Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:07 PM BST

PDB ID	:	5OAR
Title	:	Crystal structure of native beta-N-acetylhexosaminidase isolated from Aspergillus oryzae
Authors	:	Skerlova, J.; Rezacova, P.; Brynda, J.; Pachl, P.; Otwinowski, Z.; Vanek, O.
Deposited on	:	2017-06-23
Resolution	:	2.30 Å(reported)

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

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

The following versions of software and data (see references ①) were used in the production of this report:

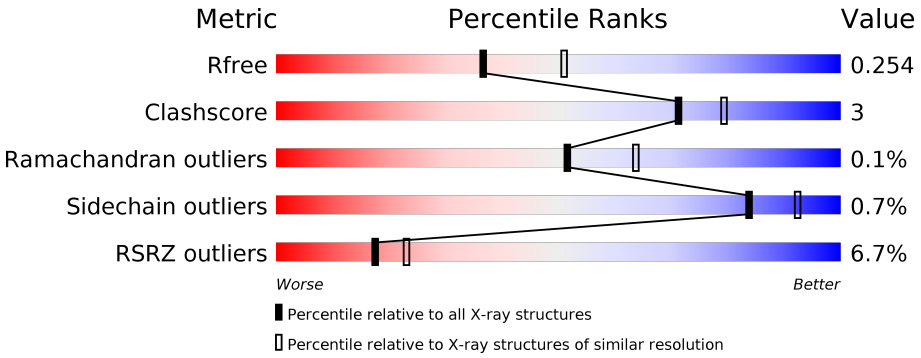
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	78	4% 86% 6% 8%
1	C	78	3% 87% 6% 6%
2	B	499	6% 93% 7%
2	D	499	8% 87% 12%
3	E	3	33% 67%
3	G	3	100%

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Mol	Chain	Length	Quality of chain
4	F	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	F	2	-	-	-	X
6	NAG	D	704	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9552 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.

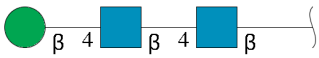
- Molecule 1 is a protein called Beta-hexosaminidase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	72	Total	C	N	O	0	0	0
			542	345	92	105			
1	C	73	Total	C	N	O	0	0	0
			549	350	93	106			

- Molecule 2 is a protein called Beta-hexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	497	Total	C	N	O	S	0	0	0
			4007	2542	680	769	16			
2	D	498	Total	C	N	O	S	0	0	0
			4017	2547	682	772	16			

- Molecule 3 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.

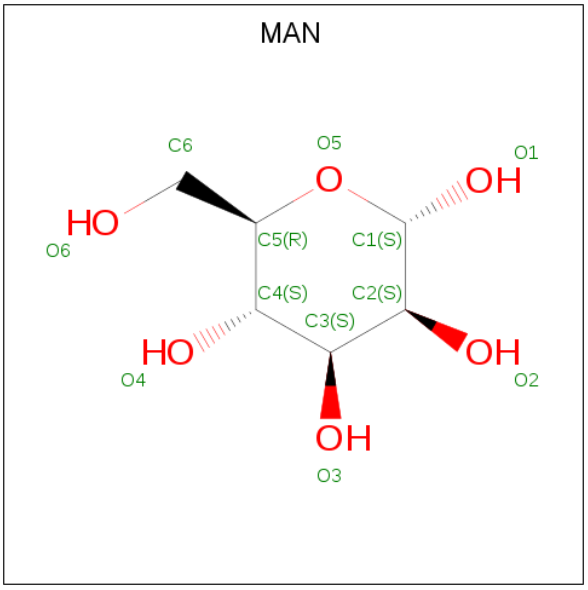


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

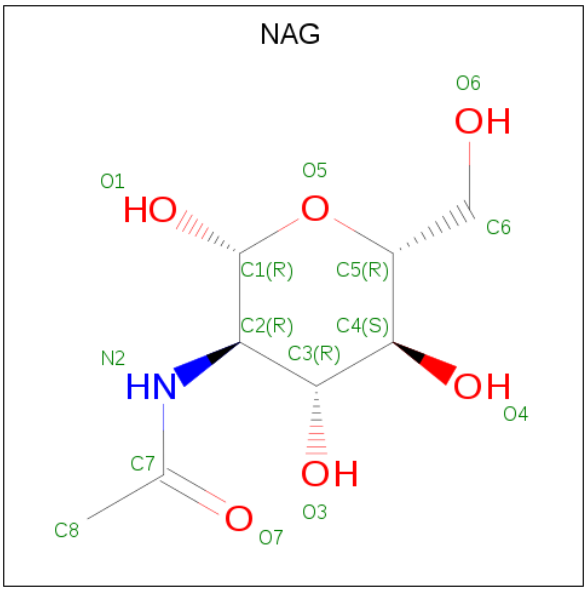
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



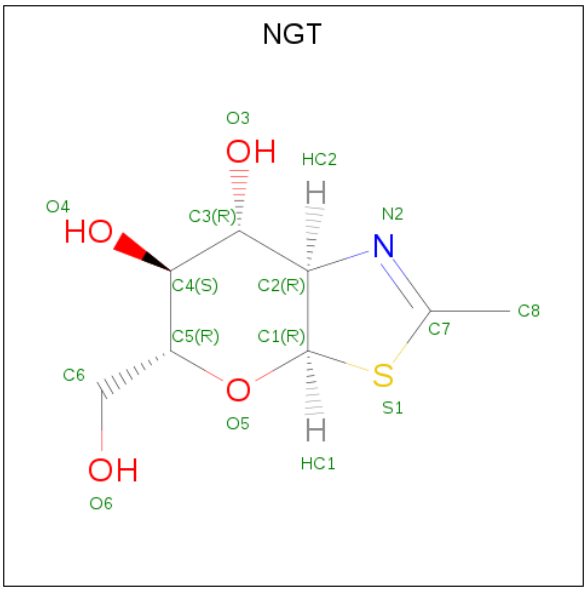
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	A	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRA HYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: $C_8H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

