Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 10:16 AM BST

PDB ID	:	1GQL
Title	:	Structure of Pseudomonas cellulosa alpha-D-glucuronidase complexed with glucuronic acid and xylotriose
Authors	:	Nurizzo, D.; Nagy, T.; Gilbert, H.J.; Davies, G.J.
Deposited on	:	2001-11-26
Resolution	:	1.67 Å(reported)

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	:	2.13.1
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 ⓘ

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

The reported resolution of this entry is 1.67 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	Percentile Ranks	Value
Rfree		0.175
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		1.4%
RSRZ outliers		3.3%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
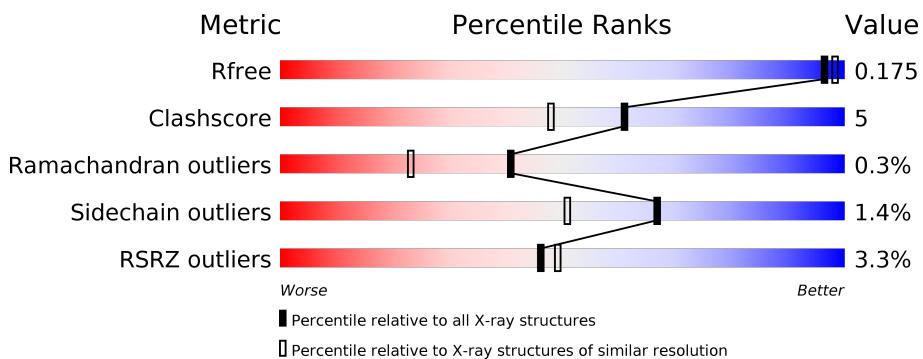
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	708	3%　89%　9% ·
1	B	708	3%　90%　8% ··
2	C	2	50%　50%
2	D	2	50%　50%
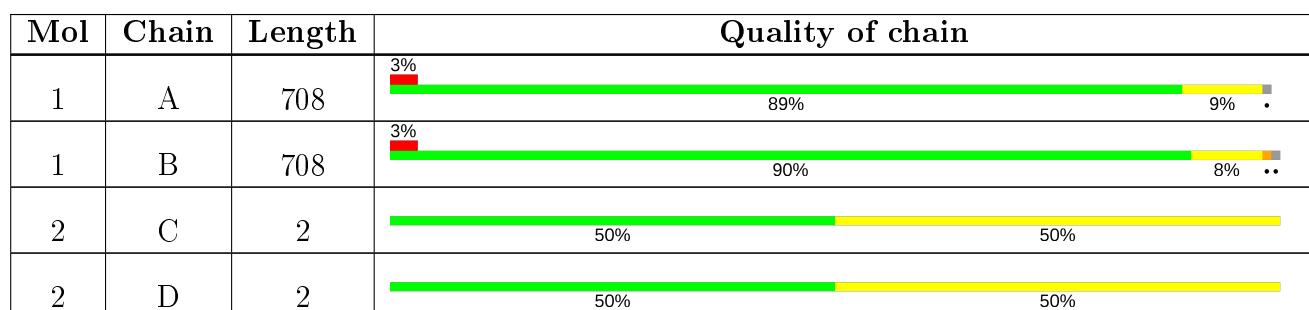
2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12936 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 ALPHA-D-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total 5714	C 3648	N 1013	O 1035	S 18	0	17	0
1	B	700	Total 5700	C 3642	N 1007	O 1033	S 18	0	20	0

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-1)-beta-D-xylopyranose.
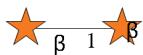
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total 11	C 6	O 5	0	0	1
2	D	2	Total 11	C 6	O 5	0	0	1

- Molecule 3 is beta-D-glucopyranuronic acid (three-letter code: BDP) (formula: $C_6H_{10}O_7$).
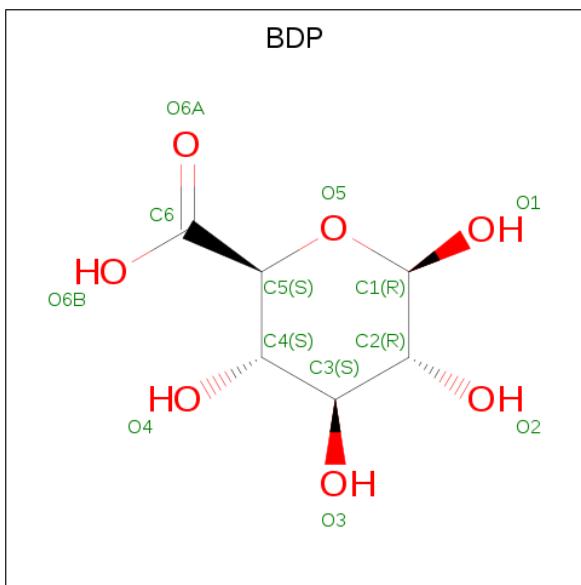
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2		0	0
4	A	1	Total 4	C 2	O 2		0	0
4	A	1	Total 4	C 2	O 2		0	0
4	B	1	Total 4	C 2	O 2		0	0
4	B	1	Total 4	C 2	O 2		0	0
4	B	1	Total 4	C 2	O 2		0	0
4	B	1	Total 4	C 2	O 2		0	0
4	B	1	Total 4	C 2	O 2		0	0
4	B	1	Total 4	C 2	O 2		0	0

- Molecule 5 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total 4	Co 4	0	0
5	A	4	Total 4	Co 4	0	4

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	705	Total 705	O 705	0	0
6	B	717	Total 717	O 717	0	0

