Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:58 PM UTC

PDB ID	:	3WO4 / pdb_00003wo4
Title	:	Crystal structure of the IL-18 signaling ternary complex
Authors	:	Tsutsumi, N.; Kimura, T.; Arita, K.; Ariyoshi, M.; Ohnishi, H.; Kondo, N.; Shirakawa, M.; Kato, Z.; Tochio, H.
Deposited on	:	2013-12-19
Resolution	:	3.10 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 ⓘ 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 ⓘ) were used in the production of this report:

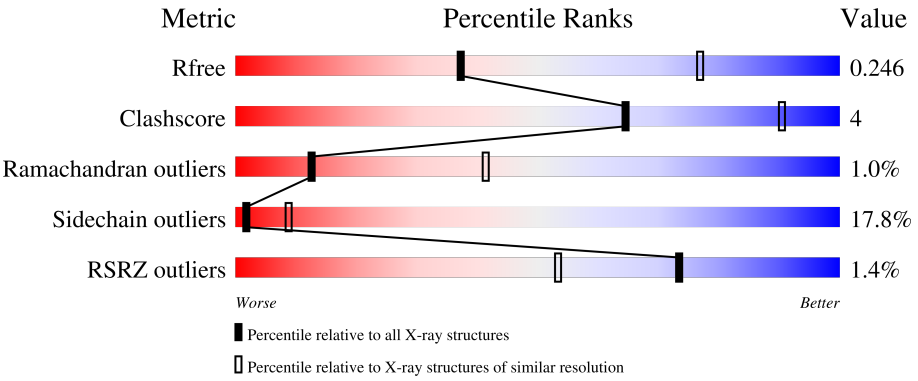
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	157	68% 31% ·
2	B	312	72% 21% · ·
3	C	344	3% 60% 16% · 22%
4	D	3	67% 33%
5	E	5	100%

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Mol	Chain	Length	Quality of chain
6	F	3	100%
7	G	2	50% 50%
7	J	2	100%
8	H	4	75% 25%
9	I	4	50% 50%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 6030 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 Interleukin-18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1266	796	209	251	10			

- Molecule 2 is a protein called Interleukin-18 receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	301	Total	C	N	O	S	0	1	0
			2375	1499	406	456	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q13478
B	-1	PRO	-	expression tag	UNP Q13478

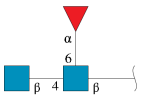
- Molecule 3 is a protein called Interleukin-18 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2022	1263	347	402	10			

There are 2 discrepancies between the modelled and reference sequences:

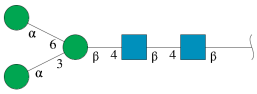
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP O95256
C	-1	PRO	-	expression tag	UNP O95256

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



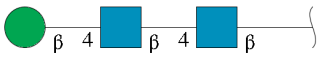
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	3	Total C N O 38 22 2 14	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(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
5	E	5	Total C N O 61 34 2 25	0	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(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
6	F	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 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
7	G	2	Total C N O 28 16 2 10	0	0	0

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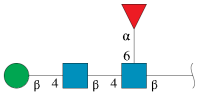
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	J	2	Total C N O 28 16 2 10	0	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

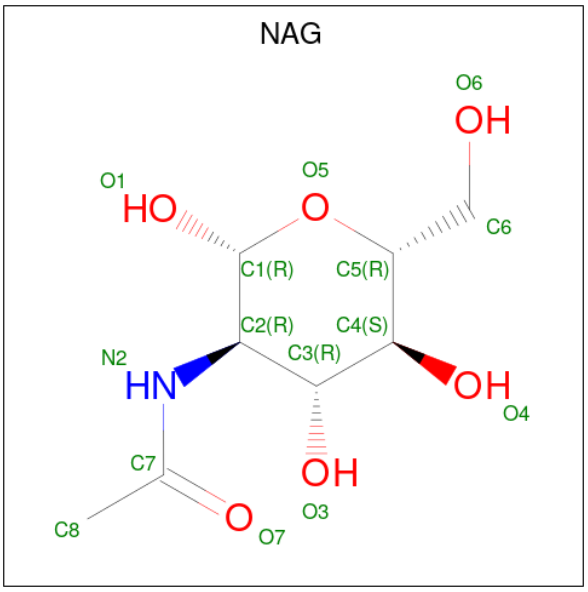


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	4	Total C N O 49 28 2 19	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(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
9	I	4	Total C N O 50 28 2 20	0	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total Cl 1 1	0	0

- Molecule 12 is water.

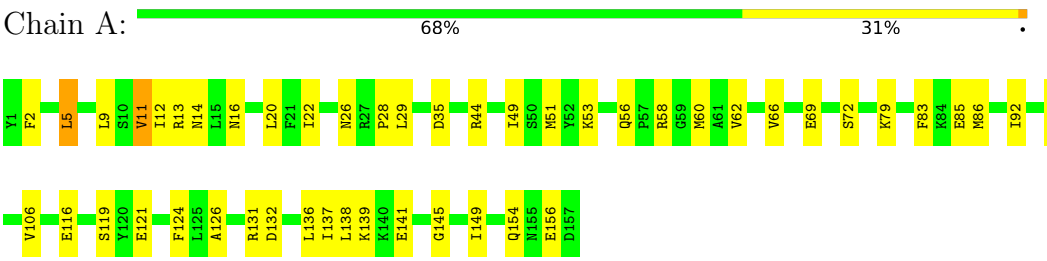
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	14	Total O 14 14	0	0
12	B	7	Total O 7 7	0	0
12	C	10	Total O 10 10	0	0

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.

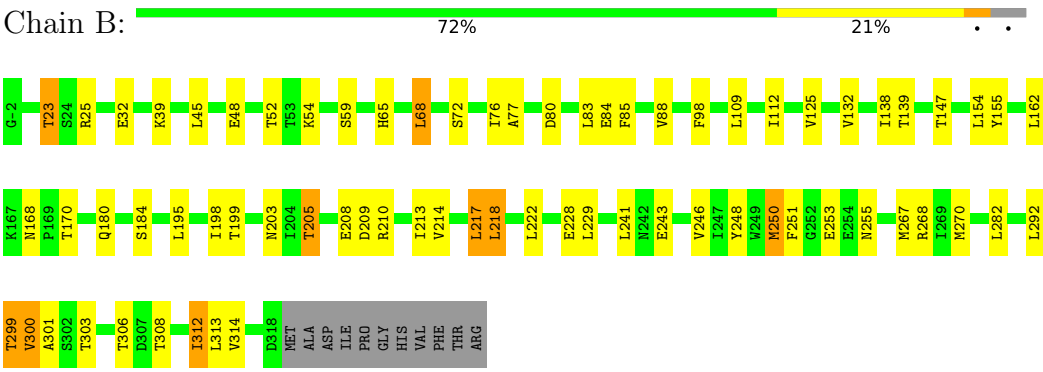
• Molecule 1: Interleukin-18

Chain A:



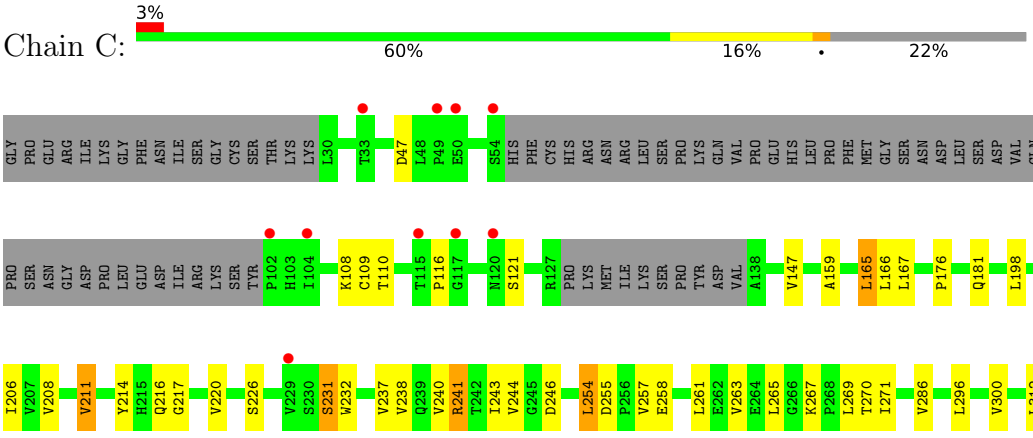
• Molecule 2: Interleukin-18 receptor 1

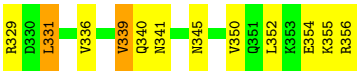
Chain B:



• Molecule 3: Interleukin-18 receptor accessory protein

Chain C:



