Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:51 AM EDT

PDB ID	:	1QK2
Title	:	WILD TYPE CEL6A WITH A NON-HYDROLYSABLE CELLOTETRAOSE
Authors	:	Zou, J.-Y.; Jones, T.A.
Deposited on	:	1999-07-09
Resolution	:	2.00 Å(reported)

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

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

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

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

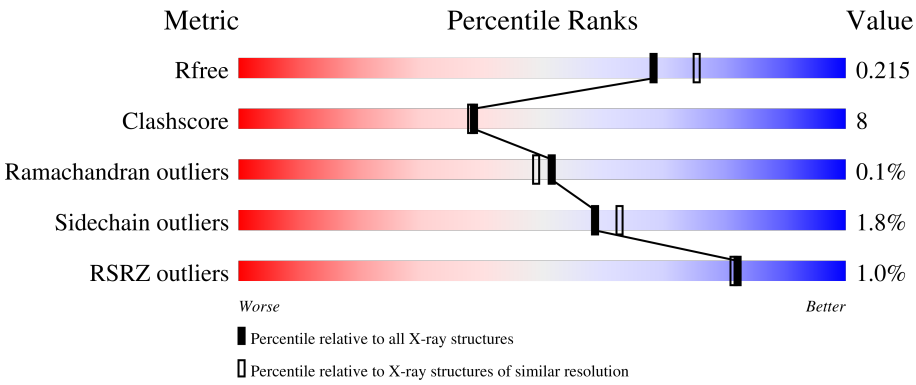
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	363	% 85% 14% .
1	B	363	% 85% 14% .
2	C	4	25% 50% 25%
2	D	4	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	3	X	-	-	-
2	GLC	C	4	X	-	-	-
2	GLC	D	3	X	-	-	-
2	GLC	D	4	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6341 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.

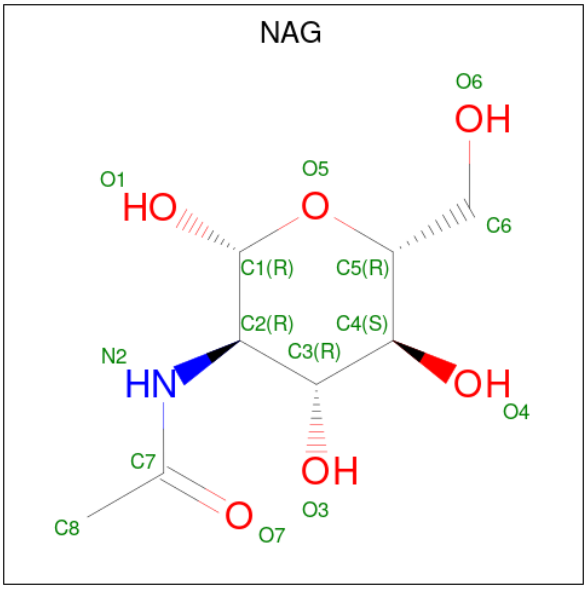
- Molecule 1 is a protein called CELLOBIOHYDROLASE CEL6A (FORMERLY CALLED CBH II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2747	1743	463	531	10	0	0	0
1	B	363	2747	1743	463	531	10	0	0	0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-methyl beta-D-glucopyranoside.

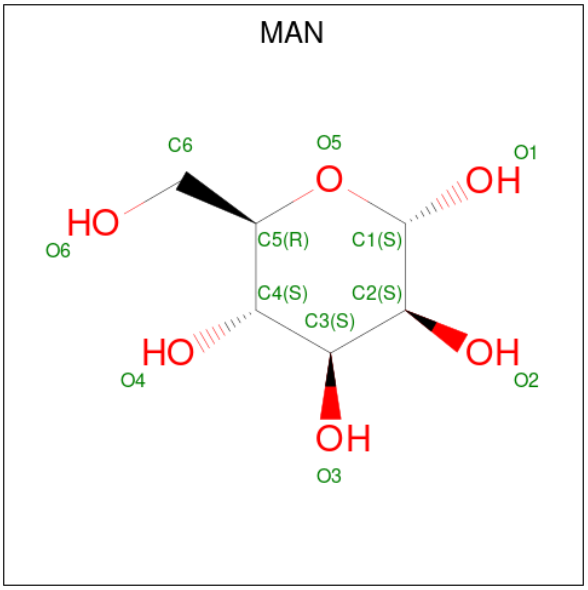
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	C	4	46	25	20	1	0	0	0
2	D	4	46	25	20	1	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

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

- Molecule 5 is water.