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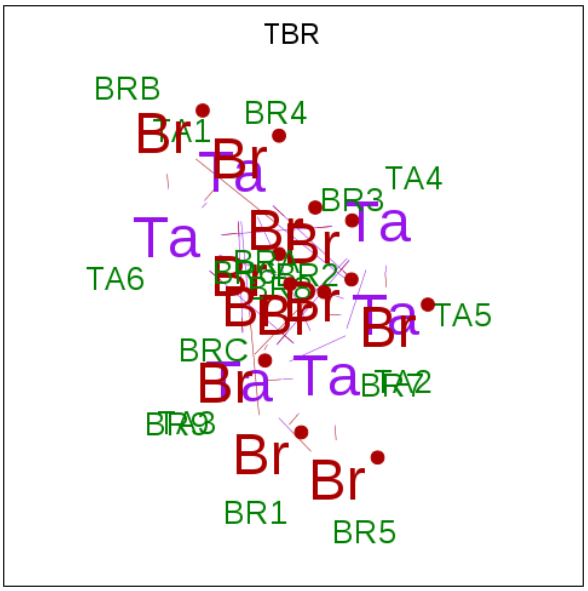
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	7	Total	Cl	0	0
			7	7		
8	D	4	Total	Cl	0	1
			5	5		

- Molecule 9 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	Br	Ta	0	0
			18	12	6		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	14	Total	O	0	0
			14	14		
10	B	96	Total	O	0	2
			98	98		

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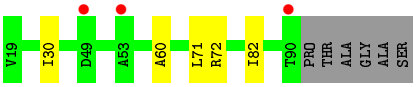
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	10	Total O 10 10	0	0
10	D	57	Total O 57 57	0	0

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: Beta-hexosaminidase

Chain A:

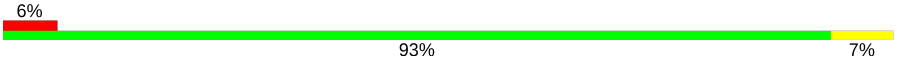


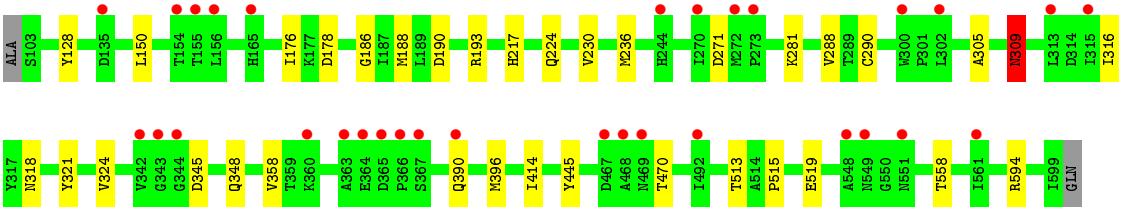
- Molecule 1: Beta-hexosaminidase

Chain C:

- Molecule 2: Beta-hexosaminidase

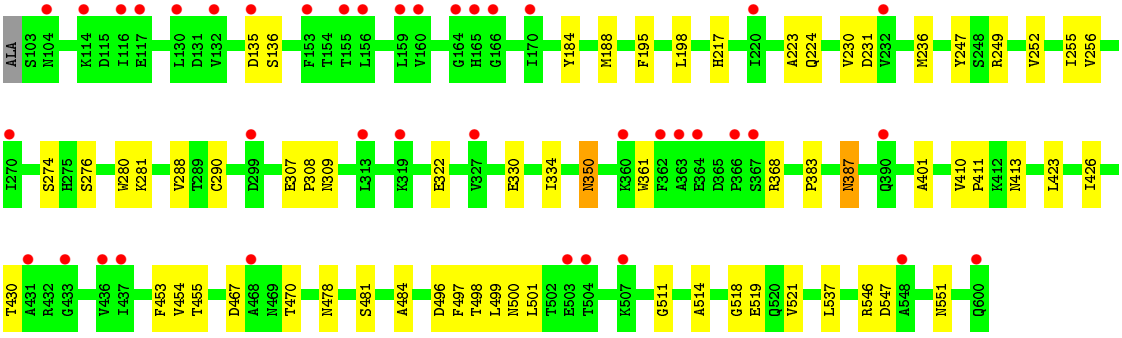
Chain B:





- Molecule 2: Beta-hexosaminidase

Chain D:

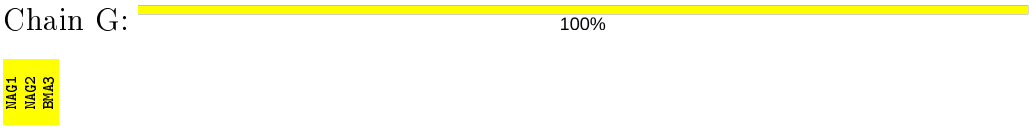


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

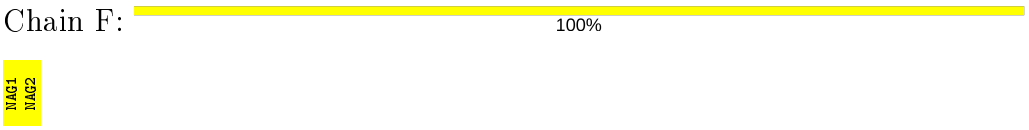
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.75Å 105.75Å 285.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.37 – 2.30 24.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	72.8 (23.37-2.30) 81.3 (24.93-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.241 0.210 , 0.254	Depositor DCC
R_{free} test set	3031 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9552	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, TBR, NGT, 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	0.64	0/559	0.68	0/770
1	C	0.58	0/567	0.68	0/782
2	B	0.61	0/4126	0.68	0/5645
2	D	0.55	0/4136	0.62	0/5657
All	All	0.59	0/9388	0.66	0/12854

