



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 01:36 AM BST

PDB ID : 6QWN
Title : Protein peptide complex
Authors : Moussu, S.; Caroline, C.; Santos-Fernandez, G.; Wehrle, S.; Grossniklaus, U.;
Santiago, J.
Deposited on : 2019-03-05
Resolution : 3.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

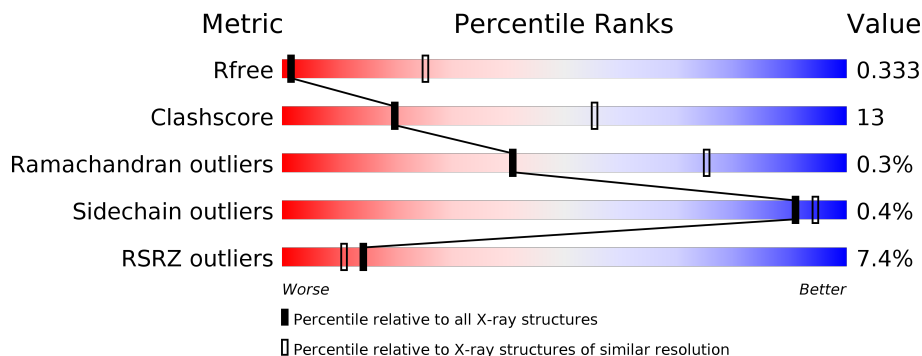
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 on 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	A	379	
1	B	379	
1	C	379	
1	D	379	
1	E	379	
2	F	56	

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Mol	Chain	Length	Quality of chain
2	G	56	
2	H	56	
2	I	56	
2	J	56	
3	K	4	
4	L	2	
5	M	3	
6	N	2	
7	O	3	

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
3	MAN	K	4	-	-	-	X
4	NAG	L	2	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15070 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 Pollen-specific leucine-rich repeat extensin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2585	1649	429	493	14	0	0	0
1	B	338	2601	1659	432	496	14	0	0	0
1	C	338	2612	1667	432	500	13	0	0	0
1	D	336	2589	1653	430	493	13	0	0	0
1	E	322	2489	1590	414	472	13	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	initiating methionine	UNP Q9LJ64
A	30	GLU	-	expression tag	UNP Q9LJ64
A	401	LEU	-	expression tag	UNP Q9LJ64
A	402	GLU	-	expression tag	UNP Q9LJ64
A	403	GLY	-	expression tag	UNP Q9LJ64
A	404	SER	-	expression tag	UNP Q9LJ64
A	405	GLU	-	expression tag	UNP Q9LJ64
A	406	ASN	-	expression tag	UNP Q9LJ64
A	407	LEU	-	expression tag	UNP Q9LJ64
B	29	MET	-	initiating methionine	UNP Q9LJ64
B	30	GLU	-	expression tag	UNP Q9LJ64
B	401	LEU	-	expression tag	UNP Q9LJ64
B	402	GLU	-	expression tag	UNP Q9LJ64
B	403	GLY	-	expression tag	UNP Q9LJ64
B	404	SER	-	expression tag	UNP Q9LJ64
B	405	GLU	-	expression tag	UNP Q9LJ64
B	406	ASN	-	expression tag	UNP Q9LJ64
B	407	LEU	-	expression tag	UNP Q9LJ64
C	29	MET	-	initiating methionine	UNP Q9LJ64

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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	GLU	-	expression tag	UNP Q9LJ64
C	401	LEU	-	expression tag	UNP Q9LJ64
C	402	GLU	-	expression tag	UNP Q9LJ64
C	403	GLY	-	expression tag	UNP Q9LJ64
C	404	SER	-	expression tag	UNP Q9LJ64
C	405	GLU	-	expression tag	UNP Q9LJ64
C	406	ASN	-	expression tag	UNP Q9LJ64
C	407	LEU	-	expression tag	UNP Q9LJ64
D	29	MET	-	initiating methionine	UNP Q9LJ64
D	30	GLU	-	expression tag	UNP Q9LJ64
D	401	LEU	-	expression tag	UNP Q9LJ64
D	402	GLU	-	expression tag	UNP Q9LJ64
D	403	GLY	-	expression tag	UNP Q9LJ64
D	404	SER	-	expression tag	UNP Q9LJ64
D	405	GLU	-	expression tag	UNP Q9LJ64
D	406	ASN	-	expression tag	UNP Q9LJ64
D	407	LEU	-	expression tag	UNP Q9LJ64
E	29	MET	-	initiating methionine	UNP Q9LJ64
E	30	GLU	-	expression tag	UNP Q9LJ64
E	401	LEU	-	expression tag	UNP Q9LJ64
E	402	GLU	-	expression tag	UNP Q9LJ64
E	403	GLY	-	expression tag	UNP Q9LJ64
E	404	SER	-	expression tag	UNP Q9LJ64
E	405	GLU	-	expression tag	UNP Q9LJ64
E	406	ASN	-	expression tag	UNP Q9LJ64
E	407	LEU	-	expression tag	UNP Q9LJ64

- Molecule 2 is a protein called Protein RALF-like 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	47	Total	C	N	O	S	0	0	0
			403	244	90	65	4			
2	G	47	Total	C	N	O	S	0	0	0
			403	244	90	65	4			
2	H	47	Total	C	N	O	S	0	0	0
			403	244	90	65	4			
2	I	47	Total	C	N	O	S	0	0	0
			403	244	90	65	4			
2	J	47	Total	C	N	O	S	0	0	0
			356	219	70	63	4			

There are 10 discrepancies between the modelled and reference sequences:

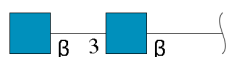
Chain	Residue	Modelled	Actual	Comment	Reference
F	1052	MET	-	initiating methionine	UNP Q9FZA0
F	1053	GLY	-	expression tag	UNP Q9FZA0
G	1052	MET	-	initiating methionine	UNP Q9FZA0
G	1053	GLY	-	expression tag	UNP Q9FZA0
H	1052	MET	-	initiating methionine	UNP Q9FZA0
H	1053	GLY	-	expression tag	UNP Q9FZA0
I	1052	MET	-	initiating methionine	UNP Q9FZA0
I	1053	GLY	-	expression tag	UNP Q9FZA0
J	1052	MET	-	initiating methionine	UNP Q9FZA0
J	1053	GLY	-	expression tag	UNP Q9FZA0

- Molecule 3 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.



