Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 10:58 AM EST

PDB ID	:	1NWU
Title	:	Crystal structure of human cartilage gp39 (HC-gp39) in complex with chitotetraose
Authors	:	Fusetti, F.; Pijning, T.; Kalk, K.H.; Bos, E.; Dijkstra, B.W.
Deposited on	:	2003-02-06
Resolution	:	2.20 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:

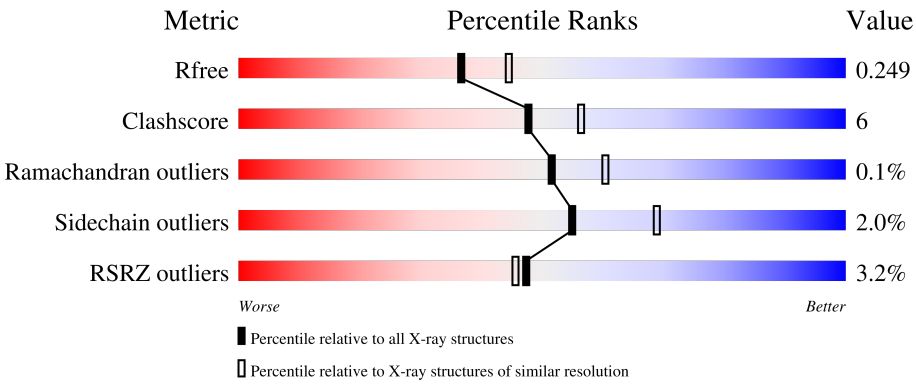
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	362	2%, 88%, 11%
1	B	362	6%, 88%, 12%
1	C	362	3%, 87%, 12%
1	D	362	2%, 88%, 11%
2	E	2	50%, 50%

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Mol	Chain	Length	Quality of chain
2	G	2	50% 50%
2	I	2	100%
2	K	2	50% 50%
3	F	4	50% 50%
3	J	4	50% 50%
3	L	4	25% 25% 50%
4	H	4	25% 75%

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
2	NAG	I	2	-	-	-	X
3	NAG	J	2	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12115 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 Chitinase-3 like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2839	1816	483	529	11	0	0	0
1	B	362	2839	1816	483	529	11	0	0	0
1	C	362	2839	1816	483	529	11	0	0	0
1	D	362	2839	1816	483	529	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	conflict	UNP P36222
B	311	ILE	THR	conflict	UNP P36222
C	311	ILE	THR	conflict	UNP P36222
D	311	ILE	THR	conflict	UNP P36222

- 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
			Total	C	N	O			
2	E	2	28	16	2	10	0	0	0
2	G	2	28	16	2	10	0	0	0
2	I	2	28	16	2	10	0	0	0

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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	F	4	57	32	4	21	0	0	0
3	J	4	57	32	4	21	0	0	0
3	L	4	57	32	4	21	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	4	57	32	4	21	0	0	0

- Molecule 5 is water.

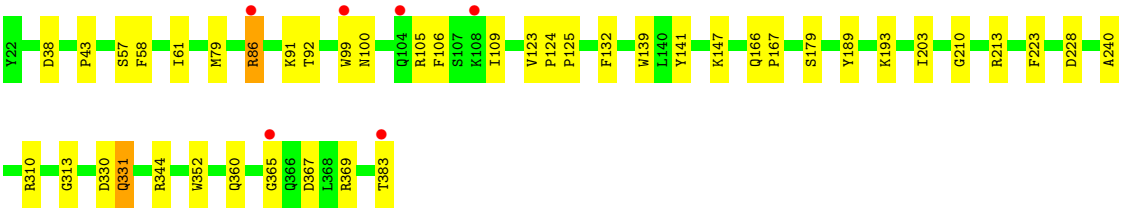
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	125	125	125	0	0
5	B	74	74	74	0	0
5	C	90	90	90	0	0
5	D	130	130	130	0	0

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.

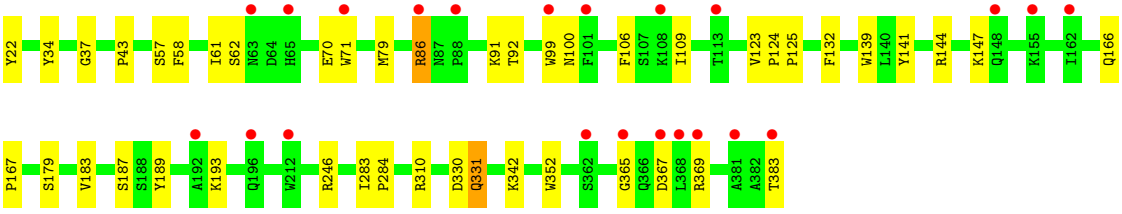
• Molecule 1: Chitinase-3 like protein 1

Chain A:



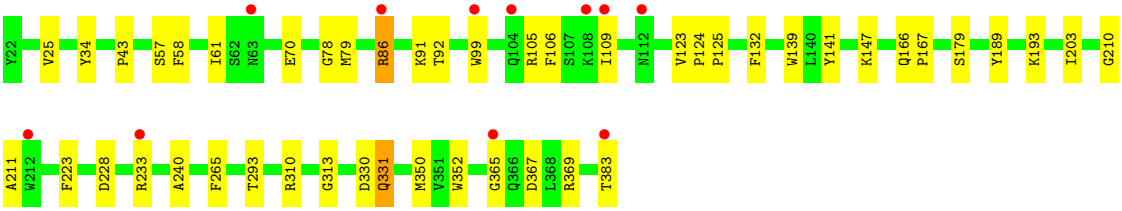
• Molecule 1: Chitinase-3 like protein 1

Chain B:



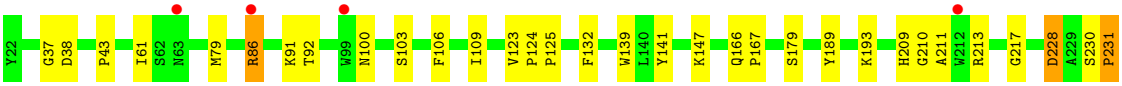
• Molecule 1: Chitinase-3 like protein 1

Chain C:



• Molecule 1: Chitinase-3 like protein 1

Chain D:



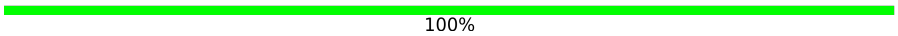
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain G:

• 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 K:

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

Chain F:

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

Chain J:

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

Chain L:

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	128.71Å 128.71Å 108.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.99 – 2.20 41.98 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.99-2.20) 99.6 (41.98-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	8.02 (at 2.06Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.245 0.231 , 0.249	Depositor DCC
R_{free} test set	12502 reflections (11.67%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12115	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, NDG

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	0.36	0/2915	0.62	2/3952 (0.1%)
1	B	0.36	0/2915	0.62	2/3952 (0.1%)
1	C	0.36	0/2915	0.78	3/3952 (0.1%)
1	D	0.36	0/2915	0.63	2/3952 (0.1%)
All	All	0.36	0/11660	0.67	9/15808 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	369	ARG	NE-CZ-NH2	-20.85	109.88	120.30
1	C	369	ARG	NE-CZ-NH1	20.48	130.54	120.30
1	C	369	ARG	CD-NE-CZ	10.25	137.94	123.60
1	A	369	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	D	369	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	369	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	369	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	D	369	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	B	369	ARG	NE-CZ-NH1	6.50	123.55	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2839	0	2742	31	0
1	B	2839	0	2742	31	0
1	C	2839	0	2742	31	0
1	D	2839	0	2742	33	0
2	E	28	0	25	0	0
2	G	28	0	25	1	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
3	F	57	0	50	7	0
3	J	57	0	50	12	0
3	L	57	0	50	6	0
4	H	57	0	47	6	0
5	A	125	0	0	3	0
5	B	74	0	0	3	0
5	C	90	0	0	1	0
5	D	130	0	0	4	0
All	All	12115	0	11265	141	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 6.