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	542	0	518	4	0
1	C	549	0	525	3	0
2	B	4007	0	3745	21	0
2	D	4017	0	3754	40	0
3	E	39	0	34	0	0
3	G	39	0	34	0	0
4	F	28	0	25	0	0
5	A	33	0	30	0	0
5	C	33	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	0	0
6	D	14	0	13	0	0
7	B	14	0	13	0	0
7	D	14	0	13	1	0
8	B	7	0	0	0	0
8	D	5	0	0	1	0
9	D	18	0	0	1	0
10	A	14	0	0	0	0
10	B	98	0	0	0	0
10	C	10	0	0	0	0
10	D	57	0	0	3	0
All	All	9552	0	8747	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (63) 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:224:GLN:HA	2:B:309:ASN:OD1	1.87	0.74
2:D:454:VAL:HG13	10:D:841:HOH:O	1.94	0.68
1:C:38:LYS:NZ	2:D:136:SER:O	2.32	0.62
2:B:190:ASP:OD2	2:B:193:ARG:HG2	2.02	0.60
2:D:188:MET:HA	2:D:217:HIS:O	2.02	0.58
1:A:60:ALA:CB	2:B:150:LEU:HD22	2.34	0.58
2:B:316:ILE:HG12	2:B:358:VAL:HG22	1.86	0.56
1:A:30:ILE:HG13	2:B:176:ILE:HG12	1.88	0.55
2:D:308:PRO:O	2:D:309:ASN:HB3	2.06	0.55
2:B:230:VAL:HG21	2:B:236:MET:HE1	1.88	0.54
2:D:426:ILE:O	2:D:430:THR:HG22	2.08	0.54
2:D:223:ALA:C	2:D:309:ASN:OD1	2.47	0.53
2:B:281:LYS:HB3	2:B:288:VAL:HG21	1.90	0.53
2:B:396:MET:HE2	2:B:414:ILE:HD13	1.90	0.52
2:D:467:ASP:OD2	2:D:470:THR:OG1	2.26	0.52
2:D:514:ALA:HB2	2:D:537:LEU:HD22	1.90	0.52
2:B:390:GLN:H	2:B:390:GLN:CD	2.13	0.52
2:D:411:PRO:C	2:D:413:ASN:H	2.13	0.52
2:D:401:ALA:HB2	2:D:410:VAL:HG21	1.93	0.50
2:D:252:VAL:O	2:D:256:VAL:HG23	2.12	0.49
2:D:281:LYS:HB3	2:D:288:VAL:HG21	1.95	0.49
2:B:193:ARG:NH1	2:B:519:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:478:ASN:HB2	2:D:481:SER:O	2.13	0.48
2:B:128:TYR:CE1	2:B:178:ASP:HB3	2.49	0.47
2:B:186:GLY:O	2:B:513:THR:HA	2.15	0.47
2:D:195:PHE:CE1	2:D:247:TYR:CZ	3.03	0.47
2:D:547:ASP:OD1	2:D:551:ASN:N	2.48	0.47
2:D:230:VAL:HG21	2:D:236:MET:CE	2.44	0.46
2:B:188:MET:HG3	2:B:217:HIS:CG	2.51	0.46
2:D:198:LEU:HD22	2:D:255:ILE:HD11	1.97	0.46
2:D:499:LEU:HD23	2:D:500:ASN:N	2.30	0.46
2:D:322:GLU:HB2	9:D:705:TBR:BRA	2.71	0.46
2:D:361:TRP:CH2	2:D:368:ARG:HD3	2.52	0.45
2:D:184:TYR:O	2:D:511:GLY:HA3	2.16	0.45
2:D:453:PHE:CE2	2:D:519:GLU:HG2	2.51	0.45
2:D:276:SER:HB3	2:D:280:TRP:CD1	2.52	0.45
2:D:307:GLU:OE2	7:D:706:NGT:HC4	2.17	0.45
2:D:518:GLY:HA2	2:D:521:VAL:HB	1.99	0.45
2:D:383:PRO:O	2:D:387:ASN:HB2	2.16	0.45
2:D:135:ASP:N	2:D:135:ASP:OD1	2.46	0.44
2:B:321:TYR:HA	2:B:324:VAL:HG22	1.98	0.44
1:C:71:LEU:O	1:C:72:ARG:C	2.56	0.44
2:D:274:SER:N	10:D:805:HOH:O	2.49	0.44
2:D:276:SER:HA	10:D:831:HOH:O	2.18	0.44
2:B:305:ALA:HA	2:B:348:GLN:HG3	1.99	0.44
2:B:445:TYR:CE1	2:B:515:PRO:HG2	2.53	0.43
1:A:71:LEU:O	1:A:72:ARG:C	2.56	0.43
2:D:423:LEU:HD21	2:D:497:PHE:HA	2.00	0.43
2:D:231:ASP:N	2:D:330:GLU:OE2	2.39	0.43
2:D:481:SER:HB3	2:D:484:ALA:HB2	2.00	0.42
2:D:230:VAL:HG21	2:D:236:MET:HE3	1.99	0.42
2:D:498:THR:HA	2:D:501:LEU:HD12	2.01	0.42
2:D:350:ASN:N	2:D:350:ASN:OD1	2.52	0.42
2:D:368:ARG:NH1	8:D:709[A]:CL:CL	2.90	0.42
1:A:82:ILE:HD13	2:B:594:ARG:HG2	2.01	0.41
2:D:249:ARG:CZ	2:D:334:ILE:HG22	2.50	0.41
2:B:230:VAL:HB	2:B:236:MET:HE3	2.03	0.41
2:B:271:ASP:OD2	2:B:345:ASP:OD1	2.39	0.41
1:C:74:VAL:O	1:C:75:PRO:C	2.59	0.41
2:D:224:GLN:N	2:D:309:ASN:OD1	2.54	0.41
2:B:558:THR:HG23	2:D:455:THR:HG21	2.03	0.40
2:D:496:ASP:CG	2:D:546:ARG:HH21	2.25	0.40
2:B:188:MET:HA	2:B:217:HIS:O	2.22	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	70/78 (90%)	67 (96%)	3 (4%)	0	100 100
1	C	71/78 (91%)	68 (96%)	3 (4%)	0	100 100
2	B	495/499 (99%)	478 (97%)	16 (3%)	1 (0%)	47 58
2	D	496/499 (99%)	472 (95%)	24 (5%)	0	100 100
All	All	1132/1154 (98%)	1085 (96%)	46 (4%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	309	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	57/60 (95%)	57 (100%)	0	100 100
1	C	58/60 (97%)	58 (100%)	0	100 100
2	B	436/437 (100%)	432 (99%)	4 (1%)	78 89
2	D	437/437 (100%)	434 (99%)	3 (1%)	84 92
All	All	988/994 (99%)	981 (99%)	7 (1%)	84 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	290	CYS
2	B	309	ASN
2	B	318	ASN
2	B	470	THR
2	D	290	CYS
2	D	350	ASN
2	D	387	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	318	ASN
2	D	387	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	C	103	1	11,11,12	0.85	0	15,15,17	1.22	2 (13%)
6	NAG	D	704	2	14,14,15	0.52	0	17,19,21	1.26	2 (11%)
5	MAN	A	103	1	11,11,12	0.68	0	15,15,17	1.39	2 (13%)
6	NAG	B	706	2	14,14,15	0.60	0	17,19,21	1.42	2 (11%)
3	NAG	G	2	3	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	MAN	A	101	1	11,11,12	0.85	0	15,15,17	1.34	2 (13%)
5	MAN	C	101	1	11,11,12	0.80	0	15,15,17	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E	1	3,2	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
3	NAG	G	1	3,2	14,14,15	0.43	0	17,19,21	1.83	6 (35%)
5	MAN	C	102	1	11,11,12	0.57	0	15,15,17	1.13	1 (6%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	1.79	3 (17%)
5	MAN	A	102	1	11,11,12	0.70	0	15,15,17	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	C	103	1	-	0/2/19/22	0/1/1/1
6	NAG	D	704	2	-	1/6/23/26	0/1/1/1
5	MAN	A	103	1	-	2/2/19/22	0/1/1/1
6	NAG	B	706	2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
5	MAN	A	101	1	-	0/2/19/22	0/1/1/1
5	MAN	C	101	1	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,2	-	4/6/23/26	0/1/1/1
5	MAN	C	102	1	-	0/2/19/22	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
5	MAN	A	102	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C1-O5-C5	5.02	118.99	112.19
5	A	103	MAN	C1-O5-C5	3.89	117.46	112.19
3	E	1	NAG	C1-O5-C5	3.79	117.33	112.19
3	G	1	NAG	C8-C7-N2	3.68	122.32	116.10
5	C	102	MAN	C1-O5-C5	3.45	116.87	112.19
3	G	1	NAG	C1-O5-C5	3.39	116.78	112.19
5	A	101	MAN	C1-C2-C3	3.35	113.78	109.67
5	C	103	MAN	C1-C2-C3	3.32	113.75	109.67
6	D	704	NAG	C1-O5-C5	3.27	116.62	112.19
3	G	1	NAG	O5-C1-C2	-2.85	106.79	111.29
5	A	103	MAN	C1-C2-C3	2.79	113.09	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	706	NAG	C4-C3-C2	-2.77	106.97	111.02
6	B	706	NAG	C1-O5-C5	2.69	115.84	112.19
3	E	1	NAG	O4-C4-C3	-2.57	104.40	110.35
3	E	2	NAG	C8-C7-N2	2.57	120.44	116.10
3	G	1	NAG	O5-C5-C6	2.38	110.93	107.20
5	A	101	MAN	O5-C5-C6	2.30	110.82	107.20
3	G	1	NAG	C1-C2-N2	2.22	114.27	110.49
3	G	1	NAG	O7-C7-C8	-2.10	118.16	122.06
6	D	704	NAG	O5-C1-C2	-2.08	108.00	111.29
3	G	2	NAG	O5-C1-C2	-2.07	108.02	111.29
3	E	2	NAG	O5-C5-C4	2.05	115.82	110.83
5	C	103	MAN	O5-C5-C6	2.03	110.39	107.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	706	NAG	C3-C2-N2-C7
5	A	103	MAN	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
5	A	103	MAN	C4-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
6	B	706	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
6	D	704	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	1.79	3 (17%)
3	BMA	E	3	3	11,11,12	0.57	0	15,15,17	0.92	0
4	NAG	F	1	2,4	14,14,15	0.52	0	17,19,21	1.60	4 (23%)
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	2.17	6 (35%)
3	NAG	G	1	3,2	14,14,15	0.43	0	17,19,21	1.83	6 (35%)
3	NAG	G	2	3	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
3	BMA	G	3	3	11,11,12	0.61	0	15,15,17	1.32	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2	NAG	C1-O5-C5	5.05	119.04	112.19
3	E	2	NAG	C1-O5-C5	5.02	118.99	112.19
3	E	1	NAG	C1-O5-C5	3.79	117.33	112.19
3	G	1	NAG	C8-C7-N2	3.68	122.32	116.10
4	F	1	NAG	C8-C7-N2	3.43	121.90	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	O5-C1-C2	-3.40	105.92	111.29
3	G	1	NAG	C1-O5-C5	3.39	116.78	112.19
4	F	2	NAG	C8-C7-N2	3.29	121.67	116.10
4	F	2	NAG	C4-C3-C2	-3.25	106.26	111.02
4	F	1	NAG	C3-C4-C5	2.91	115.42	110.24
4	F	2	NAG	O7-C7-C8	-2.90	116.67	122.06
3	G	1	NAG	O5-C1-C2	-2.85	106.79	111.29
3	G	3	BMA	C1-C2-C3	2.78	113.08	109.67
3	G	3	BMA	C3-C4-C5	2.76	115.17	110.24
3	E	1	NAG	O4-C4-C3	-2.57	104.40	110.35
3	E	2	NAG	C8-C7-N2	2.57	120.44	116.10
4	F	2	NAG	O5-C5-C4	2.49	116.89	110.83
4	F	1	NAG	O7-C7-C8	-2.46	117.49	122.06
3	G	1	NAG	O5-C5-C6	2.38	110.93	107.20
3	G	1	NAG	C1-C2-N2	2.22	114.27	110.49
4	F	2	NAG	C1-C2-N2	2.13	114.13	110.49
3	G	1	NAG	O7-C7-C8	-2.10	118.16	122.06
3	G	2	NAG	O5-C1-C2	-2.07	108.02	111.29
3	E	2	NAG	O5-C5-C4	2.05	115.82	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

