



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:11 AM UTC

PDB ID : 1DWJ / pdb_00001dwj
Title : study on radiation damage on a cryocooled crystal. Refined part 6: structure after a radiation dose of 54×10^{15} photons/mm²
Authors : Burmeister, W.P.
Deposited on : 1999-12-05
Resolution : 2.40 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

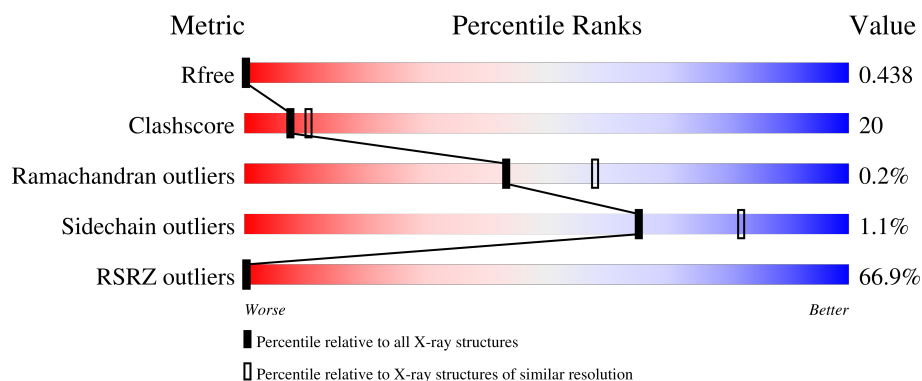
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	67% 69%30%.
2	A	2	100%
2	D	2	100%
3	B	5	20%80%
4	C	7	29%29%43%

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	MAN	C	6	-	-	X	-
8	GOL	M	1023	-	-	-	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:

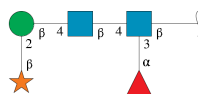
Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

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



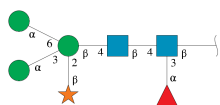
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



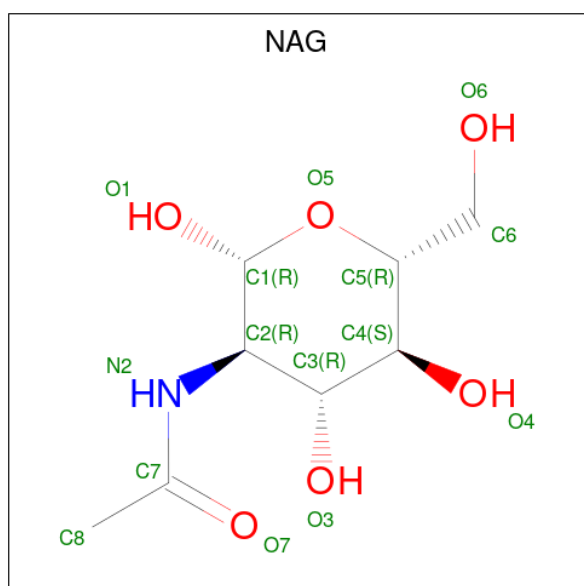
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			58	33	2	23			

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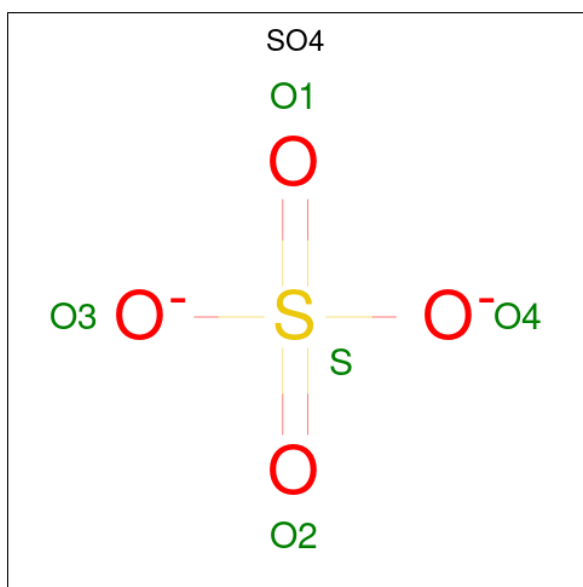
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		

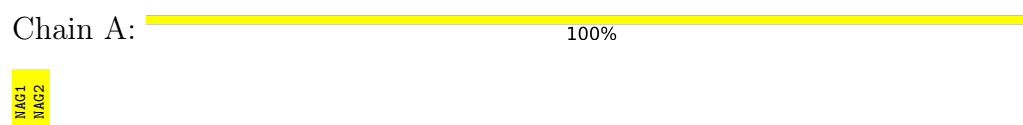
3 Residue-property plots

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



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

Chain D:  100%

MAG1
MAG2

- 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:  20% 80%

MAG1
MAG2
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:  29% 29% 43%

MAG1
MAG2
BMA3
XYP4
MANG
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 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.40) 97.2 (15.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.186 , 0.245 0.408 , 0.438	Depositor DCC
R_{free} test set	2570 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: BMA, XYP, GOL, NAG, MAN, ZN, SO4, FUC

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	0.98	3/4291 (0.1%)	1.05	14/5835 (0.2%)

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	2	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	257	ILE	CA-CB	9.03	1.64	1.53
1	M	227	ALA	CA-CB	-5.59	1.44	1.53
1	M	350	MET	CG-SD	5.06	1.93	1.80

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	253	GLY	CA-C-N	7.42	127.58	120.31
1	M	253	GLY	C-N-CA	7.42	127.58	120.31
1	M	402	ASN	CA-C-N	6.59	126.77	120.31
1	M	402	ASN	C-N-CA	6.59	126.77	120.31
1	M	323	ASP	N-CA-C	-5.95	106.15	113.41
1	M	191	VAL	CB-CA-C	-5.88	108.12	114.35
1	M	217	GLY	N-CA-C	5.83	118.33	111.63
1	M	331	PHE	N-CA-C	5.70	116.08	108.38
1	M	445	LYS	N-CA-C	5.54	117.40	111.36
1	M	191	VAL	N-CA-CB	5.49	113.96	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	190	SER	N-CA-C	5.49	116.95	110.97
1	M	485	ASP	N-CA-C	5.41	118.74	110.20
1	M	18	ASP	N-CA-C	-5.32	105.53	112.23
1	M	210	VAL	N-CA-C	-5.05	105.50	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	M	360[A]	ILE	CB
1	M	360[B]	ILE	CB

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	215	TYR	Sidechain
1	M	401	TYR	Sidechain
1	M	446	GLU	Mainchain
1	M	463	TYR	Sidechain
1	M	482	ASN	Mainchain
1	M	94	TYR	Sidechain
1	M	97	SER	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	3838	154	8
2	A	28	0	25	0	0
2	D	28	0	25	2	0
3	B	58	0	42	0	0
4	C	80	0	60	11	0
5	M	84	0	78	9	0
6	M	1	0	0	0	1
7	M	40	0	0	1	0
8	M	30	0	40	1	0
9	M	788	0	0	87	15
All	All	5220	0	4108	170	23

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 20.

