



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 11:46 pm GMT

PDB ID : 1E71
Title : MYROSINASE FROM SINAPIS ALBA with bound 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 ⓘ 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 : 4.02b-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

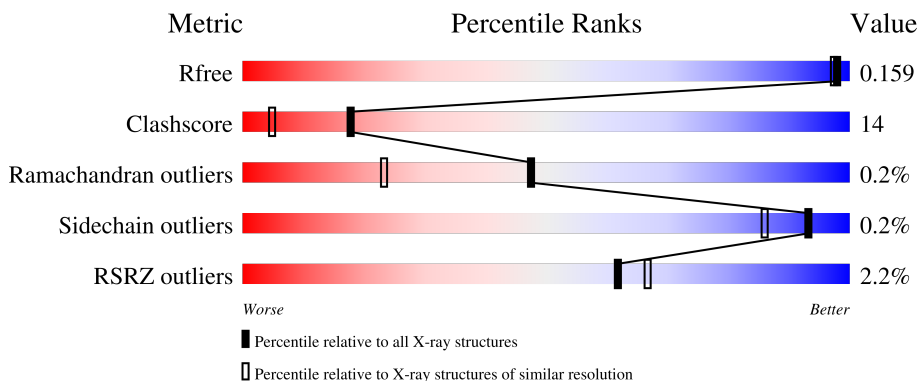
1 Overall quality at a glance

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 $\leq 5\%$. 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	 2% 86% 12%
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	931	-	-	X	-
5	NAG	M	961	-	-	-	X
5	NAG	M	971	-	-	-	X
9	SO4	M	1506	-	-	X	-
9	SO4	M	1511	-	-	X	-

2 Entry composition [i](#)

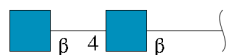
There are 10 unique types of molecules in this entry. The entry contains 5214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

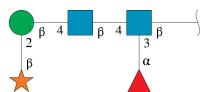
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	499	4082	2618	660	788	16	0	21	0

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



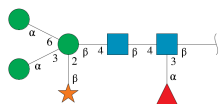
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	2	28	16	2	10	0	0	0

- 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.



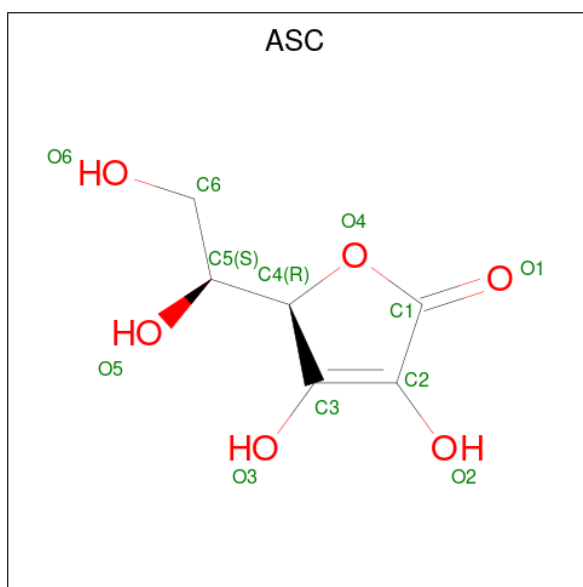
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
4	C	7	80	45	2	33	0	0	0

- 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
5	M	1	14	8	1	5	0	0
5	M	1	14	8	1	5	0	0
5	M	1	14	8	1	5	0	0
5	M	1	14	8	1	5	0	0
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
6	M	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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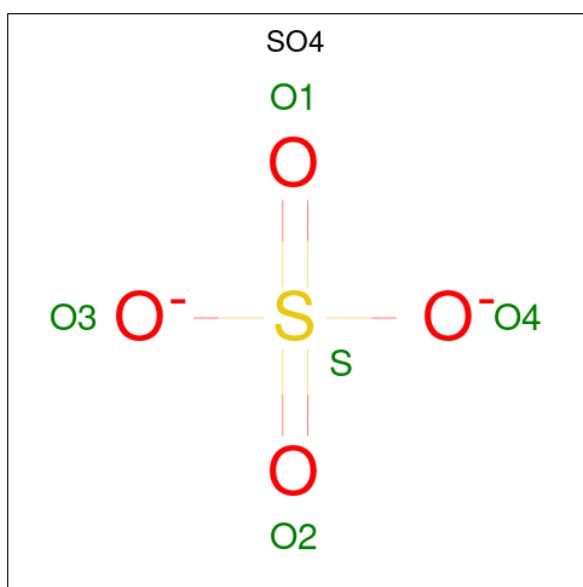
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			6	3	3		
7	M	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

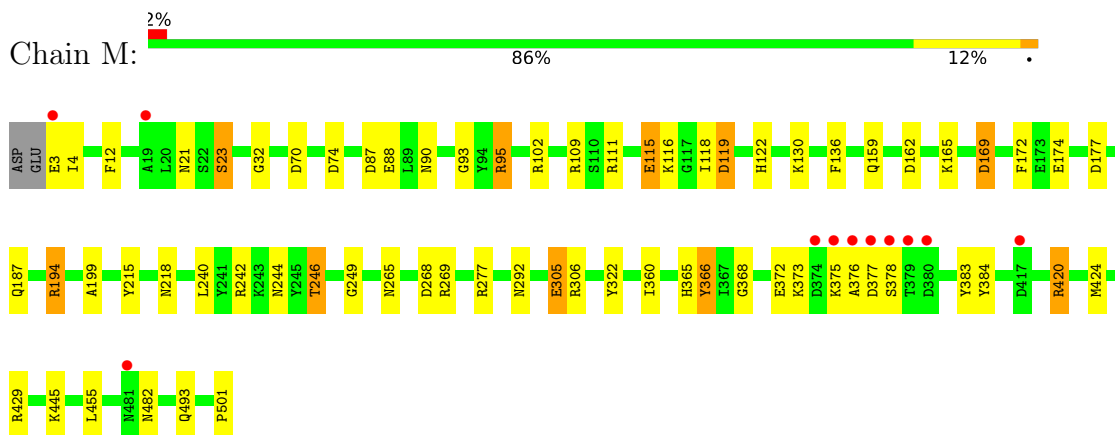
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	798	Total	O	0	0
			798	798		

3 Residue-property plots [i](#)

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

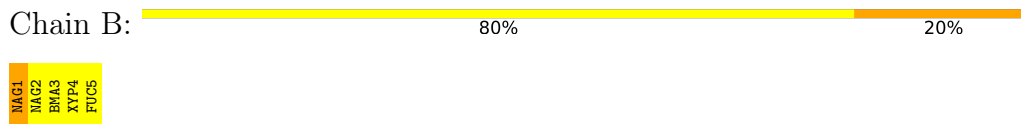
- Molecule 1: MYROSINASE MA1



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



- 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-(1-6)]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



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 – 1.50 9.99 – 1.52	Depositor EDS
% Data completeness (in resolution range)	89.7 (10.00-1.50) 92.7 (9.99-1.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.51Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.127 , 0.152 0.138 , 0.159	Depositor DCC
R_{free} test set	5441 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5214	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, XYP, ASC, NAG, MAN, ZN, FUC, BMA, GOL

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	0.74	1/4290 (0.0%)	1.43	53/5833 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	501	PRO	N-CD	6.60	1.57	1.47