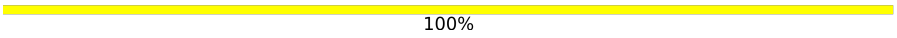


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

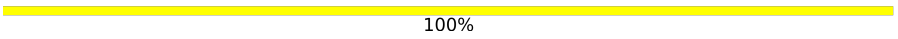
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

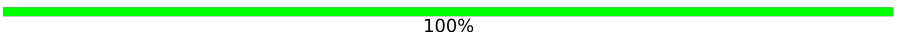


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.56Å 111.56Å 134.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.00 – 3.10 42.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.0 (42.00-3.10) 84.9 (42.00-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.39 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.188 , 0.232 0.198 , 0.246	Depositor DCC
R_{free} test set	884 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å^2)	58.9	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6030	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: BMA, NAG, CL, FUC, MAN

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	0.88	0/1287	1.21	5/1726 (0.3%)
2	B	0.81	0/2433	1.23	6/3310 (0.2%)
3	C	0.83	0/2057	1.25	8/2800 (0.3%)
All	All	0.83	0/5777	1.24	19/7836 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	132	ASP	CA-CB-CG	7.84	120.44	112.60
2	B	164	GLU	CA-C-N	6.15	131.10	122.36
2	B	164	GLU	C-N-CA	6.15	131.10	122.36
3	C	341	ASN	CA-CB-CG	5.90	118.50	112.60
3	C	217	GLY	N-CA-C	5.77	118.41	110.56
2	B	203	ASN	CA-CB-CG	5.47	118.07	112.60
3	C	345	ASN	CA-CB-CG	5.46	118.06	112.60
3	C	231	SER	CA-C-N	5.37	128.72	120.82
3	C	231	SER	C-N-CA	5.37	128.72	120.82
1	A	16	ASN	N-CA-C	-5.31	106.67	112.72
1	A	14	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	35	ASP	CA-C-N	5.28	127.30	120.44
1	A	35	ASP	C-N-CA	5.28	127.30	120.44
3	C	255	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	85	PHE	CA-CB-CG	5.18	118.98	113.80
2	B	48	GLU	CA-C-N	5.16	127.49	120.63
2	B	48	GLU	C-N-CA	5.16	127.49	120.63
3	C	198	LEU	CA-C-N	5.01	127.00	120.28
3	C	198	LEU	C-N-CA	5.01	127.00	120.28

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	1266	0	1237	14	0
2	B	2375	0	2231	18	0
3	C	2022	0	1857	17	0
4	D	38	0	34	0	0
5	E	61	0	52	0	0
6	F	39	0	34	0	0
7	G	28	0	25	0	0
7	J	28	0	25	0	0
8	H	49	0	43	0	0
9	I	50	0	43	0	0
10	B	28	0	26	0	0
10	C	14	0	13	0	0
11	C	1	0	0	0	0
12	A	14	0	0	1	0
12	B	7	0	0	0	0
12	C	10	0	0	0	0
All	All	6030	0	5620	45	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 (45) 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)
2:B:295:LEU:HD12	2:B:312:ILE:HD11	1.64	0.80
2:B:180:GLN:HG3	2:B:205:THR:HA	1.77	0.67
2:B:301:ALA:HA	2:B:306:THR:HG22	1.79	0.64
3:C:216:GLN:HG3	3:C:241:ARG:HA	1.84	0.59
2:B:54:LYS:HB3	2:B:98:PHE:HE1	1.68	0.58
2:B:217:LEU:HD13	2:B:300:VAL:HG22	1.85	0.58
1:A:56:GLN:HG3	1:A:58:ARG:HH11	1.68	0.57
3:C:267:LYS:O	3:C:326:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HD3	2:B:250:MET:HE3	1.88	0.54
2:B:23:THR:HG23	2:B:39:LYS:H	1.71	0.53
1:A:11:VAL:HG13	1:A:154:GLN:HB3	1.91	0.53
3:C:165:LEU:HB3	3:C:211:VAL:HG21	1.91	0.53
2:B:299:THR:HG22	2:B:308:THR:HG23	1.92	0.52
3:C:286:VAL:O	3:C:339:VAL:HA	2.10	0.52
3:C:201:GLU:HG2	3:C:206:ILE:HG23	1.91	0.51
2:B:155:TYR:HB2	2:B:184:SER:HB2	1.91	0.51
1:A:28:PRO:HB3	1:A:83:PHE:HE2	1.75	0.51
3:C:263:VAL:O	3:C:354:GLU:HA	2.10	0.51
2:B:139:THR:HA	2:B:170:THR:HG22	1.94	0.50
2:B:77:ALA:HB3	2:B:84:GLU:HB2	1.93	0.49
3:C:232:TRP:CD1	3:C:232:TRP:H	2.30	0.49
1:A:2:PHE:HB2	1:A:92:ILE:HB	1.95	0.48
1:A:44:ARG:NH2	12:A:202:HOH:O	2.45	0.48
3:C:159:ALA:HB3	3:C:176:PRO:HA	1.97	0.47
3:C:220:VAL:HG22	3:C:237:VAL:HG22	1.96	0.46
2:B:251:PHE:HB3	2:B:296:TYR:HD1	1.80	0.46
3:C:121:SER:HB3	3:C:147:VAL:HG12	1.97	0.46
2:B:164:GLU:CD	2:B:166:ASN:HD22	2.23	0.45
1:A:96:LYS:HB3	1:A:119:SER:HA	1.98	0.44
1:A:145:GLY:HA2	3:C:214:TYR:CE2	2.52	0.44
2:B:218:LEU:HD12	3:C:254:LEU:HA	1.99	0.44
1:A:53:LYS:HE2	2:B:248:TYR:HB2	1.98	0.44
1:A:126:ALA:HB2	1:A:149:ILE:HG22	2.00	0.43
1:A:5:LEU:HD13	1:A:53:LYS:HG3	2.01	0.43
2:B:246:VAL:HG13	2:B:301:ALA:HB3	2.01	0.42
3:C:226:SER:HA	3:C:231:SER:HA	2.02	0.42
1:A:12:ILE:HD11	1:A:49:ILE:HD11	2.01	0.42
1:A:56:GLN:HG3	1:A:58:ARG:NH1	2.34	0.41
3:C:108:LYS:C	3:C:110:THR:H	2.27	0.41
2:B:312:ILE:HG22	2:B:314:VAL:HG23	2.03	0.41
3:C:265:LEU:HA	3:C:326:VAL:HG13	2.02	0.41
2:B:68:LEU:HD13	2:B:68:LEU:HA	1.92	0.40
3:C:263:VAL:CG1	3:C:326:VAL:HG11	2.52	0.40
1:A:116:GLU:HB2	1:A:124:PHE:CE2	2.57	0.40
3:C:328:GLN:HA	3:C:331:LEU:HD22	2.03	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	155/157 (99%)	142 (92%)	12 (8%)	1 (1%)	21 52
2	B	300/312 (96%)	278 (93%)	18 (6%)	4 (1%)	9 35
3	C	264/344 (77%)	237 (90%)	25 (10%)	2 (1%)	16 47
All	All	719/813 (88%)	657 (91%)	55 (8%)	7 (1%)	12 41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	116	PRO
2	B	72	SER
2	B	80	ASP
2	B	166	ASN
2	B	209	ASP
1	A	60	MET
3	C	109	CYS

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	145/148 (98%)	118 (81%)	27 (19%)	1 8
2	B	263/288 (91%)	213 (81%)	50 (19%)	1 7
3	C	212/321 (66%)	179 (84%)	33 (16%)	2 12
All	All	620/757 (82%)	510 (82%)	110 (18%)	2 9

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LEU
1	A	11	VAL
1	A	13	ARG
1	A	20	LEU
1	A	22	ILE
1	A	26	ASN
1	A	29	LEU
1	A	51	MET
1	A	62	VAL
1	A	66	VAL
1	A	69	GLU
1	A	72	SER
1	A	79	LYS
1	A	85	GLU
1	A	86	MET
1	A	95	THR
1	A	99	ILE
1	A	106	VAL
1	A	121	GLU
1	A	131	ARG
1	A	136	LEU
1	A	137	ILE
1	A	138	LEU
1	A	139	LYS
1	A	141	GLU
1	A	156	GLU
2	B	23	THR
2	B	25	ARG
2	B	32	GLU
2	B	45	LEU
2	B	52	THR
2	B	59	SER
2	B	65	HIS
2	B	68	LEU
2	B	76	ILE
2	B	83	LEU
2	B	88	VAL
2	B	109	LEU
2	B	112	ILE
2	B	125	VAL
2	B	132	VAL

