Full wwPDB X-ray Structure Validation Report

Apr 21, 2024 – 09:22 am BST

PDB ID	:	1GQJ
Title	:	Structure of Pseudomonas cellulosa alpha-D-glucuronidase complexed with xylobiose
Authors	:	Nurizzo, D.; Nagy, T.; Gilbert, H.J.; Davies, G.J.
Deposited on	:	2001-11-26
Resolution	:	1.90 Å(reported)

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

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

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

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

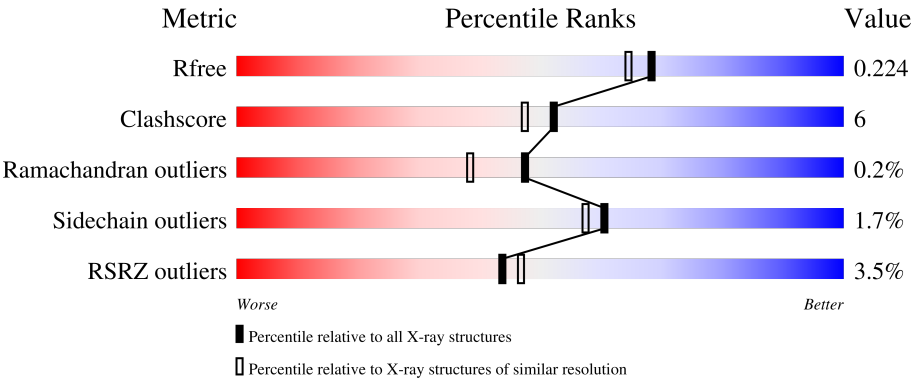
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	708	4% 83% 16%
1	B	708	3% 89% 11%
2	C	2	100%
2	D	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
2	XYP	C	1[B]	X	-	-	-
2	XYP	D	1[B]	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12991 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.

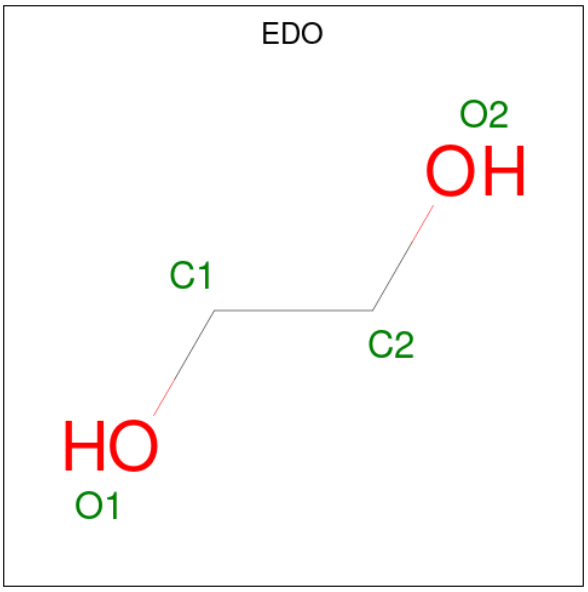
- Molecule 1 is a protein called ALPHA-D-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	17	0
			5741	3662	1018	1041	20			
1	B	708	Total	C	N	O	S	0	21	0
			5753	3669	1019	1046	19			

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	O		0	1	0
			29	15	14				
2	D	2	Total	C	O		0	1	0
			29	15	14				

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 5 is water.

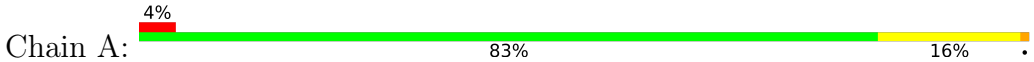
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	684	Total O 684 684	0	62
5	B	699	Total O 699 699	0	54

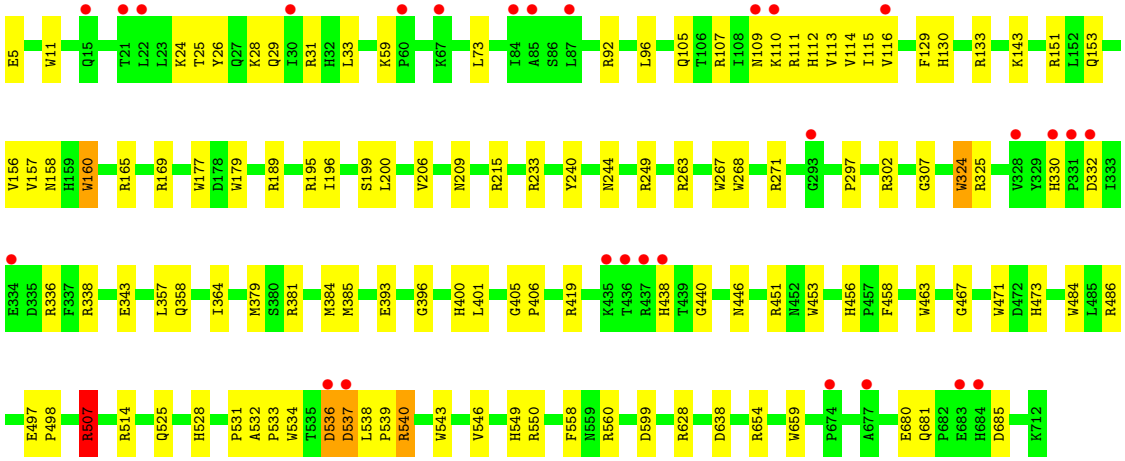
3 Residue-property plots

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

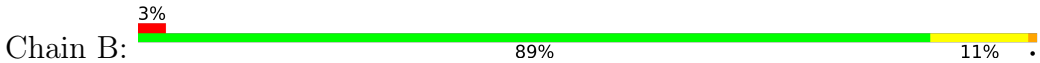
Chain A:

