



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2022 – 06:44 PM JST

PDB ID : 7EXR
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

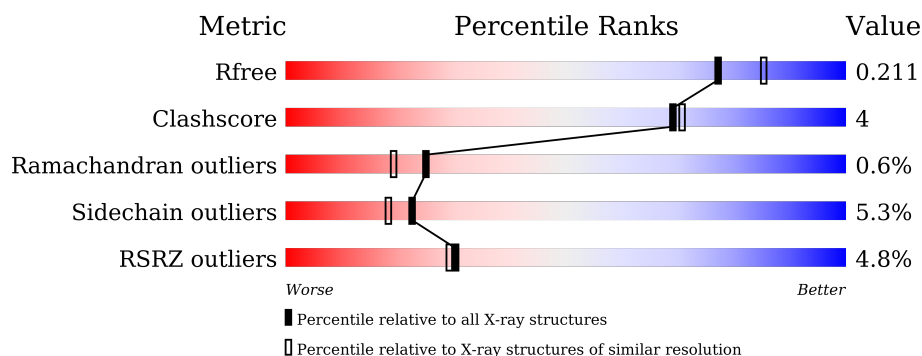
1 Overall quality at a glance

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}	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 $\leq 5\%$. 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	<div> <div>6%</div> <div>84%</div> <div>10%</div> <div>..</div> </div>
1	B	749	<div> <div>3%</div> <div>82%</div> <div>11%</div> <div>..</div> </div>
2	C	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
2	D	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TTV	C	1	X	-	-	X
2	ZCD	C	3	X	-	-	-
2	TTV	D	1	X	-	-	-
2	ZCD	D	3	X	-	-	-

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.

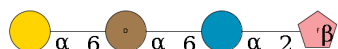
- Molecule 1 is a protein called Probable galactinol–sucrose galactosyltransferase 6.

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-idopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-psicofuranose.



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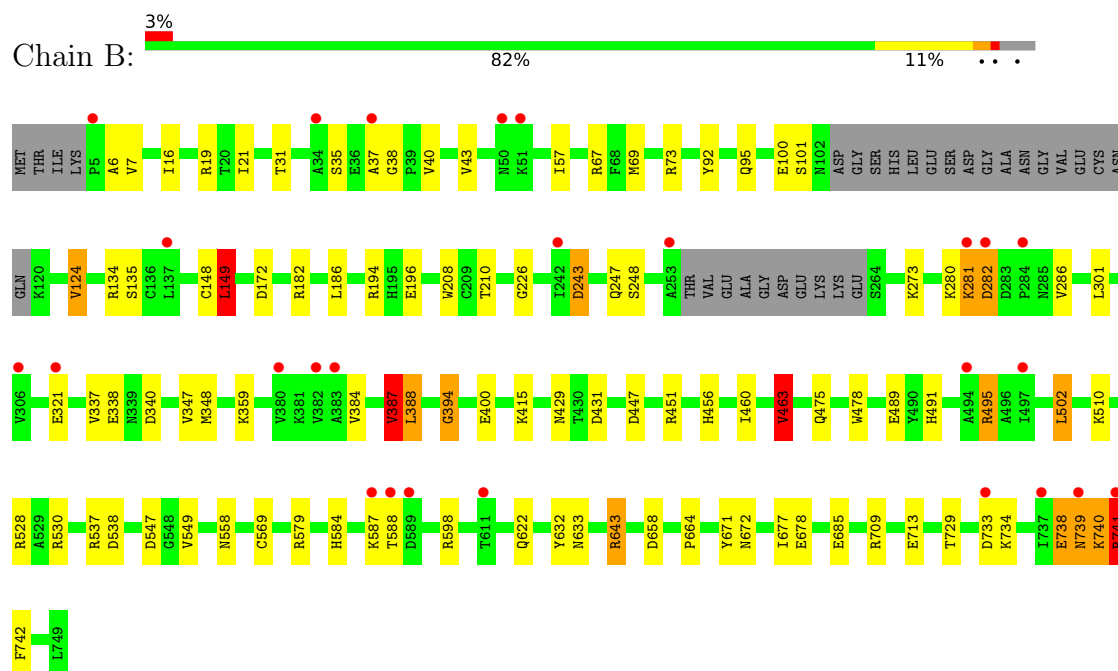
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total 216	O 216	0	0