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Mol	Chain	Res	Type
2	B	138	ILE
2	B	147	THR
2	B	154	LEU
2	B	162	LEU
2	B	163	LEU
2	B	164	GLU
2	B	168	ASN
2	B	195	LEU
2	B	198	ILE
2	B	199	THR
2	B	205	THR
2	B	208	GLU
2	B	210	ARG
2	B	213	ILE
2	B	214	VAL
2	B	217	LEU
2	B	218	LEU
2	B	222	LEU
2	B	228	GLU
2	B	229	LEU
2	B	241	LEU
2	B	243	GLU
2	B	250	MET
2	B	253	GLU
2	B	255	ASN
2	B	267	MET
2	B	268	ARG
2	B	270	MET
2	B	282	LEU
2	B	292	LEU
2	B	299	THR
2	B	300	VAL
2	B	303	THR
2	B	312	ILE
2	B	313	LEU
3	C	47	ASP
3	C	165	LEU
3	C	166	LEU
3	C	167	LEU
3	C	181	GLN
3	C	203	SER
3	C	208	VAL

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Mol	Chain	Res	Type
3	C	211	VAL
3	C	238	VAL
3	C	240	VAL
3	C	241	ARG
3	C	243	ILE
3	C	244	VAL
3	C	246	ASP
3	C	254	LEU
3	C	257	VAL
3	C	258	GLU
3	C	261	LEU
3	C	269	LEU
3	C	270	THR
3	C	271	ILE
3	C	296	LEU
3	C	300	VAL
3	C	312	LEU
3	C	329	ARG
3	C	331	LEU
3	C	336	VAL
3	C	339	VAL
3	C	340	GLN
3	C	350	VAL
3	C	352	LEU
3	C	355	LYS
3	C	356	ARG

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	78	ASN
1	A	114	GLN
2	B	124	GLN
2	B	168	ASN
2	B	180	GLN
2	B	191	HIS
2	B	192	ASN
2	B	212	ASN
2	B	255	ASN
2	B	277	HIS
3	C	106	GLN
3	C	204	ASN

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Mol	Chain	Res	Type
3	C	239	GLN
3	C	320	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

23 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	$\#\|Z\| > 2$
4	NAG	D	1	2,4	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	D	2	4	14,14,15	0.29	0	17,19,21	0.56	0
4	FUC	D	3	4	10,10,11	0.44	0	14,14,16	0.79	1 (7%)
5	NAG	E	1	5,2	14,14,15	0.28	0	17,19,21	0.73	1 (5%)
5	NAG	E	2	5	14,14,15	0.35	0	17,19,21	1.64	4 (23%)
5	BMA	E	3	5	11,11,12	0.33	0	15,15,17	0.86	1 (6%)
5	MAN	E	4	5	11,11,12	0.51	0	15,15,17	1.48	2 (13%)
5	MAN	E	5	5	11,11,12	0.39	0	15,15,17	1.01	1 (6%)
6	NAG	F	1	2,6	14,14,15	0.30	0	17,19,21	1.31	1 (5%)
6	NAG	F	2	6	14,14,15	0.38	0	17,19,21	1.68	4 (23%)
6	BMA	F	3	6	11,11,12	0.37	0	15,15,17	0.83	1 (6%)
7	NAG	G	1	2,7	14,14,15	0.31	0	17,19,21	1.00	1 (5%)
7	NAG	G	2	7	14,14,15	0.34	0	17,19,21	0.38	0
8	NAG	H	1	2,8	14,14,15	0.30	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	H	2	8	14,14,15	0.32	0	17,19,21	0.51	0
8	BMA	H	3	8	11,11,12	0.34	0	15,15,17	0.60	0
8	FUC	H	4	8	10,10,11	0.55	0	14,14,16	0.95	2 (14%)
9	NAG	I	1	3,9	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
9	NAG	I	2	9	14,14,15	0.32	0	17,19,21	0.73	0
9	BMA	I	3	9	11,11,12	0.30	0	15,15,17	0.49	0
9	MAN	I	4	9	11,11,12	0.40	0	15,15,17	0.79	1 (6%)
7	NAG	J	1	7,3	14,14,15	0.31	0	17,19,21	0.44	0
7	NAG	J	2	7	14,14,15	0.29	0	17,19,21	0.64	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
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1
5	NAG	E	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	1/2/19/22	0/1/1/1
6	NAG	F	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
8	NAG	H	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	H	2	8	-	1/6/23/26	0/1/1/1
8	BMA	H	3	8	-	0/2/19/22	0/1/1/1
8	FUC	H	4	8	-	-	0/1/1/1
9	NAG	I	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1
9	MAN	I	4	9	-	0/2/19/22	0/1/1/1
7	NAG	J	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	4	MAN	C1-O5-C5	4.92	118.78	112.19
6	F	2	NAG	C1-O5-C5	4.74	118.54	112.19
6	F	1	NAG	O5-C1-C2	-4.58	104.20	111.29
5	E	2	NAG	C1-O5-C5	4.54	118.27	112.19
5	E	5	MAN	C1-O5-C5	3.55	116.94	112.19
6	F	2	NAG	O4-C4-C5	3.23	117.28	109.32
5	E	2	NAG	O5-C1-C2	2.90	115.78	111.29
6	F	3	BMA	C1-O5-C5	2.80	115.94	112.19
7	G	1	NAG	O5-C1-C2	-2.73	107.07	111.29
5	E	2	NAG	O4-C4-C3	2.67	116.68	110.38
6	F	2	NAG	C1-C2-N2	2.65	114.61	110.43
5	E	3	BMA	C1-O5-C5	2.65	115.74	112.19
5	E	2	NAG	O4-C4-C5	2.55	115.60	109.32
5	E	4	MAN	C1-C2-C3	2.38	113.11	109.64
4	D	3	FUC	C1-O5-C5	2.33	118.47	112.97
8	H	4	FUC	C1-O5-C5	2.31	118.42	112.97
8	H	4	FUC	C1-C2-C3	2.25	112.92	109.64
9	I	4	MAN	C1-O5-C5	2.20	115.14	112.19
9	I	1	NAG	C1-O5-C5	2.15	115.07	112.19
5	E	1	NAG	C1-O5-C5	2.13	115.04	112.19
6	F	2	NAG	O4-C4-C3	2.09	115.31	110.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

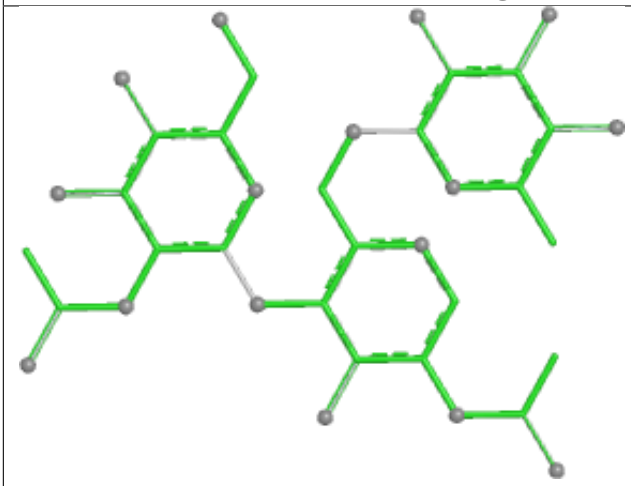
Mol	Chain	Res	Type	Atoms
7	G	2	NAG	O5-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
5	E	5	MAN	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
8	H	2	NAG	C1-C2-N2-C7
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

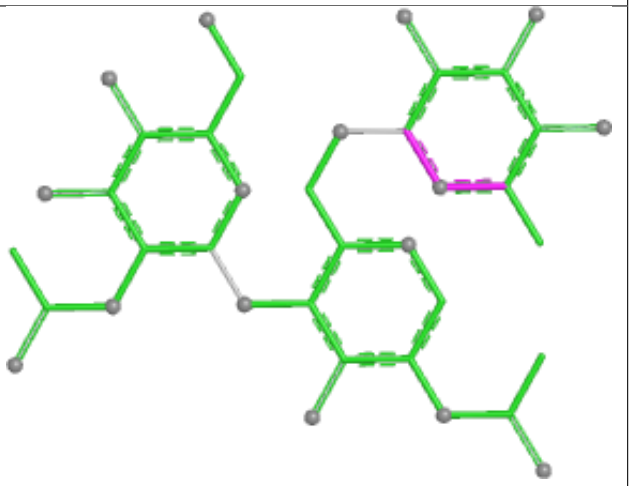
No monomer is involved in short contacts.