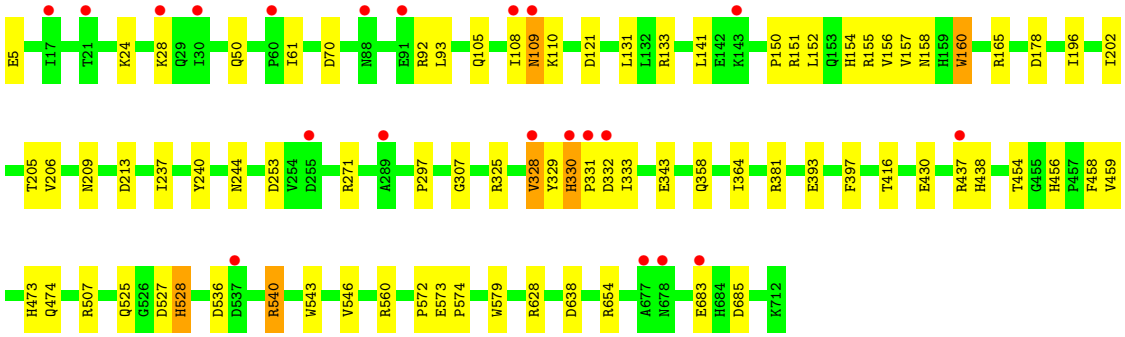




• Molecule 1: ALPHA-D-GLUCURONIDASE

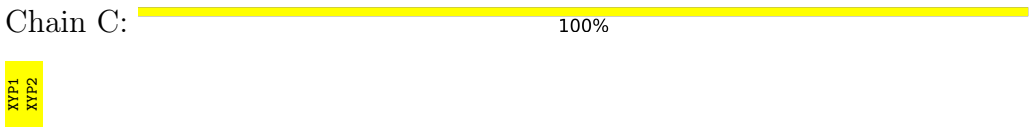
Chain B:



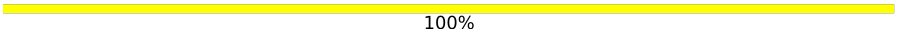


• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain C:



• Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain D: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.56Å 74.61Å 87.45Å 115.23° 93.15° 109.17°	Depositor
Resolution (Å)	20.00 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-1.90) 94.9 (19.99-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.172 , 0.221 0.182 , 0.224	Depositor DCC
R_{free} test set	830 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12991	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.94% 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: EDO, CO, XYP

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	0.92	12/5992 (0.2%)	1.13	54/8146 (0.7%)
1	B	0.76	3/6026 (0.0%)	0.94	16/8194 (0.2%)
All	All	0.84	15/12018 (0.1%)	1.04	70/16340 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	TRP	NE1-CE2	9.09	1.49	1.37
1	B	579	TRP	NE1-CE2	8.96	1.49	1.37
1	A	463	TRP	NE1-CE2	8.84	1.49	1.37
1	B	160	TRP	NE1-CE2	8.75	1.49	1.37
1	A	534	TRP	NE1-CE2	8.74	1.49	1.37
1	B	543	TRP	NE1-CE2	8.74	1.49	1.37
1	A	177	TRP	NE1-CE2	6.55	1.46	1.37
1	A	267	TRP	NE1-CE2	6.39	1.45	1.37
1	A	471	TRP	NE1-CE2	6.28	1.45	1.37
1	A	179	TRP	NE1-CE2	6.27	1.45	1.37
1	A	484	TRP	NE1-CE2	5.93	1.45	1.37
1	A	453	TRP	NE1-CE2	5.81	1.45	1.37
1	A	268	TRP	NE1-CE2	5.75	1.45	1.37
1	A	324	TRP	NE1-CE2	5.69	1.45	1.37
1	A	160	TRP	NE1-CE2	5.53	1.44	1.37

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	685	ASP	CB-CG-OD2	9.18	126.56	118.30
1	A	325	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	271	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	381	ARG	NE-CZ-NH2	-8.36	116.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	507	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	92	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	189	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	419	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	514	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	486	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	107[A]	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	107[B]	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	302	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	249	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	338	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	213	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	263	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	338	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	381	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	233	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	195	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	169	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	165	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	233	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	263	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	107[A]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	107[B]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	451	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	514	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	628	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	31	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	133	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	133	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	195	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	419	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	654	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	178	ASP	CB-CG-OD2	6.12	123.80	118.30
1	B	560	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	151	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	336	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	486	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	271	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	92	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	654	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	92	ARG	NE-CZ-NH1	5.81	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	302	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	121	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	70	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	451	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	215	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	599	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	507	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	638	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	638	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	628	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	336	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	165	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	381[A]	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	381[B]	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	654	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	253	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	271	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	397	PHE	CB-CG-CD1	5.15	124.40	120.80
1	A	189	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	685	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	560	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	165	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	560	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	5741	0	5580	63	0
1	B	5753	0	5588	64	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
3	A	24	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	36	3	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	684	0	0	9	0
5	B	699	0	0	5	0
All	All	12991	0	11240	127	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 6.

