



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2026 – 06:26 PM EDT

PDB ID : 9YOC / pdb_00009yoc
Title : Crystal structure of integrin α 4b1 headpiece
Authors : Monroy, M.F.; Lin, F.Y.; Qiao, Q.
Deposited on : 2025-10-13
Resolution : 2.90 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

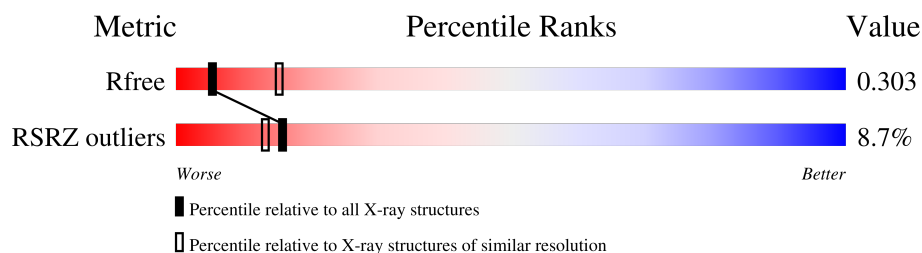
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16404 atoms, of which 8062 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 Integrin alpha-4, Integrin alpha-V heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	588	Total	C	H	N	O	S	0	0	0
			8985	2861	4448	788	866	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PHE	TYR	conflict	UNP P13612
A	589	GLY	-	expression tag	UNP P06756
A	590	GLY	-	expression tag	UNP P06756
A	591	SER	-	expression tag	UNP P06756
A	592	GLU	-	expression tag	UNP P06756
A	593	ASN	-	expression tag	UNP P06756
A	594	LEU	-	expression tag	UNP P06756
A	595	TYR	-	expression tag	UNP P06756
A	596	PHE	-	expression tag	UNP P06756
A	597	GLN	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	461	Total	C	H	N	O	S	0	0	0
			6935	2193	3416	595	703	28			

There are 27 discrepancies between the modelled and reference sequences:

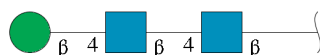
Chain	Residue	Modelled	Actual	Comment	Reference
B	195	THR	SER	conflict	UNP P05556
B	465	CYS	-	expression tag	UNP P05556
B	466	GLU	-	expression tag	UNP P05556
B	467	GLY	-	expression tag	UNP P05556
B	468	ALA	-	expression tag	UNP P05556
B	469	CYS	-	expression tag	UNP P05556

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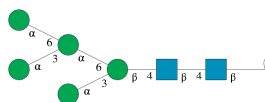
Chain	Residue	Modelled	Actual	Comment	Reference
B	470	ARG	-	expression tag	UNP P05556
B	471	CYS	-	expression tag	UNP P05556
B	472	ASN	-	expression tag	UNP P05556
B	473	GLU	-	expression tag	UNP P05556
B	474	GLY	-	expression tag	UNP P05556
B	475	ARG	-	expression tag	UNP P05556
B	476	VAL	-	expression tag	UNP P05556
B	477	GLY	-	expression tag	UNP P05556
B	478	ARG	-	expression tag	UNP P05556
B	479	HIS	-	expression tag	UNP P05556
B	480	CYS	-	expression tag	UNP P05556
B	481	GLU	-	expression tag	UNP P05556
B	482	GLY	-	expression tag	UNP P05556
B	483	GLY	-	expression tag	UNP P05556
B	484	SER	-	expression tag	UNP P05556
B	485	GLU	-	expression tag	UNP P05556
B	486	ASN	-	expression tag	UNP P05556
B	487	LEU	-	expression tag	UNP P05556
B	488	TYR	-	expression tag	UNP P05556
B	489	PHE	-	expression tag	UNP P05556
B	490	GLN	-	expression tag	UNP P05556

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	H	N	O	0	0	0
			136	46	53	2	35			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

