	D	248	SER
1	D	258	LYS
1	D	278	SER
1	D	291	LYS
1	D	292	THR
1	D	301	LEU
1	D	311	LEU
1	D	354	PHE
1	D	358	VAL
1	D	362	GLU
1	D	371	THR
1	D	416	TRP
1	D	481	VAL

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Mol	Chain	Res	Type
1	D	485	ARG
1	D	513	ARG
1	D	516	LYS
1	D	519	GLN
1	D	561	SER
1	D	591	LYS
1	D	646	THR
1	D	660	LEU
1	D	678	LEU
1	D	680	ASN
1	D	683	LEU
1	D	684	GLU
1	D	686	LEU
1	D	703	ARG
1	D	707	LEU
1	D	710	ILE
1	D	713	SER
1	D	715	LEU
1	D	730	LYS
1	D	731	LEU
1	D	736	ASP
1	D	761	GLN
1	D	776	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	556	HIS
1	A	597	GLN
1	D	556	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	13/13 (100%)	5 (38%)	2 (15%)
2	C	13/13 (100%)	3 (23%)	2 (15%)
All	All	26/26 (100%)	8 (30%)	4 (15%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	3	G
2	B	9	A
2	B	12	C
2	B	13	C
2	C	2	C
2	C	9	A
2	C	12	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	A
2	B	2	C
2	C	1	A
2	C	8	G

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)

12 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.84	1 (7%)	17,19,21	1.30	2 (11%)
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	1.31	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.58	0	17,19,21	1.46	3 (17%)
3	NAG	F	2	3	14,14,15	0.52	0	17,19,21	0.94	0
3	NAG	G	1	1,3	14,14,15	0.66	0	17,19,21	1.24	3 (17%)
3	NAG	G	2	3	14,14,15	0.54	0	17,19,21	1.19	3 (17%)
3	NAG	H	1	1,3	14,14,15	0.65	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	H	2	3	14,14,15	0.71	0	17,19,21	1.53	4 (23%)
3	NAG	I	1	1,3	14,14,15	0.52	0	17,19,21	0.94	1 (5%)
3	NAG	I	2	3	14,14,15	0.62	0	17,19,21	1.12	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.72	0	17,19,21	1.77	2 (11%)
3	NAG	J	2	3	14,14,15	0.61	0	17,19,21	1.01	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	2.12	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1	NAG	C3-C4-C5	-4.34	102.50	110.24
3	J	1	NAG	O5-C5-C6	4.17	113.74	107.20
3	E	2	NAG	C1-O5-C5	3.65	117.13	112.19
3	H	2	NAG	C1-O5-C5	3.54	116.99	112.19
3	F	1	NAG	C2-N2-C7	-3.39	118.07	122.90
3	I	2	NAG	O5-C5-C6	3.26	112.31	107.20
3	E	1	NAG	C3-C4-C5	-2.89	105.09	110.24
3	H	2	NAG	O3-C3-C2	-2.76	103.75	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	O5-C5-C6	2.71	111.45	107.20
3	J	2	NAG	C2-N2-C7	-2.65	119.13	122.90
3	I	1	NAG	O5-C5-C6	2.56	111.21	107.20
3	F	1	NAG	C3-C4-C5	-2.48	105.81	110.24
3	G	2	NAG	O4-C4-C5	2.45	115.37	109.30
3	G	2	NAG	C1-O5-C5	2.30	115.31	112.19
3	E	1	NAG	C1-C2-N2	2.27	114.36	110.49
3	H	2	NAG	O4-C4-C3	2.23	115.50	110.35
3	F	1	NAG	O5-C5-C4	-2.21	105.45	110.83
3	G	2	NAG	O3-C3-C2	-2.15	105.02	109.47
3	G	1	NAG	C1-O5-C5	2.08	115.01	112.19
3	G	1	NAG	O7-C7-C8	-2.04	118.26	122.06
3	H	2	NAG	O4-C4-C5	2.02	114.31	109.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

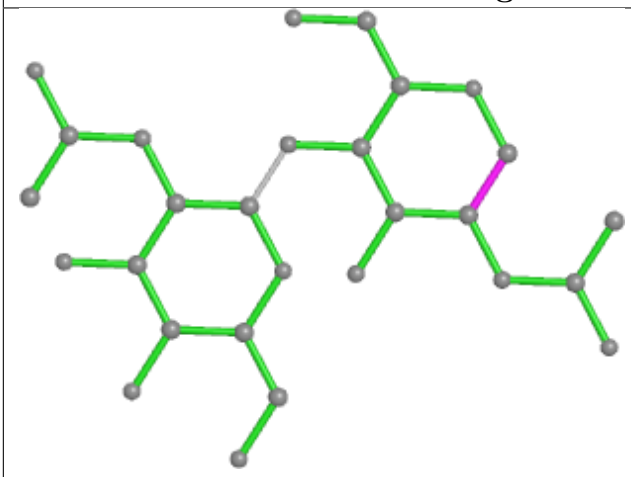
There are no ring outliers.

3 monomers are involved in 3 short contacts:

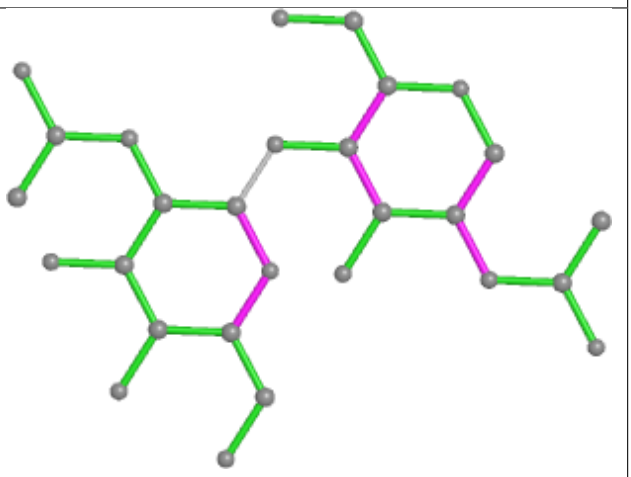
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	I	1	NAG	1	0
3	H	1	NAG	1	0

