



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:06 AM UTC

PDB ID : 7EXR / pdb_00007exr
Title : Crystal structure of alkaline alpha-galactosidase D383A mutant from *Arabidopsis thaliana* complexed with Stachyose.
Authors : Chuankhayan, P.; Guan, H.H.; Lin, C.C.; Chen, N.C.; Huang, Y.C.; Yoshimura, M.; Nakagawa, A.; Lee, R.H.; Chen, C.J.
Deposited on : 2021-05-28
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

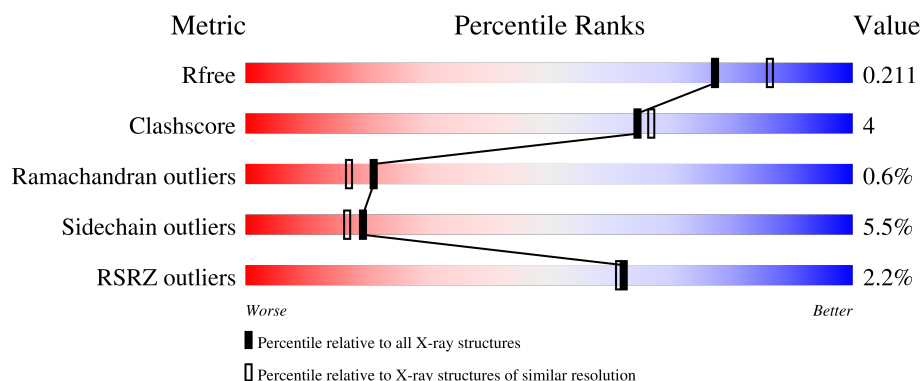
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	749	3% 84% 10% ...
1	B	749	% 83% 11% ...
2	C	4	25% 75%
2	D	4	25% 75%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11874 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.

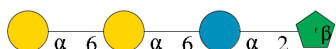
- Molecule 1 is a protein called Probable galactinol–sucrose galactosyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	718	Total	C	N	O	S	0	0	0
			5620	3573	969	1049	29			
1	A	718	Total	C	N	O	S	0	0	0
			5620	3573	969	1049	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	302	ARG	LYS	conflict	UNP Q8RX87
B	383	ALA	ASP	engineered mutation	UNP Q8RX87
A	302	ARG	LYS	conflict	UNP Q8RX87
A	383	ALA	ASP	engineered mutation	UNP Q8RX87

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	D	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	328	Total	O	0	0
			328	328		

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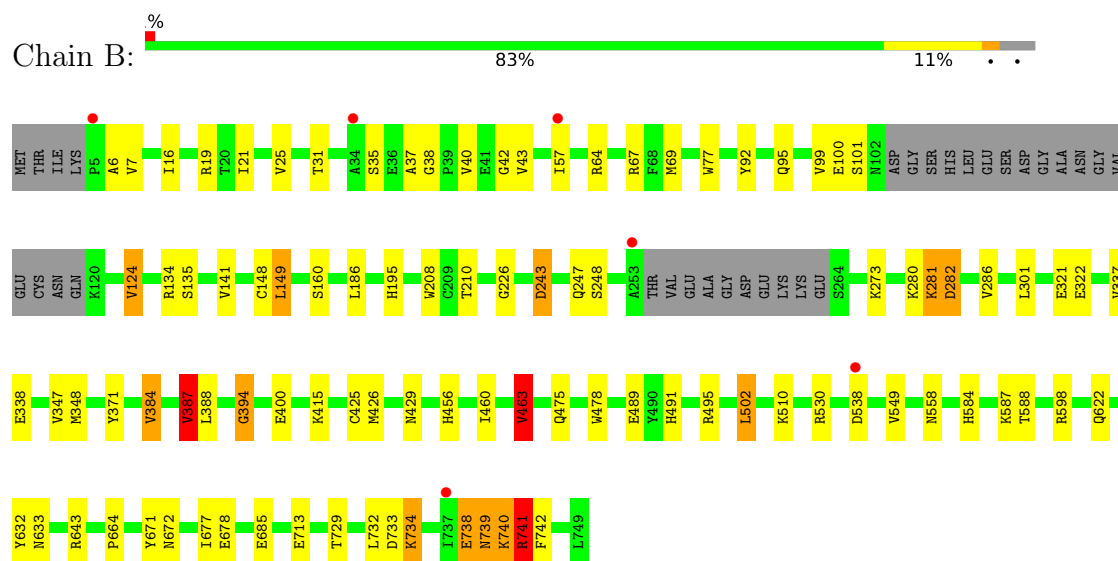
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total 216	O 216	0	0

