



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:59 AM UTC

PDB ID : 1E70 / pdb_00001e70
Title : 2-F-glucosylated MYROSINASE FROM SINAPIS ALBA
Authors : Burmeister, W.P.
Deposited on : 2000-08-23
Resolution : 1.65 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

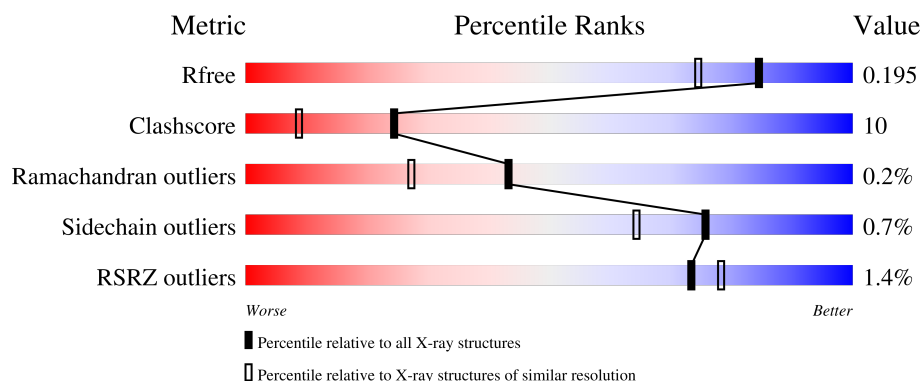
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	501	76% 22% .
2	A	2	50% 50%
3	B	5	60% 40%
4	C	6	50% 50%

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	3	X	-	-	-
5	NAG	M	961	X	-	-	-
5	NAG	M	991	X	-	-	-
8	SO4	M	1505	-	-	X	-
8	SO4	M	1510	-	-	X	-
9	GOL	M	1513	-	X	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5196 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.

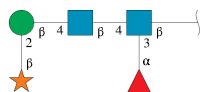
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	22	0
			4086	2622	660	788	16			

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



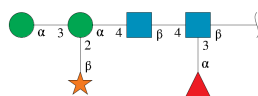
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



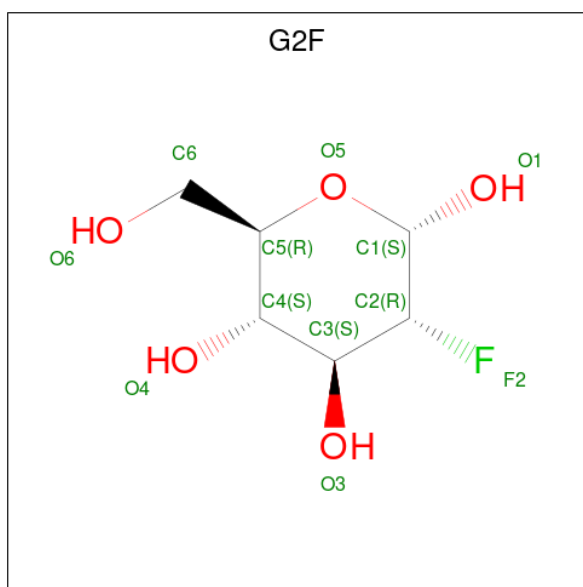
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	6	Total	C	N	O	0	0	0
			69	39	2	28			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
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 2-deoxy-2-fluoro-alpha-D-glucopyranose (CCD ID: G2F) (formula: $C_6H_{11}FO_5$).

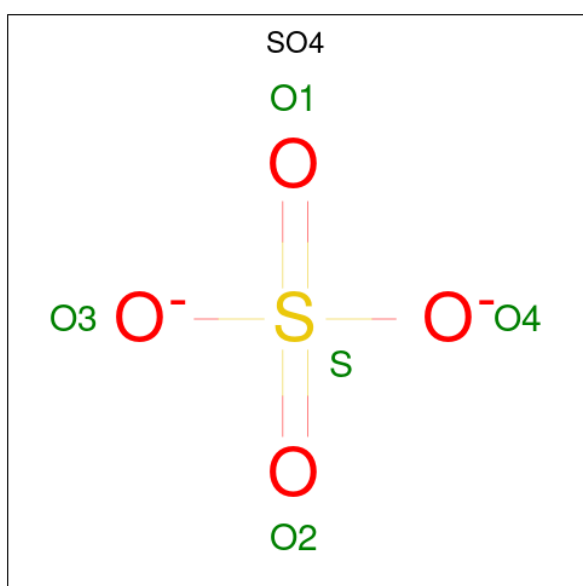


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	F	O	0	0
			11	6	1	4		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

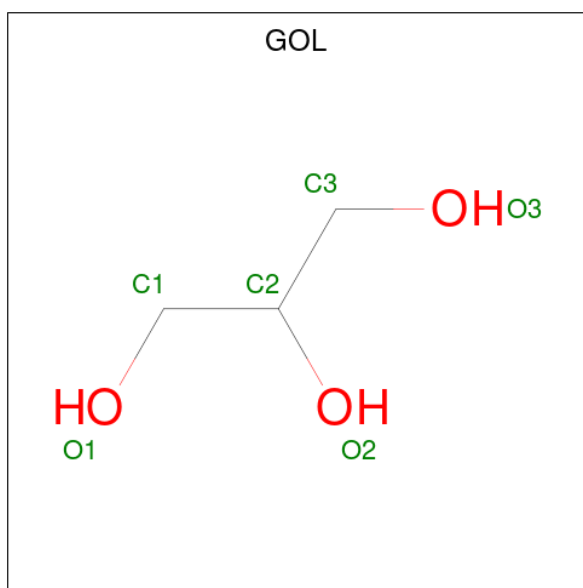
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Zn	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 7 3 4	0	1
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0

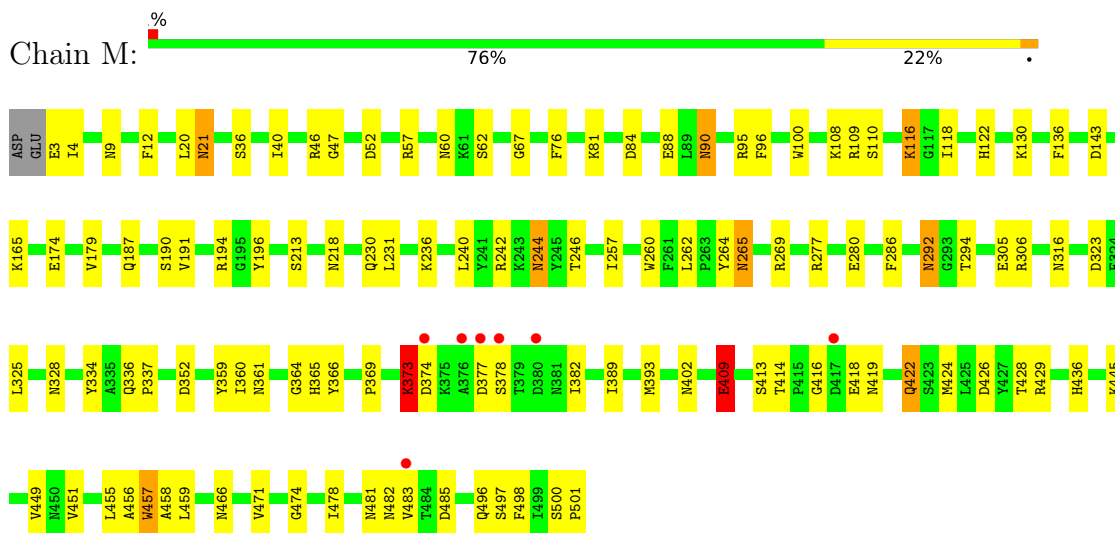
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	794	Total 794	O 794	0	0