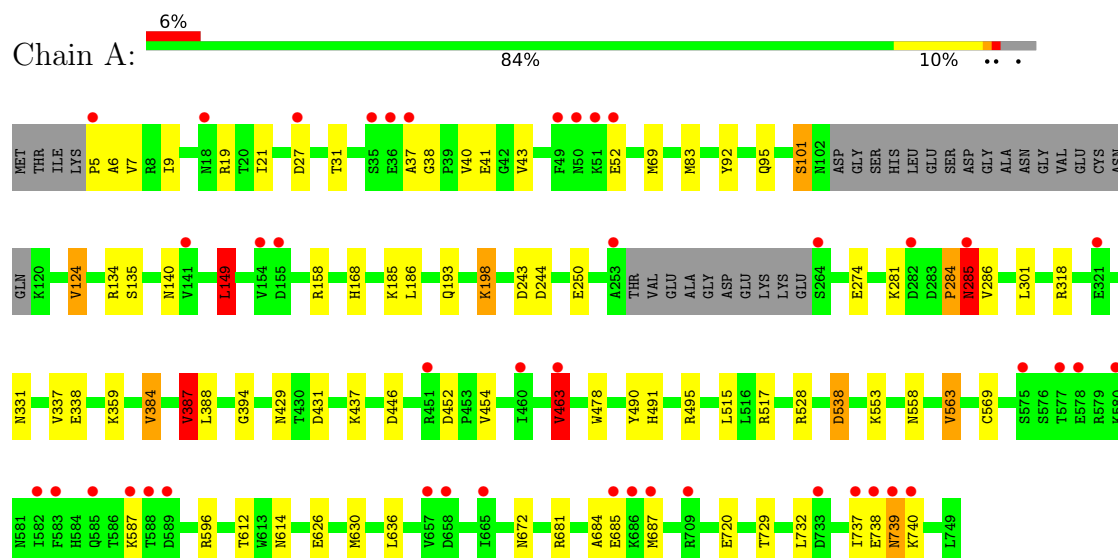
3 Residue-property plots [i](#)

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

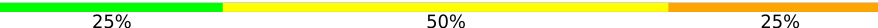


- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-idopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-psicofuranose

Chain C: 



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

Chain D: 



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 29.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.00) 99.8 (29.84-2.00)	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 (4.96%)	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)	0.36 , 41.5	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: TTV, GLA, GLC, ZCD

