



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:50 AM UTC

PDB ID : 3U14 / pdb_00003u14
Title : Structure of D50A-fructofuranosidase from Schwanniomyces occidentalis complexed with inulin
Authors : Sainz-Polo, M.A.; Sanz-Aparicio, J.
Deposited on : 2011-09-29
Resolution : 2.24 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

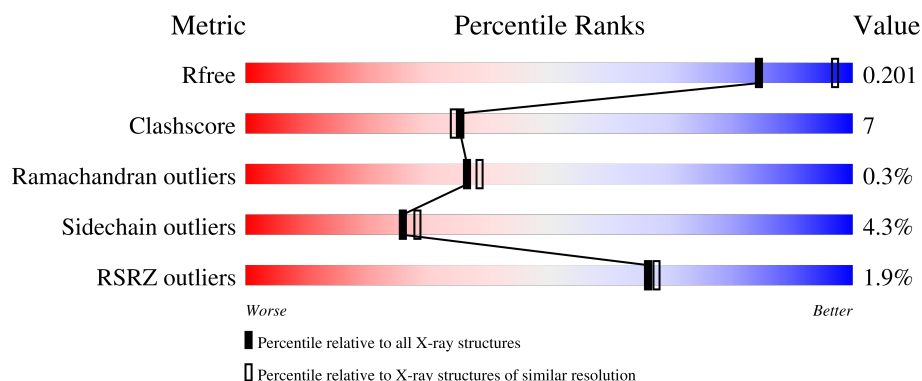
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	535	2% 77% 16% • 5%
1	B	535	2% 78% 16% • 5%
2	C	6	33% 50% 17%
2	D	6	33% 67%

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	FRU	C	1	X	-	-	-
2	FRU	D	1	X	-	-	-

2 Entry composition [i](#)

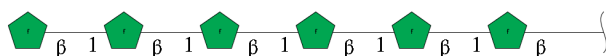
There are 4 unique types of molecules in this entry. The entry contains 9123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructofuranosidase.

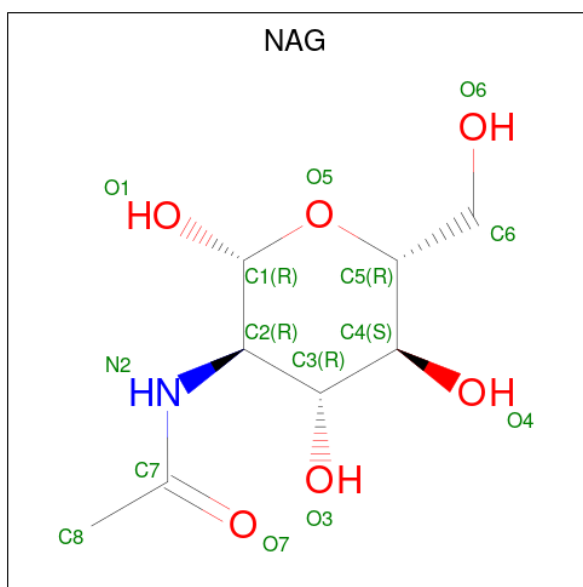
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4131	2656	677	792	6			
1	B	509	Total	C	N	O	S	0	0	0
			4131	2656	677	792	6			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	6	Total	C	O	0	0	0
			66	36	30			
2	D	6	Total	C	O	0	0	0
			66	36	30			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

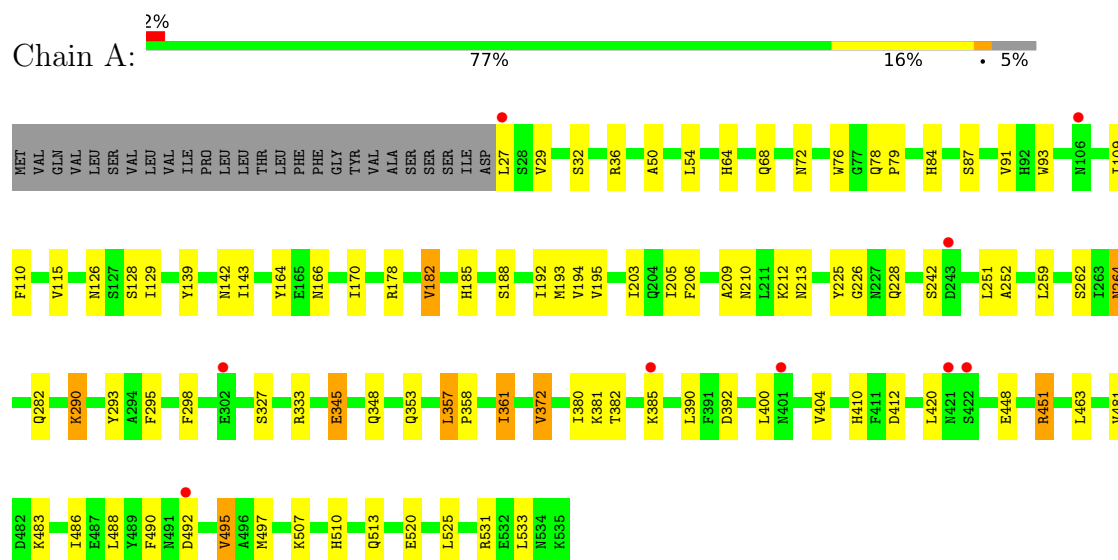
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	298	Total	O	0	0
			298	298		
4	B	319	Total	O	0	0
			319	319		

