Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 01:12 PM UTC

PDB ID	:	3ZE0 / pdb_00003ze0
Title	:	Integrin alphaIIB beta3 headpiece and RGD peptide complex
Authors	:	Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on	:	2012-12-03
Resolution	:	2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

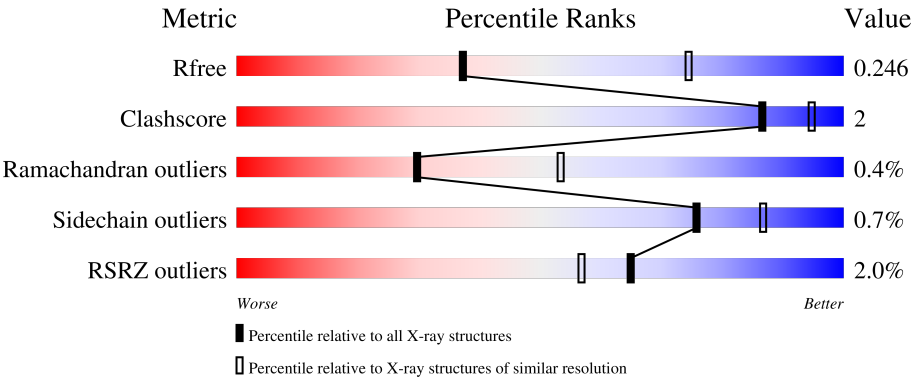
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



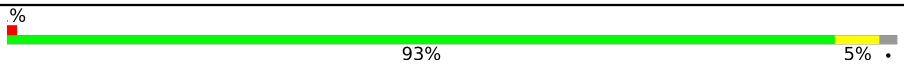
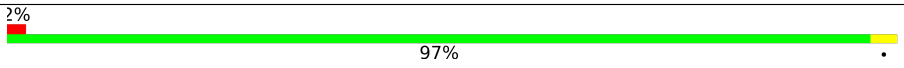
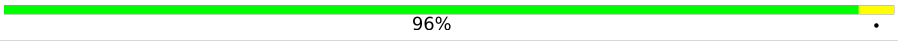
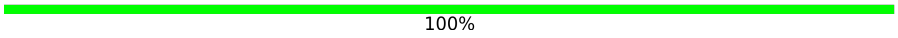
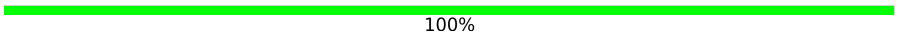
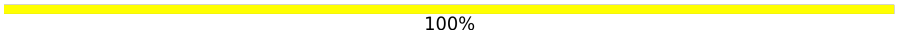
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	457	95%
1	C	457	95%
2	B	472	3% 91% 7%
2	D	472	4% 92% 8%
3	E	221	3% 91% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	I	6	
5	J	6	
6	G	4	
6	M	4	
7	K	2	
7	N	2	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 41622 atoms, of which 20222 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 INTEGRIN ALPHA-IIB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	H	N	O	S	0	5	0
			6868	2235	3355	604	666	8			
1	C	453	Total	C	H	N	O	S	0	2	0
			6795	2214	3311	600	662	8			

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	465	Total	C	H	N	O	S	6	1	0
			7098	2238	3506	613	708	33			
2	D	469	Total	C	H	N	O	S	14	1	0
			7146	2252	3526	619	715	34			

- Molecule 3 is a protein called 10E5 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			

- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

- Molecule 5 is a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	0	0
			75	22	34	9	10			
5	J	6	Total	C	H	N	O	2	0	0
			75	22	34	9	10			

- Molecule 6 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.



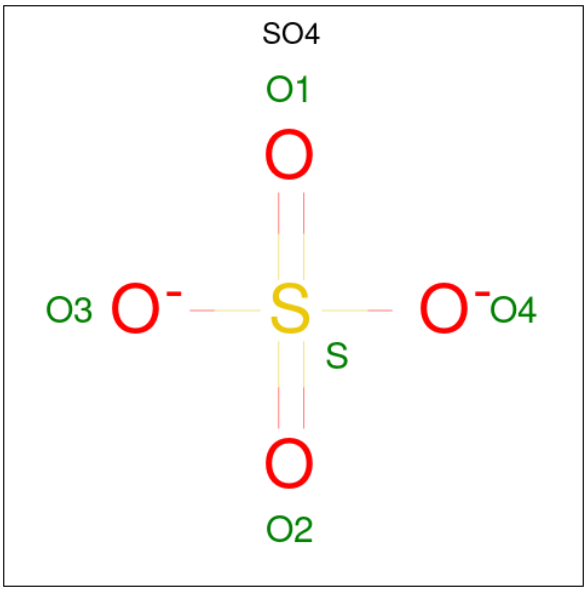
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			
6	M	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- 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	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	N	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	L	1	Total O S 5 4 1	0	0

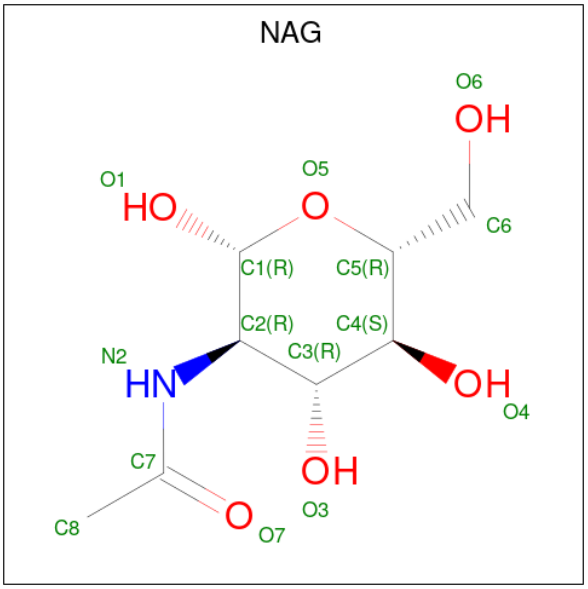
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	4	Total Ca 4 4	0	0
9	C	4	Total Ca 4 4	0	0

- Molecule 10 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	3	Total Mn 3 3	0	0
10	D	3	Total Mn 3 3	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C H N O 27 8 13 1 5	0	0
11	D	1	Total C H N O 27 8 13 1 5	0	0

- Molecule 12 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	160	Total O 160 160	0	0
13	B	71	Total O 71 71	0	0
13	C	51	Total O 51 51	0	0
13	D	26	Total O 26 26	0	0
13	E	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

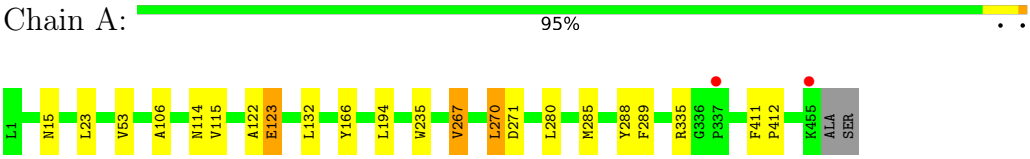
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	F	1	Total O 1 1	0	0
13	H	8	Total O 8 8	0	0
13	I	2	Total O 2 2	0	0
13	J	1	Total O 1 1	0	0
13	L	6	Total O 6 6	0	0

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.