All (170) 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)
9:M:3053:HOH:O	4:C:6:MAN:O6	1.55	1.22
1:M:15:GLY:HA3	9:M:2027:HOH:O	1.06	1.20
9:M:3055:HOH:O	4:C:6:MAN:H61	1.01	1.19
9:M:3066:HOH:O	2:D:2:NAG:H83	1.44	1.17
1:M:428:THR:HG23	9:M:2608:HOH:O	1.44	1.17
1:M:431:ASP:OD1	9:M:2612:HOH:O	1.63	1.13
1:M:215:TYR:O	9:M:2342:HOH:O	1.64	1.12
1:M:71:THR:HG23	9:M:2118:HOH:O	1.51	1.07
5:M:961:NAG:H61	9:M:3056:HOH:O	1.59	1.02
1:M:15:GLY:CA	9:M:2027:HOH:O	1.72	1.00
1:M:215:TYR:HB2	9:M:2093:HOH:O	1.60	0.99
1:M:379:THR:HG22	9:M:2542:HOH:O	0.80	0.97
1:M:246:THR:HG22	9:M:2360:HOH:O	1.66	0.95
5:M:961:NAG:C6	9:M:3056:HOH:O	2.14	0.95
1:M:6:CYS:HG	1:M:438:CYS:HG	1.16	0.91
1:M:379:THR:HG23	9:M:2537:HOH:O	1.74	0.87
1:M:15:GLY:C	9:M:2027:HOH:O	2.03	0.83
1:M:20[B]:LEU:HG	1:M:498:PHE:HE2	1.44	0.82
1:M:70:ASP:OD2	9:M:2114:HOH:O	1.96	0.82
1:M:10:LEU:CD2	9:M:2020:HOH:O	2.27	0.81
4:C:3:BMA:H61	4:C:6:MAN:H5	1.63	0.81
9:M:3053:HOH:O	4:C:6:MAN:C6	2.18	0.80
1:M:150:ASP:OD2	9:M:2270:HOH:O	2.00	0.80
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE2	2.17	0.79
4:C:3:BMA:H61	4:C:6:MAN:C5	2.13	0.79
1:M:373:LYS:NZ	9:M:2528:HOH:O	2.15	0.78
1:M:14:CYS:HG	1:M:434:CYS:HG	0.79	0.77
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.67	0.76
1:M:130:LYS:HB3	9:M:2246:HOH:O	1.85	0.76
1:M:10:LEU:HD23	9:M:2020:HOH:O	1.86	0.75
1:M:462[B]:ASN:OD1	9:M:2635:HOH:O	2.05	0.73
1:M:337:PRO:O	1:M:338[B]:SER:HB3	1.79	0.72
1:M:165:LYS:HZ1	5:M:931:NAG:H82	1.55	0.71
1:M:278:MET:HE1	9:M:2323:HOH:O	1.90	0.71
1:M:365:HIS:HE1	9:M:2519:HOH:O	1.75	0.69
1:M:215:TYR:CA	9:M:2342:HOH:O	2.40	0.69
1:M:20[B]:LEU:HG	1:M:498:PHE:CE2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:59:PRO:HB3	9:M:2091:HOH:O	1.95	0.66
1:M:333:GLN:OE1	1:M:357:LEU:HD13	1.95	0.66
1:M:327:LEU:HD12	1:M:393:MET:HE1	1.77	0.66
1:M:111:ARG:C	9:M:2204:HOH:O	2.39	0.65
1:M:200:LEU:HB3	9:M:2328:HOH:O	1.96	0.65
1:M:240:LEU:HD13	5:M:931:NAG:H83	1.77	0.65
1:M:191:VAL:HG23	9:M:2326:HOH:O	1.98	0.64
1:M:428:THR:N	9:M:2608:HOH:O	2.20	0.64
4:C:3:BMA:C6	4:C:6:MAN:C5	2.76	0.64
1:M:126[B]:SER:OG	9:M:2236:HOH:O	2.15	0.63
1:M:208:PRO:HA	9:M:2335:HOH:O	1.97	0.63
1:M:81:LYS:HD2	9:M:2665:HOH:O	1.99	0.63
9:M:3055:HOH:O	4:C:3:BMA:H61	1.99	0.62
1:M:7:GLN:NE2	9:M:2009:HOH:O	2.32	0.62
9:M:3053:HOH:O	4:C:6:MAN:C5	2.45	0.62
1:M:205:ARG:O	1:M:206:CYS:HB3	1.98	0.62
4:C:3:BMA:C6	4:C:6:MAN:H5	2.30	0.62
1:M:484:THR:HB	9:M:2664:HOH:O	2.01	0.61
1:M:10:LEU:HD22	9:M:2020:HOH:O	1.95	0.60
1:M:116:LYS:HE3	9:M:2074:HOH:O	2.01	0.60
1:M:194:ARG:NH2	9:M:2328:HOH:O	2.34	0.60
1:M:501:PRO:HB2	5:M:901:NAG:H82	1.83	0.60
1:M:414:THR:HG22	9:M:2609:HOH:O	2.02	0.59
1:M:497:THR:HG23	9:M:2682:HOH:O	2.03	0.59
1:M:7:GLN:NE2	1:M:13:THR:OG1	2.36	0.59
1:M:342[A]:VAL:HG13	9:M:2345:HOH:O	2.02	0.59
1:M:472:ARG:NE	9:M:2651:HOH:O	2.36	0.58
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.84	0.58
1:M:9:ASN:HB2	9:M:3080:HOH:O	2.03	0.58
1:M:39:GLN:HG2	1:M:463:TYR:O	2.03	0.58
1:M:421:ASN:ND2	9:M:2600:HOH:O	2.37	0.58
1:M:445:LYS:HE2	9:M:2619:HOH:O	2.04	0.58
1:M:378:SER:HB3	9:M:2528:HOH:O	2.03	0.57
9:M:3040:HOH:O	4:C:7:FUC:H2	2.03	0.57
1:M:256:MET:HE2	1:M:287:MET:HG2	1.85	0.57
1:M:61:LYS:HE2	9:M:2337:HOH:O	2.04	0.57
1:M:165:LYS:NZ	5:M:931:NAG:H82	2.20	0.57
1:M:88[B]:GLU:HG3	9:M:2147:HOH:O	2.05	0.56
5:M:961:NAG:H62	9:M:3056:HOH:O	1.92	0.55
1:M:360[B]:ILE:CG2	1:M:364:GLY:HA2	2.37	0.54
8:M:1024:GOL:H11	9:M:2291:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:259:ARG:HG3	1:M:282:PHE:CE2	2.43	0.53
1:M:215:TYR:HB2	9:M:2342:HOH:O	2.09	0.53
1:M:449[B]:VAL:HG23	1:M:451:VAL:HG23	1.90	0.53
1:M:130:LYS:HG2	9:M:2247:HOH:O	2.09	0.52
1:M:115:GLU:HA	1:M:115:GLU:OE1	2.09	0.52
1:M:188:LEU:HD12	1:M:256:MET:SD	2.49	0.52
1:M:55:THR:HG22	1:M:62[B]:SER:OG	2.10	0.52
1:M:38:TYR:HE1	1:M:52:ASP:OD1	1.93	0.51
1:M:71:THR:CG2	9:M:2118:HOH:O	2.30	0.51
1:M:360[B]:ILE:HG22	1:M:361:ASN:O	2.10	0.51
1:M:449[B]:VAL:CG2	1:M:451:VAL:HG23	2.40	0.51
1:M:428:THR:CB	9:M:2608:HOH:O	2.57	0.51
9:M:3053:HOH:O	4:C:6:MAN:O4	1.90	0.51
1:M:259:ARG:HG2	9:M:2466:HOH:O	2.11	0.51
1:M:477:TYR:HE1	9:M:2651:HOH:O	1.94	0.50
1:M:207:SER:HB2	1:M:210:VAL:HG23	1.94	0.50
1:M:471:VAL:HG11	9:M:2587:HOH:O	2.11	0.50
1:M:95:ARG:NH1	1:M:409:GLU:HG3	2.27	0.49
1:M:215:TYR:OH	9:M:2341:HOH:O	2.15	0.49
1:M:409:GLU:HG2	1:M:457:TRP:CE3	2.48	0.48
1:M:116:LYS:HA	1:M:116:LYS:HD2	1.61	0.47
1:M:328:ASN:CG	1:M:409:GLU:HB2	2.39	0.47
1:M:285:TRP:CD1	1:M:299:MET:HE1	2.50	0.47
1:M:269:ARG:NH2	9:M:2397:HOH:O	2.44	0.47
1:M:365:HIS:CE1	2:D:1:NAG:H62	2.49	0.47
1:M:259:ARG:HG3	1:M:282:PHE:CZ	2.50	0.47
1:M:387:LYS:HE3	9:M:2552:HOH:O	2.15	0.46
1:M:88[B]:GLU:CD	9:M:2154:HOH:O	2.58	0.46
1:M:4:ILE:HG21	9:M:2618:HOH:O	2.16	0.46
1:M:103:ILE:HD11	1:M:167:TYR:HE1	1.80	0.46
1:M:336:GLN:HB2	1:M:337:PRO:HD2	1.98	0.46
1:M:194:ARG:HD2	7:M:1009:SO4:O1	2.16	0.45
1:M:186:ASN:HA	1:M:255:THR:HB	1.99	0.45
1:M:241:TYR:OH	1:M:250:GLY:HA3	2.16	0.45
1:M:363[B]:SER:HB3	9:M:2505:HOH:O	2.17	0.45
1:M:388:GLY:O	1:M:392:VAL:HG23	2.16	0.45
1:M:30[B]:ILE:CD1	9:M:2085:HOH:O	2.64	0.45
1:M:327:LEU:HD12	1:M:393:MET:CE	2.46	0.45
1:M:501:PRO:HB2	5:M:901:NAG:C8	2.47	0.45
1:M:374:ASP:HB3	1:M:377:ASP:O	2.17	0.44
1:M:260:TRP:O	1:M:332:THR:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360[B]:ILE:HG21	1:M:364:GLY:HA2	1.99	0.44
1:M:95:ARG:HA	1:M:136:PHE:O	2.17	0.44
1:M:377:ASP:O	1:M:380:ASP:HB2	2.17	0.44
1:M:424:MET:HE1	9:M:2673:HOH:O	2.16	0.44
1:M:342[B]:VAL:HG11	9:M:2434:HOH:O	2.17	0.44
1:M:294:THR:HG22	9:M:2416:HOH:O	2.18	0.44
1:M:373:LYS:NZ	1:M:378:SER:OG	2.49	0.44
1:M:397:LYS:HD2	1:M:449[B]:VAL:HG12	2.00	0.44
1:M:467:LYS:HE3	9:M:2640:HOH:O	2.18	0.44
1:M:48:LEU:N	9:M:2081:HOH:O	2.27	0.43
1:M:149:GLN:O	1:M:153:GLU:HA	2.19	0.43
1:M:130:LYS:HE3	9:M:2235:HOH:O	2.17	0.43
1:M:459:LEU:HD13	9:M:2166:HOH:O	2.18	0.43
1:M:215:TYR:HA	9:M:2342:HOH:O	2.15	0.43
1:M:360[B]:ILE:HG23	1:M:364:GLY:C	2.44	0.43
1:M:426:ASP:OD2	1:M:429:ARG:NH1	2.48	0.43
1:M:39:GLN:O	1:M:462[A]:ASN:HB2	2.19	0.42
1:M:165:LYS:NZ	5:M:931:NAG:C8	2.80	0.42
1:M:381:ASN:ND2	9:M:2528:HOH:O	2.49	0.42
1:M:144:LEU:HD11	1:M:160:ILE:HD11	2.00	0.42
1:M:379:THR:CG2	9:M:2542:HOH:O	1.71	0.42
1:M:53:GLY:C	9:M:2089:HOH:O	2.62	0.42
1:M:199:ALA:HB2	1:M:214:CYS:SG	2.61	0.41
1:M:399:LYS:O	1:M:399:LYS:HG3	2.19	0.41
1:M:457:TRP:HA	1:M:458:ALA:HA	1.90	0.41
1:M:363[A]:SER:HB2	9:M:2505:HOH:O	2.20	0.41
1:M:131:LYS:HD3	1:M:131:LYS:HA	1.82	0.41
1:M:368:GLY:HA3	1:M:384:TYR:O	2.20	0.41
1:M:337:PRO:O	1:M:338[B]:SER:CB	2.55	0.41
1:M:472:ARG:CZ	9:M:2651:HOH:O	2.67	0.41
1:M:279:LYS:NZ	9:M:2407:HOH:O	2.50	0.41
1:M:378:SER:C	1:M:380:ASP:H	2.29	0.41
1:M:214:CYS:HB2	9:M:2335:HOH:O	2.20	0.41
1:M:413:SER:HB3	1:M:473:PHE:CE1	2.55	0.41
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	0.41
1:M:139:LEU:HD23	1:M:139:LEU:HA	1.86	0.41
1:M:6:CYS:CB	1:M:438:CYS:HG	2.33	0.40
1:M:399:LYS:HG2	1:M:400:TYR:CE2	2.55	0.40
1:M:428:THR:CG2	9:M:2608:HOH:O	2.25	0.40
1:M:46:ARG:NE	9:M:2077:HOH:O	2.50	0.40