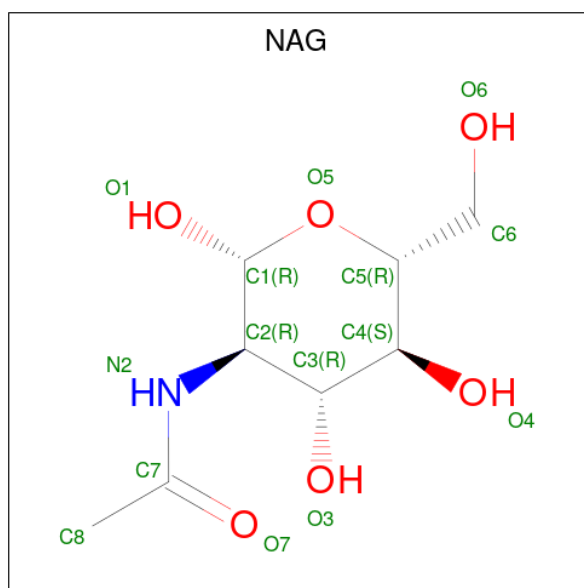


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	4	Total	C	H	N	O	0	0	0
			88	28	38	2	20			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Ca 3 3	0	0
6	B	2	Total Ca 2 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	B	1	Total	C	H	N	O	0	0
			24	8	10	1	5		
7	B	1	Total	C	H	N	O	0	0
			24	8	10	1	5		
7	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	15	Total	O	0	0
			15	15		
9	B	9	Total	O	0	0
			9	9		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.94Å 109.67Å 130.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.65 – 2.90 70.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.65-2.90) 99.8 (70.65-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.270 , 0.301 0.272 , 0.303	Depositor DCC
R_{free} test set	1784 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16404	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 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
3	NAG	C	1	3,1	14,14,15	0.29	0	17,19,21	0.44	0
3	NAG	C	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	BMA	C	3	3	11,11,12	0.58	0	15,15,17	0.77	0
4	NAG	D	1	1,4	14,14,15	0.81	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	D	2	4	14,14,15	0.92	1 (7%)	17,19,21	0.93	1 (5%)
4	BMA	D	3	4	11,11,12	0.76	0	15,15,17	0.77	0
4	MAN	D	4	4	11,11,12	1.04	1 (9%)	15,15,17	1.12	1 (6%)
4	MAN	D	5	4	11,11,12	0.70	0	15,15,17	1.39	1 (6%)
4	MAN	D	6	4	11,11,12	1.26	2 (18%)	15,15,17	2.13	2 (13%)
4	MAN	D	7	4	11,11,12	0.59	0	15,15,17	1.22	1 (6%)
5	NAG	E	1	5,1	14,14,15	0.33	0	17,19,21	0.39	0
5	NAG	E	2	5	14,14,15	0.21	0	17,19,21	0.52	0
5	BMA	E	3	5	11,11,12	0.54	0	15,15,17	0.86	0
5	MAN	E	4	5	11,11,12	0.60	0	15,15,17	1.14	2 (13%)

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
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	O5-C1	-3.09	1.38	1.43
4	D	1	NAG	O5-C1	-3.01	1.38	1.43
4	D	6	MAN	C1-C2	2.87	1.59	1.52
4	D	4	MAN	O5-C1	-2.70	1.39	1.43
4	D	6	MAN	O5-C1	2.17	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6	MAN	C1-O5-C5	7.26	121.92	112.19
4	D	5	MAN	C1-O5-C5	4.02	117.58	112.19
4	D	7	MAN	C1-O5-C5	3.59	117.00	112.19
5	E	4	MAN	C1-O5-C5	3.18	116.45	112.19
4	D	1	NAG	C1-O5-C5	-2.85	108.37	112.19
4	D	4	MAN	O2-C2-C3	-2.44	105.10	110.15
5	E	4	MAN	O2-C2-C3	-2.33	105.32	110.15
4	D	2	NAG	C1-O5-C5	-2.25	109.18	112.19
4	D	6	MAN	C1-C2-C3	2.16	112.78	109.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

