



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:42 PM UTC

PDB ID : 9K1G / pdb_00009k1g
Title : COMPLEX STRUCTURE OF ENDO-1,3-FUCANASE (FUN174Sb) FROM
GH174 FAMILY WITH FUCOTETRAOSE
Authors : Chen, G.N.; Chang, Y.G.
Deposited on : 2024-10-16
Resolution : 2.50 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

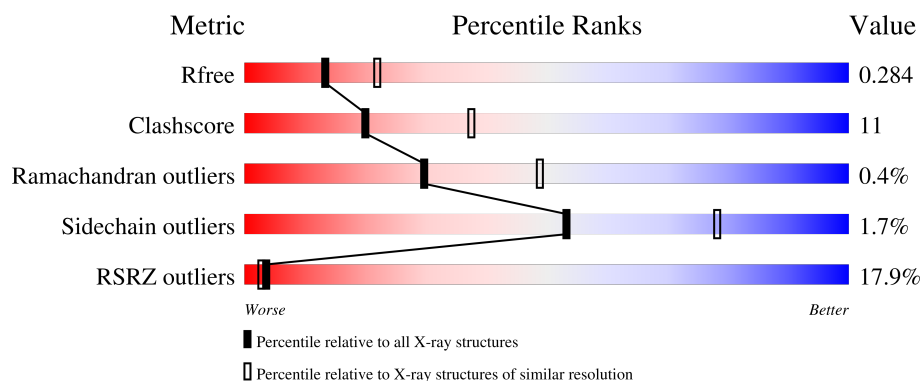
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	497	17% 68% 21% • 10%
1	B	497	16% 67% 23% 10%
2	C	4	25% 75%
2	D	4	50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7600 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 endo-1.3-fucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3510	2259	584	653	14			
1	B	449	Total	C	N	O	S	0	0	0
			3509	2258	584	653	14			

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-fucopyranose-(1-3)-alpha-L-fucopyranose-(1-3)-2,4-di-O-sulfo-alpha-L-fucopyranose-(1-3)-2-O-sulfo-alpha-L-fucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	S	0	0	0
			57	24	29	4			
2	D	4	Total	C	O	S	0	0	0
			57	24	29	4			

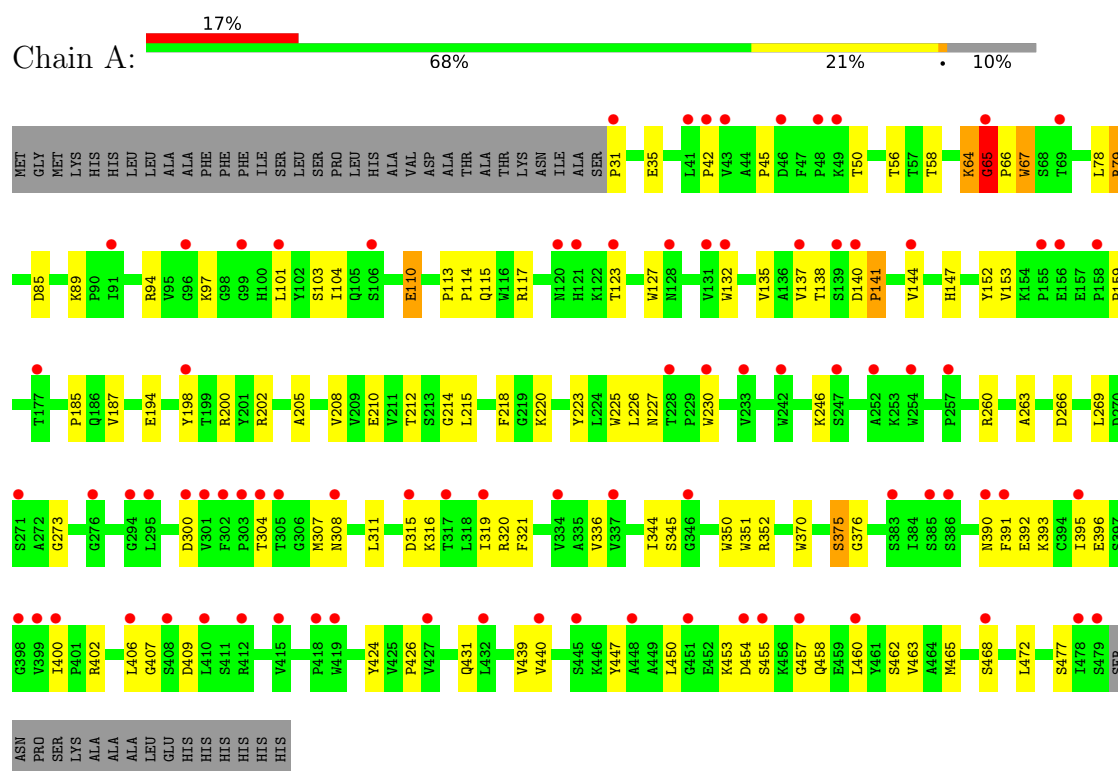
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total	O	0	0
			236	236		
3	B	231	Total	O	0	0
			231	231		