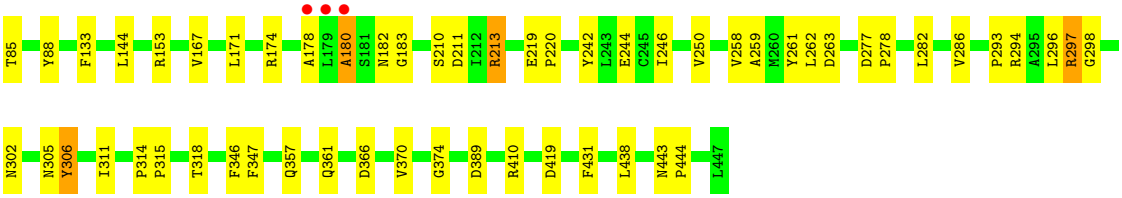
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	278	278	278	0	0
			Total	O		
5	B	267	267	267	0	0

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.

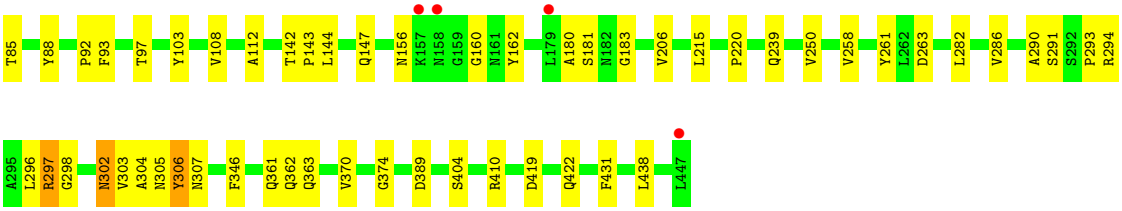
• Molecule 1: CELLOBIOHYDROLASE CEL6A (FORMERLY CALLED CBH II)

Chain A:



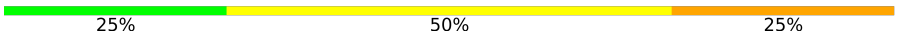
• Molecule 1: CELLOBIOHYDROLASE CEL6A (FORMERLY CALLED CBH II)

Chain B:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-methyl beta-D-glucopyranoside

Chain C:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-methyl beta-D-glucopyranoside

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.83Å 74.70Å 91.84Å 90.00° 104.12° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 40.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-2.00) 95.1 (40.00-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.00Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.189 , 0.222 0.182 , 0.215	Depositor DCC
R_{free} test set	1283 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6341	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0612e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, GLC, NAG, SGC, MGL

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	0.32	0/2823	0.57	0/3870
1	B	0.31	0/2823	0.58	0/3870
All	All	0.32	0/5646	0.58	0/7740