All (23) 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:2272:HOH:O	9:M:2272:HOH:O[3_656]	1.10	1.10
9:M:2010:HOH:O	9:M:2505:HOH:O[4_576]	1.43	0.77
9:M:2546:HOH:O	9:M:2546:HOH:O[4_576]	1.44	0.76
9:M:2017:HOH:O	9:M:2017:HOH:O[4_576]	1.63	0.57
9:M:2252:HOH:O	9:M:2252:HOH:O[4_576]	1.63	0.57
9:M:2408:HOH:O	9:M:3103:HOH:O[6_564]	1.63	0.57
1:M:373:LYS:CE	1:M:373:LYS:CE[4_576]	1.66	0.54
9:M:2241:HOH:O	9:M:2523:HOH:O[4_576]	1.67	0.53
9:M:2240:HOH:O	9:M:2240:HOH:O[4_576]	1.76	0.44
1:M:373:LYS:CD	1:M:373:LYS:NZ[4_576]	1.78	0.42
9:M:2108:HOH:O	9:M:2124:HOH:O[3_656]	1.83	0.37
1:M:45:GLY:N	1:M:57:ARG:O[3_656]	1.90	0.30
9:M:2173:HOH:O	9:M:2365:HOH:O[6_564]	1.92	0.28
9:M:2238:HOH:O	9:M:2613:HOH:O[4_576]	1.96	0.24
1:M:373:LYS:CG	1:M:373:LYS:NZ[4_576]	2.02	0.18
9:M:2058:HOH:O	9:M:2106:HOH:O[3_656]	2.02	0.18
1:M:106:ARG:CD	1:M:153:GLU:OE2[3_656]	2.07	0.13
9:M:2210:HOH:O	9:M:2339:HOH:O[3_656]	2.09	0.11
1:M:11:PRO:CG	9:M:2511:HOH:O[4_576]	2.11	0.09
9:M:2017:HOH:O	9:M:2018:HOH:O[4_576]	2.12	0.08
1:M:106:ARG:NE	1:M:153:GLU:OE2[3_656]	2.17	0.03
1:M:373:LYS:CE	1:M:373:LYS:NZ[4_576]	2.18	0.02

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%)	498 (96%)	19 (4%)	1 (0%)	43 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	456/435 (105%)	450 (99%)	6 (1%)	61 80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	110	SER
1	M	116	LYS
1	M	183	LEU
1	M	268	ASP
1	M	360[A]	ILE
1	M	360[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	39	GLN
1	M	80	GLN
1	M	146	GLN
1	M	230	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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	0.52	0	17,19,21	0.84	1 (5%)
2	NAG	A	2	2	14,14,15	1.08	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	B	1	3,1	14,14,15	0.60	0	17,19,21	0.88	1 (5%)
3	NAG	B	2	3	14,14,15	0.80	0	17,19,21	0.63	0
3	BMA	B	3	3	11,11,12	1.23	1 (9%)	15,15,17	0.67	0
3	XYP	B	4	3	9,9,10	0.87	0	10,12,14	1.34	1 (10%)
3	FUC	B	5	3	10,10,11	1.18	1 (10%)	14,14,16	0.75	0
4	NAG	C	1	4,1	14,14,15	0.64	0	17,19,21	0.84	0
4	NAG	C	2	4	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
4	BMA	C	3	4	11,11,12	1.00	1 (9%)	15,15,17	0.99	1 (6%)
4	XYP	C	4	4	9,9,10	0.73	0	10,12,14	1.14	1 (10%)
4	MAN	C	5	4	11,11,12	0.83	0	15,15,17	0.53	0
4	MAN	C	6	4	11,11,12	0.99	1 (9%)	15,15,17	1.39	1 (6%)
4	FUC	C	7	4	10,10,11	0.96	0	14,14,16	1.31	2 (14%)
2	NAG	D	1	2,1	14,14,15	0.58	0	17,19,21	0.49	0
2	NAG	D	2	2	14,14,15	0.81	0	17,19,21	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	1/2/19/22	0/1/1/1
4	MAN	C	6	4	-	2/2/19/22	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	NAG	C1-C2	2.85	1.56	1.52
3	B	5	FUC	C2-C3	2.65	1.56	1.52
4	C	3	BMA	C2-C3	-2.56	1.48	1.52
3	B	3	BMA	C4-C5	2.47	1.58	1.53
4	C	6	MAN	C2-C3	2.39	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	6	MAN	C6-C5-C4	4.15	123.21	113.02
3	B	4	XYP	C1-C2-C3	3.50	114.74	109.64
4	C	4	XYP	C5-C4-C3	3.10	114.16	109.64
4	C	2	NAG	C3-C4-C5	2.64	115.03	110.23
4	C	7	FUC	C2-C3-C4	-2.58	106.32	110.86
4	C	7	FUC	C1-C2-C3	-2.56	105.92	109.64
3	B	1	NAG	C8-C7-N2	-2.28	112.33	116.12
2	A	2	NAG	C2-N2-C7	2.08	125.69	122.90
4	C	3	BMA	O5-C5-C6	-2.04	103.69	107.66
2	A	1	NAG	C8-C7-N2	-2.02	112.77	116.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	6	MAN	C4-C5-C6-O6
4	C	6	MAN	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6