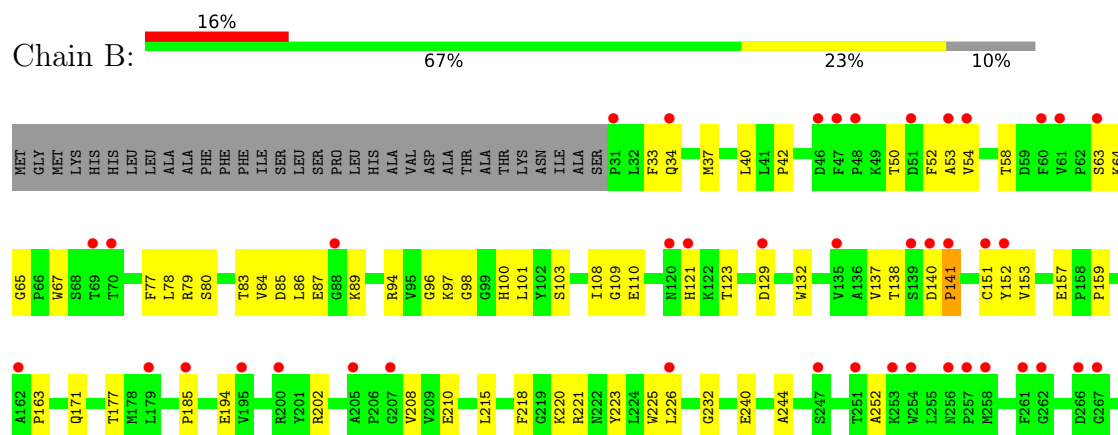
3 Residue-property plots [i](#)

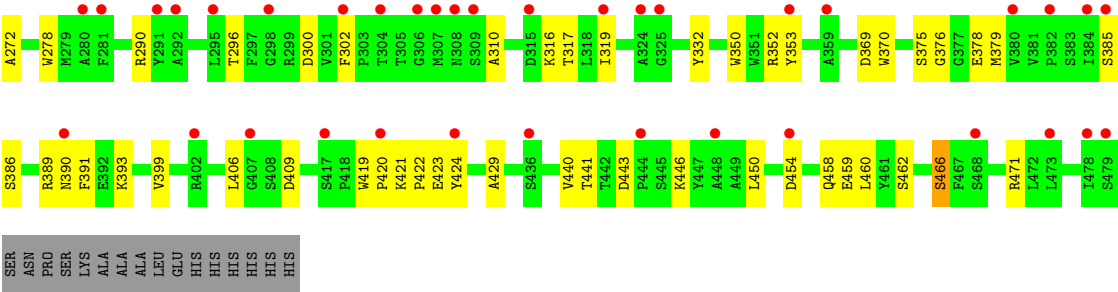
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: endo-1.3-fucanase



- Molecule 1: endo-1.3-fucanase





● Molecule 2: 2-O-sulfo-alpha-L-fucopyranose-(1-3)-alpha-L-fucopyranose-(1-3)-2,4-di-O-sulfo-alpha-L-fucopyranose-(1-3)-2-O-sulfo-alpha-L-fucopyranose



● Molecule 2: 2-O-sulfo-alpha-L-fucopyranose-(1-3)-alpha-L-fucopyranose-(1-3)-2,4-di-O-sulfo-alpha-L-fucopyranose-(1-3)-2-O-sulfo-alpha-L-fucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.63Å 92.05Å 75.81Å 90.00° 104.53° 90.00°	Depositor
Resolution (Å)	36.66 – 2.50 36.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.66-2.50) 91.8 (36.66-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.245 , 0.286 0.246 , 0.284	Depositor DCC
R_{free} test set	2000 reflections (6.93%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	1.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.1	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	0.87	EDS
Total number of atoms	7600	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: X2Y, FUC, X6Y

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	0.28	2/3621 (0.1%)	0.38	3/4938 (0.1%)
1	B	0.23	0/3620	0.36	0/4937
All	All	0.26	2/7241 (0.0%)	0.37	3/9875 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLY	CA-C	-6.47	1.42	1.51
1	A	64	LYS	N-CA	-5.04	1.40	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	GLY	CA-C-N	-5.81	112.58	119.84
1	A	65	GLY	C-N-CA	-5.81	112.58	119.84
1	A	67	TRP	N-CA-C	5.06	117.99	109.95

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	3510	0	3374	82	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3509	0	3372	74	0
2	C	57	0	9	3	0
2	D	57	0	9	2	0
3	A	236	0	0	14	0
3	B	231	0	0	14	0
All	All	7600	0	6764	158	1