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 (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	2747	0	2606	38	0
1	B	2747	0	2606	45	0
2	C	46	0	41	1	0
2	D	46	0	41	1	0
3	A	28	0	26	1	0
3	B	28	0	26	0	0
4	A	77	0	70	0	0
4	B	77	0	70	2	0
5	A	278	0	0	1	0
5	B	267	0	0	3	0
All	All	6341	0	5486	85	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 8.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:HD3	1:B:389:ASP:OD2	1.67	0.95
1:B:302:ASN:OD1	1:B:307:ASN:HB2	1.81	0.81
1:B:305:ASN:ND2	1:B:306:TYR:H	1.82	0.77
1:B:305:ASN:HD22	1:B:306:TYR:H	1.30	0.76
1:B:302:ASN:ND2	1:B:305:ASN:HB3	2.01	0.76
1:A:297:ARG:HD3	1:A:389:ASP:OD2	1.89	0.72
1:A:305:ASN:ND2	1:A:306:TYR:H	1.88	0.72
1:A:180:ALA:HB1	1:A:410:ARG:HA	1.72	0.71
5:B:2096:HOH:O	2:D:1:MGL:H73	1.92	0.68
1:B:143:PRO:O	1:B:147:GLN:HG3	1.94	0.67
1:A:305:ASN:HD22	1:A:306:TYR:H	1.42	0.66
1:B:180:ALA:HB1	1:B:410:ARG:HA	1.79	0.65
1:B:85:THR:HG21	4:B:503:MAN:H3	1.79	0.63
1:A:315:PRO:HG2	1:A:318:THR:HG23	1.80	0.62
1:B:261:TYR:CE2	1:B:297:ARG:HG2	2.36	0.60
1:A:183:GLY:HA3	5:A:2076:HOH:O	2.03	0.59
1:B:302:ASN:HD21	1:B:307:ASN:H	1.51	0.57
1:A:298:GLY:HA3	1:A:346:PHE:O	2.04	0.57
1:A:242:TYR:O	1:A:246:ILE:HG12	2.04	0.57
1:B:250:VAL:HG12	1:B:293:PRO:HG2	1.85	0.57
1:B:404:SER:CB	1:B:422:GLN:HG2	2.37	0.55
1:A:250:VAL:HG21	1:A:296:LEU:HD22	1.89	0.55
1:A:88:TYR:HB3	1:A:213:ARG:NH1	2.23	0.54
1:A:374:GLY:HA2	1:A:438:LEU:HA	1.88	0.54
1:B:294:ARG:HH11	1:B:294:ARG:HG2	1.73	0.54
1:B:362:GLN:HG3	1:B:419:ASP:HB3	1.89	0.53
1:B:261:TYR:CZ	1:B:297:ARG:HG2	2.44	0.52
1:B:294:ARG:HG2	1:B:294:ARG:NH1	2.25	0.52
1:A:294:ARG:C	1:A:294:ARG:HD3	2.31	0.51
1:B:361:GLN:HG3	1:B:370:VAL:HG11	1.92	0.51
1:B:93:PHE:CE2	1:B:215:LEU:HD13	2.45	0.51
1:A:182:ASN:OD1	1:A:410:ARG:HG3	2.10	0.51
1:A:261:TYR:CE2	1:A:297:ARG:HG2	2.46	0.50
1:B:250:VAL:HG11	1:B:296:LEU:HD22	1.94	0.49
1:A:315:PRO:HG2	1:A:318:THR:CG2	2.42	0.49
1:B:181:SER:O	1:B:410:ARG:HD2	2.12	0.49
1:A:294:ARG:HD3	1:A:294:ARG:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLN:NE2	5:B:2117:HOH:O	2.47	0.48
1:A:153:ARG:HD3	1:A:211:ASP:OD2	2.14	0.48
1:B:250:VAL:CG1	1:B:293:PRO:HG2	2.44	0.47
1:B:298:GLY:HA3	1:B:346:PHE:O	2.13	0.47
1:B:220:PRO:HA	1:B:263:ASP:CG	2.35	0.47
1:A:220:PRO:HA	1:A:263:ASP:CG	2.35	0.47
1:A:277:ASP:HB3	1:A:278:PRO:HD3	1.97	0.46
1:B:374:GLY:HA2	1:B:438:LEU:HA	1.96	0.46
1:A:297:ARG:O	1:A:297:ARG:HG3	2.15	0.46
2:C:2:SGC:S4	2:C:3:GLC:C6	3.04	0.45
1:A:171:LEU:HG	1:A:219:GLU:CD	2.36	0.45
1:B:183:GLY:HA3	5:B:2063:HOH:O	2.16	0.45
1:A:244:GLU:HA	3:A:501:NAG:H4	1.99	0.44
1:B:297:ARG:O	1:B:297:ARG:HG3	2.17	0.44
1:B:303:VAL:O	1:B:304:ALA:HB3	2.18	0.44
1:B:97:THR:O	1:B:162:TYR:HA	2.18	0.44
1:A:85:THR:HA	1:A:210:SER:O	2.17	0.44
1:A:258:VAL:HG12	1:A:259:ALA:N	2.32	0.44
1:B:290:ALA:O	1:B:291:SER:HB2	2.17	0.43
1:B:142:THR:N	1:B:143:PRO:CD	2.81	0.43
1:A:178:ALA:C	1:A:180:ALA:H	2.21	0.43
1:A:282:LEU:O	1:A:286:VAL:HG23	2.19	0.43
1:B:108:VAL:O	1:B:112:ALA:HB3	2.19	0.43
1:B:156:ASN:HA	1:B:160:GLY:CA	2.49	0.42
1:B:306:TYR:CD1	1:B:306:TYR:N	2.86	0.42
1:A:443:ASN:HA	1:A:444:PRO:C	2.38	0.42
1:B:88:TYR:O	1:B:294:ARG:NH2	2.53	0.42
1:A:302:ASN:OD1	1:A:305:ASN:HB3	2.19	0.42
1:B:294:ARG:HG2	1:B:294:ARG:O	2.19	0.42
1:A:311:ILE:HG21	1:A:357:GLN:HG3	2.02	0.42
1:B:92:PRO:CD	1:B:297:ARG:HD2	2.50	0.41
1:B:97:THR:HG21	4:B:504:MAN:H5	2.01	0.41
1:A:347:PHE:N	1:A:347:PHE:CD1	2.88	0.41
1:B:92:PRO:HD3	1:B:297:ARG:HD2	2.02	0.41
1:B:363:GLN:OE1	1:B:363:GLN:HA	2.21	0.41
1:B:103:TYR:CD1	1:B:144:LEU:HD21	2.56	0.41
1:A:366:ASP:OD2	1:A:419:ASP:OD2	2.39	0.40
1:B:220:PRO:HA	1:B:263:ASP:CB	2.51	0.40
1:A:180:ALA:HB1	1:A:410:ARG:CA	2.46	0.40
1:B:142:THR:OG1	1:B:143:PRO:HD3	2.22	0.40
1:A:133:PHE:HB3	1:A:167:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:HG11	1:B:258:VAL:CG2	2.52	0.40
1:B:282:LEU:O	1:B:286:VAL:HG23	2.21	0.40
1:A:171:LEU:O	1:A:174:ARG:HB2	2.21	0.40
1:A:258:VAL:CG1	1:A:259:ALA:N	2.84	0.40
1:A:314:PRO:HA	1:A:315:PRO:HD2	1.96	0.40
1:A:250:VAL:HG22	1:A:293:PRO:HG2	2.02	0.40
1:A:361:GLN:HG3	1:A:370:VAL:HG11	2.04	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	361/363 (99%)	346 (96%)	14 (4%)	1 (0%)	41	37
1	B	361/363 (99%)	347 (96%)	14 (4%)	0	100	100
All	All	722/726 (99%)	693 (96%)	28 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ALA