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

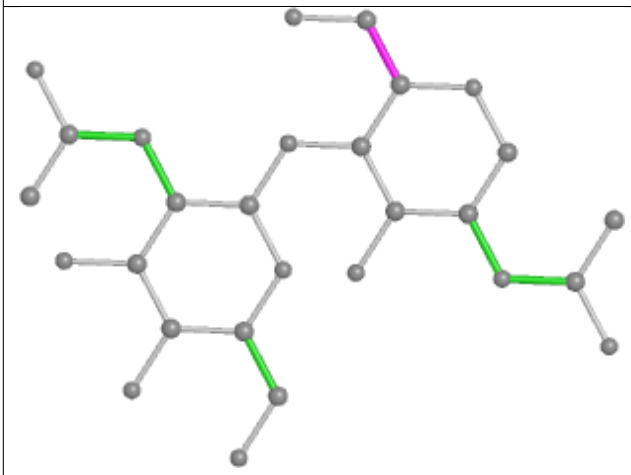
Oligosaccharide Chain E



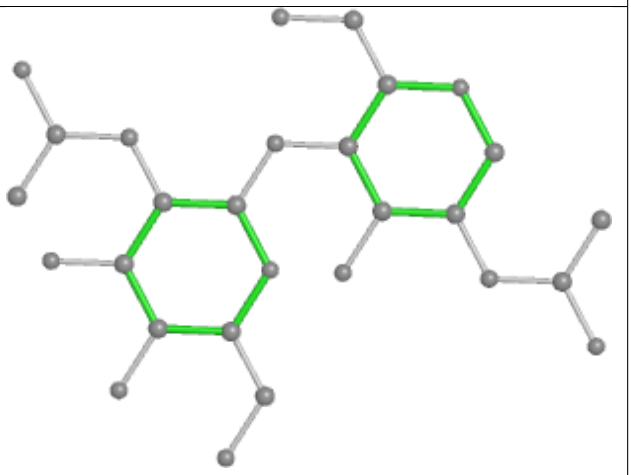
Bond lengths



Bond angles

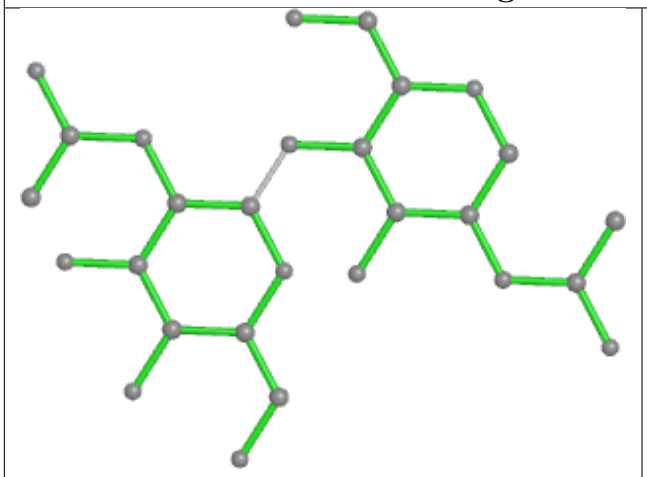


Torsions

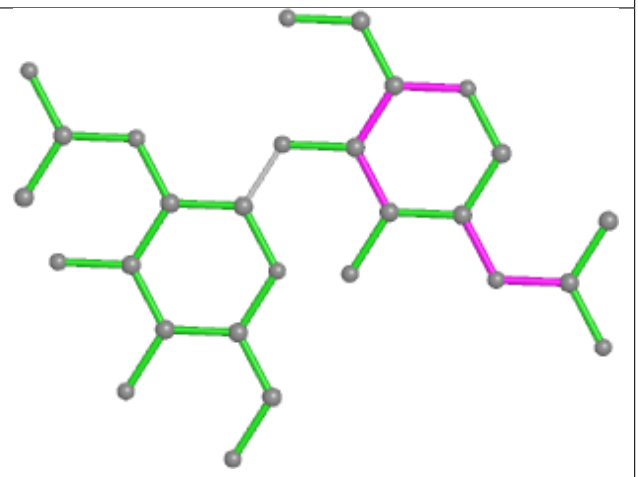


Rings

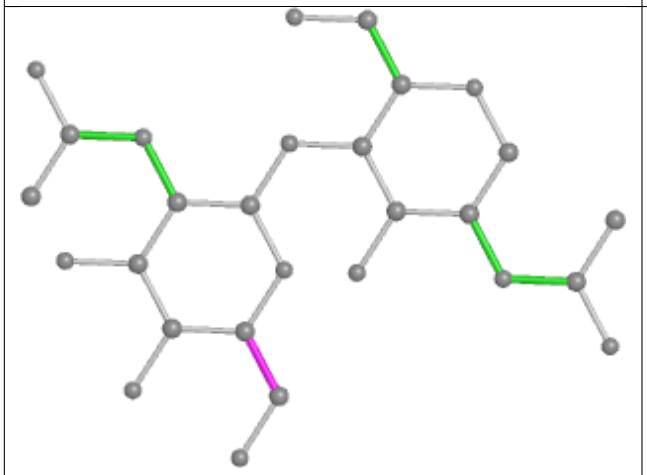
Oligosaccharide Chain F



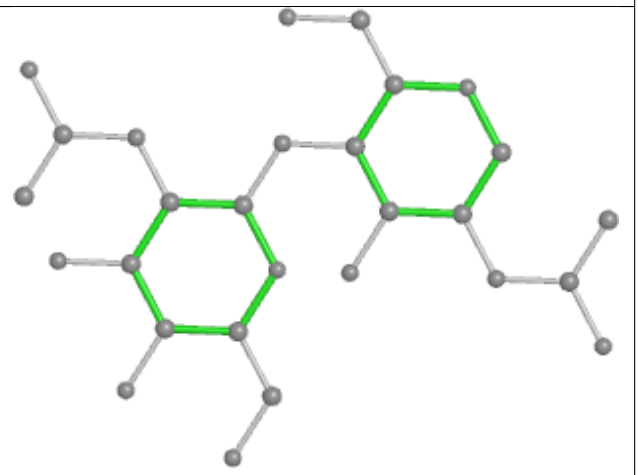
Bond lengths



Bond angles

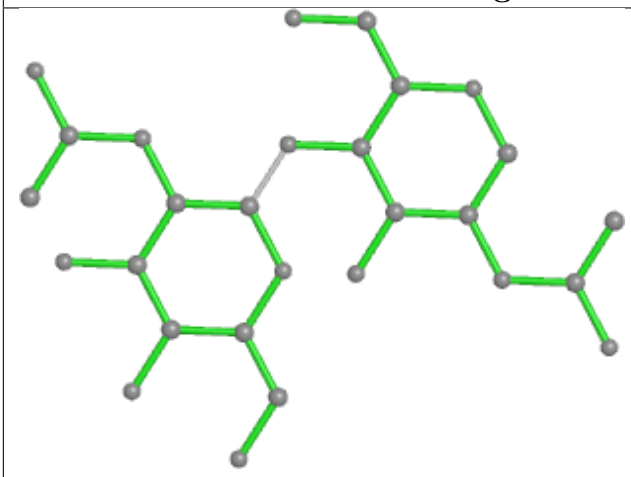


Torsions

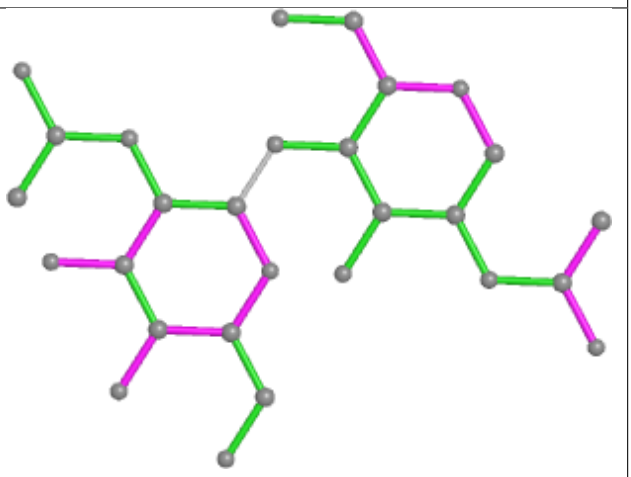


Rings

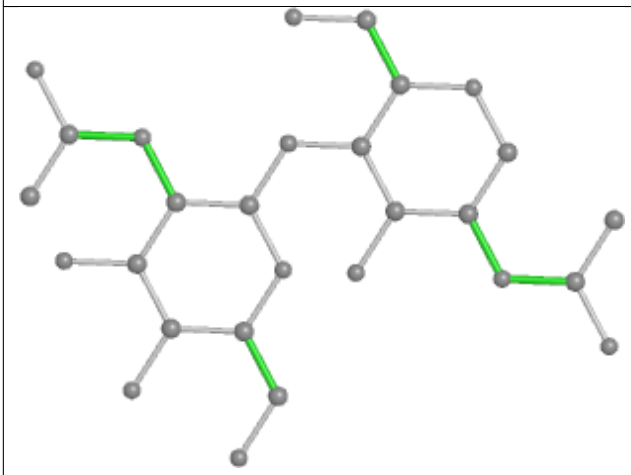