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 11.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLY:HA3	1:B:110:GLU:HB2	1.65	0.77
1:A:137:VAL:HB	1:A:225:TRP:HB3	1.66	0.77
1:B:98:GLY:O	3:B:501:HOH:O	2.06	0.74
1:A:450:LEU:HD12	1:A:460:LEU:HB3	1.71	0.72
1:A:101:LEU:HB3	1:A:132:TRP:HB2	1.71	0.72
1:B:129:ASP:OD2	1:B:152:TYR:OH	2.07	0.70
1:B:215:LEU:HD22	1:B:226:LEU:HD22	1.77	0.67
1:B:157:GLU:O	3:B:503:HOH:O	2.13	0.66
1:B:109:GLY:O	3:B:502:HOH:O	2.15	0.65
1:B:63:SER:HB2	1:B:67:TRP:HE1	1.60	0.65
1:B:350:TRP:HB3	1:B:379:MET:HG3	1.79	0.65
1:A:58:THR:HG22	1:A:79:ARG:HB2	1.79	0.64
1:A:260:ARG:NH1	3:A:514:HOH:O	2.30	0.64
1:B:378:GLU:O	3:B:505:HOH:O	2.16	0.63
1:B:300:ASP:OD2	1:B:316:LYS:HB2	2.00	0.62
1:A:390:ASN:H	1:A:393:LYS:HB2	1.65	0.61
1:A:212:THR:HG23	1:A:352:ARG:HB2	1.82	0.61
1:B:64:LYS:O	1:B:65:GLY:C	2.44	0.61
1:B:42:PRO:HG3	1:B:350:TRP:CD2	2.35	0.60
1:A:450:LEU:HD21	1:A:462:SER:HB3	1.83	0.60
1:B:65:GLY:HA3	1:B:110:GLU:CB	2.32	0.59
1:B:310:ALA:O	3:B:504:HOH:O	2.15	0.59
1:A:300:ASP:OD2	1:A:316:LYS:HB2	2.02	0.59
1:A:375:SER:OG	1:A:376:GLY:N	2.33	0.59
1:B:429:ALA:HB3	1:B:471:ARG:HB2	1.83	0.59
1:A:42:PRO:HG2	1:A:350:TRP:CD2	2.38	0.59
1:A:246:LYS:NZ	3:A:534:HOH:O	2.36	0.59
1:B:53:ALA:O	3:B:506:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:GLU:OE1	1:B:290:ARG:NH2	2.32	0.58
1:B:94:ARG:HB2	1:B:103:SER:HB3	1.86	0.58
1:B:421:LYS:HB3	1:B:422:PRO:HD2	1.86	0.57
1:A:64:LYS:O	1:A:65:GLY:C	2.46	0.57
1:B:137:VAL:HB	1:B:225:TRP:HB3	1.87	0.57
1:A:210:GLU:OE2	3:A:501:HOH:O	2.18	0.56
1:A:198:TYR:HB2	1:A:214:GLY:HA3	1.88	0.56
1:A:198:TYR:O	1:A:214:GLY:N	2.32	0.56
1:B:109:GLY:N	3:B:502:HOH:O	2.39	0.56
1:B:458:GLN:NE2	3:B:527:HOH:O	2.30	0.55
1:A:187:VAL:HG11	1:A:465:MET:HE3	1.89	0.54
1:A:94:ARG:HB2	1:A:103:SER:HB3	1.89	0.54
1:A:42:PRO:HG2	1:A:350:TRP:CE2	2.43	0.54
1:A:304:THR:HA	1:A:307:MET:HE3	1.88	0.54
1:B:232:GLY:HA3	1:B:332:TYR:HE1	1.73	0.53
1:B:390:ASN:HB3	1:B:393:LYS:HB2	1.90	0.53
1:B:390:ASN:OD1	1:B:391:PHE:N	2.42	0.53
1:A:392:GLU:OE2	1:A:392:GLU:HA	2.09	0.52
1:B:406:LEU:HD23	1:B:440:VAL:HB	1.91	0.52
1:A:113:PRO:O	1:A:115:GLN:NE2	2.36	0.52
1:A:200:ARG:NE	3:A:544:HOH:O	2.42	0.52
1:A:208:VAL:HG11	1:A:370:TRP:CE2	2.45	0.52
1:B:390:ASN:OD1	3:B:507:HOH:O	2.18	0.52
1:A:138:THR:HB	1:A:223:TYR:CD2	2.45	0.51
1:A:140:ASP:HB3	1:A:141:PRO:HD3	1.91	0.51
1:A:311:LEU:HD12	3:A:623:HOH:O	2.10	0.51
1:B:409:ASP:OD1	1:B:441:THR:OG1	2.26	0.51
1:B:140:ASP:HB3	1:B:141:PRO:HD3	1.93	0.51
1:B:462:SER:O	1:B:466:SER:OG	2.20	0.51
1:A:395:ILE:HG12	1:A:400:ILE:HD11	1.92	0.50
1:A:391:PHE:O	1:A:395:ILE:HG13	2.10	0.50
1:B:151:CYS:HA	1:B:185:PRO:HA	1.94	0.50
1:A:135:VAL:HG11	2:C:1:X6Y:C6	2.41	0.49
1:B:202:ARG:HB3	1:B:210:GLU:HB3	1.94	0.49
1:B:208:VAL:HG11	1:B:370:TRP:CE2	2.47	0.49
1:A:65:GLY:O	1:A:66:PRO:C	2.54	0.49
1:B:375:SER:OG	1:B:376:GLY:N	2.45	0.49
1:B:244:ALA:HA	1:B:252:ALA:HA	1.95	0.49
1:A:101:LEU:HD22	1:A:132:TRP:HD1	1.78	0.48
1:B:450:LEU:HD12	1:B:460:LEU:HB3	1.94	0.48
1:A:103:SER:O	3:A:502:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TRP:HE3	1:A:114:PRO:HA	1.78	0.48
1:B:278:TRP:HB3	1:B:296:THR:HG22	1.95	0.48
1:B:386:SER:HB3	1:B:419:TRP:CH2	2.48	0.48
1:A:56:THR:OG1	1:A:79:ARG:NH1	2.47	0.48
1:A:153:VAL:HG11	1:A:159:PRO:HA	1.96	0.48
1:B:153:VAL:HG11	1:B:159:PRO:HA	1.94	0.48
1:A:147:HIS:CD2	1:A:185:PRO:HB3	2.49	0.47
1:B:54:VAL:O	1:B:171:GLN:NE2	2.38	0.47
1:B:220:LYS:HB3	1:B:220:LYS:HE3	1.71	0.47
1:A:311:LEU:HD21	1:A:344:ILE:HG12	1.95	0.47
