



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:25 PM EDT

PDB ID : 1DWH / pdb_00001dwh
Title : Study on radiation damage on a cryocooled crystal. Part 4: Structure after irradiation with 27.2×10^{15} photons/mm²
Authors : Burmeister, W.P.
Deposited on : 1999-12-05
Resolution : 2.00 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

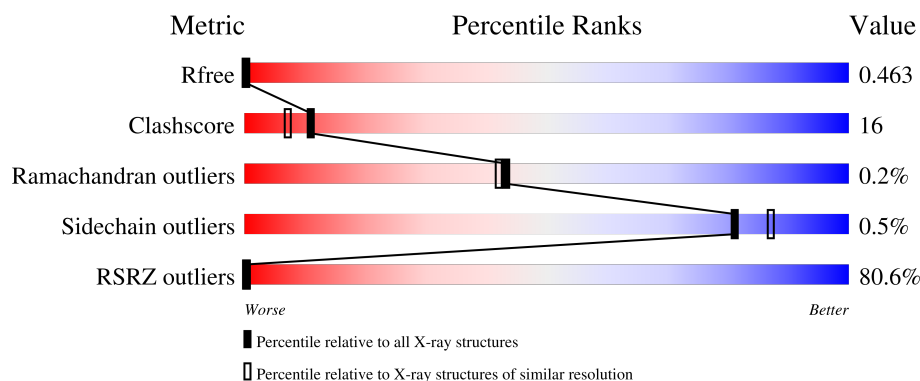
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	499	81% 80%18%.
2	A	2	50%50%
2	D	2	50%50%
3	B	5	100%
4	C	7	71%29%

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
4	BMA	C	3	-	-	X	-
4	MAN	C	6	X	X	X	-
5	NAG	M	931	-	-	X	-
5	NAG	M	961	X	-	-	-
7	SO4	M	1003	-	-	X	-
7	SO4	M	1004	-	-	X	-
7	SO4	M	1006	-	X	-	-
7	SO4	M	1009	-	X	X	X
8	GOL	M	1010	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5220 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 MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	21	0
			4083	2619	660	788	16			

There is a discrepancy between the modelled and reference sequences:

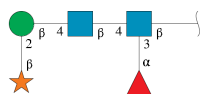
Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



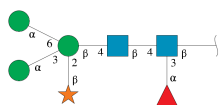
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



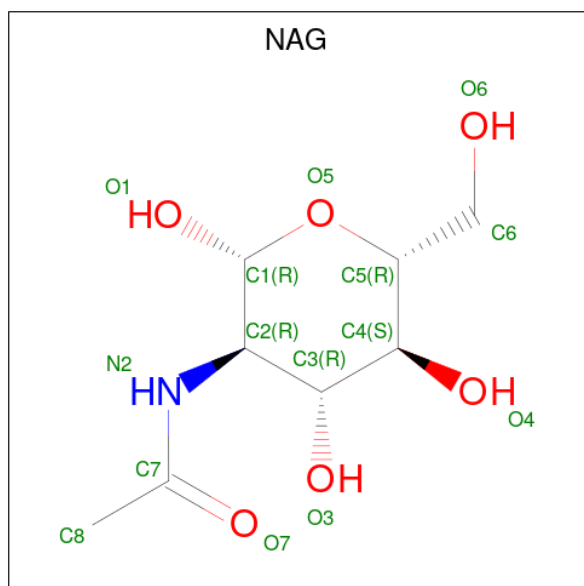
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			58	33	2	23			

- Molecule 4 is an oligosaccharide called beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	7	Total	C	N	O	0	0	0
			80	45	2	33			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		

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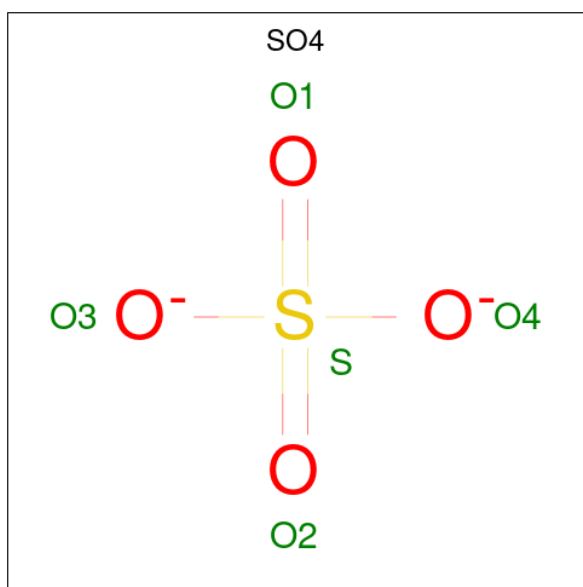
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Zn	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



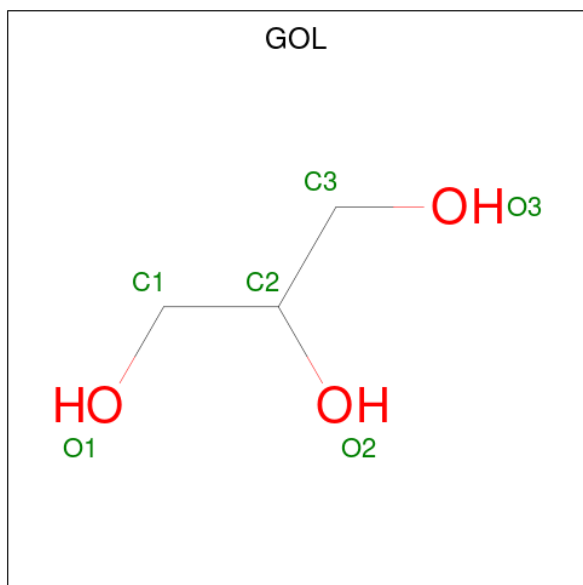
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		
8	M	1	Total	C	O	0	0
			6	3	3		

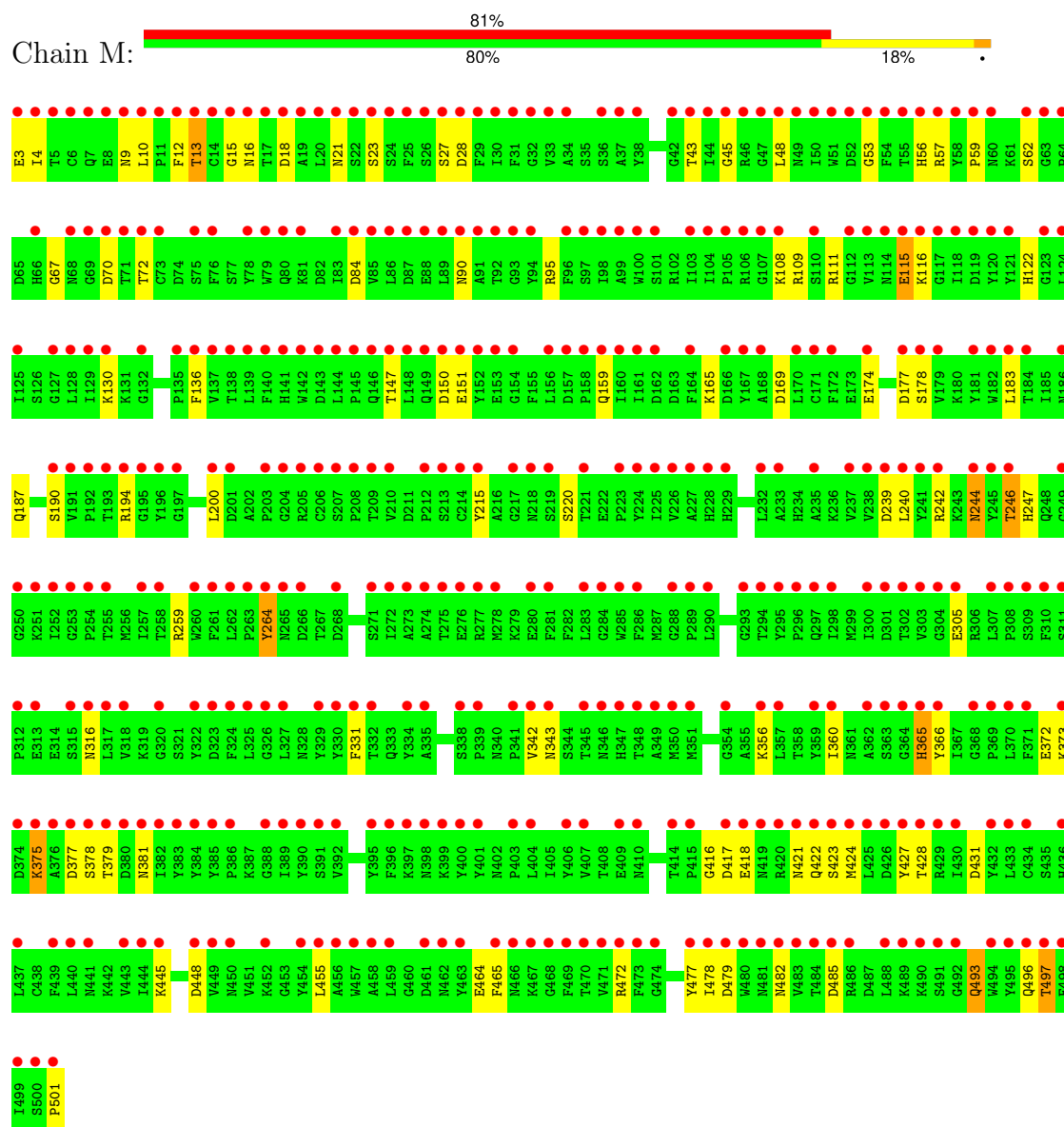
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	788	Total	O	0	0
			788	788		

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: MYROSINASE MA1



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  50% 50%

NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

NAG1
NAG2

- Molecule 3: beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

NAG1
NAG2
BMA3
XYP4
FUC5

- Molecule 4: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  71% 29%

NAG1
NAG2
BMA3
XYP4
MAN5
MAN6
FUC7

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 15.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.00) 97.6 (15.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.205 , 0.217 0.443 , 0.463	Depositor DCC
R_{free} test set	2573 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: GOL, BMA, SO4, FUC, ZN, NAG, XYP, MAN

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	M	1.25	16/4291 (0.4%)	1.34	41/5835 (0.7%)

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	M	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	264	TYR	CZ-OH	16.26	1.72	1.38
1	M	16	ASN	CG-ND2	14.88	1.64	1.33
1	M	13	THR	C-O	-12.91	1.04	1.24
1	M	264	TYR	CE1-CZ	-11.67	1.10	1.38
1	M	356	LYS	CE-NZ	-9.33	1.21	1.49
1	M	501	PRO	CA-C	6.86	1.67	1.52
1	M	423	SER	CB-OG	6.44	1.55	1.42
1	M	416	GLY	C-O	-6.22	1.17	1.24
1	M	242	ARG	NE-CZ	6.04	1.39	1.33
1	M	178	SER	CB-OG	5.84	1.53	1.42
1	M	147	THR	CB-OG1	5.48	1.52	1.43
1	M	246	THR	CB-CG2	-5.41	1.34	1.52
1	M	242	ARG	CD-NE	-5.38	1.38	1.46
1	M	497	THR	C-O	-5.38	1.17	1.24
1	M	501	PRO	N-CD	5.24	1.55	1.47
1	M	247	HIS	CE1-NE2	5.07	1.37	1.32