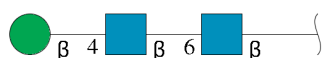
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	K	4	50	28	2	20	0	0	0

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



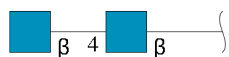
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	L	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	M	3	39	22	2	15	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



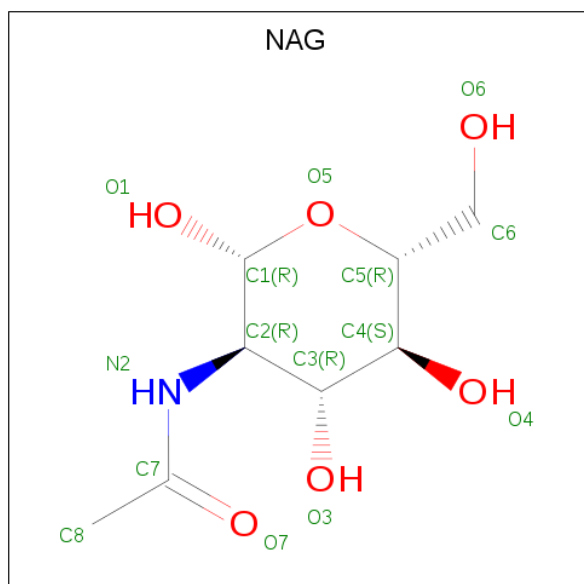
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	N	2	28	16	2	10	0	0	0

- Molecule 7 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
			Total	C	N	O			
7	O	3	39	22	2	15	39	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

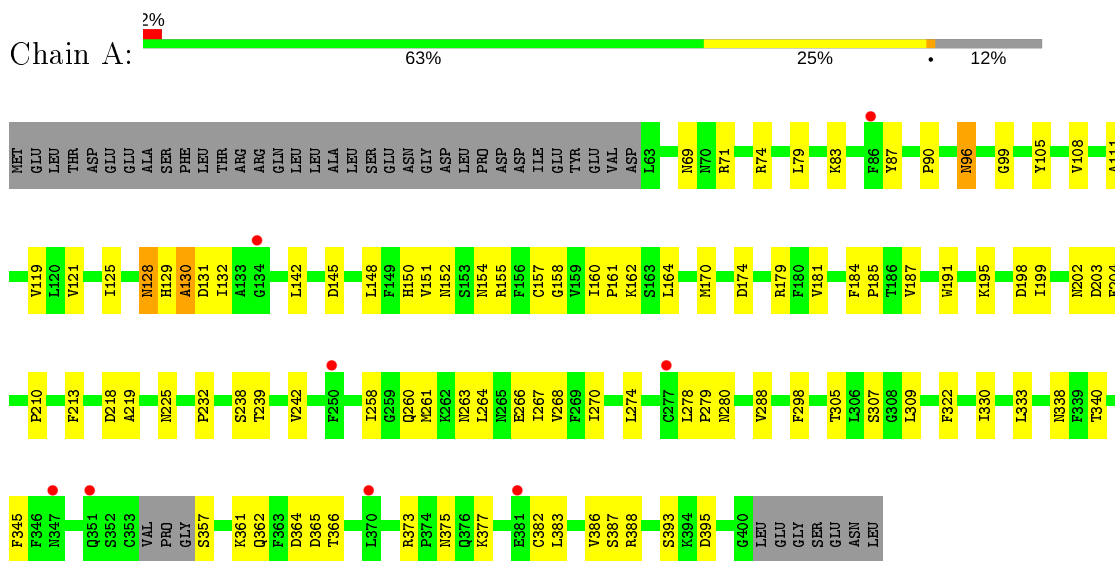


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 14	C 8	N 1	O 5	0	0
8	D	1	Total 14	C 8	N 1	O 5	0	0
8	D	1	Total 14	C 8	N 1	O 5	0	0

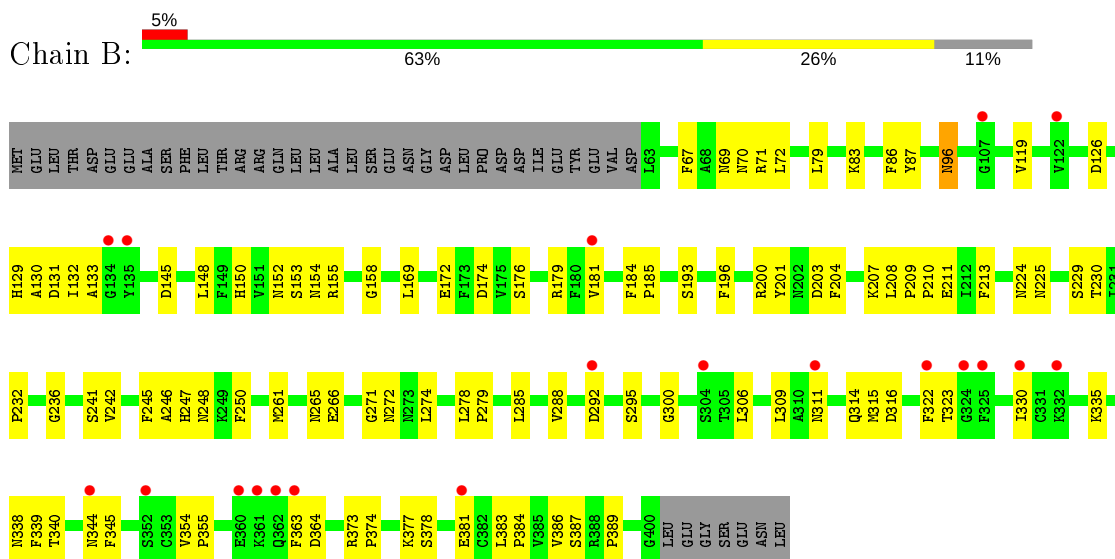
3 Residue-property plots [i](#)

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.

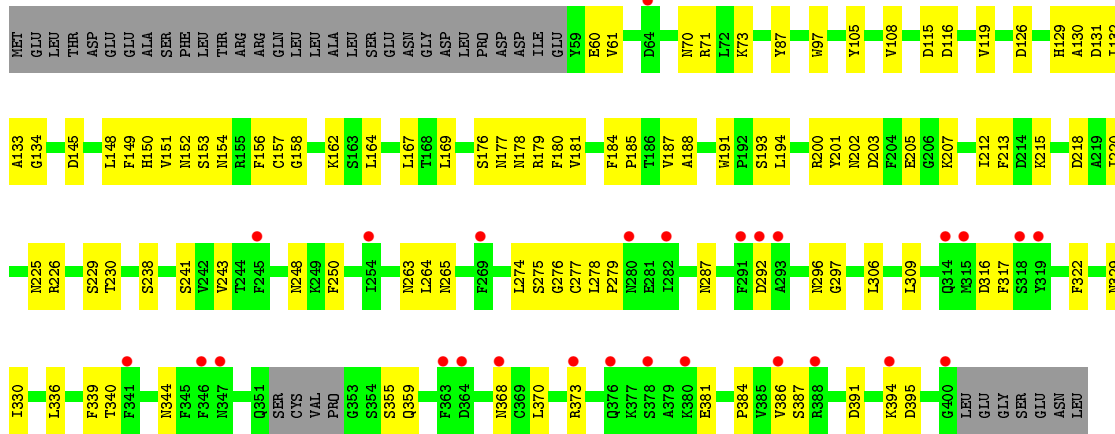
- Molecule 1: Pollen-specific leucine-rich repeat extensin-like protein 1