3 Residue-property plots ⓘ

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: ALPHA-D-GLUCURONIDASE
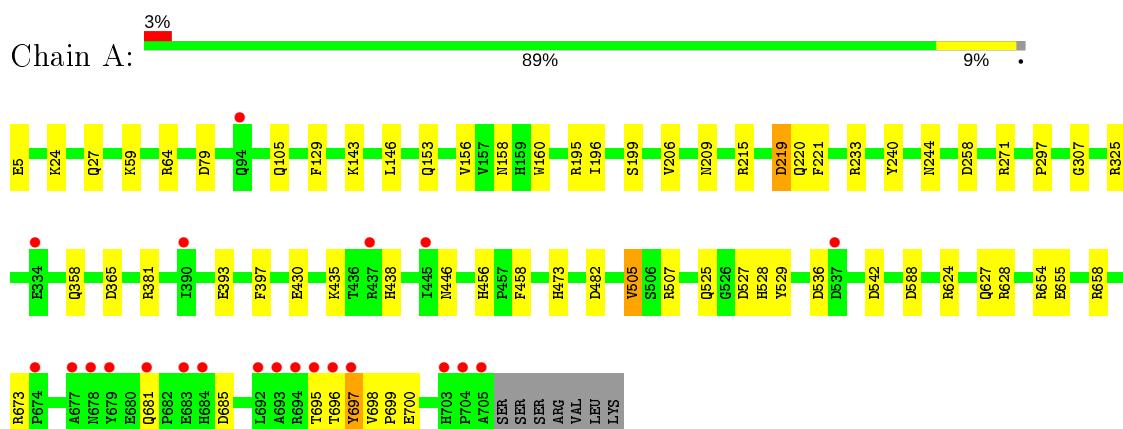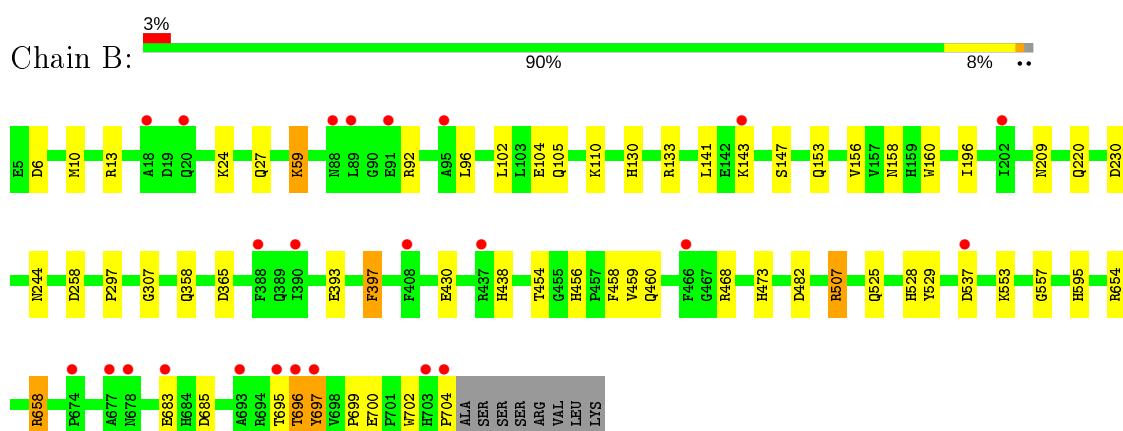
Chain A:

• Molecule 1: ALPHA-D-GLUCURONIDASE

Chain B:

• Molecule 2: beta-D-xylopyranose-(1-1)-beta-D-xylopyranose

Chain C:

• Molecule 2: beta-D-xylopyranose-(1-1)-beta-D-xylopyranose

Chain D:

XYP1 XYP2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.26Å 74.32Å 87.27Å 115.15° 92.94° 109.24°	Depositor
Resolution (Å)	20.00 – 1.67 37.71 – 1.67	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-1.67) 94.1 (37.71-1.67)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.35 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.146 , 0.172 0.155 , 0.175	Depositor DCC
R_{free} test set	1256 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.9	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12936	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: XYP, CO, BDP, EDO

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	0.72	0/5946	0.92	22/8088 (0.3%)
1	B	0.73	0/5957	0.93	19/8103 (0.2%)
All	All	0.73	0/11903	0.93	41/16191 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	685	ASP	CB-CG-OD2	9.55	126.89	118.30
1	B	258	ASP	CB-CG-OD1	8.10	125.59	118.30
1	A	685	ASP	CB-CG-OD2	7.97	125.47	118.30
1	B	92	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	325	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	397	PHE	CB-CG-CD1	6.71	125.50	120.80
1	A	628	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	527	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	381	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	468	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	654	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	654	ARG	NE-CZ-NH1	6.22	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	588	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	628	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	536	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	658[A]	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	658[B]	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	482	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	195	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	233	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	542	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	271	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	13	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	397	PHE	CB-CG-CD1	5.64	124.75	120.80
1	B	6	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	658[A]	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	658[B]	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	537	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	230	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	258	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	133	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	110	LYS	CD-CE-NZ	5.41	124.14	111.70
1	A	79	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	468	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	64	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	381	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	654	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	219	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	673	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	482	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	507	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	697	TYR	Mainchain
1	B	695	THR	Peptide

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	5714	0	5537	67	0
1	B	5700	0	5530	38	0
2	C	11	0	0	0	0
2	D	11	0	0	0	0
3	A	13	0	9	0	0
3	B	13	0	9	0	0
4	A	20	0	30	2	0
4	B	24	0	36	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	705	0	0	7	0
6	B	717	0	0	10	0
All	All	12936	0	11151	103	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 5.