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	109	ARG	NE-CZ-NH2	-18.34	111.13	120.30
1	M	242	ARG	NE-CZ-NH2	-14.39	113.10	120.30
1	M	115	GLU	OE1-CD-OE2	-13.46	107.15	123.30
1	M	109	ARG	NH1-CZ-NH2	10.20	130.62	119.40
1	M	482	ASN	CB-CG-OD1	8.58	138.76	121.60
1	M	420	ARG	CD-NE-CZ	8.56	135.58	123.60
1	M	269	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	M	366[A]	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	M	366[B]	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	M	95	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	M	366[A]	TYR	CB-CG-CD1	7.64	125.58	121.00
1	M	366[B]	TYR	CB-CG-CD1	7.64	125.58	121.00
1	M	429	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	M	277	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	M	246	THR	OG1-CB-CG2	-7.20	93.44	110.00
1	M	70	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	M	194	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	M	268	ASP	CB-CG-OD1	7.00	124.60	118.30
1	M	87	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	M	482	ASN	CA-CB-CG	-6.96	98.08	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	88[A]	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	M	88[B]	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	M	172	PHE	CB-CG-CD2	-6.61	116.17	120.80
1	M	269	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	M	87	ASP	CB-CG-OD1	6.41	124.07	118.30
1	M	372	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	M	306	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	M	429	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	M	102	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	M	95	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	M	215	TYR	CB-CG-CD1	-6.14	117.31	121.00
1	M	162	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	M	162	ASP	CB-CG-OD1	5.88	123.60	118.30
1	M	169[A]	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	M	169[B]	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	M	115	GLU	CG-CD-OE2	5.68	129.67	118.30
1	M	12	PHE	CB-CG-CD2	5.67	124.77	120.80
1	M	111	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	M	102	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	M	306	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	M	383	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	M	242	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	M	199	ALA	N-CA-CB	5.35	117.59	110.10
1	M	23	SER	CA-CB-OG	-5.29	96.93	111.20
1	M	322	TYR	CG-CD1-CE1	-5.27	117.08	121.30
1	M	109	ARG	CD-NE-CZ	-5.26	116.24	123.60
1	M	177	ASP	CB-CG-OD1	5.25	123.02	118.30
1	M	119	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	M	215	TYR	CG-CD1-CE1	-5.13	117.19	121.30
1	M	305[A]	GLU	CB-CG-CD	5.06	127.87	114.20
1	M	305[B]	GLU	CB-CG-CD	5.06	127.87	114.20
1	M	372	GLU	CG-CD-OE2	5.03	128.37	118.30
1	M	74	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4082	0	3836	85	0
2	A	28	0	25	4	0
3	B	58	0	42	5	0
4	C	80	0	57	19	0
5	M	84	0	77	18	0
6	M	12	0	7	1	0
7	M	31	0	38	2	0
8	M	1	0	0	0	0
9	M	40	0	0	7	0
10	M	798	0	0	31	0
All	All	5214	0	4082	109	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 14.

