



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:56 PM UTC

PDB ID : 1DWF / pdb_00001dwf
Title : Study on radiation damage on a cryocooled crystal. Part 2: Structure after irradiation with 9.1×10^{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

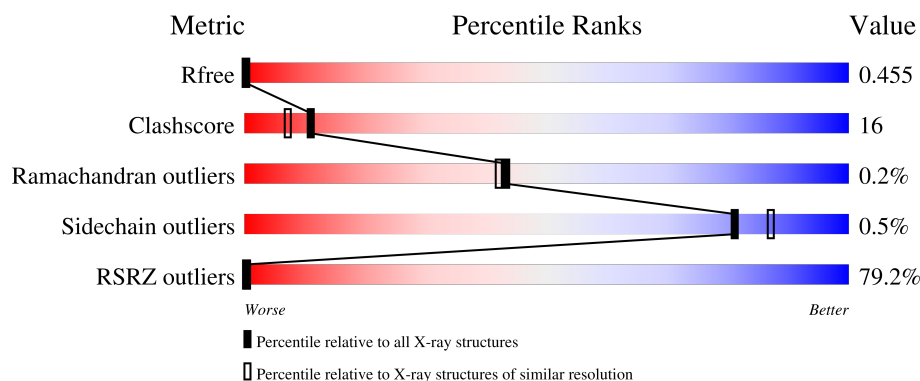
1 Overall quality at a glance

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	79% 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	1506	-	-	X	-
5	NAG	M	1519	X	-	-	-
7	SO4	M	1526	-	-	X	-
7	SO4	M	1527	-	-	X	-
7	SO4	M	1529	-	X	-	-
7	SO4	M	1532	-	X	X	X
8	GOL	M	1533	-	-	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:

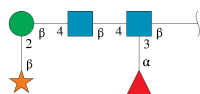
Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

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



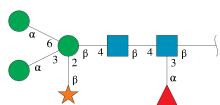
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



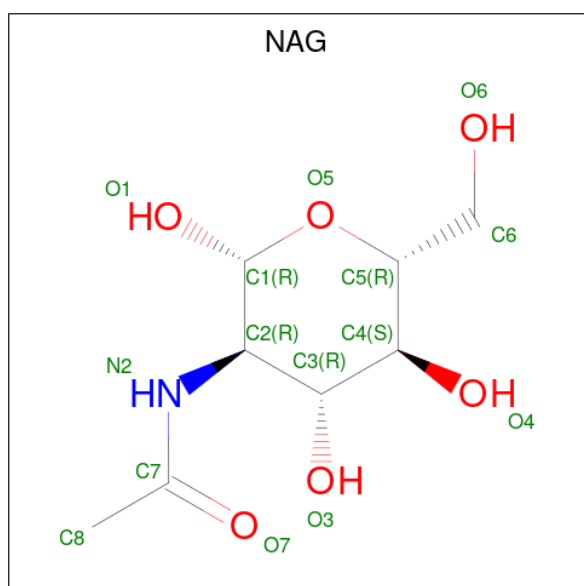
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			58	33	2	23			

- 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: C₈H₁₅NO₆).



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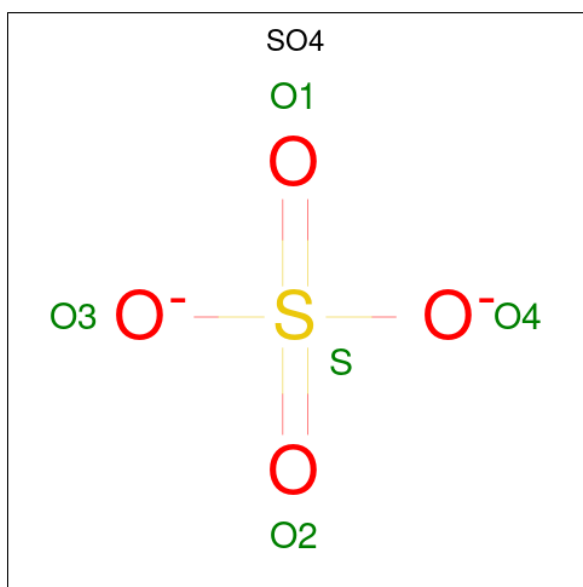
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		

- 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).



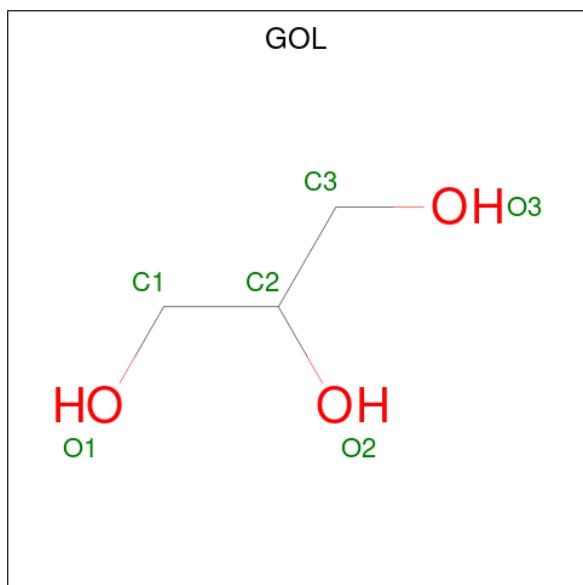
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

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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		

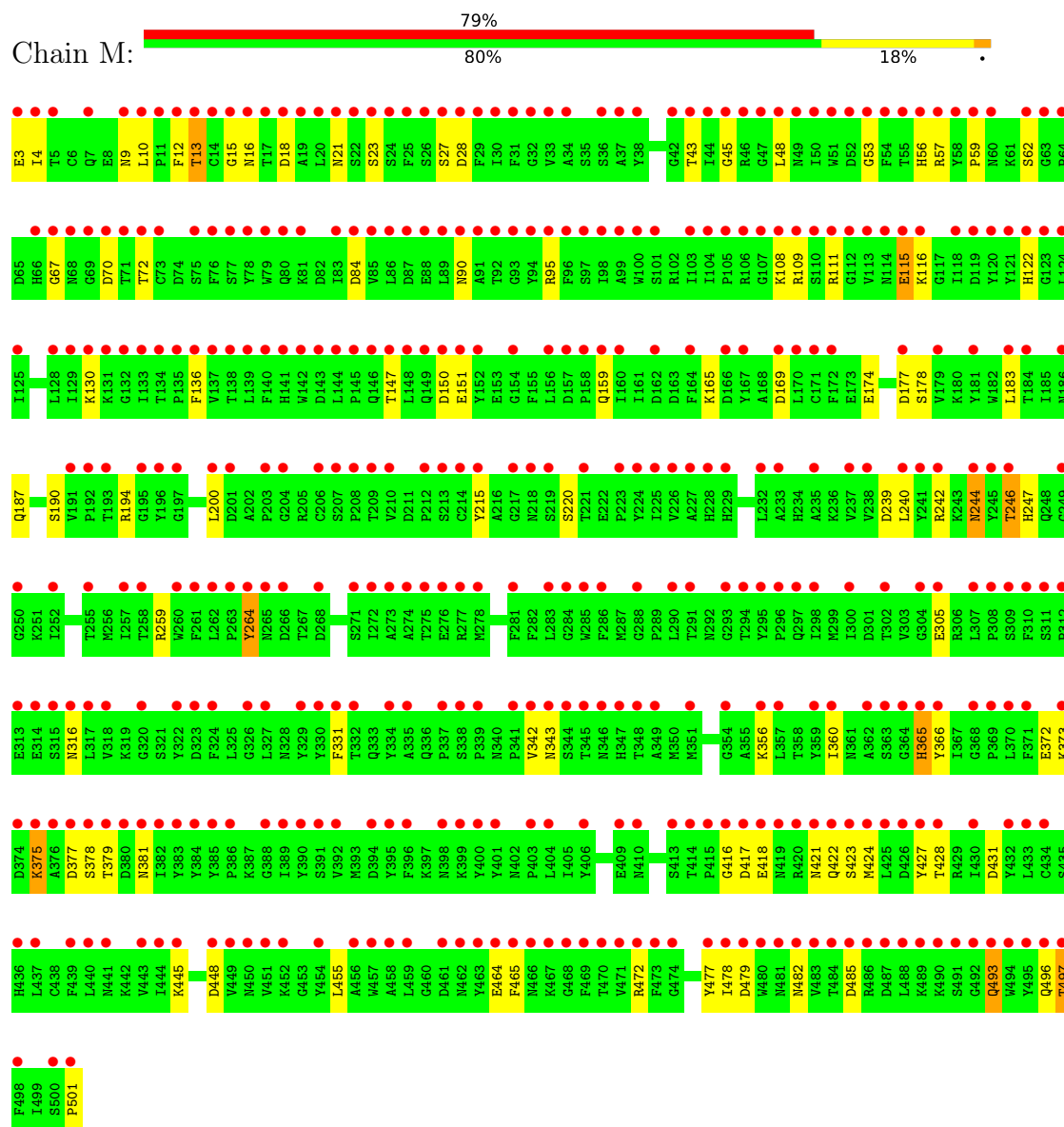
- Molecule 9 is water.