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	482	ASN	CA-CB-CG	-12.47	100.13	112.60
1	M	482	ASN	OD1-CG-ND2	-10.79	111.81	122.60
1	M	264	TYR	CE1-CZ-CE2	9.03	138.36	120.30
1	M	16	ASN	CA-CB-CG	-8.60	104.00	112.60
1	M	115	GLU	OE1-CD-OE2	-7.46	105.00	122.90
1	M	377	ASP	O-C-N	-7.37	113.70	123.14
1	M	448	ASP	CB-CG-OD2	-7.34	101.51	118.40
1	M	421	ASN	CA-C-O	-7.21	112.78	120.42
1	M	246	THR	OG1-CB-CG2	-7.00	95.31	109.30
1	M	109	ARG	NE-CZ-NH1	-6.88	114.62	121.50
1	M	478	ILE	CB-CG1-CD1	6.82	128.13	113.80
1	M	239	ASP	CA-CB-CG	6.80	119.40	112.60
1	M	264	TYR	OH-CZ-CE2	-6.70	99.82	119.90
1	M	482	ASN	CB-CG-OD1	6.64	134.09	120.80
1	M	496	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	M	448	ASP	OD1-CG-OD2	6.26	137.92	122.90
1	M	418	GLU	CA-C-O	-6.24	114.76	121.56
1	M	377	ASP	CA-C-O	6.14	128.76	120.47
1	M	422	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	M	497	THR	OG1-CB-CG2	-6.03	97.24	109.30
1	M	264	TYR	CZ-CE2-CD2	-6.01	108.77	119.60
1	M	493	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	M	316	ASN	OD1-CG-ND2	5.90	128.50	122.60
1	M	244	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	M	18	ASP	CA-C-O	-5.75	113.36	119.97
1	M	23	SER	CA-CB-OG	-5.68	99.74	111.10
1	M	416	GLY	N-CA-C	-5.68	108.42	114.67
1	M	365	HIS	CB-CG-ND1	5.65	131.17	122.70
1	M	372	GLU	CG-CD-OE2	5.65	131.39	118.40
1	M	417	ASP	CA-CB-CG	5.61	118.21	112.60
1	M	183	LEU	CD1-CG-CD2	5.59	123.09	110.80
1	M	109	ARG	NH1-CZ-NH2	5.54	126.50	119.30
1	M	84	ASP	CA-CB-CG	5.48	118.08	112.60
1	M	423	SER	CA-CB-OG	-5.31	100.49	111.10
1	M	485	ASP	CA-CB-CG	5.30	117.90	112.60
1	M	72	THR	CB-CA-C	5.28	120.92	110.42
1	M	479	ASP	CA-CB-CG	5.21	117.81	112.60
1	M	343	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	M	177	ASP	CA-CB-CG	-5.15	107.45	112.60
1	M	27	SER	CA-CB-OG	-5.10	100.90	111.10
1	M	190	SER	N-CA-C	5.01	116.56	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	13	THR	Mainchain

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	M	4083	0	3835	106	4
2	A	28	0	24	3	0
2	D	28	0	25	1	0
3	B	58	0	42	0	0
4	C	80	0	58	9	0
5	M	84	0	77	17	0
6	M	1	0	0	0	1
7	M	40	0	0	10	0
8	M	30	0	39	4	0
9	M	788	0	0	78	17
All	All	5220	0	4100	137	21

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 16.

All (137) 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:M:244:ASN:HD21	5:M:931:NAG:C1	0.96	1.56
1:M:21:ASN:HD21	5:M:901:NAG:C1	0.90	1.52
1:M:264:TYR:OH	1:M:264:TYR:CZ	1.72	1.42
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.57	1.37
8:M:1010:GOL:C1	9:M:3089:HOH:O	1.71	1.34
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	2.14	1.30
1:M:15:GLY:HA3	9:M:2032:HOH:O	1.25	1.28
1:M:427:TYR:HE2	9:M:2614:HOH:O	1.19	1.25
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.33	1.24
1:M:428:THR:HG23	9:M:2617:HOH:O	1.27	1.24
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE2	2.22	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:NAG:C3	2:A:1:NAG:O3	1.89	1.19
1:M:477:TYR:HE1	9:M:2659:HOH:O	1.21	1.18
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE2	1.78	1.17
1:M:431:ASP:OD1	9:M:2620:HOH:O	1.66	1.10
1:M:477:TYR:CE1	9:M:2659:HOH:O	1.94	1.08
8:M:1010:GOL:H11	9:M:3089:HOH:O	1.27	1.08
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE2	2.33	1.07
1:M:215:TYR:O	9:M:2355:HOH:O	1.69	1.07
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD2	1.92	1.05
8:M:1010:GOL:C2	9:M:3089:HOH:O	1.91	1.04
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	2.03	1.03
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE2	1.91	1.02
1:M:427:TYR:CE2	9:M:2614:HOH:O	1.95	1.01
7:M:1004:SO4:O2	7:M:1009:SO4:S	2.19	1.00
1:M:165:LYS:NZ	5:M:931:NAG:H82	1.76	0.99
5:M:961:NAG:H61	9:M:3056:HOH:O	1.62	0.98
1:M:259:ARG:HG2	9:M:2483:HOH:O	1.64	0.96
1:M:165:LYS:HZ1	5:M:931:NAG:H82	1.24	0.96
1:M:472:ARG:CZ	9:M:2659:HOH:O	2.12	0.95
1:M:246:THR:HG22	9:M:2377:HOH:O	1.66	0.94
1:M:150:ASP:OD2	9:M:2277:HOH:O	1.88	0.91
1:M:379:THR:HG23	9:M:2548:HOH:O	1.71	0.90
1:M:53:GLY:O	9:M:2097:HOH:O	1.90	0.89
4:C:3:BMA:H61	4:C:6:MAN:C6	2.03	0.89
7:M:1004:SO4:O2	7:M:1009:SO4:O2	1.91	0.88
1:M:130:LYS:HB3	9:M:2253:HOH:O	1.72	0.88
4:C:3:BMA:H61	4:C:6:MAN:H61	1.55	0.88
1:M:215:TYR:HB2	9:M:2102:HOH:O	1.72	0.86
1:M:130:LYS:HG3	9:M:2243:HOH:O	1.76	0.84
1:M:15:GLY:CA	9:M:2032:HOH:O	1.93	0.84
1:M:21:ASN:HD21	5:M:901:NAG:C2	1.88	0.83
1:M:151:GLU:OE1	9:M:2279:HOH:O	1.97	0.82
4:C:3:BMA:C6	4:C:6:MAN:H61	2.11	0.81
1:M:381:ASN:ND2	9:M:2554:HOH:O	2.14	0.79
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD2	2.61	0.78
7:M:1009:SO4:O1	9:M:3087:HOH:O	2.00	0.78
1:M:70:ASP:HB3	9:M:2078:HOH:O	1.83	0.76
9:M:3062:HOH:O	2:D:2:NAG:H83	1.86	0.76
4:C:3:BMA:C6	4:C:6:MAN:C6	2.65	0.74
1:M:373:LYS:NZ	9:M:2554:HOH:O	2.21	0.74
1:M:130:LYS:HB3	9:M:2091:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	2.22	0.74
1:M:90:ASN:ND2	5:M:911:NAG:C2	2.53	0.72
1:M:264:TYR:OH	1:M:264:TYR:CE2	2.42	0.71
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE2	2.24	0.71
1:M:9:ASN:HB2	9:M:3077:HOH:O	1.91	0.70
1:M:116:LYS:HG2	9:M:2225:HOH:O	1.92	0.70
9:M:3019:HOH:O	2:A:1:NAG:O3	2.10	0.70
1:M:472:ARG:NE	9:M:2659:HOH:O	2.20	0.70
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CZ	2.67	0.69
1:M:493:GLN:NE2	9:M:2681:HOH:O	2.24	0.69
7:M:1004:SO4:S	7:M:1009:SO4:O3	2.51	0.68
1:M:45:GLY:HA2	9:M:2085:HOH:O	1.93	0.68
1:M:70:ASP:OD2	9:M:2125:HOH:O	2.11	0.68
7:M:1003:SO4:O2	9:M:3069:HOH:O	2.14	0.66
1:M:115:GLU:HG3	9:M:2223:HOH:O	1.95	0.66
4:C:3:BMA:H61	4:C:6:MAN:H62	1.76	0.66
1:M:111:ARG:O	9:M:2213:HOH:O	2.14	0.66
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.78	0.65
1:M:90:ASN:CG	5:M:911:NAG:C1	2.68	0.65
1:M:472:ARG:NH2	9:M:2659:HOH:O	2.26	0.65
1:M:220[A]:SER:OG	9:M:2359:HOH:O	2.15	0.64
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.80	0.64
7:M:1003:SO4:O4	9:M:3069:HOH:O	2.16	0.63
1:M:200:LEU:HB3	9:M:2336:HOH:O	1.98	0.63
1:M:115:GLU:CD	9:M:2223:HOH:O	2.42	0.63
7:M:1004:SO4:O2	7:M:1009:SO4:O3	2.15	0.63
1:M:21:ASN:CG	5:M:901:NAG:C1	2.67	0.61
8:M:1010:GOL:O2	9:M:3089:HOH:O	2.01	0.61
7:M:1004:SO4:O1	7:M:1009:SO4:O3	2.20	0.60
1:M:365:HIS:HE1	9:M:2532:HOH:O	1.83	0.60
1:M:342[A]:VAL:HG13	9:M:2359:HOH:O	2.02	0.60
7:M:1004:SO4:S	7:M:1009:SO4:S	3.00	0.59
1:M:45:GLY:HA2	9:M:2086:HOH:O	2.03	0.58
1:M:159:GLN:NE2	9:M:2288:HOH:O	2.36	0.58
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.33	0.58
1:M:90:ASN:ND2	5:M:911:NAG:O5	2.36	0.58
1:M:115:GLU:OE2	9:M:2223:HOH:O	2.17	0.57
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.40	0.56
1:M:194:ARG:NH1	7:M:1009:SO4:O4	2.40	0.55
1:M:331:PHE:CD1	9:M:2483:HOH:O	2.53	0.55
9:M:3055:HOH:O	4:C:3:BMA:C6	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:GLY:C	9:M:2032:HOH:O	2.34	0.54
1:M:21:ASN:ND2	5:M:901:NAG:C2	2.58	0.54
1:M:424:MET:HE3	9:M:2681:HOH:O	2.06	0.54
1:M:4:ILE:HD11	1:M:445:LYS:CD	2.39	0.52
1:M:244:ASN:HD21	5:M:931:NAG:C2	1.98	0.52
9:M:3053:HOH:O	4:C:6:MAN:C4	2.58	0.52
1:M:472:ARG:HG2	9:M:2658:HOH:O	2.11	0.51
2:A:1:NAG:O3	2:A:1:NAG:C2	2.56	0.51
1:M:21:ASN:ND2	5:M:901:NAG:O5	2.40	0.51
1:M:130:LYS:CB	9:M:2253:HOH:O	2.43	0.51
1:M:28:ASP:HA	9:M:2053:HOH:O	2.10	0.51
1:M:115:GLU:CG	9:M:2223:HOH:O	2.56	0.50
1:M:360[A]:ILE:HG23	9:M:2518:HOH:O	2.10	0.50
1:M:10:LEU:HD23	9:M:2023:HOH:O	2.12	0.49
1:M:108:LYS:HD2	9:M:2298:HOH:O	2.12	0.49
1:M:70:ASP:CB	9:M:2078:HOH:O	2.51	0.48
1:M:360[A]:ILE:CG2	9:M:2518:HOH:O	2.61	0.48
1:M:95:ARG:HA	1:M:136:PHE:O	2.14	0.47
1:M:59:PRO:HB3	9:M:2100:HOH:O	2.14	0.47
9:M:3053:HOH:O	4:C:6:MAN:C5	2.62	0.47
4:C:3:BMA:O6	4:C:6:MAN:C6	2.49	0.46
1:M:12:PHE:HD2	9:M:2023:HOH:O	2.00	0.45
1:M:111:ARG:C	9:M:2213:HOH:O	2.58	0.45
1:M:165:LYS:CE	5:M:931:NAG:H82	2.46	0.45
1:M:53:GLY:C	9:M:2097:HOH:O	2.52	0.44
1:M:373:LYS:NZ	1:M:378:SER:OG	2.46	0.44
1:M:45:GLY:CA	9:M:2085:HOH:O	2.57	0.44
1:M:122:HIS:HE1	1:M:174:GLU:O	1.99	0.44
1:M:95:ARG:HB2	1:M:455:LEU:HD13	2.00	0.43
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:OH	2.05	0.43
1:M:497:THR:HG23	9:M:2689:HOH:O	2.19	0.42
1:M:59:PRO:HG3	9:M:2117:HOH:O	2.19	0.42
1:M:244:ASN:ND2	5:M:931:NAG:O5	2.42	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	0.42
1:M:12:PHE:N	9:M:2023:HOH:O	2.26	0.42
1:M:62[B]:SER:OG	1:M:67:GLY:O	2.31	0.41
5:M:961:NAG:C6	9:M:3056:HOH:O	2.41	0.41
1:M:244:ASN:ND2	5:M:931:NAG:C2	2.68	0.41
1:M:464:GLU:O	1:M:465:PHE:C	2.64	0.41
1:M:48:LEU:N	9:M:2090:HOH:O	2.35	0.40