All (127) 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:384[B]:MET:SD	1:A:384[B]:MET:CE	2.03	1.45
1:A:536:ASP:OD1	1:A:546:VAL:HG21	1.62	1.00
1:B:330[A]:HIS:CE1	1:B:332:ASP:HB2	1.97	0.99
1:A:536:ASP:O	1:A:537:ASP:OD1	1.83	0.97
1:A:550[A]:ARG:NH2	1:A:558:PHE:CZ	2.38	0.91
1:B:527:ASP:O	1:B:528:HIS:HB2	1.69	0.91
1:B:109:ASN:O	1:B:110:LYS:HB3	1.78	0.83
1:A:531:PRO:HG3	1:A:659:TRP:HA	1.60	0.81
1:A:525:GLN:HE22	1:A:528:HIS:HE1	1.31	0.79
1:B:330[A]:HIS:CD2	1:B:331:PRO:HD2	2.18	0.79
1:B:330[A]:HIS:NE2	1:B:332:ASP:HB2	1.98	0.78
1:B:330[A]:HIS:CE1	1:B:332:ASP:H	2.06	0.74
1:A:5:GLU:N	5:A:2004[A]:HOH:O	2.19	0.74
1:A:357:LEU:HD23	1:A:384[B]:MET:HE1	1.70	0.74
1:A:550[A]:ARG:NH2	1:A:558:PHE:CE2	2.57	0.72
1:A:536:ASP:OD1	1:A:546:VAL:CG2	2.38	0.70
1:B:108:ILE:O	1:B:109:ASN:OD1	2.10	0.70
1:A:324:TRP:HB3	5:A:2379:HOH:O	1.92	0.70
1:A:537:ASP:O	1:A:537:ASP:CG	2.28	0.69
1:B:151:ARG:HH12	1:B:474:GLN:HE21	1.37	0.69
1:B:527:ASP:O	1:B:528:HIS:CB	2.42	0.67
1:A:357:LEU:HD23	1:A:384[B]:MET:CE	2.25	0.66
1:B:196:ILE:HD11	3:B:1716:EDO:H22	1.78	0.66
1:A:525:GLN:NE2	1:A:528:HIS:HE1	1.93	0.65
1:B:330[A]:HIS:CE1	1:B:332:ASP:CB	2.76	0.64
1:B:154:HIS:HE1	1:B:438:HIS:HD2	1.46	0.64
1:B:456:HIS:HD2	1:B:458:PHE:H	1.48	0.60
1:A:109:ASN:O	1:A:110:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASN:O	1:B:110:LYS:CB	2.47	0.60
1:A:153[B]:GLN:OE1	1:A:438:HIS:HA	2.02	0.59
1:A:297:PRO:HG3	1:A:307:GLY:HA3	1.84	0.59
1:A:200:LEU:HD13	1:A:467:GLY:HA3	1.86	0.58
1:A:196:ILE:HD11	3:A:1716:EDO:H22	1.86	0.58
1:A:406:PRO:HG2	5:A:2478:HOH:O	2.03	0.57
1:A:332:ASP:HB3	5:A:2355:HOH:O	2.03	0.57
1:B:573[B]:GLU:HB3	1:B:574:PRO:HD3	1.86	0.57
1:A:456:HIS:HD2	1:A:458:PHE:H	1.53	0.57
1:B:329:TYR:CD1	1:B:329:TYR:N	2.71	0.57
1:B:330[A]:HIS:HE1	1:B:332:ASP:HB2	1.64	0.57
1:B:536[B]:ASP:OD1	1:B:546:VAL:HG21	2.06	0.56
1:A:5:GLU:N	5:A:2001:HOH:O	2.38	0.56
1:B:330[A]:HIS:HD2	1:B:331:PRO:HD2	1.69	0.56
1:B:573[A]:GLU:HB2	1:B:574:PRO:HD3	1.88	0.56
1:B:5:GLU:N	5:B:2004:HOH:O	2.38	0.55
1:B:330[A]:HIS:CE1	1:B:332:ASP:N	2.73	0.55
1:A:158:ASN:HD21	1:A:358:GLN:HE22	1.55	0.55
1:A:206:VAL:HG22	1:A:240:TYR:HB2	1.89	0.55
1:B:152:LEU:O	1:B:155:ARG:NH1	2.38	0.55
1:A:156[B]:VAL:HG22	1:A:157:VAL:O	2.06	0.55
1:A:160:TRP:H	1:A:446:ASN:ND2	2.05	0.55
1:B:330[A]:HIS:NE2	1:B:332:ASP:CB	2.69	0.54
1:B:108:ILE:HG22	1:B:109:ASN:CG	2.28	0.54
1:B:331:PRO:HB3	1:B:540:ARG:HH11	1.73	0.54
1:B:108:ILE:HG22	1:B:109:ASN:ND2	2.24	0.53
1:B:525:GLN:NE2	1:B:528:HIS:HE1	2.06	0.53
1:B:525:GLN:HE22	1:B:528:HIS:HE1	1.56	0.53
1:B:297:PRO:HG3	1:B:307:GLY:HA3	1.91	0.53
1:A:73:LEU:HD12	1:A:114:VAL:O	2.09	0.52
1:A:550[A]:ARG:CZ	1:A:558:PHE:CE2	2.93	0.52
1:A:393:GLU:OE2	1:A:528:HIS:HD2	1.92	0.52
1:B:196:ILE:HG13	3:B:1716:EDO:H11	1.91	0.52
1:B:393:GLU:OE2	1:B:528:HIS:HD2	1.93	0.51
1:A:497:GLU:HB3	1:A:498:PRO:HD3	1.93	0.51