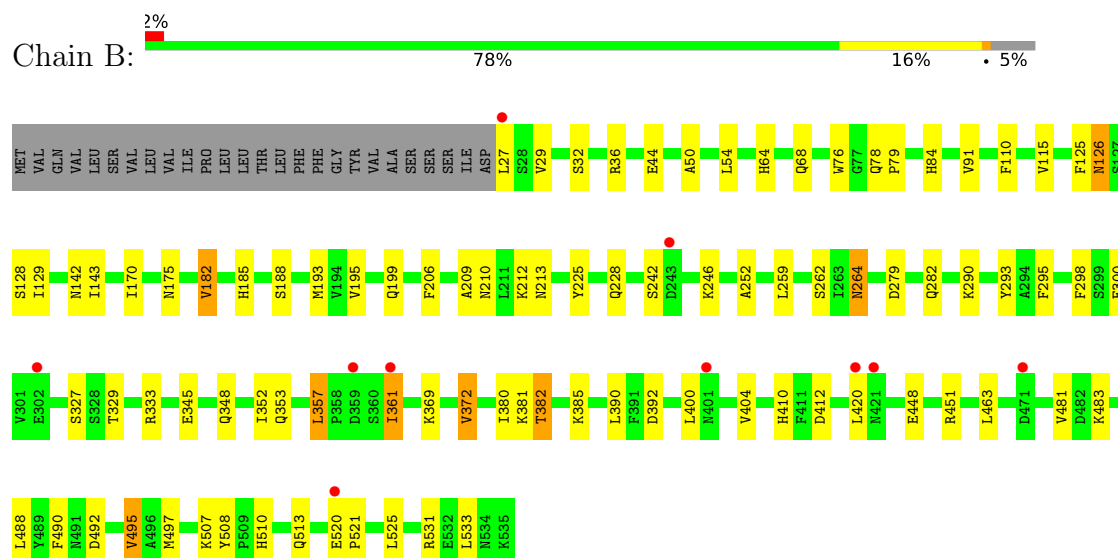
3 Residue-property plots [i](#)

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: Fructofuranosidase



• Molecule 1: Fructofuranosidase



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

Chain C:  33% 50% 17%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-beta-D-fructofuranose

Chain D:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.98Å 107.67Å 96.46Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.24 50.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.24) 98.2 (50.00-2.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.194 , 0.231 (Not available) , 0.201	Depositor DCC
R_{free} test set	3263 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.040 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9123	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: FRU, NAG

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	0.63	1/4252 (0.0%)	0.86	8/5791 (0.1%)
1	B	0.62	1/4252 (0.0%)	0.84	6/5791 (0.1%)
All	All	0.63	2/8504 (0.0%)	0.85	14/11582 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	TYR	C-O	-6.62	1.15	1.23
1	B	225	TYR	C-O	-6.27	1.16	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	225	TYR	O-C-N	-8.24	113.64	122.96
1	B	520	GLU	CA-C-N	-7.15	110.91	119.84
1	B	520	GLU	C-N-CA	-7.15	110.91	119.84
1	A	225	TYR	N-CA-C	-6.85	100.34	110.48
1	A	225	TYR	CA-C-N	-6.85	107.98	121.41
1	A	225	TYR	C-N-CA	-6.85	107.98	121.41
1	B	50	ALA	N-CA-C	5.94	116.43	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLY	N-CA-C	-5.74	99.57	113.18
1	A	520	GLU	CA-C-N	-5.47	113.01	119.84
1	A	520	GLU	C-N-CA	-5.47	113.01	119.84
1	B	125	PHE	N-CA-C	5.21	117.46	109.07
1	A	50	ALA	N-CA-C	5.07	116.08	109.64
1	B	126	ASN	CB-CA-C	-5.04	100.38	110.42
1	B	175	ASN	N-CA-CB	-5.01	102.62	110.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	ALA	Peptide
1	B	209	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4131	0	3919	62	0
1	B	4131	0	3918	58	0
2	C	66	0	59	2	0
2	D	66	0	59	1	0
3	A	56	0	52	3	0
3	B	56	0	51	0	0
4	A	298	0	0	7	0
4	B	319	0	0	6	0
All	All	9123	0	8058	122	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 7.