All (21) 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)
6:M:1001:ZN:ZN	6:M:1001:ZN:ZN[3_656]	1.10	1.10
9:M:2279:HOH:O	9:M:2279:HOH:O[3_656]	1.10	1.10
9:M:2009:HOH:O	9:M:2520:HOH:O[4_576]	1.36	0.84
9:M:2248:HOH:O	9:M:2534:HOH:O[4_576]	1.37	0.83
9:M:2247:HOH:O	9:M:2247:HOH:O[4_576]	1.42	0.78
9:M:2555:HOH:O	9:M:2555:HOH:O[4_576]	1.44	0.76
9:M:2018:HOH:O	9:M:2018:HOH:O[4_576]	1.63	0.57
9:M:2258:HOH:O	9:M:2258:HOH:O[4_576]	1.63	0.57
9:M:2385:HOH:O	9:M:2426:HOH:O[6_565]	1.71	0.49
9:M:2116:HOH:O	9:M:2132:HOH:O[3_656]	1.76	0.44
9:M:2245:HOH:O	9:M:2621:HOH:O[4_576]	1.90	0.30
1:M:45:GLY:N	1:M:57:ARG:O[3_656]	1.95	0.25
9:M:2523:HOH:O	9:M:2622:HOH:O[4_576]	2.01	0.19
1:M:375:LYS:O	1:M:375:LYS:CD[4_576]	2.04	0.16
9:M:2388:HOH:O	9:M:2441:HOH:O[6_565]	2.06	0.14
1:M:379:THR:CG2	9:M:2603:HOH:O[4_576]	2.07	0.13
9:M:2018:HOH:O	9:M:2019:HOH:O[4_576]	2.08	0.12
1:M:43:THR:OG1	1:M:56:HIS:O[3_656]	2.10	0.10
9:M:2047:HOH:O	9:M:2127:HOH:O[3_656]	2.10	0.10
9:M:3057:HOH:O	9:M:2085:HOH:O[3_656]	2.12	0.08
9:M:3077:HOH:O	9:M:3077:HOH:O[4_576]	2.12	0.08

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	M	518/499 (104%)	504 (97%)	13 (2%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

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	M	456/435 (105%)	454 (100%)	2 (0%)	84	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU
1	M	375	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	122	HIS
1	M	230	GLN
1	M	244	ASN
1	M	365	HIS
1	M	402	ASN
1	M	410	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](#)

16 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	NAG	A	1	2,1	14,14,15	5.90	7 (50%)	17,19,21	3.46	9 (52%)
2	NAG	A	2	2	14,14,15	2.98	4 (28%)	17,19,21	4.02	9 (52%)
3	NAG	B	1	1,3	14,14,15	0.59	0	17,19,21	2.03	5 (29%)
3	NAG	B	2	3	14,14,15	1.06	1 (7%)	17,19,21	1.36	2 (11%)
3	BMA	B	3	3	11,11,12	1.83	2 (18%)	15,15,17	1.74	6 (40%)
3	XYP	B	4	3	9,9,10	1.30	1 (11%)	10,12,14	2.51	4 (40%)
3	FUC	B	5	3	10,10,11	1.65	3 (30%)	14,14,16	1.97	4 (28%)
4	NAG	C	1	4,1	14,14,15	1.93	3 (21%)	17,19,21	2.47	4 (23%)
4	NAG	C	2	4	14,14,15	1.53	3 (21%)	17,19,21	1.65	5 (29%)
4	BMA	C	3	4	11,11,12	2.41	2 (18%)	15,15,17	4.55	9 (60%)
4	XYP	C	4	4	9,9,10	1.87	4 (44%)	10,12,14	2.15	4 (40%)
4	MAN	C	5	4	11,11,12	1.97	2 (18%)	15,15,17	2.53	8 (53%)
4	MAN	C	6	4	11,11,12	3.13	7 (63%)	15,15,17	7.21	12 (80%)
4	FUC	C	7	4	10,10,11	2.66	5 (50%)	14,14,16	1.65	2 (14%)
2	NAG	D	1	2,1	14,14,15	2.41	3 (21%)	17,19,21	2.56	3 (17%)
2	NAG	D	2	2	14,14,15	1.46	3 (21%)	17,19,21	2.62	10 (58%)

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	NAG	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	XYP	B	4	3	-	-	0/1/1/1
3	FUC	B	5	3	-	-	0/1/1/1
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	MAN	C	6	4	1/1/4/5	1/2/19/22	0/1/1/1
4	FUC	C	7	4	-	-	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O3-C3	18.86	1.89	1.43
4	C	6	MAN	O5-C5	8.17	1.59	1.43
2	A	1	NAG	O7-C7	7.59	1.40	1.23
2	A	2	NAG	O5-C5	7.39	1.57	1.43
2	D	1	NAG	O7-C7	-6.60	1.08	1.23
4	C	3	BMA	C2-C3	-6.35	1.42	1.52
2	A	2	NAG	C6-C5	-6.16	1.31	1.51
4	C	1	NAG	C1-C2	-5.28	1.45	1.52
2	A	1	NAG	C7-N2	-5.12	1.17	1.34
4	C	7	FUC	C4-C5	4.86	1.63	1.52
4	C	5	MAN	O5-C5	4.84	1.52	1.43
4	C	7	FUC	C2-C3	4.63	1.59	1.52
2	D	1	NAG	C8-C7	4.50	1.59	1.50
2	A	2	NAG	C4-C5	-4.49	1.43	1.53
2	A	1	NAG	C3-C2	3.96	1.60	1.52
3	B	3	BMA	C2-C3	-3.80	1.46	1.52
4	C	2	NAG	C3-C2	-3.48	1.45	1.52
4	C	3	BMA	C4-C5	3.45	1.60	1.53
4	C	7	FUC	O4-C4	3.33	1.51	1.43
4	C	6	MAN	C2-C3	3.31	1.57	1.52
4	C	5	MAN	C4-C5	3.22	1.59	1.53
2	D	2	NAG	C1-C2	3.16	1.56	1.52
2	A	1	NAG	C4-C5	3.09	1.59	1.53
2	A	1	NAG	O5-C5	3.06	1.49	1.43
4	C	6	MAN	O4-C4	3.00	1.50	1.43
4	C	4	XYP	C2-C3	2.97	1.57	1.52
3	B	3	BMA	O5-C5	2.93	1.49	1.43
4	C	4	XYP	O3-C3	2.74	1.49	1.43
2	A	1	NAG	O4-C4	2.65	1.49	1.43
3	B	5	FUC	C2-C3	2.64	1.56	1.52
4	C	4	XYP	O5-C5	2.60	1.47	1.43
4	C	6	MAN	C1-C2	2.57	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	C2-N2	-2.50	1.42	1.46
3	B	2	NAG	C1-C2	2.43	1.55	1.52
4	C	1	NAG	O5-C1	-2.43	1.39	1.43
4	C	2	NAG	O7-C7	2.36	1.28	1.23
4	C	7	FUC	C1-C2	2.36	1.57	1.52
4	C	6	MAN	C6-C5	-2.33	1.44	1.51
3	B	5	FUC	O5-C5	2.32	1.48	1.43
4	C	2	NAG	C1-C2	2.29	1.55	1.52
3	B	5	FUC	O2-C2	2.28	1.48	1.43
2	D	2	NAG	C4-C5	2.27	1.57	1.53
2	D	1	NAG	O5-C1	-2.19	1.40	1.43
3	B	4	XYP	C4-C3	2.16	1.55	1.52
2	A	2	NAG	C3-C2	-2.11	1.48	1.52
4	C	6	MAN	O5-C1	2.10	1.47	1.43
4	C	6	MAN	C4-C3	2.03	1.57	1.52
4	C	7	FUC	C4-C3	-2.02	1.47	1.52
2	D	2	NAG	C8-C7	2.02	1.54	1.50
4	C	4	XYP	O5-C1	-2.01	1.39	1.43