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

3 Residue-property plots

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%

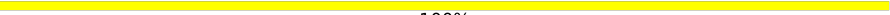
NAG1
NAG2

- 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)	17.40 – 2.00 17.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (17.40-2.00) 98.3 (17.40-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.70 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.169 , 0.180 0.441 , 0.455	Depositor DCC
R_{free} test set	2570 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: SO4, FUC, XYP, ZN, GOL, MAN, NAG, BMA

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	9	0
8	M	30	0	39	4	0
9	M	788	0	0	78	17
All	All	5220	0	4100	136	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 (136) 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:1506:NAG:C1	0.96	1.56
1:M:21:ASN:HD21	5:M:1502: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:1533:GOL:C1	9:M:3026: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:1533:GOL:H11	9:M:3026: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:1533:GOL:C2	9:M:3026: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:1527:SO4:O2	7:M:1532:SO4:S	2.19	1.00
1:M:165:LYS:NZ	5:M:1506:NAG:H82	1.76	0.99
5:M:1519:NAG:H61	9:M:1056: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:1506: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
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:1502: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:1532:SO4:O1	9:M:3024:HOH:O	2.00	0.78
1:M:70:ASP:HB3	9:M:2078:HOH:O	1.83	0.76
9:M:1062: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
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:90:ASN:ND2	5:M:1503: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:3014:HOH:O	1.91	0.70
1:M:116:LYS:HG2	9:M:2225:HOH:O	1.92	0.70
9:M:1019: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:1527:SO4:S	7:M:1532: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:1526:SO4:O2	9:M:3006: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:1503: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:1526:SO4:O4	9:M:3006: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:1527:SO4:O2	7:M:1532:SO4:O3	2.15	0.63
1:M:21:ASN:CG	5:M:1502:NAG:C1	2.67	0.61
8:M:1533:GOL:O2	9:M:3026:HOH:O	2.01	0.61
7:M:1527:SO4:O1	7:M:1532: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:1527:SO4:S	7:M:1532: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:1503: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:1532:SO4:O4	2.40	0.55
1:M:331:PHE:CD1	9:M:2483:HOH:O	2.53	0.55
9:M:1055:HOH:O	4:C:3:BMA:C6	2.47	0.55
1:M:15:GLY:C	9:M:2032:HOH:O	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:21:ASN:ND2	5:M:1502: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:1506:NAG:C2	1.98	0.52
9:M:1053: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:1502: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:1053: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:1506: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:1506: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:1519:NAG:C6	9:M:1056:HOH:O	2.41	0.41
1:M:244:ASN:ND2	5:M:1506: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:1524:ZN:ZN	6:M:1524: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:1057:HOH:O	9:M:2085:HOH:O[3_656]	2.12	0.08
9:M:3014:HOH:O	9:M:3014:HOH:O[4_576]	2.12	0.08

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	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	3,1	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	3,1	-	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:

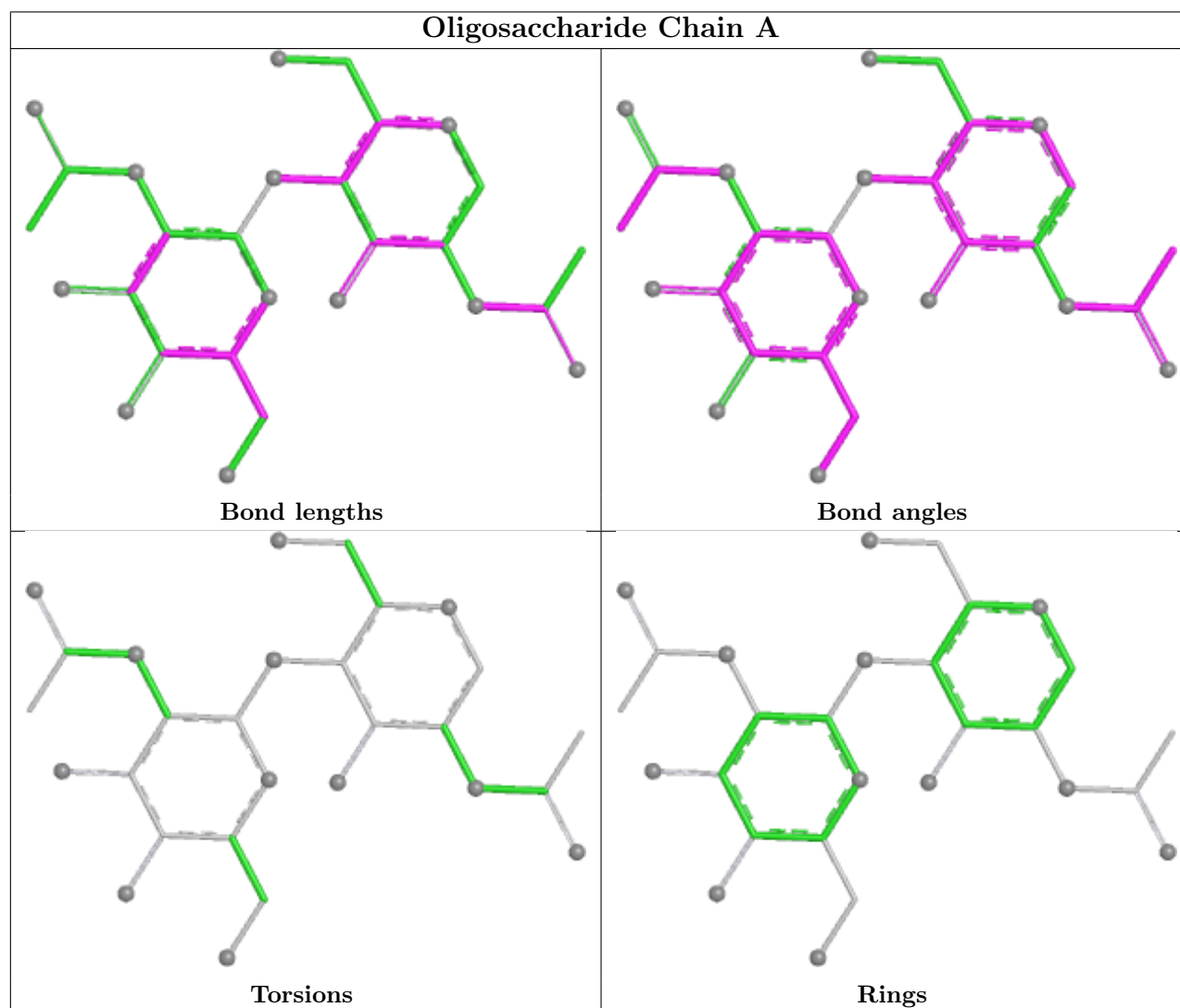
Mol	Chain	Res	Type	Atoms
4	C	6	MAN	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6