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 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



- Molecule 4: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]alpha-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



MAG1
MAG2
MAN3
XYF4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	135.30Å 137.20Å 80.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65 10.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	82.3 (10.00-1.65) 81.8 (10.00-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.195 0.177 , 0.195	Depositor DCC
R_{free} test set	3755 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5196	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, SO4, ZN, GOL, NAG, MAN, G2F, XYP, 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	0.94	3/4299 (0.1%)	1.77	94/5845 (1.6%)

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	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	501	PRO	N-CD	5.53	1.55	1.47
1	M	426	ASP	CG-OD2	5.39	1.35	1.25
1	M	500	SER	C-O	-5.01	1.18	1.24

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	457	TRP	CA-C-O	-11.25	107.86	121.36
1	M	9	ASN	CA-CB-CG	10.85	123.45	112.60
1	M	457	TRP	O-C-N	-10.16	111.68	123.06
1	M	482	ASN	CA-CB-CG	-9.32	103.28	112.60
1	M	361	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	M	213[A]	SER	CA-C-O	-9.11	108.34	119.18
1	M	213[B]	SER	CA-C-O	-9.11	108.34	119.18
1	M	190	SER	N-CA-C	8.89	120.75	111.14
1	M	60	ASN	OD1-CG-ND2	-8.59	114.01	122.60
1	M	109	ARG	NH1-CZ-NH2	8.40	130.22	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	90	ASN	OD1-CG-ND2	-8.37	114.23	122.60
1	M	280	GLU	O-C-N	-8.30	113.13	122.09
1	M	90	ASN	CB-CG-OD1	8.20	137.20	120.80
1	M	482	ASN	CB-CG-OD1	8.19	137.18	120.80
1	M	482	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	M	292	ASN	CA-CB-CG	-7.90	104.70	112.60
1	M	458	ALA	N-CA-C	7.40	121.89	110.42
1	M	109	ARG	NE-CZ-NH2	-7.30	112.63	119.20
1	M	316	ASN	OD1-CG-ND2	7.12	129.72	122.60
1	M	426	ASP	O-C-N	-6.84	113.24	122.68
1	M	286	PHE	CA-CB-CG	-6.76	107.04	113.80
1	M	21	ASN	CA-CB-CG	-6.72	105.88	112.60
1	M	478	ILE	CB-CG1-CD1	6.70	127.86	113.80
1	M	100	TRP	O-C-N	-6.66	115.16	122.09
1	M	500	SER	O-C-N	6.57	127.28	121.37
1	M	428	THR	O-C-N	6.56	130.34	122.27
1	M	414	THR	O-C-N	-6.38	116.32	121.80
1	M	474	GLY	N-CA-C	6.37	120.35	112.14
1	M	179	VAL	O-C-N	6.23	130.54	122.94
1	M	374	ASP	CA-CB-CG	6.12	118.72	112.60
1	M	294	THR	CA-C-O	-6.11	113.98	121.06
1	M	456	ALA	O-C-N	6.10	129.86	122.96
1	M	426	ASP	CB-CG-OD1	6.10	132.43	118.40
1	M	402	ASN	CA-C-O	6.09	125.17	120.48
1	M	179	VAL	CA-C-O	-6.07	113.55	120.65
1	M	426	ASP	N-CA-CB	-6.05	102.82	110.45
1	M	457	TRP	N-CA-CB	6.05	120.27	110.41
1	M	196	TYR	O-C-N	6.00	128.76	122.23
1	M	191	VAL	CA-C-O	5.98	122.70	118.69
1	M	231	LEU	O-C-N	5.90	128.37	122.12
1	M	265	ASN	CA-CB-CG	-5.86	106.75	112.60
1	M	57	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	M	466	ASN	OD1-CG-ND2	5.84	128.44	122.60
1	M	36	SER	O-C-N	-5.80	116.54	123.27
1	M	57	ARG	NH1-CZ-NH2	5.79	126.83	119.30
1	M	496	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	M	230	GLN	O-C-N	-5.73	116.17	122.07
1	M	483	VAL	N-CA-C	5.72	121.24	109.34
1	M	213[A]	SER	O-C-N	5.65	130.43	122.41
1	M	213[B]	SER	O-C-N	5.65	130.43	122.41
1	M	373	LYS	CB-CA-C	5.63	118.83	109.53
1	M	323	ASP	CA-C-O	5.60	125.74	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	426	ASP	CA-C-O	5.60	130.72	122.38
1	M	361	ASN	CB-CG-OD1	5.57	131.95	120.80
1	M	482	ASN	CB-CG-ND2	-5.56	108.06	116.40
1	M	265	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	M	76	PHE	CA-CB-CG	-5.54	108.26	113.80
1	M	485	ASP	CA-CB-CG	5.53	118.13	112.60
1	M	292	ASN	N-CA-CB	-5.50	103.72	110.98
1	M	52	ASP	N-CA-C	-5.49	105.21	111.14
1	M	40	ILE	N-CA-C	5.49	118.91	113.53
1	M	369	PRO	CA-C-O	5.45	129.06	122.08
1	M	352	ASP	O-C-N	-5.41	115.89	122.22
1	M	46	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	M	422	GLN	O-C-N	5.38	127.83	122.12
1	M	369	PRO	O-C-N	-5.37	116.44	123.00
1	M	409[A]	GLU	CB-CG-CD	5.34	121.68	112.60
1	M	409[B]	GLU	CB-CG-CD	5.34	121.68	112.60
1	M	416	GLY	N-CA-C	-5.34	107.70	114.16
1	M	496	GLN	CG-CD-NE2	5.31	124.36	116.40
1	M	436	HIS	CA-CB-CG	-5.30	108.50	113.80
1	M	20[A]	LEU	CA-C-O	5.28	126.64	120.20
1	M	20[B]	LEU	CA-C-O	5.28	126.64	120.20
1	M	90	ASN	CB-CG-ND2	-5.28	108.48	116.40
1	M	306	ARG	CD-NE-CZ	5.25	131.75	124.40
1	M	143	ASP	CA-CB-CG	5.23	117.83	112.60
1	M	481	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	M	257	ILE	N-CA-C	-5.22	101.07	108.58
1	M	294	THR	O-C-N	5.21	129.32	123.27
1	M	325	LEU	O-C-N	5.21	129.50	123.30
1	M	96	PHE	CA-C-N	-5.16	114.71	122.81
1	M	96	PHE	C-N-CA	-5.16	114.71	122.81
1	M	242	ARG	CD-NE-CZ	5.14	131.60	124.40
1	M	429	ARG	O-C-N	-5.13	115.56	122.23
1	M	12	PHE	CA-CB-CG	-5.12	108.68	113.80
1	M	497	SER	CA-CB-OG	-5.12	100.87	111.10
1	M	264	TYR	CA-C-O	5.11	126.15	120.63
1	M	244	ASN	CA-CB-CG	-5.11	107.50	112.60
1	M	316	ASN	CB-CG-ND2	-5.10	108.75	116.40
1	M	419	ASN	CA-CB-CG	5.08	117.68	112.60
1	M	277	ARG	N-CA-CB	5.07	117.57	110.12
1	M	100	TRP	CA-C-O	5.05	126.31	120.90
1	M	47	GLY	O-C-N	5.03	127.13	122.81
1	M	457	TRP	N-CA-C	-5.02	102.34	110.32