All (103) 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:A:658[B]:ARG:HH12	1:A:696:THR:CB	1.06	1.55
1:A:658[B]:ARG:NH1	1:A:696:THR:CB	1.82	1.38
1:A:658[B]:ARG:NH1	1:A:696:THR:HB	1.53	1.07
1:A:658[B]:ARG:HH12	1:A:696:THR:CG2	1.68	1.05
1:A:658[B]:ARG:HH22	1:A:696:THR:CG2	1.70	1.05
1:A:658[B]:ARG:CZ	1:A:696:THR:OG1	2.05	1.04
1:A:529[B]:TYR:OH	1:A:655[B]:GLU:OE2	1.75	1.03
1:A:658[B]:ARG:NH1	1:A:696:THR:OG1	1.92	1.00
1:A:658[B]:ARG:HH12	1:A:696:THR:HB	0.85	0.99
1:A:529[B]:TYR:OH	1:A:655[B]:GLU:CD	2.00	0.98
1:A:529[B]:TYR:OH	1:A:655[B]:GLU:OE1	1.82	0.97
1:A:696:THR:HG23	6:B:2265:HOH:O	1.64	0.96
1:A:525:GLN:HE22	1:A:528:HIS:HE1	1.15	0.93
1:A:658[B]:ARG:NH2	1:A:696:THR:CG2	2.32	0.92
1:B:525:GLN:HE22	1:B:528:HIS:HE1	1.18	0.91
1:A:658[B]:ARG:NH2	1:A:696:THR:HG21	1.92	0.85
1:A:529[B]:TYR:CZ	1:A:655[B]:GLU:OE1	2.31	0.84
1:B:658[B]:ARG:NH2	6:B:2668:HOH:O	2.10	0.83
1:A:658[B]:ARG:HH22	1:A:696:THR:HG23	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658[B]:ARG:NH1	1:A:696:THR:CG2	2.31	0.83
1:A:658[B]:ARG:CZ	1:A:696:THR:HG21	2.08	0.83
1:A:658[B]:ARG:NH2	1:A:696:THR:OG1	2.11	0.82
1:A:529[A]:TYR:HE2	1:A:696:THR:HG22	1.45	0.80
1:A:658[B]:ARG:NH1	1:A:696:THR:HG21	1.97	0.78
1:A:658[B]:ARG:CZ	1:A:696:THR:CB	2.57	0.78
1:A:658[B]:ARG:CZ	1:A:696:THR:CG2	2.65	0.74
1:A:456:HIS:HD2	1:A:458:PHE:H	1.36	0.73
1:A:529[A]:TYR:CE2	1:A:696:THR:HG22	2.26	0.70
1:A:699:PRO:HG2	6:A:2540:HOH:O	1.93	0.69
1:B:525:GLN:NE2	1:B:528:HIS:HE1	1.90	0.69
1:A:525:GLN:HE22	1:A:528:HIS:CE1	2.06	0.68
1:A:697:TYR:O	6:A:2690:HOH:O	2.09	0.68
1:A:525:GLN:NE2	1:A:528:HIS:HE1	1.89	0.68
1:B:456:HIS:HD2	1:B:458:PHE:H	1.42	0.67
1:A:529[B]:TYR:CZ	1:A:655[B]:GLU:CD	2.69	0.66
1:A:5:GLU:N	6:A:2001:HOH:O	2.28	0.66
1:B:153:GLN:HE22	1:B:438:HIS:HD2	1.43	0.64
1:A:529[A]:TYR:HE2	1:A:696:THR:CG2	2.10	0.63
1:B:525:GLN:HE22	1:B:528:HIS:CE1	2.10	0.63
1:A:529[B]:TYR:CZ	1:A:655[B]:GLU:OE2	2.51	0.63
1:B:196:ILE:HD11	4:B:1709:EDO:H22	1.84	0.60
1:B:696[B]:THR:O	1:B:697:TYR:C	2.40	0.59
1:A:698:VAL:HG12	1:A:700[B]:GLU:HG2	1.86	0.57
1:A:215[B]:ARG:NH1	1:B:696[B]:THR:HG22	2.19	0.57
1:B:196:ILE:HG13	4:B:1709:EDO:H11	1.87	0.56
1:A:529[B]:TYR:CE2	1:A:655[B]:GLU:OE2	2.59	0.56
1:A:658[B]:ARG:NH2	1:A:696:THR:CB	2.68	0.55
1:A:196:ILE:HG13	4:A:1710:EDO:H11	1.87	0.55
1:A:220:GLN:NE2	6:A:2280:HOH:O	2.40	0.55
1:A:393:GLU:OE2	1:A:528:HIS:HD2	1.91	0.54
1:A:160:TRP:H	1:A:446:ASN:ND2	2.05	0.54
1:B:105:GLN:NE2	1:B:143:LYS:H	2.06	0.54
1:A:696:THR:HA	6:B:2265:HOH:O	2.08	0.54
1:B:557:GLY:O	1:B:595:HIS:HD2	1.91	0.54
1:A:105:GLN:NE2	1:A:143:LYS:H	2.05	0.54
1:B:700[B]:GLU:HG3	1:B:702:TRP:O	2.08	0.53
1:A:430:GLU:OE1	1:A:473:HIS:HE1	1.91	0.53
1:A:525:GLN:NE2	1:A:528:HIS:CE1	2.73	0.53
1:B:393:GLU:OE2	1:B:528:HIS:HD2	1.92	0.53
1:A:158:ASN:HD21	1:A:358:GLN:HE22	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASN:HD21	1:B:358:GLN:HE22	1.57	0.52
1:B:525:GLN:NE2	1:B:528:HIS:CE1	2.74	0.52
1:A:196:ILE:HD11	4:A:1710:EDO:H22	1.93	0.51
1:A:505[B]:VAL:HG23	6:A:2516:HOH:O	2.10	0.51
1:B:430:GLU:OE1	1:B:473:HIS:HE1	1.95	0.49
1:B:153:GLN:HE22	1:B:438:HIS:CD2	2.28	0.49
1:A:658[B]:ARG:HH22	1:A:696:THR:CB	2.24	0.49
1:A:695:THR:HG21	6:B:2053:HOH:O	2.12	0.48
1:A:297:PRO:HG3	1:A:307:GLY:HA3	1.94	0.48
1:A:456:HIS:HE1	6:A:2447:HOH:O	1.97	0.48
1:A:160:TRP:H	1:A:446:ASN:HD21	1.60	0.47
1:B:456:HIS:HE1	6:B:2434:HOH:O	1.96	0.47
1:A:215[B]:ARG:NH1	1:B:696[B]:THR:CG2	2.77	0.47
1:B:397:PHE:CZ	1:B:529[B]:TYR:HB2	2.50	0.47
1:B:473:HIS:HD2	6:B:2487:HOH:O	1.96	0.47
1:B:196:ILE:CD1	4:B:1709:EDO:H22	2.45	0.46
1:B:96:LEU:HD21	1:B:147:SER:HB2	1.97	0.46
1:A:658[B]:ARG:NH1	1:A:696:THR:HG1	2.08	0.46
1:B:24:LYS:NZ	1:B:27:GLN:HE22	2.14	0.46
1:B:699:PRO:HG3	6:B:2535:HOH:O	2.17	0.45
1:B:702:TRP:CH2	1:B:704:PRO:HA	2.52	0.45
1:A:160:TRP:HA	1:A:209:ASN:HA	1.99	0.45
1:A:153[B]:GLN:OE1	1:A:438:HIS:HA	2.16	0.45
1:A:529[A]:TYR:CE2	1:A:696:THR:CG2	2.94	0.44
1:B:220:GLN:NE2	6:B:2268:HOH:O	2.45	0.44
1:A:24:LYS:NZ	1:A:27:GLN:HE22	2.14	0.44
1:B:59:LYS:HE2	6:B:2051:HOH:O	2.17	0.44
1:B:10[B]:MET:SD	1:B:460:GLN:HG2	2.57	0.44
1:A:129:PHE:CG	1:A:199:SER:HA	2.53	0.43
1:A:206:VAL:HG22	1:A:240:TYR:HB2	2.00	0.43
1:A:215[B]:ARG:HD3	1:A:221:PHE:CE2	2.53	0.43
1:B:699:PRO:CG	6:B:2535:HOH:O	2.65	0.43
1:B:102[B]:LEU:HD21	1:B:104:GLU:HB2	2.00	0.43
1:B:393:GLU:OE2	1:B:528:HIS:CD2	2.72	0.43
1:B:153:GLN:NE2	1:B:438:HIS:HA	2.35	0.42
1:A:473:HIS:HD2	6:A:2459:HOH:O	2.02	0.42
1:A:393:GLU:OE2	1:A:528:HIS:CD2	2.71	0.42
1:B:160:TRP:HA	1:B:209:ASN:HA	2.02	0.42
1:B:130:HIS:CE1	4:B:1711:EDO:H12	2.55	0.42
1:B:297:PRO:HG3	1:B:307:GLY:HA3	2.03	0.41
1:B:454:THR:HB	1:B:459:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ARG:HA	1:A:627:GLN:HE21	1.86	0.41
1:A:695:THR:O	1:A:695:THR:HG22	2.21	0.41