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	2/5754 (0.0%)	0.99	20/7793 (0.3%)
1	B	0.96	4/5754 (0.1%)	1.10	39/7793 (0.5%)
All	All	0.94	6/11508 (0.1%)	1.04	59/15586 (0.4%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ASN	C-N	-17.88	0.93	1.34
1	A	284	PRO	C-N	-15.40	0.98	1.34
1	B	538	ASP	CB-CG	-6.68	1.37	1.51
1	B	196	GLU	CD-OE1	5.75	1.31	1.25
1	B	569	CYS	CB-SG	-5.30	1.73	1.81
1	B	394	GLY	N-CA	5.11	1.53	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	ARG	NE-CZ-NH2	-16.89	111.85	120.30
1	B	530	ARG	NE-CZ-NH1	16.51	128.56	120.30
1	A	284	PRO	O-C-N	11.94	141.81	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	PRO	CA-C-N	-9.46	96.38	117.20
1	A	285	ASN	O-C-N	-8.70	108.78	122.70
1	B	182	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	387	VAL	CB-CA-C	-8.09	96.03	111.40
1	A	124	VAL	CB-CA-C	-7.74	96.70	111.40
1	B	547	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	563	VAL	CB-CA-C	-7.47	97.20	111.40
1	B	463	VAL	CA-CB-CG1	7.42	122.04	110.90
1	A	149	LEU	CA-CB-CG	7.24	131.95	115.30
1	B	149	LEU	CA-CB-CG	7.20	131.85	115.30
1	B	124	VAL	CB-CA-C	-7.15	97.81	111.40
1	A	387	VAL	CB-CA-C	-7.09	97.93	111.40
1	B	348	MET	CG-SD-CE	-6.97	89.04	100.20
1	B	172	ASP	CB-CG-OD1	6.88	124.50	118.30
1	B	124	VAL	CG1-CB-CG2	6.88	121.91	110.90
1	B	538	ASP	CB-CA-C	-6.78	96.85	110.40
1	B	387	VAL	CG1-CB-CG2	6.51	121.31	110.90
1	B	124	VAL	CA-CB-CG2	6.20	120.20	110.90
1	B	537	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	387	VAL	CA-CB-CG2	6.14	120.12	110.90
1	B	340	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	463	VAL	CG1-CB-CG2	6.06	120.59	110.90
1	B	738	GLU	C-N-CA	6.06	136.84	121.70
1	B	709	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	517	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	658	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	285	ASN	CA-C-N	6.00	130.41	117.20
1	B	37	ALA	CA-C-N	5.92	128.05	116.20
1	B	451	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	73	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	B	194	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	643	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	643	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	463	VAL	CG1-CB-CG2	5.75	120.10	110.90
1	A	387	VAL	CG1-CB-CG2	5.73	120.08	110.90
1	B	530	ARG	CD-NE-CZ	5.72	131.61	123.60
1	B	37	ALA	N-CA-C	5.68	126.35	111.00
1	B	658	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	B	340	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	388	LEU	CB-CG-CD1	5.50	120.35	111.00
1	A	614	ASN	CB-CA-C	-5.48	99.44	110.40
1	B	447	ASP	CB-CG-OD1	5.47	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	681	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	285	ASN	C-N-CA	5.34	135.06	121.70
1	B	182	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	446	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	528	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	244	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	579	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	495	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	528	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	73	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	563	VAL	CG1-CB-CG2	5.07	119.02	110.90
1	B	738	GLU	CA-C-N	5.07	128.35	117.20
1	A	517	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	528	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	37	0
1	B	5620	0	5539	43	0
2	C	45	0	19	3	0
2	D	45	0	19	0	0
3	A	216	0	0	4	0
3	B	328	0	0	9	0
All	All	11874	0	11114	82	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 (82) 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:TTV:C5	2:C:1:TTV:O5	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
1:B:584:HIS:HD2	3:B:979:HOH:O	1.75	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:A:515:LEU:HD23	1:A:515:LEU:C	2.18	0.64
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:GLC:H62	2:C:3:ZCD:C5	2.41	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
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
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:95:GLN:NE2	1:A:134:ARG:HH21	2.05	0.45
1:B:685:GLU:H	1:B:685:GLU:CD	2.19	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: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: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: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 [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	712/749 (95%)	673 (94%)	33 (5%)	6 (1%)	19	13
1	B	712/749 (95%)	680 (96%)	29 (4%)	3 (0%)	34	30
All	All	1424/1498 (95%)	1353 (95%)	62 (4%)	9 (1%)	25	19

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 [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	614/640 (96%)	582 (95%)	32 (5%)	23	19
1	B	614/640 (96%)	581 (95%)	33 (5%)	22	18
All	All	1228/1280 (96%)	1163 (95%)	65 (5%)	22	18

All (65) 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	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	359	LYS
1	B	387	VAL
1	B	388	LEU
1	B	400	GLU
1	B	431	ASP
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
1	B	713	GLU
1	B	729	THR
1	B	733	ASP
1	B	734	LYS
1	B	739	ASN
1	B	741	ARG