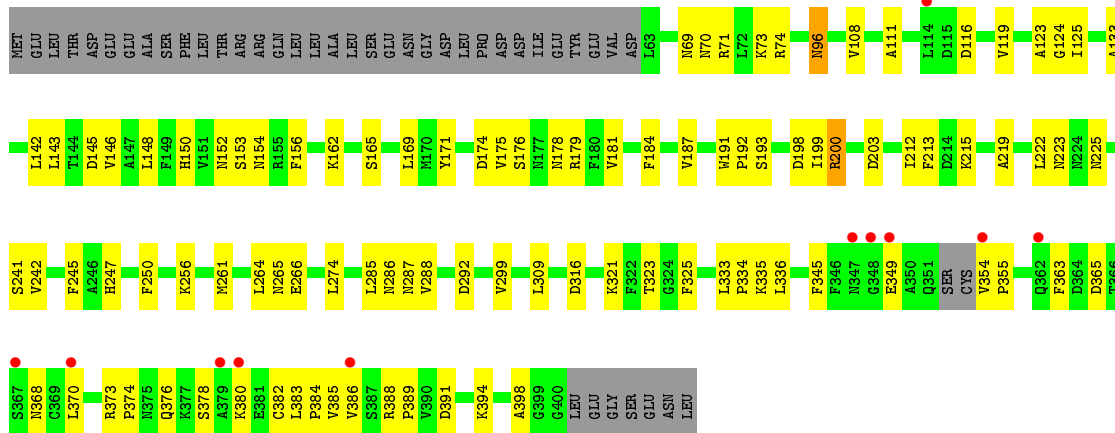
- Molecule 1: Pollen-specific leucine-rich repeat extensin-like protein 1



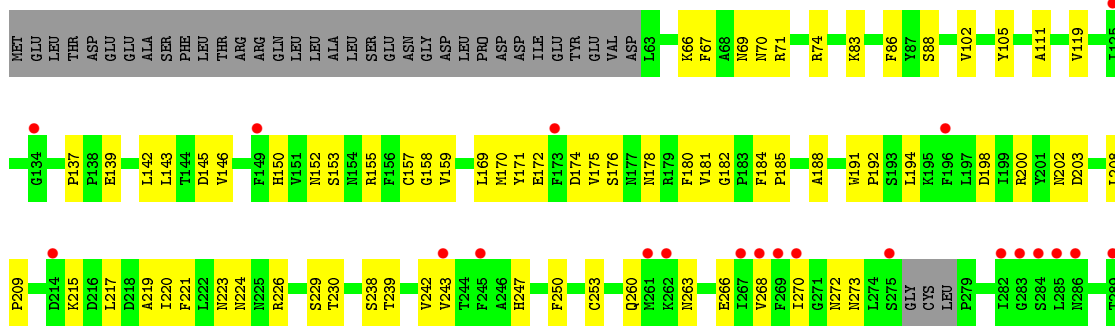
- Molecule 1: Pollen-specific leucine-rich repeat extensin-like protein 1

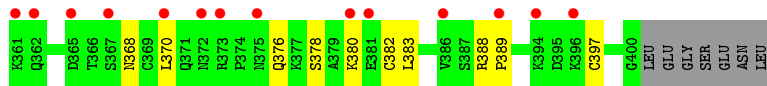
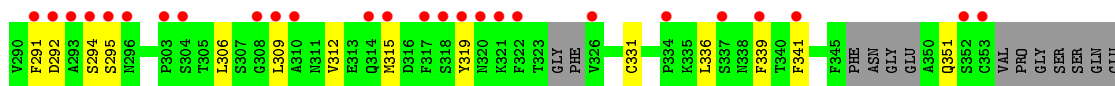


• Molecule 1: Pollen-specific leucine-rich repeat extensin-like protein 1



• Molecule 1: Pollen-specific leucine-rich repeat extensin-like protein 1





- Molecule 2: Protein RALF-like 4



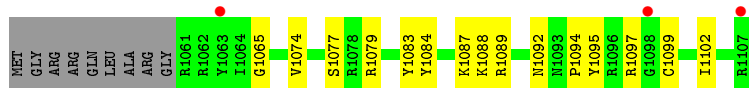
- Molecule 2: Protein RALF-like 4



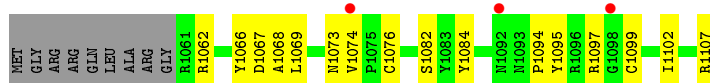
- Molecule 2: Protein RALF-like 4



- Molecule 2: Protein RALF-like 4



- Molecule 2: Protein RALF-like 4




- Molecule 3: 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



MAG1
MAG2
EMAS
MAN4

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2
EMAS

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50%

MAG1
MAG2

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2
EMAS

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.84Å 114.09Å 146.98Å 90.00° 116.25° 90.00°	Depositor
Resolution (Å)	49.44 – 3.89 49.46 – 3.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.44-3.89) 99.9 (49.46-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.46	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.282 , 0.329 0.285 , 0.333	Depositor DCC
R_{free} test set	1409 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	126.7	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.038 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h$ + $1/2^*k-l$ 0.048 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-$ $1/2^*k-l$	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15070	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	A	0.26	0/2647	0.49	0/3588
1	B	0.26	0/2665	0.48	1/3614 (0.0%)
1	C	0.26	0/2675	0.49	0/3626
1	D	0.26	0/2652	0.49	0/3595
1	E	0.26	0/2546	0.50	0/3447
2	F	0.25	0/411	0.46	0/546
2	G	0.25	0/411	0.47	0/546
2	H	0.32	0/411	0.55	0/546
2	I	0.25	0/411	0.46	0/546
2	J	0.26	0/364	0.61	0/492
All	All	0.26	0/15193	0.49	1/20546 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	LEU	CA-CB-CG	5.77	128.57	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASN	Peptide

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	A	2585	0	2489	66	0
1	B	2601	0	2503	76	0
1	C	2612	0	2510	78	0
1	D	2589	0	2492	76	0
1	E	2489	0	2409	69	0
2	F	403	0	400	12	0
2	G	403	0	400	8	0
2	H	403	0	400	14	0
2	I	403	0	400	13	0
2	J	356	0	312	14	0
3	K	50	0	43	0	0
4	L	28	0	25	0	0
5	M	39	0	34	0	0
6	N	28	0	25	0	0
7	O	39	0	34	0	0
8	A	14	0	13	0	0
8	D	28	0	26	1	0
All	All	15070	0	14515	372	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 13.

The worst 5 of 372 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:D:373:ARG:HD3	1:D:374:PRO:HD2	1.59	0.84
1:B:130:ALA:O	1:B:154:ASN:ND2	2.12	0.81
1:C:306:LEU:HD11	1:C:330:ILE:HG12	1.64	0.80
1:E:250:PHE:HB2	1:E:272:ASN:HD21	1.46	0.80
1:D:365:ASP:OD1	1:D:368:ASN:ND2	2.15	0.79

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	A	331/379 (87%)	289 (87%)	41 (12%)	1 (0%)	41	75
1	B	336/379 (89%)	301 (90%)	35 (10%)	0	100	100
1	C	334/379 (88%)	299 (90%)	34 (10%)	1 (0%)	41	75
1	D	332/379 (88%)	297 (90%)	33 (10%)	2 (1%)	25	63
1	E	312/379 (82%)	274 (88%)	37 (12%)	1 (0%)	41	75
2	F	45/56 (80%)	36 (80%)	9 (20%)	0	100	100
2	G	45/56 (80%)	38 (84%)	6 (13%)	1 (2%)	6	38
2	H	45/56 (80%)	32 (71%)	13 (29%)	0	100	100
2	I	45/56 (80%)	35 (78%)	10 (22%)	0	100	100
2	J	45/56 (80%)	36 (80%)	9 (20%)	0	100	100
All	All	1870/2175 (86%)	1637 (88%)	227 (12%)	6 (0%)	41	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	247	HIS
1	C	131	ASP
2	G	1092	ASN
1	D	345	PHE
1	E	188	ALA