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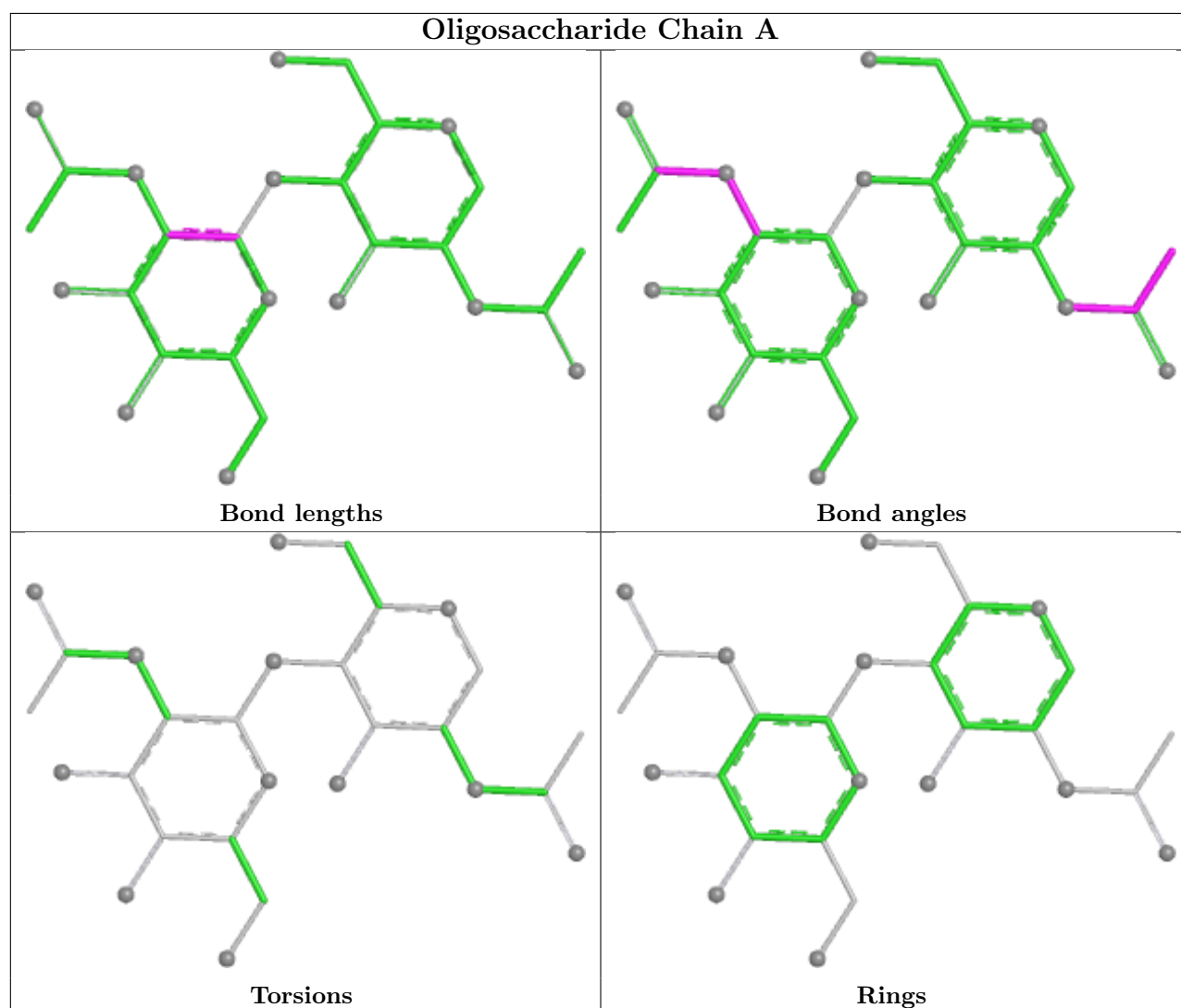
Mol	Chain	Res	Type	Atoms
4	C	5	MAN	C4-C5-C6-O6

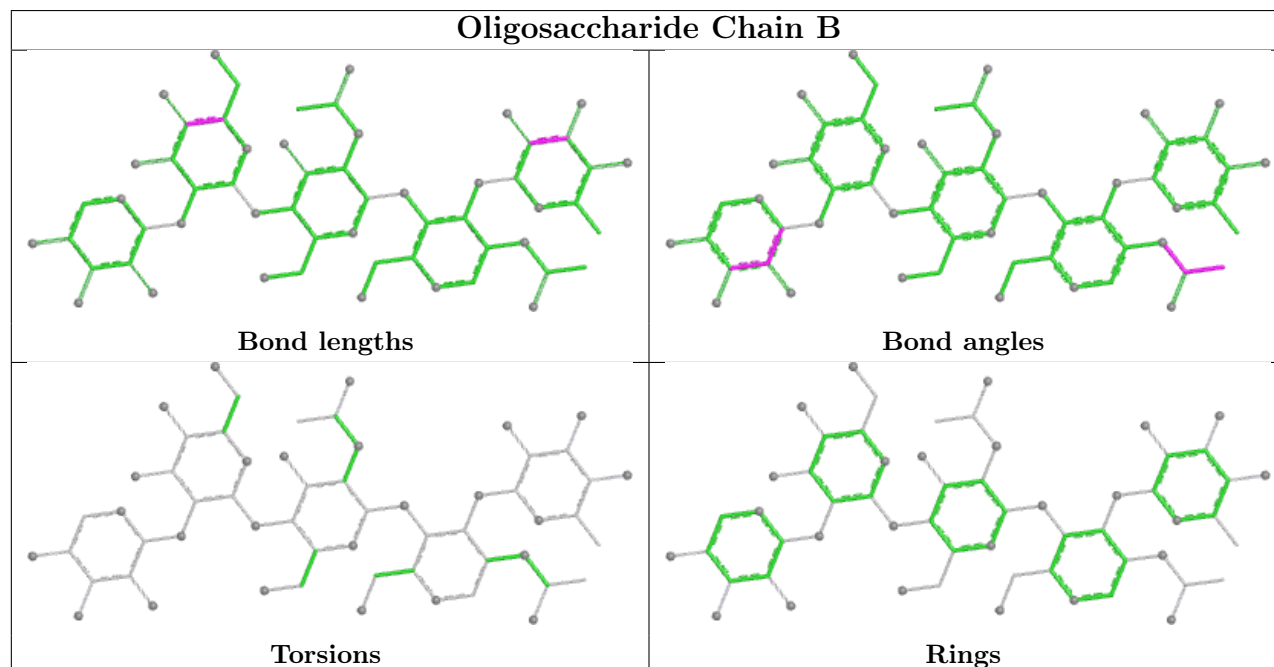
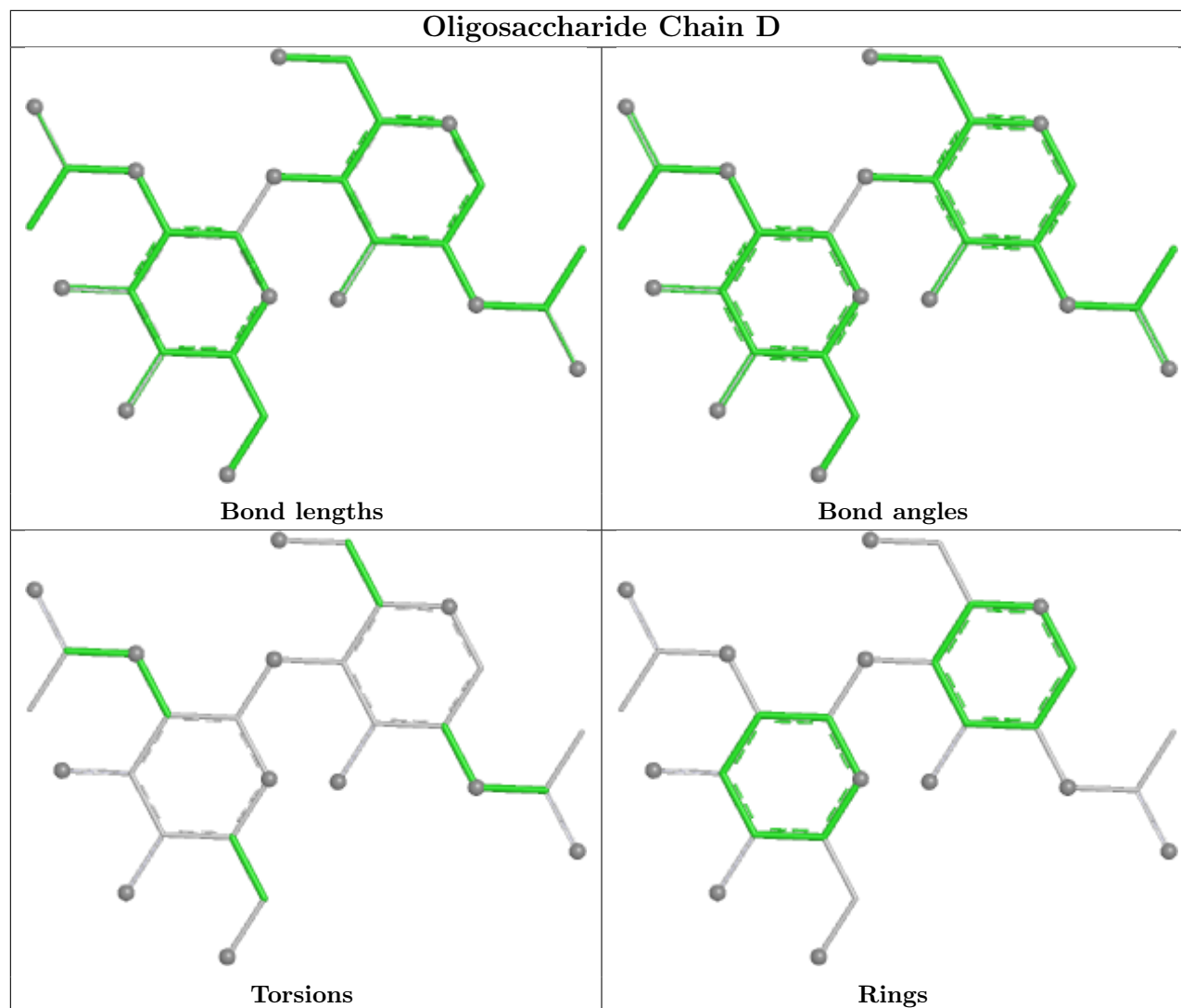
There are no ring outliers.