1:B:328[A]:VAL:CG2	1:B:343[A]:GLU:HG3	2.41	0.50
1:A:396:GLY:HA3	1:A:400:HIS:CG	2.46	0.50
1:B:108:ILE:HG22	1:B:109:ASN:OD1	2.12	0.50
1:A:196:ILE:HG13	3:A:1716:EDO:H11	1.93	0.49
1:B:196:ILE:CD1	3:B:1716:EDO:H22	2.41	0.49
1:B:131:LEU:HD12	5:B:2156:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:HA	5:A:2379:HOH:O	2.13	0.49
1:A:357:LEU:HB3	1:A:384[B]:MET:HE2	1.95	0.49
1:B:330[A]:HIS:CE1	1:B:332:ASP:CA	2.96	0.48
1:A:160:TRP:H	1:A:446:ASN:HD21	1.61	0.48
1:A:540:ARG:HD3	1:A:543:TRP:CE2	2.49	0.48
1:A:456:HIS:HE1	5:A:2413:HOH:O	1.97	0.47
1:A:115:ILE:O	1:A:115:ILE:HG13	2.14	0.47
1:B:156[B]:VAL:HG22	1:B:157:VAL:O	2.15	0.47
1:B:150:PRO:HB2	1:B:155:ARG:NH1	2.30	0.47
1:A:26:TYR:HA	1:A:29:GLN:HE21	1.80	0.46
1:B:330[A]:HIS:CD2	1:B:331:PRO:CD	2.95	0.46
1:A:105:GLN:NE2	1:A:143:LYS:H	2.13	0.46
1:A:112:HIS:C	1:A:113:VAL:HG13	2.36	0.46
1:B:473:HIS:HD2	5:B:2418:HOH:O	1.98	0.46
1:A:393:GLU:OE2	1:A:528:HIS:CD2	2.69	0.46
1:B:540:ARG:HH11	1:B:540:ARG:HD2	1.59	0.46
1:B:108:ILE:C	1:B:109:ASN:CG	2.75	0.45
1:A:25:THR:O	1:A:29:GLN:HG3	2.16	0.45
1:A:379:MET:HG3	1:A:384[B]:MET:HE1	1.99	0.45
1:B:158:ASN:HD21	1:B:358:GLN:HE22	1.65	0.45
1:B:160:TRP:HA	1:B:209:ASN:HA	1.99	0.45
1:A:33[B]:LEU:HD23	1:A:73:LEU:HB3	1.99	0.44
1:A:330:HIS:CD2	1:A:343:GLU:OE2	2.71	0.44
1:A:405:GLY:N	1:A:406:PRO:CD	2.80	0.44
1:B:628:ARG:NH2	5:B:2602:HOH:O	2.37	0.44
1:A:116:VAL:HG12	1:A:116:VAL:O	2.17	0.44
1:A:109:ASN:O	1:A:110:LYS:CB	2.64	0.44
1:A:384[B]:MET:CE	1:A:384[B]:MET:CG	2.95	0.43
1:B:131:LEU:CD1	5:B:2156:HOH:O	2.67	0.43
1:B:416:THR:O	1:B:572:PRO:HG2	2.17	0.43
1:A:29:GLN:HG2	5:A:2125:HOH:O	2.17	0.43
1:A:129:PHE:CG	1:A:199:SER:HA	2.53	0.43
1:A:546:VAL:HA	1:A:549:HIS:NE2	2.34	0.43
1:B:205[B]:THR:HG23	1:B:237:ILE:CG2	2.48	0.43
1:B:50:GLN:HG3	1:B:61:ILE:O	2.19	0.43
1:B:206:VAL:HG22	1:B:240:TYR:HB2	2.01	0.43
1:B:24:LYS:O	1:B:28:LYS:HG2	2.19	0.42
1:B:133:ARG:HH11	1:B:133:ARG:HD3	1.60	0.42
1:B:325:ARG:HH11	1:B:325:ARG:HD3	1.59	0.42
1:B:430:GLU:OE1	1:B:473:HIS:HE1	2.01	0.42
1:A:401:LEU:C	1:A:401:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:HIS:HD2	5:A:2458:HOH:O	2.02	0.42
1:A:507:ARG:C	1:A:507:ARG:HD3	2.39	0.42
1:B:205[B]:THR:HG23	1:B:237:ILE:HG21	2.01	0.42
1:A:538:LEU:O	1:A:539:PRO:C	2.58	0.42
1:A:160:TRP:HA	1:A:209:ASN:HA	2.03	0.41
1:A:130:HIS:CE1	3:A:1715:EDO:H12	2.56	0.41
1:A:532:ALA:N	1:A:533:PRO:HD3	2.35	0.41
1:B:155:ARG:O	1:B:202[B]:ILE:HG23	2.21	0.41
1:A:385[B]:MET:HE2	1:A:440:GLY:HA3	2.03	0.40
1:A:24:LYS:O	1:A:28:LYS:HG2	2.21	0.40
1:B:393:GLU:OE2	1:B:528:HIS:CD2	2.73	0.40
1:B:454:THR:HB	1:B:459:VAL:HB	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	723/708 (102%)	703 (97%)	19 (3%)	1 (0%)	51	42
1	B	727/708 (103%)	702 (97%)	23 (3%)	2 (0%)	41	31
All	All	1450/1416 (102%)	1405 (97%)	42 (3%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	528	HIS
1	A	364	ILE
1	B	364	ILE

