Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2023 – 04:40 am GMT

PDB ID	:	1E73
Title	:	2-F-glucosylated MYROSINASE FROM SINAPIS ALBA with bound L-ascorbate
Authors	:	Burmeister, W.P.
Deposited on	:	2000-08-23
Resolution	:	1.50 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 (i) 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 (i)) were used in the production of this report:

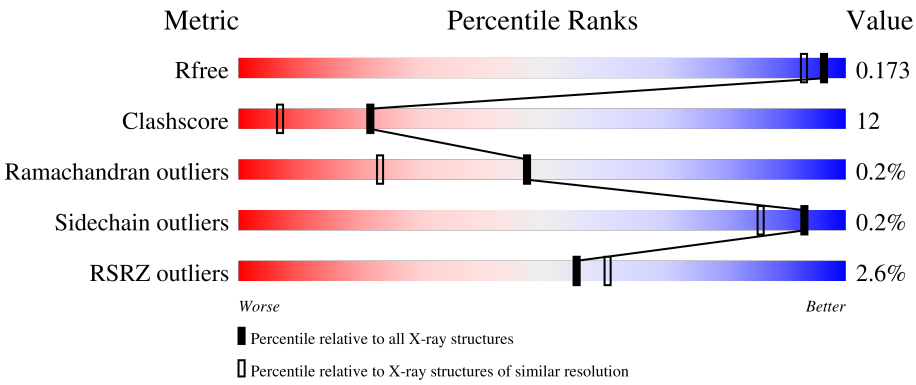
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	3%, 84%, 14%, .
2	A	2	50%, 50%
3	B	5	80%, 20%
4	C	7	57%, 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	BMA	C	3	-	-	X	-
4	MAN	C	6	X	-	X	X
5	NAG	M	961	X	-	-	X
5	NAG	M	971	-	-	-	X
5	NAG	M	991	-	-	-	X
8	SO4	M	1504	-	-	X	-
8	SO4	M	1509	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 5216 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.

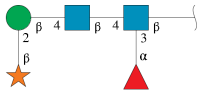
- Molecule 1 is a protein called MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	499	4082	2618	660	788	16	0	21	0

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

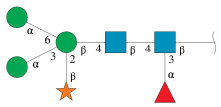
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	2	28	16	2	10	0	0	0

- 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.



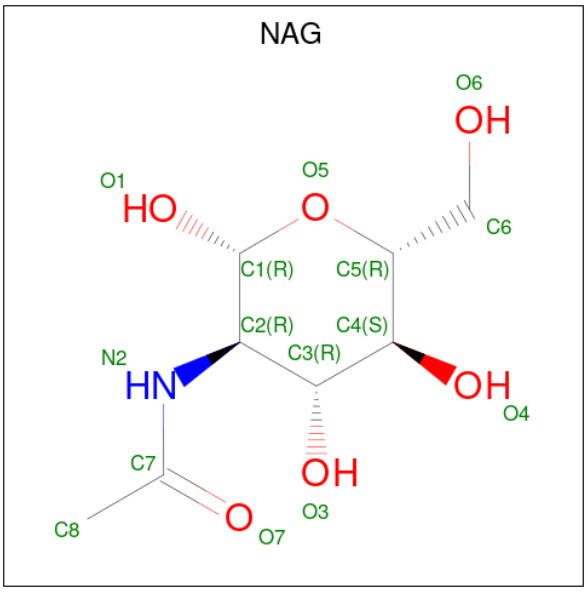
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	5	58	33	2	23	0	0	0

- 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.



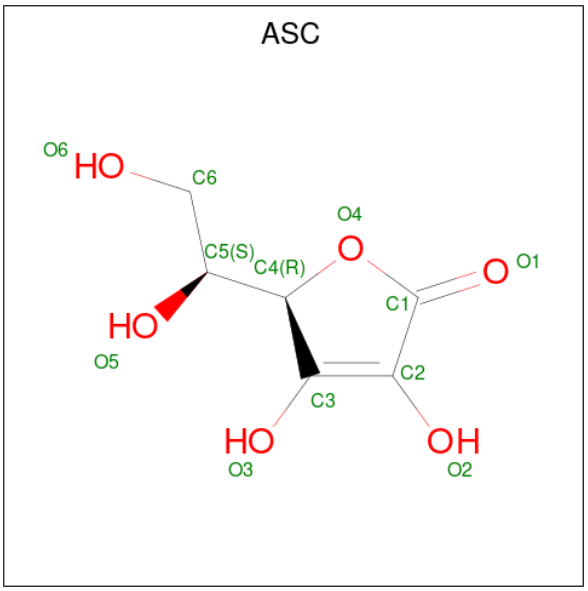
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	C	7	80	45	2	33	0	0	0

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



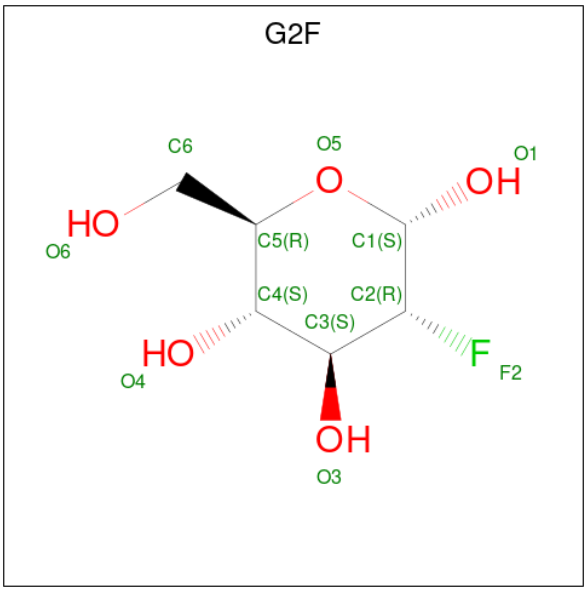
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0
			Total	C	N	O		
5	M	1	14	8	1	5	0	0

- Molecule 6 is ASCORBIC ACID (three-letter code: ASC) (formula: $C_6H_8O_6$).



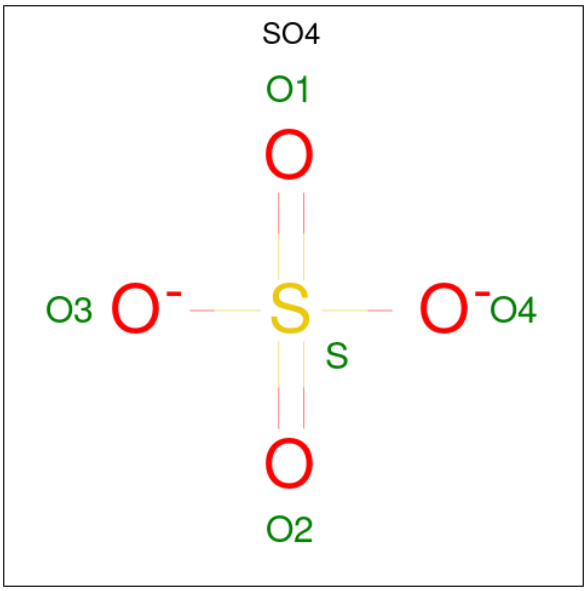
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	M	1	12	6	6	0	0

- Molecule 7 is 2-deoxy-2-fluoro-alpha-D-glucopyranose (three-letter code: G2F) (formula: $C_6H_{11}FO_5$).