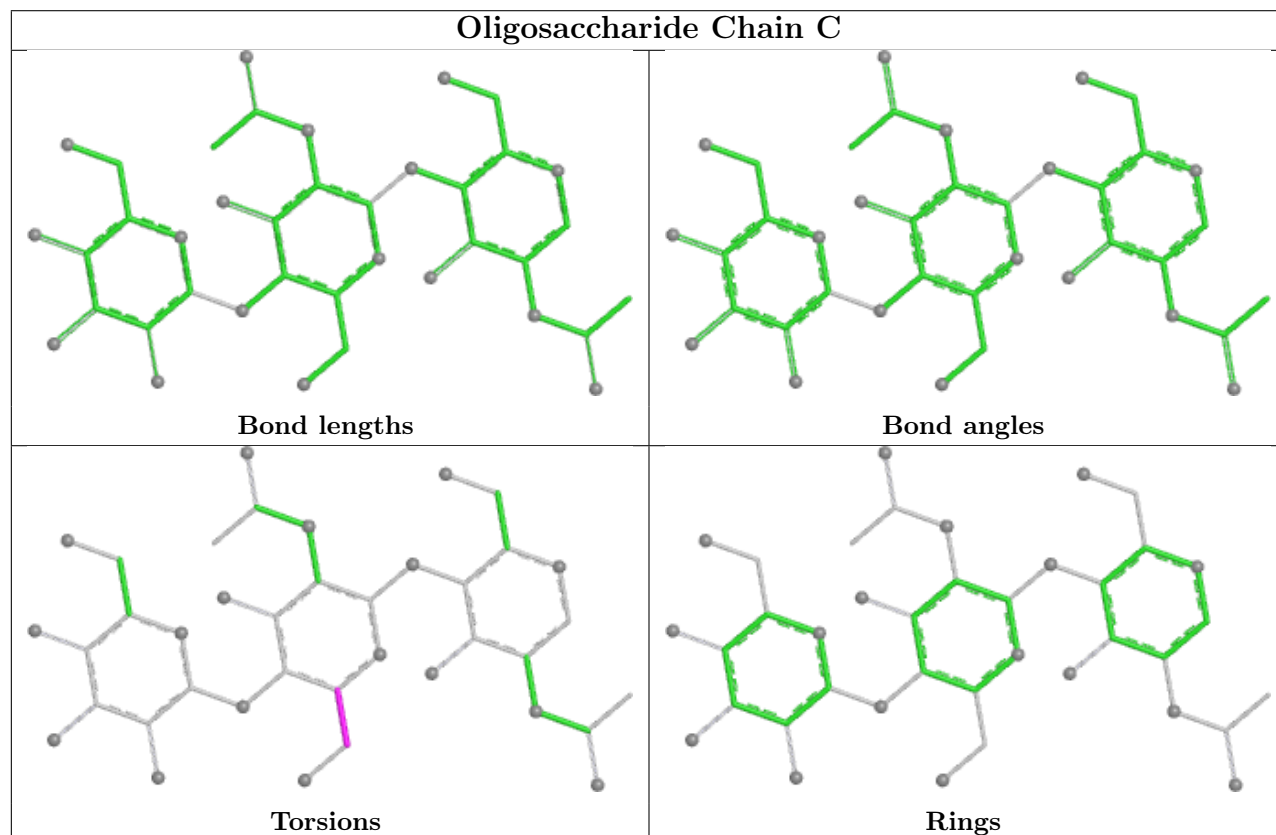
Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
4	D	4	MAN	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6