1:B:34:GLN:HA	1:B:37:MET:HG3	1.97	0.47
1:B:369:ASP:OD2	3:B:508:HOH:O	2.20	0.47
1:A:144:VAL:N	3:A:526:HOH:O	2.48	0.47
1:A:308:ASN:HB3	1:A:311:LEU:HD12	1.96	0.47
1:B:83:THR:OG1	1:B:84:VAL:N	2.45	0.47
1:B:101:LEU:HB3	1:B:132:TRP:HB2	1.96	0.47
1:A:67:TRP:CE3	1:A:114:PRO:HA	2.50	0.47
1:A:431:GLN:HG2	1:A:468:SER:HB2	1.96	0.46
1:A:393:LYS:HA	1:A:396:GLU:HG2	1.95	0.46
1:B:33:PHE:CE2	1:B:389:ARG:HD3	2.50	0.46
1:B:78:LEU:HB2	1:B:97:LYS:HA	1.98	0.46
1:A:407:GLY:C	1:A:409:ASP:H	2.23	0.46
1:B:443:ASP:OD2	1:B:446:LYS:HB2	2.16	0.46
1:A:127:TRP:HE3	3:A:505:HOH:O	1.98	0.46
1:A:439:VAL:HG21	1:A:447:TYR:CZ	2.51	0.45
1:B:121:HIS:O	1:B:123:THR:N	2.41	0.45
1:B:141:PRO:HG3	1:B:221:ARG:NH1	2.32	0.45
1:A:406:LEU:HD23	1:A:440:VAL:HB	1.97	0.45
2:D:2:X2Y:O8	2:D:3:FUC:H5	2.16	0.45
1:A:104:ILE:O	1:A:110:GLU:HA	2.17	0.45
1:A:205:ALA:HB3	1:A:208:VAL:HB	1.98	0.45
1:B:353:TYR:O	3:B:509:HOH:O	2.21	0.45
2:C:2:X2Y:O8	2:C:3:FUC:H5	2.17	0.45
1:A:101:LEU:HD21	1:A:104:ILE:HG13	1.99	0.44
1:A:269:LEU:HG	1:A:320:ARG:HG2	1.99	0.44
1:B:108:ILE:HG13	3:B:502:HOH:O	2.16	0.44
1:A:78:LEU:HB2	1:A:97:LYS:HA	2.00	0.44
1:B:50:THR:HB	1:B:52:PHE:HE1	1.83	0.44
1:A:194:GLU:HA	1:A:218:PHE:CZ	2.53	0.44
1:A:220:LYS:O	1:A:345:SER:OG	2.33	0.44
1:A:263:ALA:HB1	1:A:266:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.71	0.44
1:A:65:GLY:HA3	1:A:110:GLU:HG3	2.00	0.43
1:A:152:TYR:CE2	1:A:185:PRO:HB2	2.52	0.43
1:A:351:TRP:CE3	1:A:376:GLY:HA3	2.53	0.43
1:A:31:PRO:HD2	3:A:703:HOH:O	2.18	0.43
1:A:230:TRP:CE3	1:A:336:VAL:HB	2.53	0.43
1:B:406:LEU:HD23	1:B:406:LEU:HA	1.83	0.43
1:A:45:PRO:O	1:A:202:ARG:NH2	2.50	0.43
1:A:152:TYR:CD2	1:A:185:PRO:HB2	2.54	0.43
1:B:40:LEU:HD13	1:B:420:PRO:HD2	2.00	0.43
1:B:422:PRO:O	1:B:423:GLU:HG2	2.19	0.43
1:A:227:ASN:HD22	1:A:230:TRP:HB2	1.84	0.43
1:A:273:GLY:O	3:A:504:HOH:O	2.21	0.43
1:A:454:ASP:HB3	1:A:458:GLN:H	1.84	0.43
1:B:352:ARG:HG2	3:B:509:HOH:O	2.18	0.42
1:A:319:ILE:HG22	1:A:321:PHE:CD2	2.54	0.42
1:B:194:GLU:HA	1:B:218:PHE:CZ	2.54	0.42
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.66	0.42
1:B:97:LYS:HE2	1:B:163:PRO:HA	2.01	0.42
1:A:426:PRO:HB2	1:A:472:LEU:HD11	2.01	0.42
1:A:117:ARG:NH2	3:A:559:HOH:O	2.52	0.42
1:A:215:LEU:HD22	1:A:226:LEU:HD22	2.02	0.42
1:A:300:ASP:OD2	1:A:316:LYS:HE3	2.20	0.42
1:B:399:VAL:O	1:B:471:ARG:NH1	2.51	0.42
1:B:86:LEU:HB2	1:B:87:GLU:OE2	2.20	0.41
1:B:272:ALA:HB2	1:B:317:THR:HB	2.02	0.41
1:A:230:TRP:CZ2	2:C:1:X6Y:O2	2.73	0.41
1:B:85:ASP:OD2	1:B:89:LYS:HB2	2.20	0.41
1:A:453:LYS:HD2	1:A:458:GLN:O	2.21	0.41
1:B:138:THR:HB	1:B:223:TYR:CD2	2.54	0.41
1:B:77:PHE:N	3:B:519:HOH:O	2.53	0.41
1:A:395:ILE:HG22	1:A:402:ARG:HD2	2.01	0.41
1:B:225:TRP:CD1	2:D:3:FUC:H62	2.55	0.41
1:A:123:THR:O	3:A:507:HOH:O	2.22	0.41
1:A:202:ARG:HB3	1:A:210:GLU:HB3	2.02	0.41
1:A:85:ASP:OD2	1:A:89:LYS:HB2	2.21	0.41
1:B:77:PHE:HE1	1:B:80:SER:HB3	1.86	0.41
1:B:350:TRP:CZ3	1:B:376:GLY:HA2	2.55	0.41
1:B:421:LYS:HD3	1:B:424:TYR:CE2	2.56	0.40
1:A:304:THR:O	1:A:307:MET:HB3	2.21	0.40
1:B:58:THR:HG22	1:B:79:ARG:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLY:HA3	1:B:100:HIS:CE1	2.56	0.40
1:B:244:ALA:HB2	1:B:278:TRP:CE2	2.56	0.40
1:A:307:MET:N	3:A:562:HOH:O	2.53	0.40
1:A:424:TYR:CE1	1:A:477:SER:HB2	2.56	0.40
1:B:42:PRO:HG3	1:B:350:TRP:CE3	2.57	0.40
1:A:447:TYR:OH	3:A:503:HOH:O	2.21	0.40
1:B:302:PHE:H	1:B:302:PHE:HD1	1.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:OE2	1:A:260:ARG:NH1[2_555]	2.19	0.01