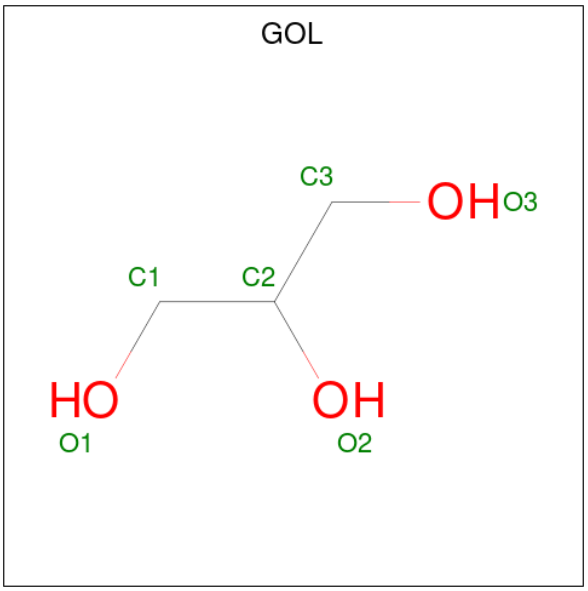
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
7	M	1	11	6	1	4	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is water.

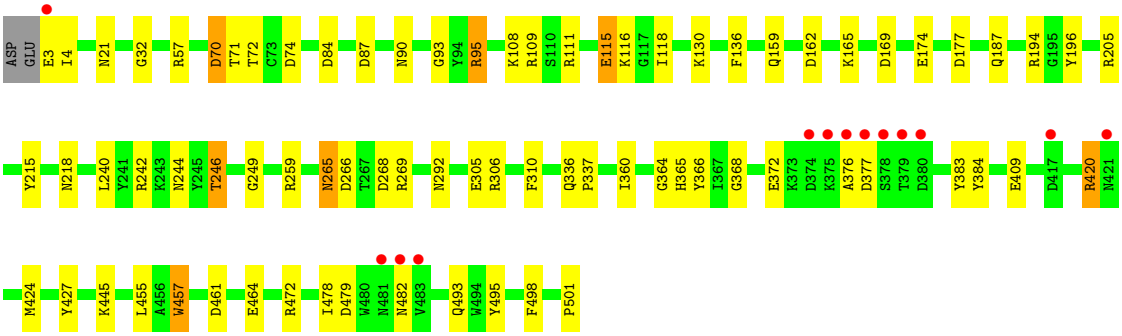
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	M	795	795	795	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYROSINASE MA1

Chain M:

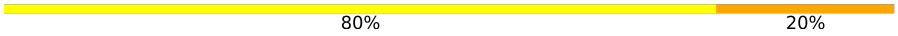


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

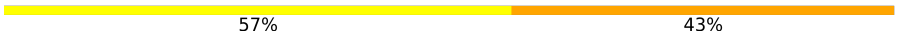
• Molecule 3: beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



• 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:



4 Data and refinement statistics (i)

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 – 1.50 9.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	79.8 (10.00-1.50) 79.8 (9.99-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.134 , 0.167 0.146 , 0.173	Depositor DCC
R_{free} test set	4838 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.50 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, GOL, MAN, NAG, G2F, SO4, ZN, XYP, ASC, 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	0.72	3/4290 (0.1%)	1.35	37/5833 (0.6%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	409	GLU	CD-OE1	6.98	1.33	1.25
1	M	501	PRO	N-CD	6.39	1.56	1.47
1	M	464	GLU	CD-OE1	5.25	1.31	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	109	ARG	NE-CZ-NH2	-17.81	111.40	120.30
1	M	242	ARG	NE-CZ-NH2	-13.79	113.41	120.30
1	M	70	ASP	CB-CG-OD2	-11.61	107.85	118.30
1	M	95	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	M	109	ARG	NH1-CZ-NH2	8.88	129.17	119.40
1	M	383	TYR	CB-CG-CD2	-8.29	116.02	121.00
1	M	269	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	M	482	ASN	CB-CG-OD1	7.71	137.02	121.60
1	M	115	GLU	OE1-CD-OE2	-7.68	114.08	123.30
1	M	420	ARG	CD-NE-CZ	7.67	134.34	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	259	ARG	NE-CZ-NH1	-7.53	116.54	120.30
1	M	74	ASP	CB-CG-OD1	6.98	124.58	118.30
1	M	269	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	M	87	ASP	CB-CG-OD1	6.71	124.33	118.30
1	M	372	GLU	OE1-CD-OE2	-6.69	115.27	123.30
1	M	71	THR	OG1-CB-CG2	-6.68	94.64	110.00
1	M	479	ASP	CB-CG-OD1	6.59	124.23	118.30
1	M	162	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	M	265	ASN	CB-CG-OD1	6.59	134.78	121.60
1	M	57	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	M	482	ASN	CA-CB-CG	-6.30	99.53	113.40
1	M	162	ASP	CB-CG-OD1	6.24	123.92	118.30
1	M	177	ASP	CB-CG-OD1	6.19	123.88	118.30
1	M	427	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	M	215	TYR	CB-CG-CD1	-5.94	117.43	121.00
1	M	495	TYR	CB-CG-CD1	5.92	124.55	121.00
1	M	372	GLU	CG-CD-OE2	5.92	130.13	118.30
1	M	472	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	M	310	PHE	CB-CG-CD1	-5.83	116.72	120.80
1	M	457	TRP	O-C-N	-5.80	113.42	122.70
1	M	84	ASP	CB-CG-OD1	5.76	123.49	118.30
1	M	246	THR	OG1-CB-CG2	-5.67	96.97	110.00
1	M	306	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	M	266	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	M	268	ASP	CB-CG-OD2	5.35	123.12	118.30
1	M	72	THR	CA-CB-CG2	5.30	119.82	112.40
1	M	310	PHE	CB-CG-CD2	5.29	124.51	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	457	TRP	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	4082	0	3835	74	0
2	A	28	0	25	4	0
3	B	58	0	42	4	0
4	C	80	0	57	18	0
5	M	84	0	77	11	0
6	M	12	0	7	1	0
7	M	11	0	9	1	0
8	M	40	0	0	5	0
9	M	25	0	30	2	0
10	M	1	0	0	0	0
11	M	795	0	0	28	0
All	All	5216	0	4082	96	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 12.