All (109) 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:90:ASN:HD21	5:M:911:NAG:C1	0.94	1.57
1:M:21:ASN:HD21	5:M:901:NAG:C1	0.95	1.56
1:M:244:ASN:HD21	5:M:931:NAG:C1	0.97	1.56
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.40	1.55
1:M:292:ASN:HD21	4:C:1:NAG:C1	0.91	1.53
1:M:218:ASN:HD21	2:A:1:NAG:C1	0.91	1.52
1:M:265:ASN:HD21	3:B:1:NAG:C1	0.92	1.52
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	1.97	1.46
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE1	1.58	1.37
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.37	1.23
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE1	2.22	1.23
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE1	2.19	1.19
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	1.96	1.06
10:M:2739:HOH:O	4:C:6:MAN:H61	1.56	1.05
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD1	1.94	1.02
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE1	1.93	1.02
1:M:246:THR:HG22	10:M:2386:HOH:O	1.62	0.98
1:M:165:LYS:NZ	5:M:931:NAG:H82	1.78	0.98
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	2.00	0.97
4:C:3:BMA:H61	4:C:6:MAN:C6	1.98	0.93
6:M:995:ASC:H4	10:M:2757:HOH:O	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3:BMA:H61	4:C:6:MAN:H62	1.53	0.89
4:C:3:BMA:C6	4:C:6:MAN:C6	2.54	0.86
4:C:3:BMA:C6	4:C:6:MAN:H61	2.08	0.84
1:M:165:LYS:HZ1	5:M:931:NAG:H82	1.39	0.83
1:M:265:ASN:HD21	3:B:1:NAG:C2	1.91	0.81
1:M:21:ASN:HD21	5:M:901:NAG:C2	1.90	0.80
1:M:116:LYS:HG2	10:M:2229:HOH:O	1.82	0.80
1:M:218:ASN:HD21	2:A:1:NAG:C2	1.93	0.79
10:M:2739:HOH:O	4:C:3:BMA:C4	2.31	0.78
1:M:130:LYS:HG3	10:M:2251:HOH:O	1.84	0.77
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD1	2.63	0.76
9:M:1506:SO4:S	9:M:1511:SO4:O3	2.44	0.76
1:M:377:ASP:HB3	10:M:2558:HOH:O	1.87	0.74
1:M:130:LYS:HB3	10:M:2098:HOH:O	1.88	0.74
4:C:3:BMA:O6	4:C:6:MAN:C6	2.33	0.73
10:M:2748:HOH:O	4:C:6:MAN:C5	2.37	0.71
1:M:244:ASN:HD21	5:M:931:NAG:C2	1.97	0.71
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE1	2.24	0.70
10:M:2739:HOH:O	4:C:3:BMA:C5	2.40	0.69
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:OH	1.90	0.68
1:M:90:ASN:HD21	5:M:911:NAG:C2	2.00	0.68
9:M:1511:SO4:O1	10:M:2789:HOH:O	2.12	0.67
1:M:130:LYS:HB3	10:M:2262:HOH:O	1.94	0.66
1:M:218:ASN:ND2	2:A:1:NAG:C2	2.56	0.66
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CZ	2.62	0.66
4:C:3:BMA:C6	4:C:6:MAN:H62	2.22	0.66
1:M:376:ALA:O	1:M:377:ASP:OD1	2.15	0.64
4:C:3:BMA:H61	4:C:6:MAN:H61	1.68	0.63
1:M:365:HIS:HD2	10:M:2254:HOH:O	1.81	0.62
9:M:1506:SO4:O2	9:M:1511:SO4:S	2.58	0.62
9:M:1506:SO4:O1	9:M:1511:SO4:O3	2.18	0.61
1:M:90:ASN:ND2	5:M:911:NAG:C2	2.59	0.61
1:M:365:HIS:HE1	10:M:2541:HOH:O	1.83	0.60
1:M:265:ASN:ND2	3:B:1:NAG:C2	2.59	0.59
1:M:493:GLN:NE2	10:M:2691:HOH:O	2.34	0.59
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.37	0.59
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.85	0.58
1:M:165:LYS:HZ2	5:M:931:NAG:H82	1.67	0.58
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.32	0.57
1:M:292:ASN:ND2	4:C:1:NAG:C2	2.62	0.57
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:244:ASN:ND2	5:M:931:NAG:O5	2.37	0.56
1:M:115:GLU:HG3	10:M:2226:HOH:O	2.04	0.55
1:M:4:ILE:HD11	1:M:445:LYS:CD	2.36	0.55
1:M:115:GLU:CD	10:M:2226:HOH:O	2.46	0.55
1:M:115:GLU:OE2	10:M:2226:HOH:O	2.19	0.54
1:M:21:ASN:CG	5:M:901:NAG:C1	2.70	0.53
1:M:265:ASN:CG	3:B:1:NAG:C1	2.68	0.53
4:C:3:BMA:O6	4:C:6:MAN:H61	2.04	0.53
1:M:218:ASN:ND2	2:A:1:NAG:O5	2.39	0.52
1:M:265:ASN:ND2	3:B:1:NAG:O5	2.37	0.51
1:M:376:ALA:C	1:M:377:ASP:OD1	2.49	0.51
1:M:292:ASN:CG	4:C:1:NAG:C1	2.71	0.50
1:M:95:ARG:HB2	1:M:455:LEU:HD13	1.95	0.49
1:M:360[A]:ILE:HG23	10:M:2528:HOH:O	2.12	0.48
1:M:95:ARG:HA	1:M:136:PHE:O	2.14	0.48
1:M:373:LYS:NZ	1:M:378:SER:OG	2.43	0.48
1:M:21:ASN:ND2	5:M:901:NAG:C2	2.62	0.47
1:M:420:ARG:O	1:M:424:MET:HG2	2.14	0.46
10:M:2750:HOH:O	4:C:6:MAN:C6	2.63	0.46
1:M:360[A]:ILE:CG2	10:M:2528:HOH:O	2.63	0.46
9:M:1506:SO4:O2	9:M:1511:SO4:O3	2.34	0.45
1:M:292:ASN:ND2	4:C:1:NAG:O5	2.38	0.45
1:M:32:GLY:HA3	1:M:93:GLY:O	2.16	0.45
1:M:159:GLN:NE2	10:M:2305:HOH:O	2.49	0.45
1:M:90:ASN:ND2	5:M:911:NAG:O5	2.42	0.44
9:M:1506:SO4:S	9:M:1511:SO4:S	3.15	0.44
1:M:118[B]:ILE:HD12	1:M:174:GLU:HG3	1.99	0.44
1:M:115:GLU:CG	10:M:2226:HOH:O	2.65	0.44
1:M:122:HIS:HE1	1:M:174:GLU:O	2.00	0.43
1:M:375:LYS:CE	10:M:2555:HOH:O	2.66	0.43
1:M:119:ASP:OD1	10:M:2226:HOH:O	2.21	0.42
1:M:194:ARG:NH1	9:M:1511:SO4:O4	2.53	0.42
1:M:165:LYS:CE	5:M:931:NAG:H82	2.47	0.42
7:M:1512:GOL:H11	10:M:2790:HOH:O	2.19	0.42
1:M:249:GLY:HA3	7:M:1514:GOL:H31	2.01	0.41
1:M:240:LEU:HD13	5:M:931:NAG:H83	2.02	0.41
1:M:368:GLY:HA3	1:M:384:TYR:O	2.20	0.41
5:M:931:NAG:H81	10:M:2379:HOH:O	2.19	0.41
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:HE1	1.56	0.41
1:M:116:LYS:HB3	1:M:116:LYS:HE3	1.97	0.41
1:M:375:LYS:HE2	10:M:2555:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:2749:HOH:O	4:C:6:MAN:C6	2.68	0.41
1:M:240:LEU:CD1	5:M:931:NAG:H83	2.51	0.41
1:M:424:MET:HE3	10:M:2691:HOH:O	2.21	0.41
1:M:21:ASN:OD1	1:M:23:SER:HB2	2.22	0.40
10:M:2748:HOH:O	4:C:6:MAN:C4	2.69	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	1.60	4 (28%)	17,19,21	3.29	8 (47%)
2	NAG	A	2	2	14,14,15	1.31	1 (7%)	17,19,21	4.57	10 (58%)
3	NAG	B	1	3,1	14,14,15	0.87	0	17,19,21	2.51	5 (29%)
3	NAG	B	2	3	14,14,15	1.12	1 (7%)	17,19,21	1.37	3 (17%)
3	BMA	B	3	3	11,11,12	1.99	3 (27%)	15,15,17	1.84	5 (33%)