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

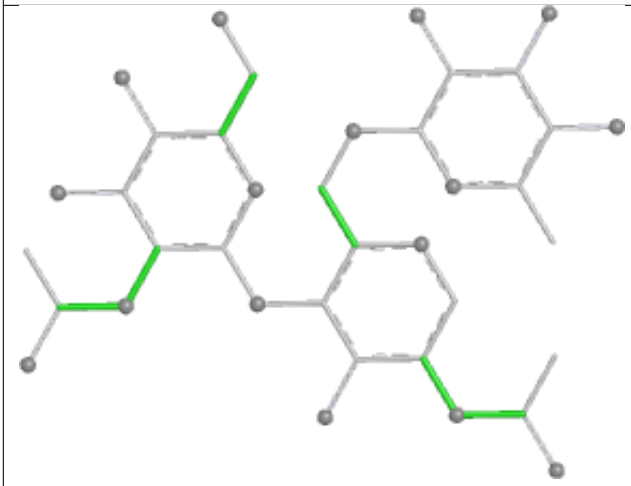
Oligosaccharide Chain D



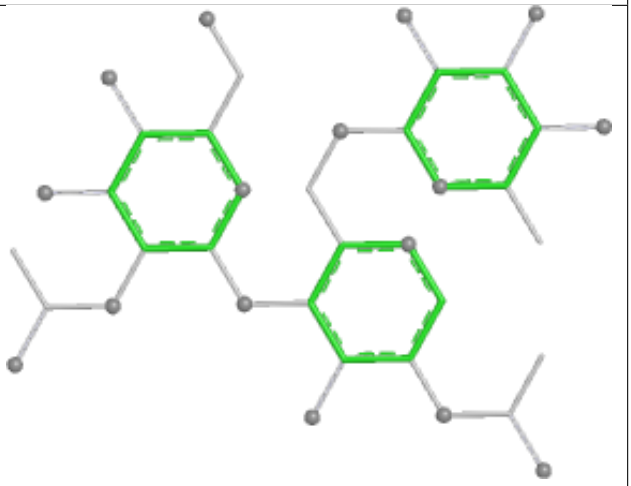
Bond lengths



Bond angles

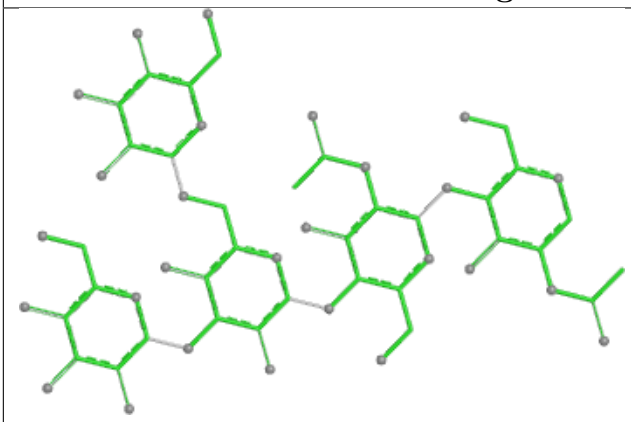


Torsions

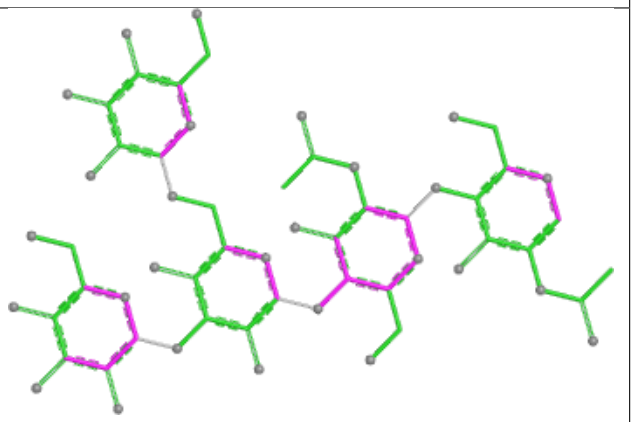


Rings

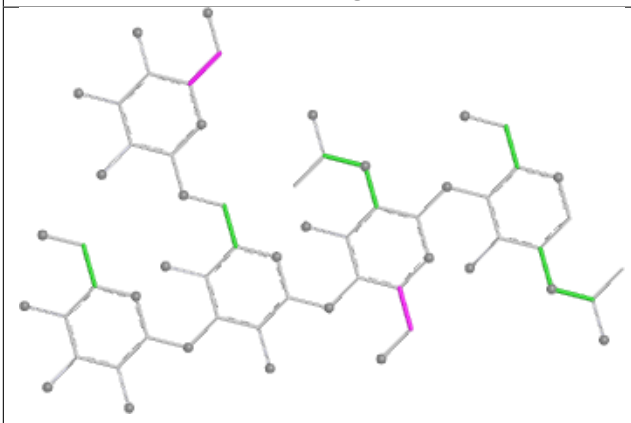
Oligosaccharide Chain E



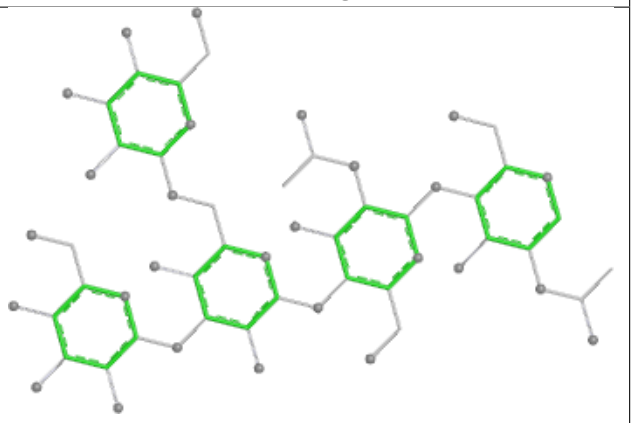
Bond lengths



Bond angles

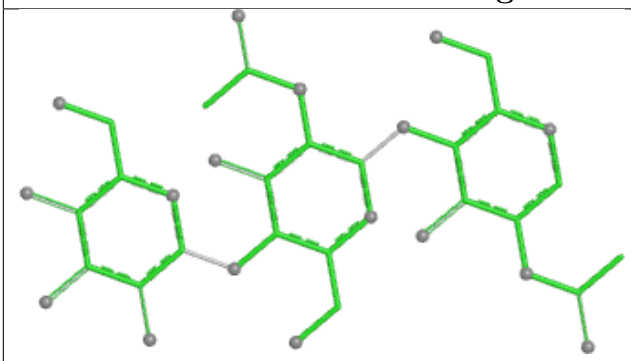


Torsions

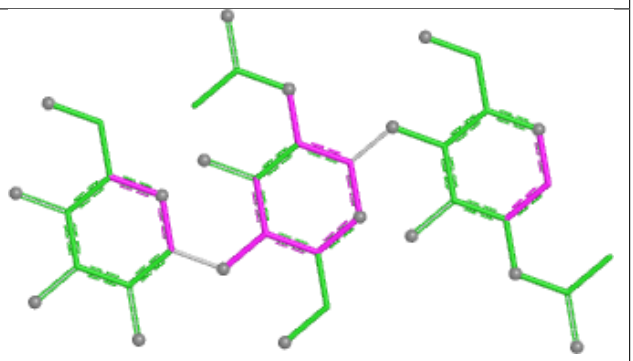


Rings

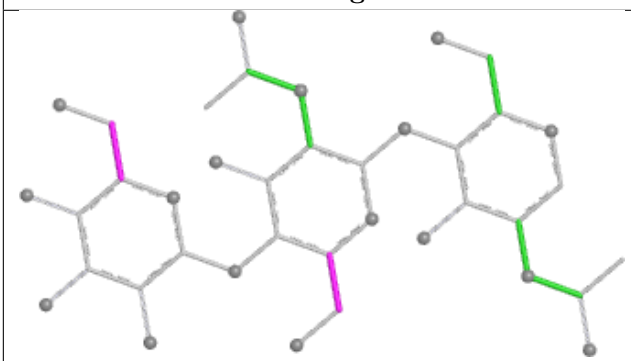
Oligosaccharide Chain F



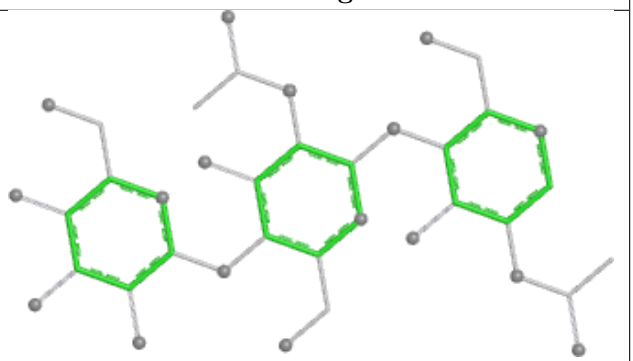
Bond lengths



Bond angles

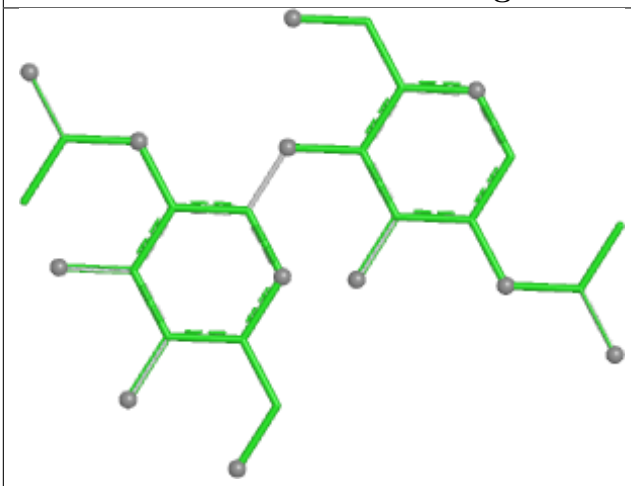


Torsions

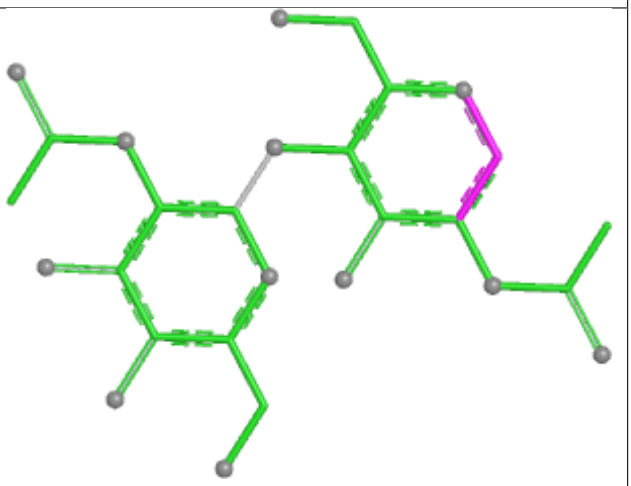


Rings

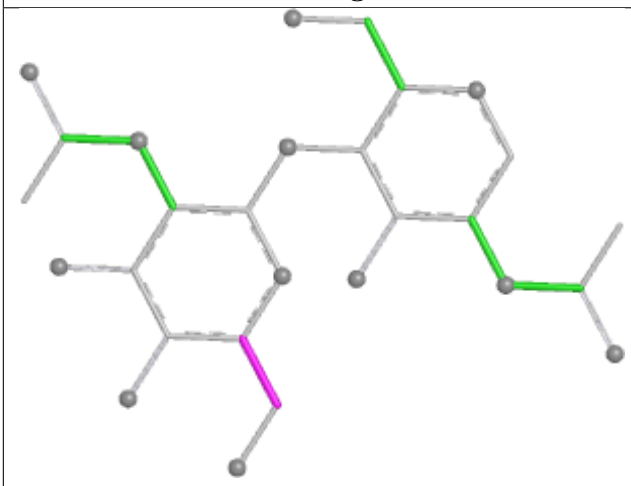
Oligosaccharide Chain G



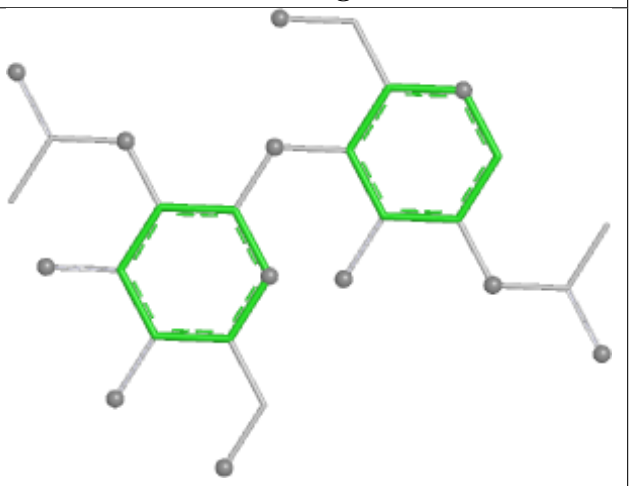
Bond lengths



Bond angles

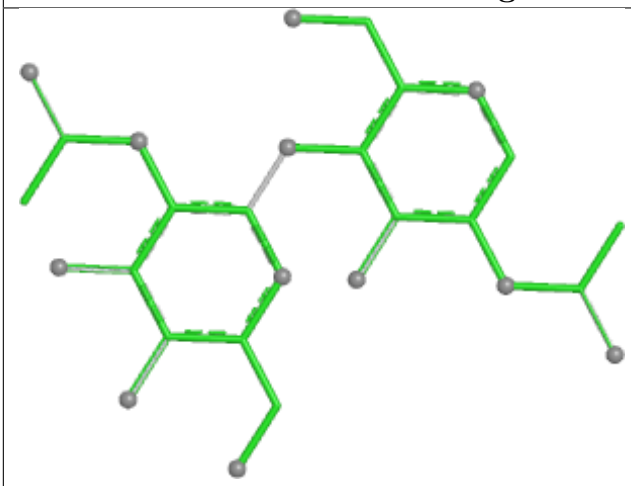


Torsions

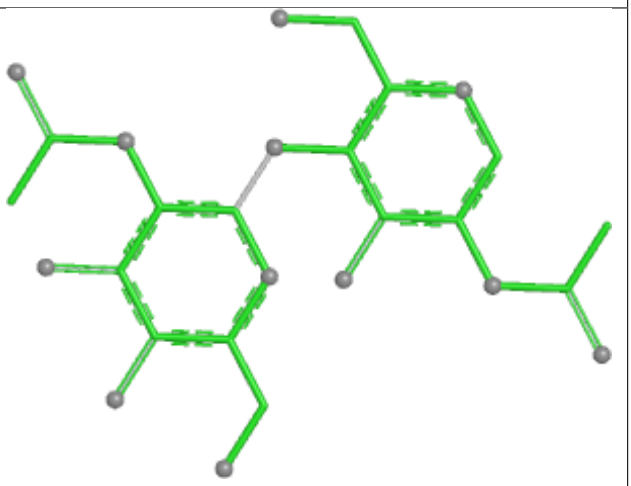


Rings

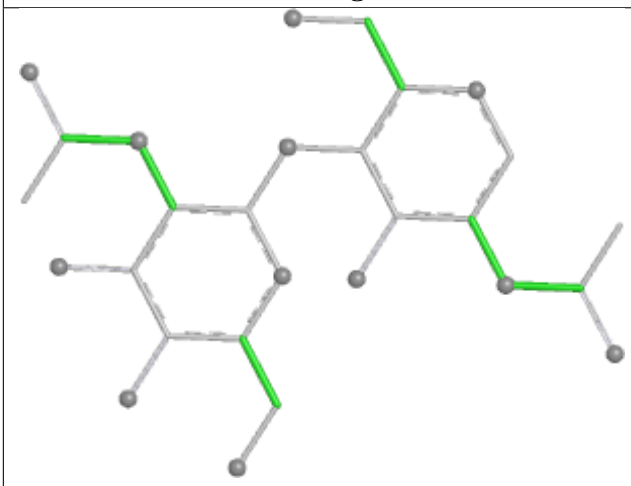
Oligosaccharide Chain J



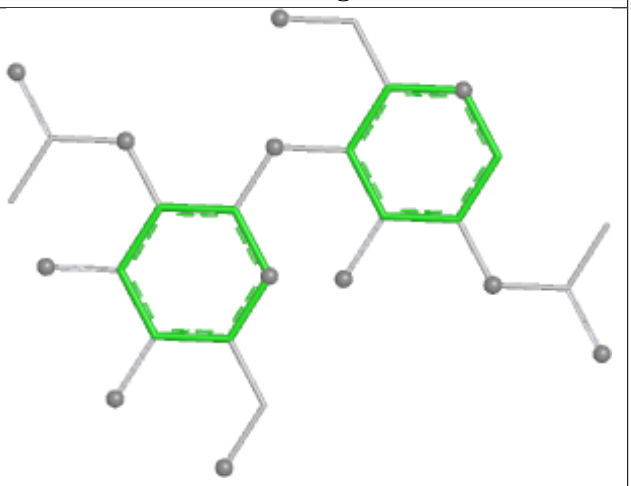
Bond lengths



Bond angles

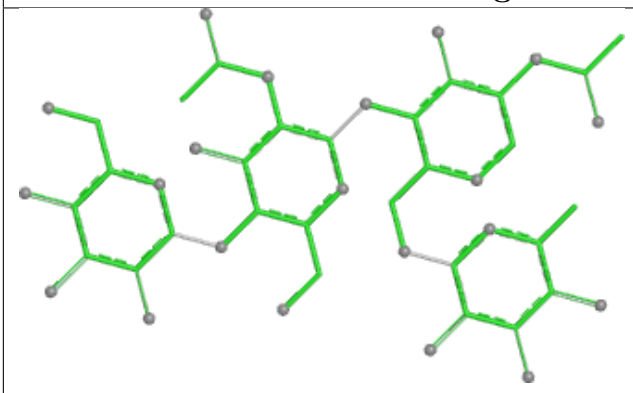


Torsions

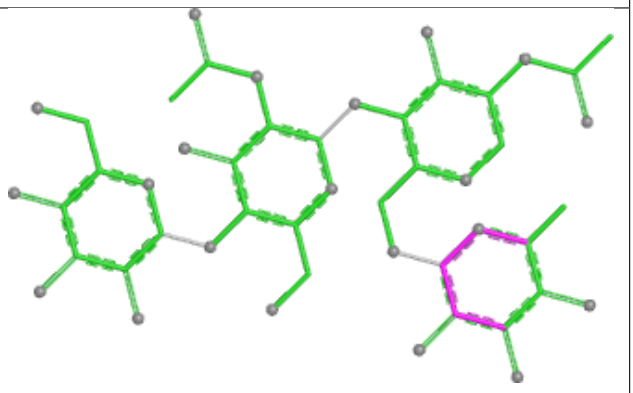


Rings