All (96) 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	1.30	1.60
1:M:90:ASN:HD21	5:M:911:NAG:C1	0.95	1.60
1:M:244:ASN:HD21	5:M:931:NAG:C1	0.96	1.60
1:M:292:ASN:HD21	4:C:1:NAG:C1	0.94	1.59
1:M:21:ASN:HD21	5:M:901:NAG:C1	0.95	1.57
1:M:265:ASN:HD21	3:B:1:NAG:C1	0.93	1.56
1:M:218:ASN:HD21	2:A:1:NAG:C1	0.92	1.53
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	1.95	1.46
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE1	1.62	1.33
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.30	1.29
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE1	2.22	1.23
11:M:2741:HOH:O	4:C:6:MAN:H61	1.46	1.15
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE1	2.23	1.11
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD1	1.95	1.00
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	1.99	0.99
4:C:3:BMA:C6	4:C:6:MAN:H61	1.92	0.99
4:C:3:BMA:H61	4:C:6:MAN:H61	1.42	0.98
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE1	1.98	0.97
1:M:246:THR:HG22	11:M:2391:HOH:O	1.69	0.91
1:M:165:LYS:NZ	5:M:931:NAG:H82	1.86	0.90
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	2.08	0.88
4:C:3:BMA:H61	4:C:6:MAN:C6	2.04	0.87
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD1	2.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:995:ASC:H4	11:M:2348:HOH:O	1.82	0.79
1:M:377:ASP:HB3	11:M:2567:HOH:O	1.85	0.76
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE1	2.19	0.76
4:C:3:BMA:C6	4:C:6:MAN:C6	2.63	0.75
1:M:265:ASN:HD21	3:B:1:NAG:C2	1.97	0.74
11:M:2751:HOH:O	4:C:6:MAN:H62	1.89	0.72
11:M:2741:HOH:O	4:C:3:BMA:C5	2.38	0.72
11:M:2750:HOH:O	4:C:6:MAN:C5	2.38	0.70
1:M:165:LYS:HZ2	5:M:931:NAG:H82	1.56	0.70
1:M:218:ASN:HD21	2:A:1:NAG:C2	1.97	0.68
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CZ	2.61	0.68
1:M:130:LYS:HG3	11:M:2257:HOH:O	1.93	0.68
1:M:376:ALA:O	1:M:377:ASP:OD1	2.12	0.67
1:M:130:LYS:HB3	11:M:2268:HOH:O	1.96	0.65
8:M:1504:SO4:O2	8:M:1509:SO4:O2	2.14	0.64
1:M:424:MET:HE3	11:M:2695:HOH:O	1.98	0.63
8:M:1504:SO4:S	8:M:1509:SO4:O3	2.58	0.62
1:M:130:LYS:HB3	11:M:2269:HOH:O	1.98	0.62
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.34	0.62
11:M:2741:HOH:O	4:C:3:BMA:C4	2.48	0.62
11:M:2751:HOH:O	4:C:6:MAN:C6	2.48	0.62
1:M:116:LYS:HG2	11:M:2234:HOH:O	2.01	0.60
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.83	0.60
1:M:115:GLU:HG3	11:M:2229:HOH:O	2.02	0.59
1:M:218:ASN:ND2	2:A:1:NAG:C2	2.62	0.59
4:C:3:BMA:O6	4:C:6:MAN:H61	2.03	0.58
11:M:2741:HOH:O	4:C:3:BMA:C6	2.52	0.58
1:M:365:HIS:HE1	11:M:2549:HOH:O	1.85	0.57
1:M:376:ALA:C	1:M:377:ASP:OD1	2.43	0.57
1:M:165:LYS:HZ1	5:M:931:NAG:H82	1.66	0.57
1:M:265:ASN:ND2	3:B:1:NAG:C2	2.62	0.57
1:M:21:ASN:HD21	5:M:901:NAG:C2	2.00	0.56
1:M:365:HIS:HD2	11:M:2258:HOH:O	1.87	0.56
1:M:90:ASN:ND2	5:M:911:NAG:C2	2.64	0.56
1:M:244:ASN:ND2	5:M:931:NAG:O5	2.39	0.55
1:M:292:ASN:ND2	4:C:1:NAG:C2	2.66	0.54
11:M:2741:HOH:O	4:C:6:MAN:C6	2.26	0.53
1:M:265:ASN:ND2	3:B:1:NAG:O5	2.36	0.53
1:M:4:ILE:HD11	1:M:445:LYS:CD	2.40	0.52
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.37	0.51
1:M:95:ARG:HB2	1:M:455:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.94	0.50
9:M:1510:GOL:H11	11:M:2786:HOH:O	2.10	0.50
1:M:218:ASN:ND2	2:A:1:NAG:O5	2.42	0.48
8:M:1504:SO4:O1	8:M:1509:SO4:O3	2.32	0.48
1:M:108:LYS:CE	11:M:2203:HOH:O	2.62	0.47
7:M:999:G2F:H2	11:M:2757:HOH:O	2.14	0.47
1:M:95:ARG:HA	1:M:136:PHE:O	2.15	0.46
8:M:1504:SO4:O2	8:M:1509:SO4:S	2.73	0.46
4:C:3:BMA:H61	4:C:6:MAN:H62	1.91	0.46
1:M:420:ARG:O	1:M:424:MET:HG2	2.16	0.46
1:M:118[B]:ILE:HD12	1:M:174:GLU:HG3	1.97	0.46
1:M:493:GLN:NE2	11:M:2695:HOH:O	2.48	0.45
1:M:249:GLY:HA3	9:M:1512:GOL:H31	1.98	0.45
1:M:108:LYS:HE3	1:M:111:ARG:NH2	2.32	0.45
1:M:115:GLU:CD	11:M:2229:HOH:O	2.56	0.44
1:M:292:ASN:ND2	4:C:1:NAG:O5	2.38	0.44
1:M:194:ARG:NH1	8:M:1509:SO4:O4	2.48	0.44
11:M:2741:HOH:O	4:C:3:BMA:H61	2.18	0.43
1:M:336:GLN:HB2	1:M:337:PRO:HD2	2.01	0.43
1:M:461:ASP:O	1:M:478:ILE:HD12	2.19	0.43
1:M:32:GLY:HA3	1:M:93:GLY:O	2.19	0.42
1:M:360[A]:ILE:HD11	1:M:364:GLY:HA2	2.02	0.42
1:M:21:ASN:ND2	5:M:901:NAG:C2	2.70	0.42
1:M:196:TYR:CE2	1:M:205:ARG:HD3	2.55	0.42
1:M:108:LYS:HE2	11:M:2320:HOH:O	2.19	0.42
1:M:21:ASN:HA	1:M:498:PHE:CD2	2.55	0.41
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:OH	2.05	0.41
1:M:159:GLN:NE2	11:M:2313:HOH:O	2.53	0.41
1:M:368:GLY:HA3	1:M:384:TYR:O	2.21	0.41
1:M:70:ASP:HB3	11:M:2091:HOH:O	2.22	0.40
1:M:165:LYS:CE	5:M:931:NAG:H82	2.50	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	518/501 (103%)	504 (97%)	13 (2%)	1 (0%)	47 23

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	456/437 (104%)	455 (100%)	1 (0%)	93 86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU

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	90	ASN
1	M	218	ASN
1	M	244	ASN
1	M	265	ASN
1	M	292	ASN
1	M	365	HIS

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)

14 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	1.41	3 (21%)	17,19,21	3.00	8 (47%)
2	NAG	A	2	2	14,14,15	1.18	0	17,19,21	3.58	8 (47%)
3	NAG	B	1	3,1	14,14,15	0.89	1 (7%)	17,19,21	2.86	7 (41%)
3	NAG	B	2	3	14,14,15	1.10	1 (7%)	17,19,21	1.31	2 (11%)
3	BMA	B	3	3	11,11,12	2.17	3 (27%)	15,15,17	1.95	4 (26%)
3	XYP	B	4	3	9,9,10	0.90	0	10,12,14	2.24	3 (30%)
3	FUC	B	5	3	10,10,11	1.50	2 (20%)	14,14,16	1.94	3 (21%)
4	NAG	C	1	4,1	14,14,15	1.42	2 (14%)	17,19,21	3.18	9 (52%)
4	NAG	C	2	4	14,14,15	1.56	2 (14%)	17,19,21	2.50	6 (35%)
4	BMA	C	3	4	11,11,12	2.17	2 (18%)	15,15,17	5.99	12 (80%)
4	XYP	C	4	4	9,9,10	1.29	1 (11%)	10,12,14	2.59	4 (40%)
4	MAN	C	5	4	11,11,12	1.39	2 (18%)	15,15,17	2.07	4 (26%)
4	MAN	C	6	4	11,11,12	2.97	4 (36%)	15,15,17	6.40	12 (80%)
4	FUC	C	7	4	10,10,11	1.97	3 (30%)	14,14,16	2.82	8 (57%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	6	MAN	C2-C3	5.92	1.61	1.52
4	C	3	BMA	C2-C3	-5.47	1.44	1.52
3	B	3	BMA	C2-C3	-5.35	1.44	1.52
4	C	6	MAN	O5-C5	5.03	1.53	1.43
4	C	2	NAG	C1-C2	4.15	1.58	1.52
4	C	6	MAN	C1-C2	4.01	1.61	1.52
4	C	6	MAN	O5-C1	3.60	1.49	1.43
4	C	3	BMA	O3-C3	3.39	1.50	1.43
4	C	7	FUC	C6-C5	3.35	1.59	1.51
3	B	3	BMA	C4-C5	3.31	1.60	1.53
4	C	1	NAG	O5-C5	3.10	1.49	1.43
4	C	7	FUC	C2-C3	2.99	1.56	1.52
3	B	5	FUC	C2-C3	2.76	1.56	1.52
4	C	2	NAG	C3-C2	-2.75	1.46	1.52
4	C	5	MAN	O5-C5	2.56	1.48	1.43
2	A	1	NAG	O5-C5	2.54	1.48	1.43
3	B	5	FUC	O5-C5	2.51	1.48	1.43
2	A	1	NAG	O4-C4	2.49	1.48	1.43
4	C	1	NAG	C3-C2	2.44	1.57	1.52
4	C	7	FUC	O2-C2	2.42	1.48	1.43
2	A	1	NAG	C3-C2	2.40	1.57	1.52
3	B	2	NAG	C1-C2	2.27	1.55	1.52
3	B	3	BMA	O5-C5	2.27	1.48	1.43
3	B	1	NAG	C3-C2	2.24	1.57	1.52
4	C	4	XYP	O5-C5	2.14	1.47	1.42
4	C	5	MAN	C4-C5	2.08	1.57	1.53