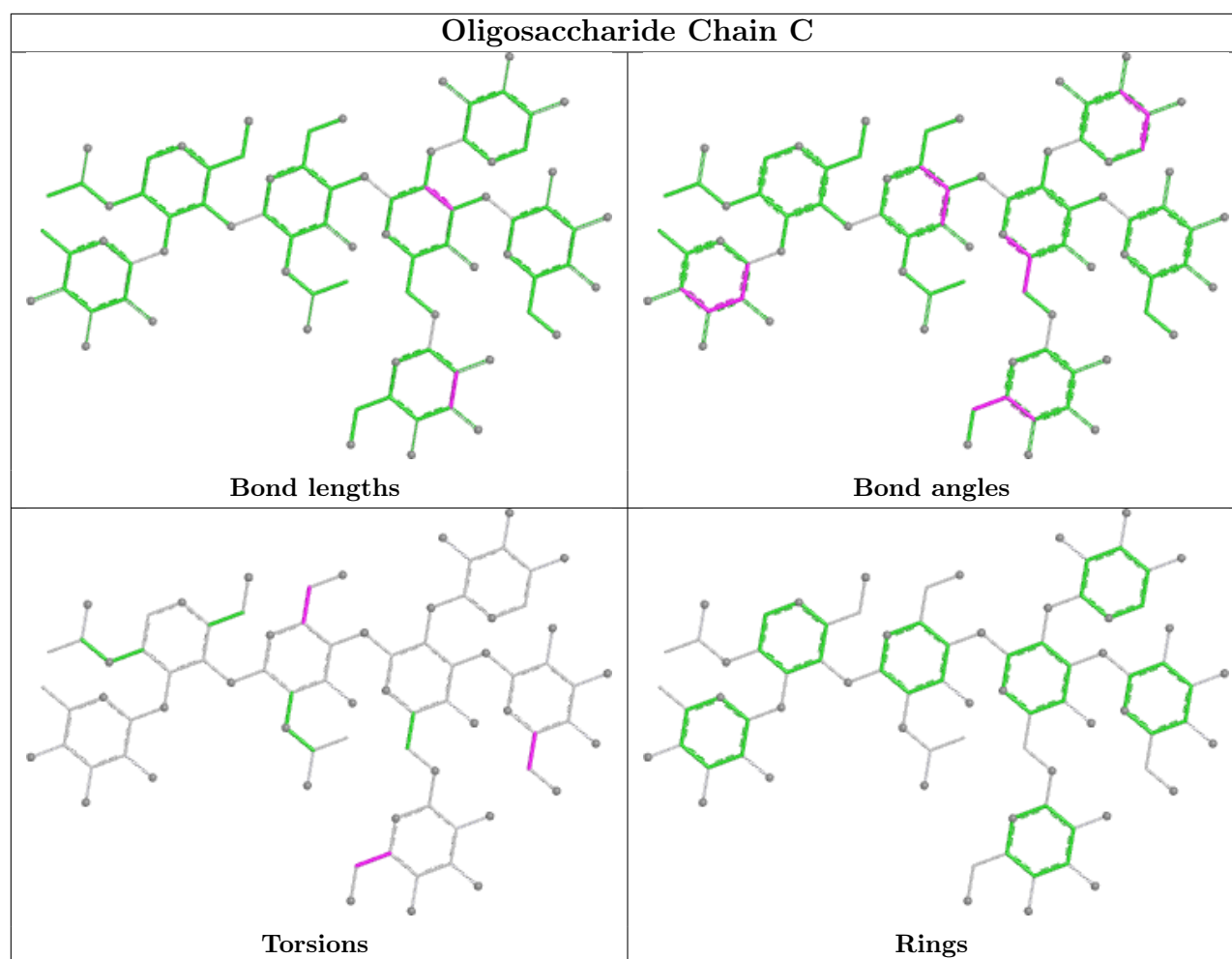
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	6	MAN	9	0
4	C	3	BMA	5	0
2	D	2	NAG	1	0
2	D	1	NAG	1	0
4	C	7	FUC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	SO4	M	1004	-	4,4,4	0.30	0	6,6,6	0.32	0
8	GOL	M	1020	-	5,5,5	0.45	0	5,5,5	0.71	0
7	SO4	M	1009	-	4,4,4	0.42	0	6,6,6	0.20	0
8	GOL	M	1023	-	5,5,5	0.40	0	5,5,5	0.40	0
7	SO4	M	1003	-	4,4,4	0.28	0	6,6,6	0.13	0
7	SO4	M	1007	-	4,4,4	0.20	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	991	1	14,14,15	0.83	0	17,19,21	0.89	1 (5%)
8	GOL	M	1021	-	5,5,5	0.36	0	5,5,5	0.23	0
5	NAG	M	961	1	14,14,15	0.89	0	17,19,21	0.91	1 (5%)
5	NAG	M	911	1	14,14,15	0.81	0	17,19,21	0.68	0
7	SO4	M	1008	-	4,4,4	0.32	0	6,6,6	0.12	0
8	GOL	M	1024	-	5,5,5	0.61	0	5,5,5	0.31	0
7	SO4	M	1005	-	4,4,4	0.31	0	6,6,6	0.21	0
7	SO4	M	1002	-	4,4,4	0.39	0	6,6,6	0.17	0
5	NAG	M	901	1	14,14,15	0.66	0	17,19,21	0.86	0
5	NAG	M	971	1	14,14,15	1.34	2 (14%)	17,19,21	0.61	0
7	SO4	M	1006	-	4,4,4	0.41	0	6,6,6	0.21	0
8	GOL	M	1010	-	5,5,5	0.15	0	5,5,5	0.51	0
5	NAG	M	931	1	14,14,15	0.71	0	17,19,21	1.21	1 (5%)

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	1024	-	-	0/4/4/4	-
8	GOL	M	1010	-	-	4/4/4/4	-
8	GOL	M	1020	-	-	0/4/4/4	-
5	NAG	M	901	1	-	0/6/23/26	0/1/1/1
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	-	2/6/23/26	0/1/1/1
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
5	NAG	M	971	1	-	2/6/23/26	0/1/1/1
5	NAG	M	931	1	-	2/6/23/26	0/1/1/1
8	GOL	M	1023	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	971	NAG	C1-C2	3.16	1.56	1.52
5	M	971	NAG	C4-C5	2.60	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	931	NAG	C2-N2-C7	3.61	127.74	122.90
5	M	991	NAG	C4-C3-C2	-2.74	107.01	111.02
5	M	961	NAG	C8-C7-N2	-2.21	112.45	116.12

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	1010	GOL	O1-C1-C2-C3
5	M	971	NAG	C4-C5-C6-O6
5	M	931	NAG	C8-C7-N2-C2
5	M	931	NAG	O7-C7-N2-C2
5	M	971	NAG	O5-C5-C6-O6
8	M	1010	GOL	O1-C1-C2-O2
8	M	1010	GOL	C1-C2-C3-O3
5	M	961	NAG	C4-C5-C6-O6
5	M	961	NAG	O5-C5-C6-O6
8	M	1010	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1009	SO4	1	0
5	M	961	NAG	3	0
8	M	1024	GOL	1	0
5	M	901	NAG	2	0
5	M	931	NAG	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%)	2.47	334 (66%) 0 0	23, 36, 48, 77	54 (10%)