All (122) 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:451:ARG:NH1	4:A:740:HOH:O	1.82	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASP:HB2	4:A:792:HOH:O	1.65	0.94
1:B:210:ASN:HD22	1:B:213:ASN:HD22	1.06	0.93
1:B:210:ASN:ND2	1:B:213:ASN:HD22	1.69	0.90
1:A:210:ASN:HD22	1:A:213:ASN:HD22	1.22	0.88
1:A:357:LEU:HD23	1:A:361:ILE:HD13	1.55	0.87
1:B:78:GLN:HE22	1:B:142:ASN:HD22	1.22	0.84
1:B:488:LEU:HD12	1:B:497:MET:CE	2.07	0.84
1:A:210:ASN:ND2	1:A:213:ASN:HD22	1.76	0.84
1:B:357:LEU:HD23	1:B:361:ILE:HD13	1.60	0.82
1:A:78:GLN:HE22	1:A:142:ASN:HD22	1.24	0.82
1:A:488:LEU:HD12	1:A:497:MET:CE	2.10	0.81
1:A:259:LEU:O	1:A:290:LYS:HE3	1.82	0.79
1:A:64:HIS:HD2	1:A:84:HIS:NE2	1.80	0.78
1:B:64:HIS:HD2	1:B:84:HIS:NE2	1.82	0.77
1:B:68:GLN:HE22	1:B:110:PHE:HA	1.49	0.77
1:A:193:MET:HE3	1:A:195:VAL:CG1	2.17	0.75
1:B:488:LEU:HD12	1:B:497:MET:HE2	1.68	0.75
1:A:193:MET:HE3	1:A:195:VAL:HG11	1.69	0.74
1:B:126:ASN:HB2	1:B:129:ILE:HG12	1.67	0.74
3:A:1072:NAG:O7	3:A:1072:NAG:H3	1.87	0.74
1:A:488:LEU:HD12	1:A:497:MET:HE2	1.71	0.73
1:B:193:MET:HE3	1:B:195:VAL:CG1	2.19	0.72
1:A:490:PHE:HD1	1:A:495:VAL:HG22	1.55	0.70
1:B:210:ASN:HB3	1:B:212:LYS:H	1.57	0.70
1:B:300:GLU:OE2	4:B:847:HOH:O	2.11	0.69
1:A:410:HIS:HD2	1:A:412:ASP:OD1	1.75	0.69
1:B:492:ASP:HB2	4:B:612:HOH:O	1.93	0.69
1:B:490:PHE:HD1	1:B:495:VAL:HG22	1.56	0.68
1:B:78:GLN:NE2	1:B:142:ASN:HD22	1.92	0.67
1:B:282:GLN:HE22	1:B:348:GLN:HE21	1.42	0.67
1:B:410:HIS:HD2	1:B:412:ASP:OD1	1.78	0.66
1:B:210:ASN:ND2	1:B:213:ASN:ND2	2.42	0.66
1:B:193:MET:HE3	1:B:195:VAL:HG11	1.78	0.65
1:A:210:ASN:HB3	1:A:212:LYS:H	1.62	0.64
1:B:282:GLN:HE22	1:B:348:GLN:NE2	1.96	0.62
1:A:126:ASN:HB2	1:A:129:ILE:HG12	1.81	0.62
1:A:193:MET:HE2	1:A:206:PHE:CD2	2.35	0.62
1:A:252:ALA:HB1	1:A:293:TYR:CE1	2.35	0.61
1:B:488:LEU:HD12	1:B:497:MET:HE3	1.81	0.61
1:A:68:GLN:HE22	1:A:110:PHE:HA	1.66	0.60
1:B:126:ASN:HB3	1:B:128:SER:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:O	1:B:290:LYS:HE3	2.03	0.58
1:B:262:SER:HB2	1:B:293:TYR:CD1	2.38	0.58
1:A:64:HIS:CD2	1:A:84:HIS:NE2	2.68	0.57
1:A:345:GLU:HB2	1:B:199:GLN:HE21	1.70	0.57
1:A:488:LEU:HD12	1:A:497:MET:HE3	1.84	0.56
1:A:282:GLN:HE22	1:A:348:GLN:NE2	2.03	0.56
1:A:264:ASN:ND2	1:A:295:PHE:H	2.04	0.56
1:B:64:HIS:CD2	1:B:84:HIS:NE2	2.70	0.56
1:A:228:GLN:NE2	4:A:671:HOH:O	2.23	0.56
1:A:262:SER:HB2	1:A:293:TYR:CD1	2.41	0.56
1:A:282:GLN:HE22	1:A:348:GLN:HE21	1.54	0.55
1:A:451:ARG:CZ	4:A:740:HOH:O	2.41	0.54
1:B:185:HIS:HD2	1:B:188:SER:OG	1.90	0.54
1:B:252:ALA:HB1	1:B:293:TYR:CE1	2.42	0.54
1:B:410:HIS:CD2	1:B:412:ASP:OD1	2.61	0.53
1:A:392:ASP:OD1	1:A:531:ARG:HD3	2.09	0.52
1:B:392:ASP:OD1	1:B:531:ARG:HD3	2.10	0.52
1:B:78:GLN:HE22	1:B:142:ASN:ND2	2.01	0.51
1:A:170:ILE:HD12	1:A:193:MET:HE1	1.91	0.51
1:A:210:ASN:ND2	1:A:213:ASN:ND2	2.52	0.51
1:A:264:ASN:HD21	1:A:295:PHE:H	1.56	0.51
1:B:91:VAL:HG11	1:B:361:ILE:HD11	1.93	0.51
1:B:420:LEU:HB2	1:B:507:LYS:HE3	1.92	0.51
1:B:264:ASN:HD21	1:B:295:PHE:H	1.60	0.50
1:A:91:VAL:HG11	1:A:361:ILE:HD11	1.93	0.50
1:B:78:GLN:HA	1:B:79:PRO:C	2.37	0.50
1:A:410:HIS:CD2	1:A:412:ASP:OD1	2.60	0.49
1:B:68:GLN:NE2	1:B:110:PHE:HA	2.24	0.49
1:B:210:ASN:HD22	1:B:213:ASN:ND2	1.90	0.49
1:A:78:GLN:NE2	1:A:142:ASN:HD22	2.02	0.49
1:A:78:GLN:HA	1:A:79:PRO:C	2.38	0.49
1:B:382:THR:HG22	4:B:786:HOH:O	2.14	0.48
1:A:372:VAL:HG22	1:A:525:LEU:HB2	1.96	0.48
1:A:72:ASN:OD1	3:A:1072:NAG:H2	2.14	0.47
1:B:54:LEU:HB3	1:B:298:PHE:CD2	2.49	0.47
1:A:126:ASN:ND2	4:A:562:HOH:O	2.48	0.47
2:C:5:FRU:H11	2:C:6:FRU:H12	1.68	0.47
1:A:32:SER:HA	1:A:36:ARG:HB2	1.97	0.47
1:B:246:LYS:NZ	1:B:279:ASP:OD2	2.47	0.47
1:A:185:HIS:HE1	4:A:748:HOH:O	1.98	0.46
1:A:126:ASN:HB3	1:A:128:SER:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PRO:HD2	1:A:361:ILE:HD12	1.98	0.46
1:B:264:ASN:ND2	1:B:295:PHE:H	2.14	0.46
1:B:115:VAL:HG11	1:B:182:VAL:HG22	1.97	0.46
1:B:463:LEU:HD21	1:B:495:VAL:HG13	1.98	0.45
1:A:76:TRP:HE1	2:C:6:FRU:HO6	1.64	0.45
1:A:333:ARG:HH11	1:A:353:GLN:NE2	2.15	0.45
1:A:420:LEU:HB2	1:A:507:LYS:HE3	1.99	0.45
1:B:44:GLU:HG2	4:B:837:HOH:O	2.18	0.44
1:A:115:VAL:HG11	1:A:182:VAL:HG22	2.00	0.44
1:A:510:HIS:HB3	4:A:729:HOH:O	2.18	0.44
1:B:193:MET:HE2	1:B:206:PHE:CD2	2.53	0.43
1:B:228:GLN:NE2	4:B:672:HOH:O	2.27	0.43
1:B:369:LYS:HD2	1:B:380:ILE:HD12	2.01	0.43
1:A:486:ILE:HD11	1:A:488:LEU:HD21	2.01	0.43
3:A:1072:NAG:O7	3:A:1072:NAG:C3	2.61	0.43
1:A:54:LEU:HB3	1:A:298:PHE:CD2	2.54	0.43
1:B:170:ILE:HD12	1:B:193:MET:HE1	2.01	0.43
1:A:182:VAL:HA	1:A:192:ILE:O	2.19	0.43
1:A:194:VAL:HG12	1:A:205:ILE:HG12	1.99	0.43
1:B:372:VAL:HG22	1:B:525:LEU:HB2	2.01	0.43
1:A:390:LEU:HG	1:A:533:LEU:HB2	2.01	0.42
1:B:381:LYS:HG2	1:B:513:GLN:HG2	2.00	0.42
1:B:382:THR:CG2	4:B:786:HOH:O	2.67	0.42
1:A:87:SER:HB2	1:A:93:TRP:CE3	2.55	0.42
1:B:32:SER:HA	1:B:36:ARG:HB2	2.02	0.42
1:B:76:TRP:HE1	2:D:6:FRU:HO6	1.68	0.42
1:B:390:LEU:HG	1:B:533:LEU:HB2	2.02	0.42
1:A:178:ARG:HH22	1:A:228:GLN:NE2	2.17	0.42
1:B:372:VAL:HG21	1:B:380:ILE:HD11	2.02	0.42
1:A:381:LYS:HG2	1:A:513:GLN:HG2	2.01	0.41
1:B:508:TYR:O	1:B:510:HIS:HD2	2.03	0.41
1:A:185:HIS:HD2	1:A:188:SER:OG	2.03	0.41
1:A:164:TYR:CE2	1:A:166:ASN:HB2	2.55	0.41
1:A:36:ARG:O	1:A:483:LYS:HD3	2.21	0.41
1:A:372:VAL:HG21	1:A:380:ILE:HD11	2.01	0.41
1:B:333:ARG:HH11	1:B:353:GLN:NE2	2.19	0.40
1:A:109:ILE:HG23	1:A:139:TYR:CD1	2.56	0.40
1:A:203:ILE:HD11	1:A:251:LEU:HD13	2.03	0.40
1:B:36:ARG:O	1:B:483:LYS:HD3	2.21	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	507/535 (95%)	477 (94%)	29 (6%)	1 (0%)	43	48
1	B	507/535 (95%)	475 (94%)	30 (6%)	2 (0%)	30	30
All	All	1014/1070 (95%)	952 (94%)	59 (6%)	3 (0%)	36	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	B	327	SER
1	B	521	PRO