All (141) 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)
3:J:2:NAG:H4	3:J:3:NAG:H62	1.42	0.99
1:A:86:ARG:HH11	1:A:86:ARG:HB3	1.32	0.95
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.32	0.94
1:C:86:ARG:HH11	1:C:86:ARG:HB3	1.33	0.92
1:D:86:ARG:HH11	1:D:86:ARG:HB3	1.32	0.90
3:J:1:NAG:H62	3:J:2:NAG:H82	1.59	0.83
3:F:2:NAG:O3	3:F:3:NAG:H4	1.82	0.80
1:A:92:THR:HG22	1:A:132:PHE:HD1	1.54	0.73
5:A:470:HOH:O	3:F:2:NAG:H83	1.86	0.73
1:B:92:THR:HG22	1:B:132:PHE:HD1	1.54	0.72
1:D:92:THR:HG22	1:D:132:PHE:HD1	1.55	0.72
1:B:86:ARG:HB3	1:B:86:ARG:NH1	2.05	0.71
1:B:92:THR:HG22	1:B:132:PHE:CD1	2.26	0.71
1:C:92:THR:HG22	1:C:132:PHE:HD1	1.55	0.70
1:A:92:THR:HG22	1:A:132:PHE:CD1	2.25	0.70
1:C:92:THR:HG22	1:C:132:PHE:CD1	2.27	0.70
1:D:86:ARG:HB3	1:D:86:ARG:NH1	2.06	0.70
1:D:92:THR:HG22	1:D:132:PHE:CD1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HB3	1:A:86:ARG:NH1	2.05	0.69
3:J:2:NAG:C4	3:J:3:NAG:H62	2.20	0.69
1:C:86:ARG:HB3	1:C:86:ARG:NH1	2.06	0.69
1:B:61:ILE:HG21	1:B:109:ILE:HD13	1.77	0.67
1:C:61:ILE:HG21	1:C:109:ILE:HD13	1.76	0.66
1:A:61:ILE:HG21	1:A:109:ILE:HD13	1.78	0.66
1:D:61:ILE:HG21	1:D:109:ILE:HD13	1.77	0.65
3:L:2:NAG:O3	3:L:3:NAG:H4	1.98	0.64
1:A:331:GLN:NE2	5:A:535:HOH:O	2.32	0.61
1:C:86:ARG:HH11	1:C:86:ARG:CB	2.11	0.61
1:A:310:ARG:NH2	1:A:330:ASP:OD2	2.32	0.61
1:B:86:ARG:HH11	1:B:86:ARG:CB	2.10	0.61
3:J:2:NAG:H4	3:J:3:NAG:C6	2.24	0.60
1:B:166:GLN:N	1:B:167:PRO:HD2	2.17	0.60
1:C:166:GLN:N	1:C:167:PRO:HD2	2.17	0.59
1:A:86:ARG:HH11	1:A:86:ARG:CB	2.11	0.59
1:D:166:GLN:N	1:D:167:PRO:HD2	2.18	0.59
1:D:310:ARG:NH2	1:D:330:ASP:OD2	2.36	0.59
1:A:166:GLN:N	1:A:167:PRO:HD2	2.17	0.59
1:A:124:PRO:HB2	1:A:125:PRO:HD3	1.85	0.59
1:C:310:ARG:NH2	1:C:330:ASP:OD2	2.36	0.59
3:J:1:NAG:C6	3:J:2:NAG:H82	2.32	0.59
1:D:124:PRO:HB2	1:D:125:PRO:HD3	1.85	0.58
1:C:211:ALA:N	1:C:265:PHE:HE1	2.02	0.58
1:B:310:ARG:NH2	1:B:330:ASP:OD2	2.37	0.57
1:C:124:PRO:HB2	1:C:125:PRO:HD3	1.86	0.57
1:D:86:ARG:HH11	1:D:86:ARG:CB	2.10	0.57
4:H:2:NAG:O3	4:H:3:NAG:H4	2.05	0.56
1:D:123:VAL:HB	1:D:124:PRO:HD3	1.87	0.56
1:D:352:TRP:CZ3	3:L:3:NAG:H83	2.40	0.56
1:C:123:VAL:HB	1:C:124:PRO:HD3	1.89	0.55
4:H:2:NAG:O4	4:H:3:NAG:H4	2.05	0.54
1:C:78:GLY:HA3	1:D:167:PRO:HB2	1.89	0.54
1:B:22:TYR:CZ	1:B:342:LYS:HG2	2.43	0.54
1:B:43:PRO:HB2	1:B:79:MET:HB3	1.89	0.54
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.89	0.53
1:A:352:TRP:CE3	3:F:3:NAG:H83	2.44	0.53
1:C:43:PRO:HB2	1:C:79:MET:HB3	1.90	0.53
1:B:123:VAL:HB	1:B:124:PRO:HD3	1.91	0.53
1:B:352:TRP:CZ3	4:H:3:NAG:H83	2.42	0.53
1:B:124:PRO:HB2	1:B:125:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LYS:HE3	1:B:189:TYR:O	2.09	0.53
1:C:352:TRP:CZ2	3:J:3:NAG:H3	2.45	0.52
1:A:43:PRO:HB2	1:A:79:MET:HB3	1.91	0.52
1:B:139:TRP:O	1:B:141:TYR:HA	2.10	0.52
1:D:141:TYR:CE2	1:D:179:SER:HB2	2.45	0.52
1:A:139:TRP:O	1:A:141:TYR:HA	2.10	0.51
1:B:183:VAL:HG23	5:B:434:HOH:O	2.10	0.51
1:C:141:TYR:CE2	1:C:179:SER:HB2	2.45	0.51
1:A:99:TRP:CE3	3:F:2:NAG:H3	2.45	0.51
1:D:43:PRO:HB2	1:D:79:MET:HB3	1.91	0.51
1:A:147:LYS:HE3	1:A:189:TYR:O	2.11	0.51
1:C:139:TRP:O	1:C:141:TYR:HA	2.11	0.50
1:B:141:TYR:CE2	1:B:179:SER:HB2	2.47	0.50
1:A:344:ARG:NH2	5:A:418:HOH:O	2.44	0.49
1:D:139:TRP:O	1:D:141:TYR:HA	2.12	0.49
1:D:100:ASN:ND2	3:L:4:NDG:H6C2	2.28	0.49
1:D:147:LYS:HE3	1:D:189:TYR:O	2.12	0.48
1:B:365:GLY:C	1:B:367:ASP:H	2.16	0.48
1:A:210:GLY:O	1:A:213:ARG:HG3	2.13	0.48
1:D:365:GLY:C	1:D:367:ASP:H	2.16	0.48
1:A:365:GLY:C	1:A:367:ASP:H	2.17	0.48
1:B:37:GLY:HA3	5:B:456:HOH:O	2.13	0.48
1:B:71:TRP:HD1	5:B:467:HOH:O	1.97	0.48
1:A:141:TYR:CE2	1:A:179:SER:HB2	2.49	0.47
1:D:37:GLY:HA3	5:D:450:HOH:O	2.14	0.47
1:C:147:LYS:HE3	1:C:189:TYR:O	2.14	0.47
3:J:3:NAG:O3	3:J:4:NDG:H6C1	2.13	0.47
1:C:99:TRP:CD2	3:J:2:NAG:H3	2.49	0.47
1:C:293:THR:HG21	3:J:4:NDG:H8C2	1.95	0.47
1:D:228:ASP:HB2	5:D:463:HOH:O	2.14	0.47
1:C:365:GLY:C	1:C:367:ASP:H	2.17	0.47
4:H:3:NAG:H61	4:H:4:NDG:N2	2.28	0.47
1:C:57:SER:HA	1:C:58:PHE:HA	1.69	0.46
3:L:2:NAG:O4	3:L:3:NAG:H4	2.13	0.46
1:A:383:THR:HG22	1:A:383:THR:O	2.16	0.46
1:D:210:GLY:C	1:D:265:PHE:HE1	2.19	0.46
1:A:99:TRP:CH2	3:F:1:NAG:H61	2.51	0.46
1:B:57:SER:HA	1:B:58:PHE:HA	1.69	0.46
1:D:344:ARG:NH2	5:D:445:HOH:O	2.49	0.46
1:B:62:SER:HA	2:G:1:NAG:O6	2.16	0.46
1:A:100:ASN:ND2	3:F:4:NDG:H6C2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:SER:HB2	5:D:516:HOH:O	2.16	0.45
1:B:331:GLN:H	1:B:331:GLN:HE21	1.65	0.45
1:A:57:SER:HA	1:A:58:PHE:HA	1.69	0.45
1:C:383:THR:HG22	1:C:383:THR:O	2.17	0.45
1:A:38:ASP:HB3	1:A:360:GLN:HE21	1.83	0.44
1:B:383:THR:HG22	1:B:383:THR:O	2.17	0.44
1:D:38:ASP:HB3	1:D:360:GLN:HE21	1.81	0.44
1:D:383:THR:O	1:D:383:THR:HG22	2.17	0.44
1:B:99:TRP:CH2	4:H:1:NDG:H6C1	2.52	0.44
3:J:2:NAG:O3	3:J:3:NAG:H4	2.17	0.44
1:D:331:GLN:HE21	1:D:331:GLN:H	1.66	0.44
3:J:1:NAG:H62	3:J:2:NAG:C8	2.39	0.44
1:A:203:ILE:HD11	1:A:240:ALA:HB1	2.00	0.44
1:B:100:ASN:ND2	4:H:4:NDG:H6C2	2.33	0.43
1:C:25:VAL:O	1:C:350:MET:HA	2.18	0.43
1:D:230:SER:HA	1:D:231:PRO:HD3	1.88	0.43
1:C:331:GLN:NE2	5:C:465:HOH:O	2.51	0.43
1:A:331:GLN:HE21	1:A:331:GLN:H	1.67	0.43
1:D:100:ASN:CG	3:L:4:NDG:H6C2	2.39	0.42
1:A:99:TRP:CD2	3:F:2:NAG:H3	2.55	0.42
1:C:331:GLN:HE21	1:C:331:GLN:H	1.67	0.42
1:D:211:ALA:N	1:D:265:PHE:HE1	2.16	0.42
1:A:105:ARG:NH1	1:A:105:ARG:HB3	2.35	0.42
1:C:203:ILE:HD11	1:C:240:ALA:HB1	2.01	0.42
3:L:2:NAG:H4	3:L:3:NAG:O6	2.19	0.42
1:A:223:PHE:HB2	1:A:313:GLY:O	2.19	0.42
1:C:223:PHE:HB2	1:C:313:GLY:O	2.20	0.42
1:B:92:THR:CG2	1:B:132:PHE:CD1	3.02	0.41
1:D:209:HIS:CE1	1:D:213:ARG:HD3	2.56	0.41
1:B:34:TYR:OH	1:B:70:GLU:HG3	2.21	0.41
1:C:99:TRP:CH2	3:J:1:NAG:H61	2.55	0.41
1:D:209:HIS:CD2	1:D:217:GLY:HA3	2.55	0.41
1:C:34:TYR:OH	1:C:70:GLU:HG3	2.21	0.41
1:D:38:ASP:CA	1:D:360:GLN:HE21	2.33	0.41
1:A:310:ARG:HH22	1:A:330:ASP:CG	2.25	0.41
1:B:283:ILE:HA	1:B:284:PRO:HD3	1.96	0.41
1:B:246:ARG:O	1:B:246:ARG:HG2	2.20	0.40
1:C:105:ARG:HB3	1:C:105:ARG:NH1	2.35	0.40
1:C:210:GLY:C	1:C:265:PHE:HE1	2.23	0.40
1:B:144:ARG:HA	1:B:187:SER:O	2.20	0.40
1:D:352:TRP:HA	1:D:353:ALA:HA	1.86	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	360/362 (99%)	352 (98%)	8 (2%)	0	100	100
1	B	360/362 (99%)	349 (97%)	11 (3%)	0	100	100
1	C	360/362 (99%)	350 (97%)	10 (3%)	0	100	100
1	D	360/362 (99%)	349 (97%)	10 (3%)	1 (0%)	41	46
All	All	1440/1448 (99%)	1400 (97%)	39 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	231	PRO