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	284/284 (100%)	278 (98%)	6 (2%)	53	57
1	B	284/284 (100%)	280 (99%)	4 (1%)	67	72
All	All	568/568 (100%)	558 (98%)	10 (2%)	59	63

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	213	ARG
1	A	262	LEU
1	A	297	ARG
1	A	306	TYR
1	A	431	PHE
1	B	297	ARG
1	B	302	ASN
1	B	306	TYR
1	B	431	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	237	ASN
1	A	281	GLN
1	A	305	ASN
1	A	319	GLN
1	A	382	ASN
1	B	147	GLN
1	B	158	ASN
1	B	239	GLN
1	B	305	ASN
1	B	307	ASN
1	B	422	GLN
1	B	441	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)

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	$\#\|Z\| > 2$
2	MGL	C	1	2	13,13,13	0.68	0	18,18,18	0.88	1 (5%)
2	SGC	C	2	2	10,11,12	0.43	0	12,15,17	0.75	0
2	GLC	C	3	2	11,11,12	0.54	0	15,15,17	1.18	2 (13%)
2	GLC	C	4	2	11,11,12	0.43	0	15,15,17	0.65	0
2	MGL	D	1	2	13,13,13	0.66	0	18,18,18	0.51	0
2	SGC	D	2	2	10,11,12	0.50	0	12,15,17	0.87	0
2	GLC	D	3	2	11,11,12	0.57	0	15,15,17	1.36	2 (13%)
2	GLC	D	4	2	11,11,12	0.44	0	15,15,17	0.65	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
2	MGL	C	1	2	-	4/4/24/24	0/1/1/1
2	SGC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	GLC	C	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MGL	D	1	2	-	2/4/24/24	0/1/1/1
2	SGC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLC	D	4	2	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	GLC	C1-O5-C5	3.50	116.93	112.19
2	D	3	GLC	O5-C5-C6	2.89	111.73	107.20
2	C	3	GLC	O5-C5-C6	2.78	111.56	107.20
2	C	3	GLC	C1-O5-C5	2.71	115.87	112.19
2	C	1	MGL	O1-C1-C2	2.52	111.10	108.15

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	GLC	C1
2	C	4	GLC	C1
2	D	3	GLC	C1
2	D	4	GLC	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	MGL	O5-C1-O1-C7
2	C	1	MGL	C2-C1-O1-C7
2	C	1	MGL	C4-C5-C6-O6
2	C	1	MGL	O5-C5-C6-O6
2	D	1	MGL	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
2	D	1	MGL	O5-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6