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	6	MAN	C1-O5-C5	-16.05	90.67	112.19
4	C	6	MAN	C6-C5-C4	12.27	143.14	113.02
4	C	3	BMA	O4-C4-C5	10.08	134.15	109.32
4	C	6	MAN	O5-C5-C6	-9.98	88.23	107.66
2	A	2	NAG	C3-C4-C5	8.86	126.30	110.23
4	C	6	MAN	O4-C4-C5	8.79	130.98	109.32
2	A	2	NAG	C1-O5-C5	-7.78	101.75	112.19
2	A	1	NAG	O3-C3-C2	-7.58	93.66	109.40
4	C	3	BMA	O5-C5-C6	-7.36	93.34	107.66
4	C	6	MAN	O5-C5-C4	6.92	127.67	110.83
2	D	1	NAG	O7-C7-N2	6.86	134.11	121.98
2	A	2	NAG	O5-C5-C4	-6.65	94.65	110.83
2	D	1	NAG	C8-C7-N2	-6.38	105.54	116.12
2	A	1	NAG	C1-O5-C5	-6.36	103.67	112.19
4	C	6	MAN	O4-C4-C3	-6.26	95.62	110.38
4	C	6	MAN	C2-C3-C4	-6.06	100.20	110.86
4	C	1	NAG	O5-C1-C2	6.00	120.57	111.29
4	C	3	BMA	O4-C4-C3	-5.85	96.58	110.38
4	C	1	NAG	C1-O5-C5	-5.74	104.50	112.19
4	C	3	BMA	C6-C5-C4	5.71	127.05	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O4-C4-C5	-5.28	96.32	109.32
2	A	2	NAG	O5-C1-C2	4.80	118.72	111.29
4	C	3	BMA	O2-C2-C3	-4.79	100.22	110.15
4	C	7	FUC	C1-C2-C3	-4.76	102.72	109.64
4	C	6	MAN	C1-C2-C3	4.73	116.53	109.64
3	B	4	XYP	C5-C4-C3	-4.69	102.81	109.64
3	B	5	FUC	O3-C3-C2	-4.69	100.48	110.05
4	C	5	MAN	C1-C2-C3	4.58	116.31	109.64
2	D	2	NAG	C1-C2-N2	-4.53	103.29	110.43
3	B	1	NAG	C1-O5-C5	-4.49	106.17	112.19
4	C	3	BMA	C1-C2-C3	-4.46	103.16	109.64
4	C	6	MAN	O6-C6-C5	4.31	126.02	111.33
4	C	3	BMA	O5-C5-C4	-4.27	100.44	110.83
2	D	2	NAG	O5-C1-C2	-4.25	104.72	111.29
2	A	1	NAG	C4-C3-C2	-4.20	104.86	111.02
2	A	2	NAG	O3-C3-C4	4.05	119.92	110.38
4	C	4	XYP	C5-C4-C3	-4.00	103.83	109.64
2	A	1	NAG	O7-C7-C8	-3.96	114.99	122.05
3	B	4	XYP	O2-C2-C3	-3.92	102.03	110.15
3	B	1	NAG	C2-N2-C7	-3.88	117.70	122.90
4	C	5	MAN	C3-C4-C5	-3.75	103.44	110.23
2	D	2	NAG	C2-N2-C7	-3.74	117.89	122.90
4	C	5	MAN	O5-C5-C6	-3.72	100.42	107.66
2	A	2	NAG	C4-C3-C2	-3.70	105.59	111.02
4	C	3	BMA	C3-C4-C5	3.55	116.67	110.23
3	B	4	XYP	O3-C3-C2	-3.50	102.91	110.05
4	C	5	MAN	C2-C3-C4	-3.47	104.77	110.86
4	C	4	XYP	C4-C3-C2	-3.42	106.86	110.92
4	C	5	MAN	O2-C2-C3	-3.37	103.16	110.15
2	A	2	NAG	O6-C6-C5	-3.37	99.85	111.33
3	B	5	FUC	C1-C2-C3	-3.37	104.74	109.64
4	C	6	MAN	C3-C4-C5	-3.29	104.27	110.23
2	A	1	NAG	O5-C5-C4	-3.28	102.85	110.83
2	D	2	NAG	C1-O5-C5	-3.26	107.81	112.19
3	B	5	FUC	O2-C2-C3	-3.25	103.43	110.15
2	D	1	NAG	C2-N2-C7	-3.24	118.56	122.90
4	C	1	NAG	O5-C5-C6	-3.23	101.37	107.66
2	A	1	NAG	O4-C4-C3	-3.17	102.91	110.38
2	D	2	NAG	O5-C5-C4	-3.15	103.16	110.83
3	B	3	BMA	O5-C5-C6	-3.15	101.54	107.66
2	A	2	NAG	O5-C5-C6	-3.14	101.54	107.66
2	A	1	NAG	O3-C3-C4	-3.12	103.03	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C2-N2-C7	-3.08	118.77	122.90
4	C	6	MAN	O5-C1-C2	-3.05	103.51	110.79
3	B	3	BMA	C2-C3-C4	3.02	116.17	110.86
2	D	2	NAG	C6-C5-C4	-2.93	105.83	113.02
2	D	2	NAG	C3-C4-C5	-2.89	105.00	110.23
2	D	2	NAG	O4-C4-C3	-2.85	103.67	110.38
3	B	4	XYP	C1-C2-C3	2.84	113.78	109.64
2	A	1	NAG	C8-C7-N2	2.68	120.56	116.12
4	C	3	BMA	C1-O5-C5	-2.66	108.62	112.19
4	C	4	XYP	O4-C4-C3	-2.63	104.70	110.15
3	B	1	NAG	C1-C2-N2	-2.62	106.30	110.43
3	B	1	NAG	C8-C7-N2	-2.56	111.87	116.12
4	C	2	NAG	O4-C4-C3	-2.56	104.34	110.38
4	C	2	NAG	C2-N2-C7	-2.56	119.47	122.90
4	C	5	MAN	O2-C2-C1	2.55	115.06	109.22
4	C	2	NAG	O5-C1-C2	-2.40	107.58	111.29
3	B	3	BMA	O3-C3-C4	2.38	115.98	110.38
4	C	5	MAN	C6-C5-C4	-2.36	107.22	113.02
4	C	6	MAN	O2-C2-C1	-2.30	103.96	109.22
4	C	4	XYP	O2-C2-C3	-2.29	105.41	110.15
3	B	1	NAG	O5-C1-C2	-2.24	107.82	111.29
2	A	2	NAG	C8-C7-N2	-2.23	112.43	116.12
3	B	3	BMA	O5-C5-C4	-2.22	105.42	110.83
3	B	2	NAG	O4-C4-C3	-2.22	105.15	110.38
4	C	1	NAG	C2-N2-C7	2.20	125.86	122.90
3	B	5	FUC	O3-C3-C4	-2.18	105.25	110.38
4	C	7	FUC	C6-C5-C4	-2.16	109.13	113.08
2	D	2	NAG	O3-C3-C2	2.14	113.86	109.40
4	C	5	MAN	C1-O5-C5	2.14	115.06	112.19
4	C	2	NAG	C8-C7-N2	-2.13	112.59	116.12
2	D	2	NAG	C4-C3-C2	-2.10	107.94	111.02
4	C	2	NAG	C1-O5-C5	-2.06	109.42	112.19
3	B	3	BMA	O4-C4-C5	2.03	114.33	109.32
3	B	3	BMA	C3-C4-C5	2.02	113.89	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	6	MAN	C5

All (2) torsion outliers are listed below:

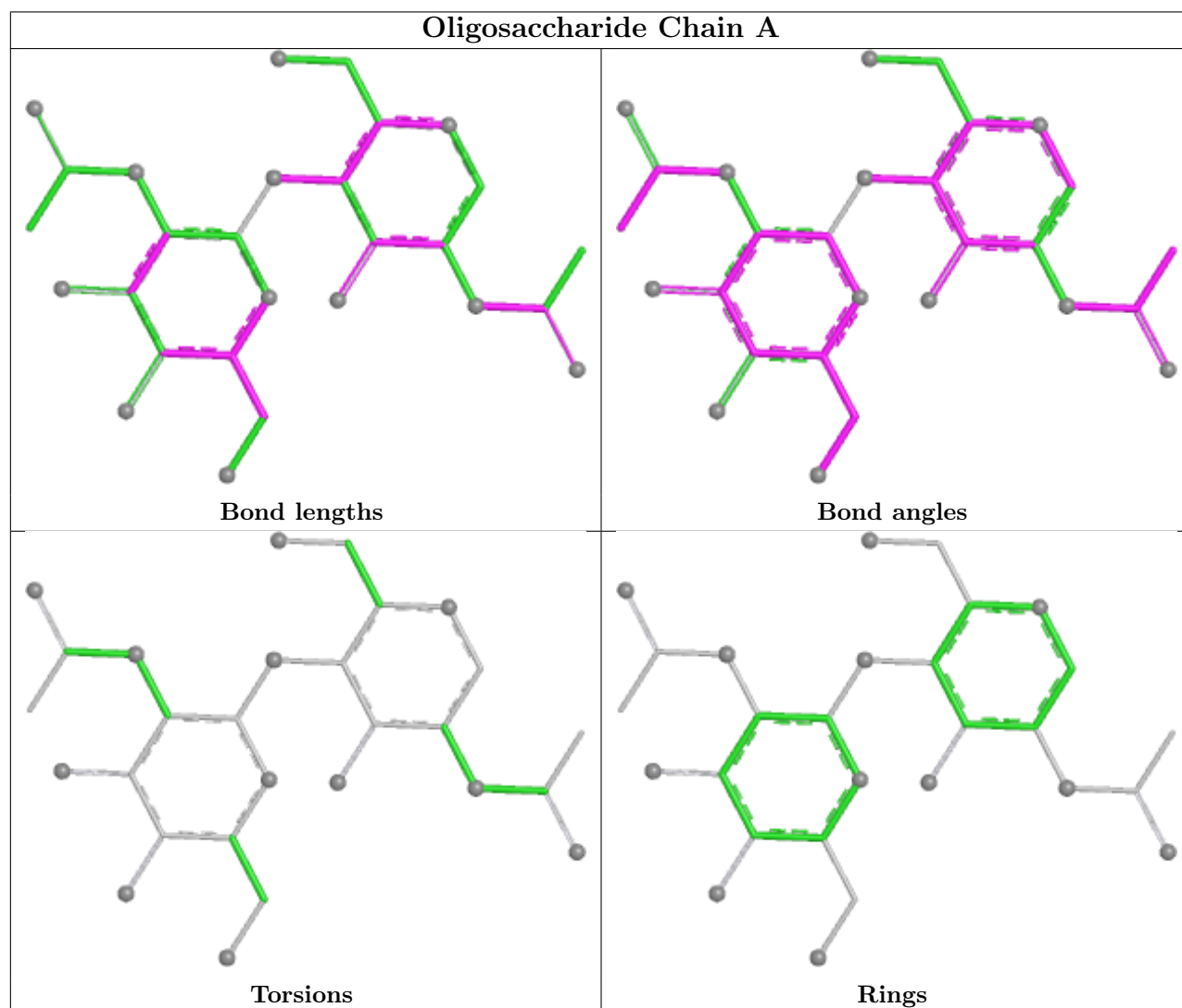
Mol	Chain	Res	Type	Atoms
4	C	6	MAN	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6