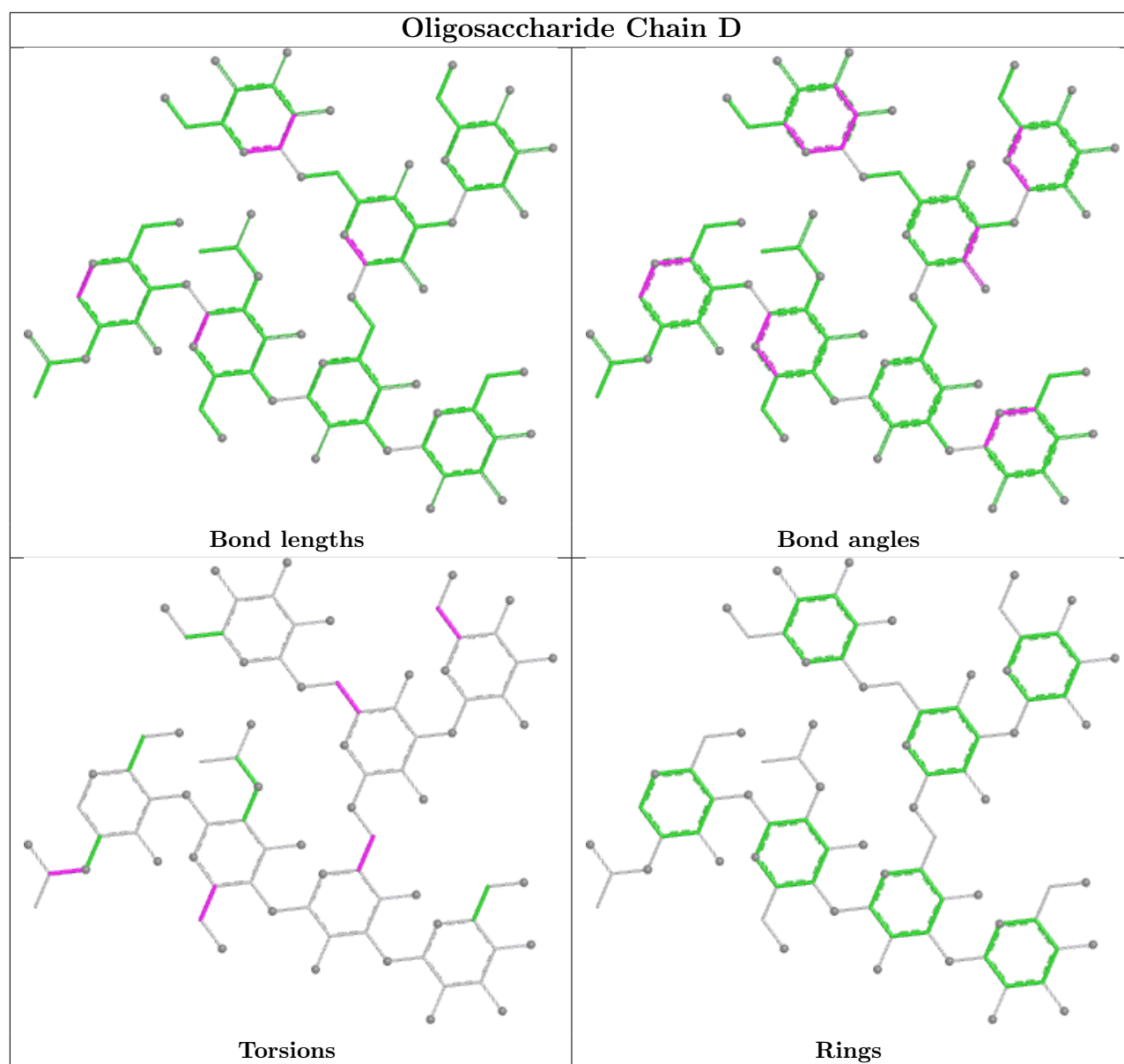
There are no ring outliers.