3	XYP	B	4	3	9,9,10	0.94	0	10,12,14	2.07	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	B	5	3	10,10,11	1.50	1 (10%)	14,14,16	2.04	5 (35%)
4	NAG	C	1	4,1	14,14,15	1.34	3 (21%)	17,19,21	3.08	7 (41%)
4	NAG	C	2	4	14,14,15	1.21	2 (14%)	17,19,21	1.91	4 (23%)
4	BMA	C	3	4	11,11,12	2.27	3 (27%)	15,15,17	5.65	11 (73%)
4	XYP	C	4	4	9,9,10	1.37	1 (11%)	10,12,14	3.89	5 (50%)
4	MAN	C	5	4	11,11,12	1.26	2 (18%)	15,15,17	2.84	7 (46%)
4	MAN	C	6	4	11,11,12	2.60	4 (36%)	15,15,17	6.86	12 (80%)
4	FUC	C	7	4	10,10,11	1.87	4 (40%)	14,14,16	2.44	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	XYP	B	4	3	-	-	0/1/1/1
3	FUC	B	5	3	-	-	0/1/1/1
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	1/2/19/22	0/1/1/1
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	2/2/19/22	0/1/1/1
4	FUC	C	7	4	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	BMA	C2-C3	-6.33	1.43	1.52
4	C	6	MAN	O5-C5	5.14	1.53	1.43
3	B	3	BMA	C2-C3	-4.84	1.45	1.52
4	C	6	MAN	C1-C2	4.16	1.61	1.52
4	C	6	MAN	C2-C3	3.96	1.58	1.52
4	C	6	MAN	O5-C1	3.25	1.48	1.43
3	B	5	FUC	C2-C3	3.13	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	7	FUC	C2-C3	3.05	1.57	1.52
2	A	1	NAG	O5-C5	3.01	1.49	1.43
3	B	3	BMA	C4-C5	2.84	1.59	1.53
4	C	4	XYP	C2-C3	2.65	1.56	1.52
4	C	7	FUC	O5-C1	-2.62	1.39	1.43
4	C	3	BMA	C4-C5	2.60	1.58	1.53
4	C	2	NAG	C3-C2	-2.58	1.47	1.52
2	A	1	NAG	O7-C7	-2.48	1.17	1.23
4	C	5	MAN	O5-C5	2.42	1.48	1.43
4	C	1	NAG	C2-N2	-2.41	1.42	1.46
3	B	2	NAG	C1-C2	2.38	1.55	1.52
2	A	1	NAG	O4-C4	2.37	1.48	1.43
4	C	7	FUC	C1-C2	2.30	1.57	1.52
2	A	1	NAG	C3-C2	2.29	1.57	1.52
4	C	3	BMA	O3-C3	2.25	1.48	1.43
4	C	2	NAG	C1-C2	2.22	1.55	1.52
4	C	1	NAG	O5-C5	2.21	1.47	1.43
4	C	1	NAG	C1-C2	-2.16	1.49	1.52
4	C	7	FUC	C6-C5	2.14	1.56	1.51
3	B	3	BMA	O5-C1	2.13	1.47	1.43
4	C	5	MAN	C4-C5	2.11	1.57	1.53
2	A	2	NAG	C3-C2	-2.07	1.48	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	C1-O5-C5	-13.80	93.49	112.19
4	C	6	MAN	C1-O5-C5	-12.74	94.93	112.19
4	C	6	MAN	O4-C4-C5	12.46	140.25	109.30
4	C	3	BMA	O4-C4-C5	11.40	137.61	109.30
4	C	3	BMA	C6-C5-C4	9.67	135.66	113.00
2	A	1	NAG	C1-O5-C5	-9.54	99.27	112.19
4	C	6	MAN	O5-C5-C4	9.37	133.62	110.83
4	C	6	MAN	O5-C5-C6	-9.29	92.64	107.20
4	C	1	NAG	C1-O5-C5	-8.53	100.63	112.19
4	C	3	BMA	O4-C4-C3	-8.46	90.79	110.35
4	C	6	MAN	C6-C5-C4	7.74	131.13	113.00
4	C	3	BMA	O5-C5-C6	-7.52	95.41	107.20
4	C	4	XYP	C1-C2-C3	7.50	118.89	109.67
4	C	3	BMA	C3-C4-C5	7.26	123.20	110.24
4	C	5	MAN	C1-C2-C3	7.02	118.29	109.67
4	C	6	MAN	O5-C1-C2	-6.86	100.18	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4	XYP	C4-C3-C2	-6.56	103.14	110.92
3	B	1	NAG	C1-O5-C5	-6.27	103.70	112.19
2	A	2	NAG	O5-C5-C4	-6.07	96.06	110.83
2	A	2	NAG	O5-C5-C6	-5.97	97.85	107.20
4	C	7	FUC	C1-C2-C3	-5.92	102.39	109.67
2	A	1	NAG	C2-N2-C7	-5.76	114.71	122.90
4	C	1	NAG	O5-C1-C2	5.54	120.04	111.29
4	C	4	XYP	C5-C4-C3	-5.34	103.10	109.67
3	B	1	NAG	C2-N2-C7	-5.05	115.71	122.90
3	B	4	XYP	C1-C2-C3	4.95	115.75	109.67
4	C	6	MAN	C1-C2-C3	4.67	115.41	109.67
2	A	2	NAG	O5-C1-C2	4.62	118.58	111.29
2	A	2	NAG	C6-C5-C4	-4.59	102.26	113.00
4	C	3	BMA	O2-C2-C3	-4.49	101.14	110.14
4	C	3	BMA	O5-C5-C4	-4.48	99.93	110.83
4	C	6	MAN	C2-C3-C4	-4.38	103.31	110.89
2	A	2	NAG	C2-N2-C7	-4.36	116.70	122.90
3	B	5	FUC	O2-C2-C3	-4.18	101.77	110.14
4	C	2	NAG	C2-N2-C7	-4.13	117.02	122.90
4	C	6	MAN	O2-C2-C1	-4.12	100.72	109.15
4	C	6	MAN	O3-C3-C2	4.09	117.83	109.99
4	C	1	NAG	O5-C5-C6	-4.05	100.85	107.20
3	B	5	FUC	C1-C2-C3	-4.04	104.70	109.67
4	C	6	MAN	O4-C4-C3	-3.89	101.35	110.35
4	C	5	MAN	O2-C2-C1	3.85	117.02	109.15
2	A	1	NAG	C8-C7-N2	-3.78	109.70	116.10
3	B	1	NAG	C1-C2-N2	-3.72	104.14	110.49
4	C	5	MAN	C2-C3-C4	-3.69	104.51	110.89
4	C	2	NAG	C8-C7-N2	-3.66	109.91	116.10
3	B	3	BMA	C2-C3-C4	3.60	117.12	110.89
3	B	3	BMA	O3-C3-C2	3.47	116.64	109.99
4	C	7	FUC	O2-C2-C1	-3.44	102.11	109.15
4	C	6	MAN	O6-C6-C5	3.44	123.10	111.29
2	A	1	NAG	O4-C4-C5	-3.36	100.96	109.30
4	C	7	FUC	C6-C5-C4	-3.27	107.03	113.07
4	C	3	BMA	C1-C2-C3	-3.27	105.64	109.67
4	C	5	MAN	C3-C4-C5	-3.04	104.82	110.24
4	C	2	NAG	O4-C4-C3	-2.95	103.53	110.35
4	C	5	MAN	O2-C2-C3	-2.88	104.37	110.14
4	C	4	XYP	O2-C2-C3	-2.87	104.39	110.14
2	A	2	NAG	O6-C6-C5	-2.84	101.54	111.29
4	C	4	XYP	O3-C3-C4	2.82	115.39	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	BMA	O5-C5-C4	-2.73	104.18	110.83
3	B	1	NAG	C8-C7-N2	-2.71	111.50	116.10
4	C	7	FUC	C1-O5-C5	2.68	118.85	112.78
3	B	5	FUC	O3-C3-C2	-2.67	104.88	109.99
4	C	5	MAN	C6-C5-C4	-2.67	106.76	113.00
4	C	1	NAG	C3-C4-C5	-2.65	105.51	110.24
2	A	2	NAG	C3-C4-C5	2.64	114.94	110.24
3	B	3	BMA	O3-C3-C4	2.61	116.38	110.35
2	A	1	NAG	O3-C3-C2	-2.60	104.08	109.47
4	C	3	BMA	C2-C3-C4	-2.59	106.42	110.89
4	C	1	NAG	O7-C7-C8	2.53	126.75	122.06
3	B	2	NAG	O6-C6-C5	-2.52	102.63	111.29
2	A	1	NAG	C1-C2-N2	-2.52	106.19	110.49
3	B	2	NAG	O3-C3-C2	-2.51	104.27	109.47
2	A	1	NAG	O5-C5-C6	-2.51	103.27	107.20
3	B	1	NAG	O7-C7-N2	2.43	126.42	121.95
4	C	3	BMA	C1-O5-C5	-2.42	108.92	112.19
3	B	4	XYP	O2-C2-C3	-2.36	105.41	110.14
3	B	5	FUC	O3-C3-C4	-2.36	104.89	110.35
4	C	1	NAG	C6-C5-C4	-2.36	107.48	113.00
2	A	2	NAG	O3-C3-C4	2.34	115.75	110.35
4	C	2	NAG	O4-C4-C5	-2.33	103.51	109.30
4	C	5	MAN	O4-C4-C3	2.32	115.71	110.35
4	C	3	BMA	O2-C2-C1	2.31	113.88	109.15
2	A	1	NAG	O7-C7-C8	2.29	126.31	122.06
4	C	1	NAG	O3-C3-C2	-2.29	104.74	109.47
3	B	3	BMA	O5-C5-C6	-2.18	103.78	107.20
2	A	2	NAG	O4-C4-C3	-2.17	105.32	110.35
3	B	4	XYP	O3-C3-C2	-2.10	105.98	109.99
3	B	5	FUC	C3-C4-C5	2.07	112.99	109.77
3	B	2	NAG	O5-C5-C6	-2.00	104.07	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	6	MAN	C5