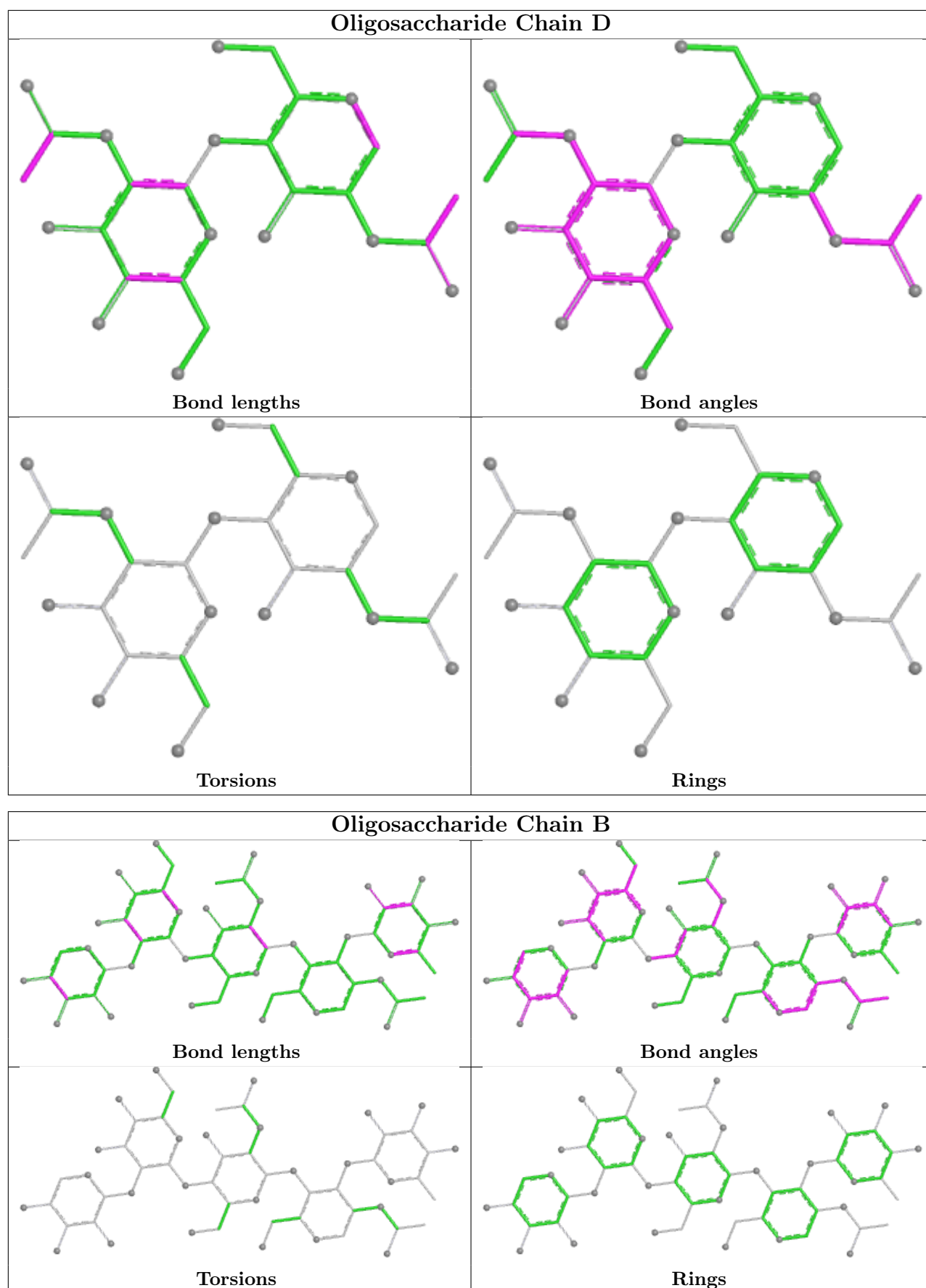
There are no ring outliers.

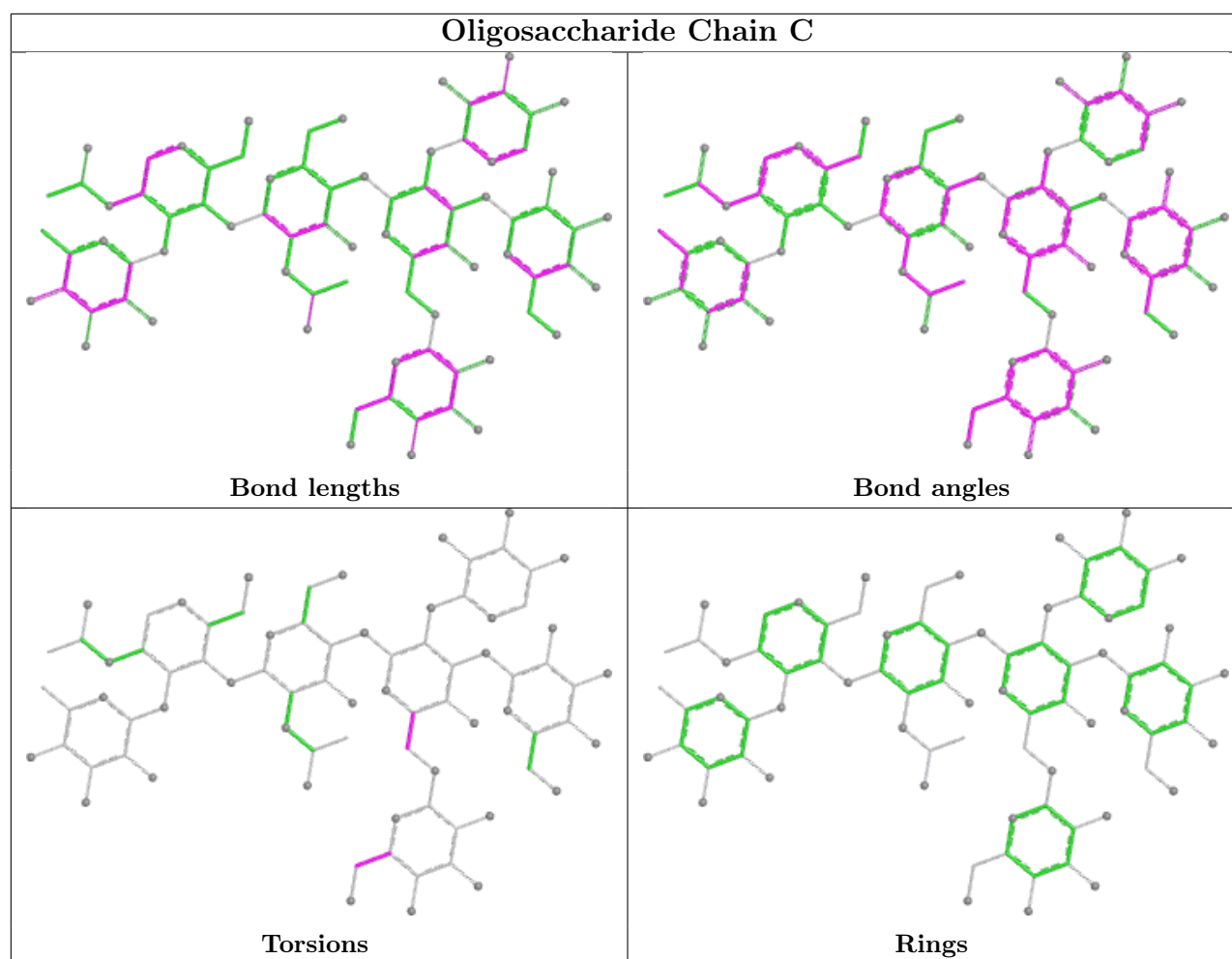
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
4	C	6	MAN	8	0
2	A	1	NAG	3	0
4	C	3	BMA	7	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](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GOL	M	1010	-	5,5,5	0.68	0	5,5,5	1.21	1 (20%)
7	SO4	M	1008	-	4,4,4	0.81	0	6,6,6	0.35	0
7	SO4	M	1005	-	4,4,4	0.27	0	6,6,6	0.32	0
8	GOL	M	1020	-	5,5,5	1.28	1 (20%)	5,5,5	1.12	0
5	NAG	M	961	1	14,14,15	1.40	2 (14%)	17,19,21	2.84	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	M	1023	-	5,5,5	0.66	0	5,5,5	1.19	1 (20%)
5	NAG	M	931	1	14,14,15	2.01	5 (35%)	17,19,21	8.34	13 (76%)
7	SO4	M	1009	-	4,4,4	1.53	1 (25%)	6,6,6	2.76	5 (83%)
5	NAG	M	911	1	14,14,15	1.72	2 (14%)	17,19,21	2.16	5 (29%)
5	NAG	M	971	1	14,14,15	1.36	1 (7%)	17,19,21	2.50	8 (47%)
7	SO4	M	1004	-	4,4,4	1.42	1 (25%)	6,6,6	1.31	1 (16%)
5	NAG	M	991	1	14,14,15	1.26	1 (7%)	17,19,21	1.97	5 (29%)
8	GOL	M	1021	-	5,5,5	0.94	0	5,5,5	1.15	1 (20%)
7	SO4	M	1002	-	4,4,4	0.88	0	6,6,6	1.39	1 (16%)
7	SO4	M	1006	-	4,4,4	1.88	1 (25%)	6,6,6	2.46	3 (50%)
8	GOL	M	1024	-	5,5,5	0.87	0	5,5,5	1.37	1 (20%)
7	SO4	M	1007	-	4,4,4	1.10	0	6,6,6	1.36	1 (16%)
5	NAG	M	901	1	14,14,15	1.21	1 (7%)	17,19,21	2.06	5 (29%)
7	SO4	M	1003	-	4,4,4	0.57	0	6,6,6	0.51	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
8	GOL	M	1023	-	-	0/4/4/4	-
8	GOL	M	1010	-	-	4/4/4/4	-
5	NAG	M	971	1	-	4/6/23/26	0/1/1/1
8	GOL	M	1024	-	-	0/4/4/4	-
5	NAG	M	931	1	-	2/6/23/26	0/1/1/1
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
5	NAG	M	901	1	-	0/6/23/26	0/1/1/1
8	GOL	M	1020	-	-	0/4/4/4	-
5	NAG	M	991	1	-	0/6/23/26	0/1/1/1
8	GOL	M	1021	-	-	0/4/4/4	-
5	NAG	M	961	1	1/1/5/7	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	911	NAG	O5-C5	4.36	1.51	1.43
5	M	971	NAG	O7-C7	-4.20	1.13	1.23
5	M	931	NAG	O7-C7	-3.99	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	991	NAG	O7-C7	-3.84	1.14	1.23
7	M	1006	SO4	O2-S	3.57	1.66	1.44
5	M	911	NAG	O7-C7	-3.48	1.15	1.23
5	M	931	NAG	C1-C2	-3.43	1.47	1.52
5	M	961	NAG	O7-C7	-3.41	1.15	1.23
5	M	931	NAG	O4-C4	2.88	1.50	1.43
5	M	901	NAG	O7-C7	-2.85	1.16	1.23
5	M	931	NAG	C2-N2	-2.69	1.41	1.46
7	M	1004	SO4	O1-S	2.59	1.60	1.44
7	M	1009	SO4	O1-S	2.47	1.59	1.44
5	M	961	NAG	C2-N2	2.26	1.50	1.46
8	M	1020	GOL	O1-C1	2.17	1.51	1.42
5	M	931	NAG	O5-C1	-2.06	1.40	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	931	NAG	C2-N2-C7	22.97	153.68	122.90
5	M	931	NAG	O5-C1-C2	15.06	134.59	111.29
5	M	931	NAG	C8-C7-N2	14.70	140.50	116.12
5	M	931	NAG	O7-C7-N2	-8.72	106.58	121.98
5	M	961	NAG	C1-O5-C5	8.53	123.61	112.19
5	M	931	NAG	C1-O5-C5	-6.73	103.16	112.19
5	M	911	NAG	C1-O5-C5	-6.30	103.74	112.19
5	M	901	NAG	C1-O5-C5	-6.18	103.90	112.19
5	M	971	NAG	O5-C1-C2	-6.04	101.95	111.29
5	M	931	NAG	O7-C7-C8	-5.21	112.77	122.05
5	M	961	NAG	C1-C2-N2	-4.75	102.95	110.43
5	M	991	NAG	C4-C3-C2	-4.60	104.28	111.02
5	M	961	NAG	O3-C3-C2	-4.28	100.50	109.40
5	M	931	NAG	C3-C4-C5	3.81	117.13	110.23
7	M	1009	SO4	O4-S-O3	3.76	129.27	108.54
5	M	991	NAG	O3-C3-C2	-3.75	101.62	109.40
5	M	911	NAG	C4-C3-C2	-3.71	105.59	111.02
7	M	1006	SO4	O3-S-O2	-3.53	91.08	109.56
7	M	1009	SO4	O3-S-O1	-3.50	91.24	109.56
5	M	971	NAG	O5-C5-C4	-3.48	102.37	110.83
5	M	931	NAG	O4-C4-C5	-3.47	100.79	109.32
5	M	971	NAG	O5-C5-C6	-3.30	101.24	107.66
5	M	961	NAG	O4-C4-C5	-3.23	101.36	109.32
5	M	971	NAG	O4-C4-C3	3.16	117.82	110.38
5	M	931	NAG	O5-C5-C6	-3.08	101.66	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1006	SO4	O2-S-O1	-3.07	87.42	109.06
7	M	1009	SO4	O2-S-O1	-2.99	88.00	109.06
5	M	991	NAG	O5-C1-C2	2.92	115.80	111.29
5	M	971	NAG	O3-C3-C2	-2.82	103.55	109.40
5	M	991	NAG	C1-C2-N2	-2.80	106.02	110.43
5	M	901	NAG	O5-C5-C4	-2.80	104.02	110.83
8	M	1024	GOL	C3-C2-C1	-2.76	101.68	111.80
5	M	901	NAG	O5-C1-C2	2.68	115.44	111.29
5	M	971	NAG	C1-O5-C5	2.67	115.77	112.19
5	M	931	NAG	O4-C4-C3	-2.54	104.40	110.38
5	M	971	NAG	C2-N2-C7	2.53	126.30	122.90
5	M	931	NAG	C1-C2-N2	2.51	114.39	110.43
7	M	1006	SO4	O4-S-O1	2.48	122.53	109.56
5	M	931	NAG	C4-C3-C2	-2.48	107.39	111.02
7	M	1004	SO4	O4-S-O3	2.47	122.18	108.54
7	M	1009	SO4	O4-S-O1	-2.46	96.69	109.56
5	M	911	NAG	O5-C5-C6	-2.46	102.87	107.66
5	M	991	NAG	O5-C5-C4	-2.39	105.02	110.83
5	M	911	NAG	O5-C5-C4	-2.37	105.05	110.83
7	M	1002	SO4	O3-S-O2	2.36	121.88	109.56
7	M	1007	SO4	O4-S-O1	2.35	121.83	109.56
8	M	1010	GOL	O2-C2-C1	2.34	118.87	109.18
5	M	971	NAG	O7-C7-C8	2.30	126.15	122.05
8	M	1023	GOL	C3-C2-C1	-2.16	103.88	111.80
5	M	901	NAG	C4-C3-C2	-2.14	107.88	111.02
7	M	1009	SO4	O3-S-O2	2.08	120.41	109.56
5	M	901	NAG	O5-C5-C6	-2.06	103.66	107.66
5	M	911	NAG	O3-C3-C2	-2.05	105.13	109.40
8	M	1021	GOL	O2-C2-C3	2.00	117.48	109.18
5	M	931	NAG	O5-C5-C4	-2.00	105.95	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	961	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	931	NAG	C8-C7-N2-C2
8	M	1010	GOL	O1-C1-C2-O2
8	M	1010	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	M	931	NAG	O7-C7-N2-C2
5	M	971	NAG	O5-C5-C6-O6
5	M	971	NAG	C4-C5-C6-O6
8	M	1010	GOL	C1-C2-C3-O3
8	M	1010	GOL	O2-C2-C3-O3
5	M	971	NAG	O7-C7-N2-C2
5	M	971	NAG	C8-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1010	GOL	4	0
5	M	961	NAG	2	0
5	M	931	NAG	7	0
7	M	1009	SO4	8	0
5	M	911	NAG	3	0
7	M	1004	SO4	6	0
5	M	901	NAG	5	0
7	M	1003	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	M	499/499 (100%)	2.83	402 (80%) 0 0	13, 19, 32, 60	44 (8%)