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	605/588 (103%)	593 (98%)	12 (2%)	55	51
1	B	609/588 (104%)	597 (98%)	12 (2%)	55	51
All	All	1214/1176 (103%)	1190 (98%)	24 (2%)	60	51

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	96	LEU
1	A	111	ARG
1	A	244	ASN
1	A	507	ARG
1	A	536	ASP
1	A	537	ASP
1	A	540	ARG
1	A	680[A]	GLU
1	A	680[B]	GLU
1	A	681[A]	GLN
1	A	681[B]	GLN
1	B	93	LEU
1	B	109	ASN
1	B	141	LEU
1	B	244	ASN
1	B	328[A]	VAL
1	B	328[B]	VAL
1	B	330[A]	HIS
1	B	330[B]	HIS
1	B	437	ARG
1	B	507	ARG
1	B	540	ARG
1	B	683	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	27	GLN
1	A	29	GLN
1	A	58	ASN
1	A	105	GLN
1	A	244	ASN
1	A	358	GLN
1	A	446	ASN
1	A	456	HIS
1	A	473	HIS
1	A	512	ASN
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	154	HIS
1	B	244	ASN
1	B	266	GLN
1	B	358	GLN
1	B	438	HIS
1	B	456	HIS
1	B	473	HIS
1	B	474	GLN
1	B	501	GLN
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)

6 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	XYP	C	1[A]	2	10,10,10	1.87	1 (10%)	14,14,14	0.98	0
2	XYP	C	1[B]	2	10,10,10	1.73	1 (10%)	14,14,14	0.97	0
2	XYP	C	2	2	9,9,10	1.54	1 (11%)	10,12,14	1.34	2 (20%)
2	XYP	D	1[A]	2	10,10,10	2.04	1 (10%)	14,14,14	1.03	0
2	XYP	D	1[B]	2	10,10,10	1.58	1 (10%)	14,14,14	1.11	1 (7%)
2	XYP	D	2	2	9,9,10	1.18	1 (11%)	10,12,14	1.42	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	1[A]	2	-	-	0/1/1/1
2	XYP	C	1[B]	2	1/1/4/4	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	D	1[A]	2	-	-	0/1/1/1
2	XYP	D	1[B]	2	1/1/4/4	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1[A]	XYP	O5-C1	-5.91	1.34	1.43
2	C	1[A]	XYP	O5-C1	-5.51	1.35	1.43
2	C	1[B]	XYP	O5-C1	-5.13	1.36	1.43
2	D	1[B]	XYP	O5-C1	-4.49	1.36	1.43
2	C	2	XYP	O5-C1	-3.69	1.35	1.42
2	D	2	XYP	O5-C1	-2.70	1.37	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	XYP	C4-C3-C2	-3.05	107.30	110.92
2	C	2	XYP	C4-C3-C2	-2.29	108.20	110.92
2	C	2	XYP	C1-C2-C3	2.11	112.26	109.67
2	D	1[B]	XYP	C5-O5-C1	2.07	116.18	112.71

All (2) chirality outliers are listed below:

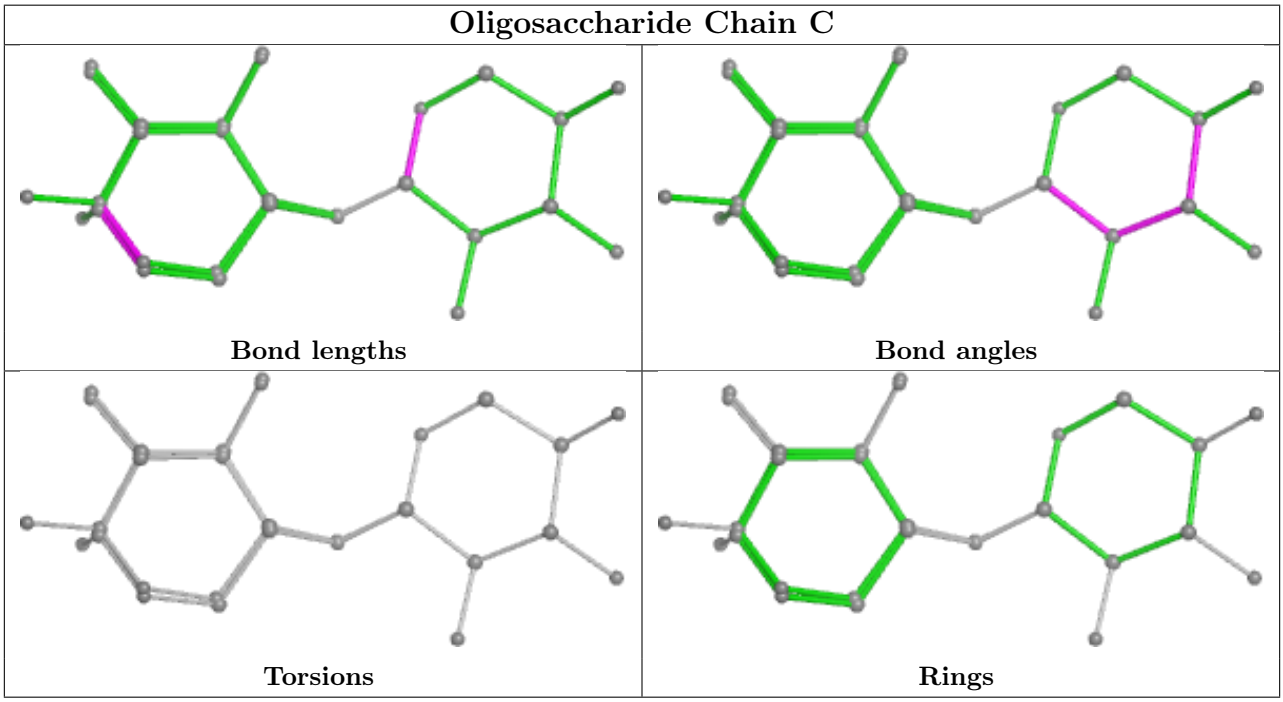
Mol	Chain	Res	Type	Atom
2	C	1[B]	XYP	C1
2	D	1[B]	XYP	C1