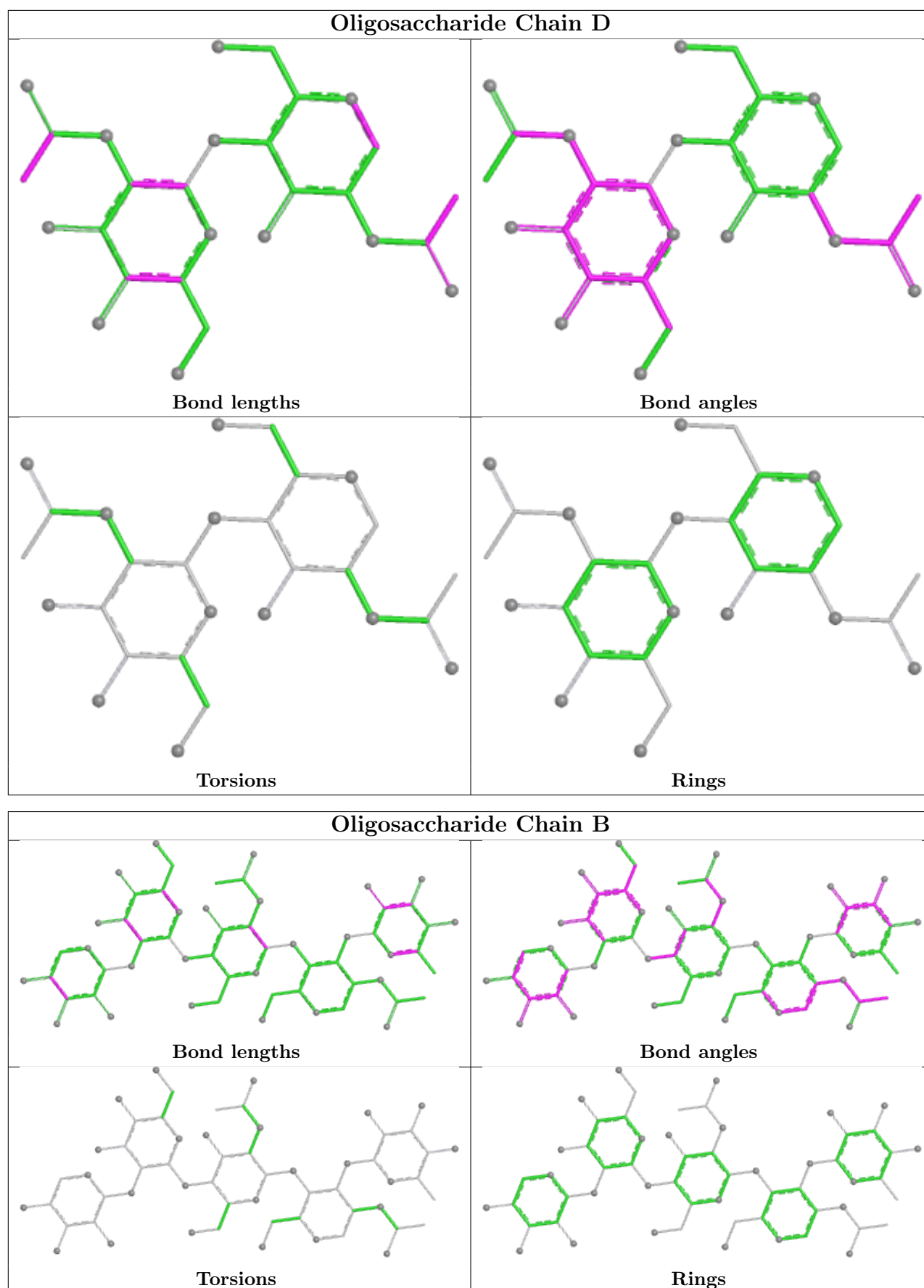
There are no ring outliers.