All (402) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	212	PRO	6.3
1	M	378	SER	6.1
1	M	23	SER	6.1
1	M	12	PHE	6.0
1	M	345	THR	5.8
1	M	364	GLY	5.8
1	M	138	THR	5.7
1	M	374	ASP	5.5
1	M	305[A]	GLU	5.4
1	M	326	GLY	5.3
1	M	469	PHE	5.1
1	M	497	THR	5.0
1	M	43	THR	5.0
1	M	376	ALA	4.9
1	M	380	ASP	4.8
1	M	313	GLU	4.7
1	M	9	ASN	4.7
1	M	404	LEU	4.7
1	M	223	PRO	4.7
1	M	4	ILE	4.7
1	M	335	ALA	4.6
1	M	492	GLY	4.6
1	M	363[A]	SER	4.6
1	M	150	ASP	4.5
1	M	377	ASP	4.5
1	M	480	TRP	4.5
1	M	152	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	M	390	TYR	4.5
1	M	18	ASP	4.5
1	M	375	LYS	4.5
1	M	409	GLU	4.5
1	M	349	ALA	4.5
1	M	245	TYR	4.4
1	M	450	ASN	4.4
1	M	89	LEU	4.4
1	M	167	TYR	4.3
1	M	112	GLY	4.3
1	M	388	GLY	4.3
1	M	419	ASN	4.3
1	M	28	ASP	4.3
1	M	20[A]	LEU	4.3
1	M	42	GLY	4.3
1	M	421	ASN	4.3
1	M	52	ASP	4.2
1	M	53	GLY	4.2
1	M	132	GLY	4.2
1	M	197	GLY	4.2
1	M	300	ILE	4.2
1	M	3	GLU	4.2
1	M	143	ASP	4.2
1	M	203	PRO	4.2
1	M	457	TRP	4.2
1	M	206	CYS	4.2
1	M	27	SER	4.1
1	M	448	ASP	4.1
1	M	99	ALA	4.1
1	M	400	TYR	4.1
1	M	63	GLY	4.1
1	M	154	GLY	4.1
1	M	482	ASN	4.0
1	M	262	LEU	4.0
1	M	465	PHE	4.0
1	M	50	ILE	4.0
1	M	195	GLY	4.0
1	M	304	GLY	4.0
1	M	417	ASP	4.0
1	M	339	PRO	3.9
1	M	140	PHE	3.9
1	M	365	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	M	341	PRO	3.9
1	M	432	TYR	3.8
1	M	213[A]	SER	3.8
1	M	274	ALA	3.8
1	M	10	LEU	3.8
1	M	55	THR	3.8
1	M	318	VAL	3.8
1	M	142	TRP	3.8
1	M	37	ALA	3.8
1	M	183	LEU	3.8
1	M	25	PHE	3.8
1	M	330	TYR	3.8
1	M	210	VAL	3.8
1	M	458	ALA	3.7
1	M	17	THR	3.7
1	M	293	GLY	3.7
1	M	219	SER	3.7
1	M	381	ASN	3.7
1	M	30[A]	ILE	3.7
1	M	36	SER	3.7
1	M	196	TYR	3.7
1	M	16	ASN	3.7
1	M	311	SER	3.7
1	M	423	SER	3.7
1	M	151	GLU	3.7
1	M	209	THR	3.7
1	M	79	TRP	3.6
1	M	115	GLU	3.6
1	M	396	PHE	3.6
1	M	275	THR	3.6
1	M	403	PRO	3.6
1	M	257	ILE	3.6
1	M	298	ILE	3.6
1	M	45	GLY	3.6
1	M	284	GLY	3.6
1	M	179	VAL	3.6
1	M	235	ALA	3.6
1	M	415	PRO	3.6
1	M	418	GLU	3.6
1	M	491	SER	3.6
1	M	443	VAL	3.5
1	M	371	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	145	PRO	3.5
1	M	359	TYR	3.5
1	M	221	THR	3.5
1	M	83	ILE	3.5
1	M	478	ILE	3.5
1	M	320	GLY	3.5
1	M	215	TYR	3.5
1	M	420	ARG	3.5
1	M	118[A]	ILE	3.4
1	M	164	PHE	3.4
1	M	357	LEU	3.4
1	M	264	TYR	3.4
1	M	5	THR	3.4
1	M	147	THR	3.4
1	M	249	GLY	3.4
1	M	490	LYS	3.4
1	M	401	TYR	3.4
1	M	33	VAL	3.4
1	M	226	VAL	3.4
1	M	22	SER	3.4
1	M	162	ASP	3.4
1	M	343	ASN	3.4
1	M	379	THR	3.4
1	M	98	ILE	3.4
1	M	170	LEU	3.4
1	M	310	PHE	3.4
1	M	474	GLY	3.3
1	M	470	THR	3.3
1	M	238	VAL	3.3
1	M	144	LEU	3.3
1	M	283	LEU	3.3
1	M	268	ASP	3.3
1	M	449[A]	VAL	3.3
1	M	225	ILE	3.3
1	M	430	ILE	3.3
1	M	434	CYS	3.2
1	M	129	ILE	3.2
1	M	201	ASP	3.2
1	M	47	GLY	3.2
1	M	436	HIS	3.2
1	M	468	GLY	3.2
1	M	73	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	100	TRP	3.2
1	M	362	ALA	3.2
1	M	441	ASN	3.2
1	M	444	ILE	3.2
1	M	149	GLN	3.2
1	M	294	THR	3.2
1	M	414	THR	3.2
1	M	15	GLY	3.2
1	M	308	PRO	3.2
1	M	7	GLN	3.2
1	M	94	TYR	3.2
1	M	160	ILE	3.2
1	M	461	ASP	3.2
1	M	501	PRO	3.2
1	M	356	LYS	3.2
1	M	159	GLN	3.2
1	M	113	VAL	3.1
1	M	148	LEU	3.1
1	M	58	TYR	3.1
1	M	241	TYR	3.1
1	M	347	HIS	3.1
1	M	76	PHE	3.1
1	M	103	ILE	3.1
1	M	80	GLN	3.1
1	M	399	LYS	3.1
1	M	97	SER	3.1
1	M	329	TYR	3.1
1	M	54	PHE	3.1
1	M	263	PRO	3.1
1	M	137	VAL	3.1
1	M	370	LEU	3.1
1	M	338[A]	SER	3.1
1	M	395	TYR	3.0
1	M	71	THR	3.0
1	M	255	THR	3.0
1	M	466	ASN	3.0
1	M	386	PRO	3.0
1	M	157	ASP	3.0
1	M	467	LYS	3.0
1	M	48	LEU	3.0
1	M	114	ASN	3.0
1	M	204	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	217	GLY	3.0
1	M	368	GLY	3.0
1	M	184	THR	3.0
1	M	428	THR	3.0
1	M	295	TYR	3.0
1	M	406	TYR	3.0
1	M	342[A]	VAL	3.0
1	M	93	GLY	3.0
1	M	156	LEU	3.0
1	M	317	LEU	3.0
1	M	437	LEU	3.0
1	M	250	GLY	3.0
1	M	87	ASP	3.0
1	M	494	TRP	3.0
1	M	57	ARG	2.9
1	M	200	LEU	2.9
1	M	290	LEU	2.9
1	M	258	THR	2.9
1	M	66	HIS	2.9
1	M	266	ASP	2.9
1	M	297	GLN	2.9
1	M	498	PHE	2.9
1	M	34	ALA	2.9
1	M	186	ASN	2.9
1	M	139	LEU	2.9
1	M	56	HIS	2.9
1	M	224	TYR	2.9
1	M	334	TYR	2.9
1	M	90	ASN	2.9
1	M	425	LEU	2.9
1	M	141	HIS	2.9
1	M	13	THR	2.9
1	M	46	ARG	2.9
1	M	92	THR	2.9
1	M	424	MET	2.9
1	M	11	PRO	2.9
1	M	91	ALA	2.9
1	M	51	TRP	2.9
1	M	471	VAL	2.8
1	M	96	PHE	2.8
1	M	360[A]	ILE	2.8
1	M	389	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	32	GLY	2.8
1	M	327	LEU	2.8
1	M	237	VAL	2.8
1	M	260	TRP	2.8
1	M	312	PRO	2.8
1	M	272	ILE	2.8
1	M	489	LYS	2.8
1	M	49	ASN	2.8
1	M	166	ASP	2.8
1	M	479	ASP	2.8
1	M	64	PRO	2.8
1	M	104	ILE	2.8
1	M	21	ASN	2.7
1	M	346	ASN	2.7
1	M	62[A]	SER	2.7
1	M	439	PHE	2.7
1	M	373	LYS	2.7
1	M	427	TYR	2.7
1	M	495	TYR	2.7
1	M	265	ASN	2.7
1	M	316	ASN	2.7
1	M	382	ILE	2.7
1	M	101[A]	SER	2.7
1	M	108	LYS	2.7
1	M	128	LEU	2.7
1	M	38	TYR	2.7
1	M	120	TYR	2.7
1	M	26	SER	2.7
1	M	285	TRP	2.7
1	M	281	PHE	2.7
1	M	124	LEU	2.7
1	M	177	ASP	2.7
1	M	426	ASP	2.7
1	M	107	GLY	2.7
1	M	240	LEU	2.6
1	M	348	THR	2.6
1	M	105	PRO	2.6
1	M	181	TYR	2.6
1	M	191	VAL	2.6
1	M	14	CYS	2.6
1	M	171	CYS	2.6
1	M	192	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	78	TYR	2.6
1	M	383	TYR	2.6
1	M	88[A]	GLU	2.6
1	M	456	ALA	2.6
1	M	158	PRO	2.6
1	M	307	LEU	2.6
1	M	60	ASN	2.6
1	M	246	THR	2.6
1	M	473	PHE	2.5
1	M	44	ILE	2.5
1	M	121	TYR	2.5
1	M	354	GLY	2.5
1	M	459	LEU	2.5
1	M	125	ILE	2.5
1	M	410	ASN	2.5
1	M	84	ASP	2.5
1	M	72	THR	2.5
1	M	229	HIS	2.5
1	M	253	GLY	2.5
1	M	472	ARG	2.5
1	M	500	SER	2.5
1	M	433	LEU	2.5
1	M	331	PHE	2.5
1	M	244	ASN	2.5
1	M	252	ILE	2.5
1	M	366[A]	TYR	2.4
1	M	384	TYR	2.4
1	M	296	PRO	2.4
1	M	233	ALA	2.4
1	M	146	GLN	2.4
1	M	496	GLN	2.4
1	M	85	VAL	2.4
1	M	322	TYR	2.4
1	M	19	ALA	2.4
1	M	130	LYS	2.4
1	M	488	LEU	2.4
1	M	68	ASN	2.4
1	M	172	PHE	2.4
1	M	286	PHE	2.4
1	M	70	ASP	2.4
1	M	485	ASP	2.4
1	M	315	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	385	TYR	2.4
1	M	463	TYR	2.4
1	M	227	ALA	2.4
1	M	86	LEU	2.4
1	M	280	GLU	2.4
1	M	261	PHE	2.4
1	M	190	SER	2.4
1	M	484	THR	2.4
1	M	454	TYR	2.3
1	M	398	ASN	2.3
1	M	69	GLY	2.3
1	M	106	ARG	2.3
1	M	24	SER	2.3
1	M	75	SER	2.3
1	M	161	ILE	2.3
1	M	391	SER	2.3
1	M	254	PRO	2.3
1	M	422	GLN	2.3
1	M	232	LEU	2.3
1	M	242	ARG	2.3
1	M	486	ARG	2.3
1	M	397	LYS	2.3
1	M	29	PHE	2.3
1	M	276	GLU	2.3
1	M	332	THR	2.3
1	M	214	CYS	2.3
1	M	273	ALA	2.3
1	M	323	ASP	2.3
1	M	351	MET	2.3
1	M	392	VAL	2.3
1	M	208	PRO	2.3
1	M	369	PRO	2.3
1	M	462[A]	ASN	2.3
1	M	301	ASP	2.3
1	M	117	GLY	2.3
1	M	174	GLU	2.2
1	M	271[A]	SER	2.2
1	M	205	ARG	2.2
1	M	277	ARG	2.2
1	M	481	ASN	2.2
1	M	452	LYS	2.2
1	M	119	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	440	LEU	2.2
1	M	182	TRP	2.2
1	M	194	ARG	2.2
1	M	59	PRO	2.2
1	M	8	GLU	2.2
1	M	153	GLU	2.2
1	M	207	SER	2.2
1	M	218	ASN	2.2
1	M	136	PHE	2.2
1	M	278	MET	2.2
1	M	228	HIS	2.1
1	M	168	ALA	2.1
1	M	429	ARG	2.1
1	M	110	SER	2.1
1	M	116	LYS	2.1
1	M	193	THR	2.1
1	M	289	PRO	2.1
1	M	324	PHE	2.1
1	M	499	ILE	2.1
1	M	309[A]	SER	2.1
1	M	325	LEU	2.1
1	M	455	LEU	2.1
1	M	239	ASP	2.1
1	M	123	GLY	2.1
1	M	31	PHE	2.1
1	M	483	VAL	2.1
1	M	81	LYS	2.1
1	M	445	LYS	2.1
1	M	477	TYR	2.1
1	M	288	GLY	2.1
1	M	303	VAL	2.1
1	M	302	THR	2.0
1	M	127	GLY	2.0
1	M	407	VAL	2.0
1	M	178	SER	2.0
1	M	350	MET	2.0
1	M	6	CYS	2.0
1	M	251	LYS	2.0
1	M	135	PRO	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](#)