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	716/708 (101%)	699 (98%)	16 (2%)	1 (0%)	51	32
1	B	718/708 (101%)	697 (97%)	17 (2%)	4 (1%)	25	10
All	All	1434/1416 (101%)	1396 (97%)	33 (2%)	5 (0%)	41	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	696[A]	THR
1	B	696[B]	THR
1	B	365	ASP
1	B	697	TYR
1	A	365	ASP

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	597/588 (102%)	586 (98%)	11 (2%)	59	40
1	B	600/588 (102%)	592 (99%)	8 (1%)	69	54
All	All	1197/1176 (102%)	1178 (98%)	19 (2%)	67	46

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	146	LEU
1	A	156[A]	VAL
1	A	156[B]	VAL
1	A	219	ASP
1	A	244	ASN
1	A	435	LYS
1	A	505[A]	VAL
1	A	505[B]	VAL
1	A	507	ARG
1	A	681	GLN
1	B	59	LYS
1	B	141	LEU
1	B	156[A]	VAL
1	B	156[B]	VAL
1	B	244	ASN
1	B	507	ARG
1	B	553	LYS
1	B	683	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	27	GLN
1	A	32	HIS
1	A	105	GLN
1	A	158	ASN
1	A	244	ASN
1	A	392	GLN
1	A	446	ASN
1	A	456	HIS
1	A	473	HIS
1	A	512	ASN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	528	HIS
1	A	618	GLN
1	A	627	GLN
1	B	27	GLN
1	B	105	GLN
1	B	153	GLN
1	B	154	HIS
1	B	244	ASN
1	B	358	GLN
1	B	392	GLN
1	B	438	HIS
1	B	456	HIS
1	B	473	HIS
1	B	512	ASN
1	B	525	GLN
1	B	528	HIS
1	B	595	HIS
1	B	618	GLN
1	B	627	GLN
1	B	681	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

4 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
2	XYP	C	1	2	1,1,10	0.10	0	-		
2	XYP	C	2	2	9,9,10	1.45	1 (11%)	10,12,14	1.41	1 (10%)
2	XYP	D	1	2	1,1,10	0.19	0	-		
2	XYP	D	2	2	9,9,10	1.59	1 (11%)	10,12,14	1.24	1 (10%)

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	XYP	C	2	2	-	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	XYP	O5-C1	-4.42	1.34	1.42
2	C	2	XYP	O5-C1	-3.84	1.35	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	XYP	C4-C3-C2	-2.85	107.54	110.92
2	D	2	XYP	C5-O5-C1	2.78	115.81	111.52

There are no chirality outliers.