All (3) 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

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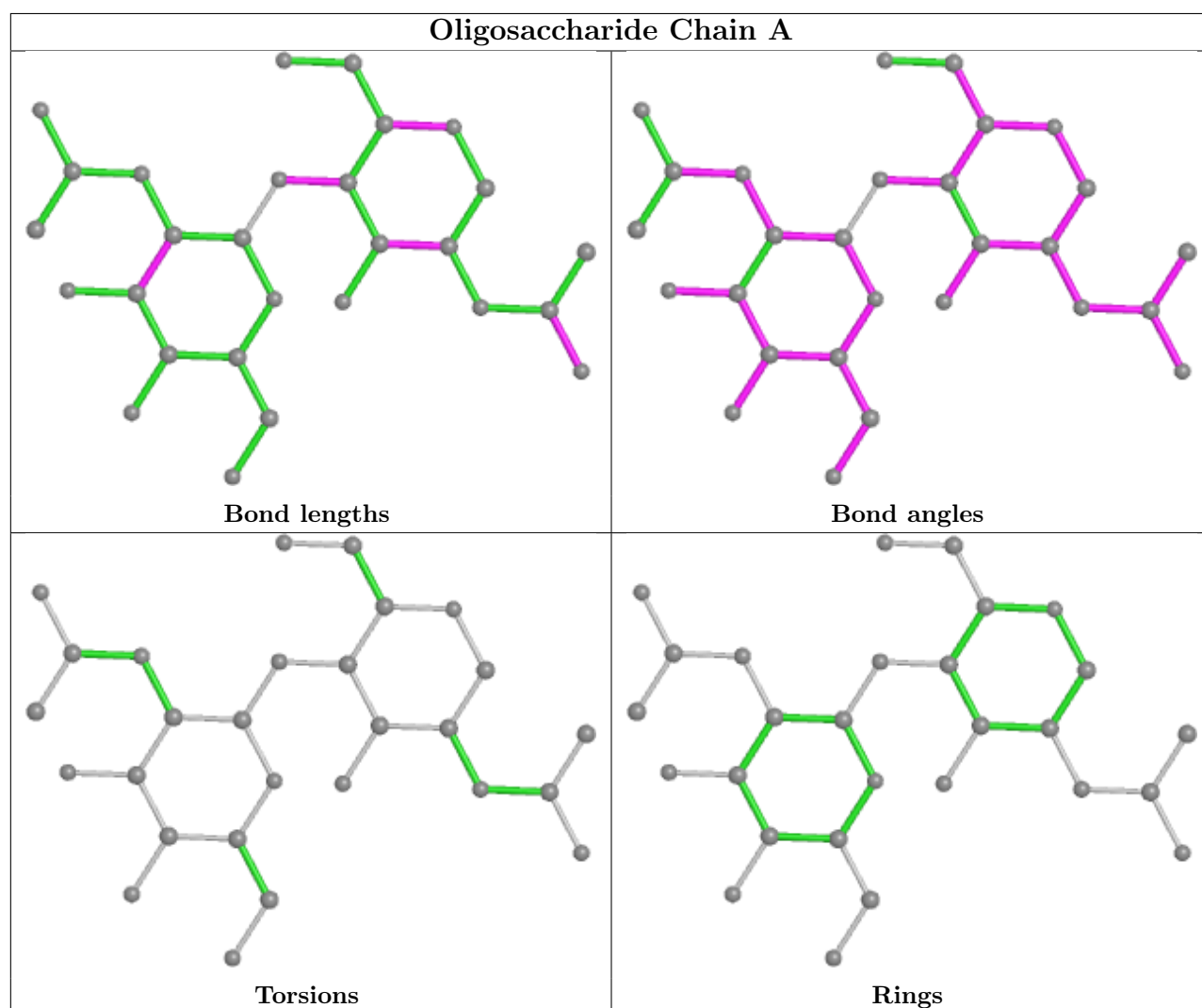
Mol	Chain	Res	Type	Atoms
4	C	6	MAN	C4-C5-C6-O6

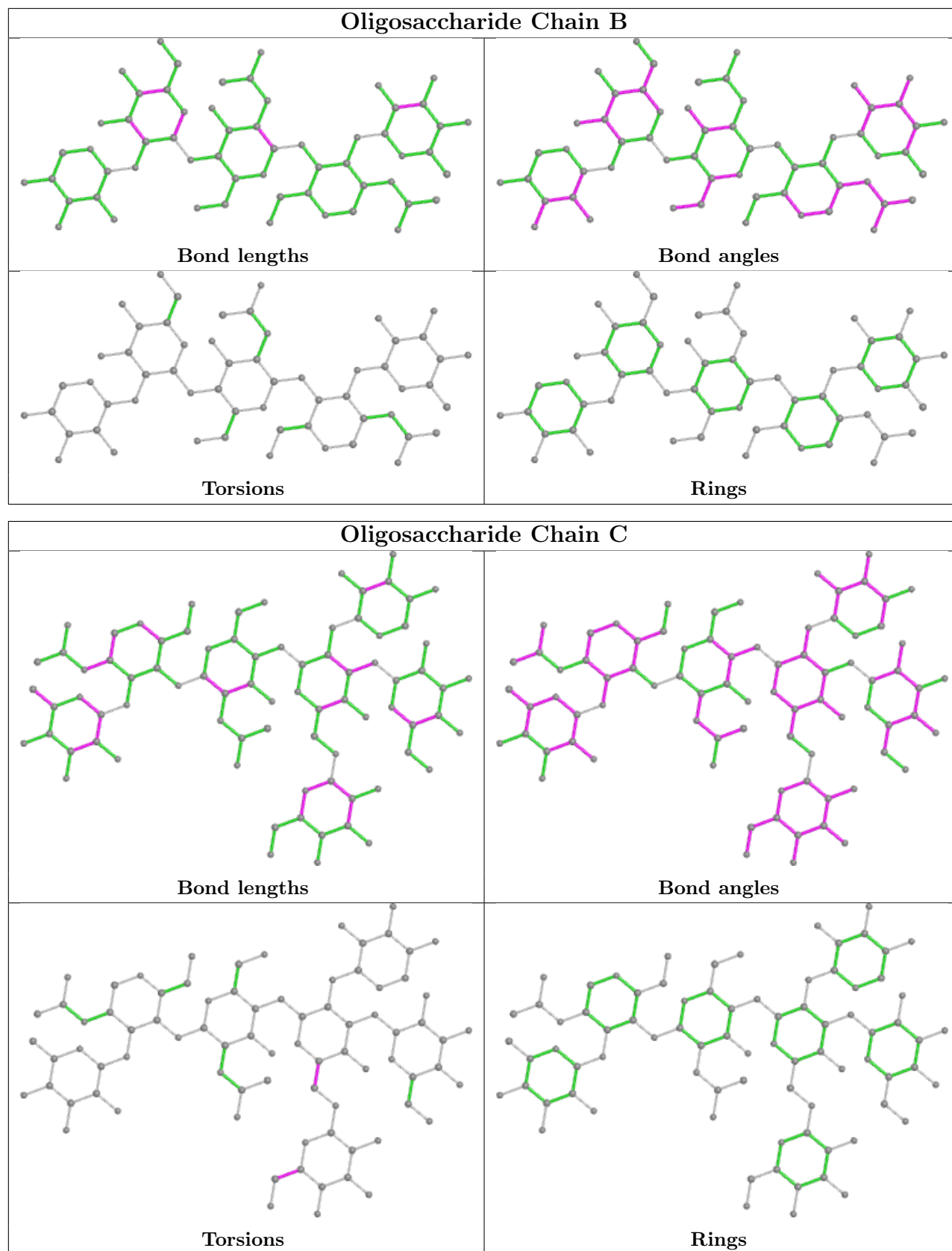
There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	5	0
4	C	6	MAN	13	0
4	C	3	BMA	10	0
4	C	1	NAG	4	0
2	A	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.