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	447/497 (90%)	419 (94%)	25 (6%)	3 (1%)	18	34
1	B	447/497 (90%)	418 (94%)	28 (6%)	1 (0%)	43	63
All	All	894/994 (90%)	837 (94%)	53 (6%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLY
1	B	141	PRO
1	A	141	PRO
1	A	457	GLY

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	376/418 (90%)	369 (98%)	7 (2%)	50	76
1	B	376/418 (90%)	370 (98%)	6 (2%)	55	79
All	All	752/836 (90%)	739 (98%)	13 (2%)	53	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	79	ARG
1	A	110	GLU
1	A	315	ASP
1	A	375	SER
1	A	455	SER
1	A	463	VAL
1	B	177	THR
1	B	319	ILE
1	B	385	SER
1	B	454	ASP
1	B	459	GLU
1	B	466	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	105	GLN
1	A	147	HIS
1	A	186	GLN
1	A	222	ASN
1	A	227	ASN
1	A	235	GLN
1	A	274	ASN
1	A	286	GLN

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Mol	Chain	Res	Type
1	B	100	HIS
1	B	105	GLN
1	B	167	GLN

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	X6Y	C	1	2	15,15,15	1.46	2 (13%)	20,23,23	1.82	4 (20%)
2	X2Y	C	2	2	18,18,19	1.99	5 (27%)	20,28,30	1.17	2 (10%)
2	FUC	C	3	2	10,10,11	1.59	3 (30%)	14,14,16	0.99	0
2	X6Y	C	4	2	14,14,15	1.74	5 (35%)	16,21,23	1.73	3 (18%)
2	X6Y	D	1	2	15,15,15	1.30	2 (13%)	20,23,23	1.68	7 (35%)
2	X2Y	D	2	2	18,18,19	1.91	5 (27%)	20,28,30	1.28	3 (15%)
2	FUC	D	3	2	10,10,11	1.55	3 (30%)	14,14,16	0.93	1 (7%)
2	X6Y	D	4	2	14,14,15	1.69	5 (35%)	16,21,23	1.67	5 (31%)

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	X6Y	C	1	2	-	3/5/25/25	0/1/1/1
2	X2Y	C	2	2	-	3/10/27/30	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	X6Y	C	4	2	-	2/5/22/25	0/1/1/1
2	X6Y	D	1	2	-	0/5/25/25	0/1/1/1
2	X2Y	D	2	2	-	4/10/27/30	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	X6Y	D	4	2	-	1/5/22/25	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	X2Y	O5-C5	4.17	1.51	1.43
2	C	2	X2Y	O2-C2	-4.05	1.41	1.47
2	D	2	X2Y	O5-C5	3.78	1.51	1.43
2	D	2	X2Y	O2-C2	-3.69	1.41	1.47
2	C	4	X6Y	O2-C2	-3.46	1.42	1.47
2	D	2	X2Y	O4-S2	3.35	1.67	1.57
2	C	2	X2Y	O4-S2	3.19	1.66	1.57
2	D	4	X6Y	O2-C2	-3.02	1.42	1.47
2	C	1	X6Y	C3-C4	-2.89	1.44	1.52
2	D	4	X6Y	O5-C5	2.85	1.49	1.43
2	C	2	X2Y	O2-S1	2.82	1.65	1.57
2	C	3	FUC	C2-C3	-2.79	1.48	1.52
2	D	2	X2Y	O2-S1	2.76	1.65	1.57
2	C	2	X2Y	C3-C4	-2.70	1.44	1.52
2	C	3	FUC	O5-C1	2.69	1.48	1.43
2	D	3	FUC	O5-C1	2.63	1.48	1.43
2	D	3	FUC	C2-C3	-2.48	1.48	1.52
2	D	1	X6Y	O2-S1	2.39	1.64	1.57
2	C	4	X6Y	O5-C5	2.33	1.48	1.43
2	D	4	X6Y	C3-C4	-2.32	1.46	1.52
2	D	2	X2Y	C3-C4	-2.32	1.46	1.52
2	D	1	X6Y	O3-C3	2.24	1.48	1.43
2	D	4	X6Y	O2-S1	2.24	1.64	1.57
2	D	3	FUC	O5-C5	2.24	1.48	1.43
2	C	1	X6Y	O2-S1	2.22	1.64	1.57
2	C	4	X6Y	C3-C4	-2.21	1.46	1.52
2	C	4	X6Y	O2-S1	2.16	1.63	1.57
2	C	4	X6Y	C3-C2	-2.16	1.48	1.53
2	C	3	FUC	O5-C5	2.14	1.47	1.43
2	D	4	X6Y	C3-C2	-2.04	1.48	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	X6Y	C1-O5-C5	-4.29	107.69	114.37
2	D	4	X6Y	O8-S1-O6	-3.85	97.41	112.24
2	C	4	X6Y	O2-C2-C3	3.62	112.01	106.95
2	C	4	X6Y	O8-S1-O6	-3.55	98.55	112.24
2	C	1	X6Y	O3-C3-C4	-3.54	102.03	110.38
2	C	1	X6Y	C6-C5-C4	-3.49	106.69	113.08
2	C	4	X6Y	O7-S1-O2	3.48	114.38	106.37
2	D	1	X6Y	O8-S1-O6	-3.42	99.06	112.24
2	D	2	X2Y	O6-S1-O2	3.13	113.57	106.37
2	D	1	X6Y	C1-O5-C5	-3.12	109.52	114.37
2	D	4	X6Y	O2-C2-C3	2.76	110.81	106.95
2	C	2	X2Y	O6-S1-O8	-2.71	99.06	108.56
2	D	1	X6Y	O4-C4-C5	-2.53	104.15	109.74
2	D	1	X6Y	C3-C4-C5	2.42	113.49	109.81
2	D	1	X6Y	O7-S1-O2	2.41	111.91	106.37
2	D	2	X2Y	O6-S1-O8	-2.38	100.22	108.56
2	C	1	X6Y	O8-S1-O6	-2.35	103.16	112.24
2	D	4	X6Y	C6-C5-C4	-2.30	108.87	113.08
2	D	2	X2Y	O11-S2-O4	2.27	111.59	106.37
2	D	1	X6Y	C6-C5-C4	-2.23	109.01	113.08
2	D	3	FUC	C6-C5-C4	-2.14	109.16	113.08
2	C	2	X2Y	O11-S2-O4	2.11	111.22	106.37
2	D	1	X6Y	C4-C3-C2	2.10	114.44	109.68
2	D	4	X6Y	O7-S1-O2	2.03	111.03	106.37
2	D	4	X6Y	C4-C3-C2	-2.01	106.59	110.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	X6Y	C3-C2-O2-S1
2	D	2	X2Y	C4-O4-S2-O10
2	D	4	X6Y	C1-C2-O2-S1
2	C	1	X6Y	C2-O2-S1-O6
2	C	1	X6Y	C2-O2-S1-O8
2	C	2	X2Y	C4-O4-S2-O9
2	C	2	X2Y	C4-O4-S2-O10
2	D	2	X2Y	C4-O4-S2-O9
2	C	1	X6Y	C2-O2-S1-O7
2	C	2	X2Y	C4-O4-S2-O11
2	D	2	X2Y	C2-O2-S1-O6