There are no torsion outliers.

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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
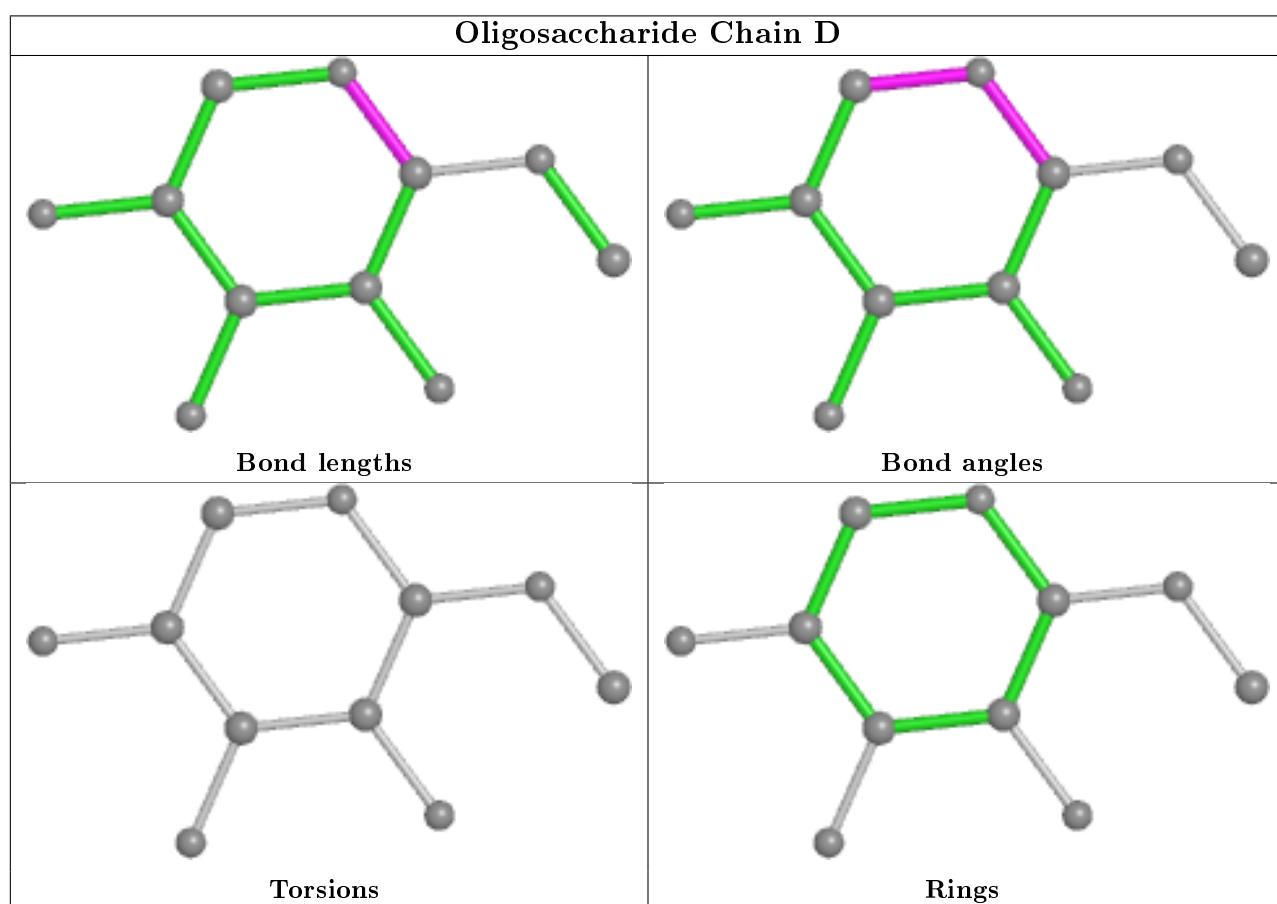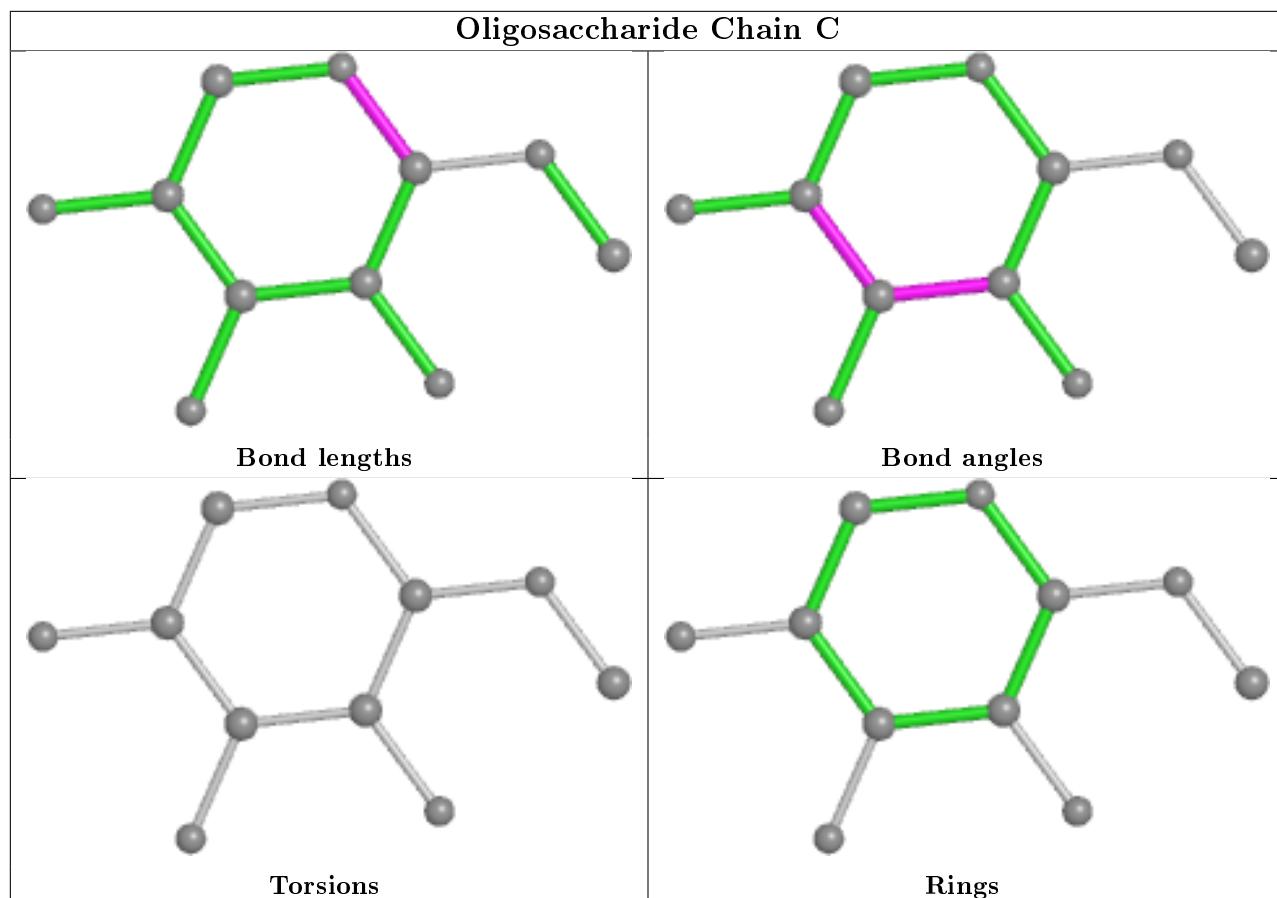
5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	#$\|Z\| > 2$
4	EDO	B	1709	-	3,3,3	0.38	0	2,2,2	0.65	0
3	BDP	A	1706	-	10,13,13	0.50	0	15,19,19	1.45	3 (20%)
4	EDO	A	1708	-	3,3,3	0.38	0	2,2,2	0.65	0
4	EDO	B	1708	-	3,3,3	0.17	0	2,2,2	0.56	0
3	BDP	B	1705	-	10,13,13	0.64	0	15,19,19	1.28	2 (13%)
4	EDO	A	1709	-	3,3,3	0.25	0	2,2,2	0.52	0
4	EDO	A	1711	-	3,3,3	0.35	0	2,2,2	0.42	0
4	EDO	B	1707	-	3,3,3	0.43	0	2,2,2	1.08	0
4	EDO	A	1707	-	3,3,3	0.48	0	2,2,2	0.72	0
4	EDO	B	1706	-	3,3,3	0.37	0	2,2,2	0.51	0
4	EDO	B	1710	-	3,3,3	0.39	0	2,2,2	0.51	0
4	EDO	A	1710	-	3,3,3	0.42	0	2,2,2	0.44	0
4	EDO	B	1711	-	3,3,3	0.43	0	2,2,2	0.31	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	EDO	B	1709	-	-	0/1/1/1	-
3	BDP	A	1706	-	-	0/0/24/24	0/1/1/1
4	EDO	A	1708	-	-	0/1/1/1	-
4	EDO	B	1708	-	-	1/1/1/1	-
3	BDP	B	1705	-	-	0/0/24/24	0/1/1/1
4	EDO	A	1709	-	-	0/1/1/1	-