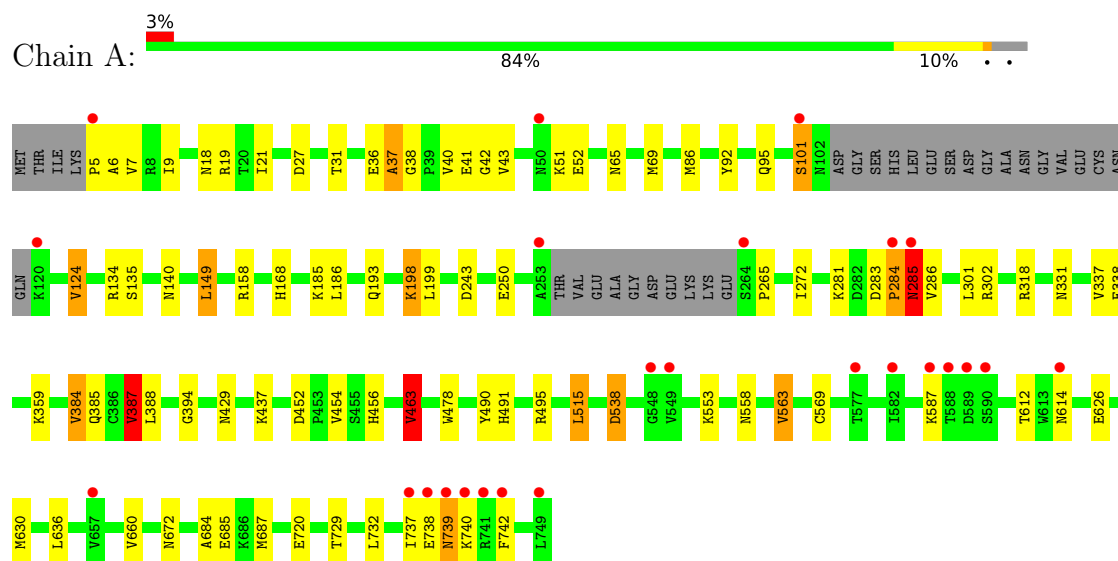
3 Residue-property plots [i](#)

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: Probable galactinol–sucrose galactosyltransferase 6



- Molecule 1: Probable galactinol–sucrose galactosyltransferase 6



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain C:  25% 75%

FRU1
GLC2
GLA3
GLA4

- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain D:  25% 75%

FRU1
GLC2
GLA3
GLA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.59Å 103.75Å 182.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.00) 99.7 (30.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.167 , 0.206 0.176 , 0.211	Depositor DCC
R_{free} test set	6172 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11874	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GLA, GLC, FRU