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	409[A]	GLU	Sidechain
1	M	409[B]	GLU	Sidechain
1	M	457	TRP	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	4086	0	3841	68	0
2	A	28	0	25	4	0
3	B	58	0	42	4	0
4	C	69	0	49	6	0
5	M	84	0	77	8	0
6	M	11	0	9	2	0
7	M	1	0	0	0	0
8	M	40	0	0	3	0
9	M	25	0	30	2	0
10	M	794	0	0	18	0
All	All	5196	0	4073	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (78) 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:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.24	1.70
1:M:21:ASN:HD21	5:M:901:NAG:C1	1.00	1.63
1:M:292:ASN:HD21	4:C:1:NAG:C1	1.00	1.62
1:M:265:ASN:HD21	3:B:1:NAG:C1	0.97	1.61
1:M:90:ASN:HD21	5:M:911:NAG:C1	0.97	1.58
1:M:218:ASN:HD21	2:A:1:NAG:C1	0.94	1.55
1:M:244:ASN:HD21	5:M:931:NAG:C1	1.00	1.52
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	1.91	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE1	1.54	1.39
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE1	2.19	1.18
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE1	2.30	1.14
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.43	1.14
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD1	1.88	1.07
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	1.98	0.94
1:M:246:THR:HG22	10:M:2392:HOH:O	1.69	0.90
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE1	2.01	0.87
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	2.10	0.83
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD1	2.63	0.74
1:M:165:LYS:NZ	5:M:931:NAG:H82	2.02	0.74
1:M:130:LYS:HG3	10:M:2253:HOH:O	1.89	0.72
1:M:165:LYS:HZ2	5:M:931:NAG:H82	1.55	0.71
1:M:130:LYS:HB3	10:M:2264:HOH:O	1.92	0.69
1:M:409[B]:GLU:CD	6:M:999:G2F:C1	2.66	0.68
10:M:2741:HOH:O	4:C:3:MAN:C4	2.43	0.66
10:M:2741:HOH:O	4:C:3:MAN:C5	2.42	0.66
1:M:218:ASN:HD21	2:A:1:NAG:C2	2.00	0.63
1:M:95:ARG:HB2	1:M:455:LEU:HD13	1.83	0.61
1:M:118[B]:ILE:HD12	1:M:174:GLU:HG3	1.81	0.61
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.36	0.61
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CE2	2.35	0.61
1:M:449[B]:VAL:HG23	1:M:451:VAL:HG23	1.84	0.60
10:M:2741:HOH:O	4:C:3:MAN:C6	2.50	0.60
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE2	2.76	0.59
1:M:108:LYS:HE3	1:M:110:SER:OG	2.04	0.57
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.87	0.56
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE1	2.35	0.55
1:M:365:HIS:HE1	10:M:2552:HOH:O	1.89	0.55
1:M:409[A]:GLU:CD	6:M:999:G2F:C1	2.80	0.54
1:M:90:ASN:ND2	5:M:911:NAG:C2	2.66	0.54
1:M:194:ARG:HD2	8:M:1510:SO4:O1	2.10	0.52
1:M:218:ASN:ND2	2:A:1:NAG:C2	2.68	0.52
1:M:122:HIS:HE1	1:M:174:GLU:O	1.93	0.52
5:M:991:NAG:H61	10:M:2682:HOH:O	2.11	0.51
1:M:265:ASN:ND2	3:B:1:NAG:O5	2.41	0.51
1:M:360[A]:ILE:HD11	1:M:364:GLY:HA2	1.91	0.51
1:M:265:ASN:ND2	3:B:1:NAG:C2	2.69	0.50
9:M:1511:GOL:H11	10:M:2786:HOH:O	2.13	0.48
10:M:2453:HOH:O	4:C:5:MAN:H61	2.14	0.48
8:M:1505:SO4:O2	8:M:1510:SO4:O2	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:165:LYS:HD2	1:M:236:LYS:HE3	1.94	0.48
1:M:240:LEU:HA	5:M:931:NAG:H83	1.97	0.47
1:M:373:LYS:NZ	1:M:378:SER:OG	2.42	0.47
1:M:218:ASN:ND2	2:A:1:NAG:O5	2.43	0.47
1:M:418:GLU:HB3	1:M:422:GLN:HB2	1.96	0.46
1:M:292:ASN:ND2	4:C:1:NAG:O5	2.38	0.46
1:M:365:HIS:HD2	10:M:2256:HOH:O	1.98	0.45
1:M:336:GLN:HB2	1:M:337:PRO:HD2	1.98	0.45
1:M:424:MET:HE3	10:M:2695:HOH:O	2.16	0.45
9:M:1511:GOL:H31	10:M:2427:HOH:O	2.16	0.45
1:M:359:TYR:CZ	1:M:382:ILE:HG23	2.52	0.45
1:M:95:ARG:HA	1:M:136:PHE:O	2.17	0.45
10:M:2424:HOH:O	3:B:2:NAG:H82	2.17	0.45
1:M:328:ASN:CG	1:M:409[B]:GLU:HG3	2.43	0.44
1:M:459:LEU:HD23	1:M:459:LEU:C	2.43	0.44
1:M:269:ARG:NH2	10:M:2426:HOH:O	2.51	0.43
1:M:262:LEU:O	1:M:334:TYR:HA	2.18	0.43
1:M:389:ILE:O	1:M:393:MET:HG2	2.19	0.42
1:M:116:LYS:HG2	10:M:2234:HOH:O	2.20	0.42
1:M:21:ASN:HA	1:M:498:PHE:CD2	2.55	0.42
1:M:413:SER:HB2	1:M:471:VAL:HB	2.01	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.50	0.41
1:M:260:TRP:CE3	1:M:260:TRP:HA	2.55	0.41
1:M:84:ASP:O	1:M:88[B]:GLU:HG3	2.20	0.41
1:M:81:LYS:HD2	10:M:2167:HOH:O	2.21	0.41
1:M:377:ASP:HA	10:M:2568:HOH:O	2.20	0.41
8:M:1505:SO4:O1	8:M:1510:SO4:O3	2.38	0.41
1:M:62[B]:SER:OG	1:M:67:GLY:O	2.33	0.40

There are no symmetry-related clashes.