Oligosaccharide Chain G



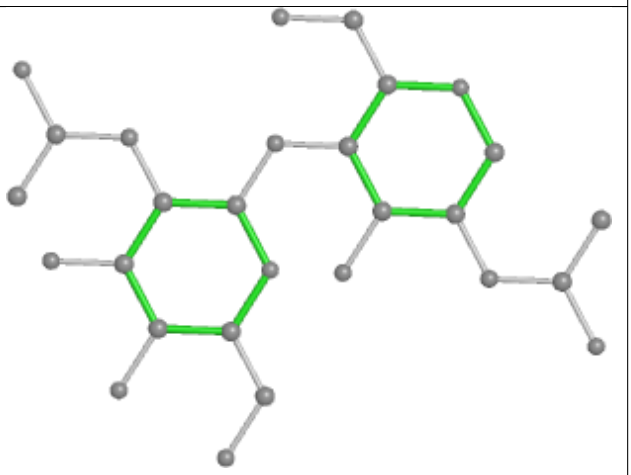
Bond lengths



Bond angles

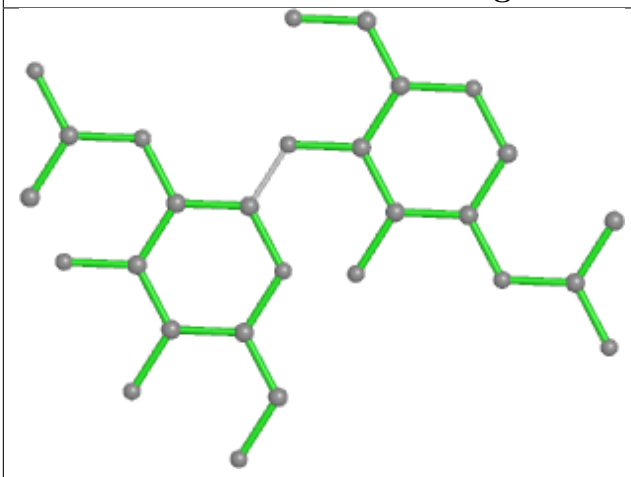


Torsions

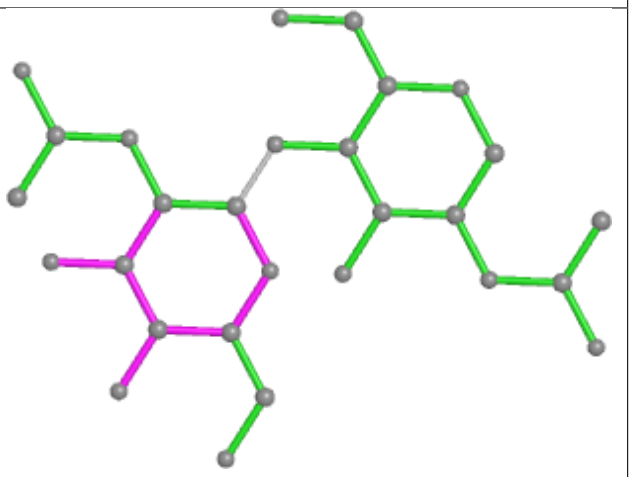


Rings

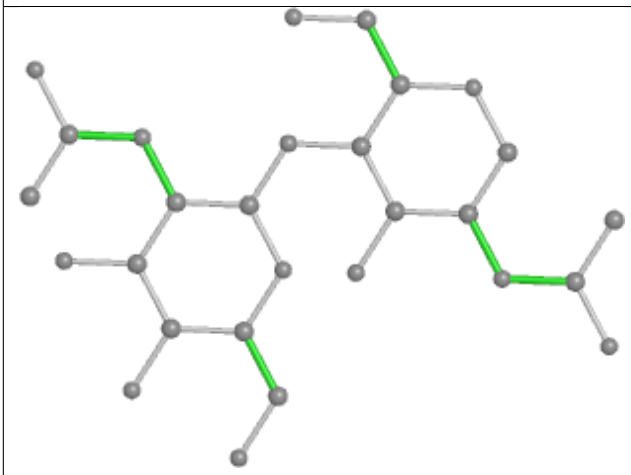
Oligosaccharide Chain H



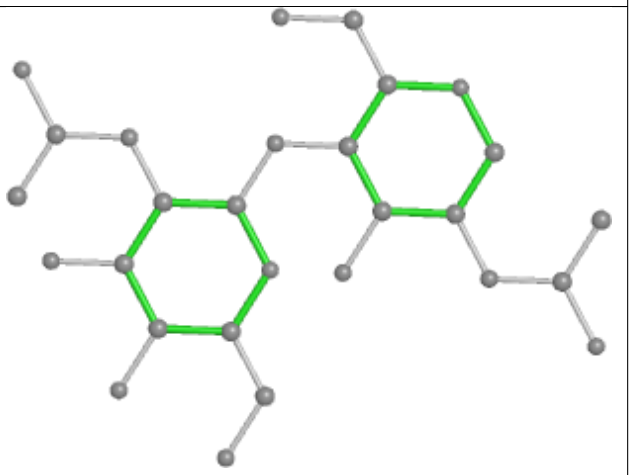
Bond lengths



Bond angles

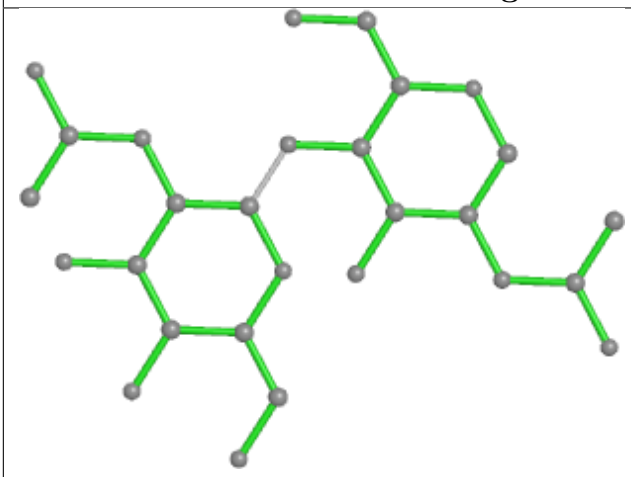


Torsions

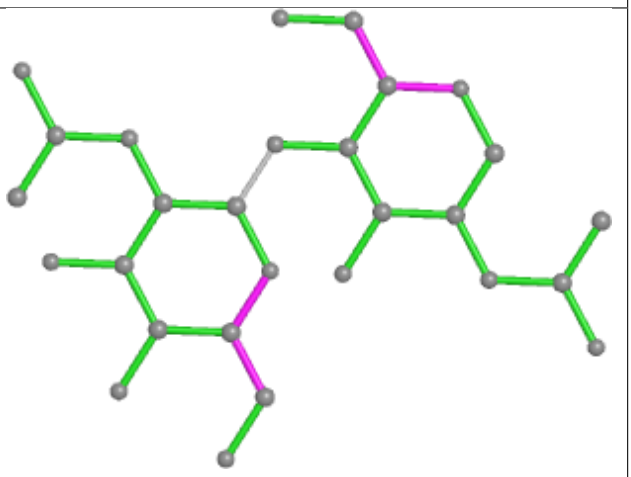


Rings

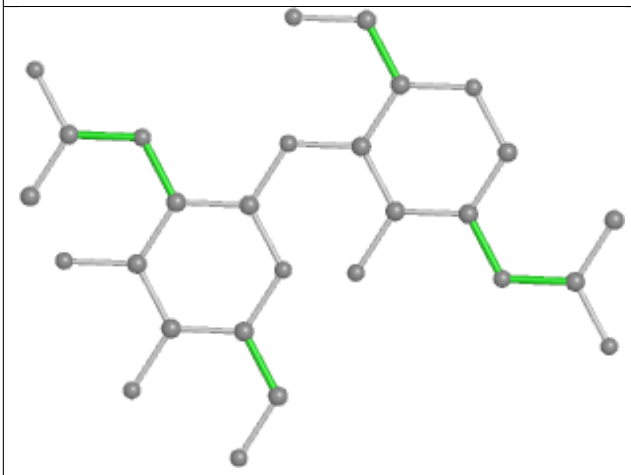
Oligosaccharide Chain I



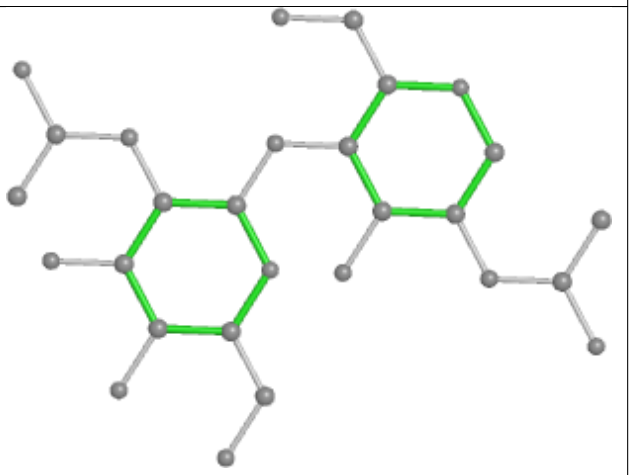
Bond lengths