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	SO4	M	1504	-	4,4,4	0.64	0	6,6,6	1.00	0
5	NAG	M	911	1	14,14,15	1.26	1 (7%)	17,19,21	2.10	4 (23%)
5	NAG	M	961	1	14,14,15	1.36	1 (7%)	17,19,21	2.59	5 (29%)
9	SO4	M	1505	-	4,4,4	0.62	0	6,6,6	0.39	0
9	SO4	M	1509	-	4,4,4	0.80	0	6,6,6	1.19	1 (16%)
7	GOL	M	1513[B]	-	5,5,5	0.91	0	5,5,5	2.53	2 (40%)
9	SO4	M	1510	-	4,4,4	0.64	0	6,6,6	0.34	0
5	NAG	M	991	1	14,14,15	1.25	1 (7%)	17,19,21	2.00	5 (29%)
7	GOL	M	1502	-	5,5,5	0.51	0	5,5,5	1.19	1 (20%)
5	NAG	M	901	1	14,14,15	1.14	1 (7%)	17,19,21	2.31	5 (29%)
7	GOL	M	1514	-	5,5,5	0.43	0	5,5,5	1.41	1 (20%)
9	SO4	M	1508	-	4,4,4	1.25	1 (25%)	6,6,6	1.66	1 (16%)
7	GOL	M	1515	-	5,5,5	0.57	0	5,5,5	1.68	2 (40%)
9	SO4	M	1507	-	4,4,4	0.46	0	6,6,6	0.53	0
9	SO4	M	1506	9	4,4,4	1.11	0	6,6,6	1.48	2 (33%)
7	GOL	M	1513[A]	-	5,5,5	0.91	0	5,5,5	1.57	1 (20%)
5	NAG	M	971	1	14,14,15	1.37	1 (7%)	17,19,21	3.56	6 (35%)
5	NAG	M	931	1	14,14,15	1.78	3 (21%)	17,19,21	8.35	10 (58%)
9	SO4	M	1511	9	4,4,4	1.20	1 (25%)	6,6,6	2.15	2 (33%)
6	ASC	M	995	-	12,12,12	4.69	9 (75%)	17,17,17	3.63	8 (47%)
7	GOL	M	1512	-	5,5,5	0.48	0	5,5,5	0.76	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
7	GOL	M	1512	-	-	4/4/4/4	-
7	GOL	M	1502	-	-	0/4/4/4	-
7	GOL	M	1513[B]	-	-	2/4/4/4	-
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
5	NAG	M	901	1	-	0/6/23/26	0/1/1/1
5	NAG	M	961	1	-	0/6/23/26	0/1/1/1
7	GOL	M	1514	-	-	0/4/4/4	-
7	GOL	M	1513[A]	-	-	0/4/4/4	-
7	GOL	M	1515	-	-	1/4/4/4	-
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
6	ASC	M	995	-	-	0/6/22/22	0/1/1/1
5	NAG	M	991	1	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	995	ASC	C2-C1	8.92	1.65	1.45
6	M	995	ASC	O1-C1	-8.49	1.03	1.21
6	M	995	ASC	O4-C1	5.78	1.44	1.36
6	M	995	ASC	C4-C3	4.69	1.57	1.50
6	M	995	ASC	O4-C4	-4.60	1.37	1.45
5	M	911	NAG	O7-C7	-3.94	1.14	1.23
5	M	971	NAG	O7-C7	-3.88	1.14	1.23
5	M	931	NAG	O7-C7	-3.85	1.14	1.23
5	M	991	NAG	O7-C7	-3.82	1.14	1.23
6	M	995	ASC	O3-C3	3.79	1.45	1.33
5	M	931	NAG	C2-N2	-3.73	1.40	1.46
5	M	961	NAG	O7-C7	-3.53	1.15	1.23
5	M	901	NAG	O7-C7	-3.28	1.15	1.23
6	M	995	ASC	C2-C3	2.76	1.42	1.35
6	M	995	ASC	O2-C2	-2.76	1.24	1.33
5	M	931	NAG	C8-C7	-2.61	1.45	1.50
9	M	1508	SO4	O2-S	2.41	1.59	1.46
6	M	995	ASC	C5-C4	2.06	1.56	1.53
9	M	1511	SO4	O1-S	2.05	1.57	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	931	NAG	C2-N2-C7	27.95	162.71	122.90
5	M	931	NAG	C8-C7-N2	12.60	137.43	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	995	ASC	O4-C1-C2	-9.94	101.02	109.86
5	M	931	NAG	O7-C7-N2	-8.75	105.87	121.95
5	M	971	NAG	C1-O5-C5	8.67	123.94	112.19
5	M	931	NAG	C1-O5-C5	-7.94	101.44	112.19
5	M	961	NAG	C1-O5-C5	7.49	122.34	112.19
5	M	931	NAG	O5-C1-C2	7.40	122.97	111.29
5	M	971	NAG	O5-C1-C2	-7.14	100.02	111.29
5	M	971	NAG	O5-C5-C6	-7.11	96.06	107.20
5	M	911	NAG	C1-O5-C5	-6.74	103.06	112.19
6	M	995	ASC	C4-O4-C1	6.38	116.46	109.25
5	M	991	NAG	C4-C3-C2	-5.56	102.87	111.02
5	M	901	NAG	C1-O5-C5	-5.38	104.90	112.19
6	M	995	ASC	O1-C1-C2	5.32	137.71	129.37
5	M	961	NAG	C1-C2-N2	-5.17	101.65	110.49
7	M	1513[B]	GOL	O1-C1-C2	4.45	131.53	110.20
5	M	901	NAG	O5-C1-C2	4.08	117.73	111.29
5	M	971	NAG	O3-C3-C2	-3.62	101.97	109.47
9	M	1511	SO4	O4-S-O3	3.56	124.24	109.06
5	M	931	NAG	C1-C2-N2	3.54	116.53	110.49
5	M	901	NAG	O5-C5-C4	-3.43	102.47	110.83
6	M	995	ASC	O2-C2-C1	3.35	130.92	122.37
7	M	1513[A]	GOL	O2-C2-C1	3.28	123.59	109.12
7	M	1513[B]	GOL	O2-C2-C1	3.28	123.59	109.12
5	M	901	NAG	O3-C3-C2	-3.28	102.67	109.47
5	M	901	NAG	C4-C3-C2	-3.28	106.21	111.02
6	M	995	ASC	O4-C4-C3	3.27	107.08	103.71
5	M	971	NAG	O5-C5-C4	-2.96	103.62	110.83
5	M	931	NAG	O7-C7-C8	-2.90	116.67	122.06
5	M	931	NAG	O5-C5-C4	-2.90	103.78	110.83
5	M	961	NAG	O4-C4-C5	-2.87	102.17	109.30
5	M	931	NAG	C3-C4-C5	2.83	115.29	110.24
5	M	991	NAG	O5-C1-C2	2.77	115.67	111.29
5	M	991	NAG	O3-C3-C2	-2.73	103.82	109.47
5	M	911	NAG	O3-C3-C2	-2.71	103.87	109.47
6	M	995	ASC	O3-C3-C2	2.70	139.38	132.29
9	M	1506	SO4	O4-S-O3	2.69	120.56	109.06
5	M	971	NAG	O4-C4-C3	2.64	116.45	110.35
6	M	995	ASC	O2-C2-C3	-2.63	120.59	128.44
9	M	1509	SO4	O4-S-O1	2.51	122.40	109.31
5	M	991	NAG	C1-C2-N2	-2.49	106.24	110.49
7	M	1515	GOL	C3-C2-C1	-2.47	102.11	111.70
7	M	1514	GOL	O2-C2-C3	2.47	119.99	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1511	SO4	O2-S-O1	-2.44	91.43	109.43
5	M	931	NAG	O4-C4-C5	-2.32	103.54	109.30
5	M	961	NAG	O3-C3-C2	-2.30	104.70	109.47
9	M	1508	SO4	O3-S-O2	-2.22	97.71	109.31
7	M	1515	GOL	O3-C3-C2	-2.20	99.65	110.20
9	M	1506	SO4	O3-S-O2	-2.20	97.83	109.31
5	M	991	NAG	O5-C5-C4	-2.18	105.52	110.83
5	M	911	NAG	O5-C5-C4	-2.13	105.65	110.83
5	M	961	NAG	C6-C5-C4	-2.13	108.02	113.00
7	M	1502	GOL	O3-C3-C2	2.09	120.24	110.20
5	M	911	NAG	C4-C3-C2	-2.03	108.04	111.02
6	M	995	ASC	C6-C5-C4	2.03	115.34	111.86