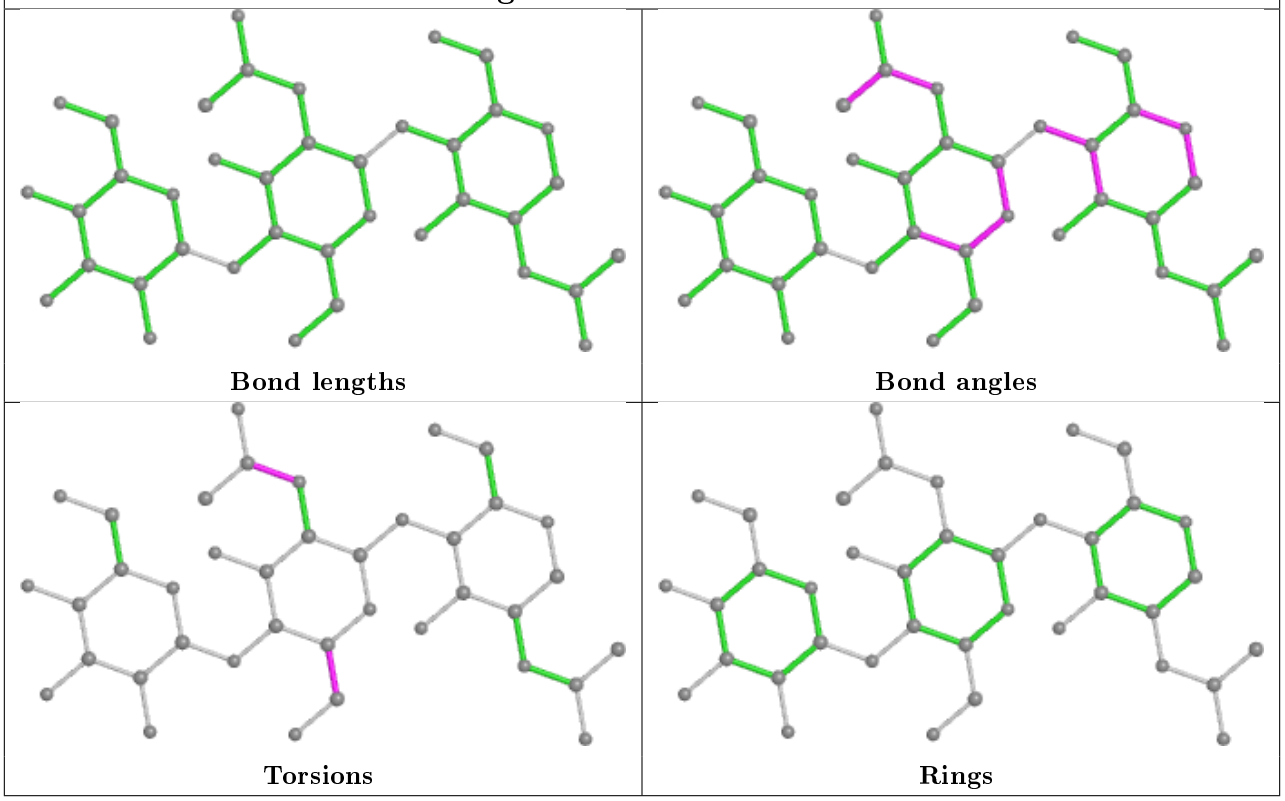
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