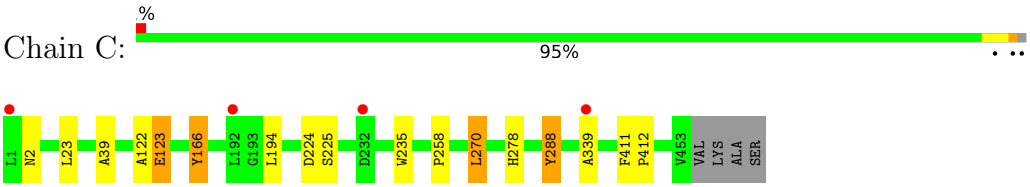
• Molecule 1: INTEGRIN ALPHA-IIB

Chain A:



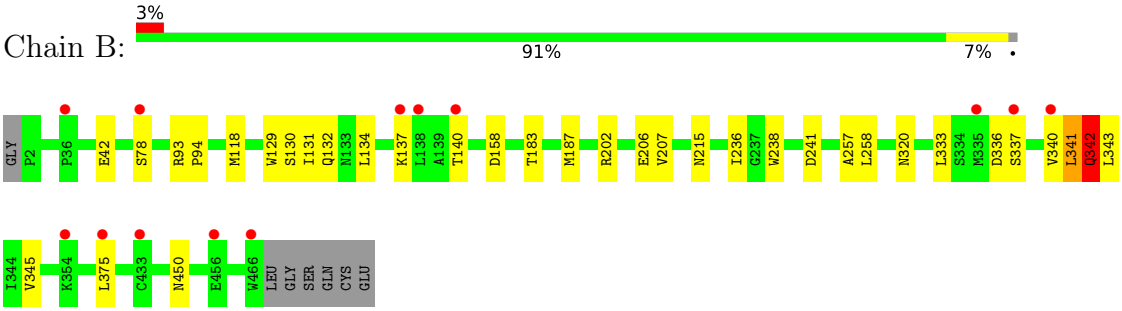
• Molecule 1: INTEGRIN ALPHA-IIB

Chain C:



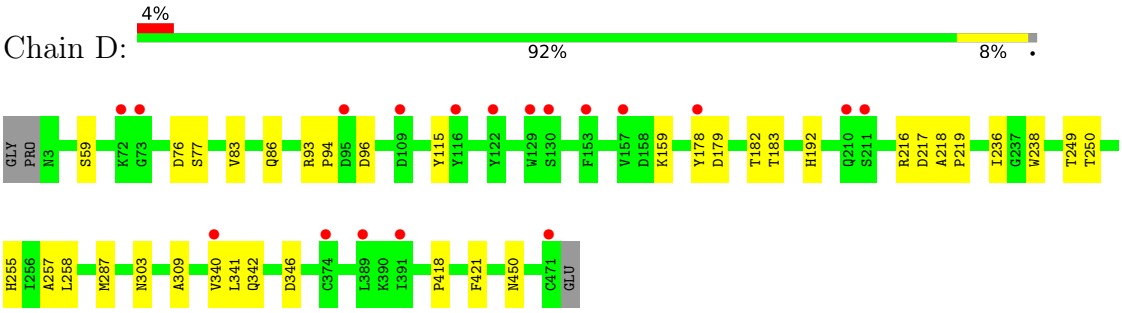
• Molecule 2: INTEGRIN BETA-3

Chain B:



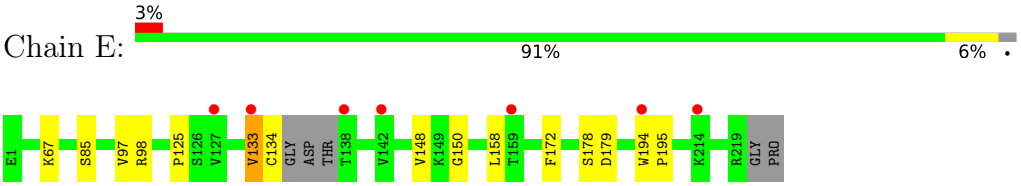
• Molecule 2: INTEGRIN BETA-3

Chain D:



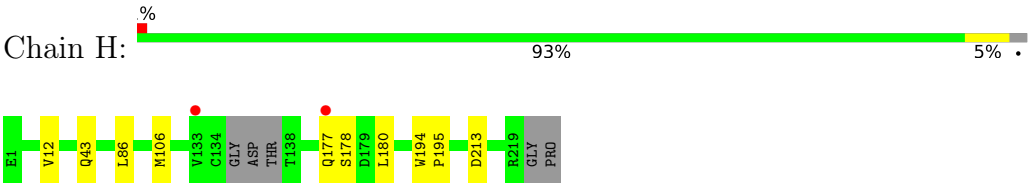
• Molecule 3: 10E5 FAB HEAVY CHAIN

Chain E:



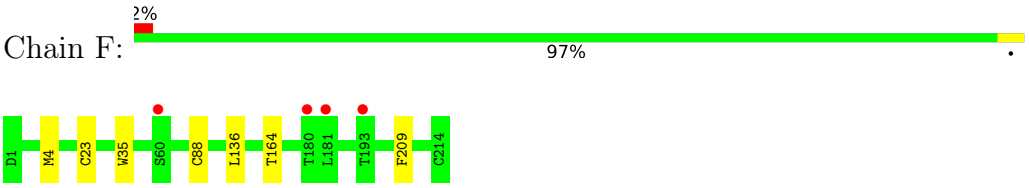
• Molecule 3: 10E5 FAB HEAVY CHAIN

Chain H:



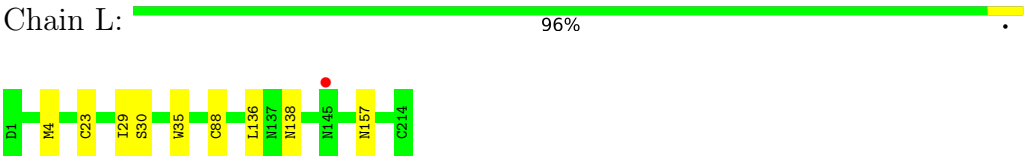
• Molecule 4: 10E5 FAB LIGHT CHAIN

Chain F:



• Molecule 4: 10E5 FAB LIGHT CHAIN

Chain L:



• Molecule 5: RGD PEPTIDE

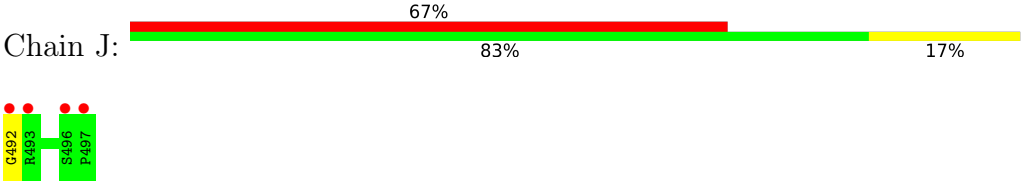
Chain I:



There are no outlier residues recorded for this chain.