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	6	MAN	C1-O5-C5	-11.89	96.08	112.19
4	C	3	BMA	C6-C5-C4	11.20	139.24	113.00
4	C	6	MAN	C6-C5-C4	10.98	138.73	113.00
4	C	3	BMA	O4-C4-C5	10.37	135.05	109.30
2	A	2	NAG	C1-O5-C5	-10.23	98.34	112.19
4	C	6	MAN	O4-C4-C5	10.04	134.22	109.30
4	C	3	BMA	O5-C5-C6	-9.50	92.31	107.20
4	C	6	MAN	O5-C5-C6	-9.13	92.89	107.20
2	A	1	NAG	C1-O5-C5	-8.05	101.29	112.19
4	C	1	NAG	C1-O5-C5	-8.04	101.30	112.19
4	C	6	MAN	O5-C1-C2	-7.45	99.27	110.77
4	C	3	BMA	O4-C4-C3	-7.02	94.13	110.35
4	C	6	MAN	O5-C5-C4	6.54	126.73	110.83
4	C	3	BMA	C3-C4-C5	6.16	121.23	110.24
4	C	7	FUC	C1-C2-C3	-6.08	102.19	109.67
3	B	1	NAG	C2-N2-C7	-6.04	114.31	122.90
4	C	4	XYP	C4-C3-C2	-5.90	103.92	110.92
3	B	1	NAG	C1-O5-C5	-5.54	104.69	112.19
4	C	3	BMA	C1-O5-C5	-5.51	104.73	112.19
4	C	3	BMA	C2-C3-C4	-5.35	101.64	110.89
3	B	5	FUC	O2-C2-C3	-5.27	99.59	110.14
3	B	3	BMA	O3-C3-C2	5.24	120.02	109.99
2	A	1	NAG	C2-N2-C7	-5.18	115.53	122.90
3	B	1	NAG	C8-C7-N2	-5.02	107.59	116.10
4	C	7	FUC	C6-C5-C4	-4.90	104.02	113.07
4	C	3	BMA	O3-C3-C2	-4.86	100.69	109.99
4	C	2	NAG	C2-N2-C7	-4.79	116.08	122.90
3	B	4	XYP	C1-C2-C3	4.69	115.43	109.67
4	C	6	MAN	C2-C3-C4	-4.62	102.90	110.89
4	C	1	NAG	O5-C1-C2	4.55	118.48	111.29
2	A	2	NAG	O5-C1-C2	4.54	118.45	111.29
2	A	1	NAG	C8-C7-N2	-4.53	108.42	116.10
2	A	2	NAG	O5-C5-C6	-4.42	100.27	107.20
4	C	2	NAG	O4-C4-C3	-4.32	100.37	110.35
2	A	2	NAG	O5-C5-C4	-4.31	100.35	110.83
4	C	5	MAN	C1-C2-C3	4.28	114.93	109.67
4	C	2	NAG	O4-C4-C5	-4.24	98.76	109.30
4	C	2	NAG	C8-C7-N2	-4.23	108.93	116.10
4	C	1	NAG	O5-C5-C6	-4.16	100.68	107.20
4	C	5	MAN	C2-C3-C4	-4.13	103.75	110.89
4	C	3	BMA	O2-C2-C3	-3.91	102.30	110.14
4	C	1	NAG	C4-C3-C2	-3.69	105.61	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	NAG	C8-C7-N2	-3.66	109.90	116.10
3	B	4	XYP	O2-C2-C3	-3.66	102.81	110.14
4	C	6	MAN	O6-C6-C5	3.60	123.65	111.29
2	A	2	NAG	C8-C7-N2	-3.49	110.20	116.10
4	C	4	XYP	C1-C2-C3	3.47	113.93	109.67
4	C	1	NAG	O7-C7-C8	3.43	128.42	122.06
2	A	2	NAG	C6-C5-C4	-3.39	105.05	113.00
4	C	2	NAG	O5-C1-C2	-3.34	106.01	111.29
4	C	6	MAN	O2-C2-C1	-3.34	102.32	109.15
2	A	1	NAG	O4-C4-C5	-3.33	101.03	109.30
4	C	3	BMA	O5-C5-C4	-3.32	102.75	110.83
3	B	1	NAG	C1-C2-N2	-3.28	104.88	110.49
4	C	7	FUC	C1-O5-C5	3.24	120.12	112.78
4	C	7	FUC	C2-C3-C4	3.18	116.40	110.89
4	C	4	XYP	C5-C4-C3	-3.13	105.82	109.67
3	B	1	NAG	O7-C7-N2	3.04	127.55	121.95
2	A	2	NAG	O6-C6-C5	-3.03	100.91	111.29
4	C	6	MAN	O4-C4-C3	-2.98	103.46	110.35
4	C	3	BMA	O2-C2-C1	2.98	115.25	109.15
4	C	4	XYP	O2-C2-C3	-2.92	104.30	110.14
2	A	1	NAG	O3-C3-C2	-2.89	103.49	109.47
3	B	4	XYP	O3-C3-C2	-2.82	104.58	109.99
4	C	6	MAN	O3-C3-C4	-2.81	103.86	110.35
4	C	3	BMA	C1-C2-C3	-2.80	106.23	109.67
2	A	1	NAG	C1-C2-N2	-2.73	105.82	110.49
2	A	2	NAG	C2-N2-C7	-2.71	119.05	122.90
3	B	3	BMA	O5-C5-C4	-2.66	104.35	110.83
4	C	7	FUC	O2-C2-C1	-2.64	103.74	109.15
2	A	1	NAG	O7-C7-N2	2.64	126.80	121.95
4	C	5	MAN	C3-C4-C5	-2.63	105.55	110.24
4	C	7	FUC	O3-C3-C4	-2.62	104.30	110.35
4	C	6	MAN	O2-C2-C3	-2.53	105.07	110.14
4	C	1	NAG	O3-C3-C4	-2.52	104.52	110.35
4	C	2	NAG	O5-C5-C4	-2.42	104.94	110.83
3	B	5	FUC	O3-C3-C2	-2.41	105.37	109.99
3	B	3	BMA	O5-C5-C6	-2.40	103.44	107.20
3	B	5	FUC	C1-C2-C3	-2.36	106.77	109.67
4	C	7	FUC	O2-C2-C3	-2.36	105.42	110.14
3	B	1	NAG	O4-C4-C3	-2.35	104.91	110.35
4	C	5	MAN	O2-C2-C3	-2.31	105.51	110.14
3	B	2	NAG	O7-C7-N2	2.29	126.17	121.95
4	C	1	NAG	C1-C2-N2	-2.28	106.60	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	NAG	O3-C3-C2	-2.23	104.85	109.47
4	C	7	FUC	O5-C5-C6	-2.22	102.54	107.33
3	B	1	NAG	C4-C3-C2	-2.21	107.78	111.02
3	B	3	BMA	C2-C3-C4	2.07	114.48	110.89
3	B	2	NAG	O3-C3-C2	-2.00	105.32	109.47
2	A	1	NAG	O4-C4-C3	-2.00	105.72	110.35