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Mol	Chain	Res	Type
1	A	19	ARG
1	A	27	ASP
1	A	40	VAL
1	A	52	GLU
1	A	69	MET
1	A	83	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	274	GLU
1	A	281	LYS
1	A	286	VAL
1	A	301	LEU
1	A	331	ASN
1	A	337	VAL
1	A	359	LYS
1	A	387	VAL
1	A	388	LEU
1	A	431	ASP
1	A	463	VAL
1	A	563	VAL
1	A	587	LYS
1	A	596	ARG
1	A	612	THR
1	A	626	GLU
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	HIS
1	B	95	GLN
1	B	168	HIS
1	B	175	GLN
1	B	193	GLN
1	B	385	GLN

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Mol	Chain	Res	Type
1	B	456	HIS
1	B	558	ASN
1	B	584	HIS
1	B	633	ASN
1	A	56	HIS
1	A	95	GLN
1	A	142	ASN
1	A	168	HIS
1	A	175	GLN
1	A	193	GLN
1	A	385	GLN
1	A	456	HIS
1	A	558	ASN
1	A	633	ASN
1	A	739	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	TTV	C	1	2	11,12,12	5.18	5 (45%)	10,18,18	1.16	1 (10%)
2	GLC	C	2	2	11,11,12	2.12	3 (27%)	15,15,17	2.02	4 (26%)
2	ZCD	C	3	2	11,11,12	1.72	3 (27%)	15,15,17	2.09	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLA	C	4	2	11,11,12	1.94	2 (18%)	15,15,17	0.92	1 (6%)
2	TTV	D	1	2	11,12,12	5.00	5 (45%)	10,18,18	1.10	1 (10%)
2	GLC	D	2	2	11,11,12	1.80	2 (18%)	15,15,17	2.78	5 (33%)
2	ZCD	D	3	2	11,11,12	1.23	1 (9%)	15,15,17	1.41	2 (13%)
2	GLA	D	4	2	11,11,12	0.96	0	15,15,17	0.77	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	TTV	C	1	2	1/1/4/4	3/5/24/24	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	ZCD	C	3	2	2/2/4/5	1/2/19/22	0/1/1/1
2	GLA	C	4	2	-	0/2/19/22	0/1/1/1
2	TTV	D	1	2	1/1/4/4	3/5/24/24	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	ZCD	D	3	2	2/2/4/5	1/2/19/22	0/1/1/1
2	GLA	D	4	2	-	0/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	TTV	C4-C5	-9.73	1.28	1.53
2	D	1	TTV	C4-C5	-9.41	1.28	1.53
2	C	1	TTV	O5-C5	9.01	1.63	1.43
2	D	1	TTV	O5-C5	8.84	1.63	1.43
2	C	1	TTV	O5-C2	8.58	1.56	1.43
2	D	1	TTV	O5-C2	8.22	1.56	1.43
2	C	4	GLA	C2-C3	-5.22	1.44	1.52
2	C	1	TTV	O2-C2	5.18	1.49	1.40
2	D	1	TTV	O2-C2	4.73	1.48	1.40
2	D	2	GLC	O5-C1	4.38	1.50	1.43
2	C	2	GLC	O5-C1	4.25	1.50	1.43
2	C	2	GLC	C2-C3	-4.14	1.46	1.52
2	C	1	TTV	C4-C3	3.95	1.69	1.52
2	D	1	TTV	C4-C3	3.69	1.68	1.52
2	C	3	ZCD	O5-C1	3.22	1.48	1.43
2	D	2	GLC	O5-C5	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	GLA	O5-C1	2.30	1.47	1.43
2	C	3	ZCD	O3-C3	2.29	1.48	1.43
2	C	2	GLC	O3-C3	2.22	1.48	1.43
2	C	3	ZCD	C2-C3	-2.18	1.49	1.52
2	D	3	ZCD	O5-C5	2.09	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	O3-C3-C4	-6.20	96.02	110.35
2	D	2	GLC	O3-C3-C2	5.84	121.18	109.99
2	D	2	GLC	O2-C2-C3	4.16	118.47	110.14
2	C	3	ZCD	C1-C2-C3	4.08	114.68	109.67
2	C	2	GLC	O5-C5-C4	4.07	120.72	110.83
2	C	3	ZCD	C3-C4-C5	3.85	117.11	110.24
2	C	2	GLC	C1-O5-C5	3.78	117.31	112.19
2	C	2	GLC	C6-C5-C4	-3.37	105.12	113.00
2	D	3	ZCD	O5-C5-C6	-3.29	102.04	107.20
2	C	3	ZCD	O3-C3-C2	-3.05	104.16	109.99
2	D	2	GLC	O5-C5-C6	2.93	111.80	107.20
2	C	2	GLC	C3-C4-C5	2.71	115.08	110.24
2	D	2	GLC	O2-C2-C1	-2.50	104.04	109.15
2	C	3	ZCD	O5-C5-C6	-2.36	103.51	107.20
2	C	3	ZCD	O4-C4-C5	-2.17	103.90	109.30
2	D	1	TTV	O4-C4-C3	-2.12	105.80	112.15
2	C	4	GLA	O2-C2-C1	-2.09	104.89	109.15
2	D	3	ZCD	C1-O5-C5	2.01	114.91	112.19
2	C	1	TTV	O2-C2-O5	2.01	113.38	109.50