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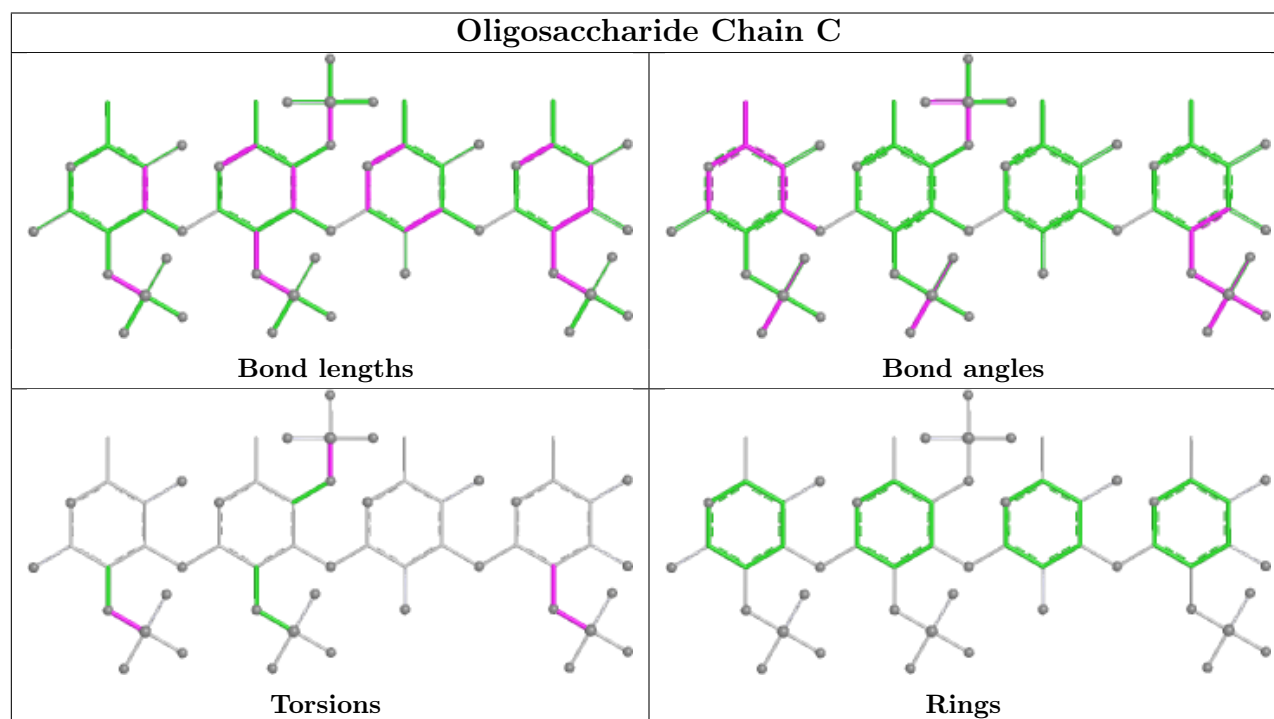
Mol	Chain	Res	Type	Atoms
2	D	2	X2Y	C4-O4-S2-O11
2	C	4	X6Y	C2-O2-S1-O6