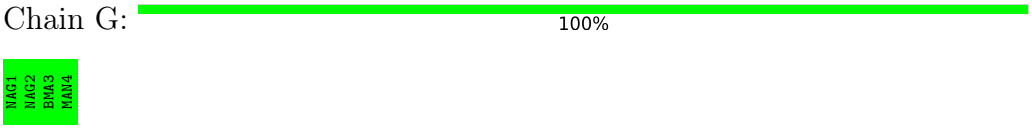
• Molecule 5: RGD PEPTIDE

Chain J:



• Molecule 6: 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 G:



• Molecule 6: 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

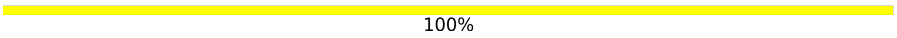
Chain M:





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

Chain K:





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

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	259.64Å 144.68Å 104.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.95 48.31 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.31-2.95) 99.6 (48.31-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.243 0.191 , 0.246	Depositor DCC
R_{free} test set	1071 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 85.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41622	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: MAN, MN, SO4, CA, CL, BMA, 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	0.28	0/3625	0.65	0/4940
1	C	0.26	0/3587	0.62	2/4888 (0.0%)
2	B	0.26	0/3662	0.66	1/4965 (0.0%)
2	D	0.25	0/3686	0.60	0/4997
3	E	0.25	0/1684	0.60	0/2305
3	H	0.25	0/1684	0.59	0/2305
4	F	0.23	0/1673	0.56	0/2269
4	L	0.24	0/1673	0.59	0/2269
5	I	0.30	0/41	0.66	0/52
5	J	0.26	0/41	0.63	0/52
All	All	0.26	0/21356	0.62	3/29042 (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	B	342	GLN	N-CA-C	-7.92	103.40	113.23
1	C	39	ALA	CA-C-N	5.14	124.85	119.82
1	C	39	ALA	C-N-CA	5.14	124.85	119.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3513	3355	3364	13	0
1	C	3484	3311	3320	10	0
2	B	3592	3506	3512	21	0
2	D	3620	3526	3531	19	0
3	E	1642	1597	1600	8	0
3	H	1642	1597	1600	5	0
4	F	1637	1550	1553	5	0
4	L	1637	1550	1553	5	0
5	I	41	34	34	0	0
5	J	41	34	34	1	0
6	G	50	43	43	0	0
6	M	50	43	43	0	0
7	K	28	25	25	1	0
7	N	28	25	25	1	0
8	A	15	0	0	1	0
8	C	5	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	B	3	0	0	0	0
10	D	3	0	0	0	0
11	B	14	13	13	0	0
11	D	14	13	13	1	0
12	C	1	0	0	0	0
13	A	160	0	0	3	1
13	B	71	0	0	0	0
13	C	51	0	0	0	1
13	D	26	0	0	1	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	H	8	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	1	0
13	L	6	0	0	1	0
All	All	21400	20222	20263	87	1

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 2.