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

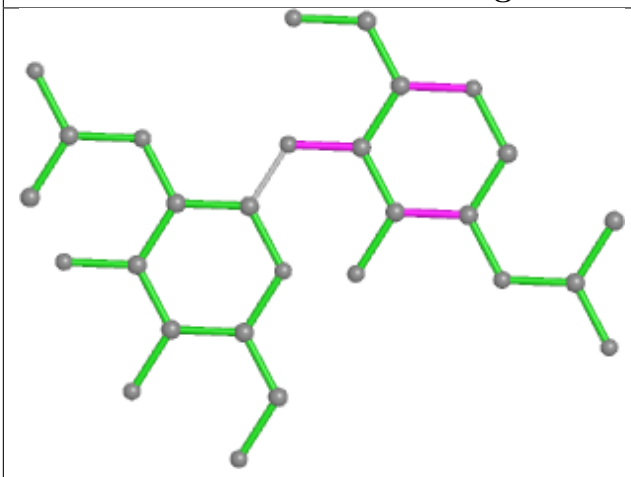
There are no ring outliers.

5 monomers are involved in 26 short contacts:

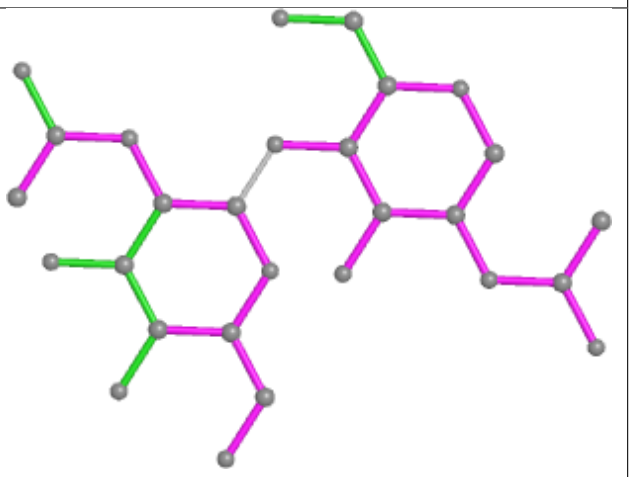
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	4	0
4	C	3	BMA	10	0
4	C	1	NAG	3	0
4	C	6	MAN	11	0
3	B	1	NAG	4	0