There are no ring outliers.

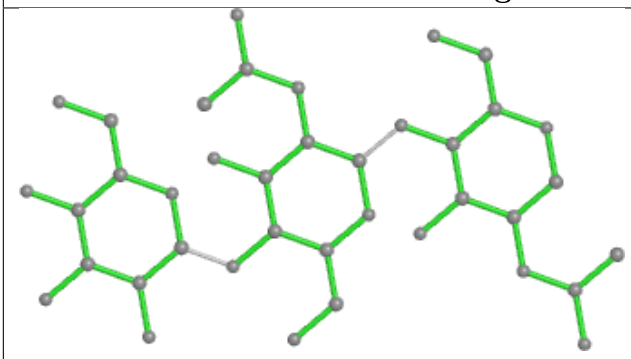
No monomer is involved in short contacts.

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

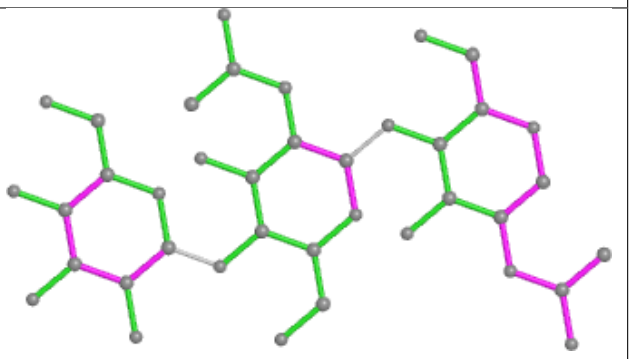
Oligosaccharide Chain E



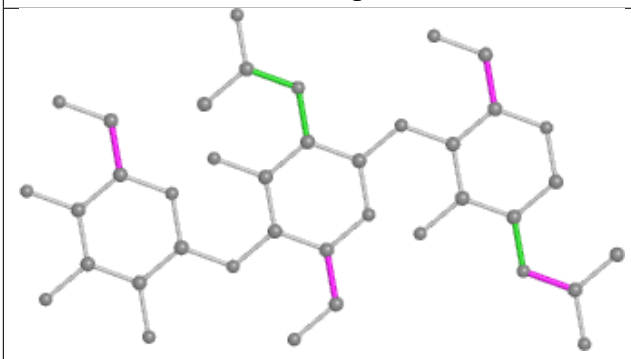
Oligosaccharide Chain G



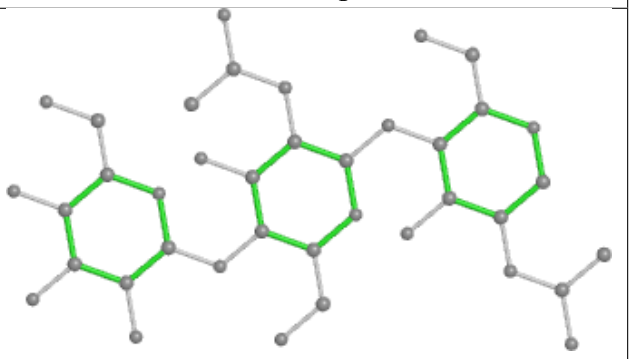
Bond lengths



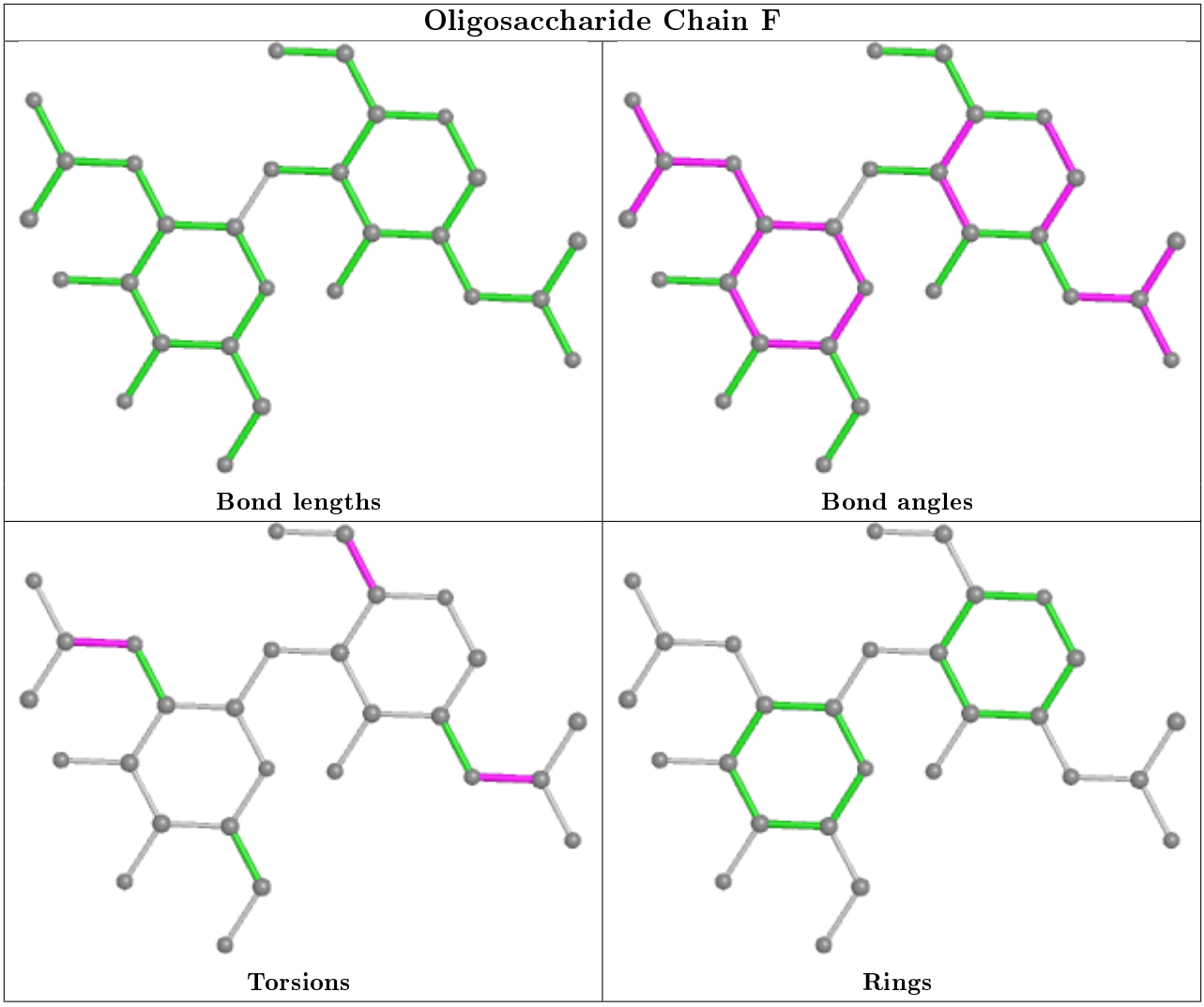
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
5	MAN	C	103	1	11,11,12	0.85	0	15,15,17	1.22	2 (13%)
5	MAN	A	103	1	11,11,12	0.68	0	15,15,17	1.39	2 (13%)
6	NAG	B	706	2	14,14,15	0.60	0	17,19,21	1.42	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	A	101	1	11,11,12	0.85	0	15,15,17	1.34	2 (13%)
7	NGT	D	706	-	13,15,15	3.78	1 (7%)	12,22,22	1.19	2 (16%)
7	NGT	B	707	-	13,15,15	3.53	1 (7%)	12,22,22	1.32	2 (16%)
6	NAG	D	704	2	14,14,15	0.52	0	17,19,21	1.26	2 (11%)
5	MAN	C	101	1	11,11,12	0.80	0	15,15,17	0.99	0
9	TBR	D	705	-	0,36,36	0.00	-	-		
5	MAN	C	102	1	11,11,12	0.57	0	15,15,17	1.13	1 (6%)
5	MAN	A	102	1	11,11,12	0.70	0	15,15,17	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	C	103	1	-	0/2/19/22	0/1/1/1
5	MAN	A	103	1	-	2/2/19/22	0/1/1/1
6	NAG	B	706	2	-	2/6/23/26	0/1/1/1
5	MAN	A	101	1	-	0/2/19/22	0/1/1/1
7	NGT	D	706	-	-	2/2/30/30	0/2/2/2
7	NGT	B	707	-	-	0/2/30/30	0/2/2/2
6	NAG	D	704	2	-	1/6/23/26	0/1/1/1
5	MAN	C	101	1	-	0/2/19/22	0/1/1/1
5	MAN	C	102	1	-	0/2/19/22	0/1/1/1
5	MAN	A	102	1	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	706	NGT	C7-S1	-13.45	1.65	1.77
7	B	707	NGT	C7-S1	-12.58	1.66	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	103	MAN	C1-O5-C5	3.89	117.46	112.19
5	C	102	MAN	C1-O5-C5	3.45	116.87	112.19
5	A	101	MAN	C1-C2-C3	3.35	113.78	109.67
5	C	103	MAN	C1-C2-C3	3.32	113.75	109.67
6	D	704	NAG	C1-O5-C5	3.27	116.62	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	707	NGT	C8-C7-S1	2.93	123.37	118.96
5	A	103	MAN	C1-C2-C3	2.79	113.09	109.67
6	B	706	NAG	C4-C3-C2	-2.77	106.97	111.02
7	D	706	NGT	C8-C7-S1	2.70	123.03	118.96
6	B	706	NAG	C1-O5-C5	2.69	115.84	112.19
7	D	706	NGT	C1-O5-C5	2.38	116.98	112.58
7	B	707	NGT	C1-O5-C5	2.35	116.91	112.58
5	A	101	MAN	O5-C5-C6	2.30	110.82	107.20
6	D	704	NAG	O5-C1-C2	-2.08	108.00	111.29
5	C	103	MAN	O5-C5-C6	2.03	110.39	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	706	NAG	C3-C2-N2-C7
5	A	103	MAN	O5-C5-C6-O6
5	A	103	MAN	C4-C5-C6-O6
6	B	706	NAG	O5-C5-C6-O6