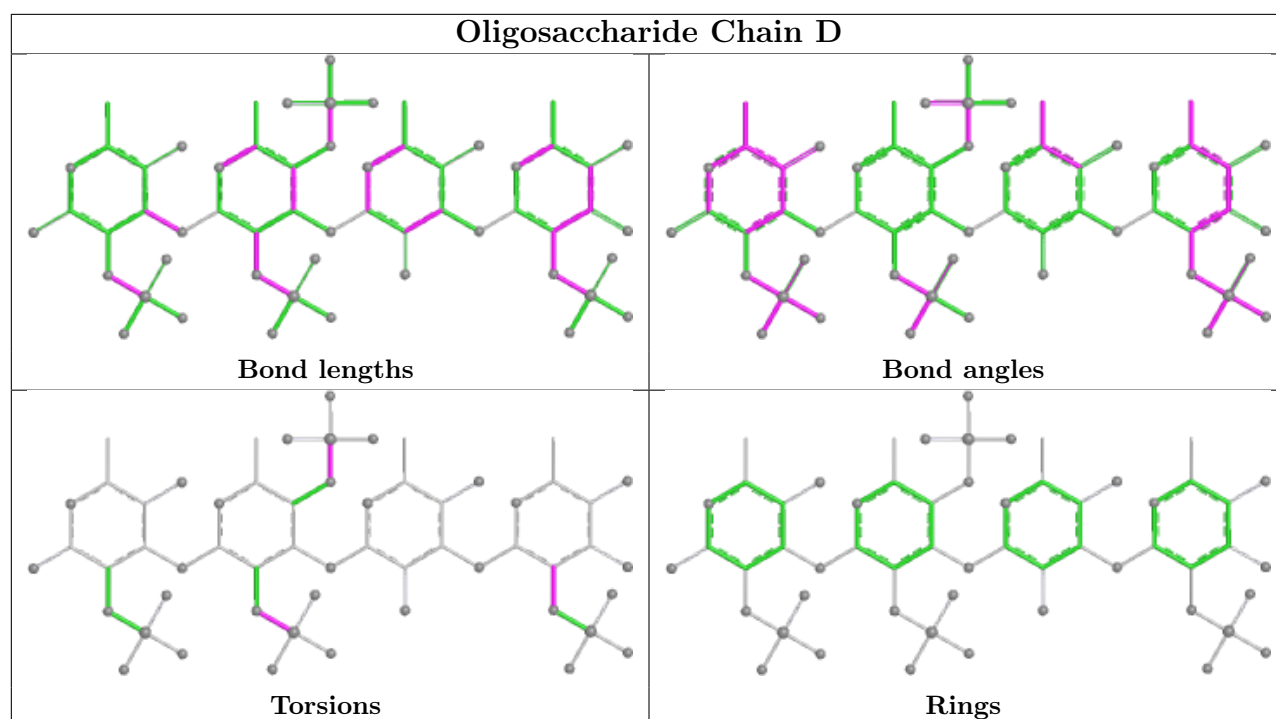
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	FUC	1	0
2	C	2	X2Y	1	0
2	D	2	X2Y	1	0
2	D	3	FUC	2	0
2	C	1	X6Y	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](#)

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, 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	449/497 (90%)	1.34	83 (18%) 3 2	17, 27, 44, 55	0
1	B	449/497 (90%)	1.33	78 (17%) 4 3	15, 27, 41, 56	0
All	All	898/994 (90%)	1.34	161 (17%) 3 3	15, 27, 43, 56	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	PHE	6.1
1	B	257	PRO	4.2
1	B	120	ASN	4.2
1	A	46	ASP	3.8
1	B	380	VAL	3.7
1	A	65	GLY	3.7
1	A	294	GLY	3.6
1	B	256	ASN	3.6
1	B	298	GLY	3.6
1	A	120	ASN	3.5
1	A	257	PRO	3.5
1	B	48	PRO	3.5
1	A	41	LEU	3.4
1	B	306	GLY	3.4
1	B	247	SER	3.3
1	A	334	VAL	3.3
1	B	267	GLY	3.2
1	B	140	ASP	3.1
1	B	473	LEU	3.1
1	A	305	THR	3.1
1	B	266	ASP	3.1
1	A	400	ILE	3.1
1	A	440	VAL	3.1
1	B	384	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	448	ALA	3.0
1	A	158	PRO	3.0
1	B	31	PRO	3.0
1	A	302	PHE	3.0
1	A	140	ASP	3.0
1	A	398	GLY	3.0
1	B	304	THR	2.9
1	A	271	SER	2.9
1	A	427	VAL	2.9
1	A	198	TYR	2.9
1	A	123	THR	2.9
1	A	303	PRO	2.9
1	B	302	PHE	2.9
1	A	385	SER	2.8
1	A	408	SER	2.8
1	B	151	CYS	2.8
1	B	307	MET	2.8
1	A	121	HIS	2.8
1	A	233	VAL	2.8
1	B	292	ALA	2.8
1	B	254	TRP	2.8
1	B	353	TYR	2.8
1	B	454	ASP	2.8
1	A	460	LEU	2.7
1	B	141	PRO	2.7
1	B	258	MET	2.7
1	A	48	PRO	2.7
1	A	399	VAL	2.7
1	B	61	VAL	2.7
1	B	60	PHE	2.6
1	B	420	PRO	2.6
1	B	139	SER	2.6
1	A	177	THR	2.6
1	B	88	GLY	2.6
1	A	42	PRO	2.6
1	B	280	ALA	2.6
1	B	309	SER	2.6
1	A	49	LYS	2.6
1	B	54	VAL	2.6
1	A	252	ALA	2.6
1	A	479	SER	2.6
1	A	99	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	457	GLY	2.5
1	A	317	THR	2.5
1	A	43	VAL	2.5
1	A	390	ASN	2.5
1	B	207	GLY	2.5
1	B	308	ASN	2.5
1	B	205	ALA	2.5
1	B	319	ILE	2.5
1	A	254	TRP	2.5
1	B	281	PHE	2.4
1	A	308	ASN	2.4
1	B	53	ALA	2.4
1	A	418	PRO	2.4
1	B	478	ILE	2.4
1	B	200	ARG	2.4
1	B	51	ASP	2.4
1	B	261	PHE	2.4
1	B	359	ALA	2.4
1	B	162	ALA	2.4
1	A	156	GLU	2.4
1	B	179	LEU	2.3
1	B	291	TYR	2.3
1	A	415	VAL	2.3
1	B	382	PRO	2.3
1	A	386	SER	2.3
1	B	129	ASP	2.3
1	B	424	TYR	2.3
1	A	445	SER	2.3
1	B	34	GLN	2.3
1	B	325	GLY	2.3
1	B	468	SER	2.3
1	B	152	TYR	2.3
1	A	128	ASN	2.3
1	A	139	SER	2.3
1	B	479	SER	2.3
1	B	70	THR	2.2
1	A	91	ILE	2.2
1	A	101	LEU	2.2
1	A	455	SER	2.2
1	A	419	TRP	2.2
1	A	137	VAL	2.2
1	A	144	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	185	PRO	2.2
1	A	346	GLY	2.2
1	B	195	VAL	2.2
1	A	448	ALA	2.2
1	A	319	ILE	2.2
1	A	478	ILE	2.2
1	A	383	SER	2.2
1	A	468	SER	2.2
1	A	454	ASP	2.2
1	A	132	TRP	2.2
1	A	242	TRP	2.2
1	A	131	VAL	2.2
1	A	304	THR	2.2
1	B	385	SER	2.2
1	A	301	VAL	2.1
1	B	324	ALA	2.1
1	A	228	THR	2.1
1	A	295	LEU	2.1
1	A	432	LEU	2.1
1	A	451	GLY	2.1
1	B	251	THR	2.1
1	A	247	SER	2.1
1	A	31	PRO	2.1
1	A	155	PRO	2.1
1	A	391	PHE	2.1
1	B	390	ASN	2.1
1	A	69	THR	2.1
1	B	226	LEU	2.1
1	B	262	GLY	2.1
1	B	46	ASP	2.1
1	B	253	LYS	2.1
1	B	444	PRO	2.1
1	B	295	LEU	2.1
1	B	407	GLY	2.1
1	A	315	ASP	2.1
1	A	410	LEU	2.1
1	A	276	GLY	2.1
1	A	106	SER	2.1
1	B	417	SER	2.1
1	B	121	HIS	2.1
1	B	135	VAL	2.0
1	B	402	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	230	TRP	2.0
1	A	300	ASP	2.0
1	B	315	ASP	2.0
1	B	436	SER	2.0
1	A	337	VAL	2.0
1	A	412	ARG	2.0
1	A	406	LEU	2.0
1	A	96	GLY	2.0
1	A	395	ILE	2.0
1	B	69	THR	2.0
1	B	63	SER	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](#)