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	519/501 (104%)	503 (97%)	15 (3%)	1 (0%)	43 27

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	457/437 (105%)	454 (99%)	3 (1%)	76 64

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU
1	M	116	LYS
1	M	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	90	ASN
1	M	122	HIS
1	M	146	GLN
1	M	187	GLN
1	M	218	ASN
1	M	230	GLN
1	M	244	ASN
1	M	265	ASN
1	M	292	ASN
1	M	297	GLN
1	M	328	ASN
1	M	365	HIS

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Mol	Chain	Res	Type
1	M	402	ASN
1	M	410	ASN

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 ⓘ

13 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	1.57	4 (28%)	17,19,21	3.36	9 (52%)
2	NAG	A	2	2	14,14,15	1.01	0	17,19,21	2.51	8 (47%)
3	NAG	B	1	3,1	14,14,15	1.21	2 (14%)	17,19,21	4.16	11 (64%)
3	NAG	B	2	3	14,14,15	1.24	2 (14%)	17,19,21	1.54	3 (17%)
3	BMA	B	3	3	11,11,12	1.83	2 (18%)	15,15,17	1.31	2 (13%)
3	XYP	B	4	3	9,9,10	0.79	0	10,12,14	2.70	3 (30%)
3	FUC	B	5	3	10,10,11	1.49	2 (20%)	14,14,16	1.85	6 (42%)
4	NAG	C	1	4,1	14,14,15	1.24	1 (7%)	17,19,21	2.89	5 (29%)
4	NAG	C	2	4	14,14,15	1.48	2 (14%)	17,19,21	2.41	6 (35%)
4	MAN	C	3	4	11,11,12	1.95	3 (27%)	15,15,17	6.21	10 (66%)
4	XYP	C	4	4	9,9,10	1.34	1 (11%)	10,12,14	3.59	5 (50%)
4	MAN	C	5	4	11,11,12	1.21	2 (18%)	15,15,17	1.80	5 (33%)
4	FUC	C	6	4	10,10,11	1.72	3 (30%)	14,14,16	2.25	7 (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
2	NAG	A	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	A	2	2	-	1/6/23/26	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	MAN	C	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	FUC	C	6	4	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	MAN	C2-C3	-4.47	1.45	1.52
3	B	3	BMA	C2-C3	-4.12	1.46	1.52
4	C	6	FUC	C2-C3	3.60	1.58	1.52
4	C	3	MAN	O5-C1	3.49	1.49	1.43
3	B	3	BMA	C4-C5	3.24	1.59	1.53
4	C	2	NAG	C1-C2	3.17	1.56	1.52
2	A	1	NAG	O5-C5	3.04	1.49	1.43
3	B	1	NAG	C3-C2	3.03	1.58	1.52
4	C	2	NAG	C3-C2	-2.91	1.46	1.52
4	C	1	NAG	O5-C5	2.88	1.49	1.43
4	C	3	MAN	O3-C3	2.57	1.49	1.43
2	A	1	NAG	C3-C2	2.55	1.57	1.52
3	B	2	NAG	O7-C7	2.47	1.28	1.23
4	C	6	FUC	C6-C5	2.42	1.57	1.51
4	C	5	MAN	O5-C5	2.36	1.48	1.43
3	B	2	NAG	C1-C2	2.35	1.55	1.52
2	A	1	NAG	C8-C7	2.31	1.55	1.50
3	B	5	FUC	C2-C3	2.30	1.56	1.52
3	B	1	NAG	O5-C5	2.27	1.47	1.43
2	A	1	NAG	O7-C7	-2.16	1.18	1.23
4	C	5	MAN	C4-C3	2.15	1.57	1.52
4	C	6	FUC	O2-C2	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	FUC	C6-C5	2.06	1.56	1.51
4	C	4	XYP	C2-C3	2.01	1.55	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	MAN	C6-C5-C4	12.49	143.68	113.02
4	C	3	MAN	O4-C4-C5	10.04	134.06	109.32
4	C	3	MAN	C1-O5-C5	-9.69	99.20	112.19
2	A	1	NAG	C1-O5-C5	-8.53	100.75	112.19
4	C	3	MAN	C3-C4-C5	8.25	125.19	110.23
4	C	1	NAG	O5-C1-C2	8.18	123.95	111.29
3	B	1	NAG	C8-C7-N2	-7.93	102.97	116.12
3	B	1	NAG	C1-O5-C5	-7.73	101.83	112.19
4	C	3	MAN	O5-C5-C6	-7.44	93.19	107.66
3	B	1	NAG	C2-N2-C7	-6.98	113.55	122.90
4	C	4	XYP	C4-C3-C2	-6.56	103.13	110.92
4	C	4	XYP	O3-C3-C4	6.42	123.16	110.05
3	B	4	XYP	C1-C2-C3	6.37	118.91	109.64
3	B	1	NAG	C4-C3-C2	-6.27	101.83	111.02
2	A	2	NAG	C1-O5-C5	-6.21	103.87	112.19
2	A	1	NAG	C8-C7-N2	-5.92	106.31	116.12
4	C	3	MAN	O4-C4-C3	-5.66	97.03	110.38
4	C	3	MAN	C2-C3-C4	-5.57	101.07	110.86
4	C	1	NAG	C1-O5-C5	-5.54	104.76	112.19
3	B	1	NAG	O7-C7-N2	5.39	131.50	121.98
4	C	2	NAG	O4-C4-C5	-5.08	96.81	109.32
2	A	1	NAG	O7-C7-N2	5.07	130.94	121.98
3	B	4	XYP	O2-C2-C3	-4.81	100.19	110.15
4	C	6	FUC	C1-C2-C3	-4.77	102.70	109.64
4	C	2	NAG	O4-C4-C3	-4.72	99.25	110.38
4	C	3	MAN	O2-C2-C3	-4.38	101.09	110.15
4	C	4	XYP	O4-C4-C3	3.88	118.19	110.15
2	A	2	NAG	O5-C5-C4	-3.87	101.40	110.83
3	B	1	NAG	C1-C2-N2	-3.77	104.48	110.43
4	C	1	NAG	C8-C7-N2	-3.74	109.91	116.12
4	C	6	FUC	C6-C5-C4	-3.72	106.28	113.08
4	C	2	NAG	C2-N2-C7	-3.65	118.01	122.90
3	B	2	NAG	O7-C7-N2	-3.54	115.73	121.98
4	C	4	XYP	O4-C4-C5	3.43	117.08	109.22
4	C	5	MAN	O2-C2-C3	-3.41	103.08	110.15
2	A	1	NAG	C2-N2-C7	-3.41	118.33	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	O5-C1-C2	3.36	116.49	111.29
4	C	4	XYP	O2-C2-C3	-3.35	103.21	110.15
2	A	1	NAG	C1-C2-N2	-3.30	105.23	110.43
4	C	3	MAN	O3-C3-C2	-3.21	103.50	110.05
3	B	5	FUC	C6-C5-C4	-3.19	107.25	113.08
3	B	1	NAG	O5-C5-C4	-3.14	103.18	110.83
2	A	1	NAG	C4-C3-C2	-3.14	106.42	111.02
3	B	5	FUC	O3-C3-C2	-2.98	103.96	110.05
4	C	6	FUC	O3-C3-C2	-2.98	103.97	110.05
4	C	2	NAG	C8-C7-N2	-2.97	111.19	116.12
4	C	2	NAG	O5-C5-C4	-2.86	103.86	110.83
2	A	2	NAG	O5-C5-C6	-2.85	102.11	107.66
3	B	1	NAG	O3-C3-C2	-2.83	103.52	109.40
4	C	5	MAN	C2-C3-C4	-2.82	105.91	110.86
4	C	3	MAN	C1-C2-C3	-2.80	105.57	109.64
2	A	1	NAG	O4-C4-C3	-2.79	103.81	110.38
2	A	2	NAG	O3-C3-C2	-2.72	103.76	109.40
4	C	2	NAG	O5-C1-C2	-2.68	107.14	111.29
4	C	1	NAG	O5-C5-C6	-2.62	102.57	107.66
2	A	1	NAG	O3-C3-C2	-2.60	104.00	109.40
2	A	1	NAG	O4-C4-C5	-2.55	103.04	109.32
3	B	5	FUC	O2-C2-C3	-2.53	104.90	110.15
4	C	1	NAG	C3-C4-C5	2.51	114.78	110.23
4	C	5	MAN	C1-C2-C3	2.46	113.22	109.64
4	C	6	FUC	O3-C3-C4	-2.44	104.63	110.38
4	C	5	MAN	O2-C2-C1	-2.37	103.80	109.22
2	A	2	NAG	O6-C6-C5	-2.36	103.29	111.33
3	B	1	NAG	C6-C5-C4	2.35	118.79	113.02
2	A	2	NAG	C6-C5-C4	-2.34	107.28	113.02
4	C	6	FUC	C1-O5-C5	2.30	118.39	112.97
3	B	3	BMA	O2-C2-C1	2.30	114.48	109.22
3	B	5	FUC	O4-C4-C5	-2.29	104.68	109.74
3	B	4	XYP	O3-C3-C4	2.27	114.69	110.05
2	A	2	NAG	C8-C7-N2	-2.27	112.36	116.12
3	B	3	BMA	C1-O5-C5	-2.25	109.17	112.19
3	B	5	FUC	O5-C5-C6	-2.23	102.57	107.40
3	B	1	NAG	O4-C4-C3	-2.22	105.15	110.38
3	B	1	NAG	C3-C4-C5	2.19	114.20	110.23
3	B	5	FUC	C1-C2-C3	-2.18	106.47	109.64
3	B	2	NAG	O5-C5-C6	-2.17	103.43	107.66
4	C	6	FUC	O2-C2-C1	-2.17	104.27	109.22
3	B	2	NAG	O7-C7-C8	-2.16	118.21	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	6	FUC	O2-C2-C3	-2.12	105.77	110.15
4	C	5	MAN	C3-C4-C5	-2.06	106.50	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	3	MAN	C1