4	EDO	A	1711	-	-	0/1/1/1	-
4	EDO	B	1707	-	-	1/1/1/1	-
4	EDO	A	1707	-	-	0/1/1/1	-
4	EDO	B	1706	-	-	0/1/1/1	-
4	EDO	B	1710	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1710	-	-	0/1/1/1	-
4	EDO	B	1711	-	-	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})
3	A	1706	BDP	C1-C2-C3	2.98	116.51	110.31
3	B	1705	BDP	O1-C1-O5	-2.65	102.43	110.38
3	B	1705	BDP	C1-C2-C3	2.40	115.29	110.31
3	A	1706	BDP	C1-O5-C5	2.36	115.84	112.31
3	A	1706	BDP	O1-C1-O5	-2.27	103.57	110.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1710	EDO	O1-C1-C2-O2
4	B	1708	EDO	O1-C1-C2-O2
4	B	1707	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1709	EDO	3	0
4	A	1710	EDO	2	0
4	B	1711	EDO	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(Å²)	Q<0.9
1	A	701/708 (99%)	0.26	22 (3%)	49	51	9, 14, 29, 45	1 (0%)
1	B	700/708 (98%)	0.23	24 (3%)	45	48	9, 14, 29, 45	0
All	All	1401/1416 (98%)	0.24	46 (3%)	46	49	9, 14, 29, 45	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	705	ALA	7.3
1	A	695	THR	6.9
1	B	696[A]	THR	6.5
1	A	437	ARG	5.7
1	A	696	THR	5.5
1	B	695	THR	5.1
1	A	692	LEU	4.7
1	A	537	ASP	4.6