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	1.28	3/5754 (0.1%)	1.16	21/7793 (0.3%)
1	B	1.25	12/5754 (0.2%)	1.18	25/7793 (0.3%)
All	All	1.27	15/11508 (0.1%)	1.17	46/15586 (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	2
1	B	0	2
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ASN	C-N	-35.17	0.93	1.33
1	A	284	PRO	C-N	-25.05	0.98	1.33
1	B	530	ARG	C-O	-6.96	1.15	1.24
1	B	734	LYS	CA-C	-6.17	1.45	1.52
1	B	195	HIS	C-O	-5.85	1.16	1.24
1	B	538	ASP	CB-CG	-5.73	1.37	1.52
1	B	37	ALA	CA-C	5.61	1.60	1.52
1	B	463	VAL	N-CA	5.55	1.52	1.46
1	B	371	TYR	CA-C	5.53	1.59	1.52
1	B	322	GLU	CA-C	5.50	1.59	1.52
1	B	64	ARG	CA-C	-5.50	1.45	1.52
1	B	99	VAL	C-O	-5.37	1.18	1.24
1	A	265	PRO	CA-C	5.33	1.58	1.52
1	B	394	GLY	N-CA	5.12	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	425	CYS	C-O	-5.08	1.18	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	PRO	O-C-N	14.89	141.81	122.89
1	B	37	ALA	N-CA-C	10.46	126.35	113.17
1	B	387	VAL	CB-CA-C	-10.41	96.03	112.16
1	A	285	ASN	O-C-N	-10.38	108.78	122.59
1	A	124	VAL	CB-CA-C	-10.13	96.70	110.98
1	A	285	ASN	CA-C-N	10.02	135.06	122.43
1	A	285	ASN	C-N-CA	10.02	135.06	122.43
1	A	387	VAL	CB-CA-C	-9.67	97.93	112.05
1	B	124	VAL	CB-CA-C	-9.34	97.81	110.98
1	B	738	GLU	CA-C-N	8.41	136.84	121.70
1	B	738	GLU	C-N-CA	8.41	136.84	121.70
1	A	37	ALA	N-CA-C	8.20	122.85	113.01
1	B	530	ARG	NE-CZ-NH2	-8.16	111.85	119.20
1	B	25	VAL	CA-C-N	-7.76	112.71	120.31
1	B	25	VAL	C-N-CA	-7.76	112.71	120.31
1	A	563	VAL	CB-CA-C	-7.55	97.20	110.71
1	A	387	VAL	N-CA-CB	7.35	122.07	110.54
1	B	530	ARG	NE-CZ-NH1	7.06	128.56	121.50
1	B	463	VAL	CA-CB-CG1	6.84	122.04	110.40
1	B	538	ASP	CB-CA-C	-6.82	96.85	110.42
1	A	742	PHE	N-CA-C	-6.79	99.43	109.81
1	B	42	GLY	N-CA-C	-6.67	100.72	111.59
1	B	387	VAL	N-CA-CB	6.59	121.91	110.65
1	A	283	ASP	CA-C-N	-6.47	113.30	119.90
1	A	283	ASP	C-N-CA	-6.47	113.30	119.90
1	B	463	VAL	CB-CA-C	6.26	119.89	111.88
1	B	160	SER	N-CA-C	6.21	118.85	109.23
1	A	463	VAL	N-CA-CB	-6.01	102.87	110.57
1	B	124	VAL	N-CA-CB	5.94	120.37	110.86
1	A	385	GLN	N-CA-C	5.77	117.65	111.36
1	B	124	VAL	CA-CB-CG2	5.77	120.20	110.40
1	B	387	VAL	CA-CB-CG2	5.72	120.12	110.40
1	B	734	LYS	N-CA-C	-5.68	100.67	109.24
1	B	463	VAL	N-CA-CB	-5.64	104.25	110.51
1	A	199	LEU	CA-C-N	-5.62	114.47	120.03
1	A	199	LEU	C-N-CA	-5.62	114.47	120.03
1	A	614	ASN	CB-CA-C	-5.52	99.44	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	741	ARG	N-CA-C	5.47	122.45	110.80
1	B	348	MET	CG-SD-CE	-5.39	89.04	100.90
1	A	614	ASN	N-CA-C	5.37	122.25	110.80
1	A	42	GLY	N-CA-C	-5.36	101.42	111.66
1	A	456	HIS	N-CA-C	5.19	116.75	111.14
1	B	530	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	18	ASN	N-CA-C	5.09	118.76	112.24
1	B	124	VAL	CG1-CB-CG2	5.05	121.91	110.80
1	B	37	ALA	O-C-N	-5.00	116.09	122.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	GLY	Peptide
1	A	684	ALA	Peptide
1	B	394	GLY	Peptide
1	B	740	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5620	0	5537	40	0
1	B	5620	0	5539	44	0
2	C	45	0	39	4	0
2	D	45	0	39	0	0
3	A	216	0	0	4	0
3	B	328	0	0	9	0
All	All	11874	0	11154	87	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 4.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:FRU:O5	2:C:1:FRU:C5	1.63	1.17
1:B:95:GLN:HE21	1:B:134:ARG:HH21	1.21	0.88
1:B:210:THR:OG1	3:B:801:HOH:O	1.91	0.88
1:B:738:GLU:HB3	1:B:739:ASN:HB2	1.57	0.85
1:A:284:PRO:O	1:A:285:ASN:CB	2.28	0.82
1:A:284:PRO:O	1:A:285:ASN:HB2	1.81	0.81
1:A:95:GLN:HE21	1:A:134:ARG:HH21	1.27	0.79
1:B:273:LYS:O	3:B:802:HOH:O	1.99	0.79
1:B:247:GLN:NE2	3:B:803:HOH:O	2.20	0.75
1:A:558:ASN:HD21	1:A:672:ASN:HD21	1.34	0.72