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	298/302 (99%)	292 (98%)	6 (2%)	55	69
1	B	298/302 (99%)	293 (98%)	5 (2%)	60	74
1	C	298/302 (99%)	291 (98%)	7 (2%)	50	63
1	D	298/302 (99%)	292 (98%)	6 (2%)	55	69
All	All	1192/1208 (99%)	1168 (98%)	24 (2%)	55	69

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	91	LYS
1	A	106	PHE
1	A	193	LYS
1	A	228	ASP
1	A	331	GLN
1	B	86	ARG
1	B	91	LYS
1	B	106	PHE
1	B	193	LYS
1	B	331	GLN
1	C	86	ARG
1	C	91	LYS
1	C	106	PHE
1	C	193	LYS
1	C	228	ASP
1	C	233	ARG
1	C	331	GLN
1	D	86	ARG
1	D	91	LYS
1	D	106	PHE
1	D	193	LYS
1	D	228	ASP
1	D	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	A	331	GLN
1	A	345	GLN
1	A	360	GLN
1	B	331	GLN
1	B	345	GLN
1	C	100	ASN
1	C	331	GLN
1	C	345	GLN
1	C	360	GLN
1	D	100	ASN
1	D	331	GLN
1	D	345	GLN

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Mol	Chain	Res	Type
1	D	360	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	0.47	0	17,19,21	0.73	1 (5%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.60	0
3	NAG	F	1	3	15,15,15	0.53	0	21,21,21	0.73	0
3	NAG	F	2	3	14,14,15	0.64	0	17,19,21	0.68	0
3	NAG	F	3	3	14,14,15	1.02	1 (7%)	17,19,21	1.09	1 (5%)
3	NDG	F	4	3	14,14,15	0.75	1 (7%)	17,19,21	0.90	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
2	NAG	G	2	2	14,14,15	0.56	0	17,19,21	0.66	0
4	NDG	H	1	4	15,15,15	0.58	0	21,21,21	0.63	0
4	NAG	H	2	4	14,14,15	0.69	0	17,19,21	0.71	1 (5%)
4	NAG	H	3	4	14,14,15	1.03	1 (7%)	17,19,21	1.15	1 (5%)
4	NDG	H	4	4	14,14,15	0.75	0	17,19,21	0.79	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.53	0	17,19,21	0.68	0
2	NAG	I	2	2	14,14,15	0.59	0	17,19,21	0.62	0
3	NAG	J	1	3	15,15,15	0.55	0	21,21,21	0.65	0
3	NAG	J	2	3	14,14,15	0.64	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	J	3	3	14,14,15	0.82	0	17,19,21	0.97	1 (5%)
3	NDG	J	4	3	14,14,15	0.71	0	17,19,21	0.77	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.55	0	17,19,21	0.61	0
2	NAG	K	2	2	14,14,15	0.52	0	17,19,21	0.79	1 (5%)
3	NAG	L	1	3	15,15,15	0.54	0	21,21,21	0.62	0
3	NAG	L	2	3	14,14,15	0.70	0	17,19,21	0.73	0
3	NAG	L	3	3	14,14,15	1.07	1 (7%)	17,19,21	1.12	1 (5%)
3	NDG	L	4	3	14,14,15	0.76	1 (7%)	17,19,21	0.86	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
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	3	-	0/6/26/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	3	3	-	2/6/23/26	0/1/1/1
3	NDG	F	4	3	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
4	NDG	H	1	4	-	2/6/26/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	3	4	-	0/6/23/26	0/1/1/1
4	NDG	H	4	4	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3	-	2/6/26/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	3	3	-	1/6/23/26	0/1/1/1
3	NDG	J	4	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3	-	0/6/26/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	3	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	L	4	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	3	NAG	C1-C2	2.40	1.55	1.52
3	L	3	NAG	C1-C2	2.34	1.55	1.52
3	F	3	NAG	C1-C2	2.16	1.55	1.52
3	L	4	NDG	C1-C2	2.09	1.55	1.52
3	F	4	NDG	C1-C2	2.01	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	NAG	C2-N2-C7	-2.42	119.46	122.90
3	L	3	NAG	C2-N2-C7	-2.35	119.56	122.90
2	K	2	NAG	C2-N2-C7	-2.31	119.61	122.90
4	H	3	NAG	C2-N2-C7	-2.31	119.62	122.90
3	F	4	NDG	C2-N2-C7	-2.30	119.62	122.90
3	J	4	NDG	C2-N2-C7	-2.28	119.66	122.90
3	J	3	NAG	C1-O5-C5	2.24	115.22	112.19
2	G	1	NAG	C2-N2-C7	-2.21	119.76	122.90
2	E	1	NAG	C2-N2-C7	-2.17	119.81	122.90
4	H	4	NDG	C2-N2-C7	-2.15	119.84	122.90
3	L	4	NDG	C2-N2-C7	-2.14	119.86	122.90
4	H	2	NAG	C2-N2-C7	-2.07	119.96	122.90

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	J	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
3	F	3	NAG	C8-C7-N2-C2
3	F	3	NAG	O7-C7-N2-C2
3	J	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
4	H	4	NDG	C8-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	4	NDG	C4-C5-C6-O6
3	F	2	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O7-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
3	L	4	NDG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	H	4	NDG	O7-C7-N2-C2
3	J	4	NDG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	L	4	NDG	O7-C7-N2-C2
2	K	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	L	3	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	H	1	NDG	C8-C7-N2-C2
3	J	3	NAG	O5-C5-C6-O6
3	L	3	NAG	O5-C5-C6-O6
4	H	1	NDG	O7-C7-N2-C2
2	I	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	4	NDG	2	0

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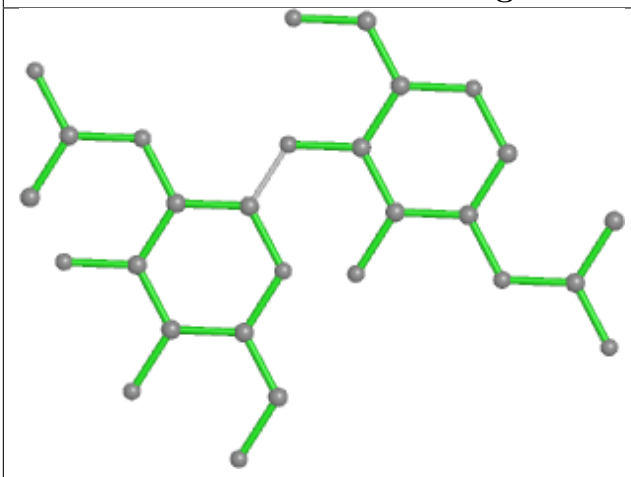
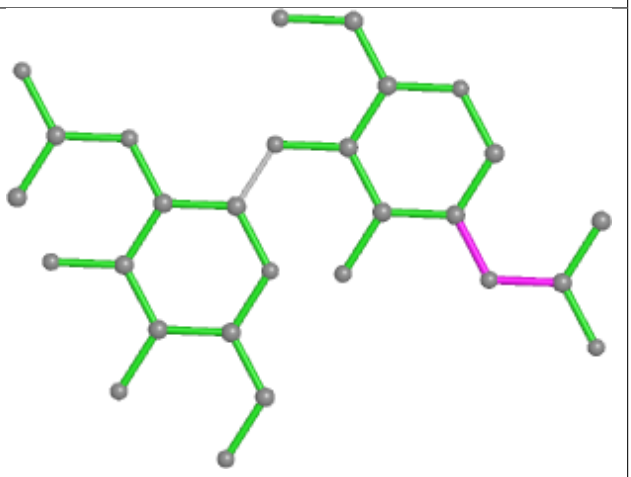
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NDG	1	0
2	G	1	NAG	1	0
4	H	4	NDG	2	0
3	F	1	NAG	1	0
4	H	3	NAG	4	0
3	F	4	NDG	1	0
3	L	3	NAG	4	0
3	L	2	NAG	3	0
3	J	1	NAG	4	0
3	J	4	NDG	2	0
4	H	2	NAG	2	0
3	J	3	NAG	6	0
3	J	2	NAG	8	0
3	F	3	NAG	2	0
3	F	2	NAG	4	0