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	TTV	C3
2	C	3	ZCD	C2
2	C	3	ZCD	C3
2	D	1	TTV	C3
2	D	3	ZCD	C2
2	D	3	ZCD	C3

All (9) torsion outliers are listed below:

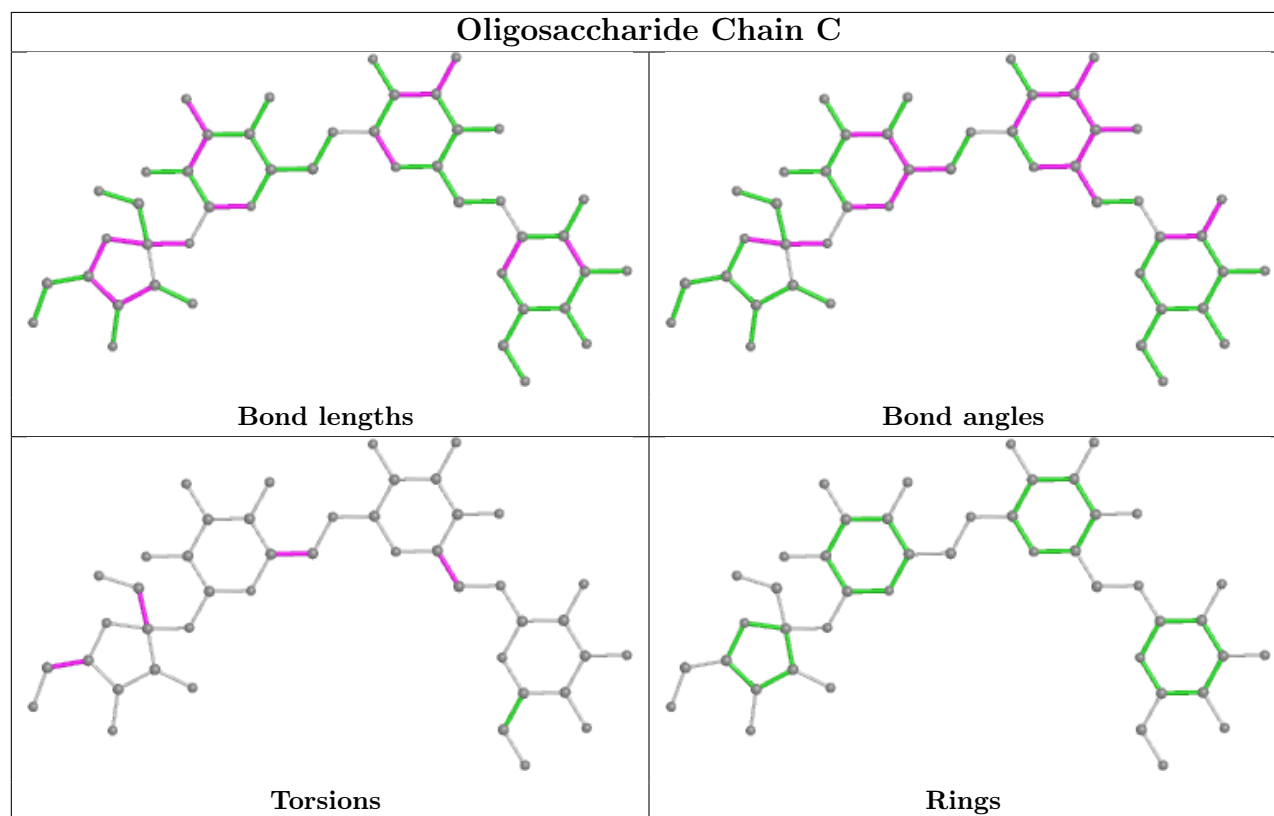
Mol	Chain	Res	Type	Atoms
2	D	1	TTV	O1-C1-C2-O2
2	C	1	TTV	O5-C5-C6-O6
2	D	1	TTV	O1-C1-C2-O5
2	C	2	GLC	C4-C5-C6-O6
2	C	1	TTV	C4-C5-C6-O6
2	C	3	ZCD	O5-C5-C6-O6
2	D	3	ZCD	O5-C5-C6-O6
2	D	1	TTV	O1-C1-C2-C3
2	C	1	TTV	O1-C1-C2-O5