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	A	292/331 (88%)	291 (100%)	1 (0%)	92	95
1	B	294/331 (89%)	293 (100%)	1 (0%)	92	95
1	C	294/331 (89%)	294 (100%)	0	100	100
1	D	292/331 (88%)	289 (99%)	3 (1%)	76	86
1	E	282/331 (85%)	282 (100%)	0	100	100
2	F	42/48 (88%)	42 (100%)	0	100	100
2	G	42/48 (88%)	42 (100%)	0	100	100
2	H	42/48 (88%)	41 (98%)	1 (2%)	49	69
2	I	42/48 (88%)	41 (98%)	1 (2%)	49	69
2	J	33/48 (69%)	33 (100%)	0	100	100
All	All	1655/1895 (87%)	1648 (100%)	7 (0%)	91	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	96	ASN
2	I	1089	ARG
1	D	200	ARG
1	B	96	ASN
1	D	325	PHE

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

Mol	Chain	Res	Type
1	A	128	ASN
1	A	263	ASN
1	B	247	HIS
1	E	70	ASN

5.3.3 RNA ⓘ

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
3	NAG	K	1	1,3	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	K	2	3	14,14,15	0.28	0	17,19,21	0.67	0
3	BMA	K	3	3	11,11,12	0.62	0	15,15,17	0.87	0
3	MAN	K	4	3	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
4	NAG	L	1	1,4	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
4	NAG	L	2	4	14,14,15	0.34	0	17,19,21	1.18	2 (11%)
5	NAG	M	1	1,5	14,14,15	0.31	0	17,19,21	0.86	1 (5%)
5	NAG	M	2	5	14,14,15	0.33	0	17,19,21	0.85	2 (11%)
5	BMA	M	3	5	11,11,12	0.89	1 (9%)	15,15,17	0.91	1 (6%)
6	NAG	N	1	1,6	14,14,15	0.30	0	17,19,21	0.87	1 (5%)
6	NAG	N	2	6	14,14,15	0.27	0	17,19,21	0.62	0
7	NAG	O	1	1,7	14,14,15	0.30	0	17,19,21	0.57	0
7	NAG	O	2	7	14,14,15	0.28	0	17,19,21	0.75	0
7	BMA	O	3	7	11,11,12	0.59	0	15,15,17	0.80	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
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
7	NAG	O	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	3	BMA	C1-C2	2.33	1.57	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C1-O5-C5	3.05	116.33	112.19
4	L	1	NAG	O3-C3-C2	2.66	114.96	109.47
6	N	1	NAG	C1-O5-C5	2.42	115.47	112.19
3	K	4	MAN	C1-O5-C5	2.35	115.38	112.19
5	M	2	NAG	O4-C4-C3	-2.28	105.08	110.35

There are no chirality outliers.

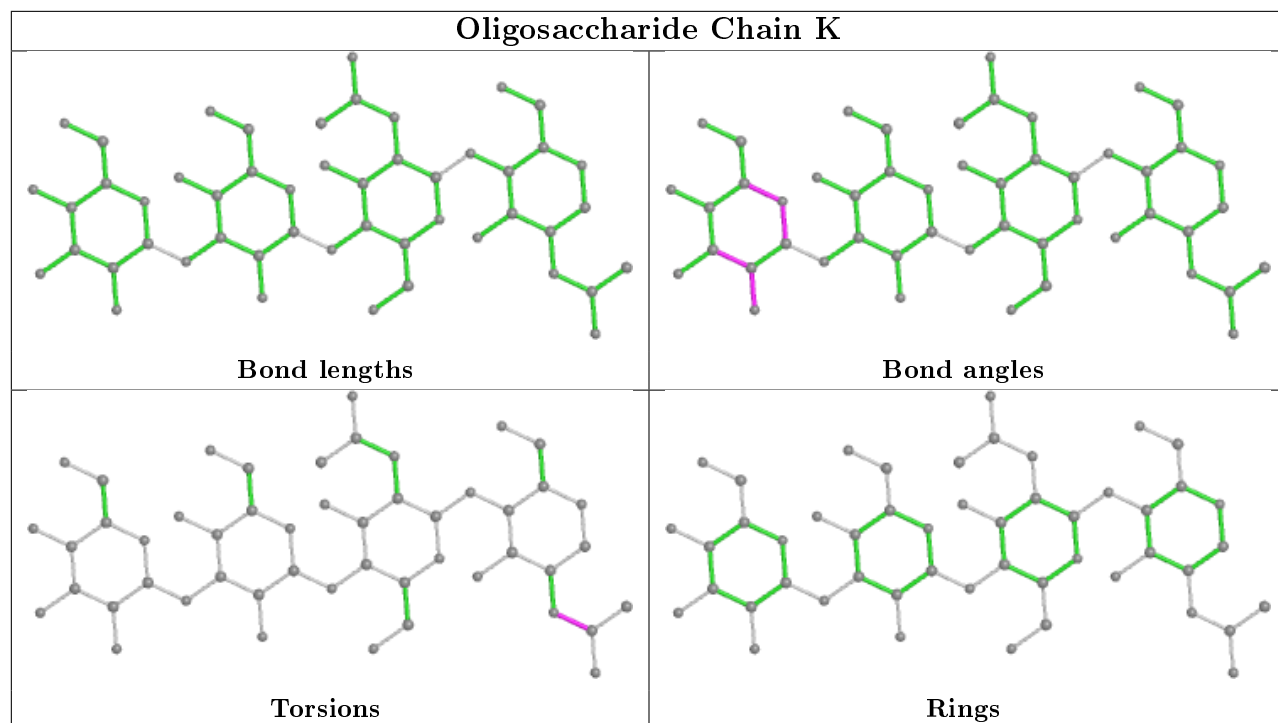
5 of 15 torsion outliers are listed below:

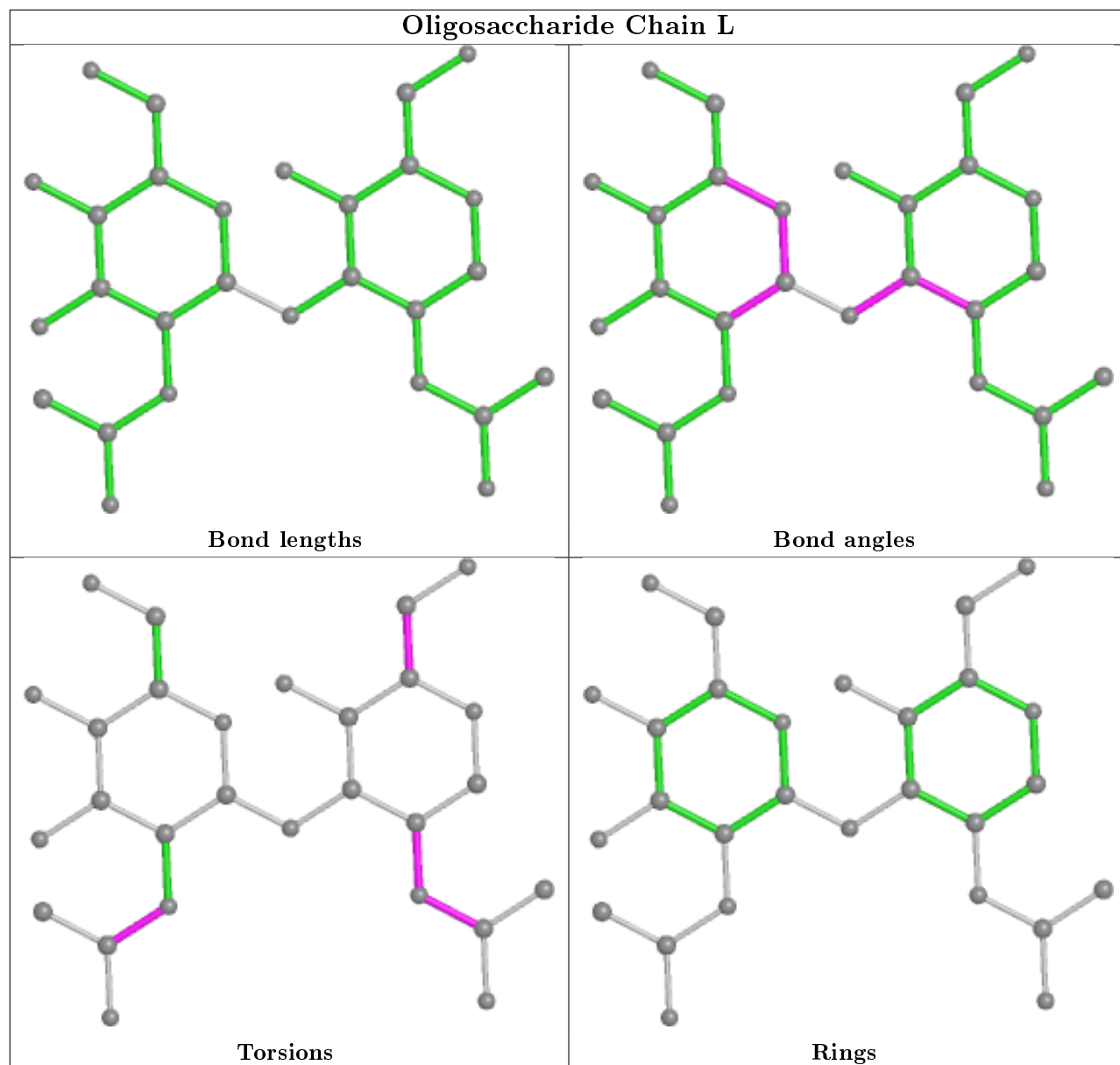
Mol	Chain	Res	Type	Atoms
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
6	N	1	NAG	O5-C5-C6-O6

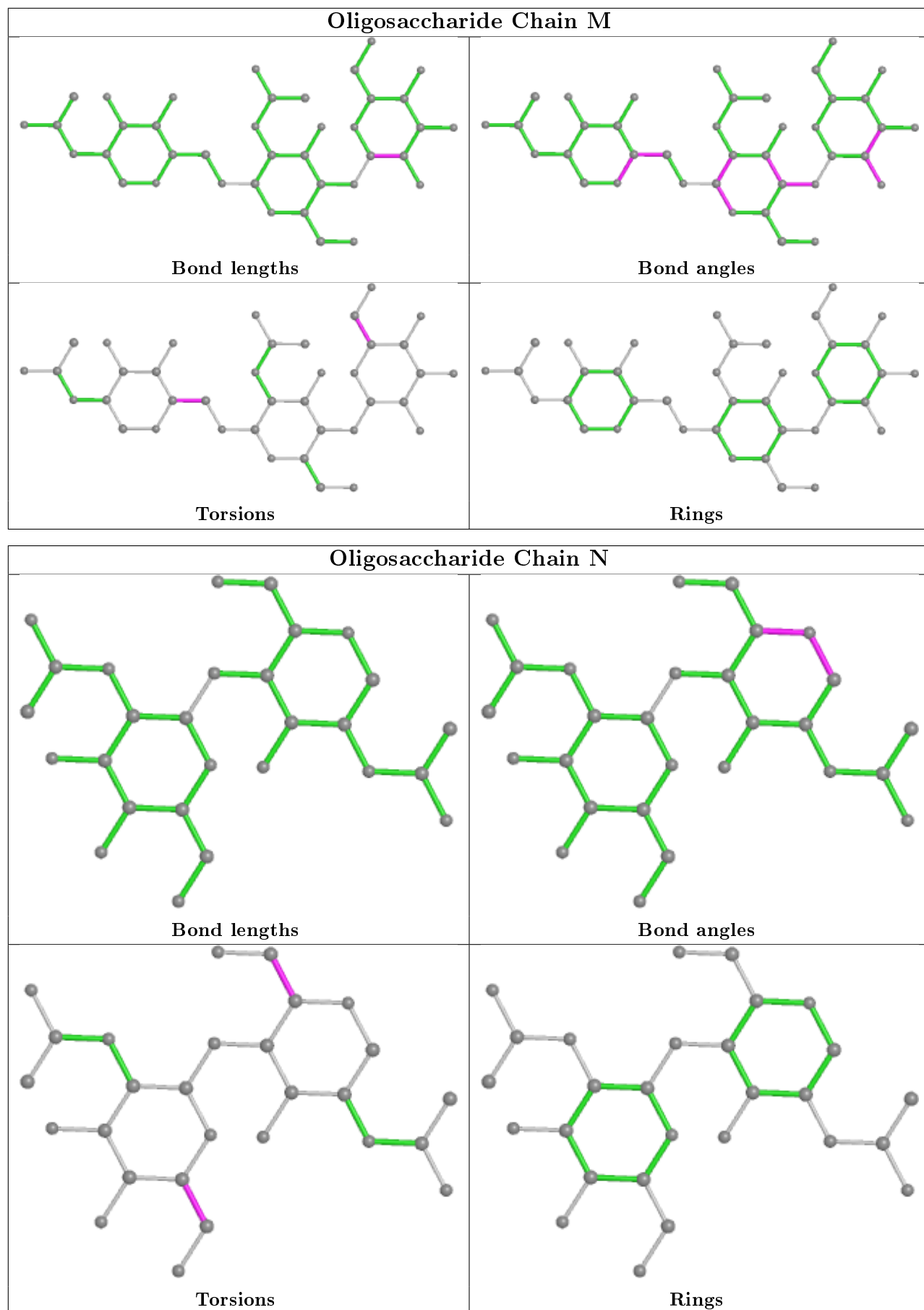
There are no ring outliers.