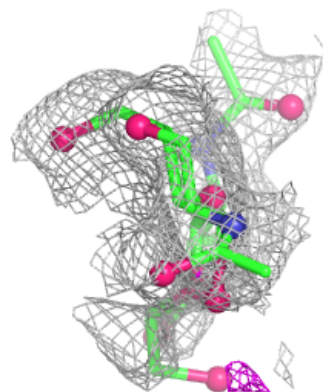
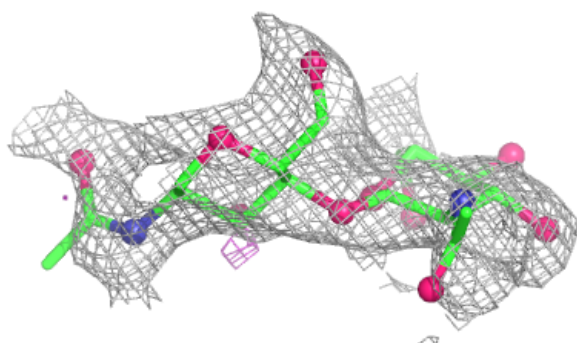
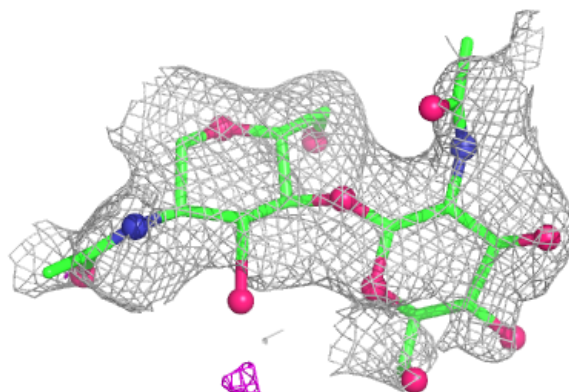
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	1	14/15	-	-	23,28,36,41	0
2	NAG	A	2	14/15	-	-	41,49,61,64	0
4	BMA	C	3	11/12	0.34	0.25	30,35,40,51	0
4	XYP	C	4	9/10	0.43	0.18	37,42,48,68	0
3	NAG	B	2	14/15	0.49	0.21	25,31,37,42	0
4	NAG	C	1	14/15	0.60	0.22	21,24,30,33	0
3	BMA	B	3	11/12	-	-	42,47,53,57	0
3	XYP	B	4	9/10	-	-	46,52,56,58	0
3	FUC	B	5	10/11	-	-	28,36,44,52	0
3	NAG	B	1	14/15	0.61	0.18	19,26,31,31	0
2	NAG	D	1	14/15	0.64	0.18	13,21,25,27	0
2	NAG	D	2	14/15	0.69	0.15	30,36,54,61	0
4	NAG	C	2	14/15	0.69	0.17	24,27,32,36	0
4	MAN	C	5	11/12	-	-	29,43,56,60	0
4	MAN	C	6	11/12	-	-	37,47,59,59	0
4	FUC	C	7	10/11	-	-	23,26,37,37	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.