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	460/484 (95%)	440 (96%)	20 (4%)	26	28
1	B	460/484 (95%)	440 (96%)	20 (4%)	26	28
All	All	920/968 (95%)	880 (96%)	40 (4%)	26	28

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	29	VAL
1	A	143	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	VAL
1	A	242	SER
1	A	264	ASN
1	A	290	LYS
1	A	345	GLU
1	A	357	LEU
1	A	361	ILE
1	A	372	VAL
1	A	382	THR
1	A	385	LYS
1	A	400	LEU
1	A	404	VAL
1	A	448	GLU
1	A	451	ARG
1	A	463	LEU
1	A	481	VAL
1	A	495	VAL
1	B	27	LEU
1	B	29	VAL
1	B	143	ILE
1	B	182	VAL
1	B	242	SER
1	B	264	ASN
1	B	329	THR
1	B	345	GLU
1	B	352	ILE
1	B	357	LEU
1	B	361	ILE
1	B	372	VAL
1	B	382	THR
1	B	385	LYS
1	B	400	LEU
1	B	404	VAL
1	B	448	GLU
1	B	451	ARG
1	B	481	VAL
1	B	495	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	HIS
1	A	68	GLN
1	A	78	GLN
1	A	104	HIS
1	A	126	ASN
1	A	166	ASN
1	A	185	HIS
1	A	199	GLN
1	A	210	ASN
1	A	227	ASN
1	A	264	ASN
1	A	282	GLN
1	A	348	GLN
1	A	353	GLN
1	A	354	ASN
1	A	362	ASN
1	A	376	ASN
1	A	401	ASN
1	A	410	HIS
1	A	513	GLN
1	B	52	ASN
1	B	64	HIS
1	B	68	GLN
1	B	78	GLN
1	B	118	HIS
1	B	185	HIS
1	B	199	GLN
1	B	210	ASN
1	B	264	ASN
1	B	282	GLN
1	B	348	GLN
1	B	353	GLN
1	B	354	ASN
1	B	362	ASN
1	B	376	ASN
1	B	401	ASN
1	B	410	HIS
1	B	435	GLN
1	B	513	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 ⓘ

12 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	11,11,12	2.91	2 (18%)	15,15,18	5.33	5 (33%)
2	FRU	C	2	2	11,11,12	0.41	0	15,15,18	0.70	0
2	FRU	C	3	2	11,11,12	0.29	0	15,15,18	0.77	0
2	FRU	C	4	2	11,11,12	0.46	0	15,15,18	1.29	2 (13%)
2	FRU	C	5	2	11,11,12	0.29	0	15,15,18	0.78	0
2	FRU	C	6	2	11,11,12	0.38	0	15,15,18	0.94	1 (6%)
2	FRU	D	1	2	11,11,12	2.76	2 (18%)	15,15,18	5.46	5 (33%)
2	FRU	D	2	2	11,11,12	0.31	0	15,15,18	0.79	0
2	FRU	D	3	2	11,11,12	0.38	0	15,15,18	0.69	0
2	FRU	D	4	2	11,11,12	0.43	0	15,15,18	1.34	1 (6%)
2	FRU	D	5	2	11,11,12	0.34	0	15,15,18	0.97	1 (6%)
2	FRU	D	6	2	11,11,12	0.31	0	15,15,18	0.81	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	1/1/4/4	1/4/20/24	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	C	2	2	-	2/4/20/24	0/1/1/1
2	FRU	C	3	2	-	0/4/20/24	0/1/1/1
2	FRU	C	4	2	-	0/4/20/24	0/1/1/1
2	FRU	C	5	2	-	2/4/20/24	0/1/1/1
2	FRU	C	6	2	-	2/4/20/24	0/1/1/1
2	FRU	D	1	2	1/1/4/4	3/4/20/24	0/1/1/1
2	FRU	D	2	2	-	2/4/20/24	0/1/1/1
2	FRU	D	3	2	-	0/4/20/24	0/1/1/1
2	FRU	D	4	2	-	2/4/20/24	0/1/1/1
2	FRU	D	5	2	-	4/4/20/24	0/1/1/1
2	FRU	D	6	2	-	0/4/20/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	FRU	C1-C2	-8.05	1.24	1.51
2	D	1	FRU	C1-C2	-7.69	1.26	1.51
2	C	1	FRU	O1-C1	-4.94	1.21	1.42
2	D	1	FRU	O1-C1	-4.62	1.23	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	FRU	O1-C1-C2	18.96	175.90	111.33
2	C	1	FRU	O1-C1-C2	18.25	173.48	111.33
2	C	1	FRU	O5-C2-C1	6.45	122.86	109.22
2	D	1	FRU	O5-C2-C1	6.38	122.71	109.22
2	C	1	FRU	O5-C2-C3	5.19	115.45	105.15
2	D	1	FRU	O5-C2-C3	4.75	114.59	105.15
2	D	1	FRU	C1-C2-C3	3.21	122.68	115.10
2	C	1	FRU	C3-C4-C5	2.98	108.36	102.61
2	D	4	FRU	C6-C5-C4	-2.97	108.07	115.10
2	C	1	FRU	C1-C2-C3	2.75	121.59	115.10
2	D	1	FRU	C3-C4-C5	2.68	107.79	102.61
2	C	4	FRU	C6-C5-C4	-2.45	109.32	115.10
2	D	5	FRU	C6-C5-C4	-2.29	109.69	115.10
2	C	6	FRU	O5-C2-C1	2.15	113.76	109.22
2	C	4	FRU	C3-C4-C5	2.01	106.50	102.61