All (3) torsion outliers are listed below:

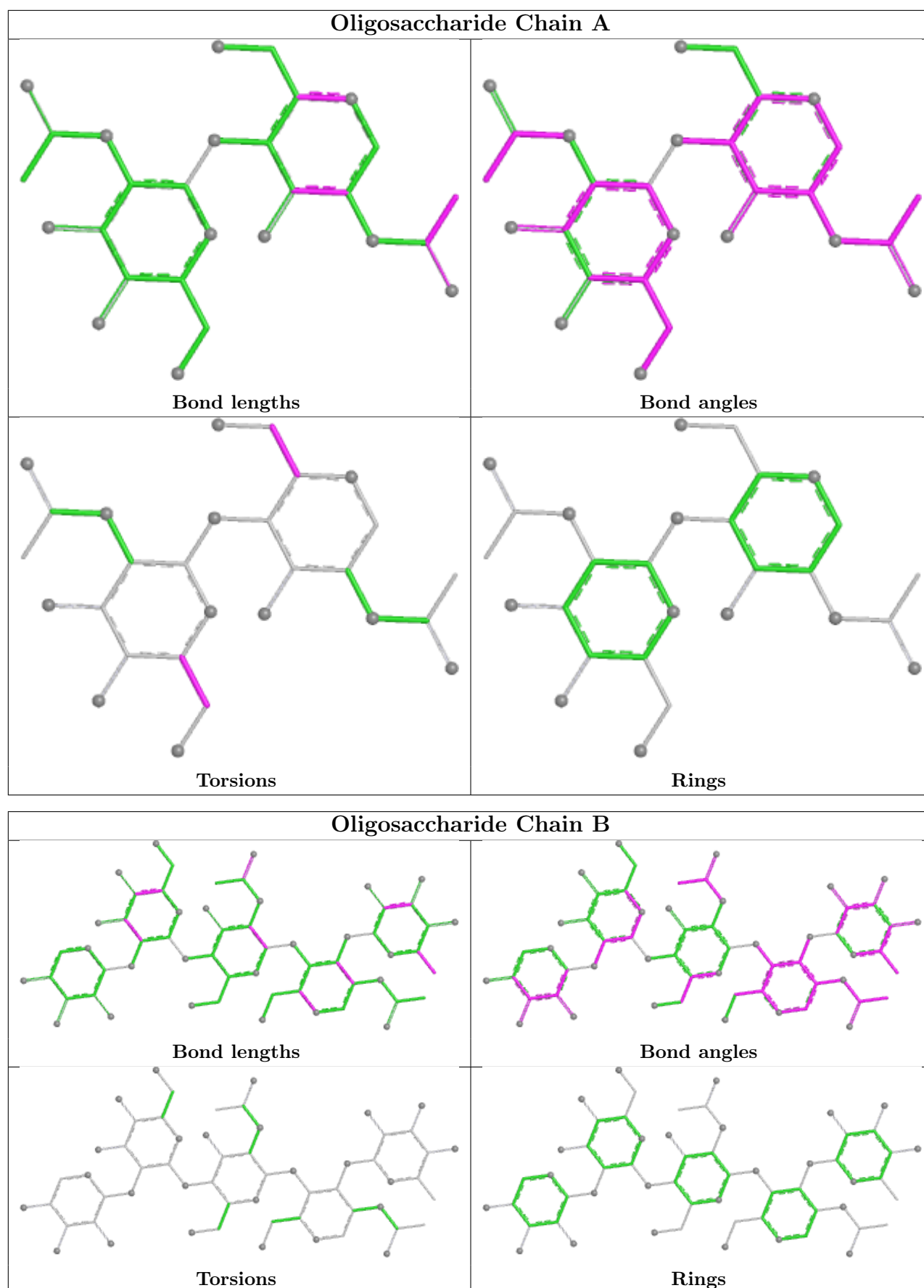
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