1	B	537	ASP	4.2
1	A	703	HIS	4.0
1	A	683	GLU	3.7
1	B	437	ARG	3.6
1	B	703	HIS	3.6
1	B	683	GLU	3.6
1	A	94	GLN	3.5
1	A	677	ALA	3.4
1	A	697	TYR	3.4
1	B	677	ALA	3.4
1	A	678	ASN	3.3
1	B	91	GLU	3.2
1	B	88	ASN	3.2
1	A	674	PRO	3.2
1	B	704	PRO	3.1
1	A	693[A]	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	694	ARG	3.0
1	B	466	PHE	2.9
1	B	89	LEU	2.9
1	B	95	ALA	2.7
1	A	704	PRO	2.7
1	B	693[A]	ALA	2.6
1	B	143	LYS	2.5
1	A	390	ILE	2.5
1	B	674	PRO	2.4
1	A	445	ILE	2.4
1	B	202[A]	ILE	2.4
1	B	390	ILE	2.4
1	B	20	GLN	2.3
1	B	408	PHE	2.3
1	B	697	TYR	2.2
1	B	388	PHE	2.1
1	A	681	GLN	2.1
1	A	684	HIS	2.1
1	A	679	TYR	2.1
1	B	18	ALA	2.0
1	A	334	GLU	2.0
1	B	678	ASN	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYP	D	1	2/10	0.84	0.35	17,17,17,23	2
2	XYP	C	1	2/10	0.87	0.36	18,18,18,25	2
2	XYP	C	2	9/10	0.96	0.07	17,18,20,21	0
2	XYP	D	2	9/10	0.96	0.08	15,17,19,22	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.
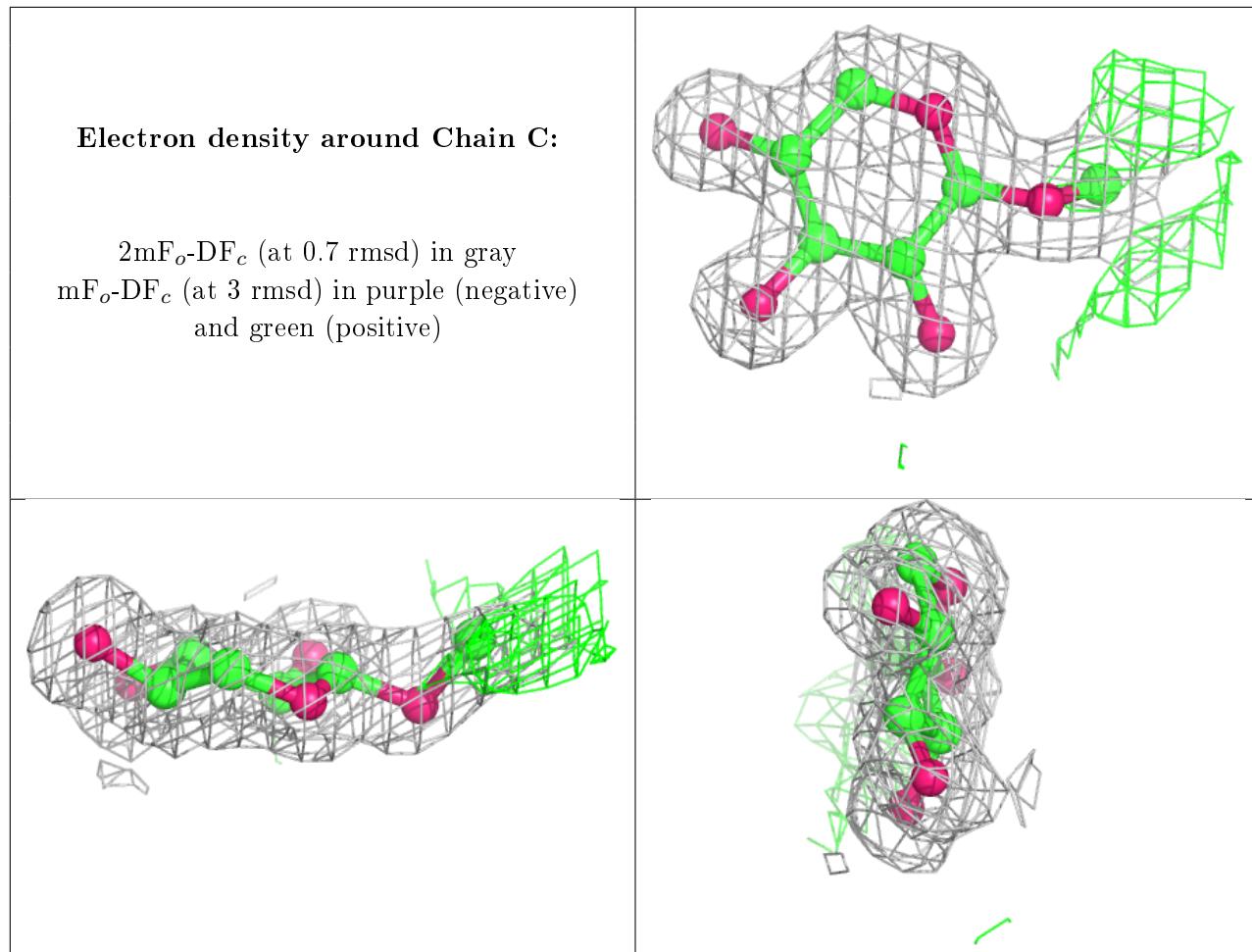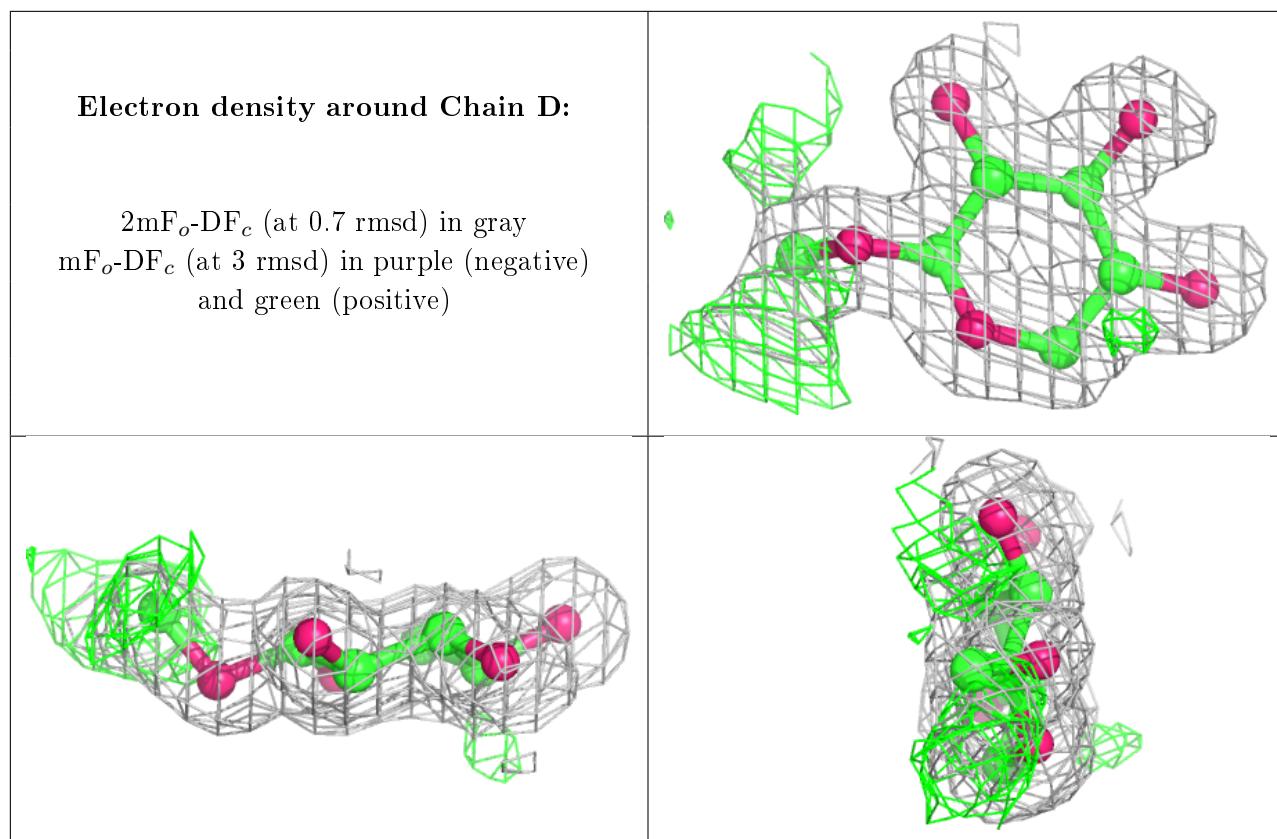
Electron density around Chain C:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 ⓘ