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	1512	GOL	O1-C1-C2-O2
7	M	1512	GOL	O1-C1-C2-C3
7	M	1512	GOL	C1-C2-C3-O3
7	M	1513[B]	GOL	O1-C1-C2-C3
5	M	971	NAG	O5-C5-C6-O6
5	M	931	NAG	C8-C7-N2-C2
5	M	931	NAG	O7-C7-N2-C2
7	M	1512	GOL	O2-C2-C3-O3
5	M	971	NAG	C4-C5-C6-O6
7	M	1515	GOL	O1-C1-C2-C3
7	M	1513[B]	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	911	NAG	4	0
5	M	901	NAG	4	0
7	M	1514	GOL	1	0
9	M	1506	SO4	5	0
5	M	931	NAG	10	0
9	M	1511	SO4	7	0
6	M	995	ASC	1	0
7	M	1512	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%)	-0.35	11 (2%) 62 67	10, 14, 27, 54	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	6.4
1	M	377	ASP	6.2
1	M	375	LYS	4.3
1	M	380	ASP	4.2
1	M	417	ASP	3.5
1	M	3	GLU	3.4
1	M	378	SER	2.9
1	M	374	ASP	2.8
1	M	481	ASN	2.7
1	M	379	THR	2.2
1	M	19	ALA	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.

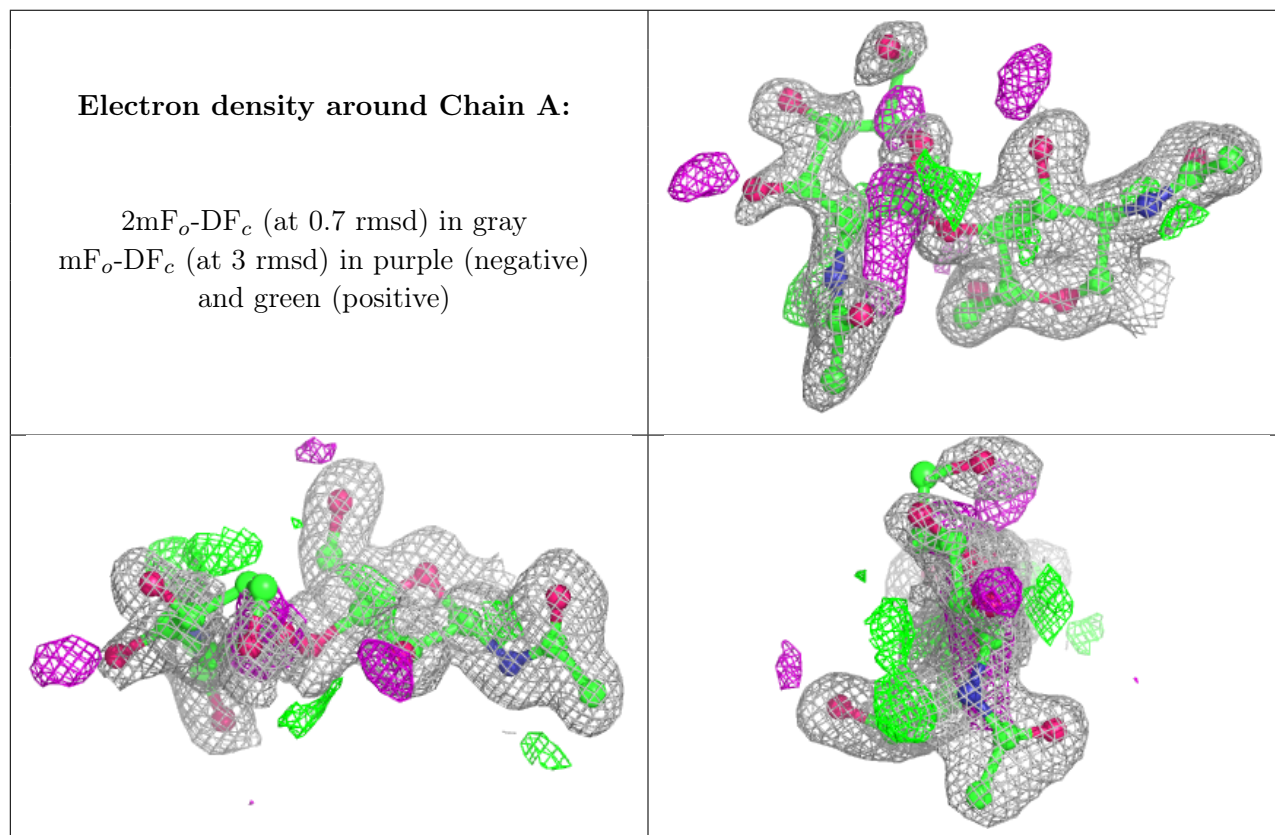
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	2	14/15	0.47	0.34	37,42,51,52	0