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

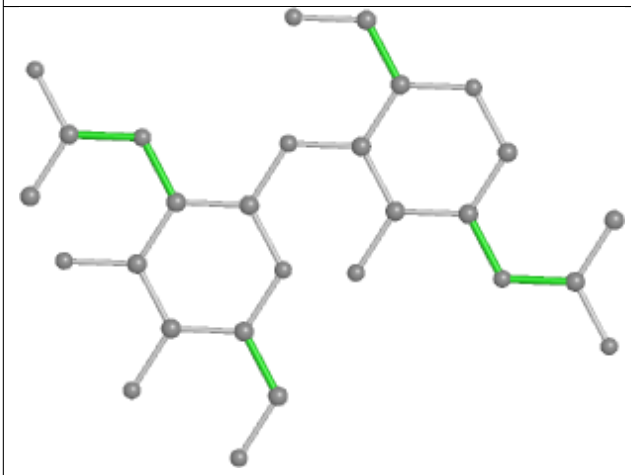
Oligosaccharide Chain A



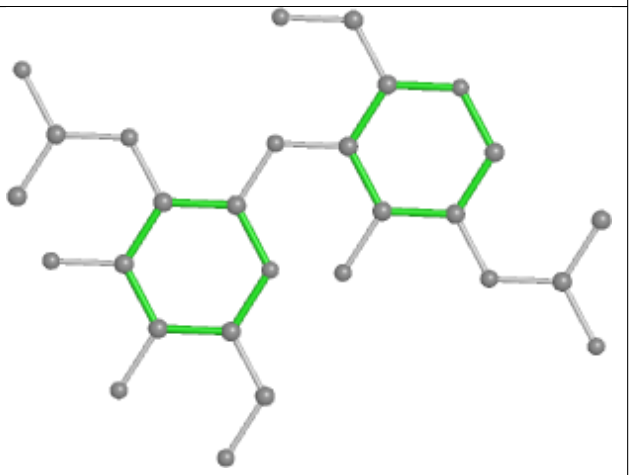
Bond lengths



Bond angles

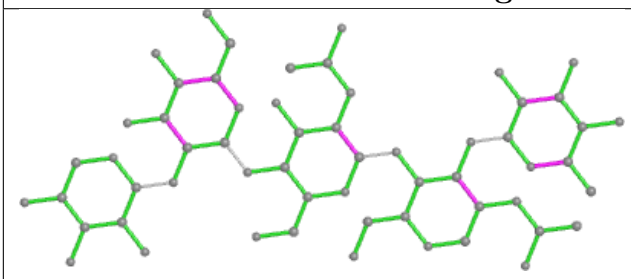


Torsions

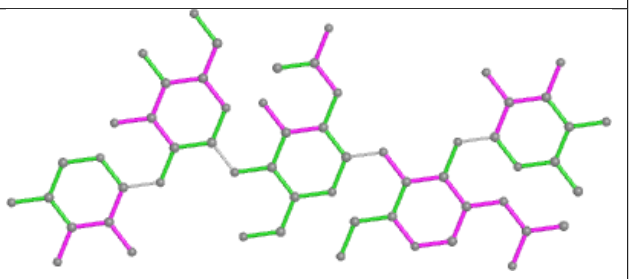


Rings

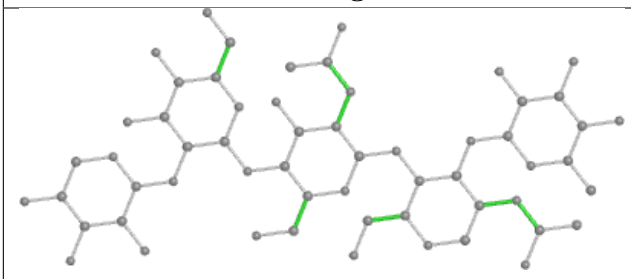
Oligosaccharide Chain B



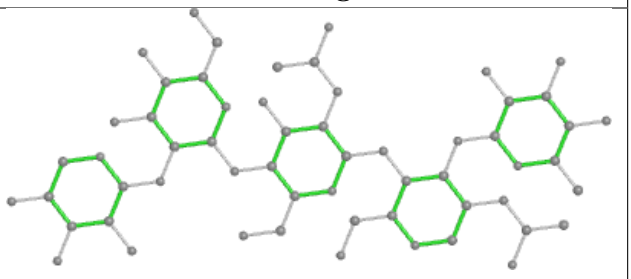
Bond lengths



Bond angles

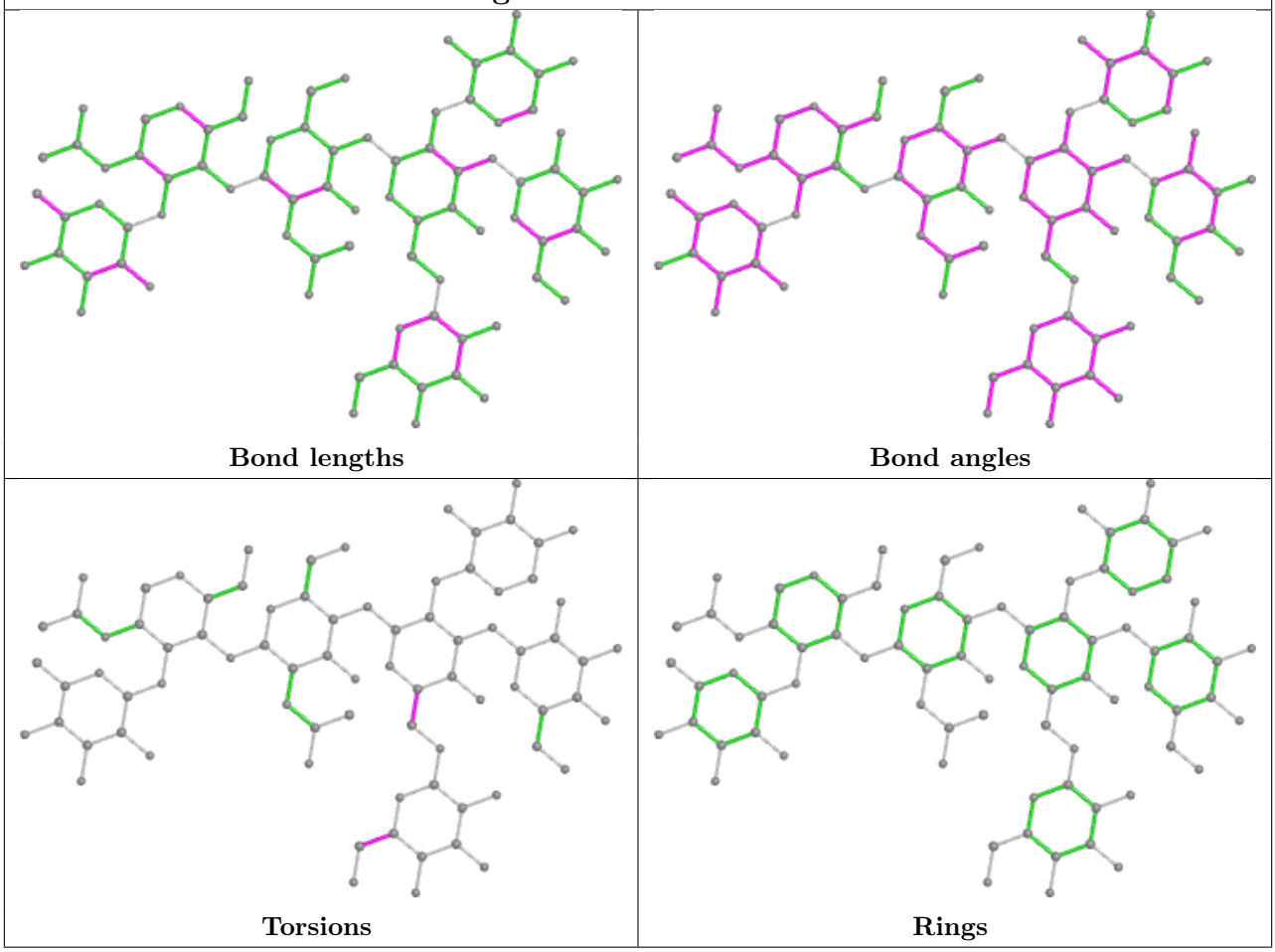


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	$\#\|Z\| > 2$
9	GOL	M	1511[B]	-	5,5,5	0.88	0	5,5,5	2.62	2 (40%)
5	NAG	M	901	1	14,14,15	1.19	1 (7%)	17,19,21	2.07	5 (29%)
5	NAG	M	911	1	14,14,15	1.30	1 (7%)	17,19,21	2.00	6 (35%)
8	SO4	M	1502	-	4,4,4	0.55	0	6,6,6	0.87	0
9	GOL	M	1512	-	5,5,5	0.66	0	5,5,5	1.74	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SO4	M	1509	-	4,4,4	0.82	0	6,6,6	1.03	1 (16%)
9	GOL	M	1511[A]	-	5,5,5	0.83	0	5,5,5	1.60	1 (20%)
7	G2F	M	999	1	11,11,12	1.41	2 (18%)	10,15,17	2.17	3 (30%)
8	SO4	M	1503	-	4,4,4	0.69	0	6,6,6	0.32	0
6	ASC	M	995	-	12,12,12	4.52	8 (66%)	17,17,17	2.31	5 (29%)
8	SO4	M	1505	-	4,4,4	0.29	0	6,6,6	0.59	0
8	SO4	M	1504	-	4,4,4	0.92	0	6,6,6	0.84	0
5	NAG	M	991	1	14,14,15	1.34	1 (7%)	17,19,21	2.01	6 (35%)
5	NAG	M	961	1	14,14,15	1.43	2 (14%)	17,19,21	2.77	6 (35%)
8	SO4	M	1507	-	4,4,4	0.88	0	6,6,6	0.87	0
9	GOL	M	1513	-	5,5,5	0.54	0	5,5,5	1.50	1 (20%)
8	SO4	M	1506	-	4,4,4	0.92	0	6,6,6	1.10	0
5	NAG	M	931	1	14,14,15	1.81	3 (21%)	17,19,21	9.27	10 (58%)
5	NAG	M	971	1	14,14,15	1.37	1 (7%)	17,19,21	2.79	5 (29%)
8	SO4	M	1508	-	4,4,4	0.63	0	6,6,6	0.35	0
9	GOL	M	1510	-	5,5,5	0.43	0	5,5,5	0.56	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
5	NAG	M	991	1	-	0/6/23/26	0/1/1/1
9	GOL	M	1511[A]	-	-	0/4/4/4	-
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
5	NAG	M	931	1	-	3/6/23/26	0/1/1/1
9	GOL	M	1510	-	-	4/4/4/4	-
7	G2F	M	999	1	-	0/2/19/22	0/1/1/1
9	GOL	M	1511[B]	-	-	2/4/4/4	-
9	GOL	M	1513	-	-	1/4/4/4	-
6	ASC	M	995	-	-	0/6/22/22	0/1/1/1
5	NAG	M	901	1	-	0/6/23/26	0/1/1/1
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
9	GOL	M	1512	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	995	ASC	C2-C1	8.97	1.66	1.45
6	M	995	ASC	O1-C1	-8.34	1.04	1.21
6	M	995	ASC	C4-C3	5.69	1.58	1.50
6	M	995	ASC	O4-C1	5.03	1.43	1.36
5	M	931	NAG	O7-C7	-4.38	1.13	1.23
5	M	971	NAG	O7-C7	-4.05	1.14	1.23
5	M	911	NAG	O7-C7	-3.84	1.14	1.23
5	M	931	NAG	C2-N2	-3.62	1.40	1.46
5	M	991	NAG	O7-C7	-3.61	1.15	1.23
5	M	901	NAG	O7-C7	-3.54	1.15	1.23
5	M	961	NAG	O7-C7	-3.48	1.15	1.23
6	M	995	ASC	O3-C3	3.34	1.43	1.33
6	M	995	ASC	C5-C4	3.13	1.58	1.53
7	M	999	G2F	C2-C3	2.97	1.55	1.51
5	M	961	NAG	C2-N2	2.61	1.50	1.46
6	M	995	ASC	C2-C3	2.40	1.41	1.35
7	M	999	G2F	C6-C5	2.29	1.59	1.51
6	M	995	ASC	O4-C4	-2.27	1.41	1.45
5	M	931	NAG	C8-C7	-2.15	1.46	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	931	NAG	C2-N2-C7	34.94	172.66	122.90
5	M	961	NAG	C1-O5-C5	9.36	124.87	112.19
5	M	971	NAG	C1-O5-C5	7.43	122.26	112.19
5	M	931	NAG	O7-C7-N2	-7.38	108.38	121.95
5	M	931	NAG	C1-O5-C5	-7.27	102.34	112.19
5	M	931	NAG	C8-C7-N2	7.06	128.05	116.10
5	M	971	NAG	O5-C1-C2	-5.92	101.94	111.29
6	M	995	ASC	O4-C1-C2	-5.64	104.85	109.86
5	M	931	NAG	O5-C1-C2	4.78	118.84	111.29
5	M	931	NAG	C1-C2-N2	4.69	118.50	110.49
9	M	1511[B]	GOL	O1-C1-C2	4.65	132.51	110.20
5	M	971	NAG	O5-C5-C6	-4.55	100.07	107.20
5	M	991	NAG	C4-C3-C2	-4.55	104.35	111.02
7	M	999	G2F	O5-C5-C6	-4.40	100.31	107.20