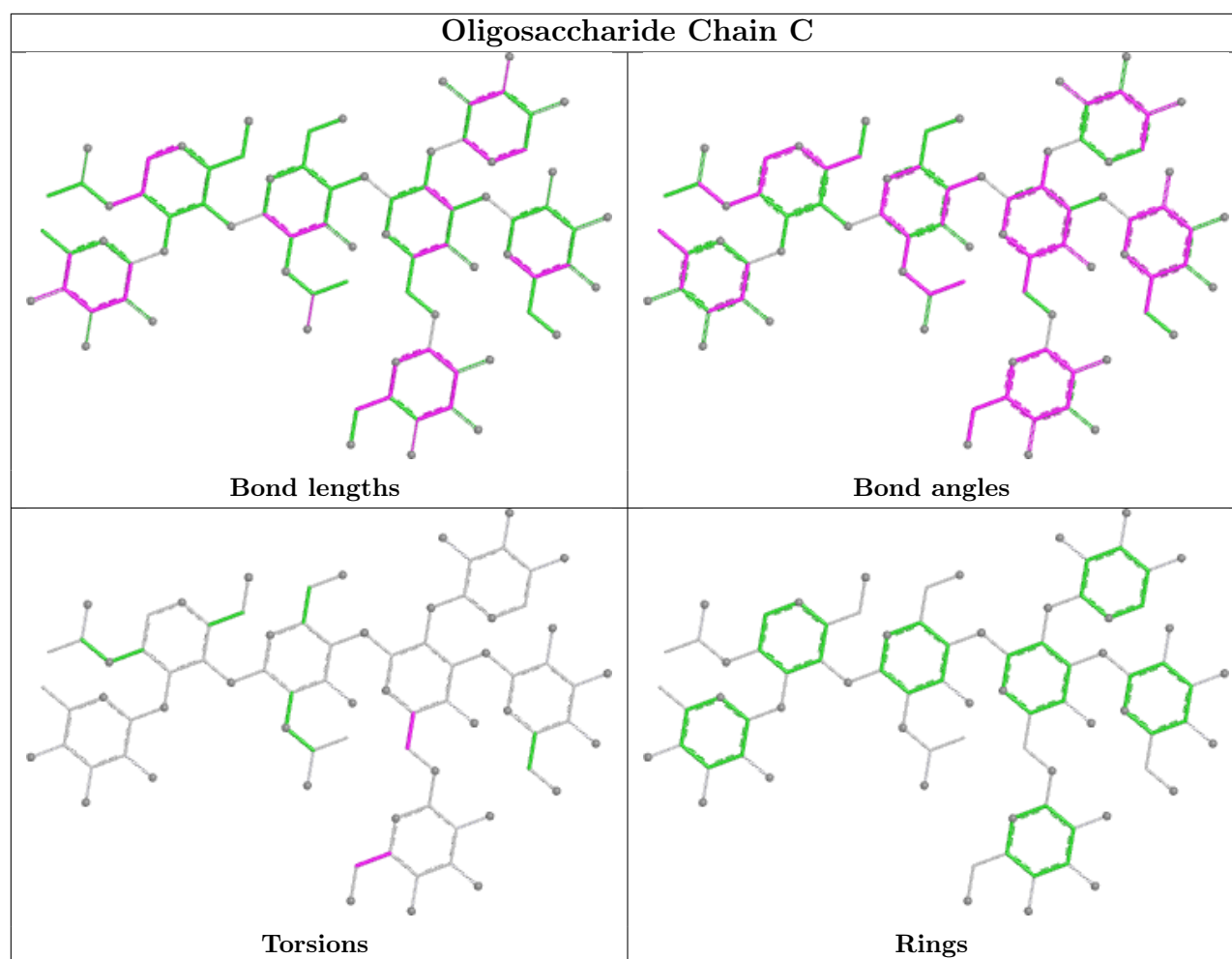
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
4	C	6	MAN	8	0
4	C	3	BMA	7	0
2	A	1	NAG	3	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$
5	NAG	M	1506	1	14,14,15	2.01	5 (35%)	17,19,21	8.34	13 (76%)
5	NAG	M	1503	1	14,14,15	1.72	2 (14%)	17,19,21	2.16	5 (29%)
5	NAG	M	1520	1	14,14,15	1.36	1 (7%)	17,19,21	2.50	8 (47%)
7	SO4	M	1527	7	4,4,4	1.42	1 (25%)	6,6,6	1.31	1 (16%)
8	GOL	M	1535	-	5,5,5	0.94	0	5,5,5	1.15	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	1502	1	14,14,15	1.21	1 (7%)	17,19,21	2.06	5 (29%)
5	NAG	M	1523	1	14,14,15	1.26	1 (7%)	17,19,21	1.97	5 (29%)
7	SO4	M	1525	-	4,4,4	0.88	0	6,6,6	1.39	1 (16%)
7	SO4	M	1528	-	4,4,4	0.27	0	6,6,6	0.32	0
7	SO4	M	1530	-	4,4,4	1.10	0	6,6,6	1.36	1 (16%)
8	GOL	M	1537	-	5,5,5	0.87	0	5,5,5	1.37	1 (20%)
7	SO4	M	1532	7	4,4,4	1.53	1 (25%)	6,6,6	2.76	5 (83%)
8	GOL	M	1534	-	5,5,5	1.28	1 (20%)	5,5,5	1.12	0
7	SO4	M	1531	-	4,4,4	0.81	0	6,6,6	0.35	0
7	SO4	M	1526	-	4,4,4	0.57	0	6,6,6	0.51	0
5	NAG	M	1519	1	14,14,15	1.40	2 (14%)	17,19,21	2.84	4 (23%)
8	GOL	M	1536	-	5,5,5	0.66	0	5,5,5	1.19	1 (20%)
8	GOL	M	1533	-	5,5,5	0.68	0	5,5,5	1.21	1 (20%)
7	SO4	M	1529	-	4,4,4	1.88	1 (25%)	6,6,6	2.46	3 (50%)

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
5	NAG	M	1506	1	-	2/6/23/26	0/1/1/1
5	NAG	M	1503	1	-	0/6/23/26	0/1/1/1
5	NAG	M	1520	1	-	4/6/23/26	0/1/1/1
8	GOL	M	1536	-	-	0/4/4/4	-
8	GOL	M	1535	-	-	0/4/4/4	-
5	NAG	M	1502	1	-	0/6/23/26	0/1/1/1
5	NAG	M	1523	1	-	0/6/23/26	0/1/1/1
8	GOL	M	1537	-	-	0/4/4/4	-
5	NAG	M	1519	1	1/1/5/7	0/6/23/26	0/1/1/1
8	GOL	M	1533	-	-	4/4/4/4	-
8	GOL	M	1534	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1503	NAG	O5-C5	4.36	1.51	1.43
5	M	1520	NAG	O7-C7	-4.20	1.13	1.23
5	M	1506	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	1523	NAG	O7-C7	-3.84	1.14	1.23
7	M	1529	SO4	O2-S	3.57	1.66	1.44
5	M	1503	NAG	O7-C7	-3.48	1.15	1.23
5	M	1506	NAG	C1-C2	-3.43	1.47	1.52
5	M	1519	NAG	O7-C7	-3.41	1.15	1.23
5	M	1506	NAG	O4-C4	2.88	1.50	1.43
5	M	1502	NAG	O7-C7	-2.85	1.16	1.23
5	M	1506	NAG	C2-N2	-2.69	1.41	1.46
7	M	1527	SO4	O1-S	2.59	1.60	1.44
7	M	1532	SO4	O1-S	2.47	1.59	1.44
5	M	1519	NAG	C2-N2	2.26	1.50	1.46
8	M	1534	GOL	O1-C1	2.17	1.51	1.42
5	M	1506	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	1506	NAG	C2-N2-C7	22.97	153.68	122.90
5	M	1506	NAG	O5-C1-C2	15.06	134.59	111.29
5	M	1506	NAG	C8-C7-N2	14.70	140.50	116.12
5	M	1506	NAG	O7-C7-N2	-8.72	106.58	121.98
5	M	1519	NAG	C1-O5-C5	8.53	123.61	112.19
5	M	1506	NAG	C1-O5-C5	-6.73	103.16	112.19
5	M	1503	NAG	C1-O5-C5	-6.30	103.74	112.19
5	M	1502	NAG	C1-O5-C5	-6.18	103.90	112.19
5	M	1520	NAG	O5-C1-C2	-6.04	101.95	111.29
5	M	1506	NAG	O7-C7-C8	-5.21	112.77	122.05
5	M	1519	NAG	C1-C2-N2	-4.75	102.95	110.43
5	M	1523	NAG	C4-C3-C2	-4.60	104.28	111.02
5	M	1519	NAG	O3-C3-C2	-4.28	100.50	109.40
5	M	1506	NAG	C3-C4-C5	3.81	117.13	110.23
7	M	1532	SO4	O4-S-O3	3.76	129.27	108.54
5	M	1523	NAG	O3-C3-C2	-3.75	101.62	109.40
5	M	1503	NAG	C4-C3-C2	-3.71	105.59	111.02
7	M	1529	SO4	O3-S-O2	-3.53	91.08	109.56
7	M	1532	SO4	O3-S-O1	-3.50	91.24	109.56
5	M	1520	NAG	O5-C5-C4	-3.48	102.37	110.83
5	M	1506	NAG	O4-C4-C5	-3.47	100.79	109.32
5	M	1520	NAG	O5-C5-C6	-3.30	101.24	107.66
5	M	1519	NAG	O4-C4-C5	-3.23	101.36	109.32
5	M	1520	NAG	O4-C4-C3	3.16	117.82	110.38
5	M	1506	NAG	O5-C5-C6	-3.08	101.66	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1529	SO4	O2-S-O1	-3.07	87.42	109.06
7	M	1532	SO4	O2-S-O1	-2.99	88.00	109.06
5	M	1523	NAG	O5-C1-C2	2.92	115.80	111.29
5	M	1520	NAG	O3-C3-C2	-2.82	103.55	109.40
5	M	1523	NAG	C1-C2-N2	-2.80	106.02	110.43
5	M	1502	NAG	O5-C5-C4	-2.80	104.02	110.83
8	M	1537	GOL	C3-C2-C1	-2.76	101.68	111.80
5	M	1502	NAG	O5-C1-C2	2.68	115.44	111.29
5	M	1520	NAG	C1-O5-C5	2.67	115.77	112.19
5	M	1506	NAG	O4-C4-C3	-2.54	104.40	110.38
5	M	1520	NAG	C2-N2-C7	2.53	126.30	122.90
5	M	1506	NAG	C1-C2-N2	2.51	114.39	110.43
7	M	1529	SO4	O4-S-O1	2.48	122.53	109.56
5	M	1506	NAG	C4-C3-C2	-2.48	107.39	111.02
7	M	1527	SO4	O4-S-O3	2.47	122.18	108.54
7	M	1532	SO4	O4-S-O1	-2.46	96.69	109.56
5	M	1503	NAG	O5-C5-C6	-2.46	102.87	107.66
5	M	1523	NAG	O5-C5-C4	-2.39	105.02	110.83
5	M	1503	NAG	O5-C5-C4	-2.37	105.05	110.83
7	M	1525	SO4	O3-S-O2	2.36	121.88	109.56
7	M	1530	SO4	O4-S-O1	2.35	121.83	109.56
8	M	1533	GOL	O2-C2-C1	2.34	118.87	109.18
5	M	1520	NAG	O7-C7-C8	2.30	126.15	122.05
8	M	1536	GOL	C3-C2-C1	-2.16	103.88	111.80
5	M	1502	NAG	C4-C3-C2	-2.14	107.88	111.02
7	M	1532	SO4	O3-S-O2	2.08	120.41	109.56
5	M	1502	NAG	O5-C5-C6	-2.06	103.66	107.66
5	M	1503	NAG	O3-C3-C2	-2.05	105.13	109.40
8	M	1535	GOL	O2-C2-C3	2.00	117.48	109.18
5	M	1506	NAG	O5-C5-C4	-2.00	105.95	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1519	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1506	NAG	C8-C7-N2-C2
8	M	1533	GOL	O1-C1-C2-O2
8	M	1533	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	M	1506	NAG	O7-C7-N2-C2
5	M	1520	NAG	O5-C5-C6-O6
5	M	1520	NAG	C4-C5-C6-O6
8	M	1533	GOL	C1-C2-C3-O3
8	M	1533	GOL	O2-C2-C3-O3
5	M	1520	NAG	O7-C7-N2-C2
5	M	1520	NAG	C8-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1506	NAG	7	0
5	M	1503	NAG	3	0
7	M	1527	SO4	5	0
5	M	1502	NAG	5	0
7	M	1532	SO4	7	0
7	M	1526	SO4	2	0
5	M	1519	NAG	2	0
8	M	1533	GOL	4	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%)	2.77	395 (79%) 0 0	8, 13, 26, 54	23 (4%)