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

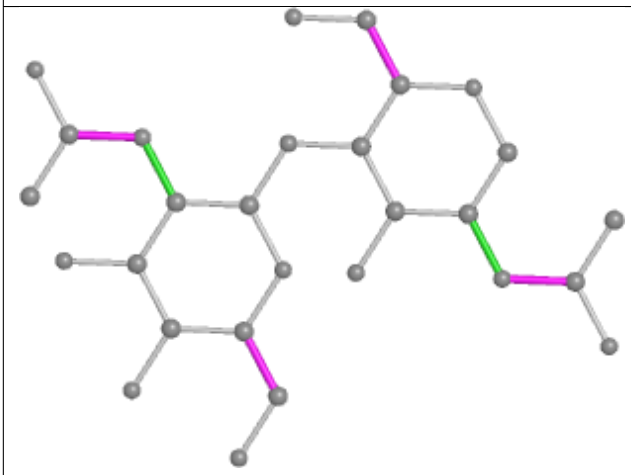
Oligosaccharide Chain E



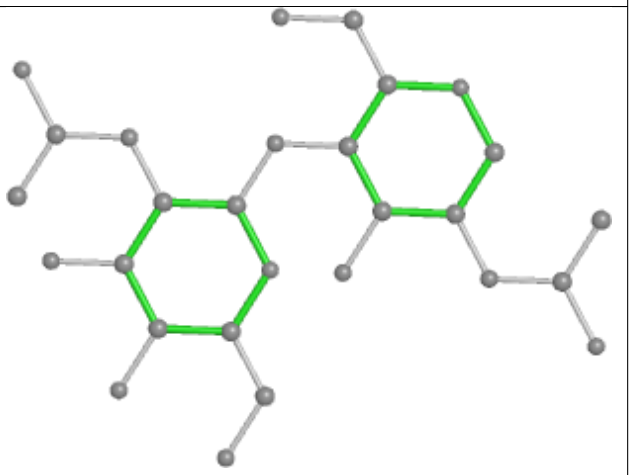
Bond lengths



Bond angles

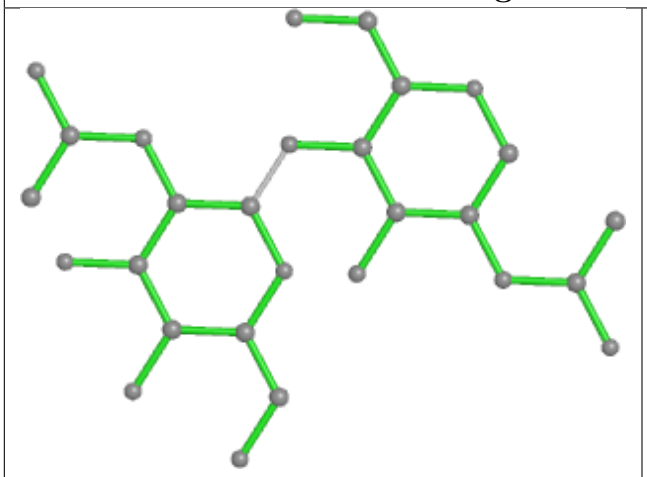


Torsions

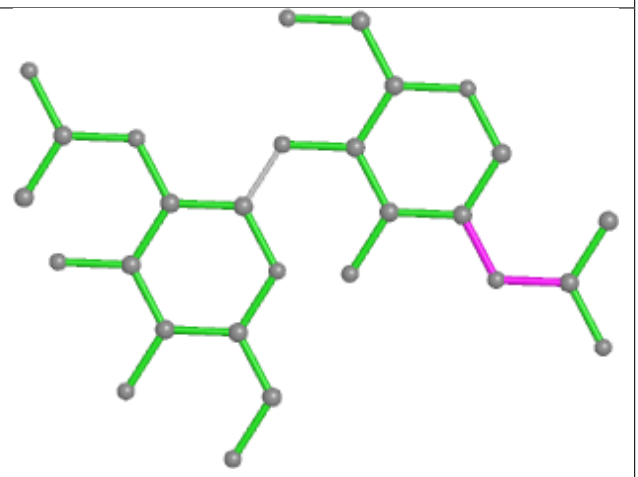


Rings

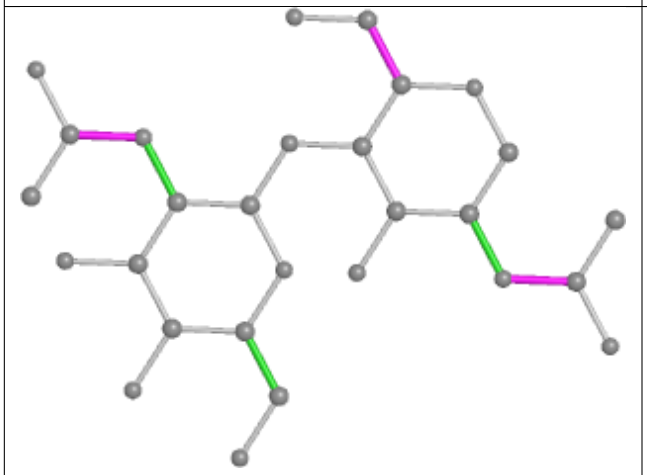
Oligosaccharide Chain G



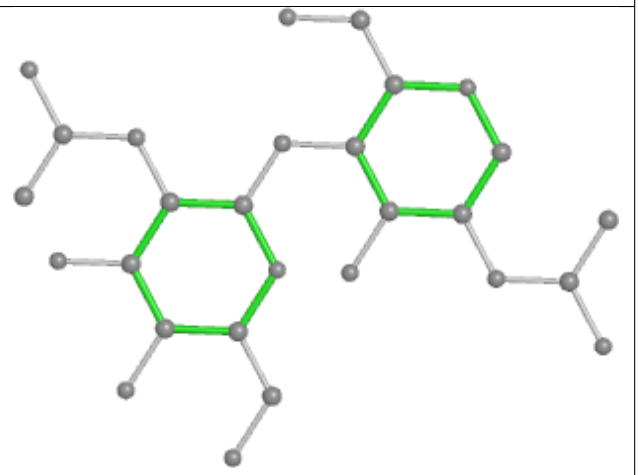
Bond lengths



Bond angles

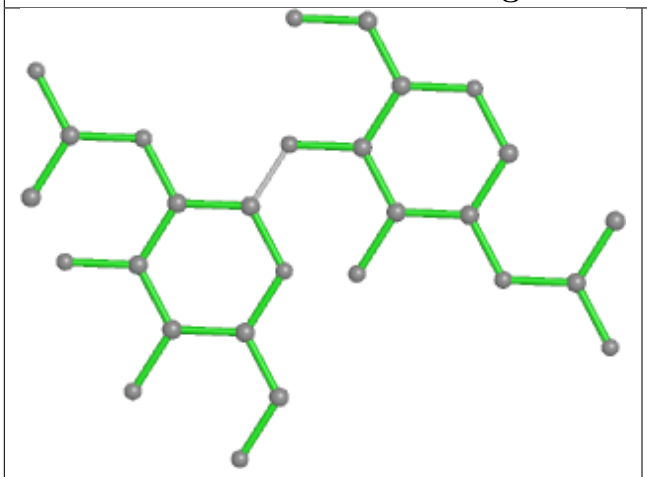


Torsions

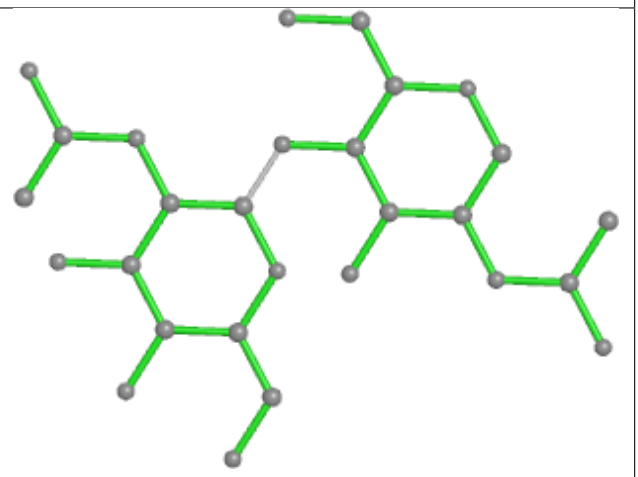


Rings

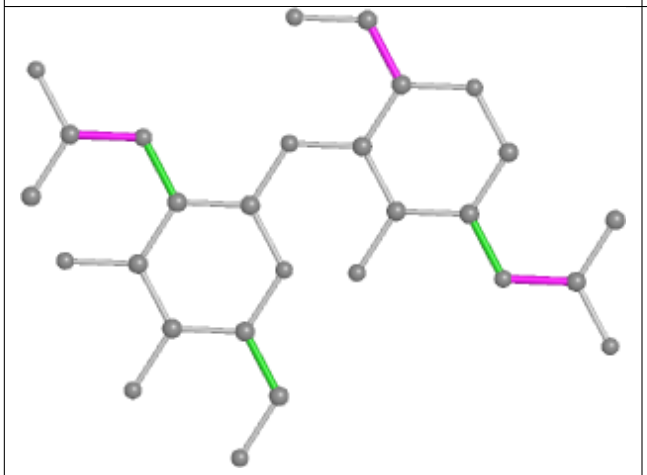
Oligosaccharide Chain I



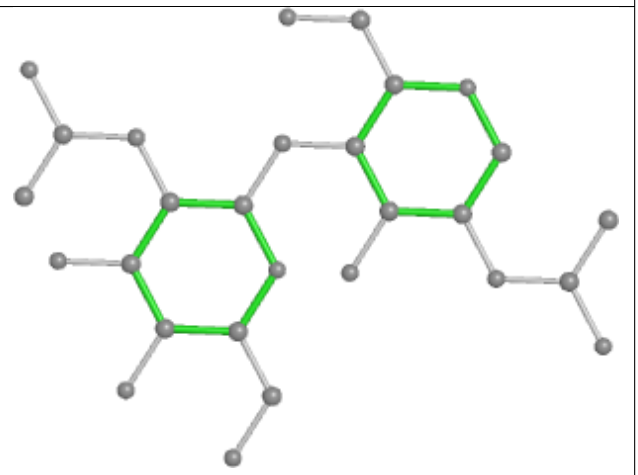
Bond lengths



Bond angles

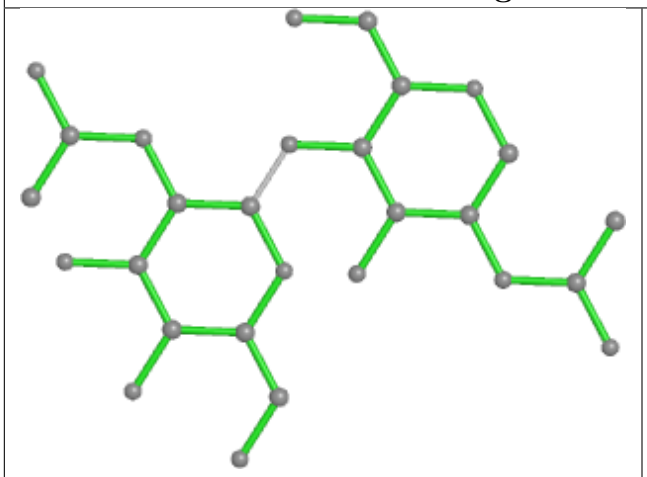


Torsions

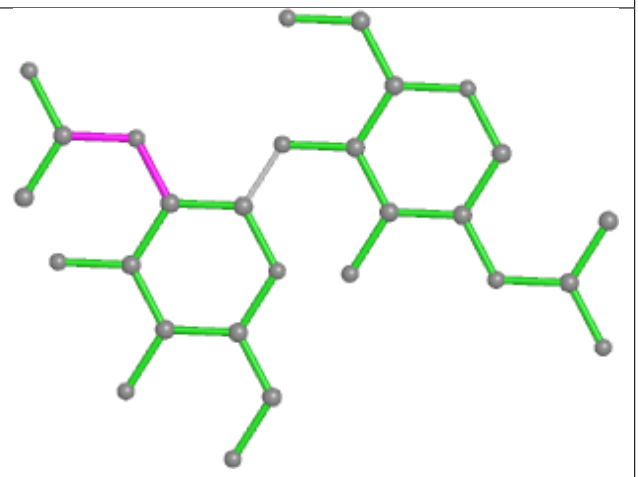


Rings

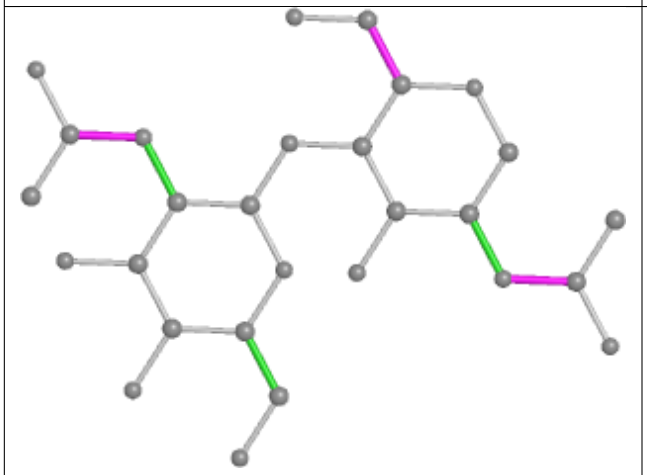
Oligosaccharide Chain K



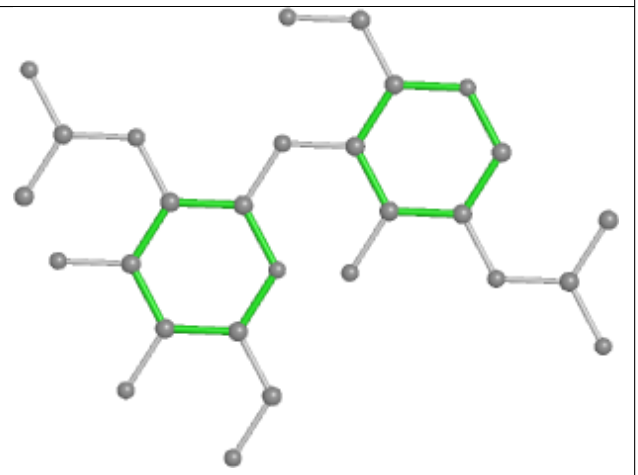
Bond lengths



Bond angles

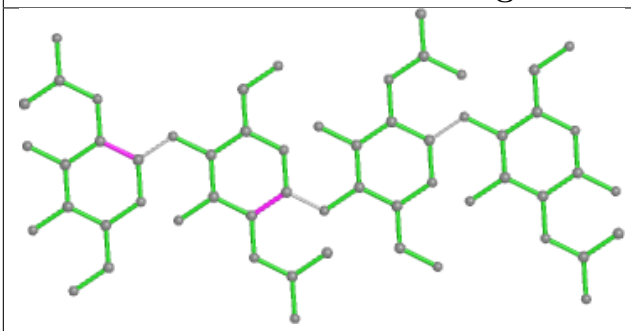


Torsions