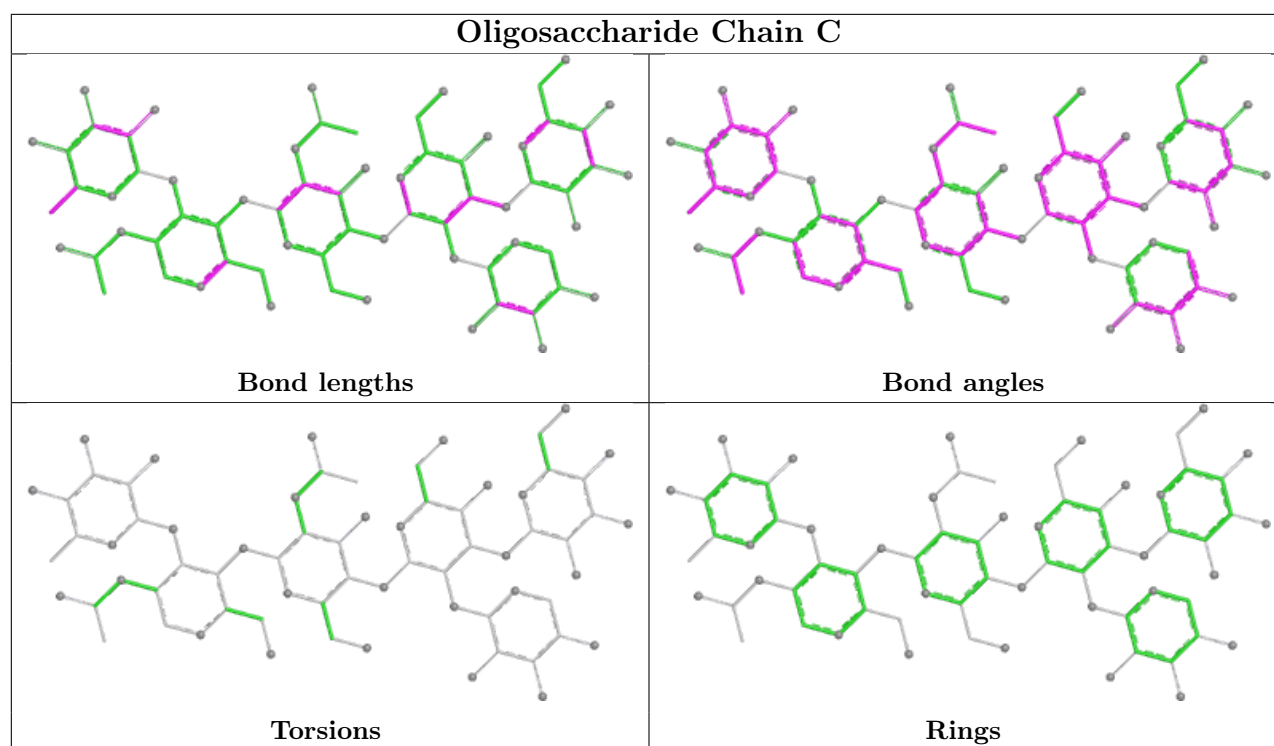
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	4	0
3	B	2	NAG	1	0
3	B	1	NAG	3	0
4	C	5	MAN	1	0
4	C	1	NAG	2	0
4	C	3	MAN	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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SO4	M	1503	-	4,4,4	0.56	0	6,6,6	0.36	0
9	GOL	M	1512[B]	-	5,5,5	0.75	0	5,5,5	2.23	2 (40%)
5	NAG	M	911	1	14,14,15	1.20	1 (7%)	17,19,21	1.99	5 (29%)
8	SO4	M	1507	-	4,4,4	0.83	0	6,6,6	1.32	1 (16%)
8	SO4	M	1510	-	4,4,4	0.61	0	6,6,6	0.40	0
5	NAG	M	971	1	14,14,15	1.35	1 (7%)	17,19,21	1.37	2 (11%)
9	GOL	M	1511	-	5,5,5	0.33	0	5,5,5	0.57	0
8	SO4	M	1508	-	4,4,4	0.81	0	6,6,6	0.67	0
5	NAG	M	931	1	14,14,15	1.73	2 (14%)	17,19,21	8.14	10 (58%)
8	SO4	M	1506	-	4,4,4	0.55	0	6,6,6	1.42	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	M	1509	-	4,4,4	0.70	0	6,6,6	0.22	0
8	SO4	M	1505	-	4,4,4	0.68	0	6,6,6	0.33	0
9	GOL	M	1514	-	5,5,5	0.26	0	5,5,5	0.84	0
5	NAG	M	961	1	14,14,15	1.50	2 (14%)	17,19,21	2.51	5 (29%)
9	GOL	M	1513	-	5,5,5	4.09	4 (80%)	5,5,5	2.61	3 (60%)
5	NAG	M	991	1	14,14,15	1.32	1 (7%)	17,19,21	1.96	6 (35%)
5	NAG	M	901	1	14,14,15	1.09	1 (7%)	17,19,21	1.65	5 (29%)
9	GOL	M	1512[A]	-	5,5,5	0.77	0	5,5,5	1.90	1 (20%)
8	SO4	M	1504	-	4,4,4	0.67	0	6,6,6	0.30	0
6	G2F	M	999	-	11,11,12	1.86	2 (18%)	12,15,17	4.15	6 (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
9	GOL	M	1514	-	-	1/4/4/4	-
5	NAG	M	961	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	M	971	1	-	2/6/23/26	0/1/1/1
9	GOL	M	1511	-	-	0/4/4/4	-
9	GOL	M	1513	-	-	3/4/4/4	-
5	NAG	M	991	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	M	901	1	-	2/6/23/26	0/1/1/1
9	GOL	M	1512[A]	-	-	0/4/4/4	-
9	GOL	M	1512[B]	-	-	2/4/4/4	-
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
6	G2F	M	999	-	-	0/2/19/22	0/1/1/1
5	NAG	M	931	1	-	3/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1513	GOL	O2-C2	6.51	1.62	1.43
5	M	931	NAG	O7-C7	-4.43	1.13	1.23
9	M	1513	GOL	O1-C1	4.24	1.60	1.42
5	M	971	NAG	O7-C7	-4.06	1.14	1.23
6	M	999	G2F	C2-C3	4.06	1.57	1.51
5	M	961	NAG	O7-C7	-3.97	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	911	NAG	O7-C7	-3.79	1.14	1.23
9	M	1513	GOL	C1-C2	3.71	1.65	1.51
5	M	991	NAG	O7-C7	-3.65	1.15	1.23
5	M	901	NAG	O7-C7	-3.13	1.16	1.23
9	M	1513	GOL	C3-C2	3.02	1.63	1.51
5	M	961	NAG	C2-N2	2.76	1.50	1.46
5	M	931	NAG	C2-N2	-2.74	1.41	1.46
6	M	999	G2F	O5-C1	2.72	1.48	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	931	NAG	C2-N2-C7	30.76	164.12	122.90
6	M	999	G2F	F2-C2-C1	-10.99	99.61	108.26
5	M	931	NAG	O5-C1-C2	8.72	124.78	111.29
5	M	961	NAG	C1-O5-C5	7.99	122.89	112.19
5	M	931	NAG	O7-C7-N2	-6.54	110.43	121.98
6	M	999	G2F	C1-O5-C5	-5.16	105.27	112.19
5	M	911	NAG	C4-C3-C2	-4.92	103.81	111.02
6	M	999	G2F	C2-C3-C4	-4.29	104.42	109.59
5	M	971	NAG	O5-C1-C2	-4.22	104.76	111.29
5	M	961	NAG	C1-C2-N2	-4.19	103.83	110.43
9	M	1512[A]	GOL	O2-C2-C1	3.99	125.69	109.18
9	M	1512[B]	GOL	O2-C2-C1	3.99	125.69	109.18
5	M	991	NAG	C4-C3-C2	-3.96	105.21	111.02
6	M	999	G2F	O5-C5-C6	-3.91	100.05	107.66
5	M	991	NAG	O5-C1-C2	3.86	117.26	111.29
6	M	999	G2F	C3-C4-C5	-3.83	103.29	110.23
5	M	931	NAG	O7-C7-C8	3.74	128.72	122.05
9	M	1513	GOL	O3-C3-C2	3.73	127.16	110.38
5	M	901	NAG	C1-O5-C5	-3.48	107.52	112.19
5	M	931	NAG	C4-C3-C2	-3.46	105.95	111.02
5	M	901	NAG	O5-C1-C2	3.29	116.38	111.29
5	M	911	NAG	C1-O5-C5	-3.15	107.97	112.19
5	M	991	NAG	C2-N2-C7	-3.11	118.73	122.90
9	M	1513	GOL	C3-C2-C1	2.93	122.56	111.80
5	M	931	NAG	C8-C7-N2	2.85	120.85	116.12
5	M	911	NAG	O3-C3-C2	-2.77	103.66	109.40
9	M	1513	GOL	O1-C1-C2	2.73	122.67	110.38
5	M	901	NAG	C4-C3-C2	-2.69	107.07	111.02
5	M	911	NAG	O5-C5-C4	-2.68	104.32	110.83
9	M	1512[B]	GOL	O1-C1-C2	2.64	122.24	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	991	NAG	C1-O5-C5	2.60	115.66	112.19
5	M	961	NAG	C4-C3-C2	2.47	114.64	111.02
5	M	971	NAG	O5-C5-C4	-2.40	104.98	110.83
5	M	991	NAG	O5-C5-C4	-2.38	105.04	110.83
8	M	1506	SO4	O4-S-O3	-2.36	95.51	108.54
5	M	931	NAG	C1-O5-C5	-2.36	109.02	112.19
5	M	931	NAG	O4-C4-C5	-2.36	103.52	109.32
5	M	931	NAG	C3-C4-C5	2.34	114.48	110.23
5	M	931	NAG	O5-C5-C4	-2.31	105.20	110.83
8	M	1507	SO4	O3-S-O1	2.28	121.49	109.56
5	M	901	NAG	O3-C3-C4	2.16	115.46	110.38
5	M	901	NAG	O3-C3-C2	-2.15	104.93	109.40
5	M	961	NAG	C8-C7-N2	-2.15	112.56	116.12
5	M	911	NAG	C2-N2-C7	2.10	125.71	122.90
5	M	961	NAG	O3-C3-C2	-2.05	105.15	109.40
6	M	999	G2F	C6-C5-C4	2.02	117.99	113.02
5	M	991	NAG	C6-C5-C4	-2.02	108.06	113.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	961	NAG	C1
5	M	991	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	1512[B]	GOL	O1-C1-C2-C3
5	M	971	NAG	O5-C5-C6-O6
5	M	971	NAG	C4-C5-C6-O6
5	M	931	NAG	O5-C5-C6-O6
5	M	901	NAG	C4-C5-C6-O6
5	M	901	NAG	O5-C5-C6-O6
5	M	931	NAG	C4-C5-C6-O6
5	M	991	NAG	O5-C5-C6-O6
9	M	1513	GOL	O1-C1-C2-C3
9	M	1514	GOL	O1-C1-C2-C3
9	M	1512[B]	GOL	O1-C1-C2-O2
9	M	1513	GOL	O1-C1-C2-O2
5	M	931	NAG	C3-C2-N2-C7
5	M	991	NAG	C4-C5-C6-O6
9	M	1513	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	911	NAG	2	0
8	M	1510	SO4	3	0
9	M	1511	GOL	2	0
5	M	931	NAG	4	0
8	M	1505	SO4	2	0
5	M	991	NAG	1	0
5	M	901	NAG	1	0
6	M	999	G2F	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	M	499/501 (99%)	-0.32	7 (1%) 73 78	15, 25, 39, 66	22 (4%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	374	ASP	5.8
1	M	376	ALA	5.5
1	M	378	SER	4.1
1	M	380	ASP	3.2
1	M	417	ASP	3.0
1	M	377	ASP	2.8
1	M	483	VAL	2.1