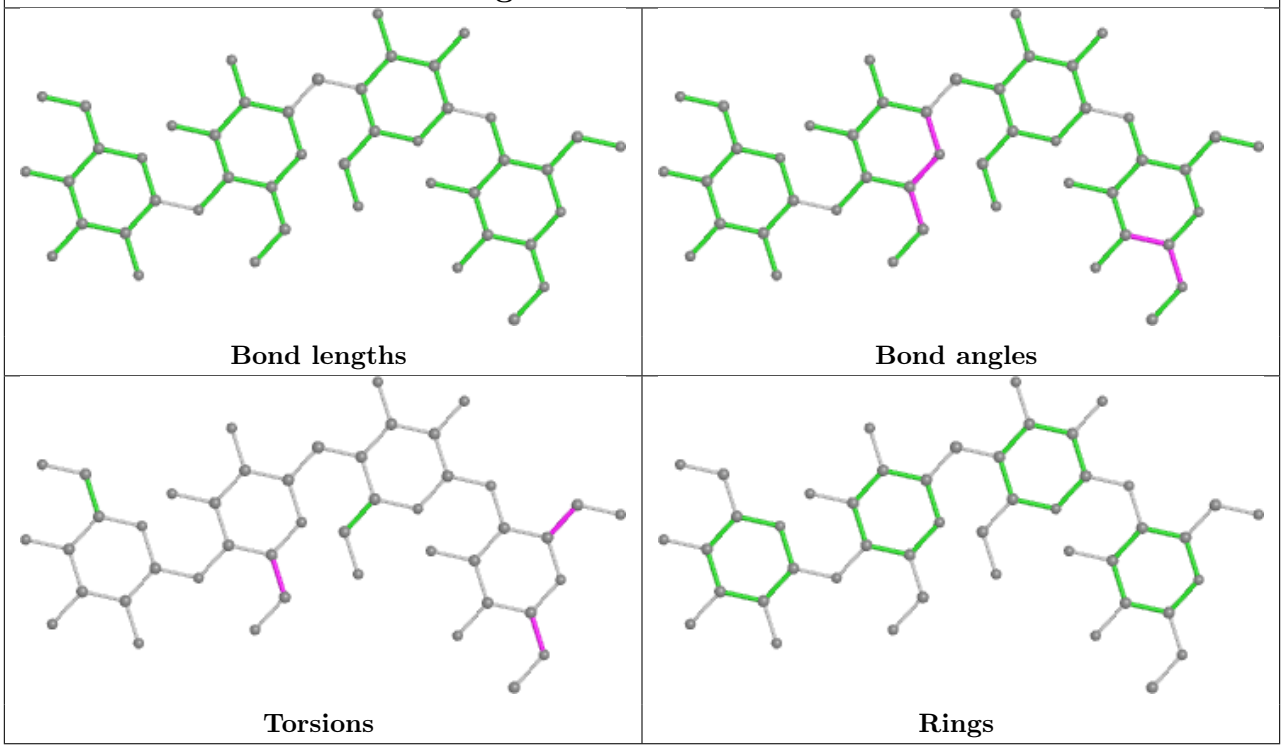
There are no ring outliers.

3 monomers are involved in 2 short contacts:

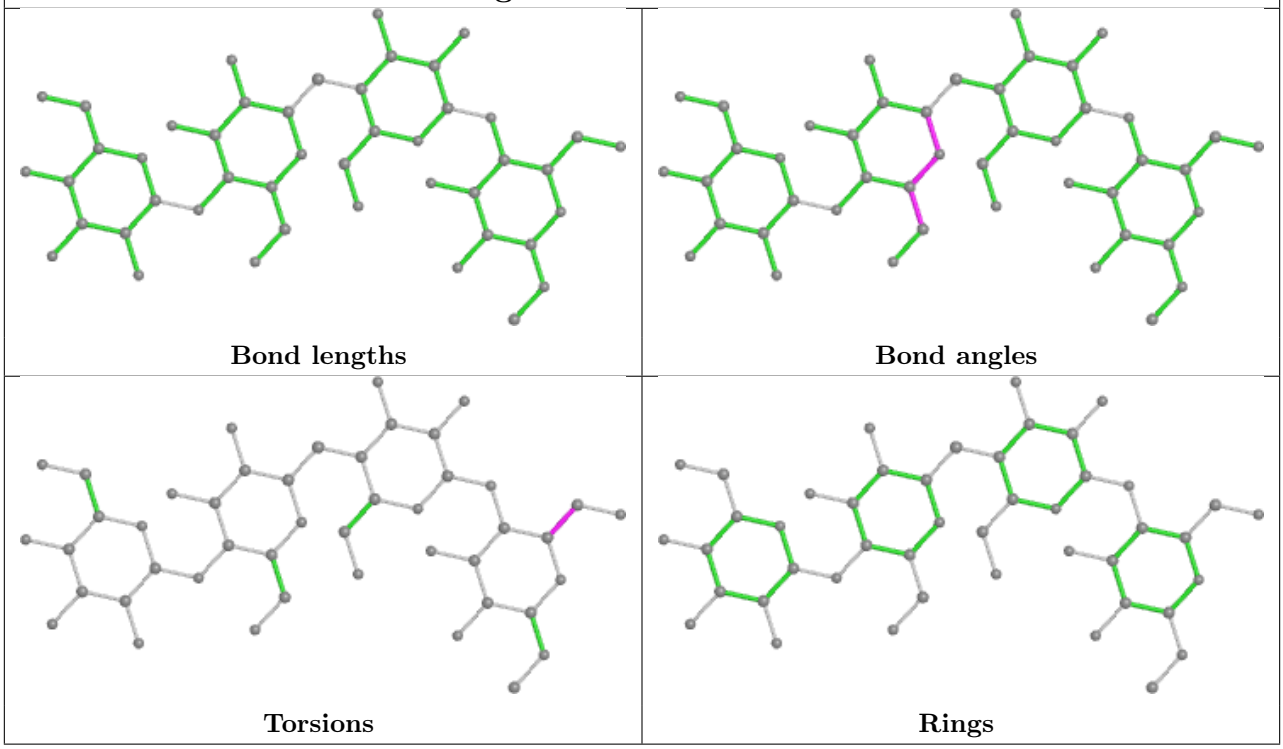
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	MGL	1	0
2	C	2	SGC	1	0
2	C	3	GLC	1	0