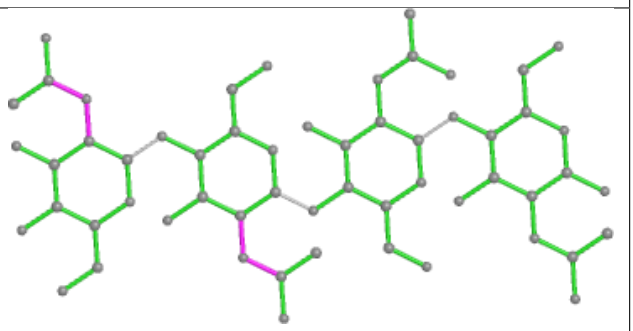


Rings

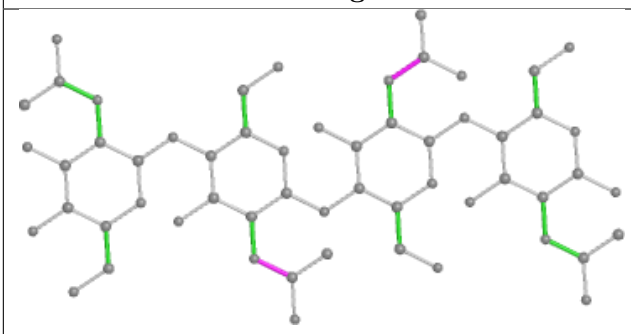
Oligosaccharide Chain F



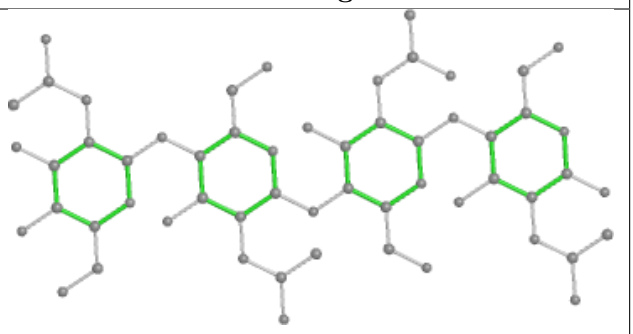
Bond lengths



Bond angles

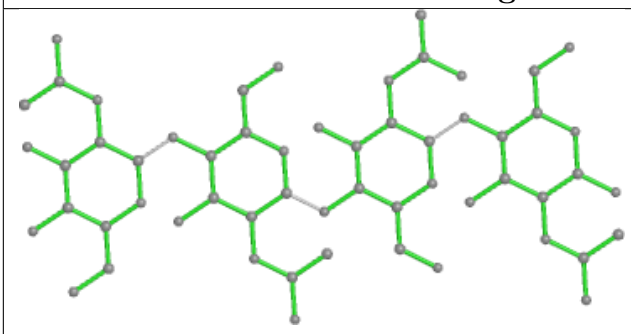


Torsions

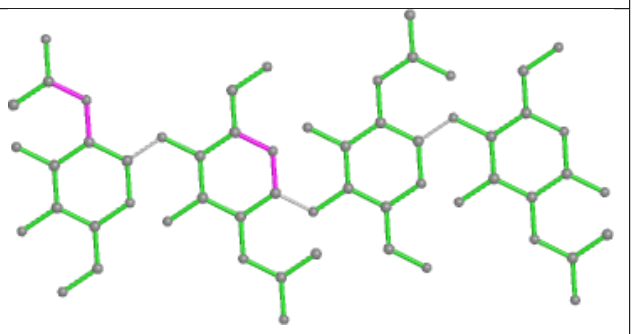


Rings

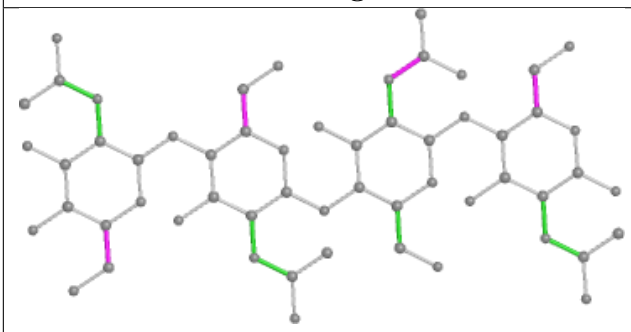
Oligosaccharide Chain J



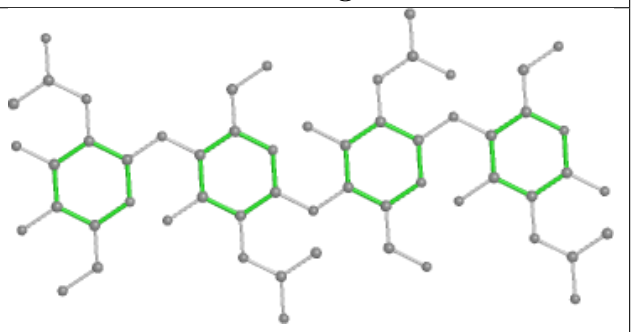
Bond lengths



Bond angles

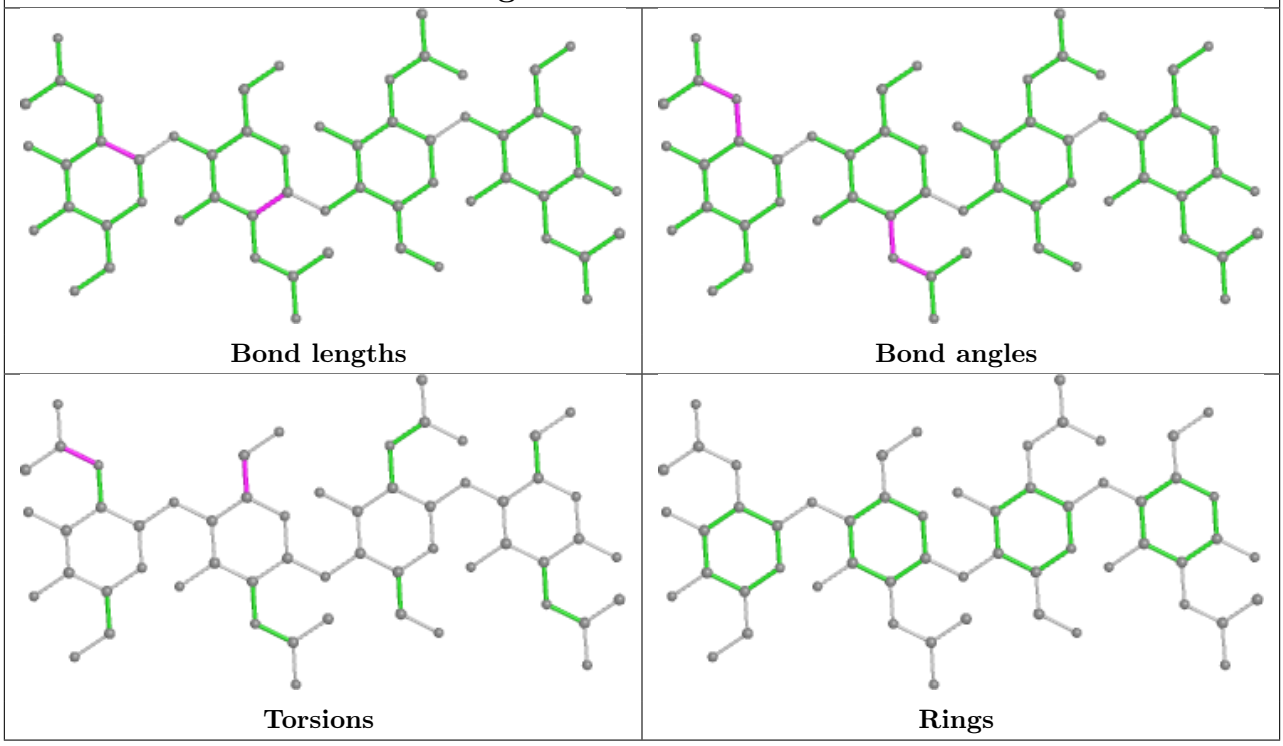


Torsions

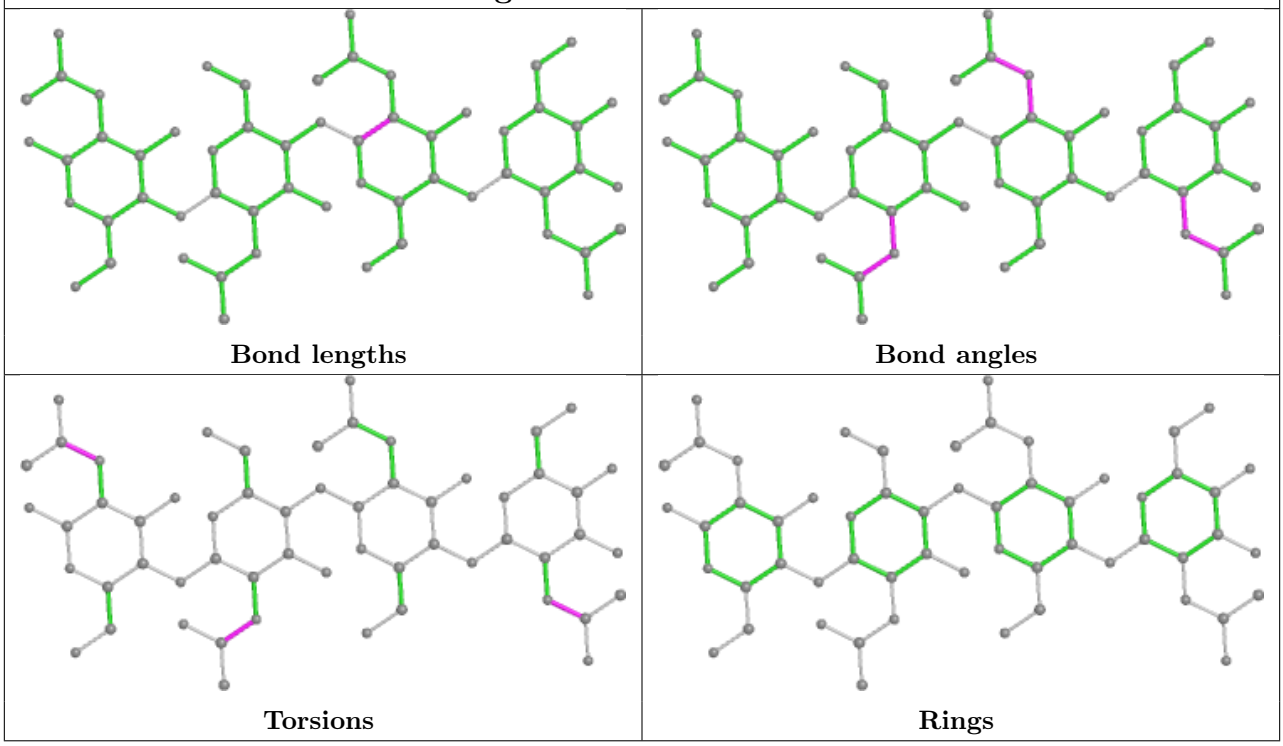


Rings

Oligosaccharide Chain L



Oligosaccharide Chain H



5.6 Ligand geometry (i)

There are no ligands in this entry.

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	362/362 (100%)	-0.15	6 (1%)	70	68	26, 40, 63, 78	0
1	B	362/362 (100%)	0.10	22 (6%)	21	20	28, 44, 64, 78	0
1	C	362/362 (100%)	-0.03	11 (3%)	50	48	25, 42, 65, 78	0
1	D	362/362 (100%)	-0.16	8 (2%)	62	59	26, 40, 64, 78	0
All	All	1448/1448 (100%)	-0.06	47 (3%)	47	45	25, 41, 64, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	383	THR	5.3