Bond angles

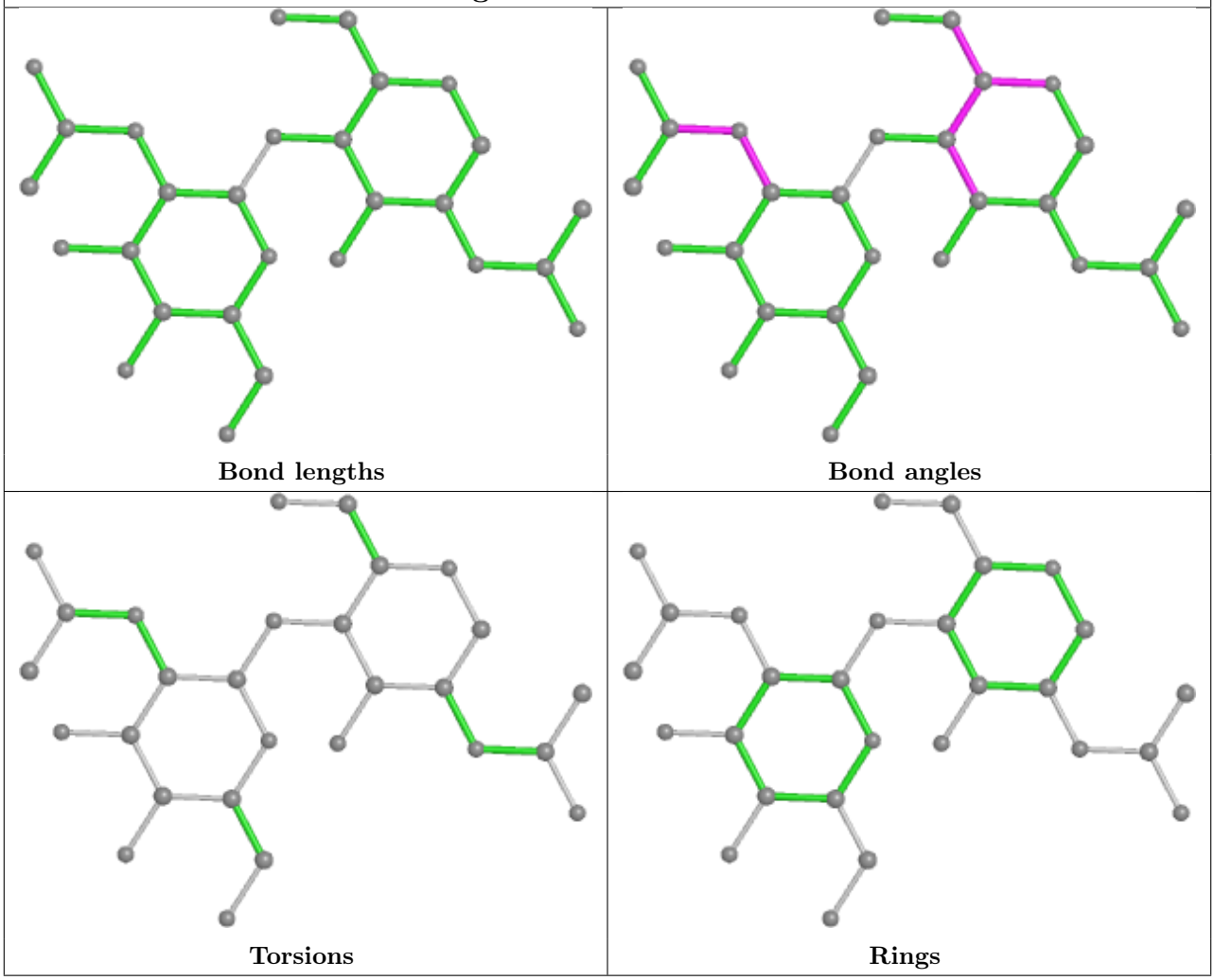


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
4	NAG	D	916	1	14,14,15	0.60	0	17,19,21	1.47	3 (17%)
4	NAG	D	903	1	14,14,15	0.58	0	17,19,21	0.90	0
4	NAG	A	904	1	14,14,15	0.62	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	904	1	14,14,15	0.50	0	17,19,21	1.24	2 (11%)
4	NAG	D	912	1	14,14,15	0.58	0	17,19,21	1.19	2 (11%)
4	NAG	A	909	-	14,14,15	0.76	1 (7%)	17,19,21	1.53	3 (17%)
4	NAG	A	915	1	14,14,15	0.48	0	17,19,21	0.89	2 (11%)
4	NAG	A	914	-	14,14,15	0.48	0	17,19,21	1.02	0
4	NAG	D	905	1	14,14,15	0.64	0	17,19,21	1.07	1 (5%)
4	NAG	A	903	1	14,14,15	0.46	0	17,19,21	1.52	3 (17%)
4	NAG	A	906	1	14,14,15	0.50	0	17,19,21	1.31	3 (17%)
4	NAG	D	914	1	14,14,15	0.49	0	17,19,21	0.84	0
4	NAG	A	905	1	14,14,15	0.46	0	17,19,21	1.24	1 (5%)
4	NAG	D	908	1	14,14,15	0.62	0	17,19,21	1.25	2 (11%)
4	NAG	A	910	1	14,14,15	0.45	0	17,19,21	1.51	1 (5%)
4	NAG	D	913	1	14,14,15	0.51	0	17,19,21	1.13	2 (11%)
4	NAG	D	909	1	14,14,15	0.60	0	17,19,21	1.72	3 (17%)
4	NAG	D	917	1	14,14,15	0.49	0	17,19,21	1.43	3 (17%)
4	NAG	A	911	1	14,14,15	0.58	0	17,19,21	1.01	1 (5%)
4	NAG	D	915	1	14,14,15	0.64	0	17,19,21	1.44	3 (17%)