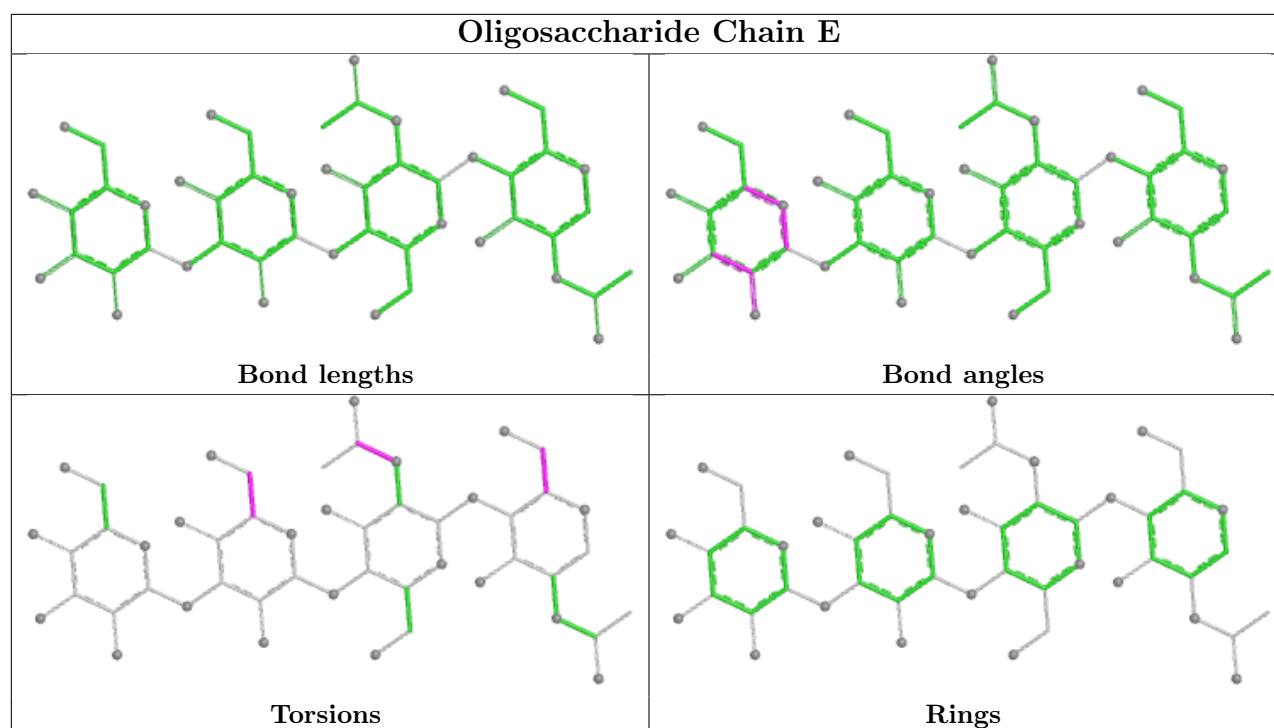
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	0	1

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







4.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	2005	1	14,14,15	0.34	0	17,19,21	1.08	1 (5%)
7	NAG	B	2005	-	14,14,15	0.28	0	17,19,21	0.35	0
7	NAG	B	2004	2	14,14,15	0.45	0	17,19,21	0.76	1 (5%)
7	NAG	A	2004	-	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
7	NAG	B	2006	2	14,14,15	1.05	2 (14%)	17,19,21	0.97	2 (11%)
7	NAG	A	2006	1	14,14,15	0.81	1 (7%)	17,19,21	1.10	2 (11%)