All (87) 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:D:250:THR:OG1	13:D:4007:HOH:O	2.11	0.69
1:C:224:ASP:OD1	1:C:225:SER:N	2.30	0.64
2:B:118:MET:SD	2:B:131:ILE:HD13	2.40	0.61
2:D:115:TYR:OH	2:D:192:HIS:ND1	2.27	0.60
1:A:122:ALA:O	1:A:123:GLU:HB2	2.05	0.56
2:B:257:ALA:O	2:B:258:LEU:HB2	2.06	0.55
2:D:76:ASP:OD1	2:D:77:SER:N	2.40	0.55
2:B:130:SER:O	2:B:341:LEU:CD1	2.57	0.53
1:C:122:ALA:O	1:C:123:GLU:HB2	2.08	0.53
1:A:122:ALA:O	1:A:123:GLU:CB	2.57	0.52
11:D:3099:NAG:O6	7:N:2:NAG:O6	2.13	0.52
3:H:194:TRP:CG	3:H:195:PRO:HA	2.44	0.52
3:H:43:GLN:N	3:H:43:GLN:OE1	2.42	0.51
2:B:131:ILE:HD12	2:B:207:VAL:HG13	1.92	0.51
2:D:342:GLN:NE2	2:D:346:ASP:OD2	2.43	0.51
8:A:1456:SO4:O3	13:A:4152:HOH:O	2.19	0.50
2:B:340:VAL:O	2:B:341:LEU:CB	2.60	0.50
2:B:342:GLN:O	2:B:345:VAL:N	2.44	0.50
1:A:267:VAL:HG12	1:A:289:PHE:CE1	2.47	0.50
3:H:177:GLN:N	3:H:180:LEU:O	2.45	0.50
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.41	0.49
2:D:450:ASN:O	2:D:450:ASN:ND2	2.47	0.48
1:C:122:ALA:O	1:C:123:GLU:CB	2.62	0.48
2:B:129:TRP:CE3	2:B:130:SER:HA	2.49	0.48
2:B:450:ASN:O	2:B:450:ASN:ND2	2.47	0.48
1:A:194:LEU:HD12	1:A:194:LEU:C	2.39	0.48
2:D:257:ALA:O	2:D:258:LEU:HB2	2.14	0.47
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.46	0.47
2:B:340:VAL:O	2:B:341:LEU:HB2	2.14	0.47
5:J:492:GLY:N	13:J:4001:HOH:O	2.46	0.47
2:D:182:THR:OG1	2:D:183:THR:N	2.48	0.47
1:A:15[B]:ASN:ND2	13:A:4009:HOH:O	2.48	0.46
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.51	0.46
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.97	0.46
1:A:53:VAL:HG21	1:A:106:ALA:CB	2.46	0.46
2:D:83:VAL:O	2:D:86:GLN:NE2	2.49	0.45
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.98	0.45
2:D:159:LYS:NZ	2:D:287:MET:O	2.41	0.45
2:B:118:MET:SD	2:B:131:ILE:HG21	2.57	0.45
1:C:411:PHE:HB3	1:C:412:PRO:CD	2.47	0.45
3:H:213:ASP:OD1	3:H:213:ASP:N	2.49	0.45
2:D:178:TYR:CG	2:D:179:ASP:N	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:133:VAL:O	3:E:134:CYS:SG	2.74	0.44
1:A:15[A]:ASN:ND2	13:A:4008:HOH:O	2.49	0.44
2:B:333:LEU:HA	2:B:340:VAL:HG13	2.00	0.44
1:C:258:PRO:HB2	1:C:288:TYR:CD2	2.52	0.44
3:E:194:TRP:CG	3:E:195:PRO:HA	2.53	0.44
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.48	0.44
7:K:1:NAG:O3	7:K:2:NAG:O5	2.31	0.44
2:B:42:GLU:OE1	2:B:42:GLU:N	2.51	0.44
1:C:2:ASN:OD1	1:C:2:ASN:N	2.50	0.44
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.98	0.44
1:A:132:LEU:HD12	1:A:132:LEU:N	2.33	0.43
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.54	0.43
1:A:411:PHE:HB3	1:A:412:PRO:CD	2.49	0.43
2:B:340:VAL:O	2:B:341:LEU:HG	2.18	0.43
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.54	0.43
1:A:285:MET:SD	2:B:320:ASN:HB3	2.59	0.43
3:E:67:LYS:NZ	3:E:85:SER:O	2.51	0.43
2:B:78:SER:OG	2:B:241:ASP:CG	2.62	0.43
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.53	0.43
1:C:278[A]:HIS:CD2	1:C:339:ALA:HB1	2.53	0.43
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.54	0.43
2:B:158:ASP:HB3	2:B:187:MET:CE	2.49	0.43
1:A:114:ASN:OD1	1:A:115:VAL:N	2.52	0.43
4:L:29:ILE:O	4:L:30:SER:C	2.61	0.42
2:D:340:VAL:HG13	2:D:341:LEU:N	2.34	0.42
3:E:178:SER:O	3:E:179:ASP:HB2	2.20	0.42
1:A:271:ASP:OD1	1:A:271:ASP:C	2.62	0.42
2:D:59:SER:OG	2:D:96:ASP:OD2	2.26	0.42
4:L:4:MET:HE3	4:L:23:CYS:SG	2.59	0.42
1:C:166:TYR:CE1	2:D:216:ARG:HD3	2.54	0.42
2:D:249:THR:HG22	2:D:309:ALA:HB3	2.02	0.42
4:F:4:MET:HE3	4:F:23:CYS:SG	2.60	0.42
4:F:136:LEU:HD12	4:F:136:LEU:N	2.35	0.41
2:B:134:LEU:HA	2:B:137:LYS:CD	2.51	0.41
2:B:236:ILE:HG21	2:B:238:TRP:CE2	2.55	0.41
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.03	0.41
2:B:336:ASP:O	2:B:337:SER:OG	2.25	0.41
1:C:194:LEU:C	1:C:194:LEU:HD12	2.46	0.41
2:D:236:ILE:HG21	2:D:238:TRP:CE2	2.56	0.41
3:E:158:LEU:HD23	3:E:158:LEU:C	2.46	0.41
4:L:157:ASN:ND2	13:L:4006:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:136:LEU:N	4:L:136:LEU:HD12	2.36	0.40
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.56	0.40
3:E:97:VAL:HG12	3:E:98:ARG:N	2.37	0.40
4:F:209:PHE:CD1	4:F:209:PHE:C	3.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:4052:HOH:O	13:C:4041:HOH:O[1_554]	2.12	0.08

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	458/457 (100%)	440 (96%)	17 (4%)	1 (0%)	43	66
1	C	453/457 (99%)	428 (94%)	24 (5%)	1 (0%)	43	66
2	B	464/472 (98%)	435 (94%)	26 (6%)	3 (1%)	21	45
2	D	468/472 (99%)	436 (93%)	30 (6%)	2 (0%)	30	53
3	E	212/221 (96%)	197 (93%)	13 (6%)	2 (1%)	14	34
3	H	212/221 (96%)	196 (92%)	15 (7%)	1 (0%)	24	49
4	F	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
4	L	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	24	49
5	I	4/6 (67%)	4 (100%)	0	0	100	100
5	J	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2699/2740 (98%)	2541 (94%)	147 (5%)	11 (0%)	30	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	341	LEU
1	A	123	GLU
2	B	343	LEU
2	B	375	LEU
1	C	123	GLU
2	D	303[A]	ASN
2	D	303[B]	ASN
4	L	138	ASN
3	H	178	SER
3	E	150	GLY
3	E	133	VAL

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	368/364 (101%)	361 (98%)	7 (2%)	50 71
1	C	363/364 (100%)	359 (99%)	4 (1%)	65 80
2	B	413/417 (99%)	408 (99%)	5 (1%)	63 79
2	D	416/417 (100%)	416 (100%)	0	100 100
3	E	187/190 (98%)	187 (100%)	0	100 100
3	H	187/190 (98%)	186 (100%)	1 (0%)	81 90
4	F	188/188 (100%)	188 (100%)	0	100 100
4	L	188/188 (100%)	188 (100%)	0	100 100
5	I	4/4 (100%)	4 (100%)	0	100 100
5	J	4/4 (100%)	4 (100%)	0	100 100
All	All	2318/2326 (100%)	2301 (99%)	17 (1%)	76 87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	267	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	270	LEU
1	A	280	LEU
1	A	288	TYR
1	A	335	ARG
2	B	132	GLN
2	B	140	THR
2	B	183	THR
2	B	215	ASN
2	B	342	GLN
1	C	23	LEU
1	C	166	TYR
1	C	270	LEU
1	C	288	TYR
3	H	106	MET

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	197	GLN
1	A	338	HIS
2	B	303	ASN
2	B	376	ASN
2	B	450	ASN
1	C	15	ASN
1	C	85	GLN
1	C	158	ASN
1	C	333	GLN
2	D	210	GLN
2	D	301	GLN
2	D	450	ASN
3	E	170	HIS
4	F	190	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
6	NAG	G	1	2,6	14,14,15	0.53	0	17,19,21	0.74	0
6	NAG	G	2	6	14,14,15	0.57	0	17,19,21	0.73	0
6	BMA	G	3	6	11,11,12	0.61	0	15,15,17	0.74	0
6	MAN	G	4	6	11,11,12	0.61	0	15,15,17	0.59	0
7	NAG	K	1	2,7	14,14,15	0.59	0	17,19,21	0.80	0
7	NAG	K	2	7	14,14,15	0.51	0	17,19,21	0.55	0
6	NAG	M	1	2,6	14,14,15	0.51	0	17,19,21	0.68	0
6	NAG	M	2	6	14,14,15	0.53	0	17,19,21	0.57	0
6	BMA	M	3	6	11,11,12	0.66	0	15,15,17	0.78	1 (6%)
6	MAN	M	4	6	11,11,12	0.64	0	15,15,17	0.58	0
7	NAG	N	1	2,7	14,14,15	0.59	0	17,19,21	0.87	0
7	NAG	N	2	7	14,14,15	0.52	0	17,19,21	0.56	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
6	NAG	G	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
6	NAG	M	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
7	NAG	N	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	3	BMA	C1-C2-C3	2.10	112.70	109.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	2	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O5-C5-C6-O6
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2