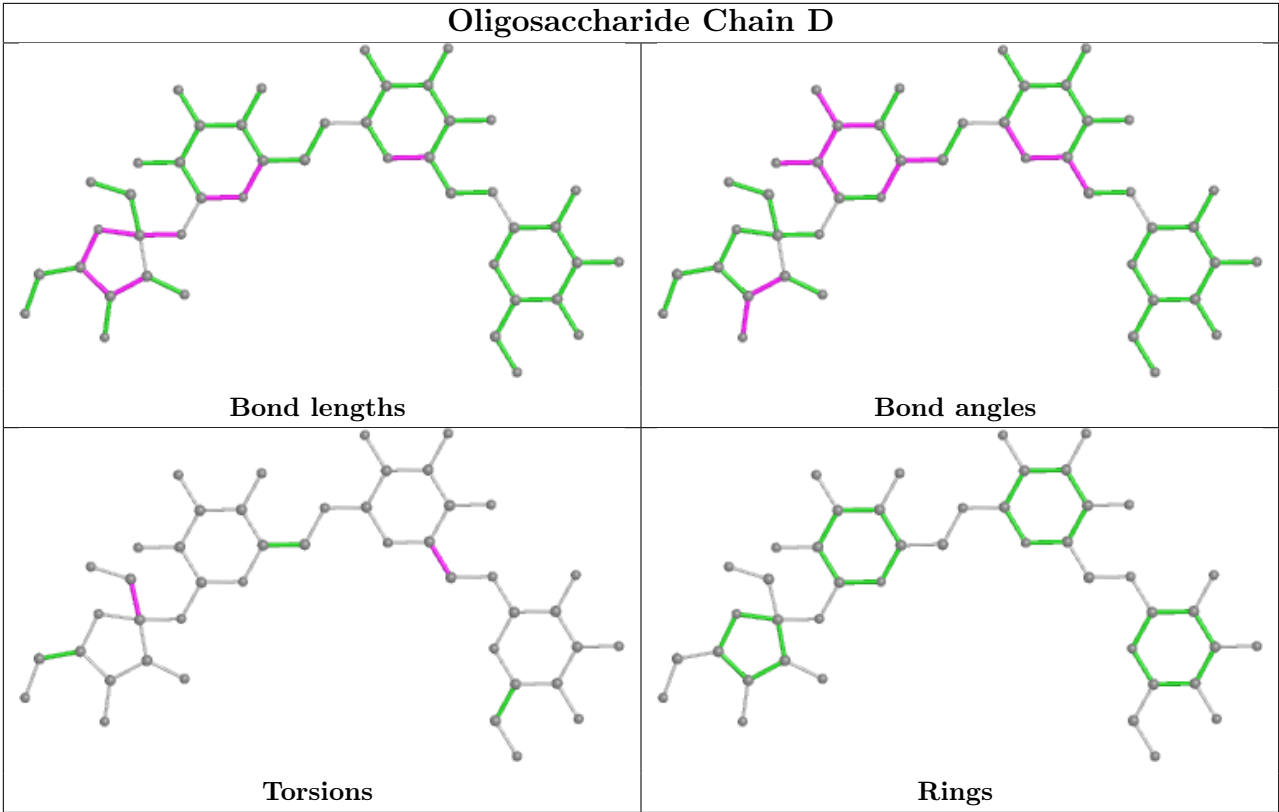
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	ZCD	1	0
2	C	1	TTV	1	0
2	C	2	GLC	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.12	43 (5%) 21 20	27, 42, 74, 122	0
1	B	718/749 (95%)	-0.07	26 (3%) 42 42	25, 34, 60, 99	0
All	All	1436/1498 (95%)	0.03	69 (4%) 30 29	25, 39, 69, 122	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	10.0
1	A	285	ASN	5.4
1	A	658	ASP	5.4
1	A	50	ASN	4.7
1	A	588	THR	4.6
1	A	36	GLU	4.5
1	B	281	LYS	4.5
1	A	577	THR	4.2
1	A	739	ASN	4.1
1	A	51	LYS	4.1
1	A	282	ASP	4.0
1	A	589	ASP	3.9
1	A	737	ILE	3.9
1	A	740	LYS	3.9
1	A	738	GLU	3.9
1	B	282	ASP	3.8
1	A	37	ALA	3.7
1	A	578	GLU	3.7
1	A	657	VAL	3.7
1	A	733	ASP	3.6
1	B	737	ILE	3.5
1	A	585	GLN	3.5
1	B	306	VAL	3.4
1	A	18	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	589	ASP	3.2
1	B	284	PRO	3.1
1	B	34	ALA	3.0
1	B	587	LYS	2.9
1	B	739	ASN	2.9
1	A	49	PHE	2.8
1	A	582	ILE	2.8
1	B	611	THR	2.8
1	B	382	VAL	2.7
1	B	588	THR	2.7
1	A	687	MET	2.6
1	B	37	ALA	2.6
1	A	583	PHE	2.6
1	A	665	ILE	2.6
1	B	380	VAL	2.6
1	B	5	PRO	2.5
1	A	27	ASP	2.5
1	A	5	PRO	2.5
1	B	733	ASP	2.5
1	A	52	GLU	2.5
1	A	686	LYS	2.4
1	B	51	LYS	2.4
1	A	141	VAL	2.4
1	B	50	ASN	2.4
1	A	587	LYS	2.4
1	B	253	ALA	2.3
1	A	154	VAL	2.3
1	A	35	SER	2.3
1	A	685	GLU	2.3
1	B	242	ILE	2.3
1	A	580	LYS	2.2
1	A	709	ARG	2.2
1	A	155	ASP	2.2
1	A	264	SER	2.2
1	B	497	ILE	2.1
1	B	321	GLU	2.1
1	B	741	ARG	2.1
1	A	321	GLU	2.1
1	A	575	SER	2.1
1	B	383	ALA	2.1
1	B	137	LEU	2.0
1	B	494	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	451	ARG	2.0
1	A	460	ILE	2.0
1	A	463	VAL	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](#)