7	D	706	NGT	C4-C5-C6-O6
7	D	706	NGT	O5-C5-C6-O6
6	D	704	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	706	NGT	1	0
9	D	705	TBR	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	72/78 (92%)	0.06	3 (4%)	36	43	34, 45, 75, 87	0
1	C	73/78 (93%)	0.26	2 (2%)	54	62	43, 60, 84, 93	0
2	B	497/499 (99%)	0.18	31 (6%)	20	26	29, 44, 67, 90	0
2	D	498/499 (99%)	0.54	40 (8%)	12	16	36, 61, 90, 117	0
All	All	1140/1154 (98%)	0.34	76 (6%)	17	23	29, 52, 84, 117	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	156	LEU	5.2
2	B	300	TRP	5.1
2	D	360	LYS	5.0
2	D	363	ALA	4.9
2	D	600	GLN	4.8
2	B	548	ALA	4.1
2	D	135	ASP	4.0
2	B	468	ALA	3.7
2	D	366	PRO	3.7
2	D	504	THR	3.6
2	D	166	GLY	3.5
2	B	366	PRO	3.5
2	D	165	HIS	3.5
2	D	390	GLN	3.5
2	D	367	SER	3.3
2	B	469	ASN	3.2
2	B	165	HIS	3.2
2	D	114	LYS	3.2
2	B	342	VAL	3.1
2	D	159	LEU	3.1
1	A	90	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	433	GLY	3.0
2	D	153	PHE	3.0
2	B	363	ALA	2.9
2	B	367	SER	2.9
2	B	272	MET	2.9
2	D	319	LYS	2.8
2	D	299	ASP	2.8
2	B	273	PRO	2.8
2	B	492	ILE	2.8
2	D	437	ILE	2.8
2	D	164	GLY	2.7
2	B	549	ASN	2.7
2	B	313	LEU	2.7
2	D	507	LYS	2.7
1	A	49	ASP	2.5
2	B	364	GLU	2.5
2	B	390	GLN	2.5
2	D	436	VAL	2.5
2	D	220	ILE	2.5
2	B	365	ASP	2.5
2	D	132	VAL	2.4
2	B	156	LEU	2.4
2	D	313	LEU	2.4
1	C	53	ALA	2.4
2	D	155	THR	2.4
2	D	170	ILE	2.3
2	D	503	GLU	2.3
2	B	344	GLY	2.3
2	B	135	ASP	2.3
2	D	116	ILE	2.3
2	D	160	VAL	2.2
2	D	232	VAL	2.2
2	D	270	ILE	2.2
2	D	130	LEU	2.2
2	D	362	PHE	2.2
2	B	561	ILE	2.2
2	D	117	GLU	2.2
2	D	104	ASN	2.2
2	B	155	THR	2.2
2	B	315	ILE	2.2
2	D	327	VAL	2.2
2	B	154	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	431	ALA	2.1
2	D	468	ALA	2.1
2	B	467	ASP	2.1
2	B	360	LYS	2.1
2	D	548	ALA	2.1
2	B	270	ILE	2.1
2	B	551	ASN	2.1
2	B	302	LEU	2.1
1	A	53	ALA	2.1
2	D	364	GLU	2.1
2	B	244	HIS	2.0
1	C	34	SER	2.0
2	B	343	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	D	704	14/15	0.71	0.41	71,97,104,109	0
6	NAG	B	706	14/15	0.75	0.32	69,77,86,89	0
3	NAG	G	2	14/15	0.76	0.31	79,98,106,106	0
3	NAG	E	2	14/15	0.79	0.30	67,85,94,99	0
5	MAN	A	103	11/12	0.80	0.33	76,84,86,88	0
3	NAG	G	1	14/15	0.84	0.22	68,75,90,98	0
5	MAN	C	103	11/12	0.88	0.40	56,69,75,77	0
5	MAN	A	101	11/12	0.88	0.19	50,55,61,61	0
5	MAN	C	101	11/12	0.92	0.17	46,50,62,71	0
5	MAN	A	102	11/12	0.92	0.25	55,58,60,60	0
3	NAG	E	1	14/15	0.94	0.15	56,66,69,76	0
5	MAN	C	102	11/12	0.94	0.19	46,50,56,60	0