1:A:9:ILE:HD12	1:A:31:THR:HG21	1.70	0.72
2:C:2:GLC:H62	2:C:3:GLA:H5	1.73	0.70
1:B:584:HIS:HD2	3:B:979:HOH:O	1.75	0.69
1:A:515:LEU:HD23	1:A:515:LEU:C	2.18	0.69
1:B:558:ASN:HD21	1:B:672:ASN:HD21	1.39	0.69
1:A:250:GLU:OE1	1:A:318:ARG:HD3	1.96	0.65
1:B:35:SER:O	1:B:38:GLY:HA2	1.98	0.63
1:B:95:GLN:HE22	1:B:429:ASN:HA	1.64	0.63
1:B:475:GLN:HG3	3:B:804:HOH:O	1.98	0.63
1:B:738:GLU:HB3	1:B:739:ASN:CB	2.29	0.63
1:B:7:VAL:HG13	1:B:16:ILE:CD1	2.31	0.61
1:B:243:ASP:N	3:B:801:HOH:O	2.32	0.60
1:A:31:THR:HB	1:A:43:VAL:CG1	2.32	0.58
1:A:720:GLU:HB2	1:A:729:THR:HG22	1.88	0.56
1:B:739:ASN:O	1:B:741:ARG:N	2.39	0.56
1:A:463:VAL:HG13	1:A:478:TRP:CE2	2.41	0.56
1:A:92:TYR:CE1	1:A:338:GLU:HG2	2.41	0.55
1:A:95:GLN:HE22	1:A:429:ASN:HA	1.70	0.55
1:A:384:VAL:O	1:A:387:VAL:HG22	2.08	0.53
3:A:1008:HOH:O	2:C:2:GLC:H61	2.07	0.53
1:B:491:HIS:HD1	1:B:495:ARG:HH12	1.56	0.53
1:B:31:THR:HB	1:B:43:VAL:HG22	1.91	0.52
1:B:678:GLU:HG3	1:B:742:PHE:CE1	2.46	0.51
1:B:7:VAL:HG13	1:B:16:ILE:HD13	1.91	0.51
1:B:463:VAL:HG13	1:B:478:TRP:CD2	2.46	0.51
1:A:5:PRO:O	1:A:7:VAL:N	2.44	0.51
1:A:490:TYR:OH	1:A:569:CYS:HB3	2.10	0.51
1:B:685:GLU:H	1:B:685:GLU:CD	2.19	0.50
1:A:198:LYS:HD3	3:A:802:HOH:O	2.10	0.50
1:A:37:ALA:N	1:A:38:GLY:HA2	2.26	0.49
1:A:538:ASP:OD2	1:A:553:LYS:NZ	2.45	0.49
1:A:630:MET:SD	1:A:636:LEU:HB2	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:VAL:O	1:B:387:VAL:HG22	2.13	0.48
1:B:415:LYS:HG3	1:A:437:LYS:HB2	1.95	0.48
1:A:452:ASP:OD1	1:A:454:VAL:HG12	2.14	0.48
1:B:456:HIS:HE1	3:B:1057:HOH:O	1.96	0.48
1:A:491:HIS:O	1:A:495:ARG:HG2	2.14	0.48
1:B:664:PRO:HB2	1:B:677:ILE:HD13	1.96	0.47
1:B:19:ARG:HD3	1:B:101:SER:HB3	1.97	0.47
1:A:463:VAL:HG13	1:A:478:TRP:CD2	2.49	0.47
2:C:2:GLC:H62	2:C:3:GLA:C5	2.41	0.47
1:B:281:LYS:O	1:B:282:ASP:HB2	2.14	0.47
1:A:384:VAL:O	1:A:384:VAL:HG12	2.15	0.47
1:B:281:LYS:O	1:B:282:ASP:CB	2.63	0.46
1:B:16:ILE:HG13	1:B:21:ILE:HG13	1.97	0.46
1:A:739:ASN:H	1:A:740:LYS:HA	1.80	0.46
1:A:491:HIS:HD1	1:A:495:ARG:HH12	1.62	0.46
1:A:515:LEU:C	1:A:515:LEU:CD2	2.89	0.46
1:A:95:GLN:NE2	1:A:134:ARG:HH21	2.05	0.45
1:B:135:SER:OG	1:B:149:LEU:HD13	2.17	0.45
1:B:456:HIS:HD2	1:B:491:HIS:NE2	2.14	0.45
1:A:250:GLU:OE2	1:A:318:ARG:NH1	2.51	0.44
1:B:135:SER:HA	1:B:148:CYS:O	2.16	0.44
1:A:135:SER:OG	1:A:149:LEU:HD13	2.18	0.44
1:B:19:ARG:CD	1:B:101:SER:HB3	2.48	0.43
1:A:737:ILE:O	1:A:739:ASN:ND2	2.52	0.43
1:B:208:TRP:CH2	1:B:226:GLY:HA3	2.53	0.43
1:B:31:THR:HB	1:B:43:VAL:CG2	2.48	0.43
1:B:77:TRP:CD2	1:B:426:MET:HE2	2.54	0.43
1:A:198:LYS:CD	3:A:802:HOH:O	2.66	0.42
1:A:140:ASN:HB2	3:A:884:HOH:O	2.19	0.42
1:A:558:ASN:ND2	1:A:672:ASN:HD21	2.10	0.42
1:A:185:LYS:NZ	1:A:193:GLN:HE21	2.18	0.42
1:B:495:ARG:HB3	1:B:502:LEU:HD22	2.00	0.42
1:B:598:ARG:NH1	1:B:632:TYR:OH	2.53	0.42
1:B:280:LYS:HG2	1:B:286:VAL:HB	2.01	0.42
1:B:92:TYR:CE1	1:B:338:GLU:HG2	2.55	0.41
1:A:65:ASN:OD1	1:A:86:MET:HE1	2.20	0.41
1:B:489:GLU:OE1	1:B:671:TYR:OH	2.38	0.41
1:B:67:ARG:NH1	1:B:100:GLU:OE1	2.54	0.41
1:A:31:THR:HB	1:A:43:VAL:HG11	2.02	0.41
1:B:248:SER:HB2	3:B:802:HOH:O	2.19	0.41
1:B:584:HIS:HE1	3:B:870:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:GLU:HB2	1:B:740:LYS:N	2.36	0.41
1:A:134:ARG:C	1:A:134:ARG:HD3	2.46	0.40
1:A:21:ILE:HD11	1:A:101:SER:HB3	2.04	0.40
1:A:41:GLU:O	1:A:168:HIS:HD2	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	712/749 (95%)	673 (94%)	33 (5%)	6 (1%)	16	11
1	B	712/749 (95%)	680 (96%)	29 (4%)	3 (0%)	30	27
All	All	1424/1498 (95%)	1353 (95%)	62 (4%)	9 (1%)	21	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	ASP
1	B	741	ARG
1	A	6	ALA
1	A	285	ASN
1	A	685	GLU
1	B	6	ALA
1	A	738	GLU
1	A	538	ASP
1	A	384	VAL