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	378	SER	6.8
1	M	376	ALA	6.4
1	M	212	PRO	6.4
1	M	345	THR	6.2
1	M	23	SER	6.0
1	M	380	ASP	6.0
1	M	469	PHE	5.8
1	M	4	ILE	5.7
1	M	375	LYS	5.7
1	M	305[A]	GLU	5.5
1	M	112	GLY	5.5
1	M	138	THR	5.4
1	M	374	ASP	5.3
1	M	421	ASN	5.3
1	M	388	GLY	5.1
1	M	419	ASN	5.0
1	M	335	ALA	4.9
1	M	497	THR	4.9
1	M	12	PHE	4.8
1	M	349	ALA	4.8
1	M	43	THR	4.7
1	M	478	ILE	4.7
1	M	313	GLU	4.6
1	M	364	GLY	4.5
1	M	245	TYR	4.5
1	M	363[A]	SER	4.5
1	M	379	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	M	415	PRO	4.5
1	M	9	ASN	4.5
1	M	16	ASN	4.4
1	M	417	ASP	4.4
1	M	409	GLU	4.4
1	M	28	ASP	4.4
1	M	152	TYR	4.4
1	M	17	THR	4.4
1	M	458	ALA	4.3
1	M	18	ASP	4.3
1	M	219	SER	4.3
1	M	480	TRP	4.2
1	M	492	GLY	4.2
1	M	213[A]	SER	4.2
1	M	89	LEU	4.2
1	M	210	VAL	4.2
1	M	339	PRO	4.2
1	M	377	ASP	4.2
1	M	197	GLY	4.1
1	M	482	ASN	4.1
1	M	470	THR	4.1
1	M	457	TRP	4.1
1	M	371	PHE	4.1
1	M	63	GLY	4.0
1	M	448	ASP	4.0
1	M	404	LEU	4.0
1	M	206	CYS	4.0
1	M	132	GLY	4.0
1	M	465	PHE	3.9
1	M	36	SER	3.9
1	M	420	ARG	3.9
1	M	195	GLY	3.9
1	M	209	THR	3.9
1	M	79	TRP	3.9
1	M	390	TYR	3.9
1	M	423	SER	3.9
1	M	55	THR	3.9
1	M	300	ILE	3.8
1	M	27	SER	3.8
1	M	479	ASP	3.8
1	M	50	ILE	3.8
1	M	215	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	3	GLU	3.8
1	M	37	ALA	3.8
1	M	147	THR	3.8
1	M	42	GLY	3.8
1	M	418	GLU	3.8
1	M	450	ASN	3.8
1	M	262	LEU	3.8
1	M	80	GLN	3.8
1	M	167	TYR	3.7
1	M	183	LEU	3.7
1	M	25	PHE	3.7
1	M	83	ILE	3.7
1	M	115	GLU	3.7
1	M	501	PRO	3.6
1	M	15	GLY	3.6
1	M	53	GLY	3.6
1	M	275	THR	3.6
1	M	264	TYR	3.6
1	M	396	PHE	3.6
1	M	196	TYR	3.6
1	M	20[A]	LEU	3.6
1	M	58	TYR	3.6
1	M	129	ILE	3.5
1	M	310	PHE	3.5
1	M	26	SER	3.5
1	M	471	VAL	3.5
1	M	444	ILE	3.5
1	M	343	ASN	3.5
1	M	223	PRO	3.5
1	M	283	LEU	3.5
1	M	94	TYR	3.5
1	M	142	TRP	3.5
1	M	145	PRO	3.5
1	M	326	GLY	3.5
1	M	318	VAL	3.5
1	M	64	PRO	3.4
1	M	357	LEU	3.4
1	M	414	THR	3.4
1	M	298	ILE	3.4
1	M	341	PRO	3.4
1	M	22	SER	3.4
1	M	154	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	249	GLY	3.4
1	M	66	HIS	3.4
1	M	401	TYR	3.4
1	M	92	THR	3.4
1	M	203	PRO	3.4
1	M	30[A]	ILE	3.4
1	M	356	LYS	3.4
1	M	365	HIS	3.4
1	M	330	TYR	3.4
1	M	52	ASP	3.4
1	M	235	ALA	3.4
1	M	140	PHE	3.4
1	M	400	TYR	3.3
1	M	191	VAL	3.3
1	M	304	GLY	3.3
1	M	164	PHE	3.3
1	M	45	GLY	3.3
1	M	98	ILE	3.3
1	M	156	LEU	3.3
1	M	443	VAL	3.2
1	M	151	GLU	3.2
1	M	10	LEU	3.2
1	M	362	ALA	3.2
1	M	78	TYR	3.2
1	M	334	TYR	3.2
1	M	48	LEU	3.2
1	M	284	GLY	3.2
1	M	354	GLY	3.2
1	M	468	GLY	3.2
1	M	449[A]	VAL	3.2
1	M	103	ILE	3.2
1	M	144	LEU	3.2
1	M	170	LEU	3.2
1	M	359	TYR	3.2
1	M	338[A]	SER	3.2
1	M	293	GLY	3.2
1	M	200	LEU	3.1
1	M	360[A]	ILE	3.1
1	M	5	THR	3.1
1	M	368	GLY	3.1
1	M	403	PRO	3.1
1	M	60	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	33	VAL	3.1
1	M	162	ASP	3.1
1	M	260	TRP	3.1
1	M	160	ILE	3.1
1	M	432	TYR	3.1
1	M	54	PHE	3.1
1	M	434	CYS	3.1
1	M	51	TRP	3.1
1	M	490	LYS	3.1
1	M	47	GLY	3.1
1	M	320	GLY	3.1
1	M	381	ASN	3.1
1	M	84	ASP	3.1
1	M	274	ALA	3.1
1	M	113	VAL	3.1
1	M	311	SER	3.1
1	M	100	TRP	3.0
1	M	13	THR	3.0
1	M	441	ASN	3.0
1	M	485	ASP	3.0
1	M	91	ALA	3.0
1	M	265	ASN	3.0
1	M	484	THR	3.0
1	M	150	ASP	3.0
1	M	73	CYS	3.0
1	M	75	SER	3.0
1	M	97	SER	3.0
1	M	128	LEU	3.0
1	M	491	SER	3.0
1	M	474	GLY	3.0
1	M	11	PRO	3.0
1	M	424	MET	3.0
1	M	226	VAL	3.0
1	M	346	ASN	3.0
1	M	257	ILE	3.0
1	M	430	ILE	3.0
1	M	143	ASP	3.0
1	M	266	ASP	3.0
1	M	46	ARG	2.9
1	M	99	ALA	2.9
1	M	437	LEU	2.9
1	M	118[A]	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	119	ASP	2.9
1	M	436	HIS	2.9
1	M	308	PRO	2.9
1	M	297	GLN	2.9
1	M	498	PHE	2.9
1	M	88[A]	GLU	2.9
1	M	148	LEU	2.9
1	M	177	ASP	2.9
1	M	208	PRO	2.9
1	M	38	TYR	2.9
1	M	130	LYS	2.9
1	M	489	LYS	2.9
1	M	70	ASP	2.9
1	M	29	PHE	2.9
1	M	49	ASN	2.9
1	M	90	ASN	2.9
1	M	157	ASP	2.8
1	M	179	VAL	2.8
1	M	466	ASN	2.8
1	M	481	ASN	2.8
1	M	76	PHE	2.8
1	M	159	GLN	2.8
1	M	34	ALA	2.8
1	M	71	THR	2.8
1	M	57	ARG	2.8
1	M	422	GLN	2.8
1	M	473	PHE	2.8
1	M	62[A]	SER	2.8
1	M	500	SER	2.8
1	M	461	ASP	2.8
1	M	204	GLY	2.8
1	M	281	PHE	2.8
1	M	221	THR	2.8
1	M	467	LYS	2.8
1	M	14	CYS	2.8
1	M	389	ILE	2.8
1	M	114	ASN	2.7
1	M	229	HIS	2.7
1	M	93	GLY	2.7
1	M	241	TYR	2.7
1	M	295	TYR	2.7
1	M	149	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	342[A]	VAL	2.7
1	M	87	ASP	2.7
1	M	250	GLY	2.7
1	M	428	THR	2.7
1	M	312	PRO	2.7
1	M	238	VAL	2.7
1	M	101[A]	SER	2.7
1	M	201	ASP	2.7
1	M	494	TRP	2.7
1	M	108	LYS	2.7
1	M	290	LEU	2.7
1	M	59	PRO	2.7
1	M	316	ASN	2.7
1	M	483	VAL	2.7
1	M	141	HIS	2.6
1	M	307	LEU	2.6
1	M	495	TYR	2.6
1	M	331	PHE	2.6
1	M	373	LYS	2.6
1	M	329	TYR	2.6
1	M	237	VAL	2.6
1	M	56	HIS	2.6
1	M	255	THR	2.6
1	M	456	ALA	2.6
1	M	105	PRO	2.6
1	M	370	LEU	2.6
1	M	487	ASP	2.6
1	M	104	ILE	2.6
1	M	120	TYR	2.6
1	M	225	ILE	2.6
1	M	382	ILE	2.6
1	M	107	GLY	2.6
1	M	116	LYS	2.6
1	M	192	PRO	2.6
1	M	426	ASP	2.6
1	M	285	TRP	2.6
1	M	44	ILE	2.5
1	M	121	TYR	2.5
1	M	383	TYR	2.5
1	M	384	TYR	2.5
1	M	106	ARG	2.5
1	M	110	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	207	SER	2.5
1	M	493	GLN	2.5
1	M	136	PHE	2.5
1	M	125	ILE	2.5
1	M	137	VAL	2.5
1	M	477	TYR	2.5
1	M	21	ASN	2.5
1	M	398	ASN	2.5
1	M	268	ASP	2.5
1	M	294	THR	2.5
1	M	344[A]	SER	2.5
1	M	416	GLY	2.5
1	M	181	TYR	2.5
1	M	395	TYR	2.5
1	M	459	LEU	2.5
1	M	81	LYS	2.5
1	M	347	HIS	2.5
1	M	399	LYS	2.5
1	M	69	GLY	2.5
1	M	217	GLY	2.5
1	M	85	VAL	2.4
1	M	392	VAL	2.4
1	M	496	GLN	2.4
1	M	24	SER	2.4
1	M	315	SER	2.4
1	M	386	PRO	2.4
1	M	278	MET	2.4
1	M	124	LEU	2.4
1	M	425	LEU	2.4
1	M	486	ARG	2.4
1	M	272	ILE	2.4
1	M	214	CYS	2.4
1	M	366[A]	TYR	2.4
1	M	72	THR	2.4
1	M	158	PRO	2.4
1	M	233	ALA	2.4
1	M	445	LYS	2.4
1	M	427	TYR	2.4
1	M	139	LEU	2.4
1	M	327	LEU	2.4
1	M	67	GLY	2.4
1	M	123	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	244	ASN	2.4
1	M	288	GLY	2.4
1	M	302	THR	2.4
1	M	135	PRO	2.4
1	M	463	TYR	2.3
1	M	96	PHE	2.3
1	M	439	PHE	2.3
1	M	68	ASN	2.3
1	M	488	LEU	2.3
1	M	369	PRO	2.3
1	M	227	ALA	2.3
1	M	166	ASP	2.3
1	M	240	LEU	2.3
1	M	406	TYR	2.3
1	M	440	LEU	2.3
1	M	77	SER	2.3
1	M	31	PHE	2.3
1	M	172	PHE	2.3
1	M	146	GLN	2.3
1	M	462[A]	ASN	2.3
1	M	86	LEU	2.3
1	M	224	TYR	2.3
1	M	276	GLU	2.2
1	M	309[A]	SER	2.2
1	M	391	SER	2.2
1	M	286	PHE	2.2
1	M	184	THR	2.2
1	M	263	PRO	2.2
1	M	271[A]	SER	2.2
1	M	131	LYS	2.2
1	M	252	ILE	2.2
1	M	258	THR	2.2
1	M	291	THR	2.2
1	M	332	THR	2.2
1	M	337	PRO	2.2
1	M	348	THR	2.2
1	M	323	ASP	2.2
1	M	351	MET	2.2
1	M	171	CYS	2.2
1	M	242	ARG	2.2
1	M	472	ARG	2.2
1	M	134	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	296	PRO	2.2
1	M	433	LEU	2.2
1	M	277	ARG	2.2
1	M	322	TYR	2.2
1	M	454	TYR	2.2
1	M	246	THR	2.2
1	M	19	ALA	2.1
1	M	95	ARG	2.1
1	M	169[A]	ASP	2.1
1	M	394	ASP	2.1
1	M	7	GLN	2.1
1	M	232	LEU	2.1
1	M	317	LEU	2.1
1	M	452	LYS	2.1
1	M	413	SER	2.1
1	M	410	ASN	2.1
1	M	273	ALA	2.1
1	M	314	GLU	2.1
1	M	464	GLU	2.1
1	M	218	ASN	2.1
1	M	111	ARG	2.1
1	M	385	TYR	2.1
1	M	32	GLY	2.1
1	M	133	ILE	2.1
1	M	261	PHE	2.1
1	M	186	ASN	2.0
1	M	109	ARG	2.0
1	M	193	THR	2.0
1	M	324	PHE	2.0
1	M	451	VAL	2.0
1	M	122	HIS	2.0
1	M	228	HIS	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,