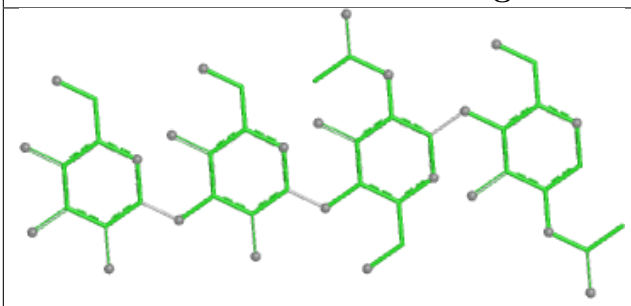
There are no ring outliers.

3 monomers are involved in 2 short contacts:

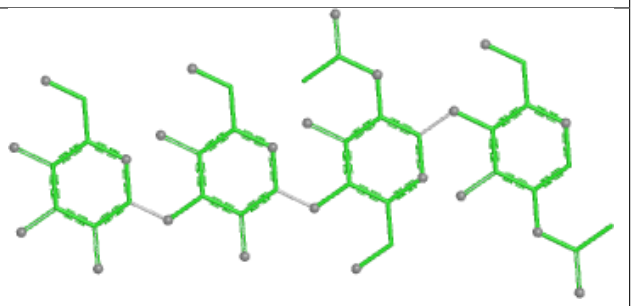
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	1	NAG	1	0
7	N	2	NAG	1	0
7	K	2	NAG	1	0