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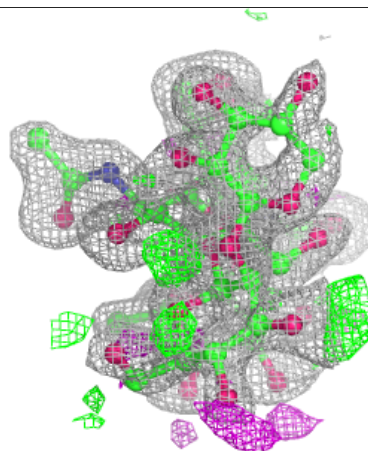
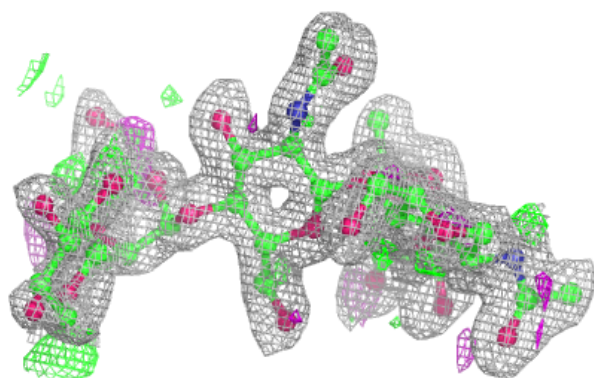
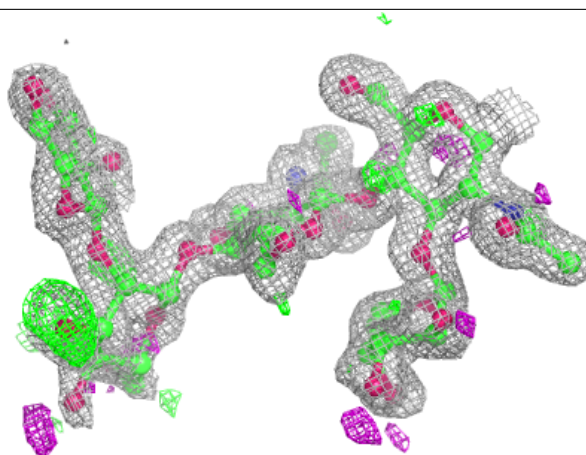
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	XYP	C	4	9/10	0.49	0.34	37,40,44,46	0
4	MAN	C	5	11/12	0.54	0.36	27,39,44,45	0
4	MAN	C	6	11/12	0.60	0.48	38,44,50,53	0
3	BMA	B	3	11/12	0.65	0.31	36,39,43,46	0
3	XYP	B	4	9/10	0.73	0.32	40,43,44,45	0
4	BMA	C	3	11/12	0.81	0.12	23,29,32,36	0
4	FUC	C	7	10/11	0.86	0.14	21,23,26,27	0
3	FUC	B	5	10/11	0.89	0.18	28,32,35,36	0
4	NAG	C	2	14/15	0.91	0.11	21,23,29,32	0
2	NAG	A	1	14/15	0.91	0.08	19,24,29,31	0
3	NAG	B	2	14/15	0.92	0.10	25,28,33,34	0
4	NAG	C	1	14/15	0.92	0.09	18,19,22,25	0
3	NAG	B	1	14/15	0.93	0.09	18,21,24,24	0

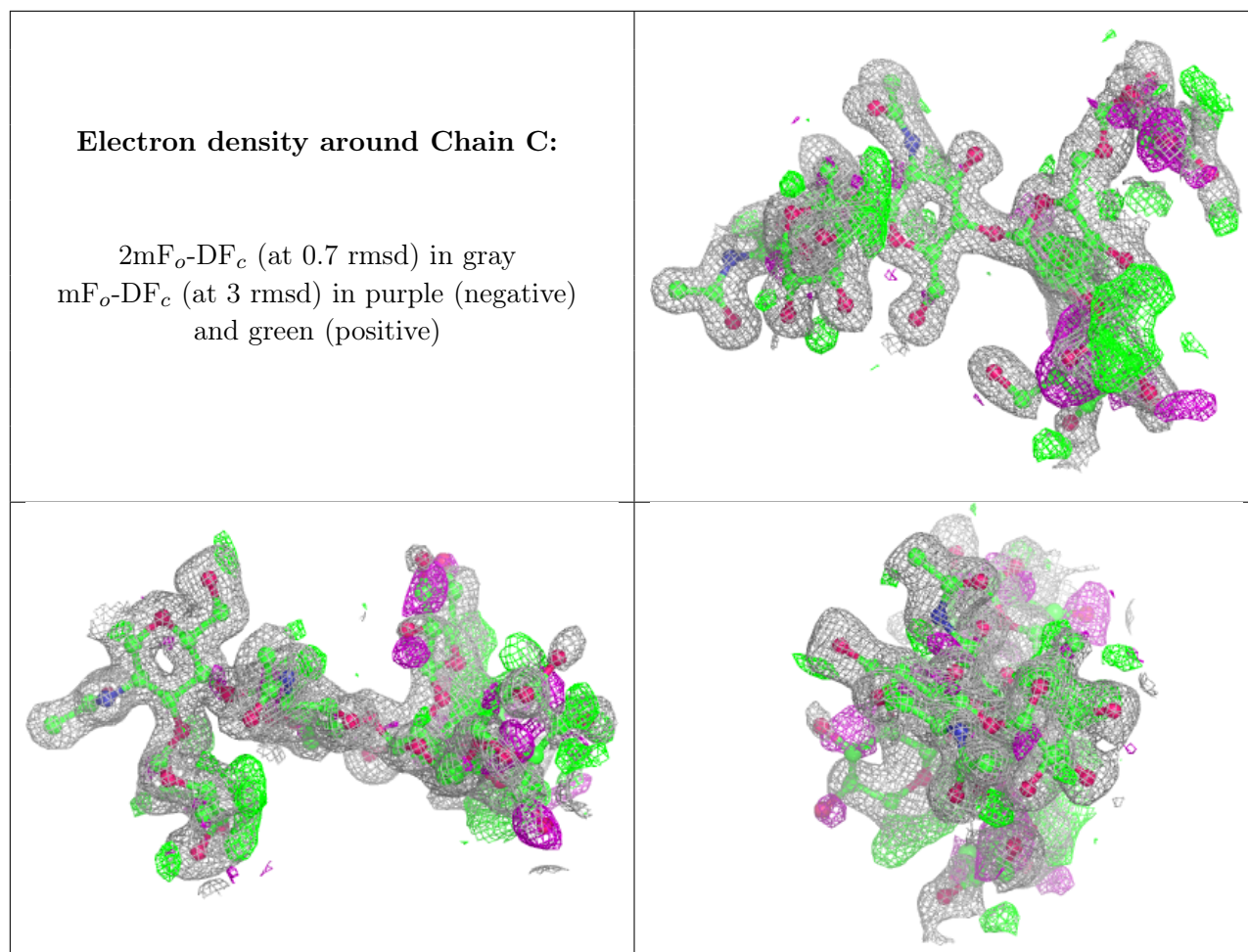
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain B:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	M	971	14/15	0.43	0.49	56,63,66,66	0
9	SO4	M	1509	5/5	0.53	0.26	27,33,34,36	5
7	GOL	M	1512	6/6	0.56	0.24	37,39,40,40	6
5	NAG	M	931	14/15	0.57	0.35	38,45,49,50	0
5	NAG	M	961	14/15	0.63	0.43	36,41,52,52	0
5	NAG	M	991	14/15	0.68	0.40	35,38,48,49	0
9	SO4	M	1508	5/5	0.69	0.31	29,32,36,36	5
7	GOL	M	1515	6/6	0.71	0.23	33,35,36,38	6
9	SO4	M	1506	5/5	0.72	0.30	25,32,33,35	5
5	NAG	M	901	14/15	0.77	0.16	30,35,37,40	0
9	SO4	M	1510	5/5	0.82	0.22	38,38,39,39	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	M	911	14/15	0.84	0.17	25,28,31,31	0
9	SO4	M	1511	5/5	0.84	0.33	39,39,42,42	1
7	GOL	M	1513[A]	6/6	0.88	0.14	12,15,17,17	2
7	GOL	M	1513[B]	6/6	0.88	0.14	12,15,17,17	2
6	ASC	M	995	12/12	0.89	0.12	17,20,22,23	0
7	GOL	M	1514	6/6	0.92	0.11	15,19,24,30	6
9	SO4	M	1505	5/5	0.93	0.16	23,27,30,30	5
7	GOL	M	1502	6/6	0.96	0.09	14,19,23,23	0
9	SO4	M	1504	5/5	0.98	0.15	22,23,27,28	5
9	SO4	M	1507	5/5	0.99	0.04	17,18,23,25	0
8	ZN	M	1503	1/1	1.00	0.03	11,11,11,11	1

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.