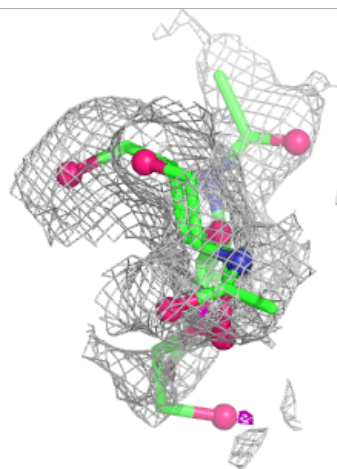
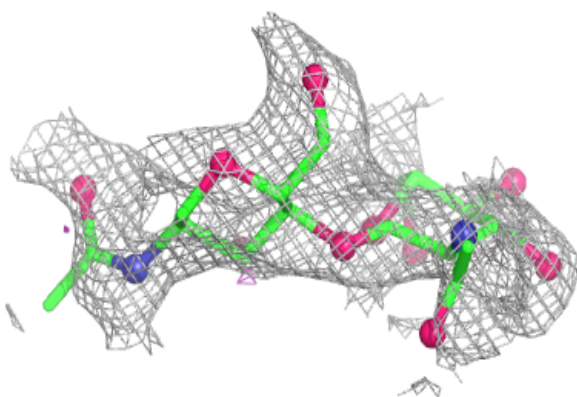
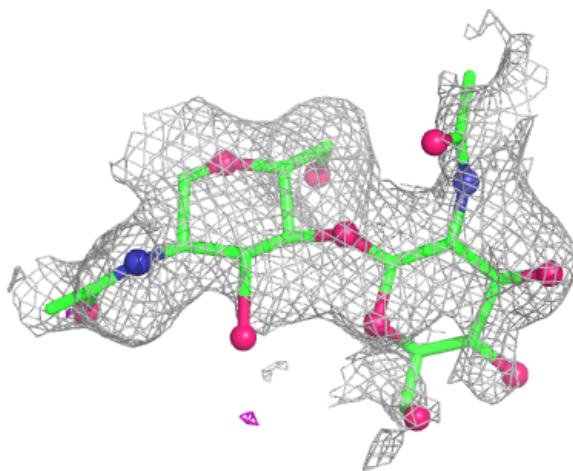
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	17,21,30,35	0
2	NAG	A	2	14/15	-	-	35,43,55,57	0
4	BMA	C	3	11/12	0.34	0.27	23,28,33,45	0
4	XYP	C	4	9/10	0.41	0.21	30,36,41,61	0
3	NAG	B	2	14/15	0.45	0.22	19,25,31,36	0
3	NAG	B	1	14/15	0.58	0.19	13,20,25,25	0
3	BMA	B	3	11/12	-	-	36,41,46,51	0
3	XYP	B	4	9/10	-	-	39,46,50,52	0
3	FUC	B	5	10/11	-	-	22,30,37,46	0
4	NAG	C	1	14/15	0.60	0.23	15,18,24,27	0
2	NAG	D	1	14/15	0.64	0.19	7,14,19,21	0
4	NAG	C	2	14/15	0.68	0.17	18,21,26,30	0
2	NAG	D	2	14/15	0.69	0.15	24,29,47,54	0
4	MAN	C	5	11/12	-	-	23,37,49,54	0
4	MAN	C	6	11/12	-	-	31,41,52,53	0
4	FUC	C	7	10/11	-	-	17,19,31,31	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.