5	M	901	NAG	C1-O5-C5	-4.38	106.26	112.19
5	M	911	NAG	C1-O5-C5	-4.31	106.36	112.19
5	M	901	NAG	O5-C1-C2	4.22	117.96	111.29
6	M	995	ASC	O4-C1-O1	4.18	126.19	121.25
5	M	991	NAG	O5-C1-C2	4.12	117.80	111.29
7	M	999	G2F	C3-C4-C5	-3.80	103.45	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	995	ASC	C4-O4-C1	3.79	113.53	109.25
5	M	961	NAG	C1-C2-N2	-3.47	104.55	110.49
5	M	911	NAG	O5-C5-C4	-3.45	102.44	110.83
9	M	1511[A]	GOL	O2-C2-C1	3.33	123.80	109.12
9	M	1511[B]	GOL	O2-C2-C1	3.33	123.80	109.12
5	M	911	NAG	C4-C3-C2	-3.27	106.22	111.02
5	M	901	NAG	O5-C5-C4	-3.18	103.10	110.83
5	M	911	NAG	O3-C3-C2	-3.09	103.08	109.47
5	M	931	NAG	O5-C5-C4	-3.08	103.34	110.83
5	M	931	NAG	C3-C4-C5	3.05	115.68	110.24
6	M	995	ASC	O4-C4-C3	2.90	106.70	103.71
5	M	931	NAG	C4-C3-C2	-2.79	106.93	111.02
5	M	901	NAG	C4-C3-C2	-2.74	107.00	111.02
7	M	999	G2F	O5-C5-C4	-2.72	104.21	110.83
5	M	901	NAG	O3-C3-C2	-2.63	104.02	109.47
5	M	961	NAG	O5-C1-C2	2.59	115.38	111.29
9	M	1513	GOL	O3-C3-C2	-2.51	98.16	110.20
5	M	991	NAG	O5-C5-C4	-2.51	104.72	110.83
5	M	971	NAG	O3-C3-C2	-2.42	104.45	109.47
5	M	991	NAG	O3-C3-C2	-2.40	104.50	109.47
5	M	971	NAG	O5-C5-C4	-2.35	105.11	110.83
5	M	961	NAG	O3-C3-C2	-2.35	104.61	109.47
5	M	911	NAG	C8-C7-N2	-2.32	112.17	116.10
5	M	991	NAG	C6-C5-C4	-2.29	107.63	113.00
5	M	961	NAG	O4-C4-C5	-2.28	103.64	109.30
5	M	931	NAG	O4-C4-C5	-2.28	103.65	109.30
5	M	961	NAG	C2-N2-C7	-2.27	119.68	122.90
9	M	1512	GOL	O1-C1-C2	2.23	120.88	110.20
6	M	995	ASC	O2-C2-C1	2.18	127.94	122.37
5	M	991	NAG	C2-N2-C7	-2.12	119.88	122.90
9	M	1512	GOL	O2-C2-C3	2.08	118.30	109.12
5	M	911	NAG	O6-C6-C5	2.03	118.26	111.29
8	M	1509	SO4	O4-S-O3	2.02	117.69	109.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	961	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	931	NAG	C8-C7-N2-C2
5	M	931	NAG	O7-C7-N2-C2
9	M	1510	GOL	O1-C1-C2-C3
9	M	1510	GOL	C1-C2-C3-O3
9	M	1511[B]	GOL	O1-C1-C2-O2
9	M	1511[B]	GOL	O1-C1-C2-C3
5	M	971	NAG	O5-C5-C6-O6
9	M	1510	GOL	O1-C1-C2-O2
5	M	971	NAG	C4-C5-C6-O6
5	M	931	NAG	C1-C2-N2-C7
9	M	1512	GOL	C1-C2-C3-O3
9	M	1513	GOL	O1-C1-C2-C3
9	M	1510	GOL	O2-C2-C3-O3
9	M	1512	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	901	NAG	3	0
5	M	911	NAG	2	0
9	M	1512	GOL	1	0
8	M	1509	SO4	5	0
7	M	999	G2F	1	0
6	M	995	ASC	1	0
8	M	1504	SO4	4	0
5	M	931	NAG	6	0
9	M	1510	GOL	1	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%)	-0.46	13 (2%) 56 61	10, 14, 28, 54	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	7.9
1	M	377	ASP	7.3
1	M	375	LYS	4.5
1	M	380	ASP	3.9
1	M	374	ASP	3.4
1	M	3	GLU	3.3
1	M	483	VAL	3.3
1	M	417	ASP	3.3
1	M	481	ASN	3.0
1	M	378	SER	2.7
1	M	379	THR	2.3
1	M	421	ASN	2.3
1	M	482	ASN	2.2

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)

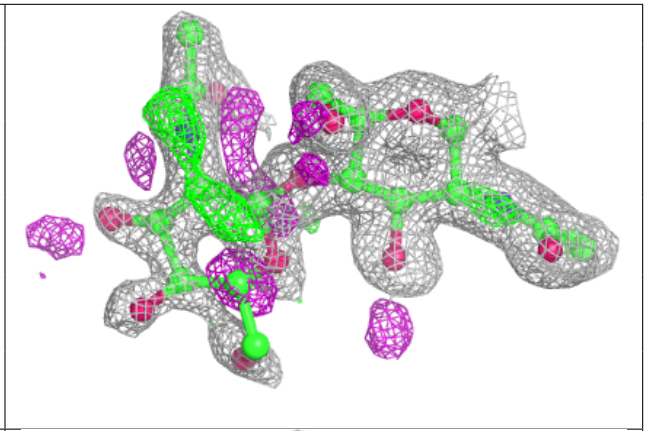
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

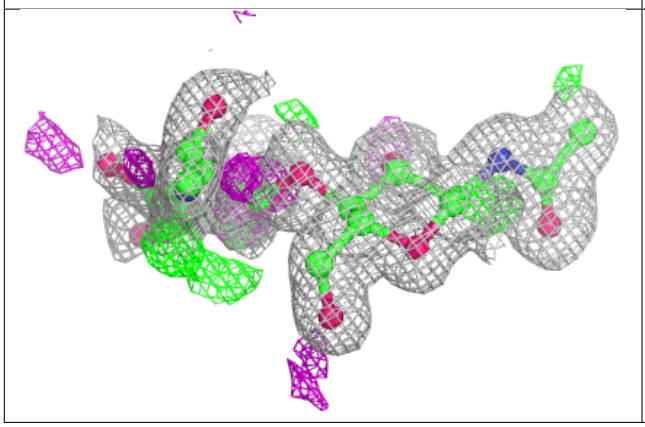
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	XYP	C	4	9/10	0.42	0.34	39,42,45,46	0
4	MAN	C	5	11/12	0.47	0.39	30,41,45,46	0
2	NAG	A	2	14/15	0.57	0.31	37,42,49,50	0
4	MAN	C	6	11/12	0.60	0.53	40,45,49,52	0
3	XYP	B	4	9/10	0.70	0.33	42,43,44,46	0
3	BMA	B	3	11/12	0.72	0.30	37,39,42,45	0
4	BMA	C	3	11/12	0.79	0.15	25,32,35,38	0
4	FUC	C	7	10/11	0.81	0.16	24,25,28,30	0
4	NAG	C	2	14/15	0.87	0.13	22,24,29,32	0
3	FUC	B	5	10/11	0.88	0.17	28,32,35,36	0
3	NAG	B	2	14/15	0.90	0.10	25,28,33,35	0
2	NAG	A	1	14/15	0.92	0.08	19,23,28,31	0
3	NAG	B	1	14/15	0.94	0.08	18,21,24,24	0
4	NAG	C	1	14/15	0.94	0.08	18,20,22,24	0