1	B	86	ARG	4.3
1	B	365	GLY	4.2
1	A	383	THR	4.0
1	D	99	TRP	3.9
1	B	383	THR	3.9
1	C	108	LYS	3.8
1	C	383	THR	3.7
1	B	113	THR	3.6
1	C	365	GLY	3.6
1	D	212	TRP	3.5
1	B	212	TRP	3.4
1	B	192	ALA	3.3
1	B	99	TRP	3.3
1	A	365	GLY	3.3
1	B	381	ALA	3.2
1	B	162	ILE	3.1
1	A	86	ARG	3.1
1	C	86	ARG	2.9
1	B	88	PRO	2.9
1	B	196	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLN	2.8
1	D	86	ARG	2.7
1	A	108	LYS	2.7
1	B	63	ASN	2.6
1	D	63	ASN	2.6
1	C	112	ASN	2.6
1	B	108	LYS	2.6
1	B	368	LEU	2.4
1	B	101	PHE	2.4
1	B	65	HIS	2.3
1	B	155	LYS	2.3
1	C	104	GLN	2.3
1	C	212	TRP	2.3
1	B	367	ASP	2.3
1	C	63	ASN	2.2
1	B	71	TRP	2.2
1	D	365	GLY	2.2
1	C	233	ARG	2.2
1	C	109	ILE	2.1
1	B	362	SER	2.1
1	C	99	TRP	2.1
1	D	382	ALA	2.1
1	B	369	ARG	2.1
1	D	366	GLN	2.1
1	A	99	TRP	2.0
1	B	148	GLN	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, 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	L	2	14/15	0.59	0.35	67,70,72,72	0
3	NAG	L	1	15/15	0.60	0.28	62,71,72,72	0