5.3.2 Protein sidechains ⓘ

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	614/640 (96%)	580 (94%)	34 (6%)	19	17
1	B	614/640 (96%)	581 (95%)	33 (5%)	20	17
All	All	1228/1280 (96%)	1161 (94%)	67 (6%)	19	17

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	VAL
1	B	57	ILE
1	B	69	MET
1	B	124	VAL
1	B	141	VAL
1	B	149	LEU
1	B	186	LEU
1	B	243	ASP
1	B	281	LYS
1	B	301	LEU
1	B	321	GLU
1	B	337	VAL
1	B	347	VAL
1	B	384	VAL
1	B	387	VAL
1	B	388	LEU
1	B	400	GLU
1	B	460	ILE
1	B	463	VAL
1	B	502	LEU
1	B	510	LYS
1	B	549	VAL
1	B	587	LYS
1	B	588	THR
1	B	622	GLN
1	B	633	ASN
1	B	643	ARG

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Mol	Chain	Res	Type
1	B	713	GLU
1	B	729	THR
1	B	732	LEU
1	B	733	ASP
1	B	734	LYS
1	B	739	ASN
1	A	19	ARG
1	A	27	ASP
1	A	36	GLU
1	A	40	VAL
1	A	51	LYS
1	A	52	GLU
1	A	69	MET
1	A	101	SER
1	A	124	VAL
1	A	149	LEU
1	A	158	ARG
1	A	186	LEU
1	A	198	LYS
1	A	243	ASP
1	A	272	ILE
1	A	281	LYS
1	A	286	VAL
1	A	301	LEU
1	A	302	ARG
1	A	331	ASN
1	A	337	VAL
1	A	359	LYS
1	A	387	VAL
1	A	388	LEU
1	A	463	VAL
1	A	515	LEU
1	A	563	VAL
1	A	587	LYS
1	A	612	THR
1	A	626	GLU
1	A	660	VAL
1	A	687	MET
1	A	732	LEU
1	A	739	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	56	HIS
1	B	95	GLN
1	B	168	HIS
1	B	193	GLN
1	B	385	GLN
1	B	404	GLN
1	B	456	HIS
1	B	558	ASN
1	B	581	ASN
1	B	584	HIS
1	A	56	HIS
1	A	95	GLN
1	A	138	GLN
1	A	142	ASN
1	A	168	HIS
1	A	175	GLN
1	A	187	HIS
1	A	193	GLN
1	A	385	GLN
1	A	404	GLN
1	A	456	HIS
1	A	558	ASN
1	A	581	ASN
1	A	633	ASN
1	A	739	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	FRU	C	1	2	11,12,12	5.12	5 (45%)	10,18,18	1.17	1 (10%)
2	GLC	C	2	2	11,11,12	2.05	3 (27%)	15,15,17	1.98	4 (26%)
2	GLA	C	3	2	11,11,12	1.67	4 (36%)	15,15,17	1.96	5 (33%)
2	GLA	C	4	2	11,11,12	1.87	2 (18%)	15,15,17	0.84	0
2	FRU	D	1	2	11,12,12	4.94	5 (45%)	10,18,18	1.08	1 (10%)
2	GLC	D	2	2	11,11,12	1.76	2 (18%)	15,15,17	2.61	5 (33%)
2	GLA	D	3	2	11,11,12	1.22	1 (9%)	15,15,17	1.32	2 (13%)
2	GLA	D	4	2	11,11,12	0.95	0	15,15,17	0.74	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	FRU	C	1	2	-	3/5/24/24	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	GLA	C	3	2	-	1/2/19/22	0/1/1/1
2	GLA	C	4	2	-	0/2/19/22	0/1/1/1
2	FRU	D	1	2	-	3/5/24/24	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLA	D	3	2	-	1/2/19/22	0/1/1/1
2	GLA	D	4	2	-	0/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	FRU	C4-C5	-9.80	1.28	1.53
2	D	1	FRU	C4-C5	-9.48	1.28	1.53
2	C	1	FRU	O5-C5	8.95	1.63	1.43
2	D	1	FRU	O5-C5	8.78	1.63	1.43
2	C	1	FRU	O5-C2	8.22	1.56	1.43
2	D	1	FRU	O5-C2	7.87	1.56	1.43
2	C	1	FRU	O2-C2	5.12	1.49	1.40
2	C	4	GLA	C2-C3	-5.00	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	FRU	O2-C2	4.67	1.48	1.40
2	D	2	GLC	O5-C1	4.18	1.50	1.43
2	C	1	FRU	C4-C3	4.11	1.69	1.53
2	C	2	GLC	O5-C1	4.05	1.50	1.43
2	C	2	GLC	C2-C3	-3.96	1.46	1.52
2	D	1	FRU	C4-C3	3.84	1.68	1.53
2	C	3	GLA	O5-C1	3.07	1.48	1.43
2	D	2	GLC	O5-C5	2.92	1.49	1.43
2	C	4	GLA	O5-C1	2.20	1.47	1.43
2	C	3	GLA	O3-C3	2.18	1.48	1.43
2	D	3	GLA	O5-C5	2.18	1.47	1.43
2	C	2	GLC	O3-C3	2.12	1.48	1.43
2	C	3	GLA	C2-C3	-2.08	1.49	1.52
2	C	3	GLA	O5-C5	2.05	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	O3-C3-C4	-6.09	96.02	110.38
2	D	2	GLC	O3-C3-C2	5.45	121.18	110.05
2	C	2	GLC	O5-C5-C4	4.07	120.72	110.83
2	D	2	GLC	O2-C2-C3	4.02	118.47	110.15
2	C	2	GLC	C1-O5-C5	3.83	117.31	112.19
2	C	3	GLA	C3-C4-C5	3.80	117.11	110.23
2	C	3	GLA	C1-C2-C3	3.46	114.68	109.64
2	C	2	GLC	C6-C5-C4	-3.22	105.12	113.02
2	C	3	GLA	O3-C3-C2	-2.89	104.16	110.05
2	D	3	GLA	O5-C5-C6	-2.89	102.04	107.66
2	C	2	GLC	C3-C4-C5	2.67	115.08	110.23
2	D	2	GLC	O2-C2-C1	-2.27	104.04	109.22
2	C	3	GLA	O4-C4-C5	-2.20	103.90	109.32
2	C	3	GLA	O5-C5-C6	-2.13	103.51	107.66
2	D	2	GLC	O5-C5-C6	2.13	111.80	107.66
2	D	1	FRU	O4-C4-C3	-2.12	105.80	112.16
2	C	1	FRU	O2-C2-O5	2.11	113.38	109.33
2	D	3	GLA	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	FRU	O1-C1-C2-O2