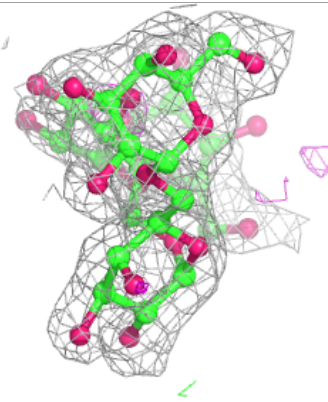
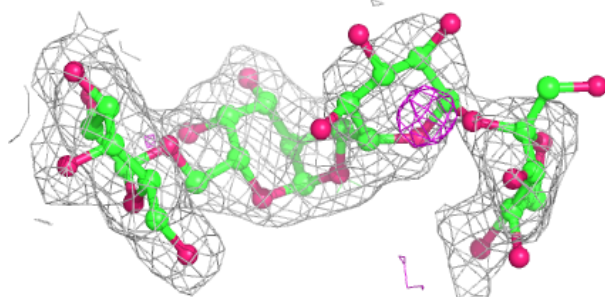
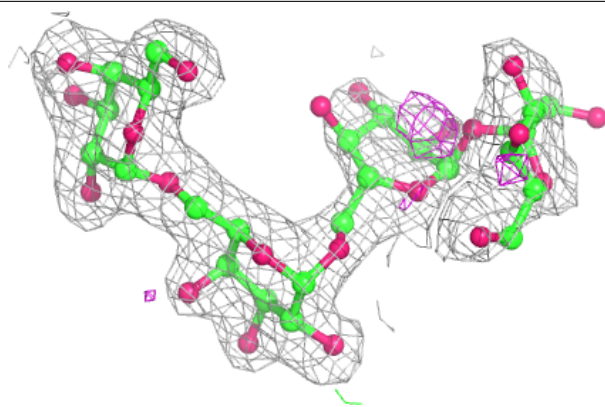
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TTV	C	1	12/12	0.78	0.47	76,94,107,113	0
2	GLC	C	2	11/12	0.84	0.38	59,81,91,94	0
2	GLC	D	2	11/12	0.88	0.25	40,52,60,63	0
2	TTV	D	1	12/12	0.90	0.39	56,70,72,83	0
2	ZCD	D	3	11/12	0.94	0.09	25,31,35,37	0
2	ZCD	C	3	11/12	0.95	0.10	33,46,49,54	0
2	GLA	C	4	11/12	0.98	0.09	30,32,34,36	0
2	GLA	D	4	11/12	0.98	0.13	24,26,29,30	0