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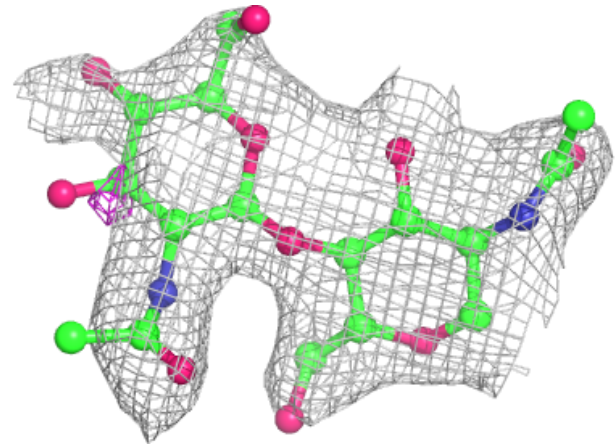
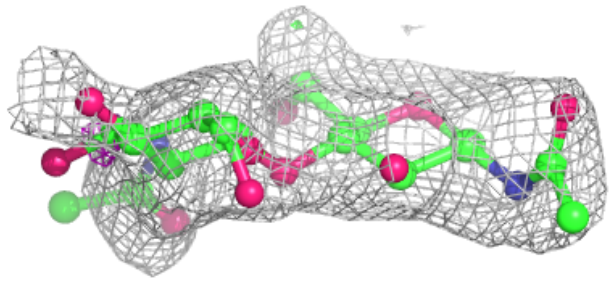
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	L	3	14/15	0.64	0.19	57,62,64,65	0
4	NAG	H	3	14/15	0.65	0.24	63,66,68,68	0
4	NDG	H	1	15/15	0.68	0.26	67,69,71,73	0
3	NDG	L	4	14/15	0.70	0.18	48,55,57,57	0
3	NAG	F	2	14/15	0.70	0.28	63,67,68,69	0
3	NAG	F	1	15/15	0.70	0.29	61,67,70,70	0
4	NAG	H	2	14/15	0.71	0.21	66,69,71,72	0
3	NDG	F	4	14/15	0.73	0.15	45,54,55,56	0
2	NAG	I	2	14/15	0.73	0.49	80,83,85,85	0
3	NAG	J	2	14/15	0.74	0.22	63,68,72,72	0
3	NAG	J	3	14/15	0.74	0.20	52,57,58,60	0
2	NAG	E	2	14/15	0.74	0.39	76,78,80,81	0
4	NDG	H	4	14/15	0.75	0.18	65,66,67,67	0
3	NAG	J	1	15/15	0.76	0.26	71,74,76,76	0
3	NAG	F	3	14/15	0.77	0.18	54,60,65,66	0
2	NAG	K	2	14/15	0.80	0.41	74,76,79,79	0
3	NDG	J	4	14/15	0.83	0.14	51,57,59,60	0
2	NAG	G	1	14/15	0.84	0.16	67,70,74,77	0
2	NAG	E	1	14/15	0.86	0.18	62,66,69,72	0
2	NAG	I	1	14/15	0.87	0.18	65,70,72,77	0
2	NAG	G	2	14/15	0.88	0.46	80,83,85,85	0
2	NAG	K	1	14/15	0.89	0.12	58,60,64,69	0

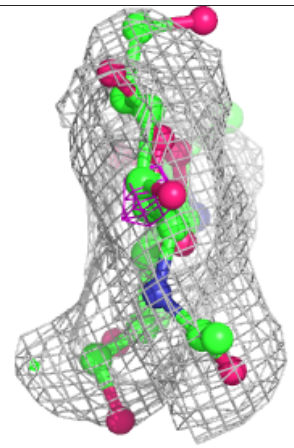
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

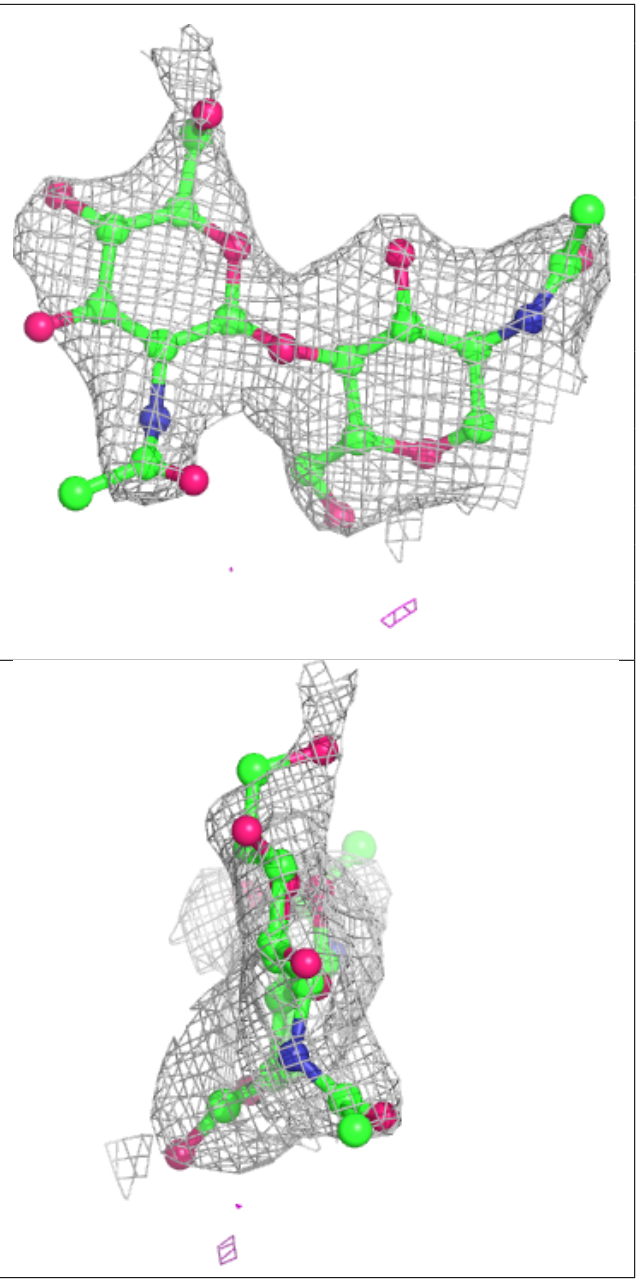






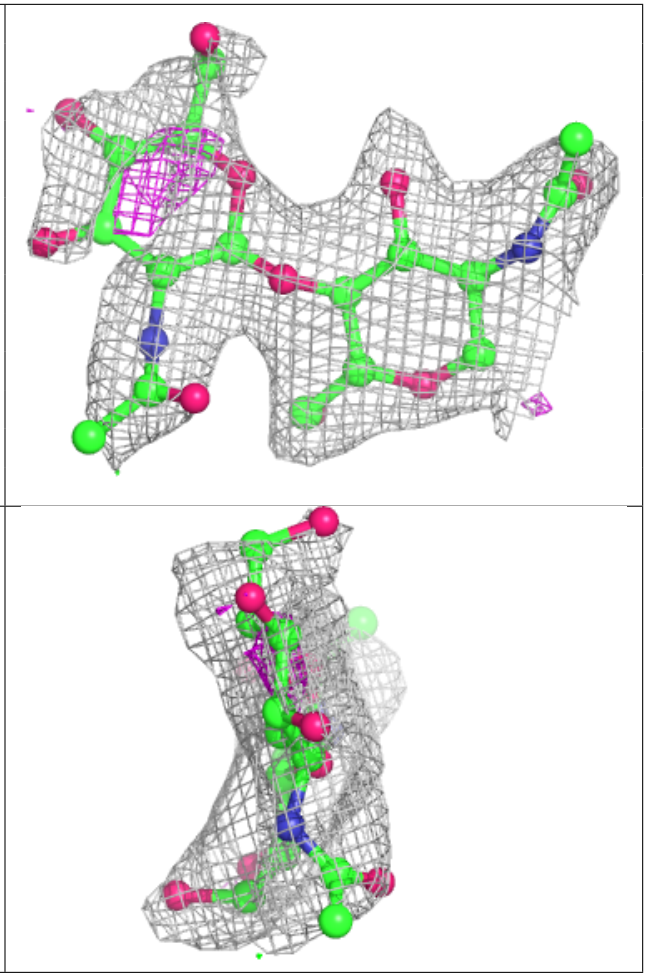
Electron density around Chain G:

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



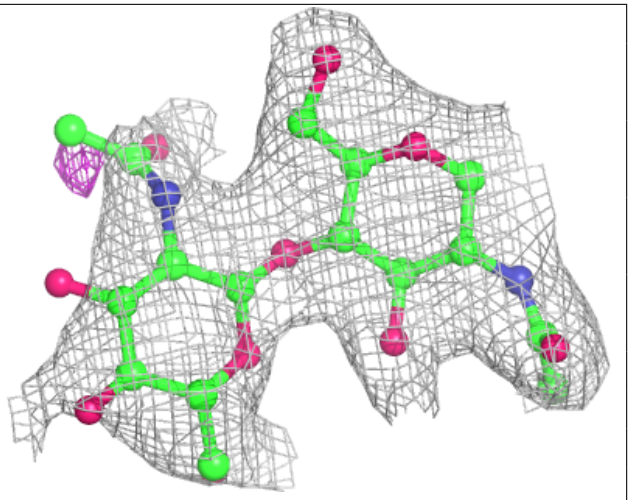
Electron density around Chain I:

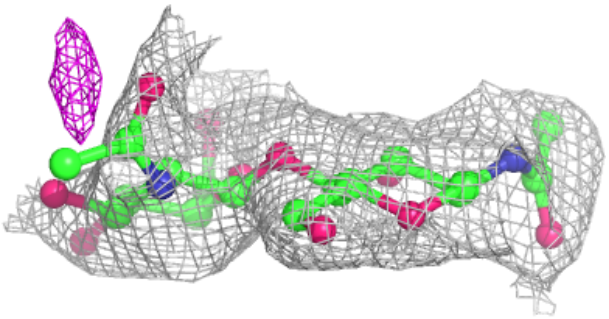
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

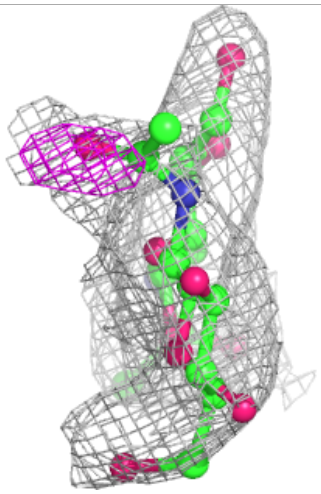


Electron density around Chain K:

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

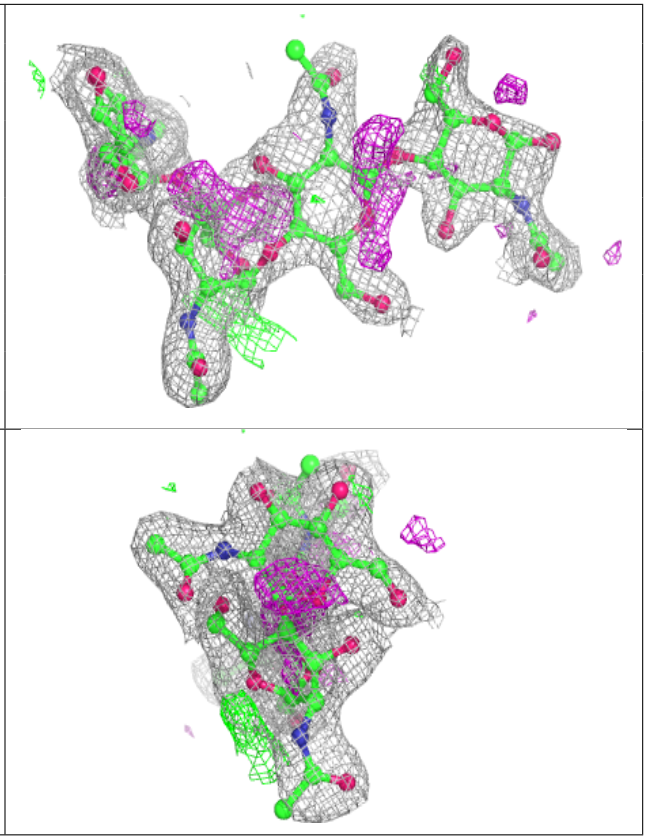


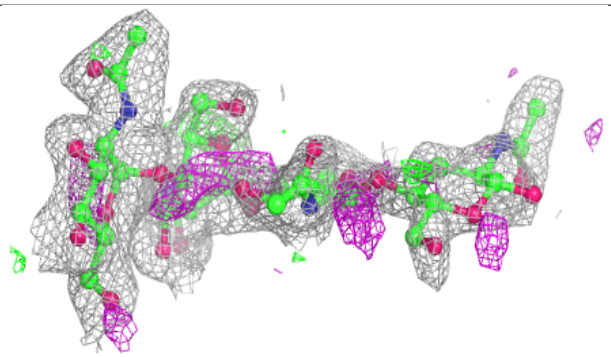




Electron density around Chain F:

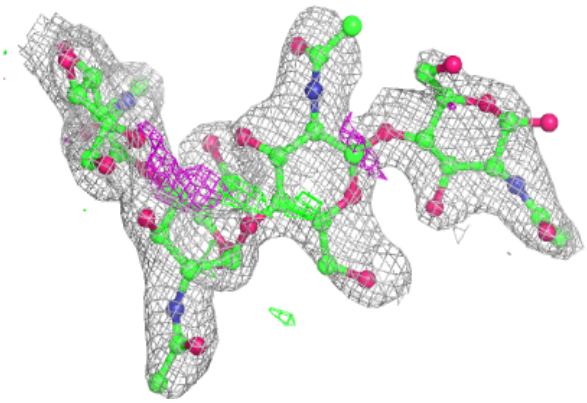
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

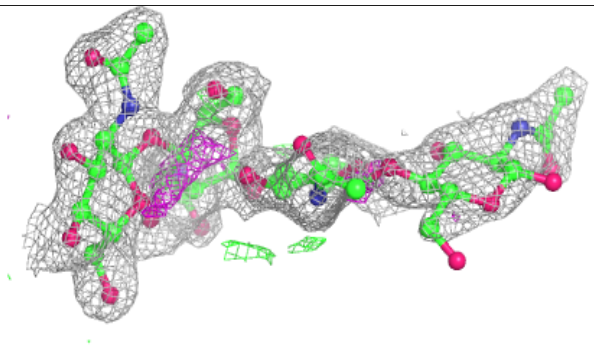


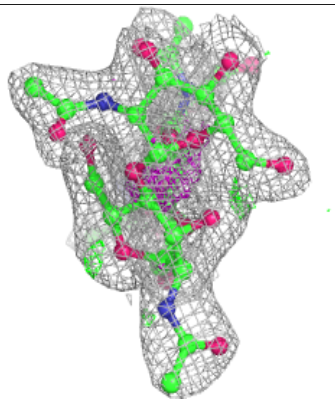


Electron density around Chain J:

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







Electron density around Chain L:

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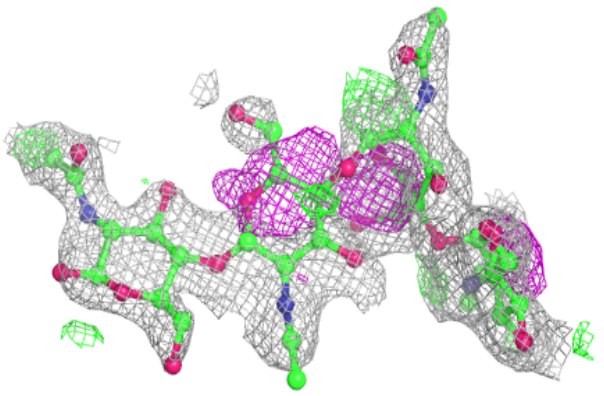
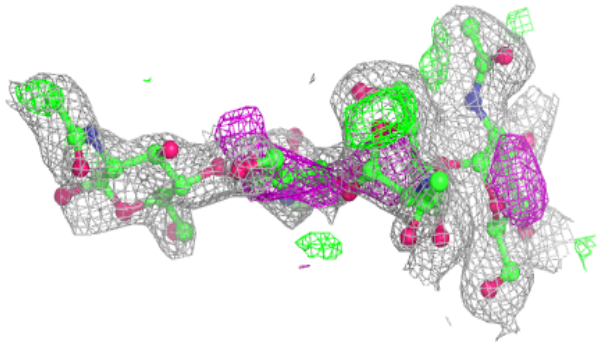
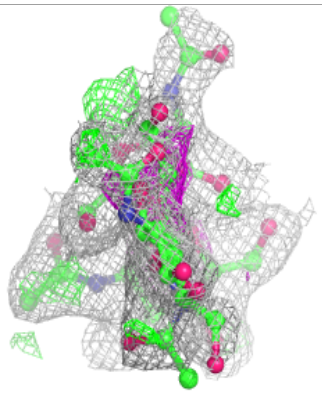
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

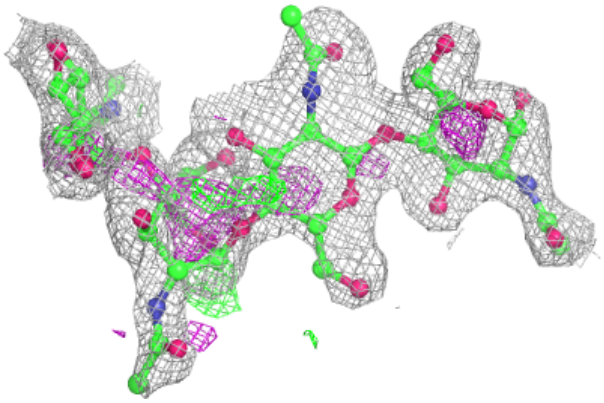


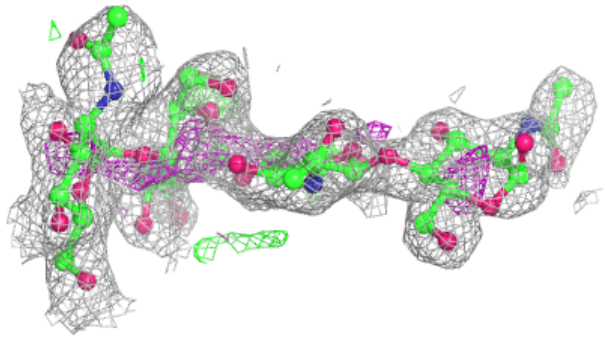


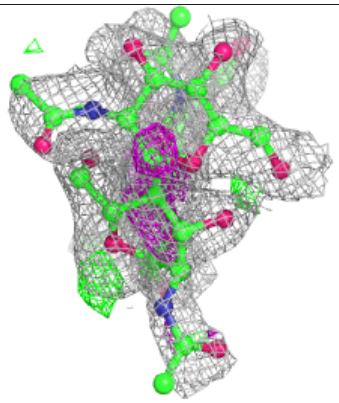


Electron density around Chain H:

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







6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.