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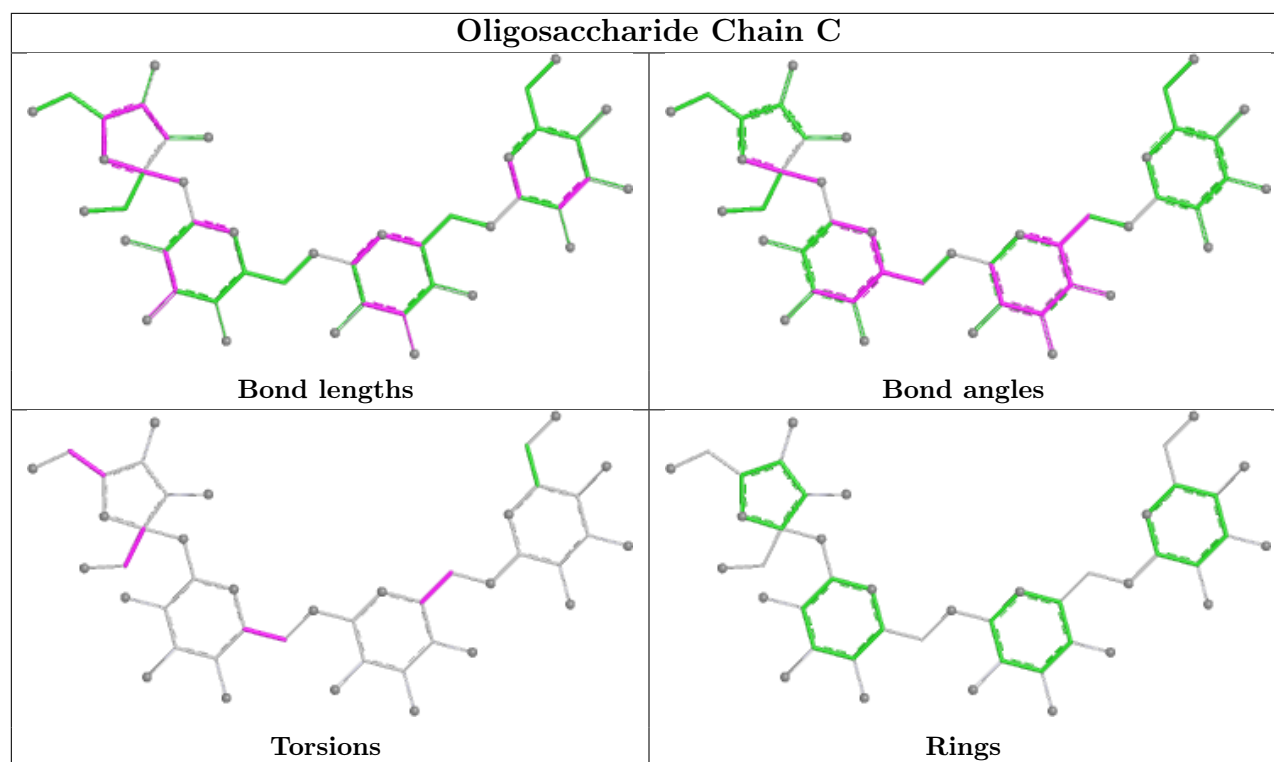
Mol	Chain	Res	Type	Atoms
2	C	1	FRU	O5-C5-C6-O6
2	D	1	FRU	O1-C1-C2-O5
2	C	1	FRU	C4-C5-C6-O6
2	C	3	GLA	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	3	GLA	O5-C5-C6-O6
2	D	1	FRU	O1-C1-C2-C3
2	C	1	FRU	O1-C1-C2-O5