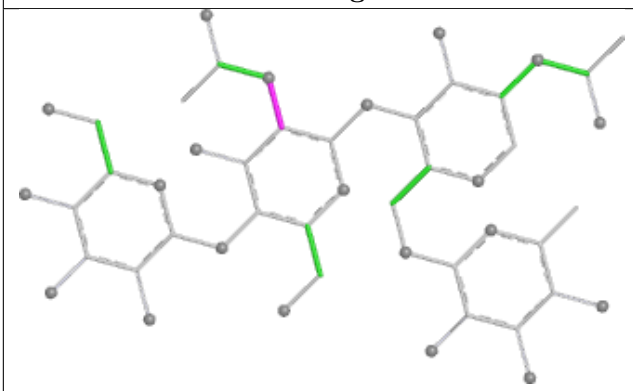
Oligosaccharide Chain H



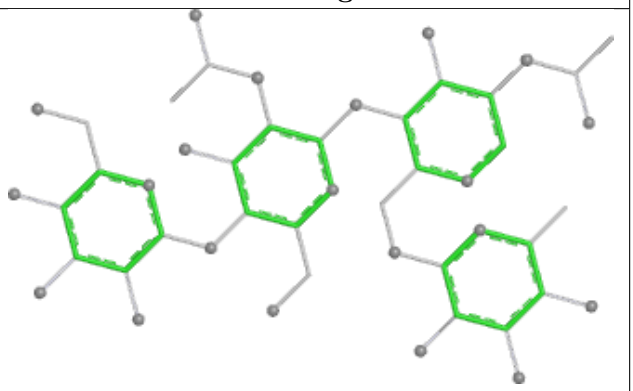
Bond lengths



Bond angles

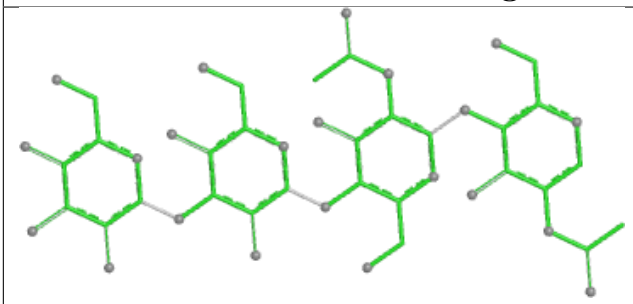


Torsions

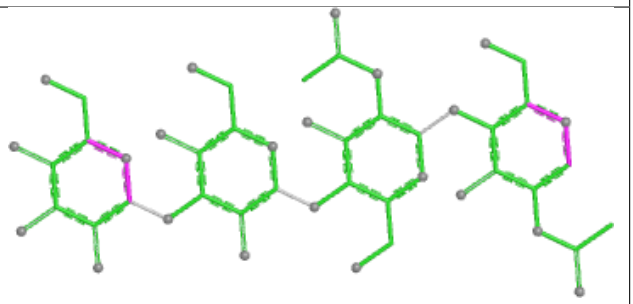


Rings

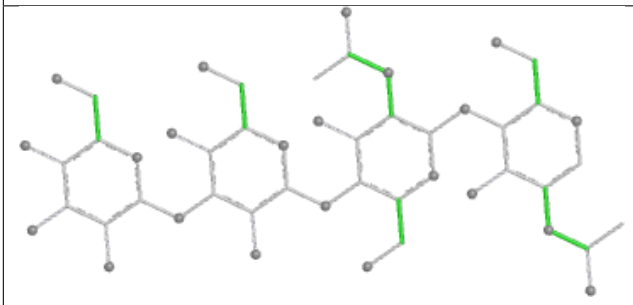
Oligosaccharide Chain I



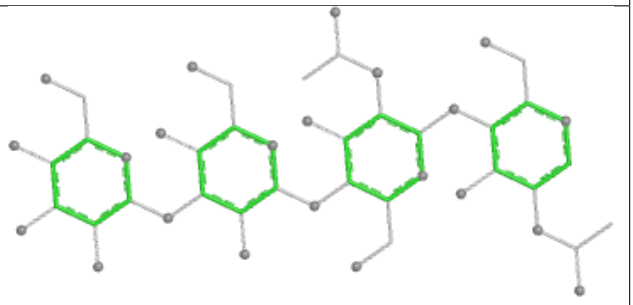
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	B	901	2	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
10	NAG	C	901	3	14,14,15	0.30	0	17,19,21	0.53	0
10	NAG	B	902	2	14,14,15	0.32	0	17,19,21	0.61	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
10	NAG	B	901	2	-	1/6/23/26	0/1/1/1
10	NAG	C	901	3	-	0/6/23/26	0/1/1/1
10	NAG	B	902	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	901	NAG	C1-O5-C5	2.11	115.01	112.19
10	B	902	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	901	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	157/157 (100%)	-0.41	0 100 100	30, 48, 80, 109	0
2	B	301/312 (96%)	-0.06	0 100 100	36, 74, 118, 151	1 (0%)
3	C	270/344 (78%)	0.19	10 (3%) 45 25	38, 80, 145, 164	0
All	All	728/813 (89%)	-0.04	10 (1%) 73 53	30, 68, 136, 164	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	104	ILE	3.5
3	C	102	PRO	3.4
3	C	54	SER	3.3
3	C	33	THR	3.1
3	C	117	GLY	2.6
3	C	120	ASN	2.6
3	C	49	PRO	2.3