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	FRU	C2
2	D	1	FRU	C2

All (18) torsion outliers are listed below:

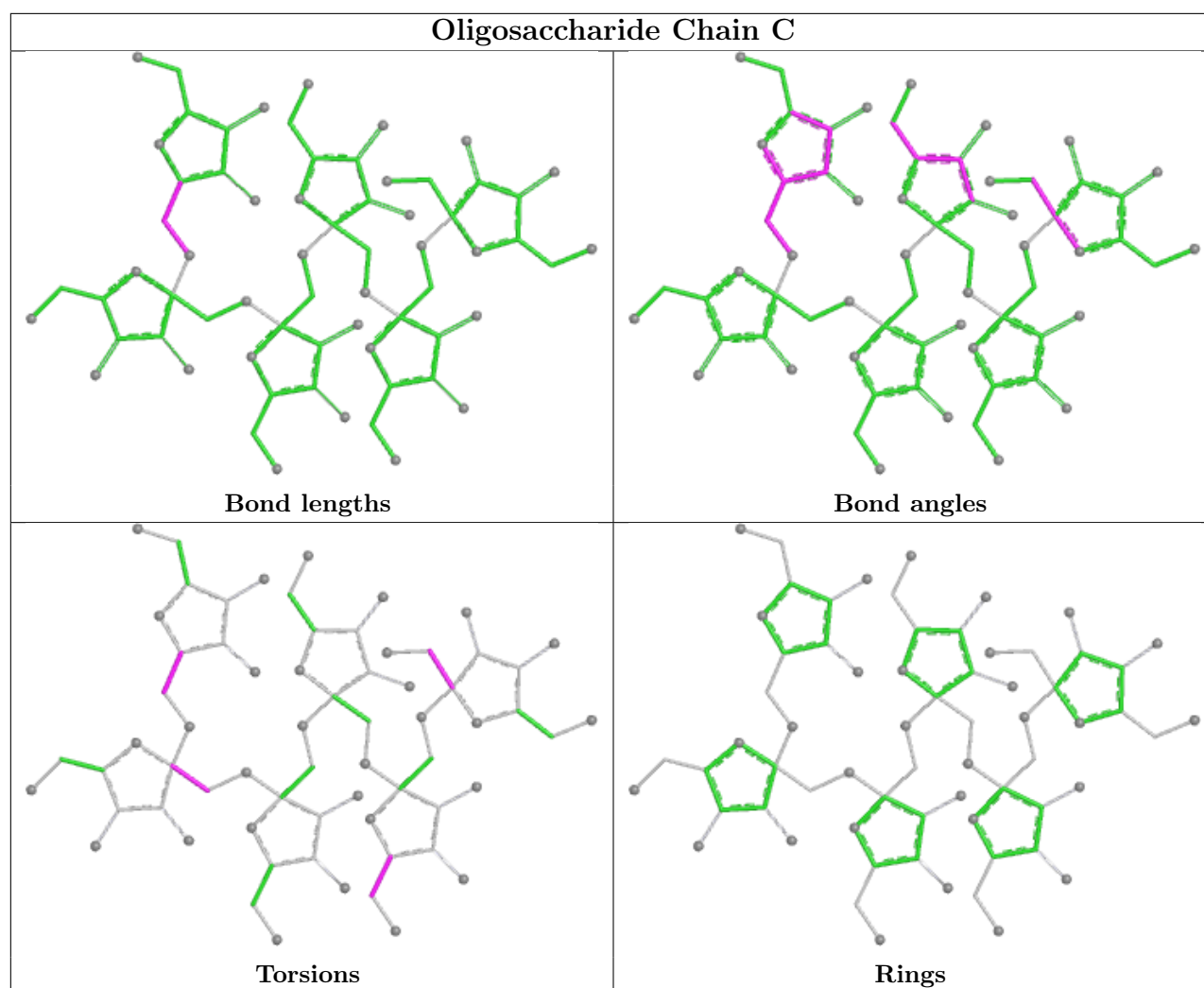
Mol	Chain	Res	Type	Atoms
2	D	1	FRU	O5-C5-C6-O6
2	D	2	FRU	O5-C5-C6-O6
2	C	1	FRU	O1-C1-C2-C3
2	D	1	FRU	O1-C1-C2-C3
2	D	1	FRU	C4-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6
2	C	5	FRU	O5-C5-C6-O6
2	D	5	FRU	O5-C5-C6-O6
2	D	5	FRU	C4-C5-C6-O6
2	C	5	FRU	C4-C5-C6-O6
2	C	6	FRU	O1-C1-C2-O5
2	D	4	FRU	C4-C5-C6-O6
2	C	6	FRU	O1-C1-C2-C3
2	D	5	FRU	O1-C1-C2-C3
2	D	5	FRU	O1-C1-C2-O5
2	C	2	FRU	O1-C1-C2-O5
2	D	4	FRU	O5-C5-C6-O6
2	C	2	FRU	O1-C1-C2-C3