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

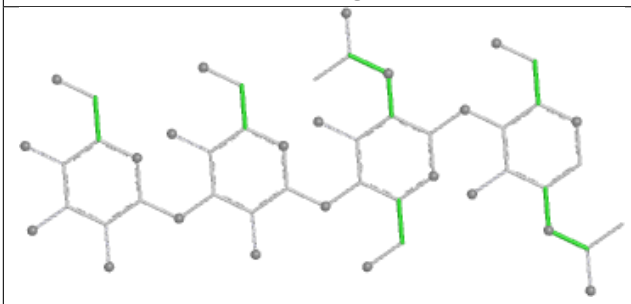
Oligosaccharide Chain G



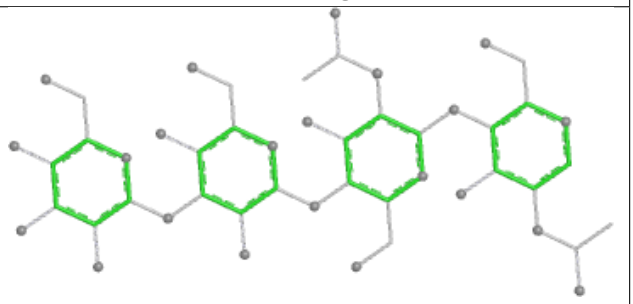
Bond lengths



Bond angles

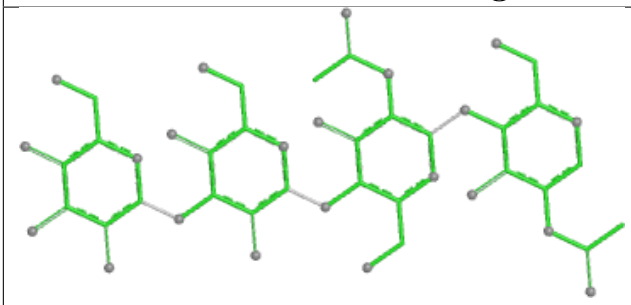


Torsions

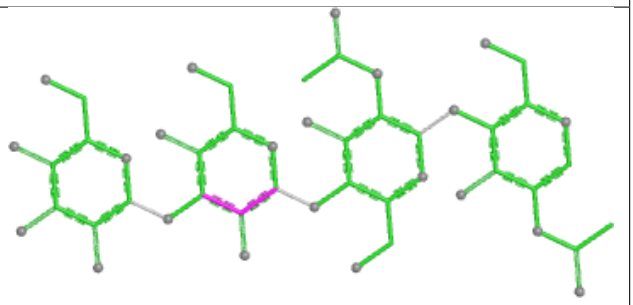


Rings

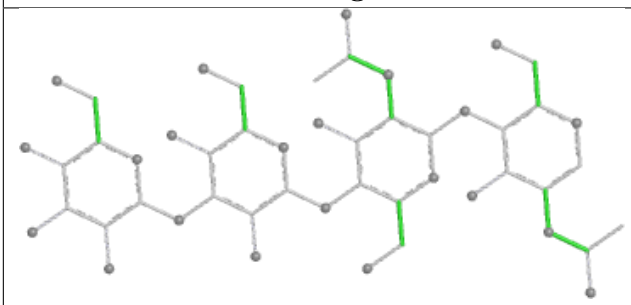
Oligosaccharide Chain M



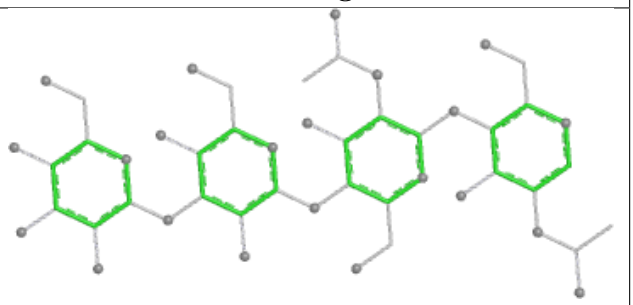
Bond lengths



Bond angles

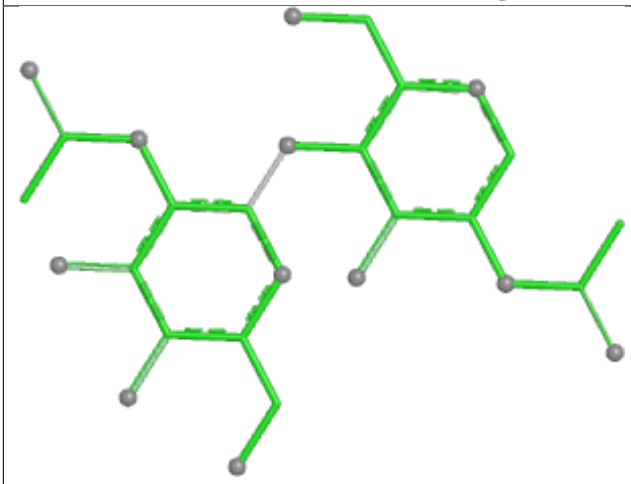


Torsions

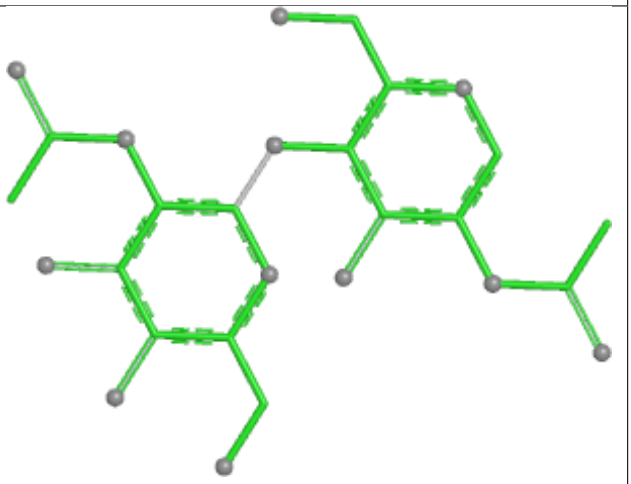


Rings

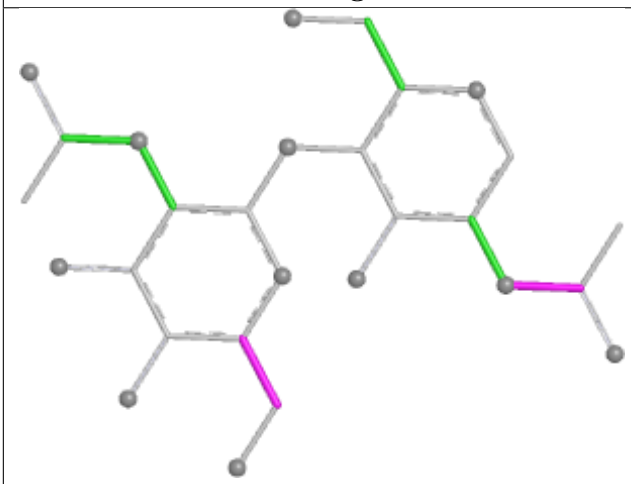
Oligosaccharide Chain K



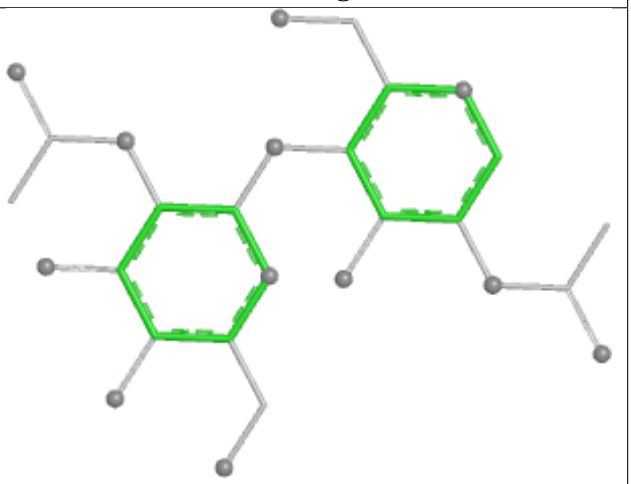
Bond lengths



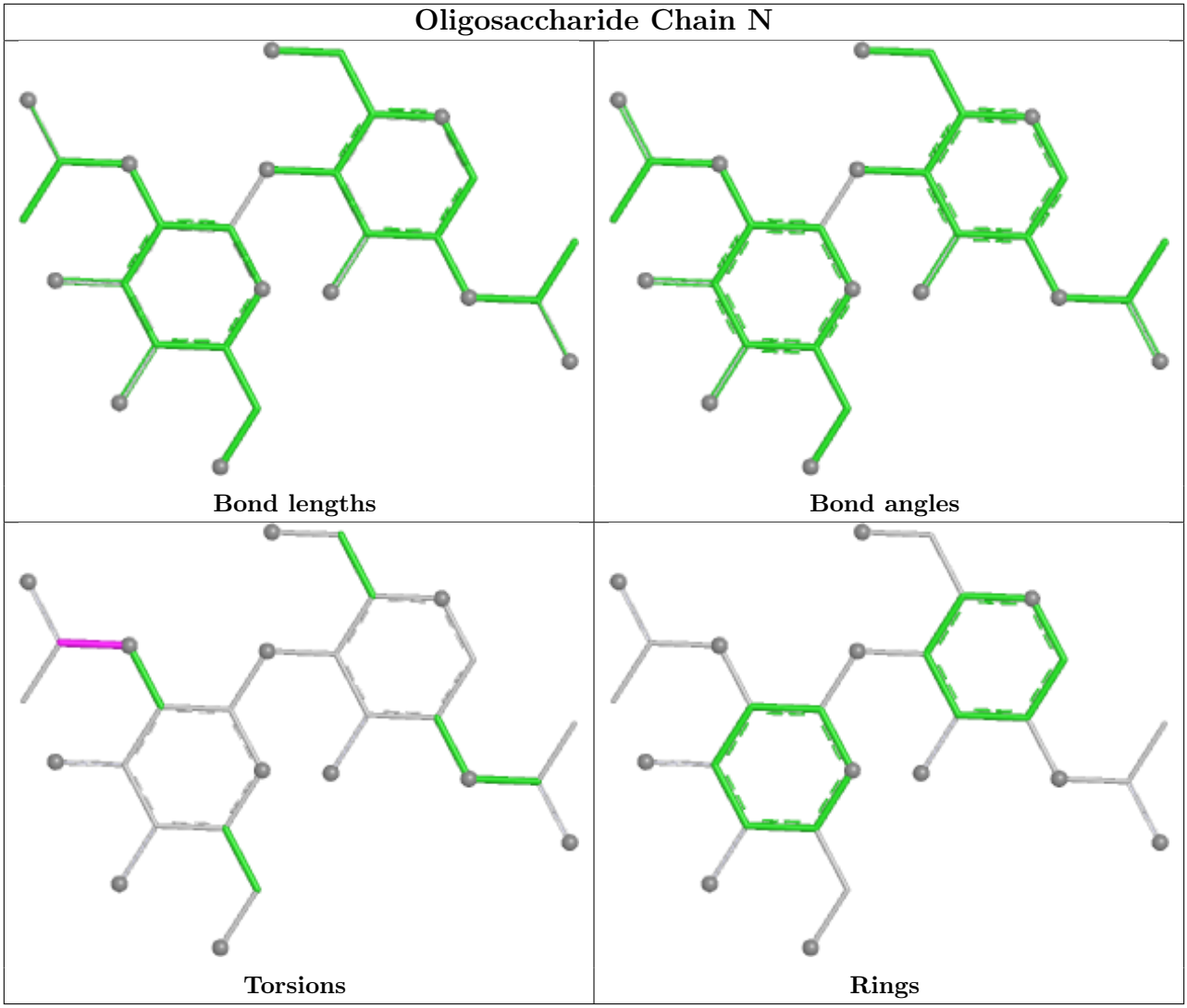
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 15 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SO4	A	1457	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	A	1458	-	4,4,4	0.23	0	6,6,6	0.06	0
8	SO4	C	1454	-	4,4,4	0.24	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	L	1215	-	4,4,4	0.24	0	6,6,6	0.07	0
11	NAG	D	3099	2	14,14,15	0.50	0	17,19,21	0.56	0
8	SO4	A	1456	-	4,4,4	0.24	0	6,6,6	0.08	0
11	NAG	B	3099	2	14,14,15	0.51	0	17,19,21	0.63	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
11	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
11	NAG	D	3099	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	3099	NAG	1	0
8	A	1456	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	455/457 (99%)	-0.53	2 (0%) 88 86	20, 45, 83, 156	5 (1%)
1	C	453/457 (99%)	-0.07	4 (0%) 81 76	38, 82, 131, 183	2 (0%)
2	B	465/472 (98%)	0.02	13 (2%) 55 47	25, 90, 190, 234	2 (0%)
2	D	469/472 (99%)	0.53	18 (3%) 44 36	47, 123, 192, 248	3 (0%)
3	E	216/221 (97%)	0.58	7 (3%) 50 43	94, 150, 206, 233	0
3	H	216/221 (97%)	0.10	2 (0%) 81 76	54, 113, 187, 224	0
4	F	214/214 (100%)	0.42	4 (1%) 66 58	93, 154, 227, 305	0
4	L	214/214 (100%)	0.04	1 (0%) 87 83	56, 104, 142, 250	0
5	I	6/6 (100%)	0.64	0 100 100	42, 64, 97, 101	0