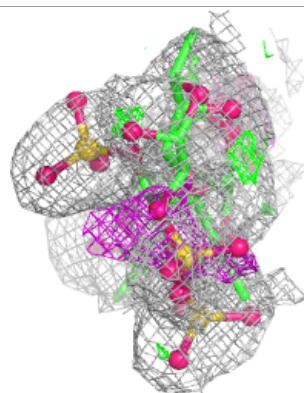
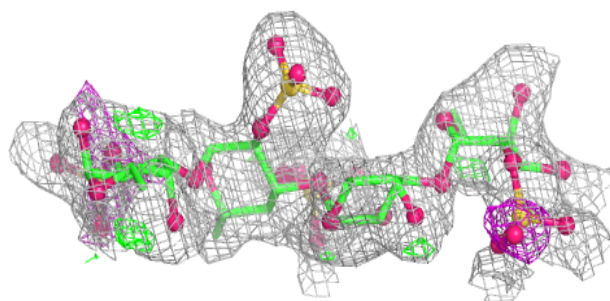
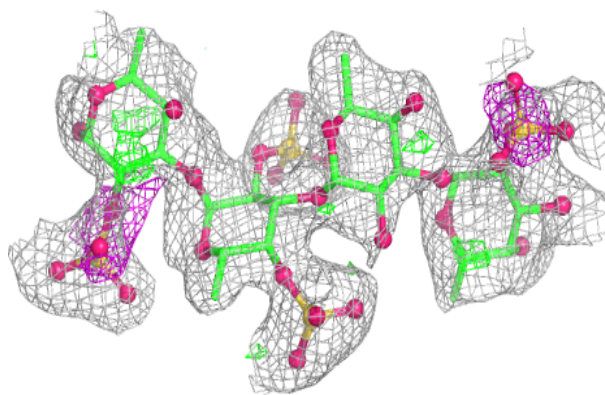
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	X6Y	C	4	14/15	0.54	0.20	29,37,48,54	0
2	X6Y	C	1	15/15	0.55	0.21	23,30,42,44	0
2	X6Y	D	1	15/15	0.57	0.22	29,35,52,63	0
2	X6Y	D	4	14/15	0.62	0.20	23,29,40,46	0
2	FUC	C	3	10/11	0.71	0.16	22,29,32,33	0
2	FUC	D	3	10/11	0.78	0.12	21,24,26,27	0
2	X2Y	C	2	18/19	0.92	0.11	20,26,29,31	0
2	X2Y	D	2	18/19	0.93	0.10	21,27,29,35	0

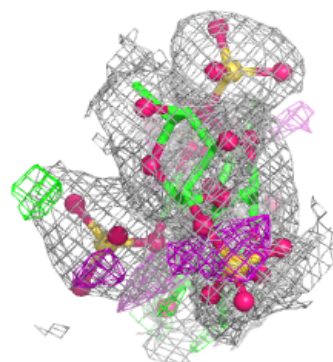
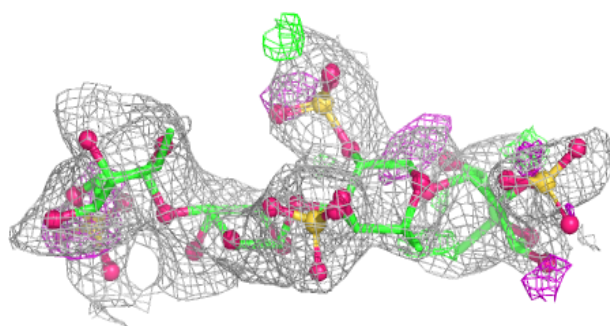
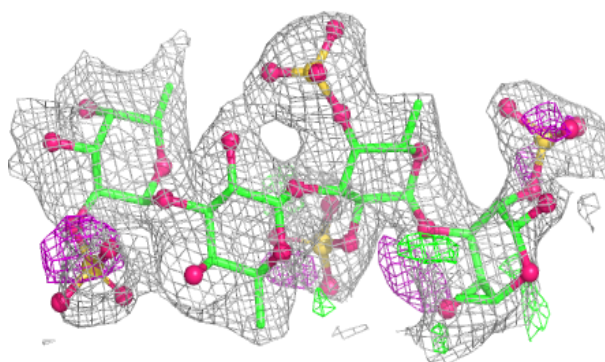
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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.