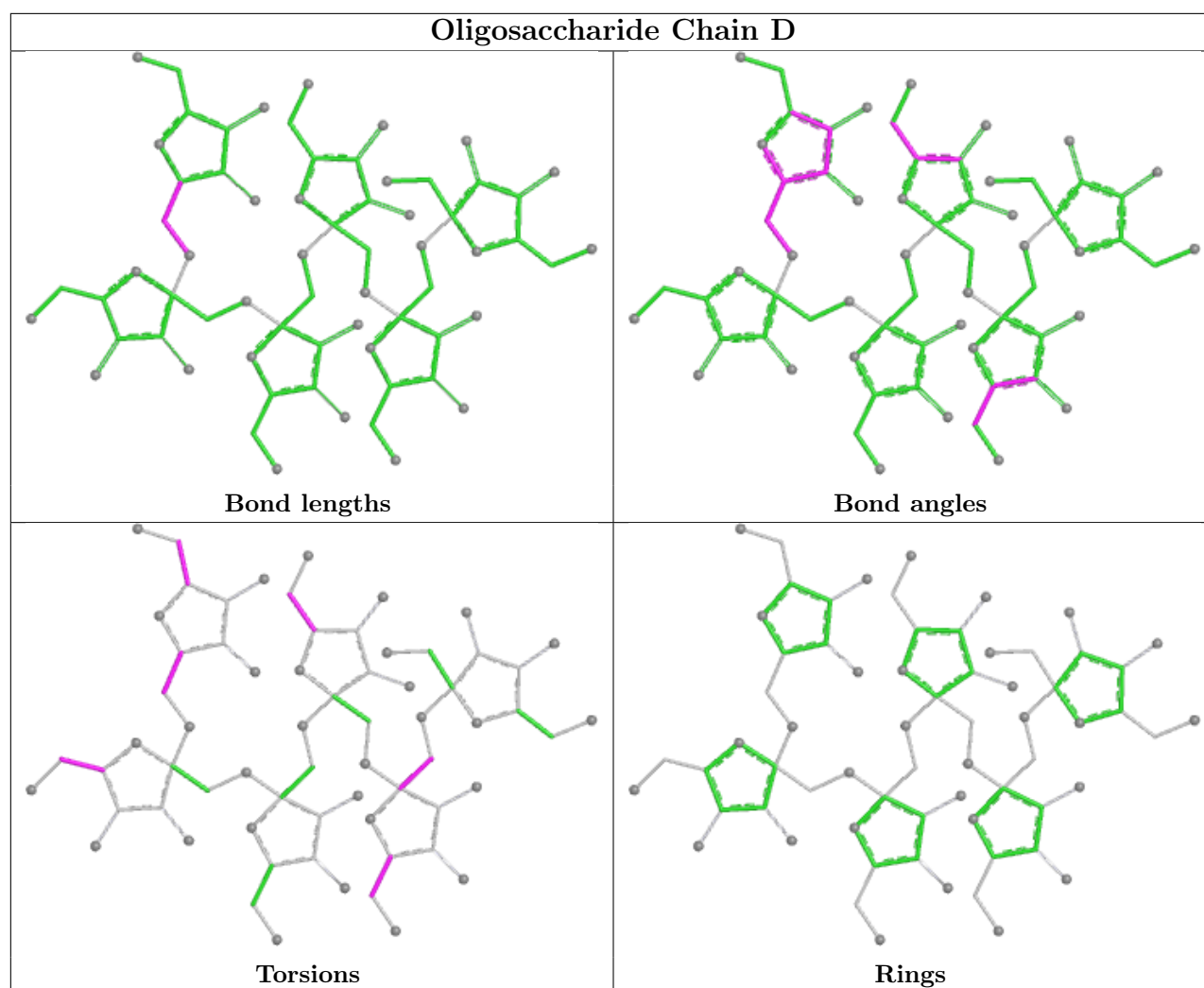
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	FRU	2	0
2	C	5	FRU	1	0
2	D	6	FRU	1	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](#)

8 ligands 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	$\# Z > 2$
3	NAG	B	1394	1	14,14,15	0.84	1 (7%)	17,19,21	1.65	5 (29%)
3	NAG	A	1072	1	14,14,15	0.56	0	17,19,21	0.62	0
3	NAG	B	1219	1	14,14,15	1.72	2 (14%)	17,19,21	2.68	6 (35%)
3	NAG	B	1126	1	14,14,15	1.81	6 (42%)	17,19,21	1.85	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1219	1	14,14,15	0.58	0	17,19,21	1.64	2 (11%)
3	NAG	A	1394	1	14,14,15	0.85	1 (7%)	17,19,21	2.86	3 (17%)
3	NAG	B	1334	1	14,14,15	1.81	1 (7%)	17,19,21	2.07	4 (23%)
3	NAG	A	1334	1	14,14,15	1.77	1 (7%)	17,19,21	2.55	7 (41%)