3	C	50	GLU	2.0
3	C	229	VAL	2.0
3	C	115	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

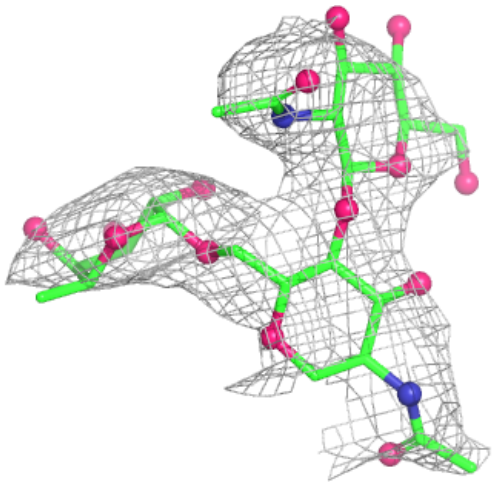
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

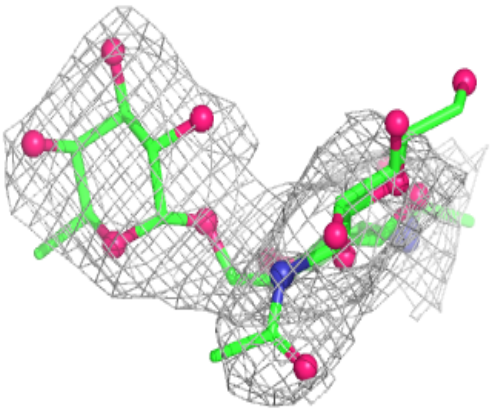
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	E	4	11/12	0.16	0.15	171,175,182,184	0
8	BMA	H	3	11/12	0.25	0.13	132,138,143,144	0
6	BMA	F	3	11/12	0.28	0.13	143,146,148,149	0
5	MAN	E	5	11/12	0.45	0.14	175,179,184,185	0
9	BMA	I	3	11/12	0.57	0.17	174,177,182,183	0
9	NAG	I	2	14/15	0.58	0.15	162,171,174,175	0
5	BMA	E	3	11/12	0.61	0.15	158,168,174,179	0
9	NAG	I	1	14/15	0.61	0.14	162,167,170,171	0
4	NAG	D	2	14/15	0.67	0.12	150,155,162,162	0
6	NAG	F	2	14/15	0.71	0.14	118,129,138,142	0
8	FUC	H	4	10/11	0.74	0.15	90,93,95,95	0
7	NAG	J	2	14/15	0.74	0.11	114,116,119,121	0
9	MAN	I	4	11/12	0.76	0.15	180,184,187,188	0
4	NAG	D	1	14/15	0.80	0.11	129,136,143,147	0
7	NAG	G	2	14/15	0.83	0.14	118,126,130,131	0
8	NAG	H	2	14/15	0.83	0.12	106,112,120,125	0
7	NAG	G	1	14/15	0.85	0.10	107,112,115,118	0
5	NAG	E	2	14/15	0.86	0.14	132,139,148,153	0
8	NAG	H	1	14/15	0.86	0.11	82,88,93,101	0
7	NAG	J	1	14/15	0.86	0.10	94,98,103,109	0
4	FUC	D	3	10/11	0.87	0.13	140,141,144,145	0
6	NAG	F	1	14/15	0.88	0.14	97,101,107,116	0
5	NAG	E	1	14/15	0.89	0.13	113,120,126,129	0