5	J	6/6 (100%)	2.99	4 (66%) 0 0	19, 28, 89, 120	3 (50%)
All	All	2714/2740 (99%)	0.09	55 (2%) 65 57	19, 100, 192, 305	15 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	493	ARG	7.1
4	F	181	LEU	4.3
2	B	466	TRP	3.7
5	J	492	GLY	3.4
5	J	497	PRO	3.4
2	B	137	LYS	3.4
1	C	1	LEU	3.3
1	A	455	LYS	3.2
2	D	122	TYR	3.1
2	D	211	SER	2.9
3	E	138	THR	2.9
4	F	193	THR	2.9
1	A	337	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	129	TRP	2.8
2	D	109	ASP	2.8
2	D	471	CYS	2.7
2	B	78	SER	2.7
3	E	142	VAL	2.7
2	D	340	VAL	2.6
5	J	496	SER	2.6
2	B	140	THR	2.6
1	C	232	ASP	2.6
1	C	339	ALA	2.6
2	B	36	PRO	2.6
2	D	116	TYR	2.5
2	B	375	LEU	2.4
2	B	340	VAL	2.4
3	H	133	VAL	2.4
3	E	159	THR	2.4
2	B	335	MET	2.4
2	B	433	CYS	2.3
2	D	130	SER	2.3
2	B	138	LEU	2.3
3	E	133	VAL	2.3
3	H	177	GLN	2.3
2	B	337	SER	2.2
2	D	73	GLY	2.2
2	D	153	PHE	2.2
2	D	72	LYS	2.2
2	D	95	ASP	2.2
2	D	210	GLN	2.2
4	F	180	THR	2.2
3	E	194	TRP	2.2
3	E	127	VAL	2.1
2	D	178	TYR	2.1
2	B	456	GLU	2.1
2	D	389	LEU	2.1
2	D	374	CYS	2.1
4	F	60	SER	2.1
2	B	354	LYS	2.1
1	C	192	LEU	2.1
4	L	145	ASN	2.0
2	D	391	ILE	2.0
3	E	214	LYS	2.0
2	D	157	VAL	2.0

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

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

6.3 Carbohydrates (i)

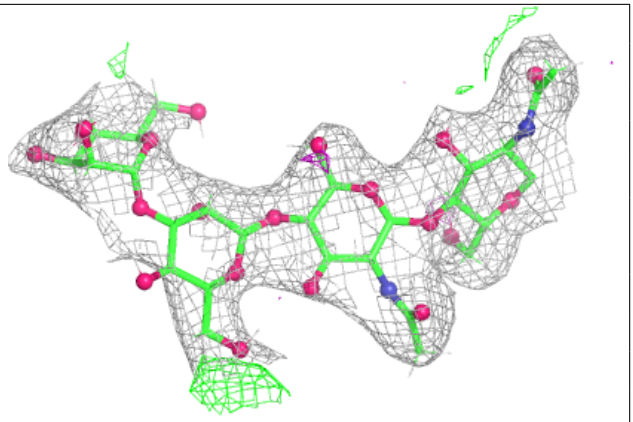
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

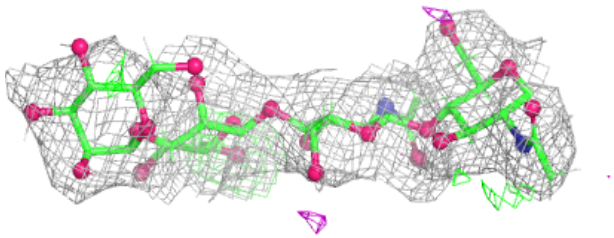
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	G	1	14/15	-	-	28,45,64,85	0
6	NAG	G	2	14/15	-	-	66,92,116,124	0
6	BMA	G	3	11/12	-	-	98,137,174,181	0
6	MAN	G	4	11/12	-	-	112,141,170,172	0
7	NAG	N	2	14/15	0.19	0.14	148,177,206,217	0
6	BMA	M	3	11/12	0.39	0.12	151,175,210,210	0
6	MAN	M	4	11/12	0.40	0.15	164,181,216,218	0
7	NAG	N	1	14/15	0.76	0.11	120,157,185,191	0
6	NAG	M	2	14/15	0.89	0.08	86,119,155,164	0
7	NAG	K	2	14/15	0.89	0.08	116,166,203,209	0
6	NAG	M	1	14/15	0.94	0.10	65,88,111,111	0
7	NAG	K	1	14/15	0.96	0.07	102,132,164,164	0