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
4	NAG	D	916	1	-	2/6/23/26	0/1/1/1
4	NAG	D	903	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	3/6/23/26	0/1/1/1
4	NAG	D	904	1	-	4/6/23/26	0/1/1/1
4	NAG	D	912	1	-	1/6/23/26	0/1/1/1
4	NAG	A	909	-	-	0/6/23/26	0/1/1/1
4	NAG	A	915	1	-	2/6/23/26	0/1/1/1
4	NAG	A	914	-	-	1/6/23/26	0/1/1/1
4	NAG	D	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1	-	2/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	D	914	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	D	908	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	910	1	-	2/6/23/26	0/1/1/1
4	NAG	D	913	1	-	0/6/23/26	0/1/1/1
4	NAG	D	909	1	-	0/6/23/26	0/1/1/1
4	NAG	D	917	1	-	2/6/23/26	0/1/1/1
4	NAG	A	911	1	-	1/6/23/26	0/1/1/1
4	NAG	D	915	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	909	NAG	O5-C1	-2.08	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	910	NAG	C1-O5-C5	4.96	118.91	112.19
4	A	909	NAG	O5-C1-C2	-4.62	104.00	111.29
4	A	903	NAG	C1-O5-C5	4.39	118.14	112.19
4	D	909	NAG	C2-N2-C7	-4.12	117.03	122.90
4	D	916	NAG	C1-O5-C5	3.96	117.56	112.19
4	D	909	NAG	C1-O5-C5	3.76	117.29	112.19
4	D	904	NAG	C1-O5-C5	3.74	117.26	112.19
4	A	906	NAG	C1-O5-C5	3.63	117.11	112.19
4	D	915	NAG	C2-N2-C7	-3.61	117.76	122.90
4	A	905	NAG	C1-O5-C5	3.45	116.86	112.19
4	D	917	NAG	C1-O5-C5	3.19	116.51	112.19
4	D	916	NAG	O5-C1-C2	3.16	116.27	111.29
4	D	917	NAG	O5-C5-C6	3.12	112.10	107.20
4	D	913	NAG	C1-O5-C5	2.93	116.17	112.19
4	D	908	NAG	C1-O5-C5	2.92	116.15	112.19
4	A	906	NAG	O5-C5-C6	2.82	111.63	107.20
4	D	913	NAG	O5-C5-C6	2.79	111.57	107.20
4	D	908	NAG	C2-N2-C7	-2.74	119.00	122.90
4	D	909	NAG	O5-C1-C2	-2.59	107.20	111.29
4	D	915	NAG	O4-C4-C5	2.54	115.60	109.30
4	D	905	NAG	C2-N2-C7	-2.52	119.31	122.90
4	A	911	NAG	O5-C5-C6	2.48	111.09	107.20
4	D	904	NAG	O5-C5-C6	2.47	111.07	107.20
4	A	903	NAG	C4-C3-C2	-2.41	107.48	111.02
4	D	912	NAG	O5-C1-C2	-2.41	107.49	111.29
4	D	917	NAG	O3-C3-C2	2.26	114.14	109.47
4	A	903	NAG	O5-C5-C6	2.25	110.73	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	909	NAG	C1-O5-C5	-2.25	109.15	112.19
4	D	915	NAG	C8-C7-N2	2.22	119.86	116.10
4	A	909	NAG	C3-C4-C5	2.18	114.13	110.24
4	A	915	NAG	O5-C5-C6	2.13	110.54	107.20
4	A	906	NAG	C6-C5-C4	-2.09	108.12	113.00
4	A	915	NAG	C1-O5-C5	2.07	115.00	112.19
4	D	916	NAG	C1-C2-N2	-2.07	106.96	110.49
4	D	912	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	904	NAG	C8-C7-N2-C2
4	D	904	NAG	O7-C7-N2-C2
4	D	917	NAG	O5-C5-C6-O6
4	D	917	NAG	C4-C5-C6-O6
4	A	915	NAG	C8-C7-N2-C2
4	D	904	NAG	C4-C5-C6-O6
4	A	915	NAG	O7-C7-N2-C2
4	A	904	NAG	C8-C7-N2-C2
4	D	904	NAG	O5-C5-C6-O6
4	A	914	NAG	O5-C5-C6-O6
4	D	912	NAG	O5-C5-C6-O6
4	A	910	NAG	C8-C7-N2-C2
4	A	904	NAG	O7-C7-N2-C2
4	A	910	NAG	O7-C7-N2-C2
4	D	916	NAG	C4-C5-C6-O6
4	A	903	NAG	C8-C7-N2-C2
4	D	916	NAG	O5-C5-C6-O6
4	A	904	NAG	C4-C5-C6-O6
4	A	903	NAG	O7-C7-N2-C2
4	A	911	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	NAG	1	0
4	A	909	NAG	2	0
4	A	914	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	917	NAG	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	709/709 (100%)	0.14	21 (2%) 50 57	15, 38, 64, 121	0
1	D	709/709 (100%)	0.04	11 (1%) 72 77	15, 31, 57, 105	0
2	B	13/13 (100%)	-0.05	0 100 100	27, 34, 55, 71	0
2	C	13/13 (100%)	-0.46	1 (7%) 13 17	29, 32, 54, 72	0
All	All	1444/1444 (100%)	0.08	33 (2%) 60 67	15, 34, 62, 121	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	GLY	4.7
1	D	554	TYR	4.2
1	D	776	MET	3.8
1	A	339	VAL	3.8
1	A	282	ASN	3.7
1	D	282	ASN	3.5
1	D	775	ALA	3.3
1	A	554	TYR	3.2
1	A	140	TRP	2.8
1	A	764	GLY	2.8
1	A	283	LYS	2.7
1	D	762	GLN	2.7
1	A	121	TRP	2.6
1	A	119	PRO	2.6
1	A	147	PHE	2.6
1	D	773	ASP	2.5
1	A	775	ALA	2.5
1	D	771	ASP	2.5
1	A	334	LEU	2.5
1	A	591	LYS	2.5
1	A	345	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	331	HIS	2.4
1	A	367	LEU	2.2
1	A	762	GLN	2.2
1	D	772	PHE	2.2
1	D	308	LEU	2.2
2	C	1	A	2.2
1	A	142	ILE	2.2
1	A	144	GLU	2.1
1	A	776	MET	2.1
1	A	264	PHE	2.1
1	A	118	LEU	2.1
1	D	327	TRP	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)

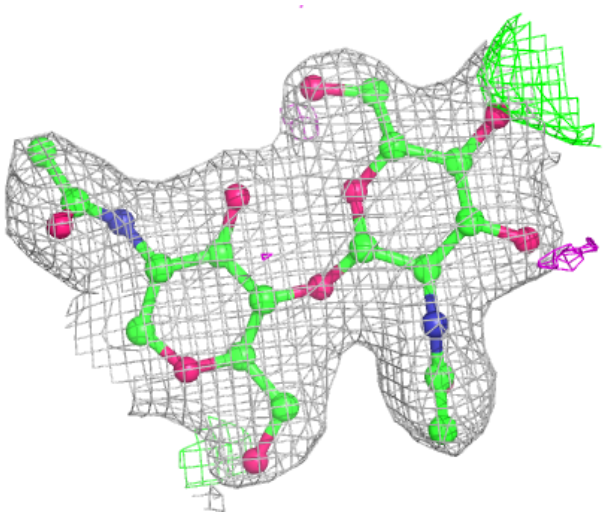
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

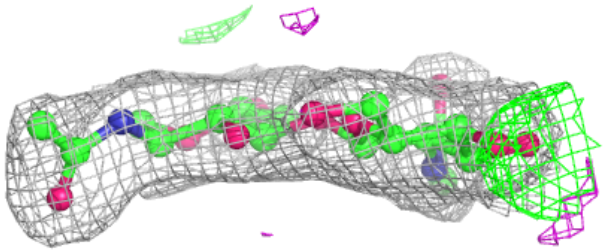
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.86	0.14	33,40,45,51	0
3	NAG	I	2	14/15	0.87	0.15	33,47,53,59	0
3	NAG	E	2	14/15	0.90	0.12	29,35,38,39	0
3	NAG	H	2	14/15	0.91	0.12	23,30,35,35	0
3	NAG	F	2	14/15	0.91	0.13	44,51,60,66	0
3	NAG	J	2	14/15	0.91	0.14	42,49,61,65	0
3	NAG	G	1	14/15	0.94	0.10	28,34,41,42	0
3	NAG	J	1	14/15	0.95	0.11	18,27,39,43	0
3	NAG	F	1	14/15	0.95	0.13	19,31,45,56	0
3	NAG	I	1	14/15	0.97	0.10	24,33,45,48	0
3	NAG	E	1	14/15	0.97	0.13	27,33,38,39	0
3	NAG	H	1	14/15	0.98	0.11	15,25,32,34	0

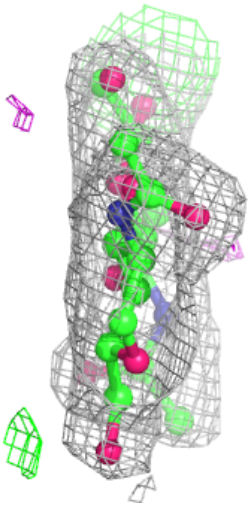
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