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	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
7	NAG	B	2005	-	-	2/6/23/26	0/1/1/1
7	NAG	B	2004	2	-	3/6/23/26	0/1/1/1
7	NAG	A	2004	-	-	2/6/23/26	0/1/1/1
7	NAG	B	2006	2	-	2/6/23/26	0/1/1/1
7	NAG	A	2006	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2006	NAG	C1-C2	2.84	1.56	1.52
7	A	2006	NAG	C1-C2	-2.81	1.48	1.52
7	B	2006	NAG	O5-C1	2.56	1.48	1.43
7	A	2004	NAG	O5-C1	-2.10	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2005	NAG	C1-O5-C5	3.68	117.12	112.19
7	A	2006	NAG	C1-O5-C5	2.63	115.72	112.19
7	B	2006	NAG	C1-O5-C5	2.43	115.44	112.19
7	B	2006	NAG	C1-C2-N2	2.34	114.12	110.43
7	B	2004	NAG	C1-O5-C5	-2.18	109.27	112.19
7	A	2006	NAG	C4-C3-C2	-2.14	107.88	111.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2004	NAG	C8-C7-N2-C2
7	B	2004	NAG	O7-C7-N2-C2
7	B	2006	NAG	C8-C7-N2-C2
7	B	2006	NAG	O7-C7-N2-C2
7	A	2005	NAG	O5-C5-C6-O6
7	A	2005	NAG	C4-C5-C6-O6
7	A	2004	NAG	O5-C5-C6-O6
7	A	2004	NAG	C4-C5-C6-O6
7	B	2005	NAG	C3-C2-N2-C7
7	B	2005	NAG	C1-C2-N2-C7
7	B	2004	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	588/597 (98%)	0.64	45 (7%)	19 16	42, 76, 131, 229	0
2	B	461/490 (94%)	0.83	46 (9%)	12 10	51, 104, 164, 218	0
All	All	1049/1087 (96%)	0.73	91 (8%)	16 13	42, 87, 151, 229	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	172	VAL	5.7
2	B	471	CYS	5.1
1	A	421	ARG	4.6
2	B	3	THR	4.5
2	B	183	LEU	4.4
2	B	469	CYS	4.4
1	A	275	ALA	4.2
2	B	150	MET	4.1
2	B	86	LEU	3.5
1	A	34	LEU	3.4
1	A	359	GLN	3.3
2	B	458	HIS	3.3
1	A	445	SER	3.3
2	B	275	LEU	3.3
2	B	167	PHE	3.2
1	A	282	LEU	3.2
1	A	272	TYR	3.2
2	B	92	THR	3.1
2	B	223	GLY	3.1
2	B	21	ALA	3.1
1	A	27	SER	3.1
2	B	155	ARG	3.0
1	A	318	MET	3.0
1	A	379	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	446	CYS	2.9
2	B	468	ALA	2.8
1	A	36	VAL	2.8
2	B	11	ASN	2.8
2	B	40	THR	2.7
1	A	500	ALA	2.6
2	B	4	GLU	2.6
1	A	19	PHE	2.6
2	B	399	SER	2.6
1	A	446	ILE	2.6
1	A	497	GLN	2.6
1	A	416	ALA	2.6
1	A	35	LEU	2.6
1	A	422	SER	2.5
1	A	74	GLY	2.5
1	A	356	GLY	2.5
2	B	10	ALA	2.5
2	B	116	LYS	2.5
1	A	269	LEU	2.5
1	A	290	LEU	2.5
1	A	402	SER	2.5
1	A	149	PRO	2.5
1	A	420	PHE	2.5
2	B	386	ASN	2.5
1	A	225	GLY	2.4
2	B	293	TYR	2.4
2	B	427	PRO	2.4
2	B	186	PRO	2.4
1	A	504	ALA	2.4
1	A	192	LEU	2.4
1	A	458	GLY	2.4
2	B	29	THR	2.4
2	B	417	LYS	2.3
2	B	76	THR	2.3
1	A	498	LYS	2.3
2	B	75	VAL	2.3
1	A	352	ASP	2.3
2	B	182	LYS	2.3
2	B	349	GLN	2.3
2	B	347	VAL	2.3
2	B	328	LEU	2.2
1	A	234	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	341	ASN	2.2
2	B	385	VAL	2.2
2	B	235	ILE	2.2
1	A	547	PRO	2.2
1	A	419	ALA	2.2
2	B	319	GLU	2.1
1	A	55	ILE	2.1
2	B	33	PHE	2.1
2	B	156	ILE	2.1
1	A	395	SER	2.1
1	A	521	SER	2.1
2	B	248	ARG	2.1
2	B	273	ILE	2.1
1	A	513	SER	2.0
2	B	105	SER	2.0
1	A	71	LEU	2.0
2	B	464	PHE	2.0
1	A	60	ILE	2.0
2	B	112	THR	2.0
1	A	230	GLN	2.0
2	B	77	ASN	2.0
2	B	192	ASN	2.0
1	A	255	GLU	2.0
1	A	195	TYR	2.0
1	A	340	VAL	2.0