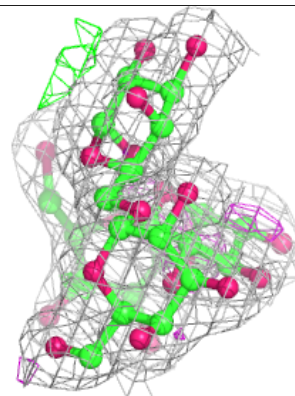
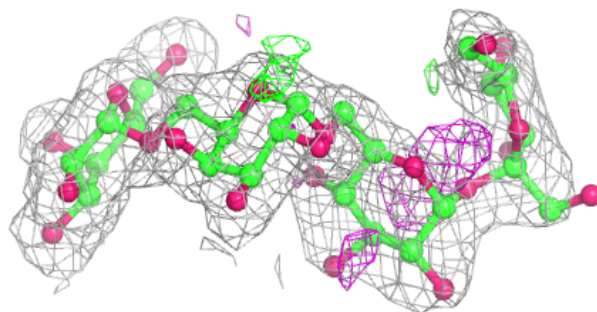
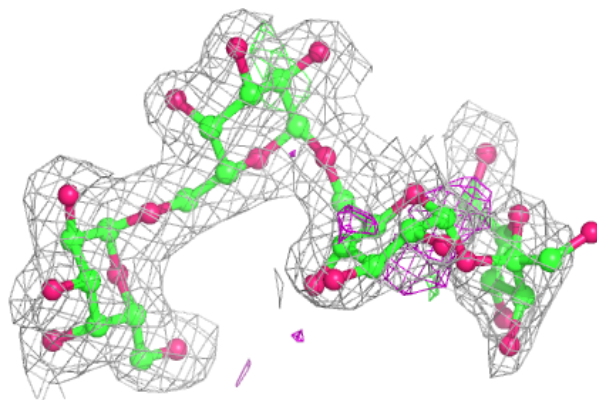
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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.