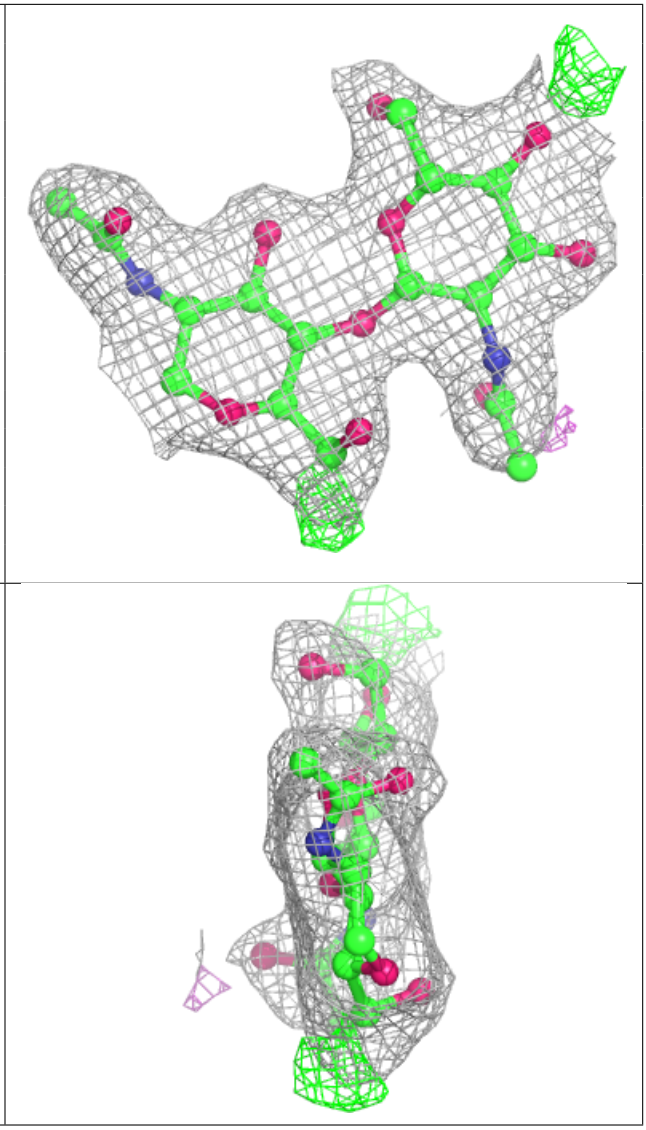






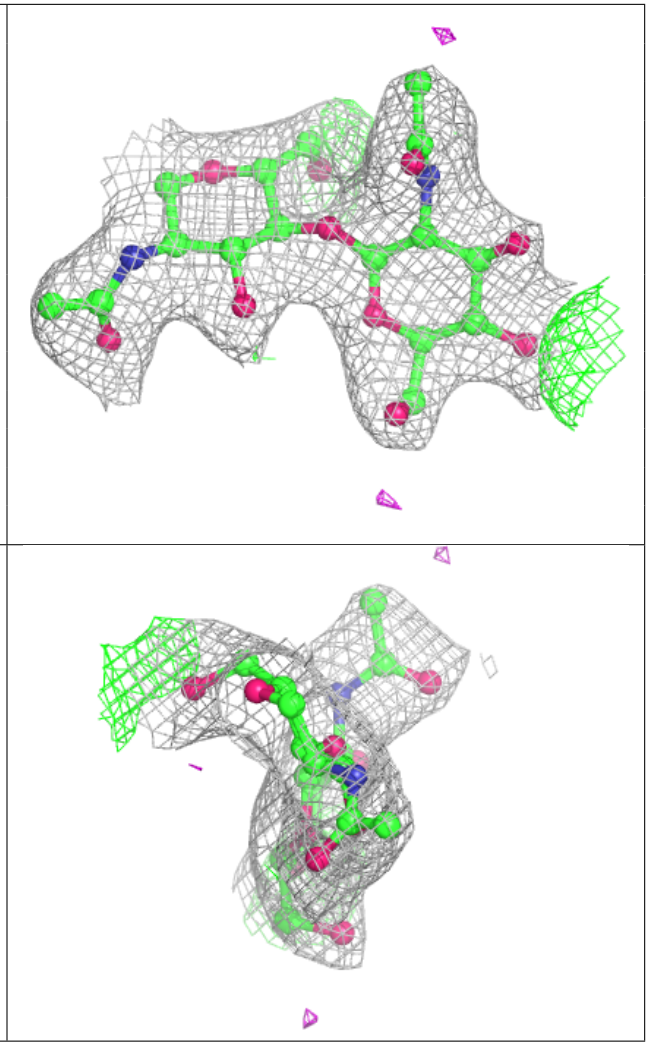
Electron density around Chain F:

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



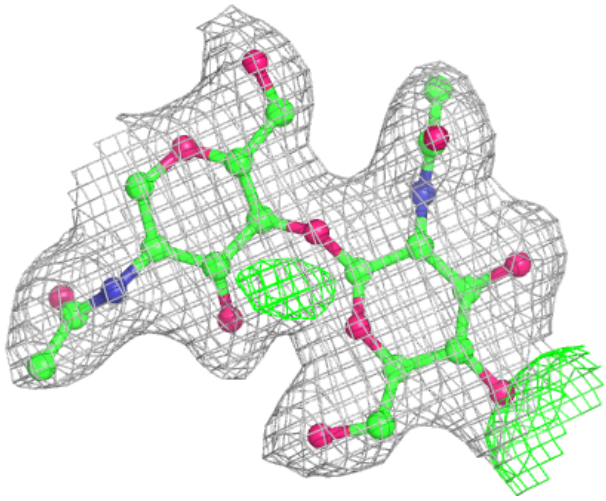
Electron density around Chain G:

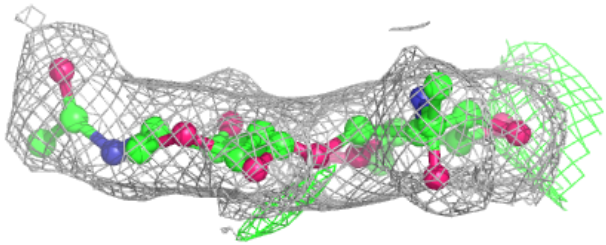
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

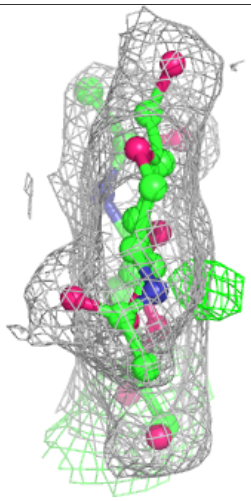


Electron density around Chain H:

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

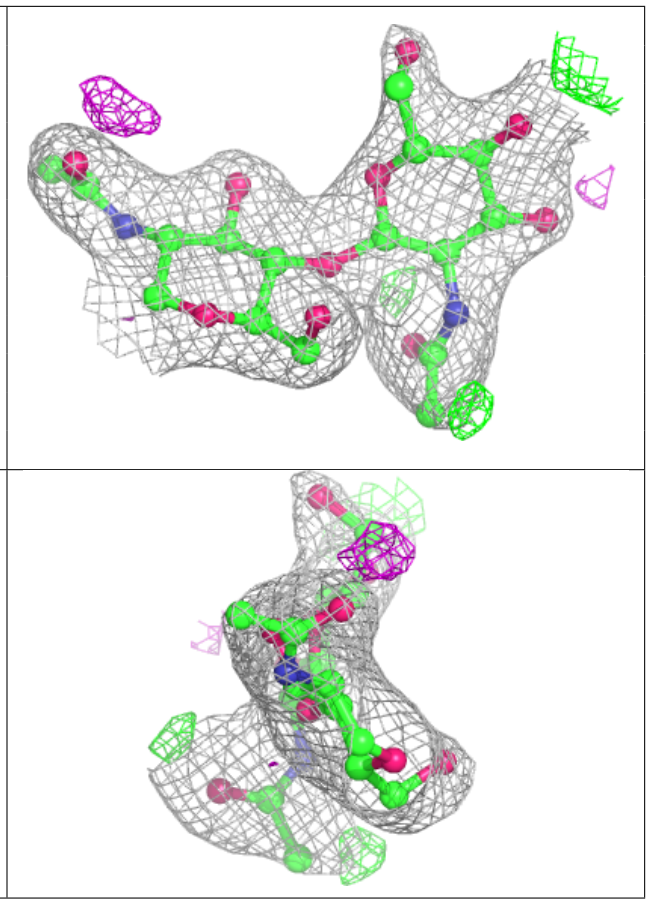


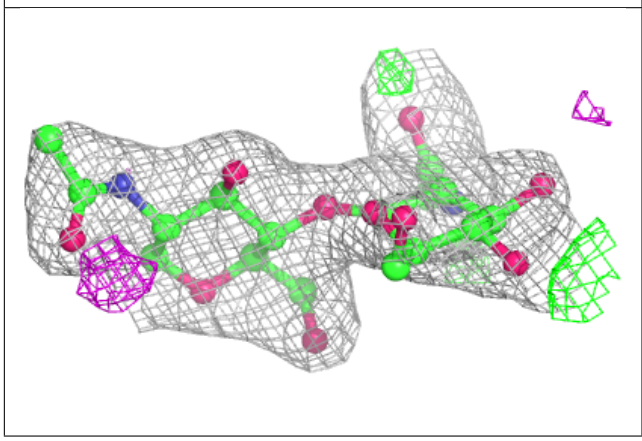




Electron density around Chain I:

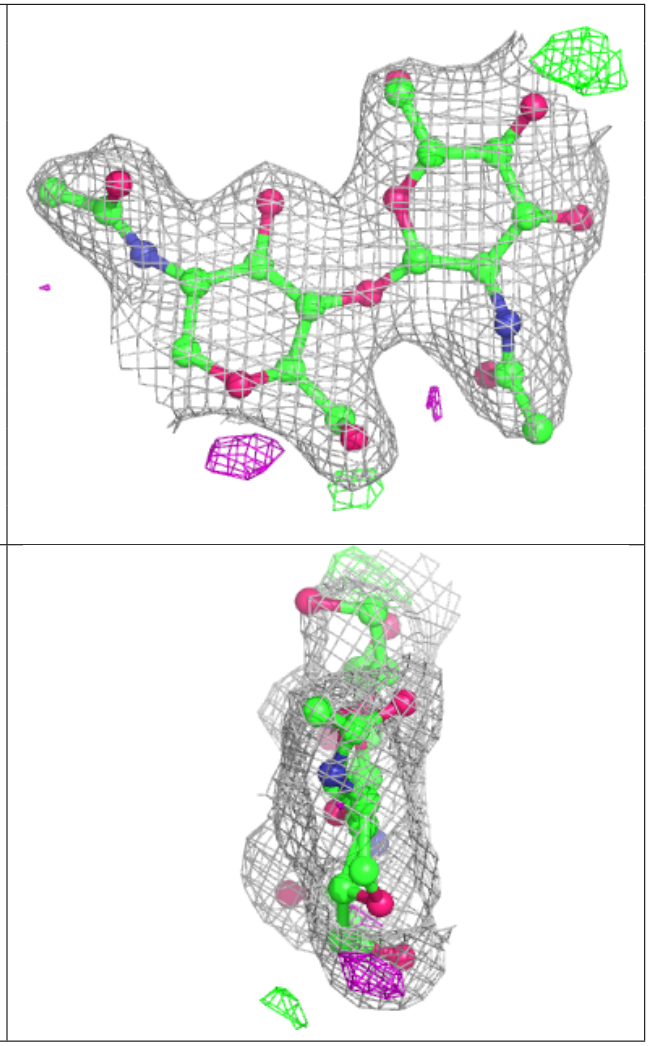
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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)



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
4	NAG	A	915	14/15	0.77	0.42	68,73,80,82	0
4	NAG	A	914	14/15	0.79	0.15	63,73,82,83	0
4	NAG	A	903	14/15	0.82	0.11	62,70,82,82	0
4	NAG	A	910	14/15	0.83	0.21	40,57,65,69	0
4	NAG	A	909	14/15	0.84	0.17	34,54,61,61	0
4	NAG	A	905	14/15	0.85	0.17	28,44,55,61	0
4	NAG	D	903	14/15	0.85	0.15	51,63,71,74	0
4	NAG	D	908	14/15	0.86	0.17	52,62,76,77	0
4	NAG	D	904	14/15	0.87	0.13	41,61,67,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	916	14/15	0.87	0.20	63,71,87,89	0
4	NAG	D	913	14/15	0.88	0.12	35,55,65,73	0
4	NAG	D	905	14/15	0.88	0.19	24,40,50,57	0
4	NAG	A	906	14/15	0.92	0.10	38,46,51,53	0
4	NAG	D	917	14/15	0.92	0.13	39,49,57,62	0
4	NAG	D	909	14/15	0.93	0.14	26,32,38,40	0
4	NAG	A	911	14/15	0.94	0.14	46,54,57,63	0
4	NAG	D	915	14/15	0.94	0.10	16,39,45,52	0
4	NAG	A	904	14/15	0.94	0.23	46,56,64,64	0
4	NAG	D	912	14/15	0.94	0.13	26,36,45,47	0
4	NAG	D	914	14/15	0.95	0.16	23,31,35,40	0

6.5 Other polymers (i)

There are no such residues in this entry.