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	NAG	B	1394	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1072	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1219	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1126	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1219	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1394	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1334	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1334	1	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1334	NAG	O5-C1	-6.52	1.32	1.43
3	A	1334	NAG	O5-C1	-6.09	1.33	1.43
3	B	1219	NAG	O5-C1	-5.09	1.35	1.43
3	B	1219	NAG	C1-C2	3.59	1.57	1.52
3	B	1126	NAG	O5-C1	-2.89	1.38	1.43
3	A	1394	NAG	C1-C2	2.81	1.56	1.52
3	B	1126	NAG	C2-N2	-2.62	1.41	1.46
3	B	1394	NAG	C1-C2	2.55	1.55	1.52
3	B	1126	NAG	O7-C7	-2.47	1.17	1.23
3	B	1126	NAG	C1-C2	2.36	1.55	1.52
3	B	1126	NAG	C7-N2	-2.18	1.27	1.34
3	B	1126	NAG	O4-C4	-2.09	1.37	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1394	NAG	C1-O5-C5	10.12	125.75	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1219	NAG	O5-C1-C2	-7.51	99.67	111.29
3	A	1334	NAG	C1-O5-C5	-6.74	103.15	112.19
3	B	1334	NAG	C1-O5-C5	-5.58	104.71	112.19
3	A	1219	NAG	C1-O5-C5	5.17	119.11	112.19
3	B	1126	NAG	O5-C5-C6	4.83	117.06	107.66
3	A	1334	NAG	C2-N2-C7	-4.53	116.83	122.90
3	B	1219	NAG	O5-C5-C6	4.39	116.20	107.66
3	A	1334	NAG	O5-C5-C6	3.61	114.69	107.66
3	A	1394	NAG	C1-C2-N2	3.61	116.12	110.43
3	B	1126	NAG	O3-C3-C2	3.55	116.78	109.40
3	B	1219	NAG	C1-C2-N2	3.55	116.02	110.43
3	B	1394	NAG	C3-C4-C5	-3.20	104.42	110.23
3	B	1334	NAG	C4-C3-C2	-3.18	106.36	111.02
3	B	1334	NAG	C2-N2-C7	-3.10	118.74	122.90
3	B	1126	NAG	O5-C1-C2	-2.94	106.74	111.29
3	B	1394	NAG	C2-N2-C7	2.81	126.67	122.90
3	B	1219	NAG	C1-O5-C5	-2.79	108.45	112.19
3	A	1394	NAG	O5-C5-C6	2.66	112.83	107.66
3	B	1126	NAG	C1-C2-N2	-2.32	106.78	110.43
3	B	1219	NAG	O3-C3-C2	2.31	114.20	109.40
3	A	1334	NAG	C4-C3-C2	-2.31	107.64	111.02
3	B	1219	NAG	C3-C4-C5	-2.28	106.09	110.23
3	B	1394	NAG	C1-O5-C5	2.26	115.22	112.19
3	A	1334	NAG	O5-C5-C4	2.25	116.31	110.83
3	A	1334	NAG	C3-C4-C5	2.24	114.30	110.23
3	A	1219	NAG	O5-C1-C2	2.18	114.67	111.29
3	B	1394	NAG	C4-C3-C2	2.16	114.18	111.02
3	B	1394	NAG	O5-C5-C6	2.11	111.77	107.66
3	B	1334	NAG	O3-C3-C2	2.06	113.67	109.40
3	A	1334	NAG	O4-C4-C3	-2.04	105.58	110.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1072	NAG	C3-C2-N2-C7
3	A	1334	NAG	O5-C5-C6-O6
3	A	1219	NAG	C4-C5-C6-O6
3	A	1219	NAG	O5-C5-C6-O6
3	B	1334	NAG	O5-C5-C6-O6
3	B	1334	NAG	C4-C5-C6-O6
3	A	1334	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1394	NAG	O5-C5-C6-O6
3	A	1394	NAG	C4-C5-C6-O6
3	A	1072	NAG	C4-C5-C6-O6
3	A	1072	NAG	O5-C5-C6-O6
3	B	1394	NAG	C4-C5-C6-O6
3	B	1126	NAG	O5-C5-C6-O6
3	A	1072	NAG	C1-C2-N2-C7
3	B	1394	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1072	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	509/535 (95%)	-0.30	9 (1%) 67 69	6, 14, 31, 46	0
1	B	509/535 (95%)	-0.30	10 (1%) 65 66	6, 14, 31, 46	0
All	All	1018/1070 (95%)	-0.30	19 (1%) 66 68	6, 14, 31, 46	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LEU	5.6
1	A	27	LEU	5.0
1	A	302	GLU	4.1
1	B	243	ASP	3.5
1	B	302	GLU	3.0
1	B	420	LEU	2.9
1	A	422	SER	2.8
1	B	520	GLU	2.8
1	A	243	ASP	2.6
1	B	401	ASN	2.5
1	B	471	ASP	2.3
1	B	361	ILE	2.3
1	A	492	ASP	2.1
1	B	359	ASP	2.1
1	A	401	ASN	2.1
1	A	106	ASN	2.1
1	A	421	ASN	2.1
1	B	421	ASN	2.0
1	A	385	LYS	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 ⓘ

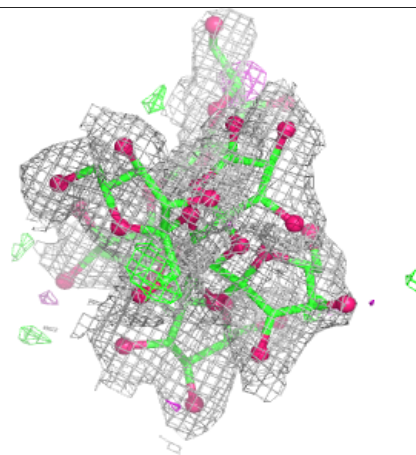
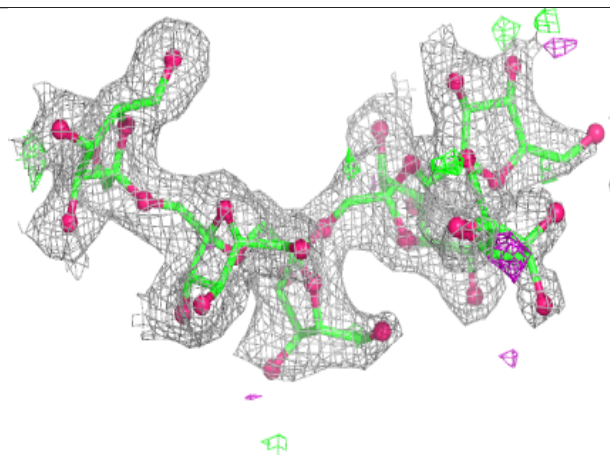
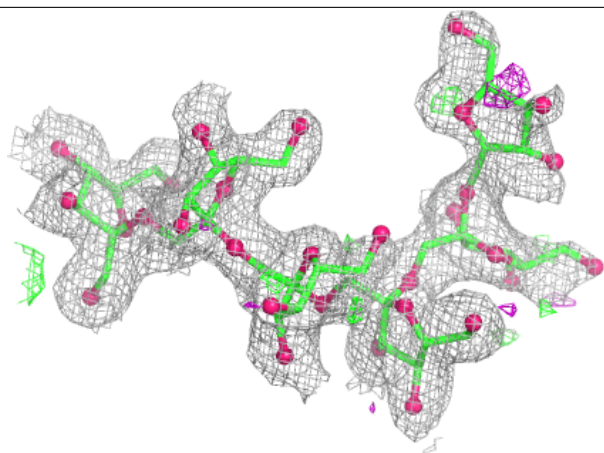
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