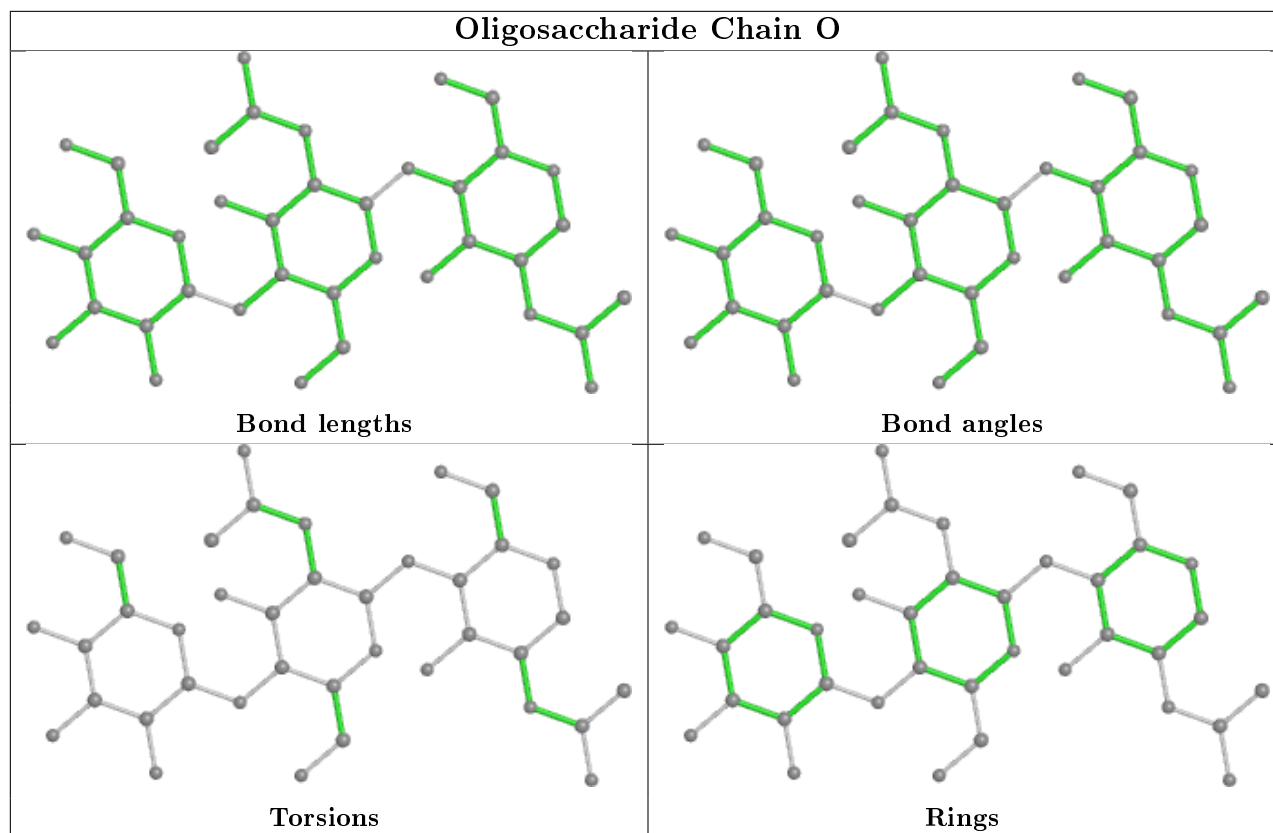
No monomer is involved in short contacts.

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](#)

3 ligands 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	$\# Z > 2$
8	NAG	A	501	1	14,14,15	0.28	0	17,19,21	0.64	0
8	NAG	D	502	1	14,14,15	0.30	0	17,19,21	0.71	0
8	NAG	D	501	1	14,14,15	0.30	0	17,19,21	0.77	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
8	NAG	A	501	1	-	4/6/23/26	0/1/1/1
8	NAG	D	502	1	-	2/6/23/26	0/1/1/1
8	NAG	D	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	501	NAG	C8-C7-N2-C2
8	A	501	NAG	O7-C7-N2-C2
8	D	501	NAG	O7-C7-N2-C2
8	D	501	NAG	C8-C7-N2-C2
8	A	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	NAG	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	A	335/379 (88%)	0.34	8 (2%) 59 48	64, 105, 151, 181	0
1	B	338/379 (89%)	0.42	20 (5%) 22 17	68, 112, 159, 199	0
1	C	338/379 (89%)	0.61	27 (7%) 12 10	63, 122, 179, 200	0
1	D	336/379 (88%)	0.33	11 (3%) 46 36	81, 114, 155, 171	0
1	E	322/379 (84%)	0.97	61 (18%) 1 1	112, 162, 202, 241	0
2	F	47/56 (83%)	0.56	6 (12%) 3 4	89, 118, 143, 152	0
2	G	47/56 (83%)	0.37	1 (2%) 63 53	90, 121, 151, 160	0
2	H	47/56 (83%)	0.22	0 100 100	92, 124, 150, 168	0
2	I	47/56 (83%)	0.60	3 (6%) 19 14	98, 136, 163, 181	0
2	J	47/56 (83%)	0.53	3 (6%) 19 14	134, 169, 186, 190	0
All	All	1904/2175 (87%)	0.52	140 (7%) 14 11	63, 123, 183, 241	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	348	GLY	6.2
1	C	314	GLN	6.1
1	E	262	LYS	5.9
1	E	269	PHE	5.9
2	I	1107	ARG	5.4

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

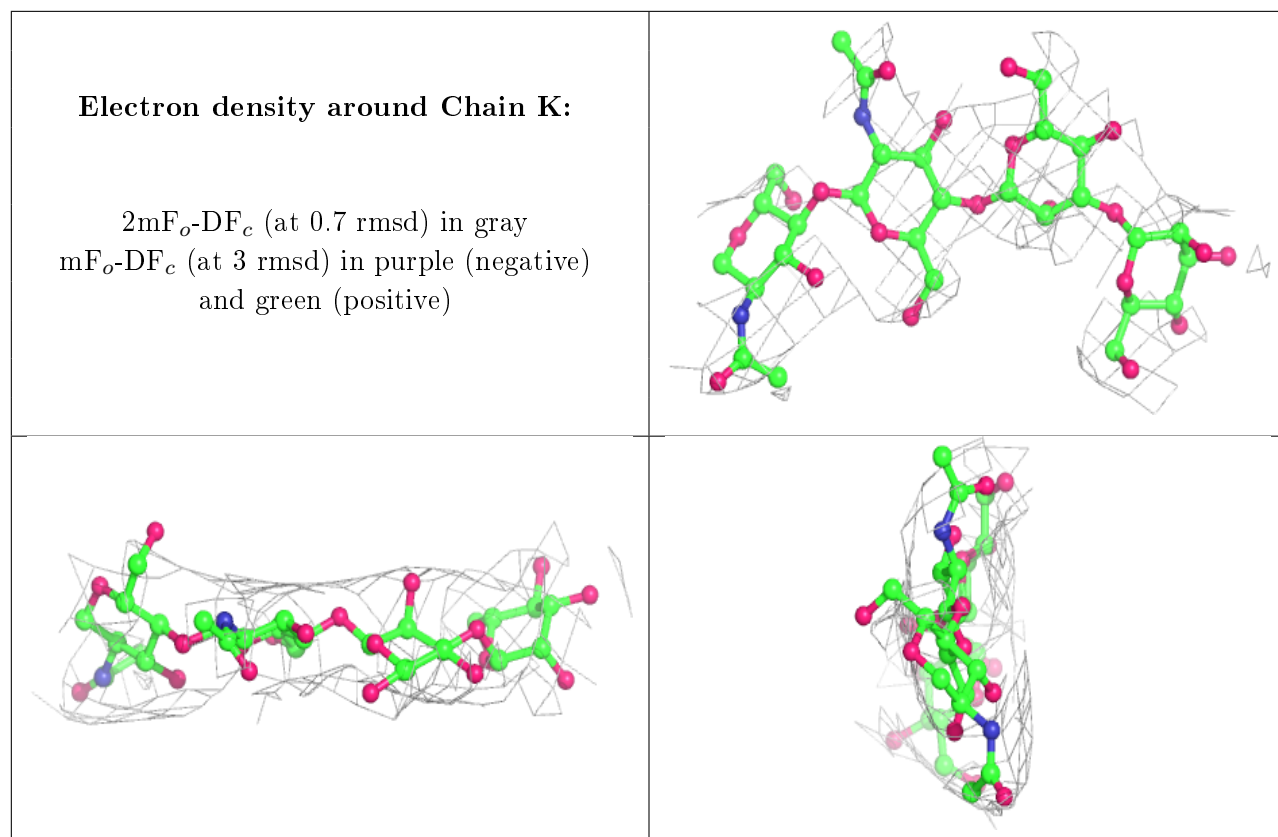
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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.