6.3 Carbohydrates (i)

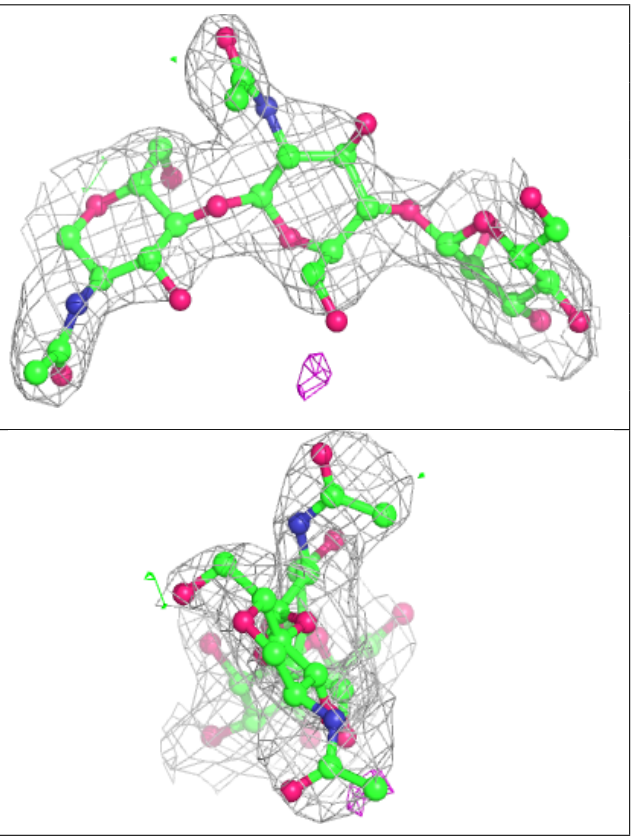
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