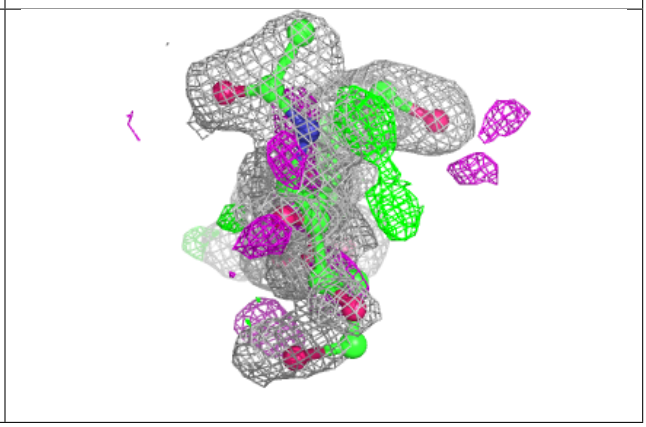
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

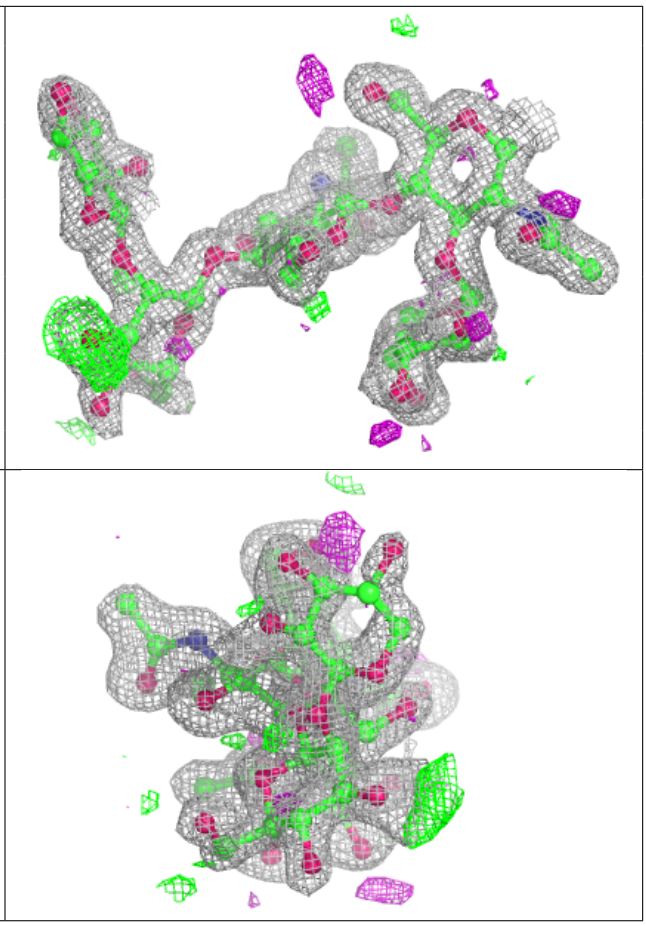






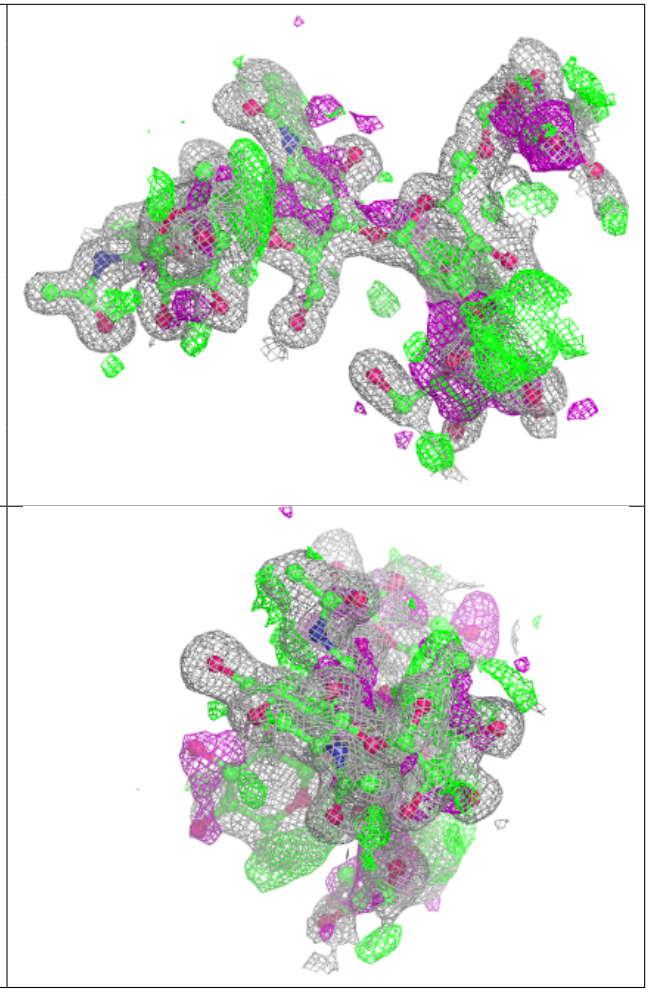
Electron density around Chain B:

$2mF_o$-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 (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
5	NAG	M	991	14/15	0.44	0.54	38,41,49,50	0
9	GOL	M	1510	6/6	0.49	0.24	38,40,40,40	6
5	NAG	M	971	14/15	0.53	0.52	57,62,65,66	0
9	GOL	M	1513	6/6	0.56	0.31	36,38,38,41	6
5	NAG	M	931	14/15	0.57	0.29	38,45,48,50	0
5	NAG	M	961	14/15	0.61	0.50	39,42,52,53	0
8	SO4	M	1507	5/5	0.63	0.23	30,34,35,35	5
8	SO4	M	1506	5/5	0.66	0.33	32,34,37,37	5
8	SO4	M	1504	5/5	0.73	0.34	31,34,36,38	5
5	NAG	M	901	14/15	0.74	0.17	32,35,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SO4	M	1508	5/5	0.81	0.28	40,40,40,40	5
5	NAG	M	911	14/15	0.82	0.17	24,27,31,32	0
9	GOL	M	1511[B]	6/6	0.89	0.13	14,16,18,18	2
9	GOL	M	1511[A]	6/6	0.89	0.13	14,16,18,18	2
8	SO4	M	1509	5/5	0.90	0.34	42,43,45,45	1
7	G2F	M	999	11/12	0.91	0.10	18,26,31,33	0
9	GOL	M	1512	6/6	0.92	0.11	17,23,26,31	6
8	SO4	M	1503	5/5	0.95	0.12	22,25,28,29	5
6	ASC	M	995	12/12	0.96	0.07	16,17,19,19	0
8	SO4	M	1502	5/5	0.98	0.16	23,23,27,29	5
8	SO4	M	1505	5/5	0.99	0.04	18,19,22,25	0
10	ZN	M	1515	1/1	1.00	0.03	11,11,11,11	1

6.5 Other polymers (i)

There are no such residues in this entry.