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	EDO	B	1710	4/4	0.85	0.17	36,42,42,45	0
4	EDO	B	1707	4/4	0.92	0.15	16,21,26,38	0
4	EDO	B	1708	4/4	0.94	0.10	19,26,26,26	0
4	EDO	B	1711	4/4	0.94	0.12	16,18,19,20	0
4	EDO	A	1711	4/4	0.95	0.14	16,24,27,30	0
3	BDP	A	1706	13/13	0.97	0.09	8,12,14,16	0
4	EDO	A	1707	4/4	0.97	0.12	11,12,14,14	0
4	EDO	A	1709	4/4	0.97	0.07	17,17,18,19	0
4	EDO	A	1710	4/4	0.97	0.09	13,14,17,17	0
4	EDO	A	1708	4/4	0.97	0.08	17,17,21,25	0
4	EDO	B	1709	4/4	0.98	0.09	12,13,18,18	0
3	BDP	B	1705	13/13	0.98	0.07	7,11,12,13	0
4	EDO	B	1706	4/4	0.98	0.16	12,12,13,13	0
5	CO	A	1714[A]	1/1	0.99	0.07	17,17,17,17	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CO	B	1717	1/1	0.99	0.07	21,21,21,21	1
5	CO	A	1716[A]	1/1	0.99	0.09	20,20,20,20	1
5	CO	B	1715	1/1	1.00	0.09	14,14,14,14	1
5	CO	B	1714	1/1	1.00	0.05	16,16,16,16	1
5	CO	A	1717[A]	1/1	1.00	0.10	16,16,16,16	1
5	CO	A	1715[A]	1/1	1.00	0.07	13,13,13,13	1
5	CO	B	1716	1/1	1.00	0.08	17,17,17,17	1

6.5 Other polymers (i)

There are no such residues in this entry.