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	23	SER	6.0
1	M	150	ASP	5.7
1	M	364	GLY	5.6
1	M	374	ASP	5.0
1	M	53	GLY	4.9
1	M	138	THR	4.9
1	M	345	THR	4.8
1	M	84	ASP	4.8
1	M	55	THR	4.7
1	M	378	SER	4.6
1	M	390	TYR	4.6
1	M	62[A]	SER	4.6
1	M	212	PRO	4.6
1	M	154	GLY	4.6
1	M	418	GLU	4.5
1	M	43	THR	4.5
1	M	137	VAL	4.4
1	M	326	GLY	4.4
1	M	18	ASP	4.4
1	M	36	SER	4.4
1	M	363[A]	SER	4.3
1	M	449[A]	VAL	4.3
1	M	301	ASP	4.3
1	M	461	ASP	4.2
1	M	491	SER	4.2
1	M	201	ASP	4.2
1	M	469	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	143	ASP	4.1
1	M	112	GLY	4.1
1	M	335	ALA	4.1
1	M	404	LEU	4.1
1	M	27	SER	4.0
1	M	128	LEU	4.0
1	M	304	GLY	3.9
1	M	305[A]	GLU	3.9
1	M	12	PHE	3.9
1	M	28	ASP	3.9
1	M	87	ASP	3.9
1	M	223	PRO	3.9
1	M	441	ASN	3.9
1	M	450	ASN	3.9
1	M	253	GLY	3.9
1	M	420	ARG	3.8
1	M	480	TRP	3.8
1	M	365	HIS	3.8
1	M	458	ALA	3.8
1	M	245	TYR	3.8
1	M	149	GLN	3.8
1	M	206	CYS	3.8
1	M	42	GLY	3.8
1	M	388	GLY	3.8
1	M	196	TYR	3.8
1	M	377	ASP	3.8
1	M	97	SER	3.7
1	M	101[A]	SER	3.7
1	M	423	SER	3.7
1	M	349	ALA	3.7
1	M	275	THR	3.7
1	M	164	PHE	3.7
1	M	370	LEU	3.7
1	M	262	LEU	3.7
1	M	268	ASP	3.7
1	M	13	THR	3.6
1	M	311	SER	3.6
1	M	45	GLY	3.6
1	M	482	ASN	3.6
1	M	376	ALA	3.6
1	M	52	ASP	3.6
1	M	166	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	318	VAL	3.6
1	M	33	VAL	3.5
1	M	330	TYR	3.5
1	M	50	ILE	3.5
1	M	263	PRO	3.5
1	M	167	TYR	3.5
1	M	338[A]	SER	3.5
1	M	209	THR	3.5
1	M	329	TYR	3.5
1	M	313	GLU	3.4
1	M	17	THR	3.4
1	M	414	THR	3.4
1	M	213[A]	SER	3.4
1	M	21	ASN	3.4
1	M	497	THR	3.4
1	M	132	GLY	3.4
1	M	99	ALA	3.4
1	M	334	TYR	3.4
1	M	3	GLU	3.4
1	M	410	ASN	3.4
1	M	37	ALA	3.4
1	M	152	TYR	3.4
1	M	432	TYR	3.4
1	M	9	ASN	3.4
1	M	5	THR	3.4
1	M	89	LEU	3.4
1	M	208	PRO	3.4
1	M	67	GLY	3.4
1	M	249	GLY	3.4
1	M	151	GLU	3.4
1	M	142	TRP	3.3
1	M	71	THR	3.3
1	M	63	GLY	3.3
1	M	492	GLY	3.3
1	M	409	GLU	3.3
1	M	70	ASP	3.3
1	M	274	ALA	3.3
1	M	375	LYS	3.3
1	M	238	VAL	3.3
1	M	359	TYR	3.2
1	M	444	ILE	3.2
1	M	57	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	11	PRO	3.2
1	M	49	ASN	3.2
1	M	197	GLY	3.2
1	M	474	GLY	3.2
1	M	391	SER	3.1
1	M	426	ASP	3.1
1	M	10	LEU	3.1
1	M	80	GLN	3.1
1	M	439	PHE	3.1
1	M	93	GLY	3.1
1	M	171	CYS	3.1
1	M	494	TRP	3.1
1	M	90	ASN	3.1
1	M	419	ASN	3.1
1	M	221	THR	3.1
1	M	470	THR	3.1
1	M	183	LEU	3.1
1	M	293	GLY	3.1
1	M	427	TYR	3.0
1	M	224	TYR	3.0
1	M	145	PRO	3.0
1	M	265	ASN	3.0
1	M	346	ASN	3.0
1	M	489	LYS	3.0
1	M	100	TRP	3.0
1	M	235	ALA	3.0
1	M	264	TYR	3.0
1	M	296	PRO	3.0
1	M	75	SER	3.0
1	M	85	VAL	2.9
1	M	382	ILE	2.9
1	M	218	ASN	2.9
1	M	298	ILE	2.9
1	M	300	ILE	2.9
1	M	184	THR	2.9
1	M	181	TYR	2.9
1	M	383	TYR	2.9
1	M	160	ILE	2.9
1	M	257	ILE	2.9
1	M	226	VAL	2.9
1	M	240	LEU	2.9
1	M	79	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	239	ASP	2.9
1	M	396	PHE	2.9
1	M	424	MET	2.9
1	M	252	ILE	2.9
1	M	64	PRO	2.9
1	M	20[A]	LEU	2.9
1	M	96	PHE	2.9
1	M	381	ASN	2.8
1	M	448	ASP	2.8
1	M	462[A]	ASN	2.8
1	M	34	ALA	2.8
1	M	327	LEU	2.8
1	M	399	LYS	2.8
1	M	126[A]	SER	2.8
1	M	443	VAL	2.8
1	M	352	ASP	2.8
1	M	465	PHE	2.8
1	M	457	TRP	2.8
1	M	58	TYR	2.8
1	M	366[A]	TYR	2.7
1	M	106	ARG	2.7
1	M	73	CYS	2.7
1	M	214	CYS	2.7
1	M	25	PHE	2.7
1	M	129	ILE	2.7
1	M	430	ILE	2.7
1	M	403	PRO	2.7
1	M	51	TRP	2.7
1	M	215	TYR	2.7
1	M	219	SER	2.7
1	M	22	SER	2.7
1	M	179	VAL	2.7
1	M	317	LEU	2.7
1	M	341	PRO	2.7
1	M	415	PRO	2.7
1	M	194	ARG	2.7
1	M	351	MET	2.7
1	M	141	HIS	2.7
1	M	162	ASP	2.6
1	M	195	GLY	2.6
1	M	192	PRO	2.6
1	M	174	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	120	TYR	2.6
1	M	147	THR	2.6
1	M	463	TYR	2.6
1	M	180	LYS	2.6
1	M	54	PHE	2.6
1	M	140	PHE	2.6
1	M	478	ILE	2.6
1	M	362	ALA	2.6
1	M	229	HIS	2.6
1	M	395	TYR	2.6
1	M	485	ASP	2.6
1	M	360[A]	ILE	2.6
1	M	499	ILE	2.6
1	M	207	SER	2.6
1	M	65	ASP	2.6
1	M	118[A]	ILE	2.6
1	M	56	HIS	2.6
1	M	108	LYS	2.6
1	M	400	TYR	2.6
1	M	312	PRO	2.5
1	M	380	ASP	2.5
1	M	468	GLY	2.5
1	M	172	PHE	2.5
1	M	347	HIS	2.5
1	M	353	ALA	2.5
1	M	284	GLY	2.5
1	M	98	ILE	2.5
1	M	258	THR	2.5
1	M	38	TYR	2.5
1	M	69	GLY	2.5
1	M	113	VAL	2.5
1	M	92	THR	2.5
1	M	320	GLY	2.5
1	M	44	ILE	2.5
1	M	331	PHE	2.5
1	M	421	ASN	2.5
1	M	271[A]	SER	2.5
1	M	308	PRO	2.4
1	M	339	PRO	2.4
1	M	241	TYR	2.4
1	M	406	TYR	2.4
1	M	156	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	290	LEU	2.4
1	M	19	ALA	2.4
1	M	59	PRO	2.4
1	M	127	GLY	2.4
1	M	169[A]	ASP	2.4
1	M	266	ASP	2.4
1	M	386	PRO	2.4
1	M	103	ILE	2.4
1	M	200	LEU	2.4
1	M	191	VAL	2.4
1	M	124	LEU	2.4
1	M	385	TYR	2.4
1	M	498	PHE	2.4
1	M	481	ASN	2.4
1	M	294	THR	2.3
1	M	83	ILE	2.3
1	M	389	ILE	2.3
1	M	437	LEU	2.3
1	M	46	ARG	2.3
1	M	368	GLY	2.3
1	M	416	GLY	2.3
1	M	486	ARG	2.3
1	M	434	CYS	2.3
1	M	473	PHE	2.3
1	M	490	LYS	2.3
1	M	121	TYR	2.3
1	M	16	ASN	2.3
1	M	182	TRP	2.3
1	M	228	HIS	2.3
1	M	225	ILE	2.3
1	M	405	ILE	2.3
1	M	74	ASP	2.3
1	M	323	ASP	2.3
1	M	429	ARG	2.3
1	M	32	GLY	2.3
1	M	159	GLN	2.3
1	M	283	LEU	2.3
1	M	357	LEU	2.3
1	M	130	LYS	2.3
1	M	276	GLU	2.3
1	M	259	ARG	2.3
1	M	144	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	397	LYS	2.2
1	M	433	LEU	2.2
1	M	471	VAL	2.2
1	M	459	LEU	2.2
1	M	157	ASP	2.2
1	M	322	TYR	2.2
1	M	495	TYR	2.2
1	M	47	GLY	2.2
1	M	117	GLY	2.2
1	M	204	GLY	2.2
1	M	178	SER	2.2
1	M	260	TRP	2.2
1	M	328	ASN	2.2
1	M	4	ILE	2.2
1	M	30[A]	ILE	2.2
1	M	153	GLU	2.2
1	M	394	ASP	2.2
1	M	203	PRO	2.2
1	M	369	PRO	2.2
1	M	91	ALA	2.1
1	M	202	ALA	2.1
1	M	48	LEU	2.1
1	M	123	GLY	2.1
1	M	332	THR	2.1
1	M	350	MET	2.1
1	M	496	GLN	2.1
1	M	361	ASN	2.1
1	M	217	GLY	2.1
1	M	8	GLU	2.1
1	M	277	ARG	2.1
1	M	177	ASP	2.1
1	M	261	PHE	2.1
1	M	104	ILE	2.1
1	M	356	LYS	2.1
1	M	198	SER	2.1
1	M	231	LEU	2.1
1	M	250	GLY	2.1
1	M	161	ILE	2.1
1	M	384	TYR	2.1
1	M	105	PRO	2.1
1	M	122	HIS	2.1
1	M	136	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	168	ALA	2.0
1	M	68	ASN	2.0
1	M	232	LEU	2.0
1	M	343	ASN	2.0
1	M	280	GLU	2.0
1	M	288	GLY	2.0
1	M	40	ILE	2.0
1	M	428	THR	2.0
1	M	135	PRO	2.0
1	M	371	PHE	2.0
1	M	447	LYS	2.0
1	M	337	PRO	2.0
1	M	78	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