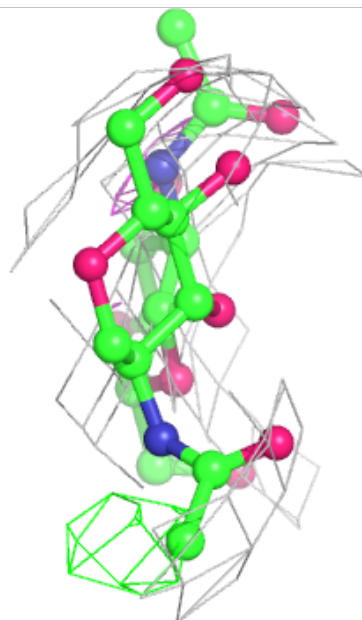
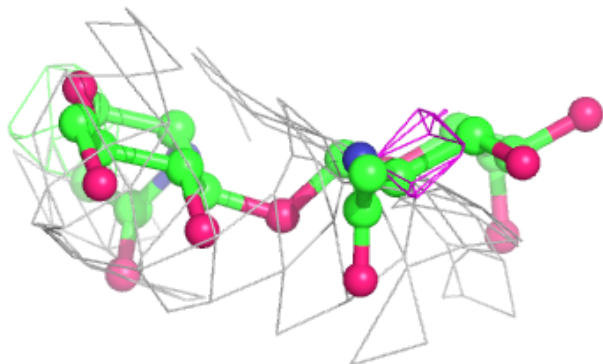
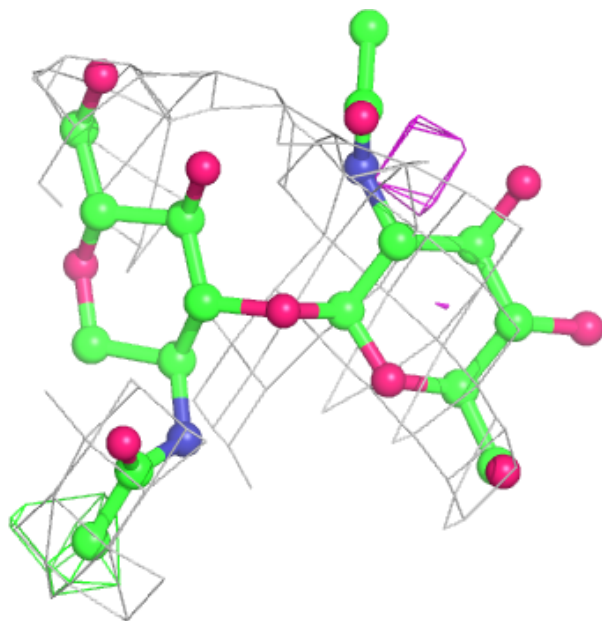
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	K	1	14/15	0.89	0.24	129,138,146,149	0
7	NAG	O	1	14/15	-	-	123,128,130,131	14
5	BMA	M	3	11/12	0.57	0.39	136,169,178,180	0
5	NAG	M	2	14/15	0.73	0.28	157,174,185,193	0
3	NAG	K	2	14/15	0.87	0.26	130,149,161,162	0
7	NAG	O	2	14/15	-	-	114,117,123,130	14
5	NAG	M	1	14/15	0.62	0.34	145,163,167,168	0
3	MAN	K	4	11/12	0.68	0.54	129,156,163,165	0
4	NAG	L	2	14/15	0.69	0.52	186,204,218,229	0
4	NAG	L	1	14/15	0.81	0.22	120,153,175,180	0
3	BMA	K	3	11/12	0.82	0.26	132,152,162,168	0
6	NAG	N	1	14/15	0.84	0.24	139,159,171,173	0
7	BMA	O	3	11/12	-	-	110,111,112,113	11
6	NAG	N	2	14/15	0.80	0.30	141,168,192,195	0

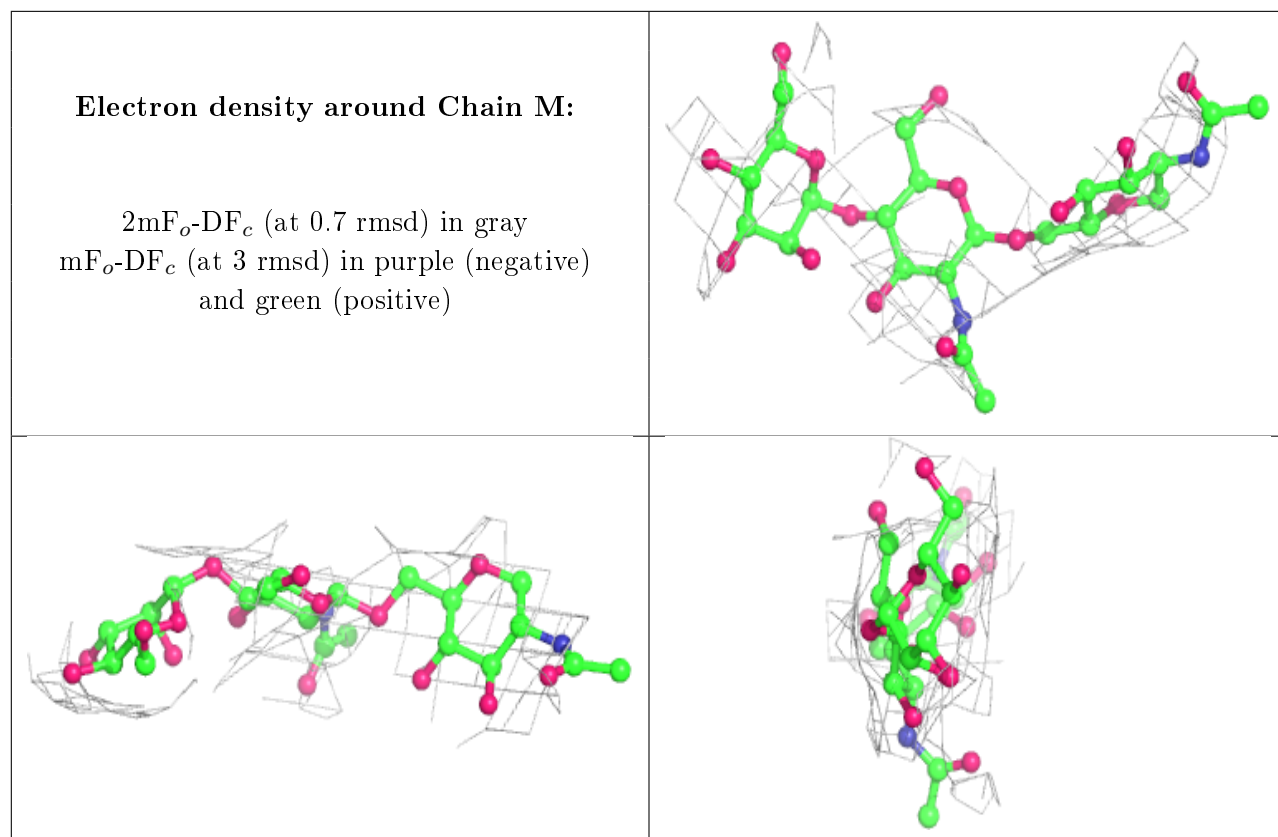
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain L:

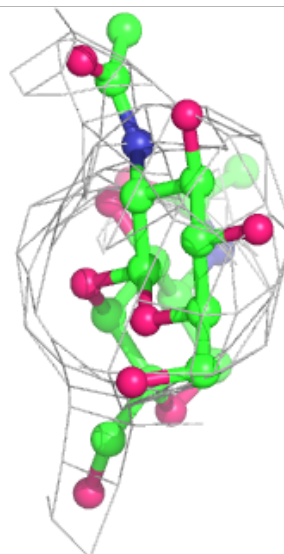
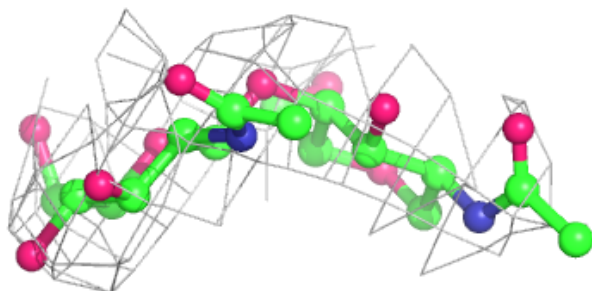
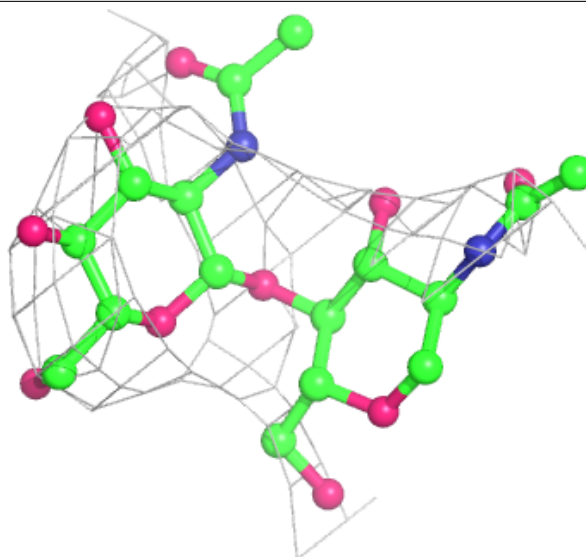
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

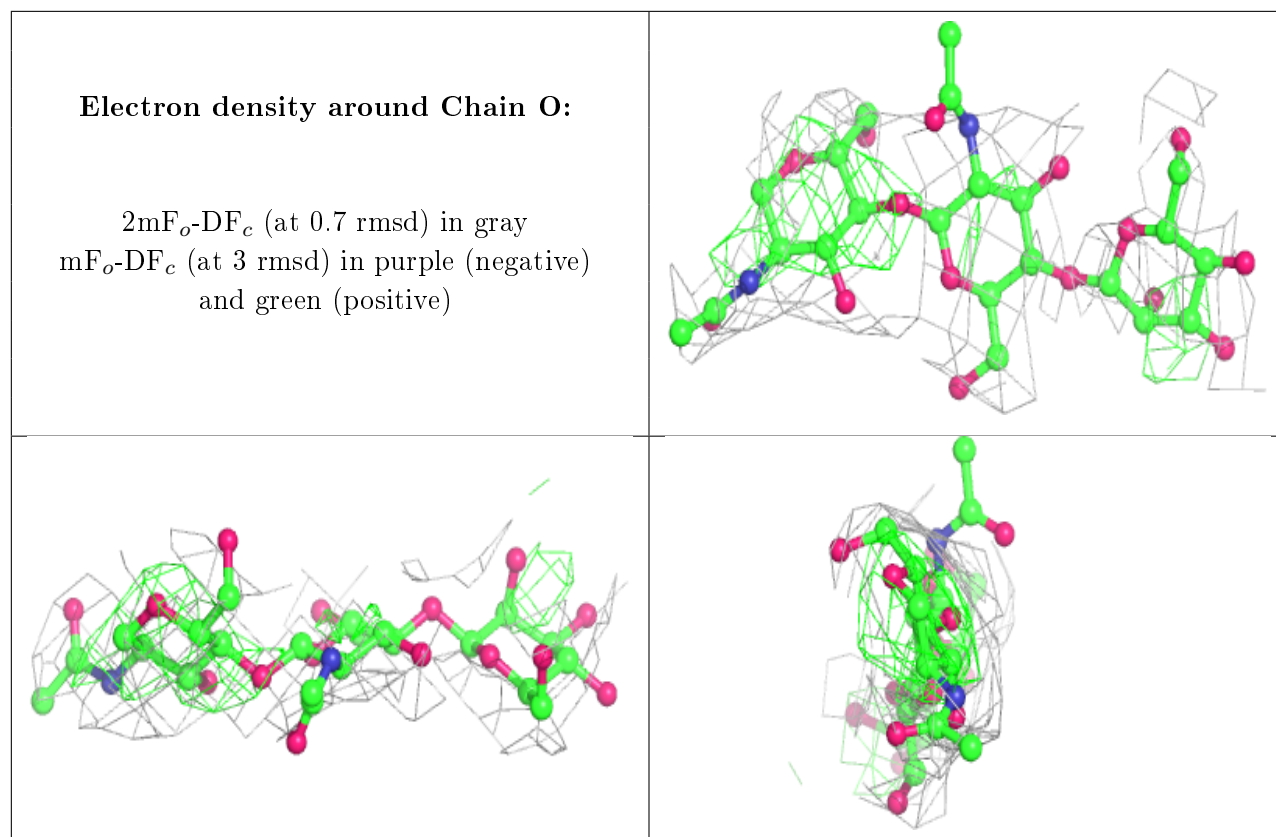




Electron density around Chain N:

$2mF_o-DF_c$ (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
8	NAG	D	502	14/15	0.63	0.37	109,138,153,155	0
8	NAG	A	501	14/15	0.70	0.36	133,148,158,162	0
8	NAG	D	501	14/15	0.81	0.32	92,122,128,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.