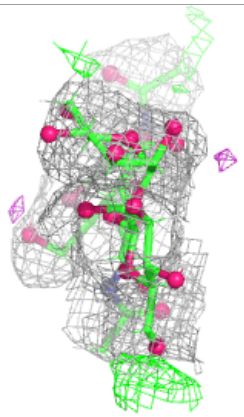
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

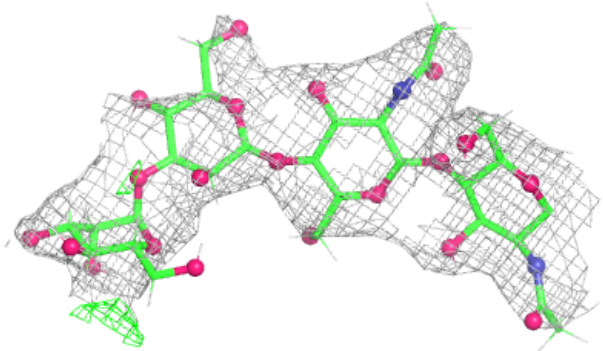


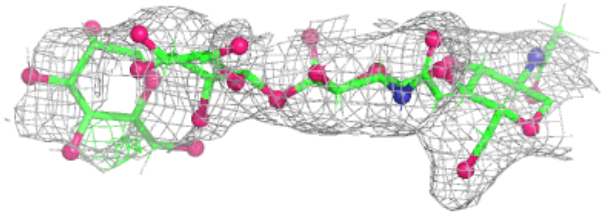


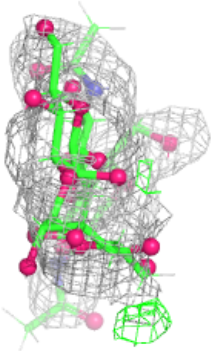


Electron density around Chain M:

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

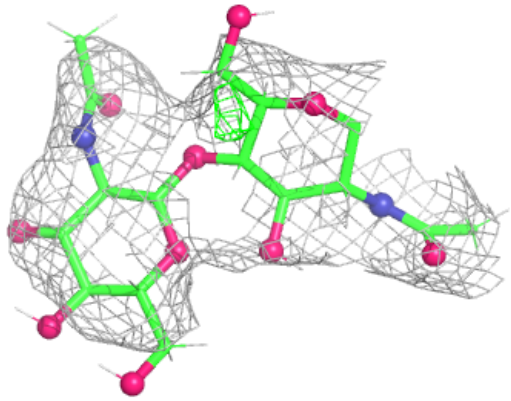


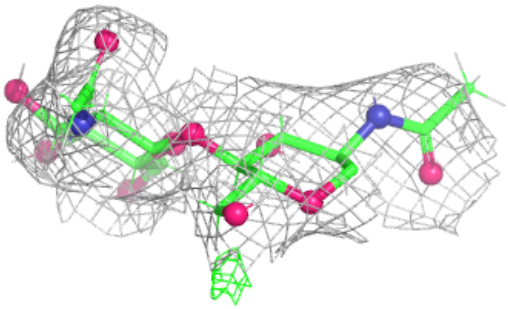


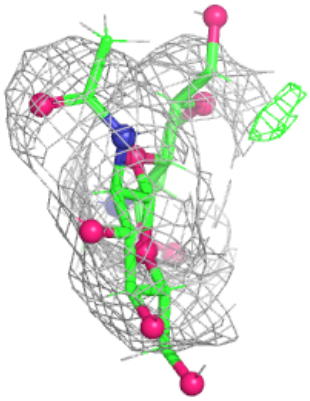


Electron density around Chain K:

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

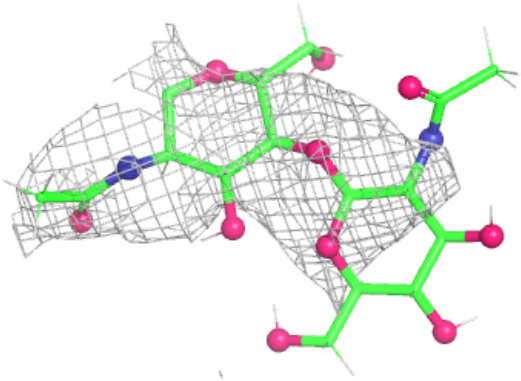


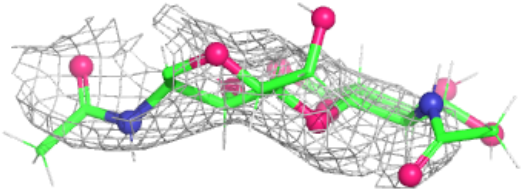


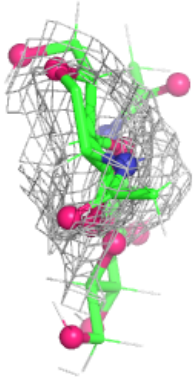


Electron density around Chain N:

$2mF_o$-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, 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
11	NAG	D	3099	14/15	0.47	0.13	130,164,195,198	0
11	NAG	B	3099	14/15	0.76	0.12	114,153,183,188	0
8	SO4	L	1215	5/5	0.82	0.10	134,136,137,142	0
8	SO4	C	1454	5/5	0.83	0.18	137,139,143,148	0
10	MN	D	2002	1/1	0.86	0.20	205,205,205,205	0
8	SO4	A	1456	5/5	0.91	0.14	75,98,98,117	0
8	SO4	A	1457	5/5	0.93	0.22	97,98,113,136	0
8	SO4	A	1458	5/5	0.94	0.14	135,143,150,167	0
10	MN	D	2003	1/1	0.98	0.04	104,104,104,104	0
10	MN	D	2001	1/1	0.98	0.04	101,101,101,101	0
9	CA	C	2004	1/1	0.98	0.04	111,111,111,111	0
12	CL	C	1455	1/1	0.98	0.10	72,72,72,72	0
9	CA	C	2005	1/1	0.99	0.03	90,90,90,90	0
9	CA	C	2006	1/1	0.99	0.03	69,69,69,69	0
9	CA	C	2007	1/1	0.99	0.03	65,65,65,65	0
10	MN	B	2002	1/1	0.99	0.03	65,65,65,65	0
9	CA	A	2006	1/1	0.99	0.02	38,38,38,38	0
9	CA	A	2005	1/1	1.00	0.04	40,40,40,40	0
10	MN	B	2001	1/1	1.00	0.05	42,42,42,42	0
9	CA	A	2004	1/1	1.00	0.02	49,49,49,49	0
10	MN	B	2003	1/1	1.00	0.02	51,51,51,51	0
9	CA	A	2007	1/1	1.00	0.01	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.