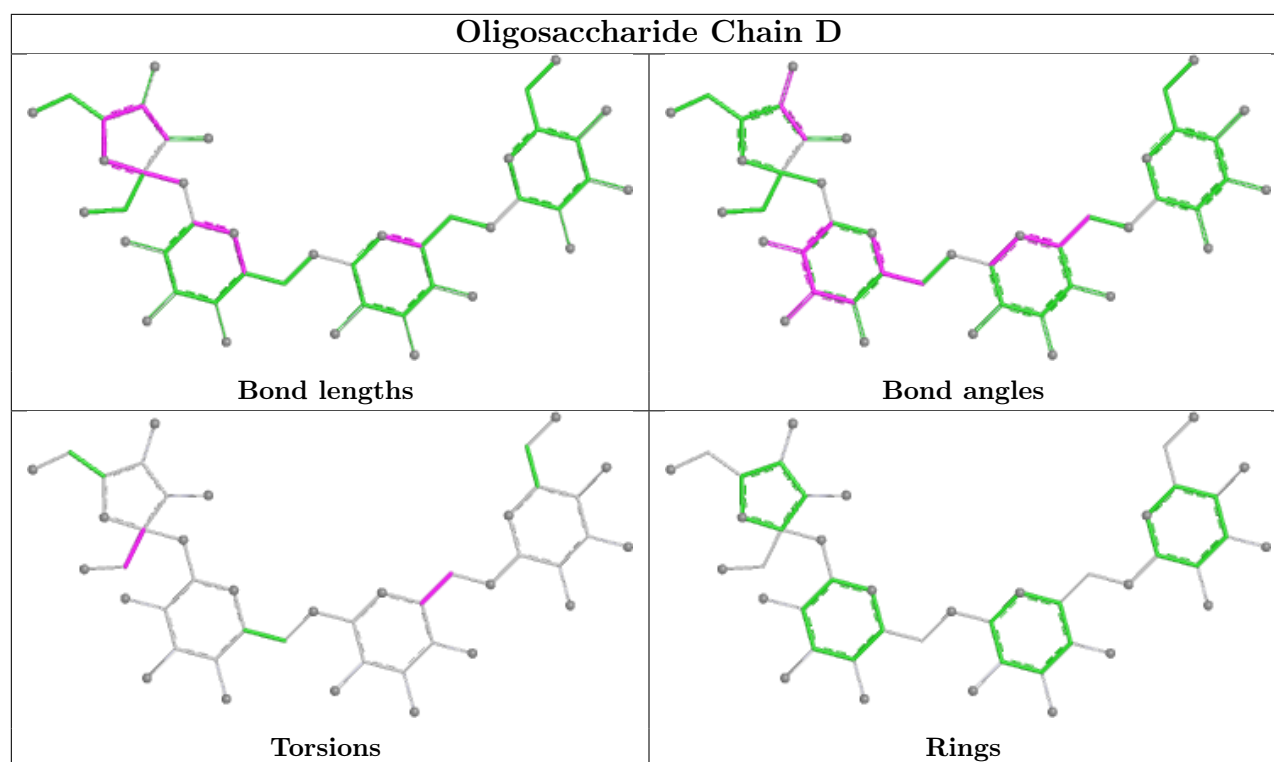
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	3	0
2	C	1	FRU	1	0
2	C	3	GLA	2	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.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	284:PRO	C	285:ASN	N	0.98
1	A	285:ASN	C	286:VAL	N	0.92

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, 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	718/749 (95%)	0.08	25 (3%) 47 46	27, 42, 74, 122	0
1	B	718/749 (95%)	-0.26	6 (0%) 82 82	25, 34, 60, 99	0
All	All	1436/1498 (95%)	-0.09	31 (2%) 62 61	25, 39, 69, 122	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	6.4
1	A	285	ASN	5.0
1	A	749	LEU	4.6
1	A	588	THR	4.5
1	A	742	PHE	3.3
1	B	5	PRO	3.3
1	A	284	PRO	3.2
1	A	657	VAL	2.9
1	B	538	ASP	2.9
1	A	737	ILE	2.9
1	A	264	SER	2.8
1	A	120	LYS	2.7
1	B	253	ALA	2.7
1	B	57	ILE	2.7
1	A	5	PRO	2.5
1	B	737	ILE	2.4
1	A	740	LYS	2.4
1	A	614	ASN	2.3
1	A	582	ILE	2.3
1	A	577	THR	2.3
1	A	589	ASP	2.3
1	A	549	VAL	2.2
1	A	739	ASN	2.2
1	A	101	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	587	LYS	2.2
1	A	738	GLU	2.2
1	B	34	ALA	2.2
1	A	741	ARG	2.1
1	A	50	ASN	2.1
1	A	590	SER	2.1
1	A	548	GLY	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](#)