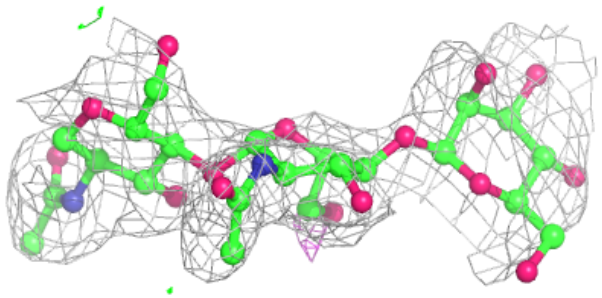
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	E	3	11/12	0.70	0.27	88,97,101,102	0
3	BMA	G	3	11/12	0.70	0.35	96,110,118,119	0
4	NAG	F	2	14/15	0.74	0.52	87,108,114,117	0
3	NAG	G	2	14/15	0.76	0.31	79,98,106,106	0
3	NAG	E	2	14/15	0.79	0.30	67,85,94,99	0
3	NAG	G	1	14/15	0.84	0.22	68,75,90,98	0
4	NAG	F	1	14/15	0.87	0.28	67,75,86,99	0
3	NAG	E	1	14/15	0.94	0.15	56,66,69,76	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:

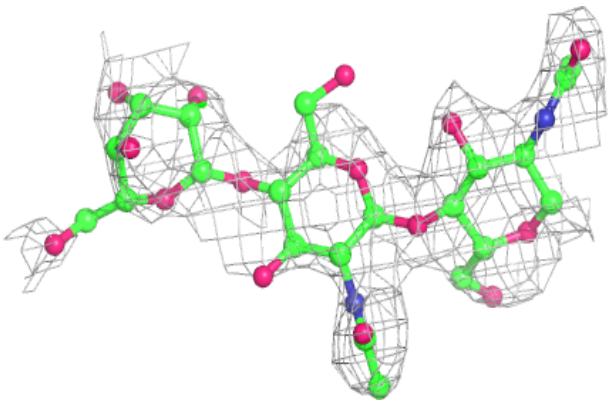
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

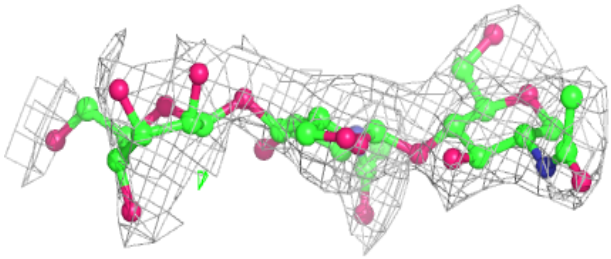


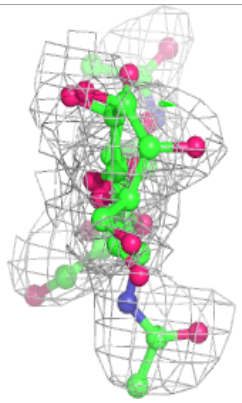


Electron density around Chain G:

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

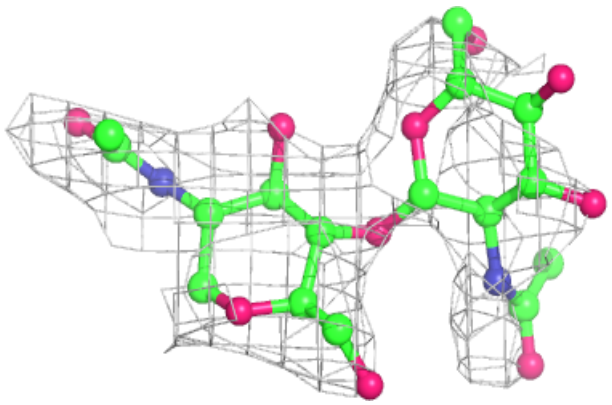


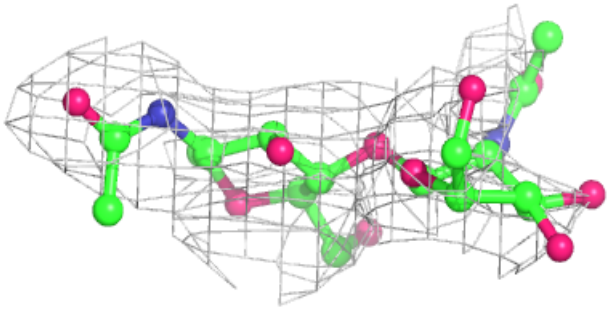


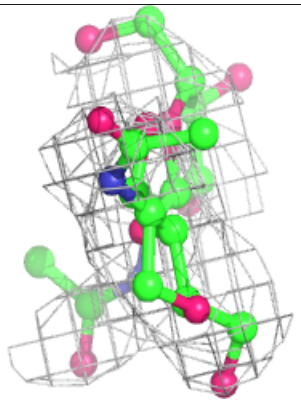


Electron density around Chain F:

$2mF_o$-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
6	NAG	D	704	14/15	0.71	0.41	71,97,104,109	0
6	NAG	B	706	14/15	0.75	0.32	69,77,86,89	0
5	MAN	A	103	11/12	0.80	0.33	76,84,86,88	0
8	CL	D	709[A]	1/1	0.81	0.11	52,52,52,52	1
8	CL	D	709[B]	1/1	0.81	0.11	54,54,54,54	1
7	NGT	D	706	14/14	0.84	0.26	62,74,78,78	14
7	NGT	B	707	14/14	0.86	0.22	55,61,66,68	14
5	MAN	A	101	11/12	0.88	0.19	50,55,61,61	0
5	MAN	C	103	11/12	0.88	0.40	56,69,75,77	0
8	CL	B	712	1/1	0.89	0.09	62,62,62,62	0
8	CL	B	708	1/1	0.91	0.30	69,69,69,69	0
5	MAN	A	102	11/12	0.92	0.25	55,58,60,60	0
8	CL	B	710	1/1	0.92	0.07	59,59,59,59	0
5	MAN	C	101	11/12	0.92	0.17	46,50,62,71	0
8	CL	B	713	1/1	0.93	0.06	76,76,76,76	0
8	CL	D	710	1/1	0.93	0.07	50,50,50,50	0
8	CL	D	708	1/1	0.93	0.14	52,52,52,52	0
9	TBR	D	705	18/18	0.94	0.16	64,74,79,80	18
8	CL	B	714	1/1	0.94	0.09	54,54,54,54	0
8	CL	D	707	1/1	0.94	0.16	37,37,37,37	1
5	MAN	C	102	11/12	0.94	0.19	46,50,56,60	0
8	CL	B	711	1/1	0.95	0.15	47,47,47,47	0
8	CL	B	709	1/1	0.97	0.04	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.