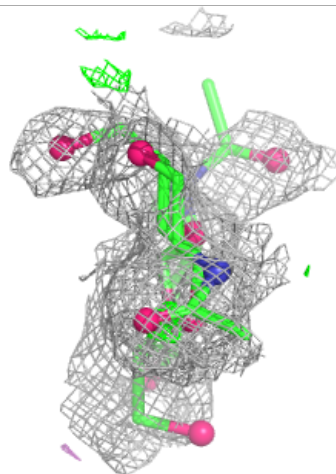
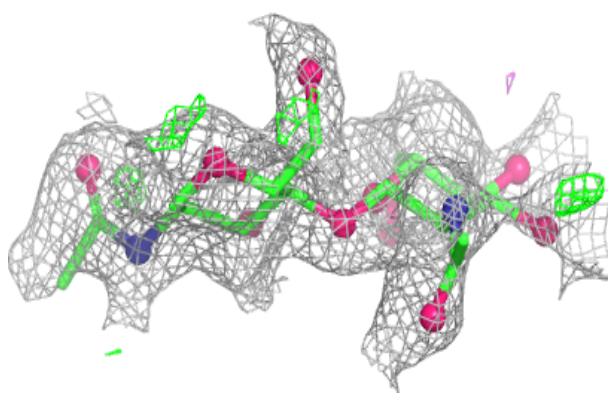
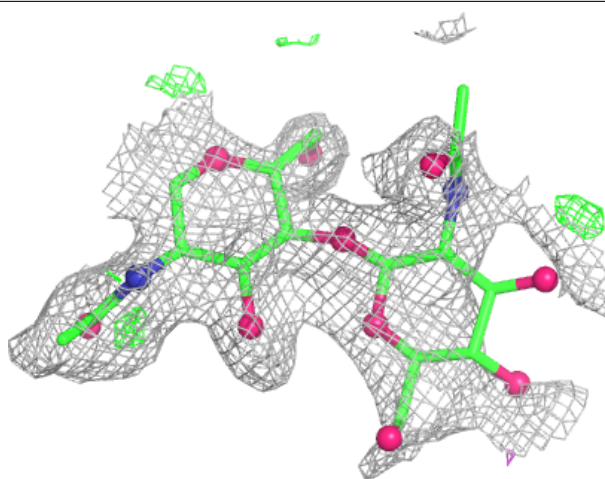
Electron density around Chain A:

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



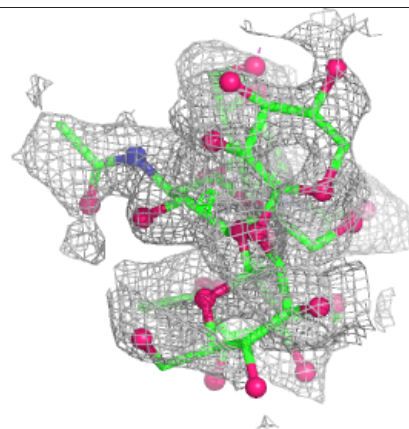
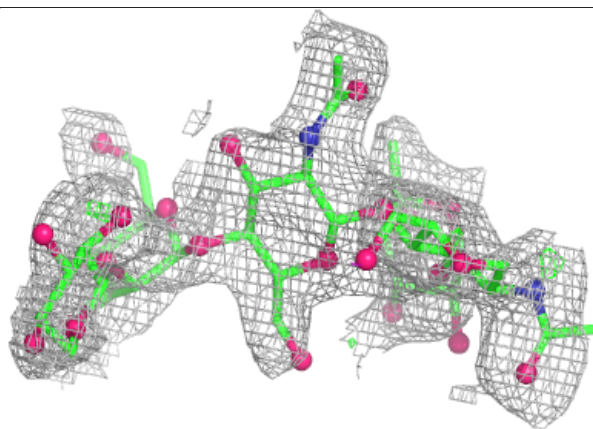
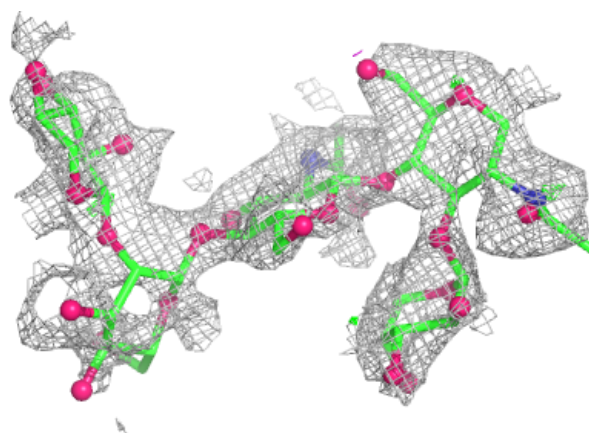
Electron density around Chain D:

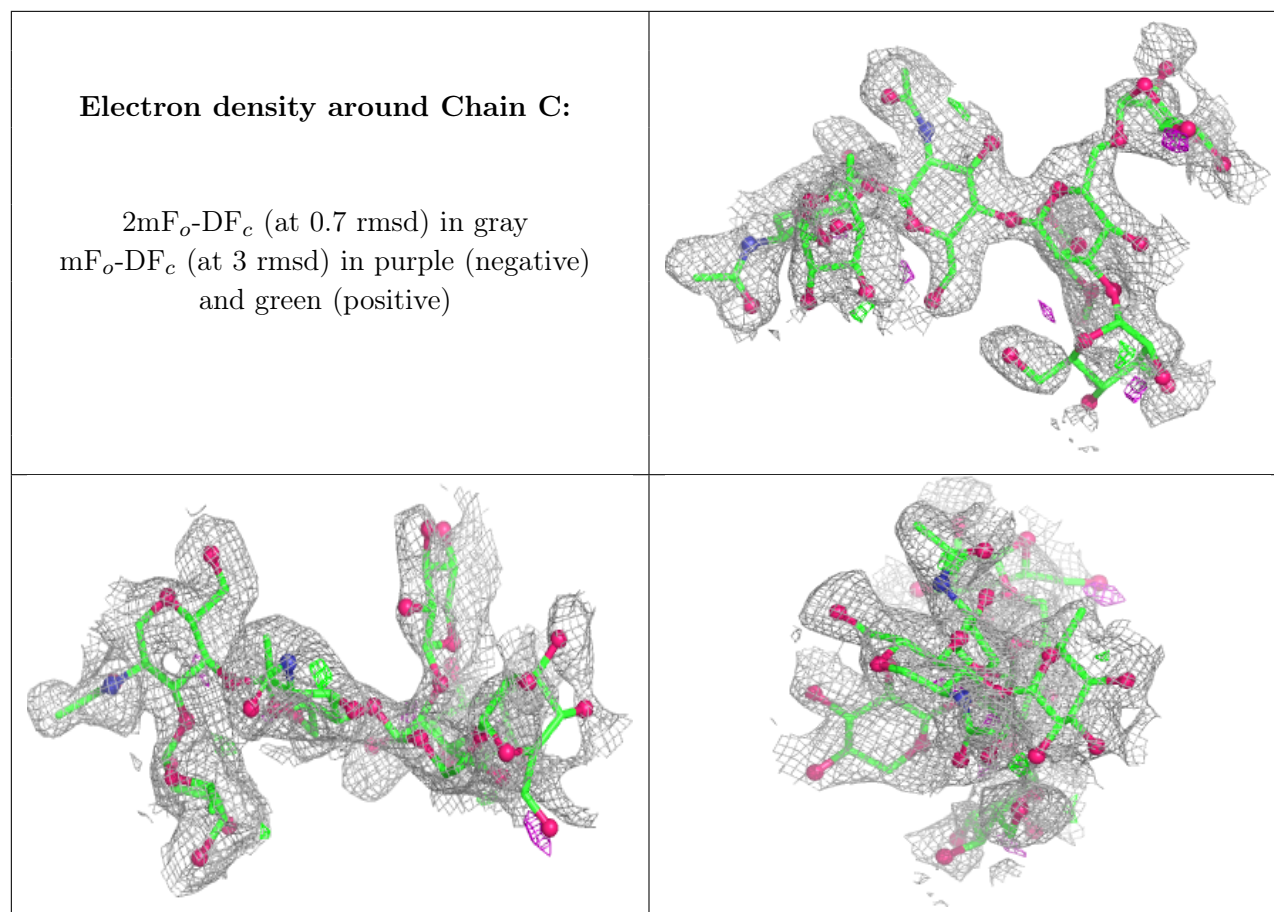
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	Q<0.9
8	GOL	M	1533	6/6	0.32	0.33	34,40,42,49	6
5	NAG	M	1523	14/15	0.47	0.25	32,38,51,54	0
5	NAG	M	1502	14/15	0.48	0.24	23,32,44,46	0
5	NAG	M	1519	14/15	0.49	0.24	41,48,60,66	0
5	NAG	M	1520	14/15	0.49	0.32	54,62,68,68	0
7	SO4	M	1526	5/5	0.53	0.26	23,26,33,34	5
7	SO4	M	1532	5/5	0.53	0.43	36,38,44,57	1
5	NAG	M	1506	14/15	0.53	0.21	33,40,46,47	0
8	GOL	M	1534	6/6	0.56	0.21	3,12,16,16	1
5	NAG	M	1503	14/15	0.57	0.19	22,25,34,43	0
8	GOL	M	1536	6/6	0.59	0.33	29,29,41,43	6
7	SO4	M	1531	5/5	0.64	0.28	31,33,36,37	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	M	1537	6/6	0.64	0.14	13,14,20,20	0
7	SO4	M	1528	5/5	0.69	0.20	15,19,24,27	0
8	GOL	M	1535	6/6	0.70	0.14	9,19,24,29	6
7	SO4	M	1527	5/5	0.71	0.16	12,26,28,32	5
7	SO4	M	1525	5/5	0.78	0.24	24,27,30,35	5
7	SO4	M	1530	5/5	0.79	0.17	11,31,32,35	5
6	ZN	M	1524	1/1	0.80	0.15	34,34,34,34	0
7	SO4	M	1529	5/5	0.81	0.27	24,28,32,33	5

6.5 Other polymers [i](#)

There are no such residues in this entry.