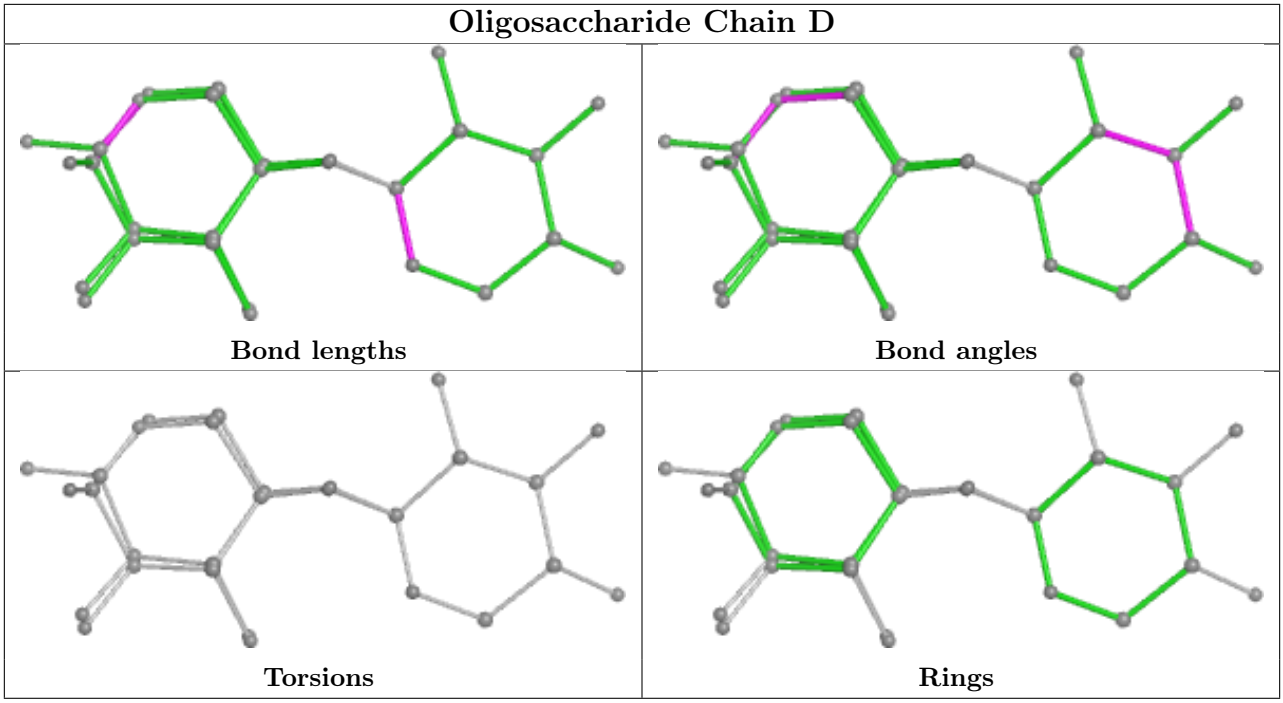
There are no torsion outliers.

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.





5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	EDO	B	1718	-	3,3,3	0.27	0	2,2,2	0.70	0
3	EDO	A	1715	-	3,3,3	0.24	0	2,2,2	0.51	0
3	EDO	B	1716	-	3,3,3	0.45	0	2,2,2	0.15	0
3	EDO	B	1714	-	3,3,3	0.35	0	2,2,2	1.04	0
3	EDO	A	1714	-	3,3,3	0.34	0	2,2,2	0.75	0
3	EDO	B	1715	-	3,3,3	0.32	0	2,2,2	0.43	0
3	EDO	A	1717	-	3,3,3	0.32	0	2,2,2	0.51	0
3	EDO	A	1718	-	3,3,3	0.40	0	2,2,2	0.18	0
3	EDO	B	1713	-	3,3,3	0.42	0	2,2,2	0.62	0
3	EDO	A	1716	-	3,3,3	0.44	0	2,2,2	0.25	0
3	EDO	B	1717	-	3,3,3	0.33	0	2,2,2	0.53	0
3	EDO	A	1713	-	3,3,3	0.24	0	2,2,2	0.70	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
3	EDO	B	1718	-	-	0/1/1/1	-
3	EDO	A	1715	-	-	0/1/1/1	-
3	EDO	B	1716	-	-	0/1/1/1	-
3	EDO	B	1714	-	-	0/1/1/1	-
3	EDO	A	1714	-	-	0/1/1/1	-
3	EDO	B	1715	-	-	1/1/1/1	-
3	EDO	A	1717	-	-	0/1/1/1	-
3	EDO	A	1718	-	-	0/1/1/1	-
3	EDO	B	1713	-	-	0/1/1/1	-
3	EDO	A	1716	-	-	0/1/1/1	-
3	EDO	B	1717	-	-	1/1/1/1	-
3	EDO	A	1713	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1715	EDO	O1-C1-C2-O2
3	B	1717	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
3	A	1715	EDO	1	0
3	B	1716	EDO	3	0
3	A	1716	EDO	2	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	708/708 (100%)	0.18	28 (3%)	38	41	12, 18, 33, 47	0
1	B	708/708 (100%)	0.15	21 (2%)	50	53	12, 18, 32, 46	0
All	All	1416/1416 (100%)	0.17	49 (3%)	44	47	12, 18, 33, 47	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	ARG	5.8
1	A	537	ASP	5.1
1	B	330[A]	HIS	4.8
1	B	437	ARG	4.7
1	B	332	ASP	4.5
1	A	435	LYS	4.4
1	B	537	ASP	4.1
1	A	674	PRO	4.1
1	B	328[A]	VAL	3.9
1	A	332	ASP	3.8
1	B	677	ALA	3.6
1	A	683	GLU	3.6
1	A	331	PRO	3.6
1	B	88	ASN	3.5
1	A	330	HIS	3.1
1	A	110	LYS	3.0
1	B	30[A]	ILE	3.0
1	A	293	GLY	3.0
1	A	60	PRO	3.0
1	A	677	ALA	2.9
1	B	143[A]	LYS	2.9
1	B	683	GLU	2.9
1	A	116	VAL	2.9
1	A	684	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	109	ASN	2.8
1	B	331	PRO	2.8
1	A	21	THR	2.8
1	A	536	ASP	2.7
1	A	67	LYS	2.7
1	A	438	HIS	2.6
1	A	87	LEU	2.5
1	B	60	PRO	2.5
1	A	328	VAL	2.5
1	B	91	GLU	2.4
1	A	334	GLU	2.3
1	A	22	LEU	2.3
1	A	436	THR	2.3
1	B	17	ILE	2.3
1	B	108	ILE	2.3
1	A	30[A]	ILE	2.2
1	B	255	ASP	2.2
1	B	289	ALA	2.2
1	B	678	ASN	2.2
1	A	84[A]	ILE	2.1
1	A	109	ASN	2.1
1	B	21	THR	2.0
1	A	15	GLN	2.0
1	B	28	LYS	2.0
1	A	85	ALA	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYP	C	1[A]	10/10	0.95	0.12	23,25,26,26	10
2	XYP	C	1[B]	10/10	0.95	0.12	22,23,23,24	10
2	XYP	C	2	9/10	0.95	0.10	19,20,23,24	0