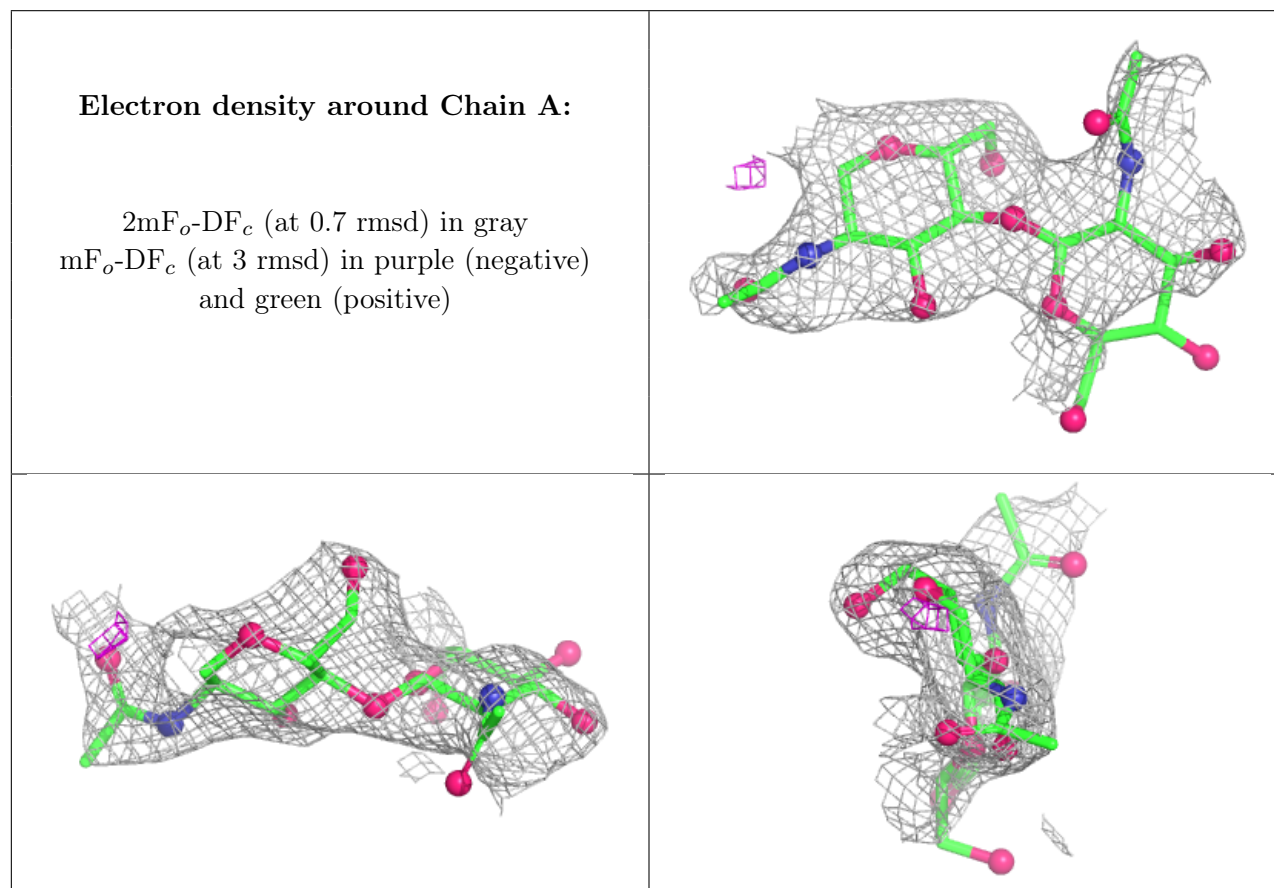
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	40,45,53,58	0
2	NAG	A	2	14/15	-	-	58,66,78,81	0
4	BMA	C	3	11/12	0.46	0.21	47,52,57,68	0
4	XYP	C	4	9/10	0.49	0.14	54,59,65,85	0
3	NAG	B	2	14/15	0.52	0.19	42,48,54,59	0
4	NAG	C	2	14/15	0.63	0.16	41,44,49,53	0
3	BMA	B	3	11/12	-	-	59,64,70,74	0
3	XYP	B	4	9/10	-	-	63,69,73,75	0
3	FUC	B	5	10/11	-	-	45,53,60,69	0
4	NAG	C	1	14/15	0.66	0.19	38,41,47,50	0
3	NAG	B	1	14/15	0.72	0.14	36,43,48,48	0
2	NAG	D	1	14/15	0.72	0.15	30,38,42,44	0
2	NAG	D	2	14/15	0.77	0.12	47,52,71,78	0
4	MAN	C	5	11/12	-	-	46,60,73,77	0
4	MAN	C	6	11/12	-	-	54,64,76,76	0

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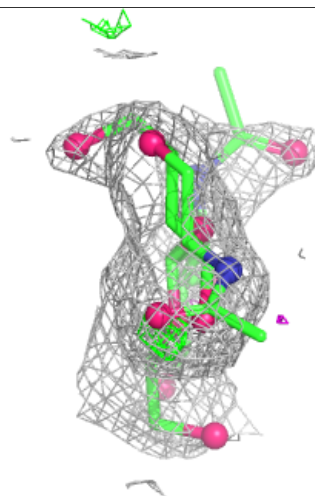
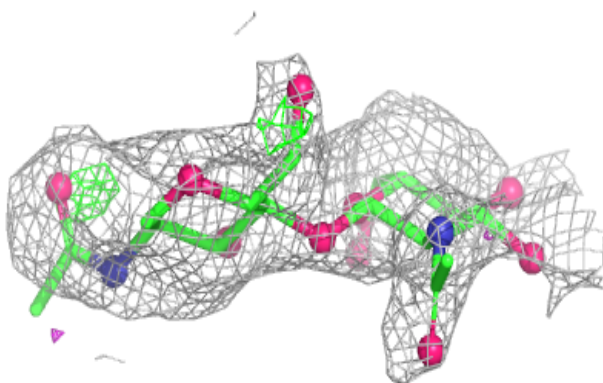
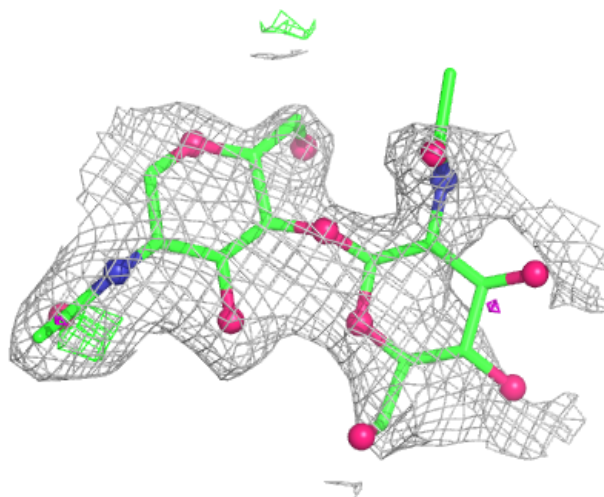
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FUC	C	7	10/11	-	-	40,43,54,54	0

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.