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 C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MAN	B	504	1	11,11,12	0.58	0	15,15,17	0.72	0
3	NAG	A	502	1	14,14,15	0.50	0	17,19,21	0.88	1 (5%)
4	MAN	A	503	1	11,11,12	0.52	0	15,15,17	0.76	0
3	NAG	A	501	1	14,14,15	0.47	0	17,19,21	0.84	1 (5%)
4	MAN	A	507	1	11,11,12	0.52	0	15,15,17	0.70	0
4	MAN	A	508	1	11,11,12	0.50	0	15,15,17	0.81	1 (6%)
4	MAN	A	509	1	11,11,12	0.50	0	15,15,17	0.70	0
4	MAN	B	507	1	11,11,12	0.47	0	15,15,17	0.68	0
4	MAN	B	509	1	11,11,12	0.53	0	15,15,17	0.68	0
4	MAN	A	506	1	11,11,12	0.56	0	15,15,17	0.72	0
4	MAN	B	506	1	11,11,12	0.48	0	15,15,17	0.80	1 (6%)
4	MAN	A	505	1	11,11,12	0.50	0	15,15,17	0.71	0
4	MAN	A	504	1	11,11,12	0.47	0	15,15,17	0.76	1 (6%)
3	NAG	B	501	1	14,14,15	0.50	0	17,19,21	0.80	0
4	MAN	B	503	1	11,11,12	0.48	0	15,15,17	0.77	1 (6%)
4	MAN	B	505	1	11,11,12	0.54	0	15,15,17	0.79	1 (6%)
4	MAN	B	508	1	11,11,12	0.46	0	15,15,17	0.75	1 (6%)
3	NAG	B	502	1	14,14,15	0.46	0	17,19,21	0.75	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	MAN	B	504	1	-	2/2/19/22	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	MAN	A	503	1	-	1/2/19/22	0/1/1/1
3	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	MAN	A	507	1	-	0/2/19/22	0/1/1/1
4	MAN	A	508	1	-	2/2/19/22	0/1/1/1
4	MAN	A	509	1	-	0/2/19/22	0/1/1/1
4	MAN	B	507	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	509	1	-	2/2/19/22	0/1/1/1
4	MAN	A	506	1	-	2/2/19/22	0/1/1/1
4	MAN	B	506	1	-	0/2/19/22	0/1/1/1
4	MAN	A	505	1	-	0/2/19/22	0/1/1/1
4	MAN	A	504	1	-	2/2/19/22	0/1/1/1
3	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	MAN	B	503	1	-	2/2/19/22	0/1/1/1
4	MAN	B	505	1	-	0/2/19/22	0/1/1/1
4	MAN	B	508	1	-	0/2/19/22	0/1/1/1
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	508	MAN	C1-O5-C5	2.36	115.39	112.19
4	A	504	MAN	C1-O5-C5	2.34	115.37	112.19
4	B	506	MAN	C1-O5-C5	2.23	115.21	112.19
3	A	502	NAG	C2-N2-C7	-2.15	119.84	122.90
4	B	503	MAN	C1-O5-C5	2.12	115.07	112.19
4	B	508	MAN	C1-O5-C5	2.06	114.98	112.19
4	B	505	MAN	C1-O5-C5	2.01	114.92	112.19
3	A	501	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	MAN	O5-C5-C6-O6
4	B	504	MAN	O5-C5-C6-O6
4	B	503	MAN	C4-C5-C6-O6
4	B	504	MAN	C4-C5-C6-O6
4	A	504	MAN	C4-C5-C6-O6
4	A	504	MAN	O5-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
4	A	503	MAN	O5-C5-C6-O6
4	A	508	MAN	C4-C5-C6-O6
4	B	509	MAN	C4-C5-C6-O6
4	A	506	MAN	C4-C5-C6-O6
4	A	506	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	508	MAN	O5-C5-C6-O6
4	B	509	MAN	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	MAN	1	0
3	A	501	NAG	1	0
4	B	503	MAN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	363/363 (100%)	-0.32	3 (0%)	86	85	8, 16, 27, 44	0
1	B	363/363 (100%)	-0.39	4 (1%)	80	79	6, 15, 27, 43	0
All	All	726/726 (100%)	-0.36	7 (0%)	82	81	6, 15, 27, 44	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	LEU	6.2
1	A	180	ALA	4.3
1	A	178	ALA	4.0
1	B	158	ASN	3.8
1	B	179	LEU	2.9
1	B	447	LEU	2.4
1	B	157	LYS	2.1