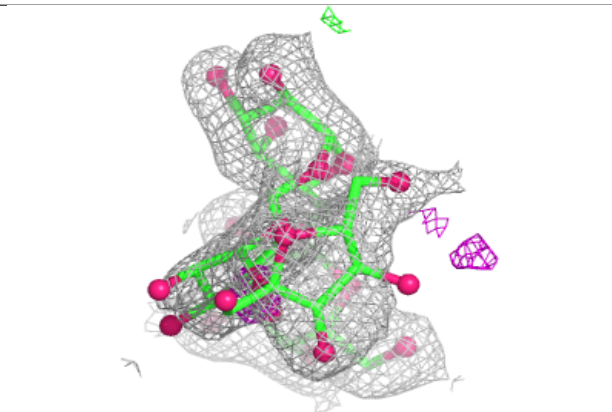
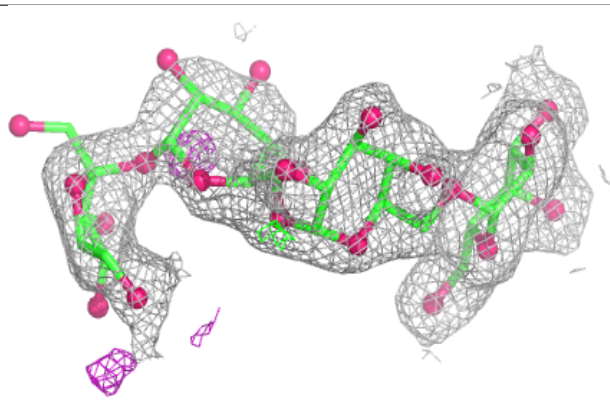
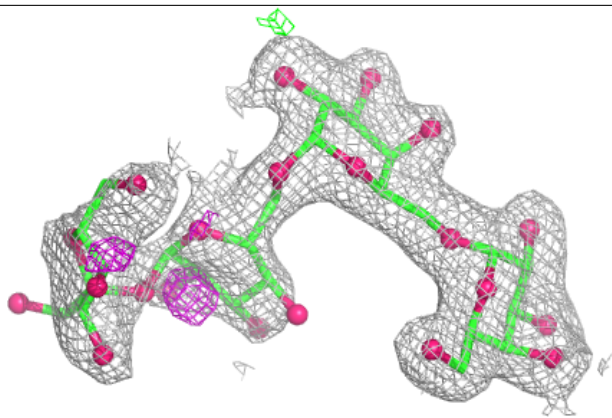
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FRU	C	1	12/12	0.63	0.12	76,94,107,113	0
2	FRU	D	1	12/12	0.78	0.12	56,70,72,83	0
2	GLC	D	2	11/12	0.88	0.12	40,52,60,63	0
2	GLC	C	2	11/12	0.90	0.11	59,81,91,94	0
2	GLA	C	3	11/12	0.94	0.07	33,46,49,54	0
2	GLA	D	3	11/12	0.95	0.06	25,31,35,37	0
2	GLA	C	4	11/12	0.98	0.06	30,32,34,36	0
2	GLA	D	4	11/12	0.98	0.07	24,26,29,30	0

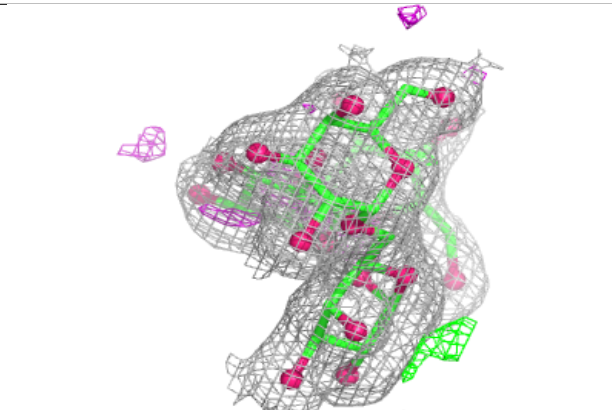
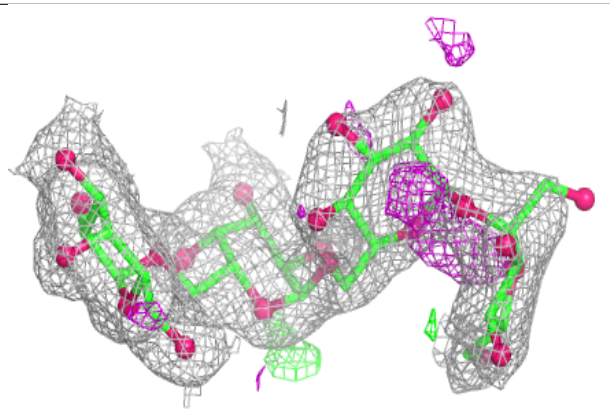
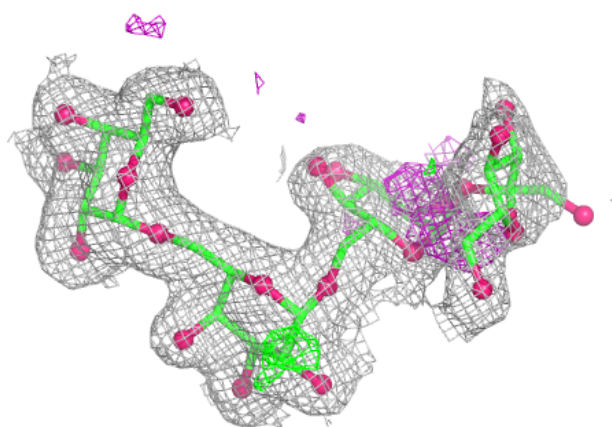
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.