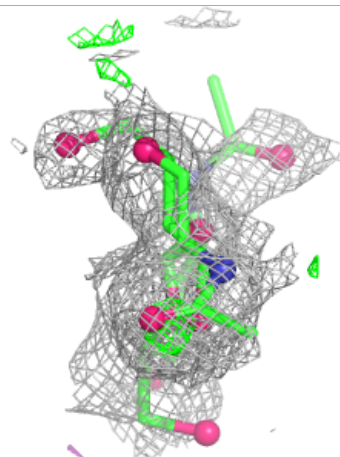
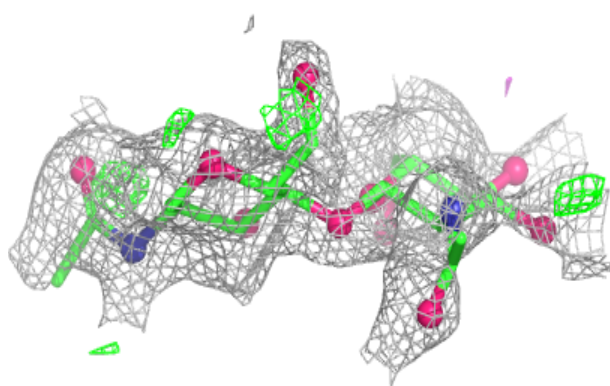
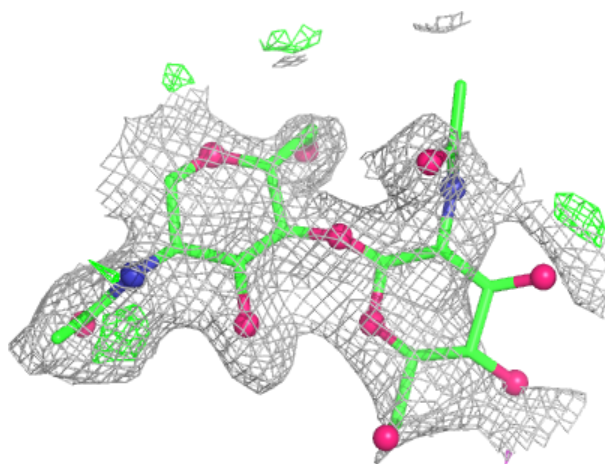
Electron density around Chain A:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



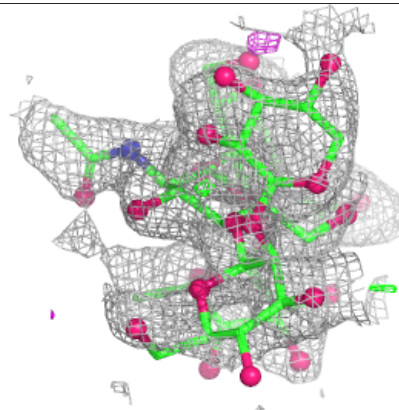
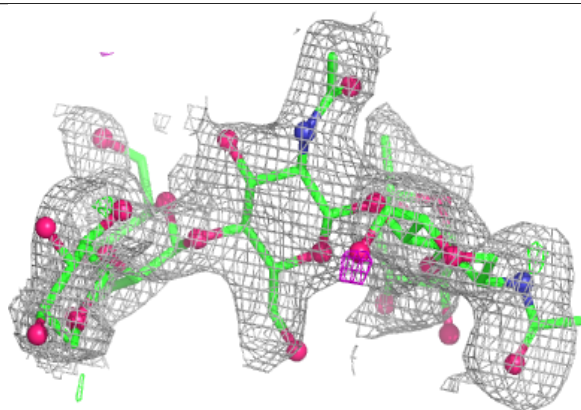
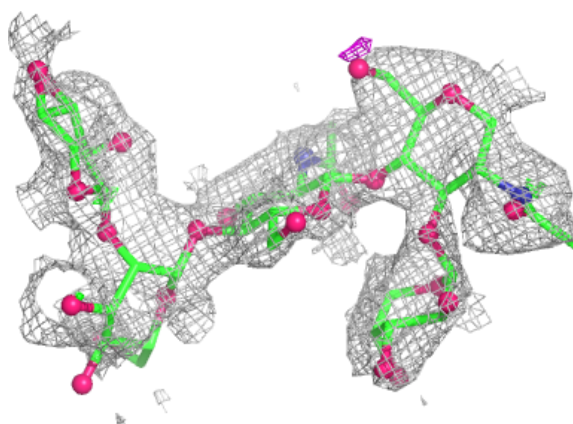
Electron density around Chain D:

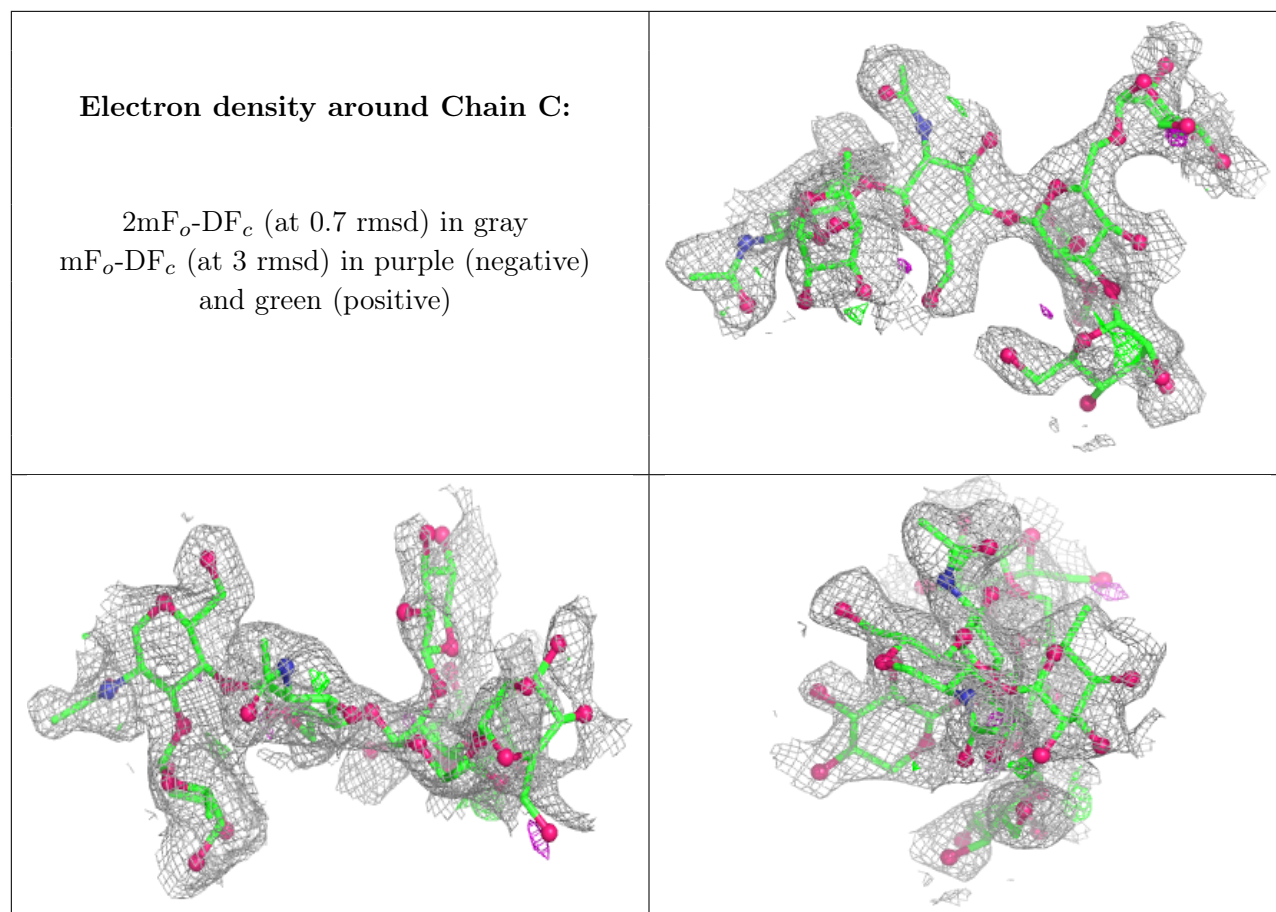
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain B:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
8	GOL	M	1010	6/6	0.33	0.33	40,46,48,55	6
5	NAG	M	991	14/15	0.45	0.23	39,44,57,61	0
5	NAG	M	971	14/15	0.47	0.29	60,68,74,74	0
7	SO4	M	1009	5/5	0.48	0.41	42,44,50,64	1
5	NAG	M	901	14/15	0.49	0.23	30,39,50,52	0
8	GOL	M	1023	6/6	0.50	0.37	35,36,47,49	6
8	GOL	M	1020	6/6	0.52	0.23	10,18,22,23	1
5	NAG	M	961	14/15	0.53	0.20	47,55,66,72	0
5	NAG	M	931	14/15	0.54	0.19	39,46,53,53	0
7	SO4	M	1003	5/5	0.56	0.25	29,32,40,41	5
5	NAG	M	911	14/15	0.63	0.18	29,32,40,49	0
8	GOL	M	1024	6/6	0.63	0.15	20,21,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	M	1021	6/6	0.64	0.14	15,25,30,35	6
7	SO4	M	1008	5/5	0.68	0.27	37,40,42,43	5
7	SO4	M	1005	5/5	0.69	0.21	22,25,31,33	0
7	SO4	M	1007	5/5	0.74	0.18	17,37,38,41	5
7	SO4	M	1002	5/5	0.75	0.22	30,33,36,41	5
7	SO4	M	1006	5/5	0.78	0.29	30,35,38,39	5
7	SO4	M	1004	5/5	0.79	0.14	18,32,34,39	5
6	ZN	M	1001	1/1	0.84	0.15	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.