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MGL	C	1	13/13	0.69	0.25	31,32,36,36	0
2	GLC	C	3	11/12	0.80	0.18	26,28,29,29	0

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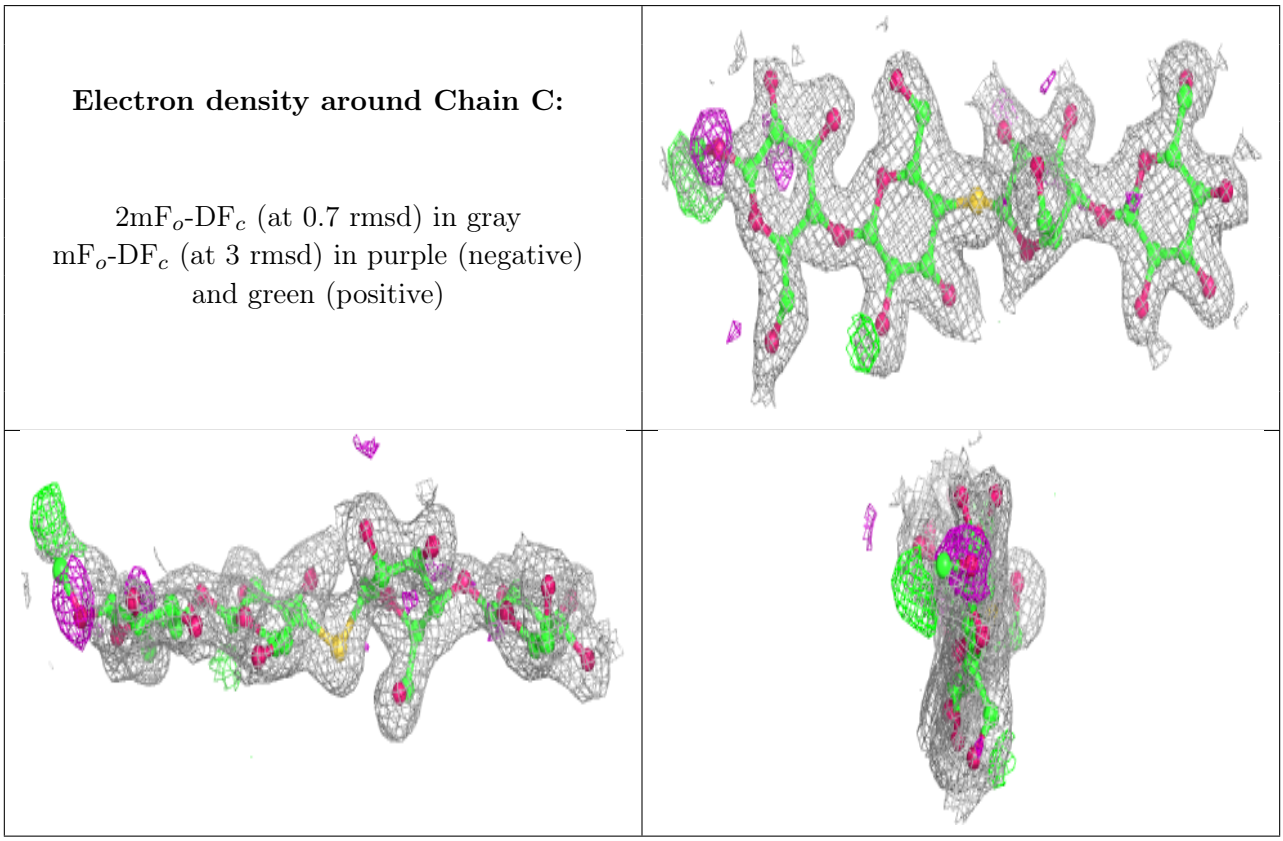
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	4	11/12	0.84	0.16	25,30,31,31	0
2	GLC	D	3	11/12	0.87	0.19	31,32,32,32	0
2	SGC	C	2	11/12	0.87	0.13	29,30,30,31	0
2	SGC	D	2	11/12	0.89	0.11	27,28,28,31	0
2	GLC	C	4	11/12	0.90	0.12	17,22,24,24	0
2	MGL	D	1	13/13	0.94	0.10	24,25,27,27	0