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.

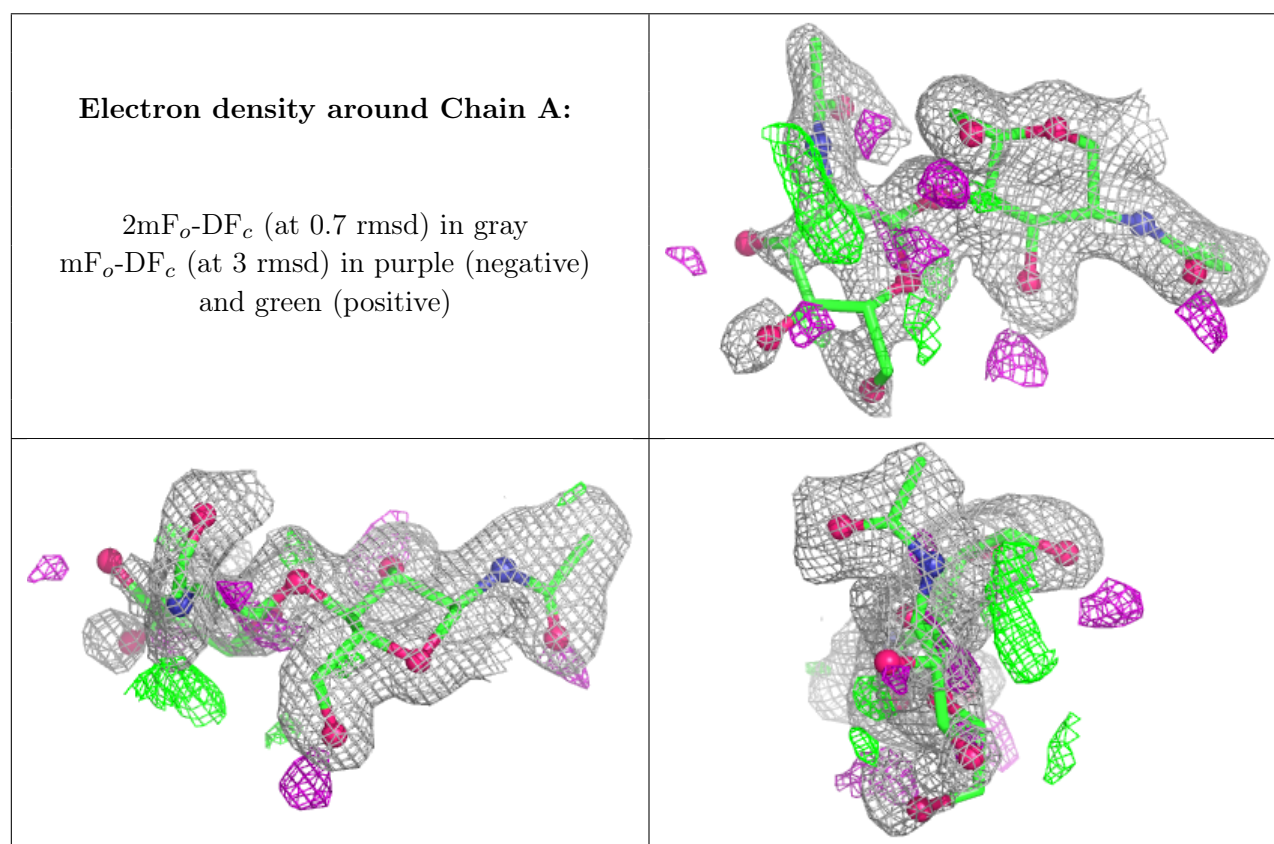
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	29,34,38,42	0
2	NAG	A	2	14/15	-	-	49,52,56,58	0
4	XYP	C	4	9/10	0.67	0.14	56,59,60,62	0
3	NAG	B	2	14/15	0.72	0.13	39,43,48,49	0
3	BMA	B	3	11/12	-	-	53,57,59,59	0