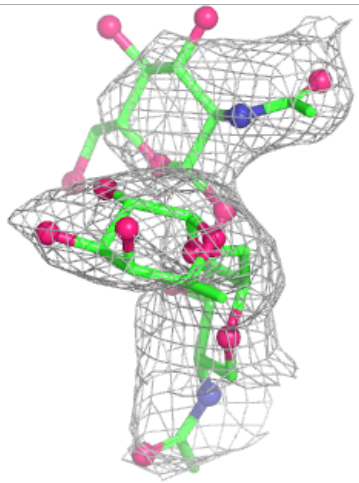
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

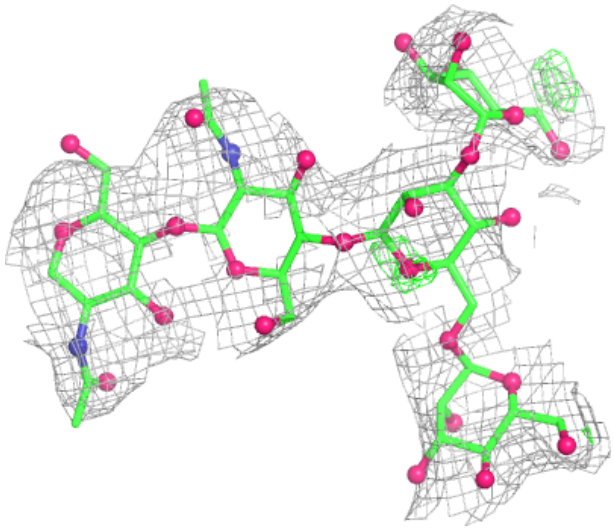


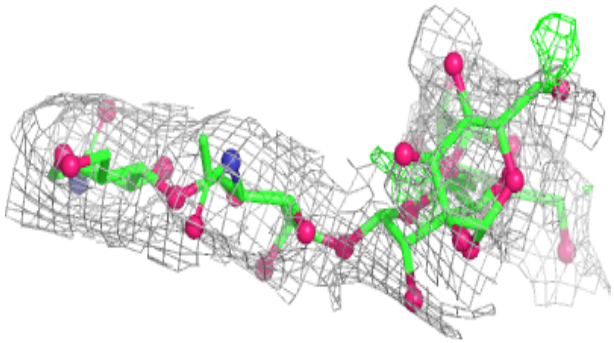


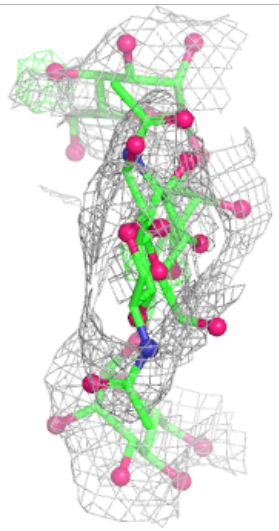


Electron density around Chain E:

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

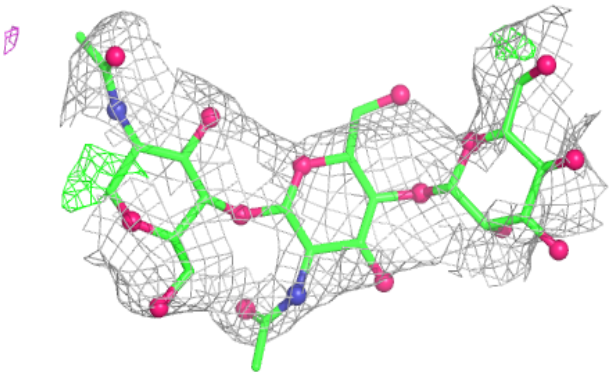


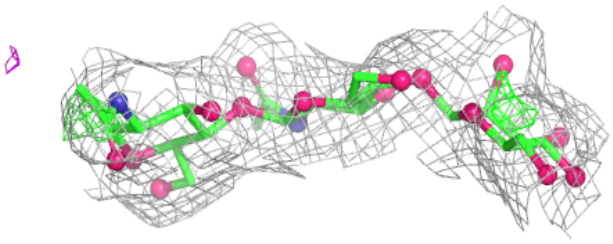


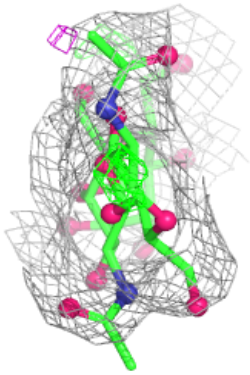


Electron density around Chain F:

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

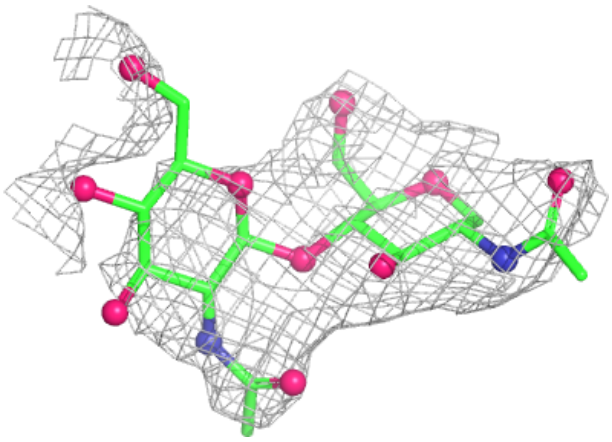


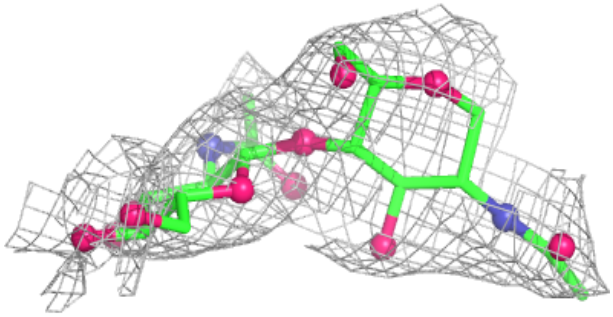


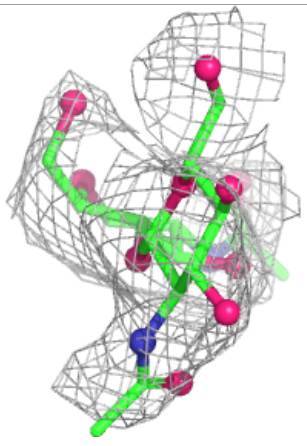


Electron density around Chain G:

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

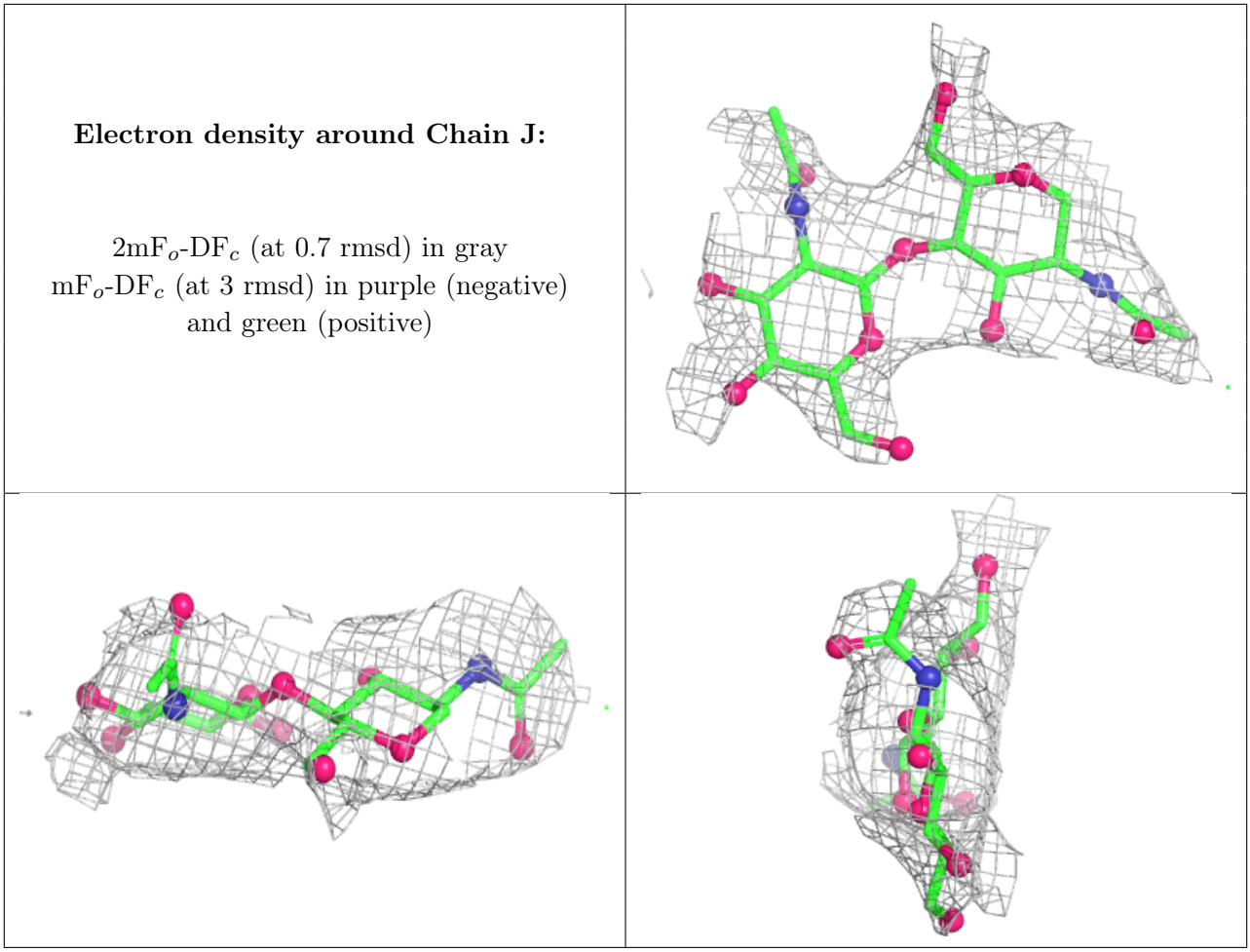






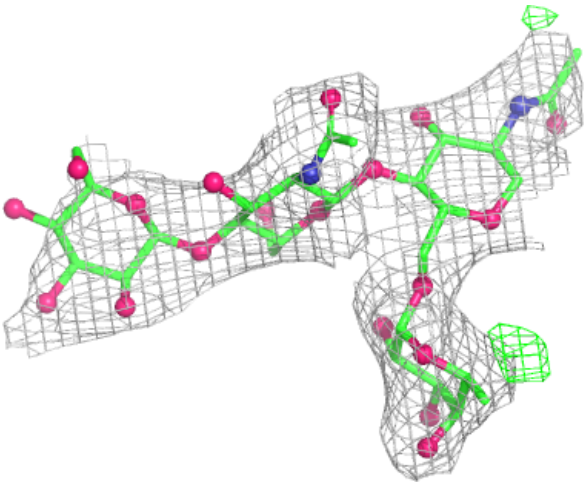
Electron density around Chain J:

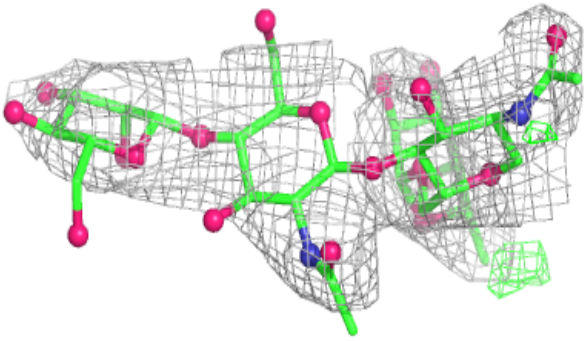
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

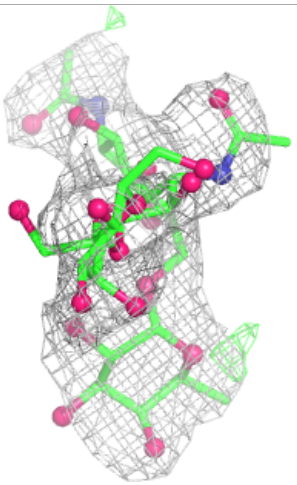


Electron density around Chain H:

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

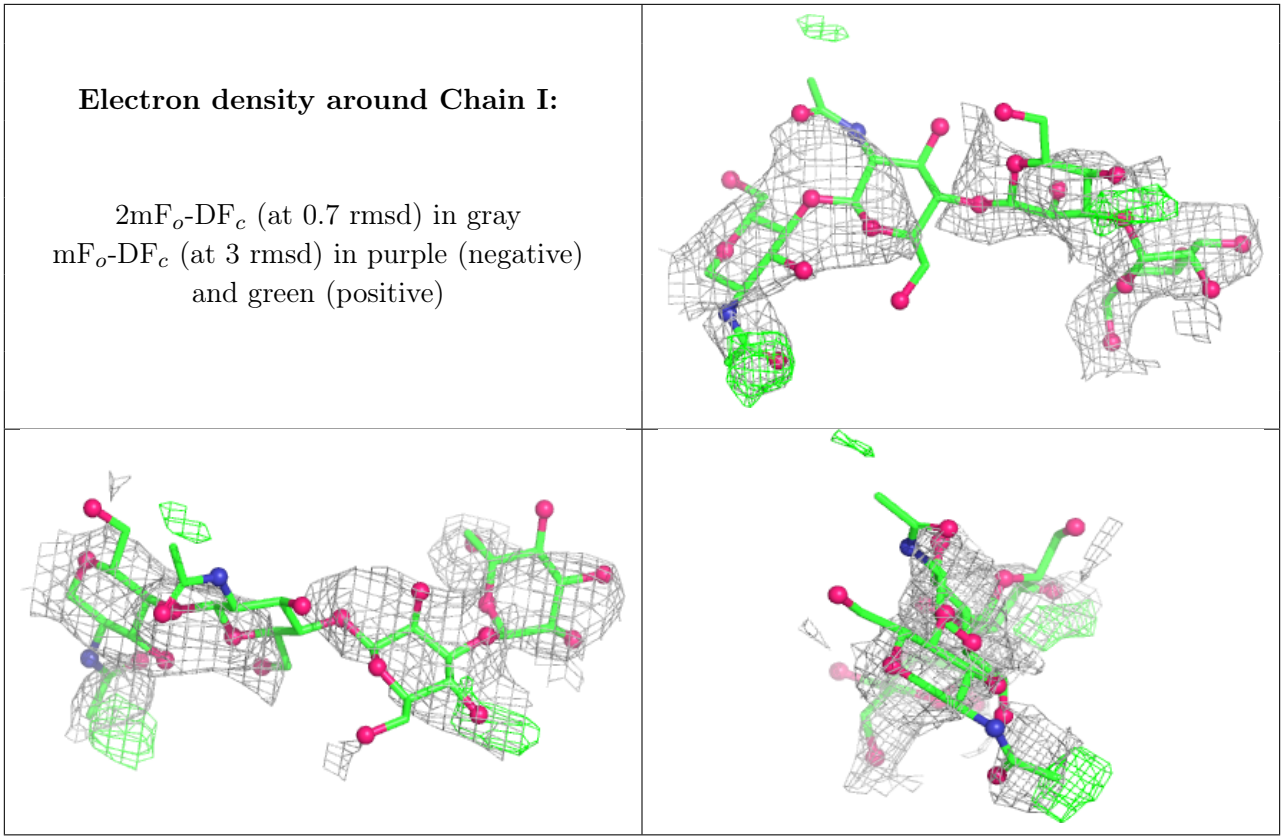






Electron density around Chain I:

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



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
10	NAG	B	901	14/15	0.21	0.18	146,149,153,156	0
10	NAG	C	901	14/15	0.43	0.15	180,182,186,188	0
10	NAG	B	902	14/15	0.54	0.11	124,132,140,143	0
11	CL	C	908	1/1	0.97	0.15	55,55,55,55	0

6.5 Other polymers

There are no such residues in this entry.