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

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

5.3 Carbohydrates ⓘ

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

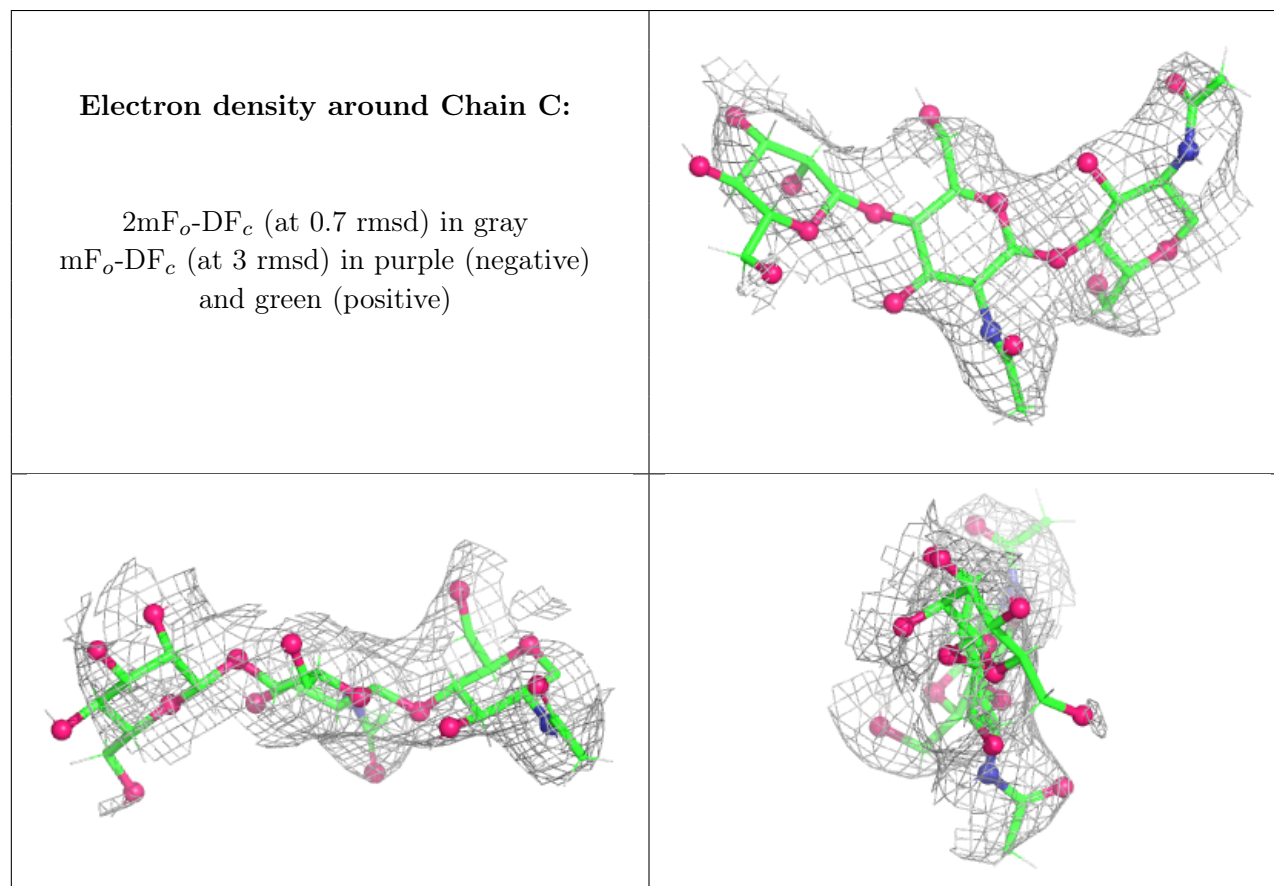
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	E	3	11/12	0.05	0.16	103,113,133,134	0
5	MAN	E	4	11/12	0.24	0.18	119,122,147,147	0
3	BMA	C	3	11/12	0.29	0.12	121,126,151,152	0

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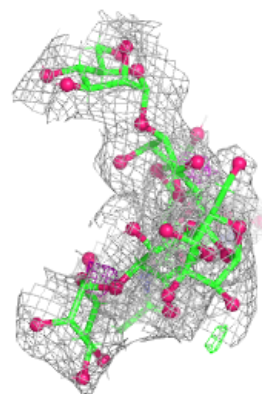
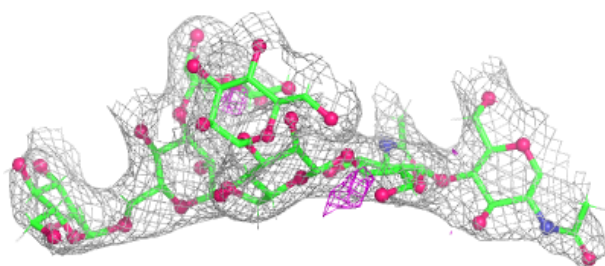
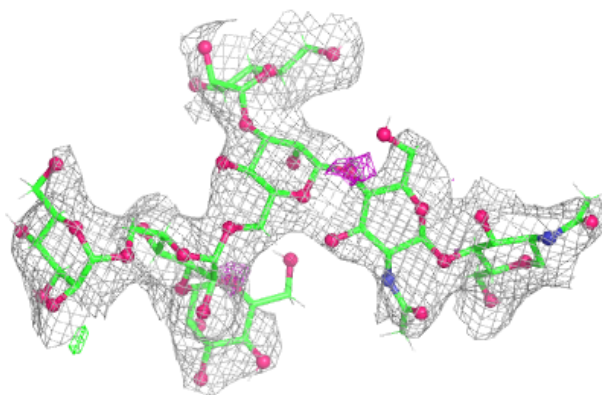
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	D	7	11/12	0.32	0.15	101,103,124,125	0
5	NAG	E	2	14/15	0.52	0.18	109,119,143,143	0
5	NAG	E	1	14/15	0.54	0.15	87,108,131,131	0
4	MAN	D	6	11/12	0.57	0.12	95,96,116,116	0
3	NAG	C	2	14/15	0.59	0.11	88,105,127,129	0
4	MAN	D	4	11/12	0.69	0.11	87,92,110,110	0
4	NAG	D	2	14/15	0.70	0.12	87,99,119,119	0
4	MAN	D	5	11/12	0.70	0.11	102,110,137,139	0
4	NAG	D	1	14/15	0.77	0.11	65,70,84,90	0
3	NAG	C	1	14/15	0.86	0.09	65,85,101,101	0
4	BMA	D	3	11/12	0.88	0.09	94,103,122,122	0