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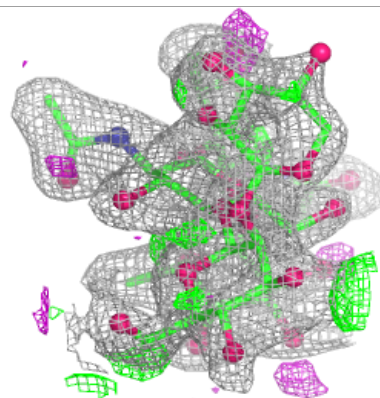
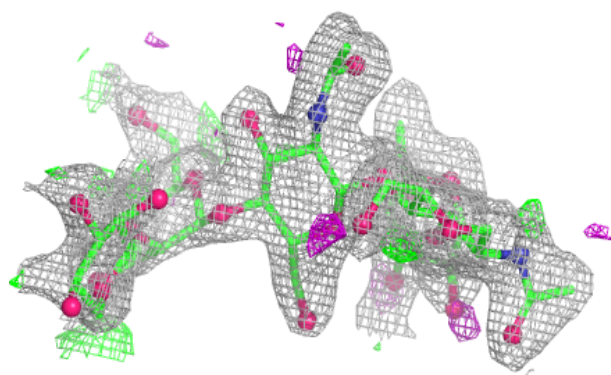
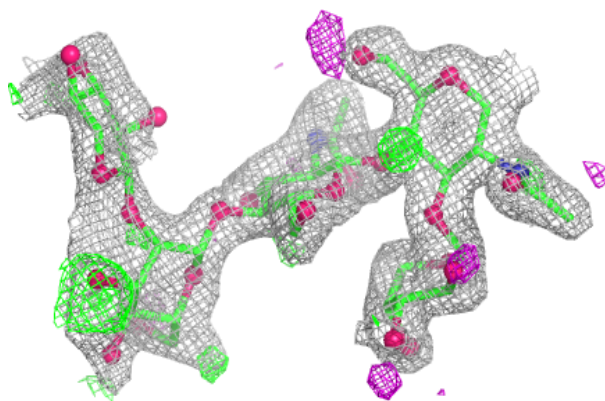
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XYP	B	4	9/10	-	-	59,60,62,62	0
3	FUC	B	5	10/11	-	-	41,43,47,49	0
4	NAG	C	2	14/15	0.85	0.10	34,37,40,42	0
4	NAG	C	1	14/15	0.89	0.08	30,32,35,36	0
4	MAN	C	3	11/12	-	-	44,48,52,54	0
3	NAG	B	1	14/15	0.90	0.09	30,33,36,36	0
4	MAN	C	5	11/12	-	-	42,55,57,57	0
4	FUC	C	6	10/11	-	-	38,39,43,43	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.

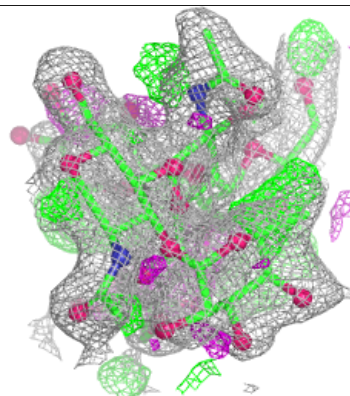
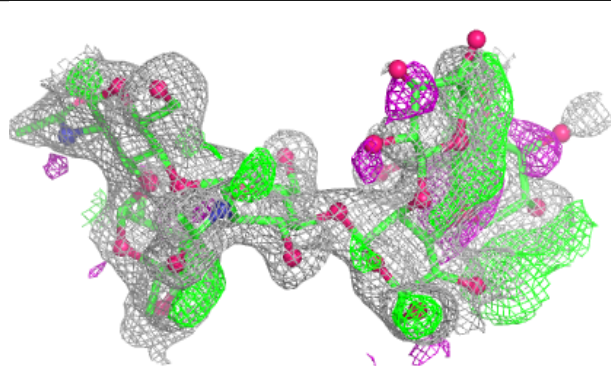
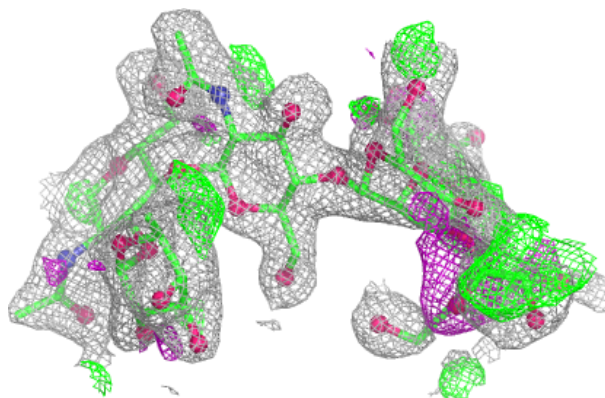


Electron density around Chain B:

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

**Electron density around Chain C:**

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



6.4 Ligands

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
5	NAG	M	991	14/15	0.51	0.15	57,58,63,64	0
5	NAG	M	961	14/15	0.53	0.14	59,63,66,67	0
8	SO4	M	1507	5/5	0.53	0.24	50,52,53,54	5
9	GOL	M	1514	6/6	0.56	0.20	57,59,59,60	6
8	SO4	M	1508	5/5	0.63	0.16	42,46,47,47	5
5	NAG	M	931	14/15	0.64	0.13	53,58,60,60	0
5	NAG	M	971	14/15	0.69	0.14	69,75,76,76	0
8	SO4	M	1505	5/5	0.73	0.17	54,56,56,58	5
9	GOL	M	1511	6/6	0.74	0.20	55,56,56,56	6
8	SO4	M	1510	5/5	0.77	0.24	62,62,63,64	1
8	SO4	M	1509	5/5	0.78	0.18	54,55,55,55	5
5	NAG	M	901	14/15	0.79	0.11	42,45,50,52	0
9	GOL	M	1513	6/6	0.80	0.24	20,26,29,36	0
5	NAG	M	911	14/15	0.86	0.09	36,40,41,45	0
8	SO4	M	1506	5/5	0.91	0.11	35,36,37,40	0
6	G2F	M	999	11/12	0.91	0.07	27,32,35,37	0
9	GOL	M	1512[A]	6/6	0.92	0.08	16,23,28,28	2
9	GOL	M	1512[B]	6/6	0.92	0.08	23,26,28,29	2
8	SO4	M	1504	5/5	0.95	0.07	36,39,41,41	5
8	SO4	M	1503	5/5	0.96	0.08	37,40,41,43	5
7	ZN	M	1502	1/1	0.99	0.02	21,21,21,21	1

6.5 Other polymers

There are no such residues in this entry.