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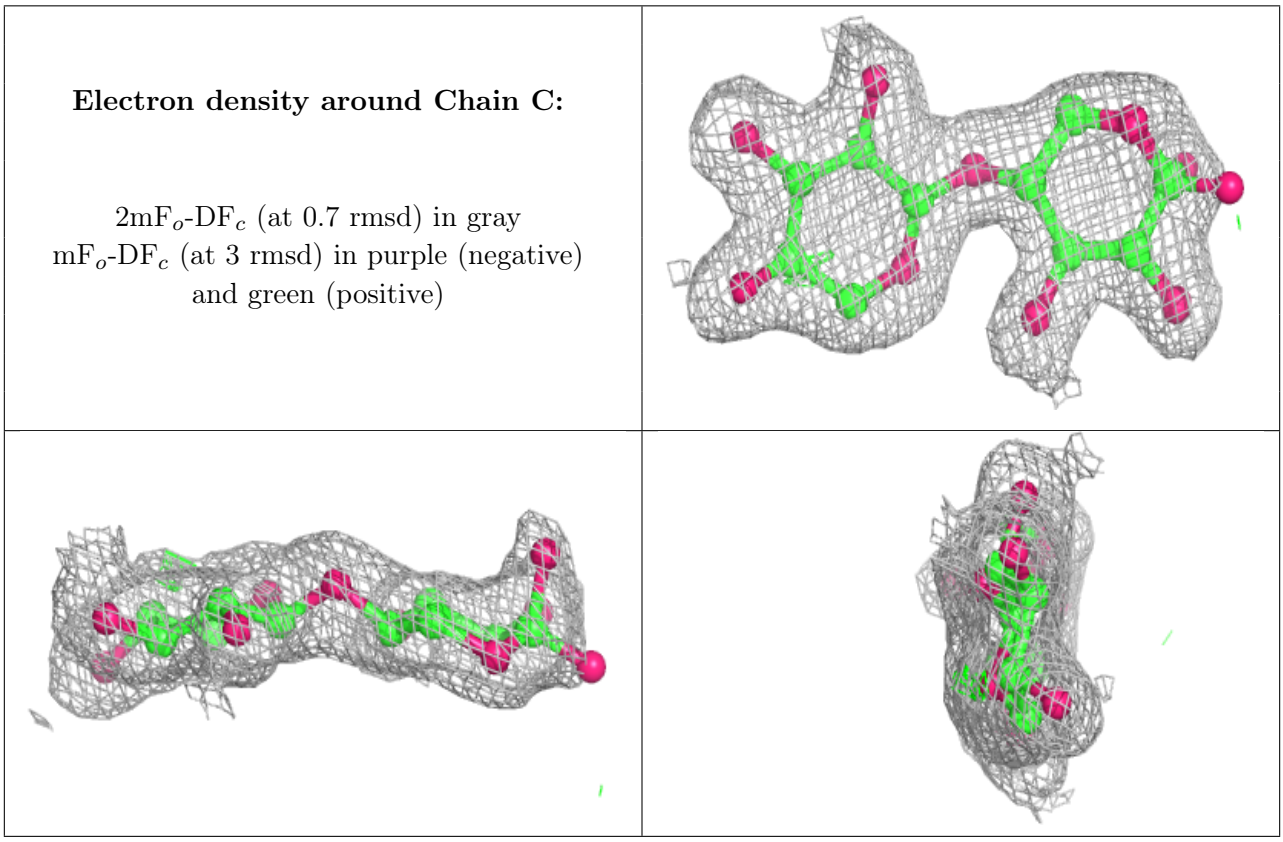
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYP	D	1[A]	10/10	0.95	0.12	25,30,31,33	10
2	XYP	D	1[B]	10/10	0.95	0.12	20,21,22,22	10
2	XYP	D	2	9/10	0.97	0.09	16,18,21,21	0

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.