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

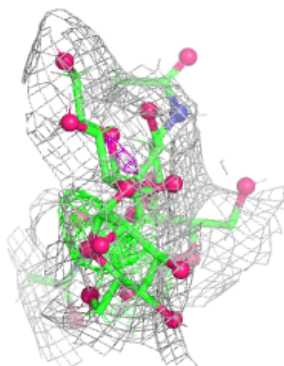
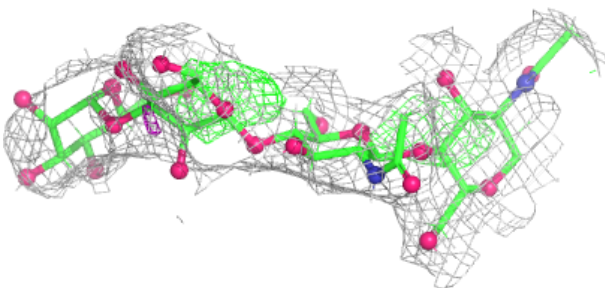
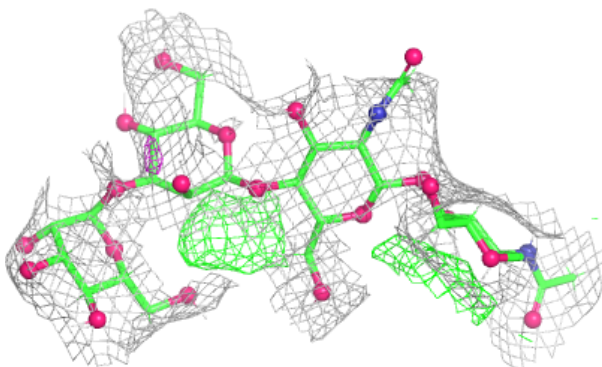


Electron density around Chain D:

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

**Electron density around Chain E:**

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



5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	2006	14/15	0.10	0.17	75,96,123,123	0
7	NAG	B	2004	14/15	0.19	0.16	65,96,116,116	0
7	NAG	A	2006	14/15	0.34	0.15	70,104,126,130	0
7	NAG	A	2005	14/15	0.45	0.16	68,86,103,107	0
7	NAG	A	2004	14/15	0.52	0.13	113,117,140,141	0
7	NAG	B	2005	14/15	0.67	0.11	65,73,88,88	0
6	CA	A	2003	1/1	0.95	0.06	65,65,65,65	0
6	CA	B	2002	1/1	0.95	0.05	167,167,167,167	0
6	CA	A	2001	1/1	0.97	0.05	65,65,65,65	0
6	CA	A	2002	1/1	0.98	0.04	74,74,74,74	0
6	CA	B	2003	1/1	0.98	0.04	65,65,65,65	0
8	MG	B	2001	1/1	0.98	0.04	65,65,65,65	0

5.5 Other polymers [i](#)

There are no such residues in this entry.