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.

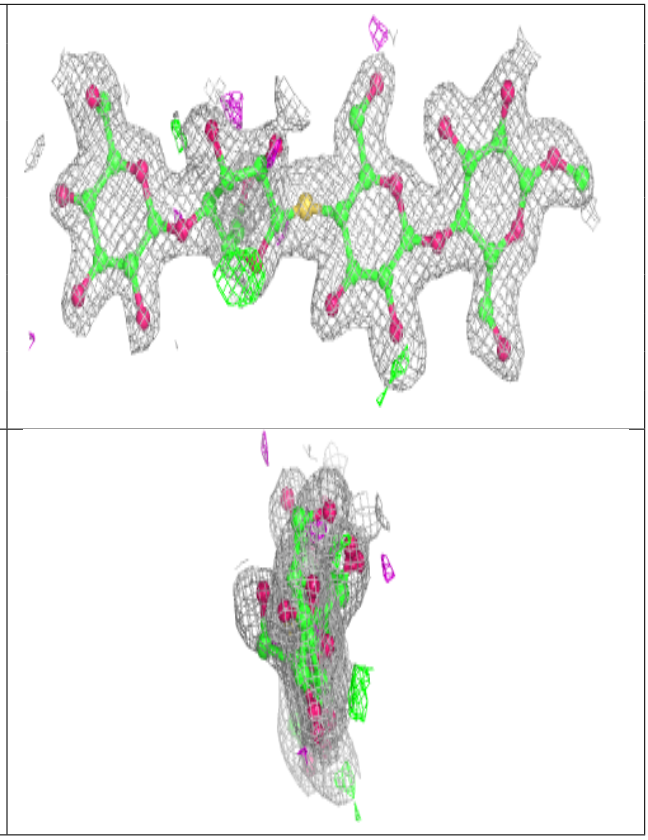
Electron density around Chain C:

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 D:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	A	503	11/12	0.57	0.37	38,41,42,43	0
4	MAN	B	503	11/12	0.69	0.24	34,37,38,39	0
4	MAN	B	509	11/12	0.70	0.36	33,36,37,38	0
4	MAN	B	504	11/12	0.79	0.22	26,29,31,32	0
4	MAN	B	508	11/12	0.80	0.17	35,37,38,38	0
4	MAN	A	504	11/12	0.85	0.17	24,26,29,33	0
3	NAG	A	501	14/15	0.86	0.18	33,35,36,37	0
4	MAN	A	509	11/12	0.87	0.16	29,30,31,32	0
4	MAN	B	507	11/12	0.88	0.12	26,28,29,29	0
4	MAN	A	505	11/12	0.90	0.10	21,23,24,25	0
4	MAN	B	505	11/12	0.91	0.12	23,24,25,28	0
4	MAN	B	506	11/12	0.93	0.13	20,22,24,26	0
3	NAG	B	501	14/15	0.93	0.14	24,25,26,27	0
4	MAN	A	506	11/12	0.94	0.10	18,18,21,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	A	507	11/12	0.94	0.09	21,22,23,26	0
3	NAG	B	502	14/15	0.95	0.09	19,21,22,23	0
3	NAG	A	502	14/15	0.95	0.08	17,18,20,21	0
4	MAN	A	508	11/12	0.96	0.11	18,19,19,21	0

6.5 Other polymers (i)

There are no such residues in this entry.