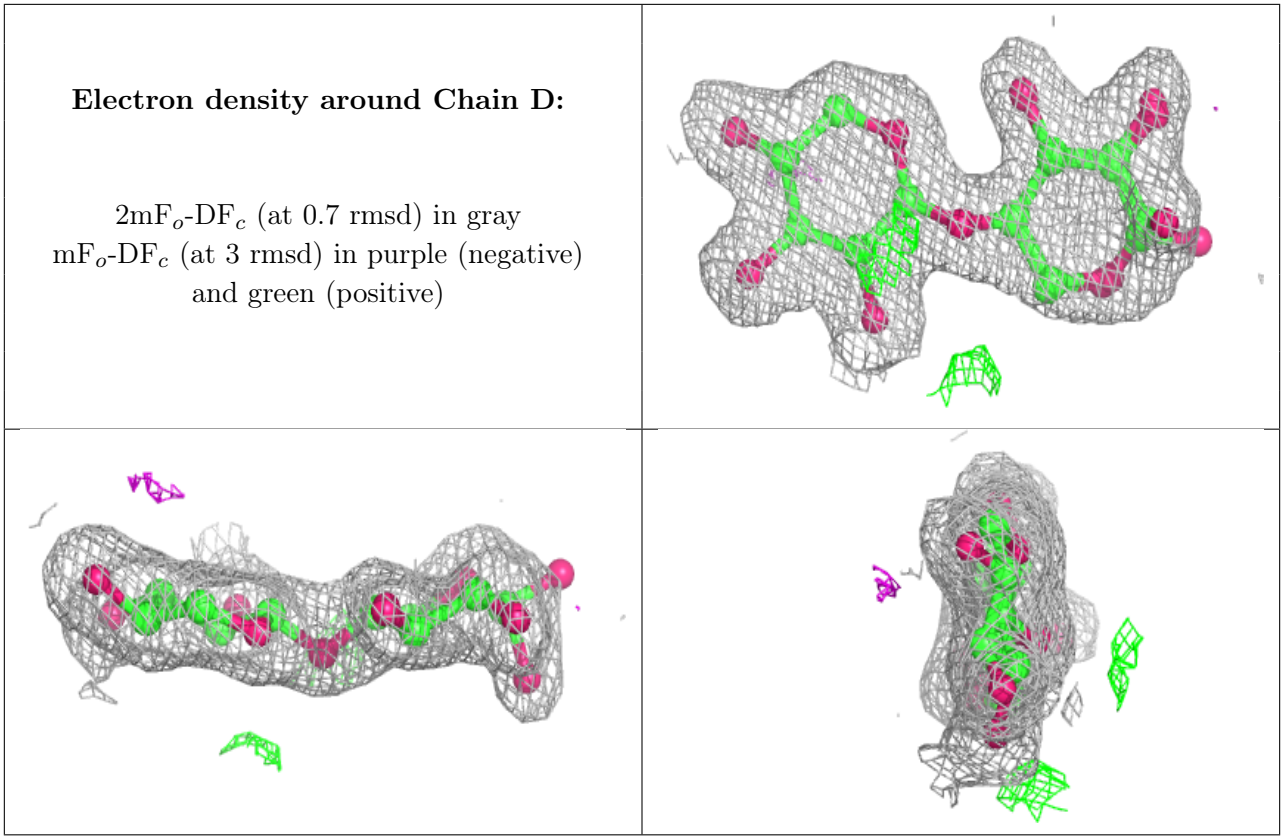
Electron density around Chain C:

$2mF_o$-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

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	EDO	B	1714	4/4	0.88	0.15	26,29,30,37	0
3	EDO	A	1718	4/4	0.90	0.21	24,32,33,33	0
3	EDO	B	1717	4/4	0.92	0.09	40,41,41,41	0
3	EDO	A	1717	4/4	0.93	0.12	30,33,35,37	0
3	EDO	B	1718	4/4	0.93	0.16	24,25,25,27	0
3	EDO	B	1715	4/4	0.94	0.10	27,28,30,32	0
3	EDO	A	1714	4/4	0.95	0.11	22,23,25,26	0
3	EDO	A	1715	4/4	0.95	0.12	22,23,23,23	0
3	EDO	B	1716	4/4	0.97	0.07	14,18,21,21	0
3	EDO	B	1713	4/4	0.98	0.09	15,15,16,16	0
3	EDO	A	1716	4/4	0.98	0.08	14,18,19,21	0
4	CO	B	1724[A]	1/1	0.98	0.09	23,23,23,23	1
4	CO	A	1721[A]	1/1	0.99	0.08	22,22,22,22	1
4	CO	A	1722[A]	1/1	0.99	0.07	20,20,20,20	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CO	A	1723[A]	1/1	0.99	0.08	22,22,22,22	1
4	CO	A	1724[A]	1/1	0.99	0.09	23,23,23,23	1
4	CO	B	1721[A]	1/1	0.99	0.05	22,22,22,22	1
4	CO	B	1722[A]	1/1	0.99	0.08	19,19,19,19	1
4	CO	B	1723[A]	1/1	0.99	0.09	20,20,20,20	1
3	EDO	A	1713	4/4	0.99	0.08	13,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.