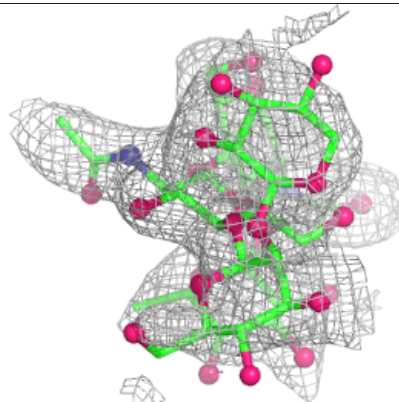
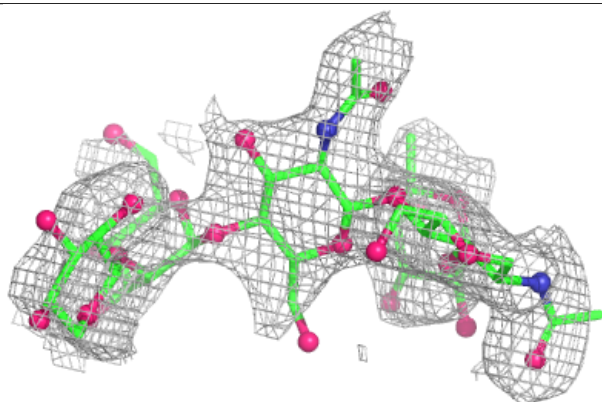
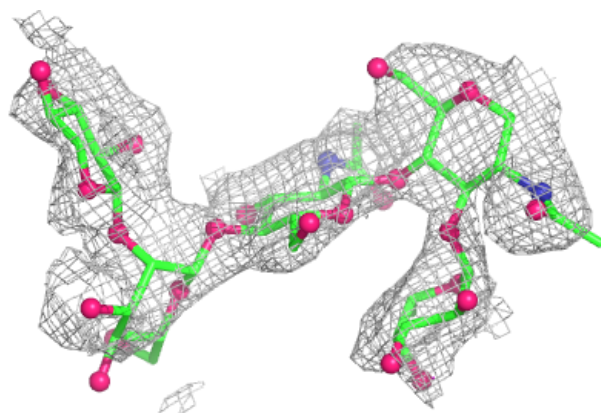
Electron density around Chain D:

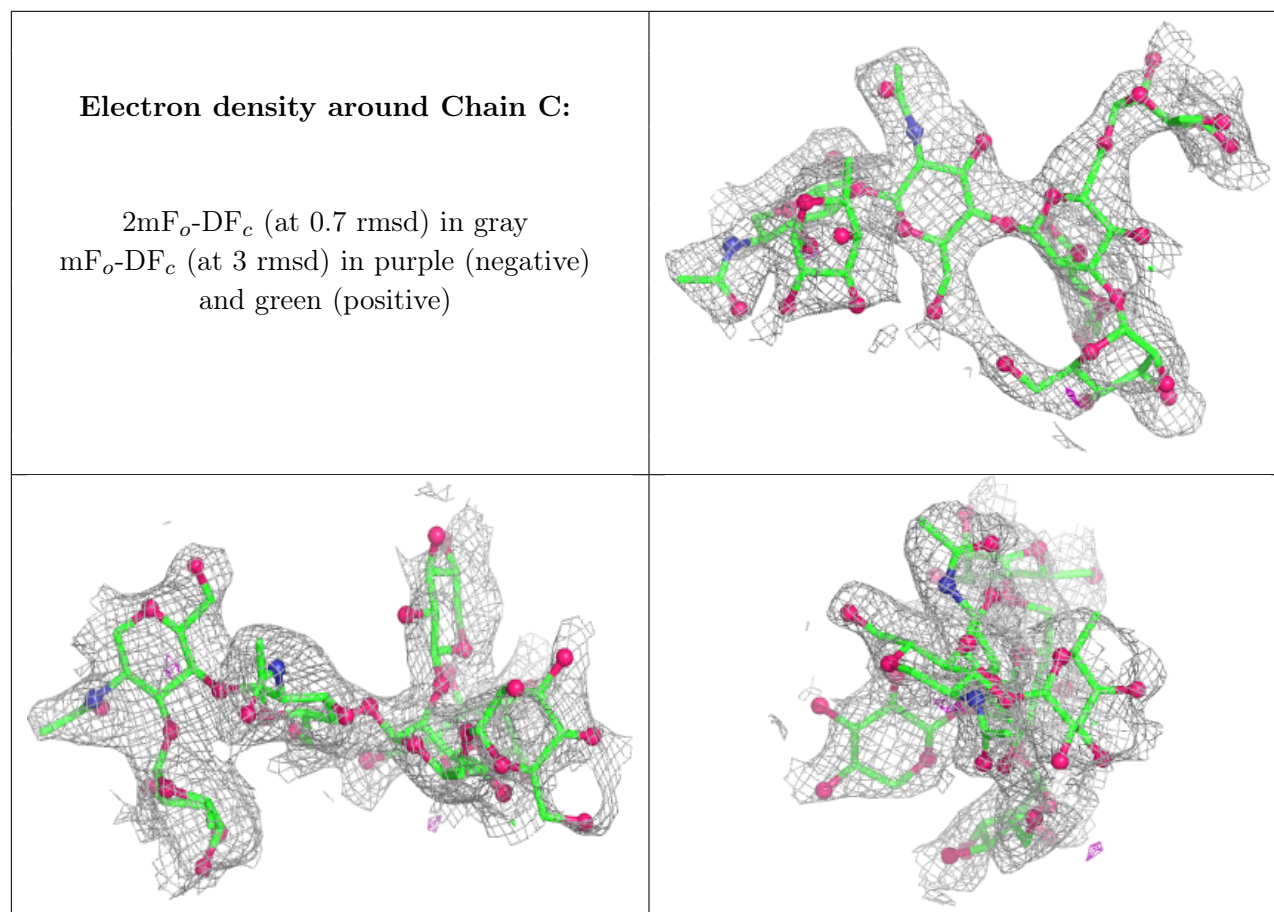
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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
7	SO4	M	1009	5/5	0.29	0.34	59,61,67,80	1
5	NAG	M	971	14/15	0.45	0.23	77,85,91,91	0
8	GOL	M	1020	6/6	0.47	0.22	27,35,39,39	1
5	NAG	M	991	14/15	0.48	0.24	56,61,74,77	0
5	NAG	M	961	14/15	0.49	0.19	64,71,83,89	0
8	GOL	M	1010	6/6	0.50	0.23	57,63,65,72	6
8	GOL	M	1023	6/6	0.50	0.40	52,53,64,66	6
5	NAG	M	931	14/15	0.53	0.20	56,63,70,70	0
7	SO4	M	1007	5/5	0.54	0.17	34,54,55,58	5
5	NAG	M	901	14/15	0.57	0.18	46,56,67,69	0
8	GOL	M	1021	6/6	0.57	0.17	32,42,47,52	6
7	SO4	M	1008	5/5	0.57	0.26	54,57,59,60	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	M	1002	5/5	0.61	0.24	47,50,53,58	5
5	NAG	M	911	14/15	0.61	0.15	46,49,57,66	0
7	SO4	M	1005	5/5	0.62	0.21	39,42,48,50	0
7	SO4	M	1003	5/5	0.62	0.21	46,49,57,57	5
8	GOL	M	1024	6/6	0.67	0.15	37,38,43,43	0
7	SO4	M	1004	5/5	0.78	0.19	35,49,51,56	5
7	SO4	M	1006	5/5	0.80	0.18	47,52,55,56	5
6	ZN	M	1001	1/1	0.89	0.16	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.