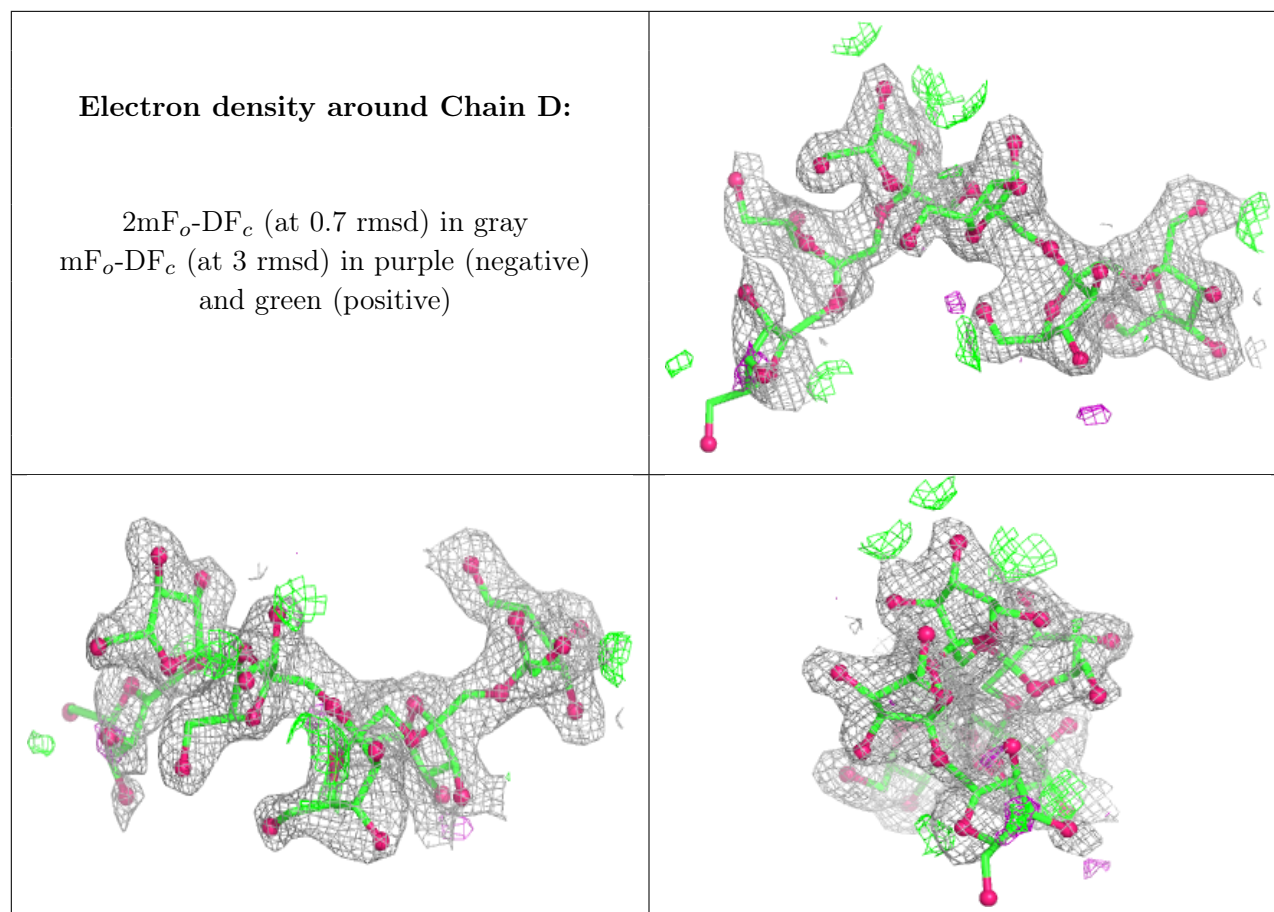
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FRU	D	1	11/12	0.55	0.22	49,58,61,62	0
2	FRU	C	1	11/12	0.66	0.20	45,56,58,58	0
2	FRU	D	2	11/12	0.85	0.12	36,45,46,47	0
2	FRU	C	2	11/12	0.87	0.14	30,41,44,46	0
2	FRU	C	4	11/12	0.87	0.12	22,29,34,37	0
2	FRU	D	4	11/12	0.87	0.12	29,32,36,36	0
2	FRU	D	3	11/12	0.90	0.09	28,31,33,33	0
2	FRU	D	5	11/12	0.91	0.10	21,28,30,33	0
2	FRU	C	5	11/12	0.93	0.08	16,20,22,25	0
2	FRU	C	3	11/12	0.93	0.08	23,26,28,28	0
2	FRU	D	6	11/12	0.96	0.07	15,19,20,20	0
2	FRU	C	6	11/12	0.97	0.06	10,12,13,15	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)





6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1072	14/15	0.67	0.18	34,38,44,44	0
3	NAG	B	1126	14/15	0.69	0.21	20,20,20,20	0
3	NAG	A	1394	14/15	0.74	0.14	33,39,43,45	0
3	NAG	A	1334	14/15	0.82	0.12	28,32,35,38	0
3	NAG	B	1394	14/15	0.83	0.11	32,36,37,38	0
3	NAG	B	1334	14/15	0.86	0.11	26,29,31,31	0
3	NAG	B	1219	14/15	0.90	0.09	19,21,25,25	0
3	NAG	A	1219	14/15	0.91	0.09	23,26,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.